



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 3, 2026 – 08:02 AM EDT

PDB ID : 4WQY / pdb_00004wqy
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with elongation factor G in the post-translocational state (without fusitic acid)
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

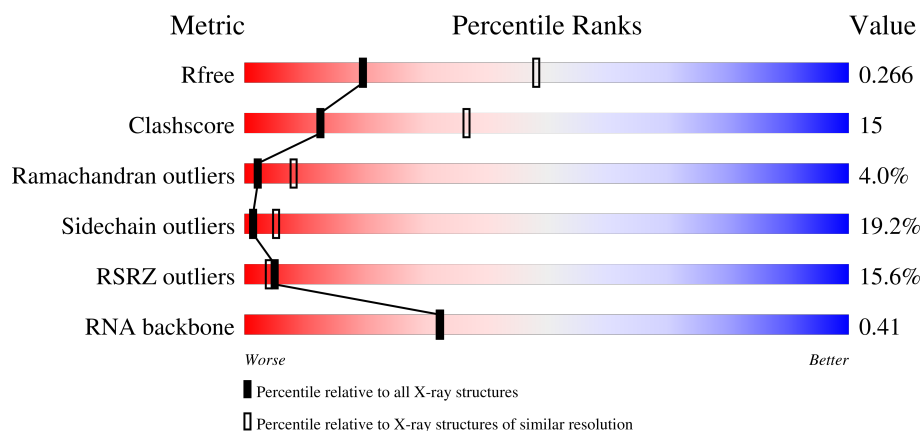
1 Overall quality at a glance

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	4% 47% 41% 9% ..
1	CA	2915	7% 45% 43% 9% .
2	AB	121	% 52% 40% 7% .
2	CB	121	4% 45% 48% 7% .

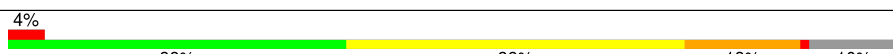
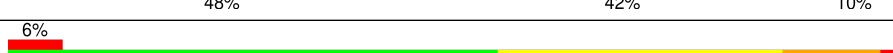
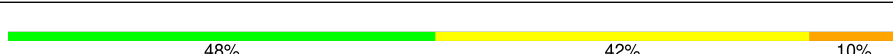
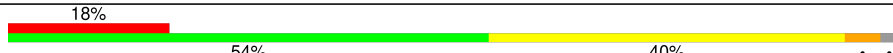
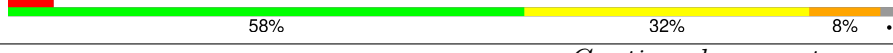
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Mol	Chain	Length	Quality of chain
3	AC	228	
3	CC	228	
4	AD	276	
4	CD	276	
5	AE	206	
5	CE	206	
6	AF	210	
6	CF	210	
7	AG	182	
7	CG	182	
8	AH	180	
8	CH	180	
9	AK	173	
9	CK	173	
10	AL	147	
10	CL	147	
11	AN	140	
11	CN	140	
12	AO	122	
12	CO	122	
13	AP	150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

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

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

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

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Mol	Chain	Length	Quality of chain
53	BT	106	
53	DT	106	
54	BU	27	
54	DU	27	
55	BV	24	
55	DV	24	
56	BX	77	
56	DX	77	
57	BZ	758	
57	DZ	758	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	CA	3071	-	-	-	X

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 305548 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	2852	Total	C	N	O	P	0	0	0
			61426	27339	11489	19747	2851			
1	CA	2848	Total	C	N	O	P	0	0	0
			61337	27299	11470	19721	2847			

- 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	139	Total	C	N	O	S	0	0	0
			1025	653	181	186	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CL	139	Total	C	N	O	S	0	0	0
			1025	653	181	186	5			

- 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	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
24	C0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BA	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	122	Total	C	N	O	S	0	0	0
			950	586	197	165	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 55 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BV	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
55	DV	6	Total	C	N	O	P	0	0	0
			128	59	27	37	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BX	76	Total	C	N	O	P	0	0	0
			1625	725	294	529	76			
56	DX	76	Total	C	N	O	P	0	0	0
			1621	723	292	529	76			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BZ	730	Total	C	N	O	S	0	0	0
			4869	3031	886	942	10			
57	DZ	730	Total	C	N	O	S	0	0	0
			4867	3029	886	942	10			

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AA	820	Total	Mg	0	0
			820	820		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AB	23	Total 23	Mg 23	0	0
58	AD	12	Total 12	Mg 12	0	0
58	AE	5	Total 5	Mg 5	0	0
58	AF	8	Total 8	Mg 8	0	0
58	AG	2	Total 2	Mg 2	0	0
58	AH	2	Total 2	Mg 2	0	0
58	AN	3	Total 3	Mg 3	0	0
58	AO	1	Total 1	Mg 1	0	0
58	AP	3	Total 3	Mg 3	0	0
58	AQ	3	Total 3	Mg 3	0	0
58	AR	2	Total 2	Mg 2	0	0
58	AU	3	Total 3	Mg 3	0	0
58	AV	5	Total 5	Mg 5	0	0
58	AW	4	Total 4	Mg 4	0	0
58	AX	1	Total 1	Mg 1	0	0
58	AZ	2	Total 2	Mg 2	0	0
58	A0	5	Total 5	Mg 5	0	0
58	A1	1	Total 1	Mg 1	0	0
58	A2	1	Total 1	Mg 1	0	0
58	A4	1	Total 1	Mg 1	0	0
58	A5	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	A6	1	Total 1	Mg 1	0	0
58	A7	5	Total 5	Mg 5	0	0
58	A8	2	Total 2	Mg 2	0	0
58	A9	1	Total 1	Mg 1	0	0
58	BA	212	Total 212	Mg 212	0	0
58	BB	1	Total 1	Mg 1	0	0
58	BD	1	Total 1	Mg 1	0	0
58	BE	1	Total 1	Mg 1	0	0
58	BF	1	Total 1	Mg 1	0	0
58	BK	1	Total 1	Mg 1	0	0
58	BL	4	Total 4	Mg 4	0	0
58	BN	2	Total 2	Mg 2	0	0
58	BT	1	Total 1	Mg 1	0	0
58	BV	1	Total 1	Mg 1	0	0
58	BX	10	Total 10	Mg 10	0	0
58	BZ	1	Total 1	Mg 1	0	0
58	CA	666	Total 666	Mg 666	0	0
58	CB	13	Total 13	Mg 13	0	0
58	CD	3	Total 3	Mg 3	0	0
58	CE	7	Total 7	Mg 7	0	0
58	CF	4	Total 4	Mg 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	CG	1	Total 1	Mg 1	0	0
58	CN	1	Total 1	Mg 1	0	0
58	CO	2	Total 2	Mg 2	0	0
58	CQ	4	Total 4	Mg 4	0	0
58	CR	1	Total 1	Mg 1	0	0
58	CU	2	Total 2	Mg 2	0	0
58	CV	2	Total 2	Mg 2	0	0
58	CY	1	Total 1	Mg 1	0	0
58	C0	1	Total 1	Mg 1	0	0
58	C1	1	Total 1	Mg 1	0	0
58	C3	1	Total 1	Mg 1	0	0
58	C7	1	Total 1	Mg 1	0	0
58	C8	1	Total 1	Mg 1	0	0
58	DA	166	Total 166	Mg 166	0	0
58	DD	1	Total 1	Mg 1	0	0
58	DE	2	Total 2	Mg 2	0	0
58	DF	1	Total 1	Mg 1	0	0
58	DJ	1	Total 1	Mg 1	0	0
58	DK	1	Total 1	Mg 1	0	0
58	DL	2	Total 2	Mg 2	0	0
58	DT	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	DZ	3	Total	Mg	0	0
			3	3		

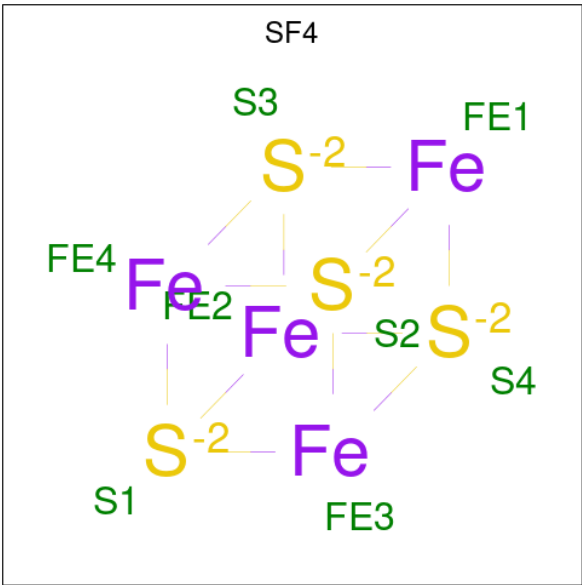
- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

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

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

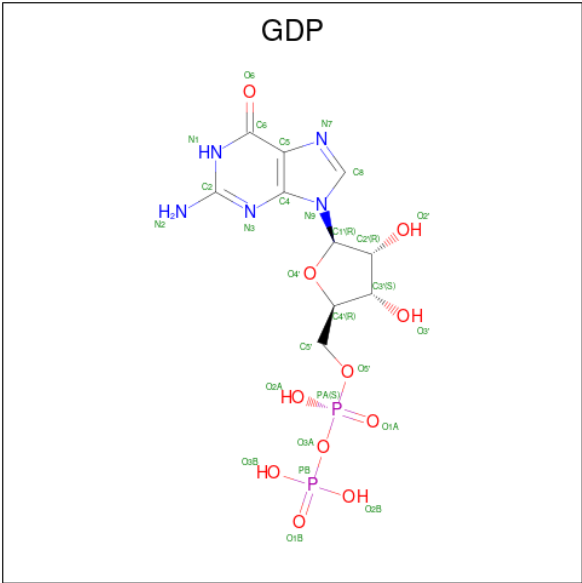
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AY	1	Total	Zn	0	0
			1	1		
60	A4	1	Total	Zn	0	0
			1	1		
60	A5	1	Total	Zn	0	0
			1	1		
60	A6	1	Total	Zn	0	0
			1	1		
60	A9	1	Total	Zn	0	0
			1	1		
60	BN	1	Total	Zn	0	0
			1	1		
60	CY	1	Total	Zn	0	0
			1	1		
60	C4	1	Total	Zn	0	0
			1	1		
60	C5	1	Total	Zn	0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

- Molecule 61 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 63 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	AA	1406	Total 1406	O 1406	0	0
63	AB	37	Total 37	O 37	0	0
63	AD	16	Total 16	O 16	0	0
63	AE	14	Total 14	O 14	0	0
63	AF	6	Total 6	O 6	0	0
63	AG	3	Total 3	O 3	0	0
63	AH	1	Total 1	O 1	0	0
63	AN	3	Total 3	O 3	0	0
63	AO	1	Total 1	O 1	0	0
63	AP	18	Total 18	O 18	0	0
63	AQ	5	Total 5	O 5	0	0
63	AR	2	Total 2	O 2	0	0
63	AS	1	Total 1	O 1	0	0
63	AT	3	Total 3	O 3	0	0
63	AU	4	Total 4	O 4	0	0
63	AV	1	Total 1	O 1	0	0
63	AW	1	Total 1	O 1	0	0
63	AX	4	Total 4	O 4	0	0
63	AZ	1	Total 1	O 1	0	0
63	A0	9	Total 9	O 9	0	0
63	A1	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	A2	1	Total 1	O 1	0	0
63	A3	2	Total 2	O 2	0	0
63	A5	4	Total 4	O 4	0	0
63	A7	4	Total 4	O 4	0	0
63	A8	9	Total 9	O 9	0	0
63	A9	1	Total 1	O 1	0	0
63	BA	203	Total 203	O 203	0	0
63	BD	3	Total 3	O 3	0	0
63	BE	2	Total 2	O 2	0	0
63	BG	1	Total 1	O 1	0	0
63	BJ	1	Total 1	O 1	0	0
63	BL	1	Total 1	O 1	0	0
63	BM	1	Total 1	O 1	0	0
63	BO	2	Total 2	O 2	0	0
63	BP	1	Total 1	O 1	0	0
63	BV	3	Total 3	O 3	0	0
63	BX	5	Total 5	O 5	0	0
63	BZ	2	Total 2	O 2	0	0
63	CA	974	Total 974	O 974	0	0
63	CB	9	Total 9	O 9	0	0
63	CD	17	Total 17	O 17	0	0

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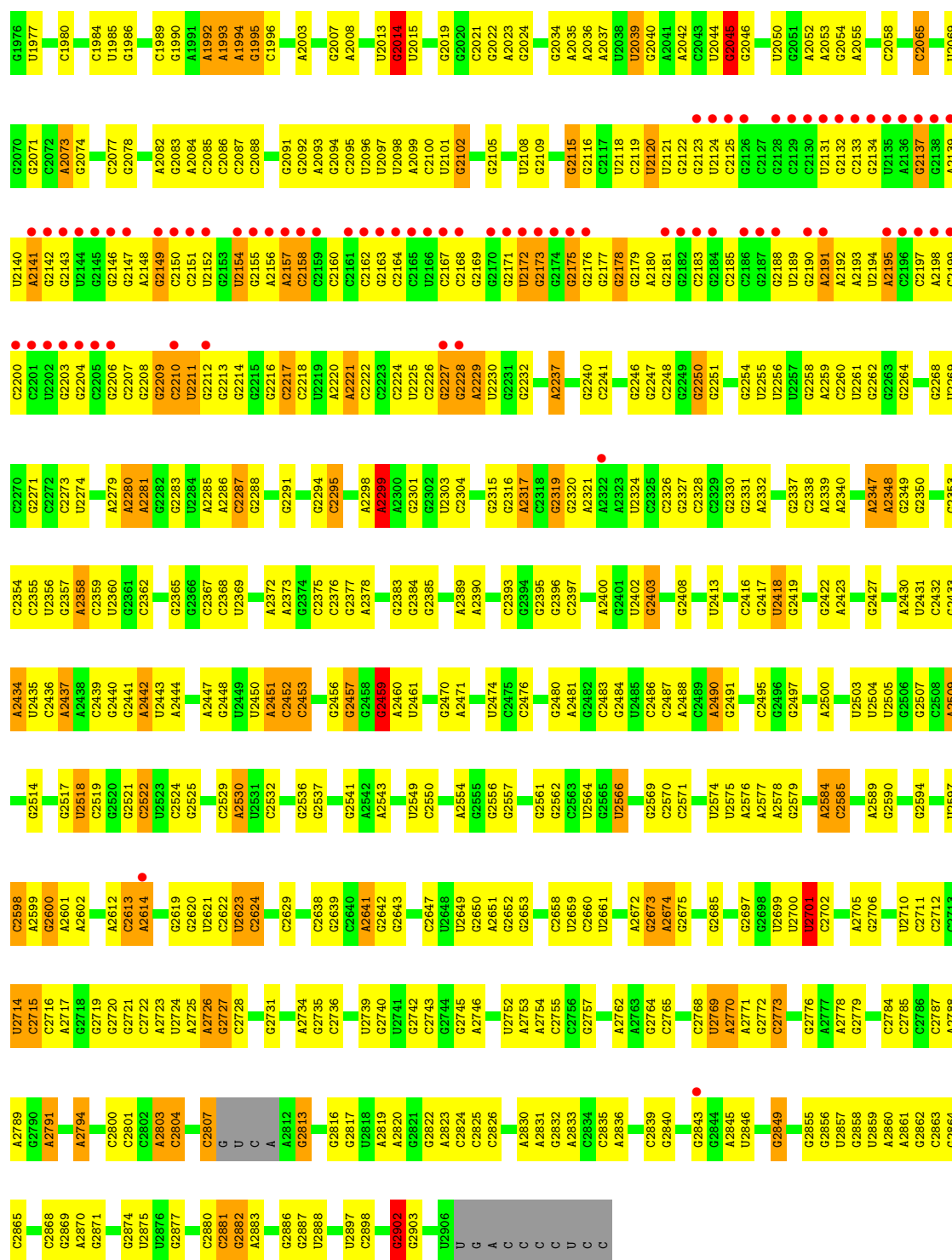
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	CE	14	Total 14	O 14	0	0
63	CF	6	Total 6	O 6	0	0
63	CN	2	Total 2	O 2	0	0
63	CP	12	Total 12	O 12	0	0
63	CQ	2	Total 2	O 2	0	0
63	CT	3	Total 3	O 3	0	0
63	CU	2	Total 2	O 2	0	0
63	CV	2	Total 2	O 2	0	0
63	CW	1	Total 1	O 1	0	0
63	CX	2	Total 2	O 2	0	0
63	CY	2	Total 2	O 2	0	0
63	C0	5	Total 5	O 5	0	0
63	C1	1	Total 1	O 1	0	0
63	C3	2	Total 2	O 2	0	0
63	C6	1	Total 1	O 1	0	0
63	C7	1	Total 1	O 1	0	0
63	C8	3	Total 3	O 3	0	0
63	DA	154	Total 154	O 154	0	0
63	DE	3	Total 3	O 3	0	0
63	DH	1	Total 1	O 1	0	0
63	DJ	1	Total 1	O 1	0	0

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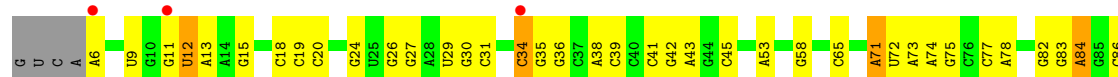
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	DK	2	Total	O	0	0
			2	2		
63	DP	1	Total	O	0	0
			1	1		
63	DT	1	Total	O	0	0
			1	1		
63	DV	1	Total	O	0	0
			1	1		
63	DZ	1	Total	O	0	0
			1	1		

A1898	A1899	G1899	C1901	C1902	C1903	U1927	C1904	A1905	A1906	C1907	A1908	A1911	A1912	G1913	C1914	G1921	A1922	A1923	G1928	G1932	U1933	A1934	A1935	C1936	U1937	A1938	U1939	A1940	A1941	A1942	G1943	G1944	U1945	C1946	A1949	A1950	G1951	G1952	U1953	A1954	G1957	A1958	A1959	A1960	C1964	U1965	U1968	C1969	U1973	A1974	A1975										
A1818	A1822	A1822	U1825	C1826	U1827	C1828	U1829	C1830	C1831	C1832	A1833	A1834	C1835	U1836	U1839	G1845	A1846	G1847	G1848	U1851	A1852	G1853	A1856	G1857	C1858	U1859	A1860	C1861	G1862	C1863	U1864	U1865	G1870	A1878	A1879	G1892	G1893	U1894	U1895	A1896	G1897	G1898	C1899	A1900	U1901	C1902	A1903	U1904	A1905	U1906	A1907	U1908	A1909	U1910	A1911	C1912	U1913	A1914	U1915	A1916	A1917
C1741	G1742	G1743	G1744	A1745	G1746	A1747	C1748	G1749	G1750	G1751	G1752	U1753	A1754	C1755	G1756	C1757	C1758	G1766	A1767	U1768	G1769	A1770	G1771	C1772	C1773	C1774	C1775	C1776	G1777	G1778	A1779	A1780	G1781	C1785	A1786	G1787	A1790	A1793	G1794	G1795	G1800	A1804	G1807	U1808	U1809	A1810	A1811	C1812	U1813	A1814	A1815	A1816	A1817								
A1655	A1656	C1657	A1660	C1663	G1670	G1671	C1672	G1676	C1677	A1678	A1679	C1680	A1681	C1682	C1683	A1684	U1685	C1686	C1687	G1694	C1695	G1698	G1699	G1700	A1701	U1706	A1712	G1713	G1714	A1715	A1716	C1717	U1718	C1719	U1720	C1722	A1723	G1729	C1730	C1731	C1732	C1733	G1734	U1735	A1736	U1739	U1740														
G1567	G1568	U1569	G1570	G1571	G1572	G1573	A1574	A1575	G1576	C1577	C1578	G	U	A	C	G1584	G1585	G1586	U1587	G1588	A1589	C1590	C1604	A1605	G1606	G1607	G1608	A1616	C1624	U1625	G1628	C1629	A1630	C1631	A1632	A1633	C1634	C1635	U1636	G1637	G1640	G1641	C1645	A1649	C1650	C1651	A1654														
A1655	A1656	C1657	A1660	C1663	G1670	G1671	C1672	G1676	C1677	A1678	A1679	C1680	A1681	C1682	C1683	A1684	U1685	C1686	C1687	G1694	C1695	G1698	G1699	G1700	A1701	U1706	A1712	G1713	G1714	A1715	A1716	C1717	U1718	C1719	U1720	C1722	A1723	G1729	C1730	C1731	C1732	C1733	G1734	U1735	A1736	U1739	U1740														
C1741	G1742	G1743	G1744	A1745	G1746	A1747	C1748	G1749	G1750	G1751	G1752	U1753	A1754	C1755	G1756	C1757	C1758	G1766	A1767	U1768	G1769	A1770	G1771	C1772	C1773	C1774	C1775	C1776	G1777	G1778	A1779	A1780	G1781	C1785	A1786	G1787	A1790	A1793	G1794	G1795	G1800	A1804	G1807	U1808	U1809	A1810	A1811	C1812	U1813	A1814	A1815	A1816	A1817								
A1818	A1822	A1822	U1825	C1826	U1827	C1828	U1829	C1830	C1831	C1832	A1833	A1834	C1835	U1836	U1839	G1845	A1846	G1847	G1848	U1851	A1852	G1853	A1856	G1857	C1858	U1859	A1860	C1861	G1862	C1863	U1864	U1865	G1870	A1878	A1879	G1892	G1893	U1894	U1895	A1896	G1897	G1898	C1899	A1900	U1901	C1902	A1903	U1904	A1905	U1906	A1907	U1908	A1909	U1910	A1911	C1912	U1913	A1914	U1915	A1916	A1917
U854	G855	G856	U857	U858	C859	U860	C861	C862	C863	C864	G865	A866	A867	A868	U869	G870	U873	U874	U875	A876	G877	U880	C881	A882	U886	C887	A888	C889	C890	C891	G892	C893	U894	G895	A896	C897	G902	C903	C904	U905	G906	G911	G912	A913	C914	G920	G921	G922	C923	U924	A925	G926	G927								

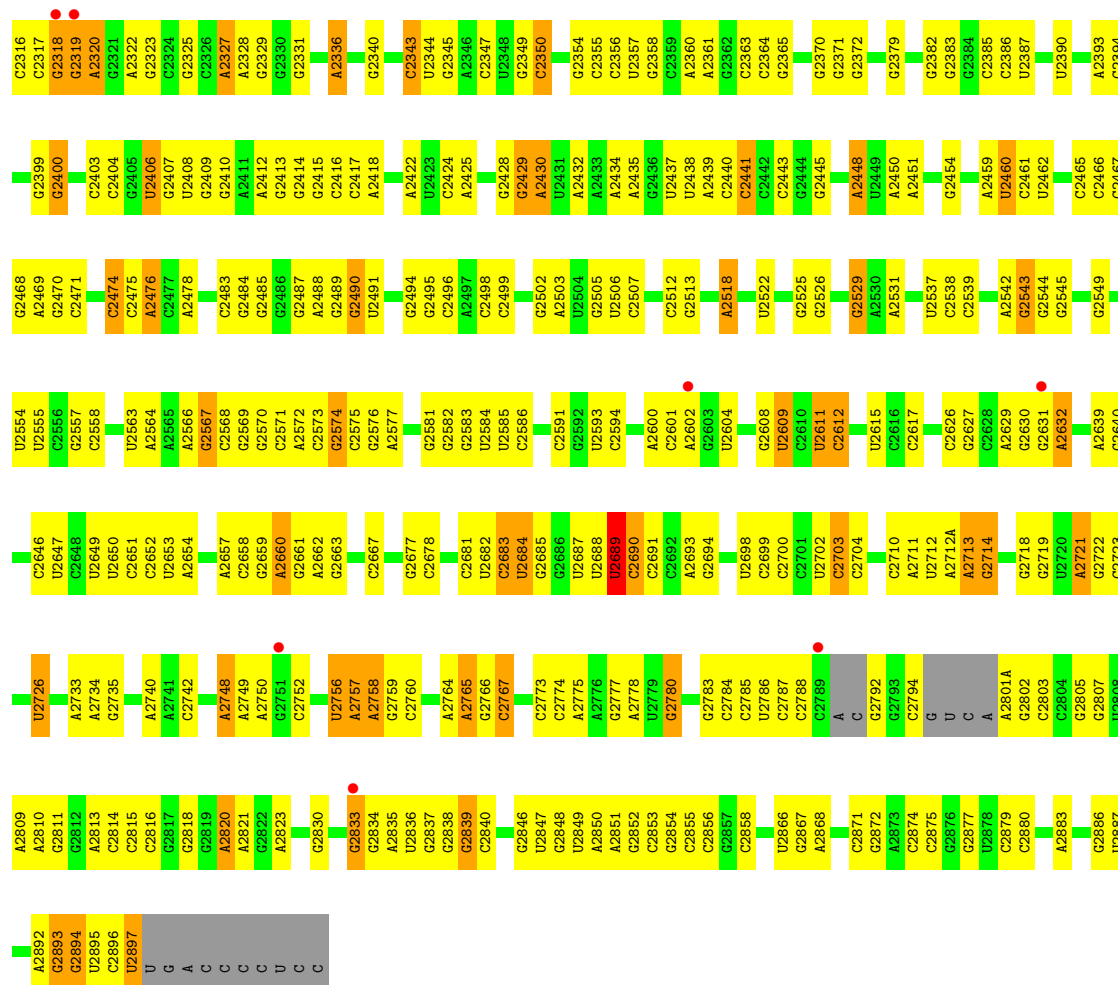


● Molecule 1: 23S Ribosomal RNA

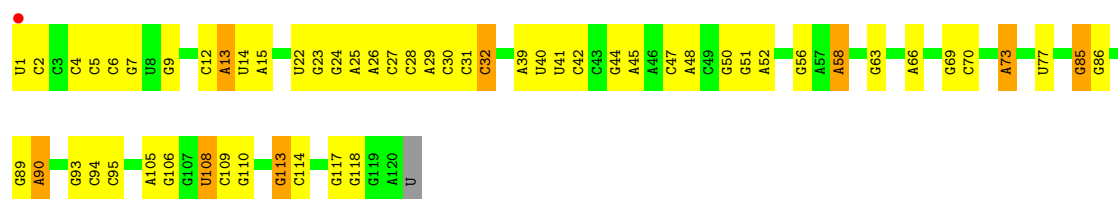




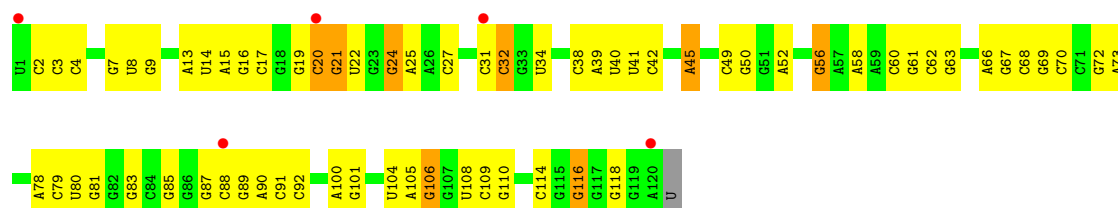


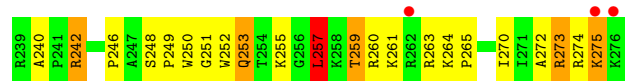


- Molecule 2: 5S Ribosomal RNA

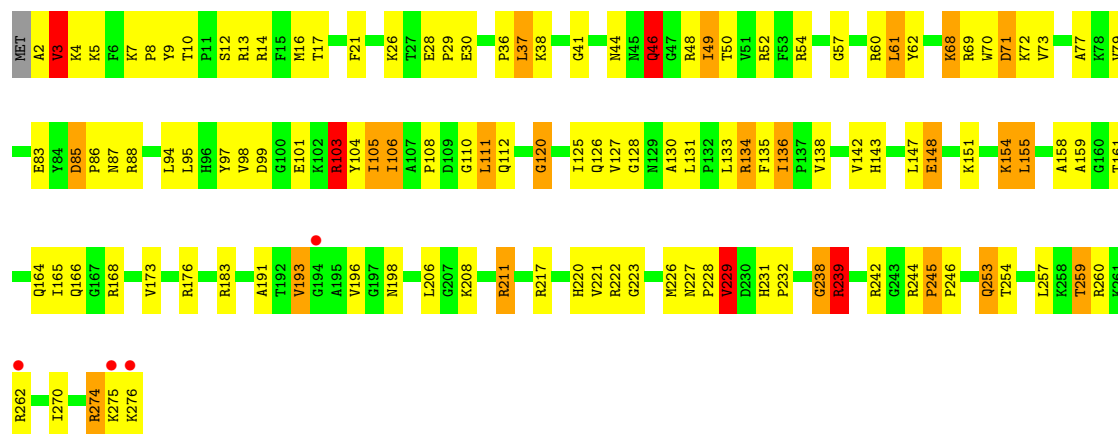


- Molecule 2: 5S Ribosomal RNA

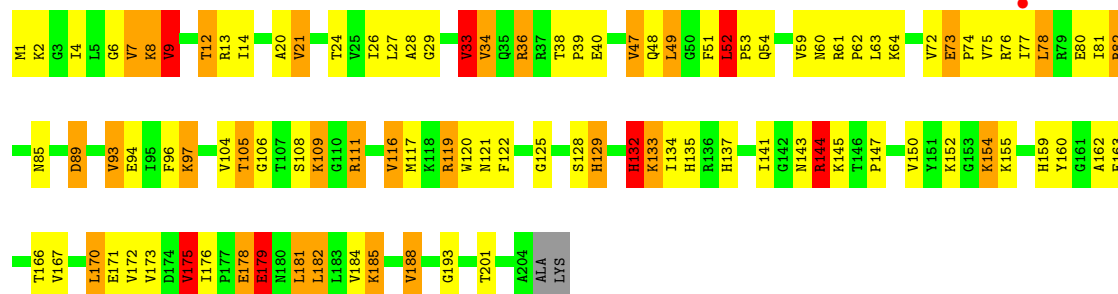




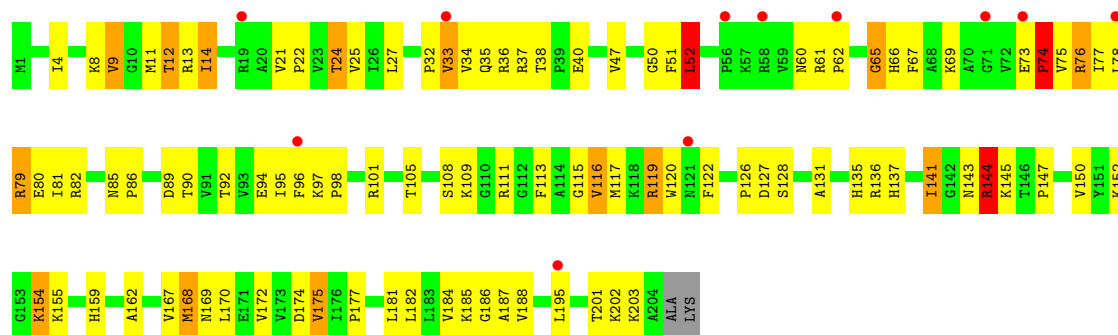
• Molecule 4: 50S ribosomal protein L2



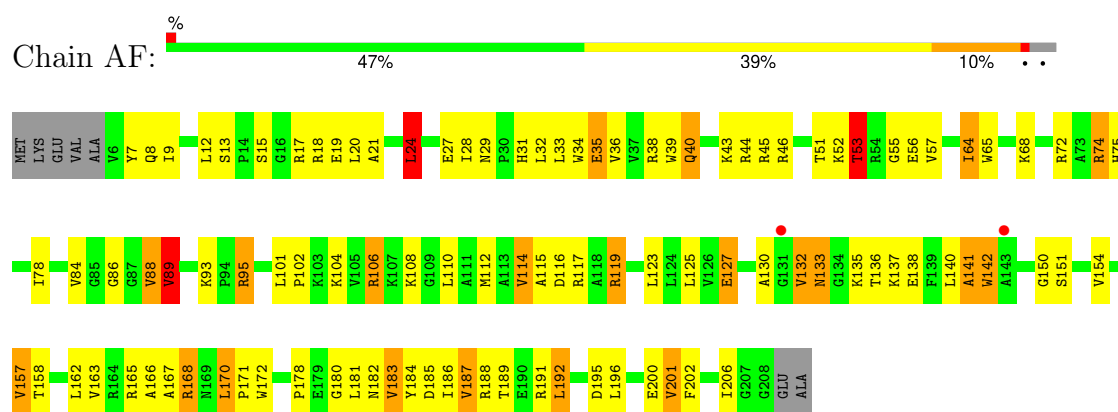
• Molecule 5: 50S ribosomal protein L3



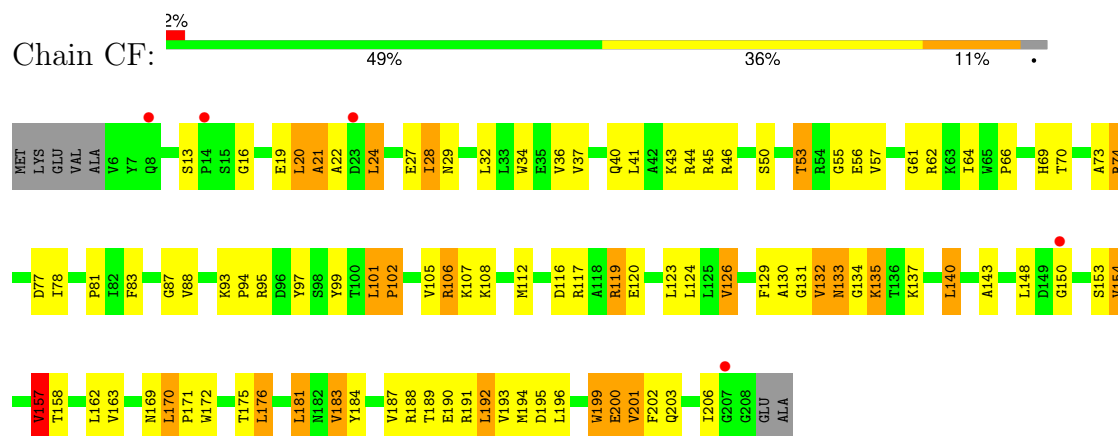
• Molecule 5: 50S ribosomal protein L3



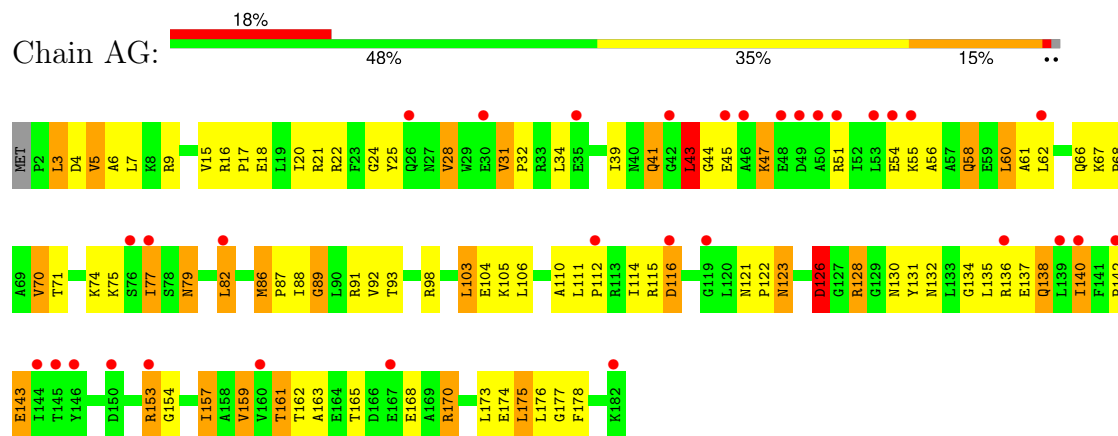
• Molecule 6: 50S ribosomal protein L4



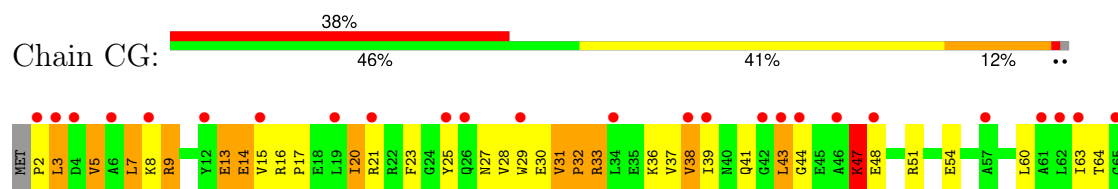
• Molecule 6: 50S ribosomal protein L4

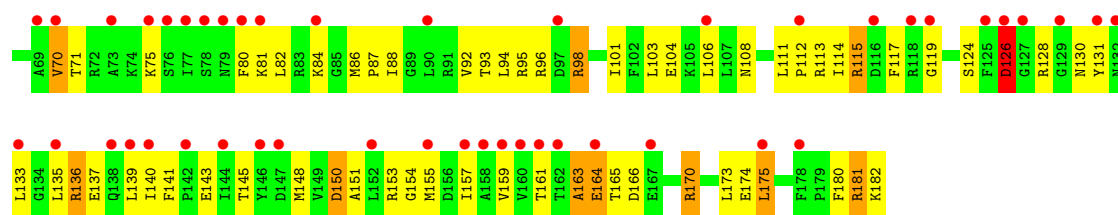


• Molecule 7: 50S ribosomal protein L5

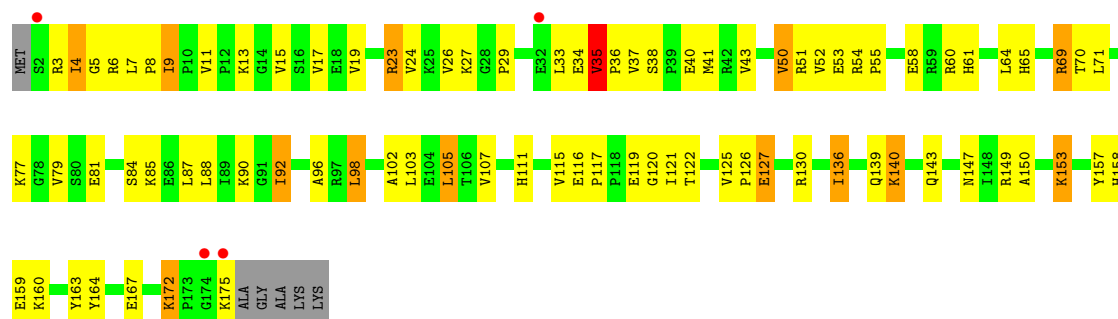


• Molecule 7: 50S ribosomal protein L5

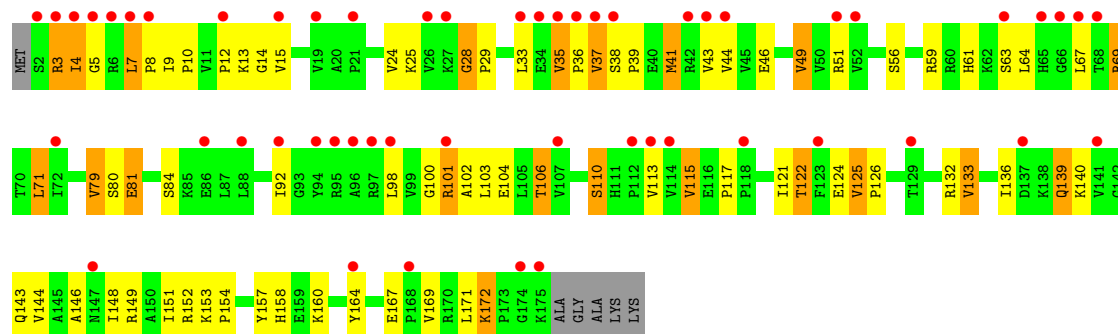




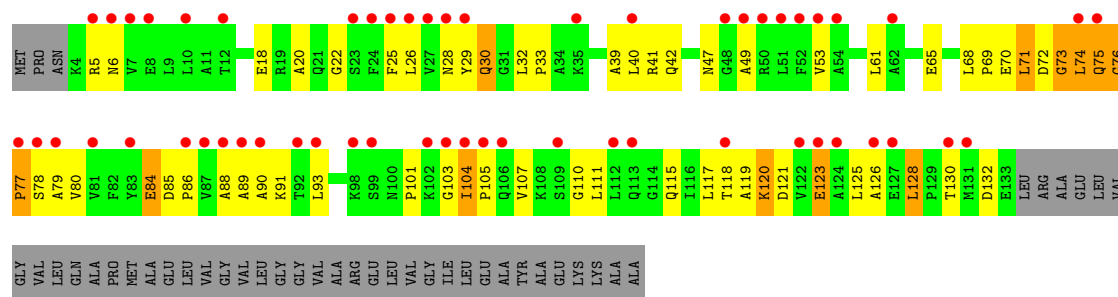
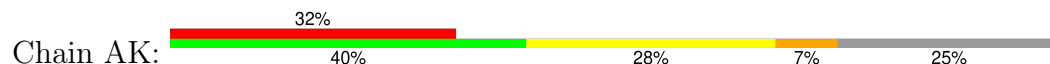
• Molecule 8: 50S ribosomal protein L6



• Molecule 8: 50S ribosomal protein L6

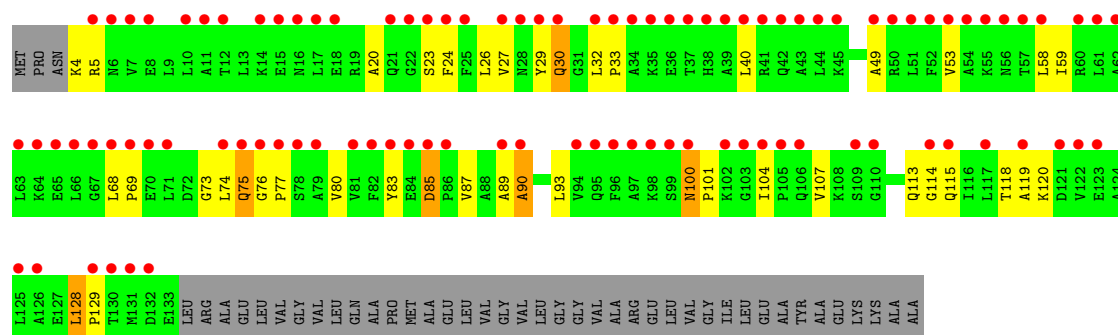


• Molecule 9: 50S ribosomal protein L10



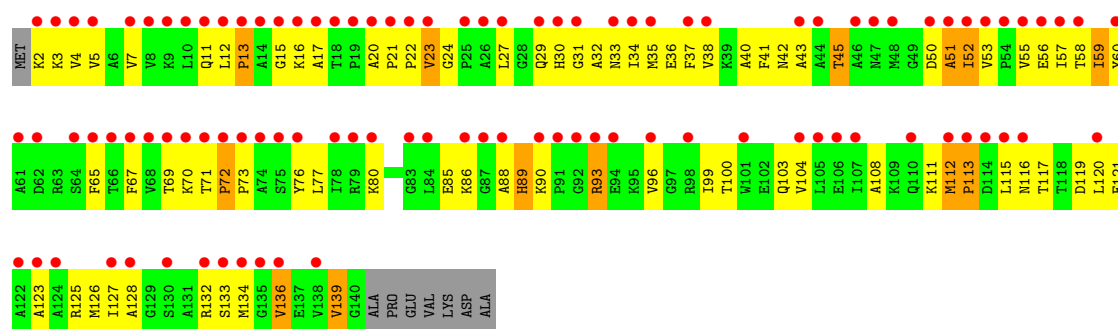
• Molecule 9: 50S ribosomal protein L10

Chain CK:



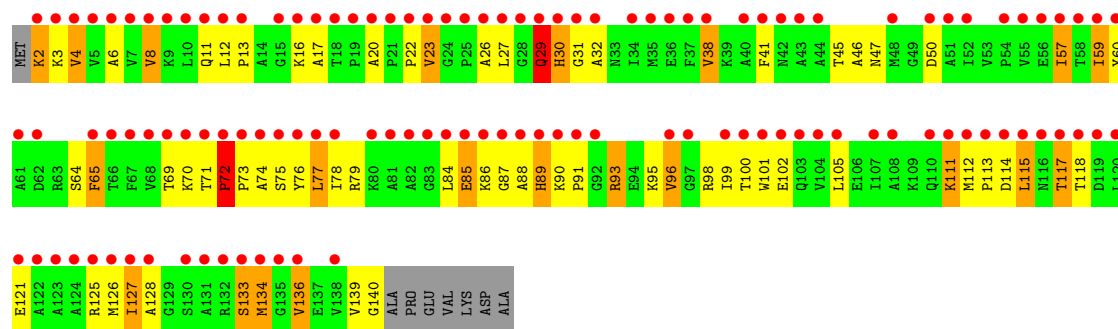
- Molecule 10: 50S ribosomal protein L11

