



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 08:39 AM UTC

PDB ID : 1VY5 / pdb_00001vy5
Title : Crystal structure of the Thermus thermophilus 70S ribosome in the post-catalysis state of peptide bond formation containing dipeptidyl-tRNA in the A site and deacylated tRNA in the P site.
Authors : Polikanov, Y.S.; Steitz, T.A.; Innis, C.A.
Deposited on : 2014-05-13
Resolution : 2.55 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

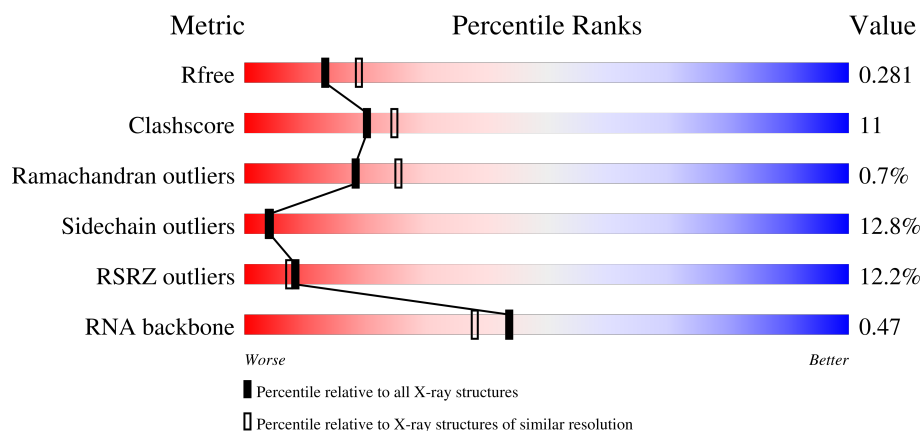
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)
RNA backbone	3983	1112 (2.80-2.28)

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	5% 51% 38% 9%
1	CA	1521	13% 45% 43% 11%
2	AB	256	27% 39% 41% 10% 10%
2	CB	256	43% 35% 41% 13% 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	

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 297141 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	1498	Total	C	N	O	P	0	0	0
			32205	14333	5970	10404	1498			
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
			1542	968	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
			1674	1050	333	284	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
			806	511	143	149	3			
6	CF	100	Total	C	N	O	S	0	0	0
			816	516	146	151	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
			983	623	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			
			714	445	138	131	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	AK	114	Total	C	N	O	S		
			829	516	155	155	3	0	0
11	CK	114	Total	C	N	O	S		
			833	519	156	155	3	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		
			930	585	185	159	1	0	0
12	CL	122	Total	C	N	O	S		
			930	585	185	159	1	0	0

- 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		
			958	592	198	166	2	0	0
13	CM	122	Total	C	N	O	S		
			950	586	197	165	2	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S		
			492	312	104	72	4	0	0
14	CN	60	Total	C	N	O	S		
			492	312	104	72	4	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		
			728	456	144	126	2	0	0
15	CO	88	Total	C	N	O	S		
			728	456	144	126	2	0	0

- 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	83	Total	C	N	O	S	0	0	0
			652	417	120	113	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
			727	446	155	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
			1607	727	288	516	73	3			
23	CW	72	Total	C	N	O	P	S	0	0	0
			1560	702	281	503	72	2			

- 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
			1625	725	294	529	76	1			
24	CX	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- 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
			2136	1349	423	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
			1061	680	186	194	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
			1135	706	230	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
			511	328	99	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	214	Total	Mg	0	0
			214	214		
57	AE	3	Total	Mg	0	0
			3	3		
57	AF	1	Total	Mg	0	0
			1	1		
57	AK	1	Total	Mg	0	0
			1	1		
57	AM	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AN	2	Total 2	Mg 2	0	0
57	AW	4	Total 4	Mg 4	0	0
57	AX	15	Total 15	Mg 15	0	0
57	AY	3	Total 3	Mg 3	0	0
57	BA	812	Total 812	Mg 812	0	0
57	BB	20	Total 20	Mg 20	0	0
57	BD	9	Total 9	Mg 9	0	0
57	BE	8	Total 8	Mg 8	0	0
57	BF	9	Total 9	Mg 9	0	0
57	BG	3	Total 3	Mg 3	0	0
57	BN	6	Total 6	Mg 6	0	0
57	BO	2	Total 2	Mg 2	0	0
57	BP	5	Total 5	Mg 5	0	0
57	BQ	5	Total 5	Mg 5	0	0
57	BR	2	Total 2	Mg 2	0	0
57	BU	8	Total 8	Mg 8	0	0
57	BV	5	Total 5	Mg 5	0	0
57	BW	4	Total 4	Mg 4	0	0
57	BX	3	Total 3	Mg 3	0	0
57	BY	1	Total 1	Mg 1	0	0
57	BZ	1	Total 1	Mg 1	0	0

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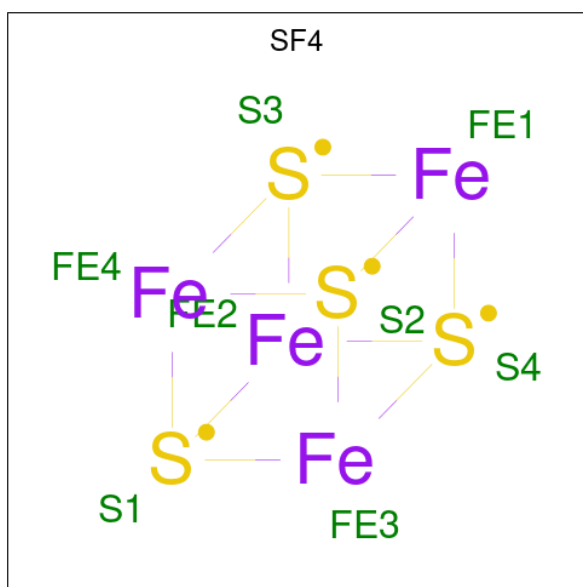
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	B0	3	Total 3	Mg 3	0	0
57	B1	1	Total 1	Mg 1	0	0
57	B2	1	Total 1	Mg 1	0	0
57	B3	2	Total 2	Mg 2	0	0
57	B4	1	Total 1	Mg 1	0	0
57	B5	1	Total 1	Mg 1	0	0
57	B6	2	Total 2	Mg 2	0	0
57	B7	5	Total 5	Mg 5	0	0
57	B8	1	Total 1	Mg 1	0	0
57	B9	1	Total 1	Mg 1	0	0
57	CA	170	Total 170	Mg 170	0	0
57	CD	1	Total 1	Mg 1	0	0
57	CE	1	Total 1	Mg 1	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	CV	1	Total 1	Mg 1	0	0
57	CW	1	Total 1	Mg 1	0	0
57	CX	3	Total 3	Mg 3	0	0
57	DA	677	Total 677	Mg 677	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DB	13	Total 13	Mg 13	0	0
57	DD	9	Total 9	Mg 9	0	0
57	DE	4	Total 4	Mg 4	0	0
57	DF	4	Total 4	Mg 4	0	0
57	DG	1	Total 1	Mg 1	0	0
57	DN	1	Total 1	Mg 1	0	0
57	DO	1	Total 1	Mg 1	0	0
57	DP	2	Total 2	Mg 2	0	0
57	DQ	4	Total 4	Mg 4	0	0
57	DR	1	Total 1	Mg 1	0	0
57	DU	2	Total 2	Mg 2	0	0
57	DV	3	Total 3	Mg 3	0	0
57	DW	4	Total 4	Mg 4	0	0
57	DX	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
60	CX	1	Total 1	K 1	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AA	227	Total 227	O 227	0	0
61	AE	2	Total 2	O 2	0	0
61	AJ	1	Total 1	O 1	0	0
61	AL	1	Total 1	O 1	0	0
61	AM	1	Total 1	O 1	0	0
61	AU	1	Total 1	O 1	0	0
61	AV	3	Total 3	O 3	0	0
61	AW	3	Total 3	O 3	0	0
61	AX	6	Total 6	O 6	0	0
61	AY	1	Total 1	O 1	0	0
61	BA	1383	Total 1383	O 1383	0	0
61	BB	36	Total 36	O 36	0	0
61	BD	12	Total 12	O 12	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	BE	14	Total 14	O 14	0	0
61	BF	8	Total 8	O 8	0	0
61	BG	3	Total 3	O 3	0	0
61	BI	1	Total 1	O 1	0	0
61	BO	4	Total 4	O 4	0	0
61	BP	16	Total 16	O 16	0	0
61	BQ	4	Total 4	O 4	0	0
61	BR	2	Total 2	O 2	0	0
61	BT	2	Total 2	O 2	0	0
61	BU	3	Total 3	O 3	0	0
61	BV	2	Total 2	O 2	0	0
61	BW	1	Total 1	O 1	0	0
61	BX	4	Total 4	O 4	0	0
61	BZ	1	Total 1	O 1	0	0
61	B0	3	Total 3	O 3	0	0
61	B1	1	Total 1	O 1	0	0
61	B3	2	Total 2	O 2	0	0
61	B5	2	Total 2	O 2	0	0
61	B6	1	Total 1	O 1	0	0
61	B7	2	Total 2	O 2	0	0
61	B8	8	Total 8	O 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	CA	185	Total 185	O 185	0	0
61	CJ	2	Total 2	O 2	0	0
61	CL	1	Total 1	O 1	0	0
61	CT	1	Total 1	O 1	0	0
61	CV	1	Total 1	O 1	0	0
61	CW	2	Total 2	O 2	0	0
61	DA	1025	Total 1025	O 1025	0	0
61	DB	9	Total 9	O 9	0	0
61	DD	19	Total 19	O 19	0	0
61	DE	11	Total 11	O 11	0	0
61	DF	3	Total 3	O 3	0	0
61	DN	2	Total 2	O 2	0	0
61	DO	1	Total 1	O 1	0	0
61	DP	16	Total 16	O 16	0	0
61	DR	1	Total 1	O 1	0	0
61	DT	3	Total 3	O 3	0	0
61	DU	2	Total 2	O 2	0	0
61	DX	3	Total 3	O 3	0	0
61	DY	2	Total 2	O 2	0	0
61	D0	3	Total 3	O 3	0	0
61	D1	1	Total 1	O 1	0	0

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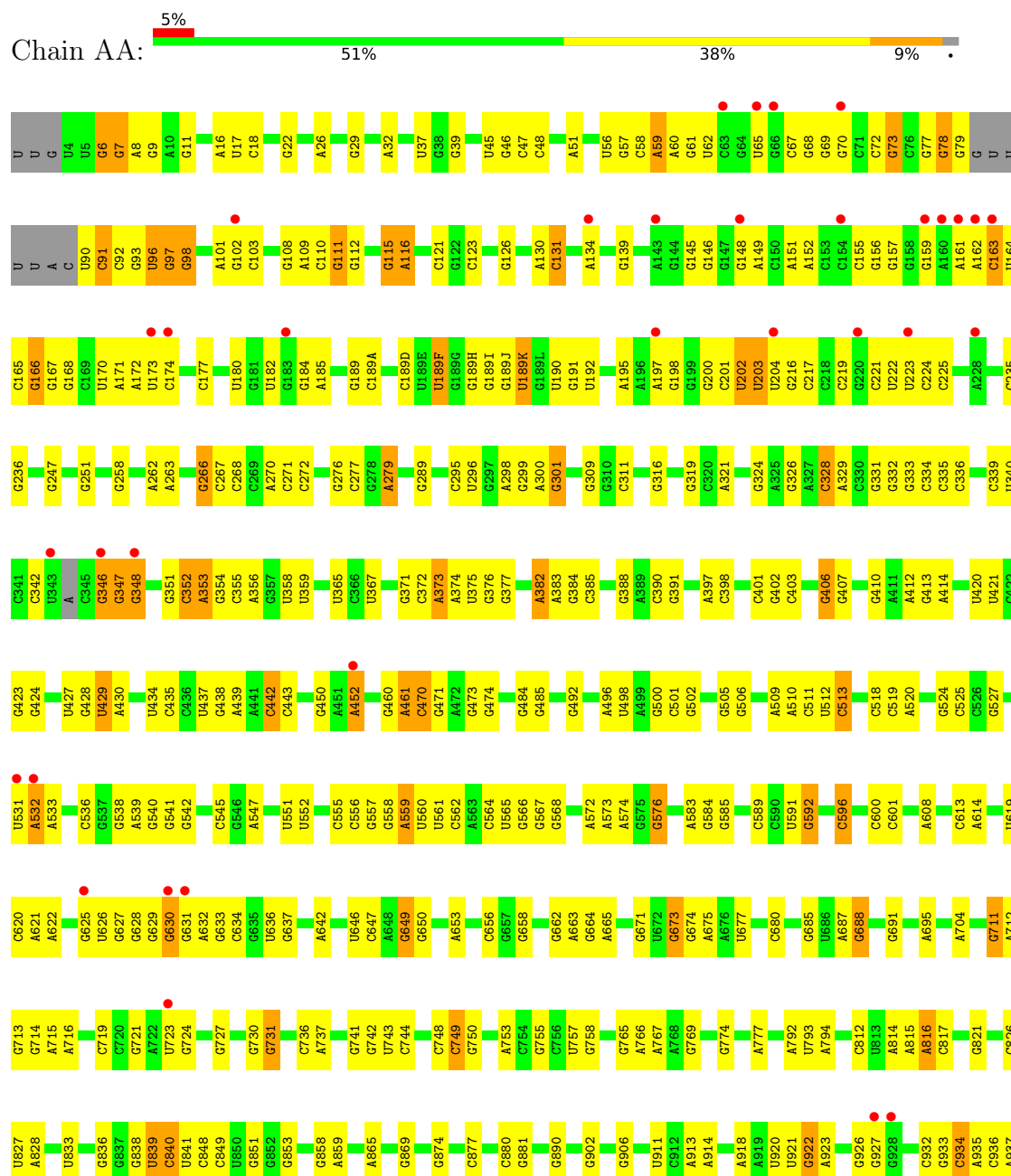
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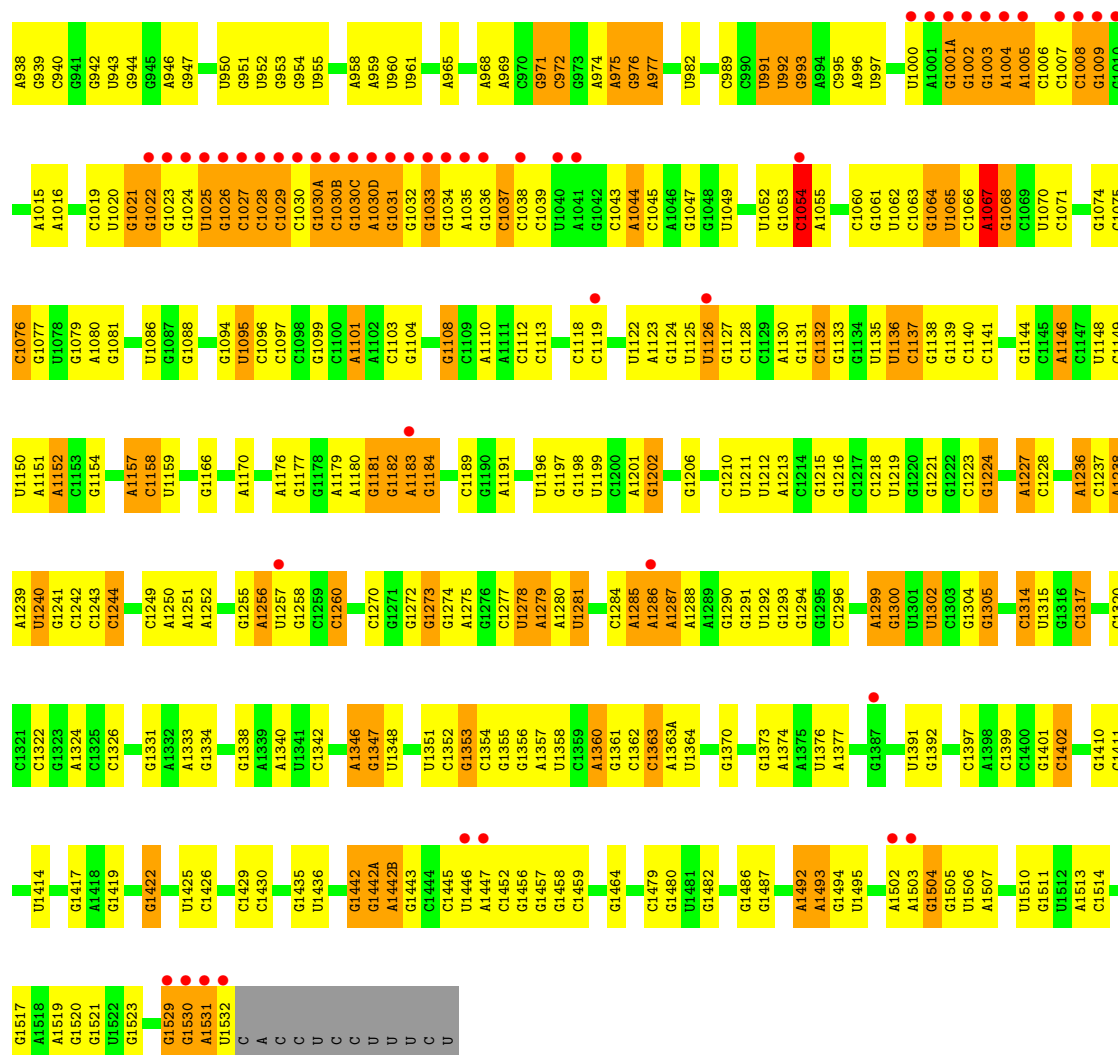
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	D3	1	Total	O	0	0
			1	1		
61	D7	3	Total	O	0	0
			3	3		
61	D8	4	Total	O	0	0
			4	4		

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.

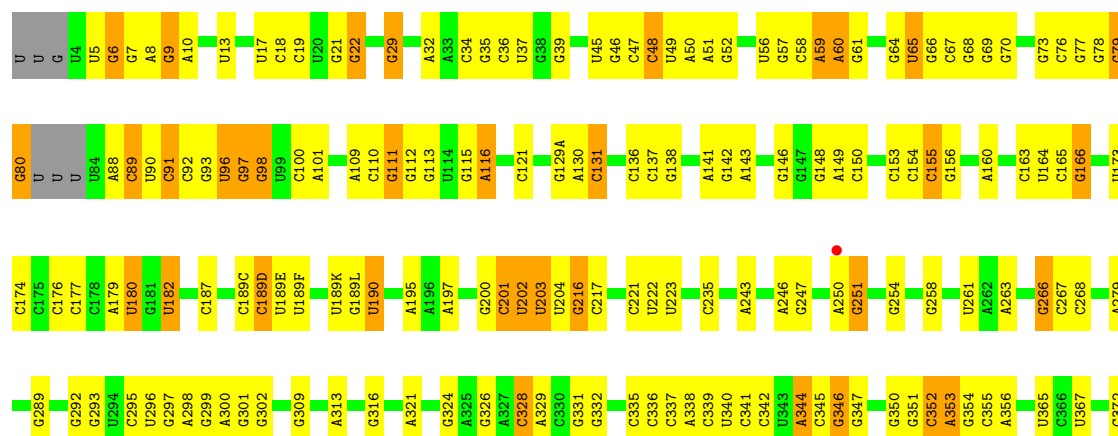
• Molecule 1: 16S Ribosomal RNA





• Molecule 1: 16S Ribosomal RNA

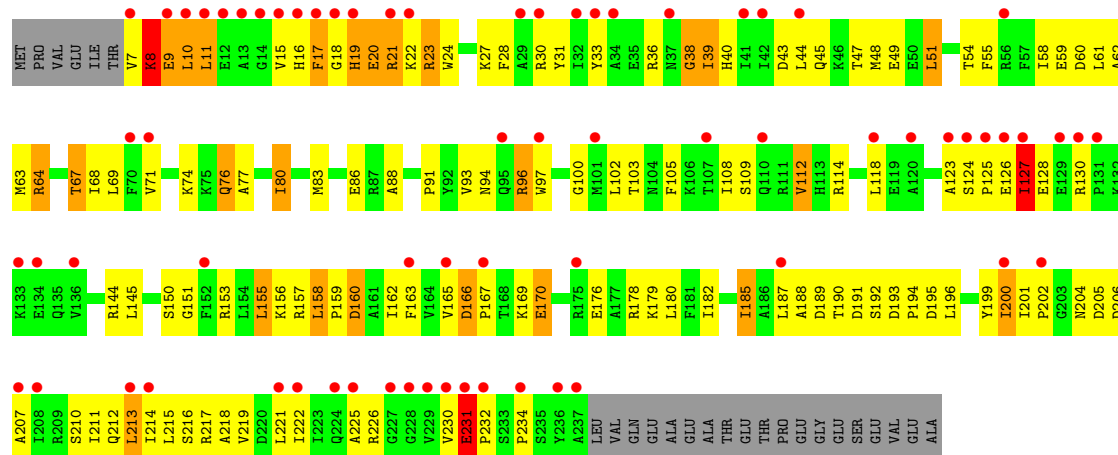
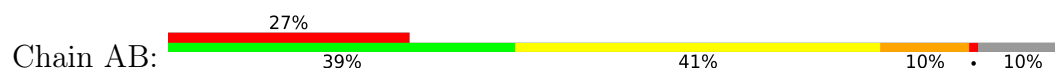
Chain CA: 13% 45% 43% 11%.



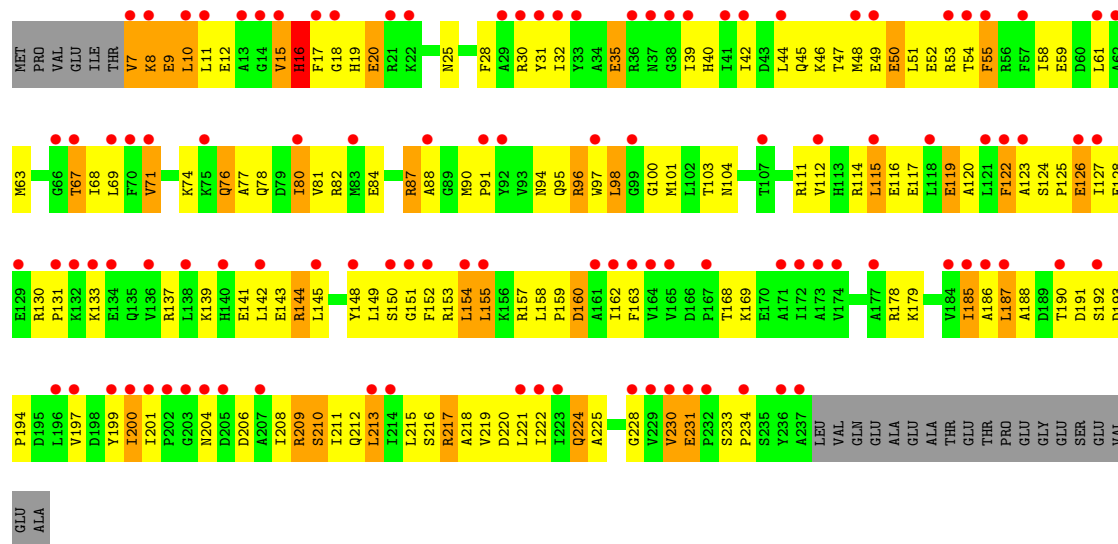
C1378	C1379	C1383	G1386	G1387	C1388	U1391	G1392	C1397	A1398	C1399	C1402	G1410	C1411	C1412	A1413	U1414	G1419	G1422	C1423	C1424	C1429	C1430	G1435	U1436	G1441	G1442	A1442B	U1446	C1447	C1452	G1456	G1457	G1469	C1479	G1480	G1486	C1487	C1490	G1491	A1492	A1493	A1494																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
U1315	G1316	C1317	A1318	A1319	C1320	C1321	C1322	G1323	A1324	C1325	C1326	C1327	C1328	G1331	A1332	A1333	G1334	G1338	A1339	A1340	U1341	C1342	G1343	C1344	U1345	C1346	C1347	U1348	A1349	U1351	C1352	G1353	C1354	A1357	U1358	C1359	A1360	G1361	C1362	A1363	U1364	G1365	C1366	C1367	G1370	G1371	U1372	G1373	A1374	A1375	U1376	A1377																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
C1249	A1179	C1116	G1050	C995	C932	A828	U646	G542	C447	A373	G447	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646	G542	C447	U646



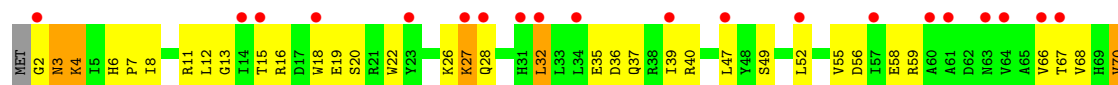
• Molecule 2: 30S ribosomal protein S2

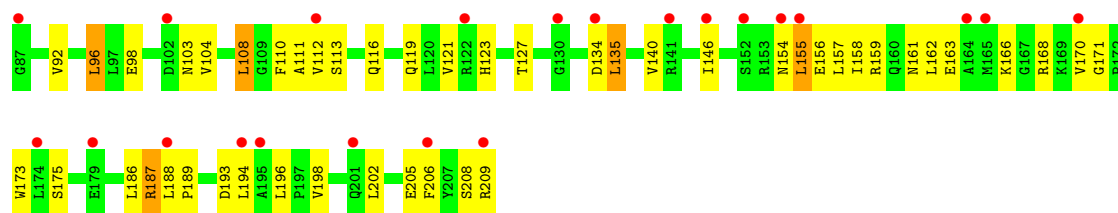


• Molecule 2: 30S ribosomal protein S2

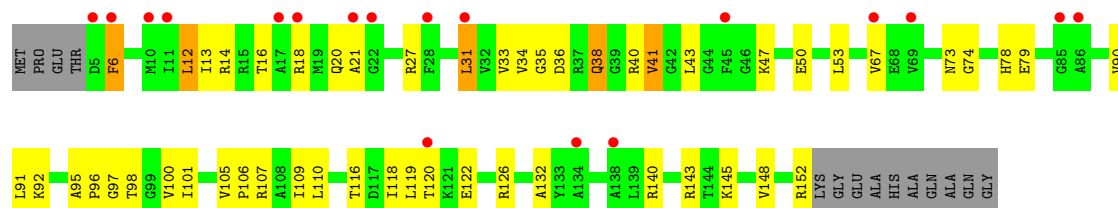


• Molecule 3: 30S ribosomal protein S3

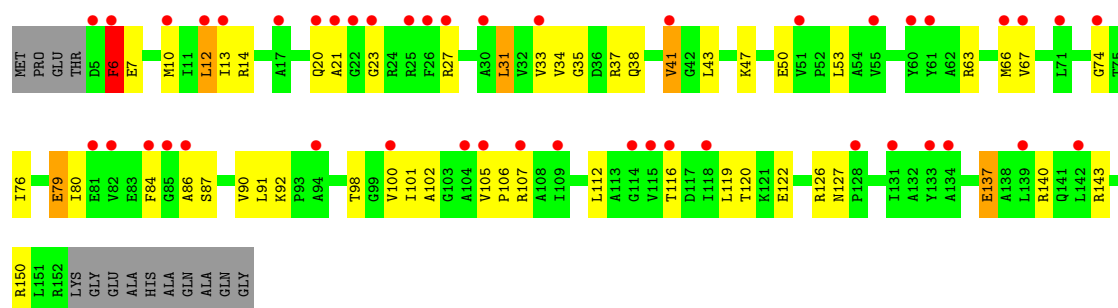




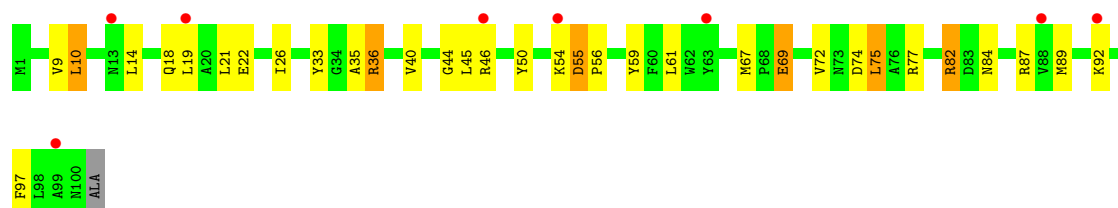
• Molecule 5: 30S ribosomal protein S5



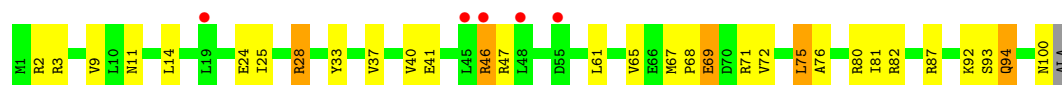
• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6

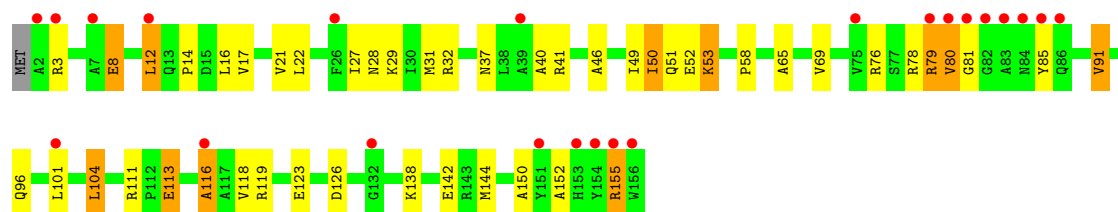


• Molecule 6: 30S ribosomal protein S6



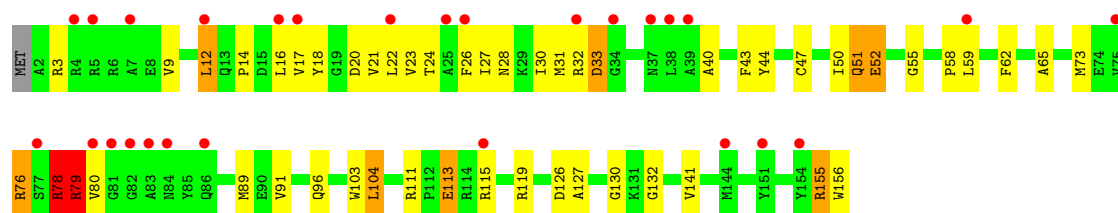
- Molecule 7: 30S ribosomal protein S7

Chain AG: 



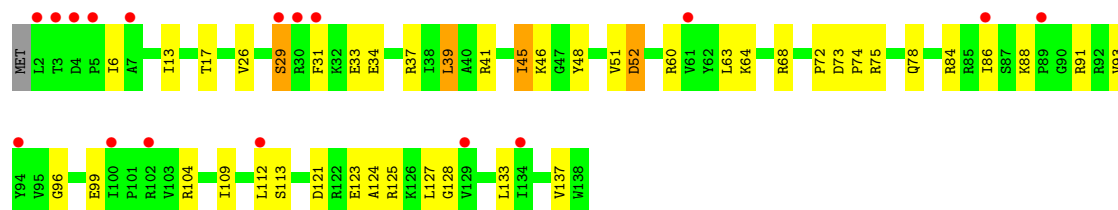
- Molecule 7: 30S ribosomal protein S7

Chain CG: 



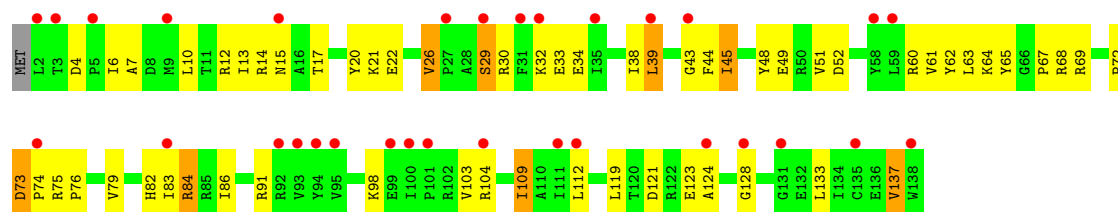
- Molecule 8: 30S ribosomal protein S8

Chain AH: 



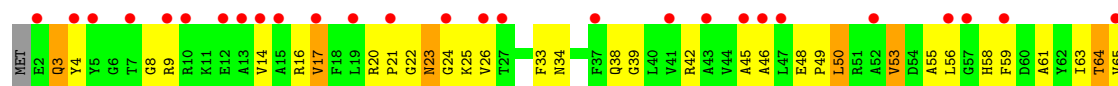
- Molecule 8: 30S ribosomal protein S8

Chain CH: 



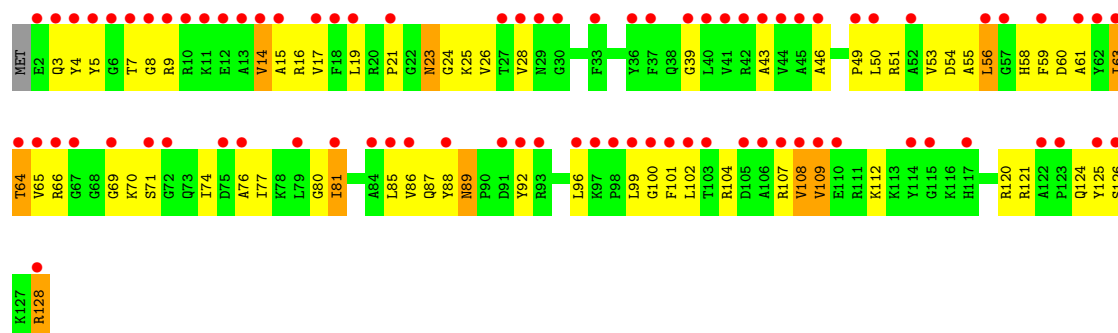
- Molecule 9: 30S ribosomal protein S9

Chain AI: 

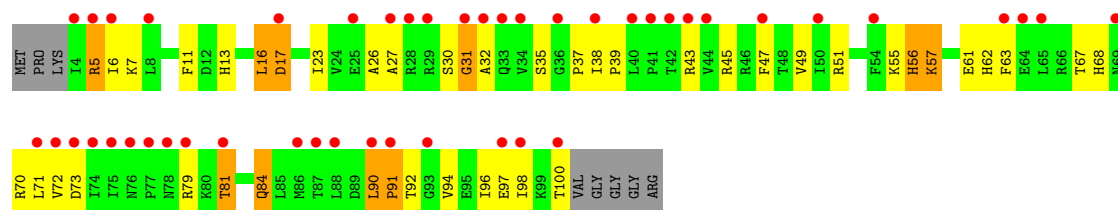




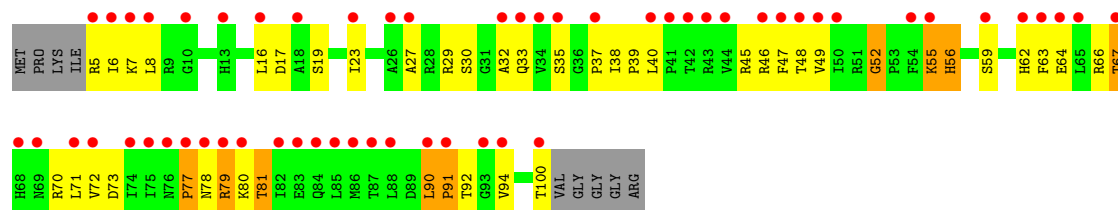
• Molecule 9: 30S ribosomal protein S9



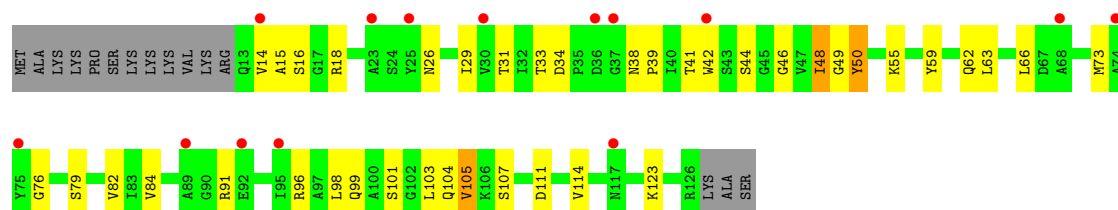
• Molecule 10: 30S ribosomal protein S10



• Molecule 10: 30S ribosomal protein S10

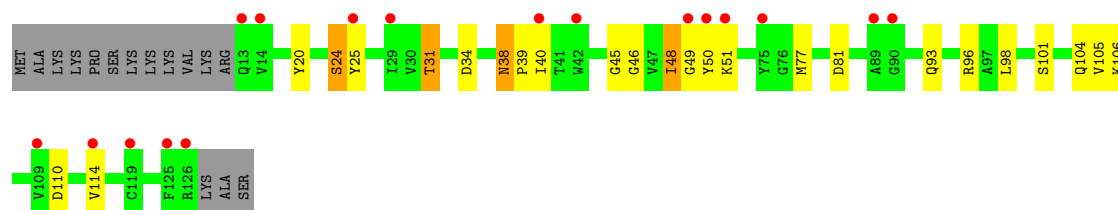


• Molecule 11: 30S ribosomal protein S11



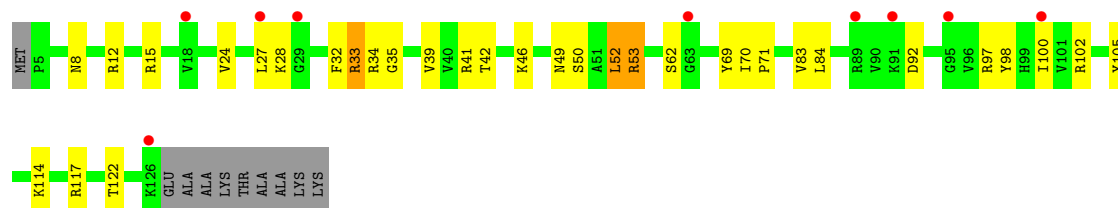
- Molecule 11: 30S ribosomal protein S11

Chain CK: 13% 69% 16% 12%



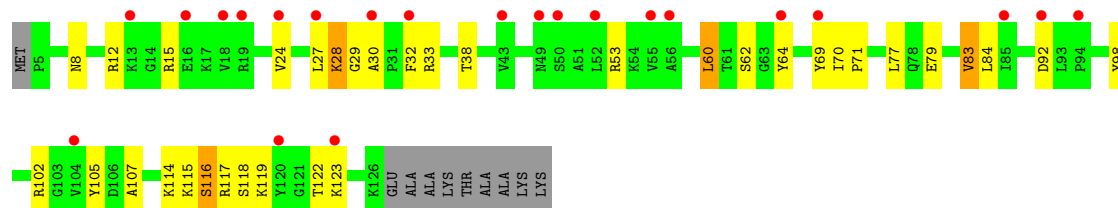
- Molecule 12: 30S ribosomal protein S12

Chain AL: 7% 67% 23% 8%



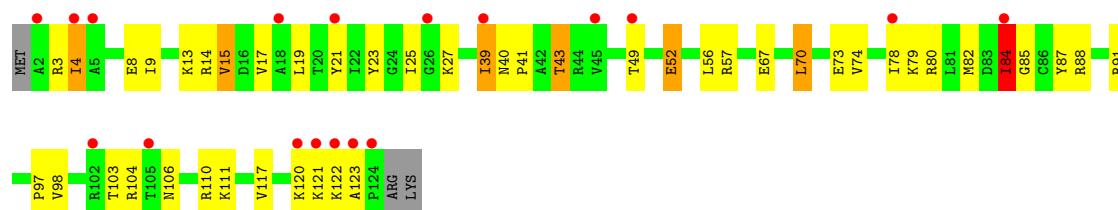
- Molecule 12: 30S ribosomal protein S12

Chain CL: 17% 66% 23% 8%



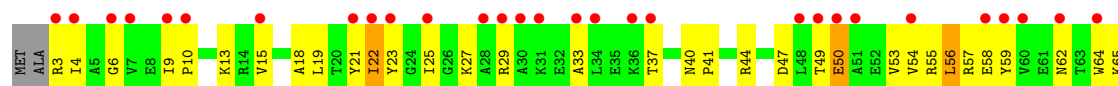
- Molecule 13: 30S ribosomal protein S13

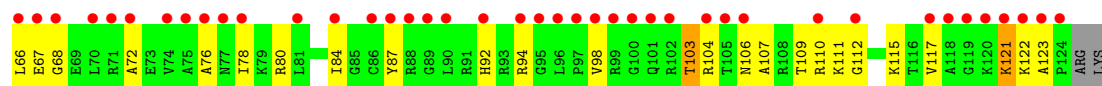
Chain AM: 14% 61% 31% 5%



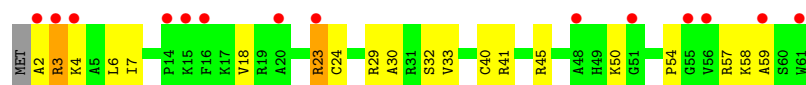
- Molecule 13: 30S ribosomal protein S13

Chain CM: 56% 51% 42%

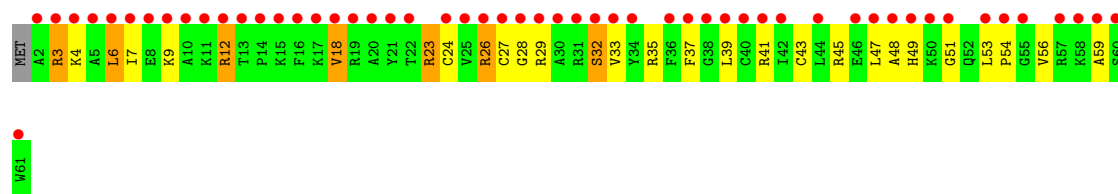
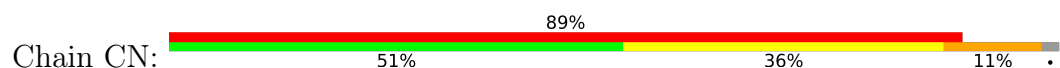




