



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2020 – 06:25 am BST

PDB ID : 6CFL
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with lysyl-CAM and bound to protein Y (YfiA) at 2.6Å resolution
Authors : Tereshchenkov, A.G.; Dobosz-Bartoszek, M.; Osterman, I.A.; Marks, J.; Sergeeva, V.A.; Kasatsky, P.; Komarova, E.S.; Stavrianidi, A.N.; Rodin, I.A.; Konevega, A.L.; Sergiev, P.V.; Sumbatyan, N.V.; Mankin, A.S.; Bogdanov, A.A.; Polikanov, Y.S.
Deposited on : 2018-02-15
Resolution : 2.60 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 ⓘ symbol.

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

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

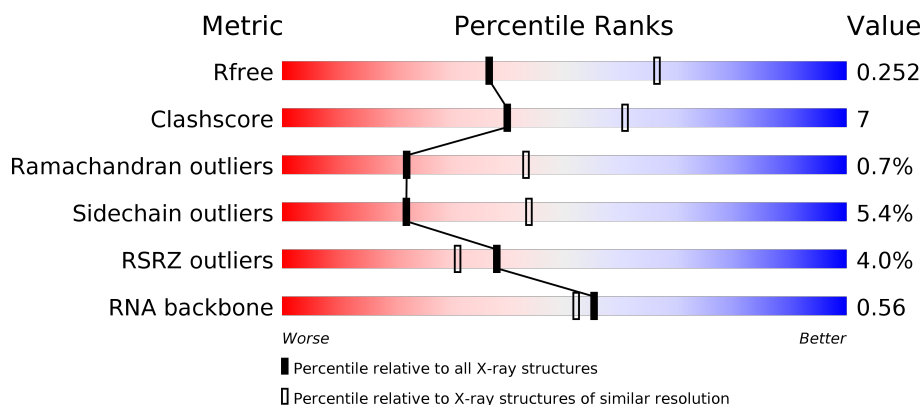
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.






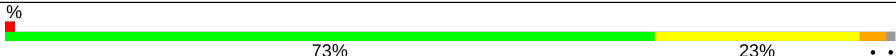



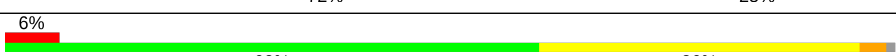



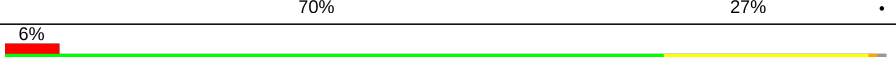

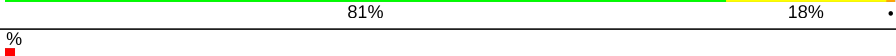
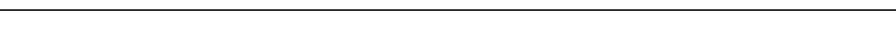




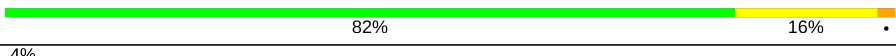

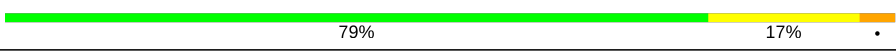



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>26%</div> <div>5%</div> </div> </div>
1	2A	2915	<div> <div>2%</div> <div> <div></div> <div>63%</div> <div>28%</div> <div>6%</div> </div> </div>
2	1B	121	<div> <div></div> <div> <div>69%</div> <div>27%</div> </div> </div>
2	2B	121	<div> <div></div> <div> <div>50%</div> <div>46%</div> </div> </div>







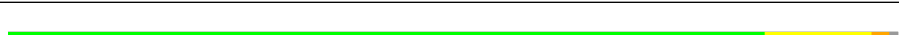
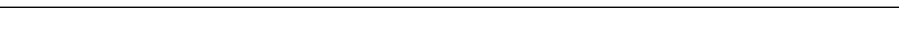
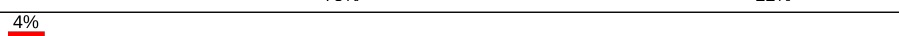


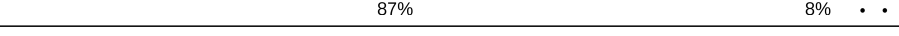









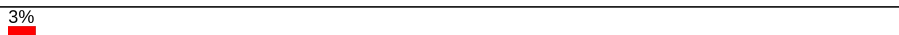
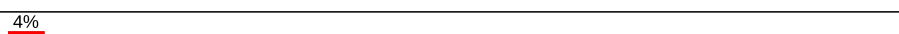
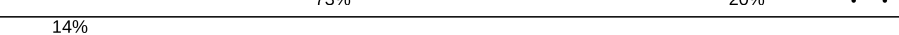
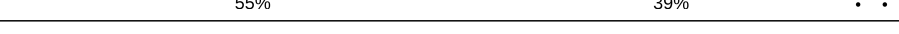
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Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118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









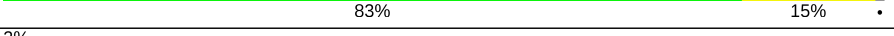


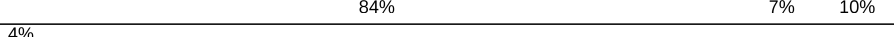

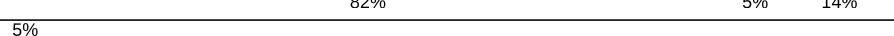
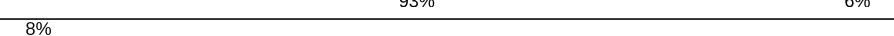
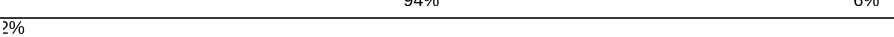
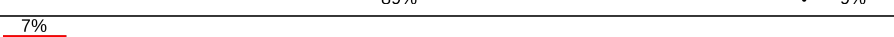

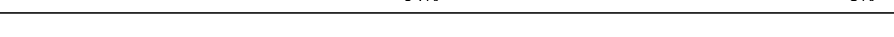
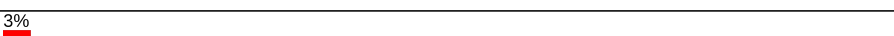

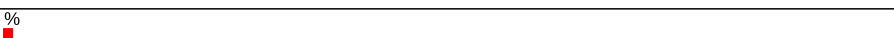
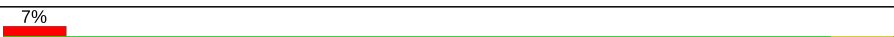


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Mol	Chain	Length	Quality of chain
15	2T	146	% 
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25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

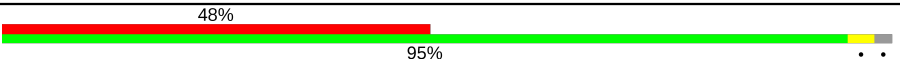


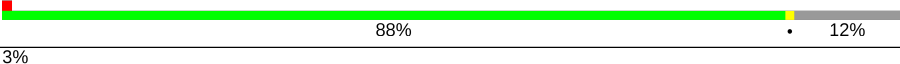
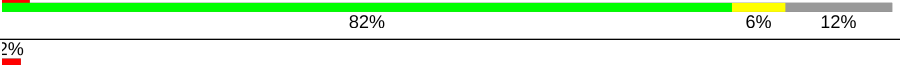
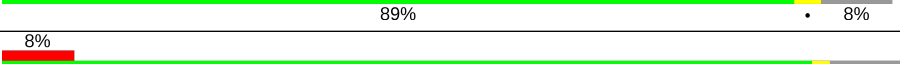
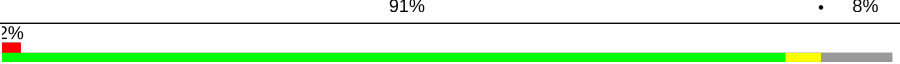
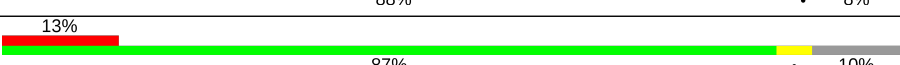
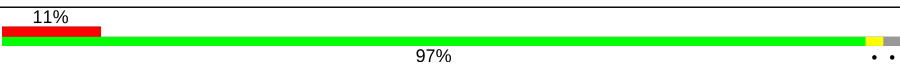
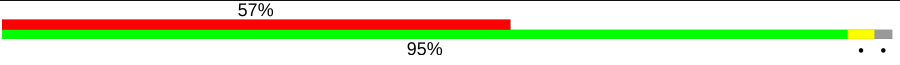
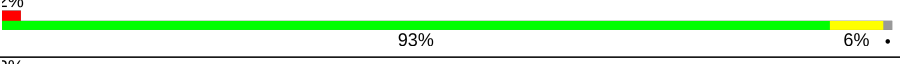
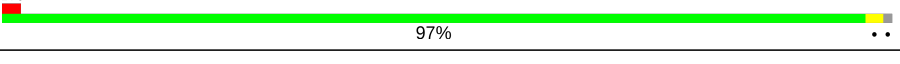


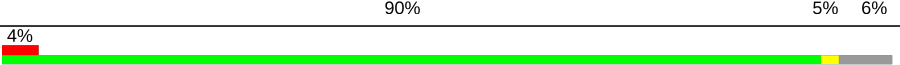
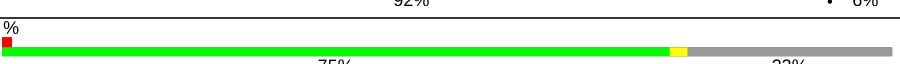
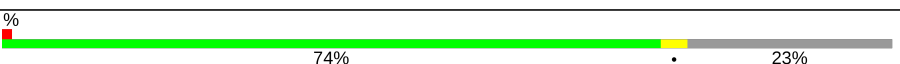
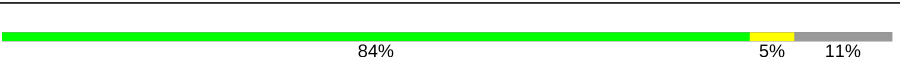




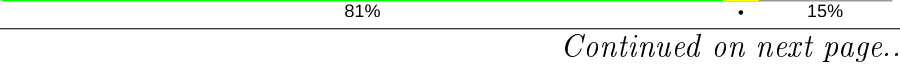


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Mol	Chain	Length	Quality of chain
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	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

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

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Mol	Chain	Length	Quality of chain
53	1y	113	
53	2y	113	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	1A	3233	-	-	-	X
54	MG	1A	3855	-	-	-	X
54	MG	1A	3900	-	-	-	X
54	MG	1A	3939	-	-	-	X
54	MG	1A	3957	-	-	-	X
54	MG	1A	3970	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 295545 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
			61869	27540	11574	19884	2871			
1	2A	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			

- 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
			2572	1145	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 L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1D	275	Total	C	N	O	S	0	0	0
			2131	1346	422	360	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 4 is a protein called 50S Ribosomal Protein L3.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1426	916	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	912	259	249	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	1H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
7	2H	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	1N	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			
9	2N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

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

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

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

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

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

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

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

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

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

- Molecule 14 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total	C	N	O	0	0	0
			877	553	175	149			
14	2S	110	Total	C	N	O	0	0	0
			870	549	173	148			

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

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

- Molecule 16 is a protein called 50S Ribosomal Protein L20.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1V	101	Total	C	N	O	S	0	0	0
			775	498	141	135	1			
17	2V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

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

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

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

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

- Molecule 20 is a protein called 50S Ribosomal Protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1Y	107	Total	C	N	O	S	0	0	0
			810	520	153	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	20	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			754	475	148	130	1			
23	21	97	Total	C	N	O	S	0	0	0
			759	478	149	131	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	12	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
24	22	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			

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

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

- Molecule 26 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			546	346	96	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			536	342	98	91	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	15	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	25	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	2a	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1842	1175	330	332	5			
33	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1558	979	305	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1665	1043	329	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1668	1047	330	284	7			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			814	516	144	151	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1229	766	241	216	6			

- Molecule 39 is a protein called 30S Ribosomal Protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1h	137	Total	C	N	O	S	0	0	0
			1098	694	210	192	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O		0	0	0
			986	625	193	168				
40	2i	126	Total	C	N	O		0	0	0
			966	613	186	167				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O		0	0	0
			719	446	142	131				
41	2j	96	Total	C	N	O		0	0	0
			710	442	137	131				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			834	520	156	155	3			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	116	Total	C	N	O	S	0	0	0
			914	564	189	159	2			
44	2m	114	Total	C	N	O	S	0	0	0
			895	550	186	157	2			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			
50	2s	83	Total	C	N	O	S	0	0	0
			645	410	118	115	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			732	449	157	124	2			
51	2t	98	Total	C	N	O	S	0	0	0
			733	451	154	126	2			

- Molecule 52 is a protein called 30S Ribosomal Protein THX.

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

- Molecule 53 is a protein called Protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1y	97	Total	C	N	O	S	0	0	0
			764	478	144	139	3			
53	2y	96	Total	C	N	O	S	0	0	0
			749	468	141	137	3			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	2E	6	Total	Mg	0	0
			6	6		
54	17	1	Total	Mg	0	0
			1	1		
54	2d	1	Total	Mg	0	0
			1	1		
54	1T	4	Total	Mg	0	0
			4	4		
54	1N	3	Total	Mg	0	0
			3	3		
54	20	2	Total	Mg	0	0
			2	2		
54	18	1	Total	Mg	0	0
			1	1		
54	1o	1	Total	Mg	0	0
			1	1		
54	2W	2	Total	Mg	0	0
			2	2		
54	2I	1	Total	Mg	0	0
			1	1		
54	13	3	Total	Mg	0	0
			3	3		
54	1f	2	Total	Mg	0	0
			2	2		
54	1P	2	Total	Mg	0	0
			2	2		
54	2B	21	Total	Mg	0	0
			21	21		
54	1q	2	Total	Mg	0	0
			2	2		
54	2a	184	Total	Mg	0	0
			184	184		
54	1k	1	Total	Mg	0	0
			1	1		
54	1E	5	Total	Mg	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1b	1	Total 1	Mg 1	0	0
54	25	1	Total 1	Mg 1	0	0
54	2F	3	Total 3	Mg 3	0	0
54	28	3	Total 3	Mg 3	0	0
54	2e	1	Total 1	Mg 1	0	0
54	1W	3	Total 3	Mg 3	0	0
54	1A	1071	Total 1071	Mg 1071	0	0
54	1t	1	Total 1	Mg 1	0	0
54	1n	2	Total 2	Mg 2	0	0
54	2P	1	Total 1	Mg 1	0	0
54	1X	2	Total 2	Mg 2	0	0
54	1y	4	Total 4	Mg 4	0	0
54	1p	1	Total 1	Mg 1	0	0
54	2T	4	Total 4	Mg 4	0	0
54	1D	13	Total 13	Mg 13	0	0
54	2N	1	Total 1	Mg 1	0	0
54	1e	3	Total 3	Mg 3	0	0
54	2G	3	Total 3	Mg 3	0	0
54	2f	1	Total 1	Mg 1	0	0
54	1V	3	Total 3	Mg 3	0	0
54	2X	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1a	260	Total 260	Mg 260	0	0
54	2Q	3	Total 3	Mg 3	0	0
54	15	3	Total 3	Mg 3	0	0
54	2j	1	Total 1	Mg 1	0	0
54	1R	2	Total 2	Mg 2	0	0
54	1G	4	Total 4	Mg 4	0	0
54	2O	3	Total 3	Mg 3	0	0
54	11	2	Total 2	Mg 2	0	0
54	1d	4	Total 4	Mg 4	0	0
54	1H	3	Total 3	Mg 3	0	0
54	21	2	Total 2	Mg 2	0	0
54	1i	1	Total 1	Mg 1	0	0
54	23	1	Total 1	Mg 1	0	0
54	2R	2	Total 2	Mg 2	0	0
54	1Z	1	Total 1	Mg 1	0	0
54	2D	6	Total 6	Mg 6	0	0
54	14	1	Total 1	Mg 1	0	0
54	1U	3	Total 3	Mg 3	0	0
54	1O	1	Total 1	Mg 1	0	0
54	19	2	Total 2	Mg 2	0	0
54	1l	2	Total 2	Mg 2	0	0

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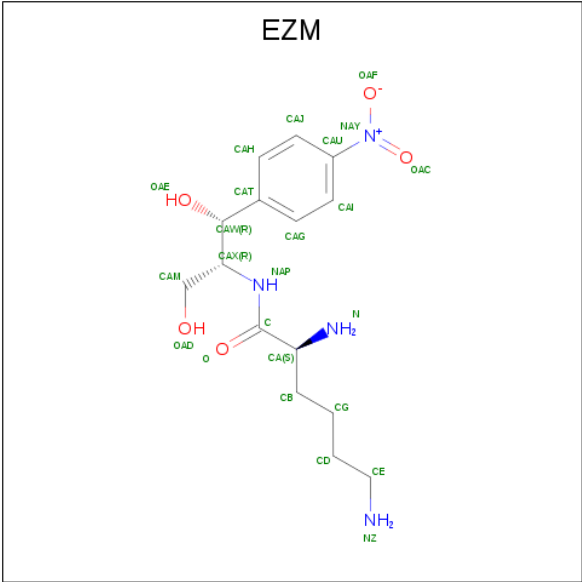
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	2V	1	Total 1	Mg 1	0	0
54	1F	10	Total 10	Mg 10	0	0
54	10	5	Total 5	Mg 5	0	0
54	1g	3	Total 3	Mg 3	0	0
54	2t	1	Total 1	Mg 1	0	0
54	1Q	4	Total 4	Mg 4	0	0
54	2A	699	Total 699	Mg 699	0	0
54	1h	2	Total 2	Mg 2	0	0
54	1B	32	Total 32	Mg 32	0	0

- Molecule 55 is POTASSIUM ION (three-letter code: K) (formula: K).

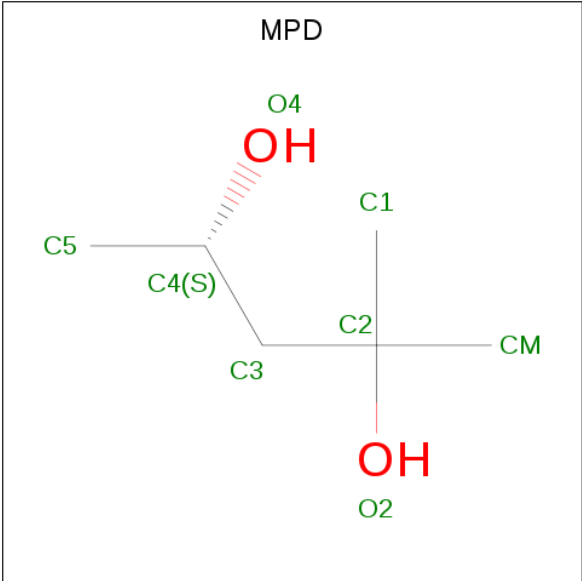
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	1A	1	Total 1	K 1	0	0
55	2A	1	Total 1	K 1	0	0

- Molecule 56 is N-[(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]-L-lysineamide (three-letter code: EZM) (formula: C₁₅H₂₄N₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
56	1A	1	Total	C	N	O	0	0
			24	15	4	5		
56	2A	1	Total	C	N	O	0	0
			24	15	4	5		

- Molecule 57 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



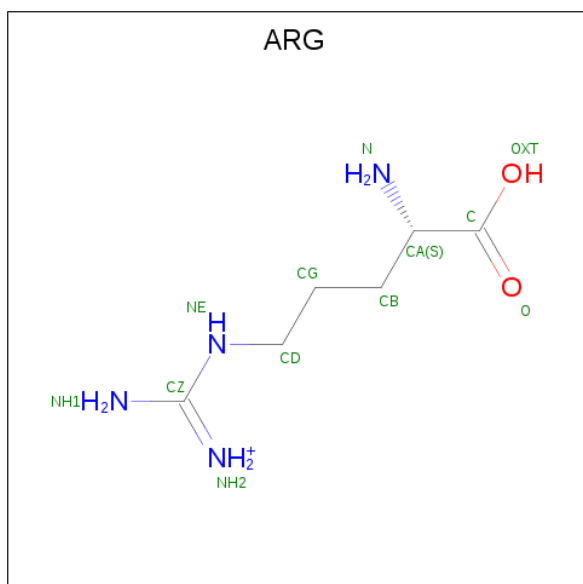
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	1A	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	1T	1	Total	C	O	0	0
			8	6	2		
57	18	1	Total	C	O	0	0
			8	6	2		
57	1a	1	Total	C	O	0	0
			8	6	2		
57	2A	1	Total	C	O	0	0
			8	6	2		
57	2A	1	Total	C	O	0	0
			8	6	2		
57	2B	1	Total	C	O	0	0
			8	6	2		

- Molecule 58 is ARGinine (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	1B	1	Total	C	N	O	0	0
			12	6	4	2		
58	1F	1	Total	C	N	O	0	0
			12	6	4	2		

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

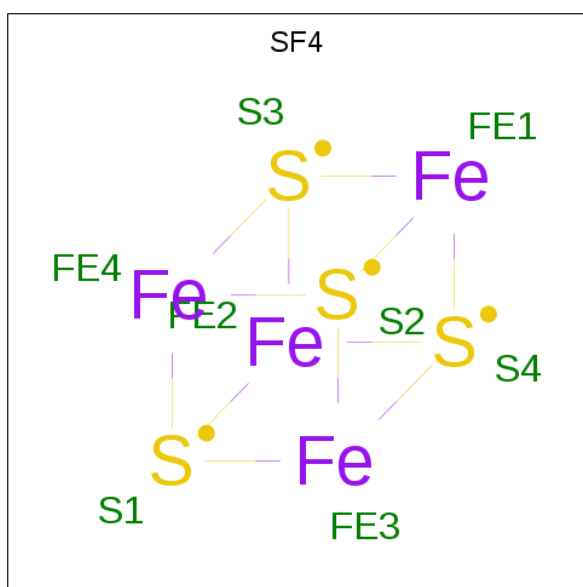
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	14	1	Total	Zn	0	0
			1	1		
59	1n	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	29	1	Total	Zn	0	0
			1	1		
59	19	1	Total	Zn	0	0
			1	1		
59	26	1	Total	Zn	0	0
			1	1		
59	25	1	Total	Zn	0	0
			1	1		
59	24	1	Total	Zn	0	0
			1	1		
59	2n	1	Total	Zn	0	0
			1	1		
59	2Y	1	Total	Zn	0	0
			1	1		
59	16	1	Total	Zn	0	0
			1	1		

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	3290	Total	O	0	0
			3290	3290		
61	1B	108	Total	O	0	0
			108	108		
61	1D	113	Total	O	0	0
			113	113		
61	1E	82	Total	O	0	0
			82	82		
61	1F	64	Total	O	0	0
			64	64		
61	1G	20	Total	O	0	0
			20	20		
61	1H	15	Total	O	0	0
			15	15		
61	1I	7	Total	O	0	0
			7	7		
61	1N	54	Total	O	0	0
			54	54		
61	1O	23	Total	O	0	0
			23	23		
61	1P	53	Total	O	0	0
			53	53		
61	1Q	46	Total	O	0	0
			46	46		
61	1R	32	Total	O	0	0
			32	32		
61	1S	13	Total	O	0	0
			13	13		
61	1T	35	Total	O	0	0
			35	35		
61	1U	42	Total	O	0	0
			42	42		
61	1V	36	Total	O	0	0
			36	36		
61	1W	26	Total	O	0	0
			26	26		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1X	23	Total 23	O 23	0	0
61	1Y	14	Total 14	O 14	0	0
61	1Z	13	Total 13	O 13	0	0
61	10	22	Total 22	O 22	0	0
61	11	25	Total 25	O 25	0	0
61	12	13	Total 13	O 13	0	0
61	13	25	Total 25	O 25	0	0
61	14	3	Total 3	O 3	0	0
61	15	24	Total 24	O 24	0	0
61	16	20	Total 20	O 20	0	0
61	17	9	Total 9	O 9	0	0
61	18	27	Total 27	O 27	0	0
61	19	6	Total 6	O 6	0	0
61	1a	343	Total 343	O 343	0	0
61	1b	1	Total 1	O 1	0	0
61	1d	8	Total 8	O 8	0	0
61	1e	6	Total 6	O 6	0	0
61	1f	3	Total 3	O 3	0	0
61	1i	1	Total 1	O 1	0	0
61	1j	2	Total 2	O 2	0	0
61	1k	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1l	4	Total 4	O 4	0	0
61	1o	4	Total 4	O 4	0	0
61	1p	3	Total 3	O 3	0	0
61	1t	1	Total 1	O 1	0	0
61	1y	4	Total 4	O 4	0	0
61	2A	1236	Total 1236	O 1236	0	0
61	2B	73	Total 73	O 73	0	0
61	2D	50	Total 50	O 50	0	0
61	2E	25	Total 25	O 25	0	0
61	2F	19	Total 19	O 19	0	0
61	2G	8	Total 8	O 8	0	0
61	2H	4	Total 4	O 4	0	0
61	2I	4	Total 4	O 4	0	0
61	2N	5	Total 5	O 5	0	0
61	2O	21	Total 21	O 21	0	0
61	2P	18	Total 18	O 18	0	0
61	2Q	26	Total 26	O 26	0	0
61	2R	15	Total 15	O 15	0	0
61	2S	5	Total 5	O 5	0	0
61	2T	10	Total 10	O 10	0	0
61	2U	14	Total 14	O 14	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2V	6	Total 6	O 6	0	0
61	2W	18	Total 18	O 18	0	0
61	2X	8	Total 8	O 8	0	0
61	2Y	3	Total 3	O 3	0	0
61	2Z	12	Total 12	O 12	0	0
61	20	12	Total 12	O 12	0	0
61	21	18	Total 18	O 18	0	0
61	22	4	Total 4	O 4	0	0
61	23	2	Total 2	O 2	0	0
61	24	2	Total 2	O 2	0	0
61	25	7	Total 7	O 7	0	0
61	26	3	Total 3	O 3	0	0
61	27	6	Total 6	O 6	0	0
61	28	13	Total 13	O 13	0	0
61	29	2	Total 2	O 2	0	0
61	2a	259	Total 259	O 259	0	0
61	2d	5	Total 5	O 5	0	0
61	2e	2	Total 2	O 2	0	0
61	2f	1	Total 1	O 1	0	0
61	2j	2	Total 2	O 2	0	0
61	2l	1	Total 1	O 1	0	0

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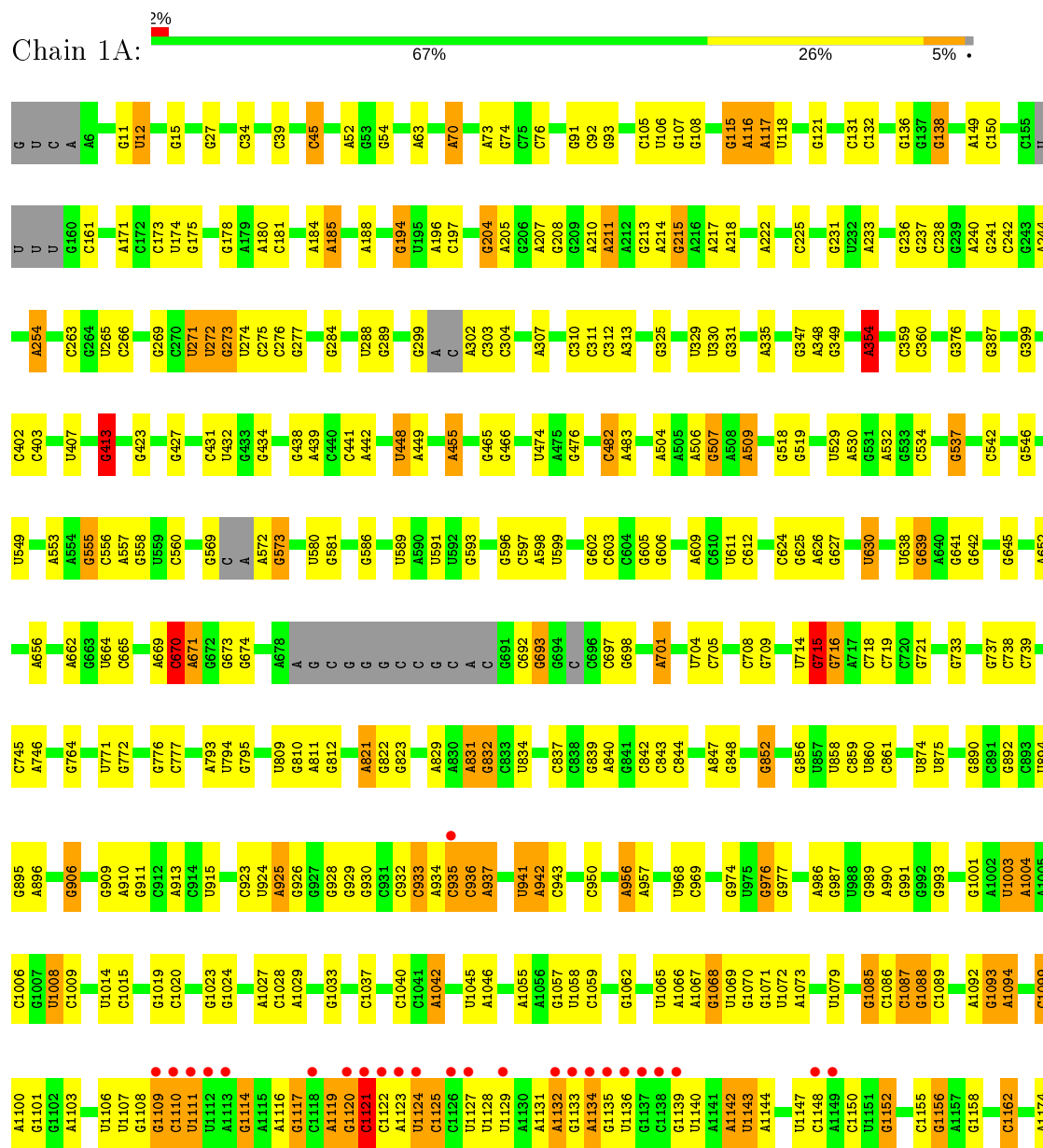
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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			1	1		
61	2o	2	Total	O	0	0
			2	2		
61	2p	1	Total	O	0	0
			1	1		
61	2q	1	Total	O	0	0
			1	1		
61	2r	5	Total	O	0	0
			5	5		
61	2s	1	Total	O	0	0
			1	1		
61	2t	1	Total	O	0	0
			1	1		
61	2u	1	Total	O	0	0
			1	1		
61	2y	1	Total	O	0	0
			1	1		

3 Residue-property plots

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

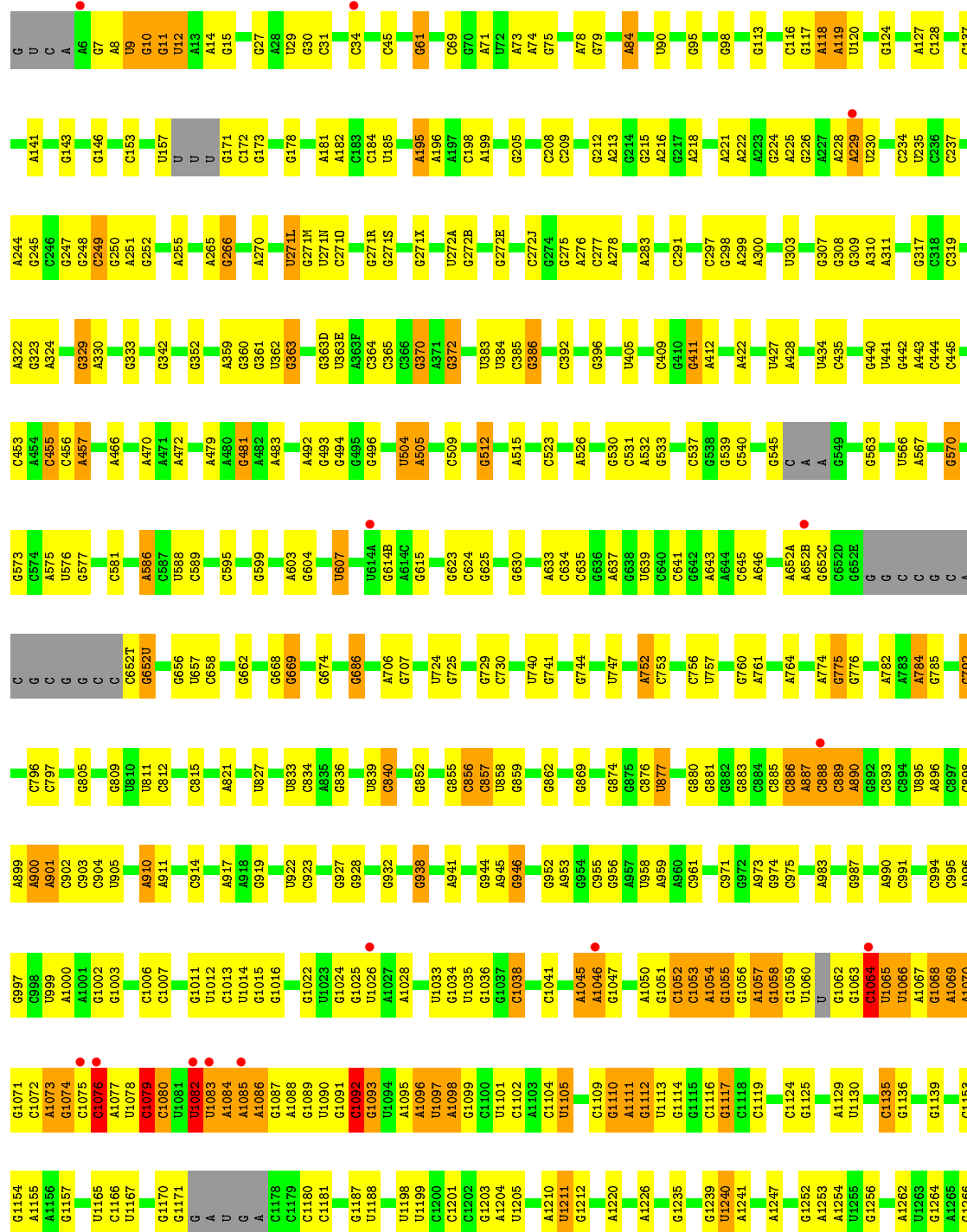
• Molecule 1: 23S Ribosomal RNA



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U2659	G2795	A2389	A2285	G2176	G2112	C1989	U1829	A1716	G1558	G1441	U1313	G1177
U2662	G2803	A2390	A2286	G2177	G2115	A1992	G1830	C1717	U1562	U1451	A1314	G1180
C2663	G2804	G2393	G2289	G2178	U2118	A1993	G1831	G1721	G1563	U1452	G1182	G1181
A2666	G2805	G2394	A2290	G2179	C2119	A1994	G1832	C1722	U1566	G1462	G1183	G1182
A2674	G2806	G2395	G2291	G2180	C2121	C2004	A1833	C1723	G1567	C1463	G1184	G1183
G2686	G2807	G2396	G2295	G2181	U2120	U2014	A1834	A1724	C1579	C1464	C1185	C1185
A2687	G2808	C2397	G2298	G2182	G2122	U2015	A1841	G1730	G	G1323	U1196	G1186
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C2695	G2810	G2417	A2299	G2184	G2124	G2019	G1845	C1732	A	C1472	A1201	A1201
U2696	G2811	U2418	A2300	G2185	C2126	G2019	G1846	G1733	U	A1324	A1324	A1324
U2697	G2812	U2419	A2301	G2186	G2127	A2035	G1847	G1734	C	G1331	G1331	G1331
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G2699	G2814	A2430	U2303	G2188	C2130	U2038	G1860	G1743	U1587	C1335	G1210	G1210
U2700	G2815	U2431	G2304	U2189	G2131	U2039	A1860	G1744	U1588	C1336	U1211	U1211
G2701	G2816	A2432	C2305	G2190	G2132	A2041	G1870	A1747	A1589	U1346	U1346	C1212
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C2703	G2818	U2434	U2307	G2192	U2134	A2043	G1874	G1750	A1605	G1485	G1217	G1217
G2704	G2819	A2435	U2308	G2193	U2135	G2044	C1874	G1751	A1616	G1486	G1218	G1218
G2828	G2820	G2436	G2316	G2194	A2136	U2044	A1878	G1766	A1617	G1487	A1219	A1219
G2829	G2821	G2437	A2317	G2195	G2137	G2045	A1879	A1767	A1618	U1358	U1220	U1220
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A2831	G2823	U2442	G2321	G2197	U2139	A2052	G1890	G1769	A1626	G1497	A1222	A1222
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C2711	G2825	A2447	G2322	G2205	A2141	G2054	G1899	G1776	G1628	U1501	C1226	C1226
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A2725	G2830	A2455	G2327	G2210	A2148	G2061	G1923	A1790	C1634	A1518	A1255	A1255
G2727	G2831	G2456	G2331	G2211	G2149	C2065	G1924	A1791	C1635	U1398	U1256	U1256
U2739	G2832	U2457	A2332	G2212	C2150	G2077	G1925	G1795	C1650	A1399	G1257	G1257
G2745	G2833	G2458	G2337	G2213	U2152	C2078	G1935	A1804	A1654	G1522	G1401	G1401
A2746	G2834	A2459	A2338	G2214	G2153	A2081	C1942	U1809	A1655	G1523	G1404	G1404
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G2764	G2837	G2462	G2341	G2217	C2158	A2084	G1952	C1812	U1685	G1539	G1411	G1411
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A2771	G2839	U2464	G2343	G2219	C2160	C2086	A1954	C1814	C1687	G1541	G1417	G1417
G2776	G2840	G2465	G2344	U2245	C2161	C2087	G1955	A1815	G1692	U1542	U1418	U1418
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G2889	G2843	A2468	G2347	U2248	C2164	G2091	A1960	C1821	A1699	U1549	A1289	A1289
C2890	G2844	G2469	A2348	G2249	C2165	G2092	U1977	A1822	A1699	C1550	G1302	G1302
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C2892	G2846	U2505	G2350	G2251	C2167	G2093	G1986	C1824	A1555	C1555		
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C2898	G2848	G2514	G2352	U2256	C2169	G2102						
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G2900	G2850	G2518			G2171							



● Molecule 1: 23S Ribosomal RNA

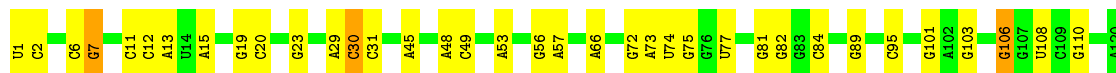


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C C C C

- Molecule 2: 5S Ribosomal RNA

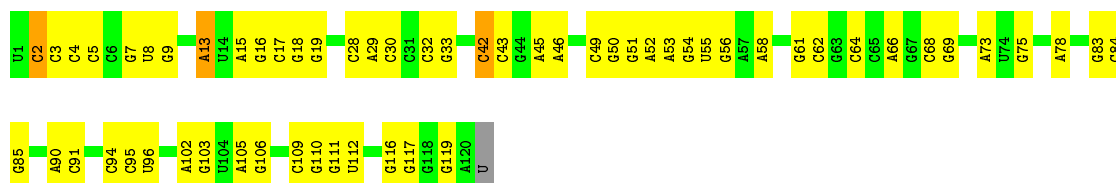
Chain 1B: 69% 27% ..



U

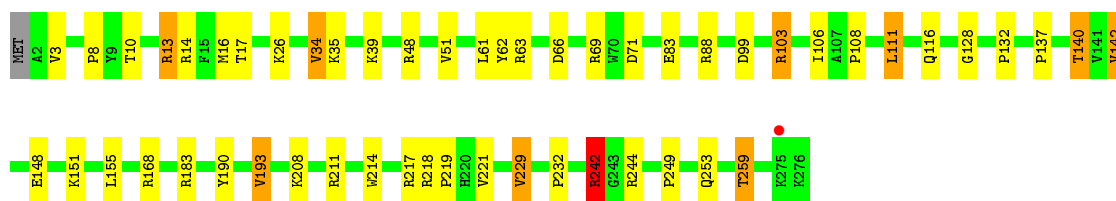
- Molecule 2: 5S Ribosomal RNA

Chain 2B: 50% 46% ..



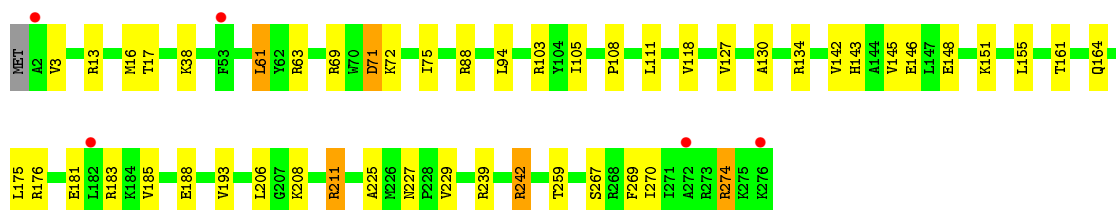
- Molecule 3: 50S ribosomal protein L2

Chain 1D: 80% 16% .



- Molecule 3: 50S ribosomal protein L2

Chain 2D: 2% 82% 16% .



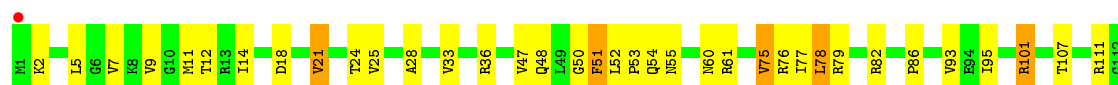
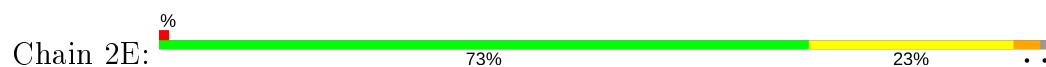
- Molecule 4: 50S Ribosomal Protein L3

Chain 1E: 76% 20% ..