Chain AL:



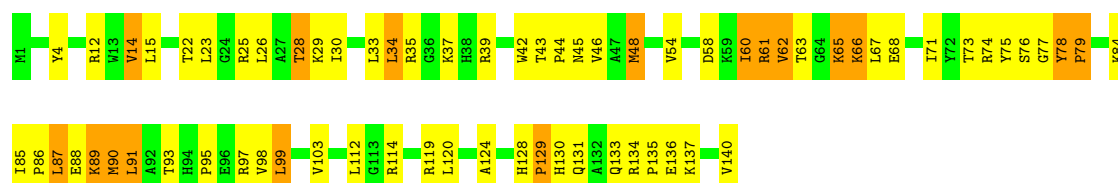
- Molecule 10: 50S ribosomal protein L11

Chain CL:

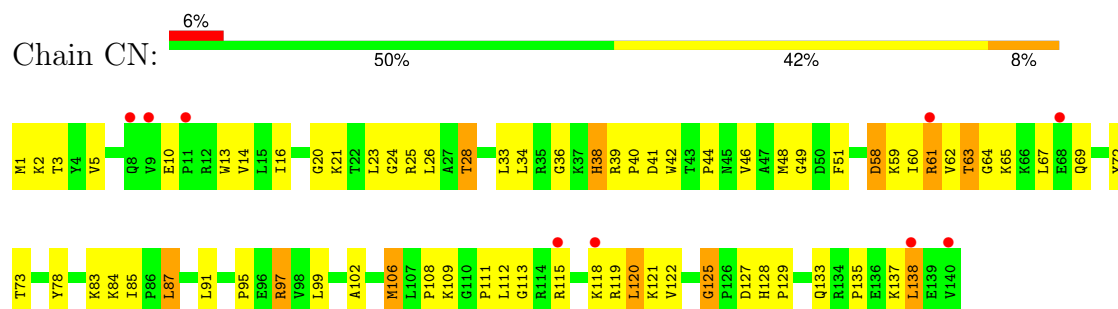


- Molecule 11: 50S ribosomal protein L13

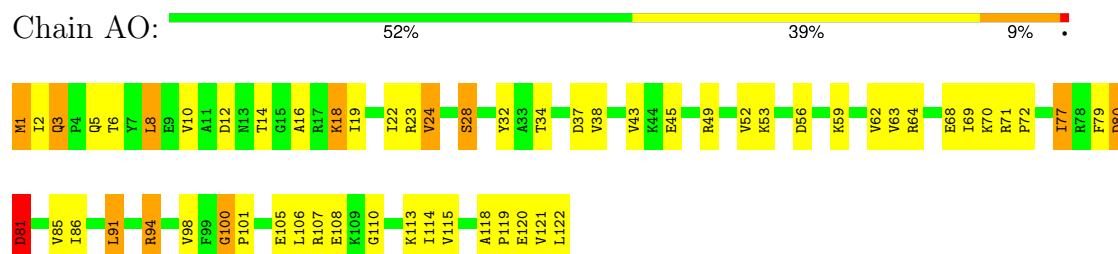
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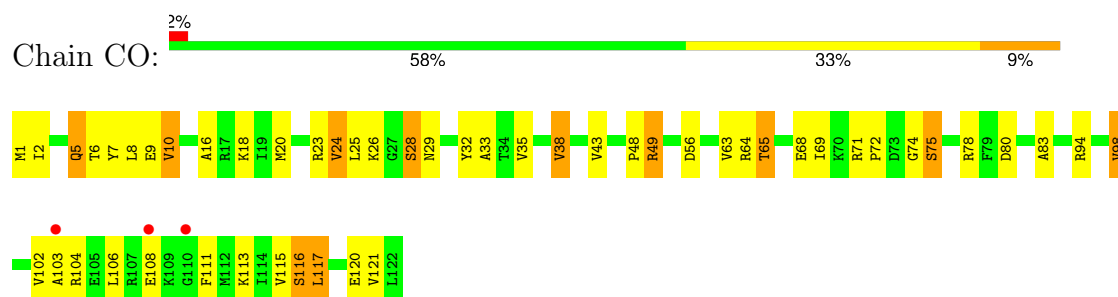
• Molecule 11: 50S ribosomal protein L13



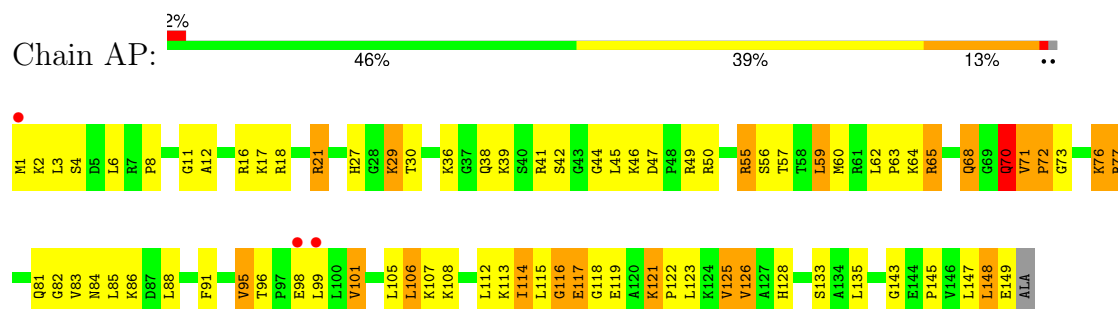
• Molecule 12: 50S ribosomal protein L14



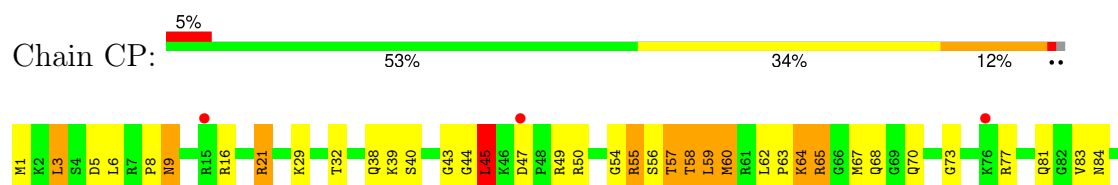
• Molecule 12: 50S ribosomal protein L14



• Molecule 13: 50S ribosomal protein L15



• Molecule 13: 50S ribosomal protein L15

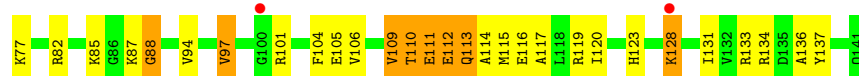




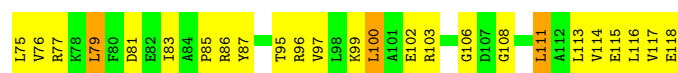
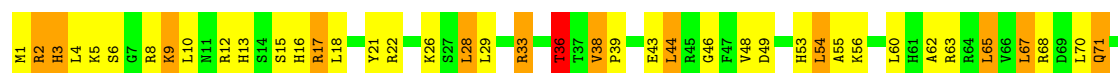
• Molecule 14: 50S ribosomal protein L16



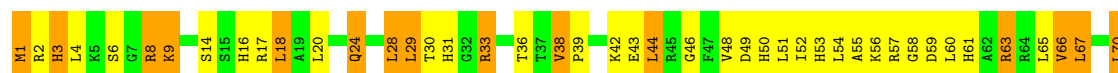
• Molecule 14: 50S ribosomal protein L16



• Molecule 15: 50S ribosomal protein L17



• Molecule 15: 50S ribosomal protein L17

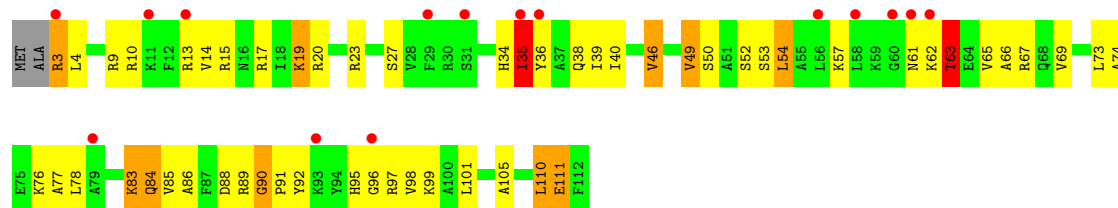


• Molecule 16: 50S ribosomal protein L18

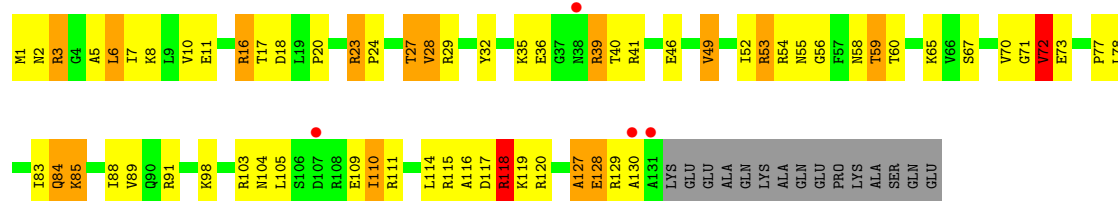




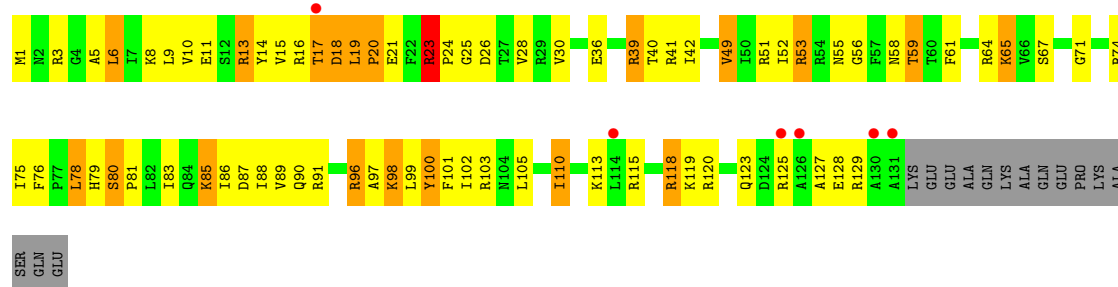
• Molecule 16: 50S ribosomal protein L18



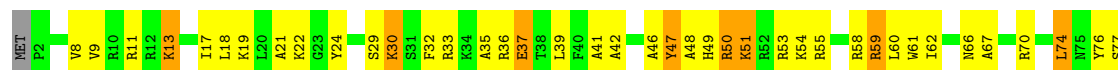
• Molecule 17: 50S ribosomal protein L19

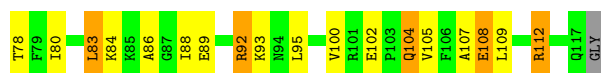


• Molecule 17: 50S ribosomal protein L19

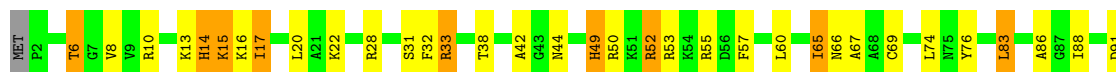


• Molecule 18: 50S ribosomal protein L20





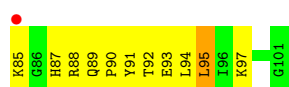
- Molecule 18: 50S ribosomal protein L20



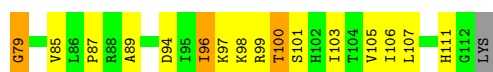
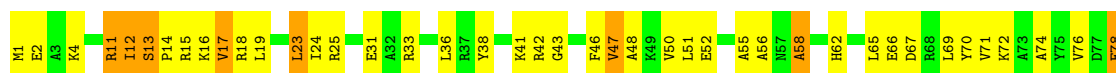
- Molecule 19: 50S ribosomal protein L21



- Molecule 19: 50S ribosomal protein L21

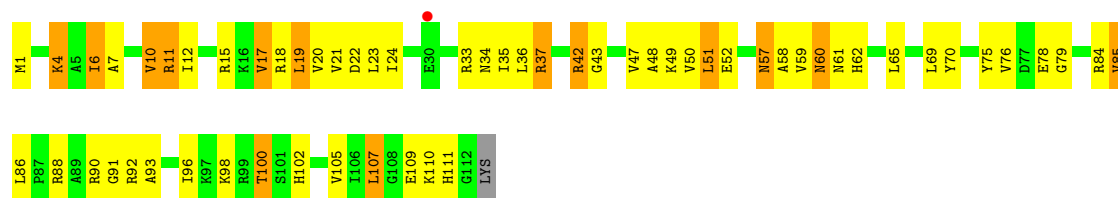


- Molecule 20: 50S ribosomal protein L22

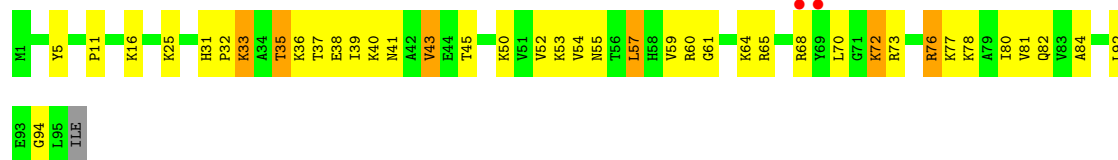


- Molecule 20: 50S ribosomal protein L22

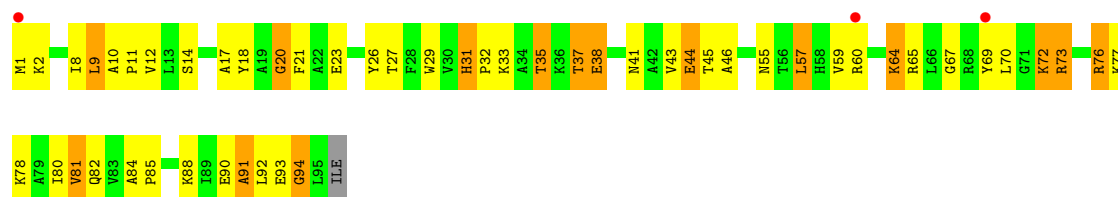




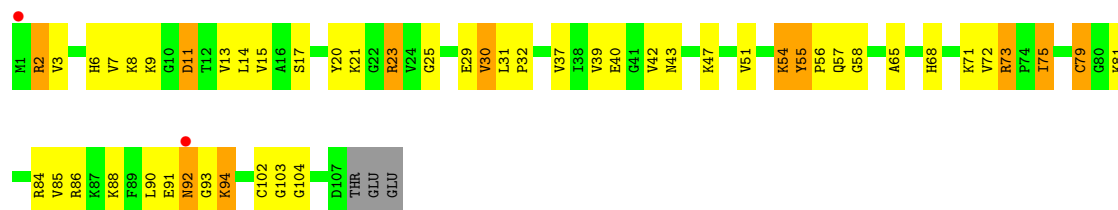
- Molecule 21: 50S ribosomal protein L23



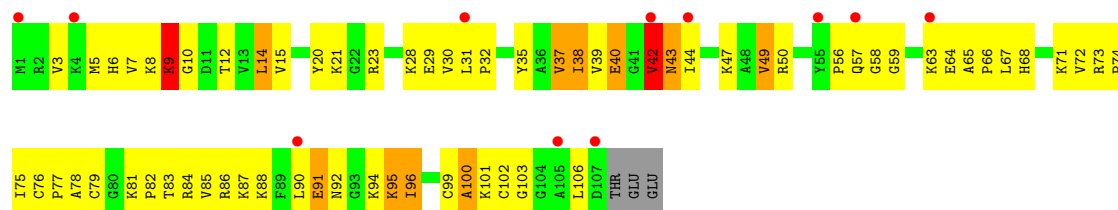
- Molecule 21: 50S ribosomal protein L23



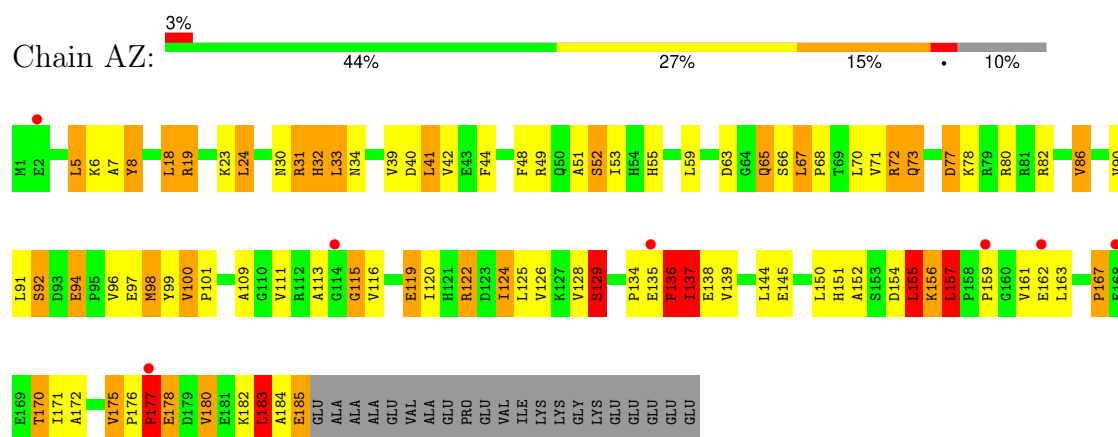
- Molecule 22: 50S ribosomal protein L24



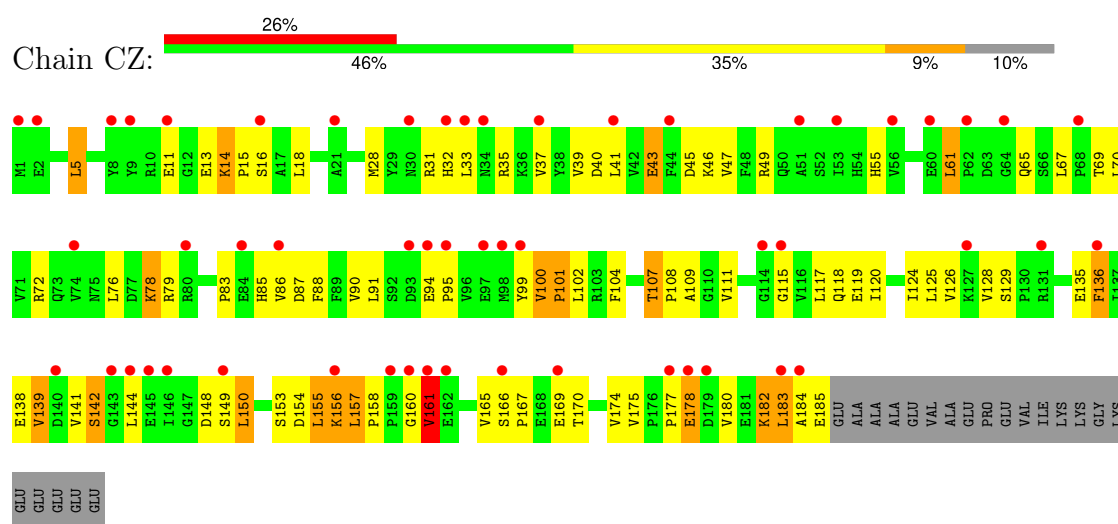
- Molecule 22: 50S ribosomal protein L24



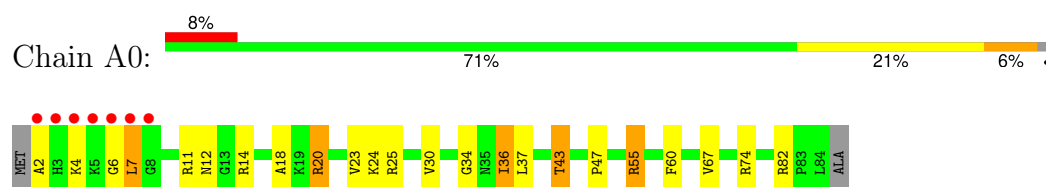
- Molecule 23: 50S ribosomal protein L25



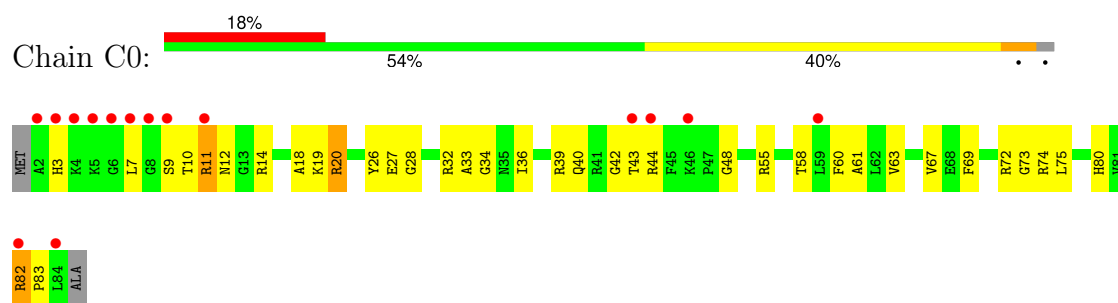
• Molecule 23: 50S ribosomal protein L25



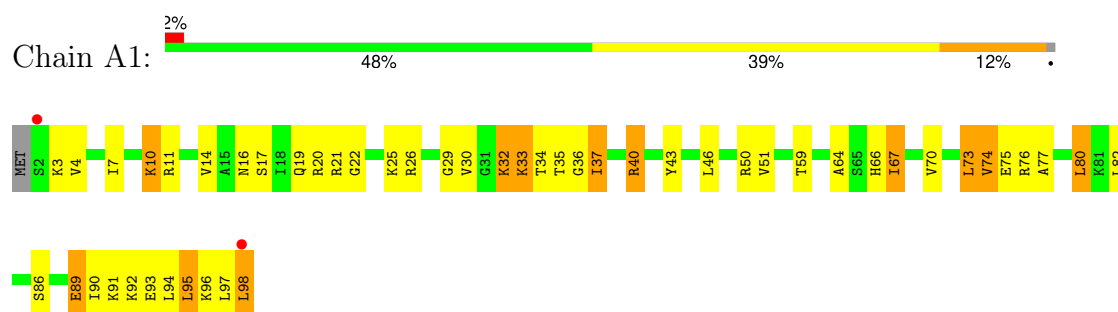
• Molecule 24: 50S ribosomal protein L27



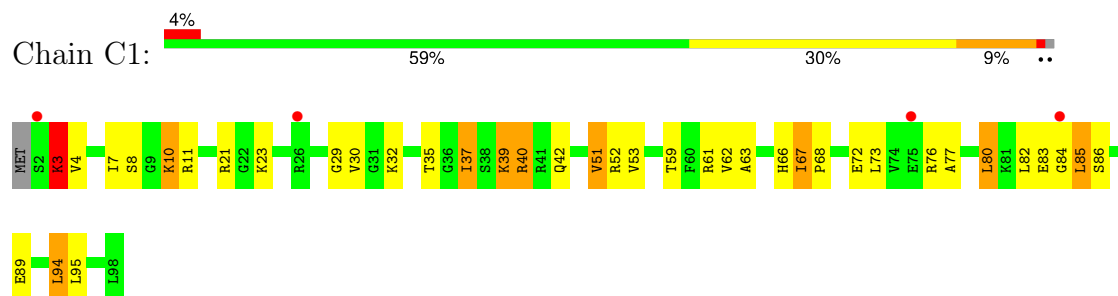
• Molecule 24: 50S ribosomal protein L27



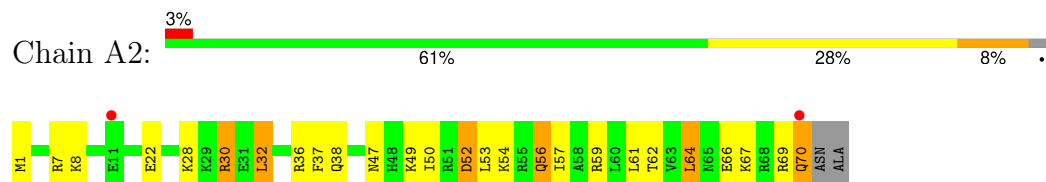
• Molecule 25: 50S ribosomal protein L28



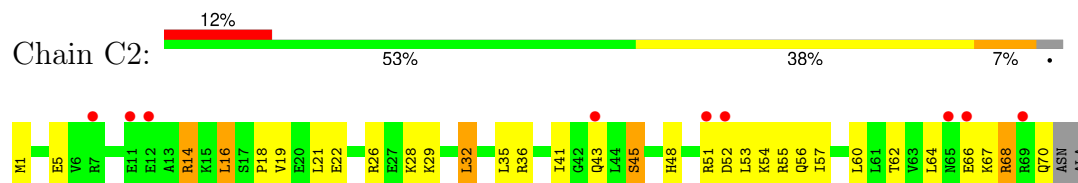
- Molecule 25: 50S ribosomal protein L28



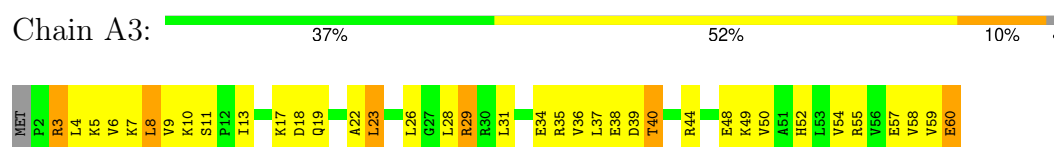
- Molecule 26: 50S ribosomal protein L29



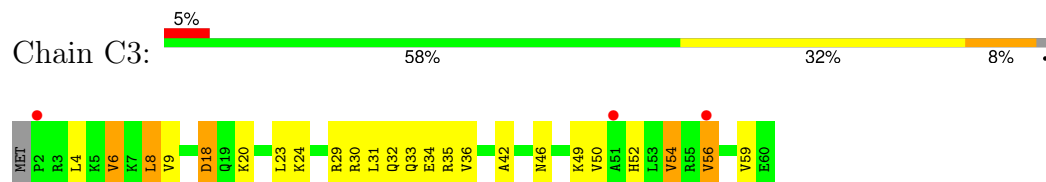
- Molecule 26: 50S ribosomal protein L29



- Molecule 27: 50S ribosomal protein L30

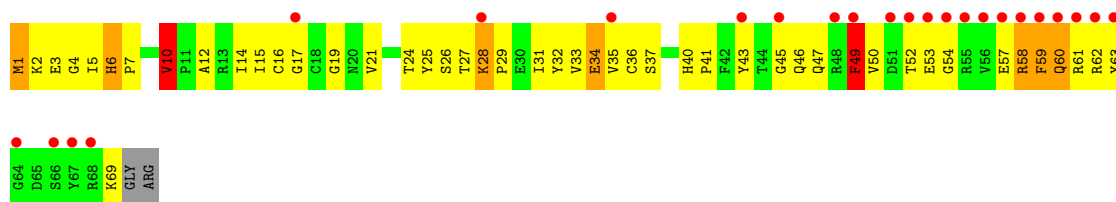


- Molecule 27: 50S ribosomal protein L30



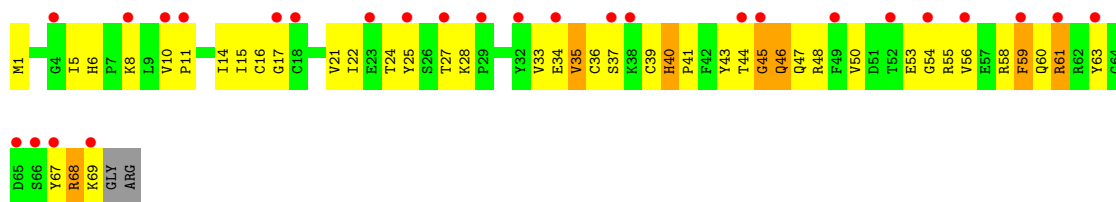
- Molecule 28: 50S ribosomal protein L31

Chain A4: 

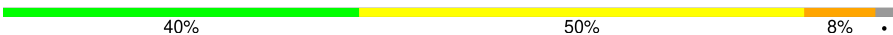


- Molecule 28: 50S ribosomal protein L31

Chain C4: 



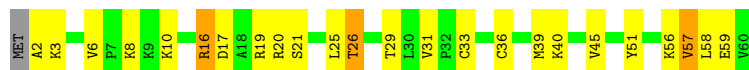
- Molecule 29: 50S ribosomal protein L32

Chain A5: 

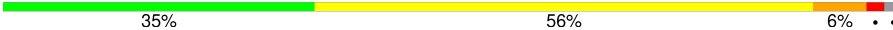


- Molecule 29: 50S ribosomal protein L32

Chain C5: 



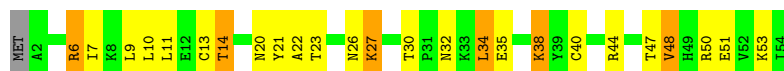
- Molecule 30: 50S ribosomal protein L33

Chain A6: 



- Molecule 30: 50S ribosomal protein L33

Chain C6: 



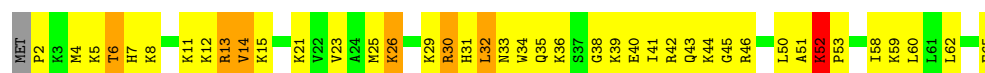
- Molecule 31: 50S ribosomal protein L34



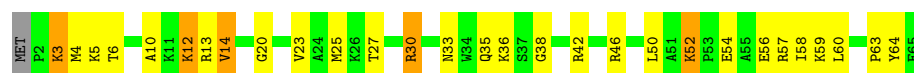
- Molecule 31: 50S ribosomal protein L34



- Molecule 32: 50S ribosomal protein L35



- Molecule 32: 50S ribosomal protein L35



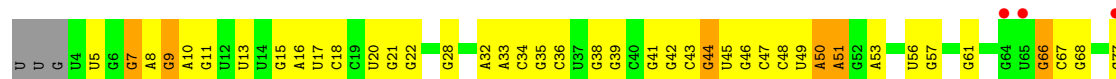
- Molecule 33: 50S ribosomal protein L36

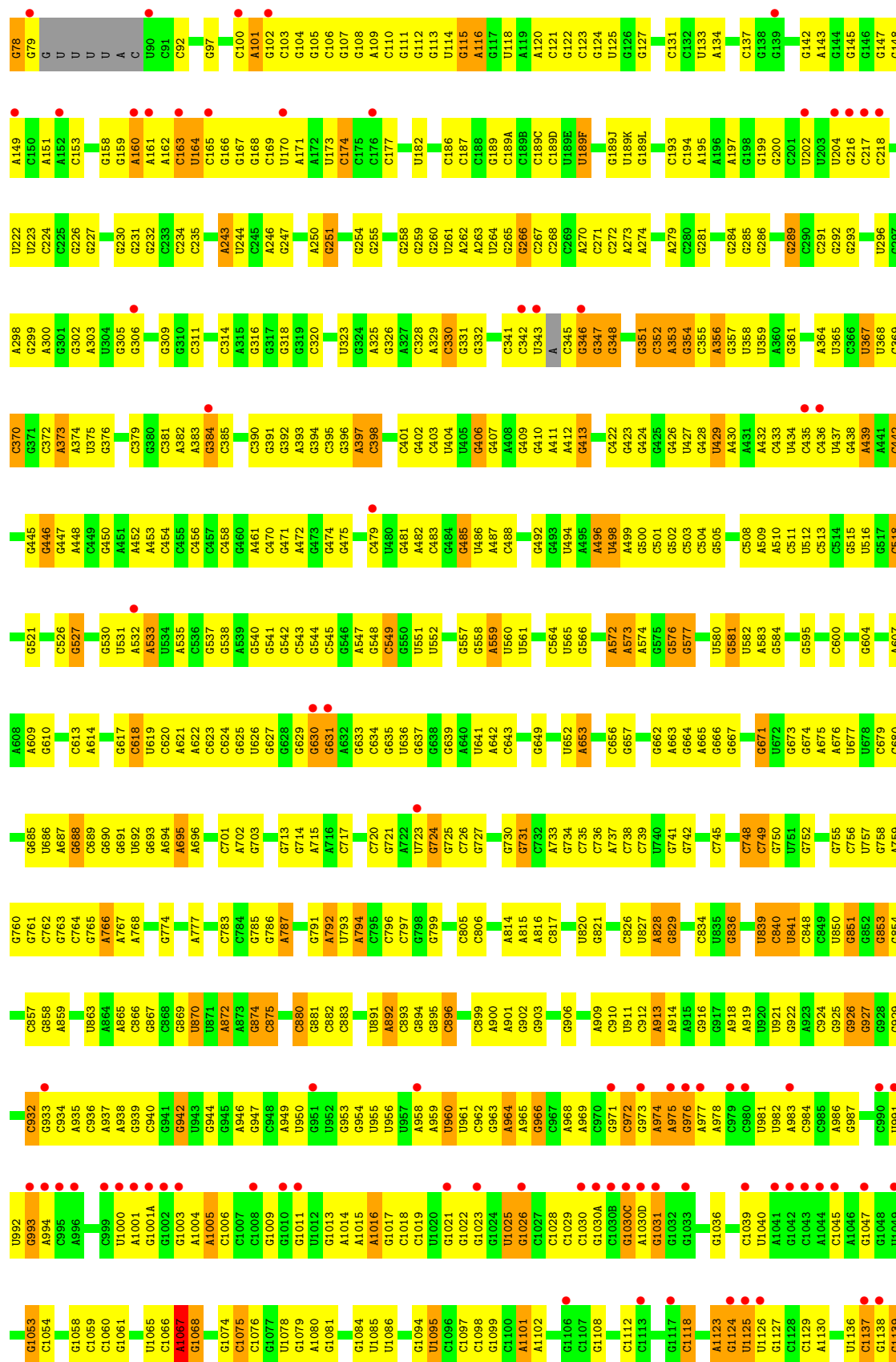


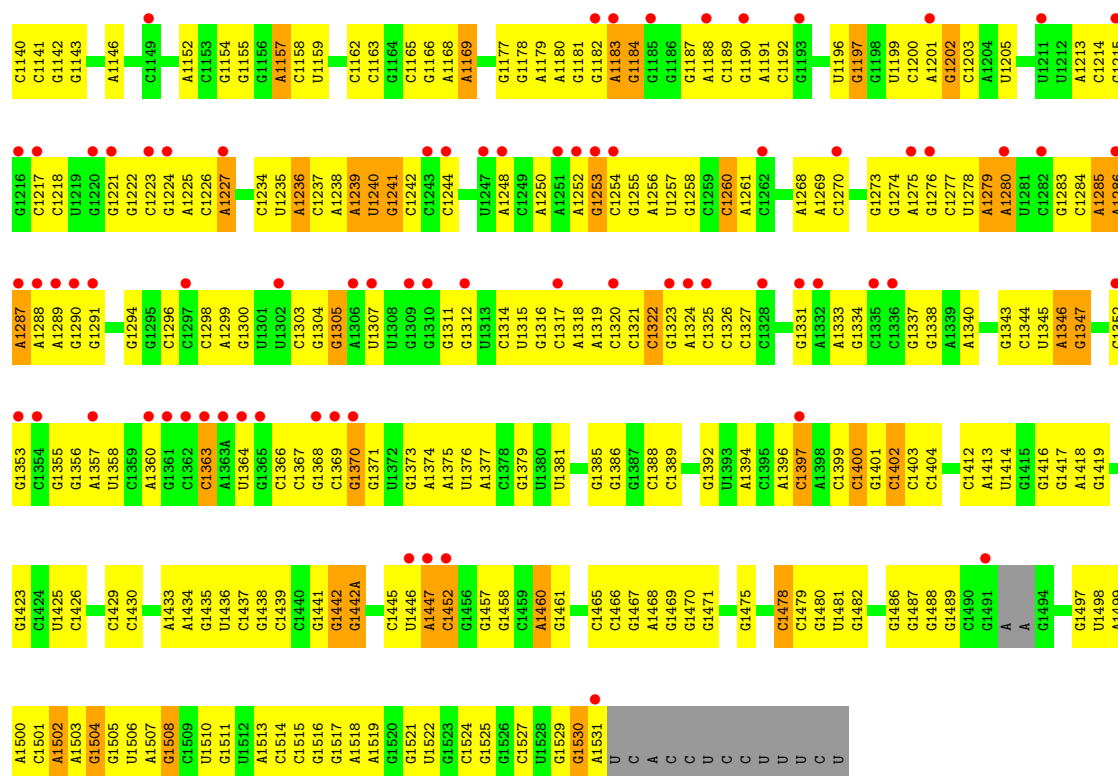
- Molecule 33: 50S ribosomal protein L36



