



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 01:30 PM UTC

PDB ID : 1VY4 / pdb_00001vy4
Title : Crystal structure of the Thermus thermophilus 70S ribosome in the pre-attack state of peptide bond formation containing acylated tRNA-substrates in the A and P sites.
Authors : Polikanov, Y.S.; Steitz, T.A.; Innis, C.A.
Deposited on : 2014-05-13
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

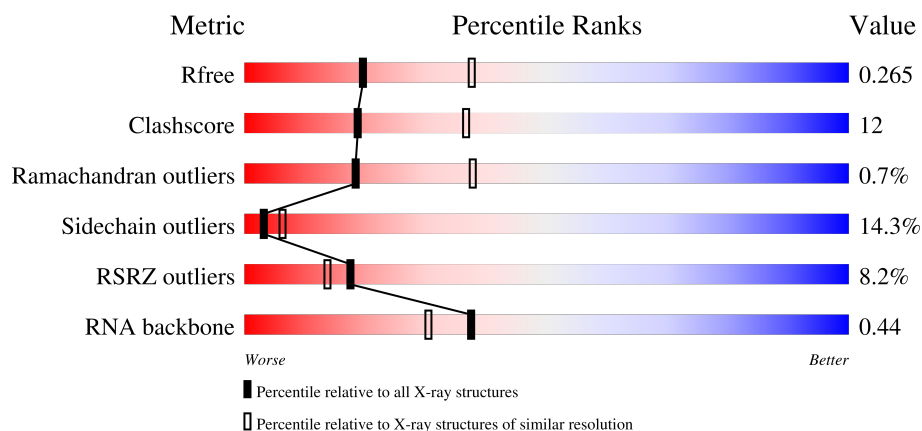
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)

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	1521	3% 49% 38% 11% .
1	CA	1521	10% 43% 42% 14% .
2	AB	256	17% 42% 38% 8% . 10%
2	CB	256	22% 36% 42% 12% . 10%

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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	24	
22	CV	24	
23	AW	76	
23	CW	76	
24	AX	77	
24	CX	77	
25	AY	76	
25	CY	76	
26	BA	2915	
26	DA	2915	
27	BB	121	
27	DB	121	

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Mol	Chain	Length	Quality of chain
28	BD	276	
28	DD	276	
29	BE	206	
29	DE	206	
30	BF	210	
30	DF	210	
31	BG	182	
31	DG	182	
32	BH	180	
32	DH	180	
33	BI	148	
33	DI	148	
34	BN	140	
34	DN	140	
35	BO	122	
35	DO	122	
36	BP	150	
36	DP	150	
37	BQ	141	
37	DQ	141	
38	BR	118	
38	DR	118	
39	BS	112	
39	DS	112	
40	BT	146	

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Mol	Chain	Length	Quality of chain
40	DT	146	
41	BU	118	
41	DU	118	
42	BV	101	
42	DV	101	
43	BW	113	
43	DW	113	
44	BX	96	
44	DX	96	
45	BY	110	
45	DY	110	
46	BZ	206	
46	DZ	206	
47	B0	85	
47	D0	85	
48	B1	98	
48	D1	98	
49	B2	72	
49	D2	72	
50	B3	60	
50	D3	60	
51	B4	71	
51	D4	71	
52	B5	60	
52	D5	60	

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Mol	Chain	Length	Quality of chain
53	B6	54	
53	D6	54	
54	B7	49	
54	D7	49	
55	B8	65	
55	D8	65	
56	B9	37	
56	D9	37	

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
25	PSU	CY	39	-	-	X	-
57	MG	DA	3079	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 297127 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 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1497	Total	C	N	O	P	0	0	0
			32185	14324	5968	10396	1497			
1	CA	1503	Total	C	N	O	P	0	0	0
			32312	14381	5990	10438	1503			

- Molecule 2 is a protein called 30S ribosomal protein S2.

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

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1552	976	302	273	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1544	970	300	273	1			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1659	1040	326	286	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1678	1052	333	286	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
5	CE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			812	514	146	149	3			
6	CF	100	Total	C	N	O	S	0	0	0
			820	518	147	152	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1231	766	243	216	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
8	CH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	0	0	0
			986	626	193	167			
9	CI	127	Total	C	N	O	0	0	0
			978	619	190	169			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	AJ	97	Total	C	N	O	0	0	0
			709	440	138	131			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	CJ	96	Total	C	N	O	0	0	0
			714	445	138	131			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	114	Total 833	C 519	N 156	O 155	S 3	0	0	0
11	CK	114	Total 833	C 519	N 156	O 155	S 3	0	0	0

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	122	Total	C	N	O	S	0	0	0
			930	585	185	159	1			
12	CL	122	Total	C	N	O	S	0	0	0
			930	585	185	159	1			

- Molecule 13 is a protein called 30S ribosomal protein S13.

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

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total 492	C 312	N 104	O 72	S 4	0	0	0
14	CN	60	Total 492	C 312	N 104	O 72	S 4	0	0	0

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			
15	CO	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
16	CP	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
17	CQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	68	Total	C	N	O	0	0	0
			555	355	108	92			
18	CR	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 19 is a protein called 30S ribosomal protein S19.

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

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
20	CT	96	Total	C	N	O	S	0	0	0
			731	449	156	124	2			

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	23	Total	C	N	O	0	0	0
			199	122	48	29			
21	CU	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 22 is a RNA chain called mRNA.

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

- Molecule 23 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	AW	74	Total	C	N	O	P	S	0	0	0
			1599	722	287	515	73	2			
23	CW	72	Total	C	N	O	P	S	0	0	0
			1552	697	280	502	72	1			

- Molecule 24 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	AX	76	Total	C	N	O	P	S	0	0	0
			1635	731	296	530	76	2			
24	CX	76	Total	C	N	O	P	S	0	0	0
			1635	731	296	530	76	2			

- Molecule 25 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
25	AY	74	Total	C	N	O	P	S	0	0	0
			1581	707	285	515	73	1			
25	CY	73	Total	C	N	O	P	S	0	0	0
			1561	698	283	507	72	1			

- Molecule 26 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BA	2819	Total	C	N	O	P	0	0	0
			60729	27026	11370	19515	2818			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	DA	2800	Total	C	N	O	P	0	0	0
			60311	26840	11284	19388	2799			

- Molecule 27 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			
27	DB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
28	DD	275	Total	C	N	O	S	0	0	0
			2142	1352	426	361	3			

- Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
29	DE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 30 is a protein called 50S ribosomal protein L4.

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

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BG	181	Total	C	N	O	S	0	0	0
			1425	914	256	251	4			
31	DG	181	Total	C	N	O	S	0	0	0
			1424	911	258	251	4			

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
32	DH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BI	146	Total	C	N	O	S	0	0	0
			1085	693	189	202	1			
33	DI	146	Total	C	N	O	S	0	0	0
			1073	688	188	196	1			

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			
34	DN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
35	DO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BP	149	Total	C	N	O	S	0	0	0
			1139	709	231	196	3			
36	DP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
37	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
38	DR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	BS	110	Total	C	N	O	0	0	0
			877	553	175	149			
39	DS	110	Total	C	N	O	0	0	0
			870	549	173	148			

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BT	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
40	DT	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
41	DU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	DV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
43	DW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
44	DX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BY	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
45	DY	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BZ	171	Total	C	N	O	S	0	0	0
			1349	862	243	242	2			
46	DZ	174	Total	C	N	O	S	0	0	0
			1360	870	243	245	2			

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
47	D0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			
48	D1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
49	D2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
50	B3	59	Total	C	N	O	0	0	0
			469	298	90	81			
50	D3	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B4	69	Total	C	N	O	S	0	0	0
			558	352	102	99	5			
51	D4	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			
52	D5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
53	D6	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
54	D7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
55	D8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
56	D9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	216	Total	Mg	0	0
			216	216		
57	AB	1	Total	Mg	0	0
			1	1		
57	AE	1	Total	Mg	0	0
			1	1		
57	AF	1	Total	Mg	0	0
			1	1		
57	AK	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AL	2	Total 2	Mg 2	0	0
57	AM	2	Total 2	Mg 2	0	0
57	AN	2	Total 2	Mg 2	0	0
57	AT	1	Total 1	Mg 1	0	0
57	AU	1	Total 1	Mg 1	0	0
57	AW	2	Total 2	Mg 2	0	0
57	AX	15	Total 15	Mg 15	0	0
57	AY	3	Total 3	Mg 3	0	0
57	BA	814	Total 814	Mg 814	0	0
57	BB	23	Total 23	Mg 23	0	0
57	BD	10	Total 10	Mg 10	0	0
57	BE	6	Total 6	Mg 6	0	0
57	BF	11	Total 11	Mg 11	0	0
57	BG	2	Total 2	Mg 2	0	0
57	BH	1	Total 1	Mg 1	0	0
57	BN	3	Total 3	Mg 3	0	0
57	BO	1	Total 1	Mg 1	0	0
57	BP	2	Total 2	Mg 2	0	0
57	BQ	2	Total 2	Mg 2	0	0
57	BR	2	Total 2	Mg 2	0	0
57	BU	4	Total 4	Mg 4	0	0

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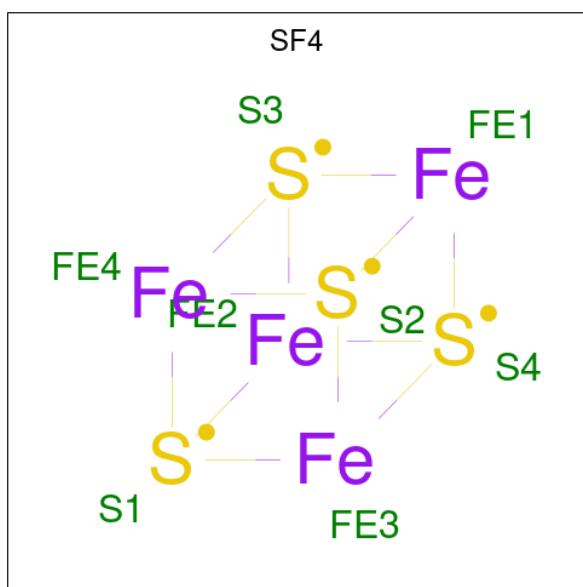
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BV	5	Total 5	Mg 5	0	0
57	BW	4	Total 4	Mg 4	0	0
57	BX	1	Total 1	Mg 1	0	0
57	BY	1	Total 1	Mg 1	0	0
57	BZ	2	Total 2	Mg 2	0	0
57	B0	2	Total 2	Mg 2	0	0
57	B2	1	Total 1	Mg 1	0	0
57	B4	1	Total 1	Mg 1	0	0
57	B5	3	Total 3	Mg 3	0	0
57	B6	2	Total 2	Mg 2	0	0
57	B7	5	Total 5	Mg 5	0	0
57	B8	2	Total 2	Mg 2	0	0
57	B9	1	Total 1	Mg 1	0	0
57	CA	169	Total 169	Mg 169	0	0
57	CD	1	Total 1	Mg 1	0	0
57	CE	2	Total 2	Mg 2	0	0
57	CF	1	Total 1	Mg 1	0	0
57	CJ	1	Total 1	Mg 1	0	0
57	CK	1	Total 1	Mg 1	0	0
57	CT	1	Total 1	Mg 1	0	0
57	CW	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CX	2	Total 2	Mg 2	0	0
57	DA	664	Total 664	Mg 664	0	0
57	DB	13	Total 13	Mg 13	0	0
57	DD	4	Total 4	Mg 4	0	0
57	DE	7	Total 7	Mg 7	0	0
57	DF	5	Total 5	Mg 5	0	0
57	DG	1	Total 1	Mg 1	0	0
57	DN	1	Total 1	Mg 1	0	0
57	DO	2	Total 2	Mg 2	0	0
57	DP	2	Total 2	Mg 2	0	0
57	DQ	3	Total 3	Mg 3	0	0
57	DR	1	Total 1	Mg 1	0	0
57	DU	1	Total 1	Mg 1	0	0
57	DV	1	Total 1	Mg 1	0	0
57	DW	1	Total 1	Mg 1	0	0
57	DY	1	Total 1	Mg 1	0	0
57	D0	1	Total 1	Mg 1	0	0
57	D3	1	Total 1	Mg 1	0	0
57	D8	1	Total 1	Mg 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	AD	1	Total	Fe	S	0	0
			8	4	4		
58	CD	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AN	1	Total	Zn	0	0
			1	1		
59	BY	1	Total	Zn	0	0
			1	1		
59	B4	1	Total	Zn	0	0
			1	1		
59	B5	1	Total	Zn	0	0
			1	1		
59	B6	1	Total	Zn	0	0
			1	1		
59	B9	1	Total	Zn	0	0
			1	1		
59	CN	1	Total	Zn	0	0
			1	1		
59	DY	1	Total	Zn	0	0
			1	1		
59	D4	1	Total	Zn	0	0
			1	1		
59	D5	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	D6	1	Total 1	Zn 1	0	0
59	D9	1	Total 1	Zn 1	0	0

- Molecule 60 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AX	1	Total 1	K 1	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AA	210	Total 210	O 210	0	0
61	AD	1	Total 1	O 1	0	0
61	AE	2	Total 2	O 2	0	0
61	AJ	1	Total 1	O 1	0	0
61	AL	2	Total 2	O 2	0	0
61	AM	2	Total 2	O 2	0	0
61	AV	2	Total 2	O 2	0	0
61	AW	4	Total 4	O 4	0	0
61	AX	4	Total 4	O 4	0	0
61	AY	1	Total 1	O 1	0	0
61	BA	1405	Total 1406	O 1406	0	1
61	BB	37	Total 37	O 37	0	0
61	BD	15	Total 15	O 15	0	0
61	BE	17	Total 17	O 17	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	BF	11	Total 11	O 11	0	0
61	BG	3	Total 3	O 3	0	0
61	BH	1	Total 1	O 1	0	0
61	BI	1	Total 1	O 1	0	0
61	BN	1	Total 1	O 1	0	0
61	BO	2	Total 2	O 2	0	0
61	BP	13	Total 13	O 13	0	0
61	BQ	4	Total 4	O 4	0	0
61	BR	2	Total 2	O 2	0	0
61	BS	2	Total 2	O 2	0	0
61	BT	2	Total 2	O 2	0	0
61	BU	4	Total 4	O 4	0	0
61	BV	2	Total 2	O 2	0	0
61	BW	3	Total 3	O 3	0	0
61	BX	3	Total 3	O 3	0	0
61	BZ	1	Total 1	O 1	0	0
61	B0	6	Total 6	O 6	0	0
61	B1	2	Total 2	O 2	0	0
61	B3	2	Total 2	O 2	0	0
61	B5	4	Total 4	O 4	0	0
61	B6	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	B7	3	Total 3	O 3	0	0
61	B8	13	Total 13	O 13	0	0
61	B9	1	Total 1	O 1	0	0
61	CA	156	Total 156	O 156	0	0
61	CE	2	Total 2	O 2	0	0
61	CH	1	Total 1	O 1	0	0
61	CJ	1	Total 1	O 1	0	0
61	CK	1	Total 1	O 1	0	0
61	CL	1	Total 1	O 1	0	0
61	CT	1	Total 1	O 1	0	0
61	CW	2	Total 2	O 2	0	0
61	CX	2	Total 2	O 2	0	0
61	CY	1	Total 1	O 1	0	0
61	DA	989	Total 989	O 989	0	0
61	DB	9	Total 9	O 9	0	0
61	DD	18	Total 18	O 18	0	0
61	DE	5	Total 5	O 5	0	0
61	DF	4	Total 4	O 4	0	0
61	DN	2	Total 2	O 2	0	0
61	DP	12	Total 12	O 12	0	0
61	DQ	1	Total 1	O 1	0	0

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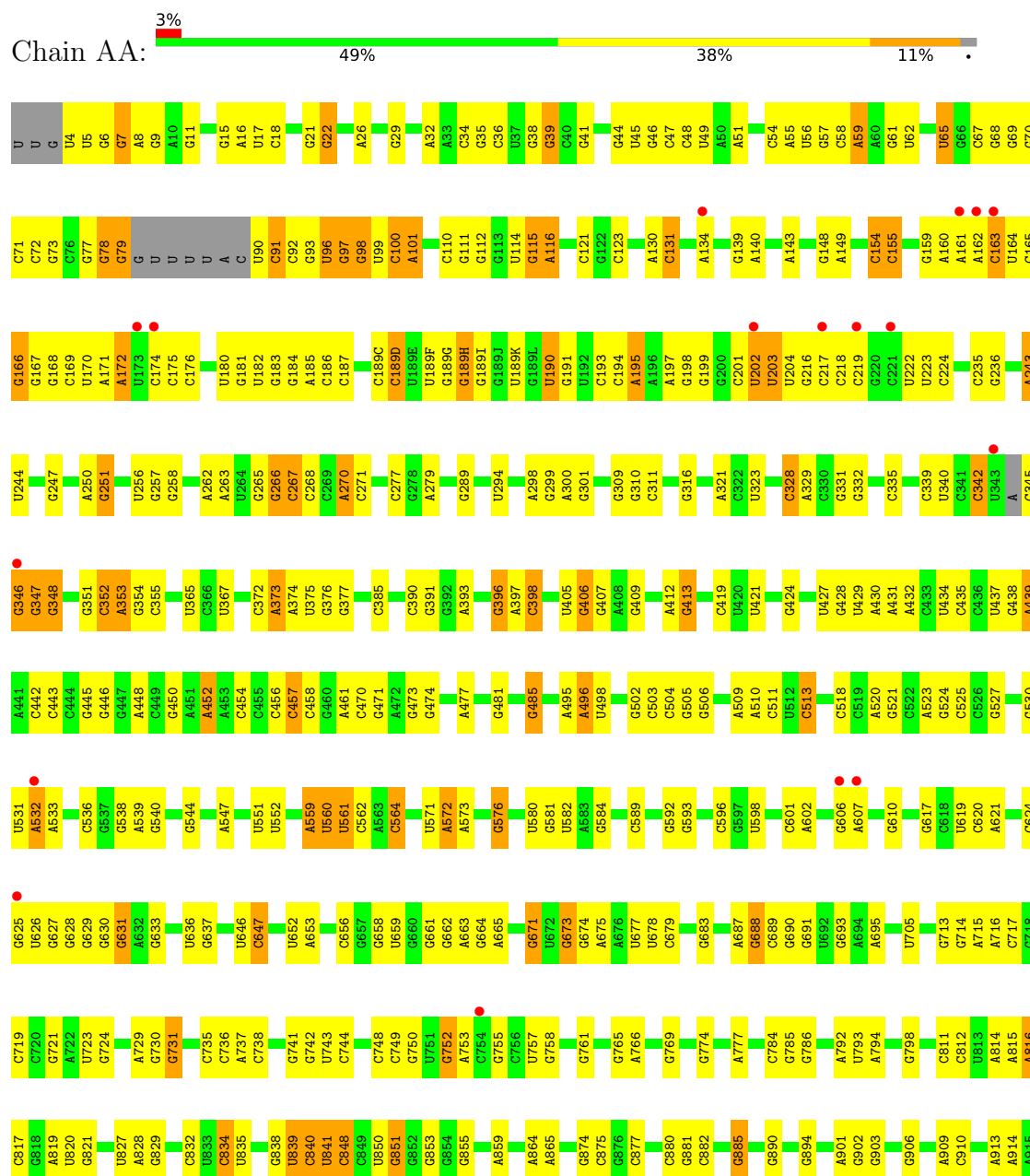
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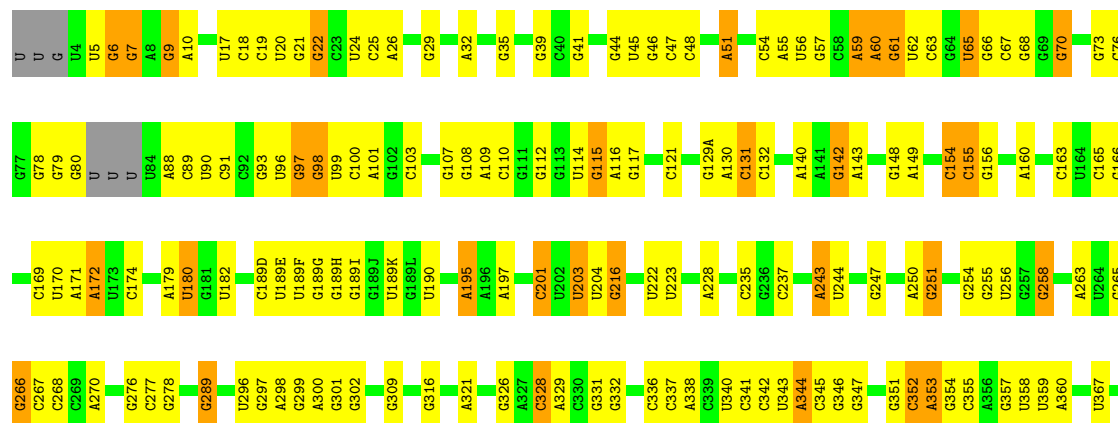
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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61	DU	1	Total 1	O 1	0	0
61	DV	1	Total 1	O 1	0	0
61	DW	1	Total 1	O 1	0	0
61	DX	2	Total 2	O 2	0	0
61	DY	1	Total 1	O 1	0	0
61	D0	4	Total 4	O 4	0	0
61	D1	1	Total 1	O 1	0	0
61	D3	2	Total 2	O 2	0	0
61	D5	1	Total 1	O 1	0	0
61	D6	1	Total 1	O 1	0	0
61	D8	3	Total 3	O 3	0	0

3 Residue-property plots

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

• Molecule 1: 16S Ribosomal RNA

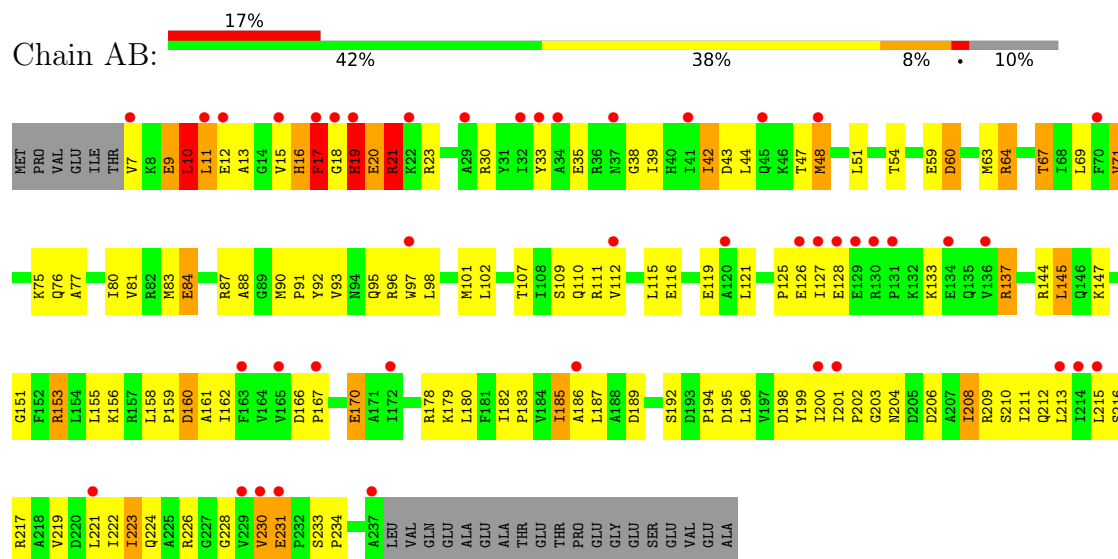




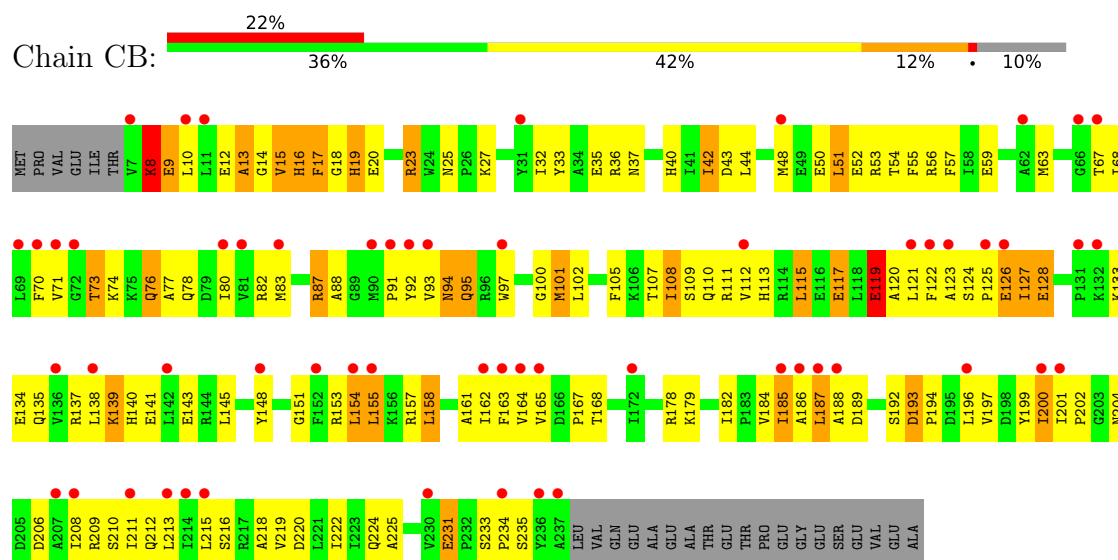




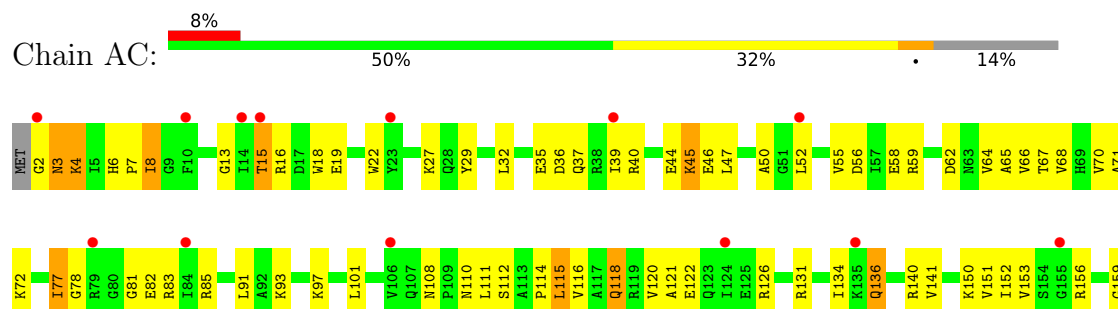
• Molecule 2: 30S ribosomal protein S2

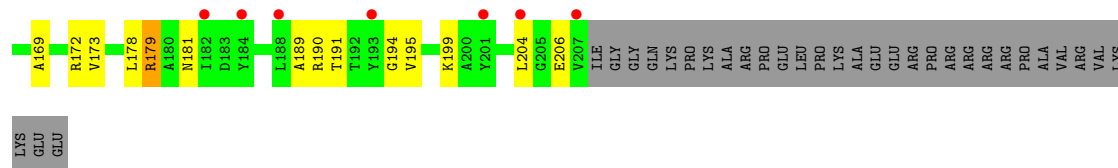


• Molecule 2: 30S ribosomal protein S2

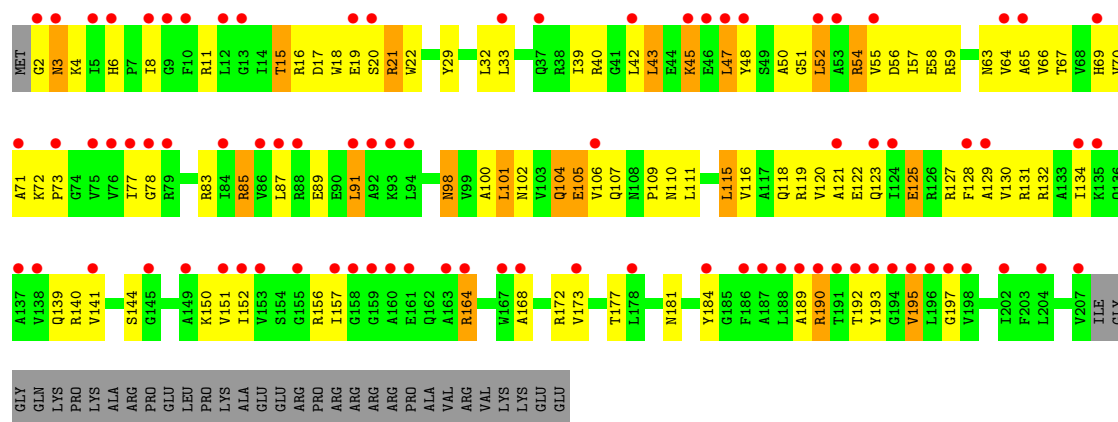


• Molecule 3: 30S ribosomal protein S3

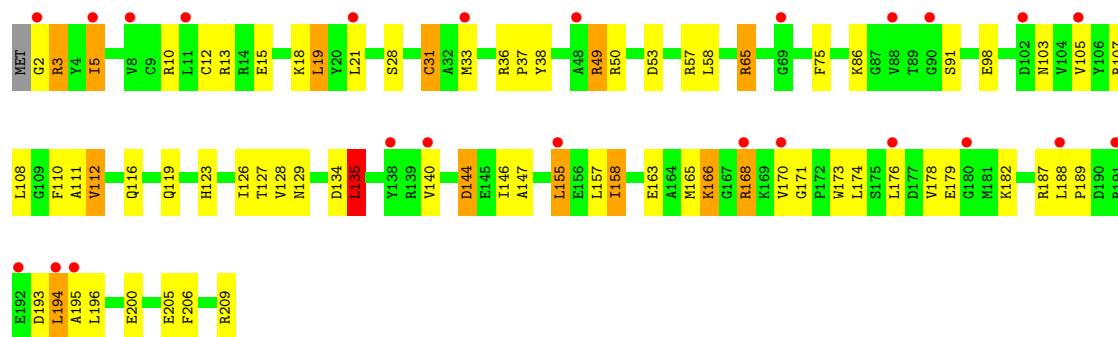




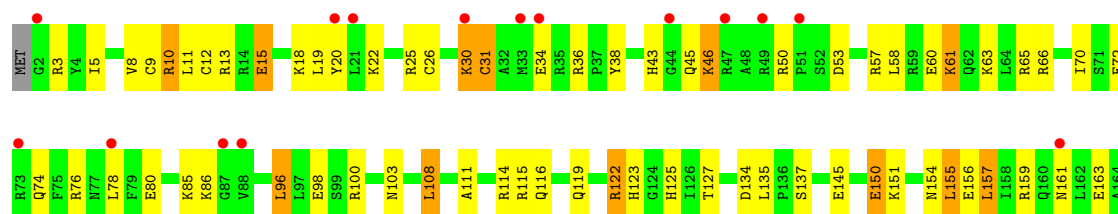
• Molecule 3: 30S ribosomal protein S3

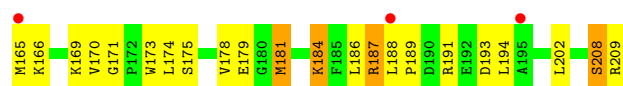


• Molecule 4: 30S ribosomal protein S4



• Molecule 4: 30S ribosomal protein S4

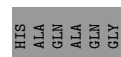
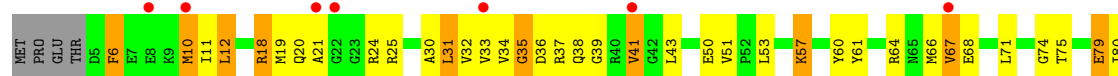




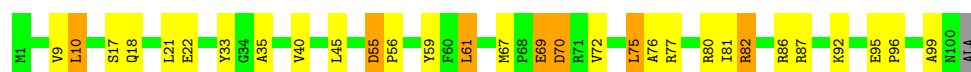
• Molecule 5: 30S ribosomal protein S5



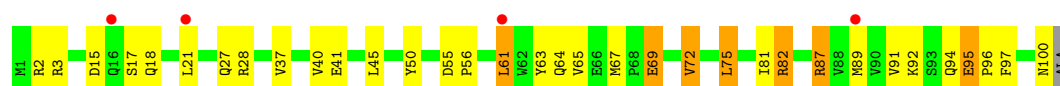
• Molecule 5: 30S ribosomal protein S5



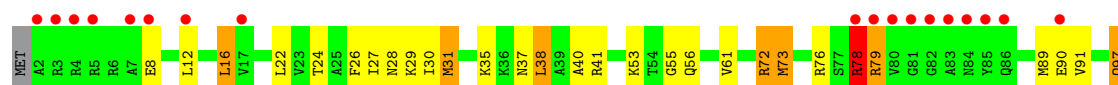
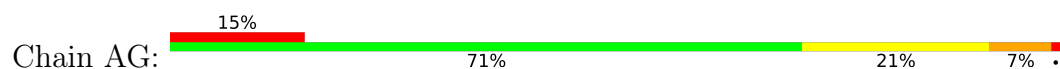
• Molecule 6: 30S ribosomal protein S6

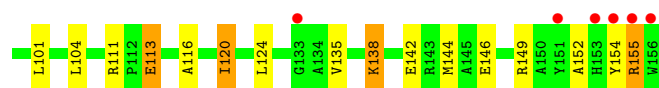


• Molecule 6: 30S ribosomal protein S6

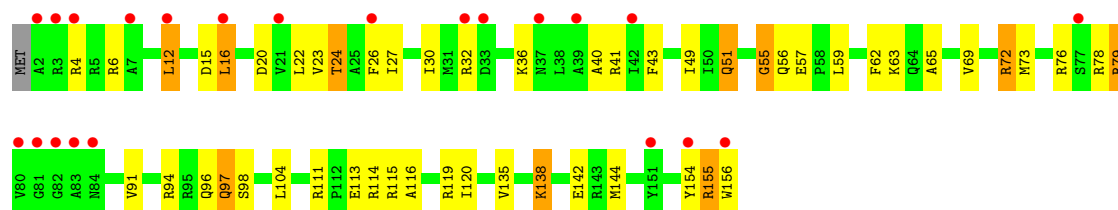


• Molecule 7: 30S ribosomal protein S7

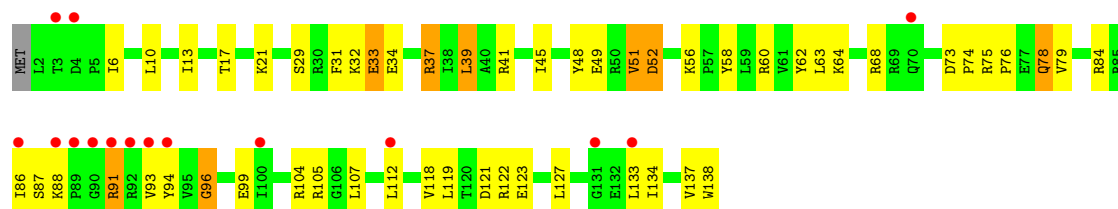




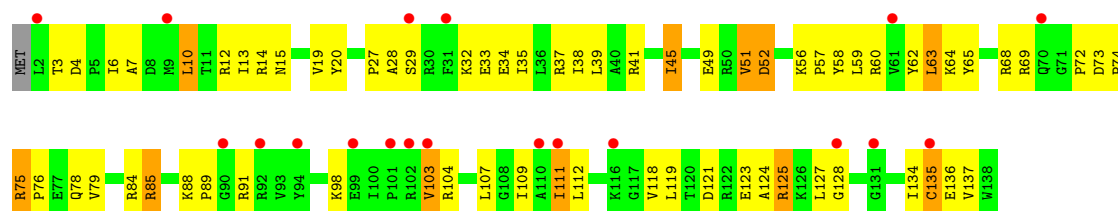
• Molecule 7: 30S ribosomal protein S7



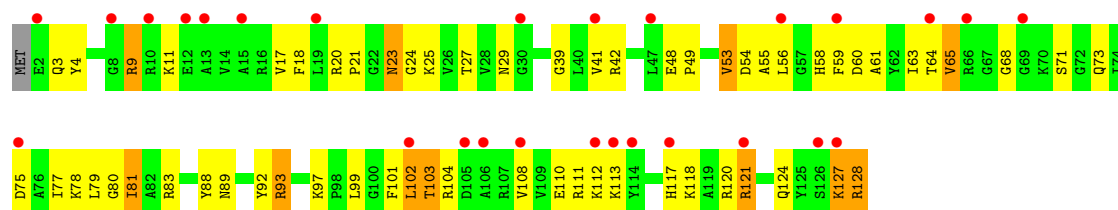
• Molecule 8: 30S ribosomal protein S8



• Molecule 8: 30S ribosomal protein S8

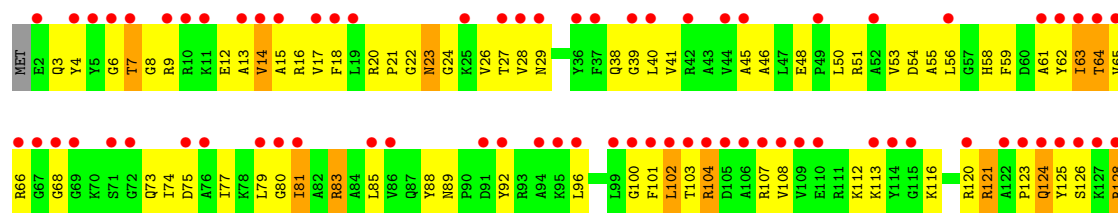


• Molecule 9: 30S ribosomal protein S9

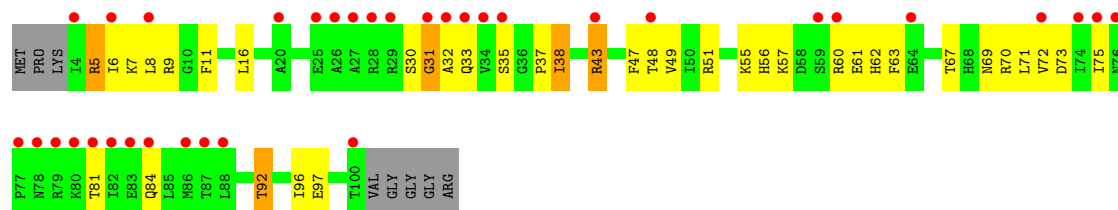


• Molecule 9: 30S ribosomal protein S9

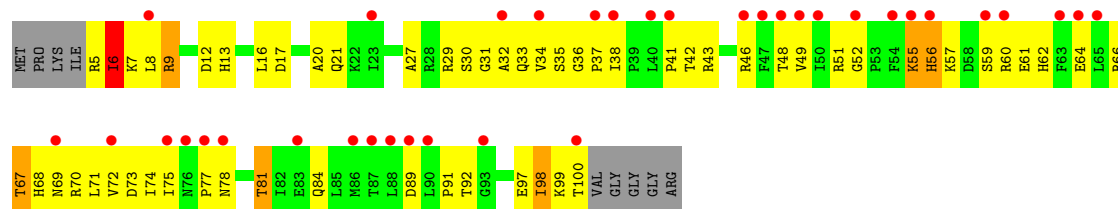




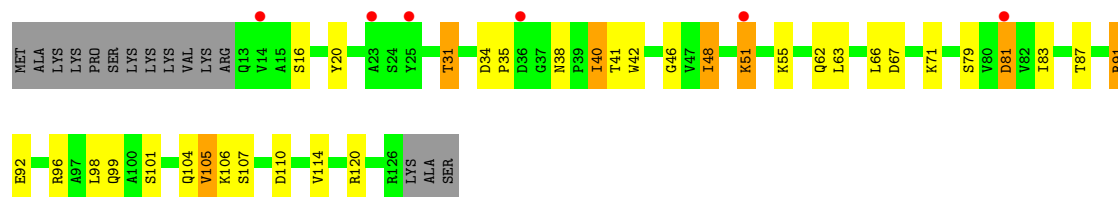
• Molecule 10: 30S ribosomal protein S10



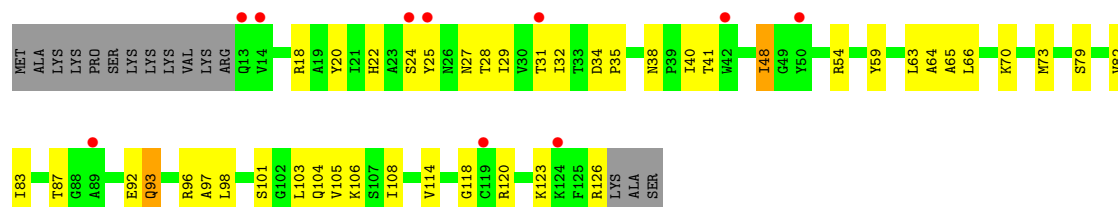
• Molecule 10: 30S ribosomal protein S10



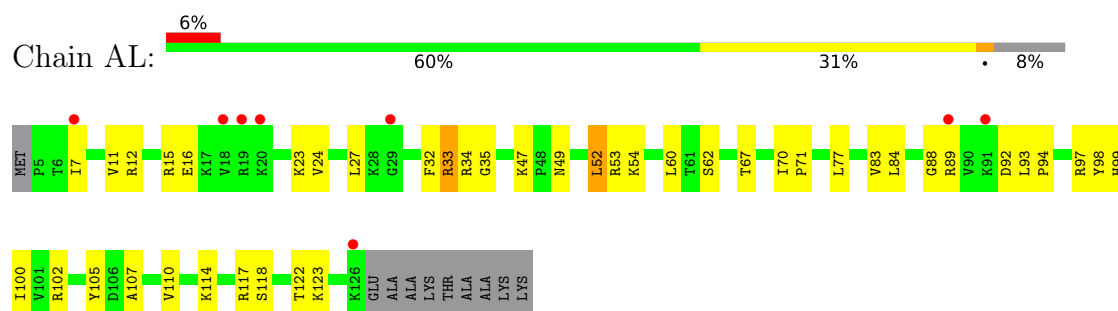
• Molecule 11: 30S ribosomal protein S11