- Molecule 4: 50S Ribosomal Protein L3



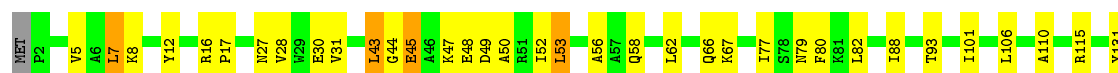
- Molecule 5: 50S ribosomal protein L4



- Molecule 5: 50S ribosomal protein L4

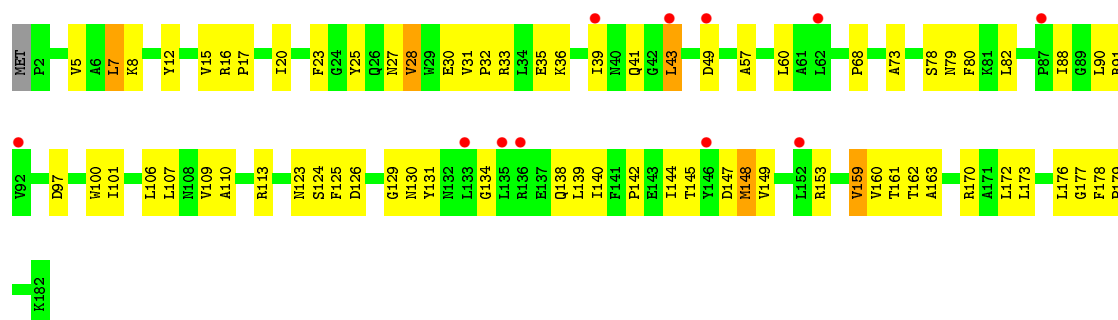


- Molecule 6: 50S ribosomal protein L5



- Molecule 6: 50S ribosomal protein L5





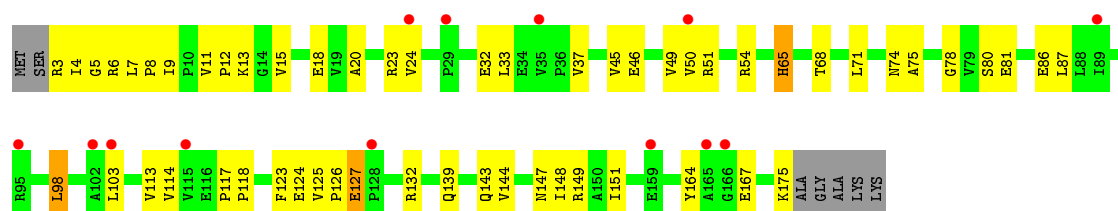
• Molecule 7: 50S ribosomal protein L6

Chain 1H: 76% 21% ..



• Molecule 7: 50S ribosomal protein L6

Chain 2H: 7% 65% 29% ..



• Molecule 8: 50S ribosomal protein L9

Chain 1I: 70% 27% ..



• Molecule 8: 50S ribosomal protein L9

Chain 2I: 6% 74% 23% ..





- Molecule 9: 50S ribosomal protein L13

Chain 1N: 81% 18%



- Molecule 9: 50S ribosomal protein L13

Chain 2N: 81% 19%



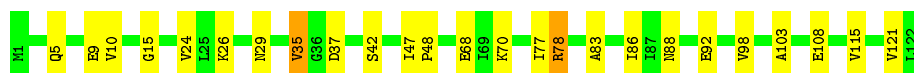
- Molecule 10: 50S ribosomal protein L14

Chain 1O: 86% 14%



- Molecule 10: 50S ribosomal protein L14

Chain 2O: 80% 19%



- Molecule 11: 50S ribosomal protein L15

Chain 1P: 81% 15%



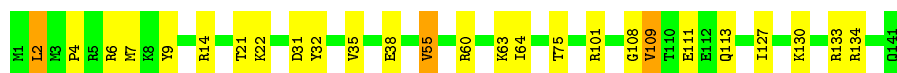
- Molecule 11: 50S ribosomal protein L15

Chain 2P: 81% 17%

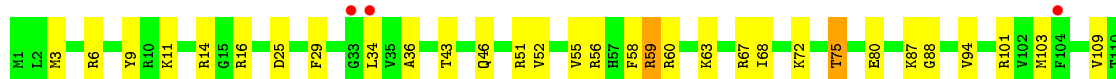
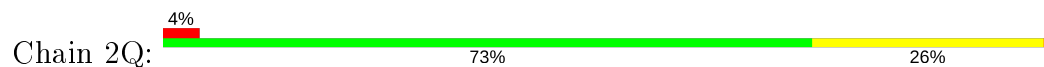


- Molecule 12: 50S ribosomal protein L16

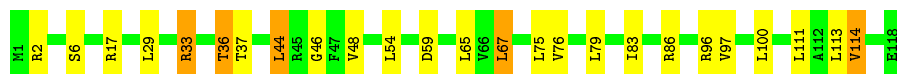
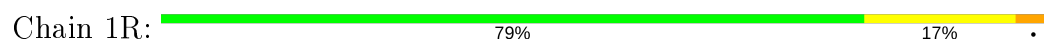
Chain 1Q: 82% 16%



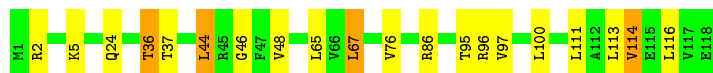
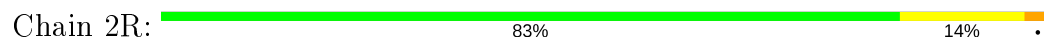
- Molecule 12: 50S ribosomal protein L16



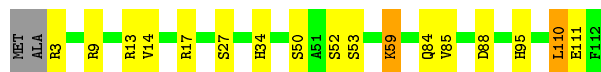
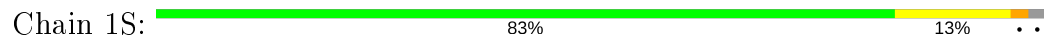
- Molecule 13: 50S ribosomal protein L17



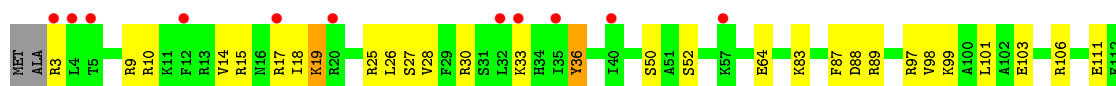
- Molecule 13: 50S ribosomal protein L17



- Molecule 14: 50S Ribosomal Protein L18



- Molecule 14: 50S Ribosomal Protein L18




- Molecule 15: 50S ribosomal protein L19



PRO
LYS
ALA
SER
GLN
GLU


- Molecule 15: 50S ribosomal protein L19

Chain 2T:  %




LYS
ALA
SER
GLN
GLU

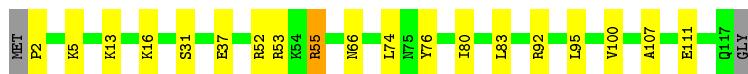
- Molecule 16: 50S Ribosomal Protein L20

Chain 1U:  %




- Molecule 16: 50S Ribosomal Protein L20

Chain 2U:  %




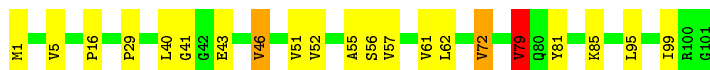
- Molecule 17: 50S ribosomal protein L21

Chain 1V:  %




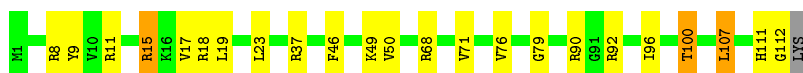
- Molecule 17: 50S ribosomal protein L21

Chain 2V:  %




- Molecule 18: 50S ribosomal protein L22

Chain 1W:  %

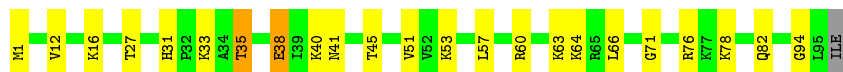


- Molecule 18: 50S ribosomal protein L22

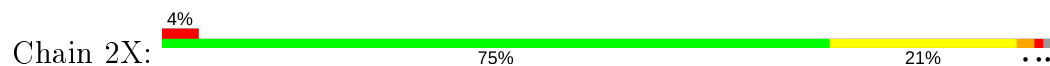
Chain 2W:  %



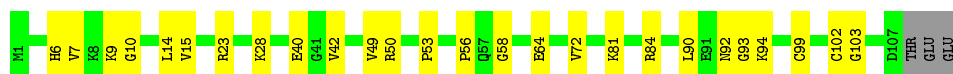
- Molecule 19: 50S ribosomal protein L23



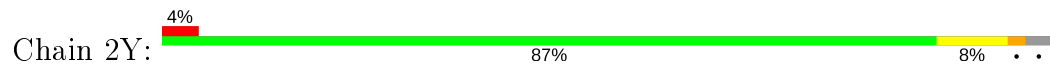
- Molecule 19: 50S ribosomal protein L23



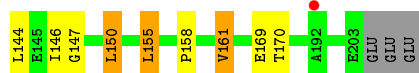
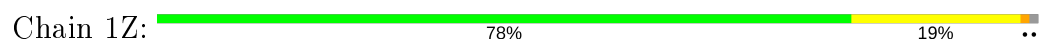
- Molecule 20: 50S Ribosomal Protein L24



- Molecule 20: 50S Ribosomal Protein L24



- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25

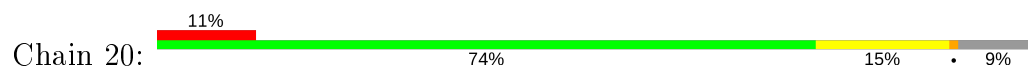




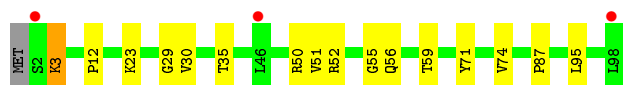
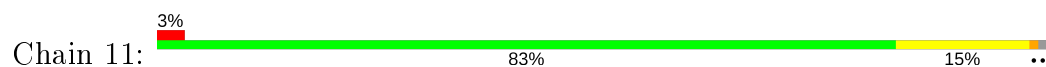
- Molecule 22: 50S ribosomal protein L27



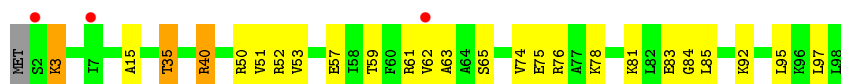
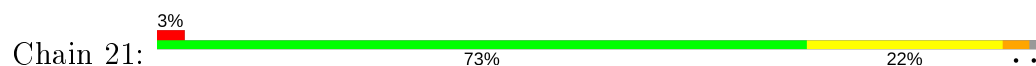
- Molecule 22: 50S ribosomal protein L27



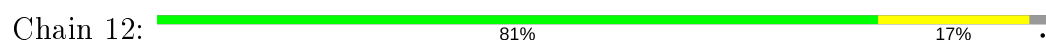
- Molecule 23: 50S ribosomal protein L28



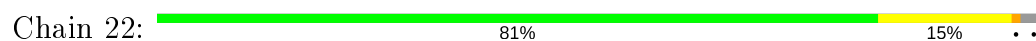
- Molecule 23: 50S ribosomal protein L28



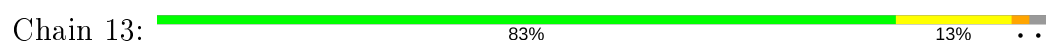
- Molecule 24: 50S ribosomal protein L29

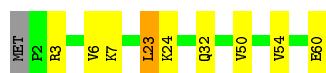


- Molecule 24: 50S ribosomal protein L29

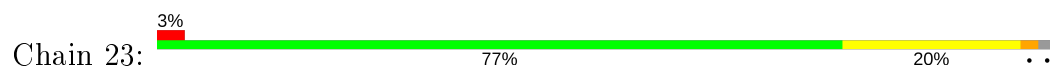


- Molecule 25: 50S ribosomal protein L30

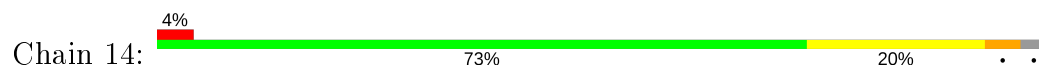




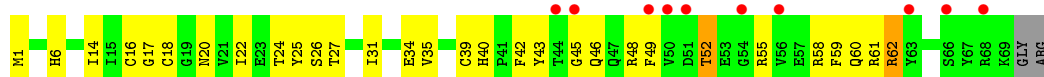
- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S Ribosomal Protein L31



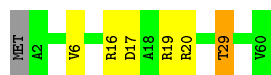
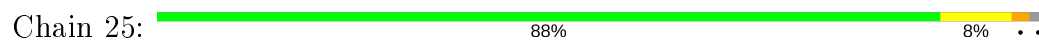
- Molecule 26: 50S Ribosomal Protein L31



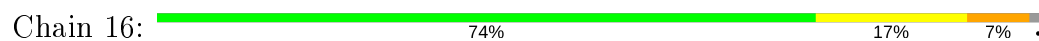
- Molecule 27: 50S ribosomal protein L32



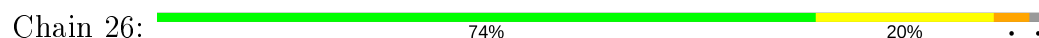
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33

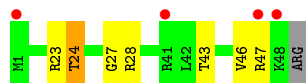
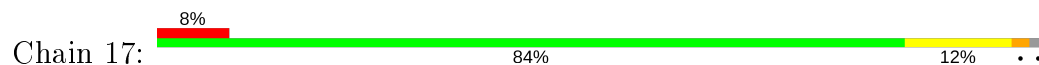


- Molecule 28: 50S ribosomal protein L33

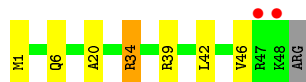
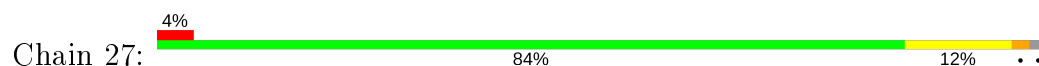




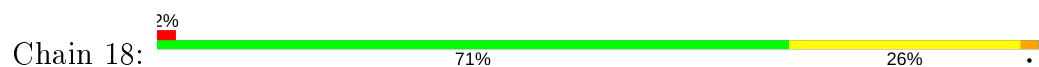
- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



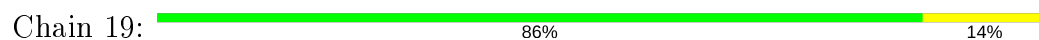
- Molecule 30: 50S ribosomal protein L35



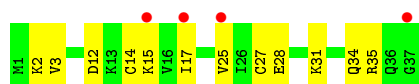
- Molecule 30: 50S ribosomal protein L35



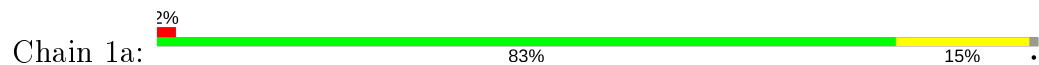
- Molecule 31: 50S ribosomal protein L36

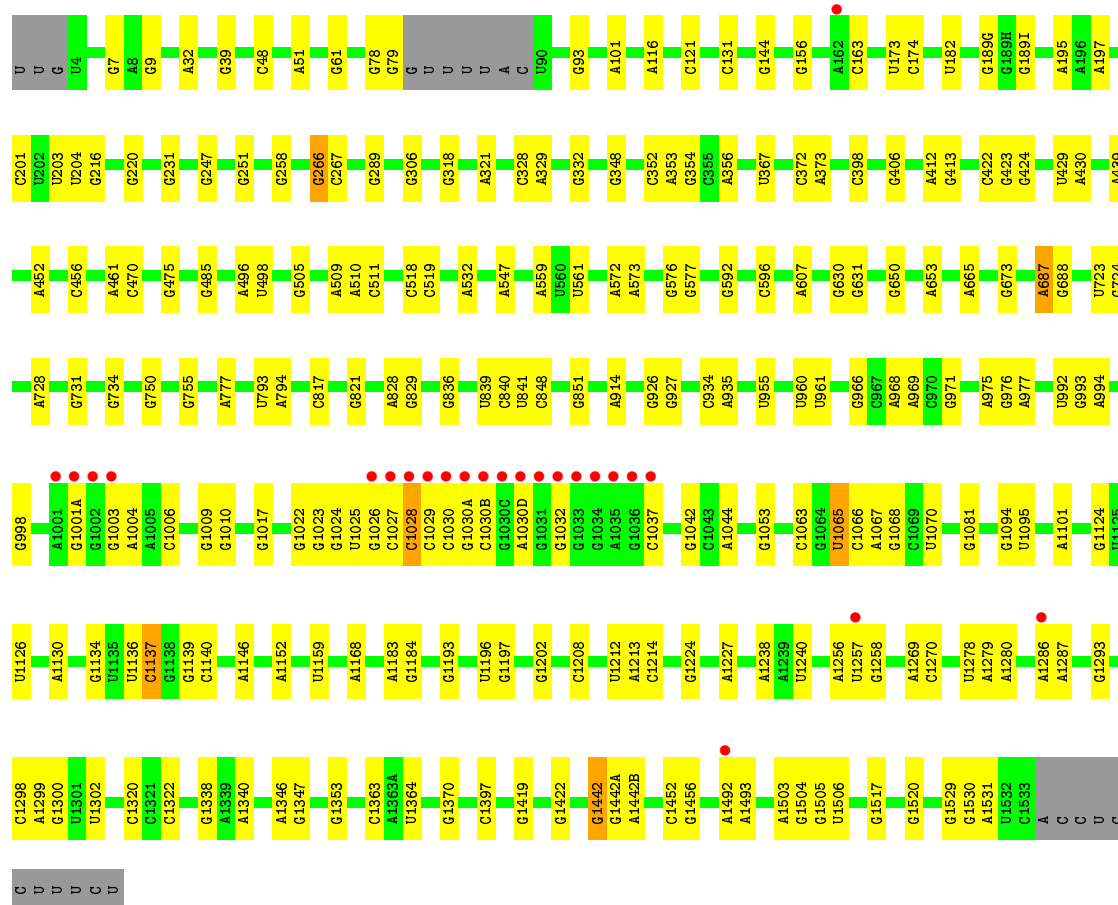


- Molecule 31: 50S ribosomal protein L36

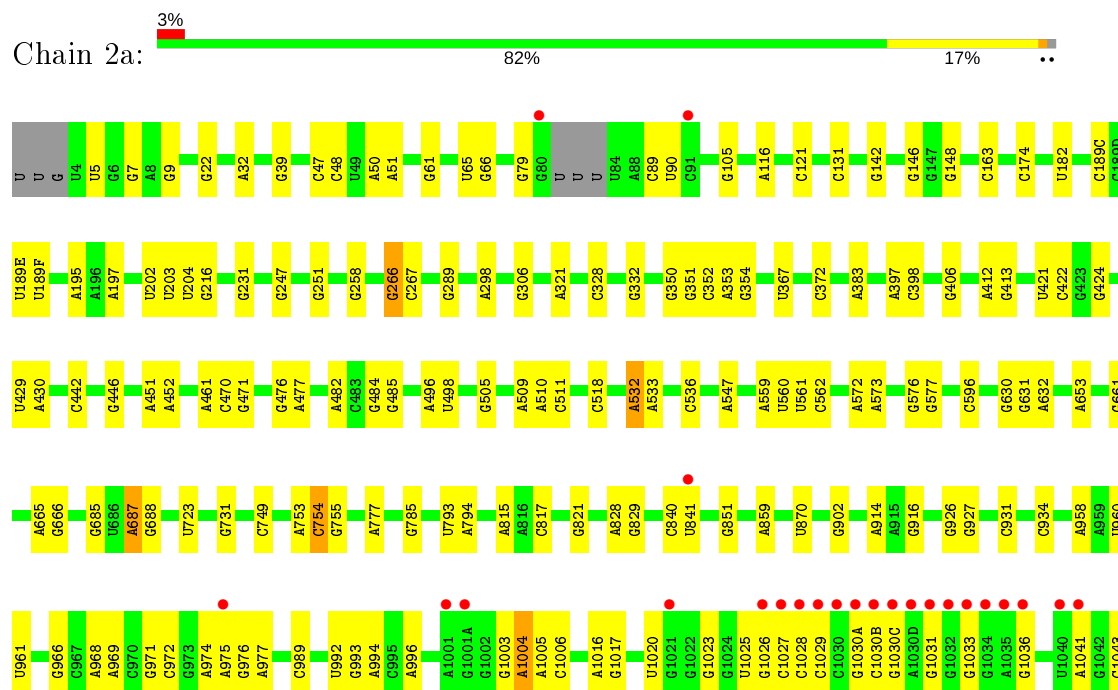


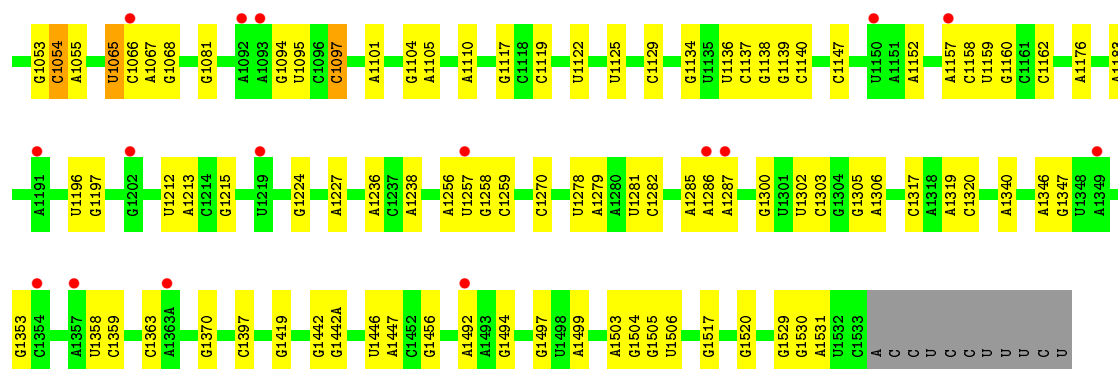
- Molecule 32: 16S Ribosomal RNA



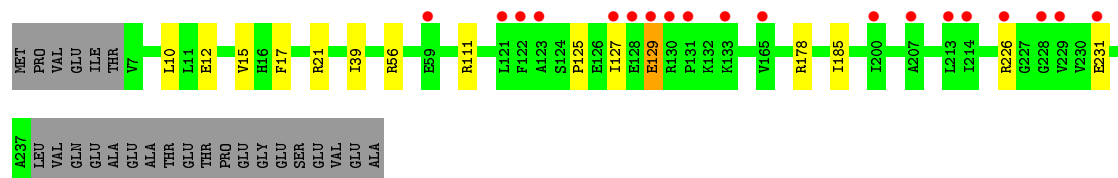
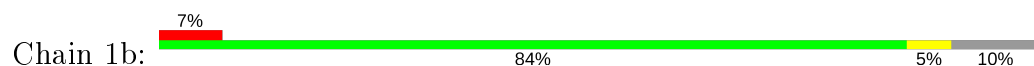


● Molecule 32: 16S Ribosomal RNA

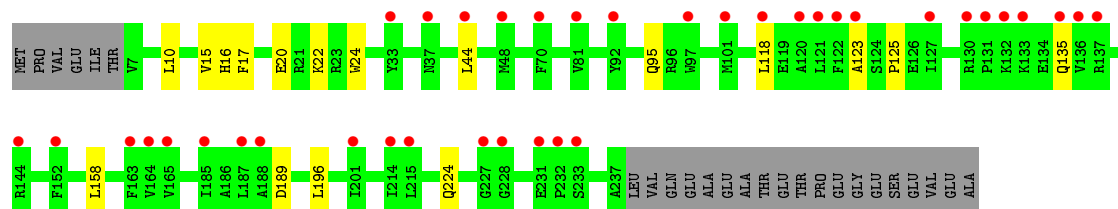
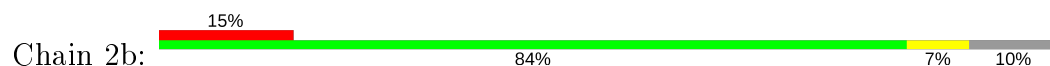




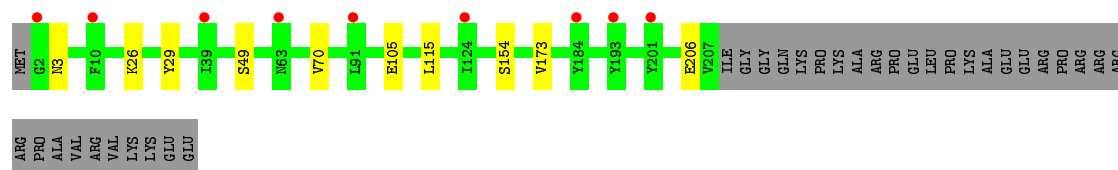
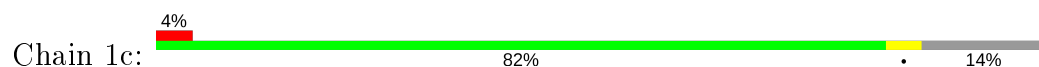
• Molecule 33: 30S ribosomal protein S2



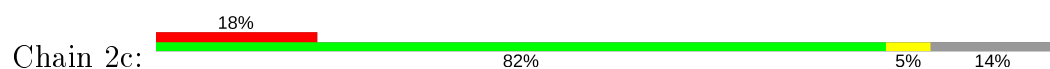
• Molecule 33: 30S ribosomal protein S2

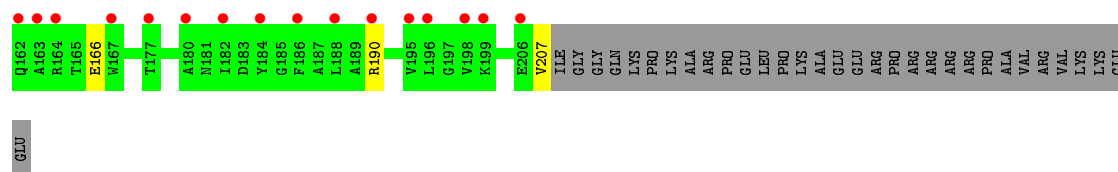


• Molecule 34: 30S ribosomal protein S3



• Molecule 34: 30S ribosomal protein S3





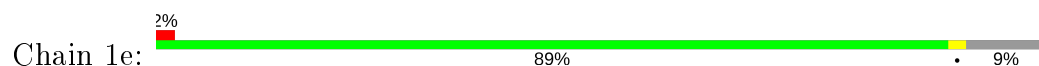
- Molecule 35: 30S ribosomal protein S4



- Molecule 35: 30S ribosomal protein S4



- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5



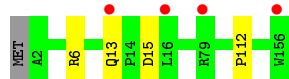
- Molecule 37: 30S ribosomal protein S6



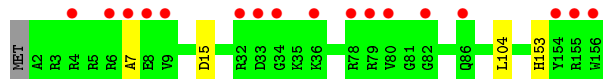
- Molecule 37: 30S ribosomal protein S6



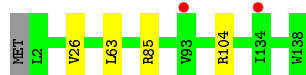
- Molecule 38: 30S ribosomal protein S7



- Molecule 38: 30S ribosomal protein S7



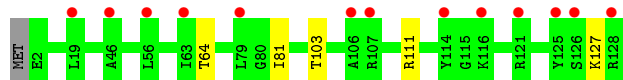
- Molecule 39: 30S Ribosomal Protein S8



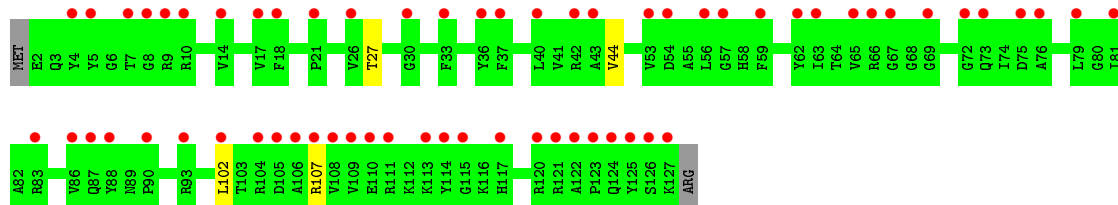
- Molecule 39: 30S Ribosomal Protein S8



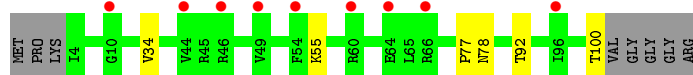
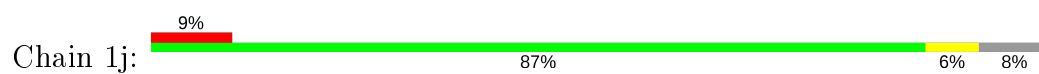
- Molecule 40: 30S ribosomal protein S9



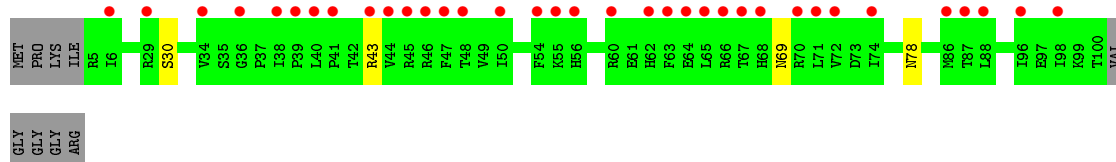
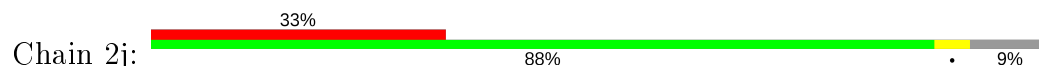
- Molecule 40: 30S ribosomal protein S9



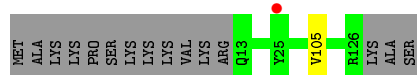
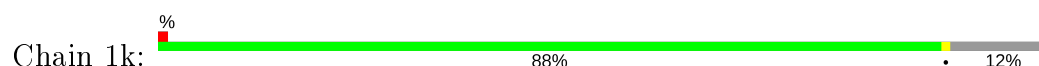
- Molecule 41: 30S ribosomal protein S10



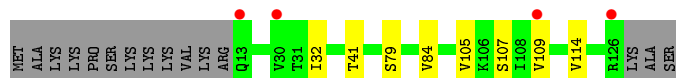
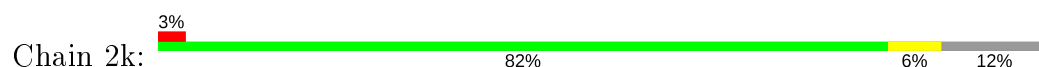
- Molecule 41: 30S ribosomal protein S10



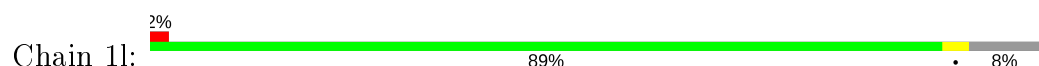
- Molecule 42: 30S ribosomal protein S11



- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12

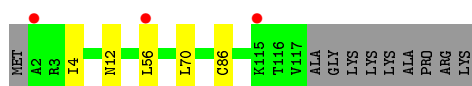


- Molecule 43: 30S ribosomal protein S12

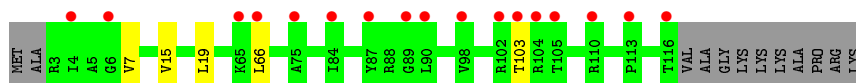
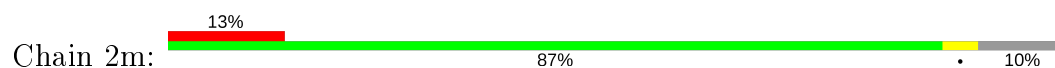


- Molecule 44: 30S ribosomal protein S13

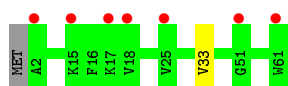




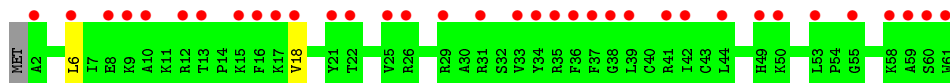
- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z



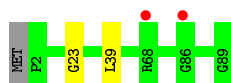
- Molecule 45: 30S ribosomal protein S14 type Z



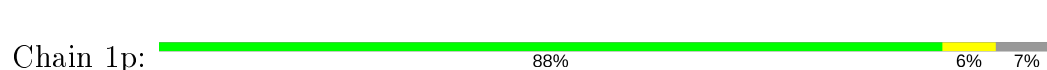
- Molecule 46: 30S ribosomal protein S15



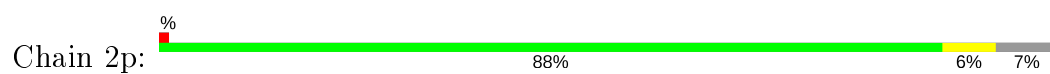
- Molecule 46: 30S ribosomal protein S15



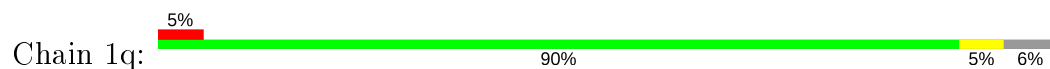
- Molecule 47: 30S ribosomal protein S16



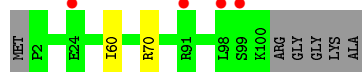
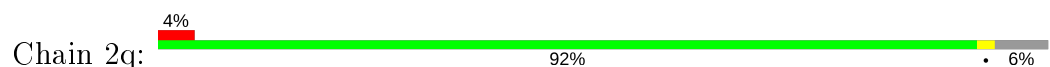
- Molecule 47: 30S ribosomal protein S16



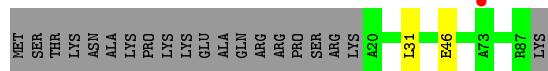
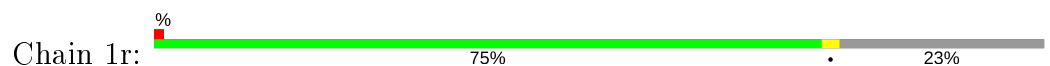
- Molecule 48: 30S ribosomal protein S17



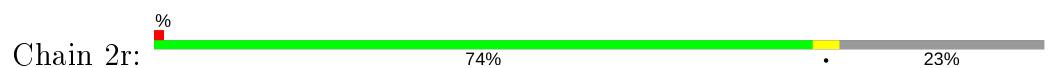
- Molecule 48: 30S ribosomal protein S17



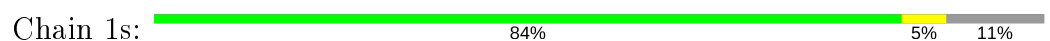
- Molecule 49: 30S ribosomal protein S18



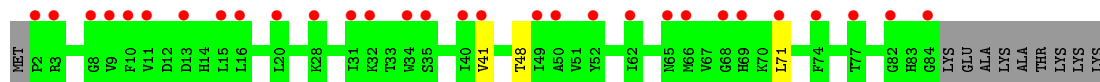
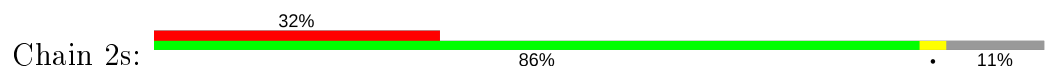
- Molecule 49: 30S ribosomal protein S18



- Molecule 50: 30S ribosomal protein S19



- Molecule 50: 30S ribosomal protein S19



- Chain 2y:
-
- 50% 83% 15%
- MET THR M3 N4 I5 T6 S7 K8 Q9 M10 E11 I12 A15 V20 L24 K29 I35 N36 P37 R38 I39 I40 I41 S42 P45 Q46 G47 F48 V49 A50 D51 A52 T53 N58 G59 V60 L61 V62 A63 S64 G65 A66 H67 D68 M69 W70 Y71 T72 A73 I74 N75 E76 L77
- I78 N79 K80 L81 E82 R83 Q84 K87 L88 K91 G92 E93 A94 A95 A98 THR SER VAL LYS ASP ALA ASN PHE VAL GLU GLU VAL GLU GLU GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.15Å 449.33Å 623.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	224.66 – 2.60 311.73 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (224.66-2.60) 99.8 (311.73-2.60)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.209 , 0.252 0.209 , 0.252	Depositor DCC
R_{free} test set	89415 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	51.3	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	295545	wwPDB-VP
Average B, all atoms (Å ²)	55.0	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.54	1/69029 (0.0%)	1.01	84/107746 (0.1%)
1	2A	0.42	0/68901	0.90	29/107544 (0.0%)
2	1B	0.45	0/2876	0.93	2/4486 (0.0%)
2	2B	0.38	0/2878	0.86	0/4490
3	1D	0.38	0/2181	0.60	1/2940 (0.0%)
3	2D	0.33	0/2186	0.54	0/2944
4	1E	0.36	0/1592	0.57	0/2149
4	2E	0.33	0/1592	0.54	0/2149
5	1F	0.37	1/1619 (0.1%)	0.58	0/2193
5	2F	0.32	0/1615	0.52	0/2188
6	1G	0.30	0/1451	0.50	0/1961
6	2G	0.32	0/1449	0.47	0/1957
7	1H	0.35	0/1356	0.51	0/1834
7	2H	0.30	0/1350	0.48	0/1826
8	1I	0.31	0/1109	0.50	0/1512
8	2I	0.28	0/1091	0.50	0/1490
9	1N	0.35	0/1148	0.54	0/1547
9	2N	0.31	0/1144	0.48	0/1543
10	1O	0.39	0/943	0.58	0/1269
10	2O	0.33	0/943	0.52	0/1269
11	1P	0.34	0/1152	0.56	0/1533
11	2P	0.33	0/1152	0.54	0/1533
12	1Q	0.35	0/1143	0.52	0/1527
12	2Q	0.31	0/1143	0.49	0/1527
13	1R	0.33	0/982	0.59	0/1312
13	2R	0.29	0/982	0.54	0/1312
14	1S	0.31	0/887	0.52	0/1180
14	2S	0.31	0/880	0.49	0/1172
15	1T	0.33	0/1105	0.55	0/1477
15	2T	0.31	0/1097	0.51	0/1468
16	1U	0.38	0/977	0.54	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.31	0/977	0.44	0/1301
17	1V	0.38	0/786	0.57	0/1053
17	2V	0.33	0/782	0.52	0/1049
18	1W	0.35	0/897	0.54	0/1205
18	2W	0.31	0/897	0.50	0/1205
19	1X	0.37	0/764	0.56	0/1025
19	2X	0.31	0/764	0.55	1/1025 (0.1%)
20	1Y	0.37	0/823	0.54	0/1099
20	2Y	0.31	0/823	0.51	0/1100
21	1Z	0.32	0/1620	0.51	0/2200
21	2Z	0.34	1/1590 (0.1%)	0.50	0/2162
22	10	0.36	0/616	0.55	0/821
22	20	0.32	0/616	0.51	0/821
23	11	0.35	0/761	0.55	0/1013
23	21	0.33	0/766	0.51	0/1018
24	12	0.31	0/590	0.51	0/781
24	22	0.31	0/594	0.42	0/785
25	13	0.33	0/474	0.55	0/635
25	23	0.30	0/469	0.49	0/630
26	14	0.34	0/559	0.54	0/754
26	24	0.37	0/549	0.56	0/741
27	15	0.39	0/473	0.68	2/639 (0.3%)
27	25	0.31	0/469	0.52	0/635
28	16	0.32	0/460	0.55	0/613
28	26	0.31	0/456	0.49	0/608
29	17	0.36	0/426	0.60	0/561
29	27	0.32	0/426	0.51	0/561
30	18	0.35	0/525	0.59	0/691
30	28	0.30	0/525	0.51	0/691
31	19	0.36	0/310	0.54	0/407
31	29	0.30	0/310	0.51	0/407
32	1a	0.39	0/35795	0.88	13/55864 (0.0%)
32	2a	0.37	0/35890	0.87	21/56012 (0.0%)
33	1b	0.30	0/1876	0.49	1/2533 (0.0%)
33	2b	0.33	0/1860	0.49	0/2518
34	1c	0.36	1/1582 (0.1%)	0.47	0/2137
34	2c	0.30	0/1566	0.49	0/2119
35	1d	0.30	0/1695	0.48	0/2274
35	2d	0.29	0/1698	0.46	0/2277
36	1e	0.32	0/1149	0.52	0/1548
36	2e	0.35	1/1149 (0.1%)	0.49	0/1548
37	1f	0.31	0/827	0.51	0/1120
37	2f	0.29	0/829	0.51	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.29	0/1254	0.42	0/1683
38	2g	0.29	0/1248	0.42	0/1676
39	1h	0.29	0/1118	0.48	0/1506
39	2h	0.28	0/1108	0.47	0/1494
40	1i	0.29	0/1005	0.51	0/1351
40	2i	0.31	0/985	0.47	0/1329
41	1j	0.30	0/732	0.50	0/993
41	2j	0.30	0/723	0.49	0/984
42	1k	0.29	0/849	0.48	0/1150
42	2k	0.30	0/848	0.52	0/1149
43	1l	0.30	0/937	0.50	0/1260
43	2l	0.28	0/937	0.52	0/1260
44	1m	0.29	0/924	0.48	0/1242
44	2m	0.30	0/905	0.47	0/1217
45	1n	0.31	0/501	0.46	0/664
45	2n	0.32	0/501	0.47	0/664
46	1o	0.30	0/739	0.46	0/985
46	2o	0.28	0/739	0.44	0/985
47	1p	0.31	0/697	0.53	0/939
47	2p	0.30	0/693	0.51	0/935
48	1q	0.30	0/836	0.49	0/1117
48	2q	0.31	0/836	0.50	0/1117
49	1r	0.29	0/560	0.49	0/746
49	2r	0.29	0/560	0.45	0/746
50	1s	0.28	0/663	0.50	0/895
50	2s	0.30	0/660	0.47	0/893
51	1t	0.28	0/734	0.45	0/969
51	2t	0.28	0/736	0.42	0/976
52	1u	0.26	0/203	0.48	0/266
52	2u	0.31	0/203	0.56	0/266
53	1y	0.29	0/776	0.49	0/1048
53	2y	0.28	0/761	0.47	0/1030
All	All	0.42	5/309937 (0.0%)	0.83	154/463223 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	1c	173	VAL	C-N	8.18	1.49	1.34
1	1A	354	A	N9-C4	-6.29	1.34	1.37
36	2e	69	VAL	C-N	6.14	1.46	1.34
21	2Z	13	GLU	C-N	5.16	1.46	1.34
5	1F	23	ASP	C-N	-5.07	1.22	1.34

