



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 7, 2022 – 07:38 PM EDT

PDB ID : 7U2I
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with mRNA, aminoacylated A-site Gly-NH-tRNA^{Gly}, aminoacylated P-site fMet-NH-tRNA^{Met}, deacylated E-site tRNA^{Gly}, and chloramphenicol at 2.55Å resolution
Authors : Syroegin, E.A.; Aleksandrova, E.V.; Polikanov, Y.S.
Deposited on : 2022-02-24
Resolution : 2.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
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)	:	2.29

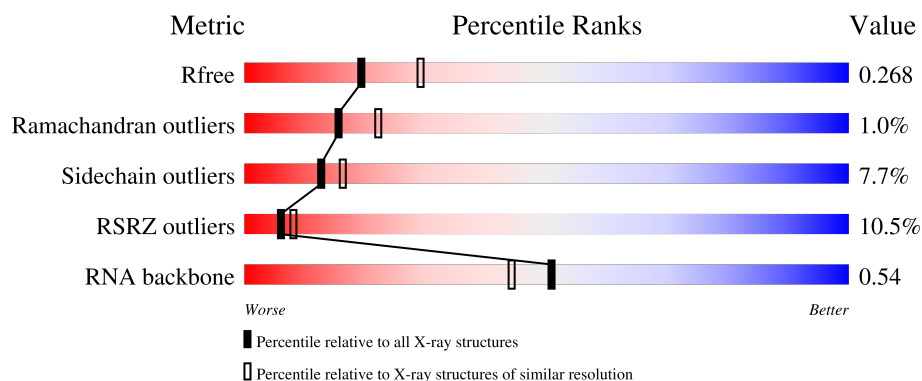
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1284 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)
RNA backbone	3102	1026 (2.88-2.20)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	<div> <div>3%</div> <div>82%</div> <div>16%</div> <div>..</div> </div>
1	2A	2915	<div> <div>4%</div> <div>79%</div> <div>17%</div> <div>.</div> </div>
2	1B	121	<div> <div>93%</div> <div>6%</div> <div>.</div> </div>
2	2B	121	<div> <div>5%</div> <div>74%</div> <div>25%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	1D	276	<div> <div></div> <div>96%</div> <div>.</div> </div>
3	2D	276	<div> <div>7%</div> <div>94%</div> <div>5%</div> </div>
4	1E	206	<div> <div>3%</div> <div>95%</div> <div>..</div> </div>
4	2E	206	<div> <div>5%</div> <div>95%</div> <div>..</div> </div>
5	1F	210	<div> <div>3%</div> <div>88%</div> <div>9%</div> </div>
5	2F	210	<div> <div>6%</div> <div>90%</div> <div>7%</div> </div>
6	1G	182	<div> <div>3%</div> <div>91%</div> <div>8%</div> </div>
6	2G	182	<div> <div>35%</div> <div>89%</div> <div>10%</div> </div>
7	1H	180	<div> <div>2%</div> <div>89%</div> <div>7%</div> </div>
7	2H	180	<div> <div>29%</div> <div>88%</div> <div>8%</div> </div>
8	1I	148	<div> <div></div> <div>89%</div> <div>9%</div> </div>
8	2I	148	<div> <div>9%</div> <div>88%</div> <div>11%</div> </div>
9	1N	140	<div> <div>2%</div> <div>94%</div> <div>6%</div> </div>
9	2N	140	<div> <div>13%</div> <div>91%</div> <div>9%</div> </div>
10	1O	122	<div> <div>2%</div> <div>98%</div> <div>.</div> </div>
10	2O	122	<div> <div>5%</div> <div>97%</div> <div>.</div> </div>
11	1P	150	<div> <div></div> <div>92%</div> <div>7%</div> </div>
11	2P	150	<div> <div>11%</div> <div>94%</div> <div>5%</div> </div>
12	1Q	141	<div> <div>2%</div> <div>97%</div> <div>.</div> </div>
12	2Q	141	<div> <div>17%</div> <div>97%</div> <div>.</div> </div>
13	1R	118	<div> <div></div> <div>93%</div> <div>7%</div> </div>
13	2R	118	<div> <div>7%</div> <div>94%</div> <div>6%</div> </div>
14	1S	112	<div> <div></div> <div>92%</div> <div>6%</div> </div>
14	2S	112	<div> <div>16%</div> <div>88%</div> <div>11%</div> </div>
15	1T	146	<div> <div></div> <div>84%</div> <div>5%</div> <div>10%</div> </div>

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

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

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Mol	Chain	Length	Quality of chain
40	2i	128	<div>59%</div> <div>90%</div> <div>9%</div>
41	1j	105	<div>20%</div> <div>80%</div> <div>12%</div> <div>8%</div>
41	2j	105	<div>39%</div> <div>76%</div> <div>15%</div> <div>9%</div>
42	1k	129	<div>8%</div> <div>79%</div> <div>9%</div> <div>12%</div>
42	2k	129	<div>19%</div> <div>82%</div> <div>6%</div> <div>12%</div>
43	1l	132	<div>15%</div> <div>88%</div> <div>5%</div> <div>8%</div>
43	2l	132	<div>22%</div> <div>85%</div> <div>8%</div> <div>8%</div>
44	1m	126	<div>10%</div> <div>88%</div> <div>9%</div> <div>..</div>
44	2m	126	<div>35%</div> <div>89%</div> <div>7%</div> <div>..</div>
45	1n	61	<div>20%</div> <div>95%</div> <div>..</div>
45	2n	61	<div>66%</div> <div>90%</div> <div>8%</div> <div>..</div>
46	1o	89	<div>4%</div> <div>92%</div> <div>7%</div> <div>..</div>
46	2o	89	<div>12%</div> <div>92%</div> <div>6%</div> <div>..</div>
47	1p	88	<div>22%</div> <div>84%</div> <div>9%</div> <div>7%</div>
47	2p	88	<div>9%</div> <div>88%</div> <div>6%</div> <div>7%</div>
48	1q	105	<div>12%</div> <div>86%</div> <div>9%</div> <div>6%</div>
48	2q	105	<div>27%</div> <div>85%</div> <div>10%</div> <div>6%</div>
49	1r	88	<div>3%</div> <div>75%</div> <div>..</div> <div>23%</div>
49	2r	88	<div>10%</div> <div>69%</div> <div>8%</div> <div>23%</div>
50	1s	93	<div>4%</div> <div>84%</div> <div>5%</div> <div>11%</div>
50	2s	93	<div>54%</div> <div>80%</div> <div>10%</div> <div>11%</div>
51	1t	106	<div>29%</div> <div>83%</div> <div>8%</div> <div>9%</div>
51	2t	106	<div>16%</div> <div>85%</div> <div>6%</div> <div>9%</div>
52	1u	27	<div>37%</div> <div>85%</div> <div>15%</div>
52	2u	27	<div>59%</div> <div>81%</div> <div>..</div> <div>15%</div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	4SU	2w	8	-	-	-	X
56	PSU	1y	55	-	-	-	X
56	5MU	2y	54	-	-	-	X
56	PSU	2y	55	-	-	-	X
57	MG	1A	3073	-	-	-	X
57	MG	1A	3235	-	-	-	X
57	MG	1A	3247	-	-	-	X
57	MG	1A	3299	-	-	-	X
57	MG	1A	3332	-	-	-	X
57	MG	1A	3418	-	-	-	X
57	MG	1A	3499	-	-	-	X
57	MG	1A	3874	-	-	-	X
57	MG	1E	310	-	-	-	X
57	MG	1U	210	-	-	-	X
57	MG	2A	3231	-	-	-	X
57	MG	2A	3255	-	-	-	X
57	MG	2A	3278	-	-	-	X
57	MG	2A	3282	-	-	-	X
57	MG	2A	3318	-	-	-	X
57	MG	2A	3323	-	-	-	X
57	MG	2A	3357	-	-	-	X
57	MG	2A	3377	-	-	-	X
57	MG	2A	3379	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	2A	3382	-	-	-	X
57	MG	2A	3617	-	-	-	X
57	MG	2A	3705	-	-	-	X
57	MG	2a	1719	-	-	-	X

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 300046 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	202	Total	C	N	O	S	0	0	0
			1583	1009	297	275	2			
5	2F	202	Total	C	N	O	S	0	0	0
			1579	1007	296	274	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 55 is a RNA chain called P-site Aminoacyl-tRNA fMet-NH-tRNAmet.

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

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

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

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

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

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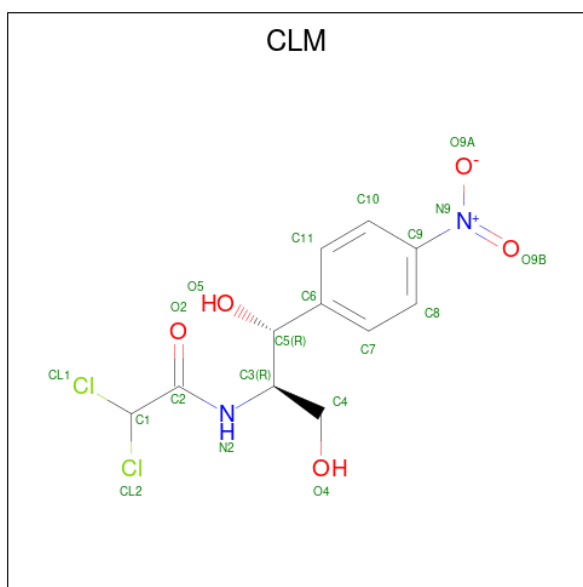
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2d	2	Total 2	Mg 2	0	0
57	2e	1	Total 1	Mg 1	0	0
57	2f	2	Total 2	Mg 2	0	0
57	2i	1	Total 1	Mg 1	0	0
57	2j	1	Total 1	Mg 1	0	0
57	2k	1	Total 1	Mg 1	0	0
57	2l	3	Total 3	Mg 3	0	0
57	2q	2	Total 2	Mg 2	0	0
57	2r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

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

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

- Molecule 59 is CHLORAMPHENICOL (three-letter code: CLM) (formula: C₁₁H₁₂Cl₂N₂O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
59	1A	1	Total	C	Cl	N	O	0
			20	11	2	2	5	
59	2A	1	Total	C	Cl	N	O	0
			20	11	2	2	5	

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

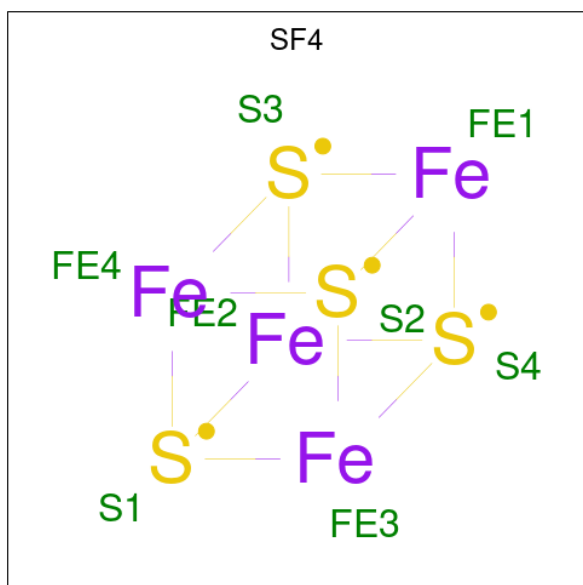
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1Y	1	Total	Zn	0	0
			1	1		
60	14	1	Total	Zn	0	0
			1	1		
60	15	1	Total	Zn	0	0
			1	1		
60	16	1	Total	Zn	0	0
			1	1		
60	19	1	Total	Zn	0	0
			1	1		
60	1n	1	Total	Zn	0	0
			1	1		
60	2Y	1	Total	Zn	0	0
			1	1		
60	24	1	Total	Zn	0	0
			1	1		
60	25	1	Total	Zn	0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

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

- Molecule 61 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 62 is water.

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

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

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

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

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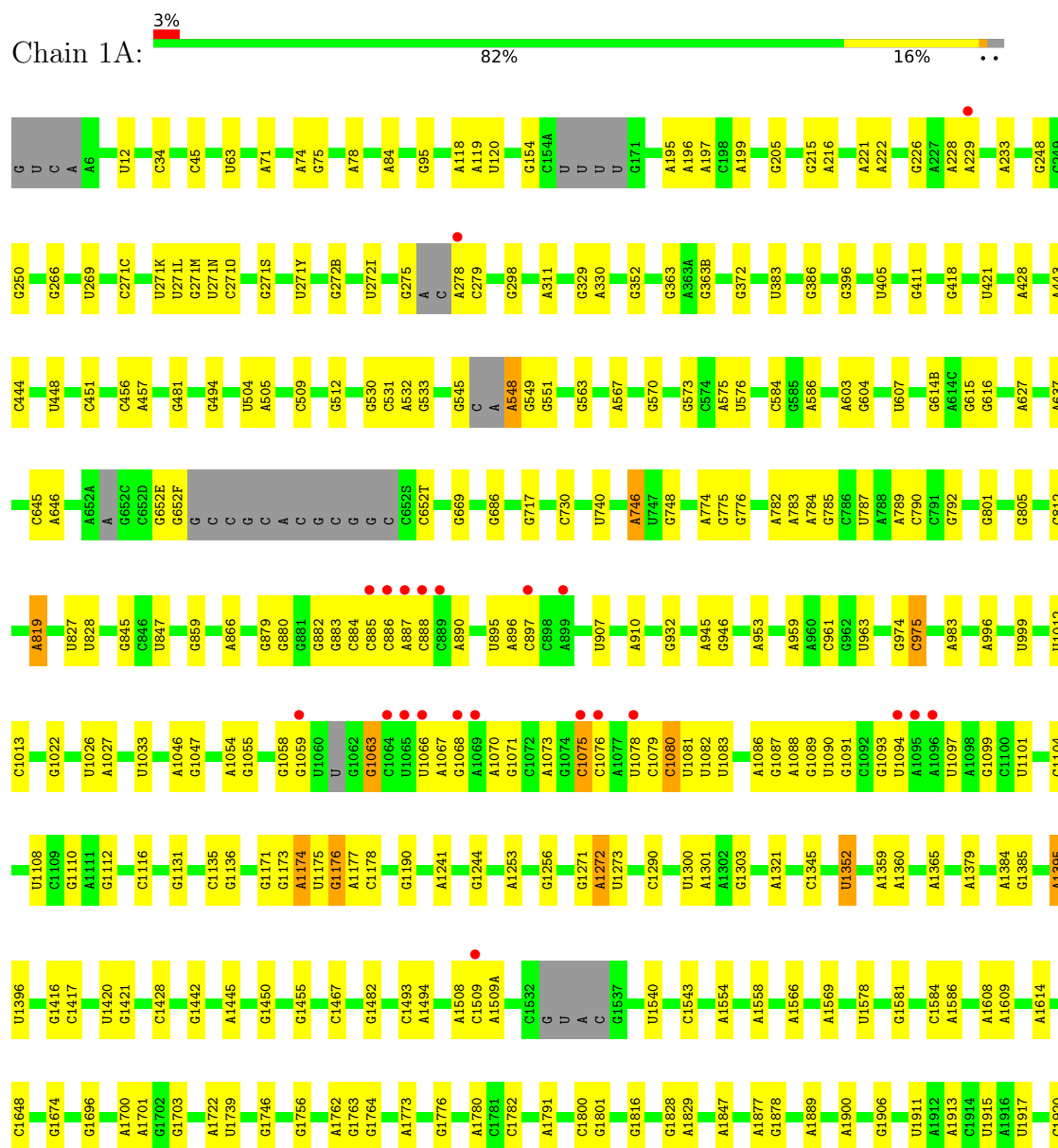
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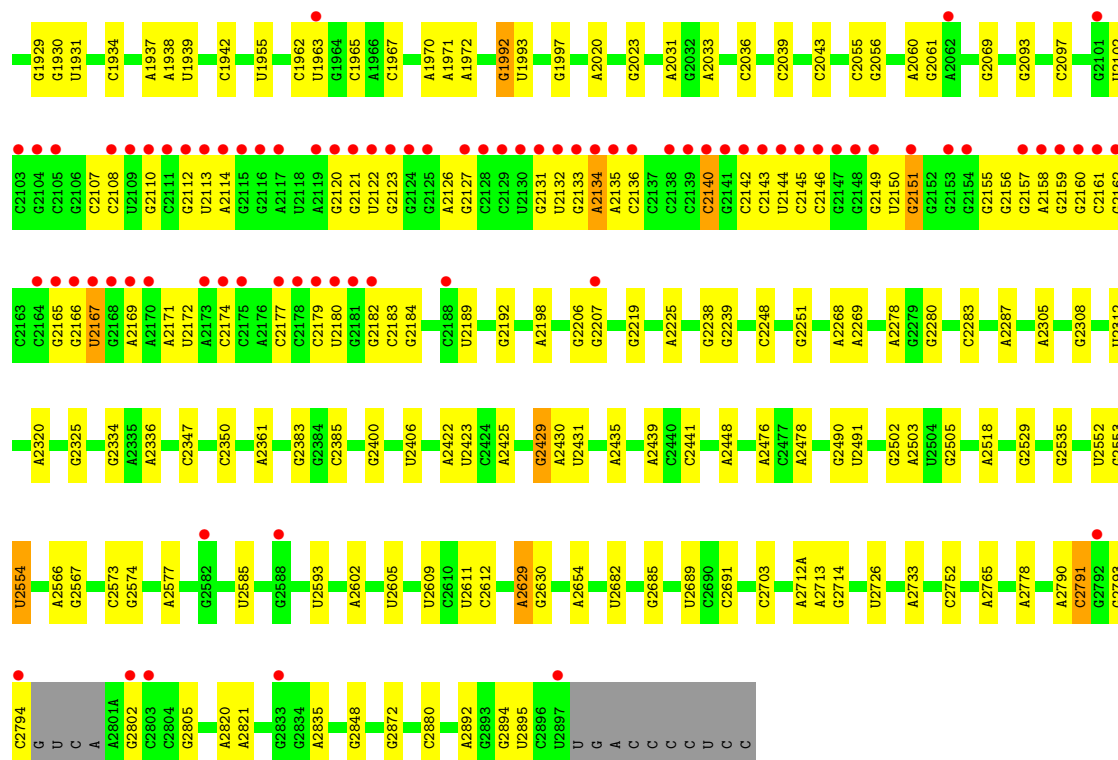
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2l	4	Total 4	O 4	0	0
62	2r	1	Total 1	O 1	0	0
62	2t	2	Total 2	O 2	0	0
62	2v	2	Total 2	O 2	0	0
62	2w	1	Total 1	O 1	0	0
62	2x	7	Total 7	O 7	0	0

3 Residue-property plots [i](#)

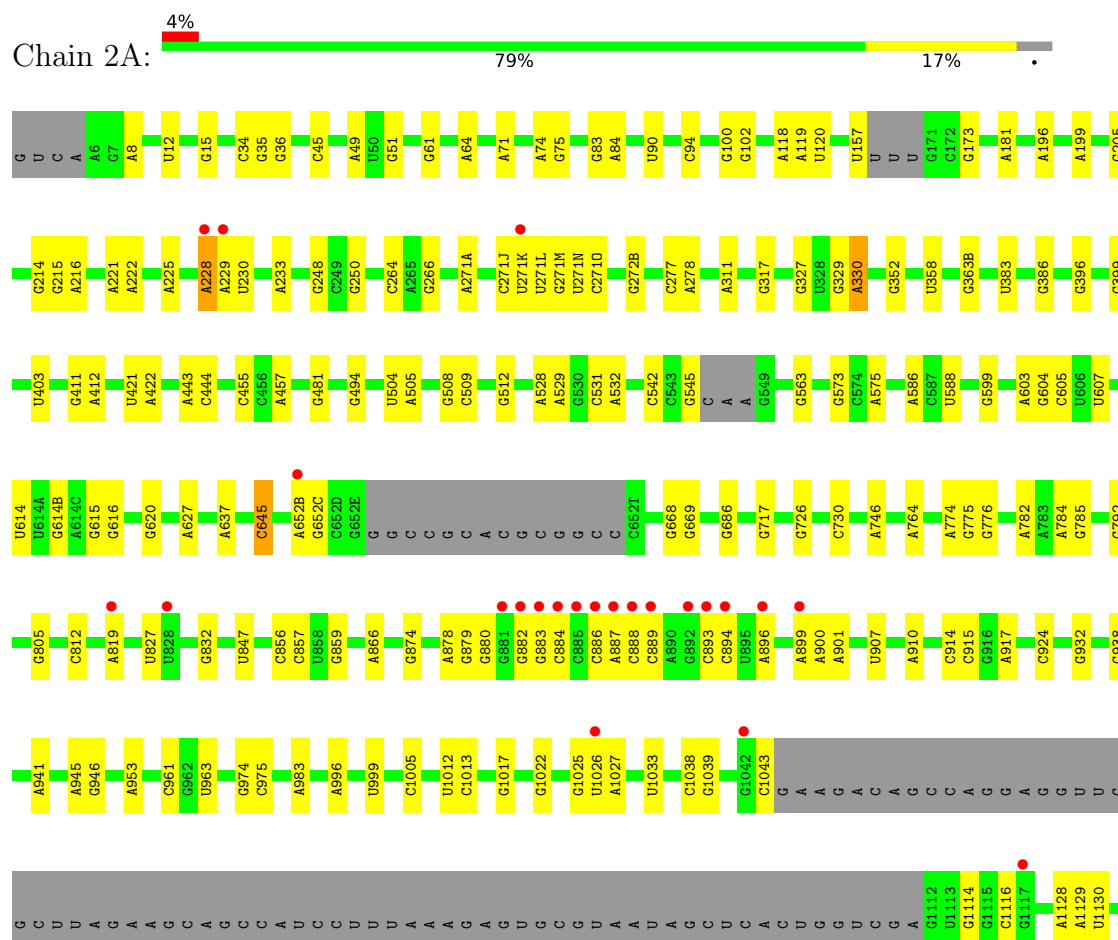
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

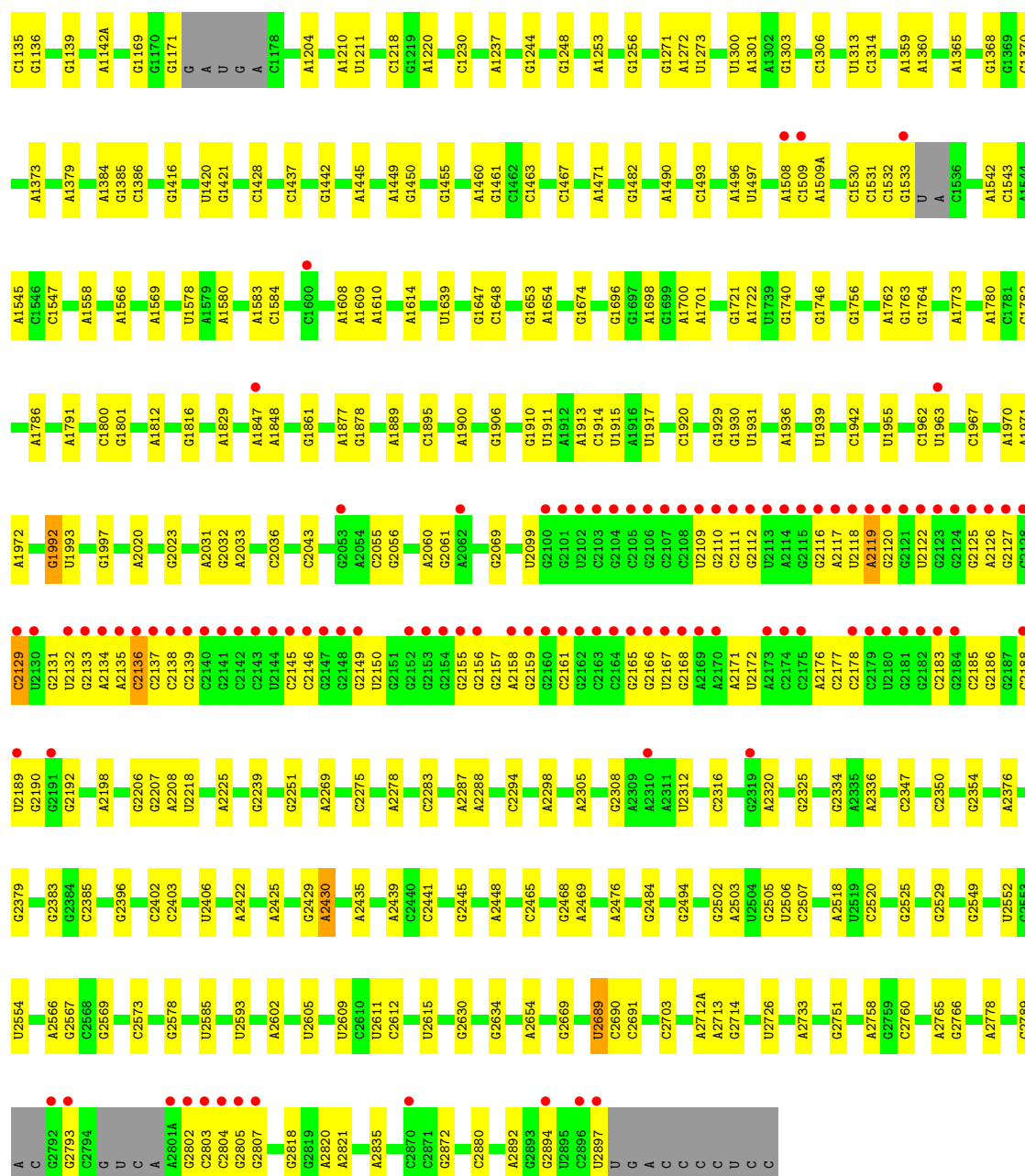
• Molecule 1: 23S Ribosomal RNA





- Molecule 1: 23S Ribosomal RNA





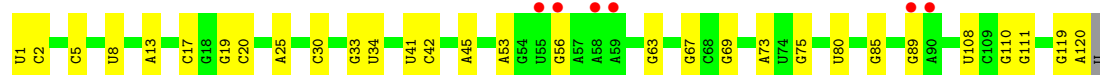
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 93% 6% .



• Molecule 2: 5S Ribosomal RNA

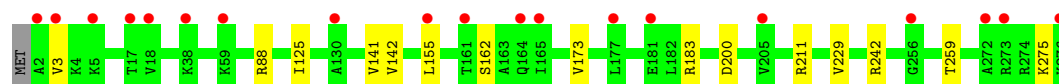
Chain 2B: 5% 74% 25% .



- Molecule 3: 50S ribosomal protein L2



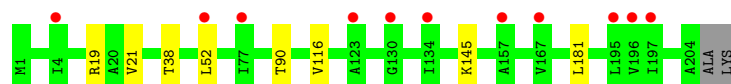
- Molecule 3: 50S ribosomal protein L2



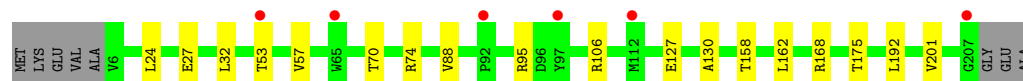
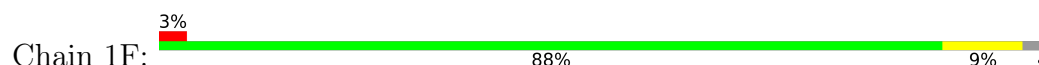
- Molecule 4: 50S ribosomal protein L3



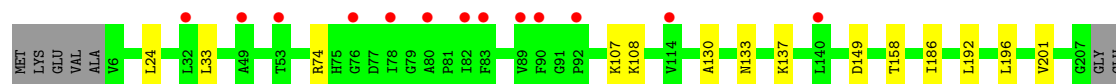
- Molecule 4: 50S ribosomal protein L3



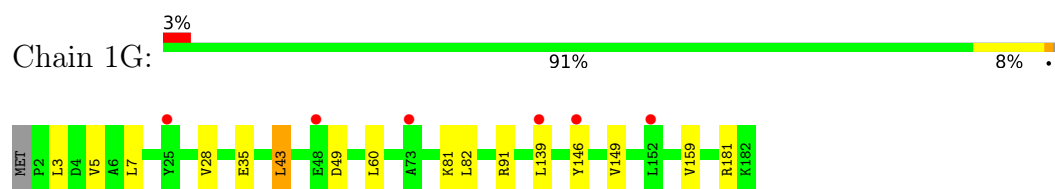
- Molecule 5: 50S ribosomal protein L4



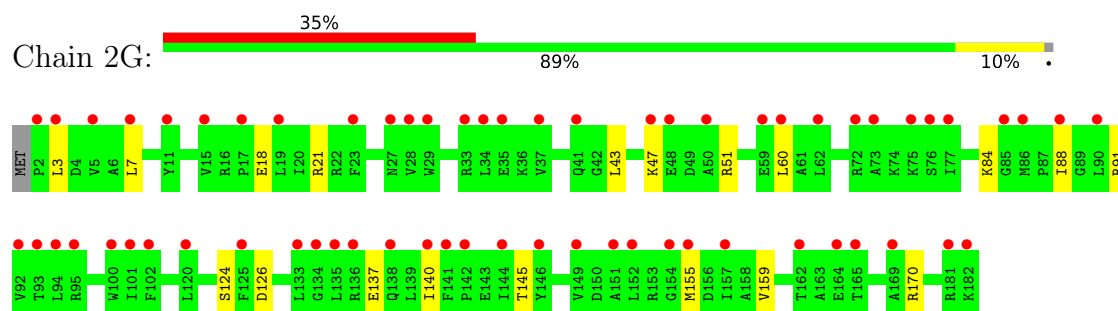
- Molecule 5: 50S ribosomal protein L4



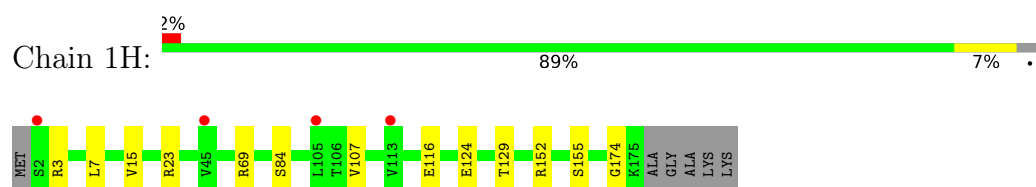
- Molecule 6: 50S ribosomal protein L5



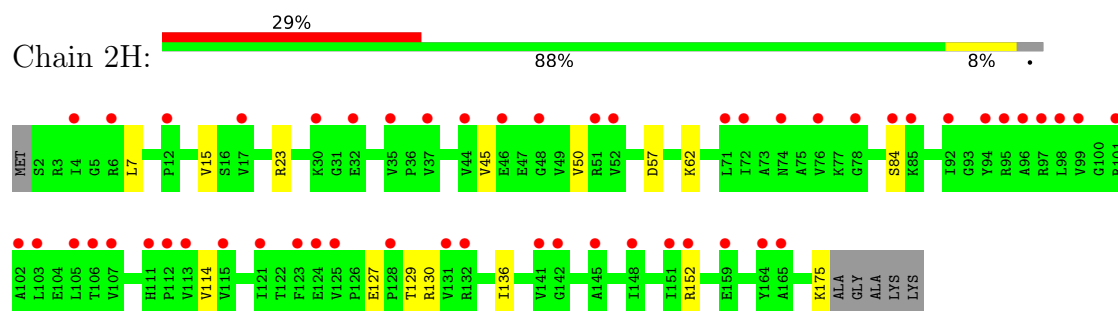
- Molecule 6: 50S ribosomal protein L5



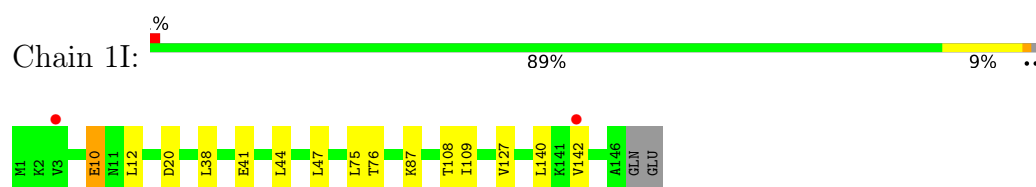
- Molecule 7: 50S ribosomal protein L6



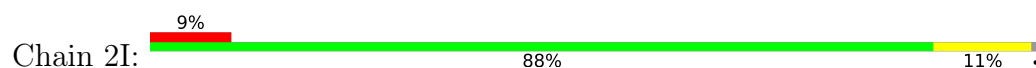
- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L9



- Molecule 8: 50S ribosomal protein L9

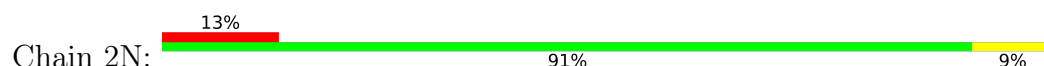




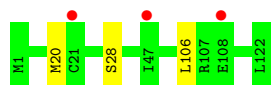
- Molecule 9: 50S ribosomal protein L13



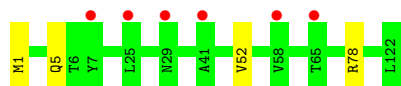
- Molecule 9: 50S ribosomal protein L13



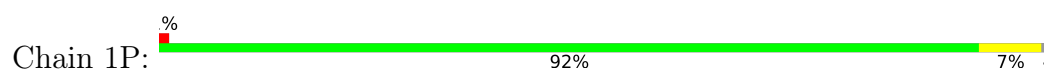
- Molecule 10: 50S ribosomal protein L14



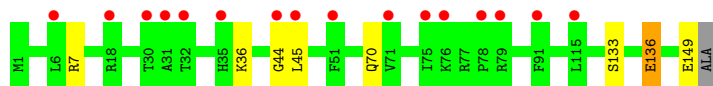
- Molecule 10: 50S ribosomal protein L14



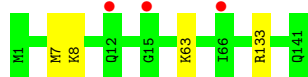
- Molecule 11: 50S ribosomal protein L15



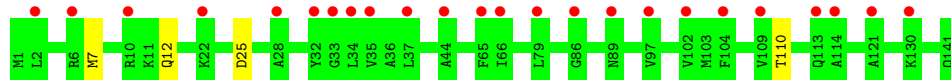
- Molecule 11: 50S ribosomal protein L15



- Molecule 12: 50S ribosomal protein L16



- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17



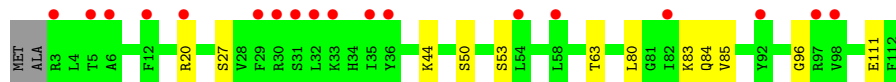
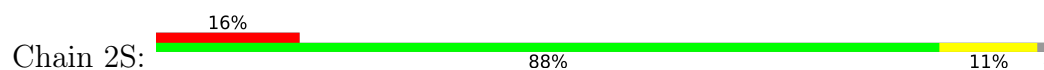
- Molecule 13: 50S ribosomal protein L17



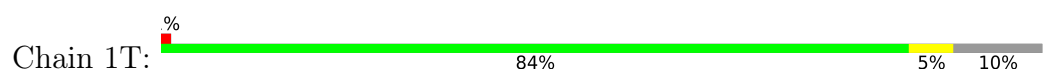
- Molecule 14: 50S ribosomal protein L18



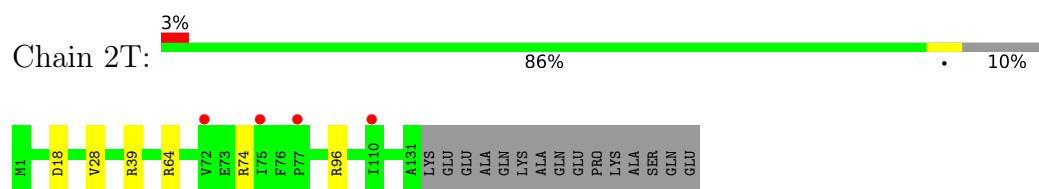
- Molecule 14: 50S ribosomal protein L18



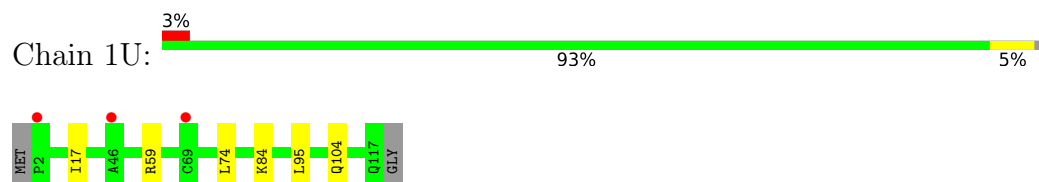
- Molecule 15: 50S ribosomal protein L19



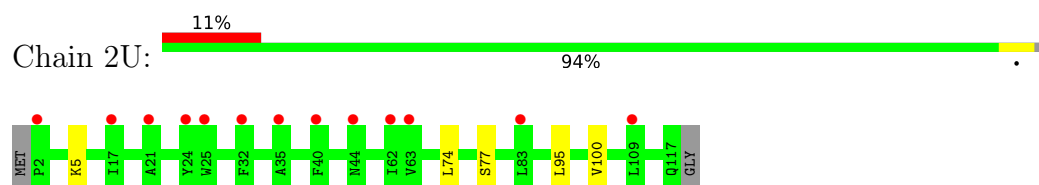
• Molecule 15: 50S ribosomal protein L19



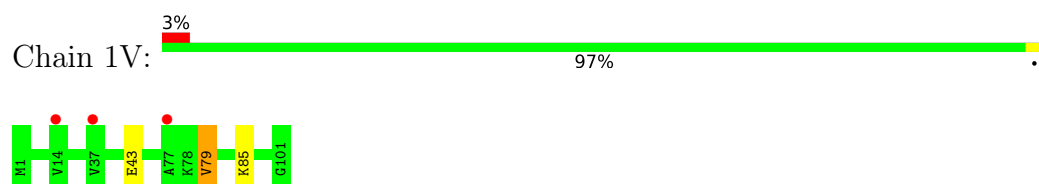
• Molecule 16: 50S ribosomal protein L20



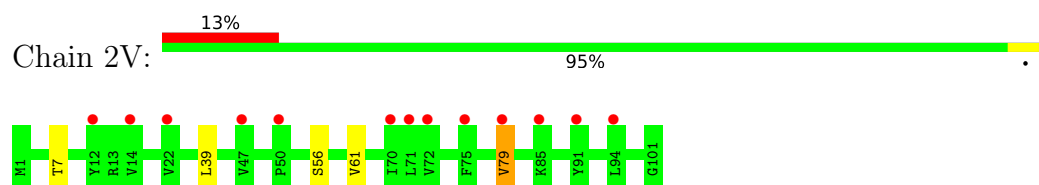
• Molecule 16: 50S ribosomal protein L20



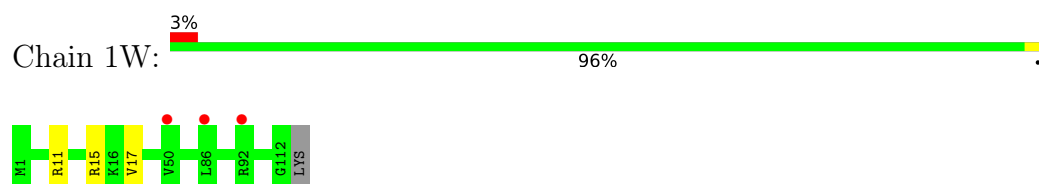
• Molecule 17: 50S ribosomal protein L21



• Molecule 17: 50S ribosomal protein L21

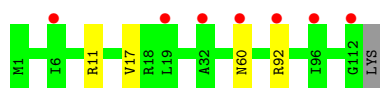


• Molecule 18: 50S ribosomal protein L22

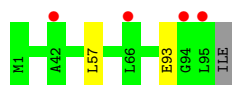


• Molecule 18: 50S ribosomal protein L22

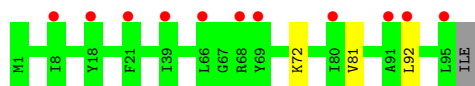




- Molecule 19: 50S ribosomal protein L23



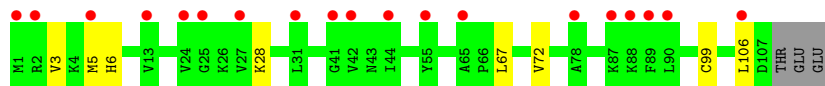
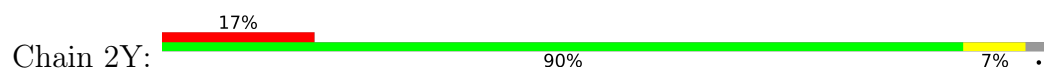
- Molecule 19: 50S ribosomal protein L23



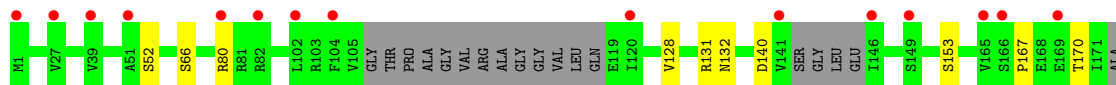
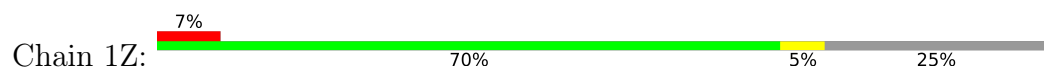
- Molecule 20: 50S ribosomal protein L24



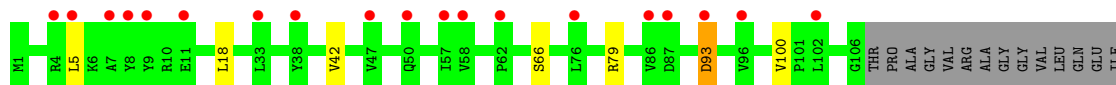
- Molecule 20: 50S ribosomal protein L24

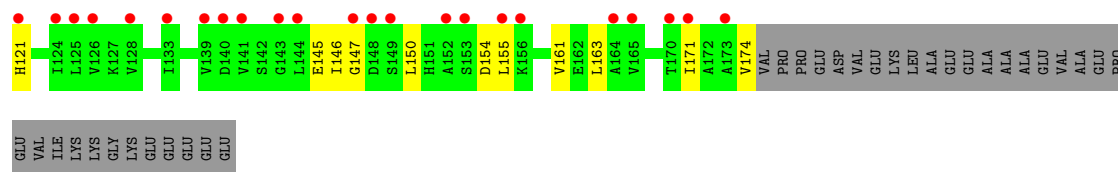


- Molecule 21: 50S ribosomal protein L25

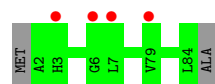


- Molecule 21: 50S ribosomal protein L25

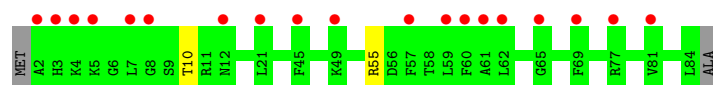




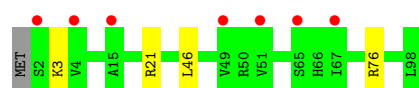
- Molecule 22: 50S ribosomal protein L27



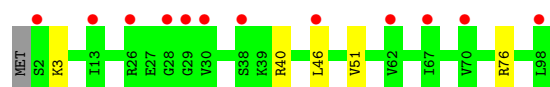
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28



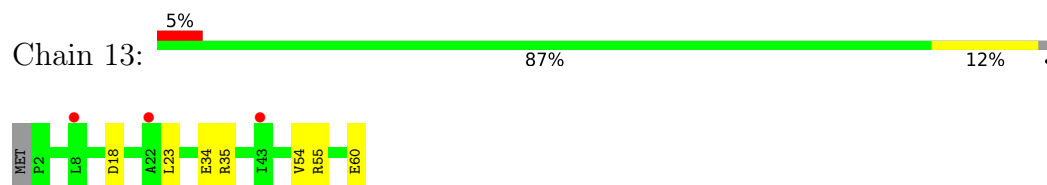
- Molecule 24: 50S ribosomal protein L29



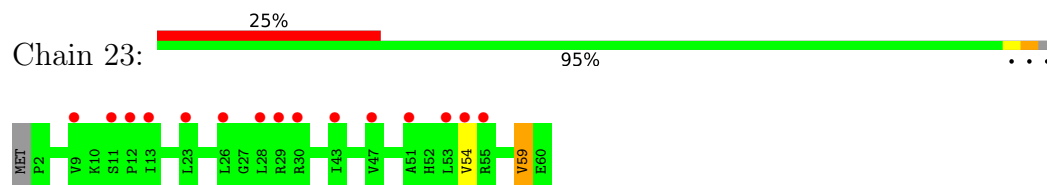
- Molecule 24: 50S ribosomal protein L29



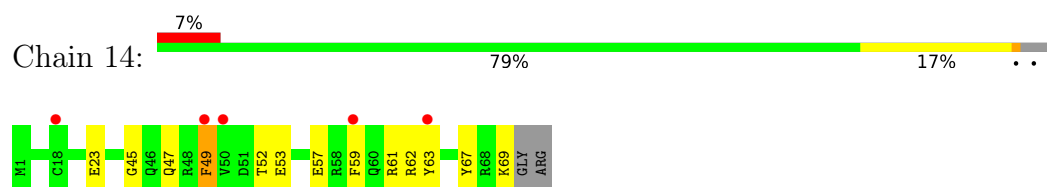
- Molecule 25: 50S ribosomal protein L30



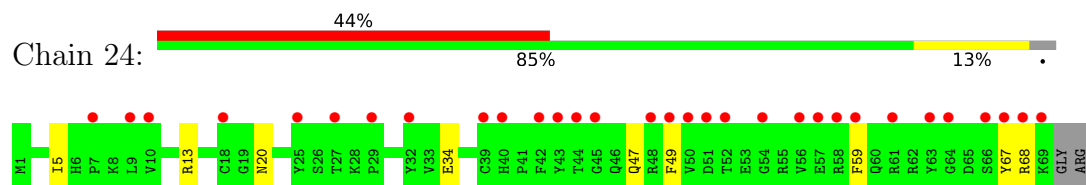
- Molecule 25: 50S ribosomal protein L30



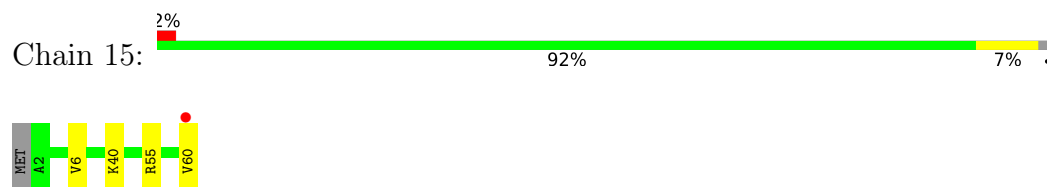
- Molecule 26: 50S ribosomal protein L31



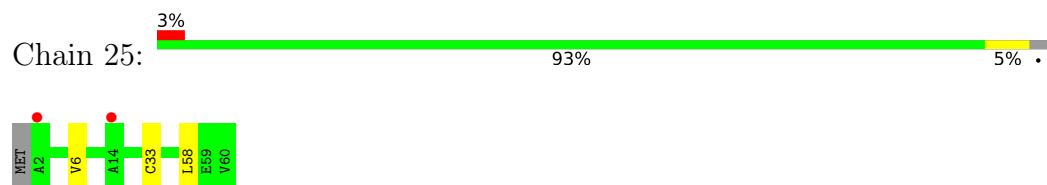
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32

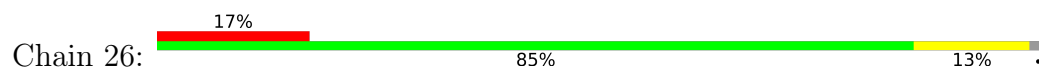


- Molecule 28: 50S ribosomal protein L33

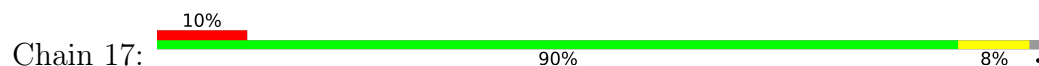




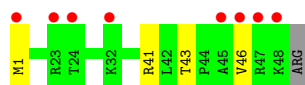
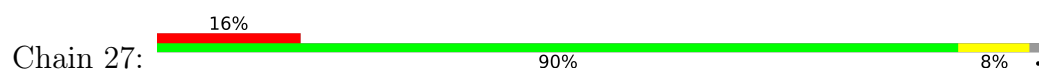
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



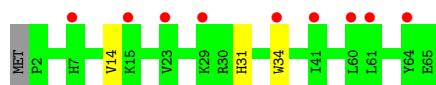
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35



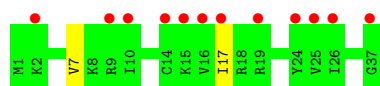
- Molecule 31: 50S ribosomal protein L36



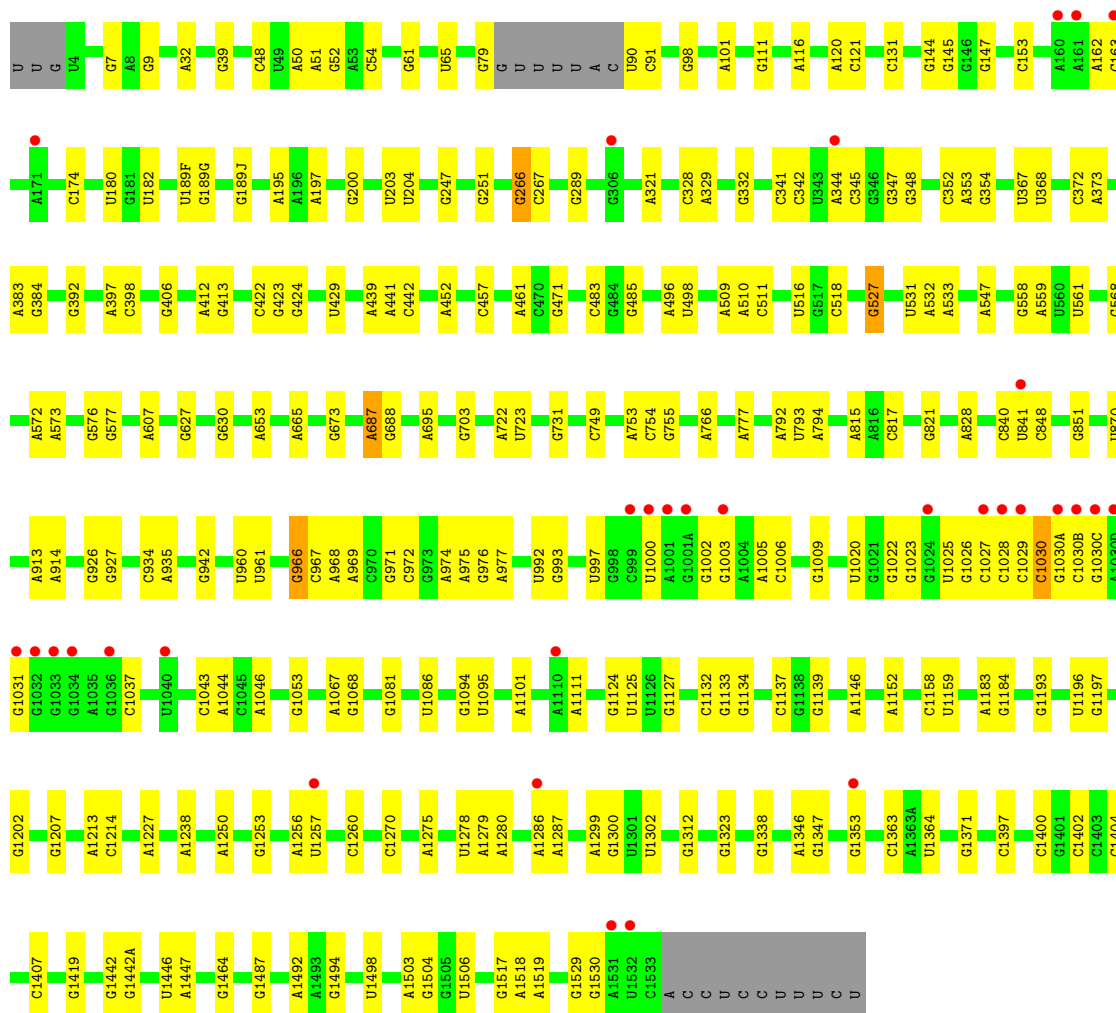
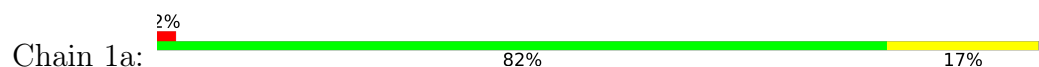
There are no outlier residues recorded for this chain.

- Molecule 31: 50S ribosomal protein L36

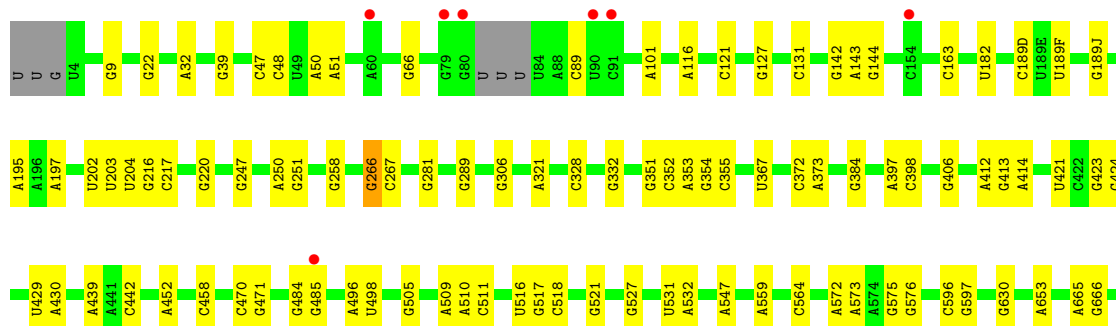
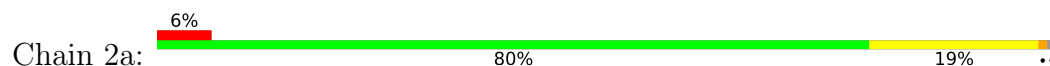


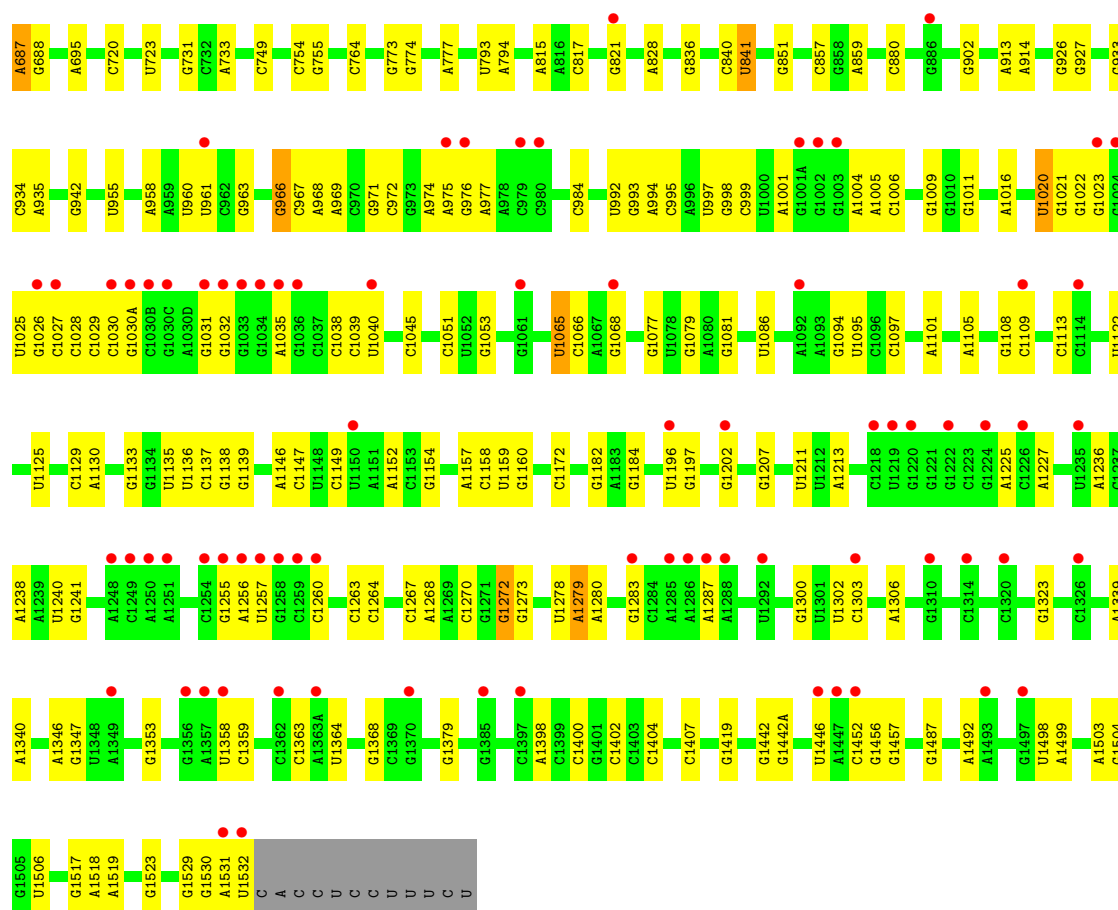


• Molecule 32: 16S Ribosomal RNA

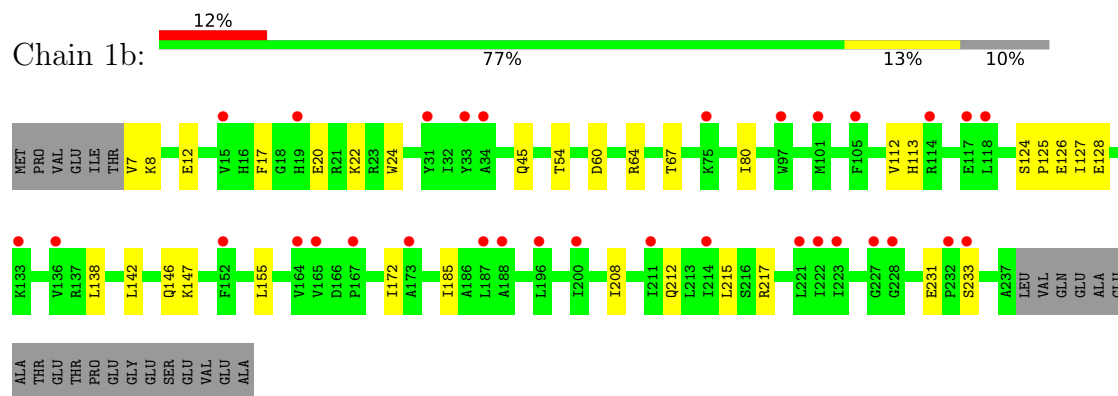


• Molecule 32: 16S Ribosomal RNA

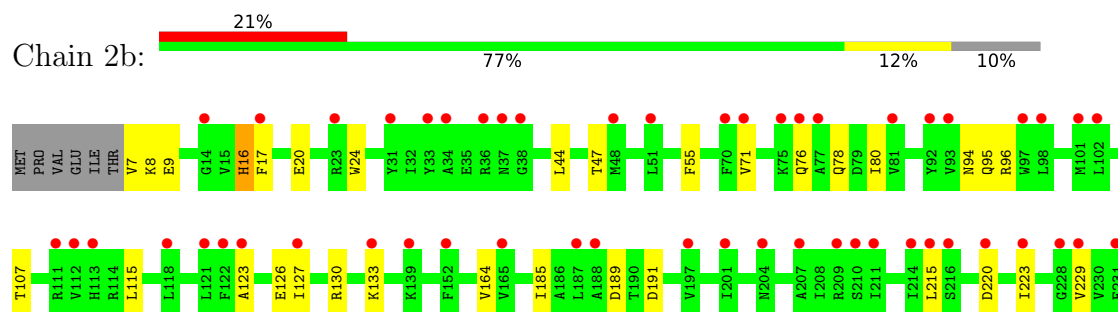


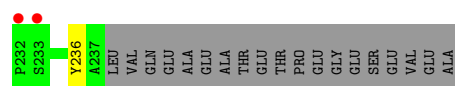


• Molecule 33: 30S ribosomal protein S2

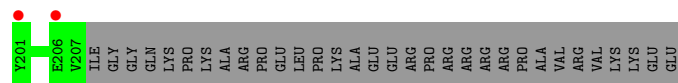
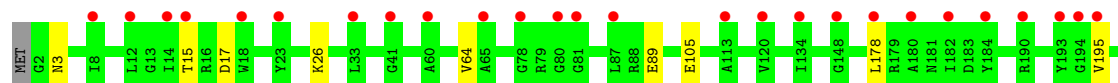
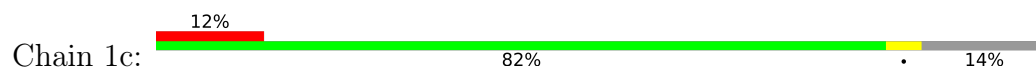


• Molecule 33: 30S ribosomal protein S2

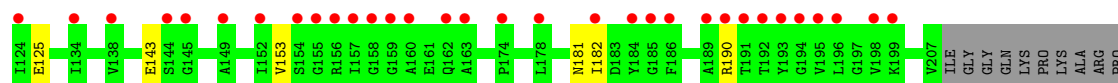
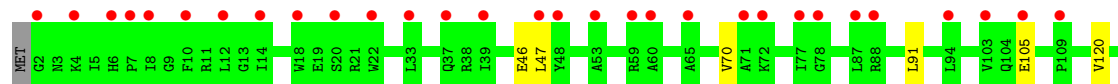
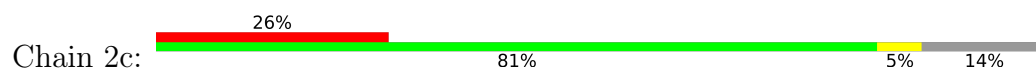




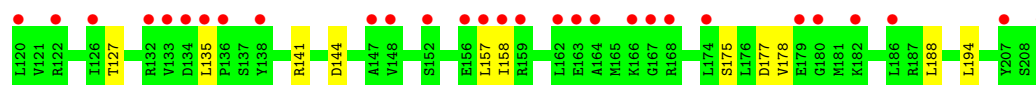
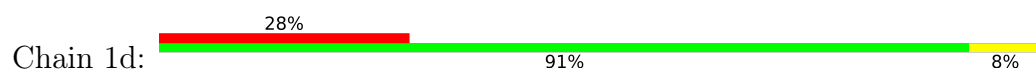
- Molecule 34: 30S ribosomal protein S3



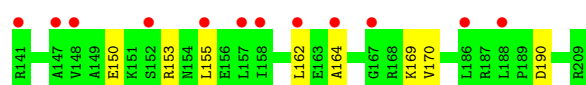
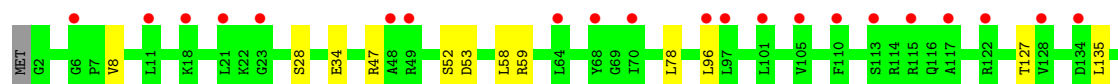
- Molecule 34: 30S ribosomal protein S3



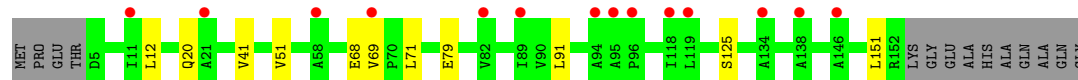
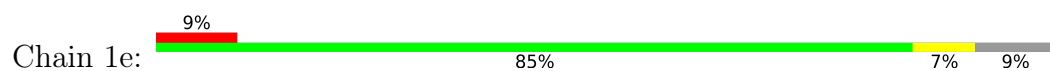
- Molecule 35: 30S ribosomal protein S4



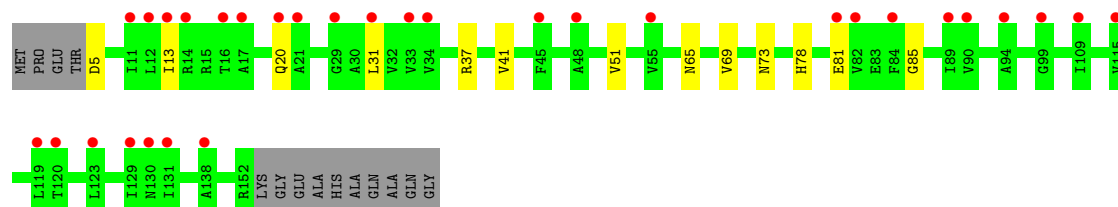
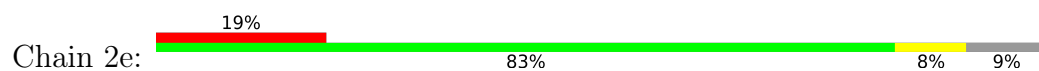
- Molecule 35: 30S ribosomal protein S4



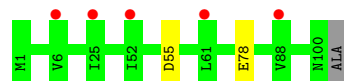
- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5



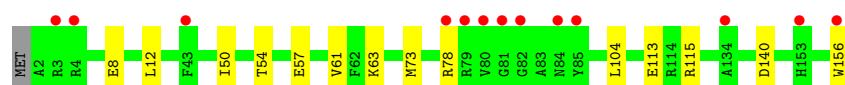
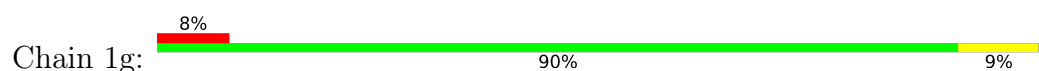
- Molecule 37: 30S ribosomal protein S6



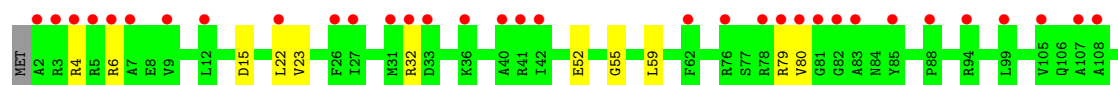
- Molecule 37: 30S ribosomal protein S6

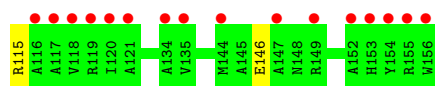


- Molecule 38: 30S ribosomal protein S7



- Molecule 38: 30S ribosomal protein S7

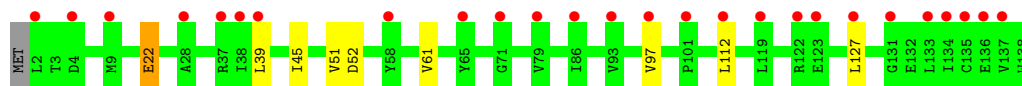
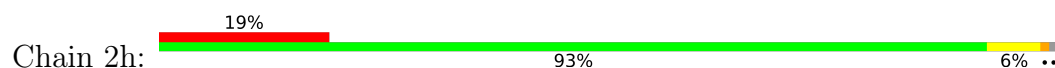