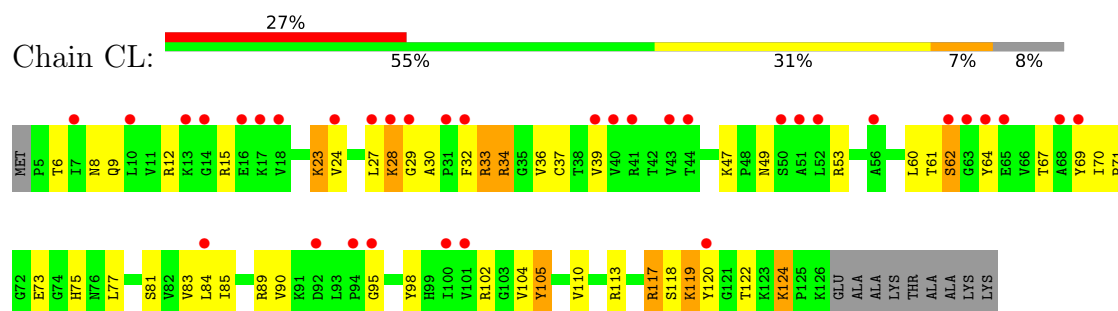
• Molecule 11: 30S ribosomal protein S11



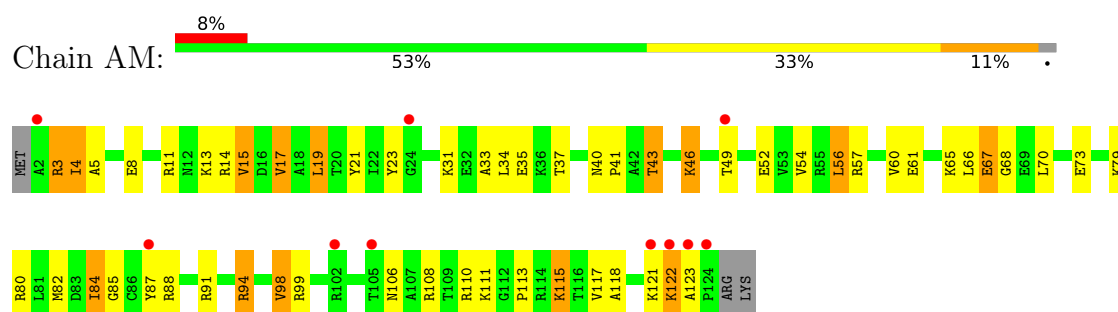
- Molecule 12: 30S ribosomal protein S12



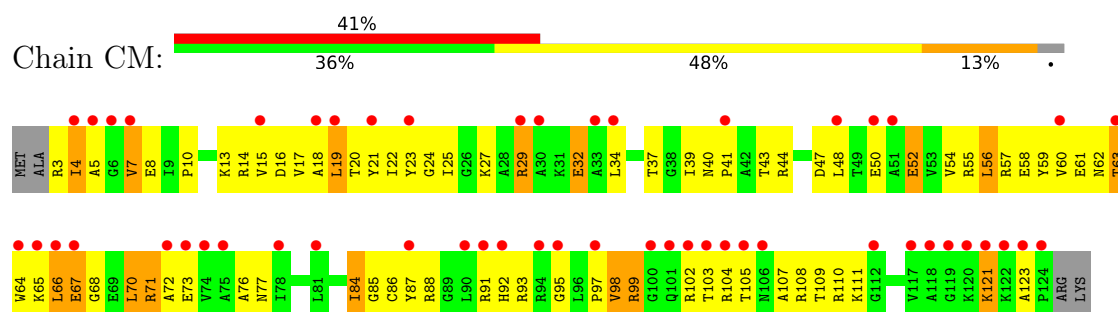
- Molecule 12: 30S ribosomal protein S12



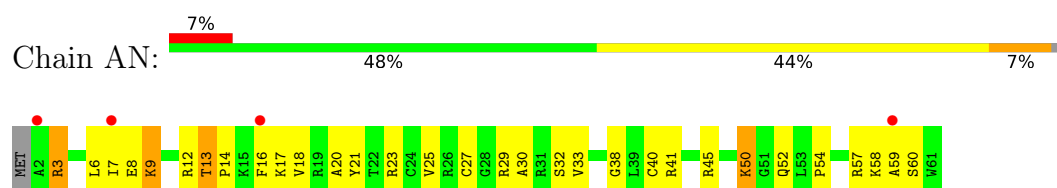
- Molecule 13: 30S ribosomal protein S13



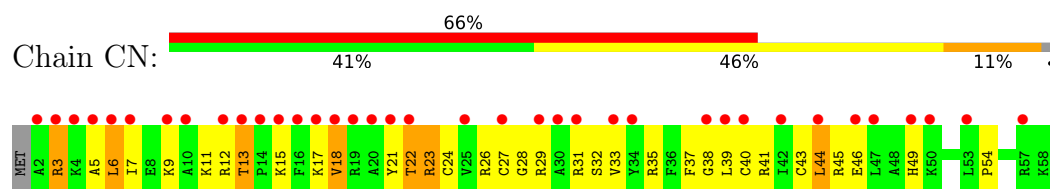
- Molecule 13: 30S ribosomal protein S13



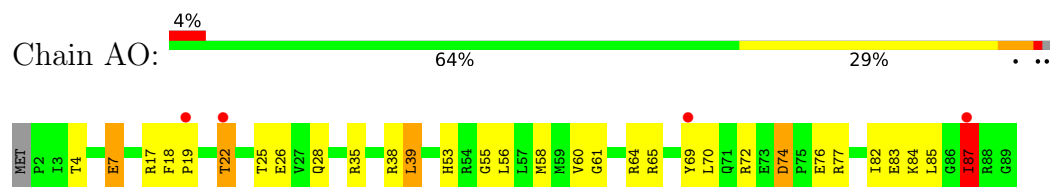
- Molecule 14: 30S ribosomal protein S14 type Z



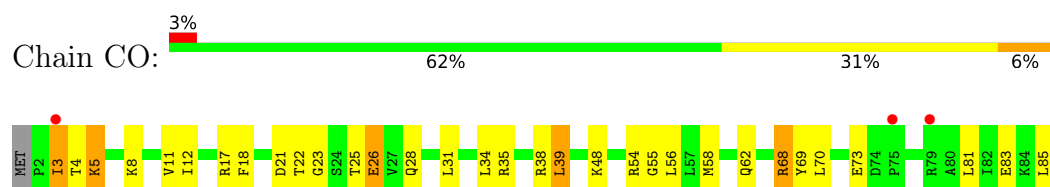
- Molecule 14: 30S ribosomal protein S14 type Z



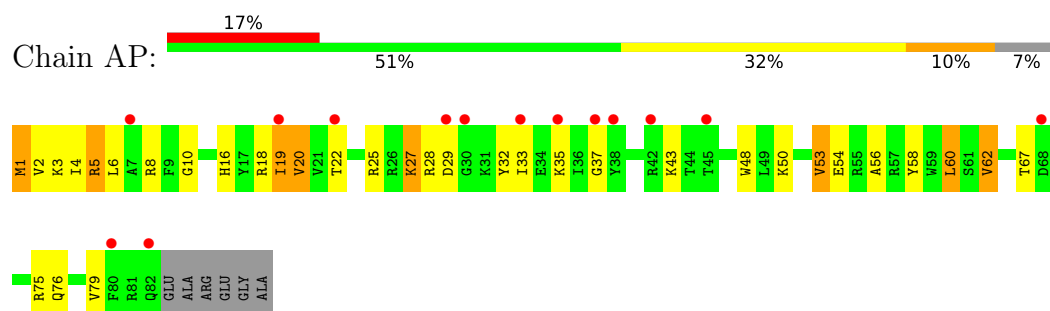
- Molecule 15: 30S ribosomal protein S15



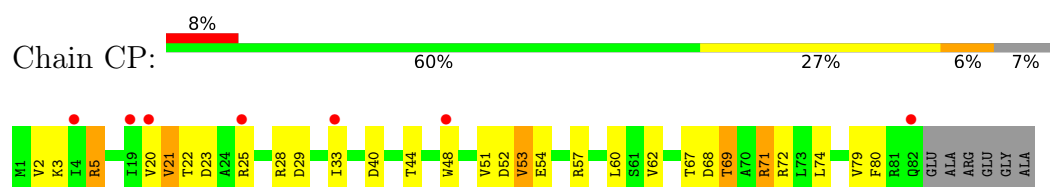
- Molecule 15: 30S ribosomal protein S15



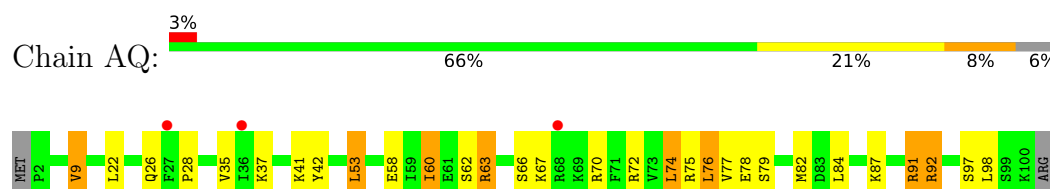
- Molecule 16: 30S ribosomal protein S16



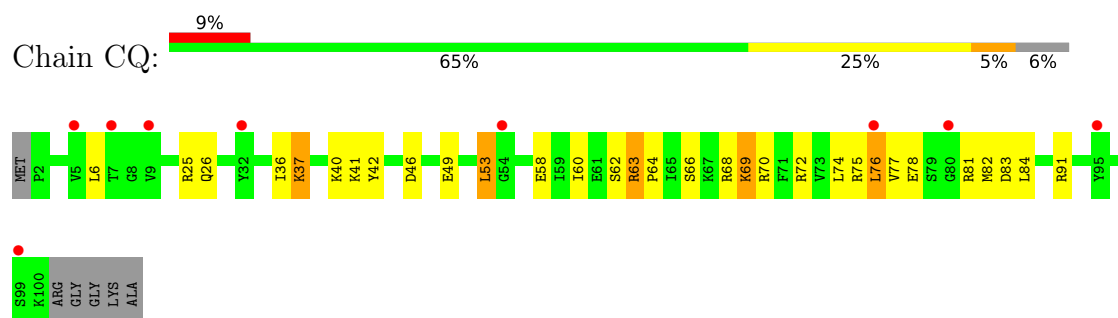
- Molecule 16: 30S ribosomal protein S16



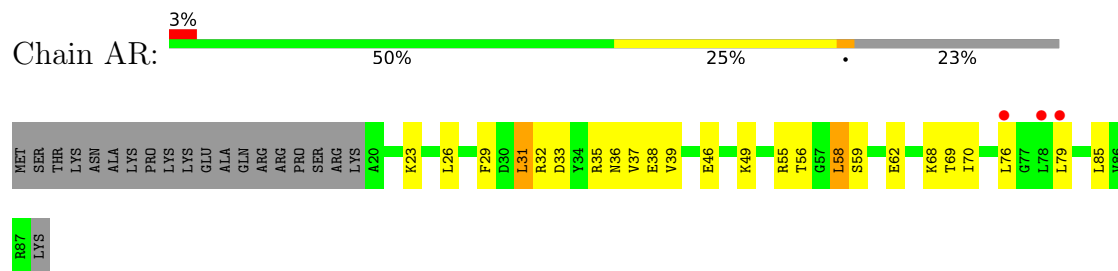
- Molecule 17: 30S ribosomal protein S17



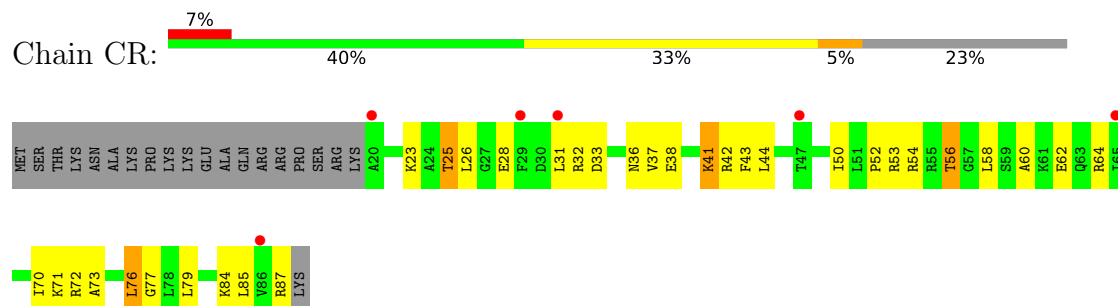
- Molecule 17: 30S ribosomal protein S17



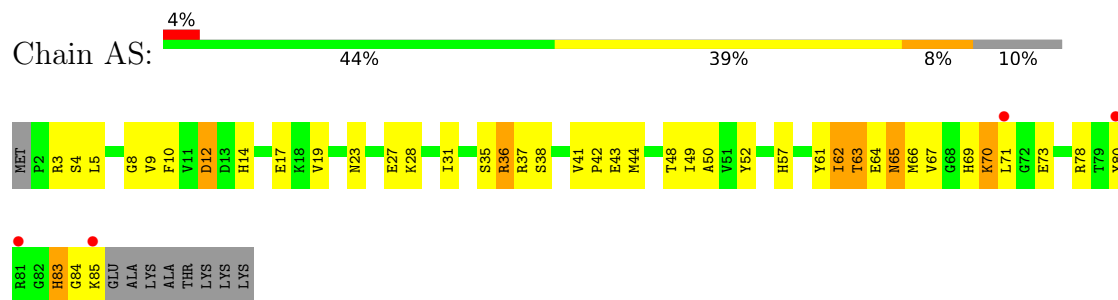
- Molecule 18: 30S ribosomal protein S18



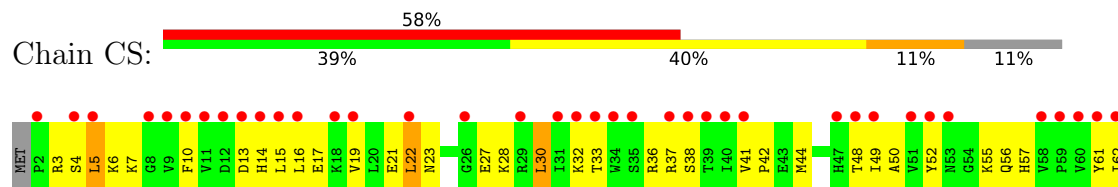
- Molecule 18: 30S ribosomal protein S18

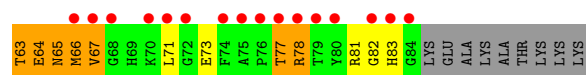


- Molecule 19: 30S ribosomal protein S19

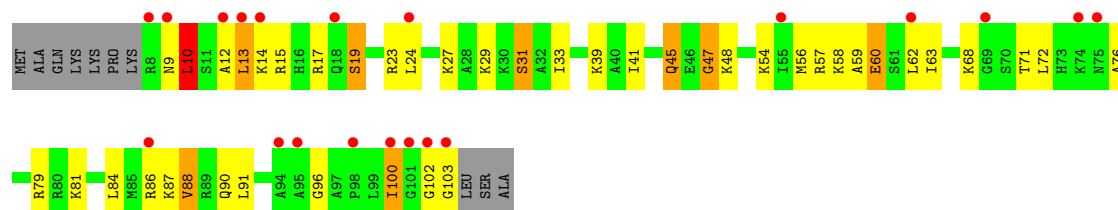


- Molecule 19: 30S ribosomal protein S19

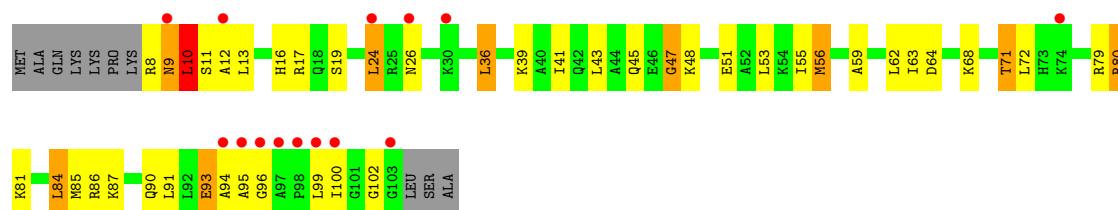




- Molecule 20: 30S ribosomal protein S20



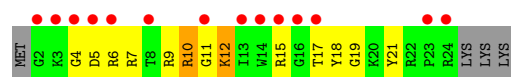
- Molecule 20: 30S ribosomal protein S20



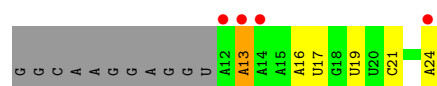
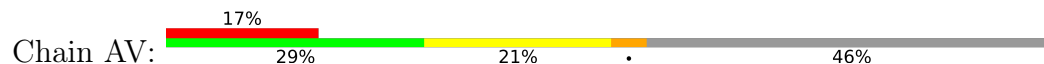
- Molecule 21: 30S ribosomal protein Thx



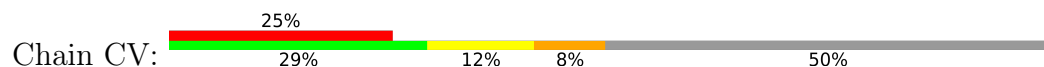
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: mRNA



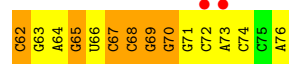
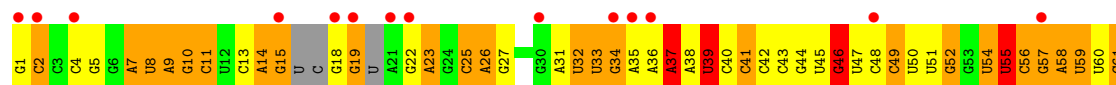
- Molecule 22: mRNA



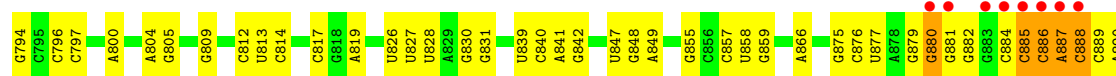
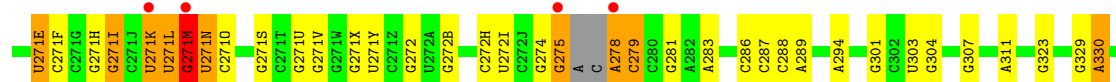




• Molecule 25: E-site tRNA



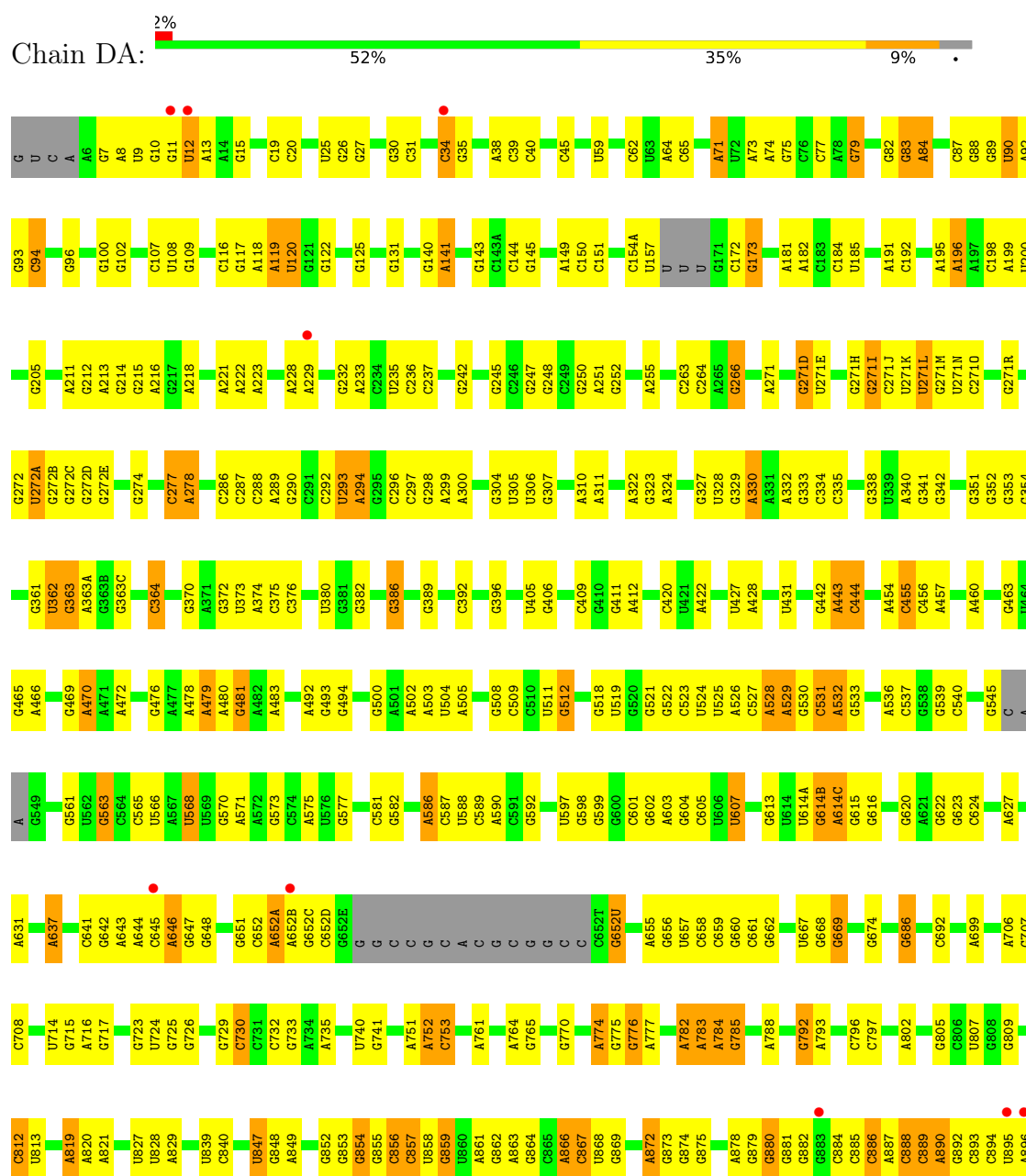
• Molecule 26: 23S Ribosomal RNA



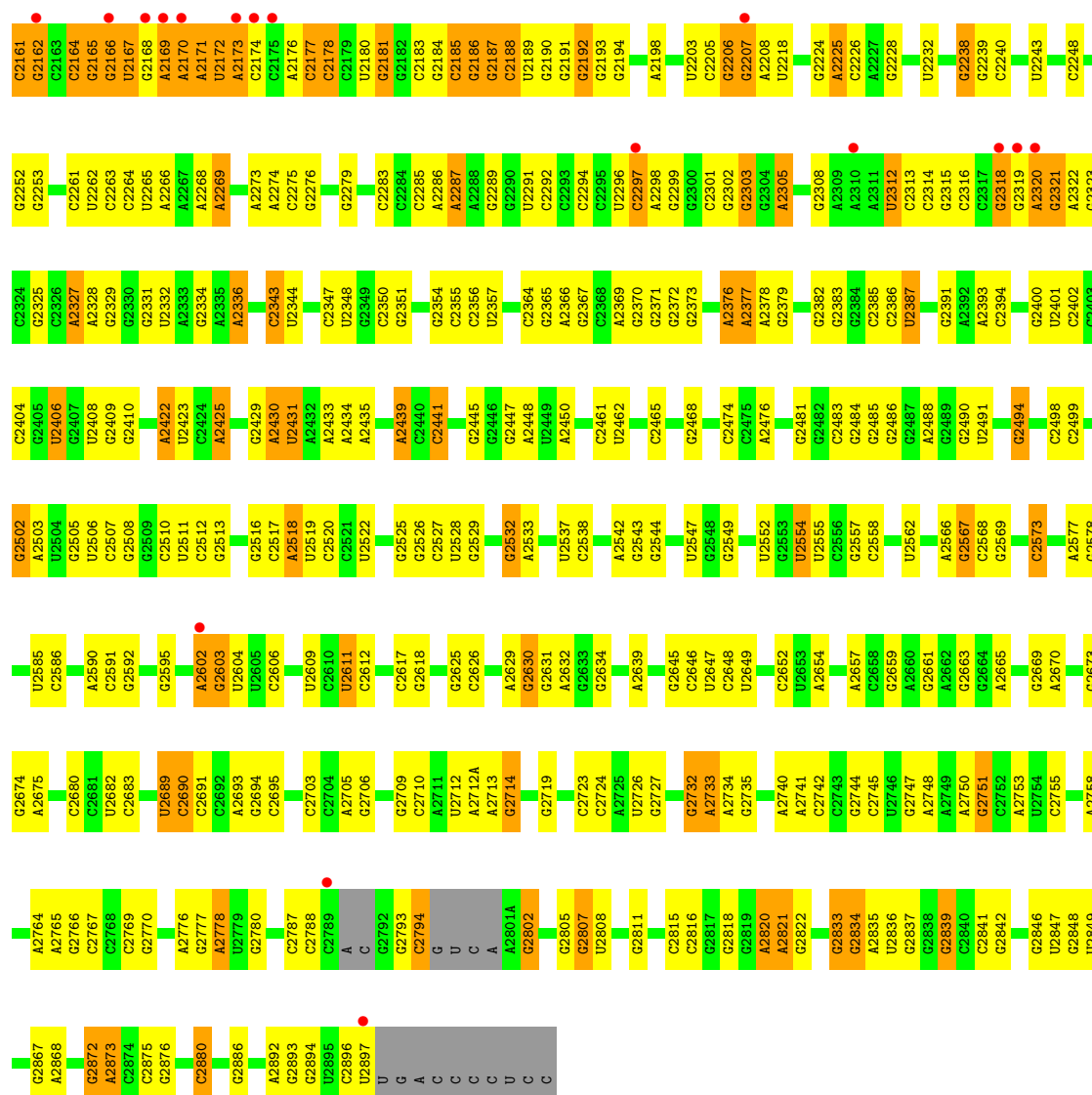
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A2418	G2313	A2199	A2134	G2056	A1937	C1797	C1686	G1537	G1428	A1279	G1154	C	A1001
U2419	G2319	C2200	A2135	G2056	A1938	U1798	U1687	G1538	G1429	U1292	A1155	A	G1002
A2422	A2320	G2206	C2137	A2059	U1939	C1800	A1689	U1540	U1431	C1293	C	C	C1005
A2425	G2325	G2207	C2138	A2060	G1948	A1803	U1693	A1542	A1434	C1297	U	U	G1006
A2428	G2326	A2208	C2140	A2062	A1952	G1814	G1696	C1543	A1434	U1300	U	U	C1007
G2429	A2327	G2208	C2141	G2067	A1953	A1815	G1697	A1554	G1441	A1301	A	A	A1009
U2430	G2328	A2225	C2142	U2068	G1954	G1816	A1698	C1557	G1442	A1302	A	A	U1012
U2431	G2329	U2233	C2143	G2069	U1955	G1817	G1699	A1558	A1445	G1303	C	A	C1013
A2435	G2330	G2234	C2144	G2070	C1958	U1818	A1701	A1566	G1447	G1310	A	A	U1019
A2439	G2331	G2238	C2145	U2074	U1968	A1825	G1702	A1566	G1448	C1314	G	G	A1020
C2440	G2332	G2239	C2146	U2075	G1964	G1828	G1703	A1569	A1449	C1315	U	U	A1021
C2441	G2333	U2243	U2150	G2080	G1967	G1839	U1709	U1578	A1450	A1342	U	U	G1022
C2442	G2334	U2244	G2151	U2086	G1968	G1840	C1711	A1579	A1452	C1345	U	U	G1025
G2445	C2340	U2245	G2152	G2087	A1969	U1941	C1712	A1580	U1453	G1187	A	A	U1026
G2446	C2342	G2246	G2153	G2087	A1970	G1842	U1713	G1581	G1455	C1187	A	A	A1027
G2447	C2343	A2247	G2154	G2093	A1971	C1843	G1714	C1467	U1352	C1201	A	A	A1028
A2448	G2344	C2260	G2155	U2096	A1972	A1847	G1721	A1584	A1353	A1204	C	C	U1033
U2449	G2345	C2261	A2158	C2097	G1992	U1851	A1722	A1587	G1470	A1204	C	C	G1034
A2450	C2346	U2262	G2159	U2098	U1993	C1852	U1739	C1588	A1471	A1210	U	U	U1035
G2468	G2347	A2268	G2160	U2099	G1996	G1958	G1745A	A1593	A1477	A1360	C	C	C1038
A2469	C2350	A2271	G2161	G2100	G1997	A1859	G1746	G1594	A1478	A1220	U	U	G1044
G2470	G2353	U2272	G2162	G2101	U2102	C1860	G1753	U1602	G1482	G1223	U	U	A1045
C2474	U2357	A2273	C2163	C2103	A2001	G1861	C1754	A1608	A1490	A1226	G1106	G1107	A1046
A2475	G2358	A2274	G2164	G2104	G2002	U1876	A1755	A1609	C1493	A1230	G1108	C1109	G1047
C2476	C2359	C2275	G2165	C2105	G2010	C1866	G1756	A1610	C1501	G1231	G1110	G1111	A1048
A2477	A2360	G2276	U2167	G2106	U2011	A1877	G1763	A1632	C1504	G1238	G1112	G1113	G1051
A2478	A2361	G2277	G2168	C2108	G2012	G1878	G1765	A1636	C1506	G1239	G1114	G1117	C1052
C2499	G2364	G2278	A2170	U2109	A2013	C1881	G1768	C1637	C1507	U1240	G	G	G
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G2505	A2366	A2280	U2172	G2111	G2014	C1883	A1773	G1649	A1395	G1252	G1128	G1129	U
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A2518	A2378	G2285	G2175	G2114	U2022	G1903	A1780	A1654	U1405	G1266	C1135	C1136	U
U2518	G2383	A2286	C2176	G2115	G2023	G1906	A1783	A1665	U1406	U1267	C1135	C1136	U
U2522	G2384	A2287	C2177	G2116	U2028	A1913	A1784	G1666	C1407	U1268	C1135	C1136	U
G2529	G2385	G2288	U2178	G2117	G2029	C1914	A1785	A1669	C1408	U1269	C1135	C1136	U
A2530	G2386	G2289	U2180	G2118	A2030	G1919	A1786	G1674	G1416	C1270	C1135	C1136	U
A2531	G2387	G2290	G2181	A2119	G2037	A1927	A1787	G1683	G1417	G1271	C1135	C1136	U
G2532	G2388	U2291	G2182	G2120	G2038	A1928	A1788	A1683	G1418	U1272	C1135	C1136	U
A2534	G2389	C2292	C2183	G2121	A2033	G1929	A1789	C1684	G1419	U1273	C1135	C1136	U
G2550	A2393	G2296	G2184	G2122	G2033	U2041	A1791	G1685	G1420	A1274	C1135	C1136	U
A2551	G2396	U2297	G2187	G2123	G2037	A2042	A1792	A1686	G1421		C1135	C1136	U
G2553	C2404	A2298	U2188	A2126	G2038	C2043	A1793	A1687			C1135	C1136	U
A2534	G2405	G2299	U2189	G2127	G2038	G2049	A1794	A1688			C1135	C1136	U
G2550	U2406	A2305	G2190	C2128	A2042		A1795	A1689			C1135	C1136	U
U2554	G2407	G2308	G2191	G2129	C2043		A1796	A1690			C1135	C1136	U
	A2411		G2192	U2130	G2043		A1797	A1691			C1135	C1136	U
			G2193	U2132	G2049		A1798	A1692			C1135	C1136	U



• Molecule 26: 23S Ribosomal RNA



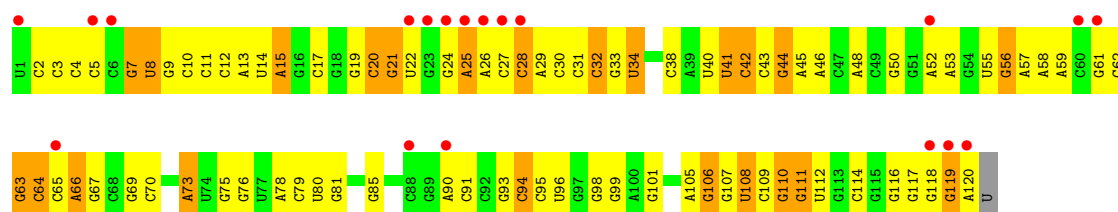




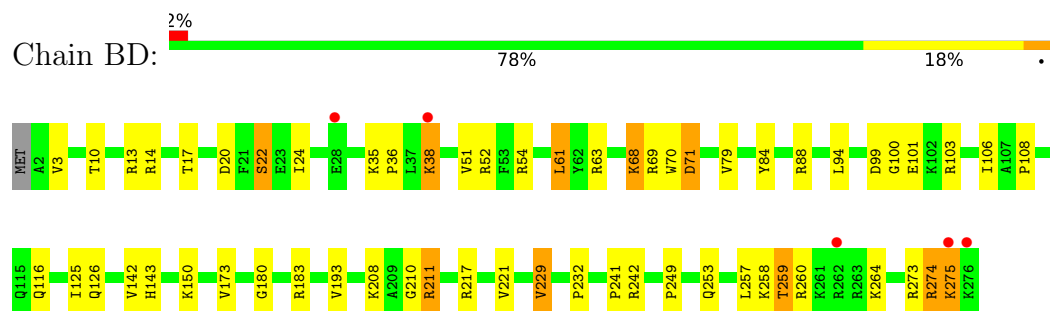
• Molecule 27: 5S Ribosomal RNA



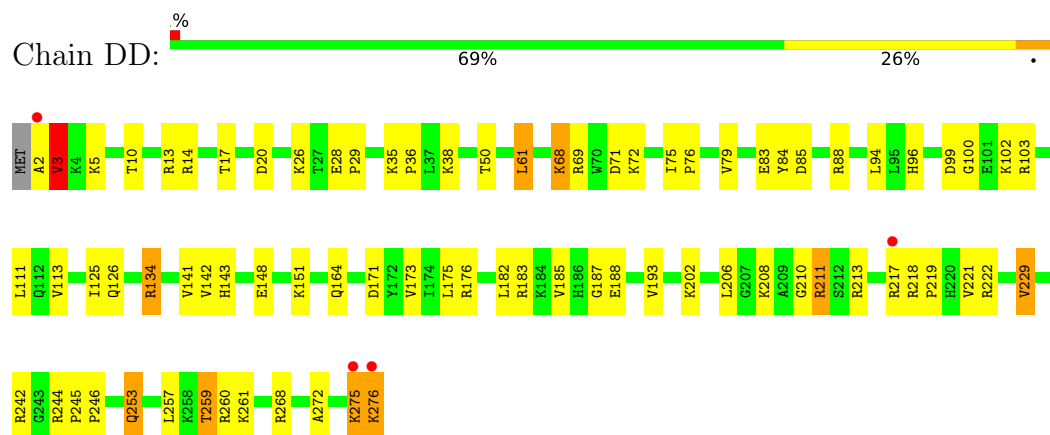
• Molecule 27: 5S Ribosomal RNA



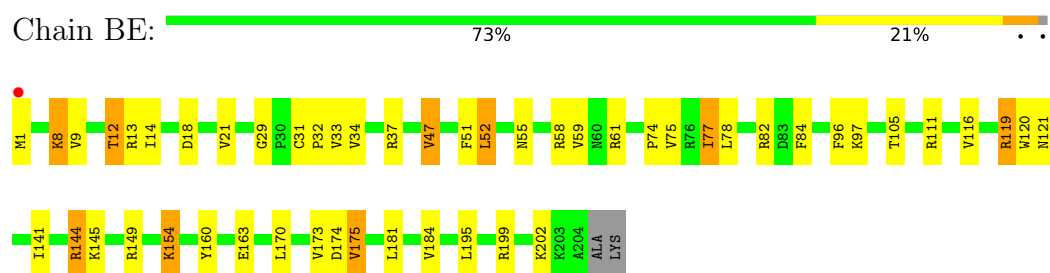
• Molecule 28: 50S ribosomal protein L2



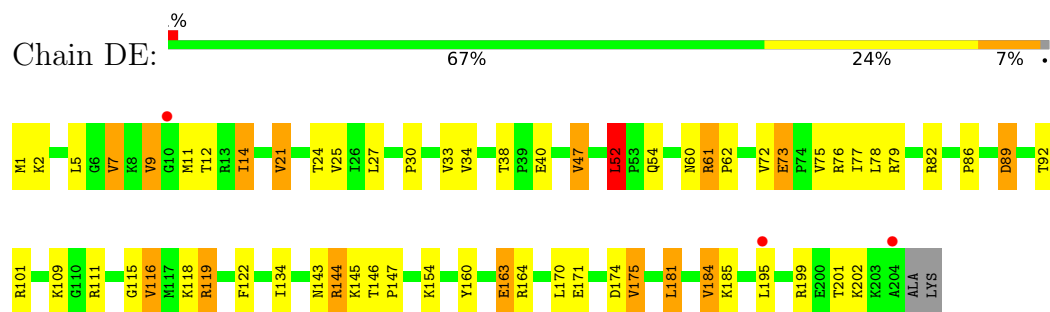
• Molecule 28: 50S ribosomal protein L2



• Molecule 29: 50S ribosomal protein L3

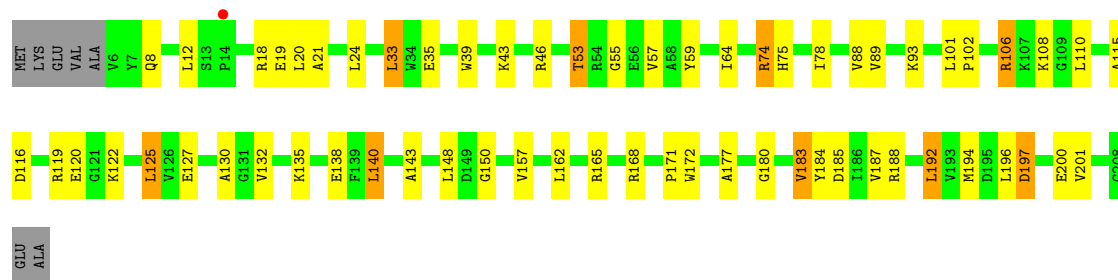


• Molecule 29: 50S ribosomal protein L3

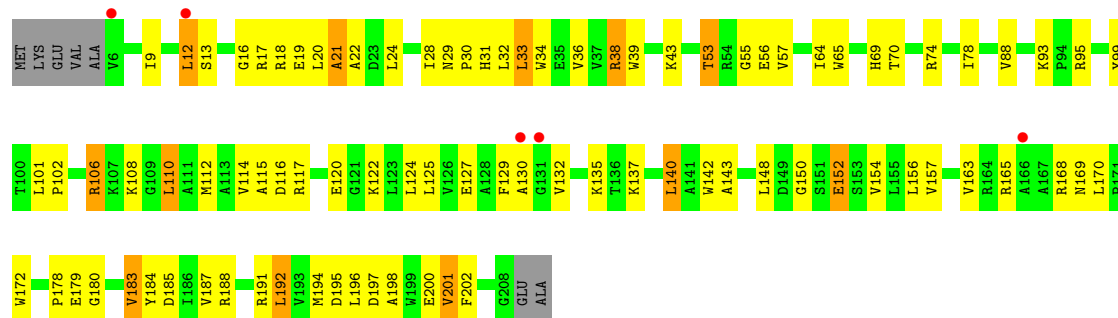


• Molecule 30: 50S ribosomal protein L4

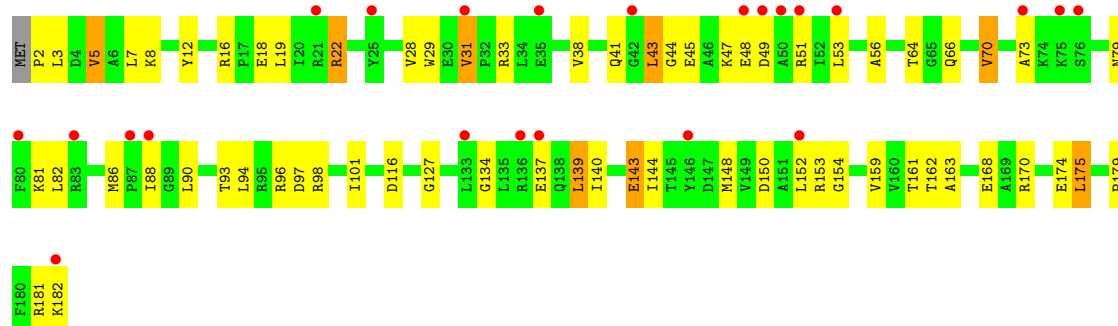




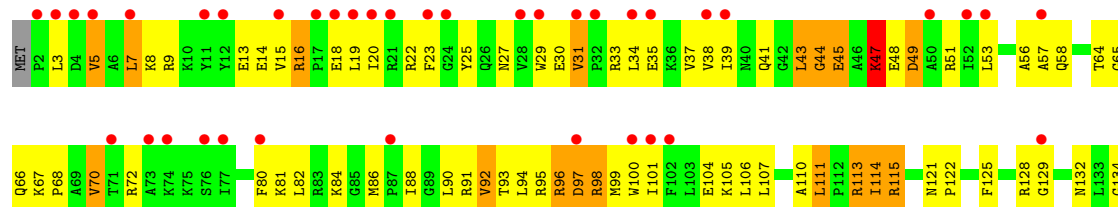
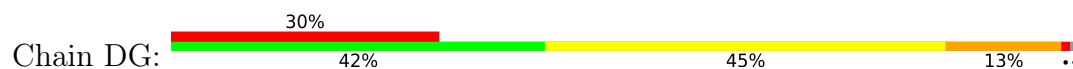
- Molecule 30: 50S ribosomal protein L4

