



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 29, 2026 – 10:53 AM UTC

PDB ID : 4WQU / pdb_00004wqu
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with elongation factor G trapped by the antibiotic dityromycin
Authors : Lin, J.; Gagnon, M.G.; Steitz, T.A.
Deposited on : 2014-10-22
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

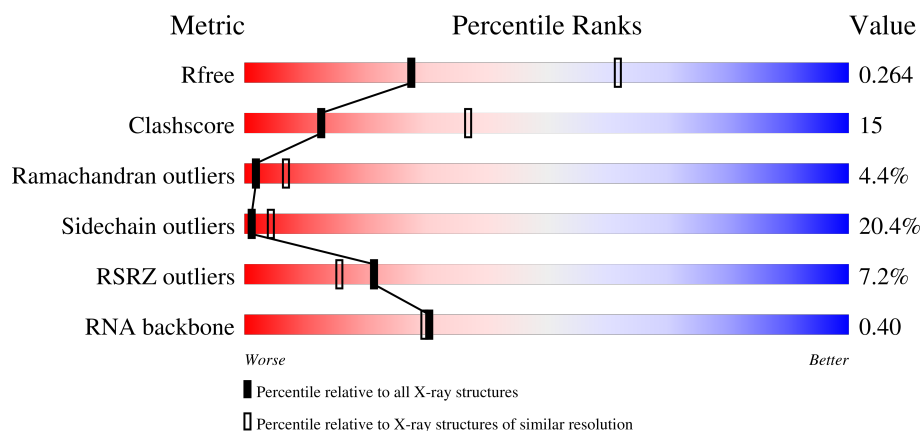
1 Overall quality at a glance

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	56% 34% 9%
1	CA	2915	2% 47% 42% 10%
2	AB	121	66% 31%
2	CB	121	4% 39% 50% 11%

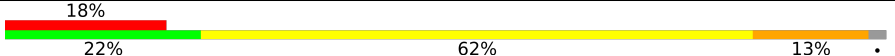
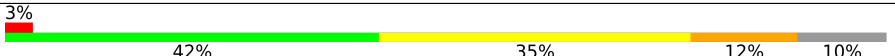
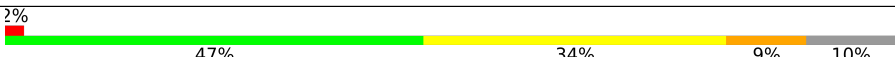
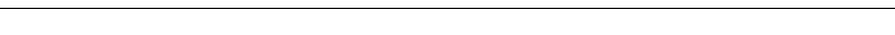
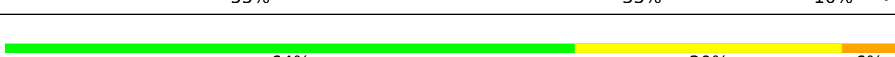
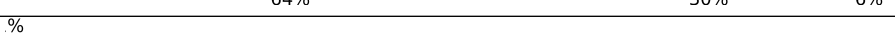
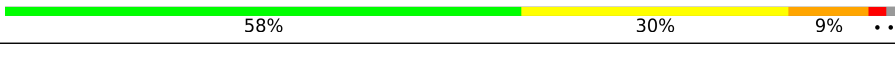
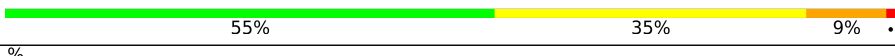
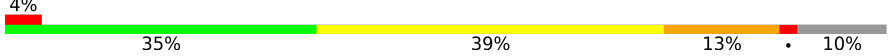
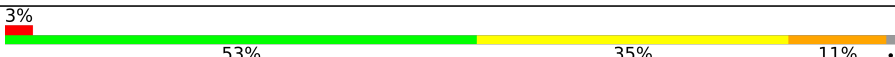
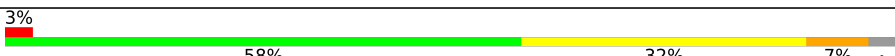
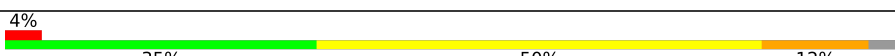
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Mol	Chain	Length	Quality of chain
3	AC	228	
3	CC	228	
4	AD	276	
4	CD	276	
5	AE	206	
5	CE	206	
6	AF	210	
6	CF	210	
7	AG	182	
7	CG	182	
8	AH	180	
8	CH	180	
9	AK	173	
9	CK	173	
10	AL	147	
10	CL	147	
11	AN	140	
11	CN	140	
12	AO	122	
12	CO	122	
13	AP	150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

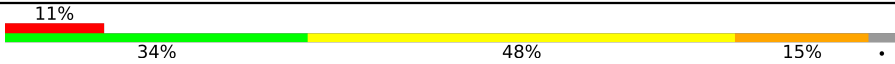
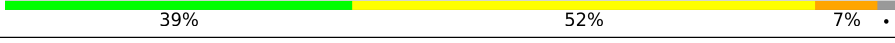
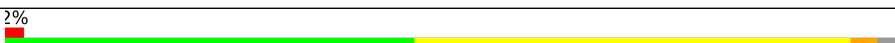
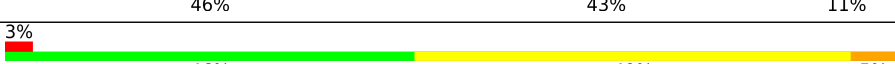
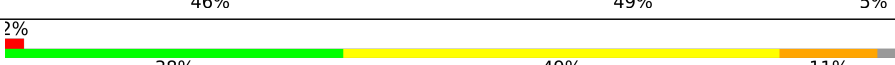
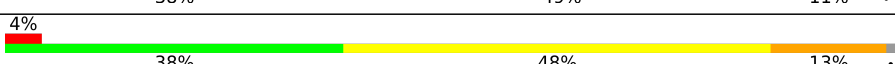
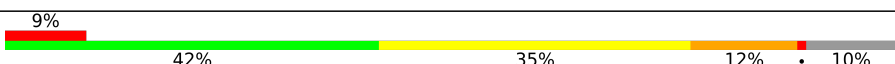
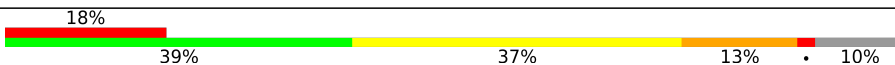
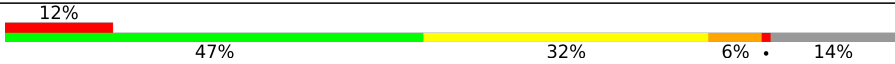
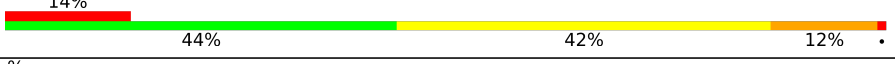
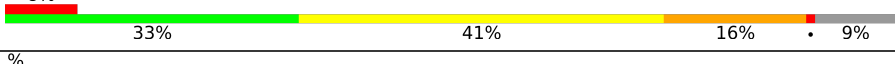
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Mol	Chain	Length	Quality of chain
15	CR	118	
16	AS	112	
16	CS	112	
17	AT	146	
17	CT	146	
18	AU	118	
18	CU	118	
19	AV	101	
19	CV	101	
20	AW	113	
20	CW	113	
21	AX	96	
21	CX	96	
22	AY	110	
22	CY	110	
23	AZ	206	
23	CZ	206	
24	A0	85	
24	C0	85	
25	A1	98	
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	18	
55	DV	18	
56	BW	76	
56	BY	76	
56	DW	76	
56	DY	76	
57	BZ	758	
57	DZ	758	
58	BX	10	
58	DX	10	

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
58	2QY	DX	10	-	-	X	-
59	MG	AA	3056	-	-	-	X
59	MG	AA	3093	-	-	-	X
59	MG	AA	3108	-	-	-	X
59	MG	AA	3717	-	-	-	X
59	MG	AA	3773	-	-	-	X
59	MG	DA	1611	-	-	-	X
61	SF4	DD	501	-	-	X	-

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 310038 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	185	Total	C	N	O	S	0	0	0
			1451	927	258	264	2			
23	CZ	185	Total	C	N	O	S	0	0	0
			1451	927	258	264	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	A0	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
24	C0	77	Total	C	N	O	S	0	0	0
			608	375	129	103	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	S	0	0	0
			469	298	90	81				
27	C3	59	Total	C	N	O	S	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	1495	Total	C	N	O	P	0	0	0
			32141	14304	5958	10384	1495			
34	DA	1501	Total	C	N	O	P	0	0	0
			32268	14361	5980	10426	1501			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	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	117	Total	C	N	O	S	0	0	0
			923	570	191	160	2			
46	DM	116	Total	C	N	O	S	0	0	0
			907	558	188	159	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	7	Total	C	N	O	P	0	0	0
			148	67	27	47	7			
55	DV	6	Total	C	N	O	P	0	0	0
			123	57	22	39	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BW	76	Total	C	N	O	P	S	0	0
			1631	731	290	532	76	2		
56	BY	74	Total	C	N	O	P	S	0	0
			1581	707	285	515	73	1		
56	DW	76	Total	C	N	O	P	S	0	0
			1631	731	290	532	76	2		
56	DY	73	Total	C	N	O	P	S	0	0
			1561	698	283	507	72	1		

- Molecule 57 is a protein called 50S ribosomal protein L9,Elongation factor G.

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

- Molecule 58 is a protein called Dityromycin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	BX	10	Total	C	N	O	0	0	0
			93	67	10	16			
58	DX	10	Total	C	N	O	0	0	0
			93	67	10	16			

- Molecule 59 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AA	821	Total	Mg	0	0
			821	821		
59	AB	23	Total	Mg	0	0
			23	23		
59	AD	12	Total	Mg	0	0
			12	12		
59	AE	5	Total	Mg	0	0
			5	5		
59	AF	8	Total	Mg	0	0
			8	8		
59	AG	2	Total	Mg	0	0
			2	2		
59	AH	1	Total	Mg	0	0
			1	1		
59	AN	3	Total	Mg	0	0
			3	3		
59	AO	1	Total	Mg	0	0
			1	1		
59	AP	4	Total	Mg	0	0
			4	4		
59	AQ	3	Total	Mg	0	0
			3	3		
59	AR	2	Total	Mg	0	0
			2	2		
59	AU	3	Total	Mg	0	0
			3	3		
59	AV	6	Total	Mg	0	0
			6	6		
59	AW	3	Total	Mg	0	0
			3	3		
59	AX	1	Total	Mg	0	0
			1	1		
59	AY	1	Total	Mg	0	0
			1	1		
59	AZ	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	A0	5	Total 5	Mg 5	0	0
59	A2	1	Total 1	Mg 1	0	0
59	A5	1	Total 1	Mg 1	0	0
59	A6	2	Total 2	Mg 2	0	0
59	A7	4	Total 4	Mg 4	0	0
59	A8	1	Total 1	Mg 1	0	0
59	A9	1	Total 1	Mg 1	0	0
59	BA	215	Total 215	Mg 215	0	0
59	BB	1	Total 1	Mg 1	0	0
59	BD	1	Total 1	Mg 1	0	0
59	BE	1	Total 1	Mg 1	0	0
59	BF	1	Total 1	Mg 1	0	0
59	BK	1	Total 1	Mg 1	0	0
59	BL	2	Total 2	Mg 2	0	0
59	BM	1	Total 1	Mg 1	0	0
59	BN	2	Total 2	Mg 2	0	0
59	BS	1	Total 1	Mg 1	0	0
59	BT	1	Total 1	Mg 1	0	0
59	BW	3	Total 3	Mg 3	0	0
59	BZ	1	Total 1	Mg 1	0	0
59	CA	664	Total 664	Mg 664	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	CB	13	Total 13	Mg 13	0	0
59	CD	4	Total 4	Mg 4	0	0
59	CE	5	Total 5	Mg 5	0	0
59	CF	4	Total 4	Mg 4	0	0
59	CG	1	Total 1	Mg 1	0	0
59	CN	1	Total 1	Mg 1	0	0
59	CO	1	Total 1	Mg 1	0	0
59	CP	1	Total 1	Mg 1	0	0
59	CQ	4	Total 4	Mg 4	0	0
59	CR	1	Total 1	Mg 1	0	0
59	CU	1	Total 1	Mg 1	0	0
59	CV	2	Total 2	Mg 2	0	0
59	CW	1	Total 1	Mg 1	0	0
59	CX	1	Total 1	Mg 1	0	0
59	C0	1	Total 1	Mg 1	0	0
59	C1	1	Total 1	Mg 1	0	0
59	C3	1	Total 1	Mg 1	0	0
59	C5	1	Total 1	Mg 1	0	0
59	C7	1	Total 1	Mg 1	0	0
59	C8	1	Total 1	Mg 1	0	0
59	DA	171	Total 171	Mg 171	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	DD	1	Total 1	Mg 1	0	0
59	DE	2	Total 2	Mg 2	0	0
59	DF	1	Total 1	Mg 1	0	0
59	DJ	1	Total 1	Mg 1	0	0
59	DK	1	Total 1	Mg 1	0	0
59	DT	1	Total 1	Mg 1	0	0
59	DW	3	Total 3	Mg 3	0	0
59	DZ	2	Total 2	Mg 2	0	0

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

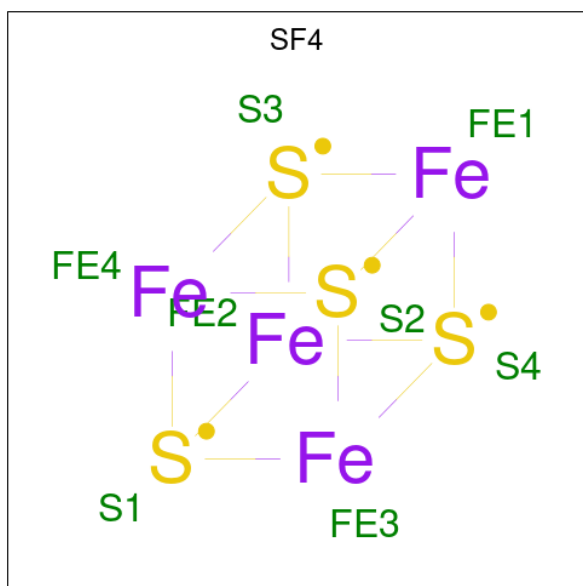
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AY	1	Total 1	Zn 1	0	0
60	A4	1	Total 1	Zn 1	0	0
60	A5	1	Total 1	Zn 1	0	0
60	A6	1	Total 1	Zn 1	0	0
60	A9	1	Total 1	Zn 1	0	0
60	BN	1	Total 1	Zn 1	0	0
60	CY	1	Total 1	Zn 1	0	0
60	C4	1	Total 1	Zn 1	0	0
60	C5	1	Total 1	Zn 1	0	0
60	C6	1	Total 1	Zn 1	0	0
60	C9	1	Total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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	DN	1	Total	Zn	0	0
			1	1		

- Molecule 61 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$).

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	AQ	4	Total	O	0	0
			4	4		
63	AR	2	Total	O	0	0
			2	2		
63	AS	1	Total	O	0	0
			1	1		
63	AT	1	Total	O	0	0
			1	1		
63	AU	4	Total	O	0	0
			4	4		
63	AV	1	Total	O	0	0
			1	1		
63	AW	1	Total	O	0	0
			1	1		
63	AX	3	Total	O	0	0
			3	3		
63	AZ	1	Total	O	0	0
			1	1		
63	A0	6	Total	O	0	0
			6	6		
63	A1	2	Total	O	0	0
			2	2		
63	A3	2	Total	O	0	0
			2	2		
63	A5	3	Total	O	0	0
			3	3		
63	A6	1	Total	O	0	0
			1	1		
63	A7	2	Total	O	0	0
			2	2		
63	A8	10	Total	O	0	0
			10	10		
63	A9	1	Total	O	0	0
			1	1		
63	BA	213	Total	O	0	0
			213	213		
63	BD	1	Total	O	0	0
			1	1		
63	BM	1	Total	O	0	0
			1	1		
63	BO	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	BP	1	Total	O	0	0
			1	1		
63	BV	1	Total	O	0	0
			1	1		
63	BW	1	Total	O	0	0
			1	1		
63	BZ	2	Total	O	0	0
			2	2		
63	CA	983	Total	O	0	0
			983	983		
63	CB	9	Total	O	0	0
			9	9		
63	CD	15	Total	O	0	0
			15	15		
63	CE	9	Total	O	0	0
			9	9		
63	CF	6	Total	O	0	0
			6	6		
63	CN	1	Total	O	0	0
			1	1		
63	CO	1	Total	O	0	0
			1	1		
63	CP	11	Total	O	0	0
			11	11		
63	CQ	2	Total	O	0	0
			2	2		
63	CT	3	Total	O	0	0
			3	3		
63	CU	2	Total	O	0	0
			2	2		
63	CV	1	Total	O	0	0
			1	1		
63	CW	1	Total	O	0	0
			1	1		
63	CX	1	Total	O	0	0
			1	1		
63	CY	2	Total	O	0	0
			2	2		
63	C0	4	Total	O	0	0
			4	4		
63	C3	2	Total	O	0	0
			2	2		

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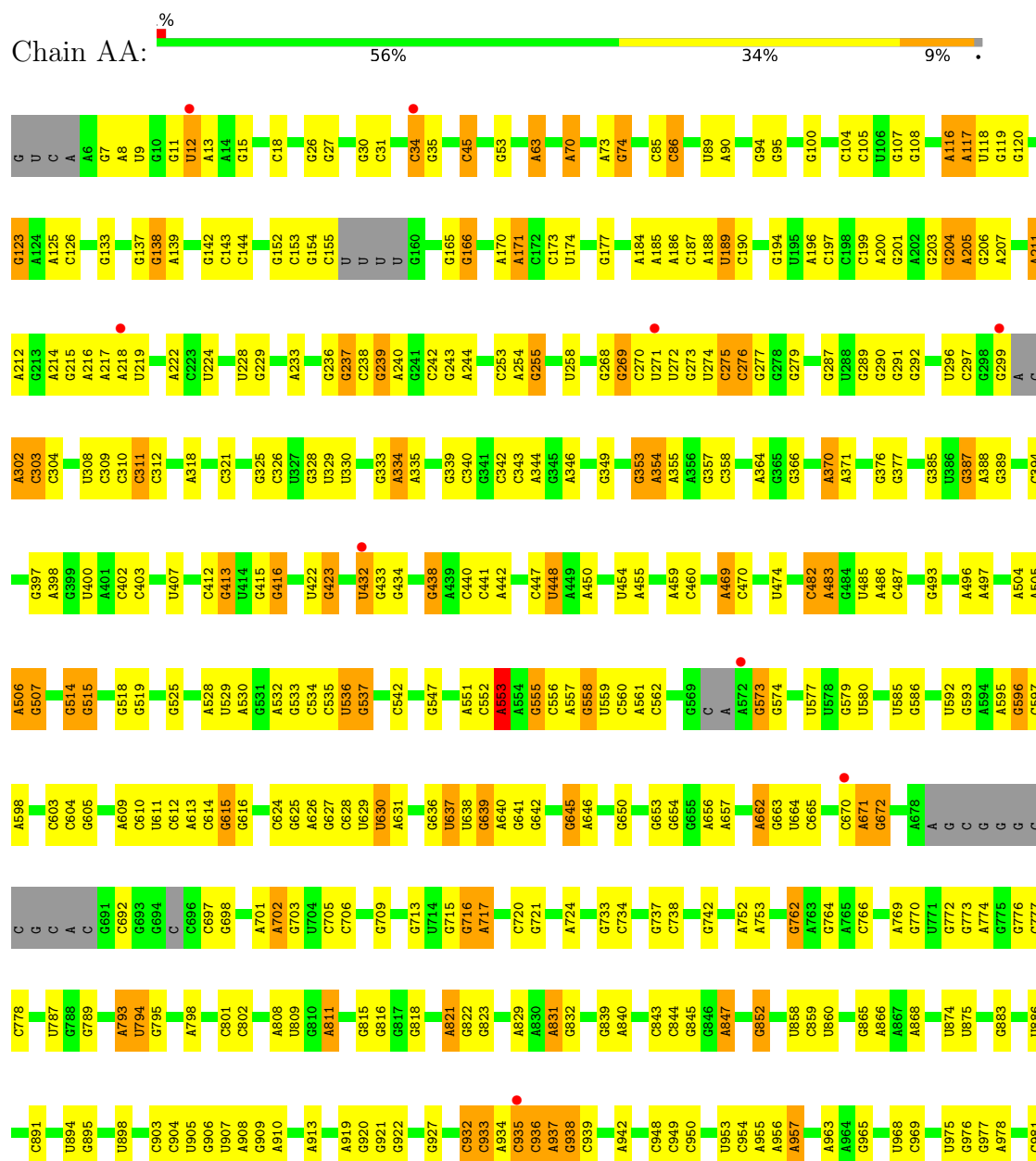
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	C5	1	Total 1	O 1	0	0
63	C7	2	Total 2	O 2	0	0
63	C8	4	Total 4	O 4	0	0
63	DA	157	Total 157	O 157	0	0
63	DD	1	Total 1	O 1	0	0
63	DE	2	Total 2	O 2	0	0
63	DH	1	Total 1	O 1	0	0
63	DJ	1	Total 1	O 1	0	0
63	DK	2	Total 2	O 2	0	0
63	DL	1	Total 1	O 1	0	0
63	DT	1	Total 1	O 1	0	0

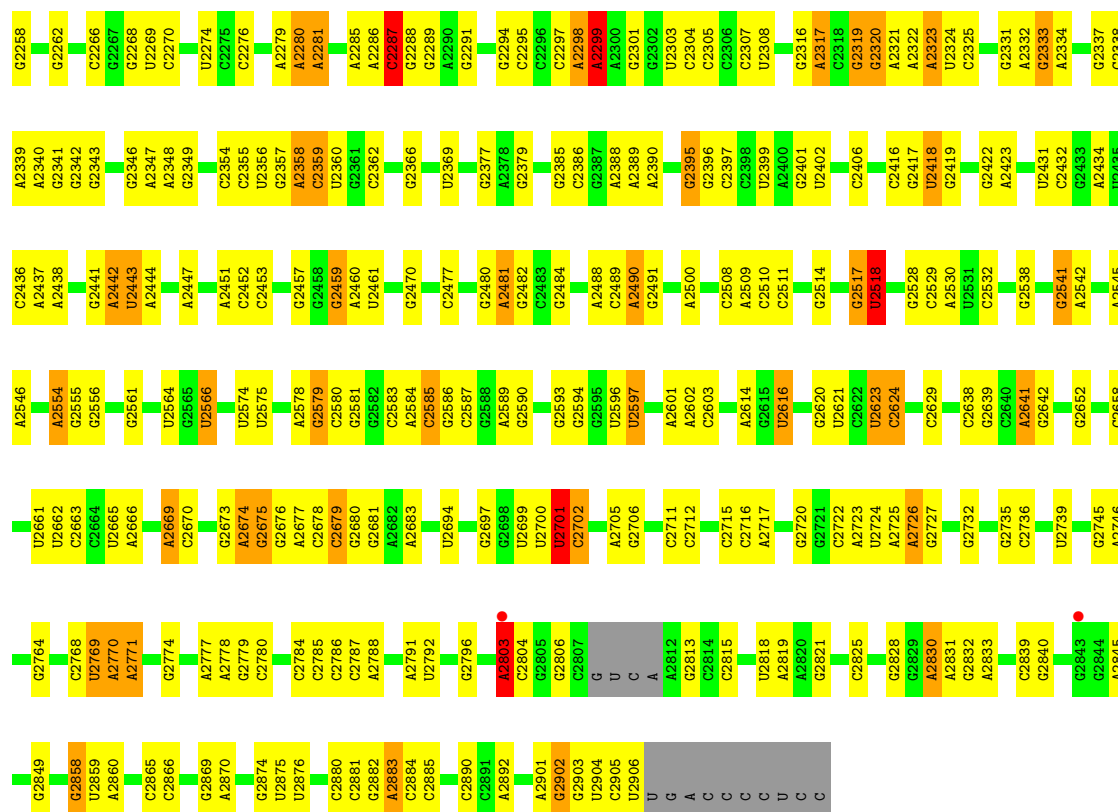
3 Residue-property plots

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.

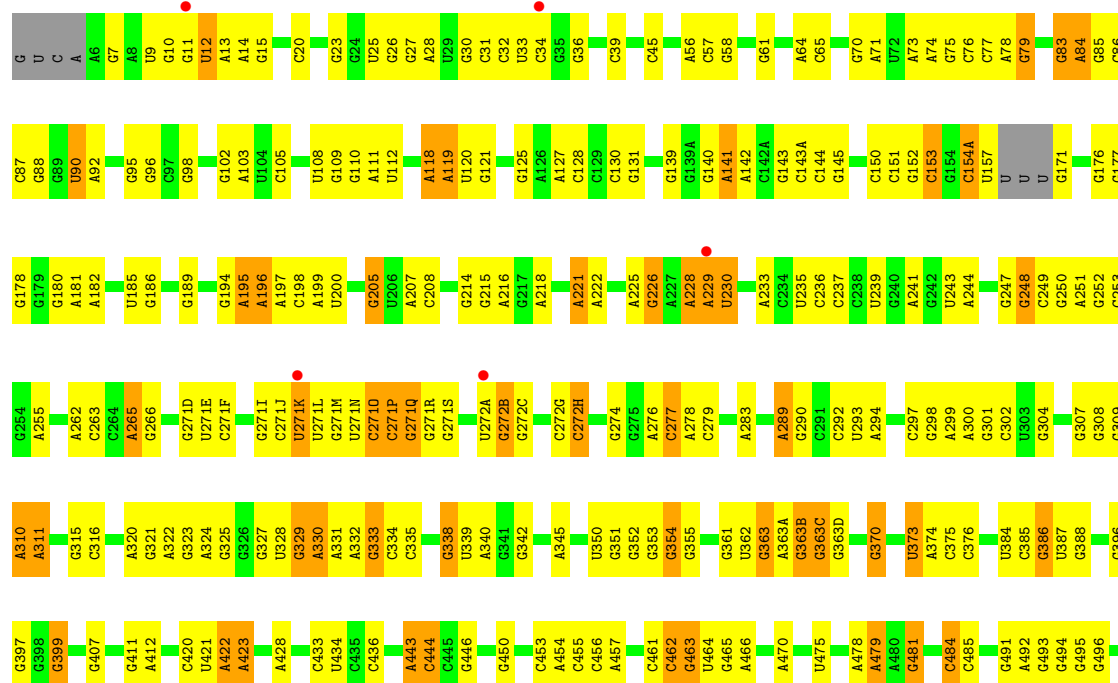
• Molecule 1: 23S Ribosomal RNA



G2184	C2021	G1794	C1695	G1586	G1506	G1417	A1315	G1221	C1138	U1072	U982
C2185	G2022	G1795	G1696	U1587	A1507	U1418	C1316	A1222	G1145	A1073	G983
G2186	A2023	A1804	G1700	G1588	G1508	G1423	G1317	C1223	A1141	A1074	A986
G2187	G2024	U1809	A1701	C1590	C1514	G1423	A1324	C1225	G1145	U1079	G989
G2188	A2027	U1810	A1711	C1594	A1518	A1425	U1328	G1228	A1149	G1080	G990
G2189	C2028	U1812	G1712	C1595	A1519	G1426	U1331	G1231	C1150	U1081	G991
G2190	U2033	A1814	G1717	C1596	G1520	A1430	G1331	G1232	U1151	G1082	G992
A2191	U2033	A1815	C1717	C1597	A1524	A1430	G1337	G1233	G1152	C1083	A998
U2194	A2036	A1816	G1721	C1598	G1525	A1438	U1338	G1234	U1154	G1087	G1001
A2195	U2044	A1817	G1722	A1600	G1526	A1439	C1339	G1235	C1155	A1002	A1002
C2196	G2045	A1822	C1722	G1600	G1529	U1440	U1340	G1236	A1157	U1003	A1004
C2197	U2050	G1823	A1723	C1604	G1530	U1441	C1343	G1237	G1158	A1092	A1005
A2198	C2054	U1825	G1725	G1606	G1531	U1442	C1346	U1243	U1159	G1093	C1006
C2199	A2055	C1826	C1730	G1607	G1532	C1450	U1347	U1244	G1160	A1094	C1012
C2200	A2055	U1827	C1731	A1613	G1533	U1451	A1348	G1246	C1170	C1095	G1013
C2201	C2054	C1828	A1736	A1614	U1534	U1452	G1349	C1246	G1171	G1097	U1014
G2204	C2058	U1829	A1737	G1615	U1535	C1453	C1352	A1249	U1176	C1098	C1015
G2205	G2058	G1830	C1738	A1616	C1539	C1454	C1352	G1251	G1177	A1100	C1016
G2206	U1953	U1831	U1739	C1624	A1540	C1455	G1355	A1255	G1178	G1101	G1019
G2207	G1955	G1832	U1740	U1625	A1541	C1462	G1356	U1256	U1179	C1102	C1020
G2208	C2065	A1834	C1741	A1626	C1544	G1463	G1360	G1261	A1180	A1103	A1026
G2209	A2064	U1843	A1744	G1628	C1548	G1464	U1369	G1261	G1181	G1104	G1105
U2211	C2065	A1846	G1746	C1629	C1550	U1466	C1361	A1265	G1183	U1106	A1029
G2212	A2073	U1847	A1747	G1631	C1551	G1470	G1370	C1270	G1184	U1107	A1030
G2213	G2074	G1853	A1748	A1632	A1554	G1471	G1374	A1271	U1186	G1109	G1035
G2214	C2077	G1854	G1749	C1633	A1554	G1472	U1375	A1272	U1187	C1110	A1036
G2215	C2077	G1857	G1750	C1635	C1555	A1473	G1376	G1273	U1188	U1111	C1037
G2216	A2079	U1857	G1752	U1636	A1556	C1474	A1377	G1274	A1189	U1112	U1113
G2217	G2079	G1887	U1753	U1644	A1557	G1475	G1384	G1275	G1195	A1113	C1040
G2218	C2085	G1888	G1764	C1645	C1558	C1476	G1385	G1278	C1196	G1114	C1041
G2219	C2086	U1870	G1765	C1645	C1559	G1480	U1386	C1279	A1116	A1042	A1047
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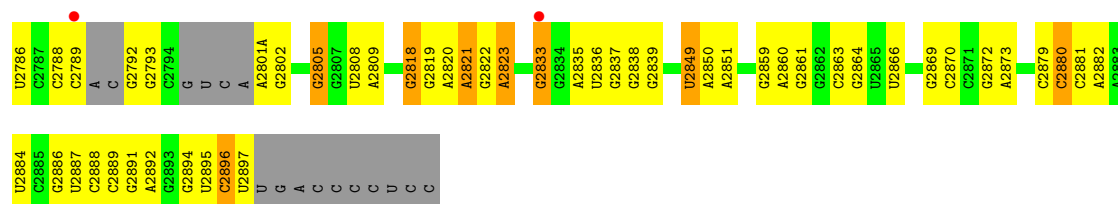


• Molecule 1: 23S Ribosomal RNA

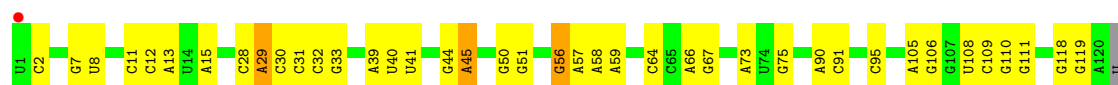




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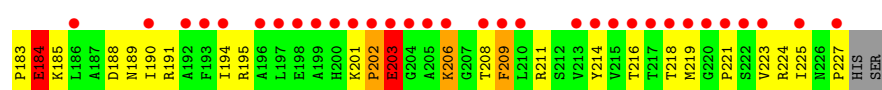
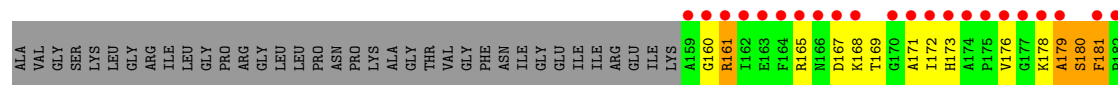
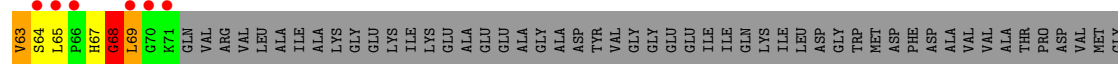
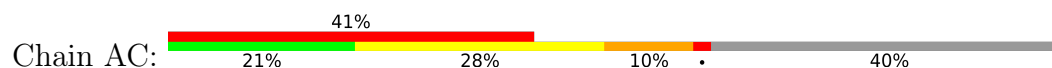
• Molecule 2: 5S Ribosomal RNA



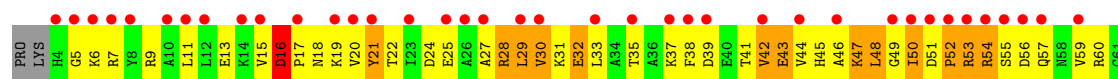
• Molecule 2: 5S Ribosomal RNA

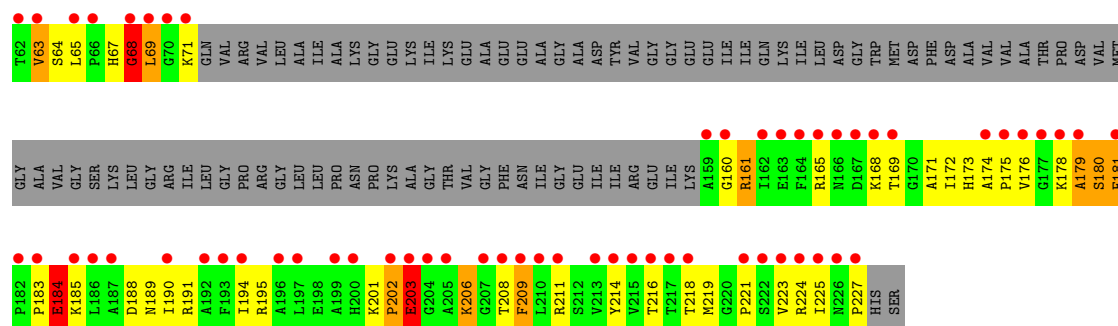


• Molecule 3: 50S ribosomal protein L1

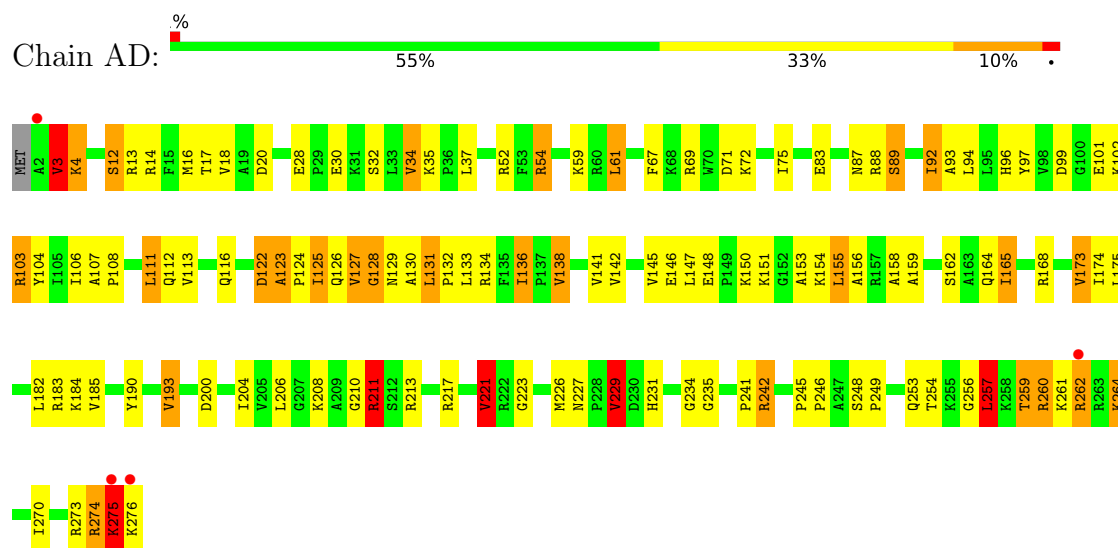


• Molecule 3: 50S ribosomal protein L1

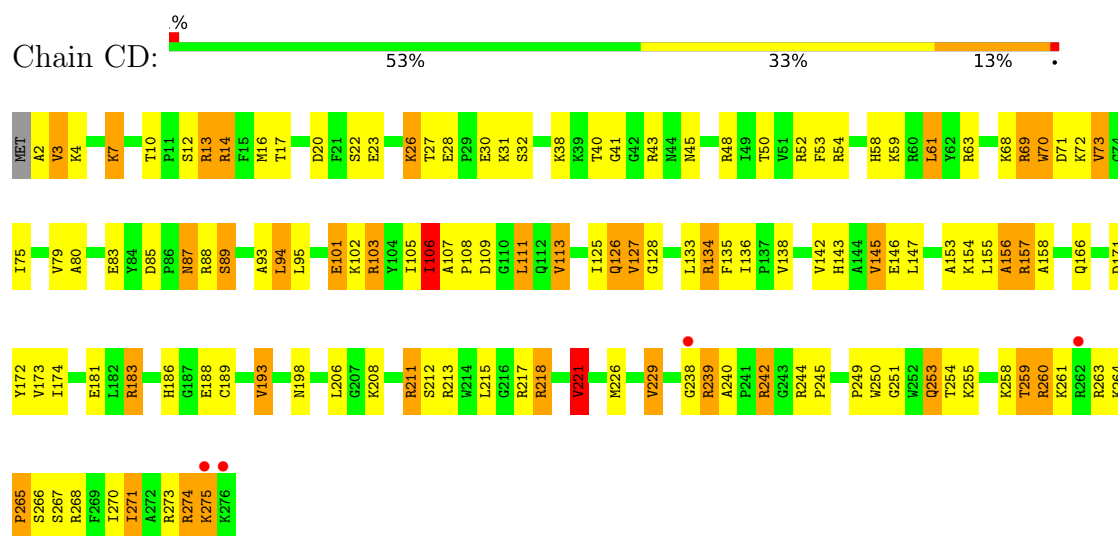




• Molecule 4: 50S ribosomal protein L2

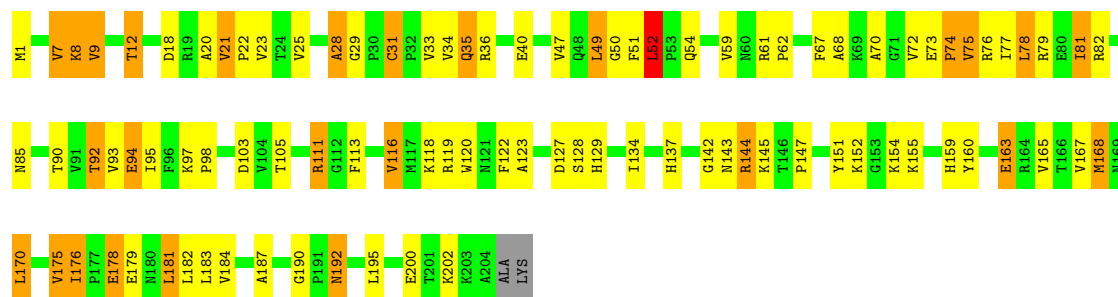


• Molecule 4: 50S ribosomal protein L2

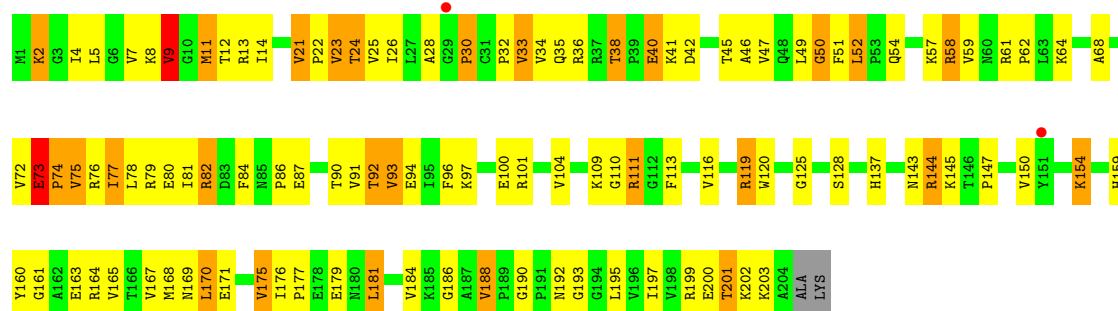


• Molecule 5: 50S ribosomal protein L3

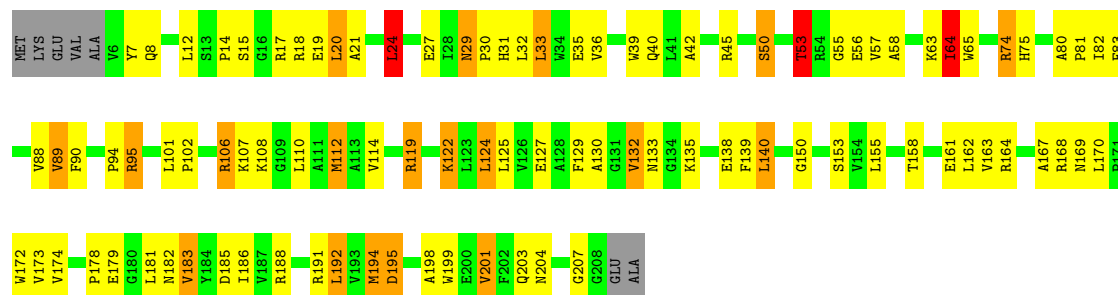




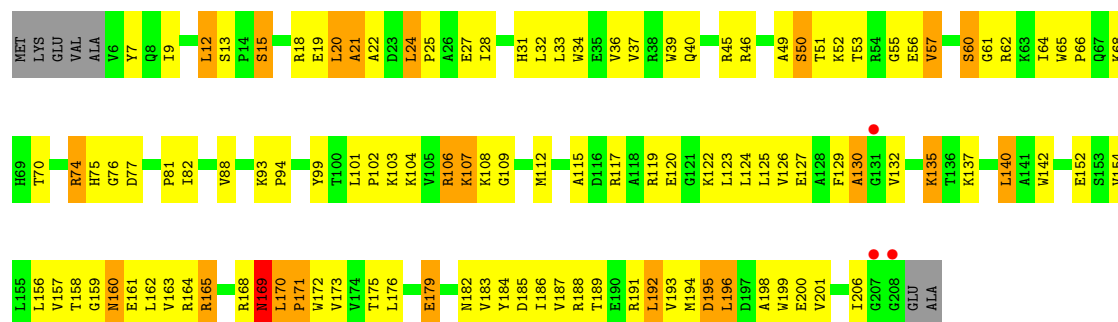
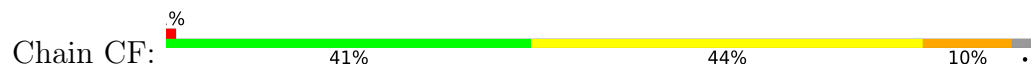
• Molecule 5: 50S ribosomal protein L3



