



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2026 – 12:34 AM EDT

PDB ID : 4V9R / pdb_00004v9r
Title : Crystal structure of antibiotic DITYROMYCIN bound to 70S ribosome
Authors : Bulkley, D.P.; Brandi, L.; Polikanov, Y.S.; Fabbretti, A.; O'Connor, M.;
Gualerzi, C.O.; Steitz, T.A.
Deposited on : 2013-12-05
Resolution : 3.00 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

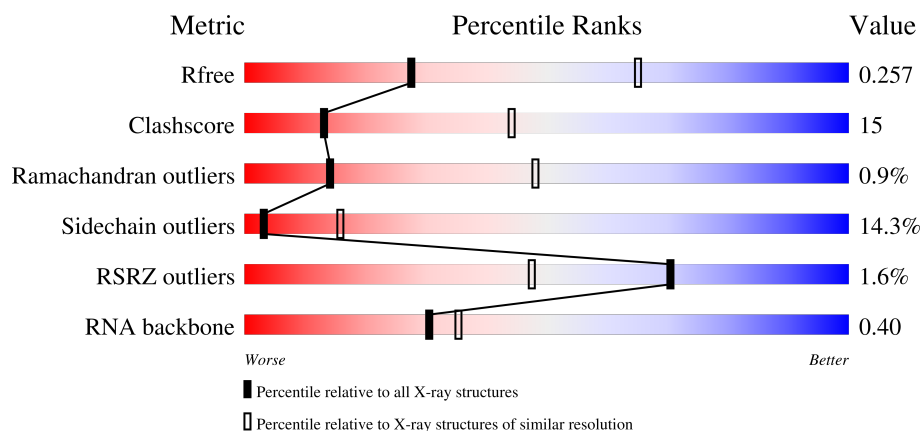
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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	1522	
1	CA	1522	
2	AB	256	
2	CB	256	

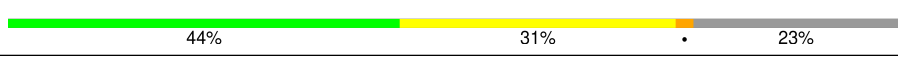
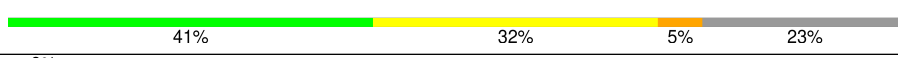
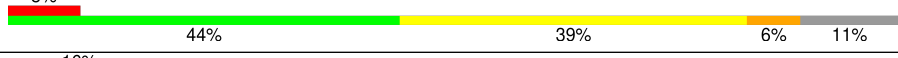
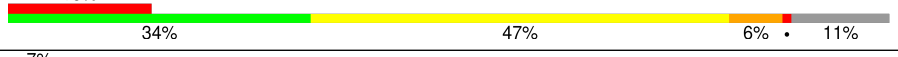
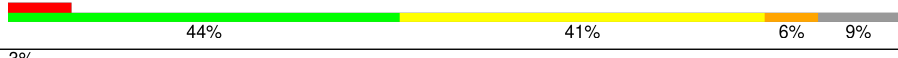
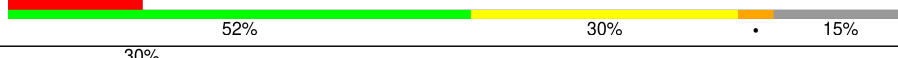
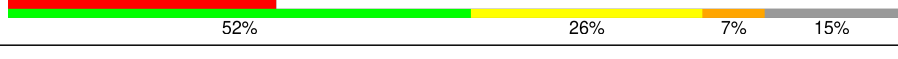
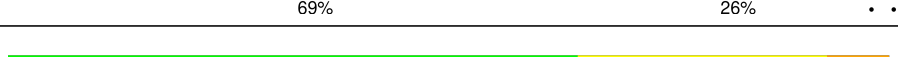
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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126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

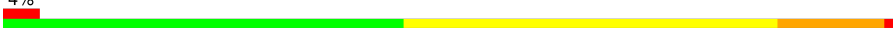
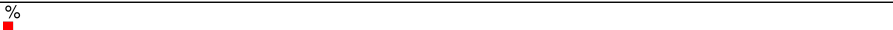
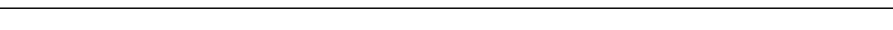
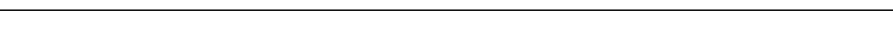
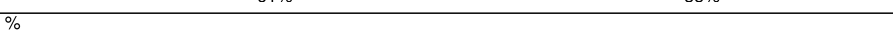
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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	24	
22	CV	24	
23	AX	77	
23	CX	77	
24	AW	10	
24	CW	10	
25	BA	2915	
25	DA	2915	
26	BB	122	
26	DB	122	
27	BD	276	
27	DD	276	

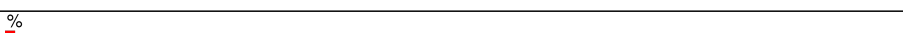
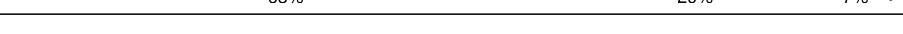
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Mol	Chain	Length	Quality of chain
28	BE	206	
28	DE	206	
29	BF	210	
29	DF	210	
30	BG	182	
30	DG	182	
31	BH	180	
31	DH	180	
32	BI	148	
32	DI	148	
33	BN	140	
33	DN	140	
34	BO	122	
34	DO	122	
35	BP	150	
35	DP	150	
36	BQ	141	
36	DQ	141	
37	BR	118	
37	DR	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	
53	D7	49	
54	B8	65	
54	D8	65	
55	B9	37	
55	D9	37	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	AA	3133	-	-	-	X
56	MG	CA	3028	-	-	-	X
56	MG	CA	3030	-	-	-	X
56	MG	CA	3053	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 286321 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
			32196	14328	5966	10404	1498			
1	CA	1503	Total	C	N	O	P	0	0	0
			32312	14381	5990	10438	1503			

- Molecule 2 is a protein called 30S Ribosomal Protein S2.

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

- Molecule 3 is a protein called 30S Ribosomal Protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1552	976	302	273	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 4 is a protein called 30S Ribosomal Protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1659	1040	326	286	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

- Molecule 5 is a protein called 30S Ribosomal Protein S5.

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

- Molecule 6 is a protein called 30S Ribosomal Protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			806	511	143	149	3			
6	CF	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 7 is a protein called 30S Ribosomal Protein S7.

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

- Molecule 8 is a protein called 30S Ribosomal Protein S8.

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

- Molecule 9 is a protein called 30S Ribosomal Protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	0	0	0
			983	623	193	167			
9	CI	127	Total	C	N	O	0	0	0
			978	619	190	169			

- Molecule 10 is a protein called 30S Ribosomal Protein S10.

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

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

- Molecule 11 is a protein called 30S Ribosomal Protein S11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	AK	114	Total	C	N	O	S		
			829	516	155	155	3	0	0
11	CK	114	Total	C	N	O	S		
			833	519	156	155	3	0	0

- Molecule 12 is a protein called 30S Ribosomal Protein S12.

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

- Molecule 13 is a protein called 30S Ribosomal Protein S13.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	AM	123	Total	C	N	O	S		
			958	592	198	166	2	0	0
13	CM	122	Total	C	N	O	S		
			950	586	197	165	2	0	0

- Molecule 14 is a protein called 30S Ribosomal Protein S14.

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	7	Total	C	N	O	P	0	0	1
			114	49	22	37	6			
22	CV	6	Total	C	N	O	P	0	0	0
			113	49	22	36	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	76	Total	C	N	O	P	0	0	0
			1623	723	294	530	76			
23	CX	76	Total	C	N	O	P	0	0	0
			1623	723	294	530	76			

- Molecule 24 is a protein called Dityromycin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	AW	10	Total	C	N	O	0	0	0
			93	67	10	16			
24	CW	10	Total	C	N	O	0	0	0
			93	67	10	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2731	Total	C	N	O	P	0	0	0
			58834	26185	11020	18899	2730			
25	DA	2714	Total	C	N	O	P	0	0	0
			58458	26018	10942	18786	2712			

- 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		0	0	0
			877	553	175	149				
38	DS	110	Total	C	N	O		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
			551	348	99	99	5			
50	D4	69	Total	C	N	O	S	0	0	0
			531	338	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	222	Total	Mg	0	0
			222	222		
56	AD	1	Total	Mg	0	0
			1	1		
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	2	Total	Mg	0	0
			2	2		
56	AN	1	Total	Mg	0	0
			1	1		
56	AS	1	Total	Mg	0	0
			1	1		
56	AV	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AX	9	Total 9	Mg 9	0	0
56	BA	739	Total 739	Mg 739	0	0
56	BB	18	Total 18	Mg 18	0	0
56	BD	12	Total 12	Mg 12	0	0
56	BE	9	Total 9	Mg 9	0	0
56	BF	6	Total 6	Mg 6	0	0
56	BG	4	Total 4	Mg 4	0	0
56	BN	6	Total 6	Mg 6	0	0
56	BO	1	Total 1	Mg 1	0	0
56	BP	4	Total 4	Mg 4	0	0
56	BQ	4	Total 4	Mg 4	0	0
56	BR	3	Total 3	Mg 3	0	0
56	BU	9	Total 9	Mg 9	0	0
56	BV	3	Total 3	Mg 3	0	0
56	BW	5	Total 5	Mg 5	0	0
56	BX	2	Total 2	Mg 2	0	0
56	BZ	1	Total 1	Mg 1	0	0
56	B0	6	Total 6	Mg 6	0	0
56	B1	2	Total 2	Mg 2	0	0
56	B2	1	Total 1	Mg 1	0	0
56	B3	3	Total 3	Mg 3	0	0

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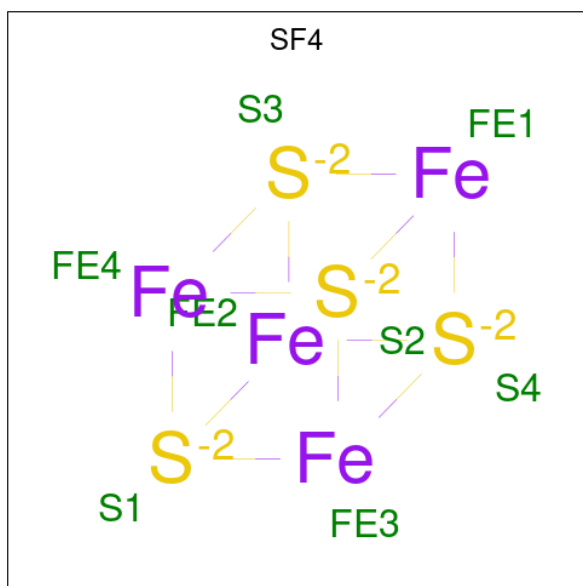
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B5	1	Total 1	Mg 1	0	0
56	B7	4	Total 4	Mg 4	0	0
56	B8	2	Total 2	Mg 2	0	0
56	B9	1	Total 1	Mg 1	0	0
56	CA	172	Total 172	Mg 172	0	0
56	CE	2	Total 2	Mg 2	0	0
56	CF	1	Total 1	Mg 1	0	0
56	CN	1	Total 1	Mg 1	0	0
56	CT	1	Total 1	Mg 1	0	0
56	CX	3	Total 3	Mg 3	0	0
56	DA	657	Total 657	Mg 657	0	0
56	DB	12	Total 12	Mg 12	0	0
56	DD	5	Total 5	Mg 5	0	0
56	DE	6	Total 6	Mg 6	0	0
56	DF	5	Total 5	Mg 5	0	0
56	DG	1	Total 1	Mg 1	0	0
56	DN	1	Total 1	Mg 1	0	0
56	DO	1	Total 1	Mg 1	0	0
56	DP	2	Total 2	Mg 2	0	0
56	DQ	4	Total 4	Mg 4	0	0
56	DR	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DU	2	Total 2	Mg 2	0	0
56	DV	3	Total 3	Mg 3	0	0
56	DW	2	Total 2	Mg 2	0	0
56	DY	1	Total 1	Mg 1	0	0
56	D3	1	Total 1	Mg 1	0	0
56	D5	2	Total 2	Mg 2	0	0
56	D8	1	Total 1	Mg 1	0	0

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

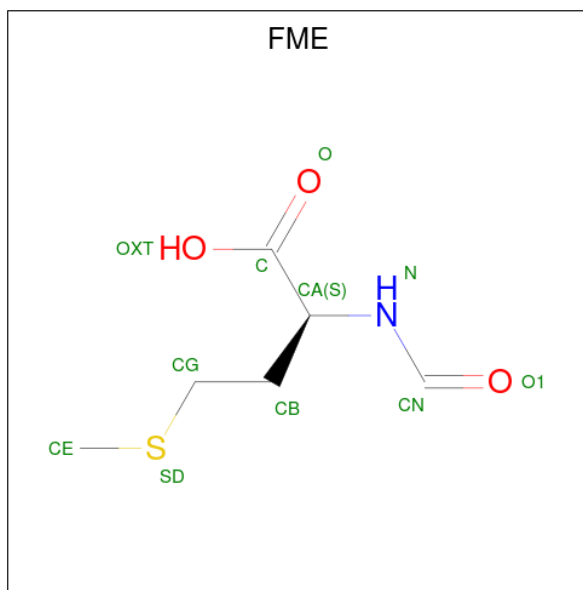


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	AD	1	Total 8	Fe 4	S 4	0	0
57	CD	1	Total 8	Fe 4	S 4	0	0

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

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

- Molecule 59 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
59	AX	1	Total	C	N	O	S	0	0
			10	6	1	2	1		
59	CX	1	Total	C	N	O	S	0	0
			10	6	1	2	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	BA	1	Total	K	0	0
			1	1		
60	DA	1	Total	K	0	0
			1	1		

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AA	147	Total	O	0	0
			147	147		
61	AD	1	Total	O	0	0
			1	1		
61	AE	2	Total	O	0	0
			2	2		
61	AJ	1	Total	O	0	0
			1	1		
61	AL	2	Total	O	0	0
			2	2		
61	AO	2	Total	O	0	0
			2	2		
61	AU	1	Total	O	0	0
			1	1		
61	AV	2	Total	O	0	0
			2	2		
61	AX	1	Total	O	0	0
			1	1		
61	BA	1086	Total	O	0	0
			1086	1086		
61	BB	26	Total	O	0	0
			26	26		
61	BD	6	Total	O	0	0
			6	6		
61	BE	13	Total	O	0	0
			13	13		
61	BF	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	BG	1	Total 1	O 1	0	0
61	BN	3	Total 3	O 3	0	0
61	BO	2	Total 2	O 2	0	0
61	BP	15	Total 15	O 15	0	0
61	BQ	3	Total 3	O 3	0	0
61	BR	1	Total 1	O 1	0	0
61	BT	2	Total 2	O 2	0	0
61	BU	5	Total 5	O 5	0	0
61	BV	2	Total 2	O 2	0	0
61	BW	4	Total 4	O 4	0	0
61	BX	4	Total 4	O 4	0	0
61	B0	4	Total 4	O 4	0	0
61	B1	2	Total 2	O 2	0	0
61	B5	2	Total 2	O 2	0	0
61	B7	1	Total 1	O 1	0	0
61	B8	7	Total 7	O 7	0	0
61	CA	186	Total 186	O 186	0	0
61	CE	2	Total 2	O 2	0	0
61	CN	1	Total 1	O 1	0	0
61	CT	1	Total 1	O 1	0	0
61	CX	2	Total 2	O 2	0	0

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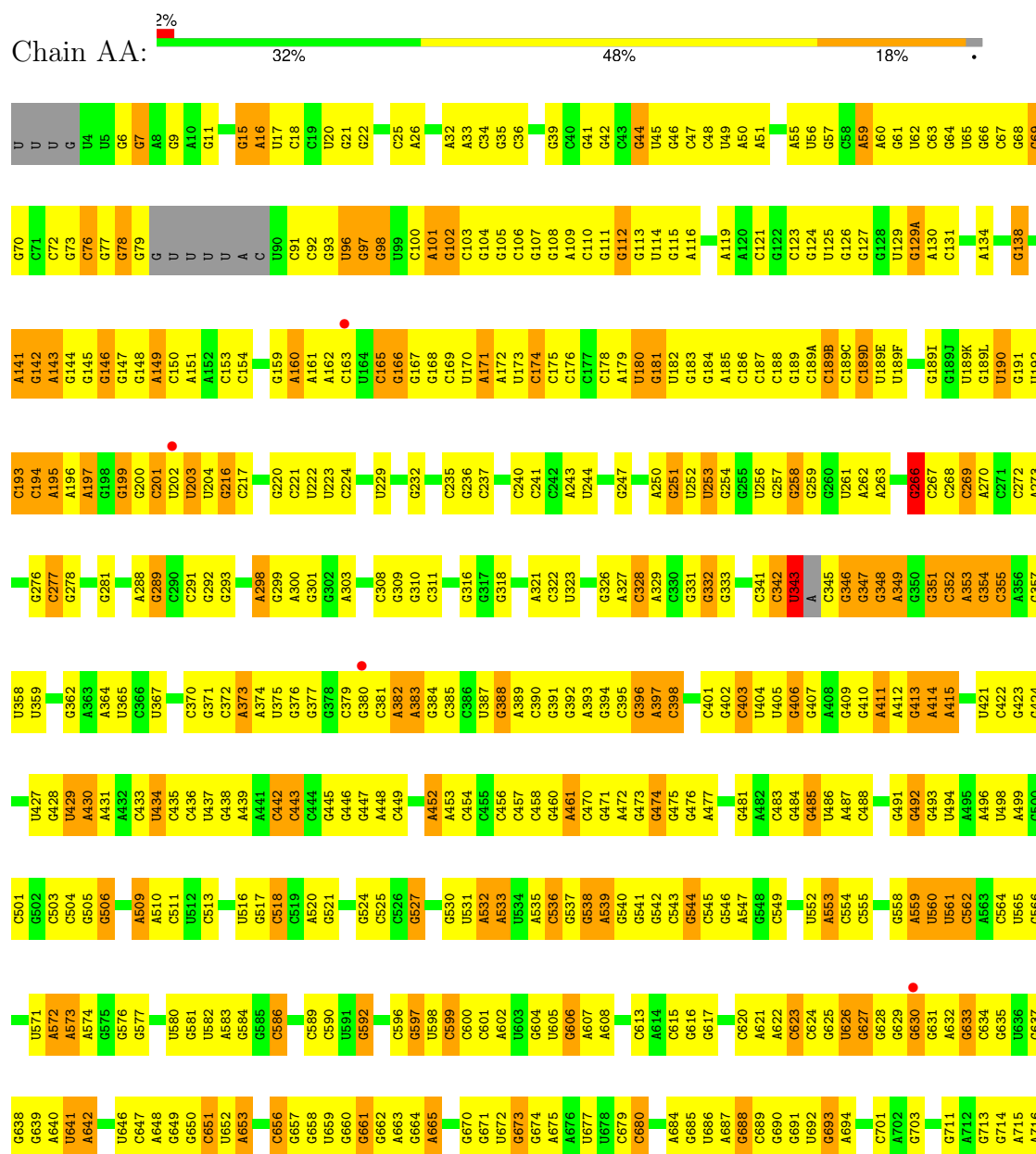
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	DA	906	Total 906	O 906	0	0
61	DB	7	Total 7	O 7	0	0
61	DD	10	Total 10	O 10	0	0
61	DE	11	Total 11	O 11	0	0
61	DF	4	Total 4	O 4	0	0
61	DO	1	Total 1	O 1	0	0
61	DP	14	Total 14	O 14	0	0
61	DQ	3	Total 3	O 3	0	0
61	DR	1	Total 1	O 1	0	0
61	DU	4	Total 4	O 4	0	0
61	DV	1	Total 1	O 1	0	0
61	DX	2	Total 2	O 2	0	0
61	DY	1	Total 1	O 1	0	0
61	D0	3	Total 3	O 3	0	0
61	D1	1	Total 1	O 1	0	0
61	D3	1	Total 1	O 1	0	0
61	D7	1	Total 1	O 1	0	0
61	D8	4	Total 4	O 4	0	0

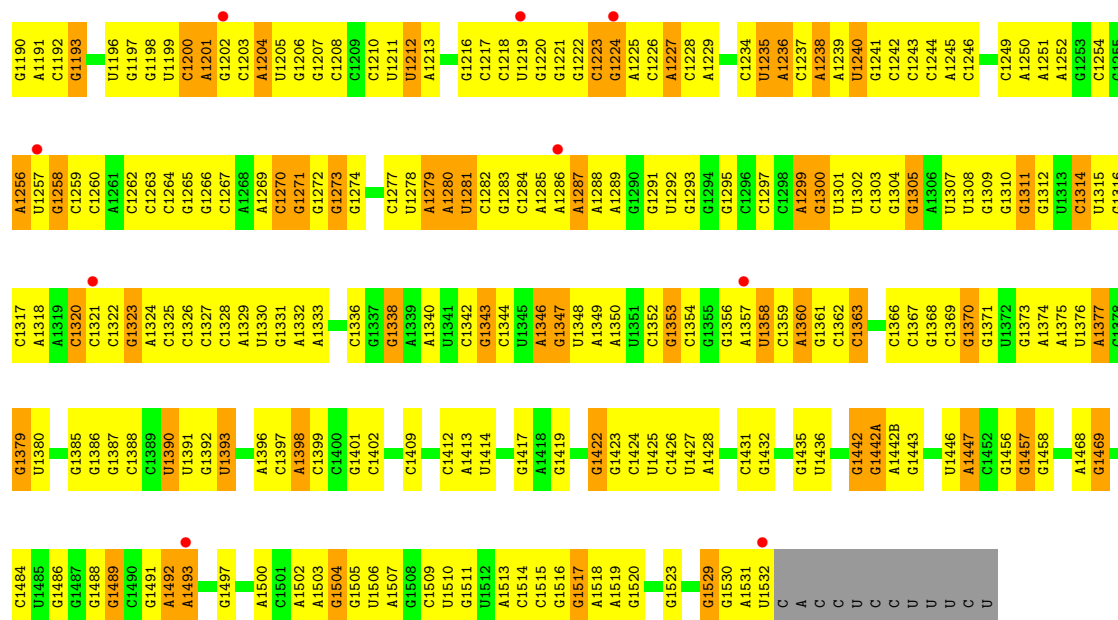
3 Residue-property plots

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.

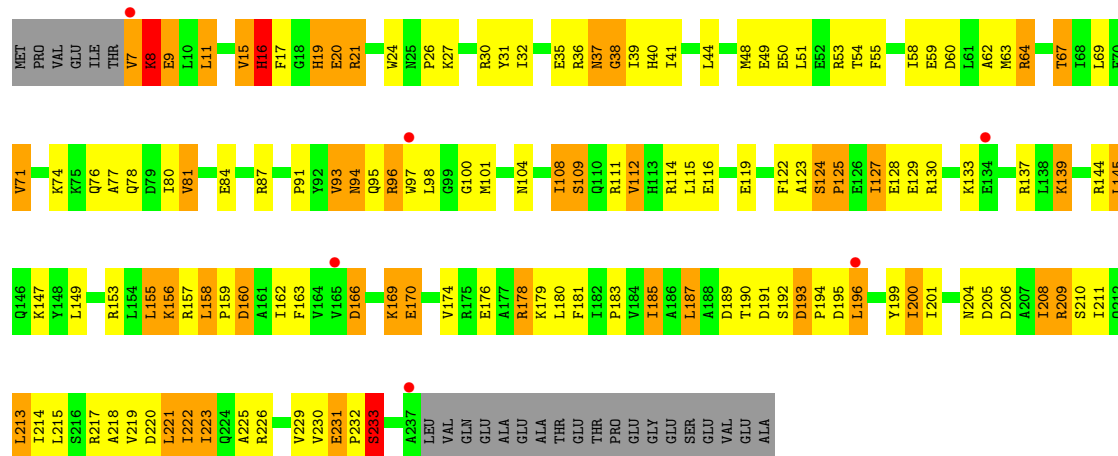
• Molecule 1: 16S Ribosomal RNA



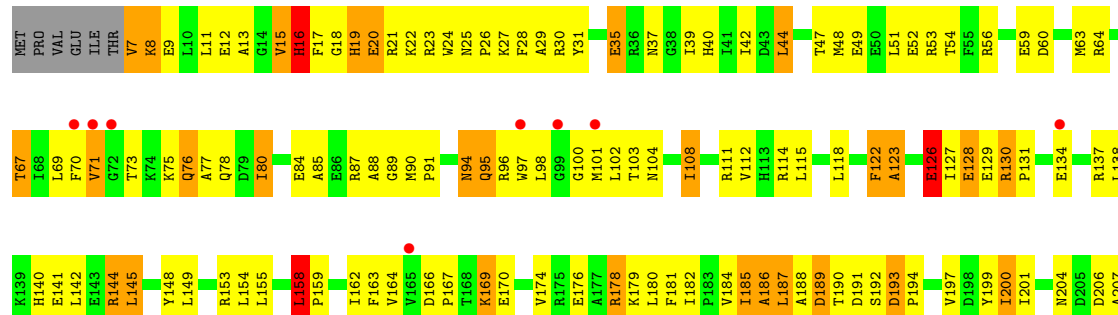
G1128	C1063	G1003	C936	G853	G772	A694	G625	C554	A477	G406	C245	U164	G78
C1129	G1064	A1004	A937	G854	G773	G700	U626	C555	C479	G407	A246	C165	G79
A1130	U1065	A1005	A938	C855	G774	G701	G627	C556	U480		G247	G166	G90
G1131	U1066	C1006	G939	C856			G628	C557					U
C1132	C1067	C1007	C940	C857	A777	A704	G629	C558	C484	G410	A250	C169	U
G1133	G1068	G1008	G941	G858	A778	G708	G630	C559	C485	A411	G251	U170	U84
G1134	G1069	G1009	G942	G859	A779	G709		U560	U486	A412	U252	A171	A88
U1135	G1010	G1010	G943	A860	C783	G710	G633	U561	U487	A413	U253	A172	C89
U1136	U1011	U1012	G944	G861	C784	G711		C562	C488	A414	G254	U173	C88
G1137	C1071	G1013	G947	C866	C785	A712	G639	A563	C489	A415	U255	C174	U90
G1138	G1072	G1014	C948	C867	C786	G713	U641	C564	C490		U256	C175	C91
G1139	U1073	A1015		C868	G714	G714	A642	U565	C491	C418	G257	G32	C92
C1140	C1074	A1016		C869	A715	A716	G643	C566	C492	C419	G258	G33	G93
C1141	C1075			G870	A716			C567	G495	U420		U178	U96
G1142	U1076	G1017	U952	U871	G792		U646	G568	A496	U421	G265	A179	U80
G1143	G1077	C1018	G953	U870	A791	C719	G647		A496	C422	G266	U180	G97
G1144	U1078	U1019	U955	A872	U793	G720	A648	U498	U498	G423	G267	G181	G98
G1145	U1079	U1020	U956	A873	A794	G721	G649	G500	A499	G424	C268	U182	
A1146	G1081	G1021	U957	G874	G795	U722	G650	C501	G500	G425	C269	C187	A101
G1147		G1022	A958	C875			G651	C502	G501	G426		C188	G102
U1148	U1084	G1023	A959	C876			G652	C503	G502	U427	G276	G189	A109
C1149	U1085	G1024	U960	C877	A802	G723	G653	C504	C503	U428	G277	C189A	C110
U1150	G1087	U1025	U961	C878	G803	G724	A654	C505	C504	U429	G278	C189B	G112
A1151	G1088	G1026		C879	U804	G727	G655	C506	C505	U430		C189C	G113
G1152	G1089	G1027		C880	C805	A728	A656	G506	G506	A431	G281	U189E	U114
C1153	U1090	C1028	A964	G881	C806	A729	C656				A282	U189F	
G1154	U1091	G1029	A965				G657	U582	A509	A432	G283		G115
G1155	C1030	C1030	C967	C885	C811	G730	U657	A583	A510	C433	G284	G189J	A116
G1156	U1093A	A1093	A968	C886	C812	C731	G658	C584	C511	U434	G285	U189K	G117
A1157	C1030B	G890	A969	C887	U813	C732	U659	C585	U512	C435	G286	U189L	
U1095	G1030C	C890	C970	C888	U814	G733	G661	C586	C513	U437	G289	C190	C121
C1096	A1030D	A900	G971	A900	A815	C735	G662	C589	C518	U438	G291	G191	G122
C1097	G1031	A901	C972	A901	A816	C736	A663	C590	C519	U439	G292	U192	C123
	G1032	G902	G973	G902	C817	A737	G664	C591	C520	A441	G293	C193	G127
G1163	G1033	G1033	A974		C818	C738	A665	C592	C442	C443	G297	C194	
G1164	A1035	A1035	G975	G906	A819	C739	G666	C596	C443	C444	G298	A196	G129A
G1165	G1036	G1036	A977	A909	U820	U740	G667	C597	C522	C445	G299	A197	A130
G1166	C1037	C1037	A978	C910	G821	G741		C597	C527	G446	G300	G198	C131
G1167	C1038	C1038	C979	C910	C826	G742	G671	U598	C528	G447	G301	G199	C137
A1169	U1039	A918	C980	A913	U827	C745	U672	C599			G302	C201	G139
A1170	C1107	A914	U981	A914	A828	C745	G673	C600	U531	C448	U304	G202	G142
G1171	G1108	A915	U982	A915	G829	C749	G674	C601	A532	C449	G305	U203	A143
C1172	A1110	G916	A983	G916	G830		A675	C602	A533	A451		U204	A144
G1173	A1111	C917	C984	G917	U831	G752	U677	U605		A452	C308	G216	G147
G1174	C1112	C1043	C985	G918	C832	A753	U678	G606	C536	A453	G309	C217	G148
			A986	A918	U833	C754	C679	A607	C537	C454	G310		C150
C1115	C1116	G1048		A919	U834	G755	C680	A608	C538	C455	G311	G220	A149
G1117	G1117	G1050	U991	U921	U835	C756	G683	A609	A539	C456	G312	C221	G149
G1118	C1118	C1051	U992	G922	G836	U757	A684	G610	C540	C457	G316	U222	A152
A1179	C1119	U1052	G993	A923	G837	G758	G685		C542	C458	A321	U223	C153
G1180	C1120	G1053	A994	G926	G838	A759	U686	C543	C543	A461	G398	G226	C154
G1181	U1121	C1084	C995	G927	U839	G760	A687	C544	C544	C470	G399	G227	
G1182	U1121	C1084			C840	A687	U619	C545	C545	A472	C400		A160
A1183	U1122	U1055	G998	C931	U841	A766	C689	C546	C546	A472	A327	C235	A161
G1184	A1056	U1056	C999	C932	C848	A767	G690	A547			C328		A162
	G1057	G1057	U1000	G933	C849	A768	G691	U552			C329	A243	C163
G1187	G1058	G1058	A1001	G934	U850	A769	U692	C623			A329	U244	
A1188	C934	C934	G1001A	C851	C770	G769	G692	C624			G402		
C1189	G1061	G1061	G1002	G852	G771		G693				U404		