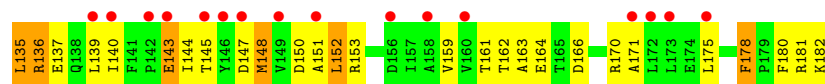


- Molecule 31: 50S ribosomal protein L5

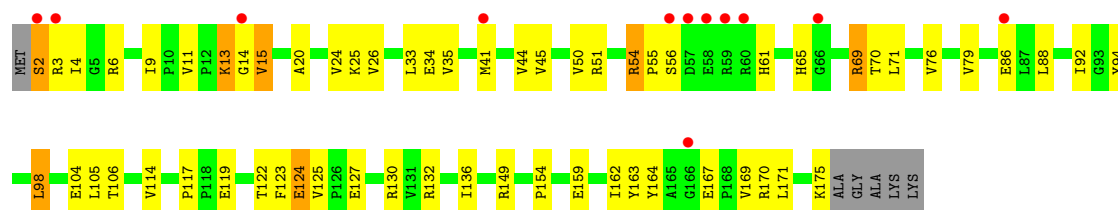


- Molecule 31: 50S ribosomal protein L5

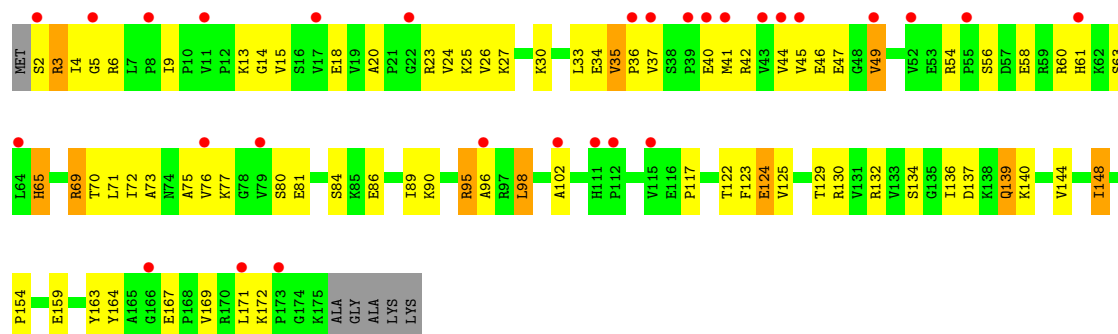




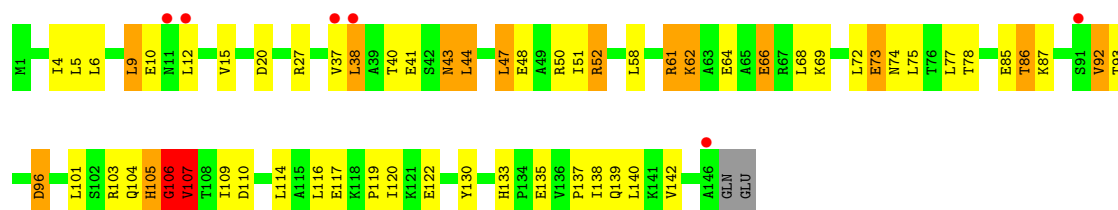
- Molecule 32: 50S ribosomal protein L6



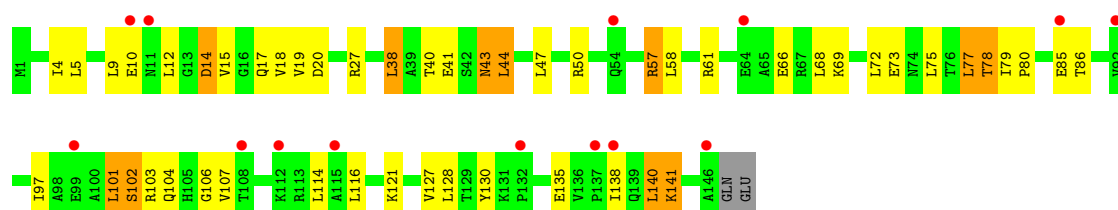
- Molecule 32: 50S ribosomal protein L6



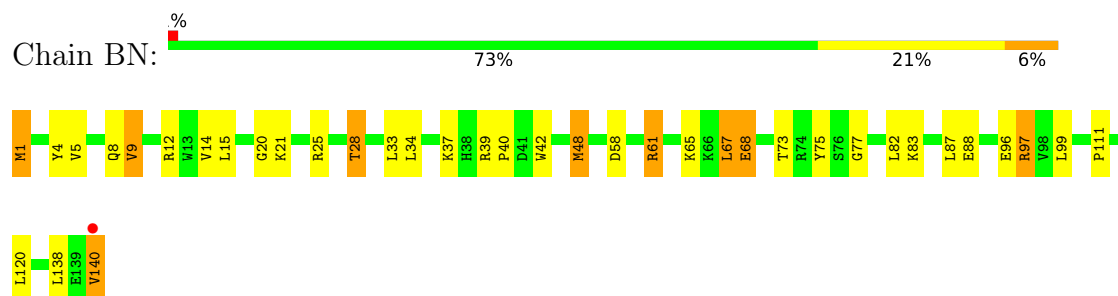
- Molecule 33: 50S ribosomal protein L9



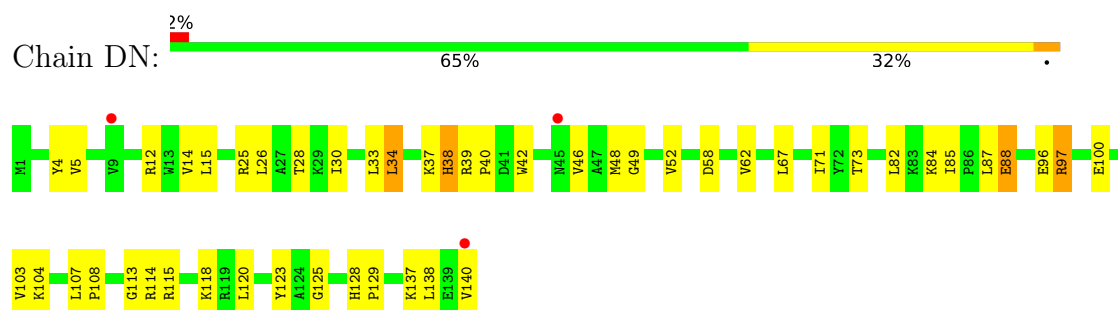
- Molecule 33: 50S ribosomal protein L9



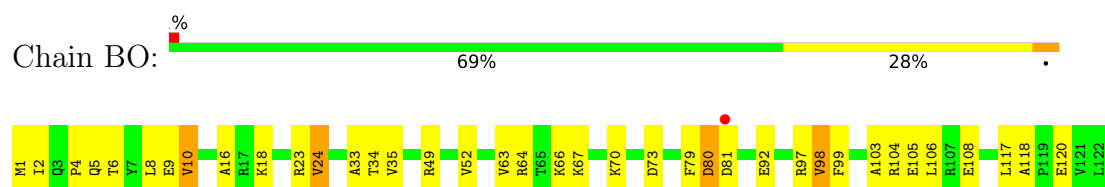
- Molecule 34: 50S ribosomal protein L13



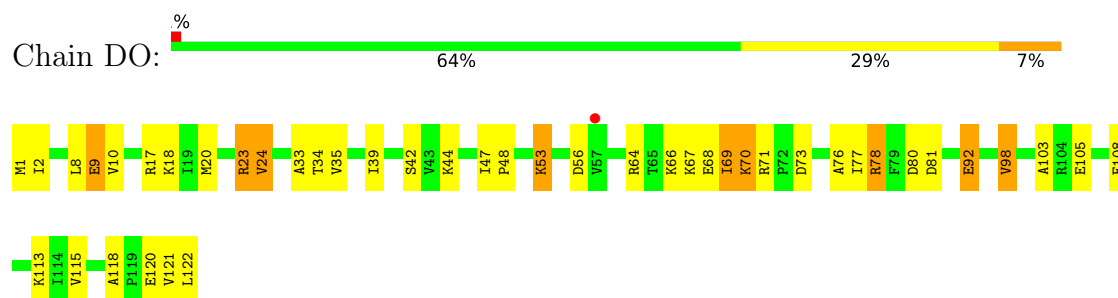
- Molecule 34: 50S ribosomal protein L13



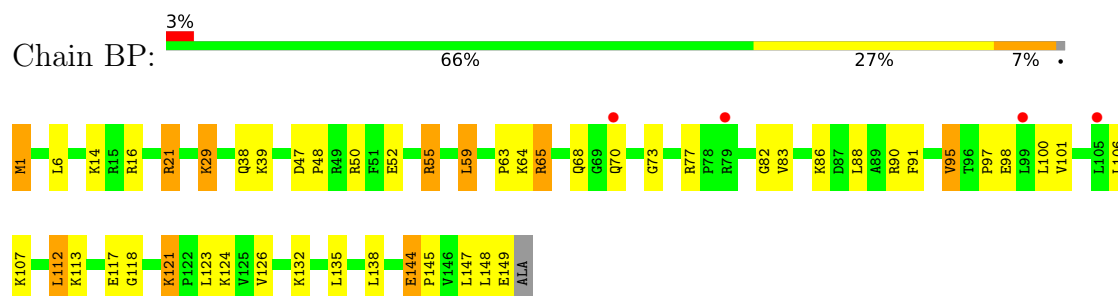
- Molecule 35: 50S ribosomal protein L14



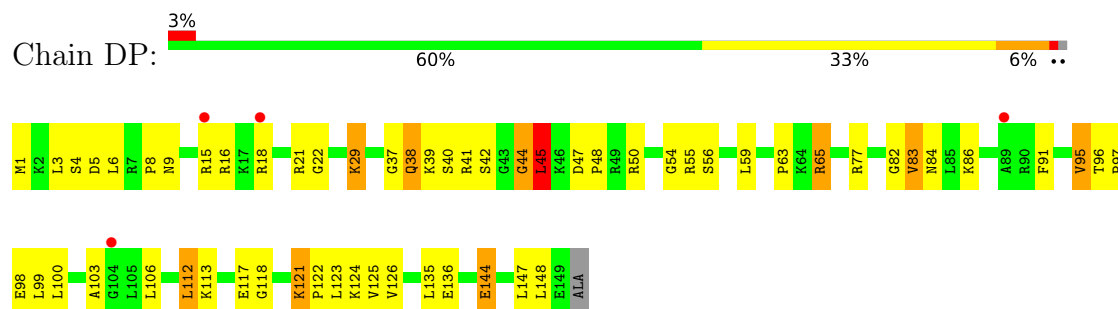
- Molecule 35: 50S ribosomal protein L14



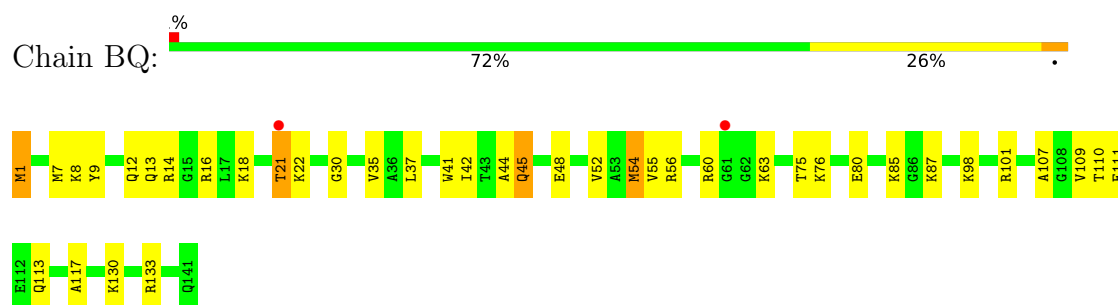
- Molecule 36: 50S ribosomal protein L15



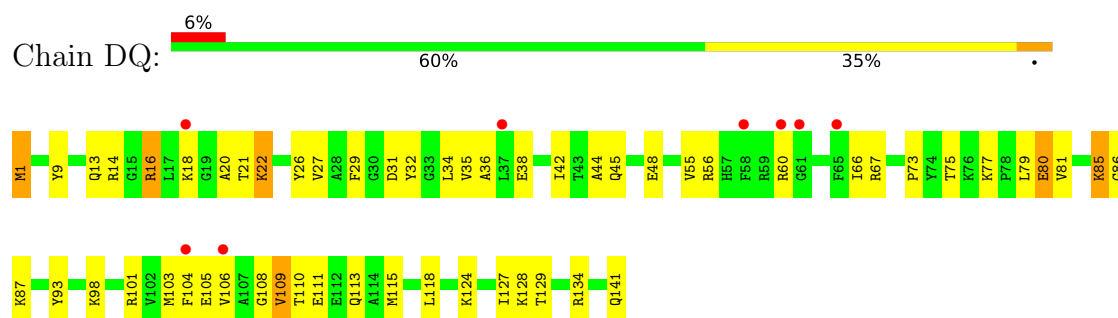
- Molecule 36: 50S ribosomal protein L15



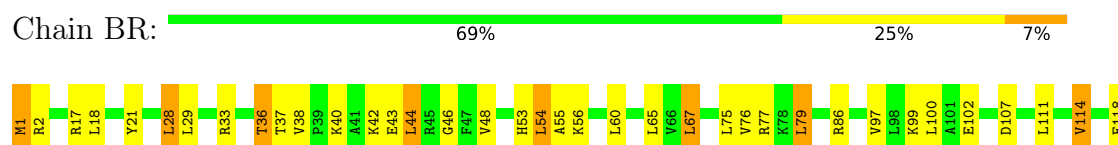
- Molecule 37: 50S ribosomal protein L16



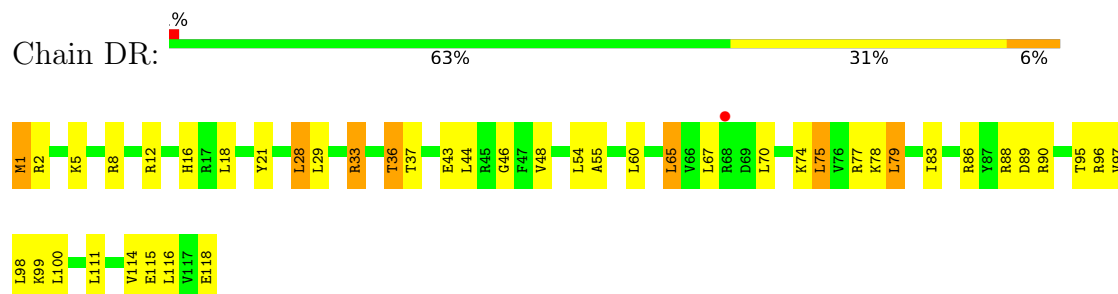
- Molecule 37: 50S ribosomal protein L16



- Molecule 38: 50S ribosomal protein L17



- Molecule 38: 50S ribosomal protein L17



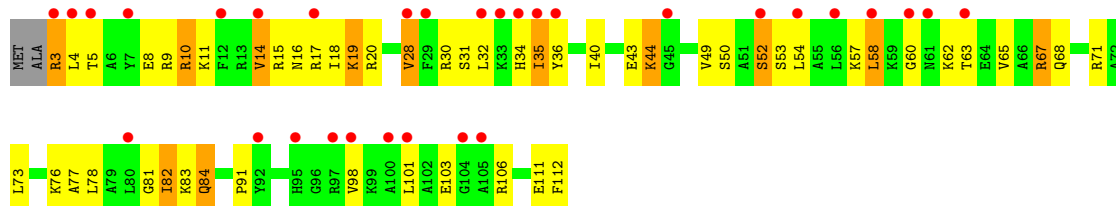
- Molecule 39: 50S ribosomal protein L18

Chain BS:  68% 23% 7% .



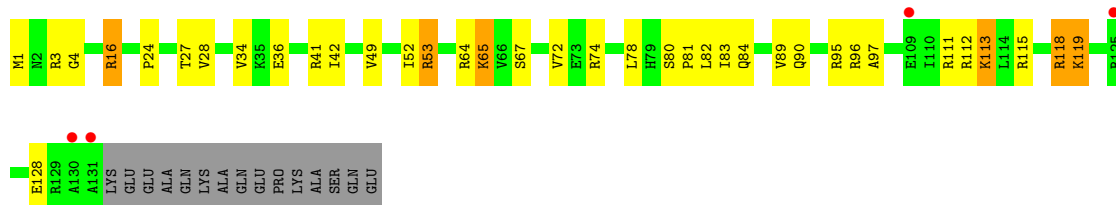
- Molecule 39: 50S ribosomal protein L18

Chain DS:  28% 51% 37% 11% .



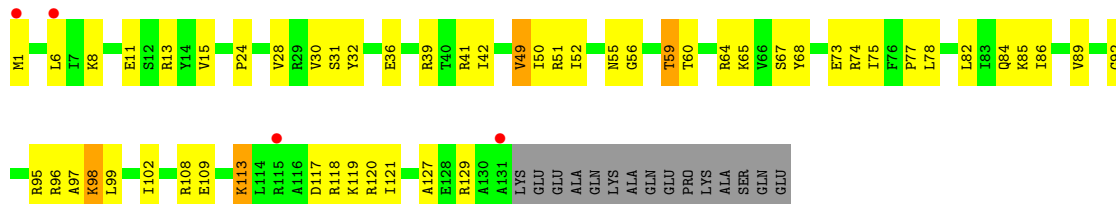
- Molecule 40: 50S ribosomal protein L19

Chain BT:  3% 64% 21% 10% .



- Molecule 40: 50S ribosomal protein L19

Chain DT:  3% 53% 34% 10% .



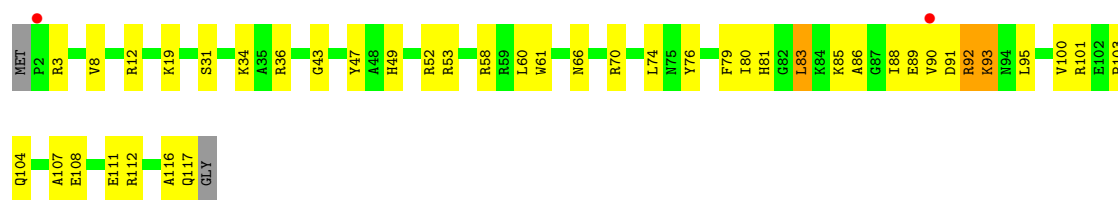
- Molecule 41: 50S ribosomal protein L20

Chain BU:  75% 22% . .



- Molecule 41: 50S ribosomal protein L20

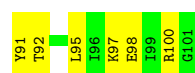
Chain DU:  2% 63% 33% . .



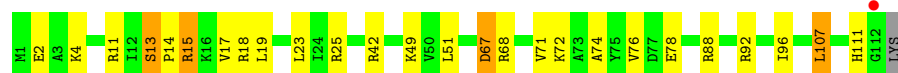
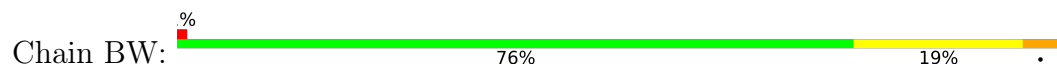
- Molecule 42: 50S ribosomal protein L21



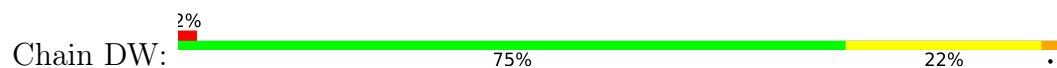
- Molecule 42: 50S ribosomal protein L21



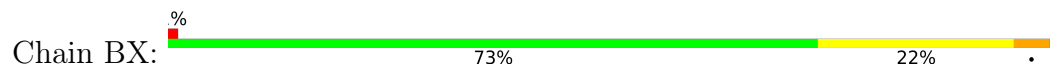
- Molecule 43: 50S ribosomal protein L22



- Molecule 43: 50S ribosomal protein L22

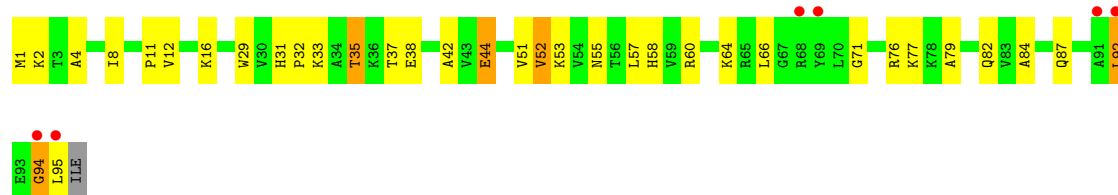


- Molecule 44: 50S ribosomal protein L23

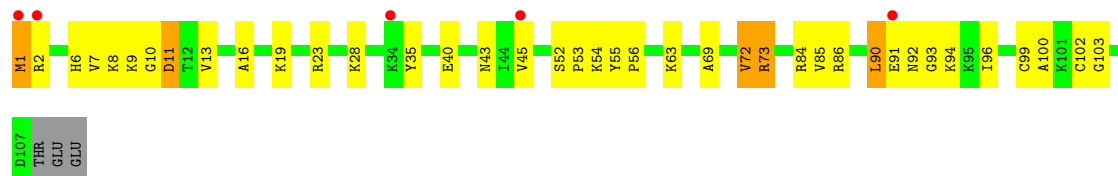


- Molecule 44: 50S ribosomal protein L23

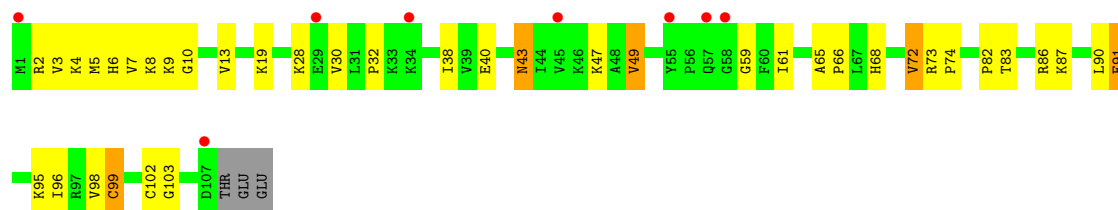




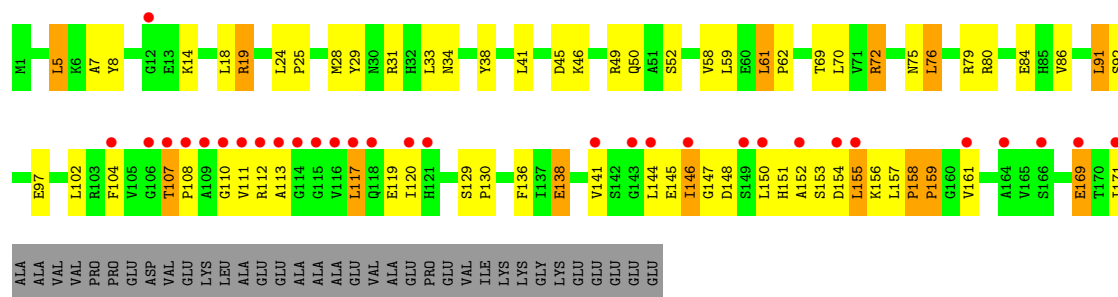
- Molecule 45: 50S ribosomal protein L24



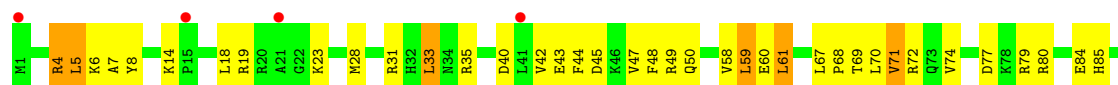
- Molecule 45: 50S ribosomal protein L24

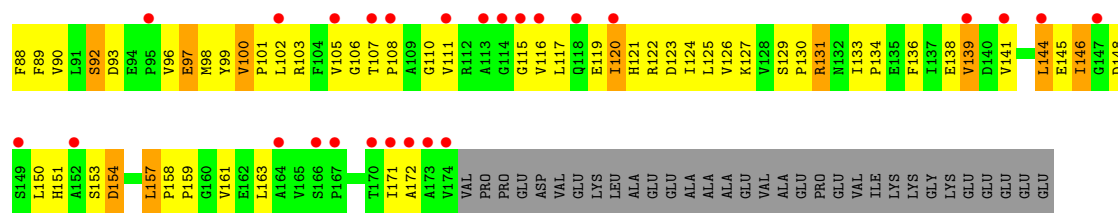


- Molecule 46: 50S ribosomal protein L25

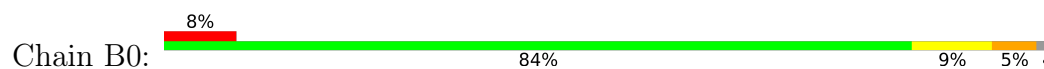


- Molecule 46: 50S ribosomal protein L25





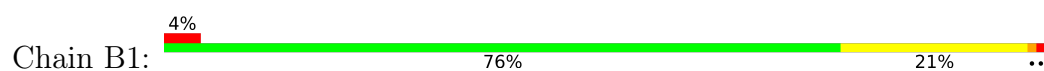
• Molecule 47: 50S ribosomal protein L27



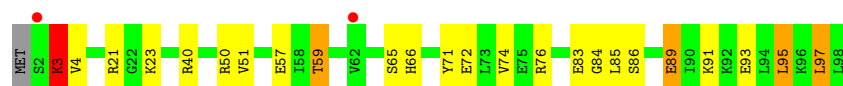
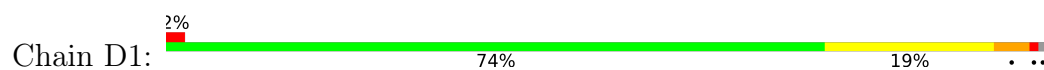
• Molecule 47: 50S ribosomal protein L27



• Molecule 48: 50S ribosomal protein L28



• Molecule 48: 50S ribosomal protein L28



• Molecule 49: 50S ribosomal protein L29

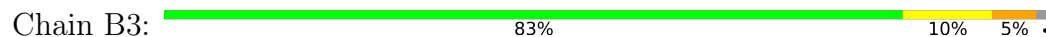


• Molecule 49: 50S ribosomal protein L29





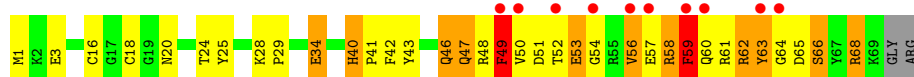
- Molecule 50: 50S ribosomal protein L30



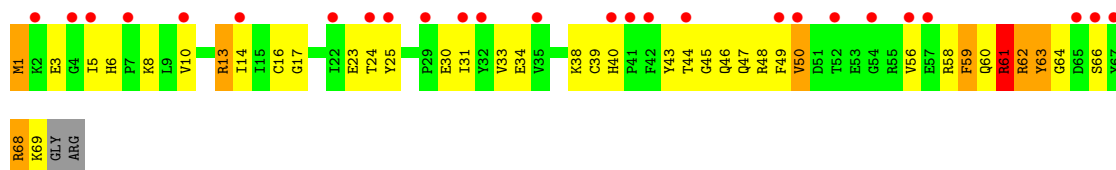
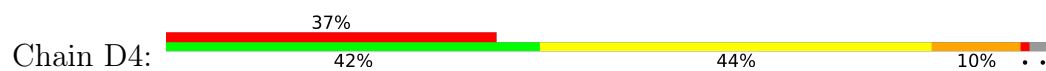
- Molecule 50: 50S ribosomal protein L30



- Molecule 51: 50S ribosomal protein L31



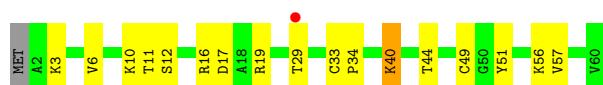
- Molecule 51: 50S ribosomal protein L31



- Molecule 52: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L33

Chain B6:  67% 22% 9% .



- Molecule 53: 50S ribosomal protein L33

Chain D6:  61% 33% . .



- Molecule 54: 50S ribosomal protein L34

Chain B7:  10% 71% 22% . .



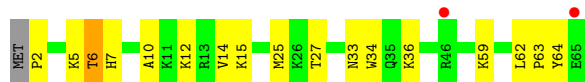
- Molecule 54: 50S ribosomal protein L34

Chain D7:  4% 65% 31% . .



- Molecule 55: 50S ribosomal protein L35

Chain B8:  3% 72% 25% . .



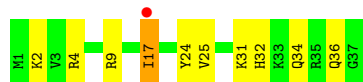
- Molecule 55: 50S ribosomal protein L35

Chain D8:  2% 65% 31% . .

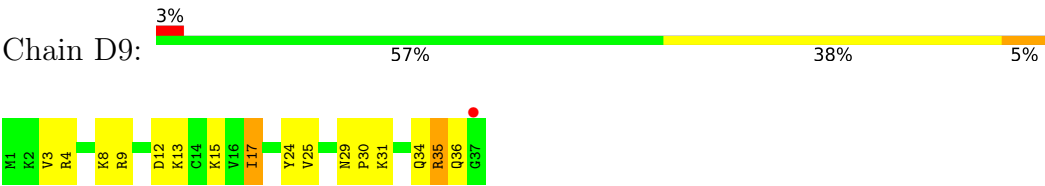


- Molecule 56: 50S ribosomal protein L36

Chain B9:  3% 73% 24% .



• Molecule 56: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.45Å 448.85Å 619.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	151.90 – 2.60 151.90 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (151.90-2.60) 99.9 (151.90-2.60)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.223 , 0.264 0.225 , 0.265	Depositor DCC
R_{free} test set	88430 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	56.4	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	297127	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 4SU, K, SF4, MG, 5MC, 31H, F3N, PSU, 7MG, MIA, ZN, 5MU

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	0.22	0/36027	0.45	2/56227 (0.0%)
1	CA	0.22	0/36170	0.47	7/56452 (0.0%)
2	AB	0.40	0/1881	1.02	10/2542 (0.4%)
2	CB	0.46	0/1860	1.07	7/2518 (0.3%)
3	AC	0.39	0/1576	0.88	2/2130 (0.1%)
3	CC	0.41	0/1568	0.97	5/2122 (0.2%)
4	AD	0.39	0/1689	0.89	3/2267 (0.1%)
4	CD	0.39	0/1708	0.92	5/2289 (0.2%)
5	AE	0.43	0/1145	0.96	4/1543 (0.3%)
5	CE	0.43	0/1149	1.01	6/1548 (0.4%)
6	AF	0.38	0/825	0.79	0/1118
6	CF	0.38	0/833	0.83	2/1128 (0.2%)
7	AG	0.37	0/1250	0.83	1/1679 (0.1%)
7	CG	0.38	0/1254	0.91	3/1683 (0.2%)
8	AH	0.37	0/1108	0.88	1/1494 (0.1%)
8	CH	0.36	0/1108	0.87	2/1494 (0.1%)
9	AI	0.38	0/1005	0.90	0/1350
9	CI	0.40	0/997	0.96	2/1343 (0.1%)
10	AJ	0.38	0/722	0.91	0/982
10	CJ	0.46	0/727	1.06	4/988 (0.4%)
11	AK	0.39	0/848	0.86	1/1149 (0.1%)
11	CK	0.38	0/848	0.90	0/1149
12	AL	0.40	0/946	0.81	0/1274
12	CL	0.37	0/946	0.93	3/1274 (0.2%)
13	AM	0.40	0/977	0.94	2/1310 (0.2%)
13	CM	0.43	0/961	0.93	1/1291 (0.1%)
14	AN	0.40	0/501	0.83	0/664
14	CN	0.42	0/501	0.88	0/664
15	AO	0.39	0/739	0.87	3/985 (0.3%)
15	CO	0.37	0/739	0.86	0/985
16	AP	0.40	0/697	0.82	0/939
16	CP	0.39	0/693	0.82	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.35	0/836	0.85	0/1117
17	CQ	0.33	0/836	0.82	0/1117
18	AR	0.36	0/560	0.81	0/746
18	CR	0.36	0/560	0.82	0/746
19	AS	0.40	0/676	0.96	0/911
19	CS	0.48	0/661	1.15	2/893 (0.2%)
20	AT	0.38	0/730	0.95	1/965 (0.1%)
20	CT	0.38	0/733	0.92	3/969 (0.3%)
21	AU	0.32	0/203	0.79	0/266
21	CU	0.36	0/203	0.92	0/266
22	AV	0.22	0/310	0.41	0/480
22	CV	0.23	0/282	0.44	0/437
23	AW	0.29	1/1577 (0.1%)	0.53	0/2454
23	CW	0.31	0/1531	0.57	0/2379
24	AX	0.27	0/1700	0.43	0/2650
24	CX	0.26	1/1700 (0.1%)	0.45	0/2650
25	AY	0.33	0/1602	0.59	0/2493
25	CY	0.32	0/1579	0.57	0/2455
26	BA	0.28	0/68013	0.46	3/106165 (0.0%)
26	DA	0.23	0/67542	0.44	1/105428 (0.0%)
27	BB	0.23	0/2878	0.45	0/4490
27	DB	0.24	0/2878	0.44	0/4490
28	BD	0.48	0/2186	0.89	1/2944 (0.0%)
28	DD	0.43	0/2192	0.90	3/2951 (0.1%)
29	BE	0.50	0/1592	0.88	0/2149
29	DE	0.42	0/1592	0.88	0/2149
30	BF	0.46	0/1619	0.87	1/2193 (0.0%)
30	DF	0.40	0/1615	0.91	3/2188 (0.1%)
31	BG	0.40	0/1450	0.88	4/1959 (0.2%)
31	DG	0.41	0/1449	1.03	7/1958 (0.4%)
32	BH	0.44	0/1356	0.93	5/1834 (0.3%)
32	DH	0.39	0/1356	0.92	1/1834 (0.1%)
33	BI	0.38	0/1100	0.94	4/1501 (0.3%)
33	DI	0.39	0/1088	0.86	0/1484
34	BN	0.47	0/1144	0.85	0/1543
34	DN	0.38	0/1144	0.90	2/1543 (0.1%)
35	BO	0.48	0/943	0.86	0/1269
35	DO	0.41	0/943	0.84	0/1269
36	BP	0.46	0/1156	0.83	0/1537
36	DP	0.40	0/1152	0.92	7/1533 (0.5%)
37	BQ	0.46	0/1143	0.80	0/1527
37	DQ	0.40	0/1143	0.81	0/1527
38	BR	0.48	0/982	0.85	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DR	0.42	0/982	0.79	0/1312
39	BS	0.40	0/887	0.91	1/1180 (0.1%)
39	DS	0.38	0/880	0.90	1/1172 (0.1%)
40	BT	0.44	0/1105	0.79	0/1477
40	DT	0.39	0/1097	0.81	0/1468
41	BU	0.49	0/977	0.84	0/1301
41	DU	0.39	0/977	0.81	0/1301
42	BV	0.46	0/782	0.84	0/1049
42	DV	0.38	0/782	0.85	0/1049
43	BW	0.50	0/897	0.88	2/1205 (0.2%)
43	DW	0.42	0/897	0.83	0/1205
44	BX	0.48	0/764	0.87	1/1025 (0.1%)
44	DX	0.41	0/764	0.89	1/1025 (0.1%)
45	BY	0.44	0/819	0.88	0/1095
45	DY	0.38	0/819	0.90	1/1095 (0.1%)
46	BZ	0.42	0/1379	0.99	5/1873 (0.3%)
46	DZ	0.39	0/1390	0.96	6/1890 (0.3%)
47	B0	0.44	0/662	0.84	1/881 (0.1%)
47	D0	0.38	0/662	0.94	3/881 (0.3%)
48	B1	0.46	0/762	0.82	0/1014
48	D1	0.41	0/762	0.79	0/1014
49	B2	0.41	0/590	0.84	1/781 (0.1%)
49	D2	0.35	0/590	0.77	0/781
50	B3	0.46	0/474	0.83	0/635
50	D3	0.35	0/469	0.89	0/630
51	B4	0.40	0/571	1.15	6/768 (0.8%)
51	D4	0.43	0/545	1.12	3/737 (0.4%)
52	B5	0.51	0/469	0.81	0/635
52	D5	0.42	0/469	0.80	0/635
53	B6	0.49	0/460	0.75	0/613
53	D6	0.37	0/456	0.75	0/608
54	B7	0.52	0/426	0.81	0/561
54	D7	0.48	0/426	0.87	0/561
55	B8	0.49	0/525	0.84	0/691
55	D8	0.38	0/525	0.79	0/691
56	B9	0.46	0/310	0.75	0/407
56	D9	0.38	0/310	0.81	0/407
All	All	0.30	2/316594 (0.0%)	0.60	156/473940 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AB	0	2
2	CB	0	1
7	AG	0	2
20	CT	0	1
33	BI	0	1
35	BO	0	1
39	BS	0	1
51	B4	0	1
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CX	8	4SU	O3'-P	5.16	1.61	1.56
23	AW	8	4SU	O3'-P	5.01	1.61	1.56

The worst 5 of 156 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	BS	60	GLY	N-CA-C	12.31	121.42	110.21
51	B4	60	GLN	N-CA-C	-9.45	101.68	113.02
2	CB	13	ALA	N-CA-C	8.91	123.72	113.02
2	AB	9	GLU	N-CA-C	8.85	122.39	110.35
13	AM	84	ILE	N-CA-C	8.80	120.59	111.00

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	231	GLU	Peptide
2	AB	9	GLU	Peptide
7	AG	78	ARG	Peptide
7	AG	79	ARG	Peptide
33	BI	9	LEU	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	32185	0	16245	538	0
1	CA	32312	0	16307	771	0
2	AB	1846	0	1867	85	0
2	CB	1825	0	1828	121	0
3	AC	1552	0	1546	61	0
3	CC	1544	0	1524	72	0
4	AD	1659	0	1676	56	0
4	CD	1678	0	1718	69	0
5	AE	1129	0	1185	31	0
5	CE	1133	0	1191	49	0
6	AF	812	0	804	20	0
6	CF	820	0	814	21	0
7	AG	1231	0	1238	24	0
7	CG	1235	0	1249	40	0
8	AH	1088	0	1126	35	0
8	CH	1088	0	1126	40	0
9	AI	986	0	995	44	0
9	CI	978	0	966	55	0
10	AJ	709	0	650	35	0
10	CJ	714	0	672	44	0
11	AK	833	0	836	21	0
11	CK	833	0	836	21	0
12	AL	930	0	980	27	0
12	CL	930	0	980	34	0
13	AM	966	0	1024	42	0
13	CM	950	0	988	73	0
14	AN	492	0	529	26	0
14	CN	492	0	529	32	0
15	AO	728	0	760	21	0
15	CO	728	0	760	23	0
16	AP	681	0	697	28	0
16	CP	677	0	686	22	0
17	AQ	823	0	891	26	0
17	CQ	823	0	891	21	0
18	AR	555	0	618	11	0
18	CR	555	0	618	26	0
19	AS	661	0	675	33	0
19	CS	646	0	644	41	0
20	AT	728	0	798	27	0
20	CT	731	0	807	28	0
21	AU	199	0	208	8	0
21	CU	199	0	208	9	0
22	AV	277	0	140	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	CV	252	0	130	6	0
23	AW	1599	0	830	42	0
23	CW	1552	0	794	53	0
24	AX	1635	0	839	23	0
24	CX	1635	0	839	36	0
25	AY	1581	0	805	85	0
25	CY	1561	0	796	94	0
26	BA	60729	0	30622	668	0
26	DA	60311	0	30412	887	0
27	BB	2573	0	1306	21	0
27	DB	2573	0	1306	79	0
28	BD	2136	0	2218	43	0
28	DD	2142	0	2229	60	0
29	BE	1559	0	1618	26	0
29	DE	1559	0	1618	41	0
30	BF	1584	0	1625	42	0
30	DF	1580	0	1619	63	0
31	BG	1425	0	1443	39	0
31	DG	1424	0	1434	93	0
32	BH	1330	0	1407	34	0
32	DH	1330	0	1407	44	0
33	BI	1085	0	1114	38	0
33	DI	1073	0	1106	22	0
34	BN	1117	0	1184	26	0
34	DN	1117	0	1184	27	0
35	BO	933	0	996	25	0
35	DO	933	0	996	32	0
36	BP	1139	0	1223	42	0
36	DP	1135	0	1212	54	0
37	BQ	1122	0	1179	30	0
37	DQ	1122	0	1179	41	0
38	BR	968	0	1033	22	0
38	DR	968	0	1033	30	0
39	BS	877	0	938	20	0
39	DS	870	0	923	35	0
40	BT	1091	0	1151	28	0
40	DT	1083	0	1136	39	0
41	BU	959	0	1019	18	0
41	DU	959	0	1018	30	0
42	BV	771	0	830	14	0
42	DV	771	0	830	25	0
43	BW	886	0	940	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DW	886	0	940	13	0
44	BX	750	0	814	15	0
44	DX	750	0	814	28	0
45	BY	806	0	881	28	0
45	DY	806	0	881	30	0
46	BZ	1349	0	1355	45	0
46	DZ	1360	0	1363	74	0
47	B0	653	0	674	14	0
47	D0	653	0	674	22	0
48	B1	755	0	826	17	0
48	D1	755	0	826	18	0
49	B2	588	0	643	13	0
49	D2	588	0	643	15	0
50	B3	469	0	518	6	0
50	D3	464	0	514	13	0
51	B4	558	0	544	39	0
51	D4	532	0	503	30	0
52	B5	455	0	465	15	0
52	D5	455	0	465	13	0
53	B6	453	0	473	12	0
53	D6	449	0	469	12	0
54	B7	418	0	467	10	0
54	D7	418	0	467	13	0
55	B8	517	0	582	17	0
55	D8	517	0	582	16	0
56	B9	307	0	335	7	0
56	D9	307	0	335	11	0
57	AA	216	0	0	0	0
57	AB	1	0	0	0	0
57	AE	1	0	0	0	0
57	AF	1	0	0	0	0
57	AK	1	0	0	0	0
57	AL	2	0	0	0	0
57	AM	2	0	0	0	0
57	AN	2	0	0	0	0
57	AT	1	0	0	0	0
57	AU	1	0	0	0	0
57	AW	2	0	0	0	0
57	AX	15	0	0	0	0
57	AY	3	0	0	0	0
57	B0	2	0	0	0	0
57	B2	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	B4	1	0	0	0	0
57	B5	3	0	0	0	0
57	B6	2	0	0	0	0
57	B7	5	0	0	0	0
57	B8	2	0	0	0	0
57	B9	1	0	0	0	0
57	BA	814	0	0	0	0
57	BB	23	0	0	0	0
57	BD	10	0	0	0	0
57	BE	6	0	0	0	0
57	BF	11	0	0	0	0
57	BG	2	0	0	0	0
57	BH	1	0	0	0	0
57	BN	3	0	0	0	0
57	BO	1	0	0	0	0
57	BP	2	0	0	0	0
57	BQ	2	0	0	0	0
57	BR	2	0	0	0	0
57	BU	4	0	0	0	0
57	BV	5	0	0	0	0
57	BW	4	0	0	0	0
57	BX	1	0	0	0	0
57	BY	1	0	0	0	0
57	BZ	2	0	0	0	0
57	CA	169	0	0	0	0
57	CD	1	0	0	0	0
57	CE	2	0	0	0	0
57	CF	1	0	0	0	0
57	CJ	1	0	0	0	0
57	CK	1	0	0	0	0
57	CT	1	0	0	0	0
57	CW	1	0	0	0	0
57	CX	2	0	0	0	0
57	D0	1	0	0	0	0
57	D3	1	0	0	0	0
57	D8	1	0	0	0	0
57	DA	664	0	0	0	0
57	DB	13	0	0	0	0
57	DD	4	0	0	0	0
57	DE	7	0	0	0	0
57	DF	5	0	0	0	0
57	DG	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	DN	1	0	0	0	0
57	DO	2	0	0	0	0
57	DP	2	0	0	0	0
57	DQ	3	0	0	0	0
57	DR	1	0	0	0	0
57	DU	1	0	0	0	0
57	DV	1	0	0	0	0
57	DW	1	0	0	0	0
57	DY	1	0	0	0	0
58	AD	8	0	0	1	0
58	CD	8	0	0	1	0
59	AN	1	0	0	0	0
59	B4	1	0	0	0	0
59	B5	1	0	0	0	0
59	B6	1	0	0	0	0
59	B9	1	0	0	0	0
59	BY	1	0	0	0	0
59	CN	1	0	0	0	0
59	D4	1	0	0	0	0
59	D5	1	0	0	0	0
59	D6	1	0	0	0	0
59	D9	1	0	0	0	0
59	DY	1	0	0	0	0
60	AX	1	0	0	0	0
61	AA	210	0	0	13	0
61	AD	1	0	0	0	0
61	AE	2	0	0	0	0
61	AJ	1	0	0	0	0
61	AL	2	0	0	1	0
61	AM	2	0	0	0	0
61	AV	2	0	0	0	0
61	AW	4	0	0	0	0
61	AX	4	0	0	0	0
61	AY	1	0	0	0	0
61	B0	6	0	0	0	0
61	B1	2	0	0	0	0
61	B3	2	0	0	0	0
61	B5	4	0	0	0	0
61	B6	2	0	0	0	0
61	B7	3	0	0	2	0
61	B8	13	0	0	0	0
61	B9	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	BA	1406	0	0	56	0
61	BB	37	0	0	1	0
61	BD	15	0	0	2	0
61	BE	17	0	0	4	0
61	BF	11	0	0	0	0
61	BG	3	0	0	0	0
61	BH	1	0	0	0	0
61	BI	1	0	0	0	0
61	BN	1	0	0	0	0
61	BO	2	0	0	0	0
61	BP	13	0	0	1	0
61	BQ	4	0	0	0	0
61	BR	2	0	0	0	0
61	BS	2	0	0	0	0
61	BT	2	0	0	0	0
61	BU	4	0	0	0	0
61	BV	2	0	0	0	0
61	BW	3	0	0	1	0
61	BX	3	0	0	0	0
61	BZ	1	0	0	0	0
61	CA	156	0	0	11	0
61	CE	2	0	0	0	0
61	CH	1	0	0	0	0
61	CJ	1	0	0	0	0
61	CK	1	0	0	0	0
61	CL	1	0	0	1	0
61	CT	1	0	0	0	0
61	CW	2	0	0	2	0
61	CX	2	0	0	0	0
61	CY	1	0	0	0	0
61	D0	4	0	0	0	0
61	D1	1	0	0	0	0
61	D3	2	0	0	0	0
61	D5	1	0	0	0	0
61	D6	1	0	0	0	0
61	D8	3	0	0	0	0
61	DA	989	0	0	44	0
61	DB	9	0	0	0	0
61	DD	18	0	0	3	0
61	DE	5	0	0	0	0
61	DF	4	0	0	0	0
61	DN	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	DP	12	0	0	4	0
61	DQ	1	0	0	0	0
61	DT	4	0	0	0	0
61	DU	1	0	0	0	0
61	DV	1	0	0	0	0
61	DW	1	0	0	0	0
61	DX	2	0	0	0	0
61	DY	1	0	0	0	0
All	All	297127	0	196404	5613	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 12.

