



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 12:05 PM UTC

PDB ID : 1VY6 / pdb_00001vy6
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in the pre-attack state of peptide bond formation containing short substrate-mimic Cytidine-Puromycin in the A site and acylated tRNA in the P site.
Authors : Polikanov, Y.S.; Steitz, T.A.; Innis, C.A.
Deposited on : 2014-05-13
Resolution : 2.90 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

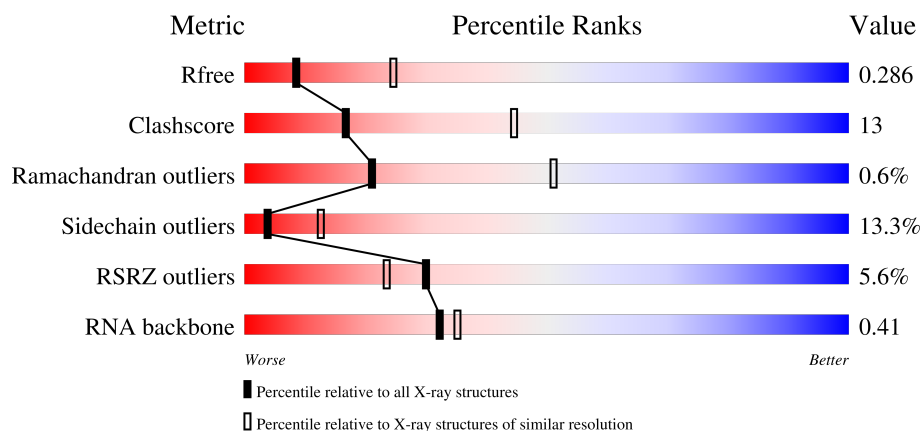
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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

Mol	Chain	Length	Quality of chain
1	AA	1521	3% 42% 42% 14% •
1	CA	1521	6% 40% 45% 14% •
2	AB	256	11% 39% 39% 10% • 10%
2	CB	256	20% 35% 45% 10% • 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	

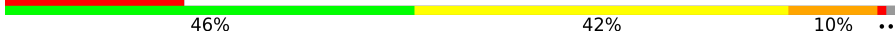
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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	24	
22	CV	24	
23	AW	2	
23	CW	2	
24	AX	77	
24	CX	77	
25	BA	2915	
25	DA	2915	
26	BB	121	
26	DB	121	
27	BD	276	
27	DD	276	

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

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Mol	Chain	Length	Quality of chain
40	DU	118	
41	BV	101	
41	DV	101	
42	BW	113	
42	DW	113	
43	BX	96	
43	DX	96	
44	BY	110	
44	DY	110	
45	BZ	206	
45	DZ	206	
46	B0	85	
46	D0	85	
47	B1	98	
47	D1	98	
48	B2	72	
48	D2	72	
49	B3	60	
49	D3	60	
50	B4	71	
50	D4	71	
51	B5	60	
51	D5	60	
52	B6	54	
52	D6	54	

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Mol	Chain	Length	Quality of chain
53	B7	49	71%22%••
53	D7	49	6% 61%31%6%•
54	B8	65	66%31%••
54	D8	65	42%52%5%•
55	B9	37	3% 84%14%•
55	D9	37	49%49%•

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 289646 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
			1670	1047	332	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 Cytidine-Puromycin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	2	Total	C	N	O	P	0	0	0
			54	31	10	12	1			
23	CW	2	Total	C	N	O	P	0	0	0
			54	31	10	12	1			

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

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

- Molecule 25 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2819	Total	C	N	O	P	0	0	0
			60729	27026	11370	19515	2818			
25	DA	2800	Total	C	N	O	P	0	0	0
			60311	26840	11284	19388	2799			

- Molecule 26 is a RNA chain called 5S Ribosomal RNA.

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

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

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BI	146	Total	C	N	O	S	0	0	0
			1085	693	189	202	1			
32	DI	146	Total	C	N	O	S	0	0	0
			1061	680	186	194	1			

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

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

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

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

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

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

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

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

- Molecule 49 is a protein called 50S ribosomal protein L30.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B4	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			
50	D4	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

- Molecule 51 is a protein called 50S ribosomal protein L32.

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

- Molecule 52 is a protein called 50S ribosomal protein L33.

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

- Molecule 53 is a protein called 50S ribosomal protein L34.

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

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B8	64	Total	C	N	O	S	0	0	0
			511	328	99	82	2			
54	D8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 55 is a protein called 50S ribosomal protein L36.

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

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	187	Total	Mg	0	0
			187	187		
56	AD	1	Total	Mg	0	0
			1	1		
56	AE	2	Total	Mg	0	0
			2	2		
56	AF	1	Total	Mg	0	0
			1	1		
56	AK	1	Total	Mg	0	0
			1	1		
56	AL	1	Total	Mg	0	0
			1	1		
56	AM	1	Total	Mg	0	0
			1	1		
56	AN	1	Total	Mg	0	0
			1	1		
56	AX	7	Total	Mg	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BA	675	Total 675	Mg 675	0	0
56	BB	18	Total 18	Mg 18	0	0
56	BD	8	Total 8	Mg 8	0	0
56	BE	6	Total 6	Mg 6	0	0
56	BF	5	Total 5	Mg 5	0	0
56	BG	3	Total 3	Mg 3	0	0
56	BH	1	Total 1	Mg 1	0	0
56	BN	2	Total 2	Mg 2	0	0
56	BO	1	Total 1	Mg 1	0	0
56	BP	4	Total 4	Mg 4	0	0
56	BQ	3	Total 3	Mg 3	0	0
56	BR	3	Total 3	Mg 3	0	0
56	BU	5	Total 5	Mg 5	0	0
56	BV	3	Total 3	Mg 3	0	0
56	BW	4	Total 4	Mg 4	0	0
56	BX	3	Total 3	Mg 3	0	0
56	BY	2	Total 2	Mg 2	0	0
56	BZ	1	Total 1	Mg 1	0	0
56	B0	5	Total 5	Mg 5	0	0
56	B3	2	Total 2	Mg 2	0	0
56	B4	1	Total 1	Mg 1	0	0

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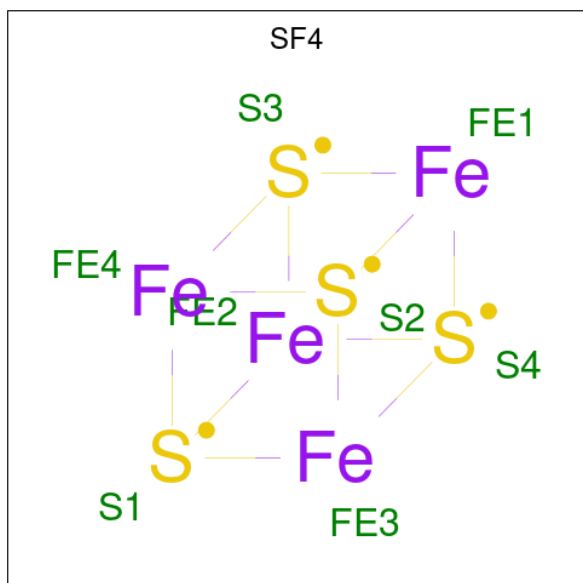
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B5	2	Total 2	Mg 2	0	0
56	B7	4	Total 4	Mg 4	0	0
56	B8	1	Total 1	Mg 1	0	0
56	B9	1	Total 1	Mg 1	0	0
56	CA	154	Total 154	Mg 154	0	0
56	CE	2	Total 2	Mg 2	0	0
56	CF	1	Total 1	Mg 1	0	0
56	CJ	1	Total 1	Mg 1	0	0
56	CK	1	Total 1	Mg 1	0	0
56	CT	1	Total 1	Mg 1	0	0
56	CX	1	Total 1	Mg 1	0	0
56	DA	595	Total 595	Mg 595	0	0
56	DB	12	Total 12	Mg 12	0	0
56	DD	2	Total 2	Mg 2	0	0
56	DE	5	Total 5	Mg 5	0	0
56	DF	3	Total 3	Mg 3	0	0
56	DG	1	Total 1	Mg 1	0	0
56	DN	1	Total 1	Mg 1	0	0
56	DP	1	Total 1	Mg 1	0	0
56	DQ	3	Total 3	Mg 3	0	0
56	DR	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DT	1	Total 1	Mg 1	0	0
56	DU	1	Total 1	Mg 1	0	0
56	DV	2	Total 2	Mg 2	0	0
56	DW	2	Total 2	Mg 2	0	0
56	DY	1	Total 1	Mg 1	0	0
56	D0	1	Total 1	Mg 1	0	0
56	D3	1	Total 1	Mg 1	0	0
56	D5	1	Total 1	Mg 1	0	0
56	D7	1	Total 1	Mg 1	0	0
56	D8	2	Total 2	Mg 2	0	0

- Molecule 57 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

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

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AN	1	Total	Zn	0	0
			1	1		
58	BY	1	Total	Zn	0	0
			1	1		
58	B4	1	Total	Zn	0	0
			1	1		
58	B5	1	Total	Zn	0	0
			1	1		
58	B6	1	Total	Zn	0	0
			1	1		
58	B9	1	Total	Zn	0	0
			1	1		
58	CN	1	Total	Zn	0	0
			1	1		
58	DY	1	Total	Zn	0	0
			1	1		
58	D4	1	Total	Zn	0	0
			1	1		
58	D5	1	Total	Zn	0	0
			1	1		
58	D6	1	Total	Zn	0	0
			1	1		
58	D9	1	Total	Zn	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AX	1	Total	K	0	0
			1	1		
59	DA	1	Total	K	0	0
			1	1		

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	AA	165	Total O 165 165	0	0
60	AJ	1	Total O 1 1	0	0
60	AL	3	Total O 3 3	0	0
60	AP	1	Total O 1 1	0	0
60	AU	1	Total O 1 1	0	0
60	AV	2	Total O 2 2	0	0
60	AW	3	Total O 3 3	0	0
60	BA	924	Total O 924 924	0	0
60	BB	27	Total O 27 27	0	0
60	BD	6	Total O 6 6	0	0
60	BE	8	Total O 8 8	0	0
60	BF	6	Total O 6 6	0	0
60	BG	1	Total O 1 1	0	0
60	BH	1	Total O 1 1	0	0
60	BN	3	Total O 3 3	0	0
60	BO	1	Total O 1 1	0	0
60	BP	14	Total O 14 14	0	0
60	BQ	2	Total O 2 2	0	0
60	BS	1	Total O 1 1	0	0
60	BT	4	Total O 4 4	0	0
60	BU	2	Total O 2 2	0	0
60	BV	5	Total O 5 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	BW	1	Total 1	O 1	0	0
60	BX	2	Total 2	O 2	0	0
60	BZ	1	Total 1	O 1	0	0
60	B0	4	Total 4	O 4	0	0
60	B1	2	Total 2	O 2	0	0
60	B2	1	Total 1	O 1	0	0
60	B3	1	Total 1	O 1	0	0
60	B5	2	Total 2	O 2	0	0
60	B7	2	Total 2	O 2	0	0
60	B8	8	Total 8	O 8	0	0
60	CA	113	Total 113	O 113	0	0
60	CE	2	Total 2	O 2	0	0
60	CJ	2	Total 2	O 2	0	0
60	CL	1	Total 1	O 1	0	0
60	CO	1	Total 1	O 1	0	0
60	CW	1	Total 1	O 1	0	0
60	CX	1	Total 1	O 1	0	0
60	DA	689	Total 689	O 689	0	0
60	DB	9	Total 9	O 9	0	0
60	DD	11	Total 11	O 11	0	0
60	DE	5	Total 5	O 5	0	0

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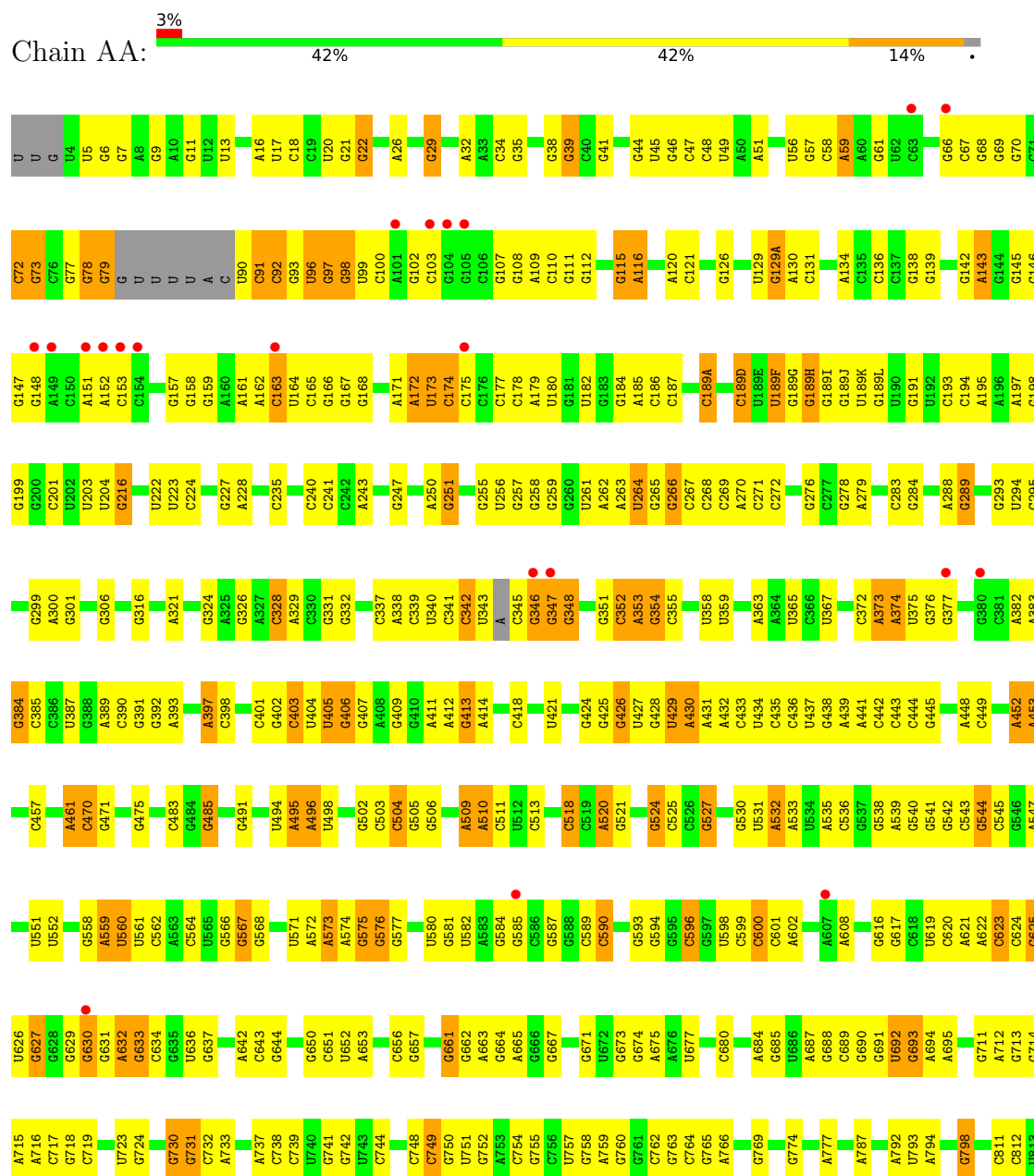
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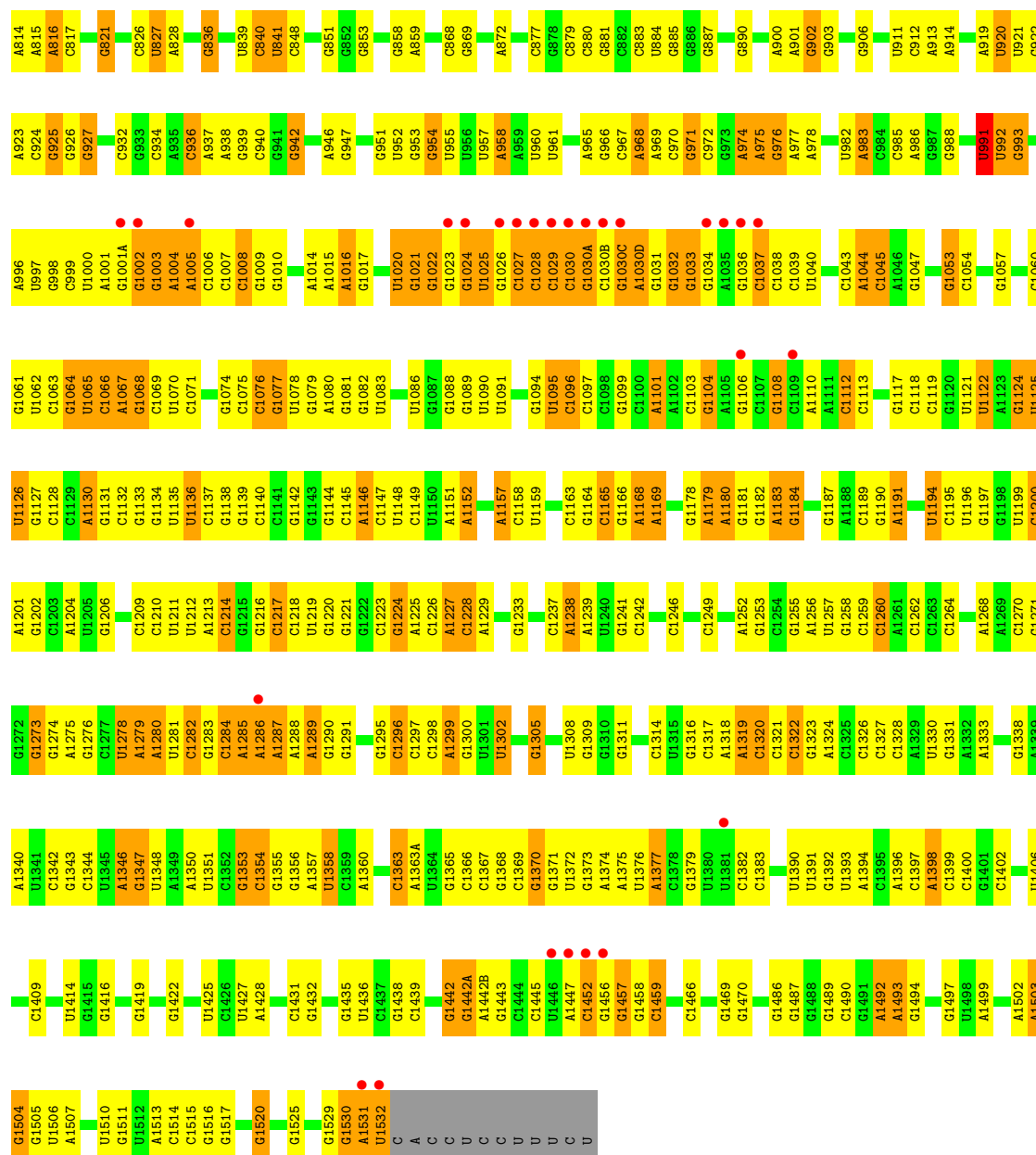
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	DF	6	Total 6	O 6	0	0
60	DO	1	Total 1	O 1	0	0
60	DP	6	Total 6	O 6	0	0
60	DU	3	Total 3	O 3	0	0
60	DV	1	Total 1	O 1	0	0
60	DW	1	Total 1	O 1	0	0
60	DX	3	Total 3	O 3	0	0
60	D0	5	Total 5	O 5	0	0
60	D1	1	Total 1	O 1	0	0
60	D3	1	Total 1	O 1	0	0
60	D8	3	Total 3	O 3	0	0

3 Residue-property plots

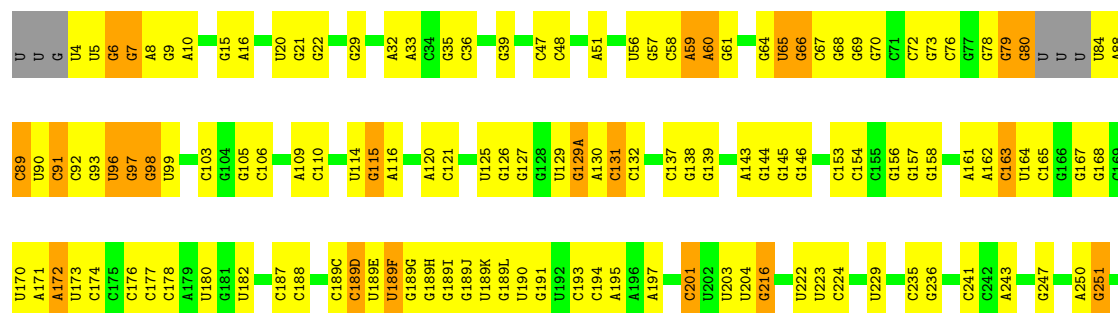
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 16S Ribosomal RNA

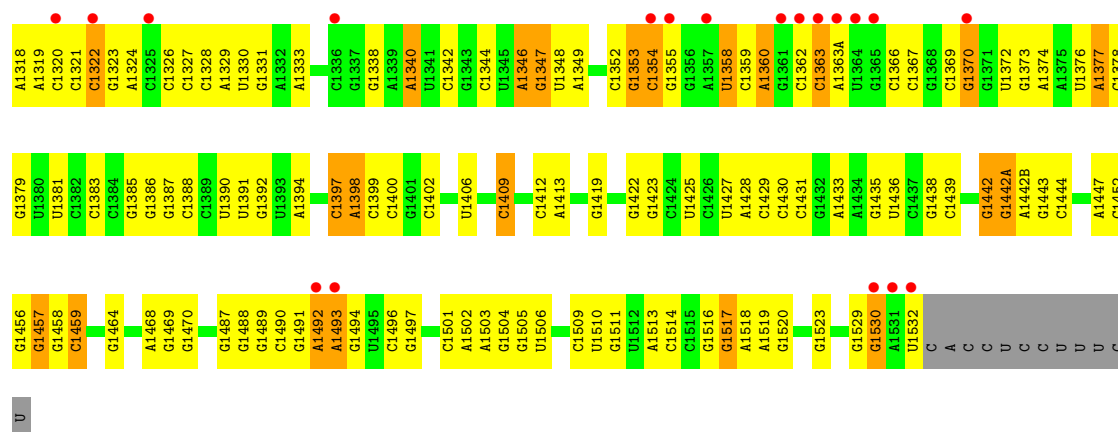




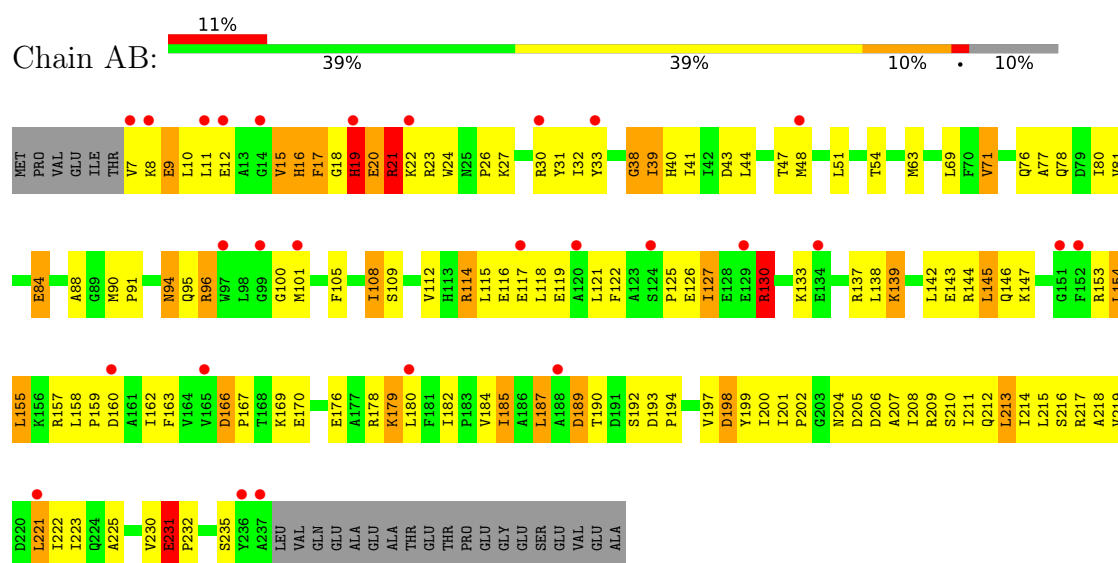
Molecule 1: 16S Ribosomal RNA



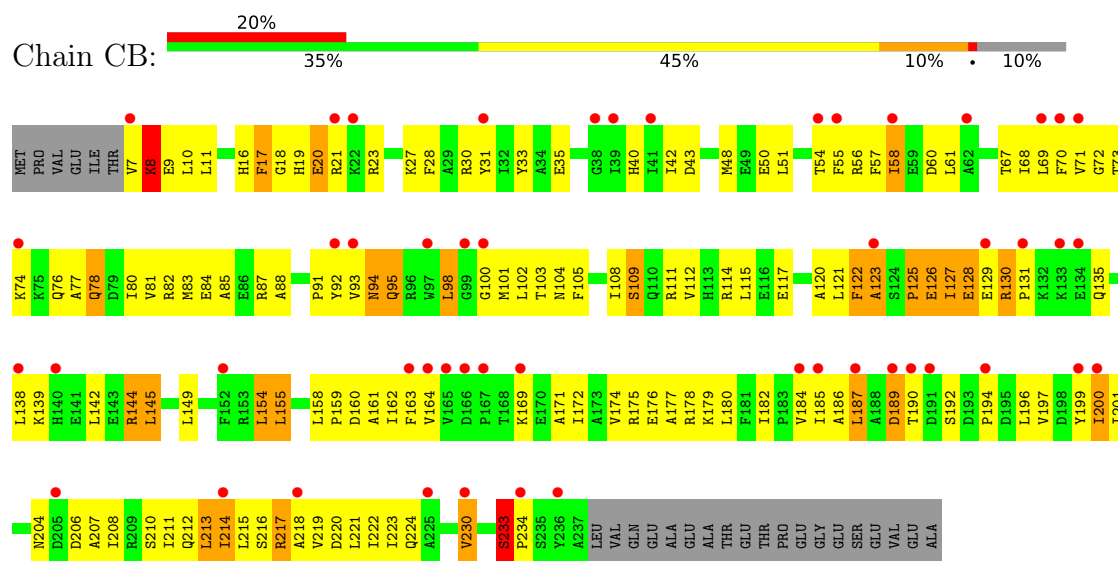
U1257	G1190	C1063	G941	C949	C754	A675	C590	A509	G495	G351	G255
G1258	A1191	G1064	G942	U950	G755	A676	U991	A510	G426	C352	U256
C1259	G1192	U1065	U943	G851	C756	A677	U992	C511	U427	C353	G257
C1260	G1193	C1066	G944	G852	U757	C679	G593	U512	G428	G354	G258
A1261	U1194	A1067	G945	G853	G758	C680	C596	C513	U429	G259	G259
C1262	C1195	G1068	A946	G854	A759	C681	C597	C514	A430	U261	G260
C1263	U1196	C1069	G947	G855	G760	G685	U997	G515	G597	U359	U262
C1264	G1197	G1070	C948	C856	C761	U686	U998	C518	C433	A360	A263
C1267	G1198	G1072	A949	C857	C762	A687	U999	C519	U434	A264	A263
A1268	U1199	U1073	U950	G858	G765	C688	C600	A520	C435	U265	G265
A1269	C1200	G1074	G951	A859	A766	C689	C601	A521	C436	G266	G266
C1270	A1201	C1075	U952	A860	A767	G690	A602	C522	U437	C366	C267
G1271	C1202	C1076	G953	A861	A768	G691	A603	A523	G438	U367	C267
G1272	C1203	G1077	G954	C862	G769	U692	A607	A524	A439	C372	C268
G1273	A1204	U1078	U955	C863	G774	A693	A608	G527	A441	A373	G276
G1274	U1205	G1079	A958	G864	A775	A694	C613	U531	C443	A374	G277
A1275	G1206	A1080	U959	U870	A776	A695	C614	A532	C444	U375	A279
G1276	G1207	G1081	U960	C875	A777	A696	A621	A533	G445	G376	G285
C1277	C1208	U1082	U961	G876	A778	U697	A622	A534	G446	G377	G286
U1278	C1209	U1083	G962	C877	A779	C698	C623	C536	A448	A382	G289
A1279	U1210	U1084	U963	G878	A780	C699	C624	C537	A449	A383	G290
A1280	C1211	U1085	G964	G879	C783	G700	C625	C538	A450	G384	G291
C1281	A1212	G1086	A965	C880	C784	C701	U626	A539	A451	A385	G292
C1282	C1213	U1087	U966	C881	C785	A702	G627	C540	C452	C386	A297
G1283	G1214	G1088	G967	U884	G786	C707	G628	G541	C453	C387	G298
G1284	U1215	U1089	U968	A889	A787	C708	G629	G542	C454	U388	A300
A1285	A1151	U1090	A969	U890	U788	C709	U630	C543	C455	A389	G306
A1286	A1152	A1092	G970	G890	A790	A712	G631	C544	G460	C390	G307
A1287	U1219	A1093	C971	U891	C791	C717	A632	C545	A461	C391	G308
C1288	G1220	G1094	G972	U892	A792	C718	G633	A547	C471	C392	G309
G1289	C1221	U1095	C973	A900	C793	G719	A642	A548	A472	A393	G317
G1290	U1222	C1096	U974	A901	A794	C720	C643	A549	G476	A397	C320
C1291	A1157	C1097	A975	G902	C797	G721	C644	C554	C483	C398	A321
U1292	C1158	U1098	G976	C906	G798	U723	C645	A559	A482	G399	C322
C1293	U1159	C1100	A977	G907	A802	G724	U646	U560	C484	C400	U323
G1294	C1162	A1101	U978	A913	A803	G725	G650	U561	C485	C401	G324
G1295	C1163	U1102	C979	A914	A815	G726	C651	C567	C486	C402	A325
C1296	G1164	C1103	U980	A915	A816	A728	U652	C568	C487	C403	G326
C1297	U1165	U1104	U981	A916	C817	C730	G653	U571	C488	U405	C328
U1298	G1166	A1105	U982	A917	C818	C731	C654	A572	C489	G407	A329
C1299	U1167	C1106	A983	A918	C819	C732	G655	A573	G490	A408	C330
G1300	A1168	U1107	U984	U920	G821	C733	U659	G575	C491	C410	G332
A1301	C1108	C1108	C985	U921	G822	C734	G660	G576	C492	A411	C335
U1302	U1109	C1109	C986	G922	G823	G735	C661	G577	A495	A412	C336
C1303	A1110	A1045	U987	A923	C824	C736	U662	U580	C496	C413	C337
G1304	U1111	U1046	U988	C924	U827	G737	G663	G581	U498	A414	A338
C1305	C1112	G1047	U989	G925	A828	C738	C664	U582	C501	C418	C342
A1306	C1113	U1048	G993	G926	U831	G739	U665	G583	C502	C419	U343
U1307	C1114	G1049	A994	G927	U832	C740	C666	G584	C503	U420	A344
G1308	C1115	U1053	C995	C928	C834	G741	U667	G585	C504	U421	C345
A1309	U1116	C1054	A996	C929	U835	G742	A665	C586	C505	C422	G346
C1310	G1117	U1055	U997	G933	U836	C743	G668	G587	C506	G423	G350
A1311	C1118	U1056	G998	C934	G837	C744	C669	G588	C507	G424	
U1312	C1119	G1057	U999	A935	G838	C745	U670	G589	C508		
G1313	A1184	U1058	U1000	C936	G839	C746	C671	G590	C509		
A1314	C1185	C1059	A1001	A937	U839	C747	U672	C591	C510		
C1315	U1121	C1060	U1002	A938	C840	C748	G673	C592	C511		
G1316	U1122	G1061	G1003	A939	U841	C749	U674	C593	C512		
C1317	A1123	U1062	C1004	G940	C842	C750	G675	C594	C513		



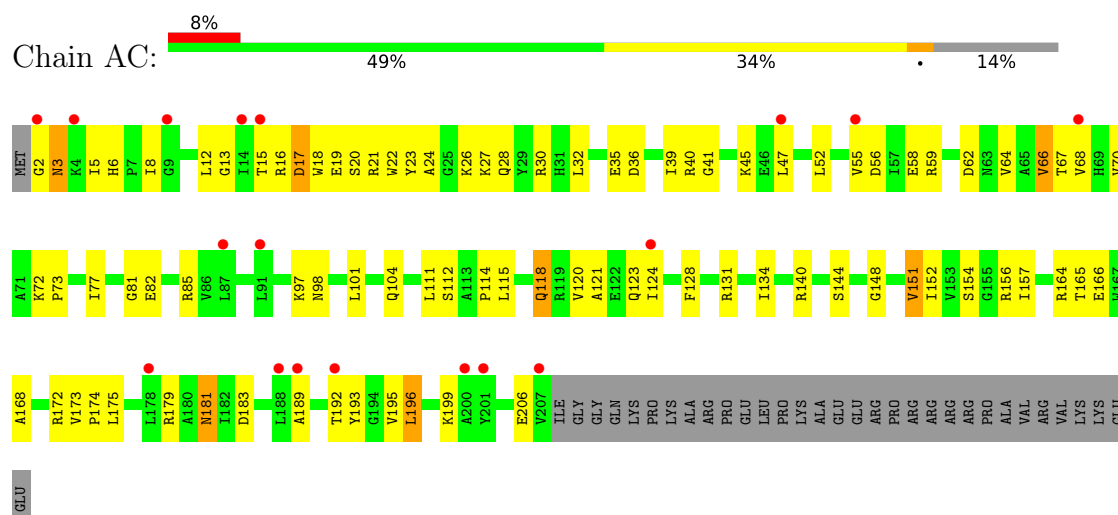
• Molecule 2: 30S ribosomal protein S2



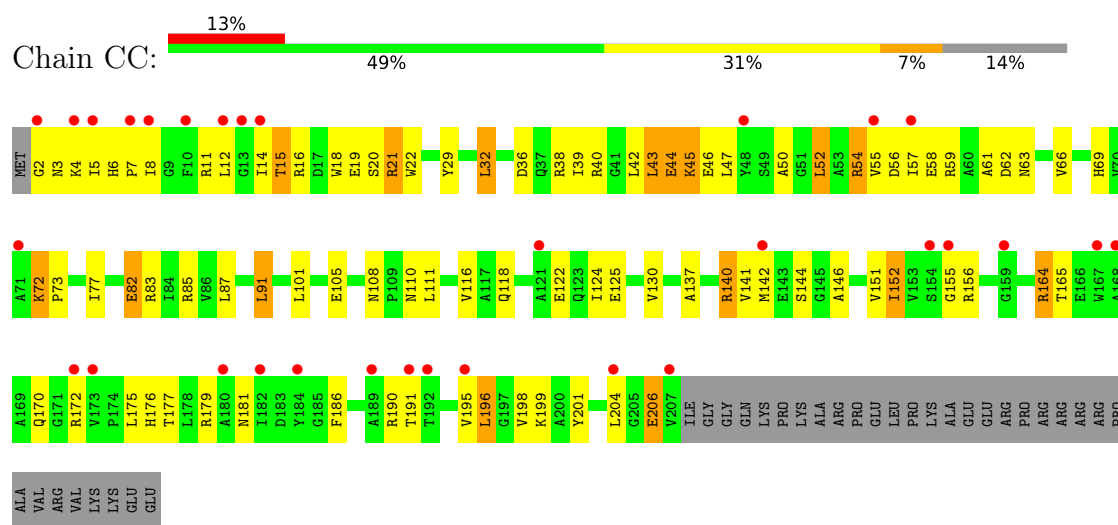
• Molecule 2: 30S ribosomal protein S2



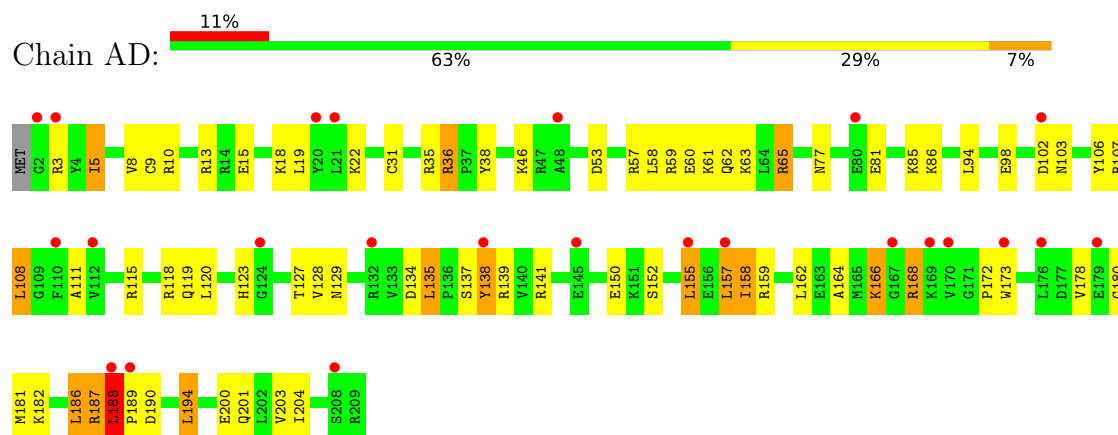
• Molecule 3: 30S ribosomal protein S3



• Molecule 3: 30S ribosomal protein S3

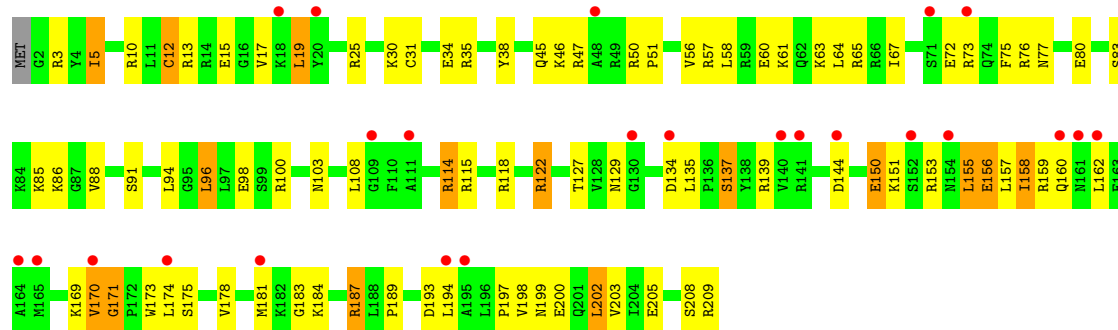


• Molecule 4: 30S ribosomal protein S4

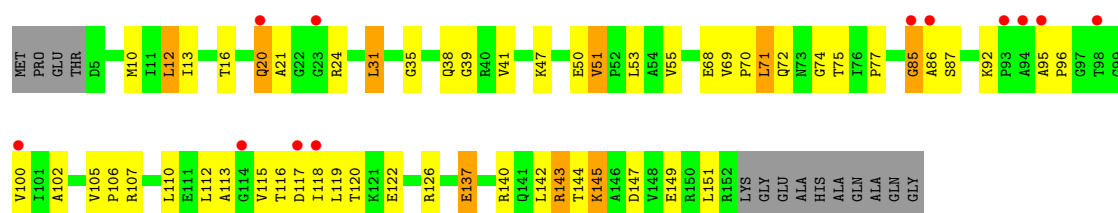


• Molecule 4: 30S ribosomal protein S4

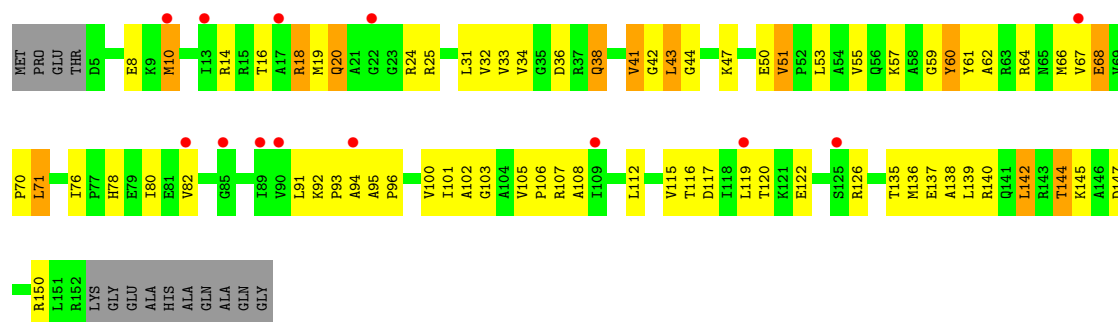




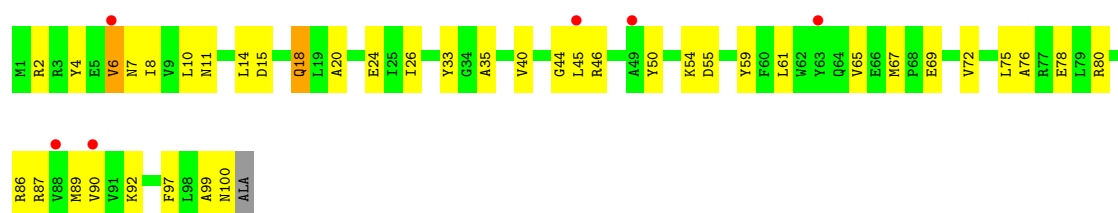
• Molecule 5: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S5