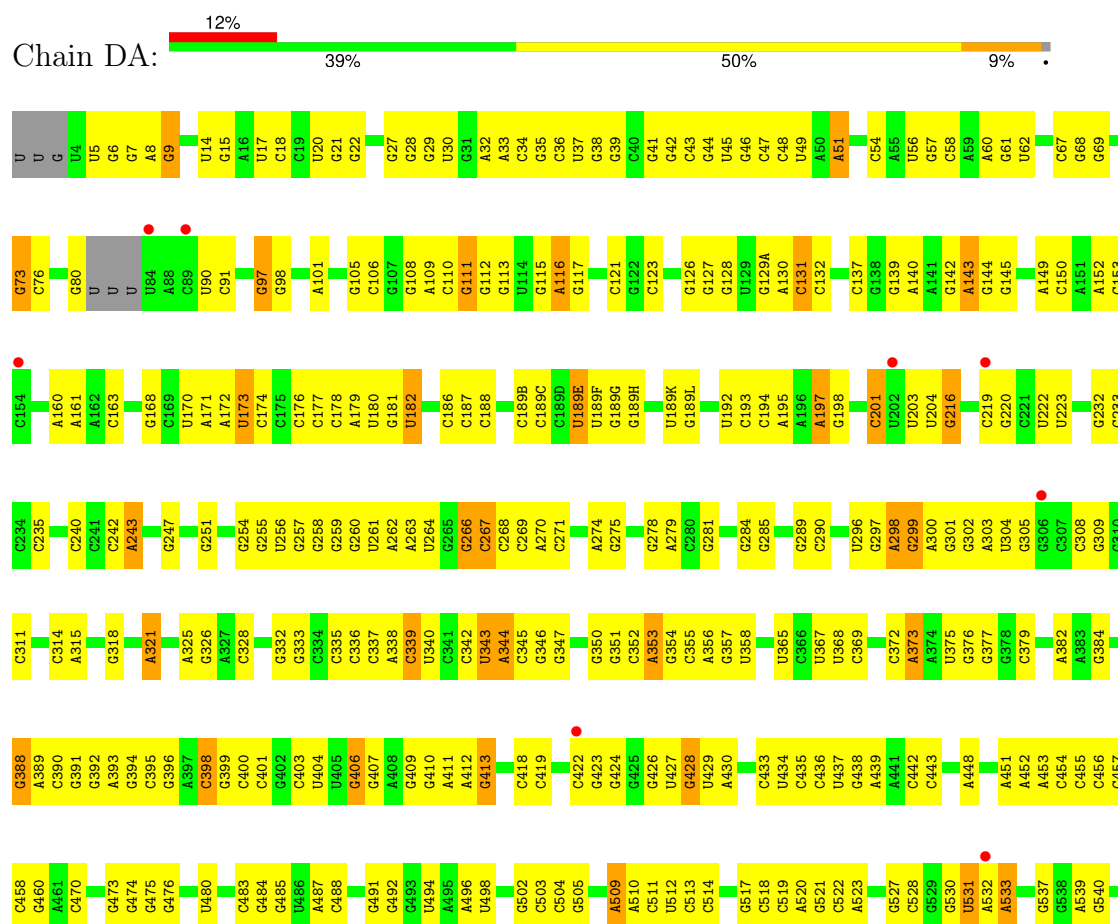
- Molecule 34: 16S Ribosomal RNA





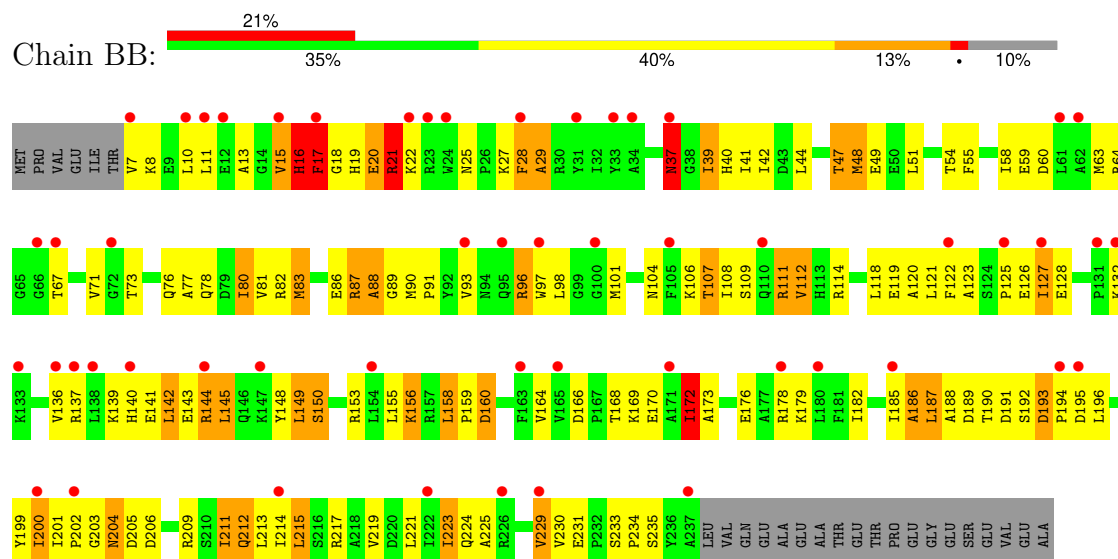


• Molecule 34: 16S Ribosomal RNA

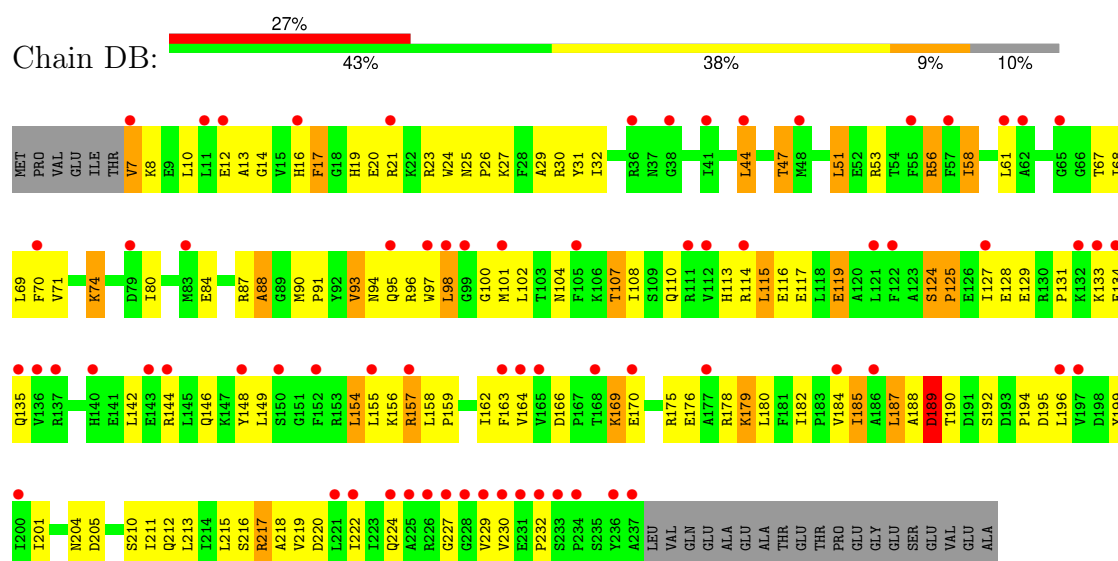




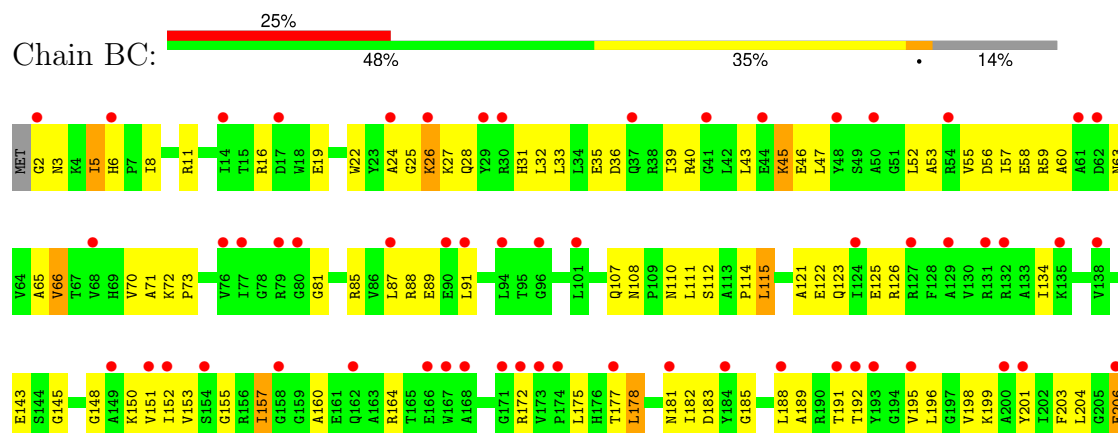
• Molecule 35: 30S ribosomal protein S2

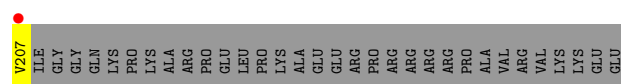


• Molecule 35: 30S ribosomal protein S2

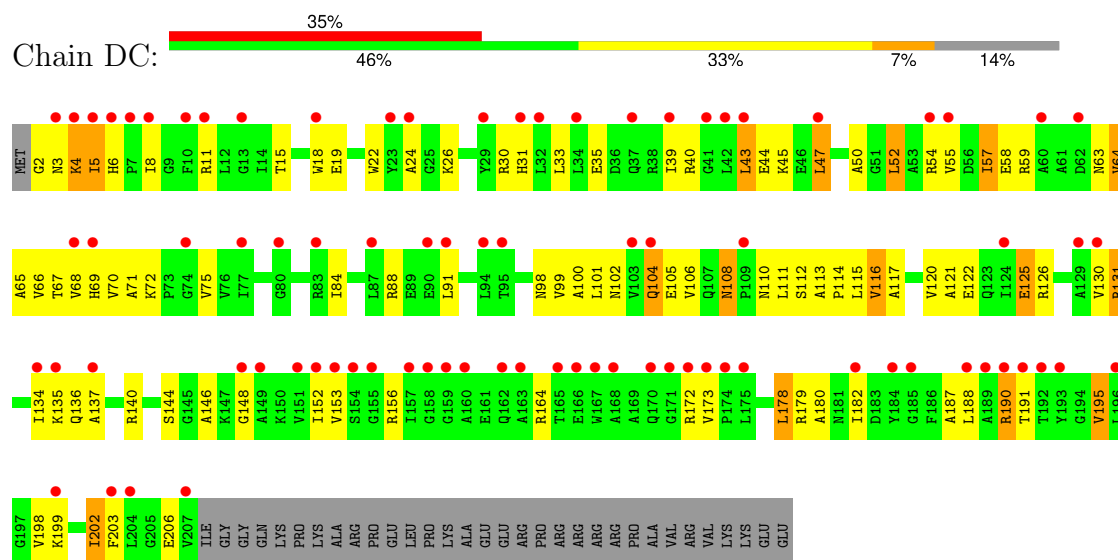


• Molecule 36: 30S ribosomal protein S3

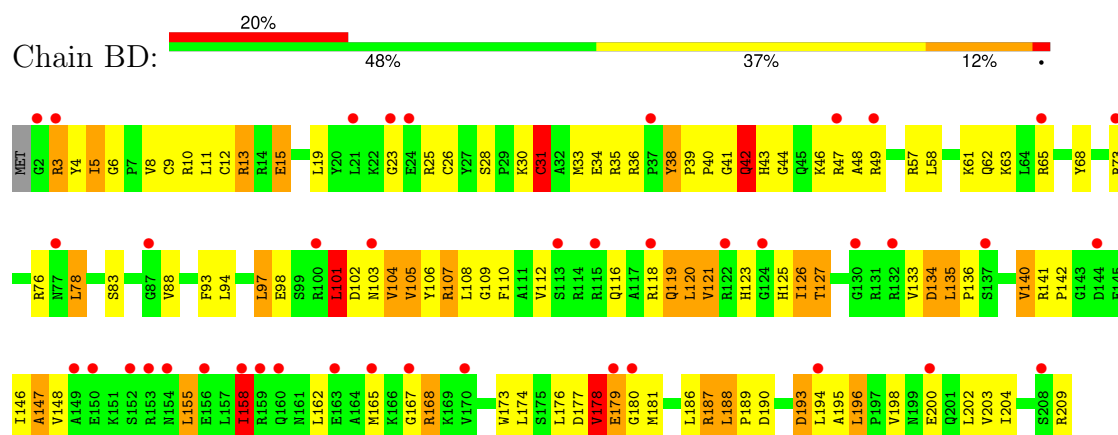




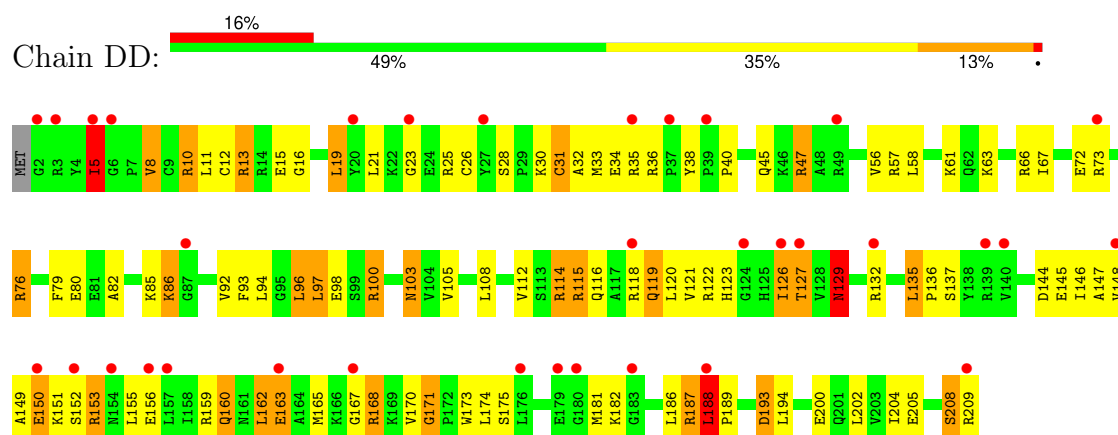
● Molecule 36: 30S ribosomal protein S3



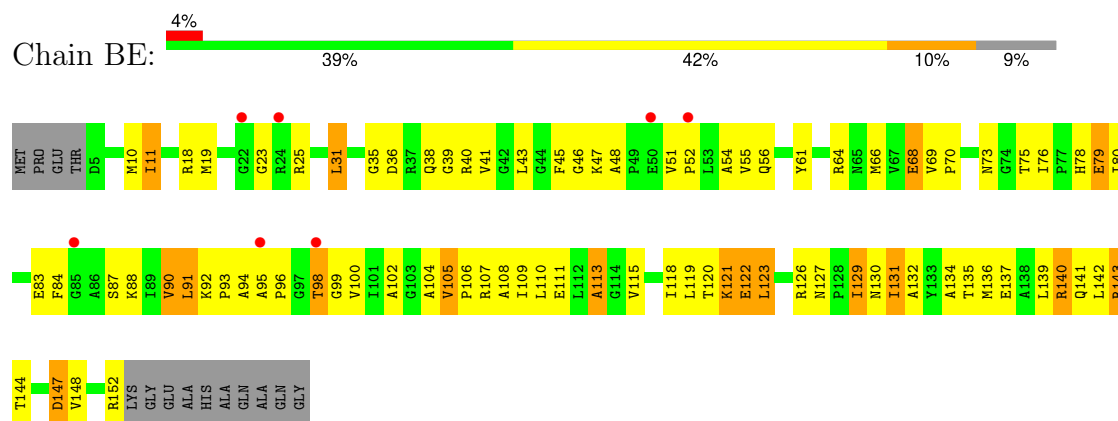
● Molecule 37: 30S ribosomal protein S4



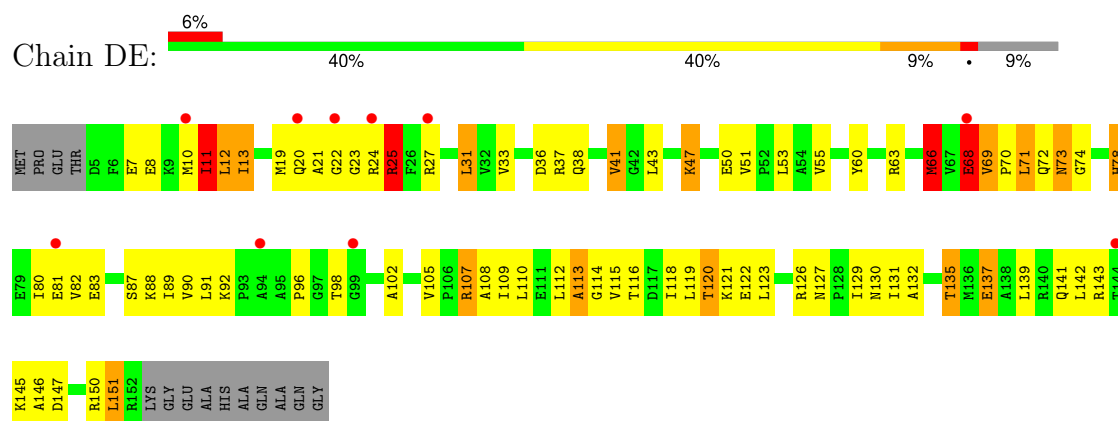
● Molecule 37: 30S ribosomal protein S4



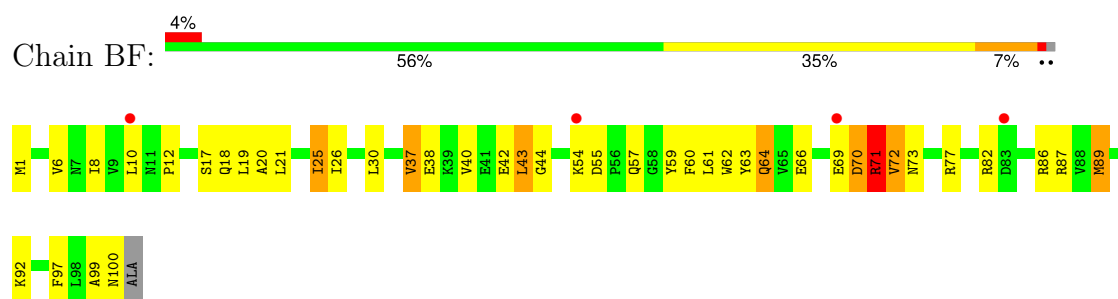
- Molecule 38: 30S ribosomal protein S5



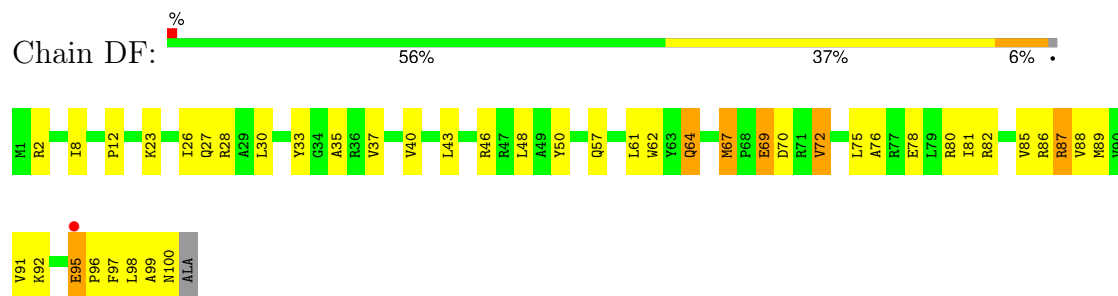
- Molecule 38: 30S ribosomal protein S5



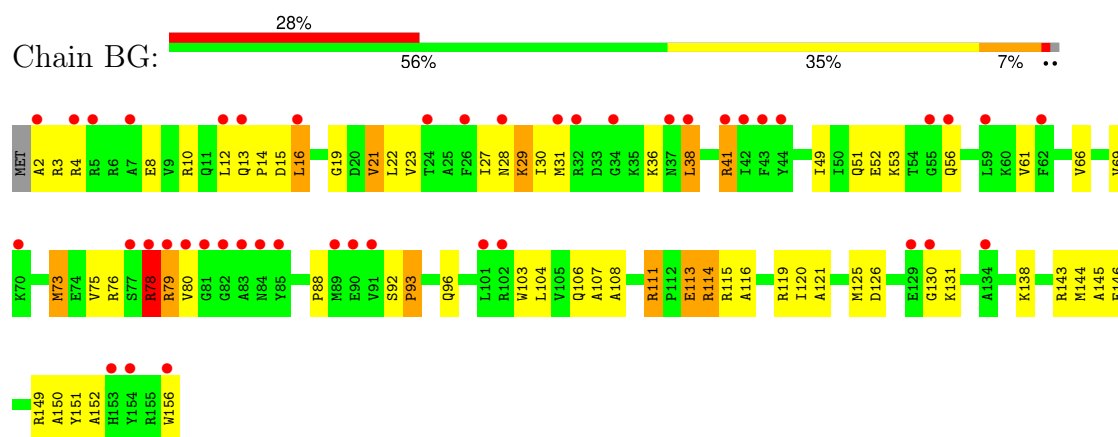
- Molecule 39: 30S ribosomal protein S6



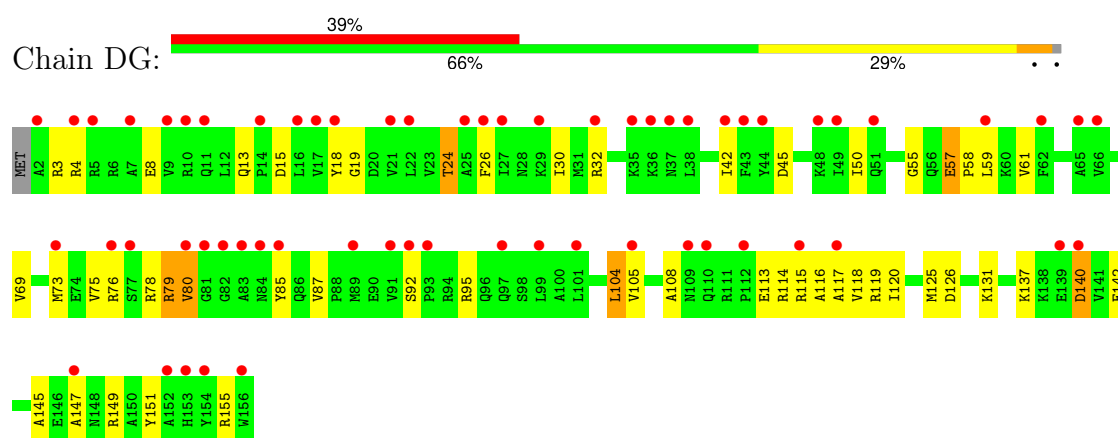
- Molecule 39: 30S ribosomal protein S6



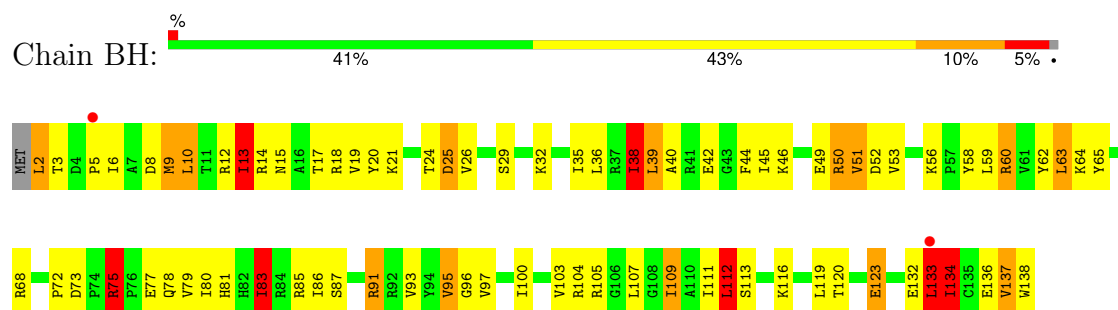
- Molecule 40: 30S ribosomal protein S7



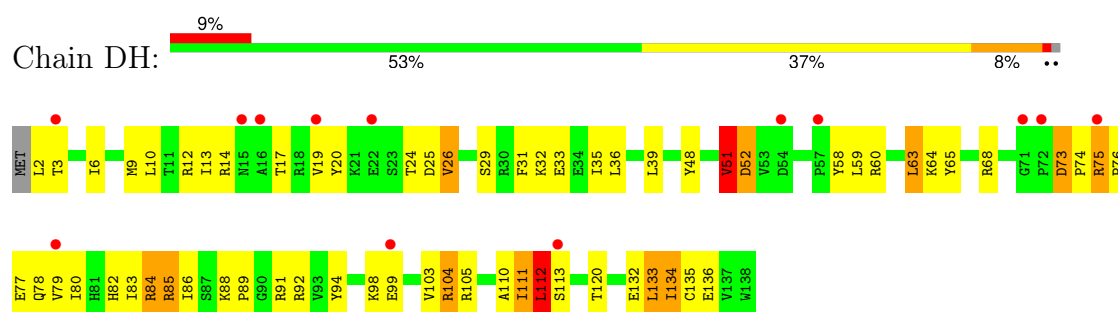
- Molecule 40: 30S ribosomal protein S7



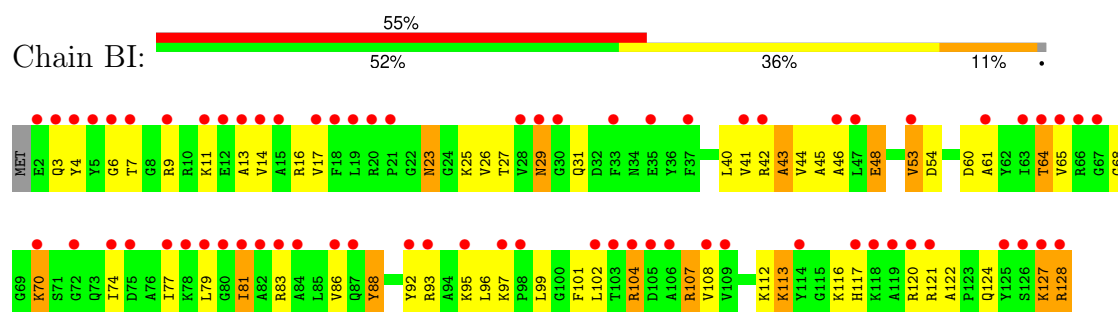
- Molecule 41: 30S ribosomal protein S8



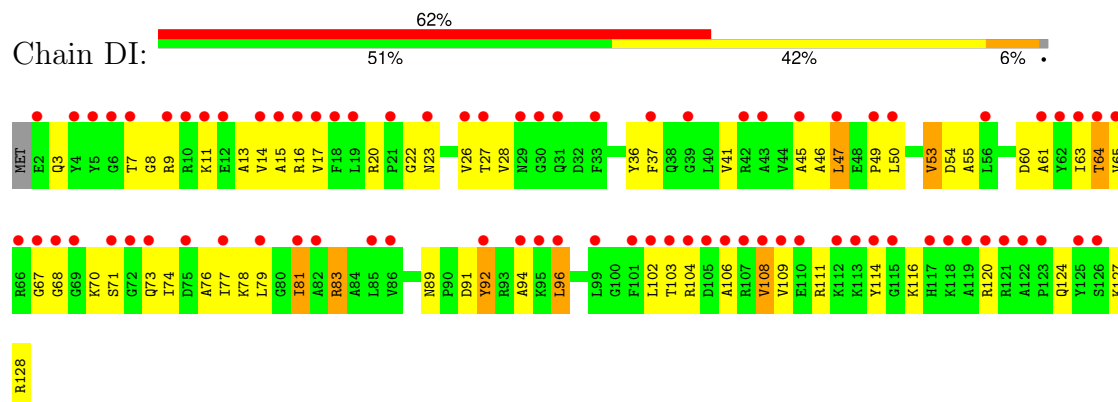
- Molecule 41: 30S ribosomal protein S8



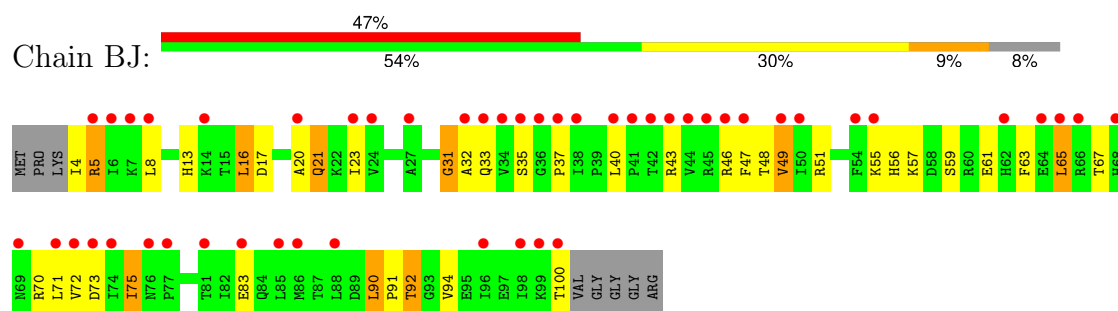
- Molecule 42: 30S ribosomal protein S9



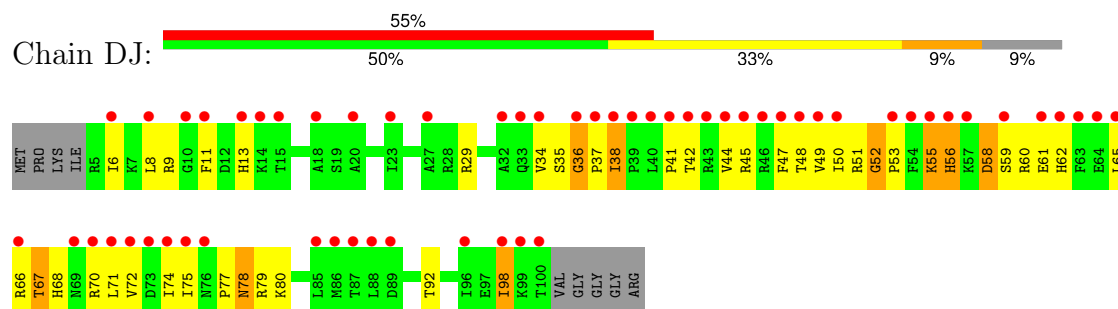
- Molecule 42: 30S ribosomal protein S9



- Molecule 43: 30S ribosomal protein S10

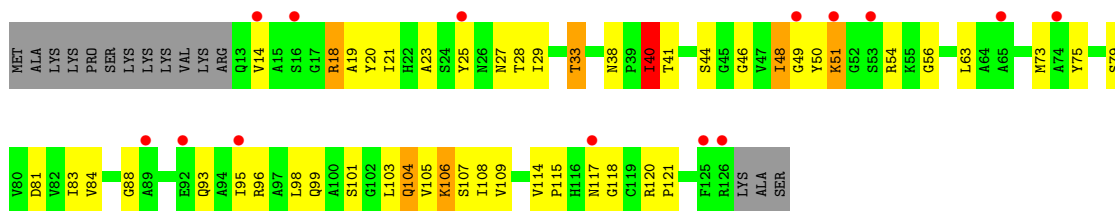


- Molecule 43: 30S ribosomal protein S10

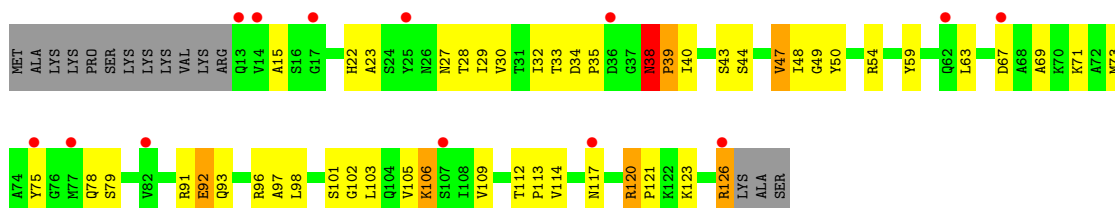


- Molecule 44: 30S ribosomal protein S11

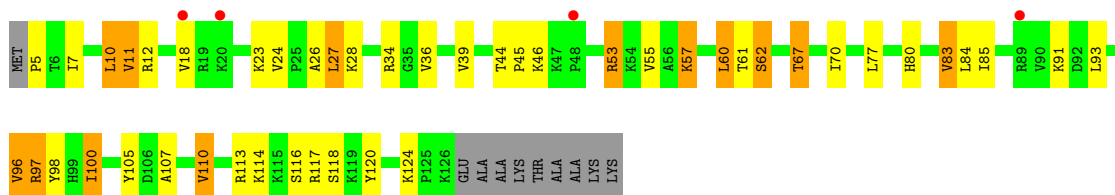




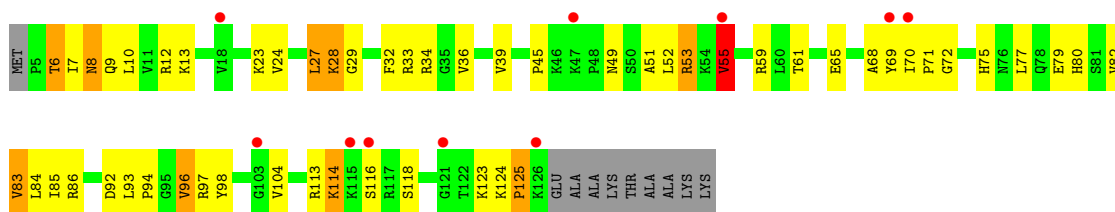
• Molecule 44: 30S ribosomal protein S11



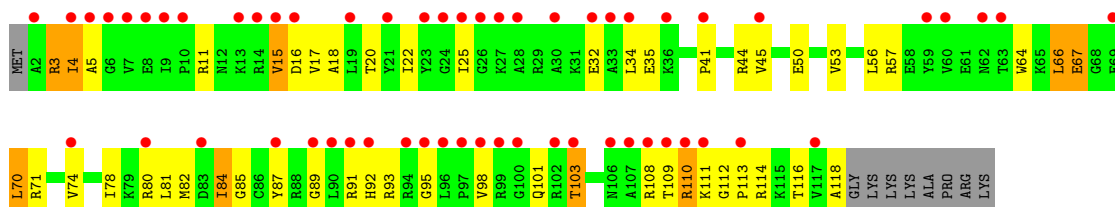
• Molecule 45: 30S ribosomal protein S12



• Molecule 45: 30S ribosomal protein S12

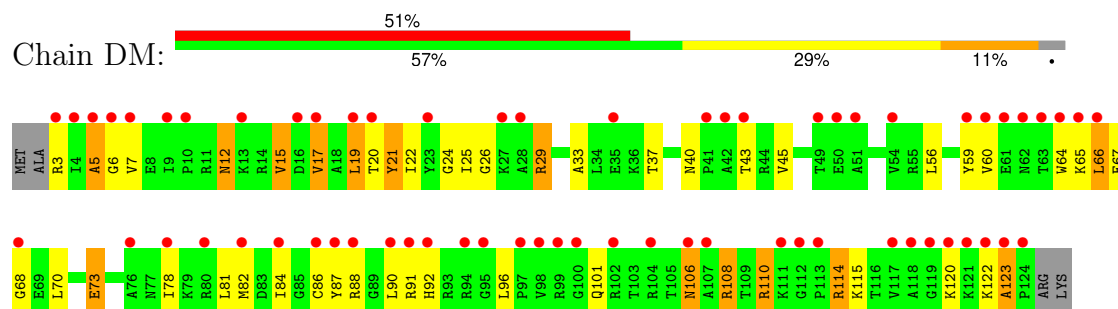


• Molecule 46: 30S ribosomal protein S13



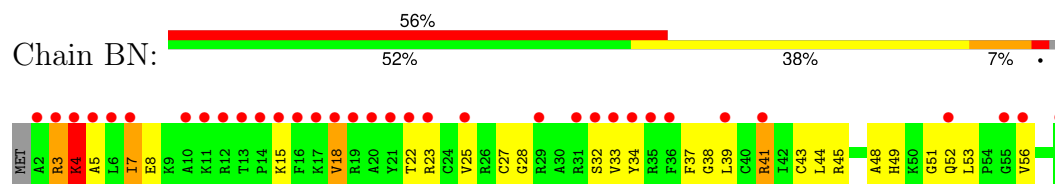
- Molecule 46: 30S ribosomal protein S13

Chain DM:



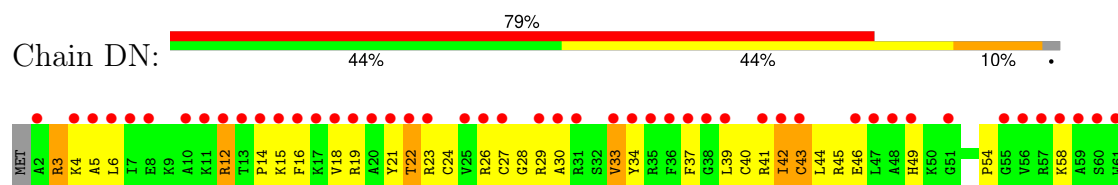
- Molecule 47: 30S ribosomal protein S14 type Z

Chain BN:



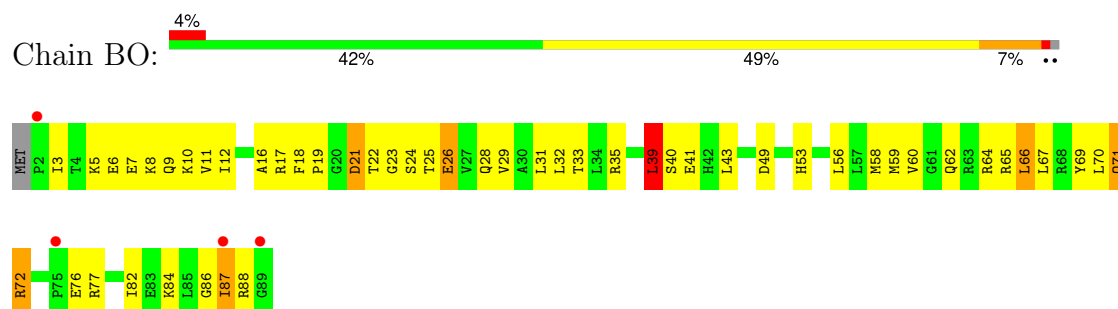
- Molecule 47: 30S ribosomal protein S14 type Z

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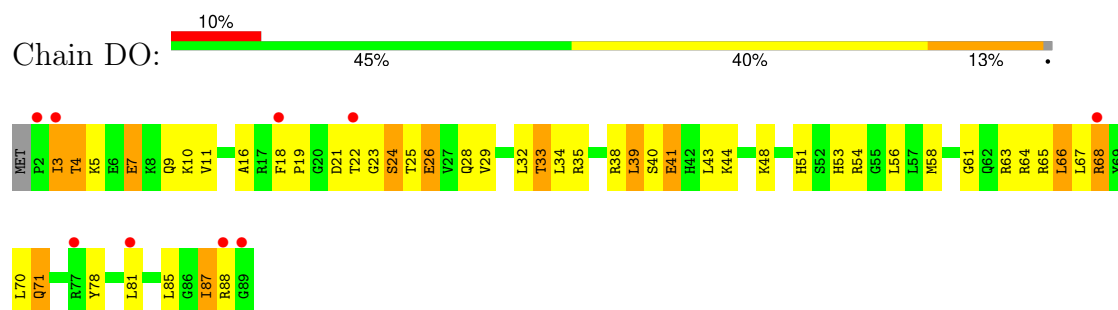
- Molecule 48: 30S ribosomal protein S15

Chain BO:

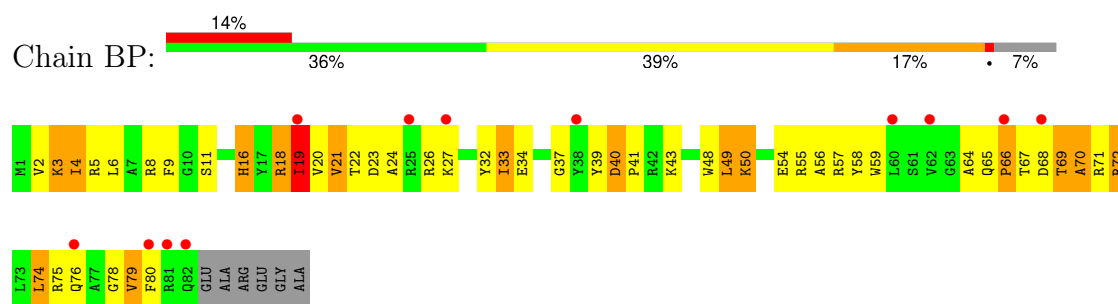


- Molecule 48: 30S ribosomal protein S15

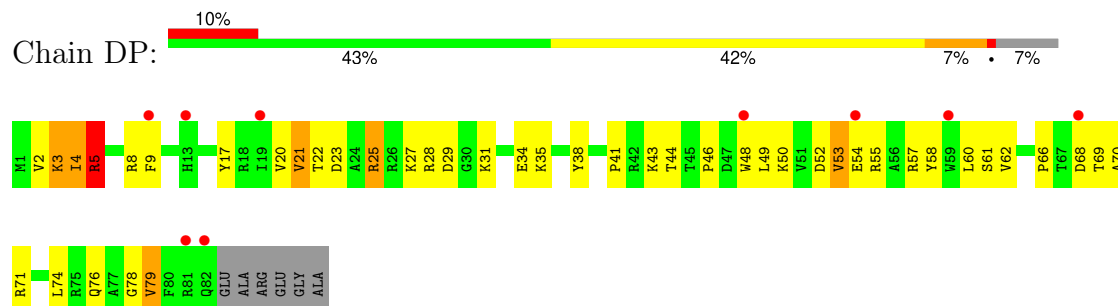
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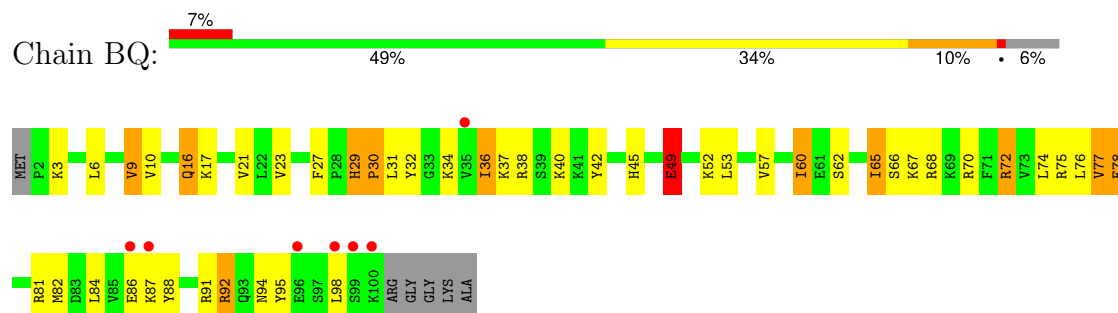
- Molecule 49: 30S ribosomal protein S16



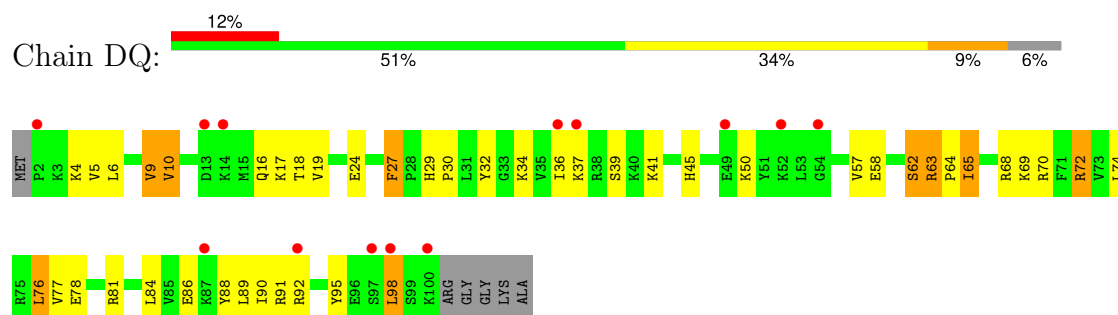
- Molecule 49: 30S ribosomal protein S16



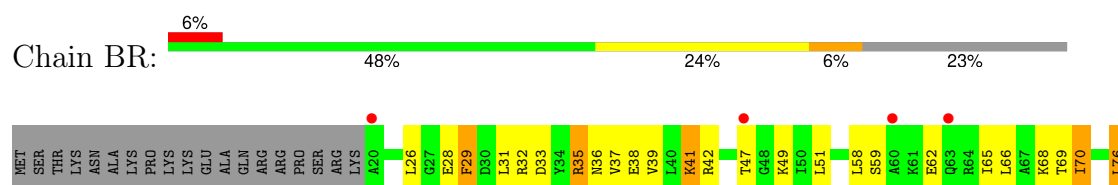
- Molecule 50: 30S ribosomal protein S17

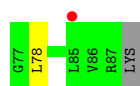


- Molecule 50: 30S ribosomal protein S17

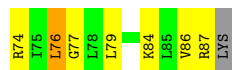
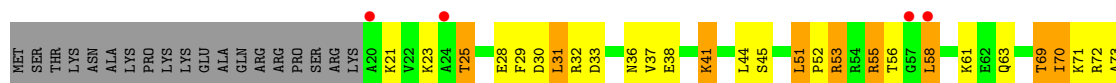


- Molecule 51: 30S ribosomal protein S18

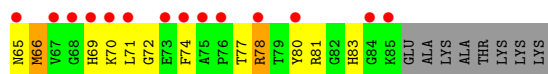
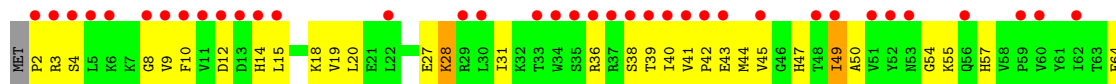
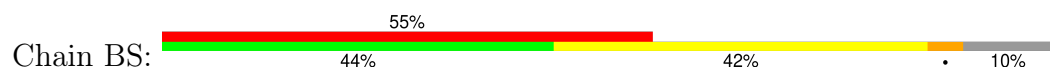




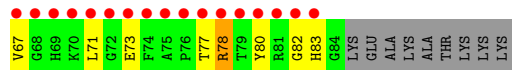
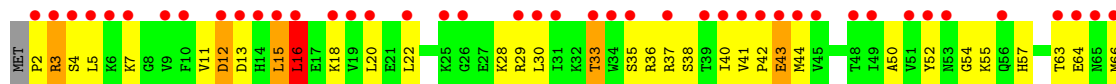
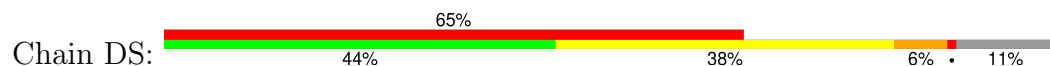
- Molecule 51: 30S ribosomal protein S18



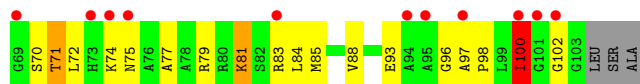
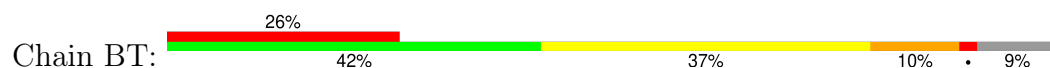
- Molecule 52: 30S ribosomal protein S19



- Molecule 52: 30S ribosomal protein S19

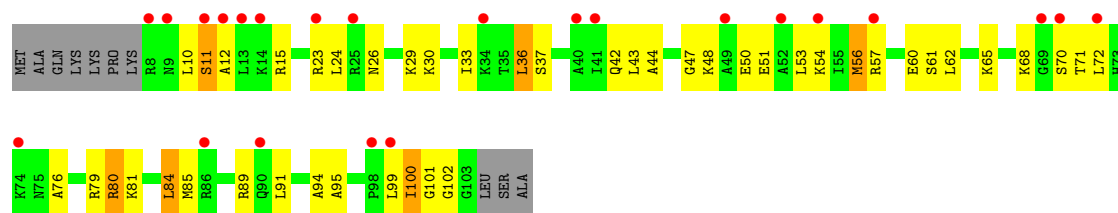


- Molecule 53: 30S ribosomal protein S20

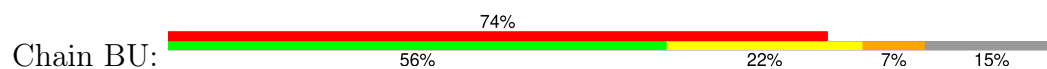


- Molecule 53: 30S ribosomal protein S20





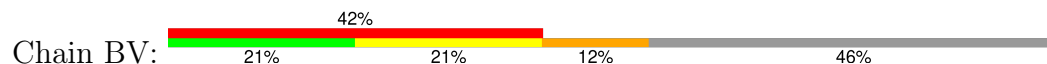
- Molecule 54: 30S ribosomal protein Thx