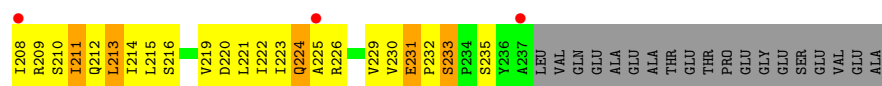


• Molecule 2: 30S Ribosomal Protein S2

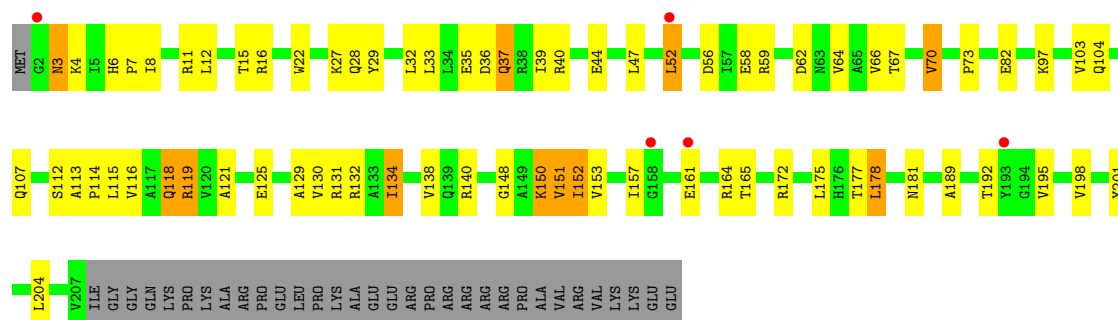


• Molecule 2: 30S Ribosomal Protein S2

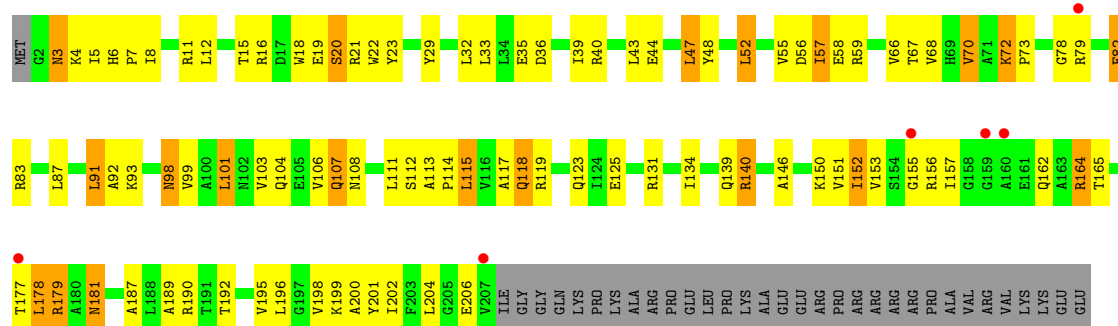




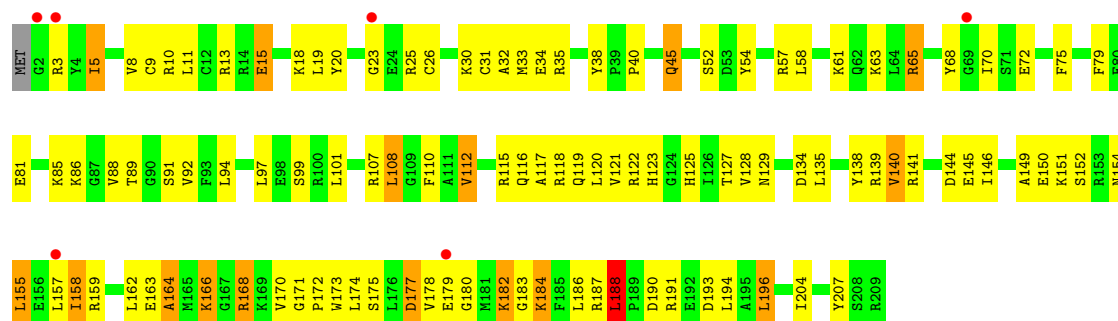
• Molecule 3: 30S Ribosomal Protein S3



• Molecule 3: 30S Ribosomal Protein S3

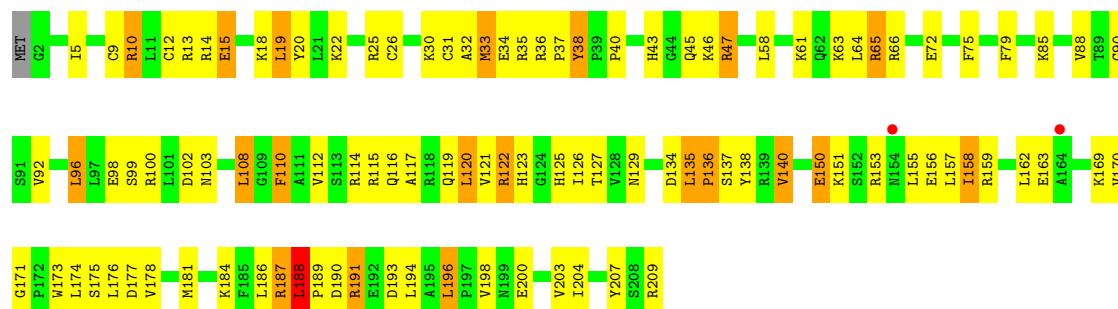


• Molecule 4: 30S Ribosomal Protein S4



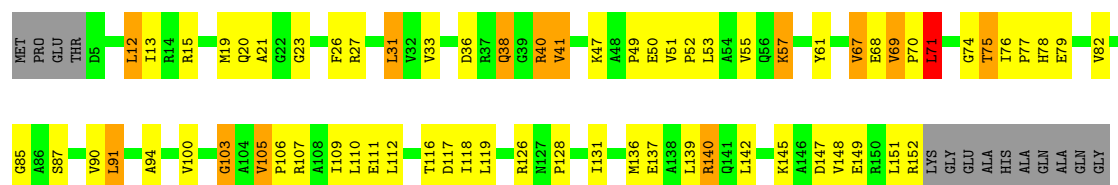
• Molecule 4: 30S Ribosomal Protein S4





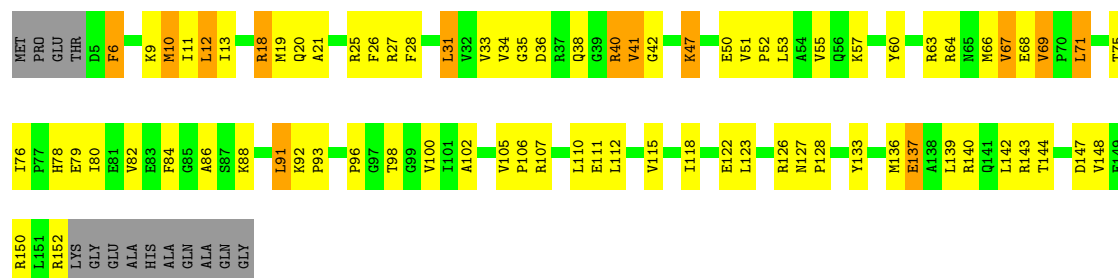
• Molecule 5: 30S Ribosomal Protein S5

Chain AE:

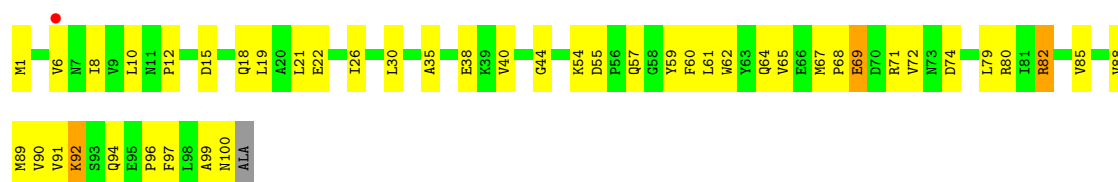


• Molecule 5: 30S Ribosomal Protein S5

Chain CE:



• Molecule 6: 30S Ribosomal Protein S6

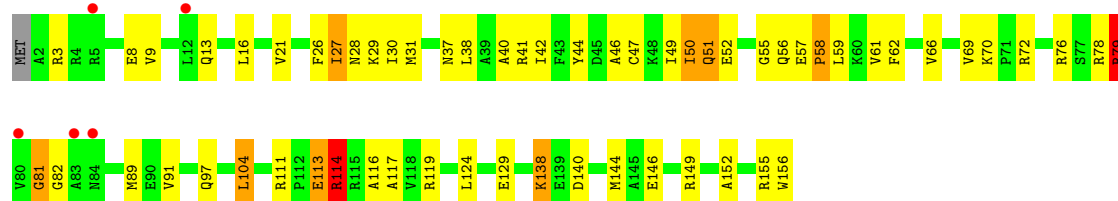


• Molecule 6: 30S Ribosomal Protein S6

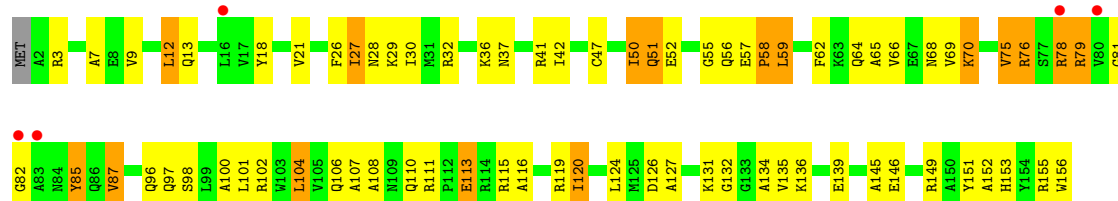
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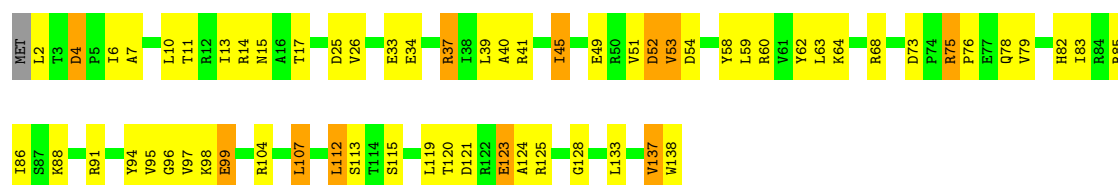
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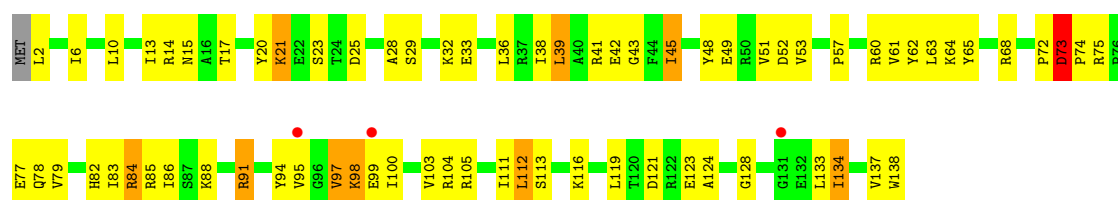
• Molecule 7: 30S Ribosomal Protein S7



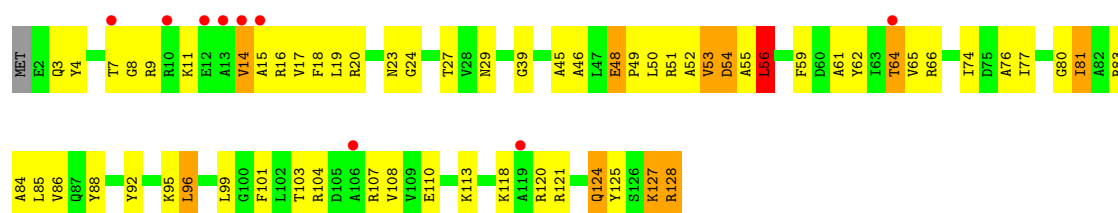
• Molecule 8: 30S Ribosomal Protein S8



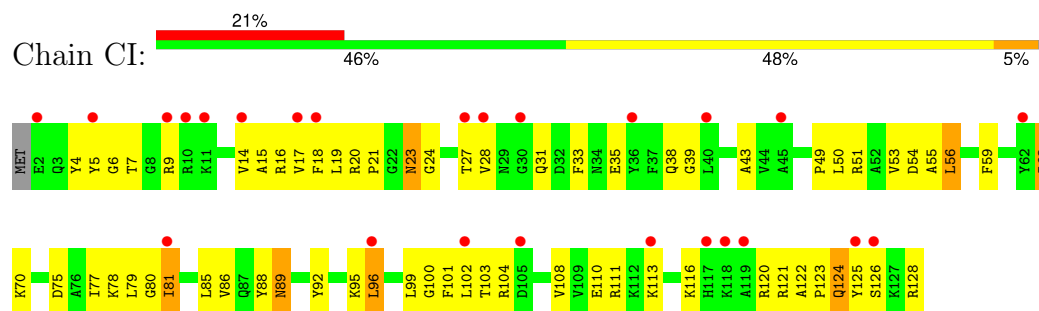
• Molecule 8: 30S Ribosomal Protein S8



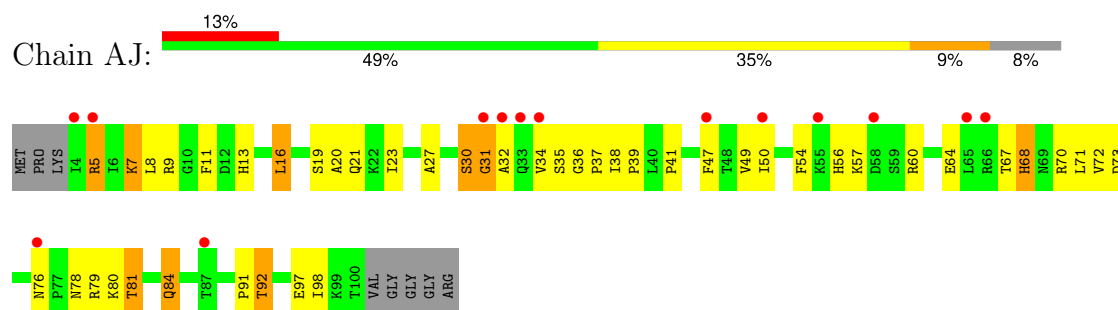
• Molecule 9: 30S Ribosomal Protein S9



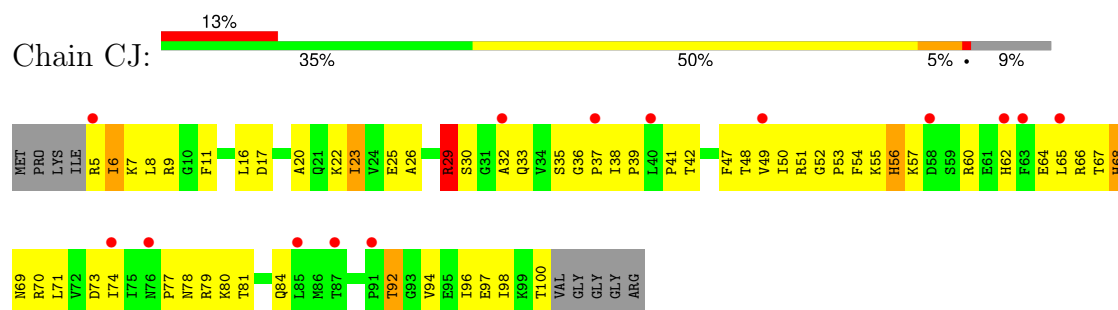
• Molecule 9: 30S Ribosomal Protein S9



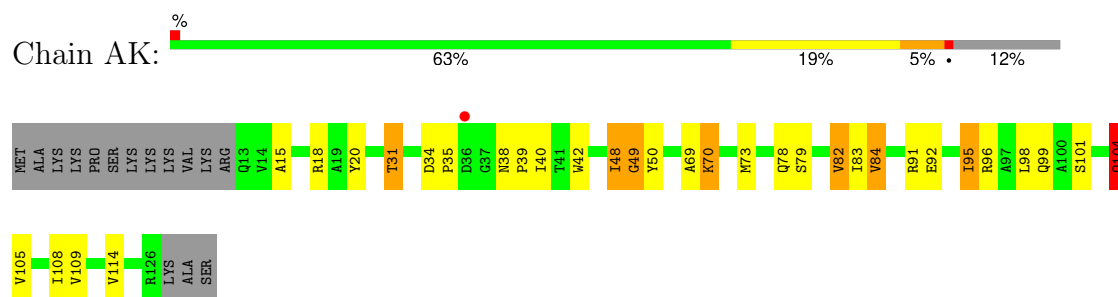
• Molecule 10: 30S Ribosomal Protein S10



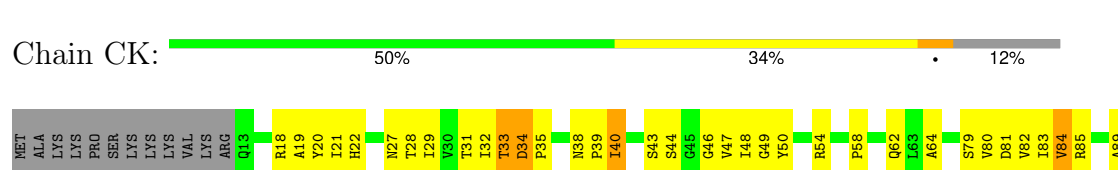
• Molecule 10: 30S Ribosomal Protein S10



• Molecule 11: 30S Ribosomal Protein S11

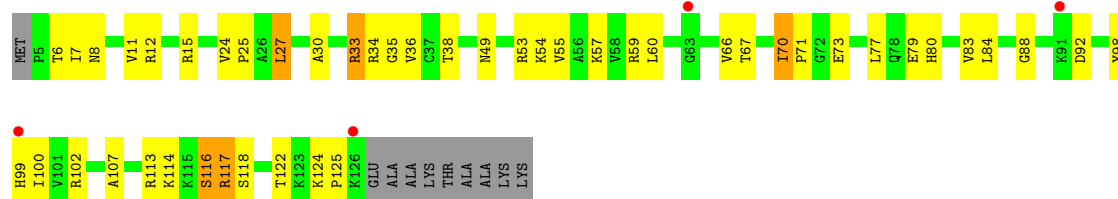


• Molecule 11: 30S Ribosomal Protein S11

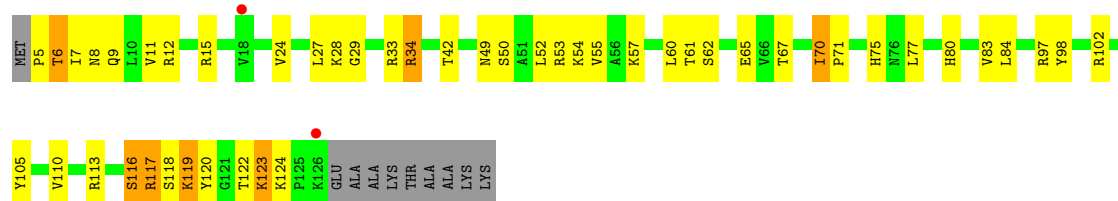




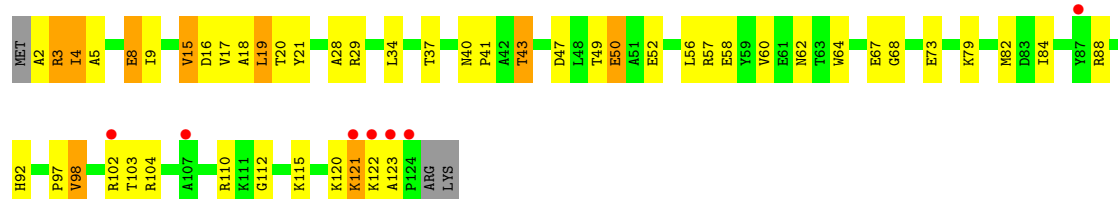
• Molecule 12: 30S Ribosomal Protein S12



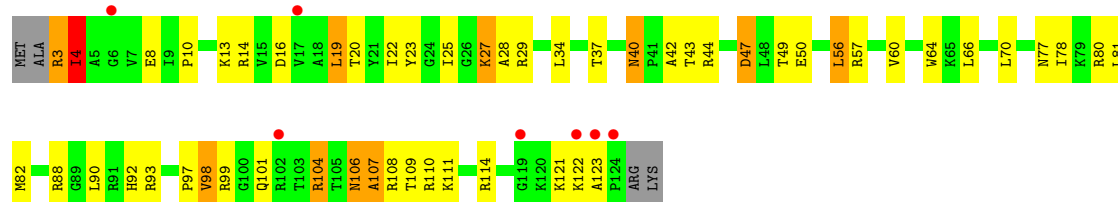
• Molecule 12: 30S Ribosomal Protein S12



• Molecule 13: 30S Ribosomal Protein S13



• Molecule 13: 30S Ribosomal Protein S13

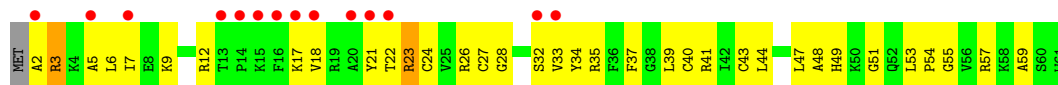
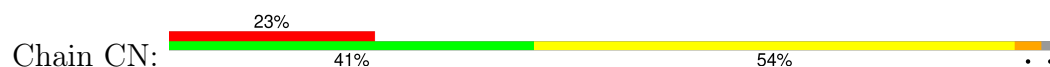


• Molecule 14: 30S Ribosomal Protein S14

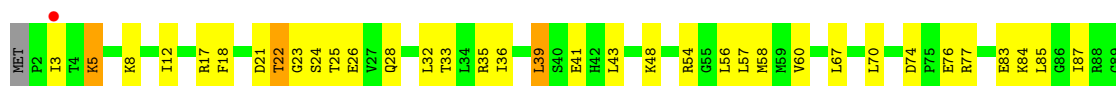




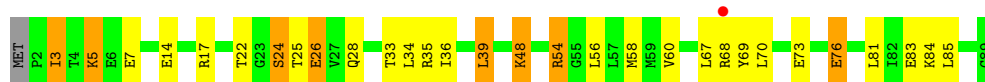
● Molecule 14: 30S Ribosomal Protein S14



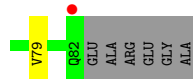
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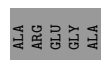
● Molecule 15: 30S Ribosomal Protein S15



● Molecule 16: 30S Ribosomal Protein S16



● Molecule 16: 30S Ribosomal Protein S16

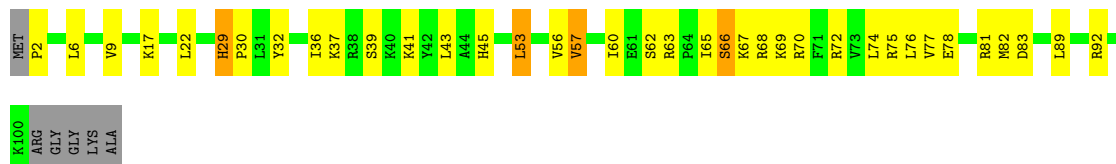


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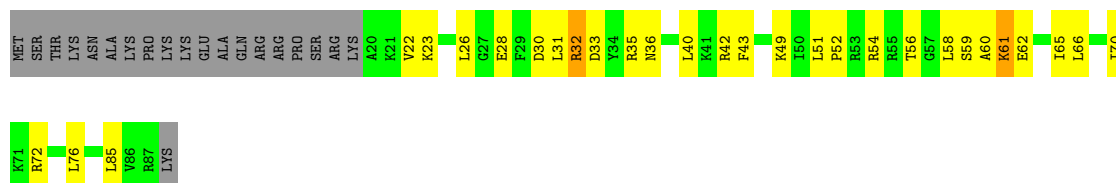