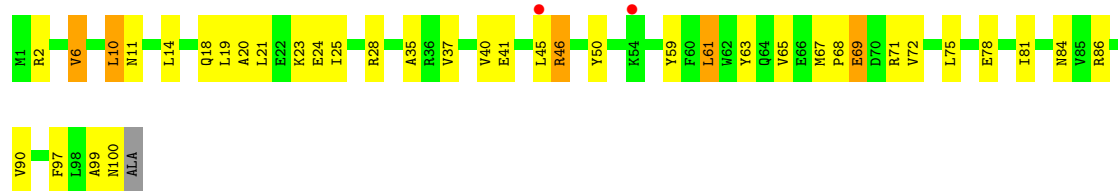


• Molecule 6: 30S ribosomal protein S6



• Molecule 6: 30S ribosomal protein S6





• Molecule 7: 30S ribosomal protein S7



• Molecule 7: 30S ribosomal protein S7



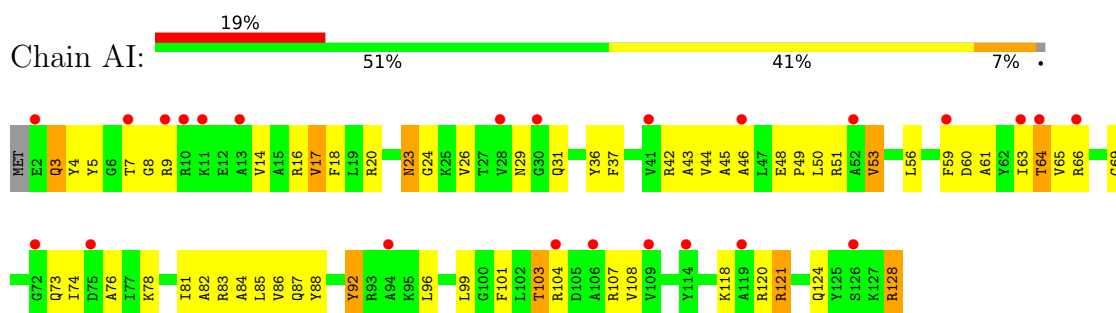
• Molecule 8: 30S ribosomal protein S8



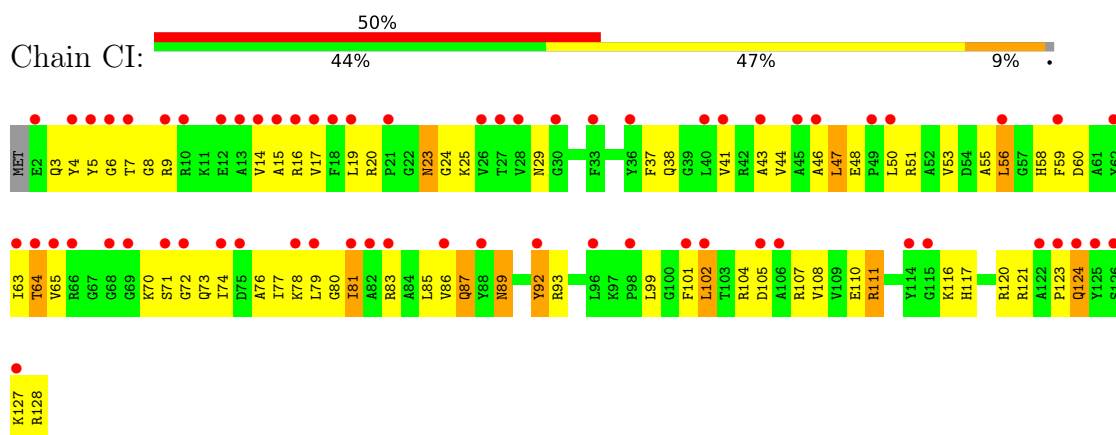
• Molecule 8: 30S ribosomal protein S8



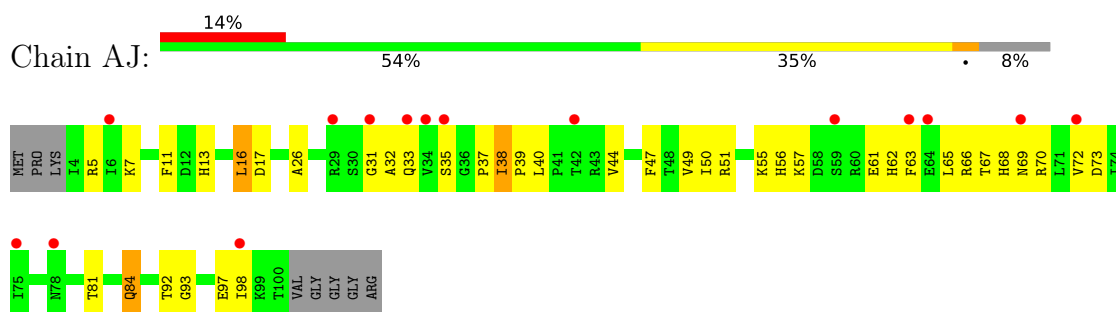
- Molecule 9: 30S ribosomal protein S9



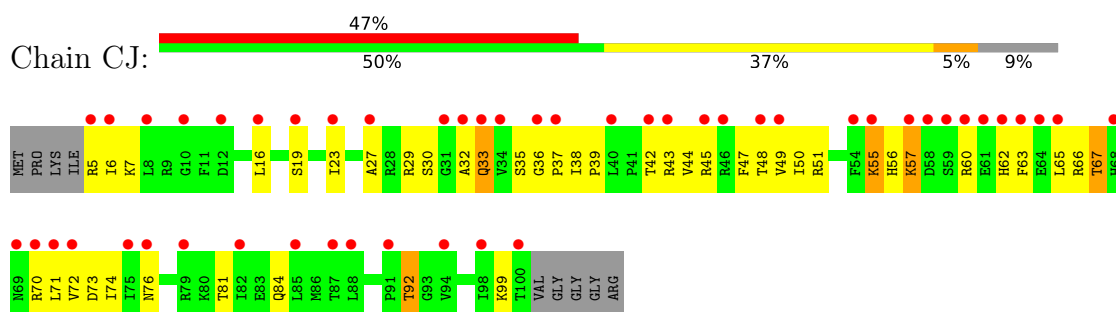
- Molecule 9: 30S ribosomal protein S9



- Molecule 10: 30S ribosomal protein S10

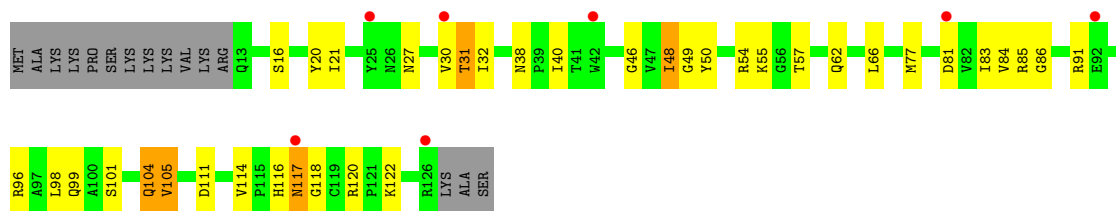


- Molecule 10: 30S ribosomal protein S10

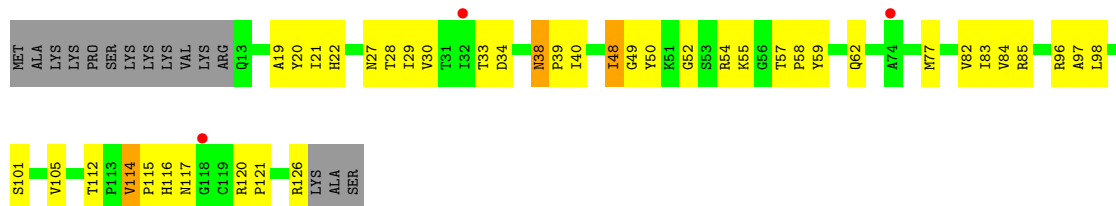


- Molecule 11: 30S ribosomal protein S11

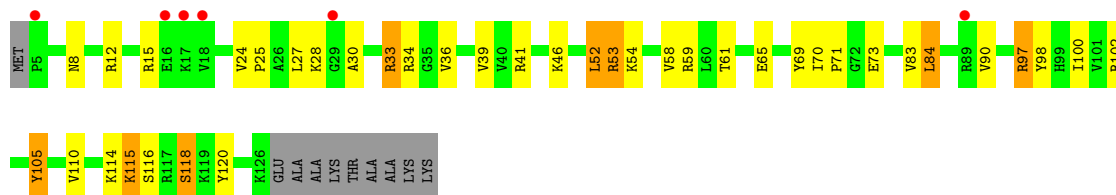




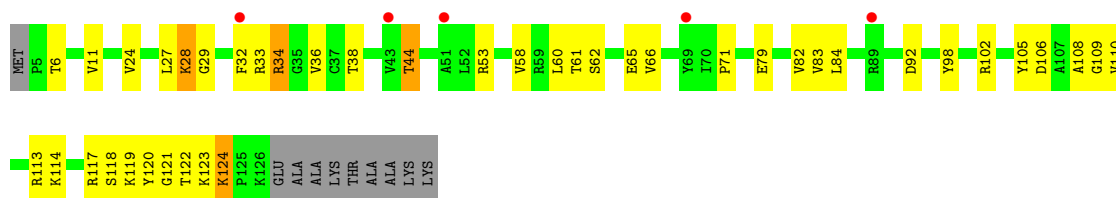
- Molecule 11: 30S ribosomal protein S11



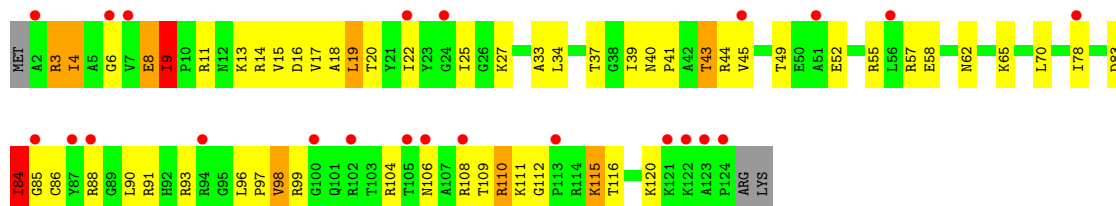
- Molecule 12: 30S ribosomal protein S12



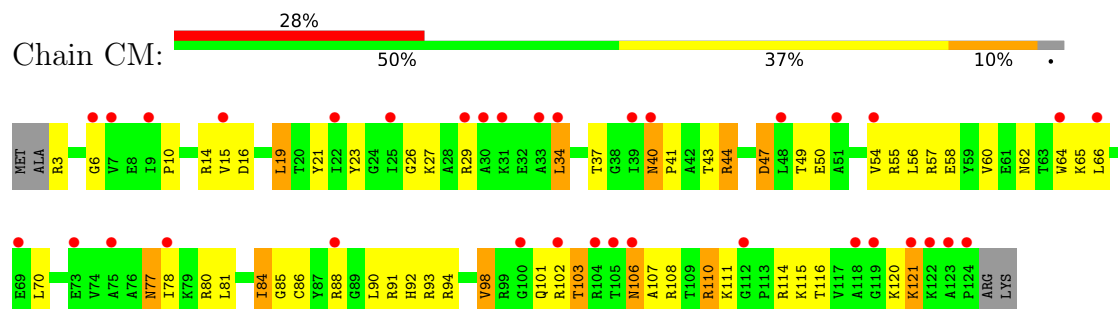
- Molecule 12: 30S ribosomal protein S12



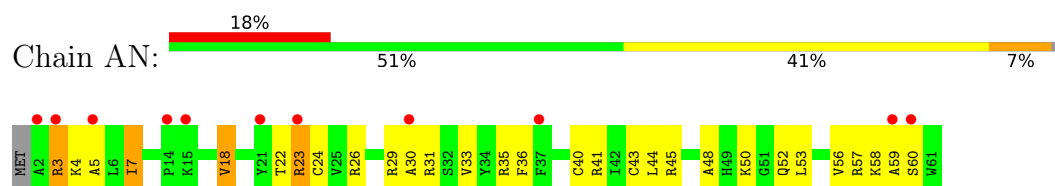
- Molecule 13: 30S ribosomal protein S13



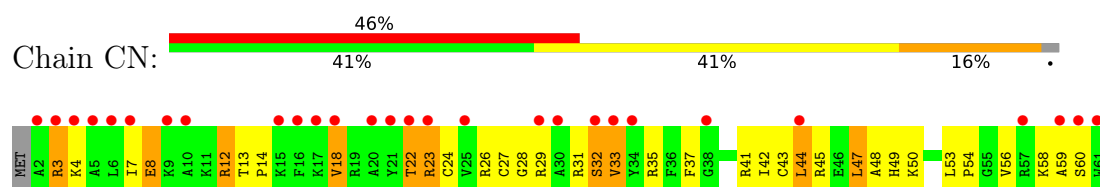
- Molecule 13: 30S ribosomal protein S13



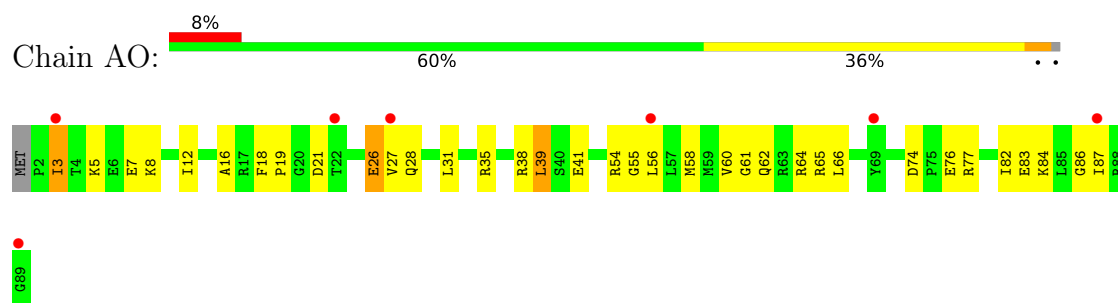
- Molecule 14: 30S ribosomal protein S14 type Z



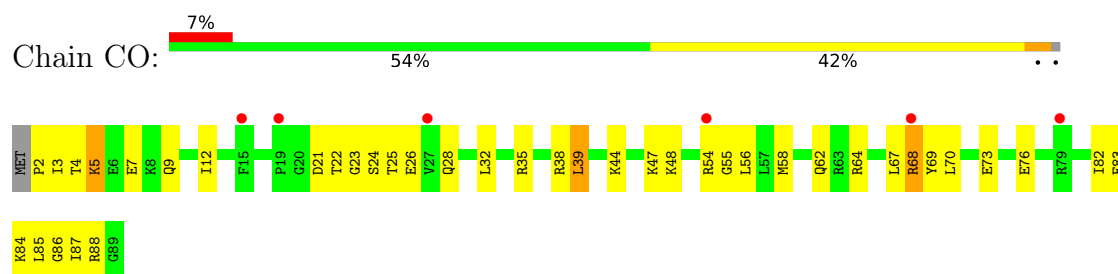
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 15: 30S ribosomal protein S15

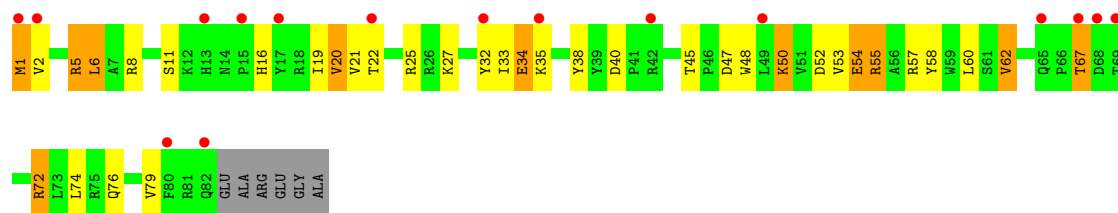


- Molecule 15: 30S ribosomal protein S15

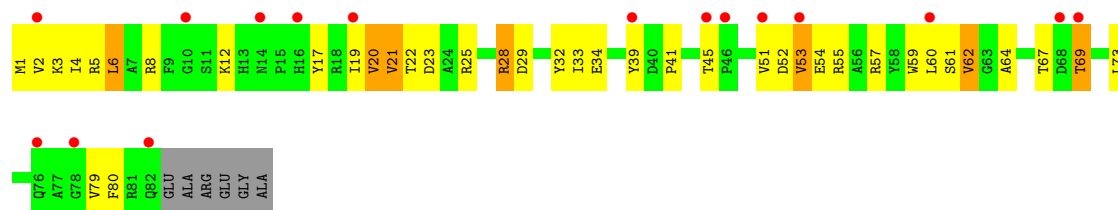


- Molecule 16: 30S ribosomal protein S16





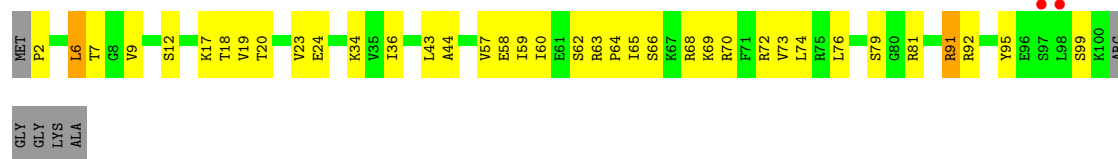
• Molecule 16: 30S ribosomal protein S16



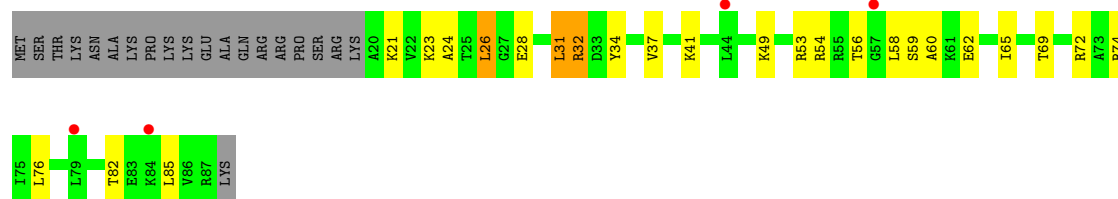
• Molecule 17: 30S ribosomal protein S17



• Molecule 17: 30S ribosomal protein S17

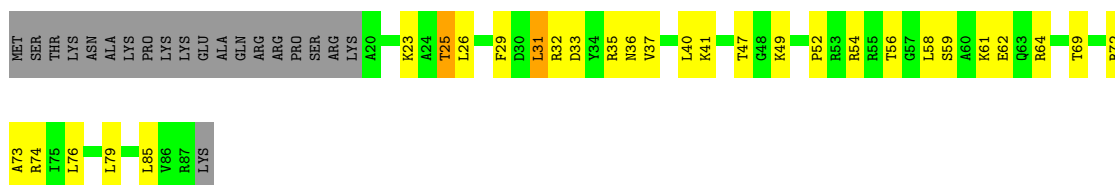


• Molecule 18: 30S ribosomal protein S18

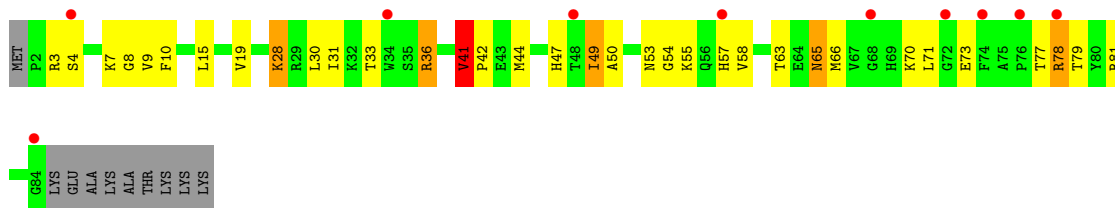


• Molecule 18: 30S ribosomal protein S18

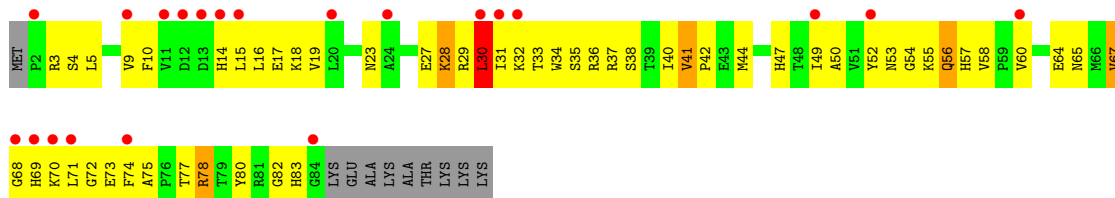




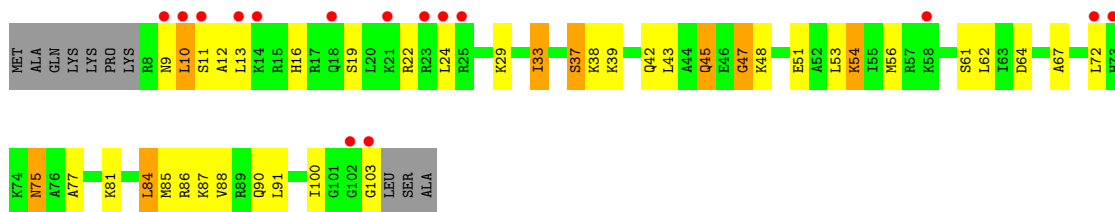
- Molecule 19: 30S ribosomal protein S19



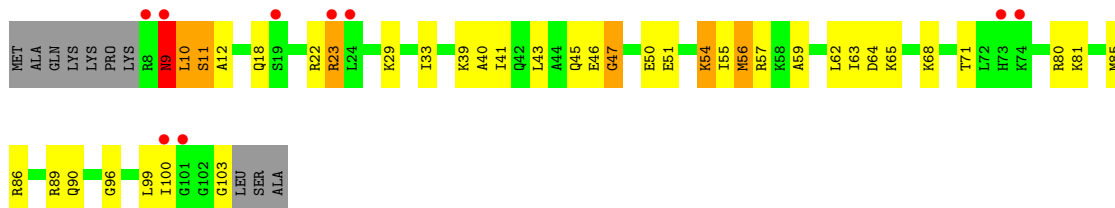
- Molecule 19: 30S ribosomal protein S19



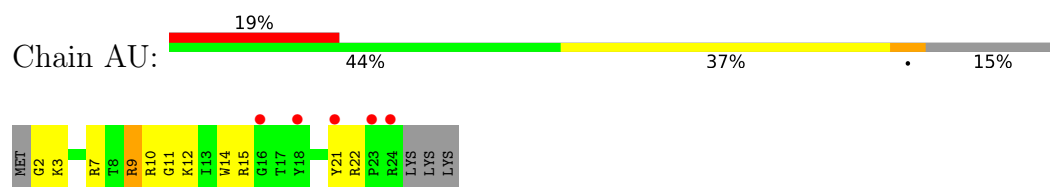
- Molecule 20: 30S ribosomal protein S20



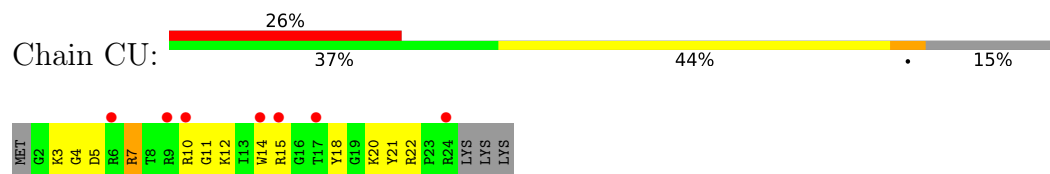
- Molecule 20: 30S ribosomal protein S20



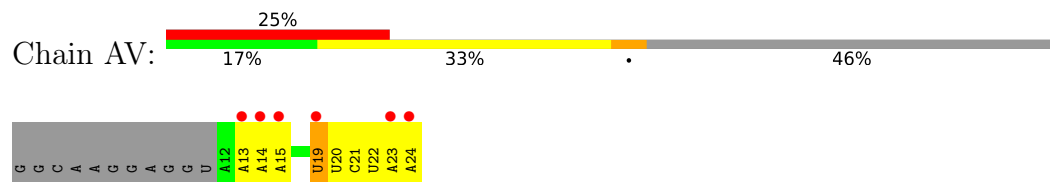
- Molecule 21: 30S ribosomal protein Thx



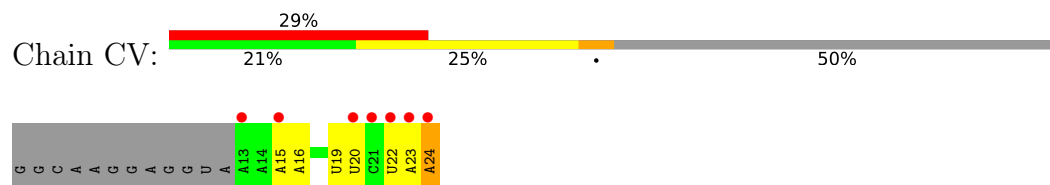
- Molecule 21: 30S ribosomal protein Thx



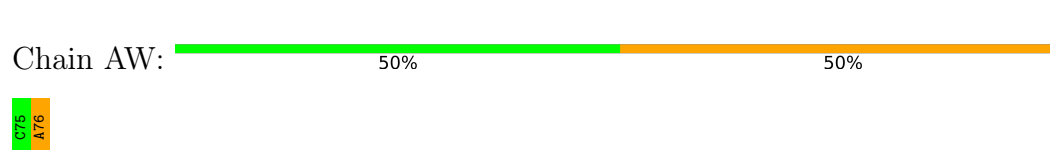
- Molecule 22: mRNA



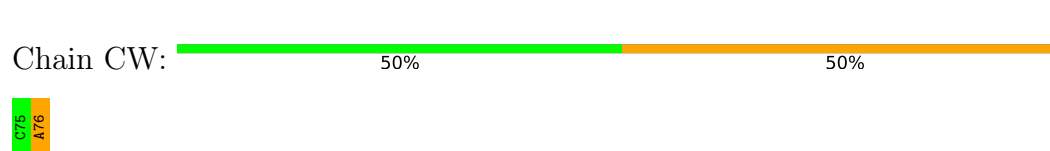
- Molecule 22: mRNA



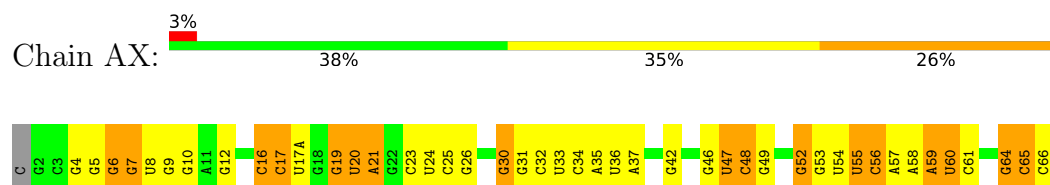
- Molecule 23: Cytidine-Puromycin



- Molecule 23: Cytidine-Puromycin



- Molecule 24: P-site tRNA





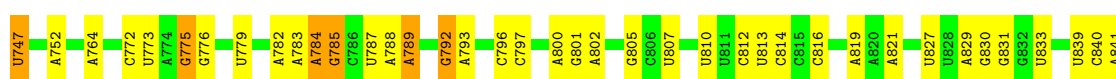
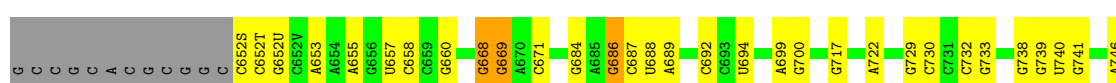
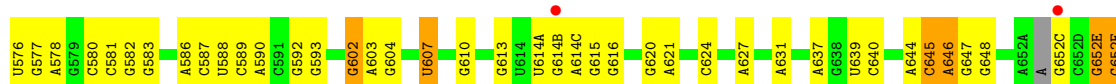
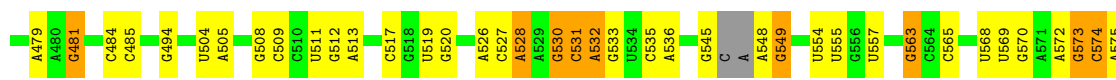
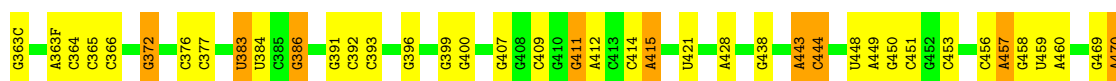
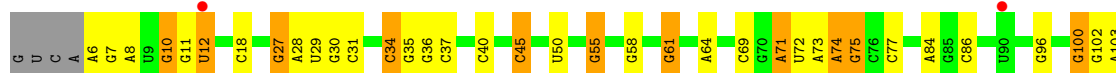
• Molecule 24: P-site tRNA