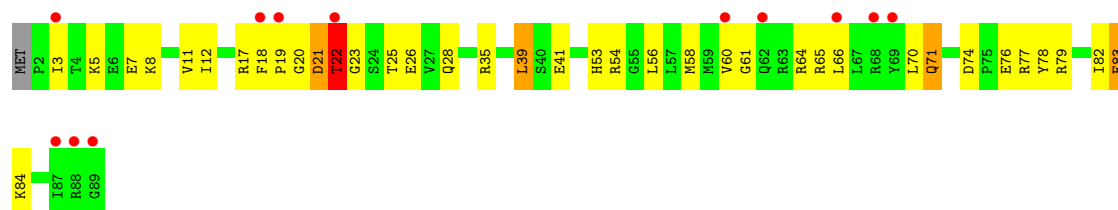
- Molecule 14: 30S ribosomal protein S14 type Z



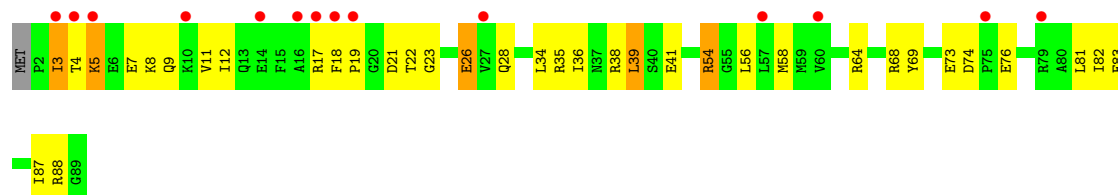
- Molecule 14: 30S ribosomal protein S14 type Z



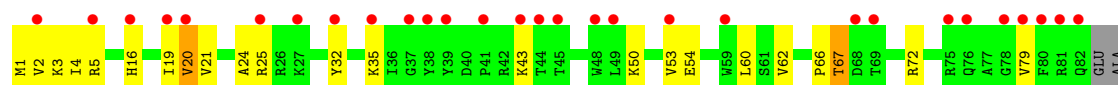
- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15

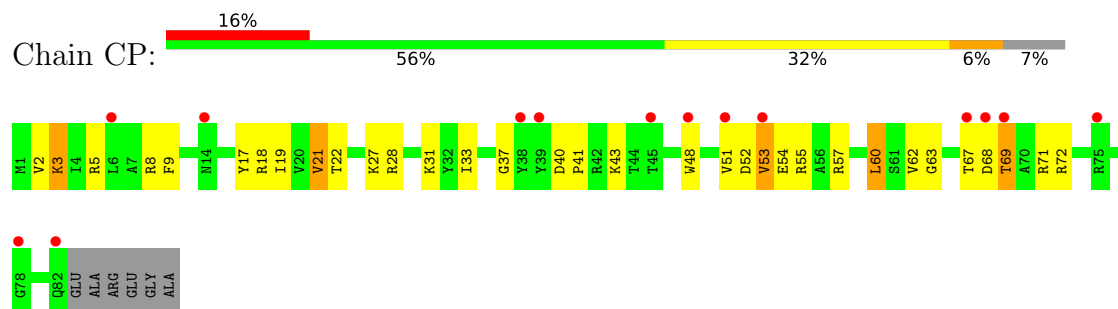


- Molecule 16: 30S ribosomal protein S16

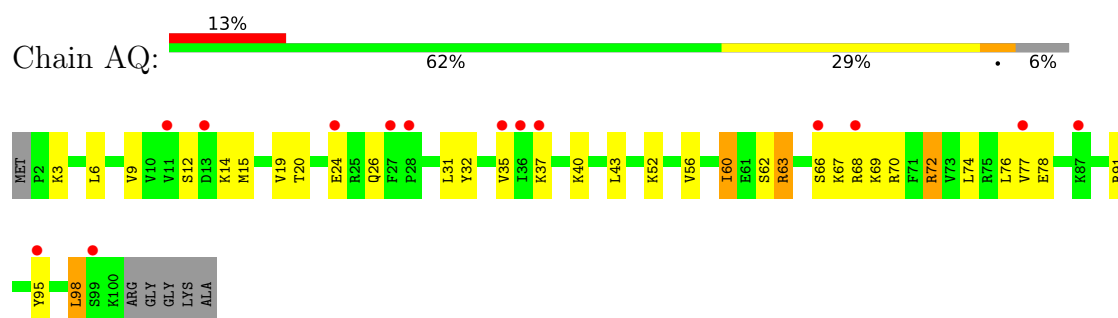


ARG
GLU
GLY
ALA

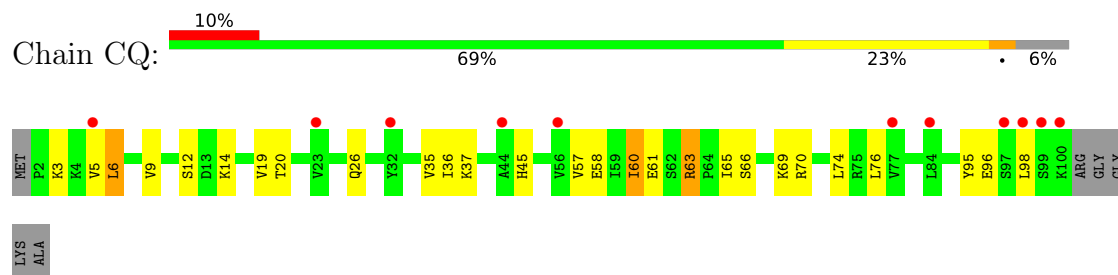
- Molecule 16: 30S ribosomal protein S16



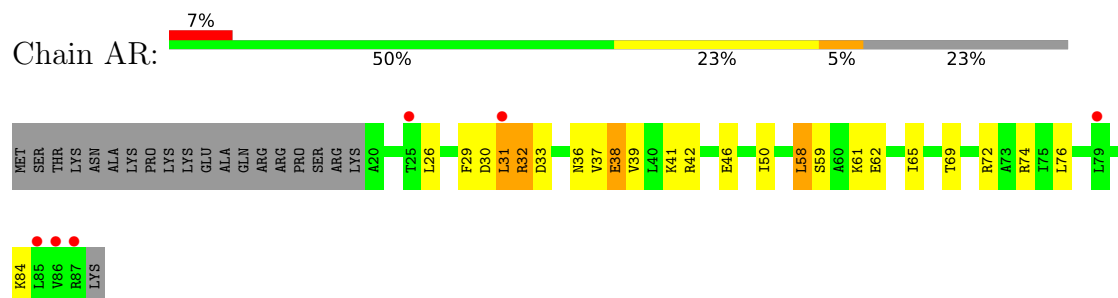
- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17

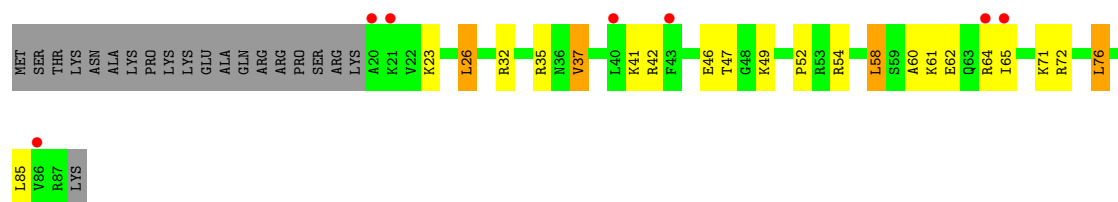


- Molecule 18: 30S ribosomal protein S18

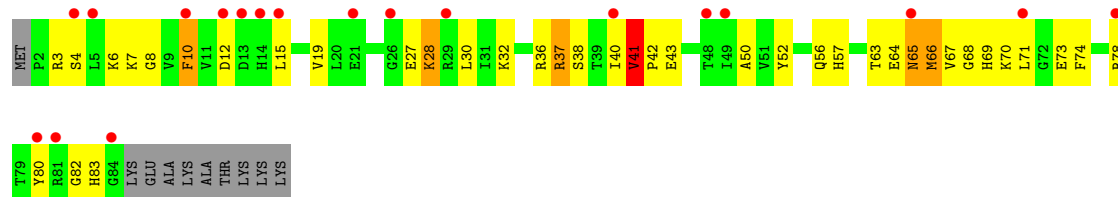


- Molecule 18: 30S ribosomal protein S18

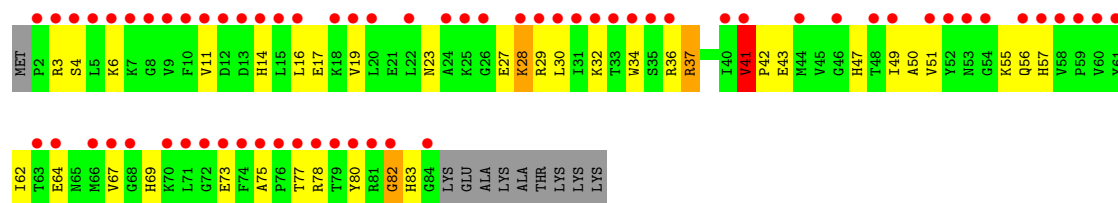
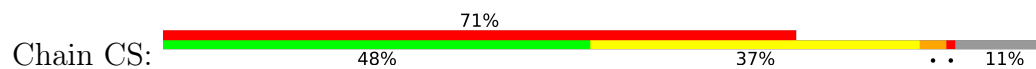




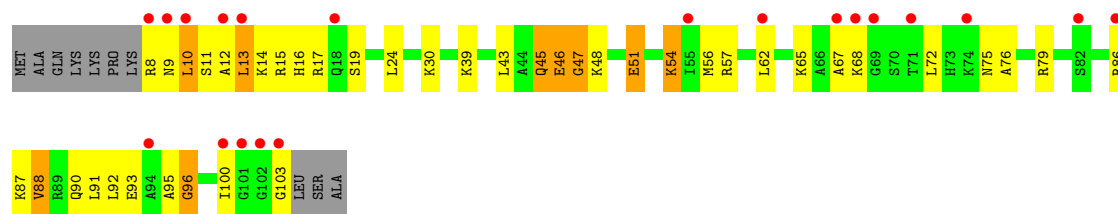
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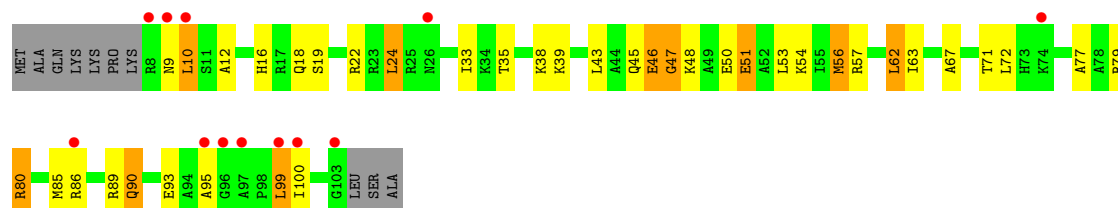
• Molecule 19: 30S ribosomal protein S19



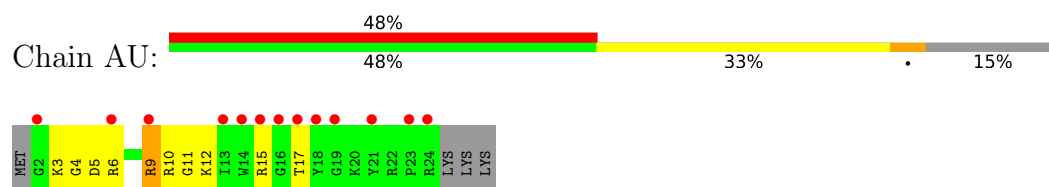
• Molecule 20: 30S ribosomal protein S20



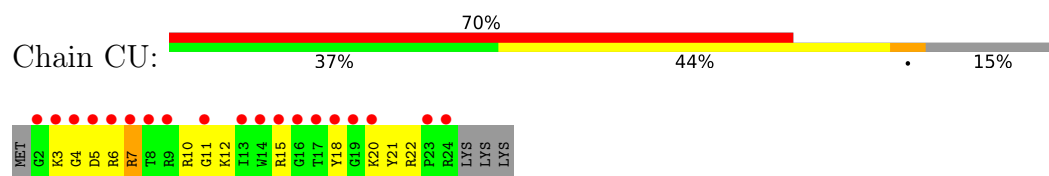
• Molecule 20: 30S ribosomal protein S20



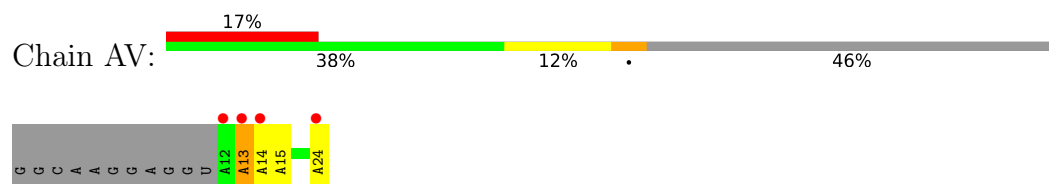
• Molecule 21: 30S ribosomal protein Thx



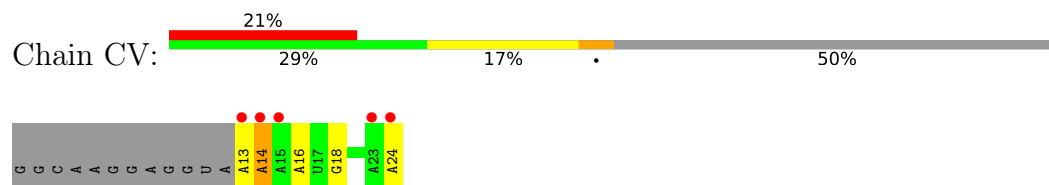
• Molecule 21: 30S ribosomal protein Thx



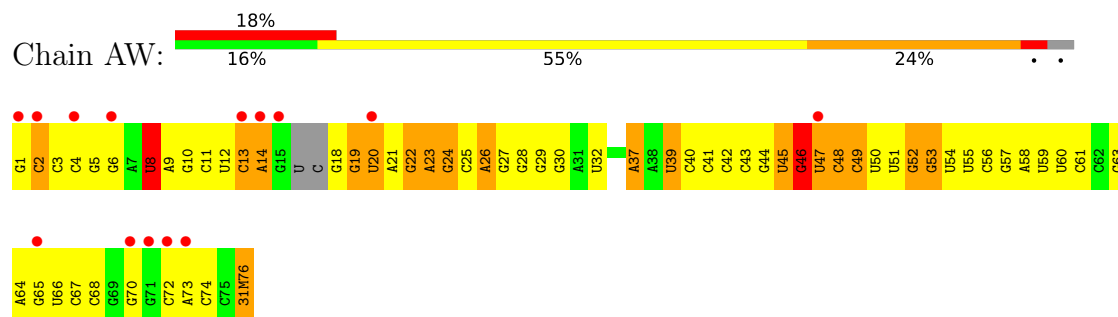
• Molecule 22: mRNA



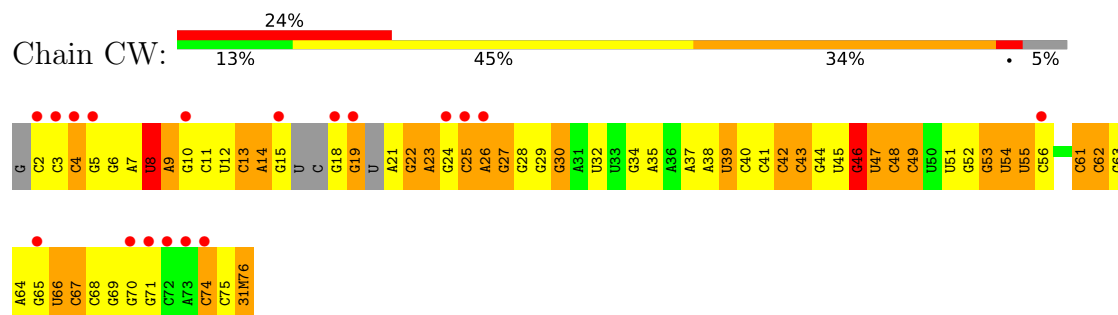
• Molecule 22: mRNA



• Molecule 23: A-site tRNA



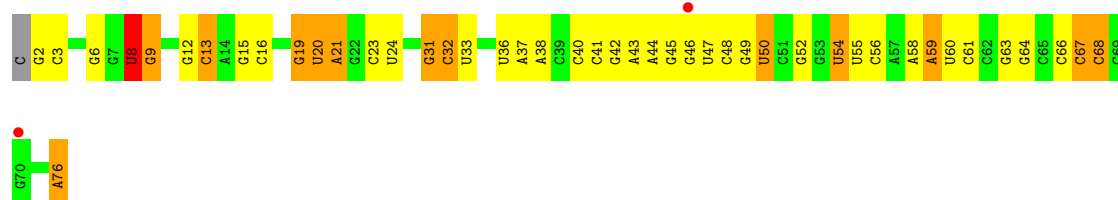
• Molecule 23: A-site tRNA



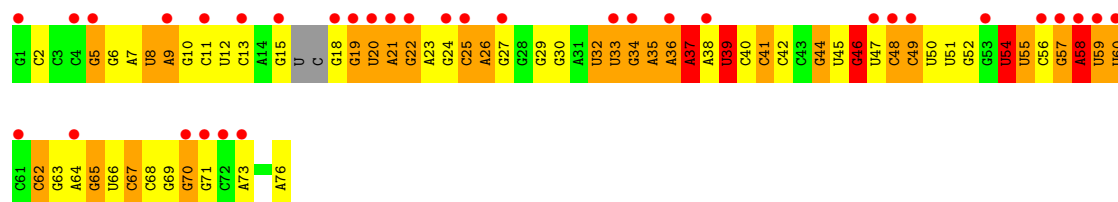
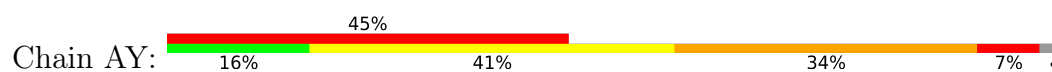
- Molecule 24: P-site tRNA



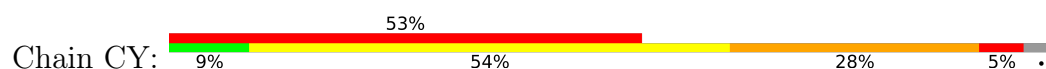
- Molecule 24: P-site tRNA



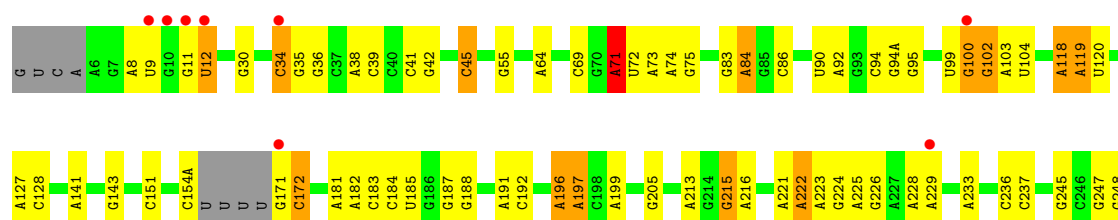
- Molecule 25: E-site tRNA

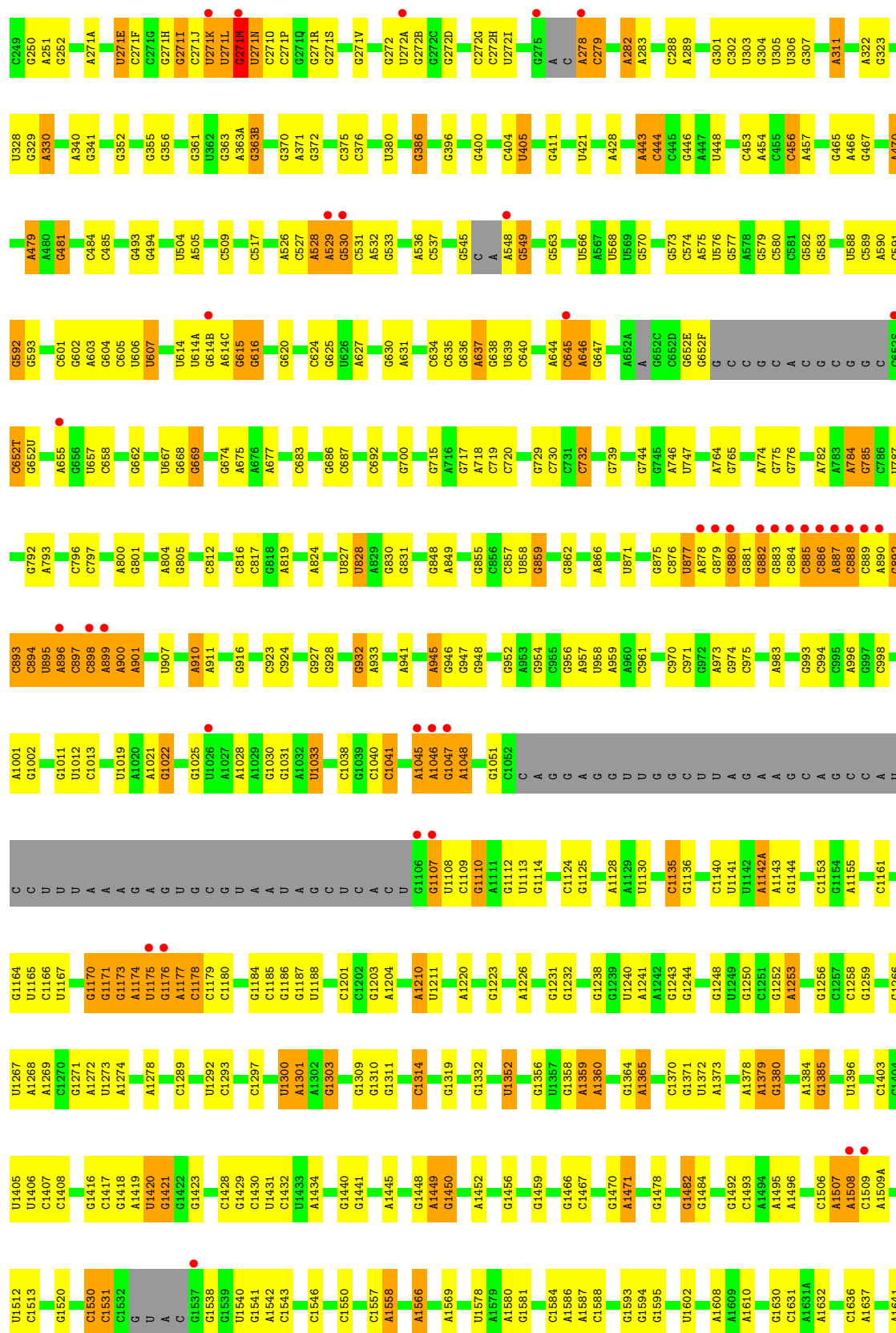


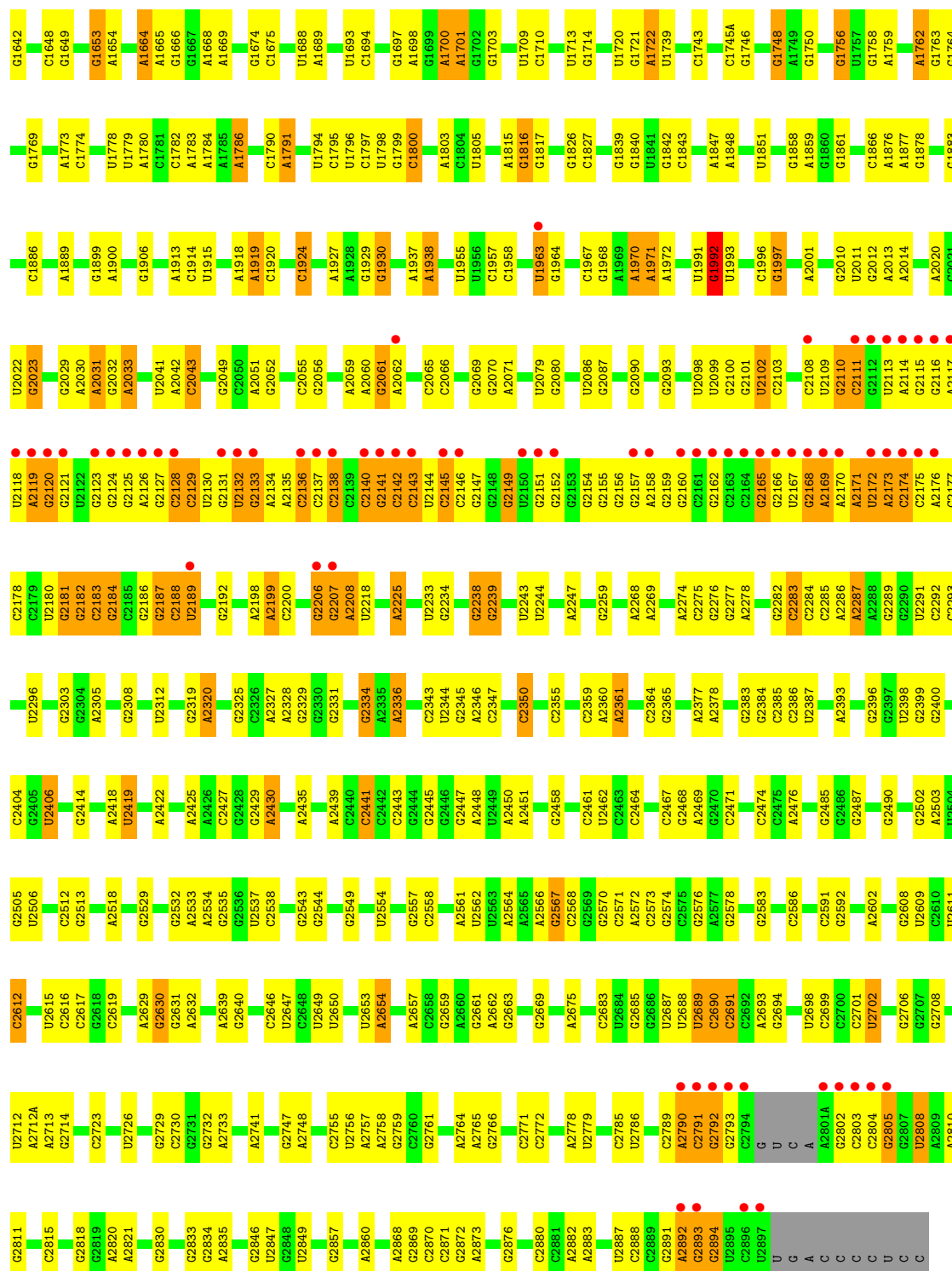
- Molecule 25: E-site tRNA



- Molecule 26: 23S Ribosomal RNA



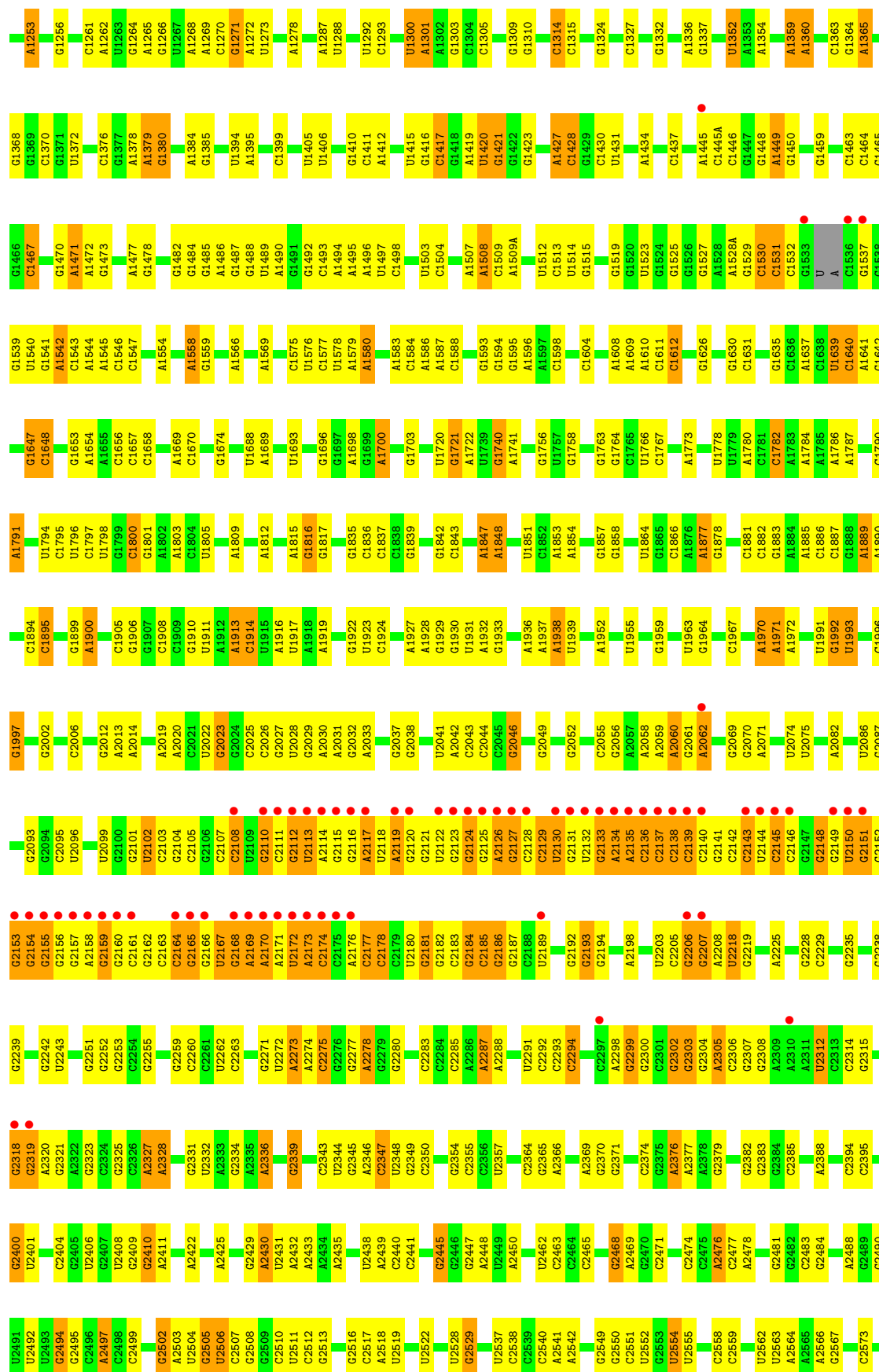


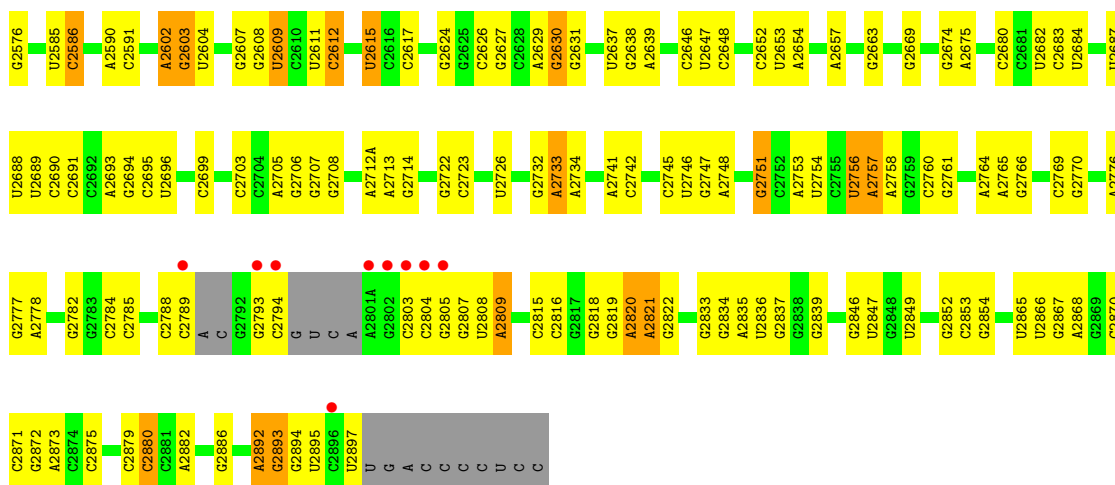


• Molecule 26: 23S Ribosomal RNA

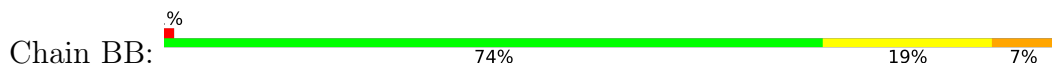


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C	C	C1038	U1038	A960	A960	G883	U803	G710	G628	C540	C453	C453	G272C	A204	G94A
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C	C	G	G	C971	C971	C889	U810	G724	U639	G	A457	A457	G272K	A103	A103
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U	U	A	A	A988	A988	C904	A880	G744	G652C	A575	A536	G437	G336	A278	A182
U	U	A	A	A988	A988	C904	A881	G744	G652D	A575	A537	G438	G337	A279	C183
U	U	A	A	A988	A988	C904	A882	G744	G652E	A575	A538	G439	G338	A280	U185
U	U	A	A	A988	A988	C904	A883	G744	G652F	A575	A539	G440	G339	A281	G178
U	U	A	A	A988	A988	C904	A884	G744	G652G	A575	A540	G441	G340	A282	A181
U	U	A	A	A988	A988	C904	A885	G744	G652H	A575	A541	G442	G341	A283	A182
U	U	A	A	A988	A988	C904	A886	G744	G652I	A575	A542	G443	G342	A284	C183
U	U	A	A	A988	A988	C904	A887	G744	G652J	A575	A543	G444	G343	A285	U185
U	U	A	A	A988	A988	C904	A888	G744	G652K	A575	A544	G445	G344	A286	G178
U	U	A	A	A988	A988	C904	A889	G744	G652L	A575	A545	G446	G345	A287	A181
U	U	A	A	A988	A988	C904	A890	G744	G652M	A575	A546	G447	G346	A288	A182
U	U	A	A	A988	A988	C904	A891	G744	G652N	A575	A547	G448	G347	A289	C183
U	U	A	A	A988	A988	C904	A892	G744	G652O	A575	A548	G449	G348	A290	U185
U	U	A	A	A988	A988	C904	A893	G744	G652P	A575	A549	G450	G349	A291	G178
U	U	A	A	A988	A988	C904	A894	G744	G652Q	A575	A550	G451	G350	A292	A181
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U	U	A	A	A988	A988	C904	A896	G744	G652S	A575	A552	G453	G352	A294	C183
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U	U	A	A	A988	A988	C904	A898	G744	G652U	A575	A554	G455	G354	A296	G178
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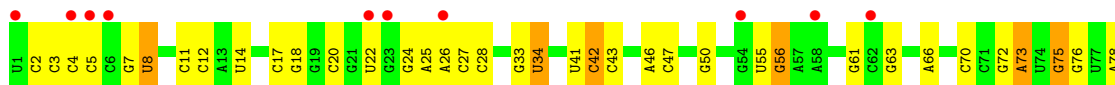




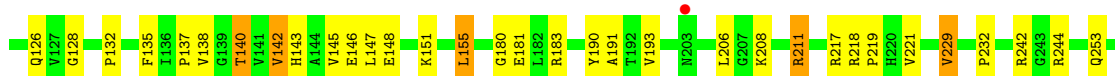
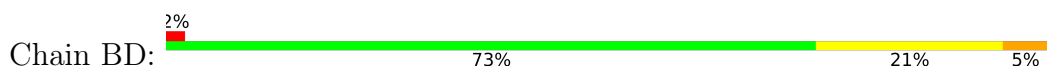
• Molecule 27: 5S Ribosomal RNA



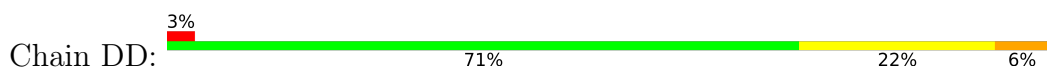
• Molecule 27: 5S Ribosomal RNA



• Molecule 28: 50S ribosomal protein L2

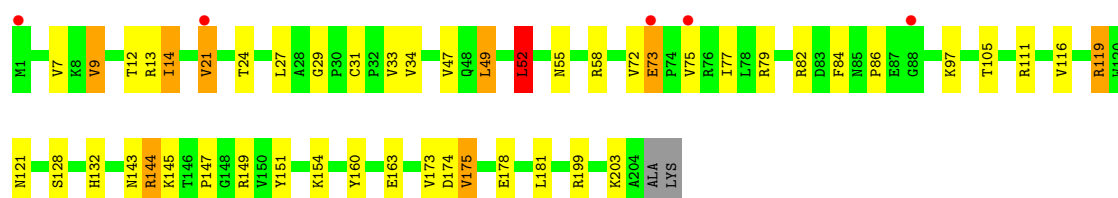
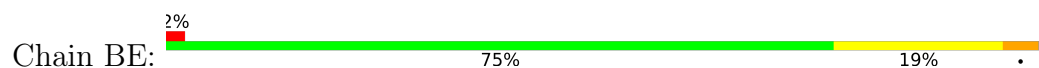


• Molecule 28: 50S ribosomal protein L2

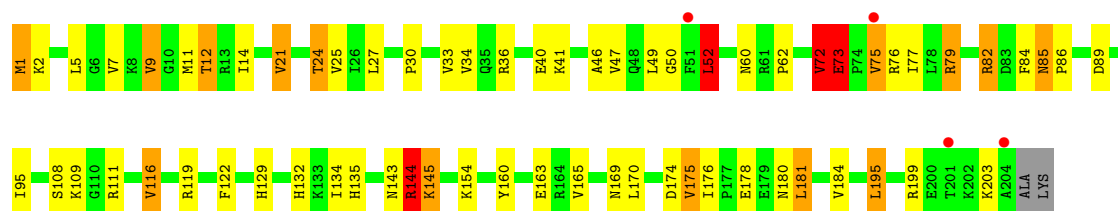




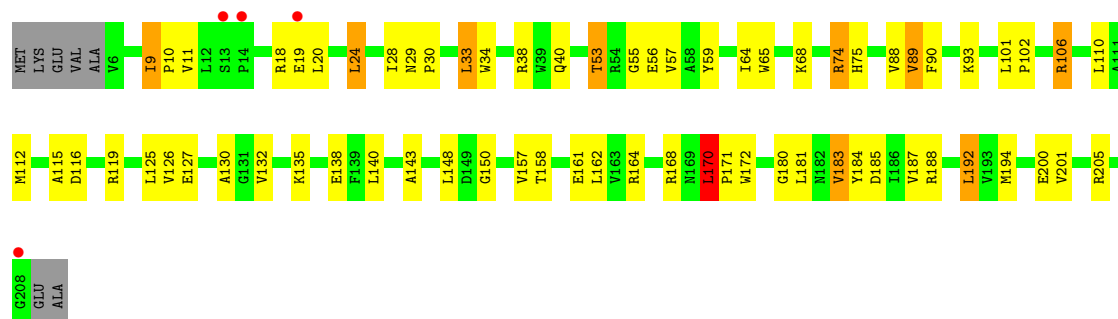
• Molecule 29: 50S ribosomal protein L3



• Molecule 29: 50S ribosomal protein L3

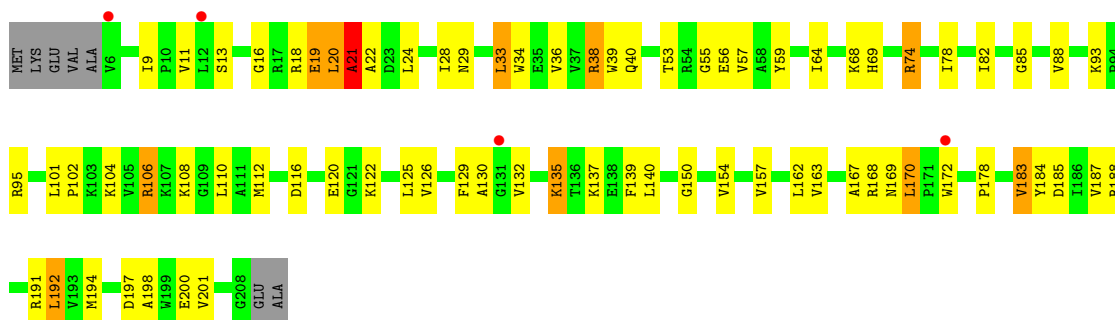


• Molecule 30: 50S ribosomal protein L4

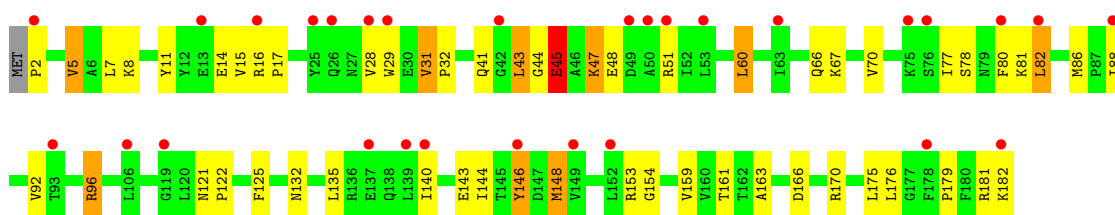


• Molecule 30: 50S ribosomal protein L4

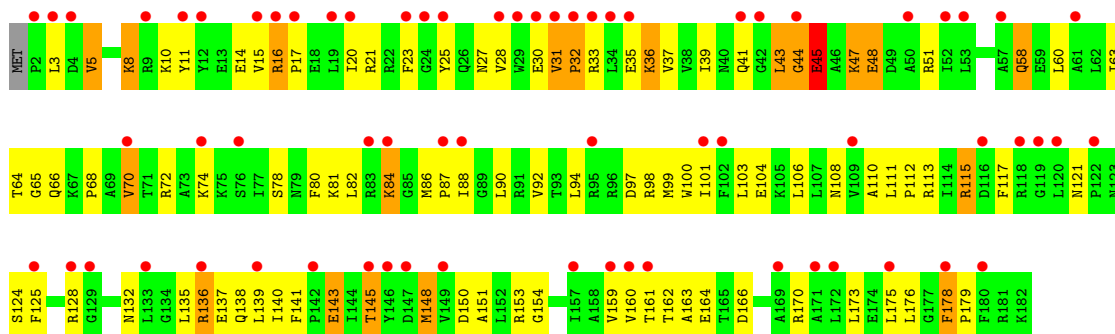
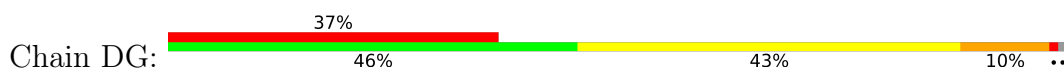