The worst 5 of 5613 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)
26:DA:2139:C:N4	26:DA:2152:G:H1	1.46	1.14
1:CA:999:C:N4	1:CA:1042:G:H1	1.48	1.12
25:AY:49:C:N4	25:AY:65:G:H1	1.51	1.09
1:CA:985:C:N4	1:CA:1220:G:H1	1.50	1.09
1:CA:998:G:H1	1:CA:1043:C:N4	1.51	1.09

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	
2	AB	229/256 (90%)	208 (91%)	13 (6%)	8 (4%)	3	4
2	CB	229/256 (90%)	208 (91%)	14 (6%)	7 (3%)	3	5
3	AC	204/239 (85%)	193 (95%)	10 (5%)	1 (0%)	24	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	CC	204/239 (85%)	191 (94%)	13 (6%)	0	100	100
4	AD	206/209 (99%)	197 (96%)	9 (4%)	0	100	100
4	CD	206/209 (99%)	200 (97%)	5 (2%)	1 (0%)	24	46
5	AE	146/162 (90%)	142 (97%)	4 (3%)	0	100	100
5	CE	146/162 (90%)	142 (97%)	3 (2%)	1 (1%)	18	38
6	AF	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
6	CF	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
7	AG	153/156 (98%)	149 (97%)	3 (2%)	1 (1%)	18	38
7	CG	153/156 (98%)	149 (97%)	3 (2%)	1 (1%)	18	38
8	AH	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
8	CH	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
9	AI	125/128 (98%)	119 (95%)	5 (4%)	1 (1%)	16	34
9	CI	125/128 (98%)	120 (96%)	4 (3%)	1 (1%)	16	34
10	AJ	95/105 (90%)	85 (90%)	8 (8%)	2 (2%)	5	11
10	CJ	94/105 (90%)	84 (89%)	6 (6%)	4 (4%)	2	2
11	AK	112/129 (87%)	107 (96%)	4 (4%)	1 (1%)	14	30
11	CK	112/129 (87%)	107 (96%)	4 (4%)	1 (1%)	14	30
12	AL	120/132 (91%)	118 (98%)	2 (2%)	0	100	100
12	CL	120/132 (91%)	117 (98%)	2 (2%)	1 (1%)	16	34
13	AM	121/126 (96%)	116 (96%)	4 (3%)	1 (1%)	16	34
13	CM	120/126 (95%)	113 (94%)	4 (3%)	3 (2%)	4	8
14	AN	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
14	CN	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
15	AO	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
15	CO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	AP	80/88 (91%)	78 (98%)	2 (2%)	0	100	100
16	CP	80/88 (91%)	78 (98%)	1 (1%)	1 (1%)	9	21
17	AQ	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
17	CQ	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
18	AR	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
18	CR	66/88 (75%)	64 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	AS	82/93 (88%)	76 (93%)	5 (6%)	1 (1%)	10	23
19	CS	81/93 (87%)	75 (93%)	6 (7%)	0	100	100
20	AT	94/106 (89%)	85 (90%)	4 (4%)	5 (5%)	1	1
20	CT	94/106 (89%)	85 (90%)	4 (4%)	5 (5%)	1	1
21	AU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
21	CU	21/27 (78%)	21 (100%)	0	0	100	100
28	BD	273/276 (99%)	263 (96%)	9 (3%)	1 (0%)	30	51
28	DD	273/276 (99%)	261 (96%)	10 (4%)	2 (1%)	18	38
29	BE	202/206 (98%)	196 (97%)	5 (2%)	1 (0%)	24	46
29	DE	202/206 (98%)	196 (97%)	5 (2%)	1 (0%)	24	46
30	BF	201/210 (96%)	197 (98%)	3 (2%)	1 (0%)	24	46
30	DF	201/210 (96%)	197 (98%)	3 (2%)	1 (0%)	24	46
31	BG	179/182 (98%)	171 (96%)	7 (4%)	1 (1%)	21	42
31	DG	179/182 (98%)	168 (94%)	8 (4%)	3 (2%)	7	15
32	BH	172/180 (96%)	166 (96%)	6 (4%)	0	100	100
32	DH	172/180 (96%)	166 (96%)	6 (4%)	0	100	100
33	BI	144/148 (97%)	132 (92%)	7 (5%)	5 (4%)	3	4
33	DI	144/148 (97%)	135 (94%)	8 (6%)	1 (1%)	18	38
34	BN	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
34	DN	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
35	BO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
35	DO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
36	BP	147/150 (98%)	142 (97%)	4 (3%)	1 (1%)	18	38
36	DP	147/150 (98%)	139 (95%)	6 (4%)	2 (1%)	9	19
37	BQ	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
37	DQ	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	18	38
38	BR	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
38	DR	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
39	BS	108/112 (96%)	106 (98%)	2 (2%)	0	100	100
39	DS	108/112 (96%)	107 (99%)	0	1 (1%)	14	30
40	BT	129/146 (88%)	123 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	DT	129/146 (88%)	126 (98%)	3 (2%)	0	100	100
41	BU	114/118 (97%)	114 (100%)	0	0	100	100
41	DU	114/118 (97%)	114 (100%)	0	0	100	100
42	BV	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	12	28
42	DV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	12	28
43	BW	110/113 (97%)	110 (100%)	0	0	100	100
43	DW	110/113 (97%)	110 (100%)	0	0	100	100
44	BX	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
44	DX	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	11	25
45	BY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
45	DY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
46	BZ	169/206 (82%)	153 (90%)	15 (9%)	1 (1%)	21	42
46	DZ	172/206 (84%)	159 (92%)	13 (8%)	0	100	100
47	B0	81/85 (95%)	81 (100%)	0	0	100	100
47	D0	81/85 (95%)	79 (98%)	1 (1%)	1 (1%)	10	23
48	B1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	25
48	D1	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11	25
49	B2	68/72 (94%)	68 (100%)	0	0	100	100
49	D2	68/72 (94%)	68 (100%)	0	0	100	100
50	B3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
50	D3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
51	B4	67/71 (94%)	54 (81%)	9 (13%)	4 (6%)	1	1
51	D4	67/71 (94%)	53 (79%)	11 (16%)	3 (4%)	2	2
52	B5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
52	D5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
53	B6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
53	D6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
54	B7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
54	D7	46/49 (94%)	45 (98%)	0	1 (2%)	5	10
55	B8	62/65 (95%)	62 (100%)	0	0	100	100
55	D8	62/65 (95%)	62 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	B9	35/37 (95%)	35 (100%)	0	0	100	100
56	D9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11410/12128 (94%)	10945 (96%)	381 (3%)	84 (1%)	18	38

5 of 84 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	17	PHE
2	AB	19	HIS
2	AB	231	GLU
9	AI	54	ASP
10	AJ	56	HIS

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	
2	AB	192/220 (87%)	153 (80%)	39 (20%)	1	2
2	CB	187/220 (85%)	151 (81%)	36 (19%)	1	2
3	AC	143/188 (76%)	126 (88%)	17 (12%)	5	10
3	CC	141/188 (75%)	116 (82%)	25 (18%)	2	3
4	AD	170/181 (94%)	147 (86%)	23 (14%)	4	7
4	CD	174/181 (96%)	146 (84%)	28 (16%)	2	4
5	AE	113/123 (92%)	99 (88%)	14 (12%)	4	9
5	CE	114/123 (93%)	98 (86%)	16 (14%)	3	6
6	AF	84/90 (93%)	74 (88%)	10 (12%)	5	10
6	CF	86/90 (96%)	71 (83%)	15 (17%)	2	3
7	AG	119/127 (94%)	97 (82%)	22 (18%)	1	3
7	CG	120/127 (94%)	103 (86%)	17 (14%)	3	6
8	AH	114/119 (96%)	100 (88%)	14 (12%)	4	9
8	CH	114/119 (96%)	92 (81%)	22 (19%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	AI	91/99 (92%)	69 (76%)	22 (24%)	1	1
9	CI	89/99 (90%)	69 (78%)	20 (22%)	1	1
10	AJ	66/92 (72%)	58 (88%)	8 (12%)	5	10
10	CJ	69/92 (75%)	59 (86%)	10 (14%)	3	6
11	AK	83/99 (84%)	74 (89%)	9 (11%)	6	13
11	CK	83/99 (84%)	71 (86%)	12 (14%)	3	6
12	AL	97/109 (89%)	88 (91%)	9 (9%)	8	18
12	CL	97/109 (89%)	84 (87%)	13 (13%)	4	7
13	AM	95/101 (94%)	78 (82%)	17 (18%)	2	3
13	CM	92/101 (91%)	75 (82%)	17 (18%)	1	3
14	AN	49/50 (98%)	40 (82%)	9 (18%)	1	3
14	CN	49/50 (98%)	37 (76%)	12 (24%)	1	1
15	AO	78/80 (98%)	69 (88%)	9 (12%)	5	11
15	CO	78/80 (98%)	67 (86%)	11 (14%)	3	6
16	AP	69/74 (93%)	54 (78%)	15 (22%)	1	2
16	CP	68/74 (92%)	60 (88%)	8 (12%)	5	10
17	AQ	94/97 (97%)	84 (89%)	10 (11%)	6	14
17	CQ	94/97 (97%)	83 (88%)	11 (12%)	5	11
18	AR	59/77 (77%)	49 (83%)	10 (17%)	2	4
18	CR	59/77 (77%)	45 (76%)	14 (24%)	1	1
19	AS	70/80 (88%)	58 (83%)	12 (17%)	2	3
19	CS	67/80 (84%)	53 (79%)	14 (21%)	1	2
20	AT	70/82 (85%)	57 (81%)	13 (19%)	1	3
20	CT	71/82 (87%)	58 (82%)	13 (18%)	2	3
21	AU	18/22 (82%)	13 (72%)	5 (28%)	0	1
21	CU	18/22 (82%)	15 (83%)	3 (17%)	2	4
28	BD	215/218 (99%)	193 (90%)	22 (10%)	7	15
28	DD	216/218 (99%)	195 (90%)	21 (10%)	8	17
29	BE	164/166 (99%)	141 (86%)	23 (14%)	3	6
29	DE	164/166 (99%)	137 (84%)	27 (16%)	2	4
30	BF	160/166 (96%)	141 (88%)	19 (12%)	5	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	DF	159/166 (96%)	139 (87%)	20 (13%)	4	9
31	BG	143/156 (92%)	126 (88%)	17 (12%)	5	10
31	DG	142/156 (91%)	112 (79%)	30 (21%)	1	2
32	BH	144/148 (97%)	128 (89%)	16 (11%)	6	12
32	DH	144/148 (97%)	122 (85%)	22 (15%)	3	5
33	BI	110/124 (89%)	85 (77%)	25 (23%)	1	1
33	DI	107/124 (86%)	79 (74%)	28 (26%)	0	1
34	BN	118/119 (99%)	97 (82%)	21 (18%)	2	3
34	DN	118/119 (99%)	99 (84%)	19 (16%)	2	4
35	BO	100/100 (100%)	91 (91%)	9 (9%)	9	20
35	DO	100/100 (100%)	86 (86%)	14 (14%)	3	6
36	BP	116/116 (100%)	100 (86%)	16 (14%)	3	7
36	DP	115/116 (99%)	101 (88%)	14 (12%)	5	10
37	BQ	111/111 (100%)	95 (86%)	16 (14%)	3	6
37	DQ	111/111 (100%)	95 (86%)	16 (14%)	3	6
38	BR	101/101 (100%)	83 (82%)	18 (18%)	2	3
38	DR	101/101 (100%)	86 (85%)	15 (15%)	3	5
39	BS	87/88 (99%)	75 (86%)	12 (14%)	3	7
39	DS	85/88 (97%)	66 (78%)	19 (22%)	1	1
40	BT	115/127 (91%)	101 (88%)	14 (12%)	5	10
40	DT	113/127 (89%)	100 (88%)	13 (12%)	5	11
41	BU	93/94 (99%)	83 (89%)	10 (11%)	6	13
41	DU	93/94 (99%)	84 (90%)	9 (10%)	8	17
42	BV	80/82 (98%)	68 (85%)	12 (15%)	3	5
42	DV	80/82 (98%)	67 (84%)	13 (16%)	2	4
43	BW	90/92 (98%)	80 (89%)	10 (11%)	6	12
43	DW	90/92 (98%)	82 (91%)	8 (9%)	9	20
44	BX	77/78 (99%)	70 (91%)	7 (9%)	9	19
44	DX	77/78 (99%)	70 (91%)	7 (9%)	9	19
45	BY	85/91 (93%)	75 (88%)	10 (12%)	5	10
45	DY	85/91 (93%)	80 (94%)	5 (6%)	18	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	BZ	145/179 (81%)	121 (83%)	24 (17%)	2	4
46	DZ	145/179 (81%)	123 (85%)	22 (15%)	3	5
47	B0	65/67 (97%)	61 (94%)	4 (6%)	16	36
47	D0	65/67 (97%)	61 (94%)	4 (6%)	16	36
48	B1	80/83 (96%)	75 (94%)	5 (6%)	16	36
48	D1	80/83 (96%)	71 (89%)	9 (11%)	5	12
49	B2	65/67 (97%)	59 (91%)	6 (9%)	8	19
49	D2	65/67 (97%)	60 (92%)	5 (8%)	12	27
50	B3	51/52 (98%)	46 (90%)	5 (10%)	7	17
50	D3	50/52 (96%)	44 (88%)	6 (12%)	5	10
51	B4	60/63 (95%)	50 (83%)	10 (17%)	2	4
51	D4	53/63 (84%)	38 (72%)	15 (28%)	0	1
52	B5	50/52 (96%)	47 (94%)	3 (6%)	17	37
52	D5	50/52 (96%)	48 (96%)	2 (4%)	28	55
53	B6	51/52 (98%)	44 (86%)	7 (14%)	3	7
53	D6	50/52 (96%)	46 (92%)	4 (8%)	11	25
54	B7	41/42 (98%)	37 (90%)	4 (10%)	7	17
54	D7	41/42 (98%)	37 (90%)	4 (10%)	7	17
55	B8	54/55 (98%)	51 (94%)	3 (6%)	19	40
55	D8	54/55 (98%)	50 (93%)	4 (7%)	13	29
56	B9	34/34 (100%)	32 (94%)	2 (6%)	18	38
56	D9	34/34 (100%)	31 (91%)	3 (9%)	9	21
All	All	9336/10066 (93%)	8004 (86%)	1332 (14%)	3	6

5 of 1332 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	CS	15	LEU
36	DP	136	GLU
21	CU	12	LYS
19	CS	7	LYS
31	DG	111	LEU

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

Mol	Chain	Res	Type
10	CJ	68	HIS
39	DS	68	GLN
13	CM	62	ASN
28	DD	253	GLN
46	DZ	75	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1494/1521 (98%)	361 (24%)	19 (1%)
1	CA	1501/1521 (98%)	371 (24%)	25 (1%)
22	AV	12/24 (50%)	3 (25%)	0
22	CV	11/24 (45%)	3 (27%)	0
23	AW	71/76 (93%)	27 (38%)	2 (2%)
23	CW	68/76 (89%)	26 (38%)	3 (4%)
24	AX	74/77 (96%)	16 (21%)	0
24	CX	74/77 (96%)	23 (31%)	0
25	AY	72/76 (94%)	38 (52%)	3 (4%)
25	CY	70/76 (92%)	37 (52%)	1 (1%)
26	BA	2812/2915 (96%)	449 (15%)	36 (1%)
26	DA	2791/2915 (95%)	564 (20%)	24 (0%)
27	BB	119/121 (98%)	13 (10%)	0
27	DB	119/121 (98%)	38 (31%)	0
All	All	9288/9620 (96%)	1969 (21%)	113 (1%)

5 of 1969 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	7	G
1	AA	9	G
1	AA	22	G
1	AA	29	G

5 of 113 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	BA	2689	U
26	DA	2422	A
1	CA	991	U
26	DA	2318	G
26	DA	1300	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
23	7MG	AW	46	23	23,26,27	1.38	4 (17%)	27,39,42	2.51	6 (22%)
23	PSU	CW	55	23	18,21,22	1.32	2 (11%)	21,30,33	2.11	4 (19%)
23	MIA	CW	37	23	21,24,32	1.60	4 (19%)	30,35,47	2.04	7 (23%)
24	31H	CX	76	57,24	31,34,35	1.35	5 (16%)	35,47,50	2.32	11 (31%)
23	MIA	AW	37	23	28,31,32	2.32	6 (21%)	38,44,47	2.67	12 (31%)
25	5MU	AY	54	25	19,22,23	1.57	6 (31%)	27,32,35	2.03	6 (22%)
25	PSU	CY	55	25	18,21,22	1.34	2 (11%)	21,30,33	2.01	4 (19%)
24	4SU	AX	8	24	18,21,22	2.26	5 (27%)	25,30,33	1.60	4 (16%)
25	4SU	CY	8	25	18,21,22	1.89	4 (22%)	25,30,33	2.48	5 (20%)
25	7MG	AY	46	25	23,26,27	1.26	2 (8%)	27,39,42	3.06	9 (33%)
24	5MU	AX	54	57,24	19,22,23	1.38	5 (26%)	27,32,35	2.05	6 (22%)
24	5MC	AX	32	24	19,22,23	1.66	3 (15%)	26,32,35	1.23	4 (15%)
25	PSU	AY	55	25	18,21,22	1.32	2 (11%)	21,30,33	2.11	5 (23%)
25	PSU	CY	39	25	18,21,22	1.55	5 (27%)	21,30,33	2.65	4 (19%)
23	F3N	CW	76	23	33,36,37	1.49	5 (15%)	41,51,54	1.73	9 (21%)
25	MIA	AY	37	25	21,24,32	1.63	4 (19%)	30,35,47	2.00	7 (23%)
24	31H	AX	76	57,24	31,34,35	1.40	5 (16%)	35,47,50	2.00	11 (31%)
23	F3N	AW	76	23	33,36,37	1.50	4 (12%)	41,51,54	1.70	8 (19%)
23	4SU	CW	8	23	18,21,22	1.73	4 (22%)	25,30,33	2.40	5 (20%)
23	PSU	CW	32	23	18,21,22	1.32	2 (11%)	21,30,33	1.99	4 (19%)
25	5MU	CY	54	25	19,22,23	1.35	4 (21%)	27,32,35	2.27	6 (22%)
25	PSU	AY	39	25	18,21,22	1.43	2 (11%)	21,30,33	1.83	4 (19%)
23	PSU	AW	55	23	18,21,22	1.43	2 (11%)	21,30,33	2.03	3 (14%)
23	PSU	CW	39	23	18,21,22	1.39	2 (11%)	21,30,33	1.70	3 (14%)
24	PSU	CX	55	24	18,21,22	1.37	2 (11%)	21,30,33	2.02	4 (19%)
25	7MG	CY	46	25	23,26,27	1.42	4 (17%)	27,39,42	2.65	9 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	4SU	AW	8	23	18,21,22	1.87	4 (22%)	25,30,33	2.06	5 (20%)
25	PSU	AY	32	25	18,21,22	1.39	2 (11%)	21,30,33	1.93	4 (19%)
25	PSU	CY	32	25	18,21,22	1.37	2 (11%)	21,30,33	1.96	4 (19%)
23	PSU	AW	39	23	18,21,22	1.37	2 (11%)	21,30,33	1.95	3 (14%)
24	PSU	AX	55	24	18,21,22	1.35	2 (11%)	21,30,33	2.11	4 (19%)
25	MIA	CY	37	25	21,24,32	1.66	4 (19%)	30,35,47	2.03	8 (26%)
24	5MC	CX	32	24	19,22,23	1.55	3 (15%)	26,32,35	1.23	4 (15%)
25	4SU	AY	8	25	18,21,22	1.76	3 (16%)	25,30,33	2.33	6 (24%)
23	5MU	AW	54	23	19,22,23	1.41	4 (21%)	27,32,35	1.90	5 (18%)
23	7MG	CW	46	23	23,26,27	1.36	4 (17%)	27,39,42	2.59	9 (33%)
23	PSU	AW	32	23,57	18,21,22	1.33	2 (11%)	21,30,33	2.04	3 (14%)
24	4SU	CX	8	24	18,21,22	2.00	6 (33%)	25,30,33	1.36	3 (12%)
24	5MU	CX	54	24	19,22,23	1.37	5 (26%)	27,32,35	2.17	6 (22%)
23	5MU	CW	54	23	19,22,23	1.41	5 (26%)	27,32,35	1.82	7 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	7MG	AW	46	23	-	4/7/37/38	0/3/3/3
23	PSU	CW	55	23	-	0/7/25/26	0/2/2/2
23	MIA	CW	37	23	-	0/7/25/34	0/3/3/3
24	31H	CX	76	57,24	-	12/22/40/41	0/3/3/3
23	MIA	AW	37	23	-	1/15/33/34	0/3/3/3
25	5MU	AY	54	25	-	4/7/25/26	0/2/2/2
25	PSU	CY	55	25	-	3/7/25/26	0/2/2/2
24	4SU	AX	8	24	-	0/7/25/26	0/2/2/2
25	4SU	CY	8	25	-	1/7/25/26	0/2/2/2
25	7MG	AY	46	25	-	4/7/37/38	0/3/3/3
24	5MU	AX	54	57,24	-	0/7/25/26	0/2/2/2
24	5MC	AX	32	24	-	0/7/25/26	0/2/2/2
25	PSU	AY	55	25	-	1/7/25/26	0/2/2/2
25	PSU	CY	39	25	-	1/7/25/26	0/2/2/2
23	F3N	CW	76	23	-	5/19/37/38	0/4/4/4
25	MIA	AY	37	25	-	3/7/25/34	0/3/3/3
24	31H	AX	76	57,24	-	7/22/40/41	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	F3N	AW	76	23	-	0/19/37/38	0/4/4/4
23	4SU	CW	8	23	-	0/7/25/26	0/2/2/2
23	PSU	CW	32	23	-	0/7/25/26	0/2/2/2
25	5MU	CY	54	25	-	2/7/25/26	0/2/2/2
25	PSU	AY	39	25	-	2/7/25/26	0/2/2/2
23	PSU	AW	55	23	-	0/7/25/26	0/2/2/2
23	PSU	CW	39	23	-	0/7/25/26	0/2/2/2
24	PSU	CX	55	24	-	0/7/25/26	0/2/2/2
25	7MG	CY	46	25	-	2/7/37/38	0/3/3/3
23	4SU	AW	8	23	-	0/7/25/26	0/2/2/2
25	PSU	AY	32	25	-	2/7/25/26	0/2/2/2
25	PSU	CY	32	25	-	2/7/25/26	0/2/2/2
23	PSU	AW	39	23	-	0/7/25/26	0/2/2/2
24	PSU	AX	55	24	-	0/7/25/26	0/2/2/2
25	MIA	CY	37	25	-	3/7/25/34	0/3/3/3
24	5MC	CX	32	24	-	0/7/25/26	0/2/2/2
25	4SU	AY	8	25	-	0/7/25/26	0/2/2/2
23	5MU	AW	54	23	-	0/7/25/26	0/2/2/2
23	7MG	CW	46	23	-	3/7/37/38	0/3/3/3
23	PSU	AW	32	23,57	-	0/7/25/26	0/2/2/2
24	4SU	CX	8	24	-	0/7/25/26	0/2/2/2
24	5MU	CX	54	24	-	0/7/25/26	0/2/2/2
23	5MU	CW	54	23	-	0/7/25/26	0/2/2/2

The worst 5 of 143 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	37	MIA	C13-C14	7.04	1.53	1.32
23	AW	37	MIA	C2-S10	-6.41	1.70	1.75
24	AX	32	5MC	C5-C4	6.00	1.48	1.44
24	AX	8	4SU	C4-N3	-5.40	1.32	1.37
24	CX	32	5MC	C5-C4	5.37	1.48	1.44

The worst 5 of 231 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	AY	46	7MG	N9-C4-N3	10.89	141.42	125.46
23	AW	46	7MG	N9-C4-N3	8.54	137.97	125.46
25	CY	39	PSU	N1-C2-N3	8.34	123.97	115.17
25	CY	46	7MG	N9-C4-N3	8.33	137.66	125.46
23	AW	37	MIA	C5-C4-N3	-8.22	118.53	127.18

There are no chirality outliers.

5 of 62 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	AW	37	MIA	C12-C13-C14-C16
24	AX	76	31H	OCN-CN-N-CA
25	AY	32	PSU	O4'-C4'-C5'-O5'
25	AY	46	7MG	C4'-C5'-O5'-P
24	CX	76	31H	C4'-C5'-O5'-P

There are no ring outliers.

27 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	CW	55	PSU	1	0
24	CX	76	31H	1	0
25	AY	54	5MU	1	0
25	CY	55	PSU	2	0
24	AX	8	4SU	1	0
25	CY	8	4SU	2	0
25	AY	46	7MG	3	0
25	AY	55	PSU	2	0
25	CY	39	PSU	8	0
23	CW	76	F3N	3	0
25	AY	37	MIA	1	0
24	AX	76	31H	1	0
23	AW	76	F3N	1	0
23	CW	8	4SU	2	0
23	CW	32	PSU	1	0
25	AY	39	PSU	2	0
23	AW	55	PSU	1	0
23	CW	39	PSU	1	0
24	CX	55	PSU	1	0
25	CY	46	7MG	4	0
23	AW	39	PSU	1	0
24	AX	55	PSU	1	0
25	CY	37	MIA	3	0
24	CX	32	5MC	1	0
25	AY	8	4SU	1	0
23	CW	46	7MG	2	0
24	CX	8	4SU	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2063 ligands modelled in this entry, 2061 are monoatomic - leaving 2 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	$\# Z > 2$
58	SF4	AD	501	4	0,12,12	-	-	-		
58	SF4	CD	501	4	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
58	SF4	AD	501	4	-	-	0/6/5/5
58	SF4	CD	501	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	AD	501	SF4	1	0
58	CD	501	SF4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	AA	1497/1521 (98%)	0.49	47 (3%)	51	45	41, 72, 93, 106	0
1	CA	1503/1521 (98%)	0.74	152 (10%)	12	9	43, 75, 94, 106	0
2	AB	231/256 (90%)	1.33	43 (18%)	3	3	68, 82, 89, 95	0
2	CB	231/256 (90%)	1.55	57 (24%)	2	1	68, 83, 90, 96	0
3	AC	206/239 (86%)	1.10	20 (9%)	13	10	69, 79, 87, 94	0
3	CC	206/239 (86%)	1.86	84 (40%)	0	0	70, 82, 90, 94	0
4	AD	208/209 (99%)	1.05	24 (11%)	9	7	57, 72, 81, 87	0
4	CD	208/209 (99%)	1.05	18 (8%)	16	12	60, 72, 81, 89	0
5	AE	148/162 (91%)	1.05	16 (10%)	11	8	58, 71, 81, 85	0
5	CE	148/162 (91%)	1.28	14 (9%)	14	10	60, 74, 83, 86	0
6	AF	100/101 (99%)	0.61	0	100	100	52, 67, 75, 85	0
6	CF	100/101 (99%)	0.95	4 (4%)	42	37	57, 71, 81, 85	0
7	AG	155/156 (99%)	1.15	24 (15%)	5	4	66, 76, 85, 96	0
7	CG	155/156 (99%)	1.27	22 (14%)	6	5	68, 77, 86, 97	0
8	AH	137/138 (99%)	0.97	15 (10%)	10	8	62, 72, 79, 83	0
8	CH	137/138 (99%)	1.23	19 (13%)	6	5	64, 74, 80, 85	0
9	AI	127/128 (99%)	1.38	27 (21%)	2	2	62, 80, 87, 89	0
9	CI	127/128 (99%)	2.32	74 (58%)	0	0	69, 82, 89, 91	0
10	AJ	97/105 (92%)	1.68	35 (36%)	1	0	66, 83, 91, 92	0
10	CJ	96/105 (91%)	1.74	36 (37%)	1	0	68, 84, 91, 93	0
11	AK	114/129 (88%)	0.89	6 (5%)	32	26	51, 70, 80, 84	0
11	CK	114/129 (88%)	1.09	10 (8%)	15	12	52, 72, 81, 85	0
12	AL	122/132 (92%)	0.54	8 (6%)	24	19	41, 56, 71, 75	0
12	CL	122/132 (92%)	1.40	35 (28%)	1	1	58, 73, 82, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
13	AM	123/126 (97%)	0.83	10 (8%)	18	14	57, 72, 83, 88	0
13	CM	122/126 (96%)	1.95	52 (42%)	0	0	69, 85, 92, 97	0
14	AN	60/61 (98%)	1.06	4 (6%)	24	19	70, 76, 83, 84	0
14	CN	60/61 (98%)	2.59	40 (66%)	0	0	73, 79, 85, 87	0
15	AO	88/89 (98%)	0.73	4 (4%)	38	32	54, 68, 79, 83	0
15	CO	88/89 (98%)	0.78	3 (3%)	48	42	56, 70, 81, 84	0
16	AP	82/88 (93%)	1.30	15 (18%)	3	3	59, 71, 79, 84	0
16	CP	82/88 (93%)	1.07	7 (8%)	16	13	59, 70, 79, 83	0
17	AQ	99/105 (94%)	0.69	3 (3%)	52	47	57, 70, 79, 84	0
17	CQ	99/105 (94%)	1.06	9 (9%)	15	11	60, 71, 79, 84	0
18	AR	68/88 (77%)	0.79	3 (4%)	39	33	59, 69, 81, 84	0
18	CR	68/88 (77%)	1.06	6 (8%)	15	12	58, 70, 81, 85	0
19	AS	84/93 (90%)	0.86	4 (4%)	35	30	70, 81, 87, 92	0
19	CS	83/93 (89%)	2.30	54 (65%)	0	0	74, 83, 90, 94	0
20	AT	96/106 (90%)	1.33	20 (20%)	2	2	59, 71, 80, 83	0
20	CT	96/106 (90%)	1.00	14 (14%)	6	4	59, 71, 80, 83	0
21	AU	23/27 (85%)	1.24	1 (4%)	40	34	70, 75, 78, 82	0
21	CU	23/27 (85%)	2.28	14 (60%)	0	0	71, 78, 81, 82	0
22	AV	13/24 (54%)	1.34	4 (30%)	1	1	58, 77, 95, 100	0
22	CV	12/24 (50%)	1.97	6 (50%)	0	0	64, 81, 93, 95	0
23	AW	66/76 (86%)	1.50	15 (22%)	2	1	66, 95, 102, 105	0
23	CW	64/76 (84%)	1.82	22 (34%)	1	1	70, 96, 101, 106	0
24	AX	71/77 (92%)	0.69	7 (9%)	13	10	42, 73, 90, 96	0
24	CX	71/77 (92%)	0.84	3 (4%)	40	35	55, 86, 95, 98	0
25	AY	67/76 (88%)	1.37	11 (16%)	4	3	44, 97, 101, 105	0
25	CY	66/76 (86%)	1.71	16 (24%)	2	1	48, 98, 102, 103	0
26	BA	2819/2915 (96%)	-0.25	86 (3%)	51	45	23, 43, 87, 106	0
26	DA	2800/2915 (96%)	-0.19	72 (2%)	57	51	27, 48, 90, 108	0
27	BB	120/121 (99%)	0.39	1 (0%)	82	80	41, 64, 76, 88	0
27	DB	120/121 (99%)	1.16	19 (15%)	5	4	48, 70, 80, 91	0
28	BD	275/276 (99%)	0.12	6 (2%)	62	57	24, 41, 58, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DD	275/276 (99%)	0.04	4 (1%) 72 68	28, 44, 61, 79	0
29	BE	204/206 (99%)	0.13	1 (0%) 87 85	23, 46, 65, 83	0
29	DE	204/206 (99%)	0.22	3 (1%) 72 68	26, 50, 67, 84	0
30	BF	203/210 (96%)	0.33	1 (0%) 87 85	25, 51, 76, 86	0
30	DF	203/210 (96%)	0.37	5 (2%) 58 52	28, 56, 78, 88	0
31	BG	181/182 (99%)	1.18	23 (12%) 8 6	55, 72, 83, 93	0
31	DG	181/182 (99%)	1.69	55 (30%) 1 1	64, 76, 85, 93	0
32	BH	174/180 (96%)	0.90	12 (6%) 23 18	50, 66, 75, 82	0
32	DH	174/180 (96%)	1.20	29 (16%) 4 3	56, 71, 79, 83	0
33	BI	146/148 (98%)	0.82	6 (4%) 41 36	49, 74, 83, 87	0
33	DI	146/148 (98%)	1.14	14 (9%) 13 10	50, 74, 83, 87	0
34	BN	140/140 (100%)	0.41	1 (0%) 84 82	29, 48, 67, 79	0
34	DN	140/140 (100%)	0.59	3 (2%) 63 58	35, 53, 70, 82	0
35	BO	122/122 (100%)	-0.24	1 (0%) 82 80	25, 40, 57, 67	0
35	DO	122/122 (100%)	0.43	1 (0%) 82 80	44, 58, 74, 79	0
36	BP	149/150 (99%)	0.40	4 (2%) 56 50	25, 55, 75, 80	0
36	DP	149/150 (99%)	0.68	4 (2%) 56 50	28, 58, 78, 83	0
37	BQ	141/141 (100%)	0.49	2 (1%) 73 69	37, 52, 68, 77	0
37	DQ	141/141 (100%)	0.79	8 (5%) 29 24	41, 58, 72, 79	0
38	BR	118/118 (100%)	-0.35	0 100 100	22, 34, 50, 59	0
38	DR	118/118 (100%)	0.19	1 (0%) 82 80	38, 53, 64, 75	0
39	BS	110/112 (98%)	0.04	0 100 100	34, 50, 64, 70	0
39	DS	110/112 (98%)	1.68	31 (28%) 1 1	70, 79, 87, 91	0
40	BT	131/146 (89%)	0.31	4 (3%) 51 45	38, 51, 73, 82	0
40	DT	131/146 (89%)	0.30	4 (3%) 51 45	40, 54, 75, 81	0
41	BU	116/118 (98%)	-0.41	0 100 100	17, 30, 50, 63	0
41	DU	116/118 (98%)	0.49	2 (1%) 69 64	40, 59, 79, 85	0
42	BV	101/101 (100%)	-0.38	0 100 100	16, 38, 58, 68	0
42	DV	101/101 (100%)	0.88	7 (6%) 23 18	44, 73, 81, 92	0
43	BW	112/113 (99%)	-0.31	1 (0%) 81 78	22, 30, 49, 83	0
43	DW	112/113 (99%)	0.24	2 (1%) 67 63	35, 50, 66, 86	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BX	95/96 (98%)	0.32	1 (1%) 78 74	31, 46, 67, 83	0
44	DX	95/96 (98%)	0.54	6 (6%) 26 20	36, 50, 68, 83	0
45	BY	107/110 (97%)	0.81	5 (4%) 36 30	42, 58, 73, 84	0
45	DY	107/110 (97%)	0.86	8 (7%) 20 16	47, 61, 75, 84	0
46	BZ	171/206 (83%)	0.80	31 (18%) 3 3	40, 66, 91, 95	0
46	DZ	174/206 (84%)	1.32	30 (17%) 4 3	69, 85, 94, 101	0
47	B0	83/85 (97%)	0.75	7 (8%) 17 13	34, 50, 67, 75	0
47	D0	83/85 (97%)	1.03	10 (12%) 9 7	40, 56, 71, 76	0
48	B1	97/98 (98%)	0.35	4 (4%) 41 36	31, 49, 72, 76	0
48	D1	97/98 (98%)	0.44	2 (2%) 63 58	34, 53, 73, 78	0
49	B2	70/72 (97%)	0.11	2 (2%) 53 48	33, 49, 64, 82	0
49	D2	70/72 (97%)	0.76	1 (1%) 73 69	58, 69, 78, 82	0
50	B3	59/60 (98%)	-0.26	0 100 100	24, 37, 63, 74	0
50	D3	59/60 (98%)	0.45	1 (1%) 69 64	52, 65, 79, 87	0
51	B4	69/71 (97%)	0.96	10 (14%) 6 4	49, 76, 89, 91	0
51	D4	69/71 (97%)	1.73	26 (37%) 1 0	74, 89, 95, 99	0
52	B5	59/60 (98%)	-0.48	1 (1%) 69 64	16, 30, 46, 68	0
52	D5	59/60 (98%)	0.12	1 (1%) 69 64	35, 49, 65, 77	0
53	B6	53/54 (98%)	-0.26	0 100 100	32, 44, 57, 72	0
53	D6	53/54 (98%)	0.64	0 100 100	49, 64, 74, 79	0
54	B7	48/49 (97%)	0.03	5 (10%) 11 9	23, 32, 58, 70	0
54	D7	48/49 (97%)	-0.04	2 (4%) 40 35	26, 35, 61, 70	0
55	B8	64/65 (98%)	0.26	2 (3%) 51 45	34, 42, 50, 65	0
55	D8	64/65 (98%)	0.40	1 (1%) 70 66	37, 46, 54, 65	0
56	B9	37/37 (100%)	0.48	1 (2%) 56 50	36, 51, 65, 73	0
56	D9	37/37 (100%)	0.75	1 (2%) 56 50	43, 55, 68, 76	0
All	All	20895/21748 (96%)	0.51	1708 (8%) 17 14	16, 64, 89, 108	0