The worst 5 of 154 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1045	U	O5'-P-OP2	-11.85	95.03	105.70
1	1A	848	G	O5'-P-OP2	-9.23	97.39	105.70
1	1A	537	G	O4'-C1'-N9	8.97	115.38	108.20
1	1A	354	A	C2-N3-C4	-8.79	106.20	110.60
32	1a	1028	C	C5-C6-N1	8.53	125.26	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61869	0	31203	510	0
1	2A	61758	0	31151	595	0
2	1B	2572	0	1305	22	0
2	2B	2573	0	1306	41	0
3	1D	2131	0	2207	37	0
3	2D	2136	0	2218	39	0
4	1E	1559	0	1618	31	0
4	2E	1559	0	1618	38	0
5	1F	1584	0	1624	31	0
5	2F	1580	0	1619	37	0
6	1G	1426	0	1445	29	0
6	2G	1424	0	1441	51	0
7	1H	1330	0	1407	23	0
7	2H	1324	0	1402	33	0
8	1I	1094	0	1127	31	0
8	2I	1076	0	1094	24	0
9	1N	1121	0	1195	11	0
9	2N	1117	0	1184	17	0
10	1O	933	0	996	13	0
10	2O	933	0	996	15	0
11	1P	1135	0	1212	26	0
11	2P	1135	0	1212	19	0
12	1Q	1122	0	1179	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	2Q	1122	0	1179	30	0
13	1R	968	0	1033	16	0
13	2R	968	0	1033	12	0
14	1S	877	0	938	13	0
14	2S	870	0	923	30	0
15	1T	1091	0	1151	19	0
15	2T	1083	0	1136	20	0
16	1U	959	0	1019	15	0
16	2U	959	0	1019	13	0
17	1V	775	0	841	13	0
17	2V	771	0	830	13	0
18	1W	886	0	940	10	0
18	2W	886	0	940	7	0
19	1X	750	0	814	16	0
19	2X	750	0	814	14	0
20	1Y	810	0	892	16	0
20	2Y	810	0	887	6	0
21	1Z	1587	0	1598	23	0
21	2Z	1557	0	1564	37	0
22	10	608	0	622	14	0
22	20	608	0	622	9	0
23	11	754	0	823	11	0
23	21	759	0	837	16	0
24	12	588	0	643	9	0
24	22	592	0	654	5	0
25	13	469	0	518	4	0
25	23	464	0	514	8	0
26	14	546	0	522	11	0
26	24	536	0	514	28	0
27	15	459	0	476	12	0
27	25	455	0	465	4	0
28	16	453	0	473	7	0
28	26	449	0	469	9	0
29	17	418	0	467	4	0
29	27	418	0	467	5	0
30	18	517	0	582	10	0
30	28	517	0	582	13	0
31	19	307	0	335	3	0
31	29	307	0	335	7	0
32	1a	32246	0	16296	0	0
32	2a	32331	0	16339	0	0
33	1b	1842	0	1862	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	2b	1825	0	1828	0	0
34	1c	1558	0	1557	0	0
34	2c	1542	0	1517	0	0
35	1d	1665	0	1687	0	0
35	2d	1668	0	1703	0	0
36	1e	1133	0	1191	0	0
36	2e	1133	0	1191	0	0
37	1f	814	0	808	0	0
37	2f	816	0	808	0	0
38	1g	1235	0	1249	0	0
38	2g	1229	0	1238	0	0
39	1h	1098	0	1143	0	0
39	2h	1088	0	1126	0	0
40	1i	986	0	990	0	0
40	2i	966	0	953	0	0
41	1j	719	0	672	0	0
41	2j	710	0	661	0	0
42	1k	834	0	838	0	0
42	2k	833	0	836	0	0
43	1l	932	0	981	0	0
43	2l	932	0	981	0	0
44	1m	914	0	954	0	0
44	2m	895	0	920	0	0
45	1n	492	0	529	0	0
45	2n	492	0	529	0	0
46	1o	728	0	760	0	0
46	2o	728	0	760	0	0
47	1p	681	0	697	0	0
47	2p	677	0	686	0	0
48	1q	823	0	891	0	0
48	2q	823	0	891	0	0
49	1r	555	0	618	0	0
49	2r	555	0	618	0	0
50	1s	648	0	658	0	0
50	2s	645	0	635	0	0
51	1t	732	0	809	0	0
51	2t	733	0	795	0	0
52	1u	199	0	208	0	0
52	2u	199	0	208	0	0
53	1y	764	0	786	0	0
53	2y	749	0	757	0	0
54	10	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	11	2	0	0	0	0
54	13	3	0	0	0	0
54	14	1	0	0	0	0
54	15	3	0	0	0	0
54	17	1	0	0	0	0
54	18	1	0	0	0	0
54	19	2	0	0	0	0
54	1A	1071	0	0	0	0
54	1B	32	0	0	0	0
54	1D	13	0	0	0	0
54	1E	5	0	0	0	0
54	1F	10	0	0	0	0
54	1G	4	0	0	0	0
54	1H	3	0	0	0	0
54	1N	3	0	0	0	0
54	1O	1	0	0	0	0
54	1P	2	0	0	0	0
54	1Q	4	0	0	0	0
54	1R	2	0	0	0	0
54	1T	4	0	0	0	0
54	1U	3	0	0	0	0
54	1V	3	0	0	0	0
54	1W	3	0	0	0	0
54	1X	2	0	0	0	0
54	1Z	1	0	0	0	0
54	1a	260	0	0	0	0
54	1b	1	0	0	0	0
54	1d	4	0	0	0	0
54	1e	3	0	0	0	0
54	1f	2	0	0	0	0
54	1g	3	0	0	0	0
54	1h	2	0	0	0	0
54	1i	1	0	0	0	0
54	1k	1	0	0	0	0
54	1l	2	0	0	0	0
54	1n	2	0	0	0	0
54	1o	1	0	0	0	0
54	1p	1	0	0	0	0
54	1q	2	0	0	0	0
54	1t	1	0	0	0	0
54	1y	4	0	0	0	0
54	20	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	21	2	0	0	0	0
54	23	1	0	0	0	0
54	25	1	0	0	0	0
54	28	3	0	0	0	0
54	2A	699	0	0	0	0
54	2B	21	0	0	0	0
54	2D	6	0	0	0	0
54	2E	6	0	0	0	0
54	2F	3	0	0	0	0
54	2G	3	0	0	0	0
54	2I	1	0	0	0	0
54	2N	1	0	0	0	0
54	2O	3	0	0	0	0
54	2P	1	0	0	0	0
54	2Q	3	0	0	0	0
54	2R	2	0	0	0	0
54	2T	4	0	0	0	0
54	2V	1	0	0	0	0
54	2W	2	0	0	0	0
54	2X	1	0	0	0	0
54	2a	184	0	0	0	0
54	2d	1	0	0	0	0
54	2e	1	0	0	0	0
54	2f	1	0	0	0	0
54	2j	1	0	0	0	0
54	2t	1	0	0	0	0
55	1A	1	0	0	0	0
55	2A	1	0	0	0	0
56	1A	24	0	0	0	0
56	2A	24	0	0	0	0
57	18	8	0	14	0	0
57	1A	8	0	14	0	0
57	1T	8	0	14	0	0
57	1a	8	0	14	0	0
57	2A	16	0	28	2	0
57	2B	8	0	14	0	0
58	1B	12	0	12	5	0
58	1F	12	0	12	4	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	0	0
60	2d	8	0	0	0	0
61	10	22	0	0	2	0
61	11	25	0	0	0	0
61	12	13	0	0	2	0
61	13	25	0	0	0	0
61	14	3	0	0	0	0
61	15	24	0	0	0	0
61	16	20	0	0	1	0
61	17	9	0	0	0	0
61	18	27	0	0	0	0
61	19	6	0	0	0	0
61	1A	3290	0	0	64	0
61	1B	108	0	0	5	0
61	1D	113	0	0	3	0
61	1E	82	0	0	4	0
61	1F	64	0	0	4	0
61	1G	20	0	0	0	0
61	1H	15	0	0	0	0
61	1I	7	0	0	0	0
61	1N	54	0	0	0	0
61	1O	23	0	0	0	0
61	1P	53	0	0	1	0
61	1Q	46	0	0	1	0
61	1R	32	0	0	0	0
61	1S	13	0	0	0	0
61	1T	35	0	0	1	0
61	1U	42	0	0	4	0
61	1V	36	0	0	3	0
61	1W	26	0	0	0	0
61	1X	23	0	0	1	0
61	1Y	14	0	0	2	0
61	1Z	13	0	0	1	0
61	1a	343	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6l	1b	1	0	0	0	0
6l	1d	8	0	0	0	0
6l	1e	6	0	0	0	0
6l	1f	3	0	0	0	0
6l	1i	1	0	0	0	0
6l	1j	2	0	0	0	0
6l	1k	1	0	0	0	0
6l	1l	4	0	0	0	0
6l	1o	4	0	0	0	0
6l	1p	3	0	0	0	0
6l	1t	1	0	0	0	0
6l	1y	4	0	0	0	0
6l	20	12	0	0	0	0
6l	21	18	0	0	1	0
6l	22	4	0	0	0	0
6l	23	2	0	0	0	0
6l	24	2	0	0	0	0
6l	25	7	0	0	0	0
6l	26	3	0	0	0	0
6l	27	6	0	0	1	0
6l	28	13	0	0	1	0
6l	29	2	0	0	0	0
6l	2A	1236	0	0	56	0
6l	2B	73	0	0	8	0
6l	2D	50	0	0	3	0
6l	2E	25	0	0	4	0
6l	2F	19	0	0	1	0
6l	2G	8	0	0	1	0
6l	2H	4	0	0	0	0
6l	2I	4	0	0	0	0
6l	2N	5	0	0	0	0
6l	2O	21	0	0	1	0
6l	2P	18	0	0	0	0
6l	2Q	26	0	0	1	0
6l	2R	15	0	0	0	0
6l	2S	5	0	0	2	0
6l	2T	10	0	0	1	0
6l	2U	14	0	0	1	0
6l	2V	6	0	0	0	0
6l	2W	18	0	0	0	0
6l	2X	8	0	0	1	0
6l	2Y	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6l	2Z	12	0	0	3	0
6l	2a	259	0	0	0	0
6l	2d	5	0	0	0	0
6l	2e	2	0	0	0	0
6l	2f	1	0	0	0	0
6l	2j	2	0	0	0	0
6l	2l	1	0	0	0	0
6l	2m	1	0	0	0	0
6l	2o	2	0	0	0	0
6l	2p	1	0	0	0	0
6l	2q	1	0	0	0	0
6l	2r	5	0	0	0	0
6l	2s	1	0	0	0	0
6l	2t	1	0	0	0	0
6l	2u	1	0	0	0	0
6l	2y	1	0	0	0	0
All	All	295545	0	194516	1938	0

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

The worst 5 of 1938 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1128:U:H3	1:1A:1132:A:N6	1.29	1.27
1:1A:2159:C:N4	1:1A:2176:G:H1	1.46	1.12
1:2A:2139:C:N4	1:2A:2152:G:H1	1.51	1.06
29:17:24:THR:HG22	29:17:27:GLY:H	1.28	0.98
1:1A:1128:U:O4	1:1A:1132:A:N1	1.97	0.98

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	258 (94%)	15 (6%)	0	100	100
3	2D	273/276 (99%)	258 (94%)	15 (6%)	0	100	100
4	1E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	29	52
4	2E	202/206 (98%)	191 (95%)	10 (5%)	1 (0%)	29	52
5	1F	201/210 (96%)	194 (96%)	6 (3%)	1 (0%)	29	52
5	2F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	29	52
6	1G	179/182 (98%)	163 (91%)	14 (8%)	2 (1%)	14	30
6	2G	179/182 (98%)	160 (89%)	14 (8%)	5 (3%)	5	7
7	1H	172/180 (96%)	164 (95%)	6 (4%)	2 (1%)	13	27
7	2H	171/180 (95%)	152 (89%)	17 (10%)	2 (1%)	13	27
8	1I	145/148 (98%)	128 (88%)	16 (11%)	1 (1%)	22	43
8	2I	144/148 (97%)	134 (93%)	8 (6%)	2 (1%)	11	22
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
9	2N	138/140 (99%)	134 (97%)	3 (2%)	1 (1%)	22	43
10	1O	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	19	39
10	2O	120/122 (98%)	111 (92%)	7 (6%)	2 (2%)	9	18
11	1P	147/150 (98%)	138 (94%)	9 (6%)	0	100	100
11	2P	147/150 (98%)	140 (95%)	6 (4%)	1 (1%)	22	43
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
12	2Q	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	22	43
13	1R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
13	2R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
14	1S	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	17	35
14	2S	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
15	1T	129/146 (88%)	124 (96%)	3 (2%)	2 (2%)	9	19
15	2T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
17	1V	99/101 (98%)	94 (95%)	3 (3%)	2 (2%)	7	14
17	2V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	15	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	14	30
19	2X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	14	30
20	1Y	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
20	2Y	105/110 (96%)	101 (96%)	3 (3%)	1 (1%)	15	32
21	1Z	201/206 (98%)	191 (95%)	10 (5%)	0	100	100
21	2Z	199/206 (97%)	187 (94%)	12 (6%)	0	100	100
22	10	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
22	20	75/85 (88%)	70 (93%)	5 (7%)	0	100	100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	30
23	21	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	14	30
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
26	14	67/71 (94%)	51 (76%)	13 (19%)	3 (4%)	2	3
26	24	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	1	1
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	196 (86%)	27 (12%)	6 (3%)	5	9
33	2b	229/256 (90%)	200 (87%)	21 (9%)	8 (4%)	3	5
34	1c	204/239 (85%)	186 (91%)	18 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	2c	204/239 (85%)	174 (85%)	26 (13%)	4 (2%)	7	14
35	1d	206/209 (99%)	195 (95%)	10 (5%)	1 (0%)	29	52
35	2d	206/209 (99%)	195 (95%)	11 (5%)	0	100	100
36	1e	146/162 (90%)	140 (96%)	6 (4%)	0	100	100
36	2e	146/162 (90%)	134 (92%)	12 (8%)	0	100	100
37	1f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
37	2f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
38	1g	153/156 (98%)	147 (96%)	5 (3%)	1 (1%)	22	43
38	2g	153/156 (98%)	143 (94%)	9 (6%)	1 (1%)	22	43
39	1h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
39	2h	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
40	1i	125/128 (98%)	108 (86%)	17 (14%)	0	100	100
40	2i	124/128 (97%)	110 (89%)	12 (10%)	2 (2%)	9	19
41	1j	95/105 (90%)	80 (84%)	12 (13%)	3 (3%)	4	6
41	2j	94/105 (90%)	80 (85%)	13 (14%)	1 (1%)	14	30
42	1k	112/129 (87%)	103 (92%)	8 (7%)	1 (1%)	17	35
42	2k	112/129 (87%)	100 (89%)	11 (10%)	1 (1%)	17	35
43	1l	119/132 (90%)	116 (98%)	3 (2%)	0	100	100
43	2l	119/132 (90%)	104 (87%)	15 (13%)	0	100	100
44	1m	114/126 (90%)	101 (89%)	12 (10%)	1 (1%)	17	35
44	2m	112/126 (89%)	100 (89%)	11 (10%)	1 (1%)	17	35
45	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
45	2n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
46	1o	86/89 (97%)	79 (92%)	5 (6%)	2 (2%)	6	11
46	2o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	13	27
47	1p	80/88 (91%)	70 (88%)	10 (12%)	0	100	100
47	2p	80/88 (91%)	73 (91%)	7 (9%)	0	100	100
48	1q	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
48	2q	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
49	1r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
49	2r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	1s	81/93 (87%)	74 (91%)	5 (6%)	2 (2%)	5	9
50	2s	81/93 (87%)	71 (88%)	10 (12%)	0	100	100
51	1t	94/106 (89%)	83 (88%)	8 (8%)	3 (3%)	4	6
51	2t	96/106 (91%)	91 (95%)	2 (2%)	3 (3%)	4	6
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	1 (5%)	1 (5%)	2	2
53	1y	95/113 (84%)	94 (99%)	1 (1%)	0	100	100
53	2y	94/113 (83%)	91 (97%)	3 (3%)	0	100	100
All	All	11629/12354 (94%)	10866 (93%)	678 (6%)	85 (1%)	22	43

5 of 85 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	47	LYS
41	1j	77	PRO
46	1o	19	PRO
4	2E	51	PHE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	214/218 (98%)	194 (91%)	20 (9%)	9	17
3	2D	215/218 (99%)	203 (94%)	12 (6%)	21	42
4	1E	164/166 (99%)	152 (93%)	12 (7%)	14	28
4	2E	164/166 (99%)	151 (92%)	13 (8%)	12	24
5	1F	160/166 (96%)	145 (91%)	15 (9%)	8	17
5	2F	159/166 (96%)	145 (91%)	14 (9%)	10	19
6	1G	144/156 (92%)	135 (94%)	9 (6%)	18	36
6	2G	142/156 (91%)	136 (96%)	6 (4%)	30	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	1H	144/148 (97%)	140 (97%)	4 (3%)	43	69
7	2H	143/148 (97%)	135 (94%)	8 (6%)	21	42
8	1I	111/124 (90%)	104 (94%)	7 (6%)	18	36
8	2I	108/124 (87%)	105 (97%)	3 (3%)	43	69
9	1N	119/119 (100%)	107 (90%)	12 (10%)	7	14
9	2N	118/119 (99%)	114 (97%)	4 (3%)	37	63
10	1O	100/100 (100%)	97 (97%)	3 (3%)	41	67
10	2O	100/100 (100%)	94 (94%)	6 (6%)	19	39
11	1P	115/116 (99%)	111 (96%)	4 (4%)	36	62
11	2P	115/116 (99%)	112 (97%)	3 (3%)	46	72
12	1Q	111/111 (100%)	104 (94%)	7 (6%)	18	36
12	2Q	111/111 (100%)	108 (97%)	3 (3%)	44	71
13	1R	101/101 (100%)	90 (89%)	11 (11%)	6	11
13	2R	101/101 (100%)	93 (92%)	8 (8%)	12	24
14	1S	87/88 (99%)	81 (93%)	6 (7%)	15	31
14	2S	85/88 (97%)	80 (94%)	5 (6%)	19	39
15	1T	115/127 (91%)	109 (95%)	6 (5%)	23	46
15	2T	113/127 (89%)	108 (96%)	5 (4%)	28	53
16	1U	93/94 (99%)	88 (95%)	5 (5%)	22	44
16	2U	93/94 (99%)	87 (94%)	6 (6%)	17	34
17	1V	81/82 (99%)	74 (91%)	7 (9%)	10	20
17	2V	80/82 (98%)	75 (94%)	5 (6%)	18	36
18	1W	90/92 (98%)	80 (89%)	10 (11%)	6	11
18	2W	90/92 (98%)	83 (92%)	7 (8%)	12	25
19	1X	77/78 (99%)	74 (96%)	3 (4%)	32	58
19	2X	77/78 (99%)	74 (96%)	3 (4%)	32	58
20	1Y	86/91 (94%)	80 (93%)	6 (7%)	15	30
20	2Y	86/91 (94%)	82 (95%)	4 (5%)	26	50
21	1Z	169/179 (94%)	156 (92%)	13 (8%)	13	25
21	2Z	165/179 (92%)	156 (94%)	9 (6%)	21	43
22	10	61/67 (91%)	58 (95%)	3 (5%)	25	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	20	61/67 (91%)	57 (93%)	4 (7%)	16	33
23	11	79/83 (95%)	77 (98%)	2 (2%)	47	73
23	21	81/83 (98%)	76 (94%)	5 (6%)	18	37
24	12	65/67 (97%)	64 (98%)	1 (2%)	65	83
24	22	66/67 (98%)	61 (92%)	5 (8%)	13	26
25	13	51/52 (98%)	48 (94%)	3 (6%)	19	39
25	23	50/52 (96%)	48 (96%)	2 (4%)	31	57
26	14	58/63 (92%)	56 (97%)	2 (3%)	37	63
26	24	54/63 (86%)	53 (98%)	1 (2%)	57	79
27	15	51/52 (98%)	47 (92%)	4 (8%)	12	25
27	25	50/52 (96%)	48 (96%)	2 (4%)	31	57
28	16	51/52 (98%)	45 (88%)	6 (12%)	5	9
28	26	50/52 (96%)	47 (94%)	3 (6%)	19	39
29	17	41/42 (98%)	37 (90%)	4 (10%)	8	15
29	27	41/42 (98%)	38 (93%)	3 (7%)	14	28
30	18	54/55 (98%)	49 (91%)	5 (9%)	9	17
30	28	54/55 (98%)	51 (94%)	3 (6%)	21	42
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	33 (97%)	1 (3%)	42	68
33	1b	191/220 (87%)	182 (95%)	9 (5%)	26	50
33	2b	187/220 (85%)	178 (95%)	9 (5%)	25	49
34	1c	144/188 (77%)	135 (94%)	9 (6%)	18	36
34	2c	140/188 (74%)	133 (95%)	7 (5%)	24	47
35	1d	171/181 (94%)	159 (93%)	12 (7%)	15	30
35	2d	172/181 (95%)	160 (93%)	12 (7%)	15	30
36	1e	114/123 (93%)	110 (96%)	4 (4%)	36	62
36	2e	114/123 (93%)	109 (96%)	5 (4%)	28	53
37	1f	85/90 (94%)	80 (94%)	5 (6%)	19	39
37	2f	85/90 (94%)	83 (98%)	2 (2%)	49	74
38	1g	120/127 (94%)	117 (98%)	3 (2%)	47	73
38	2g	119/127 (94%)	116 (98%)	3 (2%)	47	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	1h	116/119 (98%)	112 (97%)	4 (3%)	37	63
39	2h	114/119 (96%)	105 (92%)	9 (8%)	12	24
40	1i	91/99 (92%)	86 (94%)	5 (6%)	21	43
40	2i	88/99 (89%)	86 (98%)	2 (2%)	50	75
41	1j	68/92 (74%)	65 (96%)	3 (4%)	28	53
41	2j	68/92 (74%)	65 (96%)	3 (4%)	28	53
42	1k	83/99 (84%)	83 (100%)	0	100	100
42	2k	83/99 (84%)	76 (92%)	7 (8%)	11	21
43	1l	96/108 (89%)	92 (96%)	4 (4%)	30	55
43	2l	96/108 (89%)	94 (98%)	2 (2%)	53	77
44	1m	90/101 (89%)	86 (96%)	4 (4%)	28	53
44	2m	87/101 (86%)	83 (95%)	4 (5%)	27	51
45	1n	49/50 (98%)	48 (98%)	1 (2%)	55	78
45	2n	49/50 (98%)	47 (96%)	2 (4%)	30	56
46	1o	78/80 (98%)	75 (96%)	3 (4%)	33	59
46	2o	78/80 (98%)	77 (99%)	1 (1%)	69	86
47	1p	69/74 (93%)	64 (93%)	5 (7%)	14	29
47	2p	68/74 (92%)	63 (93%)	5 (7%)	13	28
48	1q	94/97 (97%)	89 (95%)	5 (5%)	22	45
48	2q	94/97 (97%)	92 (98%)	2 (2%)	53	77
49	1r	59/77 (77%)	57 (97%)	2 (3%)	37	63
49	2r	59/77 (77%)	56 (95%)	3 (5%)	24	46
50	1s	68/80 (85%)	65 (96%)	3 (4%)	28	53
50	2s	67/80 (84%)	64 (96%)	3 (4%)	27	52
51	1t	71/82 (87%)	68 (96%)	3 (4%)	30	55
51	2t	70/82 (85%)	66 (94%)	4 (6%)	20	41
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
53	1y	82/98 (84%)	82 (100%)	0	100	100
53	2y	79/98 (81%)	77 (98%)	2 (2%)	47	73
All	All	9524/10260 (93%)	9010 (95%)	514 (5%)	22	44

5 of 514 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	1h	26	VAL
4	2E	12	THR
40	2i	102	LEU
40	1i	111	ARG
48	1q	45	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 104 such sidechains are listed below:

Mol	Chain	Res	Type
48	1q	16	GLN
7	2H	74	ASN
41	2j	68	HIS
50	1s	69	HIS
3	2D	126	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2862/2915 (98%)	396 (13%)	30 (1%)
1	2A	2855/2915 (97%)	475 (16%)	38 (1%)
2	1B	119/121 (98%)	12 (10%)	0
2	2B	119/121 (98%)	16 (13%)	0
32	1a	1494/1521 (98%)	234 (15%)	0
32	2a	1498/1521 (98%)	255 (17%)	0
All	All	8947/9114 (98%)	1388 (15%)	68 (0%)

5 of 1388 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	34	C
1	1A	45	C
1	1A	54	G
1	1A	70	A
1	1A	73	A

5 of 68 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	9	U

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Mol	Chain	Res	Type
1	2A	645	C
1	2A	2321	G
1	2A	195	A
1	2A	266	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
32	M2G	2a	966	32,54	20,27,28	1.47	3 (15%)	22,40,43	2.20	6 (27%)
1	2MA	1A	2515	1,54	17,25,26	1.23	2 (11%)	19,37,40	2.04	3 (15%)
32	5MC	1a	1404	32	15,22,23	1.30	1 (6%)	19,32,35	1.18	2 (10%)
32	PSU	1a	516	32,54	17,21,22	1.42	3 (17%)	20,30,33	3.06	6 (30%)
1	2MA	2A	2503	1,54	17,25,26	1.29	2 (11%)	19,37,40	2.00	3 (15%)
1	5MU	2A	1939	1	15,22,23	1.20	2 (13%)	16,32,35	1.74	2 (12%)
32	UR3	2a	1498	32,54	14,22,23	0.73	0	15,32,35	0.69	0
32	2MG	2a	1207	32	19,26,27	1.26	2 (10%)	21,38,41	2.09	6 (28%)
32	UR3	1a	1498	32	14,22,23	0.70	0	15,32,35	0.64	0
43	0TD	2l	92	43	4,9,10	3.04	1 (25%)	3,11,13	2.92	1 (33%)
32	MA6	2a	1518	32	19,26,27	1.04	1 (5%)	18,38,41	1.70	6 (33%)
32	MA6	1a	1519	32	19,26,27	1.06	1 (5%)	18,38,41	1.62	4 (22%)
32	5MC	2a	1407	32	15,22,23	1.31	1 (6%)	19,32,35	1.40	2 (10%)
1	5MC	2A	1962	1,54	15,22,23	1.26	1 (6%)	19,32,35	1.38	3 (15%)
32	4OC	1a	1402	32	16,23,24	0.64	0	17,32,35	1.80	1 (5%)
1	4OC	2A	1920	1	15,22,24	0.70	0	17,31,35	1.29	1 (5%)
32	5MC	1a	967	32	15,22,23	1.30	1 (6%)	19,32,35	1.33	3 (15%)
1	OMG	2A	2251	1,54	18,26,27	1.20	2 (11%)	20,38,41	2.20	6 (30%)
32	MA6	1a	1518	32	19,26,27	1.01	1 (5%)	18,38,41	1.64	5 (27%)
1	OMG	1A	2263	1,54	18,26,27	1.24	2 (11%)	20,38,41	2.43	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	PSU	2a	516	32,54	17,21,22	1.59	3 (17%)	20,30,33	3.11	6 (30%)
32	5MC	1a	1400	32	15,22,23	1.33	1 (6%)	19,32,35	1.38	3 (15%)
1	5MU	2A	1915	1	15,22,23	1.07	1 (6%)	16,32,35	2.05	1 (6%)
1	5MU	1A	1961	1,54	15,22,23	0.99	1 (6%)	16,32,35	1.88	2 (12%)
1	PSU	2A	1911	1	17,21,22	1.45	2 (11%)	20,30,33	2.99	6 (30%)
32	5MC	2a	967	32	15,22,23	1.52	1 (6%)	19,32,35	1.28	2 (10%)
1	PSU	2A	2605	1	17,21,22	1.64	3 (17%)	20,30,33	3.18	6 (30%)
1	5MC	1A	1984	1,54	15,22,23	1.39	1 (6%)	19,32,35	1.22	3 (15%)
1	PSU	1A	1939	1	17,21,22	1.50	3 (17%)	20,30,33	3.09	6 (30%)
32	7MG	1a	527	32	22,26,27	1.77	4 (18%)	28,39,42	2.72	9 (32%)
32	5MC	1a	1407	32	15,22,23	1.38	1 (6%)	19,32,35	1.22	1 (5%)
32	MA6	2a	1519	32	19,26,27	1.02	1 (5%)	18,38,41	1.88	5 (27%)
32	2MG	1a	1207	32	19,26,27	1.27	2 (10%)	21,38,41	2.63	10 (47%)
1	PSU	2A	1917	1	17,21,22	1.46	3 (17%)	20,30,33	3.11	6 (30%)
43	0TD	1l	92	43	4,9,10	3.16	1 (25%)	3,11,13	5.45	1 (33%)
32	7MG	2a	527	32	22,26,27	1.76	4 (18%)	28,39,42	2.66	8 (28%)
32	4OC	2a	1402	32	16,23,24	0.65	0	17,32,35	1.53	1 (5%)
1	PSU	1A	2617	1	17,21,22	1.70	3 (17%)	20,30,33	3.30	6 (30%)
1	2MU	1A	2564	1,54	14,22,24	0.90	1 (7%)	14,31,36	0.95	1 (7%)
1	5MU	1A	1937	1	15,22,23	1.10	1 (6%)	16,32,35	1.92	1 (6%)
1	4OC	1A	1942	1	15,22,24	0.67	0	17,31,35	1.45	2 (11%)
1	5MC	1A	1964	1	15,22,23	1.28	1 (6%)	19,32,35	1.25	3 (15%)
32	M2G	1a	966	32	20,27,28	1.32	3 (15%)	22,40,43	2.14	5 (22%)
32	5MC	2a	1400	32	15,22,23	1.31	1 (6%)	19,32,35	1.45	3 (15%)
1	PSU	1A	1933	1	17,21,22	1.51	3 (17%)	20,30,33	3.07	7 (35%)
1	5MC	2A	1942	1	15,22,23	1.36	1 (6%)	19,32,35	1.35	3 (15%)
32	5MC	2a	1404	32	15,22,23	1.37	1 (6%)	19,32,35	1.31	3 (15%)
1	2MU	2A	2552	1,54	14,22,24	0.95	0	14,31,36	0.88	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	M2G	2a	966	32,54	-	0/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MA	1A	2515	1,54	-	2/3/25/26	0/3/3/3
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2
32	PSU	1a	516	32,54	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,54	-	1/3/25/26	0/3/3/3
1	5MU	2A	1939	1	-	0/5/25/26	0/2/2/2
32	UR3	2a	1498	32,54	-	0/5/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
32	UR3	1a	1498	32	-	0/5/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/3/12/14	-
32	MA6	2a	1518	32	-	1/7/29/30	0/3/3/3
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
32	5MC	2a	1407	32	-	0/5/25/26	0/2/2/2
1	5MC	2A	1962	1,54	-	2/5/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
1	4OC	2A	1920	1	-	1/7/27/30	0/2/2/2
32	5MC	1a	967	32	-	0/5/25/26	0/2/2/2
1	OMG	2A	2251	1,54	-	0/5/27/28	0/3/3/3
32	MA6	1a	1518	32	-	2/7/29/30	0/3/3/3
1	OMG	1A	2263	1,54	-	0/5/27/28	0/3/3/3
32	PSU	2a	516	32,54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/5/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/5/25/26	0/2/2/2
1	5MU	1A	1961	1,54	-	0/5/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/5/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1984	1,54	-	2/5/25/26	0/2/2/2
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	32	-	1/7/37/38	0/3/3/3
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
32	MA6	2a	1519	32	-	4/7/29/30	0/3/3/3
32	2MG	1a	1207	32	-	4/5/27/28	0/3/3/3
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/3/12/14	-
32	7MG	2a	527	32	-	1/7/37/38	0/3/3/3
32	4OC	2a	1402	32	-	4/9/29/30	0/2/2/2
1	PSU	1A	2617	1	-	0/7/25/26	0/2/2/2
1	2MU	1A	2564	1,54	-	0/7/27/28	0/2/2/2
1	5MU	1A	1937	1	-	0/5/25/26	0/2/2/2
1	4OC	1A	1942	1	-	2/7/27/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	1A	1964	1	-	0/5/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	2a	1400	32	-	2/5/25/26	0/2/2/2
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/5/25/26	0/2/2/2
1	2MU	2A	2552	1,54	-	0/7/27/28	0/2/2/2

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-6.07	1.69	1.84
43	2l	92	0TD	CB-SB	-5.79	1.70	1.84
32	2a	967	5MC	C5-C4	5.48	1.49	1.41
32	2a	527	7MG	C6-C5	5.04	1.48	1.41
1	1A	2617	PSU	C5-C1'	-4.99	1.48	1.52

The worst 5 of 176 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-9.35	83.46	101.85
32	1a	527	7MG	N3-C4-N9	8.99	138.46	126.91
1	1A	2617	PSU	N1-C2-N3	-8.92	121.34	128.43
1	2A	2605	PSU	N1-C2-N3	-8.91	121.35	128.43
1	1A	1939	PSU	N1-C2-N3	-8.82	121.42	128.43

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	2l	92	0TD	CG-CB-SB-CSB
1	1A	1984	5MC	O4'-C1'-N1-C6
1	1A	1984	5MC	C2'-C1'-N1-C6
1	2A	1962	5MC	O4'-C1'-N1-C6
1	2A	1962	5MC	C2'-C1'-N1-C6

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	1920	4OC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	1911	PSU	1	0
1	2A	1917	PSU	2	0
1	1A	1942	4OC	1	0
1	2A	2552	2MU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2456 ligands modelled in this entry, 2443 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
57	MPD	1a	1860	-	7,7,7	0.40	0	9,10,10	0.46	0
57	MPD	2B	222	-	7,7,7	0.32	0	9,10,10	0.19	0
60	SF4	2d	302	35	0,12,12	0.00	-	-	-	-
57	MPD	18	102	-	7,7,7	0.30	0	9,10,10	0.47	0
57	MPD	1A	4036	-	7,7,7	0.31	0	9,10,10	0.20	0
60	SF4	1d	501	35	0,12,12	0.00	-	-	-	-
57	MPD	2A	3692	-	7,7,7	0.34	0	9,10,10	0.33	0
56	EZM	2A	3691	-	23,24,24	3.10	3 (13%)	28,31,31	0.74	1 (3%)
56	EZM	1A	4035	-	23,24,24	1.95	3 (13%)	28,31,31	1.16	2 (7%)
57	MPD	1T	205	-	7,7,7	0.30	0	9,10,10	0.14	0
57	MPD	2A	3693	-	7,7,7	0.32	0	9,10,10	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	EZM	2A	3691	-	-	4/25/27/27	0/1/1/1
57	MPD	2B	222	-	-	2/5/5/5	-
60	SF4	2d	302	35	-	-	0/6/5/5
57	MPD	18	102	-	-	0/5/5/5	-
57	MPD	1A	4036	-	-	1/5/5/5	-
60	SF4	1d	501	35	-	-	0/6/5/5
57	MPD	2A	3692	-	-	0/5/5/5	-
57	MPD	1a	1860	-	-	2/5/5/5	-
56	EZM	1A	4035	-	-	4/25/27/27	0/1/1/1
57	MPD	1T	205	-	-	0/5/5/5	-
57	MPD	2A	3693	-	-	1/5/5/5	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2A	3691	EZM	OAC-NAY	11.74	1.42	1.22
56	2A	3691	EZM	CAT-CAW	-7.83	1.40	1.51
56	1A	4035	EZM	CAT-CAW	-7.35	1.41	1.51
56	1A	4035	EZM	CAU-NAY	-4.52	1.34	1.45
56	2A	3691	EZM	CAU-NAY	-4.38	1.34	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1A	4035	EZM	CAT-CAW-CAX	4.27	119.17	111.64
56	1A	4035	EZM	CAI-CAU-NAY	2.10	120.96	119.38
56	2A	3691	EZM	CAX-NAP-C	-2.06	119.43	123.07

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

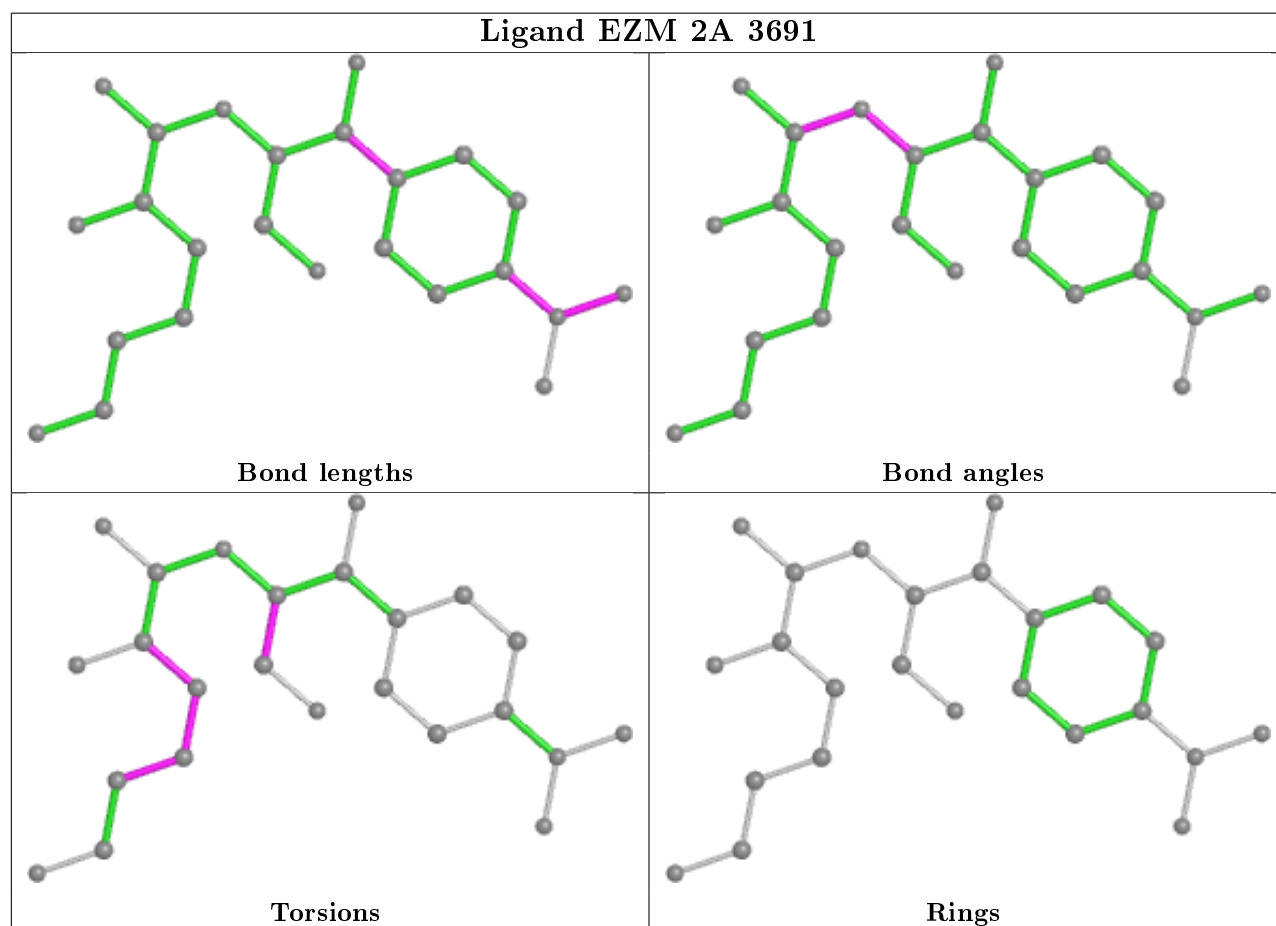
Mol	Chain	Res	Type	Atoms
57	1a	1860	MPD	C2-C3-C4-O4
56	1A	4035	EZM	CE-CD-CG-CB
56	1A	4035	EZM	CA-CB-CG-CD
56	2A	3691	EZM	CA-CB-CG-CD
56	2A	3691	EZM	OAD-CAM-CAX-CAW