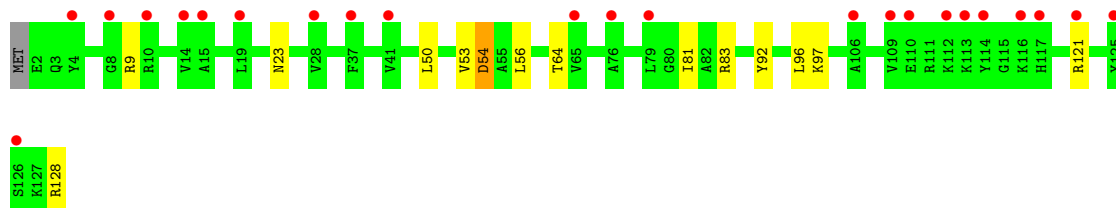
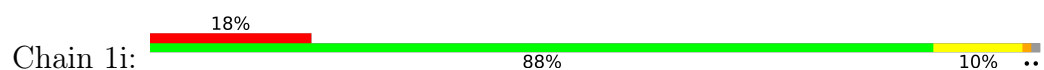
- Molecule 39: 30S ribosomal protein S8



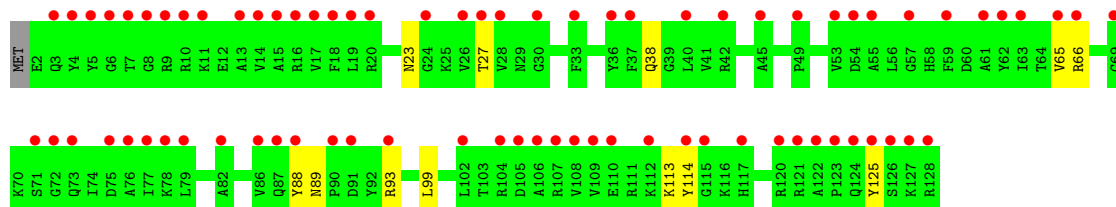
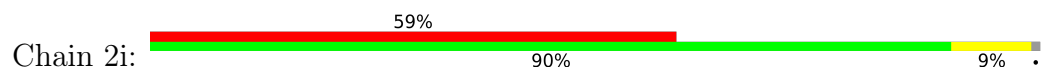
- Molecule 39: 30S ribosomal protein S8



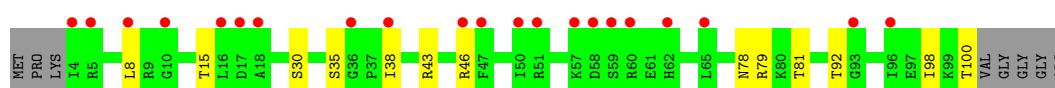
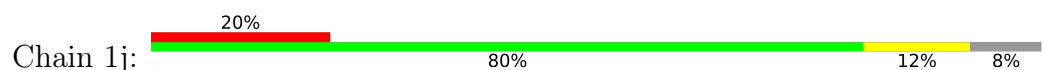
- Molecule 40: 30S ribosomal protein S9



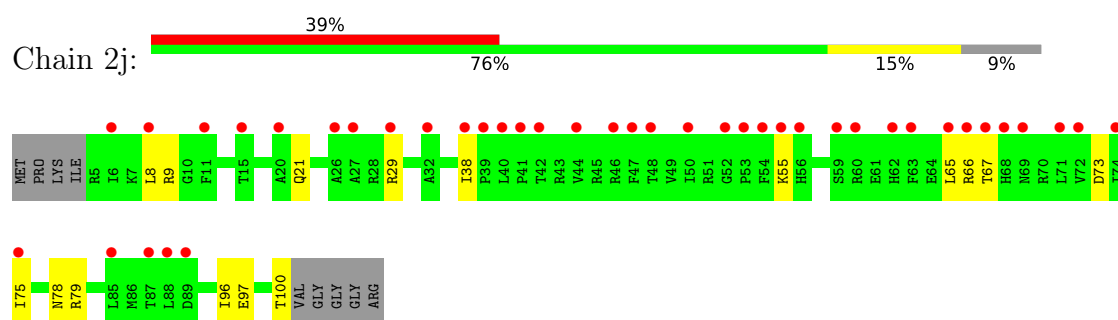
- Molecule 40: 30S ribosomal protein S9



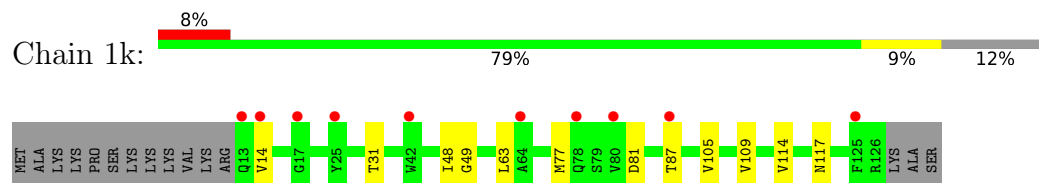
- Molecule 41: 30S ribosomal protein S10



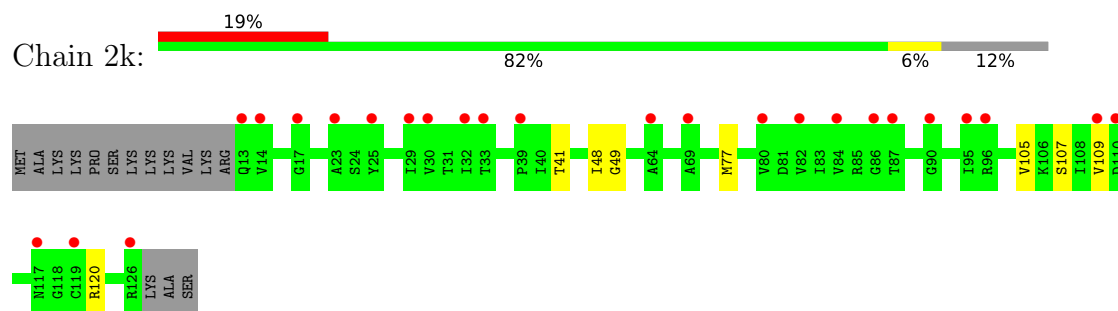
- Molecule 41: 30S ribosomal protein S10



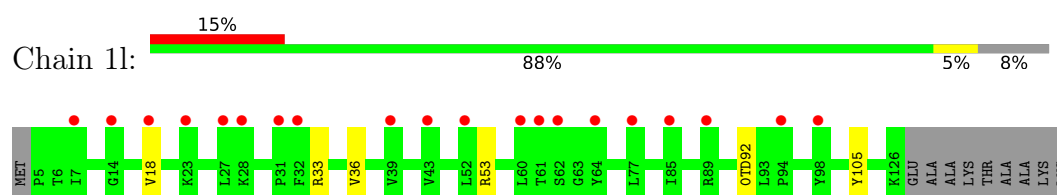
- Molecule 42: 30S ribosomal protein S11



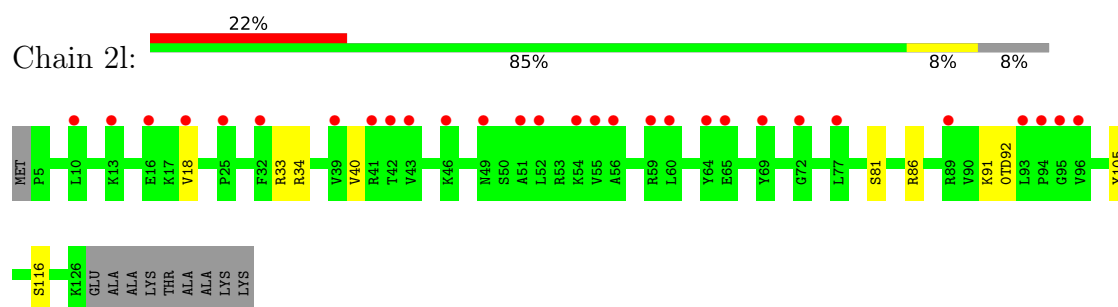
- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12

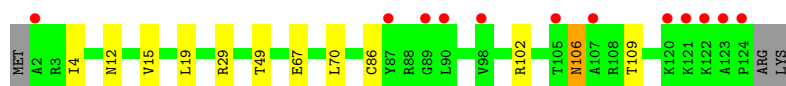


- Molecule 43: 30S ribosomal protein S12

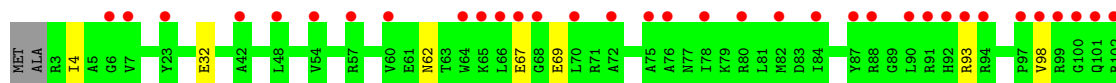
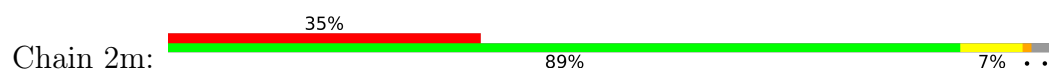


- Molecule 44: 30S ribosomal protein S13

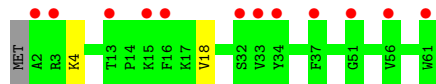




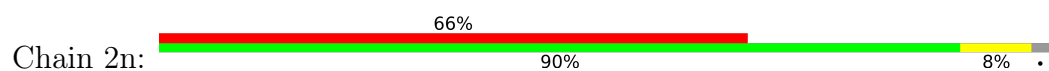
- Molecule 44: 30S ribosomal protein S13



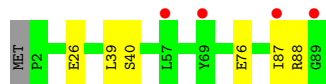
- Molecule 45: 30S ribosomal protein S14 type Z



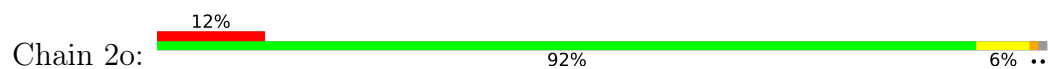
- Molecule 45: 30S ribosomal protein S14 type Z



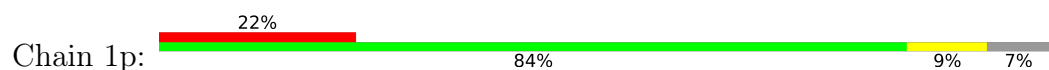
- Molecule 46: 30S ribosomal protein S15

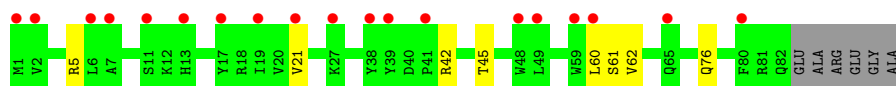


- Molecule 46: 30S ribosomal protein S15

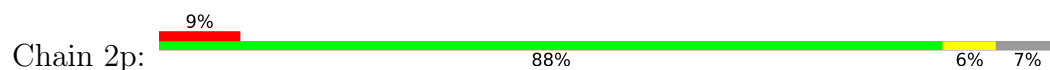


- Molecule 47: 30S ribosomal protein S16

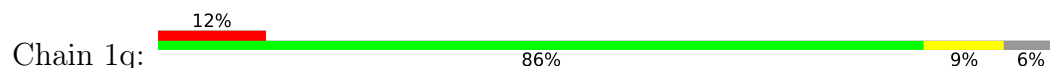




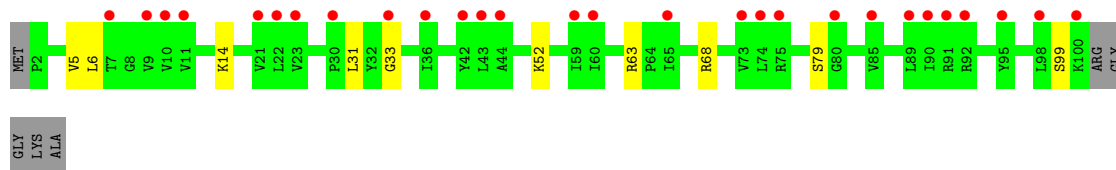
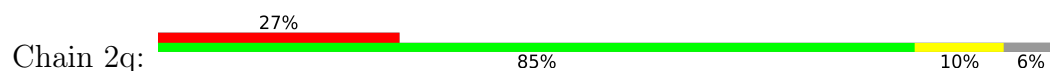
- Molecule 47: 30S ribosomal protein S16



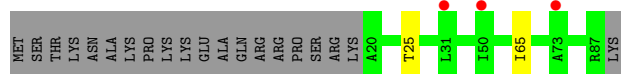
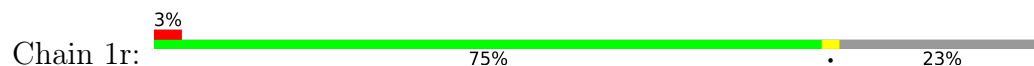
- Molecule 48: 30S ribosomal protein S17



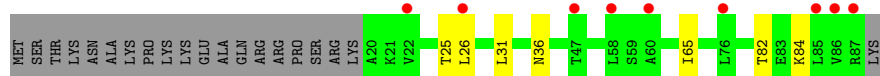
- Molecule 48: 30S ribosomal protein S17



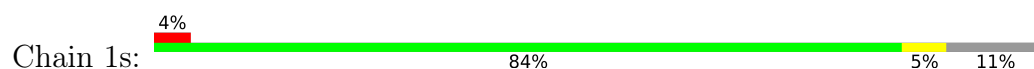
- Molecule 49: 30S ribosomal protein S18



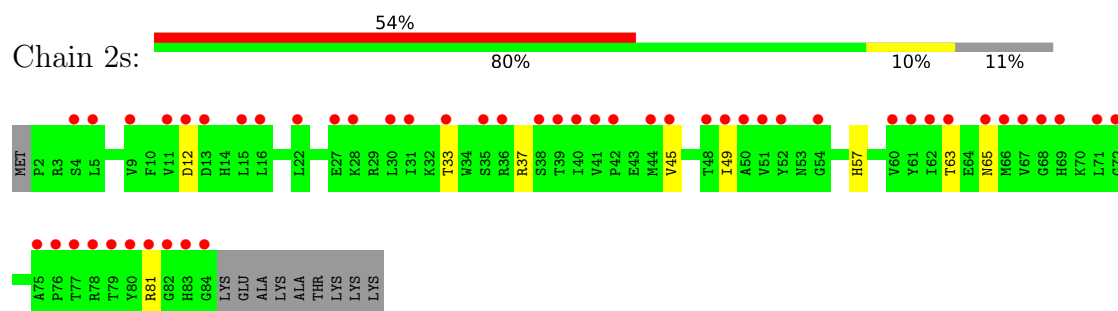
- Molecule 49: 30S ribosomal protein S18



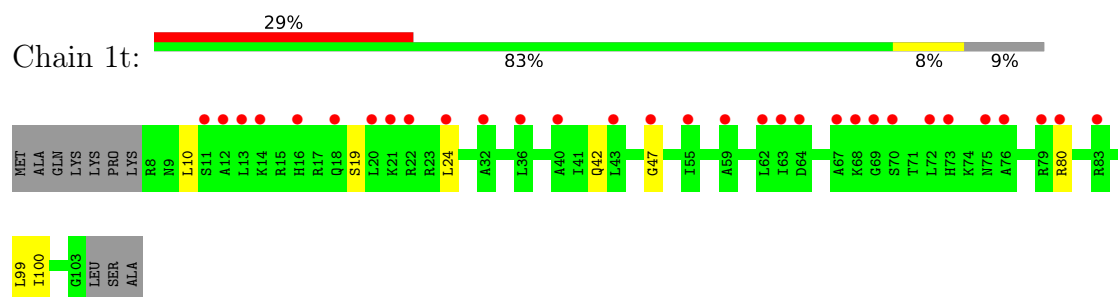
- Molecule 50: 30S ribosomal protein S19



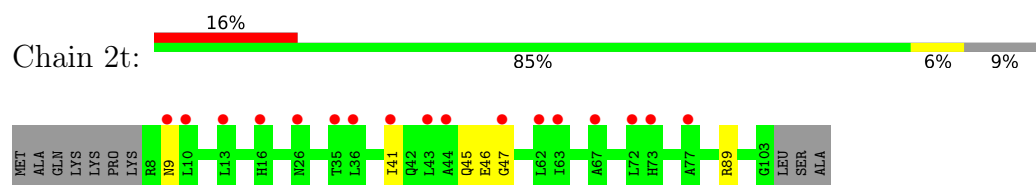
- Molecule 50: 30S ribosomal protein S19



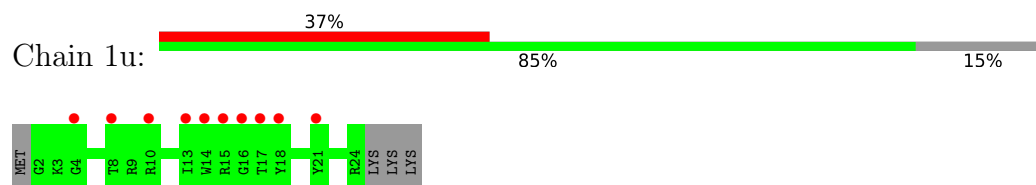
- Molecule 51: 30S ribosomal protein S20



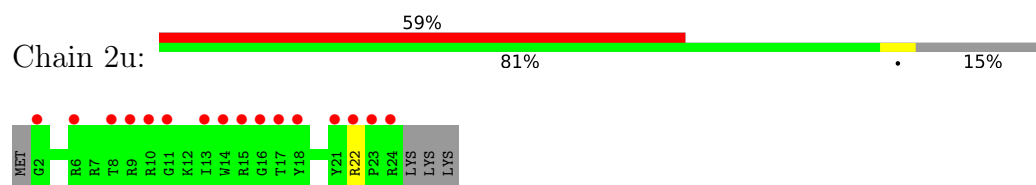
- Molecule 51: 30S ribosomal protein S20



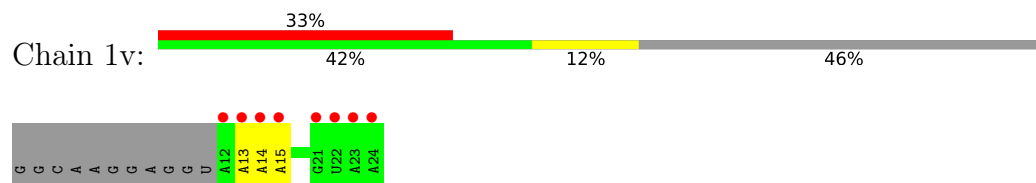
- Molecule 52: 30S ribosomal protein Thx



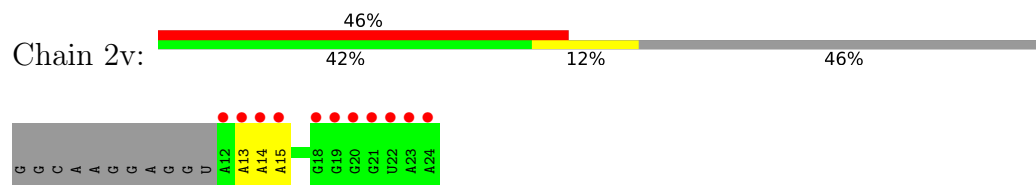
- Molecule 52: 30S ribosomal protein Thx



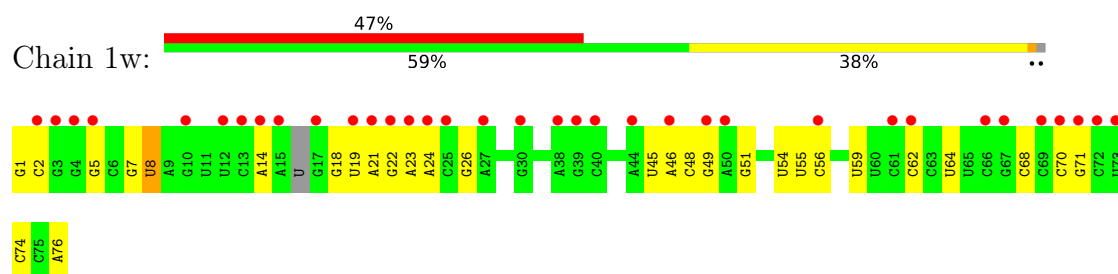
- Molecule 53: MG-mRNA



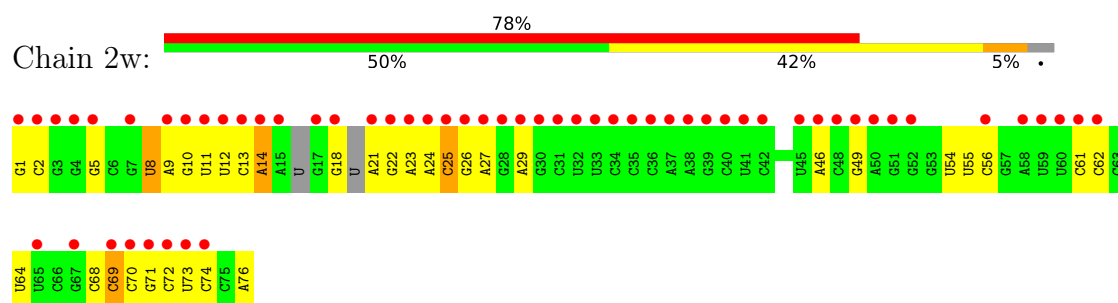
- Molecule 53: MG-mRNA



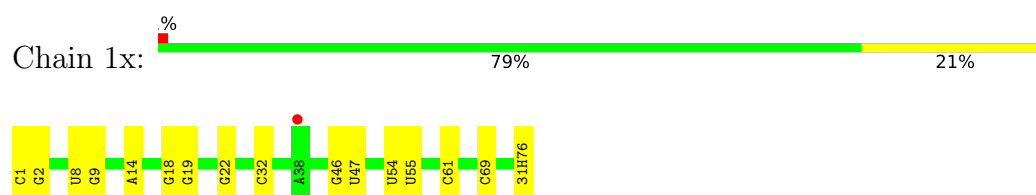
- Molecule 54: A-site Aminoacyl-tRNA Gly-NH-tRNAgly



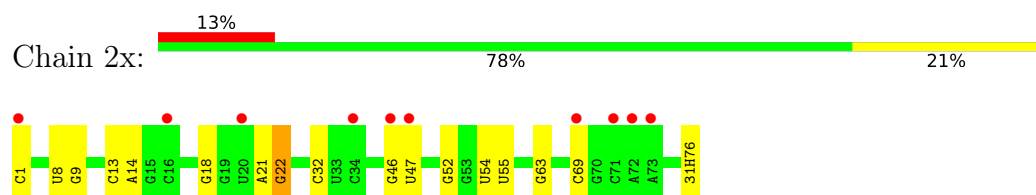
- Molecule 54: A-site Aminoacyl-tRNA Gly-NH-tRNAgly



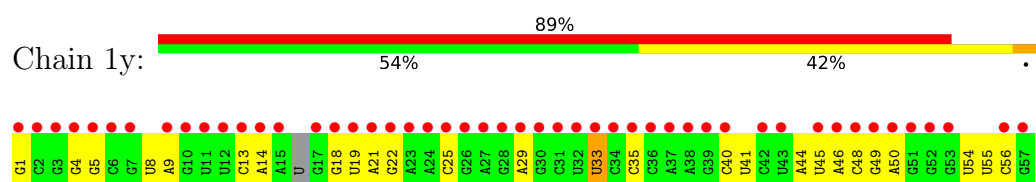
- Molecule 55: P-site Aminoacyl-tRNA fMet-NH-tRNAmet

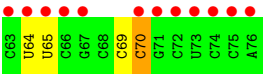


- Molecule 55: P-site Aminoacyl-tRNA fMet-NH-tRNAmet

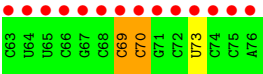


- Molecule 56: E-site Deacylated tRNAgly





● Molecule 56: E-site Deacylated tRNAgly



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.17Å 450.98Å 624.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.74 – 2.55 225.49 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.4 (153.74-2.55) 99.4 (225.49-2.55)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.223 , 0.268 0.223 , 0.268	Depositor DCC
R_{free} test set	94751 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	57.3	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	300046	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

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

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: ZN, 4OC, 2MA, K, 2MG, MA6, 5MU, PSU, 4SU, L3X, OMG, OMU, OMC, M2G, UR3, G7M, 5MC, 0TD, MG, SF4, CLM, 31H

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	0.49	0/69011	0.97	71/107720 (0.1%)
1	2A	0.38	0/67295	0.87	38/105042 (0.0%)
2	1B	0.43	1/2882 (0.0%)	0.86	0/4494
2	2B	0.39	1/2879 (0.0%)	0.83	1/4487 (0.0%)
3	1D	0.34	0/2186	0.55	0/2944
3	2D	0.31	0/2186	0.52	0/2944
4	1E	0.32	0/1592	0.55	0/2149
4	2E	0.30	0/1592	0.51	0/2149
5	1F	0.32	0/1618	0.54	0/2191
5	2F	0.29	0/1614	0.49	0/2186
6	1G	0.29	0/1448	0.48	0/1957
6	2G	0.29	0/1453	0.48	0/1963
7	1H	0.31	0/1356	0.51	0/1834
7	2H	0.27	0/1356	0.47	0/1834
8	1I	0.29	0/1112	0.49	0/1514
8	2I	0.28	0/1079	0.49	0/1475
9	1N	0.33	0/1144	0.51	0/1543
9	2N	0.27	0/1144	0.46	0/1543
10	1O	0.36	0/943	0.53	0/1269
10	2O	0.29	0/943	0.52	0/1269
11	1P	0.32	0/1152	0.58	0/1533
11	2P	0.29	0/1152	0.53	0/1533
12	1Q	0.33	0/1143	0.52	0/1527
12	2Q	0.30	0/1143	0.50	0/1527
13	1R	0.32	0/982	0.54	0/1312
13	2R	0.27	0/982	0.51	0/1312
14	1S	0.30	0/883	0.52	0/1176
14	2S	0.29	0/880	0.50	0/1172
15	1T	0.34	0/1105	0.50	0/1477
15	2T	0.29	0/1097	0.47	0/1468
16	1U	0.34	0/977	0.53	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.28	0/977	0.43	0/1301
17	1V	0.34	0/782	0.56	0/1049
17	2V	0.29	0/782	0.51	0/1049
18	1W	0.34	0/897	0.52	0/1205
18	2W	0.29	0/897	0.51	0/1205
19	1X	0.36	0/764	0.55	0/1025
19	2X	0.31	0/764	0.52	0/1025
20	1Y	0.31	0/819	0.53	0/1095
20	2Y	0.30	0/819	0.50	0/1095
21	1Z	0.29	0/1267	0.51	0/1717
21	2Z	0.29	0/1299	0.51	0/1763
22	10	0.34	0/662	0.54	0/881
22	20	0.30	0/662	0.49	0/881
23	11	0.30	0/762	0.50	0/1014
23	21	0.30	0/762	0.50	0/1014
24	12	0.29	0/590	0.47	0/781
24	22	0.25	0/590	0.41	0/781
25	13	0.32	0/474	0.53	0/635
25	23	0.26	0/469	0.45	0/630
26	14	0.30	0/565	0.57	0/761
26	24	0.29	0/545	0.50	0/737
27	15	0.32	0/469	0.58	0/635
27	25	0.30	0/469	0.48	0/635
28	16	0.32	0/460	0.54	0/613
28	26	0.28	0/456	0.49	0/608
29	17	0.34	0/426	0.54	0/561
29	27	0.30	0/426	0.47	0/561
30	18	0.30	0/525	0.52	0/691
30	28	0.28	0/525	0.48	0/691
31	19	0.32	0/310	0.50	0/407
31	29	0.27	0/310	0.53	0/407
32	1a	0.35	0/35795	0.87	15/55864 (0.0%)
32	2a	0.34	2/35886 (0.0%)	0.88	38/56005 (0.1%)
33	1b	0.29	0/1881	0.48	0/2542
33	2b	0.30	0/1860	0.49	0/2518
34	1c	0.29	0/1572	0.46	0/2126
34	2c	0.29	0/1566	0.50	0/2119
35	1d	0.28	0/1685	0.47	0/2262
35	2d	0.28	0/1704	0.45	0/2284
36	1e	0.29	0/1145	0.51	0/1543
36	2e	0.29	0/1149	0.50	0/1548
37	1f	0.27	0/823	0.47	0/1115
37	2f	0.28	0/829	0.48	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.27	0/1250	0.44	0/1679
38	2g	0.28	0/1254	0.45	0/1683
39	1h	0.28	0/1108	0.48	0/1494
39	2h	0.27	0/1108	0.47	0/1494
40	1i	0.29	0/1002	0.48	0/1346
40	2i	0.29	0/997	0.50	0/1343
41	1j	0.26	0/722	0.47	0/982
41	2j	0.29	0/727	0.52	0/988
42	1k	0.28	0/844	0.51	0/1145
42	2k	0.28	0/848	0.46	0/1149
43	1l	0.29	0/937	0.49	0/1260
43	2l	0.28	0/937	0.49	0/1260
44	1m	0.28	0/969	0.48	0/1302
44	2m	0.27	0/961	0.47	0/1291
45	1n	0.30	0/501	0.46	0/664
45	2n	0.30	0/501	0.46	0/664
46	1o	0.27	0/739	0.41	0/985
46	2o	0.26	0/739	0.42	0/985
47	1p	0.28	0/697	0.53	0/939
47	2p	0.26	0/693	0.52	0/935
48	1q	0.28	0/836	0.49	0/1117
48	2q	0.27	0/836	0.47	0/1117
49	1r	0.27	0/560	0.51	0/746
49	2r	0.27	0/560	0.48	0/746
50	1s	0.27	0/667	0.51	0/900
50	2s	0.29	0/661	0.54	0/893
51	1t	0.28	0/730	0.46	0/965
51	2t	0.30	0/729	0.43	0/965
52	1u	0.26	0/203	0.46	0/266
52	2u	0.28	0/203	0.47	0/266
53	1v	0.43	0/322	0.84	0/501
53	2v	0.40	0/322	0.88	0/501
54	1w	0.52	1/1639 (0.1%)	1.11	2/2548 (0.1%)
54	2w	0.53	1/1616 (0.1%)	1.12	8/2510 (0.3%)
55	1x	0.57	4/1723 (0.2%)	1.11	16/2684 (0.6%)
55	2x	0.51	1/1723 (0.1%)	1.05	10/2684 (0.4%)
56	1y	0.55	1/1664 (0.1%)	1.13	8/2587 (0.3%)
56	2y	0.56	1/1664 (0.1%)	1.19	9/2587 (0.3%)
All	All	0.38	13/316940 (0.0%)	0.83	216/474518 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
51	1t	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	1	C	OP3-P	-10.68	1.48	1.61
2	2B	1	U	OP3-P	-10.41	1.48	1.61
2	1B	1	U	OP3-P	-10.37	1.48	1.61
56	2y	1	G	OP3-P	-10.25	1.48	1.61
54	2w	1	G	OP3-P	-10.24	1.48	1.61
55	2x	1	C	OP3-P	-10.20	1.49	1.61
54	1w	1	G	OP3-P	-10.13	1.49	1.61
56	1y	1	G	OP3-P	-10.12	1.49	1.61
32	2a	1272	G	N1-C2	-7.19	1.31	1.37
32	2a	1272	G	C6-N1	-6.58	1.34	1.39
55	1x	14	A	C8-N7	-5.27	1.27	1.31
55	1x	22	G	N7-C5	5.22	1.42	1.39
55	1x	14	A	N7-C5	-5.13	1.36	1.39

All (216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1263	C	N1-C2-O2	20.51	131.20	118.90
32	2a	1272	G	N3-C2-N2	18.18	132.63	119.90
32	2a	1272	G	N1-C2-N2	-15.89	101.90	116.20
32	2a	1272	G	C5-C6-O6	14.92	137.55	128.60
32	2a	1263	C	C2-N3-C4	12.71	126.26	119.90
1	2A	2136	C	N1-C2-O2	11.93	126.06	118.90
55	1x	46	G	C6-N1-C2	-11.02	118.49	125.10
32	2a	1263	C	N3-C2-O2	-10.87	114.29	121.90
2	2B	80	U	O4'-C1'-N1	10.36	116.49	108.20
32	2a	1272	G	C6-N1-C2	10.12	131.17	125.10
32	2a	1263	C	C5-C6-N1	9.81	125.91	121.00
55	1x	14	A	C4-C5-C6	9.66	121.83	117.00
32	2a	1272	G	C5-C6-N1	-9.54	106.73	111.50
55	1x	14	A	C5-N7-C8	9.53	108.66	103.90
1	1A	2577	A	O5'-P-OP1	-9.31	97.32	105.70
32	1a	1030(B)	C	C2-N1-C1'	9.30	129.03	118.80
1	1A	1352	U	O5'-P-OP1	-8.82	97.76	105.70
1	1A	1063	G	C5-C6-O6	8.75	133.85	128.60
1	1A	1075	C	N1-C2-O2	8.64	124.08	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2155	G	N3-C2-N2	8.56	125.89	119.90
55	2x	46	G	C6-N1-C2	-8.45	120.03	125.10
55	2x	14	A	C4-C5-C6	8.32	121.16	117.00
1	1A	1075	C	C2-N3-C4	8.22	124.01	119.90
1	1A	512	G	O4'-C1'-N9	8.10	114.68	108.20
1	1A	801	G	O5'-P-OP2	-8.00	98.50	105.70
54	2w	14	A	C5-C6-N6	-7.98	117.31	123.70
1	1A	787	U	O5'-P-OP1	-7.88	98.60	105.70
55	1x	22	G	C5-N7-C8	-7.87	100.36	104.30
32	1a	1030(B)	C	N1-C2-O2	7.87	123.62	118.90
1	2A	2155	G	C6-N1-C2	7.86	129.81	125.10
1	1A	2682	U	O5'-P-OP2	-7.75	98.73	105.70
32	2a	1263	C	C2-N1-C1'	7.64	127.20	118.80
32	2a	1272	G	C4-N9-C1'	7.60	136.38	126.50
55	1x	14	A	C5-C6-N1	-7.53	113.93	117.70
32	2a	754	C	C2-N1-C1'	7.42	126.96	118.80
1	1A	1086	A	N1-C6-N6	-7.39	114.17	118.60
56	2y	14	A	N1-C6-N6	7.36	123.02	118.60
1	1A	1776	G	O5'-P-OP2	-7.35	99.08	105.70
32	2a	1272	G	C2-N3-C4	-7.33	108.23	111.90
56	2y	69	C	N1-C2-O2	7.30	123.28	118.90
32	1a	1030(B)	C	C6-N1-C2	-7.29	117.38	120.30
32	2a	1272	G	C8-N9-C1'	-7.25	117.58	127.00
1	2A	2136	C	C2-N3-C4	7.12	123.46	119.90
1	1A	1080	C	N1-C2-O2	7.09	123.15	118.90
56	1y	33	U	C2-N1-C1'	7.07	126.18	117.70
55	1x	22	G	C4-C5-C6	-7.05	114.57	118.80
55	1x	46	G	C5-C6-N1	7.03	115.02	111.50
56	2y	14	A	C5-C6-N6	-7.01	118.09	123.70
1	2A	1992	G	P-O3'-C3'	7.01	128.11	119.70
32	2a	1272	G	N1-C6-O6	-7.01	115.70	119.90
1	2A	2136	C	N3-C2-O2	-6.99	117.01	121.90
1	1A	1063	G	N3-C2-N2	6.96	124.77	119.90
32	2a	1263	C	C4-C5-C6	-6.94	113.93	117.40
1	1A	2248	C	O5'-P-OP2	-6.89	99.50	105.70
1	2A	1698	A	O4'-C1'-N9	6.83	113.66	108.20
1	1A	999	U	O5'-P-OP2	-6.83	99.56	105.70
1	1A	548	A	P-O3'-C3'	6.79	127.85	119.70
1	1A	2593	U	N3-C4-O4	-6.79	114.65	119.40
55	2x	14	A	C5-N7-C8	6.79	107.29	103.90
1	1A	576	U	O5'-P-OP1	-6.79	99.59	105.70
1	1A	567	A	O5'-P-OP1	-6.74	99.64	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1263	C	N1-C2-N3	-6.73	114.49	119.20
56	1y	33	U	N1-C2-O2	6.70	127.49	122.80
54	2w	14	A	N1-C6-N6	6.70	122.62	118.60
1	1A	1131	G	O4'-C1'-N9	6.69	113.55	108.20
1	1A	819	A	O5'-P-OP1	-6.68	99.69	105.70
1	1A	847	U	C2-N1-C1'	6.65	125.69	117.70
54	1w	64	U	C5-C4-O4	-6.65	121.91	125.90
1	1A	2848	G	O4'-C1'-N9	6.60	113.48	108.20
1	1A	746	A	O4'-C1'-N9	6.59	113.47	108.20
32	1a	266	G	P-O3'-C3'	6.57	127.59	119.70
1	1A	975	C	N1-C2-O2	-6.55	114.97	118.90
54	2w	21	A	N9-C4-C5	6.51	108.40	105.80
1	2A	2430	A	O5'-P-OP2	-6.40	99.94	105.70
1	2A	2689	U	N3-C2-O2	-6.37	117.74	122.20
55	1x	46	G	N3-C2-N2	-6.36	115.45	119.90
1	1A	2036	C	O5'-P-OP1	-6.34	99.99	105.70
32	1a	558	G	O5'-P-OP1	-6.33	100.00	105.70
32	2a	1263	C	C6-N1-C2	-6.33	117.77	120.30
56	2y	70	C	N1-C2-O2	6.33	122.70	118.90
1	1A	1272	A	O5'-P-OP2	-6.32	100.01	105.70
55	1x	22	G	C5-C6-N1	6.29	114.64	111.50
55	2x	14	A	C5-C6-N1	-6.29	114.56	117.70
32	1a	1030(B)	C	N3-C2-O2	-6.24	117.53	121.90
1	1A	2167	U	N3-C2-O2	-6.21	117.86	122.20
1	1A	1063	G	N1-C6-O6	-6.21	116.18	119.90
54	2w	14	A	C5-N7-C8	-6.18	100.81	103.90
1	2A	2155	G	C5-C6-O6	6.18	132.31	128.60
1	1A	548	A	OP1-P-O3'	6.13	118.69	105.20
1	1A	2134	A	P-O3'-C3'	6.13	127.05	119.70
32	1a	1030(B)	C	C6-N1-C1'	-6.09	113.49	120.80
1	2A	2689	U	P-O3'-C3'	6.06	126.97	119.70
1	1A	2554	U	O5'-P-OP1	-6.04	100.27	105.70
55	2x	22	G	C5-N7-C8	-6.04	101.28	104.30
32	2a	754	C	N1-C2-O2	6.03	122.52	118.90
1	1A	2685	G	N1-C6-O6	-6.02	116.29	119.90
1	1A	2593	U	N3-C4-C5	6.02	118.21	114.60
1	1A	226	G	O4'-C1'-N9	6.02	113.01	108.20
32	2a	1225	A	C5-C6-N6	5.98	128.49	123.70
32	2a	841	U	C2-N1-C1'	5.98	124.88	117.70
1	1A	250	G	C8-N9-C4	-5.98	104.01	106.40
1	2A	1639	U	O5'-P-OP2	-5.96	100.34	105.70
56	1y	69	C	C2-N1-C1'	5.94	125.33	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	14	A	C8-N9-C1'	-5.94	117.01	127.70
55	1x	22	G	N1-C6-O6	-5.94	116.34	119.90
32	2a	955	U	C5-C4-O4	5.92	129.45	125.90
1	2A	1204	A	O4'-C1'-N9	5.92	112.94	108.20
32	1a	1030(B)	C	C5-C6-N1	5.91	123.95	121.00
1	1A	1992	G	P-O3'-C3'	5.91	126.79	119.70
55	1x	14	A	C4-N9-C1'	5.91	136.93	126.30
32	2a	1158	C	C2-N1-C1'	5.91	125.30	118.80
1	2A	1313	U	C2-N1-C1'	5.90	124.78	117.70
32	2a	841	U	C5-C6-N1	5.88	125.64	122.70
56	1y	33	U	N3-C2-O2	-5.87	118.09	122.20
1	1A	2151	G	N3-C2-N2	5.85	124.00	119.90
55	1x	46	G	C5-C6-O6	-5.82	125.11	128.60
55	2x	22	G	C4-C5-C6	-5.82	115.31	118.80
1	2A	645	C	N1-C2-O2	5.81	122.39	118.90
1	1A	197	A	O5'-P-OP1	-5.78	100.50	105.70
1	1A	1290	C	C6-N1-C2	-5.75	118.00	120.30
32	2a	1263	C	C5-C4-N4	5.75	124.23	120.20
1	2A	1698	A	C6-C5-N7	-5.75	128.28	132.30
32	1a	754	C	C2-N1-C1'	5.72	125.10	118.80
32	1a	754	C	N1-C2-O2	5.71	122.32	118.90
1	1A	1174	A	P-O3'-C3'	5.70	126.54	119.70
32	1a	1030	C	N1-C2-O2	5.69	122.32	118.90
1	2A	1614	A	O5'-P-OP1	-5.69	100.58	105.70
54	1w	64	U	N3-C4-O4	5.69	123.38	119.40
56	2y	69	C	C2-N3-C4	5.68	122.74	119.90
32	2a	1225	A	C6-N1-C2	5.67	122.00	118.60
1	1A	740	U	O5'-P-OP2	-5.64	100.62	105.70
32	1a	90	U	N3-C2-O2	-5.62	118.26	122.20
54	2w	69	C	C2-N3-C4	5.60	122.70	119.90
32	2a	754	C	C6-N1-C1'	-5.60	114.08	120.80
1	1A	2629	A	P-O3'-C3'	5.60	126.42	119.70
1	1A	2134	A	OP1-P-O3'	5.58	117.48	105.20
54	2w	25	C	C2-N1-C1'	5.58	124.94	118.80
54	2w	14	A	C4-C5-N7	5.57	113.48	110.70
1	1A	2167	U	C2-N1-C1'	5.56	124.37	117.70
1	1A	195	A	P-O3'-C3'	5.55	126.36	119.70
1	1A	1080	C	C2-N3-C4	5.55	122.68	119.90
1	1A	1395	A	O5'-P-OP1	-5.55	100.71	105.70
1	1A	372	G	O4'-C1'-N9	5.54	112.63	108.20
1	2A	614	U	N3-C2-O2	-5.54	118.32	122.20
1	1A	2167	U	N1-C2-O2	5.53	126.67	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	955	U	C2-N3-C4	5.50	130.30	127.00
55	2x	22	G	N1-C6-O6	-5.50	116.60	119.90
1	2A	746	A	O4'-C1'-N9	5.49	112.59	108.20
1	2A	330	A	C2-N3-C4	-5.48	107.86	110.60
55	1x	14	A	C4-C5-N7	-5.47	107.96	110.70
32	2a	1158	C	N1-C2-O2	5.47	122.18	118.90
1	2A	383	U	O4'-C1'-N1	5.46	112.56	108.20
32	2a	266	G	P-O3'-C3'	5.44	126.22	119.70
1	2A	2119	A	OP1-P-O3'	5.42	117.12	105.20
32	1a	1158	C	N1-C2-O2	5.41	122.15	118.90
55	2x	46	G	N3-C2-N2	-5.41	116.11	119.90
32	2a	687	A	P-O3'-C3'	5.41	126.19	119.70
32	2a	266	G	N3-C4-C5	-5.39	125.91	128.60
1	2A	1313	U	N3-C2-O2	-5.37	118.44	122.20
32	2a	1263	C	N3-C4-N4	-5.37	114.24	118.00
32	1a	1067	A	P-O3'-C3'	5.36	126.13	119.70
1	1A	1075	C	C5-C4-N4	5.34	123.94	120.20
1	1A	2140	C	C2-N3-C4	5.34	122.57	119.90
32	2a	1020	U	N1-C2-O2	5.33	126.53	122.80
1	2A	1698	A	C4-N9-C1'	5.32	135.87	126.30
56	2y	70	C	C2-N1-C1'	5.31	124.64	118.80
55	1x	46	G	N1-C2-N3	5.29	127.08	123.90
1	1A	271(Y)	U	O4'-C1'-N1	5.28	112.42	108.20
55	2x	22	G	C5-C6-N1	5.26	114.13	111.50
55	2x	22	G	C8-N9-C1'	5.25	133.82	127.00
56	1y	70	C	C2-N1-C1'	5.24	124.56	118.80
1	1A	383	U	O4'-C1'-N1	5.23	112.38	108.20
1	2A	914	C	N1-C2-O2	5.23	122.04	118.90
1	1A	1176	G	OP1-P-O3'	5.23	116.70	105.20
1	1A	1063	G	C6-N1-C2	5.22	128.23	125.10
32	2a	841	U	N1-C2-O2	5.22	126.45	122.80
32	2a	1065	U	P-O3'-C3'	5.20	125.94	119.70
1	1A	845	G	O4'-C1'-N9	5.20	112.36	108.20
1	1A	2553	G	N3-C4-N9	5.20	129.12	126.00
1	2A	2129	C	N1-C2-O2	5.20	122.02	118.90
55	1x	22	G	C8-N9-C1'	5.19	133.74	127.00
1	1A	1174	A	OP1-P-O3'	5.18	116.60	105.20
1	1A	2791	C	C6-N1-C2	-5.17	118.23	120.30
1	2A	2177	C	C5-C6-N1	5.17	123.58	121.00
1	1A	1190	G	C5-N7-C8	5.15	106.88	104.30
1	2A	1698	A	N1-C6-N6	5.15	121.69	118.60
1	2A	847	U	C2-N1-C1'	5.14	123.87	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	214	G	O4'-C1'-N9	5.13	112.31	108.20
1	2A	1786	A	O4'-C1'-N9	5.13	112.31	108.20
1	2A	1313	U	N1-C2-O2	5.13	126.39	122.80
56	1y	64	U	C2-N3-C4	5.13	130.08	127.00
32	2a	1279	A	OP1-P-O3'	5.13	116.48	105.20
56	2y	7	G	C4-N9-C1'	5.12	133.16	126.50
1	1A	748	G	O4'-C1'-N9	5.12	112.30	108.20
1	1A	1614	A	O5'-P-OP1	-5.12	101.10	105.70
1	1A	298	G	C5-N7-C8	5.11	106.86	104.30
32	2a	913	A	P-O3'-C3'	5.10	125.81	119.70
1	2A	228	A	P-O3'-C3'	5.09	125.81	119.70
1	2A	915	C	N1-C2-O2	5.09	121.95	118.90
56	2y	7	G	C8-N9-C1'	-5.09	120.39	127.00
1	2A	2155	G	N1-C2-N3	-5.07	120.86	123.90
1	2A	914	C	N3-C2-O2	-5.06	118.36	121.90
1	1A	975	C	C5-C6-N1	-5.06	118.47	121.00
1	1A	1063	G	N1-C2-N2	-5.06	111.65	116.20
56	2y	7	G	N3-C4-N9	5.06	129.04	126.00
1	1A	2429	G	OP1-P-OP2	-5.06	112.01	119.60
1	1A	570	G	C5-C6-O6	-5.05	125.57	128.60
56	1y	69	C	C6-N1-C1'	-5.05	114.74	120.80
1	1A	1080	C	N3-C2-O2	-5.04	118.37	121.90
1	1A	783	A	N3-C4-C5	-5.04	123.27	126.80
1	2A	2593	U	N3-C4-O4	-5.04	115.87	119.40
54	2w	29	A	C5-C6-N6	5.04	127.73	123.70
32	1a	687	A	P-O3'-C3'	5.03	125.73	119.70
1	1A	1082	U	N3-C4-O4	-5.02	115.88	119.40
1	2A	512	G	O4'-C1'-N9	5.01	112.21	108.20
56	1y	64	U	C5-C4-O4	5.00	128.90	125.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	1t	99	LEU	Peptide

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	256 (94%)	16 (6%)	1 (0%)	34	46
3	2D	273/276 (99%)	256 (94%)	16 (6%)	1 (0%)	34	46
4	1E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	29	40
4	2E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	29	40
5	1F	200/210 (95%)	193 (96%)	6 (3%)	1 (0%)	29	40
5	2F	200/210 (95%)	187 (94%)	12 (6%)	1 (0%)	29	40
6	1G	179/182 (98%)	166 (93%)	11 (6%)	2 (1%)	14	19
6	2G	179/182 (98%)	150 (84%)	25 (14%)	4 (2%)	6	7
7	1H	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	25	34
7	2H	172/180 (96%)	155 (90%)	17 (10%)	0	100	100
8	1I	144/148 (97%)	128 (89%)	15 (10%)	1 (1%)	22	30
8	2I	144/148 (97%)	120 (83%)	22 (15%)	2 (1%)	11	15
9	1N	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
9	2N	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	2O	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	19	27
11	1P	147/150 (98%)	133 (90%)	12 (8%)	2 (1%)	11	15
11	2P	147/150 (98%)	131 (89%)	12 (8%)	4 (3%)	5	4
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
12	2Q	139/141 (99%)	127 (91%)	12 (9%)	0	100	100
13	1R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	1S	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
14	2S	108/112 (96%)	100 (93%)	4 (4%)	4 (4%)	3	2
15	1T	129/146 (88%)	123 (95%)	4 (3%)	2 (2%)	9	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	95 (96%)	2 (2%)	2 (2%)	7	8
17	2V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	15	22
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
19	1X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	14	19
19	2X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
20	1Y	105/110 (96%)	99 (94%)	5 (5%)	1 (1%)	15	22
20	2Y	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
21	1Z	148/206 (72%)	133 (90%)	13 (9%)	2 (1%)	11	15
21	2Z	156/206 (76%)	119 (76%)	34 (22%)	3 (2%)	8	9
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
22	20	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	14	19
23	21	95/98 (97%)	90 (95%)	4 (4%)	1 (1%)	14	19
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	10
26	14	67/71 (94%)	52 (78%)	9 (13%)	6 (9%)	1	0
26	24	67/71 (94%)	50 (75%)	15 (22%)	2 (3%)	4	3
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	46 (90%)	5 (10%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	60 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	188 (82%)	32 (14%)	9 (4%)	3	1
33	2b	229/256 (90%)	184 (80%)	37 (16%)	8 (4%)	3	2
34	1c	204/239 (85%)	193 (95%)	11 (5%)	0	100	100
34	2c	204/239 (85%)	176 (86%)	26 (13%)	2 (1%)	15	22
35	1d	206/209 (99%)	189 (92%)	16 (8%)	1 (0%)	29	40
35	2d	206/209 (99%)	190 (92%)	15 (7%)	1 (0%)	29	40
36	1e	146/162 (90%)	131 (90%)	14 (10%)	1 (1%)	22	30
36	2e	146/162 (90%)	127 (87%)	15 (10%)	4 (3%)	5	4
37	1f	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
37	2f	98/101 (97%)	98 (100%)	0	0	100	100
38	1g	153/156 (98%)	140 (92%)	12 (8%)	1 (1%)	22	30
38	2g	153/156 (98%)	139 (91%)	10 (6%)	4 (3%)	5	5
39	1h	135/138 (98%)	126 (93%)	8 (6%)	1 (1%)	22	30
39	2h	135/138 (98%)	124 (92%)	10 (7%)	1 (1%)	22	30
40	1i	125/128 (98%)	111 (89%)	12 (10%)	2 (2%)	9	12
40	2i	125/128 (98%)	108 (86%)	16 (13%)	1 (1%)	19	27
41	1j	95/105 (90%)	76 (80%)	16 (17%)	3 (3%)	4	3
41	2j	94/105 (90%)	79 (84%)	12 (13%)	3 (3%)	4	3
42	1k	112/129 (87%)	106 (95%)	3 (3%)	3 (3%)	5	4
42	2k	112/129 (87%)	101 (90%)	9 (8%)	2 (2%)	8	10
43	1l	119/132 (90%)	113 (95%)	5 (4%)	1 (1%)	19	27
43	2l	119/132 (90%)	109 (92%)	8 (7%)	2 (2%)	9	11
44	1m	121/126 (96%)	105 (87%)	14 (12%)	2 (2%)	9	11
44	2m	120/126 (95%)	107 (89%)	11 (9%)	2 (2%)	9	11
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	2n	58/61 (95%)	53 (91%)	3 (5%)	2 (3%)	3	2
46	1o	86/89 (97%)	82 (95%)	2 (2%)	2 (2%)	6	6
46	2o	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	13	17
47	1p	80/88 (91%)	70 (88%)	10 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	73 (91%)	7 (9%)	0	100	100
48	1q	97/105 (92%)	90 (93%)	6 (6%)	1 (1%)	15	22
48	2q	97/105 (92%)	86 (89%)	9 (9%)	2 (2%)	7	7
49	1r	66/88 (75%)	61 (92%)	4 (6%)	1 (2%)	10	14
49	2r	66/88 (75%)	59 (89%)	6 (9%)	1 (2%)	10	14
50	1s	81/93 (87%)	74 (91%)	7 (9%)	0	100	100
50	2s	81/93 (87%)	65 (80%)	14 (17%)	2 (2%)	5	5
51	1t	94/106 (89%)	84 (89%)	8 (8%)	2 (2%)	7	7
51	2t	94/106 (89%)	83 (88%)	10 (11%)	1 (1%)	14	19
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
All	All	11368/12128 (94%)	10432 (92%)	817 (7%)	119 (1%)	15	22

All (119) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	43	LEU
19	1X	93	GLU
21	1Z	52	SER
26	14	47	GLN
26	14	62	ARG
33	1b	17	PHE
40	1i	54	ASP
42	1k	105	VAL
44	1m	67	GLU
44	1m	106	ASN
11	2P	36	LYS
11	2P	45	LEU
23	21	3	LYS
33	2b	17	PHE
33	2b	123	ALA
38	2g	55	GLY
38	2g	80	VAL
44	2m	67	GLU
46	2o	88	ARG
50	2s	81	ARG
11	1P	38	GLN

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Mol	Chain	Res	Type
15	1T	37	GLY
17	1V	79	VAL
23	11	3	LYS
26	14	49	PHE
33	1b	155	LEU
41	1j	79	ARG
42	1k	49	GLY
42	1k	77	MET
48	1q	68	ARG
49	1r	25	THR
6	2G	84	LYS
6	2G	126	ASP
14	2S	96	GLY
17	2V	79	VAL
21	2Z	93	ASP
33	2b	8	LYS
33	2b	20	GLU
33	2b	126	GLU
35	2d	164	ALA
36	2e	65	ASN
36	2e	85	GLY
38	2g	52	GLU
41	2j	75	ILE
42	2k	49	GLY
48	2q	68	ARG
49	2r	36	ASN
50	2s	12	ASP
26	14	45	GLY
40	1i	56	LEU
41	1j	78	ASN
46	1o	87	ILE
51	1t	47	GLY
51	1t	100	ILE
5	2F	130	ALA
6	2G	47	LYS
8	2I	10	GLU
14	2S	84	GLN
26	24	49	PHE
33	2b	16	HIS
34	2c	91	LEU
36	2e	37	ARG
38	2g	4	ARG

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Mol	Chain	Res	Type
42	2k	77	MET
43	2l	91	LYS
3	1D	262	ARG
4	1E	52	LEU
11	1P	29	LYS
15	1T	55	ASN
33	1b	22	LYS
41	1j	30	SER
4	2E	52	LEU
10	2O	5	GLN
14	2S	20	ARG
14	2S	111	GLU
33	2b	78	GLN
39	2h	22	GLU
40	2i	88	TYR
41	2j	78	ASN
44	2m	106	ASN
6	1G	181	ARG
17	1V	43	GLU
26	14	53	GLU
33	1b	124	SER
33	1b	126	GLU
33	1b	231	GLU
38	1g	54	THR
43	1l	105	TYR
46	1o	88	ARG
6	2G	43	LEU
11	2P	136	GLU
21	2Z	146	ILE
33	2b	9	GLU
34	2c	181	ASN
45	2n	3	ARG
48	2q	33	GLY
51	2t	47	GLY
7	1H	174	GLY
8	1I	10	GLU
20	1Y	103	GLY
26	14	57	GLU
33	1b	8	LYS
33	1b	20	GLU
36	1e	69	VAL
8	2I	40	THR

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

5.3.2 Protein sidechains ⓘ

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%)	206 (96%)	9 (4%)	30	40
3	2D	215/218 (99%)	201 (94%)	14 (6%)	17	23
4	1E	164/166 (99%)	156 (95%)	8 (5%)	25	34
4	2E	164/166 (99%)	157 (96%)	7 (4%)	29	39
5	1F	160/166 (96%)	143 (89%)	17 (11%)	6	7
5	2F	159/166 (96%)	146 (92%)	13 (8%)	11	14
6	1G	143/156 (92%)	128 (90%)	15 (10%)	7	7
6	2G	143/156 (92%)	128 (90%)	15 (10%)	7	7
7	1H	144/148 (97%)	132 (92%)	12 (8%)	11	14
7	2H	144/148 (97%)	129 (90%)	15 (10%)	7	7
8	1I	113/124 (91%)	98 (87%)	15 (13%)	4	3
8	2I	105/124 (85%)	92 (88%)	13 (12%)	4	4
9	1N	118/119 (99%)	110 (93%)	8 (7%)	16	20
9	2N	118/119 (99%)	105 (89%)	13 (11%)	6	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	1O	100/100 (100%)	97 (97%)	3 (3%)	41	55
10	2O	100/100 (100%)	97 (97%)	3 (3%)	41	55
11	1P	115/116 (99%)	106 (92%)	9 (8%)	12	16
11	2P	115/116 (99%)	110 (96%)	5 (4%)	29	39
12	1Q	111/111 (100%)	107 (96%)	4 (4%)	35	47
12	2Q	111/111 (100%)	107 (96%)	4 (4%)	35	47
13	1R	101/101 (100%)	93 (92%)	8 (8%)	12	15
13	2R	101/101 (100%)	94 (93%)	7 (7%)	15	20
14	1S	86/88 (98%)	79 (92%)	7 (8%)	11	14
14	2S	85/88 (97%)	77 (91%)	8 (9%)	8	10
15	1T	115/127 (91%)	109 (95%)	6 (5%)	23	30
15	2T	113/127 (89%)	107 (95%)	6 (5%)	22	30
16	1U	93/94 (99%)	87 (94%)	6 (6%)	17	23
16	2U	93/94 (99%)	88 (95%)	5 (5%)	22	29
17	1V	80/82 (98%)	78 (98%)	2 (2%)	47	62
17	2V	80/82 (98%)	75 (94%)	5 (6%)	18	23
18	1W	90/92 (98%)	87 (97%)	3 (3%)	38	51
18	2W	90/92 (98%)	86 (96%)	4 (4%)	28	38
19	1X	77/78 (99%)	76 (99%)	1 (1%)	69	80
19	2X	77/78 (99%)	74 (96%)	3 (4%)	32	44
20	1Y	85/91 (93%)	80 (94%)	5 (6%)	19	25
20	2Y	85/91 (93%)	77 (91%)	8 (9%)	8	10
21	1Z	135/179 (75%)	127 (94%)	8 (6%)	19	25
21	2Z	137/179 (76%)	121 (88%)	16 (12%)	5	5
22	10	65/67 (97%)	65 (100%)	0	100	100
22	20	65/67 (97%)	63 (97%)	2 (3%)	40	54
23	11	80/83 (96%)	77 (96%)	3 (4%)	33	45
23	21	80/83 (96%)	76 (95%)	4 (5%)	24	33
24	12	65/67 (97%)	62 (95%)	3 (5%)	27	36
24	22	65/67 (97%)	61 (94%)	4 (6%)	18	24
25	13	51/52 (98%)	44 (86%)	7 (14%)	3	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	23	50/52 (96%)	48 (96%)	2 (4%)	31	43
26	14	59/63 (94%)	51 (86%)	8 (14%)	3	3
26	24	53/63 (84%)	46 (87%)	7 (13%)	4	3
27	15	50/52 (96%)	46 (92%)	4 (8%)	12	15
27	25	50/52 (96%)	47 (94%)	3 (6%)	19	25
28	16	51/52 (98%)	49 (96%)	2 (4%)	32	44
28	26	50/52 (96%)	43 (86%)	7 (14%)	3	3
29	17	41/42 (98%)	37 (90%)	4 (10%)	8	9
29	27	41/42 (98%)	37 (90%)	4 (10%)	8	9
30	18	54/55 (98%)	52 (96%)	2 (4%)	34	46
30	28	54/55 (98%)	51 (94%)	3 (6%)	21	28
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	32 (94%)	2 (6%)	19	25
33	1b	192/220 (87%)	168 (88%)	24 (12%)	4	4
33	2b	187/220 (85%)	161 (86%)	26 (14%)	3	3
34	1c	142/188 (76%)	133 (94%)	9 (6%)	18	23
34	2c	140/188 (74%)	130 (93%)	10 (7%)	14	19
35	1d	169/181 (93%)	153 (90%)	16 (10%)	8	10
35	2d	173/181 (96%)	154 (89%)	19 (11%)	6	6
36	1e	113/123 (92%)	103 (91%)	10 (9%)	10	12
36	2e	114/123 (93%)	105 (92%)	9 (8%)	12	15
37	1f	84/90 (93%)	82 (98%)	2 (2%)	49	64
37	2f	85/90 (94%)	81 (95%)	4 (5%)	26	35
38	1g	119/127 (94%)	106 (89%)	13 (11%)	6	6
38	2g	120/127 (94%)	111 (92%)	9 (8%)	13	17
39	1h	114/119 (96%)	107 (94%)	7 (6%)	18	24
39	2h	114/119 (96%)	105 (92%)	9 (8%)	12	15
40	1i	90/99 (91%)	77 (86%)	13 (14%)	3	3
40	2i	89/99 (90%)	78 (88%)	11 (12%)	4	4
41	1j	66/92 (72%)	56 (85%)	10 (15%)	3	2
41	2j	69/92 (75%)	56 (81%)	13 (19%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	1k	82/99 (83%)	73 (89%)	9 (11%)	6	6
42	2k	83/99 (84%)	77 (93%)	6 (7%)	14	18
43	1l	96/108 (89%)	92 (96%)	4 (4%)	30	40
43	2l	96/108 (89%)	89 (93%)	7 (7%)	14	18
44	1m	93/101 (92%)	82 (88%)	11 (12%)	5	5
44	2m	92/101 (91%)	83 (90%)	9 (10%)	8	9
45	1n	49/50 (98%)	47 (96%)	2 (4%)	30	41
45	2n	49/50 (98%)	46 (94%)	3 (6%)	18	24
46	1o	78/80 (98%)	74 (95%)	4 (5%)	24	32
46	2o	78/80 (98%)	72 (92%)	6 (8%)	13	16
47	1p	69/74 (93%)	61 (88%)	8 (12%)	5	5
47	2p	68/74 (92%)	63 (93%)	5 (7%)	13	18
48	1q	94/97 (97%)	86 (92%)	8 (8%)	10	13
48	2q	94/97 (97%)	86 (92%)	8 (8%)	10	13
49	1r	59/77 (77%)	58 (98%)	1 (2%)	60	75
49	2r	59/77 (77%)	53 (90%)	6 (10%)	7	8
50	1s	69/80 (86%)	64 (93%)	5 (7%)	14	18
50	2s	67/80 (84%)	60 (90%)	7 (10%)	7	7
51	1t	70/82 (85%)	65 (93%)	5 (7%)	14	19
51	2t	70/82 (85%)	65 (93%)	5 (7%)	14	19
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	17 (94%)	1 (6%)	21	28
All	All	9303/10064 (92%)	8588 (92%)	715 (8%)	13	16

All (715) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	142	VAL
3	1D	155	LEU
3	1D	211	ARG
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR

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Mol	Chain	Res	Type
3	1D	273	ARG
3	1D	275	LYS
4	1E	9	VAL
4	1E	21	VAL
4	1E	41	LYS
4	1E	89	ASP
4	1E	93	VAL
4	1E	116	VAL
4	1E	181	LEU
4	1E	184	VAL
5	1F	24	LEU
5	1F	27	GLU
5	1F	32	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	70	THR
5	1F	74	ARG
5	1F	88	VAL
5	1F	95	ARG
5	1F	106	ARG
5	1F	127	GLU
5	1F	158	THR
5	1F	162	LEU
5	1F	168	ARG
5	1F	175	THR
5	1F	192	LEU
5	1F	201	VAL
6	1G	3	LEU
6	1G	5	VAL
6	1G	7	LEU
6	1G	28	VAL
6	1G	35	GLU
6	1G	43	LEU
6	1G	49	ASP
6	1G	60	LEU
6	1G	81	LYS
6	1G	82	LEU
6	1G	91	ARG
6	1G	139	LEU
6	1G	146	TYR
6	1G	149	VAL
6	1G	159	VAL

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Mol	Chain	Res	Type
7	1H	3	ARG
7	1H	7	LEU
7	1H	15	VAL
7	1H	23	ARG
7	1H	69	ARG
7	1H	84	SER
7	1H	107	VAL
7	1H	116	GLU
7	1H	124	GLU
7	1H	129	THR
7	1H	152	ARG
7	1H	155	SER
8	1I	10	GLU
8	1I	12	LEU
8	1I	20	ASP
8	1I	38	LEU
8	1I	41	GLU
8	1I	44	LEU
8	1I	47	LEU
8	1I	75	LEU
8	1I	76	THR
8	1I	87	LYS
8	1I	108	THR
8	1I	109	ILE
8	1I	127	VAL
8	1I	140	LEU
8	1I	142	VAL
9	1N	1	MET
9	1N	14	VAL
9	1N	28	THR
9	1N	48	MET
9	1N	62	VAL
9	1N	73	THR
9	1N	96	GLU
9	1N	131	GLN
10	1O	20	MET
10	1O	28	SER
10	1O	106	LEU
11	1P	40	SER
11	1P	45	LEU
11	1P	98	GLU
11	1P	124	LYS

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Mol	Chain	Res	Type
11	1P	126	VAL
11	1P	133	SER
11	1P	147	LEU
11	1P	148	LEU
11	1P	149	GLU
12	1Q	7	MET
12	1Q	8	LYS
12	1Q	63	LYS
12	1Q	133	ARG
13	1R	6	SER
13	1R	24	GLN
13	1R	36	THR
13	1R	67	LEU
13	1R	79	LEU
13	1R	102	GLU
13	1R	111	LEU
13	1R	114	VAL
14	1S	3	ARG
14	1S	14	VAL
14	1S	25	ARG
14	1S	36	TYR
14	1S	46	VAL
14	1S	68	GLN
14	1S	69	VAL
15	1T	36	GLU
15	1T	49	VAL
15	1T	59	THR
15	1T	67	SER
15	1T	82	LEU
15	1T	128	GLU
16	1U	17	ILE
16	1U	59	ARG
16	1U	74	LEU
16	1U	84	LYS
16	1U	95	LEU
16	1U	104	GLN
17	1V	79	VAL
17	1V	85	LYS
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
19	1X	57	LEU

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Mol	Chain	Res	Type
20	1Y	31	LEU
20	1Y	43	ASN
20	1Y	88	LYS
20	1Y	98	VAL
20	1Y	99	CYS
21	1Z	66	SER
21	1Z	80	ARG
21	1Z	128	VAL
21	1Z	131	ARG
21	1Z	132	ASN
21	1Z	140	ASP
21	1Z	153	SER
21	1Z	170	THR
23	11	21	ARG
23	11	46	LEU
23	11	76	ARG
24	12	30	ARG
24	12	40	SER
24	12	55	ARG
25	13	18	ASP
25	13	23	LEU
25	13	34	GLU
25	13	35	ARG
25	13	54	VAL
25	13	55	ARG
25	13	60	GLU
26	14	23	GLU
26	14	49	PHE
26	14	52	THR
26	14	59	PHE
26	14	61	ARG
26	14	63	TYR
26	14	67	TYR
26	14	69	LYS
27	15	6	VAL
27	15	40	LYS
27	15	55	ARG
27	15	60	VAL
28	16	6	ARG
28	16	19	ARG
29	17	24	THR
29	17	41	ARG