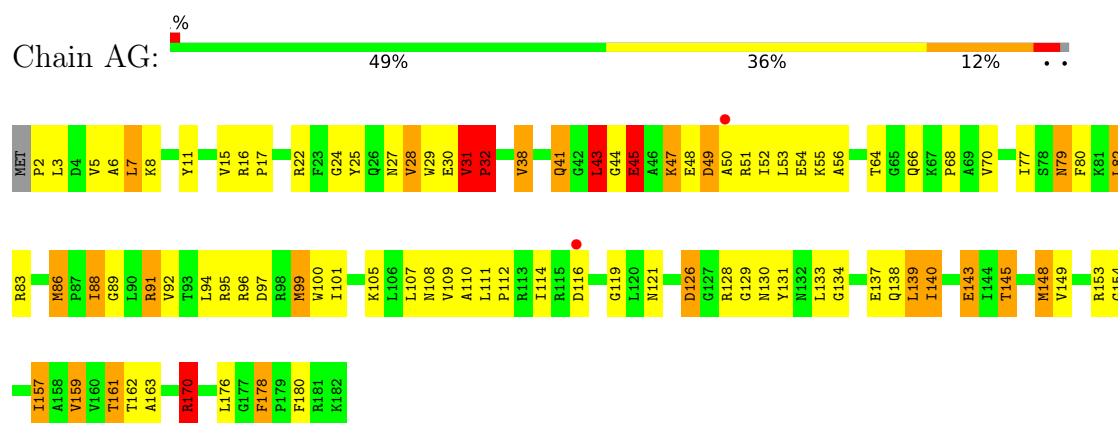
• Molecule 6: 50S ribosomal protein L4



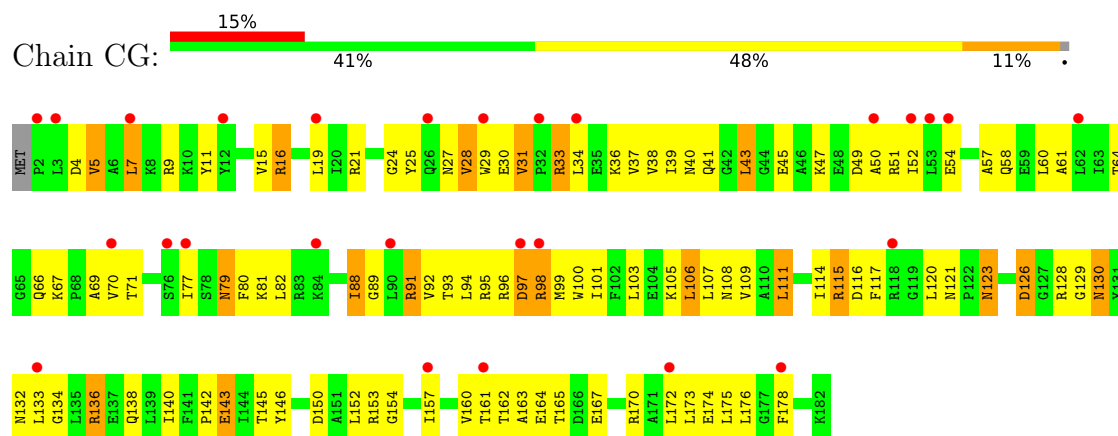
• Molecule 6: 50S ribosomal protein L4



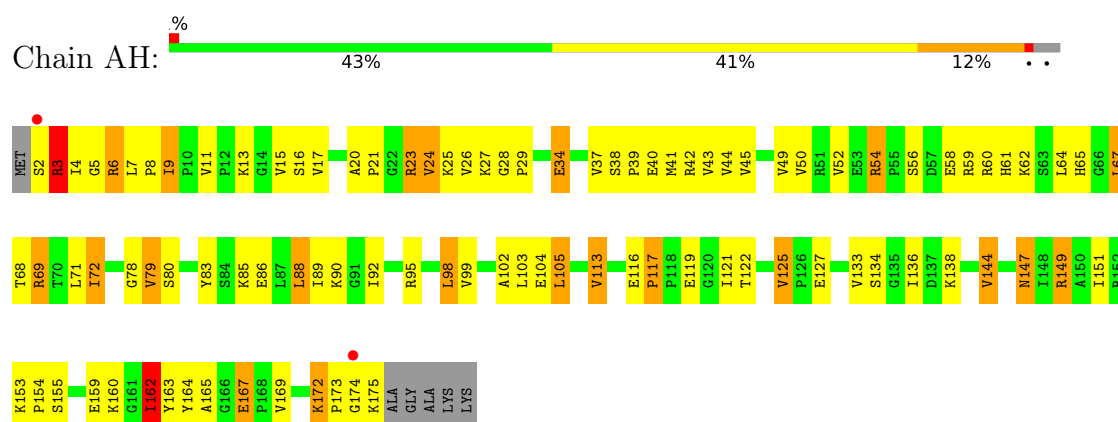
- Molecule 7: 50S ribosomal protein L5



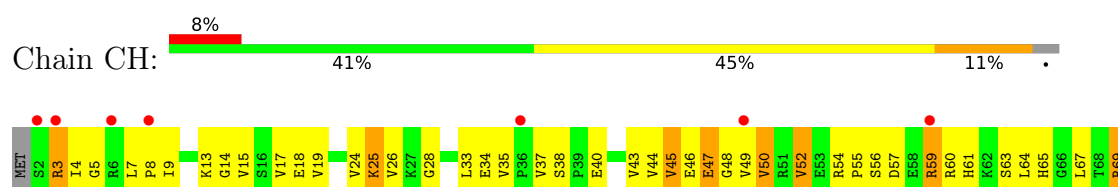
- Molecule 7: 50S ribosomal protein L5

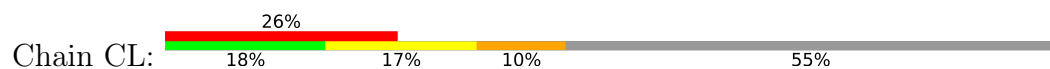


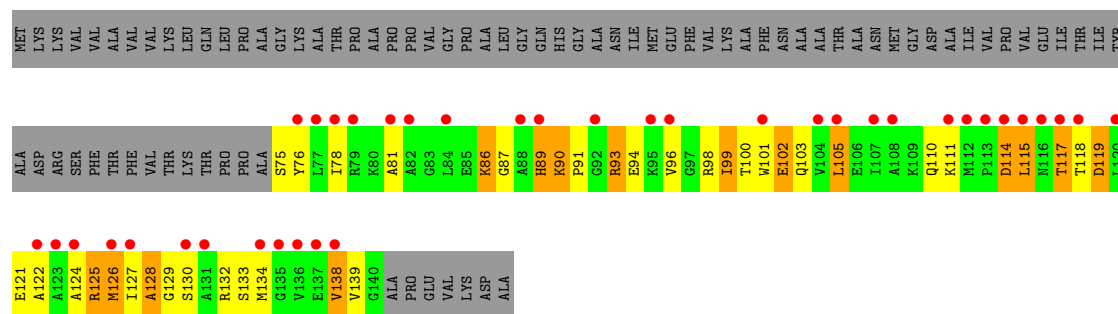
- Molecule 8: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L6







• Molecule 11: 50S ribosomal protein L13



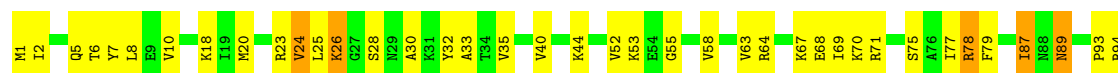
• Molecule 11: 50S ribosomal protein L13



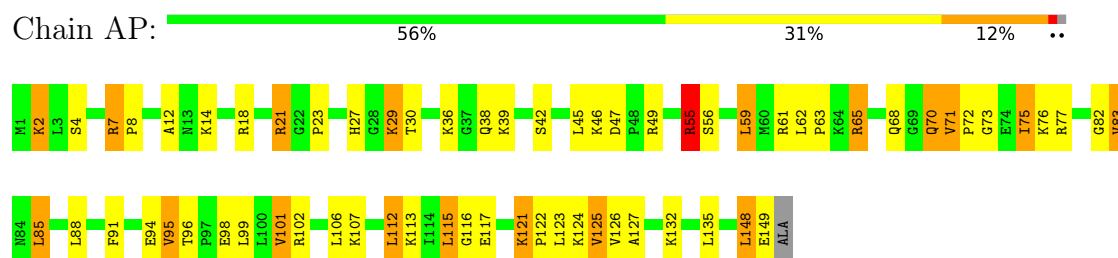
• Molecule 12: 50S ribosomal protein L14



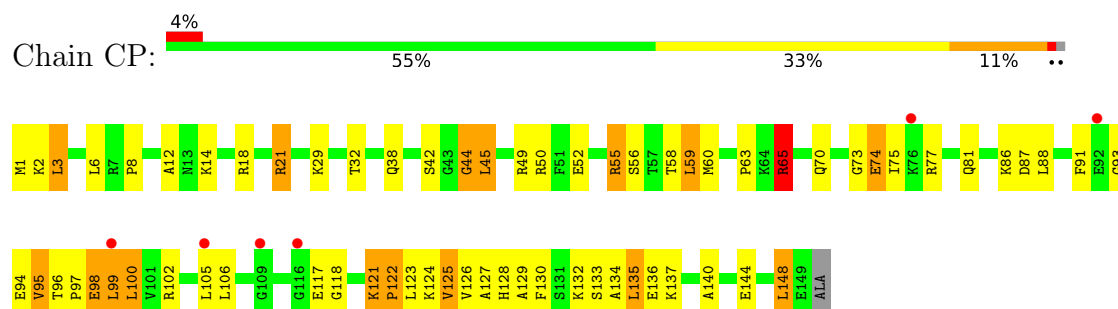
• Molecule 12: 50S ribosomal protein L14



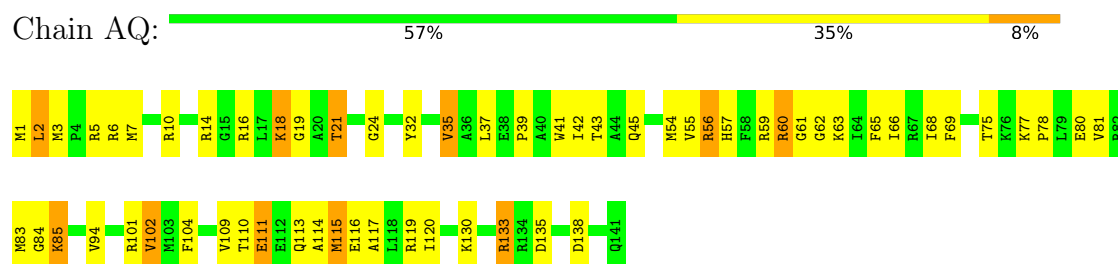
- Molecule 13: 50S ribosomal protein L15



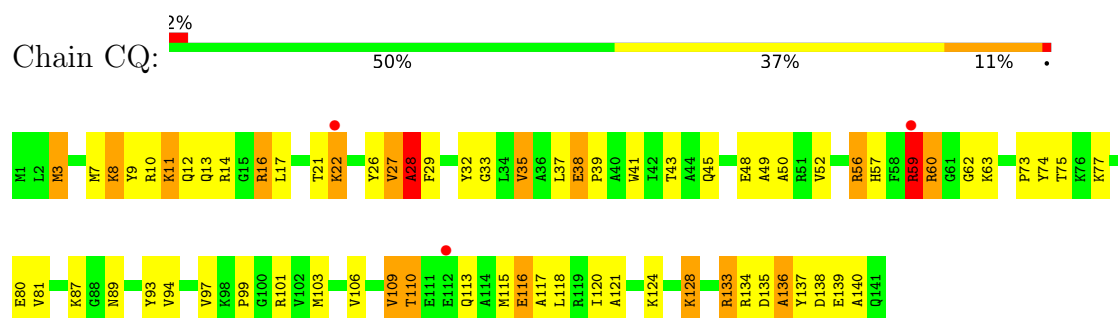
- Molecule 13: 50S ribosomal protein L15



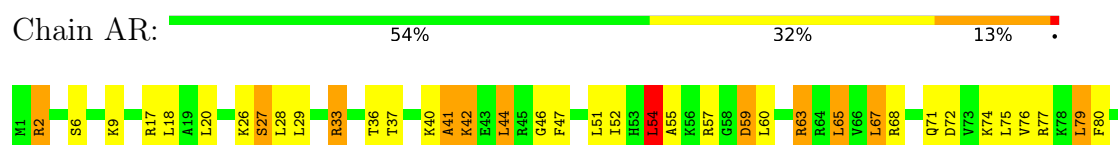
- Molecule 14: 50S ribosomal protein L16



- Molecule 14: 50S ribosomal protein L16



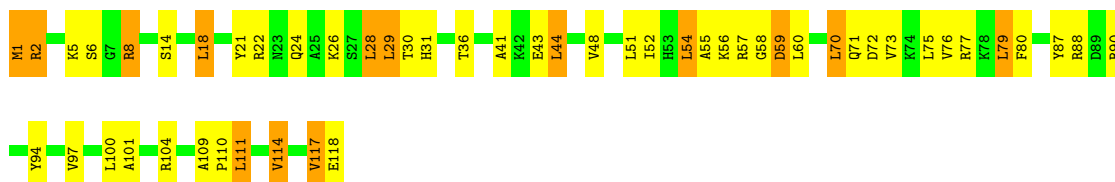
- Molecule 15: 50S ribosomal protein L17





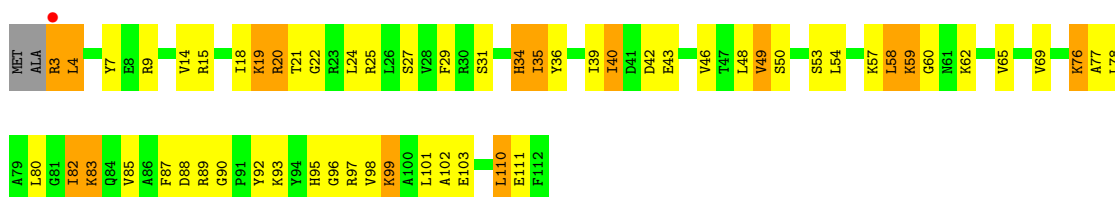
• Molecule 15: 50S ribosomal protein L17

Chain CR: 56% 32% 12%



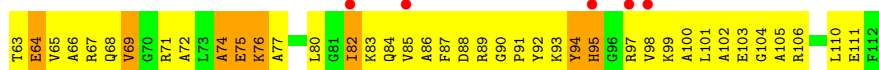
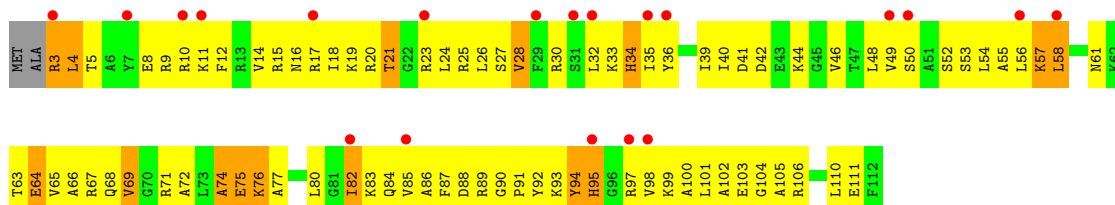
• Molecule 16: 50S ribosomal protein L18

Chain AS: 46% 39% 13%



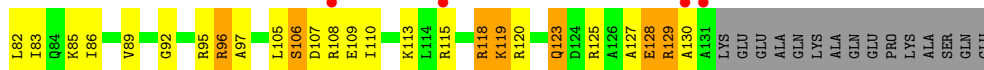
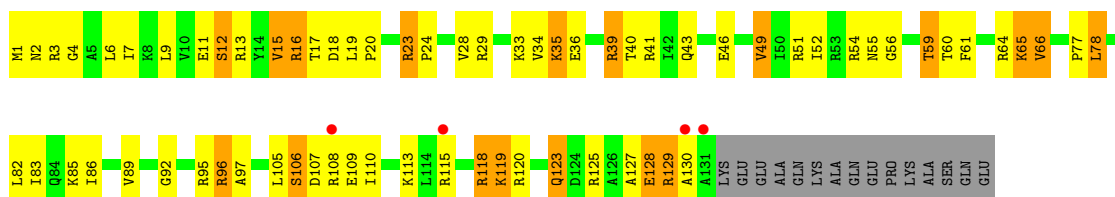
• Molecule 16: 50S ribosomal protein L18

Chain CS: 22% 62% 13%



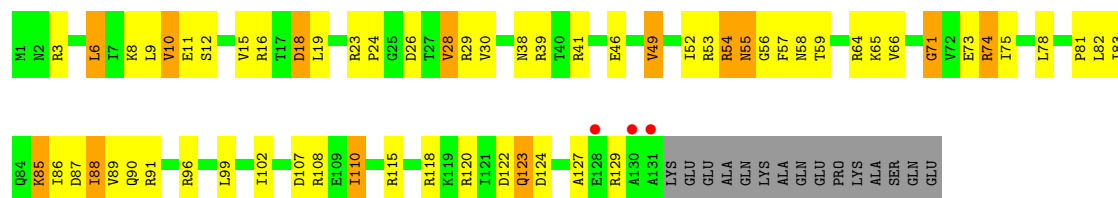
• Molecule 17: 50S ribosomal protein L19

Chain AT: 42% 35% 12% 10%



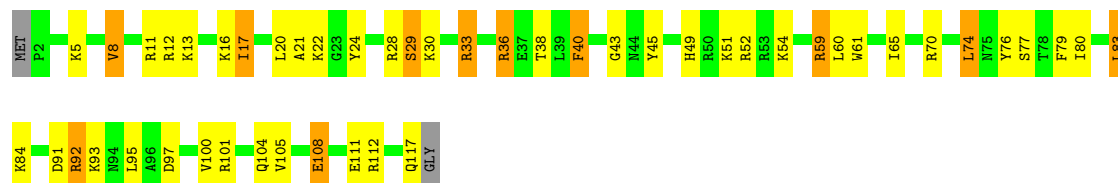
• Molecule 17: 50S ribosomal protein L19

Chain CT: 47% 34% 9% 10%



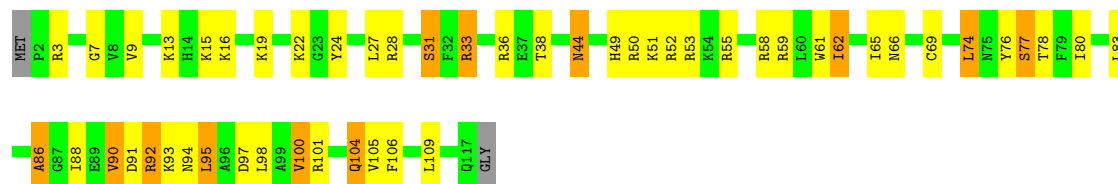
• Molecule 18: 50S ribosomal protein L20

Chain AU: 57% 32% 9% .



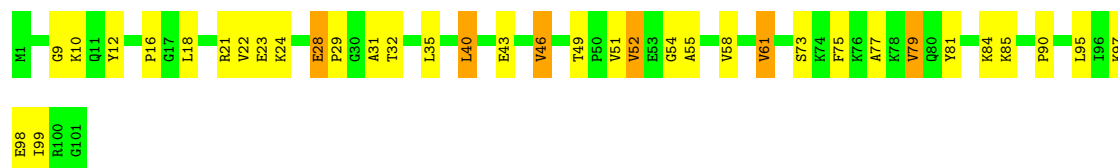
• Molecule 18: 50S ribosomal protein L20

Chain CU: 55% 33% 10% .



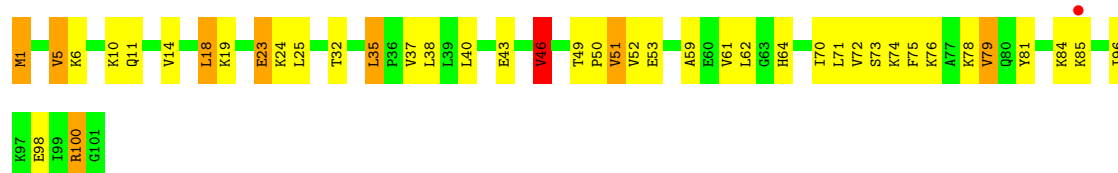
• Molecule 19: 50S ribosomal protein L21

Chain AV: 64% 30% 6% .



• Molecule 19: 50S ribosomal protein L21

Chain CV: 58% 33% 8% .



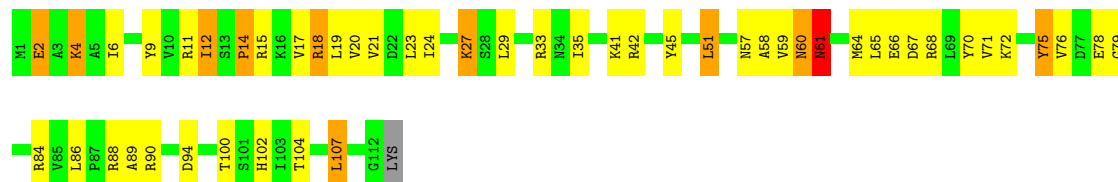
• Molecule 20: 50S ribosomal protein L22

Chain AW: 58% 30% 9% .



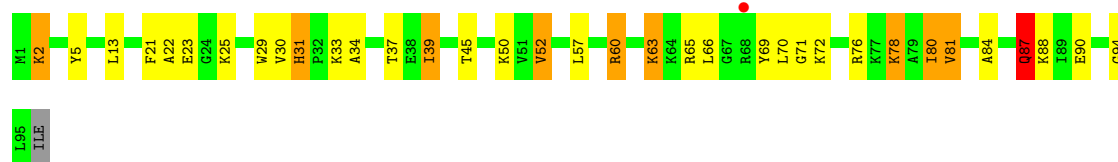
- Molecule 20: 50S ribosomal protein L22

Chain CW: 55% 35% 9% ..



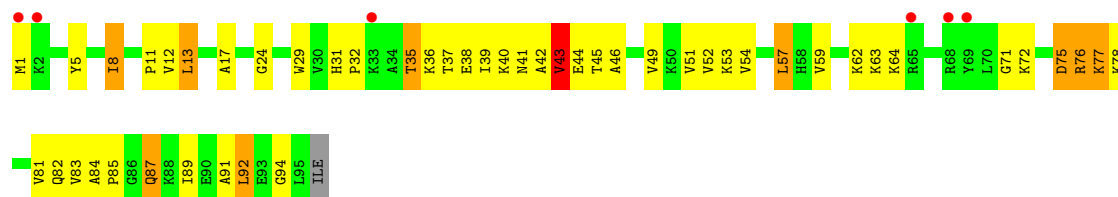
- Molecule 21: 50S ribosomal protein L23

Chain AX: 63% 26% 9% ..



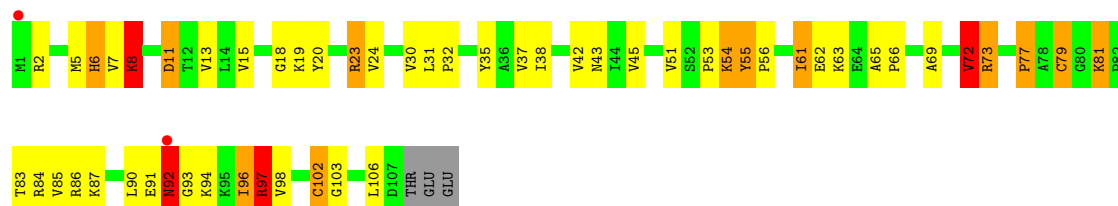
- Molecule 21: 50S ribosomal protein L23

Chain CX: 48% 41% 9% ..

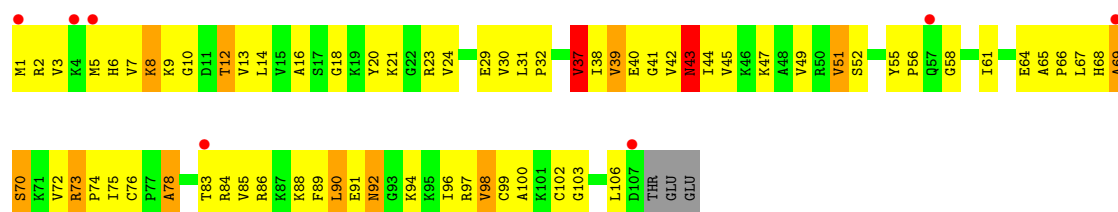


- Molecule 22: 50S ribosomal protein L24

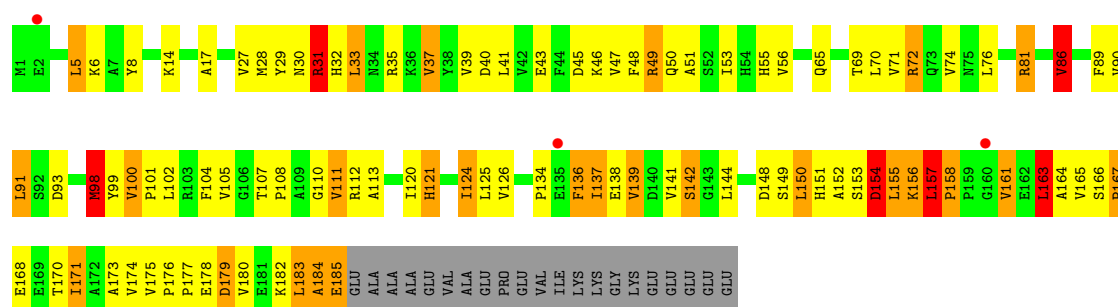
Chain AY: 48% 35% 11% ..



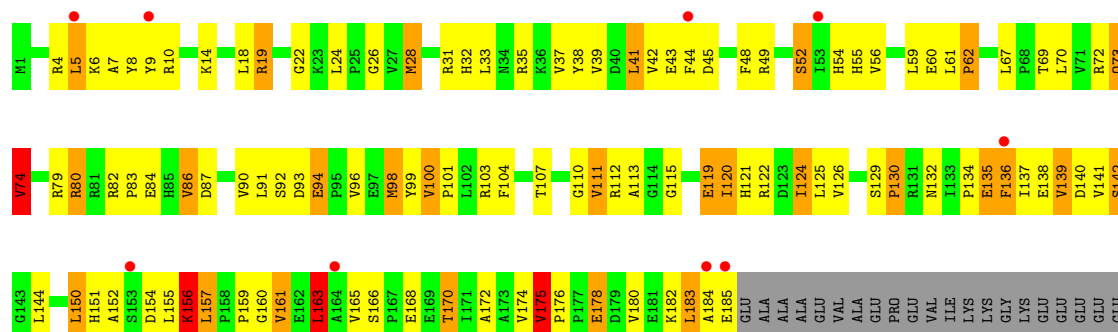
- Molecule 22: 50S ribosomal protein L24



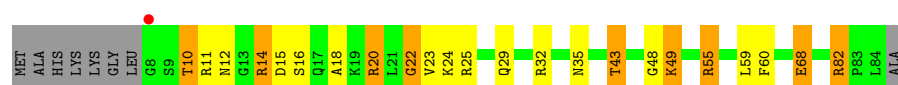
• Molecule 23: 50S ribosomal protein L25



• Molecule 23: 50S ribosomal protein L25

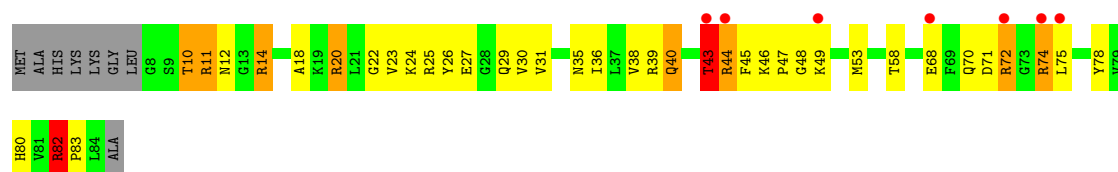


• Molecule 24: 50S ribosomal protein L27

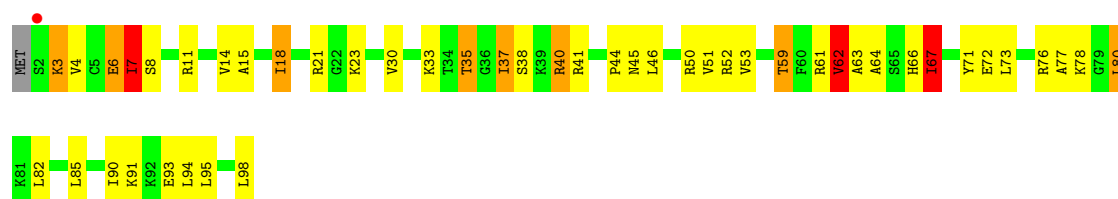


• Molecule 24: 50S ribosomal protein L27

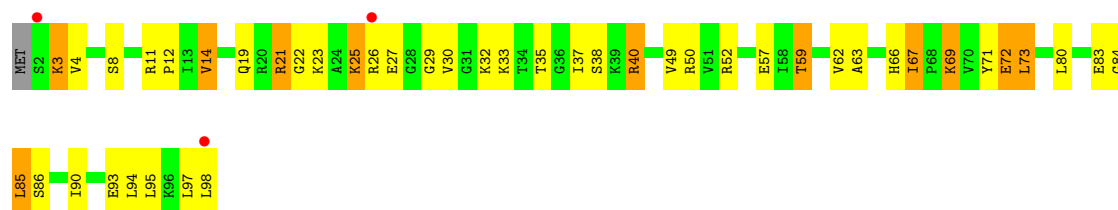




- Molecule 25: 50S ribosomal protein L28



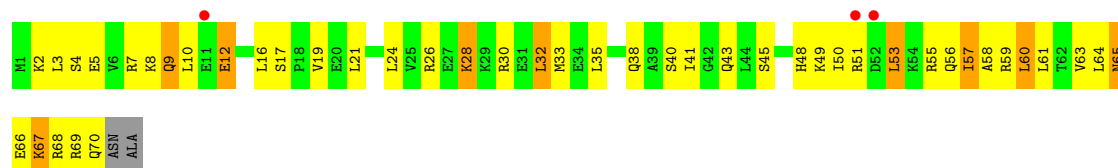
- Molecule 25: 50S ribosomal protein L28



- Molecule 26: 50S ribosomal protein L29

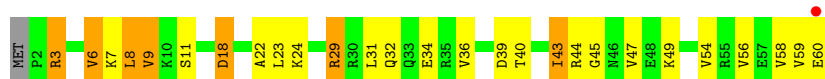


- Molecule 26: 50S ribosomal protein L29



- Molecule 27: 50S ribosomal protein L30

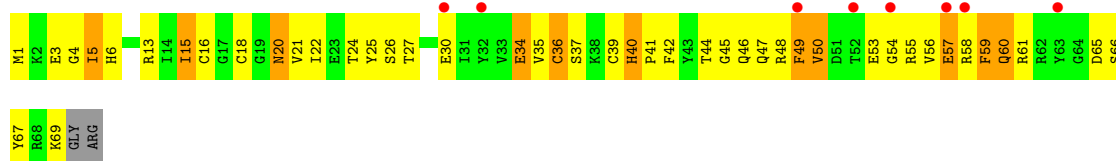




- Molecule 27: 50S ribosomal protein L30



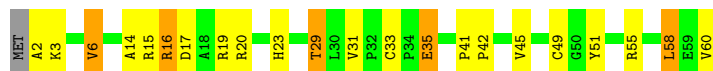
- Molecule 28: 50S ribosomal protein L31



- Molecule 28: 50S ribosomal protein L31



- Molecule 29: 50S ribosomal protein L32



- Molecule 29: 50S ribosomal protein L32



- Molecule 30: 50S ribosomal protein L33

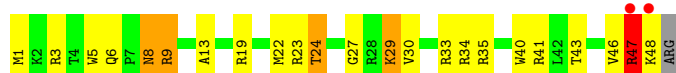




- Molecule 30: 50S ribosomal protein L33



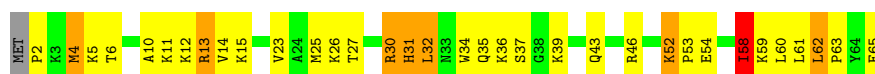
- Molecule 31: 50S ribosomal protein L34



- Molecule 31: 50S ribosomal protein L34



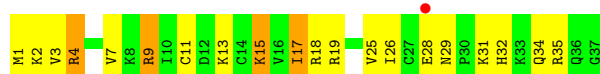
- Molecule 32: 50S ribosomal protein L35



- Molecule 32: 50S ribosomal protein L35



- Molecule 33: 50S ribosomal protein L36

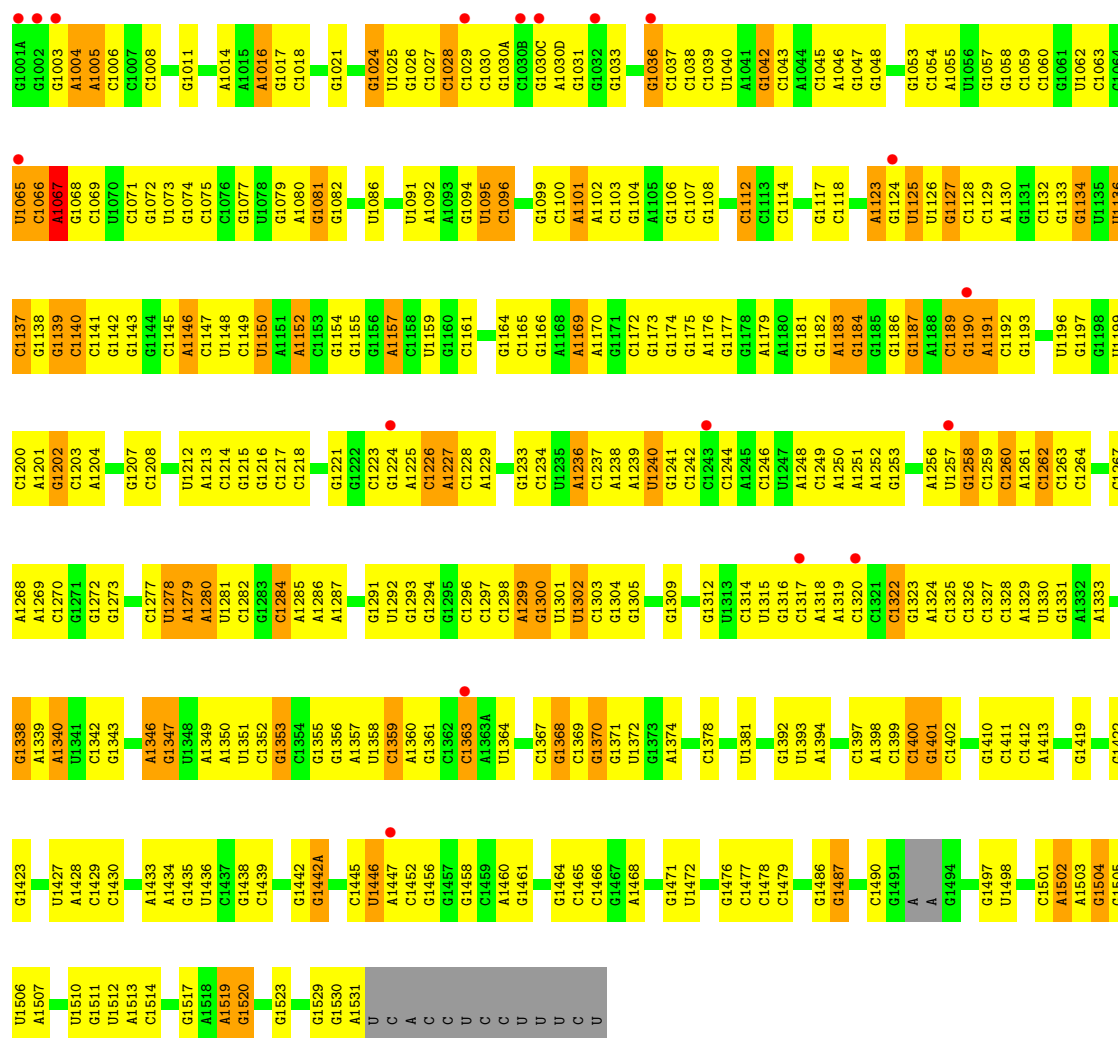


- Molecule 33: 50S ribosomal protein L36

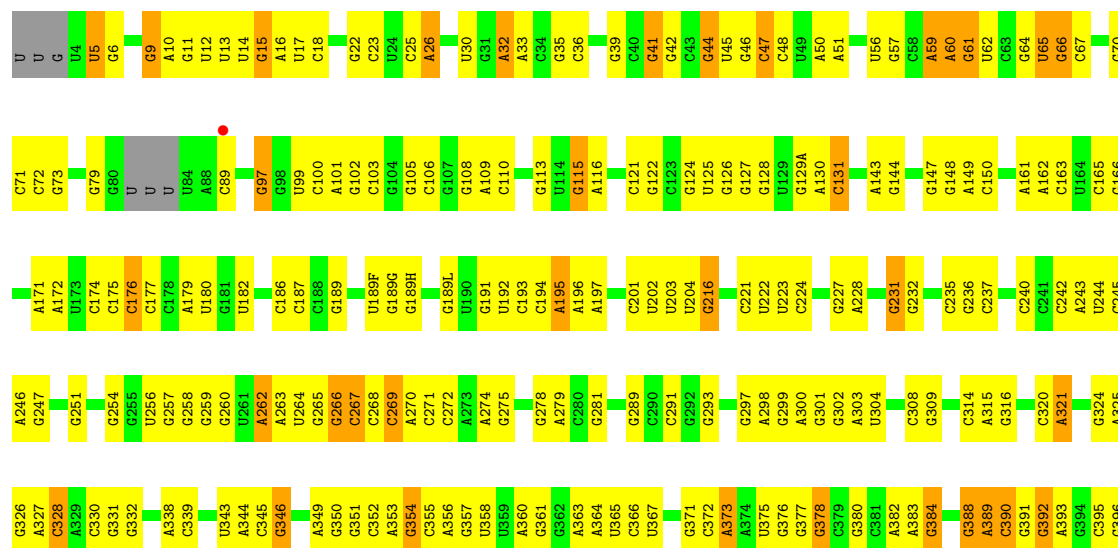


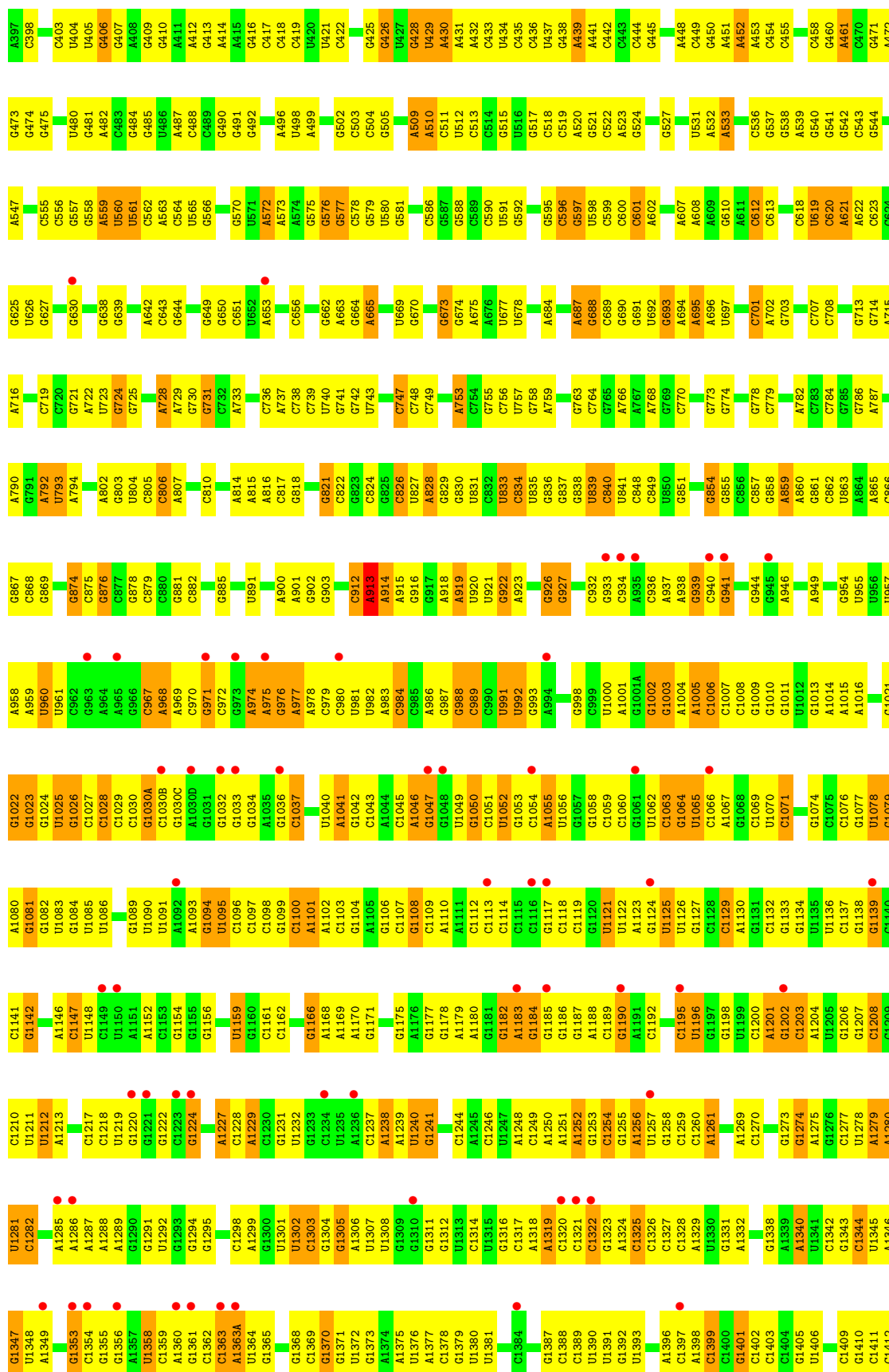
Chain BA:

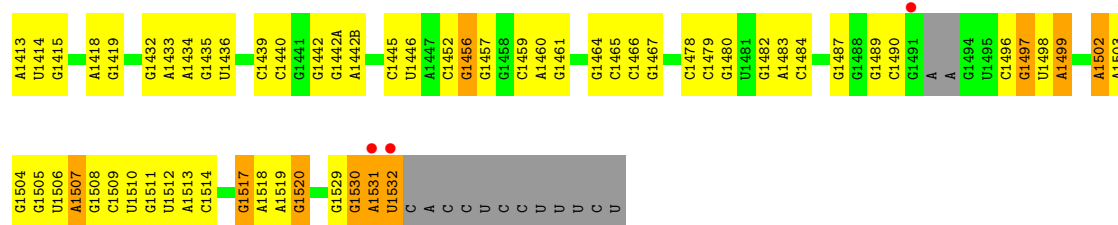




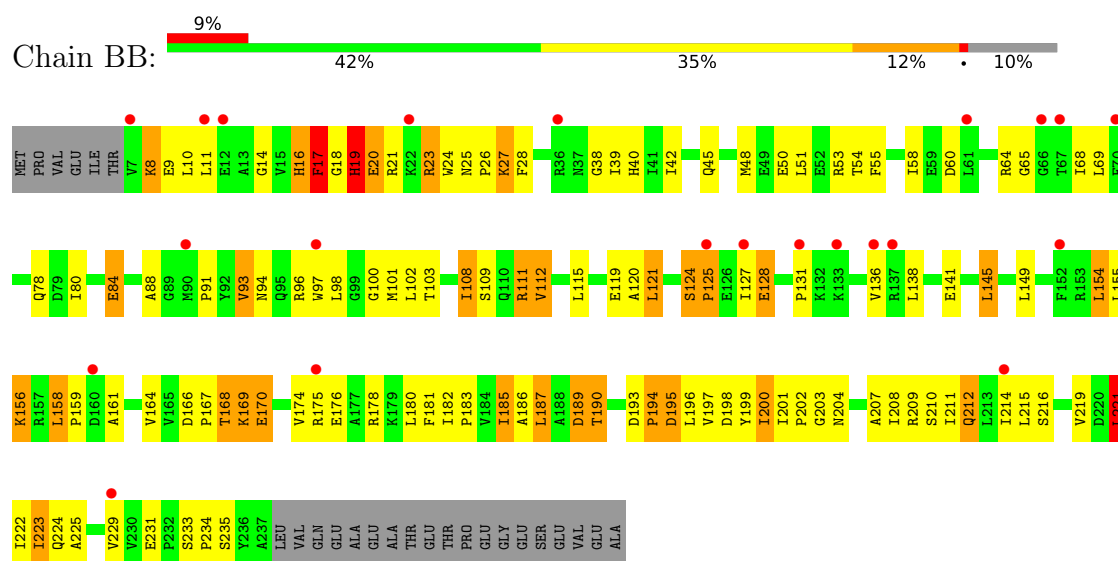
• Molecule 34: 16S Ribosomal RNA



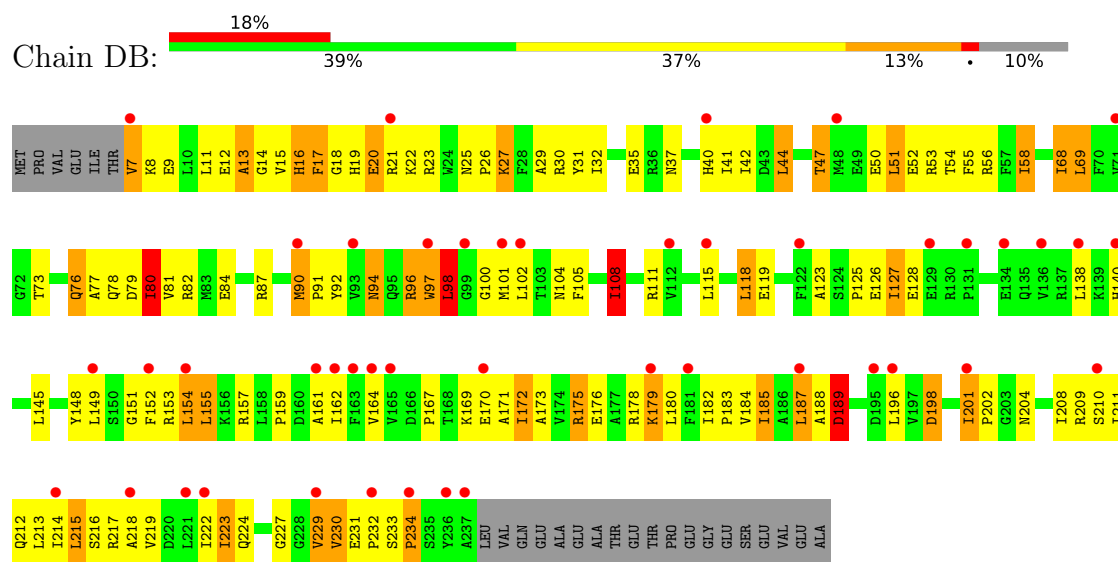




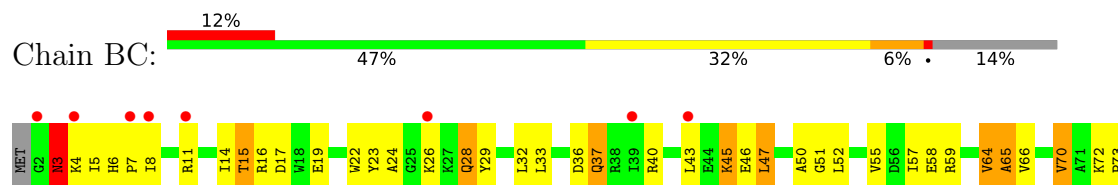
• Molecule 35: 30S ribosomal protein S2

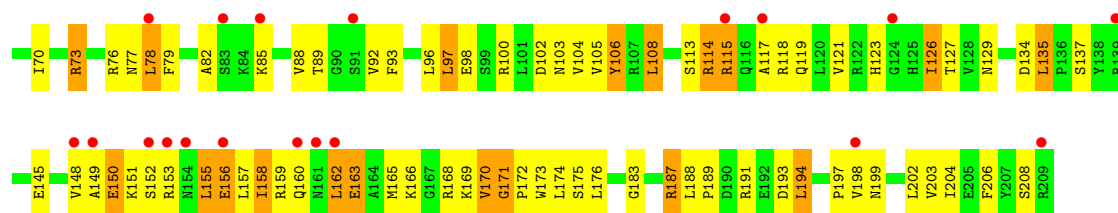


• Molecule 35: 30S ribosomal protein S2

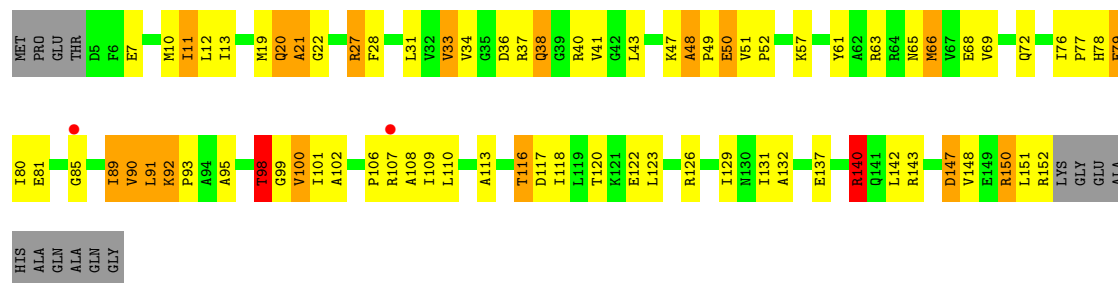


• Molecule 36: 30S ribosomal protein S3

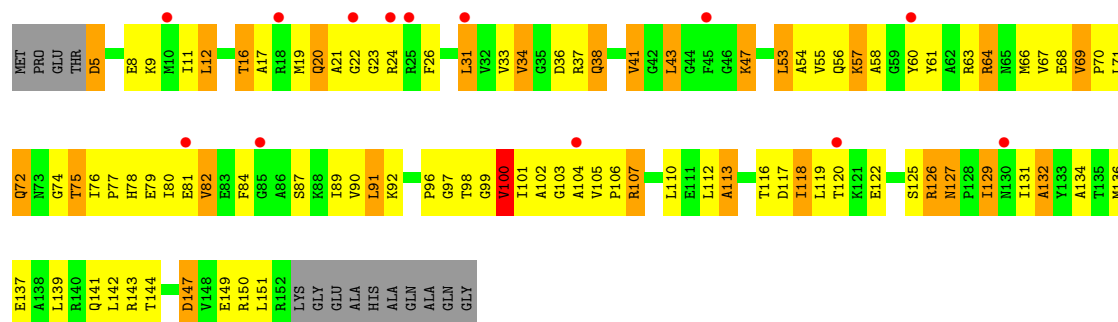




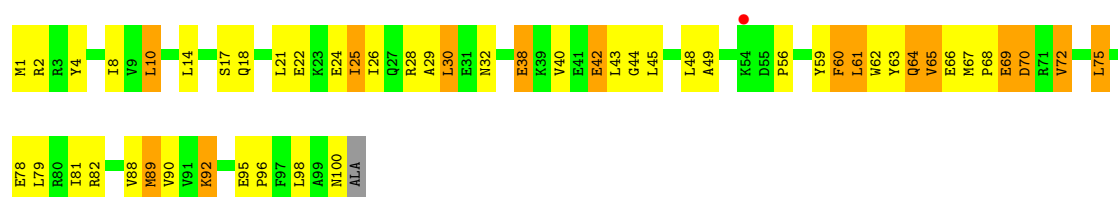
• Molecule 38: 30S ribosomal protein S5



• Molecule 38: 30S ribosomal protein S5

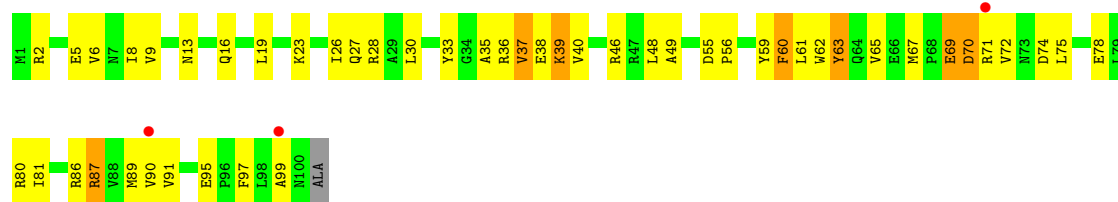


• Molecule 39: 30S ribosomal protein S6

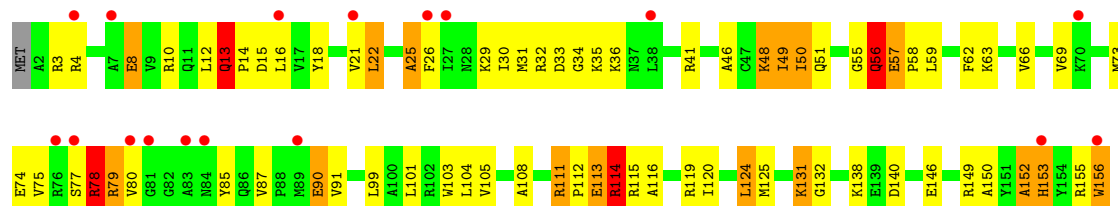


• Molecule 39: 30S ribosomal protein S6

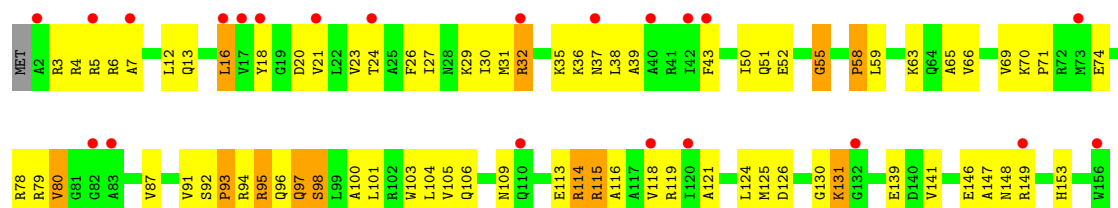




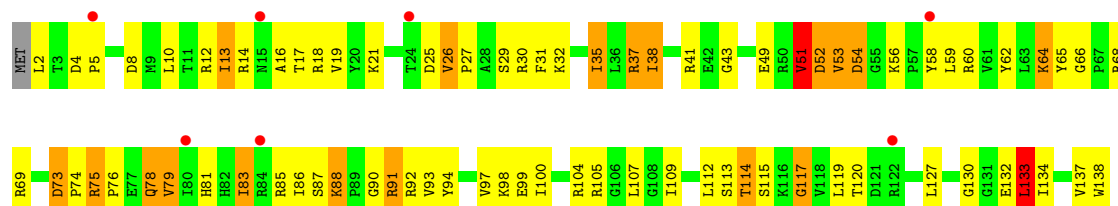
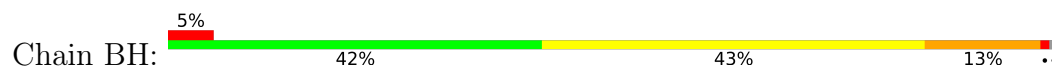
• Molecule 40: 30S ribosomal protein S7



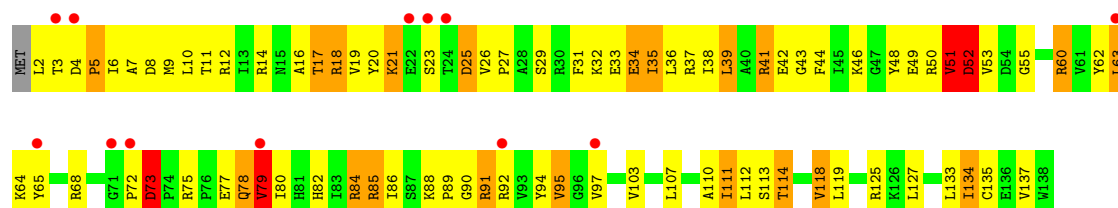
• Molecule 40: 30S ribosomal protein S7



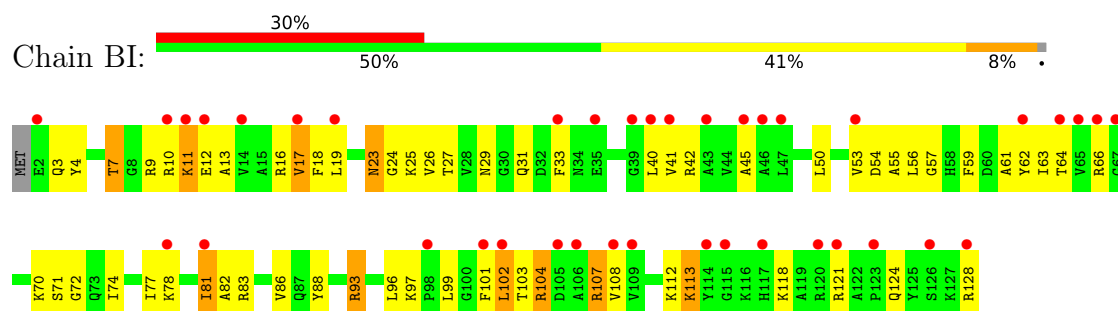
• Molecule 41: 30S ribosomal protein S8



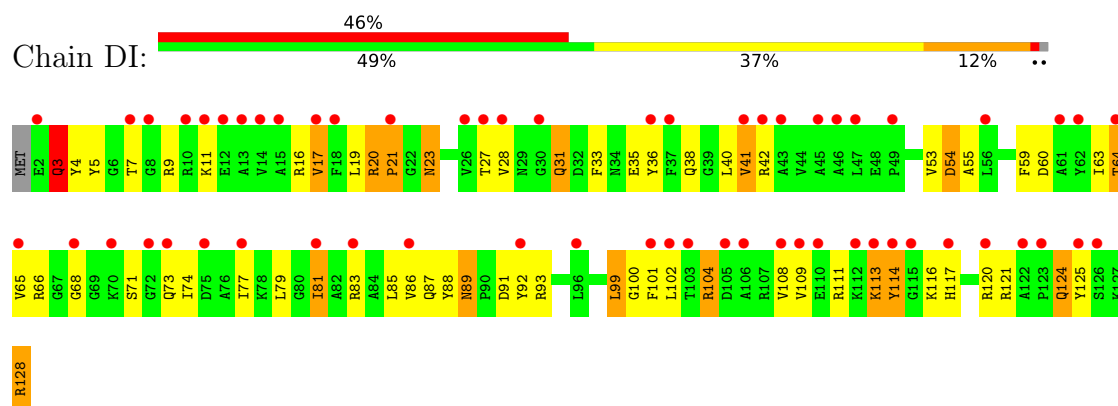
• Molecule 41: 30S ribosomal protein S8



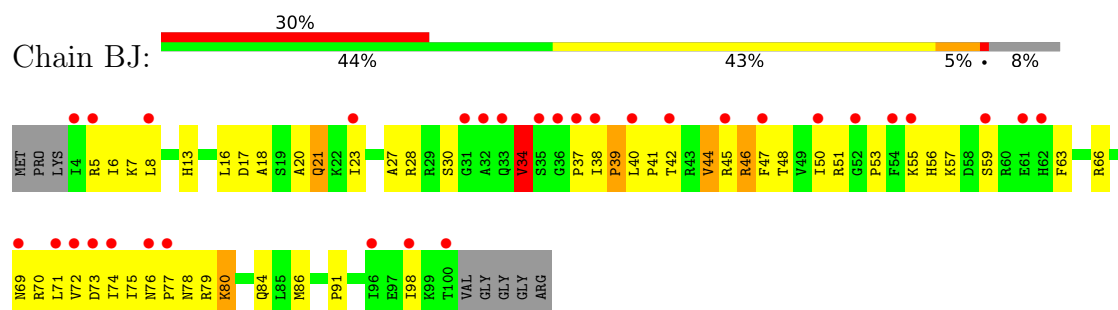
- Molecule 42: 30S ribosomal protein S9



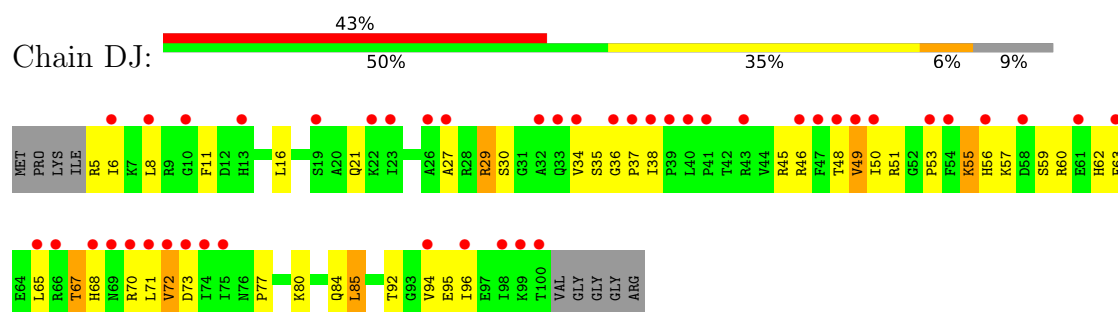
- Molecule 42: 30S ribosomal protein S9



- Molecule 43: 30S ribosomal protein S10

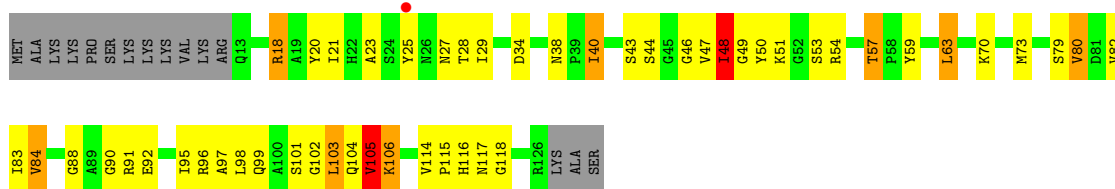


- Molecule 43: 30S ribosomal protein S10

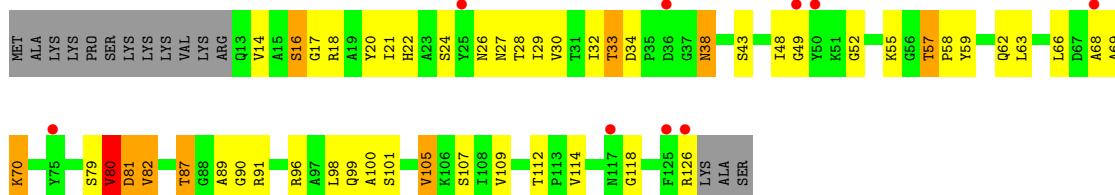


- Molecule 44: 30S ribosomal protein S11

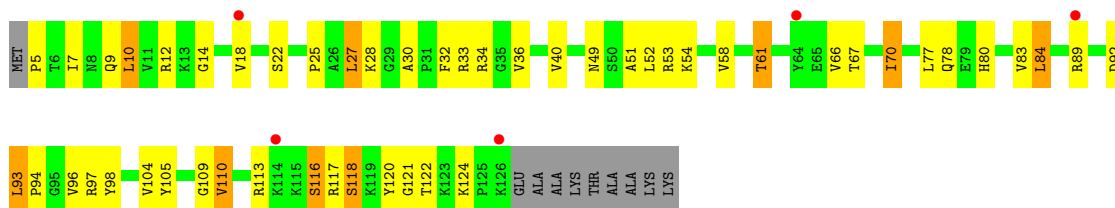




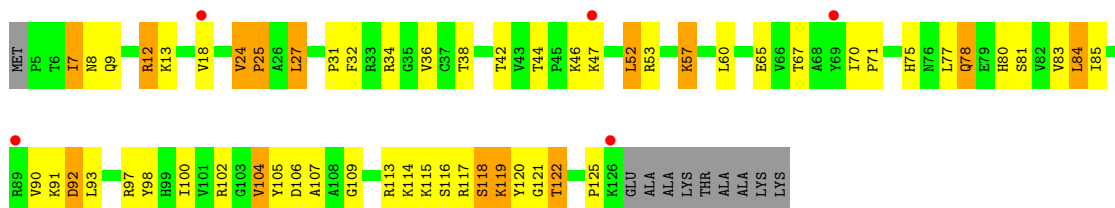
• Molecule 44: 30S ribosomal protein S11



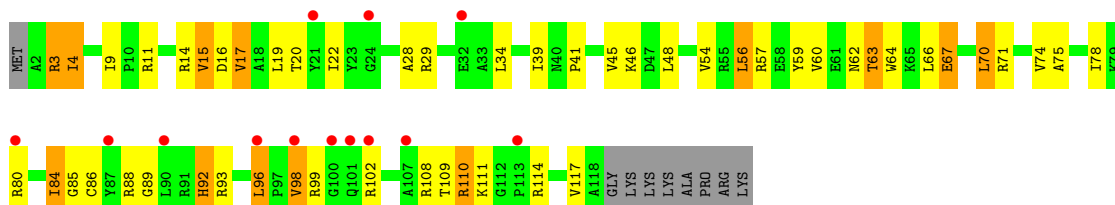
• Molecule 45: 30S ribosomal protein S12



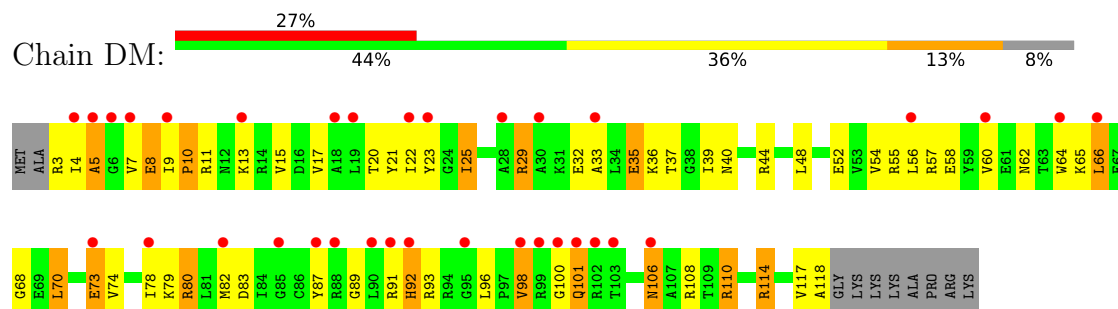
• Molecule 45: 30S ribosomal protein S12



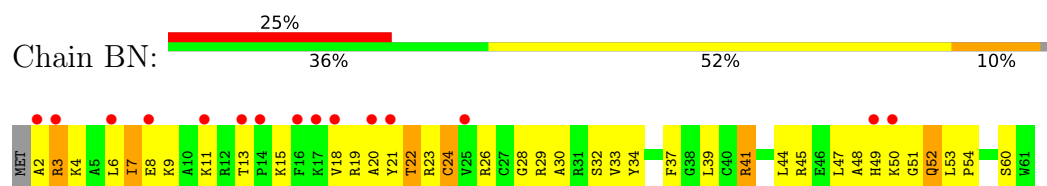
• Molecule 46: 30S ribosomal protein S13



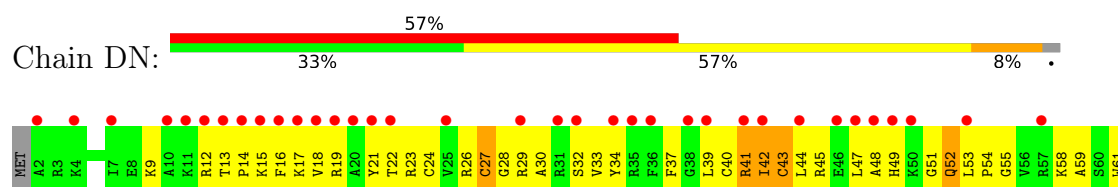
- Molecule 46: 30S ribosomal protein S13



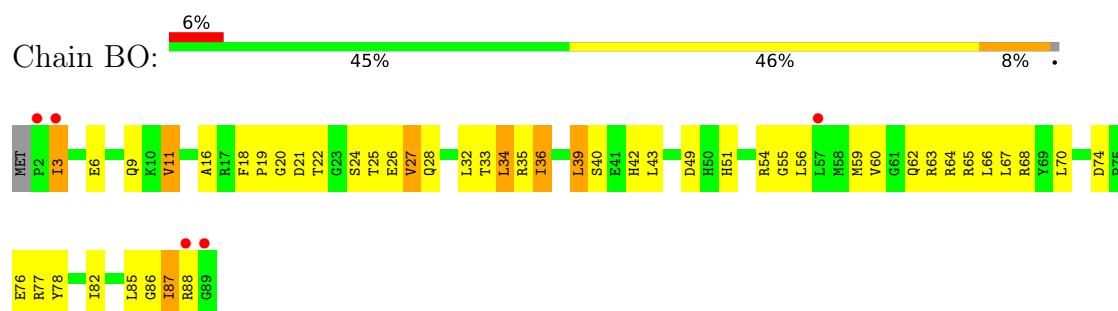
- Molecule 47: 30S ribosomal protein S14 type Z



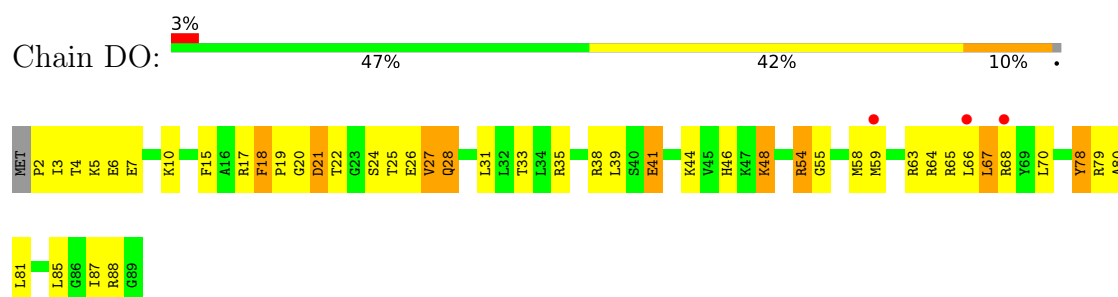
- Molecule 47: 30S ribosomal protein S14 type Z



- Molecule 48: 30S ribosomal protein S15

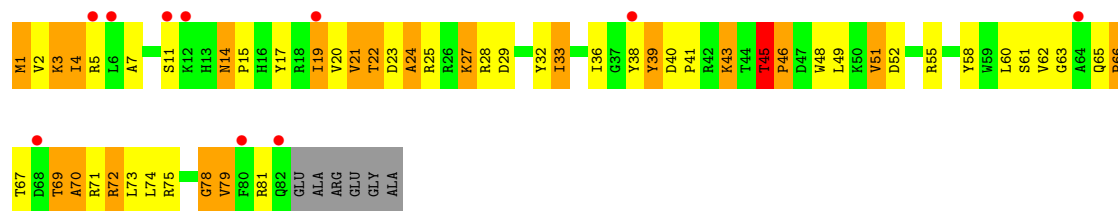


- Molecule 48: 30S ribosomal protein S15

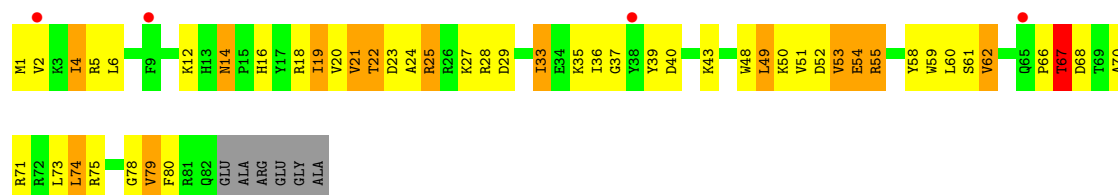


- Molecule 49: 30S ribosomal protein S16





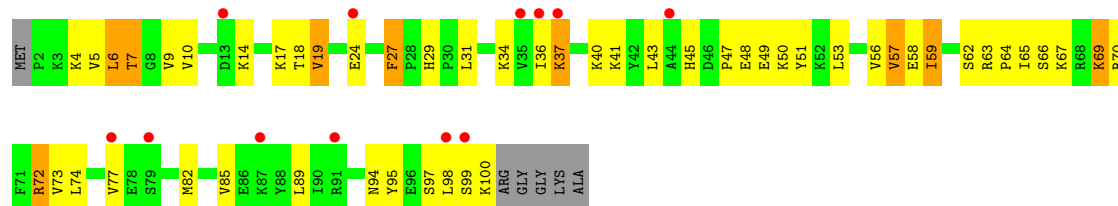
• Molecule 49: 30S ribosomal protein S16



• Molecule 50: 30S ribosomal protein S17



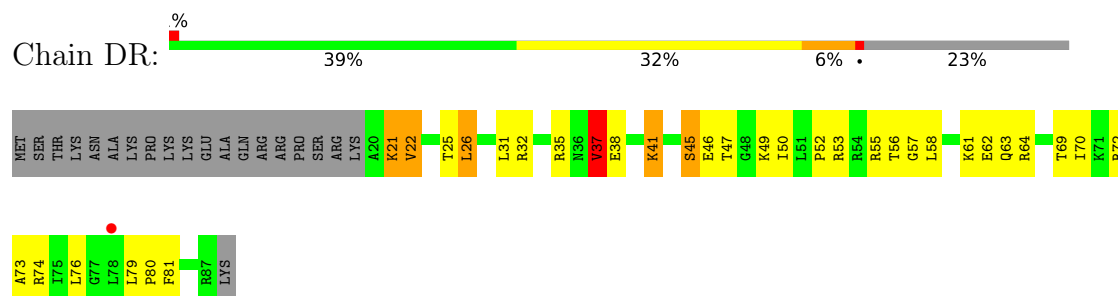
• Molecule 50: 30S ribosomal protein S17



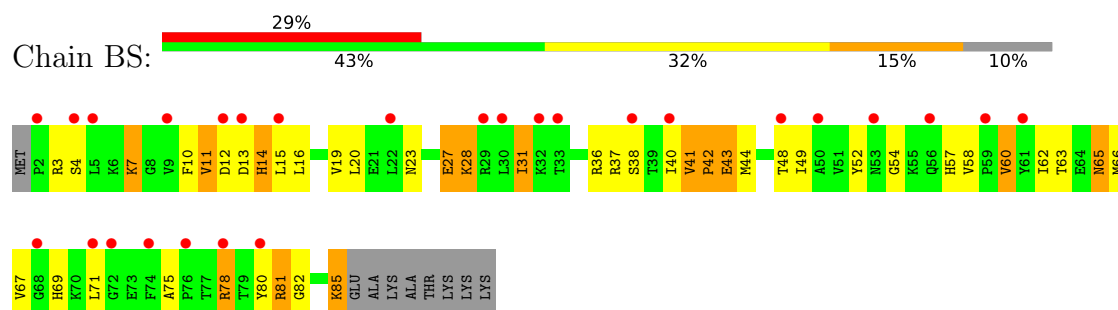
• Molecule 51: 30S ribosomal protein S18



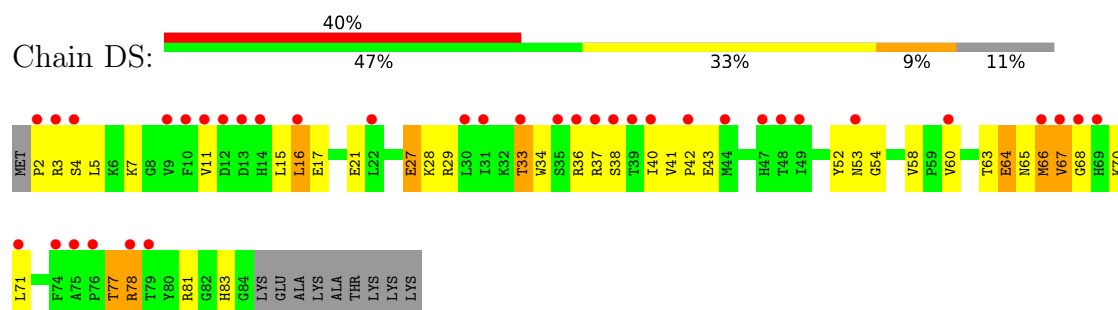
- Molecule 51: 30S ribosomal protein S18



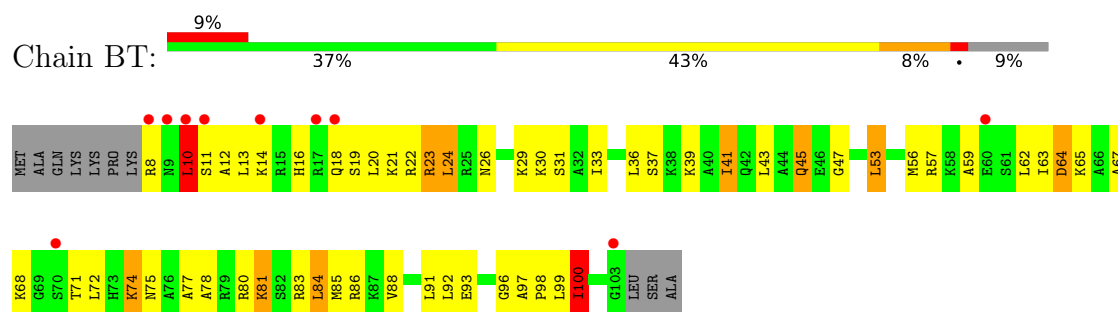
- Molecule 52: 30S ribosomal protein S19



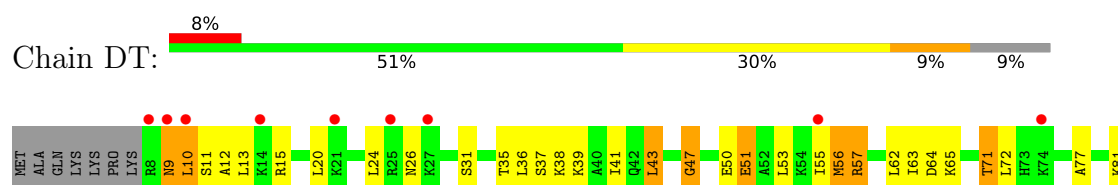
- Molecule 52: 30S ribosomal protein S19

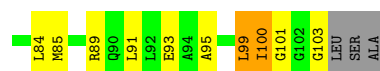


- Molecule 53: 30S ribosomal protein S20

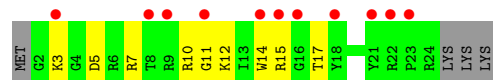
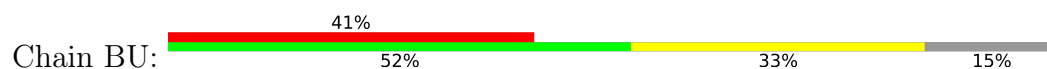


- Molecule 53: 30S ribosomal protein S20

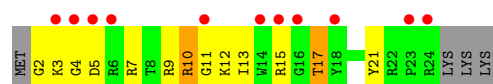




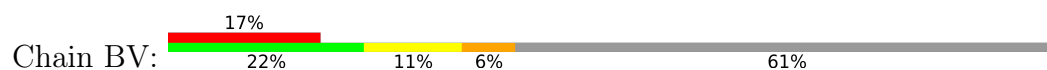
- Molecule 54: 30S ribosomal protein Thx



- Molecule 54: 30S ribosomal protein Thx



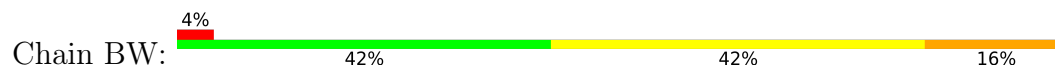
- Molecule 55: mRNA



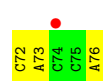
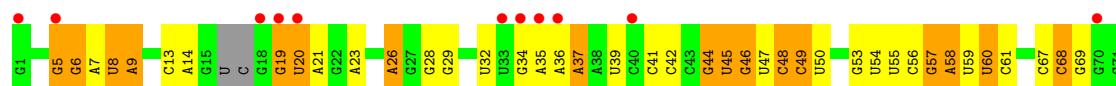
- Molecule 55: mRNA



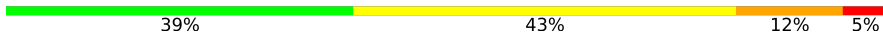
- Molecule 56: P-site tRNA

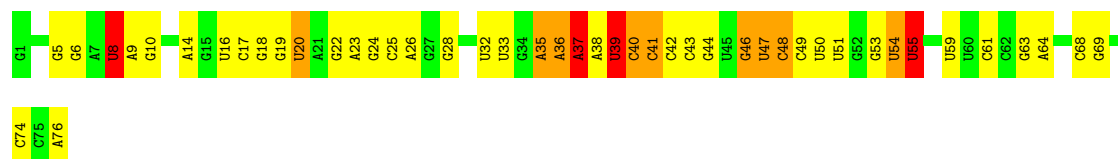


- Molecule 56: P-site tRNA

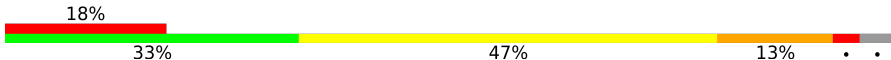


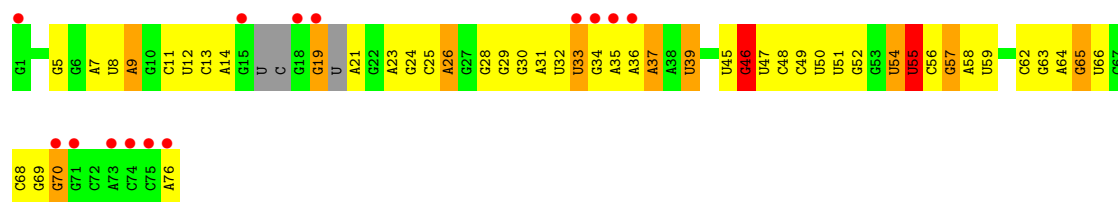
- Molecule 56: P-site tRNA

Chain DW: 

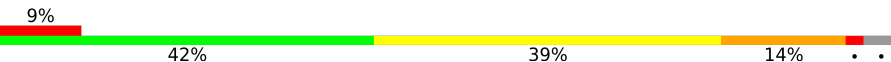


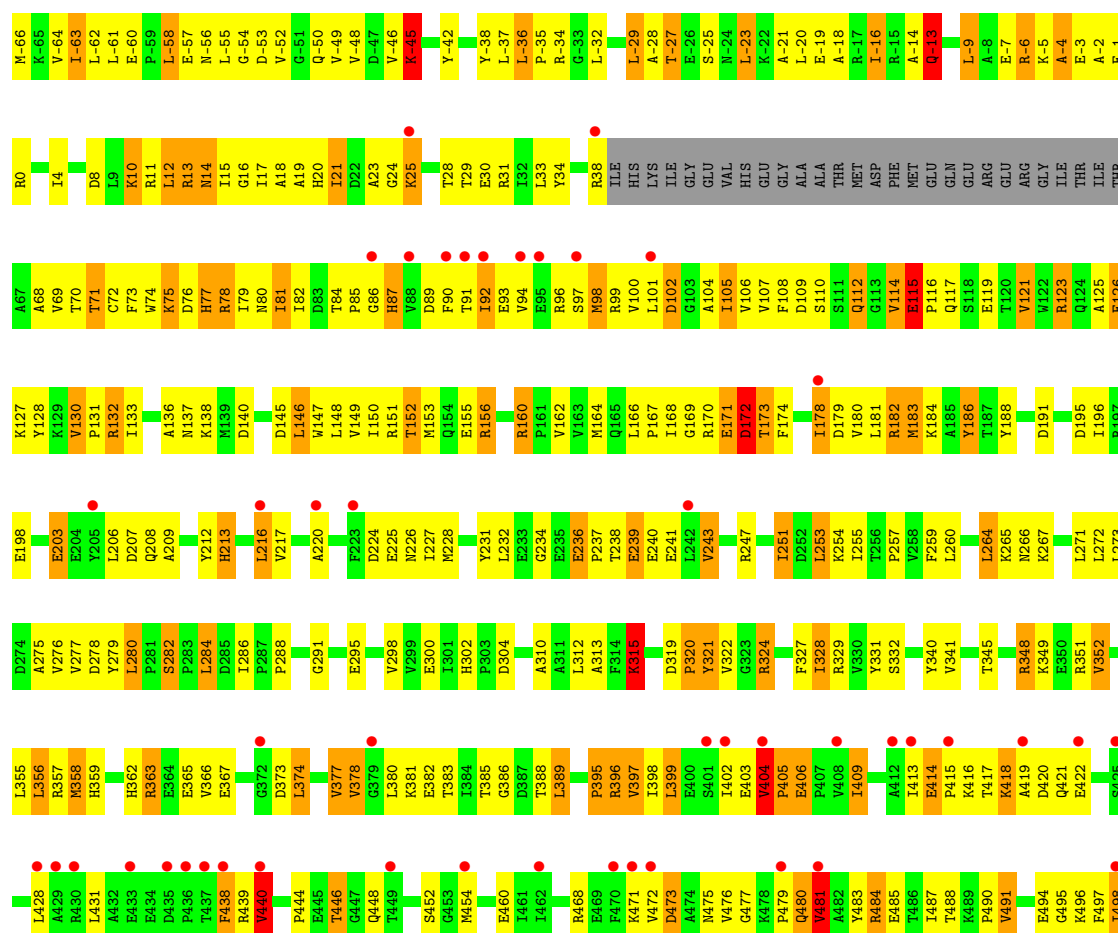
- Molecule 56: P-site tRNA

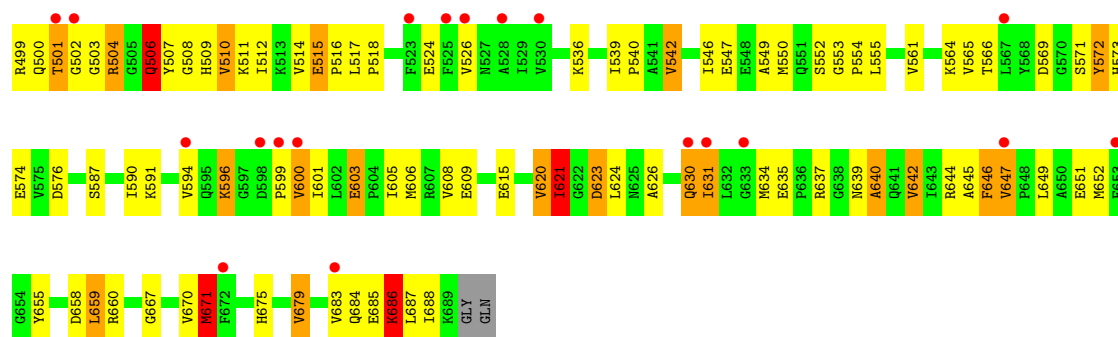
Chain DY: 



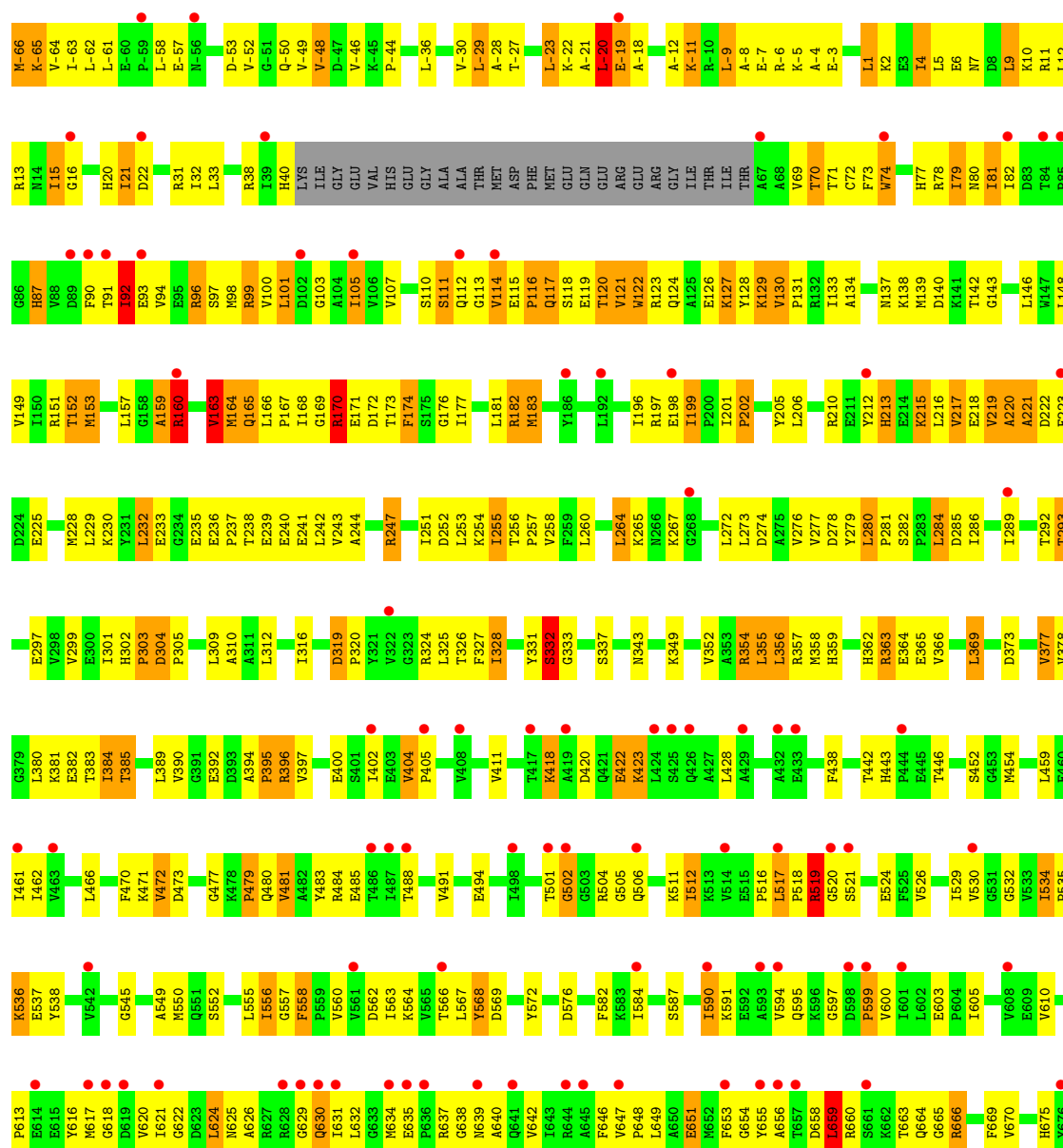
- Molecule 57: 50S ribosomal protein L9, Elongation factor G

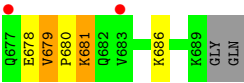
Chain BZ: 