- Molecule 54: 30S ribosomal protein Thx



- Molecule 55: mRNA



- Molecule 55: mRNA



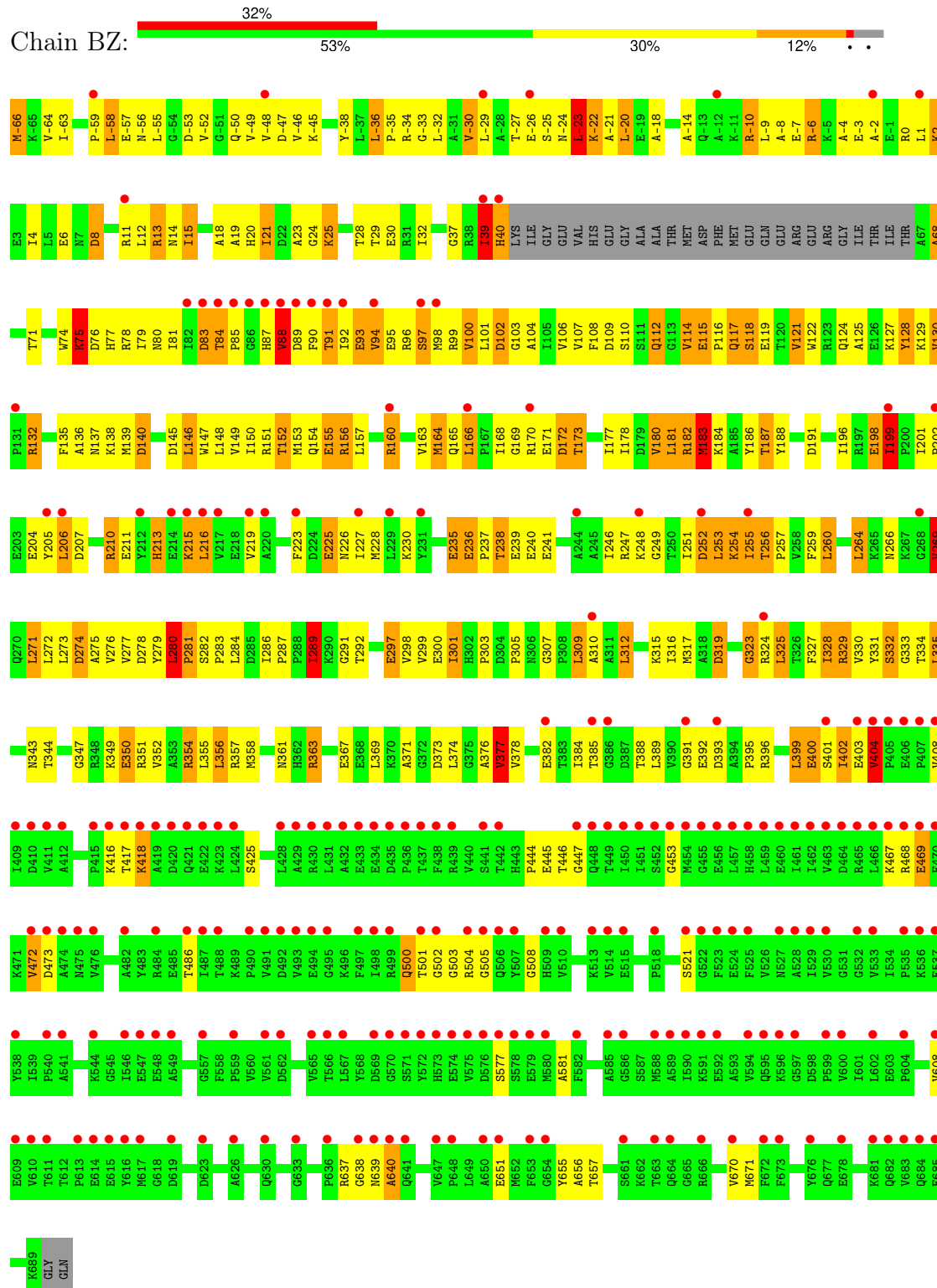
- Molecule 56: P-site tRNA



- Molecule 56: P-site tRNA

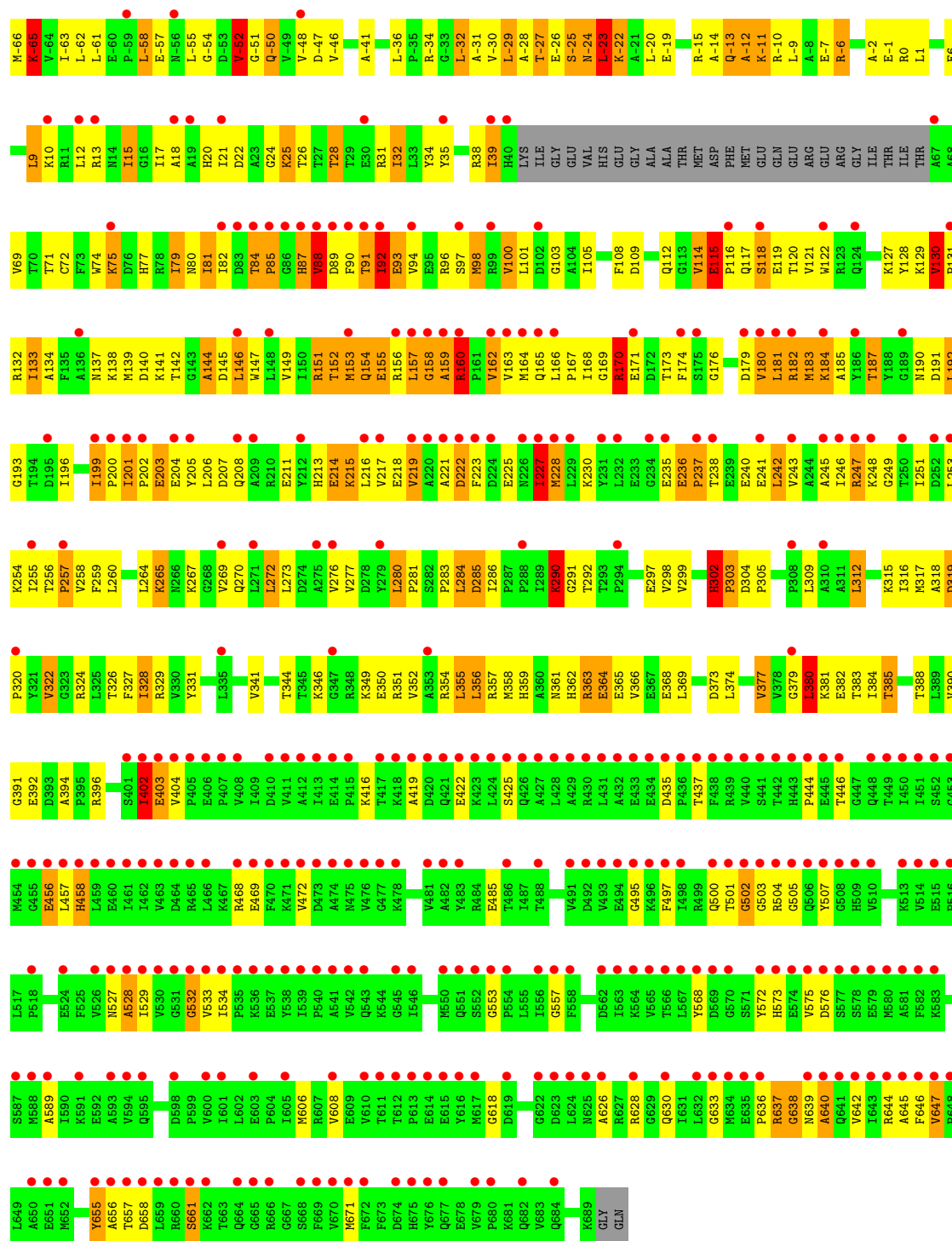


• Molecule 57: 50S ribosomal protein L9,Elongation factor G



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.48Å 448.89Å 622.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.31 – 2.80 49.31 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.8 (49.31-2.80) 96.7 (49.31-2.80)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.221 , 0.266 0.222 , 0.266	Depositor DCC
R_{free} test set	69082 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 77.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	305548	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.76	0/68792	0.95	47/107377 (0.0%)
1	CA	0.54	0/68691	0.74	7/107219 (0.0%)
2	AB	0.63	0/2878	0.90	2/4490 (0.0%)
2	CB	0.38	0/2878	0.58	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	1.17	5/2186 (0.2%)	1.49	26/2944 (0.9%)
4	CD	0.94	1/2192 (0.0%)	1.37	22/2951 (0.7%)
5	AE	1.30	9/1592 (0.6%)	1.62	31/2149 (1.4%)
5	CE	0.87	0/1592	1.26	12/2149 (0.6%)
6	AF	1.16	2/1619 (0.1%)	1.43	23/2193 (1.0%)
6	CF	0.80	0/1615	1.27	11/2188 (0.5%)
7	AG	0.74	0/1450	1.20	8/1959 (0.4%)
7	CG	0.54	0/1449	1.09	10/1958 (0.5%)
8	AH	1.05	2/1356 (0.1%)	1.40	14/1834 (0.8%)
8	CH	0.55	0/1356	1.04	10/1834 (0.5%)
9	AK	0.69	0/640	1.68	11/889 (1.2%)
9	CK	0.50	0/640	1.71	13/889 (1.5%)
10	AL	0.57	0/1044	1.10	9/1416 (0.6%)
10	CL	0.64	0/1044	1.10	15/1416 (1.1%)
11	AN	1.30	3/1144 (0.3%)	1.49	13/1543 (0.8%)
11	CN	0.72	0/1144	1.16	6/1543 (0.4%)
12	AO	1.13	1/943 (0.1%)	1.47	12/1269 (0.9%)
12	CO	0.91	0/943	1.18	1/1269 (0.1%)
13	AP	1.05	0/1156	1.39	11/1537 (0.7%)
13	CP	0.75	0/1152	1.19	8/1533 (0.5%)
14	AQ	1.21	0/1143	1.42	12/1527 (0.8%)
14	CQ	0.80	0/1143	1.17	9/1527 (0.6%)
15	AR	1.29	4/982 (0.4%)	1.41	5/1312 (0.4%)
15	CR	0.83	1/982 (0.1%)	1.16	3/1312 (0.2%)
16	AS	0.92	0/887	1.26	9/1180 (0.8%)
16	CS	0.64	0/880	1.11	2/1172 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AT	1.11	2/1105 (0.2%)	1.36	7/1477 (0.5%)
17	CT	0.81	0/1097	1.18	9/1468 (0.6%)
18	AU	1.42	4/977 (0.4%)	1.52	11/1301 (0.8%)
18	CU	0.81	0/977	1.12	3/1301 (0.2%)
19	AV	1.32	3/782 (0.4%)	1.57	14/1049 (1.3%)
19	CV	0.71	0/782	1.11	4/1049 (0.4%)
20	AW	1.43	6/897 (0.7%)	1.54	9/1205 (0.7%)
20	CW	1.02	2/897 (0.2%)	1.35	10/1205 (0.8%)
21	AX	1.22	3/764 (0.4%)	1.44	6/1025 (0.6%)
21	CX	0.86	0/764	1.34	10/1025 (1.0%)
22	AY	1.09	1/819 (0.1%)	1.47	11/1095 (1.0%)
22	CY	0.74	0/819	1.19	13/1095 (1.2%)
23	AZ	0.91	1/1483 (0.1%)	1.36	17/2017 (0.8%)
23	CZ	0.60	0/1483	1.18	12/2017 (0.6%)
24	A0	1.14	2/662 (0.3%)	1.31	3/881 (0.3%)
24	C0	0.79	0/662	1.22	5/881 (0.6%)
25	A1	1.15	1/762 (0.1%)	1.39	6/1014 (0.6%)
25	C1	0.88	1/762 (0.1%)	1.27	6/1014 (0.6%)
26	A2	1.05	0/590	1.22	2/781 (0.3%)
26	C2	0.71	0/590	1.12	3/781 (0.4%)
27	A3	1.23	0/474	1.55	7/635 (1.1%)
27	C3	0.77	0/469	1.11	1/630 (0.2%)
28	A4	0.62	1/571 (0.2%)	1.27	9/768 (1.2%)
28	C4	0.50	0/545	1.07	6/737 (0.8%)
29	A5	1.44	5/469 (1.1%)	1.64	9/635 (1.4%)
29	C5	0.87	0/469	1.32	5/635 (0.8%)
30	A6	1.09	1/460 (0.2%)	1.25	4/613 (0.7%)
30	C6	0.84	0/456	1.22	3/608 (0.5%)
31	A7	1.31	2/426 (0.5%)	1.44	1/561 (0.2%)
31	C7	0.96	0/426	1.27	3/561 (0.5%)
32	A8	1.25	0/525	1.43	2/691 (0.3%)
32	C8	0.88	0/525	1.24	3/691 (0.4%)
33	A9	1.22	1/310 (0.3%)	1.61	5/407 (1.2%)
33	C9	0.79	0/310	1.14	1/407 (0.2%)
34	BA	0.43	0/35976	0.64	4/56145 (0.0%)
34	DA	0.38	0/36119	0.59	1/56370 (0.0%)
35	BB	0.57	0/1881	1.10	16/2542 (0.6%)
35	DB	0.52	0/1860	1.02	8/2518 (0.3%)
36	BC	0.52	0/1576	0.93	0/2130
36	DC	0.51	0/1568	0.95	4/2122 (0.2%)
37	BD	0.63	0/1689	1.09	10/2267 (0.4%)
37	DD	0.61	0/1708	1.10	6/2289 (0.3%)
38	BE	0.77	0/1145	1.21	11/1543 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DE	0.73	0/1149	1.22	10/1548 (0.6%)
39	BF	0.66	0/825	1.02	1/1118 (0.1%)
39	DF	0.69	0/833	1.06	3/1128 (0.3%)
40	BG	0.54	0/1250	1.00	5/1679 (0.3%)
40	DG	0.45	0/1254	0.93	3/1683 (0.2%)
41	BH	0.77	0/1108	1.18	6/1494 (0.4%)
41	DH	0.63	0/1108	1.10	7/1494 (0.5%)
42	BI	0.51	0/1005	1.04	5/1350 (0.4%)
42	DI	0.50	0/997	0.93	1/1343 (0.1%)
43	BJ	0.49	0/722	1.09	4/982 (0.4%)
43	DJ	0.54	0/727	1.00	3/988 (0.3%)
44	BK	0.66	0/848	1.14	2/1149 (0.2%)
44	DK	0.66	0/848	1.08	4/1149 (0.3%)
45	BL	0.82	0/946	1.21	6/1274 (0.5%)
45	DL	0.71	0/946	1.12	4/1274 (0.3%)
46	BM	0.49	0/933	0.97	4/1253 (0.3%)
46	DM	0.48	0/961	0.93	2/1291 (0.2%)
47	BN	0.55	0/501	0.96	0/664
47	DN	0.47	0/501	0.79	0/664
48	BO	0.78	1/739 (0.1%)	1.15	5/985 (0.5%)
48	DO	0.71	0/739	1.12	4/985 (0.4%)
49	BP	0.71	0/697	1.17	5/939 (0.5%)
49	DP	0.65	0/693	1.13	4/935 (0.4%)
50	BQ	0.74	0/836	1.09	4/1117 (0.4%)
50	DQ	0.70	0/836	1.09	8/1117 (0.7%)
51	BR	0.67	0/560	1.10	2/746 (0.3%)
51	DR	0.69	0/560	0.99	2/746 (0.3%)
52	BS	0.44	0/676	0.90	0/911
52	DS	0.48	0/661	0.92	2/893 (0.2%)
53	BT	0.71	0/730	1.15	1/965 (0.1%)
53	DT	0.64	0/733	1.10	3/969 (0.3%)
54	BU	0.45	0/203	1.02	1/266 (0.4%)
54	DU	0.43	0/203	0.87	0/266
55	BV	0.67	0/310	0.66	0/480
55	DV	0.47	0/144	0.67	0/223
56	BX	0.54	3/1725 (0.2%)	0.72	3/2689 (0.1%)
56	DX	0.46	2/1719 (0.1%)	0.60	0/2677
57	BZ	0.84	1/4927 (0.0%)	1.31	36/6727 (0.5%)
57	DZ	0.74	1/4925 (0.0%)	1.21	37/6724 (0.6%)
All	All	0.68	72/325388 (0.0%)	0.93	840/485060 (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
4	AD	0	3
5	AE	0	1
8	AH	0	1
12	AO	0	2
21	CX	0	1
23	AZ	0	1
37	BD	0	1
53	BT	0	1
57	BZ	0	1
57	DZ	0	4
All	All	0	16

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A1	67	ILE	CA-CB	-11.79	1.48	1.54
6	AF	84	VAL	CA-CB	-9.77	1.42	1.54
19	AV	61	VAL	CA-CB	9.57	1.64	1.53
56	BX	18	G	O3'-P	7.99	1.73	1.61
56	BX	15	G	O3'-P	-7.88	1.49	1.61

The worst 5 of 840 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	CK	128	LEU	CA-C-N	17.30	141.47	119.84
9	CK	128	LEU	C-N-CA	17.30	141.47	119.84
9	AK	76	GLY	CA-C-N	16.63	140.62	119.84
9	AK	76	GLY	C-N-CA	16.63	140.62	119.84
4	AD	71	ASP	N-CA-C	-15.53	94.84	114.56

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	AD	141	VAL	Peptide
4	AD	70	TRP	Peptide
4	AD	98	VAL	Peptide
5	AE	132	HIS	Sidechain
8	AH	23	ARG	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	61426	0	30938	1079	0
1	CA	61337	0	30928	1189	0
2	AB	2573	0	1306	32	0
2	CB	2573	0	1306	45	0
3	AC	1063	0	1089	156	0
3	CC	1063	0	1091	216	0
4	AD	2136	0	2218	113	0
4	CD	2142	0	2229	86	0
5	AE	1559	0	1618	68	0
5	CE	1559	0	1618	60	0
6	AF	1584	0	1625	70	0
6	CF	1580	0	1619	81	0
7	AG	1425	0	1443	65	0
7	CG	1424	0	1434	62	0
8	AH	1330	0	1407	47	0
8	CH	1330	0	1407	50	0
9	AK	641	0	309	22	0
9	CK	641	0	309	11	0
10	AL	1025	0	1066	54	0
10	CL	1025	0	1066	51	0
11	AN	1117	0	1184	34	0
11	CN	1117	0	1184	42	0
12	AO	933	0	996	37	0
12	CO	933	0	996	29	0
13	AP	1139	0	1223	54	0
13	CP	1135	0	1212	55	0
14	AQ	1122	0	1179	55	0
14	CQ	1122	0	1179	53	0
15	AR	968	0	1033	50	0
15	CR	968	0	1033	49	0
16	AS	877	0	938	46	0
16	CS	870	0	923	37	0
17	AT	1091	0	1151	55	0
17	CT	1083	0	1136	47	0
18	AU	959	0	1019	41	0
18	CU	959	0	1018	35	0
19	AV	771	0	829	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	CV	771	0	830	30	0
20	AW	886	0	940	27	0
20	CW	886	0	940	37	0
21	AX	750	0	814	30	0
21	CX	750	0	814	40	0
22	AY	806	0	881	26	0
22	CY	806	0	881	35	0
23	AZ	1451	0	1457	64	0
23	CZ	1451	0	1457	51	0
24	A0	653	0	674	21	0
24	C0	653	0	674	26	0
25	A1	755	0	826	34	0
25	C1	755	0	826	25	0
26	A2	588	0	643	15	0
26	C2	588	0	643	20	0
27	A3	469	0	518	26	0
27	C3	464	0	514	12	0
28	A4	558	0	545	29	0
28	C4	532	0	504	21	0
29	A5	455	0	466	20	0
29	C5	455	0	465	12	0
30	A6	453	0	473	20	0
30	C6	449	0	469	16	0
31	A7	418	0	467	24	0
31	C7	418	0	467	20	0
32	A8	517	0	582	30	0
32	C8	517	0	582	26	0
33	A9	307	0	335	15	0
33	C9	307	0	335	16	0
34	BA	32141	0	16222	669	0
34	DA	32268	0	16287	689	0
35	BB	1846	0	1867	101	0
35	DB	1825	0	1828	92	0
36	BC	1552	0	1546	55	0
36	DC	1544	0	1524	53	0
37	BD	1659	0	1677	97	0
37	DD	1678	0	1719	70	0
38	BE	1129	0	1185	56	0
38	DE	1133	0	1191	66	0
39	BF	812	0	804	29	0
39	DF	820	0	814	31	0
40	BG	1231	0	1238	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	DG	1235	0	1249	24	0
41	BH	1088	0	1126	56	0
41	DH	1088	0	1126	47	0
42	BI	986	0	995	38	0
42	DI	978	0	966	43	0
43	BJ	709	0	650	31	0
43	DJ	714	0	672	38	0
44	BK	833	0	836	34	0
44	DK	833	0	836	27	0
45	BL	930	0	980	25	0
45	DL	930	0	980	42	0
46	BM	923	0	970	33	0
46	DM	950	0	988	40	0
47	BN	492	0	529	19	0
47	DN	492	0	531	34	0
48	BO	728	0	760	37	0
48	DO	728	0	760	32	0
49	BP	681	0	697	36	0
49	DP	677	0	686	28	0
50	BQ	823	0	891	29	0
50	DQ	823	0	891	37	0
51	BR	555	0	618	20	0
51	DR	555	0	618	26	0
52	BS	661	0	675	34	0
52	DS	646	0	644	30	0
53	BT	728	0	798	36	0
53	DT	731	0	807	30	0
54	BU	199	0	208	5	0
54	DU	199	0	208	8	0
55	BV	277	0	140	4	0
55	DV	128	0	67	5	0
56	BX	1625	0	829	23	0
56	DX	1621	0	826	21	0
57	BZ	4869	0	4164	261	0
57	DZ	4867	0	4166	247	0
58	A0	5	0	0	0	0
58	A1	1	0	0	0	0
58	A2	1	0	0	0	0
58	A4	1	0	0	0	0
58	A5	3	0	0	0	0
58	A6	1	0	0	0	0
58	A7	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	A8	2	0	0	0	0
58	A9	1	0	0	0	0
58	AA	820	0	0	0	0
58	AB	23	0	0	0	0
58	AD	12	0	0	0	0
58	AE	5	0	0	0	0
58	AF	8	0	0	0	0
58	AG	2	0	0	0	0
58	AH	2	0	0	0	0
58	AN	3	0	0	0	0
58	AO	1	0	0	0	0
58	AP	3	0	0	0	0
58	AQ	3	0	0	0	0
58	AR	2	0	0	0	0
58	AU	3	0	0	0	0
58	AV	5	0	0	0	0
58	AW	4	0	0	0	0
58	AX	1	0	0	0	0
58	AZ	2	0	0	0	0
58	BA	212	0	0	0	0
58	BB	1	0	0	0	0
58	BD	1	0	0	0	0
58	BE	1	0	0	0	0
58	BF	1	0	0	0	0
58	BK	1	0	0	0	0
58	BL	4	0	0	0	0
58	BN	2	0	0	0	0
58	BT	1	0	0	0	0
58	BV	1	0	0	0	0
58	BX	10	0	0	0	0
58	BZ	1	0	0	0	0
58	C0	1	0	0	0	0
58	C1	1	0	0	0	0
58	C3	1	0	0	0	0
58	C7	1	0	0	0	0
58	C8	1	0	0	0	0
58	CA	666	0	0	0	0
58	CB	13	0	0	0	0
58	CD	3	0	0	0	0
58	CE	7	0	0	0	0
58	CF	4	0	0	0	0
58	CG	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	CN	1	0	0	0	0
58	CO	2	0	0	0	0
58	CQ	4	0	0	0	0
58	CR	1	0	0	0	0
58	CU	2	0	0	0	0
58	CV	2	0	0	0	0
58	CY	1	0	0	0	0
58	DA	166	0	0	0	0
58	DD	1	0	0	0	0
58	DE	2	0	0	0	0
58	DF	1	0	0	0	0
58	DJ	1	0	0	0	0
58	DK	1	0	0	0	0
58	DL	2	0	0	0	0
58	DT	1	0	0	0	0
58	DZ	3	0	0	0	0
59	AA	1	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	0	0
61	DD	8	0	0	0	0
62	BZ	28	0	12	4	0
62	DZ	28	0	12	7	0
63	A0	9	0	0	2	0
63	A1	2	0	0	1	0
63	A2	1	0	0	0	0
63	A3	2	0	0	0	0
63	A5	4	0	0	1	0
63	A7	4	0	0	2	0
63	A8	9	0	0	3	0
63	A9	1	0	0	0	0
63	AA	1406	0	0	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	AB	37	0	0	3	0
63	AD	16	0	0	0	0
63	AE	14	0	0	3	0
63	AF	6	0	0	2	0
63	AG	3	0	0	0	0
63	AH	1	0	0	0	0
63	AN	3	0	0	0	0
63	AO	1	0	0	0	0
63	AP	18	0	0	1	0
63	AQ	5	0	0	1	0
63	AR	2	0	0	0	0
63	AS	1	0	0	0	0
63	AT	3	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	4	0	0	0	0
63	AZ	1	0	0	0	0
63	BA	203	0	0	15	0
63	BD	3	0	0	0	0
63	BE	2	0	0	0	0
63	BG	1	0	0	0	0
63	BJ	1	0	0	0	0
63	BL	1	0	0	0	0
63	BM	1	0	0	0	0
63	BO	2	0	0	0	0
63	BP	1	0	0	0	0
63	BV	3	0	0	0	0
63	BX	5	0	0	0	0
63	BZ	2	0	0	0	0
63	C0	5	0	0	0	0
63	C1	1	0	0	0	0
63	C3	2	0	0	0	0
63	C6	1	0	0	1	0
63	C7	1	0	0	0	0
63	C8	3	0	0	0	0
63	CA	974	0	0	87	0
63	CB	9	0	0	0	0
63	CD	17	0	0	0	0
63	CE	14	0	0	3	0
63	CF	6	0	0	0	0
63	CN	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	CP	12	0	0	2	0
63	CQ	2	0	0	1	0
63	CT	3	0	0	0	0
63	CU	2	0	0	1	0
63	CV	2	0	0	0	0
63	CW	1	0	0	0	0
63	CX	2	0	0	0	0
63	CY	2	0	0	1	0
63	DA	154	0	0	11	0
63	DE	3	0	0	0	0
63	DH	1	0	0	0	0
63	DJ	1	0	0	0	0
63	DK	2	0	0	0	0
63	DP	1	0	0	0	0
63	DT	1	0	0	0	0
63	DV	1	0	0	0	0
63	DZ	1	0	0	0	0
All	All	305548	0	205094	7474	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 7474 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:2128:C:H5''	3:CC:219:MET:CE	1.49	1.42
1:CA:2132:U:O2	3:CC:6:LYS:CB	1.64	1.41
1:CA:2128:C:OP1	3:CC:219:MET:CE	1.71	1.39
1:CA:2176:A:H4'	3:CC:45:HIS:CD2	1.60	1.37
1:AA:2143:G:N2	3:AC:169:THR:OG1	1.58	1.36

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	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%)	239 (88%)	28 (10%)	6 (2%)	5	19
4	CD	273/276 (99%)	234 (86%)	35 (13%)	4 (2%)	8	28
5	AE	202/206 (98%)	181 (90%)	19 (9%)	2 (1%)	12	38
5	CE	202/206 (98%)	178 (88%)	20 (10%)	4 (2%)	6	21
6	AF	201/210 (96%)	182 (90%)	15 (8%)	4 (2%)	6	21
6	CF	201/210 (96%)	181 (90%)	14 (7%)	6 (3%)	3	12
7	AG	179/182 (98%)	152 (85%)	19 (11%)	8 (4%)	2	7
7	CG	179/182 (98%)	148 (83%)	21 (12%)	10 (6%)	1	4
8	AH	172/180 (96%)	152 (88%)	17 (10%)	3 (2%)	7	25
8	CH	172/180 (96%)	149 (87%)	20 (12%)	3 (2%)	7	25
9	AK	128/173 (74%)	66 (52%)	31 (24%)	31 (24%)	0	0
9	CK	128/173 (74%)	77 (60%)	29 (23%)	22 (17%)	0	0
10	AL	137/147 (93%)	105 (77%)	24 (18%)	8 (6%)	1	4
10	CL	137/147 (93%)	97 (71%)	35 (26%)	5 (4%)	2	10
11	AN	138/140 (99%)	127 (92%)	10 (7%)	1 (1%)	18	47
11	CN	138/140 (99%)	127 (92%)	9 (6%)	2 (1%)	9	30
12	AO	120/122 (98%)	106 (88%)	13 (11%)	1 (1%)	16	44
12	CO	120/122 (98%)	108 (90%)	9 (8%)	3 (2%)	4	16
13	AP	147/150 (98%)	133 (90%)	10 (7%)	4 (3%)	4	15
13	CP	147/150 (98%)	124 (84%)	18 (12%)	5 (3%)	3	11
14	AQ	139/141 (99%)	126 (91%)	11 (8%)	2 (1%)	9	30
14	CQ	139/141 (99%)	124 (89%)	12 (9%)	3 (2%)	5	19
15	AR	116/118 (98%)	105 (90%)	9 (8%)	2 (2%)	7	25
15	CR	116/118 (98%)	100 (86%)	14 (12%)	2 (2%)	7	25
16	AS	108/112 (96%)	92 (85%)	12 (11%)	4 (4%)	2	9
16	CS	108/112 (96%)	91 (84%)	13 (12%)	4 (4%)	2	9
17	AT	129/146 (88%)	115 (89%)	13 (10%)	1 (1%)	16	44
17	CT	129/146 (88%)	118 (92%)	9 (7%)	2 (2%)	7	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AU	114/118 (97%)	106 (93%)	6 (5%)	2 (2%)	6	23
18	CU	114/118 (97%)	102 (90%)	11 (10%)	1 (1%)	14	41
19	AV	99/101 (98%)	90 (91%)	6 (6%)	3 (3%)	3	12
19	CV	99/101 (98%)	85 (86%)	9 (9%)	5 (5%)	1	5
20	AW	110/113 (97%)	99 (90%)	9 (8%)	2 (2%)	6	23
20	CW	110/113 (97%)	97 (88%)	11 (10%)	2 (2%)	6	23
21	AX	93/96 (97%)	83 (89%)	9 (10%)	1 (1%)	11	36
21	CX	93/96 (97%)	75 (81%)	14 (15%)	4 (4%)	2	7
22	AY	105/110 (96%)	90 (86%)	11 (10%)	4 (4%)	2	9
22	CY	105/110 (96%)	82 (78%)	21 (20%)	2 (2%)	6	22
23	AZ	183/206 (89%)	147 (80%)	23 (13%)	13 (7%)	1	2
23	CZ	183/206 (89%)	147 (80%)	24 (13%)	12 (7%)	1	3
24	A0	81/85 (95%)	72 (89%)	7 (9%)	2 (2%)	4	16
24	C0	81/85 (95%)	73 (90%)	7 (9%)	1 (1%)	10	34
25	A1	95/98 (97%)	90 (95%)	3 (3%)	2 (2%)	5	20
25	C1	95/98 (97%)	88 (93%)	4 (4%)	3 (3%)	3	11
26	A2	68/72 (94%)	59 (87%)	9 (13%)	0	100	100
26	C2	68/72 (94%)	60 (88%)	7 (10%)	1 (2%)	8	28
27	A3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	C3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	A4	67/71 (94%)	45 (67%)	15 (22%)	7 (10%)	0	1
28	C4	67/71 (94%)	52 (78%)	10 (15%)	5 (8%)	1	2
29	A5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
29	C5	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
30	A6	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
30	C6	51/54 (94%)	44 (86%)	6 (12%)	1 (2%)	6	21
31	A7	46/49 (94%)	41 (89%)	5 (11%)	0	100	100
31	C7	46/49 (94%)	39 (85%)	6 (13%)	1 (2%)	5	19
32	A8	62/65 (95%)	54 (87%)	5 (8%)	3 (5%)	2	6
32	C8	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
33	A9	35/37 (95%)	34 (97%)	0	1 (3%)	3	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	C9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
35	BB	229/256 (90%)	174 (76%)	42 (18%)	13 (6%)	1	4
35	DB	229/256 (90%)	176 (77%)	40 (18%)	13 (6%)	1	4
36	BC	204/239 (85%)	165 (81%)	32 (16%)	7 (3%)	3	11
36	DC	204/239 (85%)	172 (84%)	30 (15%)	2 (1%)	12	38
37	BD	206/209 (99%)	150 (73%)	42 (20%)	14 (7%)	1	2
37	DD	206/209 (99%)	165 (80%)	30 (15%)	11 (5%)	1	5
38	BE	146/162 (90%)	123 (84%)	17 (12%)	6 (4%)	2	8
38	DE	146/162 (90%)	122 (84%)	19 (13%)	5 (3%)	3	11
39	BF	98/101 (97%)	84 (86%)	10 (10%)	4 (4%)	2	8
39	DF	98/101 (97%)	86 (88%)	12 (12%)	0	100	100
40	BG	153/156 (98%)	127 (83%)	20 (13%)	6 (4%)	2	8
40	DG	153/156 (98%)	127 (83%)	19 (12%)	7 (5%)	2	6
41	BH	135/138 (98%)	111 (82%)	17 (13%)	7 (5%)	1	5
41	DH	135/138 (98%)	120 (89%)	13 (10%)	2 (2%)	8	28
42	BI	125/128 (98%)	105 (84%)	14 (11%)	6 (5%)	2	6
42	DI	125/128 (98%)	109 (87%)	15 (12%)	1 (1%)	16	44
43	BJ	95/105 (90%)	80 (84%)	12 (13%)	3 (3%)	3	11
43	DJ	94/105 (90%)	76 (81%)	9 (10%)	9 (10%)	0	1
44	BK	112/129 (87%)	94 (84%)	16 (14%)	2 (2%)	6	23
44	DK	112/129 (87%)	93 (83%)	15 (13%)	4 (4%)	2	10
45	BL	120/132 (91%)	108 (90%)	12 (10%)	0	100	100
45	DL	120/132 (91%)	109 (91%)	9 (8%)	2 (2%)	7	25
46	BM	115/126 (91%)	97 (84%)	15 (13%)	3 (3%)	4	15
46	DM	120/126 (95%)	96 (80%)	18 (15%)	6 (5%)	1	5
47	BN	58/61 (95%)	46 (79%)	10 (17%)	2 (3%)	3	11
47	DN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
48	BO	86/89 (97%)	71 (83%)	15 (17%)	0	100	100
48	DO	86/89 (97%)	72 (84%)	10 (12%)	4 (5%)	2	6
49	BP	80/88 (91%)	55 (69%)	19 (24%)	6 (8%)	1	2
49	DP	80/88 (91%)	67 (84%)	10 (12%)	3 (4%)	2	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	BQ	97/105 (92%)	87 (90%)	8 (8%)	2 (2%)	5	20
50	DQ	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
51	BR	66/88 (75%)	57 (86%)	9 (14%)	0	100	100
51	DR	66/88 (75%)	56 (85%)	9 (14%)	1 (2%)	8	28
52	BS	82/93 (88%)	71 (87%)	10 (12%)	1 (1%)	10	34
52	DS	81/93 (87%)	69 (85%)	8 (10%)	4 (5%)	1	6
53	BT	94/106 (89%)	81 (86%)	5 (5%)	8 (8%)	0	1
53	DT	94/106 (89%)	80 (85%)	10 (11%)	4 (4%)	2	7
54	BU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
54	DU	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2	6
57	BZ	726/758 (96%)	561 (77%)	115 (16%)	50 (7%)	1	2
57	DZ	726/758 (96%)	558 (77%)	113 (16%)	55 (8%)	1	2
All	All	13389/14444 (93%)	11204 (84%)	1645 (12%)	540 (4%)	2	8

5 of 540 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	42	VAL
3	AC	47	LYS
3	AC	68	GLY
3	AC	180	SER
3	AC	181	PHE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	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%)	174 (81%)	41 (19%)	1	5
4	CD	216/218 (99%)	176 (82%)	40 (18%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AE	164/166 (99%)	125 (76%)	39 (24%)	1	3
5	CE	164/166 (99%)	133 (81%)	31 (19%)	1	5
6	AF	160/166 (96%)	121 (76%)	39 (24%)	1	2
6	CF	159/166 (96%)	126 (79%)	33 (21%)	1	4
7	AG	143/156 (92%)	110 (77%)	33 (23%)	1	3
7	CG	142/156 (91%)	108 (76%)	34 (24%)	1	3
8	AH	144/148 (97%)	122 (85%)	22 (15%)	3	10
8	CH	144/148 (97%)	118 (82%)	26 (18%)	2	6
10	AL	104/111 (94%)	85 (82%)	19 (18%)	2	6
10	CL	104/111 (94%)	79 (76%)	25 (24%)	1	2
11	AN	118/119 (99%)	89 (75%)	29 (25%)	1	2
11	CN	118/119 (99%)	93 (79%)	25 (21%)	1	4
12	AO	100/100 (100%)	82 (82%)	18 (18%)	2	6
12	CO	100/100 (100%)	81 (81%)	19 (19%)	1	5
13	AP	116/116 (100%)	89 (77%)	27 (23%)	1	3
13	CP	115/116 (99%)	93 (81%)	22 (19%)	1	5
14	AQ	111/111 (100%)	90 (81%)	21 (19%)	1	5
14	CQ	111/111 (100%)	92 (83%)	19 (17%)	2	7
15	AR	101/101 (100%)	82 (81%)	19 (19%)	1	5
15	CR	101/101 (100%)	78 (77%)	23 (23%)	1	3
16	AS	87/88 (99%)	71 (82%)	16 (18%)	1	6
16	CS	85/88 (97%)	63 (74%)	22 (26%)	0	2
17	AT	115/127 (91%)	95 (83%)	20 (17%)	2	7
17	CT	113/127 (89%)	83 (74%)	30 (26%)	0	2
18	AU	93/94 (99%)	79 (85%)	14 (15%)	3	10
18	CU	93/94 (99%)	75 (81%)	18 (19%)	1	5
19	AV	80/82 (98%)	61 (76%)	19 (24%)	1	3
19	CV	80/82 (98%)	65 (81%)	15 (19%)	1	5
20	AW	90/92 (98%)	72 (80%)	18 (20%)	1	4
20	CW	90/92 (98%)	74 (82%)	16 (18%)	2	6
21	AX	77/78 (99%)	67 (87%)	10 (13%)	4	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	CX	77/78 (99%)	65 (84%)	12 (16%)	2	9
22	AY	85/91 (93%)	69 (81%)	16 (19%)	1	5
22	CY	85/91 (93%)	62 (73%)	23 (27%)	0	1
23	AZ	156/179 (87%)	120 (77%)	36 (23%)	1	3
23	CZ	156/179 (87%)	131 (84%)	25 (16%)	2	9
24	A0	65/67 (97%)	59 (91%)	6 (9%)	8	27
24	C0	65/67 (97%)	59 (91%)	6 (9%)	8	27
25	A1	80/83 (96%)	64 (80%)	16 (20%)	1	4
25	C1	80/83 (96%)	69 (86%)	11 (14%)	3	12
26	A2	65/67 (97%)	53 (82%)	12 (18%)	1	6
26	C2	65/67 (97%)	55 (85%)	10 (15%)	2	10
27	A3	51/52 (98%)	40 (78%)	11 (22%)	1	3
27	C3	50/52 (96%)	37 (74%)	13 (26%)	0	2
28	A4	60/63 (95%)	51 (85%)	9 (15%)	3	10
28	C4	53/63 (84%)	39 (74%)	14 (26%)	0	2
29	A5	50/52 (96%)	42 (84%)	8 (16%)	2	9
29	C5	50/52 (96%)	38 (76%)	12 (24%)	1	2
30	A6	51/52 (98%)	38 (74%)	13 (26%)	0	2
30	C6	50/52 (96%)	40 (80%)	10 (20%)	1	4
31	A7	41/42 (98%)	36 (88%)	5 (12%)	5	16
31	C7	41/42 (98%)	30 (73%)	11 (27%)	0	1
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%)	32 (94%)	2 (6%)	18	48
33	C9	34/34 (100%)	30 (88%)	4 (12%)	5	17
35	BB	192/220 (87%)	148 (77%)	44 (23%)	1	3
35	DB	187/220 (85%)	153 (82%)	34 (18%)	2	6
36	BC	143/188 (76%)	129 (90%)	14 (10%)	7	25
36	DC	141/188 (75%)	111 (79%)	30 (21%)	1	4
37	BD	170/181 (94%)	137 (81%)	33 (19%)	1	5
37	DD	174/181 (96%)	137 (79%)	37 (21%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BE	113/123 (92%)	96 (85%)	17 (15%)	3	10
38	DE	114/123 (93%)	91 (80%)	23 (20%)	1	4
39	BF	84/90 (93%)	69 (82%)	15 (18%)	2	6
39	DF	86/90 (96%)	75 (87%)	11 (13%)	4	15
40	BG	119/127 (94%)	95 (80%)	24 (20%)	1	4
40	DG	120/127 (94%)	106 (88%)	14 (12%)	5	18
41	BH	114/119 (96%)	86 (75%)	28 (25%)	1	2
41	DH	114/119 (96%)	94 (82%)	20 (18%)	2	7
42	BI	91/99 (92%)	73 (80%)	18 (20%)	1	5
42	DI	89/99 (90%)	73 (82%)	16 (18%)	2	6
43	BJ	66/92 (72%)	58 (88%)	8 (12%)	5	16
43	DJ	69/92 (75%)	65 (94%)	4 (6%)	18	49
44	BK	83/99 (84%)	71 (86%)	12 (14%)	3	11
44	DK	83/99 (84%)	72 (87%)	11 (13%)	4	14
45	BL	97/109 (89%)	80 (82%)	17 (18%)	2	7
45	DL	97/109 (89%)	79 (81%)	18 (19%)	1	5
46	BM	91/101 (90%)	75 (82%)	16 (18%)	2	7
46	DM	92/101 (91%)	80 (87%)	12 (13%)	4	14
47	BN	49/50 (98%)	37 (76%)	12 (24%)	1	2
47	DN	49/50 (98%)	41 (84%)	8 (16%)	2	8
48	BO	78/80 (98%)	67 (86%)	11 (14%)	3	12
48	DO	78/80 (98%)	63 (81%)	15 (19%)	1	5
49	BP	69/74 (93%)	54 (78%)	15 (22%)	1	3
49	DP	68/74 (92%)	55 (81%)	13 (19%)	1	5
50	BQ	94/97 (97%)	79 (84%)	15 (16%)	2	9
50	DQ	94/97 (97%)	86 (92%)	8 (8%)	10	31
51	BR	59/77 (77%)	50 (85%)	9 (15%)	3	10
51	DR	59/77 (77%)	45 (76%)	14 (24%)	1	3
52	BS	70/80 (88%)	62 (89%)	8 (11%)	5	19
52	DS	67/80 (84%)	57 (85%)	10 (15%)	3	10
53	BT	70/82 (85%)	52 (74%)	18 (26%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	DT	71/82 (87%)	62 (87%)	9 (13%)	4	15
54	BU	18/22 (82%)	16 (89%)	2 (11%)	6	20
54	DU	18/22 (82%)	18 (100%)	0	100	100
57	BZ	369/636 (58%)	260 (70%)	109 (30%)	0	1
57	DZ	370/636 (58%)	266 (72%)	104 (28%)	0	1
All	All	10306/11672 (88%)	8323 (81%)	1983 (19%)	1	5

5 of 1983 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
57	BZ	83	ASP
45	DL	8	ASN
7	CG	148	MET
42	DI	108	VAL
57	DZ	-6	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 209 such sidechains are listed below:

Mol	Chain	Res	Type
4	CD	116	GLN
17	CT	38	ASN
48	DO	13	GLN
5	CE	48	GLN
10	CL	103	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2845/2915 (97%)	568 (19%)	43 (1%)
1	CA	2839/2915 (97%)	584 (20%)	33 (1%)
2	AB	119/121 (98%)	25 (21%)	1 (0%)
2	CB	119/121 (98%)	23 (19%)	0
34	BA	1491/1521 (98%)	300 (20%)	18 (1%)
34	DA	1498/1521 (98%)	297 (19%)	20 (1%)
55	BV	12/24 (50%)	7 (58%)	0
55	DV	5/24 (20%)	1 (20%)	0
56	BX	75/77 (97%)	15 (20%)	1 (1%)
56	DX	75/77 (97%)	11 (14%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	9078/9316 (97%)	1831 (20%)	116 (1%)

5 of 1831 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	12	U
1	AA	13	A
1	AA	17	G
1	AA	34	C
1	AA	36	G

5 of 116 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	BA	1067	A
34	DA	1065	U
1	CA	774	A
34	DA	1064	G
34	DA	428	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	4SU	DX	8	56	18,21,22	1.72	4 (22%)	25,30,33	2.08	7 (28%)
56	5MC	BX	32	56	19,22,23	1.41	3 (15%)	26,32,35	1.13	2 (7%)
56	5MC	DX	32	56	19,22,23	2.18	2 (10%)	26,32,35	1.27	4 (15%)
56	4SU	BX	8	56	18,21,22	1.82	5 (27%)	25,30,33	2.55	7 (28%)
56	5MU	DX	54	56	19,22,23	1.38	5 (26%)	27,32,35	2.19	8 (29%)
56	PSU	BX	55	56	18,21,22	1.35	1 (5%)	21,30,33	2.22	4 (19%)
56	5MU	BX	54	56,58	19,22,23	1.59	6 (31%)	27,32,35	1.96	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	PSU	DX	55	56	18,21,22	1.41	2 (11%)	21,30,33	1.93	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	4SU	DX	8	56	-	0/7/25/26	0/2/2/2
56	5MC	BX	32	56	-	0/7/25/26	0/2/2/2
56	5MC	DX	32	56	-	0/7/25/26	0/2/2/2
56	4SU	BX	8	56	-	0/7/25/26	0/2/2/2
56	5MU	DX	54	56	-	0/7/25/26	0/2/2/2
56	PSU	BX	55	56	-	0/7/25/26	0/2/2/2
56	5MU	BX	54	56,58	-	0/7/25/26	0/2/2/2
56	PSU	DX	55	56	-	0/7/25/26	0/2/2/2

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	DX	32	5MC	C5-C4	8.29	1.50	1.44
56	BX	8	4SU	C4-S4	-5.02	1.59	1.68
56	BX	55	PSU	C6-C5	4.52	1.40	1.35
56	DX	8	4SU	C4-S4	-4.50	1.60	1.68
56	BX	32	5MC	C5-C4	4.28	1.47	1.44

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	BX	8	4SU	C4-N3-C2	-7.02	120.58	127.31
56	BX	8	4SU	C5-C4-N3	6.72	121.00	114.75
56	BX	55	PSU	N1-C2-N3	6.20	121.71	115.17
56	DX	8	4SU	C4-N3-C2	-6.07	121.50	127.31
56	DX	55	PSU	N1-C2-N3	5.87	121.36	115.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	DX	8	4SU	1	0
56	BX	32	5MC	3	0
56	BX	8	4SU	1	0
56	DX	55	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2062 ligands modelled in this entry, 2058 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	801	58	29,30,30	1.23	4 (13%)	45,47,47	1.78	6 (13%)
61	SF4	BD	501	37	0,12,12	-	-	-		
62	GDP	DZ	704	58	29,30,30	1.33	5 (17%)	45,47,47	1.78	9 (20%)
61	SF4	DD	501	37	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	801	58	-	5/16/32/32	0/3/3/3
61	SF4	BD	501	37	-	-	0/6/5/5
62	GDP	DZ	704	58	-	4/16/32/32	0/3/3/3
61	SF4	DD	501	37	-	-	0/6/5/5

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	DZ	704	GDP	C5-C4	2.96	1.46	1.38
62	DZ	704	GDP	PA-O3A	2.91	1.62	1.59
62	BZ	801	GDP	C5-C4	2.83	1.46	1.38
62	BZ	801	GDP	C5-N7	-2.62	1.33	1.39
62	DZ	704	GDP	C4-N9	-2.58	1.31	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	BZ	801	GDP	C5-C4-N3	-5.74	119.25	128.39
62	DZ	704	GDP	C5-C4-N3	-5.50	119.64	128.39
62	BZ	801	GDP	C2-N3-C4	4.97	120.86	112.30
62	DZ	704	GDP	C2-N3-C4	4.44	119.95	112.30
62	DZ	704	GDP	N9-C4-N3	3.98	133.90	125.95