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Mol	Chain	Res	Type
29	17	43	THR
29	17	46	VAL
30	18	31	HIS
30	18	34	TRP
33	1b	7	VAL
33	1b	12	GLU
33	1b	24	TRP
33	1b	45	GLN
33	1b	54	THR
33	1b	60	ASP
33	1b	64	ARG
33	1b	67	THR
33	1b	80	ILE
33	1b	112	VAL
33	1b	113	HIS
33	1b	127	ILE
33	1b	128	GLU
33	1b	138	LEU
33	1b	142	LEU
33	1b	146	GLN
33	1b	147	LYS
33	1b	172	ILE
33	1b	185	ILE
33	1b	208	ILE
33	1b	212	GLN
33	1b	215	LEU
33	1b	217	ARG
33	1b	233	SER
34	1c	3	ASN
34	1c	15	THR
34	1c	17	ASP
34	1c	26	LYS
34	1c	64	VAL
34	1c	89	GLU
34	1c	105	GLU
34	1c	178	LEU
34	1c	195	VAL
35	1d	19	LEU
35	1d	31	CYS
35	1d	88	VAL
35	1d	107	ARG
35	1d	108	LEU

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Mol	Chain	Res	Type
35	1d	127	THR
35	1d	135	LEU
35	1d	141	ARG
35	1d	144	ASP
35	1d	157	LEU
35	1d	158	ILE
35	1d	175	SER
35	1d	177	ASP
35	1d	178	VAL
35	1d	188	LEU
35	1d	194	LEU
36	1e	12	LEU
36	1e	20	GLN
36	1e	41	VAL
36	1e	51	VAL
36	1e	68	GLU
36	1e	71	LEU
36	1e	79	GLU
36	1e	91	LEU
36	1e	125	SER
36	1e	151	LEU
37	1f	55	ASP
37	1f	78	GLU
38	1g	8	GLU
38	1g	12	LEU
38	1g	50	ILE
38	1g	57	GLU
38	1g	61	VAL
38	1g	63	LYS
38	1g	73	MET
38	1g	78	ARG
38	1g	104	LEU
38	1g	113	GLU
38	1g	115	ARG
38	1g	140	ASP
38	1g	156	TRP
39	1h	39	LEU
39	1h	51	VAL
39	1h	54	ASP
39	1h	59	LEU
39	1h	99	GLU
39	1h	112	LEU

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Mol	Chain	Res	Type
39	1h	116	LYS
40	1i	9	ARG
40	1i	23	ASN
40	1i	50	LEU
40	1i	53	VAL
40	1i	54	ASP
40	1i	64	THR
40	1i	81	ILE
40	1i	83	ARG
40	1i	92	TYR
40	1i	96	LEU
40	1i	97	LYS
40	1i	121	ARG
40	1i	128	ARG
41	1j	8	LEU
41	1j	15	THR
41	1j	35	SER
41	1j	38	ILE
41	1j	43	ARG
41	1j	46	ARG
41	1j	81	THR
41	1j	92	THR
41	1j	98	ILE
41	1j	100	THR
42	1k	14	VAL
42	1k	31	THR
42	1k	48	ILE
42	1k	63	LEU
42	1k	81	ASP
42	1k	87	THR
42	1k	109	VAL
42	1k	114	VAL
42	1k	117	ASN
43	1l	18	VAL
43	1l	33	ARG
43	1l	36	VAL
43	1l	53	ARG
44	1m	4	ILE
44	1m	12	ASN
44	1m	15	VAL
44	1m	19	LEU
44	1m	29	ARG

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Mol	Chain	Res	Type
44	1m	49	THR
44	1m	70	LEU
44	1m	86	CYS
44	1m	102	ARG
44	1m	106	ASN
44	1m	109	THR
45	1n	4	LYS
45	1n	18	VAL
46	1o	26	GLU
46	1o	39	LEU
46	1o	40	SER
46	1o	76	GLU
47	1p	5	ARG
47	1p	21	VAL
47	1p	42	ARG
47	1p	45	THR
47	1p	60	LEU
47	1p	61	SER
47	1p	62	VAL
47	1p	76	GLN
48	1q	14	LYS
48	1q	31	LEU
48	1q	39	SER
48	1q	45	HIS
48	1q	52	LYS
48	1q	53	LEU
48	1q	63	ARG
48	1q	75	ARG
49	1r	65	ILE
50	1s	4	SER
50	1s	35	SER
50	1s	37	ARG
50	1s	44	MET
50	1s	48	THR
51	1t	10	LEU
51	1t	19	SER
51	1t	24	LEU
51	1t	42	GLN
51	1t	80	ARG
3	2D	3	VAL
3	2D	88	ARG
3	2D	141	VAL

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Mol	Chain	Res	Type
3	2D	142	VAL
3	2D	155	LEU
3	2D	162	SER
3	2D	173	VAL
3	2D	183	ARG
3	2D	200	ASP
3	2D	211	ARG
3	2D	229	VAL
3	2D	242	ARG
3	2D	259	THR
3	2D	275	LYS
4	2E	19	ARG
4	2E	21	VAL
4	2E	38	THR
4	2E	90	THR
4	2E	116	VAL
4	2E	145	LYS
4	2E	181	LEU
5	2F	24	LEU
5	2F	33	LEU
5	2F	74	ARG
5	2F	107	LYS
5	2F	108	LYS
5	2F	133	ASN
5	2F	137	LYS
5	2F	149	ASP
5	2F	158	THR
5	2F	186	ILE
5	2F	192	LEU
5	2F	196	LEU
5	2F	201	VAL
6	2G	3	LEU
6	2G	7	LEU
6	2G	18	GLU
6	2G	21	ARG
6	2G	51	ARG
6	2G	60	LEU
6	2G	88	ILE
6	2G	91	ARG
6	2G	124	SER
6	2G	137	GLU
6	2G	140	ILE

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Mol	Chain	Res	Type
6	2G	145	THR
6	2G	155	MET
6	2G	159	VAL
6	2G	170	ARG
7	2H	7	LEU
7	2H	15	VAL
7	2H	23	ARG
7	2H	45	VAL
7	2H	50	VAL
7	2H	57	ASP
7	2H	62	LYS
7	2H	84	SER
7	2H	114	VAL
7	2H	127	GLU
7	2H	129	THR
7	2H	130	ARG
7	2H	136	ILE
7	2H	152	ARG
7	2H	175	LYS
8	2I	14	ASP
8	2I	15	VAL
8	2I	20	ASP
8	2I	38	LEU
8	2I	61	ARG
8	2I	68	LEU
8	2I	77	LEU
8	2I	85	GLU
8	2I	96	ASP
8	2I	116	LEU
8	2I	117	GLU
8	2I	125	GLU
8	2I	127	VAL
9	2N	1	MET
9	2N	9	VAL
9	2N	14	VAL
9	2N	15	LEU
9	2N	28	THR
9	2N	38	HIS
9	2N	43	THR
9	2N	48	MET
9	2N	59	LYS
9	2N	61	ARG

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Mol	Chain	Res	Type
9	2N	62	VAL
9	2N	68	GLU
9	2N	96	GLU
10	2O	1	MET
10	2O	52	VAL
10	2O	78	ARG
11	2P	7	ARG
11	2P	70	GLN
11	2P	133	SER
11	2P	136	GLU
11	2P	149	GLU
12	2Q	7	MET
12	2Q	12	GLN
12	2Q	25	ASP
12	2Q	110	THR
13	2R	24	GLN
13	2R	36	THR
13	2R	67	LEU
13	2R	79	LEU
13	2R	95	THR
13	2R	102	GLU
13	2R	111	LEU
14	2S	27	SER
14	2S	44	LYS
14	2S	50	SER
14	2S	53	SER
14	2S	63	THR
14	2S	80	LEU
14	2S	83	LYS
14	2S	85	VAL
15	2T	18	ASP
15	2T	28	VAL
15	2T	39	ARG
15	2T	64	ARG
15	2T	74	ARG
15	2T	96	ARG
16	2U	5	LYS
16	2U	74	LEU
16	2U	77	SER
16	2U	95	LEU
16	2U	100	VAL
17	2V	7	THR

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Mol	Chain	Res	Type
17	2V	39	LEU
17	2V	56	SER
17	2V	61	VAL
17	2V	79	VAL
18	2W	11	ARG
18	2W	17	VAL
18	2W	60	ASN
18	2W	92	ARG
19	2X	72	LYS
19	2X	81	VAL
19	2X	92	LEU
20	2Y	3	VAL
20	2Y	5	MET
20	2Y	6	HIS
20	2Y	28	LYS
20	2Y	67	LEU
20	2Y	72	VAL
20	2Y	99	CYS
20	2Y	106	LEU
21	2Z	5	LEU
21	2Z	18	LEU
21	2Z	42	VAL
21	2Z	66	SER
21	2Z	79	ARG
21	2Z	93	ASP
21	2Z	100	VAL
21	2Z	121	HIS
21	2Z	145	GLU
21	2Z	150	LEU
21	2Z	154	ASP
21	2Z	155	LEU
21	2Z	161	VAL
21	2Z	163	LEU
21	2Z	171	ILE
21	2Z	174	VAL
22	20	10	THR
22	20	55	ARG
23	21	40	ARG
23	21	46	LEU
23	21	51	VAL
23	21	76	ARG
24	22	4	SER

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Mol	Chain	Res	Type
24	22	30	ARG
24	22	66	GLU
24	22	70	GLN
25	23	54	VAL
25	23	59	VAL
26	24	5	ILE
26	24	13	ARG
26	24	20	ASN
26	24	34	GLU
26	24	59	PHE
26	24	67	TYR
26	24	68	ARG
27	25	6	VAL
27	25	33	CYS
27	25	58	LEU
28	26	6	ARG
28	26	19	ARG
28	26	20	ASN
28	26	34	LEU
28	26	40	CYS
28	26	48	VAL
28	26	52	VAL
29	27	1	MET
29	27	41	ARG
29	27	43	THR
29	27	46	VAL
30	28	14	VAL
30	28	31	HIS
30	28	34	TRP
31	29	7	VAL
31	29	17	ILE
33	2b	7	VAL
33	2b	16	HIS
33	2b	24	TRP
33	2b	44	LEU
33	2b	47	THR
33	2b	55	PHE
33	2b	71	VAL
33	2b	76	GLN
33	2b	80	ILE
33	2b	94	ASN
33	2b	95	GLN

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Mol	Chain	Res	Type
33	2b	96	ARG
33	2b	107	THR
33	2b	115	LEU
33	2b	127	ILE
33	2b	130	ARG
33	2b	133	LYS
33	2b	164	VAL
33	2b	185	ILE
33	2b	189	ASP
33	2b	191	ASP
33	2b	215	LEU
33	2b	220	ASP
33	2b	223	ILE
33	2b	229	VAL
33	2b	236	TYR
34	2c	46	GLU
34	2c	47	LEU
34	2c	70	VAL
34	2c	105	GLU
34	2c	120	VAL
34	2c	125	GLU
34	2c	143	GLU
34	2c	153	VAL
34	2c	182	ILE
34	2c	190	ARG
35	2d	8	VAL
35	2d	28	SER
35	2d	34	GLU
35	2d	47	ARG
35	2d	52	SER
35	2d	53	ASP
35	2d	58	LEU
35	2d	59	ARG
35	2d	78	LEU
35	2d	96	LEU
35	2d	127	THR
35	2d	135	LEU
35	2d	150	GLU
35	2d	153	ARG
35	2d	155	LEU
35	2d	162	LEU
35	2d	169	LYS

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Mol	Chain	Res	Type
35	2d	170	VAL
35	2d	190	ASP
36	2e	5	ASP
36	2e	13	ILE
36	2e	20	GLN
36	2e	31	LEU
36	2e	41	VAL
36	2e	51	VAL
36	2e	73	ASN
36	2e	78	HIS
36	2e	81	GLU
37	2f	63	TYR
37	2f	69	GLU
37	2f	72	VAL
37	2f	81	ILE
38	2g	6	ARG
38	2g	15	ASP
38	2g	22	LEU
38	2g	23	VAL
38	2g	32	ARG
38	2g	59	LEU
38	2g	79	ARG
38	2g	115	ARG
38	2g	146	GLU
39	2h	22	GLU
39	2h	39	LEU
39	2h	45	ILE
39	2h	51	VAL
39	2h	52	ASP
39	2h	61	VAL
39	2h	97	VAL
39	2h	112	LEU
39	2h	127	LEU
40	2i	23	ASN
40	2i	27	THR
40	2i	38	GLN
40	2i	65	VAL
40	2i	66	ARG
40	2i	89	ASN
40	2i	93	ARG
40	2i	99	LEU
40	2i	113	LYS

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Mol	Chain	Res	Type
40	2i	114	TYR
40	2i	125	TYR
41	2j	8	LEU
41	2j	9	ARG
41	2j	21	GLN
41	2j	29	ARG
41	2j	38	ILE
41	2j	55	LYS
41	2j	65	LEU
41	2j	66	ARG
41	2j	67	THR
41	2j	73	ASP
41	2j	96	ILE
41	2j	97	GLU
41	2j	100	THR
42	2k	41	THR
42	2k	48	ILE
42	2k	105	VAL
42	2k	107	SER
42	2k	109	VAL
42	2k	120	ARG
43	2l	18	VAL
43	2l	33	ARG
43	2l	34	ARG
43	2l	40	VAL
43	2l	81	SER
43	2l	86	ARG
43	2l	116	SER
44	2m	4	ILE
44	2m	32	GLU
44	2m	62	ASN
44	2m	69	GLU
44	2m	93	ARG
44	2m	98	VAL
44	2m	103	THR
44	2m	106	ASN
44	2m	114	ARG
45	2n	4	LYS
45	2n	18	VAL
45	2n	33	VAL
46	2o	5	LYS
46	2o	39	LEU

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Mol	Chain	Res	Type
46	2o	60	VAL
46	2o	76	GLU
46	2o	87	ILE
46	2o	88	ARG
47	2p	20	VAL
47	2p	54	GLU
47	2p	67	THR
47	2p	73	LEU
47	2p	74	LEU
48	2q	5	VAL
48	2q	6	LEU
48	2q	14	LYS
48	2q	31	LEU
48	2q	52	LYS
48	2q	63	ARG
48	2q	79	SER
48	2q	99	SER
49	2r	25	THR
49	2r	26	LEU
49	2r	31	LEU
49	2r	65	ILE
49	2r	82	THR
49	2r	84	LYS
50	2s	33	THR
50	2s	37	ARG
50	2s	45	VAL
50	2s	49	ILE
50	2s	57	HIS
50	2s	63	THR
50	2s	65	ASN
51	2t	9	ASN
51	2t	41	ILE
51	2t	45	GLN
51	2t	46	GLU
51	2t	89	ARG
52	2u	22	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
4	1E	48	GLN
5	1F	8	GLN

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Mol	Chain	Res	Type
5	1F	69	HIS
5	1F	203	GLN
6	1G	26	GLN
7	1H	74	ASN
12	1Q	12	GLN
13	1R	71	GLN
14	1S	38	GLN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
21	1Z	55	HIS
21	1Z	73	GLN
22	10	17	GLN
22	10	70	GLN
33	1b	78	GLN
33	1b	212	GLN
34	1c	6	HIS
34	1c	176	HIS
35	1d	43	HIS
35	1d	116	GLN
35	1d	123	HIS
35	1d	160	GLN
36	1e	78	HIS
36	1e	141	GLN
37	1f	100	ASN
38	1g	28	ASN
38	1g	110	GLN
39	1h	15	ASN
40	1i	3	GLN
40	1i	31	GLN
40	1i	34	ASN
40	1i	124	GLN
41	1j	56	HIS
42	1k	78	GLN
43	1l	99	HIS
46	1o	13	GLN
46	1o	46	HIS
49	1r	63	GLN
50	1s	23	ASN
50	1s	47	HIS
50	1s	83	HIS
51	1t	90	GLN

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Mol	Chain	Res	Type
3	2D	166	GLN
4	2E	48	GLN
5	2F	69	HIS
6	2G	41	GLN
6	2G	108	ASN
10	2O	5	GLN
11	2P	27	HIS
11	2P	35	HIS
11	2P	70	GLN
12	2Q	12	GLN
14	2S	38	GLN
15	2T	58	ASN
16	2U	81	HIS
19	2X	31	HIS
21	2Z	32	HIS
21	2Z	73	GLN
30	28	35	GLN
33	2b	76	GLN
33	2b	135	GLN
33	2b	140	HIS
34	2c	6	HIS
34	2c	123	GLN
34	2c	162	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	123	HIS
35	2d	125	HIS
36	2e	72	GLN
37	2f	73	ASN
38	2g	68	ASN
38	2g	86	GLN
38	2g	148	ASN
39	2h	15	ASN
40	2i	3	GLN
40	2i	23	ASN
40	2i	58	HIS
41	2j	21	GLN
41	2j	33	GLN
42	2k	22	HIS
42	2k	117	ASN
43	2l	49	ASN
43	2l	99	HIS

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Mol	Chain	Res	Type
44	2m	40	ASN
44	2m	77	ASN
46	2o	13	GLN
49	2r	63	GLN
50	2s	57	HIS
50	2s	69	HIS
50	2s	83	HIS
51	2t	75	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2863/2915 (98%)	420 (14%)	26 (0%)
1	2A	2790/2915 (95%)	458 (16%)	24 (0%)
2	1B	119/121 (98%)	6 (5%)	0
2	2B	118/121 (97%)	28 (23%)	0
32	1a	1494/1521 (98%)	239 (15%)	0
32	2a	1498/1521 (98%)	274 (18%)	0
53	1v	12/24 (50%)	3 (25%)	0
53	2v	12/24 (50%)	3 (25%)	0
54	1w	70/74 (94%)	24 (34%)	0
54	2w	68/74 (91%)	29 (42%)	0
55	1x	75/77 (97%)	7 (9%)	0
55	2x	75/77 (97%)	9 (12%)	0
56	1y	71/74 (95%)	27 (38%)	0
56	2y	71/74 (95%)	32 (45%)	0
All	All	9336/9612 (97%)	1559 (16%)	50 (0%)

All (1559) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	63	U
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	78	A
1	1A	84	A
1	1A	95	G

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Mol	Chain	Res	Type
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	154	G
1	1A	196	A
1	1A	199	A
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	266	G
1	1A	269	U
1	1A	271(C)	C
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	271(S)	G
1	1A	272(B)	G
1	1A	272(I)	U
1	1A	275	G
1	1A	279	C
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	352	G
1	1A	363	G
1	1A	363(B)	G
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	418	G
1	1A	421	U
1	1A	428	A
1	1A	443	A

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Mol	Chain	Res	Type
1	1A	444	C
1	1A	448	U
1	1A	451	C
1	1A	456	C
1	1A	457	A
1	1A	481	G
1	1A	494	G
1	1A	504	U
1	1A	505	A
1	1A	509	C
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	551	G
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	584	C
1	1A	586	A
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	616	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(E)	G
1	1A	652(F)	G
1	1A	652(T)	C
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	774	A
1	1A	775	G
1	1A	776	G

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Mol	Chain	Res	Type
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	789	A
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	866	A
1	1A	879	G
1	1A	880	G
1	1A	882	G
1	1A	883	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	890	A
1	1A	895	U
1	1A	896	A
1	1A	897	C
1	1A	907	U
1	1A	910	A
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	959	A
1	1A	961	C
1	1A	963	U
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G

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Mol	Chain	Res	Type
1	1A	1026	U
1	1A	1027	A
1	1A	1033	U
1	1A	1046	A
1	1A	1047	G
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1059	G
1	1A	1063	G
1	1A	1066	U
1	1A	1068	G
1	1A	1070	A
1	1A	1071	G
1	1A	1073	A
1	1A	1075	C
1	1A	1076	C
1	1A	1078	U
1	1A	1079	C
1	1A	1080	C
1	1A	1081	U
1	1A	1083	U
1	1A	1087	G
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1091	G
1	1A	1093	G
1	1A	1094	U
1	1A	1097	U
1	1A	1099	G
1	1A	1101	U
1	1A	1104	C
1	1A	1108	U
1	1A	1110	G
1	1A	1112	G
1	1A	1116	C
1	1A	1135	C
1	1A	1136	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A

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Mol	Chain	Res	Type
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1241	A
1	1A	1244	G
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1321	A
1	1A	1345	C
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1384	A
1	1A	1385	G
1	1A	1395	A
1	1A	1396	U
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1467	C
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1540	U
1	1A	1543	C
1	1A	1554	A
1	1A	1558	A

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Mol	Chain	Res	Type
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1609	A
1	1A	1648	C
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1739	U
1	1A	1746	G
1	1A	1756	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1828	G
1	1A	1829	A
1	1A	1847	A
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1913	A
1	1A	1929	G
1	1A	1930	G
1	1A	1931	U
1	1A	1934	C
1	1A	1937	A

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Mol	Chain	Res	Type
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1965	C
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1992	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2033	A
1	1A	2039	C
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2069	G
1	1A	2093	G
1	1A	2097	C
1	1A	2102	U
1	1A	2107	C
1	1A	2108	C
1	1A	2110	G
1	1A	2112	G
1	1A	2113	U
1	1A	2114	A
1	1A	2120	G
1	1A	2121	G
1	1A	2122	U
1	1A	2123	G
1	1A	2126	A
1	1A	2127	G
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A

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Mol	Chain	Res	Type
1	1A	2136	C
1	1A	2140	C
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2145	C
1	1A	2146	C
1	1A	2149	G
1	1A	2150	U
1	1A	2151	G
1	1A	2155	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2160	G
1	1A	2161	C
1	1A	2162	G
1	1A	2165	G
1	1A	2166	G
1	1A	2167	U
1	1A	2169	A
1	1A	2171	A
1	1A	2172	U
1	1A	2174	C
1	1A	2177	C
1	1A	2179	C
1	1A	2180	U
1	1A	2182	G
1	1A	2184	G
1	1A	2189	U
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2269	A
1	1A	2278	A

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Mol	Chain	Res	Type
1	1A	2280	G
1	1A	2283	C
1	1A	2287	A
1	1A	2305	A
1	1A	2308	G
1	1A	2312	U
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2361	A
1	1A	2383	G
1	1A	2385	C
1	1A	2400	G
1	1A	2406	U
1	1A	2422	A
1	1A	2423	U
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2476	A
1	1A	2478	A
1	1A	2490	G
1	1A	2491	U
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A
1	1A	2529	G
1	1A	2535	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2574	G
1	1A	2585	U

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Mol	Chain	Res	Type
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2689	U
1	1A	2691	C
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2752	C
1	1A	2765	A
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2793	G
1	1A	2794	C
1	1A	2802	G
1	1A	2805	G
1	1A	2820	A
1	1A	2821	A
1	1A	2835	A
1	1A	2872	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
1	1A	2895	U
2	1B	15	A
2	1B	56	G
2	1B	65	C
2	1B	73	A
2	1B	84	C
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G

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Mol	Chain	Res	Type
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	52	G
32	1a	54	C
32	1a	61	G
32	1a	65	U
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	111	G
32	1a	116	A
32	1a	120	A
32	1a	121	C
32	1a	131	C
32	1a	144	G
32	1a	145	G
32	1a	147	G
32	1a	153	C
32	1a	162	A
32	1a	163	C
32	1a	174	C
32	1a	180	U
32	1a	182	U
32	1a	189(F)	U
32	1a	189(G)	G
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	200	G
32	1a	203	U
32	1a	204	U
32	1a	247	G
32	1a	251	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	321	A
32	1a	328	C
32	1a	329	A
32	1a	332	G

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Mol	Chain	Res	Type
32	1a	341	C
32	1a	342	C
32	1a	344	A
32	1a	345	C
32	1a	347	G
32	1a	348	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	383	A
32	1a	384	G
32	1a	392	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	422	C
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	441	A
32	1a	442	C
32	1a	452	A
32	1a	457	C
32	1a	461	A
32	1a	471	G
32	1a	483	C
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	527	G7M
32	1a	531	U
32	1a	532	A

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Mol	Chain	Res	Type
32	1a	533	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	607	A
32	1a	627	G
32	1a	630	G
32	1a	653	A
32	1a	665	A
32	1a	673	G
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	703	G
32	1a	722	A
32	1a	723	U
32	1a	731	G
32	1a	749	C
32	1a	753	A
32	1a	755	G
32	1a	766	A
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	848	C
32	1a	851	G
32	1a	870	U
32	1a	913	A
32	1a	914	A
32	1a	926	G

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Mol	Chain	Res	Type
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	942	G
32	1a	960	U
32	1a	961	U
32	1a	966	M2G
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1002	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1037	C
32	1a	1043	C
32	1a	1044	A
32	1a	1046	A
32	1a	1053	G
32	1a	1068	G

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Mol	Chain	Res	Type
32	1a	1081	G
32	1a	1086	U
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1111	A
32	1a	1124	G
32	1a	1125	U
32	1a	1127	G
32	1a	1132	C
32	1a	1133	G
32	1a	1134	G
32	1a	1137	C
32	1a	1139	G
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U
32	1a	1183	A
32	1a	1184	G
32	1a	1193	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1213	A
32	1a	1214	C
32	1a	1227	A
32	1a	1238	A
32	1a	1250	A
32	1a	1253	G
32	1a	1256	A
32	1a	1257	U
32	1a	1260	C
32	1a	1270	C
32	1a	1275	A
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U

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Mol	Chain	Res	Type
32	1a	1312	G
32	1a	1323	G
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1364	U
32	1a	1371	G
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1464	G
32	1a	1487	G
32	1a	1492	A
32	1a	1494	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
53	1v	13	A
53	1v	14	A
53	1v	15	A
54	1w	2	C
54	1w	5	G
54	1w	7	G
54	1w	8	4SU
54	1w	14	A
54	1w	18	G
54	1w	19	U
54	1w	21	A
54	1w	22	G
54	1w	23	A
54	1w	24	A
54	1w	26	G
54	1w	45	U
54	1w	46	A

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Mol	Chain	Res	Type
54	1w	48	C
54	1w	49	G
54	1w	51	G
54	1w	56	C
54	1w	59	U
54	1w	62	C
54	1w	68	C
54	1w	70	C
54	1w	71	G
54	1w	74	C
55	1x	2	G
55	1x	9	G
55	1x	18	G
55	1x	19	G
55	1x	47	U
55	1x	61	C
55	1x	69	C
56	1y	4	G
56	1y	5	G
56	1y	9	A
56	1y	13	C
56	1y	14	A
56	1y	18	G
56	1y	19	U
56	1y	21	A
56	1y	22	G
56	1y	25	C
56	1y	29	A
56	1y	33	U
56	1y	35	C
56	1y	40	C
56	1y	41	U
56	1y	44	A
56	1y	45	U
56	1y	46	A
56	1y	48	C
56	1y	49	G
56	1y	50	A
56	1y	56	C
56	1y	58	A
56	1y	59	U
56	1y	61	C

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Mol	Chain	Res	Type
56	1y	65	U
56	1y	70	C
1	2A	8	A
1	2A	12	U
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	36	G
1	2A	45	C
1	2A	49	A
1	2A	51	G
1	2A	61	G
1	2A	64	A
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	83	G
1	2A	84	A
1	2A	90	U
1	2A	94	C
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	157	U
1	2A	173	G
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	233	A
1	2A	248	G
1	2A	250	G

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Mol	Chain	Res	Type
1	2A	264	C
1	2A	266	G
1	2A	271(A)	A
1	2A	271(J)	C
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	311	A
1	2A	317	G
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	352	G
1	2A	358	U
1	2A	363(B)	G
1	2A	386	G
1	2A	396	G
1	2A	399	G
1	2A	403	U
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	422	A
1	2A	443	A
1	2A	444	C
1	2A	455	C
1	2A	457	A
1	2A	481	G
1	2A	494	G
1	2A	504	U
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	529	A
1	2A	531	C
1	2A	532	A
1	2A	542	C
1	2A	545	G

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Mol	Chain	Res	Type
1	2A	563	G
1	2A	573	G
1	2A	575	A
1	2A	586	A
1	2A	588	U
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	605	C
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	620	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	668	G
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	726	G
1	2A	730	C
1	2A	764	A
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	832	G
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	874	G
1	2A	878	A

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Mol	Chain	Res	Type
1	2A	879	G
1	2A	880	G
1	2A	882	G
1	2A	883	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	899	A
1	2A	900	A
1	2A	901	A
1	2A	907	U
1	2A	910	A
1	2A	917	A
1	2A	924	C
1	2A	932	G
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	961	C
1	2A	963	U
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	999	U
1	2A	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1027	A
1	2A	1033	U
1	2A	1038	C

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Mol	Chain	Res	Type
1	2A	1039	G
1	2A	1043	C
1	2A	1114	G
1	2A	1116	C
1	2A	1128	A
1	2A	1129	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1142(A)	A
1	2A	1169	G
1	2A	1171	G
1	2A	1210	A
1	2A	1211	U
1	2A	1218	C
1	2A	1220	A
1	2A	1230	C
1	2A	1237	A
1	2A	1244	G
1	2A	1248	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1306	C
1	2A	1314	C
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1373	A
1	2A	1379	A
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G

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Mol	Chain	Res	Type
1	2A	1420	U
1	2A	1421	G
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1461	G
1	2A	1463	C
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1496	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1533	G
1	2A	1542	A
1	2A	1543	C
1	2A	1545	A
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1583	A
1	2A	1584	C
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1647	G
1	2A	1648	C
1	2A	1654	A
1	2A	1674	G

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Mol	Chain	Res	Type
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1746	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A
1	2A	1816	G
1	2A	1829	A
1	2A	1847	A
1	2A	1848	A
1	2A	1861	G
1	2A	1877	A
1	2A	1878	G
1	2A	1889	A
1	2A	1895	C
1	2A	1900	A
1	2A	1906	G
1	2A	1910	G
1	2A	1913	A
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1931	U
1	2A	1936	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A

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Mol	Chain	Res	Type
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2036	C
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2069	G
1	2A	2099	U
1	2A	2109	U
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2116	G
1	2A	2117	A
1	2A	2118	U
1	2A	2120	G
1	2A	2122	U
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2139	C
1	2A	2145	C
1	2A	2146	C
1	2A	2149	G
1	2A	2150	U

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Mol	Chain	Res	Type
1	2A	2157	G
1	2A	2158	A
1	2A	2159	G
1	2A	2161	C
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2171	A
1	2A	2172	U
1	2A	2176	A
1	2A	2178	C
1	2A	2183	C
1	2A	2185	C
1	2A	2186	G
1	2A	2188	C
1	2A	2189	U
1	2A	2190	G
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2239	G
1	2A	2269	A
1	2A	2275	C
1	2A	2278	A
1	2A	2283	C
1	2A	2287	A
1	2A	2288	A
1	2A	2294	C
1	2A	2298	A
1	2A	2305	A
1	2A	2308	G
1	2A	2312	U
1	2A	2316	C
1	2A	2320	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A

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Mol	Chain	Res	Type
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2376	A
1	2A	2379	G
1	2A	2383	G
1	2A	2385	C
1	2A	2396	G
1	2A	2402	C
1	2A	2403	C
1	2A	2406	U
1	2A	2422	A
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2465	C
1	2A	2468	G
1	2A	2469	A
1	2A	2476	A
1	2A	2484	G
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2549	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2569	G
1	2A	2573	C
1	2A	2578	G
1	2A	2585	U

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Mol	Chain	Res	Type
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U
1	2A	2630	G
1	2A	2634	G
1	2A	2654	A
1	2A	2669	G
1	2A	2689	U
1	2A	2690	C
1	2A	2691	C
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2751	G
1	2A	2758	A
1	2A	2760	C
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2789	C
1	2A	2793	G
1	2A	2802	G
1	2A	2803	C
1	2A	2804	C
1	2A	2805	G
1	2A	2807	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2835	A
1	2A	2872	G
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	5	C

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Mol	Chain	Res	Type
2	2B	8	U
2	2B	13	A
2	2B	17	C
2	2B	19	G
2	2B	20	C
2	2B	25	A
2	2B	30	C
2	2B	33	G
2	2B	34	U
2	2B	41	U
2	2B	42	C
2	2B	45	A
2	2B	53	A
2	2B	56	G
2	2B	63	G
2	2B	67	G
2	2B	69	G
2	2B	73	A
2	2B	75	G
2	2B	85	G
2	2B	89	G
2	2B	108	U
2	2B	110	G
2	2B	111	G
2	2B	119	G
2	2B	120	A
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	66	G
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	127	G
32	2a	131	C
32	2a	142	G

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Mol	Chain	Res	Type
32	2a	143	A
32	2a	144	G
32	2a	163	C
32	2a	182	U
32	2a	189(D)	C
32	2a	189(F)	U
32	2a	189(J)	G
32	2a	195	A
32	2a	197	A
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	217	C
32	2a	220	G
32	2a	247	G
32	2a	250	A
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	281	G
32	2a	289	G
32	2a	306	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	355	C
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	414	A

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Mol	Chain	Res	Type
32	2a	421	U
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	458	C
32	2a	470	C
32	2a	471	G
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	517	G
32	2a	518	C
32	2a	521	G
32	2a	531	U
32	2a	532	A
32	2a	547	A
32	2a	559	A
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	575	G
32	2a	576	G
32	2a	596	C
32	2a	597	G
32	2a	630	G
32	2a	653	A
32	2a	665	A
32	2a	666	G
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	720	C
32	2a	723	U

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Mol	Chain	Res	Type
32	2a	731	G
32	2a	733	A
32	2a	749	C
32	2a	755	G
32	2a	764	C
32	2a	773	G
32	2a	774	G
32	2a	777	A
32	2a	793	U
32	2a	794	A
32	2a	815	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	836	G
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	857	C
32	2a	859	A
32	2a	880	C
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	933	G
32	2a	934	C
32	2a	935	A
32	2a	942	G
32	2a	958	A
32	2a	960	U
32	2a	961	U
32	2a	963	G
32	2a	966	M2G
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A

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Mol	Chain	Res	Type
32	2a	984	C
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	995	C
32	2a	997	U
32	2a	998	G
32	2a	999	C
32	2a	1001	A
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1016	A
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1032	G
32	2a	1035	A
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1045	C
32	2a	1051	C
32	2a	1053	G
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1079	G
32	2a	1081	G
32	2a	1086	U

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Mol	Chain	Res	Type
32	2a	1094	G
32	2a	1095	U
32	2a	1097	C
32	2a	1101	A
32	2a	1105	A
32	2a	1108	G
32	2a	1109	C
32	2a	1113	C
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1133	G
32	2a	1135	U
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1146	A
32	2a	1147	C
32	2a	1149	C
32	2a	1152	A
32	2a	1154	G
32	2a	1157	A
32	2a	1159	U
32	2a	1160	G
32	2a	1172	C
32	2a	1182	G
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1211	U
32	2a	1213	A
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1255	G
32	2a	1256	A
32	2a	1257	U

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Mol	Chain	Res	Type
32	2a	1260	C
32	2a	1264	C
32	2a	1267	C
32	2a	1268	A
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1283	G
32	2a	1287	A
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1306	A
32	2a	1323	G
32	2a	1339	A
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1358	U
32	2a	1359	C
32	2a	1363	C
32	2a	1364	U
32	2a	1368	G
32	2a	1379	G
32	2a	1398	A
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U
32	2a	1452	C
32	2a	1456	G
32	2a	1457	G
32	2a	1487	G
32	2a	1492	A
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U

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Mol	Chain	Res	Type
32	2a	1517	G
32	2a	1523	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	13	A
53	2v	14	A
53	2v	15	A
54	2w	2	C
54	2w	5	G
54	2w	8	4SU
54	2w	9	A
54	2w	10	G
54	2w	11	U
54	2w	12	U
54	2w	13	C
54	2w	14	A
54	2w	18	G
54	2w	22	G
54	2w	23	A
54	2w	24	A
54	2w	25	C
54	2w	26	G
54	2w	27	A
54	2w	46	A
54	2w	49	G
54	2w	56	C
54	2w	61	C
54	2w	62	C
54	2w	64	U
54	2w	68	C
54	2w	69	C
54	2w	70	C
54	2w	71	G
54	2w	72	C
54	2w	73	U
54	2w	74	C
55	2x	9	G
55	2x	13	C
55	2x	18	G
55	2x	21	A

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Mol	Chain	Res	Type
55	2x	22	G
55	2x	47	U
55	2x	52	G
55	2x	63	G
55	2x	69	C
56	2y	5	G
56	2y	7	G
56	2y	8	4SU
56	2y	9	A
56	2y	15	A
56	2y	18	G
56	2y	19	U
56	2y	21	A
56	2y	22	G
56	2y	25	C
56	2y	26	G
56	2y	27	A
56	2y	29	A
56	2y	33	U
56	2y	34	C
56	2y	37	A
56	2y	40	C
56	2y	41	U
56	2y	45	U
56	2y	46	A
56	2y	48	C
56	2y	49	G
56	2y	50	A
56	2y	52	G
56	2y	53	G
56	2y	58	A
56	2y	59	U
56	2y	61	C
56	2y	62	C
56	2y	69	C
56	2y	70	C
56	2y	73	U

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	196	A

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Mol	Chain	Res	Type
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	548	A
1	1A	746	A
1	1A	774	A
1	1A	827	U
1	1A	974	G
1	1A	1067	A
1	1A	1174	A
1	1A	1176	G
1	1A	1379	A
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1762	A
1	1A	1992	G
1	1A	2126	A
1	1A	2134	A
1	1A	2183	C
1	1A	2406	U
1	1A	2422	A
1	1A	2430	A
1	1A	2439	A
1	1A	2629	A
1	2A	196	A
1	2A	228	A
1	2A	266	G
1	2A	271(K)	U
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	774	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	1026	U
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1653	G

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Mol	Chain	Res	Type
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2156	G
1	2A	2406	U
1	2A	2689	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	4OC	1a	1402	32	20,23,24	0.76	0	26,32,35	0.94	1 (3%)
1	OMC	2A	1920	1	19,22,23	0.81	0	26,31,34	0.93	1 (3%)
32	2MG	2a	1207	32	18,26,27	0.93	1 (5%)	16,38,41	1.02	2 (12%)
32	MA6	2a	1519	32	19,26,27	0.82	0	18,38,41	1.57	2 (11%)
54	L3X	1w	76	1,54	21,28,29	1.45	4 (19%)	15,40,43	1.55	1 (6%)
1	2MA	2A	2503	57,1	17,25,26	1.05	1 (5%)	17,37,40	0.95	2 (11%)
32	UR3	2a	1498	32	19,22,23	1.01	1 (5%)	26,32,35	1.46	2 (7%)
1	PSU	1A	1911	1	18,21,22	1.36	2 (11%)	22,30,33	1.96	4 (18%)
55	31H	2x	76	55,57	28,34,35	1.07	3 (10%)	23,47,50	1.56	3 (13%)
43	0TD	2l	92	43	7,9,10	4.79	1 (14%)	6,11,13	4.98	2 (33%)
32	5MC	2a	1400	32	18,22,23	0.97	2 (11%)	26,32,35	1.19	3 (11%)
43	0TD	1l	92	43	7,9,10	4.81	1 (14%)	6,11,13	2.89	2 (33%)
1	OMU	1A	2552	1	19,22,23	1.19	2 (10%)	26,31,34	1.84	5 (19%)
54	4SU	1w	8	54	18,21,22	1.80	5 (27%)	26,30,33	1.90	5 (19%)
1	5MU	1A	1915	1	19,22,23	1.38	5 (26%)	28,32,35	2.07	5 (17%)
32	5MC	2a	967	32	18,22,23	0.92	2 (11%)	26,32,35	1.07	2 (7%)
55	4SU	2x	8	55	18,21,22	1.91	7 (38%)	26,30,33	1.31	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	5MC	2x	32	55	18,22,23	0.99	2 (11%)	26,32,35	1.29	4 (15%)
54	PSU	1w	55	57,54	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
1	5MC	1A	1962	57,1	18,22,23	0.98	2 (11%)	26,32,35	1.14	3 (11%)
1	5MC	1A	1942	1	18,22,23	0.96	2 (11%)	26,32,35	1.16	2 (7%)
32	MA6	1a	1519	32	19,26,27	0.85	0	18,38,41	1.49	2 (11%)
1	PSU	2A	1911	1	18,21,22	1.34	2 (11%)	22,30,33	1.79	3 (13%)
1	5MC	2A	1942	1	18,22,23	0.99	1 (5%)	26,32,35	1.16	3 (11%)
1	OMG	2A	2251	55,1	18,26,27	0.94	1 (5%)	19,38,41	1.14	3 (15%)
32	2MG	1a	1207	32	18,26,27	0.92	1 (5%)	16,38,41	1.20	3 (18%)
32	UR3	1a	1498	32	19,22,23	1.01	1 (5%)	26,32,35	1.54	2 (7%)
32	4OC	2a	1402	32,57	20,23,24	0.75	0	26,32,35	1.07	1 (3%)
32	5MC	2a	1404	32	18,22,23	0.98	2 (11%)	26,32,35	1.22	3 (11%)
55	5MU	1x	54	55	19,22,23	1.45	5 (26%)	28,32,35	1.97	5 (17%)
55	PSU	1x	55	55	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
32	5MC	1a	1400	32	18,22,23	0.93	2 (11%)	26,32,35	1.17	4 (15%)
32	PSU	1a	516	32	18,21,22	1.42	2 (11%)	22,30,33	1.88	3 (13%)
1	5MU	2A	1915	1	19,22,23	1.40	5 (26%)	28,32,35	2.13	6 (21%)
1	5MC	2A	1962	57,1	18,22,23	0.96	2 (11%)	26,32,35	1.16	3 (11%)
1	PSU	2A	1917	1	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	1A	2605	57,1	18,21,22	1.40	3 (16%)	22,30,33	1.80	5 (22%)
32	G7M	2a	527	32,57	20,26,27	1.22	2 (10%)	17,39,42	0.60	0
54	PSU	2w	55	57,54	18,21,22	1.33	2 (11%)	22,30,33	1.88	4 (18%)
55	31H	1x	76	55,57	28,34,35	1.05	3 (10%)	23,47,50	1.68	3 (13%)
32	5MC	1a	967	32	18,22,23	0.96	2 (11%)	26,32,35	1.08	2 (7%)
55	PSU	2x	55	55	18,21,22	1.36	2 (11%)	22,30,33	1.92	4 (18%)
32	PSU	2a	516	32	18,21,22	1.33	2 (11%)	22,30,33	1.80	3 (13%)
1	2MA	1A	2503	57,1	17,25,26	0.97	1 (5%)	17,37,40	1.09	2 (11%)
56	5MU	2y	54	56	19,22,23	1.47	4 (21%)	28,32,35	1.88	8 (28%)
32	5MC	1a	1404	32	18,22,23	0.99	2 (11%)	26,32,35	1.09	2 (7%)
55	5MU	2x	54	55	19,22,23	1.38	4 (21%)	28,32,35	2.04	6 (21%)
1	OMC	1A	1920	1	19,22,23	0.80	0	26,31,34	0.90	1 (3%)
56	PSU	1y	55	56	18,21,22	1.37	2 (11%)	22,30,33	1.95	4 (18%)
32	MA6	1a	1518	32	19,26,27	0.82	0	18,38,41	1.45	2 (11%)
32	M2G	2a	966	32	20,27,28	1.49	3 (15%)	22,40,43	1.00	2 (9%)
54	L3X	2w	76	1,54	21,28,29	1.40	4 (19%)	15,40,43	1.58	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	G7M	1a	527	32,57	20,26,27	1.20	2 (10%)	17,39,42	0.57	0
1	OMU	2A	2552	1	19,22,23	1.24	2 (10%)	26,31,34	1.66	6 (23%)
1	OMG	1A	2251	55,57,1	18,26,27	1.02	1 (5%)	19,38,41	1.09	3 (15%)
32	5MC	1a	1407	32	18,22,23	0.89	2 (11%)	26,32,35	1.18	3 (11%)
54	4SU	2w	8	54	18,21,22	1.68	4 (22%)	26,30,33	3.02	6 (23%)
55	4SU	1x	8	55	18,21,22	2.05	6 (33%)	26,30,33	1.62	7 (26%)
56	4SU	2y	8	56	18,21,22	1.70	5 (27%)	26,30,33	1.88	4 (15%)
32	MA6	2a	1518	32	19,26,27	0.79	0	18,38,41	1.46	2 (11%)
54	5MU	1w	54	54	19,22,23	1.37	4 (21%)	28,32,35	1.87	6 (21%)
56	PSU	2y	55	56	18,21,22	1.39	2 (11%)	22,30,33	1.84	3 (13%)
32	M2G	1a	966	32	20,27,28	1.41	3 (15%)	22,40,43	1.00	3 (13%)
56	4SU	1y	8	56	18,21,22	1.79	4 (22%)	26,30,33	1.65	5 (19%)
32	5MC	2a	1407	32	18,22,23	1.02	2 (11%)	26,32,35	1.23	3 (11%)
55	5MC	1x	32	55	18,22,23	0.95	2 (11%)	26,32,35	1.23	2 (7%)
54	5MU	2w	54	54	19,22,23	1.38	4 (21%)	28,32,35	1.70	6 (21%)
1	PSU	2A	2605	1	18,21,22	1.27	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	1A	1917	1	18,21,22	1.32	2 (11%)	22,30,33	1.86	3 (13%)
1	5MU	1A	1939	57,1	19,22,23	1.41	5 (26%)	28,32,35	2.28	6 (21%)
1	5MU	2A	1939	1	19,22,23	1.34	5 (26%)	28,32,35	2.35	6 (21%)
56	5MU	1y	54	56	19,22,23	1.42	5 (26%)	28,32,35	1.94	7 (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
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	2MG	2a	1207	32	-	1/5/27/28	0/3/3/3
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
54	L3X	1w	76	1,54	-	2/9/31/32	0/3/3/3
1	2MA	2A	2503	57,1	-	1/3/25/26	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
55	31H	2x	76	55,57	-	5/18/40/41	0/3/3/3
43	0TD	2l	92	43	-	2/7/12/14	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/7/12/14	-
1	OMU	1A	2552	1	-	0/9/27/28	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	57,54	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	57,1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1	-	0/5/27/28	0/3/3/3
32	2MG	1a	1207	32	-	2/5/27/28	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32,57	-	3/9/29/30	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	2/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	57,1	-	2/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	57,1	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32,57	-	2/3/25/26	0/3/3/3
54	PSU	2w	55	57,54	-	0/7/25/26	0/2/2/2
55	31H	1x	76	55,57	-	5/18/40/41	0/3/3/3
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	57,1	-	2/3/25/26	0/3/3/3
56	5MU	2y	54	56	-	3/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	0/9/27/28	0/2/2/2
56	PSU	1y	55	56	-	1/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
54	L3X	2w	76	1,54	-	2/9/31/32	0/3/3/3
32	G7M	1a	527	32,57	-	3/3/25/26	0/3/3/3
1	OMU	2A	2552	1	-	0/9/27/28	0/2/2/2
1	OMG	1A	2251	55,57,1	-	0/5/27/28	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
56	4SU	2y	8	56	-	3/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
56	PSU	2y	55	56	-	2/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
56	4SU	1y	8	56	-	1/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	57,1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
56	5MU	1y	54	56	-	0/7/25/26	0/2/2/2

All (171) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.33	1.69	1.82
43	1l	92	0TD	CB-SB	-12.22	1.69	1.82
32	2a	966	M2G	C2-N3	5.02	1.36	1.30
55	1x	8	4SU	C4-N3	-4.80	1.32	1.37
54	1w	8	4SU	C4-S4	-4.47	1.59	1.68
32	1a	966	M2G	C2-N3	4.46	1.36	1.30
54	2w	8	4SU	C4-S4	-4.43	1.60	1.68
56	2y	8	4SU	C4-S4	-4.30	1.60	1.68
55	2x	8	4SU	C4-N3	-4.27	1.33	1.37
56	1y	8	4SU	C4-S4	-4.14	1.60	1.68
55	2x	8	4SU	C4-S4	-3.98	1.60	1.68
55	1x	8	4SU	C4-S4	-3.90	1.61	1.68
56	2y	55	PSU	C6-C5	3.80	1.39	1.35
54	1w	76	L3X	O4'-C1'	3.79	1.46	1.41
56	1y	55	PSU	C6-C5	3.74	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	527	G7M	C5-C4	3.69	1.46	1.39
55	1x	8	4SU	C2-N3	-3.68	1.31	1.38
32	2a	527	G7M	C5-C4	3.63	1.46	1.39
54	1w	55	PSU	C6-C5	3.63	1.39	1.35
56	1y	8	4SU	C4-N3	-3.61	1.33	1.37
1	2A	1917	PSU	C6-C5	3.61	1.39	1.35
54	2w	55	PSU	C6-C5	3.54	1.39	1.35
32	1a	516	PSU	C6-C5	3.49	1.39	1.35
54	2w	76	L3X	O4'-C1'	3.45	1.45	1.41
32	2a	516	PSU	C6-C5	3.44	1.39	1.35
1	1A	1917	PSU	C6-C5	3.40	1.39	1.35
54	1w	8	4SU	C4-N3	-3.37	1.34	1.37
55	2x	55	PSU	C6-C5	3.30	1.39	1.35
55	1x	8	4SU	C5-C4	-3.27	1.38	1.42
1	1A	2605	PSU	C4-N3	-3.24	1.32	1.38
56	2y	54	5MU	C2-N1	3.20	1.43	1.38
55	1x	55	PSU	C6-C5	3.17	1.39	1.35
1	1A	1911	PSU	C6-C5	3.17	1.39	1.35
1	2A	2605	PSU	C6-C5	3.11	1.38	1.35
1	2A	1942	5MC	C6-C5	3.10	1.39	1.34
1	2A	1911	PSU	C6-C5	3.06	1.38	1.35
56	2y	8	4SU	C4-N3	-3.01	1.34	1.37
32	2a	1404	5MC	C6-C5	2.98	1.39	1.34
55	1x	54	5MU	C6-C5	2.97	1.39	1.34
32	1a	966	M2G	C2-N2	2.95	1.40	1.35
54	2w	8	4SU	C2-N1	2.95	1.43	1.38
1	2A	1939	5MU	C6-C5	2.90	1.39	1.34
54	1w	54	5MU	C6-C5	2.87	1.39	1.34
1	1A	1942	5MC	C6-C5	2.86	1.39	1.34
54	1w	8	4SU	C5-C4	-2.86	1.38	1.42
32	2a	1407	5MC	C6-C5	2.85	1.39	1.34
56	2y	54	5MU	C6-C5	2.84	1.39	1.34
55	2x	54	5MU	C6-C5	2.83	1.39	1.34
1	1A	1939	5MU	C6-N1	-2.82	1.33	1.38
54	1w	76	L3X	C5-C4	-2.82	1.33	1.40
32	1a	1404	5MC	C6-C5	2.80	1.39	1.34
55	2x	76	31H	C5-C4	-2.79	1.33	1.40
32	1a	967	5MC	C6-C5	2.79	1.39	1.34
56	1y	54	5MU	C6-C5	2.78	1.39	1.34
32	2a	1400	5MC	C6-C5	2.77	1.39	1.34
1	1A	1911	PSU	C4-N3	-2.75	1.33	1.38
55	2x	32	5MC	C6-C5	2.75	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1939	5MU	C4-N3	-2.74	1.33	1.38
54	2w	8	4SU	O2-C2	2.74	1.28	1.23
55	1x	54	5MU	C4-N3	-2.74	1.33	1.38
1	1A	2251	OMG	C6-N1	-2.73	1.33	1.37
55	2x	8	4SU	C2-N3	-2.72	1.33	1.38
1	2A	1915	5MU	C6-C5	2.72	1.39	1.34
55	1x	76	31H	C5-C4	-2.72	1.33	1.40
54	2w	54	5MU	C6-C5	2.72	1.39	1.34
32	1a	516	PSU	C4-N3	-2.71	1.33	1.38
55	2x	8	4SU	C5-C4	-2.70	1.39	1.42
54	2w	76	L3X	C5-C4	-2.66	1.33	1.40
55	2x	76	31H	C6-C5	-2.65	1.33	1.43
1	1A	1915	5MU	C2-N1	2.65	1.42	1.38
32	2a	967	5MC	C6-C5	2.64	1.38	1.34
32	1a	1400	5MC	C6-C5	2.63	1.38	1.34
1	2A	1911	PSU	C4-N3	-2.61	1.34	1.38
55	1x	76	31H	C6-C5	-2.59	1.33	1.43
56	1y	8	4SU	C2-N1	2.58	1.42	1.38
32	1a	1407	5MC	C6-C5	2.58	1.38	1.34
1	1A	1962	5MC	C6-C5	2.56	1.38	1.34
1	1A	1962	5MC	C6-N1	-2.56	1.33	1.38
1	2A	1962	5MC	C6-C5	2.56	1.38	1.34
54	1w	54	5MU	C2-N1	2.55	1.42	1.38
56	1y	54	5MU	C4-C5	2.55	1.49	1.44
1	1A	2552	OMU	C4-N3	-2.54	1.34	1.38
56	2y	54	5MU	C4-N3	-2.54	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.54	1.33	1.38
32	2a	966	M2G	C2-N2	2.53	1.39	1.35
1	2A	1915	5MU	C4-N3	-2.53	1.34	1.38
1	2A	1939	5MU	C4-N3	-2.53	1.34	1.38
54	1w	76	L3X	C6-C5	-2.53	1.33	1.43
1	2A	2552	OMU	C4-N3	-2.53	1.34	1.38
1	2A	2251	OMG	C6-N1	-2.51	1.34	1.37
1	2A	1917	PSU	C4-N3	-2.51	1.34	1.38
55	2x	55	PSU	C4-N3	-2.51	1.34	1.38
54	1w	55	PSU	C4-N3	-2.51	1.34	1.38
55	1x	54	5MU	C2-N1	2.50	1.42	1.38
54	2w	76	L3X	C6-C5	-2.48	1.34	1.43
55	1x	32	5MC	C6-N1	-2.47	1.33	1.38
1	1A	1939	5MU	C6-C5	2.47	1.38	1.34
1	2A	1915	5MU	C4-C5	2.47	1.48	1.44
56	1y	54	5MU	C4-N3	-2.46	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2x	54	5MU	C4-N3	-2.45	1.34	1.38
54	2w	54	5MU	C4-N3	-2.45	1.34	1.38
1	2A	2503	2MA	C2-N3	2.45	1.36	1.31
54	2w	8	4SU	C5-C4	-2.45	1.39	1.42
1	1A	1915	5MU	C6-C5	2.43	1.38	1.34
1	1A	1939	5MU	C2-N3	-2.43	1.33	1.38
32	1a	1207	2MG	C6-N1	-2.42	1.34	1.37
56	1y	8	4SU	C5-C4	-2.42	1.39	1.42
32	2a	1207	2MG	C6-N1	-2.42	1.34	1.37
55	2x	8	4SU	O2-C2	2.42	1.27	1.23
1	1A	1917	PSU	C4-N3	-2.41	1.34	1.38
1	2A	1939	5MU	C4-C5	2.41	1.48	1.44
54	2w	55	PSU	C4-N3	-2.41	1.34	1.38
55	2x	54	5MU	C2-N1	2.41	1.42	1.38
32	2a	516	PSU	C4-N3	-2.39	1.34	1.38
1	1A	1915	5MU	C4-N3	-2.39	1.34	1.38
56	2y	8	4SU	C5-C4	-2.39	1.39	1.42
55	1x	32	5MC	C6-C5	2.38	1.38	1.34
32	2a	966	M2G	C6-N1	-2.38	1.34	1.37
54	2w	54	5MU	C2-N1	2.37	1.42	1.38
1	1A	2605	PSU	C2-N3	-2.37	1.33	1.37
32	1a	527	G7M	C6-N1	-2.37	1.34	1.37
55	1x	55	PSU	C4-N3	-2.36	1.34	1.38
56	1y	55	PSU	C4-N3	-2.34	1.34	1.38
54	1w	8	4SU	C2-N1	2.34	1.42	1.38
54	1w	54	5MU	C4-C5	2.32	1.48	1.44
1	1A	1915	5MU	C4-C5	2.32	1.48	1.44
32	1a	1400	5MC	C6-N1	-2.32	1.34	1.38
1	2A	2605	PSU	C4-N3	-2.31	1.34	1.38
56	2y	8	4SU	C2-N1	2.30	1.42	1.38
1	2A	1915	5MU	C2-N1	2.28	1.42	1.38
32	1a	1404	5MC	C6-N1	-2.28	1.34	1.38
1	2A	2552	OMU	C5-C4	2.27	1.48	1.43
55	2x	54	5MU	C4-C5	2.27	1.48	1.44
56	2y	55	PSU	C4-N3	-2.26	1.34	1.38
55	2x	32	5MC	C6-N1	-2.25	1.34	1.38
56	1y	54	5MU	C2-N1	2.24	1.42	1.38
32	1a	1498	UR3	C2-N1	2.23	1.41	1.38
32	1a	967	5MC	C6-N1	-2.22	1.34	1.38
1	1A	1939	5MU	C4-C5	2.22	1.48	1.44
56	2y	54	5MU	C4-C5	2.22	1.48	1.44
54	1w	54	5MU	C4-N3	-2.22	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	527	G7M	C6-N1	-2.22	1.34	1.37
32	1a	966	M2G	C6-N1	-2.21	1.34	1.37
32	2a	1404	5MC	C6-N1	-2.20	1.34	1.38
1	2A	1915	5MU	C6-N1	-2.18	1.34	1.38
1	1A	2605	PSU	C6-C5	2.18	1.37	1.35
54	2w	76	L3X	C5-N7	-2.17	1.31	1.39
54	1w	76	L3X	C5-N7	-2.17	1.31	1.39
55	1x	8	4SU	O2-C2	2.17	1.27	1.23
32	2a	1407	5MC	C6-N1	-2.17	1.34	1.38
1	1A	2552	OMU	C5-C4	2.17	1.48	1.43
55	1x	54	5MU	C4-C5	2.16	1.48	1.44
32	2a	1400	5MC	C6-N1	-2.16	1.34	1.38
55	2x	76	31H	C5-N7	-2.15	1.31	1.39
55	1x	76	31H	C5-N7	-2.15	1.31	1.39
56	1y	54	5MU	C6-N1	-2.15	1.34	1.38
54	2w	54	5MU	C4-C5	2.13	1.48	1.44
1	2A	1939	5MU	C2-N3	-2.12	1.34	1.38
1	1A	1942	5MC	C6-N1	-2.11	1.34	1.38
56	2y	8	4SU	C2-N3	-2.10	1.34	1.38
1	1A	1915	5MU	C6-N1	-2.08	1.34	1.38
55	1x	8	4SU	C6-C5	2.08	1.39	1.35
32	2a	1498	UR3	C6-C5	2.08	1.39	1.35
32	1a	1407	5MC	C6-N1	-2.06	1.34	1.38
55	2x	8	4SU	C6-C5	2.06	1.39	1.35
55	2x	8	4SU	C2-N1	2.05	1.41	1.38
54	1w	8	4SU	C2-N3	-2.03	1.34	1.38
1	2A	1939	5MU	C6-N1	-2.02	1.34	1.38
32	2a	967	5MC	C6-N1	-2.01	1.34	1.38
55	1x	54	5MU	C2-N3	-2.01	1.34	1.38
1	1A	2503	2MA	C2-N3	2.00	1.35	1.31