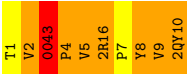


• Molecule 57: 50S ribosomal protein L9, Elongation factor G

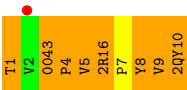




● Molecule 58: Dityromycin



● Molecule 58: Dityromycin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.84Å 450.58Å 623.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.81 – 2.80 49.81 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.5 (49.81-2.80) 94.5 (49.81-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.209 , 0.264 0.210 , 0.264	Depositor DCC
R_{free} test set	67916 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 73.5	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	0.93	EDS
Total number of atoms	310038	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% 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: 4SU, 2R1, 004, SF4, GDP, 2QZ, MVA, 7MG, 2QY, 2R3, 5MU, MIA, ZN, MG, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.75	0/69281	0.92	47/108144 (0.0%)
1	CA	0.54	0/69179	0.76	7/107984 (0.0%)
2	AB	0.63	0/2878	0.88	0/4490
2	CB	0.37	0/2878	0.62	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	1.14	5/2186 (0.2%)	1.39	19/2944 (0.6%)
4	CD	0.95	2/2192 (0.1%)	1.30	12/2951 (0.4%)
5	AE	1.17	1/1592 (0.1%)	1.54	28/2149 (1.3%)
5	CE	0.91	1/1592 (0.1%)	1.34	20/2149 (0.9%)
6	AF	1.14	1/1619 (0.1%)	1.42	14/2193 (0.6%)
6	CF	0.77	0/1615	1.17	7/2188 (0.3%)
7	AG	0.75	0/1450	1.24	16/1959 (0.8%)
7	CG	0.49	0/1449	1.03	3/1958 (0.2%)
8	AH	1.06	3/1356 (0.2%)	1.40	16/1834 (0.9%)
8	CH	0.64	0/1356	1.05	8/1834 (0.4%)
9	AK	0.59	0/640	1.53	12/889 (1.3%)
9	CK	0.48	0/640	1.62	10/889 (1.1%)
10	AL	0.48	0/503	0.96	3/673 (0.4%)
10	CL	0.53	0/503	1.13	4/673 (0.6%)
11	AN	1.14	1/1144 (0.1%)	1.33	6/1543 (0.4%)
11	CN	0.78	0/1144	1.20	6/1543 (0.4%)
12	AO	1.14	2/943 (0.2%)	1.39	8/1269 (0.6%)
12	CO	0.94	0/943	1.27	5/1269 (0.4%)
13	AP	1.02	0/1156	1.37	10/1537 (0.7%)
13	CP	0.71	0/1152	1.25	12/1533 (0.8%)
14	AQ	1.14	0/1143	1.32	9/1527 (0.6%)
14	CQ	0.79	0/1143	1.23	8/1527 (0.5%)
15	AR	1.18	2/982 (0.2%)	1.35	7/1312 (0.5%)
15	CR	0.84	0/982	1.16	1/1312 (0.1%)
16	AS	0.90	0/887	1.22	9/1180 (0.8%)
16	CS	0.59	0/880	1.07	1/1172 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AT	1.08	1/1105 (0.1%)	1.30	6/1477 (0.4%)
17	CT	0.83	0/1097	1.15	5/1468 (0.3%)
18	AU	1.31	0/977	1.39	9/1301 (0.7%)
18	CU	0.85	0/977	1.09	3/1301 (0.2%)
19	AV	1.21	2/782 (0.3%)	1.54	9/1049 (0.9%)
19	CV	0.76	0/782	1.12	2/1049 (0.2%)
20	AW	1.30	3/897 (0.3%)	1.34	7/1205 (0.6%)
20	CW	0.99	0/897	1.29	6/1205 (0.5%)
21	AX	1.17	2/764 (0.3%)	1.34	7/1025 (0.7%)
21	CX	0.82	0/764	1.19	6/1025 (0.6%)
22	AY	1.06	1/819 (0.1%)	1.46	9/1095 (0.8%)
22	CY	0.66	0/819	1.10	5/1095 (0.5%)
23	AZ	0.87	0/1483	1.31	13/2017 (0.6%)
23	CZ	0.61	1/1483 (0.1%)	1.16	11/2017 (0.5%)
24	A0	1.12	1/616 (0.2%)	1.35	3/821 (0.4%)
24	C0	0.73	0/616	1.16	6/821 (0.7%)
25	A1	1.08	1/762 (0.1%)	1.32	6/1014 (0.6%)
25	C1	0.82	0/762	1.22	6/1014 (0.6%)
26	A2	0.97	0/590	1.21	1/781 (0.1%)
26	C2	0.72	0/590	1.10	2/781 (0.3%)
27	A3	1.28	3/474 (0.6%)	1.51	6/635 (0.9%)
27	C3	0.75	0/469	1.20	3/630 (0.5%)
28	A4	0.58	0/571	1.21	7/768 (0.9%)
28	C4	0.50	0/545	1.08	4/737 (0.5%)
29	A5	1.29	2/469 (0.4%)	1.48	6/635 (0.9%)
29	C5	0.96	0/469	1.30	5/635 (0.8%)
30	A6	1.13	2/460 (0.4%)	1.32	1/613 (0.2%)
30	C6	0.79	0/456	1.04	0/608
31	A7	1.22	1/426 (0.2%)	1.27	3/561 (0.5%)
31	C7	0.96	1/426 (0.2%)	1.32	4/561 (0.7%)
32	A8	1.15	0/525	1.35	6/691 (0.9%)
32	C8	0.78	0/525	1.19	1/691 (0.1%)
33	A9	1.18	1/310 (0.3%)	1.43	4/407 (1.0%)
33	C9	0.78	0/310	1.17	1/407 (0.2%)
34	BA	0.43	0/35976	0.67	5/56145 (0.0%)
34	DA	0.38	0/36119	0.60	2/56370 (0.0%)
35	BB	0.55	0/1881	1.13	15/2542 (0.6%)
35	DB	0.51	0/1860	1.04	8/2518 (0.3%)
36	BC	0.54	0/1576	0.94	2/2130 (0.1%)
36	DC	0.51	0/1568	0.93	4/2122 (0.2%)
37	BD	0.64	1/1689 (0.1%)	1.09	9/2267 (0.4%)
37	DD	0.61	0/1708	1.12	9/2289 (0.4%)
38	BE	0.75	0/1145	1.11	4/1543 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DE	0.66	0/1149	1.19	9/1548 (0.6%)
39	BF	0.65	0/825	1.12	5/1118 (0.4%)
39	DF	0.63	0/833	1.05	3/1128 (0.3%)
40	BG	0.54	0/1250	0.99	9/1679 (0.5%)
40	DG	0.45	0/1254	0.98	3/1683 (0.2%)
41	BH	0.69	0/1108	1.19	9/1494 (0.6%)
41	DH	0.58	0/1108	1.10	5/1494 (0.3%)
42	BI	0.58	0/1005	0.99	1/1350 (0.1%)
42	DI	0.49	0/997	0.95	4/1343 (0.3%)
43	BJ	0.53	0/722	1.08	7/982 (0.7%)
43	DJ	0.49	0/727	0.96	1/988 (0.1%)
44	BK	0.73	0/848	1.18	7/1149 (0.6%)
44	DK	0.59	0/848	1.08	4/1149 (0.3%)
45	BL	0.78	0/946	1.16	6/1274 (0.5%)
45	DL	0.76	0/946	1.14	2/1274 (0.2%)
46	BM	0.52	0/933	1.03	1/1253 (0.1%)
46	DM	0.41	0/917	0.86	2/1234 (0.2%)
47	BN	0.55	0/501	1.05	2/664 (0.3%)
47	DN	0.43	0/501	0.91	0/664
48	BO	0.76	0/739	1.14	4/985 (0.4%)
48	DO	0.61	0/739	1.02	3/985 (0.3%)
49	BP	0.70	0/697	1.15	6/939 (0.6%)
49	DP	0.66	0/693	1.10	6/935 (0.6%)
50	BQ	0.69	0/836	1.12	5/1117 (0.4%)
50	DQ	0.61	0/836	1.05	3/1117 (0.3%)
51	BR	0.70	0/560	1.17	4/746 (0.5%)
51	DR	0.62	0/560	1.03	2/746 (0.3%)
52	BS	0.48	0/676	1.03	4/911 (0.4%)
52	DS	0.46	0/661	1.02	1/893 (0.1%)
53	BT	0.66	0/730	1.19	2/965 (0.2%)
53	DT	0.61	0/733	1.07	1/969 (0.1%)
54	BU	0.48	0/203	0.93	0/266
54	DU	0.48	0/203	0.95	1/266 (0.4%)
55	BV	0.36	0/165	0.61	0/254
55	DV	0.32	0/137	0.64	0/211
56	BW	0.48	0/1650	0.74	0/2569
56	BY	0.27	1/1602 (0.1%)	0.43	0/2493
56	DW	0.38	0/1650	0.59	0/2569
56	DY	0.23	0/1579	0.34	0/2455
57	BZ	0.64	0/5763	1.10	29/7804 (0.4%)
57	DZ	0.61	0/5784	1.11	41/7835 (0.5%)
58	BX	0.65	0/20	0.73	0/23
58	DX	0.72	0/20	1.46	0/23

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.65	42/329767 (0.0%)	0.91	742/491645 (0.2%)

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
5	AE	0	1
6	AF	0	1
19	AV	0	1
35	BB	0	1
57	DZ	0	1
58	BX	0	1
All	All	0	6

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	AO	24	VAL	CA-CB	12.14	1.68	1.54
8	AH	11	VAL	CA-CB	-7.32	1.47	1.54
15	AR	52	ILE	CA-CB	-7.18	1.46	1.54
29	A5	35	GLU	CA-C	-7.03	1.46	1.53
5	AE	12	THR	CA-C	-6.95	1.47	1.53

The worst 5 of 742 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	CK	76	GLY	CA-C-N	15.68	139.44	119.84
9	CK	76	GLY	C-N-CA	15.68	139.44	119.84
9	AK	76	GLY	CA-C-N	13.99	137.33	119.84
9	AK	76	GLY	C-N-CA	13.99	137.33	119.84
9	CK	128	LEU	CA-C-N	11.91	134.73	119.84

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	AE	74	PRO	Peptide
6	AF	194	MET	Peptide
19	AV	54	GLY	Peptide

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Mol	Chain	Res	Type	Group
35	BB	93	VAL	Peptide
58	BX	3	004	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	31172	862	0
1	CA	61771	0	31146	1176	0
2	AB	2573	0	1306	27	0
2	CB	2573	0	1306	57	0
3	AC	1063	0	1091	157	4
3	CC	1063	0	1090	183	17
4	AD	2136	0	2218	88	0
4	CD	2142	0	2229	89	0
5	AE	1559	0	1618	64	0
5	CE	1559	0	1618	78	0
6	AF	1584	0	1625	67	0
6	CF	1580	0	1619	79	0
7	AG	1425	0	1443	68	0
7	CG	1424	0	1434	85	0
8	AH	1330	0	1407	56	0
8	CH	1330	0	1407	54	0
9	AK	641	0	309	16	0
9	CK	641	0	309	10	0
10	AL	498	0	521	23	0
10	CL	498	0	521	29	0
11	AN	1117	0	1184	35	0
11	CN	1117	0	1184	40	0
12	AO	933	0	996	32	0
12	CO	933	0	996	28	0
13	AP	1139	0	1223	44	0
13	CP	1135	0	1212	58	0
14	AQ	1122	0	1179	39	0
14	CQ	1122	0	1179	56	0
15	AR	968	0	1033	34	0
15	CR	968	0	1033	40	0
16	AS	877	0	938	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	CS	870	0	923	68	0
17	AT	1091	0	1151	51	0
17	CT	1083	0	1136	43	0
18	AU	959	0	1019	30	0
18	CU	959	0	1018	41	0
19	AV	771	0	830	12	0
19	CV	771	0	830	25	0
20	AW	886	0	940	24	0
20	CW	886	0	940	41	0
21	AX	750	0	814	24	0
21	CX	750	0	814	28	0
22	AY	806	0	881	37	0
22	CY	806	0	882	45	0
23	AZ	1451	0	1457	64	0
23	CZ	1451	0	1457	74	0
24	A0	608	0	622	20	0
24	C0	608	0	622	27	0
25	A1	755	0	826	30	0
25	C1	755	0	826	24	0
26	A2	588	0	643	18	0
26	C2	588	0	643	31	0
27	A3	469	0	518	12	0
27	C3	464	0	514	25	0
28	A4	558	0	545	31	0
28	C4	532	0	507	30	0
29	A5	455	0	465	15	0
29	C5	455	0	465	17	0
30	A6	453	0	473	17	0
30	C6	449	0	469	21	0
31	A7	418	0	467	17	0
31	C7	418	0	467	12	0
32	A8	517	0	582	28	0
32	C8	517	0	582	25	0
33	A9	307	0	335	11	0
33	C9	307	0	335	14	0
34	BA	32141	0	16224	691	0
34	DA	32268	0	16287	744	0
35	BB	1846	0	1867	83	0
35	DB	1825	0	1828	102	0
36	BC	1552	0	1546	66	0
36	DC	1544	0	1524	65	0
37	BD	1659	0	1679	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	DD	1678	0	1719	86	0
38	BE	1129	0	1185	54	0
38	DE	1133	0	1191	69	0
39	BF	812	0	804	32	0
39	DF	820	0	814	38	0
40	BG	1231	0	1238	49	0
40	DG	1235	0	1249	54	0
41	BH	1088	0	1126	54	0
41	DH	1088	0	1126	77	0
42	BI	986	0	995	54	0
42	DI	978	0	966	55	0
43	BJ	709	0	650	32	0
43	DJ	714	0	672	32	0
44	BK	833	0	836	35	0
44	DK	833	0	836	27	0
45	BL	930	0	980	39	0
45	DL	930	0	980	47	0
46	BM	923	0	970	39	0
46	DM	907	0	934	42	0
47	BN	492	0	529	31	0
47	DN	492	0	531	46	0
48	BO	728	0	760	33	0
48	DO	728	0	760	31	0
49	BP	681	0	697	52	0
49	DP	677	0	686	37	0
50	BQ	823	0	891	35	0
50	DQ	823	0	891	35	0
51	BR	555	0	618	27	0
51	DR	555	0	618	30	0
52	BS	661	0	675	38	0
52	DS	646	0	644	34	0
53	BT	728	0	798	39	0
53	DT	731	0	807	28	0
54	BU	199	0	208	7	0
54	DU	199	0	208	9	0
55	BV	148	0	76	3	0
55	DV	123	0	66	1	0
56	BW	1631	0	839	25	0
56	BY	1581	0	805	25	0
56	DW	1631	0	839	33	0
56	DY	1561	0	796	33	0
57	BZ	5663	0	5747	286	17

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	DZ	5682	0	5766	243	4
58	BX	93	0	85	14	0
58	DX	93	0	85	15	0
59	A0	5	0	0	0	0
59	A2	1	0	0	0	0
59	A5	1	0	0	0	0
59	A6	2	0	0	0	0
59	A7	4	0	0	0	0
59	A8	1	0	0	0	0
59	A9	1	0	0	0	0
59	AA	821	0	0	0	0
59	AB	23	0	0	0	0
59	AD	12	0	0	0	0
59	AE	5	0	0	0	0
59	AF	8	0	0	0	0
59	AG	2	0	0	0	0
59	AH	1	0	0	0	0
59	AN	3	0	0	0	0
59	AO	1	0	0	0	0
59	AP	4	0	0	0	0
59	AQ	3	0	0	0	0
59	AR	2	0	0	0	0
59	AU	3	0	0	0	0
59	AV	6	0	0	0	0
59	AW	3	0	0	0	0
59	AX	1	0	0	0	0
59	AY	1	0	0	0	0
59	AZ	2	0	0	0	0
59	BA	215	0	0	0	0
59	BB	1	0	0	0	0
59	BD	1	0	0	0	0
59	BE	1	0	0	0	0
59	BF	1	0	0	0	0
59	BK	1	0	0	0	0
59	BL	2	0	0	0	0
59	BM	1	0	0	0	0
59	BN	2	0	0	0	0
59	BS	1	0	0	0	0
59	BT	1	0	0	0	0
59	BW	3	0	0	0	0
59	BZ	1	0	0	0	0
59	C0	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	C1	1	0	0	0	0
59	C3	1	0	0	0	0
59	C5	1	0	0	0	0
59	C7	1	0	0	0	0
59	C8	1	0	0	0	0
59	CA	664	0	0	0	0
59	CB	13	0	0	0	0
59	CD	4	0	0	0	0
59	CE	5	0	0	0	0
59	CF	4	0	0	0	0
59	CG	1	0	0	0	0
59	CN	1	0	0	0	0
59	CO	1	0	0	0	0
59	CP	1	0	0	0	0
59	CQ	4	0	0	0	0
59	CR	1	0	0	0	0
59	CU	1	0	0	0	0
59	CV	2	0	0	0	0
59	CW	1	0	0	0	0
59	CX	1	0	0	0	0
59	DA	171	0	0	0	0
59	DD	1	0	0	0	0
59	DE	2	0	0	0	0
59	DF	1	0	0	0	0
59	DJ	1	0	0	0	0
59	DK	1	0	0	0	0
59	DT	1	0	0	0	0
59	DW	3	0	0	0	0
59	DZ	2	0	0	0	0
60	A4	1	0	0	0	0
60	A5	1	0	0	0	0
60	A6	1	0	0	0	0
60	A9	1	0	0	0	0
60	AY	1	0	0	0	0
60	BN	1	0	0	0	0
60	C4	1	0	0	0	0
60	C5	1	0	0	0	0
60	C6	1	0	0	0	0
60	C9	1	0	0	0	0
60	CY	1	0	0	0	0
60	DN	1	0	0	0	0
61	BD	8	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	DD	8	0	0	2	0
62	BZ	28	0	12	5	0
62	DZ	28	0	12	7	0
63	A0	6	0	0	0	0
63	A1	2	0	0	0	0
63	A3	2	0	0	0	0
63	A5	3	0	0	0	0
63	A6	1	0	0	0	0
63	A7	2	0	0	1	0
63	A8	10	0	0	1	0
63	A9	1	0	0	0	0
63	AA	1413	0	0	66	0
63	AB	38	0	0	3	0
63	AD	10	0	0	2	0
63	AE	17	0	0	4	0
63	AF	11	0	0	1	0
63	AG	3	0	0	1	0
63	AH	1	0	0	0	0
63	AN	1	0	0	0	0
63	AO	3	0	0	0	0
63	AP	16	0	0	1	0
63	AQ	4	0	0	1	0
63	AR	2	0	0	0	0
63	AS	1	0	0	1	0
63	AT	1	0	0	0	0
63	AU	4	0	0	0	0
63	AV	1	0	0	0	0
63	AW	1	0	0	0	0
63	AX	3	0	0	0	0
63	AZ	1	0	0	0	0
63	BA	213	0	0	19	0
63	BD	1	0	0	0	0
63	BM	1	0	0	0	0
63	BO	1	0	0	0	0
63	BP	1	0	0	0	0
63	BV	1	0	0	0	0
63	BW	1	0	0	0	0
63	BZ	2	0	0	0	0
63	C0	4	0	0	0	0
63	C3	2	0	0	0	0
63	C5	1	0	0	0	0
63	C7	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	C8	4	0	0	0	0
63	CA	983	0	0	79	0
63	CB	9	0	0	1	0
63	CD	15	0	0	1	0
63	CE	9	0	0	1	0
63	CF	6	0	0	0	0
63	CN	1	0	0	0	0
63	CO	1	0	0	0	0
63	CP	11	0	0	2	0
63	CQ	2	0	0	1	0
63	CT	3	0	0	0	0
63	CU	2	0	0	0	0
63	CV	1	0	0	1	0
63	CW	1	0	0	0	0
63	CX	1	0	0	0	0
63	CY	2	0	0	1	0
63	DA	157	0	0	13	0
63	DD	1	0	0	0	0
63	DE	2	0	0	2	0
63	DH	1	0	0	0	0
63	DJ	1	0	0	0	0
63	DK	2	0	0	0	0
63	DL	1	0	0	0	0
63	DT	1	0	0	0	0
All	All	310038	0	209219	7561	21

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 15.

The worst 5 of 7561 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:AA:1891:G:H5''	3:AC:206:LYS:CG	1.32	1.59
1:AA:1891:G:C5'	3:AC:206:LYS:HD2	1.36	1.52
1:CA:2128:C:H5''	3:CC:219:MET:CE	1.36	1.51
1:CA:2132:U:C4	3:CC:6:LYS:HE3	1.51	1.41
1:CA:2128:C:C5'	3:CC:219:MET:HE1	1.50	1.38

The worst 5 of 21 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)
57:BZ:502:GLY:CA	3:CC:9:ARG:CD[2_655]	1.16	1.04
3:AC:9:ARG:NH2	57:DZ:504:ARG:NH1[3_654]	1.36	0.84
57:BZ:502:GLY:N	3:CC:9:ARG:CB[2_655]	1.54	0.66
57:BZ:502:GLY:N	3:CC:9:ARG:CD[2_655]	1.69	0.51
57:BZ:573:HIS:CE1	3:CC:13:GLU:OE1[2_655]	1.71	0.49

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%)	249 (91%)	19 (7%)	5 (2%)	6	23
4	CD	273/276 (99%)	234 (86%)	26 (10%)	13 (5%)	2	6
5	AE	202/206 (98%)	186 (92%)	14 (7%)	2 (1%)	12	38
5	CE	202/206 (98%)	179 (89%)	20 (10%)	3 (2%)	8	28
6	AF	201/210 (96%)	182 (90%)	18 (9%)	1 (0%)	24	55
6	CF	201/210 (96%)	177 (88%)	17 (8%)	7 (4%)	3	10
7	AG	179/182 (98%)	154 (86%)	19 (11%)	6 (3%)	3	11
7	CG	179/182 (98%)	141 (79%)	31 (17%)	7 (4%)	2	8
8	AH	172/180 (96%)	154 (90%)	15 (9%)	3 (2%)	7	25
8	CH	172/180 (96%)	144 (84%)	17 (10%)	11 (6%)	1	3
9	AK	128/173 (74%)	66 (52%)	36 (28%)	26 (20%)	0	0
9	CK	128/173 (74%)	76 (59%)	27 (21%)	25 (20%)	0	0
10	AL	64/147 (44%)	43 (67%)	17 (27%)	4 (6%)	1	3
10	CL	64/147 (44%)	42 (66%)	19 (30%)	3 (5%)	2	6
11	AN	138/140 (99%)	129 (94%)	8 (6%)	1 (1%)	18	47
11	CN	138/140 (99%)	120 (87%)	15 (11%)	3 (2%)	5	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	AO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
12	CO	120/122 (98%)	107 (89%)	10 (8%)	3 (2%)	4	16
13	AP	147/150 (98%)	130 (88%)	15 (10%)	2 (1%)	9	30
13	CP	147/150 (98%)	119 (81%)	25 (17%)	3 (2%)	6	21
14	AQ	139/141 (99%)	126 (91%)	12 (9%)	1 (1%)	18	47
14	CQ	139/141 (99%)	123 (88%)	14 (10%)	2 (1%)	9	30
15	AR	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
15	CR	116/118 (98%)	102 (88%)	11 (10%)	3 (3%)	4	15
16	AS	108/112 (96%)	88 (82%)	16 (15%)	4 (4%)	2	9
16	CS	108/112 (96%)	83 (77%)	20 (18%)	5 (5%)	2	6
17	AT	129/146 (88%)	114 (88%)	13 (10%)	2 (2%)	7	27
17	CT	129/146 (88%)	116 (90%)	11 (8%)	2 (2%)	7	27
18	AU	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
18	CU	114/118 (97%)	100 (88%)	11 (10%)	3 (3%)	4	15
19	AV	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	12	38
19	CV	99/101 (98%)	86 (87%)	10 (10%)	3 (3%)	3	12
20	AW	110/113 (97%)	104 (94%)	6 (6%)	0	100	100
20	CW	110/113 (97%)	105 (96%)	5 (4%)	0	100	100
21	AX	93/96 (97%)	85 (91%)	6 (6%)	2 (2%)	5	19
21	CX	93/96 (97%)	77 (83%)	11 (12%)	5 (5%)	1	4
22	AY	105/110 (96%)	93 (89%)	9 (9%)	3 (3%)	3	13
22	CY	105/110 (96%)	86 (82%)	14 (13%)	5 (5%)	2	6
23	AZ	183/206 (89%)	147 (80%)	24 (13%)	12 (7%)	1	3
23	CZ	183/206 (89%)	134 (73%)	33 (18%)	16 (9%)	0	1
24	A0	75/85 (88%)	70 (93%)	5 (7%)	0	100	100
24	C0	75/85 (88%)	67 (89%)	7 (9%)	1 (1%)	9	31
25	A1	95/98 (97%)	90 (95%)	5 (5%)	0	100	100
25	C1	95/98 (97%)	85 (90%)	7 (7%)	3 (3%)	3	11
26	A2	68/72 (94%)	62 (91%)	6 (9%)	0	100	100
26	C2	68/72 (94%)	60 (88%)	7 (10%)	1 (2%)	8	28
27	A3	57/60 (95%)	51 (90%)	6 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	C3	57/60 (95%)	50 (88%)	5 (9%)	2 (4%)	3	10
28	A4	67/71 (94%)	46 (69%)	12 (18%)	9 (13%)	0	0
28	C4	67/71 (94%)	43 (64%)	15 (22%)	9 (13%)	0	0
29	A5	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
29	C5	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	6	23
30	A6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
30	C6	51/54 (94%)	42 (82%)	8 (16%)	1 (2%)	6	21
31	A7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
31	C7	46/49 (94%)	41 (89%)	4 (9%)	1 (2%)	5	19
32	A8	62/65 (95%)	60 (97%)	1 (2%)	1 (2%)	7	27
32	C8	62/65 (95%)	54 (87%)	7 (11%)	1 (2%)	7	27
33	A9	35/37 (95%)	35 (100%)	0	0	100	100
33	C9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
35	BB	229/256 (90%)	182 (80%)	33 (14%)	14 (6%)	1	3
35	DB	229/256 (90%)	170 (74%)	41 (18%)	18 (8%)	1	1
36	BC	204/239 (85%)	155 (76%)	38 (19%)	11 (5%)	1	4
36	DC	204/239 (85%)	169 (83%)	29 (14%)	6 (3%)	3	13
37	BD	206/209 (99%)	166 (81%)	28 (14%)	12 (6%)	1	4
37	DD	206/209 (99%)	171 (83%)	27 (13%)	8 (4%)	2	8
38	BE	146/162 (90%)	114 (78%)	24 (16%)	8 (6%)	1	4
38	DE	146/162 (90%)	117 (80%)	22 (15%)	7 (5%)	2	6
39	BF	98/101 (97%)	84 (86%)	11 (11%)	3 (3%)	3	12
39	DF	98/101 (97%)	90 (92%)	5 (5%)	3 (3%)	3	12
40	BG	153/156 (98%)	128 (84%)	13 (8%)	12 (8%)	1	2
40	DG	153/156 (98%)	126 (82%)	22 (14%)	5 (3%)	3	11
41	BH	135/138 (98%)	110 (82%)	22 (16%)	3 (2%)	5	19
41	DH	135/138 (98%)	114 (84%)	14 (10%)	7 (5%)	1	5
42	BI	125/128 (98%)	103 (82%)	15 (12%)	7 (6%)	1	4
42	DI	125/128 (98%)	100 (80%)	21 (17%)	4 (3%)	3	11
43	BJ	95/105 (90%)	76 (80%)	12 (13%)	7 (7%)	1	2
43	DJ	94/105 (90%)	75 (80%)	16 (17%)	3 (3%)	3	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	BK	112/129 (87%)	96 (86%)	14 (12%)	2 (2%)	6	23
44	DK	112/129 (87%)	92 (82%)	16 (14%)	4 (4%)	2	10
45	BL	120/132 (91%)	108 (90%)	11 (9%)	1 (1%)	16	44
45	DL	120/132 (91%)	100 (83%)	16 (13%)	4 (3%)	3	11
46	BM	115/126 (91%)	93 (81%)	18 (16%)	4 (4%)	3	10
46	DM	114/126 (90%)	88 (77%)	17 (15%)	9 (8%)	1	1
47	BN	58/61 (95%)	46 (79%)	9 (16%)	3 (5%)	1	5
47	DN	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	3	11
48	BO	86/89 (97%)	67 (78%)	16 (19%)	3 (4%)	3	10
48	DO	86/89 (97%)	72 (84%)	10 (12%)	4 (5%)	2	6
49	BP	80/88 (91%)	54 (68%)	17 (21%)	9 (11%)	0	1
49	DP	80/88 (91%)	58 (72%)	18 (22%)	4 (5%)	1	5
50	BQ	97/105 (92%)	87 (90%)	7 (7%)	3 (3%)	3	12
50	DQ	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
51	BR	66/88 (75%)	57 (86%)	7 (11%)	2 (3%)	3	12
51	DR	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
52	BS	82/93 (88%)	64 (78%)	14 (17%)	4 (5%)	1	6
52	DS	81/93 (87%)	63 (78%)	15 (18%)	3 (4%)	2	9
53	BT	94/106 (89%)	78 (83%)	12 (13%)	4 (4%)	2	7
53	DT	94/106 (89%)	75 (80%)	13 (14%)	6 (6%)	1	3
54	BU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
54	DU	21/27 (78%)	17 (81%)	2 (10%)	2 (10%)	0	1
57	BZ	722/758 (95%)	563 (78%)	107 (15%)	52 (7%)	1	2
57	DZ	726/758 (96%)	537 (74%)	132 (18%)	57 (8%)	1	1
58	BX	3/10 (30%)	1 (33%)	0	2 (67%)	0	0
58	DX	3/10 (30%)	0	2 (67%)	1 (33%)	0	0
All	All	13227/14464 (91%)	10975 (83%)	1666 (13%)	586 (4%)	2	7

5 of 586 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%)	169 (79%)	46 (21%)	1	4
4	CD	216/218 (99%)	173 (80%)	43 (20%)	1	5
5	AE	164/166 (99%)	133 (81%)	31 (19%)	1	5
5	CE	164/166 (99%)	127 (77%)	37 (23%)	1	3
6	AF	160/166 (96%)	126 (79%)	34 (21%)	1	4
6	CF	159/166 (96%)	120 (76%)	39 (24%)	1	2
7	AG	143/156 (92%)	112 (78%)	31 (22%)	1	3
7	CG	142/156 (91%)	108 (76%)	34 (24%)	1	3
8	AH	144/148 (97%)	107 (74%)	37 (26%)	0	2
8	CH	144/148 (97%)	113 (78%)	31 (22%)	1	4
10	AL	50/111 (45%)	39 (78%)	11 (22%)	1	3
10	CL	50/111 (45%)	32 (64%)	18 (36%)	0	0
11	AN	118/119 (99%)	92 (78%)	26 (22%)	1	3
11	CN	118/119 (99%)	82 (70%)	36 (30%)	0	1
12	AO	100/100 (100%)	83 (83%)	17 (17%)	2	7
12	CO	100/100 (100%)	84 (84%)	16 (16%)	2	9
13	AP	116/116 (100%)	94 (81%)	22 (19%)	1	5
13	CP	115/116 (99%)	92 (80%)	23 (20%)	1	4
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%)	84 (76%)	27 (24%)	1	2
15	AR	101/101 (100%)	78 (77%)	23 (23%)	1	3
15	CR	101/101 (100%)	86 (85%)	15 (15%)	3	10
16	AS	87/88 (99%)	66 (76%)	21 (24%)	1	2
16	CS	85/88 (97%)	64 (75%)	21 (25%)	1	2
17	AT	115/127 (91%)	94 (82%)	21 (18%)	2	6
17	CT	113/127 (89%)	96 (85%)	17 (15%)	3	10
18	AU	93/94 (99%)	74 (80%)	19 (20%)	1	4
18	CU	93/94 (99%)	79 (85%)	14 (15%)	3	10
19	AV	80/82 (98%)	65 (81%)	15 (19%)	1	5
19	CV	80/82 (98%)	62 (78%)	18 (22%)	1	3
20	AW	90/92 (98%)	74 (82%)	16 (18%)	2	6
20	CW	90/92 (98%)	72 (80%)	18 (20%)	1	4
21	AX	77/78 (99%)	63 (82%)	14 (18%)	2	6
21	CX	77/78 (99%)	62 (80%)	15 (20%)	1	5
22	AY	85/91 (93%)	65 (76%)	20 (24%)	1	3
22	CY	85/91 (93%)	62 (73%)	23 (27%)	0	1
23	AZ	156/179 (87%)	114 (73%)	42 (27%)	0	1
23	CZ	156/179 (87%)	123 (79%)	33 (21%)	1	4
24	A0	61/67 (91%)	55 (90%)	6 (10%)	7	25
24	C0	61/67 (91%)	48 (79%)	13 (21%)	1	4
25	A1	80/83 (96%)	62 (78%)	18 (22%)	1	3
25	C1	80/83 (96%)	63 (79%)	17 (21%)	1	4
26	A2	65/67 (97%)	55 (85%)	10 (15%)	2	10
26	C2	65/67 (97%)	50 (77%)	15 (23%)	1	3
27	A3	51/52 (98%)	42 (82%)	9 (18%)	2	7
27	C3	50/52 (96%)	38 (76%)	12 (24%)	1	2
28	A4	60/63 (95%)	52 (87%)	8 (13%)	4	14
28	C4	53/63 (84%)	41 (77%)	12 (23%)	1	3
29	A5	50/52 (96%)	43 (86%)	7 (14%)	3	12
29	C5	50/52 (96%)	41 (82%)	9 (18%)	2	6

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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%)	40 (80%)	10 (20%)	1	4
31	A7	41/42 (98%)	31 (76%)	10 (24%)	1	2
31	C7	41/42 (98%)	33 (80%)	8 (20%)	1	5
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%)	29 (85%)	5 (15%)	3	10
33	C9	34/34 (100%)	31 (91%)	3 (9%)	9	29
35	BB	192/220 (87%)	150 (78%)	42 (22%)	1	3
35	DB	187/220 (85%)	145 (78%)	42 (22%)	1	3
36	BC	143/188 (76%)	122 (85%)	21 (15%)	3	10
36	DC	141/188 (75%)	104 (74%)	37 (26%)	0	2
37	BD	170/181 (94%)	135 (79%)	35 (21%)	1	4
37	DD	174/181 (96%)	136 (78%)	38 (22%)	1	3
38	BE	113/123 (92%)	85 (75%)	28 (25%)	1	2
38	DE	114/123 (93%)	80 (70%)	34 (30%)	0	1
39	BF	84/90 (93%)	68 (81%)	16 (19%)	1	5
39	DF	86/90 (96%)	73 (85%)	13 (15%)	3	10
40	BG	119/127 (94%)	93 (78%)	26 (22%)	1	3
40	DG	120/127 (94%)	103 (86%)	17 (14%)	3	12
41	BH	114/119 (96%)	87 (76%)	27 (24%)	1	3
41	DH	114/119 (96%)	84 (74%)	30 (26%)	0	2
42	BI	91/99 (92%)	76 (84%)	15 (16%)	2	8
42	DI	89/99 (90%)	66 (74%)	23 (26%)	0	2
43	BJ	66/92 (72%)	56 (85%)	10 (15%)	3	10
43	DJ	69/92 (75%)	58 (84%)	11 (16%)	2	9
44	BK	83/99 (84%)	65 (78%)	18 (22%)	1	3
44	DK	83/99 (84%)	63 (76%)	20 (24%)	1	2
45	BL	97/109 (89%)	79 (81%)	18 (19%)	1	5
45	DL	97/109 (89%)	73 (75%)	24 (25%)	1	2
46	BM	91/101 (90%)	76 (84%)	15 (16%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	DM	88/101 (87%)	73 (83%)	15 (17%)	2	7
47	BN	49/50 (98%)	38 (78%)	11 (22%)	1	3
47	DN	49/50 (98%)	42 (86%)	7 (14%)	3	11
48	BO	78/80 (98%)	69 (88%)	9 (12%)	5	18
48	DO	78/80 (98%)	61 (78%)	17 (22%)	1	3
49	BP	69/74 (93%)	53 (77%)	16 (23%)	1	3
49	DP	68/74 (92%)	52 (76%)	16 (24%)	1	3
50	BQ	94/97 (97%)	75 (80%)	19 (20%)	1	4
50	DQ	94/97 (97%)	80 (85%)	14 (15%)	3	10
51	BR	59/77 (77%)	48 (81%)	11 (19%)	1	5
51	DR	59/77 (77%)	53 (90%)	6 (10%)	7	23
52	BS	70/80 (88%)	58 (83%)	12 (17%)	2	7
52	DS	67/80 (84%)	54 (81%)	13 (19%)	1	5
53	BT	70/82 (85%)	51 (73%)	19 (27%)	0	1
53	DT	71/82 (87%)	59 (83%)	12 (17%)	2	7
54	BU	18/22 (82%)	17 (94%)	1 (6%)	19	50
54	DU	18/22 (82%)	17 (94%)	1 (6%)	19	50
57	BZ	604/636 (95%)	470 (78%)	134 (22%)	1	3
57	DZ	607/636 (95%)	491 (81%)	116 (19%)	1	5
58	BX	3/3 (100%)	3 (100%)	0	100	100
58	DX	3/3 (100%)	3 (100%)	0	100	100
All	All	10664/11678 (91%)	8485 (80%)	2179 (20%)	1	4

5 of 2179 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	DG	146	GLU
43	DJ	29	ARG
40	DG	131	LYS
57	DZ	33	LEU
42	BI	66	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 211 such sidechains are listed below:

Mol	Chain	Res	Type
8	CH	147	ASN
23	CZ	65	GLN
57	DZ	-50	GLN
12	CO	89	ASN
17	CT	58	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2865/2915 (98%)	536 (18%)	51 (1%)
1	CA	2860/2915 (98%)	615 (21%)	39 (1%)
2	AB	119/121 (98%)	15 (12%)	0
2	CB	119/121 (98%)	27 (22%)	0
34	BA	1491/1521 (98%)	331 (22%)	20 (1%)
34	DA	1498/1521 (98%)	352 (23%)	22 (1%)
55	BV	6/18 (33%)	2 (33%)	0
55	DV	5/18 (27%)	1 (20%)	0
56	BW	75/76 (98%)	16 (21%)	1 (1%)
56	BY	72/76 (94%)	24 (33%)	2 (2%)
56	DW	75/76 (98%)	24 (32%)	2 (2%)
56	DY	71/76 (93%)	23 (32%)	1 (1%)
All	All	9256/9454 (97%)	1966 (21%)	138 (1%)

5 of 1966 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	12	U
1	AA	13	A
1	AA	15	G
1	AA	34	C
1	AA	45	C

5 of 138 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	DA	115	G
34	DA	428	G
34	DA	1065	U
1	AA	2769	U
1	AA	2739	U

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

42 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$
58	2QZ	BX	1	58	7,8,9	0.67	0	7,10,12	4.73	4 (57%)
56	4SU	DW	8	56	18,21,22	1.83	5 (27%)	25,30,33	2.31	4 (16%)
58	2QY	BX	10	58	12,13,14	1.73	2 (16%)	14,16,18	4.12	6 (42%)
56	7MG	BY	46	56	23,26,27	1.30	3 (13%)	27,39,42	2.71	7 (25%)
58	004	DX	3	58	9,10,11	1.53	1 (11%)	9,12,14	1.28	1 (11%)
56	4SU	BW	8	56	18,21,22	1.49	3 (16%)	25,30,33	2.18	5 (20%)
56	PSU	DY	39	56	18,21,22	1.43	2 (11%)	21,30,33	1.97	3 (14%)
56	PSU	BW	55	56	18,21,22	1.37	1 (5%)	21,30,33	1.95	3 (14%)
58	MVA	BX	5	58	6,7,8	0.52	0	6,8,10	1.39	1 (16%)
58	2R1	DX	6	58	10,10,11	1.65	2 (20%)	8,13,15	2.10	3 (37%)
56	PSU	BY	32	56	18,21,22	1.40	2 (11%)	21,30,33	1.94	3 (14%)
56	5MU	BW	54	56	19,22,23	1.44	4 (21%)	27,32,35	1.98	7 (25%)
56	5MU	DY	54	56	19,22,23	1.44	6 (31%)	27,32,35	2.07	5 (18%)
58	MVA	DX	5	58	6,7,8	1.06	0	6,8,10	1.57	1 (16%)
58	2R3	DX	8	58	12,14,15	0.60	0	16,18,20	1.77	5 (31%)
56	PSU	BY	55	56	18,21,22	1.39	2 (11%)	21,30,33	1.98	3 (14%)
58	2R1	BX	6	58	10,10,11	2.35	3 (30%)	8,13,15	3.80	3 (37%)
56	5MU	BY	54	56	19,22,23	1.53	5 (26%)	27,32,35	2.21	8 (29%)
58	MVA	BX	9	58	6,7,8	0.77	0	6,8,10	1.50	1 (16%)
58	2QY	DX	10	58	12,13,14	1.66	1 (8%)	14,16,18	3.67	6 (42%)
56	5MU	DW	54	56	19,22,23	1.49	4 (21%)	27,32,35	2.07	7 (25%)
56	PSU	BW	39	56	18,21,22	1.37	2 (11%)	21,30,33	2.02	5 (23%)
58	2R3	BX	8	58	12,14,15	0.70	0	16,18,20	2.13	9 (56%)
56	MIA	DW	37	56	28,31,32	2.31	6 (21%)	38,44,47	2.62	13 (34%)
56	7MG	DW	46	56	23,26,27	1.30	3 (13%)	27,39,42	2.71	7 (25%)
58	004	BX	3	58	9,10,11	1.39	1 (11%)	9,12,14	1.32	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	PSU	DY	32	56	18,21,22	1.36	2 (11%)	21,30,33	1.95	4 (19%)
56	PSU	BW	32	56	18,21,22	1.34	3 (16%)	21,30,33	1.83	5 (23%)
56	MIA	BY	37	56	21,24,32	1.68	3 (14%)	30,35,47	2.03	8 (26%)
56	PSU	DY	55	56	18,21,22	1.42	2 (11%)	21,30,33	2.01	3 (14%)
56	4SU	BY	8	56	18,21,22	1.75	4 (22%)	25,30,33	2.14	6 (24%)
58	MVA	DX	9	58	6,7,8	1.14	1 (16%)	6,8,10	1.58	1 (16%)
56	PSU	BY	39	56	18,21,22	1.39	2 (11%)	21,30,33	1.93	3 (14%)
56	PSU	DW	39	56	18,21,22	1.35	2 (11%)	21,30,33	2.08	4 (19%)
56	7MG	BW	46	56	23,26,27	1.29	4 (17%)	27,39,42	2.77	7 (25%)
56	PSU	DW	55	56	18,21,22	1.40	2 (11%)	21,30,33	2.01	5 (23%)
56	MIA	BW	37	56	28,31,32	2.41	8 (28%)	38,44,47	2.62	14 (36%)
56	PSU	DW	32	56	18,21,22	1.43	3 (16%)	21,30,33	2.14	4 (19%)
58	2QZ	DX	1	58	7,8,9	0.55	0	7,10,12	4.52	3 (42%)
56	7MG	DY	46	56	23,26,27	1.24	3 (13%)	27,39,42	2.76	7 (25%)
56	4SU	DY	8	56	18,21,22	1.84	4 (22%)	25,30,33	2.35	6 (24%)
56	MIA	DY	37	56	21,24,32	1.60	4 (19%)	30,35,47	2.07	7 (23%)

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
58	2QZ	BX	1	58	-	1/8/10/12	-
56	4SU	DW	8	56	-	0/7/25/26	0/2/2/2
58	2QY	BX	10	58	-	3/5/8/10	0/1/1/1
56	7MG	BY	46	56	-	4/7/37/38	0/3/3/3
58	004	DX	3	58	-	0/4/6/8	0/1/1/1
56	4SU	BW	8	56	-	0/7/25/26	0/2/2/2
56	PSU	DY	39	56	-	2/7/25/26	0/2/2/2
56	PSU	BW	55	56	-	2/7/25/26	0/2/2/2
58	MVA	BX	5	58	-	4/6/8/10	-
58	2R1	DX	6	58	-	2/2/14/16	0/1/1/1
56	PSU	BY	32	56	-	0/7/25/26	0/2/2/2
56	5MU	BW	54	56	-	1/7/25/26	0/2/2/2
56	5MU	DY	54	56	-	2/7/25/26	0/2/2/2
58	MVA	DX	5	58	-	4/6/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	2R3	DX	8	58	-	6/11/12/14	0/1/1/1
56	PSU	BY	55	56	-	2/7/25/26	0/2/2/2
58	2R1	BX	6	58	-	0/2/14/16	0/1/1/1
56	5MU	BY	54	56	-	2/7/25/26	0/2/2/2
58	MVA	BX	9	58	-	2/6/8/10	-
58	2QY	DX	10	58	-	3/5/8/10	0/1/1/1
56	5MU	DW	54	56	-	0/7/25/26	0/2/2/2
56	PSU	BW	39	56	-	0/7/25/26	0/2/2/2
58	2R3	BX	8	58	-	6/11/12/14	0/1/1/1
56	MIA	DW	37	56	-	7/15/33/34	0/3/3/3
56	7MG	DW	46	56	-	4/7/37/38	0/3/3/3
58	004	BX	3	58	-	0/4/6/8	0/1/1/1
56	PSU	DY	32	56	-	0/7/25/26	0/2/2/2
56	PSU	BW	32	56	-	4/7/25/26	0/2/2/2
56	MIA	BY	37	56	-	2/7/25/34	0/3/3/3
56	PSU	DY	55	56	-	3/7/25/26	0/2/2/2
56	4SU	BY	8	56	-	1/7/25/26	0/2/2/2
58	MVA	DX	9	58	-	4/6/8/10	-
56	PSU	BY	39	56	-	0/7/25/26	0/2/2/2
56	PSU	DW	39	56	-	1/7/25/26	0/2/2/2
56	7MG	BW	46	56	-	1/7/37/38	0/3/3/3
56	PSU	DW	55	56	-	2/7/25/26	0/2/2/2
56	MIA	BW	37	56	-	5/15/33/34	0/3/3/3
56	PSU	DW	32	56	-	2/7/25/26	0/2/2/2
58	2QZ	DX	1	58	-	1/8/10/12	-
56	7MG	DY	46	56	-	3/7/37/38	0/3/3/3
56	4SU	DY	8	56	-	1/7/25/26	0/2/2/2
56	MIA	DY	37	56	-	3/7/25/34	0/3/3/3

The worst 5 of 105 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	BW	37	MIA	C13-C14	7.51	1.54	1.32
56	DW	37	MIA	C13-C14	7.11	1.53	1.32
56	BW	37	MIA	C2-S10	-7.10	1.69	1.75
56	DW	37	MIA	C2-S10	-5.65	1.71	1.75
56	BY	37	MIA	C5-C4	5.34	1.48	1.39

The worst 5 of 208 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	BX	1	2QZ	OG1-CB-CG2	11.46	143.95	109.68
58	DX	1	2QZ	OG1-CB-CG2	11.15	143.03	109.68
58	BX	10	2QY	CN-N-CA	-11.03	107.25	123.98
56	BW	46	7MG	N9-C4-N3	9.66	139.62	125.46
56	DY	46	7MG	N9-C4-N3	9.62	139.55	125.46

There are no chirality outliers.

5 of 90 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	BW	32	PSU	C2'-C1'-C5-C4
56	BW	32	PSU	O4'-C1'-C5-C4
56	BW	32	PSU	O4'-C1'-C5-C6
56	BW	37	MIA	N6-C12-C13-C14
56	BW	37	MIA	C12-C13-C14-C15

There are no ring outliers.