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	DZ	704	GDP	C5'-O5'-PA-O3A
62	DZ	704	GDP	C5'-O5'-PA-O2A
62	DZ	704	GDP	O4'-C4'-C5'-O5'
62	DZ	704	GDP	C3'-C4'-C5'-O5'
62	BZ	801	GDP	O4'-C4'-C5'-O5'

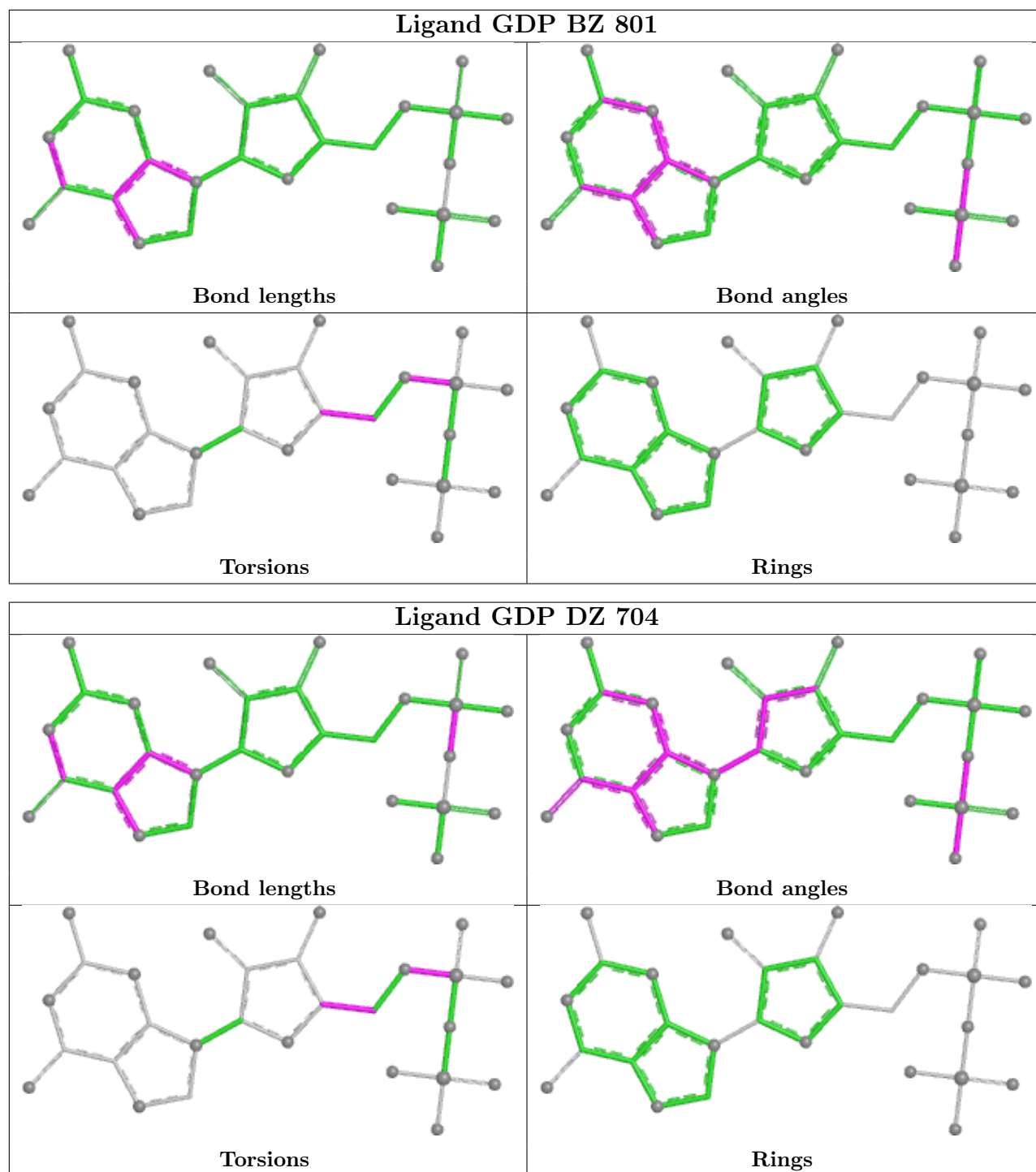
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	BZ	801	GDP	4	0
62	DZ	704	GDP	7	0

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

equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

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	2852/2915 (97%)	-0.45	117 (4%) 41 33	14, 34, 140, 350	0
1	CA	2848/2915 (97%)	0.16	197 (6%) 23 16	27, 57, 179, 341	0
2	AB	120/121 (99%)	-0.18	1 (0%) 82 75	23, 50, 72, 108	0
2	CB	120/121 (99%)	0.93	5 (4%) 40 32	64, 91, 118, 166	0
3	AC	137/228 (60%)	3.49	125 (91%) 0 0	132, 205, 251, 280	0
3	CC	137/228 (60%)	3.16	116 (84%) 0 0	144, 214, 251, 276	0
4	AD	275/276 (99%)	-0.35	3 (1%) 78 70	12, 34, 59, 136	0
4	CD	275/276 (99%)	-0.01	4 (1%) 72 63	23, 47, 73, 128	0
5	AE	204/206 (99%)	-0.42	1 (0%) 87 82	5, 33, 57, 80	0
5	CE	204/206 (99%)	0.43	11 (5%) 31 24	20, 62, 106, 135	0
6	AF	203/210 (96%)	-0.28	2 (0%) 79 72	11, 35, 77, 171	0
6	CF	203/210 (96%)	0.35	5 (2%) 58 48	21, 62, 105, 154	0
7	AG	181/182 (99%)	1.03	32 (17%) 4 3	36, 76, 134, 205	0
7	CG	181/182 (99%)	1.77	70 (38%) 1 0	72, 111, 173, 199	0
8	AH	174/180 (96%)	0.00	4 (2%) 61 51	25, 45, 68, 110	0
8	CH	174/180 (96%)	1.63	53 (30%) 1 1	63, 112, 161, 197	0
9	AK	130/173 (75%)	1.97	55 (42%) 0 0	46, 103, 172, 216	0
9	CK	130/173 (75%)	2.91	98 (75%) 0 0	74, 159, 199, 218	0
10	AL	139/147 (94%)	2.57	101 (72%) 0 0	96, 170, 224, 247	0
10	CL	139/147 (94%)	3.39	118 (84%) 0 0	126, 194, 241, 274	0
11	AN	140/140 (100%)	-0.40	0 100 100	14, 27, 59, 93	0
11	CN	140/140 (100%)	0.74	9 (6%) 25 18	32, 70, 108, 151	0
12	AO	122/122 (100%)	-0.39	0 100 100	18, 36, 61, 77	0
12	CO	122/122 (100%)	0.27	3 (2%) 58 48	36, 57, 84, 107	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AP	149/150 (99%)	-0.01	3 (2%) 65 56	11, 42, 80, 108	0
13	CP	149/150 (99%)	0.61	7 (4%) 36 29	30, 67, 115, 135	0
14	AQ	141/141 (100%)	-0.29	2 (1%) 73 64	12, 33, 54, 82	0
14	CQ	141/141 (100%)	0.73	7 (4%) 34 26	37, 69, 99, 119	0
15	AR	118/118 (100%)	-0.51	0 100 100	16, 29, 45, 54	0
15	CR	118/118 (100%)	0.33	1 (0%) 82 75	33, 55, 89, 103	0
16	AS	110/112 (98%)	0.05	0 100 100	30, 50, 80, 92	0
16	CS	110/112 (98%)	1.21	15 (13%) 7 5	46, 85, 120, 150	0
17	AT	131/146 (89%)	-0.05	4 (3%) 51 41	23, 40, 90, 169	0
17	CT	131/146 (89%)	0.59	6 (4%) 37 29	42, 65, 106, 141	0
18	AU	116/118 (98%)	-0.58	0 100 100	9, 22, 39, 87	0
18	CU	116/118 (98%)	0.62	1 (0%) 81 74	27, 65, 92, 105	0
19	AV	101/101 (100%)	-0.68	0 100 100	9, 28, 49, 73	0
19	CV	101/101 (100%)	0.59	6 (5%) 28 21	35, 78, 111, 165	0
20	AW	112/113 (99%)	-0.49	0 100 100	13, 25, 43, 110	0
20	CW	112/113 (99%)	0.15	1 (0%) 81 74	28, 49, 80, 117	0
21	AX	95/96 (98%)	-0.21	2 (2%) 63 54	15, 34, 68, 98	0
21	CX	95/96 (98%)	0.44	3 (3%) 50 40	38, 60, 85, 105	0
22	AY	107/110 (97%)	0.06	2 (1%) 66 57	23, 44, 84, 162	0
22	CY	107/110 (97%)	0.93	11 (10%) 12 9	45, 74, 115, 169	0
23	AZ	185/206 (89%)	0.36	7 (3%) 44 35	28, 56, 91, 145	0
23	CZ	185/206 (89%)	1.59	54 (29%) 1 1	61, 104, 149, 210	0
24	A0	83/85 (97%)	0.12	7 (8%) 17 12	12, 35, 83, 218	0
24	C0	83/85 (97%)	1.11	15 (18%) 3 3	42, 66, 119, 223	0
25	A1	97/98 (98%)	0.00	2 (2%) 63 54	20, 43, 78, 101	0
25	C1	97/98 (98%)	0.26	4 (4%) 41 33	30, 51, 89, 127	0
26	A2	70/72 (97%)	-0.01	2 (2%) 53 43	24, 43, 70, 121	0
26	C2	70/72 (97%)	0.82	9 (12%) 7 6	47, 71, 100, 116	0
27	A3	59/60 (98%)	-0.39	0 100 100	15, 29, 54, 99	0
27	C3	59/60 (98%)	0.94	3 (5%) 33 25	45, 72, 111, 147	0
28	A4	69/71 (97%)	1.58	24 (34%) 1 0	60, 117, 203, 232	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	C4	69/71 (97%)	1.89	27 (39%) 1 0	80, 157, 202, 217	0
29	A5	59/60 (98%)	-0.63	0 100 100	9, 25, 40, 52	0
29	C5	59/60 (98%)	0.04	0 100 100	26, 51, 89, 104	0
30	A6	53/54 (98%)	-0.41	0 100 100	22, 40, 54, 74	0
30	C6	53/54 (98%)	0.31	0 100 100	40, 59, 79, 105	0
31	A7	48/49 (97%)	-0.26	2 (4%) 40 32	13, 24, 68, 133	0
31	C7	48/49 (97%)	-0.02	4 (8%) 17 12	26, 39, 95, 118	0
32	A8	64/65 (98%)	-0.40	0 100 100	15, 28, 45, 65	0
32	C8	64/65 (98%)	0.13	0 100 100	37, 51, 71, 85	0
33	A9	37/37 (100%)	-0.27	0 100 100	23, 35, 56, 66	0
33	C9	37/37 (100%)	1.15	8 (21%) 2 2	45, 77, 95, 127	0
34	BA	1495/1521 (98%)	0.81	159 (10%) 11 8	31, 83, 186, 328	0
34	DA	1501/1521 (98%)	0.85	184 (12%) 8 6	38, 89, 195, 331	0
35	BB	231/256 (90%)	1.43	53 (22%) 2 1	42, 104, 170, 215	0
35	DB	231/256 (90%)	1.68	70 (30%) 1 1	70, 123, 177, 208	0
36	BC	206/239 (86%)	1.65	59 (28%) 1 1	56, 117, 174, 195	0
36	DC	206/239 (86%)	1.86	83 (40%) 0 0	68, 136, 180, 209	0
37	BD	208/209 (99%)	1.28	41 (19%) 3 2	44, 86, 137, 185	0
37	DD	208/209 (99%)	1.16	34 (16%) 4 4	58, 85, 135, 197	0
38	BE	148/162 (91%)	0.62	7 (4%) 36 29	34, 72, 104, 126	0
38	DE	148/162 (91%)	0.88	10 (6%) 23 17	49, 79, 116, 178	0
39	BF	100/101 (99%)	0.89	4 (4%) 42 33	55, 85, 116, 135	0
39	DF	100/101 (99%)	0.76	1 (1%) 79 72	47, 86, 117, 133	0
40	BG	155/156 (99%)	1.55	44 (28%) 1 1	67, 112, 179, 223	0
40	DG	155/156 (99%)	1.76	61 (39%) 1 0	69, 131, 189, 215	0
41	BH	137/138 (99%)	0.60	2 (1%) 72 63	47, 72, 99, 118	0
41	DH	137/138 (99%)	0.92	13 (9%) 14 10	56, 80, 109, 141	0
42	BI	127/128 (99%)	2.29	70 (55%) 0 0	64, 124, 167, 195	0
42	DI	127/128 (99%)	2.58	79 (62%) 0 0	88, 143, 190, 213	0
43	BJ	97/105 (92%)	2.20	49 (50%) 0 0	80, 129, 183, 210	0
43	DJ	96/105 (91%)	2.44	58 (60%) 0 0	90, 150, 196, 218	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BK	114/129 (88%)	0.83	14 (12%) 8 6	35, 78, 125, 148	0
44	DK	114/129 (88%)	0.93	13 (11%) 10 7	50, 89, 115, 170	0
45	BL	122/132 (92%)	0.36	4 (3%) 49 39	36, 58, 77, 111	0
45	DL	122/132 (92%)	0.74	10 (8%) 17 13	46, 70, 94, 115	0
46	BM	117/126 (92%)	2.32	57 (48%) 0 0	76, 135, 181, 201	0
46	DM	122/126 (96%)	2.47	64 (52%) 0 0	93, 150, 196, 255	0
47	BN	60/61 (98%)	2.30	34 (56%) 0 0	65, 111, 146, 169	0
47	DN	60/61 (98%)	2.94	48 (80%) 0 0	97, 138, 173, 193	0
48	BO	88/89 (98%)	0.74	4 (4%) 38 30	36, 70, 106, 119	0
48	DO	88/89 (98%)	0.79	9 (10%) 12 9	46, 70, 105, 153	0
49	BP	82/88 (93%)	1.38	12 (14%) 6 4	49, 79, 118, 168	0
49	DP	82/88 (93%)	1.12	9 (10%) 10 8	53, 77, 112, 154	0
50	BQ	99/105 (94%)	0.80	7 (7%) 22 16	44, 71, 98, 124	0
50	DQ	99/105 (94%)	0.98	13 (13%) 7 6	43, 77, 104, 115	0
51	BR	68/88 (77%)	0.84	5 (7%) 20 15	41, 79, 122, 133	0
51	DR	68/88 (77%)	0.75	4 (5%) 28 21	52, 82, 127, 143	0
52	BS	84/93 (90%)	2.56	51 (60%) 0 0	95, 144, 193, 207	0
52	DS	83/93 (89%)	2.87	60 (72%) 0 0	90, 164, 211, 224	0
53	BT	96/106 (90%)	1.50	28 (29%) 1 1	60, 83, 123, 164	0
53	DT	96/106 (90%)	1.27	23 (23%) 2 1	56, 85, 134, 156	0
54	BU	23/27 (85%)	2.90	20 (86%) 0 0	62, 116, 154, 180	0
54	DU	23/27 (85%)	2.75	14 (60%) 0 0	90, 134, 171, 184	0
55	BV	13/24 (54%)	2.63	10 (76%) 0 0	48, 85, 170, 176	0
55	DV	6/24 (25%)	2.72	3 (50%) 0 0	62, 78, 169, 197	0
56	BX	72/77 (93%)	0.62	3 (4%) 40 32	33, 76, 123, 186	0
56	DX	72/77 (93%)	0.81	7 (9%) 13 10	40, 99, 147, 161	0
57	BZ	730/758 (96%)	1.57	241 (33%) 1 1	34, 77, 135, 187	0
57	DZ	730/758 (96%)	2.01	336 (46%) 0 0	36, 100, 165, 220	0
All	All	22704/23760 (95%)	0.69	3553 (15%) 5 4	5, 70, 179, 350	0

The worst 5 of 3553 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	CL	127	ILE	12.3
46	DM	123	ALA	8.9
9	CK	57	THR	8.8
10	AL	10	LEU	8.6
57	BZ	572	TYR	8.6

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	5MC	DX	32	21/22	0.83	0.14	86,86,86,86	0
56	PSU	DX	55	20/21	0.84	0.13	95,95,95,95	0
56	5MU	DX	54	21/22	0.88	0.13	108,108,108,108	0
56	4SU	DX	8	20/21	0.89	0.12	96,96,96,96	0
56	5MU	BX	54	21/22	0.90	0.13	85,85,85,85	0
56	PSU	BX	55	20/21	0.90	0.10	74,74,74,74	0
56	5MC	BX	32	21/22	0.93	0.13	65,65,65,65	0
56	4SU	BX	8	20/21	0.94	0.10	70,70,70,70	1

