



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:32 AM UTC

PDB ID : 4WPO / pdb_00004wpo
Title : Crystal structure of the Thermus thermophilus 70S ribosome in complex with elongation factor G in the pre-translocational state
Authors : Lin, J.; Gagnon, M.G.; Steitz, T.A.
Deposited on : 2014-10-20
Resolution : 2.80 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

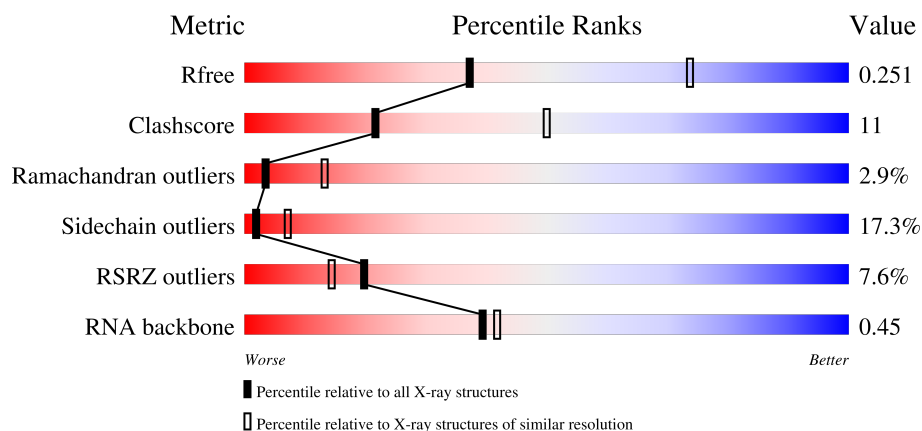
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



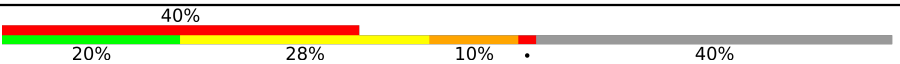
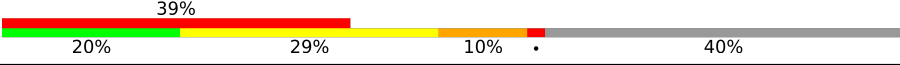
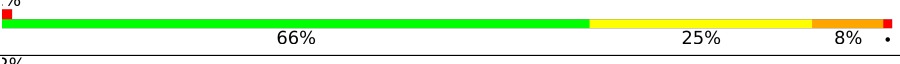
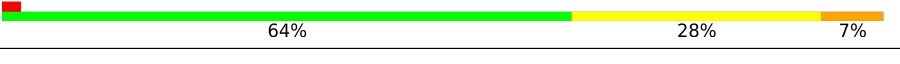
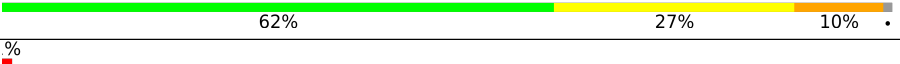
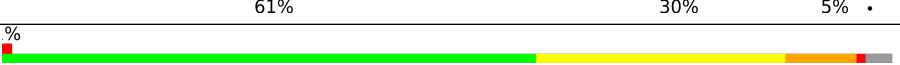
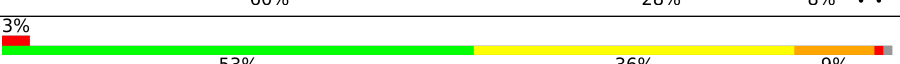
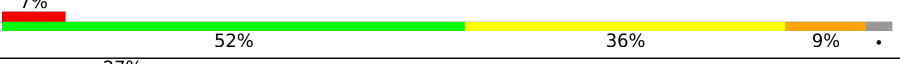
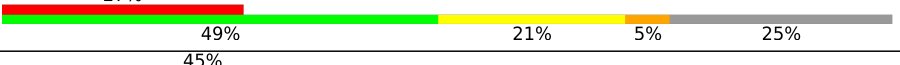
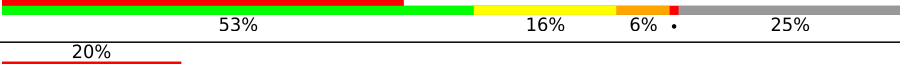
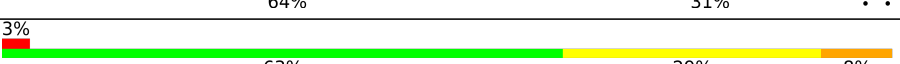
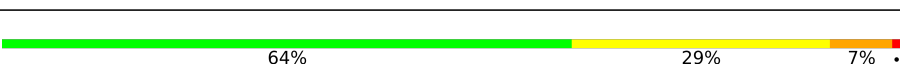
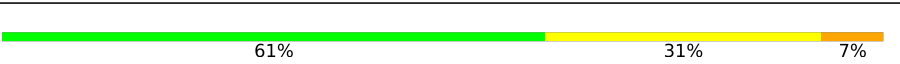
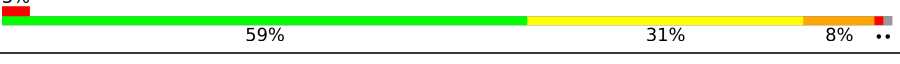
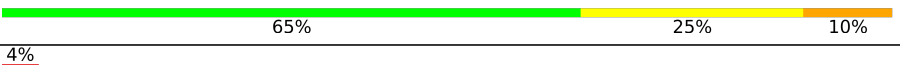
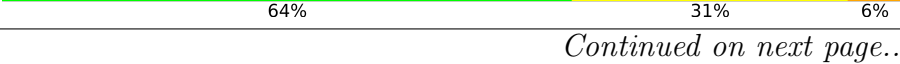
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

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

Mol	Chain	Length	Quality of chain
1	AA	2915	% 62% 30% 7% .
1	CA	2915	3% 57% 33% 8% .
2	AB	121	74% 25% .
2	CB	121	% 62% 31% 6% .

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Mol	Chain	Length	Quality of chain
3	AC	228	
3	CC	228	
4	AD	276	
4	CD	276	
5	AE	206	
5	CE	206	
6	AF	210	
6	CF	210	
7	AG	182	
7	CG	182	
8	AH	180	
8	CH	180	
9	AK	173	
9	CK	173	
10	AL	147	
10	CL	147	
11	AN	140	
11	CN	140	
12	AO	122	
12	CO	122	
13	AP	150	
13	CP	150	
14	AQ	141	
14	CQ	141	
15	AR	118	

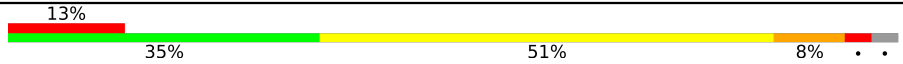
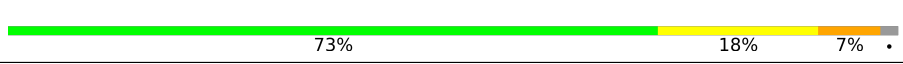
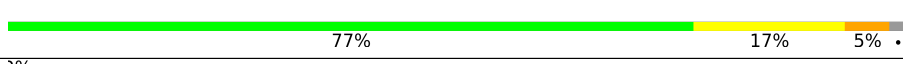
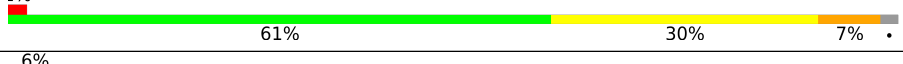
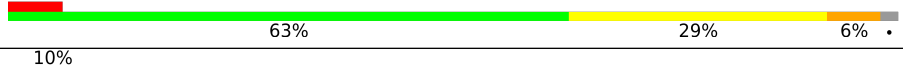
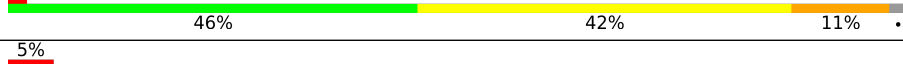
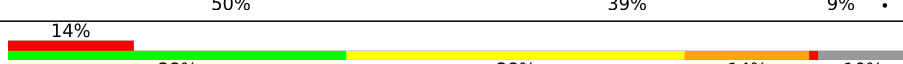
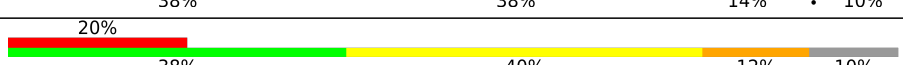
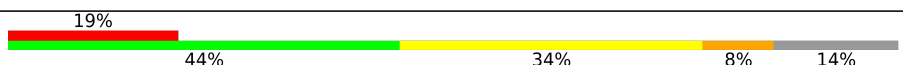
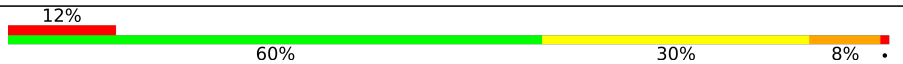
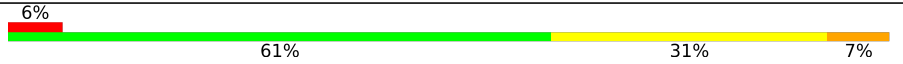
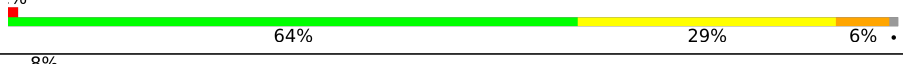
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Mol	Chain	Length	Quality of chain
15	CR	118	
16	AS	112	
16	CS	112	
17	AT	146	
17	CT	146	
18	AU	118	
18	CU	118	
19	AV	101	
19	CV	101	
20	AW	113	
20	CW	113	
21	AX	96	
21	CX	96	
22	AY	110	
22	CY	110	
23	AZ	206	
23	CZ	206	
24	A0	85	
24	C0	85	
25	A1	98	
25	C1	98	
26	A2	72	
26	C2	72	
27	A3	60	
27	C3	60	

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Mol	Chain	Length	Quality of chain
28	A4	71	
28	C4	71	
29	A5	60	
29	C5	60	
30	A6	54	
30	C6	54	
31	A7	49	
31	C7	49	
32	A8	65	
32	C8	65	
33	A9	37	
33	C9	37	
34	BA	1521	
34	DA	1521	
35	BB	256	
35	DB	256	
36	BC	239	
36	DC	239	
37	BD	209	
37	DD	209	
38	BE	162	
38	DE	162	
39	BF	101	
39	DF	101	
40	BG	156	

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Mol	Chain	Length	Quality of chain
40	DG	156	
41	BH	138	
41	DH	138	
42	BI	128	
42	DI	128	
43	BJ	105	
43	DJ	105	
44	BK	129	
44	DK	129	
45	BL	132	
45	DL	132	
46	BM	126	
46	DM	126	
47	BN	61	
47	DN	61	
48	BO	89	
48	DO	89	
49	BP	88	
49	DP	88	
50	BQ	105	
50	DQ	105	
51	BR	88	
51	DR	88	
52	BS	93	
52	DS	93	

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Mol	Chain	Length	Quality of chain
53	BT	106	
53	DT	106	
54	BU	27	
54	DU	27	
55	BV	24	
55	DV	24	
56	BW	76	
56	DW	76	
57	BX	77	
57	DX	77	
58	BY	76	
58	DY	76	
59	BZ	758	
59	DZ	758	

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
60	MG	AA	3027	-	-	-	X
60	MG	AA	3108	-	-	-	X
60	MG	AA	3183	-	-	-	X
60	MG	AA	3203	-	-	-	X
60	MG	AA	3770	-	-	-	X
60	MG	AA	3805	-	-	-	X
60	MG	BA	1800	-	-	-	X
60	MG	CA	3031	-	-	-	X
60	MG	CA	3042	-	-	-	X
60	MG	CA	3122	-	-	-	X
60	MG	CA	3220	-	-	-	X
60	MG	DA	1651	-	-	-	X

2 Entry composition

There are 65 unique types of molecules in this entry. The entry contains 313372 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	AA	2872	Total	C	N	O	P	0	0	0
			61861	27532	11574	19884	2871			
1	CA	2868	Total	C	N	O	P	0	0	0
			61771	27492	11554	19858	2867			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			
2	CB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	137	Total	C	N	O	S	0	0	0
			1063	669	201	192	1			
3	CC	137	Total	C	N	O	S	0	0	0
			1063	669	201	192	1			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AK	130	Total	C	N	O		0	0	0
			641	381	130	130				
9	CK	130	Total	C	N	O		0	0	0
			641	381	130	130				

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AZ	171	Total	C	N	O	S	0	0	0
			1349	862	243	242	2			
23	CZ	174	Total	C	N	O	S	0	0	0
			1360	870	243	245	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	A0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
24	C0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	A1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			
25	C1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	A2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	C2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	A3	59	Total	C	N	O		0	0	0
			469	298	90	81				
27	C3	59	Total	C	N	O		0	0	0
			464	296	90	78				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	A4	69	Total	C	N	O	S	0	0	0
			558	352	102	99	5			
28	C4	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	A5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			
29	C5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
30	C6	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	A7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
31	C7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	A8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
32	C8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	A9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
33	C9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BA	1497	Total	C	N	O	P	0	0	0
			32185	14324	5968	10396	1497			
34	DA	1503	Total	C	N	O	P	0	0	0
			32312	14381	5990	10438	1503			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	BR	68	Total	C	N	O	0	0	0
			555	355	108	92			
51	DR	68	Total	C	N	O	0	0	0
			555	355	108	92			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BU	23	Total	C	N	O		0	0	0
			199	122	48	29				
54	DU	23	Total	C	N	O		0	0	0
			199	122	48	29				

- Molecule 55 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BV	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
55	DV	12	Total	C	N	O	P	0	0	0
			252	115	46	80	11			

- Molecule 56 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BW	74	Total	C	N	O	P	0	0	0
			1599	722	287	515	73			
56	DW	72	Total	C	N	O	P	0	0	0
			1552	697	280	502	72			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BX	76	Total	C	N	O	P	0	0	0
			1635	731	296	530	76			
57	DX	76	Total	C	N	O	P	0	0	0
			1635	731	296	530	76			

- Molecule 58 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BY	74	Total	C	N	O	P	0	0	0
			1581	707	285	515	73			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
58	DY	73	Total	C	N	O	P	S	0	0	0
			1561	698	283	507	72	1			

- Molecule 59 is a protein called 50S ribosomal protein L9,Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	BZ	728	Total	C	N	O	S	0	0	0
			5663	3599	973	1072	19			
59	DZ	730	Total	C	N	O	S	0	0	0
			5682	3611	978	1074	19			

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AA	817	Total	Mg	0	0
			817	817		
60	AB	23	Total	Mg	0	0
			23	23		
60	AD	11	Total	Mg	0	0
			11	11		
60	AE	5	Total	Mg	0	0
			5	5		
60	AF	8	Total	Mg	0	0
			8	8		
60	AG	3	Total	Mg	0	0
			3	3		
60	AH	1	Total	Mg	0	0
			1	1		
60	AN	3	Total	Mg	0	0
			3	3		
60	AO	1	Total	Mg	0	0
			1	1		
60	AP	3	Total	Mg	0	0
			3	3		
60	AQ	3	Total	Mg	0	0
			3	3		
60	AR	2	Total	Mg	0	0
			2	2		
60	AU	4	Total	Mg	0	0
			4	4		
60	AV	4	Total	Mg	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AW	4	Total 4	Mg 4	0	0
60	AX	1	Total 1	Mg 1	0	0
60	AY	1	Total 1	Mg 1	0	0
60	AZ	1	Total 1	Mg 1	0	0
60	A0	5	Total 5	Mg 5	0	0
60	A1	2	Total 2	Mg 2	0	0
60	A2	1	Total 1	Mg 1	0	0
60	A4	1	Total 1	Mg 1	0	0
60	A5	3	Total 3	Mg 3	0	0
60	A6	2	Total 2	Mg 2	0	0
60	A7	6	Total 6	Mg 6	0	0
60	A8	2	Total 2	Mg 2	0	0
60	A9	1	Total 1	Mg 1	0	0
60	BA	213	Total 213	Mg 213	0	0
60	BB	1	Total 1	Mg 1	0	0
60	BD	1	Total 1	Mg 1	0	0
60	BE	1	Total 1	Mg 1	0	0
60	BF	1	Total 1	Mg 1	0	0
60	BK	1	Total 1	Mg 1	0	0
60	BL	2	Total 2	Mg 2	0	0
60	BM	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	BN	2	Total 2	Mg 2	0	0
60	BT	1	Total 1	Mg 1	0	0
60	BV	1	Total 1	Mg 1	0	0
60	BW	2	Total 2	Mg 2	0	0
60	BX	15	Total 15	Mg 15	0	0
60	BY	2	Total 2	Mg 2	0	0
60	BZ	1	Total 1	Mg 1	0	0
60	CA	664	Total 664	Mg 664	0	0
60	CB	13	Total 13	Mg 13	0	0
60	CD	4	Total 4	Mg 4	0	0
60	CE	6	Total 6	Mg 6	0	0
60	CF	6	Total 6	Mg 6	0	0
60	CG	1	Total 1	Mg 1	0	0
60	CN	1	Total 1	Mg 1	0	0
60	CO	2	Total 2	Mg 2	0	0
60	CP	1	Total 1	Mg 1	0	0
60	CQ	4	Total 4	Mg 4	0	0
60	CR	2	Total 2	Mg 2	0	0
60	CU	1	Total 1	Mg 1	0	0
60	CV	2	Total 2	Mg 2	0	0
60	CY	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	C0	2	Total 2	Mg 2	0	0
60	C3	1	Total 1	Mg 1	0	0
60	C5	1	Total 1	Mg 1	0	0
60	C7	1	Total 1	Mg 1	0	0
60	C8	1	Total 1	Mg 1	0	0
60	DA	168	Total 168	Mg 168	0	0
60	DD	1	Total 1	Mg 1	0	0
60	DE	2	Total 2	Mg 2	0	0
60	DF	1	Total 1	Mg 1	0	0
60	DJ	1	Total 1	Mg 1	0	0
60	DK	2	Total 2	Mg 2	0	0
60	DT	1	Total 1	Mg 1	0	0
60	DW	1	Total 1	Mg 1	0	0
60	DX	1	Total 1	Mg 1	0	0
60	DZ	1	Total 1	Mg 1	0	0

- Molecule 61 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AA	1	Total 1	K 1	0	0

- Molecule 62 is ZINC ION (CCD ID: ZN) (formula: Zn).

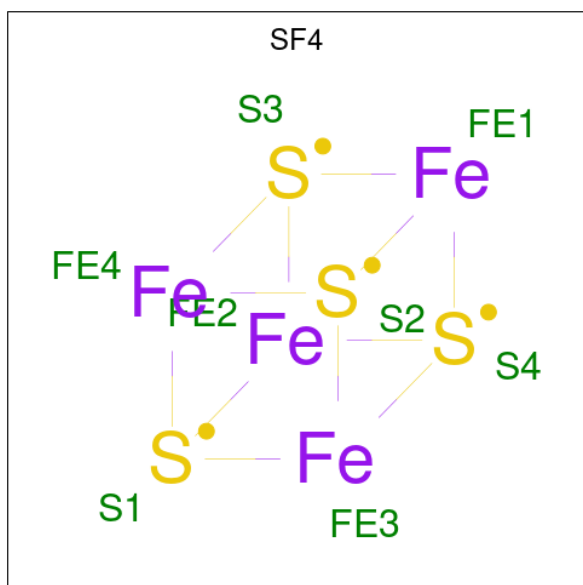
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	AY	1	Total 1	Zn 1	0	0

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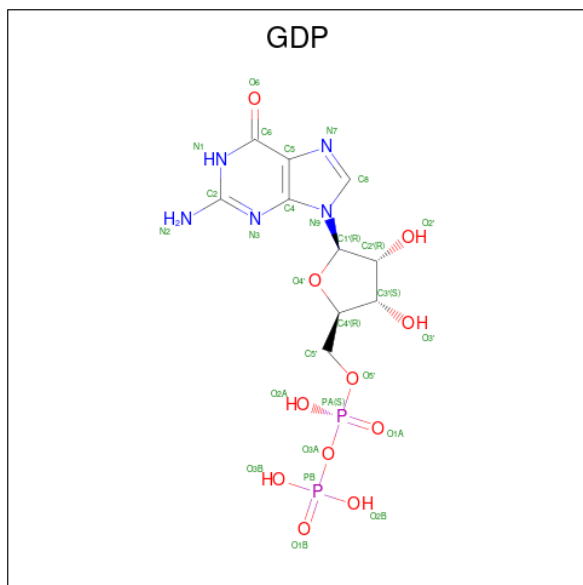
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	A4	1	Total	Zn	0	0
			1	1		
62	A5	1	Total	Zn	0	0
			1	1		
62	A6	1	Total	Zn	0	0
			1	1		
62	A9	1	Total	Zn	0	0
			1	1		
62	BN	1	Total	Zn	0	0
			1	1		
62	CY	1	Total	Zn	0	0
			1	1		
62	C4	1	Total	Zn	0	0
			1	1		
62	C5	1	Total	Zn	0	0
			1	1		
62	C6	1	Total	Zn	0	0
			1	1		
62	C9	1	Total	Zn	0	0
			1	1		
62	DN	1	Total	Zn	0	0
			1	1		

- Molecule 63 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	BD	1	Total	Fe	S	0	0
			8	4	4		
63	DD	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 64 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
64	BZ	1	Total 28	C 10	N 5	O 11	P 2	0	0
64	DZ	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 65 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
65	AA	1408	Total	O	0	0
			1408	1408		
65	AB	36	Total	O	0	0
			36	36		
65	AD	15	Total	O	0	0
			15	15		
65	AE	19	Total	O	0	0
			19	19		
65	AF	7	Total	O	0	0
			7	7		
65	AG	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
65	AH	1	Total 1	O 1	0	0
65	AN	2	Total 2	O 2	0	0
65	AO	1	Total 1	O 1	0	0
65	AP	15	Total 15	O 15	0	0
65	AQ	4	Total 4	O 4	0	0
65	AR	2	Total 2	O 2	0	0
65	AS	1	Total 1	O 1	0	0
65	AT	2	Total 2	O 2	0	0
65	AU	5	Total 5	O 5	0	0
65	AV	2	Total 2	O 2	0	0
65	AW	2	Total 2	O 2	0	0
65	AX	3	Total 3	O 3	0	0
65	AZ	1	Total 1	O 1	0	0
65	A0	6	Total 6	O 6	0	0
65	A1	1	Total 1	O 1	0	0
65	A3	1	Total 1	O 1	0	0
65	A5	3	Total 3	O 3	0	0
65	A6	2	Total 2	O 2	0	0
65	A7	4	Total 4	O 4	0	0
65	A8	10	Total 10	O 10	0	0
65	BA	212	Total 212	O 212	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
65	BD	2	Total	O	0	0
			2	2		
65	BE	2	Total	O	0	0
			2	2		
65	BL	1	Total	O	0	0
			1	1		
65	BM	1	Total	O	0	0
			1	1		
65	BV	2	Total	O	0	0
			2	2		
65	BW	3	Total	O	0	0
			3	3		
65	BX	8	Total	O	0	0
			8	8		
65	BY	1	Total	O	0	0
			1	1		
65	BZ	2	Total	O	0	0
			2	2		
65	CA	985	Total	O	0	0
			985	985		
65	CB	9	Total	O	0	0
			9	9		
65	CD	14	Total	O	0	0
			14	14		
65	CE	13	Total	O	0	0
			13	13		
65	CF	7	Total	O	0	0
			7	7		
65	CN	2	Total	O	0	0
			2	2		
65	CP	10	Total	O	0	0
			10	10		
65	CQ	1	Total	O	0	0
			1	1		
65	CR	1	Total	O	0	0
			1	1		
65	CT	3	Total	O	0	0
			3	3		
65	CU	2	Total	O	0	0
			2	2		
65	CV	1	Total	O	0	0
			1	1		

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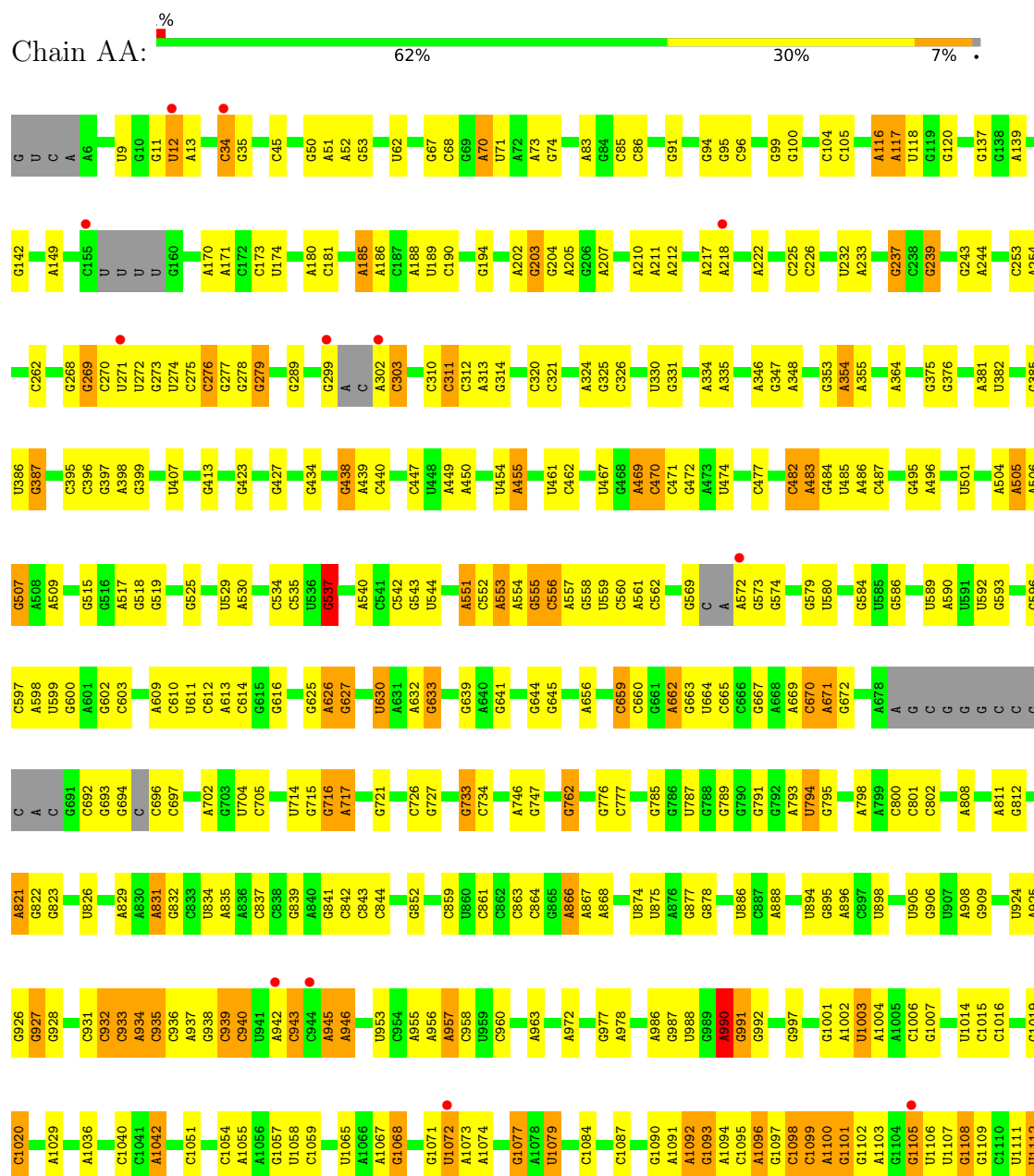
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
65	CY	1	Total	O	0	0
			1	1		
65	C0	6	Total	O	0	0
			6	6		
65	C1	2	Total	O	0	0
			2	2		
65	C3	2	Total	O	0	0
			2	2		
65	C6	1	Total	O	0	0
			1	1		
65	C7	1	Total	O	0	0
			1	1		
65	C8	3	Total	O	0	0
			3	3		
65	DA	155	Total	O	0	0
			155	155		
65	DE	4	Total	O	0	0
			4	4		
65	DJ	1	Total	O	0	0
			1	1		
65	DK	2	Total	O	0	0
			2	2		
65	DL	1	Total	O	0	0
			1	1		
65	DW	2	Total	O	0	0
			2	2		
65	DX	1	Total	O	0	0
			1	1		

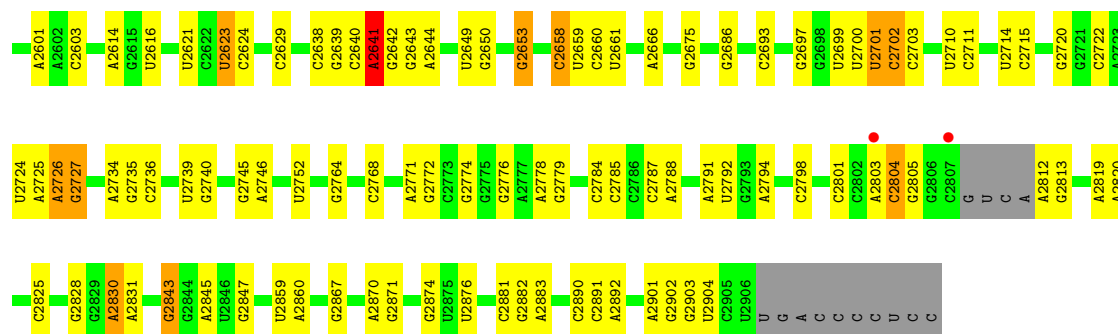
3 Residue-property plots

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

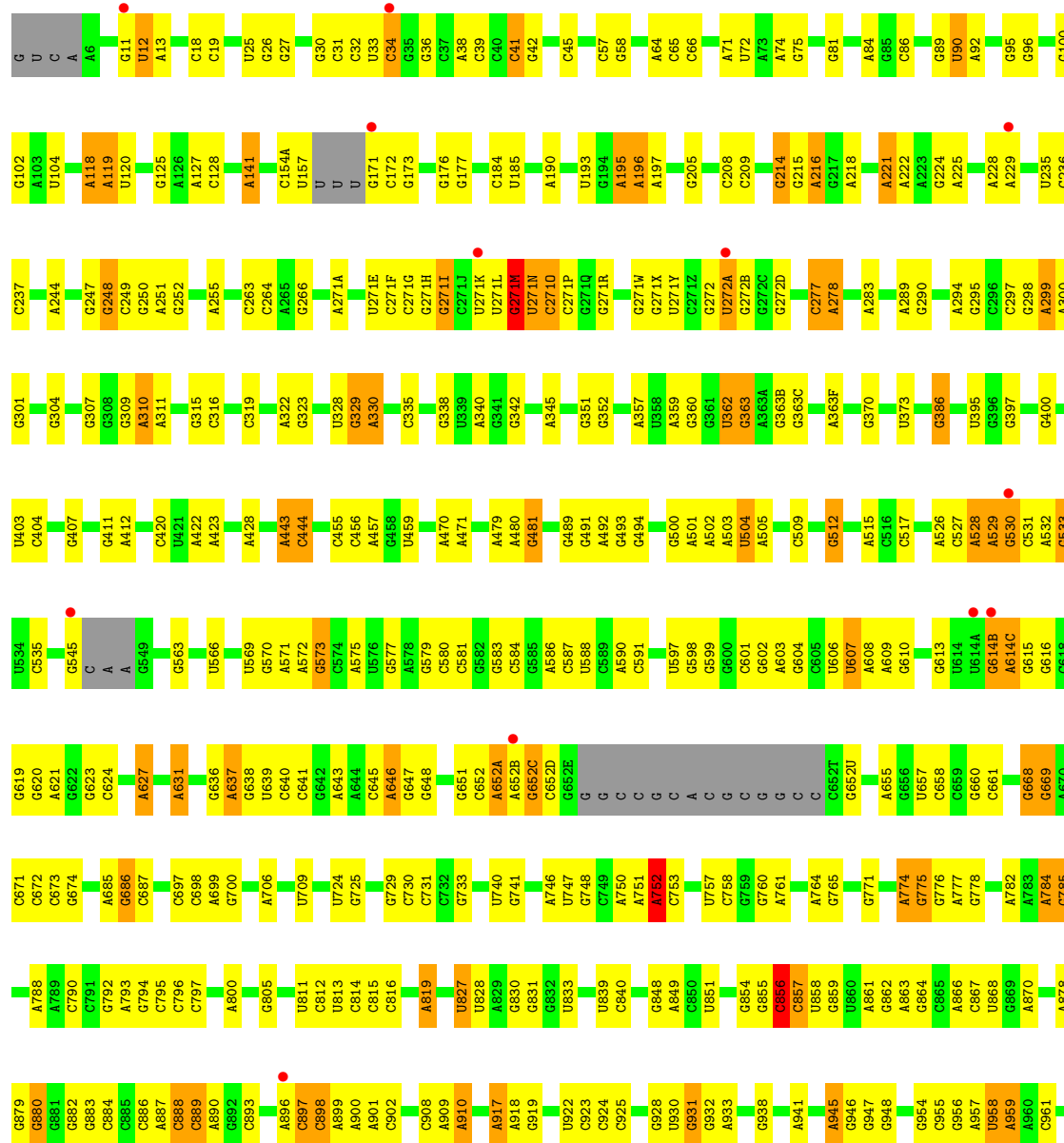
• Molecule 1: 23S Ribosomal RNA

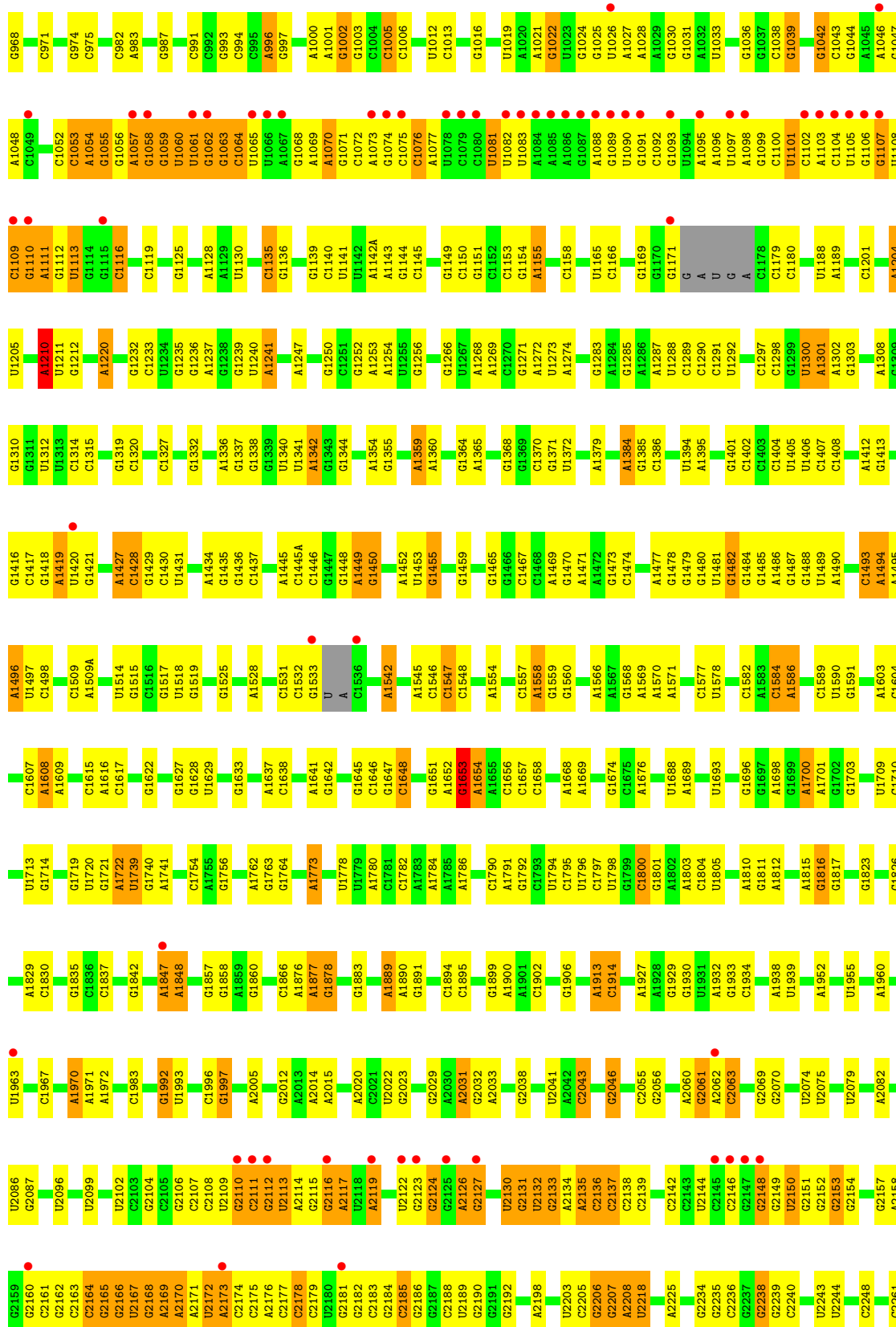


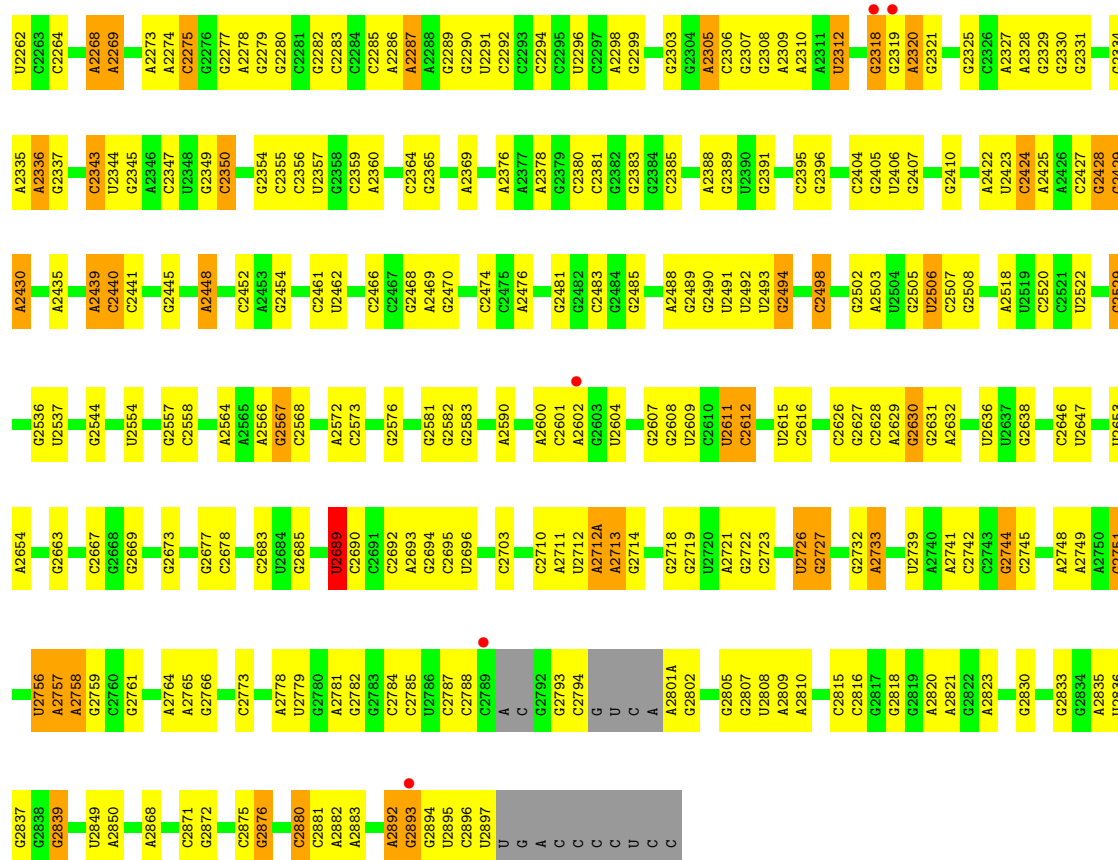
C2478	G3366	A2180	U2108	A2003	G1889	C1775	A1633	G1529	U1418	G1306	G1190	A1113
A2481	C2367	G2161	G2109	G2007	A1890	G1776	C1634	G1529	U1418	G1306	G1190	G1114
A2372	A2280	C2183	U2121	A2008	A1891	C1785	C1635	C1539	A1423	G1312	C1196	A1115
A2373	U2284	G2184	G2122	U2013	A1892	A1786	U1648	A1542	A1425	U1313	C1197	A1116
A2389	A2285	G2188	G2123	U2014	A1893	C1787	A1654	U1549	G1426	A1314	C1198	A1117
A2390	A2286	U2189	U2124	G2015	A1894	U1788	A1655	C1550	G1426	A1315	C1199	C1118
A2500	C2287	A2191	C2125	G2016	C1901	A1793	A1656	C1551	G1426	C1316	G1200	
A2501	G2288	G2128	G2128	G2019	G1905	G1794	C1657	C1552	A1430	G1317	A1201	C1121
A2504	A2290	C2129	C2130	G2020	A1906	G1795	A1654	C1553	G1431	A1318	C1210	C1122
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G2506	C2296	C2197	G2132	G2022	C1908	A1804	C1657	C1555	U1442	G1322	C1212	C1125
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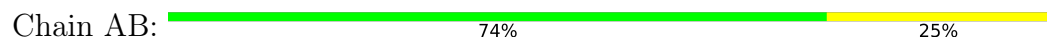
• Molecule 1: 23S Ribosomal RNA



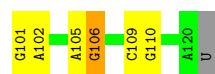
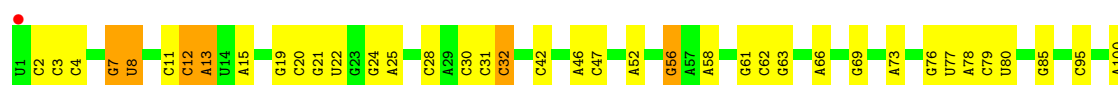