The worst 5 of 1708 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	AG	82	GLY	7.8
32	BH	2	SER	7.6

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Mol	Chain	Res	Type	RSRZ
13	CM	124	PRO	7.5
13	CM	102	ARG	7.5
13	CM	123	ALA	6.7

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
25	7MG	CY	46	24/25	0.52	0.17	87,101,108,135	0
23	7MG	AW	46	24/25	0.54	0.16	80,97,112,135	0
25	4SU	CY	8	20/21	0.58	0.15	88,102,112,128	0
23	7MG	CW	46	24/25	0.59	0.15	81,97,101,125	0
25	MIA	CY	37	22/30	0.61	0.16	79,95,102,124	0
25	7MG	AY	46	24/25	0.63	0.16	80,99,107,116	0
25	PSU	CY	55	20/21	0.65	0.21	86,100,107,118	0
25	5MU	CY	54	21/22	0.67	0.20	89,99,105,136	0
23	4SU	CW	8	20/21	0.67	0.14	85,96,117,121	0
25	PSU	CY	39	20/21	0.69	0.15	86,91,104,110	0
25	4SU	AY	8	20/21	0.69	0.14	83,95,104,129	0
23	PSU	CW	55	20/21	0.72	0.13	76,90,103,106	0
23	4SU	AW	8	20/21	0.76	0.14	83,89,107,110	0
24	4SU	CX	8	20/21	0.76	0.15	84,92,105,111	0
23	5MU	CW	54	21/22	0.77	0.13	76,87,97,99	0
25	PSU	AY	55	20/21	0.78	0.12	85,96,106,117	0
25	MIA	AY	37	22/30	0.79	0.13	79,89,101,116	0
25	5MU	AY	54	21/22	0.80	0.12	81,89,99,128	0
25	PSU	CY	32	20/21	0.81	0.12	77,91,109,114	0
23	MIA	CW	37	22/30	0.81	0.14	72,86,92,96	0
25	PSU	AY	32	20/21	0.81	0.14	76,92,107,110	0
25	PSU	AY	39	20/21	0.82	0.13	84,90,102,107	0
23	PSU	CW	39	20/21	0.83	0.13	76,85,92,95	0
23	PSU	AW	55	20/21	0.83	0.10	76,88,103,105	0
24	PSU	CX	55	20/21	0.85	0.10	81,87,92,97	0
23	PSU	AW	32	20/21	0.87	0.16	77,84,98,106	0
24	5MU	CX	54	21/22	0.88	0.11	71,85,94,104	0
23	PSU	CW	32	20/21	0.89	0.15	77,86,95,106	0
24	4SU	AX	8	20/21	0.90	0.11	59,69,79,85	0
24	31H	CX	76	32/33	0.91	0.17	48,68,88,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	5MC	CX	32	21/22	0.91	0.12	63,77,85,87	0
24	5MU	AX	54	21/22	0.91	0.11	46,72,77,86	0
23	5MU	AW	54	21/22	0.91	0.10	66,80,87,93	0
24	PSU	AX	55	20/21	0.92	0.10	52,69,77,77	0
23	F3N	CW	76	33/34	0.92	0.14	53,69,79,80	0
23	PSU	AW	39	20/21	0.93	0.10	71,82,92,93	0
23	MIA	AW	37	29/30	0.93	0.13	56,65,80,82	0
24	31H	AX	76	32/33	0.94	0.14	31,57,76,77	10
23	F3N	AW	76	33/34	0.94	0.14	44,58,72,77	0
24	5MC	AX	32	21/22	0.95	0.12	50,57,69,76	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	3086	1/1	0.39	0.29	93,93,93,93	0
57	MG	DA	3254	1/1	0.52	0.20	68,68,68,68	0
57	MG	DA	3626	1/1	0.57	0.20	81,81,81,81	0
57	MG	AA	1784	1/1	0.60	0.26	72,72,72,72	0
57	MG	DA	3079	1/1	0.60	0.42	72,72,72,72	0
57	MG	DA	3606	1/1	0.62	0.17	74,74,74,74	0
57	MG	AA	1741	1/1	0.63	0.28	86,86,86,86	0
57	MG	DA	3628	1/1	0.63	0.26	77,77,77,77	0
57	MG	CA	3153	1/1	0.64	0.19	69,69,69,69	0
57	MG	CA	3115	1/1	0.64	0.23	82,82,82,82	0
57	MG	AA	1810	1/1	0.65	0.16	86,86,86,86	0
57	MG	BA	3693	1/1	0.65	0.20	77,77,77,77	0
57	MG	CA	3108	1/1	0.68	0.25	72,72,72,72	0
57	MG	BA	3569	1/1	0.68	0.19	56,56,56,56	0
57	MG	BA	3710	1/1	0.69	0.38	65,65,65,65	0
57	MG	DA	3617	1/1	0.69	0.32	51,51,51,51	0
57	MG	AA	1755	1/1	0.70	0.16	80,80,80,80	0
57	MG	BA	3655	1/1	0.71	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
57	MG	BA	3477	1/1	0.71	0.17	68,68,68,68	0
57	MG	BA	3369	1/1	0.71	0.25	62,62,62,62	0
57	MG	DA	3545	1/1	0.71	0.13	62,62,62,62	0
57	MG	DB	3010	1/1	0.71	0.19	75,75,75,75	0
57	MG	DA	3417	1/1	0.72	0.16	52,52,52,52	0
57	MG	CA	3112	1/1	0.73	0.27	72,72,72,72	0
57	MG	BA	3442	1/1	0.73	0.27	65,65,65,65	0
57	MG	DA	3286	1/1	0.74	0.14	55,55,55,55	0
57	MG	DA	3351	1/1	0.74	0.12	56,56,56,56	0
57	MG	DA	3616	1/1	0.74	0.20	63,63,63,63	0
57	MG	CA	3143	1/1	0.74	0.18	74,74,74,74	0
57	MG	DA	3618	1/1	0.74	0.18	46,46,46,46	0
57	MG	DA	3462	1/1	0.74	0.23	50,50,50,50	0
57	MG	DA	3478	1/1	0.74	0.22	58,58,58,58	0
57	MG	DA	3486	1/1	0.74	0.12	57,57,57,57	0
57	MG	BA	3644	1/1	0.75	0.26	64,64,64,64	0
57	MG	DA	3332	1/1	0.75	0.20	46,46,46,46	0
57	MG	CA	3144	1/1	0.75	0.23	82,82,82,82	0
57	MG	AA	1601	1/1	0.75	0.22	81,81,81,81	0
57	MG	CE	202	1/1	0.75	0.14	95,95,95,95	0
57	MG	BA	3491	1/1	0.75	0.21	56,56,56,56	0
57	MG	AA	1610	1/1	0.75	0.26	81,81,81,81	0
57	MG	DA	3508	1/1	0.75	0.17	57,57,57,57	0
57	MG	DA	3516	1/1	0.76	0.18	67,67,67,67	0
57	MG	BA	3717	1/1	0.76	0.20	72,72,72,72	0
57	MG	DA	3596	1/1	0.76	0.17	69,69,69,69	0
57	MG	DA	3456	1/1	0.76	0.18	38,38,38,38	0
57	MG	CA	3089	1/1	0.76	0.22	74,74,74,74	0
57	MG	BA	3688	1/1	0.77	0.21	61,61,61,61	0
57	MG	CA	3019	1/1	0.77	0.22	68,68,68,68	0
57	MG	DA	3112	1/1	0.77	0.15	56,56,56,56	0
57	MG	DA	3135	1/1	0.77	0.18	63,63,63,63	0
57	MG	BA	3016	1/1	0.77	0.21	67,67,67,67	0
57	MG	DA	3257	1/1	0.77	0.19	44,44,44,44	0
57	MG	BA	3676	1/1	0.77	0.19	70,70,70,70	0
57	MG	BA	3712	1/1	0.77	0.18	51,51,51,51	0
57	MG	DA	3542	1/1	0.77	0.16	60,60,60,60	0
57	MG	DA	3122	1/1	0.78	0.14	60,60,60,60	0
57	MG	BA	3727	1/1	0.78	0.18	53,53,53,53	0
57	MG	BA	3747	1/1	0.78	0.20	55,55,55,55	0
57	MG	BA	3805	1/1	0.78	0.17	48,48,48,48	0
57	MG	BA	3018	1/1	0.78	0.14	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	1757	1/1	0.78	0.29	68,68,68,68	0
57	MG	AX	3007	1/1	0.79	0.30	68,68,68,68	0
57	MG	CA	3095	1/1	0.79	0.26	71,71,71,71	0
57	MG	AA	1790	1/1	0.79	0.17	81,81,81,81	0
57	MG	AA	1613	1/1	0.79	0.11	75,75,75,75	0
57	MG	BA	3204	1/1	0.79	0.32	67,67,67,67	0
57	MG	CA	3117	1/1	0.79	0.11	63,63,63,63	0
57	MG	BB	3017	1/1	0.79	0.23	81,81,81,81	0
57	MG	BA	3298	1/1	0.79	0.11	27,27,27,27	0
57	MG	DA	3645	1/1	0.79	0.12	64,64,64,64	0
57	MG	DA	3649	1/1	0.79	0.15	71,71,71,71	0
57	MG	BA	3352	1/1	0.79	0.19	68,68,68,68	0
57	MG	CA	3148	1/1	0.80	0.22	68,68,68,68	0
57	MG	BA	3041	1/1	0.80	0.21	63,63,63,63	0
57	MG	DA	3400	1/1	0.80	0.16	62,62,62,62	0
57	MG	CA	3090	1/1	0.80	0.19	76,76,76,76	0
57	MG	BA	3449	1/1	0.80	0.17	62,62,62,62	0
57	MG	BA	3680	1/1	0.80	0.18	42,42,42,42	0
57	MG	AX	3013	1/1	0.80	0.23	70,70,70,70	0
57	MG	AY	3003	1/1	0.80	0.16	79,79,79,79	0
57	MG	AW	3002	1/1	0.80	0.36	79,79,79,79	0
57	MG	CA	3070	1/1	0.80	0.27	69,69,69,69	0
57	MG	AA	1771	1/1	0.80	0.17	75,75,75,75	0
57	MG	BA	3640	1/1	0.81	0.21	57,57,57,57	0
57	MG	AA	1618	1/1	0.81	0.16	68,68,68,68	0
57	MG	CA	3125	1/1	0.81	0.22	64,64,64,64	0
57	MG	DA	3410	1/1	0.81	0.17	40,40,40,40	0
57	MG	BA	3700	1/1	0.81	0.19	36,36,36,36	0
57	MG	DA	3442	1/1	0.81	0.26	64,64,64,64	0
57	MG	DA	3444	1/1	0.81	0.13	44,44,44,44	0
57	MG	AX	3012	1/1	0.81	0.24	52,52,52,52	0
57	MG	BA	3374	1/1	0.81	0.12	50,50,50,50	0
57	MG	AA	1650	1/1	0.81	0.33	74,74,74,74	0
57	MG	CA	3160	1/1	0.81	0.21	73,73,73,73	0
57	MG	DA	3491	1/1	0.81	0.17	43,43,43,43	0
57	MG	DA	3306	1/1	0.81	0.23	65,65,65,65	0
57	MG	DA	3001	1/1	0.82	0.11	57,57,57,57	0
57	MG	DA	3016	1/1	0.82	0.23	66,66,66,66	0
57	MG	CA	3102	1/1	0.82	0.25	71,71,71,71	0
57	MG	CA	3103	1/1	0.82	0.18	73,73,73,73	0
57	MG	DA	3487	1/1	0.82	0.17	55,55,55,55	0
57	MG	BA	3561	1/1	0.82	0.16	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	1712	1/1	0.82	0.30	69,69,69,69	0
57	MG	DA	3248	1/1	0.82	0.16	58,58,58,58	0
57	MG	BA	3274	1/1	0.82	0.33	66,66,66,66	0
57	MG	BB	3019	1/1	0.82	0.17	70,70,70,70	0
57	MG	BB	3020	1/1	0.82	0.15	65,65,65,65	0
57	MG	CA	3130	1/1	0.82	0.30	64,64,64,64	0
57	MG	DA	3328	1/1	0.82	0.18	42,42,42,42	0
57	MG	CA	3131	1/1	0.82	0.24	69,69,69,69	0
57	MG	BA	3642	1/1	0.82	0.18	64,64,64,64	0
57	MG	AA	1787	1/1	0.82	0.16	49,49,49,49	0
57	MG	BA	3404	1/1	0.82	0.27	59,59,59,59	0
57	MG	DA	3630	1/1	0.82	0.20	69,69,69,69	0
57	MG	BA	3667	1/1	0.82	0.17	58,58,58,58	0
57	MG	BA	3723	1/1	0.82	0.15	30,30,30,30	0
57	MG	BA	3518	1/1	0.82	0.16	46,46,46,46	0
57	MG	DU	201	1/1	0.82	0.27	58,58,58,58	0
57	MG	AA	1705	1/1	0.83	0.30	70,70,70,70	0
57	MG	BA	3730	1/1	0.83	0.18	68,68,68,68	0
57	MG	DA	3502	1/1	0.83	0.14	48,48,48,48	0
57	MG	AA	1711	1/1	0.83	0.12	51,51,51,51	0
57	MG	DA	3305	1/1	0.83	0.10	53,53,53,53	0
57	MG	BA	3765	1/1	0.83	0.17	49,49,49,49	0
57	MG	BA	3653	1/1	0.83	0.26	57,57,57,57	0
57	MG	DA	3557	1/1	0.83	0.20	57,57,57,57	0
57	MG	DA	3572	1/1	0.83	0.19	65,65,65,65	0
57	MG	CA	3105	1/1	0.83	0.22	75,75,75,75	0
57	MG	BA	3705	1/1	0.83	0.10	59,59,59,59	0
57	MG	DA	3611	1/1	0.83	0.14	53,53,53,53	0
57	MG	BA	3563	1/1	0.83	0.14	50,50,50,50	0
57	MG	DA	3070	1/1	0.83	0.16	65,65,65,65	0
57	MG	BA	3323	1/1	0.83	0.15	57,57,57,57	0
57	MG	DA	3107	1/1	0.83	0.12	61,61,61,61	0
57	MG	CA	3009	1/1	0.83	0.16	73,73,73,73	0
57	MG	DA	3448	1/1	0.83	0.16	55,55,55,55	0
57	MG	DA	3637	1/1	0.83	0.21	72,72,72,72	0
57	MG	BA	3715	1/1	0.83	0.16	52,52,52,52	0
57	MG	BA	3632	1/1	0.83	0.23	55,55,55,55	0
57	MG	DB	3003	1/1	0.83	0.11	78,78,78,78	0
57	MG	DA	3222	1/1	0.83	0.10	58,58,58,58	0
57	MG	BA	3340	1/1	0.83	0.12	27,27,27,27	0
57	MG	BA	3769	1/1	0.84	0.15	47,47,47,47	0
57	MG	BA	3571	1/1	0.84	0.13	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BB	3014	1/1	0.84	0.18	67,67,67,67	0
57	MG	BA	3575	1/1	0.84	0.09	50,50,50,50	0
57	MG	DA	3488	1/1	0.84	0.10	53,53,53,53	0
57	MG	BA	3660	1/1	0.84	0.18	60,60,60,60	0
57	MG	DA	3146	1/1	0.84	0.10	54,54,54,54	0
57	MG	DA	3204	1/1	0.84	0.21	68,68,68,68	0
57	MG	BA	3593	1/1	0.84	0.17	55,55,55,55	0
57	MG	DA	3530	1/1	0.84	0.18	55,55,55,55	0
57	MG	DA	3539	1/1	0.84	0.13	55,55,55,55	0
57	MG	BA	3611	1/1	0.84	0.21	59,59,59,59	0
57	MG	DA	3543	1/1	0.84	0.18	64,64,64,64	0
57	MG	AX	3016	1/1	0.84	0.25	86,86,86,86	0
57	MG	CA	3036	1/1	0.84	0.22	73,73,73,73	0
57	MG	CA	3049	1/1	0.84	0.35	65,65,65,65	0
57	MG	CA	3059	1/1	0.84	0.15	75,75,75,75	0
57	MG	DA	3601	1/1	0.84	0.15	55,55,55,55	0
57	MG	BA	3074	1/1	0.84	0.24	69,69,69,69	0
57	MG	DA	3308	1/1	0.84	0.23	62,62,62,62	0
57	MG	DA	3314	1/1	0.84	0.13	43,43,43,43	0
57	MG	BA	3728	1/1	0.84	0.12	52,52,52,52	0
57	MG	AA	1688	1/1	0.84	0.26	66,66,66,66	0
57	MG	DA	3624	1/1	0.84	0.18	59,59,59,59	0
57	MG	BA	3743	1/1	0.84	0.33	47,47,47,47	0
57	MG	DA	3356	1/1	0.84	0.12	39,39,39,39	0
57	MG	CJ	5001	1/1	0.84	0.20	77,77,77,77	0
57	MG	CA	3091	1/1	0.84	0.18	69,69,69,69	0
57	MG	DA	3002	1/1	0.84	0.19	64,64,64,64	0
57	MG	BA	3694	1/1	0.84	0.19	53,53,53,53	0
57	MG	DA	3663	1/1	0.84	0.25	73,73,73,73	0
57	MG	DB	3001	1/1	0.84	0.24	63,63,63,63	0
57	MG	DA	3033	1/1	0.84	0.14	68,68,68,68	0
57	MG	DB	3004	1/1	0.84	0.23	63,63,63,63	0
57	MG	DA	3065	1/1	0.84	0.13	56,56,56,56	0
57	MG	BA	3517	1/1	0.84	0.16	33,33,33,33	0
57	MG	AA	1679	1/1	0.85	0.20	51,51,51,51	0
57	MG	BA	3734	1/1	0.85	0.14	65,65,65,65	0
57	MG	BA	3121	1/1	0.85	0.14	42,42,42,42	0
57	MG	DA	3130	1/1	0.85	0.17	52,52,52,52	0
57	MG	BA	3666	1/1	0.85	0.23	74,74,74,74	0
57	MG	CA	3107	1/1	0.85	0.14	68,68,68,68	0
57	MG	BA	3164	1/1	0.85	0.12	46,46,46,46	0
57	MG	DA	3524	1/1	0.85	0.23	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	3110	1/1	0.85	0.18	63,63,63,63	0
57	MG	DA	3538	1/1	0.85	0.16	60,60,60,60	0
57	MG	BA	3673	1/1	0.85	0.24	61,61,61,61	0
57	MG	DA	3250	1/1	0.85	0.10	50,50,50,50	0
57	MG	CA	3113	1/1	0.85	0.19	47,47,47,47	0
57	MG	BA	3377	1/1	0.85	0.18	51,51,51,51	0
57	MG	DA	3284	1/1	0.85	0.17	58,58,58,58	0
57	MG	BA	3678	1/1	0.85	0.19	67,67,67,67	0
57	MG	DA	3591	1/1	0.85	0.15	66,66,66,66	0
57	MG	BA	3572	1/1	0.85	0.15	39,39,39,39	0
57	MG	BA	3573	1/1	0.85	0.11	41,41,41,41	0
57	MG	AB	3001	1/1	0.85	0.15	77,77,77,77	0
57	MG	B0	3002	1/1	0.85	0.18	63,63,63,63	0
57	MG	CA	3002	1/1	0.85	0.22	77,77,77,77	0
57	MG	BA	3581	1/1	0.85	0.12	59,59,59,59	0
57	MG	BA	3439	1/1	0.85	0.14	36,36,36,36	0
57	MG	DA	3619	1/1	0.85	0.10	40,40,40,40	0
57	MG	CA	3030	1/1	0.85	0.25	74,74,74,74	0
57	MG	DA	3368	1/1	0.85	0.20	67,67,67,67	0
57	MG	BA	3246	1/1	0.85	0.27	55,55,55,55	0
57	MG	BA	3615	1/1	0.85	0.12	71,71,71,71	0
57	MG	DA	3415	1/1	0.85	0.16	43,43,43,43	0
57	MG	CA	3051	1/1	0.85	0.22	77,77,77,77	0
57	MG	DA	3647	1/1	0.85	0.14	52,52,52,52	0
57	MG	DA	3441	1/1	0.85	0.25	58,58,58,58	0
57	MG	AA	1717	1/1	0.85	0.24	75,75,75,75	0
57	MG	BA	3636	1/1	0.85	0.26	66,66,66,66	0
57	MG	BA	3275	1/1	0.85	0.15	66,66,66,66	0
57	MG	AA	1788	1/1	0.85	0.32	75,75,75,75	0
57	MG	AX	3008	1/1	0.85	0.28	76,76,76,76	0
57	MG	DB	3011	1/1	0.85	0.31	67,67,67,67	0
57	MG	AA	1669	1/1	0.85	0.23	69,69,69,69	0
57	MG	BA	3713	1/1	0.86	0.24	33,33,33,33	0
57	MG	CA	3146	1/1	0.86	0.20	72,72,72,72	0
57	MG	DA	3226	1/1	0.86	0.13	57,57,57,57	0
57	MG	BA	3746	1/1	0.86	0.29	78,78,78,78	0
57	MG	B6	103	1/1	0.86	0.15	52,52,52,52	0
57	MG	AL	201	1/1	0.86	0.18	63,63,63,63	0
57	MG	DA	3518	1/1	0.86	0.12	56,56,56,56	0
57	MG	CA	3164	1/1	0.86	0.18	76,76,76,76	0
57	MG	CA	3167	1/1	0.86	0.26	57,57,57,57	0
57	MG	BA	3755	1/1	0.86	0.14	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3293	1/1	0.86	0.12	61,61,61,61	0
57	MG	DA	3295	1/1	0.86	0.22	67,67,67,67	0
57	MG	CA	3013	1/1	0.86	0.29	67,67,67,67	0
57	MG	CA	3018	1/1	0.86	0.19	63,63,63,63	0
57	MG	AX	3015	1/1	0.86	0.17	51,51,51,51	0
57	MG	DA	3560	1/1	0.86	0.25	60,60,60,60	0
57	MG	CA	3022	1/1	0.86	0.22	76,76,76,76	0
57	MG	DA	3017	1/1	0.86	0.14	59,59,59,59	0
57	MG	DA	3024	1/1	0.86	0.16	61,61,61,61	0
57	MG	DA	3342	1/1	0.86	0.09	53,53,53,53	0
57	MG	DA	3344	1/1	0.86	0.13	38,38,38,38	0
57	MG	DA	3032	1/1	0.86	0.13	57,57,57,57	0
57	MG	AA	1743	1/1	0.86	0.13	66,66,66,66	0
57	MG	DA	3358	1/1	0.86	0.11	50,50,50,50	0
57	MG	DA	3366	1/1	0.86	0.12	44,44,44,44	0
57	MG	AA	1781	1/1	0.86	0.12	59,59,59,59	0
57	MG	DA	3066	1/1	0.86	0.15	58,58,58,58	0
57	MG	BA	3809	1/1	0.86	0.17	61,61,61,61	0
57	MG	BB	3009	1/1	0.86	0.10	57,57,57,57	0
57	MG	DA	3089	1/1	0.86	0.18	52,52,52,52	0
57	MG	DA	3433	1/1	0.86	0.19	59,59,59,59	0
57	MG	AA	1674	1/1	0.86	0.22	58,58,58,58	0
57	MG	CA	3124	1/1	0.86	0.19	69,69,69,69	0
57	MG	BA	3228	1/1	0.86	0.26	65,65,65,65	0
57	MG	DA	3445	1/1	0.86	0.11	52,52,52,52	0
57	MG	CA	3076	1/1	0.86	0.24	77,77,77,77	0
57	MG	CA	3082	1/1	0.86	0.34	66,66,66,66	0
57	MG	DA	3143	1/1	0.86	0.21	62,62,62,62	0
57	MG	DA	3463	1/1	0.86	0.13	44,44,44,44	0
57	MG	AA	1623	1/1	0.86	0.30	65,65,65,65	0
57	MG	DA	3190	1/1	0.86	0.21	63,63,63,63	0
57	MG	CA	3094	1/1	0.87	0.18	61,61,61,61	0
57	MG	DA	3435	1/1	0.87	0.12	44,44,44,44	0
57	MG	AA	1766	1/1	0.87	0.19	71,71,71,71	0
57	MG	BA	3796	1/1	0.87	0.14	47,47,47,47	0
57	MG	DA	3081	1/1	0.87	0.11	51,51,51,51	0
57	MG	BA	3498	1/1	0.87	0.10	45,45,45,45	0
57	MG	DA	3097	1/1	0.87	0.10	47,47,47,47	0
57	MG	DA	3098	1/1	0.87	0.14	66,66,66,66	0
57	MG	AK	3101	1/1	0.87	0.24	69,69,69,69	0
57	MG	BA	3111	1/1	0.87	0.29	53,53,53,53	0
57	MG	BA	3329	1/1	0.87	0.13	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	3109	1/1	0.87	0.12	74,74,74,74	0
57	MG	BA	3338	1/1	0.87	0.14	55,55,55,55	0
57	MG	AA	1748	1/1	0.87	0.22	64,64,64,64	0
57	MG	AA	1662	1/1	0.87	0.14	58,58,58,58	0
57	MG	BZ	301	1/1	0.87	0.09	49,49,49,49	0
57	MG	DA	3202	1/1	0.87	0.21	62,62,62,62	0
57	MG	DA	3510	1/1	0.87	0.19	64,64,64,64	0
57	MG	BA	3200	1/1	0.87	0.18	48,48,48,48	0
57	MG	CA	3121	1/1	0.87	0.21	67,67,67,67	0
57	MG	CA	3122	1/1	0.87	0.15	69,69,69,69	0
57	MG	AX	3005	1/1	0.87	0.13	65,65,65,65	0
57	MG	BA	3224	1/1	0.87	0.21	59,59,59,59	0
57	MG	BA	3394	1/1	0.87	0.19	40,40,40,40	0
57	MG	CA	3012	1/1	0.87	0.26	64,64,64,64	0
57	MG	DA	3261	1/1	0.87	0.12	39,39,39,39	0
57	MG	DA	3275	1/1	0.87	0.18	65,65,65,65	0
57	MG	DA	3553	1/1	0.87	0.18	72,72,72,72	0
57	MG	DA	3282	1/1	0.87	0.15	55,55,55,55	0
57	MG	BA	3225	1/1	0.87	0.10	46,46,46,46	0
57	MG	DA	3571	1/1	0.87	0.11	45,45,45,45	0
57	MG	BA	3604	1/1	0.87	0.14	43,43,43,43	0
57	MG	DA	3289	1/1	0.87	0.13	52,52,52,52	0
57	MG	BA	3609	1/1	0.87	0.22	56,56,56,56	0
57	MG	BA	3429	1/1	0.87	0.14	50,50,50,50	0
57	MG	CA	3152	1/1	0.87	0.18	71,71,71,71	0
57	MG	CA	3029	1/1	0.87	0.09	50,50,50,50	0
57	MG	DA	3612	1/1	0.87	0.09	58,58,58,58	0
57	MG	BA	3431	1/1	0.87	0.19	57,57,57,57	0
57	MG	BA	3722	1/1	0.87	0.24	64,64,64,64	0
57	MG	BA	3629	1/1	0.87	0.17	58,58,58,58	0
57	MG	CE	201	1/1	0.87	0.19	65,65,65,65	0
57	MG	DA	3620	1/1	0.87	0.11	53,53,53,53	0
57	MG	DA	3623	1/1	0.87	0.10	45,45,45,45	0
57	MG	DA	3334	1/1	0.87	0.23	57,57,57,57	0
57	MG	DA	3625	1/1	0.87	0.10	60,60,60,60	0
57	MG	BA	3435	1/1	0.87	0.15	53,53,53,53	0
57	MG	CA	3058	1/1	0.87	0.15	66,66,66,66	0
57	MG	BA	3006	1/1	0.87	0.14	54,54,54,54	0
57	MG	AA	1801	1/1	0.87	0.13	71,71,71,71	0
57	MG	BA	3641	1/1	0.87	0.22	68,68,68,68	0
57	MG	BA	3443	1/1	0.87	0.11	59,59,59,59	0
57	MG	BA	3272	1/1	0.87	0.25	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3393	1/1	0.87	0.12	37,37,37,37	0
57	MG	BA	3647	1/1	0.87	0.10	53,53,53,53	0
57	MG	BA	3462	1/1	0.87	0.13	53,53,53,53	0
57	MG	DA	3414	1/1	0.87	0.13	42,42,42,42	0
57	MG	DA	3035	1/1	0.87	0.09	37,37,37,37	0
57	MG	AA	1664	1/1	0.87	0.17	62,62,62,62	0
57	MG	DA	3421	1/1	0.87	0.14	56,56,56,56	0
59	ZN	D4	501	1/1	0.87	0.10	162,162,162,162	0
57	MG	DA	3396	1/1	0.88	0.16	46,46,46,46	0
57	MG	BA	3327	1/1	0.88	0.10	39,39,39,39	0
57	MG	BA	3702	1/1	0.88	0.08	39,39,39,39	0
57	MG	BA	3068	1/1	0.88	0.09	49,49,49,49	0
57	MG	CA	3057	1/1	0.88	0.19	84,84,84,84	0
57	MG	AA	1775	1/1	0.88	0.14	73,73,73,73	0
57	MG	DA	3418	1/1	0.88	0.10	47,47,47,47	0
57	MG	DA	3419	1/1	0.88	0.20	50,50,50,50	0
57	MG	DA	3056	1/1	0.88	0.12	49,49,49,49	0
57	MG	DA	3061	1/1	0.88	0.12	60,60,60,60	0
57	MG	DA	3434	1/1	0.88	0.12	60,60,60,60	0
57	MG	BA	3079	1/1	0.88	0.22	58,58,58,58	0
57	MG	BA	3351	1/1	0.88	0.13	45,45,45,45	0
57	MG	BA	3099	1/1	0.88	0.23	61,61,61,61	0
57	MG	AX	3002	1/1	0.88	0.24	71,71,71,71	0
57	MG	BA	3579	1/1	0.88	0.09	63,63,63,63	0
57	MG	DA	3087	1/1	0.88	0.15	55,55,55,55	0
57	MG	BA	3372	1/1	0.88	0.08	40,40,40,40	0
57	MG	DA	3096	1/1	0.88	0.13	68,68,68,68	0
57	MG	AA	1656	1/1	0.88	0.20	63,63,63,63	0
57	MG	BA	3594	1/1	0.88	0.15	45,45,45,45	0
57	MG	DA	3099	1/1	0.88	0.19	63,63,63,63	0
57	MG	DA	3101	1/1	0.88	0.16	56,56,56,56	0
57	MG	BA	3600	1/1	0.88	0.16	44,44,44,44	0
57	MG	BA	3375	1/1	0.88	0.12	39,39,39,39	0
57	MG	BA	3608	1/1	0.88	0.16	58,58,58,58	0
57	MG	DA	3504	1/1	0.88	0.12	52,52,52,52	0
57	MG	BA	3139	1/1	0.88	0.12	44,44,44,44	0
57	MG	AA	1625	1/1	0.88	0.27	73,73,73,73	0
57	MG	DA	3515	1/1	0.88	0.13	55,55,55,55	0
57	MG	AA	1701	1/1	0.88	0.38	73,73,73,73	0
57	MG	BA	3616	1/1	0.88	0.22	59,59,59,59	0
57	MG	DA	3523	1/1	0.88	0.09	39,39,39,39	0
57	MG	DA	3159	1/1	0.88	0.15	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3172	1/1	0.88	0.26	61,61,61,61	0
57	MG	DA	3533	1/1	0.88	0.14	56,56,56,56	0
57	MG	DA	3535	1/1	0.88	0.12	44,44,44,44	0
57	MG	BA	3416	1/1	0.88	0.13	60,60,60,60	0
57	MG	DA	3201	1/1	0.88	0.11	52,52,52,52	0
57	MG	BA	3775	1/1	0.88	0.29	39,39,39,39	0
57	MG	BA	3423	1/1	0.88	0.17	69,69,69,69	0
57	MG	DA	3219	1/1	0.88	0.15	50,50,50,50	0
57	MG	AA	1631	1/1	0.88	0.16	64,64,64,64	0
57	MG	AA	1708	1/1	0.88	0.11	60,60,60,60	0
57	MG	AA	1794	1/1	0.88	0.21	58,58,58,58	0
57	MG	DA	3570	1/1	0.88	0.10	43,43,43,43	0
57	MG	CA	3120	1/1	0.88	0.23	68,68,68,68	0
57	MG	DA	3253	1/1	0.88	0.12	54,54,54,54	0
57	MG	AA	1756	1/1	0.88	0.24	45,45,45,45	0
57	MG	DA	3594	1/1	0.88	0.15	58,58,58,58	0
57	MG	AA	1614	1/1	0.88	0.23	75,75,75,75	0
57	MG	BA	3265	1/1	0.88	0.31	72,72,72,72	0
57	MG	DA	3602	1/1	0.88	0.22	62,62,62,62	0
57	MG	AA	1655	1/1	0.88	0.09	53,53,53,53	0
57	MG	CA	3127	1/1	0.88	0.10	59,59,59,59	0
57	MG	CA	3129	1/1	0.88	0.18	69,69,69,69	0
57	MG	BO	5001	1/1	0.88	0.15	61,61,61,61	0
57	MG	DA	3287	1/1	0.88	0.18	52,52,52,52	0
57	MG	BA	3458	1/1	0.88	0.15	59,59,59,59	0
57	MG	DA	3291	1/1	0.88	0.16	36,36,36,36	0
57	MG	AA	1714	1/1	0.88	0.12	56,56,56,56	0
57	MG	B2	3001	1/1	0.88	0.11	53,53,53,53	0
57	MG	AA	1773	1/1	0.88	0.14	61,61,61,61	0
57	MG	BA	3484	1/1	0.88	0.15	40,40,40,40	0
57	MG	BA	3669	1/1	0.88	0.10	28,28,28,28	0
57	MG	DA	3311	1/1	0.88	0.09	46,46,46,46	0
57	MG	AT	3001	1/1	0.88	0.27	63,63,63,63	0
57	MG	DA	3633	1/1	0.88	0.12	58,58,58,58	0
57	MG	CA	3154	1/1	0.88	0.15	68,68,68,68	0
57	MG	BA	3497	1/1	0.88	0.12	50,50,50,50	0
57	MG	BA	3318	1/1	0.88	0.12	54,54,54,54	0
57	MG	BA	3504	1/1	0.88	0.15	56,56,56,56	0
57	MG	DA	3650	1/1	0.88	0.15	61,61,61,61	0
57	MG	DA	3657	1/1	0.88	0.21	54,54,54,54	0
57	MG	BA	3512	1/1	0.88	0.11	23,23,23,23	0
57	MG	CA	3024	1/1	0.88	0.23	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	3027	1/1	0.88	0.32	65,65,65,65	0
57	MG	CX	3001	1/1	0.88	0.22	57,57,57,57	0
57	MG	DA	3362	1/1	0.88	0.14	42,42,42,42	0
57	MG	BA	3320	1/1	0.88	0.17	55,55,55,55	0
57	MG	DF	302	1/1	0.88	0.10	53,53,53,53	0
57	MG	BA	3062	1/1	0.88	0.42	59,59,59,59	0
57	MG	CA	3032	1/1	0.88	0.19	53,53,53,53	0
57	MG	AM	3002	1/1	0.89	0.10	68,68,68,68	0
57	MG	DA	3345	1/1	0.89	0.15	58,58,58,58	0
57	MG	DA	3348	1/1	0.89	0.10	53,53,53,53	0
57	MG	B7	104	1/1	0.89	0.17	62,62,62,62	0
57	MG	BA	3507	1/1	0.89	0.18	43,43,43,43	0
57	MG	CA	3004	1/1	0.89	0.08	69,69,69,69	0
57	MG	CA	3005	1/1	0.89	0.13	73,73,73,73	0
57	MG	BA	3334	1/1	0.89	0.15	56,56,56,56	0
57	MG	BA	3199	1/1	0.89	0.30	64,64,64,64	0
57	MG	DA	3377	1/1	0.89	0.11	50,50,50,50	0
57	MG	AA	1644	1/1	0.89	0.12	56,56,56,56	0
57	MG	DA	3395	1/1	0.89	0.15	58,58,58,58	0
57	MG	CA	3014	1/1	0.89	0.16	62,62,62,62	0
57	MG	BA	3522	1/1	0.89	0.12	44,44,44,44	0
57	MG	BA	3525	1/1	0.89	0.08	43,43,43,43	0
57	MG	DA	3411	1/1	0.89	0.13	37,37,37,37	0
57	MG	DA	3413	1/1	0.89	0.15	62,62,62,62	0
57	MG	BA	3684	1/1	0.89	0.17	51,51,51,51	0
57	MG	BA	3530	1/1	0.89	0.15	33,33,33,33	0
57	MG	CA	3025	1/1	0.89	0.23	53,53,53,53	0
57	MG	DA	3041	1/1	0.89	0.14	60,60,60,60	0
57	MG	DA	3044	1/1	0.89	0.18	53,53,53,53	0
57	MG	DA	3420	1/1	0.89	0.09	49,49,49,49	0
57	MG	DA	3048	1/1	0.89	0.10	59,59,59,59	0
57	MG	DA	3431	1/1	0.89	0.18	42,42,42,42	0
57	MG	DA	3055	1/1	0.89	0.13	53,53,53,53	0
57	MG	CA	3026	1/1	0.89	0.21	66,66,66,66	0
57	MG	DA	3060	1/1	0.89	0.23	60,60,60,60	0
57	MG	BA	3538	1/1	0.89	0.10	68,68,68,68	0
57	MG	BA	3542	1/1	0.89	0.10	44,44,44,44	0
57	MG	BA	3696	1/1	0.89	0.10	46,46,46,46	0
57	MG	BA	3557	1/1	0.89	0.17	53,53,53,53	0
57	MG	DA	3072	1/1	0.89	0.10	47,47,47,47	0
57	MG	BA	3558	1/1	0.89	0.10	51,51,51,51	0
57	MG	CA	3046	1/1	0.89	0.23	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3342	1/1	0.89	0.16	67,67,67,67	0
57	MG	BA	3343	1/1	0.89	0.13	54,54,54,54	0
57	MG	BA	3202	1/1	0.89	0.10	62,62,62,62	0
57	MG	BA	3017	1/1	0.89	0.18	65,65,65,65	0
57	MG	BA	3364	1/1	0.89	0.09	47,47,47,47	0
57	MG	BA	3209	1/1	0.89	0.18	48,48,48,48	0
57	MG	DA	3497	1/1	0.89	0.19	58,58,58,58	0
57	MG	BA	3219	1/1	0.89	0.15	58,58,58,58	0
57	MG	DA	3102	1/1	0.89	0.11	40,40,40,40	0
57	MG	DA	3106	1/1	0.89	0.11	50,50,50,50	0
57	MG	AA	1620	1/1	0.89	0.19	59,59,59,59	0
57	MG	DA	3111	1/1	0.89	0.17	56,56,56,56	0
57	MG	BA	3726	1/1	0.89	0.12	31,31,31,31	0
57	MG	AA	1738	1/1	0.89	0.13	68,68,68,68	0
57	MG	AA	1651	1/1	0.89	0.25	58,58,58,58	0
57	MG	BA	3240	1/1	0.89	0.14	53,53,53,53	0
57	MG	DA	3527	1/1	0.89	0.17	52,52,52,52	0
57	MG	DA	3139	1/1	0.89	0.08	44,44,44,44	0
57	MG	BA	3245	1/1	0.89	0.10	59,59,59,59	0
57	MG	BA	3738	1/1	0.89	0.13	41,41,41,41	0
57	MG	BA	3741	1/1	0.89	0.11	57,57,57,57	0
57	MG	BA	3411	1/1	0.89	0.17	50,50,50,50	0
57	MG	DA	3541	1/1	0.89	0.20	59,59,59,59	0
57	MG	DA	3173	1/1	0.89	0.17	62,62,62,62	0
57	MG	DA	3177	1/1	0.89	0.25	58,58,58,58	0
57	MG	AA	1798	1/1	0.89	0.10	62,62,62,62	0
57	MG	DA	3196	1/1	0.89	0.19	54,54,54,54	0
57	MG	DA	3556	1/1	0.89	0.11	55,55,55,55	0
57	MG	DA	3200	1/1	0.89	0.12	41,41,41,41	0
57	MG	DA	3559	1/1	0.89	0.12	67,67,67,67	0
57	MG	BA	3248	1/1	0.89	0.21	67,67,67,67	0
57	MG	DA	3567	1/1	0.89	0.23	44,44,44,44	0
57	MG	BA	3252	1/1	0.89	0.18	36,36,36,36	0
57	MG	BA	3763	1/1	0.89	0.14	44,44,44,44	0
57	MG	DA	3212	1/1	0.89	0.29	62,62,62,62	0
57	MG	DA	3573	1/1	0.89	0.13	61,61,61,61	0
57	MG	BA	3614	1/1	0.89	0.15	53,53,53,53	0
57	MG	DA	3592	1/1	0.89	0.17	67,67,67,67	0
57	MG	CA	3111	1/1	0.89	0.10	72,72,72,72	0
57	MG	BA	3255	1/1	0.89	0.17	55,55,55,55	0
