wwPDB X-ray Structure Validation Summary Report (i)

Feb 25, 2024 – 03:04 PM EST

PDB ID	:	5HAU
Title	:	Crystal structure of antimicrobial peptide Bac7(1-19) bound to the Thermus thermophilus 70S ribosome
Authors	:	Gagnon, M.G.; Roy, R.N.; Lomakin, I.B.; Florin, T.; Mankin, A.S.; Steitz, T.A.
Deposited on	:	2015-12-30
Resolution	:	3.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

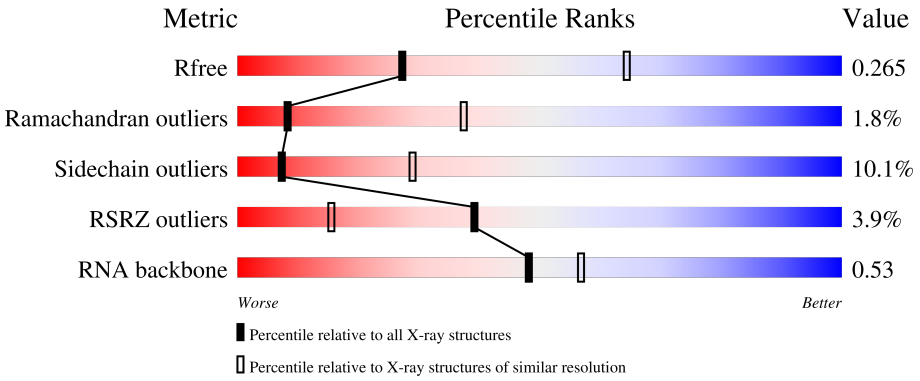
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	3% 82% 16%
1	2A	2915	3% 80% 18%
2	1B	121	91% 8%
2	2B	121	84% 15%

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Mol	Chain	Length	Quality of chain
3	1C	229	45% 51% 7% 41%
3	2C	229	48% 51% 7% 41%
4	1D	276	91% 8%
4	2D	276	92% 7%
5	1E	206	92% 7%
5	2E	206	91% 8%
6	1F	210	87% 10%
6	2F	210	89% 8%
7	1G	182	88% 12%
7	2G	182	86% 13%
8	1H	180	92% 5%
8	2H	180	87% 10%
9	1J	173	7% 64% 12% 25%
9	2J	173	12% 62% 13% 25%
10	1K	147	14% 37% 8% 54%
10	2K	147	26% 35% 10% 55%
11	1L	140	93% 7%
11	2L	140	91% 9%
12	1M	122	95% 5%
12	2M	122	91% 9%
13	1N	150	90% 9%
13	2N	150	91% 8%
14	1O	141	94% 6%
14	2O	141	92% 7%
15	1P	118	85% 15%

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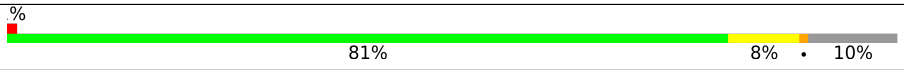
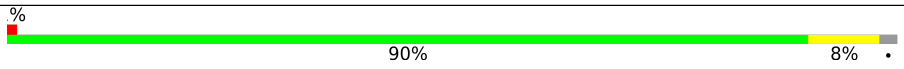
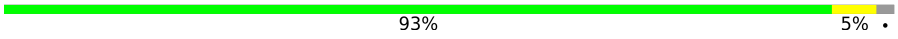
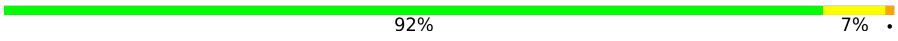
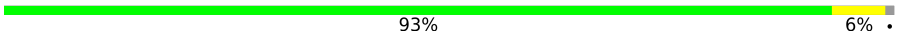
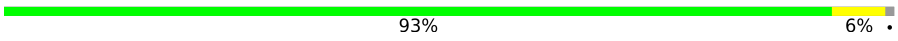
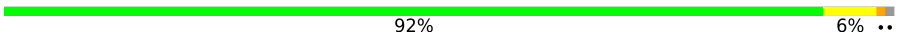
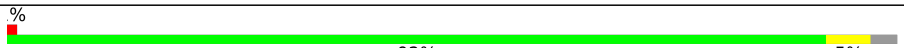
Mol	Chain	Length	Quality of chain
15	2P	118	
16	1Q	112	
16	2Q	112	
17	1R	146	
17	2R	146	
18	1S	118	
18	2S	118	
19	1T	101	
19	2T	101	
20	1U	113	
20	2U	113	
21	1V	96	
21	2V	96	
22	1W	110	
22	2W	110	
23	1X	206	
23	2X	206	
24	1Y	85	
24	2Y	85	
25	1Z	98	
25	2Z	98	
26	10	72	
26	20	72	
27	11	60	
27	21	60	

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Mol	Chain	Length	Quality of chain
28	12	71	4% 76% 20%
28	22	71	7% 76% 18%
29	13	60	90% 8%
29	23	60	88% 10%
30	14	54	89% 9%
30	24	54	89% 9%
31	15	49	94%
31	25	49	90% 8%
32	16	65	91% 8%
32	26	65	91% 8%
33	17	37	100%
33	27	37	3% 97%
34	1a	1521	2% 80% 18%
34	2a	1521	2% 81% 17%
35	1b	256	% 79% 10% 10%
35	2b	256	5% 81% 9% 10%
36	1c	239	82% 5% 14%
36	2c	239	2% 79% 8% 14%
37	1d	209	91% 8%
37	2d	209	92% 7%
38	1e	162	84% 7% 9%
38	2e	162	86% 6% 9%
39	1f	101	90% 9%
39	2f	101	92% 7%
40	1g	156	6% 93% 6%

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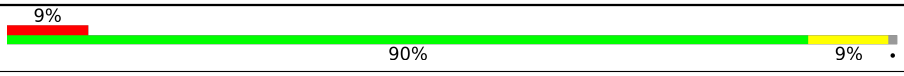
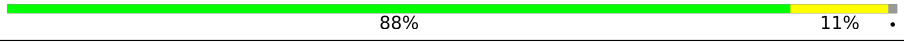
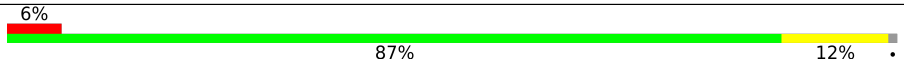
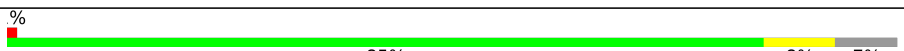
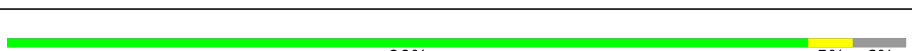
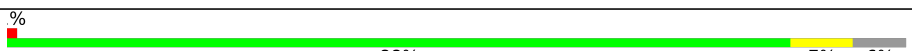
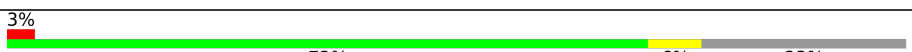
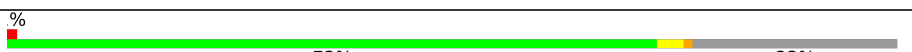
Mol	Chain	Length	Quality of chain
40	2g	156	
41	1h	138	
41	2h	138	
42	1i	128	
42	2i	128	
43	1j	105	
43	2j	105	
44	1k	129	
44	2k	129	
45	1l	132	
45	2l	132	
46	1m	126	
46	2m	126	
47	1n	61	
47	2n	61	
48	1o	89	
48	2o	89	
49	1p	88	
49	2p	88	
50	1q	105	
50	2q	105	
51	1r	88	
51	2r	88	
52	1s	93	
52	2s	93	

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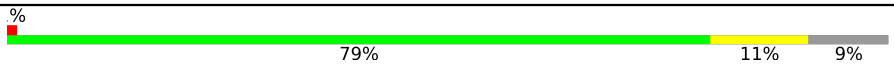
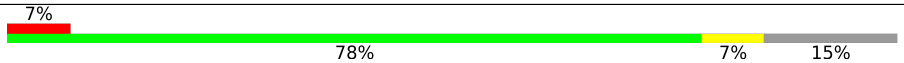
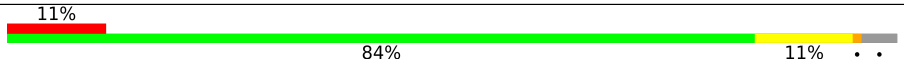
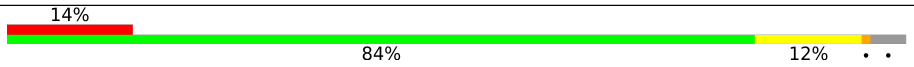
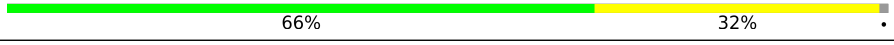
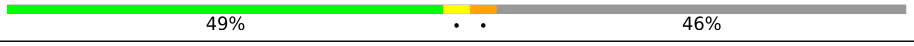
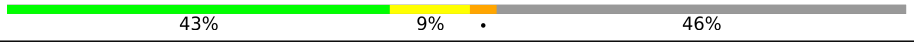
Mol	Chain	Length	Quality of chain
53	1t	106	
53	2t	106	
54	1u	27	
54	2u	27	
55	1z	758	
55	2z	758	
56	1y	24	
56	2y	24	
57	1w	77	
57	2w	77	
58	1x	35	
58	2x	35	

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
59	MG	1A	3018	-	-	-	X
59	MG	1A	3023	-	-	-	X
59	MG	1A	3104	-	-	-	X
59	MG	1A	3207	-	-	-	X
59	MG	1A	3223	-	-	-	X
59	MG	1A	3636	-	-	-	X
59	MG	1a	1622	-	-	-	X
59	MG	1a	1771	-	-	-	X
59	MG	2A	3220	-	-	-	X
59	MG	2A	3238	-	-	-	X
59	MG	2a	1603	-	-	-	X
59	MG	2a	1657	-	-	-	X
59	MG	2a	1754	-	-	-	X
60	ZN	13	103	-	-	-	X

2 Entry composition (i)

There are 63 unique types of molecules in this entry. The entry contains 306384 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	2872	Total	C	N	O	P	0	0	0
			61861	27532	11574	19884	2871			
1	2A	2868	Total	C	N	O	P	0	0	0
			61771	27492	11554	19858	2867			

- 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
			2573	1146	476	832	119			
2	2B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 3 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1C	135	Total	C	N	O	S	3	0	0
			1020	641	190	188	1			
3	2C	135	Total	C	N	O	S	3	0	0
			1020	641	190	188	1			

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	1D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
4	2D	275	Total	C	N	O	S	0	0	0
			2142	1352	426	361	3			

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
5	2E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1F	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
6	2F	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	1G	181	Total	C	N	O	S	0	0	0
			1425	914	256	251	4			
7	2G	181	Total	C	N	O	S	0	0	0
			1424	911	258	251	4			

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
8	2H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	1J	130	Total	C	N	O	0	0	0
			641	381	130	130			
9	2J	130	Total	C	N	O	0	0	0
			641	381	130	130			

- Molecule 10 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1K	67	Total	C	N	O	S	0	0	1
			499	310	94	92	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	2K	66	Total	C	N	O	S	0	0	0
			498	310	93	92	3			

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	1L	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			
11	2L	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	1M	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
12	2M	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	1N	149	Total	C	N	O	S	0	0	0
			1139	709	231	196	3			
13	2N	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	1O	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
14	2O	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1P	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
15	2P	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	1Q	110	Total	C	N	O		0	0	0
			877	553	175	149				
16	2Q	110	Total	C	N	O		0	0	0
			870	549	173	148				

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1R	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
17	2R	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	1S	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
18	2S	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	1T	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			
19	2T	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1U	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
20	2U	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1V	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
21	2V	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	1W	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
22	2W	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	1X	186	Total	C	N	O	S	0	0	0
			1460	932	259	267	2			
23	2X	186	Total	C	N	O	S	0	0	0
			1454	929	256	267	2			

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	1Y	76	Total	C	N	O	S	0	0	0
			604	373	128	102	1			
24	2Y	76	Total	C	N	O	S	0	0	0
			602	372	128	101	1			

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	1Z	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			
25	2Z	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	10	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	20	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	11	59	Total	C	N	O	0	0	0
			469	298	90	81			
27	21	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	12	69	Total	C	N	O	S	0	0	0
			558	352	102	99	5			
28	22	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	13	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			
29	23	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	14	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
30	24	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	15	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
31	25	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	16	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
32	26	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	17	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
33	27	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 34 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1a	1495	Total	C	N	O	P	0	0	0
			32141	14304	5958	10384	1495			
34	2a	1501	Total	C	N	O	P	0	0	0
			32268	14361	5980	10426	1501			

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1b	231	Total	C	N	O	S	0	0	0
			1846	1179	331	331	5			
35	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1c	206	Total	C	N	O	S	0	0	0
			1552	976	302	273	1			
36	2c	206	Total	C	N	O	S	0	0	0
			1544	970	300	273	1			

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1d	208	Total	C	N	O	S	0	0	0
			1659	1040	326	286	7			
37	2d	208	Total	C	N	O	S	0	0	0
			1678	1052	333	286	7			

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1e	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
38	2e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1f	100	Total	C	N	O	S	0	0	0
			812	514	146	149	3			
39	2f	100	Total	C	N	O	S	0	0	0
			820	518	147	152	3			

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	1g	155	Total	C	N	O	S	0	0	0
			1231	766	243	216	6			
40	2g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	1h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
41	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	1i	127	Total	C	N	O	0	0	0
			986	626	193	167			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	2i	127	Total 978	C 619	N 190	O 169	0	0	0

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	1j	97	Total 709	C 440	N 138	O 131	0	0	0
43	2j	96	Total 714	C 445	N 138	O 131	0	0	0

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1k	114	Total 833	C 519	N 156	O 155	S 3	0	0	0
44	2k	114	Total 833	C 519	N 156	O 155	S 3	0	0	0

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	1l	122	Total 930	C 585	N 185	O 159	S 1	0	0	0
45	2l	122	Total 930	C 585	N 185	O 159	S 1	0	0	0

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	1m	123	Total 966	C 598	N 200	O 166	S 2	0	0	0
46	2m	122	Total 950	C 586	N 197	O 165	S 2	0	0	0

- Molecule 47 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	1n	60	Total 492	C 312	N 104	O 72	S 4	0	0	0
47	2n	60	Total 492	C 312	N 104	O 72	S 4	0	0	0

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	1o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			
48	2o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	1p	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
49	2p	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
50	2q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	1r	68	Total	C	N	O	0	0	0
			555	355	108	92			
51	2r	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	1s	84	Total	C	N	O	S	0	0	0
			661	423	122	114	2			
52	2s	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1t	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
53	2t	96	Total	C	N	O	S	0	0	0
			731	449	156	124	2			

- Molecule 54 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	1u	23	Total	C	N	O	0	0	0
			199	122	48	29			
54	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 55 is a protein called Chimera protein of 50S ribosomal protein L9 and Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	1z	730	Total	C	N	O	S	0	0	0
			5690	3616	980	1075	19			
55	2z	730	Total	C	N	O	S	0	0	0
			5690	3616	980	1075	19			

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1y	6	Total	C	N	O	P	0	0	0
			129	58	24	41	6			
56	2y	5	Total	C	N	O	P	0	0	0
			109	49	22	33	5			

- Molecule 57 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
57	1w	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
57	2w	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 58 is a protein called Cathelicidin-3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	1x	19	Total	C	N	O	0	0	0
			168	106	43	19			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	2x	19	Total 168	C 106	N 43	O 19	0	0	0

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1A	780	Total 780	Mg 780	0	0
59	1B	24	Total 24	Mg 24	0	0
59	1D	4	Total 4	Mg 4	0	0
59	1E	6	Total 6	Mg 6	0	0
59	1F	7	Total 7	Mg 7	0	0
59	1G	2	Total 2	Mg 2	0	0
59	1H	1	Total 1	Mg 1	0	0
59	1L	2	Total 2	Mg 2	0	0
59	1M	1	Total 1	Mg 1	0	0
59	1N	2	Total 2	Mg 2	0	0
59	1O	2	Total 2	Mg 2	0	0
59	1P	2	Total 2	Mg 2	0	0
59	1S	4	Total 4	Mg 4	0	0
59	1T	1	Total 1	Mg 1	0	0
59	1U	3	Total 3	Mg 3	0	0
59	1W	1	Total 1	Mg 1	0	0
59	1X	2	Total 2	Mg 2	0	0
59	1Y	5	Total 5	Mg 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	10	2	Total Mg 2 2	0	0
59	11	1	Total Mg 1 1	0	0
59	13	3	Total Mg 3 3	0	0
59	14	1	Total Mg 1 1	0	0
59	15	2	Total Mg 2 2	0	0
59	16	2	Total Mg 2 2	0	0
59	17	2	Total Mg 2 2	0	0
59	1a	204	Total Mg 204 204	0	0
59	1b	1	Total Mg 1 1	0	0
59	1d	2	Total Mg 2 2	0	0
59	1f	1	Total Mg 1 1	0	0
59	1l	3	Total Mg 3 3	0	0
59	1t	1	Total Mg 1 1	0	0
59	1z	1	Total Mg 1 1	0	0
59	1w	6	Total Mg 6 6	0	0
59	2A	620	Total Mg 620 620	0	0
59	2B	13	Total Mg 13 13	0	0
59	2D	4	Total Mg 4 4	0	0
59	2E	4	Total Mg 4 4	0	0
59	2F	3	Total Mg 3 3	0	0
59	2G	1	Total Mg 1 1	0	0

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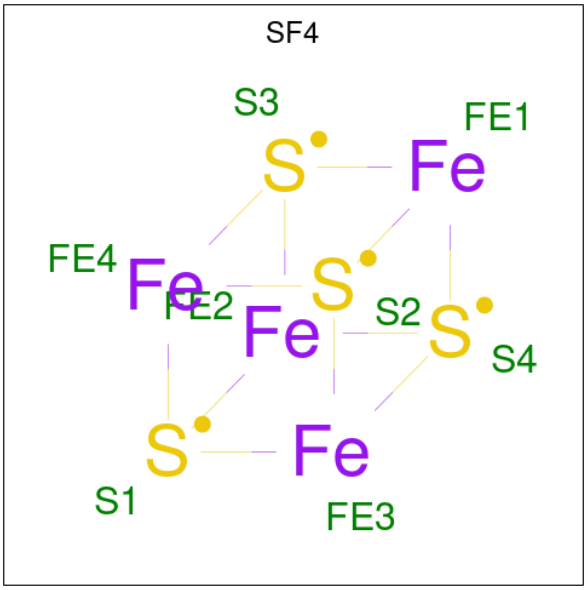
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	2M	2	Total Mg 2 2	0	0
59	2N	1	Total Mg 1 1	0	0
59	2O	2	Total Mg 2 2	0	0
59	2P	1	Total Mg 1 1	0	0
59	2R	1	Total Mg 1 1	0	0
59	2S	2	Total Mg 2 2	0	0
59	2W	1	Total Mg 1 1	0	0
59	2Y	1	Total Mg 1 1	0	0
59	23	1	Total Mg 1 1	0	0
59	26	2	Total Mg 2 2	0	0
59	2a	173	Total Mg 173 173	0	0
59	2d	1	Total Mg 1 1	0	0
59	2f	2	Total Mg 2 2	0	0
59	2j	1	Total Mg 1 1	0	0
59	2l	1	Total Mg 1 1	0	0
59	2n	1	Total Mg 1 1	0	0
59	2q	1	Total Mg 1 1	0	0
59	2t	1	Total Mg 1 1	0	0
59	2z	4	Total Mg 4 4	0	0
59	2w	4	Total Mg 4 4	0	0

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

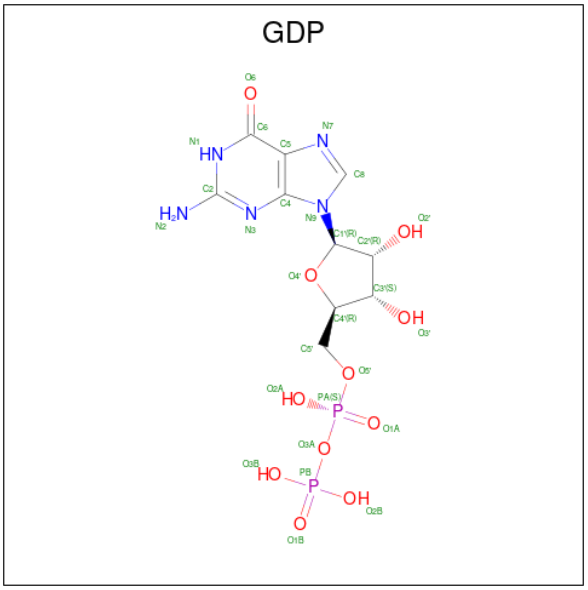
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1W	1	Total Zn 1 1	0	0
60	12	1	Total Zn 1 1	0	0
60	13	1	Total Zn 1 1	0	0
60	14	1	Total Zn 1 1	0	0
60	17	1	Total Zn 1 1	0	0
60	1n	1	Total Zn 1 1	0	0
60	2W	1	Total Zn 1 1	0	0
60	22	1	Total Zn 1 1	0	0
60	23	1	Total Zn 1 1	0	0
60	24	1	Total Zn 1 1	0	0
60	27	1	Total Zn 1 1	0	0
60	2n	1	Total Zn 1 1	0	0

- Molecule 61 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1z	1	Total C N O P 28 10 5 11 2	0	0
62	2z	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 63 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	1A	1299	Total O 1299 1299	0	0
63	1B	39	Total O 39 39	0	0
63	1D	15	Total O 15 15	0	0
63	1E	19	Total O 19 19	0	0
63	1F	12	Total O 12 12	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	1G	3	Total O 3 3	0	0
63	1H	1	Total O 1 1	0	0
63	1M	2	Total O 2 2	0	0
63	1N	12	Total O 12 12	0	0
63	1O	2	Total O 2 2	0	0
63	1P	4	Total O 4 4	0	0
63	1Q	1	Total O 1 1	0	0
63	1R	2	Total O 2 2	0	0
63	1S	4	Total O 4 4	0	0
63	1T	1	Total O 1 1	0	0
63	1U	2	Total O 2 2	0	0
63	1V	3	Total O 3 3	0	0
63	1X	2	Total O 2 2	0	0
63	1Y	4	Total O 4 4	0	0
63	1Z	1	Total O 1 1	0	0
63	11	2	Total O 2 2	0	0
63	15	2	Total O 2 2	0	0
63	16	10	Total O 10 10	0	0
63	17	1	Total O 1 1	0	0
63	1a	155	Total O 155 155	0	0
63	1d	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	1j	1	Total O 1 1	0	0
63	1l	2	Total O 2 2	0	0
63	1o	1	Total O 1 1	0	0
63	1p	2	Total O 2 2	0	0
63	1z	5	Total O 5 5	0	0
63	1w	4	Total O 4 4	0	0
63	1x	1	Total O 1 1	0	0
63	2A	650	Total O 650 650	0	0
63	2B	11	Total O 11 11	0	0
63	2D	8	Total O 8 8	0	0
63	2E	7	Total O 7 7	0	0
63	2F	5	Total O 5 5	0	0
63	2L	1	Total O 1 1	0	0
63	2M	2	Total O 2 2	0	0
63	2N	6	Total O 6 6	0	0
63	2O	3	Total O 3 3	0	0
63	2P	1	Total O 1 1	0	0
63	2R	2	Total O 2 2	0	0
63	2S	2	Total O 2 2	0	0
63	2U	1	Total O 1 1	0	0
63	2V	2	Total O 2 2	0	0

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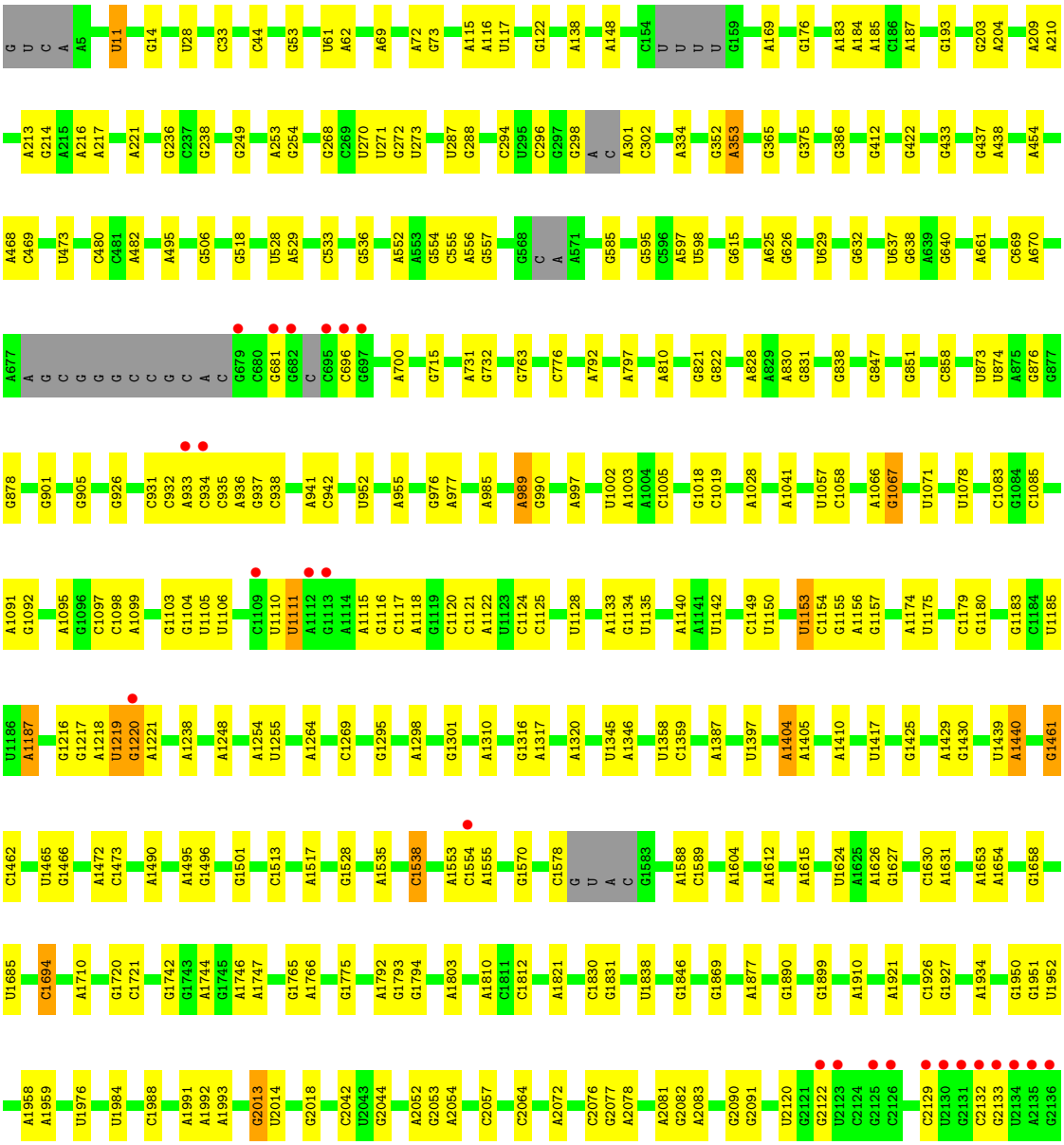
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	2W	1	Total O 1 1	0	0
63	2Y	5	Total O 5 5	0	0
63	2Z	2	Total O 2 2	0	0
63	21	2	Total O 2 2	0	0
63	24	1	Total O 1 1	0	0
63	26	3	Total O 3 3	0	0
63	2a	122	Total O 122 122	0	0
63	2f	1	Total O 1 1	0	0
63	2h	1	Total O 1 1	0	0
63	2j	1	Total O 1 1	0	0
63	2n	1	Total O 1 1	0	0
63	2t	1	Total O 1 1	0	0
63	2z	1	Total O 1 1	0	0
63	2y	1	Total O 1 1	0	0
63	2w	2	Total O 2 2	0	0

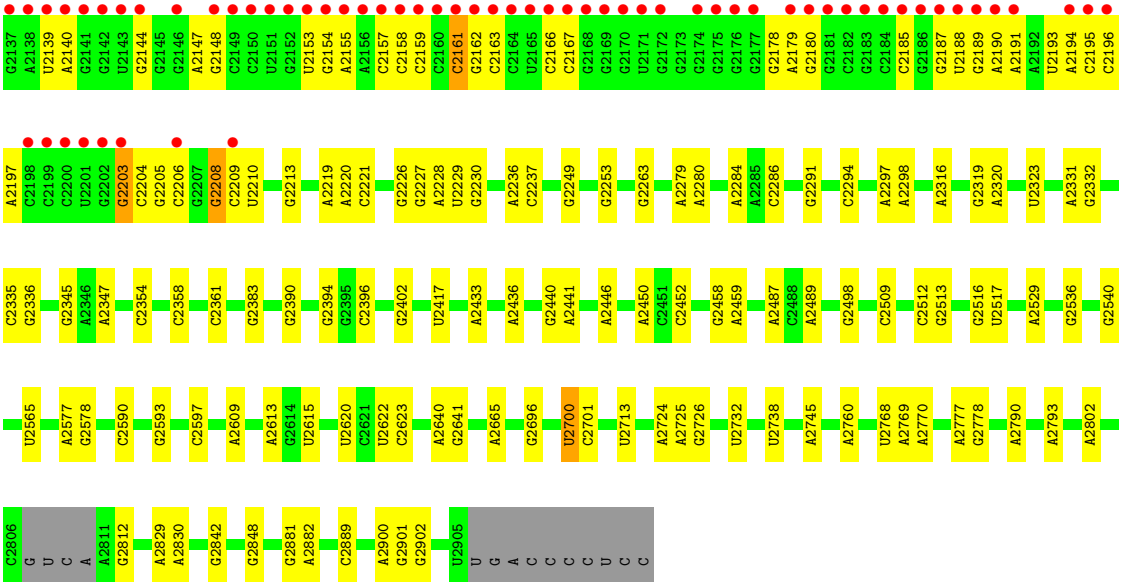
3 Residue-property plots (i)

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

- Molecule 1: 23S Ribosomal RNA

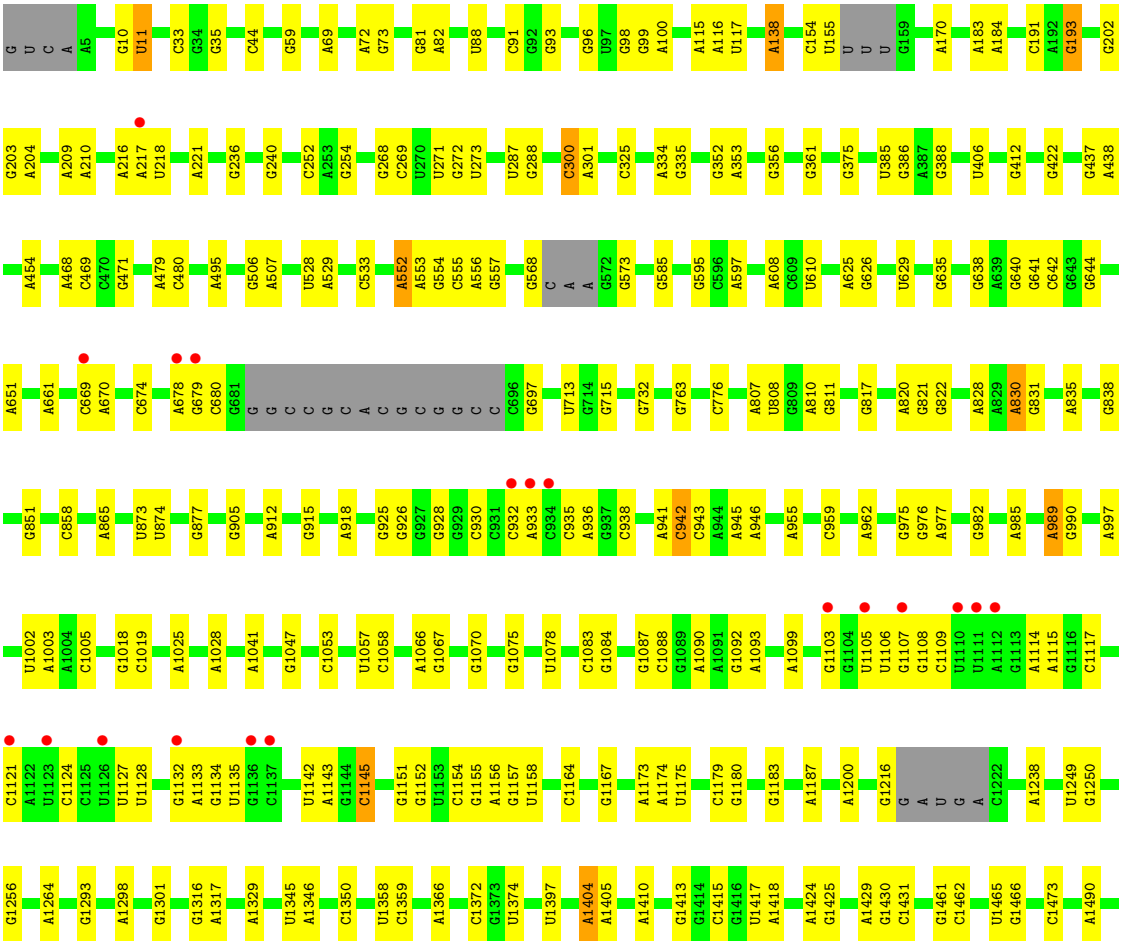
Chain 1A:

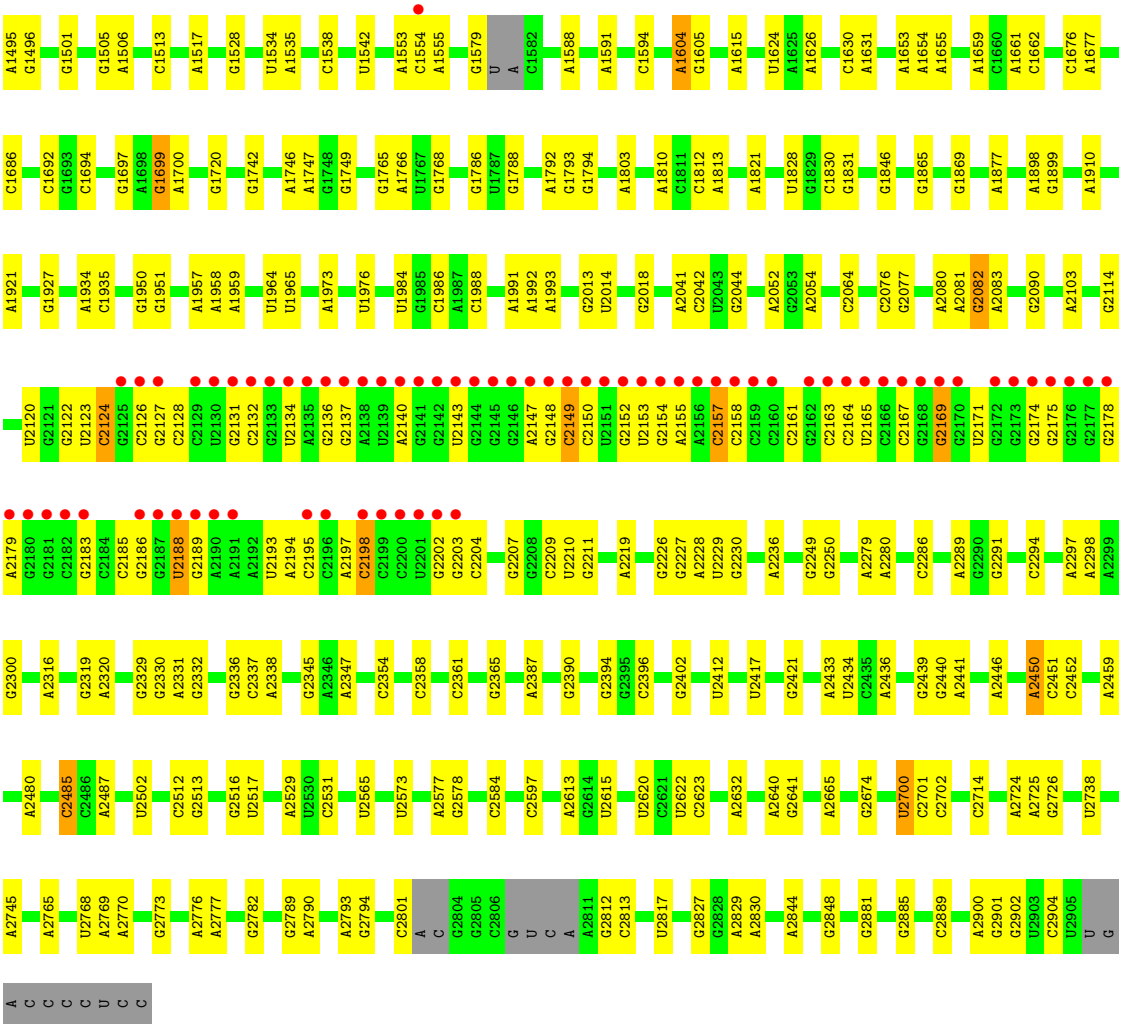




• Molecule 1: 23S Ribosomal RNA

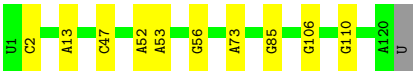
Chain 2A:





• Molecule 2: 5S Ribosomal RNA

Chain 1B:

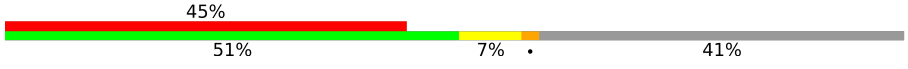


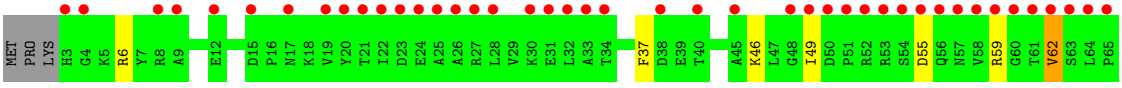
• Molecule 2: 5S Ribosomal RNA

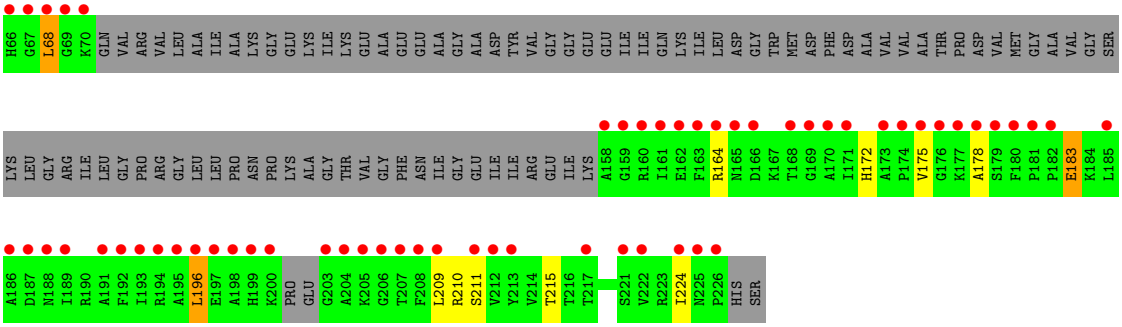
Chain 2B:

• Molecule 3: 50S ribosomal protein L1

Chain 1C:

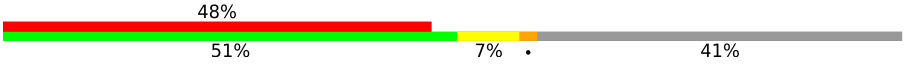


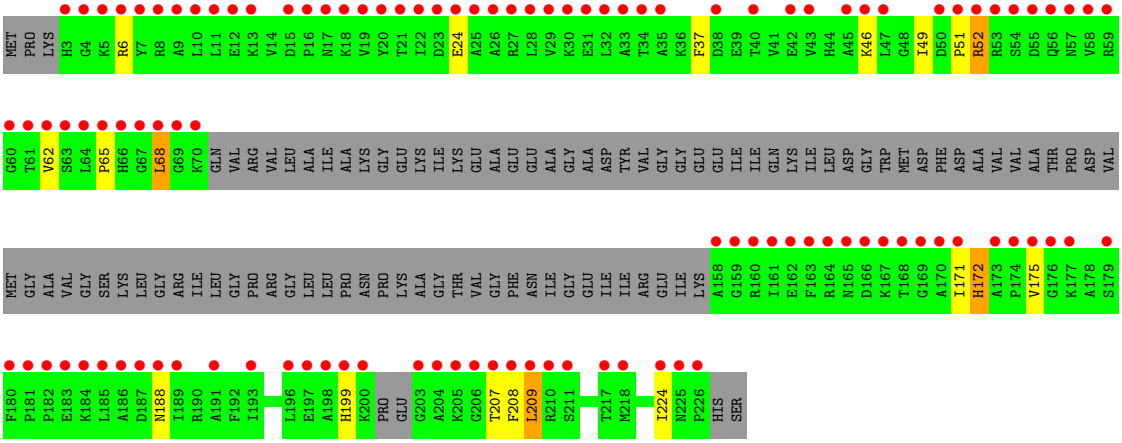




• Molecule 3: 50S ribosomal protein L1

Chain 2C:



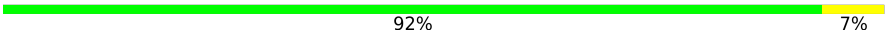


• Molecule 4: 50S ribosomal protein L2

Chain 1D:

• Molecule 4: 50S ribosomal protein L2

Chain 2D:

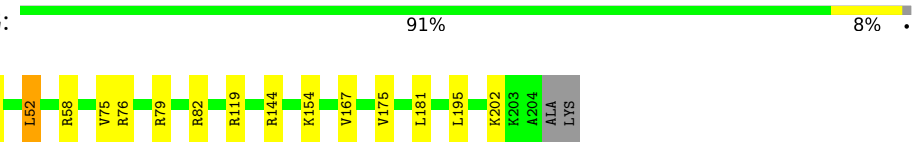


• Molecule 5: 50S ribosomal protein L3

Chain 1E:

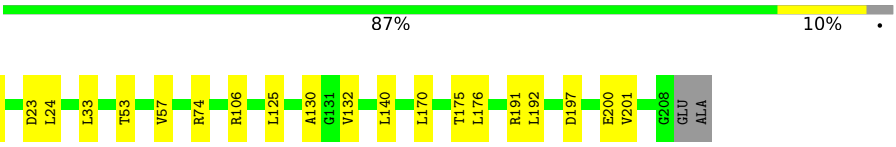
• Molecule 5: 50S ribosomal protein L3

Chain 2E:



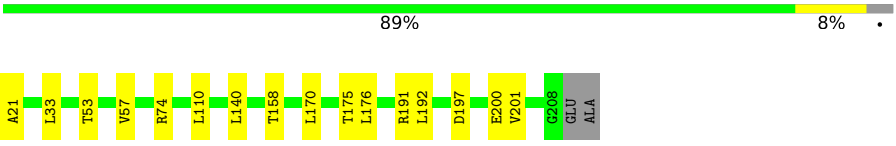
• Molecule 6: 50S ribosomal protein L4

Chain 1F:



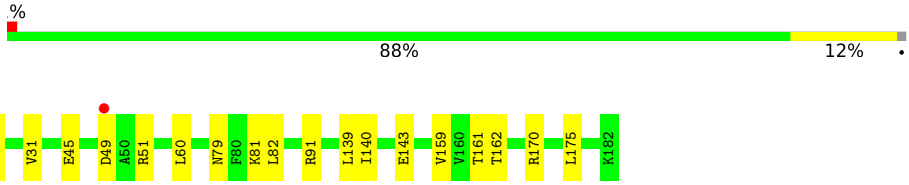
• Molecule 6: 50S ribosomal protein L4

Chain 2F:



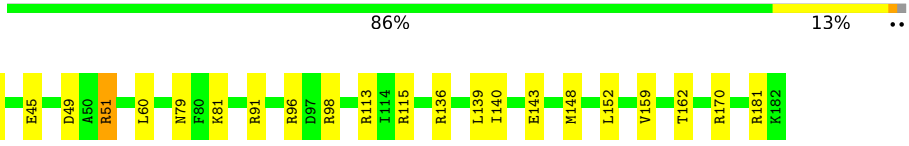
• Molecule 7: 50S ribosomal protein L5

Chain 1G:



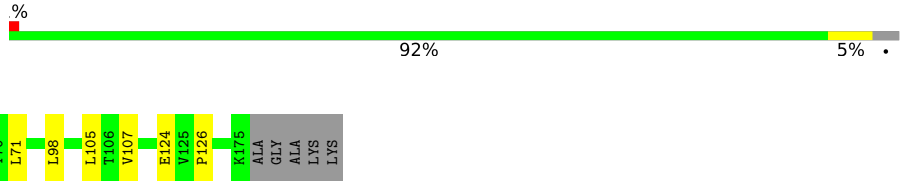
• Molecule 7: 50S ribosomal protein L5

Chain 2G:



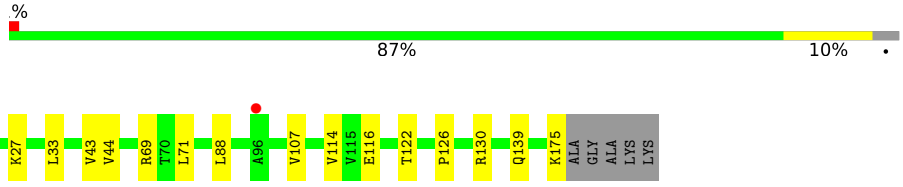
• Molecule 8: 50S ribosomal protein L6

Chain 1H:



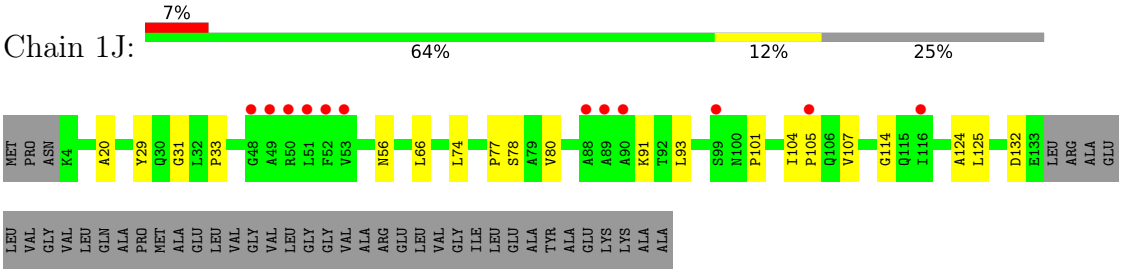
• Molecule 8: 50S ribosomal protein L6

Chain 2H:



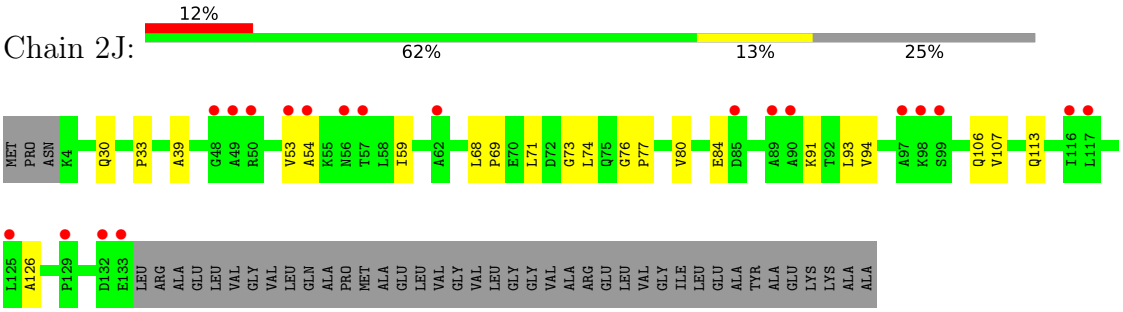
• Molecule 9: 50S ribosomal protein L10

Chain 1J:



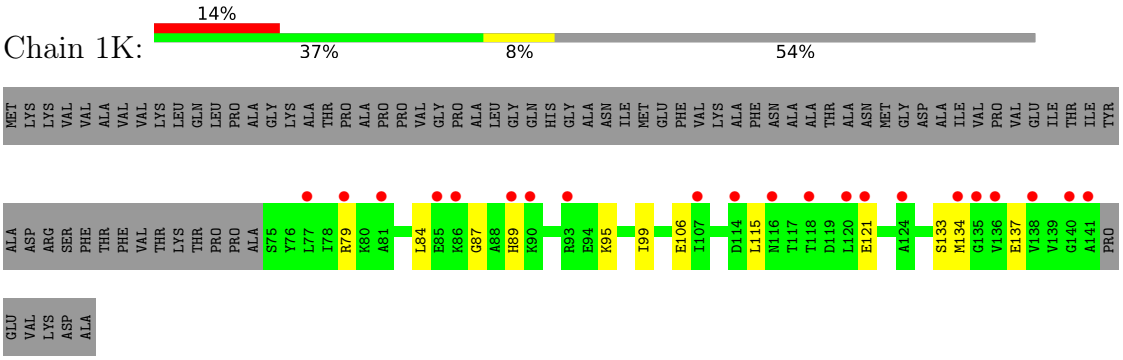
• Molecule 9: 50S ribosomal protein L10

Chain 2J:



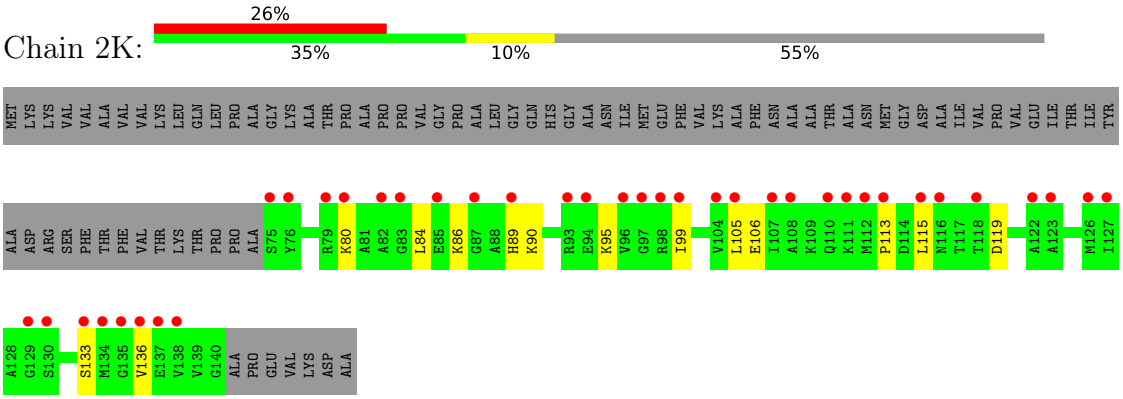
• Molecule 10: 50S ribosomal protein L11

Chain 1K:



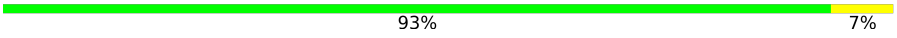
• Molecule 10: 50S ribosomal protein L11

Chain 2K:



• Molecule 11: 50S ribosomal protein L13

Chain 1L:

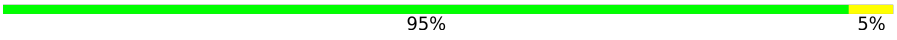


• Molecule 11: 50S ribosomal protein L13

Chain 2L:

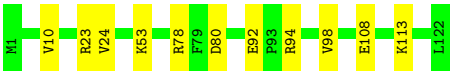
• Molecule 12: 50S ribosomal protein L14

Chain 1M:



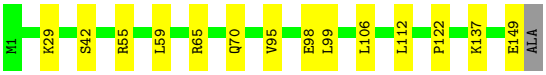
• Molecule 12: 50S ribosomal protein L14

Chain 2M:



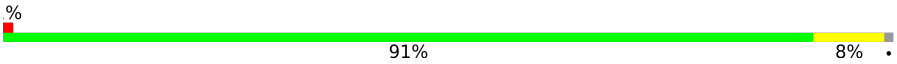
• Molecule 13: 50S ribosomal protein L15

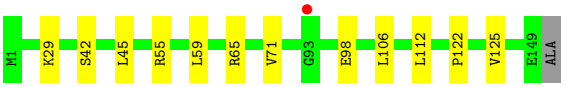
Chain 1N:



• Molecule 13: 50S ribosomal protein L15

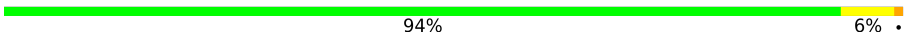
Chain 2N:





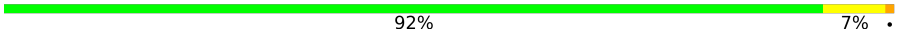
• Molecule 14: 50S ribosomal protein L16

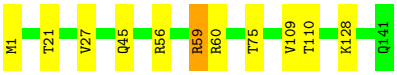
Chain 1O:



• Molecule 14: 50S ribosomal protein L16

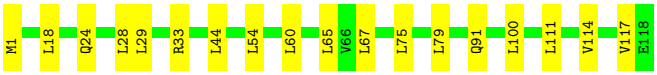
Chain 2O:





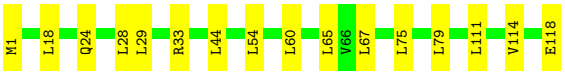
• Molecule 15: 50S ribosomal protein L17

Chain 1P:



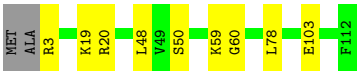
• Molecule 15: 50S ribosomal protein L17

Chain 2P:



• Molecule 16: 50S ribosomal protein L18

Chain 1Q:



• Molecule 16: 50S ribosomal protein L18

Chain 2Q:

• Molecule 17: 50S ribosomal protein L19

Chain 1R:

• Molecule 17: 50S ribosomal protein L19

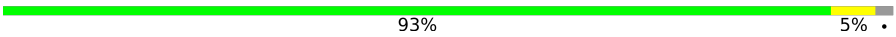
Chain 2R:

• Molecule 18: 50S ribosomal protein L20

Chain 1S:

• Molecule 18: 50S ribosomal protein L20

Chain 2S:

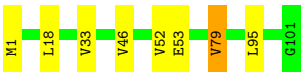


• Molecule 19: 50S ribosomal protein L21

Chain 1T:

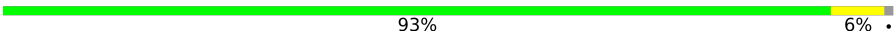
• Molecule 19: 50S ribosomal protein L21

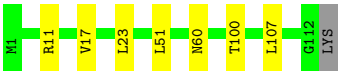
Chain 2T:



• Molecule 20: 50S ribosomal protein L22

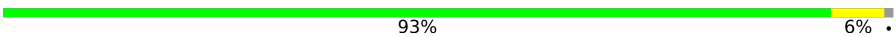
Chain 1U:

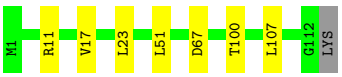




• Molecule 20: 50S ribosomal protein L22

Chain 2U:



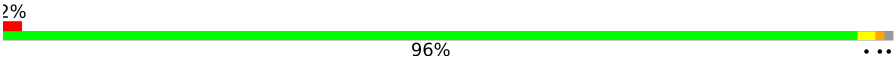


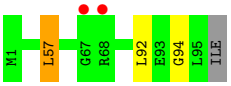
• Molecule 21: 50S ribosomal protein L23

Chain 1V:

• Molecule 21: 50S ribosomal protein L23

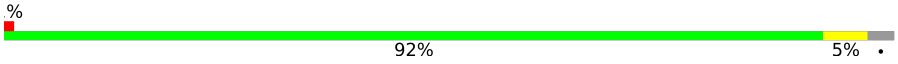
Chain 2V:





• Molecule 22: 50S ribosomal protein L24

Chain 1W:



• Molecule 22: 50S ribosomal protein L24

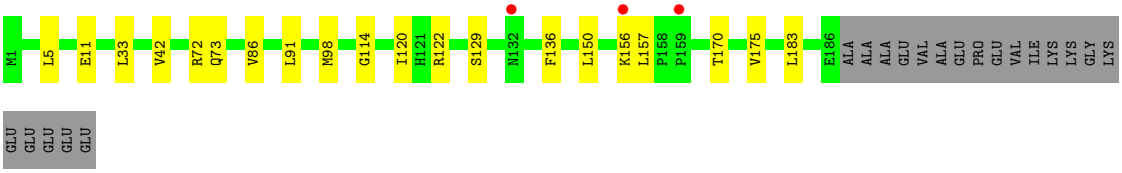
Chain 2W:

• Molecule 23: 50S ribosomal protein L25

Chain 1X:

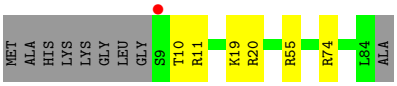
• Molecule 23: 50S ribosomal protein L25

Chain 2X:



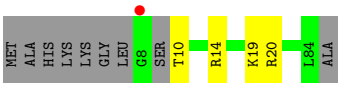
• Molecule 24: 50S ribosomal protein L27

Chain 1Y:



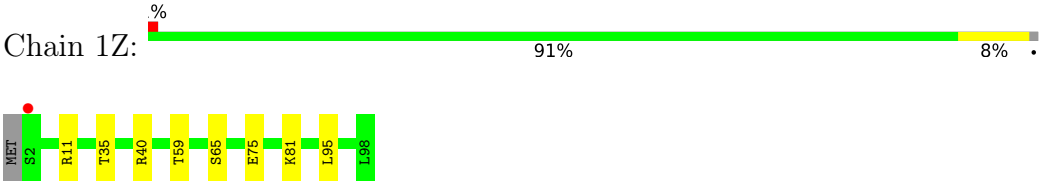
• Molecule 24: 50S ribosomal protein L27

Chain 2Y:



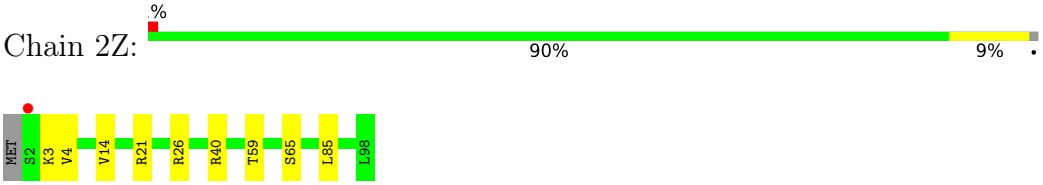
• Molecule 25: 50S ribosomal protein L28

Chain 1Z:



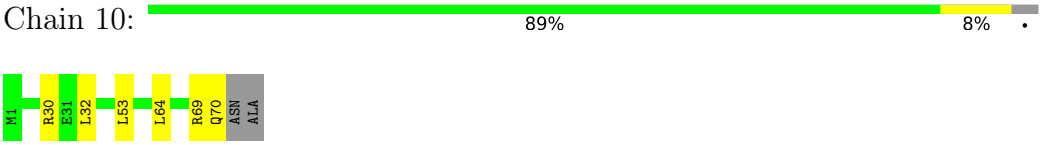
• Molecule 25: 50S ribosomal protein L28

Chain 2Z:



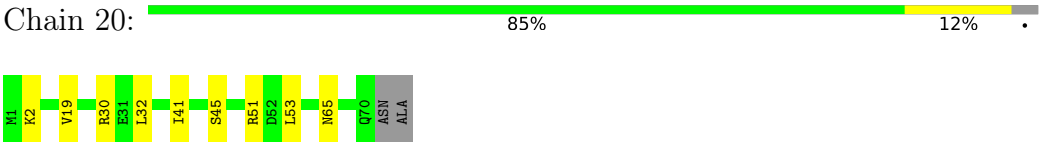
• Molecule 26: 50S ribosomal protein L29

Chain 10:



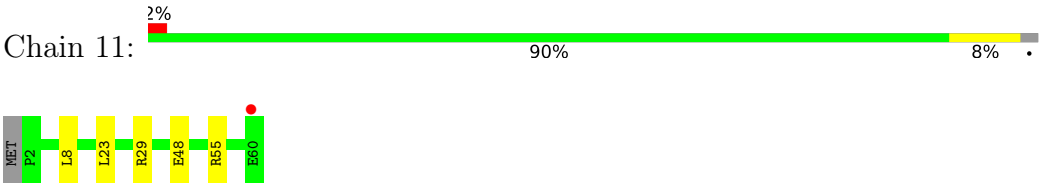
• Molecule 26: 50S ribosomal protein L29

Chain 20:



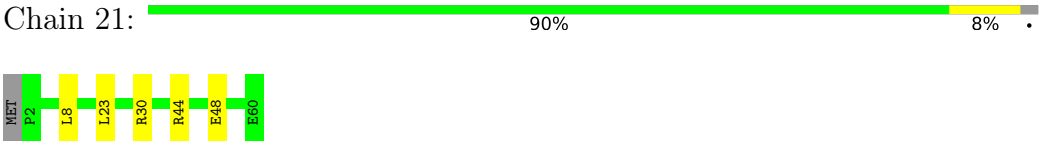
• Molecule 27: 50S ribosomal protein L30

Chain 11:



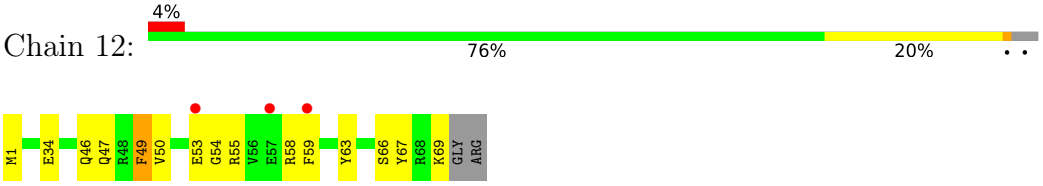
• Molecule 27: 50S ribosomal protein L30

Chain 21:



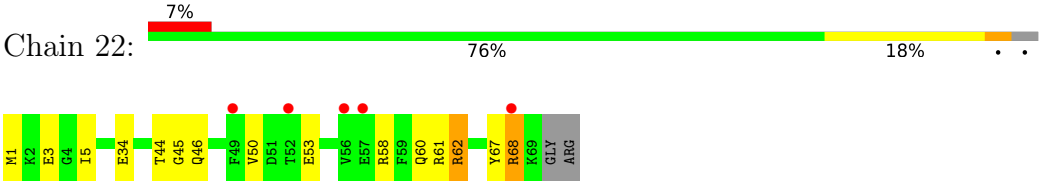
• Molecule 28: 50S ribosomal protein L31

Chain 12:



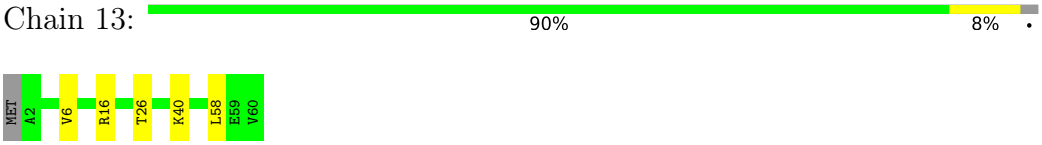
• Molecule 28: 50S ribosomal protein L31

Chain 22:



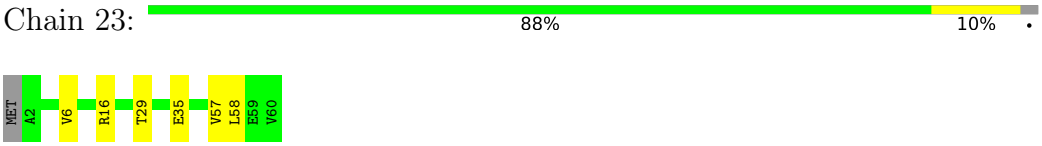
• Molecule 29: 50S ribosomal protein L32

Chain 13:



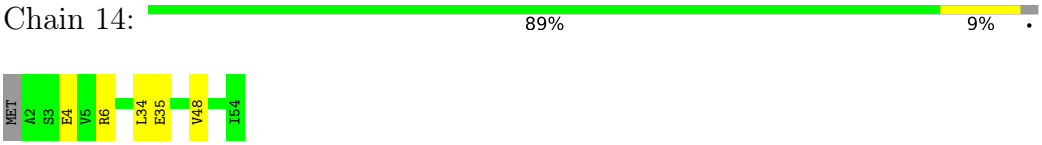
• Molecule 29: 50S ribosomal protein L32

Chain 23:



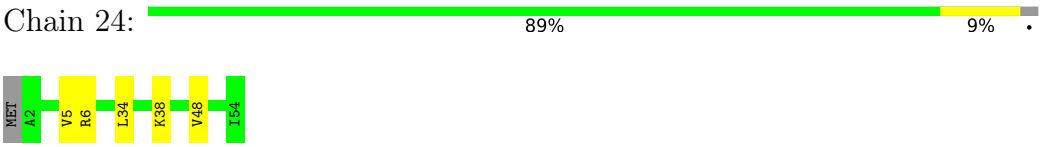
• Molecule 30: 50S ribosomal protein L33

Chain 14:



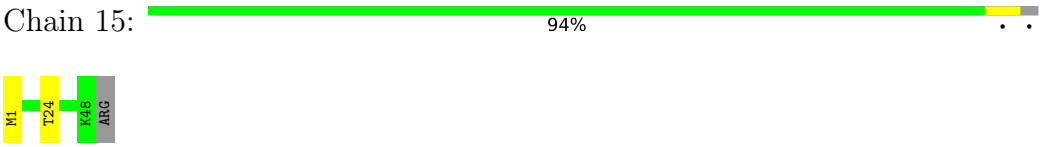
• Molecule 30: 50S ribosomal protein L33

Chain 24:



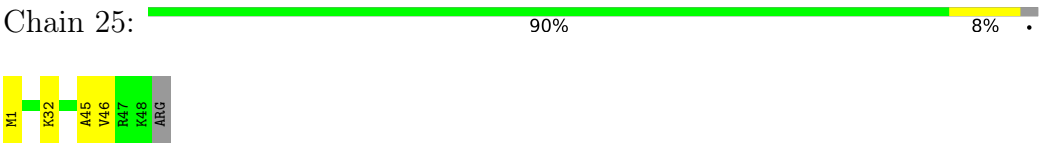
• Molecule 31: 50S ribosomal protein L34

Chain 15:



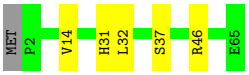
• Molecule 31: 50S ribosomal protein L34

Chain 25:



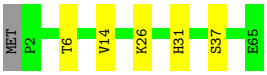
• Molecule 32: 50S ribosomal protein L35

Chain 16:



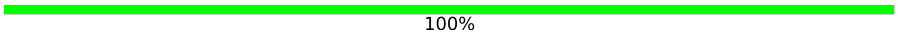
• Molecule 32: 50S ribosomal protein L35

Chain 26:



• Molecule 33: 50S ribosomal protein L36

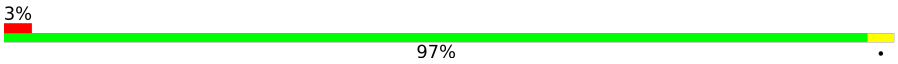
Chain 17:



There are no outlier residues recorded for this chain.

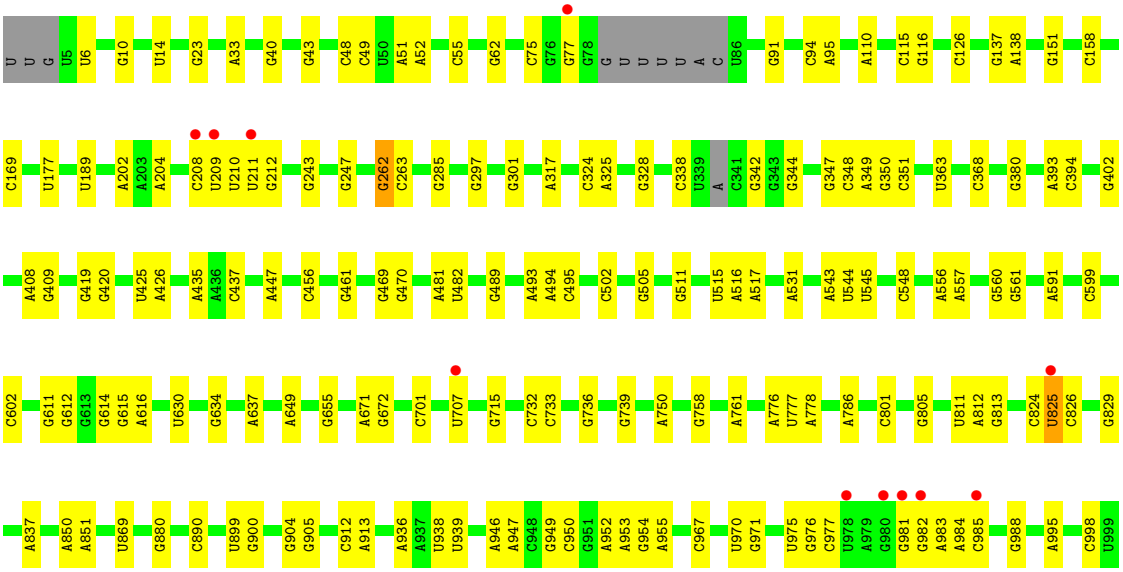
• Molecule 33: 50S ribosomal protein L36

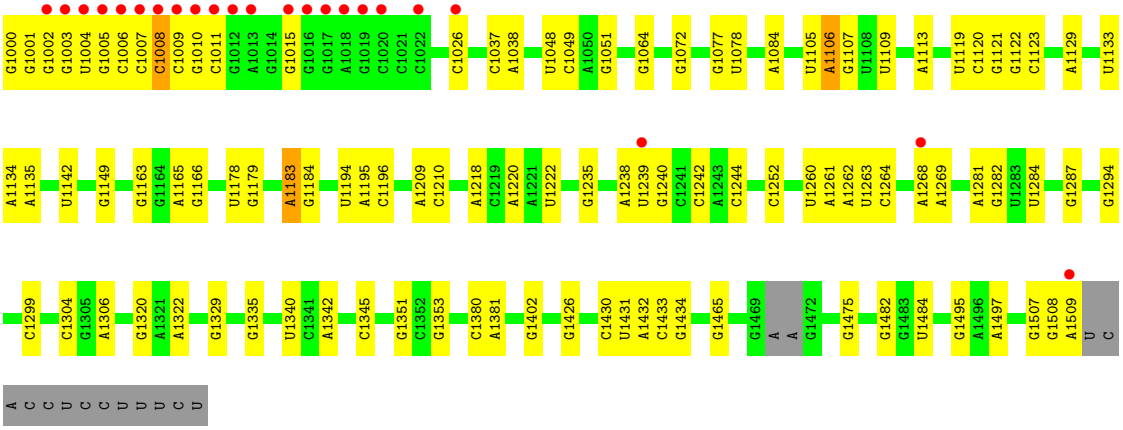
Chain 27:



• Molecule 34: 16S Ribosomal RNA

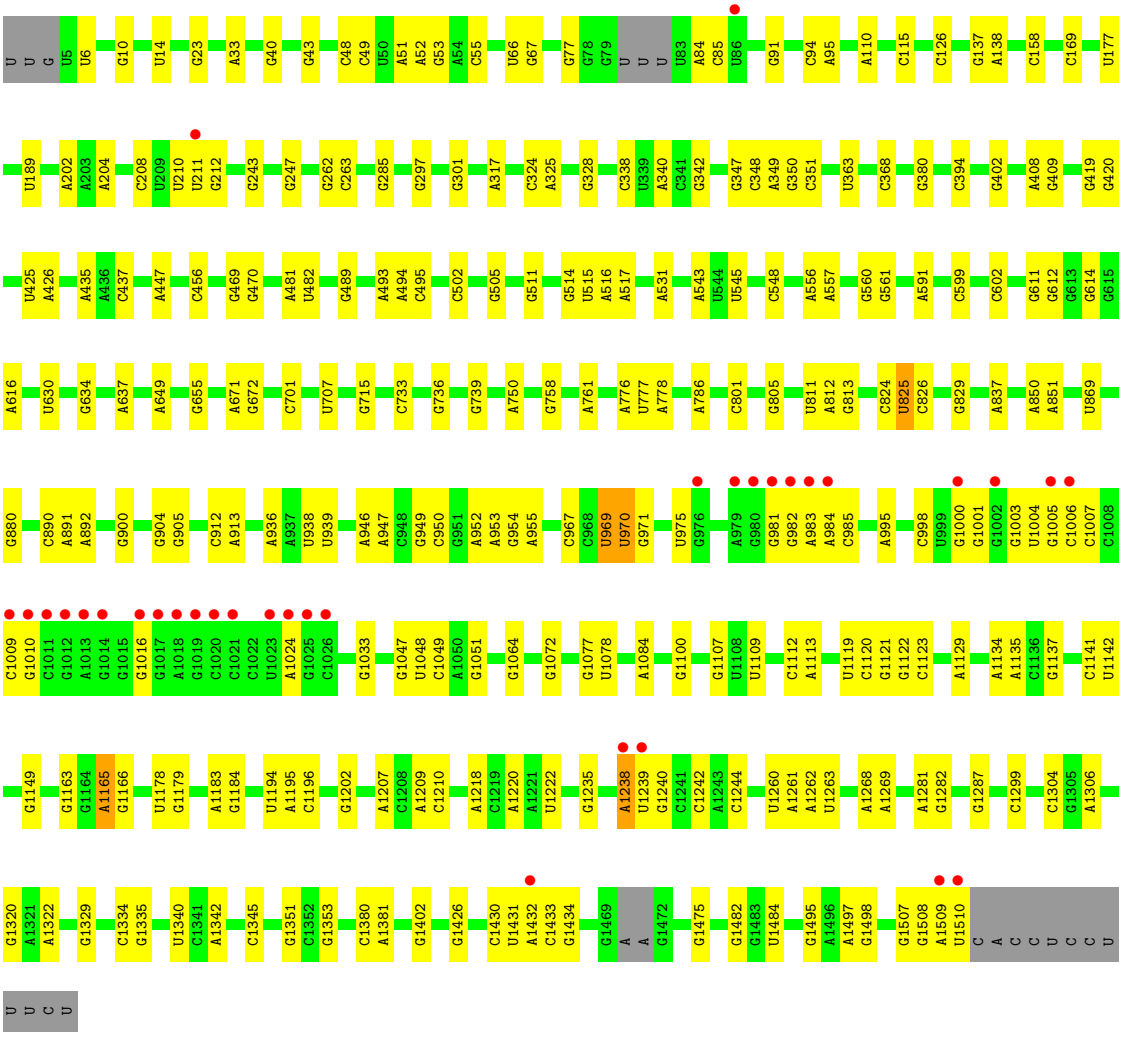
Chain 1a:





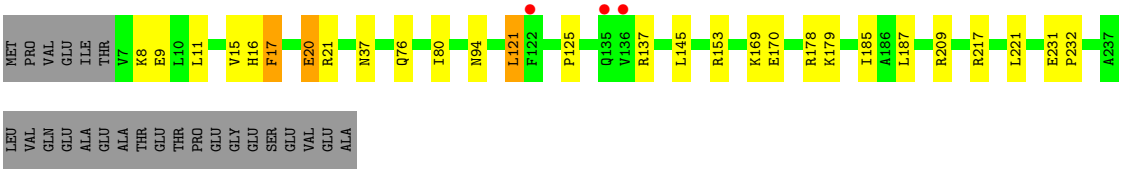
• Molecule 34: 16S Ribosomal RNA

Chain 2a:



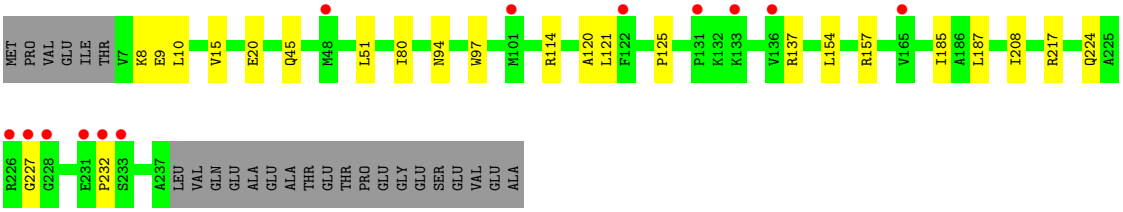
• Molecule 35: 30S ribosomal protein S2

Chain 1b:



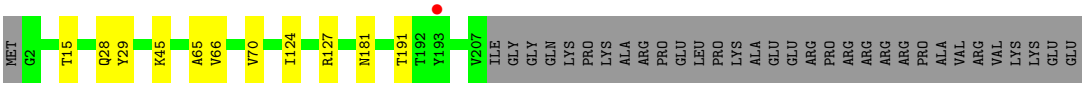
• Molecule 35: 30S ribosomal protein S2

Chain 2b:



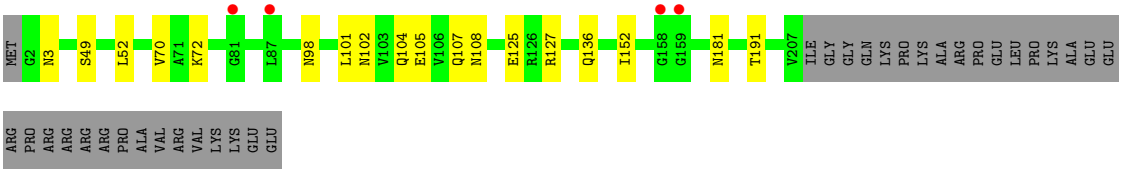
• Molecule 36: 30S ribosomal protein S3

Chain 1c:



• Molecule 36: 30S ribosomal protein S3

Chain 2c:

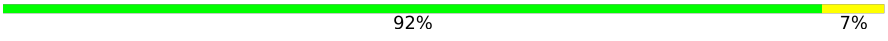


• Molecule 37: 30S ribosomal protein S4

Chain 1d:

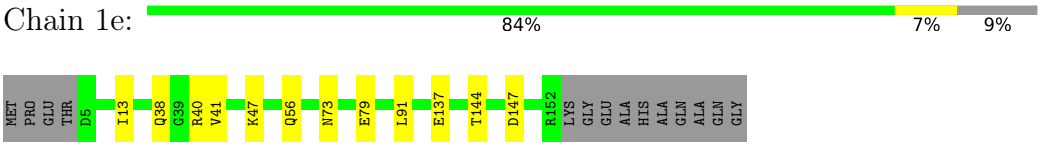
• Molecule 37: 30S ribosomal protein S4

Chain 2d:



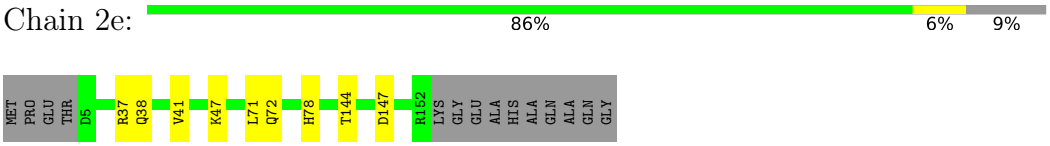
• Molecule 38: 30S ribosomal protein S5

Chain 1e:



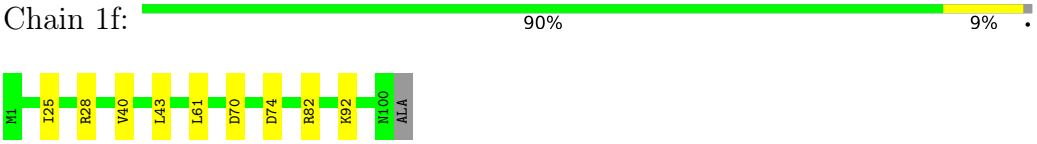
• Molecule 38: 30S ribosomal protein S5

Chain 2e:



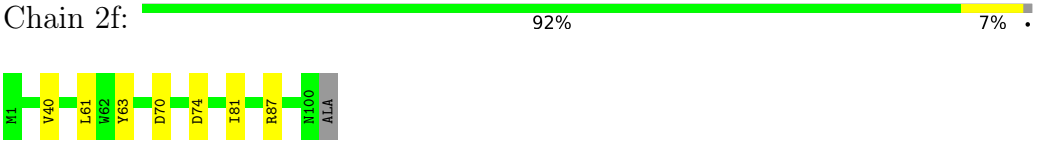
• Molecule 39: 30S ribosomal protein S6

Chain 1f:



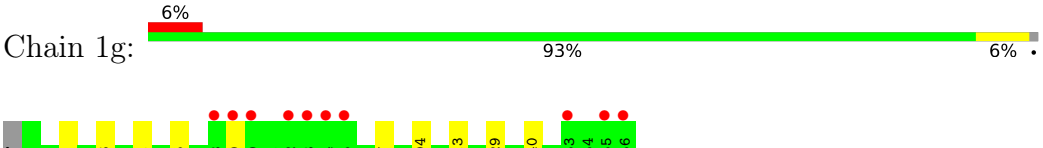
• Molecule 39: 30S ribosomal protein S6

Chain 2f:



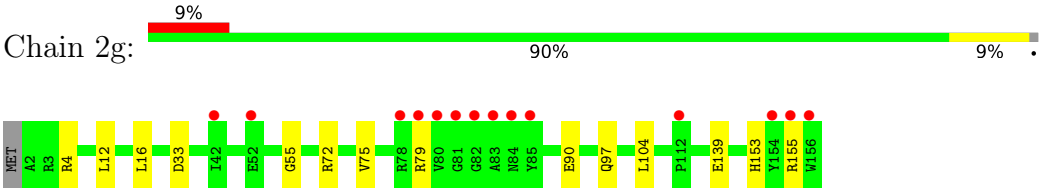
• Molecule 40: 30S ribosomal protein S7

Chain 1g:



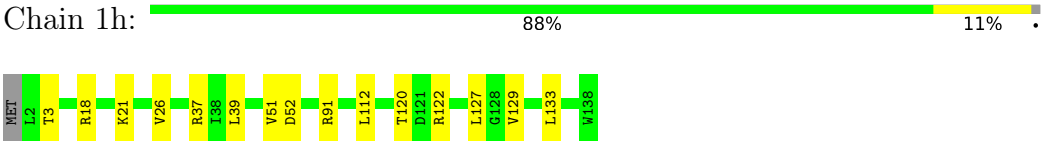
• Molecule 40: 30S ribosomal protein S7

Chain 2g:



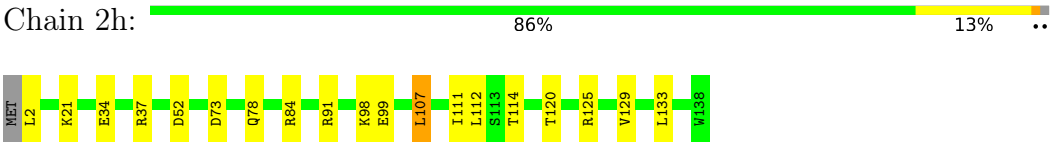
• Molecule 41: 30S ribosomal protein S8

Chain 1h:



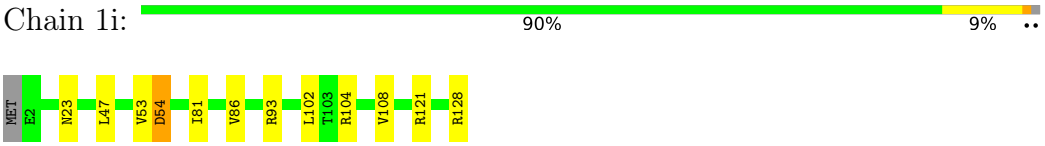
• Molecule 41: 30S ribosomal protein S8

Chain 2h:



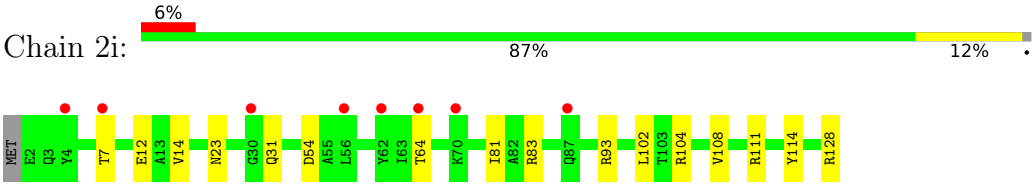
• Molecule 42: 30S ribosomal protein S9

Chain 1i:



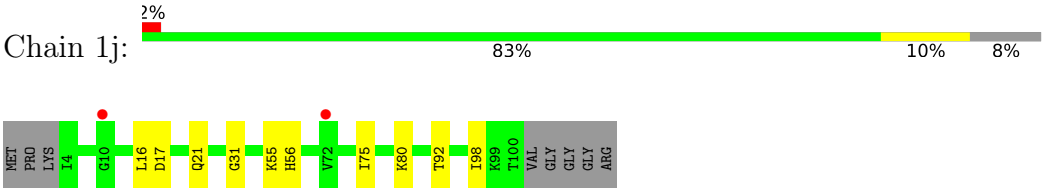
• Molecule 42: 30S ribosomal protein S9

Chain 2i:



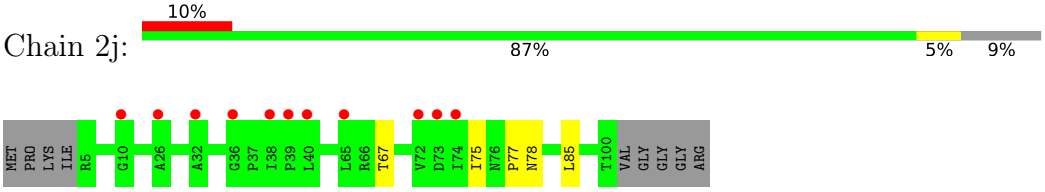
• Molecule 43: 30S ribosomal protein S10

Chain 1j:



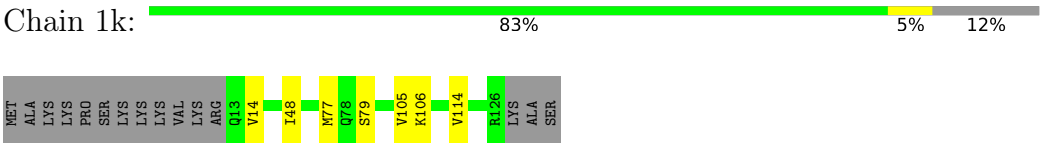
• Molecule 43: 30S ribosomal protein S10

Chain 2j:



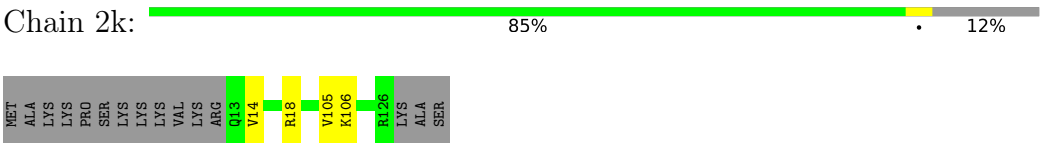
• Molecule 44: 30S ribosomal protein S11

Chain 1k:



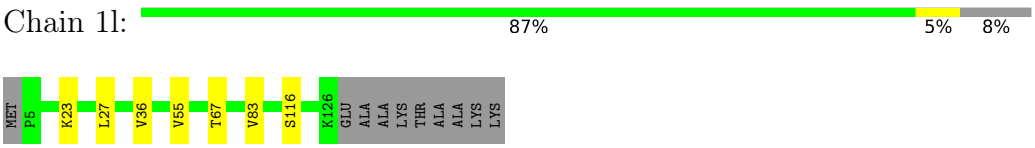
• Molecule 44: 30S ribosomal protein S11

Chain 2k:



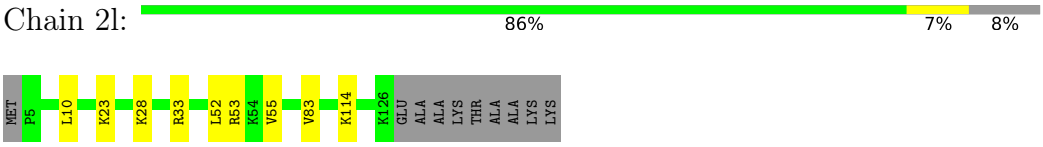
• Molecule 45: 30S ribosomal protein S12

Chain 1l:



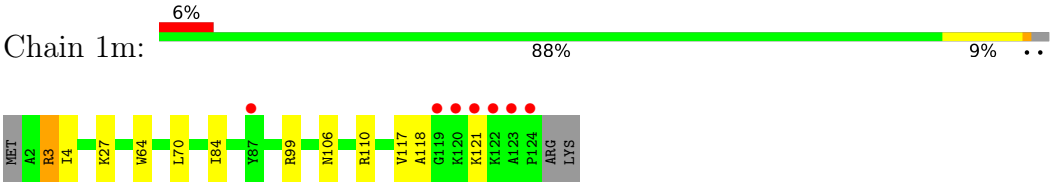
• Molecule 45: 30S ribosomal protein S12

Chain 2l:



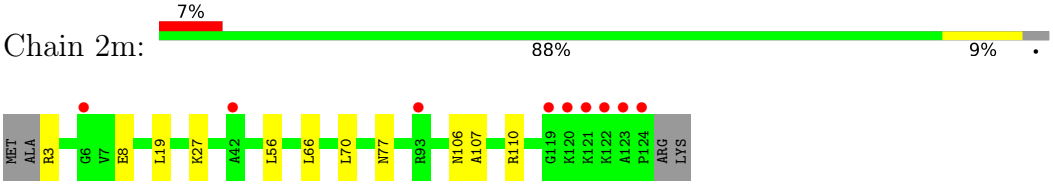
• Molecule 46: 30S ribosomal protein S13

Chain 1m:



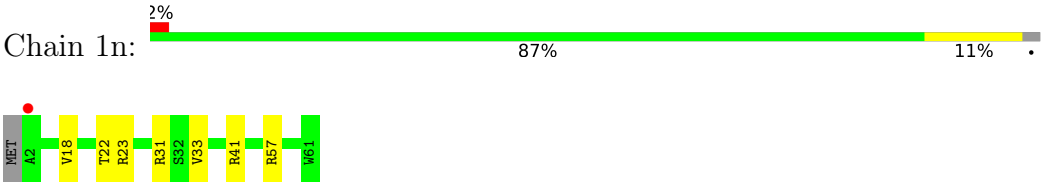
• Molecule 46: 30S ribosomal protein S13

Chain 2m:



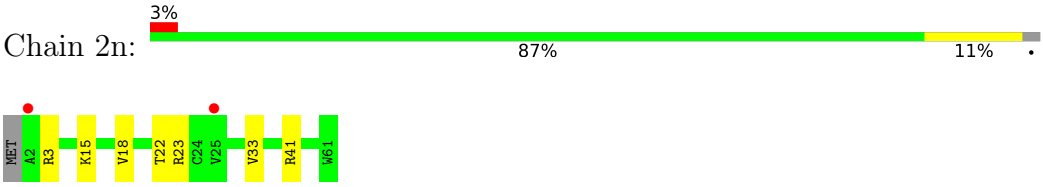
• Molecule 47: 30S ribosomal protein S14 type Z

Chain 1n:



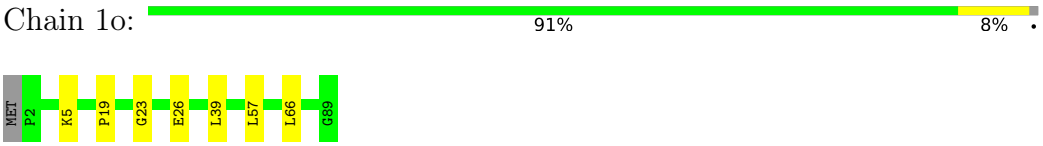
• Molecule 47: 30S ribosomal protein S14 type Z

Chain 2n:



• Molecule 48: 30S ribosomal protein S15

Chain 1o:

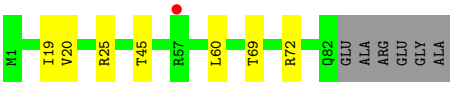


• Molecule 48: 30S ribosomal protein S15

Chain 2o:

• Molecule 49: 30S ribosomal protein S16

Chain 1p:

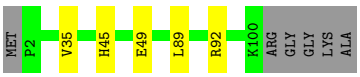


• Molecule 49: 30S ribosomal protein S16

Chain 2p:

• Molecule 50: 30S ribosomal protein S17

Chain 1q:

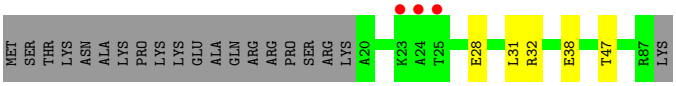


• Molecule 50: 30S ribosomal protein S17

Chain 2q:

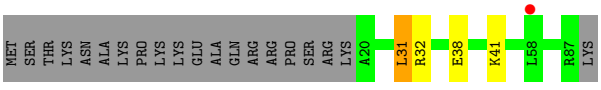
• Molecule 51: 30S ribosomal protein S18

Chain 1r:



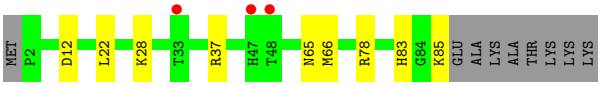
• Molecule 51: 30S ribosomal protein S18

Chain 2r:



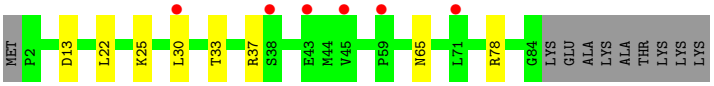
• Molecule 52: 30S ribosomal protein S19

Chain 1s:



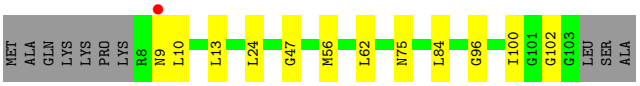
• Molecule 52: 30S ribosomal protein S19

Chain 2s:



• Molecule 53: 30S ribosomal protein S20

Chain 1t:

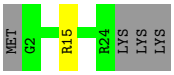


• Molecule 53: 30S ribosomal protein S20

Chain 2t:

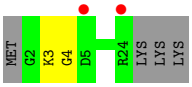
• Molecule 54: 30S ribosomal protein Thx

Chain 1u:



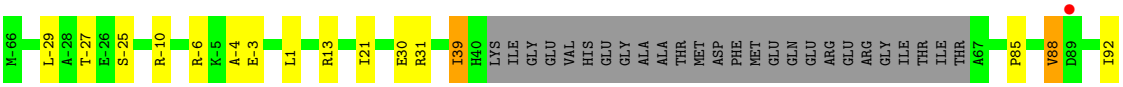
• Molecule 54: 30S ribosomal protein Thx

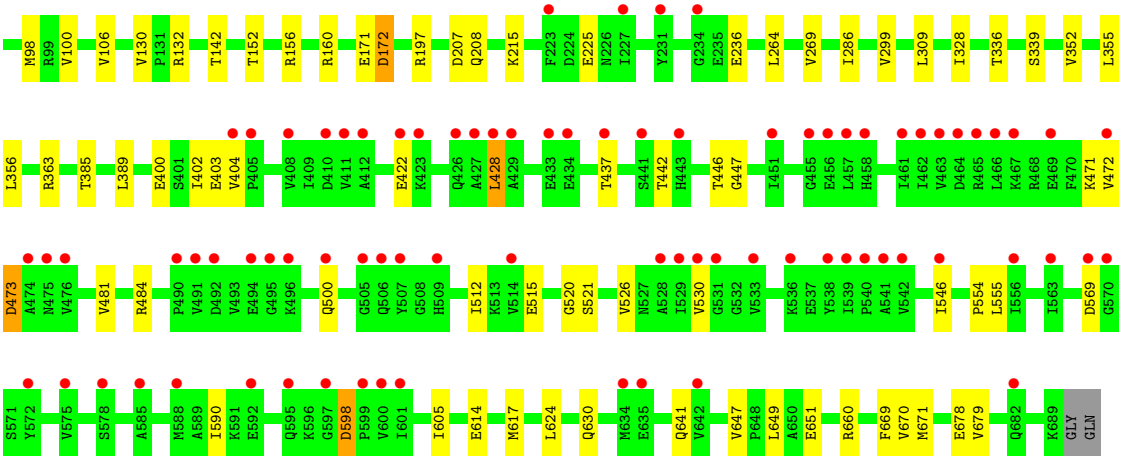
Chain 2u:



• Molecule 55: Chimera protein of 50S ribosomal protein L9 and Elongation factor G

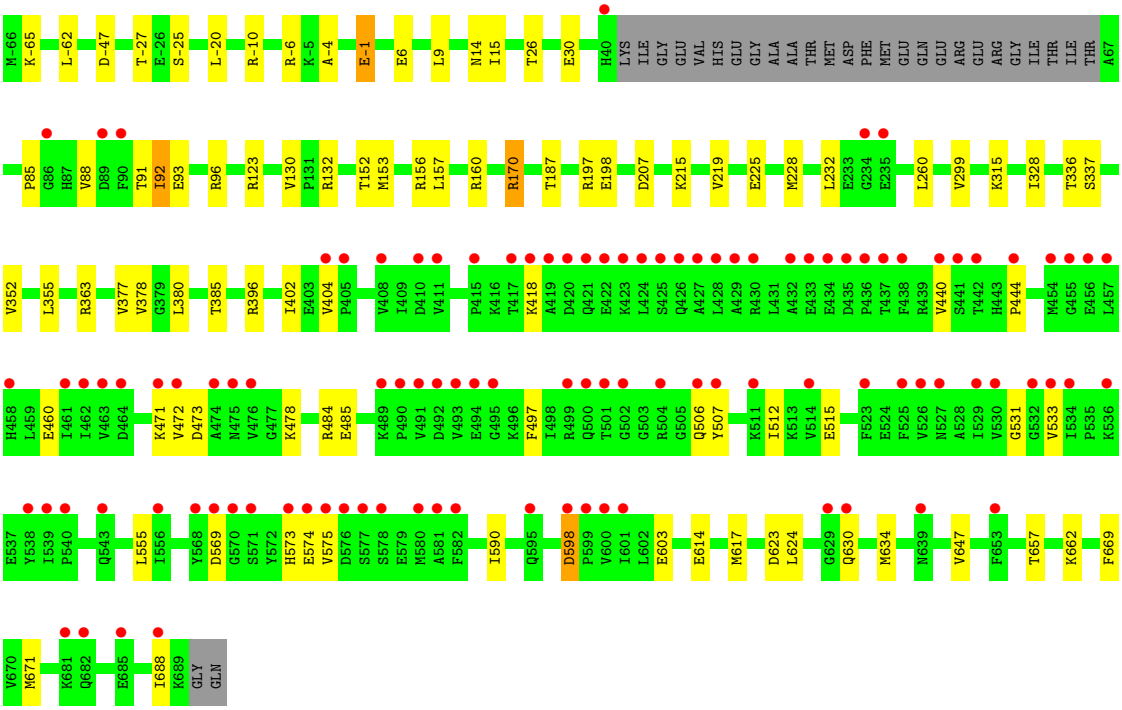
Chain 1z:





• Molecule 55: Chimera protein of 50S ribosomal protein L9 and Elongation factor G

Chain 2z:

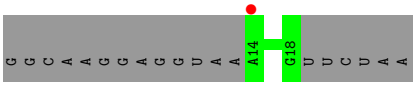


• Molecule 56: mRNA

Chain 1y:

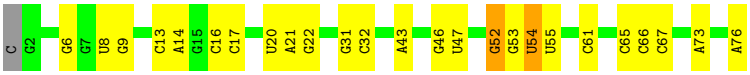
• Molecule 56: mRNA

Chain 2y:



• Molecule 57: P-site tRNA

Chain 1w:



• Molecule 57: P-site tRNA

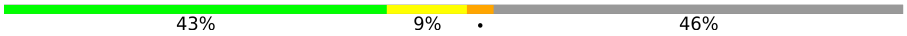
Chain 2w:

• Molecule 58: Cathelicidin-3

Chain 1x:

• Molecule 58: Cathelicidin-3

Chain 2x:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	208.78Å 449.03Å 619.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.48 – 3.00 49.48 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.48-3.00) 99.1 (49.48-3.00)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.208 , 0.265 0.208 , 0.265	Depositor DCC
R_{free} test set	57205 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	55.7	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 66.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	306384	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 4SU, 5MC, SF4, PSU, 5MU, GDP

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	0.58	4/69281 (0.0%)	0.95	75/108144 (0.1%)
1	2A	0.45	2/69179 (0.0%)	0.92	59/107984 (0.1%)
2	1B	0.47	0/2878	0.93	0/4490
2	2B	0.43	0/2878	0.92	1/4490 (0.0%)
3	1C	0.48	0/1038	0.70	2/1403 (0.1%)
3	2C	0.45	0/1038	0.68	1/1403 (0.1%)
4	1D	0.42	0/2186	0.57	0/2944
4	2D	0.36	0/2192	0.57	0/2951
5	1E	0.42	0/1592	0.56	0/2149
5	2E	0.35	0/1592	0.55	0/2149
6	1F	0.38	0/1619	0.54	0/2193
6	2F	0.34	0/1615	0.55	0/2188
7	1G	0.31	0/1450	0.53	0/1959
7	2G	0.32	0/1449	0.56	0/1958
8	1H	0.34	0/1356	0.53	0/1834
8	2H	0.33	0/1356	0.56	0/1834
9	1J	0.28	0/640	0.59	0/889
9	2J	0.29	0/640	0.55	1/889 (0.1%)
10	1K	0.35	0/504	0.58	0/675
10	2K	0.46	0/503	0.66	0/673
11	1L	0.38	0/1144	0.53	0/1543
11	2L	0.31	0/1144	0.53	0/1543
12	1M	0.40	0/943	0.57	0/1269
12	2M	0.37	0/943	0.54	0/1269
13	1N	0.37	0/1156	0.57	0/1537
13	2N	0.34	0/1152	0.57	0/1533
14	1O	0.41	0/1143	0.52	0/1527
14	2O	0.35	0/1143	0.54	0/1527
15	1P	0.38	0/982	0.59	0/1312
15	2P	0.33	0/982	0.55	0/1312
16	1Q	0.35	0/887	0.57	0/1180
16	2Q	0.33	0/880	0.58	1/1172 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	1R	0.37	0/1105	0.53	0/1477
17	2R	0.33	0/1097	0.54	0/1468
18	1S	0.42	0/977	0.55	0/1301
18	2S	0.32	0/977	0.48	0/1301
19	1T	0.38	0/782	0.54	0/1049
19	2T	0.32	0/782	0.53	0/1049
20	1U	0.39	0/897	0.53	0/1205
20	2U	0.35	0/897	0.52	0/1205
21	1V	0.38	0/764	0.58	1/1025 (0.1%)
21	2V	0.33	0/764	0.55	1/1025 (0.1%)
22	1W	0.39	0/819	0.58	0/1095
22	2W	0.34	0/819	0.56	0/1095
23	1X	0.34	0/1492	0.55	0/2029
23	2X	0.34	0/1486	0.57	0/2022
24	1Y	0.38	0/612	0.57	0/816
24	2Y	0.33	0/609	0.51	0/810
25	1Z	0.37	0/762	0.51	0/1014
25	2Z	0.33	0/762	0.53	0/1014
26	10	0.33	0/590	0.54	0/781
26	20	0.33	0/590	0.51	0/781
27	11	0.41	0/474	0.54	0/635
27	21	0.33	0/469	0.56	0/630
28	12	0.34	0/571	0.64	0/768
28	22	0.37	0/545	0.58	0/737
29	13	0.42	0/469	0.58	0/635
29	23	0.36	0/469	0.53	0/635
30	14	0.46	0/460	0.52	0/613
30	24	0.41	0/456	0.52	0/608
31	15	0.38	0/426	0.54	0/561
31	25	0.34	0/426	0.58	0/561
32	16	0.40	0/525	0.58	0/691
32	26	0.33	0/525	0.52	0/691
33	17	0.43	0/310	0.54	0/407
33	27	0.33	0/310	0.48	0/407
34	1a	0.40	0/35976	0.89	14/56145 (0.0%)
34	2a	0.39	0/36119	0.89	18/56370 (0.0%)
35	1b	0.33	0/1881	0.59	0/2542
35	2b	0.34	0/1860	0.56	0/2518
36	1c	0.29	0/1576	0.50	0/2130
36	2c	0.33	0/1568	0.53	0/2122
37	1d	0.31	0/1689	0.52	0/2267
37	2d	0.30	0/1708	0.54	1/2289 (0.0%)
38	1e	0.32	0/1145	0.52	0/1543

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	2e	0.31	0/1149	0.56	0/1548
39	1f	0.32	0/825	0.53	0/1118
39	2f	0.32	0/833	0.49	0/1128
40	1g	0.29	0/1250	0.48	0/1679
40	2g	0.31	0/1254	0.52	0/1683
41	1h	0.30	0/1108	0.52	0/1494
41	2h	0.29	0/1108	0.55	1/1494 (0.1%)
42	1i	0.30	0/1005	0.51	0/1350
42	2i	0.33	0/997	0.55	0/1343
43	1j	0.29	0/722	0.59	0/982
43	2j	0.33	0/727	0.52	0/988
44	1k	0.33	0/848	0.52	0/1149
44	2k	0.29	0/848	0.52	0/1149
45	1l	0.32	0/946	0.50	0/1274
45	2l	0.33	0/946	0.58	0/1274
46	1m	0.30	0/977	0.55	0/1310
46	2m	0.30	0/961	0.54	0/1291
47	1n	0.31	0/501	0.56	0/664
47	2n	0.31	0/501	0.55	0/664
48	1o	0.32	0/739	0.53	0/985
48	2o	0.31	0/739	0.52	0/985
49	1p	0.30	0/697	0.51	0/939
49	2p	0.30	0/693	0.50	0/935
50	1q	0.33	0/836	0.50	0/1117
50	2q	0.31	0/836	0.50	0/1117
51	1r	0.29	0/560	0.55	1/746 (0.1%)
51	2r	0.31	0/560	0.55	1/746 (0.1%)
52	1s	0.29	0/676	0.53	0/911
52	2s	0.32	0/661	0.60	0/893
53	1t	0.31	0/730	0.54	0/965
53	2t	0.28	0/733	0.49	0/969
54	1u	0.29	0/203	0.54	0/266
54	2u	0.30	0/203	0.48	0/266
55	1z	0.35	0/5792	0.59	1/7844 (0.0%)
55	2z	0.36	0/5792	0.58	0/7844
56	1y	0.47	0/144	0.96	0/222
56	2y	0.59	0/122	1.17	0/188
57	1w	0.57	2/1725 (0.1%)	1.15	22/2689 (0.8%)
57	2w	0.53	0/1725	1.17	20/2689 (0.7%)
58	1x	0.40	0/175	0.68	0/238
58	2x	0.38	0/175	0.98	1/238 (0.4%)
All	All	0.44	8/327047 (0.0%)	0.83	222/487364 (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
28	12	0	1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1187	A	N9-C4	-10.39	1.31	1.37
1	1A	1066	A	N9-C4	-6.00	1.34	1.37
57	1w	22	G	N7-C5	5.90	1.42	1.39
1	1A	353	A	N9-C4	-5.88	1.34	1.37
57	1w	46	G	C6-N1	5.85	1.43	1.39

The worst 5 of 222 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	1w	46	G	C6-N1-C2	-11.71	118.07	125.10
57	2w	46	G	C6-N1-C2	-10.97	118.52	125.10
1	1A	1149	C	OP1-P-O3'	-10.93	81.15	105.20
57	1w	22	G	C5-N7-C8	-10.78	98.91	104.30
57	2w	22	G	C5-N7-C8	-10.15	99.22	104.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	12	59	PHE	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	1C	129/229 (56%)	96 (74%)	25 (19%)	8 (6%)	1 8
3	2C	129/229 (56%)	96 (74%)	26 (20%)	7 (5%)	2 11
4	1D	273/276 (99%)	258 (94%)	12 (4%)	3 (1%)	14 50
4	2D	273/276 (99%)	253 (93%)	16 (6%)	4 (2%)	10 42
5	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	29 68
5	2E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	29 68
6	1F	201/210 (96%)	192 (96%)	8 (4%)	1 (0%)	29 68
6	2F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	29 68
7	1G	179/182 (98%)	162 (90%)	16 (9%)	1 (1%)	25 64
7	2G	179/182 (98%)	160 (89%)	16 (9%)	3 (2%)	9 39
8	1H	172/180 (96%)	159 (92%)	12 (7%)	1 (1%)	25 64
8	2H	172/180 (96%)	159 (92%)	12 (7%)	1 (1%)	25 64
9	1J	128/173 (74%)	71 (56%)	37 (29%)	20 (16%)	0 1
9	2J	128/173 (74%)	81 (63%)	26 (20%)	21 (16%)	0 1
10	1K	65/147 (44%)	52 (80%)	11 (17%)	2 (3%)	4 23
10	2K	64/147 (44%)	45 (70%)	17 (27%)	2 (3%)	4 23
11	1L	138/140 (99%)	135 (98%)	3 (2%)	0	100 100
11	2L	138/140 (99%)	134 (97%)	3 (2%)	1 (1%)	22 60
12	1M	120/122 (98%)	114 (95%)	6 (5%)	0	100 100
12	2M	120/122 (98%)	113 (94%)	7 (6%)	0	100 100
13	1N	147/150 (98%)	139 (95%)	6 (4%)	2 (1%)	11 43
13	2N	147/150 (98%)	139 (95%)	5 (3%)	3 (2%)	7 34
14	1O	139/141 (99%)	129 (93%)	9 (6%)	1 (1%)	22 60
14	2O	139/141 (99%)	126 (91%)	11 (8%)	2 (1%)	11 43
15	1P	116/118 (98%)	109 (94%)	7 (6%)	0	100 100
15	2P	116/118 (98%)	110 (95%)	6 (5%)	0	100 100
16	1Q	108/112 (96%)	97 (90%)	9 (8%)	2 (2%)	8 36
16	2Q	108/112 (96%)	98 (91%)	8 (7%)	2 (2%)	8 36
17	1R	129/146 (88%)	118 (92%)	9 (7%)	2 (2%)	9 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
17	2R	129/146 (88%)	123 (95%)	6 (5%)	0	100 100
18	1S	114/118 (97%)	113 (99%)	1 (1%)	0	100 100
18	2S	114/118 (97%)	113 (99%)	1 (1%)	0	100 100
19	1T	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15 53
19	2T	99/101 (98%)	91 (92%)	6 (6%)	2 (2%)	7 34
20	1U	110/113 (97%)	108 (98%)	2 (2%)	0	100 100
20	2U	110/113 (97%)	109 (99%)	1 (1%)	0	100 100
21	1V	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	14 50
21	2V	93/96 (97%)	90 (97%)	2 (2%)	1 (1%)	14 50
22	1W	105/110 (96%)	92 (88%)	12 (11%)	1 (1%)	15 53
22	2W	105/110 (96%)	95 (90%)	10 (10%)	0	100 100
23	1X	184/206 (89%)	164 (89%)	17 (9%)	3 (2%)	9 40
23	2X	184/206 (89%)	161 (88%)	20 (11%)	3 (2%)	9 40
24	1Y	74/85 (87%)	72 (97%)	2 (3%)	0	100 100
24	2Y	73/85 (86%)	70 (96%)	3 (4%)	0	100 100
25	1Z	95/98 (97%)	90 (95%)	4 (4%)	1 (1%)	14 50
25	2Z	95/98 (97%)	89 (94%)	5 (5%)	1 (1%)	14 50
26	10	68/72 (94%)	64 (94%)	3 (4%)	1 (2%)	10 42
26	20	68/72 (94%)	66 (97%)	2 (3%)	0	100 100
27	11	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
27	21	57/60 (95%)	52 (91%)	5 (9%)	0	100 100
28	12	67/71 (94%)	51 (76%)	13 (19%)	3 (4%)	2 14
28	22	67/71 (94%)	49 (73%)	12 (18%)	6 (9%)	1 3
29	13	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
29	23	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
30	14	51/54 (94%)	50 (98%)	1 (2%)	0	100 100
30	24	51/54 (94%)	50 (98%)	1 (2%)	0	100 100
31	15	46/49 (94%)	45 (98%)	1 (2%)	0	100 100
31	25	46/49 (94%)	44 (96%)	0	2 (4%)	2 15
32	16	62/65 (95%)	60 (97%)	2 (3%)	0	100 100
32	26	62/65 (95%)	60 (97%)	2 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	17	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	27	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
35	1b	229/256 (90%)	193 (84%)	27 (12%)	9 (4%)	3	17
35	2b	229/256 (90%)	193 (84%)	28 (12%)	8 (4%)	3	20
36	1c	204/239 (85%)	181 (89%)	20 (10%)	3 (2%)	10	42
36	2c	204/239 (85%)	185 (91%)	14 (7%)	5 (2%)	5	28
37	1d	206/209 (99%)	184 (89%)	22 (11%)	0	100	100
37	2d	206/209 (99%)	182 (88%)	24 (12%)	0	100	100
38	1e	146/162 (90%)	133 (91%)	13 (9%)	0	100	100
38	2e	146/162 (90%)	134 (92%)	11 (8%)	1 (1%)	22	60
39	1f	98/101 (97%)	92 (94%)	5 (5%)	1 (1%)	15	53
39	2f	98/101 (97%)	92 (94%)	5 (5%)	1 (1%)	15	53
40	1g	153/156 (98%)	139 (91%)	13 (8%)	1 (1%)	22	60
40	2g	153/156 (98%)	140 (92%)	9 (6%)	4 (3%)	5	27
41	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
41	2h	135/138 (98%)	126 (93%)	8 (6%)	1 (1%)	22	60
42	1i	125/128 (98%)	109 (87%)	15 (12%)	1 (1%)	19	57
42	2i	125/128 (98%)	109 (87%)	15 (12%)	1 (1%)	19	57
43	1j	95/105 (90%)	81 (85%)	9 (10%)	5 (5%)	2	11
43	2j	94/105 (90%)	83 (88%)	8 (8%)	3 (3%)	4	22
44	1k	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	17	55
44	2k	112/129 (87%)	102 (91%)	9 (8%)	1 (1%)	17	55
45	1l	120/132 (91%)	114 (95%)	6 (5%)	0	100	100
45	2l	120/132 (91%)	112 (93%)	7 (6%)	1 (1%)	19	57
46	1m	121/126 (96%)	107 (88%)	12 (10%)	2 (2%)	9	39
46	2m	120/126 (95%)	106 (88%)	13 (11%)	1 (1%)	19	57
47	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
47	2n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
48	1o	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	6	30
48	2o	86/89 (97%)	79 (92%)	5 (6%)	2 (2%)	6	30
49	1p	80/88 (91%)	75 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
49	2p	80/88 (91%)	75 (94%)	5 (6%)	0	100 100
50	1q	97/105 (92%)	89 (92%)	8 (8%)	0	100 100
50	2q	97/105 (92%)	90 (93%)	7 (7%)	0	100 100
51	1r	66/88 (75%)	65 (98%)	1 (2%)	0	100 100
51	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100 100
52	1s	82/93 (88%)	70 (85%)	12 (15%)	0	100 100
52	2s	81/93 (87%)	70 (86%)	8 (10%)	3 (4%)	3 19
53	1t	94/106 (89%)	85 (90%)	5 (5%)	4 (4%)	2 15
53	2t	94/106 (89%)	87 (93%)	5 (5%)	2 (2%)	7 33
54	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100 100
54	2u	21/27 (78%)	17 (81%)	2 (10%)	2 (10%)	0 3
55	1z	726/758 (96%)	610 (84%)	92 (13%)	24 (3%)	4 21
55	2z	726/758 (96%)	609 (84%)	95 (13%)	22 (3%)	4 24
58	1x	17/35 (49%)	16 (94%)	0	1 (6%)	1 9
58	2x	17/35 (49%)	13 (76%)	1 (6%)	3 (18%)	0 0
All	All	13263/14516 (91%)	11963 (90%)	1067 (8%)	233 (2%)	8 37