All (238) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-11.53	81.58	102.44
54	2w	8	4SU	C4-N3-C2	-9.18	118.42	127.34
54	2w	8	4SU	C5-C4-N3	7.34	121.50	114.69
54	2w	8	4SU	C5-C4-S4	-6.75	115.78	124.47
55	2x	55	PSU	N1-C2-N3	6.16	122.11	115.13
32	2a	1498	UR3	C4-N3-C2	-6.13	118.80	124.56
56	1y	55	PSU	N1-C2-N3	6.11	122.05	115.13
43	1l	92	0TD	CSB-SB-CB	-6.09	91.42	102.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1498	UR3	C4-N3-C2	-6.02	118.89	124.56
1	2A	1917	PSU	N1-C2-N3	6.00	121.93	115.13
1	1A	1911	PSU	N1-C2-N3	5.99	121.92	115.13
1	2A	1939	5MU	C4-N3-C2	-5.96	119.64	127.35
55	1x	55	PSU	N1-C2-N3	5.95	121.87	115.13
32	1a	516	PSU	N1-C2-N3	5.95	121.87	115.13
54	1w	55	PSU	N1-C2-N3	5.91	121.83	115.13
1	1A	2605	PSU	N1-C2-N3	5.80	121.71	115.13
1	1A	2552	OMU	N3-C2-N1	5.78	122.57	114.89
1	2A	2605	PSU	N1-C2-N3	5.75	121.65	115.13
56	2y	55	PSU	N1-C2-N3	5.74	121.63	115.13
1	2A	1911	PSU	N1-C2-N3	5.70	121.59	115.13
32	2a	516	PSU	N1-C2-N3	5.70	121.58	115.13
54	2w	55	PSU	N1-C2-N3	5.67	121.56	115.13
54	1w	8	4SU	C5-C4-N3	5.67	119.95	114.69
1	1A	1917	PSU	N1-C2-N3	5.67	121.55	115.13
1	1A	1939	5MU	C4-N3-C2	-5.66	120.02	127.35
55	1x	76	31H	N3-C2-N1	-5.65	119.85	128.68
54	2w	76	L3X	N3-C2-N1	-5.64	119.87	128.68
55	2x	76	31H	N3-C2-N1	-5.48	120.11	128.68
54	1w	76	L3X	N3-C2-N1	-5.47	120.12	128.68
1	2A	1939	5MU	N3-C2-N1	5.41	122.07	114.89
1	2A	1915	5MU	C4-N3-C2	-5.39	120.38	127.35
56	2y	8	4SU	C4-N3-C2	-5.26	122.23	127.34
1	2A	1939	5MU	C5-C4-N3	5.12	119.68	115.31
54	1w	8	4SU	C4-N3-C2	-5.11	122.38	127.34
56	2y	8	4SU	C5-C4-N3	5.09	119.41	114.69
1	1A	1915	5MU	C4-N3-C2	-5.07	120.79	127.35
1	1A	1939	5MU	C5-C4-N3	5.05	119.62	115.31
32	2a	1518	MA6	N3-C2-N1	-4.96	120.92	128.68
55	1x	54	5MU	N3-C2-N1	4.94	121.45	114.89
55	2x	54	5MU	C4-N3-C2	-4.94	120.96	127.35
32	1a	1518	MA6	N3-C2-N1	-4.93	120.97	128.68
32	2a	1519	MA6	N3-C2-N1	-4.92	121.00	128.68
1	2A	2552	OMU	N3-C2-N1	4.88	121.37	114.89
1	2A	1915	5MU	N3-C2-N1	4.88	121.37	114.89
1	2A	1915	5MU	C5-C4-N3	4.88	119.48	115.31
55	2x	54	5MU	N3-C2-N1	4.86	121.34	114.89
55	1x	54	5MU	C4-N3-C2	-4.78	121.16	127.35
1	1A	1915	5MU	N3-C2-N1	4.77	121.22	114.89
32	1a	1519	MA6	N3-C2-N1	-4.76	121.24	128.68
1	1A	1939	5MU	N3-C2-N1	4.75	121.19	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1939	5MU	C5-C6-N1	-4.71	118.49	123.34
56	1y	54	5MU	C4-N3-C2	-4.68	121.29	127.35
1	1A	1939	5MU	C5-C6-N1	-4.68	118.53	123.34
56	1y	8	4SU	C5-C4-N3	4.60	118.95	114.69
1	2A	1939	5MU	O4-C4-C5	-4.58	119.59	124.90
1	1A	1939	5MU	O4-C4-C5	-4.58	119.59	124.90
54	2w	8	4SU	O2-C2-N1	-4.54	116.75	122.79
1	1A	1915	5MU	C5-C4-N3	4.45	119.11	115.31
55	2x	54	5MU	O4-C4-C5	-4.41	119.79	124.90
55	2x	54	5MU	C5-C4-N3	4.40	119.07	115.31
56	1y	54	5MU	N3-C2-N1	4.37	120.69	114.89
54	1w	54	5MU	C4-N3-C2	-4.37	121.69	127.35
54	1w	54	5MU	N3-C2-N1	4.33	120.64	114.89
1	1A	1915	5MU	O4-C4-C5	-4.33	119.88	124.90
56	1y	54	5MU	C5-C4-N3	4.32	119.00	115.31
1	1A	2552	OMU	C4-N3-C2	-4.30	120.90	126.58
54	1w	54	5MU	O4-C4-C5	-4.29	119.93	124.90
1	1A	1911	PSU	C4-N3-C2	-4.26	120.20	126.34
1	2A	1915	5MU	O4-C4-C5	-4.23	119.99	124.90
1	2A	2605	PSU	C4-N3-C2	-4.23	120.25	126.34
55	1x	8	4SU	C6-C5-C4	-4.20	116.31	119.95
56	1y	8	4SU	C4-N3-C2	-4.14	123.32	127.34
56	1y	55	PSU	O2-C2-N1	-4.13	118.24	122.79
55	1x	54	5MU	C5-C4-N3	4.13	118.83	115.31
56	2y	54	5MU	N3-C2-N1	4.03	120.23	114.89
56	2y	55	PSU	O2-C2-N1	-4.00	118.38	122.79
55	1x	32	5MC	C5-C6-N1	-3.99	119.23	123.34
56	2y	54	5MU	C5-C4-N3	3.99	118.71	115.31
55	2x	55	PSU	C4-N3-C2	-3.98	120.60	126.34
54	1w	54	5MU	C5-C4-N3	3.95	118.69	115.31
1	2A	2552	OMU	C4-N3-C2	-3.93	121.40	126.58
54	2w	55	PSU	O2-C2-N1	-3.92	118.47	122.79
54	2w	54	5MU	O4-C4-C5	-3.92	120.36	124.90
55	1x	54	5MU	O4-C4-C5	-3.91	120.38	124.90
1	1A	1917	PSU	C4-N3-C2	-3.89	120.73	126.34
54	2w	8	4SU	N3-C2-N1	3.89	120.06	114.89
1	1A	2605	PSU	C4-N3-C2	-3.85	120.79	126.34
56	2y	54	5MU	C4-N3-C2	-3.84	122.38	127.35
32	1a	516	PSU	C4-N3-C2	-3.80	120.86	126.34
56	2y	54	5MU	O4-C4-C5	-3.80	120.50	124.90
1	2A	1917	PSU	C4-N3-C2	-3.80	120.87	126.34
55	2x	32	5MC	C5-C6-N1	-3.78	119.45	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	8	4SU	O2-C2-N1	3.77	127.80	122.79
1	2A	1911	PSU	C4-N3-C2	-3.75	120.93	126.34
1	2A	1962	5MC	C5-C6-N1	-3.75	119.48	123.34
1	1A	1911	PSU	O2-C2-N1	-3.75	118.66	122.79
56	1y	55	PSU	C4-N3-C2	-3.72	120.97	126.34
1	2A	1915	5MU	C5-C6-N1	-3.71	119.52	123.34
56	2y	8	4SU	N3-C2-N1	3.71	119.81	114.89
1	1A	1942	5MC	C5-C6-N1	-3.69	119.54	123.34
54	2w	54	5MU	N3-C2-N1	3.69	119.79	114.89
54	2w	54	5MU	C5-C4-N3	3.69	118.46	115.31
54	1w	55	PSU	C4-N3-C2	-3.68	121.03	126.34
54	2w	54	5MU	C4-N3-C2	-3.68	122.59	127.35
32	2a	1400	5MC	C5-C6-N1	-3.67	119.56	123.34
32	2a	1404	5MC	C5-C6-N1	-3.67	119.56	123.34
32	2a	516	PSU	C4-N3-C2	-3.66	121.06	126.34
1	2A	1939	5MU	O2-C2-N1	-3.63	117.96	122.79
55	1x	54	5MU	C5-C6-N1	-3.60	119.63	123.34
55	2x	8	4SU	C5-C4-N3	3.59	118.02	114.69
55	1x	55	PSU	C4-N3-C2	-3.57	121.19	126.34
55	1x	55	PSU	O2-C2-N1	-3.56	118.87	122.79
32	2a	1407	5MC	C5-C6-N1	-3.55	119.69	123.34
32	1a	1407	5MC	C5-C6-N1	-3.51	119.73	123.34
54	2w	55	PSU	C4-N3-C2	-3.47	121.33	126.34
54	1w	55	PSU	O2-C2-N1	-3.47	118.97	122.79
1	1A	2552	OMU	O2-C2-N1	-3.46	118.19	122.79
32	2a	967	5MC	C5-C6-N1	-3.45	119.79	123.34
56	1y	54	5MU	O4-C4-C5	-3.43	120.92	124.90
1	2A	1942	5MC	C5-C6-N1	-3.43	119.81	123.34
32	1a	1400	5MC	C5-C6-N1	-3.41	119.83	123.34
55	2x	55	PSU	O2-C2-N1	-3.40	119.04	122.79
55	1x	76	31H	O4'-C1'-C2'	-3.39	101.97	106.93
56	2y	55	PSU	C4-N3-C2	-3.36	121.50	126.34
32	1a	967	5MC	C5-C6-N1	-3.34	119.91	123.34
54	1w	8	4SU	C5-C4-S4	-3.33	120.18	124.47
1	1A	1917	PSU	O2-C2-N1	-3.31	119.15	122.79
56	1y	54	5MU	C5-C6-N1	-3.31	119.94	123.34
56	2y	54	5MU	C1'-N1-C2	3.30	123.55	117.57
55	2x	76	31H	O4'-C1'-C2'	-3.30	102.11	106.93
32	2a	516	PSU	O2-C2-N1	-3.28	119.18	122.79
32	2a	1519	MA6	C4-C5-N7	-3.23	106.03	109.40
55	2x	54	5MU	C5-C6-N1	-3.21	120.04	123.34
1	2A	1917	PSU	O2-C2-N1	-3.18	119.29	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1939	5MU	O2-C2-N1	-3.17	118.57	122.79
32	1a	516	PSU	O2-C2-N1	-3.16	119.32	122.79
32	1a	1519	MA6	C4-C5-N7	-3.15	106.11	109.40
1	1A	1915	5MU	C5-C6-N1	-3.10	120.15	123.34
1	2A	2605	PSU	O2-C2-N1	-3.09	119.39	122.79
32	2a	1407	5MC	C5-C4-N3	-3.05	118.38	121.67
32	1a	1404	5MC	C5-C6-N1	-3.03	120.22	123.34
43	2l	92	0TD	OD2-CG-CB	3.02	119.67	113.15
56	2y	8	4SU	C5-C4-S4	-3.00	120.60	124.47
1	1A	1962	5MC	C5-C6-N1	-2.95	120.30	123.34
54	1w	8	4SU	N3-C2-N1	2.95	118.81	114.89
1	2A	1911	PSU	O2-C2-N1	-2.95	119.55	122.79
55	2x	8	4SU	C6-C5-C4	-2.89	117.45	119.95
32	2a	1518	MA6	C4-C5-N7	-2.87	106.40	109.40
56	1y	8	4SU	N3-C2-N1	2.84	118.66	114.89
56	1y	8	4SU	C1'-N1-C2	2.83	122.69	117.57
1	1A	1962	5MC	CM5-C5-C6	-2.81	119.09	122.85
55	1x	8	4SU	C5-C4-N3	2.80	117.29	114.69
32	1a	1404	5MC	C5-C4-N3	-2.80	118.66	121.67
32	1a	1207	2MG	C8-N7-C5	2.78	108.28	102.99
43	1l	92	0TD	OD2-CG-CB	2.77	119.12	113.15
1	2A	1942	5MC	C5-C4-N3	-2.68	118.78	121.67
1	1A	1962	5MC	C5-C4-N3	-2.66	118.80	121.67
56	2y	54	5MU	C1'-N1-C6	-2.63	116.75	121.12
32	2a	1404	5MC	C5-C4-N3	-2.60	118.86	121.67
32	1a	1400	5MC	C5-C4-N3	-2.60	118.87	121.67
55	1x	32	5MC	C5-C4-N3	-2.56	118.91	121.67
54	2w	8	4SU	S4-C4-N3	2.55	122.72	120.21
54	1w	54	5MU	C5-C6-N1	-2.55	120.71	123.34
32	1a	1402	4OC	C6-C5-C4	2.54	120.07	116.96
55	2x	8	4SU	C1'-N1-C2	2.54	122.17	117.57
32	1a	1518	MA6	C4-C5-N7	-2.54	106.75	109.40
55	1x	8	4SU	C1'-N1-C2	2.52	122.13	117.57
1	1A	1942	5MC	C5-C4-N3	-2.51	118.97	121.67
32	2a	1207	2MG	C8-N7-C5	2.51	107.77	102.99
55	2x	32	5MC	C5-C4-N3	-2.50	118.98	121.67
1	2A	2552	OMU	C5-C4-N3	2.50	118.58	114.84
1	2A	2251	OMG	C5-C6-N1	2.49	118.35	113.95
1	2A	2503	2MA	C5-C6-N1	2.49	118.31	114.02
55	2x	32	5MC	O2-C2-N3	-2.49	118.28	122.33
1	1A	2251	OMG	C8-N7-C5	2.46	107.67	102.99
32	1a	1207	2MG	CM2-N2-C2	-2.45	118.45	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2552	OMU	C2'-C1'-N1	-2.45	109.47	114.22
56	2y	54	5MU	O2-C2-N3	-2.45	116.94	121.50
54	2w	54	5MU	C5-C6-N1	-2.44	120.83	123.34
1	2A	2251	OMG	O6-C6-C5	-2.43	119.62	124.37
54	1w	8	4SU	C1'-N1-C2	2.43	121.96	117.57
56	1y	54	5MU	C5M-C5-C4	2.41	121.42	118.77
1	1A	2503	2MA	C8-N7-C5	2.40	107.57	102.99
1	2A	1915	5MU	O2-C2-N1	-2.39	119.60	122.79
1	2A	1962	5MC	C5-C4-N3	-2.39	119.09	121.67
1	1A	2503	2MA	C5-C6-N1	2.37	118.11	114.02
55	1x	8	4SU	S4-C4-N3	-2.36	117.89	120.21
32	2a	1407	5MC	O2-C2-N3	-2.34	118.53	122.33
32	1a	1407	5MC	CM5-C5-C6	-2.34	119.73	122.85
32	1a	1407	5MC	C5-C4-N3	-2.34	119.15	121.67
1	2A	2552	OMU	O2-C2-N1	-2.33	119.69	122.79
54	2w	55	PSU	C6-C5-C4	-2.33	116.57	118.20
32	2a	1400	5MC	C5-C4-N3	-2.32	119.17	121.67
1	2A	2503	2MA	C8-N7-C5	2.32	107.41	102.99
1	2A	2251	OMG	C8-N7-C5	2.32	107.41	102.99
56	2y	54	5MU	C5-C6-N1	-2.32	120.95	123.34
55	2x	54	5MU	O2-C2-N1	-2.32	119.70	122.79
1	1A	2605	PSU	C5-C6-N1	-2.31	118.64	122.11
1	1A	2552	OMU	O4-C4-C5	-2.30	121.11	125.16
1	2A	1920	OMC	O2-C2-N3	-2.30	118.59	122.33
1	1A	2251	OMG	C5-C6-N1	2.30	118.01	113.95
32	2a	967	5MC	C5-C4-N3	-2.30	119.20	121.67
32	2a	966	M2G	C8-N7-C5	2.28	107.34	102.99
32	2a	1498	UR3	C3U-N3-C4	2.28	121.15	117.89
32	2a	1402	4OC	C6-C5-C4	2.28	119.75	116.96
32	1a	1400	5MC	O2-C2-N3	-2.27	118.64	122.33
1	1A	1920	OMC	O2-C2-N3	-2.27	118.64	122.33
32	1a	966	M2G	C5-C6-N1	2.25	117.93	113.95
1	1A	2605	PSU	O2-C2-N1	-2.24	120.33	122.79
55	1x	8	4SU	C4-N3-C2	2.23	129.51	127.34
32	2a	1400	5MC	O2-C2-N3	-2.22	118.72	122.33
32	1a	1207	2MG	C5-C6-N1	2.22	117.88	113.95
32	1a	967	5MC	C5-C4-N3	-2.21	119.29	121.67
1	2A	2552	OMU	O4-C4-C5	-2.18	121.33	125.16
1	1A	2552	OMU	C5-C4-N3	2.18	118.10	114.84
1	2A	1942	5MC	O2-C2-N3	-2.16	118.82	122.33
32	1a	966	M2G	O6-C6-C5	-2.15	120.17	124.37
1	1A	1911	PSU	C5-C6-N1	-2.15	118.89	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	966	M2G	C8-N7-C5	2.14	107.07	102.99
56	1y	8	4SU	C5-C4-S4	-2.13	121.72	124.47
55	1x	8	4SU	O2-C2-N3	-2.09	117.61	121.50
1	2A	1962	5MC	CM5-C5-C6	-2.09	120.06	122.85
55	2x	8	4SU	S4-C4-N3	-2.08	118.16	120.21
32	1a	1400	5MC	CM5-C5-C6	-2.08	120.07	122.85
54	1w	54	5MU	O2-C2-N1	-2.07	120.03	122.79
32	2a	966	M2G	C5-C6-N1	2.07	117.61	113.95
56	1y	54	5MU	O2-C2-N1	-2.07	120.04	122.79
55	2x	76	31H	O2'-C2'-C3'	2.06	116.20	111.16
32	2a	1207	2MG	C5-C6-N1	2.06	117.58	113.95
32	2a	1404	5MC	O2-C2-N3	-2.05	118.99	122.33
32	1a	1498	UR3	C1'-N1-C2	2.05	120.45	116.99
1	1A	2605	PSU	O2-C2-N3	-2.04	117.96	121.82
55	2x	55	PSU	C5-C6-N1	-2.03	119.06	122.11
1	1A	2251	OMG	O6-C6-C5	-2.03	120.40	124.37
54	2w	54	5MU	C1'-N1-C2	2.01	121.21	117.57
56	1y	55	PSU	O4'-C1'-C2'	2.01	107.97	105.14
55	2x	32	5MC	CM5-C5-C6	-2.00	120.17	122.85
55	1x	76	31H	C3'-N3'-C	-2.00	120.19	123.21

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	527	G7M	C3'-C4'-C5'-O5'
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1207	2MG	N3-C2-N2-CM2
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
43	2l	92	0TD	CA-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB
54	2w	76	L3X	C3'-C4'-C5'-O5'
54	2w	76	L3X	O4'-C4'-C5'-O5'
55	1x	76	31H	C3'-C4'-C5'-O5'
55	1x	76	31H	C-CA-CB-CG
55	1x	76	31H	N-CA-CB-CG
56	2y	8	4SU	C3'-C4'-C5'-O5'
56	2y	8	4SU	O4'-C4'-C5'-O5'
56	2y	55	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
55	2x	76	31H	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
55	2x	76	31H	O4'-C4'-C5'-O5'
56	2y	55	PSU	O4'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
1	2A	1962	5MC	O4'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'
55	1x	55	PSU	O4'-C4'-C5'-O5'
55	1x	76	31H	O4'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C4'-C5'-O5'
1	2A	1962	5MC	C3'-C4'-C5'-O5'
32	1a	527	G7M	O4'-C4'-C5'-O5'
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	2a	527	G7M	O4'-C4'-C5'-O5'
55	1x	55	PSU	C3'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
55	2x	76	31H	CB-CG-SD-CE
32	1a	1400	5MC	C3'-C4'-C5'-O5'
55	1x	76	31H	C4'-C5'-O5'-P
55	2x	76	31H	C4'-C5'-O5'-P
32	2a	1519	MA6	C4'-C5'-O5'-P
1	1A	2503	2MA	C4'-C5'-O5'-P
32	1a	1519	MA6	C4'-C5'-O5'-P
56	2y	8	4SU	C4'-C5'-O5'-P
56	2y	54	5MU	C2'-C1'-N1-C6
56	1y	55	PSU	O4'-C1'-C5-C4
32	1a	527	G7M	C4'-C5'-O5'-P
56	2y	54	5MU	C2'-C1'-N1-C2
32	1a	967	5MC	O4'-C4'-C5'-O5'
54	1w	76	L3X	O4'-C4'-C5'-O5'
32	2a	1400	5MC	C2'-C1'-N1-C6
43	1l	92	0TD	CG-CB-SB-CSB
56	1y	8	4SU	C2'-C1'-N1-C2
1	1A	2503	2MA	O4'-C4'-C5'-O5'
56	2y	54	5MU	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C2'-C1'-N1-C2
32	2a	1400	5MC	O4'-C1'-N1-C6
55	2x	76	31H	CB-CA-N-CN
54	1w	76	L3X	C2'-C3'-N3'-C

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	CLM	2A	3863	-	19,20,20	1.01	1 (5%)	23,27,27	1.04	2 (8%)
61	SF4	1d	501	35	0,12,12	-	-	-		
61	SF4	2d	303	35	0,12,12	-	-	-		
59	CLM	1A	4097	-	19,20,20	0.97	2 (10%)	23,27,27	1.23	2 (8%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1A	4097	CLM	C6-C5	-2.41	1.48	1.51
59	2A	3863	CLM	C6-C5	-2.36	1.48	1.51
59	1A	4097	CLM	C9-N9	-2.28	1.39	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	1A	4097	CLM	O5-C5-C6	-3.41	103.76	111.19
59	2A	3863	CLM	C6-C5-C3	2.75	116.48	111.64
59	1A	4097	CLM	C6-C5-C3	2.63	116.27	111.64
59	2A	3863	CLM	O5-C5-C6	-2.01	106.82	111.19

There are no chirality outliers.

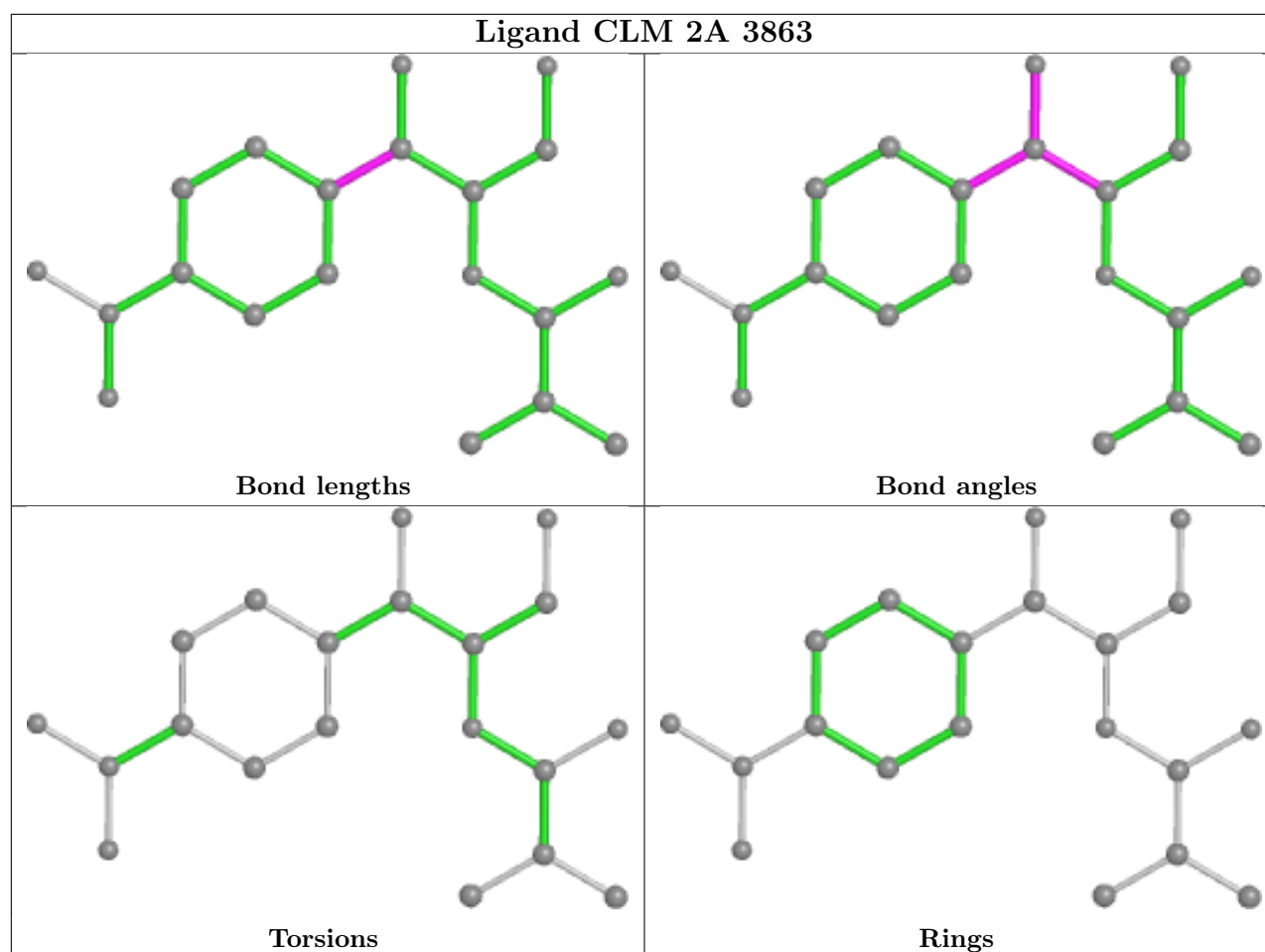
All (2) torsion outliers are listed below:

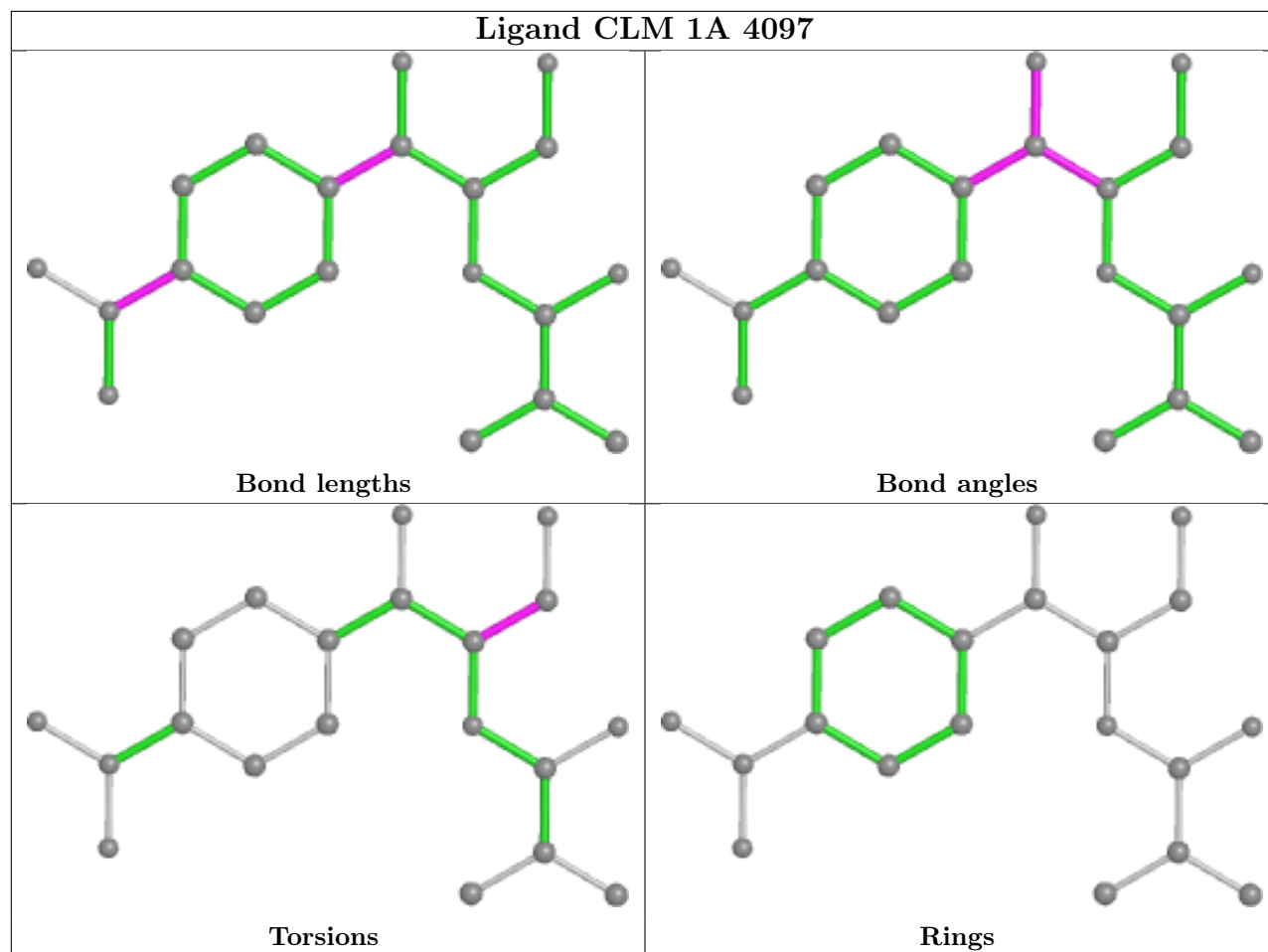
Mol	Chain	Res	Type	Atoms
59	1A	4097	CLM	N2-C3-C4-O4
59	1A	4097	CLM	C5-C3-C4-O4

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	0.94	102 (3%) 42 49	23, 38, 94, 106	0
1	2A	2789/2915 (95%)	0.69	125 (4%) 33 40	34, 60, 92, 105	0
2	1B	120/121 (99%)	0.58	0 100 100	31, 52, 67, 87	0
2	2B	120/121 (99%)	0.35	6 (5%) 28 34	65, 79, 87, 91	0
3	1D	275/276 (99%)	0.96	4 (1%) 73 79	24, 40, 54, 72	0
3	2D	275/276 (99%)	0.99	19 (6%) 16 20	33, 53, 66, 81	0
4	1E	204/206 (99%)	0.87	7 (3%) 45 52	20, 42, 61, 73	0
4	2E	204/206 (99%)	0.78	11 (5%) 25 30	36, 60, 71, 83	0
5	1F	202/210 (96%)	0.84	6 (2%) 50 57	21, 45, 68, 80	0
5	2F	202/210 (96%)	0.73	13 (6%) 19 22	39, 70, 80, 86	0
6	1G	181/182 (99%)	0.69	6 (3%) 46 53	43, 61, 75, 86	0
6	2G	181/182 (99%)	1.70	63 (34%) 0 0	70, 79, 85, 91	0
7	1H	174/180 (96%)	0.69	4 (2%) 60 67	40, 54, 66, 72	0
7	2H	174/180 (96%)	1.61	53 (30%) 0 0	70, 81, 88, 95	0
8	1I	146/148 (98%)	0.37	2 (1%) 75 81	43, 73, 81, 84	0
8	2I	146/148 (98%)	0.62	14 (9%) 8 10	59, 74, 81, 84	0
9	1N	140/140 (100%)	0.97	3 (2%) 63 70	27, 40, 60, 72	0
9	2N	140/140 (100%)	1.05	18 (12%) 3 4	47, 66, 77, 84	0
10	1O	122/122 (100%)	0.86	3 (2%) 57 63	32, 42, 60, 66	0
10	2O	122/122 (100%)	0.75	6 (4%) 29 35	45, 59, 71, 75	0
11	1P	149/150 (99%)	0.78	1 (0%) 87 90	23, 48, 67, 74	0
11	2P	149/150 (99%)	0.88	16 (10%) 6 7	41, 69, 82, 87	0
12	1Q	141/141 (100%)	0.97	3 (2%) 63 70	26, 43, 58, 72	0
12	2Q	141/141 (100%)	1.14	24 (17%) 1 1	48, 67, 76, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.97	0 100 100	27, 37, 50, 60	0
13	2R	118/118 (100%)	0.82	8 (6%) 17 20	42, 55, 64, 71	0
14	1S	110/112 (98%)	0.73	1 (0%) 84 88	41, 52, 63, 67	0
14	2S	110/112 (98%)	0.98	18 (16%) 1 1	64, 74, 80, 83	0
15	1T	131/146 (89%)	0.73	2 (1%) 73 79	32, 47, 68, 79	0
15	2T	131/146 (89%)	0.68	4 (3%) 49 56	51, 61, 76, 80	0
16	1U	116/118 (98%)	1.03	3 (2%) 56 62	23, 33, 49, 61	0
16	2U	116/118 (98%)	1.01	13 (11%) 5 7	48, 62, 75, 79	0
17	1V	101/101 (100%)	0.87	3 (2%) 50 57	26, 42, 58, 70	0
17	2V	101/101 (100%)	0.89	13 (12%) 3 4	47, 70, 76, 87	0
18	1W	112/113 (99%)	1.01	3 (2%) 54 61	27, 35, 53, 75	0
18	2W	112/113 (99%)	0.95	7 (6%) 20 23	41, 51, 69, 90	0
19	1X	95/96 (98%)	0.96	4 (4%) 36 42	29, 40, 64, 81	0
19	2X	95/96 (98%)	0.94	11 (11%) 4 6	48, 62, 77, 86	0
20	1Y	107/110 (97%)	0.71	1 (0%) 84 88	38, 51, 68, 79	0
20	2Y	107/110 (97%)	1.26	19 (17%) 1 1	63, 71, 80, 86	0
21	1Z	154/206 (74%)	0.82	15 (9%) 7 9	42, 64, 85, 88	0
21	2Z	160/206 (77%)	1.53	42 (26%) 0 0	64, 80, 89, 93	0
22	10	83/85 (97%)	0.97	4 (4%) 30 37	29, 40, 57, 64	0
22	20	83/85 (97%)	1.43	19 (22%) 0 0	46, 65, 74, 80	0
23	11	97/98 (98%)	0.93	7 (7%) 15 18	28, 47, 71, 74	0
23	21	97/98 (98%)	1.01	12 (12%) 4 5	40, 59, 74, 78	0
24	12	70/72 (97%)	0.74	0 100 100	38, 50, 62, 73	0
24	22	70/72 (97%)	0.69	5 (7%) 16 19	61, 71, 77, 79	0
25	13	59/60 (98%)	0.97	3 (5%) 28 33	28, 39, 58, 70	0
25	23	59/60 (98%)	1.24	15 (25%) 0 0	58, 67, 75, 79	0
26	14	69/71 (97%)	0.64	5 (7%) 15 18	53, 76, 86, 88	0
26	24	69/71 (97%)	2.12	31 (44%) 0 0	78, 85, 90, 94	0
27	15	59/60 (98%)	1.07	1 (1%) 70 76	21, 35, 51, 59	0
27	25	59/60 (98%)	0.79	2 (3%) 45 52	39, 53, 68, 75	0
28	16	53/54 (98%)	0.92	1 (1%) 66 73	33, 45, 59, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	1.13	9 (16%) 1 1	55, 64, 70, 71	0
29	17	48/49 (97%)	1.21	5 (10%) 6 8	24, 31, 53, 64	0
29	27	48/49 (97%)	1.55	8 (16%) 1 1	34, 44, 64, 76	0
30	18	64/65 (98%)	0.94	1 (1%) 72 78	27, 37, 45, 57	0
30	28	64/65 (98%)	1.15	9 (14%) 2 3	45, 58, 64, 68	0
31	19	37/37 (100%)	0.75	0 100 100	33, 42, 56, 63	0
31	29	37/37 (100%)	1.72	12 (32%) 0 0	61, 68, 74, 80	0
32	1a	1488/1521 (97%)	0.46	32 (2%) 62 68	38, 69, 92, 102	0
32	2a	1491/1521 (98%)	0.57	85 (5%) 23 28	52, 79, 94, 104	0
33	1b	231/256 (90%)	0.88	32 (13%) 2 3	66, 78, 85, 90	0
33	2b	231/256 (90%)	1.28	54 (23%) 0 0	73, 84, 89, 94	0
34	1c	206/239 (86%)	0.85	28 (13%) 3 3	59, 73, 82, 88	0
34	2c	206/239 (86%)	1.45	62 (30%) 0 0	76, 84, 88, 92	0
35	1d	208/209 (99%)	1.34	59 (28%) 0 0	59, 70, 78, 81	0
35	2d	208/209 (99%)	1.01	33 (15%) 1 2	63, 74, 81, 85	0
36	1e	148/162 (91%)	0.87	14 (9%) 8 10	49, 66, 74, 77	0
36	2e	148/162 (91%)	1.19	31 (20%) 1 0	67, 77, 83, 86	0
37	1f	100/101 (99%)	0.61	5 (5%) 28 34	60, 70, 77, 80	0
37	2f	100/101 (99%)	0.34	4 (4%) 38 45	62, 73, 79, 80	0
38	1g	155/156 (99%)	0.64	13 (8%) 11 13	63, 73, 83, 89	0
38	2g	155/156 (99%)	1.55	49 (31%) 0 0	73, 80, 86, 91	0
39	1h	137/138 (99%)	0.88	14 (10%) 6 8	59, 67, 74, 77	0
39	2h	137/138 (99%)	1.08	26 (18%) 1 1	69, 77, 82, 86	0
40	1i	127/128 (99%)	1.03	23 (18%) 1 1	56, 77, 83, 85	0
40	2i	127/128 (99%)	2.83	76 (59%) 0 0	73, 84, 89, 92	0
41	1j	97/105 (92%)	1.07	21 (21%) 0 0	62, 78, 84, 86	0
41	2j	96/105 (91%)	1.82	41 (42%) 0 0	72, 84, 89, 93	0
42	1k	114/129 (88%)	0.84	10 (8%) 10 11	45, 68, 77, 86	0
42	2k	114/129 (88%)	1.28	25 (21%) 0 0	57, 74, 82, 84	0
43	1l	121/132 (91%)	1.03	20 (16%) 1 1	50, 60, 69, 81	0
43	2l	121/132 (91%)	1.38	29 (23%) 0 0	61, 72, 78, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.95	12 (9%) 7 9	60, 72, 80, 91	0
44	2m	122/126 (96%)	1.74	44 (36%) 0 0	73, 82, 88, 93	0
45	1n	60/61 (98%)	1.32	12 (20%) 1 1	60, 70, 76, 78	0
45	2n	60/61 (98%)	3.18	40 (66%) 0 0	77, 84, 89, 90	0
46	1o	88/89 (98%)	0.60	4 (4%) 33 40	51, 66, 76, 78	0
46	2o	88/89 (98%)	0.93	11 (12%) 3 5	64, 74, 81, 84	0
47	1p	82/88 (93%)	1.25	19 (23%) 0 0	56, 72, 78, 81	0
47	2p	82/88 (93%)	0.98	8 (9%) 7 9	62, 71, 78, 83	0
48	1q	99/105 (94%)	1.07	13 (13%) 3 4	54, 69, 77, 80	0
48	2q	99/105 (94%)	1.47	28 (28%) 0 0	64, 74, 80, 87	0
49	1r	68/88 (77%)	0.61	3 (4%) 34 41	57, 68, 75, 78	0
49	2r	68/88 (77%)	0.94	9 (13%) 3 4	68, 75, 80, 82	0
50	1s	83/93 (89%)	0.70	4 (4%) 30 37	67, 75, 82, 84	0
50	2s	83/93 (89%)	2.72	50 (60%) 0 0	78, 86, 91, 94	0
51	1t	96/106 (90%)	1.40	31 (32%) 0 0	64, 72, 79, 82	0
51	2t	96/106 (90%)	1.15	17 (17%) 1 1	60, 72, 82, 84	0
52	1u	23/27 (85%)	1.77	10 (43%) 0 0	65, 71, 76, 79	0
52	2u	23/27 (85%)	3.13	16 (69%) 0 0	76, 81, 85, 86	0
53	1v	13/24 (54%)	2.32	8 (61%) 0 0	50, 71, 91, 94	0
53	2v	13/24 (54%)	3.82	11 (84%) 0 0	72, 85, 99, 101	0
54	1w	69/74 (93%)	2.61	35 (50%) 0 0	49, 93, 100, 101	0
54	2w	68/74 (91%)	3.99	58 (85%) 0 0	66, 96, 100, 101	0
55	1x	72/77 (93%)	0.51	1 (1%) 75 81	30, 68, 84, 88	0
55	2x	72/77 (93%)	0.91	10 (13%) 2 3	50, 82, 91, 97	0
56	1y	70/74 (94%)	5.67	66 (94%) 0 0	60, 98, 103, 105	0
56	2y	70/74 (94%)	6.59	70 (100%) 0 0	70, 99, 104, 104	0
All	All	20885/21740 (96%)	0.96	2201 (10%) 6 8	20, 66, 89, 106	0

All (2201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	1m	124	PRO	21.8
44	2m	124	PRO	16.2

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Mol	Chain	Res	Type	RSRZ
56	2y	36	C	14.9
56	1y	35	C	14.8
38	2g	80	VAL	13.0
56	1y	21	A	11.7
44	1m	123	ALA	11.6
56	2y	33	U	11.6
56	1y	34	C	11.4
56	1y	36	C	11.2
54	2w	71	G	11.1
54	1w	70	C	11.0
56	2y	74	C	10.9
45	2n	25	VAL	10.8
53	2v	24	A	10.8
56	1y	23	A	10.6
56	1y	24	A	10.6
54	1w	71	G	10.5
56	2y	37	A	10.3
56	2y	66	C	10.2
45	2n	39	LEU	10.2
20	2Y	1	MET	10.1
56	1y	38	A	10.0
56	1y	22	G	10.0
54	2w	72	C	10.0
3	2D	2	ALA	10.0
56	2y	1	G	10.0
54	2w	31	C	9.9
56	1y	71	G	9.9
40	2i	109	VAL	9.8
56	2y	35	C	9.8
1	1A	2145	C	9.5
6	2G	3	LEU	9.4
56	2y	21	A	9.4
56	1y	39	G	9.4
56	2y	29	A	9.4
56	1y	2	C	9.4
1	2A	2112	G	9.4
1	2A	2113	U	9.3
56	2y	57	G	9.2
56	2y	34	C	9.2
40	2i	66	ARG	9.1
44	2m	123	ALA	9.0
40	2i	14	VAL	8.9

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Mol	Chain	Res	Type	RSRZ
40	2i	72	GLY	8.9
1	2A	2117	A	8.8
45	1n	2	ALA	8.6
56	2y	18	G	8.5
56	2y	39	G	8.5
56	2y	52	G	8.4
56	1y	3	G	8.3
56	2y	72	C	8.3
56	1y	5	G	8.2
1	1A	2146	C	8.2
54	1w	4	G	8.2
38	1g	80	VAL	8.1
56	1y	13	C	8.1
56	2y	5	G	8.0
45	2n	34	TYR	8.0
54	2w	70	C	7.9
54	1w	3	G	7.9
22	20	3	HIS	7.8
56	2y	56	C	7.8
56	1y	75	C	7.8
56	2y	2	C	7.7
1	1A	2129	C	7.7
6	2G	29	TRP	7.6
34	2c	159	GLY	7.6
56	2y	75	C	7.5
40	2i	5	TYR	7.5
40	2i	76	ALA	7.5
21	2Z	153	SER	7.5
56	2y	42	C	7.5
1	2A	2110	G	7.5
56	2y	58	A	7.4
50	2s	80	TYR	7.4
50	2s	82	GLY	7.4
33	2b	92	TYR	7.3
1	1A	2141	G	7.3
56	2y	73	U	7.3
26	24	51	ASP	7.3
56	2y	17	G	7.3
1	1A	2115	G	7.3
56	2y	67	G	7.3
1	2A	2111	C	7.3
33	2b	165	VAL	7.2

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Mol	Chain	Res	Type	RSRZ
40	2i	36	TYR	7.2
1	1A	2130	U	7.2
56	2y	64	U	7.2
56	1y	14	A	7.1
26	24	63	TYR	7.1
1	2A	2147	G	7.1
1	2A	2115	G	7.1
56	1y	30	G	7.1
1	1A	2140	C	7.1
56	2y	28	G	7.1
56	2y	46	A	7.0
56	2y	53	G	7.0
54	2w	4	G	7.0
1	2A	2114	A	7.0
1	2A	2127	G	6.9
1	2A	2133	G	6.9
32	2a	1030(B)	C	6.9
56	2y	51	G	6.9
1	1A	2160	G	6.8
56	2y	38	A	6.8
34	2c	155	GLY	6.8
1	1A	2181	G	6.8
1	2A	2138	C	6.8
21	2Z	144	LEU	6.8
56	1y	37	A	6.8
1	2A	2802	G	6.8
1	2A	2146	C	6.8
33	2b	81	VAL	6.8
54	1w	69	C	6.8
1	2A	2141	G	6.8
1	2A	2160	G	6.8
54	2w	2	C	6.8
7	2H	128	PRO	6.8
1	2A	2142	C	6.7
52	2u	11	GLY	6.7
1	2A	2116	G	6.7
1	1A	2131	G	6.7
56	2y	49	G	6.7
56	2y	19	U	6.7
56	2y	15	A	6.6
56	1y	1	G	6.6
50	2s	84	GLY	6.5

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Mol	Chain	Res	Type	RSRZ
56	1y	33	U	6.5
45	2n	53	LEU	6.5
45	2n	55	GLY	6.5
56	1y	27	A	6.5
38	2g	156	TRP	6.5
1	2A	2128	C	6.5
45	2n	37	PHE	6.5
56	2y	32	U	6.5
1	1A	2159	G	6.5
56	1y	74	C	6.4
1	2A	2104	G	6.4
56	2y	50	A	6.4
1	2A	2139	C	6.4
53	2v	23	A	6.4
56	2y	26	G	6.4
54	2w	39	G	6.4
56	1y	29	A	6.4
56	2y	45	U	6.4
50	2s	79	THR	6.3
34	2c	198	VAL	6.3
56	2y	71	G	6.3
54	2w	30	G	6.3
54	2w	49	G	6.3
43	2l	55	VAL	6.3
56	1y	4	G	6.3
44	2m	102	ARG	6.2
35	1d	138	TYR	6.2
1	1A	2147	G	6.2
52	2u	16	GLY	6.2
36	2e	90	VAL	6.2
41	2j	44	VAL	6.2
56	1y	12	U	6.2
44	2m	122	LYS	6.2
54	2w	1	G	6.2
54	2w	3	G	6.1
32	2a	1532	U	6.1
50	2s	63	THR	6.1
34	2c	160	ALA	6.1
7	2H	102	ALA	6.1
1	2A	2170	A	6.1
56	2y	13	C	6.1
56	2y	23	A	6.1

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Mol	Chain	Res	Type	RSRZ
56	1y	70	C	6.1
1	2A	2145	C	6.0
40	2i	7	THR	6.0
1	1A	2112	G	6.0
1	2A	2129	C	6.0
54	2w	13	C	6.0
56	2y	62	C	6.0
1	2A	2123	G	6.0
56	2y	68	C	6.0
56	1y	15	A	5.9
21	2Z	141	VAL	5.9
21	2Z	149	SER	5.9
38	2g	32	ARG	5.9
45	2n	38	GLY	5.8
56	2y	4	G	5.8
36	2e	123	LEU	5.8
1	2A	2169	A	5.8
31	29	37	GLY	5.8
50	2s	12	ASP	5.8
32	2a	1035	A	5.8
56	1y	32	U	5.7
54	2w	50	A	5.7
40	2i	102	LEU	5.7
26	24	49	PHE	5.7
1	2A	888	C	5.7
56	1y	25	C	5.7
56	2y	61	C	5.7
1	1A	2144	U	5.7
21	2Z	155	LEU	5.7
52	2u	14	TRP	5.6
3	2D	276	LYS	5.6
14	2S	32	LEU	5.6
56	1y	49	G	5.6
40	2i	114	TYR	5.6
50	2s	49	ILE	5.6
40	2i	126	SER	5.6
1	1A	2132	U	5.6
1	1A	2180	U	5.6
56	2y	63	C	5.6
50	2s	48	THR	5.6
53	1v	13	A	5.6
7	2H	113	VAL	5.6

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Mol	Chain	Res	Type	RSRZ
6	2G	140	ILE	5.6
56	2y	30	G	5.5
23	21	2	SER	5.5
56	2y	31	C	5.5
1	2A	2167	U	5.5
40	2i	9	ARG	5.5
41	2j	47	PHE	5.5
44	2m	120	LYS	5.5
38	1g	79	ARG	5.5
1	2A	2174	C	5.5
56	2y	6	C	5.5
54	1w	13	C	5.5
44	2m	78	ILE	5.5
38	2g	5	ARG	5.4
56	1y	59	U	5.4
1	2A	2162	G	5.4
40	2i	19	LEU	5.4
1	1A	2113	U	5.4
1	1A	2803	C	5.4
54	1w	72	C	5.4
38	1g	81	GLY	5.3
56	2y	43	U	5.3
34	2c	157	ILE	5.3
56	2y	3	G	5.3
29	27	48	LYS	5.3
1	1A	2133	G	5.3
53	2v	13	A	5.3
54	1w	14	A	5.3
38	1g	82	GLY	5.3
50	2s	50	ALA	5.3
45	2n	29	ARG	5.3
50	2s	9	VAL	5.3
1	1A	2164	C	5.3
1	1A	2161	C	5.3
1	2A	2159	G	5.3
1	2A	2144	U	5.2
21	2Z	139	VAL	5.2
1	1A	2174	C	5.2
56	1y	42	C	5.2
1	1A	2110	G	5.2
40	2i	65	VAL	5.2
56	1y	19	U	5.2

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Mol	Chain	Res	Type	RSRZ
33	1b	227	GLY	5.2
56	1y	72	C	5.2
40	2i	115	GLY	5.2
1	1A	2158	A	5.1
52	2u	24	ARG	5.1
40	1i	126	SER	5.1
35	1d	135	LEU	5.1
54	2w	25	C	5.1
1	2A	2154	G	5.1
56	1y	62	C	5.1
42	2k	29	ILE	5.1
22	20	45	PHE	5.1
56	2y	10	G	5.1
21	1Z	149	SER	5.1
1	2A	2175	C	5.0
1	1A	1096	A	5.0
1	2A	2135	A	5.0
54	2w	18	G	5.0
6	2G	135	LEU	5.0
56	1y	50	A	5.0
56	2y	12	U	5.0
32	2a	1202	G	5.0
7	2H	78	GLY	5.0
26	24	45	GLY	5.0
1	2A	886	C	5.0
50	2s	42	PRO	5.0
54	2w	10	G	5.0
44	1m	2	ALA	5.0
35	1d	157	LEU	5.0
41	2j	88	LEU	5.0
6	2G	37	VAL	5.0
34	2c	184	TYR	5.0
56	2y	25	C	5.0
14	2S	58	LEU	4.9
41	2j	72	VAL	4.9
1	2A	885	C	4.9
50	2s	35	SER	4.9
1	1A	2120	G	4.9
1	1A	2792	G	4.9
1	2A	2181	G	4.9
32	1a	1030(A)	G	4.9
51	1t	72	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
50	2s	67	VAL	4.9
1	1A	2116	G	4.9
19	2X	95	LEU	4.9
41	2j	67	THR	4.9
54	1w	10	G	4.9
1	2A	2103	C	4.9
56	2y	14	A	4.9
6	2G	28	VAL	4.9
44	2m	84	ILE	4.9
32	2a	1034	G	4.9
21	2Z	148	ASP	4.8
1	2A	2155	G	4.8
28	26	52	VAL	4.8
54	2w	38	A	4.8
21	2Z	156	LYS	4.8
33	2b	214	ILE	4.8
1	1A	2188	C	4.8
3	2D	38	LYS	4.8
34	2c	60	ALA	4.8
32	1a	1001(A)	G	4.8
7	2H	35	VAL	4.8
38	2g	4	ARG	4.8
40	2i	73	GLN	4.8
56	1y	53	G	4.8
38	2g	41	ARG	4.8
48	2q	92	ARG	4.8
40	2i	125	TYR	4.7
56	2y	65	U	4.7
38	2g	79	ARG	4.7
52	2u	6	ARG	4.7
33	2b	34	ALA	4.7
32	2a	1531	A	4.7
43	2l	32	PHE	4.7
45	2n	43	CYS	4.7
56	1y	17	G	4.7
50	2s	71	LEU	4.7
1	2A	2179	C	4.7
54	2w	11	U	4.7
45	2n	35	ARG	4.7
34	2c	124	ILE	4.7
41	2j	6	ILE	4.7
54	2w	28	G	4.7

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Mol	Chain	Res	Type	RSRZ
1	2A	2180	U	4.7
1	2A	2105	C	4.7
40	2i	121	ARG	4.7
1	1A	2169	A	4.7
7	2H	105	LEU	4.7
1	1A	2114	A	4.6
29	27	47	ARG	4.6
21	2Z	96	VAL	4.6
40	1i	109	VAL	4.6
32	2a	1030(A)	G	4.6
54	2w	56	C	4.6
56	1y	45	U	4.6
40	2i	17	VAL	4.6
54	2w	26	G	4.6
56	1y	9	A	4.6
19	2X	92	LEU	4.6
39	2h	112	LEU	4.6
36	2e	20	GLN	4.6
50	2s	77	THR	4.6
14	2S	92	TYR	4.6
50	2s	41	VAL	4.6
23	11	2	SER	4.6
7	2H	123	PHE	4.6
34	1c	182	ILE	4.6
56	1y	10	G	4.6
11	2P	79	ARG	4.6
12	2Q	37	LEU	4.6
38	2g	78	ARG	4.6
54	2w	61	C	4.5
45	2n	31	ARG	4.5
48	1q	98	LEU	4.5
32	2a	1287	A	4.5
56	2y	24	A	4.5
33	2b	48	MET	4.5
36	2e	12	LEU	4.5
1	1A	2123	G	4.5
1	2A	2182	G	4.5
32	2a	1033	G	4.5
40	2i	124	GLN	4.5
6	2G	73	ALA	4.5
40	2i	127	LYS	4.5
41	1j	47	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	1A	2117	A	4.5
32	1a	1001	A	4.5
43	2l	51	ALA	4.5
56	2y	70	C	4.5
38	1g	156	TRP	4.5
40	2i	33	PHE	4.5
34	2c	158	GLY	4.5
41	2j	62	HIS	4.5
54	2w	32	U	4.5
56	2y	41	U	4.5
27	15	60	VAL	4.5
29	17	46	VAL	4.5
7	2H	103	LEU	4.5
56	2y	69	C	4.5
1	2A	2166	G	4.5
33	2b	232	PRO	4.5
34	1c	193	TYR	4.4
56	1y	46	A	4.4
6	2G	181	ARG	4.4
32	2a	91	C	4.4
33	2b	97	TRP	4.4
31	29	16	VAL	4.4
44	2m	119	GLY	4.4
56	2y	44	A	4.4
50	2s	52	TYR	4.4
1	2A	883	G	4.4
32	2a	1150	U	4.4
40	2i	26	VAL	4.4
45	2n	56	VAL	4.4
33	2b	201	ILE	4.4
54	1w	66	C	4.4
1	1A	2121	G	4.4
45	2n	26	ARG	4.4
33	2b	37	ASN	4.4
36	2e	33	VAL	4.4
1	2A	2793	G	4.4
34	2c	8	ILE	4.3
56	1y	11	U	4.3
33	1b	118	LEU	4.3
1	2A	2120	G	4.3
1	2A	2148	G	4.3
38	1g	4	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
14	2S	54	LEU	4.3
1	2A	2152	G	4.3
38	2g	22	LEU	4.3
38	2g	117	ALA	4.3
32	2a	1036	G	4.3
56	1y	48	C	4.3
41	2j	20	ALA	4.3
40	2i	63	ILE	4.3
34	2c	88	ARG	4.3
50	2s	38	SER	4.3
1	2A	2125	G	4.3
1	2A	2168	G	4.3
51	1t	73	HIS	4.3
1	2A	2188	C	4.3
40	2i	106	ALA	4.3
50	2s	81	ARG	4.3
50	2s	30	LEU	4.3
6	2G	50	ALA	4.3
1	1A	2175	C	4.2
1	1A	2794	C	4.2
54	1w	61	C	4.2
39	2h	2	LEU	4.2
48	1q	36	ILE	4.2
1	1A	888	C	4.2
54	2w	14	A	4.2
56	2y	40	C	4.2
48	2q	22	LEU	4.2
38	2g	154	TYR	4.2
38	2g	42	ILE	4.2
1	2A	2804	C	4.2
56	2y	22	G	4.2
35	1d	2	GLY	4.2
40	2i	105	ASP	4.2
34	2c	154	SER	4.2
41	2j	40	LEU	4.2
1	2A	2143	C	4.2
1	2A	2106	G	4.2
34	1c	206	GLU	4.2
45	2n	54	PRO	4.2
40	2i	10	ARG	4.2
1	2A	1026	U	4.2
56	1y	31	C	4.2

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Mol	Chain	Res	Type	RSRZ
56	2y	27	A	4.2
44	2m	42	ALA	4.2
56	1y	57	G	4.2
56	1y	64	U	4.2
45	2n	50	LYS	4.2
29	27	46	VAL	4.2
35	1d	207	TYR	4.2
56	1y	18	G	4.1
34	2c	87	LEU	4.1
40	2i	8	GLY	4.1
40	2i	90	PRO	4.1
43	2l	94	PRO	4.1
45	2n	46	GLU	4.1
26	24	59	PHE	4.1
14	2S	20	ARG	4.1
51	1t	22	ARG	4.1
1	2A	2189	U	4.1
38	2g	81	GLY	4.1
54	2w	73	U	4.1
56	1y	28	G	4.1
52	2u	23	PRO	4.1
21	2Z	170	THR	4.1
26	24	56	VAL	4.1
1	2A	884	C	4.1
41	2j	38	ILE	4.1
54	2w	15	A	4.1
12	2Q	33	GLY	4.1
50	2s	66	MET	4.1
14	2S	35	ILE	4.1
20	2Y	55	TYR	4.1
50	1s	71	LEU	4.1
20	2Y	5	MET	4.1
26	24	50	VAL	4.1
48	1q	27	PHE	4.1
44	2m	87	TYR	4.1
33	1b	101	MET	4.1
33	2b	216	SER	4.1
35	1d	3	ARG	4.1
32	1a	1028	C	4.1
54	2w	60	U	4.1
38	2g	105	VAL	4.1
48	2q	91	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
50	2s	22	LEU	4.0
1	2A	2109	U	4.0
56	1y	60	U	4.0
1	2A	2140	C	4.0
7	2H	111	HIS	4.0
56	1y	61	C	4.0
7	2H	124	GLU	4.0
7	2H	37	VAL	4.0
43	2l	43	VAL	4.0
41	1j	10	GLY	4.0
54	2w	36	C	4.0
43	2l	60	LEU	4.0
1	1A	2109	U	4.0
40	2i	4	TYR	4.0
1	1A	2128	C	4.0
32	1a	1257	U	4.0
26	24	67	TYR	4.0
34	2c	186	PHE	4.0
41	1j	16	LEU	4.0
45	2n	42	ILE	4.0
26	24	32	TYR	4.0
49	2r	86	VAL	4.0
1	1A	2143	C	4.0
39	1h	35	ILE	4.0
54	2w	17	G	4.0
54	2w	37	A	4.0
26	24	44	THR	4.0
40	2i	27	THR	4.0
44	2m	93	ARG	4.0
48	2q	10	VAL	4.0
33	2b	233	SER	4.0
1	2A	2136	C	3.9
52	2u	10	ARG	3.9
1	1A	2134	A	3.9
21	2Z	152	ALA	3.9
6	2G	11	TYR	3.9
44	2m	92	HIS	3.9
33	2b	215	LEU	3.9
45	2n	57	ARG	3.9
1	1A	1064	C	3.9
40	1i	125	TYR	3.9
32	2a	1257	U	3.9

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Mol	Chain	Res	Type	RSRZ
36	2e	16	THR	3.9
54	1w	56	C	3.9
40	2i	107	ARG	3.9
54	2w	24	A	3.9
11	2P	51	PHE	3.9
32	2a	1250	A	3.9
45	2n	33	VAL	3.9
7	2H	51	ARG	3.9
35	2d	122	ARG	3.9
22	20	5	LYS	3.9
53	2v	12	A	3.9
54	2w	29	A	3.9
34	2c	71	ALA	3.9
34	2c	194	GLY	3.9
40	2i	117	HIS	3.9
32	2a	1259	C	3.9
33	2b	93	VAL	3.9
6	2G	7	LEU	3.9
7	2H	98	LEU	3.9
54	1w	67	G	3.8
56	1y	67	G	3.8
56	2y	7	G	3.8
7	2H	6	ARG	3.8
36	2e	99	GLY	3.8
41	2j	63	PHE	3.8
54	2w	21	A	3.8
45	2n	58	LYS	3.8
53	2v	20	G	3.8
34	2c	193	TYR	3.8
39	2h	134	ILE	3.8
52	2u	13	ILE	3.8
54	1w	19	U	3.8
34	2c	185	GLY	3.8
48	2q	73	VAL	3.8
33	2b	118	LEU	3.8
41	2j	65	LEU	3.8
54	1w	62	C	3.8
26	24	39	CYS	3.8
53	2v	14	A	3.8
54	2w	27	A	3.8
54	2w	46	A	3.8
42	2k	30	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
43	2l	39	VAL	3.8
12	2Q	32	TYR	3.8
52	2u	17	THR	3.8
17	2V	50	PRO	3.8
35	1d	152	SER	3.8
1	2A	2132	U	3.8
1	2A	2134	A	3.8
22	20	4	LYS	3.8
54	2w	9	A	3.8
7	2H	165	ALA	3.8
1	2A	2149	G	3.8
32	1a	1032	G	3.8
51	1t	69	GLY	3.8
33	1b	165	VAL	3.8
34	2c	195	VAL	3.8
53	2v	15	A	3.8
21	2Z	57	ILE	3.7
25	23	29	ARG	3.7
33	2b	70	PHE	3.7
1	1A	2139	C	3.7
55	2x	47	U	3.7
45	2n	12	ARG	3.7
22	20	2	ALA	3.7
43	2l	64	TYR	3.7
33	2b	75	LYS	3.7
1	2A	2121	G	3.7
35	2d	117	ALA	3.7
38	2g	82	GLY	3.7
53	1v	14	A	3.7
35	2d	141	ARG	3.7
1	1A	1076	C	3.7
54	2w	42	C	3.7
7	2H	71	LEU	3.7
50	2s	5	LEU	3.7
36	2e	115	VAL	3.7
56	1y	52	G	3.7
51	1t	79	ARG	3.7
40	1i	79	LEU	3.7
18	2W	60	ASN	3.7
20	2Y	42	VAL	3.7
1	2A	2191	G	3.7
56	1y	51	G	3.7

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Mol	Chain	Res	Type	RSRZ
6	2G	152	LEU	3.7
7	2H	101	ARG	3.7
33	2b	220	ASP	3.7
35	2d	164	ALA	3.7
41	2j	26	ALA	3.7
51	1t	12	ALA	3.7
6	2G	17	PRO	3.6
31	29	17	ILE	3.6
1	2A	2102	U	3.6
40	1i	113	LYS	3.6
50	2s	69	HIS	3.6
48	2q	9	VAL	3.6
32	2a	1061	G	3.6
1	2A	2161	C	3.6
40	1i	117	HIS	3.6
31	29	24	TYR	3.6
42	2k	25	TYR	3.6
36	2e	14	ARG	3.6
41	2j	66	ARG	3.6
56	1y	26	G	3.6
1	1A	2178	C	3.6
26	24	40	HIS	3.6
44	2m	90	LEU	3.6
48	2q	42	TYR	3.6
30	28	29	LYS	3.6
44	2m	6	GLY	3.6
21	2Z	11	GLU	3.6
1	1A	2165	G	3.6
40	2i	16	ARG	3.6
55	2x	16	C	3.6
35	1d	21	LEU	3.6
40	2i	24	GLY	3.6
48	2q	80	GLY	3.6
35	1d	70	ILE	3.6
41	2j	74	ILE	3.6
1	1A	1078	U	3.6
41	2j	68	HIS	3.6
7	2H	107	VAL	3.6
17	2V	72	VAL	3.6
47	2p	38	TYR	3.6
7	2H	159	GLU	3.5
48	2q	98	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
54	2w	67	G	3.5
44	2m	64	TRP	3.5
6	2G	77	ILE	3.5
8	2I	88	ILE	3.5
1	1A	1065	U	3.5
6	2G	62	LEU	3.5
21	2Z	140	ASP	3.5
7	2H	52	VAL	3.5
41	2j	50	ILE	3.5
47	2p	19	ILE	3.5
28	26	10	LEU	3.5
20	2Y	24	VAL	3.5
29	27	1	MET	3.5
32	1a	1030(B)	C	3.5
34	1c	8	ILE	3.5
34	2c	190	ARG	3.5
54	2w	22	G	3.5
44	2m	66	LEU	3.5
45	2n	44	LEU	3.5
2	2B	59	A	3.5
6	2G	146	TYR	3.5
26	24	43	TYR	3.5
21	1Z	104	PHE	3.5
45	2n	7	ILE	3.5
46	2o	89	GLY	3.5
33	1b	97	TRP	3.5
46	2o	57	LEU	3.5
51	2t	13	LEU	3.5
1	2A	2101	G	3.5
51	2t	77	ALA	3.5
1	2A	2801(A)	A	3.5
3	2D	3	VAL	3.5
40	2i	75	ASP	3.5
1	2A	2803	C	3.5
55	2x	1	C	3.5
41	2j	55	LYS	3.5
51	1t	63	ILE	3.5
51	2t	41	ILE	3.5
1	2A	2118	U	3.5
55	2x	20	U	3.5
34	1c	87	LEU	3.5
41	2j	85	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
34	1c	180	ALA	3.5
1	2A	882	G	3.5
54	2w	5	G	3.5
26	24	64	GLY	3.5
30	28	41	ILE	3.4
50	2s	27	GLU	3.4
49	2r	76	LEU	3.4
46	2o	60	VAL	3.4
50	2s	51	VAL	3.4
52	1u	13	ILE	3.4
1	1A	2167	U	3.4
10	2O	41	ALA	3.4
40	2i	49	PRO	3.4
40	2i	93	ARG	3.4
34	2c	152	ILE	3.4
1	2A	2122	U	3.4
39	1h	59	LEU	3.4
49	2r	58	LEU	3.4
33	1b	233	SER	3.4
35	1d	23	GLY	3.4
42	2k	86	GLY	3.4
29	17	47	ARG	3.4
1	1A	2182	G	3.4
12	2Q	114	ALA	3.4
48	2q	100	LYS	3.4
56	1y	63	C	3.4
7	2H	94	TYR	3.4
35	1d	122	ARG	3.4
40	2i	13	ALA	3.4
1	2A	899	A	3.4
32	2a	1357	A	3.4
1	1A	2168	G	3.4
56	1y	66	C	3.4
6	2G	133	LEU	3.4
12	2Q	66	ILE	3.4
36	2e	109	ILE	3.4
46	1o	57	LEU	3.4
12	2Q	113	GLN	3.4
38	2g	85	TYR	3.4
39	2h	28	ALA	3.4
40	2i	88	TYR	3.4
45	1n	13	THR	3.4

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Mol	Chain	Res	Type	RSRZ
48	1q	28	PRO	3.4
1	1A	2148	G	3.4
53	2v	21	G	3.4
56	2y	48	C	3.4
7	2H	132	ARG	3.4
35	1d	19	LEU	3.3
9	2N	108	PRO	3.3
34	2c	48	TYR	3.3
33	1b	133	LYS	3.3
44	1m	122	LYS	3.3
43	2l	59	ARG	3.3
32	1a	1286	A	3.3
32	2a	1260	C	3.3
34	2c	162	GLN	3.3
45	2n	51	GLY	3.3
1	1A	2166	G	3.3
1	2A	2124	G	3.3
7	1H	2	SER	3.3
32	2a	1220	G	3.3
53	2v	19	G	3.3
39	1h	133	LEU	3.3
41	2j	8	LEU	3.3
41	2j	71	LEU	3.3
41	1j	57	LYS	3.3
42	2k	64	ALA	3.3
54	2w	12	U	3.3
40	2i	62	TYR	3.3
40	2i	128	ARG	3.3
44	2m	91	ARG	3.3
9	2N	9	VAL	3.3
1	1A	2142	C	3.3
34	2c	4	LYS	3.3
6	2G	120	LEU	3.3
8	2I	75	LEU	3.3
40	2i	37	PHE	3.3
40	1i	15	ALA	3.3
35	1d	180	GLY	3.3
1	2A	2126	A	3.3
34	2c	182	ILE	3.3
51	1t	76	ALA	3.3
21	2Z	147	GLY	3.3
32	1a	1030(C)	G	3.3

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Mol	Chain	Res	Type	RSRZ
54	1w	5	G	3.3
6	2G	5	VAL	3.3
35	1d	163	GLU	3.3
22	20	69	PHE	3.3
36	2e	84	PHE	3.3
44	2m	72	ALA	3.3
56	2y	11	U	3.3
40	2i	30	GLY	3.3
7	2H	125	VAL	3.3
9	2N	82	LEU	3.3
22	20	7	LEU	3.3
40	1i	37	PHE	3.3
45	2n	13	THR	3.3
52	1u	17	THR	3.3
1	1A	1509	C	3.3
36	2e	130	ASN	3.3
36	2e	81	GLU	3.3
40	2i	20	ARG	3.3
8	2I	29	TYR	3.3
48	2q	95	TYR	3.3
7	2H	115	VAL	3.3
45	2n	61	TRP	3.3
48	2q	21	VAL	3.3
52	1u	14	TRP	3.3
32	1a	1033	G	3.2
36	2e	119	LEU	3.2
51	1t	20	LEU	3.2
35	2d	167	GLY	3.2
1	1A	889	C	3.2
1	1A	2136	C	3.2
1	1A	2179	C	3.2
32	2a	1288	A	3.2
45	2n	11	LYS	3.2
52	1u	21	TYR	3.2
25	23	54	VAL	3.2
21	2Z	5	LEU	3.2
34	2c	33	LEU	3.2
51	2t	43	LEU	3.2
34	2c	163	ALA	3.2
6	2G	157	ILE	3.2
20	2Y	44	ILE	3.2
32	1a	1000	U	3.2

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Mol	Chain	Res	Type	RSRZ
38	2g	120	ILE	3.2
56	1y	73	U	3.2
51	1t	18	GLN	3.2
7	2H	44	VAL	3.2
23	2l	28	GLY	3.2
33	2b	98	LEU	3.2
34	2c	145	GLY	3.2
38	2g	12	LEU	3.2
44	1m	89	GLY	3.2
50	2s	68	GLY	3.2
38	2g	2	ALA	3.2
45	2n	36	PHE	3.2
50	1s	4	SER	3.2
39	1h	2	LEU	3.2
54	1w	49	G	3.2
22	10	3	HIS	3.2
42	2k	17	GLY	3.2
1	2A	2183	C	3.2
33	1b	164	VAL	3.2
40	2i	108	VAL	3.2
45	1n	33	VAL	3.2
47	1p	17	TYR	3.2
32	1a	1531	A	3.2
56	1y	58	A	3.2
26	24	27	THR	3.2
34	2c	189	ALA	3.2
35	1d	115	ARG	3.2
38	2g	31	MET	3.2
51	2t	9	ASN	3.2
4	2E	196	VAL	3.2
7	2H	131	VAL	3.2
32	2a	1001(A)	G	3.2
38	2g	135	VAL	3.2
40	1i	14	VAL	3.2
48	2q	23	VAL	3.2
1	2A	889	C	3.2
50	2s	33	THR	3.2
51	2t	72	LEU	3.2
1	1A	278	A	3.2
34	2c	156	ARG	3.2
38	2g	94	ARG	3.2
56	2y	76	A	3.2

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Mol	Chain	Res	Type	RSRZ
37	2f	52	ILE	3.2
56	2y	59	U	3.2
26	24	66	SER	3.2
36	2e	29	GLY	3.2
29	17	48	LYS	3.2
44	2m	65	LYS	3.2
50	2s	28	LYS	3.2
42	2k	126	ARG	3.2
40	2i	15	ALA	3.1
43	2l	52	LEU	3.2
1	1A	887	A	3.1
1	1A	2170	A	3.1
39	2h	38	ILE	3.1
53	1v	12	A	3.1
50	2s	72	GLY	3.1
33	1b	232	PRO	3.1
47	1p	41	PRO	3.1
46	2o	68	ARG	3.1
4	2E	195	LEU	3.1
33	2b	187	LEU	3.1
35	1d	120	LEU	3.1
43	1l	64	TYR	3.1
1	2A	2130	U	3.1
12	2Q	86	GLY	3.1
21	1Z	166	SER	3.1
1	2A	892	G	3.1
22	20	12	ASN	3.1
32	1a	999	C	3.1
39	1h	38	ILE	3.1
6	2G	100	TRP	3.1
8	2I	35	LEU	3.1
26	24	52	THR	3.1
1	1A	1963	U	3.1
41	1j	62	HIS	3.1
51	1t	80	ARG	3.1
1	2A	2173	A	3.1
38	2g	83	ALA	3.1
1	1A	1094	U	3.1
35	1d	166	LYS	3.1
54	1w	39	G	3.1
12	2Q	121	ALA	3.1
26	24	57	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
29	27	45	ALA	3.1
34	1c	15	THR	3.1
41	1j	5	ARG	3.1
41	1j	60	ARG	3.1
6	2G	86	MET	3.1
34	1c	14	ILE	3.1
34	2c	199	LYS	3.1
35	1d	156	GLU	3.1
38	2g	119	ARG	3.1
50	2s	36	ARG	3.1
32	2a	1286	A	3.1
41	2j	48	THR	3.1
35	1d	104	VAL	3.1
6	2G	2	PRO	3.1
43	1l	85	ILE	3.1
1	2A	2108	C	3.1
7	2H	142	GLY	3.1
22	20	65	GLY	3.1
32	2a	1362	C	3.1
39	2h	131	GLY	3.1
35	1d	147	ALA	3.1
38	2g	116	ALA	3.1
38	2g	121	ALA	3.1
50	2s	75	ALA	3.1
32	2a	1256	A	3.0
38	2g	33	ASP	3.0
40	2i	123	PRO	3.0
44	2m	101	GLN	3.0
40	2i	77	ILE	3.0
41	1j	38	ILE	3.0
54	2w	52	G	3.0
56	1y	7	G	3.0
18	2W	112	GLY	3.0
44	2m	68	GLY	3.0
25	23	53	LEU	3.0
54	2w	48	C	3.0
33	2b	122	PHE	3.0
1	1A	2162	G	3.0
43	2l	72	GLY	3.0
40	2i	110	GLU	3.0
33	2b	210	SER	3.0
35	2d	147	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
40	2i	40	LEU	3.0
40	2i	54	ASP	3.0
1	1A	886	C	3.0
6	2G	155	MET	3.0
39	2h	9	MET	3.0
1	1A	2135	A	3.0
1	2A	887	A	3.0
54	1w	24	A	3.0
42	1k	25	TYR	3.0
34	2c	6	HIS	3.0
32	2a	1283	G	3.0
50	2s	13	ASP	3.0
50	2s	15	LEU	3.0
8	2I	3	VAL	3.0
44	2m	97	PRO	3.0
32	2a	1249	C	3.0
54	2w	40	C	3.0
39	1h	134	ILE	3.0
39	2h	71	GLY	3.0
52	2u	2	GLY	3.0
1	1A	899	A	3.0
38	2g	6	ARG	3.0
40	1i	116	LYS	3.0
44	2m	104	ARG	3.0
36	2e	17	ALA	3.0
41	1j	8	LEU	3.0
32	2a	1031	G	3.0
48	2q	11	VAL	3.0
34	1c	41	GLY	3.0
1	2A	2896	C	3.0
43	2l	13	LYS	3.0
54	1w	2	C	3.0
19	2X	8	ILE	3.0
1	2A	229	A	3.0
52	2u	18	TYR	3.0
53	1v	24	A	3.0
11	2P	45	LEU	3.0
47	1p	59	TRP	3.0
31	29	2	LYS	3.0
6	2G	95	ARG	3.0
9	2N	69	GLN	3.0
1	2A	2100	G	3.0