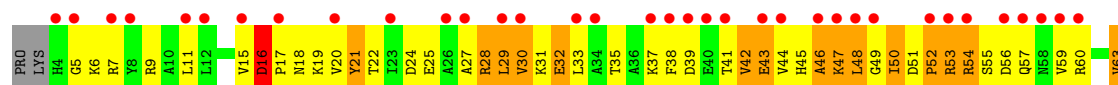
• Molecule 2: 5S Ribosomal RNA

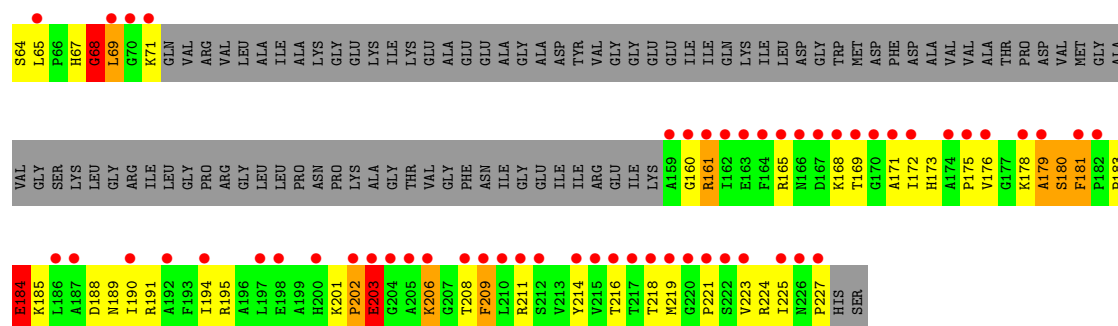


• Molecule 2: 5S Ribosomal RNA

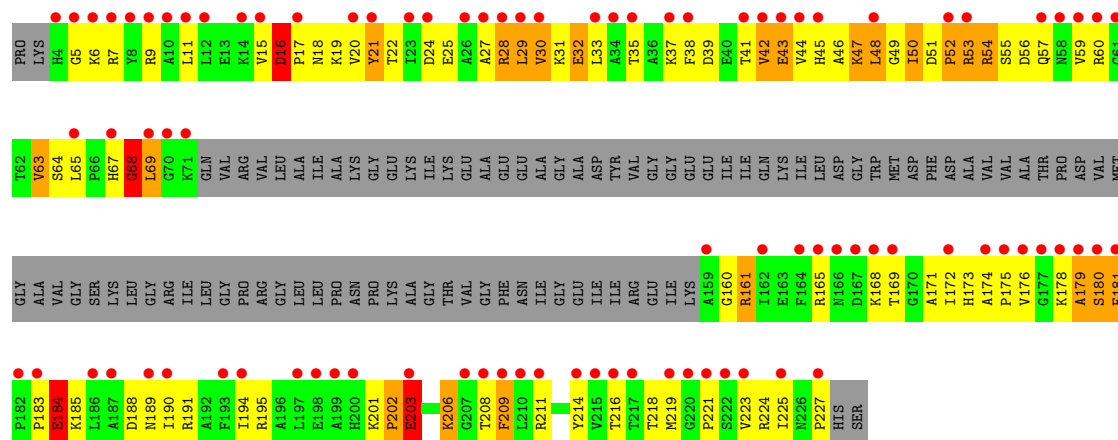


• Molecule 3: 50S ribosomal protein L1

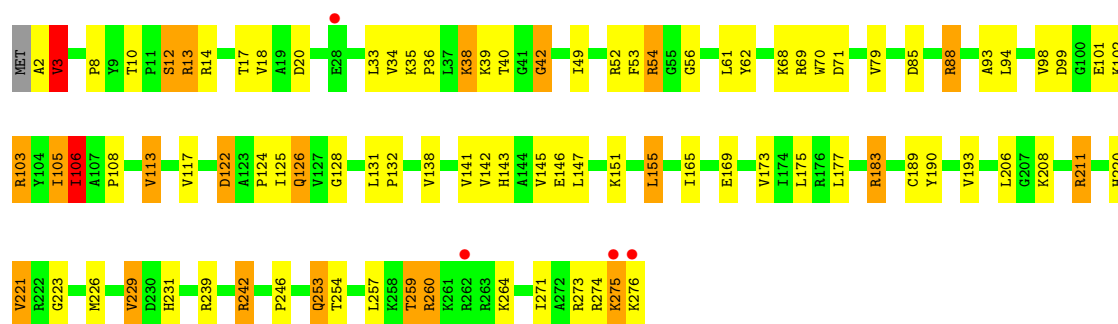




- Molecule 3: 50S ribosomal protein L1

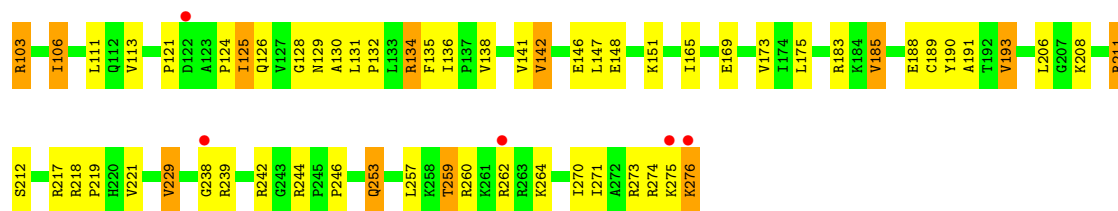


- Molecule 4: 50S ribosomal protein L2



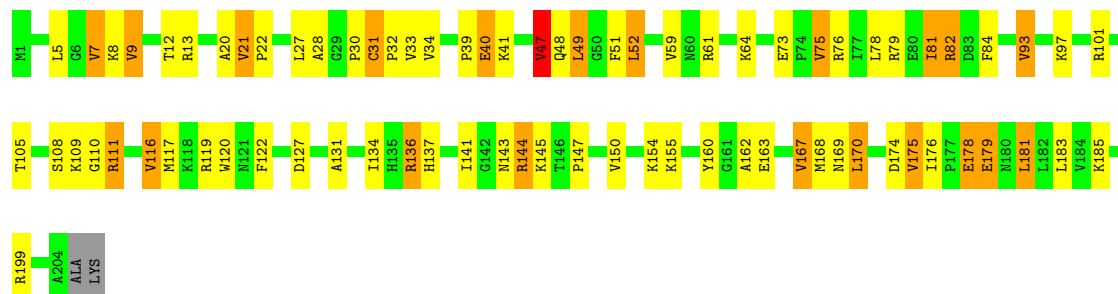
- Molecule 4: 50S ribosomal protein L2





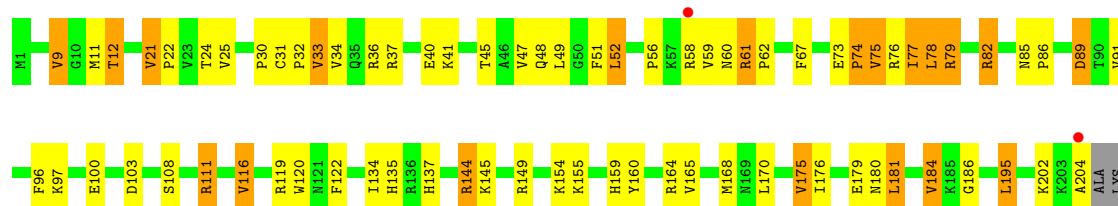
• Molecule 5: 50S ribosomal protein L3

Chain AE: 62% 27% 10%



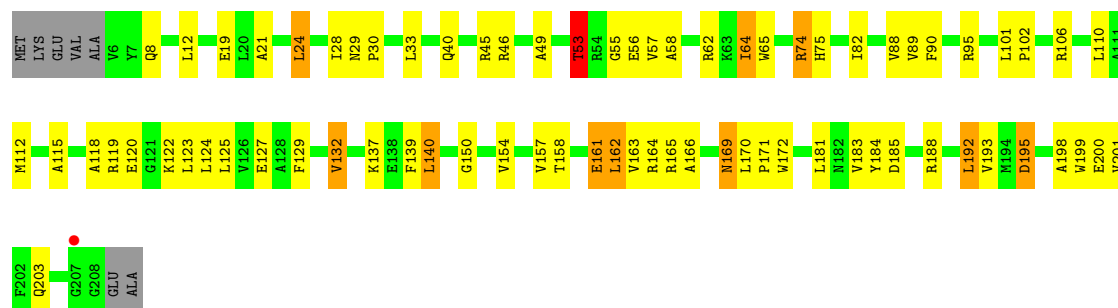
• Molecule 5: 50S ribosomal protein L3

Chain CE: 63% 27% 10%



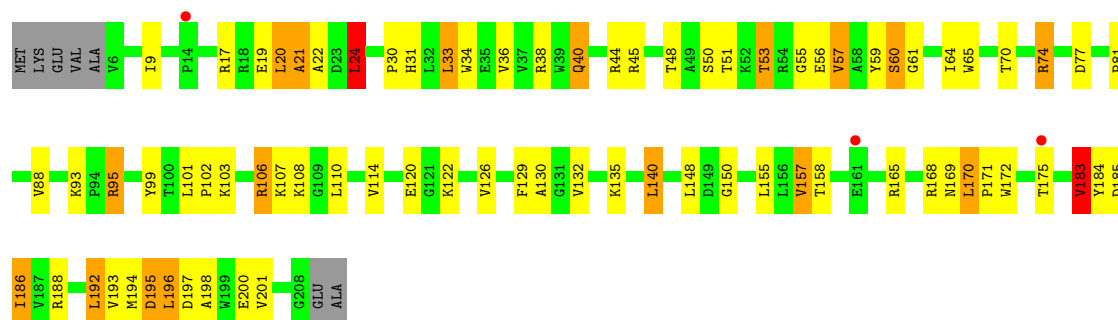
• Molecule 6: 50S ribosomal protein L4

Chain AF: 61% 30% 5%

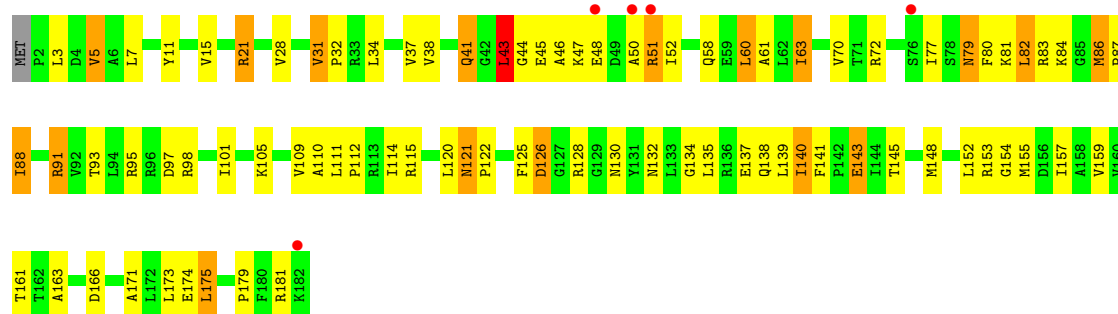


• Molecule 6: 50S ribosomal protein L4

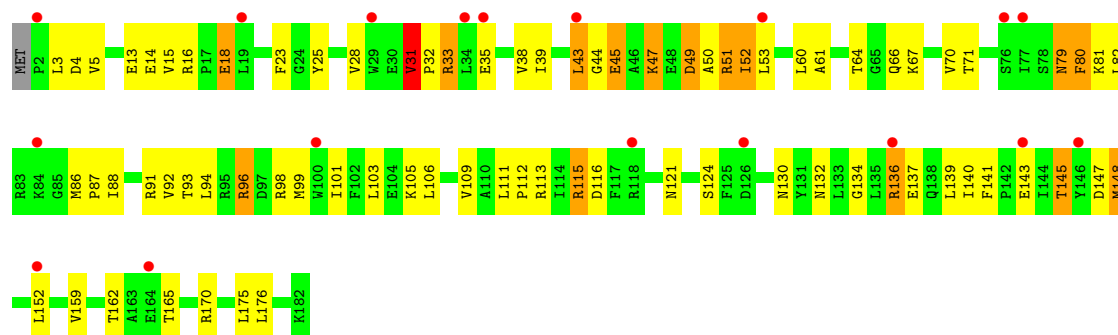
Chain CF: 60% 28% 8%



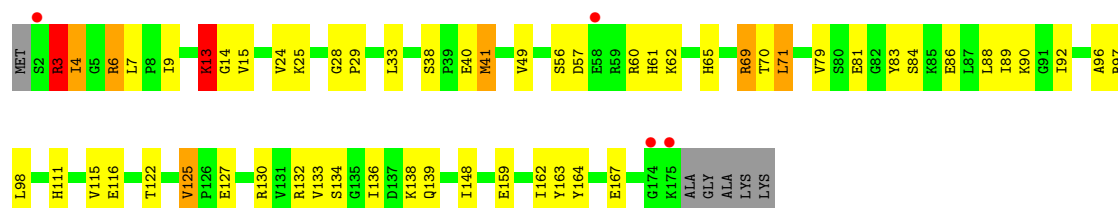
• Molecule 7: 50S ribosomal protein L5



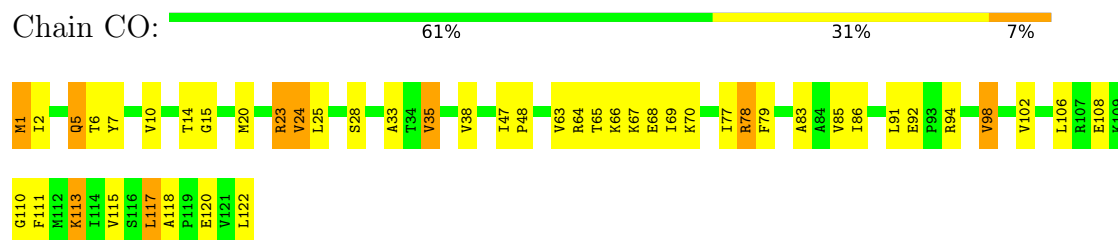
• Molecule 7: 50S ribosomal protein L5



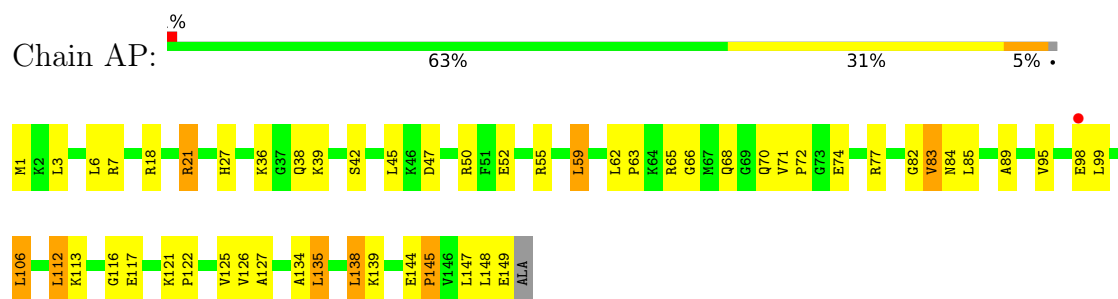
• Molecule 8: 50S ribosomal protein L6



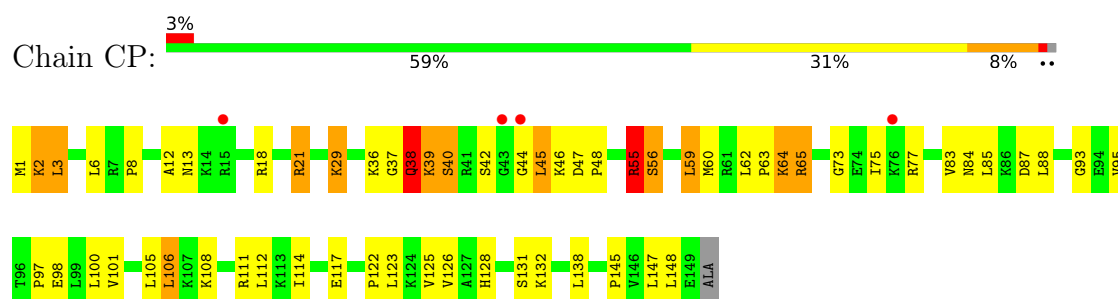
• Molecule 8: 50S ribosomal protein L6



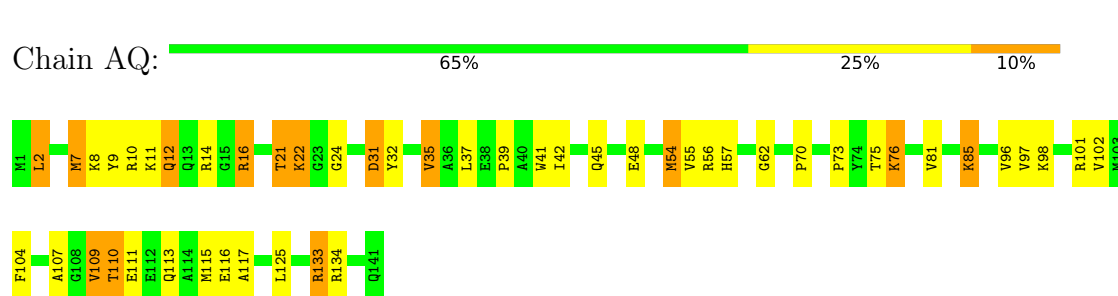
• Molecule 13: 50S ribosomal protein L15



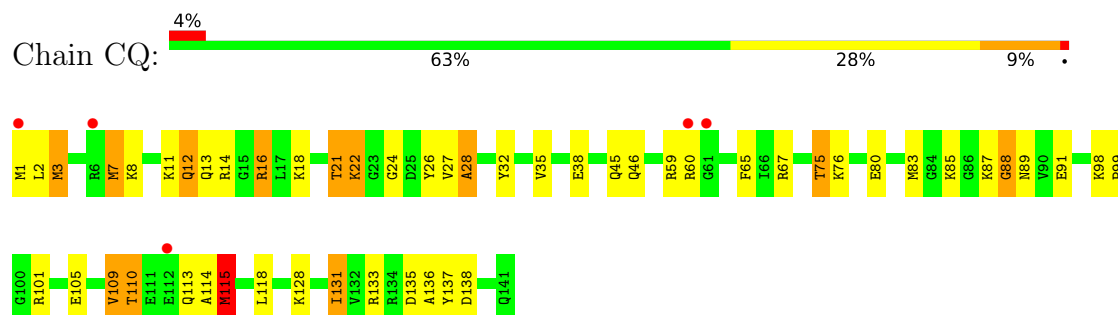
• Molecule 13: 50S ribosomal protein L15



• Molecule 14: 50S ribosomal protein L16

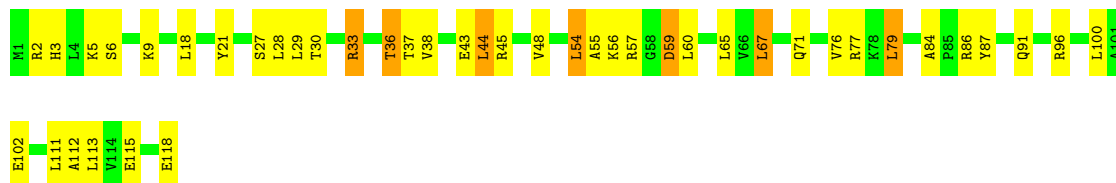


• Molecule 14: 50S ribosomal protein L16



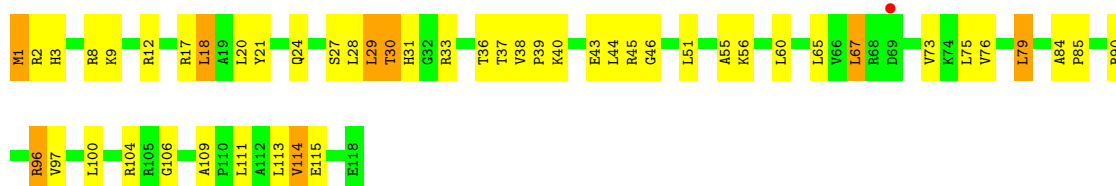
- Molecule 15: 50S ribosomal protein L17

Chain AR: 



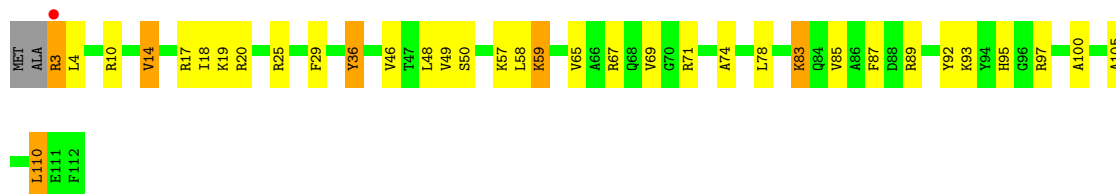
- Molecule 15: 50S ribosomal protein L17

Chain CR: 



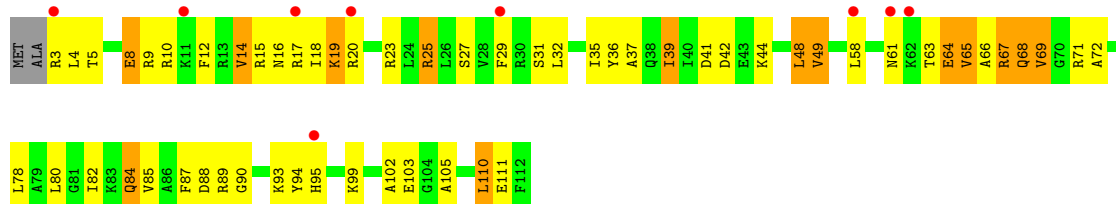
- Molecule 16: 50S ribosomal protein L18

Chain AS: 



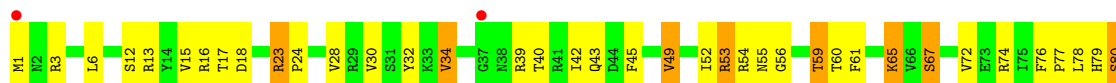
- Molecule 16: 50S ribosomal protein L18

Chain CS: 



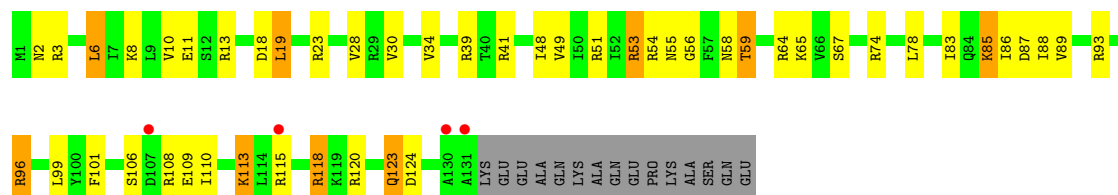
- Molecule 17: 50S ribosomal protein L19

Chain AT: 

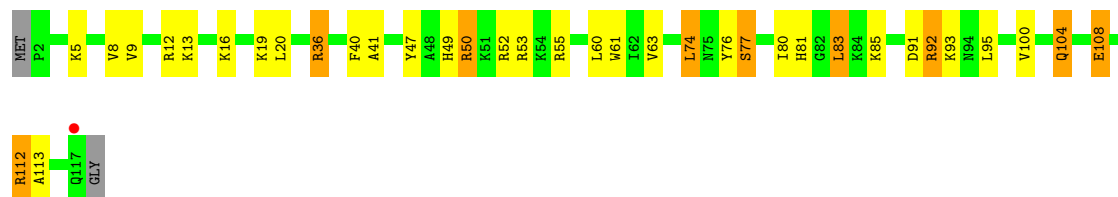




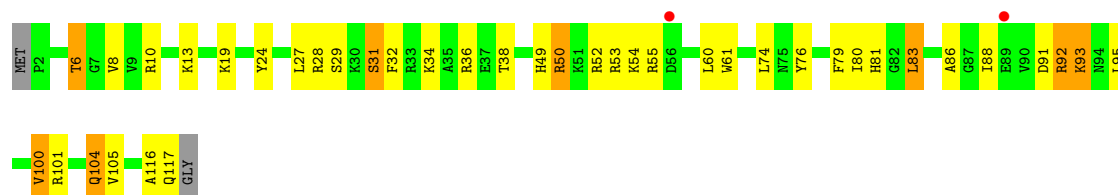
• Molecule 17: 50S ribosomal protein L19



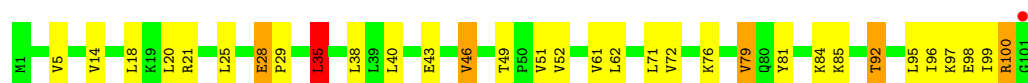
• Molecule 18: 50S ribosomal protein L20



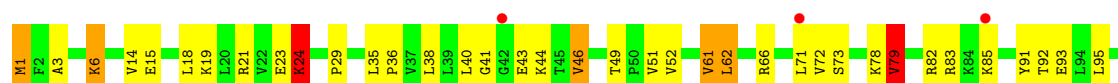
• Molecule 18: 50S ribosomal protein L20



• Molecule 19: 50S ribosomal protein L21

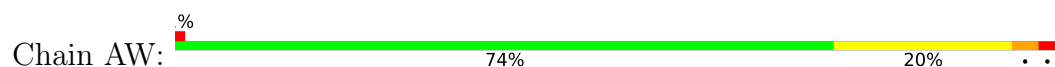


• Molecule 19: 50S ribosomal protein L21

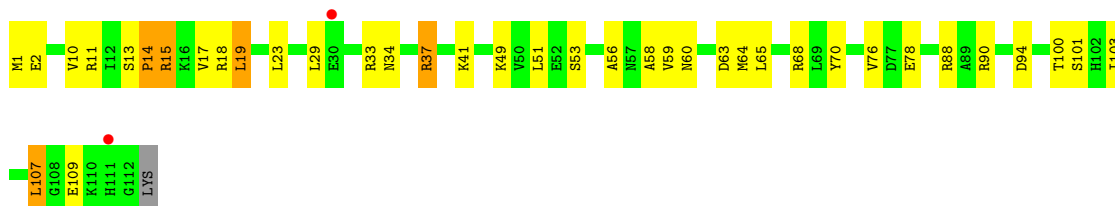




- Molecule 20: 50S ribosomal protein L22



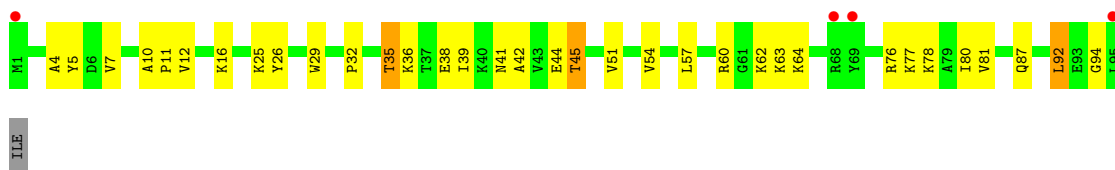
- Molecule 20: 50S ribosomal protein L22



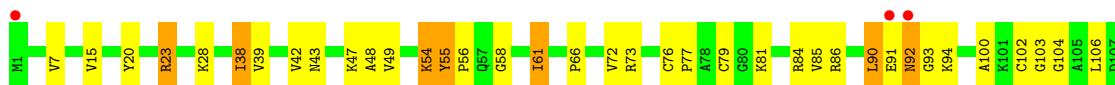
- Molecule 21: 50S ribosomal protein L23



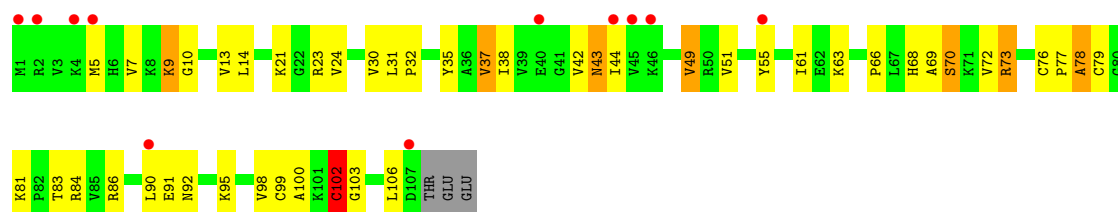
- Molecule 21: 50S ribosomal protein L23



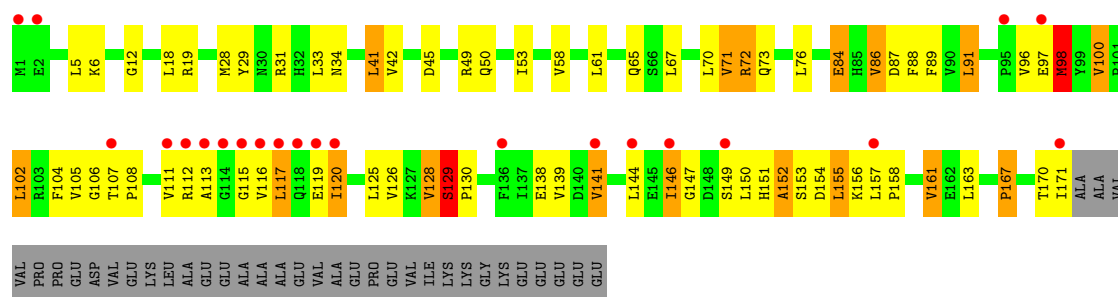
- Molecule 22: 50S ribosomal protein L24



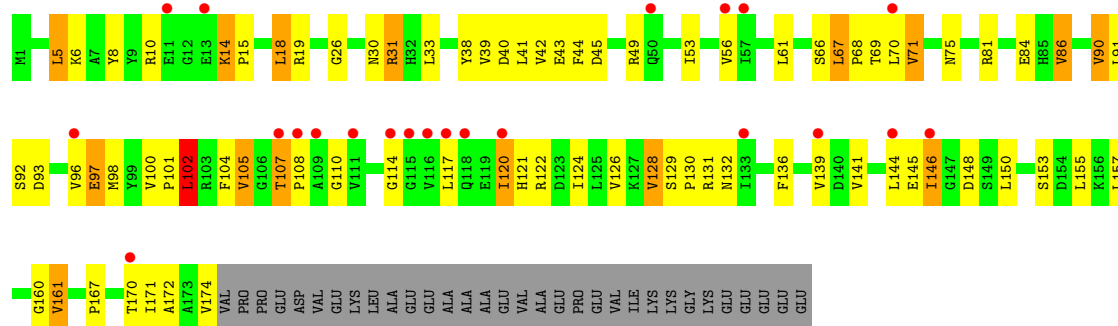
- Molecule 22: 50S ribosomal protein L24



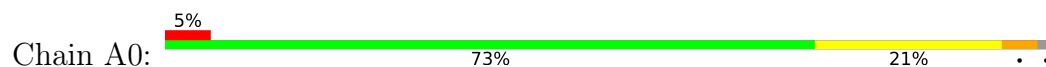
• Molecule 23: 50S ribosomal protein L25



• Molecule 23: 50S ribosomal protein L25

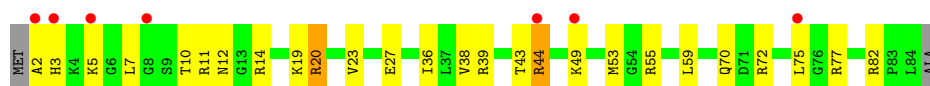


• Molecule 24: 50S ribosomal protein L27



• Molecule 24: 50S ribosomal protein L27

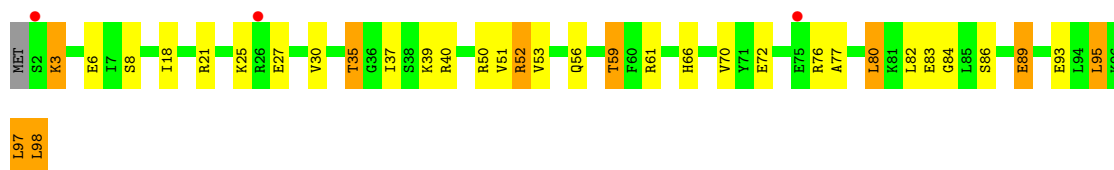




- Molecule 25: 50S ribosomal protein L28



- Molecule 25: 50S ribosomal protein L28



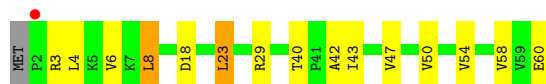
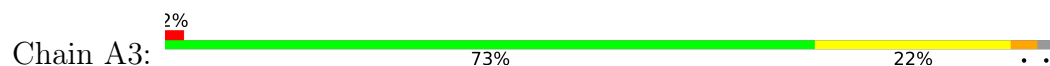
- Molecule 26: 50S ribosomal protein L29



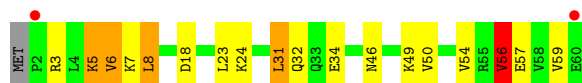
- Molecule 26: 50S ribosomal protein L29



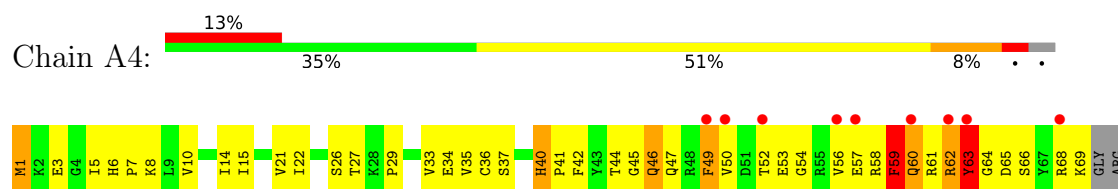
- Molecule 27: 50S ribosomal protein L30



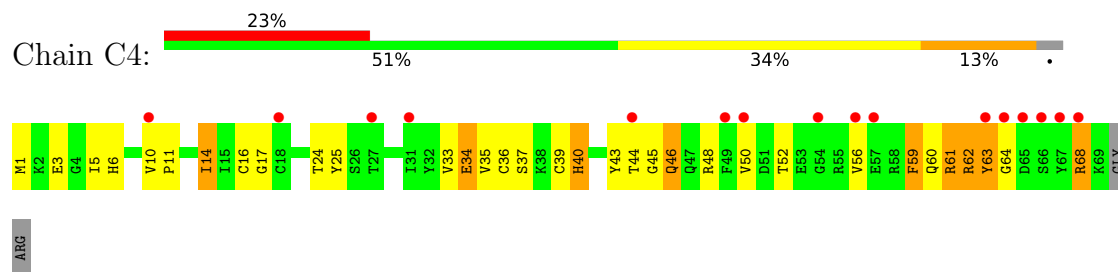
- Molecule 27: 50S ribosomal protein L30



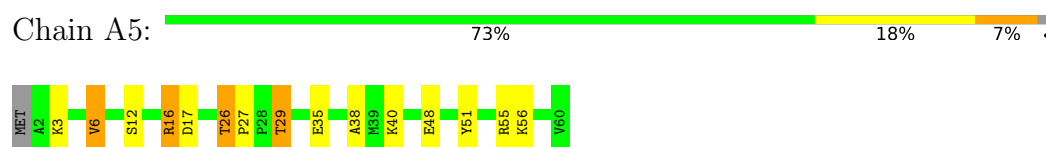
- Molecule 28: 50S ribosomal protein L31



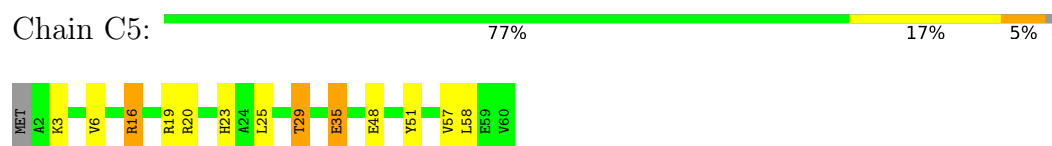
- Molecule 28: 50S ribosomal protein L31



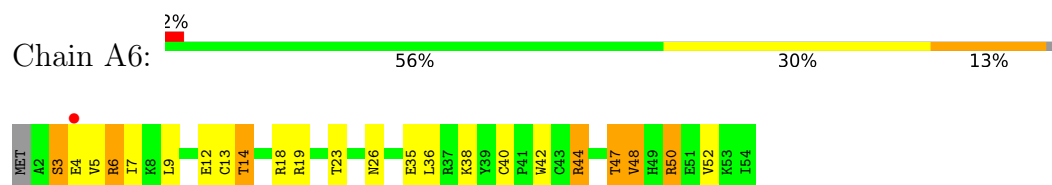
- Molecule 29: 50S ribosomal protein L32



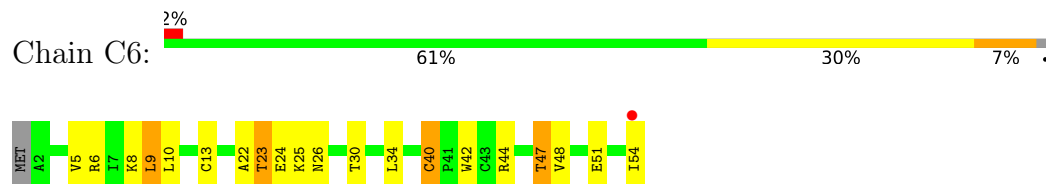
- Molecule 29: 50S ribosomal protein L32



- Molecule 30: 50S ribosomal protein L33



- Molecule 30: 50S ribosomal protein L33

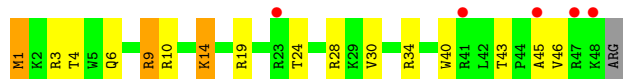


- Molecule 31: 50S ribosomal protein L34

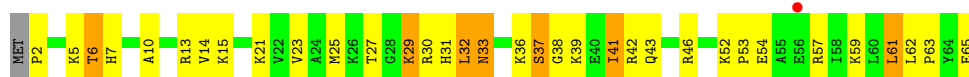




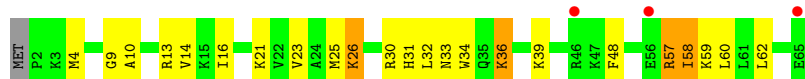
- Molecule 31: 50S ribosomal protein L34



- Molecule 32: 50S ribosomal protein L35



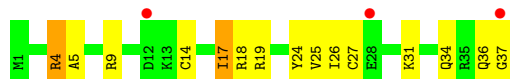
- Molecule 32: 50S ribosomal protein L35



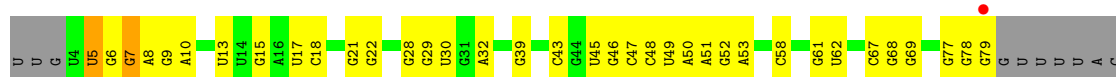
- Molecule 33: 50S ribosomal protein L36

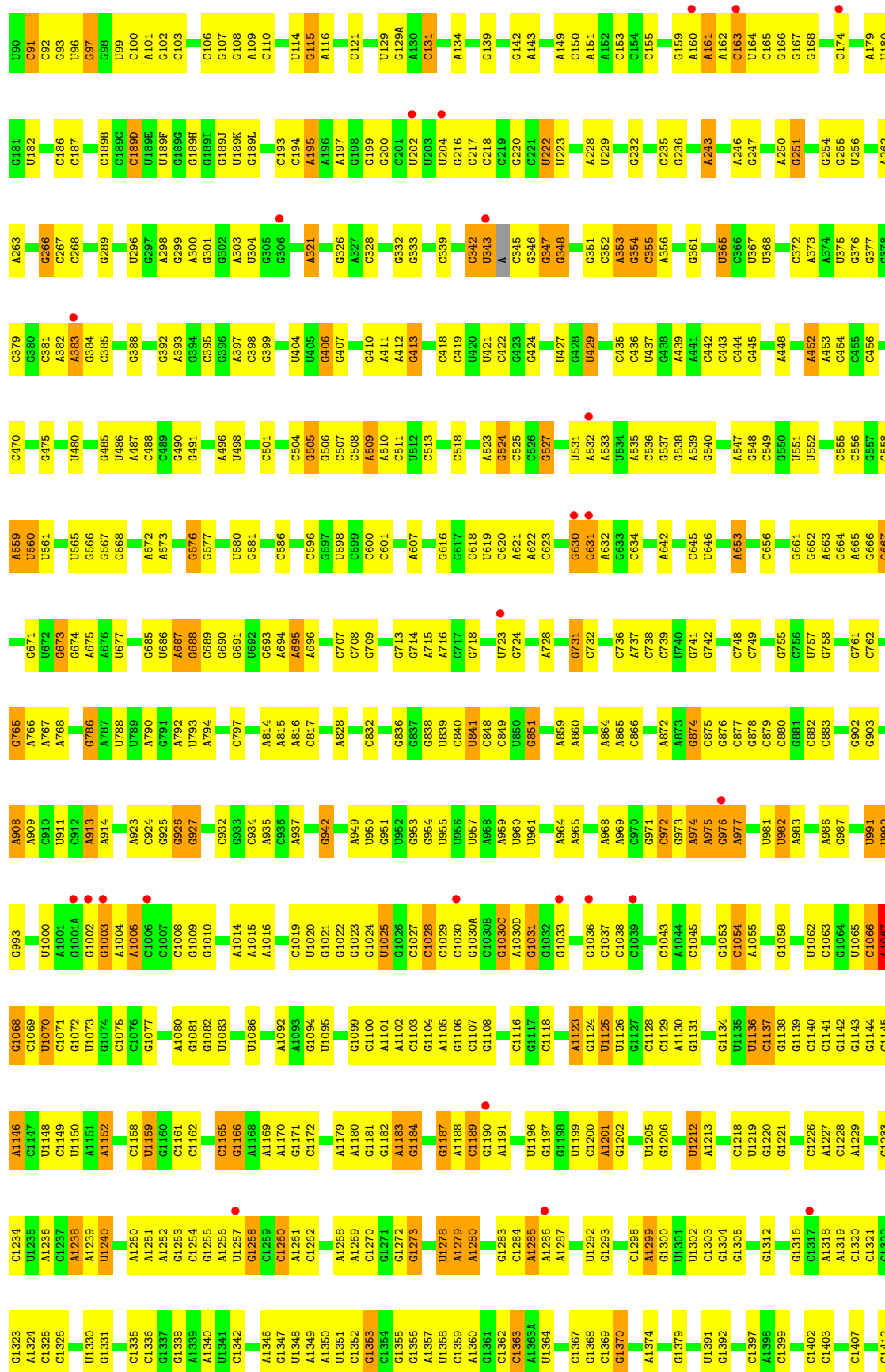


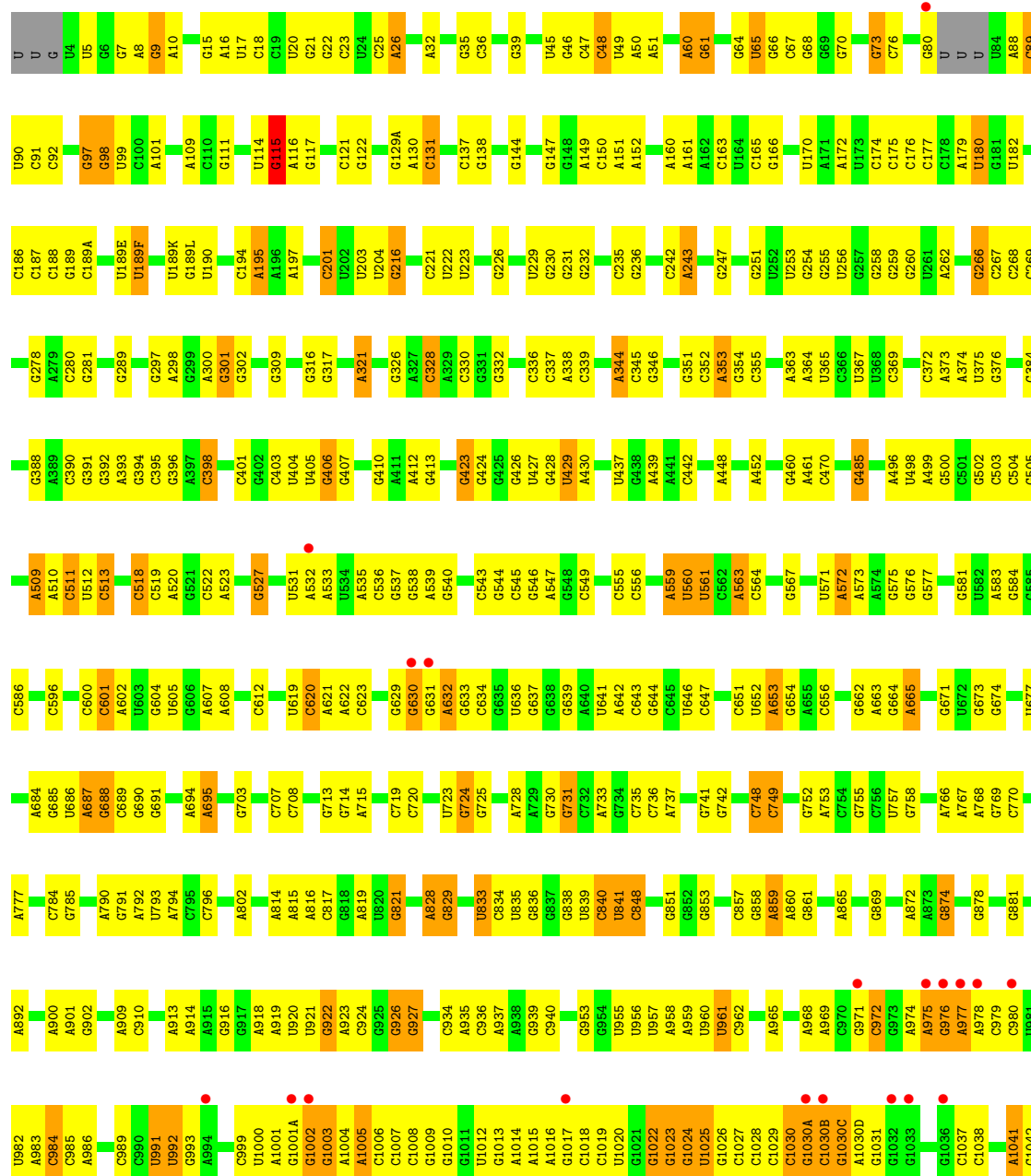
- Molecule 33: 50S ribosomal protein L36

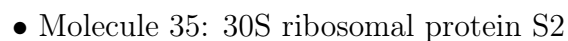
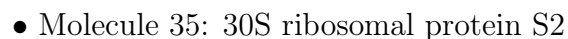