57	MG	DA	3227	1/1	0.89	0.14	56,56,56,56	0
57	MG	DA	3232	1/1	0.89	0.32	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3234	1/1	0.89	0.21	54,54,54,54	0
57	MG	DA	3236	1/1	0.89	0.20	55,55,55,55	0
57	MG	AA	1629	1/1	0.89	0.45	68,68,68,68	0
57	MG	BA	3786	1/1	0.89	0.15	51,51,51,51	0
57	MG	BA	3794	1/1	0.89	0.10	37,37,37,37	0
57	MG	CA	3119	1/1	0.89	0.19	59,59,59,59	0
57	MG	BA	3625	1/1	0.89	0.08	33,33,33,33	0
57	MG	BA	3798	1/1	0.89	0.14	22,22,22,22	0
57	MG	DA	3265	1/1	0.89	0.19	57,57,57,57	0
57	MG	DA	3269	1/1	0.89	0.14	50,50,50,50	0
57	MG	AA	1747	1/1	0.89	0.13	55,55,55,55	0
57	MG	BA	3087	1/1	0.89	0.22	43,43,43,43	0
57	MG	BB	3001	1/1	0.89	0.22	68,68,68,68	0
57	MG	BB	3004	1/1	0.89	0.24	69,69,69,69	0
57	MG	AA	1624	1/1	0.89	0.35	66,66,66,66	0
57	MG	BA	3277	1/1	0.89	0.18	52,52,52,52	0
57	MG	DA	3644	1/1	0.89	0.29	58,58,58,58	0
57	MG	BA	3282	1/1	0.89	0.23	57,57,57,57	0
57	MG	DA	3646	1/1	0.89	0.13	56,56,56,56	0
57	MG	CA	3139	1/1	0.89	0.15	81,81,81,81	0
57	MG	CA	3142	1/1	0.89	0.15	50,50,50,50	0
57	MG	DA	3302	1/1	0.89	0.18	53,53,53,53	0
57	MG	BA	3286	1/1	0.89	0.14	44,44,44,44	0
57	MG	BA	3100	1/1	0.89	0.19	61,61,61,61	0
57	MG	BF	306	1/1	0.89	0.28	49,49,49,49	0
57	MG	BG	202	1/1	0.89	0.09	52,52,52,52	0
57	MG	BA	3103	1/1	0.89	0.29	63,63,63,63	0
57	MG	DA	3315	1/1	0.89	0.08	44,44,44,44	0
57	MG	AF	3001	1/1	0.89	0.13	50,50,50,50	0
57	MG	DB	3012	1/1	0.89	0.26	66,66,66,66	0
57	MG	AA	1685	1/1	0.89	0.19	62,62,62,62	0
57	MG	DG	3001	1/1	0.89	0.22	66,66,66,66	0
57	MG	DP	201	1/1	0.89	0.23	69,69,69,69	0
57	MG	DQ	3003	1/1	0.89	0.18	62,62,62,62	0
57	MG	AA	1785	1/1	0.89	0.17	72,72,72,72	0
57	MG	CA	3161	1/1	0.89	0.09	76,76,76,76	0
57	MG	AA	1713	1/1	0.90	0.20	67,67,67,67	0
57	MG	DA	3422	1/1	0.90	0.16	62,62,62,62	0
57	MG	DA	3430	1/1	0.90	0.14	47,47,47,47	0
57	MG	BA	3570	1/1	0.90	0.15	31,31,31,31	0
57	MG	DA	3153	1/1	0.90	0.08	44,44,44,44	0
57	MG	DA	3154	1/1	0.90	0.11	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3158	1/1	0.90	0.17	56,56,56,56	0
57	MG	AX	3011	1/1	0.90	0.14	60,60,60,60	0
57	MG	BA	3419	1/1	0.90	0.13	25,25,25,25	0
57	MG	BA	3699	1/1	0.90	0.17	67,67,67,67	0
57	MG	CA	3137	1/1	0.90	0.23	78,78,78,78	0
57	MG	BA	3117	1/1	0.90	0.28	38,38,38,38	0
57	MG	CA	3141	1/1	0.90	0.11	62,62,62,62	0
57	MG	DA	3459	1/1	0.90	0.14	49,49,49,49	0
57	MG	DA	3199	1/1	0.90	0.35	62,62,62,62	0
57	MG	AA	1663	1/1	0.90	0.07	50,50,50,50	0
57	MG	DA	3470	1/1	0.90	0.10	61,61,61,61	0
57	MG	AA	1692	1/1	0.90	0.25	65,65,65,65	0
57	MG	DA	3481	1/1	0.90	0.12	40,40,40,40	0
57	MG	BA	3296	1/1	0.90	0.14	55,55,55,55	0
57	MG	BA	3436	1/1	0.90	0.11	57,57,57,57	0
57	MG	AA	1806	1/1	0.90	0.31	74,74,74,74	0
57	MG	DA	3217	1/1	0.90	0.23	57,57,57,57	0
57	MG	AA	1767	1/1	0.90	0.16	67,67,67,67	0
57	MG	AY	3001	1/1	0.90	0.23	63,63,63,63	0
57	MG	AA	1816	1/1	0.90	0.18	59,59,59,59	0
57	MG	CA	3155	1/1	0.90	0.11	57,57,57,57	0
57	MG	BA	3452	1/1	0.90	0.10	56,56,56,56	0
57	MG	DA	3514	1/1	0.90	0.14	47,47,47,47	0
57	MG	AA	1718	1/1	0.90	0.16	66,66,66,66	0
57	MG	CA	3162	1/1	0.90	0.12	79,79,79,79	0
57	MG	DA	3238	1/1	0.90	0.14	48,48,48,48	0
57	MG	BA	3205	1/1	0.90	0.36	57,57,57,57	0
57	MG	BA	3463	1/1	0.90	0.17	56,56,56,56	0
57	MG	CA	3169	1/1	0.90	0.14	62,62,62,62	0
57	MG	AA	1723	1/1	0.90	0.10	63,63,63,63	0
57	MG	DA	3256	1/1	0.90	0.12	51,51,51,51	0
57	MG	BA	3623	1/1	0.90	0.11	43,43,43,43	0
57	MG	CF	3001	1/1	0.90	0.16	51,51,51,51	0
57	MG	BA	3337	1/1	0.90	0.15	44,44,44,44	0
57	MG	AA	1731	1/1	0.90	0.21	56,56,56,56	0
57	MG	CA	3039	1/1	0.90	0.30	64,64,64,64	0
57	MG	AA	1643	1/1	0.90	0.22	58,58,58,58	0
57	MG	DA	3005	1/1	0.90	0.21	54,54,54,54	0
57	MG	DA	3012	1/1	0.90	0.08	43,43,43,43	0
57	MG	BA	3633	1/1	0.90	0.13	57,57,57,57	0
57	MG	BA	3024	1/1	0.90	0.27	58,58,58,58	0
57	MG	CA	3052	1/1	0.90	0.13	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3749	1/1	0.90	0.12	52,52,52,52	0
57	MG	BA	3637	1/1	0.90	0.09	38,38,38,38	0
57	MG	DA	3301	1/1	0.90	0.12	63,63,63,63	0
57	MG	AA	1654	1/1	0.90	0.31	65,65,65,65	0
57	MG	BA	3346	1/1	0.90	0.09	39,39,39,39	0
57	MG	CA	3073	1/1	0.90	0.20	55,55,55,55	0
57	MG	DA	3585	1/1	0.90	0.12	55,55,55,55	0
57	MG	BA	3239	1/1	0.90	0.16	47,47,47,47	0
57	MG	DA	3052	1/1	0.90	0.07	49,49,49,49	0
57	MG	DA	3593	1/1	0.90	0.10	60,60,60,60	0
57	MG	DA	3313	1/1	0.90	0.09	39,39,39,39	0
57	MG	CA	3077	1/1	0.90	0.23	60,60,60,60	0
57	MG	DA	3600	1/1	0.90	0.09	72,72,72,72	0
57	MG	BA	3774	1/1	0.90	0.14	27,27,27,27	0
57	MG	DA	3317	1/1	0.90	0.09	54,54,54,54	0
57	MG	DA	3605	1/1	0.90	0.14	45,45,45,45	0
57	MG	DA	3057	1/1	0.90	0.10	44,44,44,44	0
57	MG	DA	3608	1/1	0.90	0.19	57,57,57,57	0
57	MG	DA	3331	1/1	0.90	0.16	47,47,47,47	0
57	MG	AN	502	1/1	0.90	0.32	62,62,62,62	0
57	MG	CA	3087	1/1	0.90	0.08	57,57,57,57	0
57	MG	DA	3063	1/1	0.90	0.17	47,47,47,47	0
57	MG	BA	3646	1/1	0.90	0.15	50,50,50,50	0
57	MG	BA	3792	1/1	0.90	0.15	52,52,52,52	0
57	MG	BA	3066	1/1	0.90	0.29	58,58,58,58	0
57	MG	DA	3621	1/1	0.90	0.29	52,52,52,52	0
57	MG	AA	1603	1/1	0.90	0.10	64,64,64,64	0
57	MG	DA	3074	1/1	0.90	0.13	59,59,59,59	0
57	MG	AW	3001	1/1	0.90	0.12	59,59,59,59	0
57	MG	BA	3656	1/1	0.90	0.15	45,45,45,45	0
57	MG	BA	3527	1/1	0.90	0.11	24,24,24,24	0
57	MG	AA	1786	1/1	0.90	0.14	69,69,69,69	0
57	MG	DA	3376	1/1	0.90	0.10	51,51,51,51	0
57	MG	BA	3535	1/1	0.90	0.11	39,39,39,39	0
57	MG	DA	3641	1/1	0.90	0.12	46,46,46,46	0
57	MG	DA	3642	1/1	0.90	0.23	62,62,62,62	0
57	MG	DA	3390	1/1	0.90	0.14	58,58,58,58	0
57	MG	DA	3391	1/1	0.90	0.12	45,45,45,45	0
57	MG	DA	3392	1/1	0.90	0.20	53,53,53,53	0
57	MG	AA	1710	1/1	0.90	0.18	64,64,64,64	0
57	MG	AA	1647	1/1	0.90	0.21	44,44,44,44	0
57	MG	BA	3674	1/1	0.90	0.27	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BB	3018	1/1	0.90	0.09	54,54,54,54	0
57	MG	DA	3401	1/1	0.90	0.14	69,69,69,69	0
57	MG	DA	3403	1/1	0.90	0.08	49,49,49,49	0
57	MG	DB	3002	1/1	0.90	0.26	63,63,63,63	0
57	MG	DA	3406	1/1	0.90	0.19	70,70,70,70	0
57	MG	DA	3407	1/1	0.90	0.09	58,58,58,58	0
57	MG	BA	3268	1/1	0.90	0.18	54,54,54,54	0
57	MG	BA	3396	1/1	0.90	0.14	25,25,25,25	0
57	MG	BB	3022	1/1	0.90	0.14	60,60,60,60	0
57	MG	DB	3013	1/1	0.90	0.16	66,66,66,66	0
57	MG	DE	3004	1/1	0.90	0.10	31,31,31,31	0
57	MG	BE	301	1/1	0.90	0.11	31,31,31,31	0
57	MG	BA	3400	1/1	0.90	0.15	39,39,39,39	0
57	MG	BA	3682	1/1	0.90	0.10	60,60,60,60	0
57	MG	AA	1641	1/1	0.90	0.24	65,65,65,65	0
57	MG	BY	502	1/1	0.90	0.17	46,46,46,46	0
57	MG	D0	101	1/1	0.90	0.22	71,71,71,71	0
57	MG	BA	3687	1/1	0.90	0.15	64,64,64,64	0
57	MG	DA	3142	1/1	0.91	0.08	51,51,51,51	0
57	MG	AA	1732	1/1	0.91	0.19	63,63,63,63	0
57	MG	DA	3424	1/1	0.91	0.13	41,41,41,41	0
57	MG	DA	3426	1/1	0.91	0.11	49,49,49,49	0
57	MG	AA	1671	1/1	0.91	0.10	60,60,60,60	0
57	MG	BA	3102	1/1	0.91	0.24	57,57,57,57	0
57	MG	AA	1739	1/1	0.91	0.36	72,72,72,72	0
57	MG	DA	3156	1/1	0.91	0.22	52,52,52,52	0
57	MG	AA	1699	1/1	0.91	0.28	58,58,58,58	0
57	MG	AA	1605	1/1	0.91	0.13	50,50,50,50	0
57	MG	DA	3167	1/1	0.91	0.21	40,40,40,40	0
57	MG	BA	3685	1/1	0.91	0.29	61,61,61,61	0
57	MG	AY	3002	1/1	0.91	0.14	52,52,52,52	0
57	MG	AA	1782	1/1	0.91	0.14	54,54,54,54	0
57	MG	DA	3455	1/1	0.91	0.14	64,64,64,64	0
57	MG	DA	3184	1/1	0.91	0.16	52,52,52,52	0
57	MG	BA	3145	1/1	0.91	0.21	48,48,48,48	0
57	MG	DA	3194	1/1	0.91	0.14	48,48,48,48	0
57	MG	CA	3133	1/1	0.91	0.15	82,82,82,82	0
57	MG	BA	3577	1/1	0.91	0.17	58,58,58,58	0
57	MG	BA	3279	1/1	0.91	0.23	52,52,52,52	0
57	MG	BA	3147	1/1	0.91	0.22	36,36,36,36	0
57	MG	BA	3283	1/1	0.91	0.33	57,57,57,57	0
57	MG	AA	1617	1/1	0.91	0.08	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3597	1/1	0.91	0.14	55,55,55,55	0
57	MG	DA	3214	1/1	0.91	0.08	51,51,51,51	0
57	MG	DA	3492	1/1	0.91	0.09	48,48,48,48	0
57	MG	CA	3145	1/1	0.91	0.19	65,65,65,65	0
57	MG	BA	3598	1/1	0.91	0.12	33,33,33,33	0
57	MG	BA	3175	1/1	0.91	0.23	57,57,57,57	0
57	MG	CA	3149	1/1	0.91	0.17	54,54,54,54	0
57	MG	CA	3007	1/1	0.91	0.18	51,51,51,51	0
57	MG	DA	3513	1/1	0.91	0.11	69,69,69,69	0
57	MG	BA	3601	1/1	0.91	0.18	40,40,40,40	0
57	MG	DA	3233	1/1	0.91	0.28	65,65,65,65	0
57	MG	BA	3177	1/1	0.91	0.19	46,46,46,46	0
57	MG	BA	3716	1/1	0.91	0.23	45,45,45,45	0
57	MG	BA	3315	1/1	0.91	0.10	40,40,40,40	0
57	MG	CA	3015	1/1	0.91	0.18	64,64,64,64	0
57	MG	DA	3249	1/1	0.91	0.17	65,65,65,65	0
57	MG	DA	3529	1/1	0.91	0.11	76,76,76,76	0
57	MG	CA	3016	1/1	0.91	0.09	48,48,48,48	0
57	MG	DA	3532	1/1	0.91	0.12	48,48,48,48	0
57	MG	CA	3017	1/1	0.91	0.14	54,54,54,54	0
57	MG	BA	3190	1/1	0.91	0.26	54,54,54,54	0
57	MG	BA	3196	1/1	0.91	0.25	56,56,56,56	0
57	MG	BA	3197	1/1	0.91	0.28	58,58,58,58	0
57	MG	AA	1684	1/1	0.91	0.08	54,54,54,54	0
57	MG	AA	1749	1/1	0.91	0.14	50,50,50,50	0
57	MG	BA	3470	1/1	0.91	0.10	57,57,57,57	0
57	MG	CT	3001	1/1	0.91	0.17	60,60,60,60	0
57	MG	DA	3552	1/1	0.91	0.11	34,34,34,34	0
57	MG	BA	3732	1/1	0.91	0.15	33,33,33,33	0
57	MG	DA	3554	1/1	0.91	0.08	50,50,50,50	0
57	MG	CX	3002	1/1	0.91	0.10	67,67,67,67	0
57	MG	BA	3733	1/1	0.91	0.10	42,42,42,42	0
57	MG	BA	3333	1/1	0.91	0.13	57,57,57,57	0
57	MG	DA	3288	1/1	0.91	0.14	39,39,39,39	0
57	MG	DA	3563	1/1	0.91	0.10	70,70,70,70	0
57	MG	DA	3004	1/1	0.91	0.26	53,53,53,53	0
57	MG	BA	3735	1/1	0.91	0.14	50,50,50,50	0
57	MG	CA	3035	1/1	0.91	0.13	53,53,53,53	0
57	MG	BA	3737	1/1	0.91	0.09	34,34,34,34	0
57	MG	BA	3626	1/1	0.91	0.14	50,50,50,50	0
57	MG	DA	3577	1/1	0.91	0.09	60,60,60,60	0
57	MG	DA	3578	1/1	0.91	0.10	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3023	1/1	0.91	0.12	58,58,58,58	0
57	MG	CA	3040	1/1	0.91	0.16	56,56,56,56	0
57	MG	CA	3041	1/1	0.91	0.14	57,57,57,57	0
57	MG	AA	1753	1/1	0.91	0.17	55,55,55,55	0
57	MG	BA	3487	1/1	0.91	0.10	54,54,54,54	0
57	MG	DA	3595	1/1	0.91	0.09	57,57,57,57	0
57	MG	CA	3050	1/1	0.91	0.45	73,73,73,73	0
57	MG	AA	1719	1/1	0.91	0.13	63,63,63,63	0
57	MG	BA	3027	1/1	0.91	0.44	64,64,64,64	0
57	MG	CA	3055	1/1	0.91	0.26	63,63,63,63	0
57	MG	DA	3324	1/1	0.91	0.09	54,54,54,54	0
57	MG	DA	3327	1/1	0.91	0.13	45,45,45,45	0
57	MG	DA	3607	1/1	0.91	0.10	64,64,64,64	0
57	MG	AA	1789	1/1	0.91	0.19	60,60,60,60	0
57	MG	BA	3751	1/1	0.91	0.19	37,37,37,37	0
57	MG	BA	3752	1/1	0.91	0.07	34,34,34,34	0
57	MG	DA	3614	1/1	0.91	0.15	55,55,55,55	0
57	MG	DA	3059	1/1	0.91	0.13	50,50,50,50	0
57	MG	DA	3335	1/1	0.91	0.15	49,49,49,49	0
57	MG	DA	3336	1/1	0.91	0.08	49,49,49,49	0
57	MG	DA	3341	1/1	0.91	0.10	55,55,55,55	0
57	MG	CA	3063	1/1	0.91	0.15	65,65,65,65	0
57	MG	BA	3058	1/1	0.91	0.11	54,54,54,54	0
57	MG	BA	3757	1/1	0.91	0.16	43,43,43,43	0
57	MG	BA	3505	1/1	0.91	0.15	53,53,53,53	0
57	MG	BA	3764	1/1	0.91	0.19	66,66,66,66	0
57	MG	DA	3067	1/1	0.91	0.19	63,63,63,63	0
57	MG	DA	3627	1/1	0.91	0.16	57,57,57,57	0
57	MG	AA	1722	1/1	0.91	0.19	57,57,57,57	0
57	MG	BA	3768	1/1	0.91	0.14	57,57,57,57	0
57	MG	DA	3363	1/1	0.91	0.13	50,50,50,50	0
57	MG	DA	3634	1/1	0.91	0.12	68,68,68,68	0
57	MG	AA	1658	1/1	0.91	0.28	64,64,64,64	0
57	MG	DA	3367	1/1	0.91	0.12	49,49,49,49	0
57	MG	BA	3348	1/1	0.91	0.09	37,37,37,37	0
57	MG	DA	3643	1/1	0.91	0.12	54,54,54,54	0
57	MG	DA	3369	1/1	0.91	0.10	55,55,55,55	0
57	MG	AA	1761	1/1	0.91	0.16	70,70,70,70	0
57	MG	DA	3086	1/1	0.91	0.10	47,47,47,47	0
57	MG	DA	3379	1/1	0.91	0.08	46,46,46,46	0
57	MG	BA	3781	1/1	0.91	0.10	56,56,56,56	0
57	MG	BA	3785	1/1	0.91	0.19	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3653	1/1	0.91	0.10	33,33,33,33	0
57	MG	BA	3231	1/1	0.91	0.10	57,57,57,57	0
57	MG	CA	3099	1/1	0.91	0.15	64,64,64,64	0
57	MG	BA	3790	1/1	0.91	0.23	66,66,66,66	0
57	MG	BA	3358	1/1	0.91	0.11	52,52,52,52	0
57	MG	AA	1659	1/1	0.91	0.30	65,65,65,65	0
57	MG	BA	3365	1/1	0.91	0.09	51,51,51,51	0
57	MG	DB	3005	1/1	0.91	0.14	68,68,68,68	0
57	MG	DB	3007	1/1	0.91	0.16	67,67,67,67	0
57	MG	BA	3662	1/1	0.91	0.13	62,62,62,62	0
57	MG	AX	3010	1/1	0.91	0.40	68,68,68,68	0
57	MG	DA	3110	1/1	0.91	0.12	49,49,49,49	0
57	MG	BA	3242	1/1	0.91	0.50	55,55,55,55	0
57	MG	BA	3668	1/1	0.91	0.13	75,75,75,75	0
57	MG	DF	301	1/1	0.91	0.11	48,48,48,48	0
57	MG	DA	3114	1/1	0.91	0.14	51,51,51,51	0
57	MG	DA	3115	1/1	0.91	0.11	55,55,55,55	0
57	MG	DN	5001	1/1	0.91	0.08	63,63,63,63	0
57	MG	DA	3120	1/1	0.91	0.34	56,56,56,56	0
57	MG	AA	1804	1/1	0.91	0.18	70,70,70,70	0
57	MG	BB	3006	1/1	0.91	0.12	62,62,62,62	0
57	MG	BA	3672	1/1	0.91	0.18	44,44,44,44	0
57	MG	BA	3094	1/1	0.91	0.14	52,52,52,52	0
57	MG	BA	3690	1/1	0.92	0.08	39,39,39,39	0
57	MG	DA	3147	1/1	0.92	0.12	44,44,44,44	0
57	MG	BE	306	1/1	0.92	0.07	38,38,38,38	0
57	MG	BA	3410	1/1	0.92	0.08	55,55,55,55	0
57	MG	BA	3288	1/1	0.92	0.11	44,44,44,44	0
57	MG	BA	3414	1/1	0.92	0.07	54,54,54,54	0
57	MG	BA	3289	1/1	0.92	0.12	49,49,49,49	0
57	MG	DA	3160	1/1	0.92	0.13	62,62,62,62	0
57	MG	DA	3166	1/1	0.92	0.23	55,55,55,55	0
57	MG	BA	3290	1/1	0.92	0.14	57,57,57,57	0
57	MG	B0	3001	1/1	0.92	0.14	47,47,47,47	0
57	MG	DA	3446	1/1	0.92	0.15	50,50,50,50	0
57	MG	BA	3420	1/1	0.92	0.10	25,25,25,25	0
57	MG	DA	3449	1/1	0.92	0.08	34,34,34,34	0
57	MG	DA	3454	1/1	0.92	0.09	43,43,43,43	0
57	MG	BA	3704	1/1	0.92	0.16	26,26,26,26	0
57	MG	CA	3136	1/1	0.92	0.15	48,48,48,48	0
57	MG	DA	3457	1/1	0.92	0.07	44,44,44,44	0
57	MG	DA	3187	1/1	0.92	0.12	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AM	3001	1/1	0.92	0.06	66,66,66,66	0
57	MG	DA	3191	1/1	0.92	0.14	54,54,54,54	0
57	MG	DA	3468	1/1	0.92	0.11	62,62,62,62	0
57	MG	AA	1602	1/1	0.92	0.10	68,68,68,68	0
57	MG	CA	3140	1/1	0.92	0.13	57,57,57,57	0
57	MG	BA	3711	1/1	0.92	0.20	44,44,44,44	0
57	MG	DA	3485	1/1	0.92	0.11	56,56,56,56	0
57	MG	CA	3003	1/1	0.92	0.10	58,58,58,58	0
57	MG	BA	3584	1/1	0.92	0.08	55,55,55,55	0
57	MG	BA	3301	1/1	0.92	0.15	62,62,62,62	0
57	MG	DA	3490	1/1	0.92	0.09	33,33,33,33	0
57	MG	CA	3006	1/1	0.92	0.10	68,68,68,68	0
57	MG	BA	3433	1/1	0.92	0.10	27,27,27,27	0
57	MG	DA	3493	1/1	0.92	0.09	51,51,51,51	0
57	MG	DA	3495	1/1	0.92	0.07	50,50,50,50	0
57	MG	CA	3008	1/1	0.92	0.25	47,47,47,47	0
57	MG	BA	3081	1/1	0.92	0.24	48,48,48,48	0
57	MG	CA	3150	1/1	0.92	0.15	65,65,65,65	0
57	MG	CA	3011	1/1	0.92	0.34	66,66,66,66	0
57	MG	AA	1764	1/1	0.92	0.16	66,66,66,66	0
57	MG	BA	3438	1/1	0.92	0.11	35,35,35,35	0
57	MG	AA	1609	1/1	0.92	0.18	63,63,63,63	0
57	MG	CA	3159	1/1	0.92	0.26	62,62,62,62	0
57	MG	BA	3441	1/1	0.92	0.10	39,39,39,39	0
57	MG	BA	3215	1/1	0.92	0.19	37,37,37,37	0
57	MG	DA	3520	1/1	0.92	0.10	57,57,57,57	0
57	MG	DA	3237	1/1	0.92	0.13	59,59,59,59	0
57	MG	BA	3096	1/1	0.92	0.28	60,60,60,60	0
57	MG	DA	3241	1/1	0.92	0.14	55,55,55,55	0
57	MG	DA	3243	1/1	0.92	0.08	48,48,48,48	0
57	MG	BA	3446	1/1	0.92	0.07	59,59,59,59	0
57	MG	AU	101	1/1	0.92	0.12	56,56,56,56	0
57	MG	AA	1805	1/1	0.92	0.08	48,48,48,48	0
57	MG	BA	3014	1/1	0.92	0.10	35,35,35,35	0
57	MG	BA	3621	1/1	0.92	0.18	43,43,43,43	0
57	MG	DA	3255	1/1	0.92	0.13	47,47,47,47	0
57	MG	DA	3540	1/1	0.92	0.07	50,50,50,50	0
57	MG	BA	3460	1/1	0.92	0.08	52,52,52,52	0
57	MG	AA	1676	1/1	0.92	0.10	58,58,58,58	0
57	MG	BA	3107	1/1	0.92	0.28	57,57,57,57	0
57	MG	BA	3468	1/1	0.92	0.08	45,45,45,45	0
57	MG	DA	3549	1/1	0.92	0.10	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	3031	1/1	0.92	0.24	58,58,58,58	0
57	MG	DA	3270	1/1	0.92	0.15	42,42,42,42	0
57	MG	AA	1807	1/1	0.92	0.14	68,68,68,68	0
57	MG	DA	3281	1/1	0.92	0.08	36,36,36,36	0
57	MG	CA	3033	1/1	0.92	0.20	54,54,54,54	0
57	MG	AA	1707	1/1	0.92	0.16	57,57,57,57	0
57	MG	DA	3285	1/1	0.92	0.10	50,50,50,50	0
57	MG	BA	3019	1/1	0.92	0.20	54,54,54,54	0
57	MG	DA	3006	1/1	0.92	0.10	41,41,41,41	0
57	MG	DA	3568	1/1	0.92	0.10	43,43,43,43	0
57	MG	CA	3037	1/1	0.92	0.10	53,53,53,53	0
57	MG	BA	3129	1/1	0.92	0.12	54,54,54,54	0
57	MG	BA	3638	1/1	0.92	0.20	65,65,65,65	0
57	MG	BA	3753	1/1	0.92	0.13	68,68,68,68	0
57	MG	DA	3576	1/1	0.92	0.16	67,67,67,67	0
57	MG	CA	3042	1/1	0.92	0.10	57,57,57,57	0
57	MG	AX	3006	1/1	0.92	0.13	68,68,68,68	0
57	MG	BA	3496	1/1	0.92	0.11	51,51,51,51	0
57	MG	DA	3587	1/1	0.92	0.08	51,51,51,51	0
57	MG	DA	3588	1/1	0.92	0.10	59,59,59,59	0
57	MG	DA	3590	1/1	0.92	0.11	51,51,51,51	0
57	MG	BA	3761	1/1	0.92	0.09	36,36,36,36	0
57	MG	BA	3349	1/1	0.92	0.09	34,34,34,34	0
57	MG	BA	3026	1/1	0.92	0.14	60,60,60,60	0
57	MG	DA	3045	1/1	0.92	0.12	51,51,51,51	0
57	MG	DA	3046	1/1	0.92	0.20	56,56,56,56	0
57	MG	BA	3645	1/1	0.92	0.08	47,47,47,47	0
57	MG	DA	3597	1/1	0.92	0.14	48,48,48,48	0
57	MG	BA	3500	1/1	0.92	0.11	57,57,57,57	0
57	MG	AA	1811	1/1	0.92	0.18	49,49,49,49	0
57	MG	DA	3318	1/1	0.92	0.08	45,45,45,45	0
57	MG	BA	3773	1/1	0.92	0.23	32,32,32,32	0
57	MG	DA	3325	1/1	0.92	0.24	45,45,45,45	0
57	MG	DA	3326	1/1	0.92	0.09	46,46,46,46	0
57	MG	CA	3060	1/1	0.92	0.16	71,71,71,71	0
57	MG	CA	3061	1/1	0.92	0.12	66,66,66,66	0
57	MG	CA	3062	1/1	0.92	0.15	64,64,64,64	0
57	MG	BA	3651	1/1	0.92	0.12	66,66,66,66	0
57	MG	CA	3069	1/1	0.92	0.19	58,58,58,58	0
57	MG	BA	3153	1/1	0.92	0.11	45,45,45,45	0
57	MG	BA	3267	1/1	0.92	0.18	61,61,61,61	0
57	MG	DA	3337	1/1	0.92	0.09	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3508	1/1	0.92	0.10	20,20,20,20	0
57	MG	DA	3069	1/1	0.92	0.10	43,43,43,43	0
57	MG	BA	3154	1/1	0.92	0.09	52,52,52,52	0
57	MG	DA	3071	1/1	0.92	0.10	47,47,47,47	0
57	MG	CA	3078	1/1	0.92	0.23	65,65,65,65	0
57	MG	DA	3350	1/1	0.92	0.10	31,31,31,31	0
57	MG	BA	3789	1/1	0.92	0.12	47,47,47,47	0
57	MG	DA	3352	1/1	0.92	0.07	34,34,34,34	0
57	MG	DA	3078	1/1	0.92	0.07	47,47,47,47	0
57	MG	CA	3084	1/1	0.92	0.24	56,56,56,56	0
57	MG	BA	3366	1/1	0.92	0.10	52,52,52,52	0
57	MG	DA	3636	1/1	0.92	0.10	62,62,62,62	0
57	MG	BA	3030	1/1	0.92	0.14	39,39,39,39	0
57	MG	AA	1689	1/1	0.92	0.33	71,71,71,71	0
57	MG	BA	3057	1/1	0.92	0.09	48,48,48,48	0
57	MG	BA	3276	1/1	0.92	0.17	44,44,44,44	0
57	MG	BA	3803	1/1	0.92	0.21	55,55,55,55	0
57	MG	BA	3376	1/1	0.92	0.09	29,29,29,29	0
57	MG	BA	3185	1/1	0.92	0.08	33,33,33,33	0
57	MG	CA	3100	1/1	0.92	0.17	59,59,59,59	0
57	MG	DA	3385	1/1	0.92	0.10	60,60,60,60	0
57	MG	CA	3101	1/1	0.92	0.13	65,65,65,65	0
57	MG	DA	3104	1/1	0.92	0.10	57,57,57,57	0
57	MG	BA	3812	1/1	0.92	0.12	42,42,42,42	0
57	MG	BA	3379	1/1	0.92	0.07	35,35,35,35	0
57	MG	AA	1670	1/1	0.92	0.22	67,67,67,67	0
57	MG	BB	3005	1/1	0.92	0.18	51,51,51,51	0
57	MG	DA	3399	1/1	0.92	0.10	59,59,59,59	0
57	MG	AA	1779	1/1	0.92	0.14	59,59,59,59	0
57	MG	AA	1696	1/1	0.92	0.11	83,83,83,83	0
57	MG	DB	3006	1/1	0.92	0.07	55,55,55,55	0
57	MG	BA	3681	1/1	0.92	0.19	61,61,61,61	0
57	MG	DA	3116	1/1	0.92	0.18	53,53,53,53	0
57	MG	BA	3401	1/1	0.92	0.14	26,26,26,26	0
57	MG	AA	1796	1/1	0.92	0.16	64,64,64,64	0
57	MG	DA	3123	1/1	0.92	0.21	54,54,54,54	0
57	MG	DD	303	1/1	0.92	0.20	51,51,51,51	0
57	MG	DA	3126	1/1	0.92	0.19	59,59,59,59	0
57	MG	DE	3007	1/1	0.92	0.10	58,58,58,58	0
57	MG	DA	3127	1/1	0.92	0.15	52,52,52,52	0
57	MG	DA	3129	1/1	0.92	0.21	56,56,56,56	0
57	MG	BA	3565	1/1	0.92	0.13	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3131	1/1	0.92	0.10	49,49,49,49	0
57	MG	BA	3568	1/1	0.92	0.16	24,24,24,24	0
57	MG	CA	3116	1/1	0.92	0.24	57,57,57,57	0
57	MG	BA	3407	1/1	0.92	0.08	32,32,32,32	0
57	MG	BD	3003	1/1	0.92	0.10	37,37,37,37	0
57	MG	DA	3423	1/1	0.92	0.14	37,37,37,37	0
57	MG	DA	3010	1/1	0.93	0.06	41,41,41,41	0
57	MG	BA	3618	1/1	0.93	0.09	35,35,35,35	0
57	MG	BA	3619	1/1	0.93	0.07	28,28,28,28	0
57	MG	DA	3480	1/1	0.93	0.10	58,58,58,58	0
57	MG	DA	3245	1/1	0.93	0.26	58,58,58,58	0
57	MG	DA	3482	1/1	0.93	0.17	60,60,60,60	0
57	MG	AA	1700	1/1	0.93	0.16	71,71,71,71	0
57	MG	BA	3622	1/1	0.93	0.11	43,43,43,43	0
57	MG	BA	3176	1/1	0.93	0.14	55,55,55,55	0
57	MG	DA	3252	1/1	0.93	0.07	50,50,50,50	0
57	MG	DA	3026	1/1	0.93	0.22	50,50,50,50	0
57	MG	BA	3316	1/1	0.93	0.12	54,54,54,54	0
57	MG	AA	1642	1/1	0.93	0.25	59,59,59,59	0
57	MG	DA	3034	1/1	0.93	0.08	42,42,42,42	0
57	MG	BA	3627	1/1	0.93	0.15	56,56,56,56	0
57	MG	AA	1604	1/1	0.93	0.12	58,58,58,58	0
57	MG	DA	3499	1/1	0.93	0.12	52,52,52,52	0
57	MG	DA	3042	1/1	0.93	0.12	49,49,49,49	0
57	MG	AA	1657	1/1	0.93	0.14	64,64,64,64	0
57	MG	DA	3506	1/1	0.93	0.13	55,55,55,55	0
57	MG	DA	3507	1/1	0.93	0.09	59,59,59,59	0
57	MG	BA	3194	1/1	0.93	0.20	39,39,39,39	0
57	MG	DA	3273	1/1	0.93	0.15	62,62,62,62	0
57	MG	DA	3512	1/1	0.93	0.07	37,37,37,37	0
57	MG	DA	3274	1/1	0.93	0.13	40,40,40,40	0
57	MG	BA	3028	1/1	0.93	0.17	37,37,37,37	0
57	MG	BA	3332	1/1	0.93	0.12	54,54,54,54	0
57	MG	BA	3476	1/1	0.93	0.11	48,48,48,48	0
57	MG	CA	3066	1/1	0.93	0.19	48,48,48,48	0
57	MG	AA	1678	1/1	0.93	0.17	47,47,47,47	0
57	MG	BA	3481	1/1	0.93	0.11	54,54,54,54	0
57	MG	CA	3071	1/1	0.93	0.18	56,56,56,56	0
57	MG	CA	3072	1/1	0.93	0.21	62,62,62,62	0
57	MG	AA	1606	1/1	0.93	0.09	54,54,54,54	0
57	MG	BA	3045	1/1	0.93	0.17	39,39,39,39	0
57	MG	DA	3292	1/1	0.93	0.07	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3064	1/1	0.93	0.07	46,46,46,46	0
57	MG	BA	3052	1/1	0.93	0.20	50,50,50,50	0
57	MG	BA	3055	1/1	0.93	0.17	37,37,37,37	0
57	MG	AA	1646	1/1	0.93	0.28	58,58,58,58	0
57	MG	BA	3648	1/1	0.93	0.17	58,58,58,58	0
57	MG	BA	3804	1/1	0.93	0.07	36,36,36,36	0
57	MG	AA	1634	1/1	0.93	0.17	64,64,64,64	0
57	MG	BA	3806	1/1	0.93	0.17	43,43,43,43	0
57	MG	BA	3213	1/1	0.93	0.13	43,43,43,43	0
57	MG	BA	3347	1/1	0.93	0.10	38,38,38,38	0
57	MG	AA	1686	1/1	0.93	0.12	61,61,61,61	0
57	MG	BA	3506	1/1	0.93	0.16	61,61,61,61	0
57	MG	BA	3064	1/1	0.93	0.09	45,45,45,45	0
57	MG	DA	3555	1/1	0.93	0.14	46,46,46,46	0
57	MG	AA	1754	1/1	0.93	0.14	58,58,58,58	0
57	MG	BA	3067	1/1	0.93	0.15	43,43,43,43	0
57	MG	BA	3513	1/1	0.93	0.22	50,50,50,50	0
57	MG	AX	3003	1/1	0.93	0.12	56,56,56,56	0
57	MG	BA	3360	1/1	0.93	0.16	37,37,37,37	0
57	MG	DA	3566	1/1	0.93	0.14	37,37,37,37	0
57	MG	BA	3519	1/1	0.93	0.11	45,45,45,45	0
57	MG	AA	1648	1/1	0.93	0.20	56,56,56,56	0
57	MG	DA	3569	1/1	0.93	0.12	45,45,45,45	0
57	MG	AA	1637	1/1	0.93	0.17	61,61,61,61	0
57	MG	AA	1797	1/1	0.93	0.19	59,59,59,59	0
57	MG	AA	1665	1/1	0.93	0.16	55,55,55,55	0
57	MG	BE	303	1/1	0.93	0.10	43,43,43,43	0
57	MG	BA	3532	1/1	0.93	0.17	55,55,55,55	0
57	MG	BA	3243	1/1	0.93	0.38	44,44,44,44	0
57	MG	BF	307	1/1	0.93	0.11	34,34,34,34	0
57	MG	DA	3580	1/1	0.93	0.12	62,62,62,62	0
57	MG	BA	3093	1/1	0.93	0.19	41,41,41,41	0
57	MG	DA	3347	1/1	0.93	0.08	35,35,35,35	0
57	MG	AX	3009	1/1	0.93	0.31	65,65,65,65	0
57	MG	BP	3001	1/1	0.93	0.13	34,34,34,34	0
57	MG	DA	3117	1/1	0.93	0.13	56,56,56,56	0
57	MG	DA	3118	1/1	0.93	0.09	39,39,39,39	0
57	MG	BR	5001	1/1	0.93	0.13	50,50,50,50	0
57	MG	DA	3357	1/1	0.93	0.08	33,33,33,33	0
57	MG	AA	1693	1/1	0.93	0.30	76,76,76,76	0
57	MG	BA	3249	1/1	0.93	0.13	53,53,53,53	0
57	MG	BZ	302	1/1	0.93	0.11	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3559	1/1	0.93	0.11	26,26,26,26	0
57	MG	DA	3128	1/1	0.93	0.33	56,56,56,56	0
57	MG	BA	3691	1/1	0.93	0.06	43,43,43,43	0
57	MG	BA	3250	1/1	0.93	0.25	68,68,68,68	0
57	MG	B4	502	1/1	0.93	0.07	70,70,70,70	0
57	MG	AA	1763	1/1	0.93	0.06	79,79,79,79	0
57	MG	BA	3564	1/1	0.93	0.06	44,44,44,44	0
57	MG	DA	3380	1/1	0.93	0.07	66,66,66,66	0
57	MG	CA	3001	1/1	0.93	0.10	59,59,59,59	0
57	MG	DA	3389	1/1	0.93	0.13	59,59,59,59	0
57	MG	AA	1720	1/1	0.93	0.21	55,55,55,55	0
57	MG	BA	3263	1/1	0.93	0.30	60,60,60,60	0
57	MG	AA	1721	1/1	0.93	0.12	57,57,57,57	0
57	MG	BA	3266	1/1	0.93	0.10	44,44,44,44	0
57	MG	AX	3014	1/1	0.93	0.24	61,61,61,61	0
57	MG	BA	3408	1/1	0.93	0.10	51,51,51,51	0
57	MG	BA	3106	1/1	0.93	0.12	52,52,52,52	0
57	MG	BA	3270	1/1	0.93	0.26	56,56,56,56	0
57	MG	CA	3147	1/1	0.93	0.14	70,70,70,70	0
57	MG	DA	3161	1/1	0.93	0.21	50,50,50,50	0
57	MG	DA	3165	1/1	0.93	0.24	55,55,55,55	0
57	MG	BA	3413	1/1	0.93	0.09	37,37,37,37	0
57	MG	DA	3408	1/1	0.93	0.12	55,55,55,55	0