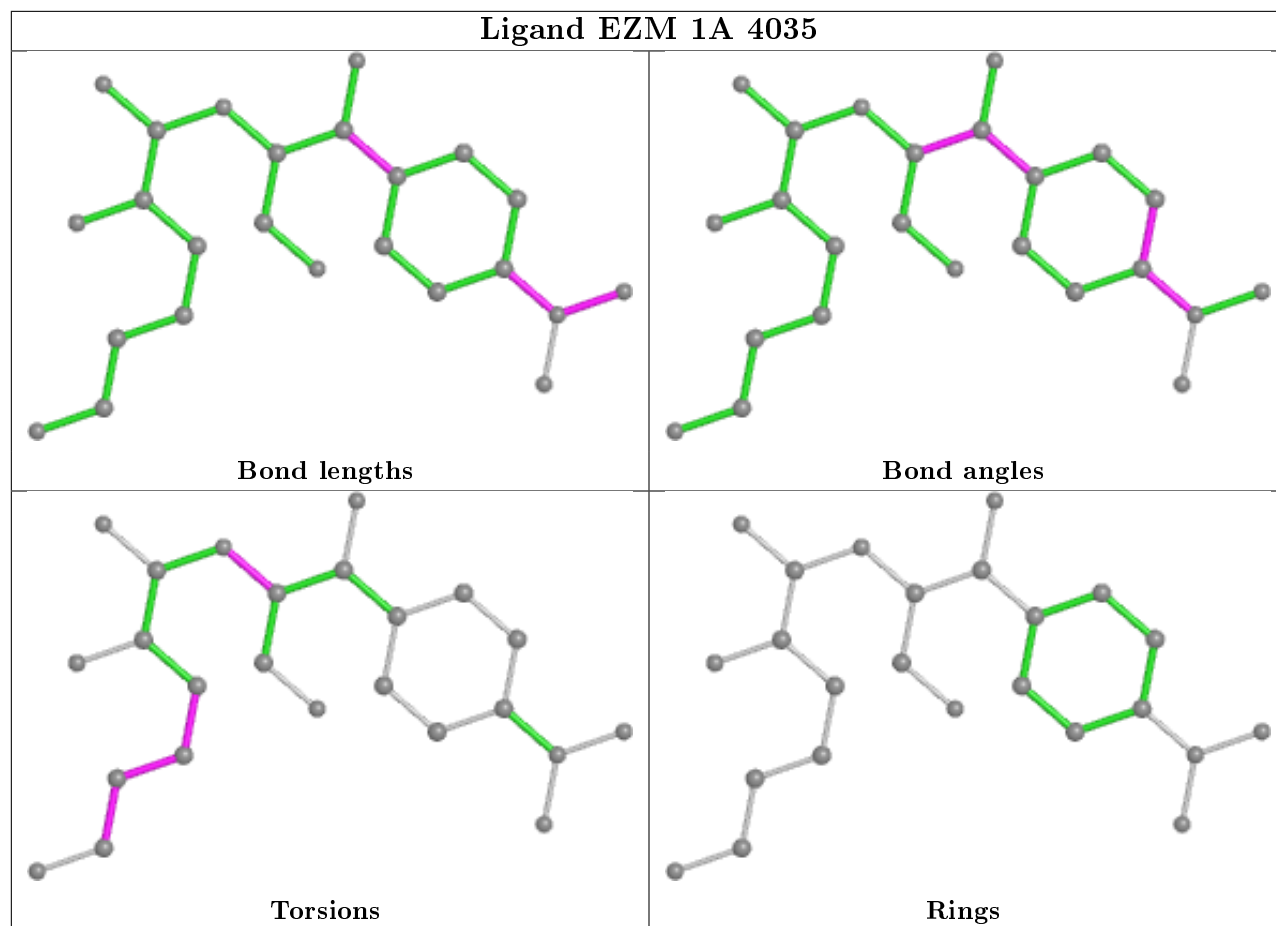
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	2A	3692	MPD	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2861/2915 (98%)	0.31	55 (1%) 66 62	16, 32, 88, 100	0
1	2A	2856/2915 (97%)	0.11	68 (2%) 59 53	28, 52, 90, 101	0
2	1B	120/121 (99%)	-0.05	0 100 100	27, 46, 60, 76	0
2	2B	120/121 (99%)	-0.21	0 100 100	56, 74, 82, 87	0
3	1D	275/276 (99%)	0.45	1 (0%) 92 91	19, 34, 48, 67	0
3	2D	275/276 (99%)	0.51	5 (1%) 68 64	29, 47, 60, 75	0
4	1E	204/206 (99%)	0.36	0 100 100	16, 35, 56, 69	0
4	2E	204/206 (99%)	0.34	3 (1%) 73 70	31, 51, 68, 74	0
5	1F	203/210 (96%)	0.29	0 100 100	17, 38, 66, 81	0
5	2F	203/210 (96%)	0.13	0 100 100	30, 60, 74, 83	0
6	1G	181/182 (99%)	-0.00	0 100 100	44, 57, 72, 81	0
6	2G	181/182 (99%)	0.52	11 (6%) 21 16	69, 77, 83, 89	0
7	1H	174/180 (96%)	0.10	0 100 100	34, 49, 62, 67	0
7	2H	173/180 (96%)	0.70	13 (7%) 14 10	63, 75, 81, 86	0
8	1I	147/148 (99%)	-0.01	0 100 100	37, 67, 77, 84	0
8	2I	146/148 (98%)	0.21	9 (6%) 20 15	53, 70, 79, 82	0
9	1N	140/140 (100%)	0.28	0 100 100	22, 34, 55, 71	0
9	2N	140/140 (100%)	0.31	2 (1%) 75 71	41, 59, 71, 79	0
10	1O	122/122 (100%)	0.38	0 100 100	25, 36, 55, 61	0
10	2O	122/122 (100%)	0.19	0 100 100	40, 51, 65, 70	0
11	1P	149/150 (99%)	0.18	1 (0%) 87 86	17, 40, 60, 74	0
11	2P	149/150 (99%)	0.38	4 (2%) 54 48	33, 62, 76, 80	0
12	1Q	141/141 (100%)	0.25	0 100 100	24, 36, 48, 66	0
12	2Q	141/141 (100%)	0.42	5 (3%) 44 36	38, 58, 69, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.37	0 100 100	23, 32, 45, 53	0
13	2R	118/118 (100%)	0.29	0 100 100	34, 48, 59, 67	0
14	1S	110/112 (98%)	0.09	0 100 100	35, 47, 59, 66	0
14	2S	110/112 (98%)	0.45	11 (10%) 7 4	59, 70, 76, 80	0
15	1T	131/146 (89%)	0.23	0 100 100	30, 41, 64, 74	0
15	2T	131/146 (89%)	0.30	2 (1%) 73 70	45, 55, 71, 77	0
16	1U	116/118 (98%)	0.38	0 100 100	19, 26, 40, 57	0
16	2U	116/118 (98%)	0.33	0 100 100	35, 53, 68, 78	0
17	1V	101/101 (100%)	0.22	0 100 100	20, 36, 53, 61	0
17	2V	101/101 (100%)	0.18	0 100 100	35, 64, 73, 76	0
18	1W	112/113 (99%)	0.33	0 100 100	21, 27, 47, 77	0
18	2W	112/113 (99%)	0.39	0 100 100	35, 45, 63, 79	0
19	1X	95/96 (98%)	0.33	0 100 100	24, 35, 60, 69	0
19	2X	95/96 (98%)	0.55	4 (4%) 36 29	44, 56, 70, 77	0
20	1Y	107/110 (97%)	0.16	0 100 100	33, 45, 62, 70	0
20	2Y	107/110 (97%)	0.49	4 (3%) 41 34	54, 64, 74, 80	0
21	1Z	203/206 (98%)	0.06	1 (0%) 91 89	33, 53, 68, 78	0
21	2Z	201/206 (97%)	0.26	7 (3%) 44 36	60, 71, 78, 83	0
22	10	77/85 (90%)	0.31	0 100 100	24, 33, 49, 58	0
22	20	77/85 (90%)	0.80	9 (11%) 4 3	45, 57, 67, 72	0
23	11	97/98 (98%)	0.55	3 (3%) 49 42	25, 40, 62, 70	0
23	21	97/98 (98%)	0.69	3 (3%) 49 42	37, 52, 70, 73	0
24	12	70/72 (97%)	0.14	0 100 100	34, 46, 57, 79	0
24	22	70/72 (97%)	0.26	0 100 100	52, 65, 71, 74	0
25	13	59/60 (98%)	0.36	0 100 100	22, 32, 57, 67	0
25	23	59/60 (98%)	0.51	2 (3%) 45 38	47, 56, 70, 78	0
26	14	69/71 (97%)	-0.01	3 (4%) 35 28	52, 70, 83, 89	0
26	24	69/71 (97%)	0.69	10 (14%) 2 1	75, 82, 87, 92	0
27	15	59/60 (98%)	0.40	0 100 100	18, 28, 44, 57	0
27	25	59/60 (98%)	0.26	0 100 100	29, 46, 59, 68	0
28	16	53/54 (98%)	0.11	0 100 100	27, 38, 52, 58	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.23	0 100 100	50, 56, 65, 68	0
29	17	48/49 (97%)	0.59	4 (8%) 11 8	15, 25, 53, 61	0
29	27	48/49 (97%)	0.69	2 (4%) 36 29	28, 38, 58, 67	0
30	18	64/65 (98%)	0.42	1 (1%) 72 68	24, 31, 38, 53	0
30	28	64/65 (98%)	0.76	2 (3%) 49 42	42, 51, 59, 66	0
31	19	37/37 (100%)	0.35	0 100 100	25, 36, 52, 55	0
31	29	37/37 (100%)	0.94	4 (10%) 5 3	53, 60, 70, 72	0
32	1a	1488/1521 (97%)	-0.04	24 (1%) 72 68	34, 63, 87, 100	0
32	2a	1492/1521 (98%)	0.13	40 (2%) 54 48	42, 72, 89, 98	0
33	1b	231/256 (90%)	0.55	19 (8%) 11 8	58, 73, 82, 86	0
33	2b	231/256 (90%)	0.88	38 (16%) 1 1	68, 79, 84, 89	0
34	1c	206/239 (86%)	0.53	9 (4%) 34 27	56, 68, 77, 82	0
34	2c	206/239 (86%)	1.07	44 (21%) 0 0	68, 77, 82, 84	0
35	1d	208/209 (99%)	0.38	10 (4%) 30 24	51, 66, 75, 82	0
35	2d	208/209 (99%)	0.73	17 (8%) 11 8	57, 67, 76, 81	0
36	1e	148/162 (91%)	0.37	3 (2%) 65 60	45, 60, 69, 76	0
36	2e	148/162 (91%)	0.62	12 (8%) 12 8	55, 68, 75, 86	0
37	1f	100/101 (99%)	0.15	0 100 100	47, 62, 70, 74	0
37	2f	100/101 (99%)	-0.04	0 100 100	52, 64, 72, 77	0
38	1g	155/156 (99%)	0.24	4 (2%) 56 50	57, 66, 74, 81	0
38	2g	155/156 (99%)	0.62	17 (10%) 5 3	67, 74, 80, 84	0
39	1h	137/138 (99%)	0.41	2 (1%) 73 70	51, 63, 70, 75	0
39	2h	137/138 (99%)	0.61	9 (6%) 18 13	60, 69, 74, 79	0
40	1i	127/128 (99%)	0.74	13 (10%) 6 4	58, 72, 80, 82	0
40	2i	126/128 (98%)	2.01	62 (49%) 0 0	70, 79, 83, 85	0
41	1j	97/105 (92%)	0.73	9 (9%) 8 6	54, 73, 82, 84	0
41	2j	96/105 (91%)	1.57	35 (36%) 0 0	71, 80, 85, 87	0
42	1k	114/129 (88%)	0.30	1 (0%) 84 82	41, 60, 69, 74	0
42	2k	114/129 (88%)	0.55	4 (3%) 44 36	52, 66, 76, 82	0
43	1l	121/132 (91%)	0.26	2 (1%) 70 66	44, 55, 67, 72	0
43	2l	121/132 (91%)	0.53	11 (9%) 9 6	53, 62, 70, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/126 (92%)	0.06	3 (2%) 56 50	53, 68, 74, 77	0
44	2m	114/126 (90%)	0.81	17 (14%) 2 1	71, 79, 83, 84	0
45	1n	60/61 (98%)	1.09	7 (11%) 4 3	55, 65, 74, 81	0
45	2n	60/61 (98%)	2.33	35 (58%) 0 0	71, 77, 82, 86	0
46	1o	88/89 (98%)	0.32	2 (2%) 60 54	43, 61, 71, 77	0
46	2o	88/89 (98%)	0.57	2 (2%) 60 54	55, 67, 76, 81	0
47	1p	82/88 (93%)	0.57	0 100 100	58, 66, 76, 82	0
47	2p	82/88 (93%)	0.38	1 (1%) 79 76	56, 65, 74, 78	0
48	1q	99/105 (94%)	0.56	5 (5%) 28 22	53, 63, 70, 73	0
48	2q	99/105 (94%)	0.54	4 (4%) 38 31	55, 64, 73, 77	0
49	1r	68/88 (77%)	0.21	1 (1%) 73 70	53, 59, 72, 79	0
49	2r	68/88 (77%)	0.23	1 (1%) 73 70	57, 67, 75, 79	0
50	1s	83/93 (89%)	-0.04	0 100 100	61, 70, 78, 80	0
50	2s	83/93 (89%)	1.64	30 (36%) 0 0	73, 81, 85, 87	0
51	1t	96/106 (90%)	0.74	11 (11%) 4 3	56, 67, 75, 80	0
51	2t	98/106 (92%)	0.43	3 (3%) 49 42	54, 65, 76, 79	0
52	1u	23/27 (85%)	0.94	2 (8%) 10 7	59, 66, 70, 74	0
52	2u	23/27 (85%)	1.91	10 (43%) 0 0	71, 75, 79, 80	0
53	1y	97/113 (85%)	0.68	5 (5%) 27 21	46, 56, 69, 74	0
53	2y	96/113 (84%)	2.31	57 (59%) 0 0	61, 72, 79, 82	0
All	All	20766/21468 (96%)	0.33	830 (3%) 38 31	15, 59, 82, 101	0