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	DA	1624	1/1	0.28	0.21	115,115,115,115	0
58	MG	DZ	701	1/1	0.29	0.19	112,112,112,112	0
58	MG	CA	3140	1/1	0.39	0.34	122,122,122,122	0
58	MG	DA	1753	1/1	0.43	0.21	83,83,83,83	0
58	MG	CA	3296	1/1	0.53	0.19	80,80,80,80	0
58	MG	BA	3025	1/1	0.53	0.20	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	BA	3169	1/1	0.55	0.26	130,130,130,130	0
58	MG	CA	3494	1/1	0.55	0.27	88,88,88,88	0
58	MG	CB	3013	1/1	0.55	0.21	96,96,96,96	0
58	MG	CA	3002	1/1	0.56	0.37	112,112,112,112	0
58	MG	BA	3203	1/1	0.56	0.20	83,83,83,83	0
58	MG	CA	3238	1/1	0.56	0.19	85,85,85,85	0
58	MG	CA	3209	1/1	0.57	0.19	82,82,82,82	0
58	MG	CA	3509	1/1	0.58	0.14	96,96,96,96	0
58	MG	DA	1752	1/1	0.58	0.20	79,79,79,79	0
58	MG	AA	3026	1/1	0.58	0.14	83,83,83,83	0
58	MG	DA	1602	1/1	0.58	0.31	95,95,95,95	0
58	MG	BA	3035	1/1	0.59	0.38	99,99,99,99	0
58	MG	BA	3052	1/1	0.59	0.29	102,102,102,102	0
58	MG	BA	3106	1/1	0.59	0.19	93,93,93,93	0
58	MG	BA	3155	1/1	0.60	0.09	96,96,96,96	0
58	MG	CA	3553	1/1	0.62	0.15	88,88,88,88	0
58	MG	DA	1734	1/1	0.64	0.13	78,78,78,78	0
58	MG	AA	3614	1/1	0.64	0.16	103,103,103,103	0
58	MG	CA	3072	1/1	0.64	0.38	93,93,93,93	0
58	MG	DK	5001	1/1	0.64	0.15	101,101,101,101	0
58	MG	DA	1729	1/1	0.64	0.36	79,79,79,79	0
58	MG	BA	3173	1/1	0.66	0.34	113,113,113,113	0
58	MG	CA	3081	1/1	0.66	0.32	85,85,85,85	0
58	MG	DA	1714	1/1	0.66	0.12	78,78,78,78	0
58	MG	BA	3017	1/1	0.67	0.16	133,133,133,133	0
58	MG	DE	202	1/1	0.67	0.17	93,93,93,93	0
58	MG	DA	1690	1/1	0.67	0.15	85,85,85,85	0
58	MG	CA	3576	1/1	0.67	0.11	71,71,71,71	0
58	MG	BA	3103	1/1	0.68	0.25	85,85,85,85	0
58	MG	CA	3149	1/1	0.68	0.20	63,63,63,63	0
58	MG	CA	3046	1/1	0.68	0.31	113,113,113,113	0
58	MG	BL	3001	1/1	0.69	0.33	80,80,80,80	0
58	MG	CA	3141	1/1	0.69	0.24	97,97,97,97	0
58	MG	CA	3592	1/1	0.69	0.14	93,93,93,93	0
58	MG	AA	3784	1/1	0.69	0.29	73,73,73,73	0
58	MG	CA	3008	1/1	0.69	0.39	98,98,98,98	0
58	MG	AA	3679	1/1	0.70	0.12	64,64,64,64	0
58	MG	BA	3110	1/1	0.70	0.29	103,103,103,103	0
58	MG	CA	3482	1/1	0.70	0.10	89,89,89,89	0
58	MG	BA	3088	1/1	0.70	0.22	68,68,68,68	0
58	MG	AA	3752	1/1	0.70	0.15	64,64,64,64	1
58	MG	CA	3292	1/1	0.71	0.29	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	BA	3048	1/1	0.71	0.11	75,75,75,75	0
58	MG	CA	3297	1/1	0.72	0.19	83,83,83,83	0
58	MG	CA	3305	1/1	0.72	0.13	90,90,90,90	0
58	MG	CA	3645	1/1	0.72	0.39	79,79,79,79	0
58	MG	BA	3140	1/1	0.73	0.14	91,91,91,91	0
58	MG	DA	1659	1/1	0.73	0.15	87,87,87,87	0
58	MG	AA	3690	1/1	0.73	0.16	69,69,69,69	0
58	MG	AA	3745	1/1	0.73	0.18	84,84,84,84	0
58	MG	AA	3611	1/1	0.73	0.12	55,55,55,55	0
58	MG	BA	3069	1/1	0.73	0.21	82,82,82,82	0
58	MG	CA	3619	1/1	0.73	0.18	79,79,79,79	0
58	MG	CA	3623	1/1	0.73	0.17	69,69,69,69	0
58	MG	CA	3114	1/1	0.73	0.26	94,94,94,94	0
58	MG	BA	3119	1/1	0.73	0.15	79,79,79,79	0
58	MG	BX	107	1/1	0.73	0.10	67,67,67,67	0
58	MG	CA	3541	1/1	0.74	0.24	71,71,71,71	0
58	MG	CA	3067	1/1	0.74	0.30	83,83,83,83	0
58	MG	BA	3160	1/1	0.74	0.14	61,61,61,61	0
58	MG	BA	3117	1/1	0.74	0.12	65,65,65,65	0
58	MG	AA	3248	1/1	0.74	0.32	72,72,72,72	0
58	MG	AA	3711	1/1	0.75	0.22	74,74,74,74	0
58	MG	AA	3274	1/1	0.75	0.22	88,88,88,88	0
58	MG	BA	3033	1/1	0.75	0.20	52,52,52,52	0
58	MG	CA	3057	1/1	0.75	0.14	84,84,84,84	0
58	MG	DZ	702	1/1	0.75	0.16	61,61,61,61	0
58	MG	CA	3587	1/1	0.76	0.18	81,81,81,81	0
58	MG	CA	3628	1/1	0.76	0.23	76,76,76,76	0
58	MG	CA	3510	1/1	0.76	0.15	93,93,93,93	0
58	MG	CA	3648	1/1	0.76	0.14	77,77,77,77	0
58	MG	CA	3616	1/1	0.76	0.20	71,71,71,71	0
58	MG	BA	3059	1/1	0.76	0.29	76,76,76,76	0
58	MG	DA	1675	1/1	0.77	0.09	77,77,77,77	0
58	MG	BA	3081	1/1	0.77	0.36	82,82,82,82	0
58	MG	CA	3555	1/1	0.77	0.14	80,80,80,80	0
58	MG	CA	3031	1/1	0.77	0.16	74,74,74,74	0
58	MG	CA	3106	1/1	0.77	0.11	79,79,79,79	0
58	MG	CB	3006	1/1	0.77	0.12	82,82,82,82	0
58	MG	AA	3017	1/1	0.77	0.22	78,78,78,78	0
58	MG	DA	1764	1/1	0.77	0.20	72,72,72,72	0
58	MG	CA	3596	1/1	0.77	0.17	77,77,77,77	0
58	MG	BA	3179	1/1	0.77	0.18	78,78,78,78	0
58	MG	DA	1635	1/1	0.77	0.14	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	BA	3196	1/1	0.77	0.18	84,84,84,84	0
58	MG	BA	3112	1/1	0.78	0.29	70,70,70,70	0
58	MG	CA	3527	1/1	0.78	0.15	81,81,81,81	0
58	MG	CA	3071	1/1	0.78	0.41	84,84,84,84	0
58	MG	DA	1749	1/1	0.78	0.20	80,80,80,80	0
58	MG	DA	1615	1/1	0.78	0.28	85,85,85,85	0
58	MG	CA	3545	1/1	0.78	0.24	61,61,61,61	0
58	MG	BA	3158	1/1	0.78	0.19	63,63,63,63	0
58	MG	AA	3246	1/1	0.78	0.34	98,98,98,98	0
58	MG	DJ	5001	1/1	0.78	0.15	105,105,105,105	0
58	MG	AA	3633	1/1	0.78	0.24	75,75,75,75	0
58	MG	AA	3270	1/1	0.78	0.20	80,80,80,80	0
58	MG	DA	1704	1/1	0.78	0.26	128,128,128,128	0
58	MG	CA	3124	1/1	0.79	0.29	87,87,87,87	0
58	MG	CA	3034	1/1	0.79	0.22	100,100,100,100	0
58	MG	CA	3043	1/1	0.79	0.35	101,101,101,101	0
58	MG	BA	3187	1/1	0.79	0.11	59,59,59,59	0
58	MG	CA	3647	1/1	0.79	0.28	82,82,82,82	0
58	MG	BA	3095	1/1	0.79	0.14	99,99,99,99	0
58	MG	AZ	301	1/1	0.79	0.19	98,98,98,98	0
58	MG	CA	3275	1/1	0.79	0.17	67,67,67,67	0
58	MG	A4	502	1/1	0.79	0.14	120,120,120,120	0
58	MG	AA	3680	1/1	0.79	0.14	58,58,58,58	0
58	MG	AA	3196	1/1	0.79	0.16	50,50,50,50	0
58	MG	AA	3778	1/1	0.79	0.13	55,55,55,55	0
58	MG	CA	3455	1/1	0.79	0.13	78,78,78,78	0
58	MG	AA	3201	1/1	0.79	0.19	91,91,91,91	0
58	MG	DA	1673	1/1	0.80	0.15	61,61,61,61	0
58	MG	BA	3188	1/1	0.80	0.11	86,86,86,86	0
58	MG	DA	1685	1/1	0.80	0.13	52,52,52,52	0
58	MG	DA	1686	1/1	0.80	0.16	101,101,101,101	0
58	MG	AA	3109	1/1	0.80	0.50	124,124,124,124	0
58	MG	BA	3030	1/1	0.80	0.18	62,62,62,62	0
58	MG	BA	3092	1/1	0.80	0.22	86,86,86,86	0
58	MG	CB	3001	1/1	0.80	0.20	96,96,96,96	0
58	MG	CA	3094	1/1	0.80	0.41	83,83,83,83	0
58	MG	CA	3074	1/1	0.81	0.21	91,91,91,91	0
58	MG	BA	3071	1/1	0.81	0.28	93,93,93,93	0
58	MG	BA	3199	1/1	0.81	0.12	68,68,68,68	0
58	MG	CA	3583	1/1	0.81	0.15	78,78,78,78	0
58	MG	BA	3177	1/1	0.81	0.14	73,73,73,73	0
58	MG	AA	3354	1/1	0.81	0.18	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3377	1/1	0.81	0.10	64,64,64,64	0
58	MG	CA	3049	1/1	0.81	0.11	78,78,78,78	0
58	MG	CA	3461	1/1	0.81	0.21	107,107,107,107	0
58	MG	DA	1707	1/1	0.81	0.21	69,69,69,69	0
58	MG	BA	3182	1/1	0.81	0.13	80,80,80,80	0
58	MG	CA	3490	1/1	0.81	0.30	78,78,78,78	0
58	MG	DA	1733	1/1	0.81	0.23	81,81,81,81	0
58	MG	CA	3059	1/1	0.81	0.26	76,76,76,76	0
58	MG	BX	108	1/1	0.81	0.13	78,78,78,78	0
58	MG	CA	3154	1/1	0.81	0.17	77,77,77,77	0
58	MG	CA	3650	1/1	0.81	0.11	67,67,67,67	0
58	MG	AA	3122	1/1	0.81	0.26	67,67,67,67	0
58	MG	CA	3535	1/1	0.81	0.16	79,79,79,79	0
58	MG	CB	3008	1/1	0.81	0.09	58,58,58,58	0
58	MG	CA	3539	1/1	0.81	0.22	77,77,77,77	0
58	MG	BA	3007	1/1	0.81	0.21	75,75,75,75	0
58	MG	CA	3241	1/1	0.81	0.22	74,74,74,74	0
58	MG	BN	503	1/1	0.82	0.24	66,66,66,66	0
58	MG	CA	3239	1/1	0.82	0.16	74,74,74,74	0
58	MG	AA	3442	1/1	0.82	0.20	64,64,64,64	0
58	MG	BA	3002	1/1	0.82	0.13	91,91,91,91	0
58	MG	DA	1641	1/1	0.82	0.10	79,79,79,79	0
58	MG	DA	1656	1/1	0.82	0.20	91,91,91,91	0
58	MG	BA	3054	1/1	0.82	0.15	77,77,77,77	0
58	MG	DA	1670	1/1	0.82	0.17	81,81,81,81	0
58	MG	AA	3237	1/1	0.82	0.18	63,63,63,63	0
58	MG	CA	3100	1/1	0.82	0.11	90,90,90,90	0
58	MG	BA	3060	1/1	0.82	0.24	82,82,82,82	0
58	MG	CA	3315	1/1	0.82	0.26	76,76,76,76	0
58	MG	CA	3324	1/1	0.82	0.12	66,66,66,66	0
58	MG	DA	1695	1/1	0.82	0.17	88,88,88,88	0
58	MG	CA	3610	1/1	0.82	0.24	98,98,98,98	0
58	MG	AA	3775	1/1	0.82	0.14	45,45,45,45	0
58	MG	CA	3119	1/1	0.82	0.08	55,55,55,55	0
58	MG	AA	3689	1/1	0.82	0.12	55,55,55,55	0
58	MG	CA	3624	1/1	0.82	0.16	72,72,72,72	0
58	MG	CA	3481	1/1	0.82	0.16	55,55,55,55	0
58	MG	DA	1744	1/1	0.82	0.27	90,90,90,90	0
58	MG	CA	3644	1/1	0.82	0.13	66,66,66,66	0
58	MG	AA	3641	1/1	0.82	0.39	76,76,76,76	0
58	MG	AN	3001	1/1	0.82	0.28	83,83,83,83	0
58	MG	CA	3143	1/1	0.82	0.15	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3500	1/1	0.82	0.11	82,82,82,82	0
58	MG	BA	3090	1/1	0.82	0.18	90,90,90,90	0
58	MG	AA	3658	1/1	0.82	0.15	60,60,60,60	0
58	MG	BL	3003	1/1	0.82	0.12	79,79,79,79	0
58	MG	CA	3225	1/1	0.82	0.27	79,79,79,79	0
58	MG	CA	3200	1/1	0.83	0.21	72,72,72,72	0
58	MG	CA	3351	1/1	0.83	0.10	83,83,83,83	0
58	MG	AA	3099	1/1	0.83	0.10	57,57,57,57	0
58	MG	CA	3429	1/1	0.83	0.21	62,62,62,62	1
58	MG	CA	3216	1/1	0.83	0.17	74,74,74,74	0
58	MG	DA	1699	1/1	0.83	0.21	123,123,123,123	0
58	MG	CA	3663	1/1	0.83	0.16	73,73,73,73	0
58	MG	AA	3364	1/1	0.83	0.25	79,79,79,79	0
58	MG	CA	3475	1/1	0.83	0.25	75,75,75,75	0
58	MG	A8	5001	1/1	0.83	0.21	57,57,57,57	0
58	MG	BA	3093	1/1	0.83	0.16	65,65,65,65	0
58	MG	AA	3616	1/1	0.83	0.12	37,37,37,37	1
58	MG	DA	1603	1/1	0.83	0.12	81,81,81,81	0
58	MG	BA	3055	1/1	0.83	0.10	54,54,54,54	0
58	MG	AA	3729	1/1	0.83	0.15	58,58,58,58	0
58	MG	AA	3806	1/1	0.83	0.12	60,60,60,60	0
58	MG	AB	3014	1/1	0.83	0.14	67,67,67,67	0
58	MG	AB	3017	1/1	0.83	0.15	76,76,76,76	0
58	MG	CA	3627	1/1	0.83	0.25	101,101,101,101	0
58	MG	AA	3095	1/1	0.83	0.51	110,110,110,110	0
58	MG	DA	1672	1/1	0.83	0.25	100,100,100,100	0
58	MG	CA	3638	1/1	0.83	0.18	78,78,78,78	0
58	MG	AA	3461	1/1	0.84	0.14	64,64,64,64	0
58	MG	AA	3476	1/1	0.84	0.16	68,68,68,68	0
58	MG	DA	1642	1/1	0.84	0.13	76,76,76,76	0
58	MG	BA	3200	1/1	0.84	0.10	63,63,63,63	0
58	MG	CA	3379	1/1	0.84	0.18	86,86,86,86	0
58	MG	AA	3608	1/1	0.84	0.09	29,29,29,29	0
58	MG	CA	3173	1/1	0.84	0.27	81,81,81,81	0
58	MG	CA	3195	1/1	0.84	0.21	69,69,69,69	0
58	MG	CA	3466	1/1	0.84	0.14	65,65,65,65	0
58	MG	AA	3794	1/1	0.84	0.26	68,68,68,68	0
58	MG	AA	3803	1/1	0.84	0.11	62,62,62,62	0
58	MG	AA	3652	1/1	0.84	0.12	74,74,74,74	0
58	MG	CA	3486	1/1	0.84	0.25	81,81,81,81	0
58	MG	AA	3727	1/1	0.84	0.14	66,66,66,66	0
58	MG	CA	3086	1/1	0.84	0.15	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3344	1/1	0.84	0.17	85,85,85,85	0
58	MG	DA	1709	1/1	0.84	0.10	44,44,44,44	0
58	MG	AB	3023	1/1	0.84	0.28	74,74,74,74	0
58	MG	CA	3242	1/1	0.84	0.11	63,63,63,63	0
58	MG	DA	1732	1/1	0.84	0.10	80,80,80,80	0
58	MG	CA	3245	1/1	0.84	0.23	77,77,77,77	0
58	MG	CA	3274	1/1	0.84	0.21	73,73,73,73	0
58	MG	DA	1742	1/1	0.84	0.12	77,77,77,77	0
58	MG	AD	308	1/1	0.84	0.13	70,70,70,70	0
58	MG	AA	3664	1/1	0.84	0.14	55,55,55,55	0
58	MG	CA	3116	1/1	0.84	0.17	75,75,75,75	0
58	MG	CE	307	1/1	0.84	0.09	65,65,65,65	0
58	MG	DA	1761	1/1	0.84	0.11	75,75,75,75	0
58	MG	AA	3100	1/1	0.84	0.13	60,60,60,60	0
58	MG	AA	3766	1/1	0.84	0.10	70,70,70,70	0
58	MG	DA	1607	1/1	0.84	0.34	82,82,82,82	0
58	MG	BA	3195	1/1	0.84	0.16	73,73,73,73	0
58	MG	CA	3577	1/1	0.84	0.14	43,43,43,43	1
58	MG	DA	1629	1/1	0.84	0.16	73,73,73,73	0
58	MG	AA	3640	1/1	0.85	0.12	74,74,74,74	0
58	MG	CA	3537	1/1	0.85	0.20	67,67,67,67	0
58	MG	CA	3077	1/1	0.85	0.12	81,81,81,81	0
58	MG	DA	1628	1/1	0.85	0.07	69,69,69,69	0
58	MG	AA	3310	1/1	0.85	0.10	57,57,57,57	0
58	MG	DA	1634	1/1	0.85	0.17	71,71,71,71	0
58	MG	CA	3543	1/1	0.85	0.11	70,70,70,70	0
58	MG	BA	3154	1/1	0.85	0.12	94,94,94,94	0
58	MG	CA	3255	1/1	0.85	0.18	95,95,95,95	0
58	MG	BA	3082	1/1	0.85	0.15	69,69,69,69	0
58	MG	CA	3099	1/1	0.85	0.27	82,82,82,82	0
58	MG	BV	101	1/1	0.85	0.20	110,110,110,110	0
58	MG	BX	101	1/1	0.85	0.09	78,78,78,78	0
58	MG	AA	3683	1/1	0.85	0.23	65,65,65,65	0
58	MG	CA	3588	1/1	0.85	0.13	68,68,68,68	0
58	MG	DA	1683	1/1	0.85	0.27	70,70,70,70	0
58	MG	AA	3491	1/1	0.85	0.13	33,33,33,33	0
58	MG	CA	3118	1/1	0.85	0.19	67,67,67,67	0
58	MG	BA	3163	1/1	0.85	0.12	52,52,52,52	0
58	MG	CA	3611	1/1	0.85	0.17	58,58,58,58	0
58	MG	CA	3337	1/1	0.85	0.19	68,68,68,68	0
58	MG	AA	3762	1/1	0.85	0.10	58,58,58,58	0
58	MG	DA	1705	1/1	0.85	0.20	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AB	3001	1/1	0.85	0.32	85,85,85,85	0
58	MG	AB	3004	1/1	0.85	0.26	87,87,87,87	0
58	MG	CA	3412	1/1	0.85	0.12	58,58,58,58	0
58	MG	DA	1728	1/1	0.85	0.16	85,85,85,85	0
58	MG	BA	3096	1/1	0.85	0.12	64,64,64,64	0
58	MG	CA	3437	1/1	0.85	0.14	74,74,74,74	0
58	MG	BA	3101	1/1	0.85	0.21	60,60,60,60	0
58	MG	CA	3151	1/1	0.85	0.12	54,54,54,54	0
58	MG	BA	3006	1/1	0.85	0.12	71,71,71,71	0
58	MG	CA	3156	1/1	0.85	0.11	84,84,84,84	0
58	MG	BA	3104	1/1	0.85	0.16	76,76,76,76	0
58	MG	DA	1751	1/1	0.85	0.14	69,69,69,69	0
58	MG	CA	3181	1/1	0.85	0.31	108,108,108,108	0
58	MG	AA	3539	1/1	0.85	0.22	63,63,63,63	0
58	MG	CA	3060	1/1	0.85	0.16	60,60,60,60	0
58	MG	BA	3010	1/1	0.85	0.14	68,68,68,68	0
58	MG	CA	3210	1/1	0.85	0.32	93,93,93,93	0
58	MG	CA	3068	1/1	0.85	0.20	72,72,72,72	0
58	MG	CF	301	1/1	0.85	0.18	62,62,62,62	0
58	MG	BA	3062	1/1	0.85	0.48	81,81,81,81	0
58	MG	AA	3106	1/1	0.85	0.14	80,80,80,80	0
58	MG	DA	1620	1/1	0.86	0.10	69,69,69,69	0
58	MG	CA	3246	1/1	0.86	0.33	77,77,77,77	0
58	MG	AA	3264	1/1	0.86	0.17	77,77,77,77	0
58	MG	CA	3004	1/1	0.86	0.28	64,64,64,64	0
58	MG	AA	3001	1/1	0.86	0.10	36,36,36,36	0
58	MG	CA	3546	1/1	0.86	0.07	79,79,79,79	0
58	MG	BA	3039	1/1	0.86	0.30	78,78,78,78	0
58	MG	BA	3176	1/1	0.86	0.10	61,61,61,61	0
58	MG	CA	3563	1/1	0.86	0.16	92,92,92,92	0
58	MG	CA	3042	1/1	0.86	0.43	96,96,96,96	0
58	MG	DA	1668	1/1	0.86	0.15	82,82,82,82	0
58	MG	CA	3129	1/1	0.86	0.14	69,69,69,69	0
58	MG	CA	3579	1/1	0.86	0.12	83,83,83,83	0
58	MG	BA	3045	1/1	0.86	0.21	75,75,75,75	0
58	MG	AA	3113	1/1	0.86	0.31	97,97,97,97	0
58	MG	CA	3048	1/1	0.86	0.23	85,85,85,85	0
58	MG	DA	1684	1/1	0.86	0.19	63,63,63,63	0
58	MG	CA	3341	1/1	0.86	0.10	48,48,48,48	0
58	MG	CA	3146	1/1	0.86	0.22	80,80,80,80	0
58	MG	AA	3057	1/1	0.86	0.10	56,56,56,56	0
58	MG	AA	3148	1/1	0.86	0.16	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3153	1/1	0.86	0.16	55,55,55,55	0
58	MG	CA	3413	1/1	0.86	0.18	79,79,79,79	0
58	MG	A7	103	1/1	0.86	0.25	48,48,48,48	0
58	MG	BA	3056	1/1	0.86	0.22	67,67,67,67	0
58	MG	CA	3448	1/1	0.86	0.16	78,78,78,78	0
58	MG	CA	3169	1/1	0.86	0.19	55,55,55,55	0
58	MG	DA	1718	1/1	0.86	0.19	72,72,72,72	0
58	MG	DA	1720	1/1	0.86	0.14	64,64,64,64	0
58	MG	BA	3107	1/1	0.86	0.11	59,59,59,59	0
58	MG	BA	3057	1/1	0.86	0.17	89,89,89,89	0
58	MG	CA	3468	1/1	0.86	0.29	80,80,80,80	0
58	MG	CA	3190	1/1	0.86	0.19	68,68,68,68	0
58	MG	AA	3538	1/1	0.86	0.13	91,91,91,91	0
58	MG	AA	3192	1/1	0.86	0.14	41,41,41,41	0
58	MG	AA	3649	1/1	0.86	0.16	90,90,90,90	0
58	MG	AA	3651	1/1	0.86	0.12	49,49,49,49	0
58	MG	CA	3078	1/1	0.86	0.12	66,66,66,66	0
58	MG	CA	3498	1/1	0.86	0.19	71,71,71,71	0
58	MG	AB	3002	1/1	0.86	0.17	58,58,58,58	0
58	MG	DA	1754	1/1	0.86	0.10	66,66,66,66	0
58	MG	AA	3590	1/1	0.86	0.22	23,23,23,23	1
58	MG	CA	3090	1/1	0.86	0.16	79,79,79,79	0
58	MG	CQ	204	1/1	0.86	0.16	79,79,79,79	0
58	MG	CA	3515	1/1	0.86	0.16	73,73,73,73	0
58	MG	AA	3598	1/1	0.86	0.09	61,61,61,61	0
58	MG	AA	3756	1/1	0.86	0.14	61,61,61,61	0
58	MG	BA	3161	1/1	0.86	0.17	87,87,87,87	0
58	MG	CA	3285	1/1	0.87	0.20	59,59,59,59	0
58	MG	AA	3695	1/1	0.87	0.11	44,44,44,44	0
58	MG	BA	3074	1/1	0.87	0.09	66,66,66,66	0
58	MG	CA	3127	1/1	0.87	0.20	94,94,94,94	0
58	MG	AA	3807	1/1	0.87	0.12	65,65,65,65	0
58	MG	DA	1640	1/1	0.87	0.22	74,74,74,74	0
58	MG	CA	3308	1/1	0.87	0.13	50,50,50,50	0
58	MG	CA	3557	1/1	0.87	0.24	82,82,82,82	0
58	MG	DA	1648	1/1	0.87	0.21	90,90,90,90	0
58	MG	CA	3135	1/1	0.87	0.27	84,84,84,84	0
58	MG	DA	1657	1/1	0.87	0.17	72,72,72,72	0
58	MG	BA	3014	1/1	0.87	0.11	97,97,97,97	0
58	MG	CA	3045	1/1	0.87	0.27	65,65,65,65	0
58	MG	AA	3813	1/1	0.87	0.12	57,57,57,57	0
58	MG	BA	3089	1/1	0.87	0.27	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3375	1/1	0.87	0.12	74,74,74,74	0
58	MG	AA	3635	1/1	0.87	0.17	60,60,60,60	0
58	MG	AA	3375	1/1	0.87	0.17	57,57,57,57	0
58	MG	CA	3593	1/1	0.87	0.11	82,82,82,82	0
58	MG	CA	3407	1/1	0.87	0.10	70,70,70,70	0
58	MG	AA	3423	1/1	0.87	0.12	65,65,65,65	0
58	MG	DA	1688	1/1	0.87	0.12	57,57,57,57	0
58	MG	AA	3740	1/1	0.87	0.21	92,92,92,92	0
58	MG	CA	3066	1/1	0.87	0.11	50,50,50,50	0
58	MG	AA	3580	1/1	0.87	0.13	39,39,39,39	0
58	MG	BA	3191	1/1	0.87	0.12	74,74,74,74	0
58	MG	AB	3018	1/1	0.87	0.14	81,81,81,81	0
58	MG	CA	3189	1/1	0.87	0.22	58,58,58,58	0
58	MG	BA	3047	1/1	0.87	0.24	71,71,71,71	0
58	MG	AA	3437	1/1	0.87	0.10	55,55,55,55	0
58	MG	BA	3051	1/1	0.87	0.20	71,71,71,71	0
58	MG	AA	3441	1/1	0.87	0.14	46,46,46,46	0
58	MG	BA	3109	1/1	0.87	0.13	79,79,79,79	0
58	MG	CA	3082	1/1	0.87	0.15	66,66,66,66	0
58	MG	CA	3487	1/1	0.87	0.19	68,68,68,68	0
58	MG	CA	3223	1/1	0.87	0.27	75,75,75,75	0
58	MG	AF	304	1/1	0.87	0.09	41,41,41,41	0
58	MG	DA	1739	1/1	0.87	0.15	76,76,76,76	0
58	MG	CA	3495	1/1	0.87	0.22	62,62,62,62	0
58	MG	AA	3601	1/1	0.87	0.09	59,59,59,59	0
58	MG	CB	3012	1/1	0.87	0.23	74,74,74,74	0
58	MG	AA	3206	1/1	0.87	0.19	62,62,62,62	0
58	MG	CA	3098	1/1	0.87	0.11	79,79,79,79	0
58	MG	AA	3200	1/1	0.87	0.11	52,52,52,52	0
58	MG	CG	3001	1/1	0.87	0.22	81,81,81,81	0
58	MG	DA	1760	1/1	0.87	0.08	71,71,71,71	0
58	MG	BA	3136	1/1	0.87	0.14	70,70,70,70	0
58	MG	CA	3523	1/1	0.87	0.17	62,62,62,62	0
58	MG	AA	3239	1/1	0.87	0.13	69,69,69,69	0
58	MG	AA	3193	1/1	0.87	0.27	72,72,72,72	0
58	MG	AA	3627	1/1	0.87	0.22	72,72,72,72	0
58	MG	AA	3527	1/1	0.87	0.08	21,21,21,21	0
58	MG	DA	1621	1/1	0.87	0.07	58,58,58,58	0
58	MG	AA	3222	1/1	0.88	0.22	61,61,61,61	0
58	MG	AA	3478	1/1	0.88	0.11	40,40,40,40	0
58	MG	BA	3115	1/1	0.88	0.21	86,86,86,86	0
58	MG	AA	3612	1/1	0.88	0.20	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3360	1/1	0.88	0.19	111,111,111,111	0
58	MG	AA	3027	1/1	0.88	0.30	77,77,77,77	0
58	MG	AA	3621	1/1	0.88	0.17	39,39,39,39	0
58	MG	DA	1650	1/1	0.88	0.17	57,57,57,57	0
58	MG	CA	3389	1/1	0.88	0.17	81,81,81,81	0
58	MG	CA	3390	1/1	0.88	0.15	74,74,74,74	0
58	MG	AA	3709	1/1	0.88	0.15	53,53,53,53	0
58	MG	DA	1663	1/1	0.88	0.15	63,63,63,63	0
58	MG	AA	3622	1/1	0.88	0.18	46,46,46,46	0
58	MG	BA	3157	1/1	0.88	0.15	67,67,67,67	0
58	MG	DA	1671	1/1	0.88	0.26	72,72,72,72	0
58	MG	CA	3606	1/1	0.88	0.11	51,51,51,51	0
58	MG	CA	3608	1/1	0.88	0.15	70,70,70,70	0
58	MG	BA	3058	1/1	0.88	0.23	69,69,69,69	0
58	MG	DA	1676	1/1	0.88	0.10	75,75,75,75	0
58	MG	CA	3159	1/1	0.88	0.15	68,68,68,68	0
58	MG	AA	3159	1/1	0.88	0.26	97,97,97,97	0
58	MG	CA	3617	1/1	0.88	0.21	52,52,52,52	0
58	MG	AA	3321	1/1	0.88	0.12	69,69,69,69	0
58	MG	AA	3634	1/1	0.88	0.11	57,57,57,57	1
58	MG	AA	3562	1/1	0.88	0.10	57,57,57,57	0
58	MG	DA	1691	1/1	0.88	0.17	74,74,74,74	0
58	MG	CA	3063	1/1	0.88	0.20	66,66,66,66	0
58	MG	BA	3170	1/1	0.88	0.08	71,71,71,71	0
58	MG	DA	1700	1/1	0.88	0.12	62,62,62,62	0
58	MG	CA	3479	1/1	0.88	0.11	56,56,56,56	0
58	MG	AZ	302	1/1	0.88	0.19	66,66,66,66	0
58	MG	BA	3073	1/1	0.88	0.27	74,74,74,74	0
58	MG	AA	3579	1/1	0.88	0.15	53,53,53,53	0
58	MG	AA	3753	1/1	0.88	0.16	72,72,72,72	0
58	MG	AA	3336	1/1	0.88	0.11	53,53,53,53	0
58	MG	AA	3758	1/1	0.88	0.24	81,81,81,81	0
58	MG	DA	1724	1/1	0.88	0.11	77,77,77,77	0
58	MG	AA	3647	1/1	0.88	0.16	71,71,71,71	0
58	MG	AA	3266	1/1	0.88	0.21	74,74,74,74	0
58	MG	AA	3774	1/1	0.88	0.22	78,78,78,78	0
58	MG	AA	3592	1/1	0.88	0.10	63,63,63,63	0
58	MG	BA	3197	1/1	0.88	0.08	75,75,75,75	0
58	MG	DA	1737	1/1	0.88	0.24	78,78,78,78	0
58	MG	CD	301	1/1	0.88	0.24	79,79,79,79	0
58	MG	CE	304	1/1	0.88	0.14	65,65,65,65	0
58	MG	BA	3016	1/1	0.88	0.09	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3593	1/1	0.88	0.13	51,51,51,51	0
58	MG	AA	3345	1/1	0.88	0.09	67,67,67,67	0
58	MG	CO	201	1/1	0.88	0.11	61,61,61,61	0
58	MG	BA	3205	1/1	0.88	0.07	68,68,68,68	0
58	MG	AA	3347	1/1	0.88	0.12	40,40,40,40	0
58	MG	AA	3668	1/1	0.88	0.09	38,38,38,38	0
58	MG	DA	1606	1/1	0.88	0.10	72,72,72,72	0
58	MG	DA	1763	1/1	0.88	0.17	94,94,94,94	0
58	MG	BN	502	1/1	0.88	0.07	64,64,64,64	0
58	MG	DA	1765	1/1	0.88	0.09	64,64,64,64	0
58	MG	AA	3804	1/1	0.88	0.12	65,65,65,65	0
58	MG	AA	3672	1/1	0.88	0.22	32,32,32,32	1
58	MG	BA	3108	1/1	0.88	0.11	49,49,49,49	0
58	MG	CA	3548	1/1	0.88	0.11	116,116,116,116	0
58	MG	AA	3674	1/1	0.88	0.16	74,74,74,74	0
58	MG	CA	3564	1/1	0.89	0.11	75,75,75,75	0
58	MG	CA	3570	1/1	0.89	0.09	41,41,41,41	0
58	MG	CA	3070	1/1	0.89	0.26	82,82,82,82	0
58	MG	CA	3166	1/1	0.89	0.19	61,61,61,61	0
58	MG	CA	3387	1/1	0.89	0.15	62,62,62,62	0
58	MG	CA	3580	1/1	0.89	0.13	79,79,79,79	0
58	MG	BA	3075	1/1	0.89	0.20	56,56,56,56	0
58	MG	BA	3137	1/1	0.89	0.09	73,73,73,73	0
58	MG	CA	3400	1/1	0.89	0.11	73,73,73,73	0
58	MG	CA	3406	1/1	0.89	0.19	89,89,89,89	0
58	MG	CA	3174	1/1	0.89	0.18	65,65,65,65	0
58	MG	DA	1664	1/1	0.89	0.19	59,59,59,59	0
58	MG	DA	1665	1/1	0.89	0.10	64,64,64,64	0
58	MG	AA	3443	1/1	0.89	0.09	61,61,61,61	0
58	MG	CA	3185	1/1	0.89	0.13	66,66,66,66	0
58	MG	CA	3607	1/1	0.89	0.08	67,67,67,67	0
58	MG	A7	101	1/1	0.89	0.28	64,64,64,64	0
58	MG	AA	3760	1/1	0.89	0.07	27,27,27,27	0
58	MG	AA	3444	1/1	0.89	0.15	73,73,73,73	0
58	MG	CA	3613	1/1	0.89	0.24	96,96,96,96	0
58	MG	AA	3660	1/1	0.89	0.16	68,68,68,68	0
58	MG	CA	3204	1/1	0.89	0.08	58,58,58,58	0
58	MG	CA	3205	1/1	0.89	0.10	71,71,71,71	0
58	MG	BA	3004	1/1	0.89	0.17	64,64,64,64	0
58	MG	BX	103	1/1	0.89	0.26	87,87,87,87	0
58	MG	BA	3053	1/1	0.89	0.15	69,69,69,69	0
58	MG	BA	3094	1/1	0.89	0.09	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3631	1/1	0.89	0.20	66,66,66,66	0
58	MG	BX	109	1/1	0.89	0.13	78,78,78,78	0
58	MG	CA	3229	1/1	0.89	0.24	61,61,61,61	0
58	MG	BA	3164	1/1	0.89	0.09	60,60,60,60	0
58	MG	BA	3167	1/1	0.89	0.11	85,85,85,85	0
58	MG	CA	3108	1/1	0.89	0.27	106,106,106,106	0
58	MG	AA	3455	1/1	0.89	0.12	56,56,56,56	0
58	MG	CA	3013	1/1	0.89	0.20	61,61,61,61	0
58	MG	CA	3499	1/1	0.89	0.10	65,65,65,65	0
58	MG	DA	1719	1/1	0.89	0.15	66,66,66,66	0
58	MG	AA	3335	1/1	0.89	0.09	40,40,40,40	0
58	MG	DA	1723	1/1	0.89	0.07	68,68,68,68	0
58	MG	CB	3007	1/1	0.89	0.25	64,64,64,64	0
58	MG	CA	3504	1/1	0.89	0.16	69,69,69,69	0
58	MG	CB	3009	1/1	0.89	0.12	64,64,64,64	0
58	MG	AA	3362	1/1	0.89	0.14	67,67,67,67	0
58	MG	CA	3271	1/1	0.89	0.19	84,84,84,84	0
58	MG	BA	3013	1/1	0.89	0.14	75,75,75,75	0
58	MG	AA	3119	1/1	0.89	0.15	62,62,62,62	0
58	MG	CA	3279	1/1	0.89	0.11	89,89,89,89	0
58	MG	CA	3530	1/1	0.89	0.17	78,78,78,78	0
58	MG	AD	302	1/1	0.89	0.16	46,46,46,46	0
58	MG	CN	5001	1/1	0.89	0.12	76,76,76,76	0
58	MG	AA	3675	1/1	0.89	0.12	40,40,40,40	0
58	MG	BA	3184	1/1	0.89	0.07	49,49,49,49	0
58	MG	CA	3540	1/1	0.89	0.11	70,70,70,70	0
58	MG	AA	3481	1/1	0.89	0.08	50,50,50,50	0
58	MG	DA	1604	1/1	0.89	0.08	72,72,72,72	0
58	MG	BA	3065	1/1	0.89	0.15	57,57,57,57	0
58	MG	AA	3249	1/1	0.89	0.13	62,62,62,62	0
58	MG	CA	3148	1/1	0.89	0.24	77,77,77,77	0
58	MG	BA	3070	1/1	0.89	0.12	72,72,72,72	0
58	MG	AA	3681	1/1	0.89	0.11	63,63,63,63	0
58	MG	AA	3518	1/1	0.89	0.08	19,19,19,19	0
58	MG	BA	3037	1/1	0.89	0.12	64,64,64,64	0
58	MG	DL	3001	1/1	0.89	0.12	57,57,57,57	0
58	MG	BA	3131	1/1	0.89	0.09	76,76,76,76	0
58	MG	DA	1632	1/1	0.89	0.17	69,69,69,69	0
58	MG	CA	3237	1/1	0.90	0.27	75,75,75,75	0
58	MG	AA	3631	1/1	0.90	0.21	68,68,68,68	0
58	MG	CA	3506	1/1	0.90	0.07	61,61,61,61	0
58	MG	BA	3149	1/1	0.90	0.18	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	BA	3028	1/1	0.90	0.20	90,90,90,90	0
58	MG	CA	3511	1/1	0.90	0.11	74,74,74,74	0
58	MG	CA	3514	1/1	0.90	0.11	63,63,63,63	0
58	MG	BA	3077	1/1	0.90	0.28	86,86,86,86	0
58	MG	CA	3516	1/1	0.90	0.20	105,105,105,105	0
58	MG	BX	104	1/1	0.90	0.08	69,69,69,69	0
58	MG	CA	3526	1/1	0.90	0.09	75,75,75,75	0
58	MG	AA	3272	1/1	0.90	0.22	69,69,69,69	0
58	MG	CA	3248	1/1	0.90	0.10	58,58,58,58	0
58	MG	DA	1626	1/1	0.90	0.28	72,72,72,72	0
58	MG	CA	3532	1/1	0.90	0.10	58,58,58,58	0
58	MG	AA	3488	1/1	0.90	0.09	23,23,23,23	0
58	MG	CA	3260	1/1	0.90	0.13	69,69,69,69	0
58	MG	AA	3060	1/1	0.90	0.20	64,64,64,64	0
58	MG	AA	3761	1/1	0.90	0.09	48,48,48,48	0
58	MG	DA	1637	1/1	0.90	0.20	67,67,67,67	0
58	MG	AA	3029	1/1	0.90	0.16	50,50,50,50	0
58	MG	AA	3107	1/1	0.90	0.20	48,48,48,48	0
58	MG	CA	3128	1/1	0.90	0.23	60,60,60,60	0
58	MG	AH	3002	1/1	0.90	0.17	77,77,77,77	0
58	MG	CA	3130	1/1	0.90	0.14	68,68,68,68	0
58	MG	DA	1651	1/1	0.90	0.11	70,70,70,70	0
58	MG	DA	1655	1/1	0.90	0.27	73,73,73,73	0
58	MG	CA	3549	1/1	0.90	0.13	61,61,61,61	0
58	MG	CA	3024	1/1	0.90	0.25	87,87,87,87	0
58	MG	CA	3139	1/1	0.90	0.10	63,63,63,63	0
58	MG	DA	1661	1/1	0.90	0.07	62,62,62,62	0
58	MG	DA	1662	1/1	0.90	0.15	70,70,70,70	0
58	MG	CA	3025	1/1	0.90	0.22	75,75,75,75	0
58	MG	AA	3773	1/1	0.90	0.31	36,36,36,36	0
58	MG	AA	3349	1/1	0.90	0.25	39,39,39,39	0
58	MG	CA	3565	1/1	0.90	0.09	90,90,90,90	0
58	MG	AA	3431	1/1	0.90	0.13	56,56,56,56	0
58	MG	CA	3573	1/1	0.90	0.18	64,64,64,64	0
58	MG	CA	3339	1/1	0.90	0.15	62,62,62,62	0
58	MG	AA	3547	1/1	0.90	0.09	30,30,30,30	0
58	MG	AA	3699	1/1	0.90	0.18	38,38,38,38	1
58	MG	CA	3358	1/1	0.90	0.15	78,78,78,78	0
58	MG	DA	1677	1/1	0.90	0.22	80,80,80,80	0
58	MG	CA	3582	1/1	0.90	0.09	96,96,96,96	0
58	MG	CA	3374	1/1	0.90	0.16	56,56,56,56	0
58	MG	AA	3015	1/1	0.90	0.20	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	BA	3181	1/1	0.90	0.08	47,47,47,47	0
58	MG	DA	1687	1/1	0.90	0.11	66,66,66,66	0
58	MG	AA	3801	1/1	0.90	0.09	89,89,89,89	0
58	MG	AA	3653	1/1	0.90	0.09	67,67,67,67	0
58	MG	BA	3186	1/1	0.90	0.16	67,67,67,67	0
58	MG	CA	3160	1/1	0.90	0.30	74,74,74,74	0
58	MG	CA	3396	1/1	0.90	0.24	64,64,64,64	0
58	MG	AA	3717	1/1	0.90	0.08	56,56,56,56	0
58	MG	BA	3005	1/1	0.90	0.26	64,64,64,64	0
58	MG	CA	3172	1/1	0.90	0.09	53,53,53,53	0
58	MG	DA	1706	1/1	0.90	0.12	85,85,85,85	0
58	MG	CA	3408	1/1	0.90	0.10	54,54,54,54	0
58	MG	AA	3574	1/1	0.90	0.09	47,47,47,47	0
58	MG	BA	3194	1/1	0.90	0.08	60,60,60,60	0
58	MG	CA	3424	1/1	0.90	0.14	51,51,51,51	0
58	MG	CA	3175	1/1	0.90	0.24	60,60,60,60	0
58	MG	AA	3577	1/1	0.90	0.13	36,36,36,36	0
58	MG	CA	3445	1/1	0.90	0.20	91,91,91,91	0
58	MG	AA	3737	1/1	0.90	0.12	75,75,75,75	0
58	MG	CA	3629	1/1	0.90	0.20	73,73,73,73	0
58	MG	BA	3116	1/1	0.90	0.14	82,82,82,82	0
58	MG	CA	3634	1/1	0.90	0.10	75,75,75,75	0
58	MG	AA	3821	1/1	0.90	0.13	58,58,58,58	0
58	MG	CA	3639	1/1	0.90	0.28	79,79,79,79	0
58	MG	DA	1736	1/1	0.90	0.13	78,78,78,78	0
58	MG	AA	3477	1/1	0.90	0.10	57,57,57,57	0
58	MG	DA	1738	1/1	0.90	0.11	78,78,78,78	0
58	MG	CA	3196	1/1	0.90	0.14	58,58,58,58	0
58	MG	DA	1740	1/1	0.90	0.12	79,79,79,79	0
58	MG	CA	3198	1/1	0.90	0.18	62,62,62,62	0
58	MG	BA	3125	1/1	0.90	0.14	63,63,63,63	0
58	MG	AA	3440	1/1	0.90	0.15	51,51,51,51	0
58	MG	CA	3652	1/1	0.90	0.14	84,84,84,84	0
58	MG	CA	3657	1/1	0.90	0.13	62,62,62,62	0
58	MG	BA	3210	1/1	0.90	0.11	68,68,68,68	0
58	MG	CA	3483	1/1	0.90	0.16	68,68,68,68	0
58	MG	CB	3003	1/1	0.90	0.12	76,76,76,76	0
58	MG	CA	3484	1/1	0.90	0.16	67,67,67,67	0
58	MG	CA	3485	1/1	0.90	0.10	74,74,74,74	0
58	MG	BA	3135	1/1	0.90	0.28	80,80,80,80	0
58	MG	BA	3072	1/1	0.90	0.28	75,75,75,75	0
58	MG	DA	1766	1/1	0.90	0.13	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3088	1/1	0.90	0.13	65,65,65,65	0
58	MG	CA	3493	1/1	0.90	0.29	105,105,105,105	0
58	MG	CA	3089	1/1	0.90	0.22	73,73,73,73	0
58	MG	BL	3004	1/1	0.90	0.18	67,67,67,67	0
58	MG	CA	3227	1/1	0.90	0.29	68,68,68,68	0
58	MG	AA	3629	1/1	0.90	0.20	74,74,74,74	0
58	MG	AA	3234	1/1	0.91	0.21	77,77,77,77	0
58	MG	AA	3553	1/1	0.91	0.15	60,60,60,60	0
58	MG	CA	3473	1/1	0.91	0.20	70,70,70,70	0
58	MG	AA	3181	1/1	0.91	0.24	94,94,94,94	0
58	MG	CA	3478	1/1	0.91	0.14	73,73,73,73	0
58	MG	BA	3031	1/1	0.91	0.09	61,61,61,61	0
58	MG	AA	3186	1/1	0.91	0.18	41,41,41,41	0
58	MG	CE	306	1/1	0.91	0.25	99,99,99,99	0
58	MG	BA	3034	1/1	0.91	0.13	61,61,61,61	0
58	MG	CA	3020	1/1	0.91	0.10	61,61,61,61	0
58	MG	CA	3179	1/1	0.91	0.13	55,55,55,55	0
58	MG	AA	3703	1/1	0.91	0.13	41,41,41,41	1
58	MG	BA	3124	1/1	0.91	0.09	71,71,71,71	0
58	MG	CQ	202	1/1	0.91	0.10	66,66,66,66	0
58	MG	AA	3816	1/1	0.91	0.14	91,91,91,91	0
58	MG	CA	3488	1/1	0.91	0.09	69,69,69,69	0
58	MG	CA	3489	1/1	0.91	0.09	53,53,53,53	0
58	MG	BA	3126	1/1	0.91	0.11	59,59,59,59	0
58	MG	DA	1605	1/1	0.91	0.20	75,75,75,75	0
58	MG	CA	3038	1/1	0.91	0.07	46,46,46,46	0
58	MG	AA	3705	1/1	0.91	0.11	57,57,57,57	0
58	MG	AA	3576	1/1	0.91	0.11	69,69,69,69	0
58	MG	CA	3199	1/1	0.91	0.07	36,36,36,36	0
58	MG	BA	3046	1/1	0.91	0.15	60,60,60,60	0
58	MG	AA	3036	1/1	0.91	0.10	49,49,49,49	0
58	MG	AA	3713	1/1	0.91	0.11	47,47,47,47	0
58	MG	CA	3206	1/1	0.91	0.16	104,104,104,104	0
58	MG	BA	3144	1/1	0.91	0.10	53,53,53,53	0
58	MG	CA	3051	1/1	0.91	0.40	64,64,64,64	0
58	MG	CA	3211	1/1	0.91	0.20	72,72,72,72	0
58	MG	CA	3053	1/1	0.91	0.17	57,57,57,57	0
58	MG	AB	3006	1/1	0.91	0.18	70,70,70,70	0
58	MG	AA	3452	1/1	0.91	0.14	67,67,67,67	0
58	MG	CA	3520	1/1	0.91	0.25	83,83,83,83	0
58	MG	AA	3721	1/1	0.91	0.13	76,76,76,76	0
58	MG	AA	3071	1/1	0.91	0.14	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3232	1/1	0.91	0.23	65,65,65,65	0
58	MG	AB	3019	1/1	0.91	0.11	64,64,64,64	0
58	MG	AA	3645	1/1	0.91	0.23	78,78,78,78	0
58	MG	AA	3736	1/1	0.91	0.09	35,35,35,35	0
58	MG	AD	307	1/1	0.91	0.10	56,56,56,56	0
58	MG	AA	3083	1/1	0.91	0.10	27,27,27,27	1
58	MG	CA	3243	1/1	0.91	0.29	110,110,110,110	0
58	MG	BA	3166	1/1	0.91	0.07	58,58,58,58	0
58	MG	AD	309	1/1	0.91	0.12	37,37,37,37	0
58	MG	CA	3247	1/1	0.91	0.15	55,55,55,55	0
58	MG	AD	311	1/1	0.91	0.12	55,55,55,55	0
58	MG	CA	3547	1/1	0.91	0.10	66,66,66,66	0
58	MG	CA	3249	1/1	0.91	0.19	64,64,64,64	0
58	MG	BA	3064	1/1	0.91	0.09	78,78,78,78	0
58	MG	CA	3257	1/1	0.91	0.16	65,65,65,65	0
58	MG	AD	312	1/1	0.91	0.38	58,58,58,58	0
58	MG	BA	3067	1/1	0.91	0.19	73,73,73,73	0
58	MG	CA	3083	1/1	0.91	0.09	70,70,70,70	0
58	MG	BA	3068	1/1	0.91	0.11	87,87,87,87	0
58	MG	AA	3111	1/1	0.91	0.18	79,79,79,79	0
58	MG	CA	3569	1/1	0.91	0.10	54,54,54,54	0
58	MG	AA	3359	1/1	0.91	0.09	49,49,49,49	0
58	MG	CA	3286	1/1	0.91	0.19	90,90,90,90	0
58	MG	AA	3112	1/1	0.91	0.10	46,46,46,46	0
58	MG	AU	203	1/1	0.91	0.18	56,56,56,56	0
58	MG	DA	1689	1/1	0.91	0.12	80,80,80,80	0
58	MG	CA	3096	1/1	0.91	0.20	63,63,63,63	0
58	MG	BA	3185	1/1	0.91	0.20	111,111,111,111	0
58	MG	AA	3600	1/1	0.91	0.15	57,57,57,57	0
58	MG	DA	1697	1/1	0.91	0.20	65,65,65,65	0
58	MG	AA	3480	1/1	0.91	0.12	54,54,54,54	0
58	MG	CA	3585	1/1	0.91	0.09	80,80,80,80	0
58	MG	CA	3101	1/1	0.91	0.34	77,77,77,77	0
58	MG	AA	3607	1/1	0.91	0.21	59,59,59,59	0
58	MG	CA	3591	1/1	0.91	0.15	77,77,77,77	0
58	MG	A5	104	1/1	0.91	0.10	60,60,60,60	0
58	MG	BA	3080	1/1	0.91	0.08	52,52,52,52	0
58	MG	DA	1710	1/1	0.91	0.09	79,79,79,79	0
58	MG	DA	1711	1/1	0.91	0.12	70,70,70,70	0
58	MG	CA	3344	1/1	0.91	0.09	36,36,36,36	0
58	MG	AA	3759	1/1	0.91	0.12	63,63,63,63	0
58	MG	AA	3172	1/1	0.91	0.39	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	BA	3083	1/1	0.91	0.22	68,68,68,68	0
58	MG	A7	104	1/1	0.91	0.16	44,44,44,44	1
58	MG	CA	3376	1/1	0.91	0.16	70,70,70,70	0
58	MG	CA	3126	1/1	0.91	0.24	71,71,71,71	0
58	MG	AA	3216	1/1	0.91	0.08	36,36,36,36	0
58	MG	DA	1730	1/1	0.91	0.12	75,75,75,75	0