23 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	DW	8	4SU	1	0
58	BX	10	2QY	1	0
58	DX	3	004	1	0
58	BX	5	MVA	2	0
58	DX	6	2R1	2	0
58	DX	5	MVA	2	0
58	DX	8	2R3	2	0
58	BX	6	2R1	5	0
58	BX	9	MVA	2	0
58	DX	10	2QY	9	0
56	DW	54	5MU	1	0
58	BX	8	2R3	2	0
56	DW	37	MIA	2	0
58	BX	3	004	4	0
56	BW	32	PSU	1	0
56	DY	55	PSU	2	0
56	BY	8	4SU	1	0
58	DX	9	MVA	4	0
56	DW	39	PSU	6	0
56	DW	55	PSU	1	0
56	BW	37	MIA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	DX	1	2QZ	2	0
56	DY	46	7MG	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2056 ligands modelled in this entry, 2052 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
62	GDP	BZ	702	59	29,30,30	1.18	2 (6%)	45,47,47	1.66	8 (17%)
62	GDP	DZ	703	59	29,30,30	1.25	3 (10%)	45,47,47	1.68	6 (13%)
61	SF4	DD	501	37	0,12,12	-	-	-		
61	SF4	BD	501	-	0,12,12	-	-	-		

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
62	GDP	BZ	702	59	-	3/16/32/32	0/3/3/3
62	GDP	DZ	703	59	-	1/16/32/32	0/3/3/3
61	SF4	DD	501	37	-	-	0/6/5/5
61	SF4	BD	501	-	-	-	0/6/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	BZ	702	GDP	C5-C4	3.41	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	DZ	703	GDP	C5-C4	3.29	1.47	1.38
62	BZ	702	GDP	C5-N7	-2.38	1.34	1.39
62	DZ	703	GDP	C4-N9	-2.25	1.32	1.38
62	DZ	703	GDP	C6-N1	-2.13	1.34	1.38

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	DZ	703	GDP	C5-C4-N3	-5.05	120.35	128.39
62	BZ	702	GDP	C5-C4-N3	-5.03	120.38	128.39
62	DZ	703	GDP	C2-N3-C4	4.36	119.80	112.30
62	BZ	702	GDP	N9-C4-N3	4.16	134.27	125.95
62	DZ	703	GDP	N9-C4-N3	4.09	134.13	125.95

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	BZ	702	GDP	C5'-O5'-PA-O3A
62	BZ	702	GDP	C5'-O5'-PA-O1A
62	BZ	702	GDP	C5'-O5'-PA-O2A
62	DZ	703	GDP	C5'-O5'-PA-O1A

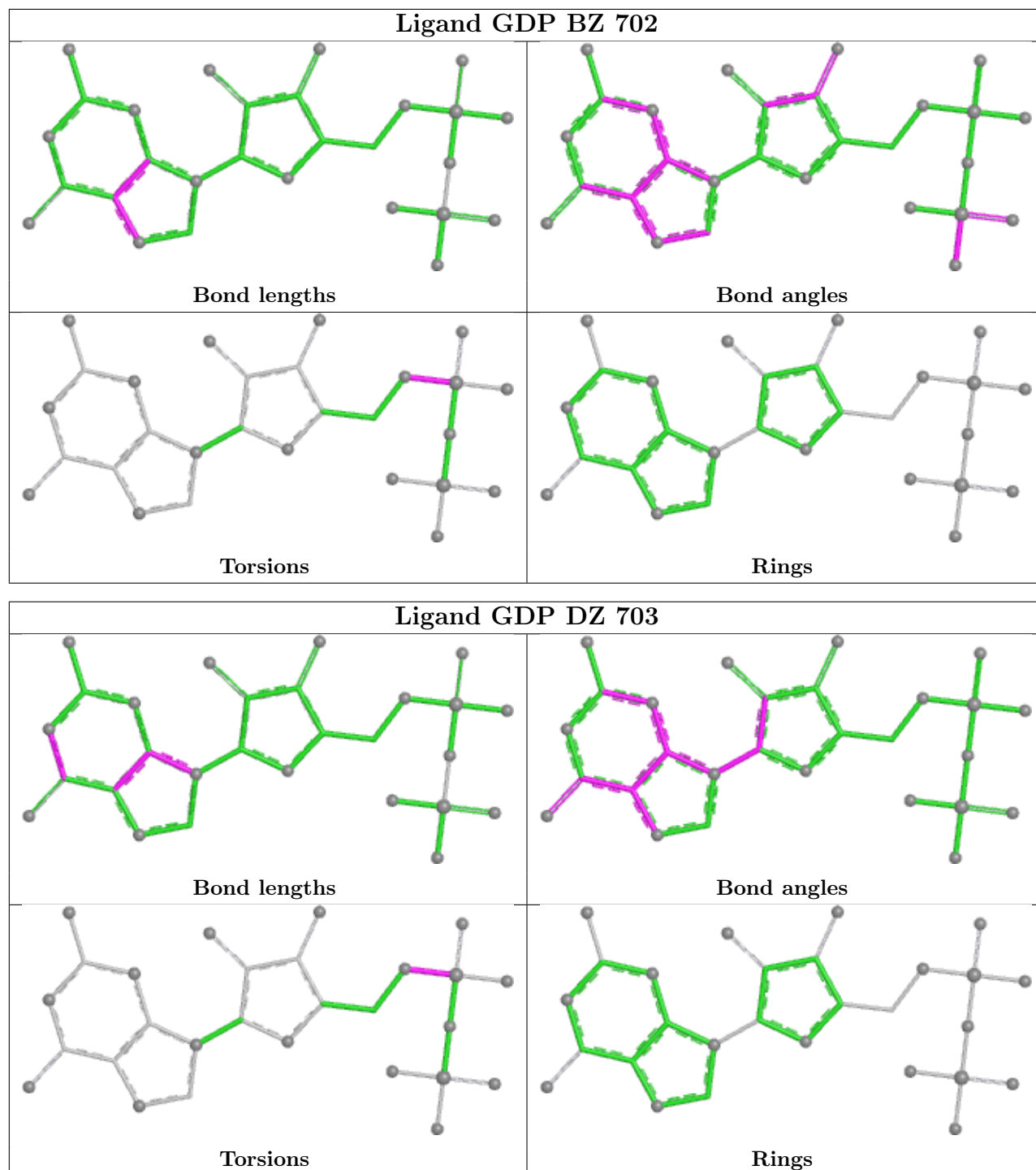
There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	BZ	702	GDP	5	0
62	DZ	703	GDP	7	0
61	DD	501	SF4	2	0
61	BD	501	SF4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	2872/2915 (98%)	-0.84	40 (1%) 73 64	13, 31, 166, 310	0
1	CA	2868/2915 (98%)	-0.32	71 (2%) 58 48	23, 54, 175, 327	0
2	AB	120/121 (99%)	-0.71	1 (0%) 82 75	23, 46, 65, 111	0
2	CB	120/121 (99%)	0.58	5 (4%) 40 32	54, 103, 145, 177	0
3	AC	137/228 (60%)	2.68	94 (68%) 0 0	89, 187, 231, 259	0
3	CC	137/228 (60%)	2.84	98 (71%) 0 0	142, 205, 249, 270	0
4	AD	275/276 (99%)	-0.59	4 (1%) 72 63	8, 30, 56, 122	0
4	CD	275/276 (99%)	-0.25	4 (1%) 72 63	13, 43, 76, 133	0
5	AE	204/206 (99%)	-0.65	0 100 100	7, 30, 60, 99	0
5	CE	204/206 (99%)	-0.23	2 (0%) 79 72	15, 51, 85, 143	0
6	AF	203/210 (96%)	-0.60	0 100 100	5, 31, 75, 140	0
6	CF	203/210 (96%)	0.13	3 (1%) 72 63	20, 66, 122, 158	0
7	AG	181/182 (99%)	0.14	2 (1%) 78 70	33, 66, 114, 178	0
7	CG	181/182 (99%)	1.20	27 (14%) 5 4	73, 124, 181, 208	0
8	AH	174/180 (96%)	-0.31	2 (1%) 78 70	21, 45, 72, 198	0
8	CH	174/180 (96%)	0.72	14 (8%) 18 13	51, 90, 139, 171	0
9	AK	130/173 (75%)	1.59	35 (26%) 1 1	65, 130, 195, 217	0
9	CK	130/173 (75%)	1.99	54 (41%) 0 0	84, 161, 205, 230	0
10	AL	66/147 (44%)	1.91	22 (33%) 1 1	109, 180, 227, 243	0
10	CL	66/147 (44%)	2.51	38 (57%) 0 0	104, 180, 226, 260	0
11	AN	140/140 (100%)	-0.68	1 (0%) 84 77	11, 27, 54, 96	0
11	CN	140/140 (100%)	0.03	1 (0%) 84 77	35, 58, 92, 142	0
12	AO	122/122 (100%)	-0.66	0 100 100	16, 35, 64, 91	0
12	CO	122/122 (100%)	-0.28	0 100 100	28, 48, 80, 94	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AP	149/150 (99%)	-0.49	0 100 100	8, 37, 77, 126	0
13	CP	149/150 (99%)	0.37	6 (4%) 42 33	26, 73, 123, 155	0
14	AQ	141/141 (100%)	-0.59	0 100 100	9, 31, 53, 97	0
14	CQ	141/141 (100%)	0.23	3 (2%) 63 54	18, 62, 94, 145	0
15	AR	118/118 (100%)	-0.77	0 100 100	13, 27, 51, 75	0
15	CR	118/118 (100%)	-0.23	0 100 100	25, 49, 73, 106	0
16	AS	110/112 (98%)	-0.25	1 (0%) 81 74	24, 46, 74, 86	0
16	CS	110/112 (98%)	1.38	20 (18%) 3 2	59, 95, 139, 166	0
17	AT	131/146 (89%)	-0.25	4 (3%) 51 41	20, 39, 93, 218	0
17	CT	131/146 (89%)	0.06	3 (2%) 61 51	35, 56, 103, 151	0
18	AU	116/118 (98%)	-0.88	0 100 100	7, 22, 38, 87	0
18	CU	116/118 (98%)	0.09	0 100 100	31, 55, 88, 107	0
19	AV	101/101 (100%)	-0.88	0 100 100	10, 27, 56, 76	0
19	CV	101/101 (100%)	0.05	1 (0%) 79 72	28, 68, 101, 162	0
20	AW	112/113 (99%)	-0.77	0 100 100	10, 23, 47, 145	0
20	CW	112/113 (99%)	-0.19	0 100 100	26, 44, 74, 159	0
21	AX	95/96 (98%)	-0.45	1 (1%) 78 70	12, 33, 63, 107	0
21	CX	95/96 (98%)	0.37	6 (6%) 26 19	36, 62, 97, 173	0
22	AY	107/110 (97%)	-0.29	2 (1%) 66 57	18, 42, 88, 117	0
22	CY	107/110 (97%)	0.63	7 (6%) 25 18	48, 80, 124, 170	0
23	AZ	185/206 (89%)	-0.06	3 (1%) 70 61	27, 55, 94, 136	0
23	CZ	185/206 (89%)	0.81	9 (4%) 35 27	52, 97, 144, 173	0
24	A0	77/85 (90%)	-0.58	1 (1%) 75 66	9, 31, 53, 82	0
24	C0	77/85 (90%)	0.65	7 (9%) 15 11	27, 67, 104, 127	0
25	A1	97/98 (98%)	-0.40	1 (1%) 79 72	15, 38, 79, 97	0
25	C1	97/98 (98%)	0.17	3 (3%) 51 41	30, 55, 94, 139	0
26	A2	70/72 (97%)	-0.16	2 (2%) 53 43	14, 43, 63, 135	0
26	C2	70/72 (97%)	0.64	3 (4%) 40 31	47, 78, 109, 151	0
27	A3	59/60 (98%)	-0.62	1 (1%) 69 60	10, 26, 50, 110	0
27	C3	59/60 (98%)	0.30	2 (3%) 48 39	31, 62, 102, 162	0
28	A4	69/71 (97%)	0.77	8 (11%) 9 7	47, 101, 187, 216	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	C4	69/71 (97%)	1.26	11 (15%) 5 4	86, 158, 194, 226	0
29	A5	59/60 (98%)	-0.79	0 100 100	11, 22, 48, 66	0
29	C5	59/60 (98%)	-0.29	0 100 100	16, 46, 81, 120	0
30	A6	53/54 (98%)	-0.48	0 100 100	17, 35, 61, 75	0
30	C6	53/54 (98%)	0.21	0 100 100	40, 62, 85, 101	0
31	A7	48/49 (97%)	-0.53	2 (4%) 40 32	11, 20, 52, 99	0
31	C7	48/49 (97%)	-0.03	4 (8%) 17 12	23, 35, 95, 120	0
32	A8	64/65 (98%)	-0.72	0 100 100	13, 26, 39, 61	0
32	C8	64/65 (98%)	0.05	1 (1%) 70 61	26, 53, 71, 93	0
33	A9	37/37 (100%)	-0.42	1 (2%) 56 46	19, 32, 61, 65	0
33	C9	37/37 (100%)	0.39	1 (2%) 56 46	43, 61, 90, 101	0
34	BA	1495/1521 (98%)	0.22	23 (1%) 72 63	23, 81, 179, 326	0
34	DA	1501/1521 (98%)	0.46	65 (4%) 40 31	39, 93, 206, 304	0
35	BB	231/256 (90%)	0.89	22 (9%) 14 10	52, 103, 165, 193	0
35	DB	231/256 (90%)	1.34	45 (19%) 3 2	66, 134, 196, 226	0
36	BC	206/239 (86%)	1.03	29 (14%) 6 5	72, 113, 168, 187	0
36	DC	206/239 (86%)	1.48	53 (25%) 1 1	88, 150, 194, 221	0
37	BD	208/209 (99%)	1.13	37 (17%) 4 3	53, 90, 140, 180	0
37	DD	208/209 (99%)	0.95	29 (13%) 6 5	52, 87, 132, 197	0
38	BE	148/162 (91%)	0.33	2 (1%) 73 64	36, 71, 108, 150	0
38	DE	148/162 (91%)	0.80	13 (8%) 15 11	42, 88, 131, 177	0
39	BF	100/101 (99%)	0.44	1 (1%) 79 72	42, 80, 123, 144	0
39	DF	100/101 (99%)	0.56	3 (3%) 52 42	48, 90, 133, 146	0
40	BG	155/156 (99%)	0.80	17 (10%) 10 8	65, 100, 155, 193	0
40	DG	155/156 (99%)	1.10	22 (14%) 6 5	79, 130, 177, 212	0
41	BH	137/138 (99%)	0.57	7 (5%) 33 25	44, 72, 105, 119	0
41	DH	137/138 (99%)	0.84	12 (8%) 15 11	51, 90, 124, 159	0
42	BI	127/128 (99%)	1.58	39 (30%) 1 1	58, 114, 168, 190	0
42	DI	127/128 (99%)	2.03	59 (46%) 0 0	78, 153, 189, 243	0
43	BJ	97/105 (92%)	1.67	32 (32%) 1 1	74, 121, 172, 194	0
43	DJ	96/105 (91%)	1.96	45 (46%) 0 0	75, 158, 198, 215	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BK	114/129 (88%)	0.25	1 (0%) 81 74	29, 73, 115, 125	0
44	DK	114/129 (88%)	0.66	9 (7%) 18 13	59, 92, 138, 168	0
45	BL	122/132 (92%)	0.24	5 (4%) 41 33	26, 60, 88, 110	0
45	DL	122/132 (92%)	0.55	5 (4%) 41 33	40, 70, 99, 142	0
46	BM	117/126 (92%)	0.92	13 (11%) 10 7	62, 107, 151, 187	0
46	DM	116/126 (92%)	1.63	34 (29%) 1 1	64, 154, 201, 235	0
47	BN	60/61 (98%)	1.55	15 (25%) 2 1	59, 109, 151, 171	0
47	DN	60/61 (98%)	2.27	35 (58%) 0 0	94, 141, 190, 208	0
48	BO	88/89 (98%)	0.35	5 (5%) 29 22	34, 68, 106, 139	0
48	DO	88/89 (98%)	0.58	3 (3%) 48 39	49, 81, 115, 139	0
49	BP	82/88 (93%)	0.94	10 (12%) 8 6	45, 80, 125, 150	0
49	DP	82/88 (93%)	0.74	4 (4%) 35 27	48, 76, 108, 120	0
50	BQ	99/105 (94%)	0.34	5 (5%) 33 25	43, 71, 103, 118	0
50	DQ	99/105 (94%)	0.79	12 (12%) 8 6	46, 79, 116, 148	0
51	BR	68/88 (77%)	0.27	1 (1%) 72 63	44, 71, 115, 135	0
51	DR	68/88 (77%)	0.54	1 (1%) 72 63	57, 89, 127, 146	0
52	BS	84/93 (90%)	1.63	27 (32%) 1 1	64, 126, 168, 222	0
52	DS	83/93 (89%)	2.01	37 (44%) 0 0	98, 162, 210, 220	0
53	BT	96/106 (90%)	0.82	10 (10%) 11 8	49, 84, 117, 159	0
53	DT	96/106 (90%)	0.76	9 (9%) 14 10	47, 81, 126, 145	0
54	BU	23/27 (85%)	1.93	11 (47%) 0 0	59, 99, 112, 154	0
54	DU	23/27 (85%)	2.42	11 (47%) 0 0	78, 132, 157, 179	0
55	BV	7/18 (38%)	1.50	3 (42%) 0 0	60, 68, 174, 188	0
55	DV	6/18 (33%)	1.98	3 (50%) 0 0	87, 94, 180, 202	0
56	BW	69/76 (90%)	-0.15	3 (4%) 40 31	37, 69, 117, 208	0
56	BY	67/76 (88%)	1.14	12 (17%) 3 3	74, 230, 278, 300	0
56	DW	69/76 (90%)	0.29	0 100 100	46, 106, 150, 254	0
56	DY	66/76 (86%)	1.36	14 (21%) 2 2	141, 280, 312, 332	0
57	BZ	728/758 (96%)	0.70	66 (9%) 15 11	37, 96, 187, 244	0
57	DZ	730/758 (96%)	0.89	90 (12%) 8 6	27, 112, 210, 259	0
58	BX	3/10 (30%)	0.69	0 100 100	81, 81, 81, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
58	DX	3/10 (30%)	1.10	1 (33%) 1 1	78, 78, 80, 81	0
All	All	22705/23918 (94%)	0.20	1642 (7%) 21 16	5, 69, 187, 332	0

The worst 5 of 1642 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
42	DI	106	ALA	11.1
25	C1	2	SER	10.3
3	CC	213	VAL	7.5
36	BC	2	GLY	7.4
10	CL	127	ILE	7.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	PSU	DY	39	20/21	0.37	0.15	291,291,291,291	0
56	5MU	DY	54	21/22	0.38	0.15	303,303,303,303	0
56	PSU	BY	32	20/21	0.45	0.14	226,226,226,226	0
56	PSU	DY	32	20/21	0.51	0.19	275,275,275,275	0
56	7MG	BY	46	24/25	0.55	0.13	276,276,276,276	0
56	PSU	BY	55	20/21	0.57	0.13	243,243,243,243	0
56	PSU	BY	39	20/21	0.61	0.15	197,197,197,197	0
56	PSU	DY	55	20/21	0.61	0.16	252,252,252,252	0
56	MIA	DY	37	22/30	0.62	0.19	271,271,271,271	0
56	5MU	BY	54	21/22	0.64	0.14	246,246,246,246	0
56	MIA	BY	37	22/30	0.70	0.15	186,186,186,186	0
58	MVA	BX	5	8/9	0.72	0.17	82,82,82,82	0
56	4SU	BY	8	20/21	0.74	0.09	239,239,239,239	0
58	2R1	DX	6	10/11	0.76	0.12	81,81,81,81	0
56	4SU	DY	8	20/21	0.78	0.09	277,277,277,277	0
56	7MG	DW	46	24/25	0.78	0.13	124,124,124,124	0
58	2R1	BX	6	10/11	0.79	0.14	82,82,82,82	1
56	7MG	DY	46	24/25	0.79	0.12	266,266,266,266	0
56	5MU	DW	54	21/22	0.81	0.11	95,95,95,95	1
58	004	DX	3	10/11	0.82	0.13	81,81,81,81	0
56	PSU	DW	32	20/21	0.82	0.15	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	PSU	DW	55	20/21	0.84	0.09	92,92,92,92	0
56	PSU	DW	39	20/21	0.84	0.15	112,112,112,112	1
58	MVA	BX	9	8/9	0.85	0.16	82,82,82,82	0
56	7MG	BW	46	24/25	0.86	0.12	76,76,76,76	3
58	004	BX	3	10/11	0.87	0.12	82,82,82,82	0
56	PSU	BW	55	20/21	0.88	0.08	79,79,79,79	0
56	4SU	DW	8	20/21	0.88	0.09	103,103,103,103	0
58	2QY	BX	10	13/14	0.88	0.12	82,82,82,82	0
58	2QY	DX	10	13/14	0.88	0.10	81,81,81,81	0
58	2R3	BX	8	14/15	0.89	0.10	82,82,82,82	0
58	MVA	DX	5	8/9	0.89	0.11	81,81,81,81	0
56	5MU	BW	54	21/22	0.89	0.09	80,80,80,80	0
56	MIA	DW	37	29/30	0.89	0.14	109,109,109,109	0
56	MIA	BW	37	29/30	0.91	0.11	79,79,79,79	0
58	MVA	DX	9	8/9	0.91	0.10	81,81,81,81	0
58	2QZ	BX	1	9/10	0.91	0.12	82,82,82,82	0
56	PSU	BW	32	20/21	0.91	0.10	73,73,73,73	1
58	2QZ	DX	1	9/10	0.93	0.13	81,81,81,81	0
56	4SU	BW	8	20/21	0.94	0.07	60,60,60,60	1
58	2R3	DX	8	14/15	0.94	0.09	81,81,81,81	0
56	PSU	BW	39	20/21	0.95	0.09	65,65,65,65	0