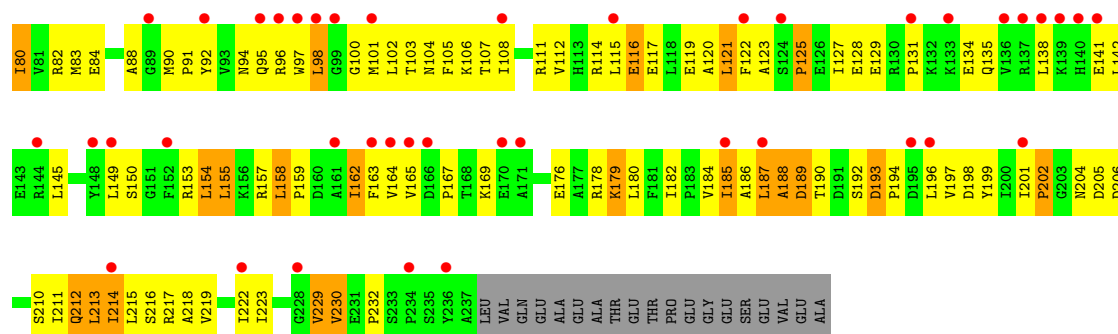
- Molecule 34: 16S Ribosomal RNA



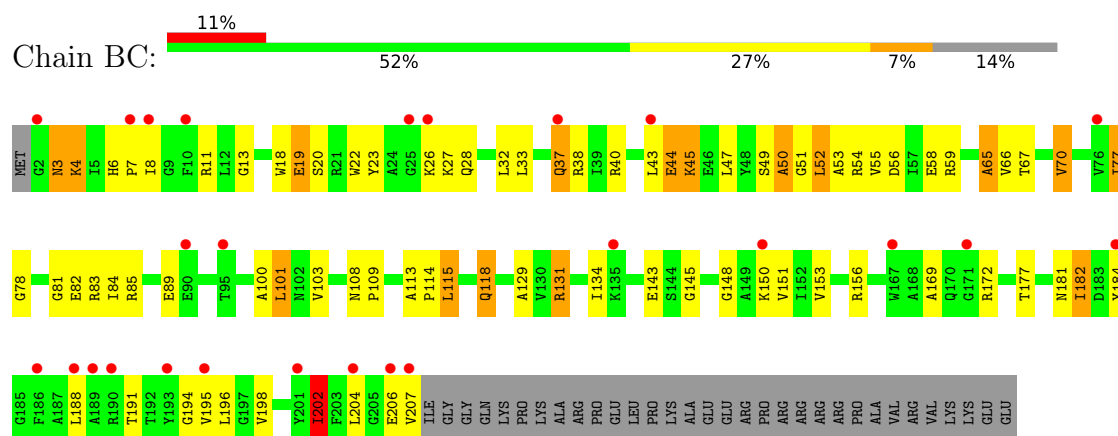




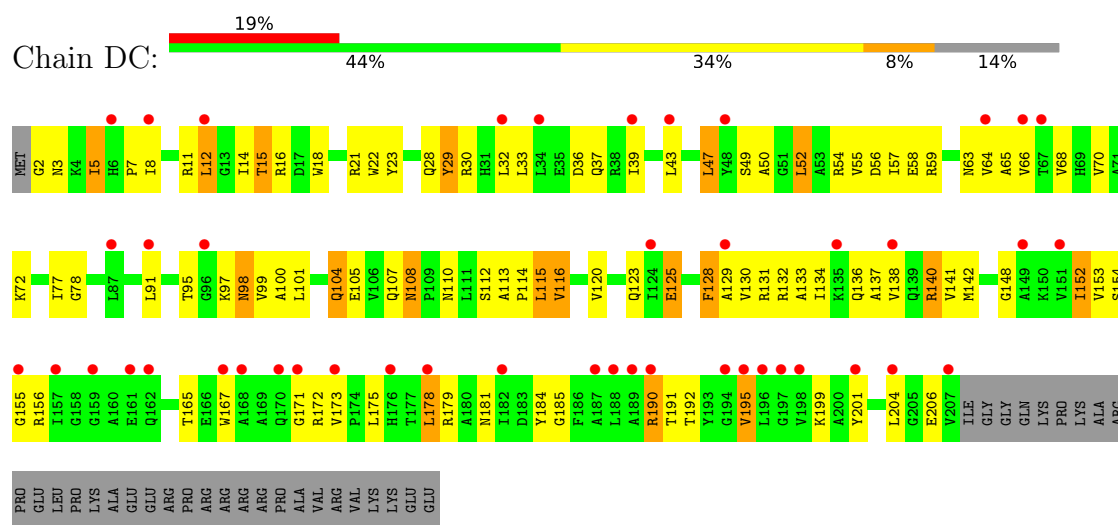




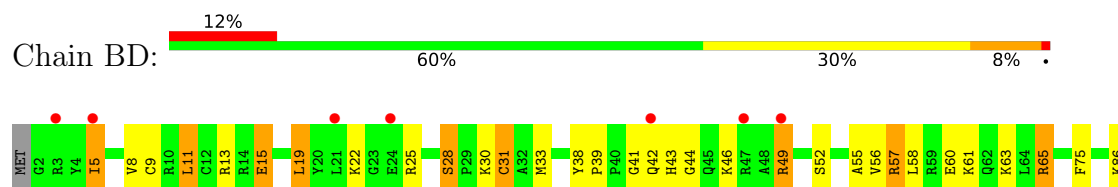
• Molecule 36: 30S ribosomal protein S3

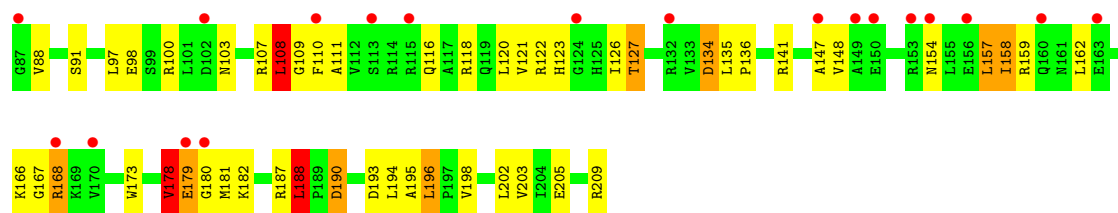


• Molecule 36: 30S ribosomal protein S3

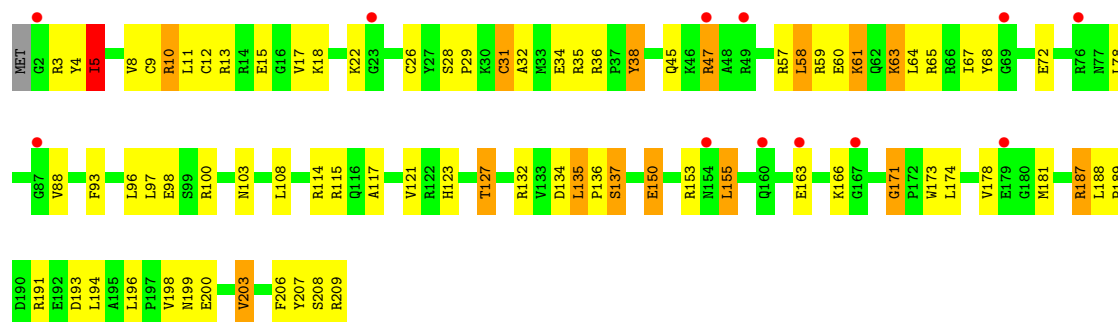


• Molecule 37: 30S ribosomal protein S4

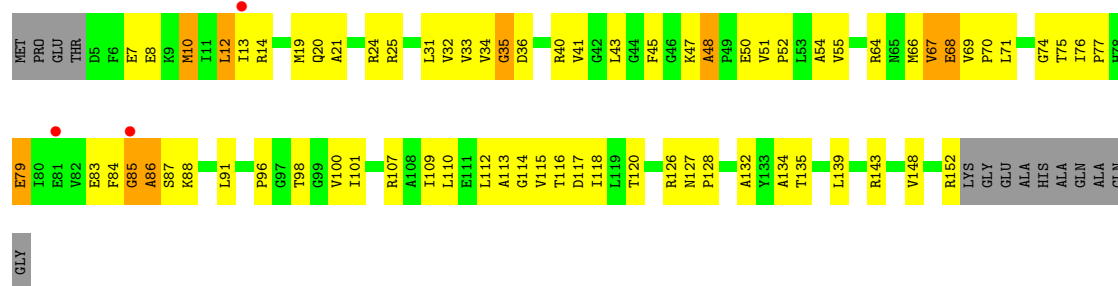




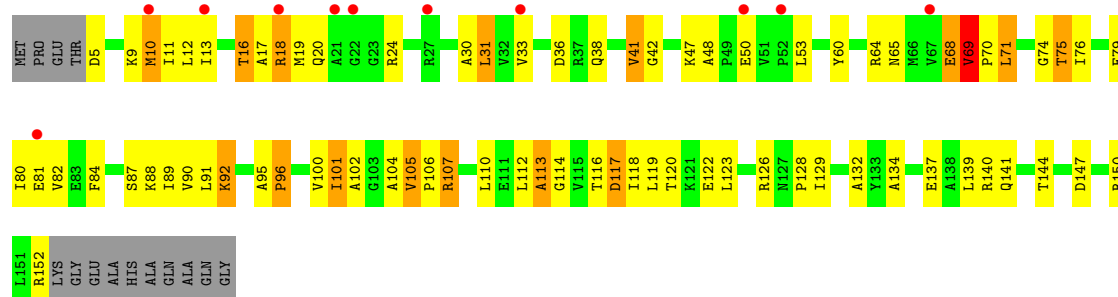
• Molecule 37: 30S ribosomal protein S4



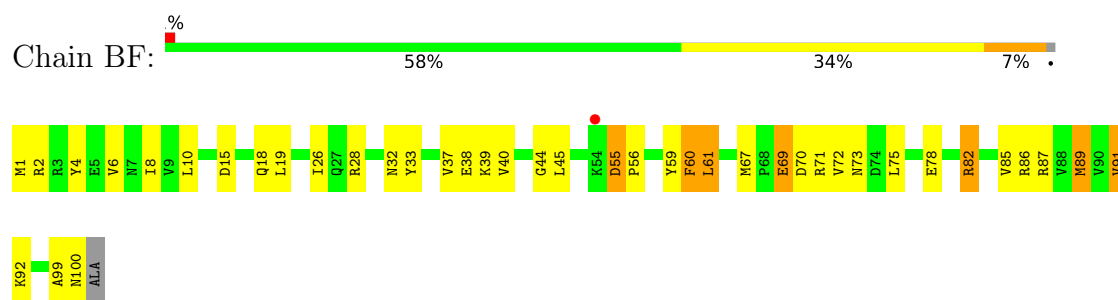
• Molecule 38: 30S ribosomal protein S5



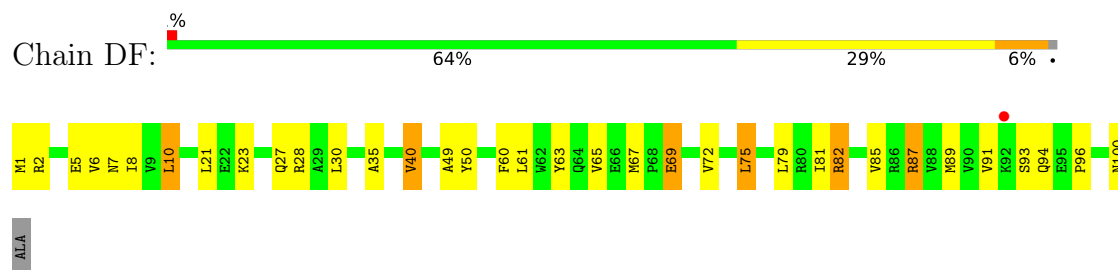
• Molecule 38: 30S ribosomal protein S5



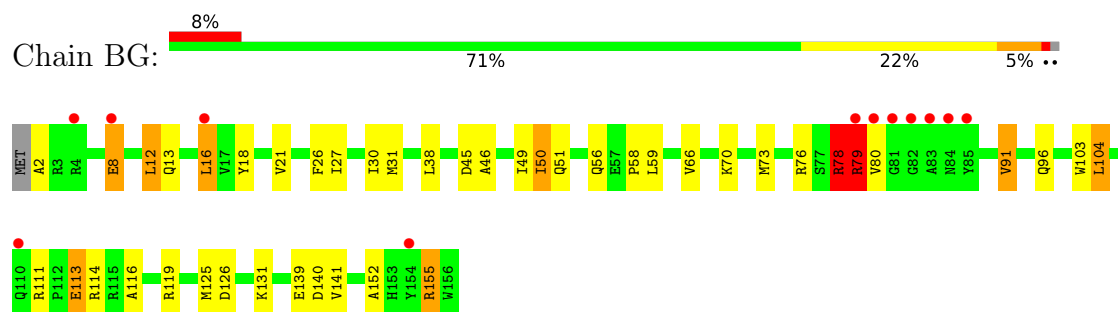
• Molecule 39: 30S ribosomal protein S6



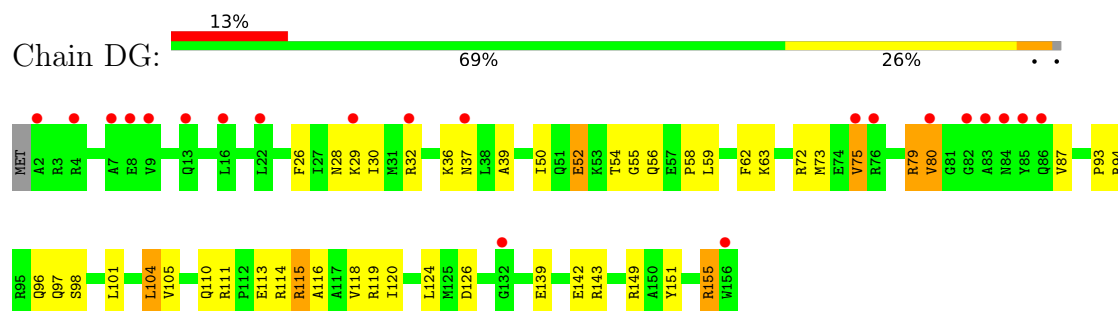
• Molecule 39: 30S ribosomal protein S6



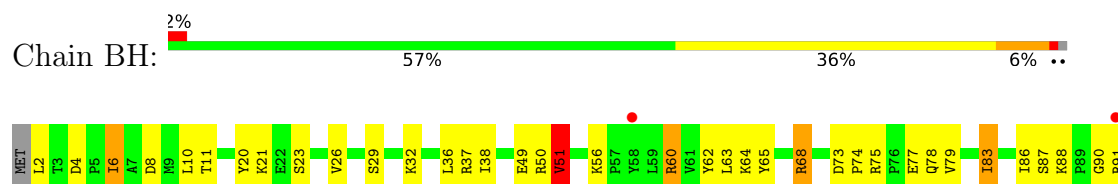
• Molecule 40: 30S ribosomal protein S7

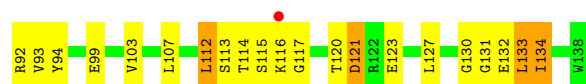


• Molecule 40: 30S ribosomal protein S7

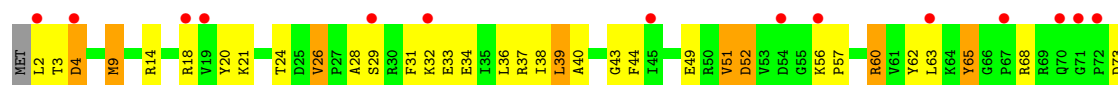


• Molecule 41: 30S ribosomal protein S8

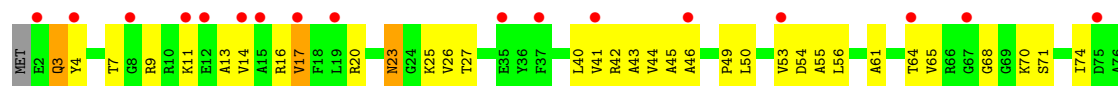




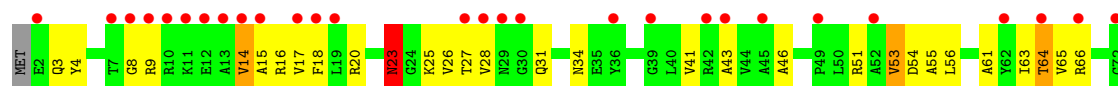
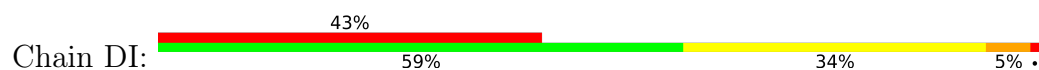
- Molecule 41: 30S ribosomal protein S8



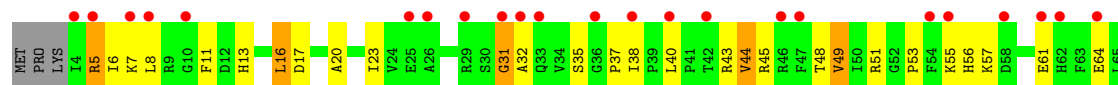
- Molecule 42: 30S ribosomal protein S9



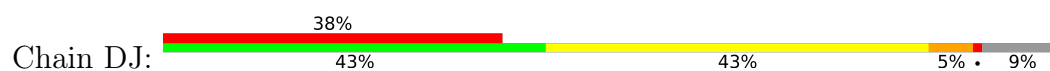
- Molecule 42: 30S ribosomal protein S9

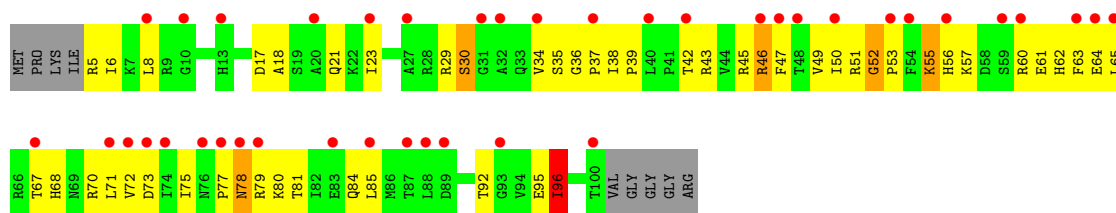


- Molecule 43: 30S ribosomal protein S10

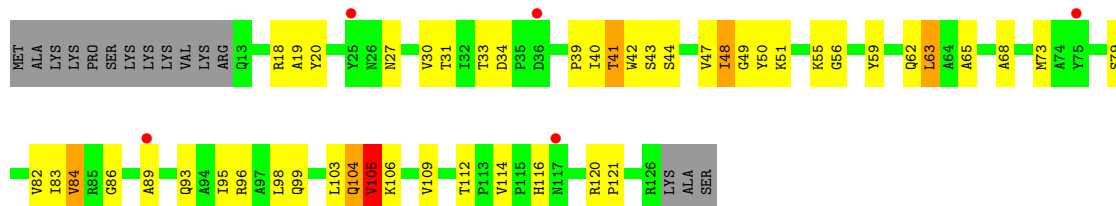


- Molecule 43: 30S ribosomal protein S10

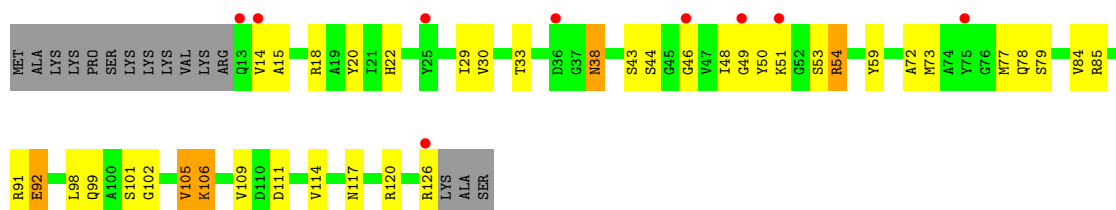




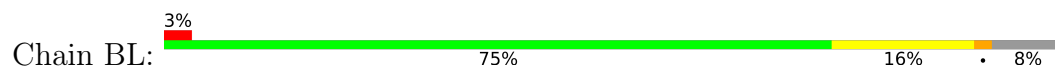
- Molecule 44: 30S ribosomal protein S11



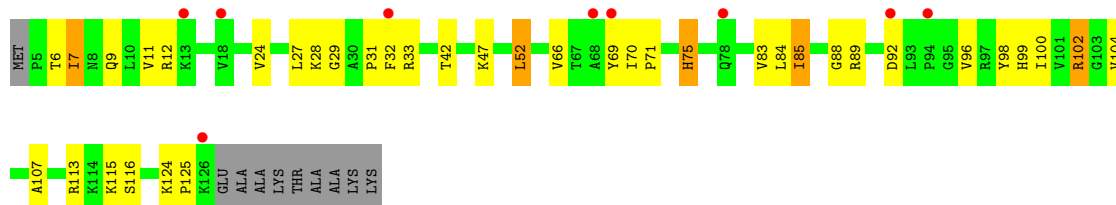
- Molecule 44: 30S ribosomal protein S11



- Molecule 45: 30S ribosomal protein S12

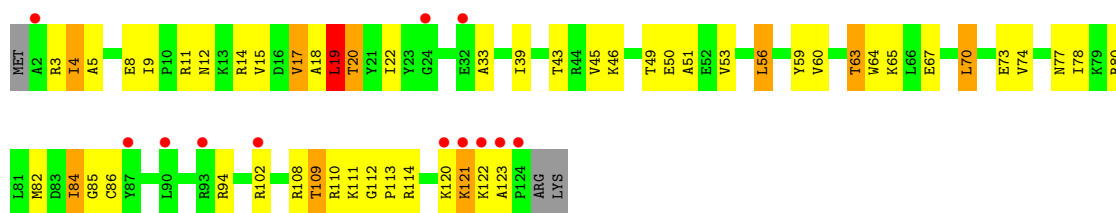


- Molecule 45: 30S ribosomal protein S12

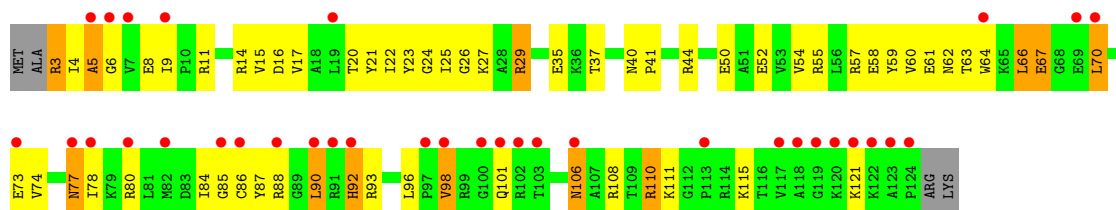


- Molecule 46: 30S ribosomal protein S13

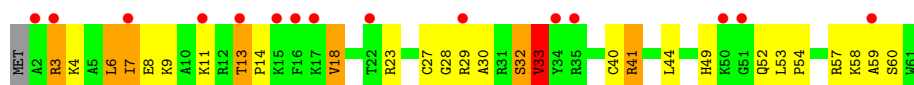




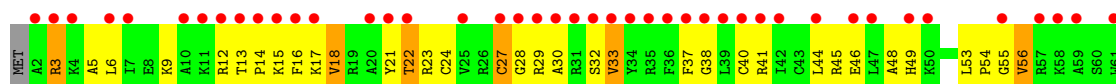
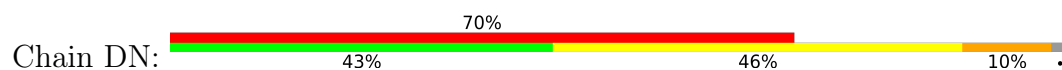
• Molecule 46: 30S ribosomal protein S13



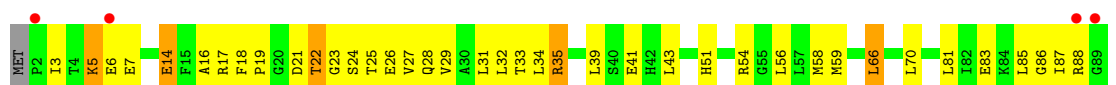
• Molecule 47: 30S ribosomal protein S14 type Z



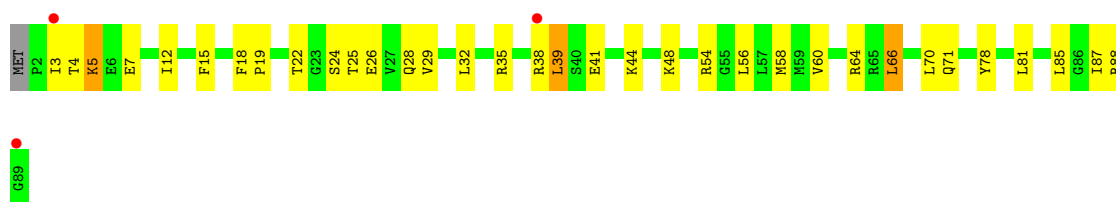
• Molecule 47: 30S ribosomal protein S14 type Z



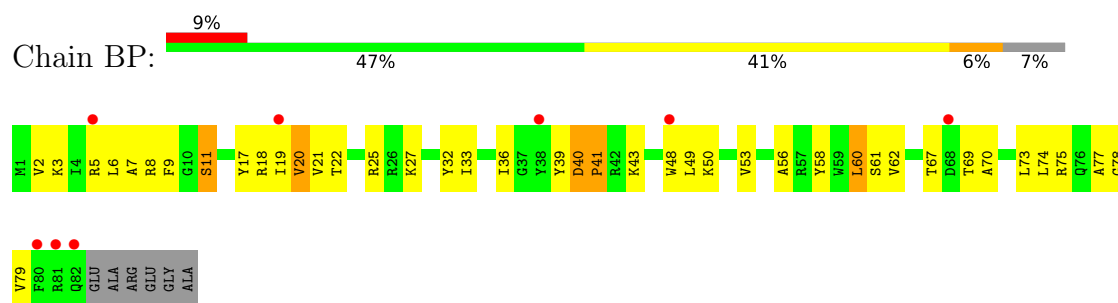
• Molecule 48: 30S ribosomal protein S15



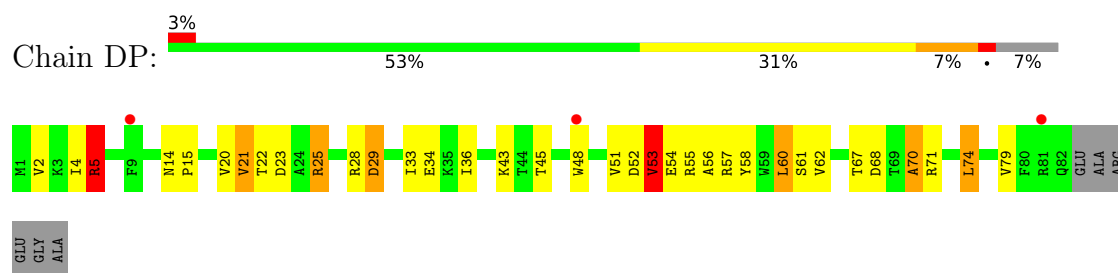
• Molecule 48: 30S ribosomal protein S15



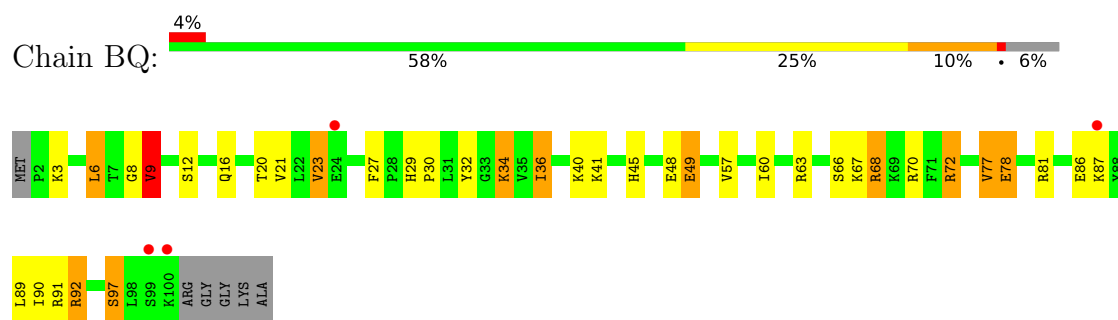
- Molecule 49: 30S ribosomal protein S16



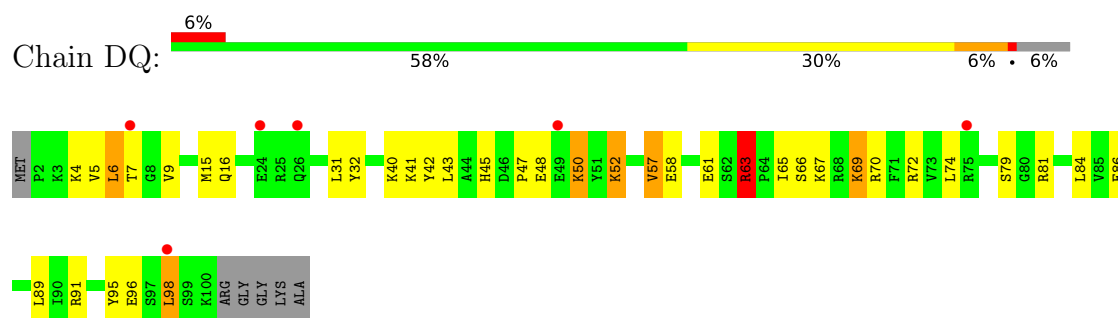
- Molecule 49: 30S ribosomal protein S16



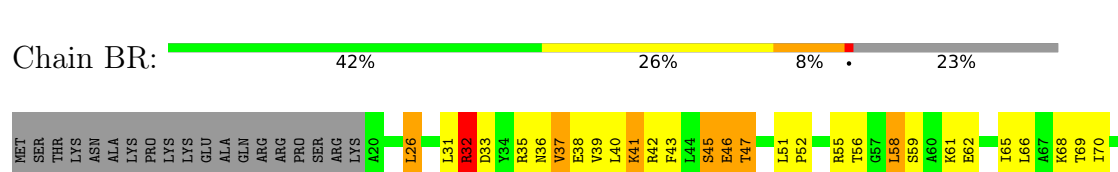
- Molecule 50: 30S ribosomal protein S17

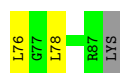


- Molecule 50: 30S ribosomal protein S17

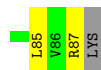
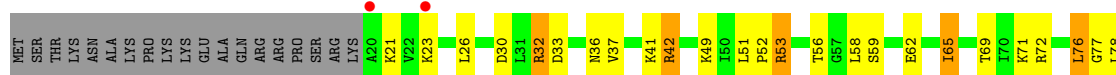


- Molecule 51: 30S ribosomal protein S18

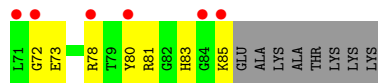
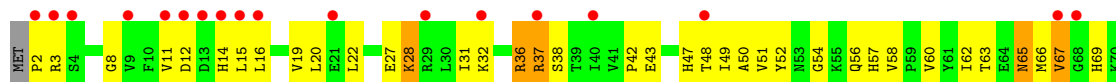




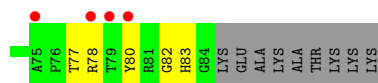
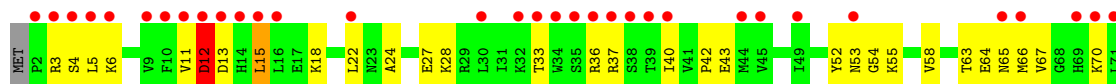
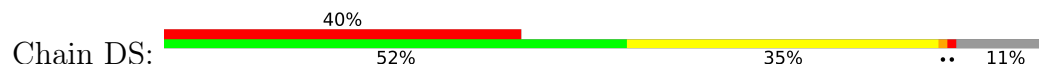
- Molecule 51: 30S ribosomal protein S18



- Molecule 52: 30S ribosomal protein S19



- Molecule 52: 30S ribosomal protein S19

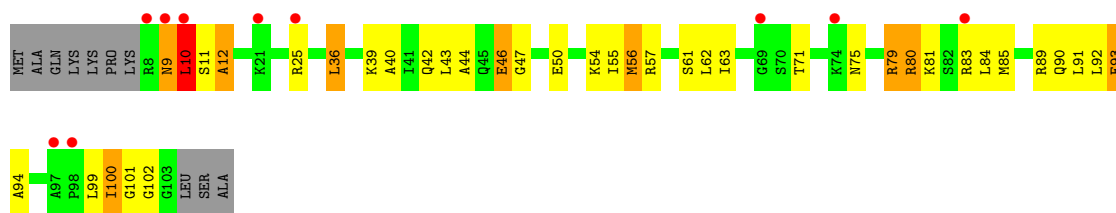


- Molecule 53: 30S ribosomal protein S20

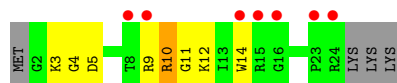


- Molecule 53: 30S ribosomal protein S20

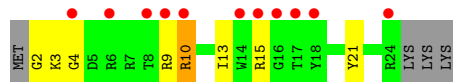
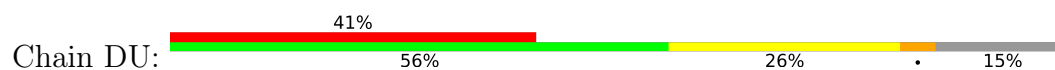




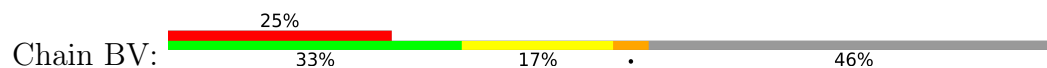
- Molecule 54: 30S ribosomal protein Thx



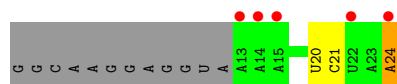
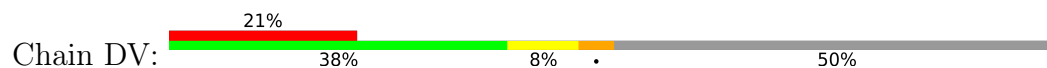
- Molecule 54: 30S ribosomal protein Thx



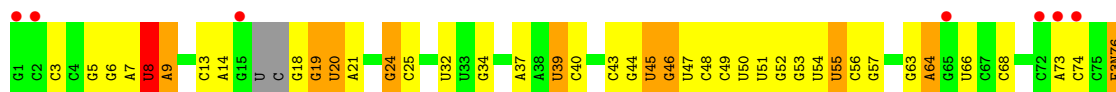
- Molecule 55: mRNA



- Molecule 55: mRNA

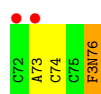


- Molecule 56: A-site tRNA



- Molecule 56: A-site tRNA

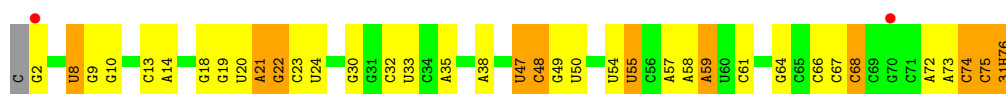




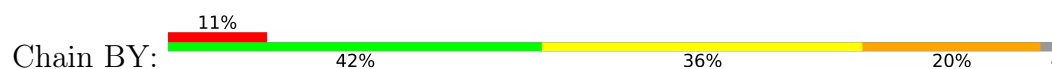
• Molecule 57: P-site tRNA



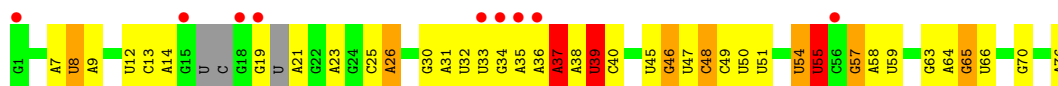
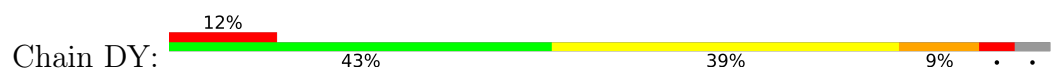
• Molecule 57: P-site tRNA



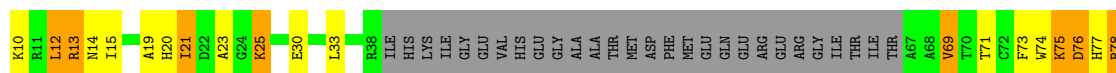
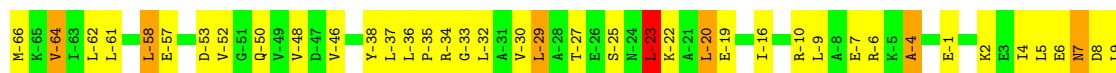
• Molecule 58: E-site tRNA

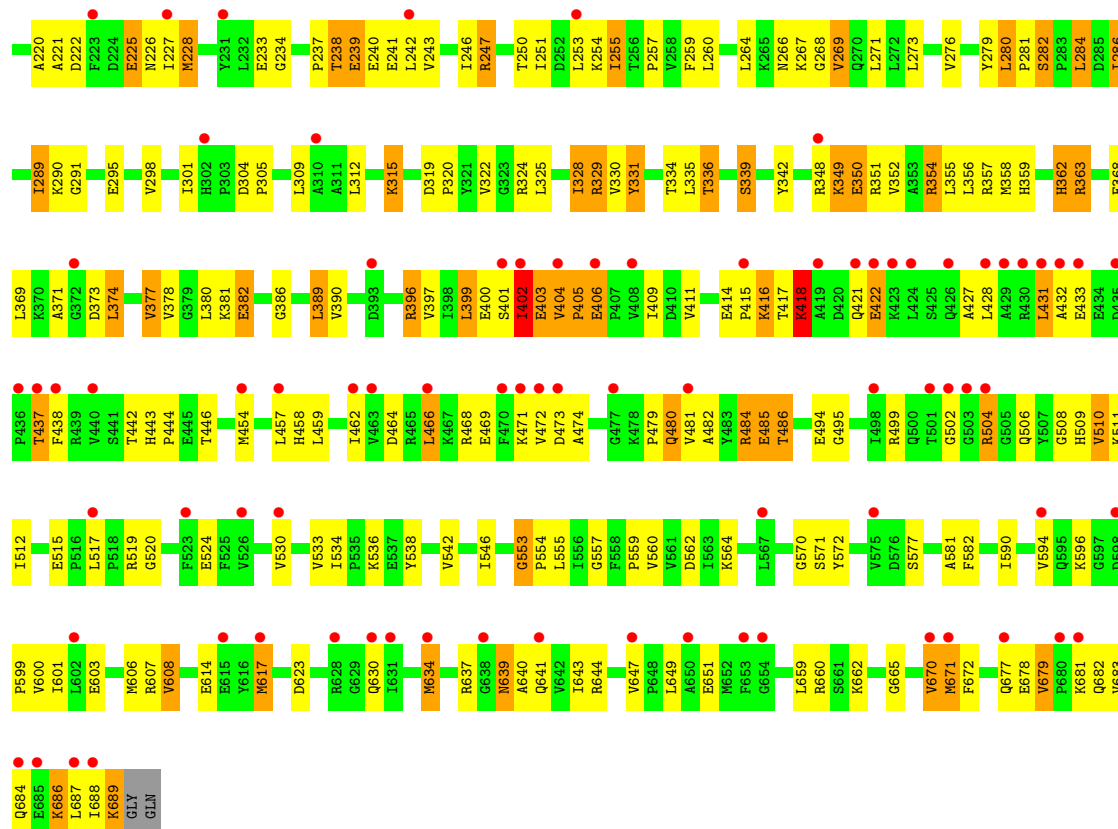


• Molecule 58: E-site tRNA

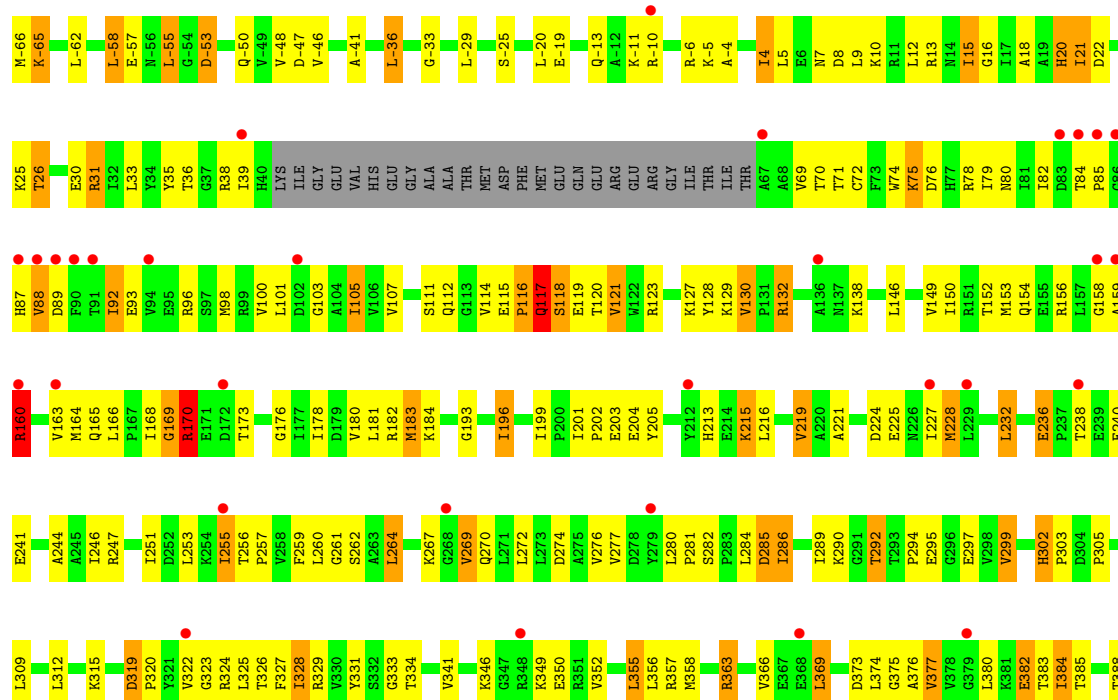


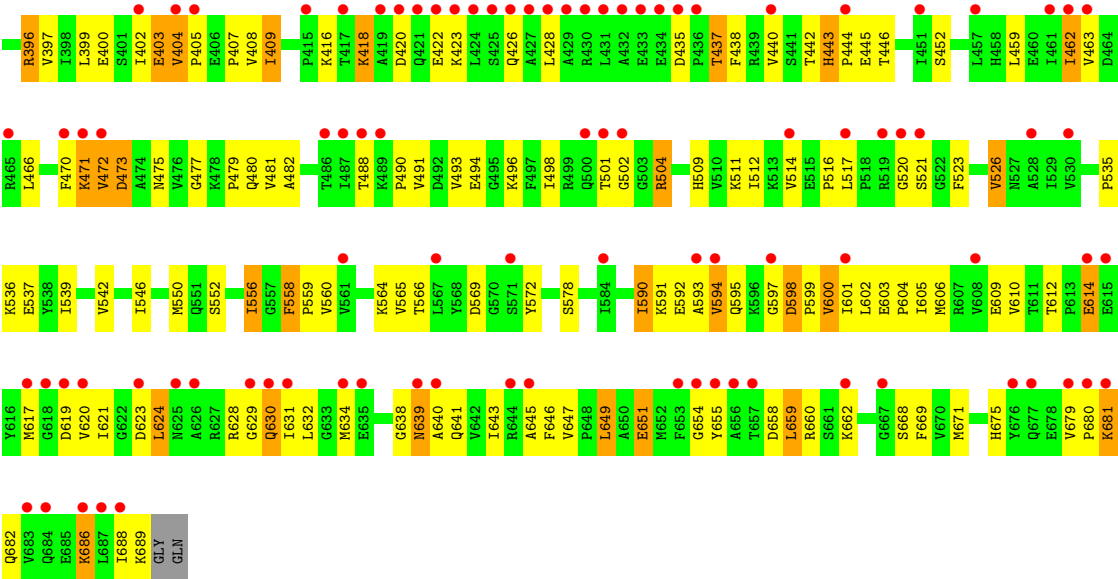
• Molecule 59: 50S ribosomal protein L9, Elongation factor G





● Molecule 59: 50S ribosomal protein L9, Elongation factor G





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.89Å 449.03Å 622.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 2.80 49.63 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.63-2.80) 99.2 (49.63-2.80)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.202 , 0.252 0.203 , 0.251	Depositor DCC
R_{free} test set	71166 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	54.8	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 66.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	313372	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% 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: MG, PSU, 5MC, 31H, 7MG, 5MU, GDP, K, SF4, MIA, ZN, 4SU, F3N