58	MG	A9	502	1/1	0.91	0.21	58,58,58,58	0
58	MG	AA	3174	1/1	0.91	0.33	62,62,62,62	0
58	MG	BA	3209	1/1	0.91	0.12	79,79,79,79	0
58	MG	CA	3392	1/1	0.91	0.08	63,63,63,63	0
58	MG	CA	3394	1/1	0.91	0.06	84,84,84,84	0
58	MG	AA	3673	1/1	0.91	0.14	66,66,66,66	0
58	MG	CA	3136	1/1	0.91	0.22	64,64,64,64	0
58	MG	CA	3403	1/1	0.91	0.14	70,70,70,70	0
58	MG	BA	3212	1/1	0.91	0.16	73,73,73,73	0
58	MG	CA	3635	1/1	0.91	0.11	79,79,79,79	0
58	MG	CA	3636	1/1	0.91	0.17	65,65,65,65	0
58	MG	BD	502	1/1	0.91	0.22	80,80,80,80	0
58	MG	AA	3767	1/1	0.91	0.13	66,66,66,66	0
58	MG	AA	3292	1/1	0.91	0.18	71,71,71,71	0
58	MG	AA	3223	1/1	0.91	0.19	54,54,54,54	0
58	MG	CA	3646	1/1	0.91	0.08	75,75,75,75	0
58	MG	CA	3422	1/1	0.91	0.19	74,74,74,74	0
58	MG	BA	3098	1/1	0.91	0.14	78,78,78,78	0
58	MG	CA	3649	1/1	0.91	0.12	94,94,94,94	0
58	MG	AA	3319	1/1	0.91	0.11	66,66,66,66	0
58	MG	CA	3433	1/1	0.91	0.20	61,61,61,61	0
58	MG	CA	3656	1/1	0.91	0.24	96,96,96,96	0
58	MG	AA	3232	1/1	0.91	0.20	79,79,79,79	0
58	MG	AA	3624	1/1	0.91	0.15	70,70,70,70	0
58	MG	BA	3015	1/1	0.91	0.23	87,87,87,87	0
58	MG	AA	3626	1/1	0.91	0.09	58,58,58,58	0
58	MG	AA	3688	1/1	0.91	0.09	29,29,29,29	0
62	GDP	DZ	704	28/28	0.91	0.10	80,80,80,80	0
58	MG	AA	3513	1/1	0.92	0.09	58,58,58,58	0
58	MG	CA	3654	1/1	0.92	0.07	29,29,29,29	0
58	MG	BA	3099	1/1	0.92	0.25	70,70,70,70	0
58	MG	BT	3001	1/1	0.92	0.23	60,60,60,60	0
58	MG	CA	3417	1/1	0.92	0.09	48,48,48,48	0
58	MG	BA	3100	1/1	0.92	0.21	74,74,74,74	0
58	MG	AA	3243	1/1	0.92	0.10	66,66,66,66	0
58	MG	CB	3004	1/1	0.92	0.15	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	BA	3008	1/1	0.92	0.13	61,61,61,61	0
58	MG	CA	3432	1/1	0.92	0.18	96,96,96,96	0
58	MG	AA	3519	1/1	0.92	0.09	32,32,32,32	0
58	MG	BA	3105	1/1	0.92	0.12	60,60,60,60	0
58	MG	BA	3011	1/1	0.92	0.07	76,76,76,76	0
58	MG	CA	3167	1/1	0.92	0.17	43,43,43,43	0
58	MG	AA	3244	1/1	0.92	0.21	69,69,69,69	0
58	MG	AA	3129	1/1	0.92	0.19	57,57,57,57	0
58	MG	AA	3358	1/1	0.92	0.10	61,61,61,61	0
58	MG	AA	3137	1/1	0.92	0.06	49,49,49,49	0
58	MG	CA	3472	1/1	0.92	0.12	45,45,45,45	0
58	MG	AA	3655	1/1	0.92	0.09	59,59,59,59	0
58	MG	CA	3017	1/1	0.92	0.09	45,45,45,45	0
58	MG	BA	3020	1/1	0.92	0.07	51,51,51,51	0
58	MG	CO	202	1/1	0.92	0.12	52,52,52,52	0
58	MG	CQ	201	1/1	0.92	0.17	63,63,63,63	0
58	MG	BA	3021	1/1	0.92	0.08	37,37,37,37	0
58	MG	CA	3187	1/1	0.92	0.14	67,67,67,67	0
58	MG	BA	3022	1/1	0.92	0.06	46,46,46,46	0
58	MG	CA	3026	1/1	0.92	0.16	79,79,79,79	0
58	MG	CA	3194	1/1	0.92	0.11	61,61,61,61	0
58	MG	AA	3199	1/1	0.92	0.12	55,55,55,55	0
58	MG	BA	3027	1/1	0.92	0.12	75,75,75,75	0
58	MG	AA	3785	1/1	0.92	0.13	70,70,70,70	0
58	MG	DA	1611	1/1	0.92	0.11	74,74,74,74	0
58	MG	AA	3793	1/1	0.92	0.10	60,60,60,60	0
58	MG	DA	1617	1/1	0.92	0.11	63,63,63,63	0
58	MG	AA	3024	1/1	0.92	0.18	55,55,55,55	0
58	MG	CA	3201	1/1	0.92	0.17	52,52,52,52	0
58	MG	AA	3796	1/1	0.92	0.14	19,19,19,19	1
58	MG	AA	3564	1/1	0.92	0.11	48,48,48,48	0
58	MG	AA	3802	1/1	0.92	0.11	54,54,54,54	0
58	MG	AA	3363	1/1	0.92	0.07	28,28,28,28	0
58	MG	DA	1630	1/1	0.92	0.12	56,56,56,56	0
58	MG	DA	1631	1/1	0.92	0.15	59,59,59,59	0
58	MG	CA	3050	1/1	0.92	0.07	43,43,43,43	0
58	MG	AA	3669	1/1	0.92	0.07	34,34,34,34	0
58	MG	CA	3215	1/1	0.92	0.16	39,39,39,39	0
58	MG	BA	3148	1/1	0.92	0.10	67,67,67,67	0
58	MG	DA	1639	1/1	0.92	0.29	83,83,83,83	0
58	MG	CA	3055	1/1	0.92	0.21	37,37,37,37	0
58	MG	AA	3265	1/1	0.92	0.16	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3058	1/1	0.92	0.08	48,48,48,48	0
58	MG	AA	3149	1/1	0.92	0.15	67,67,67,67	0
58	MG	AA	3381	1/1	0.92	0.09	26,26,26,26	0
58	MG	AA	3404	1/1	0.92	0.10	43,43,43,43	0
58	MG	DA	1652	1/1	0.92	0.10	58,58,58,58	0
58	MG	AA	3414	1/1	0.92	0.07	55,55,55,55	0
58	MG	AA	3421	1/1	0.92	0.12	70,70,70,70	0
58	MG	CA	3240	1/1	0.92	0.09	58,58,58,58	0
58	MG	AA	3269	1/1	0.92	0.25	84,84,84,84	0
58	MG	AA	3596	1/1	0.92	0.07	54,54,54,54	0
58	MG	CA	3531	1/1	0.92	0.10	58,58,58,58	0
58	MG	AA	3597	1/1	0.92	0.14	40,40,40,40	0
58	MG	CA	3534	1/1	0.92	0.12	79,79,79,79	0
58	MG	AA	3202	1/1	0.92	0.09	63,63,63,63	0
58	MG	AA	3435	1/1	0.92	0.09	37,37,37,37	0
58	MG	CA	3538	1/1	0.92	0.12	69,69,69,69	0
58	MG	AA	3156	1/1	0.92	0.18	63,63,63,63	0
58	MG	AA	3605	1/1	0.92	0.10	40,40,40,40	1
58	MG	CA	3080	1/1	0.92	0.17	56,56,56,56	0
58	MG	DA	1674	1/1	0.92	0.11	72,72,72,72	0
58	MG	CA	3250	1/1	0.92	0.13	76,76,76,76	0
58	MG	CA	3253	1/1	0.92	0.10	56,56,56,56	0
58	MG	AB	3022	1/1	0.92	0.07	56,56,56,56	0
58	MG	BA	3174	1/1	0.92	0.07	69,69,69,69	0
58	MG	AA	3606	1/1	0.92	0.15	64,64,64,64	0
58	MG	AA	3273	1/1	0.92	0.17	52,52,52,52	0
58	MG	AA	3211	1/1	0.92	0.28	86,86,86,86	0
58	MG	AA	3277	1/1	0.92	0.32	78,78,78,78	0
58	MG	AA	3285	1/1	0.92	0.09	44,44,44,44	0
58	MG	AA	3002	1/1	0.92	0.11	54,54,54,54	0
58	MG	AA	3718	1/1	0.92	0.12	47,47,47,47	0
58	MG	CA	3287	1/1	0.92	0.10	55,55,55,55	0
58	MG	CA	3566	1/1	0.92	0.12	41,41,41,41	1
58	MG	DA	1696	1/1	0.92	0.19	64,64,64,64	0
58	MG	CA	3288	1/1	0.92	0.12	63,63,63,63	0
58	MG	CA	3097	1/1	0.92	0.17	65,65,65,65	0
58	MG	CA	3293	1/1	0.92	0.07	26,26,26,26	0
58	MG	CA	3294	1/1	0.92	0.15	71,71,71,71	0
58	MG	AA	3719	1/1	0.92	0.12	41,41,41,41	0
58	MG	AF	307	1/1	0.92	0.13	61,61,61,61	0
58	MG	AA	3019	1/1	0.92	0.10	57,57,57,57	0
58	MG	DA	1708	1/1	0.92	0.17	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3618	1/1	0.92	0.10	49,49,49,49	0
58	MG	CA	3311	1/1	0.92	0.09	48,48,48,48	0
58	MG	CA	3102	1/1	0.92	0.16	76,76,76,76	0
58	MG	BA	3192	1/1	0.92	0.09	65,65,65,65	0
58	MG	CA	3334	1/1	0.92	0.19	72,72,72,72	0
58	MG	CA	3590	1/1	0.92	0.12	62,62,62,62	0
58	MG	AQ	202	1/1	0.92	0.06	29,29,29,29	0
58	MG	BA	3076	1/1	0.92	0.10	42,42,42,42	0
58	MG	AA	3316	1/1	0.92	0.16	59,59,59,59	0
58	MG	DA	1725	1/1	0.92	0.13	64,64,64,64	0
58	MG	DA	1726	1/1	0.92	0.08	61,61,61,61	0
58	MG	AA	3028	1/1	0.92	0.16	55,55,55,55	0
58	MG	CA	3598	1/1	0.92	0.10	66,66,66,66	0
58	MG	CA	3600	1/1	0.92	0.06	39,39,39,39	0
58	MG	CA	3349	1/1	0.92	0.14	54,54,54,54	0
58	MG	BA	3198	1/1	0.92	0.20	68,68,68,68	0
58	MG	AA	3229	1/1	0.92	0.10	54,54,54,54	0
58	MG	CA	3359	1/1	0.92	0.10	44,44,44,44	0
58	MG	CA	3361	1/1	0.92	0.11	48,48,48,48	0
58	MG	CA	3366	1/1	0.92	0.10	47,47,47,47	0
58	MG	CA	3367	1/1	0.92	0.20	59,59,59,59	0
58	MG	CA	3125	1/1	0.92	0.12	47,47,47,47	0
58	MG	AA	3330	1/1	0.92	0.11	66,66,66,66	0
58	MG	CA	3622	1/1	0.92	0.20	51,51,51,51	0
58	MG	DA	1746	1/1	0.92	0.11	77,77,77,77	0
58	MG	AA	3068	1/1	0.92	0.13	53,53,53,53	0
58	MG	AA	3748	1/1	0.92	0.11	56,56,56,56	0
58	MG	CA	3378	1/1	0.92	0.08	78,78,78,78	0
58	MG	BA	3208	1/1	0.92	0.10	81,81,81,81	0
58	MG	CA	3380	1/1	0.92	0.14	63,63,63,63	0
58	MG	CA	3385	1/1	0.92	0.14	70,70,70,70	0
58	MG	AA	3185	1/1	0.92	0.17	65,65,65,65	0
58	MG	CA	3134	1/1	0.92	0.20	69,69,69,69	0
58	MG	AA	3341	1/1	0.92	0.08	15,15,15,15	0
58	MG	BA	3211	1/1	0.92	0.10	59,59,59,59	0
58	MG	CA	3138	1/1	0.92	0.27	70,70,70,70	0
58	MG	CA	3395	1/1	0.92	0.07	53,53,53,53	0
58	MG	AA	3101	1/1	0.92	0.16	51,51,51,51	0
58	MG	CA	3397	1/1	0.92	0.08	59,59,59,59	0
58	MG	AA	3757	1/1	0.92	0.12	43,43,43,43	0
58	MG	DT	3001	1/1	0.92	0.20	66,66,66,66	0
58	MG	AA	3069	1/1	0.92	0.10	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3492	1/1	0.92	0.08	61,61,61,61	0
58	MG	DZ	703	1/1	0.92	0.08	56,56,56,56	0
59	K	AA	3818	1/1	0.92	0.13	87,87,87,87	0
58	MG	AA	3493	1/1	0.92	0.17	44,44,44,44	0
58	MG	CA	3069	1/1	0.93	0.12	56,56,56,56	0
58	MG	CA	3228	1/1	0.93	0.20	51,51,51,51	0
58	MG	AA	3051	1/1	0.93	0.19	34,34,34,34	0
58	MG	BA	3172	1/1	0.93	0.09	55,55,55,55	0
58	MG	CD	302	1/1	0.93	0.07	76,76,76,76	0
58	MG	CA	3235	1/1	0.93	0.30	70,70,70,70	0
58	MG	AA	3754	1/1	0.93	0.06	40,40,40,40	0
58	MG	AA	3453	1/1	0.93	0.13	54,54,54,54	0
58	MG	AA	3134	1/1	0.93	0.18	67,67,67,67	0
58	MG	AA	3079	1/1	0.93	0.29	63,63,63,63	0
58	MG	AA	3464	1/1	0.93	0.14	59,59,59,59	0
58	MG	AA	3284	1/1	0.93	0.16	43,43,43,43	0
58	MG	AV	205	1/1	0.93	0.07	37,37,37,37	0
58	MG	AA	3145	1/1	0.93	0.05	38,38,38,38	0
58	MG	CA	3496	1/1	0.93	0.17	64,64,64,64	0
58	MG	AA	3018	1/1	0.93	0.31	75,75,75,75	0
58	MG	CU	3001	1/1	0.93	0.22	91,91,91,91	0
58	MG	A1	101	1/1	0.93	0.10	54,54,54,54	0
58	MG	A2	3001	1/1	0.93	0.07	50,50,50,50	0
58	MG	CA	3501	1/1	0.93	0.09	63,63,63,63	0
58	MG	AA	3373	1/1	0.93	0.17	57,57,57,57	0
58	MG	AA	3088	1/1	0.93	0.21	73,73,73,73	0
58	MG	CA	3508	1/1	0.93	0.10	57,57,57,57	0
58	MG	DA	1609	1/1	0.93	0.09	45,45,45,45	0
58	MG	BA	3078	1/1	0.93	0.19	66,66,66,66	0
58	MG	DA	1613	1/1	0.93	0.27	70,70,70,70	0
58	MG	AA	3771	1/1	0.93	0.18	38,38,38,38	1
58	MG	AA	3482	1/1	0.93	0.10	64,64,64,64	0
58	MG	AA	3110	1/1	0.93	0.06	50,50,50,50	0
58	MG	AA	3609	1/1	0.93	0.08	71,71,71,71	0
58	MG	BA	3085	1/1	0.93	0.18	49,49,49,49	0
58	MG	CA	3517	1/1	0.93	0.10	77,77,77,77	0
58	MG	CA	3518	1/1	0.93	0.06	61,61,61,61	0
58	MG	CA	3519	1/1	0.93	0.15	62,62,62,62	0
58	MG	AA	3399	1/1	0.93	0.13	39,39,39,39	0
58	MG	CA	3521	1/1	0.93	0.16	77,77,77,77	0
58	MG	CA	3522	1/1	0.93	0.09	59,59,59,59	0
58	MG	CA	3103	1/1	0.93	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
58	MG	BA	3001	1/1	0.93	0.09	55,55,55,55	0
58	MG	BA	3202	1/1	0.93	0.09	62,62,62,62	0
58	MG	DA	1638	1/1	0.93	0.10	74,74,74,74	0
58	MG	AA	3780	1/1	0.93	0.08	41,41,41,41	0
58	MG	AA	3093	1/1	0.93	0.30	52,52,52,52	0
58	MG	CA	3290	1/1	0.93	0.10	53,53,53,53	0
58	MG	CA	3117	1/1	0.93	0.30	73,73,73,73	0
58	MG	DA	1643	1/1	0.93	0.10	55,55,55,55	0
58	MG	BA	3206	1/1	0.93	0.12	62,62,62,62	0
58	MG	CA	3536	1/1	0.93	0.10	75,75,75,75	0
58	MG	AA	3165	1/1	0.93	0.08	56,56,56,56	0
58	MG	CA	3121	1/1	0.93	0.23	60,60,60,60	0
58	MG	AA	3788	1/1	0.93	0.18	60,60,60,60	0
58	MG	CA	3300	1/1	0.93	0.14	66,66,66,66	0
58	MG	AA	3789	1/1	0.93	0.16	52,52,52,52	0
58	MG	DA	1658	1/1	0.93	0.06	63,63,63,63	0
58	MG	CA	3542	1/1	0.93	0.09	82,82,82,82	0
58	MG	DA	1660	1/1	0.93	0.10	70,70,70,70	0
58	MG	AA	3416	1/1	0.93	0.09	25,25,25,25	0
58	MG	AA	3209	1/1	0.93	0.15	59,59,59,59	0
58	MG	AA	3422	1/1	0.93	0.07	23,23,23,23	0
58	MG	AA	3332	1/1	0.93	0.10	44,44,44,44	0
58	MG	CA	3332	1/1	0.93	0.11	50,50,50,50	0
58	MG	AA	3253	1/1	0.93	0.11	65,65,65,65	0
58	MG	CA	3551	1/1	0.93	0.07	57,57,57,57	0
58	MG	AA	3625	1/1	0.93	0.10	63,63,63,63	0
58	MG	AA	3030	1/1	0.93	0.14	31,31,31,31	1
58	MG	CA	3556	1/1	0.93	0.19	66,66,66,66	0
58	MG	AA	3543	1/1	0.93	0.12	62,62,62,62	0
58	MG	CA	3342	1/1	0.93	0.11	69,69,69,69	0
58	MG	BA	3018	1/1	0.93	0.08	72,72,72,72	0
58	MG	AA	3213	1/1	0.93	0.14	50,50,50,50	1
58	MG	DA	1680	1/1	0.93	0.15	56,56,56,56	0
58	MG	AA	3808	1/1	0.93	0.15	33,33,33,33	1
58	MG	CA	3352	1/1	0.93	0.08	46,46,46,46	0
58	MG	CA	3357	1/1	0.93	0.15	57,57,57,57	0
58	MG	BX	102	1/1	0.93	0.15	67,67,67,67	0
58	MG	AA	3811	1/1	0.93	0.10	53,53,53,53	0
58	MG	BA	3023	1/1	0.93	0.28	75,75,75,75	0
58	MG	CA	3362	1/1	0.93	0.16	57,57,57,57	0
58	MG	CA	3364	1/1	0.93	0.10	65,65,65,65	0
58	MG	BX	105	1/1	0.93	0.11	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3630	1/1	0.93	0.10	58,58,58,58	0
58	MG	CA	3369	1/1	0.93	0.09	58,58,58,58	0
58	MG	AA	3714	1/1	0.93	0.16	55,55,55,55	1
58	MG	AA	3819	1/1	0.93	0.08	44,44,44,44	0
58	MG	AA	3096	1/1	0.93	0.21	81,81,81,81	0
58	MG	CA	3155	1/1	0.93	0.24	69,69,69,69	0
58	MG	AA	3268	1/1	0.93	0.29	61,61,61,61	0
58	MG	CA	3157	1/1	0.93	0.18	68,68,68,68	0
58	MG	CA	3595	1/1	0.93	0.07	69,69,69,69	0
58	MG	BA	3120	1/1	0.93	0.16	78,78,78,78	0
58	MG	AA	3016	1/1	0.93	0.19	57,57,57,57	0
58	MG	AA	3041	1/1	0.93	0.33	75,75,75,75	0
58	MG	CA	3601	1/1	0.93	0.08	73,73,73,73	0
58	MG	CA	3605	1/1	0.93	0.12	63,63,63,63	0
58	MG	DA	1716	1/1	0.93	0.10	75,75,75,75	0
58	MG	DA	1717	1/1	0.93	0.13	74,74,74,74	0
58	MG	CA	3388	1/1	0.93	0.12	68,68,68,68	0
58	MG	CA	3018	1/1	0.93	0.14	62,62,62,62	0
58	MG	CA	3168	1/1	0.93	0.14	58,58,58,58	0
58	MG	CA	3609	1/1	0.93	0.12	64,64,64,64	0
58	MG	AB	3005	1/1	0.93	0.16	67,67,67,67	0
58	MG	BA	3128	1/1	0.93	0.11	47,47,47,47	0
58	MG	BA	3130	1/1	0.93	0.07	49,49,49,49	0
58	MG	BA	3036	1/1	0.93	0.24	72,72,72,72	0
58	MG	AA	3726	1/1	0.93	0.08	37,37,37,37	0
58	MG	CA	3033	1/1	0.93	0.20	88,88,88,88	0
58	MG	DA	1731	1/1	0.93	0.14	82,82,82,82	0
58	MG	CA	3180	1/1	0.93	0.29	74,74,74,74	0
58	MG	BA	3038	1/1	0.93	0.08	65,65,65,65	0
58	MG	AB	3008	1/1	0.93	0.16	51,51,51,51	0
58	MG	CA	3625	1/1	0.93	0.13	53,53,53,53	0
58	MG	BA	3043	1/1	0.93	0.18	65,65,65,65	0
58	MG	CA	3410	1/1	0.93	0.11	40,40,40,40	0
58	MG	AA	3638	1/1	0.93	0.08	45,45,45,45	0
58	MG	CA	3044	1/1	0.93	0.10	52,52,52,52	0
58	MG	BA	3147	1/1	0.93	0.09	84,84,84,84	0
58	MG	CA	3420	1/1	0.93	0.10	58,58,58,58	0
58	MG	AB	3016	1/1	0.93	0.09	33,33,33,33	0
58	MG	DA	1747	1/1	0.93	0.20	78,78,78,78	0
58	MG	AA	3226	1/1	0.93	0.20	73,73,73,73	0
58	MG	CA	3428	1/1	0.93	0.08	55,55,55,55	0
58	MG	BA	3150	1/1	0.93	0.11	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3430	1/1	0.93	0.16	71,71,71,71	0
58	MG	AA	3732	1/1	0.93	0.13	41,41,41,41	0
58	MG	DA	1755	1/1	0.93	0.19	71,71,71,71	0
58	MG	DA	1757	1/1	0.93	0.12	73,73,73,73	0
58	MG	DA	1759	1/1	0.93	0.07	64,64,64,64	0
58	MG	AA	3448	1/1	0.93	0.06	17,17,17,17	0
58	MG	AB	3020	1/1	0.93	0.11	53,53,53,53	0
58	MG	CA	3203	1/1	0.93	0.29	76,76,76,76	0
58	MG	AB	3021	1/1	0.93	0.17	60,60,60,60	0
58	MG	AA	3643	1/1	0.93	0.09	47,47,47,47	0
58	MG	CA	3457	1/1	0.93	0.15	58,58,58,58	0
58	MG	DE	201	1/1	0.93	0.12	82,82,82,82	0
58	MG	AA	3738	1/1	0.93	0.11	28,28,28,28	0
58	MG	BA	3162	1/1	0.93	0.09	54,54,54,54	0
58	MG	AA	3449	1/1	0.93	0.13	53,53,53,53	0
58	MG	CA	3665	1/1	0.93	0.15	55,55,55,55	0
58	MG	AA	3451	1/1	0.93	0.11	53,53,53,53	1
58	MG	CA	3064	1/1	0.93	0.12	51,51,51,51	0
58	MG	AA	3747	1/1	0.93	0.13	62,62,62,62	0
58	MG	CA	3476	1/1	0.93	0.12	54,54,54,54	0
58	MG	AA	3583	1/1	0.93	0.16	64,64,64,64	0
60	ZN	C4	501	1/1	0.93	0.06	192,192,192,192	0
58	MG	AA	3588	1/1	0.93	0.18	54,54,54,54	0
58	MG	AA	3236	1/1	0.94	0.22	37,37,37,37	1
58	MG	CA	3402	1/1	0.94	0.14	67,67,67,67	0
58	MG	CA	3150	1/1	0.94	0.13	63,63,63,63	0
58	MG	AE	302	1/1	0.94	0.15	68,68,68,68	0
58	MG	CA	3651	1/1	0.94	0.14	51,51,51,51	0
58	MG	AF	302	1/1	0.94	0.21	31,31,31,31	1
58	MG	BB	3001	1/1	0.94	0.23	76,76,76,76	0
58	MG	AA	3615	1/1	0.94	0.06	55,55,55,55	0
58	MG	AA	3462	1/1	0.94	0.12	70,70,70,70	0
58	MG	CA	3659	1/1	0.94	0.22	104,104,104,104	0
58	MG	AG	202	1/1	0.94	0.07	73,73,73,73	0
58	MG	CA	3414	1/1	0.94	0.07	39,39,39,39	0
58	MG	CA	3666	1/1	0.94	0.22	62,62,62,62	0
58	MG	CA	3415	1/1	0.94	0.09	52,52,52,52	0
58	MG	CB	3002	1/1	0.94	0.07	64,64,64,64	0
58	MG	AH	3001	1/1	0.94	0.18	50,50,50,50	0
58	MG	AA	3177	1/1	0.94	0.13	51,51,51,51	0
58	MG	AA	3179	1/1	0.94	0.17	78,78,78,78	0
58	MG	CA	3423	1/1	0.94	0.12	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AP	201	1/1	0.94	0.16	66,66,66,66	0
58	MG	AP	203	1/1	0.94	0.10	41,41,41,41	0
58	MG	CB	3010	1/1	0.94	0.09	53,53,53,53	0
58	MG	AA	3116	1/1	0.94	0.16	75,75,75,75	0
58	MG	AU	201	1/1	0.94	0.11	44,44,44,44	0
58	MG	CA	3431	1/1	0.94	0.20	51,51,51,51	0
58	MG	AA	3743	1/1	0.94	0.13	80,80,80,80	0
58	MG	CE	303	1/1	0.94	0.17	53,53,53,53	0
58	MG	AV	204	1/1	0.94	0.17	37,37,37,37	0
58	MG	CA	3435	1/1	0.94	0.07	28,28,28,28	0
58	MG	AA	3184	1/1	0.94	0.07	36,36,36,36	0
58	MG	AW	3001	1/1	0.94	0.20	50,50,50,50	0
58	MG	CF	303	1/1	0.94	0.10	50,50,50,50	0
58	MG	AW	3004	1/1	0.94	0.21	64,64,64,64	0
58	MG	AA	3004	1/1	0.94	0.10	24,24,24,24	0
58	MG	CA	3183	1/1	0.94	0.11	25,25,25,25	0
58	MG	CA	3184	1/1	0.94	0.28	85,85,85,85	0
58	MG	CA	3001	1/1	0.94	0.20	71,71,71,71	0
58	MG	CA	3467	1/1	0.94	0.08	54,54,54,54	0
58	MG	CQ	203	1/1	0.94	0.08	59,59,59,59	0
58	MG	BA	3097	1/1	0.94	0.17	66,66,66,66	0
58	MG	CA	3470	1/1	0.94	0.13	69,69,69,69	0
58	MG	CV	202	1/1	0.94	0.18	85,85,85,85	0
58	MG	AA	3014	1/1	0.94	0.12	44,44,44,44	0
58	MG	CA	3006	1/1	0.94	0.08	65,65,65,65	0
58	MG	AA	3125	1/1	0.94	0.16	63,63,63,63	0
58	MG	AA	3128	1/1	0.94	0.16	71,71,71,71	0
58	MG	AA	3489	1/1	0.94	0.07	63,63,63,63	0
58	MG	CA	3197	1/1	0.94	0.23	63,63,63,63	0
58	MG	DA	1608	1/1	0.94	0.11	58,58,58,58	0
58	MG	A5	101	1/1	0.94	0.10	43,43,43,43	1
58	MG	AA	3262	1/1	0.94	0.14	49,49,49,49	0
58	MG	AA	3632	1/1	0.94	0.07	45,45,45,45	0
58	MG	AA	3194	1/1	0.94	0.17	60,60,60,60	0
58	MG	DA	1616	1/1	0.94	0.08	51,51,51,51	0
58	MG	AA	3082	1/1	0.94	0.08	38,38,38,38	0
58	MG	AA	3496	1/1	0.94	0.07	58,58,58,58	0
58	MG	CA	3032	1/1	0.94	0.24	67,67,67,67	0
58	MG	AA	3637	1/1	0.94	0.17	64,64,64,64	0
58	MG	CA	3208	1/1	0.94	0.16	69,69,69,69	0
58	MG	AA	3500	1/1	0.94	0.09	55,55,55,55	0
58	MG	CA	3491	1/1	0.94	0.12	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3035	1/1	0.94	0.16	58,58,58,58	0
58	MG	AA	3765	1/1	0.94	0.13	61,61,61,61	0
58	MG	CA	3213	1/1	0.94	0.12	68,68,68,68	0
58	MG	CA	3214	1/1	0.94	0.16	43,43,43,43	0
58	MG	CA	3039	1/1	0.94	0.18	69,69,69,69	0
58	MG	BA	3113	1/1	0.94	0.13	60,60,60,60	0
58	MG	CA	3218	1/1	0.94	0.10	50,50,50,50	0
58	MG	CA	3222	1/1	0.94	0.10	53,53,53,53	0
58	MG	AA	3639	1/1	0.94	0.17	71,71,71,71	0
58	MG	CA	3224	1/1	0.94	0.14	64,64,64,64	0
58	MG	AA	3509	1/1	0.94	0.14	48,48,48,48	0
58	MG	AA	3769	1/1	0.94	0.16	56,56,56,56	0
58	MG	DA	1644	1/1	0.94	0.17	64,64,64,64	0
58	MG	DA	1646	1/1	0.94	0.16	57,57,57,57	0
58	MG	AA	3770	1/1	0.94	0.32	39,39,39,39	0
58	MG	AA	3511	1/1	0.94	0.21	56,56,56,56	0
58	MG	BA	3121	1/1	0.94	0.07	59,59,59,59	0
58	MG	CA	3233	1/1	0.94	0.14	56,56,56,56	0
58	MG	DA	1654	1/1	0.94	0.17	57,57,57,57	0
58	MG	AA	3365	1/1	0.94	0.11	54,54,54,54	0
58	MG	AA	3372	1/1	0.94	0.18	61,61,61,61	0
58	MG	AA	3197	1/1	0.94	0.17	49,49,49,49	0
58	MG	AA	3103	1/1	0.94	0.19	48,48,48,48	0
58	MG	CA	3056	1/1	0.94	0.14	61,61,61,61	0
58	MG	AA	3529	1/1	0.94	0.09	28,28,28,28	0
58	MG	AA	3783	1/1	0.94	0.10	52,52,52,52	0
58	MG	BA	3132	1/1	0.94	0.12	61,61,61,61	0
58	MG	BA	3133	1/1	0.94	0.09	68,68,68,68	0
58	MG	AA	3062	1/1	0.94	0.28	66,66,66,66	0
58	MG	AA	3385	1/1	0.94	0.08	28,28,28,28	0
58	MG	DA	1667	1/1	0.94	0.25	61,61,61,61	0
58	MG	BA	3019	1/1	0.94	0.14	55,55,55,55	0
58	MG	AA	3144	1/1	0.94	0.15	47,47,47,47	0
58	MG	BA	3143	1/1	0.94	0.14	79,79,79,79	0
58	MG	AA	3544	1/1	0.94	0.12	52,52,52,52	0
58	MG	AA	3546	1/1	0.94	0.08	53,53,53,53	1
58	MG	AA	3661	1/1	0.94	0.20	43,43,43,43	0
58	MG	CA	3258	1/1	0.94	0.12	40,40,40,40	0
58	MG	AA	3271	1/1	0.94	0.10	55,55,55,55	0
58	MG	CA	3261	1/1	0.94	0.11	47,47,47,47	0
58	MG	BA	3026	1/1	0.94	0.20	57,57,57,57	0
58	MG	CA	3076	1/1	0.94	0.26	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3799	1/1	0.94	0.13	48,48,48,48	0
58	MG	CA	3544	1/1	0.94	0.09	66,66,66,66	0
58	MG	CA	3278	1/1	0.94	0.07	48,48,48,48	0
58	MG	AA	3665	1/1	0.94	0.14	83,83,83,83	0
58	MG	CA	3282	1/1	0.94	0.07	31,31,31,31	0
58	MG	CA	3284	1/1	0.94	0.07	48,48,48,48	0
58	MG	AA	3085	1/1	0.94	0.10	30,30,30,30	0
58	MG	AA	3204	1/1	0.94	0.12	55,55,55,55	0
58	MG	DA	1694	1/1	0.94	0.19	65,65,65,65	0
58	MG	BA	3032	1/1	0.94	0.09	47,47,47,47	0
58	MG	AA	3419	1/1	0.94	0.12	26,26,26,26	0
58	MG	AA	3572	1/1	0.94	0.10	49,49,49,49	0
58	MG	AA	3108	1/1	0.94	0.12	74,74,74,74	0
58	MG	CA	3559	1/1	0.94	0.07	75,75,75,75	0
58	MG	DA	1701	1/1	0.94	0.17	64,64,64,64	0
58	MG	AA	3063	1/1	0.94	0.27	66,66,66,66	0
58	MG	AA	3809	1/1	0.94	0.16	60,60,60,60	0
58	MG	CA	3295	1/1	0.94	0.08	69,69,69,69	0
58	MG	CA	3091	1/1	0.94	0.20	63,63,63,63	0
58	MG	CA	3567	1/1	0.94	0.15	49,49,49,49	0
58	MG	CA	3092	1/1	0.94	0.27	107,107,107,107	0
58	MG	CA	3299	1/1	0.94	0.21	54,54,54,54	0
58	MG	CA	3093	1/1	0.94	0.12	68,68,68,68	0
58	MG	DA	1712	1/1	0.94	0.08	51,51,51,51	0
58	MG	DA	1713	1/1	0.94	0.15	74,74,74,74	0
58	MG	CA	3575	1/1	0.94	0.07	78,78,78,78	0
58	MG	AA	3278	1/1	0.94	0.07	35,35,35,35	0
58	MG	AA	3429	1/1	0.94	0.17	42,42,42,42	0
58	MG	BA	3042	1/1	0.94	0.09	69,69,69,69	0
58	MG	AA	3089	1/1	0.94	0.07	33,33,33,33	0
58	MG	AA	3064	1/1	0.94	0.06	35,35,35,35	0
58	MG	CA	3331	1/1	0.94	0.13	43,43,43,43	0
58	MG	AA	3436	1/1	0.94	0.08	52,52,52,52	0
58	MG	BA	3175	1/1	0.94	0.14	78,78,78,78	0
58	MG	AA	3215	1/1	0.94	0.08	56,56,56,56	0
58	MG	AA	3438	1/1	0.94	0.05	19,19,19,19	0
58	MG	CA	3105	1/1	0.94	0.13	45,45,45,45	0
58	MG	BA	3049	1/1	0.94	0.07	36,36,36,36	0
58	MG	BA	3050	1/1	0.94	0.21	67,67,67,67	0
58	MG	CA	3345	1/1	0.94	0.14	87,87,87,87	0
58	MG	CA	3113	1/1	0.94	0.13	60,60,60,60	0
58	MG	AA	3298	1/1	0.94	0.10	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3698	1/1	0.94	0.10	62,62,62,62	0
58	MG	CA	3355	1/1	0.94	0.11	59,59,59,59	0
58	MG	CA	3602	1/1	0.94	0.09	78,78,78,78	0
58	MG	CA	3604	1/1	0.94	0.07	74,74,74,74	0
58	MG	AA	3160	1/1	0.94	0.19	50,50,50,50	0
58	MG	DA	1741	1/1	0.94	0.19	68,68,68,68	0
58	MG	AA	3700	1/1	0.94	0.14	48,48,48,48	0
58	MG	AA	3052	1/1	0.94	0.28	63,63,63,63	0
58	MG	CA	3120	1/1	0.94	0.17	127,127,127,127	0
58	MG	AA	3704	1/1	0.94	0.08	76,76,76,76	0
58	MG	BA	3190	1/1	0.94	0.17	89,89,89,89	0
58	MG	AA	3317	1/1	0.94	0.13	57,57,57,57	0
58	MG	CA	3612	1/1	0.94	0.19	74,74,74,74	0
58	MG	AA	3168	1/1	0.94	0.10	64,64,64,64	0
58	MG	CA	3368	1/1	0.94	0.18	64,64,64,64	0
58	MG	BA	3193	1/1	0.94	0.10	70,70,70,70	0
58	MG	AA	3447	1/1	0.94	0.23	75,75,75,75	0
58	MG	AA	3171	1/1	0.94	0.11	53,53,53,53	0
58	MG	BA	3061	1/1	0.94	0.22	67,67,67,67	0
58	MG	CA	3131	1/1	0.94	0.25	70,70,70,70	0
58	MG	CA	3132	1/1	0.94	0.14	61,61,61,61	0
58	MG	CA	3626	1/1	0.94	0.08	62,62,62,62	0
58	MG	AA	3325	1/1	0.94	0.07	65,65,65,65	0
58	MG	BA	3063	1/1	0.94	0.19	51,51,51,51	0
58	MG	DD	502	1/1	0.94	0.16	61,61,61,61	0
58	MG	AA	3715	1/1	0.94	0.15	54,54,54,54	0
58	MG	AA	3056	1/1	0.94	0.12	61,61,61,61	0
58	MG	CA	3633	1/1	0.94	0.07	61,61,61,61	0
58	MG	AA	3231	1/1	0.94	0.15	41,41,41,41	0
58	MG	AD	303	1/1	0.94	0.13	70,70,70,70	0
58	MG	DL	3002	1/1	0.94	0.08	74,74,74,74	0
58	MG	AA	3115	1/1	0.94	0.09	15,15,15,15	0
58	MG	CA	3637	1/1	0.94	0.09	79,79,79,79	0
58	MG	CA	3142	1/1	0.94	0.17	54,54,54,54	0
58	MG	AA	3610	1/1	0.94	0.09	51,51,51,51	0
58	MG	CA	3145	1/1	0.94	0.20	66,66,66,66	0
58	MG	AA	3175	1/1	0.94	0.21	60,60,60,60	0
58	MG	AA	3460	1/1	0.94	0.10	71,71,71,71	0
58	MG	AA	3303	1/1	0.95	0.09	53,53,53,53	0
58	MG	CB	3011	1/1	0.95	0.21	51,51,51,51	0
58	MG	AA	3730	1/1	0.95	0.07	38,38,38,38	0
58	MG	CA	3471	1/1	0.95	0.09	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3523	1/1	0.95	0.12	27,27,27,27	0
58	MG	AA	3733	1/1	0.95	0.08	66,66,66,66	0
58	MG	CD	303	1/1	0.95	0.07	35,35,35,35	0
58	MG	CA	3226	1/1	0.95	0.18	64,64,64,64	0
58	MG	AA	3734	1/1	0.95	0.16	65,65,65,65	0
58	MG	CE	305	1/1	0.95	0.09	41,41,41,41	0
58	MG	BA	3165	1/1	0.95	0.07	61,61,61,61	0
58	MG	AA	3735	1/1	0.95	0.11	21,21,21,21	0
58	MG	CA	3073	1/1	0.95	0.11	53,53,53,53	0
58	MG	CF	302	1/1	0.95	0.22	63,63,63,63	0
58	MG	AA	3189	1/1	0.95	0.06	11,11,11,11	0
58	MG	CA	3234	1/1	0.95	0.13	58,58,58,58	0
58	MG	AA	3430	1/1	0.95	0.08	25,25,25,25	0
58	MG	CA	3236	1/1	0.95	0.10	52,52,52,52	0
58	MG	AA	3531	1/1	0.95	0.06	52,52,52,52	0
58	MG	AD	310	1/1	0.95	0.13	44,44,44,44	0
58	MG	AA	3739	1/1	0.95	0.17	74,74,74,74	0
58	MG	AA	3191	1/1	0.95	0.14	44,44,44,44	0
58	MG	AA	3741	1/1	0.95	0.09	45,45,45,45	0
58	MG	AE	305	1/1	0.95	0.07	29,29,29,29	0
58	MG	CU	3002	1/1	0.95	0.15	63,63,63,63	0
58	MG	CA	3492	1/1	0.95	0.09	52,52,52,52	0
58	MG	C0	101	1/1	0.95	0.10	64,64,64,64	0
58	MG	C8	5001	1/1	0.95	0.17	48,48,48,48	0
58	MG	DA	1601	1/1	0.95	0.14	59,59,59,59	0
58	MG	AA	3154	1/1	0.95	0.14	56,56,56,56	0
58	MG	AA	3155	1/1	0.95	0.19	48,48,48,48	0
58	MG	AA	3080	1/1	0.95	0.13	33,33,33,33	0
58	MG	AG	201	1/1	0.95	0.09	49,49,49,49	0
58	MG	AA	3324	1/1	0.95	0.06	32,32,32,32	0
58	MG	BA	3066	1/1	0.95	0.17	53,53,53,53	0
58	MG	AA	3750	1/1	0.95	0.06	14,14,14,14	0
58	MG	AA	3158	1/1	0.95	0.09	35,35,35,35	0
58	MG	CA	3503	1/1	0.95	0.11	49,49,49,49	1
58	MG	AA	3552	1/1	0.95	0.12	51,51,51,51	0
58	MG	DA	1614	1/1	0.95	0.18	70,70,70,70	0
58	MG	CA	3505	1/1	0.95	0.07	60,60,60,60	0
58	MG	AA	3328	1/1	0.95	0.05	17,17,17,17	0
58	MG	AA	3045	1/1	0.95	0.44	43,43,43,43	0
58	MG	CA	3259	1/1	0.95	0.20	56,56,56,56	0
58	MG	AQ	201	1/1	0.95	0.28	51,51,51,51	0
58	MG	DA	1622	1/1	0.95	0.06	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	DA	1623	1/1	0.95	0.26	77,77,77,77	0
58	MG	AA	3023	1/1	0.95	0.09	37,37,37,37	0
58	MG	CA	3512	1/1	0.95	0.07	64,64,64,64	0
58	MG	DA	1627	1/1	0.95	0.21	48,48,48,48	0
58	MG	CA	3264	1/1	0.95	0.06	60,60,60,60	0
58	MG	CA	3269	1/1	0.95	0.11	54,54,54,54	0
58	MG	AA	3164	1/1	0.95	0.16	37,37,37,37	0
58	MG	CA	3273	1/1	0.95	0.11	54,54,54,54	0
58	MG	AA	3445	1/1	0.95	0.09	59,59,59,59	0
58	MG	AA	3250	1/1	0.95	0.11	62,62,62,62	0
58	MG	AA	3252	1/1	0.95	0.09	46,46,46,46	0
58	MG	AA	3032	1/1	0.95	0.12	37,37,37,37	0
58	MG	AA	3764	1/1	0.95	0.10	54,54,54,54	0
58	MG	CA	3112	1/1	0.95	0.08	70,70,70,70	0
58	MG	AX	101	1/1	0.95	0.23	72,72,72,72	0
58	MG	BA	3201	1/1	0.95	0.11	68,68,68,68	0
58	MG	AA	3167	1/1	0.95	0.18	29,29,29,29	0
58	MG	AA	3581	1/1	0.95	0.07	27,27,27,27	0
58	MG	AA	3662	1/1	0.95	0.15	58,58,58,58	0
58	MG	DA	1645	1/1	0.95	0.18	61,61,61,61	0
58	MG	BA	3086	1/1	0.95	0.23	51,51,51,51	0
58	MG	BA	3087	1/1	0.95	0.11	70,70,70,70	0
58	MG	DA	1649	1/1	0.95	0.10	60,60,60,60	0
58	MG	AA	3263	1/1	0.95	0.32	71,71,71,71	0
58	MG	CA	3122	1/1	0.95	0.10	43,43,43,43	0
58	MG	AA	3587	1/1	0.95	0.08	59,59,59,59	0
58	MG	AA	3203	1/1	0.95	0.15	46,46,46,46	0
58	MG	BA	3091	1/1	0.95	0.24	72,72,72,72	0
58	MG	AA	3127	1/1	0.95	0.16	52,52,52,52	0
58	MG	CA	3302	1/1	0.95	0.09	84,84,84,84	0
58	MG	A6	101	1/1	0.95	0.10	64,64,64,64	0
58	MG	AA	3670	1/1	0.95	0.08	31,31,31,31	0
58	MG	AA	3458	1/1	0.95	0.07	70,70,70,70	0
58	MG	AA	3169	1/1	0.95	0.21	61,61,61,61	0
58	MG	CA	3317	1/1	0.95	0.06	51,51,51,51	0
58	MG	AA	3267	1/1	0.95	0.10	49,49,49,49	0
58	MG	CA	3326	1/1	0.95	0.07	39,39,39,39	0
58	MG	CA	3328	1/1	0.95	0.13	52,52,52,52	0
58	MG	DA	1666	1/1	0.95	0.15	47,47,47,47	0
58	MG	CA	3329	1/1	0.95	0.07	57,57,57,57	0
58	MG	AA	3208	1/1	0.95	0.14	26,26,26,26	1
58	MG	DA	1669	1/1	0.95	0.07	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3676	1/1	0.95	0.13	64,64,64,64	0
58	MG	AA	3055	1/1	0.95	0.13	34,34,34,34	0
58	MG	CA	3137	1/1	0.95	0.09	51,51,51,51	0
58	MG	AA	3599	1/1	0.95	0.10	52,52,52,52	0
58	MG	AA	3468	1/1	0.95	0.11	51,51,51,51	0
58	MG	AA	3790	1/1	0.95	0.09	48,48,48,48	0
58	MG	AA	3792	1/1	0.95	0.09	27,27,27,27	0
58	MG	AA	3474	1/1	0.95	0.08	50,50,50,50	0
58	MG	CA	3347	1/1	0.95	0.07	33,33,33,33	0
58	MG	BX	106	1/1	0.95	0.07	55,55,55,55	0
58	MG	CA	3572	1/1	0.95	0.18	76,76,76,76	0
58	MG	CA	3144	1/1	0.95	0.25	56,56,56,56	0
58	MG	BA	3009	1/1	0.95	0.18	58,58,58,58	0
58	MG	CA	3354	1/1	0.95	0.07	46,46,46,46	0
58	MG	AA	3685	1/1	0.95	0.09	47,47,47,47	0
58	MG	CA	3147	1/1	0.95	0.15	58,58,58,58	0
58	MG	AA	3603	1/1	0.95	0.07	35,35,35,35	0
58	MG	BX	110	1/1	0.95	0.08	57,57,57,57	0
58	MG	AA	3797	1/1	0.95	0.08	39,39,39,39	0
58	MG	AA	3033	1/1	0.95	0.29	34,34,34,34	0
58	MG	CA	3003	1/1	0.95	0.21	44,44,44,44	0
58	MG	AA	3020	1/1	0.95	0.07	23,23,23,23	0
58	MG	CA	3005	1/1	0.95	0.22	56,56,56,56	0
58	MG	BA	3114	1/1	0.95	0.21	55,55,55,55	0
58	MG	AA	3693	1/1	0.95	0.17	60,60,60,60	0
58	MG	DA	1702	1/1	0.95	0.14	73,73,73,73	0
58	MG	CA	3010	1/1	0.95	0.09	40,40,40,40	0
58	MG	AA	3094	1/1	0.95	0.09	29,29,29,29	0
58	MG	CA	3162	1/1	0.95	0.17	63,63,63,63	0
58	MG	CA	3597	1/1	0.95	0.11	51,51,51,51	0
58	MG	CA	3165	1/1	0.95	0.12	41,41,41,41	0
58	MG	CA	3599	1/1	0.95	0.10	69,69,69,69	0
58	MG	CA	3014	1/1	0.95	0.14	62,62,62,62	0
58	MG	CA	3016	1/1	0.95	0.18	79,79,79,79	0
58	MG	AA	3696	1/1	0.95	0.21	76,76,76,76	0
58	MG	CA	3603	1/1	0.95	0.05	48,48,48,48	0
58	MG	AA	3805	1/1	0.95	0.18	40,40,40,40	1
58	MG	AA	3697	1/1	0.95	0.12	69,69,69,69	0
58	MG	AA	3366	1/1	0.95	0.06	52,52,52,52	0
58	MG	AA	3367	1/1	0.95	0.08	50,50,50,50	0
58	MG	AA	3176	1/1	0.95	0.09	49,49,49,49	0
58	MG	CA	3391	1/1	0.95	0.04	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	DA	1721	1/1	0.95	0.10	65,65,65,65	0
58	MG	DA	1722	1/1	0.95	0.07	58,58,58,58	0
58	MG	CA	3178	1/1	0.95	0.10	34,34,34,34	0
58	MG	CA	3393	1/1	0.95	0.07	35,35,35,35	0
58	MG	BA	3024	1/1	0.95	0.23	63,63,63,63	0
58	MG	BA	3127	1/1	0.95	0.11	50,50,50,50	0
58	MG	CA	3615	1/1	0.95	0.19	65,65,65,65	0
58	MG	AA	3484	1/1	0.95	0.12	35,35,35,35	0
58	MG	CA	3182	1/1	0.95	0.10	47,47,47,47	0
58	MG	CA	3399	1/1	0.95	0.09	63,63,63,63	0
58	MG	CA	3621	1/1	0.95	0.20	65,65,65,65	0
58	MG	AA	3138	1/1	0.95	0.09	54,54,54,54	0
58	MG	CA	3401	1/1	0.95	0.14	60,60,60,60	0
58	MG	DA	1735	1/1	0.95	0.09	70,70,70,70	0
58	MG	AA	3140	1/1	0.95	0.05	56,56,56,56	0
58	MG	CA	3036	1/1	0.95	0.08	42,42,42,42	0
58	MG	CA	3037	1/1	0.95	0.10	57,57,57,57	0
58	MG	AA	3817	1/1	0.95	0.21	57,57,57,57	0
58	MG	AA	3707	1/1	0.95	0.16	31,31,31,31	1
58	MG	CA	3191	1/1	0.95	0.14	84,84,84,84	0
58	MG	AA	3490	1/1	0.95	0.06	50,50,50,50	0
58	MG	AA	3225	1/1	0.95	0.10	34,34,34,34	0
58	MG	DA	1745	1/1	0.95	0.09	69,69,69,69	0
58	MG	AA	3280	1/1	0.95	0.09	46,46,46,46	0
58	MG	BA	3138	1/1	0.95	0.14	62,62,62,62	0
58	MG	DA	1748	1/1	0.95	0.18	66,66,66,66	0
58	MG	AA	3281	1/1	0.95	0.21	60,60,60,60	0
58	MG	DA	1750	1/1	0.95	0.08	71,71,71,71	0
58	MG	CA	3418	1/1	0.95	0.10	39,39,39,39	0
58	MG	BA	3141	1/1	0.95	0.08	49,49,49,49	0
58	MG	AA	3282	1/1	0.95	0.14	39,39,39,39	0
58	MG	AA	3716	1/1	0.95	0.06	63,63,63,63	0
58	MG	BA	3146	1/1	0.95	0.13	65,65,65,65	0
58	MG	CA	3052	1/1	0.95	0.24	69,69,69,69	0
58	MG	DA	1758	1/1	0.95	0.13	64,64,64,64	0
58	MG	AA	3623	1/1	0.95	0.06	43,43,43,43	0
58	MG	CA	3054	1/1	0.95	0.19	68,68,68,68	0
58	MG	CA	3207	1/1	0.95	0.21	55,55,55,55	0
58	MG	AB	3010	1/1	0.95	0.11	51,51,51,51	1
58	MG	AA	3074	1/1	0.95	0.16	59,59,59,59	0
58	MG	CA	3434	1/1	0.95	0.10	68,68,68,68	0
58	MG	AA	3078	1/1	0.95	0.14	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3436	1/1	0.95	0.06	53,53,53,53	0
58	MG	AA	3286	1/1	0.95	0.07	53,53,53,53	0
58	MG	CA	3443	1/1	0.95	0.18	66,66,66,66	0
58	MG	BA	3044	1/1	0.95	0.09	56,56,56,56	0
58	MG	BA	3156	1/1	0.95	0.09	36,36,36,36	0
58	MG	CA	3062	1/1	0.95	0.27	65,65,65,65	0
58	MG	CA	3456	1/1	0.95	0.07	46,46,46,46	0
58	MG	AA	3097	1/1	0.95	0.12	61,61,61,61	0
58	MG	CA	3459	1/1	0.95	0.06	48,48,48,48	0
58	MG	CA	3217	1/1	0.95	0.10	66,66,66,66	0
58	MG	CA	3463	1/1	0.95	0.08	50,50,50,50	0
58	MG	CA	3464	1/1	0.95	0.15	47,47,47,47	0
58	MG	AA	3021	1/1	0.95	0.10	39,39,39,39	0
60	ZN	DN	501	1/1	0.95	0.07	127,127,127,127	0
58	MG	CA	3221	1/1	0.95	0.10	76,76,76,76	0
58	MG	AA	3131	1/1	0.96	0.10	36,36,36,36	0
58	MG	CA	3664	1/1	0.96	0.13	55,55,55,55	0
58	MG	BA	3111	1/1	0.96	0.32	72,72,72,72	0
58	MG	AA	3276	1/1	0.96	0.26	50,50,50,50	0
58	MG	CA	3202	1/1	0.96	0.20	58,58,58,58	0
58	MG	AA	3132	1/1	0.96	0.14	53,53,53,53	0
58	MG	A0	103	1/1	0.96	0.09	54,54,54,54	0
58	MG	A0	105	1/1	0.96	0.07	36,36,36,36	0