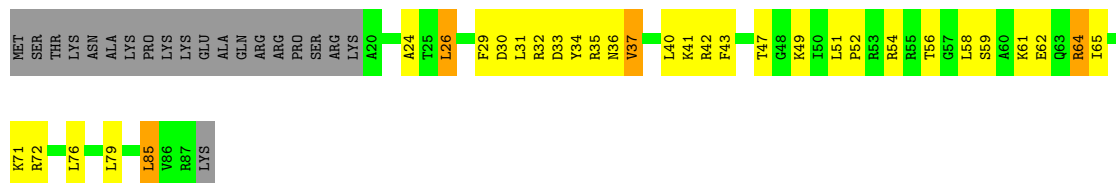
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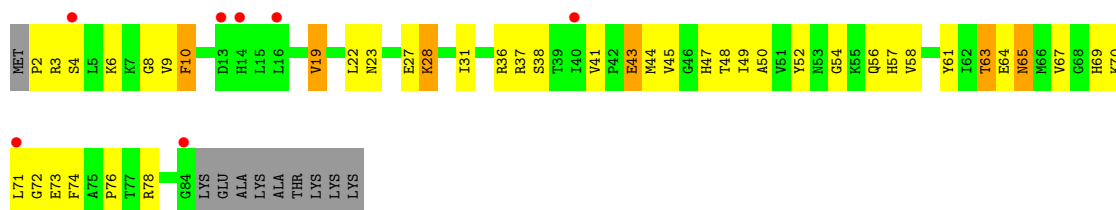
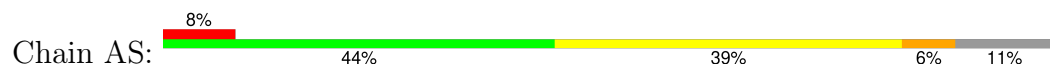
• Molecule 18: 30S Ribosomal Protein S18



• Molecule 18: 30S Ribosomal Protein S18

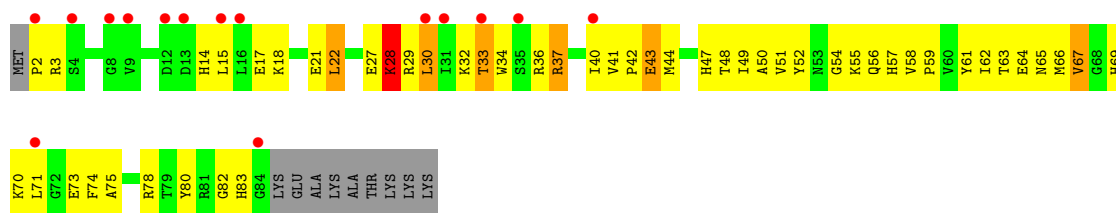


• Molecule 19: 30S Ribosomal Protein S19

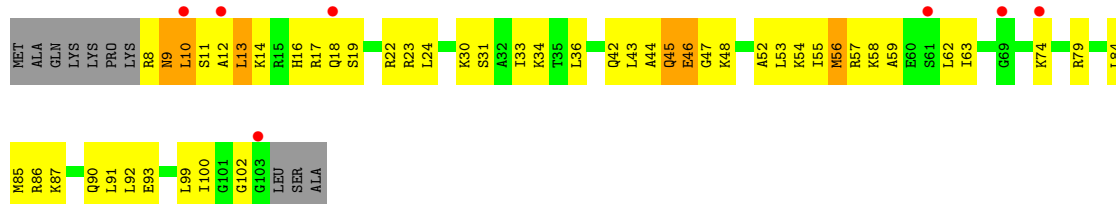


• Molecule 19: 30S Ribosomal Protein S19

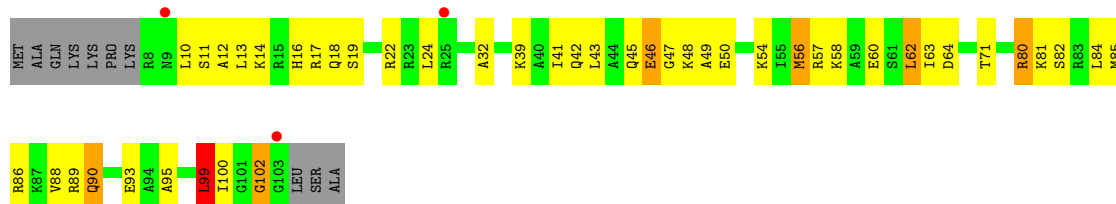




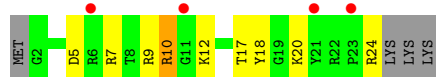
● Molecule 20: 30S Ribosomal Protein S20



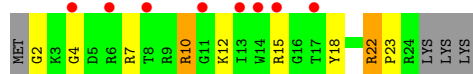
● Molecule 20: 30S Ribosomal Protein S20



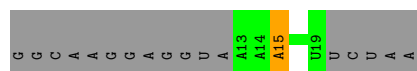
● Molecule 21: 30S Ribosomal Protein THX



● Molecule 21: 30S Ribosomal Protein THX



● Molecule 22: mRNA



- Molecule 22: mRNA

Chain CV: 

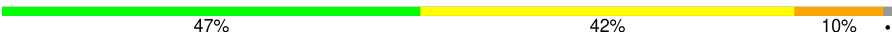


- Molecule 23: P-site tRNA

Chain AX: 



- Molecule 23: P-site tRNA

Chain CX: 



- Molecule 24: Dityromycin

Chain AW: 



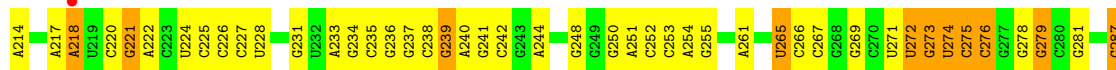
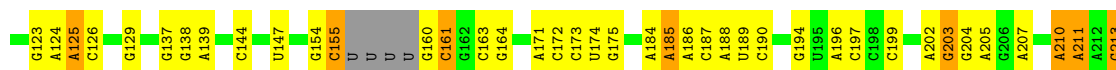
- Molecule 24: Dityromycin

Chain CW: 



- Molecule 25: 23S Ribosomal RNA

Chain BA: 

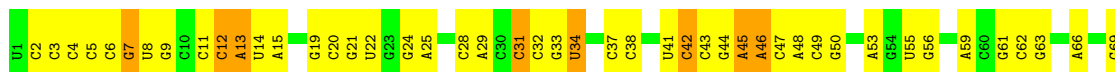




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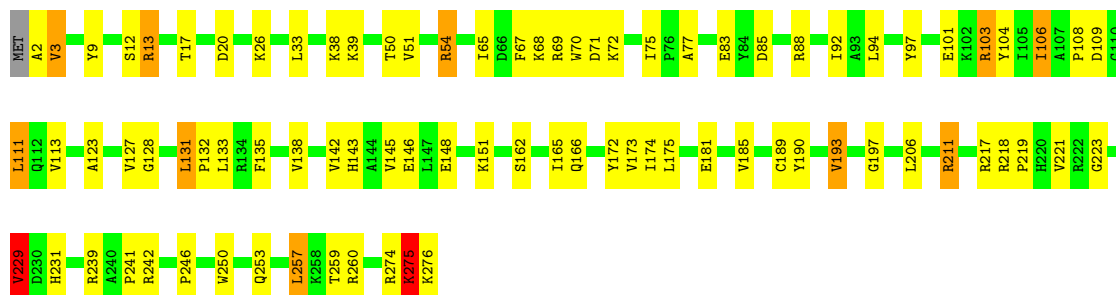






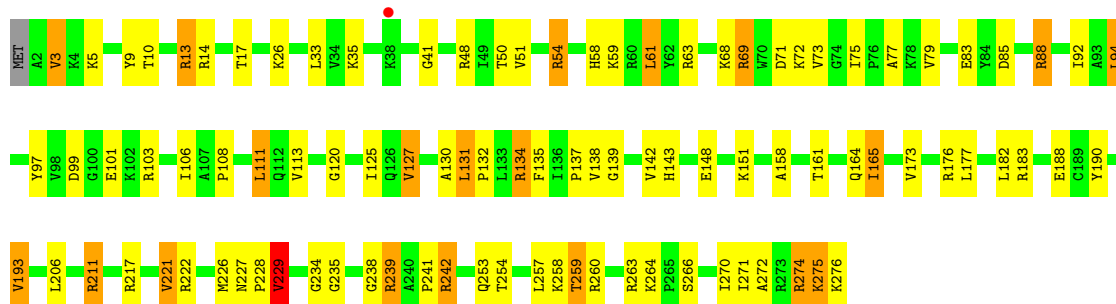
• Molecule 27: 50S Ribosomal Protein L2

Chain BD: 69% 26%



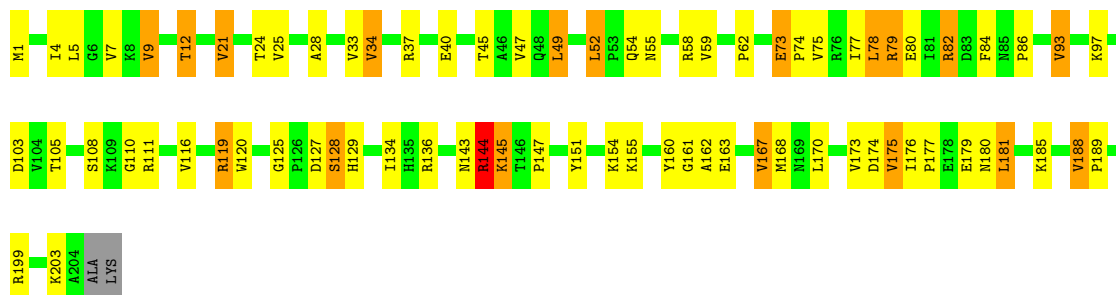
• Molecule 27: 50S Ribosomal Protein L2

Chain DD: 64% 28% 7%



• Molecule 28: 50S Ribosomal Protein L3

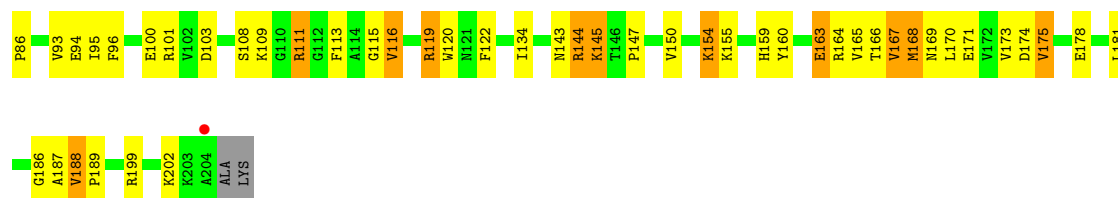
Chain BE: 62% 28% 9%



• Molecule 28: 50S Ribosomal Protein L3

Chain DE: 57% 33% 8%

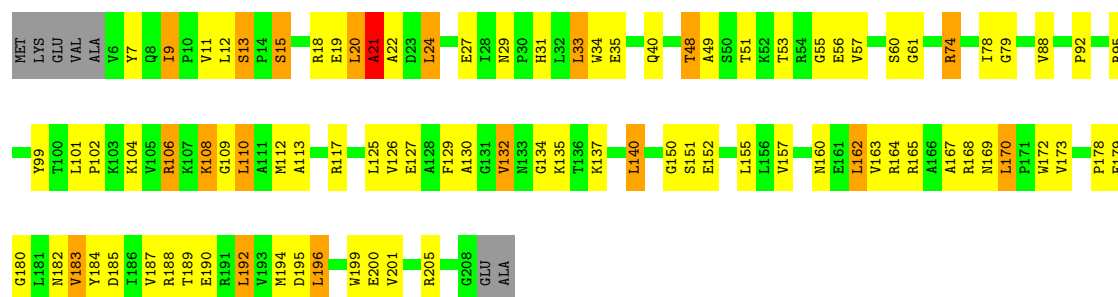




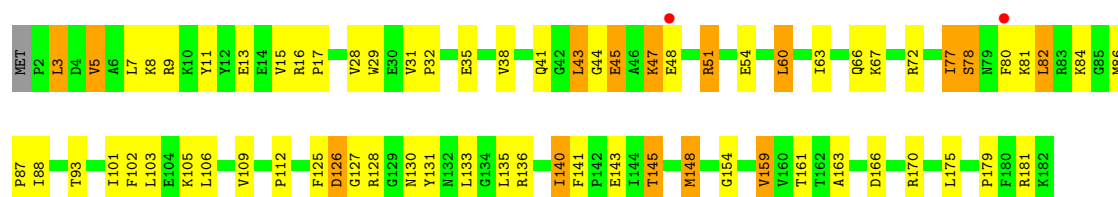
• Molecule 29: 50S Ribosomal Protein L4



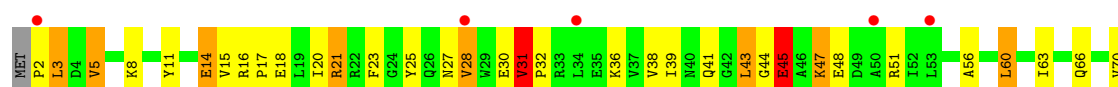
• Molecule 29: 50S Ribosomal Protein L4

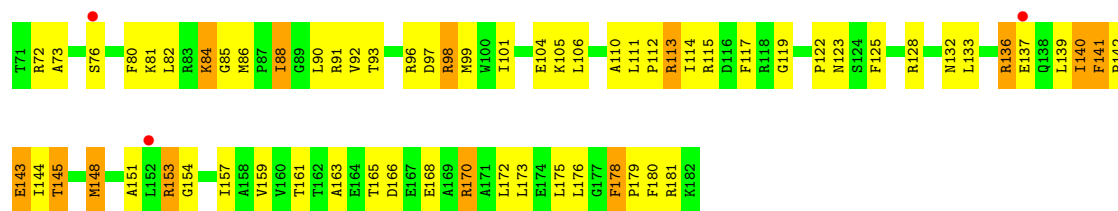


• Molecule 30: 50S Ribosomal Protein L5

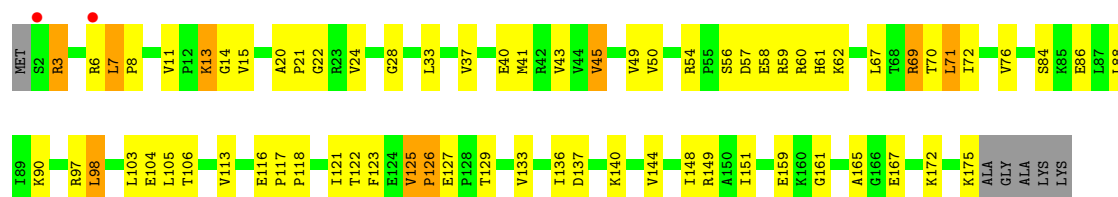


• Molecule 30: 50S Ribosomal Protein L5

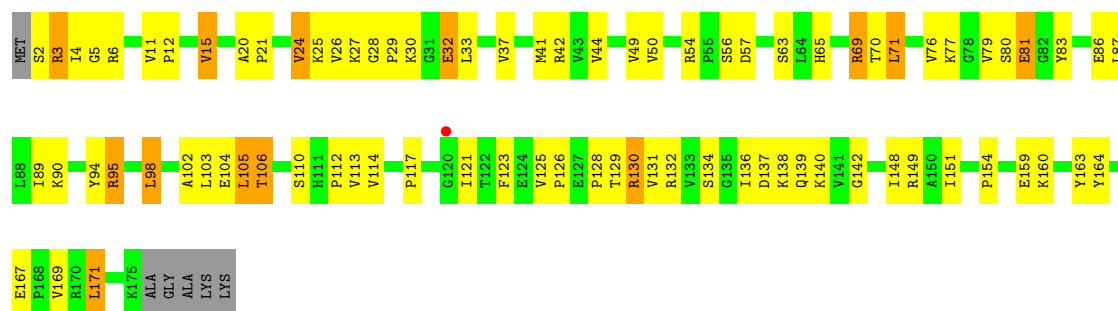




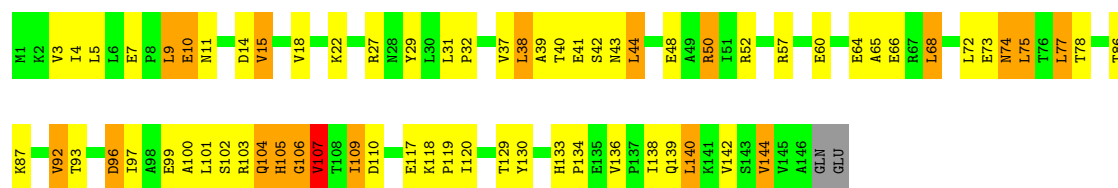
● Molecule 31: 50S Ribosomal Protein L6



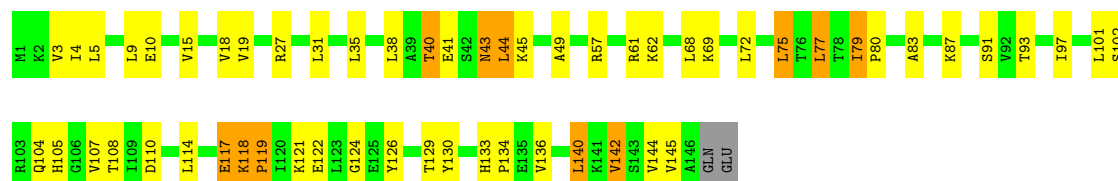
● Molecule 31: 50S Ribosomal Protein L6



● Molecule 32: 50S Ribosomal Protein L9

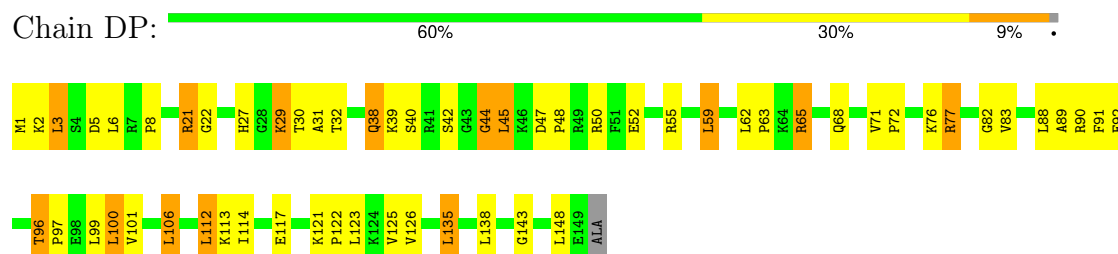


● Molecule 32: 50S Ribosomal Protein L9

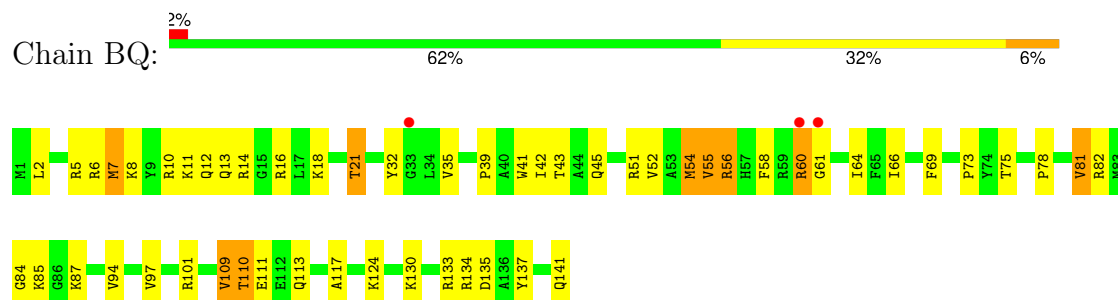


L106	M1	L117	R15	L121	K29	L135	R30	L148	L62	Q68	L82	V95	L100	L110	L126	L136	L144	L154	L164	L174	L184	L194	L204	L214	L224	L234	L244	L254	L264	L274	L284	L294	L304	L314	L324	L334	L344	L354	L364	L374	L384	L394	L404	L414	L424	L434	L444	L454	L464	L474	L484	L494	L504	L514	L524	L534	L544	L554	L564	L574	L584	L594	L604	L614	L624	L634	L644	L654	L664	L674	L684	L694	L704	L714	L724	L734	L744	L754	L764	L774	L784	L794	L804	L814	L824	L834	L844	L854	L864	L874	L884	L894	L904	L914	L924	L934	L944	L954	L964	L974	L984	L994	L1004	L1014	L1024	L1034	L1044	L1054	L1064	L1074	L1084	L1094	L1104	L1114	L1124	L1134	L1144	L1154	L1164	L1174	L1184	L1194	L1204	L1214	L1224	L1234	L1244	L1254	L1264	L1274	L1284	L1294	L1304	L1314	L1324	L1334	L1344	L1354	L1364	L1374	L1384	L1394	L1404	L1414	L1424	L1434	L1444	L1454	L1464	L1474	L1484	L1494	L1504	L1514	L1524	L1534	L1544	L1554	L1564	L1574	L1584	L1594	L1604	L1614	L1624	L1634	L1644	L1654	L1664	L1674	L1684	L1694	L1704	L1714	L1724	L1734	L1744	L1754	L1764	L1774	L1784	L1794	L1804	L1814	L1824	L1834	L1844	L1854	L1864	L1874	L1884	L1894	L1904	L1914	L1924	L1934	L1944	L1954	L1964	L1974	L1984	L1994	L2004	L2014	L2024	L2034	L2044	L2054	L2064	L2074	L2084	L2094	L2104	L2114	L2124	L2134	L2144	L2154	L2164	L2174	L2184	L2194	L2204	L2214	L2224	L2234	L2244	L2254	L2264	L2274	L2284	L2294	L2304	L2314	L2324	L2334	L2344	L2354	L2364	L2374	L2384	L2394	L2404	L2414	L2424	L2434	L2444	L2454	L2464	L2474	L2484	L2494	L2504	L2514	L2524	L2534	L2544	L2554	L2564	L2574	L2584	L2594	L2604	L2614	L2624	L2634	L2644	L2654	L2664	L2674	L2684	L2694	L2704	L2714	L2724	L2734	L2744	L2754	L2764	L2774	L2784	L2794	L2804	L2814	L2824	L2834	L2844	L2854	L2864	L2874	L2884	L2894	L2904	L2914	L2924	L2934	L2944	L2954	L2964	L2974	L2984	L2994	L3004	L3014	L3024	L3034	L3044	L3054	L3064	L3074	L3084	L3094	L3104	L3114	L3124	L3134	L3144	L3154	L3164	L3174	L3184	L3194	L3204	L3214	L3224	L3234	L3244	L3254	L3264	L3274	L3284	L3294	L3304	L3314	L3324	L3334	L3344	L3354	L3364	L3374	L3384	L3394	L3404	L3414	L3424	L3434	L3444	L3454	L3464	L3474	L3484	L3494	L3504	L3514	L3524	L3534	L3544	L3554	L3564	L3574	L3584	L3594	L3604	L3614	L3624	L3634	L3644	L3654	L3664	L3674	L3684	L3694	L3704	L3714	L3724	L3734	L3744	L3754	L3764	L3774	L3784	L3794	L3804	L3814	L3824	L3834	L3844	L3854	L3864	L3874	L3884	L3894	L3904	L3914	L3924	L3934	L3944	L3954	L3964	L3974	L3984	L3994	L4004	L4014	L4024	L4034	L4044	L4054	L4064	L4074	L4084	L4094	L4104	L4114	L4124	L4134	L4144	L4154	L4164	L4174	L4184	L4194	L4204	L4214	L4224	L4234	L4244	L4254	L4264	L4274	L4284	L4294	L4304	L4314	L4324	L4334	L4344	L4354	L4364	L4374	L4384	L4394	L4404	L4414	L4424	L4434	L4444	L4454	L4464	L4474	L4484	L4494	L4504	L4514	L4524	L4534	L4544	L4554	L4564	L4574	L4584	L4594	L4604	L4614	L4624	L46
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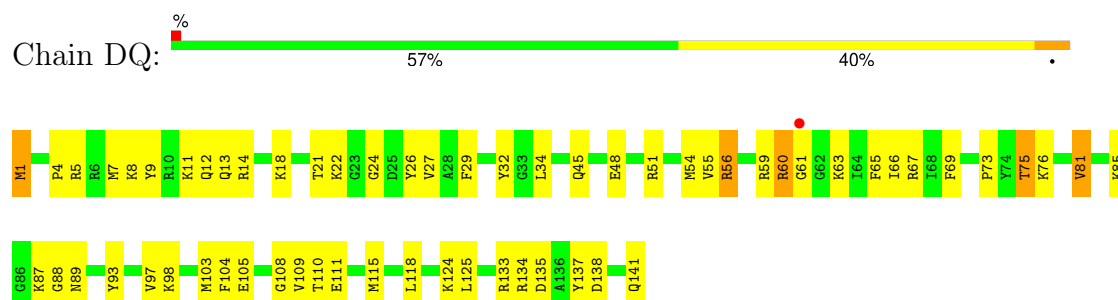
- Molecule 35: 50S Ribosomal Protein L15



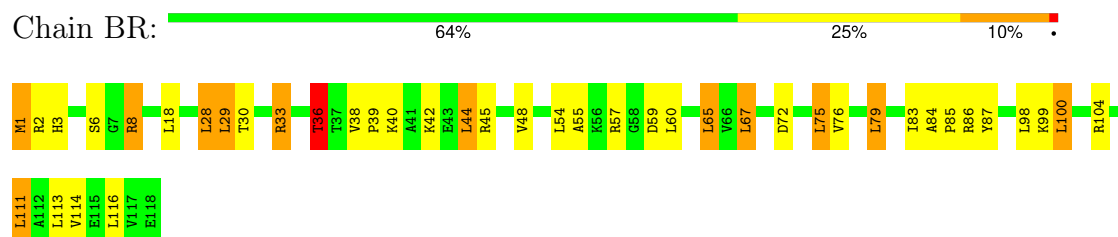
- Molecule 36: 50S Ribosomal Protein L16



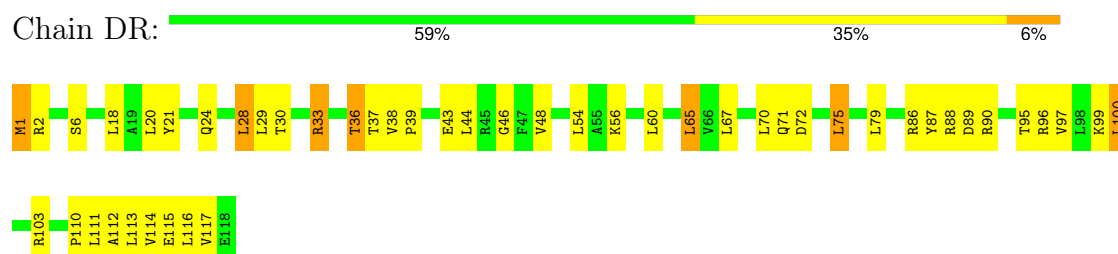
- Molecule 36: 50S Ribosomal Protein L16



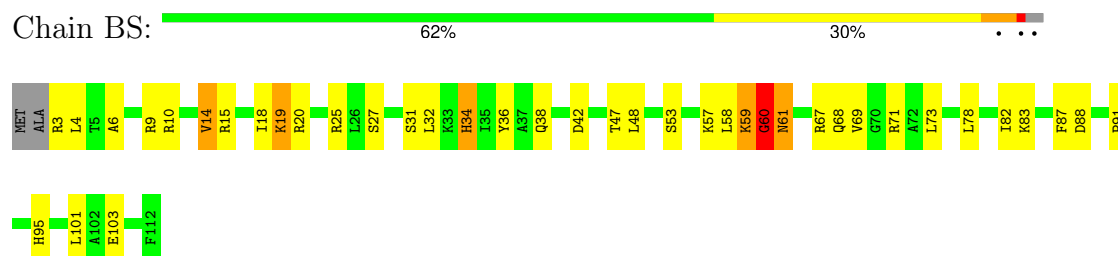
- Molecule 37: 50S Ribosomal Protein L17