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
59	MG	DA	1718	1/1	0.23	0.19	101,101,101,101	0
59	MG	BA	1776	1/1	0.27	0.18	97,97,97,97	0
59	MG	CB	3013	1/1	0.33	0.16	100,100,100,100	0
59	MG	BA	1790	1/1	0.39	0.17	96,96,96,96	0
59	MG	DA	1757	1/1	0.43	0.27	111,111,111,111	0
59	MG	CA	3624	1/1	0.51	0.22	118,118,118,118	0
59	MG	BA	1691	1/1	0.55	0.22	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	3773	1/1	0.55	0.63	35,35,35,35	1
59	MG	BA	1616	1/1	0.55	0.22	122,122,122,122	0
59	MG	DA	1754	1/1	0.55	0.28	120,120,120,120	0
59	MG	BB	3001	1/1	0.55	0.27	91,91,91,91	0
59	MG	CA	3363	1/1	0.58	0.13	88,88,88,88	0
59	MG	AA	3056	1/1	0.58	0.45	96,96,96,96	0
59	MG	DA	1609	1/1	0.59	0.13	89,89,89,89	0
59	MG	AA	3277	1/1	0.59	0.24	99,99,99,99	0
59	MG	CA	3488	1/1	0.60	0.25	88,88,88,88	0
59	MG	CA	3620	1/1	0.60	0.24	96,96,96,96	0
59	MG	BA	1660	1/1	0.61	0.24	82,82,82,82	0
59	MG	CA	3289	1/1	0.62	0.14	65,65,65,65	0
59	MG	AA	3418	1/1	0.62	0.12	74,74,74,74	0
59	MG	CA	3566	1/1	0.64	0.17	30,30,30,30	1
59	MG	DA	1710	1/1	0.65	0.10	104,104,104,104	0
59	MG	BL	201	1/1	0.65	0.12	84,84,84,84	0
59	MG	CA	3579	1/1	0.65	0.14	65,65,65,65	0
59	MG	AA	3643	1/1	0.65	0.23	84,84,84,84	0
59	MG	CA	3545	1/1	0.66	0.20	86,86,86,86	0
59	MG	DA	1738	1/1	0.66	0.14	95,95,95,95	0
59	MG	CA	3304	1/1	0.67	0.14	67,67,67,67	0
59	MG	CA	3546	1/1	0.67	0.14	88,88,88,88	0
59	MG	AA	3717	1/1	0.67	0.50	68,68,68,68	0
59	MG	CQ	202	1/1	0.67	0.27	74,74,74,74	0
59	MG	BA	1673	1/1	0.67	0.14	80,80,80,80	0
59	MG	AA	3747	1/1	0.68	0.16	85,85,85,85	0
59	MG	AA	3347	1/1	0.68	0.13	88,88,88,88	0
59	MG	DA	1611	1/1	0.68	0.41	89,89,89,89	0
59	MG	AA	3296	1/1	0.68	0.18	67,67,67,67	0
59	MG	AA	3617	1/1	0.69	0.10	77,77,77,77	0
59	MG	AA	3780	1/1	0.69	0.11	72,72,72,72	0
59	MG	DA	1749	1/1	0.69	0.12	77,77,77,77	0
59	MG	CA	3089	1/1	0.69	0.25	87,87,87,87	0
59	MG	CA	3444	1/1	0.69	0.09	67,67,67,67	0
59	MG	DA	1631	1/1	0.70	0.10	74,74,74,74	0
59	MG	BA	1741	1/1	0.70	0.10	88,88,88,88	0
59	MG	AA	3242	1/1	0.70	0.21	85,85,85,85	0
59	MG	CA	3557	1/1	0.70	0.21	76,76,76,76	0
59	MG	CA	3560	1/1	0.70	0.23	79,79,79,79	0
59	MG	CA	3485	1/1	0.70	0.10	85,85,85,85	0
59	MG	BA	1786	1/1	0.70	0.15	82,82,82,82	0
59	MG	AA	3629	1/1	0.71	0.18	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	CA	3096	1/1	0.71	0.37	125,125,125,125	0
59	MG	BA	1707	1/1	0.71	0.13	72,72,72,72	0
59	MG	AA	3464	1/1	0.72	0.17	66,66,66,66	0
59	MG	AA	3040	1/1	0.72	0.24	113,113,113,113	0
59	MG	AA	3678	1/1	0.72	0.17	77,77,77,77	0
59	MG	AA	3619	1/1	0.72	0.12	47,47,47,47	0
59	MG	CA	3125	1/1	0.72	0.38	78,78,78,78	0
59	MG	BA	1812	1/1	0.72	0.19	79,79,79,79	0
59	MG	CA	3535	1/1	0.73	0.22	77,77,77,77	0
59	MG	CA	3172	1/1	0.73	0.25	81,81,81,81	0
59	MG	CA	3055	1/1	0.73	0.16	77,77,77,77	0
59	MG	BA	1675	1/1	0.73	0.20	100,100,100,100	0
59	MG	CA	3350	1/1	0.73	0.13	82,82,82,82	0
59	MG	AA	3781	1/1	0.73	0.17	72,72,72,72	0
59	MG	BA	1775	1/1	0.73	0.17	90,90,90,90	0
59	MG	CA	3460	1/1	0.73	0.33	104,104,104,104	0
59	MG	CA	3127	1/1	0.73	0.22	94,94,94,94	0
59	MG	DA	1756	1/1	0.73	0.23	86,86,86,86	0
59	MG	CA	3139	1/1	0.73	0.22	126,126,126,126	0
59	MG	DA	1769	1/1	0.73	0.21	74,74,74,74	0
59	MG	BA	1657	1/1	0.74	0.26	78,78,78,78	0
59	MG	AA	3232	1/1	0.74	0.18	58,58,58,58	0
59	MG	BA	1719	1/1	0.74	0.14	62,62,62,62	0
59	MG	A0	101	1/1	0.74	0.12	69,69,69,69	0
59	MG	AA	3122	1/1	0.74	0.33	99,99,99,99	0
59	MG	BA	1679	1/1	0.74	0.21	59,59,59,59	0
59	MG	CA	3587	1/1	0.75	0.10	70,70,70,70	0
59	MG	AA	3625	1/1	0.75	0.18	51,51,51,51	0
59	MG	BA	1694	1/1	0.75	0.28	83,83,83,83	0
59	MG	AA	3480	1/1	0.75	0.23	88,88,88,88	0
59	MG	CA	3149	1/1	0.75	0.24	100,100,100,100	0
59	MG	CA	3100	1/1	0.75	0.29	81,81,81,81	0
59	MG	CA	3583	1/1	0.75	0.13	80,80,80,80	0
59	MG	CA	3586	1/1	0.75	0.31	93,93,93,93	0
59	MG	DT	3001	1/1	0.75	0.23	60,60,60,60	0
59	MG	DA	1727	1/1	0.76	0.08	61,61,61,61	0
59	MG	CQ	204	1/1	0.76	0.15	74,74,74,74	0
59	MG	CA	3376	1/1	0.76	0.12	78,78,78,78	0
59	MG	AA	3275	1/1	0.76	0.39	89,89,89,89	0
59	MG	CA	3646	1/1	0.76	0.14	91,91,91,91	0
59	MG	DA	1663	1/1	0.76	0.22	91,91,91,91	0
59	MG	AA	3269	1/1	0.76	0.23	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	CA	3467	1/1	0.76	0.32	77,77,77,77	0
59	MG	BA	1758	1/1	0.77	0.26	76,76,76,76	0
59	MG	DA	1715	1/1	0.77	0.18	79,79,79,79	0
59	MG	CA	3235	1/1	0.77	0.16	78,78,78,78	0
59	MG	CQ	201	1/1	0.77	0.18	72,72,72,72	0
59	MG	DA	1732	1/1	0.77	0.11	85,85,85,85	0
59	MG	AA	3016	1/1	0.77	0.20	64,64,64,64	0
59	MG	DA	1740	1/1	0.77	0.17	68,68,68,68	0
59	MG	CA	3108	1/1	0.77	0.22	78,78,78,78	0
59	MG	AA	3219	1/1	0.77	0.18	61,61,61,61	0
59	MG	AA	3481	1/1	0.77	0.19	78,78,78,78	0
59	MG	CA	3066	1/1	0.77	0.15	69,69,69,69	0
59	MG	DA	1762	1/1	0.77	0.18	61,61,61,61	0
59	MG	BA	1670	1/1	0.77	0.13	69,69,69,69	0
59	MG	DA	1668	1/1	0.77	0.31	65,65,65,65	0
59	MG	DW	503	1/1	0.77	0.19	85,85,85,85	0
59	MG	CA	3619	1/1	0.78	0.14	40,40,40,40	0
59	MG	CA	3240	1/1	0.78	0.24	71,71,71,71	0
59	MG	CA	3244	1/1	0.78	0.25	89,89,89,89	0
59	MG	CA	3246	1/1	0.78	0.26	57,57,57,57	0
59	MG	AA	3708	1/1	0.78	0.26	61,61,61,61	0
59	MG	AA	3093	1/1	0.78	0.68	92,92,92,92	0
59	MG	CA	3093	1/1	0.78	0.39	75,75,75,75	0
59	MG	CA	3357	1/1	0.78	0.13	66,66,66,66	0
59	MG	AA	3622	1/1	0.78	0.17	60,60,60,60	0
59	MG	CA	3007	1/1	0.78	0.25	92,92,92,92	0
59	MG	AA	3700	1/1	0.78	0.12	70,70,70,70	0
59	MG	DA	1635	1/1	0.78	0.21	75,75,75,75	0
59	MG	DA	1655	1/1	0.78	0.24	83,83,83,83	0
59	MG	CA	3236	1/1	0.78	0.36	81,81,81,81	0
59	MG	CA	3237	1/1	0.78	0.15	94,94,94,94	0
59	MG	AA	3583	1/1	0.79	0.13	63,63,63,63	0
59	MG	BA	1628	1/1	0.79	0.20	87,87,87,87	0
59	MG	DA	1724	1/1	0.79	0.15	70,70,70,70	0
59	MG	CA	3032	1/1	0.79	0.28	100,100,100,100	0
59	MG	CA	3050	1/1	0.79	0.21	75,75,75,75	0
59	MG	CA	3395	1/1	0.79	0.25	50,50,50,50	0
59	MG	CA	3408	1/1	0.79	0.11	58,58,58,58	0
59	MG	DA	1746	1/1	0.79	0.12	81,81,81,81	0
59	MG	BA	1671	1/1	0.79	0.36	101,101,101,101	0
59	MG	BA	1748	1/1	0.79	0.10	63,63,63,63	0
59	MG	CA	3465	1/1	0.79	0.25	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	1755	1/1	0.79	0.10	86,86,86,86	0
59	MG	CA	3295	1/1	0.79	0.17	66,66,66,66	0
59	MG	AA	3108	1/1	0.79	0.45	101,101,101,101	0
59	MG	DA	1708	1/1	0.79	0.20	77,77,77,77	0
59	MG	CA	3516	1/1	0.79	0.16	79,79,79,79	0
59	MG	AA	3571	1/1	0.80	0.19	94,94,94,94	0
59	MG	CA	3323	1/1	0.80	0.21	87,87,87,87	0
59	MG	AA	3642	1/1	0.80	0.17	71,71,71,71	0
59	MG	BA	1733	1/1	0.80	0.20	78,78,78,78	0
59	MG	AA	3776	1/1	0.80	0.10	69,69,69,69	0
59	MG	CA	3146	1/1	0.80	0.33	82,82,82,82	0
59	MG	AA	3246	1/1	0.80	0.10	52,52,52,52	0
59	MG	AA	3202	1/1	0.80	0.17	61,61,61,61	0
59	MG	CA	3186	1/1	0.80	0.20	77,77,77,77	0
59	MG	AA	3323	1/1	0.80	0.09	64,64,64,64	0
59	MG	CA	3065	1/1	0.80	0.23	56,56,56,56	0
59	MG	DA	1733	1/1	0.80	0.20	92,92,92,92	0
59	MG	DA	1737	1/1	0.80	0.15	69,69,69,69	0
59	MG	CA	3644	1/1	0.80	0.20	66,66,66,66	0
59	MG	BA	1612	1/1	0.80	0.17	92,92,92,92	0
59	MG	CB	3001	1/1	0.80	0.16	72,72,72,72	0
59	MG	CA	3078	1/1	0.80	0.21	57,57,57,57	0
59	MG	AA	3198	1/1	0.80	0.19	63,63,63,63	0
59	MG	CA	3492	1/1	0.80	0.15	59,59,59,59	0
59	MG	CA	3507	1/1	0.80	0.18	83,83,83,83	0
59	MG	DA	1604	1/1	0.80	0.18	80,80,80,80	0
59	MG	AA	3536	1/1	0.80	0.17	66,66,66,66	0
59	MG	BA	1697	1/1	0.80	0.32	99,99,99,99	0
59	MG	BA	1800	1/1	0.80	0.18	77,77,77,77	0
59	MG	AA	3660	1/1	0.81	0.16	61,61,61,61	0
59	MG	CA	3539	1/1	0.81	0.15	90,90,90,90	0
59	MG	BA	1603	1/1	0.81	0.17	61,61,61,61	0
59	MG	AA	3266	1/1	0.81	0.50	90,90,90,90	0
59	MG	CF	301	1/1	0.81	0.17	61,61,61,61	0
59	MG	BA	1721	1/1	0.81	0.09	66,66,66,66	0
59	MG	AA	3274	1/1	0.81	0.15	75,75,75,75	0
59	MG	BA	1625	1/1	0.81	0.20	86,86,86,86	0
59	MG	AA	3267	1/1	0.81	0.11	53,53,53,53	0
59	MG	CA	3223	1/1	0.81	0.09	59,59,59,59	0
59	MG	BA	1648	1/1	0.81	0.08	74,74,74,74	0
59	MG	DA	1748	1/1	0.81	0.11	70,70,70,70	0
59	MG	DA	1623	1/1	0.81	0.13	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	1753	1/1	0.81	0.30	79,79,79,79	0
59	MG	CA	3494	1/1	0.81	0.14	97,97,97,97	0
59	MG	CA	3594	1/1	0.81	0.08	73,73,73,73	0
59	MG	CA	3506	1/1	0.81	0.12	63,63,63,63	0
59	MG	AA	3644	1/1	0.81	0.21	56,56,56,56	0
59	MG	BA	1767	1/1	0.81	0.11	96,96,96,96	0
59	MG	DA	1674	1/1	0.81	0.20	77,77,77,77	0
59	MG	CA	3638	1/1	0.81	0.24	76,76,76,76	0
59	MG	CA	3428	1/1	0.82	0.14	58,58,58,58	0
59	MG	CA	3069	1/1	0.82	0.43	81,81,81,81	0
59	MG	AA	3542	1/1	0.82	0.13	58,58,58,58	0
59	MG	DA	1704	1/1	0.82	0.11	49,49,49,49	0
59	MG	BA	1792	1/1	0.82	0.17	80,80,80,80	0
59	MG	CA	3605	1/1	0.82	0.19	70,70,70,70	0
59	MG	AA	3719	1/1	0.82	0.15	59,59,59,59	0
59	MG	BA	1619	1/1	0.82	0.11	59,59,59,59	0
59	MG	AA	3737	1/1	0.82	0.10	54,54,54,54	0
59	MG	AB	3017	1/1	0.82	0.10	59,59,59,59	0
59	MG	CA	3111	1/1	0.82	0.23	79,79,79,79	0
59	MG	BA	1634	1/1	0.82	0.26	64,64,64,64	0
59	MG	AD	301	1/1	0.82	0.18	57,57,57,57	0
59	MG	CA	3035	1/1	0.82	0.38	69,69,69,69	0
59	MG	CA	3530	1/1	0.82	0.23	71,71,71,71	0
59	MG	AA	3063	1/1	0.82	0.15	54,54,54,54	0
59	MG	BA	1659	1/1	0.82	0.21	67,67,67,67	0
59	MG	CA	3542	1/1	0.82	0.14	87,87,87,87	0
59	MG	CA	3155	1/1	0.82	0.29	112,112,112,112	0
59	MG	BA	1782	1/1	0.82	0.11	47,47,47,47	0
59	MG	DA	1755	1/1	0.82	0.32	88,88,88,88	0
59	MG	AA	3441	1/1	0.82	0.18	58,58,58,58	0
59	MG	CA	3202	1/1	0.82	0.23	73,73,73,73	0
59	MG	CA	3411	1/1	0.82	0.13	57,57,57,57	0
59	MG	CA	3420	1/1	0.82	0.19	69,69,69,69	0
59	MG	DA	1638	1/1	0.82	0.15	80,80,80,80	0
59	MG	CA	3581	1/1	0.82	0.12	38,38,38,38	0
59	MG	BA	1601	1/1	0.83	0.13	95,95,95,95	0
59	MG	CA	3591	1/1	0.83	0.10	60,60,60,60	0
59	MG	BA	1693	1/1	0.83	0.17	76,76,76,76	0
59	MG	BA	1764	1/1	0.83	0.10	71,71,71,71	0
59	MG	DA	1676	1/1	0.83	0.16	74,74,74,74	0
59	MG	DA	1677	1/1	0.83	0.15	78,78,78,78	0
59	MG	DA	1678	1/1	0.83	0.20	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	3706	1/1	0.83	0.24	41,41,41,41	1
59	MG	CA	3117	1/1	0.83	0.20	67,67,67,67	0
59	MG	CA	3622	1/1	0.83	0.13	50,50,50,50	0
59	MG	CA	3502	1/1	0.83	0.27	90,90,90,90	0
59	MG	CA	3124	1/1	0.83	0.23	65,65,65,65	0
59	MG	BA	1610	1/1	0.83	0.15	78,78,78,78	0
59	MG	CA	3126	1/1	0.83	0.15	62,62,62,62	0
59	MG	AA	3235	1/1	0.83	0.25	93,93,93,93	0
59	MG	CA	3044	1/1	0.83	0.19	89,89,89,89	0
59	MG	BA	1778	1/1	0.83	0.10	54,54,54,54	0
59	MG	AA	3018	1/1	0.83	0.60	67,67,67,67	0
59	MG	AA	3582	1/1	0.83	0.23	76,76,76,76	0
59	MG	CA	3164	1/1	0.83	0.23	64,64,64,64	0
59	MG	AA	3495	1/1	0.83	0.15	35,35,35,35	0
59	MG	CA	3184	1/1	0.83	0.26	77,77,77,77	0
59	MG	AA	3133	1/1	0.83	0.21	50,50,50,50	0
59	MG	DA	1618	1/1	0.83	0.29	91,91,91,91	0
59	MG	BA	1797	1/1	0.83	0.14	59,59,59,59	0
59	MG	DA	1629	1/1	0.83	0.17	59,59,59,59	0
59	MG	CA	3203	1/1	0.83	0.10	73,73,73,73	0
59	MG	AA	3756	1/1	0.83	0.09	49,49,49,49	0
59	MG	BA	1811	1/1	0.83	0.13	77,77,77,77	0
59	MG	DA	1639	1/1	0.83	0.14	69,69,69,69	0
59	MG	DA	1643	1/1	0.83	0.17	79,79,79,79	0
59	MG	DA	1634	1/1	0.84	0.23	66,66,66,66	0
59	MG	BA	1704	1/1	0.84	0.20	71,71,71,71	0
59	MG	CA	3565	1/1	0.84	0.11	95,95,95,95	0
59	MG	CA	3398	1/1	0.84	0.14	67,67,67,67	0
59	MG	CA	3070	1/1	0.84	0.13	60,60,60,60	0
59	MG	AA	3212	1/1	0.84	0.24	81,81,81,81	0
59	MG	AA	3758	1/1	0.84	0.23	43,43,43,43	1
59	MG	AA	3425	1/1	0.84	0.16	77,77,77,77	0
59	MG	CA	3204	1/1	0.84	0.10	54,54,54,54	0
59	MG	DA	1675	1/1	0.84	0.48	70,70,70,70	0
59	MG	CA	3216	1/1	0.84	0.21	79,79,79,79	0
59	MG	BA	1662	1/1	0.84	0.24	70,70,70,70	0
59	MG	BA	1669	1/1	0.84	0.20	66,66,66,66	0
59	MG	CA	3470	1/1	0.84	0.17	74,74,74,74	0
59	MG	BA	1744	1/1	0.84	0.12	57,57,57,57	0
59	MG	AA	3141	1/1	0.84	0.09	68,68,68,68	0
59	MG	BA	1614	1/1	0.84	0.17	72,72,72,72	0
59	MG	CA	3634	1/1	0.84	0.12	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BS	101	1/1	0.84	0.09	79,79,79,79	0
59	MG	CA	3643	1/1	0.84	0.09	79,79,79,79	0
59	MG	DA	1730	1/1	0.84	0.17	71,71,71,71	0
59	MG	CA	3501	1/1	0.84	0.17	74,74,74,74	0
59	MG	AA	3653	1/1	0.84	0.10	60,60,60,60	0
59	MG	CA	3649	1/1	0.84	0.18	51,51,51,51	0
59	MG	AA	3157	1/1	0.84	0.22	91,91,91,91	0
59	MG	AA	3677	1/1	0.84	0.20	69,69,69,69	0
59	MG	DA	1742	1/1	0.84	0.11	72,72,72,72	0
59	MG	CE	301	1/1	0.84	0.16	53,53,53,53	0
59	MG	CA	3508	1/1	0.84	0.09	52,52,52,52	0
59	MG	CA	3129	1/1	0.84	0.14	64,64,64,64	0
59	MG	DA	1750	1/1	0.84	0.14	67,67,67,67	0
59	MG	CA	3518	1/1	0.84	0.11	65,65,65,65	0
59	MG	CA	3314	1/1	0.84	0.12	57,57,57,57	0
59	MG	AA	3607	1/1	0.84	0.14	60,60,60,60	1
59	MG	CA	3538	1/1	0.84	0.14	72,72,72,72	0
59	MG	AD	308	1/1	0.84	0.14	65,65,65,65	0
59	MG	BA	1644	1/1	0.84	0.15	74,74,74,74	0
59	MG	BA	1780	1/1	0.84	0.12	60,60,60,60	0
59	MG	CA	3367	1/1	0.84	0.14	63,63,63,63	0
59	MG	AA	3754	1/1	0.84	0.16	64,64,64,64	0
59	MG	CA	3294	1/1	0.85	0.06	72,72,72,72	0
59	MG	BA	1646	1/1	0.85	0.24	66,66,66,66	0
59	MG	AA	3651	1/1	0.85	0.17	77,77,77,77	0
59	MG	AA	3206	1/1	0.85	0.25	106,106,106,106	0
59	MG	AA	3068	1/1	0.85	0.32	73,73,73,73	0
59	MG	CA	3333	1/1	0.85	0.17	68,68,68,68	0
59	MG	CA	3340	1/1	0.85	0.16	66,66,66,66	0
59	MG	CA	3341	1/1	0.85	0.12	73,73,73,73	0
59	MG	CA	3555	1/1	0.85	0.07	71,71,71,71	0
59	MG	AE	305	1/1	0.85	0.18	48,48,48,48	0
59	MG	AA	3675	1/1	0.85	0.12	64,64,64,64	0
59	MG	CA	3134	1/1	0.85	0.17	71,71,71,71	0
59	MG	CA	3135	1/1	0.85	0.23	59,59,59,59	0
59	MG	A7	104	1/1	0.85	0.09	55,55,55,55	0
59	MG	CA	3379	1/1	0.85	0.10	83,83,83,83	0
59	MG	CA	3389	1/1	0.85	0.17	59,59,59,59	0
59	MG	CA	3392	1/1	0.85	0.11	43,43,43,43	0
59	MG	DA	1692	1/1	0.85	0.12	53,53,53,53	0
59	MG	DA	1694	1/1	0.85	0.12	106,106,106,106	0
59	MG	AA	3676	1/1	0.85	0.10	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	CA	3148	1/1	0.85	0.26	62,62,62,62	0
59	MG	DA	1709	1/1	0.85	0.13	70,70,70,70	0
59	MG	CA	3038	1/1	0.85	0.31	97,97,97,97	0
59	MG	DA	1713	1/1	0.85	0.08	49,49,49,49	0
59	MG	CA	3042	1/1	0.85	0.27	65,65,65,65	0
59	MG	CA	3612	1/1	0.85	0.28	83,83,83,83	0
59	MG	DA	1722	1/1	0.85	0.10	77,77,77,77	0
59	MG	AA	3755	1/1	0.85	0.29	78,78,78,78	0
59	MG	AA	3453	1/1	0.85	0.14	39,39,39,39	0
59	MG	CA	3432	1/1	0.85	0.16	32,32,32,32	0
59	MG	AA	3213	1/1	0.85	0.33	76,76,76,76	0
59	MG	BA	1676	1/1	0.85	0.24	61,61,61,61	0
59	MG	DA	1736	1/1	0.85	0.10	78,78,78,78	0
59	MG	AA	3769	1/1	0.85	0.15	63,63,63,63	0
59	MG	AA	3680	1/1	0.85	0.20	79,79,79,79	0
59	MG	BA	1781	1/1	0.85	0.09	63,63,63,63	0
59	MG	CA	3076	1/1	0.85	0.24	64,64,64,64	0
59	MG	AA	3189	1/1	0.85	0.20	62,62,62,62	0
59	MG	CA	3226	1/1	0.85	0.24	52,52,52,52	0
59	MG	AA	3138	1/1	0.85	0.09	38,38,38,38	0
59	MG	BA	1788	1/1	0.85	0.35	79,79,79,79	0
59	MG	AA	3096	1/1	0.85	0.17	59,59,59,59	0
59	MG	BA	1699	1/1	0.85	0.07	72,72,72,72	0
59	MG	CA	3107	1/1	0.85	0.20	77,77,77,77	0
59	MG	AA	3787	1/1	0.85	0.13	82,82,82,82	0
59	MG	CA	3510	1/1	0.85	0.17	95,95,95,95	0
59	MG	DA	1605	1/1	0.85	0.14	105,105,105,105	0
59	MG	CA	3511	1/1	0.85	0.10	81,81,81,81	0
59	MG	AA	3796	1/1	0.85	0.19	78,78,78,78	0
59	MG	DA	1614	1/1	0.85	0.09	65,65,65,65	0
59	MG	DA	1610	1/1	0.86	0.21	71,71,71,71	0
59	MG	CA	3524	1/1	0.86	0.10	52,52,52,52	0
59	MG	BA	1783	1/1	0.86	0.15	57,57,57,57	0
59	MG	AA	3715	1/1	0.86	0.23	33,33,33,33	1
59	MG	AA	3344	1/1	0.86	0.11	22,22,22,22	0
59	MG	A2	3001	1/1	0.86	0.11	53,53,53,53	0
59	MG	AA	3775	1/1	0.86	0.27	25,25,25,25	1
59	MG	DA	1632	1/1	0.86	0.21	57,57,57,57	0
59	MG	CA	3194	1/1	0.86	0.10	52,52,52,52	0
59	MG	CA	3378	1/1	0.86	0.16	97,97,97,97	0
59	MG	BA	1795	1/1	0.86	0.07	59,59,59,59	0
59	MG	AA	3614	1/1	0.86	0.14	50,50,50,50	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	1641	1/1	0.86	0.10	74,74,74,74	0
59	MG	AA	3273	1/1	0.86	0.09	90,90,90,90	0
59	MG	DA	1652	1/1	0.86	0.14	80,80,80,80	0
59	MG	CA	3205	1/1	0.86	0.11	81,81,81,81	0
59	MG	DA	1659	1/1	0.86	0.26	78,78,78,78	0
59	MG	DA	1662	1/1	0.86	0.23	75,75,75,75	0
59	MG	BA	1664	1/1	0.86	0.10	56,56,56,56	0
59	MG	CA	3573	1/1	0.86	0.11	65,65,65,65	0
59	MG	CA	3222	1/1	0.86	0.15	57,57,57,57	0
59	MG	CA	3104	1/1	0.86	0.17	80,80,80,80	0
59	MG	CA	3414	1/1	0.86	0.14	34,34,34,34	1
59	MG	BA	1668	1/1	0.86	0.09	69,69,69,69	0
59	MG	CA	3230	1/1	0.86	0.24	49,49,49,49	0
59	MG	DA	1690	1/1	0.86	0.19	73,73,73,73	0
59	MG	CA	3233	1/1	0.86	0.12	59,59,59,59	0
59	MG	CA	3433	1/1	0.86	0.10	82,82,82,82	0
59	MG	DA	1698	1/1	0.86	0.20	97,97,97,97	0
59	MG	CA	3603	1/1	0.86	0.16	49,49,49,49	0
59	MG	AA	3740	1/1	0.86	0.17	61,61,61,61	0
59	MG	CA	3606	1/1	0.86	0.29	73,73,73,73	0
59	MG	CA	3610	1/1	0.86	0.11	69,69,69,69	0
59	MG	CA	3456	1/1	0.86	0.11	54,54,54,54	0
59	MG	CA	3614	1/1	0.86	0.11	62,62,62,62	0
59	MG	DA	1717	1/1	0.86	0.19	95,95,95,95	0
59	MG	CA	3615	1/1	0.86	0.12	28,28,28,28	0
59	MG	AA	3098	1/1	0.86	0.26	51,51,51,51	0
59	MG	AA	3792	1/1	0.86	0.08	48,48,48,48	0
59	MG	CA	3238	1/1	0.86	0.18	69,69,69,69	0
59	MG	AA	3315	1/1	0.86	0.23	65,65,65,65	0
59	MG	CA	3626	1/1	0.86	0.16	61,61,61,61	0
59	MG	CA	3474	1/1	0.86	0.14	59,59,59,59	0
59	MG	AA	3814	1/1	0.86	0.26	72,72,72,72	0
59	MG	AA	3181	1/1	0.86	0.23	79,79,79,79	0
59	MG	CA	3249	1/1	0.86	0.10	61,61,61,61	0
59	MG	DA	1739	1/1	0.86	0.14	73,73,73,73	0
59	MG	CA	3256	1/1	0.86	0.19	65,65,65,65	0
59	MG	CA	3647	1/1	0.86	0.10	85,85,85,85	0
59	MG	DA	1743	1/1	0.86	0.11	59,59,59,59	0
59	MG	AB	3021	1/1	0.86	0.21	65,65,65,65	0
59	MG	CA	3041	1/1	0.86	0.24	61,61,61,61	0
59	MG	CA	3504	1/1	0.86	0.12	79,79,79,79	0
59	MG	BA	1687	1/1	0.86	0.23	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	CE	305	1/1	0.86	0.06	58,58,58,58	0
59	MG	AA	3586	1/1	0.86	0.20	74,74,74,74	0
59	MG	CP	201	1/1	0.86	0.08	62,62,62,62	1
59	MG	CA	3307	1/1	0.86	0.11	60,60,60,60	0
59	MG	CA	3509	1/1	0.86	0.08	83,83,83,83	0
59	MG	CA	3047	1/1	0.86	0.19	84,84,84,84	0
59	MG	BA	1638	1/1	0.86	0.17	66,66,66,66	0
59	MG	DE	201	1/1	0.86	0.15	84,84,84,84	0
59	MG	AA	3711	1/1	0.86	0.29	43,43,43,43	1
59	MG	BA	1695	1/1	0.86	0.10	83,83,83,83	0
59	MG	BA	1724	1/1	0.87	0.11	67,67,67,67	0
59	MG	AA	3786	1/1	0.87	0.09	53,53,53,53	0
59	MG	CA	3057	1/1	0.87	0.19	60,60,60,60	0
59	MG	AA	3186	1/1	0.87	0.12	48,48,48,48	0
59	MG	BA	1645	1/1	0.87	0.12	74,74,74,74	0
59	MG	CA	3067	1/1	0.87	0.13	63,63,63,63	0
59	MG	AA	3705	1/1	0.87	0.23	53,53,53,53	1
59	MG	AA	3150	1/1	0.87	0.14	45,45,45,45	0
59	MG	DA	1622	1/1	0.87	0.14	60,60,60,60	0
59	MG	AA	3194	1/1	0.87	0.21	82,82,82,82	0
59	MG	BA	1658	1/1	0.87	0.31	66,66,66,66	0
59	MG	CA	3254	1/1	0.87	0.15	85,85,85,85	0
59	MG	AA	3337	1/1	0.87	0.12	75,75,75,75	0
59	MG	CA	3273	1/1	0.87	0.11	58,58,58,58	0
59	MG	CA	3532	1/1	0.87	0.13	49,49,49,49	0
59	MG	CA	3288	1/1	0.87	0.14	49,49,49,49	0
59	MG	CA	3537	1/1	0.87	0.16	59,59,59,59	0
59	MG	DA	1640	1/1	0.87	0.27	77,77,77,77	0
59	MG	BA	1772	1/1	0.87	0.10	66,66,66,66	0
59	MG	BA	1774	1/1	0.87	0.13	50,50,50,50	0
59	MG	DA	1644	1/1	0.87	0.15	94,94,94,94	0
59	MG	DA	1649	1/1	0.87	0.27	69,69,69,69	0
59	MG	AB	3020	1/1	0.87	0.15	62,62,62,62	0
59	MG	DA	1654	1/1	0.87	0.26	63,63,63,63	0
59	MG	AA	3712	1/1	0.87	0.29	70,70,70,70	0
59	MG	AA	3486	1/1	0.87	0.13	67,67,67,67	0
59	MG	BA	1779	1/1	0.87	0.13	85,85,85,85	0
59	MG	BA	1665	1/1	0.87	0.20	73,73,73,73	0
59	MG	CA	3112	1/1	0.87	0.21	69,69,69,69	0
59	MG	CA	3563	1/1	0.87	0.11	75,75,75,75	0
59	MG	CA	3116	1/1	0.87	0.21	52,52,52,52	0
59	MG	AA	3626	1/1	0.87	0.12	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	3493	1/1	0.87	0.09	77,77,77,77	0
59	MG	AG	202	1/1	0.87	0.08	54,54,54,54	0
59	MG	AA	3195	1/1	0.87	0.26	69,69,69,69	0
59	MG	AA	3516	1/1	0.87	0.15	65,65,65,65	0
59	MG	AA	3128	1/1	0.87	0.31	89,89,89,89	0
59	MG	DA	1695	1/1	0.87	0.14	63,63,63,63	0
59	MG	AA	3367	1/1	0.87	0.13	60,60,60,60	0
59	MG	BA	1602	1/1	0.87	0.19	79,79,79,79	0
59	MG	BA	1682	1/1	0.87	0.29	70,70,70,70	0
59	MG	CA	3596	1/1	0.87	0.10	51,51,51,51	0
59	MG	CA	3598	1/1	0.87	0.07	65,65,65,65	0
59	MG	BA	1683	1/1	0.87	0.22	71,71,71,71	0
59	MG	BA	1810	1/1	0.87	0.09	82,82,82,82	0
59	MG	AA	3409	1/1	0.87	0.14	60,60,60,60	0
59	MG	AA	3169	1/1	0.87	0.19	35,35,35,35	0
59	MG	CA	3157	1/1	0.87	0.19	81,81,81,81	0
59	MG	AA	3664	1/1	0.87	0.14	62,62,62,62	0
59	MG	CA	3165	1/1	0.87	0.19	57,57,57,57	0
59	MG	BE	3001	1/1	0.87	0.08	78,78,78,78	0
59	MG	AA	3055	1/1	0.87	0.26	65,65,65,65	0
59	MG	CA	3621	1/1	0.87	0.11	61,61,61,61	0
59	MG	AA	3435	1/1	0.87	0.11	52,52,52,52	0
59	MG	CA	3442	1/1	0.87	0.30	74,74,74,74	0
59	MG	AA	3288	1/1	0.87	0.13	39,39,39,39	0
59	MG	CA	3633	1/1	0.87	0.12	68,68,68,68	0
59	MG	BA	1623	1/1	0.87	0.15	67,67,67,67	0
59	MG	CA	3034	1/1	0.87	0.24	77,77,77,77	0
59	MG	AA	3608	1/1	0.87	0.13	60,60,60,60	0
59	MG	AA	3611	1/1	0.87	0.14	47,47,47,47	0
59	MG	CA	3212	1/1	0.87	0.28	84,84,84,84	0
59	MG	BA	1714	1/1	0.87	0.21	74,74,74,74	0
59	MG	CA	3478	1/1	0.87	0.12	65,65,65,65	0
59	MG	CA	3656	1/1	0.87	0.23	63,63,63,63	0
59	MG	CA	3480	1/1	0.87	0.11	50,50,50,50	0
59	MG	CB	3005	1/1	0.87	0.18	63,63,63,63	0
59	MG	CA	3481	1/1	0.87	0.11	64,64,64,64	0
59	MG	CA	3217	1/1	0.87	0.17	62,62,62,62	0
59	MG	BA	1716	1/1	0.87	0.14	86,86,86,86	0
59	MG	CA	3490	1/1	0.87	0.09	50,50,50,50	0
59	MG	BA	1631	1/1	0.87	0.11	71,71,71,71	0
59	MG	DJ	5001	1/1	0.87	0.09	82,82,82,82	0
59	MG	DK	5001	1/1	0.87	0.10	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	3698	1/1	0.87	0.07	41,41,41,41	0
59	MG	CA	3499	1/1	0.87	0.19	62,62,62,62	0
59	MG	DZ	701	1/1	0.87	0.10	72,72,72,72	0
59	MG	CA	3072	1/1	0.88	0.12	66,66,66,66	0
59	MG	CA	3075	1/1	0.88	0.16	90,90,90,90	0
59	MG	BA	1713	1/1	0.88	0.23	68,68,68,68	0
59	MG	AA	3771	1/1	0.88	0.16	60,60,60,60	0
59	MG	CA	3577	1/1	0.88	0.10	51,51,51,51	1
59	MG	CA	3080	1/1	0.88	0.15	75,75,75,75	0
59	MG	CA	3081	1/1	0.88	0.15	63,63,63,63	0
59	MG	AA	3051	1/1	0.88	0.30	48,48,48,48	0
59	MG	DA	1646	1/1	0.88	0.08	57,57,57,57	0
59	MG	CA	3221	1/1	0.88	0.19	65,65,65,65	0
59	MG	AA	3066	1/1	0.88	0.14	51,51,51,51	0
59	MG	BA	1803	1/1	0.88	0.12	64,64,64,64	0
59	MG	CA	3224	1/1	0.88	0.22	59,59,59,59	0
59	MG	CA	3098	1/1	0.88	0.10	70,70,70,70	0
59	MG	BA	1805	1/1	0.88	0.12	71,71,71,71	0
59	MG	AA	3415	1/1	0.88	0.18	62,62,62,62	0
59	MG	DA	1665	1/1	0.88	0.11	63,63,63,63	0
59	MG	BA	1609	1/1	0.88	0.08	62,62,62,62	0
59	MG	DA	1669	1/1	0.88	0.12	65,65,65,65	0
59	MG	BA	1727	1/1	0.88	0.11	77,77,77,77	0
59	MG	CA	3608	1/1	0.88	0.21	50,50,50,50	1
59	MG	AA	3027	1/1	0.88	0.37	75,75,75,75	0
59	MG	CA	3477	1/1	0.88	0.14	69,69,69,69	0
59	MG	AA	3627	1/1	0.88	0.10	76,76,76,76	0
59	MG	DA	1679	1/1	0.88	0.12	70,70,70,70	0
59	MG	DA	1683	1/1	0.88	0.13	58,58,58,58	0
59	MG	CA	3239	1/1	0.88	0.10	69,69,69,69	0
59	MG	CA	3114	1/1	0.88	0.24	66,66,66,66	0
59	MG	CA	3241	1/1	0.88	0.18	72,72,72,72	0
59	MG	CA	3486	1/1	0.88	0.13	81,81,81,81	0
59	MG	AA	3314	1/1	0.88	0.13	57,57,57,57	0
59	MG	AA	3630	1/1	0.88	0.34	72,72,72,72	0
59	MG	CA	3001	1/1	0.88	0.16	64,64,64,64	0
59	MG	CA	3628	1/1	0.88	0.10	54,54,54,54	0
59	MG	CA	3003	1/1	0.88	0.21	62,62,62,62	0
59	MG	AA	3640	1/1	0.88	0.10	68,68,68,68	0
59	MG	AA	3551	1/1	0.88	0.08	39,39,39,39	0
59	MG	CA	3284	1/1	0.88	0.18	75,75,75,75	0
59	MG	AA	3427	1/1	0.88	0.06	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	3215	1/1	0.88	0.19	59,59,59,59	0
59	MG	AA	3124	1/1	0.88	0.30	62,62,62,62	0
59	MG	BA	1633	1/1	0.88	0.25	63,63,63,63	0
59	MG	DA	1728	1/1	0.88	0.09	71,71,71,71	0
59	MG	CA	3296	1/1	0.88	0.09	79,79,79,79	0
59	MG	CA	3298	1/1	0.88	0.21	57,57,57,57	0
59	MG	CA	3140	1/1	0.88	0.25	63,63,63,63	0
59	MG	CB	3011	1/1	0.88	0.20	56,56,56,56	0
59	MG	CB	3012	1/1	0.88	0.14	62,62,62,62	0
59	MG	CA	3514	1/1	0.88	0.22	64,64,64,64	0
59	MG	CA	3515	1/1	0.88	0.07	54,54,54,54	0
59	MG	AA	3450	1/1	0.88	0.08	58,58,58,58	0
59	MG	AA	3601	1/1	0.88	0.10	61,61,61,61	0
59	MG	AA	3010	1/1	0.88	0.18	46,46,46,46	0
59	MG	AA	3061	1/1	0.88	0.17	59,59,59,59	0
59	MG	AF	307	1/1	0.88	0.18	76,76,76,76	0
59	MG	CA	3534	1/1	0.88	0.07	73,73,73,73	0
59	MG	AA	3241	1/1	0.88	0.17	65,65,65,65	0
59	MG	CA	3536	1/1	0.88	0.13	84,84,84,84	0
59	MG	BA	1698	1/1	0.88	0.18	63,63,63,63	0
59	MG	CA	3171	1/1	0.88	0.16	56,56,56,56	0
59	MG	BA	1654	1/1	0.88	0.14	76,76,76,76	0
59	MG	CA	3180	1/1	0.88	0.19	62,62,62,62	0
59	MG	DA	1761	1/1	0.88	0.12	72,72,72,72	0
59	MG	AA	3357	1/1	0.88	0.13	55,55,55,55	0
59	MG	AA	3365	1/1	0.88	0.20	77,77,77,77	0
59	MG	DA	1770	1/1	0.88	0.09	63,63,63,63	0
59	MG	CA	3553	1/1	0.88	0.12	90,90,90,90	0
59	MG	DA	1624	1/1	0.88	0.07	82,82,82,82	0
59	MG	DA	1626	1/1	0.88	0.14	71,71,71,71	0
59	MG	CA	3190	1/1	0.88	0.16	66,66,66,66	0
59	MG	CA	3193	1/1	0.88	0.15	89,89,89,89	0
59	MG	BA	1711	1/1	0.88	0.10	61,61,61,61	0
59	MG	CA	3219	1/1	0.89	0.14	42,42,42,42	0
59	MG	BA	1808	1/1	0.89	0.10	54,54,54,54	0
59	MG	CA	3576	1/1	0.89	0.08	71,71,71,71	0
59	MG	AA	3603	1/1	0.89	0.24	76,76,76,76	0
59	MG	BA	1717	1/1	0.89	0.13	78,78,78,78	0
59	MG	BA	1718	1/1	0.89	0.06	63,63,63,63	0
59	MG	CA	3441	1/1	0.89	0.16	56,56,56,56	0
59	MG	BA	1663	1/1	0.89	0.13	43,43,43,43	0
59	MG	CA	3229	1/1	0.89	0.12	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	CA	3589	1/1	0.89	0.14	71,71,71,71	0
59	MG	CA	3454	1/1	0.89	0.08	81,81,81,81	0
59	MG	CA	3593	1/1	0.89	0.18	61,61,61,61	0
59	MG	AA	3604	1/1	0.89	0.17	81,81,81,81	0
59	MG	CA	3113	1/1	0.89	0.15	38,38,38,38	0
59	MG	AA	3180	1/1	0.89	0.22	69,69,69,69	0
59	MG	BA	1666	1/1	0.89	0.18	61,61,61,61	0
59	MG	CA	3604	1/1	0.89	0.07	62,62,62,62	0
59	MG	BA	1667	1/1	0.89	0.16	74,74,74,74	0
59	MG	CA	3120	1/1	0.89	0.17	42,42,42,42	0
59	MG	DA	1672	1/1	0.89	0.09	77,77,77,77	0
59	MG	AA	3251	1/1	0.89	0.21	56,56,56,56	0
59	MG	AA	3530	1/1	0.89	0.14	20,20,20,20	1
59	MG	AA	3240	1/1	0.89	0.15	69,69,69,69	0
59	MG	BA	1754	1/1	0.89	0.12	49,49,49,49	0
59	MG	AA	3615	1/1	0.89	0.17	43,43,43,43	0
59	MG	BA	1672	1/1	0.89	0.24	65,65,65,65	0
59	MG	CA	3040	1/1	0.89	0.29	79,79,79,79	0
59	MG	AA	3736	1/1	0.89	0.11	59,59,59,59	0
59	MG	CA	3264	1/1	0.89	0.16	60,60,60,60	0
59	MG	CA	3268	1/1	0.89	0.20	52,52,52,52	0
59	MG	CA	3495	1/1	0.89	0.13	70,70,70,70	0
59	MG	AA	3800	1/1	0.89	0.10	35,35,35,35	0
59	MG	CA	3043	1/1	0.89	0.17	61,61,61,61	0
59	MG	AA	3375	1/1	0.89	0.14	48,48,48,48	0
59	MG	CA	3636	1/1	0.89	0.10	64,64,64,64	0
59	MG	CA	3046	1/1	0.89	0.14	68,68,68,68	0
59	MG	CA	3639	1/1	0.89	0.22	61,61,61,61	0
59	MG	CA	3291	1/1	0.89	0.17	48,48,48,48	0
59	MG	AA	3739	1/1	0.89	0.09	38,38,38,38	0
59	MG	CA	3645	1/1	0.89	0.10	69,69,69,69	0
59	MG	BA	1630	1/1	0.89	0.17	61,61,61,61	0
59	MG	AA	3140	1/1	0.89	0.23	62,62,62,62	0
59	MG	AA	3565	1/1	0.89	0.13	44,44,44,44	0
59	MG	BA	1689	1/1	0.89	0.36	71,71,71,71	0
59	MG	AA	3466	1/1	0.89	0.19	76,76,76,76	0
59	MG	CB	3003	1/1	0.89	0.09	65,65,65,65	0
59	MG	AD	307	1/1	0.89	0.21	86,86,86,86	0
59	MG	AA	3278	1/1	0.89	0.17	60,60,60,60	0
59	MG	CA	3517	1/1	0.89	0.11	62,62,62,62	0
59	MG	AA	3339	1/1	0.89	0.12	49,49,49,49	0
59	MG	CA	3521	1/1	0.89	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
59	MG	CA	3335	1/1	0.89	0.17	66,66,66,66	0
59	MG	CA	3529	1/1	0.89	0.09	68,68,68,68	0
59	MG	CA	3189	1/1	0.89	0.14	50,50,50,50	0
59	MG	AA	3692	1/1	0.89	0.10	36,36,36,36	1
59	MG	CA	3343	1/1	0.89	0.09	32,32,32,32	0
59	MG	CQ	203	1/1	0.89	0.15	54,54,54,54	0
59	MG	AA	3761	1/1	0.89	0.40	92,92,92,92	0
59	MG	DA	1752	1/1	0.89	0.20	52,52,52,52	0
59	MG	BA	1789	1/1	0.89	0.14	72,72,72,72	0
59	MG	CA	3199	1/1	0.89	0.17	55,55,55,55	0
59	MG	CA	3200	1/1	0.89	0.12	51,51,51,51	0
59	MG	BA	1652	1/1	0.89	0.09	59,59,59,59	0
59	MG	CA	3540	1/1	0.89	0.08	54,54,54,54	0
59	MG	AZ	302	1/1	0.89	0.10	55,55,55,55	0
59	MG	BA	1706	1/1	0.89	0.10	63,63,63,63	0
59	MG	AA	3767	1/1	0.89	0.19	67,67,67,67	0
59	MG	CA	3207	1/1	0.89	0.19	75,75,75,75	0
59	MG	DA	1771	1/1	0.89	0.09	60,60,60,60	0
59	MG	CA	3210	1/1	0.89	0.18	62,62,62,62	0
59	MG	AA	3628	1/1	0.89	0.12	70,70,70,70	0
59	MG	CA	3406	1/1	0.89	0.09	77,77,77,77	0
59	MG	AA	3281	1/1	0.89	0.24	75,75,75,75	0
59	MG	AA	3203	1/1	0.89	0.07	59,59,59,59	0
59	MG	DA	1633	1/1	0.89	0.21	55,55,55,55	0
59	MG	CA	3368	1/1	0.90	0.10	44,44,44,44	0
59	MG	AE	302	1/1	0.90	0.11	57,57,57,57	0
59	MG	BA	1739	1/1	0.90	0.11	62,62,62,62	0
59	MG	AA	3057	1/1	0.90	0.11	46,46,46,46	0
59	MG	BA	1661	1/1	0.90	0.24	63,63,63,63	0
59	MG	CA	3571	1/1	0.90	0.07	45,45,45,45	0
59	MG	DA	1637	1/1	0.90	0.17	68,68,68,68	0
59	MG	CA	3572	1/1	0.90	0.17	70,70,70,70	0
59	MG	AA	3541	1/1	0.90	0.10	74,74,74,74	0
59	MG	BA	1749	1/1	0.90	0.11	61,61,61,61	0
59	MG	AA	3170	1/1	0.90	0.14	54,54,54,54	0
59	MG	AR	202	1/1	0.90	0.08	28,28,28,28	0
59	MG	BA	1756	1/1	0.90	0.07	85,85,85,85	0
59	MG	AA	3101	1/1	0.90	0.39	68,68,68,68	0
59	MG	CA	3585	1/1	0.90	0.12	36,36,36,36	1
59	MG	CA	3412	1/1	0.90	0.13	59,59,59,59	0
59	MG	BA	1763	1/1	0.90	0.12	76,76,76,76	0
59	MG	AA	3556	1/1	0.90	0.13	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	A0	105	1/1	0.90	0.05	30,30,30,30	0
59	MG	DA	1660	1/1	0.90	0.07	80,80,80,80	0
59	MG	DA	1661	1/1	0.90	0.13	66,66,66,66	0
59	MG	AA	3106	1/1	0.90	0.09	33,33,33,33	0
59	MG	A6	101	1/1	0.90	0.16	60,60,60,60	0
59	MG	A6	103	1/1	0.90	0.26	72,72,72,72	0
59	MG	A7	103	1/1	0.90	0.17	55,55,55,55	0
59	MG	AA	3683	1/1	0.90	0.12	62,62,62,62	0
59	MG	AA	3688	1/1	0.90	0.09	25,25,25,25	0
59	MG	CA	3455	1/1	0.90	0.22	49,49,49,49	0
59	MG	AA	3772	1/1	0.90	0.26	61,61,61,61	1
59	MG	AA	3184	1/1	0.90	0.16	75,75,75,75	0
59	MG	BA	1605	1/1	0.90	0.13	73,73,73,73	0
59	MG	CA	3092	1/1	0.90	0.36	79,79,79,79	0
59	MG	AA	3139	1/1	0.90	0.16	60,60,60,60	0
59	MG	CA	3228	1/1	0.90	0.27	59,59,59,59	0
59	MG	AA	3699	1/1	0.90	0.15	71,71,71,71	0
59	MG	AA	3070	1/1	0.90	0.36	81,81,81,81	0
59	MG	AA	3467	1/1	0.90	0.14	49,49,49,49	0
59	MG	CA	3101	1/1	0.90	0.20	84,84,84,84	0
59	MG	AA	3782	1/1	0.90	0.09	44,44,44,44	0
59	MG	AA	3783	1/1	0.90	0.25	53,53,53,53	1
59	MG	BA	1620	1/1	0.90	0.09	52,52,52,52	0
59	MG	AA	3633	1/1	0.90	0.12	48,48,48,48	0
59	MG	BA	1696	1/1	0.90	0.10	98,98,98,98	0
59	MG	CA	3635	1/1	0.90	0.10	48,48,48,48	0
59	MG	AA	3635	1/1	0.90	0.07	49,49,49,49	0
59	MG	CA	3242	1/1	0.90	0.22	82,82,82,82	0
59	MG	AA	3109	1/1	0.90	0.12	56,56,56,56	0
59	MG	DA	1721	1/1	0.90	0.07	80,80,80,80	0
59	MG	CA	3500	1/1	0.90	0.13	75,75,75,75	0
59	MG	CA	3115	1/1	0.90	0.28	67,67,67,67	0
59	MG	AA	3065	1/1	0.90	0.21	62,62,62,62	0
59	MG	AA	3153	1/1	0.90	0.16	59,59,59,59	0
59	MG	CA	3118	1/1	0.90	0.14	65,65,65,65	0
59	MG	AA	3414	1/1	0.90	0.06	37,37,37,37	0
59	MG	CA	3654	1/1	0.90	0.20	90,90,90,90	0
59	MG	AA	3816	1/1	0.90	0.25	66,66,66,66	0
59	MG	CA	3270	1/1	0.90	0.18	76,76,76,76	0
59	MG	AA	3817	1/1	0.90	0.09	75,75,75,75	0
59	MG	CA	3278	1/1	0.90	0.08	58,58,58,58	0
59	MG	BD	502	1/1	0.90	0.23	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	1640	1/1	0.90	0.17	52,52,52,52	0
59	MG	CA	3128	1/1	0.90	0.17	50,50,50,50	0
59	MG	AA	3819	1/1	0.90	0.14	35,35,35,35	1
59	MG	CA	3133	1/1	0.90	0.13	85,85,85,85	0