58	MG	CB	3005	1/1	0.96	0.24	61,61,61,61	0
58	MG	AA	3195	1/1	0.96	0.10	43,43,43,43	0
58	MG	CA	3041	1/1	0.96	0.18	31,31,31,31	0
58	MG	CA	3441	1/1	0.96	0.18	56,56,56,56	0
58	MG	CA	3442	1/1	0.96	0.19	75,75,75,75	0
58	MG	AA	3751	1/1	0.96	0.05	26,26,26,26	0
58	MG	AA	3279	1/1	0.96	0.10	51,51,51,51	0
58	MG	AA	3081	1/1	0.96	0.08	56,56,56,56	0
58	MG	CA	3449	1/1	0.96	0.08	42,42,42,42	0
58	MG	CA	3451	1/1	0.96	0.05	47,47,47,47	0
58	MG	CA	3452	1/1	0.96	0.07	62,62,62,62	0
58	MG	CA	3453	1/1	0.96	0.15	59,59,59,59	0
58	MG	CA	3454	1/1	0.96	0.07	38,38,38,38	0
58	MG	AA	3370	1/1	0.96	0.12	57,57,57,57	0
58	MG	BA	3122	1/1	0.96	0.07	58,58,58,58	0
58	MG	BA	3123	1/1	0.96	0.07	54,54,54,54	0
58	MG	CA	3458	1/1	0.96	0.12	46,46,46,46	0
58	MG	AA	3371	1/1	0.96	0.11	59,59,59,59	0
58	MG	AA	3235	1/1	0.96	0.10	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3136	1/1	0.96	0.21	66,66,66,66	0
58	MG	AA	3494	1/1	0.96	0.07	33,33,33,33	1
58	MG	AA	3283	1/1	0.96	0.18	59,59,59,59	0
58	MG	AA	3379	1/1	0.96	0.06	30,30,30,30	0
58	MG	AA	3198	1/1	0.96	0.07	36,36,36,36	0
58	MG	CA	3469	1/1	0.96	0.08	61,61,61,61	0
58	MG	AA	3763	1/1	0.96	0.14	62,62,62,62	0
58	MG	AA	3382	1/1	0.96	0.07	38,38,38,38	1
58	MG	AA	3238	1/1	0.96	0.15	55,55,55,55	0
58	MG	CR	201	1/1	0.96	0.06	51,51,51,51	0
58	MG	AA	3515	1/1	0.96	0.05	18,18,18,18	0
58	MG	AA	3517	1/1	0.96	0.09	18,18,18,18	0
58	MG	CA	3061	1/1	0.96	0.24	74,74,74,74	0
58	MG	CA	3477	1/1	0.96	0.10	54,54,54,54	0
58	MG	C1	101	1/1	0.96	0.09	67,67,67,67	0
58	MG	C7	101	1/1	0.96	0.07	47,47,47,47	0
58	MG	AA	3642	1/1	0.96	0.10	41,41,41,41	0
58	MG	AA	3394	1/1	0.96	0.05	18,18,18,18	0
58	MG	CA	3480	1/1	0.96	0.09	44,44,44,44	0
58	MG	AA	3034	1/1	0.96	0.14	56,56,56,56	0
58	MG	AA	3646	1/1	0.96	0.11	57,57,57,57	0
58	MG	BA	3012	1/1	0.96	0.05	29,29,29,29	0
58	MG	AA	3401	1/1	0.96	0.10	33,33,33,33	0
58	MG	AA	3241	1/1	0.96	0.15	64,64,64,64	0
58	MG	AA	3777	1/1	0.96	0.05	20,20,20,20	0
58	MG	AA	3405	1/1	0.96	0.06	54,54,54,54	0
58	MG	DA	1610	1/1	0.96	0.10	45,45,45,45	0
58	MG	AA	3779	1/1	0.96	0.12	61,61,61,61	0
58	MG	DA	1612	1/1	0.96	0.07	38,38,38,38	0
58	MG	AA	3411	1/1	0.96	0.06	41,41,41,41	0
58	MG	AA	3532	1/1	0.96	0.12	60,60,60,60	0
58	MG	CA	3075	1/1	0.96	0.09	52,52,52,52	0
58	MG	AA	3654	1/1	0.96	0.13	65,65,65,65	0
58	MG	AA	3296	1/1	0.96	0.06	18,18,18,18	0
58	MG	DA	1618	1/1	0.96	0.10	47,47,47,47	0
58	MG	DA	1619	1/1	0.96	0.18	62,62,62,62	0
58	MG	AA	3787	1/1	0.96	0.14	50,50,50,50	0
58	MG	AA	3297	1/1	0.96	0.05	20,20,20,20	0
58	MG	AA	3542	1/1	0.96	0.06	45,45,45,45	0
58	MG	CA	3251	1/1	0.96	0.07	47,47,47,47	0
58	MG	AA	3035	1/1	0.96	0.12	59,59,59,59	0
58	MG	CA	3254	1/1	0.96	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
58	MG	AA	3139	1/1	0.96	0.11	49,49,49,49	0
58	MG	AA	3305	1/1	0.96	0.12	53,53,53,53	0
58	MG	CA	3087	1/1	0.96	0.14	35,35,35,35	0
58	MG	AA	3309	1/1	0.96	0.10	44,44,44,44	0
58	MG	BA	3029	1/1	0.96	0.08	54,54,54,54	0
58	MG	CA	3507	1/1	0.96	0.09	71,71,71,71	0
58	MG	DA	1633	1/1	0.96	0.19	60,60,60,60	0
58	MG	AA	3666	1/1	0.96	0.14	62,62,62,62	0
58	MG	AA	3667	1/1	0.96	0.12	29,29,29,29	0
58	MG	DA	1636	1/1	0.96	0.17	64,64,64,64	0
58	MG	CA	3265	1/1	0.96	0.12	55,55,55,55	0
58	MG	CA	3266	1/1	0.96	0.09	58,58,58,58	0
58	MG	AA	3548	1/1	0.96	0.05	29,29,29,29	0
58	MG	CA	3513	1/1	0.96	0.13	66,66,66,66	0
58	MG	AA	3550	1/1	0.96	0.07	52,52,52,52	0
58	MG	CA	3272	1/1	0.96	0.06	34,34,34,34	0
58	MG	AA	3428	1/1	0.96	0.12	41,41,41,41	0
58	MG	AA	3671	1/1	0.96	0.10	57,57,57,57	0
58	MG	AA	3047	1/1	0.96	0.05	31,31,31,31	0
58	MG	CA	3276	1/1	0.96	0.07	51,51,51,51	0
58	MG	DA	1647	1/1	0.96	0.07	49,49,49,49	0
58	MG	CA	3277	1/1	0.96	0.07	42,42,42,42	0
58	MG	AA	3554	1/1	0.96	0.07	40,40,40,40	0
58	MG	AA	3555	1/1	0.96	0.06	49,49,49,49	0
58	MG	BA	3178	1/1	0.96	0.09	63,63,63,63	0
58	MG	CA	3524	1/1	0.96	0.10	54,54,54,54	0
58	MG	DA	1653	1/1	0.96	0.05	29,29,29,29	0
58	MG	CA	3525	1/1	0.96	0.12	40,40,40,40	0
58	MG	AA	3560	1/1	0.96	0.08	39,39,39,39	0
58	MG	BA	3180	1/1	0.96	0.06	41,41,41,41	0
58	MG	AA	3311	1/1	0.96	0.09	34,34,34,34	0
58	MG	CA	3104	1/1	0.96	0.13	60,60,60,60	0
58	MG	AA	3677	1/1	0.96	0.04	40,40,40,40	0
58	MG	CA	3289	1/1	0.96	0.14	51,51,51,51	0
58	MG	AA	3810	1/1	0.96	0.15	62,62,62,62	0
58	MG	CA	3107	1/1	0.96	0.07	54,54,54,54	0
58	MG	AA	3563	1/1	0.96	0.11	49,49,49,49	1
58	MG	CA	3109	1/1	0.96	0.15	59,59,59,59	0
58	MG	CA	3111	1/1	0.96	0.12	62,62,62,62	0
58	MG	AA	3812	1/1	0.96	0.08	57,57,57,57	0
58	MG	AA	3247	1/1	0.96	0.34	68,68,68,68	0
58	MG	AA	3814	1/1	0.96	0.11	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3115	1/1	0.96	0.19	37,37,37,37	0
58	MG	BA	3189	1/1	0.96	0.08	66,66,66,66	0
58	MG	CA	3303	1/1	0.96	0.08	45,45,45,45	0
58	MG	AA	3565	1/1	0.96	0.07	17,17,17,17	0
58	MG	AA	3682	1/1	0.96	0.05	51,51,51,51	0
58	MG	AA	3569	1/1	0.96	0.06	15,15,15,15	0
58	MG	CA	3314	1/1	0.96	0.11	50,50,50,50	0
58	MG	AA	3173	1/1	0.96	0.22	71,71,71,71	0
58	MG	CA	3552	1/1	0.96	0.06	34,34,34,34	0
58	MG	DA	1679	1/1	0.96	0.10	60,60,60,60	0
58	MG	CA	3316	1/1	0.96	0.05	60,60,60,60	0
58	MG	DA	1681	1/1	0.96	0.15	46,46,46,46	0
58	MG	DA	1682	1/1	0.96	0.11	52,52,52,52	0
58	MG	AA	3142	1/1	0.96	0.06	41,41,41,41	0
58	MG	CA	3320	1/1	0.96	0.08	66,66,66,66	0
58	MG	CA	3323	1/1	0.96	0.08	45,45,45,45	0
58	MG	AA	3575	1/1	0.96	0.10	30,30,30,30	0
58	MG	CA	3560	1/1	0.96	0.17	56,56,56,56	0
58	MG	AA	3205	1/1	0.96	0.12	56,56,56,56	0
58	MG	AA	3691	1/1	0.96	0.17	87,87,87,87	0
58	MG	AA	3692	1/1	0.96	0.09	51,51,51,51	0
58	MG	AA	3143	1/1	0.96	0.12	28,28,28,28	0
58	MG	DA	1692	1/1	0.96	0.09	53,53,53,53	0
58	MG	DA	1693	1/1	0.96	0.08	60,60,60,60	0
58	MG	AA	3207	1/1	0.96	0.19	37,37,37,37	0
58	MG	AA	3254	1/1	0.96	0.12	35,35,35,35	0
58	MG	CA	3336	1/1	0.96	0.08	60,60,60,60	0
58	MG	CA	3571	1/1	0.96	0.08	77,77,77,77	0
58	MG	AB	3015	1/1	0.96	0.04	38,38,38,38	0
58	MG	AA	3261	1/1	0.96	0.27	69,69,69,69	0
58	MG	AA	3582	1/1	0.96	0.06	37,37,37,37	0
58	MG	CA	3133	1/1	0.96	0.05	29,29,29,29	0
58	MG	AA	3058	1/1	0.96	0.13	35,35,35,35	0
58	MG	CA	3578	1/1	0.96	0.13	38,38,38,38	0
58	MG	BA	3207	1/1	0.96	0.09	66,66,66,66	0
58	MG	CA	3346	1/1	0.96	0.06	40,40,40,40	0
58	MG	CA	3581	1/1	0.96	0.08	51,51,51,51	0
58	MG	AA	3585	1/1	0.96	0.09	63,63,63,63	0
58	MG	AA	3701	1/1	0.96	0.09	33,33,33,33	0
58	MG	CA	3584	1/1	0.96	0.08	43,43,43,43	0
58	MG	AA	3586	1/1	0.96	0.10	65,65,65,65	0
58	MG	CA	3586	1/1	0.96	0.06	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3333	1/1	0.96	0.09	66,66,66,66	0
58	MG	AA	3334	1/1	0.96	0.07	58,58,58,58	0
58	MG	AA	3706	1/1	0.96	0.18	29,29,29,29	1
58	MG	AA	3446	1/1	0.96	0.06	59,59,59,59	0
58	MG	BF	3001	1/1	0.96	0.23	71,71,71,71	0
58	MG	AD	306	1/1	0.96	0.09	41,41,41,41	0
58	MG	CA	3594	1/1	0.96	0.17	74,74,74,74	0
58	MG	BL	3002	1/1	0.96	0.07	49,49,49,49	0
58	MG	AA	3591	1/1	0.96	0.09	66,66,66,66	0
58	MG	AA	3104	1/1	0.96	0.05	13,13,13,13	0
58	MG	AA	3210	1/1	0.96	0.18	63,63,63,63	0
58	MG	AA	3338	1/1	0.96	0.05	29,29,29,29	0
58	MG	DA	1727	1/1	0.96	0.06	57,57,57,57	0
58	MG	AA	3121	1/1	0.96	0.11	46,46,46,46	0
58	MG	AA	3342	1/1	0.96	0.07	4,4,4,4	0
58	MG	BA	3079	1/1	0.96	0.05	35,35,35,35	0
58	MG	AE	301	1/1	0.96	0.06	19,19,19,19	0
58	MG	AA	3073	1/1	0.96	0.07	25,25,25,25	0
58	MG	AE	304	1/1	0.96	0.07	40,40,40,40	0
58	MG	AA	3153	1/1	0.96	0.12	67,67,67,67	0
58	MG	CA	3158	1/1	0.96	0.09	54,54,54,54	0
58	MG	AA	3456	1/1	0.96	0.05	32,32,32,32	0
58	MG	CA	3381	1/1	0.96	0.10	68,68,68,68	0
58	MG	AF	303	1/1	0.96	0.10	43,43,43,43	0
58	MG	CA	3386	1/1	0.96	0.18	63,63,63,63	0
58	MG	AA	3602	1/1	0.96	0.20	47,47,47,47	0
58	MG	CA	3163	1/1	0.96	0.12	45,45,45,45	0
58	MG	AF	306	1/1	0.96	0.18	48,48,48,48	0
58	MG	AA	3457	1/1	0.96	0.13	65,65,65,65	0
58	MG	AF	308	1/1	0.96	0.07	55,55,55,55	0
58	MG	CA	3618	1/1	0.96	0.09	37,37,37,37	0
58	MG	AA	3048	1/1	0.96	0.10	33,33,33,33	0
58	MG	AA	3728	1/1	0.96	0.08	48,48,48,48	0
58	MG	CA	3171	1/1	0.96	0.10	45,45,45,45	0
58	MG	AA	3061	1/1	0.96	0.05	26,26,26,26	0
58	MG	AA	3350	1/1	0.96	0.08	32,32,32,32	0
58	MG	AA	3351	1/1	0.96	0.07	29,29,29,29	0
58	MG	CA	3398	1/1	0.96	0.06	58,58,58,58	0
58	MG	AN	3003	1/1	0.96	0.07	45,45,45,45	0
58	MG	AA	3463	1/1	0.96	0.10	46,46,46,46	0
58	MG	CA	3012	1/1	0.96	0.09	58,58,58,58	0
58	MG	AA	3353	1/1	0.96	0.12	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3466	1/1	0.96	0.07	59,59,59,59	0
58	MG	CA	3015	1/1	0.96	0.17	82,82,82,82	0
58	MG	AA	3007	1/1	0.96	0.08	20,20,20,20	0
58	MG	AQ	203	1/1	0.96	0.13	40,40,40,40	0
58	MG	AR	5001	1/1	0.96	0.06	32,32,32,32	0
58	MG	AA	3470	1/1	0.96	0.07	28,28,28,28	0
58	MG	CA	3021	1/1	0.96	0.09	27,27,27,27	0
58	MG	CA	3022	1/1	0.96	0.06	35,35,35,35	0
58	MG	AA	3355	1/1	0.96	0.05	57,57,57,57	0
58	MG	CA	3416	1/1	0.96	0.07	34,34,34,34	0
58	MG	CA	3192	1/1	0.96	0.22	65,65,65,65	0
58	MG	CA	3193	1/1	0.96	0.10	57,57,57,57	0
58	MG	CA	3419	1/1	0.96	0.13	40,40,40,40	0
58	MG	AA	3224	1/1	0.96	0.10	26,26,26,26	0
58	MG	CA	3421	1/1	0.96	0.14	69,69,69,69	0
58	MG	AA	3040	1/1	0.96	0.17	45,45,45,45	0
58	MG	CA	3653	1/1	0.96	0.12	25,25,25,25	0
58	MG	CA	3028	1/1	0.96	0.08	42,42,42,42	0
58	MG	AA	3619	1/1	0.96	0.09	37,37,37,37	0
60	ZN	A4	501	1/1	0.96	0.06	133,133,133,133	0
58	MG	CA	3425	1/1	0.96	0.11	54,54,54,54	0
58	MG	AA	3130	1/1	0.96	0.16	70,70,70,70	0
62	GDP	BZ	801	28/28	0.96	0.07	52,52,52,52	0
58	MG	CA	3661	1/1	0.96	0.13	60,60,60,60	0
58	MG	BA	3040	1/1	0.97	0.10	48,48,48,48	0
58	MG	BA	3041	1/1	0.97	0.07	53,53,53,53	0
58	MG	AA	3098	1/1	0.97	0.06	24,24,24,24	0
58	MG	CE	301	1/1	0.97	0.14	64,64,64,64	0
58	MG	AA	3467	1/1	0.97	0.07	44,44,44,44	0
58	MG	CA	3256	1/1	0.97	0.12	40,40,40,40	0
58	MG	CA	3095	1/1	0.97	0.15	86,86,86,86	0
58	MG	AA	3702	1/1	0.97	0.17	46,46,46,46	1
58	MG	AA	3123	1/1	0.97	0.07	53,53,53,53	0
58	MG	CA	3474	1/1	0.97	0.05	52,52,52,52	0
58	MG	AA	3124	1/1	0.97	0.20	43,43,43,43	0
58	MG	AB	3009	1/1	0.97	0.08	55,55,55,55	0
58	MG	CA	3262	1/1	0.97	0.13	64,64,64,64	0
58	MG	CA	3263	1/1	0.97	0.10	29,29,29,29	0
58	MG	AA	3012	1/1	0.97	0.15	34,34,34,34	0
58	MG	AB	3012	1/1	0.97	0.06	30,30,30,30	1
58	MG	AA	3240	1/1	0.97	0.20	60,60,60,60	0
58	MG	CA	3268	1/1	0.97	0.12	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3287	1/1	0.97	0.12	46,46,46,46	0
58	MG	CA	3270	1/1	0.97	0.18	66,66,66,66	0
58	MG	AA	3289	1/1	0.97	0.07	26,26,26,26	0
58	MG	AA	3479	1/1	0.97	0.07	53,53,53,53	0
58	MG	AA	3290	1/1	0.97	0.20	63,63,63,63	0
58	MG	AA	3291	1/1	0.97	0.08	44,44,44,44	0
58	MG	CY	502	1/1	0.97	0.11	54,54,54,54	0
58	MG	AA	3025	1/1	0.97	0.16	41,41,41,41	0
58	MG	AA	3483	1/1	0.97	0.04	44,44,44,44	0
58	MG	C3	101	1/1	0.97	0.07	69,69,69,69	0
58	MG	CA	3110	1/1	0.97	0.10	51,51,51,51	0
58	MG	AA	3293	1/1	0.97	0.12	32,32,32,32	0
58	MG	AA	3295	1/1	0.97	0.12	46,46,46,46	0
58	MG	CA	3280	1/1	0.97	0.10	38,38,38,38	0
58	MG	CA	3281	1/1	0.97	0.05	34,34,34,34	0
58	MG	AD	301	1/1	0.97	0.23	44,44,44,44	0
58	MG	CA	3497	1/1	0.97	0.08	63,63,63,63	0
58	MG	CA	3283	1/1	0.97	0.08	49,49,49,49	0
58	MG	AA	3613	1/1	0.97	0.06	54,54,54,54	0
58	MG	AA	3376	1/1	0.97	0.06	18,18,18,18	0
58	MG	AD	304	1/1	0.97	0.07	18,18,18,18	0
58	MG	CA	3502	1/1	0.97	0.07	69,69,69,69	0
58	MG	AD	305	1/1	0.97	0.21	64,64,64,64	0
58	MG	BA	3204	1/1	0.97	0.10	68,68,68,68	0
58	MG	AA	3723	1/1	0.97	0.06	19,19,19,19	0
58	MG	AA	3377	1/1	0.97	0.04	20,20,20,20	0
58	MG	AA	3378	1/1	0.97	0.07	18,18,18,18	0
58	MG	AA	3617	1/1	0.97	0.12	30,30,30,30	0
58	MG	CA	3123	1/1	0.97	0.14	66,66,66,66	0
58	MG	AA	3042	1/1	0.97	0.06	36,36,36,36	0
58	MG	AA	3102	1/1	0.97	0.13	50,50,50,50	0
58	MG	AA	3731	1/1	0.97	0.13	31,31,31,31	0
58	MG	AA	3166	1/1	0.97	0.13	57,57,57,57	0
58	MG	AA	3299	1/1	0.97	0.08	21,21,21,21	0
58	MG	CA	3301	1/1	0.97	0.07	58,58,58,58	0
58	MG	AA	3498	1/1	0.97	0.05	45,45,45,45	0
58	MG	BE	3001	1/1	0.97	0.04	59,59,59,59	0
58	MG	CA	3304	1/1	0.97	0.06	53,53,53,53	0
58	MG	AA	3390	1/1	0.97	0.07	47,47,47,47	0
58	MG	BK	201	1/1	0.97	0.12	56,56,56,56	0
58	MG	AA	3505	1/1	0.97	0.07	55,55,55,55	0
58	MG	CA	3312	1/1	0.97	0.07	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3313	1/1	0.97	0.07	51,51,51,51	0
58	MG	AA	3507	1/1	0.97	0.10	31,31,31,31	0
58	MG	AA	3391	1/1	0.97	0.05	42,42,42,42	0
58	MG	AA	3628	1/1	0.97	0.11	53,53,53,53	0
58	MG	AA	3301	1/1	0.97	0.05	22,22,22,22	0
58	MG	CA	3529	1/1	0.97	0.09	79,79,79,79	0
58	MG	CA	3318	1/1	0.97	0.04	45,45,45,45	0
58	MG	AA	3043	1/1	0.97	0.12	32,32,32,32	0
58	MG	CA	3322	1/1	0.97	0.05	32,32,32,32	0
58	MG	AA	3059	1/1	0.97	0.12	49,49,49,49	0
58	MG	AA	3744	1/1	0.97	0.11	77,77,77,77	0
58	MG	CA	3325	1/1	0.97	0.13	39,39,39,39	0
58	MG	AA	3403	1/1	0.97	0.04	18,18,18,18	0
58	MG	CA	3327	1/1	0.97	0.06	33,33,33,33	0
58	MG	AA	3306	1/1	0.97	0.06	47,47,47,47	0
58	MG	AA	3307	1/1	0.97	0.10	6,6,6,6	0
58	MG	AA	3749	1/1	0.97	0.14	55,55,55,55	0
58	MG	AO	5001	1/1	0.97	0.05	53,53,53,53	0
58	MG	CA	3333	1/1	0.97	0.07	41,41,41,41	0
58	MG	AA	3520	1/1	0.97	0.08	23,23,23,23	0
58	MG	CA	3335	1/1	0.97	0.10	43,43,43,43	0
58	MG	AA	3636	1/1	0.97	0.07	24,24,24,24	0
58	MG	AA	3522	1/1	0.97	0.05	30,30,30,30	0
58	MG	AA	3410	1/1	0.97	0.10	46,46,46,46	0
58	MG	AA	3526	1/1	0.97	0.15	38,38,38,38	0
58	MG	AA	3105	1/1	0.97	0.19	31,31,31,31	0
58	MG	AA	3413	1/1	0.97	0.09	36,36,36,36	0
58	MG	AU	202	1/1	0.97	0.24	44,44,44,44	0
58	MG	AA	3044	1/1	0.97	0.13	34,34,34,34	0
58	MG	AV	201	1/1	0.97	0.15	19,19,19,19	0
58	MG	CA	3348	1/1	0.97	0.09	58,58,58,58	0
58	MG	CA	3558	1/1	0.97	0.04	47,47,47,47	0
58	MG	AA	3006	1/1	0.97	0.13	52,52,52,52	0
58	MG	CA	3350	1/1	0.97	0.13	39,39,39,39	0
58	MG	CA	3561	1/1	0.97	0.07	55,55,55,55	1
58	MG	AA	3536	1/1	0.97	0.07	15,15,15,15	0
58	MG	CA	3009	1/1	0.97	0.16	67,67,67,67	0
58	MG	CA	3353	1/1	0.97	0.05	66,66,66,66	0
58	MG	BA	3102	1/1	0.97	0.25	56,56,56,56	0
58	MG	CA	3011	1/1	0.97	0.07	46,46,46,46	0
58	MG	CA	3356	1/1	0.97	0.05	41,41,41,41	0
58	MG	AA	3313	1/1	0.97	0.08	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3164	1/1	0.97	0.12	38,38,38,38	0
58	MG	AW	3002	1/1	0.97	0.06	52,52,52,52	0
58	MG	CA	3360	1/1	0.97	0.10	43,43,43,43	0
58	MG	AW	3003	1/1	0.97	0.10	55,55,55,55	0
58	MG	DA	1678	1/1	0.97	0.10	57,57,57,57	0
58	MG	AA	3315	1/1	0.97	0.09	34,34,34,34	0
58	MG	AA	3648	1/1	0.97	0.10	38,38,38,38	0
58	MG	CA	3365	1/1	0.97	0.14	29,29,29,29	0
58	MG	AA	3540	1/1	0.97	0.04	29,29,29,29	0
58	MG	AA	3005	1/1	0.97	0.09	61,61,61,61	0
58	MG	A0	101	1/1	0.97	0.12	51,51,51,51	0
58	MG	A0	102	1/1	0.97	0.09	43,43,43,43	0
58	MG	CA	3370	1/1	0.97	0.07	56,56,56,56	0
58	MG	AA	3010	1/1	0.97	0.22	66,66,66,66	0
58	MG	CA	3023	1/1	0.97	0.08	45,45,45,45	0
58	MG	A0	104	1/1	0.97	0.08	41,41,41,41	0
58	MG	AA	3425	1/1	0.97	0.06	49,49,49,49	0
58	MG	AA	3768	1/1	0.97	0.13	96,96,96,96	0
58	MG	CA	3027	1/1	0.97	0.09	47,47,47,47	0
58	MG	AA	3318	1/1	0.97	0.19	53,53,53,53	0
58	MG	CA	3030	1/1	0.97	0.07	57,57,57,57	0
58	MG	AA	3257	1/1	0.97	0.06	26,26,26,26	0
58	MG	AA	3258	1/1	0.97	0.04	13,13,13,13	0
58	MG	CA	3186	1/1	0.97	0.26	58,58,58,58	0
58	MG	A5	102	1/1	0.97	0.10	47,47,47,47	0
58	MG	AA	3259	1/1	0.97	0.06	20,20,20,20	0
58	MG	AA	3260	1/1	0.97	0.12	23,23,23,23	0
58	MG	AA	3086	1/1	0.97	0.11	53,53,53,53	0
58	MG	AA	3663	1/1	0.97	0.15	60,60,60,60	0
58	MG	AA	3049	1/1	0.97	0.08	51,51,51,51	0
58	MG	AA	3065	1/1	0.97	0.07	28,28,28,28	0
58	MG	CA	3040	1/1	0.97	0.14	64,64,64,64	0
58	MG	AA	3556	1/1	0.97	0.07	37,37,37,37	0
58	MG	AA	3781	1/1	0.97	0.17	52,52,52,52	1
58	MG	AA	3782	1/1	0.97	0.12	72,72,72,72	0
58	MG	BA	3003	1/1	0.97	0.05	51,51,51,51	0
58	MG	AA	3439	1/1	0.97	0.10	33,33,33,33	0
58	MG	AA	3178	1/1	0.97	0.19	61,61,61,61	0
58	MG	CA	3047	1/1	0.97	0.09	60,60,60,60	0
58	MG	DA	1715	1/1	0.97	0.08	49,49,49,49	0
58	MG	BA	3134	1/1	0.97	0.15	62,62,62,62	0
58	MG	CA	3404	1/1	0.97	0.06	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3405	1/1	0.97	0.06	53,53,53,53	0
58	MG	CA	3614	1/1	0.97	0.18	89,89,89,89	0
58	MG	AA	3066	1/1	0.97	0.07	48,48,48,48	0
58	MG	AA	3786	1/1	0.97	0.11	57,57,57,57	0
58	MG	AA	3011	1/1	0.97	0.13	39,39,39,39	0
58	MG	CA	3409	1/1	0.97	0.16	61,61,61,61	0
58	MG	AA	3218	1/1	0.97	0.16	49,49,49,49	0
58	MG	CA	3620	1/1	0.97	0.07	34,34,34,34	0
58	MG	BA	3139	1/1	0.97	0.07	54,54,54,54	0
58	MG	AA	3337	1/1	0.97	0.05	10,10,10,10	0
58	MG	AA	3570	1/1	0.97	0.06	18,18,18,18	0
58	MG	AA	3221	1/1	0.97	0.12	55,55,55,55	0
58	MG	CA	3212	1/1	0.97	0.07	37,37,37,37	0
58	MG	AA	3339	1/1	0.97	0.08	41,41,41,41	0
58	MG	AA	3037	1/1	0.97	0.09	44,44,44,44	0
58	MG	AA	3795	1/1	0.97	0.06	49,49,49,49	0
58	MG	AA	3146	1/1	0.97	0.06	34,34,34,34	0
58	MG	AA	3678	1/1	0.97	0.12	32,32,32,32	0
58	MG	CA	3632	1/1	0.97	0.12	54,54,54,54	0
58	MG	AA	3798	1/1	0.97	0.07	32,32,32,32	0
58	MG	CA	3219	1/1	0.97	0.24	52,52,52,52	0
58	MG	CA	3220	1/1	0.97	0.09	30,30,30,30	0
58	MG	BA	3151	1/1	0.97	0.11	63,63,63,63	0
58	MG	CA	3427	1/1	0.97	0.15	53,53,53,53	0
58	MG	BA	3152	1/1	0.97	0.08	58,58,58,58	0
58	MG	CA	3065	1/1	0.97	0.04	41,41,41,41	0
58	MG	CA	3640	1/1	0.97	0.12	57,57,57,57	0
58	MG	CA	3641	1/1	0.97	0.08	54,54,54,54	0
58	MG	CA	3643	1/1	0.97	0.05	57,57,57,57	0
58	MG	AA	3117	1/1	0.97	0.11	50,50,50,50	0
58	MG	AA	3450	1/1	0.97	0.07	48,48,48,48	0
58	MG	AA	3187	1/1	0.97	0.06	36,36,36,36	0
58	MG	AA	3346	1/1	0.97	0.06	45,45,45,45	0
58	MG	AA	3188	1/1	0.97	0.05	31,31,31,31	0
58	MG	BA	3159	1/1	0.97	0.04	55,55,55,55	0
58	MG	CA	3231	1/1	0.97	0.22	50,50,50,50	0
58	MG	AA	3684	1/1	0.97	0.05	28,28,28,28	0
58	MG	CA	3438	1/1	0.97	0.06	49,49,49,49	0
58	MG	AA	3228	1/1	0.97	0.08	55,55,55,55	0
58	MG	AA	3686	1/1	0.97	0.12	70,70,70,70	0
58	MG	AA	3687	1/1	0.97	0.05	46,46,46,46	0
58	MG	AA	3584	1/1	0.97	0.05	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	DA	1762	1/1	0.97	0.05	53,53,53,53	0
58	MG	CA	3658	1/1	0.97	0.16	50,50,50,50	0
58	MG	CA	3446	1/1	0.97	0.10	39,39,39,39	0
58	MG	CA	3660	1/1	0.97	0.09	38,38,38,38	0
58	MG	AA	3275	1/1	0.97	0.11	56,56,56,56	0
58	MG	AA	3053	1/1	0.97	0.05	13,13,13,13	0
58	MG	CA	3450	1/1	0.97	0.07	66,66,66,66	0
58	MG	CA	3079	1/1	0.97	0.05	46,46,46,46	0
58	MG	DF	3001	1/1	0.97	0.07	49,49,49,49	0
58	MG	AA	3352	1/1	0.97	0.08	51,51,51,51	0
58	MG	AA	3230	1/1	0.97	0.16	49,49,49,49	0
58	MG	AA	3190	1/1	0.97	0.14	40,40,40,40	0
58	MG	AA	3815	1/1	0.97	0.18	53,53,53,53	0
58	MG	CA	3244	1/1	0.97	0.07	40,40,40,40	0
58	MG	CA	3084	1/1	0.97	0.22	86,86,86,86	0
58	MG	AA	3152	1/1	0.97	0.07	49,49,49,49	0
58	MG	AA	3120	1/1	0.97	0.09	43,43,43,43	0
58	MG	CA	3460	1/1	0.97	0.09	49,49,49,49	0
58	MG	AA	3072	1/1	0.97	0.20	40,40,40,40	0
58	MG	CA	3462	1/1	0.97	0.13	43,43,43,43	0
58	MG	AA	3595	1/1	0.97	0.07	42,42,42,42	0
61	SF4	DD	501	8/8	0.97	0.06	90,90,90,90	0
58	MG	AA	3465	1/1	0.97	0.05	40,40,40,40	0
58	MG	CA	3465	1/1	0.97	0.07	46,46,46,46	0
58	MG	AA	3545	1/1	0.98	0.06	15,15,15,15	0
58	MG	AA	3161	1/1	0.98	0.05	54,54,54,54	0
58	MG	AA	3162	1/1	0.98	0.08	58,58,58,58	0
58	MG	AA	3046	1/1	0.98	0.09	35,35,35,35	0
58	MG	AA	3549	1/1	0.98	0.10	58,58,58,58	0
58	MG	AA	3300	1/1	0.98	0.08	51,51,51,51	0
58	MG	AA	3551	1/1	0.98	0.04	46,46,46,46	0
58	MG	CA	3372	1/1	0.98	0.06	53,53,53,53	0
58	MG	BA	3153	1/1	0.98	0.06	48,48,48,48	0
58	MG	AA	3356	1/1	0.98	0.05	33,33,33,33	0
58	MG	AA	3090	1/1	0.98	0.09	50,50,50,50	0
58	MG	AA	3302	1/1	0.98	0.15	56,56,56,56	0
58	MG	AA	3091	1/1	0.98	0.10	34,34,34,34	0
58	MG	AA	3361	1/1	0.98	0.12	28,28,28,28	0
58	MG	AA	3557	1/1	0.98	0.06	39,39,39,39	0
58	MG	AA	3559	1/1	0.98	0.10	50,50,50,50	0
58	MG	CA	3554	1/1	0.98	0.04	67,67,67,67	0
58	MG	AA	3092	1/1	0.98	0.06	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3561	1/1	0.98	0.06	56,56,56,56	0
58	MG	DA	1625	1/1	0.98	0.04	42,42,42,42	0
58	MG	AA	3227	1/1	0.98	0.17	31,31,31,31	0
58	MG	AA	3008	1/1	0.98	0.05	18,18,18,18	0
58	MG	AA	3070	1/1	0.98	0.16	33,33,33,33	0
58	MG	AA	3170	1/1	0.98	0.08	39,39,39,39	0
58	MG	AA	3567	1/1	0.98	0.08	26,26,26,26	0
58	MG	AA	3568	1/1	0.98	0.06	51,51,51,51	0
58	MG	AA	3013	1/1	0.98	0.13	34,34,34,34	0
58	MG	AA	3368	1/1	0.98	0.05	39,39,39,39	0
58	MG	AA	3369	1/1	0.98	0.07	27,27,27,27	0
58	MG	AA	3573	1/1	0.98	0.05	31,31,31,31	0
58	MG	AA	3312	1/1	0.98	0.09	52,52,52,52	0
58	MG	AA	3126	1/1	0.98	0.24	26,26,26,26	0
58	MG	CA	3230	1/1	0.98	0.07	50,50,50,50	0
58	MG	AA	3820	1/1	0.98	0.13	30,30,30,30	1
58	MG	AA	3314	1/1	0.98	0.08	28,28,28,28	0
58	MG	CA	3574	1/1	0.98	0.05	53,53,53,53	0
58	MG	AA	3233	1/1	0.98	0.09	51,51,51,51	0
58	MG	CA	3085	1/1	0.98	0.13	62,62,62,62	0
58	MG	AA	3147	1/1	0.98	0.33	37,37,37,37	0
58	MG	AB	3003	1/1	0.98	0.12	50,50,50,50	0
58	MG	AA	3694	1/1	0.98	0.05	47,47,47,47	0
58	MG	BA	3183	1/1	0.98	0.04	60,60,60,60	0
58	MG	AA	3031	1/1	0.98	0.11	22,22,22,22	1
58	MG	AA	3050	1/1	0.98	0.15	53,53,53,53	0
58	MG	AB	3007	1/1	0.98	0.09	45,45,45,45	0
58	MG	CA	3411	1/1	0.98	0.07	31,31,31,31	0
58	MG	AA	3150	1/1	0.98	0.07	62,62,62,62	0
58	MG	AA	3151	1/1	0.98	0.05	14,14,14,14	0
58	MG	AA	3322	1/1	0.98	0.05	33,33,33,33	0
58	MG	AB	3011	1/1	0.98	0.05	31,31,31,31	0
58	MG	AA	3323	1/1	0.98	0.03	21,21,21,21	0
58	MG	AB	3013	1/1	0.98	0.08	53,53,53,53	0
58	MG	AA	3469	1/1	0.98	0.05	42,42,42,42	0
58	MG	AA	3383	1/1	0.98	0.09	34,34,34,34	0
58	MG	AA	3473	1/1	0.98	0.04	17,17,17,17	0
58	MG	AA	3589	1/1	0.98	0.08	38,38,38,38	0
58	MG	AA	3084	1/1	0.98	0.15	41,41,41,41	0
58	MG	AA	3475	1/1	0.98	0.05	60,60,60,60	0
58	MG	AA	3388	1/1	0.98	0.06	17,17,17,17	0
58	MG	AA	3708	1/1	0.98	0.11	32,32,32,32	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3426	1/1	0.98	0.07	51,51,51,51	0
58	MG	AA	3067	1/1	0.98	0.05	50,50,50,50	0
58	MG	AA	3710	1/1	0.98	0.16	32,32,32,32	1
58	MG	AA	3594	1/1	0.98	0.11	27,27,27,27	0
58	MG	AA	3712	1/1	0.98	0.13	36,36,36,36	1
58	MG	AA	3326	1/1	0.98	0.05	59,59,59,59	0
58	MG	AA	3327	1/1	0.98	0.04	13,13,13,13	0
58	MG	AA	3395	1/1	0.98	0.06	22,22,22,22	0
58	MG	AA	3396	1/1	0.98	0.07	16,16,16,16	0
58	MG	AA	3397	1/1	0.98	0.03	15,15,15,15	0
58	MG	AA	3398	1/1	0.98	0.05	17,17,17,17	0
58	MG	CA	3267	1/1	0.98	0.07	39,39,39,39	0
58	MG	AA	3180	1/1	0.98	0.10	72,72,72,72	0
58	MG	CA	3439	1/1	0.98	0.04	46,46,46,46	0
58	MG	CA	3440	1/1	0.98	0.06	39,39,39,39	0
58	MG	AA	3485	1/1	0.98	0.04	15,15,15,15	0
58	MG	AA	3722	1/1	0.98	0.05	11,11,11,11	0
58	MG	AA	3486	1/1	0.98	0.08	28,28,28,28	0
58	MG	CA	3444	1/1	0.98	0.03	37,37,37,37	0
58	MG	AA	3725	1/1	0.98	0.11	39,39,39,39	0
58	MG	AA	3604	1/1	0.98	0.06	65,65,65,65	0
58	MG	CA	3447	1/1	0.98	0.09	62,62,62,62	0
58	MG	AA	3487	1/1	0.98	0.06	39,39,39,39	0
58	MG	AA	3400	1/1	0.98	0.09	33,33,33,33	0
58	MG	AF	301	1/1	0.98	0.10	43,43,43,43	0
58	MG	AA	3329	1/1	0.98	0.04	17,17,17,17	0
58	MG	AA	3402	1/1	0.98	0.05	27,27,27,27	0
58	MG	AA	3242	1/1	0.98	0.06	28,28,28,28	0
58	MG	AF	305	1/1	0.98	0.09	40,40,40,40	0
58	MG	AA	3331	1/1	0.98	0.15	34,34,34,34	0
58	MG	CA	3630	1/1	0.98	0.09	61,61,61,61	0
58	MG	BA	3084	1/1	0.98	0.06	80,80,80,80	0
58	MG	AA	3114	1/1	0.98	0.11	62,62,62,62	0
58	MG	AA	3408	1/1	0.98	0.06	44,44,44,44	0
58	MG	AA	3495	1/1	0.98	0.12	50,50,50,50	0
58	MG	AA	3409	1/1	0.98	0.07	30,30,30,30	0
58	MG	DA	1703	1/1	0.98	0.04	68,68,68,68	0
58	MG	AA	3497	1/1	0.98	0.09	51,51,51,51	0
58	MG	AA	3182	1/1	0.98	0.05	23,23,23,23	1
58	MG	AA	3499	1/1	0.98	0.04	35,35,35,35	0
58	MG	AA	3245	1/1	0.98	0.06	28,28,28,28	1
58	MG	AA	3501	1/1	0.98	0.06	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3742	1/1	0.98	0.10	39,39,39,39	1
58	MG	CA	3642	1/1	0.98	0.09	53,53,53,53	0
58	MG	BZ	800	1/1	0.98	0.09	44,44,44,44	0
58	MG	AP	202	1/1	0.98	0.16	31,31,31,31	0
58	MG	AA	3620	1/1	0.98	0.05	42,42,42,42	0
58	MG	AA	3502	1/1	0.98	0.05	24,24,24,24	0
58	MG	CA	3298	1/1	0.98	0.09	42,42,42,42	0
58	MG	AA	3503	1/1	0.98	0.05	52,52,52,52	0
58	MG	AA	3746	1/1	0.98	0.05	28,28,28,28	0
58	MG	AA	3504	1/1	0.98	0.08	62,62,62,62	0
58	MG	CA	3007	1/1	0.98	0.06	27,27,27,27	0
58	MG	AR	5002	1/1	0.98	0.20	40,40,40,40	0
58	MG	AA	3183	1/1	0.98	0.08	75,75,75,75	0
58	MG	CA	3152	1/1	0.98	0.06	49,49,49,49	0
58	MG	CA	3306	1/1	0.98	0.05	61,61,61,61	0
58	MG	AA	3506	1/1	0.98	0.04	32,32,32,32	0
58	MG	CA	3309	1/1	0.98	0.04	40,40,40,40	0
58	MG	AA	3075	1/1	0.98	0.04	13,13,13,13	0
58	MG	AA	3415	1/1	0.98	0.07	30,30,30,30	0
58	MG	AA	3510	1/1	0.98	0.08	47,47,47,47	0
58	MG	AA	3087	1/1	0.98	0.14	49,49,49,49	0
58	MG	AA	3512	1/1	0.98	0.06	11,11,11,11	0
58	MG	AA	3418	1/1	0.98	0.09	30,30,30,30	0
58	MG	AA	3214	1/1	0.98	0.21	39,39,39,39	1
58	MG	CA	3161	1/1	0.98	0.05	40,40,40,40	0
58	MG	CA	3319	1/1	0.98	0.06	33,33,33,33	0
58	MG	AA	3420	1/1	0.98	0.08	12,12,12,12	0
58	MG	CA	3321	1/1	0.98	0.05	30,30,30,30	0
58	MG	CA	3019	1/1	0.98	0.05	27,27,27,27	0
58	MG	AA	3135	1/1	0.98	0.18	62,62,62,62	0
58	MG	AA	3340	1/1	0.98	0.13	58,58,58,58	0
58	MG	AA	3288	1/1	0.98	0.05	25,25,25,25	0
58	MG	AA	3521	1/1	0.98	0.05	37,37,37,37	0
58	MG	AA	3424	1/1	0.98	0.05	17,17,17,17	0
58	MG	DA	1743	1/1	0.98	0.11	60,60,60,60	0
58	MG	AA	3251	1/1	0.98	0.08	33,33,33,33	1
58	MG	CA	3170	1/1	0.98	0.08	32,32,32,32	0
58	MG	CA	3330	1/1	0.98	0.06	29,29,29,29	0
58	MG	AA	3525	1/1	0.98	0.07	26,26,26,26	0
58	MG	AA	3427	1/1	0.98	0.07	34,34,34,34	0
58	MG	AA	3343	1/1	0.98	0.13	65,65,65,65	0
58	MG	CA	3029	1/1	0.98	0.05	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CE	302	1/1	0.98	0.09	46,46,46,46	0
58	MG	AA	3528	1/1	0.98	0.06	25,25,25,25	0
58	MG	CA	3176	1/1	0.98	0.05	41,41,41,41	0
58	MG	CA	3177	1/1	0.98	0.11	50,50,50,50	0
58	MG	CA	3338	1/1	0.98	0.05	41,41,41,41	0
58	MG	DA	1756	1/1	0.98	0.15	68,68,68,68	0
58	MG	AA	3644	1/1	0.98	0.06	49,49,49,49	0
58	MG	CA	3340	1/1	0.98	0.03	35,35,35,35	0
58	MG	AA	3077	1/1	0.98	0.09	92,92,92,92	0
58	MG	AA	3530	1/1	0.98	0.06	15,15,15,15	0
58	MG	CF	304	1/1	0.98	0.05	54,54,54,54	0
58	MG	CA	3343	1/1	0.98	0.07	46,46,46,46	0
58	MG	AA	3217	1/1	0.98	0.09	46,46,46,46	0
58	MG	AA	3118	1/1	0.98	0.17	36,36,36,36	1
58	MG	AA	3534	1/1	0.98	0.05	22,22,22,22	0
58	MG	BA	3129	1/1	0.98	0.10	52,52,52,52	0
58	MG	AA	3650	1/1	0.98	0.06	59,59,59,59	0
58	MG	AA	3432	1/1	0.98	0.06	28,28,28,28	0
58	MG	A7	105	1/1	0.98	0.07	44,44,44,44	0
58	MG	AA	3537	1/1	0.98	0.05	35,35,35,35	0
58	MG	A8	5002	1/1	0.98	0.05	30,30,30,30	0
58	MG	AA	3433	1/1	0.98	0.06	18,18,18,18	0
58	MG	CV	201	1/1	0.98	0.04	69,69,69,69	0
58	MG	AA	3434	1/1	0.98	0.07	22,22,22,22	0
58	MG	AA	3255	1/1	0.98	0.16	40,40,40,40	0
58	MG	AA	3656	1/1	0.98	0.09	55,55,55,55	0
58	MG	CA	3528	1/1	0.98	0.03	38,38,38,38	0
58	MG	AA	3657	1/1	0.98	0.09	51,51,51,51	1
58	MG	AA	3541	1/1	0.98	0.04	29,29,29,29	0
58	MG	AA	3294	1/1	0.98	0.06	65,65,65,65	0
60	ZN	BN	501	1/1	0.98	0.04	121,121,121,121	0
58	MG	BA	3142	1/1	0.98	0.04	47,47,47,47	0
58	MG	CA	3533	1/1	0.98	0.08	52,52,52,52	0
61	SF4	BD	501	8/8	0.98	0.04	79,79,79,79	0
58	MG	AA	3256	1/1	0.98	0.08	54,54,54,54	0
58	MG	AA	3220	1/1	0.98	0.04	34,34,34,34	0
58	MG	CA	3363	1/1	0.98	0.07	42,42,42,42	0
58	MG	AA	3791	1/1	0.99	0.08	15,15,15,15	0
58	MG	AV	202	1/1	0.99	0.03	40,40,40,40	0
58	MG	AV	203	1/1	0.99	0.07	34,34,34,34	1
58	MG	AA	3133	1/1	0.99	0.06	30,30,30,30	0
58	MG	AA	3459	1/1	0.99	0.06	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3571	1/1	0.99	0.05	14,14,14,14	0
58	MG	CA	3550	1/1	0.99	0.03	54,54,54,54	1
58	MG	CA	3291	1/1	0.99	0.10	40,40,40,40	0
58	MG	AA	3374	1/1	0.99	0.10	17,17,17,17	0
58	MG	AA	3357	1/1	0.99	0.06	27,27,27,27	0
58	MG	AA	3022	1/1	0.99	0.08	9,9,9,9	0
58	MG	AA	3533	1/1	0.99	0.08	24,24,24,24	0
58	MG	AA	3219	1/1	0.99	0.04	4,4,4,4	0
58	MG	AA	3535	1/1	0.99	0.06	27,27,27,27	0
58	MG	AA	3578	1/1	0.99	0.04	34,34,34,34	0
58	MG	AA	3163	1/1	0.99	0.15	45,45,45,45	0
58	MG	AA	3755	1/1	0.99	0.09	29,29,29,29	0
58	MG	AA	3038	1/1	0.99	0.09	10,10,10,10	0
58	MG	AA	3380	1/1	0.99	0.04	15,15,15,15	0
58	MG	AA	3406	1/1	0.99	0.08	50,50,50,50	0
58	MG	CA	3188	1/1	0.99	0.02	36,36,36,36	0
58	MG	AA	3407	1/1	0.99	0.03	19,19,19,19	0
58	MG	BA	3145	1/1	0.99	0.03	37,37,37,37	0
58	MG	CA	3568	1/1	0.99	0.03	40,40,40,40	0
58	MG	CA	3307	1/1	0.99	0.04	39,39,39,39	0
58	MG	AA	3054	1/1	0.99	0.08	38,38,38,38	0
58	MG	AA	3039	1/1	0.99	0.06	44,44,44,44	0
58	MG	CA	3371	1/1	0.99	0.11	46,46,46,46	0
58	MG	CA	3310	1/1	0.99	0.06	29,29,29,29	0
58	MG	CA	3373	1/1	0.99	0.07	42,42,42,42	0
58	MG	AE	303	1/1	0.99	0.02	17,17,17,17	0
58	MG	AA	3471	1/1	0.99	0.03	34,34,34,34	0
58	MG	CA	3252	1/1	0.99	0.05	51,51,51,51	0
58	MG	AA	3472	1/1	0.99	0.03	25,25,25,25	0
58	MG	AA	3003	1/1	0.99	0.02	19,19,19,19	0
58	MG	A7	102	1/1	0.99	0.07	39,39,39,39	0
58	MG	AA	3384	1/1	0.99	0.04	28,28,28,28	0
58	MG	AA	3720	1/1	0.99	0.04	59,59,59,59	0
58	MG	CA	3382	1/1	0.99	0.02	37,37,37,37	0
58	MG	CA	3383	1/1	0.99	0.04	40,40,40,40	0
58	MG	CA	3384	1/1	0.99	0.10	44,44,44,44	0
58	MG	CA	3655	1/1	0.99	0.10	52,52,52,52	0
58	MG	AA	3508	1/1	0.99	0.07	13,13,13,13	0
58	MG	AA	3348	1/1	0.99	0.08	31,31,31,31	0
58	MG	AA	3386	1/1	0.99	0.04	18,18,18,18	0
58	MG	CA	3589	1/1	0.99	0.03	35,35,35,35	0
58	MG	AA	3387	1/1	0.99	0.04	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	3212	1/1	0.99	0.07	31,31,31,31	1
58	MG	CA	3662	1/1	0.99	0.13	48,48,48,48	0
58	MG	AA	3772	1/1	0.99	0.07	22,22,22,22	1
58	MG	AA	3417	1/1	0.99	0.10	42,42,42,42	0
58	MG	AA	3514	1/1	0.99	0.10	35,35,35,35	0
58	MG	AA	3389	1/1	0.99	0.09	34,34,34,34	0
58	MG	AA	3516	1/1	0.99	0.04	20,20,20,20	0
58	MG	DA	1698	1/1	0.99	0.08	76,76,76,76	0
58	MG	AN	3002	1/1	0.99	0.03	26,26,26,26	0
58	MG	AA	3304	1/1	0.99	0.05	30,30,30,30	0
58	MG	AA	3320	1/1	0.99	0.09	23,23,23,23	0
58	MG	BA	3168	1/1	0.99	0.03	57,57,57,57	0
58	MG	AA	3558	1/1	0.99	0.07	18,18,18,18	0
58	MG	AA	3392	1/1	0.99	0.06	21,21,21,21	0
58	MG	BA	3171	1/1	0.99	0.08	61,61,61,61	0
58	MG	AA	3393	1/1	0.99	0.06	26,26,26,26	0
58	MG	AA	3157	1/1	0.99	0.12	40,40,40,40	1
58	MG	BA	3118	1/1	0.99	0.05	43,43,43,43	0
60	ZN	A9	501	1/1	0.99	0.03	41,41,41,41	0
58	MG	AA	3009	1/1	0.99	0.04	23,23,23,23	0
58	MG	AA	3454	1/1	0.99	0.05	49,49,49,49	0
60	ZN	C6	501	1/1	0.99	0.02	60,60,60,60	0
60	ZN	C9	501	1/1	0.99	0.07	93,93,93,93	0
58	MG	AA	3524	1/1	0.99	0.12	29,29,29,29	0
58	MG	AA	3076	1/1	0.99	0.03	8,8,8,8	0
58	MG	AA	3566	1/1	0.99	0.05	28,28,28,28	0
58	MG	AA	3426	1/1	0.99	0.06	33,33,33,33	0
58	MG	AA	3141	1/1	0.99	0.05	51,51,51,51	0
58	MG	AA	3800	1/1	1.00	0.04	30,30,30,30	0
58	MG	AA	3308	1/1	1.00	0.04	28,28,28,28	0
60	ZN	CY	501	1/1	1.00	0.02	92,92,92,92	0
58	MG	AA	3776	1/1	1.00	0.03	40,40,40,40	0
60	ZN	C5	101	1/1	1.00	0.04	66,66,66,66	0
58	MG	AA	3724	1/1	1.00	0.04	22,22,22,22	0
58	MG	AA	3412	1/1	1.00	0.07	20,20,20,20	0
58	MG	CA	3562	1/1	1.00	0.04	36,36,36,36	0
60	ZN	AY	501	1/1	1.00	0.02	63,63,63,63	0
58	MG	AA	3659	1/1	1.00	0.04	14,14,14,14	0
60	ZN	A5	103	1/1	1.00	0.01	36,36,36,36	0
60	ZN	A6	102	1/1	1.00	0.02	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.