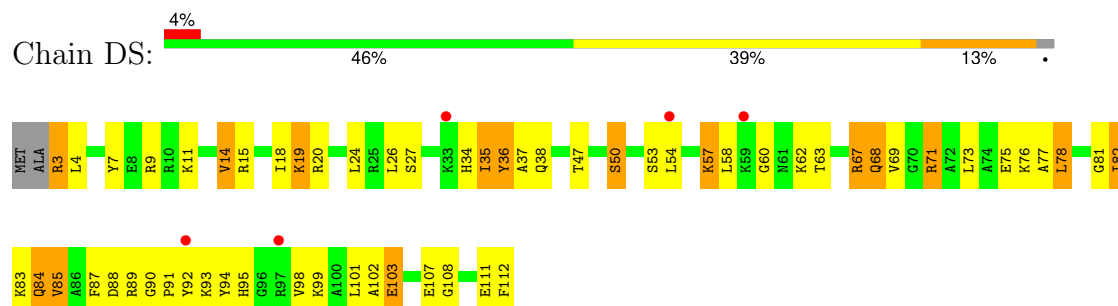
- Molecule 37: 50S Ribosomal Protein L17



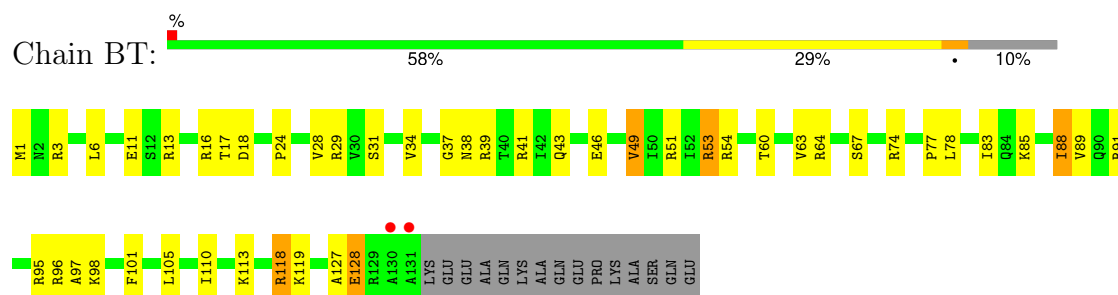
- Molecule 38: 50S Ribosomal Protein L18



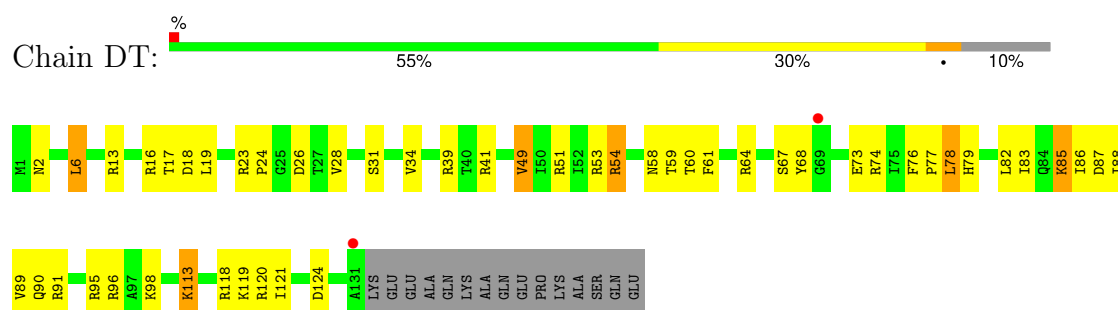
- Molecule 38: 50S Ribosomal Protein L18



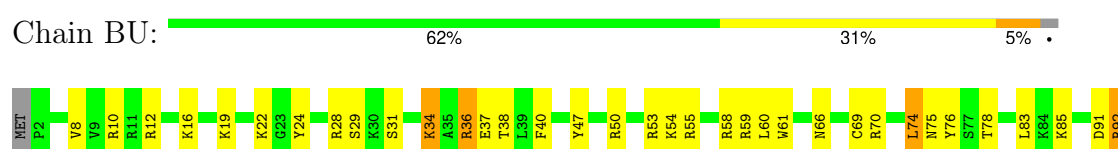
- Molecule 39: 50S Ribosomal Protein L19



- Molecule 39: 50S Ribosomal Protein L19



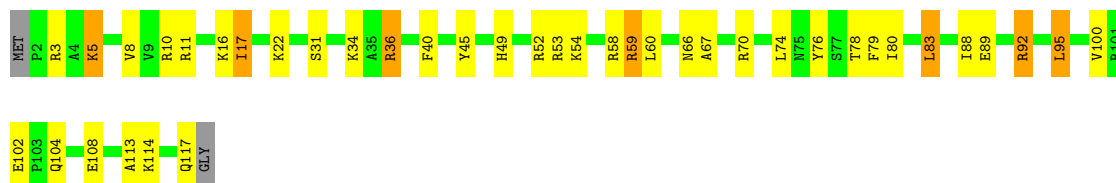
- Molecule 40: 50S Ribosomal Protein L20





• Molecule 40: 50S Ribosomal Protein L20

Chain DU: 64% 28% 6% •



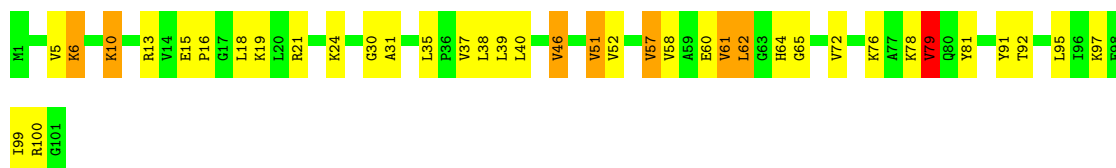
• Molecule 41: 50S Ribosomal Protein L21

Chain BV: 72% 21% 6% •



• Molecule 41: 50S Ribosomal Protein L21

Chain DV: 62% 30% 7% •



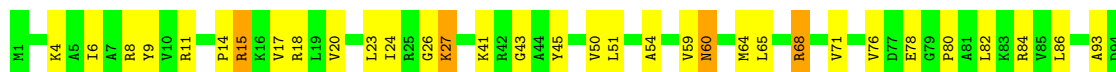
• Molecule 42: 50S Ribosomal Protein L22

Chain BW: % 74% 19% 6% •



• Molecule 42: 50S Ribosomal Protein L22

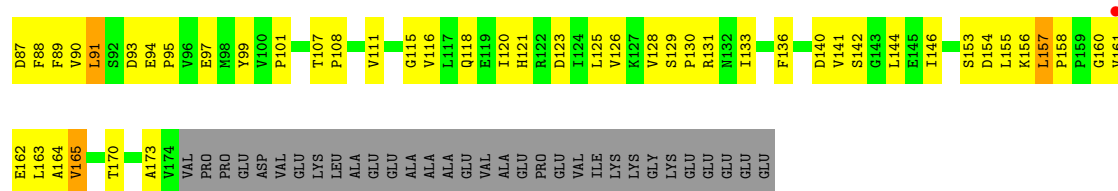
Chain DW: 63% 31% 5% •



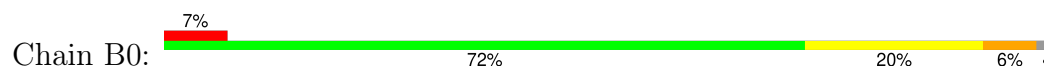
• Molecule 43: 50S Ribosomal Protein L23

Chain BX: % 71% 26% ••

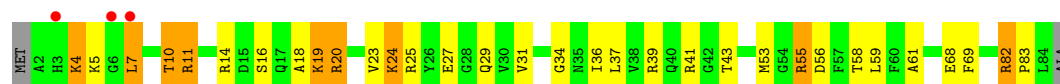




- Molecule 46: 50S Ribosomal Protein L27



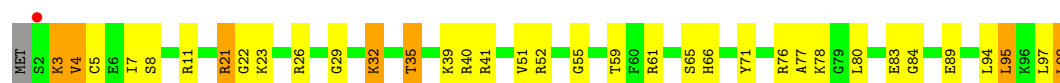
- Molecule 46: 50S Ribosomal Protein L27



- Molecule 47: 50S Ribosomal Protein L28



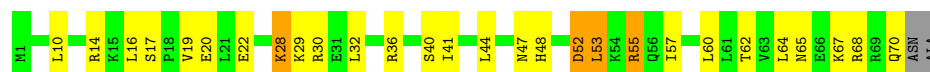
- Molecule 47: 50S Ribosomal Protein L28



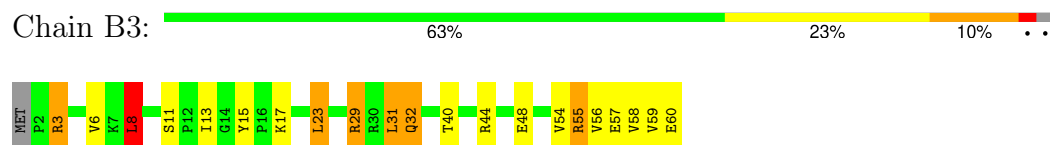
- Molecule 48: 50S Ribosomal Protein L29



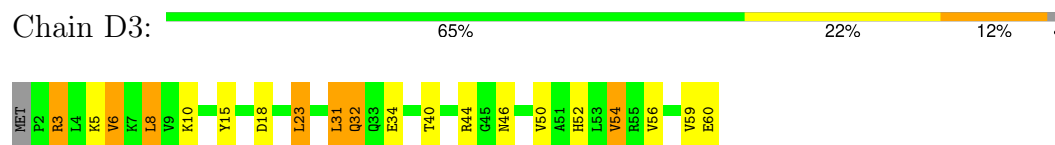
- Molecule 48: 50S Ribosomal Protein L29



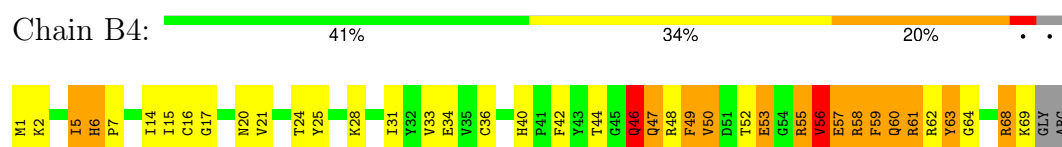
- Molecule 49: 50S Ribosomal Protein L30



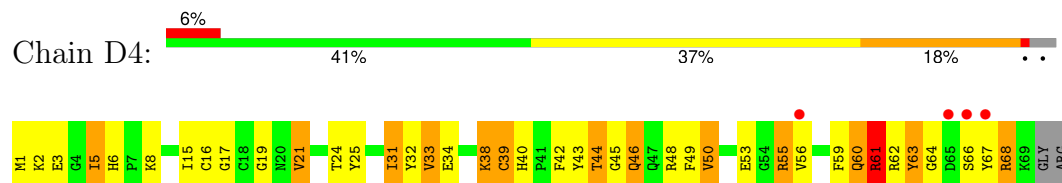
- Molecule 49: 50S Ribosomal Protein L30



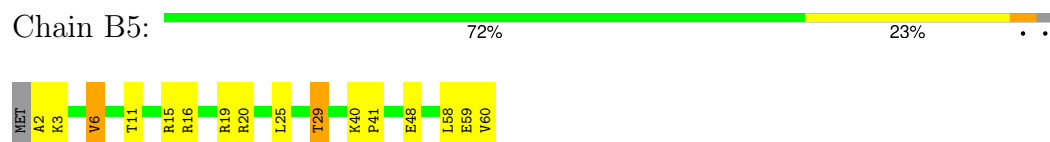
- Molecule 50: 50S Ribosomal Protein L31



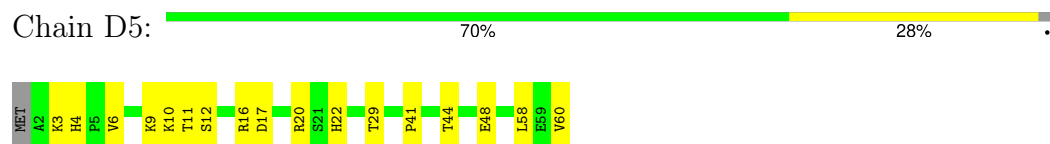
- Molecule 50: 50S Ribosomal Protein L31



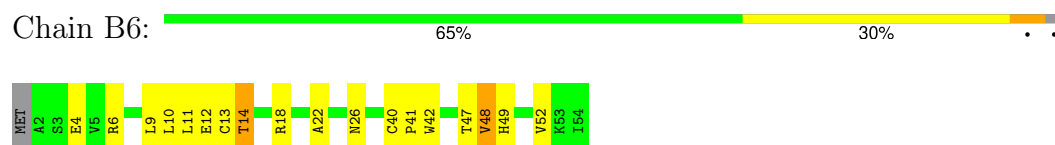
- Molecule 51: 50S Ribosomal Protein L32



- Molecule 51: 50S Ribosomal Protein L32

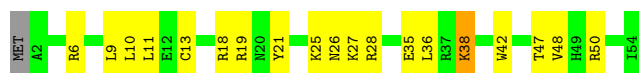


- Molecule 52: 50S Ribosomal Protein L33



- Molecule 52: 50S Ribosomal Protein L33





- Molecule 53: 50S Ribosomal Protein L34



- Molecule 53: 50S Ribosomal Protein L34



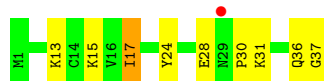
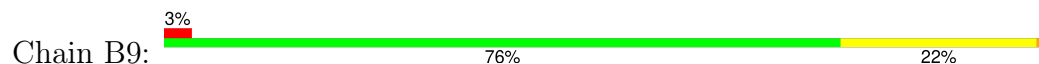
- Molecule 54: 50S Ribosomal Protein L35



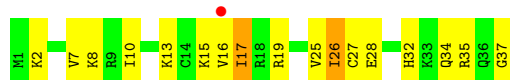
- Molecule 54: 50S Ribosomal Protein L35



- 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	210.08Å 449.83Å 619.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.74 – 3.00 49.74 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.74-3.00) 98.8 (49.74-3.00)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.24	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.203 , 0.259 0.203 , 0.257	Depositor DCC
R_{free} test set	57319 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	66.8	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	286321	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% 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: FME, 2R1, MVA, ZN, 004, 2QY, SF4, K, 2R3, 2QZ, MG

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	0.42	1/36038 (0.0%)	0.66	6/56244 (0.0%)
1	CA	0.41	0/36170	0.65	12/56452 (0.0%)
2	AB	0.61	0/1881	1.21	23/2542 (0.9%)
2	CB	0.70	0/1860	1.20	17/2518 (0.7%)
3	AC	0.62	0/1576	1.02	1/2130 (0.0%)
3	CC	0.64	0/1566	1.10	6/2119 (0.3%)
4	AD	0.63	0/1689	1.13	5/2267 (0.2%)
4	CD	0.63	0/1704	1.07	8/2284 (0.4%)
5	AE	0.62	0/1145	1.11	9/1543 (0.6%)
5	CE	0.66	0/1149	1.21	9/1548 (0.6%)
6	AF	0.61	0/819	0.97	1/1111 (0.1%)
6	CF	0.68	0/829	1.03	1/1123 (0.1%)
7	AG	0.59	0/1250	1.02	4/1679 (0.2%)
7	CG	0.60	0/1254	1.16	7/1683 (0.4%)
8	AH	0.60	0/1108	1.06	2/1494 (0.1%)
8	CH	0.56	0/1108	1.11	3/1494 (0.2%)
9	AI	0.61	0/1002	1.06	2/1346 (0.1%)
9	CI	0.72	0/997	1.09	3/1343 (0.2%)
10	AJ	0.71	0/722	1.12	3/982 (0.3%)
10	CJ	0.72	0/727	1.10	3/988 (0.3%)
11	AK	0.57	0/844	1.05	7/1145 (0.6%)
11	CK	0.58	0/848	1.01	4/1149 (0.3%)
12	AL	0.63	0/946	1.13	2/1274 (0.2%)
12	CL	0.64	0/946	1.03	1/1274 (0.1%)
13	AM	0.61	0/969	1.08	3/1302 (0.2%)
13	CM	0.64	0/961	1.07	4/1291 (0.3%)
14	AN	0.54	0/501	1.05	2/664 (0.3%)
14	CN	0.62	0/501	1.06	1/664 (0.2%)
15	AO	0.63	0/739	1.07	3/985 (0.3%)
15	CO	0.59	0/739	1.03	0/985
16	AP	0.62	0/697	1.06	3/939 (0.3%)
16	CP	0.66	0/693	0.98	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.61	0/836	0.95	0/1117
17	CQ	0.59	0/836	1.02	2/1117 (0.2%)
18	AR	0.61	0/560	1.03	1/746 (0.1%)
18	CR	0.58	0/560	0.95	0/746
19	AS	0.62	0/667	1.05	2/900 (0.2%)
19	CS	0.70	0/661	1.15	2/893 (0.2%)
20	AT	0.59	0/730	1.21	2/965 (0.2%)
20	CT	0.57	0/729	1.02	1/965 (0.1%)
21	AU	0.53	0/203	0.98	0/266
21	CU	0.64	0/203	1.05	2/266 (0.8%)
22	AV	0.52	0/127	0.65	0/198
22	CV	0.51	0/126	0.65	0/195
23	AX	0.42	0/1813	0.64	1/2825 (0.0%)
23	CX	0.45	0/1813	0.75	1/2825 (0.0%)
24	AW	0.45	0/20	0.87	0/23
24	CW	0.32	0/20	0.55	0/23
25	BA	0.58	0/65892	0.69	5/102850 (0.0%)
25	DA	0.45	0/65466	0.67	2/102184 (0.0%)
26	BB	0.46	0/2878	0.62	0/4490
26	DB	0.48	0/2878	0.69	0/4490
27	BD	0.90	0/2186	1.14	6/2944 (0.2%)
27	DD	0.78	0/2186	1.11	7/2944 (0.2%)
28	BE	0.90	0/1592	1.16	7/2149 (0.3%)
28	DE	0.73	0/1592	1.20	7/2149 (0.3%)
29	BF	0.93	1/1619 (0.1%)	1.09	8/2193 (0.4%)
29	DF	0.65	0/1615	1.18	9/2188 (0.4%)
30	BG	0.61	0/1450	1.03	5/1959 (0.3%)
30	DG	0.65	0/1449	1.20	9/1958 (0.5%)
31	BH	0.81	0/1356	1.15	11/1834 (0.6%)
31	DH	0.66	0/1356	1.10	5/1834 (0.3%)
32	BI	0.65	0/1100	1.04	5/1501 (0.3%)
32	DI	0.66	0/1076	1.11	6/1471 (0.4%)
33	BN	0.88	0/1144	1.10	2/1543 (0.1%)
33	DN	0.68	0/1144	1.15	10/1543 (0.6%)
34	BO	0.85	0/943	1.08	0/1269
34	DO	0.73	0/943	1.08	0/1269
35	BP	0.83	0/1152	1.05	1/1533 (0.1%)
35	DP	0.67	0/1152	1.17	8/1533 (0.5%)
36	BQ	0.89	0/1143	1.12	2/1527 (0.1%)
36	DQ	0.72	0/1143	1.10	2/1527 (0.1%)
37	BR	0.87	1/982 (0.1%)	1.04	2/1312 (0.2%)
37	DR	0.69	0/982	0.94	0/1312
38	BS	0.69	0/887	1.05	3/1180 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DS	0.64	0/880	1.09	2/1172 (0.2%)
39	BT	0.78	0/1105	1.08	3/1477 (0.2%)
39	DT	0.68	0/1097	1.06	1/1468 (0.1%)
40	BU	0.89	0/977	1.07	2/1301 (0.2%)
40	DU	0.66	0/977	0.97	0/1301
41	BV	0.87	0/782	1.01	0/1049
41	DV	0.69	0/782	1.00	0/1049
42	BW	0.99	1/897 (0.1%)	1.06	1/1205 (0.1%)
42	DW	0.79	1/897 (0.1%)	1.09	0/1205
43	BX	0.89	0/764	0.98	0/1025
43	DX	0.66	0/764	1.12	5/1025 (0.5%)
44	BY	0.87	0/819	1.12	3/1095 (0.3%)
44	DY	0.68	0/819	1.12	3/1095 (0.3%)
45	BZ	0.72	0/1379	1.17	12/1873 (0.6%)
45	DZ	0.66	0/1390	1.10	11/1890 (0.6%)
46	B0	0.78	0/662	1.09	2/881 (0.2%)
46	D0	0.64	0/662	1.14	3/881 (0.3%)
47	B1	0.88	1/762 (0.1%)	1.11	4/1014 (0.4%)
47	D1	0.68	0/762	1.02	0/1014
48	B2	0.83	0/590	1.12	0/781
48	D2	0.57	0/590	0.95	0/781
49	B3	0.84	0/474	1.19	6/635 (0.9%)
49	D3	0.63	0/469	1.05	2/630 (0.3%)
50	B4	0.67	0/564	1.31	8/759 (1.1%)
50	D4	0.80	0/544	1.32	4/735 (0.5%)
51	B5	0.92	0/469	1.14	0/635
51	D5	0.75	0/469	1.07	2/635 (0.3%)
52	B6	0.78	0/460	0.89	0/613
52	D6	0.67	0/456	0.97	0/608
53	B7	0.97	0/426	1.02	1/561 (0.2%)
53	D7	0.76	0/426	1.01	0/561
54	B8	0.91	0/519	1.00	0/684
54	D8	0.69	0/525	1.01	0/691
55	B9	0.88	0/310	1.02	0/407
55	D9	0.67	0/310	1.12	0/407
All	All	0.56	6/305966 (0.0%)	0.81	366/457396 (0.1%)

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	3
4	CD	0	1
7	AG	0	1
9	AI	0	1
19	CS	0	1
23	CX	1	0
24	AW	0	1
24	CW	0	1
27	DD	0	1
38	BS	0	1
44	BY	0	1
45	BZ	0	1
50	B4	0	1
50	D4	0	1
All	All	1	15

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	BR	38	VAL	CA-CB	-7.72	1.50	1.54
47	B1	67	ILE	CA-CB	-6.61	1.50	1.54
29	BF	84	VAL	CA-CB	-6.23	1.46	1.54
42	DW	103	ILE	CA-CB	-5.46	1.47	1.54
1	AA	343	U	C4-O4	5.11	1.33	1.23

The worst 5 of 366 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	CX	76	A	O4'-C1'-N9	17.86	135.29	108.50
8	CH	73	ASP	CA-C-N	11.99	132.99	120.04
8	CH	73	ASP	C-N-CA	11.99	132.99	120.04
50	B4	60	GLN	N-CA-C	-10.28	100.41	113.16
7	CG	79	ARG	N-CA-C	10.02	123.53	108.31

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	CX	76	A	C1'

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	231	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	AB	8	LYS	Peptide
2	AB	9	GLU	Peptide
7	AG	79	ARG	Peptide
9	AI	52	ALA	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32196	0	16250	915	0
1	CA	32312	0	16307	1009	0
2	AB	1846	0	1867	109	0
2	CB	1825	0	1828	122	0
3	AC	1552	0	1546	52	0
3	CC	1542	0	1517	83	0
4	AD	1659	0	1676	90	0
4	CD	1674	0	1714	89	0
5	AE	1129	0	1185	44	0
5	CE	1133	0	1191	58	0
6	AF	806	0	793	36	0
6	CF	816	0	808	26	0
7	AG	1231	0	1238	33	0
7	CG	1235	0	1249	53	0
8	AH	1088	0	1126	45	0
8	CH	1088	0	1126	57	0
9	AI	983	0	986	47	0
9	CI	978	0	966	57	0
10	AJ	709	0	650	42	0
10	CJ	714	0	672	58	0
11	AK	829	0	825	17	0
11	CK	833	0	836	27	0
12	AL	930	0	980	35	0
12	CL	930	0	980	40	0
13	AM	958	0	1002	35	0
13	CM	950	0	988	54	0
14	AN	492	0	529	26	0
14	CN	492	0	529	32	0
15	AO	728	0	760	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	CO	728	0	760	26	0
16	AP	681	0	697	36	0
16	CP	677	0	686	31	0
17	AQ	823	0	891	21	0
17	CQ	823	0	891	27	0
18	AR	555	0	618	25	0
18	CR	555	0	618	22	0
19	AS	652	0	662	43	0
19	CS	646	0	644	52	0
20	AT	728	0	798	37	0
20	CT	727	0	796	29	0
21	AU	199	0	208	7	0
21	CU	199	0	208	8	0
22	AV	114	0	54	1	0
22	CV	113	0	54	1	0
23	AX	1623	0	823	23	0
23	CX	1623	0	823	22	0
24	AW	93	0	84	10	0
24	CW	93	0	84	10	0
25	BA	58834	0	29666	844	0
25	DA	58458	0	29481	1173	0
26	BB	2573	0	1306	36	0
26	DB	2573	0	1306	66	0
27	BD	2136	0	2218	62	0
27	DD	2136	0	2218	75	0
28	BE	1559	0	1618	57	0
28	DE	1559	0	1618	65	0
29	BF	1584	0	1625	39	0
29	DF	1580	0	1619	67	0
30	BG	1425	0	1443	42	0
30	DG	1424	0	1434	92	0
31	BH	1330	0	1407	37	0
31	DH	1330	0	1407	51	0
32	BI	1085	0	1114	45	0
32	DI	1061	0	1080	28	0
33	BN	1117	0	1183	20	0
33	DN	1117	0	1184	25	0
34	BO	933	0	996	31	0
34	DO	933	0	996	31	0
35	BP	1135	0	1212	43	0
35	DP	1135	0	1212	50	0
36	BQ	1122	0	1179	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	DQ	1122	0	1179	42	0
37	BR	968	0	1033	26	0
37	DR	968	0	1032	29	0
38	BS	877	0	938	30	0
38	DS	870	0	923	45	0
39	BT	1091	0	1151	36	0
39	DT	1083	0	1136	38	0
40	BU	959	0	1019	28	0
40	DU	959	0	1019	28	0
41	BV	771	0	830	16	0
41	DV	771	0	830	23	0
42	BW	886	0	940	15	0
42	DW	886	0	940	26	0
43	BX	750	0	814	20	0
43	DX	750	0	814	23	0
44	BY	806	0	881	25	0
44	DY	806	0	881	28	0
45	BZ	1349	0	1355	45	0
45	DZ	1360	0	1363	57	0
46	B0	653	0	674	19	0
46	D0	653	0	674	32	0
47	B1	755	0	826	19	0
47	D1	755	0	826	20	0
48	B2	588	0	643	15	0
48	D2	588	0	643	18	0
49	B3	469	0	518	12	0
49	D3	464	0	514	11	0
50	B4	551	0	532	42	0
50	D4	531	0	502	41	0
51	B5	455	0	465	13	0
51	D5	455	0	465	11	0
52	B6	453	0	473	10	0
52	D6	449	0	469	13	0
53	B7	418	0	467	10	0
53	D7	418	0	467	9	0
54	B8	511	0	571	33	0
54	D8	517	0	582	24	0
55	B9	307	0	335	7	0
55	D9	307	0	335	14	0
56	AA	222	0	0	0	0
56	AD	1	0	0	0	0
56	AF	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	AK	1	0	0	0	0
56	AL	1	0	0	0	0
56	AM	2	0	0	0	0
56	AN	1	0	0	0	0
56	AS	1	0	0	0	0
56	AV	1	0	0	0	0
56	AX	9	0	0	0	0
56	B0	6	0	0	0	0
56	B1	2	0	0	0	0
56	B2	1	0	0	0	0
56	B3	3	0	0	0	0
56	B5	1	0	0	0	0
56	B7	4	0	0	0	0
56	B8	2	0	0	0	0
56	B9	1	0	0	0	0
56	BA	739	0	0	0	0
56	BB	18	0	0	0	0
56	BD	12	0	0	0	0
56	BE	9	0	0	0	0
56	BF	6	0	0	0	0
56	BG	4	0	0	0	0
56	BN	6	0	0	0	0
56	BO	1	0	0	0	0
56	BP	4	0	0	0	0
56	BQ	4	0	0	0	0
56	BR	3	0	0	0	0
56	BU	9	0	0	0	0
56	BV	3	0	0	0	0
56	BW	5	0	0	0	0
56	BX	2	0	0	0	0
56	BZ	1	0	0	0	0
56	CA	172	0	0	0	0
56	CE	2	0	0	0	0
56	CF	1	0	0	0	0
56	CN	1	0	0	0	0
56	CT	1	0	0	0	0
56	CX	3	0	0	0	0
56	D3	1	0	0	0	0
56	D5	2	0	0	0	0
56	D8	1	0	0	0	0
56	DA	657	0	0	0	0
56	DB	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DD	5	0	0	0	0
56	DE	6	0	0	0	0
56	DF	5	0	0	0	0
56	DG	1	0	0	0	0
56	DN	1	0	0	0	0
56	DO	1	0	0	0	0
56	DP	2	0	0	0	0
56	DQ	4	0	0	0	0
56	DR	1	0	0	0	0
56	DU	2	0	0	0	0
56	DV	3	0	0	0	0
56	DW	2	0	0	0	0
56	DY	1	0	0	0	0
57	AD	8	0	0	1	0
57	CD	8	0	0	1	0
58	AN	1	0	0	0	0
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	10	0	10	1	0
59	CX	10	0	10	3	0
60	BA	1	0	0	0	0
60	DA	1	0	0	0	0
61	AA	147	0	0	23	0
61	AD	1	0	0	0	0
61	AE	2	0	0	0	0
61	AJ	1	0	0	0	0
61	AL	2	0	0	0	0
61	AO	2	0	0	0	0
61	AU	1	0	0	1	0
61	AV	2	0	0	0	0
61	AX	1	0	0	0	0
61	B0	4	0	0	0	0
61	B1	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	B5	2	0	0	0	0
61	B7	1	0	0	1	0
61	B8	7	0	0	1	0
61	BA	1086	0	0	94	0
61	BB	26	0	0	2	0
61	BD	6	0	0	0	0
61	BE	13	0	0	3	0
61	BF	5	0	0	0	0
61	BG	1	0	0	0	0
61	BN	3	0	0	0	0
61	BO	2	0	0	0	0
61	BP	15	0	0	2	0
61	BQ	3	0	0	1	0
61	BR	1	0	0	0	0
61	BT	2	0	0	0	0
61	BU	5	0	0	0	0
61	BV	2	0	0	0	0
61	BW	4	0	0	0	0
61	BX	4	0	0	1	0
61	CA	186	0	0	24	0
61	CE	2	0	0	0	0
61	CN	1	0	0	0	0
61	CT	1	0	0	0	0
61	CX	2	0	0	0	0
61	D0	3	0	0	1	0
61	D1	1	0	0	0	0
61	D3	1	0	0	0	0
61	D7	1	0	0	0	0
61	D8	4	0	0	0	0
61	DA	906	0	0	117	0
61	DB	7	0	0	0	0
61	DD	10	0	0	0	0
61	DE	11	0	0	1	0
61	DF	4	0	0	0	0
61	DO	1	0	0	0	0
61	DP	14	0	0	2	0
61	DQ	3	0	0	1	0
61	DR	1	0	0	0	0
61	DU	4	0	0	0	0
61	DV	1	0	0	0	0
61	DX	2	0	0	1	0
61	DY	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	286321	0	191124	6816	0