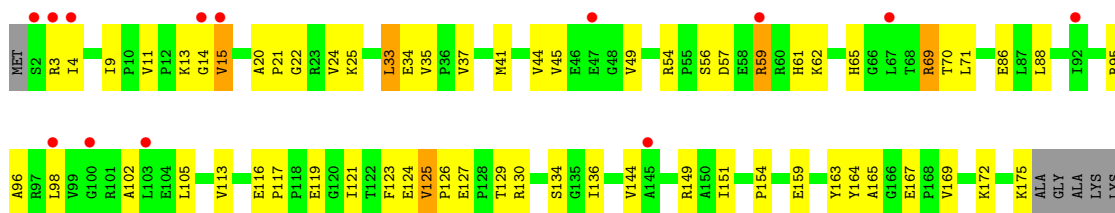
• Molecule 31: 50S ribosomal protein L5



• Molecule 31: 50S ribosomal protein L5

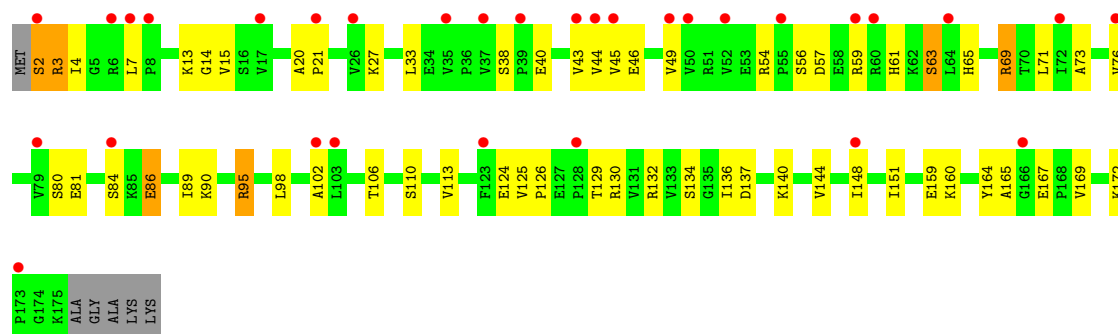


• Molecule 32: 50S ribosomal protein L6

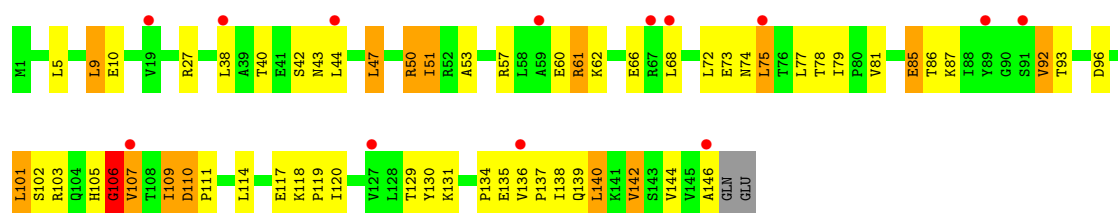


• Molecule 32: 50S ribosomal protein L6

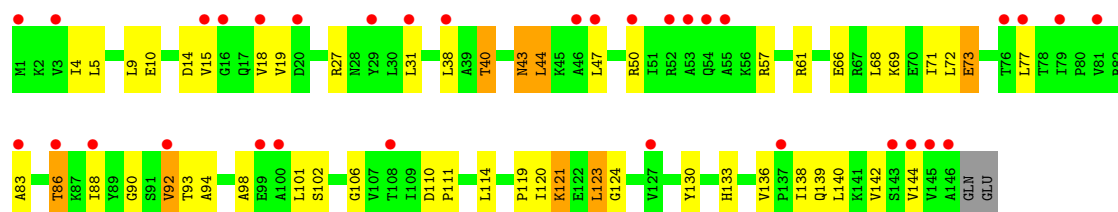




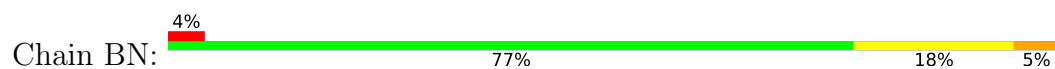
• Molecule 33: 50S ribosomal protein L9



• Molecule 33: 50S ribosomal protein L9



• Molecule 34: 50S ribosomal protein L13

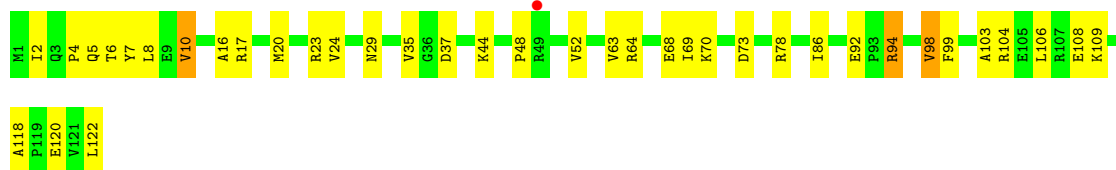
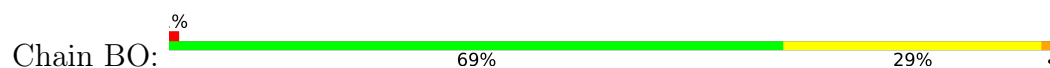


• Molecule 34: 50S ribosomal protein L13

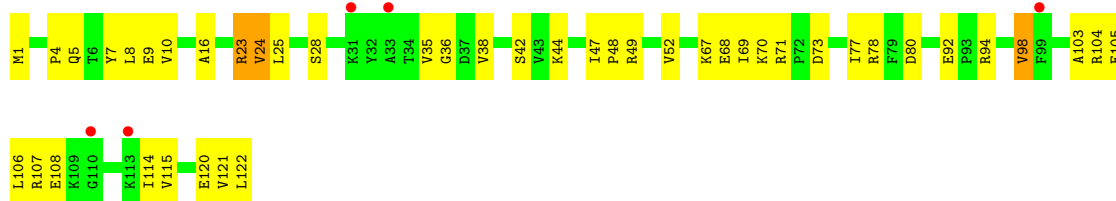




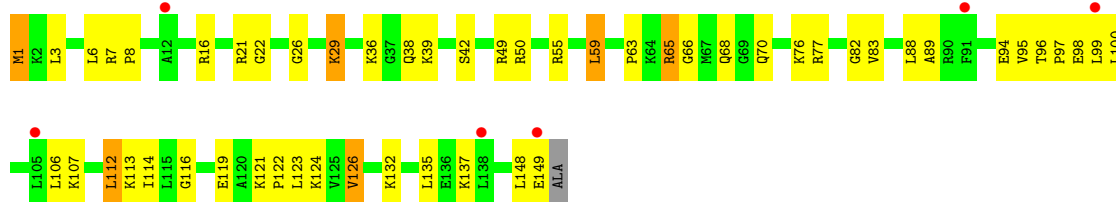
- Molecule 35: 50S ribosomal protein L14



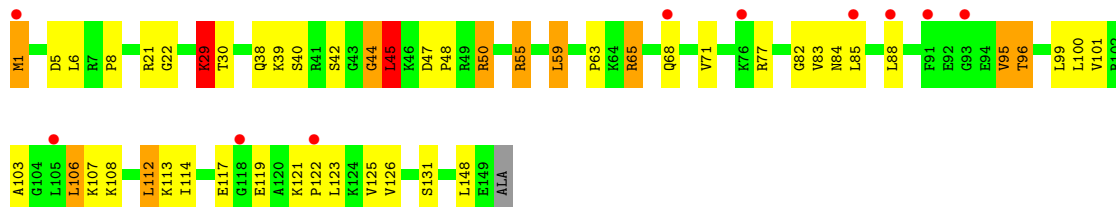
- Molecule 35: 50S ribosomal protein L14



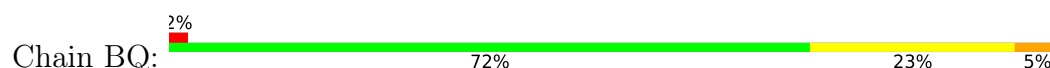
- Molecule 36: 50S ribosomal protein L15

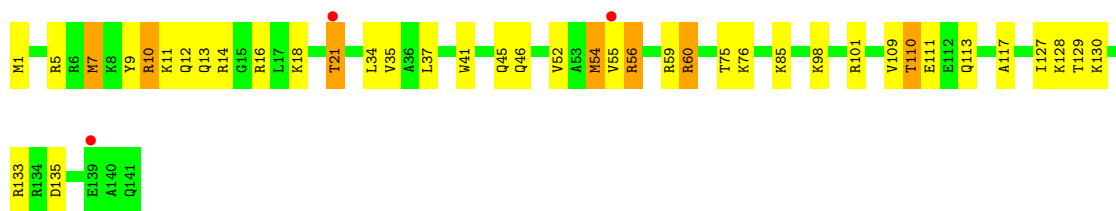


- Molecule 36: 50S ribosomal protein L15

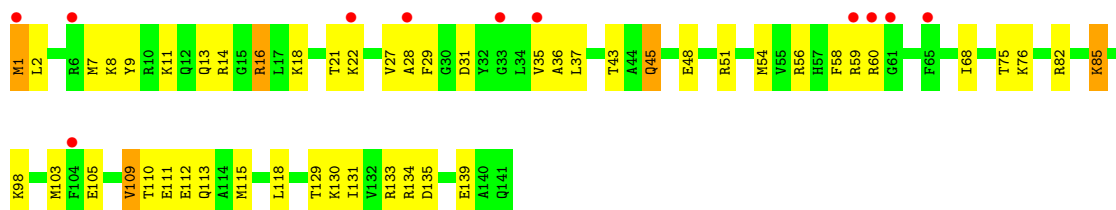


- Molecule 37: 50S ribosomal protein L16

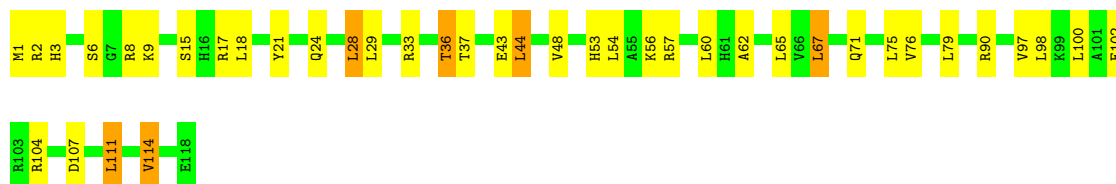




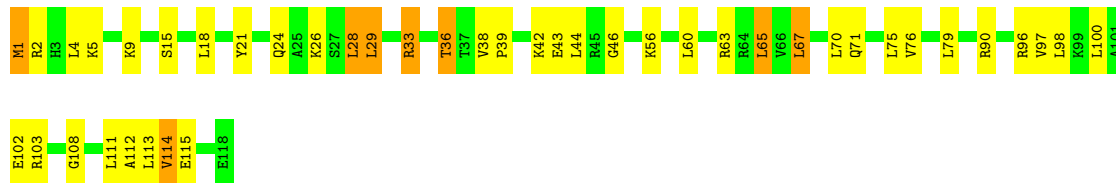
- Molecule 37: 50S ribosomal protein L16



- Molecule 38: 50S ribosomal protein L17



- Molecule 38: 50S ribosomal protein L17

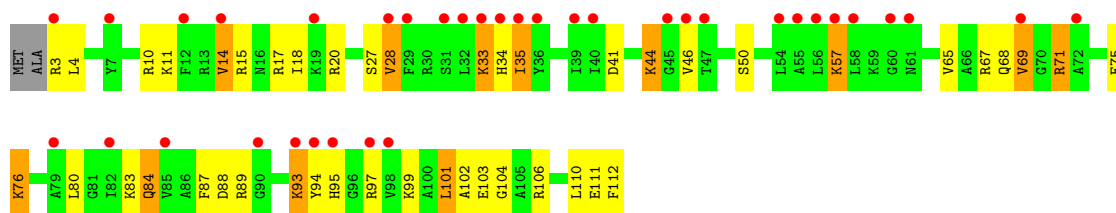


- Molecule 39: 50S ribosomal protein L18

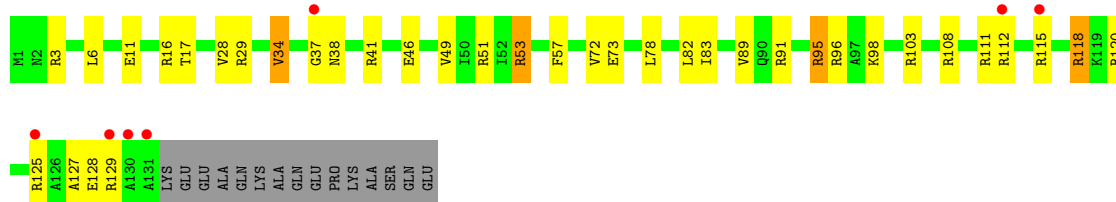


- Molecule 39: 50S ribosomal protein L18

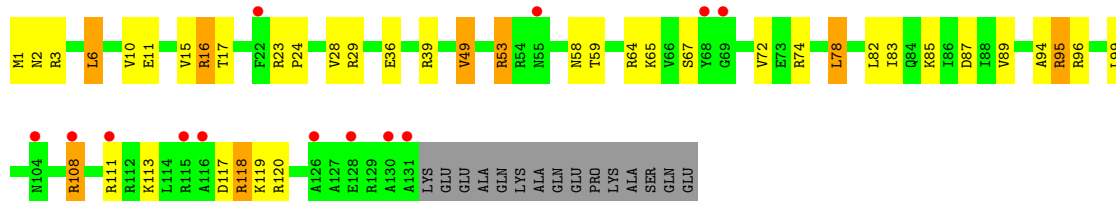




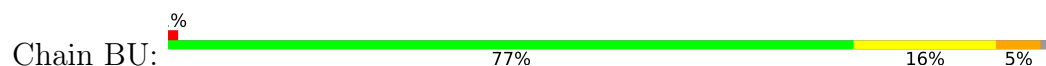
- Molecule 40: 50S ribosomal protein L19



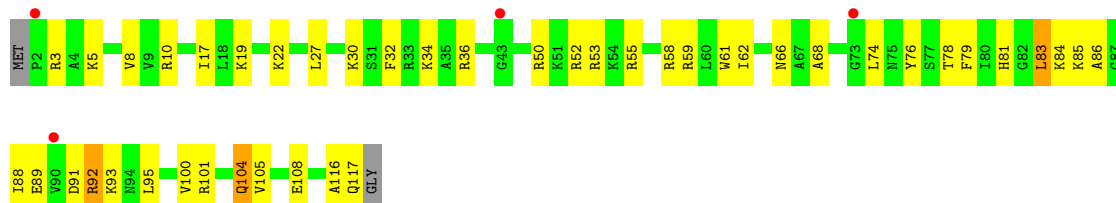
- Molecule 40: 50S ribosomal protein L19



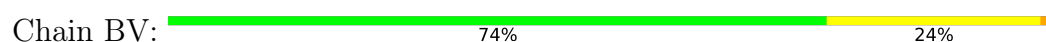
- Molecule 41: 50S ribosomal protein L20

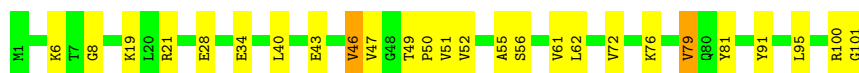


- Molecule 41: 50S ribosomal protein L20

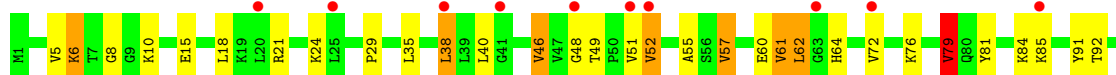


- Molecule 42: 50S ribosomal protein L21

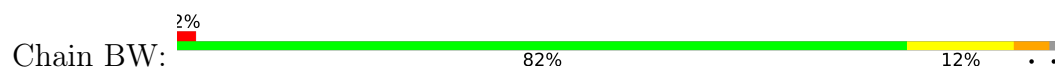




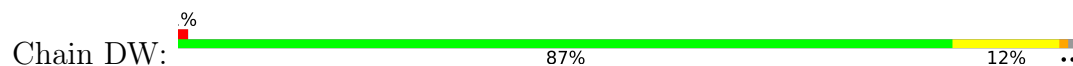
- Molecule 42: 50S ribosomal protein L21



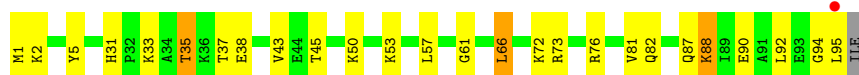
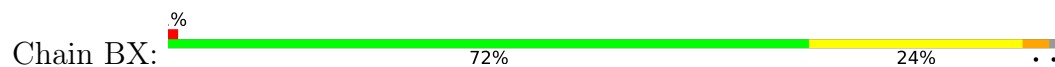
- Molecule 43: 50S ribosomal protein L22



- Molecule 43: 50S ribosomal protein L22



- Molecule 44: 50S ribosomal protein L23

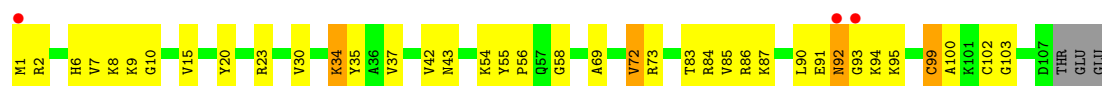


- Molecule 44: 50S ribosomal protein L23

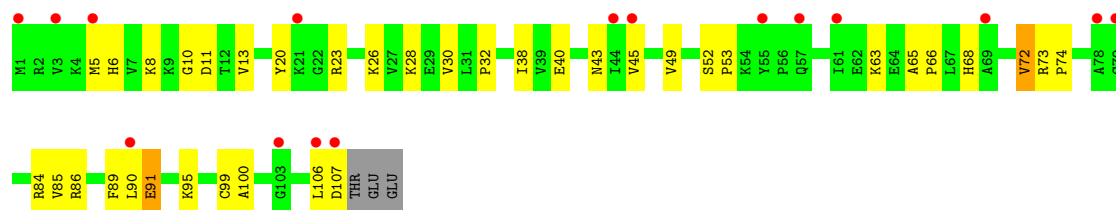


- Molecule 45: 50S ribosomal protein L24

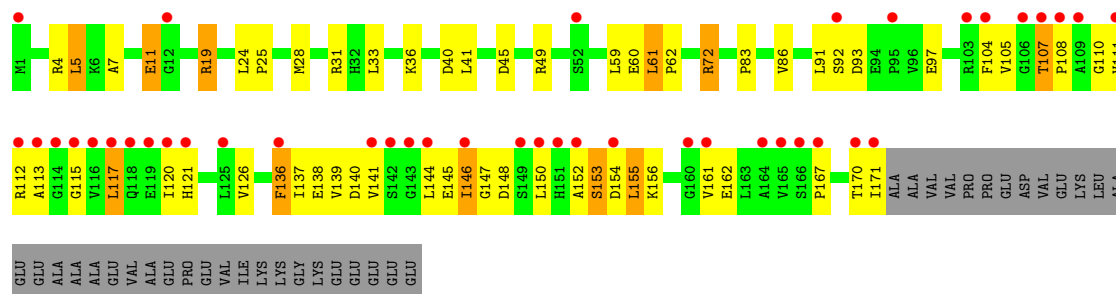




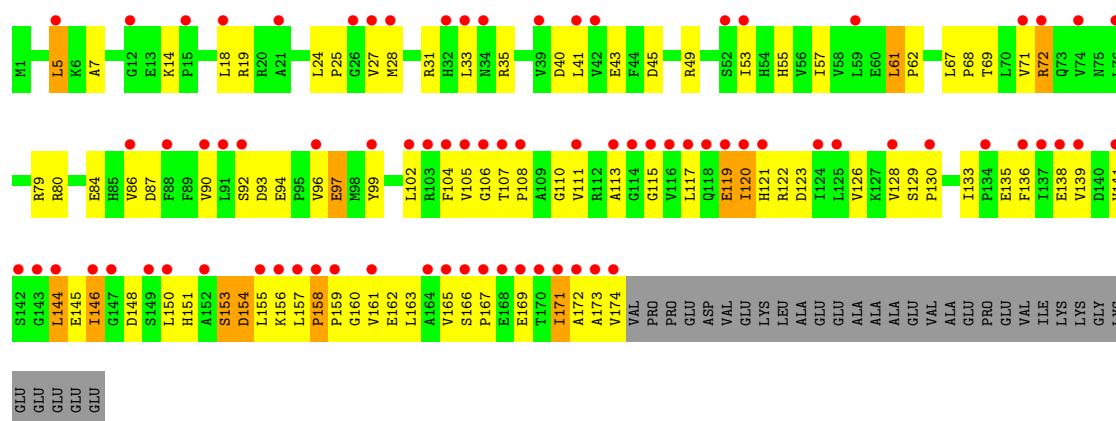
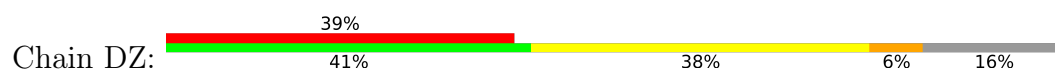
- Molecule 45: 50S ribosomal protein L24



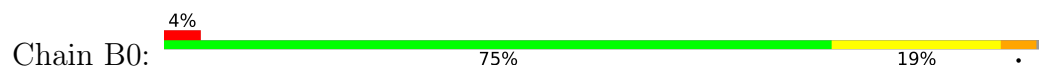
- Molecule 46: 50S ribosomal protein L25



- Molecule 46: 50S ribosomal protein L25



- Molecule 47: 50S ribosomal protein L27

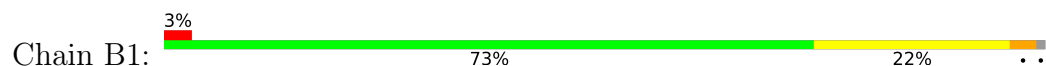




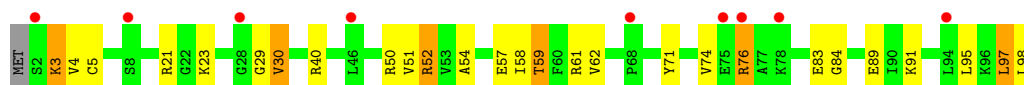
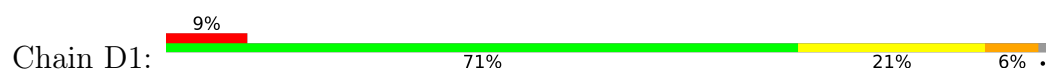
- Molecule 47: 50S ribosomal protein L27



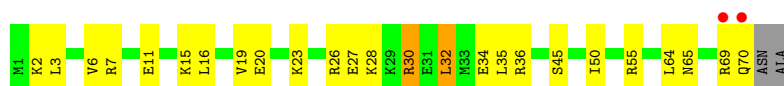
- Molecule 48: 50S ribosomal protein L28



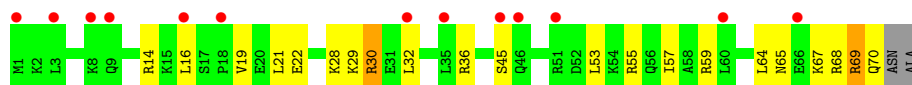
- Molecule 48: 50S ribosomal protein L28



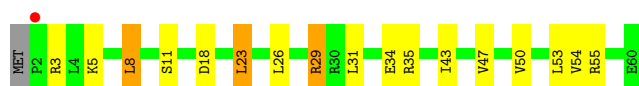
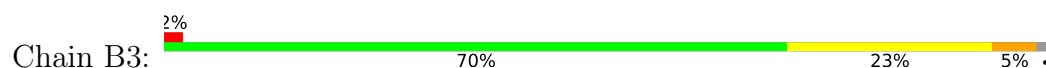
- Molecule 49: 50S ribosomal protein L29



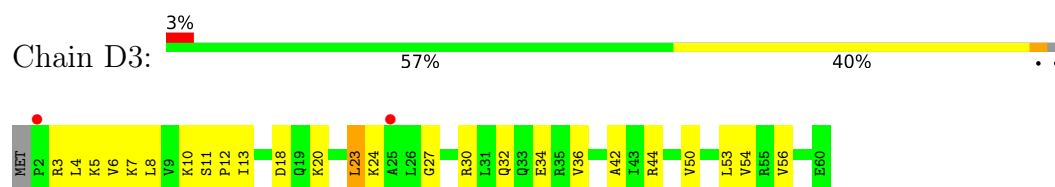
- Molecule 49: 50S ribosomal protein L29



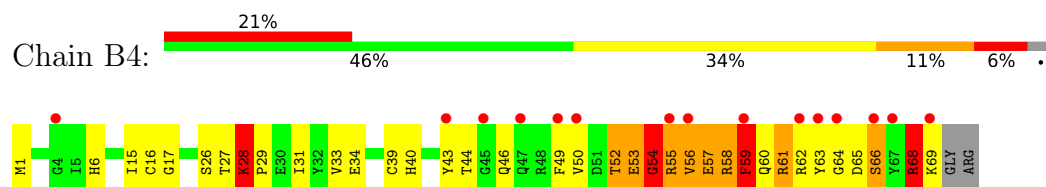
- Molecule 50: 50S ribosomal protein L30



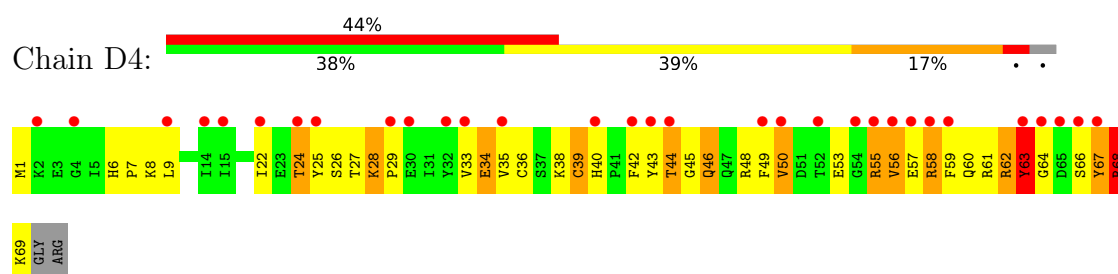
- Molecule 50: 50S ribosomal protein L30



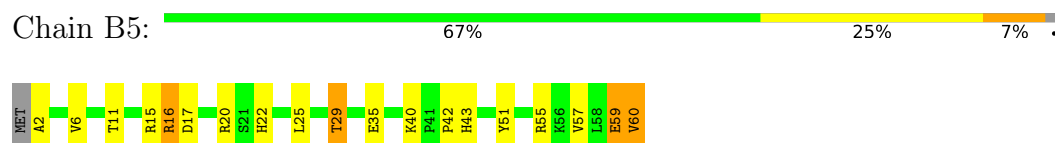
- Molecule 51: 50S ribosomal protein L31



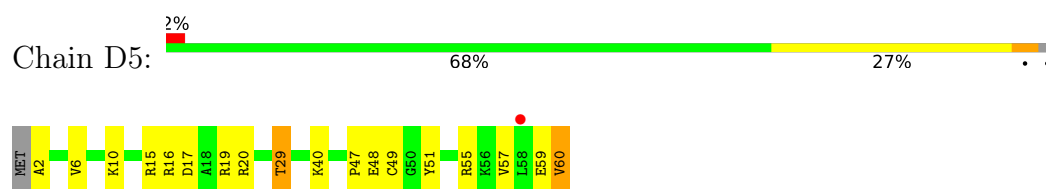
- Molecule 51: 50S ribosomal protein L31



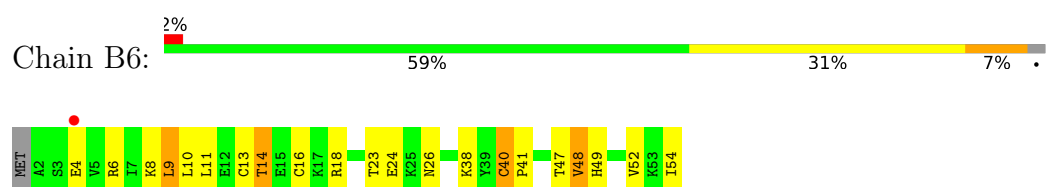
- Molecule 52: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L32

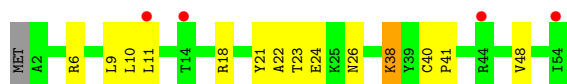


- Molecule 53: 50S ribosomal protein L33

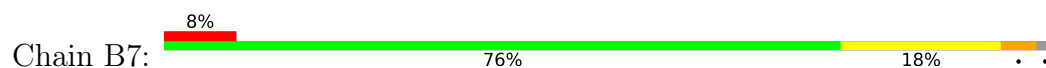


- Molecule 53: 50S ribosomal protein L33

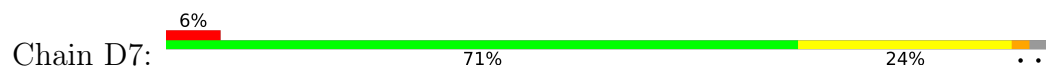




- Molecule 54: 50S ribosomal protein L34



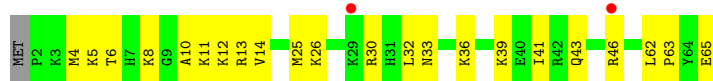
- Molecule 54: 50S ribosomal protein L34



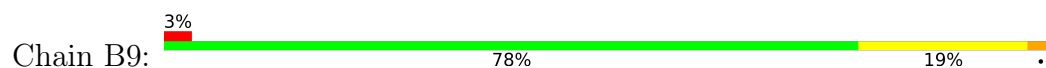
- Molecule 55: 50S ribosomal protein L35



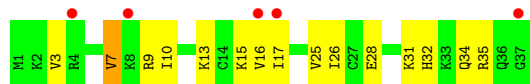
- Molecule 55: 50S ribosomal protein L35



- Molecule 56: 50S ribosomal protein L36



- 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	209.32Å 450.06Å 622.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.51 – 2.55 152.51 – 2.55	Depositor EDS
% Data completeness (in resolution range)	95.8 (152.51-2.55) 95.8 (152.51-2.55)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.233 , 0.280 0.235 , 0.281	Depositor DCC
R_{free} test set	90444 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	297141	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% 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, SF4, 5MU, 7MG, K, MG, PSU, ZN, 31M, 5MC, MIA

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	0.21	0/36049	0.44	4/56261 (0.0%)
1	CA	0.22	0/36170	0.47	11/56452 (0.0%)
2	AB	0.40	0/1881	1.01	11/2542 (0.4%)
2	CB	0.44	0/1860	1.04	6/2518 (0.2%)
3	AC	0.39	0/1576	0.87	1/2130 (0.0%)
3	CC	0.43	0/1566	1.01	10/2119 (0.5%)
4	AD	0.39	0/1689	0.90	2/2267 (0.1%)
4	CD	0.38	0/1704	0.87	2/2284 (0.1%)
5	AE	0.42	0/1145	0.92	1/1543 (0.1%)
5	CE	0.43	0/1149	1.05	9/1548 (0.6%)
6	AF	0.36	0/819	0.76	0/1111
6	CF	0.38	0/829	0.81	0/1123
7	AG	0.37	0/1250	0.87	1/1679 (0.1%)
7	CG	0.37	0/1254	0.93	4/1683 (0.2%)
8	AH	0.37	0/1108	0.85	0/1494
8	CH	0.35	0/1108	0.89	2/1494 (0.1%)
9	AI	0.40	0/1002	0.90	2/1346 (0.1%)
9	CI	0.41	0/997	0.92	1/1343 (0.1%)
10	AJ	0.40	0/722	0.99	4/982 (0.4%)
10	CJ	0.44	0/727	1.01	5/988 (0.5%)
11	AK	0.39	0/844	0.90	2/1145 (0.2%)
11	CK	0.39	0/848	0.88	2/1149 (0.2%)
12	AL	0.38	0/946	0.82	1/1274 (0.1%)
12	CL	0.37	0/946	0.88	3/1274 (0.2%)
13	AM	0.39	0/969	0.98	2/1302 (0.2%)
13	CM	0.40	0/961	0.94	4/1291 (0.3%)
14	AN	0.38	0/501	0.80	0/664
14	CN	0.40	0/501	0.87	1/664 (0.2%)
15	AO	0.38	0/739	0.88	2/985 (0.2%)
15	CO	0.38	0/739	0.83	0/985
16	AP	0.38	0/697	0.83	0/939
16	CP	0.40	0/693	0.83	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.36	0/836	0.80	0/1117
17	CQ	0.33	0/836	0.79	0/1117
18	AR	0.36	0/560	0.83	0/746
18	CR	0.36	0/560	0.79	0/746
19	AS	0.39	0/667	0.94	4/900 (0.4%)
19	CS	0.45	0/661	1.05	3/893 (0.3%)
20	AT	0.37	0/730	0.94	2/965 (0.2%)
20	CT	0.38	0/729	0.82	0/965
21	AU	0.33	0/203	0.80	0/266
21	CU	0.38	0/203	0.91	0/266
22	AV	0.21	0/310	0.37	0/480
22	CV	0.25	0/282	0.48	0/437
23	AW	0.28	0/1577	0.52	0/2454
23	CW	0.35	0/1531	0.62	0/2379
24	AX	0.27	0/1725	0.45	0/2689
24	CX	0.24	0/1725	0.43	0/2689
25	AY	0.35	1/1602 (0.1%)	0.65	1/2493 (0.0%)
25	CY	0.35	1/1579 (0.1%)	0.61	0/2455
26	BA	0.27	0/68013	0.46	4/106165 (0.0%)
26	DA	0.23	0/67542	0.45	0/105428
27	BB	0.23	0/2878	0.43	0/4490
27	DB	0.24	0/2878	0.46	0/4490
28	BD	0.48	0/2186	0.92	6/2944 (0.2%)
28	DD	0.43	0/2186	0.89	5/2944 (0.2%)
29	BE	0.49	0/1592	0.90	2/2149 (0.1%)
29	DE	0.45	0/1592	0.98	8/2149 (0.4%)
30	BF	0.46	0/1619	0.85	4/2193 (0.2%)
30	DF	0.41	0/1615	0.92	3/2188 (0.1%)
31	BG	0.41	0/1450	0.90	5/1959 (0.3%)
31	DG	0.42	0/1449	1.03	9/1958 (0.5%)
32	BH	0.43	0/1356	0.86	1/1834 (0.1%)
32	DH	0.41	0/1356	0.93	3/1834 (0.2%)
33	BI	0.40	0/1100	0.95	7/1501 (0.5%)
33	DI	0.40	0/1076	0.91	3/1471 (0.2%)
34	BN	0.43	0/1144	0.89	2/1543 (0.1%)
34	DN	0.39	0/1144	0.98	8/1543 (0.5%)
35	BO	0.46	0/943	0.84	0/1269
35	DO	0.41	0/943	0.82	0/1269
36	BP	0.46	0/1152	0.85	2/1533 (0.1%)
36	DP	0.39	0/1152	0.93	5/1533 (0.3%)
37	BQ	0.44	0/1143	0.81	0/1527
37	DQ	0.40	0/1143	0.84	0/1527
38	BR	0.47	0/982	0.85	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DR	0.40	0/982	0.78	0/1312
39	BS	0.40	0/887	0.87	1/1180 (0.1%)
39	DS	0.39	0/880	0.96	1/1172 (0.1%)
40	BT	0.41	0/1105	0.79	0/1477
40	DT	0.38	0/1097	0.82	0/1468
41	BU	0.51	0/977	0.82	0/1301
41	DU	0.39	0/977	0.82	0/1301
42	BV	0.49	0/782	0.83	1/1049 (0.1%)
42	DV	0.39	0/782	0.83	0/1049
43	BW	0.51	0/897	0.89	2/1205 (0.2%)
43	DW	0.42	0/897	0.85	0/1205
44	BX	0.47	0/764	0.86	0/1025
44	DX	0.40	0/764	0.85	0/1025
45	BY	0.42	0/819	0.90	1/1095 (0.1%)
45	DY	0.37	0/819	0.87	1/1095 (0.1%)
46	BZ	0.42	0/1379	0.98	5/1873 (0.3%)
46	DZ	0.38	0/1390	0.98	12/1890 (0.6%)
47	B0	0.43	0/662	0.85	2/881 (0.2%)
47	D0	0.34	0/662	0.82	2/881 (0.2%)
48	B1	0.46	0/762	0.87	0/1014
48	D1	0.41	0/762	0.79	0/1014
49	B2	0.42	0/590	0.86	0/781
49	D2	0.35	0/590	0.74	0/781
50	B3	0.46	0/474	0.88	2/635 (0.3%)
50	D3	0.34	0/469	0.85	0/630
51	B4	0.46	0/571	1.19	10/768 (1.3%)
51	D4	0.49	0/545	1.24	8/737 (1.1%)
52	B5	0.52	0/469	0.79	0/635
52	D5	0.43	0/469	0.76	0/635
53	B6	0.45	0/460	0.77	2/613 (0.3%)
53	D6	0.37	0/456	0.72	0/608
54	B7	0.51	0/426	0.82	1/561 (0.2%)
54	D7	0.48	0/426	0.88	0/561
55	B8	0.46	0/519	0.86	0/684
55	D8	0.40	0/525	0.80	0/691
56	B9	0.42	0/310	0.83	0/407
56	D9	0.36	0/310	0.84	0/407
All	All	0.30	2/316594 (0.0%)	0.60	231/473970 (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	4
7	AG	0	2
7	CG	0	1
20	CT	0	1
28	BD	0	1
39	BS	0	1
51	B4	0	2
51	D4	0	1
All	All	0	13

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	AY	8	4SU	O3'-P	5.64	1.61	1.56
25	CY	8	4SU	O3'-P	5.11	1.61	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	B4	60	GLN	N-CA-C	-8.56	103.89	112.97
2	AB	9	GLU	N-CA-C	8.30	123.36	109.76
7	CG	79	ARG	N-CA-C	8.20	122.37	108.67
8	CH	73	ASP	CA-C-N	8.11	128.31	119.87
8	CH	73	ASP	C-N-CA	8.11	128.31	119.87