5 of 233 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	1C	175	VAL
3	1C	224	ILE
6	1F	130	ALA
7	1G	51	ARG
8	1H	126	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	1C	103/181 (57%)	89 (86%)	14 (14%)	3 17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	2C	103/181 (57%)	88 (85%)	15 (15%)	3 15
4	1D	215/218 (99%)	195 (91%)	20 (9%)	9 33
4	2D	216/218 (99%)	200 (93%)	16 (7%)	13 44
5	1E	164/166 (99%)	151 (92%)	13 (8%)	12 41
5	2E	164/166 (99%)	147 (90%)	17 (10%)	7 27
6	1F	160/166 (96%)	141 (88%)	19 (12%)	5 22
6	2F	159/166 (96%)	143 (90%)	16 (10%)	7 29
7	1G	143/156 (92%)	123 (86%)	20 (14%)	3 16
7	2G	142/156 (91%)	119 (84%)	23 (16%)	2 12
8	1H	144/148 (97%)	136 (94%)	8 (6%)	21 56
8	2H	144/148 (97%)	127 (88%)	17 (12%)	5 22
10	1K	50/111 (45%)	40 (80%)	10 (20%)	1 7
10	2K	50/111 (45%)	38 (76%)	12 (24%)	0 3
11	1L	118/119 (99%)	108 (92%)	10 (8%)	10 38
11	2L	118/119 (99%)	107 (91%)	11 (9%)	9 33
12	1M	100/100 (100%)	94 (94%)	6 (6%)	19 53
12	2M	100/100 (100%)	89 (89%)	11 (11%)	6 25
13	1N	116/116 (100%)	104 (90%)	12 (10%)	7 28
13	2N	115/116 (99%)	106 (92%)	9 (8%)	12 42
14	1O	111/111 (100%)	102 (92%)	9 (8%)	11 40
14	2O	111/111 (100%)	101 (91%)	10 (9%)	9 35
15	1P	101/101 (100%)	83 (82%)	18 (18%)	2 9
15	2P	101/101 (100%)	85 (84%)	16 (16%)	2 12
16	1Q	87/88 (99%)	80 (92%)	7 (8%)	12 40
16	2Q	85/88 (97%)	75 (88%)	10 (12%)	5 22
17	1R	115/127 (91%)	103 (90%)	12 (10%)	7 27
17	2R	113/127 (89%)	102 (90%)	11 (10%)	8 31
18	1S	93/94 (99%)	83 (89%)	10 (11%)	6 26
18	2S	93/94 (99%)	87 (94%)	6 (6%)	17 50
19	1T	80/82 (98%)	70 (88%)	10 (12%)	4 20
19	2T	80/82 (98%)	73 (91%)	7 (9%)	10 36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	1U	90/92 (98%)	83 (92%)	7 (8%)	12 42
20	2U	90/92 (98%)	83 (92%)	7 (8%)	12 42
21	1V	77/78 (99%)	71 (92%)	6 (8%)	12 42
21	2V	77/78 (99%)	75 (97%)	2 (3%)	46 78
22	1W	85/91 (93%)	80 (94%)	5 (6%)	19 54
22	2W	85/91 (93%)	76 (89%)	9 (11%)	6 26
23	1X	157/179 (88%)	140 (89%)	17 (11%)	6 26
23	2X	156/179 (87%)	139 (89%)	17 (11%)	6 25
24	1Y	61/67 (91%)	55 (90%)	6 (10%)	8 30
24	2Y	60/67 (90%)	56 (93%)	4 (7%)	16 49
25	1Z	80/83 (96%)	73 (91%)	7 (9%)	10 36
25	2Z	80/83 (96%)	72 (90%)	8 (10%)	7 29
26	10	65/67 (97%)	60 (92%)	5 (8%)	13 42
26	20	65/67 (97%)	56 (86%)	9 (14%)	3 17
27	11	51/52 (98%)	46 (90%)	5 (10%)	8 30
27	21	50/52 (96%)	45 (90%)	5 (10%)	7 29
28	12	60/63 (95%)	48 (80%)	12 (20%)	1 7
28	22	53/63 (84%)	42 (79%)	11 (21%)	1 5
29	13	50/52 (96%)	45 (90%)	5 (10%)	7 29
29	23	50/52 (96%)	44 (88%)	6 (12%)	5 22
30	14	51/52 (98%)	46 (90%)	5 (10%)	8 30
30	24	50/52 (96%)	45 (90%)	5 (10%)	7 29
31	15	41/42 (98%)	39 (95%)	2 (5%)	25 61
31	25	41/42 (98%)	39 (95%)	2 (5%)	25 61
32	16	54/55 (98%)	49 (91%)	5 (9%)	9 33
32	26	54/55 (98%)	49 (91%)	5 (9%)	9 33
33	17	34/34 (100%)	34 (100%)	0	100 100
33	27	34/34 (100%)	33 (97%)	1 (3%)	42 76
35	1b	192/220 (87%)	170 (88%)	22 (12%)	5 24
35	2b	187/220 (85%)	171 (91%)	16 (9%)	10 37
36	1c	143/188 (76%)	135 (94%)	8 (6%)	21 56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
36	2c	141/188 (75%)	128 (91%)	13 (9%)	9 34
37	1d	170/181 (94%)	153 (90%)	17 (10%)	7 29
37	2d	174/181 (96%)	158 (91%)	16 (9%)	9 34
38	1e	113/123 (92%)	101 (89%)	12 (11%)	6 26
38	2e	114/123 (93%)	106 (93%)	8 (7%)	15 47
39	1f	84/90 (93%)	76 (90%)	8 (10%)	8 32
39	2f	86/90 (96%)	80 (93%)	6 (7%)	15 47
40	1g	119/127 (94%)	110 (92%)	9 (8%)	13 43
40	2g	120/127 (94%)	110 (92%)	10 (8%)	11 39
41	1h	114/119 (96%)	99 (87%)	15 (13%)	4 18
41	2h	114/119 (96%)	96 (84%)	18 (16%)	2 12
42	1i	91/99 (92%)	79 (87%)	12 (13%)	4 18
42	2i	89/99 (90%)	74 (83%)	15 (17%)	2 11
43	1j	66/92 (72%)	61 (92%)	5 (8%)	13 43
43	2j	69/92 (75%)	67 (97%)	2 (3%)	42 76
44	1k	83/99 (84%)	77 (93%)	6 (7%)	14 45
44	2k	83/99 (84%)	80 (96%)	3 (4%)	35 70
45	1l	97/109 (89%)	90 (93%)	7 (7%)	14 45
45	2l	97/109 (89%)	89 (92%)	8 (8%)	11 39
46	1m	95/101 (94%)	84 (88%)	11 (12%)	5 23
46	2m	92/101 (91%)	82 (89%)	10 (11%)	6 25
47	1n	49/50 (98%)	42 (86%)	7 (14%)	3 15
47	2n	49/50 (98%)	42 (86%)	7 (14%)	3 15
48	1o	78/80 (98%)	73 (94%)	5 (6%)	17 51
48	2o	78/80 (98%)	70 (90%)	8 (10%)	7 28
49	1p	69/74 (93%)	62 (90%)	7 (10%)	7 29
49	2p	68/74 (92%)	59 (87%)	9 (13%)	4 18
50	1q	94/97 (97%)	89 (95%)	5 (5%)	22 58
50	2q	94/97 (97%)	87 (93%)	7 (7%)	13 44
51	1r	59/77 (77%)	55 (93%)	4 (7%)	16 48
51	2r	59/77 (77%)	55 (93%)	4 (7%)	16 48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
52	1s	70/80 (88%)	61 (87%)	9 (13%)	4 19
52	2s	67/80 (84%)	62 (92%)	5 (8%)	13 43
53	1t	70/82 (85%)	62 (89%)	8 (11%)	5 24
53	2t	71/82 (87%)	65 (92%)	6 (8%)	10 38
54	1u	18/22 (82%)	17 (94%)	1 (6%)	21 56
54	2u	18/22 (82%)	18 (100%)	0	100 100
55	1z	609/636 (96%)	538 (88%)	71 (12%)	5 22
55	2z	609/636 (96%)	534 (88%)	75 (12%)	4 21
58	1x	19/34 (56%)	17 (90%)	2 (10%)	7 27
58	2x	19/34 (56%)	18 (95%)	1 (5%)	22 58
All	All	10695/11742 (91%)	9614 (90%)	1081 (10%)	7 29

5 of 1081 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	2i	64	THR
46	2m	56	LEU
42	2i	31	GLN
55	2z	315	LYS
43	1j	16	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 160 such sidechains are listed below:

Mol	Chain	Res	Type
35	2b	94	ASN
45	2l	78	GLN
36	2c	3	ASN
38	2e	130	ASN
55	2z	77	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	434 (15%)	24 (0%)
1	2A	2860/2915 (98%)	515 (18%)	22 (0%)
2	1B	119/121 (98%)	10 (8%)	1 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2B	119/121 (98%)	17 (14%)	0
34	1a	1491/1521 (98%)	266 (17%)	0
34	2a	1498/1521 (98%)	258 (17%)	0
56	1y	5/24 (20%)	0	0
56	2y	4/24 (16%)	0	0
57	1w	75/77 (97%)	19 (25%)	0
57	2w	75/77 (97%)	18 (24%)	0
All	All	9111/9316 (97%)	1537 (16%)	47 (0%)

5 of 1537 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	11	U
1	1A	14	G
1	1A	28	U
1	1A	33	C
1	1A	44	C

5 of 47 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	552	A
1	2A	1425	G
1	2A	810	A
1	2A	1087	G
1	2A	1699	G

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

8 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	$\#\|Z\| > 2$
57	5MU	2w	54	57	19,22,23	1.40	4 (21%)	28,32,35	2.16	6 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
57	4SU	1w	8	57	18,21,22	2.03	4 (22%)	26,30,33	1.42	5 (19%)
57	PSU	1w	55	57	18,21,22	1.31	2 (11%)	22,30,33	1.83	4 (18%)
57	4SU	2w	8	57	18,21,22	1.96	4 (22%)	26,30,33	1.21	3 (11%)
57	5MU	1w	54	57	19,22,23	1.46	5 (26%)	28,32,35	1.86	6 (21%)
57	5MC	2w	32	57	18,22,23	1.02	2 (11%)	26,32,35	1.27	3 (11%)
57	5MC	1w	32	57	18,22,23	1.02	2 (11%)	26,32,35	1.17	2 (7%)
57	PSU	2w	55	57	18,21,22	1.41	2 (11%)	22,30,33	2.01	4 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	5MU	2w	54	57	-	0/7/25/26	0/2/2/2
57	4SU	1w	8	57	-	0/7/25/26	0/2/2/2
57	PSU	1w	55	57	-	0/7/25/26	0/2/2/2
57	4SU	2w	8	57	-	0/7/25/26	0/2/2/2
57	5MU	1w	54	57	-	2/7/25/26	0/2/2/2
57	5MC	2w	32	57	-	0/7/25/26	0/2/2/2
57	5MC	1w	32	57	-	0/7/25/26	0/2/2/2
57	PSU	2w	55	57	-	0/7/25/26	0/2/2/2

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	2w	8	4SU	C4-N3	-4.91	1.32	1.37
57	1w	8	4SU	C4-N3	-4.82	1.32	1.37
57	1w	8	4SU	C4-S4	-4.06	1.60	1.68
57	2w	8	4SU	C4-S4	-3.84	1.61	1.68
57	1w	8	4SU	C2-N3	-3.65	1.31	1.38

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	2w	55	PSU	N1-C2-N3	6.38	122.35	115.13
57	1w	55	PSU	N1-C2-N3	5.53	121.40	115.13
57	2w	54	5MU	C4-N3-C2	-5.49	120.24	127.35
57	2w	54	5MU	N3-C2-N1	5.11	121.67	114.89
57	2w	54	5MU	C5-C4-N3	4.70	119.32	115.31

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	1w	54	5MU	O4'-C4'-C5'-O5'
57	1w	54	5MU	C3'-C4'-C5'-O5'

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 1945 ligands modelled in this entry, 1941 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	$\#\|Z\| > 2$
62	GDP	2z	702	59	24,30,30	0.94	1 (4%)	30,47,47	1.25	3 (10%)
61	SF4	1d	501	37	0,12,12	-	-	-		
61	SF4	2d	501	37	0,12,12	-	-	-		
62	GDP	1z	701	59	24,30,30	0.92	1 (4%)	30,47,47	1.43	3 (10%)

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
61	SF4	1d	501	37	-	-	0/6/5/5
62	GDP	2z	702	59	-	4/12/32/32	0/3/3/3
61	SF4	2d	501	37	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	GDP	1z	701	59	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	1z	701	GDP	C6-N1	-2.48	1.34	1.37
62	2z	702	GDP	C6-N1	-2.27	1.34	1.37

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
62	1z	701	GDP	PA-O3A-PB	-5.01	115.63	132.83
62	2z	702	GDP	PA-O3A-PB	-4.03	118.98	132.83
62	1z	701	GDP	C8-N7-C5	2.39	107.54	102.99
62	2z	702	GDP	O4'-C1'-C2'	-2.38	103.45	106.93
62	1z	701	GDP	C5-C6-N1	2.34	118.08	113.95

There are no chirality outliers.

All (4) torsion outliers are listed below:

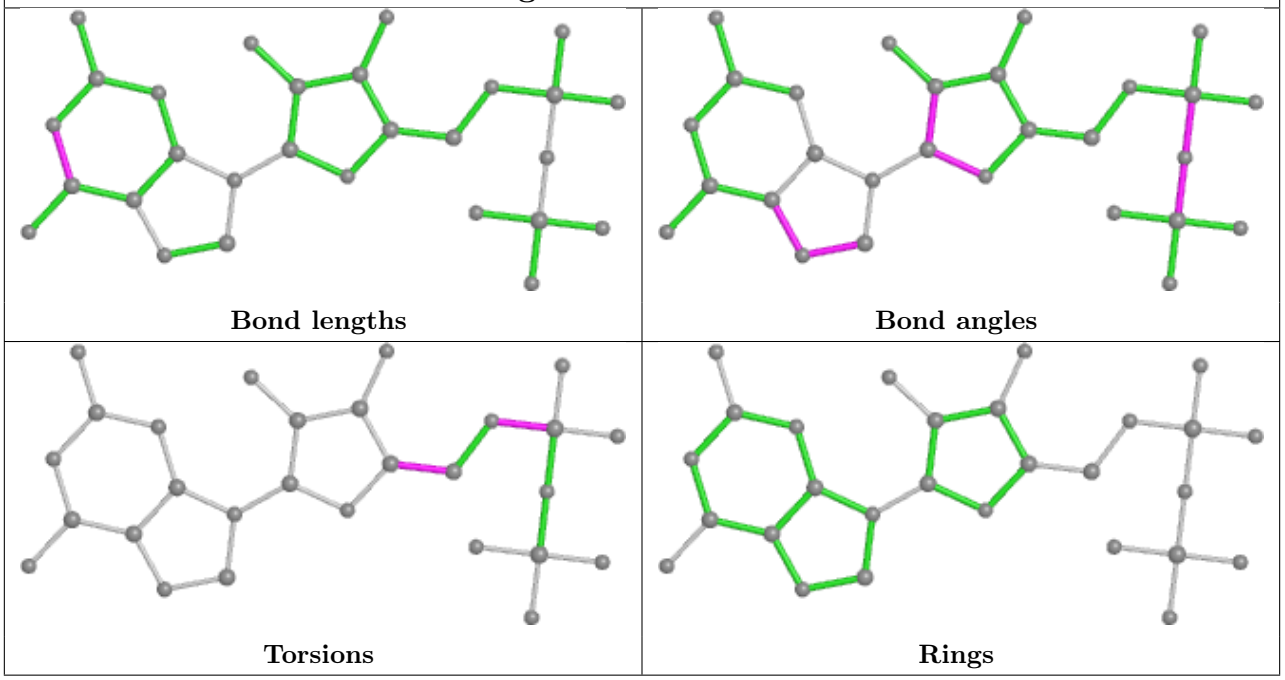
Mol	Chain	Res	Type	Atoms
62	2z	702	GDP	O4'-C4'-C5'-O5'
62	2z	702	GDP	C3'-C4'-C5'-O5'
62	2z	702	GDP	C5'-O5'-PA-O3A
62	2z	702	GDP	C5'-O5'-PA-O2A

There are no ring outliers.

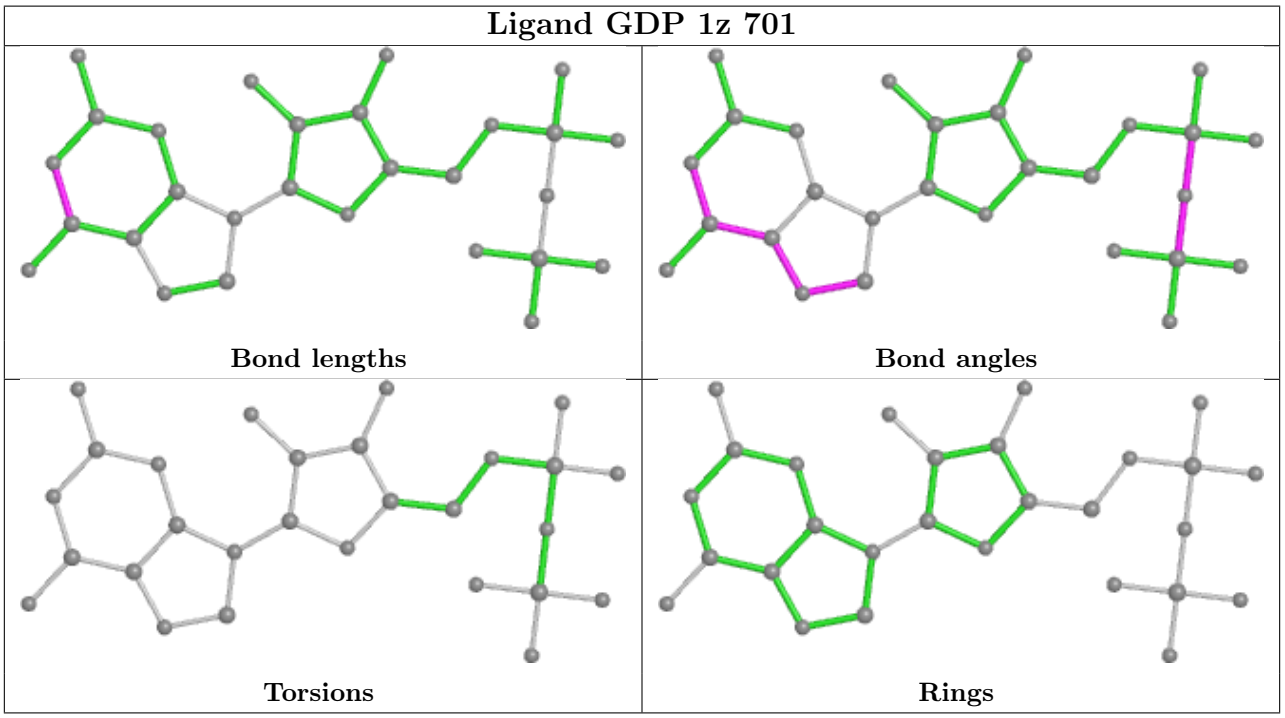
No monomer is involved in short contacts.

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

Ligand GDP 2z 702



Ligand GDP 1z 701



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1A	2872/2915 (98%)	-0.12	87 (3%) 50 22	20, 43, 93, 111	0
1	2A	2868/2915 (98%)	-0.29	90 (3%) 49 21	22, 46, 97, 112	0
2	1B	120/121 (99%)	-0.37	0 100 100	37, 57, 71, 82	0
2	2B	120/121 (99%)	-0.41	0 100 100	43, 62, 74, 83	0
3	1C	135/229 (58%)	3.52	102 (75%) 0 0	82, 99, 105, 108	2 (1%)
3	2C	135/229 (58%)	3.83	111 (82%) 0 0	82, 100, 104, 108	2 (1%)
4	1D	275/276 (99%)	-0.50	0 100 100	23, 41, 57, 85	0
4	2D	275/276 (99%)	-0.58	0 100 100	24, 42, 58, 84	0
5	1E	204/206 (99%)	-0.44	0 100 100	23, 44, 63, 75	0
5	2E	204/206 (99%)	-0.48	0 100 100	22, 48, 65, 77	0
6	1F	203/210 (96%)	-0.39	0 100 100	22, 51, 72, 89	0
6	2F	203/210 (96%)	-0.42	0 100 100	25, 54, 73, 88	0
7	1G	181/182 (99%)	-0.40	1 (0%) 89 72	50, 66, 81, 88	0
7	2G	181/182 (99%)	-0.19	0 100 100	55, 69, 82, 90	0
8	1H	174/180 (96%)	-0.33	1 (0%) 89 72	45, 62, 75, 81	0
8	2H	174/180 (96%)	0.27	1 (0%) 89 72	50, 66, 78, 83	0
9	1J	130/173 (75%)	0.45	12 (9%) 9 3	65, 82, 95, 100	0
9	2J	130/173 (75%)	1.04	20 (15%) 2 1	70, 88, 100, 104	0
10	1K	67/147 (45%)	1.68	21 (31%) 0 0	79, 94, 100, 102	0
10	2K	66/147 (44%)	2.51	38 (57%) 0 0	87, 95, 101, 104	0
11	1L	140/140 (100%)	-0.43	0 100 100	31, 44, 65, 82	0
11	2L	140/140 (100%)	-0.37	0 100 100	33, 49, 67, 81	0
12	1M	122/122 (100%)	-0.43	0 100 100	27, 46, 64, 71	0
12	2M	122/122 (100%)	-0.50	0 100 100	30, 47, 66, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1N	149/150 (99%)	-0.32	0 100 100	24, 53, 76, 84	0
13	2N	149/150 (99%)	-0.13	1 (0%) 87 69	27, 56, 77, 88	0
14	1O	141/141 (100%)	-0.37	0 100 100	32, 48, 61, 74	0
14	2O	141/141 (100%)	-0.60	0 100 100	35, 51, 65, 76	0
15	1P	118/118 (100%)	-0.41	0 100 100	27, 40, 54, 66	0
15	2P	118/118 (100%)	-0.45	0 100 100	29, 43, 58, 68	0
16	1Q	110/112 (98%)	-0.32	0 100 100	44, 56, 71, 76	0
16	2Q	110/112 (98%)	-0.17	0 100 100	47, 60, 73, 78	0
17	1R	131/146 (89%)	-0.41	1 (0%) 86 65	33, 50, 72, 84	0
17	2R	131/146 (89%)	-0.53	0 100 100	34, 52, 73, 82	0
18	1S	116/118 (98%)	-0.65	1 (0%) 84 63	15, 31, 47, 71	0
18	2S	116/118 (98%)	-0.43	0 100 100	37, 56, 70, 74	0
19	1T	101/101 (100%)	-0.58	0 100 100	21, 35, 57, 72	0
19	2T	101/101 (100%)	-0.26	0 100 100	33, 65, 78, 83	0
20	1U	112/113 (99%)	-0.58	0 100 100	19, 32, 54, 85	0
20	2U	112/113 (99%)	-0.39	0 100 100	35, 49, 65, 82	0
21	1V	95/96 (98%)	-0.52	0 100 100	23, 39, 60, 84	0
21	2V	95/96 (98%)	-0.21	2 (2%) 63 34	40, 59, 76, 84	0
22	1W	107/110 (97%)	-0.28	1 (0%) 84 63	39, 57, 74, 81	0
22	2W	107/110 (97%)	0.23	2 (1%) 66 37	44, 61, 76, 85	0
23	1X	186/206 (90%)	-0.40	0 100 100	44, 65, 77, 85	0
23	2X	186/206 (90%)	-0.01	3 (1%) 72 44	50, 68, 80, 88	0
24	1Y	76/85 (89%)	-0.51	1 (1%) 77 51	20, 36, 58, 67	0
24	2Y	76/85 (89%)	-0.12	1 (1%) 77 51	38, 56, 69, 79	0
25	1Z	97/98 (98%)	-0.31	1 (1%) 82 59	24, 44, 67, 75	0
25	2Z	97/98 (98%)	-0.25	1 (1%) 82 59	31, 56, 77, 81	0
26	10	70/72 (97%)	-0.31	0 100 100	44, 57, 69, 81	0
26	20	70/72 (97%)	-0.34	0 100 100	46, 60, 70, 81	0
27	11	59/60 (98%)	-0.23	1 (1%) 70 41	30, 45, 63, 76	0
27	21	59/60 (98%)	0.05	0 100 100	34, 49, 68, 79	0
28	12	69/71 (97%)	0.12	3 (4%) 35 13	61, 81, 93, 98	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	22	69/71 (97%)	0.18	5 (7%) 15 4	66, 82, 95, 99	0
29	13	59/60 (98%)	-0.47	0 100 100	24, 40, 57, 63	0
29	23	59/60 (98%)	-0.52	0 100 100	27, 42, 62, 68	0
30	14	53/54 (98%)	-0.40	0 100 100	37, 47, 59, 64	0
30	24	53/54 (98%)	-0.38	0 100 100	40, 49, 61, 65	0
31	15	48/49 (97%)	-0.33	0 100 100	23, 29, 58, 72	0
31	25	48/49 (97%)	-0.38	0 100 100	30, 40, 66, 78	0
32	16	64/65 (98%)	-0.56	0 100 100	20, 33, 44, 61	0
32	26	64/65 (98%)	-0.34	0 100 100	37, 50, 60, 72	0
33	17	37/37 (100%)	-0.05	0 100 100	36, 49, 59, 65	0
33	27	37/37 (100%)	-0.19	1 (2%) 54 26	39, 53, 63, 68	0
34	1a	1495/1521 (98%)	-0.12	34 (2%) 60 31	40, 72, 96, 109	0
34	2a	1501/1521 (98%)	-0.12	34 (2%) 60 31	42, 73, 96, 109	0
35	1b	231/256 (90%)	0.01	3 (1%) 77 51	67, 82, 91, 100	0
35	2b	231/256 (90%)	0.17	13 (5%) 24 8	68, 83, 93, 103	0
36	1c	206/239 (86%)	0.05	1 (0%) 91 75	68, 80, 90, 95	0
36	2c	206/239 (86%)	0.24	4 (1%) 66 37	71, 81, 90, 95	0
37	1d	208/209 (99%)	-0.24	0 100 100	56, 73, 83, 92	0
37	2d	208/209 (99%)	-0.25	0 100 100	58, 73, 82, 92	0
38	1e	148/162 (91%)	-0.33	0 100 100	54, 68, 77, 83	0
38	2e	148/162 (91%)	-0.19	0 100 100	56, 70, 78, 85	0
39	1f	100/101 (99%)	-0.43	0 100 100	54, 70, 79, 85	0
39	2f	100/101 (99%)	-0.23	0 100 100	56, 71, 81, 84	0
40	1g	155/156 (99%)	0.11	10 (6%) 18 5	70, 78, 89, 94	0
40	2g	155/156 (99%)	0.35	14 (9%) 9 3	69, 79, 91, 96	0
41	1h	137/138 (99%)	-0.19	0 100 100	58, 70, 79, 85	0
41	2h	137/138 (99%)	-0.17	0 100 100	60, 71, 78, 85	0
42	1i	127/128 (99%)	0.16	0 100 100	62, 82, 89, 94	0
42	2i	127/128 (99%)	0.63	8 (6%) 20 6	66, 83, 90, 94	0
43	1j	97/105 (92%)	0.28	2 (2%) 63 34	66, 84, 92, 94	0
43	2j	96/105 (91%)	0.77	11 (11%) 4 1	68, 85, 93, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1k	114/129 (88%)	-0.25	0 100 100	53, 69, 80, 84	0
44	2k	114/129 (88%)	-0.05	0 100 100	54, 71, 82, 85	0
45	1l	122/132 (92%)	-0.34	0 100 100	50, 60, 70, 75	0
45	2l	122/132 (92%)	-0.31	0 100 100	49, 61, 70, 75	0
46	1m	123/126 (97%)	0.27	7 (5%) 23 8	65, 78, 90, 105	0
46	2m	122/126 (96%)	0.57	9 (7%) 14 4	70, 83, 94, 105	0
47	1n	60/61 (98%)	-0.07	1 (1%) 70 41	69, 79, 84, 86	0
47	2n	60/61 (98%)	0.35	2 (3%) 46 20	70, 81, 85, 89	0
48	1o	88/89 (98%)	-0.16	0 100 100	52, 67, 79, 87	0
48	2o	88/89 (98%)	-0.05	0 100 100	51, 68, 78, 87	0
49	1p	82/88 (93%)	0.01	1 (1%) 79 54	54, 69, 79, 85	0
49	2p	82/88 (93%)	0.03	0 100 100	54, 69, 79, 84	0
50	1q	99/105 (94%)	-0.21	0 100 100	54, 67, 76, 83	0
50	2q	99/105 (94%)	-0.04	1 (1%) 82 59	55, 67, 77, 85	0
51	1r	68/88 (77%)	0.19	3 (4%) 34 13	57, 69, 82, 90	0
51	2r	68/88 (77%)	0.14	1 (1%) 73 46	60, 70, 81, 90	0
52	1s	84/93 (90%)	0.65	3 (3%) 42 17	76, 84, 92, 95	0
52	2s	83/93 (89%)	0.84	6 (7%) 15 4	75, 85, 92, 94	0
53	1t	96/106 (90%)	0.05	1 (1%) 82 59	60, 70, 80, 85	0
53	2t	96/106 (90%)	-0.04	0 100 100	59, 70, 81, 84	0
54	1u	23/27 (85%)	0.50	0 100 100	70, 77, 81, 82	0
54	2u	23/27 (85%)	1.00	2 (8%) 10 3	70, 78, 82, 84	0
55	1z	730/758 (96%)	0.38	82 (11%) 5 1	52, 79, 96, 105	0
55	2z	730/758 (96%)	0.56	108 (14%) 2 1	47, 81, 99, 108	0
56	1y	6/24 (25%)	0.58	0 100 100	61, 67, 93, 95	0
56	2y	5/24 (20%)	0.86	1 (20%) 1 0	64, 66, 89, 96	0
57	1w	72/77 (93%)	-0.20	0 100 100	32, 64, 78, 97	0
57	2w	72/77 (93%)	-0.09	0 100 100	33, 66, 79, 98	0
58	1x	19/35 (54%)	-0.31	0 100 100	35, 42, 64, 65	0
58	2x	19/35 (54%)	-0.14	0 100 100	36, 45, 65, 65	0
All	All	22619/23832 (94%)	-0.07	871 (3%) 39 15	15, 63, 94, 112	4 (0%)