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

The worst 5 of 6816 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1129:C:N4	1:AA:1143:G:H1	1.46	1.12
1:CA:1002:G:H1	1:CA:1038:C:N4	1.48	1.09
1:AA:348:G:H2'	1:AA:349:A:H5'	1.30	1.06
2:AB:185:ILE:HG22	2:AB:199:TYR:HB2	1.39	1.04
2:CB:16:HIS:HB2	2:CB:204:ASN:HB3	1.36	1.03

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	229/256 (90%)	201 (88%)	23 (10%)	5 (2%)	5	26
2	CB	229/256 (90%)	201 (88%)	21 (9%)	7 (3%)	3	19
3	AC	204/239 (85%)	182 (89%)	20 (10%)	2 (1%)	12	45
3	CC	204/239 (85%)	181 (89%)	21 (10%)	2 (1%)	12	45
4	AD	206/209 (99%)	184 (89%)	20 (10%)	2 (1%)	12	45
4	CD	206/209 (99%)	185 (90%)	18 (9%)	3 (2%)	8	35
5	AE	146/162 (90%)	136 (93%)	8 (6%)	2 (1%)	9	36
5	CE	146/162 (90%)	134 (92%)	12 (8%)	0	100	100
6	AF	98/101 (97%)	94 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	CF	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
7	AG	153/156 (98%)	137 (90%)	15 (10%)	1 (1%)	18	53
7	CG	153/156 (98%)	139 (91%)	13 (8%)	1 (1%)	18	53
8	AH	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
8	CH	135/138 (98%)	131 (97%)	3 (2%)	1 (1%)	18	53
9	AI	125/128 (98%)	112 (90%)	10 (8%)	3 (2%)	4	24
9	CI	125/128 (98%)	115 (92%)	8 (6%)	2 (2%)	7	34
10	AJ	95/105 (90%)	84 (88%)	8 (8%)	3 (3%)	3	18
10	CJ	94/105 (90%)	84 (89%)	8 (8%)	2 (2%)	5	27
11	AK	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	14	48
11	CK	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	14	48
12	AL	120/132 (91%)	117 (98%)	3 (2%)	0	100	100
12	CL	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
13	AM	121/126 (96%)	113 (93%)	7 (6%)	1 (1%)	16	50
13	CM	120/126 (95%)	113 (94%)	6 (5%)	1 (1%)	16	50
14	AN	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
14	CN	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
15	AO	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
15	CO	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	AP	80/88 (91%)	74 (92%)	6 (8%)	0	100	100
16	CP	80/88 (91%)	73 (91%)	6 (8%)	1 (1%)	9	38
17	AQ	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
17	CQ	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
18	AR	66/88 (75%)	60 (91%)	5 (8%)	1 (2%)	8	35
18	CR	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
19	AS	81/93 (87%)	76 (94%)	5 (6%)	0	100	100
19	CS	81/93 (87%)	74 (91%)	7 (9%)	0	100	100
20	AT	94/106 (89%)	84 (89%)	9 (10%)	1 (1%)	11	43
20	CT	94/106 (89%)	86 (92%)	5 (5%)	3 (3%)	3	18
21	AU	21/27 (78%)	17 (81%)	4 (19%)	0	100	100
21	CU	21/27 (78%)	18 (86%)	3 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	AW	3/10 (30%)	0	2 (67%)	1 (33%)	0	0
24	CW	3/10 (30%)	1 (33%)	1 (33%)	1 (33%)	0	0
27	BD	273/276 (99%)	260 (95%)	12 (4%)	1 (0%)	30	65
27	DD	273/276 (99%)	258 (94%)	13 (5%)	2 (1%)	18	53
28	BE	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	24	60
28	DE	202/206 (98%)	195 (96%)	4 (2%)	3 (2%)	8	35
29	BF	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	24	60
29	DF	201/210 (96%)	195 (97%)	4 (2%)	2 (1%)	12	45
30	BG	179/182 (98%)	167 (93%)	9 (5%)	3 (2%)	7	32
30	DG	179/182 (98%)	161 (90%)	14 (8%)	4 (2%)	5	26
31	BH	172/180 (96%)	165 (96%)	6 (4%)	1 (1%)	21	56
31	DH	172/180 (96%)	164 (95%)	7 (4%)	1 (1%)	21	56
32	BI	144/148 (97%)	124 (86%)	14 (10%)	6 (4%)	2	13
32	DI	144/148 (97%)	124 (86%)	17 (12%)	3 (2%)	5	27
33	BN	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
33	DN	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	18	53
34	BO	120/122 (98%)	116 (97%)	3 (2%)	1 (1%)	16	50
34	DO	120/122 (98%)	117 (98%)	2 (2%)	1 (1%)	16	50
35	BP	147/150 (98%)	138 (94%)	8 (5%)	1 (1%)	18	53
35	DP	147/150 (98%)	135 (92%)	9 (6%)	3 (2%)	6	28
36	BQ	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	18	53
36	DQ	139/141 (99%)	129 (93%)	9 (6%)	1 (1%)	18	53
37	BR	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	14	48
37	DR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
38	BS	108/112 (96%)	103 (95%)	4 (4%)	1 (1%)	14	48
38	DS	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	14	48
39	BT	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
39	DT	129/146 (88%)	127 (98%)	2 (2%)	0	100	100
40	BU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
40	DU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
41	BV	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	12	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	DV	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	12	45
42	BW	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
42	DW	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
43	BX	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
43	DX	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
44	BY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
44	DY	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
45	BZ	169/206 (82%)	150 (89%)	18 (11%)	1 (1%)	21	56
45	DZ	172/206 (84%)	162 (94%)	10 (6%)	0	100	100
46	B0	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	10	40
46	D0	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	10	40
47	B1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	43
47	D1	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11	43
48	B2	68/72 (94%)	68 (100%)	0	0	100	100
48	D2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
49	B3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
49	D3	57/60 (95%)	57 (100%)	0	0	100	100
50	B4	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1	4
50	D4	67/71 (94%)	52 (78%)	8 (12%)	7 (10%)	0	2
51	B5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
51	D5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
52	B6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
52	D6	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
53	B7	46/49 (94%)	46 (100%)	0	0	100	100
53	D7	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	5	26
54	B8	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
54	D8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
55	B9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
55	D9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
All	All	11415/12148 (94%)	10659 (93%)	648 (6%)	108 (1%)	14	48

5 of 108 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	125	PRO
3	AC	107	GLN
4	AD	166	LYS
9	AI	54	ASP
10	AJ	31	GLY

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%)	147 (77%)	45 (23%)	1	4
2	CB	187/220 (85%)	148 (79%)	39 (21%)	1	7
3	AC	143/188 (76%)	122 (85%)	21 (15%)	3	15
3	CC	140/188 (74%)	118 (84%)	22 (16%)	2	13
4	AD	170/181 (94%)	146 (86%)	24 (14%)	3	16
4	CD	173/181 (96%)	145 (84%)	28 (16%)	2	12
5	AE	113/123 (92%)	100 (88%)	13 (12%)	5	24
5	CE	114/123 (93%)	98 (86%)	16 (14%)	3	16
6	AF	83/90 (92%)	75 (90%)	8 (10%)	8	31
6	CF	85/90 (94%)	77 (91%)	8 (9%)	8	32
7	AG	119/127 (94%)	92 (77%)	27 (23%)	1	5
7	CG	120/127 (94%)	97 (81%)	23 (19%)	1	8
8	AH	114/119 (96%)	95 (83%)	19 (17%)	2	12
8	CH	114/119 (96%)	97 (85%)	17 (15%)	3	15
9	AI	90/99 (91%)	75 (83%)	15 (17%)	2	12
9	CI	89/99 (90%)	77 (86%)	12 (14%)	4	18
10	AJ	66/92 (72%)	57 (86%)	9 (14%)	3	17
10	CJ	69/92 (75%)	62 (90%)	7 (10%)	7	29
11	AK	82/99 (83%)	73 (89%)	9 (11%)	6	25
11	CK	83/99 (84%)	72 (87%)	11 (13%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	97/109 (89%)	85 (88%)	12 (12%)	4	20
12	CL	97/109 (89%)	83 (86%)	14 (14%)	3	15
13	AM	93/101 (92%)	81 (87%)	12 (13%)	4	19
13	CM	92/101 (91%)	77 (84%)	15 (16%)	2	12
14	AN	49/50 (98%)	39 (80%)	10 (20%)	1	7
14	CN	49/50 (98%)	40 (82%)	9 (18%)	1	9
15	AO	78/80 (98%)	69 (88%)	9 (12%)	5	24
15	CO	78/80 (98%)	67 (86%)	11 (14%)	3	16
16	AP	69/74 (93%)	61 (88%)	8 (12%)	5	23
16	CP	68/74 (92%)	61 (90%)	7 (10%)	7	28
17	AQ	94/97 (97%)	87 (93%)	7 (7%)	13	42
17	CQ	94/97 (97%)	85 (90%)	9 (10%)	8	31
18	AR	59/77 (77%)	54 (92%)	5 (8%)	10	36
18	CR	59/77 (77%)	51 (86%)	8 (14%)	3	17
19	AS	69/80 (86%)	63 (91%)	6 (9%)	9	35
19	CS	67/80 (84%)	58 (87%)	9 (13%)	4	18
20	AT	70/82 (85%)	59 (84%)	11 (16%)	2	13
20	CT	70/82 (85%)	61 (87%)	9 (13%)	4	19
21	AU	18/22 (82%)	15 (83%)	3 (17%)	2	12
21	CU	18/22 (82%)	15 (83%)	3 (17%)	2	12
24	AW	3/3 (100%)	2 (67%)	1 (33%)	0	1
24	CW	3/3 (100%)	2 (67%)	1 (33%)	0	1
27	BD	215/218 (99%)	194 (90%)	21 (10%)	7	30
27	DD	215/218 (99%)	187 (87%)	28 (13%)	4	19
28	BE	164/166 (99%)	135 (82%)	29 (18%)	2	10
28	DE	164/166 (99%)	135 (82%)	29 (18%)	2	10
29	BF	160/166 (96%)	134 (84%)	26 (16%)	2	12
29	DF	159/166 (96%)	133 (84%)	26 (16%)	2	12
30	BG	143/156 (92%)	120 (84%)	23 (16%)	2	12
30	DG	142/156 (91%)	119 (84%)	23 (16%)	2	12
31	BH	144/148 (97%)	125 (87%)	19 (13%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	DH	144/148 (97%)	126 (88%)	18 (12%)	4	20
32	BI	110/124 (89%)	84 (76%)	26 (24%)	1	4
32	DI	104/124 (84%)	84 (81%)	20 (19%)	1	8
33	BN	118/119 (99%)	97 (82%)	21 (18%)	2	10
33	DN	118/119 (99%)	98 (83%)	20 (17%)	2	11
34	BO	100/100 (100%)	90 (90%)	10 (10%)	7	29
34	DO	100/100 (100%)	85 (85%)	15 (15%)	3	14
35	BP	115/116 (99%)	99 (86%)	16 (14%)	3	17
35	DP	115/116 (99%)	98 (85%)	17 (15%)	3	15
36	BQ	111/111 (100%)	98 (88%)	13 (12%)	5	23
36	DQ	111/111 (100%)	99 (89%)	12 (11%)	6	26
37	BR	101/101 (100%)	82 (81%)	19 (19%)	1	9
37	DR	101/101 (100%)	82 (81%)	19 (19%)	1	9
38	BS	87/88 (99%)	75 (86%)	12 (14%)	3	17
38	DS	85/88 (97%)	66 (78%)	19 (22%)	1	5
39	BT	115/127 (91%)	101 (88%)	14 (12%)	5	21
39	DT	113/127 (89%)	100 (88%)	13 (12%)	5	24
40	BU	93/94 (99%)	80 (86%)	13 (14%)	3	16
40	DU	93/94 (99%)	78 (84%)	15 (16%)	2	12
41	BV	80/82 (98%)	65 (81%)	15 (19%)	1	9
41	DV	80/82 (98%)	64 (80%)	16 (20%)	1	7
42	BW	90/92 (98%)	79 (88%)	11 (12%)	5	21
42	DW	90/92 (98%)	79 (88%)	11 (12%)	5	21
43	BX	77/78 (99%)	71 (92%)	6 (8%)	11	39
43	DX	77/78 (99%)	71 (92%)	6 (8%)	11	39
44	BY	85/91 (93%)	77 (91%)	8 (9%)	8	32
44	DY	85/91 (93%)	79 (93%)	6 (7%)	13	43
45	BZ	145/179 (81%)	124 (86%)	21 (14%)	3	15
45	DZ	145/179 (81%)	127 (88%)	18 (12%)	4	20
46	B0	65/67 (97%)	61 (94%)	4 (6%)	16	49
46	D0	65/67 (97%)	59 (91%)	6 (9%)	8	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	B1	80/83 (96%)	70 (88%)	10 (12%)	4	20
47	D1	80/83 (96%)	67 (84%)	13 (16%)	2	12
48	B2	65/67 (97%)	56 (86%)	9 (14%)	3	17
48	D2	65/67 (97%)	56 (86%)	9 (14%)	3	17
49	B3	51/52 (98%)	40 (78%)	11 (22%)	1	6
49	D3	50/52 (96%)	41 (82%)	9 (18%)	2	10
50	B4	59/63 (94%)	48 (81%)	11 (19%)	1	9
50	D4	53/63 (84%)	43 (81%)	10 (19%)	1	9
51	B5	50/52 (96%)	44 (88%)	6 (12%)	5	22
51	D5	50/52 (96%)	47 (94%)	3 (6%)	17	50
52	B6	51/52 (98%)	47 (92%)	4 (8%)	11	39
52	D6	50/52 (96%)	46 (92%)	4 (8%)	11	38
53	B7	41/42 (98%)	37 (90%)	4 (10%)	7	30
53	D7	41/42 (98%)	37 (90%)	4 (10%)	7	30
54	B8	53/55 (96%)	49 (92%)	4 (8%)	12	41
54	D8	54/55 (98%)	51 (94%)	3 (6%)	19	52
55	B9	34/34 (100%)	33 (97%)	1 (3%)	37	70
55	D9	34/34 (100%)	31 (91%)	3 (9%)	9	35
All	All	9325/10072 (93%)	7991 (86%)	1334 (14%)	3	16

5 of 1334 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	CT	24	LEU
36	DQ	110	THR
27	DD	165	ILE
19	CS	65	ASN
30	DG	145	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 146 such sidechains are listed below:

Mol	Chain	Res	Type
28	DE	85	ASN
52	D6	20	ASN
29	DF	169	ASN

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Mol	Chain	Res	Type
38	DS	68	GLN
30	BG	26	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1495/1522 (98%)	422 (28%)	24 (1%)
1	CA	1501/1522 (98%)	423 (28%)	30 (1%)
22	AV	4/24 (16%)	1 (25%)	0
22	CV	4/24 (16%)	1 (25%)	0
23	AX	75/77 (97%)	18 (24%)	0
23	CX	75/77 (97%)	19 (25%)	0
25	BA	2722/2915 (93%)	533 (19%)	41 (1%)
25	DA	2704/2915 (92%)	529 (19%)	35 (1%)
26	BB	119/122 (97%)	21 (17%)	0
26	DB	119/122 (97%)	23 (19%)	1 (0%)
All	All	8818/9320 (94%)	1990 (22%)	131 (1%)

5 of 1990 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	9	G
1	AA	15	G
1	AA	16	A
1	AA	22	G

5 of 131 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	DA	1427	A
25	DA	1608	A
26	DB	45	A
25	BA	1466	U
25	BA	1321	A

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

14 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	MVA	CW	9	24	6,7,8	0.89	0	6,8,10	1.10	0
24	004	AW	3	24	9,10,11	1.20	1 (11%)	9,12,14	1.16	0
24	2QY	CW	10	24	12,13,14	2.04	2 (16%)	14,16,18	3.56	3 (21%)
24	004	CW	3	24	9,10,11	1.35	1 (11%)	9,12,14	0.68	0
24	2R3	CW	8	24	12,14,15	0.71	0	16,18,20	2.15	6 (37%)
24	2R1	CW	6	24	10,10,11	1.82	3 (30%)	8,13,15	3.68	3 (37%)
24	2QZ	CW	1	24	7,8,9	0.83	0	7,10,12	3.69	2 (28%)
24	2R3	AW	8	24	12,14,15	0.81	0	16,18,20	2.05	7 (43%)
24	MVA	AW	9	24	6,7,8	0.38	0	6,8,10	0.94	1 (16%)
24	MVA	CW	5	24	6,7,8	0.81	0	6,8,10	1.51	2 (33%)
24	2R1	AW	6	24	10,10,11	2.43	4 (40%)	8,13,15	4.19	3 (37%)
24	2QY	AW	10	24	12,13,14	1.94	2 (16%)	14,16,18	3.62	6 (42%)
24	2QZ	AW	1	24	7,8,9	0.41	0	7,10,12	2.50	1 (14%)
24	MVA	AW	5	24	6,7,8	0.57	0	6,8,10	1.28	0

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	MVA	CW	9	24	-	5/6/8/10	-
24	004	AW	3	24	-	1/4/6/8	0/1/1/1
24	2QY	CW	10	24	-	1/5/8/10	0/1/1/1
24	004	CW	3	24	-	0/4/6/8	0/1/1/1
24	2R3	CW	8	24	-	6/11/12/14	0/1/1/1
24	2R1	CW	6	24	-	0/2/14/16	0/1/1/1
24	2QZ	CW	1	24	-	1/8/10/12	-
24	2R3	AW	8	24	-	6/11/12/14	0/1/1/1
24	MVA	AW	9	24	-	5/6/8/10	-
24	MVA	CW	5	24	-	5/6/8/10	-
24	2R1	AW	6	24	-	1/2/14/16	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	2QY	AW	10	24	-	3/5/8/10	0/1/1/1
24	2QZ	AW	1	24	-	3/8/10/12	-
24	MVA	AW	5	24	-	2/6/8/10	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CW	10	2QY	C-CA	6.08	1.53	1.43
24	AW	10	2QY	C-CA	5.76	1.53	1.43
24	AW	6	2R1	OD1-CG1	4.61	1.56	1.42
24	AW	6	2R1	CA-N	4.13	1.46	1.36
24	CW	6	2R1	CA-N	3.84	1.45	1.36

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AW	6	2R1	OD2-CG2-CB	-10.70	92.15	111.99
24	CW	10	2QY	CN-N-CA	-9.76	109.17	123.98
24	AW	10	2QY	CN-N-CA	-9.66	109.33	123.98
24	CW	1	2QZ	OG1-CB-CG2	9.20	137.20	109.68
24	CW	6	2R1	OD2-CG2-CB	-8.95	95.40	111.99

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AW	1	2QZ	N-CA-CB-OG1
24	AW	5	MVA	CB-CA-N-CN
24	AW	8	2R3	N-CA-CB-OB
24	AW	8	2R3	N-CA-CB-CG
24	AW	8	2R3	C-CA-CB-OB

There are no ring outliers.

14 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	CW	9	MVA	3	0
24	AW	3	004	1	0
24	CW	10	2QY	4	0
24	CW	3	004	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	CW	8	2R3	2	0
24	CW	6	2R1	1	0
24	CW	1	2QZ	3	0
24	AW	8	2R3	4	0
24	AW	9	MVA	3	0
24	CW	5	MVA	1	0
24	AW	6	2R1	3	0
24	AW	10	2QY	3	0
24	AW	1	2QZ	2	0
24	AW	5	MVA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1991 ligands modelled in this entry, 1987 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
57	SF4	CD	501	4	0,12,12	-	-	-		
59	FME	CX	101	23	8,9,10	0.82	0	8,9,11	1.37	1 (12%)
57	SF4	AD	501	4	0,12,12	-	-	-		
59	FME	AX	101	23	8,9,10	0.94	0	8,9,11	1.49	2 (25%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	FME	CX	101	23	-	1/7/9/11	-
57	SF4	AD	501	4	-	-	0/6/5/5
59	FME	AX	101	23	-	2/7/9/11	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	AX	101	FME	CA-N-CN	-2.47	119.03	122.82
59	CX	101	FME	CA-N-CN	-2.33	119.25	122.82
59	AX	101	FME	CB-CA-N	2.31	114.72	110.52

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	AX	101	FME	O1-CN-N-CA
59	CX	101	FME	O1-CN-N-CA
59	AX	101	FME	CB-CG-SD-CE