Chain CX: 36% 38% 25%

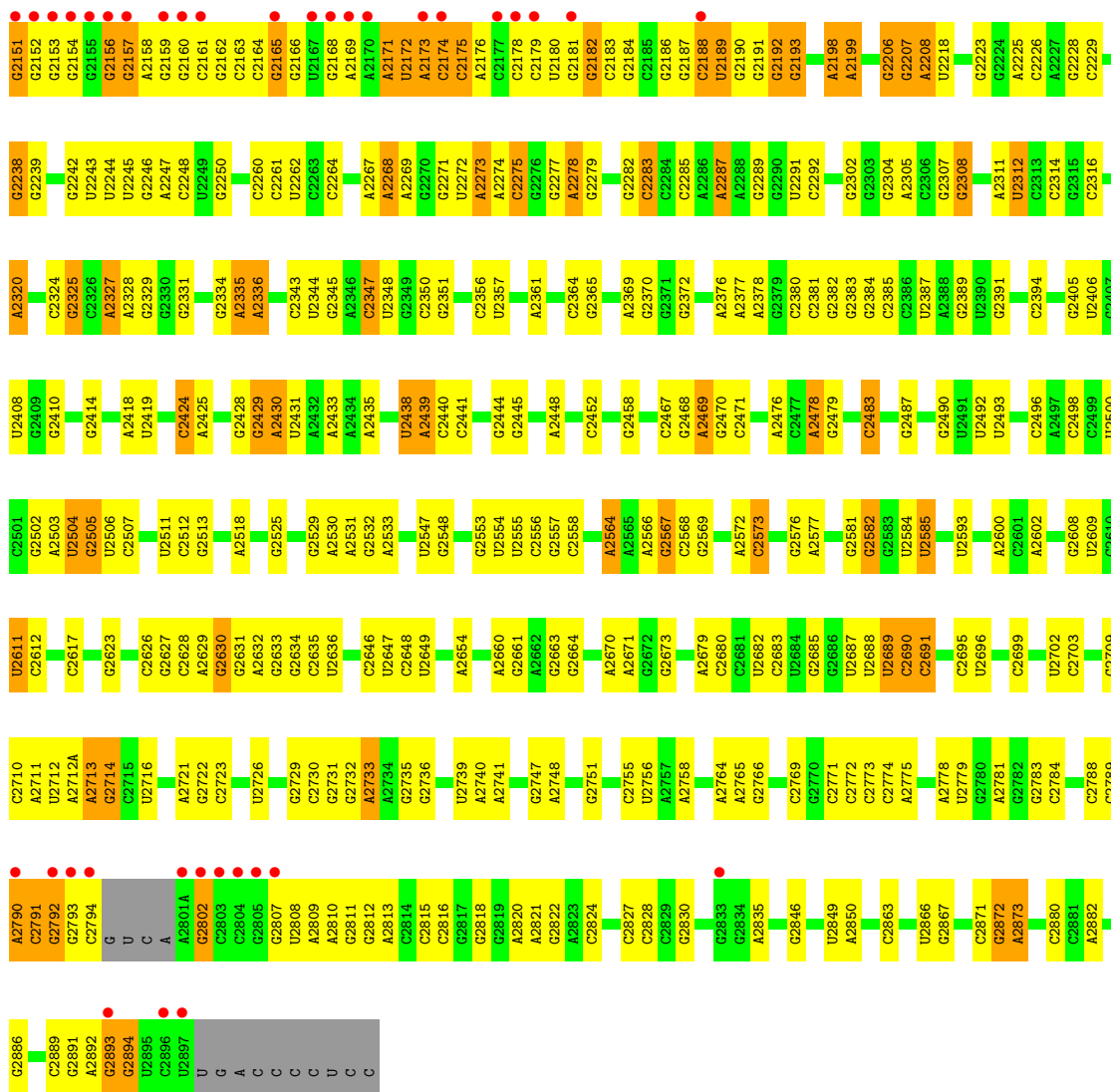


• Molecule 25: 23S Ribosomal RNA

Chain BA: 3% 54% 34% 9%

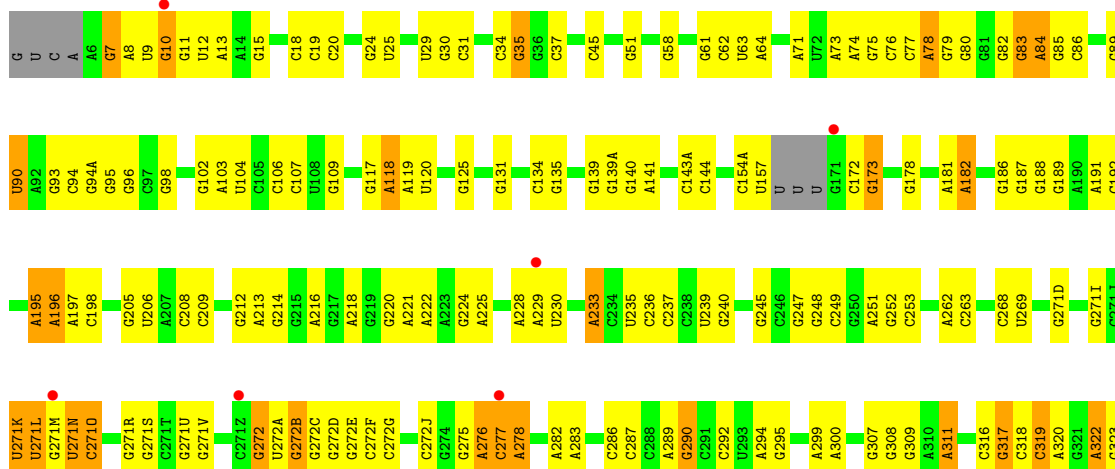






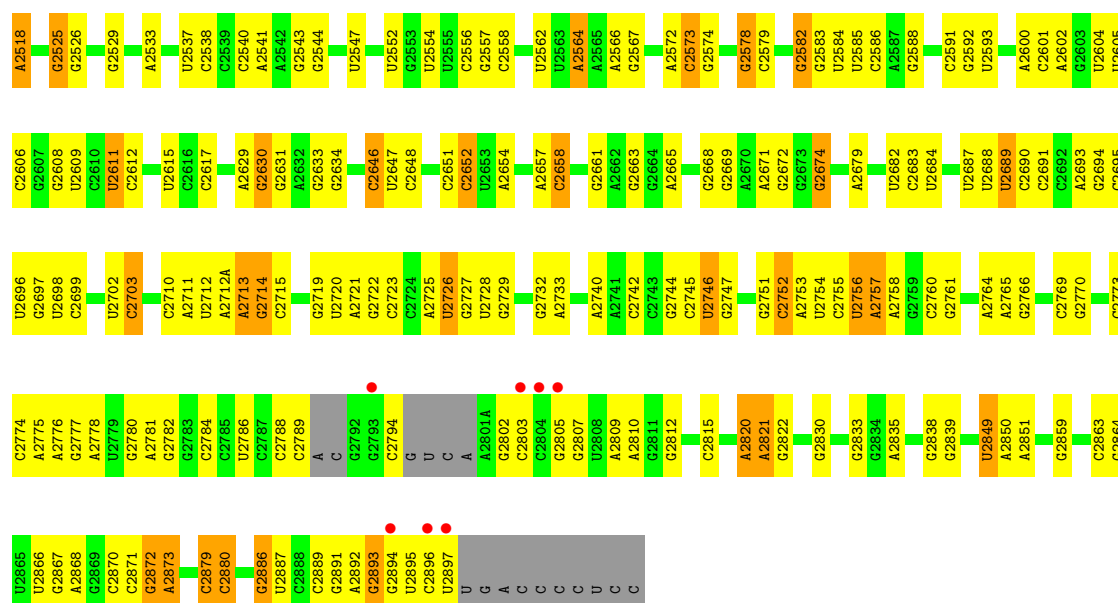
• Molecule 25: 23S Ribosomal RNA

Chain DA: 2% 44% 41% 11% •



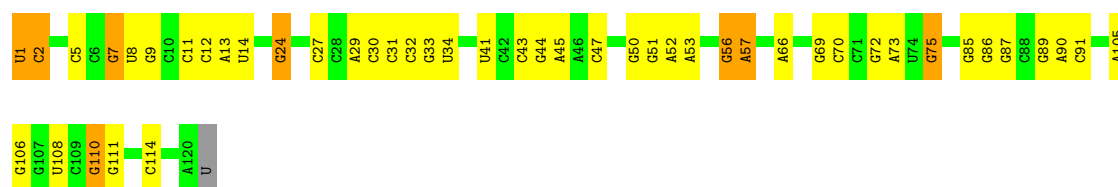
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G1216	G1219	G1220	G1221	C1221A	C1224	G1225	A1226	G1227	G1228	G1229	G1230	G1231	G1232	C1233	U1234	G1235	G1239	U1240	A1241	A1242	G1243	G1244	G1245	A1246	A1247	G1248	U1249	G1250	C1251	G1252	A1253	A1254	U1255	G1256	G1260	C1261	U1263	G1264	A1265	G1266	A1269	C1270	G1271	A1272	U1273	A1274	A1275	U1276	G1277	A1278	U1288		
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G2421	G2277	G2221	G2277	G2221	G2055	C1978	G1859	G1666	C1597	G1529	A1448
G2422	G2278	G2222	G2278	G2222	G2056	A1979	A1877	G1667	C1598	C1530	G1450
G2423	G2279	G2223	G2279	G2223	G2057	G1980	G1878	G1668	C1599	C1531	C1450A
G2424	G2280	G2224	G2280	G2224	G2058	U1981	A1879	G1669	C1600	G1532	C1451
G2425	G2281	G2225	G2281	G2225	A2059	C1982	C1880	G1670	G1601	G1533	
G2426	G2282	G2226	G2282	G2226	G2060	U1983	C1881	A1674	U		G1459
G2427	G2283	G2227	G2283	G2227	G2061	C1984	A1882	G1675	A	C1536	C1462
G2428	G2284	G2228	G2284	G2228	G2062	U1985	G1883	G1676	C1608	C1537	C1463
G2429	G2285	G2229	G2285	G2229	G2063	A1986	A1884	A1677	A1609	G1538	C1464
A2430	G2286	G2230	G2286	G2230	G2064	U1987	G1885	G1678	C1610	G1465	
A2431	A2287	G2231	A2287	G2231	G2065	C1988	A1886	G1679	C1611	G1466	
A2432	G2288	G2232	G2288	G2232	G2066	U1989	A1887	G1680	C1612	U1540	
A2433	G2289	G2233	G2289	G2233	G2067	A1990	A1888	G1681	G1613	A1542	
A2434	G2290	G2234	G2290	G2234	G2068	U1991	A1889	G1682			
A2435	G2291	G2235	G2291	G2235	G2069	A1992	A1890	G1683			
G2436	G2292	G2236	G2292	G2236	G2070	C1993	A1891	G1684			
U2437	G2293	G2237	G2293	G2237	G2071	U1994	A1892	G1685			
U2438	G2294	G2238	G2294	G2238	G2072	A1995	A1893	G1686			
A2439	G2295	G2239	G2295	G2239	G2073	U1996	A1894	G1687			
A2440	U2296	G2240	U2296	G2240	G2074	G1997	A1895	G1688			
G2441	C2297	A2375	C2297	A2375	U2075	U1998	C1896	G1689			
G2442	A2298	G2375	A2298	G2375	G2076		C1897				
G2443	G2299	A2376	G2299	A2376	G2077		C1898				
G2444					G2078		C1899				



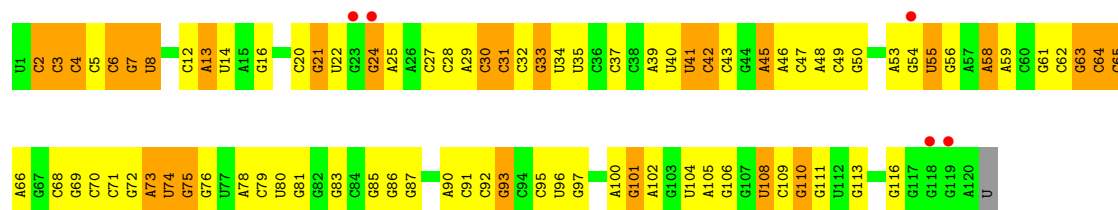
• Molecule 26: 5S Ribosomal RNA

Chain BB: 60% 32% 7% .



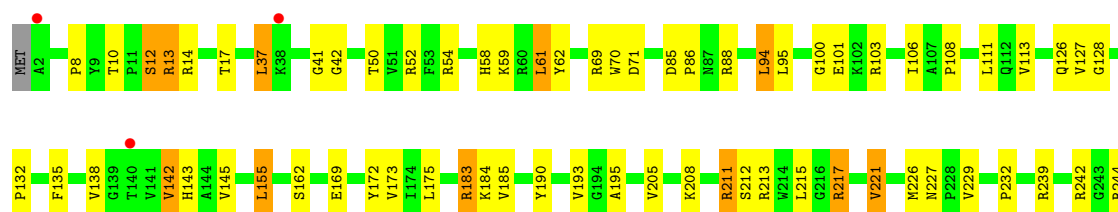
• Molecule 26: 5S Ribosomal RNA

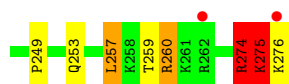
Chain DB: 4% 29% 48% 22% .



• Molecule 27: 50S ribosomal protein L2

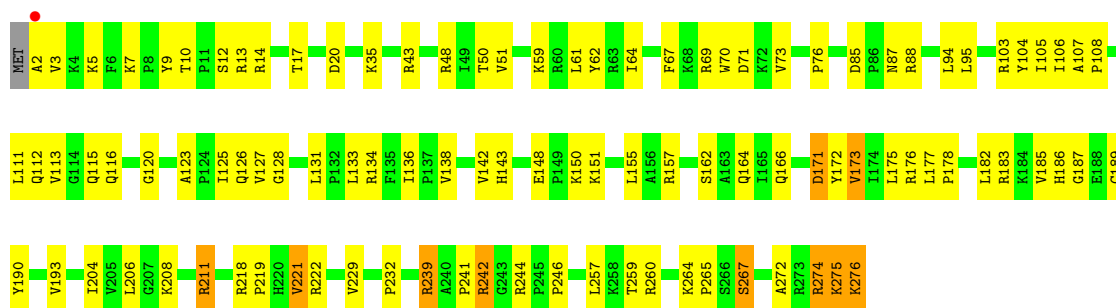
Chain BD: 2% 72% 22% 5% .





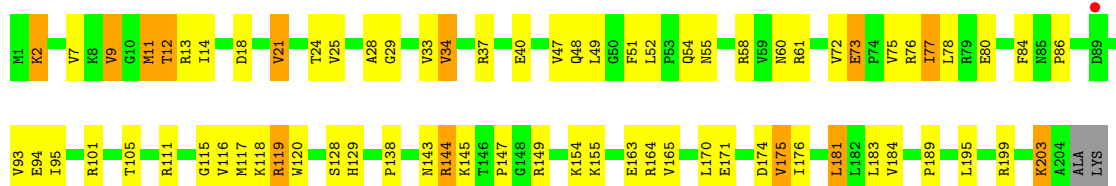
- Molecule 27: 50S ribosomal protein L2

Chain DD: 62% 34%



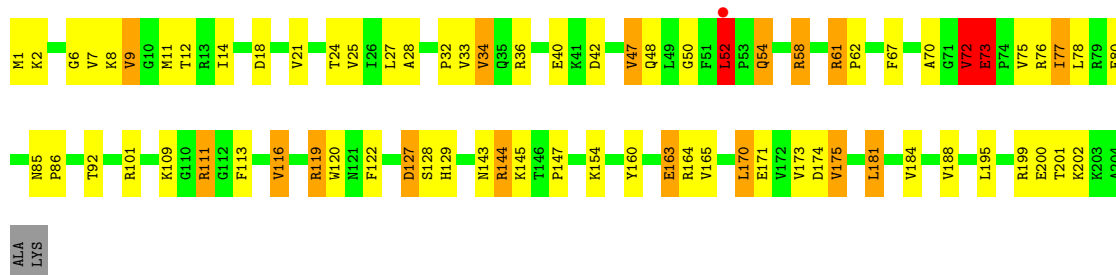
- Molecule 28: 50S ribosomal protein L3

Chain BE: 64% 29% 6%



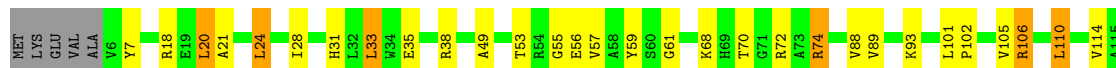
- Molecule 28: 50S ribosomal protein L3

Chain DE: 63% 27% 8%



- Molecule 29: 50S ribosomal protein L4

Chain BF: 68% 25%

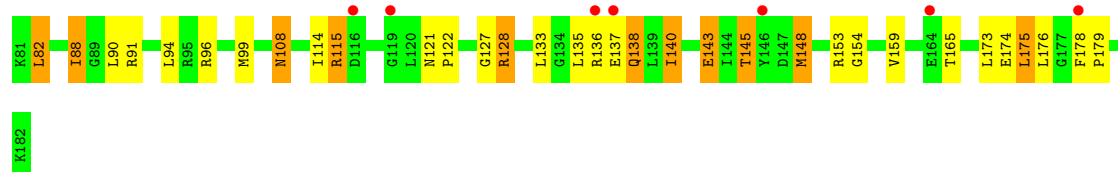




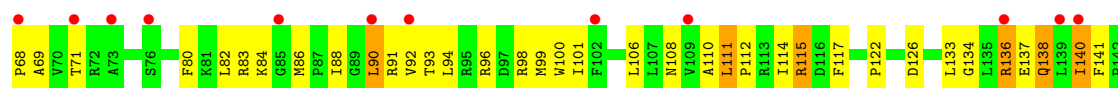
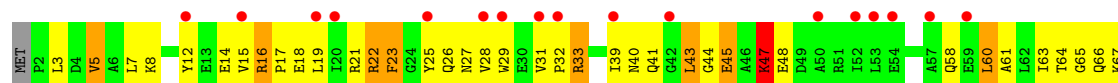
- Molecule 29: 50S ribosomal protein L4



- Molecule 30: 50S ribosomal protein L5

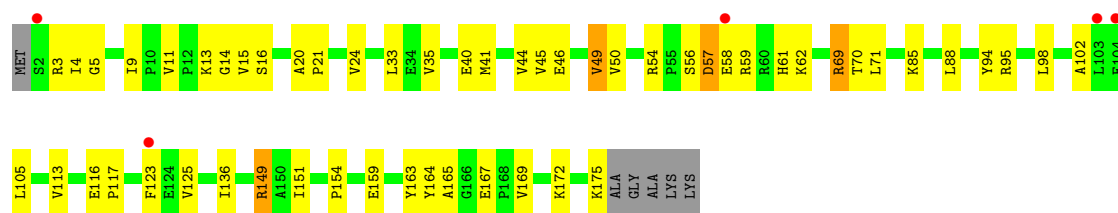


- Molecule 30: 50S ribosomal protein L5

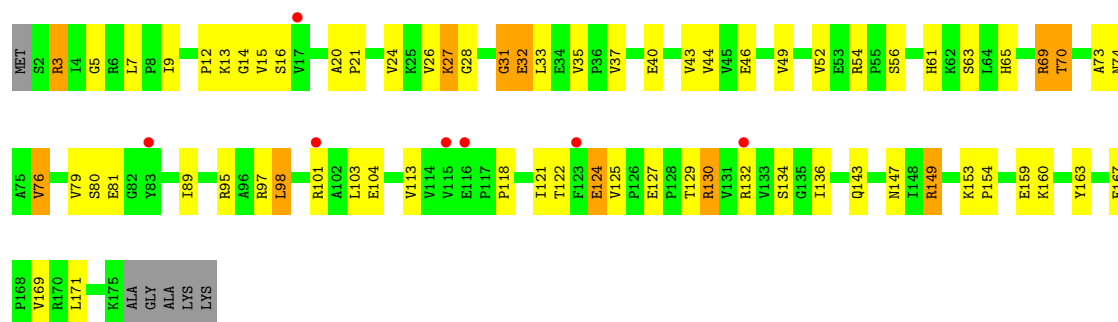


- Molecule 31: 50S ribosomal protein L6

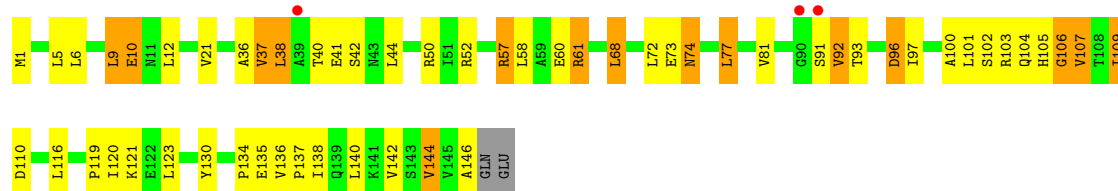




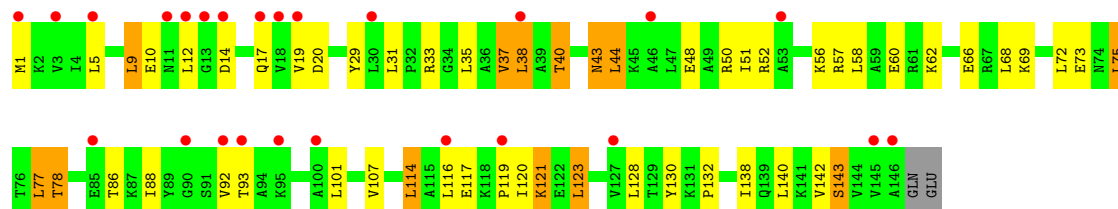
• Molecule 31: 50S ribosomal protein L6



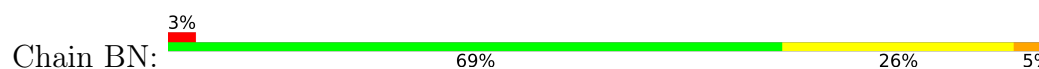
• Molecule 32: 50S ribosomal protein L9

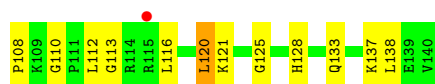


• Molecule 32: 50S ribosomal protein L9



• Molecule 33: 50S ribosomal protein L13

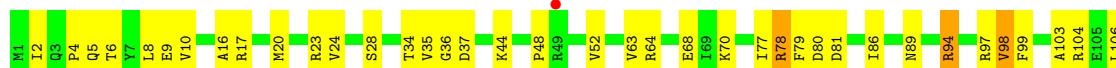




- Molecule 33: 50S ribosomal protein L13



- Molecule 34: 50S ribosomal protein L14



- Molecule 34: 50S ribosomal protein L14

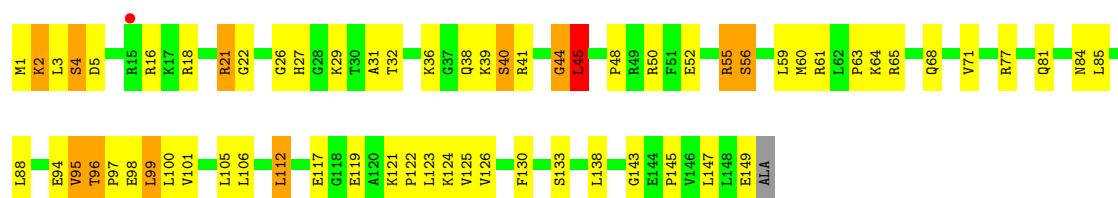


- Molecule 35: 50S ribosomal protein L15

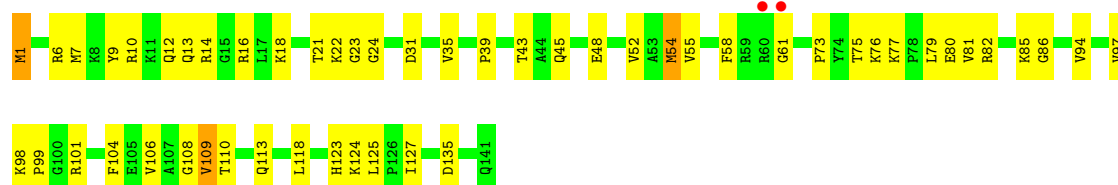


- Molecule 35: 50S ribosomal protein L15

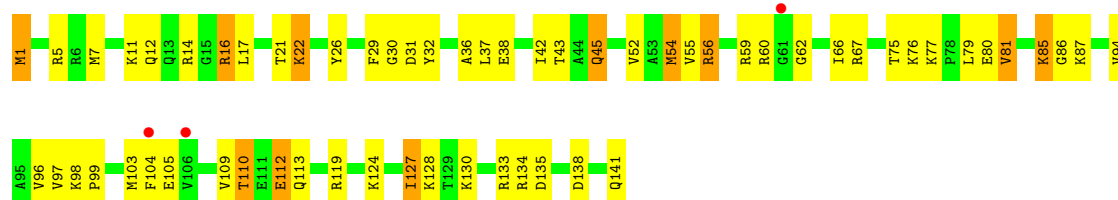




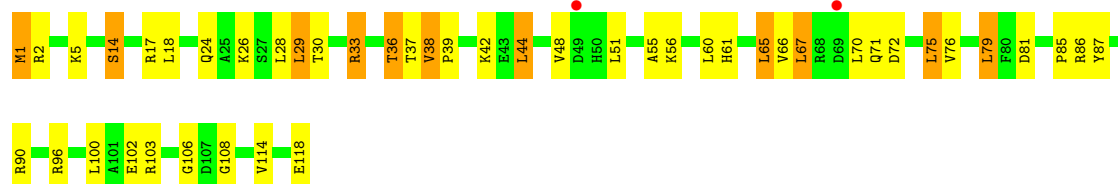
• Molecule 36: 50S ribosomal protein L16



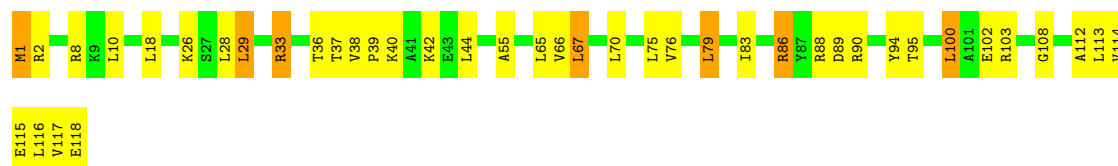
• Molecule 36: 50S ribosomal protein L16



• Molecule 37: 50S ribosomal protein L17



• Molecule 37: 50S ribosomal protein L17



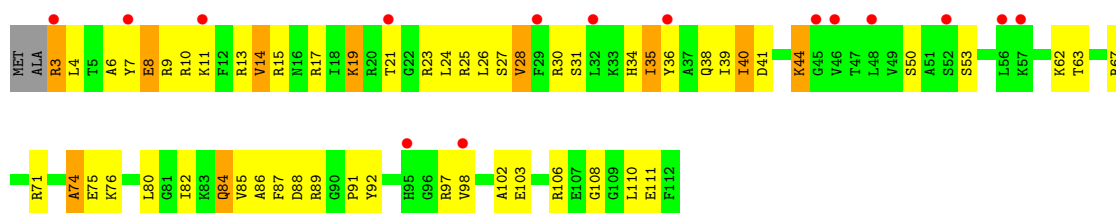
• Molecule 38: 50S ribosomal protein L18

Chain BS:  66% 28%



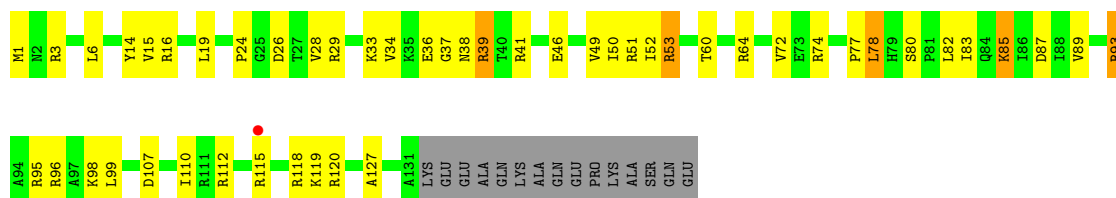
• Molecule 38: 50S ribosomal protein L18

Chain DS:  13% 47% 42% 9%



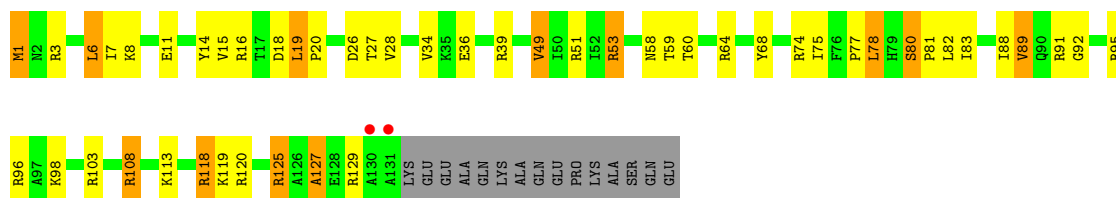
• Molecule 39: 50S ribosomal protein L19

Chain BT:  56% 30% 10%



• Molecule 39: 50S ribosomal protein L19

Chain DT:  55% 26% 8% 10%



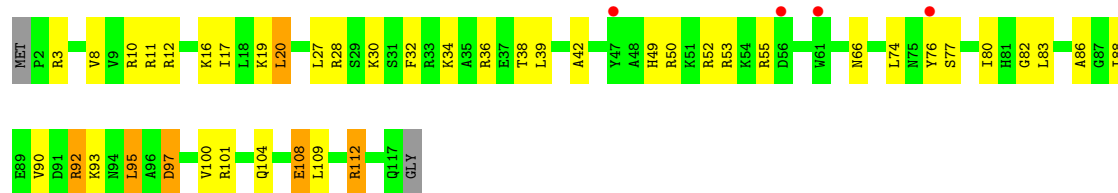
• Molecule 40: 50S ribosomal protein L20

Chain BU:  76% 19%



• Molecule 40: 50S ribosomal protein L20

Chain DU:  3% 62% 31% 5%



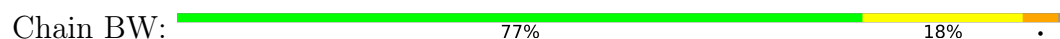
- Molecule 41: 50S ribosomal protein L21



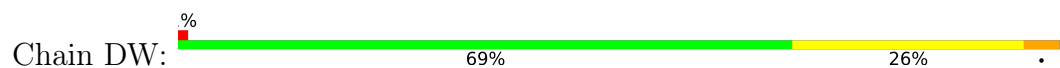
- Molecule 41: 50S ribosomal protein L21



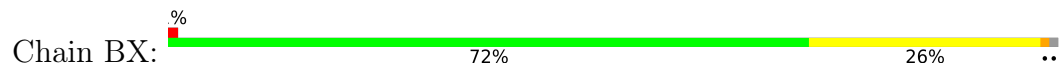
- Molecule 42: 50S ribosomal protein L22



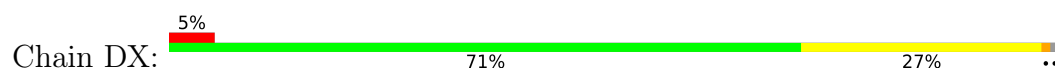
- Molecule 42: 50S ribosomal protein L22



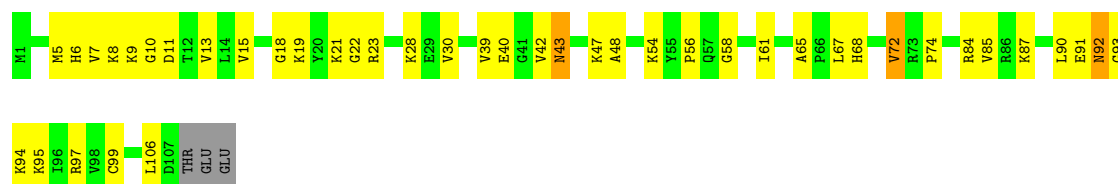
- Molecule 43: 50S ribosomal protein L23



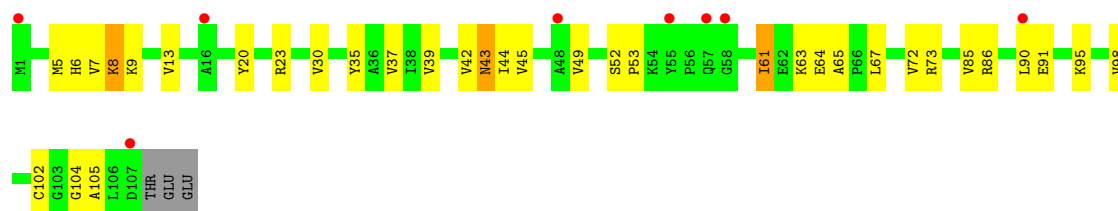
- Molecule 43: 50S ribosomal protein L23



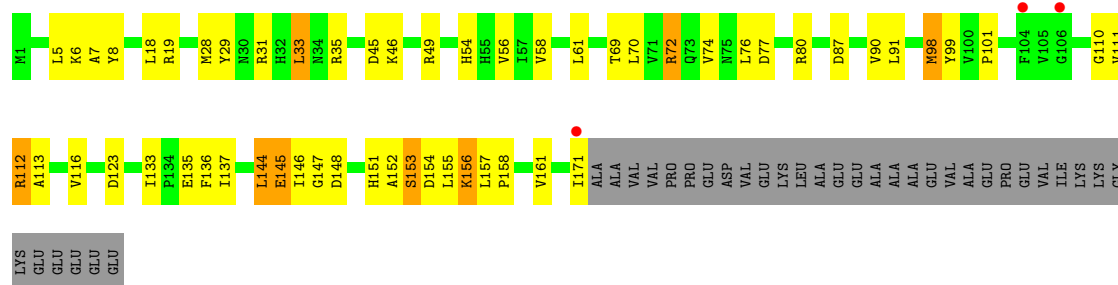
• Molecule 44: 50S ribosomal protein L24



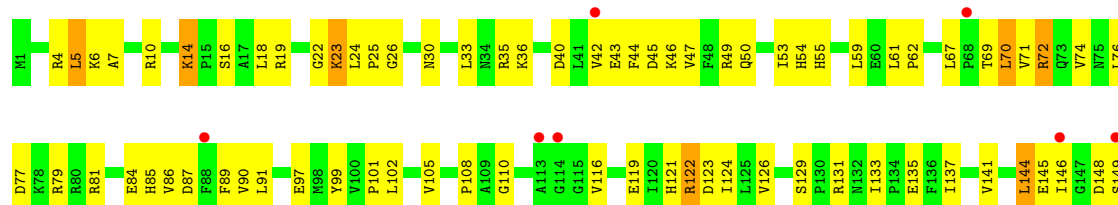
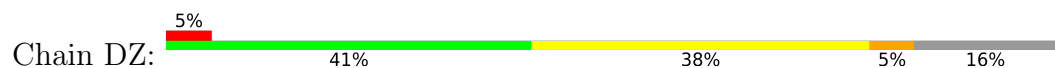
• Molecule 44: 50S ribosomal protein L24

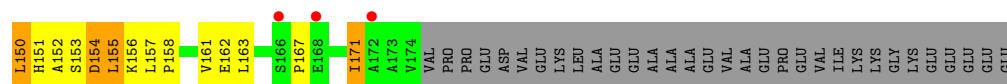


• Molecule 45: 50S ribosomal protein L25



• Molecule 45: 50S ribosomal protein L25

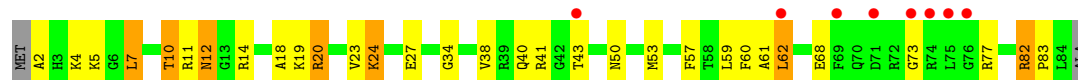




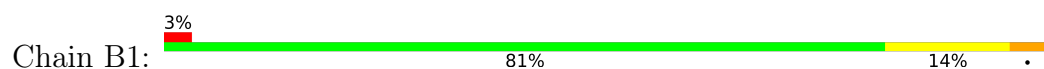
- Molecule 46: 50S ribosomal protein L27



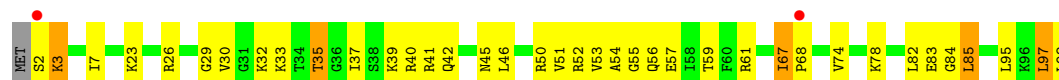
- Molecule 46: 50S ribosomal protein L27



- Molecule 47: 50S ribosomal protein L28



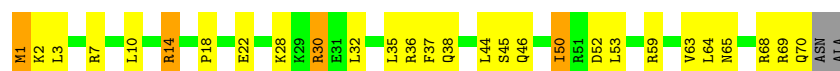
- Molecule 47: 50S ribosomal protein L28



- Molecule 48: 50S ribosomal protein L29

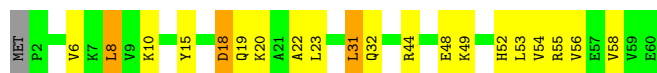


- Molecule 48: 50S ribosomal protein L29



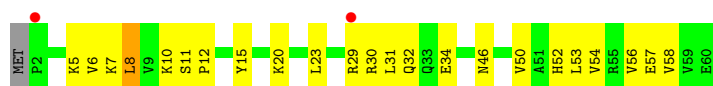
- Molecule 49: 50S ribosomal protein L30

Chain B3:  65% 28% 5% .



- Molecule 49: 50S ribosomal protein L30

Chain D3:  3% 60% 37% ..



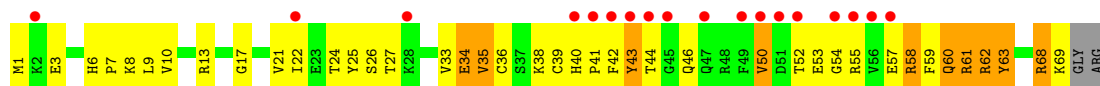
- Molecule 50: 50S ribosomal protein L31

Chain B4:  11% 48% 30% 18% ..



- Molecule 50: 50S ribosomal protein L31

Chain D4:  25% 39% 44% 14% .



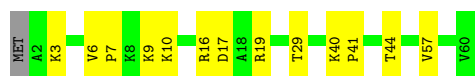
- Molecule 51: 50S ribosomal protein L32

Chain B5:  65% 30% ..



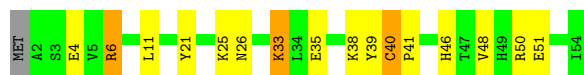
- Molecule 51: 50S ribosomal protein L32

Chain D5:  77% 22% .



- Molecule 52: 50S ribosomal protein L33

Chain B6:  69% 24% 6% .