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	18	GLY	Peptide
2	AB	231	GLU	Peptide
2	AB	8	LYS	Peptide
2	AB	9	GLU	Peptide
7	AG	78	ARG	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32205	0	16254	503	0
1	CA	32312	0	16307	665	0
2	AB	1846	0	1867	97	0
2	CB	1825	0	1828	105	0
3	AC	1552	0	1546	55	0
3	CC	1542	0	1517	82	0
4	AD	1659	0	1676	73	0
4	CD	1674	0	1714	63	0
5	AE	1129	0	1185	34	0
5	CE	1133	0	1191	34	0
6	AF	806	0	793	26	0
6	CF	816	0	808	20	0
7	AG	1231	0	1238	30	0
7	CG	1235	0	1249	37	0
8	AH	1088	0	1126	27	0
8	CH	1088	0	1126	41	0
9	AI	983	0	986	47	0
9	CI	978	0	966	48	0
10	AJ	709	0	650	35	0
10	CJ	714	0	672	36	0
11	AK	829	0	825	20	0
11	CK	833	0	836	17	0
12	AL	930	0	980	24	0
12	CL	930	0	980	27	0
13	AM	958	0	1002	31	0
13	CM	950	0	988	40	0
14	AN	492	0	529	16	0
14	CN	492	0	529	33	0
15	AO	728	0	760	21	0
15	CO	728	0	760	30	0
16	AP	681	0	697	12	0
16	CP	677	0	686	23	0
17	AQ	823	0	891	22	0
17	CQ	823	0	891	15	0
18	AR	555	0	618	19	0
18	CR	555	0	618	16	0
19	AS	652	0	662	31	0
19	CS	646	0	644	39	0
20	AT	728	0	798	33	0
20	CT	727	0	796	27	0
21	AU	199	0	208	9	0
21	CU	199	0	208	10	0
22	AV	277	0	140	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	CV	252	0	130	7	0
23	AW	1607	0	839	55	0
23	CW	1560	0	803	56	0
24	AX	1625	0	828	31	0
24	CX	1625	0	828	30	0
25	AY	1581	0	805	95	0
25	CY	1561	0	796	79	0
26	BA	60729	0	30621	675	0
26	DA	60311	0	30409	889	0
27	BB	2573	0	1306	21	0
27	DB	2573	0	1306	50	0
28	BD	2136	0	2218	53	0
28	DD	2136	0	2218	63	0
29	BE	1559	0	1618	30	0
29	DE	1559	0	1618	47	0
30	BF	1584	0	1625	51	0
30	DF	1580	0	1619	53	0
31	BG	1425	0	1443	39	0
31	DG	1424	0	1434	68	0
32	BH	1330	0	1407	28	0
32	DH	1330	0	1407	30	0
33	BI	1085	0	1114	43	0
33	DI	1061	0	1080	26	0
34	BN	1117	0	1183	16	0
34	DN	1117	0	1184	29	0
35	BO	933	0	996	22	0
35	DO	933	0	996	28	0
36	BP	1135	0	1212	39	0
36	DP	1135	0	1212	43	0
37	BQ	1122	0	1179	32	0
37	DQ	1122	0	1179	36	0
38	BR	968	0	1033	18	0
38	DR	968	0	1033	29	0
39	BS	877	0	938	23	0
39	DS	870	0	923	34	0
40	BT	1091	0	1151	28	0
40	DT	1083	0	1136	31	0
41	BU	959	0	1019	20	0
41	DU	959	0	1019	38	0
42	BV	771	0	830	13	0
42	DV	771	0	830	25	0
43	BW	886	0	939	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DW	886	0	940	10	0
44	BX	750	0	814	17	0
44	DX	750	0	814	23	0
45	BY	806	0	881	23	0
45	DY	806	0	881	27	0
46	BZ	1349	0	1355	45	0
46	DZ	1360	0	1363	63	0
47	B0	653	0	674	14	0
47	D0	653	0	674	20	0
48	B1	755	0	826	20	0
48	D1	755	0	826	18	0
49	B2	588	0	643	12	0
49	D2	588	0	643	12	0
50	B3	469	0	518	9	0
50	D3	464	0	514	13	0
51	B4	558	0	544	24	0
51	D4	532	0	503	34	0
52	B5	455	0	465	12	0
52	D5	455	0	465	12	0
53	B6	453	0	473	12	0
53	D6	449	0	469	8	0
54	B7	418	0	467	9	0
54	D7	418	0	467	10	0
55	B8	511	0	571	23	0
55	D8	517	0	582	13	0
56	B9	307	0	335	7	0
56	D9	307	0	335	13	0
57	AA	214	0	0	0	0
57	AE	3	0	0	0	0
57	AF	1	0	0	0	0
57	AK	1	0	0	0	0
57	AM	1	0	0	0	0
57	AN	2	0	0	0	0
57	AW	4	0	0	0	0
57	AX	15	0	0	0	0
57	AY	3	0	0	0	0
57	B0	3	0	0	0	0
57	B1	1	0	0	0	0
57	B2	1	0	0	0	0
57	B3	2	0	0	0	0
57	B4	1	0	0	0	0
57	B5	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	B6	2	0	0	0	0
57	B7	5	0	0	0	0
57	B8	1	0	0	0	0
57	B9	1	0	0	0	0
57	BA	812	0	0	0	0
57	BB	20	0	0	0	0
57	BD	9	0	0	0	0
57	BE	8	0	0	0	0
57	BF	9	0	0	0	0
57	BG	3	0	0	0	0
57	BN	6	0	0	0	0
57	BO	2	0	0	0	0
57	BP	5	0	0	0	0
57	BQ	5	0	0	0	0
57	BR	2	0	0	0	0
57	BU	8	0	0	0	0
57	BV	5	0	0	0	0
57	BW	4	0	0	0	0
57	BX	3	0	0	0	0
57	BY	1	0	0	0	0
57	BZ	1	0	0	0	0
57	CA	170	0	0	0	0
57	CD	1	0	0	0	0
57	CE	1	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	CV	1	0	0	0	0
57	CW	1	0	0	0	0
57	CX	3	0	0	1	0
57	D0	1	0	0	0	0
57	D3	1	0	0	0	0
57	D8	1	0	0	0	0
57	DA	677	0	0	0	0
57	DB	13	0	0	0	0
57	DD	9	0	0	0	0
57	DE	4	0	0	0	0
57	DF	4	0	0	0	0
57	DG	1	0	0	0	0
57	DN	1	0	0	0	0
57	DO	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	DP	2	0	0	0	0
57	DQ	4	0	0	0	0
57	DR	1	0	0	0	0
57	DU	2	0	0	0	0
57	DV	3	0	0	0	0
57	DW	4	0	0	0	0
57	DX	1	0	0	0	0
57	DY	1	0	0	0	0
58	AD	8	0	0	0	0
58	CD	8	0	0	0	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
60	CX	1	0	0	0	0
61	AA	227	0	0	17	0
61	AE	2	0	0	0	0
61	AJ	1	0	0	0	0
61	AL	1	0	0	1	0
61	AM	1	0	0	0	0
61	AU	1	0	0	1	0
61	AV	3	0	0	0	0
61	AW	3	0	0	0	0
61	AX	6	0	0	2	0
61	AY	1	0	0	0	0
61	B0	3	0	0	0	0
61	B1	1	0	0	0	0
61	B3	2	0	0	0	0
61	B5	2	0	0	0	0
61	B6	1	0	0	0	0
61	B7	2	0	0	0	0
61	B8	8	0	0	1	0
61	BA	1383	0	0	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	BB	36	0	0	1	0
61	BD	12	0	0	1	0
61	BE	14	0	0	4	0
61	BF	8	0	0	0	0
61	BG	3	0	0	0	0
61	BI	1	0	0	0	0
61	BO	4	0	0	0	0
61	BP	16	0	0	3	0
61	BQ	4	0	0	0	0
61	BR	2	0	0	0	0
61	BT	2	0	0	0	0
61	BU	3	0	0	0	0
61	BV	2	0	0	0	0
61	BW	1	0	0	0	0
61	BX	4	0	0	0	0
61	BZ	1	0	0	0	0
61	CA	185	0	0	17	0
61	CJ	2	0	0	1	0
61	CL	1	0	0	0	0
61	CT	1	0	0	0	0
61	CV	1	0	0	0	0
61	CW	2	0	0	0	0
61	D0	3	0	0	0	0
61	D1	1	0	0	0	0
61	D3	1	0	0	1	0
61	D7	3	0	0	0	0
61	D8	4	0	0	0	0
61	DA	1025	0	0	79	0
61	DB	9	0	0	0	0
61	DD	19	0	0	4	0
61	DE	11	0	0	0	0
61	DF	3	0	0	0	0
61	DN	2	0	0	1	0
61	DO	1	0	0	0	0
61	DP	16	0	0	2	0
61	DR	1	0	0	0	0
61	DT	3	0	0	0	0
61	DU	2	0	0	0	0
61	DX	3	0	0	0	0
61	DY	2	0	0	0	0
All	All	297141	0	196251	5318	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 11.

The worst 5 of 5318 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)
25:CY:7:A:N6	25:CY:66:U:H3	1.37	1.21
25:AY:49:C:N4	25:AY:65:G:H1	1.44	1.16
26:DA:2139:C:N4	26:DA:2152:G:H1	1.42	1.16
1:CA:1000:U:H3	1:CA:1041:A:N6	1.44	1.15
1:CA:1002:G:H1	1:CA:1038:C:N4	1.48	1.12

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%)	14 (6%)	7 (3%)	3	2
2	CB	229/256 (90%)	206 (90%)	16 (7%)	7 (3%)	3	2
3	AC	204/239 (85%)	195 (96%)	8 (4%)	1 (0%)	24	34
3	CC	204/239 (85%)	189 (93%)	15 (7%)	0	100	100
4	AD	206/209 (99%)	197 (96%)	7 (3%)	2 (1%)	12	17
4	CD	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	24	34
5	AE	146/162 (90%)	142 (97%)	4 (3%)	0	100	100
5	CE	146/162 (90%)	140 (96%)	6 (4%)	0	100	100
6	AF	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
6	CF	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
7	AG	153/156 (98%)	144 (94%)	5 (3%)	4 (3%)	4	3
7	CG	153/156 (98%)	144 (94%)	8 (5%)	1 (1%)	18	25
8	AH	135/138 (98%)	134 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	CH	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
9	AI	125/128 (98%)	117 (94%)	8 (6%)	0	100	100
9	CI	125/128 (98%)	119 (95%)	5 (4%)	1 (1%)	16	22
10	AJ	95/105 (90%)	85 (90%)	6 (6%)	4 (4%)	2	1
10	CJ	94/105 (90%)	85 (90%)	4 (4%)	5 (5%)	1	0
11	AK	112/129 (87%)	104 (93%)	6 (5%)	2 (2%)	6	7
11	CK	112/129 (87%)	103 (92%)	7 (6%)	2 (2%)	6	7
12	AL	120/132 (91%)	117 (98%)	3 (2%)	0	100	100
12	CL	120/132 (91%)	118 (98%)	2 (2%)	0	100	100
13	AM	121/126 (96%)	116 (96%)	5 (4%)	0	100	100
13	CM	120/126 (95%)	113 (94%)	7 (6%)	0	100	100
14	AN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
14	CN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
15	AO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
15	CO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	AP	80/88 (91%)	79 (99%)	1 (1%)	0	100	100
16	CP	80/88 (91%)	78 (98%)	1 (1%)	1 (1%)	9	12
17	AQ	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
17	CQ	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
18	AR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
18	CR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
19	AS	81/93 (87%)	73 (90%)	7 (9%)	1 (1%)	10	13
19	CS	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
20	AT	94/106 (89%)	87 (93%)	3 (3%)	4 (4%)	2	1
20	CT	94/106 (89%)	88 (94%)	3 (3%)	3 (3%)	3	2
21	AU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
21	CU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
28	BD	273/276 (99%)	264 (97%)	8 (3%)	1 (0%)	30	39
28	DD	273/276 (99%)	263 (96%)	8 (3%)	2 (1%)	18	25
29	BE	202/206 (98%)	196 (97%)	5 (2%)	1 (0%)	24	34
29	DE	202/206 (98%)	196 (97%)	4 (2%)	2 (1%)	12	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	BF	201/210 (96%)	200 (100%)	0	1 (0%)	24	34
30	DF	201/210 (96%)	199 (99%)	0	2 (1%)	12	17
31	BG	179/182 (98%)	170 (95%)	8 (4%)	1 (1%)	21	29
31	DG	179/182 (98%)	171 (96%)	5 (3%)	3 (2%)	7	8
32	BH	172/180 (96%)	168 (98%)	3 (2%)	1 (1%)	21	29
32	DH	172/180 (96%)	166 (96%)	5 (3%)	1 (1%)	21	29
33	BI	144/148 (97%)	130 (90%)	11 (8%)	3 (2%)	5	5
33	DI	144/148 (97%)	133 (92%)	10 (7%)	1 (1%)	18	25
34	BN	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
34	DN	138/140 (99%)	135 (98%)	2 (1%)	1 (1%)	18	25
35	BO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
35	DO	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
36	BP	147/150 (98%)	140 (95%)	6 (4%)	1 (1%)	18	25
36	DP	147/150 (98%)	138 (94%)	7 (5%)	2 (1%)	9	11
37	BQ	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
37	DQ	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	18	25
38	BR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
38	DR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
39	BS	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	14	20
39	DS	108/112 (96%)	105 (97%)	2 (2%)	1 (1%)	14	20
40	BT	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
40	DT	129/146 (88%)	127 (98%)	2 (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%)	6 (6%)	0	100	100
42	DV	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	12	17
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%)	89 (96%)	4 (4%)	0	100	100
44	DX	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
45	BY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	DY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
46	BZ	169/206 (82%)	153 (90%)	15 (9%)	1 (1%)	21	29
46	DZ	172/206 (84%)	161 (94%)	11 (6%)	0	100	100
47	B0	81/85 (95%)	81 (100%)	0	0	100	100
47	D0	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
48	B1	95/98 (97%)	94 (99%)	0	1 (1%)	11	15
48	D1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	15
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%)	53 (79%)	11 (16%)	3 (4%)	2	1
51	D4	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1	0
52	B5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
52	D5	57/60 (95%)	53 (93%)	4 (7%)	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%)	46 (100%)	0	0	100	100
54	D7	46/49 (94%)	45 (98%)	0	1 (2%)	5	5
55	B8	62/65 (95%)	62 (100%)	0	0	100	100
55	D8	62/65 (95%)	62 (100%)	0	0	100	100
56	B9	35/37 (95%)	35 (100%)	0	0	100	100
56	D9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11409/12128 (94%)	10908 (96%)	416 (4%)	85 (1%)	18	25

5 of 85 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	126	GLU
7	AG	80	VAL
20	AT	10	LEU
20	AT	96	GLY
28	BD	275	LYS

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	1
2	CB	187/220 (85%)	148 (79%)	39 (21%)	1	1
3	AC	143/188 (76%)	116 (81%)	27 (19%)	1	1
3	CC	140/188 (74%)	119 (85%)	21 (15%)	3	2
4	AD	170/181 (94%)	149 (88%)	21 (12%)	4	4
4	CD	173/181 (96%)	153 (88%)	20 (12%)	5	6
5	AE	113/123 (92%)	104 (92%)	9 (8%)	11	15
5	CE	114/123 (93%)	102 (90%)	12 (10%)	6	8
6	AF	83/90 (92%)	72 (87%)	11 (13%)	4	4
6	CF	85/90 (94%)	77 (91%)	8 (9%)	8	10
7	AG	119/127 (94%)	106 (89%)	13 (11%)	6	7
7	CG	120/127 (94%)	107 (89%)	13 (11%)	6	7
8	AH	114/119 (96%)	101 (89%)	13 (11%)	5	6
8	CH	114/119 (96%)	99 (87%)	15 (13%)	4	4
9	AI	90/99 (91%)	72 (80%)	18 (20%)	1	1
9	CI	89/99 (90%)	75 (84%)	14 (16%)	2	2
10	AJ	66/92 (72%)	57 (86%)	9 (14%)	3	3
10	CJ	69/92 (75%)	63 (91%)	6 (9%)	9	13
11	AK	82/99 (83%)	75 (92%)	7 (8%)	10	13
11	CK	83/99 (84%)	76 (92%)	7 (8%)	10	14
12	AL	97/109 (89%)	92 (95%)	5 (5%)	21	32
12	CL	97/109 (89%)	92 (95%)	5 (5%)	21	32
13	AM	93/101 (92%)	79 (85%)	14 (15%)	3	2
13	CM	92/101 (91%)	77 (84%)	15 (16%)	2	2
14	AN	49/50 (98%)	42 (86%)	7 (14%)	3	3
14	CN	49/50 (98%)	41 (84%)	8 (16%)	2	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	AO	78/80 (98%)	65 (83%)	13 (17%)	2	2
15	CO	78/80 (98%)	70 (90%)	8 (10%)	7	8
16	AP	69/74 (93%)	59 (86%)	10 (14%)	3	2
16	CP	68/74 (92%)	60 (88%)	8 (12%)	5	5
17	AQ	94/97 (97%)	81 (86%)	13 (14%)	3	3
17	CQ	94/97 (97%)	84 (89%)	10 (11%)	6	7
18	AR	59/77 (77%)	52 (88%)	7 (12%)	5	5
18	CR	59/77 (77%)	51 (86%)	8 (14%)	3	3
19	AS	69/80 (86%)	62 (90%)	7 (10%)	7	8
19	CS	67/80 (84%)	61 (91%)	6 (9%)	9	11
20	AT	70/82 (85%)	61 (87%)	9 (13%)	4	4
20	CT	70/82 (85%)	58 (83%)	12 (17%)	2	1
21	AU	18/22 (82%)	16 (89%)	2 (11%)	6	6
21	CU	18/22 (82%)	16 (89%)	2 (11%)	6	6
28	BD	215/218 (99%)	193 (90%)	22 (10%)	7	8
28	DD	215/218 (99%)	191 (89%)	24 (11%)	6	6
29	BE	164/166 (99%)	142 (87%)	22 (13%)	4	3
29	DE	164/166 (99%)	138 (84%)	26 (16%)	2	2
30	BF	160/166 (96%)	140 (88%)	20 (12%)	4	4
30	DF	159/166 (96%)	136 (86%)	23 (14%)	3	2
31	BG	143/156 (92%)	128 (90%)	15 (10%)	6	8
31	DG	142/156 (91%)	121 (85%)	21 (15%)	3	2
32	BH	144/148 (97%)	125 (87%)	19 (13%)	4	4
32	DH	144/148 (97%)	125 (87%)	19 (13%)	4	4
33	BI	110/124 (89%)	87 (79%)	23 (21%)	1	1
33	DI	104/124 (84%)	87 (84%)	17 (16%)	2	2
34	BN	118/119 (99%)	99 (84%)	19 (16%)	2	2
34	DN	118/119 (99%)	102 (86%)	16 (14%)	3	3
35	BO	100/100 (100%)	91 (91%)	9 (9%)	9	11
35	DO	100/100 (100%)	90 (90%)	10 (10%)	7	9
36	BP	115/116 (99%)	99 (86%)	16 (14%)	3	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	DP	115/116 (99%)	100 (87%)	15 (13%)	4	4
37	BQ	111/111 (100%)	97 (87%)	14 (13%)	4	4
37	DQ	111/111 (100%)	97 (87%)	14 (13%)	4	4
38	BR	101/101 (100%)	80 (79%)	21 (21%)	1	1
38	DR	101/101 (100%)	83 (82%)	18 (18%)	2	1
39	BS	87/88 (99%)	77 (88%)	10 (12%)	5	6
39	DS	85/88 (97%)	71 (84%)	14 (16%)	2	2
40	BT	115/127 (91%)	103 (90%)	12 (10%)	7	8
40	DT	113/127 (89%)	100 (88%)	13 (12%)	5	6
41	BU	93/94 (99%)	84 (90%)	9 (10%)	8	9
41	DU	93/94 (99%)	84 (90%)	9 (10%)	8	9
42	BV	80/82 (98%)	68 (85%)	12 (15%)	3	2
42	DV	80/82 (98%)	65 (81%)	15 (19%)	1	1
43	BW	90/92 (98%)	81 (90%)	9 (10%)	7	9
43	DW	90/92 (98%)	84 (93%)	6 (7%)	15	21
44	BX	77/78 (99%)	70 (91%)	7 (9%)	9	11
44	DX	77/78 (99%)	69 (90%)	8 (10%)	7	8
45	BY	85/91 (93%)	76 (89%)	9 (11%)	6	7
45	DY	85/91 (93%)	78 (92%)	7 (8%)	10	14
46	BZ	145/179 (81%)	128 (88%)	17 (12%)	5	6
46	DZ	145/179 (81%)	123 (85%)	22 (15%)	3	2
47	B0	65/67 (97%)	61 (94%)	4 (6%)	16	24
47	D0	65/67 (97%)	61 (94%)	4 (6%)	16	24
48	B1	80/83 (96%)	74 (92%)	6 (8%)	12	17
48	D1	80/83 (96%)	68 (85%)	12 (15%)	3	2
49	B2	65/67 (97%)	56 (86%)	9 (14%)	3	3
49	D2	65/67 (97%)	57 (88%)	8 (12%)	4	4
50	B3	51/52 (98%)	45 (88%)	6 (12%)	5	5
50	D3	50/52 (96%)	44 (88%)	6 (12%)	5	5
51	B4	60/63 (95%)	47 (78%)	13 (22%)	1	1
51	D4	53/63 (84%)	43 (81%)	10 (19%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	B5	50/52 (96%)	43 (86%)	7 (14%)	3	3
52	D5	50/52 (96%)	44 (88%)	6 (12%)	5	5
53	B6	51/52 (98%)	45 (88%)	6 (12%)	5	5
53	D6	50/52 (96%)	47 (94%)	3 (6%)	17	26
54	B7	41/42 (98%)	38 (93%)	3 (7%)	13	18
54	D7	41/42 (98%)	36 (88%)	5 (12%)	5	4
55	B8	53/55 (96%)	47 (89%)	6 (11%)	5	6
55	D8	54/55 (98%)	47 (87%)	7 (13%)	4	4
56	B9	34/34 (100%)	33 (97%)	1 (3%)	37	55
56	D9	34/34 (100%)	32 (94%)	2 (6%)	18	27
All	All	9320/10066 (93%)	8123 (87%)	1197 (13%)	4	4

5 of 1197 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	DG	140	ILE
48	D1	89	GLU
33	DI	40	THR
31	DG	136	ARG
39	DS	14	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 153 such sidechains are listed below:

Mol	Chain	Res	Type
28	DD	126	GLN
44	DX	82	GLN
29	DE	85	ASN
35	DO	89	ASN
47	D0	35	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1495/1521 (98%)	307 (20%)	25 (1%)
1	CA	1501/1521 (98%)	317 (21%)	28 (1%)
22	AV	12/24 (50%)	3 (25%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	CV	11/24 (45%)	2 (18%)	0
23	AW	71/76 (93%)	30 (42%)	2 (2%)
23	CW	68/76 (89%)	32 (47%)	2 (2%)
24	AX	75/77 (97%)	16 (21%)	0
24	CX	75/77 (97%)	21 (28%)	0
25	AY	72/76 (94%)	37 (51%)	4 (5%)
25	CY	70/76 (92%)	33 (47%)	1 (1%)
26	BA	2811/2915 (96%)	450 (16%)	34 (1%)
26	DA	2791/2915 (95%)	553 (19%)	30 (1%)
27	BB	119/121 (98%)	14 (11%)	0
27	DB	119/121 (98%)	17 (14%)	0
All	All	9290/9620 (96%)	1832 (19%)	126 (1%)

5 of 1832 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	7	G
1	AA	9	G
1	AA	22	G
1	AA	29	G

5 of 126 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	BA	2181	G
26	DA	1427	A
1	CA	532	A
26	DA	1420	U
26	DA	2126	A

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

38 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
24	5MC	AX	32	24	19,22,23	1.69	3 (15%)	26,32,35	1.28	3 (11%)
23	PSU	AW	39	23	18,21,22	1.40	2 (11%)	21,30,33	1.85	4 (19%)
25	PSU	AY	55	25	18,21,22	1.37	3 (16%)	21,30,33	2.34	6 (28%)
23	PSU	AW	55	23	18,21,22	1.39	2 (11%)	21,30,33	1.95	3 (14%)
25	MIA	CY	37	25	21,24,32	1.65	4 (19%)	30,35,47	2.01	9 (30%)
25	PSU	AY	32	25	18,21,22	1.38	2 (11%)	21,30,33	2.01	4 (19%)
23	MIA	AW	37	23	28,31,32	2.30	7 (25%)	38,44,47	2.73	13 (34%)
24	PSU	CX	55	24	18,21,22	1.35	2 (11%)	21,30,33	2.00	4 (19%)
25	7MG	AY	46	25	23,26,27	1.29	3 (13%)	27,39,42	2.94	7 (25%)
23	PSU	CW	55	23	18,21,22	1.37	2 (11%)	21,30,33	2.11	3 (14%)
25	PSU	CY	32	25	18,21,22	1.38	2 (11%)	21,30,33	1.99	4 (19%)
24	4SU	CX	8	24	18,21,22	2.04	6 (33%)	25,30,33	1.37	4 (16%)
23	4SU	CW	8	23	18,21,22	1.67	4 (22%)	25,30,33	2.41	5 (20%)
25	5MU	AY	54	25	19,22,23	1.49	5 (26%)	27,32,35	2.16	7 (25%)
25	5MU	CY	54	25	19,22,23	1.34	4 (21%)	27,32,35	2.19	6 (22%)
23	5MU	AW	54	23	19,22,23	1.39	5 (26%)	27,32,35	1.93	6 (22%)
23	5MU	CW	54	23	19,22,23	1.34	4 (21%)	27,32,35	2.00	7 (25%)
23	7MG	CW	46	23	23,26,27	1.41	4 (17%)	27,39,42	2.51	6 (22%)
25	4SU	AY	8	25	18,21,22	1.87	5 (27%)	25,30,33	2.06	5 (20%)
25	PSU	CY	55	25	18,21,22	1.46	4 (22%)	21,30,33	2.45	6 (28%)
24	5MU	AX	54	24,57	19,22,23	1.43	5 (26%)	27,32,35	1.96	5 (18%)
25	MIA	AY	37	25	21,24,32	1.63	4 (19%)	30,35,47	2.02	8 (26%)
23	PSU	AW	32	23	18,21,22	1.36	2 (11%)	21,30,33	2.01	4 (19%)
23	4SU	AW	8	23	18,21,22	1.80	4 (22%)	25,30,33	2.15	5 (20%)
24	PSU	AX	55	24,57	18,21,22	1.33	2 (11%)	21,30,33	2.06	4 (19%)
24	4SU	AX	8	24	18,21,22	2.28	5 (27%)	25,30,33	1.72	6 (24%)
24	5MC	CX	32	24	19,22,23	1.64	3 (15%)	26,32,35	1.17	3 (11%)
23	31M	AW	76	23	41,44,45	1.46	6 (14%)	50,61,64	1.72	11 (22%)
23	31M	CW	76	23	41,44,45	1.38	5 (12%)	50,61,64	1.66	10 (20%)
25	7MG	CY	46	25	23,26,27	1.42	5 (21%)	27,39,42	2.67	9 (33%)
23	PSU	CW	39	23	18,21,22	1.35	2 (11%)	21,30,33	1.86	4 (19%)
23	MIA	CW	37	23	21,24,32	1.60	4 (19%)	30,35,47	2.04	7 (23%)
24	5MU	CX	54	24	19,22,23	1.39	5 (26%)	27,32,35	2.30	6 (22%)
25	PSU	AY	39	25	18,21,22	1.57	4 (22%)	21,30,33	1.95	5 (23%)
25	PSU	CY	39	25	18,21,22	1.44	3 (16%)	21,30,33	2.33	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PSU	CW	32	23	18,21,22	1.34	2 (11%)	21,30,33	1.99	3 (14%)
23	7MG	AW	46	23	23,26,27	1.36	3 (13%)	27,39,42	2.63	7 (25%)
25	4SU	CY	8	25	18,21,22	1.72	4 (22%)	25,30,33	3.08	6 (24%)

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
24	5MC	AX	32	24	-	0/7/25/26	0/2/2/2
23	PSU	AW	39	23	-	0/7/25/26	0/2/2/2
25	PSU	AY	55	25	-	2/7/25/26	0/2/2/2
23	PSU	AW	55	23	-	0/7/25/26	0/2/2/2
25	MIA	CY	37	25	-	3/7/25/34	0/3/3/3
25	PSU	AY	32	25	-	1/7/25/26	0/2/2/2
23	MIA	AW	37	23	-	1/15/33/34	0/3/3/3
24	PSU	CX	55	24	-	1/7/25/26	0/2/2/2
25	7MG	AY	46	25	-	2/7/37/38	0/3/3/3
23	PSU	CW	55	23	-	0/7/25/26	0/2/2/2
25	PSU	CY	32	25	-	1/7/25/26	0/2/2/2
24	4SU	CX	8	24	-	0/7/25/26	0/2/2/2
23	4SU	CW	8	23	-	0/7/25/26	0/2/2/2
25	5MU	AY	54	25	-	2/7/25/26	0/2/2/2
25	5MU	CY	54	25	-	2/7/25/26	0/2/2/2
23	5MU	AW	54	23	-	0/7/25/26	0/2/2/2
23	5MU	CW	54	23	-	0/7/25/26	0/2/2/2
23	7MG	CW	46	23	-	3/7/37/38	0/3/3/3
25	4SU	AY	8	25	-	1/7/25/26	0/2/2/2
25	PSU	CY	55	25	-	4/7/25/26	0/2/2/2
24	5MU	AX	54	24,57	-	0/7/25/26	0/2/2/2
25	MIA	AY	37	25	-	2/7/25/34	0/3/3/3
23	PSU	AW	32	23	-	0/7/25/26	0/2/2/2
23	4SU	AW	8	23	-	0/7/25/26	0/2/2/2
24	PSU	AX	55	24,57	-	0/7/25/26	0/2/2/2
24	4SU	AX	8	24	-	0/7/25/26	0/2/2/2
24	5MC	CX	32	24	-	0/7/25/26	0/2/2/2
23	31M	AW	76	23	-	8/31/49/50	0/4/4/4
23	31M	CW	76	23	-	11/31/49/50	0/4/4/4

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

The worst 5 of 141 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	37	MIA	C13-C14	6.94	1.53	1.32
23	AW	37	MIA	C2-S10	-6.49	1.70	1.75
24	AX	32	5MC	C5-C4	6.12	1.48	1.44
24	CX	32	5MC	C5-C4	5.90	1.48	1.44
24	AX	8	4SU	C4-N3	-5.37	1.32	1.37

The worst 5 of 218 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	AY	46	7MG	N9-C4-N3	10.29	140.54	125.46
23	AW	37	MIA	C12-C13-C14	-9.12	110.65	127.01
23	AW	46	7MG	N9-C4-N3	9.11	138.81	125.46
25	CY	8	4SU	C4-N3-C2	-8.94	118.75	127.31
23	CW	46	7MG	N9-C4-N3	8.27	137.58	125.46

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	AW	37	MIA	C12-C13-C14-C16
23	AW	76	31M	NM-CAM-CTM-N
23	AW	76	31M	CBM-CAM-CTM-N
23	AW	76	31M	CBM-CAM-CTM-OTM
25	AY	46	7MG	C4'-C5'-O5'-P

There are no ring outliers.

28 monomers are involved in 63 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2093 ligands modelled in this entry, 2091 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	CD	302	4	0,12,12	-	-	-		
58	SF4	AD	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	CD	302	4	-	-	0/6/5/5
58	SF4	AD	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.

No monomer is involved in short contacts.

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	1498/1521 (98%)	0.70	82 (5%) 30 30	42, 72, 93, 108	0
1	CA	1503/1521 (98%)	0.91	191 (12%) 8 7	44, 74, 94, 109	0
2	AB	231/256 (90%)	1.68	69 (29%) 1 1	72, 82, 90, 94	0
2	CB	231/256 (90%)	2.11	109 (47%) 0 0	73, 84, 90, 95	0
3	AC	206/239 (86%)	1.55	50 (24%) 2 1	68, 79, 87, 94	0
3	CC	206/239 (86%)	2.37	129 (62%) 0 0	71, 81, 89, 94	0
4	AD	208/209 (99%)	1.50	50 (24%) 2 1	57, 72, 81, 90	0
4	CD	208/209 (99%)	1.31	28 (13%) 7 5	58, 71, 80, 91	0
5	AE	148/162 (91%)	1.27	18 (12%) 8 7	58, 71, 80, 85	0
5	CE	148/162 (91%)	1.72	45 (30%) 1 0	60, 73, 81, 86	0
6	AF	100/101 (99%)	1.17	8 (8%) 18 18	56, 69, 78, 82	0
6	CF	100/101 (99%)	1.04	5 (5%) 34 33	57, 70, 78, 82	0
7	AG	155/156 (99%)	1.33	23 (14%) 5 5	65, 75, 83, 91	0
7	CG	155/156 (99%)	1.36	27 (17%) 4 3	66, 76, 84, 92	0
8	AH	137/138 (99%)	1.24	17 (12%) 8 7	62, 72, 79, 87	0
8	CH	137/138 (99%)	1.57	31 (22%) 2 2	64, 74, 80, 87	0
9	AI	127/128 (99%)	1.79	50 (39%) 1 0	65, 80, 86, 89	0
9	CI	127/128 (99%)	2.59	82 (64%) 0 0	68, 82, 88, 91	0
10	AJ	97/105 (92%)	1.97	46 (47%) 0 0	64, 82, 90, 93	0
10	CJ	96/105 (91%)	2.43	57 (59%) 0 0	67, 84, 91, 93	0
11	AK	114/129 (88%)	1.11	14 (12%) 8 7	48, 70, 79, 84	0
11	CK	114/129 (88%)	1.27	17 (14%) 5 5	51, 71, 79, 84	0
12	AL	122/132 (92%)	0.94	9 (7%) 20 19	50, 65, 73, 78	0
12	CL	122/132 (92%)	1.27	22 (18%) 3 3	53, 67, 75, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	AM	123/126 (97%)	1.28	18 (14%)	6	5	55, 70, 81, 89	0
13	CM	122/126 (96%)	2.45	70 (57%)	0	0	70, 84, 91, 99	0
14	AN	60/61 (98%)	1.69	14 (23%)	2	1	67, 74, 83, 84	0
14	CN	60/61 (98%)	3.17	54 (90%)	0	0	69, 77, 84, 88	0
15	AO	88/89 (98%)	1.23	12 (13%)	7	5	56, 67, 80, 81	0
15	CO	88/89 (98%)	1.28	14 (15%)	5	4	59, 69, 80, 83	0
16	AP	82/88 (93%)	1.78	29 (35%)	1	0	57, 71, 80, 84	0
16	CP	82/88 (93%)	1.36	14 (17%)	4	3	58, 70, 80, 84	0
17	AQ	99/105 (94%)	1.28	14 (14%)	6	5	59, 71, 80, 84	0
17	CQ	99/105 (94%)	1.13	11 (11%)	10	9	61, 71, 81, 85	0
18	AR	68/88 (77%)	0.97	6 (8%)	15	15	59, 68, 81, 83	0
18	CR	68/88 (77%)	1.21	7 (10%)	12	11	61, 70, 80, 84	0
19	AS	83/93 (89%)	1.62	19 (22%)	2	2	71, 80, 86, 95	0
19	CS	83/93 (89%)	2.82	66 (79%)	0	0	74, 82, 89, 96	0
20	AT	96/106 (90%)	1.43	20 (20%)	2	2	57, 71, 81, 85	0
20	CT	96/106 (90%)	1.24	12 (12%)	8	7	58, 70, 82, 85	0
21	AU	23/27 (85%)	2.13	13 (56%)	0	0	67, 74, 77, 81	0
21	CU	23/27 (85%)	2.66	19 (82%)	0	0	70, 75, 80, 84	0
22	AV	13/24 (54%)	1.45	4 (30%)	1	0	58, 81, 96, 99	0
22	CV	12/24 (50%)	2.05	5 (41%)	0	0	63, 84, 93, 94	0
23	AW	66/76 (86%)	1.47	14 (21%)	2	2	68, 96, 103, 105	0
23	CW	64/76 (84%)	1.75	18 (28%)	1	1	73, 97, 103, 106	0
24	AX	72/77 (93%)	0.45	2 (2%)	55	56	39, 68, 87, 91	0
24	CX	72/77 (93%)	0.92	2 (2%)	55	56	53, 82, 93, 97	0
25	AY	67/76 (88%)	2.05	34 (50%)	0	0	44, 97, 102, 105	0
25	CY	66/76 (86%)	2.26	40 (60%)	0	0	47, 97, 102, 105	0
26	BA	2819/2915 (96%)	-0.04	116 (4%)	41	42	26, 45, 89, 104	0
26	DA	2800/2915 (96%)	0.05	100 (3%)	46	47	30, 49, 90, 108	0
27	BB	120/121 (99%)	0.46	1 (0%)	82	84	40, 64, 73, 86	0
27	DB	120/121 (99%)	1.16	16 (13%)	7	6	46, 69, 76, 90	0
28	BD	275/276 (99%)	0.43	5 (1%)	67	68	27, 43, 58, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DD	275/276 (99%)	0.32	7 (2%) 58 59	29, 45, 61, 81	0
29	BE	204/206 (99%)	0.45	5 (2%) 58 59	25, 48, 66, 80	0
29	DE	204/206 (99%)	0.55	4 (1%) 65 65	29, 52, 67, 81	0
30	BF	203/210 (96%)	0.55	4 (1%) 65 65	26, 53, 76, 87	0
30	DF	203/210 (96%)	0.64	4 (1%) 65 65	30, 58, 77, 87	0
31	BG	181/182 (99%)	1.34	29 (16%) 5 4	51, 69, 81, 88	0
31	DG	181/182 (99%)	1.83	67 (37%) 1 0	56, 73, 82, 90	0
32	BH	174/180 (96%)	1.10	13 (7%) 20 19	51, 65, 75, 88	0
32	DH	174/180 (96%)	1.38	31 (17%) 4 3	55, 70, 78, 88	0
33	BI	146/148 (98%)	1.13	13 (8%) 15 14	50, 74, 82, 87	0
33	DI	146/148 (98%)	1.55	33 (22%) 2 2	52, 75, 82, 86	0
34	BN	140/140 (100%)	0.68	5 (3%) 46 47	32, 50, 67, 76	0
34	DN	140/140 (100%)	0.77	3 (2%) 63 64	36, 55, 70, 77	0
35	BO	122/122 (100%)	0.13	1 (0%) 82 84	30, 43, 59, 70	0
35	DO	122/122 (100%)	0.81	5 (4%) 41 42	45, 59, 73, 78	0
36	BP	149/150 (99%)	0.79	6 (4%) 42 43	26, 55, 75, 83	0
36	DP	149/150 (99%)	0.91	10 (6%) 24 23	30, 59, 77, 85	0
37	BQ	141/141 (100%)	0.63	3 (2%) 63 64	36, 52, 67, 80	0
37	DQ	141/141 (100%)	1.05	11 (7%) 19 18	41, 57, 70, 82	0
38	BR	118/118 (100%)	-0.02	0 100 100	25, 36, 54, 59	0
38	DR	118/118 (100%)	0.45	0 100 100	40, 54, 65, 72	0
39	BS	110/112 (98%)	0.35	0 100 100	38, 51, 65, 72	0
39	DS	110/112 (98%)	1.75	36 (32%) 1 0	63, 77, 84, 92	0
40	BT	131/146 (89%)	0.32	7 (5%) 32 31	32, 47, 69, 82	0
40	DT	131/146 (89%)	0.95	13 (9%) 13 12	48, 63, 79, 85	0
41	BU	116/118 (98%)	-0.13	1 (0%) 81 83	18, 33, 49, 59	0
41	DU	116/118 (98%)	0.88	4 (3%) 48 49	42, 61, 78, 84	0
42	BV	101/101 (100%)	-0.04	0 100 100	21, 41, 58, 67	0
42	DV	101/101 (100%)	1.15	10 (9%) 13 12	41, 71, 83, 91	0
43	BW	112/113 (99%)	-0.05	2 (1%) 67 68	23, 34, 54, 79	0
43	DW	112/113 (99%)	0.35	1 (0%) 81 83	39, 50, 67, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BX	95/96 (98%)	0.10	1 (1%) 78 79	23, 38, 61, 84	0
44	DX	95/96 (98%)	1.01	14 (14%) 6 5	43, 60, 76, 79	0
45	BY	107/110 (97%)	0.39	3 (2%) 55 56	32, 50, 69, 83	0
45	DY	107/110 (97%)	1.32	16 (14%) 5 5	57, 71, 81, 88	0
46	BZ	171/206 (83%)	1.21	42 (24%) 2 1	39, 64, 91, 95	0
46	DZ	174/206 (84%)	2.12	80 (45%) 0 0	66, 84, 94, 101	0
47	B0	83/85 (97%)	0.25	3 (3%) 46 47	27, 39, 61, 73	0
47	D0	83/85 (97%)	1.33	15 (18%) 3 3	46, 66, 75, 82	0
48	B1	97/98 (98%)	0.50	3 (3%) 51 52	30, 48, 70, 76	0
48	D1	97/98 (98%)	0.79	9 (9%) 14 13	38, 58, 74, 83	0
49	B2	70/72 (97%)	0.39	2 (2%) 53 55	34, 50, 64, 79	0
49	D2	70/72 (97%)	1.25	13 (18%) 3 2	56, 70, 80, 86	0
50	B3	59/60 (98%)	0.08	1 (1%) 69 69	24, 37, 63, 71	0
50	D3	59/60 (98%)	0.74	2 (3%) 48 49	49, 64, 79, 85	0
51	B4	69/71 (97%)	1.36	15 (21%) 2 2	54, 73, 87, 92	0
51	D4	69/71 (97%)	2.08	31 (44%) 0 0	74, 88, 94, 99	0
52	B5	59/60 (98%)	-0.20	0 100 100	20, 33, 54, 67	0
52	D5	59/60 (98%)	0.32	1 (1%) 69 69	36, 51, 67, 73	0
53	B6	53/54 (98%)	0.14	1 (1%) 66 66	31, 44, 61, 68	0
53	D6	53/54 (98%)	1.00	4 (7%) 20 19	52, 63, 76, 79	0
54	B7	48/49 (97%)	0.12	4 (8%) 17 17	21, 30, 62, 76	0
54	D7	48/49 (97%)	0.38	3 (6%) 26 25	33, 42, 61, 70	0
55	B8	64/65 (98%)	0.15	1 (1%) 70 71	25, 36, 45, 60	0
55	D8	64/65 (98%)	1.01	2 (3%) 51 52	46, 58, 66, 72	0
56	B9	37/37 (100%)	0.40	1 (2%) 56 57	31, 49, 73, 74	0
56	D9	37/37 (100%)	1.21	5 (13%) 7 5	46, 57, 73, 76	0
All	All	20897/21748 (96%)	0.77	2548 (12%) 8 7	18, 64, 89, 109	0

The worst 5 of 2548 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	AG	82	GLY	8.4
14	AN	2	ALA	8.1

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Mol	Chain	Res	Type	RSRZ
13	CM	123	ALA	7.0
13	CM	124	PRO	7.0
28	BD	276	LYS	6.8