The worst 5 of 830 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	2a	1030(B)	C	8.3
44	2m	102	ARG	7.6
1	1A	1122	C	7.4
1	1A	1137	G	7.2
32	2a	1030(A)	G	7.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	2MG	2a	1207	24/25	0.88	0.24	77,83,87,100	0
43	0TD	2l	92	10/11	0.89	0.23	60,63,68,89	0
43	0TD	1l	92	10/11	0.89	0.27	50,56,62,88	0
1	PSU	1A	1939	20/21	0.90	0.15	56,69,73,74	0
32	5MC	2a	967	21/22	0.90	0.19	62,69,79,81	0
1	5MU	1A	1937	21/22	0.90	0.16	71,76,82,90	0
1	PSU	2A	1917	20/21	0.91	0.15	70,76,84,90	0
1	5MU	2A	1915	21/22	0.91	0.17	75,81,84,94	0
1	PSU	2A	1911	20/21	0.91	0.13	64,69,79,81	0
32	M2G	2a	966	25/26	0.93	0.17	56,67,80,85	0
1	PSU	1A	1933	20/21	0.93	0.15	50,63,66,67	0
32	PSU	2a	516	20/21	0.94	0.13	67,74,77,80	0
32	2MG	1a	1207	24/25	0.94	0.16	65,69,74,76	0
1	4OC	2A	1920	21/23	0.95	0.17	60,65,71,73	0
32	MA6	2a	1518	24/25	0.95	0.18	55,61,65,67	0
32	7MG	2a	527	24/25	0.95	0.17	57,65,68,69	0
32	5MC	2a	1404	21/22	0.95	0.22	55,61,64,66	0
32	4OC	2a	1402	22/23	0.96	0.21	52,64,68,71	0
32	MA6	2a	1519	24/25	0.96	0.26	53,59,64,65	0
32	5MC	1a	967	21/22	0.96	0.19	50,57,65,68	0
32	5MC	2a	1400	21/22	0.96	0.24	62,68,71,75	0
32	5MC	2a	1407	21/22	0.96	0.15	55,62,65,71	0
32	PSU	1a	516	20/21	0.96	0.19	51,59,63,64	0
32	MA6	1a	1518	24/25	0.97	0.26	38,43,50,53	0
1	5MC	2A	1962	21/22	0.97	0.16	39,43,54,60	0
32	7MG	1a	527	24/25	0.97	0.18	44,50,54,62	0
32	5MC	1a	1407	21/22	0.97	0.20	41,50,54,58	0
1	4OC	1A	1942	21/23	0.97	0.21	42,56,60,62	0
32	M2G	1a	966	25/26	0.97	0.21	49,53,58,62	0
32	UR3	1a	1498	21/22	0.97	0.20	41,47,51,62	0
32	MA6	1a	1519	24/25	0.97	0.23	39,43,47,48	0
32	UR3	2a	1498	21/22	0.97	0.21	56,60,64,69	0
1	PSU	1A	2617	20/21	0.98	0.20	20,24,29,31	0
1	2MA	2A	2503	23/24	0.98	0.21	30,33,38,39	0
1	PSU	2A	2605	20/21	0.98	0.22	31,37,45,51	0
1	OMG	2A	2251	24/25	0.98	0.22	31,36,38,41	0
1	5MU	2A	1939	21/22	0.98	0.20	31,36,39,43	0
32	5MC	1a	1404	21/22	0.98	0.17	35,42,46,47	0
32	4OC	1a	1402	22/23	0.98	0.17	46,49,51,56	0
32	5MC	1a	1400	21/22	0.98	0.20	41,49,53,54	0
1	5MC	2A	1942	21/22	0.98	0.18	41,50,55,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	5MC	1A	1984	21/22	0.98	0.20	27,32,39,45	0
1	2MU	2A	2552	21/23	0.98	0.20	33,37,42,43	0
1	2MU	1A	2564	21/23	0.99	0.23	23,27,31,31	0
1	2MA	1A	2515	23/24	0.99	0.22	14,20,22,24	0
1	OMG	1A	2263	24/25	0.99	0.20	18,21,23,26	0
1	5MC	1A	1964	21/22	0.99	0.18	30,36,40,42	0
1	5MU	1A	1961	21/22	0.99	0.19	19,25,28,30	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3986	1/1	0.33	0.16	99,99,99,99	0
54	MG	2B	202	1/1	0.34	0.32	93,93,93,93	0
54	MG	1A	3970	1/1	0.35	0.65	73,73,73,73	0
54	MG	2a	1777	1/1	0.38	0.22	85,85,85,85	0
54	MG	1a	1837	1/1	0.39	0.12	58,58,58,58	0
54	MG	2A	3633	1/1	0.39	0.23	66,66,66,66	0
54	MG	1a	1807	1/1	0.42	0.28	76,76,76,76	0
54	MG	2B	220	1/1	0.42	0.22	81,81,81,81	0
54	MG	2A	3627	1/1	0.43	0.19	76,76,76,76	0
54	MG	2A	3661	1/1	0.44	0.19	89,89,89,89	0
54	MG	2G	3001	1/1	0.47	0.14	80,80,80,80	0
54	MG	1a	1825	1/1	0.48	0.20	64,64,64,64	0
54	MG	1A	3807	1/1	0.49	0.20	58,58,58,58	0
54	MG	2a	1618	1/1	0.50	0.22	65,65,65,65	0
54	MG	1a	1755	1/1	0.52	0.22	73,73,73,73	0
54	MG	1a	1743	1/1	0.53	0.22	81,81,81,81	0
54	MG	1B	207	1/1	0.54	0.25	65,65,65,65	0
54	MG	1A	3953	1/1	0.54	0.23	84,84,84,84	0
54	MG	1A	3949	1/1	0.55	0.17	72,72,72,72	0
54	MG	2a	1758	1/1	0.55	0.13	89,89,89,89	0
54	MG	1A	3995	1/1	0.56	0.14	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2a	1752	1/1	0.56	0.12	72,72,72,72	0
54	MG	2A	3436	1/1	0.57	0.24	76,76,76,76	0
54	MG	1A	3900	1/1	0.57	0.53	51,51,51,51	0
54	MG	1A	3987	1/1	0.58	0.24	78,78,78,78	0
54	MG	2Q	3003	1/1	0.58	0.13	63,63,63,63	0
54	MG	1A	3513	1/1	0.58	0.10	61,61,61,61	0
54	MG	2a	1765	1/1	0.58	0.15	78,78,78,78	0
54	MG	2A	3677	1/1	0.59	0.30	74,74,74,74	0
54	MG	2A	3387	1/1	0.59	0.21	56,56,56,56	0
54	MG	1E	303	1/1	0.59	0.17	65,65,65,65	0
54	MG	1A	3930	1/1	0.60	0.11	74,74,74,74	0
54	MG	2A	3261	1/1	0.60	0.32	71,71,71,71	0
54	MG	2a	1603	1/1	0.60	0.25	69,69,69,69	0
54	MG	2A	3646	1/1	0.62	0.11	72,72,72,72	0
54	MG	2a	1653	1/1	0.63	0.17	66,66,66,66	0
54	MG	2A	3648	1/1	0.63	0.18	62,62,62,62	0
54	MG	1A	3667	1/1	0.63	0.13	49,49,49,49	0
54	MG	2a	1763	1/1	0.64	0.15	63,63,63,63	0
54	MG	2A	3353	1/1	0.64	0.18	43,43,43,43	0
54	MG	1A	3809	1/1	0.64	0.20	66,66,66,66	0
54	MG	1a	1785	1/1	0.65	0.12	81,81,81,81	0
54	MG	1A	3920	1/1	0.65	0.19	69,69,69,69	0
54	MG	2a	1674	1/1	0.65	0.16	57,57,57,57	0
54	MG	2A	3670	1/1	0.66	0.09	78,78,78,78	0
54	MG	1a	1828	1/1	0.67	0.24	70,70,70,70	0
54	MG	1A	4002	1/1	0.67	0.14	54,54,54,54	0
54	MG	2A	3316	1/1	0.67	0.10	64,64,64,64	0
54	MG	2a	1772	1/1	0.67	0.12	70,70,70,70	0
54	MG	2B	203	1/1	0.67	0.20	76,76,76,76	0
54	MG	1d	502	1/1	0.67	0.14	79,79,79,79	0
54	MG	1A	3957	1/1	0.67	0.41	66,66,66,66	0
54	MG	2a	1713	1/1	0.68	0.34	67,67,67,67	0
54	MG	1A	3722	1/1	0.68	0.16	63,63,63,63	0
54	MG	2B	210	1/1	0.68	0.13	75,75,75,75	0
54	MG	2A	3675	1/1	0.68	0.17	75,75,75,75	0
54	MG	2a	1661	1/1	0.68	0.13	66,66,66,66	0
54	MG	1A	3336	1/1	0.68	0.17	56,56,56,56	0
54	MG	1A	3782	1/1	0.69	0.15	48,48,48,48	0
54	MG	2a	1664	1/1	0.69	0.19	73,73,73,73	0
54	MG	1a	1848	1/1	0.70	0.17	61,61,61,61	0
54	MG	2A	3219	1/1	0.70	0.25	67,67,67,67	0
54	MG	2A	3658	1/1	0.70	0.23	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3072	1/1	0.70	0.25	69,69,69,69	0
54	MG	1a	1653	1/1	0.70	0.13	64,64,64,64	0
54	MG	1g	3002	1/1	0.70	0.18	75,75,75,75	0
54	MG	1A	3991	1/1	0.70	0.16	66,66,66,66	0
54	MG	1A	3516	1/1	0.70	0.14	58,58,58,58	0
54	MG	1l	102	1/1	0.71	0.15	56,56,56,56	0
54	MG	2A	3173	1/1	0.71	0.14	53,53,53,53	0
54	MG	1T	201	1/1	0.71	0.18	65,65,65,65	0
54	MG	2A	3164	1/1	0.71	0.30	65,65,65,65	0
54	MG	2A	3635	1/1	0.72	0.17	62,62,62,62	0
54	MG	1A	3653	1/1	0.72	0.06	73,73,73,73	0
54	MG	1a	1752	1/1	0.72	0.21	70,70,70,70	0
54	MG	2A	3174	1/1	0.72	0.33	56,56,56,56	0
54	MG	2a	1751	1/1	0.72	0.14	57,57,57,57	0
54	MG	1A	3640	1/1	0.72	0.14	61,61,61,61	0
54	MG	1A	3988	1/1	0.72	0.29	68,68,68,68	0
54	MG	1G	3002	1/1	0.72	0.19	57,57,57,57	0
54	MG	1A	4018	1/1	0.72	0.11	29,29,29,29	0
54	MG	2a	1779	1/1	0.73	0.20	76,76,76,76	0
54	MG	1A	3599	1/1	0.73	0.22	28,28,28,28	0
54	MG	1a	1845	1/1	0.73	0.09	86,86,86,86	0
54	MG	2B	217	1/1	0.73	0.10	73,73,73,73	0
54	MG	1a	1728	1/1	0.73	0.11	52,52,52,52	0
54	MG	1A	3142	1/1	0.73	0.20	45,45,45,45	0
54	MG	2a	1771	1/1	0.73	0.30	96,96,96,96	0
54	MG	2A	3172	1/1	0.73	0.11	62,62,62,62	0
54	MG	1A	3721	1/1	0.73	0.12	59,59,59,59	0
54	MG	1a	1608	1/1	0.73	0.13	52,52,52,52	0
54	MG	1A	3990	1/1	0.73	0.10	43,43,43,43	0
54	MG	1A	3709	1/1	0.74	0.15	54,54,54,54	0
54	MG	2A	3641	1/1	0.74	0.15	83,83,83,83	0
54	MG	2A	3630	1/1	0.74	0.08	74,74,74,74	0
54	MG	1A	3679	1/1	0.74	0.19	23,23,23,23	0
54	MG	2A	3584	1/1	0.74	0.27	57,57,57,57	0
54	MG	2A	3563	1/1	0.74	0.14	78,78,78,78	0
54	MG	1P	202	1/1	0.74	0.11	77,77,77,77	0
54	MG	1a	1853	1/1	0.74	0.15	60,60,60,60	0
54	MG	2A	3002	1/1	0.74	0.15	59,59,59,59	0
54	MG	2A	3407	1/1	0.75	0.13	62,62,62,62	0
54	MG	1B	219	1/1	0.75	0.16	74,74,74,74	0
54	MG	10	104	1/1	0.75	0.14	63,63,63,63	0
54	MG	1A	3974	1/1	0.75	0.18	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3481	1/1	0.75	0.15	58,58,58,58	0
54	MG	2A	3042	1/1	0.75	0.14	51,51,51,51	0
54	MG	2A	3319	1/1	0.75	0.13	71,71,71,71	0
54	MG	2a	1635	1/1	0.76	0.16	67,67,67,67	0
54	MG	1A	3945	1/1	0.76	0.10	43,43,43,43	0
54	MG	1A	3882	1/1	0.76	0.15	57,57,57,57	0
54	MG	2A	3154	1/1	0.76	0.21	59,59,59,59	0
54	MG	2A	3660	1/1	0.76	0.11	78,78,78,78	0
54	MG	2A	3195	1/1	0.76	0.17	62,62,62,62	0
54	MG	1q	201	1/1	0.76	0.15	62,62,62,62	0
54	MG	1a	1602	1/1	0.76	0.16	73,73,73,73	0
54	MG	1A	3977	1/1	0.76	0.13	45,45,45,45	0
54	MG	1A	3992	1/1	0.77	0.13	86,86,86,86	0
54	MG	2T	3003	1/1	0.77	0.11	62,62,62,62	0
54	MG	1A	3222	1/1	0.77	0.23	69,69,69,69	0
54	MG	2a	1632	1/1	0.77	0.12	82,82,82,82	0
54	MG	2A	3615	1/1	0.77	0.19	71,71,71,71	0
54	MG	2a	1722	1/1	0.77	0.27	65,65,65,65	0
54	MG	2A	3080	1/1	0.77	0.19	51,51,51,51	0
54	MG	2A	3687	1/1	0.77	0.06	70,70,70,70	0
54	MG	1A	3941	1/1	0.77	0.14	37,37,37,37	0
54	MG	25	502	1/1	0.77	0.14	55,55,55,55	0
54	MG	2a	1604	1/1	0.77	0.26	63,63,63,63	0
54	MG	1A	3844	1/1	0.77	0.11	57,57,57,57	0
54	MG	1A	3994	1/1	0.77	0.17	53,53,53,53	0
54	MG	1a	1786	1/1	0.77	0.14	59,59,59,59	0
54	MG	1A	3582	1/1	0.77	0.11	64,64,64,64	0
54	MG	2A	3632	1/1	0.77	0.12	48,48,48,48	0
54	MG	1A	3233	1/1	0.77	0.48	53,53,53,53	0
54	MG	1A	3011	1/1	0.77	0.25	53,53,53,53	0
54	MG	1A	3628	1/1	0.77	0.10	51,51,51,51	0
54	MG	2A	3587	1/1	0.77	0.13	57,57,57,57	0
54	MG	2A	3329	1/1	0.77	0.15	38,38,38,38	0
54	MG	2A	3652	1/1	0.78	0.14	71,71,71,71	0
54	MG	2A	3663	1/1	0.78	0.14	69,69,69,69	0
54	MG	1A	3828	1/1	0.78	0.15	25,25,25,25	0
54	MG	1A	3756	1/1	0.78	0.17	45,45,45,45	0
54	MG	2a	1776	1/1	0.78	0.13	71,71,71,71	0
54	MG	1A	3855	1/1	0.78	0.41	57,57,57,57	0
54	MG	2A	3122	1/1	0.78	0.10	58,58,58,58	0
54	MG	1a	1694	1/1	0.78	0.17	55,55,55,55	0
54	MG	2a	1639	1/1	0.78	0.25	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	1707	1/1	0.78	0.16	69,69,69,69	0
54	MG	28	102	1/1	0.78	0.18	65,65,65,65	0
54	MG	2A	3668	1/1	0.78	0.14	63,63,63,63	0
54	MG	1a	1829	1/1	0.78	0.24	63,63,63,63	0
54	MG	1A	3711	1/1	0.78	0.10	29,29,29,29	0
54	MG	1y	3003	1/1	0.78	0.19	69,69,69,69	0
54	MG	2a	1622	1/1	0.78	0.14	59,59,59,59	0
54	MG	1g	3001	1/1	0.78	0.19	67,67,67,67	0
54	MG	1A	3240	1/1	0.78	0.10	77,77,77,77	0
54	MG	1A	3939	1/1	0.78	0.62	51,51,51,51	0
54	MG	1A	3894	1/1	0.78	0.17	51,51,51,51	0
54	MG	2A	3370	1/1	0.79	0.09	39,39,39,39	0
54	MG	1A	3996	1/1	0.79	0.31	70,70,70,70	0
54	MG	1A	3545	1/1	0.79	0.14	60,60,60,60	0
54	MG	2a	1724	1/1	0.79	0.18	61,61,61,61	0
54	MG	1a	1720	1/1	0.79	0.16	62,62,62,62	0
54	MG	2A	3530	1/1	0.79	0.12	74,74,74,74	0
54	MG	1A	3810	1/1	0.79	0.16	55,55,55,55	0
54	MG	1A	3596	1/1	0.79	0.14	32,32,32,32	0
54	MG	1A	3378	1/1	0.79	0.16	33,33,33,33	0
54	MG	2A	3052	1/1	0.79	0.15	41,41,41,41	0
54	MG	2F	3001	1/1	0.79	0.16	41,41,41,41	0
54	MG	2A	3669	1/1	0.79	0.23	72,72,72,72	0
54	MG	2A	3076	1/1	0.80	0.25	56,56,56,56	0
54	MG	2A	3253	1/1	0.80	0.16	61,61,61,61	0
54	MG	2A	3196	1/1	0.80	0.28	41,41,41,41	0
54	MG	1a	1656	1/1	0.80	0.15	59,59,59,59	0
54	MG	1a	1849	1/1	0.80	0.17	68,68,68,68	0
54	MG	2A	3216	1/1	0.80	0.16	53,53,53,53	0
54	MG	1A	3910	1/1	0.80	0.25	77,77,77,77	0
54	MG	2A	3354	1/1	0.80	0.18	58,58,58,58	0
54	MG	1A	3921	1/1	0.80	0.10	62,62,62,62	0
54	MG	2a	1605	1/1	0.80	0.10	60,60,60,60	0
54	MG	2A	3624	1/1	0.80	0.13	78,78,78,78	0
54	MG	1A	3271	1/1	0.80	0.27	37,37,37,37	0
54	MG	1a	1790	1/1	0.80	0.20	65,65,65,65	0
54	MG	1A	3472	1/1	0.80	0.12	54,54,54,54	0
54	MG	1a	1601	1/1	0.80	0.10	63,63,63,63	0
54	MG	2A	3399	1/1	0.80	0.17	59,59,59,59	0
54	MG	1d	504	1/1	0.80	0.13	72,72,72,72	0
54	MG	2a	1782	1/1	0.80	0.14	78,78,78,78	0
54	MG	2A	3521	1/1	0.80	0.18	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3192	1/1	0.80	0.16	50,50,50,50	0
54	MG	2a	1668	1/1	0.80	0.08	58,58,58,58	0
54	MG	1a	1838	1/1	0.80	0.08	75,75,75,75	0
54	MG	2A	3617	1/1	0.81	0.10	63,63,63,63	0
54	MG	1A	3940	1/1	0.81	0.10	72,72,72,72	0
57	MPD	2A	3692	8/8	0.81	0.32	41,48,53,56	0
54	MG	2A	3120	1/1	0.81	0.15	41,41,41,41	0
54	MG	2B	206	1/1	0.81	0.17	69,69,69,69	0
54	MG	1A	3543	1/1	0.81	0.16	39,39,39,39	0
54	MG	1A	3853	1/1	0.81	0.21	52,52,52,52	0
54	MG	1a	1792	1/1	0.81	0.15	73,73,73,73	0
54	MG	1A	3808	1/1	0.81	0.15	58,58,58,58	0
54	MG	2E	305	1/1	0.81	0.21	70,70,70,70	0
54	MG	1A	3852	1/1	0.81	0.11	62,62,62,62	0
54	MG	2a	1602	1/1	0.81	0.16	57,57,57,57	0
54	MG	1A	3081	1/1	0.81	0.28	41,41,41,41	0
54	MG	2G	3003	1/1	0.81	0.16	68,68,68,68	0
54	MG	2a	1637	1/1	0.81	0.12	76,76,76,76	0
54	MG	1A	3891	1/1	0.81	0.16	42,42,42,42	0
54	MG	1R	202	1/1	0.81	0.20	39,39,39,39	0
54	MG	1A	3790	1/1	0.81	0.19	56,56,56,56	0
54	MG	2A	3404	1/1	0.81	0.15	66,66,66,66	0
54	MG	2A	3140	1/1	0.81	0.16	53,53,53,53	0
54	MG	1A	3486	1/1	0.81	0.20	52,52,52,52	0
54	MG	1a	1795	1/1	0.81	0.21	56,56,56,56	0
54	MG	1A	3664	1/1	0.81	0.06	45,45,45,45	0
54	MG	1A	3075	1/1	0.81	0.24	40,40,40,40	0
54	MG	1A	3947	1/1	0.81	0.19	74,74,74,74	0
54	MG	2a	1679	1/1	0.81	0.15	64,64,64,64	0
54	MG	1A	3775	1/1	0.81	0.16	53,53,53,53	0
54	MG	1A	3968	1/1	0.81	0.20	48,48,48,48	0
54	MG	2A	3053	1/1	0.81	0.11	53,53,53,53	0
54	MG	1A	3164	1/1	0.81	0.15	51,51,51,51	0
54	MG	2A	3410	1/1	0.81	0.15	69,69,69,69	0
54	MG	1A	3841	1/1	0.81	0.09	56,56,56,56	0
54	MG	1a	1855	1/1	0.81	0.17	68,68,68,68	0
54	MG	2a	1781	1/1	0.81	0.13	70,70,70,70	0
54	MG	2a	1743	1/1	0.82	0.06	66,66,66,66	0
54	MG	2A	3175	1/1	0.82	0.22	45,45,45,45	0
54	MG	2A	3583	1/1	0.82	0.18	54,54,54,54	0
54	MG	2A	3397	1/1	0.82	0.20	31,31,31,31	0
54	MG	1A	3757	1/1	0.82	0.10	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1F	310	1/1	0.82	0.25	64,64,64,64	0
54	MG	1l	201	1/1	0.82	0.18	64,64,64,64	0
54	MG	1A	3263	1/1	0.82	0.13	70,70,70,70	0
54	MG	1B	221	1/1	0.82	0.14	45,45,45,45	0
54	MG	2A	3059	1/1	0.82	0.30	50,50,50,50	0
54	MG	2a	1620	1/1	0.82	0.17	71,71,71,71	0
54	MG	2a	1746	1/1	0.82	0.21	74,74,74,74	0
54	MG	2A	3621	1/1	0.82	0.14	75,75,75,75	0
54	MG	1A	3699	1/1	0.82	0.18	42,42,42,42	0
54	MG	1A	3826	1/1	0.82	0.20	25,25,25,25	0
54	MG	1a	1732	1/1	0.82	0.12	57,57,57,57	0
54	MG	1A	3173	1/1	0.82	0.15	50,50,50,50	0
58	ARG	1F	311	12/12	0.82	0.25	52,70,77,82	0
54	MG	2A	3250	1/1	0.82	0.12	71,71,71,71	0
54	MG	1A	3270	1/1	0.82	0.21	55,55,55,55	0
54	MG	1A	3919	1/1	0.82	0.14	74,74,74,74	0
54	MG	1A	3789	1/1	0.82	0.11	38,38,38,38	0
54	MG	1A	3659	1/1	0.82	0.15	32,32,32,32	0
54	MG	1A	3565	1/1	0.82	0.22	28,28,28,28	0
54	MG	1A	3797	1/1	0.82	0.13	46,46,46,46	0
54	MG	1a	1669	1/1	0.82	0.31	54,54,54,54	0
54	MG	1A	3753	1/1	0.82	0.19	49,49,49,49	0
54	MG	2A	3027	1/1	0.82	0.25	60,60,60,60	0
54	MG	2a	1766	1/1	0.82	0.12	75,75,75,75	0
54	MG	2A	3217	1/1	0.82	0.22	61,61,61,61	0
54	MG	2A	3226	1/1	0.82	0.14	72,72,72,72	0
54	MG	1A	3984	1/1	0.82	0.10	81,81,81,81	0
54	MG	1a	1636	1/1	0.82	0.16	54,54,54,54	0
54	MG	1A	3294	1/1	0.82	0.09	62,62,62,62	0
54	MG	1A	3973	1/1	0.82	0.12	67,67,67,67	0
54	MG	2A	3599	1/1	0.82	0.14	58,58,58,58	0
54	MG	1A	3878	1/1	0.82	0.12	53,53,53,53	0
54	MG	1A	3277	1/1	0.83	0.24	60,60,60,60	0
54	MG	1B	211	1/1	0.83	0.27	67,67,67,67	0
54	MG	2a	1677	1/1	0.83	0.12	75,75,75,75	0
54	MG	1a	1612	1/1	0.83	0.17	52,52,52,52	0
54	MG	2A	3637	1/1	0.83	0.06	86,86,86,86	0
54	MG	1A	3461	1/1	0.83	0.19	58,58,58,58	0
54	MG	1A	3747	1/1	0.83	0.15	67,67,67,67	0
54	MG	1a	1675	1/1	0.83	0.13	49,49,49,49	0
54	MG	1A	3460	1/1	0.83	0.15	61,61,61,61	0
54	MG	2A	3241	1/1	0.83	0.10	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2e	201	1/1	0.83	0.29	68,68,68,68	0
54	MG	1A	4000	1/1	0.83	0.15	46,46,46,46	0
54	MG	2A	3208	1/1	0.83	0.23	66,66,66,66	0
54	MG	1a	1842	1/1	0.83	0.08	79,79,79,79	0
54	MG	1B	227	1/1	0.83	0.15	64,64,64,64	0
54	MG	1a	1605	1/1	0.83	0.14	65,65,65,65	0
54	MG	1A	3692	1/1	0.83	0.16	63,63,63,63	0
54	MG	2A	3551	1/1	0.83	0.17	59,59,59,59	0
54	MG	2a	1769	1/1	0.83	0.14	84,84,84,84	0
54	MG	1A	3329	1/1	0.83	0.16	43,43,43,43	0
54	MG	2A	3293	1/1	0.83	0.15	60,60,60,60	0
54	MG	1B	225	1/1	0.83	0.10	52,52,52,52	0
54	MG	1a	1724	1/1	0.83	0.19	58,58,58,58	0
54	MG	1A	3538	1/1	0.83	0.22	51,51,51,51	0
54	MG	2a	1744	1/1	0.83	0.18	73,73,73,73	0
54	MG	1a	1643	1/1	0.83	0.08	69,69,69,69	0
54	MG	1A	4029	1/1	0.83	0.07	58,58,58,58	0
54	MG	2A	3360	1/1	0.83	0.17	52,52,52,52	0
54	MG	2A	3043	1/1	0.83	0.17	72,72,72,72	0
54	MG	1A	3470	1/1	0.83	0.10	51,51,51,51	0
54	MG	1a	1764	1/1	0.83	0.13	69,69,69,69	0
54	MG	2a	1643	1/1	0.83	0.14	75,75,75,75	0
54	MG	1A	3656	1/1	0.83	0.15	49,49,49,49	0
54	MG	2a	1723	1/1	0.83	0.12	63,63,63,63	0
54	MG	2A	3078	1/1	0.83	0.14	52,52,52,52	0
54	MG	2A	3342	1/1	0.83	0.09	32,32,32,32	0
54	MG	1A	3979	1/1	0.83	0.30	85,85,85,85	0
54	MG	1A	3182	1/1	0.83	0.22	53,53,53,53	0
54	MG	1a	1831	1/1	0.83	0.17	69,69,69,69	0
54	MG	1a	1709	1/1	0.83	0.13	50,50,50,50	0
54	MG	1A	3369	1/1	0.83	0.16	32,32,32,32	0
54	MG	2A	3453	1/1	0.83	0.13	55,55,55,55	0
54	MG	1A	3342	1/1	0.84	0.21	17,17,17,17	0
54	MG	1A	3614	1/1	0.84	0.15	58,58,58,58	0
54	MG	2A	3228	1/1	0.84	0.19	63,63,63,63	0
54	MG	2a	1731	1/1	0.84	0.34	65,65,65,65	0
54	MG	1A	3249	1/1	0.84	0.19	52,52,52,52	0
54	MG	1a	1787	1/1	0.84	0.30	60,60,60,60	0
54	MG	2a	1714	1/1	0.84	0.12	58,58,58,58	0
54	MG	1A	3616	1/1	0.84	0.11	68,68,68,68	0
54	MG	1a	1606	1/1	0.84	0.12	54,54,54,54	0
54	MG	2F	3002	1/1	0.84	0.18	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3985	1/1	0.84	0.10	70,70,70,70	0
54	MG	2a	1726	1/1	0.84	0.18	74,74,74,74	0
54	MG	1a	1702	1/1	0.84	0.11	61,61,61,61	0
54	MG	1a	1615	1/1	0.84	0.14	54,54,54,54	0
54	MG	2T	3004	1/1	0.84	0.21	61,61,61,61	0
54	MG	2A	3115	1/1	0.84	0.10	49,49,49,49	0
54	MG	2A	3074	1/1	0.84	0.19	46,46,46,46	0
54	MG	1a	1716	1/1	0.84	0.17	54,54,54,54	0
54	MG	1A	4034	1/1	0.84	0.40	58,58,58,58	0
54	MG	1A	3433	1/1	0.84	0.16	33,33,33,33	0
54	MG	1A	3230	1/1	0.84	0.10	44,44,44,44	0
54	MG	2a	1711	1/1	0.84	0.09	62,62,62,62	0
54	MG	1A	3950	1/1	0.84	0.16	60,60,60,60	0
54	MG	2A	3575	1/1	0.84	0.12	65,65,65,65	0
54	MG	2A	3688	1/1	0.84	0.13	61,61,61,61	0
54	MG	2A	3328	1/1	0.84	0.14	38,38,38,38	0
54	MG	2B	209	1/1	0.84	0.12	73,73,73,73	0
54	MG	2A	3355	1/1	0.84	0.11	52,52,52,52	0
54	MG	1A	3848	1/1	0.84	0.12	55,55,55,55	0
54	MG	2A	3262	1/1	0.84	0.17	57,57,57,57	0
54	MG	1A	3641	1/1	0.84	0.13	49,49,49,49	0
54	MG	2A	3392	1/1	0.84	0.14	71,71,71,71	0
54	MG	20	102	1/1	0.84	0.12	62,62,62,62	0
54	MG	1A	3942	1/1	0.84	0.22	41,41,41,41	0
54	MG	2A	3167	1/1	0.84	0.17	67,67,67,67	0
54	MG	1a	1620	1/1	0.84	0.11	61,61,61,61	0
54	MG	2j	8001	1/1	0.84	0.16	81,81,81,81	0
54	MG	1A	3604	1/1	0.84	0.18	53,53,53,53	0
54	MG	2A	3310	1/1	0.84	0.14	65,65,65,65	0
54	MG	1A	3091	1/1	0.84	0.19	44,44,44,44	0
54	MG	1a	1839	1/1	0.84	0.22	73,73,73,73	0
54	MG	2A	3497	1/1	0.84	0.20	69,69,69,69	0
54	MG	1a	1779	1/1	0.84	0.11	76,76,76,76	0
54	MG	1y	3001	1/1	0.84	0.33	66,66,66,66	0
54	MG	1D	313	1/1	0.85	0.17	48,48,48,48	0
54	MG	2A	3144	1/1	0.85	0.13	62,62,62,62	0
54	MG	1A	3527	1/1	0.85	0.17	37,37,37,37	0
54	MG	1A	3280	1/1	0.85	0.22	34,34,34,34	0
54	MG	1A	3228	1/1	0.85	0.24	30,30,30,30	0
54	MG	1B	213	1/1	0.85	0.15	71,71,71,71	0
54	MG	2A	3094	1/1	0.85	0.13	45,45,45,45	0
54	MG	1A	3820	1/1	0.85	0.06	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3132	1/1	0.85	0.15	63,63,63,63	0
54	MG	2a	1732	1/1	0.85	0.15	80,80,80,80	0
54	MG	2E	303	1/1	0.85	0.35	61,61,61,61	0
54	MG	1A	3541	1/1	0.85	0.21	64,64,64,64	0
54	MG	2A	3034	1/1	0.85	0.13	66,66,66,66	0
54	MG	2A	3142	1/1	0.85	0.12	66,66,66,66	0
54	MG	2A	3363	1/1	0.85	0.12	63,63,63,63	0
54	MG	1a	1754	1/1	0.85	0.13	63,63,63,63	0
54	MG	2A	3645	1/1	0.85	0.17	72,72,72,72	0
54	MG	1A	3416	1/1	0.85	0.17	48,48,48,48	0
54	MG	1A	3121	1/1	0.85	0.15	48,48,48,48	0
54	MG	1a	1750	1/1	0.85	0.12	64,64,64,64	0
54	MG	1a	1604	1/1	0.85	0.11	61,61,61,61	0
54	MG	1A	3759	1/1	0.85	0.14	48,48,48,48	0
54	MG	1A	3111	1/1	0.85	0.19	61,61,61,61	0
54	MG	1A	3754	1/1	0.85	0.17	57,57,57,57	0
54	MG	2A	3609	1/1	0.85	0.13	75,75,75,75	0
54	MG	2A	3382	1/1	0.85	0.15	63,63,63,63	0
54	MG	2a	1703	1/1	0.85	0.17	69,69,69,69	0
54	MG	1a	1616	1/1	0.85	0.13	53,53,53,53	0
54	MG	1A	3467	1/1	0.85	0.12	31,31,31,31	0
54	MG	1a	1648	1/1	0.85	0.22	57,57,57,57	0
54	MG	2B	213	1/1	0.85	0.09	70,70,70,70	0
54	MG	2A	3212	1/1	0.85	0.19	60,60,60,60	0
54	MG	2A	3057	1/1	0.85	0.45	49,49,49,49	0
54	MG	1A	3229	1/1	0.85	0.13	61,61,61,61	0
54	MG	1a	1773	1/1	0.85	0.16	67,67,67,67	0
54	MG	1A	3933	1/1	0.85	0.13	56,56,56,56	0
54	MG	2a	1616	1/1	0.85	0.12	67,67,67,67	0
54	MG	1a	1632	1/1	0.85	0.13	62,62,62,62	0
54	MG	2A	3227	1/1	0.85	0.25	59,59,59,59	0
54	MG	1A	3254	1/1	0.85	0.14	67,67,67,67	0
54	MG	2A	3087	1/1	0.85	0.15	44,44,44,44	0
54	MG	2A	3245	1/1	0.85	0.14	50,50,50,50	0
54	MG	2A	3166	1/1	0.85	0.16	62,62,62,62	0
54	MG	1A	3026	1/1	0.85	0.08	60,60,60,60	0
54	MG	1A	3250	1/1	0.85	0.22	61,61,61,61	0
54	MG	1A	3549	1/1	0.85	0.24	42,42,42,42	0
54	MG	2A	3642	1/1	0.85	0.11	63,63,63,63	0
54	MG	1A	3673	1/1	0.85	0.18	60,60,60,60	0
54	MG	1A	3779	1/1	0.85	0.10	29,29,29,29	0
54	MG	2A	3090	1/1	0.85	0.33	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3638	1/1	0.85	0.34	58,58,58,58	0
54	MG	2A	3150	1/1	0.85	0.28	59,59,59,59	0
54	MG	1a	1819	1/1	0.85	0.14	64,64,64,64	0
54	MG	2a	1612	1/1	0.85	0.10	54,54,54,54	0
54	MG	2A	3419	1/1	0.85	0.14	66,66,66,66	0
54	MG	2R	201	1/1	0.86	0.26	51,51,51,51	0
54	MG	1A	3643	1/1	0.86	0.17	36,36,36,36	0
54	MG	1a	1703	1/1	0.86	0.14	63,63,63,63	0
54	MG	2A	3537	1/1	0.86	0.18	70,70,70,70	0
54	MG	1A	3306	1/1	0.86	0.12	27,27,27,27	0
54	MG	2A	3656	1/1	0.86	0.12	69,69,69,69	0
54	MG	2A	3339	1/1	0.86	0.25	70,70,70,70	0
54	MG	1A	3553	1/1	0.86	0.23	61,61,61,61	0
54	MG	1A	3163	1/1	0.86	0.15	65,65,65,65	0
54	MG	1A	3559	1/1	0.86	0.14	48,48,48,48	0
54	MG	2A	3678	1/1	0.86	0.13	39,39,39,39	0
54	MG	1A	3368	1/1	0.86	0.14	64,64,64,64	0
54	MG	2a	1710	1/1	0.86	0.18	68,68,68,68	0
54	MG	2A	3086	1/1	0.86	0.25	67,67,67,67	0
54	MG	1A	3435	1/1	0.86	0.20	42,42,42,42	0
54	MG	2A	3446	1/1	0.86	0.16	57,57,57,57	0
54	MG	1A	3906	1/1	0.86	0.12	71,71,71,71	0
54	MG	2A	3207	1/1	0.86	0.10	61,61,61,61	0
54	MG	2A	3461	1/1	0.86	0.35	55,55,55,55	0
54	MG	1A	3751	1/1	0.86	0.10	47,47,47,47	0
54	MG	1a	1734	1/1	0.86	0.14	59,59,59,59	0
54	MG	1A	3053	1/1	0.86	0.49	32,32,32,32	0
54	MG	1A	3259	1/1	0.86	0.15	55,55,55,55	0
54	MG	1A	3078	1/1	0.86	0.19	56,56,56,56	0
54	MG	1a	1776	1/1	0.86	0.12	68,68,68,68	0
54	MG	1A	3456	1/1	0.86	0.12	34,34,34,34	0
54	MG	1a	1736	1/1	0.86	0.14	55,55,55,55	0
54	MG	2a	1640	1/1	0.86	0.17	69,69,69,69	0
54	MG	1A	3637	1/1	0.86	0.09	31,31,31,31	0
54	MG	1q	202	1/1	0.86	0.08	65,65,65,65	0
54	MG	1a	1668	1/1	0.86	0.15	56,56,56,56	0
54	MG	2a	1633	1/1	0.86	0.23	67,67,67,67	0
54	MG	1a	1843	1/1	0.86	0.15	68,68,68,68	0
54	MG	1A	3505	1/1	0.86	0.17	53,53,53,53	0
54	MG	1B	223	1/1	0.86	0.18	36,36,36,36	0
54	MG	2A	3564	1/1	0.86	0.17	59,59,59,59	0
54	MG	2A	3440	1/1	0.86	0.22	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	1835	1/1	0.86	0.19	70,70,70,70	0
54	MG	2A	3225	1/1	0.86	0.25	67,67,67,67	0
54	MG	2A	3494	1/1	0.86	0.24	50,50,50,50	0
54	MG	2A	3429	1/1	0.86	0.28	56,56,56,56	0
54	MG	2A	3213	1/1	0.86	0.14	64,64,64,64	0
54	MG	2A	3242	1/1	0.86	0.15	33,33,33,33	0
54	MG	1A	3308	1/1	0.86	0.19	62,62,62,62	0
54	MG	1A	3870	1/1	0.86	0.20	53,53,53,53	0
54	MG	2a	1614	1/1	0.86	0.14	54,54,54,54	0
54	MG	2A	3511	1/1	0.86	0.22	45,45,45,45	0
54	MG	1A	4001	1/1	0.86	0.08	56,56,56,56	0
54	MG	1l	202	1/1	0.86	0.09	72,72,72,72	0
54	MG	2a	1733	1/1	0.86	0.08	69,69,69,69	0
54	MG	1A	3864	1/1	0.86	0.32	82,82,82,82	0
54	MG	2A	3636	1/1	0.86	0.20	63,63,63,63	0
54	MG	1A	3960	1/1	0.86	0.14	48,48,48,48	0
54	MG	1A	3627	1/1	0.86	0.25	43,43,43,43	0
54	MG	2a	1654	1/1	0.86	0.14	50,50,50,50	0
54	MG	20	101	1/1	0.86	0.15	74,74,74,74	0
54	MG	2A	3273	1/1	0.86	0.16	66,66,66,66	0
54	MG	1A	3625	1/1	0.86	0.27	67,67,67,67	0
54	MG	1A	3861	1/1	0.86	0.19	42,42,42,42	0
54	MG	1A	3767	1/1	0.86	0.10	61,61,61,61	0
54	MG	2A	3654	1/1	0.86	0.13	72,72,72,72	0
54	MG	1A	3409	1/1	0.86	0.17	48,48,48,48	0
54	MG	1A	3795	1/1	0.86	0.13	41,41,41,41	0
54	MG	2B	204	1/1	0.87	0.14	63,63,63,63	0
54	MG	1a	1851	1/1	0.87	0.10	83,83,83,83	0
54	MG	2A	3465	1/1	0.87	0.14	69,69,69,69	0
54	MG	1a	1802	1/1	0.87	0.12	50,50,50,50	0
54	MG	1A	3859	1/1	0.87	0.25	44,44,44,44	0
54	MG	2A	3008	1/1	0.87	0.38	44,44,44,44	0
54	MG	2A	3591	1/1	0.87	0.31	71,71,71,71	0
54	MG	1A	3425	1/1	0.87	0.25	66,66,66,66	0
54	MG	2A	3590	1/1	0.87	0.33	64,64,64,64	0
54	MG	1a	1659	1/1	0.87	0.16	53,53,53,53	0
54	MG	2A	3277	1/1	0.87	0.26	48,48,48,48	0
54	MG	1A	3010	1/1	0.87	0.12	44,44,44,44	0
54	MG	1A	3788	1/1	0.87	0.09	38,38,38,38	0
54	MG	2A	3065	1/1	0.87	0.31	57,57,57,57	0
54	MG	1a	1808	1/1	0.87	0.17	64,64,64,64	0
54	MG	1A	3133	1/1	0.87	0.21	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3803	1/1	0.87	0.19	22,22,22,22	0
54	MG	1A	3814	1/1	0.87	0.23	45,45,45,45	0
54	MG	1A	3909	1/1	0.87	0.19	86,86,86,86	0
54	MG	1a	1644	1/1	0.87	0.29	62,62,62,62	0
54	MG	1A	3515	1/1	0.87	0.34	55,55,55,55	0
54	MG	1A	3490	1/1	0.87	0.17	66,66,66,66	0
54	MG	2a	1756	1/1	0.87	0.12	80,80,80,80	0
54	MG	1A	3573	1/1	0.87	0.16	31,31,31,31	0
54	MG	1A	3317	1/1	0.87	0.17	27,27,27,27	0
54	MG	1A	3937	1/1	0.87	0.09	80,80,80,80	0
54	MG	2A	3405	1/1	0.87	0.21	62,62,62,62	0
54	MG	2A	3576	1/1	0.87	0.17	60,60,60,60	0
54	MG	2A	3184	1/1	0.87	0.16	64,64,64,64	0
54	MG	1a	1840	1/1	0.87	0.14	62,62,62,62	0
54	MG	1B	230	1/1	0.87	0.14	60,60,60,60	0
54	MG	2A	3229	1/1	0.87	0.15	56,56,56,56	0
54	MG	1A	3097	1/1	0.87	0.17	37,37,37,37	0
54	MG	1A	3597	1/1	0.87	0.17	22,22,22,22	0
54	MG	1A	3763	1/1	0.87	0.25	42,42,42,42	0
54	MG	1a	1685	1/1	0.87	0.17	66,66,66,66	0
54	MG	2A	3224	1/1	0.87	0.15	54,54,54,54	0
54	MG	1A	3253	1/1	0.87	0.22	48,48,48,48	0
54	MG	1A	3781	1/1	0.87	0.22	61,61,61,61	0
54	MG	2A	3503	1/1	0.87	0.14	38,38,38,38	0
54	MG	1A	3096	1/1	0.87	0.17	29,29,29,29	0
54	MG	2a	1609	1/1	0.87	0.16	65,65,65,65	0
54	MG	1A	3609	1/1	0.87	0.11	55,55,55,55	0
54	MG	2A	3267	1/1	0.87	0.19	73,73,73,73	0
54	MG	2A	3409	1/1	0.87	0.13	42,42,42,42	0
54	MG	2A	3004	1/1	0.87	0.16	61,61,61,61	0
54	MG	2a	1611	1/1	0.87	0.19	63,63,63,63	0
54	MG	1A	3778	1/1	0.87	0.15	54,54,54,54	0
54	MG	2A	3552	1/1	0.87	0.09	48,48,48,48	0
54	MG	1a	1634	1/1	0.87	0.14	71,71,71,71	0
54	MG	1a	1771	1/1	0.87	0.17	59,59,59,59	0
54	MG	1A	3905	1/1	0.87	0.08	39,39,39,39	0
54	MG	2a	1656	1/1	0.87	0.12	70,70,70,70	0
54	MG	1G	3001	1/1	0.87	0.12	65,65,65,65	0
57	MPD	1A	4036	8/8	0.87	0.23	42,53,63,65	0
54	MG	2a	1685	1/1	0.88	0.12	70,70,70,70	0
54	MG	2A	3700	1/1	0.88	0.13	49,49,49,49	0
54	MG	1A	3225	1/1	0.88	0.36	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1B	206	1/1	0.88	0.26	42,42,42,42	0
54	MG	2A	3251	1/1	0.88	0.21	33,33,33,33	0
54	MG	2A	3608	1/1	0.88	0.22	70,70,70,70	0
54	MG	1A	4025	1/1	0.88	0.15	38,38,38,38	0
54	MG	1a	1746	1/1	0.88	0.13	70,70,70,70	0
54	MG	1A	3120	1/1	0.88	0.12	53,53,53,53	0
54	MG	2a	1753	1/1	0.88	0.15	63,63,63,63	0
54	MG	1A	3935	1/1	0.88	0.15	67,67,67,67	0
54	MG	2A	3162	1/1	0.88	0.21	66,66,66,66	0
54	MG	1A	3032	1/1	0.88	0.27	41,41,41,41	0
54	MG	2a	1628	1/1	0.88	0.07	83,83,83,83	0
54	MG	2A	3651	1/1	0.88	0.16	84,84,84,84	0
54	MG	2A	3649	1/1	0.88	0.09	49,49,49,49	0
54	MG	2a	1717	1/1	0.88	0.27	48,48,48,48	0
54	MG	2A	3022	1/1	0.88	0.34	52,52,52,52	0
54	MG	1A	3983	1/1	0.88	0.09	66,66,66,66	0
54	MG	2A	3019	1/1	0.88	0.16	65,65,65,65	0
54	MG	1p	8001	1/1	0.88	0.23	64,64,64,64	0
54	MG	1a	1789	1/1	0.88	0.17	64,64,64,64	0
54	MG	2a	1692	1/1	0.88	0.25	65,65,65,65	0
54	MG	1a	1780	1/1	0.88	0.10	53,53,53,53	0
54	MG	1A	3948	1/1	0.88	0.10	70,70,70,70	0
54	MG	1a	1767	1/1	0.88	0.15	55,55,55,55	0
54	MG	1A	3786	1/1	0.88	0.14	53,53,53,53	0
54	MG	2A	3083	1/1	0.88	0.12	51,51,51,51	0
54	MG	2a	1727	1/1	0.88	0.22	65,65,65,65	0
54	MG	1A	3916	1/1	0.88	0.13	56,56,56,56	0
54	MG	1A	3351	1/1	0.88	0.20	22,22,22,22	0
54	MG	1A	3598	1/1	0.88	0.23	64,64,64,64	0
54	MG	1A	3186	1/1	0.88	0.21	36,36,36,36	0
54	MG	1A	3391	1/1	0.88	0.19	70,70,70,70	0
54	MG	2A	3459	1/1	0.88	0.15	57,57,57,57	0
54	MG	2A	3278	1/1	0.88	0.20	39,39,39,39	0
54	MG	1B	217	1/1	0.88	0.11	59,59,59,59	0
54	MG	2A	3413	1/1	0.88	0.19	66,66,66,66	0
54	MG	2A	3396	1/1	0.88	0.15	54,54,54,54	0
54	MG	2a	1648	1/1	0.88	0.17	65,65,65,65	0
54	MG	1A	4040	1/1	0.88	0.17	22,22,22,22	0
54	MG	2A	3359	1/1	0.88	0.16	57,57,57,57	0
54	MG	1A	3931	1/1	0.88	0.10	71,71,71,71	0
54	MG	2A	3180	1/1	0.88	0.32	56,56,56,56	0
54	MG	1U	201	1/1	0.88	0.17	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	1658	1/1	0.88	0.21	62,62,62,62	0
54	MG	1B	202	1/1	0.88	0.26	54,54,54,54	0
54	MG	2a	1645	1/1	0.88	0.08	71,71,71,71	0
54	MG	2a	1754	1/1	0.88	0.10	85,85,85,85	0
54	MG	1A	3021	1/1	0.88	0.16	43,43,43,43	0
54	MG	1A	3079	1/1	0.88	0.38	36,36,36,36	0
54	MG	1a	1622	1/1	0.88	0.13	59,59,59,59	0
54	MG	2A	3200	1/1	0.88	0.09	50,50,50,50	0
54	MG	2A	3054	1/1	0.88	0.27	44,44,44,44	0
54	MG	1a	1836	1/1	0.88	0.18	64,64,64,64	0
54	MG	2A	3186	1/1	0.88	0.22	42,42,42,42	0
54	MG	2A	3199	1/1	0.88	0.20	49,49,49,49	0
54	MG	1A	3298	1/1	0.88	0.15	31,31,31,31	0
54	MG	2a	1601	1/1	0.88	0.12	58,58,58,58	0
54	MG	2A	3263	1/1	0.88	0.10	63,63,63,63	0
54	MG	1h	3002	1/1	0.88	0.17	74,74,74,74	0
54	MG	1a	1638	1/1	0.88	0.18	68,68,68,68	0
54	MG	2A	3248	1/1	0.88	0.11	48,48,48,48	0
54	MG	1A	3589	1/1	0.88	0.21	58,58,58,58	0
54	MG	2a	1641	1/1	0.88	0.14	78,78,78,78	0
54	MG	2A	3324	1/1	0.88	0.30	62,62,62,62	0
54	MG	2A	3438	1/1	0.88	0.19	67,67,67,67	0
54	MG	2a	1716	1/1	0.88	0.13	70,70,70,70	0
54	MG	1A	3969	1/1	0.88	0.09	61,61,61,61	0
54	MG	1A	3728	1/1	0.88	0.11	62,62,62,62	0
54	MG	1A	3130	1/1	0.88	0.12	55,55,55,55	0
54	MG	1A	3561	1/1	0.88	0.11	64,64,64,64	0
54	MG	2A	3084	1/1	0.88	0.11	52,52,52,52	0
54	MG	1A	3422	1/1	0.88	0.17	42,42,42,42	0
54	MG	2A	3271	1/1	0.88	0.21	56,56,56,56	0
54	MG	1a	1712	1/1	0.88	0.15	51,51,51,51	0
54	MG	1A	3586	1/1	0.88	0.17	39,39,39,39	0
54	MG	1A	3602	1/1	0.88	0.18	40,40,40,40	0
54	MG	2A	3433	1/1	0.88	0.10	64,64,64,64	0
54	MG	1a	1693	1/1	0.88	0.18	66,66,66,66	0
54	MG	1A	3731	1/1	0.88	0.13	51,51,51,51	0
54	MG	2A	3622	1/1	0.88	0.29	67,67,67,67	0
54	MG	1A	3600	1/1	0.88	0.14	56,56,56,56	0
54	MG	2A	3452	1/1	0.88	0.16	63,63,63,63	0
54	MG	1a	1629	1/1	0.88	0.12	38,38,38,38	0
54	MG	2a	1607	1/1	0.88	0.09	65,65,65,65	0
54	MG	1A	3508	1/1	0.88	0.12	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	1672	1/1	0.88	0.18	65,65,65,65	0
54	MG	1A	3429	1/1	0.88	0.20	37,37,37,37	0
54	MG	1A	3998	1/1	0.88	0.18	58,58,58,58	0
54	MG	2G	3002	1/1	0.88	0.17	72,72,72,72	0
54	MG	1a	1631	1/1	0.88	0.21	62,62,62,62	0
54	MG	1B	220	1/1	0.88	0.10	54,54,54,54	0
54	MG	1e	3001	1/1	0.88	0.15	65,65,65,65	0
54	MG	2A	3063	1/1	0.89	0.08	45,45,45,45	0
54	MG	1A	3333	1/1	0.89	0.12	60,60,60,60	0
54	MG	2A	3305	1/1	0.89	0.24	41,41,41,41	0
54	MG	2A	3023	1/1	0.89	0.08	32,32,32,32	0
54	MG	1A	4017	1/1	0.89	0.33	52,52,52,52	0
54	MG	10	103	1/1	0.89	0.12	42,42,42,42	0
54	MG	1A	3256	1/1	0.89	0.24	43,43,43,43	0
54	MG	2A	3239	1/1	0.89	0.13	61,61,61,61	0
54	MG	2A	3152	1/1	0.89	0.30	70,70,70,70	0
54	MG	2A	3653	1/1	0.89	0.38	50,50,50,50	0
54	MG	2A	3631	1/1	0.89	0.42	64,64,64,64	0
54	MG	1a	1737	1/1	0.89	0.16	63,63,63,63	0
54	MG	1A	3902	1/1	0.89	0.39	49,49,49,49	0
54	MG	1a	1841	1/1	0.89	0.06	68,68,68,68	0
54	MG	2A	3426	1/1	0.89	0.20	62,62,62,62	0
54	MG	1a	1677	1/1	0.89	0.13	57,57,57,57	0
54	MG	1A	3414	1/1	0.89	0.11	34,34,34,34	0
54	MG	2A	3321	1/1	0.89	0.20	39,39,39,39	0
54	MG	1A	3913	1/1	0.89	0.11	42,42,42,42	0
54	MG	1A	3630	1/1	0.89	0.14	44,44,44,44	0
54	MG	1N	203	1/1	0.89	0.07	50,50,50,50	0
54	MG	2a	1750	1/1	0.89	0.09	53,53,53,53	0
54	MG	2A	3657	1/1	0.89	0.05	82,82,82,82	0
54	MG	1f	3001	1/1	0.89	0.18	73,73,73,73	0
54	MG	2A	3414	1/1	0.89	0.17	40,40,40,40	0
54	MG	2A	3582	1/1	0.89	0.10	65,65,65,65	0
54	MG	1G	3003	1/1	0.89	0.10	60,60,60,60	0
54	MG	1A	4055	1/1	0.89	0.18	34,34,34,34	0
54	MG	1A	3927	1/1	0.89	0.14	27,27,27,27	0
54	MG	1A	3773	1/1	0.89	0.18	31,31,31,31	0
54	MG	2A	3051	1/1	0.89	0.11	54,54,54,54	0
54	MG	2A	3640	1/1	0.89	0.23	68,68,68,68	0
54	MG	1a	1678	1/1	0.89	0.20	54,54,54,54	0
54	MG	2A	3418	1/1	0.89	0.19	56,56,56,56	0
54	MG	1a	1727	1/1	0.89	0.18	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3085	1/1	0.89	0.20	68,68,68,68	0
54	MG	1A	3187	1/1	0.89	0.16	37,37,37,37	0
54	MG	2A	3484	1/1	0.89	0.15	46,46,46,46	0
54	MG	2A	3211	1/1	0.89	0.28	62,62,62,62	0
54	MG	1A	3675	1/1	0.89	0.18	55,55,55,55	0
54	MG	2a	1619	1/1	0.89	0.23	57,57,57,57	0
54	MG	2A	3171	1/1	0.89	0.16	48,48,48,48	0
54	MG	2A	3044	1/1	0.89	0.12	72,72,72,72	0
54	MG	1B	233	1/1	0.89	0.10	59,59,59,59	0
54	MG	2A	3561	1/1	0.89	0.20	52,52,52,52	0
54	MG	1a	1625	1/1	0.89	0.11	55,55,55,55	0
54	MG	1a	1768	1/1	0.89	0.10	64,64,64,64	0
54	MG	2A	3616	1/1	0.89	0.10	58,58,58,58	0
54	MG	2A	3444	1/1	0.89	0.18	37,37,37,37	0
54	MG	1a	1745	1/1	0.89	0.18	78,78,78,78	0
54	MG	1a	1718	1/1	0.89	0.19	59,59,59,59	0
54	MG	1A	3772	1/1	0.89	0.11	41,41,41,41	0
54	MG	2A	3168	1/1	0.89	0.24	65,65,65,65	0
54	MG	2A	3158	1/1	0.89	0.14	52,52,52,52	0
54	MG	2A	3592	1/1	0.89	0.22	48,48,48,48	0
54	MG	1a	1793	1/1	0.89	0.17	79,79,79,79	0
54	MG	2A	3565	1/1	0.89	0.20	35,35,35,35	0
54	MG	1a	1613	1/1	0.89	0.10	52,52,52,52	0
54	MG	2A	3603	1/1	0.89	0.13	54,54,54,54	0
54	MG	1A	3362	1/1	0.89	0.10	48,48,48,48	0
54	MG	1B	216	1/1	0.89	0.15	43,43,43,43	0
54	MG	2I	8001	1/1	0.89	0.27	59,59,59,59	0
54	MG	1A	3531	1/1	0.89	0.19	61,61,61,61	0
54	MG	1A	3029	1/1	0.89	0.10	31,31,31,31	0
54	MG	2A	3147	1/1	0.89	0.26	57,57,57,57	0
54	MG	2A	3629	1/1	0.89	0.36	79,79,79,79	0
54	MG	2A	3665	1/1	0.89	0.15	42,42,42,42	0
54	MG	2a	1613	1/1	0.89	0.09	44,44,44,44	0
54	MG	2A	3222	1/1	0.89	0.20	66,66,66,66	0
54	MG	1A	3206	1/1	0.89	0.23	43,43,43,43	0
54	MG	2R	202	1/1	0.89	0.18	46,46,46,46	0
54	MG	1A	3612	1/1	0.89	0.16	49,49,49,49	0
54	MG	2a	1761	1/1	0.89	0.12	73,73,73,73	0
59	ZN	24	501	1/1	0.89	0.04	108,108,108,108	0
54	MG	1A	3517	1/1	0.89	0.19	56,56,56,56	0
54	MG	1A	3324	1/1	0.89	0.12	31,31,31,31	0
54	MG	2A	3425	1/1	0.89	0.19	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3475	1/1	0.89	0.16	53,53,53,53	0
54	MG	2A	3455	1/1	0.89	0.23	46,46,46,46	0
54	MG	2A	3317	1/1	0.89	0.20	55,55,55,55	0
54	MG	1a	1742	1/1	0.89	0.11	80,80,80,80	0
54	MG	2A	3506	1/1	0.89	0.24	60,60,60,60	0
54	MG	1a	1757	1/1	0.89	0.27	68,68,68,68	0
54	MG	2A	3504	1/1	0.89	0.14	52,52,52,52	0
54	MG	1A	3071	1/1	0.89	0.13	35,35,35,35	0
54	MG	1d	505	1/1	0.89	0.15	81,81,81,81	0
54	MG	1a	1666	1/1	0.89	0.13	58,58,58,58	0
54	MG	2A	3001	1/1	0.89	0.14	48,48,48,48	0
54	MG	1A	3046	1/1	0.89	0.26	59,59,59,59	0
54	MG	1i	3001	1/1	0.89	0.11	64,64,64,64	0
54	MG	1A	3710	1/1	0.89	0.15	36,36,36,36	0
54	MG	2a	1659	1/1	0.89	0.12	59,59,59,59	0
54	MG	1A	3488	1/1	0.89	0.15	57,57,57,57	0
54	MG	2A	3535	1/1	0.89	0.20	56,56,56,56	0
54	MG	2A	3020	1/1	0.89	0.14	58,58,58,58	0
54	MG	2a	1755	1/1	0.89	0.05	66,66,66,66	0
54	MG	2a	1748	1/1	0.89	0.12	65,65,65,65	0
54	MG	1a	1725	1/1	0.89	0.11	70,70,70,70	0
54	MG	2A	3604	1/1	0.89	0.23	56,56,56,56	0
54	MG	2A	3374	1/1	0.90	0.13	54,54,54,54	0
54	MG	2A	3431	1/1	0.90	0.53	53,53,53,53	0
54	MG	1A	3417	1/1	0.90	0.13	35,35,35,35	0
54	MG	1A	3261	1/1	0.90	0.14	57,57,57,57	0
54	MG	1A	3742	1/1	0.90	0.11	73,73,73,73	0
54	MG	1A	3567	1/1	0.90	0.20	54,54,54,54	0
54	MG	1A	3769	1/1	0.90	0.08	50,50,50,50	0
54	MG	1a	1722	1/1	0.90	0.12	70,70,70,70	0
54	MG	1A	3239	1/1	0.90	0.11	70,70,70,70	0
54	MG	1a	1850	1/1	0.90	0.19	78,78,78,78	0
54	MG	1A	4061	1/1	0.90	0.43	41,41,41,41	0
54	MG	1A	4011	1/1	0.90	0.21	46,46,46,46	0
54	MG	1A	4056	1/1	0.90	0.44	32,32,32,32	0
54	MG	1A	3109	1/1	0.90	0.28	35,35,35,35	0
54	MG	2a	1721	1/1	0.90	0.10	67,67,67,67	0
54	MG	1A	3874	1/1	0.90	0.10	61,61,61,61	0
54	MG	1A	3420	1/1	0.90	0.15	42,42,42,42	0
54	MG	13	101	1/1	0.90	0.19	40,40,40,40	0
54	MG	1A	3445	1/1	0.90	0.12	27,27,27,27	0
54	MG	1A	3635	1/1	0.90	0.13	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	1739	1/1	0.90	0.22	71,71,71,71	0
54	MG	1A	3125	1/1	0.90	0.15	31,31,31,31	0
54	MG	2A	3179	1/1	0.90	0.49	42,42,42,42	0
54	MG	2A	3039	1/1	0.90	0.15	61,61,61,61	0
54	MG	2a	1784	1/1	0.90	0.14	80,80,80,80	0
54	MG	1a	1747	1/1	0.90	0.18	57,57,57,57	0
54	MG	1a	1854	1/1	0.90	0.26	53,53,53,53	0
54	MG	1y	3004	1/1	0.90	0.12	72,72,72,72	0
57	MPD	1a	1860	8/8	0.90	0.27	50,63,66,67	0
54	MG	1a	1730	1/1	0.90	0.12	55,55,55,55	0
54	MG	2A	3598	1/1	0.90	0.09	51,51,51,51	0
54	MG	1A	3860	1/1	0.90	0.21	53,53,53,53	0
54	MG	1A	3267	1/1	0.90	0.13	52,52,52,52	0
54	MG	2A	3696	1/1	0.90	0.12	34,34,34,34	0
54	MG	1a	1683	1/1	0.90	0.14	44,44,44,44	0
54	MG	1A	4003	1/1	0.90	0.34	55,55,55,55	0
54	MG	1A	4004	1/1	0.90	0.12	47,47,47,47	0
54	MG	1A	3506	1/1	0.90	0.18	47,47,47,47	0
54	MG	2f	3001	1/1	0.90	0.14	52,52,52,52	0
54	MG	2a	1675	1/1	0.90	0.15	57,57,57,57	0
54	MG	2A	3345	1/1	0.90	0.11	56,56,56,56	0
54	MG	1a	1758	1/1	0.90	0.12	73,73,73,73	0
54	MG	2A	3206	1/1	0.90	0.14	55,55,55,55	0
54	MG	2A	3542	1/1	0.90	0.18	62,62,62,62	0
54	MG	1A	3481	1/1	0.90	0.18	42,42,42,42	0
54	MG	1A	3307	1/1	0.90	0.15	40,40,40,40	0
54	MG	2A	3139	1/1	0.90	0.18	63,63,63,63	0
54	MG	2a	1644	1/1	0.90	0.09	70,70,70,70	0
54	MG	2A	3594	1/1	0.90	0.17	55,55,55,55	0
54	MG	2a	1642	1/1	0.90	0.17	61,61,61,61	0
54	MG	1A	3978	1/1	0.90	0.14	65,65,65,65	0
54	MG	2N	8001	1/1	0.90	0.08	62,62,62,62	0
54	MG	1A	3697	1/1	0.90	0.12	29,29,29,29	0
54	MG	2A	3103	1/1	0.90	0.27	41,41,41,41	0
54	MG	1a	1721	1/1	0.90	0.12	66,66,66,66	0
54	MG	1A	3144	1/1	0.90	0.12	40,40,40,40	0
54	MG	1A	3730	1/1	0.90	0.18	60,60,60,60	0
54	MG	1A	3897	1/1	0.90	0.13	60,60,60,60	0
54	MG	2A	3148	1/1	0.90	0.17	60,60,60,60	0
54	MG	1A	3908	1/1	0.90	0.17	44,44,44,44	0
54	MG	1O	8001	1/1	0.90	0.08	50,50,50,50	0
54	MG	1H	8002	1/1	0.90	0.18	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3702	1/1	0.90	0.12	29,29,29,29	0
54	MG	2A	3486	1/1	0.90	0.23	43,43,43,43	0
54	MG	1A	3266	1/1	0.90	0.09	70,70,70,70	0
54	MG	1A	3674	1/1	0.90	0.24	56,56,56,56	0
54	MG	17	101	1/1	0.90	0.12	47,47,47,47	0
54	MG	1A	3780	1/1	0.90	0.20	44,44,44,44	0
54	MG	1A	3857	1/1	0.90	0.18	67,67,67,67	0
54	MG	1A	3113	1/1	0.90	0.16	35,35,35,35	0
54	MG	1A	3260	1/1	0.90	0.24	51,51,51,51	0
54	MG	1A	3104	1/1	0.90	0.55	42,42,42,42	0
54	MG	1A	3943	1/1	0.90	0.06	66,66,66,66	0
54	MG	2O	8002	1/1	0.90	0.11	57,57,57,57	0
54	MG	2A	3416	1/1	0.90	0.20	58,58,58,58	0
54	MG	2A	3311	1/1	0.90	0.20	42,42,42,42	0
54	MG	1A	3399	1/1	0.90	0.09	60,60,60,60	0
54	MG	1A	4032	1/1	0.90	0.09	44,44,44,44	0
54	MG	2A	3523	1/1	0.90	0.09	75,75,75,75	0
54	MG	1A	3432	1/1	0.90	0.13	23,23,23,23	0
54	MG	1a	1741	1/1	0.90	0.11	66,66,66,66	0
54	MG	1A	3570	1/1	0.90	0.23	53,53,53,53	0
54	MG	2A	3557	1/1	0.90	0.12	60,60,60,60	0
54	MG	2A	3662	1/1	0.90	0.17	65,65,65,65	0
54	MG	1A	4028	1/1	0.90	0.12	59,59,59,59	0
54	MG	1a	1689	1/1	0.90	0.11	74,74,74,74	0
54	MG	2A	3520	1/1	0.90	0.15	70,70,70,70	0
54	MG	1A	3869	1/1	0.90	0.09	55,55,55,55	0
54	MG	2A	3549	1/1	0.90	0.15	62,62,62,62	0
54	MG	1A	3226	1/1	0.90	0.21	54,54,54,54	0
54	MG	1A	4015	1/1	0.90	0.12	61,61,61,61	0
54	MG	1A	3966	1/1	0.90	0.12	70,70,70,70	0
54	MG	2A	3318	1/1	0.90	0.26	54,54,54,54	0
54	MG	2a	1687	1/1	0.90	0.25	61,61,61,61	0
54	MG	2A	3163	1/1	0.90	0.15	59,59,59,59	0
57	MPD	1T	205	8/8	0.90	0.26	67,71,75,76	0
54	MG	2A	3126	1/1	0.90	0.29	49,49,49,49	0
54	MG	1a	1763	1/1	0.90	0.10	53,53,53,53	0
54	MG	2a	1678	1/1	0.90	0.18	63,63,63,63	0
54	MG	1A	3898	1/1	0.90	0.13	61,61,61,61	0
54	MG	2a	1745	1/1	0.90	0.16	64,64,64,64	0
54	MG	2A	3301	1/1	0.90	0.16	33,33,33,33	0
54	MG	2a	1638	1/1	0.90	0.24	75,75,75,75	0
54	MG	1A	3893	1/1	0.90	0.10	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3594	1/1	0.90	0.15	42,42,42,42	0
54	MG	1A	3177	1/1	0.90	0.34	38,38,38,38	0
54	MG	1A	3967	1/1	0.90	0.28	51,51,51,51	0
54	MG	1B	212	1/1	0.90	0.10	59,59,59,59	0
54	MG	1D	310	1/1	0.90	0.16	64,64,64,64	0
54	MG	2A	3451	1/1	0.90	0.14	70,70,70,70	0
54	MG	1A	3332	1/1	0.90	0.10	66,66,66,66	0
54	MG	1a	1760	1/1	0.90	0.11	67,67,67,67	0
54	MG	1a	1769	1/1	0.90	0.18	60,60,60,60	0
54	MG	1A	3580	1/1	0.90	0.18	42,42,42,42	0
54	MG	2a	1725	1/1	0.91	0.21	63,63,63,63	0
54	MG	1A	3212	1/1	0.91	0.19	46,46,46,46	0
54	MG	1A	3466	1/1	0.91	0.18	16,16,16,16	0
54	MG	1X	101	1/1	0.91	0.14	67,67,67,67	0
54	MG	1a	1673	1/1	0.91	0.14	60,60,60,60	0
54	MG	1A	3651	1/1	0.91	0.10	34,34,34,34	0
54	MG	1A	3707	1/1	0.91	0.21	44,44,44,44	0
54	MG	2A	3477	1/1	0.91	0.23	58,58,58,58	0
54	MG	1A	3922	1/1	0.91	0.14	67,67,67,67	0
54	MG	1A	3463	1/1	0.91	0.17	17,17,17,17	0
54	MG	1A	3176	1/1	0.91	0.43	32,32,32,32	0
54	MG	1A	3172	1/1	0.91	0.42	48,48,48,48	0
54	MG	1a	1781	1/1	0.91	0.09	68,68,68,68	0
54	MG	1A	3715	1/1	0.91	0.23	49,49,49,49	0
54	MG	1A	3514	1/1	0.91	0.10	47,47,47,47	0
54	MG	1A	3838	1/1	0.91	0.09	49,49,49,49	0
54	MG	2A	3064	1/1	0.91	0.45	50,50,50,50	0
54	MG	2A	3165	1/1	0.91	0.45	50,50,50,50	0
54	MG	1A	3036	1/1	0.91	0.17	50,50,50,50	0
54	MG	1A	3579	1/1	0.91	0.15	55,55,55,55	0
54	MG	2A	3258	1/1	0.91	0.13	45,45,45,45	0
54	MG	1A	3359	1/1	0.91	0.17	20,20,20,20	0
54	MG	1A	4013	1/1	0.91	0.52	47,47,47,47	0
54	MG	2A	3070	1/1	0.91	0.24	43,43,43,43	0
54	MG	1A	3158	1/1	0.91	0.10	52,52,52,52	0
54	MG	2A	3026	1/1	0.91	0.14	34,34,34,34	0
54	MG	1A	3681	1/1	0.91	0.32	67,67,67,67	0
54	MG	1B	231	1/1	0.91	0.15	68,68,68,68	0
54	MG	2a	1736	1/1	0.91	0.22	63,63,63,63	0
54	MG	1W	3001	1/1	0.91	0.32	42,42,42,42	0
54	MG	1f	3002	1/1	0.91	0.13	54,54,54,54	0
54	MG	1A	3521	1/1	0.91	0.13	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3843	1/1	0.91	0.10	48,48,48,48	0
54	MG	2A	3424	1/1	0.91	0.16	57,57,57,57	0
54	MG	1a	1691	1/1	0.91	0.15	41,41,41,41	0
54	MG	1A	3436	1/1	0.91	0.20	39,39,39,39	0
54	MG	1A	3385	1/1	0.91	0.21	27,27,27,27	0
54	MG	1A	3621	1/1	0.91	0.09	44,44,44,44	0
54	MG	1A	3372	1/1	0.91	0.17	18,18,18,18	0
54	MG	1A	3535	1/1	0.91	0.18	44,44,44,44	0
54	MG	13	102	1/1	0.91	0.30	59,59,59,59	0
54	MG	2A	3282	1/1	0.91	0.16	50,50,50,50	0
54	MG	1A	3057	1/1	0.91	0.14	42,42,42,42	0
54	MG	1a	1847	1/1	0.91	0.15	77,77,77,77	0
54	MG	2A	3192	1/1	0.91	0.66	34,34,34,34	0
54	MG	1A	4020	1/1	0.91	0.13	43,43,43,43	0
54	MG	1A	3575	1/1	0.91	0.11	69,69,69,69	0
54	MG	2A	3182	1/1	0.91	0.08	48,48,48,48	0
54	MG	2a	1700	1/1	0.91	0.23	62,62,62,62	0
54	MG	1A	3035	1/1	0.91	0.28	30,30,30,30	0
54	MG	2A	3352	1/1	0.91	0.42	57,57,57,57	0
54	MG	2A	3559	1/1	0.91	0.21	43,43,43,43	0
54	MG	2A	3562	1/1	0.91	0.12	59,59,59,59	0
54	MG	2A	3302	1/1	0.91	0.12	67,67,67,67	0
54	MG	2A	3367	1/1	0.91	0.22	49,49,49,49	0
54	MG	1a	1729	1/1	0.91	0.17	63,63,63,63	0
54	MG	2B	221	1/1	0.91	0.13	62,62,62,62	0
54	MG	1A	3845	1/1	0.91	0.17	53,53,53,53	0
54	MG	2A	3536	1/1	0.91	0.07	56,56,56,56	0
54	MG	2B	215	1/1	0.91	0.14	90,90,90,90	0
54	MG	2A	3046	1/1	0.91	0.12	40,40,40,40	0
54	MG	1A	3474	1/1	0.91	0.37	38,38,38,38	0
54	MG	1A	3136	1/1	0.91	0.14	27,27,27,27	0
54	MG	1D	311	1/1	0.91	0.18	53,53,53,53	0
54	MG	2A	3659	1/1	0.91	0.56	78,78,78,78	0
54	MG	1A	3402	1/1	0.91	0.10	41,41,41,41	0
54	MG	1A	3522	1/1	0.91	0.18	47,47,47,47	0
54	MG	2A	3276	1/1	0.91	0.18	45,45,45,45	0
54	MG	1A	4022	1/1	0.91	0.14	37,37,37,37	0
54	MG	1a	1759	1/1	0.91	0.30	65,65,65,65	0
54	MG	1P	201	1/1	0.91	0.38	32,32,32,32	0
54	MG	2a	1667	1/1	0.91	0.19	46,46,46,46	0
54	MG	1A	3689	1/1	0.91	0.23	47,47,47,47	0
54	MG	2A	3507	1/1	0.91	0.30	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1h	3001	1/1	0.91	0.19	46,46,46,46	0
54	MG	2a	1666	1/1	0.91	0.13	67,67,67,67	0
54	MG	2A	3628	1/1	0.91	0.24	68,68,68,68	0
54	MG	1F	301	1/1	0.91	0.21	47,47,47,47	0
54	MG	2A	3280	1/1	0.91	0.21	61,61,61,61	0
54	MG	1A	3901	1/1	0.91	0.22	35,35,35,35	0
54	MG	1A	3569	1/1	0.91	0.22	23,23,23,23	0
54	MG	1A	3072	1/1	0.91	0.39	34,34,34,34	0
54	MG	1a	1670	1/1	0.91	0.17	70,70,70,70	0
54	MG	1T	204	1/1	0.91	0.07	67,67,67,67	0
54	MG	2a	1697	1/1	0.91	0.17	57,57,57,57	0
54	MG	1A	3050	1/1	0.91	0.39	40,40,40,40	0
54	MG	2A	3585	1/1	0.91	0.24	65,65,65,65	0
54	MG	2A	3298	1/1	0.91	0.14	33,33,33,33	0
54	MG	2A	3544	1/1	0.91	0.36	52,52,52,52	0
54	MG	1A	3703	1/1	0.91	0.19	17,17,17,17	0
54	MG	1a	1711	1/1	0.91	0.18	45,45,45,45	0
54	MG	1H	8001	1/1	0.91	0.20	62,62,62,62	0
54	MG	2A	3574	1/1	0.91	0.31	50,50,50,50	0
54	MG	2A	3238	1/1	0.91	0.12	57,57,57,57	0
54	MG	1B	204	1/1	0.91	0.35	62,62,62,62	0
54	MG	1A	3316	1/1	0.91	0.19	67,67,67,67	0
54	MG	1a	1690	1/1	0.91	0.13	51,51,51,51	0
54	MG	1a	1699	1/1	0.91	0.11	57,57,57,57	0
54	MG	2A	3255	1/1	0.91	0.20	59,59,59,59	0
54	MG	2A	3391	1/1	0.91	0.18	32,32,32,32	0
54	MG	2a	1715	1/1	0.91	0.08	75,75,75,75	0
54	MG	2a	1623	1/1	0.91	0.14	70,70,70,70	0
54	MG	1A	3533	1/1	0.91	0.30	69,69,69,69	0
54	MG	1a	1782	1/1	0.91	0.13	62,62,62,62	0
54	MG	2A	3260	1/1	0.91	0.09	41,41,41,41	0
54	MG	1A	3389	1/1	0.91	0.13	47,47,47,47	0
54	MG	1a	1816	1/1	0.91	0.10	61,61,61,61	0
54	MG	2A	3626	1/1	0.91	0.51	69,69,69,69	0
54	MG	1A	3634	1/1	0.91	0.23	27,27,27,27	0
54	MG	1A	3729	1/1	0.91	0.13	31,31,31,31	0
54	MG	1A	3971	1/1	0.91	0.08	65,65,65,65	0
54	MG	2A	3589	1/1	0.91	0.13	66,66,66,66	0
54	MG	2A	3573	1/1	0.91	0.23	49,49,49,49	0
54	MG	1A	3578	1/1	0.91	0.16	44,44,44,44	0
54	MG	1A	3801	1/1	0.91	0.16	57,57,57,57	0
54	MG	1U	203	1/1	0.91	0.15	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2I	3001	1/1	0.91	0.10	60,60,60,60	0
54	MG	2A	3099	1/1	0.91	0.37	38,38,38,38	0
54	MG	2A	3151	1/1	0.91	0.19	61,61,61,61	0
54	MG	2A	3032	1/1	0.91	0.16	44,44,44,44	0
54	MG	2A	3625	1/1	0.91	0.11	66,66,66,66	0
54	MG	1A	3899	1/1	0.91	0.07	49,49,49,49	0
57	MPD	2A	3693	8/8	0.91	0.17	51,60,65,68	0
54	MG	2A	3193	1/1	0.91	0.45	39,39,39,39	0
54	MG	1a	1692	1/1	0.91	0.20	60,60,60,60	0
54	MG	1R	201	1/1	0.91	0.15	54,54,54,54	0
54	MG	2A	3294	1/1	0.91	0.15	29,29,29,29	0
54	MG	2A	3257	1/1	0.91	0.25	47,47,47,47	0
54	MG	2A	3337	1/1	0.91	0.18	42,42,42,42	0
54	MG	1A	3211	1/1	0.91	0.10	60,60,60,60	0
54	MG	1A	3777	1/1	0.91	0.14	23,23,23,23	0
54	MG	2a	1624	1/1	0.91	0.14	61,61,61,61	0
54	MG	1A	3235	1/1	0.91	0.45	27,27,27,27	0
54	MG	2A	3306	1/1	0.91	0.16	48,48,48,48	0
54	MG	2A	3427	1/1	0.91	0.18	54,54,54,54	0
54	MG	2A	3471	1/1	0.91	0.25	37,37,37,37	0
54	MG	2A	3448	1/1	0.91	0.38	66,66,66,66	0
54	MG	1a	1717	1/1	0.91	0.21	52,52,52,52	0
54	MG	2A	3420	1/1	0.91	0.21	40,40,40,40	0
54	MG	1A	3370	1/1	0.91	0.15	40,40,40,40	0
54	MG	1A	3989	1/1	0.91	0.15	51,51,51,51	0
54	MG	1a	1748	1/1	0.91	0.11	64,64,64,64	0
54	MG	1A	3413	1/1	0.91	0.21	15,15,15,15	0
54	MG	2a	1735	1/1	0.91	0.10	60,60,60,60	0
54	MG	2A	3402	1/1	0.91	0.18	54,54,54,54	0
54	MG	2D	304	1/1	0.91	0.51	52,52,52,52	0
54	MG	1H	8003	1/1	0.91	0.13	41,41,41,41	0
54	MG	2T	3002	1/1	0.91	0.09	69,69,69,69	0
54	MG	1a	1751	1/1	0.91	0.13	63,63,63,63	0
54	MG	1A	3895	1/1	0.91	0.14	27,27,27,27	0
54	MG	2A	3472	1/1	0.91	0.18	58,58,58,58	0
54	MG	1A	3725	1/1	0.91	0.20	61,61,61,61	0
54	MG	1A	3626	1/1	0.91	0.17	41,41,41,41	0
54	MG	1A	3468	1/1	0.92	0.23	51,51,51,51	0
54	MG	2A	3326	1/1	0.92	0.23	44,44,44,44	0
54	MG	2A	3183	1/1	0.92	0.15	53,53,53,53	0
54	MG	2A	3509	1/1	0.92	0.15	47,47,47,47	0
54	MG	2A	3422	1/1	0.92	0.09	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3657	1/1	0.92	0.21	27,27,27,27	0
54	MG	2D	305	1/1	0.92	0.35	40,40,40,40	0
54	MG	2A	3671	1/1	0.92	0.29	53,53,53,53	0
54	MG	2A	3467	1/1	0.92	0.14	62,62,62,62	0
54	MG	1A	3330	1/1	0.92	0.14	39,39,39,39	0
54	MG	2A	3595	1/1	0.92	0.19	48,48,48,48	0
54	MG	2A	3464	1/1	0.92	0.18	56,56,56,56	0
54	MG	1A	4043	1/1	0.92	0.35	30,30,30,30	0
54	MG	1A	3438	1/1	0.92	0.14	25,25,25,25	0
54	MG	1A	3588	1/1	0.92	0.14	49,49,49,49	0
54	MG	2B	216	1/1	0.92	0.16	67,67,67,67	0
54	MG	1b	3001	1/1	0.92	0.20	68,68,68,68	0
54	MG	1A	3337	1/1	0.92	0.12	47,47,47,47	0
54	MG	2A	3143	1/1	0.92	0.11	58,58,58,58	0
54	MG	2A	3525	1/1	0.92	0.20	42,42,42,42	0
54	MG	2a	1646	1/1	0.92	0.16	59,59,59,59	0
54	MG	2a	1712	1/1	0.92	0.19	63,63,63,63	0
54	MG	1Q	203	1/1	0.92	0.17	35,35,35,35	0
54	MG	2a	1701	1/1	0.92	0.11	63,63,63,63	0
54	MG	2A	3394	1/1	0.92	0.16	51,51,51,51	0
54	MG	1a	1803	1/1	0.92	0.11	78,78,78,78	0
54	MG	1A	3871	1/1	0.92	0.15	41,41,41,41	0
54	MG	1A	3059	1/1	0.92	0.12	33,33,33,33	0
54	MG	1a	1783	1/1	0.92	0.13	68,68,68,68	0
54	MG	2a	1780	1/1	0.92	0.05	66,66,66,66	0
54	MG	1A	3771	1/1	0.92	0.11	34,34,34,34	0
54	MG	1A	3157	1/1	0.92	0.32	36,36,36,36	0
54	MG	2a	1760	1/1	0.92	0.12	66,66,66,66	0
54	MG	1a	1663	1/1	0.92	0.20	53,53,53,53	0
54	MG	1A	3234	1/1	0.92	0.26	26,26,26,26	0
54	MG	2D	306	1/1	0.92	0.21	32,32,32,32	0
54	MG	1B	224	1/1	0.92	0.17	49,49,49,49	0
54	MG	2A	3368	1/1	0.92	0.10	41,41,41,41	0
54	MG	2A	3619	1/1	0.92	0.18	68,68,68,68	0
54	MG	1A	3993	1/1	0.92	0.17	50,50,50,50	0
54	MG	2A	3570	1/1	0.92	0.21	68,68,68,68	0
54	MG	1A	3034	1/1	0.92	0.20	43,43,43,43	0
54	MG	2A	3197	1/1	0.92	0.14	66,66,66,66	0
54	MG	1N	202	1/1	0.92	0.10	60,60,60,60	0
54	MG	2A	3047	1/1	0.92	0.11	55,55,55,55	0
54	MG	1A	3620	1/1	0.92	0.19	32,32,32,32	0
54	MG	1a	1801	1/1	0.92	0.11	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3981	1/1	0.92	0.09	53,53,53,53	0
54	MG	1a	1657	1/1	0.92	0.12	59,59,59,59	0
54	MG	1A	3151	1/1	0.92	0.49	37,37,37,37	0
54	MG	2A	3031	1/1	0.92	0.10	57,57,57,57	0
54	MG	1A	3854	1/1	0.92	0.11	64,64,64,64	0
54	MG	2B	219	1/1	0.92	0.11	73,73,73,73	0
54	MG	1A	3159	1/1	0.92	0.18	43,43,43,43	0
54	MG	1B	229	1/1	0.92	0.12	63,63,63,63	0
54	MG	1e	3002	1/1	0.92	0.25	58,58,58,58	0
54	MG	2A	3185	1/1	0.92	0.12	57,57,57,57	0
54	MG	1A	3694	1/1	0.92	0.09	27,27,27,27	0
54	MG	1a	1609	1/1	0.92	0.18	55,55,55,55	0
54	MG	2A	3190	1/1	0.92	0.36	38,38,38,38	0
54	MG	1A	3542	1/1	0.92	0.10	49,49,49,49	0
54	MG	1A	3272	1/1	0.92	0.18	42,42,42,42	0
54	MG	1a	1844	1/1	0.92	0.09	65,65,65,65	0
54	MG	2A	3611	1/1	0.92	0.22	55,55,55,55	0
54	MG	1A	3390	1/1	0.92	0.09	54,54,54,54	0
54	MG	2B	207	1/1	0.92	0.16	56,56,56,56	0
54	MG	1A	4012	1/1	0.92	0.08	41,41,41,41	0
54	MG	2A	3643	1/1	0.92	0.12	62,62,62,62	0
54	MG	1A	3426	1/1	0.92	0.19	43,43,43,43	0
54	MG	2A	3634	1/1	0.92	0.08	68,68,68,68	0
54	MG	1A	4064	1/1	0.92	0.08	40,40,40,40	0
54	MG	1A	3477	1/1	0.92	0.11	36,36,36,36	0
54	MG	2A	3336	1/1	0.92	0.16	54,54,54,54	0
54	MG	1A	3946	1/1	0.92	0.10	75,75,75,75	0
54	MG	1A	3248	1/1	0.92	0.16	45,45,45,45	0
54	MG	1A	3743	1/1	0.92	0.17	26,26,26,26	0
54	MG	2A	3488	1/1	0.92	0.35	52,52,52,52	0
54	MG	1A	3387	1/1	0.92	0.12	45,45,45,45	0
54	MG	1A	3665	1/1	0.92	0.18	40,40,40,40	0
54	MG	1A	3288	1/1	0.92	0.19	51,51,51,51	0
54	MG	1A	3118	1/1	0.92	0.43	30,30,30,30	0
54	MG	2A	3586	1/1	0.92	0.22	51,51,51,51	0
54	MG	2A	3605	1/1	0.92	0.13	52,52,52,52	0
57	MPD	18	102	8/8	0.92	0.28	22,38,39,47	0
54	MG	1A	4050	1/1	0.92	0.29	27,27,27,27	0
54	MG	1A	3623	1/1	0.92	0.11	66,66,66,66	0
54	MG	1A	3406	1/1	0.92	0.09	45,45,45,45	0
54	MG	2A	3666	1/1	0.92	0.12	71,71,71,71	0
54	MG	1A	3319	1/1	0.92	0.16	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3114	1/1	0.92	0.17	49,49,49,49	0
54	MG	2d	301	1/1	0.92	0.08	63,63,63,63	0
54	MG	2A	3554	1/1	0.92	0.15	61,61,61,61	0
54	MG	1A	3793	1/1	0.92	0.17	49,49,49,49	0
57	MPD	2B	222	8/8	0.92	0.19	62,67,73,77	0
54	MG	1A	3066	1/1	0.92	0.48	29,29,29,29	0
54	MG	2A	3369	1/1	0.92	0.10	62,62,62,62	0
54	MG	2A	3519	1/1	0.92	0.23	38,38,38,38	0
54	MG	14	502	1/1	0.92	0.11	67,67,67,67	0
54	MG	2A	3493	1/1	0.92	0.10	53,53,53,53	0
54	MG	2a	1676	1/1	0.92	0.10	57,57,57,57	0
54	MG	2A	3673	1/1	0.92	0.39	72,72,72,72	0
54	MG	2a	1690	1/1	0.92	0.12	62,62,62,62	0
54	MG	2a	1737	1/1	0.92	0.10	68,68,68,68	0
54	MG	2A	3344	1/1	0.92	0.21	42,42,42,42	0
54	MG	2A	3458	1/1	0.92	0.26	58,58,58,58	0
54	MG	2a	1768	1/1	0.92	0.17	79,79,79,79	0
54	MG	2O	8001	1/1	0.92	0.12	64,64,64,64	0
54	MG	1A	3138	1/1	0.92	0.20	38,38,38,38	0
54	MG	1A	3484	1/1	0.92	0.11	48,48,48,48	0
54	MG	1A	3661	1/1	0.92	0.12	54,54,54,54	0
54	MG	2A	3356	1/1	0.92	0.52	45,45,45,45	0
54	MG	1A	3428	1/1	0.92	0.18	17,17,17,17	0
54	MG	1A	3610	1/1	0.92	0.08	55,55,55,55	0
54	MG	1A	3380	1/1	0.92	0.20	23,23,23,23	0
54	MG	1A	4019	1/1	0.92	0.09	48,48,48,48	0
54	MG	1a	1820	1/1	0.92	0.24	58,58,58,58	0
54	MG	2A	3703	1/1	0.92	0.23	41,41,41,41	0
54	MG	1B	228	1/1	0.92	0.13	43,43,43,43	0
54	MG	1A	3155	1/1	0.92	0.12	58,58,58,58	0
54	MG	2a	1749	1/1	0.92	0.09	69,69,69,69	0
54	MG	1A	3448	1/1	0.92	0.13	44,44,44,44	0
54	MG	1A	3291	1/1	0.92	0.14	25,25,25,25	0
54	MG	1A	3295	1/1	0.92	0.18	28,28,28,28	0
54	MG	1D	307	1/1	0.92	0.45	66,66,66,66	0
54	MG	1A	3361	1/1	0.92	0.20	45,45,45,45	0
54	MG	1a	1738	1/1	0.92	0.06	72,72,72,72	0
54	MG	1A	3015	1/1	0.92	0.21	55,55,55,55	0
54	MG	1a	1647	1/1	0.92	0.18	51,51,51,51	0
54	MG	2A	3489	1/1	0.92	0.28	54,54,54,54	0
54	MG	1A	3040	1/1	0.92	0.23	51,51,51,51	0
54	MG	15	104	1/1	0.92	0.18	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3215	1/1	0.92	0.23	55,55,55,55	0
54	MG	2T	3001	1/1	0.92	0.21	58,58,58,58	0
54	MG	2A	3178	1/1	0.92	0.46	54,54,54,54	0
54	MG	1A	3571	1/1	0.92	0.14	47,47,47,47	0
54	MG	1a	1621	1/1	0.92	0.15	44,44,44,44	0
54	MG	1B	214	1/1	0.92	0.08	47,47,47,47	0
54	MG	1A	3489	1/1	0.92	0.19	58,58,58,58	0
54	MG	2a	1680	1/1	0.92	0.10	50,50,50,50	0
54	MG	1B	201	1/1	0.92	0.58	38,38,38,38	0
54	MG	2A	3685	1/1	0.92	0.26	42,42,42,42	0
54	MG	2A	3237	1/1	0.92	0.18	49,49,49,49	0
54	MG	2A	3508	1/1	0.92	0.21	53,53,53,53	0
54	MG	1A	3055	1/1	0.92	0.28	39,39,39,39	0
54	MG	2A	3401	1/1	0.92	0.10	55,55,55,55	0
54	MG	1A	3606	1/1	0.92	0.20	36,36,36,36	0
54	MG	2A	3130	1/1	0.92	0.39	39,39,39,39	0
54	MG	2A	3314	1/1	0.92	0.18	41,41,41,41	0
54	MG	2A	3539	1/1	0.92	0.17	57,57,57,57	0
54	MG	1A	3523	1/1	0.92	0.16	29,29,29,29	0
54	MG	2A	3075	1/1	0.92	0.20	46,46,46,46	0
54	MG	2A	3475	1/1	0.92	0.28	62,62,62,62	0
54	MG	2A	3161	1/1	0.92	0.19	46,46,46,46	0
54	MG	2A	3351	1/1	0.92	0.12	36,36,36,36	0
54	MG	1a	1650	1/1	0.92	0.21	35,35,35,35	0
54	MG	1n	503	1/1	0.92	0.16	58,58,58,58	0
54	MG	2A	3112	1/1	0.92	0.21	40,40,40,40	0
54	MG	2a	1681	1/1	0.92	0.12	71,71,71,71	0
54	MG	10	102	1/1	0.92	0.07	45,45,45,45	0
54	MG	2A	3533	1/1	0.92	0.19	53,53,53,53	0
54	MG	1A	3002	1/1	0.92	0.14	44,44,44,44	0
54	MG	2A	3221	1/1	0.92	0.15	52,52,52,52	0
54	MG	1A	3961	1/1	0.92	0.15	61,61,61,61	0
54	MG	1A	3760	1/1	0.93	0.11	29,29,29,29	0
54	MG	2A	3512	1/1	0.93	0.29	56,56,56,56	0
54	MG	1A	3246	1/1	0.93	0.52	40,40,40,40	0
54	MG	1a	1679	1/1	0.93	0.12	58,58,58,58	0
54	MG	2B	211	1/1	0.93	0.13	71,71,71,71	0
54	MG	2A	3415	1/1	0.93	0.16	60,60,60,60	0
54	MG	1A	3785	1/1	0.93	0.34	36,36,36,36	0
54	MG	1D	309	1/1	0.93	0.33	65,65,65,65	0
54	MG	1A	3398	1/1	0.93	0.20	36,36,36,36	0
54	MG	2A	3612	1/1	0.93	0.19	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1W	3002	1/1	0.93	0.18	43,43,43,43	0
54	MG	1y	3002	1/1	0.93	0.12	56,56,56,56	0
54	MG	1A	3458	1/1	0.93	0.11	35,35,35,35	0
54	MG	1A	3976	1/1	0.93	0.09	46,46,46,46	0
54	MG	1A	3890	1/1	0.93	0.16	60,60,60,60	0
54	MG	1A	4068	1/1	0.93	0.37	35,35,35,35	0
54	MG	1A	3868	1/1	0.93	0.13	22,22,22,22	0
54	MG	1a	1770	1/1	0.93	0.17	73,73,73,73	0
54	MG	1A	3532	1/1	0.93	0.10	38,38,38,38	0
54	MG	1A	3706	1/1	0.93	0.18	22,22,22,22	0
54	MG	1a	1822	1/1	0.93	0.23	59,59,59,59	0
54	MG	1A	3592	1/1	0.93	0.16	54,54,54,54	0
54	MG	2A	3259	1/1	0.93	0.14	33,33,33,33	0
54	MG	1A	3540	1/1	0.93	0.20	43,43,43,43	0
54	MG	1A	3265	1/1	0.93	0.12	77,77,77,77	0
54	MG	2A	3674	1/1	0.93	0.14	52,52,52,52	0
54	MG	2A	3188	1/1	0.93	0.13	67,67,67,67	0
54	MG	1A	3695	1/1	0.93	0.17	59,59,59,59	0
54	MG	1a	1633	1/1	0.93	0.13	32,32,32,32	0
54	MG	2I	8002	1/1	0.93	0.18	81,81,81,81	0
54	MG	2A	3041	1/1	0.93	0.14	41,41,41,41	0
54	MG	2A	3128	1/1	0.93	0.10	62,62,62,62	0
54	MG	2A	3272	1/1	0.93	0.16	46,46,46,46	0
54	MG	1A	3154	1/1	0.93	0.68	40,40,40,40	0