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	AA	0.63	0/69281	0.79	17/108144 (0.0%)
1	CA	0.48	0/69179	0.67	15/107984 (0.0%)
2	AB	0.52	0/2878	0.75	0/4490
2	CB	0.36	0/2878	0.57	0/4490
3	AC	0.42	0/1083	0.97	6/1460 (0.4%)
3	CC	0.42	0/1083	0.97	5/1460 (0.3%)
4	AD	0.96	0/2186	1.25	13/2944 (0.4%)
4	CD	0.82	0/2192	1.15	6/2951 (0.2%)
5	AE	0.99	0/1592	1.31	15/2149 (0.7%)
5	CE	0.80	0/1592	1.14	5/2149 (0.2%)
6	AF	0.92	1/1619 (0.1%)	1.21	8/2193 (0.4%)
6	CF	0.70	0/1615	1.10	7/2188 (0.3%)
7	AG	0.64	0/1450	1.08	6/1959 (0.3%)
7	CG	0.48	0/1449	0.97	5/1958 (0.3%)
8	AH	0.85	0/1356	1.21	11/1834 (0.6%)
8	CH	0.54	0/1356	1.01	5/1834 (0.3%)
9	AK	0.59	0/640	1.37	11/889 (1.2%)
9	CK	0.47	0/640	1.48	11/889 (1.2%)
10	AL	0.46	0/503	0.92	2/673 (0.3%)
10	CL	0.54	0/503	1.06	4/673 (0.6%)
11	AN	0.99	1/1144 (0.1%)	1.27	5/1543 (0.3%)
11	CN	0.71	0/1144	1.12	7/1543 (0.5%)
12	AO	0.94	1/943 (0.1%)	1.19	3/1269 (0.2%)
12	CO	0.82	0/943	1.09	2/1269 (0.2%)
13	AP	0.86	0/1156	1.16	3/1537 (0.2%)
13	CP	0.62	0/1152	1.13	9/1533 (0.6%)
14	AQ	0.94	0/1143	1.18	5/1527 (0.3%)
14	CQ	0.70	0/1143	1.03	3/1527 (0.2%)
15	AR	0.92	0/982	1.13	2/1312 (0.2%)
15	CR	0.76	0/982	1.01	0/1312
16	AS	0.70	0/887	1.10	1/1180 (0.1%)
16	CS	0.58	0/880	1.06	2/1172 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AT	0.93	0/1105	1.20	7/1477 (0.5%)
17	CT	0.72	0/1097	1.05	4/1468 (0.3%)
18	AU	1.05	0/977	1.18	3/1301 (0.2%)
18	CU	0.73	0/977	0.99	2/1301 (0.2%)
19	AV	0.99	0/782	1.31	4/1049 (0.4%)
19	CV	0.67	0/782	0.97	0/1049
20	AW	1.13	1/897 (0.1%)	1.17	3/1205 (0.2%)
20	CW	0.87	0/897	1.14	2/1205 (0.2%)
21	AX	0.93	0/764	1.13	2/1025 (0.2%)
21	CX	0.77	0/764	1.13	4/1025 (0.4%)
22	AY	0.89	1/819 (0.1%)	1.20	2/1095 (0.2%)
22	CY	0.65	0/819	1.07	2/1095 (0.2%)
23	AZ	0.65	0/1379	1.10	10/1873 (0.5%)
23	CZ	0.49	0/1390	1.02	10/1890 (0.5%)
24	A0	0.84	0/662	1.12	2/881 (0.2%)
24	C0	0.68	0/662	1.08	3/881 (0.3%)
25	A1	0.85	0/762	1.08	1/1014 (0.1%)
25	C1	0.77	0/762	1.03	0/1014
26	A2	0.93	0/590	1.08	3/781 (0.4%)
26	C2	0.64	0/590	0.93	0/781
27	A3	1.00	0/474	1.22	4/635 (0.6%)
27	C3	0.64	0/469	1.06	1/630 (0.2%)
28	A4	0.52	0/571	1.19	5/768 (0.7%)
28	C4	0.48	0/545	1.10	6/737 (0.8%)
29	A5	1.11	0/469	1.35	5/635 (0.8%)
29	C5	0.88	0/469	1.18	0/635
30	A6	0.96	1/460 (0.2%)	1.08	0/613
30	C6	0.73	0/456	1.09	2/608 (0.3%)
31	A7	1.06	1/426 (0.2%)	1.15	1/561 (0.2%)
31	C7	0.88	0/426	1.12	2/561 (0.4%)
32	A8	0.99	0/525	1.22	3/691 (0.4%)
32	C8	0.74	0/525	1.07	0/691
33	A9	0.97	0/310	1.28	0/407
33	C9	0.65	0/310	1.05	1/407 (0.2%)
34	BA	0.39	0/36027	0.60	5/56227 (0.0%)
34	DA	0.35	0/36170	0.56	2/56452 (0.0%)
35	BB	0.51	0/1881	1.07	16/2542 (0.6%)
35	DB	0.46	0/1860	0.99	9/2518 (0.4%)
36	BC	0.51	0/1576	0.97	5/2130 (0.2%)
36	DC	0.46	0/1568	0.93	4/2122 (0.2%)
37	BD	0.60	0/1689	1.05	7/2267 (0.3%)
37	DD	0.59	0/1708	1.03	6/2289 (0.3%)
38	BE	0.64	0/1145	1.08	4/1543 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DE	0.58	0/1149	1.12	9/1548 (0.6%)
39	BF	0.65	0/825	0.99	2/1118 (0.2%)
39	DF	0.63	0/833	0.92	1/1128 (0.1%)
40	BG	0.53	0/1250	0.97	3/1679 (0.2%)
40	DG	0.48	0/1254	0.93	1/1683 (0.1%)
41	BH	0.64	0/1108	1.06	4/1494 (0.3%)
41	DH	0.52	0/1108	1.02	4/1494 (0.3%)
42	BI	0.53	0/1005	0.96	0/1350
42	DI	0.47	0/997	0.93	1/1343 (0.1%)
43	BJ	0.54	0/722	0.94	0/982
43	DJ	0.48	0/727	1.03	4/988 (0.4%)
44	BK	0.64	0/848	1.05	0/1149
44	DK	0.64	0/848	1.12	6/1149 (0.5%)
45	BL	0.67	0/946	0.99	2/1274 (0.2%)
45	DL	0.63	0/946	0.97	0/1274
46	BM	0.54	0/977	1.10	5/1310 (0.4%)
46	DM	0.47	0/961	0.91	2/1291 (0.2%)
47	BN	0.55	0/501	1.01	3/664 (0.5%)
47	DN	0.46	0/501	0.84	0/664
48	BO	0.62	0/739	1.01	4/985 (0.4%)
48	DO	0.57	0/739	0.96	3/985 (0.3%)
49	BP	0.65	0/697	1.06	5/939 (0.5%)
49	DP	0.65	0/693	0.97	3/935 (0.3%)
50	BQ	0.63	0/836	1.00	3/1117 (0.3%)
50	DQ	0.57	0/836	1.02	3/1117 (0.3%)
51	BR	0.63	0/560	1.05	1/746 (0.1%)
51	DR	0.63	0/560	0.97	2/746 (0.3%)
52	BS	0.47	0/676	0.93	2/911 (0.2%)
52	DS	0.49	0/661	1.03	4/893 (0.4%)
53	BT	0.60	0/730	1.08	2/965 (0.2%)
53	DT	0.64	0/733	1.10	5/969 (0.5%)
54	BU	0.47	0/203	0.91	0/266
54	DU	0.45	0/203	0.91	0/266
55	BV	0.36	0/310	0.47	0/480
55	DV	0.31	0/282	0.43	0/437
56	BW	0.26	0/1577	0.38	0/2454
56	DW	0.25	0/1531	0.38	0/2379
57	BX	0.40	0/1700	0.60	0/2650
57	DX	0.42	2/1700 (0.1%)	0.55	1/2650 (0.0%)
58	BY	0.27	1/1602 (0.1%)	0.44	0/2493
58	DY	0.23	0/1579	0.34	0/2455
59	BZ	0.57	0/5763	1.03	25/7804 (0.3%)
59	DZ	0.56	0/5784	1.00	22/7835 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.57	10/333310 (0.0%)	0.81	478/497173 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	1
28	A4	0	1
35	BB	0	1
53	BT	0	1
53	DT	0	1
59	DZ	0	1
All	All	0	6

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	DX	74	C	O3'-P	-8.91	1.47	1.61
30	A6	23	THR	CA-CB	6.13	1.62	1.53
57	DX	8	4SU	O3'-P	6.05	1.62	1.56
12	AO	98	VAL	CA-CB	5.67	1.61	1.54
31	A7	13	ALA	CA-CB	-5.55	1.44	1.53

The worst 5 of 478 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	CK	68	LEU	CA-C-N	15.24	138.89	119.84
9	CK	68	LEU	C-N-CA	15.24	138.89	119.84
9	CK	76	GLY	CA-C-N	13.20	136.34	119.84
9	CK	76	GLY	C-N-CA	13.20	136.34	119.84
28	A4	60	GLN	N-CA-C	-11.01	99.86	113.18

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	A4	59	PHE	Peptide
1	AA	537	G	Sidechain
35	BB	8	LYS	Peptide

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Mol	Chain	Res	Type	Group
53	BT	9	ASN	Peptide
53	DT	9	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	61861	0	31186	662	2
1	CA	61771	0	31146	787	0
2	AB	2573	0	1306	18	0
2	CB	2573	0	1306	26	0
3	AC	1063	0	1091	144	5
3	CC	1063	0	1089	158	10
4	AD	2136	0	2218	57	0
4	CD	2142	0	2229	66	0
5	AE	1559	0	1618	50	0
5	CE	1559	0	1618	45	0
6	AF	1584	0	1625	40	0
6	CF	1580	0	1619	51	0
7	AG	1425	0	1443	52	0
7	CG	1424	0	1434	44	0
8	AH	1330	0	1407	25	0
8	CH	1330	0	1407	42	0
9	AK	641	0	309	11	0
9	CK	641	0	309	13	0
10	AL	498	0	521	18	0
10	CL	498	0	521	21	0
11	AN	1117	0	1184	26	0
11	CN	1117	0	1184	21	0
12	AO	933	0	996	27	0
12	CO	933	0	996	24	0
13	AP	1139	0	1223	35	0
13	CP	1135	0	1212	49	0
14	AQ	1122	0	1179	37	0
14	CQ	1122	0	1179	40	0
15	AR	968	0	1033	19	0
15	CR	968	0	1033	29	0
16	AS	877	0	938	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	CS	870	0	923	35	0
17	AT	1091	0	1151	33	0
17	CT	1083	0	1136	28	0
18	AU	959	0	1019	25	0
18	CU	959	0	1019	30	0
19	AV	771	0	830	13	0
19	CV	771	0	830	20	0
20	AW	886	0	940	15	0
20	CW	886	0	940	20	0
21	AX	750	0	814	20	0
21	CX	750	0	814	19	0
22	AY	806	0	881	27	0
22	CY	806	0	882	38	0
23	AZ	1349	0	1355	39	0
23	CZ	1360	0	1363	43	0
24	A0	653	0	674	20	0
24	C0	653	0	674	20	0
25	A1	755	0	826	20	0
25	C1	755	0	826	22	0
26	A2	588	0	643	10	0
26	C2	588	0	643	14	0
27	A3	469	0	518	6	0
27	C3	464	0	514	8	0
28	A4	558	0	545	25	0
28	C4	532	0	506	20	0
29	A5	455	0	465	7	0
29	C5	455	0	465	11	0
30	A6	453	0	473	14	0
30	C6	449	0	469	13	0
31	A7	418	0	467	10	0
31	C7	418	0	467	10	0
32	A8	517	0	582	23	0
32	C8	517	0	582	19	0
33	A9	307	0	335	8	0
33	C9	307	0	335	11	0
34	BA	32185	0	16245	439	0
34	DA	32312	0	16308	512	1
35	BB	1846	0	1867	83	0
35	DB	1825	0	1828	104	0
36	BC	1552	0	1546	54	0
36	DC	1544	0	1524	68	0
37	BD	1659	0	1676	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	DD	1678	0	1718	54	0
38	BE	1129	0	1185	44	0
38	DE	1133	0	1191	43	0
39	BF	812	0	804	19	0
39	DF	820	0	814	27	0
40	BG	1231	0	1238	22	0
40	DG	1235	0	1249	32	0
41	BH	1088	0	1126	40	0
41	DH	1088	0	1126	38	0
42	BI	986	0	995	40	0
42	DI	978	0	966	41	0
43	BJ	709	0	650	34	0
43	DJ	714	0	672	34	0
44	BK	833	0	836	24	0
44	DK	833	0	836	18	0
45	BL	930	0	980	10	0
45	DL	930	0	980	30	0
46	BM	966	0	1024	36	0
46	DM	950	0	988	41	0
47	BN	492	0	529	22	0
47	DN	492	0	531	34	0
48	BO	728	0	760	20	0
48	DO	728	0	760	14	0
49	BP	681	0	697	28	0
49	DP	677	0	686	22	0
50	BQ	823	0	891	26	0
50	DQ	823	0	891	22	0
51	BR	555	0	618	17	0
51	DR	555	0	618	21	0
52	BS	661	0	675	39	0
52	DS	646	0	644	28	0
53	BT	728	0	798	28	0
53	DT	731	0	807	22	0
54	BU	199	0	208	7	0
54	DU	199	0	208	5	0
55	BV	277	0	140	4	0
55	DV	252	0	130	3	0
56	BW	1599	0	830	25	0
56	DW	1552	0	794	22	0
57	BX	1635	0	838	14	0
57	DX	1635	0	839	25	0
58	BY	1581	0	805	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	DY	1561	0	796	16	0
59	BZ	5663	0	5746	260	10
59	DZ	5682	0	5766	201	6
60	A0	5	0	0	0	0
60	A1	2	0	0	0	0
60	A2	1	0	0	0	0
60	A4	1	0	0	0	0
60	A5	3	0	0	0	0
60	A6	2	0	0	0	0
60	A7	6	0	0	0	0
60	A8	2	0	0	0	0
60	A9	1	0	0	0	0
60	AA	817	0	0	0	0
60	AB	23	0	0	0	0
60	AD	11	0	0	0	0
60	AE	5	0	0	0	0
60	AF	8	0	0	0	0
60	AG	3	0	0	0	0
60	AH	1	0	0	0	0
60	AN	3	0	0	0	0
60	AO	1	0	0	0	0
60	AP	3	0	0	0	0
60	AQ	3	0	0	0	0
60	AR	2	0	0	0	0
60	AU	4	0	0	0	0
60	AV	4	0	0	0	0
60	AW	4	0	0	0	0
60	AX	1	0	0	0	0
60	AY	1	0	0	0	0
60	AZ	1	0	0	0	0
60	BA	213	0	0	0	0
60	BB	1	0	0	0	0
60	BD	1	0	0	0	0
60	BE	1	0	0	0	0
60	BF	1	0	0	0	0
60	BK	1	0	0	0	0
60	BL	2	0	0	0	0
60	BM	1	0	0	0	0
60	BN	2	0	0	0	0
60	BT	1	0	0	0	0
60	BV	1	0	0	0	0
60	BW	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	BX	15	0	0	0	0
60	BY	2	0	0	0	0
60	BZ	1	0	0	0	0
60	C0	2	0	0	0	0
60	C3	1	0	0	0	0
60	C5	1	0	0	0	0
60	C7	1	0	0	0	0
60	C8	1	0	0	0	0
60	CA	664	0	0	0	0
60	CB	13	0	0	0	0
60	CD	4	0	0	0	0
60	CE	6	0	0	0	0
60	CF	6	0	0	0	0
60	CG	1	0	0	0	0
60	CN	1	0	0	0	0
60	CO	2	0	0	0	0
60	CP	1	0	0	0	0
60	CQ	4	0	0	0	0
60	CR	2	0	0	0	0
60	CU	1	0	0	0	0
60	CV	2	0	0	0	0
60	CY	1	0	0	0	0
60	DA	168	0	0	0	0
60	DD	1	0	0	0	0
60	DE	2	0	0	0	0
60	DF	1	0	0	0	0
60	DJ	1	0	0	0	0
60	DK	2	0	0	0	0
60	DT	1	0	0	0	0
60	DW	1	0	0	0	0
60	DX	1	0	0	0	0
60	DZ	1	0	0	0	0
61	AA	1	0	0	0	0
62	A4	1	0	0	0	0
62	A5	1	0	0	0	0
62	A6	1	0	0	0	0
62	A9	1	0	0	0	0
62	AY	1	0	0	0	0
62	BN	1	0	0	0	0
62	C4	1	0	0	0	0
62	C5	1	0	0	0	0
62	C6	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	C9	1	0	0	0	0
62	CY	1	0	0	0	0
62	DN	1	0	0	0	0
63	BD	8	0	0	1	0
63	DD	8	0	0	1	0
64	BZ	28	0	12	7	0
64	DZ	28	0	12	7	0
65	A0	6	0	0	0	0
65	A1	1	0	0	0	0
65	A3	1	0	0	0	0
65	A5	3	0	0	0	0
65	A6	2	0	0	0	0
65	A7	4	0	0	1	0
65	A8	10	0	0	1	0
65	AA	1408	0	0	48	0
65	AB	36	0	0	1	0
65	AD	15	0	0	1	0
65	AE	19	0	0	1	0
65	AF	7	0	0	0	0
65	AG	3	0	0	0	0
65	AH	1	0	0	0	0
65	AN	2	0	0	0	0
65	AO	1	0	0	0	0
65	AP	15	0	0	2	0
65	AQ	4	0	0	2	0
65	AR	2	0	0	2	0
65	AS	1	0	0	0	0
65	AT	2	0	0	0	0
65	AU	5	0	0	0	0
65	AV	2	0	0	0	0
65	AW	2	0	0	0	0
65	AX	3	0	0	0	0
65	AZ	1	0	0	0	0
65	BA	212	0	0	13	0
65	BD	2	0	0	0	0
65	BE	2	0	0	0	0
65	BL	1	0	0	0	0
65	BM	1	0	0	0	0
65	BV	2	0	0	0	0
65	BW	3	0	0	0	0
65	BX	8	0	0	0	0
65	BY	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
65	BZ	2	0	0	0	0
65	C0	6	0	0	1	0
65	C1	2	0	0	0	0
65	C3	2	0	0	0	0
65	C6	1	0	0	1	0
65	C7	1	0	0	0	0
65	C8	3	0	0	0	0
65	CA	985	0	0	52	0
65	CB	9	0	0	1	0
65	CD	14	0	0	0	0
65	CE	13	0	0	1	0
65	CF	7	0	0	0	0
65	CN	2	0	0	0	0
65	CP	10	0	0	1	0
65	CQ	1	0	0	0	0
65	CR	1	0	0	0	0
65	CT	3	0	0	0	0
65	CU	2	0	0	0	0
65	CV	1	0	0	0	0
65	CY	1	0	0	0	0
65	DA	155	0	0	6	0
65	DE	4	0	0	0	0
65	DJ	1	0	0	0	0
65	DK	2	0	0	0	0
65	DL	1	0	0	0	0
65	DW	2	0	0	0	0
65	DX	1	0	0	0	0
All	All	313372	0	210866	5452	17

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 11.

The worst 5 of 5452 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:CA:1860:G:H5'	3:CC:206:LYS:CD	1.27	1.64
1:CA:1860:G:H5''	3:CC:206:LYS:CG	1.28	1.64
1:AA:1891:G:C5'	3:AC:206:LYS:HD2	1.35	1.54
1:CA:1860:G:C5'	3:CC:206:LYS:HD2	1.25	1.53
1:CA:1860:G:C5'	3:CC:206:LYS:CG	1.84	1.50

The worst 5 of 17 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:9:ARG:NH2	59:DZ:504:ARG:NH1[3_654]	0.73	1.47
59:BZ:504:ARG:NH2	3:CC:9:ARG:NE[2_655]	1.08	1.12
59:BZ:504:ARG:NH1	3:CC:9:ARG:NH1[2_655]	1.09	1.11
3:AC:6:LYS:O	59:DZ:501:THR:O[3_654]	1.74	0.46
59:BZ:504:ARG:NH1	3:CC:9:ARG:NE[2_655]	1.80	0.40

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	133/228 (58%)	90 (68%)	25 (19%)	18 (14%)	0	0
3	CC	133/228 (58%)	90 (68%)	25 (19%)	18 (14%)	0	0
4	AD	273/276 (99%)	248 (91%)	22 (8%)	3 (1%)	11	36
4	CD	273/276 (99%)	245 (90%)	25 (9%)	3 (1%)	11	36
5	AE	202/206 (98%)	189 (94%)	12 (6%)	1 (0%)	24	55
5	CE	202/206 (98%)	189 (94%)	10 (5%)	3 (2%)	8	28
6	AF	201/210 (96%)	185 (92%)	16 (8%)	0	100	100
6	CF	201/210 (96%)	189 (94%)	8 (4%)	4 (2%)	6	21
7	AG	179/182 (98%)	159 (89%)	14 (8%)	6 (3%)	3	11
7	CG	179/182 (98%)	154 (86%)	19 (11%)	6 (3%)	3	11
8	AH	172/180 (96%)	160 (93%)	11 (6%)	1 (1%)	21	51
8	CH	172/180 (96%)	153 (89%)	13 (8%)	6 (4%)	3	10
9	AK	128/173 (74%)	74 (58%)	26 (20%)	28 (22%)	0	0
9	CK	128/173 (74%)	80 (62%)	28 (22%)	20 (16%)	0	0
10	AL	64/147 (44%)	47 (73%)	13 (20%)	4 (6%)	1	3
10	CL	64/147 (44%)	44 (69%)	17 (27%)	3 (5%)	2	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	AN	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
11	CN	138/140 (99%)	126 (91%)	10 (7%)	2 (1%)	9	30
12	AO	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	16	44
12	CO	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	16	44
13	AP	147/150 (98%)	133 (90%)	12 (8%)	2 (1%)	9	30
13	CP	147/150 (98%)	129 (88%)	15 (10%)	3 (2%)	6	21
14	AQ	139/141 (99%)	128 (92%)	11 (8%)	0	100	100
14	CQ	139/141 (99%)	123 (88%)	13 (9%)	3 (2%)	5	19
15	AR	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	14	41
15	CR	116/118 (98%)	104 (90%)	11 (10%)	1 (1%)	14	41
16	AS	108/112 (96%)	99 (92%)	8 (7%)	1 (1%)	14	41
16	CS	108/112 (96%)	89 (82%)	17 (16%)	2 (2%)	6	22
17	AT	129/146 (88%)	119 (92%)	10 (8%)	0	100	100
17	CT	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
18	AU	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
18	CU	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
19	AV	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	12	38
19	CV	99/101 (98%)	90 (91%)	7 (7%)	2 (2%)	6	21
20	AW	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
20	CW	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
21	AX	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	11	36
21	CX	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	11	36
22	AY	105/110 (96%)	95 (90%)	9 (9%)	1 (1%)	12	38
22	CY	105/110 (96%)	90 (86%)	11 (10%)	4 (4%)	2	9
23	AZ	169/206 (82%)	136 (80%)	28 (17%)	5 (3%)	3	12
23	CZ	172/206 (84%)	144 (84%)	25 (14%)	3 (2%)	7	25
24	A0	81/85 (95%)	74 (91%)	6 (7%)	1 (1%)	10	34
24	C0	81/85 (95%)	76 (94%)	5 (6%)	0	100	100
25	A1	95/98 (97%)	86 (90%)	9 (10%)	0	100	100
25	C1	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	11	36
26	A2	68/72 (94%)	66 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	C2	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
27	A3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	C3	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	6	23
28	A4	67/71 (94%)	44 (66%)	16 (24%)	7 (10%)	0	1
28	C4	67/71 (94%)	49 (73%)	13 (19%)	5 (8%)	1	2
29	A5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
29	C5	57/60 (95%)	57 (100%)	0	0	100	100
30	A6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
30	C6	51/54 (94%)	45 (88%)	6 (12%)	0	100	100
31	A7	46/49 (94%)	46 (100%)	0	0	100	100
31	C7	46/49 (94%)	44 (96%)	0	2 (4%)	2	7
32	A8	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
32	C8	62/65 (95%)	58 (94%)	2 (3%)	2 (3%)	3	11
33	A9	35/37 (95%)	35 (100%)	0	0	100	100
33	C9	35/37 (95%)	35 (100%)	0	0	100	100
35	BB	229/256 (90%)	187 (82%)	29 (13%)	13 (6%)	1	4
35	DB	229/256 (90%)	177 (77%)	37 (16%)	15 (7%)	1	3
36	BC	204/239 (85%)	171 (84%)	25 (12%)	8 (4%)	2	8
36	DC	204/239 (85%)	171 (84%)	30 (15%)	3 (2%)	8	28
37	BD	206/209 (99%)	186 (90%)	16 (8%)	4 (2%)	6	22
37	DD	206/209 (99%)	180 (87%)	20 (10%)	6 (3%)	3	13
38	BE	146/162 (90%)	128 (88%)	13 (9%)	5 (3%)	3	11
38	DE	146/162 (90%)	128 (88%)	12 (8%)	6 (4%)	2	8
39	BF	98/101 (97%)	89 (91%)	7 (7%)	2 (2%)	6	21
39	DF	98/101 (97%)	91 (93%)	6 (6%)	1 (1%)	12	38
40	BG	153/156 (98%)	142 (93%)	9 (6%)	2 (1%)	9	31
40	DG	153/156 (98%)	132 (86%)	19 (12%)	2 (1%)	9	31
41	BH	135/138 (98%)	120 (89%)	12 (9%)	3 (2%)	5	19
41	DH	135/138 (98%)	121 (90%)	12 (9%)	2 (2%)	8	28
42	BI	125/128 (98%)	111 (89%)	10 (8%)	4 (3%)	3	11
42	DI	125/128 (98%)	111 (89%)	12 (10%)	2 (2%)	7	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	BJ	95/105 (90%)	81 (85%)	9 (10%)	5 (5%)	1	5
43	DJ	94/105 (90%)	77 (82%)	10 (11%)	7 (7%)	1	2
44	BK	112/129 (87%)	102 (91%)	8 (7%)	2 (2%)	6	23
44	DK	112/129 (87%)	98 (88%)	10 (9%)	4 (4%)	2	10
45	BL	120/132 (91%)	106 (88%)	13 (11%)	1 (1%)	16	44
45	DL	120/132 (91%)	109 (91%)	11 (9%)	0	100	100
46	BM	121/126 (96%)	101 (84%)	17 (14%)	3 (2%)	4	16
46	DM	120/126 (95%)	98 (82%)	13 (11%)	9 (8%)	1	2
47	BN	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	7	25
47	DN	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	7	25
48	BO	86/89 (97%)	77 (90%)	7 (8%)	2 (2%)	5	18
48	DO	86/89 (97%)	72 (84%)	12 (14%)	2 (2%)	5	18
49	BP	80/88 (91%)	66 (82%)	12 (15%)	2 (2%)	4	16
49	DP	80/88 (91%)	66 (82%)	13 (16%)	1 (1%)	9	31
50	BQ	97/105 (92%)	87 (90%)	9 (9%)	1 (1%)	12	38
50	DQ	97/105 (92%)	85 (88%)	12 (12%)	0	100	100
51	BR	66/88 (75%)	61 (92%)	4 (6%)	1 (2%)	8	28
51	DR	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
52	BS	82/93 (88%)	73 (89%)	9 (11%)	0	100	100
52	DS	81/93 (87%)	67 (83%)	12 (15%)	2 (2%)	4	16
53	BT	94/106 (89%)	78 (83%)	10 (11%)	6 (6%)	1	3
53	DT	94/106 (89%)	78 (83%)	12 (13%)	4 (4%)	2	7
54	BU	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
54	DU	21/27 (78%)	19 (90%)	1 (5%)	1 (5%)	2	6
59	BZ	722/758 (95%)	598 (83%)	92 (13%)	32 (4%)	2	7
59	DZ	726/758 (96%)	594 (82%)	97 (13%)	35 (5%)	2	6
All	All	13220/14444 (92%)	11544 (87%)	1298 (10%)	378 (3%)	3	13

5 of 378 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	42	VAL
3	AC	47	LYS

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Mol	Chain	Res	Type
3	AC	68	GLY
3	AC	180	SER
3	AC	181	PHE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AC	111/180 (62%)	100 (90%)	11 (10%)	7	24
3	CC	111/180 (62%)	100 (90%)	11 (10%)	7	24
4	AD	215/218 (99%)	180 (84%)	35 (16%)	2	8
4	CD	216/218 (99%)	177 (82%)	39 (18%)	2	6
5	AE	164/166 (99%)	134 (82%)	30 (18%)	2	6
5	CE	164/166 (99%)	135 (82%)	29 (18%)	2	6
6	AF	160/166 (96%)	132 (82%)	28 (18%)	2	7
6	CF	159/166 (96%)	130 (82%)	29 (18%)	2	6
7	AG	143/156 (92%)	115 (80%)	28 (20%)	1	5
7	CG	142/156 (91%)	112 (79%)	30 (21%)	1	4
8	AH	144/148 (97%)	124 (86%)	20 (14%)	3	12
8	CH	144/148 (97%)	116 (81%)	28 (19%)	1	5
10	AL	50/111 (45%)	44 (88%)	6 (12%)	5	17
10	CL	50/111 (45%)	43 (86%)	7 (14%)	3	12
11	AN	118/119 (99%)	94 (80%)	24 (20%)	1	4
11	CN	118/119 (99%)	91 (77%)	27 (23%)	1	3
12	AO	100/100 (100%)	83 (83%)	17 (17%)	2	7
12	CO	100/100 (100%)	79 (79%)	21 (21%)	1	4
13	AP	116/116 (100%)	96 (83%)	20 (17%)	2	7
13	CP	115/116 (99%)	93 (81%)	22 (19%)	1	5
14	AQ	111/111 (100%)	91 (82%)	20 (18%)	2	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	CQ	111/111 (100%)	93 (84%)	18 (16%)	2	8
15	AR	101/101 (100%)	80 (79%)	21 (21%)	1	4
15	CR	101/101 (100%)	82 (81%)	19 (19%)	1	5
16	AS	87/88 (99%)	69 (79%)	18 (21%)	1	4
16	CS	85/88 (97%)	66 (78%)	19 (22%)	1	3
17	AT	115/127 (91%)	92 (80%)	23 (20%)	1	4
17	CT	113/127 (89%)	91 (80%)	22 (20%)	1	5
18	AU	93/94 (99%)	76 (82%)	17 (18%)	2	6
18	CU	93/94 (99%)	80 (86%)	13 (14%)	3	12
19	AV	80/82 (98%)	63 (79%)	17 (21%)	1	4
19	CV	80/82 (98%)	65 (81%)	15 (19%)	1	5
20	AW	90/92 (98%)	78 (87%)	12 (13%)	4	14
20	CW	90/92 (98%)	78 (87%)	12 (13%)	4	14
21	AX	77/78 (99%)	69 (90%)	8 (10%)	7	22
21	CX	77/78 (99%)	70 (91%)	7 (9%)	9	28
22	AY	85/91 (93%)	73 (86%)	12 (14%)	3	12
22	CY	85/91 (93%)	74 (87%)	11 (13%)	4	14
23	AZ	145/179 (81%)	113 (78%)	32 (22%)	1	3
23	CZ	145/179 (81%)	120 (83%)	25 (17%)	2	7
24	A0	65/67 (97%)	62 (95%)	3 (5%)	24	58
24	C0	65/67 (97%)	59 (91%)	6 (9%)	8	27
25	A1	80/83 (96%)	70 (88%)	10 (12%)	4	15
25	C1	80/83 (96%)	66 (82%)	14 (18%)	2	7
26	A2	65/67 (97%)	50 (77%)	15 (23%)	1	3
26	C2	65/67 (97%)	53 (82%)	12 (18%)	1	6
27	A3	51/52 (98%)	43 (84%)	8 (16%)	2	9
27	C3	50/52 (96%)	40 (80%)	10 (20%)	1	4
28	A4	60/63 (95%)	47 (78%)	13 (22%)	1	3
28	C4	53/63 (84%)	42 (79%)	11 (21%)	1	4
29	A5	50/52 (96%)	43 (86%)	7 (14%)	3	12
29	C5	50/52 (96%)	44 (88%)	6 (12%)	5	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	A6	51/52 (98%)	37 (72%)	14 (28%)	0	1
30	C6	50/52 (96%)	44 (88%)	6 (12%)	5	17
31	A7	41/42 (98%)	35 (85%)	6 (15%)	3	11
31	C7	41/42 (98%)	37 (90%)	4 (10%)	7	25
32	A8	54/55 (98%)	43 (80%)	11 (20%)	1	4
32	C8	54/55 (98%)	47 (87%)	7 (13%)	4	14
33	A9	34/34 (100%)	30 (88%)	4 (12%)	5	17
33	C9	34/34 (100%)	30 (88%)	4 (12%)	5	17
35	BB	192/220 (87%)	144 (75%)	48 (25%)	0	2
35	DB	187/220 (85%)	154 (82%)	33 (18%)	2	7
36	BC	143/188 (76%)	121 (85%)	22 (15%)	2	10
36	DC	141/188 (75%)	114 (81%)	27 (19%)	1	5
37	BD	170/181 (94%)	145 (85%)	25 (15%)	3	10
37	DD	174/181 (96%)	151 (87%)	23 (13%)	4	14
38	BE	113/123 (92%)	103 (91%)	10 (9%)	9	29
38	DE	114/123 (93%)	92 (81%)	22 (19%)	1	5
39	BF	84/90 (93%)	72 (86%)	12 (14%)	3	11
39	DF	86/90 (96%)	73 (85%)	13 (15%)	3	10
40	BG	119/127 (94%)	97 (82%)	22 (18%)	1	6
40	DG	120/127 (94%)	112 (93%)	8 (7%)	15	42
41	BH	114/119 (96%)	95 (83%)	19 (17%)	2	8
41	DH	114/119 (96%)	90 (79%)	24 (21%)	1	4
42	BI	91/99 (92%)	73 (80%)	18 (20%)	1	5
42	DI	89/99 (90%)	72 (81%)	17 (19%)	1	5
43	BJ	66/92 (72%)	57 (86%)	9 (14%)	3	13
43	DJ	69/92 (75%)	57 (83%)	12 (17%)	2	7
44	BK	83/99 (84%)	70 (84%)	13 (16%)	2	9
44	DK	83/99 (84%)	74 (89%)	9 (11%)	6	21
45	BL	97/109 (89%)	87 (90%)	10 (10%)	7	23
45	DL	97/109 (89%)	86 (89%)	11 (11%)	5	19
46	BM	95/101 (94%)	80 (84%)	15 (16%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	DM	92/101 (91%)	75 (82%)	17 (18%)	1	6
47	BN	49/50 (98%)	39 (80%)	10 (20%)	1	4
47	DN	49/50 (98%)	40 (82%)	9 (18%)	1	6
48	BO	78/80 (98%)	63 (81%)	15 (19%)	1	5
48	DO	78/80 (98%)	65 (83%)	13 (17%)	2	8
49	BP	69/74 (93%)	57 (83%)	12 (17%)	2	7
49	DP	68/74 (92%)	56 (82%)	12 (18%)	2	7
50	BQ	94/97 (97%)	78 (83%)	16 (17%)	2	7
50	DQ	94/97 (97%)	81 (86%)	13 (14%)	3	12
51	BR	59/77 (77%)	45 (76%)	14 (24%)	1	3
51	DR	59/77 (77%)	51 (86%)	8 (14%)	3	13
52	BS	70/80 (88%)	61 (87%)	9 (13%)	4	14
52	DS	67/80 (84%)	59 (88%)	8 (12%)	5	17
53	BT	70/82 (85%)	58 (83%)	12 (17%)	2	7
53	DT	71/82 (87%)	58 (82%)	13 (18%)	2	6
54	BU	18/22 (82%)	16 (89%)	2 (11%)	6	20
54	DU	18/22 (82%)	16 (89%)	2 (11%)	6	20
59	BZ	604/636 (95%)	466 (77%)	138 (23%)	1	3
59	DZ	607/636 (95%)	480 (79%)	127 (21%)	1	4
All	All	10652/11672 (91%)	8806 (83%)	1846 (17%)	2	7

5 of 1846 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
59	BZ	614	GLU
59	DZ	277	VAL
12	CO	24	VAL
59	DZ	112	GLN
43	DJ	67	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 188 such sidechains are listed below:

Mol	Chain	Res	Type
17	CT	84	GLN

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Mol	Chain	Res	Type
39	DF	94	GLN
21	CX	31	HIS
36	DC	3	ASN
40	DG	122	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2866/2915 (98%)	481 (16%)	41 (1%)
1	CA	2860/2915 (98%)	523 (18%)	37 (1%)
2	AB	119/121 (98%)	11 (9%)	0
2	CB	119/121 (98%)	19 (15%)	0
34	BA	1494/1521 (98%)	265 (17%)	21 (1%)
34	DA	1501/1521 (98%)	285 (18%)	23 (1%)
55	BV	12/24 (50%)	3 (25%)	0
55	DV	11/24 (45%)	1 (9%)	0
56	BW	71/76 (93%)	18 (25%)	1 (1%)
56	DW	68/76 (89%)	22 (32%)	2 (2%)
57	BX	74/77 (96%)	10 (13%)	0
57	DX	74/77 (96%)	13 (17%)	0
58	BY	72/76 (94%)	20 (27%)	2 (2%)
58	DY	71/76 (93%)	21 (29%)	0
All	All	9412/9620 (97%)	1692 (17%)	127 (1%)

5 of 1692 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	12	U
1	AA	13	A
1	AA	34	C
1	AA	45	C
1	AA	62	U

5 of 127 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	BA	1201	A
34	DA	532	A
1	CA	310	A
34	DA	509	A
34	DA	992	U

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

40 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$
56	4SU	DW	8	56	18,21,22	1.77	5 (27%)	25,30,33	2.21	5 (20%)
58	PSU	BY	55	58	18,21,22	1.37	2 (11%)	21,30,33	1.95	3 (14%)
56	PSU	BW	55	56	18,21,22	1.44	3 (16%)	21,30,33	2.06	4 (19%)
56	MIA	DW	37	56	21,24,32	1.60	4 (19%)	30,35,47	2.02	7 (23%)
58	4SU	DY	8	58	18,21,22	1.84	4 (22%)	25,30,33	2.39	5 (20%)
56	PSU	DW	39	56	18,21,22	1.30	2 (11%)	21,30,33	1.93	3 (14%)
57	PSU	DX	55	57	18,21,22	1.39	2 (11%)	21,30,33	1.90	4 (19%)
58	MIA	DY	37	58	21,24,32	1.58	4 (19%)	30,35,47	2.03	8 (26%)
58	7MG	DY	46	58	23,26,27	1.29	3 (13%)	27,39,42	2.79	7 (25%)
58	PSU	DY	39	58	18,21,22	1.43	1 (5%)	21,30,33	1.99	4 (19%)
56	PSU	DW	55	56	18,21,22	1.42	2 (11%)	21,30,33	1.97	3 (14%)
57	5MC	DX	32	57	19,22,23	1.94	2 (10%)	26,32,35	1.38	4 (15%)
56	5MU	DW	54	56	19,22,23	1.41	5 (26%)	27,32,35	2.02	8 (29%)
58	PSU	DY	55	58	18,21,22	1.45	2 (11%)	21,30,33	2.03	4 (19%)
56	F3N	DW	76	1,56	33,36,37	1.44	5 (15%)	41,51,54	1.81	10 (24%)
57	31H	DX	76	57,60	31,34,35	1.38	4 (12%)	35,47,50	2.31	11 (31%)
56	7MG	DW	46	56	23,26,27	1.31	3 (13%)	27,39,42	2.56	7 (25%)
56	5MU	BW	54	56	19,22,23	1.50	4 (21%)	27,32,35	2.06	8 (29%)
58	5MU	DY	54	58	19,22,23	1.44	6 (31%)	27,32,35	2.07	6 (22%)
56	F3N	BW	76	1,56	33,36,37	1.36	5 (15%)	41,51,54	1.74	8 (19%)
58	7MG	BY	46	58	23,26,27	1.29	4 (17%)	27,39,42	2.68	7 (25%)
57	5MU	BX	54	57,60	19,22,23	1.54	5 (26%)	27,32,35	2.06	8 (29%)
57	5MU	DX	54	57	19,22,23	1.43	5 (26%)	27,32,35	2.22	8 (29%)
58	PSU	DY	32	58	18,21,22	1.36	2 (11%)	21,30,33	1.94	3 (14%)
57	4SU	BX	8	57	18,21,22	1.48	3 (16%)	25,30,33	2.27	5 (20%)
56	MIA	BW	37	56	28,31,32	2.44	6 (21%)	38,44,47	2.78	14 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	MIA	BY	37	58	21,24,32	1.67	4 (19%)	30,35,47	2.03	9 (30%)
58	PSU	BY	32	58	18,21,22	1.40	3 (16%)	21,30,33	1.90	4 (19%)
56	PSU	DW	32	56	18,21,22	1.41	3 (16%)	21,30,33	2.00	3 (14%)
57	PSU	BX	55	57	18,21,22	1.28	2 (11%)	21,30,33	2.12	5 (23%)
57	5MC	BX	32	57	19,22,23	1.37	3 (15%)	26,32,35	1.32	3 (11%)
56	4SU	BW	8	56	18,21,22	1.80	4 (22%)	25,30,33	2.20	5 (20%)
58	5MU	BY	54	58	19,22,23	1.52	4 (21%)	27,32,35	2.19	9 (33%)
57	4SU	DX	8	57	18,21,22	1.88	4 (22%)	25,30,33	2.43	4 (16%)
56	PSU	BW	32	60,56	18,21,22	1.37	2 (11%)	21,30,33	1.94	3 (14%)
58	PSU	BY	39	58	18,21,22	1.37	2 (11%)	21,30,33	1.99	3 (14%)
56	PSU	BW	39	56	18,21,22	1.37	3 (16%)	21,30,33	2.11	4 (19%)
57	31H	BX	76	57,60	31,34,35	1.39	4 (12%)	35,47,50	2.31	11 (31%)
58	4SU	BY	8	58	18,21,22	1.85	4 (22%)	25,30,33	2.23	5 (20%)
56	7MG	BW	46	56	23,26,27	1.35	3 (13%)	27,39,42	2.59	7 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	4SU	DW	8	56	-	0/7/25/26	0/2/2/2
58	PSU	BY	55	58	-	1/7/25/26	0/2/2/2
56	PSU	BW	55	56	-	0/7/25/26	0/2/2/2
56	MIA	DW	37	56	-	0/7/25/34	0/3/3/3
58	4SU	DY	8	58	-	1/7/25/26	0/2/2/2
56	PSU	DW	39	56	-	0/7/25/26	0/2/2/2
57	PSU	DX	55	57	-	1/7/25/26	0/2/2/2
58	MIA	DY	37	58	-	2/7/25/34	0/3/3/3
58	7MG	DY	46	58	-	3/7/37/38	0/3/3/3
58	PSU	DY	39	58	-	2/7/25/26	0/2/2/2
56	PSU	DW	55	56	-	0/7/25/26	0/2/2/2
57	5MC	DX	32	57	-	0/7/25/26	0/2/2/2
56	5MU	DW	54	56	-	0/7/25/26	0/2/2/2
58	PSU	DY	55	58	-	3/7/25/26	0/2/2/2
56	F3N	DW	76	1,56	-	0/19/37/38	0/4/4/4
57	31H	DX	76	57,60	-	8/22/40/41	0/3/3/3
56	7MG	DW	46	56	-	2/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	5MU	BW	54	56	-	0/7/25/26	0/2/2/2
58	5MU	DY	54	58	-	2/7/25/26	0/2/2/2
56	F3N	BW	76	1,56	-	1/19/37/38	0/4/4/4
58	7MG	BY	46	58	-	5/7/37/38	0/3/3/3
57	5MU	BX	54	57,60	-	0/7/25/26	0/2/2/2
57	5MU	DX	54	57	-	0/7/25/26	0/2/2/2
58	PSU	DY	32	58	-	0/7/25/26	0/2/2/2
57	4SU	BX	8	57	-	0/7/25/26	0/2/2/2
56	MIA	BW	37	56	-	3/15/33/34	0/3/3/3
58	MIA	BY	37	58	-	2/7/25/34	0/3/3/3
58	PSU	BY	32	58	-	0/7/25/26	0/2/2/2
56	PSU	DW	32	56	-	0/7/25/26	0/2/2/2
57	PSU	BX	55	57	-	0/7/25/26	0/2/2/2
57	5MC	BX	32	57	-	0/7/25/26	0/2/2/2
56	4SU	BW	8	56	-	0/7/25/26	0/2/2/2
58	5MU	BY	54	58	-	1/7/25/26	0/2/2/2
57	4SU	DX	8	57	-	0/7/25/26	0/2/2/2
56	PSU	BW	32	60,56	-	0/7/25/26	0/2/2/2
58	PSU	BY	39	58	-	0/7/25/26	0/2/2/2
56	PSU	BW	39	56	-	0/7/25/26	0/2/2/2
57	31H	BX	76	57,60	-	8/22/40/41	0/3/3/3
58	4SU	BY	8	58	-	1/7/25/26	0/2/2/2
56	7MG	BW	46	56	-	3/7/37/38	0/3/3/3

The worst 5 of 138 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	BW	37	MIA	C2-S10	-7.77	1.69	1.75
57	DX	32	5MC	C5-C4	7.07	1.49	1.44
56	BW	37	MIA	C13-C14	7.05	1.53	1.32
58	BY	37	MIA	C5-C4	5.28	1.48	1.39
57	DX	8	4SU	C4-S4	-5.11	1.59	1.68

The worst 5 of 239 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	DY	46	7MG	N9-C4-N3	9.87	139.93	125.46
58	BY	46	7MG	N9-C4-N3	9.18	138.92	125.46
56	BW	37	MIA	C12-C13-C14	-9.10	110.68	127.01
56	BW	46	7MG	N9-C4-N3	8.72	138.23	125.46
56	DW	46	7MG	N9-C4-N3	8.45	137.84	125.46

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	BW	37	MIA	N1-C2-S10-C11
56	BW	37	MIA	N3-C2-S10-C11
56	BW	37	MIA	C12-C13-C14-C16
57	BX	76	31H	C4'-C5'-O5'-P
57	BX	76	31H	C-CA-CB-CG

There are no ring outliers.