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Mol	Chain	Res	Type	RSRZ
32	2a	1026	G	3.0
47	1p	1	MET	3.0
40	2i	91	ASP	3.0
50	2s	40	ILE	3.0
7	2H	46	GLU	3.0
33	2b	51	LEU	3.0
35	2d	162	LEU	3.0
36	1e	94	ALA	3.0
56	2y	9	A	3.0
52	1u	10	ARG	3.0
5	2F	89	VAL	2.9
25	23	47	VAL	2.9
36	2e	34	VAL	2.9
44	2m	60	VAL	2.9
35	1d	5	ILE	2.9
56	1y	65	U	2.9
1	1A	2125	G	2.9
1	1A	2127	G	2.9
1	1A	2154	G	2.9
32	1a	1029	C	2.9
21	2Z	8	TYR	2.9
21	2Z	125	LEU	2.9
30	28	64	TYR	2.9
40	2i	122	ALA	2.9
34	1c	80	GLY	2.9
42	2k	117	ASN	2.9
54	2w	58	A	2.9
21	2Z	47	VAL	2.9
9	2N	83	LYS	2.9
33	2b	113	HIS	2.9
43	1l	23	LYS	2.9
51	2t	63	ILE	2.9
1	1A	2111	C	2.9
1	1A	1068	G	2.9
47	1p	38	TYR	2.9
49	2r	85	LEU	2.9
32	1a	161	A	2.9
33	2b	197	VAL	2.9
35	1d	118	ARG	2.9
52	2u	22	ARG	2.9
20	2Y	106	LEU	2.9
43	2l	46	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
44	1m	107	ALA	2.9
6	1G	146	TYR	2.9
34	1c	184	TYR	2.9
42	2k	80	VAL	2.9
44	2m	80	ARG	2.9
43	1l	60	LEU	2.9
6	2G	136	ARG	2.9
16	2U	24	TYR	2.9
32	1a	163	C	2.9
34	1c	120	VAL	2.9
35	1d	133	VAL	2.9
1	1A	1069	A	2.9
32	2a	1446	U	2.9
35	1d	134	ASP	2.9
36	2e	45	PHE	2.9
46	1o	89	GLY	2.9
51	1t	47	GLY	2.9
30	28	34	TRP	2.9
39	2h	101	PRO	2.9
3	2D	273	ARG	2.9
33	2b	207	ALA	2.9
34	1c	65	ALA	2.9
34	2c	47	LEU	2.9
35	1d	179	GLU	2.9
43	2l	93	LEU	2.9
47	1p	7	ALA	2.9
48	2q	89	LEU	2.9
44	2m	98	VAL	2.9
47	1p	19	ILE	2.9
54	1w	17	G	2.9
54	2w	45	U	2.9
12	2Q	79	LEU	2.9
41	1j	18	ALA	2.9
33	2b	133	LYS	2.9
46	2o	66	LEU	2.9
34	1c	201	TYR	2.9
44	2m	23	TYR	2.9
40	1i	8	GLY	2.8
45	1n	56	VAL	2.8
47	1p	21	VAL	2.8
49	2r	22	VAL	2.8
56	1y	56	C	2.8

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Mol	Chain	Res	Type	RSRZ
53	1v	22	U	2.8
6	2G	142	PRO	2.8
6	2G	162	THR	2.8
16	2U	109	LEU	2.8
37	1f	61	LEU	2.8
40	1i	19	LEU	2.8
44	2m	70	LEU	2.8
54	2w	23	A	2.8
34	1c	81	GLY	2.8
38	2g	9	VAL	2.8
5	2F	78	ILE	2.8
6	2G	141	PHE	2.8
35	1d	12	CYS	2.8
39	2h	135	CYS	2.8
1	1A	229	A	2.8
32	2a	1224	G	2.8
21	1Z	1	MET	2.8
36	2e	82	VAL	2.8
39	1h	58	TYR	2.8
43	1l	18	VAL	2.8
44	1m	98	VAL	2.8
1	1A	1066	U	2.8
11	2P	78	PRO	2.8
6	2G	144	ILE	2.8
24	22	57	ILE	2.8
42	1k	64	ALA	2.8
6	2G	19	LEU	2.8
39	2h	127	LEU	2.8
51	1t	75	ASN	2.8
28	26	42	TRP	2.8
6	2G	164	GLU	2.8
33	1b	136	VAL	2.8
51	1t	16	HIS	2.8
8	2I	4	ILE	2.8
9	2N	104	LYS	2.8
48	2q	36	ILE	2.8
54	2w	41	U	2.8
26	24	68	ARG	2.8
51	2t	35	THR	2.8
54	2w	62	C	2.8
6	2G	149	VAL	2.8
12	2Q	22	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
15	2T	72	VAL	2.8
42	2k	14	VAL	2.8
42	2k	109	VAL	2.8
43	1l	28	LYS	2.8
55	1x	38	A	2.8
16	2U	2	PRO	2.8
46	2o	64	ARG	2.8
7	2H	72	ILE	2.8
10	1O	47	ILE	2.8
48	2q	59	ILE	2.8
1	2A	894	C	2.8
19	1X	66	LEU	2.8
35	2d	11	LEU	2.8
36	2e	31	LEU	2.8
42	1k	17	GLY	2.8
51	1t	62	LEU	2.8
41	1j	59	SER	2.8
7	2H	85	LYS	2.8
33	1b	75	LYS	2.8
13	2R	68	ARG	2.8
41	2j	29	ARG	2.8
3	2D	205	VAL	2.8
12	2Q	35	VAL	2.8
39	2h	93	VAL	2.8
40	2i	86	VAL	2.8
3	2D	164	GLN	2.8
7	2H	121	ILE	2.8
6	2G	165	THR	2.8
21	2Z	7	ALA	2.8
21	2Z	171	ILE	2.8
22	20	57	PHE	2.8
33	2b	211	ILE	2.8
35	2d	158	ILE	2.8
38	1g	84	ASN	2.8
38	2g	147	ALA	2.8
41	2j	27	ALA	2.8
45	2n	22	THR	2.8
6	2G	94	LEU	2.8
32	2a	1002	G	2.8
32	2a	1030(C)	G	2.8
35	1d	11	LEU	2.8
56	1y	6	C	2.8

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Mol	Chain	Res	Type	RSRZ
35	2d	115	ARG	2.8
33	2b	112	VAL	2.7
1	1A	2122	U	2.7
32	1a	1532	U	2.7
33	2b	31	TYR	2.7
35	2d	6	GLY	2.7
56	2y	60	U	2.7
7	2H	145	ALA	2.7
49	2r	60	ALA	2.7
4	2E	52	LEU	2.7
34	2c	196	LEU	2.7
1	1A	2153	G	2.7
32	2a	1032	G	2.7
30	28	7	HIS	2.7
41	2j	39	PRO	2.7
41	2j	41	PRO	2.7
12	2Q	102	VAL	2.7
21	1Z	120	ILE	2.7
25	23	13	ILE	2.7
33	1b	33	TYR	2.7
33	1b	200	ILE	2.7
34	2c	39	ILE	2.7
35	1d	73	ARG	2.7
35	1d	159	ARG	2.7
38	1g	78	ARG	2.7
44	2m	76	ALA	2.7
6	1G	139	LEU	2.7
40	2i	79	LEU	2.7
52	2u	9	ARG	2.7
39	2h	4	ASP	2.7
14	2S	33	LYS	2.7
1	1A	2105	C	2.7
1	2A	2165	G	2.7
26	24	7	PRO	2.7
32	2a	1030	C	2.7
3	2D	256	GLY	2.7
11	2P	44	GLY	2.7
35	1d	148	VAL	2.7
35	2d	105	VAL	2.7
42	2k	82	VAL	2.7
42	2k	84	VAL	2.7
52	1u	16	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
4	1E	123	ALA	2.7
32	2a	1358	U	2.7
34	2c	53	ALA	2.7
36	1e	89	ILE	2.7
36	1e	134	ALA	2.7
21	2Z	33	LEU	2.7
26	14	59	PHE	2.7
33	1b	105	PHE	2.7
34	1c	12	LEU	2.7
35	1d	78	LEU	2.7
38	2g	62	PHE	2.7
9	2N	42	TRP	2.7
40	2i	112	LYS	2.7
28	26	20	ASN	2.7
1	2A	2137	C	2.7
26	24	58	ARG	2.7
44	2m	94	ARG	2.7
44	2m	110	ARG	2.7
54	2w	69	C	2.7
1	1A	2149	G	2.7
54	1w	30	G	2.7
3	2D	161	THR	2.7
34	2c	65	ALA	2.7
33	1b	214	ILE	2.7
33	2b	127	ILE	2.7
39	1h	112	LEU	2.7
42	2k	95	ILE	2.7
50	2s	31	ILE	2.7
45	2n	49	HIS	2.7
48	1q	45	HIS	2.7
1	1A	1095	A	2.7
12	2Q	89	ASN	2.7
40	2i	6	GLY	2.7
7	1H	113	VAL	2.7
43	1l	43	VAL	2.7
14	2S	31	SER	2.7
40	1i	76	ALA	2.7
44	2m	118	ALA	2.7
11	2P	115	LEU	2.7
21	2Z	76	LEU	2.7
44	1m	90	LEU	2.7
47	1p	6	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
49	1r	31	LEU	2.7
50	2s	62	ILE	2.7
55	2x	46	G	2.7
13	2R	69	ASP	2.7
39	1h	93	VAL	2.7
7	2H	32	GLU	2.7
38	2g	134	ALA	2.7
54	2w	74	C	2.7
22	20	77	ARG	2.7
36	2e	131	ILE	2.7
1	1A	2124	G	2.7
1	2A	2184	G	2.7
1	2A	2792	G	2.7
40	1i	114	TYR	2.7
54	2w	7	G	2.7
34	2c	22	TRP	2.7
54	1w	38	A	2.6
8	2I	46	ALA	2.6
34	2c	144	SER	2.6
41	2j	59	SER	2.6
43	1l	39	VAL	2.6
42	2k	87	THR	2.6
6	1G	152	LEU	2.6
19	1X	95	LEU	2.6
53	2v	22	U	2.6
7	2H	48	GLY	2.6
19	1X	94	GLY	2.6
33	2b	17	PHE	2.6
36	1e	11	ILE	2.6
36	2e	13	ILE	2.6
17	2V	91	TYR	2.6
34	2c	37	GLN	2.6
46	1o	69	TYR	2.6
50	2s	61	TYR	2.6
7	2H	95	ARG	2.6
39	2h	37	ARG	2.6
40	2i	42	ARG	2.6
45	1n	61	TRP	2.6
45	2n	41	ARG	2.6
47	1p	27	LYS	2.6
8	2I	18	VAL	2.6
36	1e	69	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
40	1i	41	VAL	2.6
1	2A	1847	A	2.6
2	2B	90	A	2.6
36	2e	94	ALA	2.6
4	1E	195	LEU	2.6
8	2I	38	LEU	2.6
20	2Y	31	LEU	2.6
23	2I	29	GLY	2.6
48	1q	31	LEU	2.6
1	1A	1075	C	2.6
45	2n	52	GLN	2.6
14	2S	36	TYR	2.6
26	14	63	TYR	2.6
45	1n	34	TYR	2.6
31	29	19	ARG	2.6
40	1i	121	ARG	2.6
44	1m	120	LYS	2.6
52	2u	15	ARG	2.6
1	2A	881	G	2.6
14	2S	98	VAL	2.6
17	2V	79	VAL	2.6
32	1a	1031	G	2.6
32	2a	1356	G	2.6
1	2A	2310	A	2.6
13	2R	54	LEU	2.6
22	20	62	LEU	2.6
32	1a	1030(D)	A	2.6
32	2a	1447	A	2.6
35	1d	162	LEU	2.6
51	1t	24	LEU	2.6
53	1v	23	A	2.6
7	2H	148	ILE	2.6
14	2S	29	PHE	2.6
20	2Y	89	PHE	2.6
35	1d	126	ILE	2.6
41	2j	54	PHE	2.6
6	2G	182	LYS	2.6
43	2I	54	LYS	2.6
50	2s	78	ARG	2.6
1	2A	893	C	2.6
6	1G	73	ALA	2.6
25	23	9	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
34	2c	192	THR	2.6
52	2u	8	THR	2.6
1	2A	2319	G	2.6
13	2R	67	LEU	2.6
17	2V	71	LEU	2.6
32	2a	1024	G	2.6
32	2a	1068	G	2.6
6	2G	88	ILE	2.6
17	2V	70	ILE	2.6
22	20	60	PHE	2.6
26	24	29	PRO	2.6
41	2j	75	ILE	2.6
44	2m	88	ARG	2.6
6	1G	25	TYR	2.6
19	2X	69	TYR	2.6
39	2h	58	TYR	2.6
35	2d	152	SER	2.6
38	2g	40	ALA	2.6
38	2g	118	VAL	2.6
43	2l	18	VAL	2.6
51	2t	44	ALA	2.6
1	2A	2897	U	2.6
9	2N	112	LEU	2.6
21	2Z	62	PRO	2.6
38	2g	99	LEU	2.6
1	2A	2119	A	2.6
32	2a	1251	A	2.6
26	24	69	LYS	2.6
33	2b	101	MET	2.6
44	2m	82	MET	2.6
11	2P	35	HIS	2.6
32	2a	1109	C	2.6
33	2b	204	ASN	2.6
43	2l	95	GLY	2.6
6	2G	15	VAL	2.6
17	2V	22	VAL	2.6
40	2i	28	VAL	2.6
36	1e	96	PRO	2.6
44	2m	48	LEU	2.6
7	2H	151	ILE	2.6
34	1c	134	ILE	2.6
35	1d	75	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
35	1d	158	ILE	2.6
1	1A	2101	G	2.6
32	2a	976	G	2.6
32	2a	1248	A	2.6
45	2n	45	ARG	2.6
54	1w	21	A	2.6
1	1A	885	C	2.6
51	2t	67	ALA	2.5
56	1y	40	C	2.6
9	2N	43	THR	2.5
21	2Z	86	VAL	2.5
33	2b	229	VAL	2.5
40	1i	28	VAL	2.5
13	2R	4	LEU	2.5
35	2d	18	LYS	2.5
43	1l	77	LEU	2.5
43	2l	77	LEU	2.5
56	1y	43	U	2.5
26	14	49	PHE	2.5
40	2i	18	PHE	2.5
41	1j	4	ILE	2.5
20	2Y	2	ARG	2.5
29	27	23	ARG	2.5
12	1Q	15	GLY	2.5
25	13	22	ALA	2.5
40	2i	11	LYS	2.5
42	2k	69	ALA	2.5
12	2Q	109	VAL	2.5
21	2Z	50	GLN	2.5
26	24	10	VAL	2.5
35	2d	186	LEU	2.5
39	2h	119	LEU	2.5
51	2t	36	LEU	2.5
21	2Z	143	GLY	2.5
35	2d	23	GLY	2.5
45	1n	51	GLY	2.5
47	1p	80	PHE	2.5
34	2c	72	LYS	2.5
44	2m	121	LYS	2.5
1	2A	2062	A	2.5
20	2Y	65	ALA	2.5
38	2g	7	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
7	2H	112	PRO	2.5
21	1Z	80	ARG	2.5
32	2a	80	G	2.5
44	2m	7	VAL	2.5
45	2n	18	VAL	2.5
43	2l	65	GLU	2.5
46	2o	31	LEU	2.5
54	1w	22	G	2.5
5	2F	83	PHE	2.5
14	2S	12	PHE	2.5
35	1d	86	LYS	2.5
5	2F	49	ALA	2.5
4	1E	183	LEU	2.5
12	2Q	2	LEU	2.5
35	1d	101	LEU	2.5
21	2Z	121	HIS	2.5
34	1c	78	GLY	2.5
41	1j	93	GLY	2.5
54	1w	25	C	2.5
32	1a	1034	G	2.5
41	1j	50	ILE	2.5
26	24	18	CYS	2.5
33	2b	76	GLN	2.5
3	2D	5	LYS	2.5
5	2F	53	THR	2.5
29	27	24	THR	2.5
35	1d	182	LYS	2.5
41	1j	58	ASP	2.5
4	2E	130	GLY	2.5
6	2G	60	LEU	2.5
35	1d	8	VAL	2.5
43	1l	98	TYR	2.5
51	2t	47	GLY	2.5
1	1A	2108	C	2.5
4	2E	77	ILE	2.5
44	2m	67	GLU	2.5
44	2m	99	ARG	2.5
36	2e	120	THR	2.5
21	2Z	128	VAL	2.5
34	1c	33	LEU	2.5
38	2g	153	HIS	2.5
39	2h	137	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
42	1k	80	VAL	2.5
51	2t	73	HIS	2.5
34	2c	105	GLU	2.5
48	2q	75	ARG	2.5
1	2A	819	A	2.5
11	2P	91	PHE	2.5
21	2Z	133	ILE	2.5
32	2a	1363(A)	A	2.5
54	1w	27	A	2.5
32	2a	1226	C	2.5
32	2a	1370	G	2.5
36	2e	21	ALA	2.5
6	2G	35	GLU	2.5
43	2l	16	GLU	2.5
16	1U	69	CYS	2.4
33	2b	36	ARG	2.4
7	2H	141	VAL	2.4
22	10	79	VAL	2.4
38	1g	85	TYR	2.4
40	1i	65	VAL	2.4
50	2s	4	SER	2.4
33	2b	223	ILE	2.4
32	1a	160	A	2.4
26	24	54	GLY	2.4
35	1d	41	GLY	2.4
38	2g	76	ARG	2.4
41	1j	46	ARG	2.4
42	1k	87	THR	2.4
42	2k	23	ALA	2.4
48	2q	33	GLY	2.4
50	2s	54	GLY	2.4
6	2G	138	GLN	2.4
14	2S	3	ARG	2.4
51	1t	14	LYS	2.4
1	1A	2104	G	2.4
1	1A	2207	G	2.4
1	2A	2053	G	2.4
9	2N	116	LEU	2.4
33	1b	196	LEU	2.4
12	2Q	97	VAL	2.4
21	2Z	165	VAL	2.4
43	2l	69	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
45	2n	27	CYS	2.4
3	2D	165	ILE	2.4
33	1b	222	ILE	2.4
41	2j	11	PHE	2.4
33	2b	38	GLY	2.4
33	2b	139	LYS	2.4
1	2A	652(B)	A	2.4
4	2E	123	ALA	2.4
11	2P	30	THR	2.4
33	2b	123	ALA	2.4
54	2w	34	C	2.4
34	2c	12	LEU	2.4
33	1b	15	VAL	2.4
50	2s	45	VAL	2.4
1	2A	2156	G	2.4
1	2A	2805	G	2.4
26	24	25	TYR	2.4
32	2a	90	U	2.4
6	2G	75	LYS	2.4
51	1t	21	LYS	2.4
40	2i	87	GLN	2.4
48	1q	2	PRO	2.4
16	2U	21	ALA	2.4
20	2Y	78	ALA	2.4
33	1b	173	ALA	2.4
33	2b	188	ALA	2.4
36	1e	138	ALA	2.4
48	2q	44	ALA	2.4
49	1r	73	ALA	2.4
51	2t	16	HIS	2.4
54	1w	50	A	2.4
55	2x	73	A	2.4
22	10	7	LEU	2.4
25	23	23	LEU	2.4
20	2Y	87	LYS	2.4
21	2Z	87	ASP	2.4
40	2i	71	SER	2.4
31	29	25	VAL	2.4
48	2q	85	VAL	2.4
1	1A	2897	U	2.4
14	2S	97	ARG	2.4
7	2H	74	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
36	2e	129	ILE	2.4
42	2k	32	ILE	2.4
46	2o	69	TYR	2.4
48	2q	65	ILE	2.4
6	2G	23	PHE	2.4
33	2b	152	PHE	2.4
48	1q	71	PHE	2.4
26	14	18	CYS	2.4
34	2c	7	PRO	2.4
38	2g	88	PRO	2.4
54	2w	51	G	2.4
3	2D	272	ALA	2.4
22	20	61	ALA	2.4
34	2c	191	THR	2.4
40	2i	61	ALA	2.4
44	2m	103	THR	2.4
1	2A	896	A	2.4
22	20	59	LEU	2.4
25	23	11	SER	2.4
32	2a	1397	C	2.4
26	14	50	VAL	2.4
42	2k	13	GLN	2.4
43	2l	96	VAL	2.4
32	2a	1235	U	2.4
34	2c	2	GLY	2.4
15	2T	75	ILE	2.4
21	1Z	146	ILE	2.4
31	29	10	ILE	2.4
48	2q	60	ILE	2.4
51	1t	55	ILE	2.4
38	1g	153	HIS	2.4
38	2g	26	PHE	2.4
42	2k	39	PRO	2.4
50	2s	83	HIS	2.4
40	1i	112	LYS	2.4
1	1A	2157	G	2.4
1	2A	2153	G	2.4
47	1p	48	TRP	2.4
20	2Y	90	LEU	2.4
51	2t	62	LEU	2.4
32	1a	344	A	2.4
34	2c	78	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
32	1a	841	U	2.4
11	2P	76	LYS	2.4
34	2c	134	ILE	2.4
39	2h	86	ILE	2.4
28	26	21	TYR	2.4
51	1t	83	ARG	2.4
35	2d	101	LEU	2.4
50	1s	15	LEU	2.4
51	1t	43	LEU	2.4
32	1a	1024	G	2.3
33	1b	228	GLY	2.3
7	2H	17	VAL	2.3
7	2H	99	VAL	2.3
10	2O	58	VAL	2.3
50	2s	11	VAL	2.3
1	1A	897	C	2.3
54	1w	44	A	2.3
4	2E	197	ILE	2.3
11	2P	75	ILE	2.3
34	2c	10	PHE	2.3
35	1d	132	ARG	2.3
6	2G	41	GLN	2.3
44	1m	87	TYR	2.3
35	1d	117	ALA	2.3
36	1e	95	ALA	2.3
38	2g	107	ALA	2.3
51	1t	40	ALA	2.3
44	1m	105	THR	2.3
6	2G	27	ASN	2.3
21	1Z	102	LEU	2.3
21	2Z	102	LEU	2.3
42	2k	119	CYS	2.3
32	1a	1036	G	2.3
35	2d	49	ARG	2.3
1	2A	2178	C	2.3
16	2U	17	ILE	2.3
21	2Z	124	ILE	2.3
33	1b	223	ILE	2.3
46	1o	87	ILE	2.3
16	2U	40	PHE	2.3
40	2i	59	PHE	2.3
3	2D	59	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
5	2F	80	ALA	2.3
44	2m	75	ALA	2.3
51	1t	59	ALA	2.3
47	1p	11	SER	2.3
16	2U	44	ASN	2.3
8	2I	9	LEU	2.3
43	1l	52	LEU	2.3
26	24	48	ARG	2.3
45	1n	3	ARG	2.3
39	2h	123	GLU	2.3
47	2p	48	TRP	2.3
7	2H	76	VAL	2.3
35	1d	105	VAL	2.3
36	2e	55	VAL	2.3
22	20	49	LYS	2.3
35	1d	33	MET	2.3
45	2n	40	CYS	2.3
48	1q	100	LYS	2.3
32	2a	886	G	2.3
32	2a	980	C	2.3
21	2Z	164	ALA	2.3
27	25	2	ALA	2.3
5	1F	53	THR	2.3
34	2c	20	SER	2.3
35	2d	68	TYR	2.3
51	1t	67	ALA	2.3
6	2G	154	GLY	2.3
23	21	98	LEU	2.3
25	23	30	ARG	2.3
26	24	9	LEU	2.3
33	2b	209	ARG	2.3
38	2g	3	ARG	2.3
48	2q	43	LEU	2.3
11	2P	71	VAL	2.3
43	1l	31	PRO	2.3
48	2q	30	PRO	2.3
5	1F	112	MET	2.3
32	2a	1219	U	2.3
38	2g	144	MET	2.3
7	2H	92	ILE	2.3
14	2S	82	ILE	2.3
34	2c	77	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
35	1d	67	ILE	2.3
36	2e	11	ILE	2.3
8	2I	11	ASN	2.3
12	2Q	65	PHE	2.3
34	1c	194	GLY	2.3
1	1A	1059	G	2.3
10	2O	65	THR	2.3
11	2P	32	THR	2.3
32	2a	1003	G	2.3
32	2a	1218	C	2.3
33	1b	188	ALA	2.3
39	2h	122	ARG	2.3
39	2h	136	GLU	2.3
40	2i	55	ALA	2.3
51	2t	26	ASN	2.3
41	2j	52	GLY	2.3
43	1l	14	GLY	2.3
32	1a	1003	G	2.3
32	2a	1222	G	2.3
48	1q	91	ARG	2.3
50	2s	39	THR	2.3
53	1v	21	G	2.3
54	1w	40	C	2.3
12	2Q	34	LEU	2.3
35	1d	174	LEU	2.3
35	2d	96	LEU	2.3
43	1l	27	LEU	2.3
46	2o	85	LEU	2.3
39	1h	89	PRO	2.3
8	2I	19	VAL	2.3
48	1q	10	VAL	2.3
50	2s	60	VAL	2.3
54	1w	73	U	2.3
14	2S	30	ARG	2.3
23	2I	13	ILE	2.3
35	1d	167	GLY	2.3
38	2g	149	ARG	2.3
40	2i	69	GLY	2.3
40	2i	120	ARG	2.3
11	2P	31	ALA	2.3
12	2Q	44	ALA	2.3
35	1d	61	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
35	1d	164	ALA	2.3
38	2g	152	ALA	2.3
14	2S	5	THR	2.3
21	2Z	9	TYR	2.3
32	1a	1027	C	2.3
52	2u	21	TYR	2.3
3	2D	155	LEU	2.3
19	2X	66	LEU	2.3
50	2s	16	LEU	2.3
32	2a	485	G	2.3
56	1y	76	A	2.3
5	2F	92	PRO	2.3
25	23	12	PRO	2.3
21	2Z	126	VAL	2.3
33	2b	111	ARG	2.3
34	1c	190	ARG	2.3
35	2d	148	VAL	2.3
42	1k	14	VAL	2.3
4	2E	157	ALA	2.3
21	2Z	173	ALA	2.3
35	2d	134	ASP	2.3
7	2H	106	THR	2.3
6	2G	90	LEU	2.3
33	2b	33	TYR	2.3
35	2d	64	LEU	2.3
47	1p	39	TYR	2.3
32	2a	1114	C	2.3
32	2a	1314	C	2.3
47	1p	49	LEU	2.3
1	2A	2158	A	2.2
6	2G	33	ARG	2.2
15	2T	77	PRO	2.2
23	2I	26	ARG	2.2
35	1d	136	PRO	2.2
41	2j	60	ARG	2.2
41	2j	69	ASN	2.2
43	2I	49	ASN	2.2
20	2Y	25	GLY	2.2
33	2b	228	GLY	2.2
40	2i	3	GLN	2.2
23	2I	38	SER	2.2
21	1Z	51	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
28	26	54	ILE	2.2
37	1f	25	ILE	2.2
45	2n	30	ALA	2.2
34	2c	18	TRP	2.2
42	1k	42	TRP	2.2
6	2G	34	LEU	2.2
21	1Z	82	ARG	2.2
24	22	10	LEU	2.2
24	22	24	LEU	2.2
33	1b	187	LEU	2.2
34	1c	178	LEU	2.2
34	2c	178	LEU	2.2
35	2d	157	LEU	2.2
41	1j	65	LEU	2.2
43	2l	10	LEU	2.2
47	1p	60	LEU	2.2
52	1u	18	TYR	2.2
1	1A	2177	C	2.2
1	2A	2870	C	2.2
4	2E	167	VAL	2.2
21	2Z	93	ASP	2.2
23	21	70	VAL	2.2
32	2a	975	A	2.2
37	1f	88	VAL	2.2
40	2i	53	VAL	2.2
32	1a	1040	U	2.2
45	1n	32	SER	2.2
32	2a	79	G	2.2
32	2a	1385	G	2.2
4	2E	134	ILE	2.2
7	2H	30	LYS	2.2
17	2V	85	LYS	2.2
24	22	58	ALA	2.2
27	25	14	ALA	2.2
33	1b	211	ILE	2.2
35	2d	48	ALA	2.2
40	2i	78	LYS	2.2
43	2l	56	ALA	2.2
50	1s	40	ILE	2.2
51	1t	32	ALA	2.2
12	2Q	6	ARG	2.2
41	2j	46	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
17	2V	94	LEU	2.2
23	21	46	LEU	2.2
30	28	60	LEU	2.2
30	28	61	LEU	2.2
16	1U	2	PRO	2.2
10	2O	29	ASN	2.2
44	2m	100	GLY	2.2
32	2a	1326	C	2.2
40	1i	110	GLU	2.2
54	2w	35	C	2.2
6	2G	92	VAL	2.2
39	1h	118	VAL	2.2
51	1t	68	LYS	2.2
12	2Q	28	ALA	2.2
14	2S	6	ALA	2.2
33	2b	23	ARG	2.2
35	1d	111	ALA	2.2
36	2e	48	ALA	2.2
48	2q	90	ILE	2.2
43	1l	32	PHE	2.2
1	2A	1117	G	2.2
2	2B	89	G	2.2
32	2a	1258	G	2.2
33	2b	102	LEU	2.2
47	2p	6	LEU	2.2
40	2i	57	GLY	2.2
9	2N	76	SER	2.2
1	1A	2138	C	2.2
17	1V	37	VAL	2.2
17	2V	47	VAL	2.2
22	20	81	VAL	2.2
35	1d	209	ARG	2.2
39	2h	79	VAL	2.2
40	1i	10	ARG	2.2
47	1p	2	VAL	2.2
47	2p	20	VAL	2.2
47	2p	79	VAL	2.2
49	2r	87	ARG	2.2
32	2a	961	U	2.2
1	1A	2119	A	2.2
1	2A	228	A	2.2
2	2B	58	A	2.2