- Molecule 52: 50S ribosomal protein L33



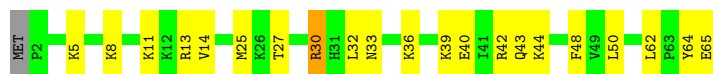
- Molecule 53: 50S ribosomal protein L34



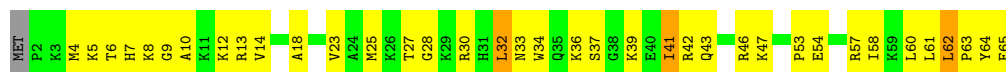
- Molecule 53: 50S ribosomal protein L34



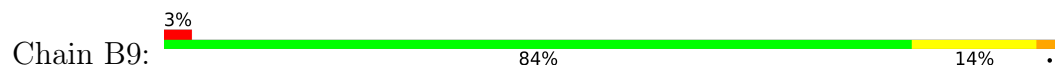
- Molecule 54: 50S ribosomal protein L35



- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 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	209.25Å 448.46Å 618.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	362.98 – 2.90 362.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.9 (362.98-2.90) 96.9 (362.98-2.90)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.231 , 0.286 0.232 , 0.286	Depositor DCC
R_{free} test set	61606 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	54.8	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 74.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	289646	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 1.87% 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: 5MC, 5MU, SF4, ZN, 31H, PPU, PSU, MG, 4SU, K

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.22	0/36049	0.44	2/56261 (0.0%)
1	CA	0.23	0/36170	0.46	5/56452 (0.0%)
2	AB	0.43	0/1881	1.04	14/2542 (0.6%)
2	CB	0.44	0/1860	1.04	12/2518 (0.5%)
3	AC	0.42	0/1576	0.85	0/2130
3	CC	0.42	0/1566	0.96	2/2119 (0.1%)
4	AD	0.41	0/1689	0.96	4/2267 (0.2%)
4	CD	0.40	0/1700	0.91	2/2280 (0.1%)
5	AE	0.41	0/1145	0.88	0/1543
5	CE	0.41	0/1149	0.97	5/1548 (0.3%)
6	AF	0.41	0/819	0.84	0/1111
6	CF	0.37	0/829	0.75	0/1123
7	AG	0.37	0/1250	0.88	2/1679 (0.1%)
7	CG	0.40	0/1254	0.99	6/1683 (0.4%)
8	AH	0.37	0/1108	0.90	2/1494 (0.1%)
8	CH	0.36	0/1108	0.88	1/1494 (0.1%)
9	AI	0.41	0/1002	0.96	2/1346 (0.1%)
9	CI	0.44	0/997	0.95	2/1343 (0.1%)
10	AJ	0.39	0/722	0.91	2/982 (0.2%)
10	CJ	0.45	0/727	0.96	0/988
11	AK	0.38	0/844	0.88	2/1145 (0.2%)
11	CK	0.39	0/848	0.89	2/1149 (0.2%)
12	AL	0.39	0/946	0.82	1/1274 (0.1%)
12	CL	0.39	0/946	0.94	5/1274 (0.4%)
13	AM	0.40	0/969	1.04	3/1302 (0.2%)
13	CM	0.45	0/961	0.96	3/1291 (0.2%)
14	AN	0.39	0/501	0.83	0/664
14	CN	0.40	0/501	0.90	0/664
15	AO	0.39	0/739	0.89	1/985 (0.1%)
15	CO	0.38	0/739	0.84	0/985
16	AP	0.39	0/697	0.86	0/939
16	CP	0.37	0/693	0.87	2/935 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.37	0/836	0.80	0/1117
17	CQ	0.34	0/836	0.84	0/1117
18	AR	0.36	0/560	0.85	0/746
18	CR	0.39	0/560	0.86	0/746
19	AS	0.37	0/667	0.94	3/900 (0.3%)
19	CS	0.46	0/661	1.09	5/893 (0.6%)
20	AT	0.40	0/730	0.96	0/965
20	CT	0.42	0/729	0.98	1/965 (0.1%)
21	AU	0.36	0/203	0.87	0/266
21	CU	0.38	0/203	0.92	0/266
22	AV	0.24	0/310	0.39	0/480
22	CV	0.25	0/282	0.43	0/437
23	AW	0.20	0/18	0.39	0/26
23	CW	0.15	0/18	0.34	0/26
24	AX	0.29	0/1700	0.48	0/2650
24	CX	0.30	0/1700	0.49	0/2650
25	BA	0.26	0/68013	0.44	1/106165 (0.0%)
25	DA	0.23	0/67542	0.44	0/105428
26	BB	0.24	0/2878	0.48	0/4490
26	DB	0.24	0/2878	0.44	0/4490
27	BD	0.48	0/2186	0.90	4/2944 (0.1%)
27	DD	0.43	0/2186	0.93	5/2944 (0.2%)
28	BE	0.44	0/1592	0.89	2/2149 (0.1%)
28	DE	0.44	0/1592	0.94	5/2149 (0.2%)
29	BF	0.47	0/1619	0.85	0/2193
29	DF	0.41	0/1615	0.94	5/2188 (0.2%)
30	BG	0.40	0/1450	0.96	5/1959 (0.3%)
30	DG	0.45	0/1449	1.10	11/1958 (0.6%)
31	BH	0.44	0/1356	0.91	1/1834 (0.1%)
31	DH	0.39	0/1356	0.96	3/1834 (0.2%)
32	BI	0.40	0/1100	0.93	2/1501 (0.1%)
32	DI	0.39	0/1076	0.91	0/1471
33	BN	0.44	0/1144	0.89	6/1543 (0.4%)
33	DN	0.42	0/1144	1.01	9/1543 (0.6%)
34	BO	0.47	0/943	0.85	0/1269
34	DO	0.44	0/943	0.85	0/1269
35	BP	0.44	0/1152	0.89	3/1533 (0.2%)
35	DP	0.39	0/1152	0.94	6/1533 (0.4%)
36	BQ	0.47	0/1143	0.82	1/1527 (0.1%)
36	DQ	0.42	0/1143	0.89	0/1527
37	BR	0.45	0/982	0.82	1/1312 (0.1%)
37	DR	0.41	0/982	0.78	0/1312
38	BS	0.43	0/887	0.87	1/1180 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DS	0.40	0/880	0.96	2/1172 (0.2%)
39	BT	0.41	0/1105	0.85	0/1477
39	DT	0.38	0/1097	0.84	2/1468 (0.1%)
40	BU	0.47	0/977	0.84	0/1301
40	DU	0.42	0/977	0.84	0/1301
41	BV	0.45	0/782	0.83	0/1049
41	DV	0.40	0/782	0.90	1/1049 (0.1%)
42	BW	0.49	0/897	0.86	2/1205 (0.2%)
42	DW	0.43	0/897	0.85	2/1205 (0.2%)
43	BX	0.48	0/764	0.84	1/1025 (0.1%)
43	DX	0.41	0/764	0.85	0/1025
44	BY	0.46	0/819	0.91	1/1095 (0.1%)
44	DY	0.40	0/819	0.94	1/1095 (0.1%)
45	BZ	0.43	0/1379	0.98	7/1873 (0.4%)
45	DZ	0.39	0/1390	1.00	8/1890 (0.4%)
46	B0	0.42	0/662	0.90	2/881 (0.2%)
46	D0	0.38	0/662	0.91	3/881 (0.3%)
47	B1	0.44	0/762	0.88	1/1014 (0.1%)
47	D1	0.40	0/762	0.85	1/1014 (0.1%)
48	B2	0.44	0/590	0.88	1/781 (0.1%)
48	D2	0.39	0/590	0.82	0/781
49	B3	0.45	0/474	0.90	0/635
49	D3	0.37	0/469	0.88	0/630
50	B4	0.50	0/565	1.23	10/761 (1.3%)
50	D4	0.49	0/545	1.13	2/737 (0.3%)
51	B5	0.48	0/469	0.80	1/635 (0.2%)
51	D5	0.44	0/469	0.81	0/635
52	B6	0.46	0/460	0.82	2/613 (0.3%)
52	D6	0.37	0/456	0.81	0/608
53	B7	0.48	0/426	0.80	0/561
53	D7	0.46	0/426	0.83	2/561 (0.4%)
54	B8	0.49	0/519	0.88	0/684
54	D8	0.38	0/525	0.89	2/691 (0.3%)
55	B9	0.42	0/310	0.78	0/407
55	D9	0.38	0/310	0.84	0/407
All	All	0.31	0/310281	0.61	216/464152 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AB	0	2
7	AG	0	1
20	CT	0	1
27	BD	0	1
38	BS	0	1
All	All	0	6

There are no bond length outliers.

The worst 5 of 216 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AM	84	ILE	N-CA-C	10.82	122.79	111.00
30	DG	178	PHE	CA-C-N	9.77	130.16	119.90
30	DG	178	PHE	C-N-CA	9.77	130.16	119.90
7	CG	79	ARG	N-CA-C	9.07	122.09	108.31
33	DN	10	GLU	CA-C-N	8.92	129.00	119.90

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	231	GLU	Peptide
2	AB	9	GLU	Peptide
7	AG	79	ARG	Peptide
27	BD	274	ARG	Peptide
38	BS	58	LEU	Peptide

5.2 Too-close contacts [i](#)

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	643	0
1	CA	32312	0	16307	730	0
2	AB	1846	0	1867	87	0
2	CB	1825	0	1828	99	0
3	AC	1552	0	1546	69	0
3	CC	1542	0	1517	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AD	1659	0	1676	66	0
4	CD	1670	0	1703	68	0
5	AE	1129	0	1185	31	0
5	CE	1133	0	1191	55	0
6	AF	806	0	793	32	0
6	CF	816	0	808	25	0
7	AG	1231	0	1238	30	0
7	CG	1235	0	1249	31	0
8	AH	1088	0	1126	26	0
8	CH	1088	0	1126	38	0
9	AI	983	0	986	52	0
9	CI	978	0	966	56	0
10	AJ	709	0	650	35	0
10	CJ	714	0	672	35	0
11	AK	829	0	825	18	0
11	CK	833	0	836	24	0
12	AL	930	0	979	32	0
12	CL	930	0	980	34	0
13	AM	958	0	1002	40	0
13	CM	950	0	988	56	0
14	AN	492	0	529	25	0
14	CN	492	0	529	36	0
15	AO	728	0	760	22	0
15	CO	728	0	760	31	0
16	AP	681	0	697	30	0
16	CP	677	0	686	28	0
17	AQ	823	0	891	23	0
17	CQ	823	0	891	22	0
18	AR	555	0	618	16	0
18	CR	555	0	618	22	0
19	AS	652	0	662	28	0
19	CS	646	0	644	53	0
20	AT	728	0	798	29	0
20	CT	727	0	796	29	0
21	AU	199	0	208	8	0
21	CU	199	0	208	12	0
22	AV	277	0	140	6	0
22	CV	252	0	130	8	0
23	AW	54	0	40	5	0
23	CW	54	0	40	7	0
24	AX	1635	0	838	33	0
24	CX	1635	0	838	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	BA	60729	0	30621	828	0
25	DA	60311	0	30408	1074	0
26	BB	2573	0	1306	30	0
26	DB	2573	0	1306	90	0
27	BD	2136	0	2218	60	0
27	DD	2136	0	2217	68	0
28	BE	1559	0	1618	55	0
28	DE	1559	0	1618	59	0
29	BF	1584	0	1625	39	0
29	DF	1580	0	1619	71	0
30	BG	1425	0	1443	45	0
30	DG	1424	0	1434	79	0
31	BH	1330	0	1407	29	0
31	DH	1330	0	1407	43	0
32	BI	1085	0	1114	40	0
32	DI	1061	0	1080	34	0
33	BN	1117	0	1184	26	0
33	DN	1117	0	1184	35	0
34	BO	933	0	996	27	0
34	DO	933	0	996	36	0
35	BP	1135	0	1212	36	0
35	DP	1135	0	1211	54	0
36	BQ	1122	0	1179	35	0
36	DQ	1122	0	1179	48	0
37	BR	968	0	1033	28	0
37	DR	968	0	1033	30	0
38	BS	877	0	938	23	0
38	DS	870	0	923	52	0
39	BT	1091	0	1151	32	0
39	DT	1083	0	1136	39	0
40	BU	959	0	1019	19	0
40	DU	959	0	1019	32	0
41	BV	771	0	830	16	0
41	DV	771	0	830	24	0
42	BW	886	0	940	11	0
42	DW	886	0	940	18	0
43	BX	750	0	814	14	0
43	DX	750	0	814	17	0
44	BY	806	0	881	31	0
44	DY	806	0	881	25	0
45	BZ	1349	0	1355	33	0
45	DZ	1360	0	1363	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	B0	653	0	674	29	0
46	D0	653	0	674	25	0
47	B1	755	0	826	12	0
47	D1	755	0	826	26	0
48	B2	588	0	643	13	0
48	D2	588	0	643	18	0
49	B3	469	0	518	9	0
49	D3	464	0	514	16	0
50	B4	552	0	533	27	0
50	D4	532	0	503	31	0
51	B5	455	0	465	12	0
51	D5	455	0	465	13	0
52	B6	453	0	473	9	0
52	D6	449	0	469	14	0
53	B7	418	0	467	13	0
53	D7	418	0	467	13	0
54	B8	511	0	571	18	0
54	D8	517	0	582	34	0
55	B9	307	0	335	4	0
55	D9	307	0	335	13	0
56	AA	187	0	0	0	0
56	AD	1	0	0	0	0
56	AE	2	0	0	0	0
56	AF	1	0	0	0	0
56	AK	1	0	0	0	0
56	AL	1	0	0	0	0
56	AM	1	0	0	0	0
56	AN	1	0	0	0	0
56	AX	7	0	0	0	0
56	B0	5	0	0	0	0
56	B3	2	0	0	0	0
56	B4	1	0	0	0	0
56	B5	2	0	0	0	0
56	B7	4	0	0	0	0
56	B8	1	0	0	0	0
56	B9	1	0	0	0	0
56	BA	675	0	0	0	0
56	BB	18	0	0	0	0
56	BD	8	0	0	0	0
56	BE	6	0	0	0	0
56	BF	5	0	0	0	0
56	BG	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BH	1	0	0	0	0
56	BN	2	0	0	0	0
56	BO	1	0	0	0	0
56	BP	4	0	0	0	0
56	BQ	3	0	0	0	0
56	BR	3	0	0	0	0
56	BU	5	0	0	0	0
56	BV	3	0	0	0	0
56	BW	4	0	0	0	0
56	BX	3	0	0	0	0
56	BY	2	0	0	0	0
56	BZ	1	0	0	0	0
56	CA	154	0	0	0	0
56	CE	2	0	0	0	0
56	CF	1	0	0	0	0
56	CJ	1	0	0	0	0
56	CK	1	0	0	0	0
56	CT	1	0	0	0	0
56	CX	1	0	0	0	0
56	D0	1	0	0	0	0
56	D3	1	0	0	0	0
56	D5	1	0	0	0	0
56	D7	1	0	0	0	0
56	D8	2	0	0	0	0
56	DA	595	0	0	0	0
56	DB	12	0	0	0	0
56	DD	2	0	0	0	0
56	DE	5	0	0	0	0
56	DF	3	0	0	0	0
56	DG	1	0	0	0	0
56	DN	1	0	0	0	0
56	DP	1	0	0	0	0
56	DQ	3	0	0	0	0
56	DR	2	0	0	0	0
56	DT	1	0	0	0	0
56	DU	1	0	0	0	0
56	DV	2	0	0	0	0
56	DW	2	0	0	0	0
56	DY	1	0	0	0	0
57	AD	8	0	0	0	0
57	CD	8	0	0	0	0
58	AN	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	B4	1	0	0	0	0
58	B5	1	0	0	0	0
58	B6	1	0	0	0	0
58	B9	1	0	0	0	0
58	BY	1	0	0	0	0
58	CN	1	0	0	0	0
58	D4	1	0	0	0	0
58	D5	1	0	0	0	0
58	D6	1	0	0	0	0
58	D9	1	0	0	0	0
58	DY	1	0	0	0	0
59	AX	1	0	0	0	0
59	DA	1	0	0	0	0
60	AA	165	0	0	12	0
60	AJ	1	0	0	0	0
60	AL	3	0	0	2	0
60	AP	1	0	0	0	0
60	AU	1	0	0	0	0
60	AV	2	0	0	0	0
60	AW	3	0	0	0	0
60	B0	4	0	0	0	0
60	B1	2	0	0	0	0
60	B2	1	0	0	0	0
60	B3	1	0	0	0	0
60	B5	2	0	0	0	0
60	B7	2	0	0	1	0
60	B8	8	0	0	2	0
60	BA	924	0	0	62	0
60	BB	27	0	0	0	0
60	BD	6	0	0	2	0
60	BE	8	0	0	0	0
60	BF	6	0	0	1	0
60	BG	1	0	0	0	0
60	BH	1	0	0	1	0
60	BN	3	0	0	0	0
60	BO	1	0	0	0	0
60	BP	14	0	0	2	0
60	BQ	2	0	0	0	0
60	BS	1	0	0	0	0
60	BT	4	0	0	1	0
60	BU	2	0	0	0	0
60	BV	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	BW	1	0	0	0	0
60	BX	2	0	0	0	0
60	BZ	1	0	0	0	0
60	CA	113	0	0	5	0
60	CE	2	0	0	0	0
60	CJ	2	0	0	1	0
60	CL	1	0	0	1	0
60	CO	1	0	0	0	0
60	CW	1	0	0	1	0
60	CX	1	0	0	1	0
60	D0	5	0	0	0	0
60	D1	1	0	0	0	0
60	D3	1	0	0	2	0
60	D8	3	0	0	0	0
60	DA	689	0	0	58	0
60	DB	9	0	0	0	0
60	DD	11	0	0	2	0
60	DE	5	0	0	1	0
60	DF	6	0	0	0	0
60	DO	1	0	0	0	0
60	DP	6	0	0	0	0
60	DU	3	0	0	0	0
60	DV	1	0	0	0	0
60	DW	1	0	0	0	0
60	DX	3	0	0	0	0
All	All	289646	0	193084	5817	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 13.

The worst 5 of 5817 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:DA:2121:G:H1	25:DA:2177:C:N4	1.35	1.23
19:CS:42:PRO:HG3	50:D4:61:ARG:HG2	1.39	1.04
1:AA:1028:C:N4	1:AA:1033:G:H1	1.56	1.01
25:DA:2128:C:H42	25:DA:2160:G:H1	1.08	1.00
25:DA:2137:C:H42	25:DA:2154:G:H1	1.05	0.99

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	229/256 (90%)	208 (91%)	18 (8%)	3 (1%)	9	32
2	CB	229/256 (90%)	206 (90%)	17 (7%)	6 (3%)	4	17
3	AC	204/239 (85%)	193 (95%)	10 (5%)	1 (0%)	24	54
3	CC	204/239 (85%)	187 (92%)	15 (7%)	2 (1%)	12	39
4	AD	206/209 (99%)	195 (95%)	9 (4%)	2 (1%)	12	39
4	CD	206/209 (99%)	194 (94%)	11 (5%)	1 (0%)	24	54
5	AE	146/162 (90%)	140 (96%)	4 (3%)	2 (1%)	9	30
5	CE	146/162 (90%)	142 (97%)	4 (3%)	0	100	100
6	AF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
6	CF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
7	AG	153/156 (98%)	148 (97%)	2 (1%)	3 (2%)	6	22
7	CG	153/156 (98%)	151 (99%)	1 (1%)	1 (1%)	18	48
8	AH	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
8	CH	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
9	AI	125/128 (98%)	118 (94%)	7 (6%)	0	100	100
9	CI	125/128 (98%)	120 (96%)	5 (4%)	0	100	100
10	AJ	95/105 (90%)	87 (92%)	7 (7%)	1 (1%)	11	36
10	CJ	94/105 (90%)	87 (93%)	5 (5%)	2 (2%)	5	21
11	AK	112/129 (87%)	104 (93%)	5 (4%)	3 (3%)	4	16
11	CK	112/129 (87%)	103 (92%)	7 (6%)	2 (2%)	6	25
12	AL	120/132 (91%)	115 (96%)	5 (4%)	0	100	100
12	CL	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
13	AM	121/126 (96%)	113 (93%)	8 (7%)	0	100	100
13	CM	120/126 (95%)	114 (95%)	5 (4%)	1 (1%)	16	44
14	AN	58/61 (95%)	55 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	CN	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
15	AO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
15	CO	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	AP	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
16	CP	80/88 (91%)	77 (96%)	2 (2%)	1 (1%)	9	32
17	AQ	97/105 (92%)	92 (95%)	4 (4%)	1 (1%)	12	39
17	CQ	97/105 (92%)	94 (97%)	3 (3%)	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%)	76 (94%)	5 (6%)	0	100	100
19	CS	81/93 (87%)	75 (93%)	6 (7%)	0	100	100
20	AT	94/106 (89%)	87 (93%)	6 (6%)	1 (1%)	11	36
20	CT	94/106 (89%)	86 (92%)	5 (5%)	3 (3%)	3	13
21	AU	21/27 (78%)	21 (100%)	0	0	100	100
21	CU	21/27 (78%)	21 (100%)	0	0	100	100
27	BD	273/276 (99%)	263 (96%)	9 (3%)	1 (0%)	30	59
27	DD	273/276 (99%)	262 (96%)	9 (3%)	2 (1%)	18	48
28	BE	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	24	54
28	DE	202/206 (98%)	193 (96%)	7 (4%)	2 (1%)	12	39
29	BF	201/210 (96%)	197 (98%)	3 (2%)	1 (0%)	24	54
29	DF	201/210 (96%)	197 (98%)	2 (1%)	2 (1%)	12	39
30	BG	179/182 (98%)	171 (96%)	7 (4%)	1 (1%)	21	51
30	DG	179/182 (98%)	167 (93%)	11 (6%)	1 (1%)	21	51
31	BH	172/180 (96%)	169 (98%)	3 (2%)	0	100	100
31	DH	172/180 (96%)	168 (98%)	4 (2%)	0	100	100
32	BI	144/148 (97%)	130 (90%)	10 (7%)	4 (3%)	4	15
32	DI	144/148 (97%)	137 (95%)	6 (4%)	1 (1%)	18	48
33	BN	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
33	DN	138/140 (99%)	135 (98%)	2 (1%)	1 (1%)	18	48
34	BO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
34	DO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	BP	147/150 (98%)	141 (96%)	6 (4%)	0	100	100
35	DP	147/150 (98%)	140 (95%)	5 (3%)	2 (1%)	9	30
36	BQ	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
36	DQ	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
37	BR	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
37	DR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
38	BS	108/112 (96%)	103 (95%)	4 (4%)	1 (1%)	14	41
38	DS	108/112 (96%)	105 (97%)	2 (2%)	1 (1%)	14	41
39	BT	129/146 (88%)	123 (95%)	4 (3%)	2 (2%)	7	27
39	DT	129/146 (88%)	125 (97%)	3 (2%)	1 (1%)	16	44
40	BU	114/118 (97%)	114 (100%)	0	0	100	100
40	DU	114/118 (97%)	114 (100%)	0	0	100	100
41	BV	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
41	DV	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
42	BW	110/113 (97%)	110 (100%)	0	0	100	100
42	DW	110/113 (97%)	110 (100%)	0	0	100	100
43	BX	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
43	DX	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
44	BY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
44	DY	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
45	BZ	169/206 (82%)	152 (90%)	16 (10%)	1 (1%)	21	51
45	DZ	172/206 (84%)	158 (92%)	14 (8%)	0	100	100
46	B0	81/85 (95%)	81 (100%)	0	0	100	100
46	D0	81/85 (95%)	79 (98%)	1 (1%)	1 (1%)	10	34
47	B1	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
47	D1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	36
48	B2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
48	D2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
49	B3	57/60 (95%)	57 (100%)	0	0	100	100
49	D3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
50	B4	67/71 (94%)	56 (84%)	9 (13%)	2 (3%)	3	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	D4	67/71 (94%)	54 (81%)	8 (12%)	5 (8%)	1	2
51	B5	57/60 (95%)	57 (100%)	0	0	100	100
51	D5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
52	B6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
52	D6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
53	B7	46/49 (94%)	46 (100%)	0	0	100	100
53	D7	46/49 (94%)	45 (98%)	0	1 (2%)	5	20
54	B8	62/65 (95%)	62 (100%)	0	0	100	100
54	D8	62/65 (95%)	62 (100%)	0	0	100	100
55	B9	35/37 (95%)	35 (100%)	0	0	100	100
55	D9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11409/12128 (94%)	10906 (96%)	432 (4%)	71 (1%)	21	51

5 of 71 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	19	HIS
2	AB	231	GLU
4	AD	166	LYS
7	AG	80	VAL
27	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%)	150 (78%)	42 (22%)	1	3
2	CB	187/220 (85%)	153 (82%)	34 (18%)	2	6
3	AC	143/188 (76%)	126 (88%)	17 (12%)	5	16
3	CC	140/188 (74%)	119 (85%)	21 (15%)	3	10
4	AD	170/181 (94%)	144 (85%)	26 (15%)	3	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CD	172/181 (95%)	144 (84%)	28 (16%)	2	8
5	AE	113/123 (92%)	98 (87%)	15 (13%)	4	12
5	CE	114/123 (93%)	96 (84%)	18 (16%)	2	8
6	AF	83/90 (92%)	77 (93%)	6 (7%)	13	39
6	CF	85/90 (94%)	76 (89%)	9 (11%)	6	22
7	AG	119/127 (94%)	104 (87%)	15 (13%)	4	14
7	CG	120/127 (94%)	107 (89%)	13 (11%)	6	21
8	AH	114/119 (96%)	100 (88%)	14 (12%)	4	15
8	CH	114/119 (96%)	101 (89%)	13 (11%)	5	18
9	AI	90/99 (91%)	75 (83%)	15 (17%)	2	7
9	CI	89/99 (90%)	70 (79%)	19 (21%)	1	4
10	AJ	66/92 (72%)	63 (96%)	3 (4%)	24	58
10	CJ	69/92 (75%)	62 (90%)	7 (10%)	7	24
11	AK	82/99 (83%)	71 (87%)	11 (13%)	4	12
11	CK	83/99 (84%)	76 (92%)	7 (8%)	10	31
12	AL	97/109 (89%)	86 (89%)	11 (11%)	5	19
12	CL	97/109 (89%)	88 (91%)	9 (9%)	8	27
13	AM	93/101 (92%)	74 (80%)	19 (20%)	1	4
13	CM	92/101 (91%)	75 (82%)	17 (18%)	1	5
14	AN	49/50 (98%)	42 (86%)	7 (14%)	3	11
14	CN	49/50 (98%)	39 (80%)	10 (20%)	1	4
15	AO	78/80 (98%)	68 (87%)	10 (13%)	4	14
15	CO	78/80 (98%)	69 (88%)	9 (12%)	5	18
16	AP	69/74 (93%)	52 (75%)	17 (25%)	1	2
16	CP	68/74 (92%)	56 (82%)	12 (18%)	2	6
17	AQ	94/97 (97%)	83 (88%)	11 (12%)	5	17
17	CQ	94/97 (97%)	84 (89%)	10 (11%)	6	22
18	AR	59/77 (77%)	51 (86%)	8 (14%)	3	12
18	CR	59/77 (77%)	51 (86%)	8 (14%)	3	12
19	AS	69/80 (86%)	60 (87%)	9 (13%)	4	13
19	CS	67/80 (84%)	57 (85%)	10 (15%)	3	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	AT	70/82 (85%)	60 (86%)	10 (14%)	3	11
20	CT	70/82 (85%)	58 (83%)	12 (17%)	2	7
21	AU	18/22 (82%)	15 (83%)	3 (17%)	2	7
21	CU	18/22 (82%)	16 (89%)	2 (11%)	6	20
27	BD	215/218 (99%)	194 (90%)	21 (10%)	7	25
27	DD	215/218 (99%)	191 (89%)	24 (11%)	6	19
28	BE	164/166 (99%)	138 (84%)	26 (16%)	2	8
28	DE	164/166 (99%)	138 (84%)	26 (16%)	2	8
29	BF	160/166 (96%)	141 (88%)	19 (12%)	5	16
29	DF	159/166 (96%)	140 (88%)	19 (12%)	5	16
30	BG	143/156 (92%)	117 (82%)	26 (18%)	2	6
30	DG	142/156 (91%)	116 (82%)	26 (18%)	2	6
31	BH	144/148 (97%)	131 (91%)	13 (9%)	9	28
31	DH	144/148 (97%)	127 (88%)	17 (12%)	5	17
32	BI	110/124 (89%)	90 (82%)	20 (18%)	2	6
32	DI	104/124 (84%)	83 (80%)	21 (20%)	1	4
33	BN	118/119 (99%)	103 (87%)	15 (13%)	4	14
33	DN	118/119 (99%)	103 (87%)	15 (13%)	4	14
34	BO	100/100 (100%)	90 (90%)	10 (10%)	7	24
34	DO	100/100 (100%)	88 (88%)	12 (12%)	5	16
35	BP	115/116 (99%)	99 (86%)	16 (14%)	3	11
35	DP	115/116 (99%)	99 (86%)	16 (14%)	3	11
36	BQ	111/111 (100%)	99 (89%)	12 (11%)	6	21
36	DQ	111/111 (100%)	94 (85%)	17 (15%)	3	9
37	BR	101/101 (100%)	83 (82%)	18 (18%)	2	6
37	DR	101/101 (100%)	87 (86%)	14 (14%)	3	11
38	BS	87/88 (99%)	79 (91%)	8 (9%)	8	27
38	DS	85/88 (97%)	74 (87%)	11 (13%)	4	13
39	BT	115/127 (91%)	103 (90%)	12 (10%)	7	23
39	DT	113/127 (89%)	97 (86%)	16 (14%)	3	11
40	BU	93/94 (99%)	84 (90%)	9 (10%)	8	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	DU	93/94 (99%)	84 (90%)	9 (10%)	8	25
41	BV	80/82 (98%)	66 (82%)	14 (18%)	2	6
41	DV	80/82 (98%)	66 (82%)	14 (18%)	2	6
42	BW	90/92 (98%)	77 (86%)	13 (14%)	3	11
42	DW	90/92 (98%)	82 (91%)	8 (9%)	9	28
43	BX	77/78 (99%)	71 (92%)	6 (8%)	11	35
43	DX	77/78 (99%)	73 (95%)	4 (5%)	21	52
44	BY	85/91 (93%)	77 (91%)	8 (9%)	8	26
44	DY	85/91 (93%)	78 (92%)	7 (8%)	10	32
45	BZ	145/179 (81%)	125 (86%)	20 (14%)	3	12
45	DZ	145/179 (81%)	125 (86%)	20 (14%)	3	12
46	B0	65/67 (97%)	60 (92%)	5 (8%)	12	35
46	D0	65/67 (97%)	60 (92%)	5 (8%)	12	35
47	B1	80/83 (96%)	75 (94%)	5 (6%)	16	45
47	D1	80/83 (96%)	70 (88%)	10 (12%)	4	15
48	B2	65/67 (97%)	60 (92%)	5 (8%)	12	35
48	D2	65/67 (97%)	55 (85%)	10 (15%)	2	9
49	B3	51/52 (98%)	44 (86%)	7 (14%)	3	12
49	D3	50/52 (96%)	45 (90%)	5 (10%)	7	24
50	B4	59/63 (94%)	44 (75%)	15 (25%)	0	2
50	D4	53/63 (84%)	38 (72%)	15 (28%)	0	1
51	B5	50/52 (96%)	44 (88%)	6 (12%)	5	16
51	D5	50/52 (96%)	48 (96%)	2 (4%)	28	62
52	B6	51/52 (98%)	46 (90%)	5 (10%)	7	25
52	D6	50/52 (96%)	45 (90%)	5 (10%)	7	24
53	B7	41/42 (98%)	38 (93%)	3 (7%)	13	38
53	D7	41/42 (98%)	36 (88%)	5 (12%)	5	16
54	B8	53/55 (96%)	49 (92%)	4 (8%)	12	37
54	D8	54/55 (98%)	48 (89%)	6 (11%)	6	20
55	B9	34/34 (100%)	33 (97%)	1 (3%)	37	71
55	D9	34/34 (100%)	30 (88%)	4 (12%)	5	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9318/10066 (93%)	8076 (87%)	1242 (13%)	4 12

5 of 1242 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	DE	175	VAL
43	DX	76	ARG
30	DG	40	ASN
28	DE	170	LEU
35	DP	4	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 155 such sidechains are listed below:

Mol	Chain	Res	Type
12	CL	78	GLN
38	DS	68	GLN
19	CS	56	GLN
29	DF	75	HIS
45	DZ	75	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1495/1521 (98%)	388 (25%)	22 (1%)
1	CA	1501/1521 (98%)	392 (26%)	24 (1%)
22	AV	12/24 (50%)	4 (33%)	0
22	CV	11/24 (45%)	4 (36%)	0
23	AW	0/2	-	-
23	CW	0/2	-	-
24	AX	74/77 (96%)	25 (33%)	1 (1%)
24	CX	74/77 (96%)	26 (35%)	1 (1%)
25	BA	2811/2915 (96%)	539 (19%)	24 (0%)
25	DA	2791/2915 (95%)	623 (22%)	29 (1%)
26	BB	120/121 (99%)	19 (15%)	3 (2%)
26	DB	119/121 (98%)	36 (30%)	0
All	All	9008/9320 (96%)	2056 (22%)	104 (1%)

5 of 2056 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	7	G
1	AA	9	G
1	AA	22	G

5 of 104 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	532	A
1	CA	1279	A
25	DA	2406	U
1	CA	748	C
1	CA	1067	A

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

12 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	4SU	AX	8	24	18,21,22	2.27	5 (27%)	25,30,33	1.65	5 (20%)
24	PSU	AX	55	24	18,21,22	1.38	3 (16%)	21,30,33	2.06	3 (14%)
24	31H	AX	76	56,24	31,34,35	1.24	3 (9%)	35,47,50	2.24	13 (37%)
24	5MC	CX	32	24	19,22,23	1.60	3 (15%)	26,32,35	1.12	2 (7%)
23	PPU	CW	76	23	37,40,41	1.30	5 (13%)	47,57,60	2.15	14 (29%)
24	31H	CX	76	24	31,34,35	1.29	3 (9%)	35,47,50	2.31	12 (34%)
23	PPU	AW	76	25,23	37,40,41	1.35	5 (13%)	47,57,60	2.24	15 (31%)
24	5MU	AX	54	56,24	19,22,23	1.37	5 (26%)	27,32,35	2.08	6 (22%)
24	5MC	AX	32	24	19,22,23	1.68	3 (15%)	26,32,35	1.31	3 (11%)
24	PSU	CX	55	24	18,21,22	1.36	2 (11%)	21,30,33	1.98	4 (19%)
24	4SU	CX	8	24	18,21,22	2.12	6 (33%)	25,30,33	1.56	5 (20%)
24	5MU	CX	54	24	19,22,23	1.28	5 (26%)	27,32,35	2.17	6 (22%)

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	4SU	AX	8	24	-	0/7/25/26	0/2/2/2
24	PSU	AX	55	24	-	1/7/25/26	0/2/2/2
24	31H	AX	76	56,24	-	5/22/40/41	0/3/3/3
24	5MC	CX	32	24	-	0/7/25/26	0/2/2/2
23	PPU	CW	76	23	-	5/25/43/44	0/4/4/4
24	31H	CX	76	24	-	10/22/40/41	0/3/3/3
23	PPU	AW	76	25,23	-	5/25/43/44	0/4/4/4
24	5MU	AX	54	56,24	-	0/7/25/26	0/2/2/2
24	5MC	AX	32	24	-	0/7/25/26	0/2/2/2
24	PSU	CX	55	24	-	1/7/25/26	0/2/2/2
24	4SU	CX	8	24	-	0/7/25/26	0/2/2/2
24	5MU	CX	54	24	-	0/7/25/26	0/2/2/2

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	32	5MC	C5-C4	6.11	1.48	1.44
24	CX	32	5MC	C5-C4	5.76	1.48	1.44
24	AX	8	4SU	C4-N3	-5.30	1.32	1.37
23	CW	76	PPU	C5-C4	5.03	1.48	1.39
23	AW	76	PPU	C5-C4	4.98	1.48	1.39

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AX	55	PSU	N1-C2-N3	6.30	121.81	115.17
24	CX	55	PSU	N1-C2-N3	6.22	121.73	115.17
23	AW	76	PPU	C5-C4-N3	-6.18	118.21	126.72
23	CW	76	PPU	C5-C4-N3	-5.95	118.52	126.72
24	AX	76	31H	N1-C2-N3	-5.94	119.59	128.58

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	AW	76	PPU	O4'-C4'-C5'-O5'
24	AX	76	31H	OCN-CN-N-CA

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Mol	Chain	Res	Type	Atoms
24	CX	76	31H	C-CA-CB-CG
24	CX	76	31H	OCN-CN-N-CA
24	CX	76	31H	CA-CB-CG-SD

There are no ring outliers.