21 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	BW	55	PSU	1	0
56	DW	37	MIA	1	0
58	DY	8	4SU	1	0
57	DX	55	PSU	1	0
58	DY	37	MIA	2	0
58	DY	39	PSU	1	0
56	DW	55	PSU	1	0
56	DW	54	5MU	1	0
58	DY	55	PSU	2	0
56	DW	76	F3N	4	0
57	DX	76	31H	3	0
56	DW	46	7MG	2	0
56	BW	76	F3N	2	0
56	DW	32	PSU	1	0
57	BX	55	PSU	1	0
57	BX	32	5MC	1	0
56	BW	8	4SU	1	0
57	DX	8	4SU	1	0
58	BY	39	PSU	1	0
56	BW	39	PSU	1	0
58	BY	8	4SU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2073 ligands modelled in this entry, 2069 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
63	SF4	DD	501	37	0,12,12	-	-	-		
63	SF4	BD	501	37	0,12,12	-	-	-		
64	GDP	BZ	702	60	29,30,30	1.29	2 (6%)	45,47,47	1.82	7 (15%)
64	GDP	DZ	702	60	29,30,30	1.19	3 (10%)	45,47,47	1.72	8 (17%)

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
63	SF4	DD	501	37	-	-	0/6/5/5
63	SF4	BD	501	37	-	-	0/6/5/5
64	GDP	BZ	702	60	-	0/16/32/32	0/3/3/3
64	GDP	DZ	702	60	-	2/16/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	BZ	702	GDP	C5-C4	3.21	1.47	1.38
64	BZ	702	GDP	C5-N7	-3.20	1.32	1.39
64	DZ	702	GDP	C5-C4	3.07	1.47	1.38
64	DZ	702	GDP	C6-N1	-2.90	1.33	1.38
64	DZ	702	GDP	C5-N7	-2.27	1.34	1.39

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	BZ	702	GDP	C5-C4-N3	-6.13	118.64	128.39
64	DZ	702	GDP	C5-C4-N3	-5.78	119.18	128.39
64	BZ	702	GDP	N9-C4-N3	4.88	135.71	125.95
64	BZ	702	GDP	C2-N3-C4	4.49	120.04	112.30
64	DZ	702	GDP	N9-C4-N3	4.43	134.80	125.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

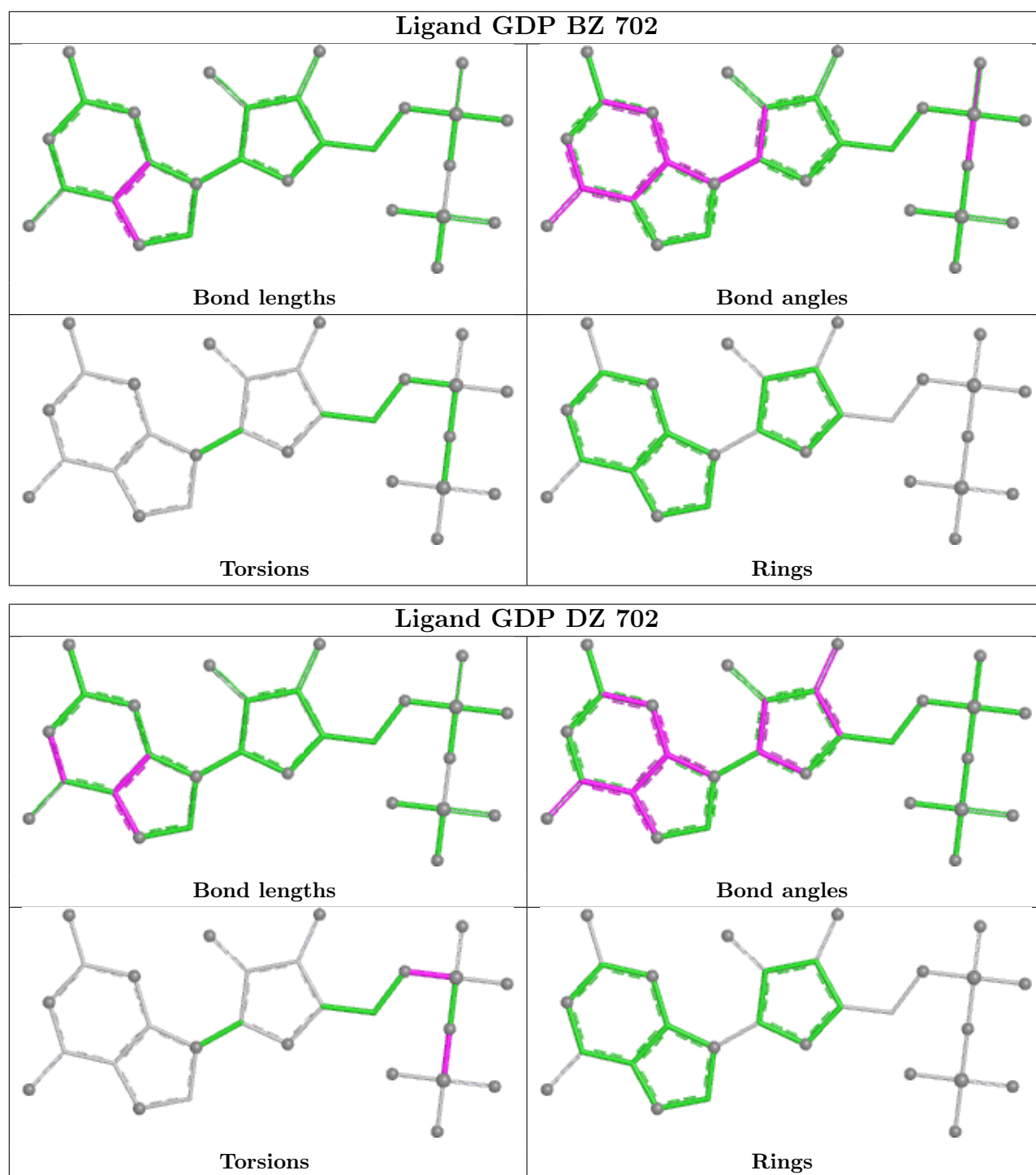
Mol	Chain	Res	Type	Atoms
64	DZ	702	GDP	PA-O3A-PB-O2B
64	DZ	702	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	DD	501	SF4	1	0
63	BD	501	SF4	1	0
64	BZ	702	GDP	7	0
64	DZ	702	GDP	7	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	AA	2872/2915 (98%)	-0.78	32 (1%) 78 70	16, 35, 152, 288	0
1	CA	2868/2915 (98%)	-0.35	79 (2%) 55 45	24, 53, 186, 314	0
2	AB	120/121 (99%)	-0.55	0 100 100	26, 52, 70, 110	0
2	CB	120/121 (99%)	0.32	1 (0%) 82 75	54, 86, 109, 176	0
3	AC	137/228 (60%)	2.51	91 (66%) 0 0	95, 162, 210, 232	0
3	CC	137/228 (60%)	2.57	90 (65%) 0 0	115, 183, 225, 239	0
4	AD	275/276 (99%)	-0.53	4 (1%) 72 63	16, 35, 58, 111	0
4	CD	275/276 (99%)	-0.17	6 (2%) 62 52	18, 45, 72, 141	0
5	AE	204/206 (99%)	-0.56	0 100 100	8, 35, 66, 99	0
5	CE	204/206 (99%)	-0.14	2 (0%) 79 72	24, 52, 86, 135	0
6	AF	203/210 (96%)	-0.41	1 (0%) 87 82	11, 36, 88, 173	0
6	CF	203/210 (96%)	0.08	3 (1%) 72 63	22, 62, 112, 162	0
7	AG	181/182 (99%)	0.34	5 (2%) 55 45	41, 71, 109, 177	0
7	CG	181/182 (99%)	0.95	18 (9%) 13 9	73, 105, 142, 189	0
8	AH	174/180 (96%)	-0.09	4 (2%) 61 51	30, 51, 79, 171	0
8	CH	174/180 (96%)	0.85	12 (6%) 23 16	44, 93, 139, 208	0
9	AK	130/173 (75%)	1.86	47 (36%) 1 0	62, 123, 186, 226	0
9	CK	130/173 (75%)	2.42	77 (59%) 0 0	103, 170, 203, 226	0
10	AL	66/147 (44%)	2.03	29 (43%) 0 0	133, 179, 216, 233	0
10	CL	66/147 (44%)	2.47	41 (62%) 0 0	115, 192, 239, 248	0
11	AN	140/140 (100%)	-0.51	2 (1%) 73 64	17, 34, 76, 106	0
11	CN	140/140 (100%)	0.13	4 (2%) 53 43	32, 59, 96, 139	0
12	AO	122/122 (100%)	-0.44	0 100 100	20, 39, 65, 93	0
12	CO	122/122 (100%)	-0.15	0 100 100	32, 51, 82, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AP	149/150 (99%)	-0.32	1 (0%) 84 77	14, 43, 81, 123	0
13	CP	149/150 (99%)	0.26	4 (2%) 56 46	29, 65, 111, 154	0
14	AQ	141/141 (100%)	-0.29	0 100 100	16, 39, 66, 96	0
14	CQ	141/141 (100%)	0.29	5 (3%) 47 38	32, 61, 91, 155	0
15	AR	118/118 (100%)	-0.64	0 100 100	17, 32, 55, 95	0
15	CR	118/118 (100%)	-0.02	1 (0%) 82 75	27, 51, 76, 96	0
16	AS	110/112 (98%)	-0.13	1 (0%) 81 74	32, 53, 79, 101	0
16	CS	110/112 (98%)	0.88	9 (8%) 17 13	52, 82, 110, 143	0
17	AT	131/146 (89%)	-0.07	6 (4%) 37 29	23, 43, 93, 159	0
17	CT	131/146 (89%)	0.11	4 (3%) 51 41	36, 57, 98, 155	0
18	AU	116/118 (98%)	-0.73	1 (0%) 81 74	15, 27, 46, 110	0
18	CU	116/118 (98%)	0.07	2 (1%) 69 60	35, 51, 81, 123	0
19	AV	101/101 (100%)	-0.73	1 (0%) 79 72	18, 34, 60, 117	0
19	CV	101/101 (100%)	0.19	3 (2%) 52 42	32, 72, 106, 137	0
20	AW	112/113 (99%)	-0.61	1 (0%) 81 74	15, 29, 55, 133	0
20	CW	112/113 (99%)	-0.11	2 (1%) 67 58	26, 47, 85, 148	0
21	AX	95/96 (98%)	-0.36	2 (2%) 63 54	22, 38, 68, 123	0
21	CX	95/96 (98%)	0.34	4 (4%) 40 32	39, 60, 92, 134	0
22	AY	107/110 (97%)	-0.06	3 (2%) 55 45	25, 47, 92, 125	0
22	CY	107/110 (97%)	0.76	11 (10%) 12 9	43, 78, 113, 169	0
23	AZ	171/206 (83%)	0.57	22 (12%) 7 6	32, 72, 142, 228	0
23	CZ	174/206 (84%)	1.15	22 (12%) 8 6	59, 106, 172, 238	0
24	A0	83/85 (97%)	-0.24	4 (4%) 35 28	16, 38, 66, 145	0
24	C0	83/85 (97%)	0.55	7 (8%) 17 12	36, 62, 94, 133	0
25	A1	97/98 (98%)	-0.17	2 (2%) 63 54	23, 43, 83, 106	0
25	C1	97/98 (98%)	0.22	3 (3%) 51 41	32, 52, 104, 118	0
26	A2	70/72 (97%)	0.06	4 (5%) 29 22	21, 46, 74, 148	0
26	C2	70/72 (97%)	0.64	4 (5%) 29 22	51, 77, 98, 119	0
27	A3	59/60 (98%)	-0.29	1 (1%) 69 60	17, 33, 62, 112	0
27	C3	59/60 (98%)	0.33	2 (3%) 48 39	42, 61, 105, 167	0
28	A4	69/71 (97%)	0.77	9 (13%) 7 6	59, 99, 181, 193	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	C4	69/71 (97%)	1.42	16 (23%) 2 1	87, 137, 192, 210	0
29	A5	59/60 (98%)	-0.76	0 100 100	14, 29, 52, 82	0
29	C5	59/60 (98%)	-0.29	0 100 100	28, 46, 76, 111	0
30	A6	53/54 (98%)	-0.31	1 (1%) 66 57	24, 41, 65, 88	0
30	C6	53/54 (98%)	0.24	1 (1%) 66 57	42, 61, 86, 102	0
31	A7	48/49 (97%)	-0.42	3 (6%) 26 19	13, 25, 62, 124	0
31	C7	48/49 (97%)	0.03	5 (10%) 11 8	25, 37, 80, 105	0
32	A8	64/65 (98%)	-0.49	1 (1%) 70 61	17, 31, 46, 68	0
32	C8	64/65 (98%)	0.06	3 (4%) 36 29	35, 51, 69, 100	0
33	A9	37/37 (100%)	-0.24	1 (2%) 56 46	23, 38, 58, 77	0
33	C9	37/37 (100%)	0.46	3 (8%) 18 13	41, 65, 95, 107	0
34	BA	1497/1521 (98%)	0.12	29 (1%) 66 57	31, 74, 166, 297	0
34	DA	1503/1521 (98%)	0.29	49 (3%) 49 39	39, 82, 173, 313	0
35	BB	231/256 (90%)	1.16	35 (15%) 5 4	61, 108, 165, 196	0
35	DB	231/256 (90%)	1.37	50 (21%) 2 2	77, 128, 182, 226	0
36	BC	206/239 (86%)	1.01	26 (12%) 8 6	59, 102, 137, 192	0
36	DC	206/239 (86%)	1.43	45 (21%) 2 2	77, 125, 169, 191	0
37	BD	208/209 (99%)	0.99	26 (12%) 8 6	50, 81, 119, 168	0
37	DD	208/209 (99%)	0.79	12 (5%) 29 22	46, 79, 111, 161	0
38	BE	148/162 (91%)	0.42	3 (2%) 65 56	47, 72, 109, 140	0
38	DE	148/162 (91%)	0.84	11 (7%) 20 15	45, 88, 128, 150	0
39	BF	100/101 (99%)	0.48	1 (1%) 79 72	45, 79, 116, 136	0
39	DF	100/101 (99%)	0.36	1 (1%) 79 72	48, 79, 103, 120	0
40	BG	155/156 (99%)	0.71	12 (7%) 19 14	57, 88, 131, 172	0
40	DG	155/156 (99%)	0.96	21 (13%) 7 5	66, 102, 142, 188	0
41	BH	137/138 (99%)	0.58	3 (2%) 62 52	44, 75, 105, 134	0
41	DH	137/138 (99%)	1.01	18 (13%) 7 6	54, 88, 126, 168	0
42	BI	127/128 (99%)	1.36	23 (18%) 3 3	50, 101, 139, 163	0
42	DI	127/128 (99%)	1.89	55 (43%) 0 0	65, 117, 158, 198	0
43	BJ	97/105 (92%)	1.73	32 (32%) 1 1	52, 112, 158, 196	0
43	DJ	96/105 (91%)	1.96	40 (41%) 0 0	68, 134, 177, 188	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BK	114/129 (88%)	0.30	5 (4%) 39 31	44, 71, 112, 128	0
44	DK	114/129 (88%)	0.46	9 (7%) 18 13	43, 80, 117, 139	0
45	BL	122/132 (92%)	0.29	4 (3%) 49 39	37, 62, 86, 113	0
45	DL	122/132 (92%)	0.64	9 (7%) 20 15	36, 72, 94, 141	0
46	BM	123/126 (97%)	1.13	12 (9%) 13 9	54, 94, 127, 213	0
46	DM	122/126 (96%)	1.68	35 (28%) 1 1	71, 124, 152, 187	0
47	BN	60/61 (98%)	1.50	15 (25%) 2 1	64, 94, 121, 137	0
47	DN	60/61 (98%)	2.64	43 (71%) 0 0	84, 121, 166, 201	0
48	BO	88/89 (98%)	0.43	4 (4%) 38 30	38, 67, 110, 141	0
48	DO	88/89 (98%)	0.57	3 (3%) 48 39	43, 76, 111, 127	0
49	BP	82/88 (93%)	0.95	8 (9%) 13 9	53, 75, 108, 131	0
49	DP	82/88 (93%)	0.59	3 (3%) 45 36	52, 70, 95, 129	0
50	BQ	99/105 (94%)	0.48	4 (4%) 42 33	42, 69, 96, 110	0
50	DQ	99/105 (94%)	0.57	6 (6%) 27 20	50, 74, 103, 123	0
51	BR	68/88 (77%)	0.39	0 100 100	47, 72, 111, 132	0
51	DR	68/88 (77%)	0.55	2 (2%) 53 43	45, 78, 114, 133	0
52	BS	84/93 (90%)	1.54	24 (28%) 1 1	64, 109, 161, 176	0
52	DS	83/93 (89%)	2.07	37 (44%) 0 0	89, 140, 184, 227	0
53	BT	96/106 (90%)	0.88	14 (14%) 6 4	52, 76, 114, 167	0
53	DT	96/106 (90%)	0.81	10 (10%) 11 8	51, 76, 116, 132	0
54	BU	23/27 (85%)	1.44	7 (30%) 1 1	56, 88, 104, 114	0
54	DU	23/27 (85%)	2.11	11 (47%) 0 0	78, 108, 129, 141	0
55	BV	13/24 (54%)	1.50	6 (46%) 0 0	48, 85, 170, 176	0
55	DV	12/24 (50%)	1.96	5 (41%) 0 0	62, 119, 169, 197	0
56	BW	66/76 (86%)	1.02	7 (10%) 11 8	62, 166, 228, 253	0
56	DW	64/76 (84%)	1.22	7 (10%) 10 8	90, 194, 235, 259	0
57	BX	71/77 (92%)	0.12	1 (1%) 73 64	33, 76, 123, 186	0
57	DX	71/77 (92%)	0.39	2 (2%) 55 45	33, 99, 147, 161	0
58	BY	67/76 (88%)	0.79	8 (11%) 9 7	38, 157, 221, 262	0
58	DY	66/76 (86%)	0.91	9 (13%) 7 5	56, 177, 227, 250	0
59	BZ	728/758 (96%)	1.04	99 (13%) 7 5	40, 106, 190, 249	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
59	DZ	730/758 (96%)	1.09	123 (16%) 4 3	37, 114, 209, 242	0
All	All	22848/24064 (94%)	0.24	1747 (7%) 20 14	8, 67, 175, 314	0

The worst 5 of 1747 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
46	BM	124	PRO	14.9
46	BM	123	ALA	9.3
47	DN	2	ALA	8.4
46	DM	122	LYS	8.3
46	DM	123	ALA	7.6

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	PSU	DY	55	20/21	0.30	0.19	222,222,222,222	0
56	7MG	DW	46	24/25	0.32	0.14	244,244,244,244	0
56	7MG	BW	46	24/25	0.40	0.14	203,203,203,203	0
56	PSU	DW	55	20/21	0.43	0.16	190,190,190,190	0
56	4SU	DW	8	20/21	0.43	0.13	225,225,225,225	0
58	5MU	BY	54	21/22	0.46	0.16	217,217,217,217	0
58	7MG	BY	46	24/25	0.52	0.12	200,200,200,200	0
56	4SU	BW	8	20/21	0.52	0.12	200,200,200,200	0
58	PSU	BY	55	20/21	0.53	0.13	205,205,205,205	0
58	5MU	DY	54	21/22	0.56	0.17	200,200,200,200	0
58	7MG	DY	46	24/25	0.57	0.13	206,206,206,206	0
58	4SU	BY	8	20/21	0.66	0.11	191,191,191,191	0
58	MIA	DY	37	22/30	0.68	0.18	156,156,156,156	0
58	PSU	DY	39	20/21	0.71	0.14	138,138,138,138	0
58	PSU	DY	32	20/21	0.71	0.13	154,154,154,154	0
58	MIA	BY	37	22/30	0.74	0.14	118,118,118,118	0
58	4SU	DY	8	20/21	0.74	0.11	193,193,193,193	0
56	PSU	BW	55	20/21	0.76	0.13	113,113,113,113	0
58	PSU	BY	32	20/21	0.76	0.12	126,126,126,126	0
56	PSU	DW	32	20/21	0.79	0.15	139,139,139,139	0
56	PSU	BW	39	20/21	0.81	0.13	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MIA	DW	37	22/30	0.82	0.12	116,116,116,116	0
58	PSU	BY	39	20/21	0.83	0.12	106,106,106,106	0
56	MIA	BW	37	29/30	0.83	0.17	95,95,95,95	1
56	PSU	DW	39	20/21	0.84	0.10	118,118,118,118	0
56	5MU	BW	54	21/22	0.84	0.13	89,89,89,89	0
56	5MU	DW	54	21/22	0.85	0.11	118,118,118,118	0
57	31H	DX	76	32/33	0.86	0.23	58,58,58,58	4
56	PSU	BW	32	20/21	0.86	0.13	110,110,110,110	0
57	5MU	BX	54	21/22	0.88	0.11	85,85,85,85	0
57	PSU	DX	55	20/21	0.88	0.09	95,95,95,95	0
57	5MU	DX	54	21/22	0.89	0.11	108,108,108,108	0
56	F3N	DW	76	33/34	0.90	0.19	75,75,75,75	1
57	5MC	DX	32	21/22	0.90	0.12	86,86,86,86	0
57	4SU	BX	8	20/21	0.90	0.10	70,70,70,70	1
57	4SU	DX	8	20/21	0.91	0.09	96,96,96,96	0
57	PSU	BX	55	20/21	0.92	0.08	74,74,74,74	0
57	31H	BX	76	32/33	0.93	0.15	58,58,58,58	4
57	5MC	BX	32	21/22	0.93	0.11	65,65,65,65	0
56	F3N	BW	76	33/34	0.96	0.12	54,54,54,54	1