The worst 5 of 871 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
46	2m	124	PRO	13.7
3	2C	165	ASN	11.9
46	1m	123	ALA	11.7
3	1C	165	ASN	11.3
3	1C	56	GLN	10.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	PSU	1w	55	20/21	0.93	0.16	53,63,72,82	0
57	PSU	2w	55	20/21	0.93	0.12	53,63,80,86	0
57	4SU	2w	8	20/21	0.94	0.16	51,68,81,83	0
57	5MU	2w	54	21/22	0.94	0.17	61,67,79,97	0
57	5MC	2w	32	21/22	0.95	0.22	52,75,83,85	0
57	4SU	1w	8	20/21	0.95	0.14	43,61,72,73	0
57	5MU	1w	54	21/22	0.96	0.13	22,55,66,75	0
57	5MC	1w	32	21/22	0.96	0.20	48,64,75,79	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1a	1771	1/1	0.33	0.79	94,94,94,94	0
59	MG	2B	206	1/1	0.41	0.27	67,67,67,67	0
60	ZN	13	103	1/1	0.48	0.52	278,278,278,278	0
59	MG	1A	3104	1/1	0.53	0.48	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1B	205	1/1	0.54	0.37	72,72,72,72	0
59	MG	2A	3238	1/1	0.54	0.42	60,60,60,60	0
59	MG	2a	1657	1/1	0.57	0.44	66,66,66,66	0
59	MG	2A	3263	1/1	0.60	0.38	69,69,69,69	0
59	MG	1A	3636	1/1	0.62	0.52	56,56,56,56	0
59	MG	1A	3509	1/1	0.63	0.15	50,50,50,50	0
59	MG	2a	1765	1/1	0.64	0.34	79,79,79,79	0
59	MG	1A	3576	1/1	0.65	0.30	51,51,51,51	0
59	MG	2a	1762	1/1	0.65	0.26	65,65,65,65	0
59	MG	2w	3003	1/1	0.66	0.20	80,80,80,80	0
59	MG	1A	3515	1/1	0.69	0.12	48,48,48,48	0
59	MG	2a	1754	1/1	0.69	0.63	61,61,61,61	0
59	MG	2A	3252	1/1	0.70	0.23	55,55,55,55	0
59	MG	1a	1622	1/1	0.70	0.40	64,64,64,64	0
59	MG	1a	1630	1/1	0.70	0.23	69,69,69,69	0
59	MG	2F	301	1/1	0.71	0.30	58,58,58,58	0
59	MG	1F	306	1/1	0.71	0.34	46,46,46,46	0
59	MG	2a	1662	1/1	0.71	0.38	62,62,62,62	0
59	MG	1A	3483	1/1	0.71	0.20	40,40,40,40	0
59	MG	2A	3326	1/1	0.72	0.27	49,49,49,49	0
59	MG	1A	3710	1/1	0.72	0.37	60,60,60,60	0
59	MG	2a	1661	1/1	0.72	0.15	67,67,67,67	0
59	MG	1a	1643	1/1	0.73	0.12	50,50,50,50	0
59	MG	1A	3226	1/1	0.74	0.28	50,50,50,50	0
59	MG	1A	3023	1/1	0.74	0.79	37,37,37,37	0
59	MG	1A	3638	1/1	0.74	0.23	89,89,89,89	0
59	MG	1A	3771	1/1	0.75	0.37	68,68,68,68	0
59	MG	2A	3330	1/1	0.75	0.19	28,28,28,28	0
59	MG	1A	3497	1/1	0.75	0.25	30,30,30,30	0
59	MG	1A	3673	1/1	0.76	0.20	70,70,70,70	0
59	MG	2B	201	1/1	0.76	0.32	62,62,62,62	0
59	MG	1A	3737	1/1	0.77	0.12	65,65,65,65	0
59	MG	1a	1686	1/1	0.77	0.31	75,75,75,75	0
59	MG	1A	3259	1/1	0.77	0.14	45,45,45,45	0
59	MG	2A	3122	1/1	0.77	0.24	42,42,42,42	0
59	MG	2A	3228	1/1	0.78	0.31	46,46,46,46	0
59	MG	2a	1603	1/1	0.78	0.74	65,65,65,65	0
59	MG	1A	3211	1/1	0.78	0.40	59,59,59,59	0
59	MG	1a	1604	1/1	0.78	0.12	51,51,51,51	0
59	MG	1a	1701	1/1	0.78	0.24	65,65,65,65	0
59	MG	2A	3311	1/1	0.78	0.31	63,63,63,63	0
59	MG	1A	3301	1/1	0.78	0.19	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1A	3321	1/1	0.78	0.17	74,74,74,74	0
59	MG	2A	3145	1/1	0.78	0.23	55,55,55,55	0
59	MG	2A	3180	1/1	0.78	0.15	56,56,56,56	0
59	MG	1A	3196	1/1	0.79	0.33	49,49,49,49	0
59	MG	2A	3220	1/1	0.79	0.46	60,60,60,60	0
59	MG	1A	3002	1/1	0.79	0.22	44,44,44,44	0
59	MG	2a	1621	1/1	0.79	0.29	66,66,66,66	0
59	MG	1A	3223	1/1	0.79	0.41	59,59,59,59	0
59	MG	1a	1799	1/1	0.79	0.29	80,80,80,80	0
59	MG	2A	3032	1/1	0.79	0.33	57,57,57,57	0
59	MG	2a	1687	1/1	0.79	0.35	48,48,48,48	0
59	MG	2a	1689	1/1	0.79	0.16	69,69,69,69	0
59	MG	2A	3273	1/1	0.79	0.18	63,63,63,63	0
59	MG	2A	3035	1/1	0.79	0.25	45,45,45,45	0
59	MG	1A	3114	1/1	0.79	0.11	43,43,43,43	0
59	MG	2A	3136	1/1	0.79	0.32	52,52,52,52	0
59	MG	1a	1684	1/1	0.79	0.17	78,78,78,78	0
59	MG	1A	3018	1/1	0.80	0.44	43,43,43,43	0
59	MG	1a	1666	1/1	0.80	0.16	49,49,49,49	0
59	MG	1a	1681	1/1	0.80	0.18	60,60,60,60	0
59	MG	2A	3432	1/1	0.80	0.08	55,55,55,55	0
59	MG	2A	3500	1/1	0.80	0.25	56,56,56,56	0
59	MG	1A	3207	1/1	0.80	0.47	45,45,45,45	0
59	MG	2A	3088	1/1	0.80	0.19	41,41,41,41	0
59	MG	2A	3094	1/1	0.80	0.26	53,53,53,53	0
59	MG	1A	3040	1/1	0.80	0.31	31,31,31,31	0
59	MG	1A	3141	1/1	0.80	0.14	46,46,46,46	0
59	MG	2A	3236	1/1	0.81	0.38	48,48,48,48	0
59	MG	1A	3072	1/1	0.81	0.39	61,61,61,61	0
59	MG	2A	3063	1/1	0.81	0.27	52,52,52,52	0
59	MG	2a	1616	1/1	0.81	0.25	57,57,57,57	0
59	MG	1A	3017	1/1	0.81	0.09	50,50,50,50	0
59	MG	2a	1640	1/1	0.81	0.11	65,65,65,65	0
59	MG	2a	1649	1/1	0.81	0.22	69,69,69,69	0
59	MG	1B	221	1/1	0.81	0.12	42,42,42,42	0
59	MG	1A	3305	1/1	0.81	0.12	42,42,42,42	0
59	MG	1A	3055	1/1	0.81	0.25	49,49,49,49	0
59	MG	1A	3403	1/1	0.81	0.19	57,57,57,57	0
59	MG	2A	3349	1/1	0.81	0.28	56,56,56,56	0
59	MG	2a	1711	1/1	0.81	0.24	76,76,76,76	0
59	MG	2A	3393	1/1	0.81	0.23	45,45,45,45	0
59	MG	1A	3760	1/1	0.81	0.39	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	2A	3002	1/1	0.81	0.20	40,40,40,40	0
59	MG	2A	3516	1/1	0.81	0.07	78,78,78,78	0
59	MG	1A	3764	1/1	0.81	0.29	33,33,33,33	0
59	MG	2a	1617	1/1	0.82	0.12	65,65,65,65	0
59	MG	1A	3505	1/1	0.82	0.18	55,55,55,55	0
59	MG	1a	1713	1/1	0.82	0.16	62,62,62,62	0
59	MG	1a	1720	1/1	0.82	0.32	54,54,54,54	0
59	MG	2A	3352	1/1	0.82	0.12	31,31,31,31	0
59	MG	2a	1658	1/1	0.82	0.23	58,58,58,58	0
59	MG	1a	1639	1/1	0.82	0.18	67,67,67,67	0
59	MG	1A	3568	1/1	0.82	0.36	54,54,54,54	0
59	MG	1A	3013	1/1	0.82	0.28	35,35,35,35	0
59	MG	2A	3507	1/1	0.82	0.20	39,39,39,39	0
59	MG	2A	3009	1/1	0.82	0.16	50,50,50,50	0
59	MG	1a	1667	1/1	0.82	0.10	67,67,67,67	0
59	MG	1A	3682	1/1	0.82	0.14	97,97,97,97	0
59	MG	1a	1610	1/1	0.82	0.17	50,50,50,50	0
59	MG	1A	3691	1/1	0.82	0.15	53,53,53,53	0
59	MG	1a	1695	1/1	0.82	0.28	49,49,49,49	0
59	MG	1A	3146	1/1	0.83	0.17	56,56,56,56	0
59	MG	1A	3118	1/1	0.83	0.30	42,42,42,42	0
59	MG	1U	202	1/1	0.83	0.27	37,37,37,37	0
59	MG	1A	3389	1/1	0.83	0.20	37,37,37,37	0
59	MG	2A	3179	1/1	0.83	0.39	50,50,50,50	0
59	MG	1a	1608	1/1	0.83	0.19	65,65,65,65	0
59	MG	2A	3186	1/1	0.83	0.22	38,38,38,38	0
59	MG	2S	202	1/1	0.83	0.18	58,58,58,58	0
59	MG	1A	3234	1/1	0.83	0.23	50,50,50,50	0
59	MG	1a	1612	1/1	0.83	0.18	41,41,41,41	0
59	MG	2A	3231	1/1	0.83	0.21	56,56,56,56	0
59	MG	1A	3717	1/1	0.83	0.35	89,89,89,89	0
59	MG	1A	3461	1/1	0.83	0.17	31,31,31,31	0
59	MG	1t	3001	1/1	0.83	0.32	54,54,54,54	0
59	MG	2a	1651	1/1	0.83	0.18	67,67,67,67	0
59	MG	1A	3580	1/1	0.83	0.32	54,54,54,54	0
59	MG	2A	3272	1/1	0.83	0.25	51,51,51,51	0
59	MG	1A	3611	1/1	0.83	0.14	46,46,46,46	0
59	MG	2A	3300	1/1	0.83	0.18	48,48,48,48	0
59	MG	2a	1673	1/1	0.83	0.33	55,55,55,55	0
59	MG	1a	1654	1/1	0.83	0.14	42,42,42,42	0
59	MG	1a	1660	1/1	0.83	0.37	59,59,59,59	0
59	MG	2A	3038	1/1	0.83	0.21	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	2a	1742	1/1	0.83	0.34	82,82,82,82	0
59	MG	1A	3139	1/1	0.83	0.15	67,67,67,67	0
59	MG	2a	1760	1/1	0.83	0.19	44,44,44,44	0
59	MG	2A	3076	1/1	0.83	0.18	45,45,45,45	0
59	MG	1A	3115	1/1	0.83	0.29	36,36,36,36	0
59	MG	2A	3419	1/1	0.83	0.20	30,30,30,30	0
59	MG	2A	3422	1/1	0.83	0.15	37,37,37,37	0
59	MG	2A	3274	1/1	0.84	0.21	56,56,56,56	0
59	MG	2A	3101	1/1	0.84	0.21	50,50,50,50	0
59	MG	2A	3301	1/1	0.84	0.12	30,30,30,30	0
59	MG	2a	1625	1/1	0.84	0.42	60,60,60,60	0
59	MG	2a	1626	1/1	0.84	0.34	57,57,57,57	0
59	MG	1G	3002	1/1	0.84	0.09	64,64,64,64	0
59	MG	1b	3001	1/1	0.84	0.16	70,70,70,70	0
59	MG	2A	3144	1/1	0.84	0.47	50,50,50,50	0
59	MG	1a	1688	1/1	0.84	0.14	60,60,60,60	0
59	MG	1A	3122	1/1	0.84	0.18	60,60,60,60	0
59	MG	2a	1659	1/1	0.84	0.22	46,46,46,46	0
59	MG	1A	3127	1/1	0.84	0.28	31,31,31,31	0
59	MG	1a	1636	1/1	0.84	0.26	62,62,62,62	0
59	MG	1A	3222	1/1	0.84	0.23	49,49,49,49	0
59	MG	1a	1741	1/1	0.84	0.26	71,71,71,71	0
59	MG	2A	3039	1/1	0.84	0.57	43,43,43,43	0
59	MG	2a	1691	1/1	0.84	0.51	64,64,64,64	0
59	MG	2A	3055	1/1	0.84	0.17	41,41,41,41	0
59	MG	2A	3237	1/1	0.84	0.14	54,54,54,54	0
59	MG	2A	3592	1/1	0.84	0.17	63,63,63,63	0
59	MG	2a	1757	1/1	0.84	0.11	64,64,64,64	0
59	MG	1a	1749	1/1	0.84	0.12	68,68,68,68	0
59	MG	1a	1757	1/1	0.84	0.12	56,56,56,56	0
59	MG	1A	3027	1/1	0.84	0.52	34,34,34,34	0
59	MG	2j	8001	1/1	0.84	0.22	65,65,65,65	0
59	MG	2w	3001	1/1	0.84	0.15	64,64,64,64	0
59	MG	2A	3091	1/1	0.84	0.31	60,60,60,60	0
59	MG	1a	1778	1/1	0.84	0.07	81,81,81,81	0
60	ZN	17	102	1/1	0.84	0.32	120,120,120,120	0
59	MG	1a	1634	1/1	0.85	0.12	48,48,48,48	0
59	MG	2a	1620	1/1	0.85	0.24	63,63,63,63	0
59	MG	2A	3280	1/1	0.85	0.29	68,68,68,68	0
59	MG	1a	1693	1/1	0.85	0.11	57,57,57,57	0
59	MG	1A	3603	1/1	0.85	0.22	65,65,65,65	0
59	MG	2a	1630	1/1	0.85	0.41	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1A	3212	1/1	0.85	0.20	40,40,40,40	0
59	MG	1a	1706	1/1	0.85	0.28	57,57,57,57	0
59	MG	1a	1707	1/1	0.85	0.20	60,60,60,60	0
59	MG	2A	3337	1/1	0.85	0.20	41,41,41,41	0
59	MG	1A	3635	1/1	0.85	0.18	72,72,72,72	0
59	MG	2A	3351	1/1	0.85	0.13	43,43,43,43	0
59	MG	2A	3210	1/1	0.85	0.08	45,45,45,45	0
59	MG	2A	3354	1/1	0.85	0.23	33,33,33,33	0
59	MG	1A	3770	1/1	0.85	0.13	68,68,68,68	0
59	MG	2A	3224	1/1	0.85	0.31	62,62,62,62	0
59	MG	1a	1739	1/1	0.85	0.20	44,44,44,44	0
59	MG	1A	3704	1/1	0.85	0.38	71,71,71,71	0
59	MG	2a	1695	1/1	0.85	0.23	61,61,61,61	0
59	MG	2A	3460	1/1	0.85	0.18	59,59,59,59	0
59	MG	2A	3068	1/1	0.85	0.29	43,43,43,43	0
59	MG	2a	1744	1/1	0.85	0.28	65,65,65,65	0
59	MG	1A	3215	1/1	0.85	0.43	37,37,37,37	0
59	MG	2A	3081	1/1	0.85	0.13	63,63,63,63	0
59	MG	2A	3241	1/1	0.85	0.13	52,52,52,52	0
59	MG	1a	1613	1/1	0.85	0.14	66,66,66,66	0
59	MG	2A	3259	1/1	0.85	0.90	72,72,72,72	0
59	MG	1a	1616	1/1	0.85	0.37	55,55,55,55	0
59	MG	2l	201	1/1	0.85	0.16	64,64,64,64	0
59	MG	2z	704	1/1	0.85	0.23	55,55,55,55	0
59	MG	2A	3265	1/1	0.85	0.56	62,62,62,62	0
59	MG	1A	3535	1/1	0.85	0.26	54,54,54,54	0
59	MG	2a	1614	1/1	0.85	0.20	49,49,49,49	0
59	MG	1A	3729	1/1	0.85	0.33	54,54,54,54	0
59	MG	1A	3019	1/1	0.86	0.24	50,50,50,50	0
59	MG	1A	3311	1/1	0.86	0.16	40,40,40,40	0
59	MG	2a	1604	1/1	0.86	0.15	51,51,51,51	0
59	MG	1a	1629	1/1	0.86	0.41	45,45,45,45	0
59	MG	1A	3506	1/1	0.86	0.26	33,33,33,33	0
59	MG	1A	3162	1/1	0.86	0.34	46,46,46,46	0
59	MG	1A	3170	1/1	0.86	0.10	61,61,61,61	0
59	MG	1B	204	1/1	0.86	0.15	51,51,51,51	0
59	MG	1a	1642	1/1	0.86	0.42	43,43,43,43	0
59	MG	1A	3180	1/1	0.86	0.23	50,50,50,50	0
59	MG	1a	1764	1/1	0.86	0.11	67,67,67,67	0
59	MG	1a	1647	1/1	0.86	0.20	73,73,73,73	0
59	MG	2A	3331	1/1	0.86	0.20	39,39,39,39	0
59	MG	2A	3170	1/1	0.86	0.30	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	2A	3176	1/1	0.86	0.15	38,38,38,38	0
59	MG	2A	3350	1/1	0.86	0.19	71,71,71,71	0
59	MG	1A	3680	1/1	0.86	0.30	46,46,46,46	0
59	MG	1A	3551	1/1	0.86	0.16	48,48,48,48	0
59	MG	1a	1800	1/1	0.86	0.44	68,68,68,68	0
59	MG	2a	1668	1/1	0.86	0.18	43,43,43,43	0
59	MG	2A	3357	1/1	0.86	0.17	27,27,27,27	0
59	MG	2a	1680	1/1	0.86	0.27	52,52,52,52	0
59	MG	1A	3437	1/1	0.86	0.09	49,49,49,49	0
59	MG	2A	3403	1/1	0.86	0.20	28,28,28,28	0
59	MG	2A	3414	1/1	0.86	0.12	42,42,42,42	0
59	MG	1H	3001	1/1	0.86	0.15	51,51,51,51	0
59	MG	2a	1703	1/1	0.86	0.15	50,50,50,50	0
59	MG	2a	1705	1/1	0.86	0.17	52,52,52,52	0
59	MG	1w	3004	1/1	0.86	0.24	49,49,49,49	0
59	MG	1A	3694	1/1	0.86	0.17	47,47,47,47	0
59	MG	1a	1683	1/1	0.86	0.15	75,75,75,75	0
59	MG	2a	1751	1/1	0.86	0.36	104,104,104,104	0
59	MG	2A	3465	1/1	0.86	0.17	22,22,22,22	0
59	MG	2A	3485	1/1	0.86	0.15	38,38,38,38	0
59	MG	2a	1759	1/1	0.86	0.32	62,62,62,62	0
59	MG	1A	3010	1/1	0.86	0.29	45,45,45,45	0
59	MG	1A	3303	1/1	0.86	0.24	48,48,48,48	0
59	MG	1a	1687	1/1	0.86	0.22	55,55,55,55	0
59	MG	2A	3581	1/1	0.86	0.19	71,71,71,71	0
59	MG	1A	3594	1/1	0.86	0.11	22,22,22,22	0
59	MG	2A	3611	1/1	0.86	0.17	59,59,59,59	0
59	MG	2z	705	1/1	0.86	0.30	67,67,67,67	0
59	MG	2A	3246	1/1	0.86	0.22	47,47,47,47	0
59	MG	1A	3596	1/1	0.86	0.14	52,52,52,52	0
59	MG	2B	210	1/1	0.86	0.15	55,55,55,55	0
59	MG	1A	3732	1/1	0.86	0.29	75,75,75,75	0
59	MG	1a	1606	1/1	0.87	0.12	63,63,63,63	0
59	MG	2A	3036	1/1	0.87	0.14	53,53,53,53	0
59	MG	2D	301	1/1	0.87	0.29	48,48,48,48	0
59	MG	1A	3036	1/1	0.87	0.28	38,38,38,38	0
59	MG	1A	3068	1/1	0.87	0.42	33,33,33,33	0
59	MG	2A	3052	1/1	0.87	0.17	47,47,47,47	0
59	MG	2A	3268	1/1	0.87	0.37	56,56,56,56	0
59	MG	2a	1607	1/1	0.87	0.12	68,68,68,68	0
59	MG	1a	1611	1/1	0.87	0.26	84,84,84,84	0
59	MG	2A	3062	1/1	0.87	0.11	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1A	3050	1/1	0.87	0.21	42,42,42,42	0
59	MG	2A	3277	1/1	0.87	0.14	69,69,69,69	0
59	MG	1A	3758	1/1	0.87	0.21	34,34,34,34	0
59	MG	2A	3292	1/1	0.87	0.14	46,46,46,46	0
59	MG	2A	3072	1/1	0.87	0.09	65,65,65,65	0
59	MG	1A	3759	1/1	0.87	0.41	46,46,46,46	0
59	MG	2A	3306	1/1	0.87	0.15	45,45,45,45	0
59	MG	1A	3076	1/1	0.87	0.09	50,50,50,50	0
59	MG	2A	3316	1/1	0.87	0.15	65,65,65,65	0
59	MG	1A	3763	1/1	0.87	0.35	38,38,38,38	0
59	MG	1a	1716	1/1	0.87	0.39	63,63,63,63	0
59	MG	1A	3357	1/1	0.87	0.14	22,22,22,22	0
59	MG	1A	3371	1/1	0.87	0.16	30,30,30,30	0
59	MG	1A	3546	1/1	0.87	0.12	54,54,54,54	0
59	MG	2A	3126	1/1	0.87	0.10	45,45,45,45	0
59	MG	1a	1744	1/1	0.87	0.24	64,64,64,64	0
59	MG	1A	3121	1/1	0.87	0.65	49,49,49,49	0
59	MG	1A	3081	1/1	0.87	0.20	56,56,56,56	0
59	MG	1a	1760	1/1	0.87	0.17	65,65,65,65	0
59	MG	2A	3359	1/1	0.87	0.12	33,33,33,33	0
59	MG	2A	3174	1/1	0.87	0.18	34,34,34,34	0
59	MG	2A	3396	1/1	0.87	0.22	24,24,24,24	0
59	MG	1B	218	1/1	0.87	0.17	65,65,65,65	0
59	MG	1a	1766	1/1	0.87	0.37	67,67,67,67	0
59	MG	2a	1725	1/1	0.87	0.12	64,64,64,64	0
59	MG	1A	3093	1/1	0.87	0.24	41,41,41,41	0
59	MG	2A	3185	1/1	0.87	0.35	33,33,33,33	0
59	MG	1a	1653	1/1	0.87	0.30	60,60,60,60	0
59	MG	2A	3441	1/1	0.87	0.38	45,45,45,45	0
59	MG	2a	1755	1/1	0.87	0.33	77,77,77,77	0
59	MG	2A	3193	1/1	0.87	0.25	51,51,51,51	0
59	MG	1a	1798	1/1	0.87	0.34	55,55,55,55	0
59	MG	1D	304	1/1	0.87	0.34	40,40,40,40	0
59	MG	1a	1659	1/1	0.87	0.22	63,63,63,63	0
59	MG	1A	3298	1/1	0.87	0.23	43,43,43,43	0
59	MG	1A	3464	1/1	0.87	0.14	43,43,43,43	0
59	MG	2A	3517	1/1	0.87	0.12	50,50,50,50	0
59	MG	2A	3538	1/1	0.87	0.30	28,28,28,28	0
59	MG	2A	3572	1/1	0.87	0.19	61,61,61,61	0
59	MG	1A	3712	1/1	0.87	0.24	80,80,80,80	0
59	MG	1A	3098	1/1	0.87	0.28	49,49,49,49	0
59	MG	1Y	104	1/1	0.87	0.20	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1A	3724	1/1	0.87	0.19	47,47,47,47	0
59	MG	2A	3142	1/1	0.88	0.20	48,48,48,48	0
59	MG	1A	3332	1/1	0.88	0.11	44,44,44,44	0
59	MG	2E	303	1/1	0.88	0.28	31,31,31,31	0
59	MG	2E	304	1/1	0.88	0.46	56,56,56,56	0
59	MG	1a	1702	1/1	0.88	0.15	51,51,51,51	0
59	MG	2F	302	1/1	0.88	0.16	46,46,46,46	0
59	MG	2A	3169	1/1	0.88	0.35	54,54,54,54	0
59	MG	1A	3544	1/1	0.88	0.22	43,43,43,43	0
59	MG	1A	3082	1/1	0.88	0.21	39,39,39,39	0
59	MG	2A	3013	1/1	0.88	0.22	55,55,55,55	0
59	MG	2a	1612	1/1	0.88	0.24	48,48,48,48	0
59	MG	2A	3022	1/1	0.88	0.09	54,54,54,54	0
59	MG	1A	3745	1/1	0.88	0.17	87,87,87,87	0
59	MG	1A	3756	1/1	0.88	0.22	30,30,30,30	0
59	MG	2A	3339	1/1	0.88	0.14	46,46,46,46	0
59	MG	1A	3670	1/1	0.88	0.16	60,60,60,60	0
59	MG	2a	1624	1/1	0.88	0.14	56,56,56,56	0
59	MG	2A	3188	1/1	0.88	0.21	41,41,41,41	0
59	MG	2A	3192	1/1	0.88	0.19	47,47,47,47	0
59	MG	2a	1627	1/1	0.88	0.38	44,44,44,44	0
59	MG	1a	1729	1/1	0.88	0.41	83,83,83,83	0
59	MG	2A	3195	1/1	0.88	0.22	53,53,53,53	0
59	MG	1A	3467	1/1	0.88	0.21	27,27,27,27	0
59	MG	2A	3211	1/1	0.88	0.29	48,48,48,48	0
59	MG	2A	3363	1/1	0.88	0.12	53,53,53,53	0
59	MG	2A	3368	1/1	0.88	0.16	56,56,56,56	0
59	MG	2A	3213	1/1	0.88	0.20	48,48,48,48	0
59	MG	2A	3218	1/1	0.88	0.18	50,50,50,50	0
59	MG	2A	3046	1/1	0.88	0.25	51,51,51,51	0
59	MG	2a	1667	1/1	0.88	0.11	65,65,65,65	0
59	MG	2A	3404	1/1	0.88	0.22	30,30,30,30	0
59	MG	1A	3475	1/1	0.88	0.15	50,50,50,50	0
59	MG	2a	1677	1/1	0.88	0.68	52,52,52,52	0
59	MG	2a	1678	1/1	0.88	0.11	51,51,51,51	0
59	MG	1a	1607	1/1	0.88	0.32	69,69,69,69	0
59	MG	2a	1686	1/1	0.88	0.16	40,40,40,40	0
59	MG	2A	3061	1/1	0.88	0.23	31,31,31,31	0
59	MG	2A	3429	1/1	0.88	0.12	56,56,56,56	0
59	MG	1A	3174	1/1	0.88	0.18	38,38,38,38	0
59	MG	1A	3157	1/1	0.88	0.18	34,34,34,34	0
59	MG	2A	3066	1/1	0.88	0.23	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1a	1759	1/1	0.88	0.18	65,65,65,65	0
59	MG	1A	3401	1/1	0.88	0.08	44,44,44,44	0
59	MG	1a	1763	1/1	0.88	0.27	55,55,55,55	0
59	MG	2a	1732	1/1	0.88	0.25	55,55,55,55	0
59	MG	1A	3193	1/1	0.88	0.17	47,47,47,47	0
59	MG	2a	1743	1/1	0.88	0.15	68,68,68,68	0
59	MG	1A	3779	1/1	0.88	0.41	39,39,39,39	0
59	MG	2A	3264	1/1	0.88	0.24	49,49,49,49	0
59	MG	2A	3520	1/1	0.88	0.17	54,54,54,54	0
59	MG	1a	1615	1/1	0.88	0.31	54,54,54,54	0
59	MG	2A	3544	1/1	0.88	0.33	53,53,53,53	0
59	MG	2A	3546	1/1	0.88	0.38	56,56,56,56	0
59	MG	2A	3550	1/1	0.88	0.23	50,50,50,50	0
59	MG	1A	3433	1/1	0.88	0.24	34,34,34,34	0
59	MG	1a	1619	1/1	0.88	0.10	51,51,51,51	0
59	MG	2A	3110	1/1	0.88	0.23	38,38,38,38	0
59	MG	2A	3593	1/1	0.88	0.10	73,73,73,73	0
59	MG	2A	3602	1/1	0.88	0.26	62,62,62,62	0
59	MG	2A	3606	1/1	0.88	0.17	29,29,29,29	0
59	MG	1A	3606	1/1	0.88	0.34	60,60,60,60	0
59	MG	2A	3618	1/1	0.88	0.22	43,43,43,43	0
59	MG	1A	3128	1/1	0.88	0.19	28,28,28,28	0
59	MG	1A	3621	1/1	0.88	0.15	21,21,21,21	0
59	MG	1A	3360	1/1	0.89	0.31	36,36,36,36	0
59	MG	2B	202	1/1	0.89	0.19	56,56,56,56	0
59	MG	1A	3362	1/1	0.89	0.26	40,40,40,40	0
59	MG	1A	3637	1/1	0.89	0.14	59,59,59,59	0
59	MG	1A	3290	1/1	0.89	0.21	34,34,34,34	0
59	MG	1A	3669	1/1	0.89	0.25	52,52,52,52	0
59	MG	2A	3276	1/1	0.89	0.17	61,61,61,61	0
59	MG	2A	3082	1/1	0.89	0.26	45,45,45,45	0
59	MG	1a	1742	1/1	0.89	0.16	43,43,43,43	0
59	MG	2N	201	1/1	0.89	0.21	42,42,42,42	0
59	MG	1A	3508	1/1	0.89	0.19	47,47,47,47	0
59	MG	2A	3092	1/1	0.89	0.20	40,40,40,40	0
59	MG	1A	3377	1/1	0.89	0.13	27,27,27,27	0
59	MG	1a	1756	1/1	0.89	0.34	67,67,67,67	0
59	MG	1A	3133	1/1	0.89	0.27	44,44,44,44	0
59	MG	2A	3115	1/1	0.89	0.31	42,42,42,42	0
59	MG	1A	3527	1/1	0.89	0.15	38,38,38,38	0
59	MG	1D	301	1/1	0.89	0.39	32,32,32,32	0
59	MG	1a	1652	1/1	0.89	0.11	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	2A	3334	1/1	0.89	0.19	54,54,54,54	0
59	MG	1A	3390	1/1	0.89	0.20	53,53,53,53	0
59	MG	1A	3046	1/1	0.89	0.27	57,57,57,57	0
59	MG	1a	1655	1/1	0.89	0.25	53,53,53,53	0
59	MG	2A	3166	1/1	0.89	0.12	43,43,43,43	0
59	MG	1a	1656	1/1	0.89	0.54	51,51,51,51	0
59	MG	1a	1657	1/1	0.89	0.28	48,48,48,48	0
59	MG	2a	1641	1/1	0.89	0.13	51,51,51,51	0
59	MG	2a	1647	1/1	0.89	0.14	61,61,61,61	0
59	MG	1A	3167	1/1	0.89	0.62	50,50,50,50	0
59	MG	1A	3412	1/1	0.89	0.17	54,54,54,54	0
59	MG	1A	3563	1/1	0.89	0.23	53,53,53,53	0
59	MG	1Y	101	1/1	0.89	0.16	51,51,51,51	0
59	MG	2A	3365	1/1	0.89	0.13	22,22,22,22	0
59	MG	2A	3367	1/1	0.89	0.15	45,45,45,45	0
59	MG	2A	3182	1/1	0.89	0.17	41,41,41,41	0
59	MG	1w	3003	1/1	0.89	0.12	54,54,54,54	0
59	MG	1A	3716	1/1	0.89	0.16	56,56,56,56	0
59	MG	2A	3397	1/1	0.89	0.15	46,46,46,46	0
59	MG	2A	3402	1/1	0.89	0.17	45,45,45,45	0
59	MG	2A	3187	1/1	0.89	0.21	55,55,55,55	0
59	MG	1a	1682	1/1	0.89	0.23	55,55,55,55	0
59	MG	2A	3007	1/1	0.89	0.14	28,28,28,28	0
59	MG	13	104	1/1	0.89	0.42	48,48,48,48	0
59	MG	1A	3213	1/1	0.89	0.16	47,47,47,47	0
59	MG	1A	3235	1/1	0.89	0.15	49,49,49,49	0
59	MG	2A	3023	1/1	0.89	0.30	34,34,34,34	0
59	MG	2A	3438	1/1	0.89	0.23	54,54,54,54	0
59	MG	2A	3212	1/1	0.89	0.23	46,46,46,46	0
59	MG	2A	3447	1/1	0.89	0.20	41,41,41,41	0
59	MG	1A	3152	1/1	0.89	0.14	24,24,24,24	0
59	MG	2A	3215	1/1	0.89	0.13	51,51,51,51	0
59	MG	2a	1735	1/1	0.89	0.13	50,50,50,50	0
59	MG	2a	1736	1/1	0.89	0.11	42,42,42,42	0
59	MG	2A	3033	1/1	0.89	0.13	50,50,50,50	0
59	MG	1A	3587	1/1	0.89	0.18	18,18,18,18	0
59	MG	2A	3221	1/1	0.89	0.22	41,41,41,41	0
59	MG	1A	3266	1/1	0.89	0.13	28,28,28,28	0
59	MG	1A	3466	1/1	0.89	0.23	26,26,26,26	0
59	MG	1a	1696	1/1	0.89	0.06	54,54,54,54	0
59	MG	2A	3042	1/1	0.89	0.12	39,39,39,39	0
59	MG	2a	1758	1/1	0.89	0.24	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	2A	3045	1/1	0.89	0.28	56,56,56,56	0
59	MG	1A	3344	1/1	0.89	0.10	42,42,42,42	0
59	MG	1A	3347	1/1	0.89	0.15	27,27,27,27	0
59	MG	2A	3054	1/1	0.89	0.28	48,48,48,48	0
59	MG	1a	1705	1/1	0.89	0.24	64,64,64,64	0
59	MG	2A	3256	1/1	0.89	0.23	48,48,48,48	0
59	MG	2A	3258	1/1	0.89	0.39	55,55,55,55	0
59	MG	2A	3595	1/1	0.89	0.17	51,51,51,51	0
59	MG	1A	3482	1/1	0.89	0.15	27,27,27,27	0
59	MG	2A	3262	1/1	0.89	0.23	51,51,51,51	0
59	MG	1A	3286	1/1	0.89	0.23	71,71,71,71	0
59	MG	1a	1618	1/1	0.89	0.29	42,42,42,42	0
59	MG	2A	3070	1/1	0.90	0.26	36,36,36,36	0
59	MG	1a	1710	1/1	0.90	0.41	42,42,42,42	0
59	MG	1A	3538	1/1	0.90	0.13	63,63,63,63	0
59	MG	2A	3078	1/1	0.90	0.19	47,47,47,47	0
59	MG	2A	3269	1/1	0.90	0.28	48,48,48,48	0
59	MG	2A	3270	1/1	0.90	0.18	52,52,52,52	0
59	MG	1A	3045	1/1	0.90	0.31	44,44,44,44	0
59	MG	1A	3696	1/1	0.90	0.13	70,70,70,70	0
59	MG	2A	3087	1/1	0.90	0.14	56,56,56,56	0
59	MG	1a	1722	1/1	0.90	0.26	78,78,78,78	0
59	MG	2M	202	1/1	0.90	0.17	55,55,55,55	0
59	MG	1A	3199	1/1	0.90	0.17	34,34,34,34	0
59	MG	2O	3002	1/1	0.90	0.26	59,59,59,59	0
59	MG	1A	3548	1/1	0.90	0.09	61,61,61,61	0
59	MG	2a	1601	1/1	0.90	0.08	68,68,68,68	0
59	MG	2A	3282	1/1	0.90	0.12	26,26,26,26	0
59	MG	2A	3291	1/1	0.90	0.09	34,34,34,34	0
59	MG	1A	3435	1/1	0.90	0.21	45,45,45,45	0
59	MG	1A	3552	1/1	0.90	0.24	47,47,47,47	0
59	MG	1A	3553	1/1	0.90	0.12	47,47,47,47	0
59	MG	1a	1748	1/1	0.90	0.44	82,82,82,82	0
59	MG	2A	3121	1/1	0.90	0.14	57,57,57,57	0
59	MG	1A	3719	1/1	0.90	0.12	68,68,68,68	0
59	MG	1A	3328	1/1	0.90	0.24	50,50,50,50	0
59	MG	2a	1623	1/1	0.90	0.12	37,37,37,37	0
59	MG	2A	3132	1/1	0.90	0.10	46,46,46,46	0
59	MG	2A	3135	1/1	0.90	0.16	45,45,45,45	0
59	MG	1A	3204	1/1	0.90	0.25	42,42,42,42	0
59	MG	1A	3255	1/1	0.90	0.23	63,63,63,63	0
59	MG	1a	1626	1/1	0.90	0.31	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1A	3083	1/1	0.90	0.38	55,55,55,55	0
59	MG	2A	3153	1/1	0.90	0.10	43,43,43,43	0
59	MG	2A	3165	1/1	0.90	0.36	44,44,44,44	0
59	MG	1A	3586	1/1	0.90	0.11	56,56,56,56	0
59	MG	1A	3746	1/1	0.90	0.24	53,53,53,53	0
59	MG	2a	1653	1/1	0.90	0.21	43,43,43,43	0
59	MG	1A	3749	1/1	0.90	0.25	54,54,54,54	0
59	MG	2A	3171	1/1	0.90	0.23	54,54,54,54	0
59	MG	1A	3263	1/1	0.90	0.19	33,33,33,33	0