59	MG	BN	503	1/1	0.90	0.07	62,62,62,62	0
59	MG	AB	3004	1/1	0.90	0.25	69,69,69,69	0
59	MG	DA	1751	1/1	0.90	0.12	64,64,64,64	0
59	MG	AA	3041	1/1	0.90	0.12	37,37,37,37	0
59	MG	AA	3652	1/1	0.90	0.10	53,53,53,53	0
59	MG	CA	3141	1/1	0.90	0.22	68,68,68,68	0
59	MG	AA	3158	1/1	0.90	0.22	68,68,68,68	0
59	MG	DA	1601	1/1	0.90	0.15	74,74,74,74	0
59	MG	CA	3020	1/1	0.90	0.10	47,47,47,47	0
59	MG	DA	1758	1/1	0.90	0.15	75,75,75,75	0
59	MG	CA	3022	1/1	0.90	0.28	69,69,69,69	0
59	MG	DA	1608	1/1	0.90	0.09	57,57,57,57	0
59	MG	DA	1767	1/1	0.90	0.08	74,74,74,74	0
59	MG	CA	3154	1/1	0.90	0.19	64,64,64,64	0
59	MG	CA	3023	1/1	0.90	0.13	68,68,68,68	0
59	MG	CA	3030	1/1	0.90	0.20	59,59,59,59	0
59	MG	CA	3159	1/1	0.90	0.15	69,69,69,69	0
59	MG	AA	3657	1/1	0.90	0.09	63,63,63,63	0
59	MG	CA	3354	1/1	0.90	0.12	49,49,49,49	0
59	MG	AA	3659	1/1	0.90	0.15	73,73,73,73	0
59	MG	BA	1726	1/1	0.90	0.10	46,46,46,46	0
59	MG	AA	3253	1/1	0.90	0.12	64,64,64,64	0
60	ZN	C4	501	1/1	0.90	0.07	194,194,194,194	0
59	MG	AA	3165	1/1	0.91	0.14	52,52,52,52	0
59	MG	CA	3348	1/1	0.91	0.14	44,44,44,44	0
59	MG	BA	1752	1/1	0.91	0.15	59,59,59,59	0
59	MG	CA	3352	1/1	0.91	0.09	79,79,79,79	0
59	MG	AA	3035	1/1	0.91	0.09	48,48,48,48	0
59	MG	DA	1619	1/1	0.91	0.17	59,59,59,59	0
59	MG	AA	3086	1/1	0.91	0.12	55,55,55,55	0
59	MG	CA	3548	1/1	0.91	0.08	90,90,90,90	0
59	MG	CA	3551	1/1	0.91	0.09	63,63,63,63	0
59	MG	AA	3174	1/1	0.91	0.21	59,59,59,59	0
59	MG	CA	3366	1/1	0.91	0.14	49,49,49,49	0
59	MG	AA	3356	1/1	0.91	0.13	80,80,80,80	0
59	MG	CA	3558	1/1	0.91	0.08	64,64,64,64	0
59	MG	CA	3559	1/1	0.91	0.09	75,75,75,75	0
59	MG	BA	1759	1/1	0.91	0.17	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	CA	3373	1/1	0.91	0.17	58,58,58,58	0
59	MG	AA	3649	1/1	0.91	0.13	62,62,62,62	0
59	MG	AA	3143	1/1	0.91	0.09	48,48,48,48	0
59	MG	CA	3059	1/1	0.91	0.13	58,58,58,58	0
59	MG	BA	1604	1/1	0.91	0.15	63,63,63,63	0
59	MG	AA	3718	1/1	0.91	0.14	42,42,42,42	0
59	MG	CA	3575	1/1	0.91	0.09	71,71,71,71	0
59	MG	BA	1606	1/1	0.91	0.22	126,126,126,126	0
59	MG	AA	3468	1/1	0.91	0.07	55,55,55,55	0
59	MG	AA	3722	1/1	0.91	0.12	37,37,37,37	0
59	MG	BA	1611	1/1	0.91	0.07	31,31,31,31	0
59	MG	BA	1678	1/1	0.91	0.13	54,54,54,54	0
59	MG	CA	3208	1/1	0.91	0.17	74,74,74,74	0
59	MG	DA	1656	1/1	0.91	0.13	63,63,63,63	0
59	MG	DA	1658	1/1	0.91	0.23	51,51,51,51	0
59	MG	AA	3724	1/1	0.91	0.11	47,47,47,47	0
59	MG	CA	3077	1/1	0.91	0.11	42,42,42,42	0
59	MG	AA	3474	1/1	0.91	0.06	18,18,18,18	1
59	MG	BA	1615	1/1	0.91	0.07	62,62,62,62	0
59	MG	AA	3363	1/1	0.91	0.10	82,82,82,82	0
59	MG	CA	3435	1/1	0.91	0.07	55,55,55,55	0
59	MG	CA	3595	1/1	0.91	0.12	70,70,70,70	0
59	MG	AB	3003	1/1	0.91	0.15	60,60,60,60	0
59	MG	DA	1670	1/1	0.91	0.10	49,49,49,49	0
59	MG	AA	3012	1/1	0.91	0.14	49,49,49,49	0
59	MG	CA	3600	1/1	0.91	0.13	86,86,86,86	0
59	MG	AB	3006	1/1	0.91	0.11	57,57,57,57	0
59	MG	CA	3094	1/1	0.91	0.13	59,59,59,59	0
59	MG	BA	1624	1/1	0.91	0.10	58,58,58,58	0
59	MG	AA	3209	1/1	0.91	0.13	62,62,62,62	0
59	MG	AA	3285	1/1	0.91	0.19	51,51,51,51	0
59	MG	AA	3378	1/1	0.91	0.19	56,56,56,56	0
59	MG	AA	3135	1/1	0.91	0.14	55,55,55,55	0
59	MG	CA	3106	1/1	0.91	0.18	66,66,66,66	0
59	MG	BA	1801	1/1	0.91	0.07	65,65,65,65	0
59	MG	CA	3616	1/1	0.91	0.22	74,74,74,74	0
59	MG	BA	1802	1/1	0.91	0.17	76,76,76,76	0
59	MG	DA	1700	1/1	0.91	0.13	61,61,61,61	0
59	MG	DA	1703	1/1	0.91	0.10	89,89,89,89	0
59	MG	AD	302	1/1	0.91	0.27	85,85,85,85	0
59	MG	BA	1700	1/1	0.91	0.22	52,52,52,52	0
59	MG	BA	1703	1/1	0.91	0.18	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	CA	3483	1/1	0.91	0.13	64,64,64,64	0
59	MG	CA	3484	1/1	0.91	0.10	78,78,78,78	0
59	MG	AA	3290	1/1	0.91	0.09	64,64,64,64	0
59	MG	CA	3630	1/1	0.91	0.10	65,65,65,65	0
59	MG	CA	3631	1/1	0.91	0.10	65,65,65,65	0
59	MG	BA	1635	1/1	0.91	0.31	65,65,65,65	0
59	MG	AA	3293	1/1	0.91	0.07	27,27,27,27	0
59	MG	BA	1814	1/1	0.91	0.09	69,69,69,69	0
59	MG	DA	1725	1/1	0.91	0.11	58,58,58,58	0
59	MG	CA	3247	1/1	0.91	0.16	39,39,39,39	0
59	MG	BA	1708	1/1	0.91	0.07	64,64,64,64	0
59	MG	AA	3252	1/1	0.91	0.08	44,44,44,44	0
59	MG	BA	1643	1/1	0.91	0.17	66,66,66,66	0
59	MG	CA	3257	1/1	0.91	0.10	35,35,35,35	0
59	MG	AA	3765	1/1	0.91	0.15	60,60,60,60	0
59	MG	BL	202	1/1	0.91	0.10	54,54,54,54	0
59	MG	AA	3118	1/1	0.91	0.22	76,76,76,76	0
59	MG	AF	308	1/1	0.91	0.12	57,57,57,57	0
59	MG	BW	502	1/1	0.91	0.12	59,59,59,59	0
59	MG	CA	3130	1/1	0.91	0.07	55,55,55,55	0
59	MG	CA	3660	1/1	0.91	0.20	60,60,60,60	0
59	MG	BW	503	1/1	0.91	0.20	60,60,60,60	0
59	MG	CB	3002	1/1	0.91	0.07	63,63,63,63	0
59	MG	BA	1647	1/1	0.91	0.25	57,57,57,57	0
59	MG	AA	3550	1/1	0.91	0.09	38,38,38,38	0
59	MG	CB	3007	1/1	0.91	0.16	52,52,52,52	0
59	MG	CB	3008	1/1	0.91	0.14	66,66,66,66	0
59	MG	CA	3293	1/1	0.91	0.12	60,60,60,60	0
59	MG	AN	3001	1/1	0.91	0.12	58,58,58,58	0
59	MG	AP	204	1/1	0.91	0.08	59,59,59,59	0
59	MG	CD	302	1/1	0.91	0.21	56,56,56,56	0
59	MG	BA	1655	1/1	0.91	0.06	59,59,59,59	0
59	MG	AQ	203	1/1	0.91	0.10	32,32,32,32	0
59	MG	DA	1759	1/1	0.91	0.08	53,53,53,53	0
59	MG	BA	1729	1/1	0.91	0.12	53,53,53,53	0
59	MG	CG	3001	1/1	0.91	0.08	65,65,65,65	0
59	MG	DA	1763	1/1	0.91	0.10	76,76,76,76	0
59	MG	CN	5001	1/1	0.91	0.08	65,65,65,65	0
59	MG	CA	3031	1/1	0.91	0.20	68,68,68,68	0
59	MG	CA	3526	1/1	0.91	0.14	58,58,58,58	0
59	MG	CA	3150	1/1	0.91	0.15	57,57,57,57	0
59	MG	AA	3102	1/1	0.91	0.23	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DE	202	1/1	0.91	0.08	100,100,100,100	0
59	MG	CA	3325	1/1	0.91	0.08	38,38,38,38	0
59	MG	AA	3694	1/1	0.91	0.07	53,53,53,53	0
59	MG	AA	3218	1/1	0.91	0.17	67,67,67,67	0
59	MG	DW	502	1/1	0.91	0.08	58,58,58,58	0
59	MG	AA	3632	1/1	0.91	0.12	54,54,54,54	0
59	MG	DA	1606	1/1	0.91	0.06	85,85,85,85	0
59	MG	AA	3440	1/1	0.91	0.09	63,63,63,63	0
59	MG	AA	3229	1/1	0.92	0.27	67,67,67,67	0
59	MG	BA	1771	1/1	0.92	0.11	65,65,65,65	0
59	MG	AF	302	1/1	0.92	0.14	47,47,47,47	0
59	MG	CV	201	1/1	0.92	0.17	117,117,117,117	0
59	MG	CX	5001	1/1	0.92	0.11	65,65,65,65	0
59	MG	AA	3646	1/1	0.92	0.12	53,53,53,53	0
59	MG	CA	3087	1/1	0.92	0.33	68,68,68,68	0
59	MG	CA	3243	1/1	0.92	0.12	58,58,58,58	0
59	MG	CA	3088	1/1	0.92	0.18	67,67,67,67	0
59	MG	AA	3558	1/1	0.92	0.07	48,48,48,48	0
59	MG	AA	3448	1/1	0.92	0.07	62,62,62,62	0
59	MG	AA	3752	1/1	0.92	0.10	42,42,42,42	0
59	MG	AA	3134	1/1	0.92	0.12	62,62,62,62	0
59	MG	CA	3520	1/1	0.92	0.10	73,73,73,73	0
59	MG	AA	3451	1/1	0.92	0.12	57,57,57,57	0
59	MG	AR	201	1/1	0.92	0.12	63,63,63,63	0
59	MG	AA	3655	1/1	0.92	0.11	55,55,55,55	0
59	MG	AX	3001	1/1	0.92	0.10	52,52,52,52	0
59	MG	AA	3160	1/1	0.92	0.07	30,30,30,30	0
59	MG	AA	3455	1/1	0.92	0.13	32,32,32,32	1
59	MG	DA	1627	1/1	0.92	0.05	77,77,77,77	0
59	MG	CA	3274	1/1	0.92	0.13	52,52,52,52	0
59	MG	A0	102	1/1	0.92	0.07	56,56,56,56	0
59	MG	CA	3280	1/1	0.92	0.07	48,48,48,48	0
59	MG	AA	3763	1/1	0.92	0.10	47,47,47,47	0
59	MG	CA	3285	1/1	0.92	0.09	63,63,63,63	0
59	MG	CA	3287	1/1	0.92	0.13	45,45,45,45	0
59	MG	DA	1636	1/1	0.92	0.24	62,62,62,62	0
59	MG	BA	1791	1/1	0.92	0.11	72,72,72,72	0
59	MG	AA	3596	1/1	0.92	0.12	65,65,65,65	0
59	MG	AA	3346	1/1	0.92	0.19	59,59,59,59	0
59	MG	BA	1796	1/1	0.92	0.16	57,57,57,57	0
59	MG	CA	3547	1/1	0.92	0.12	69,69,69,69	0
59	MG	DA	1642	1/1	0.92	0.10	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	3768	1/1	0.92	0.07	58,58,58,58	0
59	MG	BA	1798	1/1	0.92	0.11	73,73,73,73	0
59	MG	DA	1645	1/1	0.92	0.07	58,58,58,58	0
59	MG	AA	3670	1/1	0.92	0.07	54,54,54,54	0
59	MG	AA	3238	1/1	0.92	0.16	76,76,76,76	0
59	MG	CA	3119	1/1	0.92	0.32	55,55,55,55	0
59	MG	AA	3019	1/1	0.92	0.16	70,70,70,70	0
59	MG	AA	3606	1/1	0.92	0.09	34,34,34,34	0
59	MG	CA	3319	1/1	0.92	0.08	65,65,65,65	0
59	MG	AA	3208	1/1	0.92	0.27	54,54,54,54	0
59	MG	AA	3280	1/1	0.92	0.12	53,53,53,53	0
59	MG	AA	3682	1/1	0.92	0.09	31,31,31,31	0
59	MG	AA	3166	1/1	0.92	0.17	40,40,40,40	0
59	MG	BA	1608	1/1	0.92	0.22	57,57,57,57	0
59	MG	AA	3687	1/1	0.92	0.20	52,52,52,52	0
59	MG	AA	3283	1/1	0.92	0.24	43,43,43,43	0
59	MG	AA	3127	1/1	0.92	0.16	57,57,57,57	0
59	MG	AA	3693	1/1	0.92	0.16	69,69,69,69	0
59	MG	CA	3137	1/1	0.92	0.14	69,69,69,69	0
59	MG	AA	3490	1/1	0.92	0.12	27,27,27,27	0
59	MG	AA	3794	1/1	0.92	0.18	60,60,60,60	0
59	MG	AA	3695	1/1	0.92	0.10	67,67,67,67	0
59	MG	BA	1617	1/1	0.92	0.11	118,118,118,118	0
59	MG	CA	3147	1/1	0.92	0.13	55,55,55,55	0
59	MG	BA	1618	1/1	0.92	0.14	52,52,52,52	0
59	MG	CA	3590	1/1	0.92	0.11	59,59,59,59	0
59	MG	AA	3286	1/1	0.92	0.29	40,40,40,40	0
59	MG	DA	1684	1/1	0.92	0.12	69,69,69,69	0
59	MG	AA	3802	1/1	0.92	0.13	86,86,86,86	0
59	MG	AA	3803	1/1	0.92	0.14	45,45,45,45	0
59	MG	CA	3005	1/1	0.92	0.11	48,48,48,48	0
59	MG	CA	3380	1/1	0.92	0.16	59,59,59,59	0
59	MG	CA	3388	1/1	0.92	0.10	90,90,90,90	0
59	MG	AA	3249	1/1	0.92	0.16	59,59,59,59	0
59	MG	CA	3015	1/1	0.92	0.14	51,51,51,51	0
59	MG	AA	3496	1/1	0.92	0.19	31,31,31,31	0
59	MG	DA	1705	1/1	0.92	0.09	68,68,68,68	0
59	MG	DA	1706	1/1	0.92	0.13	66,66,66,66	0
59	MG	BA	1627	1/1	0.92	0.07	51,51,51,51	0
59	MG	AA	3499	1/1	0.92	0.06	48,48,48,48	0
59	MG	CA	3024	1/1	0.92	0.18	100,100,100,100	0
59	MG	CA	3409	1/1	0.92	0.13	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	CA	3176	1/1	0.92	0.23	60,60,60,60	0
59	MG	AA	3818	1/1	0.92	0.12	61,61,61,61	0
59	MG	CA	3413	1/1	0.92	0.09	39,39,39,39	0
59	MG	CA	3182	1/1	0.92	0.16	38,38,38,38	0
59	MG	CA	3419	1/1	0.92	0.08	59,59,59,59	0
59	MG	BA	1720	1/1	0.92	0.09	61,61,61,61	0
59	MG	AA	3508	1/1	0.92	0.15	43,43,43,43	0
59	MG	CA	3431	1/1	0.92	0.13	75,75,75,75	0
59	MG	CA	3033	1/1	0.92	0.20	55,55,55,55	0
59	MG	AB	3002	1/1	0.92	0.13	52,52,52,52	0
59	MG	AA	3193	1/1	0.92	0.21	40,40,40,40	0
59	MG	CA	3436	1/1	0.92	0.13	64,64,64,64	0
59	MG	CA	3037	1/1	0.92	0.31	57,57,57,57	0
59	MG	AA	3710	1/1	0.92	0.20	29,29,29,29	1
59	MG	AA	3099	1/1	0.92	0.15	53,53,53,53	0
59	MG	CA	3447	1/1	0.92	0.12	73,73,73,73	0
59	MG	CA	3451	1/1	0.92	0.14	62,62,62,62	0
59	MG	DA	1741	1/1	0.92	0.20	67,67,67,67	0
59	MG	CA	3637	1/1	0.92	0.34	61,61,61,61	0
59	MG	BA	1732	1/1	0.92	0.07	70,70,70,70	0
59	MG	BA	1639	1/1	0.92	0.23	61,61,61,61	0
59	MG	BA	1737	1/1	0.92	0.23	79,79,79,79	0
59	MG	AB	3009	1/1	0.92	0.07	50,50,50,50	0
59	MG	AA	3028	1/1	0.92	0.10	39,39,39,39	0
59	MG	BA	1742	1/1	0.92	0.09	48,48,48,48	0
59	MG	CA	3209	1/1	0.92	0.13	73,73,73,73	0
59	MG	CA	3048	1/1	0.92	0.05	47,47,47,47	0
59	MG	AB	3018	1/1	0.92	0.09	69,69,69,69	0
59	MG	CA	3213	1/1	0.92	0.18	51,51,51,51	0
59	MG	CA	3051	1/1	0.92	0.22	57,57,57,57	0
59	MG	CA	3662	1/1	0.92	0.14	33,33,33,33	0
59	MG	CA	3663	1/1	0.92	0.11	64,64,64,64	0
59	MG	CA	3054	1/1	0.92	0.14	36,36,36,36	0
59	MG	AA	3300	1/1	0.92	0.09	22,22,22,22	0
59	MG	AA	3264	1/1	0.92	0.22	51,51,51,51	0
59	MG	AA	3544	1/1	0.92	0.09	26,26,26,26	0
59	MG	CA	3061	1/1	0.92	0.14	68,68,68,68	0
59	MG	AA	3177	1/1	0.92	0.12	59,59,59,59	0
59	MG	CA	3225	1/1	0.92	0.15	64,64,64,64	0
59	MG	AD	303	1/1	0.92	0.24	58,58,58,58	0
59	MG	CA	3493	1/1	0.92	0.15	65,65,65,65	0
59	MG	AA	3641	1/1	0.92	0.09	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	3224	1/1	0.92	0.19	56,56,56,56	0
59	MG	BA	1656	1/1	0.92	0.20	75,75,75,75	0
59	MG	BA	1762	1/1	0.92	0.08	74,74,74,74	0
59	MG	CA	3073	1/1	0.92	0.09	49,49,49,49	0
59	MG	AE	301	1/1	0.92	0.11	69,69,69,69	0
59	MG	CA	3503	1/1	0.92	0.18	52,52,52,52	0
59	MG	DZ	702	1/1	0.92	0.13	57,57,57,57	0
59	MG	AA	3555	1/1	0.92	0.07	45,45,45,45	0
59	MG	DA	1603	1/1	0.93	0.08	72,72,72,72	0
59	MG	AA	3237	1/1	0.93	0.17	76,76,76,76	0
59	MG	AA	3080	1/1	0.93	0.29	61,61,61,61	0
59	MG	BA	1681	1/1	0.93	0.06	53,53,53,53	0
59	MG	DA	1607	1/1	0.93	0.07	86,86,86,86	0
59	MG	AA	3187	1/1	0.93	0.28	56,56,56,56	0
59	MG	A7	102	1/1	0.93	0.11	37,37,37,37	0
59	MG	BA	1807	1/1	0.93	0.11	61,61,61,61	0
59	MG	BA	1684	1/1	0.93	0.17	61,61,61,61	0
59	MG	CA	3122	1/1	0.93	0.13	58,58,58,58	0
59	MG	DA	1616	1/1	0.93	0.19	51,51,51,51	0
59	MG	AA	3210	1/1	0.93	0.17	59,59,59,59	1
59	MG	AA	3684	1/1	0.93	0.11	51,51,51,51	0
59	MG	DA	1620	1/1	0.93	0.16	57,57,57,57	0
59	MG	AA	3017	1/1	0.93	0.09	61,61,61,61	0
59	MG	AA	3471	1/1	0.93	0.08	56,56,56,56	0
59	MG	AA	3610	1/1	0.93	0.15	59,59,59,59	0
59	MG	DA	1625	1/1	0.93	0.08	50,50,50,50	0
59	MG	CA	3313	1/1	0.93	0.16	38,38,38,38	0
59	MG	AA	3473	1/1	0.93	0.07	53,53,53,53	0
59	MG	CA	3543	1/1	0.93	0.09	71,71,71,71	0
59	MG	AA	3791	1/1	0.93	0.14	51,51,51,51	0
59	MG	BK	201	1/1	0.93	0.09	44,44,44,44	0
59	MG	AA	3244	1/1	0.93	0.19	52,52,52,52	0
59	MG	BA	1607	1/1	0.93	0.08	64,64,64,64	0
59	MG	AA	3025	1/1	0.93	0.12	68,68,68,68	0
59	MG	CA	3336	1/1	0.93	0.10	64,64,64,64	0
59	MG	AA	3361	1/1	0.93	0.16	53,53,53,53	0
59	MG	CA	3556	1/1	0.93	0.12	62,62,62,62	0
59	MG	AA	3798	1/1	0.93	0.09	25,25,25,25	0
59	MG	AA	3618	1/1	0.93	0.10	72,72,72,72	0
59	MG	CA	3344	1/1	0.93	0.05	68,68,68,68	0
59	MG	CA	3145	1/1	0.93	0.08	76,76,76,76	0
59	MG	BZ	701	1/1	0.93	0.11	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	1705	1/1	0.93	0.14	53,53,53,53	0
59	MG	AA	3282	1/1	0.93	0.13	33,33,33,33	0
59	MG	AA	3703	1/1	0.93	0.15	56,56,56,56	0
59	MG	AA	3804	1/1	0.93	0.06	50,50,50,50	0
59	MG	DA	1650	1/1	0.93	0.15	50,50,50,50	0
59	MG	CA	3365	1/1	0.93	0.07	55,55,55,55	0
59	MG	CA	3011	1/1	0.93	0.15	63,63,63,63	0
59	MG	AA	3805	1/1	0.93	0.12	58,58,58,58	0
59	MG	CA	3016	1/1	0.93	0.16	52,52,52,52	0
59	MG	BA	1712	1/1	0.93	0.33	57,57,57,57	0
59	MG	AA	3810	1/1	0.93	0.20	67,67,67,67	0
59	MG	AA	3026	1/1	0.93	0.06	47,47,47,47	0
59	MG	AA	3492	1/1	0.93	0.08	26,26,26,26	0
59	MG	CA	3026	1/1	0.93	0.12	32,32,32,32	1
59	MG	CA	3384	1/1	0.93	0.10	55,55,55,55	0
59	MG	CA	3028	1/1	0.93	0.21	51,51,51,51	0
59	MG	DA	1666	1/1	0.93	0.19	53,53,53,53	0
59	MG	DA	1667	1/1	0.93	0.07	66,66,66,66	0
59	MG	CA	3177	1/1	0.93	0.12	29,29,29,29	0
59	MG	CA	3390	1/1	0.93	0.05	80,80,80,80	0
59	MG	CA	3178	1/1	0.93	0.09	54,54,54,54	0
59	MG	CA	3394	1/1	0.93	0.15	69,69,69,69	0
59	MG	AA	3179	1/1	0.93	0.14	45,45,45,45	1
59	MG	BA	1622	1/1	0.93	0.16	65,65,65,65	0
59	MG	CA	3402	1/1	0.93	0.10	66,66,66,66	0
59	MG	AA	3371	1/1	0.93	0.09	53,53,53,53	0
59	MG	AA	3374	1/1	0.93	0.14	49,49,49,49	0
59	MG	CA	3188	1/1	0.93	0.14	94,94,94,94	0
59	MG	AB	3001	1/1	0.93	0.15	74,74,74,74	0
59	MG	AA	3001	1/1	0.93	0.08	25,25,25,25	0
59	MG	DA	1685	1/1	0.93	0.07	46,46,46,46	0
59	MG	DA	1689	1/1	0.93	0.08	56,56,56,56	0
59	MG	AA	3714	1/1	0.93	0.14	70,70,70,70	0
59	MG	BA	1629	1/1	0.93	0.12	61,61,61,61	0
59	MG	AA	3501	1/1	0.93	0.07	49,49,49,49	0
59	MG	BA	1730	1/1	0.93	0.11	53,53,53,53	0
59	MG	CA	3421	1/1	0.93	0.15	57,57,57,57	0
59	MG	CA	3201	1/1	0.93	0.21	45,45,45,45	0
59	MG	DA	1701	1/1	0.93	0.13	68,68,68,68	0
59	MG	AA	3716	1/1	0.93	0.15	66,66,66,66	0
59	MG	BA	1632	1/1	0.93	0.09	48,48,48,48	0
59	MG	AB	3008	1/1	0.93	0.17	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	3287	1/1	0.93	0.21	43,43,43,43	0
59	MG	AA	3142	1/1	0.93	0.14	64,64,64,64	0
59	MG	CA	3625	1/1	0.93	0.11	64,64,64,64	0
59	MG	BA	1637	1/1	0.93	0.22	72,72,72,72	0
59	MG	AA	3520	1/1	0.93	0.07	17,17,17,17	0
59	MG	DA	1714	1/1	0.93	0.08	68,68,68,68	0
59	MG	BA	1747	1/1	0.93	0.09	65,65,65,65	0
59	MG	AA	3636	1/1	0.93	0.12	86,86,86,86	0
59	MG	AA	3289	1/1	0.93	0.10	53,53,53,53	0
59	MG	BA	1641	1/1	0.93	0.11	54,54,54,54	0
59	MG	BA	1642	1/1	0.93	0.11	60,60,60,60	0
59	MG	AA	3732	1/1	0.93	0.15	70,70,70,70	0
59	MG	AA	3258	1/1	0.93	0.15	68,68,68,68	0
59	MG	DA	1726	1/1	0.93	0.13	60,60,60,60	0
59	MG	AA	3263	1/1	0.93	0.16	24,24,24,24	1
59	MG	AA	3420	1/1	0.93	0.07	25,25,25,25	1
59	MG	AA	3050	1/1	0.93	0.13	28,28,28,28	0
59	MG	CA	3472	1/1	0.93	0.22	62,62,62,62	0
59	MG	AD	309	1/1	0.93	0.09	56,56,56,56	0
59	MG	DA	1734	1/1	0.93	0.05	65,65,65,65	0
59	MG	DA	1735	1/1	0.93	0.07	73,73,73,73	0
59	MG	AA	3742	1/1	0.93	0.14	68,68,68,68	0
59	MG	AA	3746	1/1	0.93	0.13	73,73,73,73	0
59	MG	AA	3298	1/1	0.93	0.09	58,58,58,58	0
59	MG	CA	3652	1/1	0.93	0.07	23,23,23,23	0
59	MG	AA	3751	1/1	0.93	0.23	61,61,61,61	0
59	MG	AA	3231	1/1	0.93	0.13	64,64,64,64	0
59	MG	CA	3658	1/1	0.93	0.17	64,64,64,64	0
59	MG	CA	3659	1/1	0.93	0.07	55,55,55,55	0
59	MG	AA	3313	1/1	0.93	0.13	39,39,39,39	0
59	MG	AA	3204	1/1	0.93	0.13	54,54,54,54	0
59	MG	AA	3446	1/1	0.93	0.17	59,59,59,59	0
59	MG	CA	3083	1/1	0.93	0.16	61,61,61,61	0
59	MG	CA	3086	1/1	0.93	0.36	85,85,85,85	0
59	MG	AN	3003	1/1	0.93	0.07	55,55,55,55	0
59	MG	CB	3004	1/1	0.93	0.09	55,55,55,55	0
59	MG	AP	203	1/1	0.93	0.08	44,44,44,44	0
59	MG	AA	3563	1/1	0.93	0.12	34,34,34,34	0
59	MG	AA	3447	1/1	0.93	0.10	56,56,56,56	0
59	MG	AA	3185	1/1	0.93	0.14	76,76,76,76	0
59	MG	CA	3245	1/1	0.93	0.24	62,62,62,62	0
59	MG	AA	3575	1/1	0.93	0.09	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	CD	301	1/1	0.93	0.12	43,43,43,43	0
59	MG	CA	3095	1/1	0.93	0.12	58,58,58,58	0
59	MG	AV	201	1/1	0.93	0.11	38,38,38,38	0
59	MG	DA	1765	1/1	0.93	0.07	64,64,64,64	0
59	MG	DA	1766	1/1	0.93	0.07	74,74,74,74	0
59	MG	CA	3253	1/1	0.93	0.10	70,70,70,70	0
59	MG	AW	3002	1/1	0.93	0.11	47,47,47,47	0
59	MG	AA	3449	1/1	0.93	0.10	50,50,50,50	0
59	MG	AY	502	1/1	0.93	0.17	60,60,60,60	0
59	MG	AZ	301	1/1	0.93	0.13	86,86,86,86	0
59	MG	BA	1793	1/1	0.93	0.07	65,65,65,65	0
59	MG	CA	3269	1/1	0.93	0.18	81,81,81,81	0
59	MG	BA	1794	1/1	0.93	0.06	38,38,38,38	0
59	MG	AA	3322	1/1	0.93	0.13	61,61,61,61	0
59	MG	CU	201	1/1	0.93	0.15	74,74,74,74	0
59	MG	AA	3270	1/1	0.93	0.22	55,55,55,55	0
59	MG	AA	3593	1/1	0.93	0.19	15,15,15,15	1
59	MG	C5	101	1/1	0.93	0.20	66,66,66,66	0
59	MG	AA	3329	1/1	0.93	0.07	40,40,40,40	1
62	GDP	DZ	703	28/28	0.93	0.08	66,66,66,66	1
59	MG	AA	3325	1/1	0.94	0.11	70,70,70,70	0
59	MG	AA	3808	1/1	0.94	0.13	72,72,72,72	0
59	MG	CB	3010	1/1	0.94	0.08	51,51,51,51	0
59	MG	AA	3148	1/1	0.94	0.22	29,29,29,29	1
59	MG	BA	1731	1/1	0.94	0.10	45,45,45,45	0
59	MG	CA	3464	1/1	0.94	0.08	36,36,36,36	0
59	MG	AA	3813	1/1	0.94	0.07	29,29,29,29	1
59	MG	AA	3599	1/1	0.94	0.07	59,59,59,59	0
59	MG	CA	3469	1/1	0.94	0.14	61,61,61,61	0
59	MG	CE	302	1/1	0.94	0.06	64,64,64,64	0
59	MG	CE	304	1/1	0.94	0.15	75,75,75,75	0
59	MG	BA	1734	1/1	0.94	0.09	61,61,61,61	0
59	MG	AA	3014	1/1	0.94	0.11	31,31,31,31	0
59	MG	BA	1738	1/1	0.94	0.05	66,66,66,66	0
59	MG	AA	3602	1/1	0.94	0.10	51,51,51,51	0
59	MG	AA	3454	1/1	0.94	0.11	61,61,61,61	0
59	MG	AA	3182	1/1	0.94	0.15	46,46,46,46	0
59	MG	CA	3056	1/1	0.94	0.07	63,63,63,63	0
59	MG	AA	3701	1/1	0.94	0.12	81,81,81,81	0
59	MG	AA	3456	1/1	0.94	0.08	56,56,56,56	0
59	MG	CA	3060	1/1	0.94	0.28	72,72,72,72	0
59	MG	AA	3704	1/1	0.94	0.09	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	3073	1/1	0.94	0.05	31,31,31,31	0
59	MG	C3	3001	1/1	0.94	0.09	72,72,72,72	0
59	MG	CA	3489	1/1	0.94	0.08	39,39,39,39	0
59	MG	AA	3220	1/1	0.94	0.08	62,62,62,62	0
59	MG	DA	1602	1/1	0.94	0.06	45,45,45,45	0
59	MG	AA	3609	1/1	0.94	0.07	58,58,58,58	0
59	MG	CA	3231	1/1	0.94	0.23	60,60,60,60	0
59	MG	CA	3232	1/1	0.94	0.21	54,54,54,54	0
59	MG	CA	3068	1/1	0.94	0.31	66,66,66,66	0
59	MG	CA	3498	1/1	0.94	0.06	49,49,49,49	0
59	MG	AA	3709	1/1	0.94	0.21	23,23,23,23	1
59	MG	AB	3014	1/1	0.94	0.09	56,56,56,56	0
59	MG	AB	3015	1/1	0.94	0.06	28,28,28,28	0
59	MG	AA	3002	1/1	0.94	0.12	57,57,57,57	0
59	MG	AA	3349	1/1	0.94	0.08	47,47,47,47	0
59	MG	DA	1615	1/1	0.94	0.06	58,58,58,58	0
59	MG	AA	3355	1/1	0.94	0.12	57,57,57,57	0
59	MG	AA	3226	1/1	0.94	0.10	46,46,46,46	0
59	MG	BA	1766	1/1	0.94	0.07	62,62,62,62	0
59	MG	CA	3079	1/1	0.94	0.07	41,41,41,41	0
59	MG	AB	3023	1/1	0.94	0.19	54,54,54,54	0
59	MG	BA	1770	1/1	0.94	0.06	54,54,54,54	0
59	MG	AA	3616	1/1	0.94	0.09	57,57,57,57	0
59	MG	CA	3513	1/1	0.94	0.10	70,70,70,70	0
59	MG	CA	3084	1/1	0.94	0.10	56,56,56,56	0
59	MG	AA	3228	1/1	0.94	0.07	32,32,32,32	0
59	MG	CA	3251	1/1	0.94	0.13	82,82,82,82	0
59	MG	DA	1630	1/1	0.94	0.27	62,62,62,62	0
59	MG	AA	3479	1/1	0.94	0.07	55,55,55,55	0
59	MG	BA	1651	1/1	0.94	0.16	55,55,55,55	0
59	MG	CA	3519	1/1	0.94	0.13	48,48,48,48	0
59	MG	AD	305	1/1	0.94	0.09	50,50,50,50	0
59	MG	AA	3046	1/1	0.94	0.12	35,35,35,35	0
59	MG	CA	3259	1/1	0.94	0.11	80,80,80,80	0
59	MG	AA	3362	1/1	0.94	0.07	46,46,46,46	0
59	MG	CA	3527	1/1	0.94	0.15	76,76,76,76	0
59	MG	CA	3528	1/1	0.94	0.08	38,38,38,38	0
59	MG	AA	3485	1/1	0.94	0.06	48,48,48,48	0
59	MG	AD	311	1/1	0.94	0.13	37,37,37,37	0
59	MG	AA	3088	1/1	0.94	0.15	39,39,39,39	0
59	MG	AA	3730	1/1	0.94	0.09	75,75,75,75	0
59	MG	CA	3099	1/1	0.94	0.20	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	1784	1/1	0.94	0.08	68,68,68,68	0
59	MG	AA	3731	1/1	0.94	0.10	51,51,51,51	0
59	MG	CA	3281	1/1	0.94	0.07	21,21,21,21	0
59	MG	BA	1787	1/1	0.94	0.12	55,55,55,55	0
59	MG	DA	1651	1/1	0.94	0.10	63,63,63,63	0
59	MG	AA	3161	1/1	0.94	0.06	43,43,43,43	0
59	MG	AA	3733	1/1	0.94	0.08	49,49,49,49	0
59	MG	AA	3162	1/1	0.94	0.22	67,67,67,67	0
59	MG	CA	3544	1/1	0.94	0.10	60,60,60,60	0
59	MG	CA	3109	1/1	0.94	0.06	35,35,35,35	0
59	MG	CA	3110	1/1	0.94	0.11	56,56,56,56	0
59	MG	AA	3370	1/1	0.94	0.08	47,47,47,47	0
59	MG	AA	3164	1/1	0.94	0.21	71,71,71,71	0
59	MG	CA	3549	1/1	0.94	0.11	70,70,70,70	0
59	MG	CA	3550	1/1	0.94	0.07	62,62,62,62	1
59	MG	DA	1664	1/1	0.94	0.05	66,66,66,66	0
59	MG	AA	3090	1/1	0.94	0.12	53,53,53,53	0
59	MG	AA	3497	1/1	0.94	0.08	44,44,44,44	0
59	MG	CA	3554	1/1	0.94	0.08	66,66,66,66	0
59	MG	AA	3743	1/1	0.94	0.15	67,67,67,67	0
59	MG	CA	3299	1/1	0.94	0.07	64,64,64,64	0
59	MG	AQ	201	1/1	0.94	0.11	48,48,48,48	0
59	MG	DA	1671	1/1	0.94	0.21	56,56,56,56	0
59	MG	AQ	202	1/1	0.94	0.14	35,35,35,35	0
59	MG	CA	3310	1/1	0.94	0.08	47,47,47,47	0
59	MG	AA	3196	1/1	0.94	0.16	55,55,55,55	0
59	MG	CA	3561	1/1	0.94	0.08	41,41,41,41	1
59	MG	AA	3114	1/1	0.94	0.09	26,26,26,26	0
59	MG	AA	3381	1/1	0.94	0.07	16,16,16,16	0
59	MG	CA	3121	1/1	0.94	0.06	49,49,49,49	0
59	MG	CA	3569	1/1	0.94	0.08	41,41,41,41	0
59	MG	AA	3385	1/1	0.94	0.10	49,49,49,49	0
59	MG	CA	3331	1/1	0.94	0.12	52,52,52,52	0
59	MG	DA	1688	1/1	0.94	0.12	51,51,51,51	0
59	MG	AV	206	1/1	0.94	0.09	33,33,33,33	0
59	MG	CA	3334	1/1	0.94	0.12	47,47,47,47	0
59	MG	AA	3753	1/1	0.94	0.08	30,30,30,30	0
59	MG	AA	3400	1/1	0.94	0.07	13,13,13,13	0
59	MG	AA	3521	1/1	0.94	0.08	19,19,19,19	0
59	MG	AA	3529	1/1	0.94	0.12	30,30,30,30	0
59	MG	DA	1699	1/1	0.94	0.10	74,74,74,74	0
59	MG	CA	3582	1/1	0.94	0.08	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	3645	1/1	0.94	0.11	58,58,58,58	0
59	MG	AA	3403	1/1	0.94	0.08	42,42,42,42	0
59	MG	CA	3347	1/1	0.94	0.07	45,45,45,45	0
59	MG	BA	1813	1/1	0.94	0.10	55,55,55,55	0
59	MG	BA	1685	1/1	0.94	0.09	50,50,50,50	0
59	MG	DA	1707	1/1	0.94	0.12	61,61,61,61	0
59	MG	BA	1815	1/1	0.94	0.18	53,53,53,53	0
59	MG	AA	3199	1/1	0.94	0.14	41,41,41,41	0
59	MG	A0	103	1/1	0.94	0.07	70,70,70,70	0
59	MG	CA	3360	1/1	0.94	0.09	38,38,38,38	0
59	MG	AA	3650	1/1	0.94	0.08	49,49,49,49	0
59	MG	BA	1692	1/1	0.94	0.18	55,55,55,55	0
59	MG	DA	1716	1/1	0.94	0.05	57,57,57,57	0
59	MG	CA	3142	1/1	0.94	0.17	61,61,61,61	0
59	MG	CA	3599	1/1	0.94	0.07	70,70,70,70	0
59	MG	DA	1719	1/1	0.94	0.17	61,61,61,61	0
59	MG	AA	3039	1/1	0.94	0.20	34,34,34,34	1
59	MG	CA	3602	1/1	0.94	0.09	84,84,84,84	0
59	MG	A5	502	1/1	0.94	0.11	51,51,51,51	0
59	MG	CA	3371	1/1	0.94	0.11	52,52,52,52	0
59	MG	BN	502	1/1	0.94	0.09	87,87,87,87	0
59	MG	CA	3375	1/1	0.94	0.16	68,68,68,68	0
59	MG	AA	3120	1/1	0.94	0.10	33,33,33,33	0
59	MG	DA	1729	1/1	0.94	0.14	49,49,49,49	0
59	MG	CA	3609	1/1	0.94	0.09	52,52,52,52	0
59	MG	AA	3172	1/1	0.94	0.13	47,47,47,47	0
59	MG	CA	3611	1/1	0.94	0.10	59,59,59,59	0
59	MG	AA	3250	1/1	0.94	0.13	123,123,123,123	0
59	MG	CA	3153	1/1	0.94	0.18	73,73,73,73	0
59	MG	CA	3381	1/1	0.94	0.07	50,50,50,50	0
59	MG	AA	3067	1/1	0.94	0.21	61,61,61,61	0
59	MG	AA	3175	1/1	0.94	0.25	63,63,63,63	0
59	MG	AA	3307	1/1	0.94	0.17	61,61,61,61	0
59	MG	AA	3176	1/1	0.94	0.16	70,70,70,70	0
59	MG	CA	3391	1/1	0.94	0.11	51,51,51,51	0
59	MG	CA	3623	1/1	0.94	0.08	64,64,64,64	0
59	MG	CA	3161	1/1	0.94	0.16	57,57,57,57	0
59	MG	AA	3667	1/1	0.94	0.12	41,41,41,41	0
59	MG	AA	3669	1/1	0.94	0.09	81,81,81,81	0
59	MG	CA	3396	1/1	0.94	0.06	39,39,39,39	0
59	MG	CA	3166	1/1	0.94	0.14	27,27,27,27	0
59	MG	CA	3399	1/1	0.94	0.06	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	3559	1/1	0.94	0.09	46,46,46,46	0
59	MG	CA	3012	1/1	0.94	0.10	65,65,65,65	0
59	MG	AA	3562	1/1	0.94	0.06	56,56,56,56	0
59	MG	AA	3785	1/1	0.94	0.10	61,61,61,61	0
59	MG	AA	3256	1/1	0.94	0.09	49,49,49,49	0
59	MG	AA	3444	1/1	0.94	0.12	66,66,66,66	0
59	MG	AA	3445	1/1	0.94	0.07	23,23,23,23	0
59	MG	CA	3642	1/1	0.94	0.20	52,52,52,52	0
59	MG	CA	3183	1/1	0.94	0.08	49,49,49,49	0
59	MG	CA	3417	1/1	0.94	0.10	56,56,56,56	0
59	MG	AA	3059	1/1	0.94	0.19	40,40,40,40	0
59	MG	AA	3321	1/1	0.94	0.11	61,61,61,61	0
59	MG	BA	1613	1/1	0.94	0.06	76,76,76,76	0
59	MG	CA	3426	1/1	0.94	0.14	38,38,38,38	0
59	MG	AA	3211	1/1	0.94	0.11	56,56,56,56	0
59	MG	CA	3430	1/1	0.94	0.17	41,41,41,41	0
59	MG	CA	3655	1/1	0.94	0.22	52,52,52,52	0
59	MG	AA	3584	1/1	0.94	0.07	17,17,17,17	0
59	MG	AA	3686	1/1	0.94	0.12	61,61,61,61	0
59	MG	AA	3145	1/1	0.94	0.11	44,44,44,44	0
59	MG	CA	3434	1/1	0.94	0.09	32,32,32,32	0
59	MG	CA	3196	1/1	0.94	0.32	68,68,68,68	0
59	MG	CA	3198	1/1	0.94	0.11	34,34,34,34	0
59	MG	BA	1722	1/1	0.94	0.14	51,51,51,51	0
59	MG	AA	3590	1/1	0.94	0.08	60,60,60,60	0
59	MG	CA	3036	1/1	0.94	0.16	32,32,32,32	0
59	MG	BA	1725	1/1	0.94	0.07	54,54,54,54	0
59	MG	AA	3690	1/1	0.94	0.10	50,50,50,50	0
59	MG	AA	3078	1/1	0.95	0.24	70,70,70,70	0
59	MG	AA	3060	1/1	0.95	0.12	20,20,20,20	0
59	MG	BW	501	1/1	0.95	0.21	47,47,47,47	0
59	MG	AA	3230	1/1	0.95	0.16	69,69,69,69	0
59	MG	AA	3405	1/1	0.95	0.15	44,44,44,44	0
59	MG	AA	3131	1/1	0.95	0.10	63,63,63,63	0
59	MG	CA	3531	1/1	0.95	0.06	47,47,47,47	0
59	MG	BA	1710	1/1	0.95	0.08	81,81,81,81	0
59	MG	DA	1612	1/1	0.95	0.10	57,57,57,57	0
59	MG	CA	3138	1/1	0.95	0.08	86,86,86,86	0
59	MG	CA	3002	1/1	0.95	0.14	28,28,28,28	0
59	MG	CA	3322	1/1	0.95	0.15	40,40,40,40	0
59	MG	AA	3613	1/1	0.95	0.07	48,48,48,48	0
59	MG	AA	3807	1/1	0.95	0.15	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	3319	1/1	0.95	0.11	58,58,58,58	0
59	MG	CA	3008	1/1	0.95	0.11	46,46,46,46	0
59	MG	CA	3541	1/1	0.95	0.12	63,63,63,63	0
59	MG	CA	3010	1/1	0.95	0.07	43,43,43,43	0
59	MG	AA	3809	1/1	0.95	0.17	57,57,57,57	0
59	MG	AA	3500	1/1	0.95	0.11	59,59,59,59	0
59	MG	CA	3338	1/1	0.95	0.09	64,64,64,64	0
59	MG	CA	3013	1/1	0.95	0.09	42,42,42,42	0
59	MG	AA	3271	1/1	0.95	0.14	34,34,34,34	0
59	MG	CA	3152	1/1	0.95	0.13	64,64,64,64	0
59	MG	AA	3081	1/1	0.95	0.12	56,56,56,56	0
59	MG	CA	3018	1/1	0.95	0.06	41,41,41,41	0
59	MG	AA	3234	1/1	0.95	0.18	36,36,36,36	0
59	MG	AA	3112	1/1	0.95	0.17	61,61,61,61	0
59	MG	CA	3351	1/1	0.95	0.08	46,46,46,46	0
59	MG	CA	3158	1/1	0.95	0.16	54,54,54,54	0
59	MG	AA	3178	1/1	0.95	0.17	48,48,48,48	0
59	MG	CA	3160	1/1	0.95	0.17	57,57,57,57	0
59	MG	CA	3358	1/1	0.95	0.14	36,36,36,36	0
59	MG	AA	3623	1/1	0.95	0.05	28,28,28,28	0
59	MG	CA	3362	1/1	0.95	0.08	43,43,43,43	0
59	MG	CA	3162	1/1	0.95	0.23	31,31,31,31	0
59	MG	AA	3431	1/1	0.95	0.10	25,25,25,25	0
59	MG	BA	1621	1/1	0.95	0.05	51,51,51,51	0
59	MG	AA	3331	1/1	0.95	0.07	15,15,15,15	0
59	MG	AA	3532	1/1	0.95	0.11	20,20,20,20	0
59	MG	AA	3535	1/1	0.95	0.06	48,48,48,48	0
59	MG	AB	3005	1/1	0.95	0.16	44,44,44,44	0
59	MG	CA	3374	1/1	0.95	0.08	60,60,60,60	0
59	MG	AA	3044	1/1	0.95	0.18	52,52,52,52	0
59	MG	AA	3136	1/1	0.95	0.15	63,63,63,63	0
59	MG	CA	3179	1/1	0.95	0.14	60,60,60,60	0
59	MG	AA	3443	1/1	0.95	0.09	33,33,33,33	0
59	MG	AA	3342	1/1	0.95	0.13	51,51,51,51	0
59	MG	BA	1736	1/1	0.95	0.10	67,67,67,67	0
59	MG	AA	3546	1/1	0.95	0.07	60,60,60,60	0
59	MG	AA	3723	1/1	0.95	0.07	49,49,49,49	0
59	MG	CA	3187	1/1	0.95	0.11	37,37,37,37	0
59	MG	AA	3547	1/1	0.95	0.13	60,60,60,60	0
59	MG	AA	3637	1/1	0.95	0.18	17,17,17,17	1
59	MG	AA	3638	1/1	0.95	0.11	71,71,71,71	0
59	MG	BA	1636	1/1	0.95	0.20	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AB	3022	1/1	0.95	0.11	61,61,61,61	0
59	MG	AA	3549	1/1	0.95	0.05	66,66,66,66	0
59	MG	CA	3197	1/1	0.95	0.12	45,45,45,45	0
59	MG	CA	3049	1/1	0.95	0.18	46,46,46,46	0
59	MG	CA	3597	1/1	0.95	0.10	58,58,58,58	0
59	MG	CA	3400	1/1	0.95	0.10	57,57,57,57	0
59	MG	AA	3116	1/1	0.95	0.24	35,35,35,35	0
59	MG	AA	3049	1/1	0.95	0.10	35,35,35,35	0
59	MG	AA	3183	1/1	0.95	0.10	58,58,58,58	0
59	MG	AA	3284	1/1	0.95	0.20	60,60,60,60	0
59	MG	AD	306	1/1	0.95	0.21	41,41,41,41	0
59	MG	DA	1681	1/1	0.95	0.20	70,70,70,70	0
59	MG	AA	3350	1/1	0.95	0.06	36,36,36,36	0
59	MG	CA	3058	1/1	0.95	0.17	67,67,67,67	0
59	MG	CA	3607	1/1	0.95	0.07	64,64,64,64	0
59	MG	DA	1687	1/1	0.95	0.25	56,56,56,56	0
59	MG	AA	3352	1/1	0.95	0.16	47,47,47,47	0
59	MG	AA	3119	1/1	0.95	0.09	47,47,47,47	0
59	MG	CA	3418	1/1	0.95	0.12	34,34,34,34	0
59	MG	AA	3744	1/1	0.95	0.07	34,34,34,34	0
59	MG	CA	3062	1/1	0.95	0.12	38,38,38,38	0
59	MG	CA	3063	1/1	0.95	0.08	34,34,34,34	0
59	MG	AA	3077	1/1	0.95	0.19	43,43,43,43	0
59	MG	CA	3215	1/1	0.95	0.12	54,54,54,54	0
59	MG	CA	3429	1/1	0.95	0.07	59,59,59,59	0
59	MG	AA	3104	1/1	0.95	0.11	54,54,54,54	0
59	MG	AE	304	1/1	0.95	0.07	52,52,52,52	0
59	MG	BA	1653	1/1	0.95	0.13	56,56,56,56	0
59	MG	AA	3748	1/1	0.95	0.07	45,45,45,45	0
59	MG	AA	3570	1/1	0.95	0.06	14,14,14,14	0
59	MG	CA	3071	1/1	0.95	0.07	45,45,45,45	0
59	MG	AF	303	1/1	0.95	0.15	39,39,39,39	0
59	MG	CA	3440	1/1	0.95	0.16	49,49,49,49	0
59	MG	AF	304	1/1	0.95	0.18	41,41,41,41	0
59	MG	AA	3217	1/1	0.95	0.17	29,29,29,29	1
59	MG	CA	3632	1/1	0.95	0.09	74,74,74,74	0
59	MG	AA	3167	1/1	0.95	0.07	45,45,45,45	0
59	MG	CA	3446	1/1	0.95	0.05	33,33,33,33	0
59	MG	AG	201	1/1	0.95	0.07	38,38,38,38	0
59	MG	AA	3656	1/1	0.95	0.18	80,80,80,80	0
59	MG	AA	3576	1/1	0.95	0.08	52,52,52,52	0
59	MG	AA	3658	1/1	0.95	0.08	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AO	5001	1/1	0.95	0.06	34,34,34,34	0
59	MG	CA	3234	1/1	0.95	0.17	50,50,50,50	0
59	MG	CA	3461	1/1	0.95	0.09	34,34,34,34	0
59	MG	CA	3462	1/1	0.95	0.10	63,63,63,63	0
59	MG	AA	3577	1/1	0.95	0.06	42,42,42,42	0
59	MG	BA	1785	1/1	0.95	0.07	62,62,62,62	0
59	MG	AA	3579	1/1	0.95	0.11	54,54,54,54	0
59	MG	CA	3648	1/1	0.95	0.16	52,52,52,52	0
59	MG	CA	3468	1/1	0.95	0.05	53,53,53,53	0
59	MG	AA	3762	1/1	0.95	0.07	23,23,23,23	0
59	MG	AA	3580	1/1	0.95	0.15	54,54,54,54	0
59	MG	AA	3168	1/1	0.95	0.07	47,47,47,47	0
59	MG	CA	3090	1/1	0.95	0.16	77,77,77,77	0
59	MG	AA	3291	1/1	0.95	0.07	45,45,45,45	0
59	MG	AA	3366	1/1	0.95	0.06	35,35,35,35	1
59	MG	AU	201	1/1	0.95	0.10	46,46,46,46	0
59	MG	AA	3673	1/1	0.95	0.07	38,38,38,38	0
59	MG	BA	1674	1/1	0.95	0.19	48,48,48,48	0