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
60	MG	DA	1686	1/1	0.15	0.17	102,102,102,102	0
60	MG	CA	3543	1/1	0.25	0.14	114,114,114,114	0
60	MG	AA	3770	1/1	0.36	0.86	57,57,57,57	1
60	MG	AA	3040	1/1	0.40	0.27	93,93,93,93	0
60	MG	CB	3008	1/1	0.44	0.29	87,87,87,87	0
60	MG	AA	3108	1/1	0.45	0.40	88,88,88,88	0
60	MG	CA	3631	1/1	0.45	0.24	88,88,88,88	0
60	MG	AA	3490	1/1	0.46	0.25	87,87,87,87	0
60	MG	BA	1709	1/1	0.49	0.25	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CA	3136	1/1	0.49	0.25	112,112,112,112	0
60	MG	CA	3550	1/1	0.51	0.20	88,88,88,88	0
60	MG	CA	3491	1/1	0.51	0.21	99,99,99,99	0
60	MG	CA	3619	1/1	0.55	0.22	78,78,78,78	0
60	MG	CA	3622	1/1	0.56	0.24	106,106,106,106	0
60	MG	CA	3616	1/1	0.56	0.25	62,62,62,62	0
60	MG	AA	3203	1/1	0.57	0.54	125,125,125,125	0
60	MG	CA	3506	1/1	0.57	0.23	120,120,120,120	0
60	MG	CA	3597	1/1	0.57	0.26	108,108,108,108	0
60	MG	BX	112	1/1	0.58	0.21	78,78,78,78	0
60	MG	CA	3575	1/1	0.58	0.20	77,77,77,77	0
60	MG	CA	3079	1/1	0.58	0.27	82,82,82,82	0
60	MG	DA	1739	1/1	0.58	0.25	85,85,85,85	0
60	MG	BA	1712	1/1	0.59	0.36	68,68,68,68	0
60	MG	CA	3664	1/1	0.59	0.24	69,69,69,69	0
60	MG	AA	3225	1/1	0.59	0.38	91,91,91,91	0
60	MG	CA	3482	1/1	0.59	0.15	89,89,89,89	0
60	MG	CA	3042	1/1	0.59	0.48	84,84,84,84	0
60	MG	CA	3073	1/1	0.61	0.19	94,94,94,94	0
60	MG	AA	3773	1/1	0.61	0.21	77,77,77,77	0
60	MG	CA	3592	1/1	0.63	0.21	87,87,87,87	0
60	MG	BK	3101	1/1	0.63	0.27	95,95,95,95	0
60	MG	AA	3438	1/1	0.63	0.20	75,75,75,75	0
60	MG	AA	3613	1/1	0.63	0.26	96,96,96,96	0
60	MG	BA	1779	1/1	0.63	0.20	82,82,82,82	0
60	MG	CA	3101	1/1	0.64	0.20	86,86,86,86	0
60	MG	BA	1691	1/1	0.64	0.27	98,98,98,98	0
60	MG	CA	3177	1/1	0.64	0.32	98,98,98,98	0
60	MG	CA	3388	1/1	0.64	0.12	97,97,97,97	0
60	MG	DA	1715	1/1	0.64	0.24	87,87,87,87	0
60	MG	BA	1706	1/1	0.64	0.22	82,82,82,82	0
60	MG	BW	101	1/1	0.65	0.25	82,82,82,82	0
60	MG	AD	307	1/1	0.66	0.36	108,108,108,108	0
60	MG	AA	3689	1/1	0.66	0.16	84,84,84,84	0
60	MG	AA	3739	1/1	0.66	0.31	90,90,90,90	0
60	MG	DA	1767	1/1	0.66	0.28	88,88,88,88	0
60	MG	CA	3481	1/1	0.67	0.18	86,86,86,86	0
60	MG	AA	3805	1/1	0.67	0.43	117,117,117,117	0
60	MG	CA	3614	1/1	0.67	0.21	79,79,79,79	0
60	MG	CA	3643	1/1	0.67	0.35	83,83,83,83	0
60	MG	CA	3524	1/1	0.67	0.24	87,87,87,87	0
60	MG	BL	201	1/1	0.68	0.10	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	DA	1671	1/1	0.68	0.40	77,77,77,77	0
60	MG	DA	1753	1/1	0.68	0.19	85,85,85,85	0
60	MG	CA	3122	1/1	0.68	0.51	95,95,95,95	0
60	MG	AA	3744	1/1	0.69	0.20	79,79,79,79	0
60	MG	CA	3206	1/1	0.69	0.29	109,109,109,109	0
60	MG	CA	3293	1/1	0.69	0.14	82,82,82,82	0
60	MG	AA	3578	1/1	0.69	0.23	71,71,71,71	0
60	MG	BA	1800	1/1	0.70	0.42	116,116,116,116	0
60	MG	AA	3783	1/1	0.70	0.22	68,68,68,68	0
60	MG	AA	3271	1/1	0.70	0.36	81,81,81,81	0
60	MG	DA	1651	1/1	0.70	0.43	86,86,86,86	0
60	MG	CA	3063	1/1	0.70	0.33	74,74,74,74	0
60	MG	BA	1740	1/1	0.71	0.13	89,89,89,89	0
60	MG	BA	1674	1/1	0.71	0.25	78,78,78,78	0
60	MG	AA	3183	1/1	0.71	0.45	89,89,89,89	0
60	MG	AA	3136	1/1	0.71	0.19	74,74,74,74	0
60	MG	AA	3221	1/1	0.71	0.26	72,72,72,72	0
60	MG	AA	3648	1/1	0.71	0.17	80,80,80,80	0
60	MG	CQ	201	1/1	0.71	0.29	85,85,85,85	0
60	MG	DX	3001	1/1	0.71	0.31	75,75,75,75	0
60	MG	AA	3098	1/1	0.72	0.27	65,65,65,65	0
60	MG	BA	1703	1/1	0.72	0.19	65,65,65,65	0
60	MG	BA	1786	1/1	0.72	0.38	79,79,79,79	0
60	MG	AA	3440	1/1	0.72	0.20	63,63,63,63	0
60	MG	AA	3582	1/1	0.72	0.25	78,78,78,78	0
60	MG	CA	3244	1/1	0.72	0.22	70,70,70,70	0
60	MG	AA	3725	1/1	0.72	0.16	42,42,42,42	0
60	MG	CA	3091	1/1	0.73	0.20	60,60,60,60	0
60	MG	CA	3478	1/1	0.73	0.21	91,91,91,91	0
60	MG	DA	1640	1/1	0.73	0.26	73,73,73,73	0
60	MG	AA	3688	1/1	0.73	0.16	76,76,76,76	0
60	MG	BA	1609	1/1	0.73	0.17	77,77,77,77	0
60	MG	BA	1638	1/1	0.73	0.31	83,83,83,83	0
60	MG	AA	3646	1/1	0.73	0.32	82,82,82,82	0
60	MG	DA	1738	1/1	0.73	0.25	100,100,100,100	0
60	MG	CA	3511	1/1	0.73	0.28	66,66,66,66	0
60	MG	AA	3710	1/1	0.73	0.14	55,55,55,55	0
60	MG	AA	3200	1/1	0.73	0.20	73,73,73,73	0
60	MG	AA	3654	1/1	0.73	0.23	81,81,81,81	0
60	MG	CE	304	1/1	0.74	0.38	74,74,74,74	0
60	MG	CA	3138	1/1	0.74	0.18	67,67,67,67	0
60	MG	DA	1626	1/1	0.74	0.34	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	1656	1/1	0.74	0.24	83,83,83,83	0
60	MG	BA	1790	1/1	0.74	0.20	87,87,87,87	0
60	MG	CA	3220	1/1	0.74	0.42	89,89,89,89	0
60	MG	CA	3094	1/1	0.74	0.33	92,92,92,92	0
60	MG	DA	1712	1/1	0.74	0.14	67,67,67,67	0
60	MG	BA	1715	1/1	0.74	0.19	90,90,90,90	0
60	MG	CA	3348	1/1	0.74	0.12	78,78,78,78	0
60	MG	AA	3026	1/1	0.74	0.17	69,69,69,69	0
60	MG	CA	3646	1/1	0.74	0.12	90,90,90,90	0
60	MG	A8	5001	1/1	0.74	0.21	66,66,66,66	0
60	MG	CA	3581	1/1	0.74	0.23	100,100,100,100	0
60	MG	AA	3489	1/1	0.75	0.20	39,39,39,39	0
60	MG	CA	3588	1/1	0.75	0.12	78,78,78,78	0
60	MG	AA	3163	1/1	0.75	0.16	73,73,73,73	0
60	MG	A0	104	1/1	0.75	0.31	81,81,81,81	0
60	MG	CA	3068	1/1	0.75	0.25	73,73,73,73	0
60	MG	AA	3329	1/1	0.75	0.23	82,82,82,82	0
60	MG	CA	3209	1/1	0.75	0.39	101,101,101,101	0
60	MG	AA	3204	1/1	0.75	0.36	83,83,83,83	0
60	MG	CA	3234	1/1	0.75	0.21	96,96,96,96	0
60	MG	DA	1719	1/1	0.75	0.20	87,87,87,87	0
60	MG	AA	3246	1/1	0.75	0.19	86,86,86,86	0
60	MG	AA	3625	1/1	0.75	0.32	88,88,88,88	0
60	MG	CA	3573	1/1	0.75	0.13	82,82,82,82	0
60	MG	BA	1722	1/1	0.75	0.17	86,86,86,86	0
60	MG	CB	3013	1/1	0.75	0.18	90,90,90,90	0
60	MG	DA	1704	1/1	0.76	0.21	83,83,83,83	0
60	MG	BX	103	1/1	0.76	0.15	88,88,88,88	0
60	MG	CA	3067	1/1	0.76	0.27	82,82,82,82	0
60	MG	CA	3542	1/1	0.76	0.18	82,82,82,82	0
60	MG	DA	1632	1/1	0.76	0.23	77,77,77,77	0
60	MG	AA	3201	1/1	0.76	0.24	71,71,71,71	0
60	MG	CA	3485	1/1	0.76	0.22	76,76,76,76	0
60	MG	CA	3376	1/1	0.76	0.21	94,94,94,94	0
60	MG	DE	201	1/1	0.76	0.36	93,93,93,93	0
60	MG	BA	1624	1/1	0.76	0.24	75,75,75,75	0
60	MG	DA	1615	1/1	0.77	0.29	87,87,87,87	0
60	MG	CA	3053	1/1	0.77	0.24	71,71,71,71	0
60	MG	AA	3579	1/1	0.77	0.14	66,66,66,66	0
60	MG	CA	3608	1/1	0.77	0.15	69,69,69,69	0
60	MG	AA	3027	1/1	0.77	0.48	85,85,85,85	0
60	MG	BA	1803	1/1	0.77	0.16	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3631	1/1	0.77	0.25	74,74,74,74	0
60	MG	BA	1610	1/1	0.77	0.13	112,112,112,112	0
60	MG	CA	3535	1/1	0.77	0.17	74,74,74,74	0
60	MG	CA	3250	1/1	0.77	0.18	69,69,69,69	0
60	MG	BA	1774	1/1	0.77	0.12	79,79,79,79	0
60	MG	AA	3664	1/1	0.77	0.23	94,94,94,94	0
60	MG	AA	3638	1/1	0.77	0.18	72,72,72,72	0
60	MG	CB	3010	1/1	0.77	0.16	67,67,67,67	0
60	MG	DA	1765	1/1	0.77	0.14	66,66,66,66	0
60	MG	CA	3007	1/1	0.77	0.23	75,75,75,75	0
60	MG	CA	3011	1/1	0.77	0.19	75,75,75,75	0
60	MG	BA	1788	1/1	0.77	0.12	79,79,79,79	0
60	MG	AA	3419	1/1	0.78	0.22	88,88,88,88	0
60	MG	CA	3194	1/1	0.78	0.38	87,87,87,87	0
60	MG	CA	3462	1/1	0.78	0.27	63,63,63,63	0
60	MG	CA	3545	1/1	0.78	0.12	93,93,93,93	0
60	MG	CA	3642	1/1	0.78	0.09	75,75,75,75	0
60	MG	BA	1605	1/1	0.78	0.15	76,76,76,76	0
60	MG	AZ	5001	1/1	0.78	0.12	67,67,67,67	0
60	MG	BA	1804	1/1	0.78	0.31	94,94,94,94	0
60	MG	CA	3484	1/1	0.78	0.21	56,56,56,56	0
60	MG	CA	3584	1/1	0.78	0.14	91,91,91,91	0
60	MG	CA	3022	1/1	0.78	0.38	76,76,76,76	0
60	MG	DA	1751	1/1	0.78	0.17	84,84,84,84	0
60	MG	BA	1670	1/1	0.78	0.19	76,76,76,76	0
60	MG	BA	1671	1/1	0.78	0.26	71,71,71,71	0
60	MG	DA	1604	1/1	0.78	0.14	90,90,90,90	0
60	MG	AA	3728	1/1	0.78	0.21	75,75,75,75	0
60	MG	DW	3001	1/1	0.78	0.15	90,90,90,90	0
60	MG	BW	102	1/1	0.78	0.16	75,75,75,75	0
60	MG	CA	3312	1/1	0.79	0.16	52,52,52,52	0
60	MG	CA	3532	1/1	0.79	0.16	59,59,59,59	0
60	MG	AA	3763	1/1	0.79	0.20	66,66,66,66	0
60	MG	AA	3765	1/1	0.79	0.11	62,62,62,62	0
60	MG	CA	3635	1/1	0.79	0.27	77,77,77,77	0
60	MG	CA	3387	1/1	0.79	0.25	73,73,73,73	0
60	MG	BY	3002	1/1	0.79	0.11	83,83,83,83	0
60	MG	CA	3183	1/1	0.79	0.28	83,83,83,83	0
60	MG	DA	1718	1/1	0.79	0.12	66,66,66,66	0
60	MG	CA	3653	1/1	0.79	0.35	102,102,102,102	0
60	MG	CA	3070	1/1	0.79	0.16	78,78,78,78	0
60	MG	AB	3022	1/1	0.79	0.14	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	DA	1749	1/1	0.79	0.24	72,72,72,72	0
60	MG	AA	3766	1/1	0.79	0.17	69,69,69,69	0
60	MG	AA	3245	1/1	0.79	0.34	79,79,79,79	0
60	MG	CA	3031	1/1	0.79	0.42	102,102,102,102	0
60	MG	CA	3095	1/1	0.79	0.19	92,92,92,92	0
60	MG	CA	3505	1/1	0.79	0.15	66,66,66,66	0
60	MG	AA	3736	1/1	0.79	0.19	74,74,74,74	0
60	MG	BX	102	1/1	0.79	0.13	78,78,78,78	0
60	MG	AA	3342	1/1	0.80	0.17	77,77,77,77	0
60	MG	DA	1607	1/1	0.80	0.35	63,63,63,63	0
60	MG	DA	1608	1/1	0.80	0.42	79,79,79,79	0
60	MG	CA	3464	1/1	0.80	0.34	78,78,78,78	0
60	MG	AB	3004	1/1	0.80	0.27	69,69,69,69	0
60	MG	CA	3591	1/1	0.80	0.13	69,69,69,69	0
60	MG	CA	3202	1/1	0.80	0.17	67,67,67,67	0
60	MG	CA	3086	1/1	0.80	0.15	65,65,65,65	0
60	MG	DA	1657	1/1	0.80	0.15	75,75,75,75	0
60	MG	AA	3630	1/1	0.80	0.22	66,66,66,66	0
60	MG	AA	3692	1/1	0.80	0.36	86,86,86,86	0
60	MG	CA	3057	1/1	0.80	0.33	77,77,77,77	0
60	MG	AN	3001	1/1	0.80	0.16	64,64,64,64	0
60	MG	CA	3111	1/1	0.80	0.28	82,82,82,82	0
60	MG	CA	3267	1/1	0.80	0.25	110,110,110,110	0
60	MG	CA	3521	1/1	0.80	0.20	59,59,59,59	0
60	MG	CA	3281	1/1	0.80	0.19	74,74,74,74	0
60	MG	CA	3527	1/1	0.80	0.19	83,83,83,83	0
60	MG	CA	3064	1/1	0.80	0.19	72,72,72,72	0
60	MG	BA	1808	1/1	0.80	0.16	80,80,80,80	0
60	MG	AA	3263	1/1	0.80	0.20	75,75,75,75	0
60	MG	CA	3361	1/1	0.80	0.12	70,70,70,70	0
60	MG	CA	3139	1/1	0.80	0.27	83,83,83,83	0
60	MG	CA	3386	1/1	0.80	0.15	79,79,79,79	0
60	MG	CA	3142	1/1	0.80	0.12	73,73,73,73	0
60	MG	AA	3621	1/1	0.80	0.10	34,34,34,34	0
60	MG	AA	3320	1/1	0.81	0.18	65,65,65,65	0
60	MG	BA	1767	1/1	0.81	0.16	73,73,73,73	0
60	MG	CA	3265	1/1	0.81	0.23	66,66,66,66	0
60	MG	CA	3497	1/1	0.81	0.21	85,85,85,85	0
60	MG	CA	3598	1/1	0.81	0.15	66,66,66,66	0
60	MG	AA	3777	1/1	0.81	0.11	58,58,58,58	0
60	MG	BA	1776	1/1	0.81	0.10	64,64,64,64	0
60	MG	CA	3507	1/1	0.81	0.22	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3157	1/1	0.81	0.35	93,93,93,93	0
60	MG	AA	3487	1/1	0.81	0.17	66,66,66,66	0
60	MG	CA	3152	1/1	0.81	0.11	67,67,67,67	0
60	MG	CA	3155	1/1	0.81	0.28	69,69,69,69	0
60	MG	AA	3753	1/1	0.81	0.15	59,59,59,59	0
60	MG	AA	3604	1/1	0.81	0.14	44,44,44,44	1
60	MG	AA	3210	1/1	0.81	0.40	106,106,106,106	0
60	MG	DA	1730	1/1	0.81	0.18	65,65,65,65	0
60	MG	DA	1734	1/1	0.81	0.26	75,75,75,75	0
60	MG	AA	3615	1/1	0.81	0.10	65,65,65,65	0
60	MG	CA	3658	1/1	0.81	0.24	62,62,62,62	0
60	MG	DA	1741	1/1	0.81	0.18	81,81,81,81	0
60	MG	CA	3661	1/1	0.81	0.15	78,78,78,78	0
60	MG	BA	1717	1/1	0.81	0.14	77,77,77,77	0
60	MG	AA	3291	1/1	0.81	0.18	84,84,84,84	0
60	MG	DA	1764	1/1	0.81	0.13	94,94,94,94	0
60	MG	CA	3572	1/1	0.81	0.15	82,82,82,82	0
60	MG	CA	3475	1/1	0.81	0.13	55,55,55,55	0
60	MG	CA	3212	1/1	0.81	0.24	78,78,78,78	0
60	MG	CA	3097	1/1	0.81	0.23	79,79,79,79	0
60	MG	BA	1737	1/1	0.81	0.09	87,87,87,87	0
60	MG	AA	3265	1/1	0.82	0.33	64,64,64,64	0
60	MG	CA	3081	1/1	0.82	0.25	69,69,69,69	0
60	MG	CA	3235	1/1	0.82	0.31	78,78,78,78	0
60	MG	BA	1657	1/1	0.82	0.32	72,72,72,72	0
60	MG	CA	3467	1/1	0.82	0.29	99,99,99,99	0
60	MG	CA	3529	1/1	0.82	0.23	69,69,69,69	0
60	MG	CA	3055	1/1	0.82	0.22	77,77,77,77	0
60	MG	AA	3802	1/1	0.82	0.12	55,55,55,55	0
60	MG	AA	3462	1/1	0.82	0.14	73,73,73,73	0
60	MG	AA	3694	1/1	0.82	0.10	49,49,49,49	0
60	MG	DA	1748	1/1	0.82	0.17	78,78,78,78	0
60	MG	DA	1611	1/1	0.82	0.12	80,80,80,80	0
60	MG	CA	3483	1/1	0.82	0.13	67,67,67,67	0
60	MG	BA	1719	1/1	0.82	0.17	75,75,75,75	0
60	MG	CA	3199	1/1	0.82	0.40	92,92,92,92	0
60	MG	BA	1633	1/1	0.82	0.27	65,65,65,65	0
60	MG	CA	3121	1/1	0.82	0.31	78,78,78,78	0
60	MG	CA	3648	1/1	0.82	0.23	78,78,78,78	0
60	MG	CA	3030	1/1	0.82	0.23	52,52,52,52	0
60	MG	AA	3109	1/1	0.82	0.17	75,75,75,75	0
60	MG	BA	1784	1/1	0.83	0.11	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CQ	203	1/1	0.83	0.20	62,62,62,62	0
60	MG	AA	3458	1/1	0.83	0.15	79,79,79,79	0
60	MG	AA	3764	1/1	0.83	0.23	48,48,48,48	0
60	MG	AA	3599	1/1	0.83	0.33	113,113,113,113	0
60	MG	CA	3410	1/1	0.83	0.17	72,72,72,72	0
60	MG	AA	3231	1/1	0.83	0.35	87,87,87,87	0
60	MG	BA	1696	1/1	0.83	0.12	84,84,84,84	0
60	MG	AA	3713	1/1	0.83	0.20	48,48,48,48	0
60	MG	A5	102	1/1	0.83	0.29	89,89,89,89	0
60	MG	CA	3195	1/1	0.83	0.10	36,36,36,36	0
60	MG	AA	3337	1/1	0.83	0.16	52,52,52,52	0
60	MG	DA	1658	1/1	0.83	0.18	89,89,89,89	0
60	MG	BA	1603	1/1	0.83	0.27	65,65,65,65	0
60	MG	DA	1673	1/1	0.83	0.21	68,68,68,68	0
60	MG	CA	3611	1/1	0.83	0.18	64,64,64,64	0
60	MG	AA	3268	1/1	0.83	0.14	80,80,80,80	0
60	MG	AA	3655	1/1	0.83	0.12	55,55,55,55	0
60	MG	CA	3618	1/1	0.83	0.16	79,79,79,79	0
60	MG	AA	3789	1/1	0.83	0.18	71,71,71,71	0
60	MG	AA	3793	1/1	0.83	0.29	76,76,76,76	0
60	MG	CA	3225	1/1	0.83	0.26	73,73,73,73	0
60	MG	CA	3092	1/1	0.83	0.26	74,74,74,74	0
60	MG	BX	105	1/1	0.83	0.14	87,87,87,87	0
60	MG	CA	3243	1/1	0.83	0.26	55,55,55,55	0
60	MG	BA	1630	1/1	0.83	0.10	61,61,61,61	0
60	MG	CA	3096	1/1	0.83	0.29	75,75,75,75	0
60	MG	AA	3121	1/1	0.83	0.19	63,63,63,63	0
60	MG	DA	1750	1/1	0.83	0.28	86,86,86,86	0
60	MG	BA	1755	1/1	0.83	0.11	92,92,92,92	0
60	MG	CA	3103	1/1	0.83	0.19	80,80,80,80	0
60	MG	CA	3283	1/1	0.83	0.15	57,57,57,57	0
60	MG	AA	3067	1/1	0.83	0.38	82,82,82,82	0
60	MG	BA	1646	1/1	0.83	0.37	71,71,71,71	0
60	MG	AA	3105	1/1	0.83	0.21	77,77,77,77	0
60	MG	AB	3021	1/1	0.83	0.14	75,75,75,75	0
60	MG	CF	303	1/1	0.83	0.14	63,63,63,63	0
60	MG	AB	3019	1/1	0.84	0.13	61,61,61,61	0
60	MG	BA	1809	1/1	0.84	0.13	74,74,74,74	0
60	MG	CA	3371	1/1	0.84	0.38	70,70,70,70	0
60	MG	BA	1629	1/1	0.84	0.20	71,71,71,71	0
60	MG	CA	3377	1/1	0.84	0.09	53,53,53,53	0
60	MG	AA	3705	1/1	0.84	0.24	29,29,29,29	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CA	3187	1/1	0.84	0.16	70,70,70,70	0
60	MG	AA	3036	1/1	0.84	0.16	63,63,63,63	0
60	MG	DA	1614	1/1	0.84	0.17	71,71,71,71	0
60	MG	CA	3393	1/1	0.84	0.21	47,47,47,47	0
60	MG	CA	3583	1/1	0.84	0.34	114,114,114,114	0
60	MG	DA	1629	1/1	0.84	0.35	79,79,79,79	0
60	MG	BA	1636	1/1	0.84	0.23	66,66,66,66	0
60	MG	CA	3442	1/1	0.84	0.19	70,70,70,70	0
60	MG	DA	1648	1/1	0.84	0.22	66,66,66,66	0
60	MG	CA	3457	1/1	0.84	0.12	60,60,60,60	0
60	MG	AA	3651	1/1	0.84	0.15	66,66,66,66	0
60	MG	AD	310	1/1	0.84	0.16	58,58,58,58	0
60	MG	CA	3089	1/1	0.84	0.39	78,78,78,78	0
60	MG	BA	1762	1/1	0.84	0.12	57,57,57,57	0
60	MG	DA	1676	1/1	0.84	0.20	69,69,69,69	0
60	MG	AA	3575	1/1	0.84	0.13	63,63,63,63	0
60	MG	CA	3613	1/1	0.84	0.18	42,42,42,42	0
60	MG	AQ	3002	1/1	0.84	0.15	79,79,79,79	0
60	MG	AX	101	1/1	0.84	0.22	78,78,78,78	0
60	MG	CA	3226	1/1	0.84	0.24	56,56,56,56	0
60	MG	AA	3450	1/1	0.84	0.13	71,71,71,71	0
60	MG	DA	1722	1/1	0.84	0.13	69,69,69,69	0
60	MG	CA	3016	1/1	0.84	0.38	69,69,69,69	0
60	MG	CA	3488	1/1	0.84	0.09	58,58,58,58	0
60	MG	AA	3002	1/1	0.84	0.17	53,53,53,53	0
60	MG	AA	3351	1/1	0.84	0.13	80,80,80,80	0
60	MG	BA	1787	1/1	0.84	0.16	64,64,64,64	0
60	MG	DA	1743	1/1	0.84	0.11	83,83,83,83	0
60	MG	CA	3645	1/1	0.84	0.11	78,78,78,78	0
60	MG	AA	3243	1/1	0.84	0.37	79,79,79,79	0
60	MG	AA	3600	1/1	0.84	0.14	70,70,70,70	0
60	MG	AA	3016	1/1	0.84	0.15	44,44,44,44	0
60	MG	CA	3519	1/1	0.84	0.18	68,68,68,68	0
60	MG	CA	3659	1/1	0.84	0.19	72,72,72,72	0
60	MG	CA	3056	1/1	0.84	0.28	83,83,83,83	0
60	MG	AA	3702	1/1	0.84	0.22	45,45,45,45	1
60	MG	AB	3014	1/1	0.84	0.14	70,70,70,70	0
60	MG	CA	3329	1/1	0.84	0.17	59,59,59,59	0
60	MG	CA	3342	1/1	0.84	0.14	84,84,84,84	0
60	MG	AA	3127	1/1	0.85	0.31	83,83,83,83	0
60	MG	CA	3043	1/1	0.85	0.19	75,75,75,75	0
60	MG	BA	1687	1/1	0.85	0.26	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CA	3534	1/1	0.85	0.13	58,58,58,58	0
60	MG	CA	3366	1/1	0.85	0.23	60,60,60,60	0
60	MG	CA	3540	1/1	0.85	0.17	71,71,71,71	0
60	MG	AA	3639	1/1	0.85	0.19	74,74,74,74	0
60	MG	CA	3373	1/1	0.85	0.24	71,71,71,71	0
60	MG	AA	3640	1/1	0.85	0.24	74,74,74,74	0
60	MG	BA	1699	1/1	0.85	0.24	70,70,70,70	0
60	MG	CA	3552	1/1	0.85	0.09	60,60,60,60	0
60	MG	CA	3181	1/1	0.85	0.18	68,68,68,68	0
60	MG	BA	1799	1/1	0.85	0.09	69,69,69,69	0
60	MG	DA	1620	1/1	0.85	0.16	68,68,68,68	0
60	MG	AA	3195	1/1	0.85	0.20	55,55,55,55	0
60	MG	BA	1704	1/1	0.85	0.20	68,68,68,68	0
60	MG	CA	3406	1/1	0.85	0.11	54,54,54,54	0
60	MG	AA	3592	1/1	0.85	0.21	67,67,67,67	0
60	MG	DA	1642	1/1	0.85	0.15	67,67,67,67	0
60	MG	CA	3587	1/1	0.85	0.17	72,72,72,72	0
60	MG	AA	3442	1/1	0.85	0.14	73,73,73,73	0
60	MG	AB	3006	1/1	0.85	0.21	84,84,84,84	0
60	MG	BA	1613	1/1	0.85	0.10	92,92,92,92	0
60	MG	AA	3324	1/1	0.85	0.11	69,69,69,69	0
60	MG	AA	3238	1/1	0.85	0.17	68,68,68,68	0
60	MG	CA	3605	1/1	0.85	0.19	72,72,72,72	0
60	MG	CA	3607	1/1	0.85	0.19	76,76,76,76	0
60	MG	DA	1695	1/1	0.85	0.17	79,79,79,79	0
60	MG	DA	1699	1/1	0.85	0.14	79,79,79,79	0
60	MG	AA	3755	1/1	0.85	0.20	77,77,77,77	0
60	MG	BA	1732	1/1	0.85	0.19	65,65,65,65	0
60	MG	BA	1736	1/1	0.85	0.15	66,66,66,66	0
60	MG	AA	3612	1/1	0.85	0.15	60,60,60,60	0
60	MG	AA	3070	1/1	0.85	0.19	68,68,68,68	0
60	MG	CA	3238	1/1	0.85	0.13	73,73,73,73	0
60	MG	DA	1729	1/1	0.85	0.15	82,82,82,82	0
60	MG	BX	113	1/1	0.85	0.07	78,78,78,78	0
60	MG	AA	3270	1/1	0.85	0.33	92,92,92,92	0
60	MG	CA	3623	1/1	0.85	0.21	71,71,71,71	0
60	MG	CA	3629	1/1	0.85	0.16	74,74,74,74	0
60	MG	CA	3098	1/1	0.85	0.33	90,90,90,90	0
60	MG	BA	1760	1/1	0.85	0.16	68,68,68,68	0
60	MG	CA	3498	1/1	0.85	0.24	68,68,68,68	0
60	MG	CA	3503	1/1	0.85	0.09	67,67,67,67	0
60	MG	AE	304	1/1	0.85	0.17	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CA	3275	1/1	0.85	0.14	73,73,73,73	0
60	MG	AA	3173	1/1	0.85	0.28	74,74,74,74	0
60	MG	AA	3353	1/1	0.85	0.15	68,68,68,68	0
60	MG	CA	3515	1/1	0.85	0.15	72,72,72,72	0
60	MG	AA	3362	1/1	0.85	0.16	69,69,69,69	0
60	MG	CA	3132	1/1	0.85	0.22	67,67,67,67	0
60	MG	AA	3283	1/1	0.85	0.20	48,48,48,48	0
60	MG	CB	3006	1/1	0.85	0.17	82,82,82,82	0
60	MG	BA	1697	1/1	0.86	0.17	80,80,80,80	0
60	MG	CA	3644	1/1	0.86	0.12	60,60,60,60	0
60	MG	CA	3204	1/1	0.86	0.28	88,88,88,88	0
60	MG	A4	502	1/1	0.86	0.07	81,81,81,81	0
60	MG	AA	3559	1/1	0.86	0.12	37,37,37,37	0
60	MG	BA	1806	1/1	0.86	0.12	63,63,63,63	0
60	MG	CA	3077	1/1	0.86	0.12	62,62,62,62	0
60	MG	BA	1807	1/1	0.86	0.20	72,72,72,72	0
60	MG	AA	3671	1/1	0.86	0.23	31,31,31,31	1
60	MG	CA	3083	1/1	0.86	0.29	80,80,80,80	0
60	MG	CA	3085	1/1	0.86	0.29	82,82,82,82	0
60	MG	CA	3237	1/1	0.86	0.24	70,70,70,70	0
60	MG	AB	3005	1/1	0.86	0.18	70,70,70,70	0
60	MG	CB	3012	1/1	0.86	0.14	74,74,74,74	0
60	MG	CA	3516	1/1	0.86	0.17	58,58,58,58	0
60	MG	AA	3247	1/1	0.86	0.22	75,75,75,75	0
60	MG	CA	3090	1/1	0.86	0.28	98,98,98,98	0
60	MG	AA	3248	1/1	0.86	0.25	79,79,79,79	0
60	MG	AB	3017	1/1	0.86	0.12	76,76,76,76	0
60	MG	AA	3460	1/1	0.86	0.26	81,81,81,81	0
60	MG	BA	1615	1/1	0.86	0.12	65,65,65,65	0
60	MG	BA	1622	1/1	0.86	0.22	64,64,64,64	0
60	MG	DA	1610	1/1	0.86	0.28	59,59,59,59	0
60	MG	BA	1623	1/1	0.86	0.21	67,67,67,67	0
60	MG	CA	3538	1/1	0.86	0.22	58,58,58,58	0
60	MG	CA	3539	1/1	0.86	0.16	72,72,72,72	0
60	MG	AA	3435	1/1	0.86	0.14	54,54,54,54	0
60	MG	CA	3311	1/1	0.86	0.14	54,54,54,54	0
60	MG	AA	3017	1/1	0.86	0.17	71,71,71,71	0
60	MG	AD	306	1/1	0.86	0.20	75,75,75,75	0
60	MG	DA	1636	1/1	0.86	0.30	77,77,77,77	0
60	MG	BA	1748	1/1	0.86	0.17	75,75,75,75	0
60	MG	CA	3113	1/1	0.86	0.41	75,75,75,75	0
60	MG	CA	3553	1/1	0.86	0.17	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CA	3560	1/1	0.86	0.15	103,103,103,103	0
60	MG	CA	3355	1/1	0.86	0.11	71,71,71,71	0
60	MG	CA	3114	1/1	0.86	0.15	59,59,59,59	0
60	MG	DA	1659	1/1	0.86	0.25	79,79,79,79	0
60	MG	DA	1668	1/1	0.86	0.14	68,68,68,68	0
60	MG	AA	3352	1/1	0.86	0.18	64,64,64,64	0
60	MG	CA	3576	1/1	0.86	0.22	91,91,91,91	0
60	MG	AD	308	1/1	0.86	0.10	54,54,54,54	0
60	MG	DA	1677	1/1	0.86	0.19	67,67,67,67	0
60	MG	CA	3582	1/1	0.86	0.10	60,60,60,60	0
60	MG	CA	3123	1/1	0.86	0.16	63,63,63,63	0
60	MG	CA	3129	1/1	0.86	0.13	76,76,76,76	0
60	MG	DA	1701	1/1	0.86	0.15	61,61,61,61	0
60	MG	CA	3021	1/1	0.86	0.34	91,91,91,91	0
60	MG	AA	3708	1/1	0.86	0.21	71,71,71,71	0
60	MG	DA	1713	1/1	0.86	0.11	59,59,59,59	0
60	MG	AE	301	1/1	0.86	0.17	65,65,65,65	0
60	MG	BA	1651	1/1	0.86	0.11	69,69,69,69	0
60	MG	CA	3032	1/1	0.86	0.31	67,67,67,67	0
60	MG	CA	3398	1/1	0.86	0.14	57,57,57,57	0
60	MG	CA	3601	1/1	0.86	0.22	61,61,61,61	0
60	MG	AA	3063	1/1	0.86	0.09	46,46,46,46	0
60	MG	CA	3409	1/1	0.86	0.21	63,63,63,63	0
60	MG	AH	201	1/1	0.86	0.29	83,83,83,83	0
60	MG	CA	3428	1/1	0.86	0.20	50,50,50,50	0
60	MG	CA	3162	1/1	0.86	0.26	57,57,57,57	0
60	MG	CA	3169	1/1	0.86	0.21	65,65,65,65	0
60	MG	CA	3173	1/1	0.86	0.26	72,72,72,72	0
60	MG	AA	3495	1/1	0.86	0.23	58,58,58,58	0
60	MG	AA	3517	1/1	0.86	0.19	44,44,44,44	0
60	MG	CA	3474	1/1	0.86	0.18	72,72,72,72	0
60	MG	AA	3530	1/1	0.86	0.11	60,60,60,60	0
60	MG	DA	1759	1/1	0.86	0.24	64,64,64,64	0
60	MG	CA	3624	1/1	0.86	0.25	76,76,76,76	0
60	MG	CA	3626	1/1	0.86	0.08	52,52,52,52	0
60	MG	AA	3732	1/1	0.86	0.14	63,63,63,63	0
60	MG	A0	101	1/1	0.86	0.15	88,88,88,88	0
60	MG	AA	3541	1/1	0.86	0.14	61,61,61,61	0
60	MG	CA	3066	1/1	0.86	0.36	69,69,69,69	0
60	MG	CA	3282	1/1	0.87	0.26	75,75,75,75	0
60	MG	AA	3066	1/1	0.87	0.17	63,63,63,63	0
60	MG	CA	3291	1/1	0.87	0.09	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CA	3523	1/1	0.87	0.10	77,77,77,77	0
60	MG	AA	3164	1/1	0.87	0.28	106,106,106,106	0
60	MG	CA	3308	1/1	0.87	0.11	35,35,35,35	0
60	MG	AA	3046	1/1	0.87	0.19	47,47,47,47	0
60	MG	CA	3531	1/1	0.87	0.10	67,67,67,67	0
60	MG	AA	3605	1/1	0.87	0.09	66,66,66,66	0
60	MG	CD	301	1/1	0.87	0.15	61,61,61,61	0
60	MG	CA	3321	1/1	0.87	0.11	65,65,65,65	0
60	MG	CF	301	1/1	0.87	0.19	61,61,61,61	0
60	MG	BA	1614	1/1	0.87	0.20	70,70,70,70	0
60	MG	CA	3131	1/1	0.87	0.13	61,61,61,61	0
60	MG	AA	3181	1/1	0.87	0.14	55,55,55,55	0
60	MG	BA	1743	1/1	0.87	0.10	60,60,60,60	0
60	MG	AA	3479	1/1	0.87	0.09	66,66,66,66	0
60	MG	CA	3365	1/1	0.87	0.16	69,69,69,69	0
60	MG	CA	3544	1/1	0.87	0.19	74,74,74,74	0
60	MG	AA	3614	1/1	0.87	0.09	66,66,66,66	0
60	MG	BA	1757	1/1	0.87	0.18	63,63,63,63	0
60	MG	AA	3251	1/1	0.87	0.16	50,50,50,50	0
60	MG	AA	3347	1/1	0.87	0.20	63,63,63,63	0
60	MG	DA	1623	1/1	0.87	0.30	70,70,70,70	0
60	MG	BA	1766	1/1	0.87	0.16	81,81,81,81	0
60	MG	AA	3624	1/1	0.87	0.13	56,56,56,56	0
60	MG	AA	3182	1/1	0.87	0.21	73,73,73,73	0
60	MG	AA	3010	1/1	0.87	0.18	68,68,68,68	0
60	MG	AA	3266	1/1	0.87	0.17	55,55,55,55	0
60	MG	CA	3578	1/1	0.87	0.10	96,96,96,96	0
60	MG	BA	1645	1/1	0.87	0.27	58,58,58,58	0
60	MG	AA	3360	1/1	0.87	0.23	72,72,72,72	0
60	MG	AA	3738	1/1	0.87	0.10	73,73,73,73	0
60	MG	BA	1653	1/1	0.87	0.18	62,62,62,62	0
60	MG	CA	3412	1/1	0.87	0.14	52,52,52,52	0
60	MG	AA	3222	1/1	0.87	0.15	58,58,58,58	0
60	MG	CA	3429	1/1	0.87	0.19	80,80,80,80	0
60	MG	DA	1672	1/1	0.87	0.19	61,61,61,61	0
60	MG	CA	3201	1/1	0.87	0.18	70,70,70,70	0
60	MG	CA	3445	1/1	0.87	0.19	70,70,70,70	0
60	MG	AA	3740	1/1	0.87	0.17	54,54,54,54	0
60	MG	DA	1678	1/1	0.87	0.29	66,66,66,66	0
60	MG	DA	1684	1/1	0.87	0.21	54,54,54,54	0
60	MG	BA	1666	1/1	0.87	0.27	70,70,70,70	0
60	MG	DA	1689	1/1	0.87	0.11	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CA	3603	1/1	0.87	0.30	93,93,93,93	0
60	MG	AA	3551	1/1	0.87	0.12	58,58,58,58	0
60	MG	AE	302	1/1	0.87	0.14	62,62,62,62	0
60	MG	AA	3747	1/1	0.87	0.16	65,65,65,65	0
60	MG	AA	3644	1/1	0.87	0.17	74,74,74,74	0
60	MG	AA	3380	1/1	0.87	0.19	75,75,75,75	0
60	MG	AA	3756	1/1	0.87	0.12	57,57,57,57	0
60	MG	DA	1717	1/1	0.87	0.18	70,70,70,70	0
60	MG	AA	3269	1/1	0.87	0.14	78,78,78,78	0
60	MG	CA	3617	1/1	0.87	0.12	41,41,41,41	0
60	MG	AA	3650	1/1	0.87	0.17	62,62,62,62	0
60	MG	DA	1724	1/1	0.87	0.22	74,74,74,74	0
60	MG	CA	3236	1/1	0.87	0.24	80,80,80,80	0
60	MG	AA	3186	1/1	0.87	0.21	53,53,53,53	0
60	MG	AA	3652	1/1	0.87	0.20	87,87,87,87	0
60	MG	DA	1735	1/1	0.87	0.18	75,75,75,75	0
60	MG	DA	1737	1/1	0.87	0.15	73,73,73,73	0
60	MG	CA	3239	1/1	0.87	0.23	76,76,76,76	0
60	MG	CA	3496	1/1	0.87	0.24	58,58,58,58	0
60	MG	BA	1705	1/1	0.87	0.16	61,61,61,61	0
60	MG	AA	3192	1/1	0.87	0.33	69,69,69,69	0
60	MG	CA	3633	1/1	0.87	0.14	85,85,85,85	0
60	MG	CA	3500	1/1	0.87	0.25	56,56,56,56	0
60	MG	CA	3638	1/1	0.87	0.27	68,68,68,68	0
60	MG	CA	3502	1/1	0.87	0.10	66,66,66,66	0
60	MG	DA	1752	1/1	0.87	0.24	73,73,73,73	0
60	MG	AA	3089	1/1	0.87	0.17	58,58,58,58	0
60	MG	AA	3199	1/1	0.87	0.24	61,61,61,61	0
60	MG	CA	3108	1/1	0.87	0.16	84,84,84,84	0
60	MG	BA	1602	1/1	0.87	0.15	75,75,75,75	0
60	MG	CA	3647	1/1	0.87	0.24	61,61,61,61	0
60	MG	DD	502	1/1	0.87	0.23	64,64,64,64	0
60	MG	CA	3280	1/1	0.87	0.10	43,43,43,43	0
60	MG	DT	3001	1/1	0.87	0.17	59,59,59,59	0
60	MG	AA	3778	1/1	0.87	0.12	68,68,68,68	0
60	MG	CA	3655	1/1	0.87	0.29	69,69,69,69	0
60	MG	CA	3249	1/1	0.88	0.17	67,67,67,67	0
60	MG	BE	3001	1/1	0.88	0.09	83,83,83,83	0
60	MG	CB	3007	1/1	0.88	0.16	57,57,57,57	0
60	MG	CA	3255	1/1	0.88	0.25	61,61,61,61	0
60	MG	CA	3261	1/1	0.88	0.12	50,50,50,50	0
60	MG	AA	3696	1/1	0.88	0.12	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3598	1/1	0.88	0.18	57,57,57,57	0
60	MG	CA	3270	1/1	0.88	0.23	69,69,69,69	0
60	MG	BL	202	1/1	0.88	0.10	56,56,56,56	0
60	MG	BV	101	1/1	0.88	0.12	78,78,78,78	0
60	MG	AA	3285	1/1	0.88	0.11	72,72,72,72	0
60	MG	CF	306	1/1	0.88	0.26	85,85,85,85	0
60	MG	BA	1626	1/1	0.88	0.14	72,72,72,72	0
60	MG	BX	101	1/1	0.88	0.16	63,63,63,63	0
60	MG	CR	201	1/1	0.88	0.16	63,63,63,63	0
60	MG	CA	3284	1/1	0.88	0.15	49,49,49,49	0
60	MG	DA	1605	1/1	0.88	0.21	59,59,59,59	0
60	MG	AA	3159	1/1	0.88	0.23	66,66,66,66	0
60	MG	CA	3536	1/1	0.88	0.15	95,95,95,95	0
60	MG	CA	3292	1/1	0.88	0.12	56,56,56,56	0
60	MG	AA	3317	1/1	0.88	0.14	56,56,56,56	0
60	MG	AF	307	1/1	0.88	0.16	69,69,69,69	0
60	MG	BX	106	1/1	0.88	0.14	85,85,85,85	0
60	MG	AA	3511	1/1	0.88	0.21	84,84,84,84	0
60	MG	AA	3715	1/1	0.88	0.11	62,62,62,62	0
60	MG	DA	1624	1/1	0.88	0.14	83,83,83,83	0
60	MG	BX	114	1/1	0.88	0.25	57,57,57,57	0
60	MG	DA	1628	1/1	0.88	0.21	69,69,69,69	0
60	MG	CA	3333	1/1	0.88	0.18	64,64,64,64	0
60	MG	BY	3001	1/1	0.88	0.14	78,78,78,78	0
60	MG	AA	3782	1/1	0.88	0.16	70,70,70,70	0
60	MG	CA	3555	1/1	0.88	0.08	59,59,59,59	0
60	MG	CA	3135	1/1	0.88	0.09	73,73,73,73	0
60	MG	CA	3569	1/1	0.88	0.18	71,71,71,71	0
60	MG	DA	1649	1/1	0.88	0.18	53,53,53,53	0
60	MG	CA	3001	1/1	0.88	0.13	81,81,81,81	0
60	MG	DA	1656	1/1	0.88	0.10	67,67,67,67	0
60	MG	AA	3724	1/1	0.88	0.14	37,37,37,37	0
60	MG	AA	3611	1/1	0.88	0.23	57,57,57,57	0
60	MG	CA	3015	1/1	0.88	0.23	66,66,66,66	0
60	MG	DA	1664	1/1	0.88	0.24	49,49,49,49	0
60	MG	DA	1667	1/1	0.88	0.37	70,70,70,70	0
60	MG	CA	3150	1/1	0.88	0.11	52,52,52,52	0
60	MG	CA	3374	1/1	0.88	0.10	74,74,74,74	0
60	MG	BA	1754	1/1	0.88	0.09	75,75,75,75	0
60	MG	AA	3137	1/1	0.88	0.23	55,55,55,55	0
60	MG	AA	3447	1/1	0.88	0.12	44,44,44,44	0
60	MG	CA	3163	1/1	0.88	0.17	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	1758	1/1	0.88	0.13	56,56,56,56	0
60	MG	DA	1679	1/1	0.88	0.17	70,70,70,70	0
60	MG	AA	3249	1/1	0.88	0.16	64,64,64,64	0
60	MG	CA	3394	1/1	0.88	0.10	54,54,54,54	0
60	MG	CA	3595	1/1	0.88	0.20	67,67,67,67	0
60	MG	CA	3397	1/1	0.88	0.12	80,80,80,80	0
60	MG	CA	3176	1/1	0.88	0.24	60,60,60,60	0
60	MG	BA	1659	1/1	0.88	0.31	68,68,68,68	0
60	MG	CA	3407	1/1	0.88	0.14	41,41,41,41	0
60	MG	BA	1763	1/1	0.88	0.10	75,75,75,75	0
60	MG	BA	1660	1/1	0.88	0.26	55,55,55,55	0
60	MG	BA	1661	1/1	0.88	0.21	59,59,59,59	0
60	MG	CA	3610	1/1	0.88	0.32	94,94,94,94	0
60	MG	CA	3190	1/1	0.88	0.16	77,77,77,77	0
60	MG	AA	3093	1/1	0.88	0.38	81,81,81,81	0
60	MG	DA	1721	1/1	0.88	0.15	60,60,60,60	0
60	MG	CA	3440	1/1	0.88	0.24	69,69,69,69	0
60	MG	AA	3656	1/1	0.88	0.13	62,62,62,62	1
60	MG	DA	1727	1/1	0.88	0.15	65,65,65,65	0
60	MG	BA	1777	1/1	0.88	0.12	76,76,76,76	0
60	MG	CA	3200	1/1	0.88	0.11	65,65,65,65	0
60	MG	BA	1601	1/1	0.88	0.09	66,66,66,66	0
60	MG	BA	1781	1/1	0.88	0.11	63,63,63,63	0
60	MG	DA	1736	1/1	0.88	0.14	63,63,63,63	0
60	MG	AA	3657	1/1	0.88	0.15	73,73,73,73	0
60	MG	CA	3205	1/1	0.88	0.17	66,66,66,66	0
60	MG	BA	1681	1/1	0.88	0.23	69,69,69,69	0
60	MG	AA	3365	1/1	0.88	0.18	55,55,55,55	0
60	MG	BA	1688	1/1	0.88	0.24	71,71,71,71	0
60	MG	CA	3213	1/1	0.88	0.12	62,62,62,62	0
60	MG	BA	1604	1/1	0.88	0.26	85,85,85,85	0
60	MG	AA	3158	1/1	0.88	0.26	50,50,50,50	0
60	MG	BA	1606	1/1	0.88	0.14	74,74,74,74	0
60	MG	AA	3474	1/1	0.88	0.13	74,74,74,74	0
60	MG	CA	3489	1/1	0.88	0.11	64,64,64,64	0
60	MG	BA	1702	1/1	0.88	0.26	56,56,56,56	0
60	MG	BA	1805	1/1	0.88	0.09	55,55,55,55	0
60	MG	AA	3412	1/1	0.88	0.08	58,58,58,58	0
60	MG	AA	3486	1/1	0.88	0.11	34,34,34,34	0
60	MG	AA	3759	1/1	0.88	0.08	29,29,29,29	0
60	MG	CA	3240	1/1	0.88	0.09	49,49,49,49	0
60	MG	AA	3175	1/1	0.88	0.19	50,50,50,50	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	1813	1/1	0.88	0.10	66,66,66,66	0
60	MG	CA	3246	1/1	0.88	0.17	79,79,79,79	0
60	MG	CO	201	1/1	0.89	0.19	72,72,72,72	0
60	MG	AA	3449	1/1	0.89	0.13	46,46,46,46	0
60	MG	CA	3050	1/1	0.89	0.18	55,55,55,55	0
60	MG	AA	3589	1/1	0.89	0.23	31,31,31,31	1
60	MG	C5	101	1/1	0.89	0.20	64,64,64,64	0
60	MG	CA	3548	1/1	0.89	0.11	53,53,53,53	0
60	MG	AP	203	1/1	0.89	0.14	70,70,70,70	0
60	MG	AA	3336	1/1	0.89	0.14	52,52,52,52	0
60	MG	BA	1667	1/1	0.89	0.10	69,69,69,69	0
60	MG	BA	1669	1/1	0.89	0.21	70,70,70,70	0
60	MG	AA	3207	1/1	0.89	0.22	67,67,67,67	0
60	MG	AA	3208	1/1	0.89	0.13	55,55,55,55	0
60	MG	CA	3570	1/1	0.89	0.11	61,61,61,61	0
60	MG	BA	1673	1/1	0.89	0.32	63,63,63,63	0
60	MG	AA	3209	1/1	0.89	0.14	64,64,64,64	0
60	MG	AA	3772	1/1	0.89	0.25	37,37,37,37	0
60	MG	BA	1684	1/1	0.89	0.18	64,64,64,64	0
60	MG	AA	3051	1/1	0.89	0.39	84,84,84,84	0
60	MG	AA	3088	1/1	0.89	0.18	42,42,42,42	0
60	MG	BA	1690	1/1	0.89	0.19	59,59,59,59	0
60	MG	DA	1634	1/1	0.89	0.21	66,66,66,66	0
60	MG	AA	3609	1/1	0.89	0.14	57,57,57,57	0
60	MG	BA	1693	1/1	0.89	0.12	69,69,69,69	0
60	MG	CA	3411	1/1	0.89	0.11	49,49,49,49	0
60	MG	AA	3130	1/1	0.89	0.15	59,59,59,59	0
60	MG	CA	3589	1/1	0.89	0.14	67,67,67,67	0
60	MG	CA	3590	1/1	0.89	0.26	78,78,78,78	0
60	MG	AA	3161	1/1	0.89	0.38	89,89,89,89	0
60	MG	CA	3218	1/1	0.89	0.31	63,63,63,63	0
60	MG	CA	3593	1/1	0.89	0.13	62,62,62,62	0
60	MG	CA	3431	1/1	0.89	0.16	80,80,80,80	0
60	MG	DA	1661	1/1	0.89	0.21	74,74,74,74	0
60	MG	AA	3788	1/1	0.89	0.24	64,64,64,64	0
60	MG	BA	1700	1/1	0.89	0.20	62,62,62,62	0
60	MG	AA	3230	1/1	0.89	0.29	55,55,55,55	0
60	MG	CA	3228	1/1	0.89	0.32	68,68,68,68	0
60	MG	CA	3232	1/1	0.89	0.15	69,69,69,69	0
60	MG	CA	3093	1/1	0.89	0.21	77,77,77,77	0
60	MG	AA	3193	1/1	0.89	0.19	63,63,63,63	0
60	MG	AA	3795	1/1	0.89	0.15	26,26,26,26	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3800	1/1	0.89	0.16	59,59,59,59	0
60	MG	AA	3494	1/1	0.89	0.08	66,66,66,66	0
60	MG	DA	1682	1/1	0.89	0.24	60,60,60,60	0
60	MG	AA	3369	1/1	0.89	0.13	59,59,59,59	0
60	MG	AA	3816	1/1	0.89	0.18	49,49,49,49	0
60	MG	CA	3102	1/1	0.89	0.15	50,50,50,50	0
60	MG	AA	3056	1/1	0.89	0.27	72,72,72,72	0