59	MG	2A	3175	1/1	0.90	0.15	44,44,44,44	0
59	MG	1A	3589	1/1	0.90	0.15	29,29,29,29	0
59	MG	1A	3468	1/1	0.90	0.20	37,37,37,37	0
59	MG	2A	3373	1/1	0.90	0.17	47,47,47,47	0
59	MG	1A	3470	1/1	0.90	0.25	28,28,28,28	0
59	MG	2A	3181	1/1	0.90	0.20	37,37,37,37	0
59	MG	1a	1802	1/1	0.90	0.16	45,45,45,45	0
59	MG	2A	3399	1/1	0.90	0.25	39,39,39,39	0
59	MG	1A	3762	1/1	0.90	0.35	25,25,25,25	0
59	MG	1A	3113	1/1	0.90	0.28	27,27,27,27	0
59	MG	1A	3605	1/1	0.90	0.18	67,67,67,67	0
59	MG	2a	1690	1/1	0.90	0.22	63,63,63,63	0
59	MG	1A	3476	1/1	0.90	0.19	29,29,29,29	0
59	MG	1A	3479	1/1	0.90	0.17	50,50,50,50	0
59	MG	1A	3776	1/1	0.90	0.30	46,46,46,46	0
59	MG	1a	1658	1/1	0.90	0.11	64,64,64,64	0
59	MG	2A	3205	1/1	0.90	0.32	58,58,58,58	0
59	MG	1A	3620	1/1	0.90	0.17	26,26,26,26	0
59	MG	2A	3439	1/1	0.90	0.18	52,52,52,52	0
59	MG	1A	3004	1/1	0.90	0.16	30,30,30,30	0
59	MG	1A	3630	1/1	0.90	0.11	51,51,51,51	0
59	MG	1B	208	1/1	0.90	0.22	38,38,38,38	0
59	MG	1A	3366	1/1	0.90	0.12	51,51,51,51	0
59	MG	1B	219	1/1	0.90	0.21	71,71,71,71	0
59	MG	1A	3179	1/1	0.90	0.20	51,51,51,51	0
59	MG	1A	3294	1/1	0.90	0.18	18,18,18,18	0
59	MG	1A	3381	1/1	0.90	0.09	23,23,23,23	0
59	MG	1A	3646	1/1	0.90	0.18	48,48,48,48	0
59	MG	1A	3653	1/1	0.90	0.17	62,62,62,62	0
59	MG	2A	3235	1/1	0.90	0.24	39,39,39,39	0
59	MG	1A	3097	1/1	0.90	0.17	55,55,55,55	0
59	MG	2A	3047	1/1	0.90	0.23	48,48,48,48	0
59	MG	1A	3217	1/1	0.90	0.24	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1A	3393	1/1	0.90	0.15	28,28,28,28	0
59	MG	1Y	103	1/1	0.90	0.83	73,73,73,73	0
59	MG	2n	502	1/1	0.90	0.65	76,76,76,76	0
59	MG	1A	3674	1/1	0.90	0.14	48,48,48,48	0
59	MG	2A	3253	1/1	0.90	0.27	53,53,53,53	0
59	MG	10	102	1/1	0.90	0.19	44,44,44,44	0
59	MG	1A	3192	1/1	0.90	0.23	47,47,47,47	0
59	MG	1A	3131	1/1	0.90	0.17	47,47,47,47	0
59	MG	1a	1709	1/1	0.90	0.49	50,50,50,50	0
60	ZN	22	501	1/1	0.90	0.04	118,118,118,118	0
59	MG	2A	3111	1/1	0.91	0.36	47,47,47,47	0
59	MG	2A	3612	1/1	0.91	0.21	46,46,46,46	0
59	MG	1a	1635	1/1	0.91	0.24	55,55,55,55	0
59	MG	2A	3119	1/1	0.91	0.21	39,39,39,39	0
59	MG	1A	3775	1/1	0.91	0.17	41,41,41,41	0
59	MG	1a	1762	1/1	0.91	0.32	62,62,62,62	0
59	MG	1A	3386	1/1	0.91	0.20	32,32,32,32	0
59	MG	1A	3665	1/1	0.91	0.10	70,70,70,70	0
59	MG	1B	202	1/1	0.91	0.27	59,59,59,59	0
59	MG	1A	3293	1/1	0.91	0.08	41,41,41,41	0
59	MG	1A	3187	1/1	0.91	0.15	48,48,48,48	0
59	MG	1A	3005	1/1	0.91	0.22	52,52,52,52	0
59	MG	2A	3303	1/1	0.91	0.10	43,43,43,43	0
59	MG	1B	209	1/1	0.91	0.14	45,45,45,45	0
59	MG	1B	213	1/1	0.91	0.14	39,39,39,39	0
59	MG	1A	3060	1/1	0.91	0.19	45,45,45,45	0
59	MG	2A	3323	1/1	0.91	0.15	50,50,50,50	0
59	MG	2a	1602	1/1	0.91	0.12	47,47,47,47	0
59	MG	1A	3124	1/1	0.91	0.21	46,46,46,46	0
59	MG	1A	3161	1/1	0.91	0.27	54,54,54,54	0
59	MG	1A	3425	1/1	0.91	0.14	68,68,68,68	0
59	MG	1A	3306	1/1	0.91	0.21	23,23,23,23	0
59	MG	1a	1663	1/1	0.91	0.20	79,79,79,79	0
59	MG	1F	304	1/1	0.91	0.13	33,33,33,33	0
59	MG	1A	3695	1/1	0.91	0.18	38,38,38,38	0
59	MG	2A	3178	1/1	0.91	0.21	50,50,50,50	0
59	MG	1a	1680	1/1	0.91	0.22	65,65,65,65	0
59	MG	1A	3561	1/1	0.91	0.10	35,35,35,35	0
59	MG	1A	3064	1/1	0.91	0.18	52,52,52,52	0
59	MG	2A	3356	1/1	0.91	0.09	58,58,58,58	0
59	MG	2A	3024	1/1	0.91	0.22	45,45,45,45	0
59	MG	2A	3030	1/1	0.91	0.17	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	2a	1629	1/1	0.91	0.09	57,57,57,57	0
59	MG	2A	3031	1/1	0.91	0.44	52,52,52,52	0
59	MG	2a	1635	1/1	0.91	0.20	40,40,40,40	0
59	MG	2a	1639	1/1	0.91	0.26	43,43,43,43	0
59	MG	1U	201	1/1	0.91	0.14	48,48,48,48	0
59	MG	1A	3237	1/1	0.91	0.14	55,55,55,55	0
59	MG	2a	1645	1/1	0.91	0.18	58,58,58,58	0
59	MG	1a	1685	1/1	0.91	0.29	51,51,51,51	0
59	MG	1A	3452	1/1	0.91	0.27	46,46,46,46	0
59	MG	1A	3246	1/1	0.91	0.15	39,39,39,39	0
59	MG	2A	3197	1/1	0.91	0.53	55,55,55,55	0
59	MG	2a	1655	1/1	0.91	0.22	63,63,63,63	0
59	MG	2a	1656	1/1	0.91	0.24	61,61,61,61	0
59	MG	1A	3331	1/1	0.91	0.26	53,53,53,53	0
59	MG	2A	3207	1/1	0.91	0.24	51,51,51,51	0
59	MG	2A	3040	1/1	0.91	0.23	45,45,45,45	0
59	MG	10	101	1/1	0.91	0.18	38,38,38,38	0
59	MG	1A	3205	1/1	0.91	0.39	56,56,56,56	0
59	MG	2a	1664	1/1	0.91	0.32	59,59,59,59	0
59	MG	2A	3410	1/1	0.91	0.15	27,27,27,27	0
59	MG	1A	3257	1/1	0.91	0.25	34,34,34,34	0
59	MG	1a	1699	1/1	0.91	0.23	60,60,60,60	0
59	MG	1a	1602	1/1	0.91	0.13	49,49,49,49	0
59	MG	2A	3426	1/1	0.91	0.29	58,58,58,58	0
59	MG	2a	1679	1/1	0.91	0.13	50,50,50,50	0
59	MG	1a	1603	1/1	0.91	0.24	69,69,69,69	0
59	MG	2a	1683	1/1	0.91	0.35	59,59,59,59	0
59	MG	1A	3112	1/1	0.91	0.12	44,44,44,44	0
59	MG	1a	1605	1/1	0.91	0.11	40,40,40,40	0
59	MG	1A	3595	1/1	0.91	0.12	49,49,49,49	0
59	MG	1A	3349	1/1	0.91	0.24	18,18,18,18	0
59	MG	1A	3744	1/1	0.91	0.15	45,45,45,45	0
59	MG	1A	3353	1/1	0.91	0.20	26,26,26,26	0
59	MG	2A	3069	1/1	0.91	0.14	50,50,50,50	0
59	MG	2A	3471	1/1	0.91	0.15	56,56,56,56	0
59	MG	2a	1708	1/1	0.91	0.13	64,64,64,64	0
59	MG	2A	3478	1/1	0.91	0.34	58,58,58,58	0
59	MG	2a	1720	1/1	0.91	0.13	63,63,63,63	0
59	MG	2A	3482	1/1	0.91	0.10	53,53,53,53	0
59	MG	1A	3260	1/1	0.91	0.17	48,48,48,48	0
59	MG	2A	3492	1/1	0.91	0.29	48,48,48,48	0
59	MG	1A	3359	1/1	0.91	0.13	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	2A	3075	1/1	0.91	0.09	46,46,46,46	0
59	MG	2A	3510	1/1	0.91	0.18	35,35,35,35	0
59	MG	2A	3515	1/1	0.91	0.23	48,48,48,48	0
59	MG	2A	3249	1/1	0.91	0.19	39,39,39,39	0
59	MG	1A	3751	1/1	0.91	0.13	43,43,43,43	0
59	MG	1a	1726	1/1	0.91	0.16	60,60,60,60	0
59	MG	2A	3528	1/1	0.91	0.25	30,30,30,30	0
59	MG	2A	3537	1/1	0.91	0.29	38,38,38,38	0
59	MG	1A	3048	1/1	0.91	0.27	32,32,32,32	0
59	MG	1A	3265	1/1	0.91	0.13	36,36,36,36	0
59	MG	2A	3083	1/1	0.91	0.24	55,55,55,55	0
59	MG	1A	3091	1/1	0.91	0.16	54,54,54,54	0
59	MG	2a	1768	1/1	0.91	0.14	64,64,64,64	0
59	MG	2A	3564	1/1	0.91	0.33	72,72,72,72	0
59	MG	1A	3274	1/1	0.91	0.18	25,25,25,25	0
59	MG	2A	3576	1/1	0.91	0.15	40,40,40,40	0
59	MG	1A	3008	1/1	0.91	0.15	31,31,31,31	0
59	MG	1A	3380	1/1	0.91	0.18	44,44,44,44	0
59	MG	2A	3266	1/1	0.91	0.18	38,38,38,38	0
59	MG	1A	3095	1/1	0.91	0.55	40,40,40,40	0
59	MG	1A	3514	1/1	0.91	0.07	43,43,43,43	0
59	MG	1A	3383	1/1	0.91	0.17	47,47,47,47	0
59	MG	2A	3609	1/1	0.91	0.12	51,51,51,51	0
59	MG	2A	3095	1/1	0.92	0.16	37,37,37,37	0
59	MG	2A	3096	1/1	0.92	0.26	55,55,55,55	0
59	MG	1A	3164	1/1	0.92	0.15	46,46,46,46	0
59	MG	2A	3104	1/1	0.92	0.15	53,53,53,53	0
59	MG	1A	3130	1/1	0.92	0.25	34,34,34,34	0
59	MG	2A	3617	1/1	0.92	0.26	62,62,62,62	0
59	MG	1a	1650	1/1	0.92	0.16	48,48,48,48	0
59	MG	1A	3453	1/1	0.92	0.19	36,36,36,36	0
59	MG	1a	1770	1/1	0.92	0.11	67,67,67,67	0
59	MG	1A	3198	1/1	0.92	0.09	60,60,60,60	0
59	MG	1A	3555	1/1	0.92	0.11	56,56,56,56	0
59	MG	2B	213	1/1	0.92	0.13	64,64,64,64	0
59	MG	1a	1781	1/1	0.92	0.13	48,48,48,48	0
59	MG	1A	3463	1/1	0.92	0.20	26,26,26,26	0
59	MG	2A	3134	1/1	0.92	0.12	36,36,36,36	0
59	MG	1A	3099	1/1	0.92	0.18	63,63,63,63	0
59	MG	1A	3230	1/1	0.92	0.23	56,56,56,56	0
59	MG	2G	3001	1/1	0.92	0.17	34,34,34,34	0
59	MG	2A	3140	1/1	0.92	0.27	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1A	3292	1/1	0.92	0.10	39,39,39,39	0
59	MG	1E	303	1/1	0.92	0.32	41,41,41,41	0
59	MG	2A	3318	1/1	0.92	0.14	42,42,42,42	0
59	MG	1d	503	1/1	0.92	0.09	80,80,80,80	0
59	MG	2A	3146	1/1	0.92	0.37	60,60,60,60	0
59	MG	2A	3148	1/1	0.92	0.18	40,40,40,40	0
59	MG	1A	3231	1/1	0.92	0.69	45,45,45,45	0
59	MG	2A	3161	1/1	0.92	0.30	47,47,47,47	0
59	MG	2a	1609	1/1	0.92	0.27	53,53,53,53	0
59	MG	2A	3163	1/1	0.92	0.21	47,47,47,47	0
59	MG	1a	1661	1/1	0.92	0.17	47,47,47,47	0
59	MG	1A	3584	1/1	0.92	0.12	62,62,62,62	0
59	MG	2A	3167	1/1	0.92	0.12	52,52,52,52	0
59	MG	2a	1618	1/1	0.92	0.13	47,47,47,47	0
59	MG	1G	3001	1/1	0.92	0.11	31,31,31,31	0
59	MG	1A	3585	1/1	0.92	0.12	52,52,52,52	0
59	MG	1a	1671	1/1	0.92	0.14	53,53,53,53	0
59	MG	2A	3173	1/1	0.92	0.12	52,52,52,52	0
59	MG	1A	3363	1/1	0.92	0.11	45,45,45,45	0
59	MG	1N	201	1/1	0.92	0.17	40,40,40,40	0
59	MG	1A	3232	1/1	0.92	0.17	47,47,47,47	0
59	MG	1A	3203	1/1	0.92	0.27	36,36,36,36	0
59	MG	2A	3026	1/1	0.92	0.21	44,44,44,44	0
59	MG	1X	3001	1/1	0.92	0.29	55,55,55,55	0
59	MG	1A	3591	1/1	0.92	0.12	47,47,47,47	0
59	MG	2A	3377	1/1	0.92	0.22	44,44,44,44	0
59	MG	1A	3726	1/1	0.92	0.28	34,34,34,34	0
59	MG	2A	3395	1/1	0.92	0.09	53,53,53,53	0
59	MG	1A	3300	1/1	0.92	0.17	47,47,47,47	0
59	MG	2A	3034	1/1	0.92	0.18	47,47,47,47	0
59	MG	1A	3153	1/1	0.92	0.33	33,33,33,33	0
59	MG	2a	1652	1/1	0.92	0.16	36,36,36,36	0
59	MG	1a	1689	1/1	0.92	0.21	22,22,22,22	0
59	MG	1A	3735	1/1	0.92	0.29	32,32,32,32	0
59	MG	1A	3176	1/1	0.92	0.16	33,33,33,33	0
59	MG	1A	3739	1/1	0.92	0.22	50,50,50,50	0
59	MG	1A	3741	1/1	0.92	0.16	50,50,50,50	0
59	MG	2A	3416	1/1	0.92	0.15	50,50,50,50	0
59	MG	2A	3417	1/1	0.92	0.15	53,53,53,53	0
59	MG	2A	3202	1/1	0.92	0.24	35,35,35,35	0
59	MG	1A	3600	1/1	0.92	0.10	33,33,33,33	0
59	MG	2a	1665	1/1	0.92	0.24	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1A	3245	1/1	0.92	0.46	31,31,31,31	0
59	MG	1A	3155	1/1	0.92	0.12	31,31,31,31	0
59	MG	2a	1670	1/1	0.92	0.15	51,51,51,51	0
59	MG	2a	1671	1/1	0.92	0.14	38,38,38,38	0
59	MG	1A	3748	1/1	0.92	0.35	67,67,67,67	0
59	MG	2A	3436	1/1	0.92	0.12	50,50,50,50	0
59	MG	1A	3308	1/1	0.92	0.13	52,52,52,52	0
59	MG	1A	3750	1/1	0.92	0.21	53,53,53,53	0
59	MG	2A	3060	1/1	0.92	0.10	36,36,36,36	0
59	MG	2A	3217	1/1	0.92	0.12	45,45,45,45	0
59	MG	2A	3456	1/1	0.92	0.07	65,65,65,65	0
59	MG	2A	3458	1/1	0.92	0.15	52,52,52,52	0
59	MG	1A	3250	1/1	0.92	0.18	51,51,51,51	0
59	MG	1a	1712	1/1	0.92	0.20	69,69,69,69	0
59	MG	2A	3469	1/1	0.92	0.17	60,60,60,60	0
59	MG	2a	1692	1/1	0.92	0.31	45,45,45,45	0
59	MG	1A	3069	1/1	0.92	0.24	39,39,39,39	0
59	MG	2A	3473	1/1	0.92	0.29	29,29,29,29	0
59	MG	2a	1704	1/1	0.92	0.15	39,39,39,39	0
59	MG	1A	3513	1/1	0.92	0.18	43,43,43,43	0
59	MG	2a	1707	1/1	0.92	0.20	49,49,49,49	0
59	MG	2A	3227	1/1	0.92	0.21	49,49,49,49	0
59	MG	1A	3181	1/1	0.92	0.27	52,52,52,52	0
59	MG	2a	1717	1/1	0.92	0.21	52,52,52,52	0
59	MG	1A	3052	1/1	0.92	0.27	40,40,40,40	0
59	MG	2a	1721	1/1	0.92	0.38	62,62,62,62	0
59	MG	2A	3232	1/1	0.92	0.10	52,52,52,52	0
59	MG	2a	1730	1/1	0.92	0.11	47,47,47,47	0
59	MG	1A	3518	1/1	0.92	0.17	59,59,59,59	0
59	MG	1A	3520	1/1	0.92	0.20	70,70,70,70	0
59	MG	1A	3405	1/1	0.92	0.14	55,55,55,55	0
59	MG	2a	1739	1/1	0.92	0.11	51,51,51,51	0
59	MG	1A	3768	1/1	0.92	0.25	50,50,50,50	0
59	MG	1A	3075	1/1	0.92	0.20	44,44,44,44	0
59	MG	2A	3079	1/1	0.92	0.08	33,33,33,33	0
59	MG	2A	3080	1/1	0.92	0.33	36,36,36,36	0
59	MG	2A	3530	1/1	0.92	0.17	40,40,40,40	0
59	MG	2A	3250	1/1	0.92	0.21	45,45,45,45	0
59	MG	2A	3251	1/1	0.92	0.26	28,28,28,28	0
59	MG	1A	3650	1/1	0.92	0.17	49,49,49,49	0
59	MG	1a	1632	1/1	0.92	0.17	63,63,63,63	0
59	MG	1A	3652	1/1	0.92	0.27	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1a	1752	1/1	0.92	0.27	75,75,75,75	0
59	MG	2A	3568	1/1	0.92	0.14	72,72,72,72	0
59	MG	1A	3333	1/1	0.92	0.15	45,45,45,45	0
59	MG	2A	3089	1/1	0.92	0.14	51,51,51,51	0
59	MG	2A	3577	1/1	0.92	0.18	56,56,56,56	0
59	MG	2A	3578	1/1	0.92	0.12	46,46,46,46	0
59	MG	2q	201	1/1	0.92	0.17	52,52,52,52	0
59	MG	2A	3090	1/1	0.92	0.18	40,40,40,40	0
59	MG	2A	3586	1/1	0.92	0.23	45,45,45,45	0
59	MG	1A	3335	1/1	0.92	0.12	46,46,46,46	0
59	MG	1A	3668	1/1	0.92	0.11	48,48,48,48	0
59	MG	2A	3594	1/1	0.92	0.14	56,56,56,56	0
59	MG	1A	3216	1/1	0.92	0.30	47,47,47,47	0
59	MG	2A	3600	1/1	0.92	0.25	47,47,47,47	0
60	ZN	2n	501	1/1	0.92	0.10	102,102,102,102	0
59	MG	2A	3604	1/1	0.93	0.16	40,40,40,40	0
59	MG	2A	3275	1/1	0.93	0.09	58,58,58,58	0
59	MG	2A	3607	1/1	0.93	0.20	32,32,32,32	0
59	MG	1A	3247	1/1	0.93	0.41	35,35,35,35	0
59	MG	1A	3686	1/1	0.93	0.12	62,62,62,62	0
59	MG	1a	1777	1/1	0.93	0.18	53,53,53,53	0
59	MG	1A	3688	1/1	0.93	0.09	89,89,89,89	0
59	MG	2A	3130	1/1	0.93	0.21	34,34,34,34	0
59	MG	2A	3620	1/1	0.93	0.14	58,58,58,58	0
59	MG	1A	3689	1/1	0.93	0.26	57,57,57,57	0
59	MG	2A	3293	1/1	0.93	0.30	44,44,44,44	0
59	MG	2A	3294	1/1	0.93	0.11	21,21,21,21	0
59	MG	2B	207	1/1	0.93	0.26	40,40,40,40	0
59	MG	1a	1786	1/1	0.93	0.27	48,48,48,48	0
59	MG	1a	1795	1/1	0.93	0.07	45,45,45,45	0
59	MG	1B	210	1/1	0.93	0.23	49,49,49,49	0
59	MG	2D	302	1/1	0.93	0.27	62,62,62,62	0
59	MG	2D	304	1/1	0.93	0.24	51,51,51,51	0
59	MG	1B	212	1/1	0.93	0.06	49,49,49,49	0
59	MG	2A	3310	1/1	0.93	0.16	55,55,55,55	0
59	MG	1A	3582	1/1	0.93	0.19	17,17,17,17	0
59	MG	1A	3041	1/1	0.93	0.18	52,52,52,52	0
59	MG	1A	3338	1/1	0.93	0.20	38,38,38,38	0
59	MG	2A	3320	1/1	0.93	0.19	40,40,40,40	0
59	MG	2A	3322	1/1	0.93	0.23	28,28,28,28	0
59	MG	1B	220	1/1	0.93	0.09	38,38,38,38	0
59	MG	1l	201	1/1	0.93	0.15	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	23	502	1/1	0.93	0.48	49,49,49,49	0
59	MG	2A	3150	1/1	0.93	0.12	37,37,37,37	0
59	MG	1l	202	1/1	0.93	0.16	47,47,47,47	0
59	MG	2A	3156	1/1	0.93	0.11	53,53,53,53	0
59	MG	2A	3160	1/1	0.93	0.21	41,41,41,41	0
59	MG	1A	3486	1/1	0.93	0.07	65,65,65,65	0
59	MG	1w	3002	1/1	0.93	0.07	51,51,51,51	0
59	MG	2a	1610	1/1	0.93	0.36	52,52,52,52	0
59	MG	2A	3164	1/1	0.93	0.18	48,48,48,48	0
59	MG	2a	1613	1/1	0.93	0.08	43,43,43,43	0
59	MG	1A	3698	1/1	0.93	0.16	33,33,33,33	0
59	MG	1D	302	1/1	0.93	0.42	39,39,39,39	0
59	MG	1A	3703	1/1	0.93	0.34	42,42,42,42	0
59	MG	1A	3006	1/1	0.93	0.15	33,33,33,33	0
59	MG	1F	302	1/1	0.93	0.49	40,40,40,40	0
59	MG	2A	3358	1/1	0.93	0.10	56,56,56,56	0
59	MG	1A	3705	1/1	0.93	0.68	56,56,56,56	0
59	MG	1A	3706	1/1	0.93	0.14	46,46,46,46	0
59	MG	1a	1679	1/1	0.93	0.42	60,60,60,60	0
59	MG	1A	3501	1/1	0.93	0.08	49,49,49,49	0
59	MG	2A	3025	1/1	0.93	0.12	42,42,42,42	0
59	MG	2a	1628	1/1	0.93	0.32	62,62,62,62	0
59	MG	1A	3502	1/1	0.93	0.19	20,20,20,20	0
59	MG	1A	3714	1/1	0.93	0.12	72,72,72,72	0
59	MG	2A	3386	1/1	0.93	0.27	43,43,43,43	0
59	MG	2A	3388	1/1	0.93	0.10	55,55,55,55	0
59	MG	1A	3346	1/1	0.93	0.20	26,26,26,26	0
59	MG	1S	3001	1/1	0.93	0.44	40,40,40,40	0
59	MG	2a	1643	1/1	0.93	0.29	39,39,39,39	0
59	MG	1T	201	1/1	0.93	0.27	40,40,40,40	0
59	MG	1A	3037	1/1	0.93	0.21	41,41,41,41	0
59	MG	2A	3398	1/1	0.93	0.15	32,32,32,32	0
59	MG	2a	1650	1/1	0.93	0.18	43,43,43,43	0
59	MG	1A	3408	1/1	0.93	0.12	55,55,55,55	0
59	MG	1A	3599	1/1	0.93	0.21	51,51,51,51	0
59	MG	2A	3037	1/1	0.93	0.15	37,37,37,37	0
59	MG	2a	1654	1/1	0.93	0.22	29,29,29,29	0
59	MG	2A	3190	1/1	0.93	0.39	34,34,34,34	0
59	MG	2A	3406	1/1	0.93	0.16	43,43,43,43	0
59	MG	1A	3134	1/1	0.93	0.15	54,54,54,54	0
59	MG	1a	1691	1/1	0.93	0.30	54,54,54,54	0
59	MG	2A	3194	1/1	0.93	0.27	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1A	3137	1/1	0.93	0.08	55,55,55,55	0
59	MG	1A	3125	1/1	0.93	0.67	39,39,39,39	0
59	MG	2A	3044	1/1	0.93	0.15	47,47,47,47	0
59	MG	1A	3733	1/1	0.93	0.32	59,59,59,59	0
59	MG	2a	1666	1/1	0.93	0.36	48,48,48,48	0
59	MG	1A	3434	1/1	0.93	0.23	48,48,48,48	0
59	MG	2A	3208	1/1	0.93	0.31	47,47,47,47	0
59	MG	2A	3209	1/1	0.93	0.23	46,46,46,46	0
59	MG	1A	3736	1/1	0.93	0.16	69,69,69,69	0
59	MG	2A	3049	1/1	0.93	0.19	38,38,38,38	0
59	MG	1a	1601	1/1	0.93	0.12	30,30,30,30	0
59	MG	2A	3444	1/1	0.93	0.15	45,45,45,45	0
59	MG	2A	3445	1/1	0.93	0.12	52,52,52,52	0
59	MG	1a	1704	1/1	0.93	0.38	54,54,54,54	0
59	MG	2a	1681	1/1	0.93	0.55	58,58,58,58	0
59	MG	2A	3448	1/1	0.93	0.14	37,37,37,37	0
59	MG	1A	3608	1/1	0.93	0.20	59,59,59,59	0
59	MG	1A	3035	1/1	0.93	0.10	38,38,38,38	0
59	MG	2a	1688	1/1	0.93	0.14	35,35,35,35	0
59	MG	1A	3612	1/1	0.93	0.25	48,48,48,48	0
59	MG	1A	3142	1/1	0.93	0.26	55,55,55,55	0
59	MG	1A	3526	1/1	0.93	0.17	47,47,47,47	0
59	MG	2A	3222	1/1	0.93	0.18	40,40,40,40	0
59	MG	1a	1711	1/1	0.93	0.19	52,52,52,52	0
59	MG	2A	3474	1/1	0.93	0.20	41,41,41,41	0
59	MG	2A	3225	1/1	0.93	0.12	45,45,45,45	0
59	MG	1A	3440	1/1	0.93	0.32	50,50,50,50	0
59	MG	1A	3269	1/1	0.93	0.13	21,21,21,21	0
59	MG	2A	3230	1/1	0.93	0.08	54,54,54,54	0
59	MG	2a	1709	1/1	0.93	0.24	68,68,68,68	0
59	MG	1A	3271	1/1	0.93	0.25	40,40,40,40	0
59	MG	2A	3501	1/1	0.93	0.20	50,50,50,50	0
59	MG	1A	3457	1/1	0.93	0.20	47,47,47,47	0
59	MG	1A	3459	1/1	0.93	0.16	30,30,30,30	0
59	MG	2A	3514	1/1	0.93	0.22	58,58,58,58	0
59	MG	2a	1727	1/1	0.93	0.10	63,63,63,63	0
59	MG	2a	1728	1/1	0.93	0.15	60,60,60,60	0
59	MG	1A	3645	1/1	0.93	0.41	40,40,40,40	0
59	MG	1a	1727	1/1	0.93	0.15	39,39,39,39	0
59	MG	1a	1614	1/1	0.93	0.09	53,53,53,53	0
59	MG	2A	3240	1/1	0.93	0.19	42,42,42,42	0
59	MG	2a	1738	1/1	0.93	0.26	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	2A	3521	1/1	0.93	0.19	69,69,69,69	0
59	MG	2A	3524	1/1	0.93	0.22	78,78,78,78	0
59	MG	1A	3319	1/1	0.93	0.20	42,42,42,42	0
59	MG	1A	3368	1/1	0.93	0.18	26,26,26,26	0
59	MG	2a	1750	1/1	0.93	0.19	49,49,49,49	0
59	MG	1a	1617	1/1	0.93	0.18	72,72,72,72	0
59	MG	1A	3651	1/1	0.93	0.11	28,28,28,28	0
59	MG	1A	3145	1/1	0.93	0.16	47,47,47,47	0
59	MG	1A	3322	1/1	0.93	0.26	42,42,42,42	0
59	MG	1a	1623	1/1	0.93	0.64	65,65,65,65	0
59	MG	1a	1753	1/1	0.93	0.12	65,65,65,65	0
59	MG	1A	3106	1/1	0.93	0.21	48,48,48,48	0
59	MG	2A	3569	1/1	0.93	0.12	60,60,60,60	0
59	MG	2a	1763	1/1	0.93	0.32	71,71,71,71	0
59	MG	2A	3570	1/1	0.93	0.34	48,48,48,48	0
59	MG	1A	3667	1/1	0.93	0.19	52,52,52,52	0
59	MG	2A	3093	1/1	0.93	0.17	28,28,28,28	0
59	MG	1a	1758	1/1	0.93	0.11	79,79,79,79	0
59	MG	1A	3560	1/1	0.93	0.14	56,56,56,56	0
59	MG	1A	3330	1/1	0.93	0.11	41,41,41,41	0
59	MG	1A	3287	1/1	0.93	0.19	22,22,22,22	0
59	MG	2A	3103	1/1	0.93	0.23	46,46,46,46	0
59	MG	1A	3565	1/1	0.93	0.12	46,46,46,46	0
59	MG	2A	3108	1/1	0.93	0.21	44,44,44,44	0
59	MG	1A	3384	1/1	0.93	0.10	25,25,25,25	0
59	MG	2A	3596	1/1	0.93	0.13	64,64,64,64	0
59	MG	1A	3219	1/1	0.93	0.32	55,55,55,55	0
59	MG	1a	1767	1/1	0.93	0.22	60,60,60,60	0
59	MG	1a	1796	1/1	0.94	0.22	55,55,55,55	0
59	MG	1A	3533	1/1	0.94	0.17	53,53,53,53	0
59	MG	1A	3178	1/1	0.94	0.31	46,46,46,46	0
59	MG	2A	3522	1/1	0.94	0.11	38,38,38,38	0
59	MG	1A	3391	1/1	0.94	0.22	55,55,55,55	0
59	MG	2A	3527	1/1	0.94	0.26	32,32,32,32	0
59	MG	1A	3392	1/1	0.94	0.14	31,31,31,31	0
59	MG	1A	3227	1/1	0.94	0.32	45,45,45,45	0
59	MG	1A	3397	1/1	0.94	0.20	49,49,49,49	0
59	MG	1A	3107	1/1	0.94	0.20	37,37,37,37	0
59	MG	1A	3718	1/1	0.94	0.22	53,53,53,53	0
59	MG	1A	3402	1/1	0.94	0.12	22,22,22,22	0
59	MG	1A	3108	1/1	0.94	0.36	38,38,38,38	0
59	MG	2A	3551	1/1	0.94	0.13	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	2A	3560	1/1	0.94	0.35	32,32,32,32	0
59	MG	2A	3561	1/1	0.94	0.25	46,46,46,46	0
59	MG	1A	3725	1/1	0.94	0.12	43,43,43,43	0
59	MG	2A	3565	1/1	0.94	0.32	25,25,25,25	0
59	MG	1A	3554	1/1	0.94	0.14	43,43,43,43	0
59	MG	2A	3001	1/1	0.94	0.29	29,29,29,29	0
59	MG	1A	3727	1/1	0.94	0.18	38,38,38,38	0
59	MG	2A	3006	1/1	0.94	0.19	29,29,29,29	0
59	MG	1A	3053	1/1	0.94	0.21	46,46,46,46	0
59	MG	1A	3730	1/1	0.94	0.27	25,25,25,25	0
59	MG	2A	3011	1/1	0.94	0.15	40,40,40,40	0
59	MG	1a	1627	1/1	0.94	0.20	50,50,50,50	0
59	MG	2A	3582	1/1	0.94	0.13	62,62,62,62	0
59	MG	2A	3583	1/1	0.94	0.12	38,38,38,38	0
59	MG	2A	3229	1/1	0.94	0.19	44,44,44,44	0
59	MG	2A	3589	1/1	0.94	0.29	50,50,50,50	0
59	MG	2A	3018	1/1	0.94	0.18	39,39,39,39	0
59	MG	1A	3313	1/1	0.94	0.07	43,43,43,43	0
59	MG	1A	3184	1/1	0.94	0.19	39,39,39,39	0
59	MG	2A	3233	1/1	0.94	0.13	41,41,41,41	0
59	MG	1A	3416	1/1	0.94	0.08	49,49,49,49	0
59	MG	1a	1633	1/1	0.94	0.10	46,46,46,46	0
59	MG	1A	3185	1/1	0.94	0.19	60,60,60,60	0
59	MG	1A	3567	1/1	0.94	0.09	63,63,63,63	0
59	MG	1A	3014	1/1	0.94	0.11	41,41,41,41	0
59	MG	1a	1638	1/1	0.94	0.20	46,46,46,46	0
59	MG	2A	3242	1/1	0.94	0.20	38,38,38,38	0
59	MG	2A	3243	1/1	0.94	0.26	39,39,39,39	0
59	MG	2A	3245	1/1	0.94	0.20	51,51,51,51	0
59	MG	1A	3243	1/1	0.94	0.12	51,51,51,51	0
59	MG	2A	3247	1/1	0.94	0.20	45,45,45,45	0
59	MG	2A	3248	1/1	0.94	0.17	49,49,49,49	0
59	MG	1a	1640	1/1	0.94	0.11	44,44,44,44	0
59	MG	1A	3742	1/1	0.94	0.28	47,47,47,47	0
59	MG	1A	3577	1/1	0.94	0.14	60,60,60,60	0
59	MG	1a	1645	1/1	0.94	0.21	45,45,45,45	0
59	MG	2B	208	1/1	0.94	0.24	58,58,58,58	0
59	MG	1A	3329	1/1	0.94	0.25	33,33,33,33	0
59	MG	2B	211	1/1	0.94	0.23	56,56,56,56	0
59	MG	2B	212	1/1	0.94	0.14	47,47,47,47	0
59	MG	2A	3254	1/1	0.94	0.25	35,35,35,35	0
59	MG	1A	3188	1/1	0.94	0.28	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1A	3190	1/1	0.94	0.21	28,28,28,28	0
59	MG	1A	3447	1/1	0.94	0.04	30,30,30,30	0
59	MG	1A	3448	1/1	0.94	0.08	41,41,41,41	0
59	MG	1A	3450	1/1	0.94	0.14	53,53,53,53	0
59	MG	1A	3030	1/1	0.94	0.22	50,50,50,50	0
59	MG	1A	3757	1/1	0.94	0.15	26,26,26,26	0
59	MG	1A	3086	1/1	0.94	0.11	31,31,31,31	0
59	MG	1A	3455	1/1	0.94	0.17	50,50,50,50	0
59	MG	1A	3456	1/1	0.94	0.21	32,32,32,32	0
59	MG	1A	3148	1/1	0.94	0.19	30,30,30,30	0
59	MG	2S	201	1/1	0.94	0.25	52,52,52,52	0
59	MG	1a	1662	1/1	0.94	0.20	58,58,58,58	0
59	MG	2W	502	1/1	0.94	0.12	45,45,45,45	0
59	MG	1A	3336	1/1	0.94	0.19	20,20,20,20	0
59	MG	26	101	1/1	0.94	0.27	33,33,33,33	0
59	MG	1a	1664	1/1	0.94	0.11	48,48,48,48	0
59	MG	1a	1665	1/1	0.94	0.20	41,41,41,41	0
59	MG	1A	3460	1/1	0.94	0.16	47,47,47,47	0
59	MG	1A	3765	1/1	0.94	0.15	58,58,58,58	0
59	MG	2A	3278	1/1	0.94	0.25	44,44,44,44	0
59	MG	1A	3337	1/1	0.94	0.22	30,30,30,30	0
59	MG	2A	3281	1/1	0.94	0.22	43,43,43,43	0
59	MG	2a	1611	1/1	0.94	0.43	70,70,70,70	0
59	MG	1a	1673	1/1	0.94	0.12	43,43,43,43	0
59	MG	2A	3285	1/1	0.94	0.09	53,53,53,53	0
59	MG	1a	1674	1/1	0.94	0.12	54,54,54,54	0
59	MG	2A	3073	1/1	0.94	0.18	28,28,28,28	0
59	MG	1a	1675	1/1	0.94	0.17	38,38,38,38	0
59	MG	1A	3090	1/1	0.94	0.22	35,35,35,35	0
59	MG	1A	3342	1/1	0.94	0.10	48,48,48,48	0
59	MG	1A	3034	1/1	0.94	0.10	50,50,50,50	0
59	MG	2a	1622	1/1	0.94	0.23	33,33,33,33	0
59	MG	1A	3200	1/1	0.94	0.15	40,40,40,40	0
59	MG	2A	3304	1/1	0.94	0.17	38,38,38,38	0
59	MG	1A	3777	1/1	0.94	0.11	45,45,45,45	0
59	MG	1A	3154	1/1	0.94	0.09	64,64,64,64	0
59	MG	1A	3024	1/1	0.94	0.07	47,47,47,47	0
59	MG	2A	3085	1/1	0.94	0.54	58,58,58,58	0