7 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AX	55	PSU	1	0
24	AX	76	31H	3	0
23	CW	76	PPU	7	0
24	CX	76	31H	4	0
23	AW	76	PPU	5	0
24	CX	55	PSU	1	0
24	CX	8	4SU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1780 ligands modelled in this entry, 1778 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	$\# Z > 2$
57	SF4	AD	501	4	0,12,12	-	-	-		
57	SF4	CD	501	4	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	SF4	AD	501	4	-	-	0/6/5/5
57	SF4	CD	501	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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%)	0.51	48 (3%)	50	41	39, 74, 94, 105	0
1	CA	1503/1521 (98%)	0.61	86 (5%)	29	23	41, 75, 94, 105	0
2	AB	231/256 (90%)	1.05	27 (11%)	9	8	65, 82, 90, 96	0
2	CB	231/256 (90%)	1.45	50 (21%)	2	2	67, 83, 92, 96	0
3	AC	206/239 (86%)	0.94	18 (8%)	16	13	67, 78, 86, 94	0
3	CC	206/239 (86%)	1.31	31 (15%)	5	4	69, 80, 87, 92	0
4	AD	208/209 (99%)	1.02	24 (11%)	9	8	57, 72, 82, 86	0
4	CD	208/209 (99%)	1.14	24 (11%)	9	8	57, 73, 82, 87	0
5	AE	148/162 (91%)	0.80	12 (8%)	18	15	55, 71, 81, 86	0
5	CE	148/162 (91%)	1.01	13 (8%)	15	13	58, 73, 82, 89	0
6	AF	100/101 (99%)	0.74	6 (6%)	27	21	55, 71, 80, 82	0
6	CF	100/101 (99%)	0.57	2 (2%)	65	56	58, 73, 80, 82	0
7	AG	155/156 (99%)	0.81	15 (9%)	13	11	67, 76, 85, 94	0
7	CG	155/156 (99%)	1.08	21 (13%)	7	5	68, 78, 86, 96	0
8	AH	137/138 (99%)	0.56	3 (2%)	62	53	62, 72, 78, 86	0
8	CH	137/138 (99%)	0.94	9 (6%)	24	19	62, 73, 80, 88	0
9	AI	127/128 (99%)	1.39	24 (18%)	3	3	64, 82, 87, 90	0
9	CI	127/128 (99%)	2.16	64 (50%)	0	0	67, 83, 89, 91	0
10	AJ	97/105 (92%)	1.21	15 (15%)	5	4	63, 80, 89, 95	0
10	CJ	96/105 (91%)	2.01	49 (51%)	0	0	70, 86, 93, 100	0
11	AK	114/129 (88%)	0.87	7 (6%)	27	21	54, 72, 81, 83	0
11	CK	114/129 (88%)	0.67	3 (2%)	57	48	56, 72, 80, 83	0
12	AL	122/132 (92%)	0.74	6 (4%)	35	27	55, 65, 75, 78	0
12	CL	122/132 (92%)	0.83	5 (4%)	41	33	57, 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%)	1.37	23 (18%) 3 3	64, 78, 86, 91	0
13	CM	122/126 (96%)	1.70	35 (28%) 1 1	68, 80, 88, 93	0
14	AN	60/61 (98%)	1.32	11 (18%) 3 3	65, 76, 83, 86	0
14	CN	60/61 (98%)	2.07	28 (46%) 0 0	69, 79, 84, 88	0
15	AO	88/89 (98%)	0.90	7 (7%) 18 15	56, 69, 80, 90	0
15	CO	88/89 (98%)	0.71	6 (6%) 23 18	56, 70, 80, 90	0
16	AP	82/88 (93%)	1.49	16 (19%) 3 2	58, 73, 83, 85	0
16	CP	82/88 (93%)	1.30	16 (19%) 3 2	58, 72, 82, 85	0
17	AQ	99/105 (94%)	1.11	7 (7%) 22 17	60, 70, 81, 85	0
17	CQ	99/105 (94%)	0.75	2 (2%) 65 56	57, 70, 80, 84	0
18	AR	68/88 (77%)	0.59	4 (5%) 28 22	60, 70, 81, 85	0
18	CR	68/88 (77%)	0.59	0 100 100	61, 72, 82, 86	0
19	AS	83/93 (89%)	1.22	10 (12%) 9 7	67, 81, 88, 96	0
19	CS	83/93 (89%)	1.52	21 (25%) 1 1	71, 83, 91, 97	0
20	AT	96/106 (90%)	1.10	15 (15%) 5 4	58, 72, 82, 89	0
20	CT	96/106 (90%)	0.95	9 (9%) 14 12	59, 72, 82, 88	0
21	AU	23/27 (85%)	1.46	5 (21%) 2 2	65, 75, 80, 86	0
21	CU	23/27 (85%)	1.78	7 (30%) 1 1	66, 76, 83, 87	0
22	AV	13/24 (54%)	1.97	6 (46%) 0 0	60, 92, 100, 100	0
22	CV	12/24 (50%)	1.91	7 (58%) 0 0	63, 93, 99, 99	0
23	AW	1/2 (50%)	-0.24	0 100 100	42, 42, 42, 42	0
23	CW	1/2 (50%)	0.94	0 100 100	59, 59, 59, 59	0
24	AX	71/77 (92%)	0.42	2 (2%) 55 46	37, 72, 84, 92	0
24	CX	71/77 (92%)	0.24	0 100 100	39, 73, 86, 92	0
25	BA	2819/2915 (96%)	-0.18	77 (2%) 56 47	23, 46, 89, 107	0
25	DA	2800/2915 (96%)	-0.14	50 (1%) 67 59	26, 50, 90, 107	0
26	BB	120/121 (99%)	0.10	0 100 100	40, 65, 76, 91	0
26	DB	120/121 (99%)	0.67	5 (4%) 40 32	44, 70, 81, 93	0
27	BD	275/276 (99%)	0.33	5 (1%) 67 59	24, 45, 61, 77	0
27	DD	275/276 (99%)	0.18	1 (0%) 88 85	27, 47, 63, 78	0
28	BE	204/206 (99%)	-0.07	1 (0%) 87 83	18, 44, 66, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DE	204/206 (99%)	0.12	1 (0%) 87 83	32, 57, 72, 86	0
29	BF	203/210 (96%)	0.30	1 (0%) 87 83	26, 55, 74, 84	0
29	DF	203/210 (96%)	0.28	0 100 100	26, 58, 75, 85	0
30	BG	181/182 (99%)	1.02	25 (13%) 6 5	56, 70, 82, 91	0
30	DG	181/182 (99%)	1.37	36 (19%) 3 2	61, 73, 85, 91	0
31	BH	174/180 (96%)	0.47	5 (2%) 53 45	51, 66, 76, 82	0
31	DH	174/180 (96%)	0.82	7 (4%) 42 34	55, 69, 80, 85	0
32	BI	146/148 (98%)	0.75	3 (2%) 63 54	46, 74, 85, 87	0
32	DI	146/148 (98%)	1.25	25 (17%) 4 3	50, 75, 84, 87	0
33	BN	140/140 (100%)	0.26	4 (2%) 53 45	33, 53, 72, 80	0
33	DN	140/140 (100%)	0.26	0 100 100	36, 56, 72, 81	0
34	BO	122/122 (100%)	-0.19	1 (0%) 82 77	25, 43, 60, 76	0
34	DO	122/122 (100%)	0.30	1 (0%) 82 77	42, 59, 73, 77	0
35	BP	149/150 (99%)	0.37	1 (0%) 84 79	27, 57, 73, 87	0
35	DP	149/150 (99%)	0.33	1 (0%) 84 79	29, 59, 76, 86	0
36	BQ	141/141 (100%)	0.36	2 (1%) 73 65	35, 53, 64, 71	0
36	DQ	141/141 (100%)	0.52	3 (2%) 63 54	38, 56, 68, 76	0
37	BR	118/118 (100%)	-0.21	2 (1%) 69 61	25, 37, 56, 66	0
37	DR	118/118 (100%)	0.24	0 100 100	40, 54, 66, 76	0
38	BS	110/112 (98%)	0.00	0 100 100	40, 52, 63, 68	0
38	DS	110/112 (98%)	1.15	15 (13%) 7 5	57, 76, 86, 92	0
39	BT	131/146 (89%)	0.00	1 (0%) 82 77	32, 50, 74, 86	0
39	DT	131/146 (89%)	0.47	2 (1%) 72 64	44, 60, 75, 85	0
40	BU	116/118 (98%)	-0.30	1 (0%) 81 75	23, 35, 55, 76	0
40	DU	116/118 (98%)	0.39	4 (3%) 48 39	41, 61, 77, 87	0
41	BV	101/101 (100%)	-0.30	0 100 100	19, 43, 64, 76	0
41	DV	101/101 (100%)	0.35	0 100 100	44, 71, 80, 88	0
42	BW	112/113 (99%)	-0.33	0 100 100	21, 38, 53, 75	0
42	DW	112/113 (99%)	0.12	1 (0%) 81 75	31, 51, 69, 85	0
43	BX	95/96 (98%)	-0.03	1 (1%) 78 71	25, 43, 64, 82	0
43	DX	95/96 (98%)	0.59	5 (5%) 32 25	43, 62, 78, 91	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BY	107/110 (97%)	0.10	0 100 100	36, 51, 69, 80	0
44	DY	107/110 (97%)	0.90	8 (7%) 20 16	55, 72, 81, 89	0
45	BZ	171/206 (83%)	0.30	3 (1%) 67 59	42, 63, 77, 92	0
45	DZ	174/206 (84%)	0.89	10 (5%) 29 23	61, 80, 90, 100	0
46	B0	83/85 (97%)	-0.07	0 100 100	16, 43, 56, 66	0
46	D0	83/85 (97%)	0.85	8 (9%) 13 11	44, 65, 74, 80	0
47	B1	97/98 (98%)	0.10	3 (3%) 51 42	27, 49, 70, 77	0
47	D1	97/98 (98%)	0.57	2 (2%) 63 54	38, 59, 75, 78	0
48	B2	70/72 (97%)	0.07	1 (1%) 73 65	37, 50, 66, 72	0
48	D2	70/72 (97%)	0.53	0 100 100	58, 70, 79, 85	0
49	B3	59/60 (98%)	-0.27	0 100 100	26, 41, 61, 72	0
49	D3	59/60 (98%)	0.29	2 (3%) 48 39	44, 64, 77, 80	0
50	B4	69/71 (97%)	1.01	8 (11%) 9 8	57, 76, 91, 94	0
50	D4	69/71 (97%)	1.55	18 (26%) 1 1	77, 87, 97, 104	0
51	B5	59/60 (98%)	-0.39	0 100 100	19, 38, 57, 78	0
51	D5	59/60 (98%)	0.04	0 100 100	31, 52, 69, 76	0
52	B6	53/54 (98%)	-0.19	0 100 100	29, 43, 60, 71	0
52	D6	53/54 (98%)	0.71	1 (1%) 66 58	50, 63, 75, 83	0
53	B7	48/49 (97%)	-0.15	0 100 100	20, 30, 53, 72	0
53	D7	48/49 (97%)	0.26	3 (6%) 26 20	35, 46, 71, 76	0
54	B8	64/65 (98%)	-0.10	0 100 100	27, 36, 47, 55	0
54	D8	64/65 (98%)	0.57	0 100 100	44, 58, 67, 75	0
55	B9	37/37 (100%)	0.18	1 (2%) 56 47	31, 52, 64, 69	0
55	D9	37/37 (100%)	0.56	0 100 100	44, 58, 67, 73	0
All	All	20634/21448 (96%)	0.42	1154 (5%) 30 23	16, 64, 87, 107	0

The worst 5 of 1154 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	CI	126	SER	7.5
13	CM	124	PRO	7.3
13	CM	123	ALA	6.9
5	CE	94	ALA	6.6
25	BA	2804	C	6.4