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Mol	Chain	Res	Type	RSRZ
3	1D	144	ALA	2.2
19	2X	91	ALA	2.2
35	2d	70	ILE	2.2
36	1e	118	ILE	2.2
39	1h	3	THR	2.2
52	1u	8	THR	2.2
55	2x	72	A	2.2
5	2F	90	PHE	2.2
3	2D	177	LEU	2.2
9	1N	82	LEU	2.2
9	2N	84	LYS	2.2
20	2Y	41	GLY	2.2
42	2k	90	GLY	2.2
43	1l	94	PRO	2.2
45	1n	15	LYS	2.2
32	2a	821	G	2.2
34	1c	18	TRP	2.2
38	2g	155	ARG	2.2
43	2l	89	ARG	2.2
35	2d	113	SER	2.2
33	2b	71	VAL	2.2
37	1f	6	VAL	2.2
54	1w	12	U	2.2
6	2G	151	ALA	2.2
7	2H	96	ALA	2.2
32	2a	979	C	2.2
36	1e	58	ALA	2.2
5	2F	82	ILE	2.2
9	2N	73	THR	2.2
16	2U	62	ILE	2.2
38	2g	36	LYS	2.2
32	1a	1110	A	2.2
45	1n	37	PHE	2.2
7	2H	12	PRO	2.2
22	10	6	GLY	2.2
33	2b	14	GLY	2.2
49	2r	26	LEU	2.2
31	29	9	ARG	2.2
7	2H	84	SER	2.2
32	2a	1023	G	2.2
2	2B	55	U	2.2
16	2U	63	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
18	1W	50	VAL	2.2
21	1Z	141	VAL	2.2
29	27	32	LYS	2.2
34	1c	195	VAL	2.2
54	2w	65	U	2.2
3	1D	191	ALA	2.2
4	1E	28	ALA	2.2
13	2R	62	ALA	2.2
1	2A	2107	C	2.2
6	2G	93	THR	2.2
23	11	67	ILE	2.2
32	2a	1254	C	2.2
38	2g	27	ILE	2.2
5	1F	207	GLY	2.2
6	2G	102	PHE	2.2
21	2Z	4	ARG	2.2
34	2c	59	ARG	2.2
14	1S	4	LEU	2.2
20	1Y	67	LEU	2.2
22	20	21	LEU	2.2
25	23	28	LEU	2.2
53	1v	15	A	2.2
21	1Z	169	GLU	2.2
33	2b	231	GLU	2.2
43	1l	62	SER	2.2
44	1m	121	LYS	2.1
21	2Z	38	TYR	2.1
50	2s	44	MET	2.1
1	1A	2151	G	2.1
1	1A	2588	G	2.1
20	2Y	13	VAL	2.1
21	1Z	39	VAL	2.1
23	11	4	VAL	2.1
30	28	23	VAL	2.1
18	2W	32	ALA	2.1
25	23	51	ALA	2.1
32	1a	306	G	2.1
32	2a	1196	U	2.1
36	1e	21	ALA	2.1
40	2i	45	ALA	2.1
41	2j	32	ALA	2.1
12	2Q	10	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
25	13	43	ILE	2.1
37	1f	52	ILE	2.1
43	1l	7	ILE	2.1
1	2A	2164	C	2.1
6	2G	59	GLU	2.1
13	2R	65	LEU	2.1
35	2d	97	LEU	2.1
36	1e	119	LEU	2.1
39	1h	119	LEU	2.1
30	28	15	LYS	2.1
32	2a	1092	A	2.1
6	2G	72	ARG	2.1
11	2P	18	ARG	2.1
1	2A	1963	U	2.1
21	1Z	165	VAL	2.1
25	23	55	ARG	2.1
33	1b	31	TYR	2.1
34	1c	23	TYR	2.1
41	2j	89	ASP	2.1
50	2s	65	ASN	2.1
6	2G	48	GLU	2.1
6	2G	169	ALA	2.1
9	2N	113	GLY	2.1
34	1c	60	ALA	2.1
54	2w	59	U	2.1
43	2l	42	THR	2.1
1	2A	1042	G	2.1
15	2T	110	ILE	2.1
18	2W	6	ILE	2.1
18	2W	96	ILE	2.1
31	29	15	LYS	2.1
31	29	26	ILE	2.1
34	2c	109	PRO	2.1
41	1j	96	ILE	2.1
41	2j	53	PRO	2.1
25	13	8	LEU	2.1
33	2b	121	LEU	2.1
35	1d	186	LEU	2.1
35	2d	21	LEU	2.1
51	2t	10	LEU	2.1
55	2x	34	C	2.1
41	2j	56	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
26	24	61	ARG	2.1
35	1d	100	ARG	2.1
4	1E	117	MET	2.1
34	1c	148	GLY	2.1
16	2U	35	ALA	2.1
21	1Z	27	VAL	2.1
32	2a	1040	U	2.1
33	2b	77	ALA	2.1
36	1e	146	ALA	2.1
37	2f	91	VAL	2.1
45	2n	2	ALA	2.1
47	2p	12	LYS	2.1
41	2j	15	THR	2.1
19	2X	39	ILE	2.1
43	2l	25	PRO	2.1
11	1P	105	LEU	2.1
35	2d	155	LEU	2.1
1	2A	1533	G	2.1
6	2G	76	SER	2.1
1	2A	1509	C	2.1
7	2H	97	ARG	2.1
41	1j	51	ARG	2.1
48	1q	66	SER	2.1
51	1t	11	SER	2.1
32	2a	1303	C	2.1
52	1u	15	ARG	2.1
12	2Q	130	LYS	2.1
20	2Y	88	LYS	2.1
54	1w	46	A	2.1
3	2D	130	ALA	2.1
9	2N	57	ALA	2.1
12	1Q	12	GLN	2.1
23	2l	62	VAL	2.1
35	1d	38	TYR	2.1
34	2c	174	PRO	2.1
42	2k	33	THR	2.1
15	1T	48	ILE	2.1
5	2F	32	LEU	2.1
10	2O	25	LEU	2.1
19	2X	68	ARG	2.1
29	17	31	LEU	2.1
51	1t	36	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	1A	2802	G	2.1
1	2A	1600	C	2.1
6	2G	85	GLY	2.1
32	2a	154	C	2.1
55	2x	69	C	2.1
3	2D	18	VAL	2.1
5	2F	114	VAL	2.1
7	1H	45	VAL	2.1
8	1I	3	VAL	2.1
8	1I	142	VAL	2.1
8	2I	92	VAL	2.1
20	2Y	27	VAL	2.1
34	1c	113	ALA	2.1
38	2g	108	ALA	2.1
39	2h	97	VAL	2.1
40	1i	106	ALA	2.1
40	2i	82	ALA	2.1
4	1E	151	TYR	2.1
9	2N	10	GLU	2.1
32	1a	171	A	2.1
32	2a	60	A	2.1
33	1b	117	GLU	2.1
35	1d	40	PRO	2.1
40	1i	4	TYR	2.1
41	2j	87	THR	2.1
54	1w	23	A	2.1
42	2k	96	ARG	2.1
44	2m	57	ARG	2.1
34	2c	14	ILE	2.1
16	2U	83	LEU	2.1
18	1W	86	LEU	2.1
19	2X	21	PHE	2.1
25	23	26	LEU	2.1
31	29	14	CYS	2.1
33	1b	152	PHE	2.1
35	1d	79	PHE	2.1
35	2d	110	PHE	2.1
38	1g	43	PHE	2.1
39	1h	39	LEU	2.1
42	1k	125	PHE	2.1
42	2k	110	ASP	2.1
45	2n	47	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
47	1p	13	HIS	2.1
5	1F	65	TRP	2.1
16	2U	25	TRP	2.1
5	2F	76	GLY	2.1
1	1A	2103	C	2.1
2	2B	56	G	2.1
38	1g	3	ARG	2.1
38	1g	134	ALA	2.1
40	2i	104	ARG	2.1
43	2l	41	ARG	2.1
17	1V	14	VAL	2.1
17	2V	14	VAL	2.1
23	1l	49	VAL	2.1
41	2j	42	THR	2.1
44	2m	54	VAL	2.1
10	2O	7	TYR	2.1
12	1Q	66	ILE	2.1
25	23	43	ILE	2.1
46	2o	50	HIS	2.1
49	1r	50	ILE	2.1
11	2P	6	LEU	2.1
17	2V	75	PHE	2.1
24	22	60	LEU	2.1
34	2c	94	LEU	2.1
39	2h	39	LEU	2.1
45	1n	16	PHE	2.1
10	1O	21	CYS	2.1
10	1O	108	GLU	2.1
28	26	13	CYS	2.1
41	1j	36	GLY	2.1
42	1k	78	GLN	2.1
33	1b	114	ARG	2.1
35	1d	168	ARG	2.1
1	2A	2163	C	2.0
33	1b	34	ALA	2.0
34	2c	149	ALA	2.0
55	2x	71	C	2.0
1	2A	271(K)	U	2.0
3	2D	17	THR	2.0
9	2N	98	VAL	2.0
30	18	14	VAL	2.0
35	1d	112	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
48	2q	7	THR	2.0
1	1A	2582	G	2.0
1	2A	2807	G	2.0
1	2A	2894	G	2.0
4	1E	77	ILE	2.0
7	2H	4	ILE	2.0
7	2H	164	TYR	2.0
19	2X	18	TYR	2.0
32	1a	1353	G	2.0
5	2F	140	LEU	2.0
6	1G	48	GLU	2.0
6	2G	101	ILE	2.0
36	2e	89	ILE	2.0
37	2f	59	TYR	2.0
48	1q	95	TYR	2.0
51	1t	70	SER	2.0
46	2o	70	LEU	2.0
6	2G	134	GLY	2.0
22	20	8	GLY	2.0
52	1u	4	GLY	2.0
54	1w	15	A	2.0
9	1N	115	ARG	2.0
29	17	41	ARG	2.0
45	2n	24	CYS	2.0
23	11	15	ALA	2.0
33	1b	167	PRO	2.0
1	2A	828	U	2.0
3	1D	205	VAL	2.0
21	2Z	58	VAL	2.0
23	11	51	VAL	2.0
32	2a	1320	C	2.0
34	2c	103	VAL	2.0
34	2c	138	VAL	2.0
35	2d	128	VAL	2.0
43	1l	61	THR	2.0
49	2r	47	THR	2.0
47	1p	65	GLN	2.0
6	2G	47	LYS	2.0
7	1H	105	LEU	2.0
19	2X	80	ILE	2.0
28	26	11	LEU	2.0
33	1b	221	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
6	2G	125	PHE	2.0
7	2H	152	ARG	2.0
9	1N	116	LEU	2.0
35	2d	188	LEU	2.0
39	2h	65	TYR	2.0
43	1l	89	ARG	2.0
48	2q	74	LEU	2.0
51	1t	13	LEU	2.0
12	2Q	104	PHE	2.0
26	24	42	PHE	2.0
32	2a	1310	G	2.0
32	2a	1497	G	2.0
1	1A	2062	A	2.0
1	1A	2173	A	2.0
32	2a	1285	A	2.0
41	1j	17	ASP	2.0
3	2D	181	GLU	2.0
16	1U	46	ALA	2.0
17	1V	77	ALA	2.0
19	1X	42	ALA	2.0
9	2N	101	HIS	2.0
28	16	13	CYS	2.0
36	2e	138	ALA	2.0
33	1b	19	HIS	2.0
42	1k	13	GLN	2.0
3	1D	173	VAL	2.0
13	2R	66	VAL	2.0
15	1T	63	VAL	2.0
18	1W	92	ARG	2.0
18	2W	92	ARG	2.0
23	11	65	SER	2.0
23	21	30	VAL	2.0
32	2a	1292	U	2.0
36	1e	82	VAL	2.0
54	2w	33	U	2.0
4	2E	4	ILE	2.0
18	2W	19	LEU	2.0
23	21	67	ILE	2.0
32	2a	1027	C	2.0
32	2a	1452	C	2.0
37	2f	14	LEU	2.0
39	2h	133	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
5	1F	97	TYR	2.0
16	2U	32	PHE	2.0
17	2V	12	TYR	2.0
28	26	39	TYR	2.0
47	2p	17	TYR	2.0
51	1t	64	ASP	2.0
1	1A	2833	G	2.0
1	2A	1508	A	2.0
32	2a	1255	G	2.0
32	2a	1349	A	2.0
32	2a	1493	A	2.0
53	2v	18	G	2.0
5	1F	92	PRO	2.0
8	2I	1	MET	2.0
50	2s	76	PRO	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	PSU	2y	55	20/21	0.55	0.58	96,103,107,108	0
56	5MU	2y	54	21/22	0.64	0.52	96,99,105,120	0
56	4SU	1y	8	20/21	0.65	0.35	92,98,101,118	0
56	4SU	2y	8	20/21	0.65	0.34	93,99,108,115	0
54	PSU	1w	55	20/21	0.71	0.33	81,90,98,98	0
56	5MU	1y	54	21/22	0.73	0.34	90,94,100,113	0
56	PSU	1y	55	20/21	0.74	0.43	94,98,104,112	0
54	5MU	2w	54	21/22	0.75	0.26	83,91,95,98	0
54	PSU	2w	55	20/21	0.76	0.35	88,94,103,103	0
54	4SU	2w	8	20/21	0.77	0.41	90,97,110,116	0
43	0TD	1l	92	10/11	0.83	0.18	54,56,61,70	0
54	5MU	1w	54	21/22	0.85	0.24	72,83,88,93	0
54	4SU	1w	8	20/21	0.86	0.25	94,96,106,110	0
32	2MG	2a	1207	24/25	0.87	0.21	82,88,96,101	0
43	0TD	2l	92	10/11	0.89	0.22	67,72,77,86	0
55	5MU	2x	54	21/22	0.89	0.28	79,86,90,97	0
32	M2G	2a	966	25/26	0.89	0.23	60,70,81,88	0
32	PSU	2a	516	20/21	0.89	0.22	76,83,88,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	PSU	2x	55	20/21	0.90	0.19	77,82,88,96	0
55	4SU	2x	8	20/21	0.91	0.18	77,81,87,88	0
55	PSU	1x	55	20/21	0.91	0.18	60,65,77,78	0
55	5MU	1x	54	21/22	0.91	0.23	65,74,76,83	0
1	PSU	2A	1917	20/21	0.92	0.22	67,75,84,85	0
32	5MC	2a	1404	21/22	0.92	0.28	54,61,67,72	0
1	PSU	1A	1917	20/21	0.92	0.18	48,56,61,64	0
1	5MU	2A	1915	21/22	0.92	0.15	75,77,81,91	0
32	5MC	2a	967	21/22	0.92	0.18	68,74,80,83	0
1	OMC	2A	1920	21/22	0.93	0.23	58,67,71,79	0
32	PSU	1a	516	20/21	0.93	0.19	62,66,72,72	0
55	5MC	2x	32	21/22	0.93	0.20	66,78,80,80	0
55	31H	2x	76	32/33	0.93	0.28	42,54,62,74	0
1	5MU	1A	1915	21/22	0.93	0.18	51,60,65,69	0
54	L3X	2w	76	26/27	0.94	0.33	52,59,63,64	0
55	4SU	1x	8	20/21	0.94	0.20	58,64,79,80	0
32	4OC	2a	1402	22/23	0.94	0.20	56,64,68,72	0
32	G7M	2a	527	24/25	0.94	0.18	65,72,80,82	0
1	PSU	2A	1911	20/21	0.94	0.17	64,69,77,81	0
32	5MC	1a	967	21/22	0.95	0.19	55,61,68,71	0
32	2MG	1a	1207	24/25	0.95	0.17	68,73,79,87	0
32	5MC	2a	1407	21/22	0.95	0.27	54,60,67,75	0
32	UR3	2a	1498	21/22	0.95	0.27	59,63,69,71	0
32	MA6	2a	1518	24/25	0.95	0.25	56,69,73,76	0
32	MA6	2a	1519	24/25	0.95	0.32	56,65,71,72	0
32	5MC	2a	1400	21/22	0.95	0.27	68,76,80,86	0
55	5MC	1x	32	21/22	0.96	0.25	51,57,64,66	0
1	5MC	2A	1962	21/22	0.96	0.21	47,51,61,72	0
55	31H	1x	76	32/33	0.96	0.25	24,38,45,54	10
1	PSU	2A	2605	20/21	0.96	0.23	39,45,51,52	0
32	M2G	1a	966	25/26	0.96	0.21	55,60,70,72	0
32	5MC	1a	1400	21/22	0.97	0.19	41,50,53,55	0
1	5MC	2A	1942	21/22	0.97	0.18	54,59,65,73	0
32	4OC	1a	1402	22/23	0.97	0.23	36,46,53,58	0
1	OMG	2A	2251	24/25	0.97	0.22	38,44,50,55	0
1	2MA	2A	2503	23/24	0.97	0.21	34,42,44,45	0
1	OMU	2A	2552	21/22	0.97	0.21	37,42,48,51	0
32	5MC	1a	1404	21/22	0.97	0.20	39,44,47,47	0
32	UR3	1a	1498	21/22	0.97	0.21	35,44,47,50	0
32	MA6	1a	1518	24/25	0.97	0.24	40,46,49,51	0
32	MA6	1a	1519	24/25	0.97	0.22	40,45,50,55	0
32	G7M	1a	527	24/25	0.97	0.23	49,54,59,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	OMC	1A	1920	21/22	0.97	0.24	37,46,49,52	0
54	L3X	1w	76	26/27	0.97	0.23	37,42,48,51	0
1	5MC	1A	1962	21/22	0.97	0.21	27,38,41,46	0
1	PSU	1A	1911	20/21	0.97	0.21	44,49,58,58	0
1	OMG	1A	2251	24/25	0.98	0.24	23,28,33,34	0
1	2MA	1A	2503	23/24	0.98	0.25	19,24,28,31	0
32	5MC	1a	1407	21/22	0.98	0.24	34,43,45,46	0
1	OMU	1A	2552	21/22	0.98	0.24	26,30,33,37	0
1	PSU	1A	2605	20/21	0.98	0.24	24,30,35,38	0
1	5MU	2A	1939	21/22	0.98	0.20	34,38,45,47	0
1	5MC	1A	1942	21/22	0.98	0.22	36,42,49,61	0
1	5MU	1A	1939	21/22	0.99	0.24	24,28,33,34	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	4077	1/1	0.03	0.15	60,60,60,60	0
57	MG	1A	3880	1/1	0.19	0.27	80,80,80,80	0
57	MG	2a	1638	1/1	0.27	0.20	84,84,84,84	0
57	MG	2q	202	1/1	0.29	0.13	81,81,81,81	0
57	MG	2a	1636	1/1	0.31	0.20	75,75,75,75	0
57	MG	2A	3757	1/1	0.34	0.19	66,66,66,66	0
57	MG	1A	3678	1/1	0.38	0.16	63,63,63,63	0
57	MG	2A	3691	1/1	0.38	0.23	74,74,74,74	0
57	MG	2A	3244	1/1	0.39	0.23	63,63,63,63	0
57	MG	2A	3377	1/1	0.42	0.59	67,67,67,67	0
57	MG	1A	3976	1/1	0.43	0.24	69,69,69,69	0
57	MG	2A	3273	1/1	0.43	0.19	75,75,75,75	0
57	MG	2w	101	1/1	0.45	0.28	83,83,83,83	0
57	MG	2A	3498	1/1	0.46	0.31	77,77,77,77	0
57	MG	1a	1703	1/1	0.48	0.28	73,73,73,73	0
57	MG	2a	1703	1/1	0.48	0.21	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1788	1/1	0.49	0.15	83,83,83,83	0
57	MG	2j	201	1/1	0.49	0.23	88,88,88,88	0
57	MG	2A	3170	1/1	0.51	0.13	84,84,84,84	0
57	MG	1w	105	1/1	0.51	0.11	88,88,88,88	0
57	MG	2A	3436	1/1	0.51	0.17	64,64,64,64	0
57	MG	2A	3371	1/1	0.52	0.32	74,74,74,74	0
57	MG	1F	303	1/1	0.52	0.27	59,59,59,59	0
57	MG	1A	3961	1/1	0.52	0.13	52,52,52,52	0
57	MG	1w	107	1/1	0.52	0.19	69,69,69,69	0
57	MG	1a	1737	1/1	0.53	0.36	83,83,83,83	0
57	MG	2A	3366	1/1	0.53	0.33	77,77,77,77	0
57	MG	2a	1610	1/1	0.53	0.18	69,69,69,69	0
57	MG	2A	3352	1/1	0.54	0.29	77,77,77,77	0
57	MG	2A	3083	1/1	0.54	0.16	62,62,62,62	0
57	MG	1A	3919	1/1	0.54	0.21	71,71,71,71	0
57	MG	2a	1736	1/1	0.55	0.15	75,75,75,75	0
57	MG	2A	3112	1/1	0.55	0.31	83,83,83,83	0
57	MG	1A	3995	1/1	0.56	0.12	56,56,56,56	0
57	MG	2a	1789	1/1	0.56	0.23	86,86,86,86	0
57	MG	1x	103	1/1	0.56	0.30	70,70,70,70	0
57	MG	1A	4064	1/1	0.56	0.27	69,69,69,69	0
57	MG	2A	3098	1/1	0.56	0.18	77,77,77,77	0
57	MG	2A	3539	1/1	0.57	0.13	62,62,62,62	0
57	MG	1A	3945	1/1	0.57	0.12	66,66,66,66	0
57	MG	1U	210	1/1	0.57	0.55	66,66,66,66	0
57	MG	1a	1665	1/1	0.57	0.15	61,61,61,61	0
57	MG	2A	3120	1/1	0.58	0.14	79,79,79,79	0
57	MG	2A	3705	1/1	0.58	0.43	79,79,79,79	0
57	MG	2A	3364	1/1	0.58	0.11	77,77,77,77	0
57	MG	2A	3337	1/1	0.59	0.17	72,72,72,72	0
57	MG	2A	3585	1/1	0.59	0.16	75,75,75,75	0
57	MG	2A	3669	1/1	0.59	0.40	83,83,83,83	0
57	MG	2A	3686	1/1	0.59	0.16	67,67,67,67	0
57	MG	1A	3446	1/1	0.59	0.24	60,60,60,60	0
57	MG	2A	3704	1/1	0.59	0.28	74,74,74,74	0
57	MG	2A	3115	1/1	0.59	0.18	77,77,77,77	0
57	MG	2A	3752	1/1	0.59	0.18	80,80,80,80	0
57	MG	1A	3479	1/1	0.59	0.39	75,75,75,75	0
57	MG	1a	1675	1/1	0.60	0.23	71,71,71,71	0
57	MG	2a	1747	1/1	0.60	0.26	77,77,77,77	0
57	MG	2a	1764	1/1	0.60	0.13	89,89,89,89	0
57	MG	1w	101	1/1	0.60	0.22	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1658	1/1	0.60	0.21	68,68,68,68	0
57	MG	2A	3710	1/1	0.60	0.20	71,71,71,71	0
57	MG	2a	1722	1/1	0.60	0.27	70,70,70,70	0
57	MG	2A	3045	1/1	0.61	0.14	74,74,74,74	0
57	MG	2A	3837	1/1	0.61	0.22	71,71,71,71	0
57	MG	2A	3215	1/1	0.61	0.23	67,67,67,67	0
57	MG	2a	1627	1/1	0.61	0.20	71,71,71,71	0
57	MG	1a	1631	1/1	0.61	0.27	75,75,75,75	0
57	MG	2A	3573	1/1	0.61	0.13	86,86,86,86	0
57	MG	1A	3554	1/1	0.61	0.28	54,54,54,54	0
57	MG	2v	103	1/1	0.61	0.19	79,79,79,79	0
57	MG	2A	3152	1/1	0.61	0.24	73,73,73,73	0
57	MG	2A	3357	1/1	0.62	1.15	63,63,63,63	0
57	MG	2A	3166	1/1	0.62	0.17	74,74,74,74	0
57	MG	2a	1727	1/1	0.62	0.24	74,74,74,74	0
57	MG	1A	3464	1/1	0.62	0.35	63,63,63,63	0
57	MG	1a	1628	1/1	0.62	0.16	58,58,58,58	0
57	MG	1a	1707	1/1	0.62	0.17	80,80,80,80	0
57	MG	2a	1787	1/1	0.62	0.20	76,76,76,76	0
57	MG	1E	310	1/1	0.62	0.54	80,80,80,80	0
57	MG	1x	107	1/1	0.62	0.17	68,68,68,68	0
57	MG	2a	1648	1/1	0.62	0.13	76,76,76,76	0
57	MG	1A	4075	1/1	0.62	0.29	58,58,58,58	0
57	MG	2a	1694	1/1	0.62	0.13	77,77,77,77	0
57	MG	1A	3938	1/1	0.63	0.21	69,69,69,69	0
57	MG	1A	3640	1/1	0.63	0.21	80,80,80,80	0
57	MG	2A	3039	1/1	0.63	0.24	70,70,70,70	0
57	MG	2A	3278	1/1	0.63	0.59	75,75,75,75	0
57	MG	2A	3672	1/1	0.64	0.19	76,76,76,76	0
57	MG	1A	3508	1/1	0.64	0.18	71,71,71,71	0
57	MG	1a	1734	1/1	0.64	0.12	80,80,80,80	0
57	MG	2A	3315	1/1	0.64	0.34	62,62,62,62	0
57	MG	2A	3850	1/1	0.64	0.23	65,65,65,65	0
57	MG	1A	3470	1/1	0.64	0.29	67,67,67,67	0
57	MG	2a	1695	1/1	0.65	0.11	80,80,80,80	0
57	MG	1A	4033	1/1	0.65	0.11	61,61,61,61	0
57	MG	1E	307	1/1	0.65	0.19	59,59,59,59	0
57	MG	2A	3810	1/1	0.65	0.18	59,59,59,59	0
57	MG	1A	3420	1/1	0.65	0.26	67,67,67,67	0
57	MG	1A	4070	1/1	0.65	0.11	70,70,70,70	0
57	MG	2a	1752	1/1	0.65	0.09	70,70,70,70	0
57	MG	1a	1677	1/1	0.65	0.16	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3214	1/1	0.65	0.16	62,62,62,62	0
57	MG	1a	1683	1/1	0.65	0.15	57,57,57,57	0
57	MG	2A	3101	1/1	0.65	0.26	74,74,74,74	0
57	MG	2A	3253	1/1	0.65	0.23	78,78,78,78	0
57	MG	2A	3426	1/1	0.65	0.25	62,62,62,62	0
57	MG	1A	3545	1/1	0.65	0.27	60,60,60,60	0
57	MG	2A	3285	1/1	0.66	0.28	62,62,62,62	0
57	MG	2A	3382	1/1	0.66	0.50	76,76,76,76	0
57	MG	2F	303	1/1	0.66	0.26	50,50,50,50	0
57	MG	1A	3798	1/1	0.66	0.12	61,61,61,61	0
57	MG	2w	104	1/1	0.66	0.20	82,82,82,82	0
57	MG	2A	3297	1/1	0.67	0.22	74,74,74,74	0
57	MG	2A	3309	1/1	0.67	0.28	63,63,63,63	0
57	MG	2A	3657	1/1	0.67	0.12	85,85,85,85	0
57	MG	2a	1767	1/1	0.67	0.12	75,75,75,75	0
57	MG	2A	3310	1/1	0.67	0.33	61,61,61,61	0
57	MG	1A	3472	1/1	0.67	0.22	67,67,67,67	0
57	MG	2A	3121	1/1	0.67	0.26	60,60,60,60	0
57	MG	2A	3277	1/1	0.67	0.25	73,73,73,73	0
57	MG	2a	1607	1/1	0.67	0.19	58,58,58,58	0
57	MG	1A	3095	1/1	0.67	0.19	61,61,61,61	0
57	MG	1A	3807	1/1	0.67	0.32	51,51,51,51	0
57	MG	2a	1721	1/1	0.68	0.19	80,80,80,80	0
57	MG	1A	3052	1/1	0.68	0.33	50,50,50,50	0
57	MG	1A	3210	1/1	0.68	0.17	79,79,79,79	0
57	MG	1A	3707	1/1	0.68	0.19	54,54,54,54	0
57	MG	1A	3925	1/1	0.68	0.14	58,58,58,58	0
57	MG	1A	4010	1/1	0.68	0.09	77,77,77,77	0
57	MG	2a	1633	1/1	0.68	0.18	62,62,62,62	0
57	MG	2A	3183	1/1	0.68	0.22	55,55,55,55	0
57	MG	1A	3219	1/1	0.68	0.22	65,65,65,65	0
57	MG	1w	104	1/1	0.68	0.20	74,74,74,74	0
57	MG	2A	3335	1/1	0.68	0.27	78,78,78,78	0
57	MG	2a	1682	1/1	0.68	0.15	65,65,65,65	0
57	MG	1A	4035	1/1	0.68	0.12	75,75,75,75	0
57	MG	2A	3342	1/1	0.68	0.31	81,81,81,81	0
57	MG	1a	1695	1/1	0.68	0.15	63,63,63,63	0
57	MG	2a	1609	1/1	0.69	0.11	78,78,78,78	0
57	MG	1a	1806	1/1	0.69	0.07	81,81,81,81	0
57	MG	2A	3712	1/1	0.69	0.12	68,68,68,68	0
57	MG	2A	3735	1/1	0.69	0.37	72,72,72,72	0
57	MG	1A	4020	1/1	0.69	0.11	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1w	103	1/1	0.69	0.29	78,78,78,78	0
57	MG	2A	3263	1/1	0.69	0.21	65,65,65,65	0
57	MG	1B	207	1/1	0.69	0.22	75,75,75,75	0
57	MG	2A	3700	1/1	0.69	0.14	59,59,59,59	0
57	MG	2a	1804	1/1	0.69	0.14	76,76,76,76	0
57	MG	1A	3480	1/1	0.69	0.36	58,58,58,58	0
57	MG	2W	201	1/1	0.69	0.20	72,72,72,72	0
57	MG	2a	1700	1/1	0.69	0.20	80,80,80,80	0
57	MG	23	102	1/1	0.69	0.33	70,70,70,70	0
57	MG	2A	3052	1/1	0.69	0.12	70,70,70,70	0
57	MG	2A	3706	1/1	0.70	0.14	76,76,76,76	0
57	MG	2A	3230	1/1	0.70	0.22	50,50,50,50	0
57	MG	1A	3321	1/1	0.70	0.22	61,61,61,61	0
57	MG	1a	1663	1/1	0.70	0.21	64,64,64,64	0
57	MG	1A	3378	1/1	0.70	0.33	50,50,50,50	0
57	MG	1U	203	1/1	0.70	0.20	60,60,60,60	0
57	MG	2A	3803	1/1	0.70	0.09	72,72,72,72	0
57	MG	2A	3187	1/1	0.70	0.26	72,72,72,72	0
57	MG	2A	3817	1/1	0.70	0.20	60,60,60,60	0
57	MG	2A	3396	1/1	0.70	0.20	57,57,57,57	0
57	MG	1A	3404	1/1	0.70	0.27	69,69,69,69	0
57	MG	2B	214	1/1	0.70	0.39	79,79,79,79	0
57	MG	2A	3435	1/1	0.70	0.31	65,65,65,65	0
57	MG	1A	3552	1/1	0.70	0.19	55,55,55,55	0
57	MG	2A	3354	1/1	0.70	0.26	79,79,79,79	0
57	MG	2x	103	1/1	0.70	0.26	81,81,81,81	0
57	MG	2y	101	1/1	0.70	0.18	78,78,78,78	0
57	MG	2a	1715	1/1	0.71	0.36	77,77,77,77	0
57	MG	23	101	1/1	0.71	0.21	78,78,78,78	0
57	MG	2A	3011	1/1	0.71	0.12	58,58,58,58	0
57	MG	1A	3405	1/1	0.71	0.30	74,74,74,74	0
57	MG	1A	3541	1/1	0.71	0.30	47,47,47,47	0
57	MG	1A	3364	1/1	0.71	0.14	58,58,58,58	0
57	MG	1a	1686	1/1	0.71	0.26	58,58,58,58	0
57	MG	2A	3087	1/1	0.71	0.24	59,59,59,59	0
57	MG	2A	3201	1/1	0.71	0.13	69,69,69,69	0
57	MG	2A	3813	1/1	0.71	0.10	61,61,61,61	0
57	MG	1A	3773	1/1	0.71	0.12	68,68,68,68	0
57	MG	2A	3383	1/1	0.71	0.21	63,63,63,63	0
57	MG	2a	1679	1/1	0.71	0.13	75,75,75,75	0
57	MG	2A	3842	1/1	0.71	0.18	76,76,76,76	0
57	MG	2a	1690	1/1	0.71	0.16	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3099	1/1	0.71	0.20	51,51,51,51	0
57	MG	1B	229	1/1	0.71	0.31	86,86,86,86	0
57	MG	1D	311	1/1	0.71	0.34	78,78,78,78	0
57	MG	1A	3073	1/1	0.71	0.46	68,68,68,68	0
57	MG	2a	1719	1/1	0.72	0.41	74,74,74,74	0
57	MG	1a	1601	1/1	0.72	0.36	72,72,72,72	0
57	MG	2A	3806	1/1	0.72	0.17	62,62,62,62	0
57	MG	2A	3682	1/1	0.72	0.16	78,78,78,78	0
57	MG	1a	1603	1/1	0.72	0.26	67,67,67,67	0
57	MG	1A	3947	1/1	0.72	0.15	55,55,55,55	0
57	MG	2A	3439	1/1	0.72	0.19	72,72,72,72	0
57	MG	2A	3447	1/1	0.72	0.17	58,58,58,58	0
57	MG	2a	1652	1/1	0.72	0.14	64,64,64,64	0
57	MG	2A	3456	1/1	0.72	0.17	62,62,62,62	0
57	MG	2A	3156	1/1	0.72	0.32	74,74,74,74	0
57	MG	2A	3339	1/1	0.72	0.29	61,61,61,61	0
57	MG	2F	307	1/1	0.72	0.25	72,72,72,72	0
57	MG	2Q	202	1/1	0.72	0.31	67,67,67,67	0
57	MG	2A	3106	1/1	0.72	0.24	71,71,71,71	0
57	MG	1A	3576	1/1	0.72	0.24	47,47,47,47	0
57	MG	2A	3392	1/1	0.72	0.28	75,75,75,75	0
57	MG	2a	1711	1/1	0.72	0.19	68,68,68,68	0
57	MG	1a	1636	1/1	0.72	0.33	89,89,89,89	0
57	MG	1A	3339	1/1	0.73	0.17	36,36,36,36	0
57	MG	2A	3290	1/1	0.73	0.14	73,73,73,73	0
57	MG	2A	3391	1/1	0.73	0.17	78,78,78,78	0
57	MG	1A	3902	1/1	0.73	0.21	40,40,40,40	0
57	MG	1A	3144	1/1	0.73	0.22	49,49,49,49	0
57	MG	2A	3190	1/1	0.73	0.14	77,77,77,77	0
57	MG	1A	3781	1/1	0.73	0.11	63,63,63,63	0
57	MG	1a	1715	1/1	0.73	0.27	51,51,51,51	0
57	MG	2A	3730	1/1	0.73	0.19	73,73,73,73	0
57	MG	1a	1725	1/1	0.73	0.13	58,58,58,58	0
57	MG	2a	1616	1/1	0.73	0.12	72,72,72,72	0
57	MG	1A	3930	1/1	0.73	0.18	47,47,47,47	0
57	MG	1A	3216	1/1	0.73	0.21	61,61,61,61	0
57	MG	1A	3481	1/1	0.73	0.15	62,62,62,62	0
57	MG	2A	3255	1/1	0.73	0.58	74,74,74,74	0
57	MG	1B	231	1/1	0.73	0.09	81,81,81,81	0
57	MG	2A	3271	1/1	0.73	0.24	77,77,77,77	0
57	MG	1t	201	1/1	0.73	0.12	69,69,69,69	0
57	MG	2a	1662	1/1	0.73	0.11	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1667	1/1	0.73	0.18	67,67,67,67	0
57	MG	2A	3063	1/1	0.73	0.17	68,68,68,68	0
57	MG	2A	3169	1/1	0.73	0.25	63,63,63,63	0
57	MG	2A	3379	1/1	0.73	0.55	67,67,67,67	0
57	MG	2A	3857	1/1	0.73	0.18	66,66,66,66	0
57	MG	1A	3999	1/1	0.74	0.19	63,63,63,63	0
57	MG	2A	3198	1/1	0.74	0.35	60,60,60,60	0
57	MG	2A	3780	1/1	0.74	0.08	75,75,75,75	0
57	MG	2A	3799	1/1	0.74	0.25	79,79,79,79	0
57	MG	2A	3597	1/1	0.74	0.16	71,71,71,71	0
57	MG	1A	3394	1/1	0.74	0.40	61,61,61,61	0
57	MG	1A	3262	1/1	0.74	0.28	56,56,56,56	0
57	MG	2a	1635	1/1	0.74	0.15	69,69,69,69	0
57	MG	1A	4025	1/1	0.74	0.20	57,57,57,57	0
57	MG	1a	1783	1/1	0.74	0.13	75,75,75,75	0
57	MG	2A	3832	1/1	0.74	0.08	55,55,55,55	0
57	MG	1a	1679	1/1	0.74	0.25	82,82,82,82	0
57	MG	2a	1653	1/1	0.74	0.19	65,65,65,65	0
57	MG	1A	3235	1/1	0.74	0.56	54,54,54,54	0
57	MG	1a	1815	1/1	0.74	0.13	74,74,74,74	0
57	MG	2A	3056	1/1	0.74	0.31	74,74,74,74	0
57	MG	1A	3338	1/1	0.74	0.30	50,50,50,50	0
57	MG	1A	3442	1/1	0.74	0.24	46,46,46,46	0
57	MG	2A	3454	1/1	0.74	0.18	63,63,63,63	0
57	MG	2A	3179	1/1	0.74	0.11	59,59,59,59	0
57	MG	1A	3392	1/1	0.74	0.20	46,46,46,46	0
57	MG	1a	1639	1/1	0.74	0.18	65,65,65,65	0
57	MG	1a	1685	1/1	0.75	0.12	73,73,73,73	0
57	MG	1A	3800	1/1	0.75	0.15	56,56,56,56	0
57	MG	1A	3525	1/1	0.75	0.34	58,58,58,58	0
57	MG	2A	3845	1/1	0.75	0.13	76,76,76,76	0
57	MG	2A	3468	1/1	0.75	0.14	62,62,62,62	0
57	MG	2A	3496	1/1	0.75	0.12	77,77,77,77	0
57	MG	1A	3831	1/1	0.75	0.27	73,73,73,73	0
57	MG	2A	3323	1/1	0.75	0.57	64,64,64,64	0
57	MG	1A	3858	1/1	0.75	0.25	62,62,62,62	0
57	MG	2a	1772	1/1	0.75	0.16	65,65,65,65	0
57	MG	1a	1647	1/1	0.75	0.22	62,62,62,62	0
57	MG	1A	3349	1/1	0.75	0.16	59,59,59,59	0
57	MG	1R	205	1/1	0.75	0.30	54,54,54,54	0
57	MG	2A	3424	1/1	0.75	0.20	88,88,88,88	0
57	MG	1A	3297	1/1	0.75	0.27	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3675	1/1	0.75	0.38	64,64,64,64	0
57	MG	1A	3484	1/1	0.75	0.22	46,46,46,46	0
57	MG	2a	1612	1/1	0.75	0.18	72,72,72,72	0
57	MG	1A	3499	1/1	0.75	0.57	58,58,58,58	0
57	MG	1A	3425	1/1	0.75	0.23	73,73,73,73	0
57	MG	1s	101	1/1	0.76	0.16	78,78,78,78	0
57	MG	1A	3886	1/1	0.76	0.19	52,52,52,52	0
57	MG	1A	3745	1/1	0.76	0.18	55,55,55,55	0
57	MG	2a	1660	1/1	0.76	0.14	67,67,67,67	0
57	MG	2A	3200	1/1	0.76	0.23	74,74,74,74	0
57	MG	2a	1664	1/1	0.76	0.19	69,69,69,69	0
57	MG	2A	3099	1/1	0.76	0.12	76,76,76,76	0
57	MG	2A	3209	1/1	0.76	0.17	72,72,72,72	0
57	MG	1A	3124	1/1	0.76	0.33	55,55,55,55	0
57	MG	2a	1683	1/1	0.76	0.12	68,68,68,68	0
57	MG	1A	3328	1/1	0.76	0.24	62,62,62,62	0
57	MG	1A	3786	1/1	0.76	0.15	42,42,42,42	0
57	MG	2A	3609	1/1	0.76	0.15	65,65,65,65	0
57	MG	2A	3231	1/1	0.76	0.67	56,56,56,56	0
57	MG	1A	3090	1/1	0.76	0.18	32,32,32,32	0
57	MG	2A	3860	1/1	0.76	0.23	66,66,66,66	0
57	MG	1A	3476	1/1	0.76	0.20	59,59,59,59	0
57	MG	1A	3509	1/1	0.76	0.23	50,50,50,50	0
57	MG	1a	1770	1/1	0.76	0.17	75,75,75,75	0
57	MG	2A	3265	1/1	0.76	0.27	65,65,65,65	0
57	MG	1A	3006	1/1	0.76	0.28	70,70,70,70	0
57	MG	20	101	1/1	0.76	0.17	74,74,74,74	0
57	MG	2A	3157	1/1	0.76	0.31	64,64,64,64	0
57	MG	18	105	1/1	0.76	0.31	52,52,52,52	0
57	MG	25	101	1/1	0.76	0.15	61,61,61,61	0
57	MG	1A	3079	1/1	0.76	0.30	64,64,64,64	0
57	MG	2A	3279	1/1	0.76	0.28	68,68,68,68	0
57	MG	2A	3421	1/1	0.76	0.28	70,70,70,70	0
57	MG	2A	3280	1/1	0.76	0.14	62,62,62,62	0
57	MG	2A	3717	1/1	0.76	0.16	47,47,47,47	0
57	MG	2a	1625	1/1	0.76	0.17	70,70,70,70	0
57	MG	2A	3282	1/1	0.76	0.51	64,64,64,64	0
57	MG	1A	3712	1/1	0.76	0.26	68,68,68,68	0
57	MG	2A	3175	1/1	0.76	0.17	58,58,58,58	0
57	MG	2A	3060	1/1	0.76	0.30	65,65,65,65	0
57	MG	1f	201	1/1	0.76	0.28	50,50,50,50	0
57	MG	2A	3788	1/1	0.76	0.08	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3661	1/1	0.77	0.17	72,72,72,72	0
57	MG	1A	4081	1/1	0.77	0.19	54,54,54,54	0
57	MG	2A	3318	1/1	0.77	0.44	72,72,72,72	0
57	MG	2a	1707	1/1	0.77	0.19	81,81,81,81	0
57	MG	2A	3812	1/1	0.77	0.14	38,38,38,38	0
57	MG	1a	1671	1/1	0.77	0.24	62,62,62,62	0
57	MG	1A	3332	1/1	0.77	0.41	51,51,51,51	0
57	MG	2A	3264	1/1	0.77	0.15	65,65,65,65	0
57	MG	1A	3371	1/1	0.77	0.19	57,57,57,57	0
57	MG	1A	3568	1/1	0.77	0.31	61,61,61,61	0
57	MG	1A	3314	1/1	0.77	0.19	54,54,54,54	0
57	MG	1A	3228	1/1	0.77	0.24	52,52,52,52	0
57	MG	1a	1629	1/1	0.77	0.23	77,77,77,77	0
57	MG	2A	3125	1/1	0.77	0.22	71,71,71,71	0
57	MG	2A	3133	1/1	0.77	0.14	57,57,57,57	0
57	MG	2A	3369	1/1	0.77	0.16	51,51,51,51	0
57	MG	2A	3370	1/1	0.77	0.24	70,70,70,70	0
57	MG	1A	3662	1/1	0.77	0.20	53,53,53,53	0
57	MG	2T	3502	1/1	0.77	0.30	76,76,76,76	0
57	MG	1A	3308	1/1	0.77	0.23	43,43,43,43	0
57	MG	1A	3551	1/1	0.77	0.35	66,66,66,66	0
57	MG	1S	203	1/1	0.77	0.28	68,68,68,68	0
57	MG	1T	201	1/1	0.77	0.32	69,69,69,69	0
57	MG	2a	1689	1/1	0.77	0.17	73,73,73,73	0
57	MG	2A	3252	1/1	0.77	0.18	71,71,71,71	0
57	MG	2a	1602	1/1	0.77	0.21	70,70,70,70	0
57	MG	1A	3491	1/1	0.78	0.26	45,45,45,45	0
57	MG	25	105	1/1	0.78	0.23	63,63,63,63	0
57	MG	1a	1682	1/1	0.78	0.18	80,80,80,80	0
57	MG	2A	3789	1/1	0.78	0.08	48,48,48,48	0
57	MG	2A	3373	1/1	0.78	0.21	66,66,66,66	0
57	MG	1A	3025	1/1	0.78	0.21	38,38,38,38	0
57	MG	1A	3252	1/1	0.78	0.14	76,76,76,76	0
57	MG	2A	3220	1/1	0.78	0.12	73,73,73,73	0
57	MG	1A	3373	1/1	0.78	0.27	45,45,45,45	0
57	MG	1R	207	1/1	0.78	0.33	45,45,45,45	0
57	MG	2A	3313	1/1	0.78	0.20	68,68,68,68	0
57	MG	1A	3376	1/1	0.78	0.36	54,54,54,54	0
57	MG	2A	3159	1/1	0.78	0.21	64,64,64,64	0
57	MG	1A	3527	1/1	0.78	0.25	50,50,50,50	0
57	MG	2A	3332	1/1	0.78	0.18	81,81,81,81	0
57	MG	2A	3701	1/1	0.78	0.22	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1B	226	1/1	0.78	0.24	67,67,67,67	0
57	MG	1A	3094	1/1	0.78	0.20	49,49,49,49	0
57	MG	13	104	1/1	0.78	0.18	52,52,52,52	0
57	MG	1A	3345	1/1	0.78	0.17	66,66,66,66	0
57	MG	2A	3266	1/1	0.78	0.20	78,78,78,78	0
57	MG	2A	3102	1/1	0.78	0.19	80,80,80,80	0
57	MG	2A	3725	1/1	0.78	0.11	58,58,58,58	0
57	MG	1a	1763	1/1	0.78	0.10	66,66,66,66	0
57	MG	1A	3117	1/1	0.78	0.24	41,41,41,41	0
57	MG	2A	3008	1/1	0.78	0.20	57,57,57,57	0
57	MG	2A	3119	1/1	0.78	0.14	61,61,61,61	0
57	MG	2A	3411	1/1	0.79	0.14	56,56,56,56	0
57	MG	2A	3732	1/1	0.79	0.10	65,65,65,65	0
57	MG	2A	3167	1/1	0.79	0.10	78,78,78,78	0
57	MG	2A	3739	1/1	0.79	0.18	55,55,55,55	0
57	MG	1I	201	1/1	0.79	0.19	66,66,66,66	0
57	MG	1A	3419	1/1	0.79	0.26	78,78,78,78	0
57	MG	2a	1654	1/1	0.79	0.28	74,74,74,74	0
57	MG	2A	3289	1/1	0.79	0.22	68,68,68,68	0
57	MG	1A	4003	1/1	0.79	0.12	51,51,51,51	0
57	MG	1A	4009	1/1	0.79	0.33	66,66,66,66	0
57	MG	1A	3169	1/1	0.79	0.30	66,66,66,66	0
57	MG	1A	4015	1/1	0.79	0.14	33,33,33,33	0
57	MG	1A	3226	1/1	0.79	0.23	46,46,46,46	0
57	MG	2A	3463	1/1	0.79	0.23	61,61,61,61	0
57	MG	2A	3192	1/1	0.79	0.23	63,63,63,63	0
57	MG	2A	3480	1/1	0.79	0.18	68,68,68,68	0
57	MG	2A	3061	1/1	0.79	0.10	76,76,76,76	0
57	MG	1Z	301	1/1	0.79	0.29	77,77,77,77	0
57	MG	2A	3328	1/1	0.79	0.21	68,68,68,68	0
57	MG	1A	3874	1/1	0.79	0.53	52,52,52,52	0
57	MG	1A	3877	1/1	0.79	0.16	72,72,72,72	0
57	MG	2A	3088	1/1	0.79	0.13	65,65,65,65	0
57	MG	1A	3439	1/1	0.79	0.17	73,73,73,73	0
57	MG	2A	3617	1/1	0.79	0.51	77,77,77,77	0
57	MG	2A	3652	1/1	0.79	0.12	49,49,49,49	0
57	MG	2a	1720	1/1	0.79	0.12	72,72,72,72	0
57	MG	1A	3441	1/1	0.79	0.26	56,56,56,56	0
57	MG	1a	1604	1/1	0.79	0.11	59,59,59,59	0
57	MG	2A	3665	1/1	0.79	0.14	73,73,73,73	0
57	MG	1A	4067	1/1	0.79	0.19	66,66,66,66	0
57	MG	1A	3702	1/1	0.79	0.20	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3340	1/1	0.79	0.32	63,63,63,63	0
57	MG	1A	3382	1/1	0.79	0.17	57,57,57,57	0
57	MG	2A	3685	1/1	0.79	0.12	64,64,64,64	0
57	MG	1A	3732	1/1	0.79	0.20	64,64,64,64	0
57	MG	2A	3257	1/1	0.79	0.30	67,67,67,67	0
57	MG	1A	3295	1/1	0.79	0.24	42,42,42,42	0
57	MG	1A	3247	1/1	0.79	0.53	62,62,62,62	0
57	MG	2a	1815	1/1	0.79	0.14	77,77,77,77	0
57	MG	1A	3299	1/1	0.79	0.43	56,56,56,56	0
57	MG	1A	3954	1/1	0.79	0.15	51,51,51,51	0
57	MG	1A	3334	1/1	0.79	0.27	49,49,49,49	0
57	MG	1A	3415	1/1	0.79	0.29	45,45,45,45	0
57	MG	1A	3985	1/1	0.79	0.19	69,69,69,69	0
57	MG	1A	3418	1/1	0.79	0.45	69,69,69,69	0
57	MG	1x	112	1/1	0.79	0.24	66,66,66,66	0
57	MG	2a	1628	1/1	0.80	0.18	68,68,68,68	0
57	MG	2A	3294	1/1	0.80	0.14	58,58,58,58	0
57	MG	1a	1793	1/1	0.80	0.22	78,78,78,78	0
57	MG	1a	1653	1/1	0.80	0.13	49,49,49,49	0
57	MG	1A	3343	1/1	0.80	0.15	58,58,58,58	0
57	MG	1A	3768	1/1	0.80	0.18	23,23,23,23	0
57	MG	2a	1649	1/1	0.80	0.21	73,73,73,73	0
57	MG	2A	3210	1/1	0.80	0.30	74,74,74,74	0
57	MG	1A	3997	1/1	0.80	0.17	64,64,64,64	0
57	MG	2A	3321	1/1	0.80	0.14	69,69,69,69	0
57	MG	2A	3465	1/1	0.80	0.20	60,60,60,60	0
57	MG	2A	3798	1/1	0.80	0.08	80,80,80,80	0
57	MG	1a	1672	1/1	0.80	0.18	66,66,66,66	0
57	MG	2A	3801	1/1	0.80	0.10	71,71,71,71	0
57	MG	2A	3324	1/1	0.80	1.06	66,66,66,66	0
57	MG	2A	3485	1/1	0.80	0.24	69,69,69,69	0
57	MG	1A	3998	1/1	0.80	0.09	64,64,64,64	0
57	MG	1A	3519	1/1	0.80	0.36	58,58,58,58	0
57	MG	2A	3527	1/1	0.80	0.21	70,70,70,70	0
57	MG	1A	4088	1/1	0.80	0.19	44,44,44,44	0
57	MG	2A	3818	1/1	0.80	0.16	43,43,43,43	0
57	MG	2A	3561	1/1	0.80	0.13	38,38,38,38	0
57	MG	10	105	1/1	0.80	0.27	65,65,65,65	0
57	MG	2A	3338	1/1	0.80	0.11	60,60,60,60	0
57	MG	1A	3520	1/1	0.80	0.30	75,75,75,75	0
57	MG	16	102	1/1	0.80	0.39	64,64,64,64	0
57	MG	1A	3592	1/1	0.80	0.25	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3316	1/1	0.80	0.17	55,55,55,55	0
57	MG	2A	3005	1/1	0.80	0.25	67,67,67,67	0
57	MG	2B	219	1/1	0.80	0.20	78,78,78,78	0
57	MG	2A	3006	1/1	0.80	0.18	68,68,68,68	0
57	MG	1A	3290	1/1	0.80	0.27	48,48,48,48	0
57	MG	1A	3530	1/1	0.80	0.26	45,45,45,45	0
57	MG	2a	1746	1/1	0.80	0.17	75,75,75,75	0
57	MG	2A	3267	1/1	0.80	0.28	59,59,59,59	0
57	MG	2A	3268	1/1	0.80	0.23	68,68,68,68	0
57	MG	2A	3018	1/1	0.80	0.17	64,64,64,64	0
57	MG	1a	1625	1/1	0.80	0.23	62,62,62,62	0
57	MG	2A	3275	1/1	0.80	0.14	77,77,77,77	0
57	MG	2A	3043	1/1	0.80	0.17	70,70,70,70	0
57	MG	1A	3413	1/1	0.80	0.12	49,49,49,49	0
57	MG	26	101	1/1	0.80	0.16	78,78,78,78	0
57	MG	1A	3494	1/1	0.80	0.24	56,56,56,56	0
57	MG	2a	1817	1/1	0.80	0.10	74,74,74,74	0
57	MG	2d	301	1/1	0.80	0.36	63,63,63,63	0
57	MG	1A	3024	1/1	0.80	0.30	64,64,64,64	0
57	MG	1A	4038	1/1	0.80	0.13	55,55,55,55	0
57	MG	2A	3406	1/1	0.80	0.29	45,45,45,45	0
57	MG	1O	204	1/1	0.80	0.14	66,66,66,66	0
57	MG	2A	3419	1/1	0.80	0.15	65,65,65,65	0
57	MG	1a	1643	1/1	0.80	0.14	73,73,73,73	0
57	MG	1A	3272	1/1	0.80	0.22	52,52,52,52	0
57	MG	2a	1643	1/1	0.81	0.20	60,60,60,60	0
57	MG	2a	1644	1/1	0.81	0.15	77,77,77,77	0
57	MG	1A	4096	1/1	0.81	0.12	59,59,59,59	0
57	MG	1A	3553	1/1	0.81	0.16	49,49,49,49	0
57	MG	2a	1650	1/1	0.81	0.13	80,80,80,80	0
57	MG	2A	3471	1/1	0.81	0.13	64,64,64,64	0
57	MG	2A	3475	1/1	0.81	0.23	68,68,68,68	0
57	MG	2A	3259	1/1	0.81	0.27	55,55,55,55	0
57	MG	1B	219	1/1	0.81	0.22	34,34,34,34	0
57	MG	1B	225	1/1	0.81	0.13	62,62,62,62	0
57	MG	2A	3349	1/1	0.81	0.22	59,59,59,59	0
57	MG	2A	3513	1/1	0.81	0.12	85,85,85,85	0
57	MG	1a	1669	1/1	0.81	0.18	54,54,54,54	0
57	MG	2a	1670	1/1	0.81	0.09	61,61,61,61	0
57	MG	13	101	1/1	0.81	0.22	49,49,49,49	0
57	MG	2a	1680	1/1	0.81	0.17	77,77,77,77	0
57	MG	1A	3885	1/1	0.81	0.19	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3363	1/1	0.81	0.22	64,64,64,64	0
57	MG	1a	1809	1/1	0.81	0.10	69,69,69,69	0
57	MG	2A	3172	1/1	0.81	0.36	60,60,60,60	0
57	MG	1A	3982	1/1	0.81	0.14	74,74,74,74	0
57	MG	2A	3069	1/1	0.81	0.14	70,70,70,70	0
57	MG	2A	3632	1/1	0.81	0.16	65,65,65,65	0
57	MG	2A	3649	1/1	0.81	0.08	59,59,59,59	0
57	MG	2A	3180	1/1	0.81	0.23	54,54,54,54	0
57	MG	1A	3500	1/1	0.81	0.30	47,47,47,47	0
57	MG	1A	3566	1/1	0.81	0.29	36,36,36,36	0
57	MG	1A	4041	1/1	0.81	0.12	59,59,59,59	0
57	MG	2A	3381	1/1	0.81	0.12	64,64,64,64	0
57	MG	2A	3097	1/1	0.81	0.20	63,63,63,63	0
57	MG	1A	4050	1/1	0.81	0.15	38,38,38,38	0
57	MG	2A	3389	1/1	0.81	0.16	69,69,69,69	0
57	MG	2a	1730	1/1	0.81	0.26	83,83,83,83	0
57	MG	1a	1605	1/1	0.81	0.15	71,71,71,71	0
57	MG	2a	1745	1/1	0.81	0.14	70,70,70,70	0
57	MG	1A	3416	1/1	0.81	0.27	44,44,44,44	0
57	MG	1A	3716	1/1	0.81	0.12	62,62,62,62	0
57	MG	1A	3004	1/1	0.81	0.18	28,28,28,28	0
57	MG	2A	3303	1/1	0.81	0.13	52,52,52,52	0
57	MG	2A	3413	1/1	0.81	0.29	70,70,70,70	0
57	MG	2a	1768	1/1	0.81	0.15	87,87,87,87	0
57	MG	1A	3834	1/1	0.81	0.17	55,55,55,55	0
57	MG	2a	1775	1/1	0.81	0.09	67,67,67,67	0
57	MG	1a	1713	1/1	0.81	0.17	73,73,73,73	0
57	MG	1A	3220	1/1	0.81	0.40	47,47,47,47	0
57	MG	2A	3227	1/1	0.81	0.15	50,50,50,50	0
57	MG	2a	1806	1/1	0.81	0.14	65,65,65,65	0
57	MG	2A	3433	1/1	0.81	0.23	69,69,69,69	0
57	MG	1a	1722	1/1	0.81	0.20	75,75,75,75	0
57	MG	2a	1822	1/1	0.81	0.23	67,67,67,67	0
57	MG	2A	3319	1/1	0.81	0.25	57,57,57,57	0
57	MG	2a	1626	1/1	0.81	0.27	74,74,74,74	0
57	MG	1A	3245	1/1	0.81	0.28	51,51,51,51	0
57	MG	2A	3238	1/1	0.81	0.12	61,61,61,61	0
57	MG	2A	3122	1/1	0.81	0.08	54,54,54,54	0
57	MG	1a	1727	1/1	0.81	0.30	53,53,53,53	0
57	MG	1A	3065	1/1	0.81	0.25	56,56,56,56	0
57	MG	2A	3777	1/1	0.81	0.15	75,75,75,75	0
57	MG	2A	3744	1/1	0.82	0.19	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1733	1/1	0.82	0.32	79,79,79,79	0
57	MG	2A	3193	1/1	0.82	0.50	65,65,65,65	0
57	MG	2A	3314	1/1	0.82	0.26	65,65,65,65	0
57	MG	1A	3214	1/1	0.82	0.24	55,55,55,55	0
57	MG	1A	3320	1/1	0.82	0.14	46,46,46,46	0
57	MG	1A	3631	1/1	0.82	0.14	62,62,62,62	0
57	MG	1A	3422	1/1	0.82	0.28	38,38,38,38	0
57	MG	1A	3147	1/1	0.82	0.22	42,42,42,42	0
57	MG	2A	3212	1/1	0.82	0.26	73,73,73,73	0
57	MG	2A	3325	1/1	0.82	0.19	79,79,79,79	0
57	MG	2A	3077	1/1	0.82	0.26	53,53,53,53	0
57	MG	2a	1671	1/1	0.82	0.15	71,71,71,71	0
57	MG	2A	3809	1/1	0.82	0.21	64,64,64,64	0
57	MG	1A	3830	1/1	0.82	0.17	61,61,61,61	0
57	MG	2A	3489	1/1	0.82	0.26	64,64,64,64	0
57	MG	1a	1790	1/1	0.82	0.09	61,61,61,61	0
57	MG	2A	3336	1/1	0.82	0.10	75,75,75,75	0
57	MG	1a	1792	1/1	0.82	0.17	70,70,70,70	0
57	MG	2A	3523	1/1	0.82	0.16	63,63,63,63	0
57	MG	1A	4048	1/1	0.82	0.14	58,58,58,58	0
57	MG	1a	1799	1/1	0.82	0.10	72,72,72,72	0
57	MG	1a	1660	1/1	0.82	0.14	66,66,66,66	0
57	MG	2A	3344	1/1	0.82	0.11	61,61,61,61	0
57	MG	1A	4049	1/1	0.82	0.15	52,52,52,52	0
57	MG	1A	3326	1/1	0.82	0.21	35,35,35,35	0
57	MG	1A	3296	1/1	0.82	0.29	51,51,51,51	0
57	MG	1h	201	1/1	0.82	0.17	66,66,66,66	0
57	MG	1A	3850	1/1	0.82	0.24	42,42,42,42	0
57	MG	1A	3978	1/1	0.82	0.22	70,70,70,70	0
57	MG	1W	202	1/1	0.82	0.39	50,50,50,50	0
57	MG	2R	202	1/1	0.82	0.16	64,64,64,64	0
57	MG	1A	3489	1/1	0.82	0.21	71,71,71,71	0
57	MG	2T	3503	1/1	0.82	0.22	52,52,52,52	0
57	MG	1A	3153	1/1	0.82	0.18	37,37,37,37	0
57	MG	1A	3129	1/1	0.82	0.28	53,53,53,53	0
57	MG	1A	3462	1/1	0.82	0.28	69,69,69,69	0
57	MG	16	101	1/1	0.82	0.13	57,57,57,57	0
57	MG	1x	105	1/1	0.82	0.21	71,71,71,71	0
57	MG	1A	3182	1/1	0.82	0.24	58,58,58,58	0
57	MG	1x	109	1/1	0.82	0.12	74,74,74,74	0
57	MG	1A	3469	1/1	0.82	0.17	64,64,64,64	0
57	MG	2A	3388	1/1	0.82	0.23	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1B	213	1/1	0.82	0.27	75,75,75,75	0
57	MG	2A	3168	1/1	0.82	0.09	76,76,76,76	0
57	MG	1a	1706	1/1	0.82	0.26	65,65,65,65	0
57	MG	2A	3281	1/1	0.82	0.20	65,65,65,65	0
57	MG	2A	3007	1/1	0.82	0.11	61,61,61,61	0
57	MG	2A	3709	1/1	0.82	0.15	43,43,43,43	0
57	MG	1A	4002	1/1	0.82	0.12	55,55,55,55	0
57	MG	1A	3889	1/1	0.82	0.12	35,35,35,35	0
57	MG	1A	3896	1/1	0.82	0.17	64,64,64,64	0
57	MG	2A	3028	1/1	0.82	0.16	48,48,48,48	0
57	MG	2A	3295	1/1	0.82	0.15	57,57,57,57	0
57	MG	1a	1615	1/1	0.82	0.17	68,68,68,68	0
57	MG	2x	102	1/1	0.82	0.14	75,75,75,75	0
57	MG	1A	3899	1/1	0.82	0.24	73,73,73,73	0
57	MG	1A	3019	1/1	0.82	0.26	50,50,50,50	0
57	MG	2A	3718	1/1	0.83	0.53	66,66,66,66	0
57	MG	2A	3414	1/1	0.83	0.37	68,68,68,68	0
57	MG	2A	3299	1/1	0.83	0.14	84,84,84,84	0
57	MG	1A	3085	1/1	0.83	0.72	34,34,34,34	0
57	MG	2A	3305	1/1	0.83	0.15	60,60,60,60	0
57	MG	1A	3402	1/1	0.83	0.21	71,71,71,71	0
57	MG	2A	3071	1/1	0.83	0.16	62,62,62,62	0
57	MG	2A	3751	1/1	0.83	0.20	50,50,50,50	0
57	MG	2A	3075	1/1	0.83	0.14	45,45,45,45	0
57	MG	1Q	205	1/1	0.83	0.28	55,55,55,55	0
57	MG	1R	202	1/1	0.83	0.24	46,46,46,46	0
57	MG	1R	204	1/1	0.83	0.29	35,35,35,35	0
57	MG	1A	3955	1/1	0.83	0.23	56,56,56,56	0
57	MG	1A	3403	1/1	0.83	0.76	65,65,65,65	0
57	MG	1S	201	1/1	0.83	0.40	43,43,43,43	0
57	MG	2A	3222	1/1	0.83	0.20	65,65,65,65	0
57	MG	1A	3970	1/1	0.83	0.20	54,54,54,54	0
57	MG	2A	3229	1/1	0.83	0.22	53,53,53,53	0
57	MG	1A	4053	1/1	0.83	0.11	59,59,59,59	0
57	MG	1A	3971	1/1	0.83	0.27	65,65,65,65	0
57	MG	2A	3235	1/1	0.83	0.39	62,62,62,62	0
57	MG	1A	3864	1/1	0.83	0.23	50,50,50,50	0
57	MG	2A	3495	1/1	0.83	0.31	72,72,72,72	0
57	MG	1A	3246	1/1	0.83	0.41	73,73,73,73	0
57	MG	1A	3440	1/1	0.83	0.13	65,65,65,65	0
57	MG	1A	3744	1/1	0.83	0.18	56,56,56,56	0
57	MG	10	108	1/1	0.83	0.28	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3345	1/1	0.83	0.20	67,67,67,67	0
57	MG	12	3702	1/1	0.83	0.20	45,45,45,45	0
57	MG	2A	3350	1/1	0.83	0.16	65,65,65,65	0
57	MG	2A	3854	1/1	0.83	0.08	61,61,61,61	0
57	MG	2A	3258	1/1	0.83	0.18	74,74,74,74	0
57	MG	1A	3082	1/1	0.83	0.30	44,44,44,44	0
57	MG	2A	3356	1/1	0.83	0.85	56,56,56,56	0
57	MG	1A	3583	1/1	0.83	0.23	67,67,67,67	0
57	MG	2A	3616	1/1	0.83	0.12	36,36,36,36	0
57	MG	2A	3132	1/1	0.83	0.26	49,49,49,49	0
57	MG	1A	3223	1/1	0.83	0.20	50,50,50,50	0
57	MG	2A	3637	1/1	0.83	0.17	47,47,47,47	0
57	MG	1A	3381	1/1	0.83	0.28	60,60,60,60	0
57	MG	2A	3367	1/1	0.83	0.13	60,60,60,60	0
57	MG	1A	3636	1/1	0.83	0.20	61,61,61,61	0
57	MG	1A	3360	1/1	0.83	0.22	77,77,77,77	0
57	MG	1B	220	1/1	0.83	0.22	72,72,72,72	0
57	MG	2A	3372	1/1	0.83	0.15	70,70,70,70	0
57	MG	1A	3907	1/1	0.83	0.16	41,41,41,41	0
57	MG	1A	3645	1/1	0.83	0.17	30,30,30,30	0
57	MG	1A	3920	1/1	0.83	0.09	64,64,64,64	0
57	MG	1a	1617	1/1	0.83	0.10	41,41,41,41	0
57	MG	1A	3804	1/1	0.83	0.18	25,25,25,25	0
57	MG	2A	3042	1/1	0.83	0.21	56,56,56,56	0
57	MG	2A	3385	1/1	0.83	0.19	74,74,74,74	0
57	MG	2a	1611	1/1	0.83	0.35	66,66,66,66	0
57	MG	2A	3173	1/1	0.83	0.28	61,61,61,61	0
57	MG	2a	1615	1/1	0.83	0.34	64,64,64,64	0
57	MG	1A	3387	1/1	0.83	0.27	51,51,51,51	0
57	MG	1a	1764	1/1	0.83	0.13	58,58,58,58	0
57	MG	1A	4030	1/1	0.83	0.14	49,49,49,49	0
57	MG	1A	3309	1/1	0.83	0.34	63,63,63,63	0
57	MG	1a	1787	1/1	0.83	0.10	77,77,77,77	0
57	MG	1A	3699	1/1	0.83	0.24	36,36,36,36	0
57	MG	2A	3062	1/1	0.83	0.12	78,78,78,78	0
57	MG	1V	207	1/1	0.84	0.30	63,63,63,63	0
57	MG	2A	3302	1/1	0.84	0.22	64,64,64,64	0
57	MG	2A	3707	1/1	0.84	0.06	64,64,64,64	0
57	MG	1B	210	1/1	0.84	0.36	71,71,71,71	0
57	MG	1W	207	1/1	0.84	0.24	33,33,33,33	0
57	MG	1X	106	1/1	0.84	0.25	83,83,83,83	0
57	MG	1A	3531	1/1	0.84	0.30	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3539	1/1	0.84	0.26	63,63,63,63	0
57	MG	2A	3720	1/1	0.84	0.38	60,60,60,60	0
57	MG	2A	3432	1/1	0.84	0.23	50,50,50,50	0
57	MG	1A	4023	1/1	0.84	0.21	53,53,53,53	0
57	MG	1A	3302	1/1	0.84	0.55	70,70,70,70	0
57	MG	1A	4026	1/1	0.84	0.11	71,71,71,71	0
57	MG	1A	3691	1/1	0.84	0.17	73,73,73,73	0
57	MG	2A	3219	1/1	0.84	0.21	63,63,63,63	0
57	MG	1a	1681	1/1	0.84	0.19	64,64,64,64	0
57	MG	1A	3449	1/1	0.84	0.35	67,67,67,67	0
57	MG	1A	3458	1/1	0.84	0.28	39,39,39,39	0
57	MG	2A	3759	1/1	0.84	0.10	67,67,67,67	0
57	MG	2A	3103	1/1	0.84	0.15	59,59,59,59	0
57	MG	18	104	1/1	0.84	0.42	47,47,47,47	0
57	MG	1A	3260	1/1	0.84	0.14	30,30,30,30	0
57	MG	2A	3472	1/1	0.84	0.14	64,64,64,64	0
57	MG	2A	3233	1/1	0.84	0.18	42,42,42,42	0
57	MG	2a	1669	1/1	0.84	0.12	70,70,70,70	0
57	MG	2A	3476	1/1	0.84	0.14	68,68,68,68	0
57	MG	2A	3234	1/1	0.84	0.80	65,65,65,65	0
57	MG	19	101	1/1	0.84	0.33	54,54,54,54	0
57	MG	1a	1699	1/1	0.84	0.27	53,53,53,53	0
57	MG	1A	3370	1/1	0.84	0.20	61,61,61,61	0
57	MG	1x	106	1/1	0.84	0.28	60,60,60,60	0
57	MG	1A	3429	1/1	0.84	0.21	48,48,48,48	0
57	MG	2A	3124	1/1	0.84	0.26	54,54,54,54	0
57	MG	2A	3816	1/1	0.84	0.09	54,54,54,54	0
57	MG	2A	3256	1/1	0.84	0.86	57,57,57,57	0
57	MG	1A	3506	1/1	0.84	0.22	58,58,58,58	0
57	MG	2a	1701	1/1	0.84	0.09	69,69,69,69	0
57	MG	1A	3430	1/1	0.84	0.17	65,65,65,65	0
57	MG	2a	1706	1/1	0.84	0.14	76,76,76,76	0
57	MG	2A	3001	1/1	0.84	0.25	62,62,62,62	0
57	MG	2A	3839	1/1	0.84	0.11	70,70,70,70	0
57	MG	2A	3566	1/1	0.84	0.16	64,64,64,64	0
57	MG	2A	3148	1/1	0.84	0.17	71,71,71,71	0
57	MG	2A	3358	1/1	0.84	0.14	62,62,62,62	0
57	MG	1a	1714	1/1	0.84	0.17	64,64,64,64	0
57	MG	2A	3155	1/1	0.84	0.18	65,65,65,65	0
57	MG	2a	1724	1/1	0.84	0.25	72,72,72,72	0
57	MG	2a	1726	1/1	0.84	0.30	76,76,76,76	0
57	MG	1A	3433	1/1	0.84	0.23	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1728	1/1	0.84	0.17	63,63,63,63	0
57	MG	2B	204	1/1	0.84	0.11	76,76,76,76	0
57	MG	2B	206	1/1	0.84	0.17	83,83,83,83	0
57	MG	2a	1739	1/1	0.84	0.24	72,72,72,72	0
57	MG	1a	1720	1/1	0.84	0.15	71,71,71,71	0
57	MG	1A	3764	1/1	0.84	0.28	33,33,33,33	0
57	MG	2D	301	1/1	0.84	0.47	52,52,52,52	0
57	MG	2E	303	1/1	0.84	0.15	74,74,74,74	0
57	MG	1a	1723	1/1	0.84	0.14	55,55,55,55	0
57	MG	2A	3641	1/1	0.84	0.12	44,44,44,44	0
57	MG	2A	3272	1/1	0.84	0.18	72,72,72,72	0
57	MG	2a	1770	1/1	0.84	0.14	70,70,70,70	0
57	MG	1a	1619	1/1	0.84	0.15	46,46,46,46	0
57	MG	1a	1623	1/1	0.84	0.12	64,64,64,64	0
57	MG	2A	3660	1/1	0.84	0.16	78,78,78,78	0
57	MG	2A	3037	1/1	0.84	0.23	71,71,71,71	0
57	MG	2a	1800	1/1	0.84	0.22	83,83,83,83	0
57	MG	2Z	301	1/1	0.84	0.15	82,82,82,82	0
57	MG	1A	3076	1/1	0.84	0.26	50,50,50,50	0
57	MG	1A	3588	1/1	0.84	0.27	53,53,53,53	0
57	MG	1A	3204	1/1	0.84	0.17	48,48,48,48	0
57	MG	1A	3616	1/1	0.84	0.24	35,35,35,35	0
57	MG	1A	3910	1/1	0.84	0.31	42,42,42,42	0
57	MG	1A	3315	1/1	0.84	0.18	60,60,60,60	0
57	MG	1A	3130	1/1	0.84	0.32	38,38,38,38	0
57	MG	2a	1605	1/1	0.84	0.30	77,77,77,77	0
57	MG	2a	1606	1/1	0.84	0.15	79,79,79,79	0
57	MG	2A	3184	1/1	0.84	0.23	62,62,62,62	0
57	MG	2A	3185	1/1	0.84	0.16	56,56,56,56	0
57	MG	1A	3482	1/1	0.84	0.25	42,42,42,42	0
57	MG	1a	1651	1/1	0.84	0.15	71,71,71,71	0
57	MG	2A	3072	1/1	0.85	0.13	67,67,67,67	0
57	MG	2A	3716	1/1	0.85	0.14	44,44,44,44	0
57	MG	2A	3197	1/1	0.85	0.19	86,86,86,86	0
57	MG	1a	1795	1/1	0.85	0.16	65,65,65,65	0
57	MG	2a	1631	1/1	0.85	0.15	63,63,63,63	0
57	MG	2A	3304	1/1	0.85	0.35	66,66,66,66	0
57	MG	1A	3522	1/1	0.85	0.31	35,35,35,35	0
57	MG	2A	3434	1/1	0.85	0.19	53,53,53,53	0
57	MG	2A	3308	1/1	0.85	0.15	68,68,68,68	0
57	MG	2A	3733	1/1	0.85	0.07	72,72,72,72	0
57	MG	1A	3148	1/1	0.85	0.71	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1645	1/1	0.85	0.21	64,64,64,64	0
57	MG	1A	3236	1/1	0.85	0.26	63,63,63,63	0
57	MG	1A	3239	1/1	0.85	0.22	47,47,47,47	0
57	MG	2A	3089	1/1	0.85	0.37	47,47,47,47	0
57	MG	2A	3095	1/1	0.85	0.21	48,48,48,48	0
57	MG	1a	1816	1/1	0.85	0.12	59,59,59,59	0
57	MG	1A	3839	1/1	0.85	0.32	67,67,67,67	0
57	MG	2A	3764	1/1	0.85	0.14	64,64,64,64	0
57	MG	2A	3770	1/1	0.85	0.47	50,50,50,50	0
57	MG	2A	3775	1/1	0.85	0.20	69,69,69,69	0
57	MG	1A	3952	1/1	0.85	0.24	49,49,49,49	0
57	MG	1A	3590	1/1	0.85	0.23	42,42,42,42	0
57	MG	2A	3226	1/1	0.85	0.20	56,56,56,56	0
57	MG	1E	306	1/1	0.85	0.21	46,46,46,46	0
57	MG	1A	3722	1/1	0.85	0.13	40,40,40,40	0
57	MG	1A	3862	1/1	0.85	0.20	61,61,61,61	0
57	MG	1A	3285	1/1	0.85	0.15	42,42,42,42	0
57	MG	1a	1690	1/1	0.85	0.23	61,61,61,61	0
57	MG	1a	1693	1/1	0.85	0.22	68,68,68,68	0
57	MG	1x	101	1/1	0.85	0.32	71,71,71,71	0
57	MG	1A	3734	1/1	0.85	0.14	65,65,65,65	0
57	MG	2a	1693	1/1	0.85	0.23	67,67,67,67	0
57	MG	2A	3241	1/1	0.85	0.73	54,54,54,54	0
57	MG	1A	3741	1/1	0.85	0.17	37,37,37,37	0
57	MG	2a	1699	1/1	0.85	0.14	71,71,71,71	0
57	MG	2A	3251	1/1	0.85	0.47	75,75,75,75	0
57	MG	1A	3120	1/1	0.85	0.49	44,44,44,44	0
57	MG	1A	4057	1/1	0.85	0.27	31,31,31,31	0
57	MG	2A	3565	1/1	0.85	0.13	38,38,38,38	0
57	MG	2A	3130	1/1	0.85	0.21	47,47,47,47	0
57	MG	2A	3131	1/1	0.85	0.23	49,49,49,49	0
57	MG	1A	3626	1/1	0.85	0.13	32,32,32,32	0
57	MG	1A	3163	1/1	0.85	0.24	52,52,52,52	0
57	MG	2A	3142	1/1	0.85	0.14	70,70,70,70	0
57	MG	2A	3610	1/1	0.85	0.19	72,72,72,72	0
57	MG	2A	3612	1/1	0.85	0.17	61,61,61,61	0
57	MG	2A	3262	1/1	0.85	0.26	63,63,63,63	0
57	MG	1A	3027	1/1	0.85	0.11	77,77,77,77	0
57	MG	1A	3174	1/1	0.85	0.17	35,35,35,35	0
57	MG	2B	211	1/1	0.85	0.27	83,83,83,83	0
57	MG	1A	3257	1/1	0.85	0.19	57,57,57,57	0
57	MG	1A	3900	1/1	0.85	0.16	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1T	203	1/1	0.85	0.18	54,54,54,54	0
57	MG	1a	1724	1/1	0.85	0.21	56,56,56,56	0
57	MG	1a	1635	1/1	0.85	0.33	79,79,79,79	0
57	MG	1A	3661	1/1	0.85	0.15	57,57,57,57	0
57	MG	1a	1637	1/1	0.85	0.11	52,52,52,52	0
57	MG	1A	3797	1/1	0.85	0.09	45,45,45,45	0
57	MG	2A	3668	1/1	0.85	0.22	50,50,50,50	0
57	MG	1V	206	1/1	0.85	0.59	60,60,60,60	0
57	MG	1a	1741	1/1	0.85	0.21	67,67,67,67	0
57	MG	2A	3674	1/1	0.85	0.12	66,66,66,66	0
57	MG	1B	202	1/1	0.85	0.30	59,59,59,59	0
57	MG	2A	3681	1/1	0.85	0.10	70,70,70,70	0
57	MG	1A	3515	1/1	0.85	0.16	61,61,61,61	0
57	MG	2a	1791	1/1	0.85	0.12	67,67,67,67	0
57	MG	2a	1794	1/1	0.85	0.14	66,66,66,66	0
57	MG	2a	1799	1/1	0.85	0.11	79,79,79,79	0
57	MG	2A	3386	1/1	0.85	0.18	69,69,69,69	0
57	MG	25	103	1/1	0.85	0.38	61,61,61,61	0
57	MG	1B	209	1/1	0.85	0.14	37,37,37,37	0
57	MG	2a	1809	1/1	0.85	0.12	74,74,74,74	0
57	MG	1a	1654	1/1	0.85	0.09	56,56,56,56	0
57	MG	2A	3693	1/1	0.85	0.14	58,58,58,58	0
57	MG	1a	1656	1/1	0.85	0.19	50,50,50,50	0
57	MG	2a	1825	1/1	0.85	0.19	72,72,72,72	0
57	MG	1X	103	1/1	0.85	0.24	46,46,46,46	0
57	MG	2A	3702	1/1	0.85	0.08	65,65,65,65	0
57	MG	1A	3391	1/1	0.85	0.46	60,60,60,60	0
57	MG	2A	3291	1/1	0.85	0.22	75,75,75,75	0
57	MG	2A	3067	1/1	0.85	0.19	43,43,43,43	0
57	MG	2w	103	1/1	0.85	0.18	75,75,75,75	0
57	MG	1a	1664	1/1	0.85	0.14	73,73,73,73	0
57	MG	2a	1614	1/1	0.85	0.21	65,65,65,65	0
57	MG	2A	3296	1/1	0.85	0.24	64,64,64,64	0
57	MG	1A	3327	1/1	0.85	0.18	44,44,44,44	0
60	ZN	14	501	1/1	0.85	0.05	106,106,106,106	0
57	MG	1A	3512	1/1	0.86	0.60	58,58,58,58	0
57	MG	1A	3981	1/1	0.86	0.13	75,75,75,75	0
57	MG	2a	1642	1/1	0.86	0.22	83,83,83,83	0
57	MG	1A	3292	1/1	0.86	0.18	59,59,59,59	0
57	MG	1A	3199	1/1	0.86	0.60	39,39,39,39	0
57	MG	2A	3178	1/1	0.86	0.12	60,60,60,60	0
57	MG	2A	3442	1/1	0.86	0.30	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3745	1/1	0.86	0.12	65,65,65,65	0
57	MG	1a	1708	1/1	0.86	0.16	68,68,68,68	0
57	MG	2A	3038	1/1	0.86	0.22	61,61,61,61	0
57	MG	1a	1709	1/1	0.86	0.29	77,77,77,77	0
57	MG	1A	3992	1/1	0.86	0.20	32,32,32,32	0
57	MG	1A	3366	1/1	0.86	0.22	48,48,48,48	0
57	MG	1A	3337	1/1	0.86	0.17	47,47,47,47	0
57	MG	2A	3189	1/1	0.86	0.54	62,62,62,62	0
57	MG	2A	3048	1/1	0.86	0.16	67,67,67,67	0
57	MG	2a	1666	1/1	0.86	0.14	59,59,59,59	0
57	MG	2A	3049	1/1	0.86	0.18	52,52,52,52	0
57	MG	1A	3623	1/1	0.86	0.20	64,64,64,64	0
57	MG	2A	3055	1/1	0.86	0.15	66,66,66,66	0
57	MG	1A	3761	1/1	0.86	0.21	29,29,29,29	0
57	MG	1B	221	1/1	0.86	0.24	64,64,64,64	0
57	MG	1A	3488	1/1	0.86	0.28	41,41,41,41	0
57	MG	2A	3204	1/1	0.86	0.13	64,64,64,64	0
57	MG	1a	1606	1/1	0.86	0.19	73,73,73,73	0
57	MG	1a	1611	1/1	0.86	0.17	70,70,70,70	0
57	MG	2A	3065	1/1	0.86	0.23	75,75,75,75	0
57	MG	1a	1732	1/1	0.86	0.15	49,49,49,49	0
57	MG	2A	3529	1/1	0.86	0.15	52,52,52,52	0
57	MG	2A	3536	1/1	0.86	0.16	63,63,63,63	0
57	MG	1a	1614	1/1	0.86	0.17	63,63,63,63	0
57	MG	2A	3559	1/1	0.86	0.24	48,48,48,48	0
57	MG	1A	3898	1/1	0.86	0.10	45,45,45,45	0
57	MG	1A	3178	1/1	0.86	0.21	29,29,29,29	0
57	MG	1B	230	1/1	0.86	0.26	73,73,73,73	0
57	MG	1A	3269	1/1	0.86	0.24	63,63,63,63	0
57	MG	1A	4012	1/1	0.86	0.19	53,53,53,53	0
57	MG	2a	1714	1/1	0.86	0.25	71,71,71,71	0
57	MG	1A	3639	1/1	0.86	0.23	62,62,62,62	0
57	MG	1A	3468	1/1	0.86	0.17	50,50,50,50	0
57	MG	2A	3347	1/1	0.86	0.41	68,68,68,68	0
57	MG	1A	4022	1/1	0.86	0.38	84,84,84,84	0
57	MG	2A	3092	1/1	0.86	0.15	40,40,40,40	0
57	MG	1A	3495	1/1	0.86	0.33	63,63,63,63	0
57	MG	2A	3631	1/1	0.86	0.19	46,46,46,46	0
57	MG	1F	306	1/1	0.86	0.16	36,36,36,36	0
57	MG	1A	3646	1/1	0.86	0.15	64,64,64,64	0
57	MG	1N	201	1/1	0.86	0.22	44,44,44,44	0
57	MG	2a	1731	1/1	0.86	0.20	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1O	202	1/1	0.86	0.15	66,66,66,66	0
57	MG	1A	3496	1/1	0.86	0.22	50,50,50,50	0
57	MG	2a	1741	1/1	0.86	0.35	62,62,62,62	0
57	MG	1A	3270	1/1	0.86	0.37	53,53,53,53	0
57	MG	1A	3806	1/1	0.86	0.24	70,70,70,70	0
57	MG	1A	4034	1/1	0.86	0.13	45,45,45,45	0
57	MG	2A	3662	1/1	0.86	0.15	70,70,70,70	0
57	MG	2a	1761	1/1	0.86	0.14	70,70,70,70	0
57	MG	2a	1763	1/1	0.86	0.11	74,74,74,74	0
57	MG	2A	3113	1/1	0.86	0.10	60,60,60,60	0
57	MG	1A	3248	1/1	0.86	0.32	68,68,68,68	0
57	MG	1A	3942	1/1	0.86	0.07	43,43,43,43	0
57	MG	1A	3501	1/1	0.86	0.15	61,61,61,61	0
57	MG	1A	4044	1/1	0.86	0.14	57,57,57,57	0
57	MG	1A	4047	1/1	0.86	0.11	42,42,42,42	0
57	MG	1A	3502	1/1	0.86	0.10	66,66,66,66	0
57	MG	2a	1788	1/1	0.86	0.13	77,77,77,77	0
57	MG	1A	3504	1/1	0.86	0.25	37,37,37,37	0
57	MG	25	104	1/1	0.86	0.19	51,51,51,51	0
57	MG	1A	3835	1/1	0.86	0.26	71,71,71,71	0
57	MG	2a	1798	1/1	0.86	0.14	81,81,81,81	0
57	MG	1V	202	1/1	0.86	0.19	31,31,31,31	0
57	MG	2A	3687	1/1	0.86	0.13	78,78,78,78	0
57	MG	2a	1604	1/1	0.86	0.30	65,65,65,65	0
57	MG	2A	3384	1/1	0.86	0.31	65,65,65,65	0
57	MG	1A	4052	1/1	0.86	0.21	50,50,50,50	0
57	MG	1A	3218	1/1	0.86	0.47	46,46,46,46	0
57	MG	1A	3959	1/1	0.86	0.20	43,43,43,43	0
57	MG	2a	1818	1/1	0.86	0.24	87,87,87,87	0
57	MG	1A	3711	1/1	0.86	0.09	67,67,67,67	0
57	MG	2a	1824	1/1	0.86	0.14	71,71,71,71	0
57	MG	2A	3274	1/1	0.86	0.35	77,77,77,77	0
57	MG	1A	3965	1/1	0.86	0.15	45,45,45,45	0
57	MG	1A	3969	1/1	0.86	0.31	52,52,52,52	0
57	MG	1A	4072	1/1	0.86	0.27	47,47,47,47	0
57	MG	1x	110	1/1	0.86	0.29	63,63,63,63	0
57	MG	1A	3029	1/1	0.86	0.20	38,38,38,38	0
57	MG	2A	3165	1/1	0.86	0.16	64,64,64,64	0
57	MG	1a	1692	1/1	0.86	0.26	86,86,86,86	0
57	MG	2x	101	1/1	0.86	0.09	60,60,60,60	0
57	MG	1A	3385	1/1	0.86	0.34	38,38,38,38	0
57	MG	2A	3288	1/1	0.86	0.12	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3863	1/1	0.86	0.15	34,34,34,34	0
57	MG	1a	1698	1/1	0.86	0.21	48,48,48,48	0
60	ZN	24	501	1/1	0.86	0.05	117,117,117,117	0
57	MG	1A	3987	1/1	0.87	0.11	52,52,52,52	0
57	MG	1a	1739	1/1	0.87	0.12	65,65,65,65	0
57	MG	2A	3430	1/1	0.87	0.12	51,51,51,51	0
57	MG	1a	1645	1/1	0.87	0.33	60,60,60,60	0
57	MG	1A	3406	1/1	0.87	0.36	37,37,37,37	0
57	MG	1A	3994	1/1	0.87	0.25	65,65,65,65	0
57	MG	1A	3018	1/1	0.87	0.18	33,33,33,33	0
57	MG	1a	1780	1/1	0.87	0.08	80,80,80,80	0
57	MG	1A	3779	1/1	0.87	0.39	68,68,68,68	0
57	MG	1A	3054	1/1	0.87	0.15	43,43,43,43	0
57	MG	1a	1659	1/1	0.87	0.18	78,78,78,78	0
57	MG	2A	3453	1/1	0.87	0.22	79,79,79,79	0
57	MG	2A	3741	1/1	0.87	0.17	67,67,67,67	0
57	MG	1A	3782	1/1	0.87	0.21	43,43,43,43	0
57	MG	2A	3312	1/1	0.87	0.53	76,76,76,76	0
57	MG	1a	1662	1/1	0.87	0.13	74,74,74,74	0
57	MG	2A	3208	1/1	0.87	0.16	68,68,68,68	0
57	MG	2a	1657	1/1	0.87	0.13	86,86,86,86	0
57	MG	1A	4000	1/1	0.87	0.12	46,46,46,46	0
57	MG	2A	3086	1/1	0.87	0.17	73,73,73,73	0
57	MG	1A	4001	1/1	0.87	0.25	46,46,46,46	0
57	MG	2A	3320	1/1	0.87	0.17	64,64,64,64	0
57	MG	2A	3213	1/1	0.87	0.79	54,54,54,54	0
57	MG	1B	204	1/1	0.87	0.30	62,62,62,62	0
57	MG	1A	3445	1/1	0.87	0.17	53,53,53,53	0
57	MG	2A	3217	1/1	0.87	0.24	58,58,58,58	0
57	MG	1B	208	1/1	0.87	0.27	62,62,62,62	0
57	MG	2a	1672	1/1	0.87	0.23	65,65,65,65	0
57	MG	2A	3795	1/1	0.87	0.17	50,50,50,50	0
57	MG	1A	3668	1/1	0.87	0.14	42,42,42,42	0
57	MG	1a	1673	1/1	0.87	0.53	68,68,68,68	0
57	MG	1e	202	1/1	0.87	0.16	53,53,53,53	0
57	MG	2A	3802	1/1	0.87	0.10	64,64,64,64	0
57	MG	1a	1674	1/1	0.87	0.16	75,75,75,75	0
57	MG	1A	3058	1/1	0.87	0.15	42,42,42,42	0
57	MG	1a	1676	1/1	0.87	0.12	70,70,70,70	0
57	MG	1A	3679	1/1	0.87	0.17	30,30,30,30	0
57	MG	1a	1678	1/1	0.87	0.20	65,65,65,65	0
57	MG	2A	3543	1/1	0.87	0.13	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3109	1/1	0.87	0.14	60,60,60,60	0
57	MG	1A	3921	1/1	0.87	0.13	41,41,41,41	0
57	MG	2a	1704	1/1	0.87	0.16	72,72,72,72	0
57	MG	1A	3682	1/1	0.87	0.18	44,44,44,44	0
57	MG	2A	3828	1/1	0.87	0.13	66,66,66,66	0
57	MG	1A	3926	1/1	0.87	0.17	32,32,32,32	0
57	MG	1w	106	1/1	0.87	0.19	73,73,73,73	0
57	MG	2A	3838	1/1	0.87	0.10	59,59,59,59	0
57	MG	1A	3301	1/1	0.87	0.29	61,61,61,61	0
57	MG	2A	3586	1/1	0.87	0.14	69,69,69,69	0
57	MG	2A	3589	1/1	0.87	0.11	42,42,42,42	0
57	MG	2A	3593	1/1	0.87	0.09	67,67,67,67	0
57	MG	2A	3355	1/1	0.87	0.20	61,61,61,61	0
57	MG	2A	3603	1/1	0.87	0.10	46,46,46,46	0
57	MG	1A	3693	1/1	0.87	0.23	50,50,50,50	0
57	MG	2B	202	1/1	0.87	0.11	64,64,64,64	0
57	MG	1A	3809	1/1	0.87	0.17	49,49,49,49	0
57	MG	2B	205	1/1	0.87	0.15	68,68,68,68	0
57	MG	1A	3089	1/1	0.87	0.28	37,37,37,37	0
57	MG	2B	210	1/1	0.87	0.15	75,75,75,75	0
57	MG	2A	3360	1/1	0.87	0.19	47,47,47,47	0
57	MG	2a	1742	1/1	0.87	0.23	65,65,65,65	0
57	MG	1A	3102	1/1	0.87	0.11	60,60,60,60	0
57	MG	2B	216	1/1	0.87	0.12	64,64,64,64	0
57	MG	1A	3584	1/1	0.87	0.20	40,40,40,40	0
57	MG	1A	3492	1/1	0.87	0.26	39,39,39,39	0
57	MG	2E	301	1/1	0.87	0.23	61,61,61,61	0
57	MG	2A	3634	1/1	0.87	0.14	62,62,62,62	0
57	MG	2E	307	1/1	0.87	0.10	60,60,60,60	0
57	MG	2E	308	1/1	0.87	0.21	39,39,39,39	0
57	MG	1A	3164	1/1	0.87	0.12	58,58,58,58	0
57	MG	2a	1769	1/1	0.87	0.26	83,83,83,83	0
57	MG	2F	306	1/1	0.87	0.26	50,50,50,50	0
57	MG	1A	3465	1/1	0.87	0.24	52,52,52,52	0
57	MG	1A	4040	1/1	0.87	0.13	58,58,58,58	0
57	MG	1A	3595	1/1	0.87	0.36	37,37,37,37	0
57	MG	1G	203	1/1	0.87	0.21	59,59,59,59	0
57	MG	2A	3659	1/1	0.87	0.10	59,59,59,59	0
57	MG	1A	3400	1/1	0.87	0.57	49,49,49,49	0
57	MG	2W	202	1/1	0.87	0.23	43,43,43,43	0
57	MG	1A	3313	1/1	0.87	0.32	54,54,54,54	0
57	MG	1a	1620	1/1	0.87	0.20	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1621	1/1	0.87	0.30	77,77,77,77	0
57	MG	2A	3164	1/1	0.87	0.14	46,46,46,46	0
57	MG	2A	3027	1/1	0.87	0.21	63,63,63,63	0
57	MG	1A	3538	1/1	0.87	0.34	54,54,54,54	0
57	MG	2a	1813	1/1	0.87	0.18	74,74,74,74	0
57	MG	1a	1719	1/1	0.87	0.21	56,56,56,56	0
57	MG	1A	3212	1/1	0.87	0.47	54,54,54,54	0
57	MG	1a	1626	1/1	0.87	0.25	64,64,64,64	0
57	MG	2a	1821	1/1	0.87	0.10	75,75,75,75	0
57	MG	1A	3133	1/1	0.87	0.17	40,40,40,40	0
57	MG	2A	3390	1/1	0.87	0.23	68,68,68,68	0
57	MG	2A	3171	1/1	0.87	0.19	61,61,61,61	0
57	MG	1A	3746	1/1	0.87	0.22	42,42,42,42	0
57	MG	2e	201	1/1	0.87	0.13	72,72,72,72	0
57	MG	2A	3395	1/1	0.87	0.43	71,71,71,71	0
57	MG	2a	1608	1/1	0.87	0.25	75,75,75,75	0
57	MG	1A	3759	1/1	0.87	0.20	26,26,26,26	0
57	MG	1A	4054	1/1	0.87	0.17	55,55,55,55	0
57	MG	2A	3408	1/1	0.87	0.27	64,64,64,64	0
57	MG	1A	3259	1/1	0.87	0.20	28,28,28,28	0
57	MG	2A	3050	1/1	0.87	0.12	61,61,61,61	0
57	MG	1A	4062	1/1	0.87	0.11	53,53,53,53	0
57	MG	2A	3182	1/1	0.87	0.15	66,66,66,66	0
57	MG	2a	1619	1/1	0.87	0.12	74,74,74,74	0
57	MG	1A	3550	1/1	0.87	0.48	53,53,53,53	0
57	MG	2A	3422	1/1	0.87	0.32	66,66,66,66	0
57	MG	1l	202	1/1	0.88	0.20	68,68,68,68	0
57	MG	2A	3457	1/1	0.88	0.26	72,72,72,72	0
57	MG	2a	1634	1/1	0.88	0.24	70,70,70,70	0
57	MG	1A	3517	1/1	0.88	0.13	49,49,49,49	0
57	MG	1A	3414	1/1	0.88	0.22	62,62,62,62	0
57	MG	2A	3216	1/1	0.88	0.15	64,64,64,64	0
57	MG	2a	1639	1/1	0.88	0.10	67,67,67,67	0
57	MG	2A	3470	1/1	0.88	0.19	64,64,64,64	0
57	MG	1A	3814	1/1	0.88	0.16	65,65,65,65	0
57	MG	2A	3748	1/1	0.88	0.13	66,66,66,66	0
57	MG	1w	102	1/1	0.88	0.23	74,74,74,74	0
57	MG	1A	3276	1/1	0.88	0.19	39,39,39,39	0
57	MG	2A	3327	1/1	0.88	0.27	71,71,71,71	0
57	MG	2A	3221	1/1	0.88	0.18	63,63,63,63	0
57	MG	2A	3760	1/1	0.88	0.17	62,62,62,62	0
57	MG	2A	3481	1/1	0.88	0.18	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3709	1/1	0.88	0.15	58,58,58,58	0
57	MG	1a	1691	1/1	0.88	0.29	78,78,78,78	0
57	MG	1A	3710	1/1	0.88	0.30	59,59,59,59	0
57	MG	2A	3778	1/1	0.88	0.13	79,79,79,79	0
57	MG	2A	3779	1/1	0.88	0.06	62,62,62,62	0
57	MG	1A	3388	1/1	0.88	0.31	47,47,47,47	0
57	MG	2A	3497	1/1	0.88	0.25	49,49,49,49	0
57	MG	1A	3957	1/1	0.88	0.13	56,56,56,56	0
57	MG	2A	3501	1/1	0.88	0.37	69,69,69,69	0
57	MG	2A	3506	1/1	0.88	0.10	74,74,74,74	0
57	MG	1x	102	1/1	0.88	0.20	52,52,52,52	0
57	MG	1E	308	1/1	0.88	0.19	30,30,30,30	0
57	MG	1A	3335	1/1	0.88	0.17	63,63,63,63	0
57	MG	1A	3960	1/1	0.88	0.18	38,38,38,38	0
57	MG	1A	3594	1/1	0.88	0.40	59,59,59,59	0
57	MG	1A	4045	1/1	0.88	0.14	64,64,64,64	0
57	MG	1A	3964	1/1	0.88	0.14	53,53,53,53	0
57	MG	2A	3550	1/1	0.88	0.11	56,56,56,56	0
57	MG	2A	3247	1/1	0.88	0.14	61,61,61,61	0
57	MG	2A	3353	1/1	0.88	0.15	73,73,73,73	0
57	MG	2A	3564	1/1	0.88	0.07	52,52,52,52	0
57	MG	2a	1696	1/1	0.88	0.16	56,56,56,56	0
57	MG	2A	3248	1/1	0.88	0.12	71,71,71,71	0
57	MG	2A	3820	1/1	0.88	0.09	47,47,47,47	0
57	MG	2A	3250	1/1	0.88	0.29	68,68,68,68	0
57	MG	1x	111	1/1	0.88	0.20	65,65,65,65	0
57	MG	2A	3581	1/1	0.88	0.10	61,61,61,61	0
57	MG	2A	3582	1/1	0.88	0.20	69,69,69,69	0
57	MG	2A	3584	1/1	0.88	0.17	67,67,67,67	0
57	MG	1A	3107	1/1	0.88	0.15	30,30,30,30	0
57	MG	1A	3860	1/1	0.88	0.27	47,47,47,47	0
57	MG	2A	3847	1/1	0.88	0.17	47,47,47,47	0
57	MG	2a	1717	1/1	0.88	0.14	63,63,63,63	0
57	MG	1A	3608	1/1	0.88	0.18	43,43,43,43	0
57	MG	2A	3144	1/1	0.88	0.26	45,45,45,45	0
57	MG	1P	205	1/1	0.88	0.24	55,55,55,55	0
57	MG	2A	3150	1/1	0.88	0.34	54,54,54,54	0
57	MG	2a	1723	1/1	0.88	0.39	66,66,66,66	0
57	MG	2A	3862	1/1	0.88	0.15	65,65,65,65	0
57	MG	1Q	203	1/1	0.88	0.26	47,47,47,47	0
57	MG	2A	3261	1/1	0.88	0.18	53,53,53,53	0
57	MG	1A	3393	1/1	0.88	0.23	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3317	1/1	0.88	0.20	49,49,49,49	0
57	MG	2B	208	1/1	0.88	0.13	65,65,65,65	0
57	MG	1A	3532	1/1	0.88	0.18	79,79,79,79	0
57	MG	1A	3628	1/1	0.88	0.11	21,21,21,21	0
57	MG	1A	3497	1/1	0.88	0.22	45,45,45,45	0
57	MG	2A	3378	1/1	0.88	0.36	69,69,69,69	0
57	MG	2A	3030	1/1	0.88	0.15	45,45,45,45	0
57	MG	1a	1726	1/1	0.88	0.21	47,47,47,47	0
57	MG	2A	3270	1/1	0.88	0.20	73,73,73,73	0
57	MG	2a	1748	1/1	0.88	0.13	70,70,70,70	0
57	MG	1A	3397	1/1	0.88	0.31	32,32,32,32	0
57	MG	2a	1757	1/1	0.88	0.08	50,50,50,50	0
57	MG	1A	3399	1/1	0.88	0.18	55,55,55,55	0
57	MG	1A	3888	1/1	0.88	0.21	32,32,32,32	0
57	MG	1a	1650	1/1	0.88	0.12	77,77,77,77	0
57	MG	1A	3197	1/1	0.88	0.44	58,58,58,58	0
57	MG	1U	202	1/1	0.88	0.30	42,42,42,42	0
57	MG	2G	201	1/1	0.88	0.21	81,81,81,81	0
57	MG	2O	201	1/1	0.88	0.20	57,57,57,57	0
57	MG	1A	3891	1/1	0.88	0.15	34,34,34,34	0
57	MG	2Q	203	1/1	0.88	0.17	46,46,46,46	0
57	MG	1a	1752	1/1	0.88	0.28	62,62,62,62	0
57	MG	2A	3177	1/1	0.88	0.23	61,61,61,61	0
57	MG	2A	3393	1/1	0.88	0.18	67,67,67,67	0
57	MG	1A	3255	1/1	0.88	0.47	57,57,57,57	0
57	MG	1A	3377	1/1	0.88	0.29	40,40,40,40	0
57	MG	2A	3676	1/1	0.88	0.50	65,65,65,65	0
57	MG	1a	1769	1/1	0.88	0.15	55,55,55,55	0
57	MG	20	102	1/1	0.88	0.12	68,68,68,68	0
57	MG	1A	3092	1/1	0.88	0.20	49,49,49,49	0
57	MG	2a	1805	1/1	0.88	0.12	71,71,71,71	0
57	MG	1A	3310	1/1	0.88	0.26	45,45,45,45	0
57	MG	1A	3151	1/1	0.88	0.46	43,43,43,43	0
57	MG	1a	1784	1/1	0.88	0.08	81,81,81,81	0
57	MG	2A	3688	1/1	0.88	0.11	59,59,59,59	0
57	MG	2A	3416	1/1	0.88	0.30	60,60,60,60	0
57	MG	1A	3511	1/1	0.88	0.15	60,60,60,60	0
57	MG	2A	3694	1/1	0.88	0.20	59,59,59,59	0
57	MG	1A	3790	1/1	0.88	0.14	48,48,48,48	0
57	MG	1A	3795	1/1	0.88	0.20	28,28,28,28	0
57	MG	1A	3567	1/1	0.88	0.12	54,54,54,54	0
57	MG	2A	3425	1/1	0.88	0.16	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3273	1/1	0.88	0.13	41,41,41,41	0
57	MG	2A	3194	1/1	0.88	0.22	58,58,58,58	0
57	MG	1B	211	1/1	0.88	0.17	54,54,54,54	0
57	MG	2A	3708	1/1	0.88	0.13	71,71,71,71	0
57	MG	1l	103	1/1	0.88	0.11	67,67,67,67	0
57	MG	2w	102	1/1	0.88	0.34	71,71,71,71	0
57	MG	1A	4014	1/1	0.88	0.22	28,28,28,28	0
57	MG	1B	214	1/1	0.88	0.14	55,55,55,55	0
57	MG	2A	3202	1/1	0.88	0.22	61,61,61,61	0
57	MG	1A	3684	1/1	0.88	0.37	81,81,81,81	0
57	MG	1A	3571	1/1	0.88	0.23	41,41,41,41	0
57	MG	2x	104	1/1	0.88	0.14	69,69,69,69	0
57	MG	1A	3486	1/1	0.88	0.24	43,43,43,43	0
58	K	1A	3570	1/1	0.88	0.14	58,58,58,58	0
57	MG	1a	1680	1/1	0.88	0.21	74,74,74,74	0
60	ZN	2Y	202	1/1	0.88	0.18	89,89,89,89	0
57	MG	1B	222	1/1	0.88	0.24	59,59,59,59	0
57	MG	2A	3740	1/1	0.89	0.07	52,52,52,52	0
57	MG	1A	3924	1/1	0.89	0.19	51,51,51,51	0
57	MG	1A	3305	1/1	0.89	0.34	52,52,52,52	0
57	MG	2A	3477	1/1	0.89	0.20	68,68,68,68	0
57	MG	2A	3479	1/1	0.89	0.13	52,52,52,52	0
57	MG	1A	3813	1/1	0.89	0.20	32,32,32,32	0
57	MG	1A	3546	1/1	0.89	0.32	61,61,61,61	0
57	MG	2A	3080	1/1	0.89	0.13	61,61,61,61	0
57	MG	1a	1794	1/1	0.89	0.09	73,73,73,73	0
57	MG	2A	3490	1/1	0.89	0.28	63,63,63,63	0
57	MG	1A	3825	1/1	0.89	0.19	55,55,55,55	0
57	MG	1A	3548	1/1	0.89	0.30	26,26,26,26	0
57	MG	1a	1802	1/1	0.89	0.13	70,70,70,70	0
57	MG	10	107	1/1	0.89	0.12	61,61,61,61	0
57	MG	1a	1807	1/1	0.89	0.04	64,64,64,64	0
57	MG	2A	3502	1/1	0.89	0.17	69,69,69,69	0
57	MG	1a	1808	1/1	0.89	0.12	56,56,56,56	0
57	MG	1A	3361	1/1	0.89	0.36	74,74,74,74	0
57	MG	2A	3228	1/1	0.89	0.21	46,46,46,46	0
57	MG	1A	3833	1/1	0.89	0.11	38,38,38,38	0
57	MG	1A	3948	1/1	0.89	0.12	40,40,40,40	0
57	MG	2A	3530	1/1	0.89	0.11	43,43,43,43	0
57	MG	1a	1826	1/1	0.89	0.16	62,62,62,62	0
57	MG	1A	4029	1/1	0.89	0.13	69,69,69,69	0
57	MG	1B	223	1/1	0.89	0.26	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1677	1/1	0.89	0.20	67,67,67,67	0
57	MG	2A	3805	1/1	0.89	0.10	56,56,56,56	0
57	MG	2A	3548	1/1	0.89	0.18	54,54,54,54	0
57	MG	1A	3060	1/1	0.89	0.24	38,38,38,38	0
57	MG	2A	3551	1/1	0.89	0.08	52,52,52,52	0
57	MG	2A	3236	1/1	0.89	0.27	68,68,68,68	0
57	MG	2A	3108	1/1	0.89	0.13	50,50,50,50	0
57	MG	2A	3240	1/1	0.89	0.52	65,65,65,65	0
57	MG	1A	3184	1/1	0.89	0.28	58,58,58,58	0
57	MG	1n	101	1/1	0.89	0.26	64,64,64,64	0
57	MG	2A	3819	1/1	0.89	0.10	58,58,58,58	0
57	MG	2a	1697	1/1	0.89	0.23	68,68,68,68	0
57	MG	2A	3569	1/1	0.89	0.11	38,38,38,38	0
57	MG	2A	3821	1/1	0.89	0.12	40,40,40,40	0
57	MG	2A	3362	1/1	0.89	0.10	70,70,70,70	0
57	MG	2A	3575	1/1	0.89	0.19	43,43,43,43	0
57	MG	1n	102	1/1	0.89	0.15	62,62,62,62	0
57	MG	18	101	1/1	0.89	0.57	60,60,60,60	0
57	MG	2A	3117	1/1	0.89	0.38	52,52,52,52	0
57	MG	2a	1709	1/1	0.89	0.14	76,76,76,76	0
57	MG	1A	3453	1/1	0.89	0.28	45,45,45,45	0
57	MG	1A	3842	1/1	0.89	0.14	52,52,52,52	0
57	MG	1A	3007	1/1	0.89	0.18	40,40,40,40	0
57	MG	2A	3592	1/1	0.89	0.09	75,75,75,75	0
57	MG	2A	3852	1/1	0.89	0.14	51,51,51,51	0
57	MG	1A	3555	1/1	0.89	0.18	58,58,58,58	0
57	MG	1A	3859	1/1	0.89	0.12	52,52,52,52	0
57	MG	1A	3225	1/1	0.89	0.32	51,51,51,51	0
57	MG	2A	3376	1/1	0.89	0.27	53,53,53,53	0
57	MG	2B	201	1/1	0.89	0.09	82,82,82,82	0
57	MG	1A	3752	1/1	0.89	0.10	38,38,38,38	0
57	MG	1A	3659	1/1	0.89	0.20	26,26,26,26	0
57	MG	1A	3121	1/1	0.89	0.24	46,46,46,46	0
57	MG	1F	305	1/1	0.89	0.30	33,33,33,33	0
57	MG	2B	207	1/1	0.89	0.21	70,70,70,70	0
57	MG	1A	3026	1/1	0.89	0.16	73,73,73,73	0
57	MG	1A	3975	1/1	0.89	0.10	60,60,60,60	0
57	MG	2a	1740	1/1	0.89	0.28	70,70,70,70	0
57	MG	1a	1618	1/1	0.89	0.13	60,60,60,60	0
57	MG	1A	3426	1/1	0.89	0.12	56,56,56,56	0
57	MG	1A	3769	1/1	0.89	0.09	65,65,65,65	0
57	MG	1N	202	1/1	0.89	0.23	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2B	220	1/1	0.89	0.15	73,73,73,73	0
57	MG	1A	3087	1/1	0.89	0.24	34,34,34,34	0
57	MG	2a	1749	1/1	0.89	0.12	62,62,62,62	0
57	MG	2a	1750	1/1	0.89	0.07	87,87,87,87	0
57	MG	2A	3653	1/1	0.89	0.56	70,70,70,70	0
57	MG	1A	3774	1/1	0.89	0.13	47,47,47,47	0
57	MG	1P	202	1/1	0.89	0.24	36,36,36,36	0
57	MG	2A	3004	1/1	0.89	0.25	61,61,61,61	0
57	MG	1a	1717	1/1	0.89	0.28	71,71,71,71	0
57	MG	1A	4061	1/1	0.89	0.21	49,49,49,49	0
57	MG	1A	3074	1/1	0.89	0.23	27,27,27,27	0
57	MG	2A	3401	1/1	0.89	0.34	53,53,53,53	0
57	MG	1Q	204	1/1	0.89	0.25	62,62,62,62	0
57	MG	1a	1632	1/1	0.89	0.20	61,61,61,61	0
57	MG	1a	1633	1/1	0.89	0.18	31,31,31,31	0
57	MG	2a	1777	1/1	0.89	0.11	75,75,75,75	0
57	MG	2a	1779	1/1	0.89	0.16	67,67,67,67	0
57	MG	1A	3471	1/1	0.89	0.29	35,35,35,35	0
57	MG	2T	3501	1/1	0.89	0.14	71,71,71,71	0
57	MG	1A	3132	1/1	0.89	0.35	43,43,43,43	0
57	MG	2A	3677	1/1	0.89	0.22	65,65,65,65	0
57	MG	2U	201	1/1	0.89	0.30	63,63,63,63	0
57	MG	2a	1795	1/1	0.89	0.23	64,64,64,64	0
57	MG	1A	4069	1/1	0.89	0.11	50,50,50,50	0
57	MG	2A	3031	1/1	0.89	0.15	53,53,53,53	0
57	MG	2A	3684	1/1	0.89	0.18	43,43,43,43	0
57	MG	1a	1729	1/1	0.89	0.23	61,61,61,61	0
57	MG	1A	3687	1/1	0.89	0.22	39,39,39,39	0
57	MG	1a	1642	1/1	0.89	0.19	70,70,70,70	0
57	MG	2A	3292	1/1	0.89	0.12	59,59,59,59	0
57	MG	1A	3789	1/1	0.89	0.25	54,54,54,54	0
57	MG	2A	3428	1/1	0.89	0.09	77,77,77,77	0
57	MG	1a	1644	1/1	0.89	0.21	67,67,67,67	0
57	MG	1A	4073	1/1	0.89	0.15	20,20,20,20	0
57	MG	1A	3103	1/1	0.89	0.15	37,37,37,37	0
57	MG	1A	3535	1/1	0.89	0.29	58,58,58,58	0
57	MG	2A	3703	1/1	0.89	0.15	68,68,68,68	0
57	MG	1a	1753	1/1	0.89	0.25	60,60,60,60	0
57	MG	1A	3695	1/1	0.89	0.24	31,31,31,31	0
57	MG	2A	3437	1/1	0.89	0.20	60,60,60,60	0
57	MG	2A	3054	1/1	0.89	0.11	68,68,68,68	0
57	MG	2I	202	1/1	0.89	0.35	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3191	1/1	0.89	0.32	68,68,68,68	0
57	MG	2v	101	1/1	0.89	0.13	72,72,72,72	0
57	MG	1A	3040	1/1	0.89	0.39	61,61,61,61	0
57	MG	1a	1765	1/1	0.89	0.17	68,68,68,68	0
57	MG	2A	3057	1/1	0.89	0.20	58,58,58,58	0
57	MG	2A	3455	1/1	0.89	0.10	52,52,52,52	0
57	MG	2A	3059	1/1	0.89	0.11	43,43,43,43	0
57	MG	1A	3358	1/1	0.89	0.15	43,43,43,43	0
57	MG	2A	3462	1/1	0.89	0.17	61,61,61,61	0
57	MG	2A	3724	1/1	0.89	0.08	68,68,68,68	0
57	MG	1A	3601	1/1	0.89	0.20	35,35,35,35	0
57	MG	1A	3603	1/1	0.89	0.22	28,28,28,28	0
57	MG	1a	1782	1/1	0.89	0.10	91,91,91,91	0
57	MG	1B	206	1/1	0.89	0.38	49,49,49,49	0
57	MG	1a	1661	1/1	0.89	0.23	67,67,67,67	0
57	MG	1A	3505	1/1	0.89	0.25	31,31,31,31	0
57	MG	2A	3727	1/1	0.90	0.20	69,69,69,69	0
57	MG	1a	1705	1/1	0.90	0.27	55,55,55,55	0
57	MG	1A	3188	1/1	0.90	0.33	44,44,44,44	0
57	MG	2A	3002	1/1	0.90	0.38	52,52,52,52	0
57	MG	2A	3464	1/1	0.90	0.39	71,71,71,71	0
57	MG	1A	3363	1/1	0.90	0.11	43,43,43,43	0
57	MG	1A	3756	1/1	0.90	0.24	18,18,18,18	0
57	MG	1A	3288	1/1	0.90	0.07	54,54,54,54	0
57	MG	1A	3319	1/1	0.90	0.18	53,53,53,53	0
57	MG	1A	3887	1/1	0.90	0.09	45,45,45,45	0
57	MG	2A	3473	1/1	0.90	0.11	71,71,71,71	0
57	MG	2a	1646	1/1	0.90	0.16	63,63,63,63	0
57	MG	1A	3762	1/1	0.90	0.21	35,35,35,35	0
57	MG	2A	3176	1/1	0.90	0.26	69,69,69,69	0
57	MG	1A	3451	1/1	0.90	0.31	43,43,43,43	0
57	MG	2A	3025	1/1	0.90	0.27	47,47,47,47	0
57	MG	1A	3064	1/1	0.90	0.25	34,34,34,34	0
57	MG	1A	3895	1/1	0.90	0.18	39,39,39,39	0
57	MG	2A	3768	1/1	0.90	0.14	43,43,43,43	0
57	MG	2A	3484	1/1	0.90	0.13	62,62,62,62	0
57	MG	2A	3771	1/1	0.90	0.19	67,67,67,67	0
57	MG	1A	3291	1/1	0.90	0.23	54,54,54,54	0
57	MG	2A	3776	1/1	0.90	0.08	52,52,52,52	0
57	MG	2A	3317	1/1	0.90	0.10	51,51,51,51	0
57	MG	1A	3053	1/1	0.90	0.12	53,53,53,53	0
57	MG	2A	3034	1/1	0.90	0.27	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3655	1/1	0.90	0.25	59,59,59,59	0
57	MG	1B	233	1/1	0.90	0.14	57,57,57,57	0
57	MG	1A	4018	1/1	0.90	0.10	32,32,32,32	0
57	MG	1A	3254	1/1	0.90	0.26	59,59,59,59	0
57	MG	1A	3660	1/1	0.90	0.21	23,23,23,23	0
57	MG	2A	3326	1/1	0.90	0.28	48,48,48,48	0
57	MG	1A	3165	1/1	0.90	0.17	33,33,33,33	0
57	MG	1A	3227	1/1	0.90	0.24	43,43,43,43	0
57	MG	2A	3526	1/1	0.90	0.08	52,52,52,52	0
57	MG	2A	3329	1/1	0.90	0.25	56,56,56,56	0
57	MG	1A	3788	1/1	0.90	0.20	89,89,89,89	0
57	MG	2A	3196	1/1	0.90	0.27	58,58,58,58	0
57	MG	2A	3534	1/1	0.90	0.10	60,60,60,60	0
57	MG	1a	1627	1/1	0.90	0.25	59,59,59,59	0
57	MG	1A	3022	1/1	0.90	0.15	46,46,46,46	0
57	MG	2a	1698	1/1	0.90	0.14	64,64,64,64	0
57	MG	1A	3233	1/1	0.90	0.17	56,56,56,56	0
57	MG	1a	1630	1/1	0.90	0.23	70,70,70,70	0
57	MG	1F	310	1/1	0.90	0.19	55,55,55,55	0
57	MG	2a	1702	1/1	0.90	0.30	80,80,80,80	0
57	MG	1F	311	1/1	0.90	0.22	48,48,48,48	0
57	MG	2A	3206	1/1	0.90	0.20	58,58,58,58	0
57	MG	1A	3923	1/1	0.90	0.19	63,63,63,63	0
57	MG	2A	3827	1/1	0.90	0.09	61,61,61,61	0
57	MG	2a	1708	1/1	0.90	0.13	70,70,70,70	0
57	MG	2A	3563	1/1	0.90	0.29	64,64,64,64	0
57	MG	2A	3829	1/1	0.90	0.16	45,45,45,45	0
57	MG	2a	1713	1/1	0.90	0.25	80,80,80,80	0
57	MG	1G	204	1/1	0.90	0.28	55,55,55,55	0
57	MG	1A	3557	1/1	0.90	0.21	66,66,66,66	0
57	MG	1A	3565	1/1	0.90	0.27	36,36,36,36	0
57	MG	1a	1771	1/1	0.90	0.22	78,78,78,78	0
57	MG	1A	3261	1/1	0.90	0.19	33,33,33,33	0
57	MG	1a	1640	1/1	0.90	0.37	71,71,71,71	0
57	MG	1A	3929	1/1	0.90	0.11	41,41,41,41	0
57	MG	2A	3070	1/1	0.90	0.25	47,47,47,47	0
57	MG	1A	3510	1/1	0.90	0.19	65,65,65,65	0
57	MG	1A	3689	1/1	0.90	0.16	26,26,26,26	0
57	MG	2A	3074	1/1	0.90	0.38	47,47,47,47	0
57	MG	2A	3859	1/1	0.90	0.13	53,53,53,53	0
57	MG	1P	204	1/1	0.90	0.11	42,42,42,42	0
57	MG	2A	3861	1/1	0.90	0.70	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1646	1/1	0.90	0.13	66,66,66,66	0
57	MG	1A	3940	1/1	0.90	0.14	46,46,46,46	0
57	MG	1Q	202	1/1	0.90	0.23	36,36,36,36	0
57	MG	2A	3085	1/1	0.90	0.15	67,67,67,67	0
57	MG	1A	3386	1/1	0.90	0.15	52,52,52,52	0
57	MG	1A	3423	1/1	0.90	0.25	67,67,67,67	0
57	MG	1A	3424	1/1	0.90	0.26	40,40,40,40	0
57	MG	1a	1801	1/1	0.90	0.13	63,63,63,63	0
57	MG	1A	3812	1/1	0.90	0.31	72,72,72,72	0
57	MG	2A	3621	1/1	0.90	0.13	53,53,53,53	0
57	MG	2A	3094	1/1	0.90	0.13	74,74,74,74	0
57	MG	1a	1804	1/1	0.90	0.17	51,51,51,51	0
57	MG	2a	1756	1/1	0.90	0.10	75,75,75,75	0
57	MG	1A	3949	1/1	0.90	0.08	57,57,57,57	0
57	MG	1A	3048	1/1	0.90	0.26	24,24,24,24	0
57	MG	1A	3265	1/1	0.90	0.07	65,65,65,65	0
57	MG	1A	3817	1/1	0.90	0.10	49,49,49,49	0
57	MG	2E	302	1/1	0.90	0.17	61,61,61,61	0
57	MG	1a	1811	1/1	0.90	0.17	76,76,76,76	0
57	MG	2E	304	1/1	0.90	0.23	65,65,65,65	0
57	MG	1A	3956	1/1	0.90	0.15	45,45,45,45	0
57	MG	1A	3586	1/1	0.90	0.21	50,50,50,50	0
57	MG	1a	1821	1/1	0.90	0.06	60,60,60,60	0
57	MG	2a	1776	1/1	0.90	0.11	60,60,60,60	0
57	MG	1A	3131	1/1	0.90	0.14	70,70,70,70	0
57	MG	1A	3589	1/1	0.90	0.32	42,42,42,42	0
57	MG	2a	1781	1/1	0.90	0.26	88,88,88,88	0
57	MG	2a	1782	1/1	0.90	0.14	59,59,59,59	0
57	MG	2a	1785	1/1	0.90	0.12	80,80,80,80	0
57	MG	1A	4068	1/1	0.90	0.18	58,58,58,58	0
57	MG	2A	3664	1/1	0.90	0.22	67,67,67,67	0
57	MG	2P	202	1/1	0.90	0.18	66,66,66,66	0
57	MG	2a	1790	1/1	0.90	0.18	67,67,67,67	0
57	MG	1U	204	1/1	0.90	0.20	38,38,38,38	0
57	MG	2a	1793	1/1	0.90	0.20	67,67,67,67	0
57	MG	1A	3521	1/1	0.90	0.19	35,35,35,35	0
57	MG	1A	3962	1/1	0.90	0.16	24,24,24,24	0
57	MG	1A	3035	1/1	0.90	0.10	47,47,47,47	0
57	MG	2A	3397	1/1	0.90	0.18	44,44,44,44	0
57	MG	1A	3312	1/1	0.90	0.29	56,56,56,56	0
57	MG	1A	4074	1/1	0.90	0.12	43,43,43,43	0
57	MG	2A	3123	1/1	0.90	0.10	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1v	101	1/1	0.90	0.23	75,75,75,75	0
57	MG	2a	1808	1/1	0.90	0.31	77,77,77,77	0
57	MG	1A	3717	1/1	0.90	0.36	60,60,60,60	0
57	MG	2A	3129	1/1	0.90	0.24	78,78,78,78	0
57	MG	2A	3415	1/1	0.90	0.08	70,70,70,70	0
57	MG	2a	1816	1/1	0.90	0.22	74,74,74,74	0
57	MG	1A	3487	1/1	0.90	0.34	50,50,50,50	0
57	MG	1A	3724	1/1	0.90	0.28	76,76,76,76	0
57	MG	2A	3420	1/1	0.90	0.28	66,66,66,66	0
57	MG	1Y	202	1/1	0.90	0.11	64,64,64,64	0
57	MG	1A	3857	1/1	0.90	0.45	42,42,42,42	0
57	MG	1A	4089	1/1	0.90	0.16	42,42,42,42	0
57	MG	1A	3529	1/1	0.90	0.15	62,62,62,62	0
57	MG	1A	3241	1/1	0.90	0.19	37,37,37,37	0
57	MG	2i	201	1/1	0.90	0.16	77,77,77,77	0
57	MG	1A	3739	1/1	0.90	0.22	22,22,22,22	0
57	MG	2A	3151	1/1	0.90	0.13	55,55,55,55	0
57	MG	2q	201	1/1	0.90	0.20	77,77,77,77	0
57	MG	1A	3157	1/1	0.90	0.23	33,33,33,33	0
57	MG	2A	3153	1/1	0.90	0.39	43,43,43,43	0
57	MG	1A	3186	1/1	0.90	0.16	39,39,39,39	0
57	MG	1A	3534	1/1	0.90	0.18	52,52,52,52	0
57	MG	2A	3284	1/1	0.90	0.34	49,49,49,49	0
57	MG	15	104	1/1	0.90	0.23	39,39,39,39	0
57	MG	2A	3287	1/1	0.90	0.16	65,65,65,65	0
57	MG	1A	3866	1/1	0.90	0.17	46,46,46,46	0
57	MG	2A	3444	1/1	0.90	0.13	62,62,62,62	0
57	MG	2A	3160	1/1	0.90	0.16	55,55,55,55	0
57	MG	2A	3161	1/1	0.90	0.17	43,43,43,43	0
57	MG	2a	1622	1/1	0.90	0.13	81,81,81,81	0
57	MG	2A	3719	1/1	0.90	0.17	70,70,70,70	0
57	MG	2A	3162	1/1	0.90	0.33	60,60,60,60	0
57	MG	1A	3869	1/1	0.90	0.14	39,39,39,39	0
57	MG	17	103	1/1	0.90	0.17	37,37,37,37	0
57	MG	1W	203	1/1	0.91	0.28	50,50,50,50	0
57	MG	2A	3488	1/1	0.91	0.25	72,72,72,72	0
57	MG	1A	4011	1/1	0.91	0.11	71,71,71,71	0
57	MG	1X	102	1/1	0.91	0.21	38,38,38,38	0
57	MG	1A	3829	1/1	0.91	0.21	52,52,52,52	0
57	MG	1A	3256	1/1	0.91	0.20	30,30,30,30	0
57	MG	2A	3331	1/1	0.91	0.31	60,60,60,60	0
57	MG	2A	3766	1/1	0.91	0.07	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3207	1/1	0.91	0.24	67,67,67,67	0
57	MG	2A	3333	1/1	0.91	0.14	76,76,76,76	0
57	MG	1A	3322	1/1	0.91	0.26	55,55,55,55	0
57	MG	1A	4016	1/1	0.91	0.17	30,30,30,30	0
57	MG	2A	3511	1/1	0.91	0.18	42,42,42,42	0
57	MG	1a	1666	1/1	0.91	0.13	71,71,71,71	0
57	MG	1Z	302	1/1	0.91	0.21	65,65,65,65	0
57	MG	2A	3079	1/1	0.91	0.37	54,54,54,54	0
57	MG	2A	3341	1/1	0.91	0.17	64,64,64,64	0
57	MG	2A	3786	1/1	0.91	0.29	64,64,64,64	0
57	MG	2a	1668	1/1	0.91	0.21	55,55,55,55	0
57	MG	2A	3528	1/1	0.91	0.10	47,47,47,47	0
57	MG	10	101	1/1	0.91	0.17	43,43,43,43	0
57	MG	2A	3793	1/1	0.91	0.13	62,62,62,62	0
57	MG	10	103	1/1	0.91	0.21	51,51,51,51	0
57	MG	2a	1674	1/1	0.91	0.20	64,64,64,64	0
57	MG	1A	3832	1/1	0.91	0.18	31,31,31,31	0
57	MG	1A	3081	1/1	0.91	0.27	46,46,46,46	0
57	MG	1A	3936	1/1	0.91	0.14	40,40,40,40	0
57	MG	2a	1681	1/1	0.91	0.10	70,70,70,70	0
57	MG	11	101	1/1	0.91	1.67	48,48,48,48	0
57	MG	1a	1818	1/1	0.91	0.07	52,52,52,52	0
57	MG	2a	1688	1/1	0.91	0.26	74,74,74,74	0
57	MG	1a	1820	1/1	0.91	0.09	65,65,65,65	0
57	MG	1A	3390	1/1	0.91	0.15	45,45,45,45	0
57	MG	1A	3359	1/1	0.91	0.22	62,62,62,62	0
57	MG	1b	302	1/1	0.91	0.11	84,84,84,84	0
57	MG	2A	3562	1/1	0.91	0.18	45,45,45,45	0
57	MG	1A	3837	1/1	0.91	0.20	52,52,52,52	0
57	MG	1A	4028	1/1	0.91	0.14	66,66,66,66	0
57	MG	1f	202	1/1	0.91	0.26	75,75,75,75	0
57	MG	2A	3232	1/1	0.91	0.34	46,46,46,46	0
57	MG	1A	3751	1/1	0.91	0.21	23,23,23,23	0
57	MG	2A	3570	1/1	0.91	0.22	53,53,53,53	0
57	MG	15	106	1/1	0.91	0.20	72,72,72,72	0
57	MG	1A	3946	1/1	0.91	0.33	72,72,72,72	0
57	MG	2A	3576	1/1	0.91	0.16	50,50,50,50	0
57	MG	2A	3580	1/1	0.91	0.12	54,54,54,54	0
57	MG	1a	1684	1/1	0.91	0.20	55,55,55,55	0
57	MG	2A	3834	1/1	0.91	0.17	33,33,33,33	0
57	MG	1A	3841	1/1	0.91	0.13	71,71,71,71	0
57	MG	1A	3202	1/1	0.91	0.14	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3847	1/1	0.91	0.07	62,62,62,62	0
57	MG	1A	3558	1/1	0.91	0.13	61,61,61,61	0
57	MG	2A	3245	1/1	0.91	0.53	71,71,71,71	0
57	MG	2A	3590	1/1	0.91	0.19	67,67,67,67	0
57	MG	2A	3246	1/1	0.91	0.24	54,54,54,54	0
57	MG	1A	3856	1/1	0.91	0.13	52,52,52,52	0
57	MG	1A	3111	1/1	0.91	0.17	46,46,46,46	0
57	MG	1A	3428	1/1	0.91	0.31	53,53,53,53	0
57	MG	1A	3331	1/1	0.91	0.23	59,59,59,59	0
57	MG	1A	3958	1/1	0.91	0.18	57,57,57,57	0
57	MG	1a	1700	1/1	0.91	0.33	59,59,59,59	0
57	MG	1A	3664	1/1	0.91	0.18	33,33,33,33	0
57	MG	1A	3767	1/1	0.91	0.19	30,30,30,30	0
57	MG	2A	3127	1/1	0.91	0.23	53,53,53,53	0
57	MG	2A	3623	1/1	0.91	0.10	60,60,60,60	0
57	MG	2a	1735	1/1	0.91	0.28	63,63,63,63	0
57	MG	1F	313	1/1	0.91	0.13	35,35,35,35	0
57	MG	1F	314	1/1	0.91	0.14	55,55,55,55	0
57	MG	1A	3395	1/1	0.91	0.70	56,56,56,56	0
57	MG	1A	3569	1/1	0.91	0.38	58,58,58,58	0
57	MG	1A	3075	1/1	0.91	0.18	32,32,32,32	0
57	MG	2A	3644	1/1	0.91	0.27	47,47,47,47	0
57	MG	1A	3333	1/1	0.91	0.28	50,50,50,50	0
57	MG	2A	3394	1/1	0.91	0.32	61,61,61,61	0
57	MG	1A	3870	1/1	0.91	0.23	40,40,40,40	0
57	MG	2A	3146	1/1	0.91	0.17	57,57,57,57	0
57	MG	1A	4060	1/1	0.91	0.14	45,45,45,45	0
57	MG	2A	3149	1/1	0.91	0.28	68,68,68,68	0
57	MG	2a	1755	1/1	0.91	0.11	70,70,70,70	0
57	MG	1O	203	1/1	0.91	0.21	66,66,66,66	0
57	MG	1a	1624	1/1	0.91	0.14	59,59,59,59	0
57	MG	1A	3579	1/1	0.91	0.35	42,42,42,42	0
57	MG	1O	205	1/1	0.91	0.21	76,76,76,76	0
57	MG	1A	3368	1/1	0.91	0.20	48,48,48,48	0
57	MG	2a	1766	1/1	0.91	0.18	73,73,73,73	0
57	MG	1A	3369	1/1	0.91	0.21	57,57,57,57	0
57	MG	2A	3671	1/1	0.91	0.15	56,56,56,56	0
57	MG	2A	3276	1/1	0.91	0.23	61,61,61,61	0
57	MG	1A	4065	1/1	0.91	0.20	62,62,62,62	0
57	MG	2A	3010	1/1	0.91	0.13	66,66,66,66	0
57	MG	2P	201	1/1	0.91	0.21	60,60,60,60	0
57	MG	1A	3002	1/1	0.91	0.33	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2Q	201	1/1	0.91	0.12	49,49,49,49	0
57	MG	1A	3043	1/1	0.91	0.34	38,38,38,38	0
57	MG	2a	1780	1/1	0.91	0.17	60,60,60,60	0
57	MG	2A	3679	1/1	0.91	0.17	57,57,57,57	0
57	MG	2A	3680	1/1	0.91	0.18	67,67,67,67	0
57	MG	2A	3020	1/1	0.91	0.18	68,68,68,68	0
57	MG	2A	3023	1/1	0.91	0.23	71,71,71,71	0
57	MG	2A	3283	1/1	0.91	0.12	61,61,61,61	0
57	MG	1A	3493	1/1	0.91	0.24	47,47,47,47	0
57	MG	1A	3336	1/1	0.91	0.16	49,49,49,49	0
57	MG	1A	3984	1/1	0.91	0.13	66,66,66,66	0
57	MG	1A	3152	1/1	0.91	0.32	44,44,44,44	0
57	MG	1A	3409	1/1	0.91	0.27	43,43,43,43	0
57	MG	1A	3412	1/1	0.91	0.14	45,45,45,45	0
57	MG	1A	3253	1/1	0.91	0.20	51,51,51,51	0
57	MG	2A	3696	1/1	0.91	0.08	70,70,70,70	0
57	MG	1a	1641	1/1	0.91	0.23	73,73,73,73	0
57	MG	2a	1801	1/1	0.91	0.19	75,75,75,75	0
57	MG	1a	1754	1/1	0.91	0.13	54,54,54,54	0
57	MG	2A	3441	1/1	0.91	0.29	64,64,64,64	0
57	MG	2A	3040	1/1	0.91	0.31	65,65,65,65	0
57	MG	2a	1807	1/1	0.91	0.22	67,67,67,67	0
57	MG	2A	3443	1/1	0.91	0.34	50,50,50,50	0
57	MG	28	102	1/1	0.91	0.23	54,54,54,54	0
57	MG	1a	1760	1/1	0.91	0.12	63,63,63,63	0
57	MG	2a	1603	1/1	0.91	0.12	83,83,83,83	0
57	MG	1A	3460	1/1	0.91	0.42	57,57,57,57	0
57	MG	2A	3298	1/1	0.91	0.10	63,63,63,63	0
57	MG	1A	3604	1/1	0.91	0.14	42,42,42,42	0
57	MG	2a	1820	1/1	0.91	0.25	69,69,69,69	0
57	MG	1A	3714	1/1	0.91	0.13	63,63,63,63	0
57	MG	1A	4095	1/1	0.91	0.14	44,44,44,44	0
57	MG	2A	3711	1/1	0.91	0.20	73,73,73,73	0
57	MG	1A	3542	1/1	0.91	0.28	59,59,59,59	0
57	MG	2A	3458	1/1	0.91	0.26	62,62,62,62	0
57	MG	2A	3051	1/1	0.91	0.17	75,75,75,75	0
57	MG	1A	3271	1/1	0.91	0.17	53,53,53,53	0
57	MG	2A	3053	1/1	0.91	0.10	57,57,57,57	0
57	MG	1a	1779	1/1	0.91	0.12	65,65,65,65	0
57	MG	2a	1617	1/1	0.91	0.16	73,73,73,73	0
57	MG	2a	1618	1/1	0.91	0.17	64,64,64,64	0
57	MG	2A	3721	1/1	0.91	0.15	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3193	1/1	0.91	0.13	42,42,42,42	0
57	MG	1a	1781	1/1	0.91	0.15	46,46,46,46	0
57	MG	1A	3547	1/1	0.91	0.41	57,57,57,57	0
57	MG	1A	3172	1/1	0.91	0.29	49,49,49,49	0
57	MG	2A	3316	1/1	0.91	0.12	51,51,51,51	0
57	MG	2a	1630	1/1	0.91	0.20	78,78,78,78	0
57	MG	1A	3823	1/1	0.91	0.14	38,38,38,38	0
57	MG	1A	3344	1/1	0.91	0.31	63,63,63,63	0
57	MG	2A	3195	1/1	0.91	0.11	69,69,69,69	0
57	MG	1a	1657	1/1	0.91	0.24	55,55,55,55	0
57	MG	1a	1658	1/1	0.91	0.20	60,60,60,60	0
58	K	2A	3451	1/1	0.91	0.12	71,71,71,71	0
57	MG	2a	1637	1/1	0.91	0.31	73,73,73,73	0
57	MG	2A	3064	1/1	0.91	0.16	59,59,59,59	0
57	MG	2A	3199	1/1	0.91	0.15	70,70,70,70	0
57	MG	1A	3908	1/1	0.92	0.20	43,43,43,43	0
57	MG	1A	3485	1/1	0.92	0.17	42,42,42,42	0
57	MG	1A	3915	1/1	0.92	0.19	38,38,38,38	0
57	MG	1A	3537	1/1	0.92	0.45	33,33,33,33	0
57	MG	1A	3348	1/1	0.92	0.45	49,49,49,49	0
57	MG	2a	1620	1/1	0.92	0.14	73,73,73,73	0
57	MG	2a	1621	1/1	0.92	0.11	68,68,68,68	0
57	MG	1S	202	1/1	0.92	0.13	44,44,44,44	0
57	MG	2a	1624	1/1	0.92	0.17	65,65,65,65	0
57	MG	1A	3185	1/1	0.92	0.09	69,69,69,69	0
57	MG	1A	3540	1/1	0.92	0.33	46,46,46,46	0
57	MG	1A	3784	1/1	0.92	0.12	40,40,40,40	0
57	MG	2A	3445	1/1	0.92	0.27	42,42,42,42	0
57	MG	1A	3357	1/1	0.92	0.18	66,66,66,66	0
57	MG	2A	3449	1/1	0.92	0.36	48,48,48,48	0
57	MG	2A	3135	1/1	0.92	0.18	38,38,38,38	0
57	MG	2A	3138	1/1	0.92	0.24	61,61,61,61	0
57	MG	1A	3435	1/1	0.92	0.14	35,35,35,35	0
57	MG	2A	3143	1/1	0.92	0.23	53,53,53,53	0
57	MG	1A	3543	1/1	0.92	0.30	41,41,41,41	0
57	MG	1U	205	1/1	0.92	0.16	38,38,38,38	0
57	MG	1U	206	1/1	0.92	0.15	37,37,37,37	0
57	MG	2a	1640	1/1	0.92	0.11	72,72,72,72	0
57	MG	2a	1641	1/1	0.92	0.14	80,80,80,80	0
57	MG	1A	3544	1/1	0.92	0.27	51,51,51,51	0
57	MG	1A	3933	1/1	0.92	0.17	58,58,58,58	0
57	MG	1A	3791	1/1	0.92	0.16	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3731	1/1	0.92	0.13	38,38,38,38	0
57	MG	1A	3647	1/1	0.92	0.18	53,53,53,53	0
57	MG	2A	3293	1/1	0.92	0.15	54,54,54,54	0
57	MG	1A	3796	1/1	0.92	0.15	43,43,43,43	0
57	MG	2A	3737	1/1	0.92	0.17	66,66,66,66	0
57	MG	1A	3086	1/1	0.92	0.28	30,30,30,30	0
57	MG	1x	104	1/1	0.92	0.07	69,69,69,69	0
57	MG	1A	3944	1/1	0.92	0.17	30,30,30,30	0
57	MG	2A	3743	1/1	0.92	0.15	40,40,40,40	0
57	MG	1A	3059	1/1	0.92	0.34	54,54,54,54	0
57	MG	2a	1659	1/1	0.92	0.26	80,80,80,80	0
57	MG	1A	3221	1/1	0.92	0.24	45,45,45,45	0
57	MG	1x	108	1/1	0.92	0.19	33,33,33,33	0
57	MG	1A	3189	1/1	0.92	0.31	43,43,43,43	0
57	MG	2A	3163	1/1	0.92	0.31	54,54,54,54	0
57	MG	2A	3754	1/1	0.92	0.13	44,44,44,44	0
57	MG	2A	3755	1/1	0.92	0.25	54,54,54,54	0
57	MG	2A	3482	1/1	0.92	0.17	56,56,56,56	0
57	MG	1A	3549	1/1	0.92	0.37	60,60,60,60	0
57	MG	2A	3307	1/1	0.92	0.09	63,63,63,63	0
57	MG	2A	3761	1/1	0.92	0.36	72,72,72,72	0
57	MG	2A	3486	1/1	0.92	0.27	52,52,52,52	0
57	MG	1A	3444	1/1	0.92	0.38	41,41,41,41	0
57	MG	2A	3767	1/1	0.92	0.15	61,61,61,61	0
57	MG	1A	3362	1/1	0.92	0.25	54,54,54,54	0
57	MG	2A	3769	1/1	0.92	0.16	43,43,43,43	0
57	MG	1A	3670	1/1	0.92	0.17	22,22,22,22	0
57	MG	1a	1697	1/1	0.92	0.28	63,63,63,63	0
57	MG	2A	3774	1/1	0.92	0.08	76,76,76,76	0
57	MG	1A	3294	1/1	0.92	0.34	35,35,35,35	0
57	MG	1A	3448	1/1	0.92	0.17	56,56,56,56	0
57	MG	10	106	1/1	0.92	0.15	56,56,56,56	0
57	MG	1A	4079	1/1	0.92	0.07	50,50,50,50	0
57	MG	1A	3088	1/1	0.92	0.26	47,47,47,47	0
57	MG	1A	3450	1/1	0.92	0.35	48,48,48,48	0
57	MG	2A	3508	1/1	0.92	0.18	76,76,76,76	0
57	MG	1A	3167	1/1	0.92	0.21	39,39,39,39	0
57	MG	12	3701	1/1	0.92	0.18	53,53,53,53	0
57	MG	2A	3790	1/1	0.92	0.17	74,74,74,74	0
57	MG	2A	3516	1/1	0.92	0.13	28,28,28,28	0
57	MG	2A	3794	1/1	0.92	0.16	68,68,68,68	0
57	MG	1A	3828	1/1	0.92	0.16	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3796	1/1	0.92	0.32	56,56,56,56	0
57	MG	1A	3688	1/1	0.92	0.21	33,33,33,33	0
57	MG	1A	3503	1/1	0.92	0.29	52,52,52,52	0
57	MG	2A	3800	1/1	0.92	0.11	76,76,76,76	0
57	MG	1A	3561	1/1	0.92	0.22	51,51,51,51	0
57	MG	1A	3452	1/1	0.92	0.51	55,55,55,55	0
57	MG	1a	1718	1/1	0.92	0.27	53,53,53,53	0
57	MG	2A	3531	1/1	0.92	0.11	53,53,53,53	0
57	MG	1A	3966	1/1	0.92	0.18	27,27,27,27	0
57	MG	2a	1716	1/1	0.92	0.22	68,68,68,68	0
57	MG	2A	3807	1/1	0.92	0.13	55,55,55,55	0
57	MG	2A	3032	1/1	0.92	0.22	50,50,50,50	0
57	MG	1A	3968	1/1	0.92	0.12	57,57,57,57	0
57	MG	2A	3540	1/1	0.92	0.14	78,78,78,78	0
57	MG	1A	3046	1/1	0.92	0.14	40,40,40,40	0
57	MG	2A	3546	1/1	0.92	0.19	48,48,48,48	0
57	MG	17	105	1/1	0.92	0.22	49,49,49,49	0
57	MG	2a	1725	1/1	0.92	0.32	75,75,75,75	0
57	MG	1A	3698	1/1	0.92	0.20	64,64,64,64	0
57	MG	1A	3150	1/1	0.92	0.32	42,42,42,42	0
57	MG	2A	3552	1/1	0.92	0.18	50,50,50,50	0
57	MG	2a	1729	1/1	0.92	0.41	73,73,73,73	0
57	MG	2A	3556	1/1	0.92	0.12	69,69,69,69	0
57	MG	1A	3836	1/1	0.92	0.19	57,57,57,57	0
57	MG	1A	3055	1/1	0.92	0.29	41,41,41,41	0
57	MG	2A	3044	1/1	0.92	0.09	62,62,62,62	0
57	MG	2a	1738	1/1	0.92	0.40	65,65,65,65	0
57	MG	1A	3207	1/1	0.92	0.19	51,51,51,51	0
57	MG	1A	3979	1/1	0.92	0.27	70,70,70,70	0
57	MG	1A	3209	1/1	0.92	0.27	46,46,46,46	0
57	MG	1A	3573	1/1	0.92	0.20	27,27,27,27	0
57	MG	1A	3844	1/1	0.92	0.15	52,52,52,52	0
57	MG	1A	3266	1/1	0.92	0.19	68,68,68,68	0
57	MG	1A	3466	1/1	0.92	0.27	58,58,58,58	0
57	MG	1a	1746	1/1	0.92	0.19	73,73,73,73	0
57	MG	2A	3849	1/1	0.92	0.11	40,40,40,40	0
57	MG	1a	1751	1/1	0.92	0.14	57,57,57,57	0
57	MG	2A	3579	1/1	0.92	0.21	57,57,57,57	0
57	MG	2a	1754	1/1	0.92	0.11	85,85,85,85	0
57	MG	1A	3989	1/1	0.92	0.18	38,38,38,38	0
57	MG	1A	3581	1/1	0.92	0.20	50,50,50,50	0
57	MG	2A	3858	1/1	0.92	0.17	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3268	1/1	0.92	0.16	42,42,42,42	0
57	MG	1a	1757	1/1	0.92	0.33	50,50,50,50	0
57	MG	1a	1759	1/1	0.92	0.21	68,68,68,68	0
57	MG	1A	3238	1/1	0.92	0.19	32,32,32,32	0
57	MG	2A	3587	1/1	0.92	0.13	61,61,61,61	0
57	MG	1B	234	1/1	0.92	0.12	72,72,72,72	0
57	MG	2B	203	1/1	0.92	0.19	79,79,79,79	0
57	MG	1D	310	1/1	0.92	0.26	28,28,28,28	0
57	MG	1a	1622	1/1	0.92	0.14	67,67,67,67	0
57	MG	2A	3218	1/1	0.92	0.20	73,73,73,73	0
57	MG	1A	3721	1/1	0.92	0.12	73,73,73,73	0
57	MG	2A	3602	1/1	0.92	0.27	51,51,51,51	0
57	MG	1A	3585	1/1	0.92	0.31	66,66,66,66	0
57	MG	1A	3379	1/1	0.92	0.30	55,55,55,55	0
57	MG	1A	3380	1/1	0.92	0.34	69,69,69,69	0
57	MG	2A	3611	1/1	0.92	0.15	46,46,46,46	0
57	MG	2A	3223	1/1	0.92	0.22	79,79,79,79	0
57	MG	2A	3224	1/1	0.92	0.41	42,42,42,42	0
57	MG	1A	3091	1/1	0.92	0.20	60,60,60,60	0
57	MG	1E	311	1/1	0.92	0.21	41,41,41,41	0
57	MG	2A	3622	1/1	0.92	0.11	66,66,66,66	0
57	MG	1A	3475	1/1	0.92	0.17	56,56,56,56	0
57	MG	2A	3627	1/1	0.92	0.10	84,84,84,84	0
57	MG	1A	3591	1/1	0.92	0.16	39,39,39,39	0
57	MG	1A	4005	1/1	0.92	0.17	23,23,23,23	0
57	MG	2A	3633	1/1	0.92	0.16	34,34,34,34	0
57	MG	1a	1786	1/1	0.92	0.13	57,57,57,57	0
57	MG	1A	3181	1/1	0.92	0.36	38,38,38,38	0
57	MG	1A	3593	1/1	0.92	0.43	71,71,71,71	0
57	MG	2a	1803	1/1	0.92	0.22	74,74,74,74	0
57	MG	2A	3643	1/1	0.92	0.76	68,68,68,68	0
57	MG	1A	3478	1/1	0.92	0.27	65,65,65,65	0
57	MG	1A	3747	1/1	0.92	0.18	45,45,45,45	0
57	MG	1A	3750	1/1	0.92	0.14	49,49,49,49	0
57	MG	1A	3108	1/1	0.92	0.23	39,39,39,39	0
57	MG	2A	3239	1/1	0.92	0.35	44,44,44,44	0
57	MG	1A	3598	1/1	0.92	0.11	63,63,63,63	0
57	MG	1A	3754	1/1	0.92	0.20	52,52,52,52	0
57	MG	2A	3242	1/1	0.92	0.42	67,67,67,67	0
57	MG	1a	1800	1/1	0.92	0.23	51,51,51,51	0
57	MG	2A	3096	1/1	0.92	0.28	51,51,51,51	0
57	MG	2V	202	1/1	0.92	0.54	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3215	1/1	0.92	0.12	53,53,53,53	0
57	MG	1N	203	1/1	0.92	0.24	44,44,44,44	0
57	MG	2A	3398	1/1	0.92	0.22	65,65,65,65	0
57	MG	1O	201	1/1	0.92	0.25	53,53,53,53	0
57	MG	1A	3016	1/1	0.92	0.30	54,54,54,54	0
57	MG	1A	3346	1/1	0.92	0.13	36,36,36,36	0
57	MG	1A	3607	1/1	0.92	0.17	38,38,38,38	0
57	MG	2A	3105	1/1	0.92	0.14	62,62,62,62	0
57	MG	1A	3533	1/1	0.92	0.27	54,54,54,54	0
57	MG	2I	203	1/1	0.92	0.08	72,72,72,72	0
57	MG	2A	3107	1/1	0.92	0.28	73,73,73,73	0
57	MG	1A	4027	1/1	0.92	0.07	64,64,64,64	0
57	MG	1A	3610	1/1	0.92	0.21	43,43,43,43	0
57	MG	2v	102	1/1	0.92	0.15	77,77,77,77	0
57	MG	27	102	1/1	0.92	0.62	53,53,53,53	0
57	MG	28	101	1/1	0.92	0.23	61,61,61,61	0
57	MG	2A	3110	1/1	0.92	0.18	61,61,61,61	0
57	MG	1A	3347	1/1	0.92	0.33	65,65,65,65	0
57	MG	1Q	201	1/1	0.92	0.39	42,42,42,42	0
57	MG	2A	3114	1/1	0.92	0.19	63,63,63,63	0
57	MG	1A	3901	1/1	0.92	0.21	35,35,35,35	0
57	MG	2A	3116	1/1	0.92	0.15	37,37,37,37	0
57	MG	2A	3427	1/1	0.92	0.34	57,57,57,57	0
57	MG	2A	3692	1/1	0.92	0.12	59,59,59,59	0
57	MG	1A	3617	1/1	0.92	0.11	70,70,70,70	0
57	MG	1a	1825	1/1	0.92	0.20	69,69,69,69	0
57	MG	1A	3906	1/1	0.92	0.22	38,38,38,38	0
57	MG	2A	3698	1/1	0.92	0.15	64,64,64,64	0
57	MG	1A	3772	1/1	0.92	0.15	39,39,39,39	0
57	MG	1A	3851	1/1	0.93	0.09	83,83,83,83	0
57	MG	2A	3756	1/1	0.93	0.42	51,51,51,51	0
57	MG	1A	3852	1/1	0.93	0.12	76,76,76,76	0
57	MG	1A	3853	1/1	0.93	0.19	26,26,26,26	0
57	MG	1a	1803	1/1	0.93	0.18	67,67,67,67	0
57	MG	1A	3963	1/1	0.93	0.14	46,46,46,46	0
57	MG	2A	3535	1/1	0.93	0.14	74,74,74,74	0
57	MG	1A	3644	1/1	0.93	0.13	32,32,32,32	0
57	MG	1A	3564	1/1	0.93	0.30	35,35,35,35	0
57	MG	1A	3318	1/1	0.93	0.31	53,53,53,53	0
57	MG	2A	3542	1/1	0.93	0.18	51,51,51,51	0
57	MG	2A	3091	1/1	0.93	0.47	50,50,50,50	0
57	MG	1V	205	1/1	0.93	0.35	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3093	1/1	0.93	0.11	69,69,69,69	0
57	MG	2A	3359	1/1	0.93	0.17	78,78,78,78	0
57	MG	1A	3278	1/1	0.93	0.31	40,40,40,40	0
57	MG	1A	3648	1/1	0.93	0.21	38,38,38,38	0
57	MG	2A	3555	1/1	0.93	0.25	59,59,59,59	0
57	MG	1A	4084	1/1	0.93	0.12	40,40,40,40	0
57	MG	2A	3557	1/1	0.93	0.15	47,47,47,47	0
57	MG	2a	1655	1/1	0.93	0.10	81,81,81,81	0
57	MG	2A	3782	1/1	0.93	0.07	55,55,55,55	0
57	MG	2A	3783	1/1	0.93	0.16	58,58,58,58	0
57	MG	1A	4086	1/1	0.93	0.15	50,50,50,50	0
57	MG	1A	3861	1/1	0.93	0.17	47,47,47,47	0
57	MG	1A	3650	1/1	0.93	0.23	36,36,36,36	0
57	MG	2a	1663	1/1	0.93	0.28	65,65,65,65	0
57	MG	1A	4090	1/1	0.93	0.33	48,48,48,48	0
57	MG	1A	3972	1/1	0.93	0.23	64,64,64,64	0
57	MG	1A	3652	1/1	0.93	0.25	41,41,41,41	0
57	MG	1A	3067	1/1	0.93	0.23	31,31,31,31	0
57	MG	1A	3865	1/1	0.93	0.08	45,45,45,45	0
57	MG	1A	3068	1/1	0.93	0.57	48,48,48,48	0
57	MG	2A	3571	1/1	0.93	0.13	45,45,45,45	0
57	MG	1A	3477	1/1	0.93	0.19	66,66,66,66	0
57	MG	1l	201	1/1	0.93	0.17	73,73,73,73	0
57	MG	2a	1675	1/1	0.93	0.11	75,75,75,75	0
57	MG	2a	1676	1/1	0.93	0.09	74,74,74,74	0
57	MG	1A	3431	1/1	0.93	0.16	44,44,44,44	0
57	MG	2a	1678	1/1	0.93	0.16	65,65,65,65	0
57	MG	1m	3001	1/1	0.93	0.12	67,67,67,67	0
57	MG	1A	3432	1/1	0.93	0.09	46,46,46,46	0
57	MG	1A	3575	1/1	0.93	0.27	44,44,44,44	0
57	MG	1a	1687	1/1	0.93	0.20	77,77,77,77	0
57	MG	1A	3192	1/1	0.93	0.26	38,38,38,38	0
57	MG	1B	212	1/1	0.93	0.23	42,42,42,42	0
57	MG	2A	3387	1/1	0.93	0.20	58,58,58,58	0
57	MG	1A	3881	1/1	0.93	0.19	29,29,29,29	0
57	MG	1A	3777	1/1	0.93	0.19	40,40,40,40	0
57	MG	1A	3993	1/1	0.93	0.24	40,40,40,40	0
57	MG	1A	3140	1/1	0.93	0.19	47,47,47,47	0
57	MG	1A	3671	1/1	0.93	0.20	30,30,30,30	0
57	MG	15	101	1/1	0.93	0.41	35,35,35,35	0
57	MG	2A	3600	1/1	0.93	0.13	58,58,58,58	0
57	MG	2A	3823	1/1	0.93	0.11	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3824	1/1	0.93	0.09	52,52,52,52	0
57	MG	1A	3996	1/1	0.93	0.17	48,48,48,48	0
57	MG	1a	1701	1/1	0.93	0.35	68,68,68,68	0
57	MG	2A	3605	1/1	0.93	0.15	62,62,62,62	0
57	MG	2A	3830	1/1	0.93	0.15	47,47,47,47	0
57	MG	2A	3128	1/1	0.93	0.07	61,61,61,61	0
57	MG	1A	3672	1/1	0.93	0.17	23,23,23,23	0
57	MG	2A	3835	1/1	0.93	0.09	56,56,56,56	0
57	MG	1A	3438	1/1	0.93	0.28	45,45,45,45	0
57	MG	1A	3785	1/1	0.93	0.09	49,49,49,49	0
57	MG	2a	1712	1/1	0.93	0.17	78,78,78,78	0
57	MG	2A	3404	1/1	0.93	0.29	48,48,48,48	0
57	MG	1A	3893	1/1	0.93	0.16	79,79,79,79	0
57	MG	1A	3049	1/1	0.93	0.23	41,41,41,41	0
57	MG	2A	3410	1/1	0.93	0.15	48,48,48,48	0
57	MG	1A	3168	1/1	0.93	0.17	40,40,40,40	0
57	MG	2A	3412	1/1	0.93	0.31	59,59,59,59	0
57	MG	2A	3630	1/1	0.93	0.24	64,64,64,64	0
57	MG	2A	3853	1/1	0.93	0.39	48,48,48,48	0
57	MG	2A	3136	1/1	0.93	0.09	68,68,68,68	0
57	MG	2A	3855	1/1	0.93	0.22	64,64,64,64	0
57	MG	2A	3269	1/1	0.93	0.25	55,55,55,55	0
57	MG	1B	232	1/1	0.93	0.21	60,60,60,60	0
57	MG	1A	3258	1/1	0.93	0.15	79,79,79,79	0
57	MG	18	106	1/1	0.93	0.34	63,63,63,63	0
57	MG	1a	1716	1/1	0.93	0.38	56,56,56,56	0
57	MG	2A	3642	1/1	0.93	0.20	57,57,57,57	0
57	MG	1A	3200	1/1	0.93	0.27	49,49,49,49	0
57	MG	1D	308	1/1	0.93	0.36	52,52,52,52	0
57	MG	2a	1733	1/1	0.93	0.09	64,64,64,64	0
57	MG	1A	3042	1/1	0.93	0.28	35,35,35,35	0
57	MG	2A	3650	1/1	0.93	0.22	81,81,81,81	0
57	MG	2A	3651	1/1	0.93	0.23	46,46,46,46	0
57	MG	1A	3028	1/1	0.93	0.23	29,29,29,29	0
57	MG	1a	1721	1/1	0.93	0.09	68,68,68,68	0
57	MG	1A	3490	1/1	0.93	0.35	54,54,54,54	0
57	MG	1A	3039	1/1	0.93	0.38	37,37,37,37	0
57	MG	2a	1744	1/1	0.93	0.17	69,69,69,69	0
57	MG	1A	3447	1/1	0.93	0.25	47,47,47,47	0
57	MG	1A	3407	1/1	0.93	0.13	37,37,37,37	0
57	MG	1A	3208	1/1	0.93	0.29	35,35,35,35	0
57	MG	2A	3017	1/1	0.93	0.17	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1E	312	1/1	0.93	0.26	58,58,58,58	0
57	MG	2A	3667	1/1	0.93	0.10	33,33,33,33	0
57	MG	2D	304	1/1	0.93	0.69	42,42,42,42	0
57	MG	2D	305	1/1	0.93	0.28	52,52,52,52	0
57	MG	1a	1728	1/1	0.93	0.32	59,59,59,59	0
57	MG	1A	3303	1/1	0.93	0.42	36,36,36,36	0
57	MG	2A	3670	1/1	0.93	0.13	60,60,60,60	0
57	MG	2a	1759	1/1	0.93	0.09	61,61,61,61	0
57	MG	2A	3438	1/1	0.93	0.20	58,58,58,58	0
57	MG	2E	305	1/1	0.93	0.18	39,39,39,39	0
57	MG	1A	3597	1/1	0.93	0.19	34,34,34,34	0
57	MG	2a	1765	1/1	0.93	0.12	46,46,46,46	0
57	MG	2A	3440	1/1	0.93	0.28	58,58,58,58	0
57	MG	2F	302	1/1	0.93	0.26	72,72,72,72	0
57	MG	1A	3177	1/1	0.93	0.18	32,32,32,32	0
57	MG	2F	304	1/1	0.93	0.28	63,63,63,63	0
57	MG	1A	3811	1/1	0.93	0.19	65,65,65,65	0
57	MG	1A	3922	1/1	0.93	0.09	30,30,30,30	0
57	MG	1A	3125	1/1	0.93	0.34	38,38,38,38	0
57	MG	2N	201	1/1	0.93	0.12	62,62,62,62	0
57	MG	1A	3021	1/1	0.93	0.17	27,27,27,27	0
57	MG	2A	3446	1/1	0.93	0.20	75,75,75,75	0
57	MG	2A	3033	1/1	0.93	0.12	41,41,41,41	0
57	MG	1a	1742	1/1	0.93	0.18	61,61,61,61	0
57	MG	2A	3035	1/1	0.93	0.25	47,47,47,47	0
57	MG	2a	1783	1/1	0.93	0.21	57,57,57,57	0
57	MG	1a	1743	1/1	0.93	0.11	65,65,65,65	0
57	MG	1F	315	1/1	0.93	0.22	54,54,54,54	0
57	MG	1A	3455	1/1	0.93	0.18	46,46,46,46	0
57	MG	2A	3689	1/1	0.93	0.09	61,61,61,61	0
57	MG	1A	3456	1/1	0.93	0.39	39,39,39,39	0
57	MG	1A	3928	1/1	0.93	0.19	46,46,46,46	0
57	MG	2U	202	1/1	0.93	0.42	51,51,51,51	0
57	MG	2A	3459	1/1	0.93	0.52	45,45,45,45	0
57	MG	1A	4031	1/1	0.93	0.11	50,50,50,50	0
57	MG	2a	1796	1/1	0.93	0.19	71,71,71,71	0
57	MG	2A	3306	1/1	0.93	0.11	69,69,69,69	0
57	MG	1A	3244	1/1	0.93	0.54	39,39,39,39	0
57	MG	1A	3609	1/1	0.93	0.19	43,43,43,43	0
57	MG	1A	3718	1/1	0.93	0.16	55,55,55,55	0
57	MG	2a	1802	1/1	0.93	0.16	76,76,76,76	0
57	MG	1A	3934	1/1	0.93	0.14	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3311	1/1	0.93	0.21	78,78,78,78	0
57	MG	23	104	1/1	0.93	0.09	60,60,60,60	0
57	MG	1A	3104	1/1	0.93	0.17	30,30,30,30	0
57	MG	1A	3080	1/1	0.93	0.36	44,44,44,44	0
57	MG	2A	3186	1/1	0.93	0.23	63,63,63,63	0
57	MG	1A	4043	1/1	0.93	0.17	25,25,25,25	0
57	MG	2A	3188	1/1	0.93	0.25	74,74,74,74	0
57	MG	2a	1814	1/1	0.93	0.07	70,70,70,70	0
57	MG	27	101	1/1	0.93	0.26	66,66,66,66	0
57	MG	1A	3723	1/1	0.93	0.10	60,60,60,60	0
57	MG	27	103	1/1	0.93	0.22	58,58,58,58	0
57	MG	1A	3463	1/1	0.93	0.33	53,53,53,53	0
57	MG	1A	3728	1/1	0.93	0.13	58,58,58,58	0
57	MG	1A	3158	1/1	0.93	0.17	56,56,56,56	0
57	MG	2A	3713	1/1	0.93	0.12	57,57,57,57	0
57	MG	1A	3421	1/1	0.93	0.30	57,57,57,57	0
57	MG	2A	3058	1/1	0.93	0.13	55,55,55,55	0
57	MG	1A	3736	1/1	0.93	0.18	44,44,44,44	0
57	MG	1A	3275	1/1	0.93	0.26	46,46,46,46	0
57	MG	2f	201	1/1	0.93	0.15	51,51,51,51	0
57	MG	1A	3556	1/1	0.93	0.23	55,55,55,55	0
57	MG	1a	1785	1/1	0.93	0.10	58,58,58,58	0
57	MG	2A	3491	1/1	0.93	0.17	70,70,70,70	0
57	MG	2A	3492	1/1	0.93	0.14	62,62,62,62	0
57	MG	1A	3950	1/1	0.93	0.12	83,83,83,83	0
57	MG	2a	1613	1/1	0.93	0.20	73,73,73,73	0
57	MG	1A	3951	1/1	0.93	0.11	63,63,63,63	0
57	MG	1A	3633	1/1	0.93	0.13	21,21,21,21	0
57	MG	2A	3066	1/1	0.93	0.19	59,59,59,59	0
57	MG	2A	3500	1/1	0.93	0.34	69,69,69,69	0
57	MG	1A	3159	1/1	0.93	0.27	33,33,33,33	0
57	MG	2A	3334	1/1	0.93	0.26	73,73,73,73	0
57	MG	2A	3068	1/1	0.93	0.63	62,62,62,62	0
57	MG	2A	3507	1/1	0.93	0.11	39,39,39,39	0
57	MG	1a	1791	1/1	0.93	0.09	71,71,71,71	0
57	MG	1A	3637	1/1	0.93	0.18	25,25,25,25	0
57	MG	1A	3846	1/1	0.93	0.11	48,48,48,48	0
57	MG	2A	3514	1/1	0.93	0.15	33,33,33,33	0
57	MG	1A	3277	1/1	0.93	0.16	48,48,48,48	0
57	MG	1A	3848	1/1	0.93	0.23	45,45,45,45	0
57	MG	2a	1629	1/1	0.93	0.11	81,81,81,81	0
57	MG	1a	1796	1/1	0.93	0.11	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3354	1/1	0.93	0.27	35,35,35,35	0
60	ZN	2n	501	1/1	0.93	0.07	106,106,106,106	0
57	MG	10	102	1/1	0.94	0.28	46,46,46,46	0
57	MG	2A	3014	1/1	0.94	0.17	46,46,46,46	0
57	MG	1A	3372	1/1	0.94	0.26	43,43,43,43	0
57	MG	2A	3518	1/1	0.94	0.18	44,44,44,44	0
57	MG	2A	3758	1/1	0.94	0.11	57,57,57,57	0
57	MG	2A	3522	1/1	0.94	0.11	52,52,52,52	0
57	MG	1A	3587	1/1	0.94	0.17	43,43,43,43	0
57	MG	1A	3084	1/1	0.94	0.24	30,30,30,30	0
57	MG	2A	3762	1/1	0.94	0.08	63,63,63,63	0
57	MG	2A	3021	1/1	0.94	0.14	29,29,29,29	0
57	MG	1B	203	1/1	0.94	0.19	37,37,37,37	0
57	MG	1A	3775	1/1	0.94	0.15	29,29,29,29	0
57	MG	1A	3980	1/1	0.94	0.09	51,51,51,51	0
57	MG	1A	3878	1/1	0.94	0.14	40,40,40,40	0
57	MG	1A	3274	1/1	0.94	0.29	36,36,36,36	0
57	MG	2a	1647	1/1	0.94	0.14	73,73,73,73	0
57	MG	2A	3340	1/1	0.94	0.15	61,61,61,61	0
57	MG	1A	3190	1/1	0.94	0.50	43,43,43,43	0
57	MG	1A	3884	1/1	0.94	0.24	28,28,28,28	0
57	MG	2a	1651	1/1	0.94	0.13	62,62,62,62	0
57	MG	1A	3673	1/1	0.94	0.26	27,27,27,27	0
57	MG	1A	3988	1/1	0.94	0.24	23,23,23,23	0
57	MG	1A	3211	1/1	0.94	0.15	38,38,38,38	0
57	MG	2A	3348	1/1	0.94	0.14	68,68,68,68	0
57	MG	2a	1656	1/1	0.94	0.22	76,76,76,76	0
57	MG	2A	3547	1/1	0.94	0.11	58,58,58,58	0
57	MG	2A	3781	1/1	0.94	0.06	64,64,64,64	0
57	MG	15	105	1/1	0.94	0.31	46,46,46,46	0
57	MG	1A	3991	1/1	0.94	0.18	26,26,26,26	0
57	MG	2A	3784	1/1	0.94	0.13	62,62,62,62	0
57	MG	1B	217	1/1	0.94	0.20	45,45,45,45	0
57	MG	1A	3783	1/1	0.94	0.17	33,33,33,33	0
57	MG	2A	3553	1/1	0.94	0.11	35,35,35,35	0
57	MG	1A	3127	1/1	0.94	0.34	36,36,36,36	0
57	MG	1A	3681	1/1	0.94	0.17	24,24,24,24	0
57	MG	1A	3234	1/1	0.94	0.18	47,47,47,47	0
57	MG	1A	3279	1/1	0.94	0.24	29,29,29,29	0
57	MG	1A	3459	1/1	0.94	0.31	58,58,58,58	0
57	MG	2A	3797	1/1	0.94	0.36	65,65,65,65	0
57	MG	1A	3596	1/1	0.94	0.30	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1735	1/1	0.94	0.26	53,53,53,53	0
57	MG	2A	3361	1/1	0.94	0.07	75,75,75,75	0
57	MG	1B	228	1/1	0.94	0.08	74,74,74,74	0
57	MG	1A	3897	1/1	0.94	0.19	31,31,31,31	0
57	MG	2A	3568	1/1	0.94	0.13	51,51,51,51	0
57	MG	1A	3213	1/1	0.94	0.31	34,34,34,34	0
57	MG	1A	3498	1/1	0.94	0.31	47,47,47,47	0
57	MG	1A	3461	1/1	0.94	0.24	42,42,42,42	0
57	MG	1A	3602	1/1	0.94	0.24	54,54,54,54	0
57	MG	1a	1608	1/1	0.94	0.31	63,63,63,63	0
57	MG	1A	3383	1/1	0.94	0.53	44,44,44,44	0
57	MG	1a	1612	1/1	0.94	0.09	77,77,77,77	0
57	MG	2a	1692	1/1	0.94	0.29	67,67,67,67	0
57	MG	1D	301	1/1	0.94	0.22	37,37,37,37	0
57	MG	1D	303	1/1	0.94	0.11	39,39,39,39	0
57	MG	1a	1616	1/1	0.94	0.13	57,57,57,57	0
57	MG	1D	307	1/1	0.94	0.25	42,42,42,42	0
57	MG	1A	3905	1/1	0.94	0.14	32,32,32,32	0
57	MG	1A	3287	1/1	0.94	0.25	37,37,37,37	0
57	MG	1A	3605	1/1	0.94	0.16	28,28,28,28	0
57	MG	2A	3588	1/1	0.94	0.11	58,58,58,58	0
57	MG	2A	3825	1/1	0.94	0.15	60,60,60,60	0
57	MG	1E	301	1/1	0.94	0.33	41,41,41,41	0
57	MG	1A	3706	1/1	0.94	0.22	39,39,39,39	0
57	MG	1A	3606	1/1	0.94	0.19	51,51,51,51	0
57	MG	1a	1772	1/1	0.94	0.10	60,60,60,60	0
57	MG	1a	1773	1/1	0.94	0.07	49,49,49,49	0
57	MG	1a	1774	1/1	0.94	0.09	54,54,54,54	0
57	MG	2A	3601	1/1	0.94	0.24	57,57,57,57	0
57	MG	1A	3912	1/1	0.94	0.22	28,28,28,28	0
57	MG	1A	3708	1/1	0.94	0.15	55,55,55,55	0
57	MG	1A	3917	1/1	0.94	0.21	54,54,54,54	0
57	MG	2A	3606	1/1	0.94	0.17	68,68,68,68	0
57	MG	2A	3608	1/1	0.94	0.19	70,70,70,70	0
57	MG	2A	3846	1/1	0.94	0.28	60,60,60,60	0
57	MG	2A	3078	1/1	0.94	0.14	59,59,59,59	0
57	MG	2A	3848	1/1	0.94	0.17	52,52,52,52	0
57	MG	1A	3810	1/1	0.94	0.13	62,62,62,62	0
57	MG	1F	302	1/1	0.94	0.24	27,27,27,27	0
57	MG	2A	3081	1/1	0.94	0.28	48,48,48,48	0
57	MG	2A	3614	1/1	0.94	0.14	60,60,60,60	0
57	MG	1A	3093	1/1	0.94	0.27	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3237	1/1	0.94	0.49	35,35,35,35	0
57	MG	1A	4024	1/1	0.94	0.16	47,47,47,47	0
57	MG	1F	307	1/1	0.94	0.17	46,46,46,46	0
57	MG	2A	3402	1/1	0.94	0.32	55,55,55,55	0
57	MG	2A	3243	1/1	0.94	0.22	62,62,62,62	0
57	MG	1A	3352	1/1	0.94	0.52	39,39,39,39	0
57	MG	1a	1789	1/1	0.94	0.08	71,71,71,71	0
57	MG	2A	3409	1/1	0.94	0.21	43,43,43,43	0
57	MG	1A	3467	1/1	0.94	0.14	34,34,34,34	0
57	MG	1A	3353	1/1	0.94	0.21	36,36,36,36	0
57	MG	2A	3636	1/1	0.94	0.18	40,40,40,40	0
57	MG	1A	3715	1/1	0.94	0.14	35,35,35,35	0
57	MG	1a	1638	1/1	0.94	0.29	60,60,60,60	0
57	MG	1A	3196	1/1	0.94	0.18	38,38,38,38	0
57	MG	1A	3927	1/1	0.94	0.17	42,42,42,42	0
57	MG	2B	209	1/1	0.94	0.13	65,65,65,65	0
57	MG	1A	3826	1/1	0.94	0.17	50,50,50,50	0
57	MG	2A	3645	1/1	0.94	0.17	52,52,52,52	0
57	MG	2B	212	1/1	0.94	0.24	62,62,62,62	0
57	MG	1a	1797	1/1	0.94	0.13	54,54,54,54	0
57	MG	2B	215	1/1	0.94	0.22	73,73,73,73	0
57	MG	1A	3620	1/1	0.94	0.20	33,33,33,33	0
57	MG	2a	1751	1/1	0.94	0.46	83,83,83,83	0
57	MG	2B	217	1/1	0.94	0.16	71,71,71,71	0
57	MG	2A	3100	1/1	0.94	0.14	30,30,30,30	0
57	MG	1A	3621	1/1	0.94	0.18	50,50,50,50	0
57	MG	2A	3423	1/1	0.94	0.19	58,58,58,58	0
57	MG	2A	3656	1/1	0.94	0.11	64,64,64,64	0
57	MG	1A	3622	1/1	0.94	0.26	60,60,60,60	0
57	MG	1A	4037	1/1	0.94	0.12	78,78,78,78	0
57	MG	2A	3104	1/1	0.94	0.42	54,54,54,54	0
57	MG	1N	205	1/1	0.94	0.36	38,38,38,38	0
57	MG	1A	3356	1/1	0.94	0.31	43,43,43,43	0
57	MG	1a	1805	1/1	0.94	0.07	58,58,58,58	0
57	MG	1a	1648	1/1	0.94	0.14	63,63,63,63	0
57	MG	2A	3666	1/1	0.94	0.11	69,69,69,69	0
57	MG	1A	3179	1/1	0.94	0.22	22,22,22,22	0
57	MG	1A	3032	1/1	0.94	0.26	25,25,25,25	0
57	MG	1A	3474	1/1	0.94	0.23	40,40,40,40	0
57	MG	2F	305	1/1	0.94	0.52	50,50,50,50	0
57	MG	1A	3731	1/1	0.94	0.30	79,79,79,79	0
57	MG	1a	1812	1/1	0.94	0.09	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1778	1/1	0.94	0.15	74,74,74,74	0
57	MG	1A	3943	1/1	0.94	0.19	28,28,28,28	0
57	MG	1P	203	1/1	0.94	0.32	29,29,29,29	0
57	MG	1a	1817	1/1	0.94	0.06	64,64,64,64	0
57	MG	1A	3632	1/1	0.94	0.19	30,30,30,30	0
57	MG	1A	3513	1/1	0.94	0.27	44,44,44,44	0
57	MG	1A	3514	1/1	0.94	0.12	68,68,68,68	0
57	MG	1A	3323	1/1	0.94	0.29	36,36,36,36	0
57	MG	1A	3263	1/1	0.94	0.23	55,55,55,55	0
57	MG	1b	301	1/1	0.94	0.12	82,82,82,82	0
57	MG	2A	3683	1/1	0.94	0.16	79,79,79,79	0
57	MG	1A	3843	1/1	0.94	0.27	53,53,53,53	0
57	MG	2A	3448	1/1	0.94	0.15	49,49,49,49	0
57	MG	1e	201	1/1	0.94	0.10	68,68,68,68	0
57	MG	1A	3051	1/1	0.94	0.24	42,42,42,42	0
57	MG	2V	201	1/1	0.94	0.35	75,75,75,75	0
57	MG	1A	4056	1/1	0.94	0.27	39,39,39,39	0
57	MG	1A	3845	1/1	0.94	0.16	62,62,62,62	0
57	MG	1a	1667	1/1	0.94	0.28	58,58,58,58	0
57	MG	2X	101	1/1	0.94	0.43	73,73,73,73	0
57	MG	1A	4058	1/1	0.94	0.12	60,60,60,60	0
57	MG	1R	206	1/1	0.94	0.30	32,32,32,32	0
57	MG	2A	3134	1/1	0.94	0.32	53,53,53,53	0
57	MG	2A	3460	1/1	0.94	0.28	54,54,54,54	0
57	MG	1A	3643	1/1	0.94	0.20	29,29,29,29	0
57	MG	23	103	1/1	0.94	0.24	56,56,56,56	0
57	MG	1A	3123	1/1	0.94	0.26	34,34,34,34	0
57	MG	1A	3329	1/1	0.94	0.34	56,56,56,56	0
57	MG	1A	3045	1/1	0.94	0.21	36,36,36,36	0
57	MG	1A	3523	1/1	0.94	0.32	40,40,40,40	0
57	MG	1A	3138	1/1	0.94	0.31	39,39,39,39	0
57	MG	1A	3139	1/1	0.94	0.21	42,42,42,42	0
57	MG	1A	3577	1/1	0.94	0.30	44,44,44,44	0
57	MG	1A	3757	1/1	0.94	0.17	45,45,45,45	0
57	MG	2a	1819	1/1	0.94	0.18	74,74,74,74	0
57	MG	2A	3300	1/1	0.94	0.11	72,72,72,72	0
57	MG	1A	4071	1/1	0.94	0.26	47,47,47,47	0
57	MG	1A	3654	1/1	0.94	0.22	52,52,52,52	0
57	MG	1U	207	1/1	0.94	0.45	37,37,37,37	0
57	MG	1A	3483	1/1	0.94	0.25	57,57,57,57	0
57	MG	1A	3658	1/1	0.94	0.21	25,25,25,25	0
57	MG	1A	3249	1/1	0.94	0.50	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3483	1/1	0.94	0.16	59,59,59,59	0
57	MG	1A	3765	1/1	0.94	0.20	44,44,44,44	0
57	MG	1a	1688	1/1	0.94	0.12	63,63,63,63	0
57	MG	1a	1689	1/1	0.94	0.37	66,66,66,66	0
57	MG	1A	3766	1/1	0.94	0.22	32,32,32,32	0
57	MG	1A	3250	1/1	0.94	0.20	69,69,69,69	0
57	MG	1A	4083	1/1	0.94	0.26	45,45,45,45	0
57	MG	2t	201	1/1	0.94	0.17	66,66,66,66	0
57	MG	1A	3306	1/1	0.94	0.25	39,39,39,39	0
57	MG	1a	1694	1/1	0.94	0.20	55,55,55,55	0
57	MG	1A	3410	1/1	0.94	0.17	42,42,42,42	0
57	MG	1A	4087	1/1	0.94	0.07	51,51,51,51	0
57	MG	1A	3868	1/1	0.94	0.52	34,34,34,34	0
57	MG	1A	3973	1/1	0.94	0.22	64,64,64,64	0
57	MG	1A	3974	1/1	0.94	0.13	51,51,51,51	0
57	MG	1A	4092	1/1	0.94	0.17	69,69,69,69	0
57	MG	1a	1702	1/1	0.94	0.31	62,62,62,62	0
57	MG	2A	3505	1/1	0.94	0.17	63,63,63,63	0
57	MG	2a	1623	1/1	0.94	0.11	73,73,73,73	0
57	MG	1Z	303	1/1	0.94	0.29	57,57,57,57	0
57	MG	2A	3174	1/1	0.94	0.22	37,37,37,37	0
57	MG	1a	1704	1/1	0.94	0.22	63,63,63,63	0
57	MG	2A	3509	1/1	0.94	0.11	53,53,53,53	0
57	MG	2A	3750	1/1	0.94	0.05	57,57,57,57	0
57	MG	2A	3510	1/1	0.94	0.09	56,56,56,56	0
57	MG	1A	4094	1/1	0.94	0.20	52,52,52,52	0
57	MG	2A	3400	1/1	0.95	0.27	47,47,47,47	0
57	MG	2A	3787	1/1	0.95	0.11	51,51,51,51	0
57	MG	1A	3696	1/1	0.95	0.21	38,38,38,38	0
57	MG	1A	3524	1/1	0.95	0.27	33,33,33,33	0
57	MG	2A	3583	1/1	0.95	0.17	32,32,32,32	0
57	MG	2A	3403	1/1	0.95	0.33	55,55,55,55	0
57	MG	1A	3109	1/1	0.95	0.50	38,38,38,38	0
57	MG	1a	1710	1/1	0.95	0.21	69,69,69,69	0
57	MG	1A	3700	1/1	0.95	0.16	26,26,26,26	0
57	MG	1A	3375	1/1	0.95	0.45	41,41,41,41	0
57	MG	1A	4051	1/1	0.95	0.17	31,31,31,31	0
57	MG	1F	308	1/1	0.95	0.32	36,36,36,36	0
57	MG	1A	3704	1/1	0.95	0.23	31,31,31,31	0
57	MG	2A	3126	1/1	0.95	0.17	49,49,49,49	0
57	MG	2A	3594	1/1	0.95	0.21	69,69,69,69	0
57	MG	1A	3879	1/1	0.95	0.09	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1610	1/1	0.95	0.16	27,27,27,27	0
57	MG	1A	3630	1/1	0.95	0.16	22,22,22,22	0
57	MG	2A	3417	1/1	0.95	0.42	62,62,62,62	0
57	MG	1A	3967	1/1	0.95	0.12	42,42,42,42	0
57	MG	2A	3604	1/1	0.95	0.10	74,74,74,74	0
57	MG	1A	3528	1/1	0.95	0.13	52,52,52,52	0
57	MG	1G	201	1/1	0.95	0.28	41,41,41,41	0
57	MG	2A	3814	1/1	0.95	0.17	51,51,51,51	0
57	MG	1A	3411	1/1	0.95	0.21	37,37,37,37	0
57	MG	1A	3792	1/1	0.95	0.17	20,20,20,20	0
57	MG	1A	3794	1/1	0.95	0.15	30,30,30,30	0
57	MG	1A	3014	1/1	0.95	0.15	28,28,28,28	0
57	MG	2A	3137	1/1	0.95	0.15	43,43,43,43	0
57	MG	1A	4063	1/1	0.95	0.24	29,29,29,29	0
57	MG	2A	3140	1/1	0.95	0.19	41,41,41,41	0
57	MG	1A	3634	1/1	0.95	0.18	41,41,41,41	0
57	MG	2A	3618	1/1	0.95	0.15	54,54,54,54	0
57	MG	2A	3431	1/1	0.95	0.18	47,47,47,47	0
57	MG	2A	3003	1/1	0.95	0.29	48,48,48,48	0
57	MG	1A	3170	1/1	0.95	0.20	28,28,28,28	0
57	MG	1A	3217	1/1	0.95	0.22	34,34,34,34	0
57	MG	2a	1684	1/1	0.95	0.17	61,61,61,61	0
57	MG	2a	1685	1/1	0.95	0.27	57,57,57,57	0
57	MG	2a	1686	1/1	0.95	0.09	81,81,81,81	0
57	MG	2A	3628	1/1	0.95	0.14	50,50,50,50	0
57	MG	2A	3833	1/1	0.95	0.15	45,45,45,45	0
57	MG	2A	3147	1/1	0.95	0.17	46,46,46,46	0
57	MG	1A	3114	1/1	0.95	0.30	36,36,36,36	0
57	MG	1A	3454	1/1	0.95	0.27	36,36,36,36	0
57	MG	1A	3041	1/1	0.95	0.16	32,32,32,32	0
57	MG	1A	3198	1/1	0.95	0.17	45,45,45,45	0
57	MG	2A	3840	1/1	0.95	0.13	71,71,71,71	0
57	MG	2A	3635	1/1	0.95	0.21	56,56,56,56	0
57	MG	1P	201	1/1	0.95	0.20	31,31,31,31	0
57	MG	1A	3457	1/1	0.95	0.30	39,39,39,39	0
57	MG	2A	3640	1/1	0.95	0.19	41,41,41,41	0
57	MG	2A	3154	1/1	0.95	0.30	56,56,56,56	0
57	MG	2A	3015	1/1	0.95	0.35	39,39,39,39	0
57	MG	2A	3016	1/1	0.95	0.16	70,70,70,70	0
57	MG	1A	3719	1/1	0.95	0.19	45,45,45,45	0
57	MG	1a	1744	1/1	0.95	0.19	56,56,56,56	0
57	MG	2A	3646	1/1	0.95	0.17	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3019	1/1	0.95	0.36	43,43,43,43	0
57	MG	2A	3856	1/1	0.95	0.17	67,67,67,67	0
57	MG	2a	1710	1/1	0.95	0.17	72,72,72,72	0
57	MG	1A	3983	1/1	0.95	0.25	51,51,51,51	0
57	MG	1a	1747	1/1	0.95	0.09	56,56,56,56	0
57	MG	2A	3450	1/1	0.95	0.13	67,67,67,67	0
57	MG	1a	1748	1/1	0.95	0.17	35,35,35,35	0
57	MG	2A	3654	1/1	0.95	0.19	74,74,74,74	0
57	MG	1A	3350	1/1	0.95	0.30	59,59,59,59	0
57	MG	1A	4076	1/1	0.95	0.14	52,52,52,52	0
57	MG	1a	1634	1/1	0.95	0.20	63,63,63,63	0
57	MG	2A	3029	1/1	0.95	0.09	62,62,62,62	0
57	MG	1A	3351	1/1	0.95	0.29	47,47,47,47	0
57	MG	1A	3986	1/1	0.95	0.12	76,76,76,76	0
57	MG	2A	3663	1/1	0.95	0.11	73,73,73,73	0
57	MG	1A	3009	1/1	0.95	0.17	27,27,27,27	0
57	MG	1A	3324	1/1	0.95	0.19	30,30,30,30	0
57	MG	1R	201	1/1	0.95	0.23	37,37,37,37	0
57	MG	1A	3300	1/1	0.95	0.19	34,34,34,34	0
57	MG	1A	4085	1/1	0.95	0.16	48,48,48,48	0
57	MG	2A	3466	1/1	0.95	0.29	39,39,39,39	0
57	MG	2B	213	1/1	0.95	0.26	62,62,62,62	0
57	MG	1a	1766	1/1	0.95	0.19	43,43,43,43	0
57	MG	2a	1732	1/1	0.95	0.27	64,64,64,64	0
57	MG	1a	1767	1/1	0.95	0.09	55,55,55,55	0
57	MG	1A	3818	1/1	0.95	0.15	27,27,27,27	0
57	MG	2A	3041	1/1	0.95	0.23	68,68,68,68	0
57	MG	2B	218	1/1	0.95	0.18	81,81,81,81	0
57	MG	1A	3653	1/1	0.95	0.24	48,48,48,48	0
57	MG	2A	3474	1/1	0.95	0.35	66,66,66,66	0
57	MG	1A	3824	1/1	0.95	0.11	40,40,40,40	0
57	MG	2A	3678	1/1	0.95	0.13	39,39,39,39	0
57	MG	2a	1743	1/1	0.95	0.19	68,68,68,68	0
57	MG	1A	3222	1/1	0.95	0.22	38,38,38,38	0
57	MG	1A	3733	1/1	0.95	0.29	48,48,48,48	0
57	MG	2A	3046	1/1	0.95	0.14	50,50,50,50	0
57	MG	2A	3047	1/1	0.95	0.14	36,36,36,36	0
57	MG	1A	3389	1/1	0.95	0.34	28,28,28,28	0
57	MG	1a	1778	1/1	0.95	0.17	59,59,59,59	0
57	MG	2E	306	1/1	0.95	0.13	34,34,34,34	0
57	MG	1A	3918	1/1	0.95	0.15	34,34,34,34	0
57	MG	1a	1649	1/1	0.95	0.11	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1753	1/1	0.95	0.13	68,68,68,68	0
57	MG	2F	301	1/1	0.95	0.45	49,49,49,49	0
57	MG	1T	202	1/1	0.95	0.20	68,68,68,68	0
57	MG	1A	3656	1/1	0.95	0.20	37,37,37,37	0
57	MG	1A	3657	1/1	0.95	0.17	32,32,32,32	0
57	MG	2a	1758	1/1	0.95	0.25	61,61,61,61	0
57	MG	1A	3740	1/1	0.95	0.16	27,27,27,27	0
57	MG	1A	3062	1/1	0.95	0.33	61,61,61,61	0
57	MG	1A	3251	1/1	0.95	0.50	45,45,45,45	0
57	MG	1A	3330	1/1	0.95	0.21	48,48,48,48	0
57	MG	1A	4004	1/1	0.95	0.22	33,33,33,33	0
57	MG	1A	3304	1/1	0.95	0.41	53,53,53,53	0
57	MG	2A	3699	1/1	0.95	0.10	65,65,65,65	0
57	MG	1A	4006	1/1	0.95	0.21	32,32,32,32	0
57	MG	1V	203	1/1	0.95	0.15	37,37,37,37	0
57	MG	2A	3499	1/1	0.95	0.28	67,67,67,67	0
57	MG	2a	1771	1/1	0.95	0.12	77,77,77,77	0
57	MG	1A	3599	1/1	0.95	0.22	43,43,43,43	0
57	MG	1A	3136	1/1	0.95	0.11	49,49,49,49	0
57	MG	2A	3203	1/1	0.95	0.11	66,66,66,66	0
57	MG	2A	3503	1/1	0.95	0.17	57,57,57,57	0
57	MG	1A	3667	1/1	0.95	0.17	34,34,34,34	0
57	MG	2T	3504	1/1	0.95	0.24	59,59,59,59	0
57	MG	1A	3137	1/1	0.95	0.19	28,28,28,28	0
57	MG	1A	4013	1/1	0.95	0.21	29,29,29,29	0
57	MG	1A	3122	1/1	0.95	0.19	47,47,47,47	0
57	MG	1a	1798	1/1	0.95	0.08	71,71,71,71	0
57	MG	1A	3434	1/1	0.95	0.23	38,38,38,38	0
57	MG	2A	3351	1/1	0.95	0.14	60,60,60,60	0
57	MG	2A	3512	1/1	0.95	0.15	63,63,63,63	0
57	MG	1A	3473	1/1	0.95	0.20	33,33,33,33	0
57	MG	1X	104	1/1	0.95	0.21	32,32,32,32	0
57	MG	2A	3515	1/1	0.95	0.15	61,61,61,61	0
57	MG	2I	101	1/1	0.95	0.85	59,59,59,59	0
57	MG	1A	3183	1/1	0.95	0.24	46,46,46,46	0
57	MG	1Y	201	1/1	0.95	0.28	50,50,50,50	0
57	MG	2A	3722	1/1	0.95	0.24	70,70,70,70	0
57	MG	1A	3675	1/1	0.95	0.19	32,32,32,32	0
57	MG	1A	4021	1/1	0.95	0.24	35,35,35,35	0
57	MG	2A	3524	1/1	0.95	0.16	45,45,45,45	0
57	MG	2A	3728	1/1	0.95	0.10	37,37,37,37	0
57	MG	2A	3729	1/1	0.95	0.16	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3677	1/1	0.95	0.26	46,46,46,46	0
57	MG	1A	3941	1/1	0.95	0.10	54,54,54,54	0
57	MG	1A	3763	1/1	0.95	0.20	31,31,31,31	0
57	MG	2A	3082	1/1	0.95	0.20	49,49,49,49	0
57	MG	1A	3160	1/1	0.95	0.18	30,30,30,30	0
57	MG	1a	1810	1/1	0.95	0.10	47,47,47,47	0
57	MG	2A	3532	1/1	0.95	0.13	44,44,44,44	0
57	MG	2a	1812	1/1	0.95	0.12	79,79,79,79	0
57	MG	1A	3367	1/1	0.95	0.20	64,64,64,64	0
57	MG	2A	3225	1/1	0.95	0.18	61,61,61,61	0
57	MG	10	104	1/1	0.95	0.65	39,39,39,39	0
57	MG	2A	3537	1/1	0.95	0.21	54,54,54,54	0
57	MG	2A	3538	1/1	0.95	0.15	53,53,53,53	0
57	MG	2A	3747	1/1	0.95	0.14	66,66,66,66	0
57	MG	2A	3368	1/1	0.95	0.17	60,60,60,60	0
57	MG	1a	1814	1/1	0.95	0.09	69,69,69,69	0
57	MG	1A	3680	1/1	0.95	0.17	63,63,63,63	0
57	MG	1A	3063	1/1	0.95	0.32	50,50,50,50	0
57	MG	2a	1823	1/1	0.95	0.21	70,70,70,70	0
57	MG	1A	3011	1/1	0.95	0.20	44,44,44,44	0
57	MG	1A	3613	1/1	0.95	0.17	34,34,34,34	0
57	MG	1A	3771	1/1	0.95	0.18	28,28,28,28	0
57	MG	2A	3549	1/1	0.95	0.19	53,53,53,53	0
57	MG	1A	3685	1/1	0.95	0.20	30,30,30,30	0
57	MG	1a	1823	1/1	0.95	0.16	63,63,63,63	0
57	MG	1a	1824	1/1	0.95	0.13	68,68,68,68	0
57	MG	2l	201	1/1	0.95	0.20	64,64,64,64	0
57	MG	2A	3380	1/1	0.95	0.34	58,58,58,58	0
57	MG	1D	305	1/1	0.95	0.24	48,48,48,48	0
57	MG	1A	3050	1/1	0.95	0.25	27,27,27,27	0
57	MG	2A	3765	1/1	0.95	0.19	58,58,58,58	0
57	MG	2r	101	1/1	0.95	0.11	84,84,84,84	0
57	MG	1A	3443	1/1	0.95	0.26	55,55,55,55	0
57	MG	2A	3558	1/1	0.95	0.12	45,45,45,45	0
57	MG	1D	309	1/1	0.95	0.14	41,41,41,41	0
57	MG	13	105	1/1	0.95	0.17	62,62,62,62	0
57	MG	2v	104	1/1	0.95	0.15	70,70,70,70	0
57	MG	1A	4036	1/1	0.95	0.13	52,52,52,52	0
57	MG	1a	1696	1/1	0.95	0.36	69,69,69,69	0
57	MG	2A	3772	1/1	0.95	0.06	68,68,68,68	0
57	MG	2A	3773	1/1	0.95	0.11	65,65,65,65	0
57	MG	1A	3953	1/1	0.95	0.21	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1D	313	1/1	0.95	0.19	36,36,36,36	0
57	MG	1A	3618	1/1	0.95	0.26	28,28,28,28	0
57	MG	1E	304	1/1	0.95	0.18	33,33,33,33	0
57	MG	1A	3776	1/1	0.95	0.16	26,26,26,26	0
57	MG	2A	3249	1/1	0.95	0.13	79,79,79,79	0
57	MG	1A	3145	1/1	0.95	0.47	28,28,28,28	0
59	CLM	2A	3863	20/20	0.95	0.29	42,47,57,60	0
57	MG	17	104	1/1	0.95	0.19	58,58,58,58	0
60	ZN	1n	103	1/1	0.95	0.17	71,71,71,71	0
57	MG	1A	4042	1/1	0.95	0.07	43,43,43,43	0
57	MG	1A	3342	1/1	0.95	0.15	71,71,71,71	0
57	MG	1A	3408	1/1	0.95	0.34	32,32,32,32	0
57	MG	2A	3260	1/1	0.96	0.20	63,63,63,63	0
57	MG	2A	3690	1/1	0.96	0.14	65,65,65,65	0
57	MG	1A	3627	1/1	0.96	0.17	37,37,37,37	0
57	MG	1A	3574	1/1	0.96	0.26	60,60,60,60	0
57	MG	1A	3629	1/1	0.96	0.16	32,32,32,32	0
57	MG	1a	1775	1/1	0.96	0.18	70,70,70,70	0
57	MG	2A	3695	1/1	0.96	0.17	52,52,52,52	0
57	MG	1A	3692	1/1	0.96	0.22	27,27,27,27	0
57	MG	1W	206	1/1	0.96	0.17	41,41,41,41	0
57	MG	1A	3071	1/1	0.96	0.54	30,30,30,30	0
57	MG	1A	3849	1/1	0.96	0.23	24,24,24,24	0
57	MG	1A	3374	1/1	0.96	0.40	48,48,48,48	0
57	MG	1B	227	1/1	0.96	0.19	39,39,39,39	0
57	MG	1A	3341	1/1	0.96	0.27	51,51,51,51	0
57	MG	1A	3134	1/1	0.96	0.20	43,43,43,43	0
57	MG	1A	3311	1/1	0.96	0.16	31,31,31,31	0
57	MG	1A	3115	1/1	0.96	0.15	41,41,41,41	0
57	MG	2A	3541	1/1	0.96	0.17	51,51,51,51	0
57	MG	2A	3399	1/1	0.96	0.23	59,59,59,59	0
57	MG	1A	3161	1/1	0.96	0.26	30,30,30,30	0
57	MG	2A	3544	1/1	0.96	0.14	47,47,47,47	0
57	MG	2A	3158	1/1	0.96	0.39	43,43,43,43	0
57	MG	1A	4032	1/1	0.96	0.17	61,61,61,61	0
57	MG	1A	3638	1/1	0.96	0.16	18,18,18,18	0
57	MG	1A	3417	1/1	0.96	0.28	41,41,41,41	0
57	MG	1A	3778	1/1	0.96	0.19	50,50,50,50	0
57	MG	2A	3407	1/1	0.96	0.30	65,65,65,65	0
57	MG	1A	3116	1/1	0.96	0.30	42,42,42,42	0
57	MG	1D	306	1/1	0.96	0.22	31,31,31,31	0
57	MG	1A	3780	1/1	0.96	0.19	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1718	1/1	0.96	0.11	72,72,72,72	0
57	MG	1A	3072	1/1	0.96	0.12	12,12,12,12	0
57	MG	1A	4039	1/1	0.96	0.12	46,46,46,46	0
57	MG	2A	3286	1/1	0.96	0.20	60,60,60,60	0
57	MG	10	109	1/1	0.96	0.21	46,46,46,46	0
57	MG	2A	3560	1/1	0.96	0.13	44,44,44,44	0
57	MG	1A	3096	1/1	0.96	0.31	41,41,41,41	0
57	MG	11	102	1/1	0.96	0.14	36,36,36,36	0
57	MG	1A	3166	1/1	0.96	0.27	38,38,38,38	0
57	MG	2A	3418	1/1	0.96	0.17	60,60,60,60	0
57	MG	1A	3284	1/1	0.96	0.39	34,34,34,34	0
57	MG	1A	3867	1/1	0.96	0.16	42,42,42,42	0
57	MG	1A	3017	1/1	0.96	0.19	52,52,52,52	0
57	MG	2A	3738	1/1	0.96	0.19	71,71,71,71	0
57	MG	13	103	1/1	0.96	0.28	42,42,42,42	0
57	MG	1A	3195	1/1	0.96	0.18	30,30,30,30	0
57	MG	1A	3100	1/1	0.96	0.33	72,72,72,72	0
57	MG	2A	3742	1/1	0.96	0.28	65,65,65,65	0
57	MG	1A	3873	1/1	0.96	0.34	42,42,42,42	0
57	MG	15	102	1/1	0.96	0.27	38,38,38,38	0
57	MG	1A	3651	1/1	0.96	0.11	64,64,64,64	0
57	MG	2A	3577	1/1	0.96	0.14	37,37,37,37	0
57	MG	1A	3875	1/1	0.96	0.14	32,32,32,32	0
57	MG	2A	3749	1/1	0.96	0.36	63,63,63,63	0
57	MG	1A	3876	1/1	0.96	0.22	37,37,37,37	0
57	MG	2V	203	1/1	0.96	0.27	68,68,68,68	0
57	MG	1A	3020	1/1	0.96	0.23	44,44,44,44	0
57	MG	1A	3427	1/1	0.96	0.22	59,59,59,59	0
57	MG	2A	3753	1/1	0.96	0.14	61,61,61,61	0
57	MG	17	102	1/1	0.96	0.16	33,33,33,33	0
57	MG	1A	3355	1/1	0.96	0.18	38,38,38,38	0
57	MG	1A	3720	1/1	0.96	0.22	27,27,27,27	0
57	MG	1a	1819	1/1	0.96	0.09	59,59,59,59	0
57	MG	1A	3224	1/1	0.96	0.21	38,38,38,38	0
57	MG	1A	3882	1/1	0.96	0.24	32,32,32,32	0
57	MG	18	102	1/1	0.96	0.20	44,44,44,44	0
57	MG	1A	3005	1/1	0.96	0.22	44,44,44,44	0
57	MG	1A	3507	1/1	0.96	0.30	40,40,40,40	0
57	MG	2A	3763	1/1	0.96	0.10	65,65,65,65	0
57	MG	1F	312	1/1	0.96	0.27	48,48,48,48	0
57	MG	2a	1760	1/1	0.96	0.04	85,85,85,85	0
57	MG	1A	3171	1/1	0.96	0.42	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1762	1/1	0.96	0.11	62,62,62,62	0
57	MG	1A	3727	1/1	0.96	0.18	54,54,54,54	0
57	MG	2A	3598	1/1	0.96	0.09	58,58,58,58	0
57	MG	2A	3599	1/1	0.96	0.13	54,54,54,54	0
57	MG	1A	3036	1/1	0.96	0.18	39,39,39,39	0
57	MG	1A	3056	1/1	0.96	0.23	46,46,46,46	0
57	MG	1G	202	1/1	0.96	0.25	58,58,58,58	0
57	MG	2a	1601	1/1	0.96	0.08	75,75,75,75	0
57	MG	1A	4066	1/1	0.96	0.19	19,19,19,19	0
57	MG	1A	3232	1/1	0.96	0.22	50,50,50,50	0
57	MG	1A	3892	1/1	0.96	0.23	24,24,24,24	0
57	MG	2a	1773	1/1	0.96	0.24	63,63,63,63	0
57	MG	2A	3452	1/1	0.96	0.20	22,22,22,22	0
57	MG	1A	3808	1/1	0.96	0.14	35,35,35,35	0
57	MG	2A	3090	1/1	0.96	0.57	57,57,57,57	0
57	MG	1A	3894	1/1	0.96	0.20	39,39,39,39	0
57	MG	1a	1613	1/1	0.96	0.23	68,68,68,68	0
57	MG	1A	3398	1/1	0.96	0.21	25,25,25,25	0
57	MG	1A	3436	1/1	0.96	0.13	53,53,53,53	0
57	MG	2A	3615	1/1	0.96	0.13	31,31,31,31	0
57	MG	2A	3330	1/1	0.96	0.48	58,58,58,58	0
57	MG	2a	1784	1/1	0.96	0.13	68,68,68,68	0
57	MG	2A	3211	1/1	0.96	0.46	72,72,72,72	0
57	MG	2a	1786	1/1	0.96	0.08	85,85,85,85	0
57	MG	1A	3735	1/1	0.96	0.14	52,52,52,52	0
57	MG	1A	3665	1/1	0.96	0.18	35,35,35,35	0
57	MG	1A	3737	1/1	0.96	0.09	65,65,65,65	0
57	MG	1A	3666	1/1	0.96	0.17	24,24,24,24	0
57	MG	2A	3624	1/1	0.96	0.26	65,65,65,65	0
57	MG	2A	3626	1/1	0.96	0.13	43,43,43,43	0
57	MG	1A	3816	1/1	0.96	0.11	37,37,37,37	0
57	MG	2A	3467	1/1	0.96	0.15	57,57,57,57	0
57	MG	2A	3629	1/1	0.96	0.09	38,38,38,38	0
57	MG	2a	1797	1/1	0.96	0.22	70,70,70,70	0
57	MG	1A	3437	1/1	0.96	0.41	50,50,50,50	0
57	MG	1A	4080	1/1	0.96	0.23	31,31,31,31	0
57	MG	1A	3203	1/1	0.96	0.14	35,35,35,35	0
57	MG	1A	3821	1/1	0.96	0.24	38,38,38,38	0
57	MG	1A	3822	1/1	0.96	0.19	29,29,29,29	0
57	MG	1A	3742	1/1	0.96	0.20	20,20,20,20	0
57	MG	2A	3343	1/1	0.96	0.11	64,64,64,64	0
57	MG	1A	3559	1/1	0.96	0.18	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3638	1/1	0.96	0.16	46,46,46,46	0
57	MG	1A	3911	1/1	0.96	0.29	37,37,37,37	0
57	MG	2A	3346	1/1	0.96	0.19	65,65,65,65	0
57	MG	1a	1736	1/1	0.96	0.17	60,60,60,60	0
57	MG	2a	1811	1/1	0.96	0.28	50,50,50,50	0
57	MG	2A	3811	1/1	0.96	0.06	50,50,50,50	0
57	MG	1A	3175	1/1	0.96	0.29	33,33,33,33	0
57	MG	1A	3612	1/1	0.96	0.16	24,24,24,24	0
57	MG	2A	3111	1/1	0.96	0.19	69,69,69,69	0
57	MG	2A	3815	1/1	0.96	0.11	46,46,46,46	0
57	MG	1A	3264	1/1	0.96	0.22	67,67,67,67	0
57	MG	2A	3647	1/1	0.96	0.13	45,45,45,45	0
57	MG	2A	3648	1/1	0.96	0.10	55,55,55,55	0
57	MG	1A	3748	1/1	0.96	0.19	58,58,58,58	0
57	MG	1A	3749	1/1	0.96	0.16	41,41,41,41	0
57	MG	2A	3487	1/1	0.96	0.28	60,60,60,60	0
57	MG	1A	3206	1/1	0.96	0.27	37,37,37,37	0
57	MG	1A	3038	1/1	0.96	0.27	32,32,32,32	0
57	MG	1B	201	1/1	0.96	0.27	63,63,63,63	0
57	MG	2A	3118	1/1	0.96	0.08	76,76,76,76	0
57	MG	1A	3044	1/1	0.96	0.20	34,34,34,34	0
57	MG	2A	3494	1/1	0.96	0.23	65,65,65,65	0
57	MG	1a	1750	1/1	0.96	0.14	43,43,43,43	0
57	MG	1A	3110	1/1	0.96	0.24	31,31,31,31	0
57	MG	2k	201	1/1	0.96	0.13	73,73,73,73	0
57	MG	1A	3755	1/1	0.96	0.26	44,44,44,44	0
57	MG	1B	205	1/1	0.96	0.17	40,40,40,40	0
57	MG	1A	3155	1/1	0.96	0.33	45,45,45,45	0
57	MG	1a	1756	1/1	0.96	0.17	50,50,50,50	0
57	MG	1A	3307	1/1	0.96	0.20	30,30,30,30	0
57	MG	2a	1661	1/1	0.96	0.10	67,67,67,67	0
57	MG	1A	3838	1/1	0.96	0.13	39,39,39,39	0
57	MG	2A	3012	1/1	0.96	0.14	47,47,47,47	0
57	MG	2A	3504	1/1	0.96	0.07	57,57,57,57	0
57	MG	2a	1665	1/1	0.96	0.22	56,56,56,56	0
57	MG	2A	3013	1/1	0.96	0.16	50,50,50,50	0
57	MG	1A	3572	1/1	0.96	0.63	33,33,33,33	0
57	MG	1A	3624	1/1	0.96	0.24	25,25,25,25	0
57	MG	1A	3625	1/1	0.96	0.14	54,54,54,54	0
57	MG	1A	3932	1/1	0.96	0.18	19,19,19,19	0
57	MG	2A	3374	1/1	0.96	0.18	67,67,67,67	0
57	MG	2A	3375	1/1	0.96	0.24	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	4017	1/1	0.96	0.17	28,28,28,28	0
57	MG	1A	3070	1/1	0.96	0.23	20,20,20,20	0
57	MG	2A	3254	1/1	0.96	0.10	81,81,81,81	0
57	MG	1B	216	1/1	0.96	0.22	53,53,53,53	0
57	MG	1A	4019	1/1	0.96	0.12	36,36,36,36	0
59	CLM	1A	4097	20/20	0.96	0.27	29,37,54,64	0
57	MG	2A	3517	1/1	0.96	0.16	69,69,69,69	0
57	MG	1B	218	1/1	0.96	0.32	49,49,49,49	0
57	MG	2A	3519	1/1	0.96	0.14	49,49,49,49	0
57	MG	2A	3520	1/1	0.96	0.12	62,62,62,62	0
57	MG	2A	3024	1/1	0.96	0.28	53,53,53,53	0
60	ZN	26	102	1/1	0.96	0.21	60,60,60,60	0
57	MG	2A	3141	1/1	0.96	0.17	59,59,59,59	0
57	MG	2A	3726	1/1	0.97	0.17	43,43,43,43	0
57	MG	2D	302	1/1	0.97	0.27	53,53,53,53	0
57	MG	2D	303	1/1	0.97	0.12	30,30,30,30	0
57	MG	1A	3914	1/1	0.97	0.19	25,25,25,25	0
57	MG	1A	3242	1/1	0.97	0.35	36,36,36,36	0
57	MG	2A	3322	1/1	0.97	0.28	57,57,57,57	0
57	MG	2a	1705	1/1	0.97	0.10	74,74,74,74	0
57	MG	2A	3084	1/1	0.97	0.19	55,55,55,55	0
57	MG	1A	3916	1/1	0.97	0.47	37,37,37,37	0
57	MG	1A	3243	1/1	0.97	0.15	26,26,26,26	0
57	MG	2A	3205	1/1	0.97	0.16	63,63,63,63	0
57	MG	2A	3734	1/1	0.97	0.05	67,67,67,67	0
57	MG	1A	3112	1/1	0.97	0.14	34,34,34,34	0
57	MG	1A	3641	1/1	0.97	0.25	25,25,25,25	0
57	MG	1A	3113	1/1	0.97	0.26	31,31,31,31	0
57	MG	1A	3703	1/1	0.97	0.18	31,31,31,31	0
57	MG	1a	1602	1/1	0.97	0.11	67,67,67,67	0
57	MG	2A	3591	1/1	0.97	0.23	65,65,65,65	0
57	MG	1A	3770	1/1	0.97	0.19	24,24,24,24	0
57	MG	1a	1711	1/1	0.97	0.29	62,62,62,62	0
57	MG	1a	1712	1/1	0.97	0.03	85,85,85,85	0
57	MG	1A	3083	1/1	0.97	0.31	46,46,46,46	0
57	MG	2A	3746	1/1	0.97	0.33	39,39,39,39	0
57	MG	1A	3001	1/1	0.97	0.15	48,48,48,48	0
57	MG	2A	3461	1/1	0.97	0.14	70,70,70,70	0
57	MG	1A	3061	1/1	0.97	0.19	45,45,45,45	0
57	MG	1A	3191	1/1	0.97	0.24	32,32,32,32	0
57	MG	1a	1609	1/1	0.97	0.11	73,73,73,73	0
57	MG	1A	4007	1/1	0.97	0.22	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2R	201	1/1	0.97	0.26	66,66,66,66	0
57	MG	1A	4091	1/1	0.97	0.07	46,46,46,46	0
57	MG	1A	4008	1/1	0.97	0.10	32,32,32,32	0
57	MG	1A	4093	1/1	0.97	0.11	52,52,52,52	0
57	MG	2A	3607	1/1	0.97	0.17	66,66,66,66	0
57	MG	1A	3280	1/1	0.97	0.24	37,37,37,37	0
57	MG	2a	1734	1/1	0.97	0.21	67,67,67,67	0
57	MG	1A	3649	1/1	0.97	0.11	43,43,43,43	0
57	MG	1A	3281	1/1	0.97	0.52	42,42,42,42	0
57	MG	2a	1737	1/1	0.97	0.32	63,63,63,63	0
57	MG	1A	3600	1/1	0.97	0.19	27,27,27,27	0
57	MG	1A	3037	1/1	0.97	0.18	20,20,20,20	0
57	MG	1A	3118	1/1	0.97	0.24	28,28,28,28	0
57	MG	1A	3286	1/1	0.97	0.12	46,46,46,46	0
57	MG	1Q	207	1/1	0.97	0.22	35,35,35,35	0
57	MG	2A	3478	1/1	0.97	0.12	68,68,68,68	0
57	MG	1A	3119	1/1	0.97	0.18	39,39,39,39	0
57	MG	2A	3619	1/1	0.97	0.17	50,50,50,50	0
57	MG	2A	3620	1/1	0.97	0.13	44,44,44,44	0
57	MG	1A	3937	1/1	0.97	0.17	30,30,30,30	0
57	MG	1R	203	1/1	0.97	0.26	38,38,38,38	0
57	MG	1A	3401	1/1	0.97	0.33	54,54,54,54	0
57	MG	1A	3143	1/1	0.97	0.12	51,51,51,51	0
57	MG	1A	3518	1/1	0.97	0.24	49,49,49,49	0
57	MG	1a	1738	1/1	0.97	0.36	62,62,62,62	0
57	MG	25	102	1/1	0.97	0.48	43,43,43,43	0
57	MG	1A	3325	1/1	0.97	0.23	52,52,52,52	0
57	MG	1A	3289	1/1	0.97	0.56	47,47,47,47	0
57	MG	1A	3101	1/1	0.97	0.17	41,41,41,41	0
57	MG	1A	3611	1/1	0.97	0.14	60,60,60,60	0
57	MG	1A	3725	1/1	0.97	0.09	53,53,53,53	0
57	MG	1B	215	1/1	0.97	0.17	43,43,43,43	0
57	MG	1A	3726	1/1	0.97	0.20	62,62,62,62	0
57	MG	2A	3493	1/1	0.97	0.18	64,64,64,64	0
57	MG	1A	3793	1/1	0.97	0.22	20,20,20,20	0
57	MG	1A	3010	1/1	0.97	0.21	34,34,34,34	0
57	MG	2A	3785	1/1	0.97	0.13	43,43,43,43	0
57	MG	1A	3008	1/1	0.97	0.21	24,24,24,24	0
57	MG	2A	3639	1/1	0.97	0.08	46,46,46,46	0
57	MG	1A	3729	1/1	0.97	0.18	28,28,28,28	0
57	MG	1A	3872	1/1	0.97	0.19	31,31,31,31	0
57	MG	1A	3730	1/1	0.97	0.15	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3791	1/1	0.97	0.09	53,53,53,53	0
57	MG	1a	1755	1/1	0.97	0.14	82,82,82,82	0
57	MG	1A	3614	1/1	0.97	0.17	15,15,15,15	0
57	MG	1V	201	1/1	0.97	0.25	30,30,30,30	0
57	MG	2a	1774	1/1	0.97	0.13	63,63,63,63	0
57	MG	1a	1758	1/1	0.97	0.16	34,34,34,34	0
57	MG	1B	224	1/1	0.97	0.19	57,57,57,57	0
57	MG	1A	3615	1/1	0.97	0.24	31,31,31,31	0
57	MG	1V	204	1/1	0.97	0.18	29,29,29,29	0
57	MG	2A	3139	1/1	0.97	0.22	57,57,57,57	0
57	MG	1A	3802	1/1	0.97	0.24	22,22,22,22	0
57	MG	1A	3293	1/1	0.97	0.50	53,53,53,53	0
57	MG	2A	3022	1/1	0.97	0.26	43,43,43,43	0
57	MG	2A	3804	1/1	0.97	0.17	48,48,48,48	0
57	MG	1A	3669	1/1	0.97	0.16	39,39,39,39	0
57	MG	2A	3655	1/1	0.97	0.16	63,63,63,63	0
57	MG	1W	201	1/1	0.97	0.16	45,45,45,45	0
57	MG	2A	3145	1/1	0.97	0.14	38,38,38,38	0
57	MG	2A	3658	1/1	0.97	0.14	44,44,44,44	0
57	MG	1a	1768	1/1	0.97	0.20	66,66,66,66	0
57	MG	1A	3047	1/1	0.97	0.23	33,33,33,33	0
57	MG	1A	3526	1/1	0.97	0.33	30,30,30,30	0
57	MG	2a	1792	1/1	0.97	0.32	66,66,66,66	0
57	MG	1a	1652	1/1	0.97	0.13	54,54,54,54	0
57	MG	1W	205	1/1	0.97	0.25	41,41,41,41	0
57	MG	1A	3149	1/1	0.97	0.38	31,31,31,31	0
57	MG	2a	1632	1/1	0.97	0.29	54,54,54,54	0
57	MG	1A	3105	1/1	0.97	0.17	50,50,50,50	0
57	MG	2A	3521	1/1	0.97	0.11	60,60,60,60	0
57	MG	1A	3230	1/1	0.97	0.28	32,32,32,32	0
57	MG	1a	1777	1/1	0.97	0.14	55,55,55,55	0
57	MG	1A	3676	1/1	0.97	0.22	31,31,31,31	0
57	MG	2A	3525	1/1	0.97	0.13	58,58,58,58	0
57	MG	1B	235	1/1	0.97	0.16	48,48,48,48	0
57	MG	1X	105	1/1	0.97	0.18	51,51,51,51	0
57	MG	1A	3298	1/1	0.97	0.07	54,54,54,54	0
57	MG	1D	302	1/1	0.97	0.34	37,37,37,37	0
57	MG	1A	3231	1/1	0.97	0.32	32,32,32,32	0
57	MG	1Y	203	1/1	0.97	0.69	52,52,52,52	0
57	MG	2A	3831	1/1	0.97	0.13	42,42,42,42	0
57	MG	2a	1810	1/1	0.97	0.14	63,63,63,63	0
57	MG	1D	304	1/1	0.97	0.24	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3533	1/1	0.97	0.49	69,69,69,69	0
57	MG	1A	4046	1/1	0.97	0.10	52,52,52,52	0
57	MG	2A	3405	1/1	0.97	0.26	60,60,60,60	0
57	MG	2A	3836	1/1	0.97	0.12	64,64,64,64	0
57	MG	1A	3815	1/1	0.97	0.30	33,33,33,33	0
57	MG	1a	1668	1/1	0.97	0.19	70,70,70,70	0
57	MG	1A	3077	1/1	0.97	0.17	31,31,31,31	0
57	MG	1a	1670	1/1	0.97	0.14	72,72,72,72	0
57	MG	2A	3841	1/1	0.97	0.17	24,24,24,24	0
57	MG	1A	3205	1/1	0.97	0.25	19,19,19,19	0
57	MG	2A	3843	1/1	0.97	0.07	58,58,58,58	0
57	MG	2A	3844	1/1	0.97	0.12	41,41,41,41	0
57	MG	1A	3580	1/1	0.97	0.11	37,37,37,37	0
57	MG	1A	3819	1/1	0.97	0.18	32,32,32,32	0
57	MG	1A	3820	1/1	0.97	0.17	27,27,27,27	0
57	MG	1A	3126	1/1	0.97	0.32	38,38,38,38	0
57	MG	2A	3545	1/1	0.97	0.10	58,58,58,58	0
57	MG	1A	3683	1/1	0.97	0.17	30,30,30,30	0
57	MG	1E	302	1/1	0.97	0.24	34,34,34,34	0
57	MG	1A	4055	1/1	0.97	0.24	31,31,31,31	0
57	MG	1A	3582	1/1	0.97	0.46	39,39,39,39	0
57	MG	1A	3066	1/1	0.97	0.26	32,32,32,32	0
57	MG	2A	3697	1/1	0.97	0.18	40,40,40,40	0
57	MG	1A	3977	1/1	0.97	0.16	55,55,55,55	0
57	MG	1A	3180	1/1	0.97	0.15	33,33,33,33	0
57	MG	1A	3267	1/1	0.97	0.28	36,36,36,36	0
57	MG	2A	3301	1/1	0.97	0.10	81,81,81,81	0
57	MG	1A	3827	1/1	0.97	0.24	50,50,50,50	0
57	MG	13	102	1/1	0.97	0.15	30,30,30,30	0
57	MG	1F	301	1/1	0.97	0.25	38,38,38,38	0
57	MG	1A	3154	1/1	0.97	0.31	34,34,34,34	0
57	MG	1A	3903	1/1	0.97	0.18	22,22,22,22	0
57	MG	2A	3429	1/1	0.97	0.19	59,59,59,59	0
57	MG	1A	3904	1/1	0.97	0.23	53,53,53,53	0
57	MG	1A	3690	1/1	0.97	0.15	26,26,26,26	0
57	MG	15	103	1/1	0.97	0.22	26,26,26,26	0
57	MG	1A	3023	1/1	0.97	0.21	16,16,16,16	0
57	MG	1A	3758	1/1	0.97	0.18	47,47,47,47	0
57	MG	2A	3567	1/1	0.97	0.14	38,38,38,38	0
57	MG	2A	3715	1/1	0.97	0.14	32,32,32,32	0
57	MG	1A	3635	1/1	0.97	0.22	32,32,32,32	0
57	MG	1A	3909	1/1	0.97	0.14	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1691	1/1	0.97	0.17	44,44,44,44	0
57	MG	1A	3012	1/1	0.97	0.12	32,32,32,32	0
60	ZN	1Y	204	1/1	0.97	0.19	60,60,60,60	0
57	MG	17	101	1/1	0.97	0.14	34,34,34,34	0
57	MG	1A	3694	1/1	0.97	0.11	42,42,42,42	0
57	MG	1A	3013	1/1	0.97	0.27	28,28,28,28	0
57	MG	1A	3913	1/1	0.97	0.15	29,29,29,29	0
57	MG	1a	1822	1/1	0.97	0.23	63,63,63,63	0
57	MG	2A	3578	1/1	0.97	0.14	45,45,45,45	0
57	MG	18	103	1/1	0.98	0.29	40,40,40,40	0
57	MG	1A	3939	1/1	0.98	0.20	37,37,37,37	0
57	MG	1A	3738	1/1	0.98	0.19	49,49,49,49	0
57	MG	1a	1776	1/1	0.98	0.18	70,70,70,70	0
57	MG	1a	1655	1/1	0.98	0.15	72,72,72,72	0
57	MG	1A	3642	1/1	0.98	0.20	31,31,31,31	0
57	MG	1A	3201	1/1	0.98	0.27	26,26,26,26	0
57	MG	1W	204	1/1	0.98	0.47	40,40,40,40	0
57	MG	1A	3855	1/1	0.98	0.23	32,32,32,32	0
57	MG	1A	3069	1/1	0.98	0.31	25,25,25,25	0
57	MG	2A	3554	1/1	0.98	0.20	39,39,39,39	0
57	MG	1A	3141	1/1	0.98	0.23	29,29,29,29	0
57	MG	1N	204	1/1	0.98	0.44	51,51,51,51	0
57	MG	1A	4082	1/1	0.98	0.26	23,23,23,23	0
57	MG	1a	1607	1/1	0.98	0.22	51,51,51,51	0
57	MG	1A	3990	1/1	0.98	0.24	40,40,40,40	0
57	MG	1A	3743	1/1	0.98	0.30	61,61,61,61	0
57	MG	1A	3142	1/1	0.98	0.25	20,20,20,20	0
57	MG	1X	107	1/1	0.98	0.18	29,29,29,29	0
57	MG	1B	236	1/1	0.98	0.20	30,30,30,30	0
57	MG	1A	3560	1/1	0.98	0.20	26,26,26,26	0
57	MG	1A	3536	1/1	0.98	0.20	38,38,38,38	0
57	MG	2A	3808	1/1	0.98	0.08	59,59,59,59	0
57	MG	1A	3562	1/1	0.98	0.21	25,25,25,25	0
57	MG	1a	1730	1/1	0.98	0.21	54,54,54,54	0
57	MG	1a	1731	1/1	0.98	0.16	55,55,55,55	0
57	MG	1A	3563	1/1	0.98	0.44	34,34,34,34	0
57	MG	1A	3240	1/1	0.98	0.28	29,29,29,29	0
57	MG	1A	3187	1/1	0.98	0.23	50,50,50,50	0
57	MG	1A	3156	1/1	0.98	0.24	26,26,26,26	0
57	MG	2A	3574	1/1	0.98	0.08	47,47,47,47	0
57	MG	1A	3516	1/1	0.98	0.21	27,27,27,27	0
57	MG	2A	3073	1/1	0.98	0.68	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3787	1/1	0.98	0.21	24,24,24,24	0
57	MG	1A	3753	1/1	0.98	0.19	59,59,59,59	0
57	MG	2A	3076	1/1	0.98	0.21	26,26,26,26	0
57	MG	1A	3003	1/1	0.98	0.17	29,29,29,29	0
57	MG	2A	3009	1/1	0.98	0.15	49,49,49,49	0
57	MG	1a	1740	1/1	0.98	0.16	61,61,61,61	0
57	MG	2A	3826	1/1	0.98	0.13	46,46,46,46	0
57	MG	1A	3384	1/1	0.98	0.19	49,49,49,49	0
57	MG	1A	3283	1/1	0.98	0.29	31,31,31,31	0
57	MG	1A	3078	1/1	0.98	0.20	26,26,26,26	0
57	MG	1A	3365	1/1	0.98	0.17	66,66,66,66	0
57	MG	2A	3365	1/1	0.98	0.14	47,47,47,47	0
57	MG	1a	1745	1/1	0.98	0.17	52,52,52,52	0
57	MG	1E	305	1/1	0.98	0.17	36,36,36,36	0
57	MG	1A	3033	1/1	0.98	0.32	30,30,30,30	0
57	MG	1a	1813	1/1	0.98	0.06	61,61,61,61	0
57	MG	2d	302	1/1	0.98	0.12	70,70,70,70	0
57	MG	1A	3760	1/1	0.98	0.17	37,37,37,37	0
57	MG	1a	1749	1/1	0.98	0.25	37,37,37,37	0
57	MG	2f	202	1/1	0.98	0.14	77,77,77,77	0
57	MG	2A	3673	1/1	0.98	0.16	41,41,41,41	0
57	MG	1A	3176	1/1	0.98	0.22	31,31,31,31	0
57	MG	2A	3595	1/1	0.98	0.13	37,37,37,37	0
57	MG	2A	3596	1/1	0.98	0.12	40,40,40,40	0
57	MG	1E	309	1/1	0.98	0.21	33,33,33,33	0
57	MG	2Y	201	1/1	0.98	0.35	56,56,56,56	0
57	MG	1A	3146	1/1	0.98	0.19	31,31,31,31	0
57	MG	1A	3663	1/1	0.98	0.20	38,38,38,38	0
57	MG	1A	3799	1/1	0.98	0.08	46,46,46,46	0
57	MG	2A	3026	1/1	0.98	0.57	54,54,54,54	0
57	MG	1A	3229	1/1	0.98	0.20	31,31,31,31	0
57	MG	1A	3883	1/1	0.98	0.20	33,33,33,33	0
57	MG	2A	3237	1/1	0.98	0.12	67,67,67,67	0
57	MG	1A	3801	1/1	0.98	0.14	19,19,19,19	0
57	MG	2a	1673	1/1	0.98	0.17	66,66,66,66	0
57	MG	2A	3851	1/1	0.98	0.14	56,56,56,56	0
57	MG	1A	3578	1/1	0.98	0.17	39,39,39,39	0
57	MG	1A	3803	1/1	0.98	0.17	47,47,47,47	0
57	MG	1A	3106	1/1	0.98	0.18	38,38,38,38	0
57	MG	1A	3805	1/1	0.98	0.30	32,32,32,32	0
57	MG	1F	309	1/1	0.98	0.20	30,30,30,30	0
57	MG	1U	209	1/1	0.98	0.30	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3036	1/1	0.98	0.22	31,31,31,31	0
57	MG	2A	3613	1/1	0.98	0.21	68,68,68,68	0
57	MG	1A	3135	1/1	0.98	0.13	36,36,36,36	0
57	MG	1A	3890	1/1	0.98	0.17	22,22,22,22	0
57	MG	1A	3034	1/1	0.98	0.35	34,34,34,34	0
57	MG	1A	3935	1/1	0.98	0.18	28,28,28,28	0
57	MG	2a	1687	1/1	0.98	0.16	68,68,68,68	0
57	MG	1A	3015	1/1	0.98	0.24	36,36,36,36	0
57	MG	1A	3030	1/1	0.98	0.25	30,30,30,30	0
57	MG	2A	3181	1/1	0.98	0.10	46,46,46,46	0
60	ZN	25	106	1/1	0.98	0.22	62,62,62,62	0
57	MG	2A	3469	1/1	0.98	0.21	37,37,37,37	0
60	ZN	29	501	1/1	0.98	0.13	68,68,68,68	0
57	MG	1A	3031	1/1	0.98	0.31	33,33,33,33	0
61	SF4	2d	303	8/8	0.98	0.15	71,81,85,99	0
57	MG	1A	3840	1/1	0.99	0.14	39,39,39,39	0
57	MG	1U	208	1/1	0.99	0.24	36,36,36,36	0
57	MG	2A	3723	1/1	0.99	0.11	46,46,46,46	0
57	MG	1A	3697	1/1	0.99	0.27	27,27,27,27	0
57	MG	1D	312	1/1	0.99	0.19	38,38,38,38	0
57	MG	2A	3625	1/1	0.99	0.16	43,43,43,43	0
57	MG	1A	4078	1/1	0.99	0.23	15,15,15,15	0
57	MG	1A	3713	1/1	0.99	0.14	15,15,15,15	0
57	MG	1A	3674	1/1	0.99	0.19	24,24,24,24	0
57	MG	1Q	206	1/1	0.99	0.38	40,40,40,40	0
57	MG	1E	303	1/1	0.99	0.32	31,31,31,31	0
57	MG	1A	4059	1/1	0.99	0.16	43,43,43,43	0
57	MG	1A	3686	1/1	0.99	0.21	26,26,26,26	0
57	MG	1A	3057	1/1	0.99	0.25	26,26,26,26	0
57	MG	1A	3701	1/1	0.99	0.14	17,17,17,17	0
57	MG	2A	3736	1/1	0.99	0.08	65,65,65,65	0
57	MG	1A	3097	1/1	0.99	0.13	32,32,32,32	0
57	MG	1A	3194	1/1	0.99	0.26	33,33,33,33	0
57	MG	2A	3572	1/1	0.99	0.17	56,56,56,56	0
57	MG	1A	3128	1/1	0.99	0.27	40,40,40,40	0
57	MG	1A	3705	1/1	0.99	0.19	33,33,33,33	0
57	MG	1A	3098	1/1	0.99	0.28	20,20,20,20	0
57	MG	1X	101	1/1	0.99	0.48	33,33,33,33	0
57	MG	1A	3619	1/1	0.99	0.26	32,32,32,32	0
57	MG	1A	3871	1/1	0.99	0.34	39,39,39,39	0
57	MG	1A	3162	1/1	0.99	0.30	35,35,35,35	0
57	MG	1F	304	1/1	0.99	0.14	35,35,35,35	0