59	MG	1B	203	1/1	0.94	0.17	43,43,43,43	0
59	MG	1A	3156	1/1	0.94	0.15	54,54,54,54	0
59	MG	2a	1634	1/1	0.94	0.28	52,52,52,52	0
59	MG	2A	3321	1/1	0.94	0.09	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	2a	1636	1/1	0.94	0.16	42,42,42,42	0
59	MG	1A	3624	1/1	0.94	0.20	48,48,48,48	0
59	MG	1A	3628	1/1	0.94	0.22	13,13,13,13	0
59	MG	2A	3325	1/1	0.94	0.18	30,30,30,30	0
59	MG	1A	3025	1/1	0.94	0.17	42,42,42,42	0
59	MG	2a	1644	1/1	0.94	0.28	50,50,50,50	0
59	MG	2A	3328	1/1	0.94	0.19	30,30,30,30	0
59	MG	1a	1692	1/1	0.94	0.28	57,57,57,57	0
59	MG	2a	1648	1/1	0.94	0.23	61,61,61,61	0
59	MG	1A	3478	1/1	0.94	0.21	28,28,28,28	0
59	MG	2A	3332	1/1	0.94	0.14	25,25,25,25	0
59	MG	1A	3159	1/1	0.94	0.34	53,53,53,53	0
59	MG	1A	3481	1/1	0.94	0.14	27,27,27,27	0
59	MG	1A	3096	1/1	0.94	0.18	47,47,47,47	0
59	MG	1A	3641	1/1	0.94	0.30	49,49,49,49	0
59	MG	2A	3102	1/1	0.94	0.05	48,48,48,48	0
59	MG	1A	3643	1/1	0.94	0.09	23,23,23,23	0
59	MG	1A	3361	1/1	0.94	0.18	30,30,30,30	0
59	MG	1A	3280	1/1	0.94	0.09	40,40,40,40	0
59	MG	2A	3109	1/1	0.94	0.26	47,47,47,47	0
59	MG	1A	3488	1/1	0.94	0.09	45,45,45,45	0
59	MG	1A	3492	1/1	0.94	0.21	48,48,48,48	0
59	MG	2a	1663	1/1	0.94	0.14	51,51,51,51	0
59	MG	1E	301	1/1	0.94	0.13	18,18,18,18	0
59	MG	2A	3362	1/1	0.94	0.17	35,35,35,35	0
59	MG	2A	3116	1/1	0.94	0.12	34,34,34,34	0
59	MG	1A	3493	1/1	0.94	0.13	41,41,41,41	0
59	MG	1E	304	1/1	0.94	0.22	58,58,58,58	0
59	MG	2a	1669	1/1	0.94	0.58	55,55,55,55	0
59	MG	1E	305	1/1	0.94	0.11	30,30,30,30	0
59	MG	2A	3124	1/1	0.94	0.27	44,44,44,44	0
59	MG	2a	1672	1/1	0.94	0.12	57,57,57,57	0
59	MG	2A	3376	1/1	0.94	0.12	41,41,41,41	0
59	MG	2a	1674	1/1	0.94	0.23	60,60,60,60	0
59	MG	2a	1675	1/1	0.94	0.21	43,43,43,43	0
59	MG	1A	3281	1/1	0.94	0.15	42,42,42,42	0
59	MG	2A	3379	1/1	0.94	0.14	48,48,48,48	0
59	MG	1A	3656	1/1	0.94	0.17	45,45,45,45	0
59	MG	1a	1719	1/1	0.94	0.24	59,59,59,59	0
59	MG	2A	3133	1/1	0.94	0.14	52,52,52,52	0
59	MG	2a	1682	1/1	0.94	0.14	42,42,42,42	0
59	MG	1A	3282	1/1	0.94	0.13	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1A	3049	1/1	0.94	0.29	41,41,41,41	0
59	MG	1A	3369	1/1	0.94	0.18	53,53,53,53	0
59	MG	2A	3138	1/1	0.94	0.46	58,58,58,58	0
59	MG	1A	3026	1/1	0.94	0.26	42,42,42,42	0
59	MG	1a	1728	1/1	0.94	0.13	44,44,44,44	0
59	MG	1A	3039	1/1	0.94	0.18	36,36,36,36	0
59	MG	1a	1732	1/1	0.94	0.17	54,54,54,54	0
59	MG	1a	1733	1/1	0.94	0.15	61,61,61,61	0
59	MG	2a	1696	1/1	0.94	0.34	40,40,40,40	0
59	MG	2a	1697	1/1	0.94	0.24	55,55,55,55	0
59	MG	2a	1698	1/1	0.94	0.18	29,29,29,29	0
59	MG	2a	1702	1/1	0.94	0.25	53,53,53,53	0
59	MG	2A	3407	1/1	0.94	0.30	32,32,32,32	0
59	MG	1P	202	1/1	0.94	0.18	36,36,36,36	0
59	MG	1A	3378	1/1	0.94	0.19	24,24,24,24	0
59	MG	1S	3002	1/1	0.94	0.55	32,32,32,32	0
59	MG	2A	3154	1/1	0.94	0.22	59,59,59,59	0
59	MG	1A	3511	1/1	0.94	0.13	37,37,37,37	0
59	MG	2A	3420	1/1	0.94	0.19	36,36,36,36	0
59	MG	2A	3159	1/1	0.94	0.43	49,49,49,49	0
59	MG	1A	3675	1/1	0.94	0.23	32,32,32,32	0
59	MG	1A	3679	1/1	0.94	0.18	55,55,55,55	0
59	MG	2A	3430	1/1	0.94	0.34	40,40,40,40	0
59	MG	1U	203	1/1	0.94	0.38	39,39,39,39	0
59	MG	1W	201	1/1	0.94	0.20	32,32,32,32	0
59	MG	2A	3437	1/1	0.94	0.12	37,37,37,37	0
59	MG	1A	3168	1/1	0.94	0.32	60,60,60,60	0
59	MG	1A	3100	1/1	0.94	0.25	38,38,38,38	0
59	MG	2A	3440	1/1	0.94	0.14	51,51,51,51	0
59	MG	1A	3684	1/1	0.94	0.18	57,57,57,57	0
59	MG	1A	3382	1/1	0.94	0.22	46,46,46,46	0
59	MG	1A	3516	1/1	0.94	0.09	27,27,27,27	0
59	MG	1A	3220	1/1	0.94	0.11	33,33,33,33	0
59	MG	2A	3172	1/1	0.94	0.14	49,49,49,49	0
59	MG	2a	1749	1/1	0.94	0.17	59,59,59,59	0
59	MG	2A	3452	1/1	0.94	0.34	52,52,52,52	0
59	MG	13	102	1/1	0.94	0.17	34,34,34,34	0
59	MG	1A	3221	1/1	0.94	0.28	38,38,38,38	0
59	MG	15	101	1/1	0.94	0.21	54,54,54,54	0
59	MG	16	102	1/1	0.94	0.24	47,47,47,47	0
59	MG	1a	1769	1/1	0.94	0.18	68,68,68,68	0
59	MG	17	103	1/1	0.94	0.17	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	2A	3472	1/1	0.94	0.21	21,21,21,21	0
59	MG	2a	1761	1/1	0.94	0.11	39,39,39,39	0
59	MG	1A	3078	1/1	0.94	0.30	45,45,45,45	0
59	MG	1a	1774	1/1	0.94	0.09	68,68,68,68	0
59	MG	2A	3477	1/1	0.94	0.10	54,54,54,54	0
59	MG	2a	1766	1/1	0.94	0.28	61,61,61,61	0
59	MG	1a	1776	1/1	0.94	0.18	66,66,66,66	0
59	MG	2A	3184	1/1	0.94	0.34	56,56,56,56	0
59	MG	1A	3079	1/1	0.94	0.19	22,22,22,22	0
59	MG	2A	3489	1/1	0.94	0.10	47,47,47,47	0
59	MG	1A	3529	1/1	0.94	0.14	53,53,53,53	0
59	MG	2z	701	1/1	0.94	0.19	76,76,76,76	0
59	MG	1a	1779	1/1	0.94	0.41	54,54,54,54	0
59	MG	1A	3530	1/1	0.94	0.22	34,34,34,34	0
59	MG	2A	3502	1/1	0.94	0.22	47,47,47,47	0
59	MG	2w	3002	1/1	0.94	0.07	52,52,52,52	0
59	MG	1a	1782	1/1	0.94	0.10	48,48,48,48	0
60	ZN	12	501	1/1	0.94	0.09	100,100,100,100	0
59	MG	1A	3531	1/1	0.94	0.17	61,61,61,61	0
59	MG	1a	1791	1/1	0.94	0.17	52,52,52,52	0
59	MG	1a	1793	1/1	0.94	0.24	53,53,53,53	0
59	MG	1A	3532	1/1	0.94	0.10	25,25,25,25	0
59	MG	1a	1740	1/1	0.95	0.33	39,39,39,39	0
59	MG	1A	3214	1/1	0.95	0.84	61,61,61,61	0
59	MG	2A	3099	1/1	0.95	0.18	58,58,58,58	0
59	MG	2A	3580	1/1	0.95	0.07	53,53,53,53	0
59	MG	2A	3100	1/1	0.95	0.21	32,32,32,32	0
59	MG	1A	3396	1/1	0.95	0.14	51,51,51,51	0
59	MG	1A	3601	1/1	0.95	0.11	33,33,33,33	0
59	MG	1A	3734	1/1	0.95	0.24	45,45,45,45	0
59	MG	1A	3602	1/1	0.95	0.15	53,53,53,53	0
59	MG	1A	3323	1/1	0.95	0.26	33,33,33,33	0
59	MG	1A	3400	1/1	0.95	0.06	66,66,66,66	0
59	MG	2A	3284	1/1	0.95	0.15	53,53,53,53	0
59	MG	1A	3738	1/1	0.95	0.48	88,88,88,88	0
59	MG	2A	3287	1/1	0.95	0.22	55,55,55,55	0
59	MG	2A	3290	1/1	0.95	0.25	25,25,25,25	0
59	MG	1A	3183	1/1	0.95	0.23	33,33,33,33	0
59	MG	2A	3114	1/1	0.95	0.46	37,37,37,37	0
59	MG	1A	3073	1/1	0.95	0.10	35,35,35,35	0
59	MG	1A	3609	1/1	0.95	0.18	26,26,26,26	0
59	MG	2A	3608	1/1	0.95	0.22	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	2A	3295	1/1	0.95	0.20	52,52,52,52	0
59	MG	2A	3296	1/1	0.95	0.11	45,45,45,45	0
59	MG	1A	3610	1/1	0.95	0.31	46,46,46,46	0
59	MG	2A	3614	1/1	0.95	0.13	53,53,53,53	0
59	MG	2A	3120	1/1	0.95	0.19	53,53,53,53	0
59	MG	1A	3261	1/1	0.95	0.06	34,34,34,34	0
59	MG	2A	3619	1/1	0.95	0.22	43,43,43,43	0
59	MG	1A	3262	1/1	0.95	0.10	53,53,53,53	0
59	MG	1A	3747	1/1	0.95	0.11	42,42,42,42	0
59	MG	2A	3308	1/1	0.95	0.22	29,29,29,29	0
59	MG	2B	204	1/1	0.95	0.17	45,45,45,45	0
59	MG	2B	205	1/1	0.95	0.30	56,56,56,56	0
59	MG	2A	3309	1/1	0.95	0.12	27,27,27,27	0
59	MG	1A	3614	1/1	0.95	0.47	43,43,43,43	0
59	MG	2A	3128	1/1	0.95	0.25	29,29,29,29	0
59	MG	1A	3617	1/1	0.95	0.12	25,25,25,25	0
59	MG	1A	3619	1/1	0.95	0.18	49,49,49,49	0
59	MG	1a	1625	1/1	0.95	0.09	53,53,53,53	0
59	MG	1A	3063	1/1	0.95	0.09	47,47,47,47	0
59	MG	1A	3752	1/1	0.95	0.20	42,42,42,42	0
59	MG	1A	3755	1/1	0.95	0.19	53,53,53,53	0
59	MG	2D	303	1/1	0.95	0.23	24,24,24,24	0
59	MG	1A	3409	1/1	0.95	0.11	29,29,29,29	0
59	MG	2A	3139	1/1	0.95	0.20	42,42,42,42	0
59	MG	2A	3327	1/1	0.95	0.22	59,59,59,59	0
59	MG	1A	3410	1/1	0.95	0.10	52,52,52,52	0
59	MG	2A	3329	1/1	0.95	0.17	46,46,46,46	0
59	MG	1A	3625	1/1	0.95	0.14	58,58,58,58	0
59	MG	2M	201	1/1	0.95	0.09	54,54,54,54	0
59	MG	1A	3186	1/1	0.95	0.23	45,45,45,45	0
59	MG	1A	3414	1/1	0.95	0.13	53,53,53,53	0
59	MG	2O	3001	1/1	0.95	0.24	42,42,42,42	0
59	MG	1a	1785	1/1	0.95	0.31	41,41,41,41	0
59	MG	2P	8001	1/1	0.95	0.09	30,30,30,30	0
59	MG	2A	3336	1/1	0.95	0.13	30,30,30,30	0
59	MG	1A	3633	1/1	0.95	0.14	23,23,23,23	0
59	MG	2A	3338	1/1	0.95	0.18	31,31,31,31	0
59	MG	2Y	8001	1/1	0.95	0.18	59,59,59,59	0
59	MG	1A	3087	1/1	0.95	0.56	48,48,48,48	0
59	MG	2A	3343	1/1	0.95	0.14	43,43,43,43	0
59	MG	26	102	1/1	0.95	0.25	47,47,47,47	0
59	MG	2A	3345	1/1	0.95	0.11	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	2A	3152	1/1	0.95	0.12	27,27,27,27	0
59	MG	1A	3135	1/1	0.95	0.18	36,36,36,36	0
59	MG	1A	3521	1/1	0.95	0.09	45,45,45,45	0
59	MG	2a	1605	1/1	0.95	0.13	40,40,40,40	0
59	MG	1A	3430	1/1	0.95	0.08	63,63,63,63	0
59	MG	1A	3270	1/1	0.95	0.16	47,47,47,47	0
59	MG	1A	3642	1/1	0.95	0.22	45,45,45,45	0
59	MG	1a	1646	1/1	0.95	0.32	43,43,43,43	0
59	MG	1a	1801	1/1	0.95	0.17	55,55,55,55	0
59	MG	1A	3773	1/1	0.95	0.14	25,25,25,25	0
59	MG	2A	3361	1/1	0.95	0.10	26,26,26,26	0
59	MG	2a	1615	1/1	0.95	0.18	43,43,43,43	0
59	MG	1A	3028	1/1	0.95	0.56	40,40,40,40	0
59	MG	1d	502	1/1	0.95	0.36	39,39,39,39	0
59	MG	1A	3119	1/1	0.95	0.45	41,41,41,41	0
59	MG	2a	1619	1/1	0.95	0.50	46,46,46,46	0
59	MG	1A	3225	1/1	0.95	0.17	39,39,39,39	0
59	MG	1A	3647	1/1	0.95	0.13	39,39,39,39	0
59	MG	2A	3369	1/1	0.95	0.30	29,29,29,29	0
59	MG	1l	203	1/1	0.95	0.18	56,56,56,56	0
59	MG	1A	3439	1/1	0.95	0.29	26,26,26,26	0
59	MG	1A	3102	1/1	0.95	0.34	43,43,43,43	0
59	MG	1A	3195	1/1	0.95	0.24	21,21,21,21	0
59	MG	2A	3381	1/1	0.95	0.16	42,42,42,42	0
59	MG	2A	3385	1/1	0.95	0.10	45,45,45,45	0
59	MG	1A	3229	1/1	0.95	0.16	51,51,51,51	0
59	MG	1w	3005	1/1	0.95	0.13	78,78,78,78	0
59	MG	2a	1632	1/1	0.95	0.12	45,45,45,45	0
59	MG	2A	3389	1/1	0.95	0.19	39,39,39,39	0
59	MG	2A	3177	1/1	0.95	0.21	15,15,15,15	0
59	MG	2A	3394	1/1	0.95	0.17	34,34,34,34	0
59	MG	1w	3006	1/1	0.95	0.19	72,72,72,72	0
59	MG	1A	3541	1/1	0.95	0.10	53,53,53,53	0
59	MG	1A	3658	1/1	0.95	0.61	38,38,38,38	0
59	MG	2a	1642	1/1	0.95	0.15	29,29,29,29	0
59	MG	2A	3003	1/1	0.95	0.14	40,40,40,40	0
59	MG	1A	3660	1/1	0.95	0.19	55,55,55,55	0
59	MG	2A	3400	1/1	0.95	0.06	46,46,46,46	0
59	MG	2A	3401	1/1	0.95	0.17	25,25,25,25	0
59	MG	1B	211	1/1	0.95	0.10	32,32,32,32	0
59	MG	1A	3350	1/1	0.95	0.25	29,29,29,29	0
59	MG	1A	3065	1/1	0.95	0.09	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	2A	3012	1/1	0.95	0.24	39,39,39,39	0
59	MG	1A	3355	1/1	0.95	0.21	27,27,27,27	0
59	MG	2A	3408	1/1	0.95	0.14	33,33,33,33	0
59	MG	1A	3550	1/1	0.95	0.12	36,36,36,36	0
59	MG	2A	3412	1/1	0.95	0.15	39,39,39,39	0
59	MG	1A	3454	1/1	0.95	0.11	52,52,52,52	0
59	MG	2A	3415	1/1	0.95	0.30	34,34,34,34	0
59	MG	1a	1670	1/1	0.95	0.19	54,54,54,54	0
59	MG	1A	3672	1/1	0.95	0.06	47,47,47,47	0
59	MG	1a	1672	1/1	0.95	0.30	43,43,43,43	0
59	MG	1A	3289	1/1	0.95	0.11	46,46,46,46	0
59	MG	2A	3421	1/1	0.95	0.11	48,48,48,48	0
59	MG	2A	3199	1/1	0.95	0.41	41,41,41,41	0
59	MG	2A	3424	1/1	0.95	0.14	23,23,23,23	0
59	MG	2A	3425	1/1	0.95	0.27	50,50,50,50	0
59	MG	2A	3201	1/1	0.95	0.34	38,38,38,38	0
59	MG	2A	3028	1/1	0.95	0.10	40,40,40,40	0
59	MG	2A	3029	1/1	0.95	0.26	24,24,24,24	0
59	MG	2A	3431	1/1	0.95	0.22	46,46,46,46	0
59	MG	2A	3206	1/1	0.95	0.32	39,39,39,39	0
59	MG	1A	3143	1/1	0.95	0.09	46,46,46,46	0
59	MG	1D	303	1/1	0.95	0.11	33,33,33,33	0
59	MG	1a	1676	1/1	0.95	0.15	42,42,42,42	0
59	MG	1A	3169	1/1	0.95	0.15	55,55,55,55	0
59	MG	1A	3123	1/1	0.95	0.23	38,38,38,38	0
59	MG	1A	3201	1/1	0.95	0.20	36,36,36,36	0
59	MG	2A	3443	1/1	0.95	0.21	52,52,52,52	0
59	MG	1A	3295	1/1	0.95	0.21	36,36,36,36	0
59	MG	1A	3683	1/1	0.95	0.16	62,62,62,62	0
59	MG	1A	3297	1/1	0.95	0.10	45,45,45,45	0
59	MG	1A	3171	1/1	0.95	0.32	50,50,50,50	0
59	MG	2a	1685	1/1	0.95	0.25	51,51,51,51	0
59	MG	1A	3299	1/1	0.95	0.12	44,44,44,44	0
59	MG	2A	3454	1/1	0.95	0.08	66,66,66,66	0
59	MG	2A	3455	1/1	0.95	0.16	47,47,47,47	0
59	MG	2A	3041	1/1	0.95	0.23	22,22,22,22	0
59	MG	1A	3238	1/1	0.95	0.23	29,29,29,29	0
59	MG	1A	3571	1/1	0.95	0.14	45,45,45,45	0
59	MG	1A	3692	1/1	0.95	0.19	45,45,45,45	0
59	MG	1M	201	1/1	0.95	0.20	48,48,48,48	0
59	MG	1A	3574	1/1	0.95	0.15	47,47,47,47	0
59	MG	1N	202	1/1	0.95	0.41	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1a	1694	1/1	0.95	0.14	39,39,39,39	0
59	MG	2a	1699	1/1	0.95	0.10	47,47,47,47	0
59	MG	2A	3053	1/1	0.95	0.29	44,44,44,44	0
59	MG	2A	3475	1/1	0.95	0.15	51,51,51,51	0
59	MG	1O	3002	1/1	0.95	0.21	27,27,27,27	0
59	MG	1P	201	1/1	0.95	0.30	52,52,52,52	0
59	MG	2A	3479	1/1	0.95	0.09	34,34,34,34	0
59	MG	2A	3480	1/1	0.95	0.07	59,59,59,59	0
59	MG	2A	3059	1/1	0.95	0.13	49,49,49,49	0
59	MG	1a	1698	1/1	0.95	0.16	45,45,45,45	0
59	MG	2a	1714	1/1	0.95	0.25	60,60,60,60	0
59	MG	2a	1716	1/1	0.95	0.18	62,62,62,62	0
59	MG	1A	3575	1/1	0.95	0.12	52,52,52,52	0
59	MG	2a	1718	1/1	0.95	0.10	50,50,50,50	0
59	MG	2A	3491	1/1	0.95	0.23	42,42,42,42	0
59	MG	1A	3241	1/1	0.95	0.34	40,40,40,40	0
59	MG	2A	3494	1/1	0.95	0.10	44,44,44,44	0
59	MG	2A	3495	1/1	0.95	0.07	56,56,56,56	0
59	MG	2A	3498	1/1	0.95	0.15	36,36,36,36	0
59	MG	2A	3499	1/1	0.95	0.12	53,53,53,53	0
59	MG	2a	1731	1/1	0.95	0.19	48,48,48,48	0
59	MG	2A	3239	1/1	0.95	0.67	50,50,50,50	0
59	MG	1A	3302	1/1	0.95	0.20	29,29,29,29	0
59	MG	2A	3064	1/1	0.95	0.29	28,28,28,28	0
59	MG	2A	3503	1/1	0.95	0.15	32,32,32,32	0
59	MG	2A	3505	1/1	0.95	0.14	46,46,46,46	0
59	MG	2a	1740	1/1	0.95	0.31	53,53,53,53	0
59	MG	1a	1703	1/1	0.95	0.21	52,52,52,52	0
59	MG	1A	3702	1/1	0.95	0.10	51,51,51,51	0
59	MG	2A	3512	1/1	0.95	0.06	63,63,63,63	0
59	MG	1A	3579	1/1	0.95	0.12	44,44,44,44	0
59	MG	1A	3033	1/1	0.95	0.43	49,49,49,49	0
59	MG	1A	3304	1/1	0.95	0.15	39,39,39,39	0
59	MG	2a	1752	1/1	0.95	0.19	64,64,64,64	0
59	MG	2a	1753	1/1	0.95	0.09	39,39,39,39	0
59	MG	1A	3244	1/1	0.95	0.17	41,41,41,41	0
59	MG	1A	3094	1/1	0.95	0.23	43,43,43,43	0
59	MG	1A	3151	1/1	0.95	0.18	36,36,36,36	0
59	MG	1A	3057	1/1	0.95	0.10	38,38,38,38	0
59	MG	1A	3110	1/1	0.95	0.27	61,61,61,61	0
59	MG	1A	3590	1/1	0.95	0.12	44,44,44,44	0
59	MG	1a	1717	1/1	0.95	0.11	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	2A	3255	1/1	0.95	0.18	37,37,37,37	0
59	MG	1A	3316	1/1	0.95	0.07	48,48,48,48	0
59	MG	11	8001	1/1	0.95	0.67	44,44,44,44	0
59	MG	2A	3540	1/1	0.95	0.40	31,31,31,31	0
59	MG	2a	1767	1/1	0.95	0.14	45,45,45,45	0
59	MG	2A	3541	1/1	0.95	0.14	49,49,49,49	0
59	MG	2a	1769	1/1	0.95	0.22	54,54,54,54	0
59	MG	1A	3593	1/1	0.95	0.17	53,53,53,53	0
59	MG	2A	3260	1/1	0.95	0.09	49,49,49,49	0
59	MG	2A	3261	1/1	0.95	0.16	27,27,27,27	0
59	MG	1A	3720	1/1	0.95	0.15	64,64,64,64	0
59	MG	2A	3552	1/1	0.95	0.29	39,39,39,39	0
59	MG	2z	703	1/1	0.95	0.17	41,41,41,41	0
59	MG	1A	3252	1/1	0.95	0.11	45,45,45,45	0
59	MG	15	102	1/1	0.95	0.12	40,40,40,40	0
59	MG	2A	3562	1/1	0.95	0.06	34,34,34,34	0
59	MG	1A	3490	1/1	0.95	0.09	64,64,64,64	0
59	MG	1a	1731	1/1	0.95	0.20	47,47,47,47	0
59	MG	1A	3029	1/1	0.95	0.62	40,40,40,40	0
59	MG	1A	3597	1/1	0.95	0.11	50,50,50,50	0
59	MG	1A	3598	1/1	0.95	0.21	48,48,48,48	0
59	MG	2A	3271	1/1	0.95	0.18	58,58,58,58	0
59	MG	2A	3573	1/1	0.95	0.25	43,43,43,43	0
59	MG	2A	3143	1/1	0.96	0.30	47,47,47,47	0
59	MG	2A	3597	1/1	0.96	0.21	43,43,43,43	0
59	MG	1A	3623	1/1	0.96	0.20	16,16,16,16	0
59	MG	2A	3601	1/1	0.96	0.25	53,53,53,53	0
59	MG	1a	1787	1/1	0.96	0.14	70,70,70,70	0
59	MG	1a	1789	1/1	0.96	0.22	43,43,43,43	0
59	MG	1a	1790	1/1	0.96	0.16	51,51,51,51	0
59	MG	2A	3149	1/1	0.96	0.30	46,46,46,46	0
59	MG	1A	3512	1/1	0.96	0.18	19,19,19,19	0
59	MG	1A	3158	1/1	0.96	0.26	29,29,29,29	0
59	MG	2A	3610	1/1	0.96	0.08	52,52,52,52	0
59	MG	1a	1794	1/1	0.96	0.08	71,71,71,71	0
59	MG	1A	3345	1/1	0.96	0.14	38,38,38,38	0
59	MG	2A	3340	1/1	0.96	0.17	44,44,44,44	0
59	MG	2A	3615	1/1	0.96	0.21	53,53,53,53	0
59	MG	2A	3341	1/1	0.96	0.26	24,24,24,24	0
59	MG	1A	3044	1/1	0.96	0.18	33,33,33,33	0
59	MG	2A	3344	1/1	0.96	0.13	49,49,49,49	0
59	MG	2A	3157	1/1	0.96	0.36	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1A	3631	1/1	0.96	0.11	48,48,48,48	0
59	MG	1A	3413	1/1	0.96	0.29	47,47,47,47	0
59	MG	1A	3517	1/1	0.96	0.26	27,27,27,27	0
59	MG	2A	3162	1/1	0.96	0.24	30,30,30,30	0
59	MG	1A	3160	1/1	0.96	0.13	36,36,36,36	0
59	MG	1A	3016	1/1	0.96	0.26	37,37,37,37	0
59	MG	1A	3766	1/1	0.96	0.09	28,28,28,28	0
59	MG	1A	3418	1/1	0.96	0.11	37,37,37,37	0
59	MG	1a	1649	1/1	0.96	0.23	52,52,52,52	0
59	MG	2A	3168	1/1	0.96	0.21	45,45,45,45	0
59	MG	1A	3522	1/1	0.96	0.12	42,42,42,42	0
59	MG	1A	3126	1/1	0.96	0.18	34,34,34,34	0
59	MG	1A	3427	1/1	0.96	0.06	30,30,30,30	0
59	MG	2A	3366	1/1	0.96	0.23	40,40,40,40	0
59	MG	1A	3774	1/1	0.96	0.40	49,49,49,49	0
59	MG	2E	301	1/1	0.96	0.25	20,20,20,20	0
59	MG	2E	302	1/1	0.96	0.14	27,27,27,27	0
59	MG	1w	3001	1/1	0.96	0.07	55,55,55,55	0
59	MG	1A	3528	1/1	0.96	0.18	49,49,49,49	0
59	MG	2A	3370	1/1	0.96	0.14	46,46,46,46	0
59	MG	2A	3372	1/1	0.96	0.09	36,36,36,36	0
59	MG	1A	3351	1/1	0.96	0.09	29,29,29,29	0
59	MG	2A	3375	1/1	0.96	0.12	28,28,28,28	0
59	MG	1A	3431	1/1	0.96	0.05	44,44,44,44	0
59	MG	1A	3352	1/1	0.96	0.14	33,33,33,33	0
59	MG	1B	201	1/1	0.96	0.16	54,54,54,54	0
59	MG	1A	3248	1/1	0.96	0.17	36,36,36,36	0
59	MG	2A	3382	1/1	0.96	0.18	34,34,34,34	0
59	MG	2A	3384	1/1	0.96	0.14	25,25,25,25	0
59	MG	1A	3354	1/1	0.96	0.18	31,31,31,31	0
59	MG	1A	3436	1/1	0.96	0.05	46,46,46,46	0
59	MG	2A	3004	1/1	0.96	0.12	53,53,53,53	0
59	MG	1A	3537	1/1	0.96	0.20	46,46,46,46	0
59	MG	2A	3391	1/1	0.96	0.13	47,47,47,47	0
59	MG	2A	3392	1/1	0.96	0.15	39,39,39,39	0
59	MG	1B	206	1/1	0.96	0.08	33,33,33,33	0
59	MG	1B	207	1/1	0.96	0.18	50,50,50,50	0
59	MG	1A	3296	1/1	0.96	0.21	17,17,17,17	0
59	MG	1A	3438	1/1	0.96	0.13	49,49,49,49	0
59	MG	2A	3189	1/1	0.96	0.37	29,29,29,29	0
59	MG	1A	3661	1/1	0.96	0.11	40,40,40,40	0
59	MG	2a	1608	1/1	0.96	0.26	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	2A	3016	1/1	0.96	0.11	48,48,48,48	0
59	MG	1A	3663	1/1	0.96	0.13	32,32,32,32	0
59	MG	1A	3542	1/1	0.96	0.23	67,67,67,67	0
59	MG	1A	3249	1/1	0.96	0.19	40,40,40,40	0
59	MG	1A	3358	1/1	0.96	0.16	30,30,30,30	0
59	MG	1A	3547	1/1	0.96	0.10	42,42,42,42	0
59	MG	1A	3442	1/1	0.96	0.09	50,50,50,50	0
59	MG	2A	3027	1/1	0.96	0.39	44,44,44,44	0
59	MG	1a	1678	1/1	0.96	0.11	48,48,48,48	0
59	MG	2A	3409	1/1	0.96	0.06	48,48,48,48	0
59	MG	1A	3445	1/1	0.96	0.12	46,46,46,46	0
59	MG	2A	3411	1/1	0.96	0.26	43,43,43,43	0
59	MG	1B	222	1/1	0.96	0.09	41,41,41,41	0
59	MG	2A	3413	1/1	0.96	0.11	30,30,30,30	0
59	MG	1B	223	1/1	0.96	0.16	46,46,46,46	0
59	MG	1A	3446	1/1	0.96	0.05	31,31,31,31	0
59	MG	1A	3012	1/1	0.96	0.18	40,40,40,40	0
59	MG	1A	3189	1/1	0.96	0.05	44,44,44,44	0
59	MG	1A	3677	1/1	0.96	0.29	58,58,58,58	0
59	MG	1A	3253	1/1	0.96	0.12	40,40,40,40	0
59	MG	1A	3165	1/1	0.96	0.08	40,40,40,40	0
59	MG	1A	3557	1/1	0.96	0.14	44,44,44,44	0
59	MG	2a	1631	1/1	0.96	0.15	48,48,48,48	0
59	MG	2A	3423	1/1	0.96	0.24	34,34,34,34	0
59	MG	2a	1633	1/1	0.96	0.14	36,36,36,36	0
59	MG	1A	3047	1/1	0.96	0.12	37,37,37,37	0
59	MG	2A	3219	1/1	0.96	0.20	43,43,43,43	0
59	MG	1A	3364	1/1	0.96	0.17	27,27,27,27	0
59	MG	2a	1637	1/1	0.96	0.23	54,54,54,54	0
59	MG	2A	3428	1/1	0.96	0.16	28,28,28,28	0
59	MG	1A	3365	1/1	0.96	0.24	39,39,39,39	0
59	MG	1F	305	1/1	0.96	0.14	36,36,36,36	0
59	MG	2A	3043	1/1	0.96	0.12	43,43,43,43	0
59	MG	1A	3258	1/1	0.96	0.13	24,24,24,24	0
59	MG	2A	3434	1/1	0.96	0.27	54,54,54,54	0
59	MG	2A	3226	1/1	0.96	0.27	34,34,34,34	0
59	MG	2a	1646	1/1	0.96	0.08	55,55,55,55	0
59	MG	1A	3147	1/1	0.96	0.17	32,32,32,32	0
59	MG	1A	3690	1/1	0.96	0.07	56,56,56,56	0
59	MG	1A	3056	1/1	0.96	0.10	30,30,30,30	0
59	MG	1A	3150	1/1	0.96	0.21	31,31,31,31	0
59	MG	2A	3050	1/1	0.96	0.05	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	2A	3051	1/1	0.96	0.15	35,35,35,35	0
59	MG	1a	1700	1/1	0.96	0.16	50,50,50,50	0
59	MG	2A	3234	1/1	0.96	0.52	56,56,56,56	0
59	MG	1A	3693	1/1	0.96	0.14	48,48,48,48	0
59	MG	1A	3374	1/1	0.96	0.15	35,35,35,35	0
59	MG	2A	3451	1/1	0.96	0.11	56,56,56,56	0
59	MG	1A	3375	1/1	0.96	0.16	12,12,12,12	0
59	MG	2A	3057	1/1	0.96	0.15	41,41,41,41	0
59	MG	2A	3058	1/1	0.96	0.13	48,48,48,48	0
59	MG	1A	3307	1/1	0.96	0.16	18,18,18,18	0
59	MG	1A	3085	1/1	0.96	0.44	55,55,55,55	0
59	MG	1A	3699	1/1	0.96	0.22	51,51,51,51	0
59	MG	2A	3461	1/1	0.96	0.07	54,54,54,54	0
59	MG	2A	3462	1/1	0.96	0.27	40,40,40,40	0
59	MG	2A	3463	1/1	0.96	0.10	45,45,45,45	0
59	MG	1A	3701	1/1	0.96	0.13	47,47,47,47	0
59	MG	2A	3466	1/1	0.96	0.09	51,51,51,51	0
59	MG	2A	3467	1/1	0.96	0.10	35,35,35,35	0
59	MG	2A	3468	1/1	0.96	0.15	55,55,55,55	0
59	MG	1a	1708	1/1	0.96	0.21	37,37,37,37	0
59	MG	1S	3003	1/1	0.96	0.58	57,57,57,57	0
59	MG	1A	3578	1/1	0.96	0.19	40,40,40,40	0
59	MG	1A	3173	1/1	0.96	0.23	48,48,48,48	0
59	MG	2a	1676	1/1	0.96	0.48	47,47,47,47	0
59	MG	1A	3007	1/1	0.96	0.16	18,18,18,18	0
59	MG	1A	3581	1/1	0.96	0.12	61,61,61,61	0
59	MG	2A	3476	1/1	0.96	0.17	61,61,61,61	0
59	MG	1A	3059	1/1	0.96	0.06	36,36,36,36	0
59	MG	1A	3708	1/1	0.96	0.18	51,51,51,51	0
59	MG	2A	3074	1/1	0.96	0.19	39,39,39,39	0
59	MG	1A	3583	1/1	0.96	0.29	39,39,39,39	0
59	MG	2a	1684	1/1	0.96	0.45	55,55,55,55	0
59	MG	2A	3481	1/1	0.96	0.09	51,51,51,51	0
59	MG	1A	3471	1/1	0.96	0.17	23,23,23,23	0
59	MG	2A	3484	1/1	0.96	0.08	38,38,38,38	0
59	MG	1A	3713	1/1	0.96	0.63	42,42,42,42	0
59	MG	2A	3486	1/1	0.96	0.16	49,49,49,49	0
59	MG	2A	3487	1/1	0.96	0.06	41,41,41,41	0
59	MG	1A	3472	1/1	0.96	0.16	47,47,47,47	0
59	MG	1A	3715	1/1	0.96	0.27	42,42,42,42	0
59	MG	2a	1694	1/1	0.96	0.08	41,41,41,41	0
59	MG	1A	3268	1/1	0.96	0.08	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1A	3202	1/1	0.96	0.38	38,38,38,38	0
59	MG	1A	3588	1/1	0.96	0.11	51,51,51,51	0
59	MG	2A	3497	1/1	0.96	0.09	41,41,41,41	0
59	MG	1A	3477	1/1	0.96	0.12	18,18,18,18	0
59	MG	2a	1701	1/1	0.96	0.13	63,63,63,63	0
59	MG	1A	3385	1/1	0.96	0.14	43,43,43,43	0
59	MG	1a	1734	1/1	0.96	0.15	36,36,36,36	0
59	MG	1a	1738	1/1	0.96	0.19	66,66,66,66	0
59	MG	1A	3721	1/1	0.96	0.10	31,31,31,31	0
59	MG	2a	1706	1/1	0.96	0.18	87,87,87,87	0
59	MG	1A	3011	1/1	0.96	0.12	28,28,28,28	0
59	MG	1A	3480	1/1	0.96	0.07	26,26,26,26	0
59	MG	1A	3387	1/1	0.96	0.23	17,17,17,17	0
59	MG	2A	3509	1/1	0.96	0.11	49,49,49,49	0
59	MG	1A	3233	1/1	0.96	0.16	51,51,51,51	0
59	MG	1a	1745	1/1	0.96	0.11	47,47,47,47	0
59	MG	1a	1746	1/1	0.96	0.06	76,76,76,76	0
59	MG	2A	3097	1/1	0.96	0.08	56,56,56,56	0
59	MG	1A	3273	1/1	0.96	0.27	37,37,37,37	0
59	MG	1A	3484	1/1	0.96	0.14	42,42,42,42	0
59	MG	2A	3519	1/1	0.96	0.06	31,31,31,31	0
59	MG	1a	1751	1/1	0.96	0.42	48,48,48,48	0
59	MG	1A	3061	1/1	0.96	0.35	21,21,21,21	0
59	MG	2a	1729	1/1	0.96	0.20	54,54,54,54	0