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	CD	501	SF4	1	0
59	CX	101	FME	3	0
57	AD	501	SF4	1	0
59	AX	101	FME	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1498/1522 (98%)	0.01	25 (1%) 69 45	39, 80, 103, 118	0
1	CA	1503/1522 (98%)	0.01	22 (1%) 72 49	41, 80, 103, 119	0
2	AB	231/256 (90%)	0.47	6 (2%) 57 34	69, 86, 97, 105	0
2	CB	231/256 (90%)	0.54	11 (4%) 35 19	70, 88, 98, 107	0
3	AC	206/239 (86%)	0.44	5 (2%) 59 36	73, 87, 95, 104	0
3	CC	206/239 (86%)	0.62	6 (2%) 53 31	72, 89, 97, 104	0
4	AD	208/209 (99%)	0.55	6 (2%) 53 31	61, 80, 90, 97	0
4	CD	208/209 (99%)	0.43	2 (0%) 79 59	61, 79, 89, 97	0
5	AE	148/162 (91%)	-0.10	0 100 100	51, 73, 82, 93	0
5	CE	148/162 (91%)	0.18	0 100 100	53, 75, 84, 96	0
6	AF	100/101 (99%)	0.11	1 (1%) 79 59	63, 77, 87, 94	0
6	CF	100/101 (99%)	0.15	0 100 100	62, 78, 87, 95	0
7	AG	155/156 (99%)	0.29	5 (3%) 50 29	74, 86, 99, 106	0
7	CG	155/156 (99%)	0.43	5 (3%) 50 29	75, 86, 99, 105	0
8	AH	137/138 (99%)	0.17	0 100 100	60, 74, 82, 89	0
8	CH	137/138 (99%)	0.32	3 (2%) 62 39	62, 75, 83, 89	0
9	AI	127/128 (99%)	0.81	9 (7%) 22 11	73, 91, 99, 101	0
9	CI	127/128 (99%)	1.33	27 (21%) 2 1	72, 93, 100, 102	0
10	AJ	97/105 (92%)	1.05	14 (14%) 6 3	73, 91, 100, 105	0
10	CJ	96/105 (91%)	1.19	14 (14%) 6 3	77, 93, 100, 104	0
11	AK	114/129 (88%)	-0.00	1 (0%) 81 61	53, 74, 87, 91	0
11	CK	114/129 (88%)	0.02	0 100 100	55, 76, 87, 92	0
12	AL	122/132 (92%)	0.24	4 (3%) 49 28	53, 68, 80, 87	0
12	CL	122/132 (92%)	0.14	2 (1%) 70 47	53, 69, 80, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	123/126 (97%)	0.40	7 (5%) 29 15	67, 85, 95, 105	0
13	CM	122/126 (96%)	0.75	7 (5%) 29 15	77, 92, 100, 109	0
14	AN	60/61 (98%)	0.85	6 (10%) 12 7	75, 87, 94, 103	0
14	CN	60/61 (98%)	1.32	14 (23%) 2 1	77, 89, 94, 100	0
15	AO	88/89 (98%)	0.17	1 (1%) 78 57	55, 72, 85, 90	0
15	CO	88/89 (98%)	0.09	1 (1%) 78 57	55, 72, 85, 91	0
16	AP	82/88 (93%)	0.66	5 (6%) 27 14	67, 78, 89, 94	0
16	CP	82/88 (93%)	0.58	3 (3%) 45 25	66, 76, 88, 94	0
17	AQ	99/105 (94%)	0.22	1 (1%) 79 59	59, 72, 83, 90	0
17	CQ	99/105 (94%)	0.18	0 100 100	58, 72, 83, 89	0
18	AR	68/88 (77%)	0.18	0 100 100	65, 73, 87, 91	0
18	CR	68/88 (77%)	0.08	0 100 100	64, 75, 87, 91	0
19	AS	83/93 (89%)	0.79	7 (8%) 17 9	77, 92, 99, 106	0
19	CS	83/93 (89%)	1.14	15 (18%) 3 2	79, 92, 101, 106	0
20	AT	96/106 (90%)	0.63	7 (7%) 21 11	62, 76, 86, 90	0
20	CT	96/106 (90%)	0.32	3 (3%) 51 30	62, 74, 86, 92	0
21	AU	23/27 (85%)	1.34	4 (17%) 4 3	73, 88, 93, 94	0
21	CU	23/27 (85%)	1.81	8 (34%) 1 1	73, 89, 92, 94	0
22	AV	7/24 (29%)	0.35	0 100 100	65, 77, 102, 104	0
22	CV	6/24 (25%)	0.46	1 (16%) 4 3	67, 78, 103, 103	0
23	AX	76/77 (98%)	-0.38	0 100 100	52, 80, 97, 105	0
23	CX	76/77 (98%)	-0.13	0 100 100	52, 82, 100, 106	0
24	AW	3/10 (30%)	0.50	0 100 100	67, 67, 82, 98	0
24	CW	3/10 (30%)	-0.32	0 100 100	67, 67, 78, 82	0
25	BA	2731/2915 (93%)	-0.69	13 (0%) 87 72	23, 44, 85, 111	0
25	DA	2714/2915 (93%)	-0.69	4 (0%) 92 86	26, 47, 85, 118	0
26	BB	120/122 (98%)	-0.27	0 100 100	42, 68, 80, 95	0
26	DB	120/122 (98%)	0.09	0 100 100	48, 74, 84, 97	0
27	BD	275/276 (99%)	-0.44	0 100 100	22, 42, 58, 77	0
27	DD	275/276 (99%)	-0.45	1 (0%) 88 76	23, 44, 60, 79	0
28	BE	204/206 (99%)	-0.42	0 100 100	23, 45, 67, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DE	204/206 (99%)	-0.39	1 (0%) 87 72	24, 47, 70, 88	0
29	BF	203/210 (96%)	-0.23	0 100 100	20, 51, 77, 94	0
29	DF	203/210 (96%)	-0.26	0 100 100	22, 54, 78, 93	0
30	BG	181/182 (99%)	0.18	2 (1%) 78 57	59, 77, 90, 103	0
30	DG	181/182 (99%)	0.59	8 (4%) 39 21	63, 80, 92, 102	0
31	BH	174/180 (96%)	0.12	2 (1%) 78 57	50, 66, 78, 84	0
31	DH	174/180 (96%)	0.31	1 (0%) 85 69	54, 71, 82, 87	0
32	BI	146/148 (98%)	-0.08	0 100 100	45, 75, 87, 92	0
32	DI	146/148 (98%)	0.17	0 100 100	48, 76, 86, 91	0
33	BN	140/140 (100%)	-0.16	1 (0%) 84 66	32, 49, 68, 80	0
33	DN	140/140 (100%)	-0.23	0 100 100	34, 53, 72, 81	0
34	BO	122/122 (100%)	-0.57	0 100 100	25, 39, 60, 78	0
34	DO	122/122 (100%)	-0.39	0 100 100	34, 52, 68, 79	0
35	BP	149/150 (99%)	-0.19	1 (0%) 84 66	26, 54, 76, 84	0
35	DP	149/150 (99%)	-0.08	0 100 100	30, 57, 79, 86	0
36	BQ	141/141 (100%)	-0.05	3 (2%) 63 40	33, 51, 65, 79	0
36	DQ	141/141 (100%)	-0.15	1 (0%) 84 66	35, 54, 70, 80	0
37	BR	118/118 (100%)	-0.53	0 100 100	22, 35, 51, 64	0
37	DR	118/118 (100%)	-0.26	0 100 100	36, 50, 64, 81	0
38	BS	110/112 (98%)	-0.30	0 100 100	38, 55, 69, 81	0
38	DS	110/112 (98%)	0.57	5 (4%) 38 20	66, 78, 90, 100	0
39	BT	131/146 (89%)	-0.30	2 (1%) 72 49	33, 45, 75, 91	0
39	DT	131/146 (89%)	-0.21	2 (1%) 72 49	44, 56, 80, 86	0
40	BU	116/118 (98%)	-0.71	0 100 100	19, 30, 50, 63	0
40	DU	116/118 (98%)	-0.10	0 100 100	39, 61, 79, 88	0
41	BV	101/101 (100%)	-0.29	0 100 100	29, 52, 70, 77	0
41	DV	101/101 (100%)	-0.31	0 100 100	32, 58, 74, 79	0
42	BW	112/113 (99%)	-0.47	1 (0%) 81 61	27, 37, 61, 94	0
42	DW	112/113 (99%)	-0.42	0 100 100	31, 40, 63, 94	0
43	BX	95/96 (98%)	-0.16	1 (1%) 78 57	32, 46, 69, 82	0
43	DX	95/96 (98%)	-0.04	0 100 100	38, 50, 72, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BY	107/110 (97%)	0.11	3 (2%) 55 32	44, 59, 77, 82	0
44	DY	107/110 (97%)	0.30	3 (2%) 55 32	46, 63, 80, 85	0
45	BZ	171/206 (83%)	0.11	2 (1%) 76 55	52, 71, 85, 93	0
45	DZ	174/206 (84%)	0.33	1 (0%) 85 69	56, 74, 87, 95	0
46	B0	83/85 (97%)	-0.13	6 (7%) 21 11	22, 40, 75, 104	0
46	D0	83/85 (97%)	0.28	3 (3%) 46 26	45, 66, 87, 98	0
47	B1	97/98 (98%)	-0.41	0 100 100	25, 42, 71, 77	0
47	D1	97/98 (98%)	-0.17	1 (1%) 79 59	35, 56, 79, 85	0
48	B2	70/72 (97%)	-0.23	0 100 100	31, 48, 64, 77	0
48	D2	70/72 (97%)	0.09	0 100 100	56, 73, 84, 86	0
49	B3	59/60 (98%)	-0.44	0 100 100	26, 38, 63, 86	0
49	D3	59/60 (98%)	-0.14	0 100 100	49, 62, 80, 93	0
50	B4	69/71 (97%)	0.27	0 100 100	64, 87, 101, 104	0
50	D4	69/71 (97%)	0.72	4 (5%) 29 15	85, 95, 104, 107	0
51	B5	59/60 (98%)	-0.75	0 100 100	14, 35, 55, 71	0
51	D5	59/60 (98%)	-0.34	0 100 100	29, 51, 70, 77	0
52	B6	53/54 (98%)	-0.38	0 100 100	40, 54, 68, 74	0
52	D6	53/54 (98%)	-0.30	0 100 100	42, 58, 68, 74	0
53	B7	48/49 (97%)	-0.39	0 100 100	26, 32, 67, 78	0
53	D7	48/49 (97%)	-0.27	1 (2%) 63 40	27, 34, 66, 79	0
54	B8	64/65 (98%)	-0.33	0 100 100	33, 43, 51, 56	0
54	D8	64/65 (98%)	-0.14	0 100 100	34, 46, 56, 60	0
55	B9	37/37 (100%)	0.14	1 (2%) 56 33	43, 52, 68, 77	0
55	D9	37/37 (100%)	0.26	1 (2%) 56 33	48, 57, 72, 78	0
All	All	20462/21468 (95%)	-0.13	333 (1%) 70 47	14, 65, 95, 119	0

The worst 5 of 333 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	CM	124	PRO	6.6
13	AM	123	ALA	6.0
13	CM	123	ALA	5.9
9	CI	11	LYS	5.2
44	BY	1	MET	5.0