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
24	4SU	CX	8	20/21	0.85	0.11	65,84,90,94	0
24	5MU	CX	54	21/22	0.86	0.12	66,78,87,98	0
24	PSU	CX	55	20/21	0.86	0.11	59,68,84,85	0
24	PSU	AX	55	20/21	0.92	0.10	57,66,78,79	0
24	5MC	CX	32	21/22	0.92	0.12	52,69,78,83	0
24	4SU	AX	8	20/21	0.93	0.10	50,63,78,79	0
24	31H	CX	76	32/33	0.93	0.12	33,54,78,89	0
24	5MC	AX	32	21/22	0.94	0.11	46,61,70,75	0
24	5MU	AX	54	21/22	0.94	0.09	55,69,75,82	0
23	PPU	CW	76	37/38	0.96	0.11	31,50,63,70	0
24	31H	AX	76	32/33	0.96	0.12	27,44,76,98	0
23	PPU	AW	76	37/38	0.97	0.09	25,33,43,45	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(Å ²)	Q<0.9
56	MG	DG	3001	1/1	0.55	0.21	81,81,81,81	0
56	MG	DA	3574	1/1	0.66	0.33	56,56,56,56	0
56	MG	CA	3138	1/1	0.69	0.17	58,58,58,58	0
56	MG	DA	3504	1/1	0.71	0.17	49,49,49,49	0
56	MG	DA	3247	1/1	0.73	0.15	49,49,49,49	0
56	MG	AA	3184	1/1	0.75	0.23	74,74,74,74	0
56	MG	AA	3056	1/1	0.75	0.29	69,69,69,69	0
56	MG	AA	3180	1/1	0.75	0.15	56,56,56,56	0
56	MG	CA	3105	1/1	0.76	0.25	84,84,84,84	0
56	MG	AA	3167	1/1	0.76	0.25	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3580	1/1	0.76	0.13	62,62,62,62	0
56	MG	DA	3478	1/1	0.77	0.25	53,53,53,53	0
56	MG	CA	3126	1/1	0.77	0.15	73,73,73,73	0
56	MG	BA	3639	1/1	0.77	0.19	64,64,64,64	0
56	MG	CA	3119	1/1	0.77	0.12	48,48,48,48	0
56	MG	DA	3326	1/1	0.78	0.13	41,41,41,41	0
56	MG	DA	3354	1/1	0.78	0.16	51,51,51,51	0
56	MG	CA	3149	1/1	0.78	0.38	66,66,66,66	0
56	MG	DA	3271	1/1	0.79	0.17	55,55,55,55	0
56	MG	AA	3055	1/1	0.79	0.20	72,72,72,72	0
56	MG	CA	3068	1/1	0.79	0.20	74,74,74,74	0
56	MG	DA	3446	1/1	0.79	0.12	46,46,46,46	0
56	MG	AF	3001	1/1	0.80	0.18	52,52,52,52	0
56	MG	CA	3140	1/1	0.80	0.23	61,61,61,61	0
56	MG	DA	3475	1/1	0.80	0.14	41,41,41,41	0
56	MG	BA	3634	1/1	0.80	0.23	41,41,41,41	0
56	MG	CA	3108	1/1	0.80	0.20	59,59,59,59	0
56	MG	BA	3569	1/1	0.80	0.17	55,55,55,55	0
56	MG	BB	3009	1/1	0.80	0.18	67,67,67,67	0
56	MG	CA	3125	1/1	0.81	0.24	71,71,71,71	0
56	MG	BA	3631	1/1	0.81	0.13	41,41,41,41	0
56	MG	DA	3103	1/1	0.81	0.08	56,56,56,56	0
56	MG	DA	3443	1/1	0.81	0.12	49,49,49,49	0
56	MG	AA	3106	1/1	0.81	0.15	50,50,50,50	0
56	MG	DA	3366	1/1	0.82	0.12	43,43,43,43	0
56	MG	DA	3416	1/1	0.82	0.13	44,44,44,44	0
56	MG	BA	3536	1/1	0.82	0.21	53,53,53,53	0
56	MG	BA	3497	1/1	0.82	0.14	34,34,34,34	0
56	MG	BA	3633	1/1	0.82	0.15	57,57,57,57	0
56	MG	BZ	3001	1/1	0.82	0.12	58,58,58,58	0
56	MG	CA	3016	1/1	0.82	0.16	68,68,68,68	0
56	MG	DA	3507	1/1	0.82	0.13	54,54,54,54	0
56	MG	DA	3566	1/1	0.82	0.15	61,61,61,61	0
56	MG	CA	3035	1/1	0.82	0.13	66,66,66,66	0
56	MG	DB	3006	1/1	0.82	0.13	55,55,55,55	0
56	MG	CA	3065	1/1	0.82	0.14	55,55,55,55	0
56	MG	DW	3002	1/1	0.82	0.11	60,60,60,60	0
56	MG	CA	3145	1/1	0.83	0.18	59,59,59,59	0
56	MG	DA	3518	1/1	0.83	0.19	53,53,53,53	0
56	MG	DA	3301	1/1	0.83	0.13	56,56,56,56	0
56	MG	DA	3302	1/1	0.83	0.10	43,43,43,43	0
56	MG	BA	3062	1/1	0.83	0.18	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3104	1/1	0.83	0.29	74,74,74,74	0
56	MG	AA	3024	1/1	0.83	0.38	60,60,60,60	0
56	MG	DY	502	1/1	0.83	0.14	51,51,51,51	0
56	MG	BA	3466	1/1	0.84	0.26	49,49,49,49	0
56	MG	AA	3049	1/1	0.84	0.14	47,47,47,47	0
56	MG	CA	3151	1/1	0.84	0.20	50,50,50,50	0
56	MG	DA	3020	1/1	0.84	0.22	50,50,50,50	0
56	MG	DA	3474	1/1	0.84	0.11	62,62,62,62	0
56	MG	DA	3090	1/1	0.84	0.10	54,54,54,54	0
56	MG	BA	3505	1/1	0.84	0.23	46,46,46,46	0
56	MG	DA	3479	1/1	0.84	0.18	63,63,63,63	0
56	MG	DA	3150	1/1	0.84	0.35	55,55,55,55	0
56	MG	AA	3181	1/1	0.84	0.17	53,53,53,53	0
56	MG	AA	3109	1/1	0.84	0.22	44,44,44,44	0
56	MG	DA	3538	1/1	0.84	0.10	39,39,39,39	0
56	MG	DA	3300	1/1	0.84	0.18	58,58,58,58	0
56	MG	AA	3160	1/1	0.84	0.12	71,71,71,71	0
56	MG	AA	3086	1/1	0.84	0.37	61,61,61,61	0
56	MG	DB	3009	1/1	0.84	0.14	60,60,60,60	0
56	MG	CA	3139	1/1	0.84	0.15	67,67,67,67	0
56	MG	DA	3343	1/1	0.84	0.23	56,56,56,56	0
56	MG	BA	3331	1/1	0.84	0.12	59,59,59,59	0
56	MG	CA	3103	1/1	0.85	0.16	52,52,52,52	0
56	MG	CA	3129	1/1	0.85	0.11	55,55,55,55	0
56	MG	CA	3011	1/1	0.85	0.17	66,66,66,66	0
56	MG	DA	3539	1/1	0.85	0.16	52,52,52,52	0
56	MG	BA	3617	1/1	0.85	0.25	66,66,66,66	0
56	MG	AA	3088	1/1	0.85	0.20	62,62,62,62	0
56	MG	BA	3632	1/1	0.85	0.25	54,54,54,54	0
56	MG	BA	3611	1/1	0.85	0.20	59,59,59,59	0
56	MG	DA	3485	1/1	0.85	0.18	60,60,60,60	0
56	MG	DA	3501	1/1	0.85	0.11	55,55,55,55	0
56	MG	DA	3381	1/1	0.85	0.20	56,56,56,56	0
56	MG	AA	3149	1/1	0.86	0.17	68,68,68,68	0
56	MG	AA	3027	1/1	0.86	0.21	71,71,71,71	0
56	MG	DA	3359	1/1	0.86	0.17	43,43,43,43	0
56	MG	BA	3043	1/1	0.86	0.20	36,36,36,36	0
56	MG	CA	3132	1/1	0.86	0.25	73,73,73,73	0
56	MG	DA	3398	1/1	0.86	0.14	51,51,51,51	0
56	MG	BA	3545	1/1	0.86	0.11	54,54,54,54	0
56	MG	BA	3557	1/1	0.86	0.18	42,42,42,42	0
56	MG	AA	3092	1/1	0.86	0.23	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3244	1/1	0.86	0.21	46,46,46,46	0
56	MG	BA	3582	1/1	0.86	0.14	31,31,31,31	0
56	MG	CA	3036	1/1	0.86	0.14	56,56,56,56	0
56	MG	BA	3583	1/1	0.86	0.12	37,37,37,37	0
56	MG	DA	3058	1/1	0.86	0.20	45,45,45,45	0
56	MG	BA	3584	1/1	0.86	0.14	44,44,44,44	0
56	MG	CA	3083	1/1	0.86	0.22	66,66,66,66	0
56	MG	DA	3135	1/1	0.86	0.12	47,47,47,47	0
56	MG	CA	3084	1/1	0.86	0.13	72,72,72,72	0
56	MG	BA	3601	1/1	0.86	0.15	50,50,50,50	0
56	MG	DA	3251	1/1	0.86	0.22	62,62,62,62	0
56	MG	DA	3557	1/1	0.86	0.13	62,62,62,62	0
56	MG	DA	3561	1/1	0.86	0.14	63,63,63,63	0
56	MG	AA	3013	1/1	0.86	0.25	58,58,58,58	0
56	MG	DA	3568	1/1	0.86	0.11	60,60,60,60	0
56	MG	DA	3274	1/1	0.86	0.13	56,56,56,56	0
56	MG	DA	3580	1/1	0.86	0.10	58,58,58,58	0
56	MG	DB	3005	1/1	0.86	0.11	56,56,56,56	0
56	MG	AA	3054	1/1	0.86	0.17	65,65,65,65	0
56	MG	BA	3483	1/1	0.86	0.14	47,47,47,47	0
56	MG	BA	3496	1/1	0.86	0.16	31,31,31,31	0
56	MG	DQ	3003	1/1	0.86	0.13	50,50,50,50	0
56	MG	DA	3309	1/1	0.86	0.13	60,60,60,60	0
56	MG	CA	3121	1/1	0.86	0.15	61,61,61,61	0
56	MG	BA	3307	1/1	0.87	0.08	63,63,63,63	0
56	MG	BA	3585	1/1	0.87	0.25	50,50,50,50	0
56	MG	BA	3510	1/1	0.87	0.19	25,25,25,25	0
56	MG	CA	3019	1/1	0.87	0.34	71,71,71,71	0
56	MG	CA	3034	1/1	0.87	0.24	67,67,67,67	0
56	MG	AA	3061	1/1	0.87	0.22	62,62,62,62	0
56	MG	BA	3395	1/1	0.87	0.10	54,54,54,54	0
56	MG	CA	3049	1/1	0.87	0.18	51,51,51,51	0
56	MG	DA	3325	1/1	0.87	0.12	54,54,54,54	0
56	MG	BA	3412	1/1	0.87	0.11	48,48,48,48	0
56	MG	CA	3067	1/1	0.87	0.19	63,63,63,63	0
56	MG	AA	3171	1/1	0.87	0.10	62,62,62,62	0
56	MG	CA	3078	1/1	0.87	0.18	66,66,66,66	0
56	MG	BA	3574	1/1	0.87	0.19	55,55,55,55	0
56	MG	DA	3022	1/1	0.87	0.19	39,39,39,39	0
56	MG	BA	3211	1/1	0.87	0.22	29,29,29,29	0
56	MG	BA	3229	1/1	0.87	0.20	54,54,54,54	0
56	MG	DA	3425	1/1	0.87	0.10	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3428	1/1	0.87	0.15	33,33,33,33	0
56	MG	DF	303	1/1	0.87	0.17	57,57,57,57	0
56	MG	DA	3437	1/1	0.87	0.15	48,48,48,48	0
56	MG	AA	3102	1/1	0.87	0.23	60,60,60,60	0
56	MG	BB	3010	1/1	0.87	0.09	77,77,77,77	0
56	MG	BB	3015	1/1	0.87	0.10	48,48,48,48	0
56	MG	DA	3467	1/1	0.88	0.14	47,47,47,47	0
56	MG	DA	3470	1/1	0.88	0.30	52,52,52,52	0
56	MG	DA	3252	1/1	0.88	0.12	53,53,53,53	0
56	MG	AA	3121	1/1	0.88	0.14	40,40,40,40	0
56	MG	AA	3003	1/1	0.88	0.12	57,57,57,57	0
56	MG	DA	3275	1/1	0.88	0.12	45,45,45,45	0
56	MG	CA	3041	1/1	0.88	0.18	67,67,67,67	0
56	MG	DA	3496	1/1	0.88	0.10	46,46,46,46	0
56	MG	CA	3133	1/1	0.88	0.19	68,68,68,68	0
56	MG	CA	3048	1/1	0.88	0.39	52,52,52,52	0
56	MG	AA	3057	1/1	0.88	0.29	67,67,67,67	0
56	MG	BB	3003	1/1	0.88	0.09	61,61,61,61	0
56	MG	DA	3526	1/1	0.88	0.14	64,64,64,64	0
56	MG	AA	3058	1/1	0.88	0.19	62,62,62,62	0
56	MG	AA	3023	1/1	0.88	0.30	71,71,71,71	0
56	MG	DA	3347	1/1	0.88	0.09	41,41,41,41	0
56	MG	BA	3553	1/1	0.88	0.49	48,48,48,48	0
56	MG	BG	3003	1/1	0.88	0.09	41,41,41,41	0
56	MG	DA	3567	1/1	0.88	0.11	41,41,41,41	0
56	MG	BA	3094	1/1	0.88	0.14	45,45,45,45	0
56	MG	DA	3373	1/1	0.88	0.09	42,42,42,42	0
56	MG	CA	3003	1/1	0.88	0.21	65,65,65,65	0
56	MG	DA	3585	1/1	0.88	0.09	37,37,37,37	0
56	MG	CA	3009	1/1	0.88	0.17	55,55,55,55	0
56	MG	BA	3612	1/1	0.88	0.18	51,51,51,51	0
56	MG	DA	3420	1/1	0.88	0.09	46,46,46,46	0
56	MG	AA	3176	1/1	0.88	0.14	60,60,60,60	0
56	MG	DA	3147	1/1	0.88	0.20	47,47,47,47	0
56	MG	DN	5001	1/1	0.88	0.12	65,65,65,65	0
56	MG	AA	3045	1/1	0.88	0.25	60,60,60,60	0
56	MG	CA	3021	1/1	0.88	0.14	52,52,52,52	0
56	MG	BA	3576	1/1	0.88	0.13	48,48,48,48	0
56	MG	AA	3042	1/1	0.89	0.20	54,54,54,54	0
56	MG	AA	3164	1/1	0.89	0.14	61,61,61,61	0
56	MG	BA	3306	1/1	0.89	0.17	54,54,54,54	0
56	MG	DA	3412	1/1	0.89	0.19	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3004	1/1	0.89	0.11	51,51,51,51	0
56	MG	AA	3016	1/1	0.89	0.16	49,49,49,49	0
56	MG	BA	3323	1/1	0.89	0.11	61,61,61,61	0
56	MG	BA	3578	1/1	0.89	0.12	59,59,59,59	0
56	MG	BA	3579	1/1	0.89	0.10	46,46,46,46	0
56	MG	BA	3036	1/1	0.89	0.13	56,56,56,56	0
56	MG	CA	3025	1/1	0.89	0.11	48,48,48,48	0
56	MG	CA	3033	1/1	0.89	0.28	52,52,52,52	0
56	MG	BA	3357	1/1	0.89	0.10	30,30,30,30	0
56	MG	DA	3066	1/1	0.89	0.13	49,49,49,49	0
56	MG	DA	3083	1/1	0.89	0.09	48,48,48,48	0
56	MG	BA	3367	1/1	0.89	0.12	49,49,49,49	0
56	MG	DA	3100	1/1	0.89	0.09	34,34,34,34	0
56	MG	BA	3387	1/1	0.89	0.21	49,49,49,49	0
56	MG	DA	3109	1/1	0.89	0.08	50,50,50,50	0
56	MG	AA	3169	1/1	0.89	0.15	71,71,71,71	0
56	MG	BA	3593	1/1	0.89	0.23	39,39,39,39	0
56	MG	BA	3401	1/1	0.89	0.14	32,32,32,32	0
56	MG	DA	3173	1/1	0.89	0.15	54,54,54,54	0
56	MG	DA	3191	1/1	0.89	0.14	53,53,53,53	0
56	MG	CA	3055	1/1	0.89	0.11	62,62,62,62	0
56	MG	BA	3605	1/1	0.89	0.08	46,46,46,46	0
56	MG	DA	3545	1/1	0.89	0.16	58,58,58,58	0
56	MG	BA	3056	1/1	0.89	0.13	46,46,46,46	0
56	MG	AA	3002	1/1	0.89	0.23	43,43,43,43	0
56	MG	BA	3469	1/1	0.89	0.09	28,28,28,28	0
56	MG	CA	3082	1/1	0.89	0.32	62,62,62,62	0
56	MG	BA	3619	1/1	0.89	0.12	30,30,30,30	0
56	MG	BA	3075	1/1	0.89	0.31	58,58,58,58	0
56	MG	BA	3495	1/1	0.89	0.23	48,48,48,48	0
56	MG	DA	3307	1/1	0.89	0.09	53,53,53,53	0
56	MG	BA	3090	1/1	0.89	0.16	44,44,44,44	0
56	MG	AA	3142	1/1	0.89	0.17	60,60,60,60	0
56	MG	DB	3007	1/1	0.89	0.09	38,38,38,38	0
56	MG	BA	3111	1/1	0.89	0.08	27,27,27,27	0
56	MG	DA	3337	1/1	0.89	0.07	42,42,42,42	0
56	MG	CA	3118	1/1	0.89	0.15	78,78,78,78	0
56	MG	BA	3192	1/1	0.89	0.26	58,58,58,58	0
56	MG	BA	3523	1/1	0.89	0.10	50,50,50,50	0
56	MG	AA	3073	1/1	0.89	0.24	50,50,50,50	0
56	MG	BA	3213	1/1	0.89	0.20	21,21,21,21	0
56	MG	BA	3609	1/1	0.90	0.10	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3399	1/1	0.90	0.08	40,40,40,40	0
56	MG	DA	3402	1/1	0.90	0.11	63,63,63,63	0
56	MG	BA	3488	1/1	0.90	0.22	36,36,36,36	0
56	MG	BA	3237	1/1	0.90	0.21	57,57,57,57	0
56	MG	DA	3067	1/1	0.90	0.24	53,53,53,53	0
56	MG	AA	3093	1/1	0.90	0.14	45,45,45,45	0
56	MG	BA	3246	1/1	0.90	0.20	56,56,56,56	0
56	MG	DA	3098	1/1	0.90	0.09	46,46,46,46	0
56	MG	BA	3503	1/1	0.90	0.13	30,30,30,30	0
56	MG	BA	3293	1/1	0.90	0.11	17,17,17,17	0
56	MG	DA	3108	1/1	0.90	0.10	46,46,46,46	0
56	MG	CA	3072	1/1	0.90	0.22	57,57,57,57	0
56	MG	BA	3044	1/1	0.90	0.15	30,30,30,30	0
56	MG	AA	3038	1/1	0.90	0.23	53,53,53,53	0
56	MG	AA	3062	1/1	0.90	0.30	58,58,58,58	0
56	MG	DA	3163	1/1	0.90	0.26	31,31,31,31	0
56	MG	DA	3166	1/1	0.90	0.16	35,35,35,35	0
56	MG	DA	3487	1/1	0.90	0.09	50,50,50,50	0
56	MG	AA	3041	1/1	0.90	0.20	52,52,52,52	0
56	MG	DA	3500	1/1	0.90	0.17	46,46,46,46	0
56	MG	BB	3005	1/1	0.90	0.18	30,30,30,30	0
56	MG	DA	3211	1/1	0.90	0.17	35,35,35,35	0
56	MG	BA	3549	1/1	0.90	0.16	57,57,57,57	0
56	MG	DA	3515	1/1	0.90	0.09	64,64,64,64	0
56	MG	BA	3350	1/1	0.90	0.14	59,59,59,59	0
56	MG	AA	3113	1/1	0.90	0.21	53,53,53,53	0
56	MG	DA	3530	1/1	0.90	0.14	60,60,60,60	0
56	MG	DA	3531	1/1	0.90	0.11	69,69,69,69	0
56	MG	BA	3567	1/1	0.90	0.09	53,53,53,53	0
56	MG	BA	3359	1/1	0.90	0.10	54,54,54,54	0
56	MG	DA	3541	1/1	0.90	0.11	57,57,57,57	0
56	MG	DA	3544	1/1	0.90	0.12	51,51,51,51	0
56	MG	AA	3085	1/1	0.90	0.23	63,63,63,63	0
56	MG	CA	3123	1/1	0.90	0.17	66,66,66,66	0
56	MG	BA	3373	1/1	0.90	0.13	41,41,41,41	0
56	MG	BA	3381	1/1	0.90	0.18	31,31,31,31	0
56	MG	AA	3010	1/1	0.90	0.20	60,60,60,60	0
56	MG	CA	3013	1/1	0.90	0.16	53,53,53,53	0
56	MG	AA	3015	1/1	0.90	0.12	56,56,56,56	0
56	MG	CA	3137	1/1	0.90	0.14	66,66,66,66	0
56	MG	DA	3584	1/1	0.90	0.13	61,61,61,61	0
56	MG	BA	3206	1/1	0.90	0.21	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3403	1/1	0.90	0.13	18,18,18,18	0
56	MG	AA	3185	1/1	0.90	0.08	64,64,64,64	0
56	MG	DA	3351	1/1	0.90	0.09	46,46,46,46	0
56	MG	BA	3415	1/1	0.90	0.15	54,54,54,54	0
56	MG	AA	3151	1/1	0.90	0.18	45,45,45,45	0
56	MG	AA	3035	1/1	0.90	0.23	65,65,65,65	0
56	MG	DA	3371	1/1	0.90	0.07	46,46,46,46	0
56	MG	DA	3017	1/1	0.90	0.25	46,46,46,46	0
56	MG	DA	3375	1/1	0.90	0.12	49,49,49,49	0
56	MG	BA	3230	1/1	0.90	0.07	40,40,40,40	0
56	MG	DA	3340	1/1	0.91	0.11	47,47,47,47	0
56	MG	CA	3120	1/1	0.91	0.17	51,51,51,51	0
56	MG	AA	3110	1/1	0.91	0.12	60,60,60,60	0
56	MG	AA	3012	1/1	0.91	0.10	64,64,64,64	0
56	MG	AA	3119	1/1	0.91	0.16	57,57,57,57	0
56	MG	BA	3235	1/1	0.91	0.09	51,51,51,51	0
56	MG	BH	3001	1/1	0.91	0.19	56,56,56,56	0
56	MG	BO	5001	1/1	0.91	0.18	62,62,62,62	0
56	MG	AA	3076	1/1	0.91	0.14	52,52,52,52	0
56	MG	BA	3404	1/1	0.91	0.16	38,38,38,38	0
56	MG	BA	3405	1/1	0.91	0.11	26,26,26,26	0
56	MG	CA	3007	1/1	0.91	0.07	50,50,50,50	0
56	MG	AA	3126	1/1	0.91	0.29	54,54,54,54	0
56	MG	AA	3006	1/1	0.91	0.11	67,67,67,67	0
56	MG	DA	3406	1/1	0.91	0.09	50,50,50,50	0
56	MG	CA	3148	1/1	0.91	0.11	57,57,57,57	0
56	MG	CA	3012	1/1	0.91	0.18	52,52,52,52	0
56	MG	BA	3423	1/1	0.91	0.11	47,47,47,47	0
56	MG	DA	3424	1/1	0.91	0.14	30,30,30,30	0
56	MG	CA	3152	1/1	0.91	0.13	75,75,75,75	0
56	MG	BA	3428	1/1	0.91	0.08	58,58,58,58	0
56	MG	CA	3018	1/1	0.91	0.10	43,43,43,43	0
56	MG	BA	3443	1/1	0.91	0.09	44,44,44,44	0
56	MG	DA	3445	1/1	0.91	0.13	48,48,48,48	0
56	MG	DA	3028	1/1	0.91	0.10	47,47,47,47	0
56	MG	BA	3278	1/1	0.91	0.08	50,50,50,50	0
56	MG	AA	3018	1/1	0.91	0.16	50,50,50,50	0
56	MG	DA	3473	1/1	0.91	0.10	50,50,50,50	0
56	MG	BA	3476	1/1	0.91	0.07	51,51,51,51	0
56	MG	DA	3070	1/1	0.91	0.30	49,49,49,49	0
56	MG	DA	3477	1/1	0.91	0.09	42,42,42,42	0
56	MG	DA	3076	1/1	0.91	0.07	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3596	1/1	0.91	0.15	56,56,56,56	0
56	MG	DA	3483	1/1	0.91	0.10	54,54,54,54	0
56	MG	DA	3484	1/1	0.91	0.12	34,34,34,34	0
56	MG	DA	3088	1/1	0.91	0.06	39,39,39,39	0
56	MG	BA	3600	1/1	0.91	0.20	68,68,68,68	0
56	MG	BA	3480	1/1	0.91	0.17	43,43,43,43	0
56	MG	BA	3604	1/1	0.91	0.07	28,28,28,28	0
56	MG	BA	3297	1/1	0.91	0.08	39,39,39,39	0
56	MG	BA	3300	1/1	0.91	0.15	39,39,39,39	0
56	MG	DA	3506	1/1	0.91	0.11	65,65,65,65	0
56	MG	CA	3050	1/1	0.91	0.21	67,67,67,67	0
56	MG	AA	3019	1/1	0.91	0.27	62,62,62,62	0
56	MG	DA	3516	1/1	0.91	0.08	61,61,61,61	0
56	MG	AA	3153	1/1	0.91	0.17	50,50,50,50	0
56	MG	CA	3066	1/1	0.91	0.21	43,43,43,43	0
56	MG	BA	3112	1/1	0.91	0.14	40,40,40,40	0
56	MG	BA	3125	1/1	0.91	0.14	51,51,51,51	0
56	MG	BA	3626	1/1	0.91	0.15	50,50,50,50	0
56	MG	CA	3077	1/1	0.91	0.18	44,44,44,44	0
56	MG	DA	3192	1/1	0.91	0.12	51,51,51,51	0
56	MG	DA	3206	1/1	0.91	0.08	50,50,50,50	0
56	MG	BA	3627	1/1	0.91	0.13	54,54,54,54	0
56	MG	DA	3552	1/1	0.91	0.17	49,49,49,49	0
56	MG	DA	3213	1/1	0.91	0.12	34,34,34,34	0
56	MG	BA	3629	1/1	0.91	0.17	60,60,60,60	0
56	MG	BA	3140	1/1	0.91	0.17	33,33,33,33	0
56	MG	BA	3507	1/1	0.91	0.11	53,53,53,53	0
56	MG	DA	3257	1/1	0.91	0.11	55,55,55,55	0
56	MG	CA	3085	1/1	0.91	0.13	52,52,52,52	0
56	MG	DA	3578	1/1	0.91	0.10	47,47,47,47	0
56	MG	DA	3272	1/1	0.91	0.10	57,57,57,57	0
56	MG	CA	3090	1/1	0.91	0.17	66,66,66,66	0
56	MG	CA	3091	1/1	0.91	0.19	66,66,66,66	0
56	MG	DB	3004	1/1	0.91	0.11	36,36,36,36	0
56	MG	BA	3171	1/1	0.91	0.09	44,44,44,44	0
56	MG	BA	3513	1/1	0.91	0.08	60,60,60,60	0
56	MG	AA	3156	1/1	0.91	0.10	61,61,61,61	0
56	MG	BA	3642	1/1	0.91	0.20	47,47,47,47	0
56	MG	DB	3012	1/1	0.91	0.13	53,53,53,53	0
56	MG	CA	3113	1/1	0.91	0.14	57,57,57,57	0
56	MG	CA	3114	1/1	0.91	0.14	80,80,80,80	0
56	MG	AA	3187	1/1	0.91	0.13	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3327	1/1	0.91	0.14	34,34,34,34	0
56	MG	DA	3328	1/1	0.91	0.13	48,48,48,48	0
56	MG	AA	3158	1/1	0.91	0.11	54,54,54,54	0
56	MG	D8	5002	1/1	0.91	0.17	64,64,64,64	0
56	MG	BD	302	1/1	0.92	0.09	45,45,45,45	0
56	MG	BA	3347	1/1	0.92	0.14	53,53,53,53	0
56	MG	BA	3130	1/1	0.92	0.09	40,40,40,40	0
56	MG	BA	3550	1/1	0.92	0.17	44,44,44,44	0
56	MG	BW	3002	1/1	0.92	0.13	57,57,57,57	0
56	MG	CA	3131	1/1	0.92	0.10	65,65,65,65	0
56	MG	DA	3346	1/1	0.92	0.10	33,33,33,33	0
56	MG	BY	502	1/1	0.92	0.08	35,35,35,35	0
56	MG	BY	503	1/1	0.92	0.07	42,42,42,42	0
56	MG	DA	3352	1/1	0.92	0.07	45,45,45,45	0
56	MG	CA	3136	1/1	0.92	0.08	53,53,53,53	0
56	MG	BA	3013	1/1	0.92	0.08	35,35,35,35	0
56	MG	DA	3360	1/1	0.92	0.09	39,39,39,39	0
56	MG	DA	3361	1/1	0.92	0.15	38,38,38,38	0
56	MG	BA	3141	1/1	0.92	0.10	45,45,45,45	0
56	MG	BA	3019	1/1	0.92	0.23	49,49,49,49	0
56	MG	BA	3023	1/1	0.92	0.10	40,40,40,40	0
56	MG	BA	3571	1/1	0.92	0.16	50,50,50,50	0
56	MG	AA	3154	1/1	0.92	0.19	51,51,51,51	0
56	MG	DA	3386	1/1	0.92	0.17	48,48,48,48	0
56	MG	BA	3575	1/1	0.92	0.08	55,55,55,55	0
56	MG	AA	3125	1/1	0.92	0.21	41,41,41,41	0
56	MG	AA	3179	1/1	0.92	0.21	63,63,63,63	0
56	MG	DA	3004	1/1	0.92	0.18	51,51,51,51	0
56	MG	DA	3409	1/1	0.92	0.22	53,53,53,53	0
56	MG	DA	3009	1/1	0.92	0.08	42,42,42,42	0
56	MG	BA	3046	1/1	0.92	0.13	29,29,29,29	0
56	MG	DA	3418	1/1	0.92	0.10	29,29,29,29	0
56	MG	AA	3112	1/1	0.92	0.19	94,94,94,94	0
56	MG	DA	3021	1/1	0.92	0.11	55,55,55,55	0
56	MG	AA	3159	1/1	0.92	0.07	56,56,56,56	0
56	MG	BA	3074	1/1	0.92	0.11	45,45,45,45	0
56	MG	DA	3432	1/1	0.92	0.18	33,33,33,33	0
56	MG	DA	3032	1/1	0.92	0.17	42,42,42,42	0
56	MG	DA	3438	1/1	0.92	0.15	38,38,38,38	0
56	MG	DA	3050	1/1	0.92	0.10	41,41,41,41	0
56	MG	DA	3052	1/1	0.92	0.08	49,49,49,49	0
56	MG	BA	3408	1/1	0.92	0.09	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3454	1/1	0.92	0.11	64,64,64,64	0
56	MG	DA	3465	1/1	0.92	0.13	38,38,38,38	0
56	MG	BA	3241	1/1	0.92	0.29	26,26,26,26	0
56	MG	AA	3004	1/1	0.92	0.15	67,67,67,67	0
56	MG	BA	3594	1/1	0.92	0.13	37,37,37,37	0
56	MG	DA	3075	1/1	0.92	0.13	41,41,41,41	0
56	MG	BA	3077	1/1	0.92	0.22	37,37,37,37	0
56	MG	BA	3254	1/1	0.92	0.12	45,45,45,45	0
56	MG	BA	3437	1/1	0.92	0.26	58,58,58,58	0
56	MG	BA	3602	1/1	0.92	0.10	31,31,31,31	0
56	MG	DA	3092	1/1	0.92	0.21	45,45,45,45	0
56	MG	BA	3265	1/1	0.92	0.27	47,47,47,47	0
56	MG	CA	3059	1/1	0.92	0.20	58,58,58,58	0
56	MG	CA	3062	1/1	0.92	0.13	57,57,57,57	0
56	MG	DA	3494	1/1	0.92	0.13	49,49,49,49	0
56	MG	BA	3449	1/1	0.92	0.08	47,47,47,47	0
56	MG	BA	3084	1/1	0.92	0.13	34,34,34,34	0
56	MG	DA	3113	1/1	0.92	0.12	41,41,41,41	0
56	MG	DA	3503	1/1	0.92	0.07	38,38,38,38	0
56	MG	DA	3118	1/1	0.92	0.17	49,49,49,49	0
56	MG	DA	3121	1/1	0.92	0.11	50,50,50,50	0
56	MG	DA	3125	1/1	0.92	0.10	47,47,47,47	0
56	MG	DA	3508	1/1	0.92	0.07	38,38,38,38	0
56	MG	DA	3510	1/1	0.92	0.14	53,53,53,53	0
56	MG	DA	3127	1/1	0.92	0.10	41,41,41,41	0
56	MG	AA	3079	1/1	0.92	0.33	49,49,49,49	0
56	MG	AA	3105	1/1	0.92	0.15	44,44,44,44	0
56	MG	CA	3071	1/1	0.92	0.30	51,51,51,51	0
56	MG	DA	3162	1/1	0.92	0.19	57,57,57,57	0
56	MG	BA	3098	1/1	0.92	0.23	56,56,56,56	0
56	MG	AA	3124	1/1	0.92	0.13	30,30,30,30	0
56	MG	BA	3624	1/1	0.92	0.13	49,49,49,49	0
56	MG	DA	3178	1/1	0.92	0.18	46,46,46,46	0
56	MG	CA	3081	1/1	0.92	0.12	56,56,56,56	0
56	MG	BA	3001	1/1	0.92	0.15	35,35,35,35	0
56	MG	DA	3201	1/1	0.92	0.13	51,51,51,51	0
56	MG	DA	3553	1/1	0.92	0.15	46,46,46,46	0
56	MG	BA	3309	1/1	0.92	0.09	32,32,32,32	0
56	MG	BA	3316	1/1	0.92	0.09	61,61,61,61	0
56	MG	DA	3563	1/1	0.92	0.11	60,60,60,60	0
56	MG	BA	3124	1/1	0.92	0.15	58,58,58,58	0
56	MG	DA	3236	1/1	0.92	0.14	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3239	1/1	0.92	0.15	56,56,56,56	0
56	MG	DA	3242	1/1	0.92	0.17	60,60,60,60	0
56	MG	CA	3086	1/1	0.92	0.17	68,68,68,68	0
56	MG	BA	3498	1/1	0.92	0.16	37,37,37,37	0
56	MG	BA	3324	1/1	0.92	0.10	53,53,53,53	0
56	MG	CA	3096	1/1	0.92	0.13	61,61,61,61	0
56	MG	DA	3592	1/1	0.92	0.30	52,52,52,52	0
56	MG	DA	3263	1/1	0.92	0.07	39,39,39,39	0
56	MG	DA	3269	1/1	0.92	0.14	43,43,43,43	0
56	MG	BA	3328	1/1	0.92	0.10	39,39,39,39	0
56	MG	BA	3329	1/1	0.92	0.09	30,30,30,30	0
56	MG	BA	3002	1/1	0.92	0.11	39,39,39,39	0
56	MG	CA	3107	1/1	0.92	0.23	56,56,56,56	0
56	MG	DE	3001	1/1	0.92	0.07	43,43,43,43	0
56	MG	BA	3675	1/1	0.92	0.25	33,33,33,33	0
56	MG	BA	3339	1/1	0.92	0.11	34,34,34,34	0
56	MG	BA	3515	1/1	0.92	0.10	25,25,25,25	0
56	MG	BA	3340	1/1	0.92	0.08	42,42,42,42	0
56	MG	BA	3524	1/1	0.92	0.08	57,57,57,57	0
56	MG	DA	3323	1/1	0.92	0.07	35,35,35,35	0
56	MG	D7	101	1/1	0.92	0.40	51,51,51,51	0
56	MG	BA	3345	1/1	0.92	0.15	41,41,41,41	0
56	MG	BU	205	1/1	0.93	0.11	53,53,53,53	0
56	MG	BV	201	1/1	0.93	0.25	36,36,36,36	0
56	MG	BA	3561	1/1	0.93	0.09	55,55,55,55	0
56	MG	BA	3565	1/1	0.93	0.12	51,51,51,51	0
56	MG	BA	3566	1/1	0.93	0.11	46,46,46,46	0
56	MG	DA	3329	1/1	0.93	0.07	48,48,48,48	0
56	MG	BA	3398	1/1	0.93	0.12	41,41,41,41	0
56	MG	B0	104	1/1	0.93	0.21	48,48,48,48	0
56	MG	BA	3064	1/1	0.93	0.15	30,30,30,30	0
56	MG	BA	3073	1/1	0.93	0.10	14,14,14,14	0
56	MG	AA	3065	1/1	0.93	0.20	48,48,48,48	0
56	MG	AA	3107	1/1	0.93	0.22	36,36,36,36	0
56	MG	CE	202	1/1	0.93	0.10	68,68,68,68	0
56	MG	CF	3001	1/1	0.93	0.11	45,45,45,45	0
56	MG	CJ	5001	1/1	0.93	0.07	60,60,60,60	0
56	MG	CK	3001	1/1	0.93	0.14	50,50,50,50	0
56	MG	CX	101	1/1	0.93	0.18	48,48,48,48	0
56	MG	DA	3365	1/1	0.93	0.07	29,29,29,29	0
56	MG	AA	3066	1/1	0.93	0.22	46,46,46,46	0
56	MG	AE	3001	1/1	0.93	0.06	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3261	1/1	0.93	0.15	53,53,53,53	0
56	MG	CA	3015	1/1	0.93	0.10	43,43,43,43	0
56	MG	BA	3416	1/1	0.93	0.12	64,64,64,64	0
56	MG	DA	3384	1/1	0.93	0.16	52,52,52,52	0
56	MG	BA	3088	1/1	0.93	0.09	42,42,42,42	0
56	MG	DA	3392	1/1	0.93	0.09	54,54,54,54	0
56	MG	DA	3025	1/1	0.93	0.09	41,41,41,41	0
56	MG	BA	3425	1/1	0.93	0.16	53,53,53,53	0
56	MG	AA	3039	1/1	0.93	0.07	45,45,45,45	0
56	MG	DA	3033	1/1	0.93	0.15	37,37,37,37	0
56	MG	DA	3408	1/1	0.93	0.11	28,28,28,28	0
56	MG	DA	3039	1/1	0.93	0.24	51,51,51,51	0
56	MG	DA	3044	1/1	0.93	0.05	47,47,47,47	0
56	MG	DA	3414	1/1	0.93	0.07	42,42,42,42	0
56	MG	DA	3047	1/1	0.93	0.17	41,41,41,41	0
56	MG	BA	3288	1/1	0.93	0.11	48,48,48,48	0
56	MG	CA	3028	1/1	0.93	0.07	52,52,52,52	0
56	MG	DA	3423	1/1	0.93	0.09	40,40,40,40	0
56	MG	CA	3029	1/1	0.93	0.18	48,48,48,48	0
56	MG	DA	3065	1/1	0.93	0.22	49,49,49,49	0
56	MG	CA	3032	1/1	0.93	0.12	68,68,68,68	0
56	MG	BA	3586	1/1	0.93	0.23	45,45,45,45	0
56	MG	BA	3588	1/1	0.93	0.12	51,51,51,51	0
56	MG	BA	3441	1/1	0.93	0.08	44,44,44,44	0
56	MG	DA	3441	1/1	0.93	0.21	45,45,45,45	0
56	MG	BA	3093	1/1	0.93	0.08	40,40,40,40	0
56	MG	DA	3444	1/1	0.93	0.20	53,53,53,53	0
56	MG	BA	3595	1/1	0.93	0.09	47,47,47,47	0
56	MG	CA	3043	1/1	0.93	0.16	60,60,60,60	0
56	MG	DA	3450	1/1	0.93	0.10	37,37,37,37	0
56	MG	DA	3089	1/1	0.93	0.20	33,33,33,33	0
56	MG	DA	3459	1/1	0.93	0.18	38,38,38,38	0
56	MG	CA	3044	1/1	0.93	0.13	56,56,56,56	0
56	MG	DA	3091	1/1	0.93	0.12	45,45,45,45	0
56	MG	DA	3469	1/1	0.93	0.16	33,33,33,33	0
56	MG	BA	3447	1/1	0.93	0.15	55,55,55,55	0
56	MG	DA	3472	1/1	0.93	0.08	53,53,53,53	0
56	MG	DA	3096	1/1	0.93	0.06	29,29,29,29	0
56	MG	DA	3097	1/1	0.93	0.07	46,46,46,46	0
56	MG	BA	3597	1/1	0.93	0.11	43,43,43,43	0
56	MG	AK	3001	1/1	0.93	0.15	43,43,43,43	0
56	MG	BA	3298	1/1	0.93	0.07	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3106	1/1	0.93	0.06	43,43,43,43	0
56	MG	DA	3481	1/1	0.93	0.07	41,41,41,41	0
56	MG	CA	3057	1/1	0.93	0.12	41,41,41,41	0
56	MG	AX	3002	1/1	0.93	0.12	56,56,56,56	0
56	MG	BA	3472	1/1	0.93	0.13	34,34,34,34	0
56	MG	BA	3106	1/1	0.93	0.11	40,40,40,40	0
56	MG	DA	3488	1/1	0.93	0.08	41,41,41,41	0
56	MG	AX	3007	1/1	0.93	0.18	60,60,60,60	0
56	MG	AA	3128	1/1	0.93	0.15	57,57,57,57	0
56	MG	AA	3131	1/1	0.93	0.10	55,55,55,55	0
56	MG	DA	3132	1/1	0.93	0.05	35,35,35,35	0
56	MG	BA	3615	1/1	0.93	0.10	42,42,42,42	0
56	MG	DA	3145	1/1	0.93	0.04	31,31,31,31	0
56	MG	BA	3616	1/1	0.93	0.10	34,34,34,34	0
56	MG	AA	3136	1/1	0.93	0.13	56,56,56,56	0
56	MG	DA	3155	1/1	0.93	0.24	45,45,45,45	0
56	MG	DA	3158	1/1	0.93	0.15	36,36,36,36	0
56	MG	BA	3016	1/1	0.93	0.24	50,50,50,50	0
56	MG	AA	3111	1/1	0.93	0.20	45,45,45,45	0
56	MG	AA	3170	1/1	0.93	0.12	54,54,54,54	0
56	MG	BA	3165	1/1	0.93	0.25	43,43,43,43	0
56	MG	BA	3334	1/1	0.93	0.10	32,32,32,32	0
56	MG	DA	3187	1/1	0.93	0.08	46,46,46,46	0
56	MG	DA	3534	1/1	0.93	0.12	54,54,54,54	0
56	MG	DA	3535	1/1	0.93	0.10	22,22,22,22	0
56	MG	BA	3028	1/1	0.93	0.08	41,41,41,41	0
56	MG	BA	3172	1/1	0.93	0.17	54,54,54,54	0
56	MG	DA	3195	1/1	0.93	0.10	38,38,38,38	0
56	MG	BA	3191	1/1	0.93	0.11	33,33,33,33	0
56	MG	AA	3147	1/1	0.93	0.09	67,67,67,67	0
56	MG	BA	3638	1/1	0.93	0.10	32,32,32,32	0
56	MG	BA	3517	1/1	0.93	0.12	40,40,40,40	0
56	MG	DA	3223	1/1	0.93	0.17	47,47,47,47	0
56	MG	DA	3559	1/1	0.93	0.10	55,55,55,55	0
56	MG	DA	3230	1/1	0.93	0.14	41,41,41,41	0
56	MG	DA	3232	1/1	0.93	0.08	38,38,38,38	0
56	MG	BA	3199	1/1	0.93	0.12	32,32,32,32	0
56	MG	BA	3673	1/1	0.93	0.10	37,37,37,37	0
56	MG	AA	3148	1/1	0.93	0.07	56,56,56,56	0
56	MG	DA	3569	1/1	0.93	0.10	55,55,55,55	0
56	MG	DA	3245	1/1	0.93	0.19	46,46,46,46	0
56	MG	BA	3532	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
56	MG	DA	3249	1/1	0.93	0.11	34,34,34,34	0
56	MG	DA	3582	1/1	0.93	0.14	38,38,38,38	0
56	MG	CA	3110	1/1	0.93	0.13	64,64,64,64	0
56	MG	BB	3004	1/1	0.93	0.11	49,49,49,49	0
56	MG	DA	3587	1/1	0.93	0.17	53,53,53,53	0
56	MG	AA	3059	1/1	0.93	0.19	54,54,54,54	0
56	MG	DA	3593	1/1	0.93	0.13	51,51,51,51	0
56	MG	DA	3259	1/1	0.93	0.17	42,42,42,42	0
56	MG	DA	3260	1/1	0.93	0.16	36,36,36,36	0
56	MG	DA	3261	1/1	0.93	0.15	49,49,49,49	0
56	MG	BB	3006	1/1	0.93	0.09	49,49,49,49	0
56	MG	AA	3051	1/1	0.93	0.17	49,49,49,49	0
56	MG	DB	3010	1/1	0.93	0.23	60,60,60,60	0
56	MG	BA	3220	1/1	0.93	0.11	31,31,31,31	0
56	MG	AA	3020	1/1	0.93	0.07	49,49,49,49	0
56	MG	DA	3273	1/1	0.93	0.11	31,31,31,31	0
56	MG	CA	3122	1/1	0.93	0.19	54,54,54,54	0
56	MG	AA	3183	1/1	0.93	0.20	55,55,55,55	0
56	MG	BE	305	1/1	0.93	0.11	51,51,51,51	0
56	MG	DT	5001	1/1	0.93	0.08	42,42,42,42	0
56	MG	BF	303	1/1	0.93	0.11	20,20,20,20	0
56	MG	BA	3554	1/1	0.93	0.14	47,47,47,47	0
56	MG	BA	3234	1/1	0.93	0.20	57,57,57,57	0
56	MG	BA	3559	1/1	0.93	0.16	52,52,52,52	0
56	MG	CA	3109	1/1	0.94	0.13	50,50,50,50	0
56	MG	BA	3087	1/1	0.94	0.06	36,36,36,36	0
56	MG	CA	3112	1/1	0.94	0.17	55,55,55,55	0
56	MG	BA	3260	1/1	0.94	0.15	49,49,49,49	0