59	MG	1A	3487	1/1	0.96	0.18	47,47,47,47	0
59	MG	1A	3276	1/1	0.96	0.23	18,18,18,18	0
59	MG	2A	3526	1/1	0.96	0.27	56,56,56,56	0
59	MG	2a	1734	1/1	0.96	0.19	70,70,70,70	0
59	MG	2A	3283	1/1	0.96	0.08	32,32,32,32	0
59	MG	2A	3105	1/1	0.96	0.09	33,33,33,33	0
59	MG	2a	1737	1/1	0.96	0.24	63,63,63,63	0
59	MG	1A	3277	1/1	0.96	0.12	36,36,36,36	0
59	MG	2A	3534	1/1	0.96	0.28	58,58,58,58	0
59	MG	2A	3535	1/1	0.96	0.06	55,55,55,55	0
59	MG	2a	1741	1/1	0.96	0.12	43,43,43,43	0
59	MG	2A	3536	1/1	0.96	0.15	50,50,50,50	0
59	MG	1A	3395	1/1	0.96	0.22	42,42,42,42	0
59	MG	2A	3289	1/1	0.96	0.15	45,45,45,45	0
59	MG	2a	1745	1/1	0.96	0.21	60,60,60,60	0
59	MG	2A	3539	1/1	0.96	0.41	41,41,41,41	0
59	MG	1A	3279	1/1	0.96	0.12	45,45,45,45	0
59	MG	1A	3604	1/1	0.96	0.15	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1A	3496	1/1	0.96	0.11	36,36,36,36	0
59	MG	1A	3740	1/1	0.96	0.07	45,45,45,45	0
59	MG	1A	3138	1/1	0.96	0.06	43,43,43,43	0
59	MG	1A	3499	1/1	0.96	0.21	39,39,39,39	0
59	MG	2a	1756	1/1	0.96	0.27	73,73,73,73	0
59	MG	1A	3399	1/1	0.96	0.12	55,55,55,55	0
59	MG	2A	3554	1/1	0.96	0.16	47,47,47,47	0
59	MG	2A	3298	1/1	0.96	0.19	42,42,42,42	0
59	MG	2A	3299	1/1	0.96	0.10	38,38,38,38	0
59	MG	1A	3236	1/1	0.96	0.68	52,52,52,52	0
59	MG	1A	3504	1/1	0.96	0.18	21,21,21,21	0
59	MG	1A	3077	1/1	0.96	0.22	38,38,38,38	0
59	MG	2A	3567	1/1	0.96	0.19	45,45,45,45	0
59	MG	2A	3125	1/1	0.96	0.10	30,30,30,30	0
59	MG	1a	1772	1/1	0.96	0.20	59,59,59,59	0
59	MG	2A	3127	1/1	0.96	0.20	38,38,38,38	0
59	MG	2A	3571	1/1	0.96	0.33	36,36,36,36	0
59	MG	1a	1773	1/1	0.96	0.27	55,55,55,55	0
59	MG	1a	1624	1/1	0.96	0.12	38,38,38,38	0
59	MG	1A	3283	1/1	0.96	0.13	33,33,33,33	0
59	MG	2A	3313	1/1	0.96	0.21	30,30,30,30	0
59	MG	2t	3001	1/1	0.96	0.35	45,45,45,45	0
59	MG	2A	3314	1/1	0.96	0.14	54,54,54,54	0
59	MG	1A	3507	1/1	0.96	0.20	21,21,21,21	0
59	MG	1A	3210	1/1	0.96	0.33	38,38,38,38	0
59	MG	2A	3319	1/1	0.96	0.28	29,29,29,29	0
59	MG	1a	1628	1/1	0.96	0.16	53,53,53,53	0
59	MG	2A	3584	1/1	0.96	0.16	40,40,40,40	0
59	MG	1a	1780	1/1	0.96	0.26	33,33,33,33	0
59	MG	2w	3004	1/1	0.96	0.28	52,52,52,52	0
59	MG	2A	3137	1/1	0.96	0.23	40,40,40,40	0
59	MG	1A	3339	1/1	0.96	0.10	30,30,30,30	0
59	MG	1A	3182	1/1	0.96	0.10	37,37,37,37	0
59	MG	1a	1783	1/1	0.96	0.23	44,44,44,44	0
60	ZN	24	501	1/1	0.96	0.18	72,72,72,72	0
59	MG	1A	3753	1/1	0.96	0.06	54,54,54,54	0
62	GDP	2z	702	28/28	0.96	0.14	50,62,73,81	0
59	MG	1A	3592	1/1	0.97	0.17	44,44,44,44	0
59	MG	1A	3415	1/1	0.97	0.20	42,42,42,42	0
59	MG	2B	203	1/1	0.97	0.07	62,62,62,62	0
59	MG	1a	1690	1/1	0.97	0.30	58,58,58,58	0
59	MG	1L	3001	1/1	0.97	0.13	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	2A	3390	1/1	0.97	0.25	36,36,36,36	0
59	MG	2A	3196	1/1	0.97	0.23	51,51,51,51	0
59	MG	1L	3002	1/1	0.97	0.13	29,29,29,29	0
59	MG	1A	3503	1/1	0.97	0.23	19,19,19,19	0
59	MG	1A	3288	1/1	0.97	0.17	45,45,45,45	0
59	MG	1A	3711	1/1	0.97	0.17	41,41,41,41	0
59	MG	2A	3203	1/1	0.97	0.38	36,36,36,36	0
59	MG	1O	3001	1/1	0.97	0.26	35,35,35,35	0
59	MG	1A	3240	1/1	0.97	0.35	37,37,37,37	0
59	MG	1A	3419	1/1	0.97	0.14	46,46,46,46	0
59	MG	1A	3421	1/1	0.97	0.14	41,41,41,41	0
59	MG	1A	3038	1/1	0.97	0.09	40,40,40,40	0
59	MG	1A	3426	1/1	0.97	0.11	57,57,57,57	0
59	MG	1A	3510	1/1	0.97	0.10	42,42,42,42	0
59	MG	1S	3004	1/1	0.97	0.26	36,36,36,36	0
59	MG	1A	3242	1/1	0.97	0.72	51,51,51,51	0
59	MG	2A	3214	1/1	0.97	0.20	41,41,41,41	0
59	MG	2F	303	1/1	0.97	0.14	40,40,40,40	0
59	MG	1A	3140	1/1	0.97	0.16	42,42,42,42	0
59	MG	2A	3216	1/1	0.97	0.25	42,42,42,42	0
59	MG	1A	3088	1/1	0.97	0.37	39,39,39,39	0
59	MG	1A	3432	1/1	0.97	0.22	47,47,47,47	0
59	MG	1A	3722	1/1	0.97	0.19	27,27,27,27	0
59	MG	2A	3048	1/1	0.97	0.21	40,40,40,40	0
59	MG	1A	3356	1/1	0.97	0.17	26,26,26,26	0
59	MG	1A	3607	1/1	0.97	0.33	27,27,27,27	0
59	MG	2A	3223	1/1	0.97	0.17	39,39,39,39	0
59	MG	1Y	102	1/1	0.97	0.07	31,31,31,31	0
59	MG	1A	3089	1/1	0.97	0.10	42,42,42,42	0
59	MG	1a	1714	1/1	0.97	0.11	48,48,48,48	0
59	MG	1a	1715	1/1	0.97	0.19	28,28,28,28	0
59	MG	1A	3172	1/1	0.97	0.19	53,53,53,53	0
59	MG	2A	3056	1/1	0.97	0.13	27,27,27,27	0
59	MG	1Y	105	1/1	0.97	0.17	57,57,57,57	0
59	MG	1a	1718	1/1	0.97	0.13	39,39,39,39	0
59	MG	1A	3206	1/1	0.97	0.18	34,34,34,34	0
59	MG	2A	3427	1/1	0.97	0.20	44,44,44,44	0
59	MG	2a	1606	1/1	0.97	0.19	24,24,24,24	0
59	MG	1A	3070	1/1	0.97	0.13	37,37,37,37	0
59	MG	1A	3731	1/1	0.97	0.23	16,16,16,16	0
59	MG	13	101	1/1	0.97	0.18	38,38,38,38	0
59	MG	1A	3144	1/1	0.97	0.32	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1A	3175	1/1	0.97	0.34	46,46,46,46	0
59	MG	2A	3065	1/1	0.97	0.27	51,51,51,51	0
59	MG	2A	3435	1/1	0.97	0.17	38,38,38,38	0
59	MG	14	101	1/1	0.97	0.08	46,46,46,46	0
59	MG	1A	3616	1/1	0.97	0.09	63,63,63,63	0
59	MG	1A	3523	1/1	0.97	0.13	35,35,35,35	0
59	MG	1A	3525	1/1	0.97	0.57	61,61,61,61	0
59	MG	17	101	1/1	0.97	0.18	45,45,45,45	0
59	MG	1a	1735	1/1	0.97	0.11	69,69,69,69	0
59	MG	2A	3442	1/1	0.97	0.13	49,49,49,49	0
59	MG	1a	1736	1/1	0.97	0.22	32,32,32,32	0
59	MG	1a	1737	1/1	0.97	0.07	40,40,40,40	0
59	MG	1A	3001	1/1	0.97	0.11	30,30,30,30	0
59	MG	2A	3446	1/1	0.97	0.06	45,45,45,45	0
59	MG	1A	3177	1/1	0.97	0.19	21,21,21,21	0
59	MG	1A	3443	1/1	0.97	0.11	49,49,49,49	0
59	MG	1A	3444	1/1	0.97	0.09	35,35,35,35	0
59	MG	1A	3254	1/1	0.97	0.29	43,43,43,43	0
59	MG	1a	1743	1/1	0.97	0.14	64,64,64,64	0
59	MG	1A	3092	1/1	0.97	0.19	48,48,48,48	0
59	MG	2A	3084	1/1	0.97	0.09	33,33,33,33	0
59	MG	2A	3457	1/1	0.97	0.07	48,48,48,48	0
59	MG	1A	3743	1/1	0.97	0.09	53,53,53,53	0
59	MG	2A	3257	1/1	0.97	0.08	49,49,49,49	0
59	MG	2A	3086	1/1	0.97	0.19	25,25,25,25	0
59	MG	1A	3629	1/1	0.97	0.12	27,27,27,27	0
59	MG	1a	1747	1/1	0.97	0.15	47,47,47,47	0
59	MG	2A	3464	1/1	0.97	0.09	60,60,60,60	0
59	MG	1A	3256	1/1	0.97	0.09	49,49,49,49	0
59	MG	1a	1609	1/1	0.97	0.23	37,37,37,37	0
59	MG	1a	1750	1/1	0.97	0.12	86,86,86,86	0
59	MG	1A	3120	1/1	0.97	0.17	31,31,31,31	0
59	MG	1A	3632	1/1	0.97	0.12	14,14,14,14	0
59	MG	2A	3470	1/1	0.97	0.09	26,26,26,26	0
59	MG	1A	3534	1/1	0.97	0.08	38,38,38,38	0
59	MG	1a	1754	1/1	0.97	0.06	42,42,42,42	0
59	MG	1A	3058	1/1	0.97	0.48	34,34,34,34	0
59	MG	1A	3536	1/1	0.97	0.26	31,31,31,31	0
59	MG	2A	3098	1/1	0.97	0.28	50,50,50,50	0
59	MG	1A	3373	1/1	0.97	0.13	37,37,37,37	0
59	MG	1A	3074	1/1	0.97	0.27	28,28,28,28	0
59	MG	1A	3539	1/1	0.97	0.16	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1A	3540	1/1	0.97	0.20	47,47,47,47	0
59	MG	1A	3309	1/1	0.97	0.13	37,37,37,37	0
59	MG	1A	3644	1/1	0.97	0.11	26,26,26,26	0
59	MG	1A	3218	1/1	0.97	0.21	58,58,58,58	0
59	MG	2A	3483	1/1	0.97	0.10	47,47,47,47	0
59	MG	2A	3279	1/1	0.97	0.28	37,37,37,37	0
59	MG	2A	3107	1/1	0.97	0.21	38,38,38,38	0
59	MG	1A	3312	1/1	0.97	0.14	30,30,30,30	0
59	MG	1A	3015	1/1	0.97	0.21	45,45,45,45	0
59	MG	2A	3488	1/1	0.97	0.25	51,51,51,51	0
59	MG	1A	3761	1/1	0.97	0.35	27,27,27,27	0
59	MG	2A	3490	1/1	0.97	0.09	32,32,32,32	0
59	MG	1A	3458	1/1	0.97	0.09	47,47,47,47	0
59	MG	2A	3112	1/1	0.97	0.24	20,20,20,20	0
59	MG	2A	3113	1/1	0.97	0.23	33,33,33,33	0
59	MG	2A	3288	1/1	0.97	0.20	34,34,34,34	0
59	MG	1A	3009	1/1	0.97	0.09	20,20,20,20	0
59	MG	1A	3318	1/1	0.97	0.16	22,22,22,22	0
59	MG	1A	3042	1/1	0.97	0.23	19,19,19,19	0
59	MG	1a	1631	1/1	0.97	0.06	41,41,41,41	0
59	MG	1A	3655	1/1	0.97	0.12	31,31,31,31	0
59	MG	1A	3767	1/1	0.97	0.05	44,44,44,44	0
59	MG	1A	3264	1/1	0.97	0.07	47,47,47,47	0
59	MG	2A	3123	1/1	0.97	0.20	39,39,39,39	0
59	MG	2A	3506	1/1	0.97	0.11	56,56,56,56	0
59	MG	2A	3297	1/1	0.97	0.09	29,29,29,29	0
59	MG	1A	3657	1/1	0.97	0.10	43,43,43,43	0
59	MG	1A	3062	1/1	0.97	0.17	17,17,17,17	0
59	MG	2A	3511	1/1	0.97	0.21	39,39,39,39	0
59	MG	1A	3772	1/1	0.97	0.17	20,20,20,20	0
59	MG	2A	3513	1/1	0.97	0.10	54,54,54,54	0
59	MG	1A	3043	1/1	0.97	0.23	23,23,23,23	0
59	MG	2A	3302	1/1	0.97	0.14	35,35,35,35	0
59	MG	1A	3326	1/1	0.97	0.14	34,34,34,34	0
59	MG	1A	3662	1/1	0.97	0.08	31,31,31,31	0
59	MG	2A	3305	1/1	0.97	0.09	46,46,46,46	0
59	MG	2A	3131	1/1	0.97	0.36	40,40,40,40	0
59	MG	2A	3307	1/1	0.97	0.11	27,27,27,27	0
59	MG	2a	1693	1/1	0.97	0.37	51,51,51,51	0
59	MG	1A	3556	1/1	0.97	0.13	57,57,57,57	0
59	MG	2A	3523	1/1	0.97	0.09	38,38,38,38	0
59	MG	1A	3327	1/1	0.97	0.14	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	2A	3525	1/1	0.97	0.25	41,41,41,41	0
59	MG	1A	3558	1/1	0.97	0.14	42,42,42,42	0
59	MG	1A	3559	1/1	0.97	0.14	44,44,44,44	0
59	MG	2a	1700	1/1	0.97	0.15	45,45,45,45	0
59	MG	1a	1792	1/1	0.97	0.11	55,55,55,55	0
59	MG	1a	1648	1/1	0.97	0.17	60,60,60,60	0
59	MG	2A	3531	1/1	0.97	0.29	38,38,38,38	0
59	MG	2A	3315	1/1	0.97	0.16	38,38,38,38	0
59	MG	1A	3224	1/1	0.97	0.42	35,35,35,35	0
59	MG	1A	3080	1/1	0.97	0.11	43,43,43,43	0
59	MG	1a	1651	1/1	0.97	0.26	54,54,54,54	0
59	MG	2A	3141	1/1	0.97	0.44	49,49,49,49	0
59	MG	1a	1797	1/1	0.97	0.25	66,66,66,66	0
59	MG	1A	3671	1/1	0.97	0.20	36,36,36,36	0
59	MG	2a	1713	1/1	0.97	0.11	43,43,43,43	0
59	MG	1A	3129	1/1	0.97	0.13	29,29,29,29	0
59	MG	2a	1715	1/1	0.97	0.14	68,68,68,68	0
59	MG	1A	3474	1/1	0.97	0.09	42,42,42,42	0
59	MG	2A	3545	1/1	0.97	0.17	38,38,38,38	0
59	MG	1A	3566	1/1	0.97	0.13	49,49,49,49	0
59	MG	1A	3021	1/1	0.97	0.18	40,40,40,40	0
59	MG	1a	1803	1/1	0.97	0.25	53,53,53,53	0
59	MG	2a	1724	1/1	0.97	0.26	52,52,52,52	0
59	MG	1a	1804	1/1	0.97	0.10	60,60,60,60	0
59	MG	2a	1726	1/1	0.97	0.17	62,62,62,62	0
59	MG	2A	3553	1/1	0.97	0.26	40,40,40,40	0
59	MG	2A	3151	1/1	0.97	0.17	29,29,29,29	0
59	MG	2A	3556	1/1	0.97	0.12	37,37,37,37	0
59	MG	2A	3557	1/1	0.97	0.18	60,60,60,60	0
59	MG	2A	3558	1/1	0.97	0.29	30,30,30,30	0
59	MG	1A	3676	1/1	0.97	0.13	51,51,51,51	0
59	MG	1A	3394	1/1	0.97	0.21	50,50,50,50	0
59	MG	1A	3570	1/1	0.97	0.23	54,54,54,54	0
59	MG	1A	3054	1/1	0.97	0.36	43,43,43,43	0
59	MG	1A	3681	1/1	0.97	0.12	30,30,30,30	0
59	MG	2A	3158	1/1	0.97	0.14	33,33,33,33	0
59	MG	1B	215	1/1	0.97	0.10	37,37,37,37	0
59	MG	1B	216	1/1	0.97	0.07	34,34,34,34	0
59	MG	1z	702	1/1	0.97	0.33	39,39,39,39	0
59	MG	1B	217	1/1	0.97	0.11	24,24,24,24	0
59	MG	1A	3572	1/1	0.97	0.13	43,43,43,43	0
59	MG	1A	3191	1/1	0.97	0.24	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	2A	3574	1/1	0.97	0.33	62,62,62,62	0
59	MG	2a	1747	1/1	0.97	0.21	39,39,39,39	0
59	MG	2a	1748	1/1	0.97	0.13	39,39,39,39	0
59	MG	2A	3575	1/1	0.97	0.17	36,36,36,36	0
59	MG	2A	3346	1/1	0.97	0.11	64,64,64,64	0
59	MG	2A	3347	1/1	0.97	0.08	51,51,51,51	0
59	MG	1A	3334	1/1	0.97	0.11	29,29,29,29	0
59	MG	1a	1669	1/1	0.97	0.21	44,44,44,44	0
59	MG	1A	3398	1/1	0.97	0.15	26,26,26,26	0
59	MG	1A	3275	1/1	0.97	0.18	51,51,51,51	0
59	MG	1A	3132	1/1	0.97	0.14	36,36,36,36	0
59	MG	2A	3355	1/1	0.97	0.24	27,27,27,27	0
59	MG	2A	3585	1/1	0.97	0.11	49,49,49,49	0
59	MG	1A	3066	1/1	0.97	0.63	43,43,43,43	0
59	MG	2A	3588	1/1	0.97	0.23	32,32,32,32	0
59	MG	1A	3194	1/1	0.97	0.34	43,43,43,43	0
59	MG	2A	3590	1/1	0.97	0.09	38,38,38,38	0
59	MG	1A	3084	1/1	0.97	0.24	29,29,29,29	0
59	MG	1A	3404	1/1	0.97	0.11	40,40,40,40	0
59	MG	2A	3360	1/1	0.97	0.19	34,34,34,34	0
59	MG	2A	3008	1/1	0.97	0.20	33,33,33,33	0
59	MG	1a	1677	1/1	0.97	0.17	36,36,36,36	0
59	MG	2A	3010	1/1	0.97	0.11	34,34,34,34	0
59	MG	2a	1772	1/1	0.97	0.17	64,64,64,64	0
59	MG	2d	502	1/1	0.97	0.21	35,35,35,35	0
59	MG	2A	3598	1/1	0.97	0.14	46,46,46,46	0
59	MG	2A	3364	1/1	0.97	0.13	30,30,30,30	0
59	MG	1A	3163	1/1	0.97	0.15	43,43,43,43	0
59	MG	1E	302	1/1	0.97	0.17	51,51,51,51	0
59	MG	1A	3406	1/1	0.97	0.13	56,56,56,56	0
59	MG	2A	3015	1/1	0.97	0.17	36,36,36,36	0
59	MG	1A	3067	1/1	0.97	0.12	43,43,43,43	0
59	MG	1A	3032	1/1	0.97	0.68	46,46,46,46	0
59	MG	2A	3183	1/1	0.97	0.18	45,45,45,45	0
59	MG	2A	3019	1/1	0.97	0.12	41,41,41,41	0
59	MG	2A	3020	1/1	0.97	0.33	37,37,37,37	0
59	MG	1A	3285	1/1	0.97	0.27	51,51,51,51	0
59	MG	2A	3613	1/1	0.97	0.18	21,21,21,21	0
59	MG	1A	3111	1/1	0.97	0.38	39,39,39,39	0
59	MG	1A	3498	1/1	0.97	0.11	70,70,70,70	0
59	MG	2A	3616	1/1	0.97	0.36	51,51,51,51	0
60	ZN	2W	501	1/1	0.97	0.06	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	2A	3380	1/1	0.97	0.10	36,36,36,36	0
60	ZN	23	501	1/1	0.97	0.15	85,85,85,85	0
59	MG	1A	3348	1/1	0.97	0.19	28,28,28,28	0
60	ZN	27	101	1/1	0.97	0.11	68,68,68,68	0
59	MG	1A	3239	1/1	0.97	0.09	49,49,49,49	0
62	GDP	1z	701	28/28	0.97	0.14	30,50,64,75	0
59	MG	2A	3191	1/1	0.97	0.22	44,44,44,44	0
59	MG	2A	3543	1/1	0.98	0.24	28,28,28,28	0
59	MG	1A	3325	1/1	0.98	0.27	64,64,64,64	0
59	MG	1a	1755	1/1	0.98	0.11	42,42,42,42	0
59	MG	1A	3428	1/1	0.98	0.18	64,64,64,64	0
59	MG	2A	3548	1/1	0.98	0.23	32,32,32,32	0
59	MG	2A	3549	1/1	0.98	0.36	31,31,31,31	0
59	MG	2A	3405	1/1	0.98	0.25	45,45,45,45	0
59	MG	1A	3429	1/1	0.98	0.12	44,44,44,44	0
59	MG	1A	3388	1/1	0.98	0.15	21,21,21,21	0
59	MG	1A	3666	1/1	0.98	0.17	32,32,32,32	0
59	MG	1A	3166	1/1	0.98	0.25	45,45,45,45	0
59	MG	2A	3555	1/1	0.98	0.39	42,42,42,42	0
59	MG	1a	1761	1/1	0.98	0.18	41,41,41,41	0
59	MG	1A	3103	1/1	0.98	0.06	40,40,40,40	0
59	MG	1A	3031	1/1	0.98	0.13	28,28,28,28	0
59	MG	1A	3071	1/1	0.98	0.30	31,31,31,31	0
59	MG	1a	1765	1/1	0.98	0.07	44,44,44,44	0
59	MG	1A	3149	1/1	0.98	0.10	36,36,36,36	0
59	MG	2A	3563	1/1	0.98	0.20	41,41,41,41	0
59	MG	1A	3284	1/1	0.98	0.14	48,48,48,48	0
59	MG	1a	1768	1/1	0.98	0.16	56,56,56,56	0
59	MG	2a	1660	1/1	0.98	0.38	36,36,36,36	0
59	MG	2A	3566	1/1	0.98	0.10	54,54,54,54	0
59	MG	2A	3418	1/1	0.98	0.13	46,46,46,46	0
59	MG	1A	3485	1/1	0.98	0.12	29,29,29,29	0
59	MG	1A	3003	1/1	0.98	0.09	29,29,29,29	0
59	MG	1A	3754	1/1	0.98	0.12	28,28,28,28	0
59	MG	1A	3101	1/1	0.98	0.11	38,38,38,38	0
59	MG	1A	3267	1/1	0.98	0.19	45,45,45,45	0
59	MG	1A	3543	1/1	0.98	0.07	61,61,61,61	0
59	MG	1A	3489	1/1	0.98	0.04	48,48,48,48	0
59	MG	1A	3545	1/1	0.98	0.20	46,46,46,46	0
59	MG	1A	3251	1/1	0.98	0.22	48,48,48,48	0
59	MG	1A	3116	1/1	0.98	0.20	40,40,40,40	0
59	MG	2A	3067	1/1	0.98	0.23	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	2A	3579	1/1	0.98	0.10	42,42,42,42	0
59	MG	1A	3208	1/1	0.98	0.32	33,33,33,33	0
59	MG	1A	3549	1/1	0.98	0.11	27,27,27,27	0
59	MG	1A	3685	1/1	0.98	0.16	60,60,60,60	0
59	MG	2A	3433	1/1	0.98	0.10	35,35,35,35	0
59	MG	2A	3071	1/1	0.98	0.05	35,35,35,35	0
59	MG	1A	3494	1/1	0.98	0.22	46,46,46,46	0
59	MG	1a	1784	1/1	0.98	0.23	37,37,37,37	0
59	MG	1A	3495	1/1	0.98	0.17	53,53,53,53	0
59	MG	1A	3291	1/1	0.98	0.20	60,60,60,60	0
59	MG	1A	3613	1/1	0.98	0.06	53,53,53,53	0
59	MG	2A	3077	1/1	0.98	0.32	40,40,40,40	0
59	MG	1a	1788	1/1	0.98	0.19	45,45,45,45	0
59	MG	1A	3769	1/1	0.98	0.14	35,35,35,35	0
59	MG	1A	3209	1/1	0.98	0.27	41,41,41,41	0
59	MG	2A	3312	1/1	0.98	0.19	60,60,60,60	0
59	MG	16	101	1/1	0.98	0.15	24,24,24,24	0
59	MG	1A	3615	1/1	0.98	0.05	59,59,59,59	0
59	MG	1A	3370	1/1	0.98	0.07	21,21,21,21	0
59	MG	1A	3340	1/1	0.98	0.14	19,19,19,19	0
59	MG	2A	3449	1/1	0.98	0.11	27,27,27,27	0
59	MG	2A	3450	1/1	0.98	0.07	45,45,45,45	0
59	MG	2A	3605	1/1	0.98	0.12	35,35,35,35	0
59	MG	2A	3198	1/1	0.98	0.40	20,20,20,20	0
59	MG	1A	3618	1/1	0.98	0.09	33,33,33,33	0
59	MG	2A	3453	1/1	0.98	0.15	21,21,21,21	0
59	MG	2A	3200	1/1	0.98	0.25	34,34,34,34	0
59	MG	1A	3500	1/1	0.98	0.12	63,63,63,63	0
59	MG	1A	3697	1/1	0.98	0.33	43,43,43,43	0
59	MG	1A	3372	1/1	0.98	0.11	19,19,19,19	0
59	MG	2A	3324	1/1	0.98	0.10	43,43,43,43	0
59	MG	2A	3459	1/1	0.98	0.08	48,48,48,48	0
59	MG	2A	3204	1/1	0.98	0.14	26,26,26,26	0
59	MG	1a	1697	1/1	0.98	0.07	61,61,61,61	0
59	MG	1A	3778	1/1	0.98	0.31	33,33,33,33	0
59	MG	1A	3449	1/1	0.98	0.15	47,47,47,47	0
59	MG	2a	1710	1/1	0.98	0.16	46,46,46,46	0
59	MG	1A	3780	1/1	0.98	0.47	31,31,31,31	0
59	MG	2a	1712	1/1	0.98	0.22	62,62,62,62	0
59	MG	1A	3700	1/1	0.98	0.06	66,66,66,66	0
59	MG	1A	3622	1/1	0.98	0.10	21,21,21,21	0
59	MG	1A	3341	1/1	0.98	0.15	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	2A	3333	1/1	0.98	0.18	35,35,35,35	0
59	MG	1A	3451	1/1	0.98	0.27	51,51,51,51	0
59	MG	1A	3407	1/1	0.98	0.09	32,32,32,32	0
59	MG	2a	1719	1/1	0.98	0.12	56,56,56,56	0
59	MG	1f	3001	1/1	0.98	0.30	39,39,39,39	0
59	MG	1A	3626	1/1	0.98	0.16	31,31,31,31	0
59	MG	2a	1722	1/1	0.98	0.21	45,45,45,45	0
59	MG	2a	1723	1/1	0.98	0.12	65,65,65,65	0
59	MG	1A	3627	1/1	0.98	0.07	34,34,34,34	0
59	MG	1A	3707	1/1	0.98	0.12	51,51,51,51	0
59	MG	1A	3562	1/1	0.98	0.06	38,38,38,38	0
59	MG	2A	3342	1/1	0.98	0.20	48,48,48,48	0
59	MG	1A	3709	1/1	0.98	0.15	41,41,41,41	0
59	MG	1A	3314	1/1	0.98	0.13	36,36,36,36	0
59	MG	1A	3315	1/1	0.98	0.09	34,34,34,34	0
59	MG	2A	3106	1/1	0.98	0.21	39,39,39,39	0
59	MG	1a	1620	1/1	0.98	0.07	40,40,40,40	0
59	MG	2a	1733	1/1	0.98	0.12	62,62,62,62	0
59	MG	2A	3348	1/1	0.98	0.10	36,36,36,36	0
59	MG	1A	3376	1/1	0.98	0.04	45,45,45,45	0
59	MG	1A	3411	1/1	0.98	0.18	21,21,21,21	0
59	MG	1A	3109	1/1	0.98	0.10	36,36,36,36	0
59	MG	1A	3569	1/1	0.98	0.13	41,41,41,41	0
59	MG	2A	3353	1/1	0.98	0.12	44,44,44,44	0
59	MG	1A	3317	1/1	0.98	0.15	33,33,33,33	0
59	MG	1A	3379	1/1	0.98	0.16	38,38,38,38	0
59	MG	1A	3197	1/1	0.98	0.21	41,41,41,41	0
59	MG	1a	1721	1/1	0.98	0.09	46,46,46,46	0
59	MG	1A	3640	1/1	0.98	0.17	41,41,41,41	0
59	MG	2A	3493	1/1	0.98	0.15	23,23,23,23	0
59	MG	2a	1746	1/1	0.98	0.21	43,43,43,43	0
59	MG	2A	3117	1/1	0.98	0.30	35,35,35,35	0
59	MG	2A	3118	1/1	0.98	0.27	35,35,35,35	0
59	MG	2R	8001	1/1	0.98	0.05	41,41,41,41	0
59	MG	2A	3496	1/1	0.98	0.36	41,41,41,41	0
59	MG	1a	1723	1/1	0.98	0.16	43,43,43,43	0
59	MG	1a	1724	1/1	0.98	0.15	18,18,18,18	0
59	MG	1a	1725	1/1	0.98	0.15	50,50,50,50	0
59	MG	1A	3573	1/1	0.98	0.11	50,50,50,50	0
59	MG	1A	3051	1/1	0.98	0.15	35,35,35,35	0
59	MG	1B	224	1/1	0.98	0.07	56,56,56,56	0
59	MG	2A	3014	1/1	0.98	0.16	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	1A	3417	1/1	0.98	0.06	51,51,51,51	0
59	MG	1a	1730	1/1	0.98	0.15	49,49,49,49	0
59	MG	2A	3244	1/1	0.98	0.35	49,49,49,49	0
59	MG	2A	3508	1/1	0.98	0.17	32,32,32,32	0
59	MG	2A	3017	1/1	0.98	0.12	47,47,47,47	0
59	MG	2A	3129	1/1	0.98	0.21	39,39,39,39	0
59	MG	2a	1764	1/1	0.98	0.21	61,61,61,61	0
59	MG	1A	3723	1/1	0.98	0.16	36,36,36,36	0
59	MG	1A	3320	1/1	0.98	0.12	35,35,35,35	0
59	MG	1A	3465	1/1	0.98	0.16	33,33,33,33	0
59	MG	2A	3378	1/1	0.98	0.22	35,35,35,35	0
59	MG	1a	1637	1/1	0.98	0.39	42,42,42,42	0
59	MG	2a	1770	1/1	0.98	0.10	59,59,59,59	0
59	MG	2a	1771	1/1	0.98	0.17	72,72,72,72	0
59	MG	1A	3136	1/1	0.98	0.16	41,41,41,41	0
59	MG	2a	1773	1/1	0.98	0.09	50,50,50,50	0
59	MG	1A	3519	1/1	0.98	0.14	21,21,21,21	0
59	MG	2A	3518	1/1	0.98	0.26	40,40,40,40	0
59	MG	1A	3728	1/1	0.98	0.21	35,35,35,35	0
59	MG	2A	3383	1/1	0.98	0.10	39,39,39,39	0
59	MG	1a	1641	1/1	0.98	0.08	49,49,49,49	0
59	MG	1A	3649	1/1	0.98	0.15	35,35,35,35	0
59	MG	1A	3420	1/1	0.98	0.14	38,38,38,38	0
59	MG	2A	3387	1/1	0.98	0.12	46,46,46,46	0
59	MG	1F	301	1/1	0.98	0.25	27,27,27,27	0
59	MG	1A	3228	1/1	0.98	0.15	44,44,44,44	0
59	MG	1F	303	1/1	0.98	0.12	45,45,45,45	0
59	MG	1A	3469	1/1	0.98	0.21	36,36,36,36	0
59	MG	1A	3422	1/1	0.98	0.13	21,21,21,21	0
59	MG	1A	3654	1/1	0.98	0.20	54,54,54,54	0
59	MG	2A	3532	1/1	0.98	0.37	35,35,35,35	0
59	MG	1F	307	1/1	0.98	0.10	19,19,19,19	0
59	MG	2A	3147	1/1	0.98	0.23	33,33,33,33	0
59	MG	1A	3524	1/1	0.98	0.14	30,30,30,30	0
59	MG	1A	3423	1/1	0.98	0.17	17,17,17,17	0
59	MG	1A	3278	1/1	0.98	0.10	37,37,37,37	0
59	MG	1A	3473	1/1	0.98	0.18	46,46,46,46	0
59	MG	1A	3659	1/1	0.98	0.36	31,31,31,31	0
59	MG	1A	3324	1/1	0.98	0.11	51,51,51,51	0
59	MG	2A	3542	1/1	0.98	0.31	36,36,36,36	0
59	MG	2a	1638	1/1	0.98	0.38	54,54,54,54	0
59	MG	2A	3547	1/1	0.99	0.25	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	2A	3335	1/1	0.99	0.22	25,25,25,25	0
59	MG	2A	3155	1/1	0.99	0.21	27,27,27,27	0
59	MG	2A	3591	1/1	0.99	0.12	31,31,31,31	0
59	MG	1A	3117	1/1	0.99	0.15	38,38,38,38	0
59	MG	2A	3371	1/1	0.99	0.13	26,26,26,26	0
59	MG	1A	3639	1/1	0.99	0.10	54,54,54,54	0
59	MG	1A	3310	1/1	0.99	0.06	39,39,39,39	0
59	MG	2A	3374	1/1	0.99	0.06	26,26,26,26	0
59	MG	1A	3105	1/1	0.99	0.22	22,22,22,22	0
59	MG	1A	3020	1/1	0.99	0.20	25,25,25,25	0
59	MG	2A	3599	1/1	0.99	0.18	46,46,46,46	0
59	MG	1A	3491	1/1	0.99	0.09	41,41,41,41	0
59	MG	2A	3021	1/1	0.99	0.13	25,25,25,25	0
59	MG	2A	3559	1/1	0.99	0.32	48,48,48,48	0
59	MG	2A	3603	1/1	0.99	0.12	50,50,50,50	0
59	MG	1A	3564	1/1	0.99	0.08	30,30,30,30	0
59	MG	1A	3678	1/1	0.99	0.08	16,16,16,16	0
59	MG	1A	3343	1/1	0.99	0.16	46,46,46,46	0
59	MG	1E	306	1/1	0.99	0.16	39,39,39,39	0
59	MG	1B	214	1/1	0.99	0.15	41,41,41,41	0
59	MG	2f	3001	1/1	0.99	0.07	40,40,40,40	0
59	MG	2f	3002	1/1	0.99	0.07	69,69,69,69	0
59	MG	1A	3272	1/1	0.99	0.11	33,33,33,33	0
59	MG	2A	3317	1/1	0.99	0.28	37,37,37,37	0
59	MG	2A	3286	1/1	0.99	0.19	30,30,30,30	0
59	MG	1A	3022	1/1	0.99	0.11	36,36,36,36	0
59	MG	2A	3529	1/1	0.99	0.14	28,28,28,28	0
59	MG	1a	1668	1/1	0.99	0.13	41,41,41,41	0
59	MG	1a	1644	1/1	0.99	0.11	33,33,33,33	0
59	MG	1a	1621	1/1	0.99	0.10	66,66,66,66	0
59	MG	2A	3533	1/1	0.99	0.35	23,23,23,23	0
59	MG	1A	3664	1/1	0.99	0.17	39,39,39,39	0
59	MG	2A	3005	1/1	0.99	0.10	27,27,27,27	0
59	MG	1A	3648	1/1	0.99	0.14	40,40,40,40	0
59	MG	1A	3441	1/1	0.99	0.14	34,34,34,34	0
60	ZN	1W	202	1/1	0.99	0.12	68,68,68,68	0
59	MG	1A	3634	1/1	0.99	0.07	20,20,20,20	0
59	MG	1a	1775	1/1	0.99	0.34	46,46,46,46	0
60	ZN	14	102	1/1	0.99	0.15	48,48,48,48	0
59	MG	1A	3462	1/1	0.99	0.25	42,42,42,42	0
60	ZN	1n	501	1/1	0.99	0.13	77,77,77,77	0
59	MG	2A	3267	1/1	0.99	0.22	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	2A	3504	1/1	0.99	0.09	33,33,33,33	0
59	MG	1X	3002	1/1	0.99	0.12	53,53,53,53	0
59	MG	1A	3687	1/1	0.99	0.17	69,69,69,69	0
59	MG	2B	209	1/1	0.99	0.18	71,71,71,71	0
59	MG	1A	3367	1/1	0.99	0.15	49,49,49,49	0
61	SF4	1d	501	8/8	0.99	0.13	61,67,75,78	0
61	SF4	2d	501	8/8	0.99	0.12	63,67,88,88	0
59	MG	1A	3424	1/1	0.99	0.19	34,34,34,34	0
59	MG	2A	3587	1/1	0.99	0.28	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.