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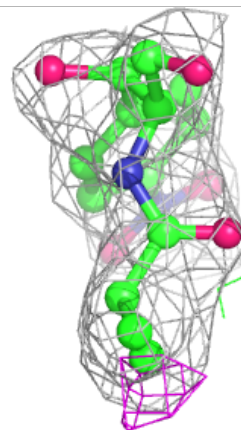
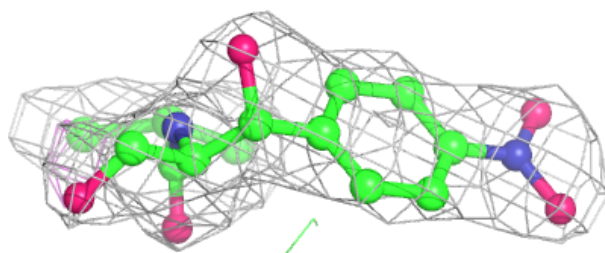
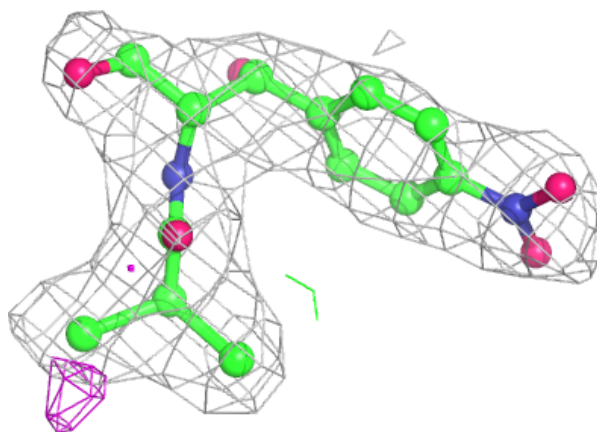
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1U	201	1/1	0.99	0.38	31,31,31,31	0
57	MG	2A	3822	1/1	0.99	0.14	41,41,41,41	0
57	MG	1A	3854	1/1	0.99	0.28	22,22,22,22	0
60	ZN	15	107	1/1	0.99	0.25	43,43,43,43	0
60	ZN	16	103	1/1	0.99	0.28	53,53,53,53	0
60	ZN	19	102	1/1	0.99	0.24	44,44,44,44	0
57	MG	2A	3714	1/1	0.99	0.22	47,47,47,47	0
57	MG	1A	3931	1/1	0.99	0.13	45,45,45,45	0
57	MG	1A	3282	1/1	0.99	0.18	31,31,31,31	0
57	MG	1a	1761	1/1	0.99	0.15	68,68,68,68	0
57	MG	1a	1762	1/1	0.99	0.11	46,46,46,46	0
57	MG	1A	3173	1/1	0.99	0.24	41,41,41,41	0
57	MG	2A	3792	1/1	0.99	0.12	72,72,72,72	0
61	SF4	1d	501	8/8	0.99	0.15	62,70,75,80	0
57	MG	1A	3396	1/1	0.99	0.49	34,34,34,34	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.