56	MG	BA	3471	1/1	0.94	0.14	35,35,35,35	0
56	MG	DA	3281	1/1	0.94	0.08	56,56,56,56	0
56	MG	DA	3288	1/1	0.94	0.12	64,64,64,64	0
56	MG	CA	3116	1/1	0.94	0.14	59,59,59,59	0
56	MG	CA	3117	1/1	0.94	0.18	42,42,42,42	0
56	MG	AX	3006	1/1	0.94	0.10	54,54,54,54	0
56	MG	DA	3306	1/1	0.94	0.06	38,38,38,38	0
56	MG	AA	3166	1/1	0.94	0.11	53,53,53,53	0
56	MG	BA	3635	1/1	0.94	0.13	63,63,63,63	0
56	MG	DA	3310	1/1	0.94	0.07	41,41,41,41	0
56	MG	DA	3316	1/1	0.94	0.17	57,57,57,57	0
56	MG	DA	3320	1/1	0.94	0.08	46,46,46,46	0
56	MG	BA	3478	1/1	0.94	0.08	47,47,47,47	0
56	MG	BA	3266	1/1	0.94	0.15	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3092	1/1	0.94	0.15	44,44,44,44	0
56	MG	BA	3645	1/1	0.94	0.07	66,66,66,66	0
56	MG	BA	3649	1/1	0.94	0.10	50,50,50,50	0
56	MG	BA	3652	1/1	0.94	0.17	49,49,49,49	0
56	MG	DA	3330	1/1	0.94	0.10	42,42,42,42	0
56	MG	BA	3654	1/1	0.94	0.21	64,64,64,64	0
56	MG	DA	3338	1/1	0.94	0.10	36,36,36,36	0
56	MG	BA	3667	1/1	0.94	0.34	38,38,38,38	0
56	MG	BA	3484	1/1	0.94	0.10	46,46,46,46	0
56	MG	BA	3283	1/1	0.94	0.16	57,57,57,57	0
56	MG	BA	3491	1/1	0.94	0.11	39,39,39,39	0
56	MG	BA	3493	1/1	0.94	0.09	40,40,40,40	0
56	MG	BA	3494	1/1	0.94	0.15	34,34,34,34	0
56	MG	BA	3285	1/1	0.94	0.12	48,48,48,48	0
56	MG	AA	3047	1/1	0.94	0.14	45,45,45,45	0
56	MG	AA	3074	1/1	0.94	0.17	38,38,38,38	0
56	MG	AA	3026	1/1	0.94	0.13	40,40,40,40	0
56	MG	BB	3017	1/1	0.94	0.09	40,40,40,40	0
56	MG	BA	3500	1/1	0.94	0.09	35,35,35,35	0
56	MG	BA	3101	1/1	0.94	0.07	30,30,30,30	0
56	MG	BE	306	1/1	0.94	0.07	32,32,32,32	0
56	MG	AA	3017	1/1	0.94	0.13	63,63,63,63	0
56	MG	BF	304	1/1	0.94	0.10	37,37,37,37	0
56	MG	BF	305	1/1	0.94	0.17	61,61,61,61	0
56	MG	DA	3003	1/1	0.94	0.24	47,47,47,47	0
56	MG	BG	3002	1/1	0.94	0.07	27,27,27,27	0
56	MG	DA	3393	1/1	0.94	0.06	48,48,48,48	0
56	MG	DA	3396	1/1	0.94	0.07	45,45,45,45	0
56	MG	AA	3081	1/1	0.94	0.13	44,44,44,44	0
56	MG	AA	3178	1/1	0.94	0.12	62,62,62,62	0
56	MG	BA	3308	1/1	0.94	0.12	52,52,52,52	0
56	MG	BP	201	1/1	0.94	0.18	36,36,36,36	0
56	MG	BP	203	1/1	0.94	0.13	47,47,47,47	0
56	MG	BA	3116	1/1	0.94	0.07	50,50,50,50	0
56	MG	DA	3410	1/1	0.94	0.21	64,64,64,64	0
56	MG	BA	3311	1/1	0.94	0.09	39,39,39,39	0
56	MG	DA	3030	1/1	0.94	0.12	30,30,30,30	0
56	MG	BA	3117	1/1	0.94	0.22	40,40,40,40	0
56	MG	BX	102	1/1	0.94	0.09	38,38,38,38	0
56	MG	DA	3419	1/1	0.94	0.15	59,59,59,59	0
56	MG	AA	3053	1/1	0.94	0.16	50,50,50,50	0
56	MG	DA	3421	1/1	0.94	0.10	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3527	1/1	0.94	0.09	40,40,40,40	0
56	MG	AA	3043	1/1	0.94	0.08	53,53,53,53	0
56	MG	B0	101	1/1	0.94	0.12	71,71,71,71	0
56	MG	B0	102	1/1	0.94	0.11	42,42,42,42	0
56	MG	DA	3431	1/1	0.94	0.13	61,61,61,61	0
56	MG	DA	3056	1/1	0.94	0.06	36,36,36,36	0
56	MG	DA	3434	1/1	0.94	0.15	41,41,41,41	0
56	MG	DA	3435	1/1	0.94	0.14	33,33,33,33	0
56	MG	BA	3126	1/1	0.94	0.13	45,45,45,45	0
56	MG	DA	3064	1/1	0.94	0.12	48,48,48,48	0
56	MG	BA	3543	1/1	0.94	0.12	47,47,47,47	0
56	MG	BA	3040	1/1	0.94	0.10	43,43,43,43	0
56	MG	BA	3136	1/1	0.94	0.07	44,44,44,44	0
56	MG	AA	3087	1/1	0.94	0.07	62,62,62,62	0
56	MG	DA	3071	1/1	0.94	0.08	36,36,36,36	0
56	MG	BA	3338	1/1	0.94	0.06	48,48,48,48	0
56	MG	DA	3452	1/1	0.94	0.14	56,56,56,56	0
56	MG	AA	3044	1/1	0.94	0.25	50,50,50,50	0
56	MG	DA	3458	1/1	0.94	0.15	34,34,34,34	0
56	MG	DA	3082	1/1	0.94	0.33	58,58,58,58	0
56	MG	DA	3460	1/1	0.94	0.08	50,50,50,50	0
56	MG	BA	3145	1/1	0.94	0.09	30,30,30,30	0
56	MG	DA	3466	1/1	0.94	0.07	38,38,38,38	0
56	MG	BA	3558	1/1	0.94	0.12	59,59,59,59	0
56	MG	BA	3344	1/1	0.94	0.09	35,35,35,35	0
56	MG	BA	3153	1/1	0.94	0.14	39,39,39,39	0
56	MG	BA	3164	1/1	0.94	0.08	37,37,37,37	0
56	MG	BA	3348	1/1	0.94	0.07	31,31,31,31	0
56	MG	DA	3093	1/1	0.94	0.11	46,46,46,46	0
56	MG	AA	3034	1/1	0.94	0.30	54,54,54,54	0
56	MG	CA	3026	1/1	0.94	0.19	44,44,44,44	0
56	MG	BA	3048	1/1	0.94	0.13	47,47,47,47	0
56	MG	BA	3050	1/1	0.94	0.15	44,44,44,44	0
56	MG	BA	3177	1/1	0.94	0.08	44,44,44,44	0
56	MG	DA	3105	1/1	0.94	0.05	36,36,36,36	0
56	MG	BA	3183	1/1	0.94	0.16	35,35,35,35	0
56	MG	BA	3186	1/1	0.94	0.12	39,39,39,39	0
56	MG	DA	3486	1/1	0.94	0.16	37,37,37,37	0
56	MG	BA	3188	1/1	0.94	0.13	39,39,39,39	0
56	MG	BA	3393	1/1	0.94	0.09	49,49,49,49	0
56	MG	DA	3492	1/1	0.94	0.09	44,44,44,44	0
56	MG	CA	3039	1/1	0.94	0.19	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3394	1/1	0.94	0.15	35,35,35,35	0
56	MG	AA	3069	1/1	0.94	0.15	50,50,50,50	0
56	MG	BA	3396	1/1	0.94	0.12	38,38,38,38	0
56	MG	DA	3131	1/1	0.94	0.10	46,46,46,46	0
56	MG	BA	3058	1/1	0.94	0.11	43,43,43,43	0
56	MG	BA	3400	1/1	0.94	0.18	45,45,45,45	0
56	MG	DA	3137	1/1	0.94	0.06	37,37,37,37	0
56	MG	AA	3157	1/1	0.94	0.08	55,55,55,55	0
56	MG	CA	3053	1/1	0.94	0.14	44,44,44,44	0
56	MG	DA	3514	1/1	0.94	0.07	40,40,40,40	0
56	MG	BA	3587	1/1	0.94	0.07	42,42,42,42	0
56	MG	DA	3152	1/1	0.94	0.11	34,34,34,34	0
56	MG	AD	502	1/1	0.94	0.27	55,55,55,55	0
56	MG	DA	3524	1/1	0.94	0.11	51,51,51,51	0
56	MG	DA	3525	1/1	0.94	0.06	44,44,44,44	0
56	MG	BA	3590	1/1	0.94	0.16	55,55,55,55	0
56	MG	DA	3529	1/1	0.94	0.13	41,41,41,41	0
56	MG	CA	3060	1/1	0.94	0.23	50,50,50,50	0
56	MG	BA	3210	1/1	0.94	0.24	24,24,24,24	0
56	MG	DA	3164	1/1	0.94	0.12	36,36,36,36	0
56	MG	DA	3165	1/1	0.94	0.14	34,34,34,34	0
56	MG	CA	3063	1/1	0.94	0.35	53,53,53,53	0
56	MG	DA	3171	1/1	0.94	0.13	51,51,51,51	0
56	MG	DA	3172	1/1	0.94	0.07	35,35,35,35	0
56	MG	DA	3543	1/1	0.94	0.11	63,63,63,63	0
56	MG	CA	3064	1/1	0.94	0.10	60,60,60,60	0
56	MG	BA	3066	1/1	0.94	0.12	48,48,48,48	0
56	MG	DA	3548	1/1	0.94	0.16	40,40,40,40	0
56	MG	DA	3549	1/1	0.94	0.07	41,41,41,41	0
56	MG	DA	3183	1/1	0.94	0.07	37,37,37,37	0
56	MG	BA	3070	1/1	0.94	0.09	30,30,30,30	0
56	MG	DA	3554	1/1	0.94	0.07	68,68,68,68	0
56	MG	BA	3217	1/1	0.94	0.19	29,29,29,29	0
56	MG	AA	3122	1/1	0.94	0.09	58,58,58,58	0
56	MG	DA	3560	1/1	0.94	0.11	51,51,51,51	0
56	MG	BA	3599	1/1	0.94	0.06	46,46,46,46	0
56	MG	DA	3198	1/1	0.94	0.11	54,54,54,54	0
56	MG	DA	3565	1/1	0.94	0.10	51,51,51,51	0
56	MG	DA	3199	1/1	0.94	0.07	52,52,52,52	0
56	MG	AA	3096	1/1	0.94	0.15	53,53,53,53	0
56	MG	BA	3422	1/1	0.94	0.10	46,46,46,46	0
56	MG	AA	3097	1/1	0.94	0.13	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	3098	1/1	0.94	0.21	48,48,48,48	0
56	MG	DA	3576	1/1	0.94	0.10	36,36,36,36	0
56	MG	DA	3217	1/1	0.94	0.06	39,39,39,39	0
56	MG	DA	3218	1/1	0.94	0.07	33,33,33,33	0
56	MG	DA	3581	1/1	0.94	0.10	53,53,53,53	0
56	MG	BA	3426	1/1	0.94	0.07	43,43,43,43	0
56	MG	DA	3226	1/1	0.94	0.07	27,27,27,27	0
56	MG	BA	3607	1/1	0.94	0.19	51,51,51,51	0
56	MG	BA	3079	1/1	0.94	0.05	46,46,46,46	0
56	MG	DA	3233	1/1	0.94	0.21	36,36,36,36	0
56	MG	DA	3234	1/1	0.94	0.10	45,45,45,45	0
56	MG	DA	3594	1/1	0.94	0.18	48,48,48,48	0
56	MG	DB	3002	1/1	0.94	0.12	50,50,50,50	0
56	MG	DA	3235	1/1	0.94	0.14	42,42,42,42	0
56	MG	BA	3429	1/1	0.94	0.13	41,41,41,41	0
56	MG	BA	3430	1/1	0.94	0.09	29,29,29,29	0
56	MG	DA	3240	1/1	0.94	0.12	54,54,54,54	0
56	MG	CA	3089	1/1	0.94	0.12	40,40,40,40	0
56	MG	BA	3081	1/1	0.94	0.14	42,42,42,42	0
56	MG	BA	3239	1/1	0.94	0.21	52,52,52,52	0
56	MG	CA	3093	1/1	0.94	0.21	72,72,72,72	0
56	MG	DE	3002	1/1	0.94	0.10	35,35,35,35	0
56	MG	CA	3094	1/1	0.94	0.16	67,67,67,67	0
56	MG	BA	3082	1/1	0.94	0.10	47,47,47,47	0
56	MG	CA	3097	1/1	0.94	0.13	67,67,67,67	0
56	MG	DQ	3001	1/1	0.94	0.06	48,48,48,48	0
56	MG	BA	3446	1/1	0.94	0.12	61,61,61,61	0
56	MG	BA	3621	1/1	0.94	0.08	30,30,30,30	0
56	MG	DV	3002	1/1	0.94	0.06	43,43,43,43	0
56	MG	AX	3003	1/1	0.94	0.19	50,50,50,50	0
56	MG	BA	3086	1/1	0.94	0.15	39,39,39,39	0
56	MG	DA	3264	1/1	0.94	0.15	47,47,47,47	0
56	MG	BA	3463	1/1	0.94	0.06	43,43,43,43	0
56	MG	BB	3014	1/1	0.95	0.08	35,35,35,35	0
56	MG	BA	3327	1/1	0.95	0.06	44,44,44,44	0
56	MG	BA	3166	1/1	0.95	0.06	35,35,35,35	0
56	MG	DA	3305	1/1	0.95	0.09	30,30,30,30	0
56	MG	AA	3134	1/1	0.95	0.22	52,52,52,52	0
56	MG	BE	303	1/1	0.95	0.15	41,41,41,41	0
56	MG	CA	3142	1/1	0.95	0.12	42,42,42,42	0
56	MG	CA	3143	1/1	0.95	0.13	42,42,42,42	0
56	MG	CA	3144	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
56	MG	BA	3330	1/1	0.95	0.16	44,44,44,44	0
56	MG	BA	3518	1/1	0.95	0.19	41,41,41,41	0
56	MG	AA	3021	1/1	0.95	0.13	41,41,41,41	0
56	MG	BA	3332	1/1	0.95	0.09	61,61,61,61	0
56	MG	BA	3526	1/1	0.95	0.13	25,25,25,25	0
56	MG	CE	201	1/1	0.95	0.14	52,52,52,52	0
56	MG	BA	3173	1/1	0.95	0.17	45,45,45,45	0
56	MG	BA	3174	1/1	0.95	0.04	29,29,29,29	0
56	MG	DA	3333	1/1	0.95	0.07	38,38,38,38	0
56	MG	BA	3533	1/1	0.95	0.08	45,45,45,45	0
56	MG	BA	3176	1/1	0.95	0.08	47,47,47,47	0
56	MG	BA	3537	1/1	0.95	0.21	58,58,58,58	0
56	MG	BA	3539	1/1	0.95	0.12	58,58,58,58	0
56	MG	BA	3540	1/1	0.95	0.13	46,46,46,46	0
56	MG	AA	3009	1/1	0.95	0.09	54,54,54,54	0
56	MG	DA	3349	1/1	0.95	0.13	46,46,46,46	0
56	MG	BV	202	1/1	0.95	0.08	36,36,36,36	0
56	MG	DA	3018	1/1	0.95	0.10	39,39,39,39	0
56	MG	DA	3353	1/1	0.95	0.06	32,32,32,32	0
56	MG	BA	3180	1/1	0.95	0.09	33,33,33,33	0
56	MG	DA	3356	1/1	0.95	0.06	31,31,31,31	0
56	MG	DA	3357	1/1	0.95	0.07	33,33,33,33	0
56	MG	BW	3004	1/1	0.95	0.13	30,30,30,30	0
56	MG	BA	3078	1/1	0.95	0.13	53,53,53,53	0
56	MG	BA	3010	1/1	0.95	0.07	33,33,33,33	0
56	MG	BA	3187	1/1	0.95	0.12	37,37,37,37	0
56	MG	BA	3012	1/1	0.95	0.09	39,39,39,39	0
56	MG	DA	3368	1/1	0.95	0.05	25,25,25,25	0
56	MG	DA	3369	1/1	0.95	0.11	45,45,45,45	0
56	MG	BA	3556	1/1	0.95	0.09	41,41,41,41	0
56	MG	BA	3352	1/1	0.95	0.07	32,32,32,32	0
56	MG	BA	3356	1/1	0.95	0.10	46,46,46,46	0
56	MG	DA	3041	1/1	0.95	0.06	35,35,35,35	0
56	MG	DA	3382	1/1	0.95	0.14	50,50,50,50	0
56	MG	DA	3043	1/1	0.95	0.08	30,30,30,30	0
56	MG	B5	503	1/1	0.95	0.20	47,47,47,47	0
56	MG	CA	3001	1/1	0.95	0.08	72,72,72,72	0
56	MG	BA	3189	1/1	0.95	0.18	26,26,26,26	0
56	MG	DA	3394	1/1	0.95	0.07	41,41,41,41	0
56	MG	AA	3174	1/1	0.95	0.12	55,55,55,55	0
56	MG	BA	3563	1/1	0.95	0.14	47,47,47,47	0
56	MG	BA	3362	1/1	0.95	0.08	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3059	1/1	0.95	0.07	33,33,33,33	0
56	MG	DA	3405	1/1	0.95	0.16	45,45,45,45	0
56	MG	DA	3062	1/1	0.95	0.19	42,42,42,42	0
56	MG	BA	3365	1/1	0.95	0.12	41,41,41,41	0
56	MG	AA	3080	1/1	0.95	0.20	39,39,39,39	0
56	MG	BA	3018	1/1	0.95	0.15	47,47,47,47	0
56	MG	BA	3374	1/1	0.95	0.07	29,29,29,29	0
56	MG	DA	3069	1/1	0.95	0.06	35,35,35,35	0
56	MG	DA	3415	1/1	0.95	0.10	40,40,40,40	0
56	MG	BA	3572	1/1	0.95	0.07	59,59,59,59	0
56	MG	DA	3417	1/1	0.95	0.10	40,40,40,40	0
56	MG	BA	3376	1/1	0.95	0.09	39,39,39,39	0
56	MG	DA	3073	1/1	0.95	0.16	51,51,51,51	0
56	MG	AA	3068	1/1	0.95	0.11	31,31,31,31	0
56	MG	BA	3384	1/1	0.95	0.07	28,28,28,28	0
56	MG	DA	3078	1/1	0.95	0.15	46,46,46,46	0
56	MG	CA	3024	1/1	0.95	0.10	64,64,64,64	0
56	MG	BA	3021	1/1	0.95	0.09	37,37,37,37	0
56	MG	BA	3390	1/1	0.95	0.10	47,47,47,47	0
56	MG	DA	3430	1/1	0.95	0.15	30,30,30,30	0
56	MG	CA	3027	1/1	0.95	0.24	64,64,64,64	0
56	MG	AA	3114	1/1	0.95	0.15	56,56,56,56	0
56	MG	BA	3581	1/1	0.95	0.05	34,34,34,34	0
56	MG	BA	3026	1/1	0.95	0.24	46,46,46,46	0
56	MG	AA	3150	1/1	0.95	0.20	51,51,51,51	0
56	MG	BA	3218	1/1	0.95	0.19	38,38,38,38	0
56	MG	AA	3116	1/1	0.95	0.13	51,51,51,51	0
56	MG	BA	3222	1/1	0.95	0.12	45,45,45,45	0
56	MG	BA	3223	1/1	0.95	0.19	51,51,51,51	0
56	MG	CA	3040	1/1	0.95	0.24	52,52,52,52	0
56	MG	BA	3224	1/1	0.95	0.12	45,45,45,45	0
56	MG	AA	3182	1/1	0.95	0.19	57,57,57,57	0
56	MG	BA	3591	1/1	0.95	0.08	36,36,36,36	0
56	MG	CA	3045	1/1	0.95	0.14	52,52,52,52	0
56	MG	DA	3456	1/1	0.95	0.08	34,34,34,34	0
56	MG	DA	3111	1/1	0.95	0.21	39,39,39,39	0
56	MG	CA	3046	1/1	0.95	0.07	41,41,41,41	0
56	MG	DA	3114	1/1	0.95	0.05	37,37,37,37	0
56	MG	CA	3047	1/1	0.95	0.21	51,51,51,51	0
56	MG	DA	3120	1/1	0.95	0.15	33,33,33,33	0
56	MG	BA	3592	1/1	0.95	0.08	52,52,52,52	0
56	MG	DA	3468	1/1	0.95	0.10	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3123	1/1	0.95	0.07	51,51,51,51	0
56	MG	BA	3042	1/1	0.95	0.08	33,33,33,33	0
56	MG	DA	3471	1/1	0.95	0.07	50,50,50,50	0
56	MG	DA	3126	1/1	0.95	0.16	42,42,42,42	0
56	MG	BA	3232	1/1	0.95	0.06	41,41,41,41	0
56	MG	DA	3128	1/1	0.95	0.07	42,42,42,42	0
56	MG	DA	3129	1/1	0.95	0.18	54,54,54,54	0
56	MG	BA	3102	1/1	0.95	0.08	49,49,49,49	0
56	MG	AA	3083	1/1	0.95	0.12	59,59,59,59	0
56	MG	BA	3107	1/1	0.95	0.05	21,21,21,21	0
56	MG	DA	3480	1/1	0.95	0.06	32,32,32,32	0
56	MG	CA	3058	1/1	0.95	0.17	56,56,56,56	0
56	MG	DA	3141	1/1	0.95	0.05	42,42,42,42	0
56	MG	DA	3144	1/1	0.95	0.06	38,38,38,38	0
56	MG	BA	3108	1/1	0.95	0.08	38,38,38,38	0
56	MG	DA	3146	1/1	0.95	0.08	34,34,34,34	0
56	MG	BA	3110	1/1	0.95	0.11	31,31,31,31	0
56	MG	BA	3242	1/1	0.95	0.23	46,46,46,46	0
56	MG	DA	3491	1/1	0.95	0.06	40,40,40,40	0
56	MG	DA	3151	1/1	0.95	0.07	34,34,34,34	0
56	MG	AA	3120	1/1	0.95	0.08	47,47,47,47	0
56	MG	AA	3100	1/1	0.95	0.14	35,35,35,35	0
56	MG	DA	3156	1/1	0.95	0.07	38,38,38,38	0
56	MG	BA	3047	1/1	0.95	0.18	41,41,41,41	0
56	MG	BA	3256	1/1	0.95	0.24	41,41,41,41	0
56	MG	BA	3435	1/1	0.95	0.11	36,36,36,36	0
56	MG	AA	3001	1/1	0.95	0.11	57,57,57,57	0
56	MG	CA	3069	1/1	0.95	0.10	34,34,34,34	0
56	MG	AA	3123	1/1	0.95	0.15	38,38,38,38	0
56	MG	DA	3509	1/1	0.95	0.06	36,36,36,36	0
56	MG	DA	3170	1/1	0.95	0.19	38,38,38,38	0
56	MG	DA	3512	1/1	0.95	0.10	36,36,36,36	0
56	MG	BA	3051	1/1	0.95	0.14	41,41,41,41	0
56	MG	CA	3073	1/1	0.95	0.18	57,57,57,57	0
56	MG	CA	3074	1/1	0.95	0.26	48,48,48,48	0
56	MG	DA	3517	1/1	0.95	0.18	47,47,47,47	0
56	MG	CA	3076	1/1	0.95	0.22	48,48,48,48	0
56	MG	DA	3520	1/1	0.95	0.08	34,34,34,34	0
56	MG	DA	3179	1/1	0.95	0.14	20,20,20,20	0
56	MG	AA	3071	1/1	0.95	0.04	36,36,36,36	0
56	MG	DA	3185	1/1	0.95	0.06	32,32,32,32	0
56	MG	BA	3268	1/1	0.95	0.30	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3079	1/1	0.95	0.30	55,55,55,55	0
56	MG	BA	3448	1/1	0.95	0.09	42,42,42,42	0
56	MG	DA	3533	1/1	0.95	0.07	60,60,60,60	0
56	MG	DA	3193	1/1	0.95	0.17	49,49,49,49	0
56	MG	DA	3194	1/1	0.95	0.10	47,47,47,47	0
56	MG	BA	3620	1/1	0.95	0.12	41,41,41,41	0
56	MG	DA	3197	1/1	0.95	0.13	38,38,38,38	0
56	MG	DA	3540	1/1	0.95	0.15	46,46,46,46	0
56	MG	AE	3002	1/1	0.95	0.10	38,38,38,38	0
56	MG	BA	3623	1/1	0.95	0.06	48,48,48,48	0
56	MG	BA	3061	1/1	0.95	0.20	44,44,44,44	0
56	MG	DA	3204	1/1	0.95	0.06	37,37,37,37	0
56	MG	BA	3137	1/1	0.95	0.12	30,30,30,30	0
56	MG	DA	3207	1/1	0.95	0.14	39,39,39,39	0
56	MG	DA	3551	1/1	0.95	0.08	52,52,52,52	0
56	MG	BA	3286	1/1	0.95	0.10	32,32,32,32	0
56	MG	DA	3212	1/1	0.95	0.17	39,39,39,39	0
56	MG	BA	3287	1/1	0.95	0.09	46,46,46,46	0
56	MG	AA	3048	1/1	0.95	0.22	42,42,42,42	0
56	MG	CA	3092	1/1	0.95	0.15	54,54,54,54	0
56	MG	DA	3222	1/1	0.95	0.06	36,36,36,36	0
56	MG	BA	3474	1/1	0.95	0.12	53,53,53,53	0
56	MG	DA	3225	1/1	0.95	0.06	33,33,33,33	0
56	MG	AA	3014	1/1	0.95	0.16	49,49,49,49	0
56	MG	BA	3296	1/1	0.95	0.06	25,25,25,25	0
56	MG	AA	3165	1/1	0.95	0.07	43,43,43,43	0
56	MG	CA	3099	1/1	0.95	0.20	57,57,57,57	0
56	MG	CA	3101	1/1	0.95	0.14	53,53,53,53	0
56	MG	DA	3571	1/1	0.95	0.14	48,48,48,48	0
56	MG	BA	3146	1/1	0.95	0.08	31,31,31,31	0
56	MG	BA	3149	1/1	0.95	0.10	50,50,50,50	0
56	MG	DA	3577	1/1	0.95	0.12	35,35,35,35	0
56	MG	DA	3237	1/1	0.95	0.09	39,39,39,39	0
56	MG	DA	3238	1/1	0.95	0.11	42,42,42,42	0
56	MG	BA	3641	1/1	0.95	0.15	33,33,33,33	0
56	MG	BA	3486	1/1	0.95	0.14	21,21,21,21	0
56	MG	BA	3643	1/1	0.95	0.07	42,42,42,42	0
56	MG	DA	3243	1/1	0.95	0.06	50,50,50,50	0
56	MG	DA	3244	1/1	0.95	0.07	48,48,48,48	0
56	MG	BA	3644	1/1	0.95	0.07	41,41,41,41	0
56	MG	BA	3301	1/1	0.95	0.09	46,46,46,46	0
56	MG	BA	3646	1/1	0.95	0.10	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DB	3001	1/1	0.95	0.13	40,40,40,40	0
56	MG	BA	3150	1/1	0.95	0.11	32,32,32,32	0
56	MG	BA	3151	1/1	0.95	0.05	34,34,34,34	0
56	MG	DA	3256	1/1	0.95	0.06	45,45,45,45	0
56	MG	BA	3069	1/1	0.95	0.06	47,47,47,47	0
56	MG	BA	3662	1/1	0.95	0.11	36,36,36,36	0
56	MG	BA	3154	1/1	0.95	0.17	40,40,40,40	0
56	MG	BA	3671	1/1	0.95	0.12	48,48,48,48	0
56	MG	BA	3156	1/1	0.95	0.12	48,48,48,48	0
56	MG	BA	3314	1/1	0.95	0.12	36,36,36,36	0
56	MG	BA	3162	1/1	0.95	0.13	39,39,39,39	0
56	MG	DE	3003	1/1	0.95	0.11	40,40,40,40	0
56	MG	DF	301	1/1	0.95	0.20	44,44,44,44	0
56	MG	BA	3318	1/1	0.95	0.07	44,44,44,44	0
56	MG	AA	3108	1/1	0.95	0.19	54,54,54,54	0
56	MG	AA	3089	1/1	0.95	0.11	36,36,36,36	0
56	MG	DP	3001	1/1	0.95	0.11	44,44,44,44	0
56	MG	BB	3007	1/1	0.95	0.09	35,35,35,35	0
56	MG	BA	3325	1/1	0.95	0.09	42,42,42,42	0
56	MG	DA	3277	1/1	0.95	0.09	48,48,48,48	0
56	MG	BA	3509	1/1	0.95	0.12	23,23,23,23	0
56	MG	DA	3286	1/1	0.95	0.07	35,35,35,35	0
56	MG	DA	3287	1/1	0.95	0.12	38,38,38,38	0
56	MG	BB	3013	1/1	0.95	0.15	57,57,57,57	0
56	MG	D8	5001	1/1	0.95	0.14	50,50,50,50	0
56	MG	DA	3292	1/1	0.95	0.12	45,45,45,45	0
56	MG	DA	3255	1/1	0.96	0.22	32,32,32,32	0
56	MG	BA	3637	1/1	0.96	0.13	24,24,24,24	0
56	MG	AA	3104	1/1	0.96	0.09	56,56,56,56	0
56	MG	CA	3115	1/1	0.96	0.06	62,62,62,62	0
56	MG	BA	3267	1/1	0.96	0.07	40,40,40,40	0
56	MG	BA	3142	1/1	0.96	0.05	40,40,40,40	0
56	MG	BA	3450	1/1	0.96	0.06	45,45,45,45	0
56	MG	BA	3451	1/1	0.96	0.06	48,48,48,48	0
56	MG	DA	3265	1/1	0.96	0.26	51,51,51,51	0
56	MG	DA	3266	1/1	0.96	0.07	46,46,46,46	0
56	MG	DA	3268	1/1	0.96	0.08	38,38,38,38	0
56	MG	BA	3458	1/1	0.96	0.07	60,60,60,60	0
56	MG	BA	3459	1/1	0.96	0.13	42,42,42,42	0
56	MG	BA	3460	1/1	0.96	0.06	57,57,57,57	0
56	MG	BA	3270	1/1	0.96	0.12	21,21,21,21	0
56	MG	BA	3271	1/1	0.96	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
56	MG	BA	3653	1/1	0.96	0.08	33,33,33,33	0
56	MG	BA	3277	1/1	0.96	0.12	32,32,32,32	0
56	MG	DA	3278	1/1	0.96	0.10	50,50,50,50	0
56	MG	CA	3130	1/1	0.96	0.15	57,57,57,57	0
56	MG	DA	3282	1/1	0.96	0.05	30,30,30,30	0
56	MG	DA	3285	1/1	0.96	0.12	52,52,52,52	0
56	MG	BA	3655	1/1	0.96	0.09	18,18,18,18	0
56	MG	BA	3659	1/1	0.96	0.10	28,28,28,28	0
56	MG	BA	3660	1/1	0.96	0.09	49,49,49,49	0
56	MG	DA	3291	1/1	0.96	0.07	38,38,38,38	0
56	MG	CA	3134	1/1	0.96	0.12	53,53,53,53	0
56	MG	DA	3295	1/1	0.96	0.07	61,61,61,61	0
56	MG	DA	3298	1/1	0.96	0.05	32,32,32,32	0
56	MG	CA	3135	1/1	0.96	0.23	62,62,62,62	0
56	MG	BA	3470	1/1	0.96	0.09	48,48,48,48	0
56	MG	BA	3057	1/1	0.96	0.06	38,38,38,38	0
56	MG	BA	3668	1/1	0.96	0.13	26,26,26,26	0
56	MG	BA	3280	1/1	0.96	0.12	48,48,48,48	0
56	MG	BA	3473	1/1	0.96	0.10	37,37,37,37	0
56	MG	DA	3308	1/1	0.96	0.08	29,29,29,29	0
56	MG	AA	3031	1/1	0.96	0.07	60,60,60,60	0
56	MG	BA	3284	1/1	0.96	0.12	41,41,41,41	0
56	MG	BA	3147	1/1	0.96	0.10	35,35,35,35	0
56	MG	BA	3148	1/1	0.96	0.06	25,25,25,25	0
56	MG	DA	3321	1/1	0.96	0.08	45,45,45,45	0
56	MG	DA	3322	1/1	0.96	0.07	23,23,23,23	0
56	MG	AL	201	1/1	0.96	0.05	63,63,63,63	0
56	MG	AM	3001	1/1	0.96	0.07	54,54,54,54	0
56	MG	BB	3008	1/1	0.96	0.10	21,21,21,21	0
56	MG	BA	3485	1/1	0.96	0.14	64,64,64,64	0
56	MG	CA	3153	1/1	0.96	0.11	37,37,37,37	0
56	MG	CA	3154	1/1	0.96	0.18	62,62,62,62	0
56	MG	BA	3292	1/1	0.96	0.11	43,43,43,43	0
56	MG	DA	3331	1/1	0.96	0.06	41,41,41,41	0
56	MG	DA	3332	1/1	0.96	0.06	43,43,43,43	0
56	MG	AA	3033	1/1	0.96	0.25	48,48,48,48	0
56	MG	BA	3295	1/1	0.96	0.08	61,61,61,61	0
56	MG	BA	3492	1/1	0.96	0.09	42,42,42,42	0
56	MG	BB	3016	1/1	0.96	0.05	24,24,24,24	0
56	MG	CT	3001	1/1	0.96	0.12	50,50,50,50	0
56	MG	DA	3344	1/1	0.96	0.14	31,31,31,31	0
56	MG	BA	3152	1/1	0.96	0.06	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	3072	1/1	0.96	0.13	39,39,39,39	0
56	MG	BD	304	1/1	0.96	0.20	28,28,28,28	0
56	MG	AX	3005	1/1	0.96	0.25	42,42,42,42	0
56	MG	DA	3011	1/1	0.96	0.08	38,38,38,38	0
56	MG	DA	3015	1/1	0.96	0.09	41,41,41,41	0
56	MG	AA	3005	1/1	0.96	0.07	37,37,37,37	0
56	MG	BA	3157	1/1	0.96	0.13	34,34,34,34	0
56	MG	BF	301	1/1	0.96	0.10	56,56,56,56	0
56	MG	BA	3158	1/1	0.96	0.12	33,33,33,33	0
56	MG	AA	3129	1/1	0.96	0.06	35,35,35,35	0
56	MG	DA	3023	1/1	0.96	0.06	37,37,37,37	0
56	MG	DA	3024	1/1	0.96	0.12	36,36,36,36	0
56	MG	BA	3163	1/1	0.96	0.07	31,31,31,31	0
56	MG	DA	3367	1/1	0.96	0.10	47,47,47,47	0
56	MG	DA	3026	1/1	0.96	0.12	34,34,34,34	0
56	MG	DA	3027	1/1	0.96	0.07	30,30,30,30	0
56	MG	DA	3370	1/1	0.96	0.13	44,44,44,44	0
56	MG	BA	3504	1/1	0.96	0.10	39,39,39,39	0
56	MG	DA	3029	1/1	0.96	0.10	40,40,40,40	0
56	MG	AA	3130	1/1	0.96	0.10	50,50,50,50	0
56	MG	DA	3377	1/1	0.96	0.11	37,37,37,37	0
56	MG	AA	3091	1/1	0.96	0.06	36,36,36,36	0
56	MG	BA	3076	1/1	0.96	0.04	29,29,29,29	0
56	MG	DA	3034	1/1	0.96	0.21	46,46,46,46	0
56	MG	DA	3038	1/1	0.96	0.05	30,30,30,30	0
56	MG	BA	3169	1/1	0.96	0.09	39,39,39,39	0
56	MG	BA	3512	1/1	0.96	0.10	45,45,45,45	0
56	MG	BQ	201	1/1	0.96	0.14	52,52,52,52	0
56	MG	BQ	203	1/1	0.96	0.19	33,33,33,33	0
56	MG	DA	3045	1/1	0.96	0.17	48,48,48,48	0
56	MG	BU	202	1/1	0.96	0.07	40,40,40,40	0
56	MG	BU	203	1/1	0.96	0.15	32,32,32,32	0
56	MG	DA	3404	1/1	0.96	0.05	46,46,46,46	0
56	MG	DA	3051	1/1	0.96	0.07	50,50,50,50	0
56	MG	BA	3317	1/1	0.96	0.08	35,35,35,35	0
56	MG	DA	3054	1/1	0.96	0.21	45,45,45,45	0
56	MG	DA	3055	1/1	0.96	0.07	34,34,34,34	0
56	MG	BA	3514	1/1	0.96	0.10	32,32,32,32	0
56	MG	BA	3003	1/1	0.96	0.05	49,49,49,49	0
56	MG	BA	3516	1/1	0.96	0.08	43,43,43,43	0
56	MG	DA	3060	1/1	0.96	0.06	45,45,45,45	0
56	MG	BA	3319	1/1	0.96	0.12	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3063	1/1	0.96	0.05	31,31,31,31	0
56	MG	BX	101	1/1	0.96	0.10	46,46,46,46	0
56	MG	BA	3005	1/1	0.96	0.06	29,29,29,29	0
56	MG	BA	3521	1/1	0.96	0.07	54,54,54,54	0
56	MG	BA	3009	1/1	0.96	0.06	34,34,34,34	0
56	MG	BA	3080	1/1	0.96	0.09	29,29,29,29	0
56	MG	BA	3525	1/1	0.96	0.07	46,46,46,46	0
56	MG	AA	3132	1/1	0.96	0.11	50,50,50,50	0
56	MG	DA	3072	1/1	0.96	0.08	33,33,33,33	0
56	MG	DA	3429	1/1	0.96	0.08	35,35,35,35	0
56	MG	AA	3133	1/1	0.96	0.06	38,38,38,38	0
56	MG	B0	105	1/1	0.96	0.08	43,43,43,43	0
56	MG	B4	502	1/1	0.96	0.05	61,61,61,61	0
56	MG	DA	3077	1/1	0.96	0.07	34,34,34,34	0
56	MG	B5	502	1/1	0.96	0.11	34,34,34,34	0
56	MG	DA	3436	1/1	0.96	0.06	27,27,27,27	0
56	MG	AA	3060	1/1	0.96	0.14	55,55,55,55	0
56	MG	BA	3182	1/1	0.96	0.13	30,30,30,30	0
56	MG	DA	3439	1/1	0.96	0.09	28,28,28,28	0
56	MG	DA	3440	1/1	0.96	0.12	52,52,52,52	0
56	MG	DA	3087	1/1	0.96	0.15	35,35,35,35	0
56	MG	AA	3135	1/1	0.96	0.07	46,46,46,46	0
56	MG	BA	3184	1/1	0.96	0.05	37,37,37,37	0
56	MG	CA	3005	1/1	0.96	0.08	42,42,42,42	0
56	MG	BA	3185	1/1	0.96	0.08	43,43,43,43	0
56	MG	DA	3447	1/1	0.96	0.07	33,33,33,33	0
56	MG	DA	3449	1/1	0.96	0.09	29,29,29,29	0
56	MG	BA	3335	1/1	0.96	0.10	40,40,40,40	0
56	MG	BA	3017	1/1	0.96	0.11	40,40,40,40	0
56	MG	DA	3094	1/1	0.96	0.09	35,35,35,35	0
56	MG	DA	3095	1/1	0.96	0.09	47,47,47,47	0
56	MG	DA	3457	1/1	0.96	0.10	38,38,38,38	0
56	MG	AA	3052	1/1	0.96	0.21	60,60,60,60	0
56	MG	AA	3175	1/1	0.96	0.19	53,53,53,53	0
56	MG	BA	3343	1/1	0.96	0.12	27,27,27,27	0
56	MG	DA	3099	1/1	0.96	0.12	37,37,37,37	0
56	MG	AA	3137	1/1	0.96	0.07	79,79,79,79	0
56	MG	DA	3101	1/1	0.96	0.08	46,46,46,46	0
56	MG	DA	3102	1/1	0.96	0.20	51,51,51,51	0
56	MG	CA	3017	1/1	0.96	0.09	41,41,41,41	0
56	MG	BA	3190	1/1	0.96	0.24	31,31,31,31	0
56	MG	BA	3555	1/1	0.96	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
56	MG	BA	3346	1/1	0.96	0.09	43,43,43,43	0
56	MG	CA	3022	1/1	0.96	0.12	34,34,34,34	0
56	MG	AA	3177	1/1	0.96	0.15	32,32,32,32	0
56	MG	DA	3112	1/1	0.96	0.08	24,24,24,24	0
56	MG	AA	3138	1/1	0.96	0.08	50,50,50,50	0
56	MG	BA	3349	1/1	0.96	0.10	46,46,46,46	0
56	MG	DA	3115	1/1	0.96	0.08	36,36,36,36	0
56	MG	DA	3117	1/1	0.96	0.16	43,43,43,43	0
56	MG	BA	3560	1/1	0.96	0.13	55,55,55,55	0
56	MG	BA	3195	1/1	0.96	0.14	47,47,47,47	0
56	MG	BA	3562	1/1	0.96	0.05	46,46,46,46	0
56	MG	DA	3122	1/1	0.96	0.14	45,45,45,45	0
56	MG	BA	3095	1/1	0.96	0.04	33,33,33,33	0
56	MG	BA	3564	1/1	0.96	0.10	29,29,29,29	0
56	MG	BA	3202	1/1	0.96	0.06	30,30,30,30	0
56	MG	BA	3205	1/1	0.96	0.14	40,40,40,40	0
56	MG	BA	3358	1/1	0.96	0.10	39,39,39,39	0
56	MG	DA	3493	1/1	0.96	0.12	45,45,45,45	0
56	MG	CA	3038	1/1	0.96	0.14	44,44,44,44	0
56	MG	DA	3495	1/1	0.96	0.12	45,45,45,45	0
56	MG	BA	3096	1/1	0.96	0.15	44,44,44,44	0
56	MG	DA	3498	1/1	0.96	0.07	48,48,48,48	0
56	MG	DA	3499	1/1	0.96	0.07	45,45,45,45	0
56	MG	BA	3361	1/1	0.96	0.09	45,45,45,45	0
56	MG	BA	3027	1/1	0.96	0.07	28,28,28,28	0
56	MG	DA	3136	1/1	0.96	0.13	36,36,36,36	0
56	MG	CA	3042	1/1	0.96	0.16	56,56,56,56	0
56	MG	DA	3505	1/1	0.96	0.05	44,44,44,44	0
56	MG	DA	3139	1/1	0.96	0.20	39,39,39,39	0
56	MG	BA	3573	1/1	0.96	0.14	44,44,44,44	0
56	MG	AA	3141	1/1	0.96	0.09	47,47,47,47	0
56	MG	BA	3031	1/1	0.96	0.24	46,46,46,46	0
56	MG	BA	3105	1/1	0.96	0.07	32,32,32,32	0
56	MG	BA	3577	1/1	0.96	0.13	57,57,57,57	0
56	MG	BA	3034	1/1	0.96	0.16	24,24,24,24	0
56	MG	BA	3375	1/1	0.96	0.21	51,51,51,51	0
56	MG	BA	3219	1/1	0.96	0.05	20,20,20,20	0
56	MG	AA	3094	1/1	0.96	0.19	49,49,49,49	0
56	MG	CA	3054	1/1	0.96	0.13	44,44,44,44	0
56	MG	BA	3383	1/1	0.96	0.06	33,33,33,33	0
56	MG	DA	3521	1/1	0.96	0.22	51,51,51,51	0
56	MG	DA	3523	1/1	0.96	0.08	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3159	1/1	0.96	0.12	31,31,31,31	0
56	MG	DA	3161	1/1	0.96	0.07	24,24,24,24	0
56	MG	CA	3056	1/1	0.96	0.19	40,40,40,40	0
56	MG	DA	3527	1/1	0.96	0.13	43,43,43,43	0
56	MG	BA	3221	1/1	0.96	0.18	41,41,41,41	0
56	MG	AA	3144	1/1	0.96	0.15	42,42,42,42	0
56	MG	BA	3388	1/1	0.96	0.04	54,54,54,54	0
56	MG	BA	3389	1/1	0.96	0.17	35,35,35,35	0
56	MG	DA	3167	1/1	0.96	0.06	51,51,51,51	0
56	MG	BA	3041	1/1	0.96	0.10	42,42,42,42	0
56	MG	DA	3536	1/1	0.96	0.06	56,56,56,56	0
56	MG	DA	3537	1/1	0.96	0.12	47,47,47,47	0
56	MG	BA	3392	1/1	0.96	0.10	41,41,41,41	0
56	MG	AA	3146	1/1	0.96	0.11	41,41,41,41	0
56	MG	BA	3226	1/1	0.96	0.25	32,32,32,32	0
56	MG	DA	3174	1/1	0.96	0.09	44,44,44,44	0
56	MG	DA	3175	1/1	0.96	0.08	47,47,47,47	0
56	MG	AA	3025	1/1	0.96	0.11	37,37,37,37	0
56	MG	AA	3036	1/1	0.96	0.12	41,41,41,41	0
56	MG	BA	3231	1/1	0.96	0.18	41,41,41,41	0
56	MG	BA	3045	1/1	0.96	0.11	34,34,34,34	0
56	MG	DA	3550	1/1	0.96	0.10	46,46,46,46	0
56	MG	DA	3186	1/1	0.96	0.06	41,41,41,41	0
56	MG	CA	3070	1/1	0.96	0.08	39,39,39,39	0
56	MG	DA	3189	1/1	0.96	0.20	31,31,31,31	0
56	MG	DA	3190	1/1	0.96	0.10	34,34,34,34	0
56	MG	DA	3555	1/1	0.96	0.10	51,51,51,51	0
56	MG	DA	3556	1/1	0.96	0.12	36,36,36,36	0
56	MG	BA	3120	1/1	0.96	0.08	44,44,44,44	0
56	MG	BA	3402	1/1	0.96	0.14	28,28,28,28	0
56	MG	BA	3598	1/1	0.96	0.12	48,48,48,48	0
56	MG	BA	3121	1/1	0.96	0.25	43,43,43,43	0
56	MG	CA	3075	1/1	0.96	0.15	53,53,53,53	0
56	MG	BA	3236	1/1	0.96	0.07	42,42,42,42	0
56	MG	AA	3037	1/1	0.96	0.06	51,51,51,51	0
56	MG	BA	3406	1/1	0.96	0.14	39,39,39,39	0
56	MG	BA	3603	1/1	0.96	0.07	49,49,49,49	0
56	MG	DA	3203	1/1	0.96	0.09	21,21,21,21	0