54	MG	2A	3600	1/1	0.93	0.08	62,62,62,62	0
54	MG	1a	1765	1/1	0.93	0.34	59,59,59,59	0
54	MG	2A	3155	1/1	0.93	0.21	60,60,60,60	0
54	MG	2A	3136	1/1	0.93	0.11	42,42,42,42	0
54	MG	1a	1772	1/1	0.93	0.09	68,68,68,68	0
54	MG	1A	3487	1/1	0.93	0.21	55,55,55,55	0
54	MG	1A	3501	1/1	0.93	0.19	59,59,59,59	0
54	MG	1A	4074	1/1	0.93	0.30	38,38,38,38	0
54	MG	1A	3645	1/1	0.93	0.32	44,44,44,44	0
54	MG	1A	3190	1/1	0.93	0.38	30,30,30,30	0
54	MG	2a	1617	1/1	0.93	0.15	45,45,45,45	0
54	MG	1A	3972	1/1	0.93	0.20	55,55,55,55	0
54	MG	1A	3242	1/1	0.93	0.11	56,56,56,56	0
54	MG	1A	3813	1/1	0.93	0.14	27,27,27,27	0
54	MG	2A	3116	1/1	0.93	0.17	28,28,28,28	0
54	MG	1A	3218	1/1	0.93	0.33	30,30,30,30	0
54	MG	2A	3602	1/1	0.93	0.15	51,51,51,51	0
54	MG	1a	1651	1/1	0.93	0.27	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2a	1698	1/1	0.93	0.11	69,69,69,69	0
54	MG	1A	3374	1/1	0.93	0.25	65,65,65,65	0
54	MG	2A	3373	1/1	0.93	0.19	53,53,53,53	0
54	MG	2A	3546	1/1	0.93	0.13	54,54,54,54	0
54	MG	1A	3431	1/1	0.93	0.14	29,29,29,29	0
54	MG	1A	3232	1/1	0.93	0.18	41,41,41,41	0
54	MG	2A	3309	1/1	0.93	0.21	46,46,46,46	0
54	MG	2A	3473	1/1	0.93	0.16	41,41,41,41	0
54	MG	2A	3447	1/1	0.93	0.15	44,44,44,44	0
54	MG	2A	3137	1/1	0.93	0.19	40,40,40,40	0
54	MG	2a	1742	1/1	0.93	0.05	59,59,59,59	0
54	MG	1A	3892	1/1	0.93	0.20	55,55,55,55	0
54	MG	1A	3805	1/1	0.93	0.16	33,33,33,33	0
54	MG	1A	3958	1/1	0.93	0.18	54,54,54,54	0
54	MG	2A	3639	1/1	0.93	0.13	58,58,58,58	0
54	MG	1V	202	1/1	0.93	0.08	52,52,52,52	0
54	MG	1A	3802	1/1	0.93	0.13	40,40,40,40	0
54	MG	2A	3268	1/1	0.93	0.22	65,65,65,65	0
54	MG	1A	3737	1/1	0.93	0.21	51,51,51,51	0
54	MG	1A	3912	1/1	0.93	0.34	50,50,50,50	0
54	MG	2X	101	1/1	0.93	0.11	56,56,56,56	0
54	MG	1A	3312	1/1	0.93	0.18	17,17,17,17	0
54	MG	10	105	1/1	0.93	0.13	64,64,64,64	0
54	MG	1a	1766	1/1	0.93	0.12	65,65,65,65	0
54	MG	1A	3584	1/1	0.93	0.47	33,33,33,33	0
54	MG	1A	3269	1/1	0.93	0.22	45,45,45,45	0
54	MG	2A	3469	1/1	0.93	0.31	53,53,53,53	0
54	MG	1A	3851	1/1	0.93	0.15	48,48,48,48	0
54	MG	2A	3478	1/1	0.93	0.27	50,50,50,50	0
54	MG	2a	1762	1/1	0.93	0.10	92,92,92,92	0
54	MG	1A	3089	1/1	0.93	0.11	43,43,43,43	0
54	MG	2A	3531	1/1	0.93	0.12	44,44,44,44	0
54	MG	1a	1812	1/1	0.93	0.17	53,53,53,53	0
54	MG	2A	3202	1/1	0.93	0.18	60,60,60,60	0
54	MG	1a	1701	1/1	0.93	0.09	66,66,66,66	0
54	MG	2A	3230	1/1	0.93	0.20	57,57,57,57	0
54	MG	1a	1626	1/1	0.93	0.12	43,43,43,43	0
54	MG	1A	3388	1/1	0.93	0.11	77,77,77,77	0
54	MG	2A	3037	1/1	0.93	0.15	63,63,63,63	0
54	MG	2A	3015	1/1	0.93	0.73	42,42,42,42	0
54	MG	1W	3003	1/1	0.93	0.17	48,48,48,48	0
54	MG	1A	3951	1/1	0.93	0.14	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3039	1/1	0.93	0.17	34,34,34,34	0
54	MG	2A	3146	1/1	0.93	0.20	42,42,42,42	0
54	MG	2A	3100	1/1	0.93	0.07	41,41,41,41	0
54	MG	1a	1832	1/1	0.93	0.20	61,61,61,61	0
54	MG	1A	3618	1/1	0.93	0.43	59,59,59,59	0
54	MG	1a	1674	1/1	0.93	0.11	65,65,65,65	0
54	MG	2a	1662	1/1	0.93	0.15	63,63,63,63	0
54	MG	2A	3613	1/1	0.93	0.18	73,73,73,73	0
54	MG	2A	3378	1/1	0.93	0.12	48,48,48,48	0
54	MG	2A	3350	1/1	0.93	0.15	46,46,46,46	0
54	MG	2A	3330	1/1	0.93	0.09	58,58,58,58	0
54	MG	1a	1630	1/1	0.93	0.13	43,43,43,43	0
54	MG	1A	4023	1/1	0.93	0.17	35,35,35,35	0
54	MG	1A	3822	1/1	0.93	0.13	47,47,47,47	0
54	MG	1A	3165	1/1	0.93	0.32	43,43,43,43	0
54	MG	1A	3982	1/1	0.93	0.07	54,54,54,54	0
54	MG	2a	1774	1/1	0.93	0.06	67,67,67,67	0
54	MG	2A	3437	1/1	0.93	0.25	58,58,58,58	0
54	MG	2A	3021	1/1	0.93	0.09	48,48,48,48	0
54	MG	2A	3045	1/1	0.93	0.21	68,68,68,68	0
54	MG	1A	3290	1/1	0.93	0.16	16,16,16,16	0
54	MG	1A	3963	1/1	0.93	0.10	49,49,49,49	0
54	MG	1A	3090	1/1	0.93	0.16	28,28,28,28	0
54	MG	2A	3247	1/1	0.93	0.13	34,34,34,34	0
54	MG	2A	3560	1/1	0.93	0.12	46,46,46,46	0
54	MG	1A	3624	1/1	0.93	0.14	64,64,64,64	0
54	MG	1A	3896	1/1	0.93	0.11	49,49,49,49	0
54	MG	1E	304	1/1	0.93	0.17	26,26,26,26	0
54	MG	1A	3792	1/1	0.93	0.12	36,36,36,36	0
54	MG	2a	1647	1/1	0.93	0.11	53,53,53,53	0
54	MG	2A	3389	1/1	0.93	0.12	47,47,47,47	0
54	MG	2A	3296	1/1	0.93	0.15	48,48,48,48	0
54	MG	2A	3050	1/1	0.93	0.53	49,49,49,49	0
54	MG	1A	3944	1/1	0.93	0.35	38,38,38,38	0
54	MG	2A	3240	1/1	0.93	0.11	35,35,35,35	0
54	MG	1A	3443	1/1	0.93	0.13	33,33,33,33	0
54	MG	2A	3474	1/1	0.93	0.24	47,47,47,47	0
54	MG	2A	3650	1/1	0.93	0.17	82,82,82,82	0
54	MG	2a	1699	1/1	0.93	0.14	58,58,58,58	0
54	MG	2A	3556	1/1	0.93	0.18	49,49,49,49	0
54	MG	1a	1811	1/1	0.93	0.13	57,57,57,57	0
54	MG	1A	3685	1/1	0.93	0.10	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	1681	1/1	0.93	0.18	67,67,67,67	0
54	MG	2a	1695	1/1	0.93	0.24	48,48,48,48	0
54	MG	2a	1650	1/1	0.93	0.19	57,57,57,57	0
54	MG	2A	3071	1/1	0.93	0.17	46,46,46,46	0
54	MG	2B	214	1/1	0.93	0.12	60,60,60,60	0
54	MG	1A	3924	1/1	0.93	0.14	44,44,44,44	0
54	MG	1A	3733	1/1	0.93	0.40	42,42,42,42	0
54	MG	1A	3519	1/1	0.93	0.17	16,16,16,16	0
54	MG	2A	3601	1/1	0.93	0.12	51,51,51,51	0
54	MG	2A	3480	1/1	0.93	0.05	52,52,52,52	0
54	MG	1A	3188	1/1	0.93	0.58	32,32,32,32	0
54	MG	2a	1608	1/1	0.93	0.11	58,58,58,58	0
54	MG	1A	3603	1/1	0.93	0.09	63,63,63,63	0
54	MG	1A	3485	1/1	0.93	0.22	30,30,30,30	0
54	MG	1A	3284	1/1	0.93	0.17	23,23,23,23	0
54	MG	1A	3755	1/1	0.93	0.16	36,36,36,36	0
54	MG	1A	3227	1/1	0.93	0.34	39,39,39,39	0
54	MG	1A	3371	1/1	0.93	0.17	24,24,24,24	0
54	MG	2A	3524	1/1	0.93	0.19	31,31,31,31	0
54	MG	2A	3366	1/1	0.93	0.12	59,59,59,59	0
54	MG	2a	1693	1/1	0.93	0.12	57,57,57,57	0
54	MG	2A	3439	1/1	0.93	0.22	59,59,59,59	0
54	MG	2A	3664	1/1	0.93	0.13	61,61,61,61	0
54	MG	1A	4027	1/1	0.93	0.43	37,37,37,37	0
54	MG	2a	1658	1/1	0.93	0.12	58,58,58,58	0
54	MG	2A	3485	1/1	0.93	0.12	50,50,50,50	0
54	MG	1A	3646	1/1	0.93	0.14	60,60,60,60	0
54	MG	1A	3752	1/1	0.93	0.12	52,52,52,52	0
54	MG	1A	3415	1/1	0.93	0.24	63,63,63,63	0
54	MG	2A	3364	1/1	0.93	0.17	57,57,57,57	0
54	MG	1A	3357	1/1	0.93	0.17	16,16,16,16	0
54	MG	1A	3696	1/1	0.93	0.16	50,50,50,50	0
54	MG	2a	1627	1/1	0.93	0.07	64,64,64,64	0
54	MG	1A	3726	1/1	0.93	0.11	46,46,46,46	0
54	MG	1a	1617	1/1	0.93	0.15	45,45,45,45	0
54	MG	2a	1634	1/1	0.93	0.19	64,64,64,64	0
54	MG	1A	3846	1/1	0.93	0.36	55,55,55,55	0
54	MG	2A	3025	1/1	0.93	0.18	43,43,43,43	0
54	MG	1A	3601	1/1	0.94	0.21	17,17,17,17	0
54	MG	2a	1688	1/1	0.94	0.20	63,63,63,63	0
54	MG	2A	3153	1/1	0.94	0.11	49,49,49,49	0
54	MG	1a	1645	1/1	0.94	0.14	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3669	1/1	0.94	0.11	39,39,39,39	0
54	MG	2A	3060	1/1	0.94	0.22	62,62,62,62	0
54	MG	1A	3678	1/1	0.94	0.21	24,24,24,24	0
54	MG	2A	3077	1/1	0.94	0.15	71,71,71,71	0
54	MG	1a	1744	1/1	0.94	0.17	66,66,66,66	0
54	MG	2A	3013	1/1	0.94	0.18	51,51,51,51	0
54	MG	2A	3491	1/1	0.94	0.26	43,43,43,43	0
54	MG	2A	3082	1/1	0.94	0.15	40,40,40,40	0
54	MG	1A	3889	1/1	0.94	0.18	54,54,54,54	0
54	MG	1A	3526	1/1	0.94	0.21	19,19,19,19	0
54	MG	2A	3017	1/1	0.94	0.18	46,46,46,46	0
54	MG	2a	1738	1/1	0.94	0.18	66,66,66,66	0
54	MG	2A	3029	1/1	0.94	0.14	63,63,63,63	0
54	MG	1B	226	1/1	0.94	0.08	46,46,46,46	0
54	MG	1A	3918	1/1	0.94	0.17	57,57,57,57	0
54	MG	1A	3421	1/1	0.94	0.18	44,44,44,44	0
54	MG	2a	1657	1/1	0.94	0.14	62,62,62,62	0
54	MG	1A	3132	1/1	0.94	0.34	48,48,48,48	0
54	MG	1A	3146	1/1	0.94	0.39	47,47,47,47	0
54	MG	1A	3363	1/1	0.94	0.13	21,21,21,21	0
54	MG	2a	1740	1/1	0.94	0.17	64,64,64,64	0
54	MG	2A	3091	1/1	0.94	0.11	48,48,48,48	0
54	MG	1a	1806	1/1	0.94	0.24	63,63,63,63	0
54	MG	2a	1636	1/1	0.94	0.11	55,55,55,55	0
54	MG	2A	3558	1/1	0.94	0.24	63,63,63,63	0
54	MG	2A	3062	1/1	0.94	0.24	47,47,47,47	0
54	MG	1A	3566	1/1	0.94	0.20	42,42,42,42	0
54	MG	1A	3806	1/1	0.94	0.16	36,36,36,36	0
54	MG	2B	212	1/1	0.94	0.22	65,65,65,65	0
54	MG	1A	3816	1/1	0.94	0.13	46,46,46,46	0
54	MG	1A	3056	1/1	0.94	0.29	43,43,43,43	0
54	MG	2A	3487	1/1	0.94	0.20	46,46,46,46	0
54	MG	1A	3539	1/1	0.94	0.17	20,20,20,20	0
54	MG	1a	1817	1/1	0.94	0.20	62,62,62,62	0
54	MG	1A	3693	1/1	0.94	0.24	60,60,60,60	0
54	MG	1A	3881	1/1	0.94	0.10	44,44,44,44	0
54	MG	2A	3408	1/1	0.94	0.11	31,31,31,31	0
54	MG	1A	3014	1/1	0.94	0.45	31,31,31,31	0
54	MG	2A	3341	1/1	0.94	0.14	35,35,35,35	0
54	MG	1A	3518	1/1	0.94	0.30	40,40,40,40	0
54	MG	1a	1640	1/1	0.94	0.19	43,43,43,43	0
54	MG	1a	1798	1/1	0.94	0.08	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	1611	1/1	0.94	0.14	55,55,55,55	0
54	MG	2A	3386	1/1	0.94	0.09	61,61,61,61	0
54	MG	2A	3380	1/1	0.94	0.22	60,60,60,60	0
54	MG	1A	3530	1/1	0.94	0.37	37,37,37,37	0
54	MG	2A	3460	1/1	0.94	0.11	32,32,32,32	0
54	MG	2A	3403	1/1	0.94	0.13	41,41,41,41	0
54	MG	1A	3825	1/1	0.94	0.16	16,16,16,16	0
54	MG	1A	4062	1/1	0.94	0.19	40,40,40,40	0
54	MG	1A	3462	1/1	0.94	0.16	49,49,49,49	0
54	MG	1A	3345	1/1	0.94	0.27	34,34,34,34	0
54	MG	2A	3092	1/1	0.94	0.10	60,60,60,60	0
54	MG	1A	3536	1/1	0.94	0.14	42,42,42,42	0
54	MG	1A	3495	1/1	0.94	0.14	35,35,35,35	0
59	ZN	2n	501	1/1	0.94	0.05	89,89,89,89	0
54	MG	2a	1757	1/1	0.94	0.11	74,74,74,74	0
54	MG	1A	3377	1/1	0.94	0.22	23,23,23,23	0
54	MG	2A	3482	1/1	0.94	0.27	46,46,46,46	0
54	MG	1A	3923	1/1	0.94	0.06	42,42,42,42	0
54	MG	2A	3124	1/1	0.94	0.11	54,54,54,54	0
54	MG	2A	3106	1/1	0.94	0.16	74,74,74,74	0
54	MG	1B	210	1/1	0.94	0.25	49,49,49,49	0
54	MG	2A	3381	1/1	0.94	0.17	29,29,29,29	0
54	MG	1A	3183	1/1	0.94	0.77	42,42,42,42	0
54	MG	2A	3372	1/1	0.94	0.18	55,55,55,55	0
54	MG	1A	3207	1/1	0.94	0.58	39,39,39,39	0
54	MG	2A	3434	1/1	0.94	0.23	44,44,44,44	0
54	MG	2B	208	1/1	0.94	0.15	61,61,61,61	0
54	MG	1A	3408	1/1	0.94	0.19	37,37,37,37	0
54	MG	1A	3106	1/1	0.94	0.28	30,30,30,30	0
54	MG	1d	503	1/1	0.94	0.12	67,67,67,67	0
54	MG	2A	3375	1/1	0.94	0.18	52,52,52,52	0
54	MG	1A	3524	1/1	0.94	0.20	54,54,54,54	0
54	MG	2A	3209	1/1	0.94	0.15	49,49,49,49	0
54	MG	1D	308	1/1	0.94	0.19	37,37,37,37	0
54	MG	1A	3834	1/1	0.94	0.14	12,12,12,12	0
54	MG	2A	3697	1/1	0.94	0.54	44,44,44,44	0
54	MG	1A	3504	1/1	0.94	0.10	56,56,56,56	0
54	MG	1a	1719	1/1	0.94	0.10	52,52,52,52	0
54	MG	2A	3011	1/1	0.94	0.15	47,47,47,47	0
54	MG	1A	3926	1/1	0.94	0.09	47,47,47,47	0
54	MG	1A	4009	1/1	0.94	0.14	17,17,17,17	0
54	MG	1A	3917	1/1	0.94	0.13	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3160	1/1	0.94	0.22	26,26,26,26	0
54	MG	1a	1654	1/1	0.94	0.07	64,64,64,64	0
54	MG	1A	3293	1/1	0.94	0.17	31,31,31,31	0
54	MG	1A	3691	1/1	0.94	0.15	23,23,23,23	0
54	MG	2A	3702	1/1	0.94	0.27	37,37,37,37	0
54	MG	1A	3128	1/1	0.94	0.09	62,62,62,62	0
54	MG	2A	3135	1/1	0.94	0.07	63,63,63,63	0
54	MG	1a	1635	1/1	0.94	0.07	69,69,69,69	0
54	MG	2A	3313	1/1	0.94	0.24	51,51,51,51	0
54	MG	1B	203	1/1	0.94	0.12	61,61,61,61	0
54	MG	1a	1639	1/1	0.94	0.24	59,59,59,59	0
54	MG	1A	3648	1/1	0.94	0.16	34,34,34,34	0
54	MG	1E	301	1/1	0.94	0.07	37,37,37,37	0
54	MG	1A	3439	1/1	0.94	0.18	17,17,17,17	0
54	MG	1A	3585	1/1	0.94	0.18	58,58,58,58	0
54	MG	2a	1682	1/1	0.94	0.14	57,57,57,57	0
54	MG	2A	3299	1/1	0.94	0.30	68,68,68,68	0
54	MG	1A	3427	1/1	0.94	0.22	48,48,48,48	0
54	MG	1a	1834	1/1	0.94	0.09	78,78,78,78	0
54	MG	1A	3214	1/1	0.94	0.10	38,38,38,38	0
54	MG	1A	3193	1/1	0.94	0.22	29,29,29,29	0
54	MG	2A	3517	1/1	0.94	0.21	46,46,46,46	0
54	MG	2A	3680	1/1	0.94	0.10	23,23,23,23	0
54	MG	1A	3449	1/1	0.94	0.09	45,45,45,45	0
54	MG	1A	3067	1/1	0.94	0.33	30,30,30,30	0
54	MG	1A	3309	1/1	0.94	0.17	28,28,28,28	0
54	MG	2A	3610	1/1	0.94	0.11	57,57,57,57	0
54	MG	1n	502	1/1	0.94	0.12	71,71,71,71	0
54	MG	1A	3020	1/1	0.94	0.39	40,40,40,40	0
54	MG	2A	3384	1/1	0.94	0.11	43,43,43,43	0
54	MG	1A	3262	1/1	0.94	0.43	76,76,76,76	0
54	MG	1A	3766	1/1	0.94	0.19	45,45,45,45	0
54	MG	2A	3450	1/1	0.94	0.20	60,60,60,60	0
54	MG	1A	3376	1/1	0.94	0.08	60,60,60,60	0
54	MG	1a	1815	1/1	0.94	0.09	70,70,70,70	0
54	MG	2A	3149	1/1	0.94	0.09	51,51,51,51	0
54	MG	1A	4058	1/1	0.94	0.27	37,37,37,37	0
54	MG	1A	3491	1/1	0.94	0.24	48,48,48,48	0
54	MG	1A	3216	1/1	0.94	0.29	42,42,42,42	0
54	MG	2A	3235	1/1	0.94	0.14	55,55,55,55	0
54	MG	1a	1660	1/1	0.94	0.16	60,60,60,60	0
54	MG	2A	3244	1/1	0.94	0.13	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3024	1/1	0.94	0.13	55,55,55,55	0
54	MG	1A	3129	1/1	0.94	0.14	29,29,29,29	0
54	MG	1A	3525	1/1	0.94	0.15	60,60,60,60	0
54	MG	1A	3331	1/1	0.94	0.09	35,35,35,35	0
54	MG	1B	208	1/1	0.94	0.31	53,53,53,53	0
54	MG	1A	3195	1/1	0.94	0.51	34,34,34,34	0
54	MG	1A	3447	1/1	0.94	0.20	47,47,47,47	0
54	MG	1A	3076	1/1	0.94	0.43	35,35,35,35	0
54	MG	2A	3205	1/1	0.94	0.09	44,44,44,44	0
54	MG	2A	3138	1/1	0.94	0.13	46,46,46,46	0
54	MG	2a	1739	1/1	0.94	0.16	66,66,66,66	0
54	MG	1A	3473	1/1	0.94	0.14	19,19,19,19	0
54	MG	2A	3449	1/1	0.94	0.09	59,59,59,59	0
54	MG	1A	3197	1/1	0.94	0.36	38,38,38,38	0
54	MG	1a	1791	1/1	0.94	0.06	67,67,67,67	0
54	MG	1A	3074	1/1	0.94	0.45	45,45,45,45	0
54	MG	28	101	1/1	0.94	0.12	59,59,59,59	0
54	MG	1A	3364	1/1	0.94	0.20	59,59,59,59	0
54	MG	1A	3787	1/1	0.94	0.18	26,26,26,26	0
54	MG	1A	4041	1/1	0.94	0.58	38,38,38,38	0
54	MG	1A	3872	1/1	0.94	0.11	54,54,54,54	0
54	MG	2A	3553	1/1	0.94	0.18	51,51,51,51	0
54	MG	1A	3647	1/1	0.94	0.21	32,32,32,32	0
54	MG	2A	3577	1/1	0.94	0.11	48,48,48,48	0
54	MG	1A	4045	1/1	0.94	0.24	32,32,32,32	0
54	MG	1A	3615	1/1	0.94	0.17	58,58,58,58	0
54	MG	2A	3079	1/1	0.94	0.15	66,66,66,66	0
54	MG	2A	3048	1/1	0.94	0.12	50,50,50,50	0
54	MG	1A	3611	1/1	0.94	0.17	37,37,37,37	0
54	MG	1A	4006	1/1	0.94	0.33	28,28,28,28	0
54	MG	1A	3185	1/1	0.94	0.19	43,43,43,43	0
54	MG	1A	3499	1/1	0.94	0.10	34,34,34,34	0
54	MG	1A	3980	1/1	0.94	0.12	47,47,47,47	0
54	MG	1A	3384	1/1	0.94	0.14	52,52,52,52	0
54	MG	2Q	3002	1/1	0.94	0.21	54,54,54,54	0
54	MG	1A	3086	1/1	0.94	0.14	35,35,35,35	0
54	MG	1A	3038	1/1	0.94	0.11	43,43,43,43	0
54	MG	19	103	1/1	0.94	0.09	62,62,62,62	0
54	MG	1a	1788	1/1	0.94	0.06	66,66,66,66	0
54	MG	2A	3210	1/1	0.94	0.16	45,45,45,45	0
54	MG	1A	3764	1/1	0.94	0.15	52,52,52,52	0
54	MG	2A	3432	1/1	0.94	0.12	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3028	1/1	0.94	0.14	62,62,62,62	0
54	MG	1A	3241	1/1	0.94	0.12	31,31,31,31	0
54	MG	2A	3694	1/1	0.94	0.54	38,38,38,38	0
54	MG	1A	3169	1/1	0.94	0.21	37,37,37,37	0
54	MG	2a	1670	1/1	0.94	0.16	68,68,68,68	0
54	MG	1A	3547	1/1	0.94	0.11	35,35,35,35	0
54	MG	1A	3401	1/1	0.94	0.16	53,53,53,53	0
54	MG	2a	1694	1/1	0.94	0.21	72,72,72,72	0
54	MG	1A	3740	1/1	0.94	0.22	44,44,44,44	0
54	MG	1A	3073	1/1	0.94	0.28	33,33,33,33	0
54	MG	1A	3198	1/1	0.94	0.24	31,31,31,31	0
54	MG	2A	3550	1/1	0.94	0.14	58,58,58,58	0
54	MG	2A	3456	1/1	0.94	0.32	58,58,58,58	0
54	MG	2A	3620	1/1	0.94	0.48	68,68,68,68	0
54	MG	2a	1629	1/1	0.94	0.19	66,66,66,66	0
54	MG	1A	3434	1/1	0.94	0.22	24,24,24,24	0
54	MG	1A	3044	1/1	0.94	0.34	22,22,22,22	0
54	MG	2A	3513	1/1	0.94	0.14	39,39,39,39	0
54	MG	1a	1665	1/1	0.94	0.26	51,51,51,51	0
54	MG	2A	3327	1/1	0.94	0.20	48,48,48,48	0
54	MG	2A	3009	1/1	0.94	0.15	71,71,71,71	0
54	MG	2a	1684	1/1	0.94	0.12	68,68,68,68	0
59	ZN	2Y	501	1/1	0.94	0.12	79,79,79,79	0
54	MG	1a	1680	1/1	0.94	0.12	55,55,55,55	0
54	MG	2A	3383	1/1	0.94	0.25	54,54,54,54	0
54	MG	1A	3379	1/1	0.94	0.17	45,45,45,45	0
54	MG	1A	3959	1/1	0.94	0.12	48,48,48,48	0
54	MG	1F	306	1/1	0.94	0.91	48,48,48,48	0
54	MG	2A	3312	1/1	0.94	0.21	69,69,69,69	0
54	MG	1A	3041	1/1	0.94	0.26	26,26,26,26	0
54	MG	2E	302	1/1	0.94	0.16	52,52,52,52	0
54	MG	2A	3332	1/1	0.94	0.28	52,52,52,52	0
54	MG	1A	3558	1/1	0.94	0.20	27,27,27,27	0
54	MG	2A	3049	1/1	0.94	0.15	36,36,36,36	0
58	ARG	1B	232	12/12	0.94	0.26	29,45,53,55	0
54	MG	2A	3169	1/1	0.94	0.14	52,52,52,52	0
54	MG	1A	3264	1/1	0.94	0.12	57,57,57,57	0
54	MG	2a	1630	1/1	0.94	0.15	78,78,78,78	0
54	MG	2A	3499	1/1	0.94	0.38	54,54,54,54	0
54	MG	1A	3221	1/1	0.94	0.11	52,52,52,52	0
54	MG	1A	3275	1/1	0.94	0.38	40,40,40,40	0
54	MG	1A	3720	1/1	0.94	0.26	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3579	1/1	0.94	0.28	56,56,56,56	0
54	MG	2a	1606	1/1	0.94	0.16	59,59,59,59	0
54	MG	1A	4007	1/1	0.94	0.35	25,25,25,25	0
54	MG	1a	1649	1/1	0.94	0.06	70,70,70,70	0
54	MG	1A	3671	1/1	0.94	0.08	36,36,36,36	0
54	MG	1A	3823	1/1	0.94	0.16	29,29,29,29	0
54	MG	1a	1799	1/1	0.94	0.19	49,49,49,49	0
54	MG	2A	3527	1/1	0.94	0.23	70,70,70,70	0
54	MG	2A	3198	1/1	0.94	0.20	43,43,43,43	0
54	MG	1a	1857	1/1	0.94	0.10	50,50,50,50	0
54	MG	1a	1805	1/1	0.94	0.27	52,52,52,52	0
54	MG	1A	3784	1/1	0.94	0.25	43,43,43,43	0
54	MG	1A	3279	1/1	0.95	0.16	20,20,20,20	0
54	MG	1A	3663	1/1	0.95	0.21	31,31,31,31	0
54	MG	1A	3062	1/1	0.95	0.09	57,57,57,57	0
54	MG	1a	1861	1/1	0.95	0.08	66,66,66,66	0
54	MG	1A	3117	1/1	0.95	0.12	40,40,40,40	0
54	MG	1A	3666	1/1	0.95	0.13	28,28,28,28	0
54	MG	1A	3866	1/1	0.95	0.12	24,24,24,24	0
54	MG	1o	3001	1/1	0.95	0.22	48,48,48,48	0
54	MG	2a	1625	1/1	0.95	0.11	37,37,37,37	0
54	MG	2A	3385	1/1	0.95	0.23	61,61,61,61	0
54	MG	1a	1852	1/1	0.95	0.31	72,72,72,72	0
54	MG	1A	3323	1/1	0.95	0.15	36,36,36,36	0
54	MG	2A	3376	1/1	0.95	0.12	57,57,57,57	0
54	MG	1A	3591	1/1	0.95	0.19	47,47,47,47	0
54	MG	2A	3545	1/1	0.95	0.20	64,64,64,64	0
54	MG	1a	1814	1/1	0.95	0.19	56,56,56,56	0
54	MG	1A	3305	1/1	0.95	0.12	49,49,49,49	0
54	MG	2A	3412	1/1	0.95	0.11	57,57,57,57	0
54	MG	1A	3583	1/1	0.95	0.23	55,55,55,55	0
54	MG	1A	3088	1/1	0.95	0.11	50,50,50,50	0
54	MG	2A	3055	1/1	0.95	0.14	53,53,53,53	0
54	MG	1A	3166	1/1	0.95	0.28	38,38,38,38	0
54	MG	2A	3682	1/1	0.95	0.16	58,58,58,58	0
54	MG	2A	3275	1/1	0.95	0.16	28,28,28,28	0
54	MG	1A	3008	1/1	0.95	0.14	34,34,34,34	0
54	MG	1A	3340	1/1	0.95	0.18	34,34,34,34	0
54	MG	2A	3606	1/1	0.95	0.36	55,55,55,55	0
54	MG	2a	1669	1/1	0.95	0.11	54,54,54,54	0
54	MG	1A	3791	1/1	0.95	0.12	43,43,43,43	0
54	MG	1D	306	1/1	0.95	0.12	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3069	1/1	0.95	0.54	45,45,45,45	0
54	MG	1a	1698	1/1	0.95	0.14	32,32,32,32	0
54	MG	2A	3466	1/1	0.95	0.29	62,62,62,62	0
54	MG	1D	312	1/1	0.95	0.50	50,50,50,50	0
54	MG	1A	3251	1/1	0.95	0.27	37,37,37,37	0
54	MG	2A	3095	1/1	0.95	0.13	57,57,57,57	0
54	MG	2A	3066	1/1	0.95	0.17	45,45,45,45	0
54	MG	1A	3167	1/1	0.95	0.15	53,53,53,53	0
54	MG	1A	3430	1/1	0.95	0.16	14,14,14,14	0
54	MG	2A	3468	1/1	0.95	0.22	56,56,56,56	0
54	MG	1A	3867	1/1	0.95	0.17	26,26,26,26	0
54	MG	2A	3098	1/1	0.95	0.18	42,42,42,42	0
54	MG	1A	3849	1/1	0.95	0.10	36,36,36,36	0
54	MG	2A	3495	1/1	0.95	0.19	32,32,32,32	0
54	MG	1A	3344	1/1	0.95	0.14	20,20,20,20	0
54	MG	1A	3131	1/1	0.95	0.15	62,62,62,62	0
54	MG	1A	3770	1/1	0.95	0.17	27,27,27,27	0
54	MG	2A	3133	1/1	0.95	0.44	48,48,48,48	0
54	MG	1e	3003	1/1	0.95	0.39	53,53,53,53	0
54	MG	2A	3291	1/1	0.95	0.14	32,32,32,32	0
54	MG	1A	3734	1/1	0.95	0.19	73,73,73,73	0
54	MG	2A	3160	1/1	0.95	0.53	54,54,54,54	0
54	MG	2A	3295	1/1	0.95	0.19	34,34,34,34	0
54	MG	2A	3243	1/1	0.95	0.08	62,62,62,62	0
54	MG	1a	1809	1/1	0.95	0.12	50,50,50,50	0
54	MG	2A	3496	1/1	0.95	0.22	54,54,54,54	0
54	MG	1A	3799	1/1	0.95	0.17	29,29,29,29	0
54	MG	2A	3490	1/1	0.95	0.28	50,50,50,50	0
54	MG	1A	3301	1/1	0.95	0.16	45,45,45,45	0
54	MG	2A	3667	1/1	0.95	0.19	62,62,62,62	0
54	MG	2A	3170	1/1	0.95	0.07	67,67,67,67	0
54	MG	1A	3745	1/1	0.95	0.24	36,36,36,36	0
54	MG	2a	1615	1/1	0.95	0.17	55,55,55,55	0
54	MG	2D	303	1/1	0.95	0.25	39,39,39,39	0
54	MG	2A	3572	1/1	0.95	0.07	66,66,66,66	0
54	MG	2A	3695	1/1	0.95	0.37	50,50,50,50	0
54	MG	1A	3684	1/1	0.95	0.20	33,33,33,33	0
54	MG	2A	3395	1/1	0.95	0.16	29,29,29,29	0
54	MG	1A	3617	1/1	0.95	0.20	22,22,22,22	0
54	MG	1A	3410	1/1	0.95	0.17	54,54,54,54	0
54	MG	2A	3201	1/1	0.95	0.12	53,53,53,53	0
54	MG	1A	3243	1/1	0.95	0.16	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3322	1/1	0.95	0.16	64,64,64,64	0
54	MG	1A	3723	1/1	0.95	0.17	61,61,61,61	0
54	MG	1A	3051	1/1	0.95	0.34	38,38,38,38	0
54	MG	1A	3761	1/1	0.95	0.22	31,31,31,31	0
54	MG	2A	3288	1/1	0.95	0.13	44,44,44,44	0
54	MG	1A	3644	1/1	0.95	0.16	39,39,39,39	0
54	MG	1A	3093	1/1	0.95	0.23	51,51,51,51	0
56	EZM	2A	3691	24/24	0.95	0.36	38,42,48,51	0
54	MG	1A	3286	1/1	0.95	0.19	22,22,22,22	0
54	MG	2P	8001	1/1	0.95	0.12	52,52,52,52	0
54	MG	2A	3234	1/1	0.95	0.29	59,59,59,59	0
54	MG	1A	3999	1/1	0.95	0.27	44,44,44,44	0
54	MG	2A	3423	1/1	0.95	0.37	56,56,56,56	0
54	MG	1A	3412	1/1	0.95	0.14	35,35,35,35	0
54	MG	2A	3232	1/1	0.95	0.88	41,41,41,41	0
54	MG	1A	3494	1/1	0.95	0.11	33,33,33,33	0
54	MG	1A	3139	1/1	0.95	0.16	48,48,48,48	0
54	MG	10	101	1/1	0.95	0.13	46,46,46,46	0
54	MG	2A	3081	1/1	0.95	0.16	54,54,54,54	0
54	MG	2A	3638	1/1	0.95	0.08	53,53,53,53	0
54	MG	2A	3441	1/1	0.95	0.27	55,55,55,55	0
54	MG	1F	307	1/1	0.95	0.10	44,44,44,44	0
54	MG	1A	3605	1/1	0.95	0.13	52,52,52,52	0
54	MG	1a	1733	1/1	0.95	0.13	62,62,62,62	0
54	MG	1A	3444	1/1	0.95	0.10	55,55,55,55	0
54	MG	1A	3102	1/1	0.95	0.24	34,34,34,34	0
54	MG	1A	3135	1/1	0.95	0.15	27,27,27,27	0
54	MG	1A	3798	1/1	0.95	0.16	27,27,27,27	0
54	MG	2A	3698	1/1	0.95	0.15	57,57,57,57	0
54	MG	1A	3356	1/1	0.95	0.16	18,18,18,18	0
54	MG	1A	3593	1/1	0.95	0.13	64,64,64,64	0
54	MG	1A	3025	1/1	0.95	0.21	24,24,24,24	0
54	MG	1A	3835	1/1	0.95	0.08	38,38,38,38	0
54	MG	1A	3682	1/1	0.95	0.13	35,35,35,35	0
54	MG	1A	3863	1/1	0.95	0.16	54,54,54,54	0
54	MG	1A	3497	1/1	0.95	0.18	40,40,40,40	0
54	MG	1A	3587	1/1	0.95	0.17	34,34,34,34	0
54	MG	1A	3954	1/1	0.95	0.14	48,48,48,48	0
54	MG	2A	3681	1/1	0.95	0.20	37,37,37,37	0
54	MG	1A	3028	1/1	0.95	0.15	32,32,32,32	0
54	MG	1X	102	1/1	0.95	0.17	34,34,34,34	0
54	MG	1A	3296	1/1	0.95	0.12	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3365	1/1	0.95	0.15	19,19,19,19	0
54	MG	1A	3334	1/1	0.95	0.16	32,32,32,32	0
54	MG	1Q	204	1/1	0.95	0.20	47,47,47,47	0
54	MG	1F	303	1/1	0.95	0.11	35,35,35,35	0
54	MG	1a	1655	1/1	0.95	0.34	61,61,61,61	0
54	MG	1A	3471	1/1	0.95	0.08	49,49,49,49	0
54	MG	2A	3567	1/1	0.95	0.13	33,33,33,33	0
54	MG	1A	3962	1/1	0.95	0.23	65,65,65,65	0
54	MG	1a	1710	1/1	0.95	0.16	59,59,59,59	0
54	MG	1a	1797	1/1	0.95	0.22	63,63,63,63	0
54	MG	1A	3285	1/1	0.95	0.16	57,57,57,57	0
54	MG	1A	3459	1/1	0.95	0.14	22,22,22,22	0
54	MG	2D	302	1/1	0.95	1.17	44,44,44,44	0
54	MG	1A	3680	1/1	0.95	0.12	54,54,54,54	0
54	MG	2A	3119	1/1	0.95	0.20	49,49,49,49	0
54	MG	1A	4026	1/1	0.95	0.31	48,48,48,48	0
54	MG	1A	3705	1/1	0.95	0.17	36,36,36,36	0
54	MG	1A	3252	1/1	0.95	0.28	29,29,29,29	0
54	MG	2A	3127	1/1	0.95	0.12	58,58,58,58	0
54	MG	1A	3395	1/1	0.95	0.11	38,38,38,38	0
54	MG	2a	1663	1/1	0.95	0.11	44,44,44,44	0
54	MG	1a	1641	1/1	0.95	0.19	46,46,46,46	0
54	MG	2A	3231	1/1	0.95	0.17	21,21,21,21	0
54	MG	2A	3333	1/1	0.95	0.21	38,38,38,38	0
54	MG	2a	1673	1/1	0.95	0.18	67,67,67,67	0
54	MG	2A	3068	1/1	0.95	0.34	41,41,41,41	0
54	MG	1A	3352	1/1	0.95	0.14	34,34,34,34	0
54	MG	1A	3343	1/1	0.95	0.15	17,17,17,17	0
54	MG	2A	3323	1/1	0.95	0.16	58,58,58,58	0
54	MG	1A	4070	1/1	0.95	0.54	42,42,42,42	0
54	MG	2A	3303	1/1	0.95	0.17	40,40,40,40	0
54	MG	2B	201	1/1	0.95	0.22	72,72,72,72	0
54	MG	2A	3338	1/1	0.95	0.17	43,43,43,43	0
54	MG	2a	1747	1/1	0.95	0.14	73,73,73,73	0
54	MG	2A	3111	1/1	0.95	0.17	59,59,59,59	0
54	MG	2a	1719	1/1	0.95	0.08	66,66,66,66	0
54	MG	1A	3175	1/1	0.95	0.69	35,35,35,35	0
54	MG	1a	1762	1/1	0.95	0.07	66,66,66,66	0
54	MG	1A	3095	1/1	0.95	0.27	32,32,32,32	0
54	MG	1A	3030	1/1	0.95	0.13	13,13,13,13	0
54	MG	2A	3457	1/1	0.95	0.18	47,47,47,47	0
54	MG	1A	3451	1/1	0.95	0.14	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3830	1/1	0.95	0.16	14,14,14,14	0
54	MG	1A	3405	1/1	0.95	0.16	20,20,20,20	0
54	MG	2A	3540	1/1	0.95	0.28	61,61,61,61	0
54	MG	1A	3713	1/1	0.95	0.19	53,53,53,53	0
54	MG	2A	3498	1/1	0.95	0.12	52,52,52,52	0
54	MG	1a	1676	1/1	0.95	0.14	54,54,54,54	0
54	MG	1A	3856	1/1	0.95	0.10	58,58,58,58	0
54	MG	1A	3875	1/1	0.95	0.07	48,48,48,48	0
54	MG	1A	3687	1/1	0.95	0.17	30,30,30,30	0
54	MG	1E	302	1/1	0.95	0.22	22,22,22,22	0
54	MG	2Q	3001	1/1	0.95	0.10	49,49,49,49	0
54	MG	1A	3327	1/1	0.95	0.11	57,57,57,57	0
54	MG	2A	3346	1/1	0.95	0.22	52,52,52,52	0
54	MG	2A	3233	1/1	0.95	0.82	53,53,53,53	0
54	MG	1A	3732	1/1	0.95	0.10	56,56,56,56	0
54	MG	1A	3302	1/1	0.95	0.13	57,57,57,57	0
54	MG	19	101	1/1	0.95	0.08	59,59,59,59	0
54	MG	1A	3122	1/1	0.95	0.43	45,45,45,45	0
54	MG	1A	3162	1/1	0.95	0.42	36,36,36,36	0
54	MG	1A	3738	1/1	0.95	0.14	45,45,45,45	0
54	MG	1a	1695	1/1	0.95	0.13	54,54,54,54	0
54	MG	2a	1621	1/1	0.95	0.12	58,58,58,58	0
54	MG	2A	3470	1/1	0.95	0.25	44,44,44,44	0
54	MG	1A	3457	1/1	0.95	0.15	39,39,39,39	0
54	MG	1A	3238	1/1	0.95	0.38	42,42,42,42	0
54	MG	1a	1823	1/1	0.95	0.11	65,65,65,65	0
54	MG	1A	3479	1/1	0.95	0.16	20,20,20,20	0
54	MG	1A	3975	1/1	0.95	0.10	65,65,65,65	0
54	MG	1A	3847	1/1	0.95	0.14	31,31,31,31	0
54	MG	1A	3938	1/1	0.95	0.14	59,59,59,59	0
54	MG	1A	3058	1/1	0.95	0.23	48,48,48,48	0
54	MG	1A	3829	1/1	0.95	0.10	25,25,25,25	0
54	MG	1A	3348	1/1	0.95	0.20	21,21,21,21	0
54	MG	2a	1759	1/1	0.95	0.14	68,68,68,68	0
54	MG	2A	3157	1/1	0.95	0.23	66,66,66,66	0
54	MG	1V	203	1/1	0.95	0.11	54,54,54,54	0
54	MG	1A	3520	1/1	0.95	0.22	51,51,51,51	0
54	MG	1a	1775	1/1	0.95	0.17	60,60,60,60	0
54	MG	1A	3257	1/1	0.95	0.15	48,48,48,48	0
54	MG	2A	3093	1/1	0.95	0.12	67,67,67,67	0
54	MG	11	101	1/1	0.95	0.10	41,41,41,41	0
54	MG	1A	3717	1/1	0.95	0.18	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3532	1/1	0.95	0.24	61,61,61,61	0
54	MG	1A	3965	1/1	0.95	0.14	52,52,52,52	0
54	MG	1A	4037	1/1	0.95	0.30	32,32,32,32	0
54	MG	1A	3299	1/1	0.95	0.23	37,37,37,37	0
54	MG	1A	3741	1/1	0.95	0.18	44,44,44,44	0
54	MG	1A	3247	1/1	0.95	0.19	31,31,31,31	0
54	MG	1A	3557	1/1	0.95	0.12	36,36,36,36	0
54	MG	1A	3903	1/1	0.95	0.30	38,38,38,38	0
54	MG	2a	1728	1/1	0.95	0.17	56,56,56,56	0
54	MG	1A	3750	1/1	0.95	0.11	19,19,19,19	0
54	MG	1A	3013	1/1	0.95	0.17	17,17,17,17	0
54	MG	1F	309	1/1	0.95	0.41	42,42,42,42	0
54	MG	1a	1731	1/1	0.95	0.16	60,60,60,60	0
54	MG	2A	3571	1/1	0.95	0.13	53,53,53,53	0
54	MG	2A	3347	1/1	0.95	0.20	32,32,32,32	0
54	MG	2t	3001	1/1	0.95	0.15	54,54,54,54	0
54	MG	1A	3577	1/1	0.95	0.07	44,44,44,44	0
54	MG	2A	3189	1/1	0.95	0.17	60,60,60,60	0
54	MG	2a	1729	1/1	0.95	0.20	53,53,53,53	0
54	MG	2A	3110	1/1	0.95	0.27	52,52,52,52	0
54	MG	1a	1796	1/1	0.95	0.17	61,61,61,61	0
54	MG	2a	1704	1/1	0.95	0.32	59,59,59,59	0
54	MG	2A	3203	1/1	0.95	0.15	57,57,57,57	0
54	MG	1A	3375	1/1	0.95	0.14	22,22,22,22	0
54	MG	2A	3596	1/1	0.95	0.21	47,47,47,47	0
54	MG	2A	3430	1/1	0.95	0.51	39,39,39,39	0
54	MG	1A	3512	1/1	0.95	0.15	48,48,48,48	0
54	MG	1A	3655	1/1	0.95	0.19	48,48,48,48	0
54	MG	2A	3187	1/1	0.95	0.14	52,52,52,52	0
54	MG	2A	3038	1/1	0.95	0.13	52,52,52,52	0
54	MG	1A	3529	1/1	0.95	0.22	35,35,35,35	0
54	MG	1A	3554	1/1	0.95	0.14	48,48,48,48	0
54	MG	2A	3030	1/1	0.95	0.17	49,49,49,49	0
54	MG	2A	3443	1/1	0.95	0.13	36,36,36,36	0
54	MG	2A	3320	1/1	0.95	0.20	60,60,60,60	0
54	MG	1A	3952	1/1	0.95	0.17	43,43,43,43	0
54	MG	1A	3581	1/1	0.96	0.25	32,32,32,32	0
54	MG	1V	201	1/1	0.96	0.14	47,47,47,47	0
54	MG	1A	3817	1/1	0.96	0.23	37,37,37,37	0
54	MG	2A	3684	1/1	0.96	0.07	53,53,53,53	0
54	MG	1A	3502	1/1	0.96	0.23	48,48,48,48	0
54	MG	2A	3145	1/1	0.96	0.12	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	4063	1/1	0.96	0.30	39,39,39,39	0
54	MG	2A	3588	1/1	0.96	0.13	42,42,42,42	0
54	MG	1A	3724	1/1	0.96	0.21	49,49,49,49	0
54	MG	1A	3877	1/1	0.96	0.11	62,62,62,62	0
54	MG	2a	1705	1/1	0.96	0.33	58,58,58,58	0
54	MG	1A	3880	1/1	0.96	0.25	44,44,44,44	0
54	MG	1A	3509	1/1	0.96	0.17	58,58,58,58	0
54	MG	1a	1778	1/1	0.96	0.11	57,57,57,57	0
54	MG	2A	3249	1/1	0.96	0.18	51,51,51,51	0
54	MG	1a	1794	1/1	0.96	0.23	61,61,61,61	0
54	MG	1A	3168	1/1	0.96	0.38	48,48,48,48	0
54	MG	1a	1774	1/1	0.96	0.14	51,51,51,51	0
54	MG	1a	1642	1/1	0.96	0.10	51,51,51,51	0
54	MG	2A	3016	1/1	0.96	0.50	45,45,45,45	0
54	MG	1A	3914	1/1	0.96	0.11	48,48,48,48	0
54	MG	1A	3049	1/1	0.96	0.25	34,34,34,34	0
54	MG	1A	3184	1/1	0.96	0.51	31,31,31,31	0
54	MG	1A	4072	1/1	0.96	0.27	36,36,36,36	0
54	MG	2a	1730	1/1	0.96	0.10	53,53,53,53	0
54	MG	1a	1706	1/1	0.96	0.12	59,59,59,59	0
54	MG	1A	3381	1/1	0.96	0.17	25,25,25,25	0
54	MG	1A	3080	1/1	0.96	0.19	51,51,51,51	0
54	MG	1A	3208	1/1	0.96	0.15	31,31,31,31	0
54	MG	2A	3101	1/1	0.96	0.30	51,51,51,51	0
54	MG	2A	3331	1/1	0.96	0.15	55,55,55,55	0
54	MG	1A	3650	1/1	0.96	0.15	51,51,51,51	0
54	MG	1A	3297	1/1	0.96	0.10	35,35,35,35	0
54	MG	1A	3452	1/1	0.96	0.12	36,36,36,36	0
54	MG	1A	3883	1/1	0.96	0.13	38,38,38,38	0
54	MG	2A	3515	1/1	0.96	0.21	45,45,45,45	0
54	MG	1A	3268	1/1	0.96	0.24	31,31,31,31	0
54	MG	1A	4065	1/1	0.96	0.18	29,29,29,29	0
54	MG	2A	3036	1/1	0.96	0.14	55,55,55,55	0
54	MG	1A	3676	1/1	0.96	0.14	50,50,50,50	0
54	MG	1A	3708	1/1	0.96	0.13	33,33,33,33	0
54	MG	1A	3590	1/1	0.96	0.12	29,29,29,29	0
54	MG	1A	3060	1/1	0.96	0.12	40,40,40,40	0
54	MG	2A	3593	1/1	0.96	0.13	39,39,39,39	0
54	MG	1A	3544	1/1	0.96	0.19	48,48,48,48	0
54	MG	2A	3689	1/1	0.96	0.20	59,59,59,59	0
54	MG	1A	3350	1/1	0.96	0.20	19,19,19,19	0
54	MG	1a	1697	1/1	0.96	0.09	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3548	1/1	0.96	0.14	41,41,41,41	0
54	MG	1t	3001	1/1	0.96	0.10	63,63,63,63	0
54	MG	1a	1846	1/1	0.96	0.17	51,51,51,51	0
54	MG	1A	3454	1/1	0.96	0.12	44,44,44,44	0
54	MG	2W	8002	1/1	0.96	0.23	66,66,66,66	0
54	MG	1A	3551	1/1	0.96	0.22	47,47,47,47	0
54	MG	1A	3116	1/1	0.96	0.09	46,46,46,46	0
54	MG	1A	3727	1/1	0.96	0.20	30,30,30,30	0
54	MG	2A	3003	1/1	0.96	0.12	31,31,31,31	0
54	MG	1A	3736	1/1	0.96	0.15	26,26,26,26	0
54	MG	2a	1672	1/1	0.96	0.18	70,70,70,70	0
54	MG	2A	3502	1/1	0.96	0.13	61,61,61,61	0
54	MG	2A	3335	1/1	0.96	0.21	53,53,53,53	0
54	MG	1A	3563	1/1	0.96	0.17	23,23,23,23	0
54	MG	2a	1741	1/1	0.96	0.24	47,47,47,47	0
54	MG	2A	3445	1/1	0.96	0.16	38,38,38,38	0
54	MG	1A	3366	1/1	0.96	0.11	35,35,35,35	0
54	MG	1A	3047	1/1	0.96	0.13	19,19,19,19	0
54	MG	1A	3311	1/1	0.96	0.11	26,26,26,26	0
54	MG	1A	4010	1/1	0.96	0.10	18,18,18,18	0
54	MG	1A	4066	1/1	0.96	0.30	33,33,33,33	0
54	MG	1Z	8001	1/1	0.96	0.12	54,54,54,54	0
54	MG	1a	1761	1/1	0.96	0.23	56,56,56,56	0
54	MG	2A	3362	1/1	0.96	0.11	51,51,51,51	0
54	MG	2A	3701	1/1	0.96	0.27	46,46,46,46	0
54	MG	1A	3904	1/1	0.96	0.31	66,66,66,66	0
54	MG	2A	3388	1/1	0.96	0.20	56,56,56,56	0
54	MG	2A	3159	1/1	0.96	0.14	45,45,45,45	0
54	MG	1A	3282	1/1	0.96	0.17	49,49,49,49	0
54	MG	2A	3286	1/1	0.96	0.17	54,54,54,54	0
54	MG	2A	3292	1/1	0.96	0.25	55,55,55,55	0
54	MG	1A	3358	1/1	0.96	0.15	17,17,17,17	0
54	MG	2a	1767	1/1	0.96	0.24	72,72,72,72	0
54	MG	1A	3202	1/1	0.96	0.51	35,35,35,35	0
54	MG	2A	3290	1/1	0.96	0.16	33,33,33,33	0
54	MG	2A	3607	1/1	0.96	0.10	72,72,72,72	0
54	MG	1A	3339	1/1	0.96	0.18	44,44,44,44	0
54	MG	1A	3712	1/1	0.96	0.13	51,51,51,51	0
54	MG	1A	3701	1/1	0.96	0.13	41,41,41,41	0
54	MG	1A	4057	1/1	0.96	0.45	29,29,29,29	0
54	MG	2A	3683	1/1	0.96	0.15	27,27,27,27	0
54	MG	1A	3550	1/1	0.96	0.14	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3796	1/1	0.96	0.24	24,24,24,24	0
54	MG	1A	3480	1/1	0.96	0.13	58,58,58,58	0
54	MG	2A	3134	1/1	0.96	0.14	40,40,40,40	0
54	MG	1A	3683	1/1	0.96	0.11	40,40,40,40	0
54	MG	2A	3358	1/1	0.96	0.13	41,41,41,41	0
54	MG	1A	3255	1/1	0.96	0.26	51,51,51,51	0
54	MG	1A	3833	1/1	0.96	0.10	50,50,50,50	0
54	MG	2a	1783	1/1	0.96	0.14	49,49,49,49	0
54	MG	2a	1720	1/1	0.96	0.12	66,66,66,66	0
54	MG	1a	1652	1/1	0.96	0.20	58,58,58,58	0
54	MG	1A	4069	1/1	0.96	0.14	28,28,28,28	0
54	MG	2A	3400	1/1	0.96	0.23	50,50,50,50	0
59	ZN	14	501	1/1	0.96	0.13	82,82,82,82	0
54	MG	1A	3283	1/1	0.96	0.26	58,58,58,58	0
54	MG	1A	3744	1/1	0.96	0.36	30,30,30,30	0
54	MG	2A	3108	1/1	0.96	0.16	57,57,57,57	0
54	MG	2A	3204	1/1	0.96	0.39	38,38,38,38	0
54	MG	1A	3004	1/1	0.96	0.24	47,47,47,47	0
54	MG	18	101	1/1	0.96	0.22	48,48,48,48	0
54	MG	2A	3476	1/1	0.96	0.20	30,30,30,30	0
54	MG	1A	3201	1/1	0.96	0.29	58,58,58,58	0
54	MG	1A	3281	1/1	0.96	0.16	39,39,39,39	0
54	MG	1A	3907	1/1	0.96	0.18	59,59,59,59	0
54	MG	1A	3865	1/1	0.96	0.10	22,22,22,22	0
54	MG	2A	3411	1/1	0.96	0.15	47,47,47,47	0
54	MG	1A	3503	1/1	0.96	0.17	31,31,31,31	0
54	MG	1A	3258	1/1	0.96	0.11	47,47,47,47	0
54	MG	2A	3357	1/1	0.96	0.16	45,45,45,45	0
54	MG	1A	3112	1/1	0.96	0.17	28,28,28,28	0
54	MG	2A	3285	1/1	0.96	0.16	30,30,30,30	0
54	MG	2A	3390	1/1	0.96	0.16	66,66,66,66	0
54	MG	1A	3437	1/1	0.96	0.18	25,25,25,25	0
54	MG	1D	305	1/1	0.96	0.16	30,30,30,30	0
54	MG	1A	3758	1/1	0.96	0.19	27,27,27,27	0
54	MG	2A	3005	1/1	0.96	0.12	43,43,43,43	0
54	MG	1a	1856	1/1	0.96	0.11	49,49,49,49	0
54	MG	1a	1804	1/1	0.96	0.07	52,52,52,52	0
54	MG	2A	3088	1/1	0.96	0.15	29,29,29,29	0
54	MG	2A	3129	1/1	0.96	0.36	47,47,47,47	0
54	MG	1A	3092	1/1	0.96	0.36	35,35,35,35	0
54	MG	1a	1661	1/1	0.96	0.26	55,55,55,55	0
54	MG	1a	1627	1/1	0.96	0.18	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	1753	1/1	0.96	0.21	57,57,57,57	0
54	MG	2A	3105	1/1	0.96	0.09	61,61,61,61	0
54	MG	1a	1662	1/1	0.96	0.17	63,63,63,63	0
54	MG	1A	3400	1/1	0.96	0.25	62,62,62,62	0
54	MG	2A	3141	1/1	0.96	0.19	53,53,53,53	0
54	MG	2a	1683	1/1	0.96	0.17	56,56,56,56	0
54	MG	1A	3929	1/1	0.96	0.16	58,58,58,58	0
54	MG	2A	3264	1/1	0.96	0.20	50,50,50,50	0
54	MG	2A	3644	1/1	0.96	0.15	53,53,53,53	0
54	MG	1A	3085	1/1	0.96	0.42	33,33,33,33	0
54	MG	1A	3393	1/1	0.96	0.15	50,50,50,50	0
54	MG	1A	3276	1/1	0.96	0.22	28,28,28,28	0
54	MG	1A	4044	1/1	0.96	0.15	25,25,25,25	0
54	MG	1a	1700	1/1	0.96	0.28	31,31,31,31	0
54	MG	2A	3454	1/1	0.96	0.18	58,58,58,58	0
54	MG	2A	3580	1/1	0.96	0.22	40,40,40,40	0
54	MG	1A	3065	1/1	0.96	0.42	41,41,41,41	0
54	MG	1A	4053	1/1	0.96	0.41	34,34,34,34	0
54	MG	1A	3440	1/1	0.96	0.11	46,46,46,46	0
54	MG	2a	1626	1/1	0.96	0.14	66,66,66,66	0
54	MG	1A	3237	1/1	0.96	0.11	55,55,55,55	0
54	MG	1A	4038	1/1	0.96	0.25	50,50,50,50	0
54	MG	1A	3441	1/1	0.96	0.14	18,18,18,18	0
54	MG	1A	3397	1/1	0.96	0.17	20,20,20,20	0
54	MG	2A	3483	1/1	0.96	0.23	62,62,62,62	0
54	MG	1F	308	1/1	0.96	0.24	52,52,52,52	0
54	MG	2A	3325	1/1	0.96	0.14	63,63,63,63	0
54	MG	1A	3607	1/1	0.96	0.25	42,42,42,42	0
54	MG	1A	3124	1/1	0.96	0.16	19,19,19,19	0
54	MG	1A	3353	1/1	0.96	0.21	34,34,34,34	0
54	MG	1A	3161	1/1	0.96	0.31	35,35,35,35	0
54	MG	2A	3114	1/1	0.96	0.16	41,41,41,41	0
54	MG	1A	3482	1/1	0.96	0.12	21,21,21,21	0
54	MG	1A	3453	1/1	0.96	0.16	38,38,38,38	0
54	MG	1A	3012	1/1	0.96	0.15	43,43,43,43	0
54	MG	1A	3140	1/1	0.96	0.16	26,26,26,26	0
54	MG	1E	305	1/1	0.96	0.17	57,57,57,57	0
54	MG	1B	205	1/1	0.96	0.15	47,47,47,47	0
54	MG	1A	3174	1/1	0.96	0.34	40,40,40,40	0
54	MG	1a	1826	1/1	0.96	0.14	47,47,47,47	0
54	MG	1a	1619	1/1	0.96	0.17	53,53,53,53	0
54	MG	1A	3213	1/1	0.96	0.53	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	1623	1/1	0.96	0.10	46,46,46,46	0
54	MG	2A	3500	1/1	0.96	0.21	43,43,43,43	0
54	MG	1A	3170	1/1	0.96	0.23	40,40,40,40	0
54	MG	2a	1671	1/1	0.96	0.08	68,68,68,68	0
54	MG	1a	1715	1/1	0.96	0.12	67,67,67,67	0
54	MG	1A	4033	1/1	0.96	0.09	48,48,48,48	0
54	MG	1a	1824	1/1	0.96	0.09	42,42,42,42	0
54	MG	2A	3007	1/1	0.96	0.26	44,44,44,44	0
54	MG	1A	3716	1/1	0.96	0.18	42,42,42,42	0
54	MG	2A	3265	1/1	0.96	0.15	37,37,37,37	0
54	MG	1A	3037	1/1	0.96	0.12	48,48,48,48	0
54	MG	1A	3179	1/1	0.96	0.16	41,41,41,41	0
54	MG	1A	3783	1/1	0.96	0.08	46,46,46,46	0
54	MG	1A	3099	1/1	0.96	0.17	55,55,55,55	0
54	MG	2A	3113	1/1	0.96	0.13	59,59,59,59	0
54	MG	1A	3217	1/1	0.96	0.15	42,42,42,42	0
54	MG	1A	3493	1/1	0.96	0.12	27,27,27,27	0
54	MG	2a	1702	1/1	0.96	0.09	69,69,69,69	0
54	MG	1a	1740	1/1	0.96	0.13	66,66,66,66	0
54	MG	2A	3252	1/1	0.96	0.14	51,51,51,51	0
54	MG	2A	3018	1/1	0.96	0.46	54,54,54,54	0
54	MG	1A	3347	1/1	0.96	0.15	27,27,27,27	0
54	MG	1A	3328	1/1	0.96	0.12	42,42,42,42	0
54	MG	1a	1859	1/1	0.96	0.12	57,57,57,57	0
54	MG	1A	3718	1/1	0.96	0.24	41,41,41,41	0
54	MG	1A	3631	1/1	0.96	0.25	48,48,48,48	0
54	MG	23	101	1/1	0.96	0.15	55,55,55,55	0
54	MG	2A	3010	1/1	0.96	0.27	37,37,37,37	0
54	MG	1A	3418	1/1	0.96	0.09	50,50,50,50	0
54	MG	1A	4014	1/1	0.96	0.30	34,34,34,34	0
54	MG	2A	3566	1/1	0.96	0.18	27,27,27,27	0
54	MG	1A	3824	1/1	0.96	0.09	11,11,11,11	0
54	MG	1A	3464	1/1	0.96	0.20	16,16,16,16	0
54	MG	2A	3061	1/1	0.96	0.48	47,47,47,47	0
54	MG	1a	1858	1/1	0.96	0.18	59,59,59,59	0
54	MG	2a	1660	1/1	0.96	0.15	69,69,69,69	0
54	MG	2A	3501	1/1	0.96	0.22	38,38,38,38	0
54	MG	2A	3526	1/1	0.96	0.22	54,54,54,54	0
54	MG	2a	1773	1/1	0.96	0.08	59,59,59,59	0
54	MG	1A	3469	1/1	0.96	0.15	18,18,18,18	0
54	MG	1A	3873	1/1	0.96	0.09	57,57,57,57	0
54	MG	1T	203	1/1	0.96	0.07	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3101	1/1	0.96	0.25	25,25,25,25	0
54	MG	2a	1709	1/1	0.96	0.23	63,63,63,63	0
54	MG	1A	3774	1/1	0.96	0.09	31,31,31,31	0
54	MG	1A	3956	1/1	0.96	0.11	48,48,48,48	0
54	MG	1a	1624	1/1	0.96	0.10	63,63,63,63	0
54	MG	2A	3033	1/1	0.96	0.07	27,27,27,27	0
54	MG	2a	1686	1/1	0.96	0.20	57,57,57,57	0
54	MG	2A	3492	1/1	0.96	0.14	48,48,48,48	0
54	MG	1A	3762	1/1	0.96	0.14	41,41,41,41	0
54	MG	1A	3423	1/1	0.96	0.16	29,29,29,29	0
54	MG	1a	1704	1/1	0.96	0.12	56,56,56,56	0
54	MG	2A	3254	1/1	0.96	0.12	43,43,43,43	0
54	MG	1a	1749	1/1	0.96	0.20	61,61,61,61	0
54	MG	1A	3077	1/1	0.96	0.34	30,30,30,30	0
54	MG	1a	1827	1/1	0.96	0.06	65,65,65,65	0
54	MG	1A	3156	1/1	0.96	0.38	41,41,41,41	0
54	MG	1A	3546	1/1	0.96	0.18	39,39,39,39	0
54	MG	1a	1667	1/1	0.96	0.27	56,56,56,56	0
54	MG	1A	3031	1/1	0.96	0.12	46,46,46,46	0
54	MG	1A	3236	1/1	0.96	0.55	43,43,43,43	0
54	MG	2a	1764	1/1	0.96	0.07	63,63,63,63	0
54	MG	1a	1618	1/1	0.97	0.09	52,52,52,52	0
54	MG	1A	3191	1/1	0.97	0.34	35,35,35,35	0
54	MG	1A	3070	1/1	0.97	0.23	25,25,25,25	0
54	MG	1A	3098	1/1	0.97	0.22	25,25,25,25	0
54	MG	1A	3338	1/1	0.97	0.16	48,48,48,48	0
54	MG	1A	3033	1/1	0.97	0.13	41,41,41,41	0
54	MG	1a	1610	1/1	0.97	0.12	49,49,49,49	0
54	MG	1a	1682	1/1	0.97	0.14	54,54,54,54	0
60	SF4	1d	501	8/8	0.97	0.15	50,59,66,73	0
54	MG	2A	3365	1/1	0.97	0.15	38,38,38,38	0
54	MG	1A	3700	1/1	0.97	0.13	27,27,27,27	0
54	MG	1A	3083	1/1	0.97	0.15	34,34,34,34	0
54	MG	2A	3568	1/1	0.97	0.17	43,43,43,43	0
54	MG	2A	3690	1/1	0.97	0.31	37,37,37,37	0
54	MG	1A	3148	1/1	0.97	0.32	26,26,26,26	0
54	MG	2A	3618	1/1	0.97	0.10	66,66,66,66	0
54	MG	1a	1818	1/1	0.97	0.11	51,51,51,51	0
54	MG	2A	3121	1/1	0.97	0.12	59,59,59,59	0
54	MG	2A	3194	1/1	0.97	0.06	53,53,53,53	0
54	MG	1a	1800	1/1	0.97	0.16	50,50,50,50	0
54	MG	1A	3314	1/1	0.97	0.10	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3110	1/1	0.97	0.08	33,33,33,33	0
54	MG	1A	3714	1/1	0.97	0.10	32,32,32,32	0
54	MG	1A	3320	1/1	0.97	0.20	15,15,15,15	0
54	MG	1A	3325	1/1	0.97	0.16	22,22,22,22	0
54	MG	1a	1821	1/1	0.97	0.11	58,58,58,58	0
54	MG	1F	305	1/1	0.97	0.33	30,30,30,30	0
54	MG	2A	3289	1/1	0.97	0.17	53,53,53,53	0
54	MG	2A	3109	1/1	0.97	0.11	60,60,60,60	0
54	MG	1A	3749	1/1	0.97	0.20	30,30,30,30	0
54	MG	2V	201	1/1	0.97	0.15	57,57,57,57	0
54	MG	2A	3117	1/1	0.97	0.38	49,49,49,49	0
54	MG	2A	3510	1/1	0.97	0.15	36,36,36,36	0
54	MG	1A	3181	1/1	0.97	0.31	24,24,24,24	0
54	MG	2A	3581	1/1	0.97	0.13	44,44,44,44	0
54	MG	1A	3842	1/1	0.97	0.23	50,50,50,50	0
54	MG	1A	3203	1/1	0.97	0.33	35,35,35,35	0
54	MG	2A	3522	1/1	0.97	0.12	53,53,53,53	0
54	MG	2A	3156	1/1	0.97	0.20	61,61,61,61	0
54	MG	1A	4005	1/1	0.97	0.06	57,57,57,57	0
54	MG	1A	3622	1/1	0.97	0.14	27,27,27,27	0
54	MG	2a	1649	1/1	0.97	0.19	50,50,50,50	0
54	MG	2a	1708	1/1	0.97	0.09	48,48,48,48	0
54	MG	1A	3009	1/1	0.97	0.12	24,24,24,24	0
54	MG	2A	3125	1/1	0.97	0.16	52,52,52,52	0
54	MG	1U	202	1/1	0.97	0.12	46,46,46,46	0
54	MG	1A	3884	1/1	0.97	0.10	25,25,25,25	0
54	MG	2A	3398	1/1	0.97	0.14	42,42,42,42	0
54	MG	1A	3220	1/1	0.97	0.24	32,32,32,32	0
54	MG	2A	3548	1/1	0.97	0.15	34,34,34,34	0
54	MG	2a	1775	1/1	0.97	0.13	78,78,78,78	0
54	MG	1A	3652	1/1	0.97	0.14	39,39,39,39	0
54	MG	2A	3578	1/1	0.97	0.21	54,54,54,54	0
54	MG	1B	209	1/1	0.97	0.12	35,35,35,35	0
54	MG	1A	3836	1/1	0.97	0.40	32,32,32,32	0
54	MG	1A	3231	1/1	0.97	0.23	29,29,29,29	0
54	MG	2A	3270	1/1	0.97	0.08	55,55,55,55	0
54	MG	1A	3568	1/1	0.97	0.20	47,47,47,47	0
54	MG	1A	3123	1/1	0.97	0.22	35,35,35,35	0
54	MG	1A	3108	1/1	0.97	0.23	34,34,34,34	0
54	MG	1A	3450	1/1	0.97	0.11	16,16,16,16	0
54	MG	1A	3633	1/1	0.97	0.43	50,50,50,50	0
54	MG	1A	3839	1/1	0.97	0.19	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3478	1/1	0.97	0.06	38,38,38,38	0
54	MG	1A	3054	1/1	0.97	0.31	25,25,25,25	0
54	MG	1A	3137	1/1	0.97	0.24	28,28,28,28	0
54	MG	1A	3812	1/1	0.97	0.15	42,42,42,42	0
54	MG	1A	3318	1/1	0.97	0.18	13,13,13,13	0
54	MG	1A	3500	1/1	0.97	0.21	33,33,33,33	0
54	MG	2A	3102	1/1	0.97	0.37	36,36,36,36	0
54	MG	2A	3304	1/1	0.97	0.18	60,60,60,60	0
54	MG	1A	3196	1/1	0.97	0.52	33,33,33,33	0
54	MG	1a	1696	1/1	0.97	0.23	56,56,56,56	0
54	MG	1A	3001	1/1	0.97	0.14	31,31,31,31	0
54	MG	1A	3084	1/1	0.97	0.14	36,36,36,36	0
54	MG	2a	1651	1/1	0.97	0.11	68,68,68,68	0
54	MG	2A	3529	1/1	0.97	0.33	64,64,64,64	0
54	MG	2A	3191	1/1	0.97	0.12	57,57,57,57	0
54	MG	1a	1664	1/1	0.97	0.14	56,56,56,56	0
54	MG	2A	3541	1/1	0.97	0.27	56,56,56,56	0
54	MG	1A	3245	1/1	0.97	0.21	12,12,12,12	0
54	MG	1a	1756	1/1	0.97	0.18	49,49,49,49	0
54	MG	1A	3354	1/1	0.97	0.19	17,17,17,17	0
54	MG	2A	3006	1/1	0.97	0.13	45,45,45,45	0
54	MG	1k	3001	1/1	0.97	0.16	42,42,42,42	0
54	MG	1A	3819	1/1	0.97	0.11	46,46,46,46	0
54	MG	2A	3655	1/1	0.97	0.23	79,79,79,79	0
54	MG	1a	1684	1/1	0.97	0.23	46,46,46,46	0
54	MG	1A	3498	1/1	0.97	0.13	28,28,28,28	0
54	MG	15	103	1/1	0.97	0.09	45,45,45,45	0
54	MG	1A	3821	1/1	0.97	0.10	40,40,40,40	0
54	MG	1B	218	1/1	0.97	0.19	39,39,39,39	0
54	MG	2E	306	1/1	0.97	0.34	42,42,42,42	0
54	MG	1A	3287	1/1	0.97	0.17	22,22,22,22	0
54	MG	1A	3811	1/1	0.97	0.17	28,28,28,28	0
54	MG	2a	1665	1/1	0.97	0.12	58,58,58,58	0
54	MG	1F	302	1/1	0.97	0.42	33,33,33,33	0
54	MG	1A	3832	1/1	0.97	0.20	22,22,22,22	0
54	MG	1a	1687	1/1	0.97	0.20	34,34,34,34	0
54	MG	2A	3284	1/1	0.97	0.15	27,27,27,27	0
54	MG	1A	3019	1/1	0.97	0.46	35,35,35,35	0
54	MG	2A	3279	1/1	0.97	0.14	51,51,51,51	0
54	MG	2F	3003	1/1	0.97	0.41	43,43,43,43	0
54	MG	2A	3417	1/1	0.97	0.21	61,61,61,61	0
54	MG	1A	3815	1/1	0.97	0.21	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3574	1/1	0.97	0.20	21,21,21,21	0
54	MG	1A	3654	1/1	0.97	0.14	24,24,24,24	0
54	MG	1A	3063	1/1	0.97	0.20	53,53,53,53	0
54	MG	1N	201	1/1	0.97	0.16	36,36,36,36	0
54	MG	1a	1686	1/1	0.97	0.10	46,46,46,46	0
54	MG	1A	3341	1/1	0.97	0.13	24,24,24,24	0
54	MG	1A	3442	1/1	0.97	0.18	16,16,16,16	0
54	MG	1A	3476	1/1	0.97	0.15	19,19,19,19	0
54	MG	1A	3115	1/1	0.97	0.31	26,26,26,26	0
54	MG	1A	3704	1/1	0.97	0.20	38,38,38,38	0
54	MG	1A	4054	1/1	0.97	0.24	34,34,34,34	0
54	MG	1A	3355	1/1	0.97	0.18	16,16,16,16	0
54	MG	1A	3564	1/1	0.97	0.19	18,18,18,18	0
54	MG	2A	3647	1/1	0.97	0.07	55,55,55,55	0
54	MG	1A	3219	1/1	0.97	0.34	31,31,31,31	0
54	MG	1A	3562	1/1	0.97	0.11	39,39,39,39	0
54	MG	2A	3371	1/1	0.97	0.18	48,48,48,48	0
54	MG	2A	3300	1/1	0.97	0.14	47,47,47,47	0
54	MG	1A	3326	1/1	0.97	0.18	27,27,27,27	0
54	MG	2A	3463	1/1	0.97	0.30	48,48,48,48	0
54	MG	1A	3800	1/1	0.97	0.19	21,21,21,21	0
54	MG	2A	3406	1/1	0.97	0.21	63,63,63,63	0
54	MG	1A	3934	1/1	0.97	0.04	76,76,76,76	0
54	MG	1A	3887	1/1	0.97	0.12	37,37,37,37	0
54	MG	28	103	1/1	0.97	0.08	46,46,46,46	0
54	MG	2A	3435	1/1	0.97	0.17	60,60,60,60	0
54	MG	1a	1628	1/1	0.97	0.14	58,58,58,58	0
54	MG	1A	3407	1/1	0.97	0.17	47,47,47,47	0
54	MG	1A	3018	1/1	0.97	0.24	23,23,23,23	0
54	MG	1A	3310	1/1	0.97	0.18	16,16,16,16	0
54	MG	2A	3283	1/1	0.97	0.20	29,29,29,29	0
54	MG	1A	3632	1/1	0.97	0.28	48,48,48,48	0
54	MG	1A	3831	1/1	0.97	0.14	39,39,39,39	0
54	MG	1T	202	1/1	0.97	0.16	58,58,58,58	0
54	MG	1A	3794	1/1	0.97	0.16	18,18,18,18	0
54	MG	1A	4049	1/1	0.97	0.16	35,35,35,35	0
56	EZM	1A	4035	24/24	0.97	0.34	21,31,39,44	0
54	MG	1A	3886	1/1	0.97	0.08	51,51,51,51	0
54	MG	1A	3141	1/1	0.97	0.11	23,23,23,23	0
54	MG	1a	1830	1/1	0.97	0.19	60,60,60,60	0
54	MG	1A	3915	1/1	0.97	0.13	17,17,17,17	0
54	MG	1A	3511	1/1	0.97	0.16	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3068	1/1	0.97	0.14	36,36,36,36	0
54	MG	1A	3315	1/1	0.97	0.12	45,45,45,45	0
54	MG	1A	3686	1/1	0.97	0.20	36,36,36,36	0
54	MG	1B	215	1/1	0.97	0.17	39,39,39,39	0
54	MG	2A	3528	1/1	0.97	0.18	54,54,54,54	0
54	MG	1a	1708	1/1	0.97	0.15	31,31,31,31	0
54	MG	2A	3104	1/1	0.97	0.14	65,65,65,65	0
54	MG	2B	205	1/1	0.97	0.11	67,67,67,67	0
54	MG	13	103	1/1	0.97	0.14	39,39,39,39	0
54	MG	1D	301	1/1	0.97	0.20	12,12,12,12	0
54	MG	1A	3292	1/1	0.97	0.18	28,28,28,28	0
54	MG	2a	1770	1/1	0.97	0.06	67,67,67,67	0
54	MG	1A	3932	1/1	0.97	0.08	53,53,53,53	0
54	MG	2A	3096	1/1	0.97	0.21	50,50,50,50	0
54	MG	1A	4067	1/1	0.97	0.27	33,33,33,33	0
54	MG	1A	3862	1/1	0.97	0.12	39,39,39,39	0
54	MG	2a	1707	1/1	0.97	0.16	48,48,48,48	0
54	MG	2A	3543	1/1	0.97	0.15	40,40,40,40	0
54	MG	2A	3014	1/1	0.97	0.39	42,42,42,42	0
54	MG	1A	3483	1/1	0.97	0.22	58,58,58,58	0
54	MG	2A	3534	1/1	0.97	0.24	60,60,60,60	0
54	MG	2A	3479	1/1	0.97	0.24	53,53,53,53	0
54	MG	1A	4051	1/1	0.97	0.17	34,34,34,34	0
54	MG	1A	3556	1/1	0.97	0.25	29,29,29,29	0
54	MG	1A	3507	1/1	0.97	0.17	32,32,32,32	0
54	MG	1A	3510	1/1	0.97	0.11	47,47,47,47	0
54	MG	1A	3061	1/1	0.97	0.13	26,26,26,26	0
54	MG	2A	3623	1/1	0.97	0.12	64,64,64,64	0
54	MG	1A	3396	1/1	0.97	0.14	46,46,46,46	0
54	MG	2a	1718	1/1	0.97	0.20	46,46,46,46	0
54	MG	2A	3428	1/1	0.97	0.15	35,35,35,35	0
54	MG	2A	3123	1/1	0.97	0.15	38,38,38,38	0
54	MG	1A	3313	1/1	0.97	0.20	23,23,23,23	0
54	MG	2a	1691	1/1	0.97	0.18	68,68,68,68	0
54	MG	1A	3087	1/1	0.97	0.15	17,17,17,17	0
54	MG	1A	3818	1/1	0.97	0.15	24,24,24,24	0
54	MG	1A	3690	1/1	0.97	0.25	37,37,37,37	0
54	MG	2A	3073	1/1	0.97	0.25	61,61,61,61	0
54	MG	1A	3199	1/1	0.97	0.35	25,25,25,25	0
54	MG	1A	3688	1/1	0.97	0.14	46,46,46,46	0
54	MG	1A	3735	1/1	0.97	0.18	48,48,48,48	0
54	MG	1A	3672	1/1	0.97	0.18	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3214	1/1	0.97	0.31	38,38,38,38	0
54	MG	1A	3189	1/1	0.97	0.51	33,33,33,33	0
54	MG	2A	3035	1/1	0.97	0.11	53,53,53,53	0
54	MG	1D	304	1/1	0.97	0.22	41,41,41,41	0
54	MG	2a	1610	1/1	0.97	0.12	48,48,48,48	0
54	MG	1A	3850	1/1	0.97	0.07	43,43,43,43	0
54	MG	2A	3181	1/1	0.97	0.42	43,43,43,43	0
54	MG	2A	3699	1/1	0.97	0.65	47,47,47,47	0
54	MG	1A	3424	1/1	0.97	0.05	42,42,42,42	0
59	ZN	29	501	1/1	0.97	0.15	68,68,68,68	0
54	MG	1A	3178	1/1	0.97	0.30	27,27,27,27	0
54	MG	2B	218	1/1	0.97	0.14	60,60,60,60	0
54	MG	2A	3349	1/1	0.97	0.13	49,49,49,49	0
54	MG	15	101	1/1	0.97	0.09	44,44,44,44	0
54	MG	1a	1607	1/1	0.97	0.10	49,49,49,49	0
54	MG	2A	3505	1/1	0.97	0.12	44,44,44,44	0
54	MG	2a	1652	1/1	0.97	0.09	71,71,71,71	0
54	MG	2A	3056	1/1	0.97	0.34	39,39,39,39	0
54	MG	1A	3662	1/1	0.97	0.08	39,39,39,39	0
54	MG	2A	3040	1/1	0.97	0.16	39,39,39,39	0
54	MG	1A	3608	1/1	0.97	0.12	36,36,36,36	0
54	MG	1A	4073	1/1	0.97	0.27	36,36,36,36	0
54	MG	1A	3145	1/1	0.97	0.20	37,37,37,37	0
54	MG	2A	3569	1/1	0.97	0.16	24,24,24,24	0
54	MG	1A	3360	1/1	0.97	0.15	18,18,18,18	0
54	MG	2A	3281	1/1	0.97	0.14	32,32,32,32	0
54	MG	1a	1735	1/1	0.97	0.13	54,54,54,54	0
54	MG	2A	3274	1/1	0.97	0.18	46,46,46,46	0
54	MG	2A	3097	1/1	0.98	0.23	46,46,46,46	0
54	MG	2A	3343	1/1	0.98	0.22	45,45,45,45	0
54	MG	1A	3403	1/1	0.98	0.10	47,47,47,47	0
54	MG	2A	3058	1/1	0.98	0.20	30,30,30,30	0
54	MG	2D	301	1/1	0.98	0.56	52,52,52,52	0
54	MG	2A	3348	1/1	0.98	0.18	70,70,70,70	0
54	MG	1A	3048	1/1	0.98	0.32	43,43,43,43	0
54	MG	1A	3386	1/1	0.98	0.14	29,29,29,29	0
54	MG	1A	3698	1/1	0.98	0.22	41,41,41,41	0
54	MG	1A	3827	1/1	0.98	0.21	49,49,49,49	0
54	MG	1A	3719	1/1	0.98	0.17	26,26,26,26	0
54	MG	1A	3016	1/1	0.98	0.19	30,30,30,30	0
54	MG	2E	301	1/1	0.98	0.18	35,35,35,35	0
54	MG	2A	3089	1/1	0.98	0.21	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3394	1/1	0.98	0.13	37,37,37,37	0
54	MG	2A	3361	1/1	0.98	0.14	30,30,30,30	0
54	MG	1A	3555	1/1	0.98	0.23	34,34,34,34	0
54	MG	2A	3421	1/1	0.98	0.13	72,72,72,72	0
54	MG	1A	3636	1/1	0.98	0.25	36,36,36,36	0
54	MG	1A	3007	1/1	0.98	0.18	32,32,32,32	0
54	MG	1A	3885	1/1	0.98	0.15	28,28,28,28	0
54	MG	1A	3496	1/1	0.98	0.12	34,34,34,34	0
54	MG	2A	3377	1/1	0.98	0.14	63,63,63,63	0
54	MG	1A	3879	1/1	0.98	0.09	47,47,47,47	0
54	MG	1A	3492	1/1	0.98	0.13	24,24,24,24	0
54	MG	1a	1705	1/1	0.98	0.13	61,61,61,61	0
54	MG	1A	3119	1/1	0.98	0.50	25,25,25,25	0
54	MG	2a	1689	1/1	0.98	0.18	58,58,58,58	0
54	MG	1A	3595	1/1	0.98	0.10	25,25,25,25	0
54	MG	1A	3147	1/1	0.98	0.32	26,26,26,26	0
54	MG	2A	3442	1/1	0.98	0.20	37,37,37,37	0
54	MG	1A	3455	1/1	0.98	0.16	57,57,57,57	0
54	MG	1A	3082	1/1	0.98	0.20	33,33,33,33	0
54	MG	1A	3005	1/1	0.98	0.20	15,15,15,15	0
54	MG	2A	3246	1/1	0.98	0.32	44,44,44,44	0
54	MG	1G	3004	1/1	0.98	0.15	37,37,37,37	0
54	MG	2A	3676	1/1	0.98	0.14	40,40,40,40	0
54	MG	1A	3094	1/1	0.98	0.53	28,28,28,28	0
54	MG	1A	3660	1/1	0.98	0.11	28,28,28,28	0
54	MG	2a	1631	1/1	0.98	0.13	63,63,63,63	0
54	MG	2A	3555	1/1	0.98	0.24	55,55,55,55	0
54	MG	1A	3552	1/1	0.98	0.27	35,35,35,35	0
54	MG	1A	3153	1/1	0.98	0.28	32,32,32,32	0
54	MG	1a	1784	1/1	0.98	0.16	59,59,59,59	0
54	MG	2a	1706	1/1	0.98	0.27	63,63,63,63	0
54	MG	1A	4008	1/1	0.98	0.17	11,11,11,11	0
54	MG	2A	3220	1/1	0.98	0.20	48,48,48,48	0
54	MG	1A	3209	1/1	0.98	0.25	36,36,36,36	0
54	MG	1A	3804	1/1	0.98	0.09	60,60,60,60	0
54	MG	1A	3649	1/1	0.98	0.15	21,21,21,21	0
54	MG	1A	4047	1/1	0.98	0.26	24,24,24,24	0
54	MG	2A	3334	1/1	0.98	0.21	45,45,45,45	0
54	MG	1A	3023	1/1	0.98	0.23	18,18,18,18	0
54	MG	1A	3936	1/1	0.98	0.15	63,63,63,63	0
54	MG	1A	3888	1/1	0.98	0.17	24,24,24,24	0
54	MG	1Q	201	1/1	0.98	0.16	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	1646	1/1	0.98	0.18	49,49,49,49	0
54	MG	2A	3315	1/1	0.98	0.19	40,40,40,40	0
54	MG	1A	3194	1/1	0.98	0.49	29,29,29,29	0
54	MG	1A	3670	1/1	0.98	0.18	45,45,45,45	0
54	MG	1A	3776	1/1	0.98	0.20	26,26,26,26	0
54	MG	1A	3642	1/1	0.98	0.19	40,40,40,40	0
54	MG	1A	3006	1/1	0.98	0.21	25,25,25,25	0
59	ZN	26	501	1/1	0.98	0.18	58,58,58,58	0
54	MG	1A	3069	1/1	0.98	0.12	27,27,27,27	0
54	MG	2A	3067	1/1	0.98	0.14	56,56,56,56	0
54	MG	1D	303	1/1	0.98	0.38	40,40,40,40	0
54	MG	2A	3393	1/1	0.98	0.10	57,57,57,57	0
54	MG	1A	3876	1/1	0.98	0.30	62,62,62,62	0
54	MG	1A	4071	1/1	0.98	0.35	33,33,33,33	0
54	MG	1A	3274	1/1	0.98	0.25	34,34,34,34	0
59	ZN	25	501	1/1	0.98	0.20	52,52,52,52	0
54	MG	1A	3346	1/1	0.98	0.21	38,38,38,38	0
54	MG	1a	1777	1/1	0.98	0.14	64,64,64,64	0
54	MG	1A	3837	1/1	0.98	0.07	41,41,41,41	0
54	MG	1A	4052	1/1	0.98	0.27	30,30,30,30	0
54	MG	1A	3658	1/1	0.98	0.22	48,48,48,48	0
54	MG	1A	3210	1/1	0.98	0.15	49,49,49,49	0
54	MG	1A	3446	1/1	0.98	0.15	22,22,22,22	0
59	ZN	1n	501	1/1	0.98	0.11	59,59,59,59	0
54	MG	1A	3928	1/1	0.98	0.17	62,62,62,62	0
59	ZN	15	102	1/1	0.98	0.20	38,38,38,38	0
54	MG	1A	3064	1/1	0.98	0.24	34,34,34,34	0
54	MG	1F	304	1/1	0.98	0.37	24,24,24,24	0
54	MG	2A	3307	1/1	0.98	0.20	37,37,37,37	0
54	MG	2A	3012	1/1	0.98	0.31	39,39,39,39	0
54	MG	1A	3180	1/1	0.98	0.18	22,22,22,22	0
54	MG	1A	3152	1/1	0.98	0.18	28,28,28,28	0
54	MG	2A	3538	1/1	0.98	0.21	60,60,60,60	0
54	MG	1A	3224	1/1	0.98	0.50	26,26,26,26	0
54	MG	2A	3379	1/1	0.98	0.15	55,55,55,55	0
54	MG	1A	3840	1/1	0.98	0.12	46,46,46,46	0
54	MG	1g	3003	1/1	0.98	0.10	52,52,52,52	0
54	MG	1A	3419	1/1	0.98	0.23	45,45,45,45	0
54	MG	1A	3022	1/1	0.98	0.19	26,26,26,26	0
54	MG	2A	3462	1/1	0.98	0.22	22,22,22,22	0
54	MG	1A	3639	1/1	0.98	0.10	27,27,27,27	0
54	MG	2A	3686	1/1	0.98	0.11	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3597	1/1	0.98	0.29	43,43,43,43	0
60	SF4	2d	302	8/8	0.98	0.12	59,71,73,91	0
54	MG	2a	1778	1/1	0.98	0.08	56,56,56,56	0
54	MG	2A	3308	1/1	0.98	0.16	29,29,29,29	0
54	MG	1A	3027	1/1	0.98	0.40	30,30,30,30	0
54	MG	1A	3100	1/1	0.98	0.43	28,28,28,28	0
54	MG	2A	3107	1/1	0.98	0.20	27,27,27,27	0
54	MG	1A	3404	1/1	0.98	0.17	18,18,18,18	0
54	MG	2A	3177	1/1	0.98	0.42	43,43,43,43	0
54	MG	2A	3218	1/1	0.98	0.17	40,40,40,40	0
54	MG	1D	302	1/1	0.98	0.18	33,33,33,33	0
54	MG	1A	4059	1/1	0.98	0.23	28,28,28,28	0
54	MG	1A	3964	1/1	0.98	0.09	68,68,68,68	0
54	MG	2A	3256	1/1	0.98	0.19	30,30,30,30	0
54	MG	1A	4060	1/1	0.98	0.26	38,38,38,38	0
54	MG	1a	1726	1/1	0.98	0.13	55,55,55,55	0
54	MG	2A	3518	1/1	0.98	0.27	60,60,60,60	0
54	MG	1A	3411	1/1	0.98	0.19	42,42,42,42	0
54	MG	1A	3997	1/1	0.98	0.16	48,48,48,48	0
54	MG	1A	3149	1/1	0.98	0.24	28,28,28,28	0
54	MG	1a	1637	1/1	0.98	0.14	51,51,51,51	0
54	MG	1A	3273	1/1	0.98	0.26	33,33,33,33	0
54	MG	1a	1671	1/1	0.98	0.43	58,58,58,58	0
54	MG	1a	1810	1/1	0.98	0.10	60,60,60,60	0
54	MG	1A	3304	1/1	0.98	0.07	41,41,41,41	0
54	MG	1A	3127	1/1	0.98	0.26	29,29,29,29	0
54	MG	2A	3614	1/1	0.98	0.20	52,52,52,52	0
54	MG	2A	3223	1/1	0.98	0.25	55,55,55,55	0
54	MG	1A	3629	1/1	0.98	0.21	49,49,49,49	0
54	MG	2E	304	1/1	0.98	0.14	26,26,26,26	0
54	MG	1A	3748	1/1	0.98	0.13	12,12,12,12	0
54	MG	1A	3244	1/1	0.98	0.17	18,18,18,18	0
54	MG	1A	3925	1/1	0.98	0.09	46,46,46,46	0
54	MG	1a	1688	1/1	0.98	0.17	36,36,36,36	0
54	MG	1A	3052	1/1	0.98	0.14	28,28,28,28	0
54	MG	2A	3131	1/1	0.98	0.16	65,65,65,65	0
54	MG	1A	3768	1/1	0.98	0.06	36,36,36,36	0
54	MG	1A	3223	1/1	0.98	0.21	27,27,27,27	0
54	MG	1A	4048	1/1	0.98	0.15	31,31,31,31	0
54	MG	1A	3215	1/1	0.98	0.13	59,59,59,59	0
54	MG	1A	3349	1/1	0.98	0.18	16,16,16,16	0
54	MG	1A	3150	1/1	0.98	0.14	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3765	1/1	0.98	0.14	14,14,14,14	0
54	MG	2A	3516	1/1	0.98	0.09	26,26,26,26	0
54	MG	1A	3043	1/1	0.98	0.32	29,29,29,29	0
54	MG	1A	3171	1/1	0.98	0.35	35,35,35,35	0
54	MG	1a	1614	1/1	0.98	0.11	63,63,63,63	0
54	MG	1A	3392	1/1	0.98	0.15	12,12,12,12	0
54	MG	1A	3619	1/1	0.98	0.08	40,40,40,40	0
54	MG	1A	3572	1/1	0.98	0.13	25,25,25,25	0
54	MG	2A	3547	1/1	0.98	0.16	31,31,31,31	0
54	MG	1A	3528	1/1	0.98	0.16	19,19,19,19	0
54	MG	1A	4024	1/1	0.98	0.29	27,27,27,27	0
54	MG	2A	3287	1/1	0.98	0.22	42,42,42,42	0
54	MG	2a	1655	1/1	0.98	0.20	61,61,61,61	0
54	MG	2A	3297	1/1	0.98	0.20	39,39,39,39	0
54	MG	1A	3300	1/1	0.98	0.08	30,30,30,30	0
54	MG	1A	4046	1/1	0.98	0.14	20,20,20,20	0
54	MG	1A	3289	1/1	0.98	0.13	20,20,20,20	0
54	MG	2O	8003	1/1	0.98	0.11	64,64,64,64	0
54	MG	2a	1696	1/1	0.98	0.21	52,52,52,52	0
54	MG	1A	3143	1/1	0.98	0.38	40,40,40,40	0
54	MG	1A	4030	1/1	0.98	0.15	33,33,33,33	0
54	MG	1a	1603	1/1	0.98	0.12	44,44,44,44	0
54	MG	1a	1714	1/1	0.98	0.11	67,67,67,67	0
54	MG	1A	3335	1/1	0.98	0.08	46,46,46,46	0
54	MG	2A	3514	1/1	0.98	0.29	43,43,43,43	0
54	MG	1A	3560	1/1	0.98	0.13	30,30,30,30	0
54	MG	2W	8001	1/1	0.98	0.30	44,44,44,44	0
54	MG	1A	3955	1/1	0.98	0.11	50,50,50,50	0
54	MG	1A	4031	1/1	0.98	0.34	38,38,38,38	0
54	MG	1A	3534	1/1	0.98	0.14	44,44,44,44	0
54	MG	1Q	202	1/1	0.99	0.17	22,22,22,22	0
54	MG	1A	3017	1/1	0.99	0.23	21,21,21,21	0
54	MG	1A	3200	1/1	0.99	0.24	24,24,24,24	0
54	MG	2A	3269	1/1	0.99	0.20	34,34,34,34	0
54	MG	1B	222	1/1	0.99	0.14	30,30,30,30	0
54	MG	1A	4042	1/1	0.99	0.31	31,31,31,31	0
59	ZN	19	102	1/1	0.99	0.24	41,41,41,41	0
54	MG	2A	3322	1/1	0.99	0.23	49,49,49,49	0
54	MG	2a	1734	1/1	0.99	0.24	46,46,46,46	0
54	MG	1A	3465	1/1	0.99	0.17	22,22,22,22	0
54	MG	1A	3321	1/1	0.99	0.13	12,12,12,12	0
54	MG	2A	3340	1/1	0.99	0.17	33,33,33,33	0