60	MG	BA	1620	1/1	0.89	0.13	60,60,60,60	0
60	MG	CA	3487	1/1	0.89	0.12	64,64,64,64	0
60	MG	BA	1621	1/1	0.89	0.30	78,78,78,78	0
60	MG	DA	1710	1/1	0.89	0.12	56,56,56,56	0
60	MG	CA	3112	1/1	0.89	0.33	76,76,76,76	0
60	MG	AA	3516	1/1	0.89	0.16	38,38,38,38	0
60	MG	BA	1730	1/1	0.89	0.20	68,68,68,68	0
60	MG	CA	3118	1/1	0.89	0.12	67,67,67,67	0
60	MG	CA	3632	1/1	0.89	0.10	55,55,55,55	0
60	MG	CA	3119	1/1	0.89	0.22	63,63,63,63	0
60	MG	DA	1720	1/1	0.89	0.09	61,61,61,61	0
60	MG	AA	3242	1/1	0.89	0.15	69,69,69,69	0
60	MG	CA	3271	1/1	0.89	0.12	59,59,59,59	0
60	MG	AA	3525	1/1	0.89	0.15	45,45,45,45	0
60	MG	AA	3061	1/1	0.89	0.35	64,64,64,64	0
60	MG	CA	3124	1/1	0.89	0.29	68,68,68,68	0
60	MG	CA	3126	1/1	0.89	0.29	71,71,71,71	0
60	MG	AA	3537	1/1	0.89	0.10	90,90,90,90	0
60	MG	CA	3512	1/1	0.89	0.09	58,58,58,58	0
60	MG	AA	3165	1/1	0.89	0.23	64,64,64,64	0
60	MG	AA	3146	1/1	0.89	0.14	53,53,53,53	0
60	MG	CA	3517	1/1	0.89	0.16	75,75,75,75	0
60	MG	AA	3147	1/1	0.89	0.22	52,52,52,52	0
60	MG	AA	3743	1/1	0.89	0.11	66,66,66,66	0
60	MG	CA	3301	1/1	0.89	0.20	56,56,56,56	0
60	MG	DA	1747	1/1	0.89	0.10	67,67,67,67	0
60	MG	CA	3663	1/1	0.89	0.20	74,74,74,74	0
60	MG	CA	3302	1/1	0.89	0.09	67,67,67,67	0
60	MG	CB	3004	1/1	0.89	0.12	70,70,70,70	0
60	MG	AA	3568	1/1	0.89	0.10	23,23,23,23	0
60	MG	AA	3573	1/1	0.89	0.08	47,47,47,47	0
60	MG	BA	1647	1/1	0.89	0.10	57,57,57,57	0
60	MG	CA	3144	1/1	0.89	0.22	84,84,84,84	0
60	MG	DA	1762	1/1	0.89	0.10	86,86,86,86	0
60	MG	CA	3146	1/1	0.89	0.32	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CA	3029	1/1	0.89	0.19	68,68,68,68	0
60	MG	CA	3338	1/1	0.89	0.12	58,58,58,58	0
60	MG	CD	302	1/1	0.89	0.17	51,51,51,51	0
60	MG	AA	3752	1/1	0.89	0.18	75,75,75,75	0
60	MG	DJ	5001	1/1	0.89	0.11	94,94,94,94	0
60	MG	AA	3156	1/1	0.89	0.13	46,46,46,46	0
60	MG	AA	3444	1/1	0.89	0.09	52,52,52,52	0
60	MG	AA	3331	1/1	0.89	0.18	61,61,61,61	0
60	MG	CA	3033	1/1	0.90	0.08	47,47,47,47	0
60	MG	CA	3127	1/1	0.90	0.17	68,68,68,68	0
60	MG	CA	3039	1/1	0.90	0.27	76,76,76,76	0
60	MG	DA	1621	1/1	0.90	0.08	69,69,69,69	0
60	MG	AF	305	1/1	0.90	0.17	42,42,42,42	0
60	MG	BA	1789	1/1	0.90	0.08	68,68,68,68	0
60	MG	CA	3134	1/1	0.90	0.22	64,64,64,64	0
60	MG	CA	3049	1/1	0.90	0.18	63,63,63,63	0
60	MG	AA	3095	1/1	0.90	0.11	58,58,58,58	0
60	MG	DA	1631	1/1	0.90	0.16	55,55,55,55	0
60	MG	CA	3052	1/1	0.90	0.13	46,46,46,46	0
60	MG	BA	1793	1/1	0.90	0.08	68,68,68,68	0
60	MG	CA	3141	1/1	0.90	0.22	51,51,51,51	0
60	MG	CA	3486	1/1	0.90	0.08	48,48,48,48	0
60	MG	BA	1798	1/1	0.90	0.17	62,62,62,62	0
60	MG	DA	1646	1/1	0.90	0.20	51,51,51,51	0
60	MG	AA	3779	1/1	0.90	0.14	41,41,41,41	0
60	MG	CA	3145	1/1	0.90	0.22	65,65,65,65	0
60	MG	AA	3150	1/1	0.90	0.24	63,63,63,63	0
60	MG	CA	3492	1/1	0.90	0.18	60,60,60,60	0
60	MG	CA	3287	1/1	0.90	0.18	43,43,43,43	0
60	MG	CA	3059	1/1	0.90	0.27	66,66,66,66	0
60	MG	CA	3151	1/1	0.90	0.23	66,66,66,66	0
60	MG	AA	3073	1/1	0.90	0.20	61,61,61,61	0
60	MG	DA	1662	1/1	0.90	0.12	51,51,51,51	0
60	MG	CA	3501	1/1	0.90	0.14	78,78,78,78	0
60	MG	CA	3300	1/1	0.90	0.13	56,56,56,56	0
60	MG	AA	3279	1/1	0.90	0.28	62,62,62,62	0
60	MG	DA	1670	1/1	0.90	0.22	74,74,74,74	0
60	MG	AV	203	1/1	0.90	0.12	39,39,39,39	0
60	MG	BA	1710	1/1	0.90	0.21	83,83,83,83	0
60	MG	AA	3282	1/1	0.90	0.31	65,65,65,65	0
60	MG	CA	3630	1/1	0.90	0.15	91,91,91,91	0
60	MG	BA	1713	1/1	0.90	0.18	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3214	1/1	0.90	0.09	47,47,47,47	0
60	MG	CA	3514	1/1	0.90	0.10	68,68,68,68	0
60	MG	CA	3634	1/1	0.90	0.16	82,82,82,82	0
60	MG	CA	3074	1/1	0.90	0.17	64,64,64,64	0
60	MG	CA	3178	1/1	0.90	0.23	54,54,54,54	0
60	MG	CA	3639	1/1	0.90	0.18	54,54,54,54	0
60	MG	CA	3640	1/1	0.90	0.10	47,47,47,47	0
60	MG	DA	1696	1/1	0.90	0.19	65,65,65,65	0
60	MG	CA	3075	1/1	0.90	0.14	51,51,51,51	0
60	MG	DA	1700	1/1	0.90	0.19	66,66,66,66	0
60	MG	AA	3059	1/1	0.90	0.30	62,62,62,62	0
60	MG	AA	3055	1/1	0.90	0.16	61,61,61,61	0
60	MG	A2	3001	1/1	0.90	0.11	62,62,62,62	0
60	MG	BA	1723	1/1	0.90	0.13	61,61,61,61	0
60	MG	AA	3298	1/1	0.90	0.09	28,28,28,28	0
60	MG	AA	3372	1/1	0.90	0.17	59,59,59,59	0
60	MG	CA	3652	1/1	0.90	0.21	79,79,79,79	0
60	MG	AA	3300	1/1	0.90	0.11	43,43,43,43	0
60	MG	AA	3745	1/1	0.90	0.17	42,42,42,42	0
60	MG	AA	3403	1/1	0.90	0.09	55,55,55,55	0
60	MG	AA	3310	1/1	0.90	0.14	37,37,37,37	0
60	MG	CA	3660	1/1	0.90	0.13	65,65,65,65	0
60	MG	AA	3028	1/1	0.90	0.17	40,40,40,40	1
60	MG	CA	3662	1/1	0.90	0.20	60,60,60,60	0
60	MG	CA	3383	1/1	0.90	0.24	66,66,66,66	0
60	MG	AA	3672	1/1	0.90	0.18	71,71,71,71	0
60	MG	DA	1733	1/1	0.90	0.09	73,73,73,73	0
60	MG	CB	3001	1/1	0.90	0.16	68,68,68,68	0
60	MG	AA	3318	1/1	0.90	0.14	64,64,64,64	0
60	MG	BA	1672	1/1	0.90	0.19	61,61,61,61	0
60	MG	AA	3160	1/1	0.90	0.26	96,96,96,96	0
60	MG	AA	3254	1/1	0.90	0.16	47,47,47,47	0
60	MG	CA	3219	1/1	0.90	0.15	57,57,57,57	0
60	MG	BA	1675	1/1	0.90	0.15	50,50,50,50	0
60	MG	DA	1742	1/1	0.90	0.14	52,52,52,52	0
60	MG	AA	3618	1/1	0.90	0.09	39,39,39,39	0
60	MG	DA	1746	1/1	0.90	0.20	67,67,67,67	0
60	MG	BA	1765	1/1	0.90	0.24	67,67,67,67	0
60	MG	BA	1682	1/1	0.90	0.20	71,71,71,71	0
60	MG	AA	3110	1/1	0.90	0.23	57,57,57,57	0
60	MG	AA	3233	1/1	0.90	0.28	85,85,85,85	0
60	MG	BA	1618	1/1	0.90	0.28	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CA	3419	1/1	0.90	0.17	55,55,55,55	0
60	MG	CA	3420	1/1	0.90	0.15	50,50,50,50	0
60	MG	DA	1754	1/1	0.90	0.10	77,77,77,77	0
60	MG	AA	3445	1/1	0.90	0.11	59,59,59,59	0
60	MG	DA	1761	1/1	0.90	0.07	68,68,68,68	0
60	MG	AA	3234	1/1	0.90	0.11	58,58,58,58	0
60	MG	CA	3023	1/1	0.90	0.11	56,56,56,56	0
60	MG	CA	3577	1/1	0.90	0.12	52,52,52,52	0
60	MG	CA	3433	1/1	0.90	0.09	45,45,45,45	0
60	MG	AA	3448	1/1	0.90	0.16	74,74,74,74	0
60	MG	DA	1606	1/1	0.90	0.08	66,66,66,66	0
60	MG	DF	3001	1/1	0.90	0.10	53,53,53,53	0
60	MG	AA	3162	1/1	0.90	0.13	35,35,35,35	0
60	MG	AE	305	1/1	0.90	0.23	44,44,44,44	0
60	MG	CA	3451	1/1	0.90	0.15	78,78,78,78	0
60	MG	BA	1625	1/1	0.90	0.19	53,53,53,53	0
60	MG	AA	3751	1/1	0.91	0.10	76,76,76,76	0
60	MG	BA	1664	1/1	0.91	0.29	64,64,64,64	0
60	MG	BA	1665	1/1	0.91	0.26	68,68,68,68	0
60	MG	AA	3094	1/1	0.91	0.35	82,82,82,82	0
60	MG	CA	3495	1/1	0.91	0.12	64,64,64,64	0
60	MG	AA	3117	1/1	0.91	0.12	64,64,64,64	0
60	MG	AA	3586	1/1	0.91	0.17	75,75,75,75	0
60	MG	AA	3358	1/1	0.91	0.09	72,72,72,72	0
60	MG	CA	3084	1/1	0.91	0.37	73,73,73,73	0
60	MG	AA	3757	1/1	0.91	0.22	67,67,67,67	0
60	MG	CA	3242	1/1	0.91	0.22	48,48,48,48	0
60	MG	BA	1796	1/1	0.91	0.11	75,75,75,75	0
60	MG	CA	3504	1/1	0.91	0.16	77,77,77,77	0
60	MG	CF	302	1/1	0.91	0.22	64,64,64,64	0
60	MG	CA	3088	1/1	0.91	0.45	85,85,85,85	0
60	MG	AA	3758	1/1	0.91	0.15	70,70,70,70	0
60	MG	CG	3001	1/1	0.91	0.21	66,66,66,66	0
60	MG	AA	3252	1/1	0.91	0.22	76,76,76,76	0
60	MG	AA	3760	1/1	0.91	0.12	50,50,50,50	0
60	MG	CA	3251	1/1	0.91	0.16	62,62,62,62	0
60	MG	CA	3513	1/1	0.91	0.19	109,109,109,109	0
60	MG	CV	201	1/1	0.91	0.12	84,84,84,84	0
60	MG	C0	102	1/1	0.91	0.07	56,56,56,56	0
60	MG	AA	3060	1/1	0.91	0.12	23,23,23,23	0
60	MG	BA	1677	1/1	0.91	0.25	57,57,57,57	0
60	MG	AA	3660	1/1	0.91	0.28	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CA	3266	1/1	0.91	0.24	67,67,67,67	0
60	MG	AA	3151	1/1	0.91	0.18	63,63,63,63	0
60	MG	AA	3670	1/1	0.91	0.16	66,66,66,66	0
60	MG	A0	105	1/1	0.91	0.09	52,52,52,52	0
60	MG	AA	3769	1/1	0.91	0.37	48,48,48,48	1
60	MG	CA	3526	1/1	0.91	0.08	69,69,69,69	0
60	MG	BA	1689	1/1	0.91	0.21	65,65,65,65	0
60	MG	AA	3309	1/1	0.91	0.15	72,72,72,72	0
60	MG	AA	3484	1/1	0.91	0.18	48,48,48,48	0
60	MG	CA	3106	1/1	0.91	0.09	45,45,45,45	0
60	MG	AA	3680	1/1	0.91	0.10	70,70,70,70	0
60	MG	CA	3285	1/1	0.91	0.07	41,41,41,41	0
60	MG	BA	1694	1/1	0.91	0.22	78,78,78,78	0
60	MG	CA	3290	1/1	0.91	0.15	61,61,61,61	0
60	MG	BN	502	1/1	0.91	0.18	64,64,64,64	0
60	MG	BN	503	1/1	0.91	0.11	61,61,61,61	0
60	MG	DA	1633	1/1	0.91	0.31	67,67,67,67	0
60	MG	AA	3001	1/1	0.91	0.15	39,39,39,39	0
60	MG	CA	3295	1/1	0.91	0.13	55,55,55,55	0
60	MG	AA	3240	1/1	0.91	0.30	39,39,39,39	0
60	MG	DA	1641	1/1	0.91	0.07	55,55,55,55	0
60	MG	AA	3691	1/1	0.91	0.10	51,51,51,51	0
60	MG	AA	3780	1/1	0.91	0.17	51,51,51,51	1
60	MG	CA	3305	1/1	0.91	0.19	64,64,64,64	0
60	MG	AA	3381	1/1	0.91	0.09	34,34,34,34	0
60	MG	AA	3015	1/1	0.91	0.30	74,74,74,74	0
60	MG	DA	1655	1/1	0.91	0.19	72,72,72,72	0
60	MG	BX	104	1/1	0.91	0.20	67,67,67,67	0
60	MG	BA	1608	1/1	0.91	0.09	52,52,52,52	0
60	MG	CA	3564	1/1	0.91	0.11	33,33,33,33	0
60	MG	AA	3695	1/1	0.91	0.12	50,50,50,50	0
60	MG	BX	110	1/1	0.91	0.22	67,67,67,67	0
60	MG	CA	3334	1/1	0.91	0.07	56,56,56,56	0
60	MG	BX	111	1/1	0.91	0.07	67,67,67,67	0
60	MG	DA	1665	1/1	0.91	0.12	57,57,57,57	0
60	MG	CA	3339	1/1	0.91	0.20	75,75,75,75	0
60	MG	AA	3408	1/1	0.91	0.09	41,41,41,41	0
60	MG	AA	3698	1/1	0.91	0.17	51,51,51,51	1
60	MG	AA	3701	1/1	0.91	0.26	62,62,62,62	0
60	MG	AA	3797	1/1	0.91	0.18	60,60,60,60	0
60	MG	CA	3363	1/1	0.91	0.10	55,55,55,55	0
60	MG	DA	1674	1/1	0.91	0.15	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3041	1/1	0.91	0.19	41,41,41,41	0
60	MG	AA	3414	1/1	0.91	0.10	43,43,43,43	0
60	MG	BA	1716	1/1	0.91	0.18	71,71,71,71	0
60	MG	AA	3021	1/1	0.91	0.15	49,49,49,49	0
60	MG	AA	3811	1/1	0.91	0.26	65,65,65,65	0
60	MG	DA	1683	1/1	0.91	0.26	60,60,60,60	0
60	MG	AA	3812	1/1	0.91	0.16	78,78,78,78	0
60	MG	AA	3177	1/1	0.91	0.09	43,43,43,43	0
60	MG	CA	3382	1/1	0.91	0.15	70,70,70,70	0
60	MG	DA	1694	1/1	0.91	0.18	60,60,60,60	0
60	MG	AA	3817	1/1	0.91	0.22	72,72,72,72	0
60	MG	AB	3001	1/1	0.91	0.13	80,80,80,80	0
60	MG	DA	1698	1/1	0.91	0.15	75,75,75,75	0
60	MG	CA	3596	1/1	0.91	0.08	75,75,75,75	0
60	MG	CA	3026	1/1	0.91	0.23	55,55,55,55	0
60	MG	BA	1628	1/1	0.91	0.22	59,59,59,59	0
60	MG	CA	3156	1/1	0.91	0.27	92,92,92,92	0
60	MG	DA	1706	1/1	0.91	0.15	70,70,70,70	0
60	MG	DA	1707	1/1	0.91	0.09	79,79,79,79	0
60	MG	DA	1709	1/1	0.91	0.14	57,57,57,57	0
60	MG	CA	3158	1/1	0.91	0.17	54,54,54,54	0
60	MG	AA	3436	1/1	0.91	0.09	31,31,31,31	0
60	MG	AA	3275	1/1	0.91	0.17	56,56,56,56	0
60	MG	CA	3399	1/1	0.91	0.13	45,45,45,45	0
60	MG	CA	3168	1/1	0.91	0.16	65,65,65,65	0
60	MG	AA	3439	1/1	0.91	0.14	43,43,43,43	0
60	MG	CA	3612	1/1	0.91	0.10	59,59,59,59	0
60	MG	CA	3170	1/1	0.91	0.34	68,68,68,68	0
60	MG	AA	3277	1/1	0.91	0.22	48,48,48,48	0
60	MG	CA	3175	1/1	0.91	0.13	59,59,59,59	0
60	MG	CA	3036	1/1	0.91	0.23	65,65,65,65	0
60	MG	DA	1725	1/1	0.91	0.13	78,78,78,78	0
60	MG	CA	3037	1/1	0.91	0.22	65,65,65,65	0
60	MG	AA	3632	1/1	0.91	0.15	97,97,97,97	0
60	MG	CA	3423	1/1	0.91	0.12	57,57,57,57	0
60	MG	CA	3427	1/1	0.91	0.15	69,69,69,69	0
60	MG	CA	3041	1/1	0.91	0.30	67,67,67,67	0
60	MG	BA	1642	1/1	0.91	0.18	59,59,59,59	0
60	MG	CA	3628	1/1	0.91	0.12	76,76,76,76	0
60	MG	BA	1756	1/1	0.91	0.17	43,43,43,43	0
60	MG	CA	3045	1/1	0.91	0.14	68,68,68,68	0
60	MG	CA	3048	1/1	0.91	0.19	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	1643	1/1	0.91	0.13	56,56,56,56	0
60	MG	AA	3633	1/1	0.91	0.13	51,51,51,51	0
60	MG	AA	3441	1/1	0.91	0.07	62,62,62,62	0
60	MG	AA	3558	1/1	0.91	0.15	72,72,72,72	0
60	MG	AA	3278	1/1	0.91	0.32	58,58,58,58	0
60	MG	CA	3463	1/1	0.91	0.27	75,75,75,75	0
60	MG	BA	1652	1/1	0.91	0.14	65,65,65,65	0
60	MG	CA	3641	1/1	0.91	0.36	59,59,59,59	0
60	MG	CA	3466	1/1	0.91	0.12	56,56,56,56	0
60	MG	AA	3642	1/1	0.91	0.17	60,60,60,60	0
60	MG	CA	3469	1/1	0.91	0.32	76,76,76,76	0
60	MG	CA	3470	1/1	0.91	0.12	55,55,55,55	0
60	MG	CA	3472	1/1	0.91	0.20	49,49,49,49	0
60	MG	AA	3180	1/1	0.91	0.11	53,53,53,53	0
60	MG	BA	1772	1/1	0.91	0.17	51,51,51,51	0
60	MG	BA	1773	1/1	0.91	0.16	69,69,69,69	0
60	MG	CA	3480	1/1	0.91	0.09	61,61,61,61	0
60	MG	CA	3654	1/1	0.91	0.30	76,76,76,76	0
60	MG	AA	3344	1/1	0.91	0.14	65,65,65,65	0
60	MG	BA	1658	1/1	0.91	0.29	68,68,68,68	0
60	MG	AA	3281	1/1	0.91	0.28	38,38,38,38	0
60	MG	AA	3228	1/1	0.91	0.20	63,63,63,63	0
60	MG	CA	3222	1/1	0.91	0.42	81,81,81,81	0
60	MG	CA	3071	1/1	0.91	0.17	53,53,53,53	0
60	MG	CA	3072	1/1	0.91	0.17	54,54,54,54	0
60	MG	AA	3809	1/1	0.92	0.09	46,46,46,46	0
60	MG	CA	3210	1/1	0.92	0.18	44,44,44,44	0
60	MG	DA	1619	1/1	0.92	0.18	50,50,50,50	0
60	MG	AA	3092	1/1	0.92	0.22	41,41,41,41	0
60	MG	AA	3637	1/1	0.92	0.12	54,54,54,54	0
60	MG	CA	3214	1/1	0.92	0.16	50,50,50,50	0
60	MG	CA	3418	1/1	0.92	0.15	53,53,53,53	0
60	MG	CA	3215	1/1	0.92	0.33	50,50,50,50	0
60	MG	AA	3813	1/1	0.92	0.21	68,68,68,68	0
60	MG	AA	3731	1/1	0.92	0.09	34,34,34,34	0
60	MG	AA	3032	1/1	0.92	0.23	62,62,62,62	0
60	MG	AA	3437	1/1	0.92	0.08	25,25,25,25	0
60	MG	AA	3276	1/1	0.92	0.20	64,64,64,64	0
60	MG	BA	1708	1/1	0.92	0.18	55,55,55,55	0
60	MG	AA	3034	1/1	0.92	0.22	84,84,84,84	0
60	MG	DA	1639	1/1	0.92	0.14	59,59,59,59	0
60	MG	AA	3341	1/1	0.92	0.17	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AB	3010	1/1	0.92	0.06	56,56,56,56	1
60	MG	BA	1627	1/1	0.92	0.11	63,63,63,63	0
60	MG	DA	1644	1/1	0.92	0.17	49,49,49,49	0
60	MG	DA	1645	1/1	0.92	0.28	58,58,58,58	0
60	MG	AB	3013	1/1	0.92	0.09	55,55,55,55	0
60	MG	AA	3194	1/1	0.92	0.20	58,58,58,58	0
60	MG	CA	3602	1/1	0.92	0.07	49,49,49,49	0
60	MG	AA	3571	1/1	0.92	0.09	53,53,53,53	0
60	MG	DA	1654	1/1	0.92	0.24	48,48,48,48	0
60	MG	BA	1632	1/1	0.92	0.26	60,60,60,60	0
60	MG	CA	3606	1/1	0.92	0.11	58,58,58,58	0
60	MG	AB	3018	1/1	0.92	0.07	76,76,76,76	0
60	MG	BX	107	1/1	0.92	0.20	69,69,69,69	0
60	MG	CA	3609	1/1	0.92	0.10	62,62,62,62	0
60	MG	DA	1660	1/1	0.92	0.19	81,81,81,81	0
60	MG	BX	109	1/1	0.92	0.23	55,55,55,55	0
60	MG	AA	3215	1/1	0.92	0.09	48,48,48,48	0
60	MG	BA	1725	1/1	0.92	0.20	52,52,52,52	0
60	MG	BA	1726	1/1	0.92	0.14	59,59,59,59	0
60	MG	BA	1727	1/1	0.92	0.24	53,53,53,53	0
60	MG	AA	3280	1/1	0.92	0.21	63,63,63,63	0
60	MG	CA	3477	1/1	0.92	0.17	65,65,65,65	0
60	MG	AA	3220	1/1	0.92	0.14	65,65,65,65	0
60	MG	CA	3260	1/1	0.92	0.10	59,59,59,59	0
60	MG	BA	1735	1/1	0.92	0.11	58,58,58,58	0
60	MG	CA	3120	1/1	0.92	0.12	47,47,47,47	0
60	MG	AA	3029	1/1	0.92	0.11	50,50,50,50	0
60	MG	CA	3003	1/1	0.92	0.20	49,49,49,49	0
60	MG	AA	3581	1/1	0.92	0.13	48,48,48,48	0
60	MG	AA	3196	1/1	0.92	0.19	48,48,48,48	0
60	MG	AA	3197	1/1	0.92	0.22	42,42,42,42	0
60	MG	AA	3080	1/1	0.92	0.26	54,54,54,54	0
60	MG	CA	3018	1/1	0.92	0.08	59,59,59,59	0
60	MG	CA	3490	1/1	0.92	0.18	81,81,81,81	0
60	MG	BA	1751	1/1	0.92	0.16	49,49,49,49	0
60	MG	DA	1690	1/1	0.92	0.08	74,74,74,74	0
60	MG	DA	1691	1/1	0.92	0.17	66,66,66,66	0
60	MG	AA	3293	1/1	0.92	0.13	68,68,68,68	0
60	MG	AA	3459	1/1	0.92	0.12	65,65,65,65	0
60	MG	BA	1655	1/1	0.92	0.17	65,65,65,65	0
60	MG	CA	3286	1/1	0.92	0.11	62,62,62,62	0
60	MG	AA	3297	1/1	0.92	0.08	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3260	1/1	0.92	0.28	67,67,67,67	0
60	MG	AF	306	1/1	0.92	0.17	54,54,54,54	0
60	MG	CA	3140	1/1	0.92	0.33	54,54,54,54	0
60	MG	AA	3675	1/1	0.92	0.10	67,67,67,67	0
60	MG	AA	3262	1/1	0.92	0.46	70,70,70,70	0
60	MG	DA	1708	1/1	0.92	0.15	67,67,67,67	0
60	MG	AA	3687	1/1	0.92	0.07	48,48,48,48	0
60	MG	BA	1662	1/1	0.92	0.13	45,45,45,45	0
60	MG	BA	1663	1/1	0.92	0.12	66,66,66,66	0
60	MG	BA	1770	1/1	0.92	0.11	62,62,62,62	0
60	MG	AA	3768	1/1	0.92	0.19	67,67,67,67	0
60	MG	AA	3100	1/1	0.92	0.12	34,34,34,34	0
60	MG	CA	3154	1/1	0.92	0.12	68,68,68,68	0
60	MG	AU	203	1/1	0.92	0.15	55,55,55,55	0
60	MG	CA	3322	1/1	0.92	0.16	41,41,41,41	0
60	MG	CA	3046	1/1	0.92	0.12	72,72,72,72	0
60	MG	CA	3331	1/1	0.92	0.24	62,62,62,62	0
60	MG	AA	3135	1/1	0.92	0.17	53,53,53,53	0
60	MG	AA	3388	1/1	0.92	0.09	55,55,55,55	0
60	MG	AA	3399	1/1	0.92	0.13	51,51,51,51	0
60	MG	CB	3002	1/1	0.92	0.12	78,78,78,78	0
60	MG	CA	3051	1/1	0.92	0.15	52,52,52,52	0
60	MG	DA	1731	1/1	0.92	0.10	51,51,51,51	0
60	MG	AA	3315	1/1	0.92	0.17	56,56,56,56	0
60	MG	AA	3101	1/1	0.92	0.34	68,68,68,68	0
60	MG	AA	3491	1/1	0.92	0.15	40,40,40,40	0
60	MG	AA	3065	1/1	0.92	0.23	51,51,51,51	0
60	MG	AA	3700	1/1	0.92	0.10	48,48,48,48	0
60	MG	CA	3058	1/1	0.92	0.39	74,74,74,74	0
60	MG	AA	3620	1/1	0.92	0.09	49,49,49,49	0
60	MG	A6	102	1/1	0.92	0.18	69,69,69,69	0
60	MG	CD	303	1/1	0.92	0.07	70,70,70,70	0
60	MG	CE	303	1/1	0.92	0.19	55,55,55,55	0
60	MG	DA	1745	1/1	0.92	0.13	54,54,54,54	0
60	MG	AA	3206	1/1	0.92	0.15	55,55,55,55	0
60	MG	BA	1794	1/1	0.92	0.17	63,63,63,63	0
60	MG	CA	3188	1/1	0.92	0.25	55,55,55,55	0
60	MG	AA	3622	1/1	0.92	0.07	52,52,52,52	0
60	MG	CA	3379	1/1	0.92	0.10	62,62,62,62	0
60	MG	AA	3498	1/1	0.92	0.08	56,56,56,56	0
60	MG	AA	3049	1/1	0.92	0.07	35,35,35,35	0
60	MG	CA	3196	1/1	0.92	0.13	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CA	3551	1/1	0.92	0.12	76,76,76,76	0
60	MG	DA	1755	1/1	0.92	0.12	69,69,69,69	0
60	MG	CA	3197	1/1	0.92	0.17	48,48,48,48	0
60	MG	AA	3421	1/1	0.92	0.13	73,73,73,73	0
60	MG	CA	3554	1/1	0.92	0.10	60,60,60,60	0
60	MG	C3	101	1/1	0.92	0.19	91,91,91,91	0
60	MG	CA	3390	1/1	0.92	0.10	42,42,42,42	0
60	MG	BA	1802	1/1	0.92	0.11	58,58,58,58	0
60	MG	DA	1768	1/1	0.92	0.09	57,57,57,57	0
60	MG	AA	3433	1/1	0.92	0.16	50,50,50,50	0
60	MG	CA	3396	1/1	0.92	0.14	59,59,59,59	0
60	MG	AA	3718	1/1	0.92	0.12	40,40,40,40	0
60	MG	AA	3803	1/1	0.92	0.15	37,37,37,37	0
60	MG	DK	202	1/1	0.92	0.09	80,80,80,80	0
60	MG	DA	1609	1/1	0.92	0.11	49,49,49,49	0
60	MG	AA	3434	1/1	0.92	0.13	58,58,58,58	0
60	MG	AA	3807	1/1	0.92	0.13	62,62,62,62	0
60	MG	BA	1801	1/1	0.93	0.10	55,55,55,55	0
60	MG	BA	1668	1/1	0.93	0.15	72,72,72,72	0
60	MG	CA	3253	1/1	0.93	0.22	61,61,61,61	0
60	MG	CA	3499	1/1	0.93	0.13	68,68,68,68	0
60	MG	AA	3492	1/1	0.93	0.09	41,41,41,41	0
60	MG	AA	3176	1/1	0.93	0.22	70,70,70,70	0
60	MG	AA	3626	1/1	0.93	0.22	59,59,59,59	0
60	MG	CA	3262	1/1	0.93	0.18	59,59,59,59	0
60	MG	AA	3628	1/1	0.93	0.15	62,62,62,62	0
60	MG	CQ	202	1/1	0.93	0.17	56,56,56,56	0
60	MG	AA	3316	1/1	0.93	0.17	64,64,64,64	0
60	MG	CQ	204	1/1	0.93	0.12	74,74,74,74	0
60	MG	AA	3140	1/1	0.93	0.09	66,66,66,66	0
60	MG	CU	201	1/1	0.93	0.16	62,62,62,62	0
60	MG	CA	3269	1/1	0.93	0.25	64,64,64,64	0
60	MG	CV	202	1/1	0.93	0.19	82,82,82,82	0
60	MG	CA	3509	1/1	0.93	0.09	52,52,52,52	0
60	MG	CA	3510	1/1	0.93	0.15	71,71,71,71	0
60	MG	AG	201	1/1	0.93	0.12	59,59,59,59	0
60	MG	DA	1602	1/1	0.93	0.09	65,65,65,65	0
60	MG	CA	3104	1/1	0.93	0.15	64,64,64,64	0
60	MG	BA	1676	1/1	0.93	0.15	39,39,39,39	0
60	MG	CA	3107	1/1	0.93	0.10	64,64,64,64	0
60	MG	BB	3001	1/1	0.93	0.19	67,67,67,67	0
60	MG	CA	3109	1/1	0.93	0.10	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BD	502	1/1	0.93	0.19	56,56,56,56	0
60	MG	AG	203	1/1	0.93	0.09	69,69,69,69	0
60	MG	AA	3503	1/1	0.93	0.10	41,41,41,41	0
60	MG	AA	3748	1/1	0.93	0.17	62,62,62,62	0
60	MG	CA	3115	1/1	0.93	0.12	71,71,71,71	0
60	MG	CA	3116	1/1	0.93	0.30	57,57,57,57	0
60	MG	BA	1683	1/1	0.93	0.13	50,50,50,50	0
60	MG	AN	3002	1/1	0.93	0.15	76,76,76,76	0
60	MG	AA	3749	1/1	0.93	0.09	30,30,30,30	0
60	MG	AQ	3001	1/1	0.93	0.19	56,56,56,56	0
60	MG	CA	3296	1/1	0.93	0.10	61,61,61,61	0
60	MG	CA	3298	1/1	0.93	0.09	68,68,68,68	0
60	MG	AA	3509	1/1	0.93	0.19	51,51,51,51	0
60	MG	AA	3634	1/1	0.93	0.15	63,63,63,63	0
60	MG	AA	3179	1/1	0.93	0.11	62,62,62,62	0
60	MG	CA	3303	1/1	0.93	0.14	52,52,52,52	0
60	MG	CA	3125	1/1	0.93	0.23	58,58,58,58	0
60	MG	BA	1692	1/1	0.93	0.26	69,69,69,69	0
60	MG	DA	1638	1/1	0.93	0.12	60,60,60,60	0
60	MG	AA	3420	1/1	0.93	0.07	26,26,26,26	0
60	MG	AA	3143	1/1	0.93	0.05	37,37,37,37	0
60	MG	CA	3320	1/1	0.93	0.16	47,47,47,47	0
60	MG	BA	1695	1/1	0.93	0.05	64,64,64,64	0
60	MG	AA	3428	1/1	0.93	0.16	36,36,36,36	0
60	MG	AA	3018	1/1	0.93	0.33	55,55,55,55	0
60	MG	AA	3531	1/1	0.93	0.14	61,61,61,61	0
60	MG	CA	3332	1/1	0.93	0.15	47,47,47,47	0
60	MG	AA	3106	1/1	0.93	0.16	43,43,43,43	0
60	MG	DA	1650	1/1	0.93	0.24	48,48,48,48	0
60	MG	CA	3556	1/1	0.93	0.07	77,77,77,77	0
60	MG	CA	3557	1/1	0.93	0.19	76,76,76,76	0
60	MG	AA	3047	1/1	0.93	0.15	40,40,40,40	0
60	MG	AA	3332	1/1	0.93	0.09	55,55,55,55	0
60	MG	AA	3333	1/1	0.93	0.05	33,33,33,33	0
60	MG	CA	3341	1/1	0.93	0.11	35,35,35,35	0
60	MG	AA	3334	1/1	0.93	0.12	62,62,62,62	0
60	MG	AA	3767	1/1	0.93	0.21	75,75,75,75	0
60	MG	CA	3351	1/1	0.93	0.08	50,50,50,50	0
60	MG	AA	3561	1/1	0.93	0.13	64,64,64,64	0
60	MG	CA	3360	1/1	0.93	0.10	52,52,52,52	0
60	MG	AA	3563	1/1	0.93	0.10	37,37,37,37	1
60	MG	CA	3579	1/1	0.93	0.09	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3033	1/1	0.93	0.23	48,48,48,48	0
60	MG	AA	3152	1/1	0.93	0.20	80,80,80,80	0
60	MG	CA	3010	1/1	0.93	0.07	49,49,49,49	0
60	MG	AA	3659	1/1	0.93	0.08	56,56,56,56	0
60	MG	AA	3050	1/1	0.93	0.14	29,29,29,29	0
60	MG	AA	3663	1/1	0.93	0.17	61,61,61,61	0
60	MG	DA	1675	1/1	0.93	0.12	61,61,61,61	0
60	MG	AA	3113	1/1	0.93	0.10	41,41,41,41	0
60	MG	BA	1612	1/1	0.93	0.11	79,79,79,79	0
60	MG	AA	3669	1/1	0.93	0.14	36,36,36,36	0
60	MG	AA	3443	1/1	0.93	0.09	58,58,58,58	0
60	MG	BA	1724	1/1	0.93	0.13	60,60,60,60	0
60	MG	AA	3024	1/1	0.93	0.21	60,60,60,60	0
60	MG	AA	3787	1/1	0.93	0.13	55,55,55,55	0
60	MG	BA	1619	1/1	0.93	0.07	54,54,54,54	0
60	MG	DA	1688	1/1	0.93	0.14	46,46,46,46	0
60	MG	AA	3346	1/1	0.93	0.09	32,32,32,32	0
60	MG	CA	3392	1/1	0.93	0.12	66,66,66,66	0
60	MG	AA	3673	1/1	0.93	0.14	58,58,58,58	0
60	MG	AA	3119	1/1	0.93	0.12	41,41,41,41	0
60	MG	AA	3096	1/1	0.93	0.20	54,54,54,54	0
60	MG	AA	3681	1/1	0.93	0.15	52,52,52,52	0
60	MG	AA	3799	1/1	0.93	0.07	45,45,45,45	0
60	MG	AA	3198	1/1	0.93	0.10	47,47,47,47	0
60	MG	CA	3403	1/1	0.93	0.13	70,70,70,70	0
60	MG	BA	1746	1/1	0.93	0.10	70,70,70,70	0
60	MG	DA	1702	1/1	0.93	0.10	58,58,58,58	0
60	MG	AA	3591	1/1	0.93	0.16	61,61,61,61	0
60	MG	CA	3191	1/1	0.93	0.17	61,61,61,61	0
60	MG	CA	3193	1/1	0.93	0.20	47,47,47,47	0
60	MG	AA	3062	1/1	0.93	0.24	60,60,60,60	0
60	MG	AA	3690	1/1	0.93	0.12	58,58,58,58	0
60	MG	AA	3595	1/1	0.93	0.10	60,60,60,60	0
60	MG	BA	1631	1/1	0.93	0.06	44,44,44,44	0
60	MG	AA	3597	1/1	0.93	0.15	58,58,58,58	0
60	MG	AA	3693	1/1	0.93	0.10	47,47,47,47	0
60	MG	CA	3426	1/1	0.93	0.12	46,46,46,46	0
60	MG	AA	3356	1/1	0.93	0.09	51,51,51,51	0
60	MG	CA	3054	1/1	0.93	0.09	50,50,50,50	0
60	MG	CA	3203	1/1	0.93	0.17	45,45,45,45	0
60	MG	CA	3430	1/1	0.93	0.14	38,38,38,38	0
60	MG	BA	1761	1/1	0.93	0.15	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	1637	1/1	0.93	0.08	64,64,64,64	0
60	MG	CA	3434	1/1	0.93	0.17	67,67,67,67	0
60	MG	AA	3099	1/1	0.93	0.10	48,48,48,48	0
60	MG	BA	1639	1/1	0.93	0.17	42,42,42,42	0
60	MG	BA	1641	1/1	0.93	0.20	56,56,56,56	0
60	MG	CA	3636	1/1	0.93	0.20	60,60,60,60	0
60	MG	AA	3134	1/1	0.93	0.23	49,49,49,49	0
60	MG	CA	3452	1/1	0.93	0.10	37,37,37,37	0
60	MG	AA	3290	1/1	0.93	0.15	78,78,78,78	0
60	MG	CA	3458	1/1	0.93	0.09	28,28,28,28	0
60	MG	CA	3460	1/1	0.93	0.14	57,57,57,57	0
60	MG	AA	3464	1/1	0.93	0.11	69,69,69,69	0
60	MG	AA	3607	1/1	0.93	0.10	39,39,39,39	0
60	MG	AA	3083	1/1	0.93	0.27	48,48,48,48	1
60	MG	CA	3069	1/1	0.93	0.17	66,66,66,66	0
60	MG	AA	3475	1/1	0.93	0.14	73,73,73,73	0
60	MG	AA	3476	1/1	0.93	0.06	50,50,50,50	0
60	MG	AA	3054	1/1	0.93	0.15	26,26,26,26	0
60	MG	CA	3471	1/1	0.93	0.18	59,59,59,59	0
60	MG	AA	3711	1/1	0.93	0.18	41,41,41,41	0
60	MG	BA	1782	1/1	0.93	0.11	72,72,72,72	0
60	MG	CA	3230	1/1	0.93	0.15	64,64,64,64	0
60	MG	CA	3476	1/1	0.93	0.12	60,60,60,60	0
60	MG	AA	3294	1/1	0.93	0.20	56,56,56,56	0
60	MG	CA	3233	1/1	0.93	0.22	52,52,52,52	0
60	MG	AA	3205	1/1	0.93	0.20	45,45,45,45	0
60	MG	AA	3616	1/1	0.93	0.06	33,33,33,33	0
60	MG	DA	1756	1/1	0.93	0.16	60,60,60,60	0
60	MG	DA	1757	1/1	0.93	0.14	77,77,77,77	0
60	MG	DA	1758	1/1	0.93	0.19	80,80,80,80	0
60	MG	AA	3721	1/1	0.93	0.09	21,21,21,21	0
60	MG	AA	3167	1/1	0.93	0.16	69,69,69,69	0
60	MG	AB	3023	1/1	0.93	0.16	63,63,63,63	0
60	MG	DA	1763	1/1	0.93	0.10	61,61,61,61	0
60	MG	AD	301	1/1	0.93	0.17	64,64,64,64	0
60	MG	AA	3619	1/1	0.93	0.09	39,39,39,39	0
60	MG	BA	1795	1/1	0.93	0.19	64,64,64,64	0
60	MG	AA	3170	1/1	0.93	0.28	44,44,44,44	1
60	MG	AA	3102	1/1	0.93	0.19	38,38,38,38	0
60	MG	CB	3011	1/1	0.93	0.19	51,51,51,51	0
60	MG	CA	3245	1/1	0.93	0.08	53,53,53,53	0
60	MG	AA	3138	1/1	0.93	0.06	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CA	3247	1/1	0.93	0.07	45,45,45,45	0
60	MG	CA	3494	1/1	0.93	0.11	58,58,58,58	0
60	MG	AA	3623	1/1	0.93	0.07	58,58,58,58	0
60	MG	CE	301	1/1	0.93	0.19	54,54,54,54	0
60	MG	CA	3207	1/1	0.94	0.27	62,62,62,62	0
60	MG	AA	3653	1/1	0.94	0.07	47,47,47,47	0
60	MG	CA	3044	1/1	0.94	0.25	64,64,64,64	0
60	MG	AA	3426	1/1	0.94	0.12	47,47,47,47	0
60	MG	AA	3111	1/1	0.94	0.14	47,47,47,47	0
60	MG	CA	3047	1/1	0.94	0.07	54,54,54,54	0
60	MG	AA	3325	1/1	0.94	0.09	78,78,78,78	0
60	MG	CA	3216	1/1	0.94	0.14	32,32,32,32	0
60	MG	BA	1607	1/1	0.94	0.07	64,64,64,64	0
60	MG	BA	1731	1/1	0.94	0.07	65,65,65,65	0
60	MG	AA	3327	1/1	0.94	0.06	36,36,36,36	0
60	MG	CA	3221	1/1	0.94	0.29	60,60,60,60	0
60	MG	AA	3141	1/1	0.94	0.10	46,46,46,46	0
60	MG	AA	3569	1/1	0.94	0.08	17,17,17,17	0
60	MG	AA	3661	1/1	0.94	0.26	78,78,78,78	0
60	MG	CE	302	1/1	0.94	0.08	31,31,31,31	0
60	MG	CA	3227	1/1	0.94	0.17	30,30,30,30	0
60	MG	BA	1738	1/1	0.94	0.14	55,55,55,55	0
60	MG	CE	305	1/1	0.94	0.12	37,37,37,37	0
60	MG	CE	306	1/1	0.94	0.07	69,69,69,69	0
60	MG	CA	3479	1/1	0.94	0.16	67,67,67,67	0
60	MG	CA	3229	1/1	0.94	0.21	48,48,48,48	0
60	MG	AA	3662	1/1	0.94	0.22	60,60,60,60	0
60	MG	CA	3231	1/1	0.94	0.25	56,56,56,56	0
60	MG	BA	1741	1/1	0.94	0.09	49,49,49,49	0
60	MG	AA	3142	1/1	0.94	0.16	50,50,50,50	0
60	MG	AA	3272	1/1	0.94	0.15	74,74,74,74	0
60	MG	CA	3060	1/1	0.94	0.13	50,50,50,50	0
60	MG	BA	1747	1/1	0.94	0.06	53,53,53,53	0
60	MG	BA	1617	1/1	0.94	0.06	64,64,64,64	0
60	MG	BA	1750	1/1	0.94	0.10	54,54,54,54	0
60	MG	AA	3667	1/1	0.94	0.09	45,45,45,45	0
60	MG	AA	3784	1/1	0.94	0.11	69,69,69,69	0
60	MG	AA	3273	1/1	0.94	0.12	57,57,57,57	0
60	MG	AA	3576	1/1	0.94	0.17	49,49,49,49	0
60	MG	AA	3078	1/1	0.94	0.19	54,54,54,54	0
60	MG	AA	3791	1/1	0.94	0.13	48,48,48,48	0
60	MG	AA	3235	1/1	0.94	0.17	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3580	1/1	0.94	0.07	26,26,26,26	0
60	MG	AA	3796	1/1	0.94	0.18	45,45,45,45	0
60	MG	AA	3005	1/1	0.94	0.13	63,63,63,63	0
60	MG	AA	3679	1/1	0.94	0.07	64,64,64,64	0
60	MG	AA	3339	1/1	0.94	0.10	18,18,18,18	0
60	MG	AA	3202	1/1	0.94	0.11	46,46,46,46	0
60	MG	CA	3257	1/1	0.94	0.08	45,45,45,45	0
60	MG	AA	3682	1/1	0.94	0.11	58,58,58,58	0
60	MG	AA	3804	1/1	0.94	0.13	70,70,70,70	0
60	MG	AA	3064	1/1	0.94	0.09	31,31,31,31	0
60	MG	DA	1617	1/1	0.94	0.10	47,47,47,47	0
60	MG	DA	1618	1/1	0.94	0.08	51,51,51,51	0
60	MG	BA	1635	1/1	0.94	0.26	62,62,62,62	0
60	MG	AA	3590	1/1	0.94	0.10	71,71,71,71	0
60	MG	AA	3808	1/1	0.94	0.08	47,47,47,47	0
60	MG	AA	3120	1/1	0.94	0.13	54,54,54,54	0
60	MG	BA	1780	1/1	0.94	0.08	44,44,44,44	0
60	MG	AA	3810	1/1	0.94	0.15	49,49,49,49	0
60	MG	CA	3273	1/1	0.94	0.08	42,42,42,42	0
60	MG	BA	1640	1/1	0.94	0.12	56,56,56,56	0
60	MG	DA	1630	1/1	0.94	0.15	51,51,51,51	0
60	MG	CA	3278	1/1	0.94	0.09	38,38,38,38	0
60	MG	CA	3518	1/1	0.94	0.11	72,72,72,72	0
60	MG	AA	3057	1/1	0.94	0.11	56,56,56,56	0
60	MG	BA	1785	1/1	0.94	0.14	69,69,69,69	0
60	MG	AA	3123	1/1	0.94	0.18	55,55,55,55	0
60	MG	AA	3596	1/1	0.94	0.10	39,39,39,39	0
60	MG	CA	3100	1/1	0.94	0.15	75,75,75,75	0
60	MG	AA	3815	1/1	0.94	0.14	72,72,72,72	0
60	MG	AA	3126	1/1	0.94	0.14	68,68,68,68	0
60	MG	CA	3530	1/1	0.94	0.10	68,68,68,68	0
60	MG	AA	3284	1/1	0.94	0.11	45,45,45,45	0
60	MG	CA	3288	1/1	0.94	0.17	39,39,39,39	0
60	MG	BA	1791	1/1	0.94	0.10	58,58,58,58	0
60	MG	AA	3455	1/1	0.94	0.14	80,80,80,80	0
60	MG	AA	3044	1/1	0.94	0.18	62,62,62,62	0
60	MG	CA	3537	1/1	0.94	0.10	64,64,64,64	0
60	MG	AA	3601	1/1	0.94	0.14	44,44,44,44	0
60	MG	AA	3602	1/1	0.94	0.11	39,39,39,39	0
60	MG	AA	3354	1/1	0.94	0.15	56,56,56,56	0
60	MG	CA	3541	1/1	0.94	0.13	58,58,58,58	0
60	MG	AA	3289	1/1	0.94	0.13	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3704	1/1	0.94	0.08	57,57,57,57	0
60	MG	AA	3461	1/1	0.94	0.11	57,57,57,57	0
60	MG	AA	3357	1/1	0.94	0.10	52,52,52,52	0
60	MG	CA	3546	1/1	0.94	0.08	59,59,59,59	0
60	MG	AA	3129	1/1	0.94	0.15	52,52,52,52	0
60	MG	DA	1663	1/1	0.94	0.11	53,53,53,53	0
60	MG	CA	3549	1/1	0.94	0.09	29,29,29,29	0
60	MG	AB	3020	1/1	0.94	0.10	66,66,66,66	0
60	MG	AA	3466	1/1	0.94	0.09	48,48,48,48	0
60	MG	AA	3250	1/1	0.94	0.20	46,46,46,46	1
60	MG	AA	3104	1/1	0.94	0.14	55,55,55,55	0
60	MG	AA	3716	1/1	0.94	0.12	63,63,63,63	0
60	MG	AA	3364	1/1	0.94	0.16	57,57,57,57	0
60	MG	BA	1811	1/1	0.94	0.14	52,52,52,52	0
60	MG	CA	3325	1/1	0.94	0.14	42,42,42,42	0
60	MG	CA	3558	1/1	0.94	0.10	49,49,49,49	1
60	MG	AA	3720	1/1	0.94	0.18	78,78,78,78	0
60	MG	CA	3561	1/1	0.94	0.10	62,62,62,62	0
60	MG	CA	3330	1/1	0.94	0.12	37,37,37,37	0
60	MG	CA	3566	1/1	0.94	0.13	47,47,47,47	0
60	MG	CA	3568	1/1	0.94	0.15	71,71,71,71	0
60	MG	AA	3213	1/1	0.94	0.22	49,49,49,49	0
60	MG	AA	3368	1/1	0.94	0.13	54,54,54,54	0
60	MG	AA	3295	1/1	0.94	0.07	24,24,24,24	0
60	MG	AA	3370	1/1	0.94	0.09	43,43,43,43	0
60	MG	AA	3190	1/1	0.94	0.21	51,51,51,51	0
60	MG	AA	3378	1/1	0.94	0.10	24,24,24,24	0
60	MG	AF	302	1/1	0.94	0.20	46,46,46,46	0
60	MG	DA	1692	1/1	0.94	0.18	49,49,49,49	0
60	MG	AF	303	1/1	0.94	0.12	46,46,46,46	0
60	MG	CA	3343	1/1	0.94	0.06	37,37,37,37	0
60	MG	AA	3379	1/1	0.94	0.08	40,40,40,40	1
60	MG	CA	3349	1/1	0.94	0.07	36,36,36,36	0
60	MG	CA	3350	1/1	0.94	0.12	74,74,74,74	0
60	MG	BA	1678	1/1	0.94	0.18	52,52,52,52	0
60	MG	AA	3258	1/1	0.94	0.12	32,32,32,32	0
60	MG	CA	3357	1/1	0.94	0.07	34,34,34,34	0
60	MG	AA	3191	1/1	0.94	0.11	57,57,57,57	0
60	MG	AA	3383	1/1	0.94	0.11	31,31,31,31	0
60	MG	CA	3143	1/1	0.94	0.15	62,62,62,62	0
60	MG	AA	3741	1/1	0.94	0.12	47,47,47,47	0
60	MG	BA	1685	1/1	0.94	0.12	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CA	3369	1/1	0.94	0.09	65,65,65,65	0
60	MG	BA	1686	1/1	0.94	0.24	58,58,58,58	0
60	MG	CA	3372	1/1	0.94	0.12	63,63,63,63	0
60	MG	DA	1714	1/1	0.94	0.19	82,82,82,82	0
60	MG	CA	3147	1/1	0.94	0.07	51,51,51,51	0
60	MG	CA	3599	1/1	0.94	0.06	75,75,75,75	0
60	MG	AA	3308	1/1	0.94	0.11	45,45,45,45	0
60	MG	AA	3019	1/1	0.94	0.10	53,53,53,53	0
60	MG	BX	108	1/1	0.94	0.14	78,78,78,78	0
60	MG	AA	3402	1/1	0.94	0.14	53,53,53,53	0
60	MG	AN	3003	1/1	0.94	0.07	52,52,52,52	0
60	MG	DA	1723	1/1	0.94	0.13	53,53,53,53	0
60	MG	AA	3068	1/1	0.94	0.23	52,52,52,52	0
60	MG	CA	3384	1/1	0.94	0.12	52,52,52,52	0
60	MG	AA	3264	1/1	0.94	0.14	54,54,54,54	0
60	MG	AA	3409	1/1	0.94	0.09	51,51,51,51	0
60	MG	AA	3025	1/1	0.94	0.13	60,60,60,60	0
60	MG	CA	3389	1/1	0.94	0.07	55,55,55,55	0
60	MG	CA	3167	1/1	0.94	0.28	68,68,68,68	0
60	MG	CA	3391	1/1	0.94	0.08	67,67,67,67	0
60	MG	BX	115	1/1	0.94	0.11	44,44,44,44	0
60	MG	AA	3526	1/1	0.94	0.07	26,26,26,26	0
60	MG	AW	3001	1/1	0.94	0.15	46,46,46,46	0
60	MG	BZ	701	1/1	0.94	0.13	58,58,58,58	0
60	MG	AA	3071	1/1	0.94	0.24	55,55,55,55	0
60	MG	DA	1740	1/1	0.94	0.14	56,56,56,56	0
60	MG	BA	1698	1/1	0.94	0.20	57,57,57,57	0
60	MG	AY	502	1/1	0.94	0.15	54,54,54,54	0