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	2R1	AW	6	10/11	0.76	0.14	66,72,84,91	0
24	MVA	AW	5	8/9	0.77	0.15	69,82,86,91	0
24	004	AW	3	10/11	0.81	0.12	67,87,95,97	0
24	2QY	CW	10	13/14	0.85	0.11	60,72,80,86	0
24	2R1	CW	6	10/11	0.86	0.12	68,82,90,91	0
24	2R3	AW	8	14/15	0.86	0.13	70,78,86,87	0
24	MVA	CW	5	8/9	0.87	0.12	76,88,91,99	0
24	MVA	CW	9	8/9	0.88	0.11	70,73,84,91	0
24	2QY	AW	10	13/14	0.90	0.10	49,70,87,100	0
24	MVA	AW	9	8/9	0.92	0.11	63,74,87,88	0
24	2QZ	AW	1	9/10	0.92	0.10	50,71,82,83	0
24	2R3	CW	8	14/15	0.93	0.08	62,69,77,78	0
24	2QZ	CW	1	9/10	0.94	0.10	63,71,80,101	0
24	004	CW	3	10/11	0.94	0.08	69,78,82,83	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	CA	3147	1/1	0.28	0.30	77,77,77,77	0
56	MG	CA	3139	1/1	0.48	0.22	76,76,76,76	0
56	MG	CA	3114	1/1	0.55	0.18	67,67,67,67	0
56	MG	AA	3180	1/1	0.58	0.29	75,75,75,75	0
56	MG	BA	3661	1/1	0.61	0.19	69,69,69,69	0
56	MG	CA	3156	1/1	0.62	0.21	80,80,80,80	0
56	MG	AA	3093	1/1	0.63	0.25	90,90,90,90	0
56	MG	CA	3142	1/1	0.65	0.21	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3164	1/1	0.65	0.16	43,43,43,43	0
56	MG	DA	3356	1/1	0.65	0.14	57,57,57,57	0
56	MG	CA	3030	1/1	0.66	0.44	74,74,74,74	0
56	MG	CA	3053	1/1	0.66	0.50	87,87,87,87	0
56	MG	AA	3164	1/1	0.66	0.28	61,61,61,61	0
56	MG	AA	3076	1/1	0.67	0.37	74,74,74,74	0
56	MG	AA	3129	1/1	0.68	0.25	77,77,77,77	0
56	MG	BA	3103	1/1	0.68	0.28	58,58,58,58	0
56	MG	AA	3072	1/1	0.68	0.20	69,69,69,69	0
56	MG	DG	3001	1/1	0.68	0.16	68,68,68,68	0
56	MG	BB	3005	1/1	0.69	0.27	62,62,62,62	0
56	MG	BA	3625	1/1	0.69	0.17	80,80,80,80	0
56	MG	CA	3161	1/1	0.69	0.15	71,71,71,71	0
56	MG	AX	108	1/1	0.70	0.26	66,66,66,66	0
56	MG	BA	3203	1/1	0.70	0.17	45,45,45,45	0
56	MG	DA	3540	1/1	0.71	0.16	76,76,76,76	0
56	MG	AA	3200	1/1	0.71	0.24	79,79,79,79	0
56	MG	AA	3021	1/1	0.72	0.18	76,76,76,76	0
56	MG	BA	3704	1/1	0.72	0.20	58,58,58,58	0
56	MG	AA	3094	1/1	0.72	0.13	78,78,78,78	0
56	MG	DA	3568	1/1	0.73	0.18	58,58,58,58	0
56	MG	DA	3619	1/1	0.73	0.17	67,67,67,67	0
56	MG	AA	3133	1/1	0.73	0.41	71,71,71,71	0
56	MG	CA	3025	1/1	0.74	0.18	102,102,102,102	0
56	MG	AA	3087	1/1	0.74	0.21	87,87,87,87	0
56	MG	DA	3567	1/1	0.74	0.15	68,68,68,68	0
56	MG	AS	3001	1/1	0.74	0.16	79,79,79,79	0
56	MG	AX	104	1/1	0.74	0.11	62,62,62,62	0
56	MG	BA	3620	1/1	0.74	0.22	57,57,57,57	0
56	MG	CA	3129	1/1	0.75	0.21	54,54,54,54	0
56	MG	AA	3002	1/1	0.75	0.14	74,74,74,74	0
56	MG	DA	3464	1/1	0.75	0.11	51,51,51,51	0
56	MG	DA	3630	1/1	0.75	0.12	67,67,67,67	0
56	MG	DB	3003	1/1	0.75	0.21	70,70,70,70	0
56	MG	AA	3022	1/1	0.75	0.19	56,56,56,56	0
56	MG	DA	3001	1/1	0.76	0.37	76,76,76,76	0
56	MG	DA	3115	1/1	0.76	0.11	64,64,64,64	0
56	MG	CA	3073	1/1	0.76	0.22	74,74,74,74	0
56	MG	DA	3436	1/1	0.76	0.11	61,61,61,61	0
56	MG	DA	3456	1/1	0.76	0.20	58,58,58,58	0
56	MG	AA	3209	1/1	0.76	0.16	66,66,66,66	0
56	MG	DA	3500	1/1	0.76	0.30	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BF	306	1/1	0.76	0.13	52,52,52,52	0
56	MG	AA	3063	1/1	0.76	0.18	57,57,57,57	0
56	MG	CA	3027	1/1	0.76	0.14	64,64,64,64	0
56	MG	DA	3602	1/1	0.76	0.17	63,63,63,63	0
56	MG	AA	3131	1/1	0.76	0.25	65,65,65,65	0
56	MG	BA	3582	1/1	0.76	0.16	52,52,52,52	0
56	MG	DA	3639	1/1	0.76	0.22	55,55,55,55	0
56	MG	CA	3061	1/1	0.76	0.36	68,68,68,68	0
56	MG	CA	3070	1/1	0.76	0.21	59,59,59,59	0
56	MG	CA	3119	1/1	0.77	0.29	73,73,73,73	0
56	MG	DA	3603	1/1	0.77	0.17	66,66,66,66	0
56	MG	BA	3711	1/1	0.77	0.28	64,64,64,64	0
56	MG	CA	3009	1/1	0.77	0.14	55,55,55,55	0
56	MG	BA	3708	1/1	0.77	0.16	38,38,38,38	0
56	MG	CA	3056	1/1	0.77	0.19	63,63,63,63	0
56	MG	CA	3117	1/1	0.77	0.11	58,58,58,58	0
56	MG	BA	3740	1/1	0.78	0.26	57,57,57,57	0
56	MG	CA	3172	1/1	0.78	0.19	65,65,65,65	0
56	MG	BA	3133	1/1	0.78	0.34	53,53,53,53	0
56	MG	DA	3462	1/1	0.78	0.19	71,71,71,71	0
56	MG	DA	3066	1/1	0.78	0.25	59,59,59,59	0
56	MG	CA	3144	1/1	0.78	0.26	84,84,84,84	0
56	MG	DA	3123	1/1	0.78	0.10	61,61,61,61	0
56	MG	DA	3220	1/1	0.78	0.06	61,61,61,61	0
56	MG	AA	3189	1/1	0.79	0.13	74,74,74,74	0
56	MG	CA	3152	1/1	0.79	0.21	45,45,45,45	0
56	MG	DA	3131	1/1	0.79	0.09	60,60,60,60	0
56	MG	DA	3141	1/1	0.79	0.22	63,63,63,63	0
56	MG	BA	3358	1/1	0.79	0.12	78,78,78,78	0
56	MG	DA	3296	1/1	0.79	0.19	65,65,65,65	0
56	MG	CA	3007	1/1	0.79	0.11	63,63,63,63	0
56	MG	AA	3115	1/1	0.79	0.27	67,67,67,67	0
56	MG	AA	3067	1/1	0.79	0.29	76,76,76,76	0
56	MG	DB	3001	1/1	0.79	0.17	80,80,80,80	0
56	MG	AA	3112	1/1	0.79	0.14	53,53,53,53	0
56	MG	CA	3091	1/1	0.79	0.11	95,95,95,95	0
56	MG	CA	3028	1/1	0.80	0.44	62,62,62,62	0
56	MG	DA	3241	1/1	0.80	0.08	74,74,74,74	0
56	MG	AA	3136	1/1	0.80	0.14	68,68,68,68	0
56	MG	AA	3117	1/1	0.80	0.18	64,64,64,64	0
56	MG	DA	3073	1/1	0.80	0.23	50,50,50,50	0
56	MG	DA	3441	1/1	0.80	0.11	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	DA	3627	1/1	0.80	0.14	52,52,52,52	0
56	MG	AA	3030	1/1	0.80	0.39	66,66,66,66	0
56	MG	CA	3060	1/1	0.80	0.27	59,59,59,59	0
56	MG	BA	3247	1/1	0.80	0.26	58,58,58,58	0
56	MG	BA	3292	1/1	0.80	0.27	59,59,59,59	0
56	MG	DA	3506	1/1	0.80	0.11	61,61,61,61	0
56	MG	BA	3636	1/1	0.81	0.13	54,54,54,54	0
56	MG	CA	3159	1/1	0.81	0.25	76,76,76,76	0
56	MG	DA	3113	1/1	0.81	0.45	61,61,61,61	0
56	MG	DA	3346	1/1	0.81	0.10	64,64,64,64	0
56	MG	BA	3510	1/1	0.81	0.24	66,66,66,66	0
56	MG	AA	3184	1/1	0.81	0.16	81,81,81,81	0
56	MG	AA	3217	1/1	0.81	0.30	64,64,64,64	0
56	MG	AD	502	1/1	0.81	0.30	56,56,56,56	0
56	MG	CA	3048	1/1	0.82	0.32	70,70,70,70	0
56	MG	DA	3414	1/1	0.82	0.18	59,59,59,59	0
56	MG	DA	3418	1/1	0.82	0.14	57,57,57,57	0
56	MG	BA	3338	1/1	0.82	0.18	62,62,62,62	0
56	MG	BA	3710	1/1	0.82	0.15	57,57,57,57	0
56	MG	AA	3127	1/1	0.82	0.20	50,50,50,50	0
56	MG	BA	3060	1/1	0.82	0.31	64,64,64,64	0
56	MG	AA	3114	1/1	0.82	0.18	73,73,73,73	0
56	MG	DA	3496	1/1	0.82	0.20	76,76,76,76	0
56	MG	BB	3014	1/1	0.82	0.17	68,68,68,68	0
56	MG	BB	3017	1/1	0.82	0.29	80,80,80,80	0
56	MG	DA	3537	1/1	0.82	0.15	74,74,74,74	0
56	MG	CA	3110	1/1	0.82	0.15	93,93,93,93	0
56	MG	DA	3554	1/1	0.82	0.06	62,62,62,62	0
56	MG	DA	3566	1/1	0.82	0.18	55,55,55,55	0
56	MG	AA	3171	1/1	0.82	0.15	77,77,77,77	0
56	MG	BA	3177	1/1	0.82	0.43	35,35,35,35	0
56	MG	AA	3023	1/1	0.82	0.13	56,56,56,56	0
56	MG	AA	3132	1/1	0.82	0.16	59,59,59,59	0
56	MG	DA	3606	1/1	0.82	0.14	58,58,58,58	0
56	MG	DA	3617	1/1	0.82	0.12	51,51,51,51	0
56	MG	BA	3693	1/1	0.82	0.22	57,57,57,57	0
56	MG	DA	3162	1/1	0.82	0.18	69,69,69,69	0
56	MG	DA	3169	1/1	0.82	0.24	58,58,58,58	0
56	MG	CA	3141	1/1	0.82	0.39	85,85,85,85	0
56	MG	DA	3642	1/1	0.82	0.21	67,67,67,67	0
56	MG	AA	3032	1/1	0.82	0.28	65,65,65,65	0
56	MG	BA	3705	1/1	0.82	0.14	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3033	1/1	0.82	0.14	64,64,64,64	0
56	MG	AA	3039	1/1	0.83	0.10	62,62,62,62	0
56	MG	AA	3162	1/1	0.83	0.17	79,79,79,79	0
56	MG	AA	3126	1/1	0.83	0.21	54,54,54,54	0
56	MG	DA	3086	1/1	0.83	0.20	43,43,43,43	0
56	MG	DA	3108	1/1	0.83	0.11	50,50,50,50	0
56	MG	AA	3016	1/1	0.83	0.10	70,70,70,70	0
56	MG	CA	3029	1/1	0.83	0.16	54,54,54,54	0
56	MG	DA	3122	1/1	0.83	0.12	60,60,60,60	0
56	MG	AA	3178	1/1	0.83	0.16	63,63,63,63	0
56	MG	CA	3136	1/1	0.83	0.25	70,70,70,70	0
56	MG	CA	3032	1/1	0.83	0.20	44,44,44,44	0
56	MG	AA	3098	1/1	0.83	0.37	76,76,76,76	0
56	MG	CA	3039	1/1	0.83	0.32	82,82,82,82	0
56	MG	DA	3171	1/1	0.83	0.26	58,58,58,58	0
56	MG	AA	3029	1/1	0.83	0.32	60,60,60,60	0
56	MG	BA	3601	1/1	0.83	0.16	61,61,61,61	0
56	MG	AA	3089	1/1	0.83	0.24	80,80,80,80	0
56	MG	AA	3196	1/1	0.83	0.33	78,78,78,78	0
56	MG	AA	3092	1/1	0.83	0.25	59,59,59,59	0
56	MG	DA	3393	1/1	0.83	0.17	35,35,35,35	0
56	MG	CA	3065	1/1	0.83	0.17	81,81,81,81	0
56	MG	BW	3001	1/1	0.83	0.13	55,55,55,55	0
56	MG	BA	3180	1/1	0.83	0.25	48,48,48,48	0
56	MG	CX	103	1/1	0.83	0.08	57,57,57,57	0
59	FME	CX	101	10/11	0.83	0.25	59,80,100,106	0
56	MG	CA	3081	1/1	0.84	0.14	72,72,72,72	0
56	MG	BA	3648	1/1	0.84	0.13	54,54,54,54	0
56	MG	AA	3106	1/1	0.84	0.29	68,68,68,68	0
56	MG	DA	3514	1/1	0.84	0.17	60,60,60,60	0
56	MG	DA	3531	1/1	0.84	0.08	44,44,44,44	0
56	MG	BA	3686	1/1	0.84	0.25	65,65,65,65	0
56	MG	BD	305	1/1	0.84	0.17	41,41,41,41	0
56	MG	DA	3549	1/1	0.84	0.19	73,73,73,73	0
56	MG	CA	3041	1/1	0.84	0.31	71,71,71,71	0
56	MG	AA	3017	1/1	0.84	0.25	57,57,57,57	0
56	MG	DA	3246	1/1	0.84	0.10	55,55,55,55	0
56	MG	CA	3135	1/1	0.84	0.20	61,61,61,61	0
56	MG	DA	3586	1/1	0.84	0.12	57,57,57,57	0
56	MG	DA	3314	1/1	0.84	0.14	56,56,56,56	0
56	MG	AA	3134	1/1	0.84	0.29	70,70,70,70	0
56	MG	AA	3045	1/1	0.84	0.26	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	DA	3613	1/1	0.84	0.20	64,64,64,64	0
56	MG	DA	3096	1/1	0.84	0.14	68,68,68,68	0
56	MG	DA	3405	1/1	0.84	0.24	53,53,53,53	0
56	MG	DA	3098	1/1	0.84	0.35	45,45,45,45	0
56	MG	BA	3616	1/1	0.84	0.18	73,73,73,73	0
56	MG	DA	3424	1/1	0.84	0.13	58,58,58,58	0
56	MG	AA	3147	1/1	0.84	0.14	51,51,51,51	0
56	MG	BA	3294	1/1	0.84	0.20	59,59,59,59	0
56	MG	BA	3716	1/1	0.84	0.20	77,77,77,77	0
56	MG	DB	3011	1/1	0.84	0.17	49,49,49,49	0
56	MG	AA	3148	1/1	0.84	0.14	72,72,72,72	0
56	MG	DA	3124	1/1	0.84	0.17	66,66,66,66	0
56	MG	CA	3122	1/1	0.85	0.18	70,70,70,70	0
56	MG	DA	3102	1/1	0.85	0.11	49,49,49,49	0
56	MG	CA	3125	1/1	0.85	0.17	64,64,64,64	0
56	MG	DA	3109	1/1	0.85	0.14	55,55,55,55	0
56	MG	CA	3127	1/1	0.85	0.12	72,72,72,72	0
56	MG	DA	3468	1/1	0.85	0.13	47,47,47,47	0
56	MG	DA	3491	1/1	0.85	0.23	55,55,55,55	0
56	MG	AA	3064	1/1	0.85	0.07	65,65,65,65	0
56	MG	BA	3465	1/1	0.85	0.12	51,51,51,51	0
56	MG	BA	3467	1/1	0.85	0.09	44,44,44,44	0
56	MG	BA	3473	1/1	0.85	0.13	55,55,55,55	0
56	MG	AA	3079	1/1	0.85	0.27	65,65,65,65	0
56	MG	BA	3538	1/1	0.85	0.13	29,29,29,29	0
56	MG	DA	3153	1/1	0.85	0.21	51,51,51,51	0
56	MG	DA	3155	1/1	0.85	0.15	50,50,50,50	0
56	MG	BA	3567	1/1	0.85	0.07	54,54,54,54	0
56	MG	DA	3557	1/1	0.85	0.13	74,74,74,74	0
56	MG	DA	3563	1/1	0.85	0.14	49,49,49,49	0
56	MG	AA	3053	1/1	0.85	0.20	56,56,56,56	0
56	MG	BA	3186	1/1	0.85	0.18	50,50,50,50	0
56	MG	DA	3212	1/1	0.85	0.17	48,48,48,48	0
56	MG	AA	3088	1/1	0.85	0.25	53,53,53,53	0
56	MG	DA	3591	1/1	0.85	0.13	67,67,67,67	0
56	MG	BA	3223	1/1	0.85	0.22	49,49,49,49	0
56	MG	AA	3025	1/1	0.85	0.11	78,78,78,78	0
56	MG	DA	3251	1/1	0.85	0.22	50,50,50,50	0
56	MG	DA	3607	1/1	0.85	0.21	68,68,68,68	0
56	MG	DA	3263	1/1	0.85	0.14	48,48,48,48	0
56	MG	BA	3248	1/1	0.85	0.33	68,68,68,68	0
56	MG	DA	3618	1/1	0.85	0.15	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	DA	3306	1/1	0.85	0.11	51,51,51,51	0
56	MG	DA	3620	1/1	0.85	0.15	66,66,66,66	0
56	MG	BA	3022	1/1	0.85	0.23	66,66,66,66	0
56	MG	DA	3333	1/1	0.85	0.09	61,61,61,61	0
56	MG	BA	3293	1/1	0.85	0.29	69,69,69,69	0
56	MG	CA	3103	1/1	0.85	0.14	101,101,101,101	0
56	MG	DA	3005	1/1	0.85	0.09	50,50,50,50	0
56	MG	BA	3667	1/1	0.85	0.18	72,72,72,72	0
56	MG	DB	3010	1/1	0.85	0.17	66,66,66,66	0
56	MG	AA	3090	1/1	0.85	0.23	64,64,64,64	0
56	MG	AA	3074	1/1	0.85	0.20	40,40,40,40	0
56	MG	DQ	3004	1/1	0.85	0.12	52,52,52,52	0
59	FME	AX	101	10/11	0.85	0.22	55,74,92,107	0
56	MG	BA	3694	1/1	0.85	0.15	48,48,48,48	0
56	MG	DA	3060	1/1	0.86	0.07	51,51,51,51	0
56	MG	BB	3001	1/1	0.86	0.17	56,56,56,56	0
56	MG	BA	3028	1/1	0.86	0.25	59,59,59,59	0
56	MG	DA	3074	1/1	0.86	0.24	60,60,60,60	0
56	MG	DA	3084	1/1	0.86	0.10	55,55,55,55	0
56	MG	BA	3597	1/1	0.86	0.14	46,46,46,46	0
56	MG	DA	3093	1/1	0.86	0.14	51,51,51,51	0
56	MG	AA	3061	1/1	0.86	0.10	57,57,57,57	0
56	MG	CA	3109	1/1	0.86	0.16	79,79,79,79	0
56	MG	BB	3018	1/1	0.86	0.15	54,54,54,54	0
56	MG	DA	3504	1/1	0.86	0.10	46,46,46,46	0
56	MG	BA	3257	1/1	0.86	0.21	56,56,56,56	0
56	MG	CA	3116	1/1	0.86	0.16	76,76,76,76	0
56	MG	BA	3289	1/1	0.86	0.17	53,53,53,53	0
56	MG	BA	3066	1/1	0.86	0.20	49,49,49,49	0
56	MG	B7	101	1/1	0.86	0.16	45,45,45,45	0
56	MG	BA	3068	1/1	0.86	0.26	43,43,43,43	0
56	MG	BA	3641	1/1	0.86	0.09	33,33,33,33	0
56	MG	AF	3001	1/1	0.86	0.16	62,62,62,62	0
56	MG	BA	3651	1/1	0.86	0.23	52,52,52,52	0
56	MG	BA	3301	1/1	0.86	0.18	44,44,44,44	0
56	MG	BA	3123	1/1	0.86	0.11	47,47,47,47	0
56	MG	AA	3020	1/1	0.86	0.09	80,80,80,80	0
56	MG	BA	3433	1/1	0.86	0.24	46,46,46,46	0
56	MG	DA	3589	1/1	0.86	0.14	65,65,65,65	0
56	MG	AA	3097	1/1	0.86	0.31	53,53,53,53	0
56	MG	DA	3596	1/1	0.86	0.22	68,68,68,68	0
56	MG	BA	3701	1/1	0.86	0.11	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3702	1/1	0.86	0.11	56,56,56,56	0
56	MG	CA	3153	1/1	0.86	0.15	85,85,85,85	0
56	MG	DA	3243	1/1	0.86	0.22	49,49,49,49	0
56	MG	DA	3608	1/1	0.86	0.23	63,63,63,63	0
56	MG	AX	105	1/1	0.86	0.20	72,72,72,72	0
56	MG	CA	3158	1/1	0.86	0.12	64,64,64,64	0
56	MG	AA	3082	1/1	0.86	0.26	52,52,52,52	0
56	MG	DA	3281	1/1	0.86	0.09	33,33,33,33	0
56	MG	DA	3289	1/1	0.86	0.21	64,64,64,64	0
56	MG	BA	3014	1/1	0.86	0.29	48,48,48,48	0
56	MG	CA	3162	1/1	0.86	0.16	60,60,60,60	0
56	MG	BA	3530	1/1	0.86	0.14	72,72,72,72	0
56	MG	CA	3168	1/1	0.86	0.28	79,79,79,79	0
56	MG	DA	3645	1/1	0.86	0.19	57,57,57,57	0
56	MG	AA	3028	1/1	0.86	0.24	72,72,72,72	0
56	MG	CE	3001	1/1	0.86	0.19	66,66,66,66	0
56	MG	DA	3361	1/1	0.86	0.18	58,58,58,58	0
56	MG	DA	3392	1/1	0.86	0.10	60,60,60,60	0
56	MG	BA	3565	1/1	0.86	0.14	75,75,75,75	0
56	MG	CA	3067	1/1	0.86	0.16	66,66,66,66	0
56	MG	D3	101	1/1	0.86	0.12	54,54,54,54	0
56	MG	BA	3224	1/1	0.86	0.15	48,48,48,48	0
56	MG	DA	3035	1/1	0.86	0.16	58,58,58,58	0
60	K	BA	3304	1/1	0.86	0.19	93,93,93,93	0
56	MG	BA	3143	1/1	0.87	0.39	41,41,41,41	0
56	MG	BA	3156	1/1	0.87	0.25	61,61,61,61	0
56	MG	BA	3173	1/1	0.87	0.17	41,41,41,41	0
56	MG	BA	3357	1/1	0.87	0.15	45,45,45,45	0
56	MG	BA	3027	1/1	0.87	0.13	53,53,53,53	0
56	MG	BA	3674	1/1	0.87	0.17	67,67,67,67	0
56	MG	BA	3369	1/1	0.87	0.14	49,49,49,49	0
56	MG	AA	3015	1/1	0.87	0.12	74,74,74,74	0
56	MG	BA	3184	1/1	0.87	0.23	51,51,51,51	0
56	MG	CA	3145	1/1	0.87	0.08	67,67,67,67	0
56	MG	DA	3534	1/1	0.87	0.12	62,62,62,62	0
56	MG	CA	3146	1/1	0.87	0.15	61,61,61,61	0
56	MG	CA	3038	1/1	0.87	0.09	54,54,54,54	0
56	MG	CA	3150	1/1	0.87	0.12	63,63,63,63	0
56	MG	AA	3078	1/1	0.87	0.31	55,55,55,55	0
56	MG	BA	3469	1/1	0.87	0.12	60,60,60,60	0
56	MG	DA	3189	1/1	0.87	0.19	55,55,55,55	0
56	MG	AA	3068	1/1	0.87	0.21	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3157	1/1	0.87	0.11	56,56,56,56	0
56	MG	DA	3224	1/1	0.87	0.23	53,53,53,53	0
56	MG	DA	3585	1/1	0.87	0.25	62,62,62,62	0
56	MG	CA	3050	1/1	0.87	0.22	54,54,54,54	0
56	MG	BA	3212	1/1	0.87	0.20	47,47,47,47	0
56	MG	CA	3054	1/1	0.87	0.23	74,74,74,74	0
56	MG	AA	3141	1/1	0.87	0.18	51,51,51,51	0
56	MG	BA	3071	1/1	0.87	0.19	55,55,55,55	0
56	MG	BA	3563	1/1	0.87	0.38	66,66,66,66	0
56	MG	DA	3287	1/1	0.87	0.08	53,53,53,53	0
56	MG	BA	3088	1/1	0.87	0.08	55,55,55,55	0
56	MG	BA	3739	1/1	0.87	0.10	50,50,50,50	0
56	MG	AA	3080	1/1	0.87	0.22	58,58,58,58	0
56	MG	BA	3119	1/1	0.87	0.12	56,56,56,56	0
56	MG	DA	3323	1/1	0.87	0.09	60,60,60,60	0
56	MG	CA	3074	1/1	0.87	0.15	56,56,56,56	0
56	MG	BA	3596	1/1	0.87	0.11	79,79,79,79	0
56	MG	DA	3621	1/1	0.87	0.16	46,46,46,46	0
56	MG	BA	3262	1/1	0.87	0.32	44,44,44,44	0
56	MG	DA	3628	1/1	0.87	0.10	38,38,38,38	0
56	MG	DA	3062	1/1	0.87	0.23	58,58,58,58	0
56	MG	DA	3367	1/1	0.87	0.19	55,55,55,55	0
56	MG	DA	3391	1/1	0.87	0.10	54,54,54,54	0
56	MG	BA	3267	1/1	0.87	0.19	56,56,56,56	0
56	MG	BA	3272	1/1	0.87	0.21	49,49,49,49	0
56	MG	AA	3219	1/1	0.87	0.16	54,54,54,54	0
56	MG	DB	3006	1/1	0.87	0.10	54,54,54,54	0
56	MG	AA	3081	1/1	0.87	0.25	46,46,46,46	0
56	MG	BA	3634	1/1	0.87	0.14	77,77,77,77	0
56	MG	BX	102	1/1	0.87	0.22	60,60,60,60	0
56	MG	DA	3095	1/1	0.87	0.22	53,53,53,53	0
56	MG	DY	502	1/1	0.87	0.13	66,66,66,66	0
56	MG	BA	3137	1/1	0.87	0.15	59,59,59,59	0
56	MG	DA	3448	1/1	0.87	0.21	67,67,67,67	0
56	MG	CA	3004	1/1	0.87	0.15	88,88,88,88	0
56	MG	DA	3460	1/1	0.87	0.13	47,47,47,47	0
56	MG	DA	3344	1/1	0.88	0.07	48,48,48,48	0
56	MG	AA	3047	1/1	0.88	0.22	59,59,59,59	0
56	MG	BA	3644	1/1	0.88	0.13	38,38,38,38	0
56	MG	CA	3160	1/1	0.88	0.14	49,49,49,49	0
56	MG	AA	3207	1/1	0.88	0.16	51,51,51,51	0
56	MG	BA	3328	1/1	0.88	0.15	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	3335	1/1	0.88	0.19	51,51,51,51	0
56	MG	CA	3034	1/1	0.88	0.26	66,66,66,66	0
56	MG	CA	3171	1/1	0.88	0.16	61,61,61,61	0
56	MG	BA	3172	1/1	0.88	0.13	54,54,54,54	0
56	MG	BA	3669	1/1	0.88	0.12	61,61,61,61	0
56	MG	CN	502	1/1	0.88	0.18	70,70,70,70	0
56	MG	AA	3100	1/1	0.88	0.18	43,43,43,43	0
56	MG	BA	3675	1/1	0.88	0.28	68,68,68,68	0
56	MG	AA	3215	1/1	0.88	0.33	77,77,77,77	0
56	MG	DA	3008	1/1	0.88	0.12	56,56,56,56	0
56	MG	BA	3039	1/1	0.88	0.15	44,44,44,44	0
56	MG	DA	3039	1/1	0.88	0.25	46,46,46,46	0
56	MG	DA	3040	1/1	0.88	0.15	45,45,45,45	0
56	MG	DA	3055	1/1	0.88	0.20	55,55,55,55	0
56	MG	DA	3057	1/1	0.88	0.17	57,57,57,57	0
56	MG	BA	3373	1/1	0.88	0.07	48,48,48,48	0
56	MG	BA	3429	1/1	0.88	0.20	55,55,55,55	0
56	MG	AA	3102	1/1	0.88	0.20	68,68,68,68	0
56	MG	BA	3064	1/1	0.88	0.10	49,49,49,49	0
56	MG	CA	3064	1/1	0.88	0.11	74,74,74,74	0
56	MG	AA	3218	1/1	0.88	0.14	73,73,73,73	0
56	MG	DA	3532	1/1	0.88	0.14	60,60,60,60	0
56	MG	BA	3204	1/1	0.88	0.12	48,48,48,48	0
56	MG	DA	3536	1/1	0.88	0.09	57,57,57,57	0
56	MG	BA	3709	1/1	0.88	0.14	77,77,77,77	0
56	MG	CA	3071	1/1	0.88	0.25	64,64,64,64	0
56	MG	BA	3209	1/1	0.88	0.22	39,39,39,39	0
56	MG	BA	3499	1/1	0.88	0.22	50,50,50,50	0
56	MG	AA	3070	1/1	0.88	0.14	68,68,68,68	0
56	MG	CA	3086	1/1	0.88	0.19	70,70,70,70	0
56	MG	BA	3717	1/1	0.88	0.13	51,51,51,51	0
56	MG	DA	3112	1/1	0.88	0.21	49,49,49,49	0
56	MG	BA	3514	1/1	0.88	0.13	49,49,49,49	0
56	MG	BA	3213	1/1	0.88	0.14	63,63,63,63	0
56	MG	BA	3070	1/1	0.88	0.10	46,46,46,46	0
56	MG	CA	3111	1/1	0.88	0.16	69,69,69,69	0
56	MG	CA	3112	1/1	0.88	0.20	69,69,69,69	0
56	MG	AA	3176	1/1	0.88	0.16	60,60,60,60	0
56	MG	DA	3134	1/1	0.88	0.13	37,37,37,37	0
56	MG	BA	3238	1/1	0.88	0.15	48,48,48,48	0
56	MG	BA	3240	1/1	0.88	0.24	54,54,54,54	0
56	MG	BA	3571	1/1	0.88	0.11	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3121	1/1	0.88	0.27	59,59,59,59	0
56	MG	BD	304	1/1	0.88	0.17	41,41,41,41	0
56	MG	DA	3170	1/1	0.88	0.09	45,45,45,45	0
56	MG	CA	3124	1/1	0.88	0.12	64,64,64,64	0
56	MG	AA	3071	1/1	0.88	0.23	60,60,60,60	0
56	MG	AA	3027	1/1	0.88	0.11	67,67,67,67	0
56	MG	BG	3003	1/1	0.88	0.14	53,53,53,53	0
56	MG	BN	3002	1/1	0.88	0.11	52,52,52,52	0
56	MG	DA	3230	1/1	0.88	0.19	61,61,61,61	0
56	MG	DA	3240	1/1	0.88	0.23	58,58,58,58	0
56	MG	BQ	3002	1/1	0.88	0.09	51,51,51,51	0
56	MG	BA	3107	1/1	0.88	0.23	60,60,60,60	0
56	MG	AX	103	1/1	0.88	0.06	57,57,57,57	0
56	MG	BA	3122	1/1	0.88	0.10	68,68,68,68	0
56	MG	DA	3255	1/1	0.88	0.17	46,46,46,46	0
56	MG	CA	3003	1/1	0.88	0.13	69,69,69,69	0
56	MG	AA	3065	1/1	0.88	0.25	50,50,50,50	0
56	MG	AA	3086	1/1	0.88	0.12	65,65,65,65	0
56	MG	CA	3008	1/1	0.88	0.35	59,59,59,59	0
56	MG	DQ	3003	1/1	0.88	0.18	58,58,58,58	0
56	MG	BA	3135	1/1	0.88	0.22	57,57,57,57	0
56	MG	CA	3021	1/1	0.88	0.16	54,54,54,54	0
56	MG	CA	3022	1/1	0.88	0.10	67,67,67,67	0
56	MG	AA	3033	1/1	0.88	0.23	68,68,68,68	0
56	MG	BA	3638	1/1	0.88	0.11	73,73,73,73	0
56	MG	DA	3336	1/1	0.88	0.12	36,36,36,36	0
56	MG	BA	3317	1/1	0.89	0.16	40,40,40,40	0
56	MG	CA	3042	1/1	0.89	0.27	69,69,69,69	0
56	MG	DA	3119	1/1	0.89	0.10	44,44,44,44	0
56	MG	DA	3121	1/1	0.89	0.10	46,46,46,46	0
56	MG	CA	3047	1/1	0.89	0.14	56,56,56,56	0
56	MG	DA	3465	1/1	0.89	0.08	41,41,41,41	0
56	MG	AA	3003	1/1	0.89	0.13	70,70,70,70	0
56	MG	BA	3604	1/1	0.89	0.20	64,64,64,64	0
56	MG	AA	3203	1/1	0.89	0.12	76,76,76,76	0
56	MG	BB	3003	1/1	0.89	0.14	40,40,40,40	0
56	MG	BA	3208	1/1	0.89	0.18	50,50,50,50	0
56	MG	BA	3621	1/1	0.89	0.11	57,57,57,57	0
56	MG	AA	3128	1/1	0.89	0.22	64,64,64,64	0
56	MG	DA	3524	1/1	0.89	0.09	51,51,51,51	0
56	MG	DA	3529	1/1	0.89	0.22	72,72,72,72	0
56	MG	DA	3157	1/1	0.89	0.29	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	3633	1/1	0.89	0.20	54,54,54,54	0
56	MG	BA	3021	1/1	0.89	0.15	62,62,62,62	0
56	MG	AA	3004	1/1	0.89	0.17	50,50,50,50	0
56	MG	BD	309	1/1	0.89	0.18	43,43,43,43	0
56	MG	BD	311	1/1	0.89	0.28	53,53,53,53	0
56	MG	CA	3072	1/1	0.89	0.19	57,57,57,57	0
56	MG	BF	303	1/1	0.89	0.18	42,42,42,42	0
56	MG	DA	3222	1/1	0.89	0.08	45,45,45,45	0
56	MG	BA	3637	1/1	0.89	0.60	52,52,52,52	0
56	MG	AA	3085	1/1	0.89	0.23	57,57,57,57	0
56	MG	DA	3235	1/1	0.89	0.17	46,46,46,46	0
56	MG	AA	3013	1/1	0.89	0.07	75,75,75,75	0
56	MG	BA	3230	1/1	0.89	0.30	70,70,70,70	0
56	MG	BA	3447	1/1	0.89	0.09	76,76,76,76	0
56	MG	DA	3587	1/1	0.89	0.16	57,57,57,57	0
56	MG	CA	3107	1/1	0.89	0.23	71,71,71,71	0
56	MG	DA	3022	1/1	0.89	0.13	41,41,41,41	0
56	MG	DA	3595	1/1	0.89	0.11	53,53,53,53	0
56	MG	DA	3029	1/1	0.89	0.17	62,62,62,62	0
56	MG	DA	3598	1/1	0.89	0.07	45,45,45,45	0
56	MG	DA	3256	1/1	0.89	0.13	41,41,41,41	0
56	MG	BA	3460	1/1	0.89	0.17	66,66,66,66	0
56	MG	AA	3056	1/1	0.89	0.24	61,61,61,61	0
56	MG	DA	3282	1/1	0.89	0.14	58,58,58,58	0
56	MG	AA	3037	1/1	0.89	0.16	53,53,53,53	0
56	MG	DA	3043	1/1	0.89	0.27	56,56,56,56	0
56	MG	BA	3149	1/1	0.89	0.13	58,58,58,58	0
56	MG	AA	3120	1/1	0.89	0.22	53,53,53,53	0
56	MG	BA	3158	1/1	0.89	0.32	43,43,43,43	0
56	MG	BA	3681	1/1	0.89	0.24	54,54,54,54	0
56	MG	DA	3326	1/1	0.89	0.16	61,61,61,61	0
56	MG	CA	3015	1/1	0.89	0.14	53,53,53,53	0
56	MG	DA	3069	1/1	0.89	0.17	49,49,49,49	0
56	MG	BA	3164	1/1	0.89	0.17	57,57,57,57	0
56	MG	DA	3637	1/1	0.89	0.17	59,59,59,59	0
56	MG	AA	3140	1/1	0.89	0.10	65,65,65,65	0
56	MG	DA	3351	1/1	0.89	0.12	58,58,58,58	0
56	MG	DA	3078	1/1	0.89	0.15	49,49,49,49	0
56	MG	DA	3646	1/1	0.89	0.08	42,42,42,42	0
56	MG	BA	3520	1/1	0.89	0.12	69,69,69,69	0
56	MG	AM	3002	1/1	0.89	0.25	60,60,60,60	0