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
23	7MG	AW	46	24/25	0.42	0.18	84,99,117,133	0
23	7MG	CW	46	24/25	0.44	0.16	79,96,109,133	0
25	7MG	CY	46	24/25	0.52	0.21	86,105,111,137	0
25	MIA	CY	37	22/30	0.54	0.18	72,95,113,138	0
23	4SU	CW	8	20/21	0.59	0.15	81,98,120,127	0
25	PSU	CY	55	20/21	0.59	0.26	94,102,110,124	0
25	4SU	CY	8	20/21	0.62	0.18	93,103,113,128	0
25	PSU	AY	55	20/21	0.64	0.17	93,101,108,122	0
25	5MU	CY	54	21/22	0.67	0.25	78,94,109,140	0
25	PSU	CY	39	20/21	0.68	0.17	79,90,116,130	0
23	4SU	AW	8	20/21	0.68	0.15	86,95,112,128	0
25	5MU	AY	54	21/22	0.69	0.15	80,96,105,131	0
25	7MG	AY	46	24/25	0.69	0.19	75,101,111,123	0
25	PSU	CY	32	20/21	0.71	0.15	80,92,101,107	0
25	4SU	AY	8	20/21	0.71	0.14	82,96,103,118	0
25	MIA	AY	37	22/30	0.75	0.15	77,90,111,119	0
23	PSU	CW	55	20/21	0.75	0.13	79,89,99,104	0
25	PSU	AY	39	20/21	0.75	0.16	78,90,117,123	0
23	5MU	CW	54	21/22	0.78	0.14	74,88,99,101	0
23	MIA	CW	37	22/30	0.80	0.13	75,85,92,100	0
23	PSU	AW	55	20/21	0.81	0.12	77,90,98,104	0
23	31M	CW	76	41/42	0.83	0.24	50,63,73,88	20
23	PSU	CW	39	20/21	0.83	0.14	78,84,97,98	0
23	PSU	CW	32	20/21	0.84	0.15	81,87,94,103	0
25	PSU	AY	32	20/21	0.84	0.15	78,93,100,106	0
24	4SU	CX	8	20/21	0.85	0.14	77,87,95,97	0
24	5MU	CX	54	21/22	0.86	0.12	70,81,89,99	0
24	PSU	CX	55	20/21	0.86	0.12	70,80,91,96	0
23	PSU	AW	32	20/21	0.86	0.15	77,83,92,98	0
23	5MU	AW	54	21/22	0.88	0.12	65,82,91,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	PSU	AW	39	20/21	0.89	0.12	73,82,95,97	0
24	5MU	AX	54	21/22	0.92	0.12	49,68,79,84	0
23	31M	AW	76	41/42	0.92	0.16	37,54,66,83	9
24	5MC	CX	32	21/22	0.92	0.14	63,76,86,88	0
24	4SU	AX	8	20/21	0.92	0.12	54,66,82,89	0
24	PSU	AX	55	20/21	0.93	0.10	50,63,73,83	0
23	MIA	AW	37	29/30	0.94	0.11	59,71,81,86	0
24	5MC	AX	32	21/22	0.95	0.11	43,53,62,78	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	DA	3448	1/1	0.54	0.40	70,70,70,70	0
57	MG	BA	3670	1/1	0.60	0.27	61,61,61,61	0
57	MG	CA	3156	1/1	0.65	0.24	73,73,73,73	0
57	MG	BA	3730	1/1	0.65	0.19	71,71,71,71	0
57	MG	BA	3721	1/1	0.66	0.35	82,82,82,82	0
57	MG	DA	3530	1/1	0.68	0.27	74,74,74,74	0
57	MG	DA	3531	1/1	0.68	0.20	61,61,61,61	0
57	MG	DA	3544	1/1	0.68	0.22	65,65,65,65	0
57	MG	BA	3757	1/1	0.70	0.19	76,76,76,76	0
57	MG	BA	3616	1/1	0.70	0.22	65,65,65,65	0
57	MG	DB	3011	1/1	0.70	0.23	72,72,72,72	0
57	MG	BA	3745	1/1	0.71	0.26	75,75,75,75	0
57	MG	DR	5001	1/1	0.71	0.25	70,70,70,70	0
57	MG	DA	3259	1/1	0.72	0.22	43,43,43,43	0
57	MG	DA	3630	1/1	0.72	0.14	61,61,61,61	0
57	MG	AA	3059	1/1	0.74	0.39	78,78,78,78	0
57	MG	BA	3658	1/1	0.74	0.29	61,61,61,61	0
57	MG	DA	3469	1/1	0.74	0.21	44,44,44,44	0
57	MG	DA	3413	1/1	0.75	0.20	48,48,48,48	0
57	MG	BA	3362	1/1	0.75	0.22	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	3707	1/1	0.75	0.21	44,44,44,44	0
57	MG	DA	3518	1/1	0.75	0.24	54,54,54,54	0
57	MG	CA	3098	1/1	0.75	0.19	65,65,65,65	0
57	MG	AA	3105	1/1	0.75	0.34	69,69,69,69	0
57	MG	CV	101	1/1	0.75	0.28	72,72,72,72	0
57	MG	AA	3199	1/1	0.75	0.26	73,73,73,73	0
57	MG	DA	3673	1/1	0.75	0.25	69,69,69,69	0
57	MG	DA	3262	1/1	0.75	0.23	65,65,65,65	0
57	MG	DA	3320	1/1	0.75	0.15	55,55,55,55	0
57	MG	BA	3728	1/1	0.76	0.24	48,48,48,48	0
57	MG	BA	3724	1/1	0.76	0.15	62,62,62,62	0
57	MG	DA	3521	1/1	0.76	0.16	58,58,58,58	0
57	MG	DB	3001	1/1	0.76	0.25	64,64,64,64	0
57	MG	BB	218	1/1	0.76	0.21	77,77,77,77	0
57	MG	CA	3070	1/1	0.76	0.24	63,63,63,63	0
57	MG	DA	3215	1/1	0.77	0.22	59,59,59,59	0
57	MG	DA	3563	1/1	0.77	0.21	74,74,74,74	0
57	MG	BA	3427	1/1	0.77	0.17	61,61,61,61	0
57	MG	DA	3632	1/1	0.77	0.17	36,36,36,36	0
57	MG	DA	3646	1/1	0.77	0.23	59,59,59,59	0
57	MG	BA	3760	1/1	0.77	0.18	44,44,44,44	0
57	MG	BA	3779	1/1	0.77	0.28	66,66,66,66	0
57	MG	DA	3408	1/1	0.77	0.13	58,58,58,58	0
57	MG	AA	3166	1/1	0.77	0.23	69,69,69,69	0
57	MG	DA	3651	1/1	0.78	0.32	75,75,75,75	0
57	MG	DA	3575	1/1	0.78	0.24	64,64,64,64	0
57	MG	BA	3794	1/1	0.78	0.22	51,51,51,51	0
57	MG	CA	3140	1/1	0.78	0.16	67,67,67,67	0
57	MG	DA	3487	1/1	0.78	0.18	62,62,62,62	0
57	MG	BA	3703	1/1	0.79	0.21	64,64,64,64	0
57	MG	DA	3256	1/1	0.79	0.22	62,62,62,62	0
57	MG	BA	3769	1/1	0.79	0.21	52,52,52,52	0
57	MG	DA	3633	1/1	0.79	0.14	58,58,58,58	0
57	MG	BA	3641	1/1	0.79	0.19	68,68,68,68	0
57	MG	BA	3602	1/1	0.79	0.12	53,53,53,53	0
57	MG	DA	3355	1/1	0.79	0.12	58,58,58,58	0
57	MG	AA	3175	1/1	0.79	0.20	63,63,63,63	0
57	MG	DA	3185	1/1	0.79	0.20	68,68,68,68	0
57	MG	DD	303	1/1	0.79	0.20	87,87,87,87	0
57	MG	DA	3415	1/1	0.79	0.24	68,68,68,68	0
57	MG	DA	3313	1/1	0.80	0.12	47,47,47,47	0
57	MG	CA	3102	1/1	0.80	0.14	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	3128	1/1	0.80	0.23	65,65,65,65	0
57	MG	DA	3607	1/1	0.80	0.17	65,65,65,65	0
57	MG	DA	3626	1/1	0.80	0.13	67,67,67,67	0
57	MG	BA	3583	1/1	0.80	0.19	45,45,45,45	0
57	MG	BA	3771	1/1	0.80	0.23	50,50,50,50	0
57	MG	AA	3020	1/1	0.80	0.20	76,76,76,76	0
57	MG	DA	3140	1/1	0.80	0.20	58,58,58,58	0
57	MG	BA	3683	1/1	0.80	0.26	73,73,73,73	0
57	MG	BA	3434	1/1	0.80	0.14	55,55,55,55	0
57	MG	CA	3039	1/1	0.80	0.15	68,68,68,68	0
57	MG	BA	3638	1/1	0.80	0.23	63,63,63,63	0
57	MG	BA	3463	1/1	0.80	0.21	48,48,48,48	0
57	MG	DA	3279	1/1	0.80	0.12	56,56,56,56	0
57	MG	CA	3136	1/1	0.81	0.24	72,72,72,72	0
57	MG	BA	3642	1/1	0.81	0.10	48,48,48,48	0
57	MG	CA	3115	1/1	0.81	0.14	63,63,63,63	0
57	MG	BA	3754	1/1	0.81	0.13	48,48,48,48	0
57	MG	DA	3335	1/1	0.81	0.16	47,47,47,47	0
57	MG	DA	3125	1/1	0.81	0.35	70,70,70,70	0
57	MG	DB	3008	1/1	0.81	0.26	67,67,67,67	0
57	MG	DA	3623	1/1	0.81	0.19	66,66,66,66	0
57	MG	DA	3362	1/1	0.81	0.13	44,44,44,44	0
57	MG	DA	3402	1/1	0.81	0.14	66,66,66,66	0
57	MG	DV	3003	1/1	0.81	0.15	65,65,65,65	0
57	MG	DA	3308	1/1	0.82	0.15	61,61,61,61	0
57	MG	AA	3204	1/1	0.82	0.14	53,53,53,53	0
57	MG	BA	3512	1/1	0.82	0.15	52,52,52,52	0
57	MG	BA	3574	1/1	0.82	0.28	66,66,66,66	0
57	MG	AX	3014	1/1	0.82	0.18	72,72,72,72	0
57	MG	DA	3608	1/1	0.82	0.20	68,68,68,68	0
57	MG	BA	3257	1/1	0.82	0.18	53,53,53,53	0
57	MG	DA	3380	1/1	0.82	0.12	55,55,55,55	0
57	MG	DA	3118	1/1	0.82	0.14	77,77,77,77	0
57	MG	BA	3302	1/1	0.82	0.34	69,69,69,69	0
57	MG	CA	3018	1/1	0.82	0.25	69,69,69,69	0
57	MG	AA	3153	1/1	0.82	0.14	74,74,74,74	0
57	MG	BA	3396	1/1	0.82	0.14	50,50,50,50	0
57	MG	DA	3462	1/1	0.82	0.21	42,42,42,42	0
57	MG	CA	3083	1/1	0.82	0.19	79,79,79,79	0
57	MG	DA	3484	1/1	0.82	0.19	62,62,62,62	0
57	MG	AA	3193	1/1	0.82	0.14	72,72,72,72	0
57	MG	BA	3654	1/1	0.82	0.15	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3274	1/1	0.82	0.17	58,58,58,58	0
57	MG	AA	3127	1/1	0.82	0.14	65,65,65,65	0
57	MG	BA	3550	1/1	0.83	0.16	36,36,36,36	0
57	MG	DA	3399	1/1	0.83	0.28	59,59,59,59	0
57	MG	AA	3196	1/1	0.83	0.13	74,74,74,74	0
57	MG	BB	215	1/1	0.83	0.18	73,73,73,73	0
57	MG	BA	3453	1/1	0.83	0.20	45,45,45,45	0
57	MG	B4	502	1/1	0.83	0.13	71,71,71,71	0
57	MG	DA	3421	1/1	0.83	0.12	50,50,50,50	0
57	MG	DA	3430	1/1	0.83	0.12	37,37,37,37	0
57	MG	AA	3002	1/1	0.83	0.26	71,71,71,71	0
57	MG	CA	3027	1/1	0.83	0.26	64,64,64,64	0
57	MG	CA	3152	1/1	0.83	0.28	76,76,76,76	0
57	MG	BA	3335	1/1	0.83	0.19	52,52,52,52	0
57	MG	CE	3001	1/1	0.83	0.11	79,79,79,79	0
57	MG	CJ	5001	1/1	0.83	0.13	73,73,73,73	0
57	MG	DA	3329	1/1	0.83	0.16	54,54,54,54	0
57	MG	CA	3066	1/1	0.83	0.28	66,66,66,66	0
57	MG	BA	3514	1/1	0.83	0.16	48,48,48,48	0
57	MG	CA	3082	1/1	0.83	0.24	79,79,79,79	0
57	MG	AA	3108	1/1	0.84	0.17	67,67,67,67	0
57	MG	BA	3631	1/1	0.84	0.13	42,42,42,42	0
57	MG	BA	3455	1/1	0.84	0.24	64,64,64,64	0
57	MG	DA	3577	1/1	0.84	0.14	58,58,58,58	0
57	MG	BB	206	1/1	0.84	0.17	47,47,47,47	0
57	MG	AA	3117	1/1	0.84	0.14	79,79,79,79	0
57	MG	DA	3614	1/1	0.84	0.10	65,65,65,65	0
57	MG	AA	3057	1/1	0.84	0.27	64,64,64,64	0
57	MG	DA	3417	1/1	0.84	0.14	52,52,52,52	0
57	MG	BA	3741	1/1	0.84	0.18	64,64,64,64	0
57	MG	AA	3026	1/1	0.84	0.23	70,70,70,70	0
57	MG	AA	3054	1/1	0.84	0.12	53,53,53,53	0
57	MG	DA	3641	1/1	0.84	0.20	69,69,69,69	0
57	MG	DA	3301	1/1	0.84	0.15	52,52,52,52	0
57	MG	CA	3153	1/1	0.84	0.28	70,70,70,70	0
57	MG	AA	3172	1/1	0.84	0.15	72,72,72,72	0
57	MG	CA	3049	1/1	0.84	0.27	63,63,63,63	0
57	MG	CA	3059	1/1	0.84	0.18	72,72,72,72	0
57	MG	BA	3225	1/1	0.84	0.30	61,61,61,61	0
57	MG	DA	3524	1/1	0.84	0.13	61,61,61,61	0
57	MG	DA	3093	1/1	0.84	0.15	62,62,62,62	0
57	MG	BA	3443	1/1	0.84	0.17	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3669	1/1	0.85	0.14	62,62,62,62	0
57	MG	DA	3470	1/1	0.85	0.15	45,45,45,45	0
57	MG	DA	3478	1/1	0.85	0.17	59,59,59,59	0
57	MG	BA	3070	1/1	0.85	0.32	59,59,59,59	0
57	MG	BA	3681	1/1	0.85	0.13	66,66,66,66	0
57	MG	BA	3128	1/1	0.85	0.15	69,69,69,69	0
57	MG	AA	3187	1/1	0.85	0.14	62,62,62,62	0
57	MG	AA	3028	1/1	0.85	0.39	76,76,76,76	0
57	MG	BA	3540	1/1	0.85	0.16	37,37,37,37	0
57	MG	AA	3170	1/1	0.85	0.13	75,75,75,75	0
57	MG	DA	3541	1/1	0.85	0.17	44,44,44,44	0
57	MG	BA	3316	1/1	0.85	0.14	66,66,66,66	0
57	MG	DA	3554	1/1	0.85	0.13	62,62,62,62	0
57	MG	AA	3197	1/1	0.85	0.16	70,70,70,70	0
57	MG	DA	3317	1/1	0.85	0.13	44,44,44,44	0
57	MG	BA	3590	1/1	0.85	0.17	50,50,50,50	0
57	MG	BA	3598	1/1	0.85	0.13	63,63,63,63	0
57	MG	AA	3004	1/1	0.85	0.11	67,67,67,67	0
57	MG	DA	3339	1/1	0.85	0.13	61,61,61,61	0
57	MG	DA	3618	1/1	0.85	0.18	53,53,53,53	0
57	MG	BA	3388	1/1	0.85	0.15	48,48,48,48	0
57	MG	CA	3146	1/1	0.85	0.27	66,66,66,66	0
57	MG	BA	3619	1/1	0.85	0.16	58,58,58,58	0
57	MG	BA	3623	1/1	0.85	0.20	55,55,55,55	0
57	MG	AA	3111	1/1	0.85	0.17	79,79,79,79	0
57	MG	AA	3209	1/1	0.85	0.12	59,59,59,59	0
57	MG	AE	202	1/1	0.85	0.16	80,80,80,80	0
57	MG	CT	3001	1/1	0.85	0.14	56,56,56,56	0
57	MG	DA	3667	1/1	0.85	0.13	50,50,50,50	0
57	MG	BA	3438	1/1	0.85	0.10	60,60,60,60	0
57	MG	BA	3652	1/1	0.85	0.25	67,67,67,67	0
57	MG	DA	3425	1/1	0.85	0.15	61,61,61,61	0
57	MG	AA	3185	1/1	0.85	0.29	82,82,82,82	0
57	MG	BA	3656	1/1	0.85	0.28	53,53,53,53	0
57	MG	AX	3016	1/1	0.85	0.19	56,56,56,56	0
57	MG	DA	3467	1/1	0.85	0.14	40,40,40,40	0
57	MG	BA	3523	1/1	0.86	0.10	48,48,48,48	0
57	MG	BA	3399	1/1	0.86	0.16	45,45,45,45	0
57	MG	BA	3419	1/1	0.86	0.16	37,37,37,37	0
57	MG	BA	3755	1/1	0.86	0.13	55,55,55,55	0
57	MG	AA	3192	1/1	0.86	0.21	71,71,71,71	0
57	MG	DA	3523	1/1	0.86	0.14	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3429	1/1	0.86	0.18	65,65,65,65	0
57	MG	AA	3031	1/1	0.86	0.27	70,70,70,70	0
57	MG	AA	3107	1/1	0.86	0.20	64,64,64,64	0
57	MG	DA	3532	1/1	0.86	0.16	69,69,69,69	0
57	MG	CA	3121	1/1	0.86	0.16	63,63,63,63	0
57	MG	BA	3680	1/1	0.86	0.18	68,68,68,68	0
57	MG	DA	3553	1/1	0.86	0.10	49,49,49,49	0
57	MG	BA	3783	1/1	0.86	0.20	56,56,56,56	0
57	MG	AA	3027	1/1	0.86	0.20	50,50,50,50	0
57	MG	BA	3811	1/1	0.86	0.15	65,65,65,65	0
57	MG	BB	202	1/1	0.86	0.27	59,59,59,59	0
57	MG	DA	3591	1/1	0.86	0.14	55,55,55,55	0
57	MG	BA	3353	1/1	0.86	0.12	50,50,50,50	0
57	MG	AA	3160	1/1	0.86	0.21	59,59,59,59	0
57	MG	CA	3159	1/1	0.86	0.25	70,70,70,70	0
57	MG	AA	3200	1/1	0.86	0.19	73,73,73,73	0
57	MG	DA	3403	1/1	0.86	0.10	57,57,57,57	0
57	MG	DA	3406	1/1	0.86	0.13	51,51,51,51	0
57	MG	BA	3470	1/1	0.86	0.10	62,62,62,62	0
57	MG	CA	3012	1/1	0.86	0.21	60,60,60,60	0
57	MG	DA	3414	1/1	0.86	0.13	43,43,43,43	0
57	MG	DA	3638	1/1	0.86	0.15	51,51,51,51	0
57	MG	BA	3636	1/1	0.86	0.12	64,64,64,64	0
57	MG	DA	3062	1/1	0.86	0.12	63,63,63,63	0
57	MG	DA	3075	1/1	0.86	0.16	59,59,59,59	0
57	MG	DA	3652	1/1	0.86	0.20	67,67,67,67	0
57	MG	DA	3662	1/1	0.86	0.19	62,62,62,62	0
57	MG	CA	3021	1/1	0.86	0.24	61,61,61,61	0
57	MG	BA	3391	1/1	0.86	0.22	63,63,63,63	0
57	MG	DA	3447	1/1	0.86	0.20	58,58,58,58	0
57	MG	CA	3037	1/1	0.86	0.33	73,73,73,73	0
57	MG	AA	3069	1/1	0.86	0.14	68,68,68,68	0
57	MG	BA	3740	1/1	0.86	0.18	28,28,28,28	0
57	MG	CA	3055	1/1	0.86	0.21	69,69,69,69	0
57	MG	DA	3230	1/1	0.86	0.17	73,73,73,73	0
57	MG	DA	3433	1/1	0.87	0.15	46,46,46,46	0
57	MG	DA	3076	1/1	0.87	0.14	58,58,58,58	0
57	MG	DA	3079	1/1	0.87	0.15	55,55,55,55	0
57	MG	BA	3548	1/1	0.87	0.10	40,40,40,40	0
57	MG	BA	3750	1/1	0.87	0.12	27,27,27,27	0
57	MG	AA	3184	1/1	0.87	0.13	60,60,60,60	0
57	MG	BA	3066	1/1	0.87	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	AA	3076	1/1	0.87	0.38	77,77,77,77	0
57	MG	DA	3194	1/1	0.87	0.13	56,56,56,56	0
57	MG	DA	3213	1/1	0.87	0.16	63,63,63,63	0
57	MG	DA	3502	1/1	0.87	0.15	55,55,55,55	0
57	MG	DA	3505	1/1	0.87	0.11	56,56,56,56	0
57	MG	AA	3091	1/1	0.87	0.20	60,60,60,60	0
57	MG	DA	3218	1/1	0.87	0.11	59,59,59,59	0
57	MG	BA	3673	1/1	0.87	0.14	55,55,55,55	0
57	MG	DA	3244	1/1	0.87	0.17	71,71,71,71	0
57	MG	BA	3212	1/1	0.87	0.19	54,54,54,54	0
57	MG	BA	3459	1/1	0.87	0.14	48,48,48,48	0
57	MG	DA	3261	1/1	0.87	0.09	49,49,49,49	0
57	MG	DA	3539	1/1	0.87	0.11	53,53,53,53	0
57	MG	CA	3090	1/1	0.87	0.16	67,67,67,67	0
57	MG	BA	3781	1/1	0.87	0.17	41,41,41,41	0
57	MG	DA	3546	1/1	0.87	0.09	71,71,71,71	0
57	MG	DA	3550	1/1	0.87	0.18	57,57,57,57	0
57	MG	DA	3276	1/1	0.87	0.15	49,49,49,49	0
57	MG	AA	3191	1/1	0.87	0.19	47,47,47,47	0
57	MG	DA	3291	1/1	0.87	0.13	44,44,44,44	0
57	MG	CA	3112	1/1	0.87	0.15	69,69,69,69	0
57	MG	BA	3686	1/1	0.87	0.23	60,60,60,60	0
57	MG	DA	3586	1/1	0.87	0.15	60,60,60,60	0
57	MG	BA	3466	1/1	0.87	0.17	49,49,49,49	0
57	MG	CA	3124	1/1	0.87	0.19	59,59,59,59	0
57	MG	DA	3318	1/1	0.87	0.12	40,40,40,40	0
57	MG	CA	3126	1/1	0.87	0.18	67,67,67,67	0
57	MG	AA	3100	1/1	0.87	0.15	65,65,65,65	0
57	MG	DA	3620	1/1	0.87	0.15	68,68,68,68	0
57	MG	BA	3486	1/1	0.87	0.15	57,57,57,57	0
57	MG	BA	3411	1/1	0.87	0.10	33,33,33,33	0
57	MG	DA	3628	1/1	0.87	0.19	76,76,76,76	0
57	MG	AA	3047	1/1	0.87	0.28	63,63,63,63	0
57	MG	CA	3149	1/1	0.87	0.14	52,52,52,52	0
57	MG	BF	308	1/1	0.87	0.10	46,46,46,46	0
57	MG	DA	3634	1/1	0.87	0.13	60,60,60,60	0
57	MG	DA	3635	1/1	0.87	0.10	38,38,38,38	0
57	MG	DA	3382	1/1	0.87	0.11	48,48,48,48	0
57	MG	BA	3304	1/1	0.87	0.18	67,67,67,67	0
57	MG	DA	3642	1/1	0.87	0.13	54,54,54,54	0
57	MG	B6	102	1/1	0.87	0.15	68,68,68,68	0
57	MG	CA	3157	1/1	0.87	0.11	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	CA	3006	1/1	0.87	0.26	64,64,64,64	0
57	MG	BA	3732	1/1	0.87	0.17	51,51,51,51	0
57	MG	DA	3409	1/1	0.87	0.12	57,57,57,57	0
57	MG	BA	3735	1/1	0.87	0.31	57,57,57,57	0
57	MG	BA	3530	1/1	0.87	0.23	49,49,49,49	0
57	MG	CA	3024	1/1	0.87	0.29	74,74,74,74	0
57	MG	CX	3003	1/1	0.87	0.17	54,54,54,54	0
57	MG	AA	3049	1/1	0.87	0.24	64,64,64,64	0
57	MG	DA	3073	1/1	0.87	0.10	42,42,42,42	0
57	MG	CA	3033	1/1	0.87	0.25	71,71,71,71	0
57	MG	BA	3418	1/1	0.88	0.10	30,30,30,30	0
57	MG	DA	3437	1/1	0.88	0.23	52,52,52,52	0
57	MG	BA	3738	1/1	0.88	0.16	43,43,43,43	0
57	MG	DA	3111	1/1	0.88	0.15	61,61,61,61	0
57	MG	CA	3051	1/1	0.88	0.18	81,81,81,81	0
57	MG	AX	3009	1/1	0.88	0.22	64,64,64,64	0
57	MG	CA	3057	1/1	0.88	0.18	76,76,76,76	0
57	MG	DA	3141	1/1	0.88	0.19	61,61,61,61	0
57	MG	DA	3181	1/1	0.88	0.12	50,50,50,50	0
57	MG	CA	3058	1/1	0.88	0.21	68,68,68,68	0
57	MG	BA	3615	1/1	0.88	0.29	68,68,68,68	0
57	MG	DA	3495	1/1	0.88	0.10	47,47,47,47	0
57	MG	BA	3424	1/1	0.88	0.17	39,39,39,39	0
57	MG	CA	3069	1/1	0.88	0.14	60,60,60,60	0
57	MG	AX	3011	1/1	0.88	0.21	78,78,78,78	0
57	MG	BA	3231	1/1	0.88	0.31	63,63,63,63	0
57	MG	BA	3238	1/1	0.88	0.25	62,62,62,62	0
57	MG	CA	3088	1/1	0.88	0.10	74,74,74,74	0
57	MG	AA	3176	1/1	0.88	0.11	67,67,67,67	0
57	MG	BA	3267	1/1	0.88	0.12	65,65,65,65	0
57	MG	AA	3177	1/1	0.88	0.09	66,66,66,66	0
57	MG	DA	3273	1/1	0.88	0.11	47,47,47,47	0
57	MG	CA	3107	1/1	0.88	0.11	80,80,80,80	0
57	MG	BA	3023	1/1	0.88	0.12	36,36,36,36	0
57	MG	BA	3648	1/1	0.88	0.17	65,65,65,65	0
57	MG	BA	3306	1/1	0.88	0.12	37,37,37,37	0
57	MG	BA	3034	1/1	0.88	0.24	56,56,56,56	0
57	MG	BA	3318	1/1	0.88	0.12	41,41,41,41	0
57	MG	DA	3309	1/1	0.88	0.09	51,51,51,51	0
57	MG	DA	3564	1/1	0.88	0.10	61,61,61,61	0
57	MG	BA	3053	1/1	0.88	0.18	54,54,54,54	0
57	MG	DA	3314	1/1	0.88	0.11	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3482	1/1	0.88	0.10	51,51,51,51	0
57	MG	DA	3588	1/1	0.88	0.12	65,65,65,65	0
57	MG	CA	3138	1/1	0.88	0.15	80,80,80,80	0
57	MG	DA	3598	1/1	0.88	0.15	61,61,61,61	0
57	MG	DA	3604	1/1	0.88	0.12	59,59,59,59	0
57	MG	BA	3342	1/1	0.88	0.09	46,46,46,46	0
57	MG	CA	3144	1/1	0.88	0.11	71,71,71,71	0
57	MG	BB	207	1/1	0.88	0.19	54,54,54,54	0
57	MG	AA	3037	1/1	0.88	0.21	55,55,55,55	0
57	MG	DA	3340	1/1	0.88	0.12	58,58,58,58	0
57	MG	AA	3036	1/1	0.88	0.17	61,61,61,61	0
57	MG	DA	3356	1/1	0.88	0.08	36,36,36,36	0
57	MG	DA	3627	1/1	0.88	0.16	63,63,63,63	0
57	MG	DA	3360	1/1	0.88	0.11	46,46,46,46	0
57	MG	BA	3387	1/1	0.88	0.09	54,54,54,54	0
57	MG	BA	3109	1/1	0.88	0.17	51,51,51,51	0
57	MG	BA	3117	1/1	0.88	0.12	59,59,59,59	0
57	MG	DA	3383	1/1	0.88	0.11	54,54,54,54	0
57	MG	DA	3388	1/1	0.88	0.16	53,53,53,53	0
57	MG	DA	3398	1/1	0.88	0.08	45,45,45,45	0
57	MG	CA	3004	1/1	0.88	0.14	66,66,66,66	0
57	MG	CA	3168	1/1	0.88	0.17	56,56,56,56	0
57	MG	BA	3545	1/1	0.88	0.15	65,65,65,65	0
57	MG	DA	3649	1/1	0.88	0.15	58,58,58,58	0
57	MG	AA	3138	1/1	0.88	0.22	71,71,71,71	0
57	MG	BA	3709	1/1	0.88	0.15	62,62,62,62	0
57	MG	DA	3655	1/1	0.88	0.09	64,64,64,64	0
57	MG	DA	3661	1/1	0.88	0.13	62,62,62,62	0
57	MG	BA	3129	1/1	0.88	0.22	58,58,58,58	0
57	MG	BA	3401	1/1	0.88	0.09	35,35,35,35	0
57	MG	DA	3669	1/1	0.88	0.16	55,55,55,55	0
57	MG	DA	3025	1/1	0.88	0.14	54,54,54,54	0
57	MG	DA	3676	1/1	0.88	0.18	67,67,67,67	0
57	MG	DA	3035	1/1	0.88	0.11	52,52,52,52	0
57	MG	BA	3179	1/1	0.88	0.11	50,50,50,50	0
57	MG	CA	3031	1/1	0.88	0.15	68,68,68,68	0
57	MG	BA	3415	1/1	0.88	0.08	28,28,28,28	0
57	MG	DP	201	1/1	0.88	0.21	70,70,70,70	0
57	MG	DA	3426	1/1	0.88	0.16	49,49,49,49	0
57	MG	BA	3594	1/1	0.88	0.10	40,40,40,40	0
57	MG	DW	3003	1/1	0.88	0.13	72,72,72,72	0
57	MG	DA	3440	1/1	0.89	0.11	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	CA	3046	1/1	0.89	0.17	69,69,69,69	0
57	MG	DA	3103	1/1	0.89	0.24	58,58,58,58	0
57	MG	DA	3451	1/1	0.89	0.12	55,55,55,55	0
57	MG	BA	3593	1/1	0.89	0.13	38,38,38,38	0
57	MG	DA	3117	1/1	0.89	0.12	52,52,52,52	0
57	MG	BA	3300	1/1	0.89	0.16	57,57,57,57	0
57	MG	BA	3596	1/1	0.89	0.10	64,64,64,64	0
57	MG	BA	3397	1/1	0.89	0.09	30,30,30,30	0
57	MG	DA	3482	1/1	0.89	0.13	50,50,50,50	0
57	MG	AA	3206	1/1	0.89	0.20	64,64,64,64	0
57	MG	BA	3608	1/1	0.89	0.14	62,62,62,62	0
57	MG	CA	3062	1/1	0.89	0.16	64,64,64,64	0
57	MG	DA	3499	1/1	0.89	0.10	53,53,53,53	0
57	MG	BA	3468	1/1	0.89	0.16	62,62,62,62	0
57	MG	CA	3067	1/1	0.89	0.28	61,61,61,61	0
57	MG	BA	3160	1/1	0.89	0.25	55,55,55,55	0
57	MG	BA	3473	1/1	0.89	0.14	56,56,56,56	0
57	MG	CA	3077	1/1	0.89	0.17	66,66,66,66	0
57	MG	DA	3231	1/1	0.89	0.12	62,62,62,62	0
57	MG	BA	3749	1/1	0.89	0.11	56,56,56,56	0
57	MG	DA	3248	1/1	0.89	0.14	56,56,56,56	0
57	MG	AA	3051	1/1	0.89	0.27	73,73,73,73	0
57	MG	BA	3624	1/1	0.89	0.17	68,68,68,68	0
57	MG	BA	3185	1/1	0.89	0.14	57,57,57,57	0
57	MG	BA	3633	1/1	0.89	0.11	49,49,49,49	0
57	MG	BA	3487	1/1	0.89	0.13	50,50,50,50	0
57	MG	CA	3104	1/1	0.89	0.15	68,68,68,68	0
57	MG	BA	3488	1/1	0.89	0.18	60,60,60,60	0
57	MG	BA	3492	1/1	0.89	0.10	46,46,46,46	0
57	MG	DA	3287	1/1	0.89	0.09	41,41,41,41	0
57	MG	DA	3290	1/1	0.89	0.18	59,59,59,59	0
57	MG	DA	3567	1/1	0.89	0.17	62,62,62,62	0
57	MG	DA	3571	1/1	0.89	0.12	56,56,56,56	0
57	MG	BA	3503	1/1	0.89	0.15	49,49,49,49	0
57	MG	DA	3295	1/1	0.89	0.18	44,44,44,44	0
57	MG	AA	3145	1/1	0.89	0.19	66,66,66,66	0
57	MG	BA	3319	1/1	0.89	0.10	46,46,46,46	0
57	MG	BA	3515	1/1	0.89	0.10	53,53,53,53	0
57	MG	BA	3796	1/1	0.89	0.12	45,45,45,45	0
57	MG	BA	3799	1/1	0.89	0.10	49,49,49,49	0
57	MG	BA	3520	1/1	0.89	0.19	61,61,61,61	0
57	MG	BA	3423	1/1	0.89	0.13	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3668	1/1	0.89	0.12	53,53,53,53	0
57	MG	DA	3615	1/1	0.89	0.16	65,65,65,65	0
57	MG	BA	3072	1/1	0.89	0.09	47,47,47,47	0
57	MG	DA	3331	1/1	0.89	0.15	37,37,37,37	0
57	MG	BA	3535	1/1	0.89	0.12	31,31,31,31	0
57	MG	DA	3625	1/1	0.89	0.09	69,69,69,69	0
57	MG	CA	3150	1/1	0.89	0.16	56,56,56,56	0
57	MG	BA	3671	1/1	0.89	0.13	63,63,63,63	0
57	MG	BA	3095	1/1	0.89	0.19	51,51,51,51	0
57	MG	BA	3679	1/1	0.89	0.16	62,62,62,62	0
57	MG	DA	3631	1/1	0.89	0.13	57,57,57,57	0
57	MG	BA	3022	1/1	0.89	0.13	60,60,60,60	0
57	MG	CA	3158	1/1	0.89	0.17	67,67,67,67	0
57	MG	BA	3243	1/1	0.89	0.17	53,53,53,53	0
57	MG	CA	3167	1/1	0.89	0.18	60,60,60,60	0
57	MG	BA	3385	1/1	0.89	0.23	59,59,59,59	0
57	MG	BA	3554	1/1	0.89	0.12	51,51,51,51	0
57	MG	BA	3700	1/1	0.89	0.10	61,61,61,61	0
57	MG	BA	3572	1/1	0.89	0.10	61,61,61,61	0
57	MG	CA	3022	1/1	0.89	0.18	78,78,78,78	0
57	MG	AX	3002	1/1	0.89	0.11	58,58,58,58	0
57	MG	DA	3001	1/1	0.89	0.09	60,60,60,60	0
57	MG	BA	3261	1/1	0.89	0.13	61,61,61,61	0
57	MG	DA	3657	1/1	0.89	0.19	63,63,63,63	0
57	MG	BA	3711	1/1	0.89	0.22	54,54,54,54	0
57	MG	DA	3410	1/1	0.89	0.10	53,53,53,53	0
57	MG	DA	3044	1/1	0.89	0.18	62,62,62,62	0
57	MG	DA	3051	1/1	0.89	0.09	48,48,48,48	0
57	MG	DA	3060	1/1	0.89	0.19	64,64,64,64	0
57	MG	BA	3712	1/1	0.89	0.25	53,53,53,53	0
57	MG	DA	3420	1/1	0.89	0.12	60,60,60,60	0
57	MG	DA	3069	1/1	0.89	0.23	57,57,57,57	0
57	MG	CA	3036	1/1	0.89	0.21	66,66,66,66	0
57	MG	DB	3013	1/1	0.89	0.21	64,64,64,64	0
57	MG	BA	3718	1/1	0.89	0.12	71,71,71,71	0
57	MG	DE	303	1/1	0.89	0.15	54,54,54,54	0
57	MG	CA	3038	1/1	0.89	0.13	58,58,58,58	0
57	MG	DA	3432	1/1	0.89	0.10	37,37,37,37	0
57	MG	AA	3134	1/1	0.89	0.12	66,66,66,66	0
57	MG	DA	3090	1/1	0.89	0.13	52,52,52,52	0
57	MG	D3	3001	1/1	0.89	0.16	57,57,57,57	0
57	MG	D8	5001	1/1	0.89	0.28	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	AA	3156	1/1	0.90	0.27	63,63,63,63	0
57	MG	BA	3471	1/1	0.90	0.15	53,53,53,53	0
57	MG	DA	3077	1/1	0.90	0.27	61,61,61,61	0
57	MG	BA	3622	1/1	0.90	0.12	48,48,48,48	0
57	MG	DA	3081	1/1	0.90	0.10	55,55,55,55	0
57	MG	BA	3375	1/1	0.90	0.14	68,68,68,68	0
57	MG	AA	3046	1/1	0.90	0.20	55,55,55,55	0
57	MG	AA	3161	1/1	0.90	0.26	65,65,65,65	0
57	MG	CA	3060	1/1	0.90	0.17	65,65,65,65	0
57	MG	AA	3017	1/1	0.90	0.26	71,71,71,71	0
57	MG	DA	3452	1/1	0.90	0.17	51,51,51,51	0
57	MG	BA	3634	1/1	0.90	0.13	62,62,62,62	0
57	MG	BA	3213	1/1	0.90	0.10	40,40,40,40	0
57	MG	BA	3005	1/1	0.90	0.09	30,30,30,30	0
57	MG	BA	3759	1/1	0.90	0.13	33,33,33,33	0
57	MG	DA	3147	1/1	0.90	0.18	56,56,56,56	0
57	MG	DA	3481	1/1	0.90	0.24	55,55,55,55	0
57	MG	DA	3149	1/1	0.90	0.07	56,56,56,56	0
57	MG	BA	3640	1/1	0.90	0.15	53,53,53,53	0
57	MG	BA	3761	1/1	0.90	0.14	59,59,59,59	0
57	MG	DA	3492	1/1	0.90	0.11	55,55,55,55	0
57	MG	BA	3764	1/1	0.90	0.12	51,51,51,51	0
57	MG	DA	3498	1/1	0.90	0.12	51,51,51,51	0
57	MG	DA	3205	1/1	0.90	0.09	56,56,56,56	0
57	MG	DA	3206	1/1	0.90	0.09	50,50,50,50	0
57	MG	DA	3207	1/1	0.90	0.17	63,63,63,63	0
57	MG	DA	3516	1/1	0.90	0.10	67,67,67,67	0
57	MG	CA	3087	1/1	0.90	0.19	67,67,67,67	0
57	MG	BA	3501	1/1	0.90	0.11	71,71,71,71	0
57	MG	AA	3136	1/1	0.90	0.17	70,70,70,70	0
57	MG	DA	3219	1/1	0.90	0.14	53,53,53,53	0
57	MG	DA	3222	1/1	0.90	0.11	57,57,57,57	0
57	MG	CA	3097	1/1	0.90	0.20	69,69,69,69	0
57	MG	BA	3647	1/1	0.90	0.11	56,56,56,56	0
57	MG	DA	3536	1/1	0.90	0.10	48,48,48,48	0
57	MG	DA	3234	1/1	0.90	0.22	63,63,63,63	0
57	MG	DA	3242	1/1	0.90	0.10	52,52,52,52	0
57	MG	BA	3504	1/1	0.90	0.10	56,56,56,56	0
57	MG	AA	3104	1/1	0.90	0.26	59,59,59,59	0
57	MG	DA	3255	1/1	0.90	0.10	51,51,51,51	0
57	MG	AA	3139	1/1	0.90	0.10	59,59,59,59	0
57	MG	CA	3109	1/1	0.90	0.14	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	DA	3556	1/1	0.90	0.17	67,67,67,67	0
57	MG	DA	3557	1/1	0.90	0.10	51,51,51,51	0
57	MG	DA	3558	1/1	0.90	0.14	61,61,61,61	0
57	MG	BA	3405	1/1	0.90	0.12	63,63,63,63	0
57	MG	BA	3409	1/1	0.90	0.09	30,30,30,30	0
57	MG	DA	3268	1/1	0.90	0.13	51,51,51,51	0
57	MG	DA	3569	1/1	0.90	0.18	49,49,49,49	0
57	MG	CA	3117	1/1	0.90	0.25	71,71,71,71	0
57	MG	CA	3118	1/1	0.90	0.31	68,68,68,68	0