59	MG	AV	203	1/1	0.95	0.08	47,47,47,47	0
59	MG	AA	3674	1/1	0.95	0.10	30,30,30,30	0
59	MG	DA	1745	1/1	0.95	0.20	50,50,50,50	0
59	MG	AW	3001	1/1	0.95	0.21	54,54,54,54	0
59	MG	CA	3487	1/1	0.95	0.16	60,60,60,60	0
59	MG	CA	3252	1/1	0.95	0.16	62,62,62,62	0
59	MG	CB	3006	1/1	0.95	0.08	71,71,71,71	0
59	MG	AA	3105	1/1	0.95	0.14	52,52,52,52	0
59	MG	BA	1799	1/1	0.95	0.10	64,64,64,64	0
59	MG	AA	3588	1/1	0.95	0.09	47,47,47,47	0
59	MG	AA	3368	1/1	0.95	0.14	49,49,49,49	0
59	MG	CA	3258	1/1	0.95	0.24	51,51,51,51	0
59	MG	AA	3294	1/1	0.95	0.10	37,37,37,37	0
59	MG	AA	3594	1/1	0.95	0.09	56,56,56,56	0
59	MG	CA	3265	1/1	0.95	0.14	61,61,61,61	0
59	MG	AA	3144	1/1	0.95	0.14	50,50,50,50	0
59	MG	BA	1806	1/1	0.95	0.11	55,55,55,55	0
59	MG	AA	3373	1/1	0.95	0.10	48,48,48,48	0
59	MG	BA	1688	1/1	0.95	0.19	61,61,61,61	0
59	MG	AA	3225	1/1	0.95	0.16	73,73,73,73	0
59	MG	CA	3277	1/1	0.95	0.15	55,55,55,55	0
59	MG	AA	3685	1/1	0.95	0.07	72,72,72,72	0
59	MG	DA	1768	1/1	0.95	0.06	59,59,59,59	0
59	MG	CA	3279	1/1	0.95	0.07	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	3171	1/1	0.95	0.14	54,54,54,54	0
59	MG	AA	3377	1/1	0.95	0.06	20,20,20,20	0
59	MG	AA	3788	1/1	0.95	0.14	61,61,61,61	0
59	MG	AA	3789	1/1	0.95	0.10	44,44,44,44	0
59	MG	CR	201	1/1	0.95	0.06	34,34,34,34	0
59	MG	AA	3790	1/1	0.95	0.23	57,57,57,57	0
59	MG	AA	3302	1/1	0.95	0.09	51,51,51,51	0
59	MG	AA	3689	1/1	0.95	0.05	35,35,35,35	0
59	MG	CA	3290	1/1	0.95	0.15	34,34,34,34	0
59	MG	AA	3605	1/1	0.95	0.17	45,45,45,45	0
59	MG	AA	3306	1/1	0.95	0.12	52,52,52,52	0
59	MG	BA	1701	1/1	0.95	0.07	54,54,54,54	0
62	GDP	BZ	702	28/28	0.95	0.07	57,57,57,57	0
59	MG	AA	3797	1/1	0.95	0.08	52,52,52,52	0
59	MG	CA	3286	1/1	0.96	0.09	58,58,58,58	0
59	MG	BM	201	1/1	0.96	0.04	62,62,62,62	0
59	MG	BA	1702	1/1	0.96	0.15	46,46,46,46	0
59	MG	CA	3505	1/1	0.96	0.05	67,67,67,67	0
59	MG	AA	3197	1/1	0.96	0.08	45,45,45,45	0
59	MG	AA	3472	1/1	0.96	0.08	42,42,42,42	0
59	MG	AA	3799	1/1	0.96	0.10	42,42,42,42	0
59	MG	CW	201	1/1	0.96	0.13	46,46,46,46	0
59	MG	CA	3131	1/1	0.96	0.09	26,26,26,26	0
59	MG	C1	101	1/1	0.96	0.10	57,57,57,57	0
59	MG	AA	3600	1/1	0.96	0.07	25,25,25,25	0
59	MG	AA	3033	1/1	0.96	0.11	55,55,55,55	0
59	MG	C7	101	1/1	0.96	0.10	56,56,56,56	0
59	MG	C8	5001	1/1	0.96	0.11	37,37,37,37	0
59	MG	AA	3079	1/1	0.96	0.07	27,27,27,27	0
59	MG	AA	3201	1/1	0.96	0.11	53,53,53,53	0
59	MG	AA	3047	1/1	0.96	0.04	29,29,29,29	0
59	MG	AA	3034	1/1	0.96	0.12	49,49,49,49	0
59	MG	CA	3004	1/1	0.96	0.15	49,49,49,49	0
59	MG	AA	3483	1/1	0.96	0.07	46,46,46,46	0
59	MG	CA	3312	1/1	0.96	0.09	38,38,38,38	0
59	MG	AA	3696	1/1	0.96	0.08	66,66,66,66	0
59	MG	CA	3144	1/1	0.96	0.13	40,40,40,40	0
59	MG	CA	3522	1/1	0.96	0.10	54,54,54,54	0
59	MG	CA	3315	1/1	0.96	0.09	47,47,47,47	0
59	MG	CA	3316	1/1	0.96	0.09	43,43,43,43	0
59	MG	BA	1715	1/1	0.96	0.07	60,60,60,60	0
59	MG	AA	3372	1/1	0.96	0.12	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	3082	1/1	0.96	0.15	60,60,60,60	0
59	MG	DA	1617	1/1	0.96	0.13	64,64,64,64	0
59	MG	AA	3488	1/1	0.96	0.07	36,36,36,36	0
59	MG	CA	3326	1/1	0.96	0.08	28,28,28,28	0
59	MG	AA	3205	1/1	0.96	0.09	42,42,42,42	0
59	MG	CA	3332	1/1	0.96	0.09	29,29,29,29	0
59	MG	AA	3083	1/1	0.96	0.14	61,61,61,61	0
59	MG	AA	3299	1/1	0.96	0.19	47,47,47,47	0
59	MG	CA	3017	1/1	0.96	0.05	30,30,30,30	0
59	MG	AA	3207	1/1	0.96	0.11	60,60,60,60	0
59	MG	BA	1723	1/1	0.96	0.06	70,70,70,70	0
59	MG	CA	3156	1/1	0.96	0.14	52,52,52,52	0
59	MG	AA	3064	1/1	0.96	0.05	32,32,32,32	0
59	MG	AA	3113	1/1	0.96	0.11	45,45,45,45	0
59	MG	AA	3386	1/1	0.96	0.08	45,45,45,45	0
59	MG	CA	3025	1/1	0.96	0.16	59,59,59,59	0
59	MG	AA	3389	1/1	0.96	0.07	25,25,25,25	0
59	MG	AA	3390	1/1	0.96	0.06	23,23,23,23	0
59	MG	AA	3620	1/1	0.96	0.05	22,22,22,22	0
59	MG	AA	3621	1/1	0.96	0.04	17,17,17,17	0
59	MG	AA	3503	1/1	0.96	0.05	54,54,54,54	0
59	MG	CA	3167	1/1	0.96	0.07	50,50,50,50	0
59	MG	CA	3168	1/1	0.96	0.20	58,58,58,58	0
59	MG	AB	3012	1/1	0.96	0.06	23,23,23,23	1
59	MG	AB	3013	1/1	0.96	0.07	53,53,53,53	0
59	MG	CA	3173	1/1	0.96	0.19	61,61,61,61	0
59	MG	AA	3395	1/1	0.96	0.07	54,54,54,54	0
59	MG	AA	3624	1/1	0.96	0.07	42,42,42,42	0
59	MG	AA	3398	1/1	0.96	0.13	31,31,31,31	0
59	MG	DA	1647	1/1	0.96	0.14	51,51,51,51	0
59	MG	AA	3254	1/1	0.96	0.13	52,52,52,52	0
59	MG	AB	3019	1/1	0.96	0.11	70,70,70,70	0
59	MG	AA	3309	1/1	0.96	0.14	46,46,46,46	0
59	MG	BA	1743	1/1	0.96	0.04	41,41,41,41	0
59	MG	CA	3564	1/1	0.96	0.14	80,80,80,80	0
59	MG	AA	3255	1/1	0.96	0.08	38,38,38,38	0
59	MG	AA	3015	1/1	0.96	0.26	57,57,57,57	0
59	MG	CA	3567	1/1	0.96	0.05	26,26,26,26	0
59	MG	CA	3377	1/1	0.96	0.07	52,52,52,52	0
59	MG	CA	3045	1/1	0.96	0.21	60,60,60,60	0
59	MG	AA	3729	1/1	0.96	0.10	41,41,41,41	0
59	MG	AA	3257	1/1	0.96	0.18	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	3533	1/1	0.96	0.09	22,22,22,22	0
59	MG	AA	3036	1/1	0.96	0.08	25,25,25,25	0
59	MG	CA	3385	1/1	0.96	0.27	61,61,61,61	0
59	MG	CA	3387	1/1	0.96	0.06	50,50,50,50	0
59	MG	AA	3634	1/1	0.96	0.17	76,76,76,76	0
59	MG	AA	3417	1/1	0.96	0.06	25,25,25,25	0
59	MG	CA	3053	1/1	0.96	0.13	32,32,32,32	0
59	MG	BA	1757	1/1	0.96	0.11	43,43,43,43	0
59	MG	AA	3261	1/1	0.96	0.10	25,25,25,25	0
59	MG	AA	3091	1/1	0.96	0.32	47,47,47,47	1
59	MG	DA	1673	1/1	0.96	0.06	82,82,82,82	0
59	MG	BA	1761	1/1	0.96	0.09	62,62,62,62	0
59	MG	AA	3092	1/1	0.96	0.18	39,39,39,39	0
59	MG	AA	3149	1/1	0.96	0.08	51,51,51,51	0
59	MG	CA	3592	1/1	0.96	0.08	64,64,64,64	0
59	MG	BA	1649	1/1	0.96	0.11	35,35,35,35	0
59	MG	BA	1765	1/1	0.96	0.13	54,54,54,54	0
59	MG	CA	3206	1/1	0.96	0.16	44,44,44,44	0
59	MG	DA	1682	1/1	0.96	0.16	52,52,52,52	0
59	MG	CA	3403	1/1	0.96	0.06	70,70,70,70	0
59	MG	CA	3404	1/1	0.96	0.08	65,65,65,65	0
59	MG	CA	3405	1/1	0.96	0.08	55,55,55,55	0
59	MG	DA	1686	1/1	0.96	0.16	56,56,56,56	0
59	MG	BA	1650	1/1	0.96	0.10	55,55,55,55	0
59	MG	AD	312	1/1	0.96	0.18	78,78,78,78	0
59	MG	CA	3601	1/1	0.96	0.05	57,57,57,57	0
59	MG	BA	1768	1/1	0.96	0.08	64,64,64,64	0
59	MG	CA	3410	1/1	0.96	0.08	25,25,25,25	0
59	MG	AA	3023	1/1	0.96	0.17	53,53,53,53	0
59	MG	AA	3094	1/1	0.96	0.26	80,80,80,80	0
59	MG	DA	1696	1/1	0.96	0.12	53,53,53,53	0
59	MG	AA	3334	1/1	0.96	0.08	63,63,63,63	0
59	MG	BA	1773	1/1	0.96	0.07	40,40,40,40	0
59	MG	CA	3416	1/1	0.96	0.07	44,44,44,44	0
59	MG	AA	3154	1/1	0.96	0.08	57,57,57,57	0
59	MG	AA	3442	1/1	0.96	0.09	23,23,23,23	0
59	MG	AA	3750	1/1	0.96	0.15	51,51,51,51	0
59	MG	AA	3338	1/1	0.96	0.06	28,28,28,28	0
59	MG	CA	3613	1/1	0.96	0.10	57,57,57,57	0
59	MG	AA	3648	1/1	0.96	0.07	41,41,41,41	0
59	MG	CA	3422	1/1	0.96	0.10	43,43,43,43	0
59	MG	AA	3155	1/1	0.96	0.18	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	3221	1/1	0.96	0.05	30,30,30,30	0
59	MG	DA	1711	1/1	0.96	0.12	60,60,60,60	0
59	MG	AA	3156	1/1	0.96	0.17	49,49,49,49	0
59	MG	AA	3123	1/1	0.96	0.12	54,54,54,54	0
59	MG	CA	3227	1/1	0.96	0.15	41,41,41,41	0
59	MG	AA	3564	1/1	0.96	0.06	44,44,44,44	0
59	MG	AA	3760	1/1	0.96	0.14	55,55,55,55	0
59	MG	CA	3082	1/1	0.96	0.15	76,76,76,76	0
59	MG	AP	201	1/1	0.96	0.20	72,72,72,72	0
59	MG	DA	1720	1/1	0.96	0.09	60,60,60,60	0
59	MG	AA	3654	1/1	0.96	0.05	67,67,67,67	0
59	MG	CA	3437	1/1	0.96	0.08	64,64,64,64	0
59	MG	DA	1723	1/1	0.96	0.06	53,53,53,53	0
59	MG	AA	3276	1/1	0.96	0.10	67,67,67,67	0
59	MG	AA	3566	1/1	0.96	0.06	56,56,56,56	0
59	MG	AA	3764	1/1	0.96	0.07	73,73,73,73	0
59	MG	AA	3567	1/1	0.96	0.07	26,26,26,26	0
59	MG	CA	3445	1/1	0.96	0.07	22,22,22,22	0
59	MG	AA	3348	1/1	0.96	0.05	53,53,53,53	0
59	MG	AA	3095	1/1	0.96	0.12	75,75,75,75	0
59	MG	CA	3448	1/1	0.96	0.09	37,37,37,37	0
59	MG	AA	3573	1/1	0.96	0.07	12,12,12,12	0
59	MG	CA	3640	1/1	0.96	0.10	43,43,43,43	0
59	MG	AA	3662	1/1	0.96	0.05	60,60,60,60	0
59	MG	AA	3006	1/1	0.96	0.08	52,52,52,52	0
59	MG	BA	1677	1/1	0.96	0.08	28,28,28,28	0
59	MG	CA	3097	1/1	0.96	0.16	66,66,66,66	0
59	MG	AA	3452	1/1	0.96	0.04	14,14,14,14	0
59	MG	AA	3668	1/1	0.96	0.10	54,54,54,54	0
59	MG	CA	3463	1/1	0.96	0.10	56,56,56,56	0
59	MG	AA	3188	1/1	0.96	0.14	31,31,31,31	0
59	MG	CA	3651	1/1	0.96	0.27	76,76,76,76	0
59	MG	AA	3777	1/1	0.96	0.06	41,41,41,41	0
59	MG	CA	3102	1/1	0.96	0.13	62,62,62,62	0
59	MG	DA	1747	1/1	0.96	0.07	48,48,48,48	0
59	MG	CA	3250	1/1	0.96	0.06	38,38,38,38	0
59	MG	CA	3103	1/1	0.96	0.16	53,53,53,53	0
59	MG	CA	3657	1/1	0.96	0.15	41,41,41,41	0
59	MG	AA	3779	1/1	0.96	0.05	22,22,22,22	0
59	MG	CA	3105	1/1	0.96	0.06	39,39,39,39	0
59	MG	CA	3473	1/1	0.96	0.08	51,51,51,51	0
59	MG	AA	3578	1/1	0.96	0.06	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	3671	1/1	0.96	0.11	19,19,19,19	0
59	MG	CA	3664	1/1	0.96	0.10	48,48,48,48	0
59	MG	AA	3672	1/1	0.96	0.06	48,48,48,48	0
59	MG	CA	3479	1/1	0.96	0.08	50,50,50,50	0
59	MG	AA	3030	1/1	0.96	0.20	24,24,24,24	1
59	MG	DA	1760	1/1	0.96	0.07	61,61,61,61	0
59	MG	AA	3129	1/1	0.96	0.07	34,34,34,34	1
59	MG	CA	3260	1/1	0.96	0.07	35,35,35,35	0
59	MG	BA	1809	1/1	0.96	0.08	61,61,61,61	0
59	MG	BA	1690	1/1	0.96	0.16	71,71,71,71	0
59	MG	A0	104	1/1	0.96	0.13	51,51,51,51	0
59	MG	AA	3163	1/1	0.96	0.14	72,72,72,72	0
59	MG	AA	3458	1/1	0.96	0.08	40,40,40,40	0
59	MG	AA	3460	1/1	0.96	0.07	27,27,27,27	0
59	MG	AA	3461	1/1	0.96	0.10	62,62,62,62	0
59	MG	CA	3491	1/1	0.96	0.04	44,44,44,44	0
59	MG	DD	502	1/1	0.96	0.18	50,50,50,50	0
59	MG	CA	3275	1/1	0.96	0.07	61,61,61,61	0
59	MG	CD	303	1/1	0.96	0.08	70,70,70,70	0
59	MG	DF	3001	1/1	0.96	0.10	54,54,54,54	0
59	MG	AA	3359	1/1	0.96	0.06	31,31,31,31	0
59	MG	AA	3233	1/1	0.96	0.14	46,46,46,46	0
59	MG	AA	3058	1/1	0.96	0.03	22,22,22,22	0
59	MG	CA	3496	1/1	0.96	0.10	56,56,56,56	0
59	MG	BF	3001	1/1	0.96	0.06	49,49,49,49	0
59	MG	CF	302	1/1	0.96	0.20	69,69,69,69	0
59	MG	CF	304	1/1	0.96	0.07	65,65,65,65	0
60	ZN	A4	501	1/1	0.96	0.04	117,117,117,117	0
59	MG	AA	3031	1/1	0.96	0.14	63,63,63,63	0
59	MG	A8	5001	1/1	0.96	0.06	30,30,30,30	0
59	MG	AA	3595	1/1	0.96	0.07	42,42,42,42	0
59	MG	AA	3612	1/1	0.97	0.05	68,68,68,68	0
59	MG	CO	5001	1/1	0.97	0.08	50,50,50,50	0
59	MG	CA	3497	1/1	0.97	0.07	45,45,45,45	0
59	MG	AA	3806	1/1	0.97	0.12	42,42,42,42	0
59	MG	CA	3297	1/1	0.97	0.10	36,36,36,36	0
59	MG	CA	3143	1/1	0.97	0.19	41,41,41,41	0
59	MG	AA	3413	1/1	0.97	0.07	25,25,25,25	0
59	MG	CA	3300	1/1	0.97	0.05	47,47,47,47	0
59	MG	CA	3301	1/1	0.97	0.07	60,60,60,60	0
59	MG	CA	3014	1/1	0.97	0.08	50,50,50,50	0
59	MG	CA	3305	1/1	0.97	0.11	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	3115	1/1	0.97	0.09	44,44,44,44	0
59	MG	C0	101	1/1	0.97	0.11	59,59,59,59	0
59	MG	CA	3308	1/1	0.97	0.04	39,39,39,39	0
59	MG	AA	3507	1/1	0.97	0.06	50,50,50,50	0
59	MG	AA	3005	1/1	0.97	0.11	64,64,64,64	0
59	MG	AA	3811	1/1	0.97	0.08	56,56,56,56	0
59	MG	AA	3812	1/1	0.97	0.06	41,41,41,41	0
59	MG	CA	3021	1/1	0.97	0.13	69,69,69,69	0
59	MG	AA	3509	1/1	0.97	0.07	40,40,40,40	0
59	MG	CA	3317	1/1	0.97	0.06	49,49,49,49	0
59	MG	CA	3318	1/1	0.97	0.05	24,24,24,24	0
59	MG	AA	3511	1/1	0.97	0.06	14,14,14,14	0
59	MG	BA	1728	1/1	0.97	0.12	47,47,47,47	0
59	MG	AA	3815	1/1	0.97	0.08	30,30,30,30	0
59	MG	AA	3514	1/1	0.97	0.06	42,42,42,42	0
59	MG	CA	3027	1/1	0.97	0.04	31,31,31,31	0
59	MG	CA	3328	1/1	0.97	0.06	35,35,35,35	0
59	MG	CA	3523	1/1	0.97	0.10	37,37,37,37	0
59	MG	CA	3330	1/1	0.97	0.08	36,36,36,36	0
59	MG	DA	1613	1/1	0.97	0.21	48,48,48,48	0
59	MG	CA	3525	1/1	0.97	0.10	23,23,23,23	0
59	MG	AA	3245	1/1	0.97	0.06	11,11,11,11	0
59	MG	CA	3029	1/1	0.97	0.10	56,56,56,56	0
59	MG	AA	3341	1/1	0.97	0.06	25,25,25,25	0
59	MG	AA	3008	1/1	0.97	0.06	26,26,26,26	0
59	MG	AA	3820	1/1	0.97	0.05	25,25,25,25	0
59	MG	BA	1735	1/1	0.97	0.13	41,41,41,41	0
59	MG	DA	1621	1/1	0.97	0.06	42,42,42,42	0
59	MG	CA	3337	1/1	0.97	0.05	20,20,20,20	0
59	MG	CA	3533	1/1	0.97	0.07	45,45,45,45	0
59	MG	AA	3524	1/1	0.97	0.07	41,41,41,41	0
59	MG	AA	3713	1/1	0.97	0.18	27,27,27,27	0
59	MG	BA	1626	1/1	0.97	0.11	41,41,41,41	0
59	MG	AA	3424	1/1	0.97	0.08	14,14,14,14	0
59	MG	DA	1628	1/1	0.97	0.04	39,39,39,39	0
59	MG	AA	3247	1/1	0.97	0.19	55,55,55,55	0
59	MG	CA	3345	1/1	0.97	0.06	46,46,46,46	0
59	MG	CA	3039	1/1	0.97	0.21	37,37,37,37	0
59	MG	CA	3174	1/1	0.97	0.26	50,50,50,50	0
59	MG	CA	3175	1/1	0.97	0.10	31,31,31,31	0
59	MG	AA	3216	1/1	0.97	0.27	38,38,38,38	0
59	MG	AA	3429	1/1	0.97	0.08	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	CA	3353	1/1	0.97	0.06	45,45,45,45	0
59	MG	AB	3007	1/1	0.97	0.04	39,39,39,39	0
59	MG	CA	3355	1/1	0.97	0.08	35,35,35,35	0
59	MG	BA	1745	1/1	0.97	0.04	46,46,46,46	0
59	MG	AA	3430	1/1	0.97	0.05	39,39,39,39	0
59	MG	CA	3359	1/1	0.97	0.04	33,33,33,33	0
59	MG	CA	3181	1/1	0.97	0.13	40,40,40,40	0
59	MG	CA	3552	1/1	0.97	0.09	30,30,30,30	0
59	MG	CA	3361	1/1	0.97	0.14	43,43,43,43	0
59	MG	AA	3100	1/1	0.97	0.10	29,29,29,29	0
59	MG	AB	3010	1/1	0.97	0.04	62,62,62,62	0
59	MG	CA	3364	1/1	0.97	0.04	22,22,22,22	0
59	MG	BA	1751	1/1	0.97	0.06	48,48,48,48	0
59	MG	CA	3185	1/1	0.97	0.09	48,48,48,48	0
59	MG	AA	3720	1/1	0.97	0.08	55,55,55,55	0
59	MG	AA	3721	1/1	0.97	0.12	40,40,40,40	0
59	MG	CA	3370	1/1	0.97	0.06	41,41,41,41	0
59	MG	AA	3432	1/1	0.97	0.13	42,42,42,42	0
59	MG	AA	3631	1/1	0.97	0.13	46,46,46,46	0
59	MG	AB	3016	1/1	0.97	0.06	34,34,34,34	0
59	MG	CA	3191	1/1	0.97	0.16	46,46,46,46	0
59	MG	CA	3192	1/1	0.97	0.03	45,45,45,45	0
59	MG	AA	3433	1/1	0.97	0.10	37,37,37,37	0
59	MG	CA	3570	1/1	0.97	0.04	36,36,36,36	0
59	MG	AA	3725	1/1	0.97	0.05	13,13,13,13	0
59	MG	CA	3195	1/1	0.97	0.18	47,47,47,47	0
59	MG	AA	3728	1/1	0.97	0.11	29,29,29,29	0
59	MG	AA	3434	1/1	0.97	0.06	17,17,17,17	0
59	MG	AA	3545	1/1	0.97	0.09	43,43,43,43	0
59	MG	AA	3191	1/1	0.97	0.03	16,16,16,16	0
59	MG	CA	3386	1/1	0.97	0.09	50,50,50,50	0
59	MG	CA	3580	1/1	0.97	0.09	76,76,76,76	0
59	MG	AA	3069	1/1	0.97	0.03	28,28,28,28	0
59	MG	AA	3121	1/1	0.97	0.08	53,53,53,53	0
59	MG	AA	3735	1/1	0.97	0.04	25,25,25,25	0
59	MG	CA	3584	1/1	0.97	0.05	32,32,32,32	0
59	MG	AA	3351	1/1	0.97	0.08	29,29,29,29	0
59	MG	CA	3064	1/1	0.97	0.07	48,48,48,48	0
59	MG	AA	3087	1/1	0.97	0.17	55,55,55,55	0
59	MG	AA	3552	1/1	0.97	0.09	63,63,63,63	0
59	MG	AA	3222	1/1	0.97	0.06	4,4,4,4	0
59	MG	DA	1680	1/1	0.97	0.09	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	3741	1/1	0.97	0.05	21,21,21,21	0
59	MG	AA	3146	1/1	0.97	0.05	29,29,29,29	0
59	MG	AA	3557	1/1	0.97	0.08	37,37,37,37	0
59	MG	AA	3021	1/1	0.97	0.07	33,33,33,33	0
59	MG	AA	3745	1/1	0.97	0.09	68,68,68,68	0
59	MG	AA	3358	1/1	0.97	0.04	45,45,45,45	0
59	MG	CA	3074	1/1	0.97	0.05	49,49,49,49	0
59	MG	AA	3009	1/1	0.97	0.04	22,22,22,22	0
59	MG	CA	3218	1/1	0.97	0.27	40,40,40,40	0
59	MG	AA	3360	1/1	0.97	0.09	22,22,22,22	0
59	MG	CA	3220	1/1	0.97	0.05	59,59,59,59	0
59	MG	DA	1693	1/1	0.97	0.06	67,67,67,67	0
59	MG	AF	301	1/1	0.97	0.10	38,38,38,38	0
59	MG	AA	3749	1/1	0.97	0.08	73,73,73,73	0
59	MG	AA	3297	1/1	0.97	0.09	27,27,27,27	0
59	MG	DA	1697	1/1	0.97	0.03	48,48,48,48	0
59	MG	AA	3259	1/1	0.97	0.12	41,41,41,41	1
59	MG	AA	3227	1/1	0.97	0.04	22,22,22,22	0
59	MG	CA	3415	1/1	0.97	0.09	34,34,34,34	0
59	MG	AA	3126	1/1	0.97	0.14	79,79,79,79	0
59	MG	DA	1702	1/1	0.97	0.08	63,63,63,63	0
59	MG	AA	3152	1/1	0.97	0.12	10,10,10,10	0
59	MG	AA	3305	1/1	0.97	0.06	25,25,25,25	0
59	MG	AH	201	1/1	0.97	0.19	64,64,64,64	0
59	MG	AA	3572	1/1	0.97	0.10	17,17,17,17	0
59	MG	AN	3002	1/1	0.97	0.08	69,69,69,69	0
59	MG	AA	3265	1/1	0.97	0.12	43,43,43,43	0
59	MG	CA	3424	1/1	0.97	0.09	66,66,66,66	0
59	MG	CA	3425	1/1	0.97	0.06	50,50,50,50	0
59	MG	AA	3075	1/1	0.97	0.10	49,49,49,49	0
59	MG	DA	1712	1/1	0.97	0.12	53,53,53,53	0
59	MG	CA	3427	1/1	0.97	0.11	37,37,37,37	0
59	MG	CA	3091	1/1	0.97	0.14	69,69,69,69	0
59	MG	AA	3459	1/1	0.97	0.11	53,53,53,53	0
59	MG	AA	3107	1/1	0.97	0.06	49,49,49,49	0
59	MG	AA	3661	1/1	0.97	0.09	41,41,41,41	1
59	MG	AA	3310	1/1	0.97	0.08	56,56,56,56	0
59	MG	AA	3462	1/1	0.97	0.04	54,54,54,54	0
59	MG	CA	3627	1/1	0.97	0.09	60,60,60,60	0
59	MG	AA	3766	1/1	0.97	0.10	54,54,54,54	0
59	MG	CA	3629	1/1	0.97	0.05	55,55,55,55	0
59	MG	AA	3665	1/1	0.97	0.15	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	3666	1/1	0.97	0.14	41,41,41,41	0
59	MG	AA	3268	1/1	0.97	0.10	66,66,66,66	0
59	MG	BA	1804	1/1	0.97	0.06	45,45,45,45	0
59	MG	AA	3062	1/1	0.97	0.10	47,47,47,47	0
59	MG	AA	3042	1/1	0.97	0.09	32,32,32,32	0
59	MG	BA	1686	1/1	0.97	0.12	36,36,36,36	0
59	MG	CA	3248	1/1	0.97	0.10	53,53,53,53	0
59	MG	DA	1731	1/1	0.97	0.07	49,49,49,49	0
59	MG	AV	204	1/1	0.97	0.09	45,45,45,45	0
59	MG	AA	3376	1/1	0.97	0.11	35,35,35,35	0
59	MG	AA	3774	1/1	0.97	0.21	25,25,25,25	1
59	MG	CA	3641	1/1	0.97	0.04	46,46,46,46	0
59	MG	CA	3449	1/1	0.97	0.04	55,55,55,55	0
59	MG	CA	3450	1/1	0.97	0.05	54,54,54,54	0
59	MG	AA	3585	1/1	0.97	0.07	35,35,35,35	0
59	MG	CA	3453	1/1	0.97	0.06	35,35,35,35	0
59	MG	AW	3003	1/1	0.97	0.06	28,28,28,28	0
59	MG	AA	3470	1/1	0.97	0.05	39,39,39,39	0
59	MG	AA	3587	1/1	0.97	0.12	28,28,28,28	0
59	MG	CA	3457	1/1	0.97	0.09	43,43,43,43	0
59	MG	DA	1744	1/1	0.97	0.07	66,66,66,66	0
59	MG	CA	3458	1/1	0.97	0.05	54,54,54,54	0
59	MG	AA	3316	1/1	0.97	0.10	36,36,36,36	0
59	MG	CA	3653	1/1	0.97	0.05	32,32,32,32	0
59	MG	AA	3318	1/1	0.97	0.09	23,23,23,23	0
59	MG	AA	3592	1/1	0.97	0.05	26,26,26,26	0
59	MG	AA	3110	1/1	0.97	0.15	52,52,52,52	0
59	MG	CA	3261	1/1	0.97	0.07	47,47,47,47	0
59	MG	CA	3263	1/1	0.97	0.07	64,64,64,64	0
59	MG	CA	3466	1/1	0.97	0.20	56,56,56,56	0
59	MG	AA	3384	1/1	0.97	0.06	22,22,22,22	0
59	MG	CA	3661	1/1	0.97	0.09	27,27,27,27	0
59	MG	AA	3272	1/1	0.97	0.05	55,55,55,55	0
59	MG	AA	3111	1/1	0.97	0.06	24,24,24,24	0
59	MG	AA	3598	1/1	0.97	0.12	51,51,51,51	0
59	MG	AA	3387	1/1	0.97	0.05	29,29,29,29	0
59	MG	CA	3272	1/1	0.97	0.14	49,49,49,49	0
59	MG	AA	3236	1/1	0.97	0.10	57,57,57,57	0
59	MG	CA	3475	1/1	0.97	0.17	50,50,50,50	0
59	MG	CA	3476	1/1	0.97	0.04	38,38,38,38	0
59	MG	DA	1764	1/1	0.97	0.05	71,71,71,71	0
59	MG	AA	3159	1/1	0.97	0.15	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	3391	1/1	0.97	0.07	19,19,19,19	0
59	MG	CA	3276	1/1	0.97	0.07	44,44,44,44	0
59	MG	CB	3009	1/1	0.97	0.12	67,67,67,67	0
59	MG	BT	3001	1/1	0.97	0.05	46,46,46,46	0
59	MG	AA	3394	1/1	0.97	0.07	39,39,39,39	0
59	MG	AA	3326	1/1	0.97	0.05	36,36,36,36	1
59	MG	AA	3327	1/1	0.97	0.04	31,31,31,31	0
59	MG	BA	1709	1/1	0.97	0.15	50,50,50,50	0
59	MG	A9	502	1/1	0.97	0.12	41,41,41,41	0
59	MG	AA	3043	1/1	0.97	0.15	45,45,45,45	0
59	MG	CD	304	1/1	0.97	0.10	28,28,28,28	0
59	MG	CA	3132	1/1	0.97	0.06	48,48,48,48	0
59	MG	AA	3029	1/1	0.97	0.10	28,28,28,28	0
59	MG	DW	501	1/1	0.97	0.14	44,44,44,44	0
59	MG	CE	303	1/1	0.97	0.17	51,51,51,51	0
59	MG	AA	3045	1/1	0.97	0.11	55,55,55,55	0
59	MG	AA	3408	1/1	0.97	0.11	41,41,41,41	0
59	MG	AA	3336	1/1	0.97	0.08	51,51,51,51	0
59	MG	AA	3697	1/1	0.97	0.07	40,40,40,40	0
60	ZN	BN	501	1/1	0.97	0.04	132,132,132,132	0
59	MG	CF	303	1/1	0.97	0.10	51,51,51,51	0
61	SF4	DD	501	8/8	0.97	0.05	82,82,82,82	1
59	MG	CA	3009	1/1	0.97	0.05	27,27,27,27	0
59	MG	AA	3411	1/1	0.97	0.04	12,12,12,12	0
59	MG	CA	3019	1/1	0.98	0.03	22,22,22,22	0
59	MG	AA	3054	1/1	0.98	0.06	21,21,21,21	0
59	MG	AA	3301	1/1	0.98	0.05	39,39,39,39	0
59	MG	AA	3498	1/1	0.98	0.12	47,47,47,47	0
59	MG	CA	3439	1/1	0.98	0.08	32,32,32,32	0
59	MG	CA	3283	1/1	0.98	0.03	31,31,31,31	0
59	MG	AA	3097	1/1	0.98	0.09	22,22,22,22	0
59	MG	AA	3353	1/1	0.98	0.07	39,39,39,39	0
59	MG	AA	3354	1/1	0.98	0.04	27,27,27,27	0
59	MG	AA	3502	1/1	0.98	0.04	29,29,29,29	1
59	MG	AA	3421	1/1	0.98	0.07	28,28,28,28	0
59	MG	AA	3504	1/1	0.98	0.03	29,29,29,29	0
59	MG	AA	3422	1/1	0.98	0.09	23,23,23,23	0
59	MG	AA	3423	1/1	0.98	0.10	16,16,16,16	0
59	MG	CA	3292	1/1	0.98	0.03	12,12,12,12	0
59	MG	DA	1648	1/1	0.98	0.10	40,40,40,40	0
59	MG	BA	1740	1/1	0.98	0.10	50,50,50,50	0
59	MG	CA	3452	1/1	0.98	0.05	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	3303	1/1	0.98	0.06	24,24,24,24	0
59	MG	AA	3510	1/1	0.98	0.05	17,17,17,17	0
59	MG	DA	1653	1/1	0.98	0.18	55,55,55,55	0
59	MG	AA	3304	1/1	0.98	0.06	47,47,47,47	0
59	MG	AA	3512	1/1	0.98	0.05	38,38,38,38	0
59	MG	AA	3426	1/1	0.98	0.07	20,20,20,20	0
59	MG	DA	1657	1/1	0.98	0.04	23,23,23,23	0
59	MG	AB	3011	1/1	0.98	0.05	29,29,29,29	0
59	MG	CA	3459	1/1	0.98	0.04	28,28,28,28	0
59	MG	AA	3515	1/1	0.98	0.07	12,12,12,12	0
59	MG	AA	3137	1/1	0.98	0.25	53,53,53,53	0
59	MG	CA	3302	1/1	0.98	0.06	37,37,37,37	0
59	MG	CA	3303	1/1	0.98	0.09	43,43,43,43	0
59	MG	CA	3617	1/1	0.98	0.07	41,41,41,41	0
59	MG	CA	3618	1/1	0.98	0.14	40,40,40,40	0
59	MG	BA	1750	1/1	0.98	0.05	55,55,55,55	0
59	MG	AA	3428	1/1	0.98	0.04	18,18,18,18	0
59	MG	CA	3306	1/1	0.98	0.04	24,24,24,24	0
59	MG	AA	3013	1/1	0.98	0.05	28,28,28,28	0
59	MG	CA	3169	1/1	0.98	0.10	34,34,34,34	0
59	MG	CA	3309	1/1	0.98	0.10	22,22,22,22	0
59	MG	CA	3170	1/1	0.98	0.04	32,32,32,32	0
59	MG	CA	3471	1/1	0.98	0.10	33,33,33,33	0
59	MG	BA	1753	1/1	0.98	0.06	48,48,48,48	0
59	MG	AA	3522	1/1	0.98	0.06	30,30,30,30	0
59	MG	AA	3523	1/1	0.98	0.03	13,13,13,13	0
59	MG	AA	3117	1/1	0.98	0.20	25,25,25,25	1
59	MG	AA	3525	1/1	0.98	0.07	35,35,35,35	0
59	MG	AA	3527	1/1	0.98	0.06	27,27,27,27	0
59	MG	AA	3528	1/1	0.98	0.06	19,19,19,19	0
59	MG	BA	1760	1/1	0.98	0.07	53,53,53,53	0
59	MG	CA	3320	1/1	0.98	0.06	36,36,36,36	0
59	MG	AA	3308	1/1	0.98	0.09	18,18,18,18	0
59	MG	CA	3482	1/1	0.98	0.09	61,61,61,61	0
59	MG	CA	3052	1/1	0.98	0.09	44,44,44,44	0
59	MG	CA	3324	1/1	0.98	0.05	26,26,26,26	0
59	MG	AA	3037	1/1	0.98	0.04	4,4,4,4	0
59	MG	AA	3734	1/1	0.98	0.09	26,26,26,26	0
59	MG	CA	3327	1/1	0.98	0.05	38,38,38,38	0
59	MG	AA	3531	1/1	0.98	0.06	24,24,24,24	0
59	MG	AA	3020	1/1	0.98	0.04	11,11,11,11	0
59	MG	AD	304	1/1	0.98	0.05	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	3311	1/1	0.98	0.06	2,2,2,2	0
59	MG	AA	3534	1/1	0.98	0.10	14,14,14,14	0
59	MG	AA	3364	1/1	0.98	0.08	23,23,23,23	0
59	MG	AA	3437	1/1	0.98	0.05	17,17,17,17	0
59	MG	AA	3537	1/1	0.98	0.10	20,20,20,20	0
59	MG	AD	310	1/1	0.98	0.08	46,46,46,46	0
59	MG	AA	3539	1/1	0.98	0.10	34,34,34,34	0
59	MG	AA	3439	1/1	0.98	0.08	37,37,37,37	0
59	MG	AA	3243	1/1	0.98	0.10	43,43,43,43	0
59	MG	BA	1777	1/1	0.98	0.12	71,71,71,71	0
59	MG	AA	3639	1/1	0.98	0.07	18,18,18,18	0
59	MG	AA	3543	1/1	0.98	0.06	32,32,32,32	0
59	MG	AA	3084	1/1	0.98	0.07	23,23,23,23	0
59	MG	AA	3085	1/1	0.98	0.11	46,46,46,46	0
59	MG	CA	3349	1/1	0.98	0.07	23,23,23,23	0
59	MG	AA	3190	1/1	0.98	0.03	24,24,24,24	0
59	MG	AA	3369	1/1	0.98	0.04	47,47,47,47	0
59	MG	AA	3548	1/1	0.98	0.04	7,7,7,7	0
59	MG	AA	3317	1/1	0.98	0.07	24,24,24,24	0
59	MG	AA	3647	1/1	0.98	0.04	43,43,43,43	0
59	MG	AA	3032	1/1	0.98	0.11	59,59,59,59	0
59	MG	CA	3512	1/1	0.98	0.07	53,53,53,53	0
59	MG	AA	3279	1/1	0.98	0.09	34,34,34,34	0
59	MG	AA	3757	1/1	0.98	0.03	14,14,14,14	0
59	MG	AA	3192	1/1	0.98	0.05	30,30,30,30	0
59	MG	AA	3759	1/1	0.98	0.05	57,57,57,57	0
59	MG	AA	3553	1/1	0.98	0.04	43,43,43,43	0
59	MG	AA	3554	1/1	0.98	0.08	40,40,40,40	0
59	MG	AA	3048	1/1	0.98	0.04	28,28,28,28	0
59	MG	CA	3085	1/1	0.98	0.07	25,25,25,25	0
59	MG	AP	202	1/1	0.98	0.21	21,21,21,21	1
59	MG	AA	3071	1/1	0.98	0.13	40,40,40,40	0
59	MG	AA	3147	1/1	0.98	0.21	40,40,40,40	1
59	MG	AA	3223	1/1	0.98	0.04	15,15,15,15	0
59	MG	CA	3369	1/1	0.98	0.07	48,48,48,48	0
59	MG	AA	3089	1/1	0.98	0.10	49,49,49,49	0
59	MG	BA	1680	1/1	0.98	0.09	40,40,40,40	0
59	MG	AA	3560	1/1	0.98	0.05	29,29,29,29	0
59	MG	AA	3561	1/1	0.98	0.06	21,21,21,21	0
59	MG	AA	3379	1/1	0.98	0.11	23,23,23,23	0
59	MG	AA	3770	1/1	0.98	0.07	43,43,43,43	0
59	MG	AU	202	1/1	0.98	0.06	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AU	203	1/1	0.98	0.12	25,25,25,25	0
59	MG	AA	3380	1/1	0.98	0.04	18,18,18,18	0
59	MG	AV	202	1/1	0.98	0.07	38,38,38,38	0
59	MG	AA	3072	1/1	0.98	0.03	19,19,19,19	0
59	MG	AA	3382	1/1	0.98	0.05	37,37,37,37	0
59	MG	AA	3383	1/1	0.98	0.05	20,20,20,20	0
59	MG	AA	3330	1/1	0.98	0.05	66,66,66,66	0
59	MG	AA	3568	1/1	0.98	0.04	15,15,15,15	0
59	MG	AA	3173	1/1	0.98	0.08	46,46,46,46	0
59	MG	AA	3333	1/1	0.98	0.06	11,11,11,11	0
59	MG	AA	3004	1/1	0.98	0.09	21,21,21,21	0
59	MG	AA	3200	1/1	0.98	0.14	30,30,30,30	0
59	MG	AA	3574	1/1	0.98	0.05	12,12,12,12	0
59	MG	CV	202	1/1	0.98	0.08	38,38,38,38	0
59	MG	AA	3007	1/1	0.98	0.03	12,12,12,12	0
59	MG	AA	3260	1/1	0.98	0.07	21,21,21,21	0
59	MG	AA	3469	1/1	0.98	0.03	32,32,32,32	0
59	MG	CA	3397	1/1	0.98	0.08	57,57,57,57	0
59	MG	AA	3392	1/1	0.98	0.07	17,17,17,17	0
59	MG	AA	3292	1/1	0.98	0.07	24,24,24,24	0
59	MG	AA	3340	1/1	0.98	0.04	3,3,3,3	0
59	MG	AA	3581	1/1	0.98	0.07	52,52,52,52	0
59	MG	AA	3681	1/1	0.98	0.04	42,42,42,42	0
59	MG	AA	3130	1/1	0.98	0.07	34,34,34,34	0
59	MG	A7	101	1/1	0.98	0.08	47,47,47,47	0
59	MG	AA	3399	1/1	0.98	0.03	16,16,16,16	0
59	MG	CA	3407	1/1	0.98	0.07	36,36,36,36	0
59	MG	AA	3795	1/1	0.98	0.12	22,22,22,22	0
59	MG	AA	3262	1/1	0.98	0.03	15,15,15,15	0
59	MG	CA	3123	1/1	0.98	0.04	29,29,29,29	0
59	MG	AA	3295	1/1	0.98	0.07	57,57,57,57	0
59	MG	CA	3255	1/1	0.98	0.08	28,28,28,28	0
59	MG	AA	3345	1/1	0.98	0.06	6,6,6,6	0
59	MG	AA	3406	1/1	0.98	0.04	20,20,20,20	0
59	MG	AA	3484	1/1	0.98	0.07	53,53,53,53	0
59	MG	CA	3568	1/1	0.98	0.04	39,39,39,39	0
59	MG	AA	3589	1/1	0.98	0.04	55,55,55,55	0
59	MG	CA	3006	1/1	0.98	0.03	22,22,22,22	0
59	MG	AA	3407	1/1	0.98	0.05	10,10,10,10	0
59	MG	AA	3691	1/1	0.98	0.05	62,62,62,62	0
59	MG	AA	3591	1/1	0.98	0.11	52,52,52,52	0
59	MG	AA	3024	1/1	0.98	0.13	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	CA	3267	1/1	0.98	0.04	38,38,38,38	0
59	MG	AA	3132	1/1	0.98	0.07	41,41,41,41	0
59	MG	AA	3410	1/1	0.98	0.10	57,57,57,57	0
59	MG	CA	3136	1/1	0.98	0.03	63,63,63,63	0
59	MG	CA	3271	1/1	0.98	0.07	48,48,48,48	0
59	MG	AA	3491	1/1	0.98	0.04	46,46,46,46	0
59	MG	AA	3052	1/1	0.98	0.07	11,11,11,11	0
59	MG	AA	3597	1/1	0.98	0.04	33,33,33,33	0
59	MG	AA	3412	1/1	0.98	0.10	39,39,39,39	0
60	ZN	DN	501	1/1	0.98	0.04	117,117,117,117	0
61	SF4	BD	501	8/8	0.98	0.04	78,78,78,78	0
59	MG	AA	3494	1/1	0.98	0.06	34,34,34,34	0
59	MG	AA	3053	1/1	0.98	0.11	19,19,19,19	0
59	MG	CA	3588	1/1	0.98	0.04	32,32,32,32	0
59	MG	CA	3321	1/1	0.99	0.06	28,28,28,28	0
59	MG	CA	3562	1/1	0.99	0.03	29,29,29,29	0
59	MG	AA	3519	1/1	0.99	0.12	27,27,27,27	0
59	MG	CA	3401	1/1	0.99	0.04	28,28,28,28	0
59	MG	AA	3343	1/1	0.99	0.06	46,46,46,46	0
59	MG	CA	3650	1/1	0.99	0.07	14,14,14,14	0
59	MG	AA	3312	1/1	0.99	0.02	23,23,23,23	0
59	MG	AA	3074	1/1	0.99	0.06	14,14,14,14	0
59	MG	AA	3702	1/1	0.99	0.10	14,14,14,14	0
59	MG	AA	3482	1/1	0.99	0.03	41,41,41,41	0
59	MG	AF	305	1/1	0.99	0.07	19,19,19,19	0
59	MG	CA	3329	1/1	0.99	0.04	21,21,21,21	0
59	MG	AF	306	1/1	0.99	0.06	36,36,36,36	0
59	MG	AA	3401	1/1	0.99	0.04	21,21,21,21	0
59	MG	CA	3574	1/1	0.99	0.04	37,37,37,37	0
59	MG	CA	3262	1/1	0.99	0.03	11,11,11,11	0
59	MG	AA	3402	1/1	0.99	0.04	27,27,27,27	0
59	MG	AA	3526	1/1	0.99	0.11	19,19,19,19	0
59	MG	CA	3578	1/1	0.99	0.05	38,38,38,38	0
59	MG	AA	3707	1/1	0.99	0.03	59,59,59,59	0
59	MG	CA	3266	1/1	0.99	0.07	36,36,36,36	0
59	MG	AA	3328	1/1	0.99	0.05	42,42,42,42	0
59	MG	AA	3404	1/1	0.99	0.08	27,27,27,27	0
59	MG	AA	3487	1/1	0.99	0.03	49,49,49,49	0
59	MG	AA	3663	1/1	0.99	0.05	11,11,11,11	0
59	MG	CA	3342	1/1	0.99	0.03	33,33,33,33	0
59	MG	AA	3125	1/1	0.99	0.06	22,22,22,22	1
59	MG	AA	3489	1/1	0.99	0.04	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	CA	3423	1/1	0.99	0.10	46,46,46,46	0
59	MG	AA	3248	1/1	0.99	0.07	22,22,22,22	0
59	MG	CA	3346	1/1	0.99	0.06	30,30,30,30	0
59	MG	AA	3821	1/1	0.99	0.09	82,82,82,82	0
59	MG	AA	3038	1/1	0.99	0.15	29,29,29,29	1
59	MG	AA	3457	1/1	0.99	0.04	30,30,30,30	0
59	MG	CA	3211	1/1	0.99	0.04	29,29,29,29	0
59	MG	AA	3332	1/1	0.99	0.04	17,17,17,17	0
59	MG	AA	3239	1/1	0.99	0.13	25,25,25,25	1
59	MG	CA	3214	1/1	0.99	0.07	22,22,22,22	0
59	MG	CA	3151	1/1	0.99	0.03	38,38,38,38	0
59	MG	CA	3282	1/1	0.99	0.05	36,36,36,36	0
59	MG	CA	3356	1/1	0.99	0.07	44,44,44,44	0
59	MG	AA	3003	1/1	0.99	0.02	8,8,8,8	0
59	MG	AA	3538	1/1	0.99	0.05	15,15,15,15	0
59	MG	CA	3438	1/1	0.99	0.04	24,24,24,24	0
59	MG	AA	3103	1/1	0.99	0.02	5,5,5,5	0
59	MG	AA	3540	1/1	0.99	0.03	36,36,36,36	0
59	MG	BA	1746	1/1	0.99	0.04	33,33,33,33	0
59	MG	AA	3436	1/1	0.99	0.03	12,12,12,12	0
59	MG	CA	3443	1/1	0.99	0.04	28,28,28,28	0
59	MG	AA	3463	1/1	0.99	0.03	15,15,15,15	0
59	MG	AA	3388	1/1	0.99	0.02	28,28,28,28	0
59	MG	AA	3726	1/1	0.99	0.06	12,12,12,12	0
59	MG	AA	3778	1/1	0.99	0.04	43,43,43,43	0
59	MG	AV	205	1/1	0.99	0.04	42,42,42,42	0
59	MG	CA	3163	1/1	0.99	0.13	30,30,30,30	0
59	MG	AA	3727	1/1	0.99	0.03	23,23,23,23	0
59	MG	AA	3465	1/1	0.99	0.06	42,42,42,42	0
59	MG	AA	3679	1/1	0.99	0.04	36,36,36,36	0
59	MG	CA	3372	1/1	0.99	0.08	35,35,35,35	0
59	MG	AA	3438	1/1	0.99	0.06	17,17,17,17	0
59	MG	AA	3320	1/1	0.99	0.08	37,37,37,37	0
59	MG	AA	3784	1/1	0.99	0.07	59,59,59,59	0
59	MG	AA	3214	1/1	0.99	0.22	58,58,58,58	1
59	MG	AA	3011	1/1	0.99	0.04	16,16,16,16	0
59	MG	AA	3505	1/1	0.99	0.04	30,30,30,30	0
59	MG	AA	3506	1/1	0.99	0.03	48,48,48,48	0
59	MG	AA	3151	1/1	0.99	0.07	62,62,62,62	0
59	MG	AA	3393	1/1	0.99	0.07	23,23,23,23	0
59	MG	CA	3382	1/1	0.99	0.07	38,38,38,38	0
59	MG	CA	3383	1/1	0.99	0.05	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	3738	1/1	0.99	0.07	24,24,24,24	0
59	MG	DA	1691	1/1	0.99	0.06	63,63,63,63	0
59	MG	AA	3419	1/1	0.99	0.06	20,20,20,20	0
59	MG	AA	3793	1/1	0.99	0.07	7,7,7,7	0
59	MG	AA	3324	1/1	0.99	0.02	15,15,15,15	0
59	MG	CA	3311	1/1	0.99	0.05	50,50,50,50	0
59	MG	BA	1769	1/1	0.99	0.05	58,58,58,58	0
59	MG	AA	3022	1/1	0.99	0.02	5,5,5,5	0
59	MG	AA	3475	1/1	0.99	0.08	45,45,45,45	0
59	MG	AA	3513	1/1	0.99	0.03	41,41,41,41	0
60	ZN	CY	501	1/1	0.99	0.03	101,101,101,101	0
59	MG	CA	3393	1/1	0.99	0.05	68,68,68,68	0
60	ZN	C5	102	1/1	0.99	0.04	66,66,66,66	0
60	ZN	C6	501	1/1	0.99	0.03	66,66,66,66	0
60	ZN	C9	501	1/1	0.99	0.03	75,75,75,75	0
59	MG	AA	3476	1/1	0.99	0.03	28,28,28,28	0
59	MG	AA	3477	1/1	0.99	0.03	14,14,14,14	0
59	MG	AA	3478	1/1	0.99	0.04	33,33,33,33	0
59	MG	AA	3517	1/1	0.99	0.03	23,23,23,23	0
59	MG	AA	3518	1/1	0.99	0.04	14,14,14,14	0
60	ZN	A6	102	1/1	1.00	0.03	40,40,40,40	0
60	ZN	A9	501	1/1	1.00	0.02	42,42,42,42	0
59	MG	AA	3397	1/1	1.00	0.05	13,13,13,13	0
59	MG	AA	3569	1/1	1.00	0.04	17,17,17,17	0
59	MG	CA	3339	1/1	1.00	0.03	24,24,24,24	0
59	MG	AA	3076	1/1	1.00	0.03	0,0,0,0	0
59	MG	AA	3335	1/1	1.00	0.08	15,15,15,15	0
59	MG	AA	3416	1/1	1.00	0.03	14,14,14,14	0
59	MG	AA	3801	1/1	1.00	0.05	27,27,27,27	0
59	MG	AA	3396	1/1	1.00	0.06	16,16,16,16	0
60	ZN	AY	501	1/1	1.00	0.01	61,61,61,61	0
59	MG	AE	303	1/1	1.00	0.09	19,19,19,19	0
60	ZN	A5	501	1/1	1.00	0.01	30,30,30,30	0

6.5 Other polymers ⓘ

There are no such residues in this entry.