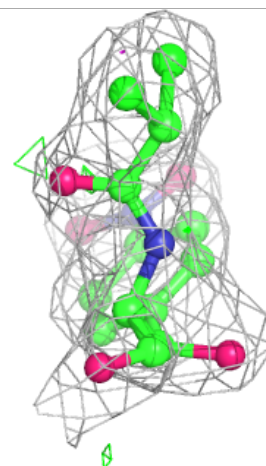
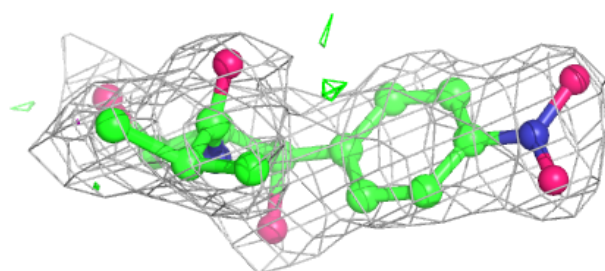
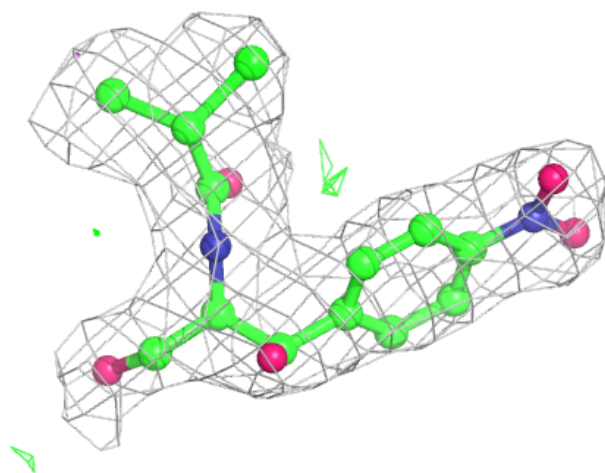
Electron density around CLM 2A 3863:

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



Electron density around CLM 1A 4097:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.