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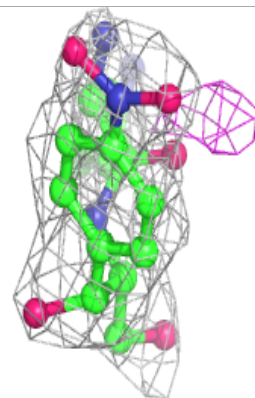
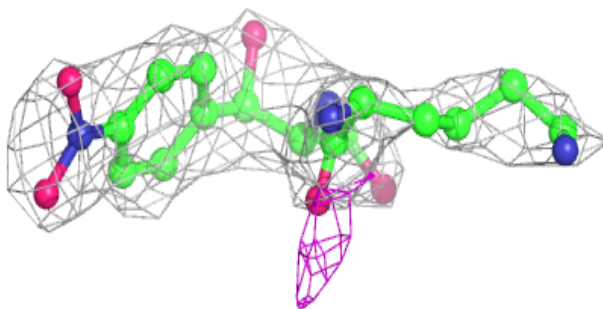
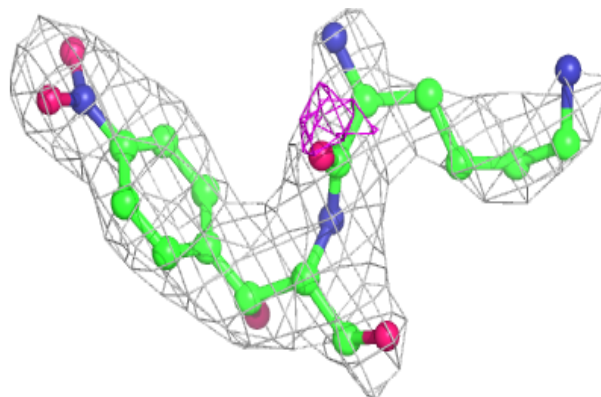
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3118	1/1	0.99	0.16	46,46,46,46	0
54	MG	1a	1713	1/1	0.99	0.15	52,52,52,52	0
54	MG	1A	4016	1/1	0.99	0.13	14,14,14,14	0
54	MG	1A	3373	1/1	0.99	0.20	20,20,20,20	0
54	MG	1A	3382	1/1	0.99	0.21	12,12,12,12	0
54	MG	1A	3858	1/1	0.99	0.20	19,19,19,19	0
54	MG	1A	3042	1/1	0.99	0.17	12,12,12,12	0
54	MG	1a	1813	1/1	0.99	0.09	53,53,53,53	0
54	MG	1A	3126	1/1	0.99	0.18	25,25,25,25	0
54	MG	1A	3205	1/1	0.99	0.42	25,25,25,25	0
59	ZN	1Y	501	1/1	0.99	0.19	46,46,46,46	0
54	MG	1A	3383	1/1	0.99	0.16	28,28,28,28	0
54	MG	1A	3739	1/1	0.99	0.09	30,30,30,30	0
54	MG	1A	3024	1/1	0.99	0.29	30,30,30,30	0
59	ZN	16	501	1/1	0.99	0.24	39,39,39,39	0
54	MG	1a	1833	1/1	0.99	0.12	29,29,29,29	0
55	K	2A	3236	1/1	0.99	0.11	28,28,28,28	0
54	MG	1A	3677	1/1	0.99	0.08	21,21,21,21	0
54	MG	1A	3045	1/1	0.99	0.21	11,11,11,11	0
55	K	1A	3278	1/1	0.99	0.10	22,22,22,22	0
54	MG	1A	3303	1/1	0.99	0.20	18,18,18,18	0
54	MG	1A	3576	1/1	0.99	0.11	36,36,36,36	0
54	MG	1A	3746	1/1	0.99	0.39	27,27,27,27	0
54	MG	1A	4021	1/1	0.99	0.14	36,36,36,36	0
54	MG	1A	3204	1/1	0.99	0.40	30,30,30,30	0
54	MG	1A	3003	1/1	0.99	0.13	19,19,19,19	0
54	MG	1A	3537	1/1	0.99	0.12	41,41,41,41	0
54	MG	2A	3176	1/1	0.99	0.23	51,51,51,51	0
54	MG	1a	1723	1/1	0.99	0.14	49,49,49,49	0
54	MG	1A	3103	1/1	0.99	0.33	27,27,27,27	0
54	MG	2A	3672	1/1	0.99	0.19	54,54,54,54	0
54	MG	1A	4039	1/1	0.99	0.21	31,31,31,31	0
54	MG	1A	3107	1/1	0.99	0.18	27,27,27,27	0
54	MG	2A	3679	1/1	0.99	0.14	58,58,58,58	0
54	MG	1A	3367	1/1	0.99	0.16	21,21,21,21	0
54	MG	1A	3134	1/1	0.99	0.42	37,37,37,37	0
54	MG	1A	3105	1/1	0.99	0.35	36,36,36,36	0
54	MG	1A	3613	1/1	0.99	0.19	59,59,59,59	0
54	MG	2A	3266	1/1	0.99	0.09	19,19,19,19	0
54	MG	1A	3911	1/1	1.00	0.16	20,20,20,20	0
54	MG	1A	3668	1/1	1.00	0.24	13,13,13,13	0