57	MG	CA	3120	1/1	0.90	0.26	64,64,64,64	0
57	MG	BA	3052	1/1	0.90	0.12	56,56,56,56	0
57	MG	BA	3812	1/1	0.90	0.22	47,47,47,47	0
57	MG	AA	3202	1/1	0.90	0.14	57,57,57,57	0
57	MG	DA	3593	1/1	0.90	0.08	40,40,40,40	0
57	MG	DA	3594	1/1	0.90	0.11	54,54,54,54	0
57	MG	AA	3008	1/1	0.90	0.32	73,73,73,73	0
57	MG	CA	3133	1/1	0.90	0.28	59,59,59,59	0
57	MG	DA	3300	1/1	0.90	0.11	45,45,45,45	0
57	MG	BA	3294	1/1	0.90	0.21	61,61,61,61	0
57	MG	DA	3609	1/1	0.90	0.09	46,46,46,46	0
57	MG	BA	3541	1/1	0.90	0.14	38,38,38,38	0
57	MG	AA	3205	1/1	0.90	0.17	51,51,51,51	0
57	MG	DA	3311	1/1	0.90	0.13	54,54,54,54	0
57	MG	AA	3146	1/1	0.90	0.10	66,66,66,66	0
57	MG	BV	202	1/1	0.90	0.14	50,50,50,50	0
57	MG	DA	3624	1/1	0.90	0.14	56,56,56,56	0
57	MG	BX	3001	1/1	0.90	0.44	48,48,48,48	0
57	MG	BA	3426	1/1	0.90	0.11	37,37,37,37	0
57	MG	B5	101	1/1	0.90	0.18	51,51,51,51	0
57	MG	DA	3321	1/1	0.90	0.08	48,48,48,48	0
57	MG	AA	3147	1/1	0.90	0.16	70,70,70,70	0
57	MG	BA	3684	1/1	0.90	0.13	68,68,68,68	0
57	MG	BA	3555	1/1	0.90	0.11	29,29,29,29	0
57	MG	DA	3338	1/1	0.90	0.23	61,61,61,61	0
57	MG	CA	3008	1/1	0.90	0.26	51,51,51,51	0
57	MG	CA	3011	1/1	0.90	0.27	61,61,61,61	0
57	MG	DA	3636	1/1	0.90	0.14	63,63,63,63	0
57	MG	DA	3637	1/1	0.90	0.29	58,58,58,58	0
57	MG	DA	3348	1/1	0.90	0.10	34,34,34,34	0
57	MG	DA	3354	1/1	0.90	0.13	44,44,44,44	0
57	MG	BA	3693	1/1	0.90	0.12	56,56,56,56	0
57	MG	DA	3643	1/1	0.90	0.12	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	3102	1/1	0.90	0.15	44,44,44,44	0
57	MG	CA	3170	1/1	0.90	0.20	58,58,58,58	0
57	MG	BA	3431	1/1	0.90	0.11	59,59,59,59	0
57	MG	DA	3371	1/1	0.90	0.14	58,58,58,58	0
57	MG	BA	3314	1/1	0.90	0.19	58,58,58,58	0
57	MG	AA	3214	1/1	0.90	0.24	73,73,73,73	0
57	MG	CA	3026	1/1	0.90	0.22	63,63,63,63	0
57	MG	CX	3002	1/1	0.90	0.12	70,70,70,70	0
57	MG	DA	3663	1/1	0.90	0.11	60,60,60,60	0
57	MG	DA	3394	1/1	0.90	0.17	65,65,65,65	0
57	MG	BA	3114	1/1	0.90	0.13	53,53,53,53	0
57	MG	CA	3029	1/1	0.90	0.21	63,63,63,63	0
57	MG	DA	3002	1/1	0.90	0.10	48,48,48,48	0
57	MG	DA	3007	1/1	0.90	0.12	50,50,50,50	0
57	MG	DB	3005	1/1	0.90	0.10	59,59,59,59	0
57	MG	DA	3010	1/1	0.90	0.08	47,47,47,47	0
57	MG	AA	3121	1/1	0.90	0.14	70,70,70,70	0
57	MG	BA	3121	1/1	0.90	0.33	64,64,64,64	0
57	MG	AA	3155	1/1	0.90	0.23	48,48,48,48	0
57	MG	BA	3601	1/1	0.90	0.07	55,55,55,55	0
57	MG	BA	3351	1/1	0.90	0.12	30,30,30,30	0
57	MG	AX	3008	1/1	0.90	0.18	70,70,70,70	0
57	MG	CA	3041	1/1	0.90	0.14	59,59,59,59	0
57	MG	DA	3071	1/1	0.90	0.14	59,59,59,59	0
57	MG	BA	3359	1/1	0.90	0.19	62,62,62,62	0
57	MG	DA	3422	1/1	0.90	0.11	46,46,46,46	0
57	MG	BA	3717	1/1	0.91	0.10	50,50,50,50	0
57	MG	DA	3431	1/1	0.91	0.15	50,50,50,50	0
57	MG	AA	3013	1/1	0.91	0.15	69,69,69,69	0
57	MG	BA	3591	1/1	0.91	0.14	35,35,35,35	0
57	MG	AA	3092	1/1	0.91	0.19	63,63,63,63	0
57	MG	BA	3725	1/1	0.91	0.10	44,44,44,44	0
57	MG	BA	3432	1/1	0.91	0.10	58,58,58,58	0
57	MG	BA	3078	1/1	0.91	0.23	51,51,51,51	0
57	MG	DA	3450	1/1	0.91	0.08	40,40,40,40	0
57	MG	CA	3052	1/1	0.91	0.14	72,72,72,72	0
57	MG	BA	3731	1/1	0.91	0.27	37,37,37,37	0
57	MG	DA	3454	1/1	0.91	0.17	56,56,56,56	0
57	MG	BA	3083	1/1	0.91	0.19	56,56,56,56	0
57	MG	DA	3465	1/1	0.91	0.12	46,46,46,46	0
57	MG	DA	3123	1/1	0.91	0.14	56,56,56,56	0
57	MG	DA	3468	1/1	0.91	0.15	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	AA	3095	1/1	0.91	0.24	60,60,60,60	0
57	MG	BA	3315	1/1	0.91	0.11	31,31,31,31	0
57	MG	DA	3473	1/1	0.91	0.10	50,50,50,50	0
57	MG	BA	3604	1/1	0.91	0.09	36,36,36,36	0
57	MG	CA	3061	1/1	0.91	0.14	66,66,66,66	0
57	MG	AA	3183	1/1	0.91	0.16	65,65,65,65	0
57	MG	DA	3155	1/1	0.91	0.26	48,48,48,48	0
57	MG	DA	3160	1/1	0.91	0.14	56,56,56,56	0
57	MG	DA	3178	1/1	0.91	0.22	50,50,50,50	0
57	MG	CA	3063	1/1	0.91	0.27	58,58,58,58	0
57	MG	CA	3064	1/1	0.91	0.16	60,60,60,60	0
57	MG	DA	3188	1/1	0.91	0.19	48,48,48,48	0
57	MG	DA	3501	1/1	0.91	0.09	37,37,37,37	0
57	MG	BA	3742	1/1	0.91	0.15	65,65,65,65	0
57	MG	BA	3613	1/1	0.91	0.35	42,42,42,42	0
57	MG	BA	3747	1/1	0.91	0.17	52,52,52,52	0
57	MG	BA	3748	1/1	0.91	0.07	29,29,29,29	0
57	MG	DA	3520	1/1	0.91	0.13	57,57,57,57	0
57	MG	DA	3208	1/1	0.91	0.17	58,58,58,58	0
57	MG	CA	3071	1/1	0.91	0.21	68,68,68,68	0
57	MG	AN	503	1/1	0.91	0.14	54,54,54,54	0
57	MG	AW	3001	1/1	0.91	0.13	60,60,60,60	0
57	MG	BA	3465	1/1	0.91	0.13	43,43,43,43	0
57	MG	AW	3003	1/1	0.91	0.17	72,72,72,72	0
57	MG	DA	3534	1/1	0.91	0.21	55,55,55,55	0
57	MG	DA	3223	1/1	0.91	0.17	50,50,50,50	0
57	MG	BA	3120	1/1	0.91	0.22	55,55,55,55	0
57	MG	AA	3097	1/1	0.91	0.38	56,56,56,56	0
57	MG	BA	3626	1/1	0.91	0.16	44,44,44,44	0
57	MG	DA	3239	1/1	0.91	0.33	56,56,56,56	0
57	MG	BA	3126	1/1	0.91	0.17	54,54,54,54	0
57	MG	DA	3552	1/1	0.91	0.12	54,54,54,54	0
57	MG	BA	3355	1/1	0.91	0.16	61,61,61,61	0
57	MG	BA	3127	1/1	0.91	0.25	57,57,57,57	0
57	MG	DA	3251	1/1	0.91	0.12	62,62,62,62	0
57	MG	AA	3023	1/1	0.91	0.10	74,74,74,74	0
57	MG	CA	3108	1/1	0.91	0.14	68,68,68,68	0
57	MG	BA	3365	1/1	0.91	0.15	62,62,62,62	0
57	MG	BA	3639	1/1	0.91	0.28	48,48,48,48	0
57	MG	DA	3566	1/1	0.91	0.09	69,69,69,69	0
57	MG	CA	3113	1/1	0.91	0.11	67,67,67,67	0
57	MG	BA	3782	1/1	0.91	0.15	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3271	1/1	0.91	0.11	48,48,48,48	0
57	MG	DA	3574	1/1	0.91	0.14	53,53,53,53	0
57	MG	CA	3116	1/1	0.91	0.11	68,68,68,68	0
57	MG	AA	3052	1/1	0.91	0.30	65,65,65,65	0
57	MG	DA	3583	1/1	0.91	0.18	51,51,51,51	0
57	MG	DA	3584	1/1	0.91	0.20	53,53,53,53	0
57	MG	BA	3788	1/1	0.91	0.12	51,51,51,51	0
57	MG	BA	3159	1/1	0.91	0.27	50,50,50,50	0
57	MG	BA	3499	1/1	0.91	0.10	58,58,58,58	0
57	MG	BA	3386	1/1	0.91	0.09	53,53,53,53	0
57	MG	AA	3040	1/1	0.91	0.10	60,60,60,60	0
57	MG	BA	3651	1/1	0.91	0.09	45,45,45,45	0
57	MG	DA	3298	1/1	0.91	0.14	59,59,59,59	0
57	MG	DA	3299	1/1	0.91	0.19	55,55,55,55	0
57	MG	AA	3041	1/1	0.91	0.17	46,46,46,46	0
57	MG	BA	3508	1/1	0.91	0.17	51,51,51,51	0
57	MG	DA	3610	1/1	0.91	0.21	64,64,64,64	0
57	MG	DA	3613	1/1	0.91	0.10	54,54,54,54	0
57	MG	AA	3003	1/1	0.91	0.12	72,72,72,72	0
57	MG	BA	3205	1/1	0.91	0.13	50,50,50,50	0
57	MG	CA	3142	1/1	0.91	0.24	69,69,69,69	0
57	MG	BA	3663	1/1	0.91	0.09	41,41,41,41	0
57	MG	DA	3621	1/1	0.91	0.08	44,44,44,44	0
57	MG	BD	302	1/1	0.91	0.11	50,50,50,50	0
57	MG	BE	301	1/1	0.91	0.08	35,35,35,35	0
57	MG	BE	308	1/1	0.91	0.12	40,40,40,40	0
57	MG	BA	3001	1/1	0.91	0.10	53,53,53,53	0
57	MG	AA	3064	1/1	0.91	0.19	60,60,60,60	0
57	MG	DA	3327	1/1	0.91	0.12	57,57,57,57	0
57	MG	BA	3218	1/1	0.91	0.17	47,47,47,47	0
57	MG	BA	3527	1/1	0.91	0.11	54,54,54,54	0
57	MG	BA	3672	1/1	0.91	0.18	43,43,43,43	0
57	MG	BA	3404	1/1	0.91	0.13	59,59,59,59	0
57	MG	CA	3161	1/1	0.91	0.11	56,56,56,56	0
57	MG	CA	3166	1/1	0.91	0.12	66,66,66,66	0
57	MG	B7	101	1/1	0.91	0.12	39,39,39,39	0
57	MG	B7	102	1/1	0.91	0.10	47,47,47,47	0
57	MG	BA	3018	1/1	0.91	0.14	56,56,56,56	0
57	MG	BA	3406	1/1	0.91	0.09	50,50,50,50	0
57	MG	AA	3065	1/1	0.91	0.24	63,63,63,63	0
57	MG	CA	3009	1/1	0.91	0.14	64,64,64,64	0
57	MG	DA	3644	1/1	0.91	0.08	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	CA	3010	1/1	0.91	0.09	56,56,56,56	0
57	MG	DA	3374	1/1	0.91	0.16	56,56,56,56	0
57	MG	AA	3033	1/1	0.91	0.09	59,59,59,59	0
57	MG	AA	3048	1/1	0.91	0.26	57,57,57,57	0
57	MG	DA	3653	1/1	0.91	0.09	52,52,52,52	0
57	MG	CX	3004	1/1	0.91	0.14	63,63,63,63	0
57	MG	CA	3014	1/1	0.91	0.21	58,58,58,58	0
57	MG	DA	3659	1/1	0.91	0.12	48,48,48,48	0
57	MG	CA	3016	1/1	0.91	0.09	57,57,57,57	0
57	MG	CA	3017	1/1	0.91	0.18	53,53,53,53	0
57	MG	BA	3244	1/1	0.91	0.14	53,53,53,53	0
57	MG	DA	3017	1/1	0.91	0.14	55,55,55,55	0
57	MG	DA	3024	1/1	0.91	0.28	59,59,59,59	0
57	MG	AA	3078	1/1	0.91	0.31	66,66,66,66	0
57	MG	BA	3695	1/1	0.91	0.13	67,67,67,67	0
57	MG	AA	3173	1/1	0.91	0.19	54,54,54,54	0
57	MG	DB	3004	1/1	0.91	0.14	55,55,55,55	0
57	MG	DA	3048	1/1	0.91	0.08	53,53,53,53	0
57	MG	DA	3411	1/1	0.91	0.15	53,53,53,53	0
57	MG	BA	3264	1/1	0.91	0.16	58,58,58,58	0
57	MG	DB	3012	1/1	0.91	0.26	61,61,61,61	0
57	MG	BA	3057	1/1	0.91	0.10	34,34,34,34	0
57	MG	DA	3061	1/1	0.91	0.10	48,48,48,48	0
57	MG	BA	3580	1/1	0.91	0.10	55,55,55,55	0
57	MG	DF	3001	1/1	0.91	0.08	44,44,44,44	0
57	MG	DA	3418	1/1	0.91	0.12	52,52,52,52	0
57	MG	DA	3067	1/1	0.91	0.23	57,57,57,57	0
57	MG	CA	3030	1/1	0.91	0.23	57,57,57,57	0
57	MG	AA	3174	1/1	0.91	0.08	50,50,50,50	0
57	MG	D0	101	1/1	0.91	0.16	71,71,71,71	0
57	MG	BA	3584	1/1	0.91	0.19	63,63,63,63	0
57	MG	BA	3714	1/1	0.91	0.10	57,57,57,57	0
59	ZN	D4	501	1/1	0.91	0.08	144,144,144,144	0
57	MG	DA	3429	1/1	0.92	0.11	41,41,41,41	0
57	MG	BA	3526	1/1	0.92	0.09	44,44,44,44	0
57	MG	DA	3087	1/1	0.92	0.24	58,58,58,58	0
57	MG	BA	3364	1/1	0.92	0.16	60,60,60,60	0
57	MG	BA	3145	1/1	0.92	0.09	44,44,44,44	0
57	MG	DA	3436	1/1	0.92	0.14	54,54,54,54	0
57	MG	DA	3095	1/1	0.92	0.28	58,58,58,58	0
57	MG	BA	3532	1/1	0.92	0.14	52,52,52,52	0
57	MG	DA	3110	1/1	0.92	0.14	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	3372	1/1	0.92	0.08	28,28,28,28	0
57	MG	DA	3112	1/1	0.92	0.17	59,59,59,59	0
57	MG	DA	3114	1/1	0.92	0.13	55,55,55,55	0
57	MG	BA	3715	1/1	0.92	0.12	63,63,63,63	0
57	MG	DA	3453	1/1	0.92	0.20	60,60,60,60	0
57	MG	BA	3154	1/1	0.92	0.11	47,47,47,47	0
57	MG	DA	3457	1/1	0.92	0.10	54,54,54,54	0
57	MG	BA	3003	1/1	0.92	0.11	60,60,60,60	0
57	MG	DA	3463	1/1	0.92	0.10	55,55,55,55	0
57	MG	BA	3720	1/1	0.92	0.16	65,65,65,65	0
57	MG	DA	3132	1/1	0.92	0.14	52,52,52,52	0
57	MG	DA	3133	1/1	0.92	0.24	50,50,50,50	0
57	MG	DA	3139	1/1	0.92	0.13	53,53,53,53	0
57	MG	AA	3198	1/1	0.92	0.15	61,61,61,61	0
57	MG	BA	3723	1/1	0.92	0.07	47,47,47,47	0
57	MG	DA	3474	1/1	0.92	0.12	51,51,51,51	0
57	MG	DA	3476	1/1	0.92	0.13	62,62,62,62	0
57	MG	BA	3177	1/1	0.92	0.12	46,46,46,46	0
57	MG	BA	3012	1/1	0.92	0.13	39,39,39,39	0
57	MG	BA	3389	1/1	0.92	0.12	55,55,55,55	0
57	MG	BA	3180	1/1	0.92	0.11	47,47,47,47	0
57	MG	DA	3485	1/1	0.92	0.15	52,52,52,52	0
57	MG	DA	3165	1/1	0.92	0.24	57,57,57,57	0
57	MG	BA	3566	1/1	0.92	0.17	67,67,67,67	0
57	MG	DA	3180	1/1	0.92	0.18	42,42,42,42	0
57	MG	DA	3497	1/1	0.92	0.09	55,55,55,55	0
57	MG	BA	3570	1/1	0.92	0.11	42,42,42,42	0
57	MG	DA	3184	1/1	0.92	0.12	47,47,47,47	0
57	MG	AA	3038	1/1	0.92	0.32	68,68,68,68	0
57	MG	BA	3186	1/1	0.92	0.20	45,45,45,45	0
57	MG	DA	3503	1/1	0.92	0.18	52,52,52,52	0
57	MG	BA	3576	1/1	0.92	0.07	57,57,57,57	0
57	MG	DA	3513	1/1	0.92	0.12	52,52,52,52	0
57	MG	DA	3197	1/1	0.92	0.11	55,55,55,55	0
57	MG	BA	3202	1/1	0.92	0.21	60,60,60,60	0
57	MG	CA	3074	1/1	0.92	0.24	64,64,64,64	0
57	MG	BA	3021	1/1	0.92	0.10	49,49,49,49	0
57	MG	CA	3078	1/1	0.92	0.12	44,44,44,44	0
57	MG	DA	3212	1/1	0.92	0.12	45,45,45,45	0
57	MG	DA	3527	1/1	0.92	0.17	60,60,60,60	0
57	MG	AA	3068	1/1	0.92	0.17	69,69,69,69	0
57	MG	BA	3587	1/1	0.92	0.11	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	DA	3216	1/1	0.92	0.27	56,56,56,56	0
57	MG	CA	3085	1/1	0.92	0.22	54,54,54,54	0
57	MG	BA	3589	1/1	0.92	0.14	27,27,27,27	0
57	MG	AA	3094	1/1	0.92	0.14	59,59,59,59	0
57	MG	DA	3540	1/1	0.92	0.08	42,42,42,42	0
57	MG	AA	3115	1/1	0.92	0.22	79,79,79,79	0
57	MG	DA	3225	1/1	0.92	0.10	49,49,49,49	0
57	MG	DA	3229	1/1	0.92	0.09	50,50,50,50	0
57	MG	BA	3592	1/1	0.92	0.14	28,28,28,28	0
57	MG	BA	3408	1/1	0.92	0.13	36,36,36,36	0
57	MG	BA	3224	1/1	0.92	0.28	65,65,65,65	0
57	MG	AA	3154	1/1	0.92	0.16	69,69,69,69	0
57	MG	BA	3229	1/1	0.92	0.16	54,54,54,54	0
57	MG	DA	3243	1/1	0.92	0.16	55,55,55,55	0
57	MG	BA	3599	1/1	0.92	0.16	43,43,43,43	0
57	MG	BA	3417	1/1	0.92	0.13	38,38,38,38	0
57	MG	CA	3110	1/1	0.92	0.10	65,65,65,65	0
57	MG	AA	3178	1/1	0.92	0.21	59,59,59,59	0
57	MG	AA	3180	1/1	0.92	0.13	73,73,73,73	0
57	MG	BA	3421	1/1	0.92	0.08	32,32,32,32	0
57	MG	BA	3064	1/1	0.92	0.09	43,43,43,43	0
57	MG	DA	3573	1/1	0.92	0.10	43,43,43,43	0
57	MG	AA	3058	1/1	0.92	0.19	59,59,59,59	0
57	MG	AA	3044	1/1	0.92	0.25	60,60,60,60	0
57	MG	BA	3258	1/1	0.92	0.07	44,44,44,44	0
57	MG	DA	3578	1/1	0.92	0.12	59,59,59,59	0
57	MG	BA	3793	1/1	0.92	0.16	40,40,40,40	0
57	MG	BA	3260	1/1	0.92	0.17	39,39,39,39	0
57	MG	CA	3125	1/1	0.92	0.12	63,63,63,63	0
57	MG	AA	3157	1/1	0.92	0.13	45,45,45,45	0
57	MG	DA	3283	1/1	0.92	0.12	51,51,51,51	0
57	MG	DA	3592	1/1	0.92	0.07	51,51,51,51	0
57	MG	BA	3073	1/1	0.92	0.16	61,61,61,61	0
57	MG	DA	3288	1/1	0.92	0.14	52,52,52,52	0
57	MG	DA	3289	1/1	0.92	0.15	53,53,53,53	0
57	MG	DA	3602	1/1	0.92	0.13	65,65,65,65	0
57	MG	BA	3800	1/1	0.92	0.08	38,38,38,38	0
57	MG	DA	3605	1/1	0.92	0.14	58,58,58,58	0
57	MG	BA	3075	1/1	0.92	0.17	45,45,45,45	0
57	MG	BA	3629	1/1	0.92	0.09	43,43,43,43	0
57	MG	BA	3630	1/1	0.92	0.13	58,58,58,58	0
57	MG	BA	3275	1/1	0.92	0.12	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	3612	1/1	0.92	0.10	62,62,62,62	0
57	MG	BA	3278	1/1	0.92	0.12	34,34,34,34	0
57	MG	BB	213	1/1	0.92	0.21	60,60,60,60	0
57	MG	DA	3302	1/1	0.92	0.14	70,70,70,70	0
57	MG	BA	3444	1/1	0.92	0.11	29,29,29,29	0
57	MG	BA	3445	1/1	0.92	0.20	63,63,63,63	0
57	MG	BB	219	1/1	0.92	0.17	67,67,67,67	0
57	MG	BA	3446	1/1	0.92	0.12	40,40,40,40	0
57	MG	BA	3285	1/1	0.92	0.13	50,50,50,50	0
57	MG	BA	3293	1/1	0.92	0.18	50,50,50,50	0
57	MG	BA	3076	1/1	0.92	0.13	43,43,43,43	0
57	MG	BG	202	1/1	0.92	0.12	41,41,41,41	0
57	MG	BN	3004	1/1	0.92	0.14	60,60,60,60	0
57	MG	BO	202	1/1	0.92	0.09	65,65,65,65	0
57	MG	BA	3460	1/1	0.92	0.21	62,62,62,62	0
57	MG	AA	3159	1/1	0.92	0.10	66,66,66,66	0
57	MG	DA	3334	1/1	0.92	0.15	52,52,52,52	0
57	MG	B2	3001	1/1	0.92	0.11	56,56,56,56	0
57	MG	DA	3337	1/1	0.92	0.09	41,41,41,41	0
57	MG	CD	301	1/1	0.92	0.17	56,56,56,56	0
57	MG	BA	3301	1/1	0.92	0.13	60,60,60,60	0
57	MG	BA	3650	1/1	0.92	0.10	52,52,52,52	0
57	MG	AA	3189	1/1	0.92	0.11	65,65,65,65	0
57	MG	DA	3351	1/1	0.92	0.10	48,48,48,48	0
57	MG	BA	3091	1/1	0.92	0.26	56,56,56,56	0
57	MG	AW	3004	1/1	0.92	0.10	49,49,49,49	0
57	MG	B7	104	1/1	0.92	0.12	48,48,48,48	0
57	MG	DA	3358	1/1	0.92	0.09	45,45,45,45	0
57	MG	B7	105	1/1	0.92	0.14	56,56,56,56	0
57	MG	BA	3310	1/1	0.92	0.17	58,58,58,58	0
57	MG	BA	3313	1/1	0.92	0.07	53,53,53,53	0
57	MG	BA	3478	1/1	0.92	0.12	58,58,58,58	0
57	MG	DA	3656	1/1	0.92	0.09	58,58,58,58	0
57	MG	BA	3667	1/1	0.92	0.17	61,61,61,61	0
57	MG	AA	3190	1/1	0.92	0.10	58,58,58,58	0
57	MG	BA	3484	1/1	0.92	0.08	54,54,54,54	0
57	MG	AA	3012	1/1	0.92	0.11	46,46,46,46	0
57	MG	BA	3113	1/1	0.92	0.19	53,53,53,53	0
57	MG	DA	3037	1/1	0.92	0.13	43,43,43,43	0
57	MG	DA	3668	1/1	0.92	0.20	60,60,60,60	0
57	MG	AA	3101	1/1	0.92	0.11	43,43,43,43	0
57	MG	DA	3672	1/1	0.92	0.29	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	DA	3400	1/1	0.92	0.08	54,54,54,54	0
57	MG	DA	3046	1/1	0.92	0.13	47,47,47,47	0
57	MG	AA	3103	1/1	0.92	0.35	73,73,73,73	0
57	MG	DB	3002	1/1	0.92	0.22	65,65,65,65	0
57	MG	DB	3003	1/1	0.92	0.09	57,57,57,57	0
57	MG	DA	3405	1/1	0.92	0.12	46,46,46,46	0
57	MG	BA	3322	1/1	0.92	0.18	52,52,52,52	0
57	MG	DA	3052	1/1	0.92	0.21	61,61,61,61	0
57	MG	DA	3054	1/1	0.92	0.27	48,48,48,48	0
57	MG	AX	3012	1/1	0.92	0.13	59,59,59,59	0
57	MG	AA	3195	1/1	0.92	0.12	57,57,57,57	0
57	MG	BA	3682	1/1	0.92	0.15	53,53,53,53	0
57	MG	DA	3066	1/1	0.92	0.10	42,42,42,42	0
57	MG	BA	3344	1/1	0.92	0.15	66,66,66,66	0
57	MG	AA	3083	1/1	0.92	0.26	57,57,57,57	0
57	MG	DQ	3004	1/1	0.92	0.13	54,54,54,54	0
57	MG	BA	3685	1/1	0.92	0.10	53,53,53,53	0
57	MG	AY	3002	1/1	0.92	0.15	56,56,56,56	0
57	MG	AA	3089	1/1	0.92	0.14	60,60,60,60	0
57	MG	BA	3002	1/1	0.92	0.10	50,50,50,50	0
57	MG	BA	3361	1/1	0.92	0.09	49,49,49,49	0
57	MG	BA	3143	1/1	0.92	0.11	45,45,45,45	0
57	MG	DA	3427	1/1	0.92	0.10	45,45,45,45	0
60	K	CX	3001	1/1	0.92	0.14	82,82,82,82	0
57	MG	BA	3767	1/1	0.93	0.12	73,73,73,73	0
57	MG	BA	3628	1/1	0.93	0.14	49,49,49,49	0
57	MG	DA	3158	1/1	0.93	0.15	60,60,60,60	0
57	MG	DA	3159	1/1	0.93	0.14	58,58,58,58	0
57	MG	AA	3088	1/1	0.93	0.27	65,65,65,65	0
57	MG	DA	3163	1/1	0.93	0.07	49,49,49,49	0
57	MG	AA	3016	1/1	0.93	0.08	63,63,63,63	0
57	MG	CA	3086	1/1	0.93	0.12	64,64,64,64	0
57	MG	BA	3780	1/1	0.93	0.09	62,62,62,62	0
57	MG	BA	3358	1/1	0.93	0.15	49,49,49,49	0
57	MG	BA	3087	1/1	0.93	0.12	42,42,42,42	0
57	MG	AY	3001	1/1	0.93	0.31	65,65,65,65	0
57	MG	BA	3228	1/1	0.93	0.24	59,59,59,59	0
57	MG	BA	3092	1/1	0.93	0.08	37,37,37,37	0
57	MG	AA	3067	1/1	0.93	0.23	57,57,57,57	0
57	MG	DA	3202	1/1	0.93	0.18	57,57,57,57	0
57	MG	BA	3366	1/1	0.93	0.08	57,57,57,57	0
57	MG	BA	3797	1/1	0.93	0.08	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	3371	1/1	0.93	0.09	35,35,35,35	0
57	MG	BA	3232	1/1	0.93	0.19	52,52,52,52	0
57	MG	BA	3802	1/1	0.93	0.29	54,54,54,54	0
57	MG	BA	3808	1/1	0.93	0.16	42,42,42,42	0
57	MG	BA	3809	1/1	0.93	0.08	63,63,63,63	0
57	MG	DA	3489	1/1	0.93	0.07	51,51,51,51	0
57	MG	DA	3490	1/1	0.93	0.12	47,47,47,47	0
57	MG	BA	3643	1/1	0.93	0.08	46,46,46,46	0
57	MG	DA	3493	1/1	0.93	0.10	66,66,66,66	0
57	MG	BA	3500	1/1	0.93	0.15	56,56,56,56	0
57	MG	AY	3003	1/1	0.93	0.12	53,53,53,53	0
57	MG	DA	3221	1/1	0.93	0.12	52,52,52,52	0
57	MG	BA	3376	1/1	0.93	0.11	48,48,48,48	0
57	MG	BA	3380	1/1	0.93	0.09	48,48,48,48	0
57	MG	BB	209	1/1	0.93	0.33	65,65,65,65	0
57	MG	BA	3506	1/1	0.93	0.10	58,58,58,58	0
57	MG	AA	3032	1/1	0.93	0.10	67,67,67,67	0
57	MG	CA	3127	1/1	0.93	0.16	62,62,62,62	0
57	MG	BA	3511	1/1	0.93	0.07	30,30,30,30	0
57	MG	DA	3236	1/1	0.93	0.24	47,47,47,47	0
57	MG	DA	3519	1/1	0.93	0.11	63,63,63,63	0
57	MG	AA	3150	1/1	0.93	0.15	57,57,57,57	0
57	MG	CA	3135	1/1	0.93	0.12	63,63,63,63	0
57	MG	DA	3522	1/1	0.93	0.15	71,71,71,71	0
57	MG	BB	220	1/1	0.93	0.10	57,57,57,57	0
57	MG	BA	3662	1/1	0.93	0.10	61,61,61,61	0
57	MG	DA	3247	1/1	0.93	0.07	45,45,45,45	0
57	MG	BA	3248	1/1	0.93	0.21	42,42,42,42	0
57	MG	DA	3249	1/1	0.93	0.15	45,45,45,45	0
57	MG	BE	305	1/1	0.93	0.15	43,43,43,43	0
57	MG	DA	3254	1/1	0.93	0.06	52,52,52,52	0
57	MG	AA	3179	1/1	0.93	0.14	69,69,69,69	0
57	MG	DA	3538	1/1	0.93	0.15	58,58,58,58	0
57	MG	BF	306	1/1	0.93	0.22	31,31,31,31	0
57	MG	BA	3517	1/1	0.93	0.11	45,45,45,45	0
57	MG	DA	3260	1/1	0.93	0.16	55,55,55,55	0
57	MG	DA	3543	1/1	0.93	0.09	53,53,53,53	0
57	MG	BG	201	1/1	0.93	0.11	58,58,58,58	0
57	MG	AA	3152	1/1	0.93	0.12	62,62,62,62	0
57	MG	DA	3547	1/1	0.93	0.17	54,54,54,54	0
57	MG	DA	3263	1/1	0.93	0.09	41,41,41,41	0
57	MG	DA	3267	1/1	0.93	0.12	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	AA	3109	1/1	0.93	0.13	62,62,62,62	0
57	MG	BA	3394	1/1	0.93	0.12	40,40,40,40	0
57	MG	BQ	3005	1/1	0.93	0.07	49,49,49,49	0
57	MG	AA	3210	1/1	0.93	0.25	59,59,59,59	0
57	MG	BV	204	1/1	0.93	0.12	49,49,49,49	0
57	MG	CA	3160	1/1	0.93	0.10	62,62,62,62	0
57	MG	BA	3263	1/1	0.93	0.17	49,49,49,49	0
57	MG	CA	3163	1/1	0.93	0.09	63,63,63,63	0
57	MG	B0	103	1/1	0.93	0.07	53,53,53,53	0
57	MG	BA	3398	1/1	0.93	0.09	32,32,32,32	0
57	MG	BA	3125	1/1	0.93	0.07	47,47,47,47	0
57	MG	BA	3537	1/1	0.93	0.10	45,45,45,45	0
57	MG	DA	3293	1/1	0.93	0.16	54,54,54,54	0
57	MG	BA	3538	1/1	0.93	0.09	40,40,40,40	0
57	MG	DA	3296	1/1	0.93	0.07	28,28,28,28	0
57	MG	AA	3093	1/1	0.93	0.10	66,66,66,66	0
57	MG	BA	3271	1/1	0.93	0.12	58,58,58,58	0
57	MG	BA	3543	1/1	0.93	0.11	37,37,37,37	0
57	MG	AA	3006	1/1	0.93	0.08	52,52,52,52	0
57	MG	CW	3001	1/1	0.93	0.16	67,67,67,67	0
57	MG	DA	3590	1/1	0.93	0.10	51,51,51,51	0
57	MG	DA	3305	1/1	0.93	0.15	50,50,50,50	0
57	MG	CA	3003	1/1	0.93	0.12	57,57,57,57	0
57	MG	AA	3070	1/1	0.93	0.11	52,52,52,52	0
57	MG	BA	3694	1/1	0.93	0.09	51,51,51,51	0
57	MG	BA	3279	1/1	0.93	0.21	43,43,43,43	0
57	MG	BA	3696	1/1	0.93	0.09	33,33,33,33	0
57	MG	DA	3316	1/1	0.93	0.09	45,45,45,45	0
57	MG	BA	3552	1/1	0.93	0.14	29,29,29,29	0
57	MG	DA	3009	1/1	0.93	0.11	48,48,48,48	0
57	MG	BA	3033	1/1	0.93	0.11	53,53,53,53	0
57	MG	DA	3015	1/1	0.93	0.20	52,52,52,52	0
57	MG	BA	3288	1/1	0.93	0.11	56,56,56,56	0
57	MG	DA	3611	1/1	0.93	0.11	48,48,48,48	0
57	MG	DA	3019	1/1	0.93	0.10	37,37,37,37	0
57	MG	BA	3560	1/1	0.93	0.07	56,56,56,56	0
57	MG	BA	3562	1/1	0.93	0.08	37,37,37,37	0
57	MG	DA	3032	1/1	0.93	0.10	48,48,48,48	0
57	MG	DA	3616	1/1	0.93	0.09	71,71,71,71	0
57	MG	BA	3413	1/1	0.93	0.09	47,47,47,47	0
57	MG	BA	3568	1/1	0.93	0.07	59,59,59,59	0
57	MG	DA	3038	1/1	0.93	0.15	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	BA	3131	1/1	0.93	0.15	58,58,58,58	0
57	MG	DA	3342	1/1	0.93	0.10	42,42,42,42	0
57	MG	AA	3118	1/1	0.93	0.11	47,47,47,47	0
57	MG	BA	3298	1/1	0.93	0.20	51,51,51,51	0
57	MG	DA	3352	1/1	0.93	0.13	63,63,63,63	0
57	MG	AA	3119	1/1	0.93	0.07	51,51,51,51	0
57	MG	BA	3153	1/1	0.93	0.15	47,47,47,47	0
57	MG	BA	3722	1/1	0.93	0.15	47,47,47,47	0
57	MG	DA	3056	1/1	0.93	0.11	51,51,51,51	0
57	MG	AA	3072	1/1	0.93	0.13	66,66,66,66	0
57	MG	BA	3303	1/1	0.93	0.18	36,36,36,36	0
57	MG	DA	3364	1/1	0.93	0.07	40,40,40,40	0
57	MG	DA	3366	1/1	0.93	0.15	42,42,42,42	0
57	MG	DA	3367	1/1	0.93	0.12	61,61,61,61	0
57	MG	DA	3368	1/1	0.93	0.16	50,50,50,50	0
57	MG	AA	3001	1/1	0.93	0.16	61,61,61,61	0
57	MG	CA	3034	1/1	0.93	0.12	59,59,59,59	0
57	MG	DA	3376	1/1	0.93	0.19	61,61,61,61	0
57	MG	BA	3061	1/1	0.93	0.11	29,29,29,29	0
57	MG	BA	3165	1/1	0.93	0.12	45,45,45,45	0
57	MG	DA	3070	1/1	0.93	0.14	58,58,58,58	0
57	MG	DA	3384	1/1	0.93	0.14	49,49,49,49	0
57	MG	BA	3311	1/1	0.93	0.16	48,48,48,48	0
57	MG	BA	3168	1/1	0.93	0.14	47,47,47,47	0
57	MG	DA	3654	1/1	0.93	0.14	56,56,56,56	0
57	MG	BA	3734	1/1	0.93	0.10	52,52,52,52	0
57	MG	BA	3172	1/1	0.93	0.08	46,46,46,46	0
57	MG	CA	3048	1/1	0.93	0.15	67,67,67,67	0
57	MG	DA	3658	1/1	0.93	0.19	62,62,62,62	0
57	MG	DA	3078	1/1	0.93	0.14	57,57,57,57	0
57	MG	AX	3004	1/1	0.93	0.16	64,64,64,64	0
57	MG	BA	3065	1/1	0.93	0.16	60,60,60,60	0
57	MG	DA	3082	1/1	0.93	0.10	47,47,47,47	0
57	MG	DA	3083	1/1	0.93	0.07	40,40,40,40	0
57	MG	AX	3007	1/1	0.93	0.10	67,67,67,67	0
57	MG	CA	3054	1/1	0.93	0.31	69,69,69,69	0
57	MG	AA	3131	1/1	0.93	0.16	71,71,71,71	0
57	MG	AA	3061	1/1	0.93	0.30	55,55,55,55	0
57	MG	DA	3098	1/1	0.93	0.10	53,53,53,53	0
57	MG	BA	3325	1/1	0.93	0.09	48,48,48,48	0
57	MG	DA	3416	1/1	0.93	0.08	50,50,50,50	0
57	MG	BA	3200	1/1	0.93	0.31	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	BA	3456	1/1	0.93	0.13	49,49,49,49	0
57	MG	BA	3337	1/1	0.93	0.11	58,58,58,58	0
57	MG	DB	3007	1/1	0.93	0.19	58,58,58,58	0
57	MG	BA	3751	1/1	0.93	0.09	26,26,26,26	0
57	MG	BA	3753	1/1	0.93	0.09	33,33,33,33	0
57	MG	DA	3424	1/1	0.93	0.08	61,61,61,61	0
57	MG	AX	3010	1/1	0.93	0.16	59,59,59,59	0
57	MG	BA	3461	1/1	0.93	0.14	62,62,62,62	0
57	MG	DA	3124	1/1	0.93	0.12	57,57,57,57	0
57	MG	BA	3462	1/1	0.93	0.12	36,36,36,36	0
57	MG	DA	3126	1/1	0.93	0.11	55,55,55,55	0
57	MG	DQ	3002	1/1	0.93	0.11	51,51,51,51	0
57	MG	DA	3130	1/1	0.93	0.17	52,52,52,52	0
57	MG	BA	3343	1/1	0.93	0.10	53,53,53,53	0
57	MG	AA	3102	1/1	0.93	0.28	59,59,59,59	0
57	MG	BA	3349	1/1	0.93	0.11	56,56,56,56	0
57	MG	DW	3004	1/1	0.93	0.09	52,52,52,52	0
57	MG	DY	502	1/1	0.93	0.07	50,50,50,50	0
57	MG	AA	3021	1/1	0.93	0.20	63,63,63,63	0
57	MG	DA	3439	1/1	0.93	0.11	42,42,42,42	0
57	MG	CA	3075	1/1	0.93	0.18	59,59,59,59	0
57	MG	DA	3443	1/1	0.93	0.12	54,54,54,54	0
57	MG	BA	3766	1/1	0.93	0.09	28,28,28,28	0
57	MG	DA	3096	1/1	0.94	0.20	42,42,42,42	0
57	MG	BA	3317	1/1	0.94	0.07	53,53,53,53	0
57	MG	AX	3015	1/1	0.94	0.11	42,42,42,42	0
57	MG	DA	3106	1/1	0.94	0.12	52,52,52,52	0
57	MG	DA	3108	1/1	0.94	0.12	52,52,52,52	0
57	MG	DA	3423	1/1	0.94	0.12	49,49,49,49	0
57	MG	CA	3053	1/1	0.94	0.07	41,41,41,41	0
57	MG	BA	3448	1/1	0.94	0.11	32,32,32,32	0
57	MG	BA	3182	1/1	0.94	0.09	55,55,55,55	0
57	MG	BA	3320	1/1	0.94	0.10	48,48,48,48	0
57	MG	BA	3321	1/1	0.94	0.18	55,55,55,55	0
57	MG	BA	3457	1/1	0.94	0.12	32,32,32,32	0
57	MG	DA	3122	1/1	0.94	0.09	49,49,49,49	0
57	MG	BA	3183	1/1	0.94	0.07	42,42,42,42	0
57	MG	BA	3603	1/1	0.94	0.08	53,53,53,53	0
57	MG	DA	3435	1/1	0.94	0.17	50,50,50,50	0
57	MG	AA	3024	1/1	0.94	0.09	54,54,54,54	0