57	MG	AA	1695	1/1	0.93	0.11	59,59,59,59	0
57	MG	AA	1639	1/1	0.93	0.12	54,54,54,54	0
57	MG	AA	1726	1/1	0.93	0.18	58,58,58,58	0
57	MG	DA	3175	1/1	0.93	0.12	41,41,41,41	0
57	MG	DA	3639	1/1	0.93	0.23	59,59,59,59	0
57	MG	DA	3640	1/1	0.93	0.22	62,62,62,62	0
57	MG	BA	3720	1/1	0.93	0.07	38,38,38,38	0
57	MG	DA	3416	1/1	0.93	0.10	52,52,52,52	0
57	MG	BA	3591	1/1	0.93	0.38	41,41,41,41	0
57	MG	AA	1812	1/1	0.93	0.16	63,63,63,63	0
57	MG	CA	3156	1/1	0.93	0.12	59,59,59,59	0
57	MG	CA	3158	1/1	0.93	0.17	55,55,55,55	0
57	MG	DA	3192	1/1	0.93	0.23	34,34,34,34	0
57	MG	AA	1814	1/1	0.93	0.20	57,57,57,57	0
57	MG	BA	3596	1/1	0.93	0.12	59,59,59,59	0
57	MG	DA	3197	1/1	0.93	0.25	59,59,59,59	0
57	MG	AA	1815	1/1	0.93	0.14	47,47,47,47	0
57	MG	DA	3662	1/1	0.93	0.20	50,50,50,50	0
57	MG	DA	3429	1/1	0.93	0.15	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3430	1/1	0.93	0.10	34,34,34,34	0
57	MG	BA	3599	1/1	0.93	0.10	60,60,60,60	0
57	MG	BA	3141	1/1	0.93	0.09	38,38,38,38	0
57	MG	DA	3203	1/1	0.93	0.21	53,53,53,53	0
57	MG	BA	3144	1/1	0.93	0.13	41,41,41,41	0
57	MG	DA	3211	1/1	0.93	0.12	51,51,51,51	0
57	MG	BA	3602	1/1	0.93	0.09	47,47,47,47	0
57	MG	DB	3008	1/1	0.93	0.17	56,56,56,56	0
57	MG	DA	3443	1/1	0.93	0.16	51,51,51,51	0
57	MG	AA	1774	1/1	0.93	0.18	51,51,51,51	0
57	MG	BA	3015	1/1	0.93	0.11	47,47,47,47	0
57	MG	BA	3740	1/1	0.93	0.16	65,65,65,65	0
57	MG	AA	1626	1/1	0.93	0.29	59,59,59,59	0
57	MG	AE	3001	1/1	0.93	0.07	63,63,63,63	0
57	MG	BA	3613	1/1	0.93	0.20	53,53,53,53	0
57	MG	BA	3293	1/1	0.93	0.09	58,58,58,58	0
57	MG	CA	3038	1/1	0.93	0.17	57,57,57,57	0
57	MG	DF	303	1/1	0.93	0.07	42,42,42,42	0
57	MG	BA	3161	1/1	0.93	0.15	44,44,44,44	0
57	MG	DA	3235	1/1	0.93	0.08	48,48,48,48	0
57	MG	AA	1777	1/1	0.93	0.08	71,71,71,71	0
57	MG	BA	3617	1/1	0.93	0.09	42,42,42,42	0
57	MG	DA	3465	1/1	0.93	0.11	42,42,42,42	0
57	MG	DV	201	1/1	0.93	0.19	58,58,58,58	0
57	MG	DA	3466	1/1	0.93	0.07	48,48,48,48	0
57	MG	D3	3001	1/1	0.93	0.13	63,63,63,63	0
57	MG	DA	3467	1/1	0.93	0.11	52,52,52,52	0
57	MG	AA	1675	1/1	0.94	0.23	61,61,61,61	0
57	MG	BA	3697	1/1	0.94	0.15	41,41,41,41	0
57	MG	B7	105	1/1	0.94	0.18	28,28,28,28	0
57	MG	B8	5002	1/1	0.94	0.21	53,53,53,53	0
57	MG	BA	3405	1/1	0.94	0.12	52,52,52,52	0
57	MG	DA	3451	1/1	0.94	0.06	55,55,55,55	0
57	MG	DA	3193	1/1	0.94	0.10	47,47,47,47	0
57	MG	BA	3165	1/1	0.94	0.14	52,52,52,52	0
57	MG	BA	3170	1/1	0.94	0.11	38,38,38,38	0
57	MG	BA	3056	1/1	0.94	0.14	46,46,46,46	0
57	MG	DA	3198	1/1	0.94	0.24	52,52,52,52	0
57	MG	DA	3461	1/1	0.94	0.08	51,51,51,51	0
57	MG	CA	3151	1/1	0.94	0.14	64,64,64,64	0
57	MG	AA	1640	1/1	0.94	0.19	54,54,54,54	0
57	MG	DA	3464	1/1	0.94	0.11	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	1698	1/1	0.94	0.12	58,58,58,58	0
57	MG	BA	3179	1/1	0.94	0.18	43,43,43,43	0
57	MG	BA	3415	1/1	0.94	0.09	35,35,35,35	0
57	MG	AA	1760	1/1	0.94	0.14	65,65,65,65	0
57	MG	DA	3208	1/1	0.94	0.23	54,54,54,54	0
57	MG	DA	3474	1/1	0.94	0.06	53,53,53,53	0
57	MG	AA	1660	1/1	0.94	0.26	51,51,51,51	0
57	MG	BA	3291	1/1	0.94	0.14	53,53,53,53	0
57	MG	BA	3422	1/1	0.94	0.09	36,36,36,36	0
57	MG	BA	3065	1/1	0.94	0.08	50,50,50,50	0
57	MG	DA	3484	1/1	0.94	0.10	46,46,46,46	0
57	MG	BA	3426	1/1	0.94	0.10	46,46,46,46	0
57	MG	DA	3220	1/1	0.94	0.27	50,50,50,50	0
57	MG	CA	3163	1/1	0.94	0.17	62,62,62,62	0
57	MG	BA	3295	1/1	0.94	0.10	23,23,23,23	0
57	MG	AA	1803	1/1	0.94	0.09	46,46,46,46	0
57	MG	DA	3230	1/1	0.94	0.09	46,46,46,46	0
57	MG	DA	3231	1/1	0.94	0.23	61,61,61,61	0
57	MG	BA	3297	1/1	0.94	0.07	42,42,42,42	0
57	MG	CD	502	1/1	0.94	0.28	53,53,53,53	0
57	MG	AA	1762	1/1	0.94	0.21	66,66,66,66	0
57	MG	CA	3020	1/1	0.94	0.10	45,45,45,45	0
57	MG	DA	3500	1/1	0.94	0.16	55,55,55,55	0
57	MG	BA	3300	1/1	0.94	0.12	53,53,53,53	0
57	MG	AA	1628	1/1	0.94	0.11	65,65,65,65	0
57	MG	BA	3437	1/1	0.94	0.18	62,62,62,62	0
57	MG	DA	3239	1/1	0.94	0.10	49,49,49,49	0
57	MG	CW	3001	1/1	0.94	0.10	66,66,66,66	0
57	MG	BA	3603	1/1	0.94	0.21	42,42,42,42	0
57	MG	BA	3306	1/1	0.94	0.10	15,15,15,15	0
57	MG	CA	3028	1/1	0.94	0.17	48,48,48,48	0
57	MG	BA	3606	1/1	0.94	0.07	36,36,36,36	0
57	MG	BA	3309	1/1	0.94	0.14	65,65,65,65	0
57	MG	BA	3313	1/1	0.94	0.12	38,38,38,38	0
57	MG	AA	1725	1/1	0.94	0.15	51,51,51,51	0
57	MG	DA	3009	1/1	0.94	0.16	61,61,61,61	0
57	MG	DA	3522	1/1	0.94	0.09	51,51,51,51	0
57	MG	BA	3078	1/1	0.94	0.26	54,54,54,54	0
57	MG	CA	3034	1/1	0.94	0.32	66,66,66,66	0
57	MG	AA	1765	1/1	0.94	0.21	65,65,65,65	0
57	MG	BA	3448	1/1	0.94	0.06	17,17,17,17	0
57	MG	BA	3748	1/1	0.94	0.27	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3267	1/1	0.94	0.07	44,44,44,44	0
57	MG	AA	1680	1/1	0.94	0.19	51,51,51,51	0
57	MG	AA	1727	1/1	0.94	0.11	50,50,50,50	0
57	MG	AA	1769	1/1	0.94	0.11	50,50,50,50	0
57	MG	AA	1770	1/1	0.94	0.07	51,51,51,51	0
57	MG	BA	3754	1/1	0.94	0.08	42,42,42,42	0
57	MG	BA	3218	1/1	0.94	0.07	45,45,45,45	0
57	MG	CA	3047	1/1	0.94	0.10	50,50,50,50	0
57	MG	CA	3048	1/1	0.94	0.08	58,58,58,58	0
57	MG	BA	3095	1/1	0.94	0.17	53,53,53,53	0
57	MG	BA	3222	1/1	0.94	0.08	42,42,42,42	0
57	MG	BA	3762	1/1	0.94	0.09	20,20,20,20	0
57	MG	AA	1702	1/1	0.94	0.20	47,47,47,47	0
57	MG	CA	3054	1/1	0.94	0.33	69,69,69,69	0
57	MG	BA	3001	1/1	0.94	0.09	43,43,43,43	0
57	MG	AA	1682	1/1	0.94	0.30	59,59,59,59	0
57	MG	BA	3767	1/1	0.94	0.11	45,45,45,45	0
57	MG	BA	3628	1/1	0.94	0.20	52,52,52,52	0
57	MG	DA	3296	1/1	0.94	0.14	60,60,60,60	0
57	MG	DA	3561	1/1	0.94	0.10	52,52,52,52	0
57	MG	BA	3010	1/1	0.94	0.20	53,53,53,53	0
57	MG	BA	3630	1/1	0.94	0.17	39,39,39,39	0
57	MG	BA	3631	1/1	0.94	0.16	46,46,46,46	0
57	MG	BA	3482	1/1	0.94	0.07	51,51,51,51	0
57	MG	CA	3064	1/1	0.94	0.31	55,55,55,55	0
57	MG	DA	3310	1/1	0.94	0.07	35,35,35,35	0
57	MG	BA	3237	1/1	0.94	0.08	44,44,44,44	0
57	MG	CA	3068	1/1	0.94	0.13	58,58,58,58	0
57	MG	BA	3485	1/1	0.94	0.11	26,26,26,26	0
57	MG	DA	3575	1/1	0.94	0.09	56,56,56,56	0
57	MG	BA	3345	1/1	0.94	0.12	51,51,51,51	0
57	MG	BA	3787	1/1	0.94	0.07	45,45,45,45	0
57	MG	AA	1737	1/1	0.94	0.11	60,60,60,60	0
57	MG	DA	3579	1/1	0.94	0.11	62,62,62,62	0
57	MG	DA	3319	1/1	0.94	0.09	33,33,33,33	0
57	MG	DA	3583	1/1	0.94	0.10	52,52,52,52	0
57	MG	BA	3492	1/1	0.94	0.06	38,38,38,38	0
57	MG	DA	3077	1/1	0.94	0.07	38,38,38,38	0
57	MG	CA	3074	1/1	0.94	0.17	60,60,60,60	0
57	MG	CA	3075	1/1	0.94	0.20	65,65,65,65	0
57	MG	AA	1622	1/1	0.94	0.15	69,69,69,69	0
57	MG	DA	3085	1/1	0.94	0.14	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	1653	1/1	0.94	0.16	54,54,54,54	0
57	MG	DA	3333	1/1	0.94	0.11	47,47,47,47	0
57	MG	BA	3110	1/1	0.94	0.08	36,36,36,36	0
57	MG	DA	3088	1/1	0.94	0.13	50,50,50,50	0
57	MG	CA	3081	1/1	0.94	0.12	44,44,44,44	0
57	MG	AA	1616	1/1	0.94	0.07	73,73,73,73	0
57	MG	BA	3801	1/1	0.94	0.10	71,71,71,71	0
57	MG	AA	1742	1/1	0.94	0.10	52,52,52,52	0
57	MG	DA	3604	1/1	0.94	0.11	61,61,61,61	0
57	MG	BA	3353	1/1	0.94	0.10	55,55,55,55	0
57	MG	AA	1687	1/1	0.94	0.22	46,46,46,46	0
57	MG	AA	1619	1/1	0.94	0.15	64,64,64,64	0
57	MG	BA	3130	1/1	0.94	0.26	48,48,48,48	0
57	MG	DA	3610	1/1	0.94	0.09	47,47,47,47	0
57	MG	DA	3349	1/1	0.94	0.10	34,34,34,34	0
57	MG	BA	3654	1/1	0.94	0.10	59,59,59,59	0
57	MG	BA	3135	1/1	0.94	0.34	56,56,56,56	0
57	MG	DA	3109	1/1	0.94	0.10	49,49,49,49	0
57	MG	CA	3097	1/1	0.94	0.21	60,60,60,60	0
57	MG	BA	3137	1/1	0.94	0.19	52,52,52,52	0
57	MG	BA	3516	1/1	0.94	0.12	46,46,46,46	0
57	MG	DA	3361	1/1	0.94	0.06	33,33,33,33	0
57	MG	AA	1645	1/1	0.94	0.21	61,61,61,61	0
57	MG	DA	3622	1/1	0.94	0.14	49,49,49,49	0
57	MG	BA	3664	1/1	0.94	0.18	69,69,69,69	0
57	MG	BA	3264	1/1	0.94	0.18	51,51,51,51	0
57	MG	AA	1691	1/1	0.94	0.27	62,62,62,62	0
57	MG	AA	1750	1/1	0.94	0.08	49,49,49,49	0
57	MG	AA	1751	1/1	0.94	0.20	53,53,53,53	0
57	MG	DA	3371	1/1	0.94	0.08	34,34,34,34	0
57	MG	DA	3375	1/1	0.94	0.15	57,57,57,57	0
57	MG	BA	3526	1/1	0.94	0.18	41,41,41,41	0
57	MG	AA	1612	1/1	0.94	0.07	63,63,63,63	0
57	MG	DA	3125	1/1	0.94	0.17	56,56,56,56	0
57	MG	BD	3002	1/1	0.94	0.10	28,28,28,28	0
57	MG	DA	3638	1/1	0.94	0.06	47,47,47,47	0
57	MG	AA	1621	1/1	0.94	0.08	44,44,44,44	0
57	MG	BA	3381	1/1	0.94	0.07	49,49,49,49	0
57	MG	BA	3383	1/1	0.94	0.07	37,37,37,37	0
57	MG	BE	304	1/1	0.94	0.11	23,23,23,23	0
57	MG	BA	3536	1/1	0.94	0.06	32,32,32,32	0
57	MG	DA	3133	1/1	0.94	0.09	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3134	1/1	0.94	0.11	52,52,52,52	0
57	MG	BA	3385	1/1	0.94	0.13	30,30,30,30	0
57	MG	DA	3397	1/1	0.94	0.09	42,42,42,42	0
57	MG	DA	3648	1/1	0.94	0.12	62,62,62,62	0
57	MG	DA	3136	1/1	0.94	0.15	48,48,48,48	0
57	MG	DA	3138	1/1	0.94	0.12	54,54,54,54	0
57	MG	BA	3386	1/1	0.94	0.06	28,28,28,28	0
57	MG	DA	3402	1/1	0.94	0.09	48,48,48,48	0
57	MG	DA	3140	1/1	0.94	0.10	64,64,64,64	0
57	MG	DA	3405	1/1	0.94	0.08	47,47,47,47	0
57	MG	BA	3549	1/1	0.94	0.11	66,66,66,66	0
57	MG	BA	3389	1/1	0.94	0.15	37,37,37,37	0
57	MG	DA	3145	1/1	0.94	0.30	48,48,48,48	0
57	MG	CA	3123	1/1	0.94	0.26	61,61,61,61	0
57	MG	BA	3686	1/1	0.94	0.08	27,27,27,27	0
57	MG	DA	3149	1/1	0.94	0.11	46,46,46,46	0
57	MG	DA	3150	1/1	0.94	0.16	50,50,50,50	0
57	MG	BP	3002	1/1	0.94	0.09	60,60,60,60	0
57	MG	CA	3126	1/1	0.94	0.09	45,45,45,45	0
57	MG	DA	3155	1/1	0.94	0.26	53,53,53,53	0
57	MG	BA	3390	1/1	0.94	0.06	31,31,31,31	0
57	MG	DA	3157	1/1	0.94	0.12	34,34,34,34	0
57	MG	DD	301	1/1	0.94	0.08	44,44,44,44	0
57	MG	BV	204	1/1	0.94	0.09	39,39,39,39	0
57	MG	BW	3004	1/1	0.94	0.10	45,45,45,45	0
57	MG	BA	3271	1/1	0.94	0.13	60,60,60,60	0
57	MG	BA	3560	1/1	0.94	0.12	63,63,63,63	0
57	MG	BA	3051	1/1	0.94	0.17	37,37,37,37	0
57	MG	BA	3692	1/1	0.94	0.08	58,58,58,58	0
57	MG	CA	3138	1/1	0.94	0.11	65,65,65,65	0
57	MG	BA	3160	1/1	0.94	0.09	49,49,49,49	0
57	MG	DO	202	1/1	0.94	0.15	60,60,60,60	0
57	MG	AA	1791	1/1	0.94	0.06	54,54,54,54	0
57	MG	DA	3174	1/1	0.94	0.17	52,52,52,52	0
57	MG	DR	3001	1/1	0.94	0.09	49,49,49,49	0
57	MG	BA	3695	1/1	0.94	0.06	40,40,40,40	0
57	MG	DA	3176	1/1	0.94	0.18	38,38,38,38	0
57	MG	B6	101	1/1	0.94	0.21	60,60,60,60	0
57	MG	DA	3179	1/1	0.94	0.10	59,59,59,59	0
57	MG	D8	5001	1/1	0.94	0.12	44,44,44,44	0
57	MG	DA	3181	1/1	0.94	0.09	49,49,49,49	0
60	K	AX	3001	1/1	0.94	0.11	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3663	1/1	0.95	0.14	50,50,50,50	0
57	MG	AA	1778	1/1	0.95	0.09	51,51,51,51	0
57	MG	DA	3425	1/1	0.95	0.14	51,51,51,51	0
57	MG	BA	3665	1/1	0.95	0.11	42,42,42,42	0
57	MG	BD	3005	1/1	0.95	0.09	44,44,44,44	0
57	MG	CA	3128	1/1	0.95	0.13	52,52,52,52	0
57	MG	BA	3524	1/1	0.95	0.12	33,33,33,33	0
57	MG	DA	3432	1/1	0.95	0.17	52,52,52,52	0
57	MG	BA	3025	1/1	0.95	0.06	43,43,43,43	0
57	MG	AA	1733	1/1	0.95	0.10	50,50,50,50	0
57	MG	BE	305	1/1	0.95	0.08	48,48,48,48	0
57	MG	DA	3437	1/1	0.95	0.14	48,48,48,48	0
57	MG	DA	3438	1/1	0.95	0.05	42,42,42,42	0
57	MG	CA	3135	1/1	0.95	0.09	59,59,59,59	0
57	MG	AA	1759	1/1	0.95	0.09	55,55,55,55	0
57	MG	BA	3670	1/1	0.95	0.16	54,54,54,54	0
57	MG	BA	3387	1/1	0.95	0.10	29,29,29,29	0
57	MG	BG	201	1/1	0.95	0.09	39,39,39,39	0
57	MG	BA	3280	1/1	0.95	0.08	25,25,25,25	0
57	MG	BN	3002	1/1	0.95	0.08	51,51,51,51	0
57	MG	DA	3183	1/1	0.95	0.17	41,41,41,41	0
57	MG	BA	3533	1/1	0.95	0.11	23,23,23,23	0
57	MG	DA	3185	1/1	0.95	0.07	51,51,51,51	0
57	MG	BA	3675	1/1	0.95	0.17	56,56,56,56	0
57	MG	DA	3189	1/1	0.95	0.12	47,47,47,47	0
57	MG	BA	3281	1/1	0.95	0.25	50,50,50,50	0
57	MG	BA	3391	1/1	0.95	0.07	41,41,41,41	0
57	MG	DA	3460	1/1	0.95	0.17	37,37,37,37	0
57	MG	BU	201	1/1	0.95	0.21	43,43,43,43	0
57	MG	BU	204	1/1	0.95	0.19	47,47,47,47	0
57	MG	AA	1636	1/1	0.95	0.18	52,52,52,52	0
57	MG	BW	3002	1/1	0.95	0.23	58,58,58,58	0
57	MG	BA	3187	1/1	0.95	0.23	38,38,38,38	0
57	MG	BA	3545	1/1	0.95	0.08	28,28,28,28	0
57	MG	BA	3683	1/1	0.95	0.07	62,62,62,62	0
57	MG	BA	3546	1/1	0.95	0.06	68,68,68,68	0
57	MG	BA	3284	1/1	0.95	0.13	57,57,57,57	0
57	MG	DA	3473	1/1	0.95	0.19	50,50,50,50	0
57	MG	BA	3552	1/1	0.95	0.15	55,55,55,55	0
57	MG	DA	3477	1/1	0.95	0.08	53,53,53,53	0
57	MG	BA	3554	1/1	0.95	0.07	51,51,51,51	0
57	MG	CA	3157	1/1	0.95	0.13	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3205	1/1	0.95	0.09	62,62,62,62	0
57	MG	BA	3285	1/1	0.95	0.10	58,58,58,58	0
57	MG	BA	3689	1/1	0.95	0.11	59,59,59,59	0
57	MG	BA	3403	1/1	0.95	0.12	33,33,33,33	0
57	MG	B7	103	1/1	0.95	0.13	40,40,40,40	0
57	MG	BA	3189	1/1	0.95	0.06	39,39,39,39	0
57	MG	AA	1783	1/1	0.95	0.10	35,35,35,35	0
57	MG	BA	3193	1/1	0.95	0.06	37,37,37,37	0
57	MG	CA	3166	1/1	0.95	0.07	55,55,55,55	0
57	MG	DA	3224	1/1	0.95	0.08	39,39,39,39	0
57	MG	BA	3562	1/1	0.95	0.09	55,55,55,55	0
57	MG	DA	3494	1/1	0.95	0.07	45,45,45,45	0
57	MG	BA	3101	1/1	0.95	0.17	37,37,37,37	0
57	MG	DA	3496	1/1	0.95	0.17	56,56,56,56	0
57	MG	BA	3036	1/1	0.95	0.09	56,56,56,56	0
57	MG	DA	3498	1/1	0.95	0.13	35,35,35,35	0
57	MG	AA	1615	1/1	0.95	0.12	51,51,51,51	0
57	MG	BA	3566	1/1	0.95	0.10	31,31,31,31	0
57	MG	BA	3105	1/1	0.95	0.12	46,46,46,46	0
57	MG	AA	1666	1/1	0.95	0.26	63,63,63,63	0
57	MG	DA	3505	1/1	0.95	0.07	51,51,51,51	0
57	MG	CK	5001	1/1	0.95	0.10	61,61,61,61	0
57	MG	BA	3049	1/1	0.95	0.12	46,46,46,46	0
57	MG	BA	3203	1/1	0.95	0.30	61,61,61,61	0
57	MG	BA	3706	1/1	0.95	0.09	47,47,47,47	0
57	MG	BA	3707	1/1	0.95	0.20	39,39,39,39	0
57	MG	BA	3709	1/1	0.95	0.31	48,48,48,48	0
57	MG	DA	3242	1/1	0.95	0.10	52,52,52,52	0
57	MG	BA	3108	1/1	0.95	0.07	42,42,42,42	0
57	MG	DA	3244	1/1	0.95	0.21	55,55,55,55	0
57	MG	DA	3003	1/1	0.95	0.15	36,36,36,36	0
57	MG	DA	3519	1/1	0.95	0.19	58,58,58,58	0
57	MG	DA	3247	1/1	0.95	0.15	49,49,49,49	0
57	MG	DA	3521	1/1	0.95	0.07	57,57,57,57	0
57	MG	BA	3109	1/1	0.95	0.11	56,56,56,56	0
57	MG	BA	3421	1/1	0.95	0.16	62,62,62,62	0
57	MG	AA	1638	1/1	0.95	0.07	60,60,60,60	0
57	MG	BA	3578	1/1	0.95	0.25	39,39,39,39	0
57	MG	DA	3528	1/1	0.95	0.10	36,36,36,36	0
57	MG	AA	1703	1/1	0.95	0.23	43,43,43,43	0
57	MG	BA	3310	1/1	0.95	0.08	26,26,26,26	0
57	MG	DA	3015	1/1	0.95	0.11	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	3021	1/1	0.95	0.24	61,61,61,61	0
57	MG	DA	3534	1/1	0.95	0.07	46,46,46,46	0
57	MG	BA	3582	1/1	0.95	0.07	31,31,31,31	0
57	MG	DA	3020	1/1	0.95	0.04	26,26,26,26	0
57	MG	DA	3262	1/1	0.95	0.10	20,20,20,20	0
57	MG	DA	3263	1/1	0.95	0.07	65,65,65,65	0
57	MG	DA	3264	1/1	0.95	0.10	51,51,51,51	0
57	MG	DA	3021	1/1	0.95	0.09	50,50,50,50	0
57	MG	DA	3022	1/1	0.95	0.27	60,60,60,60	0
57	MG	DA	3544	1/1	0.95	0.09	53,53,53,53	0
57	MG	BA	3721	1/1	0.95	0.08	47,47,47,47	0
57	MG	DA	3546	1/1	0.95	0.07	47,47,47,47	0
57	MG	BA	3112	1/1	0.95	0.17	41,41,41,41	0
57	MG	BA	3588	1/1	0.95	0.07	43,43,43,43	0
57	MG	DA	3027	1/1	0.95	0.30	43,43,43,43	0
57	MG	BA	3724	1/1	0.95	0.05	20,20,20,20	0
57	MG	DA	3279	1/1	0.95	0.07	36,36,36,36	0
57	MG	BA	3314	1/1	0.95	0.10	39,39,39,39	0
57	MG	BA	3592	1/1	0.95	0.09	65,65,65,65	0
57	MG	DA	3558	1/1	0.95	0.09	48,48,48,48	0
57	MG	DA	3283	1/1	0.95	0.06	27,27,27,27	0
57	MG	BA	3113	1/1	0.95	0.09	50,50,50,50	0
57	MG	DA	3038	1/1	0.95	0.07	56,56,56,56	0
57	MG	AA	1704	1/1	0.95	0.20	57,57,57,57	0
57	MG	BA	3595	1/1	0.95	0.12	61,61,61,61	0
57	MG	AA	1652	1/1	0.95	0.19	62,62,62,62	0
57	MG	BA	3122	1/1	0.95	0.09	35,35,35,35	0
57	MG	BA	3321	1/1	0.95	0.08	53,53,53,53	0
57	MG	BA	3736	1/1	0.95	0.07	22,22,22,22	0
57	MG	DA	3050	1/1	0.95	0.23	44,44,44,44	0
57	MG	DA	3294	1/1	0.95	0.06	40,40,40,40	0
57	MG	BA	3123	1/1	0.95	0.07	43,43,43,43	0
57	MG	BA	3325	1/1	0.95	0.09	45,45,45,45	0
57	MG	DA	3298	1/1	0.95	0.14	55,55,55,55	0
57	MG	BA	3739	1/1	0.95	0.07	21,21,21,21	0
57	MG	AA	1706	1/1	0.95	0.18	60,60,60,60	0
57	MG	DA	3303	1/1	0.95	0.11	43,43,43,43	0
57	MG	BA	3229	1/1	0.95	0.10	52,52,52,52	0
57	MG	BA	3230	1/1	0.95	0.13	58,58,58,58	0
57	MG	CA	3043	1/1	0.95	0.16	44,44,44,44	0
57	MG	CA	3045	1/1	0.95	0.24	62,62,62,62	0
57	MG	BA	3745	1/1	0.95	0.13	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3444	1/1	0.95	0.09	48,48,48,48	0
57	MG	AA	1683	1/1	0.95	0.20	62,62,62,62	0
57	MG	BA	3607	1/1	0.95	0.07	36,36,36,36	0
57	MG	DA	3068	1/1	0.95	0.18	53,53,53,53	0
57	MG	BA	3236	1/1	0.95	0.16	52,52,52,52	0
57	MG	BA	3750	1/1	0.95	0.10	46,46,46,46	0
57	MG	DA	3320	1/1	0.95	0.09	49,49,49,49	0
57	MG	BA	3132	1/1	0.95	0.09	50,50,50,50	0
57	MG	BA	3610	1/1	0.95	0.06	61,61,61,61	0
57	MG	DA	3073	1/1	0.95	0.06	33,33,33,33	0
57	MG	BA	3060	1/1	0.95	0.18	51,51,51,51	0
57	MG	DA	3076	1/1	0.95	0.20	52,52,52,52	0
57	MG	DA	3330	1/1	0.95	0.10	36,36,36,36	0
57	MG	BA	3453	1/1	0.95	0.07	50,50,50,50	0
57	MG	BA	3455	1/1	0.95	0.07	52,52,52,52	0
57	MG	BA	3136	1/1	0.95	0.28	49,49,49,49	0
57	MG	BA	3759	1/1	0.95	0.09	70,70,70,70	0
57	MG	DA	3084	1/1	0.95	0.08	44,44,44,44	0
57	MG	BA	3341	1/1	0.95	0.11	18,18,18,18	0
57	MG	DA	3613	1/1	0.95	0.11	56,56,56,56	0
57	MG	BA	3241	1/1	0.95	0.15	56,56,56,56	0
57	MG	DA	3339	1/1	0.95	0.12	52,52,52,52	0
57	MG	AA	1633	1/1	0.95	0.26	59,59,59,59	0
57	MG	BA	3466	1/1	0.95	0.12	51,51,51,51	0
57	MG	CA	3065	1/1	0.95	0.14	59,59,59,59	0
57	MG	DA	3090	1/1	0.95	0.15	50,50,50,50	0
57	MG	DA	3092	1/1	0.95	0.15	57,57,57,57	0
57	MG	DA	3094	1/1	0.95	0.05	39,39,39,39	0
57	MG	BA	3620	1/1	0.95	0.07	29,29,29,29	0
57	MG	BA	3467	1/1	0.95	0.05	46,46,46,46	0
57	MG	BA	3063	1/1	0.95	0.17	47,47,47,47	0
57	MG	AA	1795	1/1	0.95	0.08	55,55,55,55	0
57	MG	DA	3354	1/1	0.95	0.07	41,41,41,41	0
57	MG	BA	3770	1/1	0.95	0.14	49,49,49,49	0
57	MG	AA	1709	1/1	0.95	0.19	55,55,55,55	0
57	MG	DA	3103	1/1	0.95	0.10	56,56,56,56	0
57	MG	DA	3359	1/1	0.95	0.11	40,40,40,40	0
57	MG	DA	3360	1/1	0.95	0.06	31,31,31,31	0
57	MG	AA	1627	1/1	0.95	0.06	54,54,54,54	0
57	MG	AN	503	1/1	0.95	0.11	52,52,52,52	0
57	MG	BA	3152	1/1	0.95	0.13	23,23,23,23	0
57	MG	DA	3365	1/1	0.95	0.06	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3108	1/1	0.95	0.08	50,50,50,50	0
57	MG	BA	3784	1/1	0.95	0.07	52,52,52,52	0
57	MG	AA	1728	1/1	0.95	0.18	49,49,49,49	0
57	MG	AA	1799	1/1	0.95	0.10	78,78,78,78	0
57	MG	BA	3486	1/1	0.95	0.08	41,41,41,41	0
57	MG	DA	3372	1/1	0.95	0.13	53,53,53,53	0
57	MG	DA	3374	1/1	0.95	0.25	62,62,62,62	0
57	MG	BA	3788	1/1	0.95	0.09	44,44,44,44	0
57	MG	CA	3083	1/1	0.95	0.11	50,50,50,50	0
57	MG	BA	3355	1/1	0.95	0.08	35,35,35,35	0
57	MG	DA	3651	1/1	0.95	0.07	48,48,48,48	0
57	MG	AA	1800	1/1	0.95	0.12	59,59,59,59	0
57	MG	DA	3654	1/1	0.95	0.14	35,35,35,35	0
57	MG	BA	3791	1/1	0.95	0.21	49,49,49,49	0
57	MG	DA	3658	1/1	0.95	0.23	62,62,62,62	0
57	MG	DA	3660	1/1	0.95	0.27	46,46,46,46	0
57	MG	DA	3382	1/1	0.95	0.06	41,41,41,41	0
57	MG	BA	3634	1/1	0.95	0.07	55,55,55,55	0
57	MG	DA	3387	1/1	0.95	0.13	59,59,59,59	0
57	MG	DA	3388	1/1	0.95	0.10	47,47,47,47	0
57	MG	BA	3359	1/1	0.95	0.07	60,60,60,60	0
57	MG	AA	1697	1/1	0.95	0.18	65,65,65,65	0
57	MG	BA	3363	1/1	0.95	0.12	52,52,52,52	0
57	MG	BA	3799	1/1	0.95	0.10	42,42,42,42	0
57	MG	AA	1776	1/1	0.95	0.16	73,73,73,73	0
57	MG	BA	3083	1/1	0.95	0.21	60,60,60,60	0
57	MG	DB	3009	1/1	0.95	0.08	58,58,58,58	0
57	MG	BA	3167	1/1	0.95	0.17	45,45,45,45	0
57	MG	BA	3367	1/1	0.95	0.09	52,52,52,52	0
57	MG	BA	3169	1/1	0.95	0.12	50,50,50,50	0
57	MG	BA	3807	1/1	0.95	0.11	66,66,66,66	0
57	MG	BA	3370	1/1	0.95	0.17	50,50,50,50	0
57	MG	BA	3269	1/1	0.95	0.11	45,45,45,45	0
57	MG	BA	3509	1/1	0.95	0.15	50,50,50,50	0
57	MG	DE	3005	1/1	0.95	0.08	35,35,35,35	0
57	MG	DE	3006	1/1	0.95	0.12	38,38,38,38	0
57	MG	BB	3002	1/1	0.95	0.17	55,55,55,55	0
57	MG	BA	3650	1/1	0.95	0.13	45,45,45,45	0
57	MG	BA	3373	1/1	0.95	0.07	34,34,34,34	0
57	MG	DA	3141	1/1	0.95	0.10	51,51,51,51	0
57	MG	DF	304	1/1	0.95	0.05	51,51,51,51	0
57	MG	DF	305	1/1	0.95	0.23	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3409	1/1	0.95	0.10	54,54,54,54	0
57	MG	BA	3652	1/1	0.95	0.07	58,58,58,58	0
57	MG	BB	3008	1/1	0.95	0.28	59,59,59,59	0
57	MG	DA	3144	1/1	0.95	0.18	41,41,41,41	0
57	MG	CA	3114	1/1	0.95	0.17	71,71,71,71	0
57	MG	AA	1635	1/1	0.95	0.22	65,65,65,65	0
57	MG	BA	3515	1/1	0.95	0.07	27,27,27,27	0
57	MG	BB	3015	1/1	0.95	0.11	45,45,45,45	0
57	MG	DY	502	1/1	0.95	0.12	55,55,55,55	0
57	MG	BA	3171	1/1	0.95	0.20	35,35,35,35	0
57	MG	BA	3172	1/1	0.95	0.14	40,40,40,40	0
57	MG	BA	3273	1/1	0.95	0.08	45,45,45,45	0
57	MG	BA	3174	1/1	0.95	0.38	38,38,38,38	0
57	MG	BB	3021	1/1	0.95	0.07	41,41,41,41	0
57	MG	BA	3362	1/1	0.96	0.09	47,47,47,47	0
57	MG	DA	3271	1/1	0.96	0.07	30,30,30,30	0
57	MG	BA	3212	1/1	0.96	0.19	57,57,57,57	0
57	MG	CA	3096	1/1	0.96	0.12	43,43,43,43	0
57	MG	DA	3082	1/1	0.96	0.08	47,47,47,47	0
57	MG	DA	3083	1/1	0.96	0.07	41,41,41,41	0
57	MG	DA	3280	1/1	0.96	0.07	48,48,48,48	0
57	MG	BE	302	1/1	0.96	0.06	35,35,35,35	0
57	MG	CA	3098	1/1	0.96	0.09	54,54,54,54	0
57	MG	BA	3461	1/1	0.96	0.07	45,45,45,45	0
57	MG	BA	3703	1/1	0.96	0.25	28,28,28,28	0
57	MG	AA	1632	1/1	0.96	0.06	48,48,48,48	0
57	MG	AA	1694	1/1	0.96	0.06	47,47,47,47	0
57	MG	BF	301	1/1	0.96	0.19	40,40,40,40	0
57	MG	DA	3091	1/1	0.96	0.08	54,54,54,54	0
57	MG	BF	303	1/1	0.96	0.07	33,33,33,33	0
57	MG	BA	3216	1/1	0.96	0.28	39,39,39,39	0
57	MG	DA	3503	1/1	0.96	0.14	38,38,38,38	0
57	MG	BA	3155	1/1	0.96	0.09	40,40,40,40	0
57	MG	BA	3159	1/1	0.96	0.12	27,27,27,27	0
57	MG	BA	3287	1/1	0.96	0.09	27,27,27,27	0
57	MG	BH	201	1/1	0.96	0.07	56,56,56,56	0
57	MG	DA	3100	1/1	0.96	0.10	47,47,47,47	0
57	MG	BN	3001	1/1	0.96	0.09	48,48,48,48	0
57	MG	DA	3511	1/1	0.96	0.06	44,44,44,44	0
57	MG	BA	3475	1/1	0.96	0.07	49,49,49,49	0
57	MG	AA	1715	1/1	0.96	0.16	45,45,45,45	0
57	MG	BA	3223	1/1	0.96	0.07	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3714	1/1	0.96	0.06	46,46,46,46	0
57	MG	BQ	3002	1/1	0.96	0.23	46,46,46,46	0
57	MG	DA	3517	1/1	0.96	0.09	48,48,48,48	0
57	MG	BA	3480	1/1	0.96	0.07	47,47,47,47	0
57	MG	DA	3309	1/1	0.96	0.06	48,48,48,48	0
57	MG	AA	1802	1/1	0.96	0.09	54,54,54,54	0
57	MG	BA	3605	1/1	0.96	0.12	47,47,47,47	0
57	MG	BA	3719	1/1	0.96	0.08	41,41,41,41	0
57	MG	BW	3001	1/1	0.96	0.21	44,44,44,44	0
57	MG	BA	3162	1/1	0.96	0.24	41,41,41,41	0
57	MG	AA	1780	1/1	0.96	0.10	69,69,69,69	0
57	MG	BX	3001	1/1	0.96	0.09	44,44,44,44	0
57	MG	BA	3029	1/1	0.96	0.07	36,36,36,36	0
57	MG	BA	3166	1/1	0.96	0.14	33,33,33,33	0
57	MG	DA	3531	1/1	0.96	0.07	48,48,48,48	0
57	MG	DA	3323	1/1	0.96	0.10	49,49,49,49	0
57	MG	DA	3119	1/1	0.96	0.13	50,50,50,50	0
57	MG	AX	3004	1/1	0.96	0.16	61,61,61,61	0
57	MG	BA	3232	1/1	0.96	0.11	49,49,49,49	0
57	MG	BA	3612	1/1	0.96	0.10	60,60,60,60	0
57	MG	BA	3299	1/1	0.96	0.10	60,60,60,60	0
57	MG	DA	3329	1/1	0.96	0.07	47,47,47,47	0
57	MG	BA	3494	1/1	0.96	0.07	38,38,38,38	0
57	MG	B5	102	1/1	0.96	0.15	43,43,43,43	0
57	MG	BA	3034	1/1	0.96	0.19	35,35,35,35	0
57	MG	BA	3069	1/1	0.96	0.28	48,48,48,48	0
57	MG	B7	102	1/1	0.96	0.07	41,41,41,41	0
57	MG	BA	3388	1/1	0.96	0.07	25,25,25,25	0
57	MG	DA	3132	1/1	0.96	0.10	43,43,43,43	0
57	MG	DA	3551	1/1	0.96	0.13	49,49,49,49	0
57	MG	BA	3303	1/1	0.96	0.14	26,26,26,26	0
57	MG	DA	3338	1/1	0.96	0.06	44,44,44,44	0
57	MG	BA	3238	1/1	0.96	0.33	44,44,44,44	0
57	MG	AA	1630	1/1	0.96	0.11	53,53,53,53	0
57	MG	B9	502	1/1	0.96	0.07	46,46,46,46	0
57	MG	DA	3137	1/1	0.96	0.12	52,52,52,52	0
57	MG	BA	3392	1/1	0.96	0.11	26,26,26,26	0
57	MG	BA	3116	1/1	0.96	0.15	46,46,46,46	0
57	MG	BA	3395	1/1	0.96	0.10	30,30,30,30	0
57	MG	BA	3624	1/1	0.96	0.05	38,38,38,38	0
57	MG	BA	3311	1/1	0.96	0.12	56,56,56,56	0
57	MG	DA	3564	1/1	0.96	0.11	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3399	1/1	0.96	0.09	41,41,41,41	0
57	MG	BA	3312	1/1	0.96	0.07	31,31,31,31	0
57	MG	DA	3353	1/1	0.96	0.09	47,47,47,47	0
57	MG	BA	3514	1/1	0.96	0.11	43,43,43,43	0
57	MG	BA	3173	1/1	0.96	0.12	32,32,32,32	0