The following is a graphical depiction of the model fit to experimental electron density of all

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

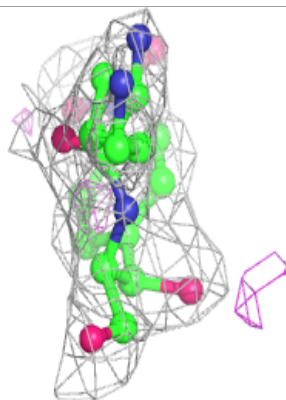
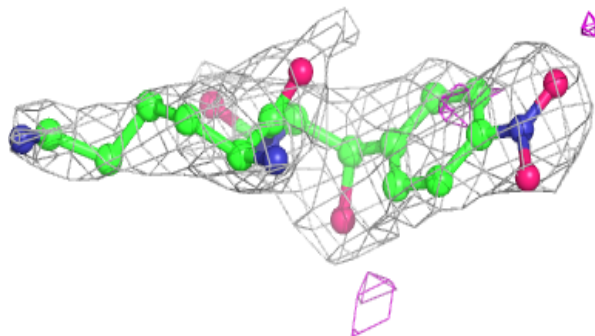
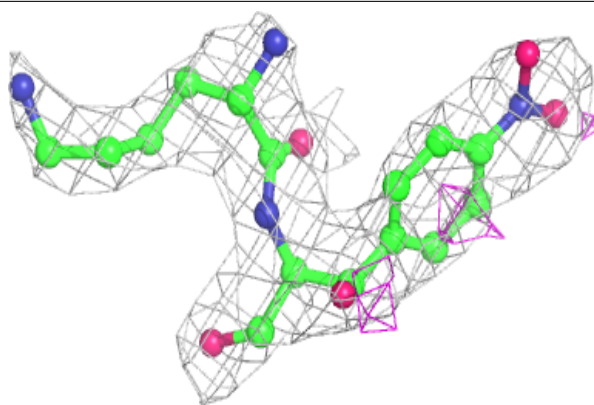
Electron density around EZM 2A 3691:

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



Electron density around EZM 1A 4035:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.