57	MG	BA	3607	1/1	0.94	0.09	38,38,38,38	0
57	MG	DA	3128	1/1	0.94	0.20	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	3025	1/1	0.94	0.10	62,62,62,62	0
57	MG	AA	3018	1/1	0.94	0.23	56,56,56,56	0
57	MG	BA	3080	1/1	0.94	0.23	60,60,60,60	0
57	MG	DA	3136	1/1	0.94	0.09	52,52,52,52	0
57	MG	DA	3138	1/1	0.94	0.17	55,55,55,55	0
57	MG	BA	3765	1/1	0.94	0.11	48,48,48,48	0
57	MG	AA	3079	1/1	0.94	0.17	68,68,68,68	0
57	MG	BA	3207	1/1	0.94	0.23	54,54,54,54	0
57	MG	CA	3073	1/1	0.94	0.17	57,57,57,57	0
57	MG	DA	3148	1/1	0.94	0.14	54,54,54,54	0
57	MG	BA	3768	1/1	0.94	0.10	47,47,47,47	0
57	MG	DA	3151	1/1	0.94	0.14	55,55,55,55	0
57	MG	DA	3153	1/1	0.94	0.18	47,47,47,47	0
57	MG	BA	3621	1/1	0.94	0.10	53,53,53,53	0
57	MG	DA	3157	1/1	0.94	0.10	47,47,47,47	0
57	MG	CA	3076	1/1	0.94	0.11	57,57,57,57	0
57	MG	BA	3770	1/1	0.94	0.10	45,45,45,45	0
57	MG	DA	3472	1/1	0.94	0.09	44,44,44,44	0
57	MG	BA	3347	1/1	0.94	0.10	44,44,44,44	0
57	MG	CA	3079	1/1	0.94	0.15	66,66,66,66	0
57	MG	DA	3164	1/1	0.94	0.12	51,51,51,51	0
57	MG	BA	3776	1/1	0.94	0.14	43,43,43,43	0
57	MG	DA	3169	1/1	0.94	0.12	47,47,47,47	0
57	MG	DA	3170	1/1	0.94	0.09	53,53,53,53	0
57	MG	BA	3778	1/1	0.94	0.08	48,48,48,48	0
57	MG	BA	3469	1/1	0.94	0.12	49,49,49,49	0
57	MG	DA	3486	1/1	0.94	0.08	47,47,47,47	0
57	MG	BA	3348	1/1	0.94	0.10	36,36,36,36	0
57	MG	AA	3213	1/1	0.94	0.18	54,54,54,54	0
57	MG	AA	3188	1/1	0.94	0.15	69,69,69,69	0
57	MG	BA	3475	1/1	0.94	0.12	42,42,42,42	0
57	MG	DA	3192	1/1	0.94	0.12	60,60,60,60	0
57	MG	DA	3494	1/1	0.94	0.10	47,47,47,47	0
57	MG	CA	3095	1/1	0.94	0.23	64,64,64,64	0
57	MG	DA	3496	1/1	0.94	0.07	53,53,53,53	0
57	MG	BA	3787	1/1	0.94	0.20	45,45,45,45	0
57	MG	DA	3198	1/1	0.94	0.14	40,40,40,40	0
57	MG	DA	3200	1/1	0.94	0.11	66,66,66,66	0
57	MG	BA	3477	1/1	0.94	0.18	61,61,61,61	0
57	MG	DA	3203	1/1	0.94	0.20	50,50,50,50	0
57	MG	AA	3062	1/1	0.94	0.27	51,51,51,51	0
57	MG	BA	3093	1/1	0.94	0.22	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	CA	3106	1/1	0.94	0.07	56,56,56,56	0
57	MG	AF	3001	1/1	0.94	0.17	44,44,44,44	0
57	MG	DA	3209	1/1	0.94	0.20	53,53,53,53	0
57	MG	DA	3210	1/1	0.94	0.14	53,53,53,53	0
57	MG	DA	3211	1/1	0.94	0.07	48,48,48,48	0
57	MG	BA	3635	1/1	0.94	0.13	58,58,58,58	0
57	MG	BA	3101	1/1	0.94	0.12	53,53,53,53	0
57	MG	DA	3214	1/1	0.94	0.28	59,59,59,59	0
57	MG	BA	3007	1/1	0.94	0.16	55,55,55,55	0
57	MG	CA	3111	1/1	0.94	0.08	64,64,64,64	0
57	MG	BA	3801	1/1	0.94	0.18	50,50,50,50	0
57	MG	BA	3106	1/1	0.94	0.10	42,42,42,42	0
57	MG	BA	3803	1/1	0.94	0.14	44,44,44,44	0
57	MG	AM	201	1/1	0.94	0.07	51,51,51,51	0
57	MG	BA	3493	1/1	0.94	0.16	58,58,58,58	0
57	MG	BA	3494	1/1	0.94	0.09	49,49,49,49	0
57	MG	DA	3228	1/1	0.94	0.22	38,38,38,38	0
57	MG	CA	3119	1/1	0.94	0.08	64,64,64,64	0
57	MG	BA	3237	1/1	0.94	0.07	45,45,45,45	0
57	MG	BA	3644	1/1	0.94	0.07	35,35,35,35	0
57	MG	CA	3122	1/1	0.94	0.21	64,64,64,64	0
57	MG	BB	205	1/1	0.94	0.22	60,60,60,60	0
57	MG	BA	3017	1/1	0.94	0.19	48,48,48,48	0
57	MG	DA	3548	1/1	0.94	0.07	60,60,60,60	0
57	MG	DA	3549	1/1	0.94	0.13	57,57,57,57	0
57	MG	BA	3239	1/1	0.94	0.12	48,48,48,48	0
57	MG	BA	3649	1/1	0.94	0.09	40,40,40,40	0
57	MG	BB	210	1/1	0.94	0.07	61,61,61,61	0
57	MG	DA	3245	1/1	0.94	0.12	54,54,54,54	0
57	MG	CA	3129	1/1	0.94	0.09	43,43,43,43	0
57	MG	CA	3132	1/1	0.94	0.15	66,66,66,66	0
57	MG	BA	3502	1/1	0.94	0.09	56,56,56,56	0
57	MG	DA	3561	1/1	0.94	0.09	57,57,57,57	0
57	MG	DA	3250	1/1	0.94	0.13	69,69,69,69	0
57	MG	CA	3134	1/1	0.94	0.17	69,69,69,69	0
57	MG	DA	3565	1/1	0.94	0.09	59,59,59,59	0
57	MG	BB	214	1/1	0.94	0.08	49,49,49,49	0
57	MG	AA	3135	1/1	0.94	0.24	65,65,65,65	0
57	MG	BA	3116	1/1	0.94	0.18	50,50,50,50	0
57	MG	CA	3139	1/1	0.94	0.24	62,62,62,62	0
57	MG	BA	3505	1/1	0.94	0.09	55,55,55,55	0
57	MG	AA	3084	1/1	0.94	0.26	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	CA	3143	1/1	0.94	0.10	64,64,64,64	0
57	MG	BA	3118	1/1	0.94	0.12	48,48,48,48	0
57	MG	DA	3265	1/1	0.94	0.10	30,30,30,30	0
57	MG	DA	3582	1/1	0.94	0.07	56,56,56,56	0
57	MG	BD	304	1/1	0.94	0.12	32,32,32,32	0
57	MG	CA	3147	1/1	0.94	0.20	64,64,64,64	0
57	MG	DA	3585	1/1	0.94	0.08	43,43,43,43	0
57	MG	CA	3148	1/1	0.94	0.16	70,70,70,70	0
57	MG	DA	3272	1/1	0.94	0.08	41,41,41,41	0
57	MG	BA	3659	1/1	0.94	0.13	61,61,61,61	0
57	MG	BE	303	1/1	0.94	0.14	51,51,51,51	0
57	MG	AA	3137	1/1	0.94	0.10	51,51,51,51	0
57	MG	BE	307	1/1	0.94	0.10	62,62,62,62	0
57	MG	AA	3005	1/1	0.94	0.18	62,62,62,62	0
57	MG	DA	3284	1/1	0.94	0.07	47,47,47,47	0
57	MG	BF	304	1/1	0.94	0.11	45,45,45,45	0
57	MG	BA	3665	1/1	0.94	0.14	49,49,49,49	0
57	MG	BA	3122	1/1	0.94	0.07	41,41,41,41	0
57	MG	BA	3024	1/1	0.94	0.18	49,49,49,49	0
57	MG	BA	3516	1/1	0.94	0.15	52,52,52,52	0
57	MG	AA	3009	1/1	0.94	0.11	57,57,57,57	0
57	MG	BN	3006	1/1	0.94	0.12	49,49,49,49	0
57	MG	AX	3003	1/1	0.94	0.10	71,71,71,71	0
57	MG	BQ	3004	1/1	0.94	0.14	42,42,42,42	0
57	MG	BA	3393	1/1	0.94	0.13	51,51,51,51	0
57	MG	BR	201	1/1	0.94	0.22	57,57,57,57	0
57	MG	BA	3268	1/1	0.94	0.10	55,55,55,55	0
57	MG	BA	3674	1/1	0.94	0.17	63,63,63,63	0
57	MG	BA	3269	1/1	0.94	0.10	53,53,53,53	0
57	MG	DA	3307	1/1	0.94	0.08	42,42,42,42	0
57	MG	BZ	3001	1/1	0.94	0.11	55,55,55,55	0
57	MG	B0	102	1/1	0.94	0.15	48,48,48,48	0
57	MG	BA	3035	1/1	0.94	0.12	39,39,39,39	0
57	MG	BA	3531	1/1	0.94	0.10	26,26,26,26	0
57	MG	BA	3273	1/1	0.94	0.14	54,54,54,54	0
57	MG	BA	3039	1/1	0.94	0.08	32,32,32,32	0
57	MG	BA	3047	1/1	0.94	0.19	60,60,60,60	0
57	MG	DA	3005	1/1	0.94	0.28	57,57,57,57	0
57	MG	DA	3006	1/1	0.94	0.07	38,38,38,38	0
57	MG	BA	3403	1/1	0.94	0.08	54,54,54,54	0
57	MG	BA	3134	1/1	0.94	0.18	48,48,48,48	0
57	MG	DA	3328	1/1	0.94	0.09	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	BA	3138	1/1	0.94	0.18	42,42,42,42	0
57	MG	BA	3139	1/1	0.94	0.26	40,40,40,40	0
57	MG	DA	3332	1/1	0.94	0.10	53,53,53,53	0
57	MG	BA	3289	1/1	0.94	0.14	56,56,56,56	0
57	MG	DA	3018	1/1	0.94	0.13	62,62,62,62	0
57	MG	BA	3290	1/1	0.94	0.21	40,40,40,40	0
57	MG	AA	3066	1/1	0.94	0.29	60,60,60,60	0
57	MG	BA	3551	1/1	0.94	0.11	36,36,36,36	0
57	MG	DA	3645	1/1	0.94	0.07	45,45,45,45	0
57	MG	DA	3030	1/1	0.94	0.06	39,39,39,39	0
57	MG	BA	3704	1/1	0.94	0.09	77,77,77,77	0
57	MG	DA	3650	1/1	0.94	0.09	67,67,67,67	0
57	MG	AX	3006	1/1	0.94	0.08	65,65,65,65	0
57	MG	BA	3296	1/1	0.94	0.18	53,53,53,53	0
57	MG	AA	3022	1/1	0.94	0.17	71,71,71,71	0
57	MG	CA	3013	1/1	0.94	0.20	69,69,69,69	0
57	MG	BA	3058	1/1	0.94	0.09	49,49,49,49	0
57	MG	BA	3156	1/1	0.94	0.24	41,41,41,41	0
57	MG	BA	3564	1/1	0.94	0.10	44,44,44,44	0
57	MG	DA	3359	1/1	0.94	0.11	47,47,47,47	0
57	MG	AA	3007	1/1	0.94	0.10	57,57,57,57	0
57	MG	DA	3660	1/1	0.94	0.20	61,61,61,61	0
57	MG	DA	3361	1/1	0.94	0.08	44,44,44,44	0
57	MG	CA	3019	1/1	0.94	0.17	65,65,65,65	0
57	MG	CA	3020	1/1	0.94	0.17	56,56,56,56	0
57	MG	AA	3112	1/1	0.94	0.22	63,63,63,63	0
57	MG	BA	3161	1/1	0.94	0.10	52,52,52,52	0
57	MG	BA	3162	1/1	0.94	0.08	38,38,38,38	0
57	MG	CA	3025	1/1	0.94	0.15	51,51,51,51	0
57	MG	DA	3372	1/1	0.94	0.12	56,56,56,56	0
57	MG	DA	3675	1/1	0.94	0.08	52,52,52,52	0
57	MG	BA	3573	1/1	0.94	0.11	51,51,51,51	0
57	MG	DA	3068	1/1	0.94	0.14	58,58,58,58	0
57	MG	DA	3378	1/1	0.94	0.21	57,57,57,57	0
57	MG	DA	3379	1/1	0.94	0.14	63,63,63,63	0
57	MG	BA	3307	1/1	0.94	0.09	29,29,29,29	0
57	MG	BA	3308	1/1	0.94	0.10	43,43,43,43	0
57	MG	BA	3579	1/1	0.94	0.10	49,49,49,49	0
57	MG	DA	3072	1/1	0.94	0.12	47,47,47,47	0
57	MG	BA	3163	1/1	0.94	0.06	55,55,55,55	0
57	MG	DA	3391	1/1	0.94	0.11	45,45,45,45	0
57	MG	BA	3729	1/1	0.94	0.10	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	DA	3396	1/1	0.94	0.07	40,40,40,40	0
57	MG	DD	307	1/1	0.94	0.26	43,43,43,43	0
57	MG	BA	3581	1/1	0.94	0.09	30,30,30,30	0
57	MG	BA	3582	1/1	0.94	0.17	74,74,74,74	0
57	MG	DF	3002	1/1	0.94	0.09	48,48,48,48	0
57	MG	DN	5001	1/1	0.94	0.10	66,66,66,66	0
57	MG	AA	3056	1/1	0.94	0.15	61,61,61,61	0
57	MG	AA	3201	1/1	0.94	0.09	52,52,52,52	0
57	MG	DQ	3003	1/1	0.94	0.09	51,51,51,51	0
57	MG	BA	3585	1/1	0.94	0.07	46,46,46,46	0
57	MG	AA	3045	1/1	0.94	0.12	58,58,58,58	0
57	MG	DU	3001	1/1	0.94	0.13	55,55,55,55	0
57	MG	DU	3002	1/1	0.94	0.13	55,55,55,55	0
57	MG	BA	3442	1/1	0.94	0.10	44,44,44,44	0
57	MG	DW	3001	1/1	0.94	0.17	54,54,54,54	0
57	MG	DA	3085	1/1	0.94	0.08	53,53,53,53	0
57	MG	CA	3047	1/1	0.94	0.13	53,53,53,53	0
57	MG	DA	3088	1/1	0.94	0.12	47,47,47,47	0
57	MG	BA	3071	1/1	0.94	0.23	59,59,59,59	0
57	MG	DA	3091	1/1	0.94	0.10	48,48,48,48	0
57	MG	DA	3092	1/1	0.94	0.08	45,45,45,45	0
57	MG	AA	3096	1/1	0.94	0.34	63,63,63,63	0
57	MG	CA	3050	1/1	0.94	0.32	61,61,61,61	0
57	MG	DA	3173	1/1	0.95	0.08	53,53,53,53	0
57	MG	DA	3175	1/1	0.95	0.07	41,41,41,41	0
57	MG	BA	3369	1/1	0.95	0.07	44,44,44,44	0
57	MG	BA	3370	1/1	0.95	0.10	39,39,39,39	0
57	MG	BA	3657	1/1	0.95	0.18	47,47,47,47	0
57	MG	BA	3509	1/1	0.95	0.09	31,31,31,31	0
57	MG	AX	3005	1/1	0.95	0.05	47,47,47,47	0
57	MG	BA	3041	1/1	0.95	0.14	40,40,40,40	0
57	MG	DA	3189	1/1	0.95	0.17	41,41,41,41	0
57	MG	BA	3513	1/1	0.95	0.09	59,59,59,59	0
57	MG	BA	3664	1/1	0.95	0.17	55,55,55,55	0
57	MG	DA	3196	1/1	0.95	0.21	49,49,49,49	0
57	MG	CA	3130	1/1	0.95	0.12	57,57,57,57	0
57	MG	BA	3242	1/1	0.95	0.12	55,55,55,55	0
57	MG	BA	3666	1/1	0.95	0.14	50,50,50,50	0
57	MG	DA	3466	1/1	0.95	0.14	41,41,41,41	0
57	MG	DA	3201	1/1	0.95	0.13	61,61,61,61	0
57	MG	AA	3011	1/1	0.95	0.26	57,57,57,57	0
57	MG	AA	3039	1/1	0.95	0.12	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	BA	3382	1/1	0.95	0.09	63,63,63,63	0
57	MG	BA	3518	1/1	0.95	0.09	44,44,44,44	0
57	MG	BA	3383	1/1	0.95	0.09	53,53,53,53	0
57	MG	AA	3163	1/1	0.95	0.16	56,56,56,56	0
57	MG	BA	3251	1/1	0.95	0.07	44,44,44,44	0
57	MG	BG	203	1/1	0.95	0.06	42,42,42,42	0
57	MG	DA	3479	1/1	0.95	0.10	43,43,43,43	0
57	MG	BA	3252	1/1	0.95	0.19	60,60,60,60	0
57	MG	CA	3145	1/1	0.95	0.09	66,66,66,66	0
57	MG	BN	3005	1/1	0.95	0.04	36,36,36,36	0
57	MG	BA	3675	1/1	0.95	0.08	67,67,67,67	0
57	MG	BA	3676	1/1	0.95	0.11	33,33,33,33	0
57	MG	BA	3529	1/1	0.95	0.12	56,56,56,56	0
57	MG	DA	3488	1/1	0.95	0.07	41,41,41,41	0
57	MG	DA	3217	1/1	0.95	0.07	38,38,38,38	0
57	MG	BA	3055	1/1	0.95	0.13	45,45,45,45	0
57	MG	AA	3132	1/1	0.95	0.08	55,55,55,55	0
57	MG	DA	3220	1/1	0.95	0.17	46,46,46,46	0
57	MG	BU	204	1/1	0.95	0.17	35,35,35,35	0
57	MG	CA	3154	1/1	0.95	0.16	56,56,56,56	0
57	MG	BA	3130	1/1	0.95	0.07	44,44,44,44	0
57	MG	DA	3224	1/1	0.95	0.17	49,49,49,49	0
57	MG	AA	3087	1/1	0.95	0.07	41,41,41,41	0
57	MG	AA	3029	1/1	0.95	0.25	53,53,53,53	0
57	MG	BA	3062	1/1	0.95	0.16	42,42,42,42	0
57	MG	BA	3266	1/1	0.95	0.14	39,39,39,39	0
57	MG	AA	3034	1/1	0.95	0.07	47,47,47,47	0
57	MG	DA	3233	1/1	0.95	0.09	53,53,53,53	0
57	MG	DA	3508	1/1	0.95	0.09	44,44,44,44	0
57	MG	DA	3510	1/1	0.95	0.18	49,49,49,49	0
57	MG	DA	3511	1/1	0.95	0.07	49,49,49,49	0
57	MG	CA	3162	1/1	0.95	0.09	66,66,66,66	0
57	MG	DA	3514	1/1	0.95	0.10	42,42,42,42	0
57	MG	AA	3071	1/1	0.95	0.08	53,53,53,53	0
57	MG	DA	3238	1/1	0.95	0.28	44,44,44,44	0
57	MG	CA	3164	1/1	0.95	0.14	60,60,60,60	0
57	MG	CA	3165	1/1	0.95	0.07	45,45,45,45	0
57	MG	AA	3035	1/1	0.95	0.23	56,56,56,56	0
57	MG	BA	3546	1/1	0.95	0.12	40,40,40,40	0
57	MG	BA	3697	1/1	0.95	0.11	61,61,61,61	0
57	MG	DA	3246	1/1	0.95	0.06	43,43,43,43	0
57	MG	BA	3147	1/1	0.95	0.09	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	3528	1/1	0.95	0.10	62,62,62,62	0
57	MG	DA	3529	1/1	0.95	0.06	38,38,38,38	0
57	MG	BA	3701	1/1	0.95	0.14	43,43,43,43	0
57	MG	BA	3549	1/1	0.95	0.19	39,39,39,39	0
57	MG	BA	3272	1/1	0.95	0.36	48,48,48,48	0
57	MG	CK	3001	1/1	0.95	0.08	45,45,45,45	0
57	MG	DA	3252	1/1	0.95	0.06	37,37,37,37	0
57	MG	B9	502	1/1	0.95	0.08	48,48,48,48	0
57	MG	CA	3001	1/1	0.95	0.14	75,75,75,75	0
57	MG	BA	3149	1/1	0.95	0.09	40,40,40,40	0
57	MG	BA	3708	1/1	0.95	0.08	50,50,50,50	0
57	MG	BA	3274	1/1	0.95	0.11	49,49,49,49	0
57	MG	CA	3007	1/1	0.95	0.09	57,57,57,57	0
57	MG	DA	3545	1/1	0.95	0.06	35,35,35,35	0
57	MG	BA	3151	1/1	0.95	0.10	52,52,52,52	0
57	MG	BA	3068	1/1	0.95	0.15	43,43,43,43	0
57	MG	AA	3073	1/1	0.95	0.10	56,56,56,56	0
57	MG	BA	3412	1/1	0.95	0.14	40,40,40,40	0
57	MG	BA	3716	1/1	0.95	0.09	65,65,65,65	0
57	MG	DA	3551	1/1	0.95	0.09	55,55,55,55	0
57	MG	DA	3269	1/1	0.95	0.10	49,49,49,49	0
57	MG	BA	3282	1/1	0.95	0.09	39,39,39,39	0
57	MG	AA	3141	1/1	0.95	0.18	61,61,61,61	0
57	MG	DA	3555	1/1	0.95	0.08	53,53,53,53	0
57	MG	CA	3015	1/1	0.95	0.17	56,56,56,56	0
57	MG	BA	3567	1/1	0.95	0.11	34,34,34,34	0
57	MG	AA	3208	1/1	0.95	0.19	60,60,60,60	0
57	MG	DA	3559	1/1	0.95	0.10	43,43,43,43	0
57	MG	DA	3277	1/1	0.95	0.09	55,55,55,55	0
57	MG	DA	3562	1/1	0.95	0.12	64,64,64,64	0
57	MG	AA	3143	1/1	0.95	0.08	60,60,60,60	0
57	MG	DA	3281	1/1	0.95	0.10	53,53,53,53	0
57	MG	DA	3021	1/1	0.95	0.06	31,31,31,31	0
57	MG	DA	3022	1/1	0.95	0.13	51,51,51,51	0
57	MG	AA	3030	1/1	0.95	0.07	60,60,60,60	0
57	MG	BA	3292	1/1	0.95	0.09	48,48,48,48	0
57	MG	DA	3570	1/1	0.95	0.10	31,31,31,31	0
57	MG	DA	3026	1/1	0.95	0.19	59,59,59,59	0
57	MG	AA	3211	1/1	0.95	0.09	47,47,47,47	0
57	MG	AA	3077	1/1	0.95	0.25	56,56,56,56	0
57	MG	DA	3292	1/1	0.95	0.10	30,30,30,30	0
57	MG	DA	3033	1/1	0.95	0.08	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3294	1/1	0.95	0.12	43,43,43,43	0
57	MG	DA	3579	1/1	0.95	0.08	48,48,48,48	0
57	MG	BA	3164	1/1	0.95	0.09	48,48,48,48	0
57	MG	AA	3181	1/1	0.95	0.16	51,51,51,51	0
57	MG	DA	3297	1/1	0.95	0.05	39,39,39,39	0
57	MG	BA	3428	1/1	0.95	0.06	46,46,46,46	0
57	MG	BA	3081	1/1	0.95	0.15	46,46,46,46	0
57	MG	DA	3587	1/1	0.95	0.09	56,56,56,56	0
57	MG	BA	3430	1/1	0.95	0.07	37,37,37,37	0
57	MG	DA	3047	1/1	0.95	0.19	49,49,49,49	0
57	MG	BA	3169	1/1	0.95	0.11	45,45,45,45	0
57	MG	DA	3303	1/1	0.95	0.07	48,48,48,48	0
57	MG	DA	3049	1/1	0.95	0.19	52,52,52,52	0
57	MG	BA	3170	1/1	0.95	0.10	38,38,38,38	0
57	MG	DA	3595	1/1	0.95	0.08	59,59,59,59	0
57	MG	CA	3032	1/1	0.95	0.29	62,62,62,62	0
57	MG	DA	3600	1/1	0.95	0.12	70,70,70,70	0
57	MG	BA	3006	1/1	0.95	0.10	48,48,48,48	0
57	MG	DA	3310	1/1	0.95	0.10	38,38,38,38	0
57	MG	BA	3173	1/1	0.95	0.10	48,48,48,48	0
57	MG	DA	3606	1/1	0.95	0.14	71,71,71,71	0
57	MG	DA	3059	1/1	0.95	0.08	43,43,43,43	0
57	MG	CA	3035	1/1	0.95	0.10	59,59,59,59	0
57	MG	BA	3439	1/1	0.95	0.06	33,33,33,33	0
57	MG	BA	3743	1/1	0.95	0.09	44,44,44,44	0
57	MG	DA	3063	1/1	0.95	0.08	54,54,54,54	0
57	MG	BA	3305	1/1	0.95	0.10	62,62,62,62	0
57	MG	BA	3746	1/1	0.95	0.12	51,51,51,51	0
57	MG	DA	3326	1/1	0.95	0.09	43,43,43,43	0
57	MG	BA	3175	1/1	0.95	0.08	20,20,20,20	0
57	MG	CA	3042	1/1	0.95	0.20	59,59,59,59	0
57	MG	AA	3113	1/1	0.95	0.09	58,58,58,58	0
57	MG	DA	3619	1/1	0.95	0.08	69,69,69,69	0
57	MG	BA	3089	1/1	0.95	0.05	19,19,19,19	0
57	MG	BA	3595	1/1	0.95	0.07	51,51,51,51	0
57	MG	DA	3622	1/1	0.95	0.08	61,61,61,61	0
57	MG	AA	3149	1/1	0.95	0.07	46,46,46,46	0
57	MG	BA	3016	1/1	0.95	0.08	38,38,38,38	0
57	MG	BA	3450	1/1	0.95	0.07	48,48,48,48	0
57	MG	AA	3055	1/1	0.95	0.11	57,57,57,57	0
57	MG	AN	502	1/1	0.95	0.34	63,63,63,63	0
57	MG	BA	3098	1/1	0.95	0.13	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	DA	3341	1/1	0.95	0.09	51,51,51,51	0
57	MG	DA	3080	1/1	0.95	0.16	55,55,55,55	0
57	MG	DA	3346	1/1	0.95	0.06	48,48,48,48	0
57	MG	BA	3191	1/1	0.95	0.11	43,43,43,43	0
57	MG	BA	3606	1/1	0.95	0.11	61,61,61,61	0
57	MG	BA	3763	1/1	0.95	0.09	24,24,24,24	0
57	MG	DA	3353	1/1	0.95	0.14	42,42,42,42	0
57	MG	BA	3193	1/1	0.95	0.15	48,48,48,48	0
57	MG	BA	3196	1/1	0.95	0.12	38,38,38,38	0
57	MG	DA	3640	1/1	0.95	0.11	43,43,43,43	0
57	MG	BA	3610	1/1	0.95	0.12	61,61,61,61	0
57	MG	BA	3100	1/1	0.95	0.11	39,39,39,39	0
57	MG	BA	3614	1/1	0.95	0.13	63,63,63,63	0
57	MG	BA	3201	1/1	0.95	0.30	62,62,62,62	0
57	MG	BA	3019	1/1	0.95	0.12	42,42,42,42	0
57	MG	BA	3618	1/1	0.95	0.11	65,65,65,65	0
57	MG	CA	3068	1/1	0.95	0.19	48,48,48,48	0
57	MG	BA	3773	1/1	0.95	0.12	52,52,52,52	0
57	MG	DA	3100	1/1	0.95	0.13	43,43,43,43	0
57	MG	BA	3775	1/1	0.95	0.14	33,33,33,33	0
57	MG	DA	3370	1/1	0.95	0.11	51,51,51,51	0
57	MG	BA	3203	1/1	0.95	0.14	40,40,40,40	0
57	MG	CA	3072	1/1	0.95	0.14	54,54,54,54	0
57	MG	BA	3204	1/1	0.95	0.08	36,36,36,36	0
57	MG	BA	3326	1/1	0.95	0.10	20,20,20,20	0
57	MG	BA	3329	1/1	0.95	0.12	60,60,60,60	0
57	MG	AA	3019	1/1	0.95	0.10	66,66,66,66	0
57	MG	DA	3116	1/1	0.95	0.25	52,52,52,52	0
57	MG	BA	3206	1/1	0.95	0.20	49,49,49,49	0
57	MG	BA	3627	1/1	0.95	0.12	56,56,56,56	0
57	MG	DA	3119	1/1	0.95	0.08	39,39,39,39	0
57	MG	DA	3385	1/1	0.95	0.10	52,52,52,52	0
57	MG	DA	3120	1/1	0.95	0.13	49,49,49,49	0
57	MG	AA	3098	1/1	0.95	0.16	55,55,55,55	0
57	MG	DA	3392	1/1	0.95	0.12	70,70,70,70	0
57	MG	CA	3081	1/1	0.95	0.05	46,46,46,46	0
57	MG	DA	3395	1/1	0.95	0.07	47,47,47,47	0
57	MG	BA	3208	1/1	0.95	0.07	44,44,44,44	0
57	MG	BA	3789	1/1	0.95	0.07	12,12,12,12	0
57	MG	BA	3790	1/1	0.95	0.11	34,34,34,34	0
57	MG	BA	3792	1/1	0.95	0.14	54,54,54,54	0
57	MG	DA	3129	1/1	0.95	0.09	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3209	1/1	0.95	0.14	54,54,54,54	0
57	MG	DA	3131	1/1	0.95	0.18	46,46,46,46	0
57	MG	BA	3345	1/1	0.95	0.08	38,38,38,38	0
57	MG	DB	3009	1/1	0.95	0.19	59,59,59,59	0
57	MG	BA	3480	1/1	0.95	0.09	35,35,35,35	0
57	MG	DA	3134	1/1	0.95	0.08	41,41,41,41	0
57	MG	CA	3093	1/1	0.95	0.08	55,55,55,55	0
57	MG	DD	301	1/1	0.95	0.10	47,47,47,47	0
57	MG	DA	3137	1/1	0.95	0.16	54,54,54,54	0
57	MG	DD	304	1/1	0.95	0.14	52,52,52,52	0
57	MG	DD	306	1/1	0.95	0.15	39,39,39,39	0
57	MG	BA	3211	1/1	0.95	0.17	55,55,55,55	0
57	MG	DD	309	1/1	0.95	0.11	59,59,59,59	0
57	MG	BA	3107	1/1	0.95	0.10	53,53,53,53	0
57	MG	DE	304	1/1	0.95	0.12	43,43,43,43	0
57	MG	BA	3485	1/1	0.95	0.09	42,42,42,42	0
57	MG	AA	3099	1/1	0.95	0.24	51,51,51,51	0
57	MG	DA	3145	1/1	0.95	0.12	43,43,43,43	0
57	MG	BA	3215	1/1	0.95	0.21	36,36,36,36	0
57	MG	AA	3120	1/1	0.95	0.09	45,45,45,45	0
57	MG	BA	3805	1/1	0.95	0.06	44,44,44,44	0
57	MG	BA	3354	1/1	0.95	0.09	48,48,48,48	0
57	MG	DA	3152	1/1	0.95	0.12	51,51,51,51	0
57	MG	BA	3027	1/1	0.95	0.06	26,26,26,26	0
57	MG	BA	3115	1/1	0.95	0.14	59,59,59,59	0
57	MG	BA	3227	1/1	0.95	0.25	57,57,57,57	0
57	MG	BA	3645	1/1	0.95	0.05	33,33,33,33	0
57	MG	DA	3428	1/1	0.95	0.14	37,37,37,37	0
57	MG	BB	204	1/1	0.95	0.09	41,41,41,41	0
57	MG	BA	3030	1/1	0.95	0.13	46,46,46,46	0
57	MG	AA	3080	1/1	0.95	0.18	58,58,58,58	0
57	MG	AA	3122	1/1	0.95	0.08	56,56,56,56	0
57	MG	BA	3119	1/1	0.95	0.11	45,45,45,45	0
57	MG	AA	3123	1/1	0.95	0.12	51,51,51,51	0
57	MG	BA	3368	1/1	0.95	0.09	40,40,40,40	0
57	MG	DA	3464	1/1	0.96	0.06	46,46,46,46	0
57	MG	BA	3050	1/1	0.96	0.06	38,38,38,38	0
57	MG	BA	3762	1/1	0.96	0.10	46,46,46,46	0
57	MG	BA	3233	1/1	0.96	0.25	56,56,56,56	0
57	MG	DA	3004	1/1	0.96	0.15	40,40,40,40	0
57	MG	BA	3236	1/1	0.96	0.11	49,49,49,49	0
57	MG	DA	3226	1/1	0.96	0.26	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	BA	3051	1/1	0.96	0.08	43,43,43,43	0
57	MG	BA	3528	1/1	0.96	0.15	56,56,56,56	0
57	MG	DA	3008	1/1	0.96	0.06	36,36,36,36	0
57	MG	AA	3130	1/1	0.96	0.09	56,56,56,56	0
57	MG	DA	3232	1/1	0.96	0.10	62,62,62,62	0
57	MG	BA	3646	1/1	0.96	0.11	42,42,42,42	0
57	MG	DA	3013	1/1	0.96	0.04	40,40,40,40	0
57	MG	AA	3010	1/1	0.96	0.15	52,52,52,52	0
57	MG	DA	3483	1/1	0.96	0.15	55,55,55,55	0
57	MG	DA	3237	1/1	0.96	0.19	56,56,56,56	0
57	MG	BA	3240	1/1	0.96	0.18	47,47,47,47	0
57	MG	AA	3060	1/1	0.96	0.13	46,46,46,46	0
57	MG	DA	3240	1/1	0.96	0.09	48,48,48,48	0
57	MG	DA	3241	1/1	0.96	0.08	45,45,45,45	0
57	MG	BA	3772	1/1	0.96	0.15	33,33,33,33	0
57	MG	BA	3324	1/1	0.96	0.12	45,45,45,45	0
57	MG	BA	3774	1/1	0.96	0.06	46,46,46,46	0
57	MG	BA	3536	1/1	0.96	0.22	49,49,49,49	0
57	MG	BA	3108	1/1	0.96	0.16	44,44,44,44	0
57	MG	AA	3133	1/1	0.96	0.16	56,56,56,56	0
57	MG	DA	3027	1/1	0.96	0.16	51,51,51,51	0
57	MG	DA	3028	1/1	0.96	0.13	52,52,52,52	0
57	MG	DA	3029	1/1	0.96	0.14	49,49,49,49	0
57	MG	BA	3328	1/1	0.96	0.14	40,40,40,40	0
57	MG	DA	3031	1/1	0.96	0.25	43,43,43,43	0
57	MG	AA	3081	1/1	0.96	0.06	48,48,48,48	0
57	MG	BA	3330	1/1	0.96	0.11	37,37,37,37	0
57	MG	BA	3331	1/1	0.96	0.11	49,49,49,49	0
57	MG	DA	3507	1/1	0.96	0.09	43,43,43,43	0
57	MG	DA	3257	1/1	0.96	0.16	50,50,50,50	0
57	MG	DA	3509	1/1	0.96	0.08	59,59,59,59	0
57	MG	DA	3036	1/1	0.96	0.07	48,48,48,48	0
57	MG	CA	3044	1/1	0.96	0.23	62,62,62,62	0
57	MG	CA	3045	1/1	0.96	0.18	54,54,54,54	0
57	MG	DA	3043	1/1	0.96	0.14	38,38,38,38	0
57	MG	DA	3515	1/1	0.96	0.15	45,45,45,45	0
57	MG	BA	3332	1/1	0.96	0.11	38,38,38,38	0
57	MG	BA	3785	1/1	0.96	0.11	59,59,59,59	0
57	MG	BA	3786	1/1	0.96	0.06	35,35,35,35	0
57	MG	BA	3249	1/1	0.96	0.06	49,49,49,49	0
57	MG	BA	3336	1/1	0.96	0.10	64,64,64,64	0
57	MG	BA	3437	1/1	0.96	0.10	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	3250	1/1	0.96	0.38	42,42,42,42	0
57	MG	BA	3171	1/1	0.96	0.21	31,31,31,31	0
57	MG	DA	3526	1/1	0.96	0.06	48,48,48,48	0
57	MG	BA	3008	1/1	0.96	0.10	47,47,47,47	0
57	MG	DA	3275	1/1	0.96	0.08	42,42,42,42	0
57	MG	BA	3256	1/1	0.96	0.07	40,40,40,40	0
57	MG	BA	3556	1/1	0.96	0.12	36,36,36,36	0
57	MG	DA	3278	1/1	0.96	0.07	43,43,43,43	0
57	MG	BA	3557	1/1	0.96	0.09	33,33,33,33	0
57	MG	DA	3533	1/1	0.96	0.07	43,43,43,43	0
57	MG	DA	3280	1/1	0.96	0.09	33,33,33,33	0
57	MG	BA	3798	1/1	0.96	0.11	28,28,28,28	0
57	MG	DA	3282	1/1	0.96	0.06	52,52,52,52	0
57	MG	AA	3015	1/1	0.96	0.11	65,65,65,65	0
57	MG	DA	3064	1/1	0.96	0.06	49,49,49,49	0
57	MG	DA	3065	1/1	0.96	0.09	43,43,43,43	0
57	MG	BA	3346	1/1	0.96	0.05	27,27,27,27	0
57	MG	BA	3174	1/1	0.96	0.07	37,37,37,37	0
57	MG	BA	3063	1/1	0.96	0.25	59,59,59,59	0
57	MG	AA	3203	1/1	0.96	0.06	59,59,59,59	0
57	MG	BA	3804	1/1	0.96	0.32	53,53,53,53	0
57	MG	BA	3451	1/1	0.96	0.07	31,31,31,31	0
57	MG	BA	3350	1/1	0.96	0.10	28,28,28,28	0
57	MG	BA	3262	1/1	0.96	0.09	41,41,41,41	0
57	MG	BA	3352	1/1	0.96	0.15	53,53,53,53	0
57	MG	BA	3178	1/1	0.96	0.07	46,46,46,46	0
57	MG	AA	3075	1/1	0.96	0.09	49,49,49,49	0
57	MG	BA	3578	1/1	0.96	0.06	46,46,46,46	0
57	MG	AA	3085	1/1	0.96	0.13	48,48,48,48	0
57	MG	BA	3687	1/1	0.96	0.09	22,22,22,22	0
57	MG	BA	3690	1/1	0.96	0.22	58,58,58,58	0
57	MG	BA	3691	1/1	0.96	0.11	55,55,55,55	0
57	MG	AA	3053	1/1	0.96	0.15	61,61,61,61	0
57	MG	DA	3306	1/1	0.96	0.15	55,55,55,55	0
57	MG	AA	3207	1/1	0.96	0.11	65,65,65,65	0
57	MG	CA	3080	1/1	0.96	0.07	49,49,49,49	0
57	MG	AA	3063	1/1	0.96	0.04	35,35,35,35	0
57	MG	DA	3089	1/1	0.96	0.21	52,52,52,52	0
57	MG	BA	3464	1/1	0.96	0.07	45,45,45,45	0
57	MG	DA	3312	1/1	0.96	0.06	54,54,54,54	0
57	MG	BB	216	1/1	0.96	0.17	51,51,51,51	0
57	MG	CA	3084	1/1	0.96	0.12	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	AA	3140	1/1	0.96	0.09	53,53,53,53	0
57	MG	BA	3190	1/1	0.96	0.10	52,52,52,52	0
57	MG	AA	3043	1/1	0.96	0.14	51,51,51,51	0
57	MG	BA	3702	1/1	0.96	0.18	51,51,51,51	0
57	MG	DA	3576	1/1	0.96	0.06	53,53,53,53	0
57	MG	BD	303	1/1	0.96	0.11	39,39,39,39	0
57	MG	DA	3322	1/1	0.96	0.17	51,51,51,51	0
57	MG	DA	3323	1/1	0.96	0.06	50,50,50,50	0
57	MG	DA	3101	1/1	0.96	0.10	49,49,49,49	0
57	MG	CA	3091	1/1	0.96	0.11	55,55,55,55	0
57	MG	CA	3092	1/1	0.96	0.05	50,50,50,50	0
57	MG	DA	3107	1/1	0.96	0.10	51,51,51,51	0
57	MG	DA	3330	1/1	0.96	0.11	45,45,45,45	0
57	MG	BA	3074	1/1	0.96	0.06	46,46,46,46	0
57	MG	DA	3109	1/1	0.96	0.05	40,40,40,40	0
57	MG	DA	3333	1/1	0.96	0.09	41,41,41,41	0
57	MG	BD	305	1/1	0.96	0.09	35,35,35,35	0
57	MG	BD	309	1/1	0.96	0.12	57,57,57,57	0
57	MG	BA	3026	1/1	0.96	0.06	41,41,41,41	0
57	MG	DA	3113	1/1	0.96	0.24	60,60,60,60	0
57	MG	CA	3101	1/1	0.96	0.13	49,49,49,49	0
57	MG	DA	3596	1/1	0.96	0.10	56,56,56,56	0
57	MG	BA	3276	1/1	0.96	0.19	54,54,54,54	0
57	MG	BE	304	1/1	0.96	0.12	42,42,42,42	0
57	MG	DA	3601	1/1	0.96	0.06	44,44,44,44	0
57	MG	CA	3105	1/1	0.96	0.15	52,52,52,52	0
57	MG	DA	3343	1/1	0.96	0.13	50,50,50,50	0
57	MG	DA	3345	1/1	0.96	0.09	44,44,44,44	0