60	MG	AA	3267	1/1	0.94	0.16	43,43,43,43	0
60	MG	CA	3179	1/1	0.94	0.15	27,27,27,27	0
60	MG	CA	3180	1/1	0.94	0.13	46,46,46,46	0
60	MG	BA	1701	1/1	0.94	0.17	47,47,47,47	0
60	MG	CA	3182	1/1	0.94	0.27	45,45,45,45	0
60	MG	AA	3641	1/1	0.94	0.11	45,45,45,45	0
60	MG	CA	3184	1/1	0.94	0.11	43,43,43,43	0
60	MG	CA	3414	1/1	0.94	0.10	50,50,50,50	0
60	MG	CA	3415	1/1	0.94	0.07	43,43,43,43	0
60	MG	CA	3417	1/1	0.94	0.09	58,58,58,58	0
60	MG	AA	3533	1/1	0.94	0.07	20,20,20,20	0
60	MG	AA	3048	1/1	0.94	0.07	39,39,39,39	0
60	MG	AA	3645	1/1	0.94	0.11	57,57,57,57	0
60	MG	AA	3323	1/1	0.94	0.09	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CA	3424	1/1	0.94	0.12	40,40,40,40	0
60	MG	A5	101	1/1	0.94	0.22	68,68,68,68	0
60	MG	AA	3761	1/1	0.94	0.16	72,72,72,72	0
60	MG	A6	101	1/1	0.94	0.11	75,75,75,75	0
60	MG	AA	3549	1/1	0.94	0.07	53,53,53,53	0
60	MG	A7	102	1/1	0.94	0.10	52,52,52,52	0
60	MG	A7	105	1/1	0.94	0.11	34,34,34,34	1
60	MG	AA	3424	1/1	0.94	0.08	48,48,48,48	0
60	MG	CA	3035	1/1	0.94	0.21	47,47,47,47	0
60	MG	CA	3438	1/1	0.94	0.14	45,45,45,45	0
60	MG	CA	3439	1/1	0.94	0.16	47,47,47,47	0
60	MG	DE	202	1/1	0.94	0.06	92,92,92,92	0
60	MG	A8	5002	1/1	0.94	0.11	45,45,45,45	0
60	MG	A9	502	1/1	0.94	0.21	52,52,52,52	0
60	MG	BA	1721	1/1	0.94	0.16	60,60,60,60	0
60	MG	AA	3553	1/1	0.94	0.10	47,47,47,47	0
60	MG	AA	3555	1/1	0.94	0.12	57,57,57,57	0
60	MG	CA	3455	1/1	0.94	0.12	37,37,37,37	0
61	K	AA	3814	1/1	0.94	0.17	87,87,87,87	0
60	MG	DA	1603	1/1	0.95	0.05	52,52,52,52	0
60	MG	AA	3149	1/1	0.95	0.12	15,15,15,15	0
60	MG	AA	3058	1/1	0.95	0.06	38,38,38,38	0
60	MG	AB	3008	1/1	0.95	0.22	46,46,46,46	0
60	MG	CA	3385	1/1	0.95	0.08	48,48,48,48	0
60	MG	AB	3009	1/1	0.95	0.10	62,62,62,62	0
60	MG	AA	3227	1/1	0.95	0.15	75,75,75,75	0
60	MG	BA	1812	1/1	0.95	0.07	47,47,47,47	0
60	MG	AA	3610	1/1	0.95	0.09	66,66,66,66	0
60	MG	DA	1613	1/1	0.95	0.23	50,50,50,50	0
60	MG	AA	3538	1/1	0.95	0.08	62,62,62,62	0
60	MG	AB	3016	1/1	0.95	0.08	47,47,47,47	0
60	MG	DA	1616	1/1	0.95	0.15	44,44,44,44	0
60	MG	AA	3539	1/1	0.95	0.09	42,42,42,42	0
60	MG	AA	3349	1/1	0.95	0.07	34,34,34,34	0
60	MG	AA	3544	1/1	0.95	0.05	16,16,16,16	0
60	MG	AA	3547	1/1	0.95	0.10	50,50,50,50	0
60	MG	AA	3311	1/1	0.95	0.12	46,46,46,46	0
60	MG	DA	1622	1/1	0.95	0.13	43,43,43,43	0
60	MG	AA	3411	1/1	0.95	0.07	21,21,21,21	0
60	MG	BT	3001	1/1	0.95	0.15	47,47,47,47	0
60	MG	CA	3400	1/1	0.95	0.08	48,48,48,48	0
60	MG	AA	3125	1/1	0.95	0.14	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3188	1/1	0.95	0.05	15,15,15,15	0
60	MG	AD	302	1/1	0.95	0.19	46,46,46,46	0
60	MG	BA	1718	1/1	0.95	0.07	48,48,48,48	0
60	MG	AD	303	1/1	0.95	0.11	31,31,31,31	0
60	MG	AA	3081	1/1	0.95	0.06	38,38,38,38	0
60	MG	AA	3683	1/1	0.95	0.10	40,40,40,40	0
60	MG	CA	3413	1/1	0.95	0.08	38,38,38,38	0
60	MG	DA	1637	1/1	0.95	0.14	61,61,61,61	0
60	MG	AA	3468	1/1	0.95	0.06	34,34,34,34	0
60	MG	AA	3762	1/1	0.95	0.12	63,63,63,63	0
60	MG	CA	3416	1/1	0.95	0.15	33,33,33,33	0
60	MG	BA	1634	1/1	0.95	0.24	71,71,71,71	0
60	MG	AD	311	1/1	0.95	0.22	63,63,63,63	0
60	MG	DA	1643	1/1	0.95	0.12	51,51,51,51	0
60	MG	AA	3168	1/1	0.95	0.12	60,60,60,60	0
60	MG	AA	3562	1/1	0.95	0.05	45,45,45,45	0
60	MG	CA	3241	1/1	0.95	0.10	69,69,69,69	0
60	MG	DA	1647	1/1	0.95	0.09	39,39,39,39	0
60	MG	AA	3261	1/1	0.95	0.17	53,53,53,53	0
60	MG	AA	3566	1/1	0.95	0.12	26,26,26,26	0
60	MG	BA	1733	1/1	0.95	0.05	57,57,57,57	0
60	MG	CA	3117	1/1	0.95	0.12	46,46,46,46	0
60	MG	AA	3627	1/1	0.95	0.13	53,53,53,53	0
60	MG	AA	3567	1/1	0.95	0.09	69,69,69,69	0
60	MG	AA	3629	1/1	0.95	0.12	51,51,51,51	0
60	MG	AA	3154	1/1	0.95	0.08	64,64,64,64	0
60	MG	BA	1739	1/1	0.95	0.07	52,52,52,52	0
60	MG	BA	1644	1/1	0.95	0.21	72,72,72,72	0
60	MG	CA	3600	1/1	0.95	0.07	60,60,60,60	0
60	MG	CA	3002	1/1	0.95	0.16	32,32,32,32	0
60	MG	AA	3425	1/1	0.95	0.12	40,40,40,40	0
60	MG	CA	3004	1/1	0.95	0.16	43,43,43,43	0
60	MG	CA	3604	1/1	0.95	0.10	54,54,54,54	0
60	MG	CA	3443	1/1	0.95	0.17	40,40,40,40	0
60	MG	CA	3005	1/1	0.95	0.17	69,69,69,69	0
60	MG	CA	3446	1/1	0.95	0.12	37,37,37,37	0
60	MG	BA	1742	1/1	0.95	0.04	45,45,45,45	0
60	MG	AA	3570	1/1	0.95	0.07	22,22,22,22	0
60	MG	AA	3699	1/1	0.95	0.12	61,61,61,61	0
60	MG	CA	3133	1/1	0.95	0.12	72,72,72,72	0
60	MG	BA	1649	1/1	0.95	0.28	56,56,56,56	0
60	MG	CA	3459	1/1	0.95	0.07	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	1650	1/1	0.95	0.18	49,49,49,49	0
60	MG	AA	3171	1/1	0.95	0.26	71,71,71,71	0
60	MG	CA	3137	1/1	0.95	0.22	64,64,64,64	0
60	MG	CA	3274	1/1	0.95	0.21	64,64,64,64	0
60	MG	DA	1681	1/1	0.95	0.10	44,44,44,44	0
60	MG	CA	3465	1/1	0.95	0.07	64,64,64,64	0
60	MG	AA	3236	1/1	0.95	0.12	61,61,61,61	0
60	MG	CA	3276	1/1	0.95	0.07	32,32,32,32	0
60	MG	DA	1685	1/1	0.95	0.13	49,49,49,49	0
60	MG	CA	3468	1/1	0.95	0.10	37,37,37,37	0
60	MG	DA	1687	1/1	0.95	0.11	60,60,60,60	0
60	MG	BA	1753	1/1	0.95	0.10	48,48,48,48	0
60	MG	AA	3636	1/1	0.95	0.14	71,71,71,71	0
60	MG	AA	3703	1/1	0.95	0.07	76,76,76,76	0
60	MG	CA	3028	1/1	0.95	0.21	60,60,60,60	0
60	MG	CA	3473	1/1	0.95	0.09	48,48,48,48	0
60	MG	AP	201	1/1	0.95	0.20	67,67,67,67	0
60	MG	AA	3363	1/1	0.95	0.18	47,47,47,47	0
60	MG	AA	3038	1/1	0.95	0.13	42,42,42,42	0
60	MG	AA	3786	1/1	0.95	0.15	57,57,57,57	0
60	MG	AQ	3003	1/1	0.95	0.13	37,37,37,37	0
60	MG	CA	3149	1/1	0.95	0.11	58,58,58,58	0
60	MG	AU	201	1/1	0.95	0.14	53,53,53,53	0
60	MG	AU	202	1/1	0.95	0.14	65,65,65,65	0
60	MG	DA	1703	1/1	0.95	0.06	59,59,59,59	0
60	MG	AA	3707	1/1	0.95	0.21	59,59,59,59	0
60	MG	CA	3153	1/1	0.95	0.16	54,54,54,54	0
60	MG	CA	3294	1/1	0.95	0.12	40,40,40,40	0
60	MG	AA	3085	1/1	0.95	0.17	80,80,80,80	0
60	MG	AA	3241	1/1	0.95	0.13	29,29,29,29	0
60	MG	AW	3004	1/1	0.95	0.09	45,45,45,45	0
60	MG	DA	1711	1/1	0.95	0.06	64,64,64,64	0
60	MG	CA	3299	1/1	0.95	0.06	42,42,42,42	0
60	MG	CA	3157	1/1	0.95	0.12	56,56,56,56	0
60	MG	CA	3651	1/1	0.95	0.15	41,41,41,41	0
60	MG	AA	3077	1/1	0.95	0.19	44,44,44,44	0
60	MG	CA	3159	1/1	0.95	0.23	42,42,42,42	0
60	MG	CA	3161	1/1	0.95	0.26	45,45,45,45	0
60	MG	AA	3712	1/1	0.95	0.11	50,50,50,50	0
60	MG	CA	3657	1/1	0.95	0.10	34,34,34,34	0
60	MG	AA	3131	1/1	0.95	0.12	39,39,39,39	0
60	MG	CA	3164	1/1	0.95	0.11	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CA	3165	1/1	0.95	0.31	58,58,58,58	0
60	MG	CA	3314	1/1	0.95	0.07	41,41,41,41	0
60	MG	CA	3317	1/1	0.95	0.08	61,61,61,61	0
60	MG	AA	3145	1/1	0.95	0.15	41,41,41,41	1
60	MG	DA	1728	1/1	0.95	0.10	53,53,53,53	0
60	MG	A0	103	1/1	0.95	0.08	67,67,67,67	0
60	MG	AA	3376	1/1	0.95	0.12	39,39,39,39	0
60	MG	AA	3717	1/1	0.95	0.13	47,47,47,47	0
60	MG	CB	3003	1/1	0.95	0.11	61,61,61,61	0
60	MG	CA	3328	1/1	0.95	0.07	40,40,40,40	0
60	MG	CB	3005	1/1	0.95	0.18	65,65,65,65	0
60	MG	A1	101	1/1	0.95	0.10	58,58,58,58	0
60	MG	AA	3296	1/1	0.95	0.10	40,40,40,40	0
60	MG	AA	3719	1/1	0.95	0.07	62,62,62,62	0
60	MG	CB	3009	1/1	0.95	0.12	66,66,66,66	0
60	MG	AA	3504	1/1	0.95	0.08	44,44,44,44	0
60	MG	AA	3507	1/1	0.95	0.12	53,53,53,53	0
60	MG	AA	3219	1/1	0.95	0.11	38,38,38,38	0
60	MG	AA	3806	1/1	0.95	0.18	56,56,56,56	0
60	MG	A7	101	1/1	0.95	0.14	41,41,41,41	0
60	MG	AA	3035	1/1	0.95	0.12	69,69,69,69	0
60	MG	AA	3512	1/1	0.95	0.08	32,32,32,32	0
60	MG	BA	1792	1/1	0.95	0.07	61,61,61,61	0
60	MG	CA	3346	1/1	0.95	0.19	48,48,48,48	0
60	MG	CA	3347	1/1	0.95	0.07	37,37,37,37	0
60	MG	CA	3062	1/1	0.95	0.06	41,41,41,41	0
60	MG	AA	3729	1/1	0.95	0.05	40,40,40,40	0
60	MG	AA	3515	1/1	0.95	0.08	27,27,27,27	0
60	MG	CA	3065	1/1	0.95	0.13	56,56,56,56	0
60	MG	CA	3192	1/1	0.95	0.22	47,47,47,47	0
60	MG	AA	3299	1/1	0.95	0.15	64,64,64,64	0
60	MG	AA	3733	1/1	0.95	0.06	40,40,40,40	0
60	MG	BA	1797	1/1	0.95	0.13	75,75,75,75	0
60	MG	AA	3079	1/1	0.95	0.05	27,27,27,27	0
60	MG	CO	202	1/1	0.95	0.10	53,53,53,53	0
60	MG	CP	201	1/1	0.95	0.07	57,57,57,57	0
60	MG	CA	3364	1/1	0.95	0.23	64,64,64,64	0
60	MG	CA	3533	1/1	0.95	0.07	63,63,63,63	0
60	MG	AA	3343	1/1	0.95	0.05	60,60,60,60	0
60	MG	CA	3198	1/1	0.95	0.23	49,49,49,49	0
60	MG	AA	3392	1/1	0.95	0.09	31,31,31,31	0
60	MG	CR	202	1/1	0.95	0.18	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3529	1/1	0.95	0.08	12,12,12,12	1
60	MG	AA	3397	1/1	0.95	0.10	41,41,41,41	0
60	MG	AB	3002	1/1	0.95	0.16	55,55,55,55	0
60	MG	CY	502	1/1	0.95	0.12	53,53,53,53	0
60	MG	DK	201	1/1	0.95	0.12	55,55,55,55	0
60	MG	C0	101	1/1	0.95	0.06	50,50,50,50	0
60	MG	AB	3003	1/1	0.95	0.07	40,40,40,40	0
60	MG	CA	3076	1/1	0.95	0.14	48,48,48,48	0
60	MG	AA	3742	1/1	0.95	0.11	68,68,68,68	0
60	MG	DZ	701	1/1	0.95	0.13	47,47,47,47	0
60	MG	CA	3078	1/1	0.95	0.07	49,49,49,49	0
62	ZN	C4	501	1/1	0.95	0.06	163,163,163,163	0
64	GDP	BZ	702	28/28	0.95	0.08	57,57,57,57	1
64	GDP	DZ	702	28/28	0.95	0.07	69,69,69,69	0
60	MG	CA	3315	1/1	0.96	0.09	44,44,44,44	0
60	MG	BA	1648	1/1	0.96	0.10	28,28,28,28	0
60	MG	AA	3429	1/1	0.96	0.09	58,58,58,58	0
60	MG	AA	3042	1/1	0.96	0.09	43,43,43,43	0
60	MG	AA	3371	1/1	0.96	0.06	21,21,21,21	0
60	MG	AA	3635	1/1	0.96	0.06	33,33,33,33	0
60	MG	CA	3326	1/1	0.96	0.09	54,54,54,54	0
60	MG	AA	3043	1/1	0.96	0.13	39,39,39,39	0
60	MG	AU	204	1/1	0.96	0.15	55,55,55,55	0
60	MG	AA	3493	1/1	0.96	0.13	56,56,56,56	0
60	MG	AV	204	1/1	0.96	0.14	46,46,46,46	0
60	MG	AA	3374	1/1	0.96	0.05	22,22,22,22	0
60	MG	CA	3621	1/1	0.96	0.10	55,55,55,55	0
60	MG	AA	3072	1/1	0.96	0.03	20,20,20,20	0
60	MG	AA	3801	1/1	0.96	0.06	39,39,39,39	0
60	MG	CA	3335	1/1	0.96	0.07	38,38,38,38	0
60	MG	DA	1652	1/1	0.96	0.10	68,68,68,68	0
60	MG	CA	3336	1/1	0.96	0.09	64,64,64,64	0
60	MG	AA	3714	1/1	0.96	0.12	44,44,44,44	0
60	MG	AA	3122	1/1	0.96	0.12	39,39,39,39	0
60	MG	BA	1752	1/1	0.96	0.05	48,48,48,48	0
60	MG	CA	3105	1/1	0.96	0.05	47,47,47,47	0
60	MG	CA	3211	1/1	0.96	0.08	19,19,19,19	0
60	MG	CA	3345	1/1	0.96	0.09	41,41,41,41	0
60	MG	AA	3153	1/1	0.96	0.12	47,47,47,47	0
60	MG	CA	3493	1/1	0.96	0.18	66,66,66,66	0
60	MG	AA	3345	1/1	0.96	0.05	34,34,34,34	0
60	MG	CA	3637	1/1	0.96	0.14	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3107	1/1	0.96	0.07	51,51,51,51	0
60	MG	DA	1666	1/1	0.96	0.14	45,45,45,45	0
60	MG	AA	3584	1/1	0.96	0.10	63,63,63,63	0
60	MG	AA	3585	1/1	0.96	0.08	60,60,60,60	0
60	MG	CA	3217	1/1	0.96	0.09	52,52,52,52	0
60	MG	A1	102	1/1	0.96	0.05	46,46,46,46	0
60	MG	AA	3226	1/1	0.96	0.08	51,51,51,51	0
60	MG	CA	3358	1/1	0.96	0.08	41,41,41,41	0
60	MG	AA	3587	1/1	0.96	0.07	44,44,44,44	0
60	MG	AA	3348	1/1	0.96	0.11	39,39,39,39	0
60	MG	CA	3013	1/1	0.96	0.11	52,52,52,52	0
60	MG	CA	3224	1/1	0.96	0.12	32,32,32,32	0
60	MG	CA	3650	1/1	0.96	0.08	42,42,42,42	0
60	MG	AA	3287	1/1	0.96	0.06	25,25,25,25	0
60	MG	DA	1680	1/1	0.96	0.10	40,40,40,40	0
60	MG	BA	1764	1/1	0.96	0.10	55,55,55,55	0
60	MG	CA	3508	1/1	0.96	0.09	74,74,74,74	0
60	MG	AA	3288	1/1	0.96	0.08	39,39,39,39	0
60	MG	AA	3446	1/1	0.96	0.05	25,25,25,25	0
60	MG	CA	3656	1/1	0.96	0.20	75,75,75,75	0
60	MG	AA	3321	1/1	0.96	0.09	45,45,45,45	0
60	MG	AA	3518	1/1	0.96	0.09	28,28,28,28	0
60	MG	CA	3024	1/1	0.96	0.35	67,67,67,67	0
60	MG	AA	3524	1/1	0.96	0.19	41,41,41,41	0
60	MG	AA	3084	1/1	0.96	0.08	27,27,27,27	0
60	MG	CA	3378	1/1	0.96	0.16	63,63,63,63	0
60	MG	BA	1679	1/1	0.96	0.10	51,51,51,51	0
60	MG	BA	1775	1/1	0.96	0.10	47,47,47,47	0
60	MG	CA	3128	1/1	0.96	0.08	31,31,31,31	0
60	MG	AA	3172	1/1	0.96	0.07	50,50,50,50	0
60	MG	DA	1697	1/1	0.96	0.14	67,67,67,67	0
60	MG	CA	3522	1/1	0.96	0.07	25,25,25,25	0
60	MG	CA	3130	1/1	0.96	0.09	57,57,57,57	0
60	MG	AA	3006	1/1	0.96	0.11	56,56,56,56	0
60	MG	AA	3451	1/1	0.96	0.13	43,43,43,43	0
60	MG	CA	3034	1/1	0.96	0.10	51,51,51,51	0
60	MG	AA	3326	1/1	0.96	0.05	22,22,22,22	0
60	MG	AA	3603	1/1	0.96	0.08	68,68,68,68	0
60	MG	DA	1705	1/1	0.96	0.10	61,61,61,61	0
60	MG	AA	3665	1/1	0.96	0.06	63,63,63,63	0
60	MG	BA	1783	1/1	0.96	0.07	61,61,61,61	0
60	MG	AA	3666	1/1	0.96	0.15	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3746	1/1	0.96	0.14	62,62,62,62	0
60	MG	AA	3532	1/1	0.96	0.09	20,20,20,20	0
60	MG	AB	3015	1/1	0.96	0.11	51,51,51,51	0
60	MG	AA	3008	1/1	0.96	0.07	28,28,28,28	0
60	MG	AA	3606	1/1	0.96	0.19	62,62,62,62	0
60	MG	CA	3254	1/1	0.96	0.08	35,35,35,35	0
60	MG	CA	3402	1/1	0.96	0.09	46,46,46,46	0
60	MG	DA	1716	1/1	0.96	0.15	56,56,56,56	0
60	MG	AA	3004	1/1	0.96	0.05	30,30,30,30	0
60	MG	CA	3256	1/1	0.96	0.14	73,73,73,73	0
60	MG	AA	3608	1/1	0.96	0.07	66,66,66,66	0
60	MG	AA	3413	1/1	0.96	0.06	34,34,34,34	0
60	MG	AA	3091	1/1	0.96	0.12	62,62,62,62	0
60	MG	AA	3676	1/1	0.96	0.05	46,46,46,46	0
60	MG	CF	304	1/1	0.96	0.05	46,46,46,46	0
60	MG	CF	305	1/1	0.96	0.06	45,45,45,45	0
60	MG	CA	3263	1/1	0.96	0.09	50,50,50,50	0
60	MG	AA	3678	1/1	0.96	0.08	62,62,62,62	0
60	MG	CN	5001	1/1	0.96	0.05	64,64,64,64	0
60	MG	AA	3416	1/1	0.96	0.09	31,31,31,31	0
60	MG	AA	3542	1/1	0.96	0.05	47,47,47,47	0
60	MG	AA	3543	1/1	0.96	0.17	84,84,84,84	0
60	MG	AD	304	1/1	0.96	0.10	46,46,46,46	0
60	MG	AA	3417	1/1	0.96	0.07	16,16,16,16	0
60	MG	CA	3272	1/1	0.96	0.09	56,56,56,56	0
60	MG	AA	3274	1/1	0.96	0.20	48,48,48,48	1
60	MG	CA	3421	1/1	0.96	0.09	39,39,39,39	0
60	MG	AA	3684	1/1	0.96	0.06	47,47,47,47	0
60	MG	AD	309	1/1	0.96	0.09	49,49,49,49	0
60	MG	CA	3061	1/1	0.96	0.11	36,36,36,36	0
60	MG	CA	3562	1/1	0.96	0.11	69,69,69,69	0
60	MG	AA	3685	1/1	0.96	0.12	58,58,58,58	0
60	MG	AA	3686	1/1	0.96	0.10	62,62,62,62	0
60	MG	DA	1744	1/1	0.96	0.11	57,57,57,57	0
60	MG	AA	3548	1/1	0.96	0.08	69,69,69,69	0
60	MG	BA	1711	1/1	0.96	0.26	63,63,63,63	0
60	MG	AA	3617	1/1	0.96	0.08	32,32,32,32	0
60	MG	C7	101	1/1	0.96	0.12	47,47,47,47	0
60	MG	DA	1601	1/1	0.96	0.09	59,59,59,59	0
60	MG	CA	3432	1/1	0.96	0.06	29,29,29,29	0
60	MG	AA	3467	1/1	0.96	0.09	54,54,54,54	0
60	MG	AA	3014	1/1	0.96	0.18	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CA	3435	1/1	0.96	0.10	55,55,55,55	0
60	MG	AA	3552	1/1	0.96	0.14	73,73,73,73	0
60	MG	AA	3472	1/1	0.96	0.11	37,37,37,37	0
60	MG	AF	304	1/1	0.96	0.11	31,31,31,31	0
60	MG	CA	3289	1/1	0.96	0.08	23,23,23,23	0
60	MG	AA	3473	1/1	0.96	0.06	57,57,57,57	0
60	MG	AA	3774	1/1	0.96	0.08	44,44,44,44	0
60	MG	DA	1760	1/1	0.96	0.09	53,53,53,53	0
60	MG	BF	3001	1/1	0.96	0.08	49,49,49,49	0
60	MG	CA	3448	1/1	0.96	0.08	64,64,64,64	0
60	MG	CA	3449	1/1	0.96	0.14	52,52,52,52	0
60	MG	AA	3556	1/1	0.96	0.09	54,54,54,54	0
60	MG	AA	3132	1/1	0.96	0.21	43,43,43,43	0
60	MG	AA	3423	1/1	0.96	0.12	53,53,53,53	0
60	MG	CA	3456	1/1	0.96	0.07	37,37,37,37	0
60	MG	AA	3697	1/1	0.96	0.09	71,71,71,71	0
60	MG	AA	3366	1/1	0.96	0.10	35,35,35,35	0
60	MG	CA	3080	1/1	0.96	0.17	78,78,78,78	0
60	MG	AA	3367	1/1	0.96	0.15	52,52,52,52	0
60	MG	CA	3461	1/1	0.96	0.05	46,46,46,46	0
60	MG	CA	3185	1/1	0.96	0.14	47,47,47,47	0
60	MG	DA	1627	1/1	0.96	0.19	48,48,48,48	0
60	MG	BA	1728	1/1	0.96	0.09	53,53,53,53	0
60	MG	AA	3480	1/1	0.96	0.14	78,78,78,78	0
60	MG	CA	3189	1/1	0.96	0.05	40,40,40,40	0
60	MG	AA	3259	1/1	0.96	0.27	27,27,27,27	0
60	MG	AA	3427	1/1	0.96	0.10	34,34,34,34	0
60	MG	CA	3087	1/1	0.96	0.21	107,107,107,107	0
60	MG	AA	3237	1/1	0.96	0.06	51,51,51,51	0
60	MG	DA	1635	1/1	0.96	0.22	61,61,61,61	0
60	MG	CA	3082	1/1	0.97	0.14	31,31,31,31	0
60	MG	AA	3482	1/1	0.97	0.11	46,46,46,46	0
60	MG	CA	3313	1/1	0.97	0.12	54,54,54,54	0
60	MG	AA	3483	1/1	0.97	0.05	21,21,21,21	0
60	MG	AA	3022	1/1	0.97	0.03	19,19,19,19	0
60	MG	CA	3316	1/1	0.97	0.06	34,34,34,34	0
60	MG	AA	3485	1/1	0.97	0.06	34,34,34,34	0
60	MG	AA	3229	1/1	0.97	0.05	33,33,33,33	0
60	MG	BA	1734	1/1	0.97	0.08	35,35,35,35	0
60	MG	AA	3792	1/1	0.97	0.16	35,35,35,35	0
60	MG	CA	3323	1/1	0.97	0.08	32,32,32,32	0
60	MG	CA	3324	1/1	0.97	0.10	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CA	3620	1/1	0.97	0.07	41,41,41,41	0
60	MG	AR	201	1/1	0.97	0.13	51,51,51,51	0
60	MG	AA	3286	1/1	0.97	0.10	48,48,48,48	0
60	MG	DA	1653	1/1	0.97	0.07	29,29,29,29	0
60	MG	AA	3794	1/1	0.97	0.09	47,47,47,47	0
60	MG	AA	3118	1/1	0.97	0.10	59,59,59,59	0
60	MG	CA	3625	1/1	0.97	0.11	46,46,46,46	0
60	MG	AA	3023	1/1	0.97	0.17	40,40,40,40	1
60	MG	AV	202	1/1	0.97	0.12	56,56,56,56	0
60	MG	AA	3572	1/1	0.97	0.07	51,51,51,51	0
60	MG	AA	3232	1/1	0.97	0.19	58,58,58,58	0
60	MG	BA	1744	1/1	0.97	0.04	48,48,48,48	0
60	MG	CA	3099	1/1	0.97	0.18	55,55,55,55	0
60	MG	AA	3184	1/1	0.97	0.14	39,39,39,39	0
60	MG	AW	3002	1/1	0.97	0.11	59,59,59,59	0
60	MG	AA	3133	1/1	0.97	0.20	92,92,92,92	1
60	MG	AA	3187	1/1	0.97	0.07	29,29,29,29	0
60	MG	AA	3373	1/1	0.97	0.08	23,23,23,23	0
60	MG	AA	3647	1/1	0.97	0.05	35,35,35,35	0
60	MG	CA	3344	1/1	0.97	0.07	27,27,27,27	0
60	MG	AA	3496	1/1	0.97	0.04	43,43,43,43	0
60	MG	AA	3649	1/1	0.97	0.05	78,78,78,78	0
60	MG	AA	3722	1/1	0.97	0.08	31,31,31,31	0
60	MG	AA	3087	1/1	0.97	0.12	62,62,62,62	0
60	MG	CA	3110	1/1	0.97	0.14	35,35,35,35	0
60	MG	AA	3501	1/1	0.97	0.07	45,45,45,45	0
60	MG	AA	3726	1/1	0.97	0.07	74,74,74,74	0
60	MG	CA	3353	1/1	0.97	0.09	48,48,48,48	0
60	MG	CA	3354	1/1	0.97	0.07	40,40,40,40	0
60	MG	CA	3008	1/1	0.97	0.15	52,52,52,52	0
60	MG	CA	3356	1/1	0.97	0.07	28,28,28,28	0
60	MG	CA	3223	1/1	0.97	0.11	46,46,46,46	0
60	MG	BA	1759	1/1	0.97	0.07	60,60,60,60	0
60	MG	CA	3359	1/1	0.97	0.10	44,44,44,44	0
60	MG	AA	3727	1/1	0.97	0.09	64,64,64,64	0
60	MG	CA	3012	1/1	0.97	0.05	41,41,41,41	0
60	MG	AA	3097	1/1	0.97	0.13	29,29,29,29	0
60	MG	AA	3377	1/1	0.97	0.05	19,19,19,19	0
60	MG	AA	3505	1/1	0.97	0.06	29,29,29,29	0
60	MG	A5	104	1/1	0.97	0.05	46,46,46,46	0
60	MG	CA	3019	1/1	0.97	0.06	23,23,23,23	0
60	MG	CA	3020	1/1	0.97	0.09	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	DA	1693	1/1	0.97	0.08	50,50,50,50	0
60	MG	AA	3338	1/1	0.97	0.09	49,49,49,49	0
60	MG	AA	3030	1/1	0.97	0.11	44,44,44,44	1
60	MG	AA	3735	1/1	0.97	0.09	30,30,30,30	0
60	MG	CA	3375	1/1	0.97	0.04	65,65,65,65	0
60	MG	BA	1769	1/1	0.97	0.12	80,80,80,80	0
60	MG	CA	3025	1/1	0.97	0.20	32,32,32,32	1
60	MG	AA	3510	1/1	0.97	0.06	13,13,13,13	0
60	MG	BA	1771	1/1	0.97	0.08	48,48,48,48	0
60	MG	CA	3520	1/1	0.97	0.05	27,27,27,27	0
60	MG	AA	3239	1/1	0.97	0.13	63,63,63,63	0
60	MG	BA	1680	1/1	0.97	0.05	50,50,50,50	0
60	MG	AA	3211	1/1	0.97	0.19	53,53,53,53	0
60	MG	AA	3593	1/1	0.97	0.06	49,49,49,49	0
60	MG	AA	3594	1/1	0.97	0.15	48,48,48,48	0
60	MG	AA	3069	1/1	0.97	0.06	32,32,32,32	0
60	MG	BA	1778	1/1	0.97	0.10	52,52,52,52	0
60	MG	AA	3384	1/1	0.97	0.05	26,26,26,26	0
60	MG	AA	3124	1/1	0.97	0.10	39,39,39,39	1
60	MG	CA	3038	1/1	0.97	0.10	26,26,26,26	0
60	MG	AB	3011	1/1	0.97	0.10	47,47,47,47	0
60	MG	CA	3040	1/1	0.97	0.09	63,63,63,63	0
60	MG	AA	3303	1/1	0.97	0.08	30,30,30,30	0
60	MG	CA	3395	1/1	0.97	0.07	60,60,60,60	0
60	MG	AA	3521	1/1	0.97	0.12	30,30,30,30	0
60	MG	AA	3394	1/1	0.97	0.08	22,22,22,22	0
60	MG	AA	3304	1/1	0.97	0.10	44,44,44,44	0
60	MG	AA	3139	1/1	0.97	0.13	64,64,64,64	0
60	MG	AA	3527	1/1	0.97	0.08	20,20,20,20	0
60	MG	CA	3148	1/1	0.97	0.05	41,41,41,41	0
60	MG	AA	3528	1/1	0.97	0.09	26,26,26,26	0
60	MG	CA	3404	1/1	0.97	0.06	46,46,46,46	0
60	MG	CA	3405	1/1	0.97	0.06	50,50,50,50	0
60	MG	DA	1726	1/1	0.97	0.12	58,58,58,58	0
60	MG	CA	3264	1/1	0.97	0.10	54,54,54,54	0
60	MG	AA	3452	1/1	0.97	0.07	53,53,53,53	0
60	MG	CA	3408	1/1	0.97	0.11	35,35,35,35	0
60	MG	AA	3453	1/1	0.97	0.08	51,51,51,51	0
60	MG	AA	3401	1/1	0.97	0.08	26,26,26,26	0
60	MG	CA	3268	1/1	0.97	0.11	46,46,46,46	0
60	MG	BA	1616	1/1	0.97	0.05	69,69,69,69	0
60	MG	AA	3456	1/1	0.97	0.09	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3216	1/1	0.97	0.07	68,68,68,68	0
60	MG	AA	3535	1/1	0.97	0.05	37,37,37,37	0
60	MG	AA	3217	1/1	0.97	0.05	50,50,50,50	0
60	MG	AA	3406	1/1	0.97	0.06	52,52,52,52	0
60	MG	AA	3350	1/1	0.97	0.11	54,54,54,54	0
60	MG	AA	3540	1/1	0.97	0.06	28,28,28,28	0
60	MG	AA	3174	1/1	0.97	0.10	39,39,39,39	0
60	MG	CA	3563	1/1	0.97	0.17	30,30,30,30	0
60	MG	CA	3279	1/1	0.97	0.11	46,46,46,46	0
60	MG	BA	1707	1/1	0.97	0.12	57,57,57,57	0
60	MG	C8	5001	1/1	0.97	0.11	43,43,43,43	0
60	MG	CA	3567	1/1	0.97	0.06	42,42,42,42	0
60	MG	AA	3312	1/1	0.97	0.08	25,25,25,25	0
60	MG	CA	3425	1/1	0.97	0.11	45,45,45,45	0
60	MG	AA	3465	1/1	0.97	0.06	49,49,49,49	0
60	MG	AA	3031	1/1	0.97	0.17	29,29,29,29	1
60	MG	AA	3012	1/1	0.97	0.07	38,38,38,38	0
60	MG	AA	3045	1/1	0.97	0.12	58,58,58,58	0
60	MG	AA	3178	1/1	0.97	0.18	50,50,50,50	0
60	MG	CA	3172	1/1	0.97	0.11	41,41,41,41	0
60	MG	BA	1714	1/1	0.97	0.11	44,44,44,44	0
60	MG	CA	3174	1/1	0.97	0.06	31,31,31,31	0
60	MG	AA	3771	1/1	0.97	0.13	40,40,40,40	0
60	MG	BA	1810	1/1	0.97	0.08	39,39,39,39	0
60	MG	CA	3437	1/1	0.97	0.09	41,41,41,41	0
60	MG	AA	3115	1/1	0.97	0.25	44,44,44,44	0
60	MG	AA	3359	1/1	0.97	0.10	31,31,31,31	0
60	MG	AA	3144	1/1	0.97	0.12	48,48,48,48	0
60	MG	CA	3441	1/1	0.97	0.06	37,37,37,37	0
60	MG	AA	3361	1/1	0.97	0.06	33,33,33,33	0
60	MG	BA	1720	1/1	0.97	0.07	51,51,51,51	0
60	MG	CA	3297	1/1	0.97	0.06	55,55,55,55	0
60	MG	AA	3477	1/1	0.97	0.05	47,47,47,47	0
60	MG	CA	3594	1/1	0.97	0.08	62,62,62,62	0
60	MG	DA	1625	1/1	0.97	0.04	38,38,38,38	0
60	MG	AA	3557	1/1	0.97	0.05	21,21,21,21	0
60	MG	AA	3478	1/1	0.97	0.06	70,70,70,70	0
60	MG	CA	3450	1/1	0.97	0.09	38,38,38,38	0
60	MG	AA	3322	1/1	0.97	0.07	37,37,37,37	0
60	MG	CA	3186	1/1	0.97	0.09	49,49,49,49	0
60	MG	CA	3453	1/1	0.97	0.06	43,43,43,43	0
60	MG	AA	3560	1/1	0.97	0.07	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CA	3304	1/1	0.97	0.08	48,48,48,48	0
60	MG	AA	3256	1/1	0.97	0.14	24,24,24,24	0
60	MG	CA	3307	1/1	0.97	0.09	31,31,31,31	0
62	ZN	DN	501	1/1	0.97	0.04	120,120,120,120	0
60	MG	AA	3785	1/1	0.97	0.12	54,54,54,54	0
60	MG	CA	3310	1/1	0.97	0.11	45,45,45,45	0
60	MG	AA	3224	1/1	0.98	0.04	26,26,26,26	0
60	MG	AA	3112	1/1	0.98	0.12	44,44,44,44	0
60	MG	AA	3643	1/1	0.98	0.06	56,56,56,56	0
60	MG	DA	1669	1/1	0.98	0.12	63,63,63,63	0
60	MG	AA	3709	1/1	0.98	0.24	39,39,39,39	0
60	MG	AA	3128	1/1	0.98	0.14	53,53,53,53	1
60	MG	AA	3519	1/1	0.98	0.06	39,39,39,39	0
60	MG	CA	3436	1/1	0.98	0.05	34,34,34,34	0
60	MG	AA	3039	1/1	0.98	0.15	34,34,34,34	0
60	MG	CA	3327	1/1	0.98	0.08	37,37,37,37	0
60	MG	AA	3522	1/1	0.98	0.06	31,31,31,31	0
60	MG	AA	3523	1/1	0.98	0.08	35,35,35,35	0
60	MG	AG	202	1/1	0.98	0.04	41,41,41,41	0
60	MG	AA	3114	1/1	0.98	0.15	55,55,55,55	0
60	MG	AA	3463	1/1	0.98	0.07	41,41,41,41	0
60	MG	CA	3444	1/1	0.98	0.10	70,70,70,70	0
60	MG	AA	3020	1/1	0.98	0.04	25,25,25,25	0
60	MG	AA	3335	1/1	0.98	0.04	14,14,14,14	0
60	MG	CA	3447	1/1	0.98	0.03	44,44,44,44	0
60	MG	AA	3301	1/1	0.98	0.11	59,59,59,59	0
60	MG	AO	5001	1/1	0.98	0.05	43,43,43,43	0
60	MG	AA	3302	1/1	0.98	0.19	58,58,58,58	0
60	MG	AP	202	1/1	0.98	0.22	35,35,35,35	0
60	MG	AA	3422	1/1	0.98	0.07	22,22,22,22	0
60	MG	AA	3469	1/1	0.98	0.07	37,37,37,37	0
60	MG	AA	3185	1/1	0.98	0.14	35,35,35,35	0
60	MG	AA	3658	1/1	0.98	0.06	25,25,25,25	0
60	MG	AA	3166	1/1	0.98	0.07	52,52,52,52	0
60	MG	AR	202	1/1	0.98	0.04	34,34,34,34	0
60	MG	CA	3574	1/1	0.98	0.05	31,31,31,31	0
60	MG	AA	3534	1/1	0.98	0.12	34,34,34,34	0
60	MG	AA	3305	1/1	0.98	0.07	38,38,38,38	0
60	MG	BA	1729	1/1	0.98	0.08	38,38,38,38	0
60	MG	AA	3306	1/1	0.98	0.05	3,3,3,3	0
60	MG	AA	3730	1/1	0.98	0.11	34,34,34,34	0
60	MG	CA	3580	1/1	0.98	0.05	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CA	3352	1/1	0.98	0.09	40,40,40,40	0
60	MG	AV	201	1/1	0.98	0.07	45,45,45,45	0
60	MG	AA	3375	1/1	0.98	0.04	16,16,16,16	0
60	MG	AA	3255	1/1	0.98	0.08	64,64,64,64	0
60	MG	CA	3586	1/1	0.98	0.14	75,75,75,75	0
60	MG	BM	201	1/1	0.98	0.05	60,60,60,60	0
60	MG	CA	3252	1/1	0.98	0.11	30,30,30,30	0
60	MG	AA	3116	1/1	0.98	0.21	36,36,36,36	0
60	MG	AA	3430	1/1	0.98	0.04	23,23,23,23	0
60	MG	BA	1654	1/1	0.98	0.04	45,45,45,45	0
60	MG	CA	3160	1/1	0.98	0.14	33,33,33,33	0
60	MG	CA	3362	1/1	0.98	0.04	20,20,20,20	0
60	MG	AA	3431	1/1	0.98	0.06	25,25,25,25	0
60	MG	CA	3258	1/1	0.98	0.08	54,54,54,54	0
60	MG	CA	3259	1/1	0.98	0.08	19,19,19,19	0
60	MG	AW	3003	1/1	0.98	0.13	38,38,38,38	0
60	MG	CA	3367	1/1	0.98	0.10	39,39,39,39	0
60	MG	CA	3368	1/1	0.98	0.07	45,45,45,45	0
60	MG	AA	3668	1/1	0.98	0.06	25,25,25,25	0
60	MG	AA	3481	1/1	0.98	0.04	53,53,53,53	0
60	MG	AA	3432	1/1	0.98	0.09	24,24,24,24	0
60	MG	CA	3166	1/1	0.98	0.10	31,31,31,31	0
60	MG	AA	3545	1/1	0.98	0.04	64,64,64,64	0
60	MG	AA	3546	1/1	0.98	0.05	36,36,36,36	0
60	MG	AA	3007	1/1	0.98	0.03	18,18,18,18	0
60	MG	AA	3674	1/1	0.98	0.03	56,56,56,56	0
60	MG	CA	3171	1/1	0.98	0.27	48,48,48,48	0
60	MG	DA	1612	1/1	0.98	0.04	46,46,46,46	0
60	MG	AA	3169	1/1	0.98	0.09	36,36,36,36	0
60	MG	CA	3380	1/1	0.98	0.07	37,37,37,37	0
60	MG	DA	1732	1/1	0.98	0.07	54,54,54,54	0
60	MG	BA	1749	1/1	0.98	0.13	52,52,52,52	0
60	MG	AA	3103	1/1	0.98	0.09	11,11,11,11	0
60	MG	AA	3677	1/1	0.98	0.11	26,26,26,26	0
60	MG	AA	3550	1/1	0.98	0.09	47,47,47,47	0
60	MG	CA	3615	1/1	0.98	0.08	33,33,33,33	0
60	MG	AA	3313	1/1	0.98	0.11	31,31,31,31	0
60	MG	AB	3007	1/1	0.98	0.03	37,37,37,37	0
60	MG	CA	3277	1/1	0.98	0.05	43,43,43,43	0
60	MG	AA	3750	1/1	0.98	0.04	26,26,26,26	0
60	MG	AA	3382	1/1	0.98	0.05	29,29,29,29	0
60	MG	AA	3488	1/1	0.98	0.08	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3554	1/1	0.98	0.04	48,48,48,48	0
60	MG	AB	3012	1/1	0.98	0.07	24,24,24,24	1
60	MG	AA	3314	1/1	0.98	0.11	43,43,43,43	0
60	MG	A7	103	1/1	0.98	0.06	39,39,39,39	0
60	MG	A7	104	1/1	0.98	0.07	49,49,49,49	0
60	MG	CA	3627	1/1	0.98	0.09	59,59,59,59	0
60	MG	AA	3052	1/1	0.98	0.11	15,15,15,15	0
60	MG	A7	106	1/1	0.98	0.06	57,57,57,57	0
60	MG	CA	3006	1/1	0.98	0.03	24,24,24,24	0
60	MG	AA	3385	1/1	0.98	0.06	24,24,24,24	0
60	MG	CA	3401	1/1	0.98	0.05	75,75,75,75	0
60	MG	AA	3037	1/1	0.98	0.04	12,12,12,12	0
60	MG	CA	3009	1/1	0.98	0.03	24,24,24,24	0
60	MG	AA	3389	1/1	0.98	0.08	46,46,46,46	0
60	MG	AA	3082	1/1	0.98	0.32	57,57,57,57	1
60	MG	AA	3155	1/1	0.98	0.15	31,31,31,31	0
60	MG	AA	3395	1/1	0.98	0.05	21,21,21,21	0
60	MG	CA	3014	1/1	0.98	0.09	58,58,58,58	0
60	MG	AA	3497	1/1	0.98	0.04	36,36,36,36	0
60	MG	AA	3009	1/1	0.98	0.04	26,26,26,26	0
60	MG	CA	3017	1/1	0.98	0.04	28,28,28,28	0
60	MG	AA	3355	1/1	0.98	0.04	19,19,19,19	0
60	MG	DA	1766	1/1	0.98	0.04	41,41,41,41	0
60	MG	AA	3074	1/1	0.98	0.14	26,26,26,26	0
60	MG	AA	3075	1/1	0.98	0.07	47,47,47,47	0
60	MG	CA	3525	1/1	0.98	0.04	30,30,30,30	0
60	MG	AA	3086	1/1	0.98	0.14	43,43,43,43	1
60	MG	AA	3404	1/1	0.98	0.07	50,50,50,50	0
60	MG	BA	1611	1/1	0.98	0.08	31,31,31,31	0
60	MG	AD	305	1/1	0.98	0.17	49,49,49,49	0
60	MG	AA	3405	1/1	0.98	0.06	27,27,27,27	0
60	MG	AA	3292	1/1	0.98	0.10	31,31,31,31	0
60	MG	CA	3027	1/1	0.98	0.02	29,29,29,29	0
60	MG	CA	3422	1/1	0.98	0.08	43,43,43,43	0
60	MG	AA	3454	1/1	0.98	0.07	27,27,27,27	0
60	MG	AA	3244	1/1	0.98	0.15	42,42,42,42	0
60	MG	AA	3577	1/1	0.98	0.06	65,65,65,65	0
62	ZN	A4	501	1/1	0.98	0.04	120,120,120,120	0
60	MG	AA	3776	1/1	0.98	0.05	21,21,21,21	0
60	MG	AA	3514	1/1	0.98	0.09	32,32,32,32	0
63	SF4	DD	501	8/8	0.98	0.04	71,71,71,71	0
60	MG	AA	3076	1/1	0.98	0.04	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CA	3318	1/1	0.98	0.07	31,31,31,31	0
60	MG	BA	1745	1/1	0.99	0.04	46,46,46,46	0
60	MG	AA	3754	1/1	0.99	0.03	25,25,25,25	0
60	MG	AA	3393	1/1	0.99	0.04	18,18,18,18	0
60	MG	AA	3513	1/1	0.99	0.08	37,37,37,37	0
60	MG	CA	3547	1/1	0.99	0.02	57,57,57,57	1
60	MG	AE	303	1/1	0.99	0.08	23,23,23,23	0
60	MG	AA	3011	1/1	0.99	0.04	27,27,27,27	0
60	MG	AA	3218	1/1	0.99	0.07	10,10,10,10	0
60	MG	AF	301	1/1	0.99	0.18	40,40,40,40	0
60	MG	AA	3340	1/1	0.99	0.03	3,3,3,3	0
60	MG	AA	3398	1/1	0.99	0.09	29,29,29,29	0
60	MG	AA	3189	1/1	0.99	0.07	31,31,31,31	0
60	MG	AA	3400	1/1	0.99	0.03	19,19,19,19	0
60	MG	AA	3520	1/1	0.99	0.07	34,34,34,34	0
60	MG	AA	3003	1/1	0.99	0.03	14,14,14,14	0
60	MG	AF	308	1/1	0.99	0.03	48,48,48,48	0
60	MG	CA	3559	1/1	0.99	0.03	30,30,30,30	0
60	MG	AA	3457	1/1	0.99	0.04	18,18,18,18	0
60	MG	AA	3212	1/1	0.99	0.16	43,43,43,43	0
60	MG	CA	3248	1/1	0.99	0.03	58,58,58,58	0
60	MG	CA	3306	1/1	0.99	0.04	39,39,39,39	0
60	MG	AA	3148	1/1	0.99	0.08	48,48,48,48	0
60	MG	CA	3565	1/1	0.99	0.06	36,36,36,36	0
60	MG	AA	3328	1/1	0.99	0.06	21,21,21,21	0
60	MG	CA	3309	1/1	0.99	0.06	50,50,50,50	0
60	MG	AA	3818	1/1	0.99	0.06	37,37,37,37	0
60	MG	AA	3253	1/1	0.99	0.08	42,42,42,42	0
60	MG	AA	3330	1/1	0.99	0.08	33,33,33,33	0
60	MG	CA	3571	1/1	0.99	0.06	52,52,52,52	0
60	MG	AA	3564	1/1	0.99	0.09	17,17,17,17	0
60	MG	BA	1768	1/1	0.99	0.09	64,64,64,64	0
60	MG	AA	3565	1/1	0.99	0.06	26,26,26,26	0
60	MG	AA	3407	1/1	0.99	0.07	22,22,22,22	0
60	MG	AA	3223	1/1	0.99	0.03	21,21,21,21	0
60	MG	CA	3381	1/1	0.99	0.08	37,37,37,37	0
60	MG	AA	3775	1/1	0.99	0.07	52,52,52,52	0
60	MG	CA	3649	1/1	0.99	0.06	15,15,15,15	0
60	MG	CA	3319	1/1	0.99	0.03	32,32,32,32	0
60	MG	AA	3013	1/1	0.99	0.06	38,38,38,38	0
60	MG	AA	3053	1/1	0.99	0.08	21,21,21,21	0
60	MG	AA	3257	1/1	0.99	0.12	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3734	1/1	0.99	0.03	23,23,23,23	0
60	MG	AA	3386	1/1	0.99	0.09	19,19,19,19	0
60	MG	CA	3585	1/1	0.99	0.04	44,44,44,44	0
60	MG	CA	3208	1/1	0.99	0.09	24,24,24,24	0
60	MG	AA	3781	1/1	0.99	0.04	49,49,49,49	0
60	MG	CA	3454	1/1	0.99	0.09	43,43,43,43	0
60	MG	AA	3499	1/1	0.99	0.05	46,46,46,46	0
60	MG	AA	3737	1/1	0.99	0.04	25,25,25,25	0
60	MG	AA	3500	1/1	0.99	0.03	27,27,27,27	0
60	MG	AA	3574	1/1	0.99	0.06	26,26,26,26	0
60	MG	AA	3536	1/1	0.99	0.04	36,36,36,36	0
60	MG	AA	3387	1/1	0.99	0.09	34,34,34,34	0
60	MG	AA	3502	1/1	0.99	0.04	41,41,41,41	0
60	MG	AA	3415	1/1	0.99	0.08	29,29,29,29	0
60	MG	AA	3790	1/1	0.99	0.07	11,11,11,11	0
60	MG	CA	3528	1/1	0.99	0.06	51,51,51,51	1
60	MG	AA	3319	1/1	0.99	0.06	28,28,28,28	0
60	MG	CA	3337	1/1	0.99	0.04	27,27,27,27	0
60	MG	AA	3090	1/1	0.99	0.06	52,52,52,52	0
60	MG	AA	3506	1/1	0.99	0.06	19,19,19,19	0
60	MG	CA	3340	1/1	0.99	0.06	38,38,38,38	0
60	MG	AA	3418	1/1	0.99	0.08	22,22,22,22	0
60	MG	AA	3583	1/1	0.99	0.07	18,18,18,18	0
60	MG	A0	102	1/1	0.99	0.03	41,41,41,41	0
60	MG	AA	3508	1/1	0.99	0.06	42,42,42,42	0
60	MG	AA	3706	1/1	0.99	0.21	26,26,26,26	1
62	ZN	BN	501	1/1	0.99	0.03	83,83,83,83	0
62	ZN	CY	501	1/1	0.99	0.03	92,92,92,92	0
60	MG	AA	3798	1/1	0.99	0.05	34,34,34,34	0
60	MG	CD	304	1/1	0.99	0.08	32,32,32,32	0
63	SF4	BD	501	8/8	0.99	0.04	67,67,67,67	0
60	MG	AA	3390	1/1	0.99	0.05	23,23,23,23	0
60	MG	AA	3391	1/1	0.99	0.06	27,27,27,27	0
60	MG	AA	3307	1/1	0.99	0.03	35,35,35,35	0
62	ZN	A5	103	1/1	1.00	0.02	40,40,40,40	0
62	ZN	A6	103	1/1	1.00	0.02	47,47,47,47	0
62	ZN	A9	501	1/1	1.00	0.03	45,45,45,45	0
60	MG	AA	3723	1/1	1.00	0.04	30,30,30,30	0
60	MG	AA	3588	1/1	1.00	0.06	33,33,33,33	0
60	MG	AA	3410	1/1	1.00	0.03	19,19,19,19	0
62	ZN	C5	102	1/1	1.00	0.02	66,66,66,66	0
62	ZN	C6	501	1/1	1.00	0.02	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
62	ZN	C9	501	1/1	1.00	0.01	70,70,70,70	0
60	MG	AA	3396	1/1	1.00	0.06	22,22,22,22	0
60	MG	AA	3470	1/1	1.00	0.01	24,24,24,24	0
60	MG	AA	3471	1/1	1.00	0.06	24,24,24,24	0
62	ZN	AY	501	1/1	1.00	0.01	68,68,68,68	0
60	MG	CA	3370	1/1	1.00	0.02	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.