56	MG	DA	3570	1/1	0.96	0.06	52,52,52,52	0
56	MG	CA	3080	1/1	0.96	0.09	41,41,41,41	0
56	MG	DA	3572	1/1	0.96	0.10	51,51,51,51	0
56	MG	DA	3573	1/1	0.96	0.16	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3407	1/1	0.96	0.10	43,43,43,43	0
56	MG	DA	3575	1/1	0.96	0.16	49,49,49,49	0
56	MG	BA	3238	1/1	0.96	0.21	47,47,47,47	0
56	MG	DA	3208	1/1	0.96	0.11	43,43,43,43	0
56	MG	DA	3210	1/1	0.96	0.06	37,37,37,37	0
56	MG	DA	3579	1/1	0.96	0.11	54,54,54,54	0
56	MG	BA	3410	1/1	0.96	0.09	43,43,43,43	0
56	MG	AA	3067	1/1	0.96	0.30	42,42,42,42	0
56	MG	BA	3240	1/1	0.96	0.18	43,43,43,43	0
56	MG	DA	3583	1/1	0.96	0.05	43,43,43,43	0
56	MG	DA	3214	1/1	0.96	0.14	30,30,30,30	0
56	MG	DA	3215	1/1	0.96	0.07	31,31,31,31	0
56	MG	AA	3101	1/1	0.96	0.29	53,53,53,53	0
56	MG	DA	3590	1/1	0.96	0.18	38,38,38,38	0
56	MG	CA	3087	1/1	0.96	0.06	33,33,33,33	0
56	MG	DA	3219	1/1	0.96	0.11	33,33,33,33	0
56	MG	DA	3220	1/1	0.96	0.08	43,43,43,43	0
56	MG	DA	3221	1/1	0.96	0.06	33,33,33,33	0
56	MG	CA	3088	1/1	0.96	0.14	41,41,41,41	0
56	MG	DB	3003	1/1	0.96	0.06	29,29,29,29	0
56	MG	BA	3127	1/1	0.96	0.06	45,45,45,45	0
56	MG	BA	3128	1/1	0.96	0.17	29,29,29,29	0
56	MG	BA	3245	1/1	0.96	0.12	27,27,27,27	0
56	MG	BA	3618	1/1	0.96	0.20	54,54,54,54	0
56	MG	BA	3129	1/1	0.96	0.10	42,42,42,42	0
56	MG	BA	3427	1/1	0.96	0.10	49,49,49,49	0
56	MG	BA	3252	1/1	0.96	0.10	51,51,51,51	0
56	MG	DD	301	1/1	0.96	0.11	43,43,43,43	0
56	MG	AA	3028	1/1	0.96	0.12	39,39,39,39	0
56	MG	CA	3098	1/1	0.96	0.14	42,42,42,42	0
56	MG	BA	3255	1/1	0.96	0.23	32,32,32,32	0
56	MG	CA	3100	1/1	0.96	0.15	56,56,56,56	0
56	MG	BA	3434	1/1	0.96	0.08	43,43,43,43	0
56	MG	CA	3102	1/1	0.96	0.16	30,30,30,30	0
56	MG	DA	3241	1/1	0.96	0.16	36,36,36,36	0
56	MG	BA	3135	1/1	0.96	0.10	36,36,36,36	0
56	MG	AA	3103	1/1	0.96	0.10	51,51,51,51	0
56	MG	BA	3630	1/1	0.96	0.08	47,47,47,47	0
56	MG	DR	202	1/1	0.96	0.06	32,32,32,32	0
56	MG	BA	3439	1/1	0.96	0.13	30,30,30,30	0
56	MG	DU	201	1/1	0.96	0.12	41,41,41,41	0
56	MG	DV	3001	1/1	0.96	0.13	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3052	1/1	0.96	0.05	27,27,27,27	0
56	MG	BA	3263	1/1	0.96	0.22	64,64,64,64	0
56	MG	BA	3444	1/1	0.96	0.08	34,34,34,34	0
56	MG	D0	5001	1/1	0.96	0.06	39,39,39,39	0
56	MG	D3	3001	1/1	0.96	0.19	70,70,70,70	0
56	MG	BA	3053	1/1	0.96	0.10	31,31,31,31	0
56	MG	DA	3253	1/1	0.96	0.05	26,26,26,26	0
56	MG	DA	3254	1/1	0.96	0.11	46,46,46,46	0
59	K	AX	3001	1/1	0.96	0.06	48,48,48,48	0
59	K	DA	3001	1/1	0.96	0.05	48,48,48,48	0
56	MG	DA	3363	1/1	0.97	0.04	36,36,36,36	0
56	MG	DA	3364	1/1	0.97	0.07	37,37,37,37	0
56	MG	BB	3018	1/1	0.97	0.05	30,30,30,30	0
56	MG	BA	3322	1/1	0.97	0.10	40,40,40,40	0
56	MG	DA	3119	1/1	0.97	0.16	37,37,37,37	0
56	MG	BD	303	1/1	0.97	0.21	37,37,37,37	0
56	MG	BA	3118	1/1	0.97	0.09	45,45,45,45	0
56	MG	BD	305	1/1	0.97	0.09	38,38,38,38	0
56	MG	BD	307	1/1	0.97	0.05	27,27,27,27	0
56	MG	BD	308	1/1	0.97	0.07	35,35,35,35	0
56	MG	DA	3374	1/1	0.97	0.07	35,35,35,35	0
56	MG	BE	301	1/1	0.97	0.11	45,45,45,45	0
56	MG	DA	3376	1/1	0.97	0.06	38,38,38,38	0
56	MG	BE	302	1/1	0.97	0.28	36,36,36,36	0
56	MG	BA	3233	1/1	0.97	0.17	41,41,41,41	0
56	MG	BA	3431	1/1	0.97	0.06	44,44,44,44	0
56	MG	DA	3130	1/1	0.97	0.24	47,47,47,47	0
56	MG	BA	3432	1/1	0.97	0.06	37,37,37,37	0
56	MG	DA	3387	1/1	0.97	0.05	53,53,53,53	0
56	MG	BA	3167	1/1	0.97	0.08	46,46,46,46	0
56	MG	DA	3133	1/1	0.97	0.06	53,53,53,53	0
56	MG	DA	3134	1/1	0.97	0.19	33,33,33,33	0
56	MG	DA	3395	1/1	0.97	0.04	41,41,41,41	0
56	MG	BA	3568	1/1	0.97	0.07	42,42,42,42	0
56	MG	DA	3397	1/1	0.97	0.05	18,18,18,18	0
56	MG	BA	3168	1/1	0.97	0.09	47,47,47,47	0
56	MG	BA	3570	1/1	0.97	0.07	36,36,36,36	0
56	MG	DA	3138	1/1	0.97	0.11	33,33,33,33	0
56	MG	BG	3001	1/1	0.97	0.10	71,71,71,71	0
56	MG	AA	3077	1/1	0.97	0.08	39,39,39,39	0
56	MG	BA	3170	1/1	0.97	0.12	34,34,34,34	0
56	MG	DA	3407	1/1	0.97	0.06	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	3099	1/1	0.97	0.17	33,33,33,33	0
56	MG	BN	3001	1/1	0.97	0.06	57,57,57,57	0
56	MG	BA	3123	1/1	0.97	0.06	36,36,36,36	0
56	MG	DA	3411	1/1	0.97	0.04	36,36,36,36	0
56	MG	DA	3149	1/1	0.97	0.14	41,41,41,41	0
56	MG	BA	3011	1/1	0.97	0.03	30,30,30,30	0
56	MG	BP	202	1/1	0.97	0.32	31,31,31,31	0
56	MG	BA	3333	1/1	0.97	0.09	35,35,35,35	0
56	MG	DA	3153	1/1	0.97	0.09	42,42,42,42	0
56	MG	AA	3152	1/1	0.97	0.11	57,57,57,57	0
56	MG	AA	3172	1/1	0.97	0.10	69,69,69,69	0
56	MG	BR	3003	1/1	0.97	0.11	39,39,39,39	0
56	MG	BA	3337	1/1	0.97	0.05	37,37,37,37	0
56	MG	DA	3422	1/1	0.97	0.05	63,63,63,63	0
56	MG	DA	3160	1/1	0.97	0.13	44,44,44,44	0
56	MG	BA	3243	1/1	0.97	0.09	45,45,45,45	0
56	MG	CA	3124	1/1	0.97	0.13	52,52,52,52	0
56	MG	BA	3014	1/1	0.97	0.14	35,35,35,35	0
56	MG	BA	3179	1/1	0.97	0.04	27,27,27,27	0
56	MG	CA	3127	1/1	0.97	0.13	49,49,49,49	0
56	MG	BA	3342	1/1	0.97	0.05	35,35,35,35	0
56	MG	AA	3078	1/1	0.97	0.08	34,34,34,34	0
56	MG	BA	3461	1/1	0.97	0.16	52,52,52,52	0
56	MG	BA	3249	1/1	0.97	0.07	48,48,48,48	0
56	MG	BA	3464	1/1	0.97	0.06	41,41,41,41	0
56	MG	BX	103	1/1	0.97	0.08	25,25,25,25	0
56	MG	BA	3251	1/1	0.97	0.08	37,37,37,37	0
56	MG	BA	3467	1/1	0.97	0.10	20,20,20,20	0
56	MG	DA	3176	1/1	0.97	0.12	29,29,29,29	0
56	MG	BA	3468	1/1	0.97	0.06	32,32,32,32	0
56	MG	DA	3442	1/1	0.97	0.18	42,42,42,42	0
56	MG	BA	3181	1/1	0.97	0.04	37,37,37,37	0
56	MG	BA	3253	1/1	0.97	0.18	47,47,47,47	0
56	MG	DA	3184	1/1	0.97	0.13	30,30,30,30	0
56	MG	AA	3063	1/1	0.97	0.19	39,39,39,39	0
56	MG	CA	3141	1/1	0.97	0.11	54,54,54,54	0
56	MG	AA	3155	1/1	0.97	0.10	61,61,61,61	0
56	MG	DA	3188	1/1	0.97	0.04	25,25,25,25	0
56	MG	BA	3131	1/1	0.97	0.06	36,36,36,36	0
56	MG	DA	3453	1/1	0.97	0.08	31,31,31,31	0
56	MG	BA	3257	1/1	0.97	0.04	29,29,29,29	0
56	MG	DA	3455	1/1	0.97	0.14	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3258	1/1	0.97	0.14	30,30,30,30	0
56	MG	CA	3146	1/1	0.97	0.05	42,42,42,42	0
56	MG	B7	3001	1/1	0.97	0.06	45,45,45,45	0
56	MG	B7	3004	1/1	0.97	0.05	34,34,34,34	0
56	MG	CA	3150	1/1	0.97	0.07	62,62,62,62	0
56	MG	DA	3461	1/1	0.97	0.10	33,33,33,33	0
56	MG	DA	3463	1/1	0.97	0.07	28,28,28,28	0
56	MG	DA	3464	1/1	0.97	0.12	46,46,46,46	0
56	MG	B8	5001	1/1	0.97	0.09	36,36,36,36	0
56	MG	B9	502	1/1	0.97	0.07	41,41,41,41	0
56	MG	BA	3259	1/1	0.97	0.12	35,35,35,35	0
56	MG	CA	3002	1/1	0.97	0.08	43,43,43,43	0
56	MG	BA	3132	1/1	0.97	0.10	25,25,25,25	0
56	MG	BA	3133	1/1	0.97	0.04	33,33,33,33	0
56	MG	BA	3360	1/1	0.97	0.07	21,21,21,21	0
56	MG	CA	3006	1/1	0.97	0.24	37,37,37,37	0
56	MG	AA	3139	1/1	0.97	0.06	36,36,36,36	0
56	MG	DA	3209	1/1	0.97	0.06	38,38,38,38	0
56	MG	CA	3008	1/1	0.97	0.22	31,31,31,31	0
56	MG	BA	3020	1/1	0.97	0.10	33,33,33,33	0
56	MG	DA	3002	1/1	0.97	0.10	33,33,33,33	0
56	MG	CA	3010	1/1	0.97	0.06	53,53,53,53	0
56	MG	BA	3487	1/1	0.97	0.10	17,17,17,17	0
56	MG	DA	3006	1/1	0.97	0.06	33,33,33,33	0
56	MG	DA	3216	1/1	0.97	0.08	37,37,37,37	0
56	MG	DA	3007	1/1	0.97	0.05	39,39,39,39	0
56	MG	BA	3606	1/1	0.97	0.09	32,32,32,32	0
56	MG	DA	3010	1/1	0.97	0.08	36,36,36,36	0
56	MG	BA	3363	1/1	0.97	0.10	29,29,29,29	0
56	MG	DA	3014	1/1	0.97	0.07	33,33,33,33	0
56	MG	DA	3489	1/1	0.97	0.13	49,49,49,49	0
56	MG	CA	3014	1/1	0.97	0.09	39,39,39,39	0
56	MG	BA	3608	1/1	0.97	0.16	45,45,45,45	0
56	MG	BA	3089	1/1	0.97	0.07	37,37,37,37	0
56	MG	DA	3019	1/1	0.97	0.06	40,40,40,40	0
56	MG	DA	3227	1/1	0.97	0.21	49,49,49,49	0
56	MG	DA	3228	1/1	0.97	0.08	51,51,51,51	0
56	MG	BA	3610	1/1	0.97	0.08	47,47,47,47	0
56	MG	BA	3366	1/1	0.97	0.06	34,34,34,34	0
56	MG	BA	3138	1/1	0.97	0.10	35,35,35,35	0
56	MG	CA	3020	1/1	0.97	0.28	46,46,46,46	0
56	MG	DA	3502	1/1	0.97	0.10	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3613	1/1	0.97	0.08	45,45,45,45	0
56	MG	BA	3614	1/1	0.97	0.05	55,55,55,55	0
56	MG	CA	3023	1/1	0.97	0.08	38,38,38,38	0
56	MG	BA	3368	1/1	0.97	0.07	42,42,42,42	0
56	MG	BA	3370	1/1	0.97	0.09	29,29,29,29	0
56	MG	AA	3064	1/1	0.97	0.18	45,45,45,45	0
56	MG	BA	3269	1/1	0.97	0.05	34,34,34,34	0
56	MG	DA	3031	1/1	0.97	0.04	21,21,21,21	0
56	MG	DA	3511	1/1	0.97	0.14	53,53,53,53	0
56	MG	BA	3054	1/1	0.97	0.14	42,42,42,42	0
56	MG	BA	3499	1/1	0.97	0.09	35,35,35,35	0
56	MG	CA	3030	1/1	0.97	0.09	41,41,41,41	0
56	MG	DA	3246	1/1	0.97	0.17	38,38,38,38	0
56	MG	DA	3035	1/1	0.97	0.12	46,46,46,46	0
56	MG	DA	3248	1/1	0.97	0.20	52,52,52,52	0
56	MG	DA	3037	1/1	0.97	0.10	40,40,40,40	0
56	MG	CA	3031	1/1	0.97	0.08	52,52,52,52	0
56	MG	BA	3193	1/1	0.97	0.19	48,48,48,48	0
56	MG	DA	3040	1/1	0.97	0.14	34,34,34,34	0
56	MG	BA	3622	1/1	0.97	0.11	45,45,45,45	0
56	MG	BA	3501	1/1	0.97	0.09	44,44,44,44	0
56	MG	BA	3502	1/1	0.97	0.10	33,33,33,33	0
56	MG	BA	3276	1/1	0.97	0.06	42,42,42,42	0
56	MG	DA	3258	1/1	0.97	0.19	49,49,49,49	0
56	MG	DA	3046	1/1	0.97	0.17	34,34,34,34	0
56	MG	DA	3532	1/1	0.97	0.06	51,51,51,51	0
56	MG	CA	3037	1/1	0.97	0.06	45,45,45,45	0
56	MG	DA	3048	1/1	0.97	0.07	41,41,41,41	0
56	MG	DA	3262	1/1	0.97	0.06	39,39,39,39	0
56	MG	DA	3049	1/1	0.97	0.04	40,40,40,40	0
56	MG	BA	3194	1/1	0.97	0.03	23,23,23,23	0
56	MG	BA	3055	1/1	0.97	0.07	13,13,13,13	0
56	MG	BA	3385	1/1	0.97	0.06	20,20,20,20	0
56	MG	DA	3267	1/1	0.97	0.15	47,47,47,47	0
56	MG	DA	3053	1/1	0.97	0.12	41,41,41,41	0
56	MG	BA	3386	1/1	0.97	0.14	32,32,32,32	0
56	MG	DA	3270	1/1	0.97	0.06	37,37,37,37	0
56	MG	BA	3197	1/1	0.97	0.10	19,19,19,19	0
56	MG	DA	3547	1/1	0.97	0.09	41,41,41,41	0
56	MG	BA	3282	1/1	0.97	0.15	31,31,31,31	0
56	MG	DA	3057	1/1	0.97	0.04	30,30,30,30	0
56	MG	BA	3144	1/1	0.97	0.12	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3201	1/1	0.97	0.07	41,41,41,41	0
56	MG	BA	3636	1/1	0.97	0.04	32,32,32,32	0
56	MG	DA	3061	1/1	0.97	0.05	35,35,35,35	0
56	MG	DA	3279	1/1	0.97	0.05	27,27,27,27	0
56	MG	BA	3391	1/1	0.97	0.08	37,37,37,37	0
56	MG	AA	3046	1/1	0.97	0.10	42,42,42,42	0
56	MG	BA	3024	1/1	0.97	0.17	32,32,32,32	0
56	MG	DA	3558	1/1	0.97	0.05	39,39,39,39	0
56	MG	BA	3025	1/1	0.97	0.10	37,37,37,37	0
56	MG	CA	3051	1/1	0.97	0.09	66,66,66,66	0
56	MG	CA	3052	1/1	0.97	0.06	39,39,39,39	0
56	MG	DA	3290	1/1	0.97	0.06	36,36,36,36	0
56	MG	DA	3564	1/1	0.97	0.05	36,36,36,36	0
56	MG	DA	3068	1/1	0.97	0.08	35,35,35,35	0
56	MG	BA	3060	1/1	0.97	0.10	42,42,42,42	0
56	MG	AA	3082	1/1	0.97	0.20	57,57,57,57	0
56	MG	DA	3296	1/1	0.97	0.05	28,28,28,28	0
56	MG	BA	3212	1/1	0.97	0.14	28,28,28,28	0
56	MG	DA	3299	1/1	0.97	0.06	50,50,50,50	0
56	MG	AA	3145	1/1	0.97	0.07	35,35,35,35	0
56	MG	BA	3214	1/1	0.97	0.14	28,28,28,28	0
56	MG	DA	3074	1/1	0.97	0.04	29,29,29,29	0
56	MG	DA	3303	1/1	0.97	0.06	43,43,43,43	0
56	MG	BA	3103	1/1	0.97	0.10	42,42,42,42	0
56	MG	BA	3651	1/1	0.97	0.05	42,42,42,42	0
56	MG	BA	3529	1/1	0.97	0.10	33,33,33,33	0
56	MG	BA	3531	1/1	0.97	0.05	41,41,41,41	0
56	MG	AA	3029	1/1	0.97	0.12	52,52,52,52	0
56	MG	BA	3030	1/1	0.97	0.45	43,43,43,43	0
56	MG	DA	3313	1/1	0.97	0.07	40,40,40,40	0
56	MG	DA	3314	1/1	0.97	0.17	54,54,54,54	0
56	MG	DA	3084	1/1	0.97	0.07	39,39,39,39	0
56	MG	DA	3317	1/1	0.97	0.09	53,53,53,53	0
56	MG	DA	3318	1/1	0.97	0.12	43,43,43,43	0
56	MG	DA	3586	1/1	0.97	0.10	47,47,47,47	0
56	MG	DA	3319	1/1	0.97	0.18	38,38,38,38	0
56	MG	DA	3588	1/1	0.97	0.10	21,21,21,21	0
56	MG	DA	3589	1/1	0.97	0.06	33,33,33,33	0
56	MG	BA	3067	1/1	0.97	0.09	34,34,34,34	0
56	MG	DA	3591	1/1	0.97	0.09	42,42,42,42	0
56	MG	BA	3302	1/1	0.97	0.10	55,55,55,55	0
56	MG	BA	3661	1/1	0.97	0.06	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3155	1/1	0.97	0.20	27,27,27,27	0
56	MG	DA	3324	1/1	0.97	0.08	52,52,52,52	0
56	MG	BA	3666	1/1	0.97	0.16	35,35,35,35	0
56	MG	AA	3095	1/1	0.97	0.13	55,55,55,55	0
56	MG	BA	3409	1/1	0.97	0.07	28,28,28,28	0
56	MG	BA	3670	1/1	0.97	0.14	34,34,34,34	0
56	MG	BA	3544	1/1	0.97	0.12	25,25,25,25	0
56	MG	BA	3033	1/1	0.97	0.08	33,33,33,33	0
56	MG	DB	3008	1/1	0.97	0.08	35,35,35,35	0
56	MG	BA	3546	1/1	0.97	0.06	57,57,57,57	0
56	MG	BB	3001	1/1	0.97	0.08	36,36,36,36	0
56	MG	DB	3011	1/1	0.97	0.06	29,29,29,29	0
56	MG	BA	3547	1/1	0.97	0.05	60,60,60,60	0
56	MG	DA	3335	1/1	0.97	0.12	36,36,36,36	0
56	MG	DD	302	1/1	0.97	0.11	39,39,39,39	0
56	MG	BA	3548	1/1	0.97	0.07	30,30,30,30	0
56	MG	BA	3072	1/1	0.97	0.10	24,24,24,24	0
56	MG	DA	3339	1/1	0.97	0.09	32,32,32,32	0
56	MG	DE	3004	1/1	0.97	0.09	48,48,48,48	0
56	MG	BA	3413	1/1	0.97	0.10	26,26,26,26	0
56	MG	DA	3341	1/1	0.97	0.07	25,25,25,25	0
56	MG	DA	3342	1/1	0.97	0.14	37,37,37,37	0
56	MG	AA	3008	1/1	0.97	0.24	55,55,55,55	0
56	MG	DA	3104	1/1	0.97	0.17	35,35,35,35	0
56	MG	BA	3227	1/1	0.97	0.06	32,32,32,32	0
56	MG	DQ	3002	1/1	0.97	0.18	38,38,38,38	0
56	MG	BA	3418	1/1	0.97	0.06	46,46,46,46	0
56	MG	DA	3348	1/1	0.97	0.07	25,25,25,25	0
56	MG	DA	3107	1/1	0.97	0.19	46,46,46,46	0
56	MG	BA	3419	1/1	0.97	0.07	20,20,20,20	0
56	MG	BB	3012	1/1	0.97	0.10	44,44,44,44	0
56	MG	DA	3110	1/1	0.97	0.12	42,42,42,42	0
56	MG	BA	3315	1/1	0.97	0.15	31,31,31,31	0
56	MG	DA	3355	1/1	0.97	0.04	36,36,36,36	0
56	MG	BA	3228	1/1	0.97	0.08	40,40,40,40	0
56	MG	BA	3113	1/1	0.97	0.18	41,41,41,41	0
56	MG	DA	3358	1/1	0.97	0.10	45,45,45,45	0
56	MG	AA	3032	1/1	0.97	0.11	42,42,42,42	0
56	MG	AA	3186	1/1	0.97	0.12	55,55,55,55	0
58	ZN	B4	501	1/1	0.97	0.06	106,106,106,106	0
58	ZN	D4	501	1/1	0.97	0.08	141,141,141,141	0
56	MG	DA	3116	1/1	0.97	0.10	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3362	1/1	0.97	0.07	43,43,43,43	0
56	MG	BA	3004	1/1	0.98	0.06	23,23,23,23	0
56	MG	BA	3203	1/1	0.98	0.13	35,35,35,35	0
56	MG	B0	103	1/1	0.98	0.07	33,33,33,33	0
56	MG	DA	3448	1/1	0.98	0.14	29,29,29,29	0
56	MG	BA	3204	1/1	0.98	0.12	35,35,35,35	0
56	MG	AA	3070	1/1	0.98	0.16	33,33,33,33	0
56	MG	DA	3451	1/1	0.98	0.05	30,30,30,30	0
56	MG	B3	101	1/1	0.98	0.12	35,35,35,35	0
56	MG	B3	102	1/1	0.98	0.15	22,22,22,22	0
56	MG	BA	3326	1/1	0.98	0.05	28,28,28,28	0
56	MG	BA	3068	1/1	0.98	0.04	39,39,39,39	0
56	MG	BA	3519	1/1	0.98	0.07	53,53,53,53	0
56	MG	BA	3520	1/1	0.98	0.06	24,24,24,24	0
56	MG	B7	3002	1/1	0.98	0.05	35,35,35,35	0
56	MG	B7	3003	1/1	0.98	0.06	28,28,28,28	0
56	MG	BA	3208	1/1	0.98	0.16	25,25,25,25	0
56	MG	BA	3522	1/1	0.98	0.06	52,52,52,52	0
56	MG	DA	3462	1/1	0.98	0.06	35,35,35,35	0
56	MG	BA	3628	1/1	0.98	0.07	38,38,38,38	0
56	MG	BA	3209	1/1	0.98	0.18	26,26,26,26	0
56	MG	BA	3022	1/1	0.98	0.04	26,26,26,26	0
56	MG	BA	3414	1/1	0.98	0.06	31,31,31,31	0
56	MG	BA	3006	1/1	0.98	0.12	36,36,36,36	0
56	MG	DA	3276	1/1	0.98	0.18	50,50,50,50	0
56	MG	BA	3099	1/1	0.98	0.20	32,32,32,32	0
56	MG	BA	3528	1/1	0.98	0.05	38,38,38,38	0
56	MG	BA	3262	1/1	0.98	0.09	24,24,24,24	0
56	MG	DA	3280	1/1	0.98	0.07	50,50,50,50	0
56	MG	BA	3007	1/1	0.98	0.03	32,32,32,32	0
56	MG	BA	3420	1/1	0.98	0.05	24,24,24,24	0
56	MG	DA	3283	1/1	0.98	0.04	38,38,38,38	0
56	MG	DA	3476	1/1	0.98	0.03	32,32,32,32	0
56	MG	DA	3284	1/1	0.98	0.04	23,23,23,23	0
56	MG	BA	3421	1/1	0.98	0.07	36,36,36,36	0
56	MG	BA	3535	1/1	0.98	0.05	47,47,47,47	0
56	MG	BA	3640	1/1	0.98	0.06	33,33,33,33	0
56	MG	BA	3264	1/1	0.98	0.15	35,35,35,35	0
56	MG	DA	3482	1/1	0.98	0.05	46,46,46,46	0
56	MG	DA	3124	1/1	0.98	0.09	29,29,29,29	0
56	MG	BA	3336	1/1	0.98	0.06	43,43,43,43	0
56	MG	BA	3538	1/1	0.98	0.14	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3294	1/1	0.98	0.04	37,37,37,37	0
56	MG	BA	3134	1/1	0.98	0.10	40,40,40,40	0
56	MG	BA	3215	1/1	0.98	0.10	32,32,32,32	0
56	MG	DA	3297	1/1	0.98	0.08	38,38,38,38	0
56	MG	DA	3490	1/1	0.98	0.06	34,34,34,34	0
56	MG	CA	3147	1/1	0.98	0.08	52,52,52,52	0
56	MG	BA	3542	1/1	0.98	0.07	51,51,51,51	0
56	MG	BA	3216	1/1	0.98	0.23	33,33,33,33	0
56	MG	BA	3650	1/1	0.98	0.04	31,31,31,31	0
56	MG	AN	502	1/1	0.98	0.18	53,53,53,53	0
56	MG	BA	3341	1/1	0.98	0.05	32,32,32,32	0
56	MG	DA	3497	1/1	0.98	0.11	45,45,45,45	0
56	MG	DA	3304	1/1	0.98	0.10	32,32,32,32	0
56	MG	AA	3168	1/1	0.98	0.14	56,56,56,56	0
56	MG	BA	3104	1/1	0.98	0.04	42,42,42,42	0
56	MG	BA	3049	1/1	0.98	0.09	43,43,43,43	0
56	MG	BA	3657	1/1	0.98	0.07	24,24,24,24	0
56	MG	BA	3658	1/1	0.98	0.06	27,27,27,27	0
56	MG	BA	3272	1/1	0.98	0.07	37,37,37,37	0
56	MG	DA	3311	1/1	0.98	0.08	43,43,43,43	0
56	MG	DA	3142	1/1	0.98	0.10	37,37,37,37	0
56	MG	DA	3143	1/1	0.98	0.05	27,27,27,27	0
56	MG	DA	3315	1/1	0.98	0.10	43,43,43,43	0
56	MG	BA	3273	1/1	0.98	0.05	29,29,29,29	0
56	MG	BA	3551	1/1	0.98	0.05	48,48,48,48	0
56	MG	BA	3274	1/1	0.98	0.08	47,47,47,47	0
56	MG	BA	3665	1/1	0.98	0.05	30,30,30,30	0
56	MG	DA	3513	1/1	0.98	0.06	32,32,32,32	0
56	MG	DA	3148	1/1	0.98	0.04	47,47,47,47	0
56	MG	BA	3175	1/1	0.98	0.10	33,33,33,33	0
56	MG	AA	3075	1/1	0.98	0.12	39,39,39,39	0
56	MG	DA	3005	1/1	0.98	0.06	26,26,26,26	0
56	MG	AX	3004	1/1	0.98	0.11	39,39,39,39	0
56	MG	DA	3519	1/1	0.98	0.05	42,42,42,42	0
56	MG	BA	3351	1/1	0.98	0.04	33,33,33,33	0
56	MG	DA	3008	1/1	0.98	0.03	38,38,38,38	0
56	MG	DA	3522	1/1	0.98	0.09	44,44,44,44	0
56	MG	BA	3279	1/1	0.98	0.07	38,38,38,38	0
56	MG	BA	3353	1/1	0.98	0.06	39,39,39,39	0
56	MG	BA	3674	1/1	0.98	0.05	54,54,54,54	0
56	MG	DA	3012	1/1	0.98	0.11	30,30,30,30	0
56	MG	DA	3013	1/1	0.98	0.06	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3528	1/1	0.98	0.04	37,37,37,37	0
56	MG	BA	3354	1/1	0.98	0.05	42,42,42,42	0
56	MG	BA	3355	1/1	0.98	0.04	31,31,31,31	0
56	MG	DA	3016	1/1	0.98	0.15	31,31,31,31	0
56	MG	DA	3336	1/1	0.98	0.08	22,22,22,22	0
56	MG	BB	3002	1/1	0.98	0.12	41,41,41,41	0
56	MG	BA	3178	1/1	0.98	0.17	26,26,26,26	0
56	MG	BA	3281	1/1	0.98	0.12	51,51,51,51	0
56	MG	DA	3168	1/1	0.98	0.11	39,39,39,39	0
56	MG	DA	3169	1/1	0.98	0.04	38,38,38,38	0
56	MG	BA	3453	1/1	0.98	0.04	27,27,27,27	0
56	MG	BA	3456	1/1	0.98	0.12	33,33,33,33	0
56	MG	BA	3457	1/1	0.98	0.06	29,29,29,29	0
56	MG	BA	3225	1/1	0.98	0.05	31,31,31,31	0
56	MG	BA	3029	1/1	0.98	0.07	12,12,12,12	0
56	MG	AA	3030	1/1	0.98	0.09	47,47,47,47	0
56	MG	BB	3011	1/1	0.98	0.05	45,45,45,45	0
56	MG	DA	3546	1/1	0.98	0.06	40,40,40,40	0
56	MG	DA	3177	1/1	0.98	0.06	52,52,52,52	0
56	MG	AA	3162	1/1	0.98	0.06	40,40,40,40	0
56	MG	BA	3032	1/1	0.98	0.04	40,40,40,40	0
56	MG	DA	3180	1/1	0.98	0.06	30,30,30,30	0
56	MG	DA	3181	1/1	0.98	0.05	40,40,40,40	0
56	MG	DA	3182	1/1	0.98	0.05	38,38,38,38	0
56	MG	BA	3015	1/1	0.98	0.04	27,27,27,27	0
56	MG	BA	3364	1/1	0.98	0.05	29,29,29,29	0
56	MG	BA	3114	1/1	0.98	0.12	34,34,34,34	0
56	MG	BA	3291	1/1	0.98	0.08	14,14,14,14	0
56	MG	AA	3050	1/1	0.98	0.04	24,24,24,24	0
56	MG	BD	301	1/1	0.98	0.11	30,30,30,30	0
56	MG	BA	3085	1/1	0.98	0.10	27,27,27,27	0
56	MG	DA	3036	1/1	0.98	0.04	38,38,38,38	0
56	MG	CA	3061	1/1	0.98	0.10	45,45,45,45	0
56	MG	DA	3562	1/1	0.98	0.06	42,42,42,42	0
56	MG	BA	3369	1/1	0.98	0.09	33,33,33,33	0
56	MG	BA	3035	1/1	0.98	0.15	21,21,21,21	0
56	MG	BA	3371	1/1	0.98	0.06	25,25,25,25	0
56	MG	BD	306	1/1	0.98	0.10	36,36,36,36	0
56	MG	DA	3196	1/1	0.98	0.06	33,33,33,33	0
56	MG	DA	3042	1/1	0.98	0.04	32,32,32,32	0
56	MG	DA	3372	1/1	0.98	0.06	21,21,21,21	0
56	MG	BA	3372	1/1	0.98	0.07	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3475	1/1	0.98	0.07	45,45,45,45	0
56	MG	DA	3200	1/1	0.98	0.08	28,28,28,28	0
56	MG	BA	3119	1/1	0.98	0.08	29,29,29,29	0
56	MG	DA	3202	1/1	0.98	0.13	24,24,24,24	0
56	MG	DA	3378	1/1	0.98	0.08	31,31,31,31	0
56	MG	DA	3380	1/1	0.98	0.04	33,33,33,33	0
56	MG	BA	3477	1/1	0.98	0.06	50,50,50,50	0
56	MG	AA	3173	1/1	0.98	0.12	32,32,32,32	0
56	MG	BE	304	1/1	0.98	0.07	13,13,13,13	0
56	MG	DA	3385	1/1	0.98	0.03	45,45,45,45	0
56	MG	BA	3038	1/1	0.98	0.06	30,30,30,30	0
56	MG	BA	3299	1/1	0.98	0.07	36,36,36,36	0
56	MG	DA	3389	1/1	0.98	0.04	42,42,42,42	0
56	MG	DA	3391	1/1	0.98	0.04	42,42,42,42	0
56	MG	BA	3377	1/1	0.98	0.07	31,31,31,31	0
56	MG	BA	3589	1/1	0.98	0.06	27,27,27,27	0
56	MG	BA	3380	1/1	0.98	0.09	17,17,17,17	0
56	MG	BA	3122	1/1	0.98	0.20	39,39,39,39	0
56	MG	BA	3382	1/1	0.98	0.09	27,27,27,27	0
56	MG	AA	3007	1/1	0.98	0.13	30,30,30,30	0
56	MG	BA	3489	1/1	0.98	0.17	41,41,41,41	0
56	MG	BA	3490	1/1	0.98	0.07	38,38,38,38	0
56	MG	DA	3400	1/1	0.98	0.17	38,38,38,38	0
56	MG	DA	3401	1/1	0.98	0.09	55,55,55,55	0
56	MG	DA	3596	1/1	0.98	0.12	54,54,54,54	0
56	MG	BA	3063	1/1	0.98	0.11	47,47,47,47	0
56	MG	DA	3403	1/1	0.98	0.04	39,39,39,39	0
56	MG	BN	3002	1/1	0.98	0.04	27,27,27,27	0
56	MG	BA	3304	1/1	0.98	0.09	43,43,43,43	0
56	MG	BA	3305	1/1	0.98	0.07	28,28,28,28	0
56	MG	BA	3091	1/1	0.98	0.14	19,19,19,19	0
56	MG	BA	3159	1/1	0.98	0.14	27,27,27,27	0
56	MG	BP	204	1/1	0.98	0.08	31,31,31,31	0
56	MG	BA	3196	1/1	0.98	0.10	17,17,17,17	0
56	MG	BQ	202	1/1	0.98	0.04	14,14,14,14	0
56	MG	BA	3160	1/1	0.98	0.09	29,29,29,29	0
56	MG	BR	3001	1/1	0.98	0.04	31,31,31,31	0
56	MG	DA	3229	1/1	0.98	0.16	38,38,38,38	0
56	MG	BR	3002	1/1	0.98	0.04	23,23,23,23	0
56	MG	DA	3231	1/1	0.98	0.05	37,37,37,37	0
56	MG	BA	3198	1/1	0.98	0.07	34,34,34,34	0
56	MG	CA	3095	1/1	0.98	0.11	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3312	1/1	0.98	0.05	18,18,18,18	0
56	MG	DE	3005	1/1	0.98	0.06	20,20,20,20	0
56	MG	BA	3313	1/1	0.98	0.06	17,17,17,17	0
56	MG	DF	302	1/1	0.98	0.05	41,41,41,41	0
56	MG	BU	204	1/1	0.98	0.12	29,29,29,29	0
56	MG	BA	3161	1/1	0.98	0.04	39,39,39,39	0
56	MG	BA	3247	1/1	0.98	0.19	48,48,48,48	0
56	MG	BA	3248	1/1	0.98	0.14	21,21,21,21	0
56	MG	DA	3426	1/1	0.98	0.07	35,35,35,35	0
56	MG	DA	3427	1/1	0.98	0.08	25,25,25,25	0
56	MG	DA	3080	1/1	0.98	0.07	29,29,29,29	0
56	MG	DR	201	1/1	0.98	0.23	36,36,36,36	0
56	MG	DA	3081	1/1	0.98	0.07	44,44,44,44	0
56	MG	BW	3001	1/1	0.98	0.05	25,25,25,25	0
56	MG	BA	3200	1/1	0.98	0.08	25,25,25,25	0
56	MG	BA	3399	1/1	0.98	0.08	42,42,42,42	0
56	MG	DA	3433	1/1	0.98	0.10	33,33,33,33	0
56	MG	DW	3001	1/1	0.98	0.09	38,38,38,38	0
56	MG	DA	3085	1/1	0.98	0.16	40,40,40,40	0
56	MG	DA	3086	1/1	0.98	0.07	41,41,41,41	0
56	MG	BA	3506	1/1	0.98	0.04	39,39,39,39	0
56	MG	CA	3106	1/1	0.98	0.14	40,40,40,40	0
56	MG	BA	3250	1/1	0.98	0.08	33,33,33,33	0
56	MG	DA	3250	1/1	0.98	0.05	37,37,37,37	0
56	MG	BA	3508	1/1	0.98	0.06	25,25,25,25	0
57	SF4	CD	501	8/8	0.98	0.04	58,71,82,82	0
56	MG	AA	3084	1/1	0.98	0.08	43,43,43,43	0
58	ZN	CN	501	1/1	0.98	0.04	82,82,82,82	0
56	MG	BA	3320	1/1	0.98	0.05	44,44,44,44	0
58	ZN	D9	501	1/1	0.98	0.06	54,54,54,54	0
56	MG	CA	3111	1/1	0.98	0.08	43,43,43,43	0
56	MG	BA	3321	1/1	0.98	0.06	53,53,53,53	0
56	MG	AA	3040	1/1	0.99	0.12	27,27,27,27	0
56	MG	AA	3127	1/1	0.99	0.09	68,68,68,68	0
56	MG	BA	3289	1/1	0.99	0.07	28,28,28,28	0
56	MG	BA	3290	1/1	0.99	0.04	36,36,36,36	0
56	MG	BA	3207	1/1	0.99	0.14	36,36,36,36	0
56	MG	BA	3083	1/1	0.99	0.09	34,34,34,34	0
56	MG	BA	3530	1/1	0.99	0.08	36,36,36,36	0
56	MG	BA	3479	1/1	0.99	0.07	45,45,45,45	0
56	MG	AA	3022	1/1	0.99	0.04	39,39,39,39	0
56	MG	BA	3481	1/1	0.99	0.09	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3534	1/1	0.99	0.09	20,20,20,20	0
56	MG	BA	3482	1/1	0.99	0.03	23,23,23,23	0
56	MG	BA	3294	1/1	0.99	0.04	32,32,32,32	0
56	MG	BF	302	1/1	0.99	0.03	45,45,45,45	0
56	MG	BA	3647	1/1	0.99	0.02	30,30,30,30	0
56	MG	DA	3413	1/1	0.99	0.07	24,24,24,24	0
56	MG	BA	3648	1/1	0.99	0.05	28,28,28,28	0
56	MG	BA	3433	1/1	0.99	0.04	33,33,33,33	0
56	MG	DA	3334	1/1	0.99	0.03	24,24,24,24	0
56	MG	BA	3065	1/1	0.99	0.08	29,29,29,29	0
56	MG	BA	3397	1/1	0.99	0.03	30,30,30,30	0
56	MG	BA	3436	1/1	0.99	0.04	35,35,35,35	0
56	MG	BA	3541	1/1	0.99	0.02	26,26,26,26	0
56	MG	AA	3090	1/1	0.99	0.10	28,28,28,28	0
56	MG	BA	3438	1/1	0.99	0.05	33,33,33,33	0
56	MG	BA	3656	1/1	0.99	0.07	12,12,12,12	0
56	MG	BA	3109	1/1	0.99	0.04	36,36,36,36	0
56	MG	BA	3440	1/1	0.99	0.05	38,38,38,38	0
56	MG	AA	3115	1/1	0.99	0.03	35,35,35,35	0
56	MG	DA	3345	1/1	0.99	0.08	33,33,33,33	0
56	MG	AA	3011	1/1	0.99	0.05	24,24,24,24	0
56	MG	AA	3140	1/1	0.99	0.05	31,31,31,31	0
56	MG	DA	3595	1/1	0.99	0.04	43,43,43,43	0
56	MG	BA	3445	1/1	0.99	0.03	22,22,22,22	0
56	MG	BA	3664	1/1	0.99	0.12	30,30,30,30	0
56	MG	DA	3350	1/1	0.99	0.09	36,36,36,36	0
56	MG	BA	3008	1/1	0.99	0.07	27,27,27,27	0
56	MG	BA	3071	1/1	0.99	0.09	32,32,32,32	0
56	MG	DA	3205	1/1	0.99	0.17	32,32,32,32	0
56	MG	BA	3303	1/1	0.99	0.06	31,31,31,31	0
56	MG	BU	201	1/1	0.99	0.11	32,32,32,32	0
56	MG	BA	3139	1/1	0.99	0.04	31,31,31,31	0
56	MG	BA	3669	1/1	0.99	0.05	29,29,29,29	0
56	MG	BA	3115	1/1	0.99	0.05	34,34,34,34	0
56	MG	DA	3140	1/1	0.99	0.09	37,37,37,37	0
56	MG	BA	3037	1/1	0.99	0.04	24,24,24,24	0
56	MG	BA	3672	1/1	0.99	0.04	46,46,46,46	0
56	MG	BA	3452	1/1	0.99	0.08	38,38,38,38	0
56	MG	BV	203	1/1	0.99	0.03	24,24,24,24	0
56	MG	BA	3275	1/1	0.99	0.05	39,39,39,39	0
56	MG	BA	3454	1/1	0.99	0.08	21,21,21,21	0
56	MG	DA	3289	1/1	0.99	0.09	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3079	1/1	0.99	0.04	54,54,54,54	0
56	MG	BW	3003	1/1	0.99	0.06	27,27,27,27	0
56	MG	BA	3455	1/1	0.99	0.03	21,21,21,21	0
56	MG	DA	3293	1/1	0.99	0.07	34,34,34,34	0
56	MG	AA	3161	1/1	0.99	0.09	66,66,66,66	0
56	MG	BA	3411	1/1	0.99	0.09	25,25,25,25	0
56	MG	BA	3143	1/1	0.99	0.15	36,36,36,36	0
56	MG	DA	3224	1/1	0.99	0.10	22,22,22,22	0
56	MG	BA	3310	1/1	0.99	0.05	35,35,35,35	0
56	MG	BA	3039	1/1	0.99	0.07	31,31,31,31	0
56	MG	BA	3511	1/1	0.99	0.05	38,38,38,38	0
56	MG	DA	3157	1/1	0.99	0.07	40,40,40,40	0
56	MG	DA	3379	1/1	0.99	0.03	26,26,26,26	0
56	MG	AA	3117	1/1	0.99	0.04	47,47,47,47	0
56	MG	BA	3462	1/1	0.99	0.03	44,44,44,44	0
56	MG	AA	3163	1/1	0.99	0.03	49,49,49,49	0
56	MG	DA	3383	1/1	0.99	0.06	47,47,47,47	0
56	MG	BA	3417	1/1	0.99	0.09	24,24,24,24	0
56	MG	BA	3625	1/1	0.99	0.05	25,25,25,25	0
56	MG	BA	3465	1/1	0.99	0.05	37,37,37,37	0
56	MG	BA	3097	1/1	0.99	0.12	53,53,53,53	0
56	MG	D5	502	1/1	0.99	0.20	36,36,36,36	0
56	MG	DA	3388	1/1	0.99	0.03	35,35,35,35	0
56	MG	AA	3118	1/1	0.99	0.11	36,36,36,36	0
56	MG	DA	3390	1/1	0.99	0.04	41,41,41,41	0
57	SF4	AD	501	8/8	0.99	0.04	50,63,78,83	0
56	MG	BA	3059	1/1	0.99	0.04	27,27,27,27	0
58	ZN	AN	501	1/1	0.99	0.04	67,67,67,67	0
58	ZN	BY	501	1/1	0.99	0.02	51,51,51,51	0
56	MG	BA	3100	1/1	0.99	0.06	29,29,29,29	0
56	MG	DA	3312	1/1	0.99	0.03	47,47,47,47	0
58	ZN	DY	501	1/1	0.99	0.04	92,92,92,92	0
56	MG	AA	3143	1/1	0.99	0.05	32,32,32,32	0
58	ZN	D5	501	1/1	0.99	0.04	67,67,67,67	0
58	ZN	D6	501	1/1	0.99	0.06	68,68,68,68	0
56	MG	AX	3008	1/1	0.99	0.08	23,23,23,23	0
56	MG	BA	3424	1/1	0.99	0.06	38,38,38,38	0
56	MG	CA	3128	1/1	0.99	0.03	39,39,39,39	0
58	ZN	B6	501	1/1	1.00	0.01	45,45,45,45	0
58	ZN	B9	501	1/1	1.00	0.03	45,45,45,45	0
56	MG	BA	3663	1/1	1.00	0.01	20,20,20,20	0
56	MG	BA	3378	1/1	1.00	0.06	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3542	1/1	1.00	0.03	30,30,30,30	0
56	MG	BA	3552	1/1	1.00	0.03	31,31,31,31	0
56	MG	BA	3379	1/1	1.00	0.05	31,31,31,31	0
56	MG	DA	3154	1/1	1.00	0.07	24,24,24,24	0
56	MG	BA	3442	1/1	1.00	0.05	20,20,20,20	0
58	ZN	B5	501	1/1	1.00	0.02	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.