57	MG	BA	3472	1/1	0.96	0.04	20,20,20,20	0
57	MG	BA	3199	1/1	0.96	0.14	46,46,46,46	0
57	MG	DA	3350	1/1	0.96	0.09	51,51,51,51	0
57	MG	BA	3710	1/1	0.96	0.09	57,57,57,57	0
57	MG	BF	301	1/1	0.96	0.09	35,35,35,35	0
57	MG	BF	302	1/1	0.96	0.11	46,46,46,46	0
57	MG	BF	303	1/1	0.96	0.33	49,49,49,49	0
57	MG	AA	3142	1/1	0.96	0.05	41,41,41,41	0
57	MG	BA	3476	1/1	0.96	0.12	55,55,55,55	0
57	MG	CA	3114	1/1	0.96	0.06	57,57,57,57	0
57	MG	BA	3713	1/1	0.96	0.07	33,33,33,33	0
57	MG	BF	309	1/1	0.96	0.10	53,53,53,53	0
57	MG	BA	3077	1/1	0.96	0.16	49,49,49,49	0
57	MG	BA	3374	1/1	0.96	0.12	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	DA	3363	1/1	0.96	0.06	29,29,29,29	0
57	MG	BA	3479	1/1	0.96	0.06	50,50,50,50	0
57	MG	DA	3135	1/1	0.96	0.07	38,38,38,38	0
57	MG	BN	3001	1/1	0.96	0.22	53,53,53,53	0
57	MG	BN	3002	1/1	0.96	0.06	39,39,39,39	0
57	MG	BN	3003	1/1	0.96	0.08	48,48,48,48	0
57	MG	CA	3123	1/1	0.96	0.07	58,58,58,58	0
57	MG	BA	3600	1/1	0.96	0.20	44,44,44,44	0
57	MG	BA	3284	1/1	0.96	0.19	43,43,43,43	0
57	MG	DA	3375	1/1	0.96	0.11	39,39,39,39	0
57	MG	DA	3142	1/1	0.96	0.07	47,47,47,47	0
57	MG	BA	3029	1/1	0.96	0.43	37,37,37,37	0
57	MG	DA	3146	1/1	0.96	0.13	55,55,55,55	0
57	MG	BA	3132	1/1	0.96	0.05	40,40,40,40	0
57	MG	BP	201	1/1	0.96	0.13	41,41,41,41	0
57	MG	BA	3381	1/1	0.96	0.10	46,46,46,46	0
57	MG	DA	3150	1/1	0.96	0.06	56,56,56,56	0
57	MG	BA	3133	1/1	0.96	0.11	45,45,45,45	0
57	MG	AA	3169	1/1	0.96	0.07	62,62,62,62	0
57	MG	DA	3389	1/1	0.96	0.08	46,46,46,46	0
57	MG	BU	201	1/1	0.96	0.10	43,43,43,43	0
57	MG	BU	202	1/1	0.96	0.16	40,40,40,40	0
57	MG	BA	3135	1/1	0.96	0.09	43,43,43,43	0
57	MG	BU	207	1/1	0.96	0.16	38,38,38,38	0
57	MG	DA	3647	1/1	0.96	0.08	54,54,54,54	0
57	MG	DA	3648	1/1	0.96	0.14	57,57,57,57	0
57	MG	CA	3137	1/1	0.96	0.09	56,56,56,56	0
57	MG	DA	3397	1/1	0.96	0.07	57,57,57,57	0
57	MG	BV	201	1/1	0.96	0.13	33,33,33,33	0
57	MG	DA	3162	1/1	0.96	0.21	50,50,50,50	0
57	MG	BA	3727	1/1	0.96	0.07	51,51,51,51	0
57	MG	DA	3401	1/1	0.96	0.05	38,38,38,38	0
57	MG	BA	3031	1/1	0.96	0.18	52,52,52,52	0
57	MG	BW	202	1/1	0.96	0.19	54,54,54,54	0
57	MG	DA	3404	1/1	0.96	0.06	48,48,48,48	0
57	MG	AA	3124	1/1	0.96	0.05	47,47,47,47	0
57	MG	BX	3002	1/1	0.96	0.10	46,46,46,46	0
57	MG	DA	3171	1/1	0.96	0.08	31,31,31,31	0
57	MG	DA	3172	1/1	0.96	0.10	62,62,62,62	0
57	MG	BA	3142	1/1	0.96	0.10	49,49,49,49	0
57	MG	AE	201	1/1	0.96	0.23	59,59,59,59	0
57	MG	DA	3664	1/1	0.96	0.13	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3666	1/1	0.96	0.06	35,35,35,35	0
57	MG	DA	3412	1/1	0.96	0.21	50,50,50,50	0
57	MG	DA	3176	1/1	0.96	0.13	41,41,41,41	0
57	MG	BA	3088	1/1	0.96	0.14	48,48,48,48	0
57	MG	DA	3671	1/1	0.96	0.21	74,74,74,74	0
57	MG	DA	3179	1/1	0.96	0.18	52,52,52,52	0
57	MG	B1	101	1/1	0.96	0.19	51,51,51,51	0
57	MG	DA	3674	1/1	0.96	0.07	37,37,37,37	0
57	MG	BA	3733	1/1	0.96	0.08	58,58,58,58	0
57	MG	BA	3392	1/1	0.96	0.13	53,53,53,53	0
57	MG	DA	3677	1/1	0.96	0.19	52,52,52,52	0
57	MG	CA	3151	1/1	0.96	0.19	59,59,59,59	0
57	MG	DA	3186	1/1	0.96	0.13	54,54,54,54	0
57	MG	AA	3171	1/1	0.96	0.07	51,51,51,51	0
57	MG	B6	101	1/1	0.96	0.10	48,48,48,48	0
57	MG	BA	3736	1/1	0.96	0.18	42,42,42,42	0
57	MG	DA	3193	1/1	0.96	0.18	57,57,57,57	0
57	MG	BA	3620	1/1	0.96	0.08	40,40,40,40	0
57	MG	BA	3739	1/1	0.96	0.16	40,40,40,40	0
57	MG	DB	3010	1/1	0.96	0.10	57,57,57,57	0
57	MG	B7	103	1/1	0.96	0.07	42,42,42,42	0
57	MG	BA	3090	1/1	0.96	0.21	53,53,53,53	0
57	MG	BA	3395	1/1	0.96	0.05	38,38,38,38	0
57	MG	BA	3217	1/1	0.96	0.07	37,37,37,37	0
57	MG	BA	3036	1/1	0.96	0.09	40,40,40,40	0
57	MG	BA	3222	1/1	0.96	0.10	37,37,37,37	0
57	MG	DA	3434	1/1	0.96	0.07	39,39,39,39	0
57	MG	AA	3126	1/1	0.96	0.07	49,49,49,49	0
57	MG	CA	3005	1/1	0.96	0.05	62,62,62,62	0
57	MG	BA	3510	1/1	0.96	0.07	46,46,46,46	0
57	MG	DA	3438	1/1	0.96	0.13	47,47,47,47	0
57	MG	AA	3090	1/1	0.96	0.24	66,66,66,66	0
57	MG	BA	3402	1/1	0.96	0.07	40,40,40,40	0
57	MG	DF	3003	1/1	0.96	0.15	43,43,43,43	0
57	MG	DA	3441	1/1	0.96	0.10	45,45,45,45	0
57	MG	CA	3169	1/1	0.96	0.07	51,51,51,51	0
57	MG	DA	3445	1/1	0.96	0.06	32,32,32,32	0
57	MG	DA	3446	1/1	0.96	0.07	45,45,45,45	0
57	MG	BA	3226	1/1	0.96	0.11	47,47,47,47	0
57	MG	BA	3155	1/1	0.96	0.22	44,44,44,44	0
57	MG	BA	3094	1/1	0.96	0.08	36,36,36,36	0
57	MG	BA	3312	1/1	0.96	0.12	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	DV	3001	1/1	0.96	0.09	70,70,70,70	0
57	MG	DV	3002	1/1	0.96	0.12	49,49,49,49	0
57	MG	BA	3043	1/1	0.96	0.07	48,48,48,48	0
57	MG	BA	3756	1/1	0.96	0.08	48,48,48,48	0
57	MG	BA	3637	1/1	0.96	0.07	39,39,39,39	0
57	MG	DA	3455	1/1	0.96	0.07	47,47,47,47	0
57	MG	DX	101	1/1	0.96	0.09	51,51,51,51	0
57	MG	DA	3456	1/1	0.96	0.07	50,50,50,50	0
57	MG	BA	3758	1/1	0.96	0.07	45,45,45,45	0
57	MG	DA	3458	1/1	0.96	0.06	52,52,52,52	0
57	MG	DA	3461	1/1	0.96	0.14	62,62,62,62	0
57	MG	AA	3128	1/1	0.96	0.07	57,57,57,57	0
60	K	AX	3001	1/1	0.96	0.08	65,65,65,65	0
57	MG	BA	3519	1/1	0.96	0.06	55,55,55,55	0
57	MG	CA	3096	1/1	0.97	0.06	44,44,44,44	0
57	MG	BA	3390	1/1	0.97	0.11	38,38,38,38	0
57	MG	BA	3123	1/1	0.97	0.14	32,32,32,32	0
57	MG	CA	3099	1/1	0.97	0.09	44,44,44,44	0
57	MG	BA	3230	1/1	0.97	0.13	53,53,53,53	0
57	MG	DA	3512	1/1	0.97	0.05	47,47,47,47	0
57	MG	BA	3617	1/1	0.97	0.13	51,51,51,51	0
57	MG	CA	3103	1/1	0.97	0.12	46,46,46,46	0
57	MG	BA	3056	1/1	0.97	0.09	40,40,40,40	0
57	MG	BO	201	1/1	0.97	0.11	50,50,50,50	0
57	MG	AA	3158	1/1	0.97	0.06	45,45,45,45	0
57	MG	DA	3104	1/1	0.97	0.08	53,53,53,53	0
57	MG	DA	3105	1/1	0.97	0.10	48,48,48,48	0
57	MG	BA	3004	1/1	0.97	0.06	33,33,33,33	0
57	MG	DA	3304	1/1	0.97	0.08	48,48,48,48	0
57	MG	BP	204	1/1	0.97	0.07	46,46,46,46	0
57	MG	BP	205	1/1	0.97	0.10	65,65,65,65	0
57	MG	DA	3525	1/1	0.97	0.09	59,59,59,59	0
57	MG	BQ	3001	1/1	0.97	0.15	45,45,45,45	0
57	MG	BQ	3002	1/1	0.97	0.12	43,43,43,43	0
57	MG	BQ	3003	1/1	0.97	0.06	49,49,49,49	0
57	MG	BA	3309	1/1	0.97	0.11	41,41,41,41	0
57	MG	AA	3116	1/1	0.97	0.07	55,55,55,55	0
57	MG	AA	3186	1/1	0.97	0.06	42,42,42,42	0
57	MG	DA	3115	1/1	0.97	0.08	40,40,40,40	0
57	MG	BA	3176	1/1	0.97	0.07	45,45,45,45	0
57	MG	BA	3625	1/1	0.97	0.10	39,39,39,39	0
57	MG	DA	3535	1/1	0.97	0.06	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	BU	203	1/1	0.97	0.09	47,47,47,47	0
57	MG	DA	3537	1/1	0.97	0.07	44,44,44,44	0
57	MG	AA	3125	1/1	0.97	0.11	37,37,37,37	0
57	MG	DA	3319	1/1	0.97	0.07	41,41,41,41	0
57	MG	AA	3014	1/1	0.97	0.07	32,32,32,32	0
57	MG	DA	3121	1/1	0.97	0.04	44,44,44,44	0
57	MG	DA	3542	1/1	0.97	0.06	24,24,24,24	0
57	MG	BA	3241	1/1	0.97	0.13	36,36,36,36	0
57	MG	AA	3162	1/1	0.97	0.06	66,66,66,66	0
57	MG	DA	3324	1/1	0.97	0.07	33,33,33,33	0
57	MG	DA	3325	1/1	0.97	0.06	35,35,35,35	0
57	MG	BV	203	1/1	0.97	0.14	38,38,38,38	0
57	MG	BA	3097	1/1	0.97	0.09	44,44,44,44	0
57	MG	BV	205	1/1	0.97	0.10	38,38,38,38	0
57	MG	BW	201	1/1	0.97	0.15	44,44,44,44	0
57	MG	BA	3181	1/1	0.97	0.15	43,43,43,43	0
57	MG	BW	204	1/1	0.97	0.09	42,42,42,42	0
57	MG	BA	3632	1/1	0.97	0.05	50,50,50,50	0
57	MG	BA	3407	1/1	0.97	0.07	47,47,47,47	0
57	MG	CA	3131	1/1	0.97	0.07	55,55,55,55	0
57	MG	BX	3003	1/1	0.97	0.07	35,35,35,35	0
57	MG	DA	3336	1/1	0.97	0.08	40,40,40,40	0
57	MG	BY	502	1/1	0.97	0.11	40,40,40,40	0
57	MG	BA	3246	1/1	0.97	0.21	39,39,39,39	0
57	MG	B0	101	1/1	0.97	0.10	36,36,36,36	0
57	MG	AA	3110	1/1	0.97	0.07	48,48,48,48	0
57	MG	BA	3410	1/1	0.97	0.07	27,27,27,27	0
57	MG	BA	3038	1/1	0.97	0.09	35,35,35,35	0
57	MG	BA	3136	1/1	0.97	0.05	30,30,30,30	0
57	MG	DA	3344	1/1	0.97	0.07	31,31,31,31	0
57	MG	B3	3002	1/1	0.97	0.10	66,66,66,66	0
57	MG	DA	3568	1/1	0.97	0.09	52,52,52,52	0
57	MG	CA	3141	1/1	0.97	0.09	92,92,92,92	0
57	MG	BA	3323	1/1	0.97	0.11	30,30,30,30	0
57	MG	AA	3164	1/1	0.97	0.08	61,61,61,61	0
57	MG	BA	3187	1/1	0.97	0.14	29,29,29,29	0
57	MG	BA	3253	1/1	0.97	0.07	55,55,55,55	0
57	MG	BA	3254	1/1	0.97	0.13	25,25,25,25	0
57	MG	BA	3420	1/1	0.97	0.08	40,40,40,40	0
57	MG	BA	3255	1/1	0.97	0.08	47,47,47,47	0
57	MG	BA	3422	1/1	0.97	0.10	33,33,33,33	0
57	MG	BA	3189	1/1	0.97	0.07	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	DA	3581	1/1	0.97	0.08	57,57,57,57	0
57	MG	B8	101	1/1	0.97	0.06	44,44,44,44	0
57	MG	BA	3534	1/1	0.97	0.09	44,44,44,44	0
57	MG	AA	3165	1/1	0.97	0.08	54,54,54,54	0
57	MG	CA	3002	1/1	0.97	0.08	63,63,63,63	0
57	MG	DA	3161	1/1	0.97	0.06	38,38,38,38	0
57	MG	BA	3140	1/1	0.97	0.05	47,47,47,47	0
57	MG	DA	3365	1/1	0.97	0.05	36,36,36,36	0
57	MG	BA	3333	1/1	0.97	0.12	38,38,38,38	0
57	MG	BA	3334	1/1	0.97	0.07	37,37,37,37	0
57	MG	BA	3653	1/1	0.97	0.12	39,39,39,39	0
57	MG	DA	3369	1/1	0.97	0.05	28,28,28,28	0
57	MG	DA	3166	1/1	0.97	0.16	55,55,55,55	0
57	MG	DA	3167	1/1	0.97	0.11	41,41,41,41	0
57	MG	DA	3168	1/1	0.97	0.10	45,45,45,45	0
57	MG	BA	3539	1/1	0.97	0.13	52,52,52,52	0
57	MG	BA	3655	1/1	0.97	0.14	50,50,50,50	0
57	MG	BA	3192	1/1	0.97	0.15	46,46,46,46	0
57	MG	BA	3141	1/1	0.97	0.20	42,42,42,42	0
57	MG	BA	3777	1/1	0.97	0.13	40,40,40,40	0
57	MG	BA	3194	1/1	0.97	0.08	47,47,47,47	0
57	MG	BA	3340	1/1	0.97	0.07	39,39,39,39	0
57	MG	DA	3177	1/1	0.97	0.16	42,42,42,42	0
57	MG	BA	3661	1/1	0.97	0.11	44,44,44,44	0
57	MG	BA	3433	1/1	0.97	0.11	32,32,32,32	0
57	MG	BA	3547	1/1	0.97	0.17	39,39,39,39	0
57	MG	BA	3341	1/1	0.97	0.08	51,51,51,51	0
57	MG	DA	3182	1/1	0.97	0.23	51,51,51,51	0
57	MG	BA	3435	1/1	0.97	0.15	45,45,45,45	0
57	MG	DA	3393	1/1	0.97	0.07	50,50,50,50	0
57	MG	BA	3436	1/1	0.97	0.06	40,40,40,40	0
57	MG	BA	3104	1/1	0.97	0.11	42,42,42,42	0
57	MG	DA	3617	1/1	0.97	0.06	56,56,56,56	0
57	MG	DA	3187	1/1	0.97	0.11	42,42,42,42	0
57	MG	BA	3105	1/1	0.97	0.07	37,37,37,37	0
57	MG	BA	3265	1/1	0.97	0.10	54,54,54,54	0
57	MG	DA	3190	1/1	0.97	0.27	54,54,54,54	0
57	MG	CA	3023	1/1	0.97	0.07	44,44,44,44	0
57	MG	BA	3144	1/1	0.97	0.08	41,41,41,41	0
57	MG	AA	3082	1/1	0.97	0.10	46,46,46,46	0
57	MG	BA	3044	1/1	0.97	0.12	20,20,20,20	0
57	MG	BA	3558	1/1	0.97	0.05	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	3028	1/1	0.97	0.05	41,41,41,41	0
57	MG	DA	3199	1/1	0.97	0.07	47,47,47,47	0
57	MG	DA	3629	1/1	0.97	0.09	62,62,62,62	0
57	MG	BA	3148	1/1	0.97	0.18	44,44,44,44	0
57	MG	BA	3561	1/1	0.97	0.05	45,45,45,45	0
57	MG	BA	3046	1/1	0.97	0.17	41,41,41,41	0
57	MG	BA	3677	1/1	0.97	0.11	60,60,60,60	0
57	MG	BA	3678	1/1	0.97	0.05	65,65,65,65	0
57	MG	BA	3563	1/1	0.97	0.09	36,36,36,36	0
57	MG	BA	3150	1/1	0.97	0.07	55,55,55,55	0
57	MG	BA	3020	1/1	0.97	0.26	53,53,53,53	0
57	MG	DA	3011	1/1	0.97	0.05	48,48,48,48	0
57	MG	DA	3639	1/1	0.97	0.22	59,59,59,59	0
57	MG	DA	3012	1/1	0.97	0.07	33,33,33,33	0
57	MG	BA	3110	1/1	0.97	0.10	41,41,41,41	0
57	MG	DA	3419	1/1	0.97	0.07	32,32,32,32	0
57	MG	DA	3014	1/1	0.97	0.07	46,46,46,46	0
57	MG	BA	3452	1/1	0.97	0.11	55,55,55,55	0
57	MG	BA	3111	1/1	0.97	0.15	54,54,54,54	0
57	MG	CA	3040	1/1	0.97	0.05	51,51,51,51	0
57	MG	BA	3571	1/1	0.97	0.08	58,58,58,58	0
57	MG	DA	3020	1/1	0.97	0.13	55,55,55,55	0
57	MG	BA	3810	1/1	0.97	0.09	41,41,41,41	0
57	MG	CA	3043	1/1	0.97	0.08	47,47,47,47	0
57	MG	BA	3454	1/1	0.97	0.09	27,27,27,27	0
57	MG	BA	3112	1/1	0.97	0.13	30,30,30,30	0
57	MG	BB	201	1/1	0.97	0.14	55,55,55,55	0
57	MG	BA	3689	1/1	0.97	0.07	42,42,42,42	0
57	MG	BB	203	1/1	0.97	0.13	43,43,43,43	0
57	MG	BA	3277	1/1	0.97	0.35	47,47,47,47	0
57	MG	BA	3575	1/1	0.97	0.10	48,48,48,48	0
57	MG	BA	3356	1/1	0.97	0.06	37,37,37,37	0
57	MG	BA	3210	1/1	0.97	0.14	49,49,49,49	0
57	MG	BB	208	1/1	0.97	0.09	45,45,45,45	0
57	MG	BA	3048	1/1	0.97	0.10	47,47,47,47	0
57	MG	BA	3360	1/1	0.97	0.06	41,41,41,41	0
57	MG	CA	3056	1/1	0.97	0.15	64,64,64,64	0
57	MG	BB	211	1/1	0.97	0.04	51,51,51,51	0
57	MG	DA	3665	1/1	0.97	0.10	42,42,42,42	0
57	MG	DA	3235	1/1	0.97	0.12	45,45,45,45	0
57	MG	DA	3444	1/1	0.97	0.05	44,44,44,44	0
57	MG	DA	3039	1/1	0.97	0.05	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	3041	1/1	0.97	0.05	38,38,38,38	0
57	MG	DA	3670	1/1	0.97	0.16	60,60,60,60	0
57	MG	BB	212	1/1	0.97	0.08	55,55,55,55	0
57	MG	BA	3281	1/1	0.97	0.29	60,60,60,60	0
57	MG	DA	3045	1/1	0.97	0.09	51,51,51,51	0
57	MG	BA	3698	1/1	0.97	0.12	31,31,31,31	0
57	MG	BA	3157	1/1	0.97	0.11	45,45,45,45	0
57	MG	BA	3283	1/1	0.97	0.09	35,35,35,35	0
57	MG	BB	217	1/1	0.97	0.05	29,29,29,29	0
57	MG	AA	3194	1/1	0.97	0.10	56,56,56,56	0
57	MG	CA	3065	1/1	0.97	0.25	49,49,49,49	0
57	MG	DA	3053	1/1	0.97	0.06	47,47,47,47	0
57	MG	AA	3168	1/1	0.97	0.06	59,59,59,59	0
57	MG	DA	3055	1/1	0.97	0.13	49,49,49,49	0
57	MG	DB	3006	1/1	0.97	0.11	57,57,57,57	0
57	MG	BA	3367	1/1	0.97	0.13	29,29,29,29	0
57	MG	DA	3057	1/1	0.97	0.07	42,42,42,42	0
57	MG	DA	3058	1/1	0.97	0.09	29,29,29,29	0
57	MG	BD	301	1/1	0.97	0.07	40,40,40,40	0
57	MG	BA	3706	1/1	0.97	0.05	53,53,53,53	0
57	MG	BA	3286	1/1	0.97	0.08	34,34,34,34	0
57	MG	BA	3287	1/1	0.97	0.06	42,42,42,42	0
57	MG	DA	3258	1/1	0.97	0.09	48,48,48,48	0
57	MG	BA	3216	1/1	0.97	0.14	37,37,37,37	0
57	MG	BD	306	1/1	0.97	0.09	38,38,38,38	0
57	MG	BD	308	1/1	0.97	0.11	46,46,46,46	0
57	MG	BA	3079	1/1	0.97	0.09	39,39,39,39	0
57	MG	DA	3475	1/1	0.97	0.10	51,51,51,51	0
57	MG	DE	301	1/1	0.97	0.15	46,46,46,46	0
57	MG	DE	302	1/1	0.97	0.12	33,33,33,33	0
57	MG	AA	3148	1/1	0.97	0.14	57,57,57,57	0
57	MG	DA	3264	1/1	0.97	0.07	40,40,40,40	0
57	MG	BE	302	1/1	0.97	0.11	39,39,39,39	0
57	MG	BA	3219	1/1	0.97	0.12	36,36,36,36	0
57	MG	BA	3220	1/1	0.97	0.09	29,29,29,29	0
57	MG	DG	3001	1/1	0.97	0.04	55,55,55,55	0
57	MG	AA	3129	1/1	0.97	0.06	47,47,47,47	0
57	MG	DO	5001	1/1	0.97	0.11	59,59,59,59	0
57	MG	BA	3378	1/1	0.97	0.04	28,28,28,28	0
57	MG	DP	202	1/1	0.97	0.06	53,53,53,53	0
57	MG	BA	3295	1/1	0.97	0.06	38,38,38,38	0
57	MG	DA	3074	1/1	0.97	0.08	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3223	1/1	0.97	0.06	41,41,41,41	0
57	MG	BA	3481	1/1	0.97	0.08	41,41,41,41	0
57	MG	BA	3297	1/1	0.97	0.08	43,43,43,43	0
57	MG	BA	3082	1/1	0.97	0.07	39,39,39,39	0
57	MG	DA	3491	1/1	0.97	0.06	51,51,51,51	0
57	MG	BA	3299	1/1	0.97	0.04	25,25,25,25	0
57	MG	BA	3054	1/1	0.97	0.14	36,36,36,36	0
57	MG	CA	3089	1/1	0.97	0.11	47,47,47,47	0
57	MG	BA	3167	1/1	0.97	0.07	41,41,41,41	0
57	MG	BA	3084	1/1	0.97	0.17	38,38,38,38	0
57	MG	DA	3084	1/1	0.97	0.09	39,39,39,39	0
57	MG	BA	3490	1/1	0.97	0.06	54,54,54,54	0
57	MG	DA	3286	1/1	0.97	0.06	42,42,42,42	0
57	MG	DA	3500	1/1	0.97	0.08	49,49,49,49	0
57	MG	DA	3086	1/1	0.97	0.04	43,43,43,43	0
59	ZN	CN	501	1/1	0.97	0.07	93,93,93,93	0
59	ZN	DY	501	1/1	0.97	0.06	96,96,96,96	0
57	MG	BA	3612	1/1	0.97	0.05	21,21,21,21	0
57	MG	CA	3094	1/1	0.97	0.19	70,70,70,70	0
57	MG	AA	3212	1/1	0.97	0.09	42,42,42,42	0
57	MG	BA	3569	1/1	0.98	0.07	49,49,49,49	0
57	MG	BA	3025	1/1	0.98	0.05	27,27,27,27	0
57	MG	BA	3137	1/1	0.98	0.18	39,39,39,39	0
57	MG	DA	3442	1/1	0.98	0.05	39,39,39,39	0
57	MG	DA	3589	1/1	0.98	0.06	68,68,68,68	0
57	MG	BA	3049	1/1	0.98	0.12	36,36,36,36	0
57	MG	BA	3744	1/1	0.98	0.10	39,39,39,39	0
57	MG	BD	307	1/1	0.98	0.11	40,40,40,40	0
57	MG	BA	3489	1/1	0.98	0.04	59,59,59,59	0
57	MG	BA	3259	1/1	0.98	0.10	25,25,25,25	0
57	MG	DA	3183	1/1	0.98	0.10	38,38,38,38	0
57	MG	DA	3449	1/1	0.98	0.10	54,54,54,54	0
57	MG	BA	3491	1/1	0.98	0.06	45,45,45,45	0
57	MG	DA	3599	1/1	0.98	0.04	36,36,36,36	0
57	MG	BA	3214	1/1	0.98	0.08	41,41,41,41	0
57	MG	BA	3660	1/1	0.98	0.06	61,61,61,61	0
57	MG	BA	3577	1/1	0.98	0.13	51,51,51,51	0
57	MG	AA	3151	1/1	0.98	0.06	45,45,45,45	0
57	MG	BE	306	1/1	0.98	0.10	26,26,26,26	0
57	MG	BA	3752	1/1	0.98	0.07	32,32,32,32	0
57	MG	DA	3191	1/1	0.98	0.08	37,37,37,37	0
57	MG	BA	3009	1/1	0.98	0.06	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3460	1/1	0.98	0.09	41,41,41,41	0
57	MG	BA	3425	1/1	0.98	0.04	40,40,40,40	0
57	MG	BA	3028	1/1	0.98	0.10	51,51,51,51	0
57	MG	DA	3195	1/1	0.98	0.05	43,43,43,43	0
57	MG	BA	3010	1/1	0.98	0.09	39,39,39,39	0
57	MG	BA	3011	1/1	0.98	0.05	35,35,35,35	0
57	MG	AA	3050	1/1	0.98	0.07	33,33,33,33	0
57	MG	BF	307	1/1	0.98	0.15	37,37,37,37	0
57	MG	BA	3221	1/1	0.98	0.05	37,37,37,37	0
57	MG	BA	3586	1/1	0.98	0.04	53,53,53,53	0
57	MG	BA	3032	1/1	0.98	0.06	47,47,47,47	0
57	MG	DA	3471	1/1	0.98	0.13	50,50,50,50	0
57	MG	BA	3146	1/1	0.98	0.07	40,40,40,40	0
57	MG	DA	3204	1/1	0.98	0.15	46,46,46,46	0
57	MG	BA	3373	1/1	0.98	0.10	48,48,48,48	0
57	MG	BA	3270	1/1	0.98	0.05	48,48,48,48	0
57	MG	BA	3013	1/1	0.98	0.07	32,32,32,32	0
57	MG	BA	3085	1/1	0.98	0.13	35,35,35,35	0
57	MG	BA	3377	1/1	0.98	0.06	44,44,44,44	0
57	MG	DA	3480	1/1	0.98	0.07	40,40,40,40	0
57	MG	BA	3184	1/1	0.98	0.22	43,43,43,43	0
57	MG	BA	3379	1/1	0.98	0.05	31,31,31,31	0
57	MG	BA	3440	1/1	0.98	0.05	42,42,42,42	0
57	MG	CA	3155	1/1	0.98	0.12	53,53,53,53	0
57	MG	BA	3441	1/1	0.98	0.05	35,35,35,35	0
57	MG	BA	3086	1/1	0.98	0.07	22,22,22,22	0
57	MG	BP	202	1/1	0.98	0.18	36,36,36,36	0
57	MG	BP	203	1/1	0.98	0.07	33,33,33,33	0
57	MG	BA	3014	1/1	0.98	0.23	42,42,42,42	0
57	MG	DA	3347	1/1	0.98	0.09	27,27,27,27	0
57	MG	BA	3059	1/1	0.98	0.12	26,26,26,26	0
57	MG	DA	3349	1/1	0.98	0.06	52,52,52,52	0
57	MG	DA	3094	1/1	0.98	0.09	50,50,50,50	0
57	MG	BA	3188	1/1	0.98	0.16	49,49,49,49	0
57	MG	BA	3521	1/1	0.98	0.07	39,39,39,39	0
57	MG	DA	3097	1/1	0.98	0.04	33,33,33,33	0
57	MG	BA	3605	1/1	0.98	0.05	43,43,43,43	0
57	MG	DA	3099	1/1	0.98	0.13	32,32,32,32	0
57	MG	BA	3522	1/1	0.98	0.06	52,52,52,52	0
57	MG	DA	3357	1/1	0.98	0.05	50,50,50,50	0
57	MG	DA	3227	1/1	0.98	0.12	41,41,41,41	0
57	MG	BA	3384	1/1	0.98	0.06	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	3525	1/1	0.98	0.08	34,34,34,34	0
57	MG	DA	3504	1/1	0.98	0.04	47,47,47,47	0
57	MG	BR	202	1/1	0.98	0.07	31,31,31,31	0
57	MG	DA	3506	1/1	0.98	0.05	42,42,42,42	0
57	MG	BA	3692	1/1	0.98	0.05	40,40,40,40	0
57	MG	BA	3447	1/1	0.98	0.07	72,72,72,72	0
57	MG	BA	3611	1/1	0.98	0.09	46,46,46,46	0
57	MG	BA	3784	1/1	0.98	0.09	33,33,33,33	0
57	MG	CF	3001	1/1	0.98	0.05	46,46,46,46	0
57	MG	BU	205	1/1	0.98	0.18	47,47,47,47	0
57	MG	BU	206	1/1	0.98	0.14	35,35,35,35	0
57	MG	BA	3152	1/1	0.98	0.07	43,43,43,43	0
57	MG	BU	208	1/1	0.98	0.18	40,40,40,40	0
57	MG	BA	3449	1/1	0.98	0.08	35,35,35,35	0
57	MG	AA	3114	1/1	0.98	0.12	59,59,59,59	0
57	MG	BA	3280	1/1	0.98	0.04	37,37,37,37	0
57	MG	BA	3699	1/1	0.98	0.07	35,35,35,35	0
57	MG	AA	3042	1/1	0.98	0.11	57,57,57,57	0
57	MG	DA	3377	1/1	0.98	0.06	38,38,38,38	0
57	MG	BA	3791	1/1	0.98	0.07	28,28,28,28	0
57	MG	DA	3003	1/1	0.98	0.09	27,27,27,27	0
57	MG	BA	3234	1/1	0.98	0.03	38,38,38,38	0
57	MG	DA	3381	1/1	0.98	0.10	56,56,56,56	0
57	MG	BW	203	1/1	0.98	0.05	44,44,44,44	0
57	MG	BA	3235	1/1	0.98	0.05	42,42,42,42	0
57	MG	AW	3002	1/1	0.98	0.11	53,53,53,53	0
57	MG	AA	3144	1/1	0.98	0.07	46,46,46,46	0
57	MG	BA	3705	1/1	0.98	0.08	62,62,62,62	0
57	MG	DA	3253	1/1	0.98	0.05	45,45,45,45	0
57	MG	DA	3390	1/1	0.98	0.08	43,43,43,43	0
57	MG	DA	3127	1/1	0.98	0.12	35,35,35,35	0
57	MG	BA	3124	1/1	0.98	0.07	19,19,19,19	0
57	MG	BA	3195	1/1	0.98	0.06	46,46,46,46	0
57	MG	BA	3338	1/1	0.98	0.05	40,40,40,40	0
57	MG	BA	3339	1/1	0.98	0.05	23,23,23,23	0
57	MG	BA	3158	1/1	0.98	0.12	41,41,41,41	0
57	MG	BA	3542	1/1	0.98	0.07	45,45,45,45	0
57	MG	BA	3197	1/1	0.98	0.09	41,41,41,41	0
57	MG	B3	3001	1/1	0.98	0.08	34,34,34,34	0
57	MG	BA	3544	1/1	0.98	0.09	44,44,44,44	0
57	MG	BA	3807	1/1	0.98	0.08	47,47,47,47	0
57	MG	DD	302	1/1	0.98	0.04	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3040	1/1	0.98	0.24	35,35,35,35	0
57	MG	BA	3400	1/1	0.98	0.05	33,33,33,33	0
57	MG	DD	305	1/1	0.98	0.04	36,36,36,36	0
57	MG	DA	3023	1/1	0.98	0.29	40,40,40,40	0
57	MG	BA	3291	1/1	0.98	0.17	33,33,33,33	0
57	MG	DD	308	1/1	0.98	0.19	48,48,48,48	0
57	MG	DA	3270	1/1	0.98	0.08	46,46,46,46	0
57	MG	DA	3407	1/1	0.98	0.03	66,66,66,66	0
57	MG	BA	3467	1/1	0.98	0.08	50,50,50,50	0
57	MG	AA	3106	1/1	0.98	0.14	57,57,57,57	0
57	MG	BA	3719	1/1	0.98	0.09	53,53,53,53	0
57	MG	CA	3100	1/1	0.98	0.06	52,52,52,52	0
57	MG	BA	3067	1/1	0.98	0.09	41,41,41,41	0
57	MG	BA	3245	1/1	0.98	0.16	34,34,34,34	0
57	MG	DF	3004	1/1	0.98	0.19	44,44,44,44	0
57	MG	BA	3096	1/1	0.98	0.23	54,54,54,54	0
57	MG	BA	3553	1/1	0.98	0.04	59,59,59,59	0
57	MG	BA	3247	1/1	0.98	0.16	25,25,25,25	0
57	MG	DA	3560	1/1	0.98	0.05	40,40,40,40	0
57	MG	DA	3034	1/1	0.98	0.08	38,38,38,38	0
57	MG	DQ	3001	1/1	0.98	0.04	47,47,47,47	0
57	MG	DA	3154	1/1	0.98	0.26	48,48,48,48	0
57	MG	BA	3042	1/1	0.98	0.10	43,43,43,43	0
57	MG	BA	3726	1/1	0.98	0.14	63,63,63,63	0
57	MG	BA	3474	1/1	0.98	0.09	55,55,55,55	0
57	MG	DA	3285	1/1	0.98	0.06	32,32,32,32	0
57	MG	BA	3069	1/1	0.98	0.11	22,22,22,22	0
57	MG	AE	203	1/1	0.98	0.13	63,63,63,63	0
57	MG	DA	3040	1/1	0.98	0.05	31,31,31,31	0
57	MG	BA	3559	1/1	0.98	0.05	47,47,47,47	0
57	MG	DA	3042	1/1	0.98	0.08	38,38,38,38	0
57	MG	DW	3002	1/1	0.98	0.07	45,45,45,45	0
57	MG	DA	3572	1/1	0.98	0.05	62,62,62,62	0
57	MG	BA	3166	1/1	0.98	0.04	38,38,38,38	0
57	MG	AX	3013	1/1	0.98	0.06	58,58,58,58	0
57	MG	BA	3045	1/1	0.98	0.15	36,36,36,36	0
57	MG	AA	3182	1/1	0.98	0.09	49,49,49,49	0
57	MG	BA	3414	1/1	0.98	0.09	41,41,41,41	0
57	MG	AK	3001	1/1	0.98	0.13	44,44,44,44	0
58	SF4	AD	501	8/8	0.98	0.06	62,68,73,86	0
58	SF4	CD	302	8/8	0.98	0.06	60,68,83,86	0
59	ZN	B4	501	1/1	0.98	0.04	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3737	1/1	0.98	0.16	43,43,43,43	0
57	MG	DA	3050	1/1	0.98	0.17	59,59,59,59	0
57	MG	BA	3416	1/1	0.98	0.07	21,21,21,21	0
59	ZN	D9	501	1/1	0.98	0.05	68,68,68,68	0
57	MG	BA	3357	1/1	0.98	0.09	25,25,25,25	0
57	MG	DA	3174	1/1	0.98	0.10	44,44,44,44	0
57	MG	BA	3037	1/1	0.99	0.14	34,34,34,34	0
57	MG	DA	3386	1/1	0.99	0.04	35,35,35,35	0
57	MG	DA	3459	1/1	0.99	0.05	47,47,47,47	0
57	MG	DA	3387	1/1	0.99	0.04	42,42,42,42	0
57	MG	DA	3102	1/1	0.99	0.09	40,40,40,40	0
57	MG	BA	3565	1/1	0.99	0.08	40,40,40,40	0
57	MG	BA	3495	1/1	0.99	0.06	37,37,37,37	0
57	MG	DA	3580	1/1	0.99	0.07	36,36,36,36	0
57	MG	BA	3496	1/1	0.99	0.08	41,41,41,41	0
57	MG	BA	3498	1/1	0.99	0.06	36,36,36,36	0
57	MG	BA	3609	1/1	0.99	0.04	39,39,39,39	0
57	MG	BA	3588	1/1	0.99	0.10	31,31,31,31	0
57	MG	BA	3483	1/1	0.99	0.06	28,28,28,28	0
57	MG	BA	3533	1/1	0.99	0.04	59,59,59,59	0
57	MG	AA	3167	1/1	0.99	0.05	57,57,57,57	0
57	MG	BA	3795	1/1	0.99	0.09	35,35,35,35	0
57	MG	BA	3198	1/1	0.99	0.19	37,37,37,37	0
57	MG	DA	3266	1/1	0.99	0.04	57,57,57,57	0
57	MG	AA	3074	1/1	0.99	0.08	50,50,50,50	0
57	MG	DA	3143	1/1	0.99	0.10	38,38,38,38	0
57	MG	DA	3144	1/1	0.99	0.05	38,38,38,38	0
57	MG	DA	3477	1/1	0.99	0.03	43,43,43,43	0
57	MG	BA	3363	1/1	0.99	0.04	22,22,22,22	0
57	MG	DA	3517	1/1	0.99	0.04	51,51,51,51	0
57	MG	DA	3597	1/1	0.99	0.03	51,51,51,51	0
57	MG	BA	3103	1/1	0.99	0.07	38,38,38,38	0
57	MG	BA	3060	1/1	0.99	0.09	30,30,30,30	0
57	MG	BA	3597	1/1	0.99	0.13	25,25,25,25	0
57	MG	BA	3015	1/1	0.99	0.05	32,32,32,32	0
57	MG	DA	3373	1/1	0.99	0.07	44,44,44,44	0
57	MG	DA	3603	1/1	0.99	0.05	41,41,41,41	0
57	MG	BA	3507	1/1	0.99	0.08	49,49,49,49	0
57	MG	BF	305	1/1	0.99	0.03	49,49,49,49	0
57	MG	BA	3688	1/1	0.99	0.07	46,46,46,46	0
57	MG	BA	3524	1/1	0.99	0.03	42,42,42,42	0
59	ZN	AN	501	1/1	0.99	0.05	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	ZN	BY	501	1/1	0.99	0.03	58,58,58,58	0
57	MG	BA	3806	1/1	0.99	0.08	30,30,30,30	0
59	ZN	B5	102	1/1	0.99	0.05	48,48,48,48	0
59	ZN	B6	103	1/1	0.99	0.05	49,49,49,49	0
59	ZN	B9	501	1/1	0.99	0.03	38,38,38,38	0
57	MG	DA	3016	1/1	0.99	0.09	50,50,50,50	0
57	MG	DA	3156	1/1	0.99	0.04	51,51,51,51	0
57	MG	AA	3086	1/1	0.99	0.08	57,57,57,57	0
59	ZN	D5	501	1/1	0.99	0.04	58,58,58,58	0
59	ZN	D6	501	1/1	0.99	0.04	71,71,71,71	0
57	MG	DA	3315	1/1	0.99	0.03	42,42,42,42	0
57	MG	BA	3458	1/1	0.99	0.05	18,18,18,18	0
57	MG	BA	3099	1/1	0.99	0.04	41,41,41,41	0
57	MG	BA	3327	1/1	1.00	0.07	38,38,38,38	0
57	MG	BA	3497	1/1	1.00	0.06	28,28,28,28	0

6.5 Other polymers ⓘ

There are no such residues in this entry.