57	MG	BA	3076	1/1	0.96	0.12	42,42,42,42	0
57	MG	BA	3037	1/1	0.96	0.09	42,42,42,42	0
57	MG	BA	3038	1/1	0.96	0.13	20,20,20,20	0
57	MG	DA	3151	1/1	0.96	0.04	37,37,37,37	0
57	MG	BA	3406	1/1	0.96	0.09	56,56,56,56	0
57	MG	BA	3520	1/1	0.96	0.12	29,29,29,29	0
57	MG	BA	3521	1/1	0.96	0.10	40,40,40,40	0
57	MG	DA	3364	1/1	0.96	0.07	45,45,45,45	0
57	MG	BA	3317	1/1	0.96	0.07	43,43,43,43	0
57	MG	DA	3581	1/1	0.96	0.09	44,44,44,44	0
57	MG	BA	3523	1/1	0.96	0.11	41,41,41,41	0
57	MG	AA	1793	1/1	0.96	0.16	63,63,63,63	0
57	MG	DA	3586	1/1	0.96	0.06	50,50,50,50	0
57	MG	BA	3178	1/1	0.96	0.07	32,32,32,32	0
57	MG	BA	3124	1/1	0.96	0.10	57,57,57,57	0
57	MG	DA	3370	1/1	0.96	0.14	59,59,59,59	0
57	MG	BA	3643	1/1	0.96	0.11	52,52,52,52	0
57	MG	DA	3162	1/1	0.96	0.16	57,57,57,57	0
57	MG	BA	3180	1/1	0.96	0.18	46,46,46,46	0
57	MG	BA	3528	1/1	0.96	0.10	36,36,36,36	0
57	MG	BA	3766	1/1	0.96	0.08	47,47,47,47	0
57	MG	DA	3169	1/1	0.96	0.22	41,41,41,41	0
57	MG	BA	3529	1/1	0.96	0.12	24,24,24,24	0
57	MG	DA	3599	1/1	0.96	0.09	48,48,48,48	0
57	MG	BA	3324	1/1	0.96	0.10	60,60,60,60	0
57	MG	BA	3184	1/1	0.96	0.08	42,42,42,42	0
57	MG	BA	3253	1/1	0.96	0.16	31,31,31,31	0
57	MG	DA	3603	1/1	0.96	0.06	65,65,65,65	0
57	MG	BA	3771	1/1	0.96	0.08	41,41,41,41	0
57	MG	BA	3328	1/1	0.96	0.07	27,27,27,27	0
57	MG	BA	3254	1/1	0.96	0.07	33,33,33,33	0
57	MG	BA	3331	1/1	0.96	0.13	53,53,53,53	0
57	MG	BA	3776	1/1	0.96	0.16	60,60,60,60	0
57	MG	DA	3609	1/1	0.96	0.09	61,61,61,61	0
57	MG	BA	3777	1/1	0.96	0.06	41,41,41,41	0
57	MG	BA	3778	1/1	0.96	0.05	40,40,40,40	0
57	MG	BA	3541	1/1	0.96	0.11	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3188	1/1	0.96	0.09	35,35,35,35	0
57	MG	BA	3782	1/1	0.96	0.09	38,38,38,38	0
57	MG	BA	3044	1/1	0.96	0.32	43,43,43,43	0
57	MG	BA	3257	1/1	0.96	0.10	43,43,43,43	0
57	MG	DA	3008	1/1	0.96	0.10	45,45,45,45	0
57	MG	BA	3659	1/1	0.96	0.08	47,47,47,47	0
57	MG	BA	3425	1/1	0.96	0.15	48,48,48,48	0
57	MG	BA	3548	1/1	0.96	0.06	35,35,35,35	0
57	MG	BA	3261	1/1	0.96	0.04	18,18,18,18	0
57	MG	BA	3427	1/1	0.96	0.09	33,33,33,33	0
57	MG	BA	3553	1/1	0.96	0.09	45,45,45,45	0
57	MG	BA	3428	1/1	0.96	0.09	51,51,51,51	0
57	MG	AA	1772	1/1	0.96	0.13	47,47,47,47	0
57	MG	BA	3088	1/1	0.96	0.13	43,43,43,43	0
57	MG	DA	3412	1/1	0.96	0.09	41,41,41,41	0
57	MG	DA	3629	1/1	0.96	0.09	57,57,57,57	0
57	MG	BA	3092	1/1	0.96	0.17	40,40,40,40	0
57	MG	DA	3631	1/1	0.96	0.07	49,49,49,49	0
57	MG	DA	3632	1/1	0.96	0.12	52,52,52,52	0
57	MG	BA	3432	1/1	0.96	0.09	32,32,32,32	0
57	MG	BA	3671	1/1	0.96	0.07	24,24,24,24	0
57	MG	DA	3635	1/1	0.96	0.07	43,43,43,43	0
57	MG	DA	3206	1/1	0.96	0.11	50,50,50,50	0
57	MG	DA	3207	1/1	0.96	0.14	48,48,48,48	0
57	MG	CA	3056	1/1	0.96	0.11	64,64,64,64	0
57	MG	DA	3210	1/1	0.96	0.06	52,52,52,52	0
57	MG	DA	3029	1/1	0.96	0.22	45,45,45,45	0
57	MG	DA	3030	1/1	0.96	0.10	44,44,44,44	0
57	MG	DA	3031	1/1	0.96	0.13	42,42,42,42	0
57	MG	BA	3802	1/1	0.96	0.10	46,46,46,46	0
57	MG	DA	3218	1/1	0.96	0.08	52,52,52,52	0
57	MG	BA	3047	1/1	0.96	0.10	43,43,43,43	0
57	MG	AL	202	1/1	0.96	0.23	56,56,56,56	0
57	MG	DA	3427	1/1	0.96	0.15	47,47,47,47	0
57	MG	DA	3428	1/1	0.96	0.06	38,38,38,38	0
57	MG	DA	3221	1/1	0.96	0.07	41,41,41,41	0
57	MG	BA	3138	1/1	0.96	0.10	43,43,43,43	0
57	MG	DA	3223	1/1	0.96	0.08	39,39,39,39	0
57	MG	AA	1608	1/1	0.96	0.18	43,43,43,43	0
57	MG	DA	3225	1/1	0.96	0.10	55,55,55,55	0
57	MG	DA	3040	1/1	0.96	0.09	28,28,28,28	0
57	MG	BA	3140	1/1	0.96	0.05	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3436	1/1	0.96	0.06	35,35,35,35	0
57	MG	AA	1808	1/1	0.96	0.09	49,49,49,49	0
57	MG	DA	3043	1/1	0.96	0.21	53,53,53,53	0
57	MG	BA	3811	1/1	0.96	0.15	48,48,48,48	0
57	MG	BA	3201	1/1	0.96	0.13	48,48,48,48	0
57	MG	BA	3814	1/1	0.96	0.11	39,39,39,39	0
57	MG	CA	3067	1/1	0.96	0.23	46,46,46,46	0
57	MG	AA	1746	1/1	0.96	0.14	56,56,56,56	0
57	MG	DA	3051	1/1	0.96	0.09	44,44,44,44	0
57	MG	DA	3447	1/1	0.96	0.18	59,59,59,59	0
57	MG	AA	1736	1/1	0.96	0.07	49,49,49,49	0
57	MG	DA	3053	1/1	0.96	0.13	47,47,47,47	0
57	MG	BB	3003	1/1	0.96	0.04	30,30,30,30	0
57	MG	AA	1673	1/1	0.96	0.08	48,48,48,48	0
57	MG	BA	3445	1/1	0.96	0.09	54,54,54,54	0
57	MG	BA	3150	1/1	0.96	0.10	39,39,39,39	0
57	MG	BA	3574	1/1	0.96	0.08	42,42,42,42	0
57	MG	DD	302	1/1	0.96	0.08	49,49,49,49	0
57	MG	BA	3447	1/1	0.96	0.13	52,52,52,52	0
57	MG	DA	3062	1/1	0.96	0.15	53,53,53,53	0
57	MG	BB	3013	1/1	0.96	0.08	39,39,39,39	0
57	MG	BA	3576	1/1	0.96	0.16	30,30,30,30	0
57	MG	BA	3354	1/1	0.96	0.08	47,47,47,47	0
57	MG	CA	3080	1/1	0.96	0.07	49,49,49,49	0
57	MG	BA	3207	1/1	0.96	0.09	36,36,36,36	0
57	MG	BA	3451	1/1	0.96	0.10	44,44,44,44	0
57	MG	BA	3278	1/1	0.96	0.42	54,54,54,54	0
57	MG	BA	3208	1/1	0.96	0.07	43,43,43,43	0
57	MG	DA	3258	1/1	0.96	0.09	45,45,45,45	0
57	MG	DA	3471	1/1	0.96	0.15	54,54,54,54	0
57	MG	DA	3472	1/1	0.96	0.07	25,25,25,25	0
57	MG	BA	3023	1/1	0.96	0.10	41,41,41,41	0
57	MG	BA	3586	1/1	0.96	0.07	55,55,55,55	0
57	MG	DA	3475	1/1	0.96	0.20	56,56,56,56	0
57	MG	DA	3476	1/1	0.96	0.07	45,45,45,45	0
57	MG	BB	3023	1/1	0.96	0.13	47,47,47,47	0
57	MG	BA	3456	1/1	0.96	0.13	37,37,37,37	0
57	MG	DA	3479	1/1	0.96	0.07	42,42,42,42	0
57	MG	DA	3075	1/1	0.96	0.12	55,55,55,55	0
57	MG	BA	3589	1/1	0.96	0.19	59,59,59,59	0
59	ZN	CN	501	1/1	0.96	0.08	100,100,100,100	0
57	MG	CA	3093	1/1	0.96	0.09	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3483	1/1	0.96	0.10	53,53,53,53	0
57	MG	BA	3585	1/1	0.97	0.08	29,29,29,29	0
57	MG	BA	3163	1/1	0.97	0.20	55,55,55,55	0
57	MG	BA	3031	1/1	0.97	0.16	36,36,36,36	0
57	MG	BA	3226	1/1	0.97	0.10	25,25,25,25	0
57	MG	DA	3509	1/1	0.97	0.06	49,49,49,49	0
57	MG	BA	3032	1/1	0.97	0.17	33,33,33,33	0
57	MG	BA	3380	1/1	0.97	0.09	40,40,40,40	0
57	MG	AA	1758	1/1	0.97	0.07	37,37,37,37	0
57	MG	DA	3148	1/1	0.97	0.09	49,49,49,49	0
57	MG	BA	3382	1/1	0.97	0.08	55,55,55,55	0
57	MG	BA	3008	1/1	0.97	0.05	28,28,28,28	0
57	MG	BA	3168	1/1	0.97	0.16	45,45,45,45	0
57	MG	DA	3152	1/1	0.97	0.05	45,45,45,45	0
57	MG	AA	1809	1/1	0.97	0.12	42,42,42,42	0
57	MG	BA	3302	1/1	0.97	0.09	49,49,49,49	0
57	MG	BA	3701	1/1	0.97	0.12	39,39,39,39	0
57	MG	BA	3488	1/1	0.97	0.04	20,20,20,20	0
57	MG	BA	3233	1/1	0.97	0.15	40,40,40,40	0
57	MG	CA	3053	1/1	0.97	0.09	41,41,41,41	0
57	MG	BB	3010	1/1	0.97	0.06	53,53,53,53	0
57	MG	BB	3011	1/1	0.97	0.08	47,47,47,47	0
57	MG	DA	3011	1/1	0.97	0.10	35,35,35,35	0
57	MG	DA	3340	1/1	0.97	0.07	27,27,27,27	0
57	MG	BB	3012	1/1	0.97	0.13	56,56,56,56	0
57	MG	DA	3164	1/1	0.97	0.16	44,44,44,44	0
57	MG	BA	3304	1/1	0.97	0.11	39,39,39,39	0
57	MG	BA	3493	1/1	0.97	0.12	38,38,38,38	0
57	MG	DA	3346	1/1	0.97	0.06	49,49,49,49	0
57	MG	BA	3305	1/1	0.97	0.06	46,46,46,46	0
57	MG	DA	3536	1/1	0.97	0.05	52,52,52,52	0
57	MG	DA	3168	1/1	0.97	0.08	44,44,44,44	0
57	MG	DA	3018	1/1	0.97	0.04	31,31,31,31	0
57	MG	DA	3019	1/1	0.97	0.06	42,42,42,42	0
57	MG	BA	3234	1/1	0.97	0.12	52,52,52,52	0
57	MG	BA	3708	1/1	0.97	0.24	33,33,33,33	0
57	MG	BA	3308	1/1	0.97	0.16	39,39,39,39	0
57	MG	BA	3235	1/1	0.97	0.11	44,44,44,44	0
57	MG	DA	3355	1/1	0.97	0.06	43,43,43,43	0
57	MG	BA	3070	1/1	0.97	0.10	41,41,41,41	0
57	MG	DA	3547	1/1	0.97	0.06	48,48,48,48	0
57	MG	DA	3548	1/1	0.97	0.07	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3025	1/1	0.97	0.18	47,47,47,47	0
57	MG	DA	3180	1/1	0.97	0.18	48,48,48,48	0
57	MG	BA	3071	1/1	0.97	0.24	59,59,59,59	0
57	MG	DA	3182	1/1	0.97	0.24	52,52,52,52	0
57	MG	BA	3398	1/1	0.97	0.12	32,32,32,32	0
57	MG	DA	3028	1/1	0.97	0.04	39,39,39,39	0
57	MG	BA	3115	1/1	0.97	0.06	33,33,33,33	0
57	MG	DA	3186	1/1	0.97	0.18	49,49,49,49	0
57	MG	BA	3072	1/1	0.97	0.13	49,49,49,49	0
57	MG	BA	3012	1/1	0.97	0.11	25,25,25,25	0
57	MG	BD	3008	1/1	0.97	0.07	45,45,45,45	0
57	MG	BD	3009	1/1	0.97	0.05	37,37,37,37	0
57	MG	BA	3119	1/1	0.97	0.08	46,46,46,46	0
57	MG	BA	3510	1/1	0.97	0.06	45,45,45,45	0
57	MG	DA	3565	1/1	0.97	0.05	52,52,52,52	0
57	MG	BA	3511	1/1	0.97	0.13	50,50,50,50	0
57	MG	BA	3120	1/1	0.97	0.12	45,45,45,45	0
57	MG	DA	3195	1/1	0.97	0.08	42,42,42,42	0
57	MG	AA	1672	1/1	0.97	0.15	45,45,45,45	0
57	MG	BA	3244	1/1	0.97	0.16	31,31,31,31	0
57	MG	BA	3319	1/1	0.97	0.08	23,23,23,23	0
57	MG	BA	3077	1/1	0.97	0.07	15,15,15,15	0
57	MG	BF	304	1/1	0.97	0.18	41,41,41,41	0
57	MG	DA	3381	1/1	0.97	0.10	40,40,40,40	0
57	MG	BF	305	1/1	0.97	0.10	36,36,36,36	0
57	MG	DA	3384	1/1	0.97	0.04	38,38,38,38	0
57	MG	BA	3042	1/1	0.97	0.05	37,37,37,37	0
57	MG	DA	3386	1/1	0.97	0.05	44,44,44,44	0
57	MG	DA	3049	1/1	0.97	0.10	47,47,47,47	0
57	MG	BA	3043	1/1	0.97	0.12	31,31,31,31	0
57	MG	BF	309	1/1	0.97	0.13	31,31,31,31	0
57	MG	BF	310	1/1	0.97	0.14	56,56,56,56	0
57	MG	BA	3181	1/1	0.97	0.04	40,40,40,40	0
57	MG	BA	3182	1/1	0.97	0.20	52,52,52,52	0
57	MG	DA	3209	1/1	0.97	0.06	49,49,49,49	0
57	MG	DA	3394	1/1	0.97	0.04	60,60,60,60	0
57	MG	BA	3326	1/1	0.97	0.05	24,24,24,24	0
57	MG	CA	3092	1/1	0.97	0.14	51,51,51,51	0
57	MG	DA	3058	1/1	0.97	0.14	61,61,61,61	0
57	MG	BA	3251	1/1	0.97	0.15	43,43,43,43	0
57	MG	DA	3215	1/1	0.97	0.16	40,40,40,40	0
57	MG	DA	3216	1/1	0.97	0.11	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3418	1/1	0.97	0.10	38,38,38,38	0
57	MG	BN	3003	1/1	0.97	0.07	38,38,38,38	0
57	MG	BA	3125	1/1	0.97	0.11	38,38,38,38	0
57	MG	BA	3126	1/1	0.97	0.22	36,36,36,36	0
57	MG	BA	3127	1/1	0.97	0.11	45,45,45,45	0
57	MG	BQ	3001	1/1	0.97	0.14	37,37,37,37	0
57	MG	BA	3188	1/1	0.97	0.16	32,32,32,32	0
57	MG	AA	1668	1/1	0.97	0.06	63,63,63,63	0
57	MG	BA	3424	1/1	0.97	0.13	31,31,31,31	0
57	MG	BA	3258	1/1	0.97	0.21	44,44,44,44	0
57	MG	CA	3104	1/1	0.97	0.14	37,37,37,37	0
57	MG	DA	3228	1/1	0.97	0.12	44,44,44,44	0
57	MG	DA	3229	1/1	0.97	0.08	38,38,38,38	0
57	MG	BV	201	1/1	0.97	0.22	31,31,31,31	0
57	MG	CA	3106	1/1	0.97	0.10	58,58,58,58	0
57	MG	BA	3744	1/1	0.97	0.07	55,55,55,55	0
57	MG	BA	3531	1/1	0.97	0.06	60,60,60,60	0
57	MG	DA	3615	1/1	0.97	0.14	62,62,62,62	0
57	MG	BA	3335	1/1	0.97	0.06	40,40,40,40	0
57	MG	AA	1661	1/1	0.97	0.27	54,54,54,54	0
57	MG	BA	3534	1/1	0.97	0.12	26,26,26,26	0
57	MG	BA	3191	1/1	0.97	0.12	40,40,40,40	0
57	MG	BA	3339	1/1	0.97	0.09	43,43,43,43	0
57	MG	DA	3080	1/1	0.97	0.04	49,49,49,49	0
57	MG	DA	3240	1/1	0.97	0.10	52,52,52,52	0
57	MG	BA	3086	1/1	0.97	0.14	42,42,42,42	0
57	MG	BA	3539	1/1	0.97	0.06	42,42,42,42	0
57	MG	BA	3540	1/1	0.97	0.07	31,31,31,31	0
57	MG	BA	3133	1/1	0.97	0.14	37,37,37,37	0
57	MG	BA	3195	1/1	0.97	0.12	36,36,36,36	0
57	MG	DA	3246	1/1	0.97	0.04	46,46,46,46	0
57	MG	B5	101	1/1	0.97	0.28	30,30,30,30	0
57	MG	BA	3543	1/1	0.97	0.11	52,52,52,52	0
57	MG	B5	104	1/1	0.97	0.08	58,58,58,58	0
57	MG	BA	3649	1/1	0.97	0.08	55,55,55,55	0
57	MG	BA	3760	1/1	0.97	0.08	50,50,50,50	0
57	MG	AA	1813	1/1	0.97	0.14	38,38,38,38	0
57	MG	DA	3439	1/1	0.97	0.07	40,40,40,40	0
57	MG	BA	3434	1/1	0.97	0.04	19,19,19,19	0
57	MG	DA	3093	1/1	0.97	0.06	47,47,47,47	0
57	MG	BA	3344	1/1	0.97	0.07	71,71,71,71	0
57	MG	BA	3048	1/1	0.97	0.08	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	B8	5001	1/1	0.97	0.08	42,42,42,42	0
57	MG	DA	3260	1/1	0.97	0.10	39,39,39,39	0
57	MG	BA	3198	1/1	0.97	0.11	44,44,44,44	0
57	MG	BA	3089	1/1	0.97	0.10	36,36,36,36	0
57	MG	CA	3132	1/1	0.97	0.10	64,64,64,64	0
57	MG	DA	3450	1/1	0.97	0.05	50,50,50,50	0
57	MG	BA	3090	1/1	0.97	0.12	38,38,38,38	0
57	MG	DA	3452	1/1	0.97	0.05	45,45,45,45	0
57	MG	CA	3134	1/1	0.97	0.15	64,64,64,64	0
57	MG	DA	3266	1/1	0.97	0.07	37,37,37,37	0
57	MG	BA	3658	1/1	0.97	0.09	61,61,61,61	0
57	MG	DA	3268	1/1	0.97	0.07	41,41,41,41	0
57	MG	DA	3652	1/1	0.97	0.12	31,31,31,31	0
57	MG	DA	3458	1/1	0.97	0.06	41,41,41,41	0
57	MG	BA	3091	1/1	0.97	0.11	42,42,42,42	0
57	MG	DA	3656	1/1	0.97	0.15	41,41,41,41	0
57	MG	DA	3105	1/1	0.97	0.07	45,45,45,45	0
57	MG	AA	1724	1/1	0.97	0.07	39,39,39,39	0
57	MG	DA	3659	1/1	0.97	0.10	41,41,41,41	0
57	MG	DA	3272	1/1	0.97	0.11	49,49,49,49	0
57	MG	DA	3661	1/1	0.97	0.06	62,62,62,62	0
57	MG	BA	3661	1/1	0.97	0.09	25,25,25,25	0
57	MG	AA	1716	1/1	0.97	0.12	50,50,50,50	0
57	MG	DA	3664	1/1	0.97	0.10	51,51,51,51	0
57	MG	BA	3022	1/1	0.97	0.04	25,25,25,25	0
57	MG	DA	3276	1/1	0.97	0.08	28,28,28,28	0
57	MG	DA	3278	1/1	0.97	0.04	39,39,39,39	0
57	MG	AA	1752	1/1	0.97	0.06	48,48,48,48	0
57	MG	DA	3469	1/1	0.97	0.05	50,50,50,50	0
57	MG	BA	3206	1/1	0.97	0.04	34,34,34,34	0
57	MG	BA	3146	1/1	0.97	0.12	41,41,41,41	0
57	MG	DA	3113	1/1	0.97	0.12	35,35,35,35	0
57	MG	AA	1607	1/1	0.97	0.10	55,55,55,55	0
57	MG	BA	3780	1/1	0.97	0.04	42,42,42,42	0
57	MG	BA	3097	1/1	0.97	0.06	41,41,41,41	0
57	MG	BA	3361	1/1	0.97	0.07	56,56,56,56	0
57	MG	BA	3210	1/1	0.97	0.12	41,41,41,41	0
57	MG	BA	3098	1/1	0.97	0.09	23,23,23,23	0
57	MG	BA	3454	1/1	0.97	0.09	46,46,46,46	0
57	MG	AA	1667	1/1	0.97	0.20	55,55,55,55	0
57	MG	DD	304	1/1	0.97	0.08	36,36,36,36	0
57	MG	BA	3214	1/1	0.97	0.30	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3124	1/1	0.97	0.11	43,43,43,43	0
57	MG	AA	1690	1/1	0.97	0.37	52,52,52,52	0
57	MG	AA	1729	1/1	0.97	0.05	35,35,35,35	0
57	MG	CA	3023	1/1	0.97	0.04	39,39,39,39	0
57	MG	BA	3677	1/1	0.97	0.07	44,44,44,44	0
57	MG	DA	3299	1/1	0.97	0.05	46,46,46,46	0
57	MG	BA	3217	1/1	0.97	0.05	50,50,50,50	0
57	MG	DA	3489	1/1	0.97	0.07	48,48,48,48	0
57	MG	BA	3793	1/1	0.97	0.10	11,11,11,11	0
57	MG	BA	3061	1/1	0.97	0.18	25,25,25,25	0
57	MG	DO	201	1/1	0.97	0.14	49,49,49,49	0
57	MG	DA	3304	1/1	0.97	0.05	42,42,42,42	0
57	MG	BA	3795	1/1	0.97	0.11	19,19,19,19	0
57	MG	DP	202	1/1	0.97	0.09	49,49,49,49	0
57	MG	DQ	3002	1/1	0.97	0.12	47,47,47,47	0
57	MG	BA	3371	1/1	0.97	0.06	49,49,49,49	0
57	MG	DA	3307	1/1	0.97	0.06	51,51,51,51	0
57	MG	BA	3797	1/1	0.97	0.24	51,51,51,51	0
57	MG	BA	3465	1/1	0.97	0.04	48,48,48,48	0
57	MG	AA	1677	1/1	0.97	0.13	43,43,43,43	0
57	MG	BA	3580	1/1	0.97	0.04	48,48,48,48	0
57	MG	BA	3002	1/1	0.97	0.12	53,53,53,53	0
57	MG	DA	3501	1/1	0.97	0.09	49,49,49,49	0
57	MG	BA	3005	1/1	0.97	0.12	44,44,44,44	0
57	MG	BA	3469	1/1	0.97	0.11	61,61,61,61	0
57	MG	DA	3316	1/1	0.97	0.18	57,57,57,57	0
57	MG	BA	3556	1/1	0.98	0.04	46,46,46,46	0
57	MG	BA	3075	1/1	0.98	0.13	24,24,24,24	0
57	MG	BA	3783	1/1	0.98	0.11	37,37,37,37	0
57	MG	AA	1649	1/1	0.98	0.07	28,28,28,28	0
57	MG	DA	3453	1/1	0.98	0.10	54,54,54,54	0
57	MG	BR	5002	1/1	0.98	0.12	50,50,50,50	0
57	MG	BA	3059	1/1	0.98	0.06	36,36,36,36	0
57	MG	DA	3095	1/1	0.98	0.18	60,60,60,60	0
57	MG	CA	3165	1/1	0.98	0.05	42,42,42,42	0
57	MG	BU	202	1/1	0.98	0.11	40,40,40,40	0
57	MG	BU	203	1/1	0.98	0.13	34,34,34,34	0
57	MG	CA	3168	1/1	0.98	0.08	41,41,41,41	0
57	MG	DA	3213	1/1	0.98	0.10	37,37,37,37	0
57	MG	BA	3368	1/1	0.98	0.12	32,32,32,32	0
57	MG	BA	3489	1/1	0.98	0.11	50,50,50,50	0
57	MG	BV	202	1/1	0.98	0.18	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BV	203	1/1	0.98	0.07	23,23,23,23	0
57	MG	BA	3490	1/1	0.98	0.04	43,43,43,43	0
57	MG	DA	3598	1/1	0.98	0.04	55,55,55,55	0
57	MG	BV	205	1/1	0.98	0.08	34,34,34,34	0
57	MG	BA	3156	1/1	0.98	0.11	35,35,35,35	0
57	MG	DA	3343	1/1	0.98	0.06	34,34,34,34	0
57	MG	BA	3157	1/1	0.98	0.07	46,46,46,46	0
57	MG	BW	3003	1/1	0.98	0.07	35,35,35,35	0
57	MG	BA	3158	1/1	0.98	0.06	41,41,41,41	0
57	MG	BA	3322	1/1	0.98	0.04	38,38,38,38	0
57	MG	BA	3639	1/1	0.98	0.13	49,49,49,49	0
57	MG	CA	3079	1/1	0.98	0.08	49,49,49,49	0
57	MG	BA	3495	1/1	0.98	0.07	43,43,43,43	0
57	MG	BA	3021	1/1	0.98	0.04	43,43,43,43	0
57	MG	BA	3011	1/1	0.98	0.05	30,30,30,30	0
57	MG	AA	1735	1/1	0.98	0.07	45,45,45,45	0
57	MG	DA	3007	1/1	0.98	0.04	30,30,30,30	0
57	MG	BA	3082	1/1	0.98	0.06	28,28,28,28	0
57	MG	CA	3085	1/1	0.98	0.08	41,41,41,41	0
57	MG	BA	3503	1/1	0.98	0.05	51,51,51,51	0
57	MG	BA	3718	1/1	0.98	0.07	47,47,47,47	0
57	MG	CA	3088	1/1	0.98	0.10	43,43,43,43	0
57	MG	DA	3014	1/1	0.98	0.06	44,44,44,44	0
57	MG	BA	3128	1/1	0.98	0.05	42,42,42,42	0
57	MG	BA	3378	1/1	0.98	0.09	39,39,39,39	0
57	MG	BA	3104	1/1	0.98	0.11	24,24,24,24	0
57	MG	BA	3046	1/1	0.98	0.04	43,43,43,43	0
57	MG	B7	101	1/1	0.98	0.04	41,41,41,41	0
57	MG	BA	3330	1/1	0.98	0.07	27,27,27,27	0
57	MG	BA	3131	1/1	0.98	0.12	44,44,44,44	0
57	MG	BA	3808	1/1	0.98	0.12	38,38,38,38	0
57	MG	BA	3084	1/1	0.98	0.06	42,42,42,42	0
57	MG	BA	3384	1/1	0.98	0.04	45,45,45,45	0
57	MG	BA	3085	1/1	0.98	0.13	31,31,31,31	0
57	MG	BA	3583	1/1	0.98	0.05	33,33,33,33	0
57	MG	BA	3134	1/1	0.98	0.16	40,40,40,40	0
57	MG	BA	3657	1/1	0.98	0.07	38,38,38,38	0
57	MG	BA	3033	1/1	0.98	0.43	31,31,31,31	0
57	MG	BA	3247	1/1	0.98	0.13	29,29,29,29	0
57	MG	DA	3378	1/1	0.98	0.06	52,52,52,52	0
57	MG	AA	1611	1/1	0.98	0.04	20,20,20,20	0
57	MG	BA	3292	1/1	0.98	0.12	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BB	3007	1/1	0.98	0.03	41,41,41,41	0
57	MG	BA	3035	1/1	0.98	0.11	49,49,49,49	0
57	MG	BA	3294	1/1	0.98	0.09	43,43,43,43	0
57	MG	DA	3036	1/1	0.98	0.07	35,35,35,35	0
57	MG	DA	3037	1/1	0.98	0.04	26,26,26,26	0
57	MG	CA	3010	1/1	0.98	0.05	49,49,49,49	0
57	MG	BA	3450	1/1	0.98	0.07	54,54,54,54	0
57	MG	BA	3004	1/1	0.98	0.14	36,36,36,36	0
57	MG	BA	3742	1/1	0.98	0.05	48,48,48,48	0
57	MG	AA	1745	1/1	0.98	0.07	36,36,36,36	0
57	MG	BA	3053	1/1	0.98	0.16	23,23,23,23	0
57	MG	BA	3114	1/1	0.98	0.06	39,39,39,39	0
57	MG	BB	3016	1/1	0.98	0.04	34,34,34,34	0
57	MG	DA	3047	1/1	0.98	0.14	45,45,45,45	0
57	MG	BA	3142	1/1	0.98	0.19	46,46,46,46	0
57	MG	BA	3054	1/1	0.98	0.14	30,30,30,30	0
57	MG	BA	3457	1/1	0.98	0.12	48,48,48,48	0
57	MG	DA	3655	1/1	0.98	0.05	38,38,38,38	0
57	MG	BA	3256	1/1	0.98	0.30	34,34,34,34	0
57	MG	BA	3459	1/1	0.98	0.07	31,31,31,31	0
57	MG	DA	3525	1/1	0.98	0.08	28,28,28,28	0
57	MG	DA	3526	1/1	0.98	0.06	52,52,52,52	0
57	MG	DA	3277	1/1	0.98	0.05	50,50,50,50	0
57	MG	BA	3402	1/1	0.98	0.05	27,27,27,27	0
57	MG	DA	3163	1/1	0.98	0.14	34,34,34,34	0
57	MG	DA	3054	1/1	0.98	0.07	27,27,27,27	0
57	MG	AA	1792	1/1	0.98	0.06	47,47,47,47	0
57	MG	BA	3350	1/1	0.98	0.04	34,34,34,34	0
57	MG	BA	3039	1/1	0.98	0.14	36,36,36,36	0
57	MG	BD	3004	1/1	0.98	0.17	28,28,28,28	0
57	MG	BA	3464	1/1	0.98	0.03	44,44,44,44	0
57	MG	DA	3170	1/1	0.98	0.08	35,35,35,35	0
57	MG	DA	3537	1/1	0.98	0.06	45,45,45,45	0
57	MG	DA	3171	1/1	0.98	0.09	40,40,40,40	0
57	MG	BD	3007	1/1	0.98	0.11	46,46,46,46	0
57	MG	BA	3756	1/1	0.98	0.05	18,18,18,18	0
57	MG	DA	3290	1/1	0.98	0.07	33,33,33,33	0
57	MG	BA	3679	1/1	0.98	0.11	52,52,52,52	0
57	MG	BD	3010	1/1	0.98	0.07	46,46,46,46	0
57	MG	BA	3260	1/1	0.98	0.08	19,19,19,19	0
57	MG	BA	3118	1/1	0.98	0.12	35,35,35,35	0
57	MG	DA	3178	1/1	0.98	0.08	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3537	1/1	0.98	0.05	43,43,43,43	0
57	MG	DA	3297	1/1	0.98	0.15	51,51,51,51	0
57	MG	DE	3001	1/1	0.98	0.26	31,31,31,31	0
57	MG	DE	3002	1/1	0.98	0.12	33,33,33,33	0
57	MG	DE	3003	1/1	0.98	0.12	43,43,43,43	0
57	MG	BA	3220	1/1	0.98	0.07	35,35,35,35	0
57	MG	DA	3550	1/1	0.98	0.04	60,60,60,60	0
57	MG	BA	3409	1/1	0.98	0.09	22,22,22,22	0
57	MG	DA	3300	1/1	0.98	0.11	38,38,38,38	0
57	MG	BA	3221	1/1	0.98	0.14	29,29,29,29	0
57	MG	BA	3357	1/1	0.98	0.04	34,34,34,34	0
57	MG	BF	302	1/1	0.98	0.17	30,30,30,30	0
57	MG	BA	3474	1/1	0.98	0.13	33,33,33,33	0
57	MG	BA	3148	1/1	0.98	0.21	38,38,38,38	0
57	MG	BA	3544	1/1	0.98	0.05	52,52,52,52	0
57	MG	BA	3183	1/1	0.98	0.18	49,49,49,49	0
57	MG	BA	3149	1/1	0.98	0.04	42,42,42,42	0
57	MG	BF	308	1/1	0.98	0.06	43,43,43,43	0
57	MG	BA	3478	1/1	0.98	0.07	54,54,54,54	0
57	MG	BA	3772	1/1	0.98	0.14	36,36,36,36	0
57	MG	BF	311	1/1	0.98	0.07	52,52,52,52	0
57	MG	BA	3073	1/1	0.98	0.04	32,32,32,32	0
57	MG	DA	3440	1/1	0.98	0.06	36,36,36,36	0
57	MG	BA	3550	1/1	0.98	0.06	50,50,50,50	0
57	MG	BA	3551	1/1	0.98	0.05	44,44,44,44	0
57	MG	DW	3001	1/1	0.98	0.07	41,41,41,41	0
57	MG	BA	3151	1/1	0.98	0.07	36,36,36,36	0
57	MG	BA	3227	1/1	0.98	0.05	33,33,33,33	0
57	MG	BA	3698	1/1	0.98	0.05	47,47,47,47	0
57	MG	BA	3779	1/1	0.98	0.03	17,17,17,17	0
58	SF4	AD	501	8/8	0.98	0.06	59,68,73,79	0
58	SF4	CD	501	8/8	0.98	0.04	64,67,74,91	0
57	MG	DA	3574	1/1	0.98	0.04	61,61,61,61	0
57	MG	DA	3322	1/1	0.98	0.09	42,42,42,42	0
57	MG	AA	1740	1/1	0.98	0.08	41,41,41,41	0
57	MG	DA	3251	1/1	0.99	0.04	40,40,40,40	0
57	MG	BA	3050	1/1	0.99	0.11	32,32,32,32	0
57	MG	BA	3040	1/1	0.99	0.20	33,33,33,33	0
57	MG	CA	3044	1/1	0.99	0.09	47,47,47,47	0
57	MG	BA	3587	1/1	0.99	0.05	46,46,46,46	0
57	MG	BA	3186	1/1	0.99	0.09	41,41,41,41	0
57	MG	BA	3013	1/1	0.99	0.04	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3590	1/1	0.99	0.07	33,33,33,33	0
57	MG	DA	3259	1/1	0.99	0.06	42,42,42,42	0
57	MG	DA	3312	1/1	0.99	0.03	42,42,42,42	0
57	MG	AA	1734	1/1	0.99	0.05	43,43,43,43	0
57	MG	BA	3555	1/1	0.99	0.08	50,50,50,50	0
57	MG	AA	1768	1/1	0.99	0.06	53,53,53,53	0
57	MG	DA	3013	1/1	0.99	0.03	39,39,39,39	0
57	MG	BA	3307	1/1	0.99	0.05	28,28,28,28	0
57	MG	BA	3412	1/1	0.99	0.03	30,30,30,30	0
57	MG	DA	3373	1/1	0.99	0.03	31,31,31,31	0
57	MG	AA	1744	1/1	0.99	0.06	44,44,44,44	0
57	MG	BA	3009	1/1	0.99	0.06	31,31,31,31	0
57	MG	DA	3321	1/1	0.99	0.09	29,29,29,29	0
57	MG	BA	3192	1/1	0.99	0.06	19,19,19,19	0
57	MG	BA	3635	1/1	0.99	0.04	42,42,42,42	0
57	MG	BA	3440	1/1	0.99	0.04	35,35,35,35	0
57	MG	AA	1730	1/1	0.99	0.10	27,27,27,27	0
57	MG	BA	3417	1/1	0.99	0.09	24,24,24,24	0
57	MG	DA	3121	1/1	0.99	0.10	40,40,40,40	0
57	MG	DA	3383	1/1	0.99	0.02	28,28,28,28	0
57	MG	BA	3393	1/1	0.99	0.06	23,23,23,23	0
57	MG	BA	3499	1/1	0.99	0.03	39,39,39,39	0
57	MG	BD	3001	1/1	0.99	0.04	34,34,34,34	0
57	MG	BA	3080	1/1	0.99	0.07	31,31,31,31	0
57	MG	DA	3562	1/1	0.99	0.03	31,31,31,31	0
57	MG	BA	3501	1/1	0.99	0.03	42,42,42,42	0
57	MG	BA	3003	1/1	0.99	0.05	33,33,33,33	0
57	MG	BA	3758	1/1	0.99	0.05	41,41,41,41	0
57	MG	BD	3006	1/1	0.99	0.06	34,34,34,34	0
57	MG	BA	3471	1/1	0.99	0.07	27,27,27,27	0
57	MG	BA	3800	1/1	0.99	0.06	29,29,29,29	0
57	MG	BA	3472	1/1	0.99	0.05	24,24,24,24	0
57	MG	CA	3118	1/1	0.99	0.11	60,60,60,60	0
57	MG	BA	3473	1/1	0.99	0.07	28,28,28,28	0
57	MG	BA	3259	1/1	0.99	0.08	25,25,25,25	0
57	MG	DA	3398	1/1	0.99	0.02	40,40,40,40	0
57	MG	BA	3211	1/1	0.99	0.09	43,43,43,43	0
57	MG	BA	3020	1/1	0.99	0.04	25,25,25,25	0
57	MG	DA	3039	1/1	0.99	0.07	38,38,38,38	0
57	MG	DQ	3001	1/1	0.99	0.05	50,50,50,50	0
57	MG	BA	3356	1/1	0.99	0.09	31,31,31,31	0
57	MG	BA	3336	1/1	0.99	0.04	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3404	1/1	0.99	0.03	43,43,43,43	0
57	MG	BA	3479	1/1	0.99	0.05	53,53,53,53	0
57	MG	BA	3262	1/1	0.99	0.26	31,31,31,31	0
57	MG	DA	3582	1/1	0.99	0.05	53,53,53,53	0
57	MG	BA	3810	1/1	0.99	0.04	35,35,35,35	0
57	MG	DA	3584	1/1	0.99	0.03	31,31,31,31	0
57	MG	BA	3729	1/1	0.99	0.04	46,46,46,46	0
57	MG	BA	3143	1/1	0.99	0.08	41,41,41,41	0
57	MG	BA	3813	1/1	0.99	0.12	29,29,29,29	0
57	MG	BA	3731	1/1	0.99	0.04	32,32,32,32	0
59	ZN	AN	501	1/1	0.99	0.04	77,77,77,77	0
59	ZN	BY	501	1/1	0.99	0.04	68,68,68,68	0
59	ZN	B4	501	1/1	0.99	0.03	118,118,118,118	0
57	MG	BA	3547	1/1	0.99	0.06	45,45,45,45	0
59	ZN	DY	501	1/1	0.99	0.03	90,90,90,90	0
57	MG	AA	1681	1/1	0.99	0.03	38,38,38,38	0
59	ZN	D5	501	1/1	0.99	0.04	57,57,57,57	0
59	ZN	D6	501	1/1	0.99	0.04	65,65,65,65	0
59	ZN	D9	501	1/1	0.99	0.03	64,64,64,64	0
57	MG	BA	3483	1/1	0.99	0.06	44,44,44,44	0
59	ZN	B6	102	1/1	1.00	0.07	50,50,50,50	0
59	ZN	B9	501	1/1	1.00	0.07	49,49,49,49	0
57	MG	BA	3397	1/1	1.00	0.04	28,28,28,28	0
57	MG	BA	3725	1/1	1.00	0.05	31,31,31,31	0
57	MG	BA	3502	1/1	1.00	0.11	30,30,30,30	0
57	MG	BA	3007	1/1	1.00	0.09	21,21,21,21	0
57	MG	BA	3567	1/1	1.00	0.11	32,32,32,32	0
57	MG	DA	3589	1/1	1.00	0.02	29,29,29,29	0
59	ZN	B5	103	1/1	1.00	0.03	40,40,40,40	0

6.5 Other polymers ⓘ

There are no such residues in this entry.