56	MG	AA	3019	1/1	0.89	0.17	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3178	1/1	0.89	0.17	51,51,51,51	0
56	MG	AA	3194	1/1	0.89	0.16	50,50,50,50	0
56	MG	DB	3012	1/1	0.89	0.22	50,50,50,50	0
56	MG	DF	304	1/1	0.89	0.24	39,39,39,39	0
56	MG	AA	3143	1/1	0.89	0.15	67,67,67,67	0
56	MG	DA	3099	1/1	0.89	0.20	39,39,39,39	0
56	MG	BA	3299	1/1	0.89	0.24	56,56,56,56	0
56	MG	BA	3300	1/1	0.89	0.18	48,48,48,48	0
56	MG	DA	3425	1/1	0.89	0.17	51,51,51,51	0
56	MG	D8	5001	1/1	0.89	0.21	53,53,53,53	0
56	MG	BA	3583	1/1	0.89	0.20	57,57,57,57	0
56	MG	BA	3094	1/1	0.89	0.19	62,62,62,62	0
56	MG	DA	3445	1/1	0.89	0.33	60,60,60,60	0
60	K	DA	3234	1/1	0.89	0.21	102,102,102,102	0
56	MG	BQ	3004	1/1	0.90	0.10	41,41,41,41	0
56	MG	DA	3079	1/1	0.90	0.09	44,44,44,44	0
56	MG	BR	203	1/1	0.90	0.14	48,48,48,48	0
56	MG	BV	3002	1/1	0.90	0.28	42,42,42,42	0
56	MG	DA	3087	1/1	0.90	0.15	43,43,43,43	0
56	MG	DA	3089	1/1	0.90	0.07	51,51,51,51	0
56	MG	DA	3431	1/1	0.90	0.15	56,56,56,56	0
56	MG	DA	3435	1/1	0.90	0.11	56,56,56,56	0
56	MG	CA	3113	1/1	0.90	0.23	84,84,84,84	0
56	MG	DA	3437	1/1	0.90	0.18	46,46,46,46	0
56	MG	BA	3477	1/1	0.90	0.17	52,52,52,52	0
56	MG	DA	3444	1/1	0.90	0.17	43,43,43,43	0
56	MG	BA	3663	1/1	0.90	0.23	73,73,73,73	0
56	MG	DA	3447	1/1	0.90	0.12	56,56,56,56	0
56	MG	B2	101	1/1	0.90	0.09	34,34,34,34	0
56	MG	DA	3452	1/1	0.90	0.23	64,64,64,64	0
56	MG	BA	3666	1/1	0.90	0.31	54,54,54,54	0
56	MG	DA	3458	1/1	0.90	0.11	47,47,47,47	0
56	MG	BA	3485	1/1	0.90	0.11	67,67,67,67	0
56	MG	DA	3106	1/1	0.90	0.29	45,45,45,45	0
56	MG	AX	106	1/1	0.90	0.10	64,64,64,64	0
56	MG	BA	3672	1/1	0.90	0.15	63,63,63,63	0
56	MG	DA	3110	1/1	0.90	0.13	46,46,46,46	0
56	MG	DA	3475	1/1	0.90	0.08	35,35,35,35	0
56	MG	DA	3477	1/1	0.90	0.28	35,35,35,35	0
56	MG	AA	3005	1/1	0.90	0.34	66,66,66,66	0
56	MG	DA	3495	1/1	0.90	0.08	53,53,53,53	0
56	MG	CA	3126	1/1	0.90	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	DA	3498	1/1	0.90	0.15	75,75,75,75	0
56	MG	BA	3512	1/1	0.90	0.12	42,42,42,42	0
56	MG	DA	3116	1/1	0.90	0.12	43,43,43,43	0
56	MG	BA	3006	1/1	0.90	0.10	46,46,46,46	0
56	MG	BA	3284	1/1	0.90	0.45	76,76,76,76	0
56	MG	DA	3523	1/1	0.90	0.08	47,47,47,47	0
56	MG	BA	3007	1/1	0.90	0.13	55,55,55,55	0
56	MG	DA	3528	1/1	0.90	0.10	33,33,33,33	0
56	MG	AA	3099	1/1	0.90	0.21	49,49,49,49	0
56	MG	BA	3696	1/1	0.90	0.13	36,36,36,36	0
56	MG	BA	3549	1/1	0.90	0.24	49,49,49,49	0
56	MG	BA	3561	1/1	0.90	0.15	39,39,39,39	0
56	MG	DA	3135	1/1	0.90	0.13	58,58,58,58	0
56	MG	AA	3182	1/1	0.90	0.09	48,48,48,48	0
56	MG	BA	3111	1/1	0.90	0.17	43,43,43,43	0
56	MG	BA	3187	1/1	0.90	0.10	53,53,53,53	0
56	MG	CA	3149	1/1	0.90	0.09	81,81,81,81	0
56	MG	BA	3196	1/1	0.90	0.17	45,45,45,45	0
56	MG	DA	3166	1/1	0.90	0.06	37,37,37,37	0
56	MG	CA	3037	1/1	0.90	0.13	45,45,45,45	0
56	MG	BA	3118	1/1	0.90	0.22	53,53,53,53	0
56	MG	AA	3009	1/1	0.90	0.27	71,71,71,71	0
56	MG	DA	3180	1/1	0.90	0.24	47,47,47,47	0
56	MG	BA	3714	1/1	0.90	0.12	72,72,72,72	0
56	MG	DA	3196	1/1	0.90	0.17	54,54,54,54	0
56	MG	DA	3200	1/1	0.90	0.22	48,48,48,48	0
56	MG	DA	3201	1/1	0.90	0.09	43,43,43,43	0
56	MG	DA	3594	1/1	0.90	0.13	63,63,63,63	0
56	MG	BA	3591	1/1	0.90	0.12	38,38,38,38	0
56	MG	CA	3043	1/1	0.90	0.14	62,62,62,62	0
56	MG	BA	3324	1/1	0.90	0.19	54,54,54,54	0
56	MG	BA	3722	1/1	0.90	0.09	49,49,49,49	0
56	MG	AA	3001	1/1	0.90	0.18	74,74,74,74	0
56	MG	AA	3150	1/1	0.90	0.27	67,67,67,67	0
56	MG	DA	3236	1/1	0.90	0.08	38,38,38,38	0
56	MG	BA	3131	1/1	0.90	0.08	31,31,31,31	0
56	MG	BA	3610	1/1	0.90	0.61	49,49,49,49	0
56	MG	BA	3038	1/1	0.90	0.19	51,51,51,51	0
56	MG	BB	3006	1/1	0.90	0.20	34,34,34,34	0
56	MG	CA	3063	1/1	0.90	0.08	57,57,57,57	0
56	MG	BA	3214	1/1	0.90	0.17	37,37,37,37	0
56	MG	AA	3095	1/1	0.90	0.23	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3003	1/1	0.90	0.07	43,43,43,43	0
56	MG	DA	3278	1/1	0.90	0.08	39,39,39,39	0
56	MG	BA	3043	1/1	0.90	0.20	33,33,33,33	0
56	MG	CA	3069	1/1	0.90	0.22	63,63,63,63	0
56	MG	DA	3015	1/1	0.90	0.18	54,54,54,54	0
56	MG	BA	3044	1/1	0.90	0.19	32,32,32,32	0
56	MG	AA	3018	1/1	0.90	0.19	51,51,51,51	0
56	MG	AA	3168	1/1	0.90	0.16	80,80,80,80	0
56	MG	DA	3655	1/1	0.90	0.18	62,62,62,62	0
56	MG	DA	3036	1/1	0.90	0.11	35,35,35,35	0
56	MG	DA	3318	1/1	0.90	0.13	47,47,47,47	0
56	MG	AA	3139	1/1	0.90	0.17	58,58,58,58	0
56	MG	BA	3163	1/1	0.90	0.13	50,50,50,50	0
56	MG	CA	3075	1/1	0.90	0.26	76,76,76,76	0
56	MG	BA	3255	1/1	0.90	0.18	53,53,53,53	0
56	MG	DE	303	1/1	0.90	0.14	36,36,36,36	0
56	MG	AA	3113	1/1	0.90	0.16	56,56,56,56	0
56	MG	BG	3004	1/1	0.90	0.14	53,53,53,53	0
56	MG	DA	3061	1/1	0.90	0.20	47,47,47,47	0
56	MG	DA	3353	1/1	0.90	0.16	54,54,54,54	0
56	MG	DV	202	1/1	0.90	0.19	45,45,45,45	0
56	MG	BA	3470	1/1	0.90	0.11	44,44,44,44	0
56	MG	CA	3106	1/1	0.90	0.22	72,72,72,72	0
56	MG	DA	3363	1/1	0.90	0.16	56,56,56,56	0
56	MG	BN	3005	1/1	0.90	0.33	63,63,63,63	0
56	MG	DA	3373	1/1	0.90	0.14	52,52,52,52	0
56	MG	CA	3108	1/1	0.90	0.11	45,45,45,45	0
56	MG	BA	3261	1/1	0.90	0.25	45,45,45,45	0
56	MG	BA	3263	1/1	0.91	0.33	35,35,35,35	0
56	MG	BA	3144	1/1	0.91	0.10	52,52,52,52	0
56	MG	AA	3026	1/1	0.91	0.15	52,52,52,52	0
56	MG	BU	202	1/1	0.91	0.47	41,41,41,41	0
56	MG	BA	3279	1/1	0.91	0.23	60,60,60,60	0
56	MG	BA	3600	1/1	0.91	0.12	54,54,54,54	0
56	MG	DA	3299	1/1	0.91	0.08	35,35,35,35	0
56	MG	BA	3150	1/1	0.91	0.18	42,42,42,42	0
56	MG	BZ	3001	1/1	0.91	0.11	47,47,47,47	0
56	MG	B1	3001	1/1	0.91	0.45	63,63,63,63	0
56	MG	AA	3084	1/1	0.91	0.21	71,71,71,71	0
56	MG	BA	3047	1/1	0.91	0.21	30,30,30,30	0
56	MG	DA	3331	1/1	0.91	0.11	27,27,27,27	0
56	MG	CA	3163	1/1	0.91	0.08	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	B7	104	1/1	0.91	0.17	55,55,55,55	0
56	MG	B8	5001	1/1	0.91	0.10	62,62,62,62	0
56	MG	CA	3169	1/1	0.91	0.16	52,52,52,52	0
56	MG	BA	3612	1/1	0.91	0.13	41,41,41,41	0
56	MG	BA	3614	1/1	0.91	0.10	48,48,48,48	0
56	MG	AA	3075	1/1	0.91	0.11	50,50,50,50	0
56	MG	AA	3096	1/1	0.91	0.21	52,52,52,52	0
56	MG	BA	3296	1/1	0.91	0.23	69,69,69,69	0
56	MG	BA	3624	1/1	0.91	0.10	73,73,73,73	0
56	MG	CA	3018	1/1	0.91	0.07	55,55,55,55	0
56	MG	CA	3019	1/1	0.91	0.09	62,62,62,62	0
56	MG	BA	3166	1/1	0.91	0.10	41,41,41,41	0
56	MG	DA	3012	1/1	0.91	0.18	52,52,52,52	0
56	MG	BA	3627	1/1	0.91	0.22	50,50,50,50	0
56	MG	DA	3018	1/1	0.91	0.17	41,41,41,41	0
56	MG	CA	3024	1/1	0.91	0.26	57,57,57,57	0
56	MG	DA	3023	1/1	0.91	0.34	64,64,64,64	0
56	MG	BA	3631	1/1	0.91	0.11	41,41,41,41	0
56	MG	DA	3031	1/1	0.91	0.15	60,60,60,60	0
56	MG	DA	3432	1/1	0.91	0.17	37,37,37,37	0
56	MG	BA	3632	1/1	0.91	0.11	55,55,55,55	0
56	MG	AA	3038	1/1	0.91	0.38	64,64,64,64	0
56	MG	AA	3187	1/1	0.91	0.08	72,72,72,72	0
56	MG	BA	3309	1/1	0.91	0.17	43,43,43,43	0
56	MG	CA	3031	1/1	0.91	0.32	55,55,55,55	0
56	MG	BA	3310	1/1	0.91	0.14	59,59,59,59	0
56	MG	AX	102	1/1	0.91	0.14	66,66,66,66	0
56	MG	BA	3318	1/1	0.91	0.11	30,30,30,30	0
56	MG	DA	3449	1/1	0.91	0.25	46,46,46,46	0
56	MG	CA	3036	1/1	0.91	0.11	56,56,56,56	0
56	MG	DA	3455	1/1	0.91	0.14	53,53,53,53	0
56	MG	BA	3643	1/1	0.91	0.10	59,59,59,59	0
56	MG	DA	3064	1/1	0.91	0.09	55,55,55,55	0
56	MG	AA	3188	1/1	0.91	0.18	52,52,52,52	0
56	MG	DA	3068	1/1	0.91	0.12	52,52,52,52	0
56	MG	BA	3647	1/1	0.91	0.08	40,40,40,40	0
56	MG	BA	3072	1/1	0.91	0.25	45,45,45,45	0
56	MG	BA	3331	1/1	0.91	0.11	61,61,61,61	0
56	MG	BA	3654	1/1	0.91	0.16	49,49,49,49	0
56	MG	CA	3044	1/1	0.91	0.14	52,52,52,52	0
56	MG	DA	3483	1/1	0.91	0.13	55,55,55,55	0
56	MG	DA	3485	1/1	0.91	0.08	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	3081	1/1	0.91	0.20	56,56,56,56	0
56	MG	BA	3656	1/1	0.91	0.12	70,70,70,70	0
56	MG	BA	3181	1/1	0.91	0.09	37,37,37,37	0
56	MG	CA	3049	1/1	0.91	0.18	51,51,51,51	0
56	MG	BA	3082	1/1	0.91	0.20	54,54,54,54	0
56	MG	DA	3090	1/1	0.91	0.20	59,59,59,59	0
56	MG	DA	3092	1/1	0.91	0.21	48,48,48,48	0
56	MG	DA	3513	1/1	0.91	0.12	58,58,58,58	0
56	MG	BA	3342	1/1	0.91	0.18	46,46,46,46	0
56	MG	DA	3521	1/1	0.91	0.11	46,46,46,46	0
56	MG	BA	3185	1/1	0.91	0.16	40,40,40,40	0
56	MG	BA	3083	1/1	0.91	0.14	33,33,33,33	0
56	MG	DA	3525	1/1	0.91	0.11	56,56,56,56	0
56	MG	DA	3097	1/1	0.91	0.14	58,58,58,58	0
56	MG	CA	3058	1/1	0.91	0.08	36,36,36,36	0
56	MG	BA	3087	1/1	0.91	0.20	48,48,48,48	0
56	MG	DA	3100	1/1	0.91	0.14	55,55,55,55	0
56	MG	BA	3673	1/1	0.91	0.17	60,60,60,60	0
56	MG	BA	3371	1/1	0.91	0.13	38,38,38,38	0
56	MG	BA	3191	1/1	0.91	0.09	56,56,56,56	0
56	MG	BA	3676	1/1	0.91	0.08	63,63,63,63	0
56	MG	DA	3542	1/1	0.91	0.10	44,44,44,44	0
56	MG	DA	3543	1/1	0.91	0.11	52,52,52,52	0
56	MG	DA	3547	1/1	0.91	0.10	47,47,47,47	0
56	MG	BA	3376	1/1	0.91	0.21	35,35,35,35	0
56	MG	DA	3111	1/1	0.91	0.20	67,67,67,67	0
56	MG	BA	3394	1/1	0.91	0.20	45,45,45,45	0
56	MG	DA	3559	1/1	0.91	0.12	47,47,47,47	0
56	MG	BA	3395	1/1	0.91	0.22	56,56,56,56	0
56	MG	BA	3405	1/1	0.91	0.10	57,57,57,57	0
56	MG	BA	3195	1/1	0.91	0.16	37,37,37,37	0
56	MG	BA	3697	1/1	0.91	0.13	63,63,63,63	0
56	MG	DA	3569	1/1	0.91	0.07	54,54,54,54	0
56	MG	DA	3571	1/1	0.91	0.17	57,57,57,57	0
56	MG	AA	3118	1/1	0.91	0.27	39,39,39,39	0
56	MG	AA	3191	1/1	0.91	0.10	56,56,56,56	0
56	MG	BA	3455	1/1	0.91	0.17	47,47,47,47	0
56	MG	BA	3099	1/1	0.91	0.32	55,55,55,55	0
56	MG	DA	3128	1/1	0.91	0.16	54,54,54,54	0
56	MG	AA	3077	1/1	0.91	0.30	67,67,67,67	0
56	MG	CA	3099	1/1	0.91	0.21	64,64,64,64	0
56	MG	BA	3466	1/1	0.91	0.09	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	3104	1/1	0.91	0.16	60,60,60,60	0
56	MG	DA	3600	1/1	0.91	0.14	73,73,73,73	0
56	MG	DA	3152	1/1	0.91	0.15	43,43,43,43	0
56	MG	BA	3105	1/1	0.91	0.28	54,54,54,54	0
56	MG	AA	3124	1/1	0.91	0.15	61,61,61,61	0
56	MG	AA	3197	1/1	0.91	0.16	64,64,64,64	0
56	MG	DA	3161	1/1	0.91	0.16	51,51,51,51	0
56	MG	DA	3611	1/1	0.91	0.14	51,51,51,51	0
56	MG	BA	3117	1/1	0.91	0.14	37,37,37,37	0
56	MG	AA	3048	1/1	0.91	0.11	52,52,52,52	0
56	MG	BA	3718	1/1	0.91	0.13	52,52,52,52	0
56	MG	BA	3478	1/1	0.91	0.20	36,36,36,36	0
56	MG	BA	3732	1/1	0.91	0.18	56,56,56,56	0
56	MG	DA	3172	1/1	0.91	0.20	46,46,46,46	0
56	MG	DA	3175	1/1	0.91	0.20	52,52,52,52	0
56	MG	AA	3036	1/1	0.91	0.14	69,69,69,69	0
56	MG	AA	3204	1/1	0.91	0.13	70,70,70,70	0
56	MG	DA	3636	1/1	0.91	0.18	64,64,64,64	0
56	MG	DA	3190	1/1	0.91	0.08	54,54,54,54	0
56	MG	DA	3194	1/1	0.91	0.34	65,65,65,65	0
56	MG	BA	3502	1/1	0.91	0.17	59,59,59,59	0
56	MG	DA	3198	1/1	0.91	0.18	34,34,34,34	0
56	MG	BA	3505	1/1	0.91	0.10	45,45,45,45	0
56	MG	BB	3004	1/1	0.91	0.22	57,57,57,57	0
56	MG	BA	3231	1/1	0.91	0.18	50,50,50,50	0
56	MG	DB	3002	1/1	0.91	0.23	72,72,72,72	0
56	MG	AA	3055	1/1	0.91	0.23	56,56,56,56	0
56	MG	DB	3004	1/1	0.91	0.14	56,56,56,56	0
56	MG	BA	3126	1/1	0.91	0.17	47,47,47,47	0
56	MG	BA	3242	1/1	0.91	0.23	45,45,45,45	0
56	MG	BA	3246	1/1	0.91	0.21	38,38,38,38	0
56	MG	BA	3535	1/1	0.91	0.16	42,42,42,42	0
56	MG	BA	3026	1/1	0.91	0.06	36,36,36,36	0
56	MG	AA	3073	1/1	0.91	0.11	63,63,63,63	0
56	MG	BA	3552	1/1	0.91	0.18	30,30,30,30	0
56	MG	DN	5001	1/1	0.91	0.07	71,71,71,71	0
56	MG	DQ	3002	1/1	0.91	0.16	51,51,51,51	0
56	MG	BA	3251	1/1	0.91	0.06	45,45,45,45	0
56	MG	BA	3252	1/1	0.91	0.28	65,65,65,65	0
56	MG	DA	3249	1/1	0.91	0.10	25,25,25,25	0
56	MG	AA	3107	1/1	0.91	0.21	44,44,44,44	0
56	MG	DA	3254	1/1	0.91	0.12	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	AA	3216	1/1	0.91	0.20	60,60,60,60	0
56	MG	BA	3139	1/1	0.91	0.22	50,50,50,50	0
56	MG	AA	3108	1/1	0.91	0.15	72,72,72,72	0
56	MG	DA	3268	1/1	0.91	0.12	42,42,42,42	0
56	MG	DA	3273	1/1	0.91	0.13	32,32,32,32	0
56	MG	BA	3273	1/1	0.92	0.29	35,35,35,35	0
56	MG	BU	208	1/1	0.92	0.13	42,42,42,42	0
56	MG	AA	3154	1/1	0.92	0.12	60,60,60,60	0
56	MG	BA	3280	1/1	0.92	0.26	44,44,44,44	0
56	MG	BA	3649	1/1	0.92	0.20	43,43,43,43	0
56	MG	BA	3061	1/1	0.92	0.21	44,44,44,44	0
56	MG	BA	3476	1/1	0.92	0.08	47,47,47,47	0
56	MG	BA	3004	1/1	0.92	0.18	45,45,45,45	0
56	MG	B3	3403	1/1	0.92	0.13	37,37,37,37	0
56	MG	BA	3657	1/1	0.92	0.11	29,29,29,29	0
56	MG	BA	3658	1/1	0.92	0.16	62,62,62,62	0
56	MG	BA	3291	1/1	0.92	0.16	44,44,44,44	0
56	MG	DA	3454	1/1	0.92	0.07	52,52,52,52	0
56	MG	CA	3131	1/1	0.92	0.07	48,48,48,48	0
56	MG	BA	3190	1/1	0.92	0.08	42,42,42,42	0
56	MG	DA	3457	1/1	0.92	0.08	44,44,44,44	0
56	MG	BA	3487	1/1	0.92	0.18	47,47,47,47	0
56	MG	AA	3135	1/1	0.92	0.17	49,49,49,49	0
56	MG	DA	3461	1/1	0.92	0.09	40,40,40,40	0
56	MG	AA	3083	1/1	0.92	0.15	56,56,56,56	0
56	MG	BA	3671	1/1	0.92	0.12	44,44,44,44	0
56	MG	DA	3126	1/1	0.92	0.14	61,61,61,61	0
56	MG	CA	3014	1/1	0.92	0.22	56,56,56,56	0
56	MG	BA	3295	1/1	0.92	0.07	30,30,30,30	0
56	MG	CA	3016	1/1	0.92	0.13	72,72,72,72	0
56	MG	DA	3478	1/1	0.92	0.06	58,58,58,58	0
56	MG	BA	3012	1/1	0.92	0.07	34,34,34,34	0
56	MG	DA	3484	1/1	0.92	0.10	47,47,47,47	0
56	MG	BA	3202	1/1	0.92	0.24	29,29,29,29	0
56	MG	DA	3487	1/1	0.92	0.06	44,44,44,44	0
56	MG	DA	3146	1/1	0.92	0.20	34,34,34,34	0
56	MG	DA	3149	1/1	0.92	0.08	47,47,47,47	0
56	MG	AA	3116	1/1	0.92	0.32	62,62,62,62	0
56	MG	AA	3111	1/1	0.92	0.08	70,70,70,70	0
56	MG	DA	3154	1/1	0.92	0.30	45,45,45,45	0
56	MG	DA	3502	1/1	0.92	0.16	48,48,48,48	0
56	MG	BA	3524	1/1	0.92	0.09	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	CA	3155	1/1	0.92	0.07	71,71,71,71	0
56	MG	BA	3075	1/1	0.92	0.19	36,36,36,36	0
56	MG	BA	3081	1/1	0.92	0.21	44,44,44,44	0
56	MG	DA	3515	1/1	0.92	0.12	57,57,57,57	0
56	MG	DA	3163	1/1	0.92	0.14	52,52,52,52	0
56	MG	BA	3311	1/1	0.92	0.27	52,52,52,52	0
56	MG	BA	3540	1/1	0.92	0.18	29,29,29,29	0
56	MG	BA	3316	1/1	0.92	0.14	51,51,51,51	0
56	MG	DA	3527	1/1	0.92	0.15	58,58,58,58	0
56	MG	AA	3173	1/1	0.92	0.06	37,37,37,37	0
56	MG	AA	3174	1/1	0.92	0.17	49,49,49,49	0
56	MG	DA	3530	1/1	0.92	0.12	57,57,57,57	0
56	MG	BA	3145	1/1	0.92	0.14	40,40,40,40	0
56	MG	AA	3198	1/1	0.92	0.08	73,73,73,73	0
56	MG	AA	3046	1/1	0.92	0.19	60,60,60,60	0
56	MG	BA	3155	1/1	0.92	0.07	56,56,56,56	0
56	MG	AA	3069	1/1	0.92	0.11	77,77,77,77	0
56	MG	DA	3195	1/1	0.92	0.13	51,51,51,51	0
56	MG	BA	3340	1/1	0.92	0.17	57,57,57,57	0
56	MG	BA	3235	1/1	0.92	0.25	44,44,44,44	0
56	MG	BA	3593	1/1	0.92	0.08	51,51,51,51	0
56	MG	CT	3001	1/1	0.92	0.19	57,57,57,57	0
56	MG	DA	3551	1/1	0.92	0.07	43,43,43,43	0
56	MG	DA	3203	1/1	0.92	0.06	48,48,48,48	0
56	MG	DA	3205	1/1	0.92	0.15	41,41,41,41	0
56	MG	DA	3558	1/1	0.92	0.15	77,77,77,77	0
56	MG	BA	3343	1/1	0.92	0.07	37,37,37,37	0
56	MG	BA	3356	1/1	0.92	0.09	33,33,33,33	0
56	MG	BA	3719	1/1	0.92	0.08	63,63,63,63	0
56	MG	DA	3223	1/1	0.92	0.09	41,41,41,41	0
56	MG	BA	3721	1/1	0.92	0.21	56,56,56,56	0
56	MG	DA	3225	1/1	0.92	0.17	64,64,64,64	0
56	MG	DA	3570	1/1	0.92	0.18	67,67,67,67	0
56	MG	BA	3599	1/1	0.92	0.09	56,56,56,56	0
56	MG	DA	3231	1/1	0.92	0.09	45,45,45,45	0
56	MG	BA	3098	1/1	0.92	0.24	42,42,42,42	0
56	MG	BA	3737	1/1	0.92	0.11	39,39,39,39	0
56	MG	AA	3121	1/1	0.92	0.21	52,52,52,52	0
56	MG	BA	3359	1/1	0.92	0.12	63,63,63,63	0
56	MG	CA	3057	1/1	0.92	0.14	40,40,40,40	0
56	MG	DA	3024	1/1	0.92	0.28	59,59,59,59	0
56	MG	BA	3607	1/1	0.92	0.15	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3250	1/1	0.92	0.11	42,42,42,42	0
56	MG	BB	3002	1/1	0.92	0.16	49,49,49,49	0
56	MG	DA	3252	1/1	0.92	0.20	36,36,36,36	0
56	MG	BA	3368	1/1	0.92	0.12	22,22,22,22	0
56	MG	CA	3062	1/1	0.92	0.33	67,67,67,67	0
56	MG	BA	3042	1/1	0.92	0.21	50,50,50,50	0
56	MG	DA	3259	1/1	0.92	0.09	45,45,45,45	0
56	MG	AA	3123	1/1	0.92	0.25	38,38,38,38	0
56	MG	DA	3612	1/1	0.92	0.17	46,46,46,46	0
56	MG	DA	3041	1/1	0.92	0.20	54,54,54,54	0
56	MG	DA	3615	1/1	0.92	0.09	57,57,57,57	0
56	MG	DA	3270	1/1	0.92	0.14	55,55,55,55	0
56	MG	BA	3167	1/1	0.92	0.40	50,50,50,50	0
56	MG	DA	3048	1/1	0.92	0.21	29,29,29,29	0
56	MG	DA	3049	1/1	0.92	0.13	56,56,56,56	0
56	MG	DA	3054	1/1	0.92	0.13	34,34,34,34	0
56	MG	DA	3622	1/1	0.92	0.10	40,40,40,40	0
56	MG	DA	3285	1/1	0.92	0.12	41,41,41,41	0
56	MG	AA	3052	1/1	0.92	0.18	58,58,58,58	0
56	MG	BB	3016	1/1	0.92	0.14	24,24,24,24	0
56	MG	DA	3631	1/1	0.92	0.15	49,49,49,49	0
56	MG	BA	3390	1/1	0.92	0.12	40,40,40,40	0
56	MG	BA	3109	1/1	0.92	0.34	62,62,62,62	0
56	MG	BA	3174	1/1	0.92	0.06	52,52,52,52	0
56	MG	BA	3253	1/1	0.92	0.29	63,63,63,63	0
56	MG	DA	3065	1/1	0.92	0.14	40,40,40,40	0
56	MG	BA	3629	1/1	0.92	0.07	51,51,51,51	0
56	MG	BA	3425	1/1	0.92	0.15	42,42,42,42	0
56	MG	CA	3079	1/1	0.92	0.07	37,37,37,37	0
56	MG	DA	3070	1/1	0.92	0.24	51,51,51,51	0
56	MG	DA	3071	1/1	0.92	0.28	46,46,46,46	0
56	MG	BD	312	1/1	0.92	0.33	72,72,72,72	0
56	MG	CA	3084	1/1	0.92	0.18	80,80,80,80	0
56	MG	DA	3075	1/1	0.92	0.16	45,45,45,45	0
56	MG	DA	3077	1/1	0.92	0.12	48,48,48,48	0
56	MG	BA	3046	1/1	0.92	0.13	52,52,52,52	0
56	MG	CA	3090	1/1	0.92	0.10	63,63,63,63	0
56	MG	DE	305	1/1	0.92	0.17	68,68,68,68	0
56	MG	BA	3112	1/1	0.92	0.20	46,46,46,46	0
56	MG	BG	3002	1/1	0.92	0.17	51,51,51,51	0
56	MG	BA	3179	1/1	0.92	0.30	53,53,53,53	0
56	MG	DP	201	1/1	0.92	0.09	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	DP	202	1/1	0.92	0.19	54,54,54,54	0
56	MG	DA	3380	1/1	0.92	0.07	40,40,40,40	0
56	MG	BA	3453	1/1	0.92	0.20	54,54,54,54	0
56	MG	BA	3114	1/1	0.92	0.25	46,46,46,46	0
56	MG	DU	3001	1/1	0.92	0.19	61,61,61,61	0
56	MG	BA	3116	1/1	0.92	0.23	30,30,30,30	0
56	MG	DW	202	1/1	0.92	0.09	53,53,53,53	0
56	MG	BP	202	1/1	0.92	0.27	47,47,47,47	0
56	MG	BA	3640	1/1	0.92	0.13	31,31,31,31	0
56	MG	DA	3416	1/1	0.92	0.19	34,34,34,34	0
56	MG	BA	3182	1/1	0.92	0.17	43,43,43,43	0
56	MG	DA	3419	1/1	0.92	0.09	53,53,53,53	0
56	MG	BR	201	1/1	0.92	0.14	44,44,44,44	0
56	MG	AA	3211	1/1	0.92	0.09	58,58,58,58	0
56	MG	BA	3148	1/1	0.93	0.38	49,49,49,49	0
56	MG	BA	3544	1/1	0.93	0.12	35,35,35,35	0
56	MG	DA	3184	1/1	0.93	0.15	54,54,54,54	0
56	MG	DA	3030	1/1	0.93	0.14	49,49,49,49	0
56	MG	AA	3181	1/1	0.93	0.17	46,46,46,46	0
56	MG	DA	3032	1/1	0.93	0.06	36,36,36,36	0
56	MG	DA	3033	1/1	0.93	0.15	41,41,41,41	0
56	MG	BA	3193	1/1	0.93	0.16	53,53,53,53	0
56	MG	BA	3018	1/1	0.93	0.10	54,54,54,54	0
56	MG	BA	3152	1/1	0.93	0.11	52,52,52,52	0
56	MG	DA	3486	1/1	0.93	0.07	52,52,52,52	0
56	MG	BA	3198	1/1	0.93	0.20	29,29,29,29	0
56	MG	CA	3088	1/1	0.93	0.09	49,49,49,49	0
56	MG	BW	3004	1/1	0.93	0.27	46,46,46,46	0
56	MG	DA	3209	1/1	0.93	0.10	44,44,44,44	0
56	MG	BA	3199	1/1	0.93	0.15	31,31,31,31	0
56	MG	DA	3214	1/1	0.93	0.12	48,48,48,48	0
56	MG	BA	3375	1/1	0.93	0.08	44,44,44,44	0
56	MG	DA	3221	1/1	0.93	0.18	56,56,56,56	0
56	MG	DA	3053	1/1	0.93	0.14	47,47,47,47	0
56	MG	DA	3507	1/1	0.93	0.16	53,53,53,53	0
56	MG	DA	3509	1/1	0.93	0.06	57,57,57,57	0
56	MG	B0	101	1/1	0.93	0.13	57,57,57,57	0
56	MG	B0	106	1/1	0.93	0.05	43,43,43,43	0
56	MG	BA	3680	1/1	0.93	0.16	62,62,62,62	0
56	MG	DA	3517	1/1	0.93	0.09	47,47,47,47	0
56	MG	DA	3520	1/1	0.93	0.07	38,38,38,38	0
56	MG	DA	3058	1/1	0.93	0.15	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	3277	1/1	0.93	0.27	45,45,45,45	0
56	MG	BA	3682	1/1	0.93	0.27	50,50,50,50	0
56	MG	BA	3201	1/1	0.93	0.21	36,36,36,36	0
56	MG	B7	103	1/1	0.93	0.16	46,46,46,46	0
56	MG	BA	3687	1/1	0.93	0.13	59,59,59,59	0
56	MG	BA	3590	1/1	0.93	0.12	23,23,23,23	0
56	MG	B9	502	1/1	0.93	0.15	49,49,49,49	0
56	MG	BA	3392	1/1	0.93	0.11	53,53,53,53	0
56	MG	BA	3154	1/1	0.93	0.14	55,55,55,55	0
56	MG	BA	3283	1/1	0.93	0.22	61,61,61,61	0
56	MG	BA	3019	1/1	0.93	0.17	42,42,42,42	0
56	MG	AA	3166	1/1	0.93	0.14	55,55,55,55	0
56	MG	CA	3010	1/1	0.93	0.11	34,34,34,34	0
56	MG	DA	3541	1/1	0.93	0.09	55,55,55,55	0
56	MG	CA	3123	1/1	0.93	0.14	75,75,75,75	0
56	MG	AN	101	1/1	0.93	0.07	64,64,64,64	0
56	MG	DA	3544	1/1	0.93	0.32	42,42,42,42	0
56	MG	AA	3007	1/1	0.93	0.08	68,68,68,68	0
56	MG	BA	3435	1/1	0.93	0.11	59,59,59,59	0
56	MG	BA	3605	1/1	0.93	0.08	35,35,35,35	0
56	MG	AA	3185	1/1	0.93	0.19	47,47,47,47	0
56	MG	DA	3555	1/1	0.93	0.11	43,43,43,43	0
56	MG	DA	3276	1/1	0.93	0.07	26,26,26,26	0
56	MG	CA	3130	1/1	0.93	0.11	59,59,59,59	0
56	MG	AA	3169	1/1	0.93	0.08	62,62,62,62	0
56	MG	AA	3101	1/1	0.93	0.20	61,61,61,61	0
56	MG	DA	3284	1/1	0.93	0.12	45,45,45,45	0
56	MG	DA	3091	1/1	0.93	0.41	50,50,50,50	0
56	MG	BA	3217	1/1	0.93	0.10	59,59,59,59	0
56	MG	DA	3288	1/1	0.93	0.10	68,68,68,68	0
56	MG	BA	3297	1/1	0.93	0.12	43,43,43,43	0
56	MG	DA	3094	1/1	0.93	0.16	26,26,26,26	0
56	MG	DA	3575	1/1	0.93	0.16	51,51,51,51	0
56	MG	BA	3618	1/1	0.93	0.18	37,37,37,37	0
56	MG	DA	3302	1/1	0.93	0.12	42,42,42,42	0
56	MG	BA	3120	1/1	0.93	0.19	56,56,56,56	0
56	MG	DA	3310	1/1	0.93	0.17	30,30,30,30	0
56	MG	AA	3043	1/1	0.93	0.28	63,63,63,63	0
56	MG	BA	3622	1/1	0.93	0.18	32,32,32,32	0
56	MG	BA	3468	1/1	0.93	0.19	45,45,45,45	0
56	MG	DA	3325	1/1	0.93	0.16	31,31,31,31	0
56	MG	BA	3734	1/1	0.93	0.15	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	DA	3328	1/1	0.93	0.20	33,33,33,33	0
56	MG	DA	3601	1/1	0.93	0.10	50,50,50,50	0
56	MG	BA	3735	1/1	0.93	0.08	47,47,47,47	0
56	MG	DA	3104	1/1	0.93	0.12	46,46,46,46	0
56	MG	DA	3604	1/1	0.93	0.06	50,50,50,50	0
56	MG	DA	3105	1/1	0.93	0.11	56,56,56,56	0
56	MG	DA	3338	1/1	0.93	0.14	58,58,58,58	0
56	MG	BA	3229	1/1	0.93	0.10	50,50,50,50	0
56	MG	CA	3151	1/1	0.93	0.10	80,80,80,80	0
56	MG	CA	3035	1/1	0.93	0.18	49,49,49,49	0
56	MG	BA	3305	1/1	0.93	0.10	48,48,48,48	0
56	MG	AA	3125	1/1	0.93	0.13	56,56,56,56	0
56	MG	AA	3175	1/1	0.93	0.12	70,70,70,70	0
56	MG	BA	3093	1/1	0.93	0.35	52,52,52,52	0
56	MG	BA	3313	1/1	0.93	0.12	56,56,56,56	0
56	MG	DA	3370	1/1	0.93	0.20	40,40,40,40	0
56	MG	BA	3479	1/1	0.93	0.12	44,44,44,44	0
56	MG	DA	3378	1/1	0.93	0.07	38,38,38,38	0
56	MG	DA	3117	1/1	0.93	0.08	46,46,46,46	0
56	MG	DA	3381	1/1	0.93	0.14	68,68,68,68	0
56	MG	DA	3387	1/1	0.93	0.09	50,50,50,50	0
56	MG	DA	3390	1/1	0.93	0.12	58,58,58,58	0
56	MG	BA	3481	1/1	0.93	0.14	41,41,41,41	0
56	MG	AA	3159	1/1	0.93	0.17	57,57,57,57	0
56	MG	DA	3638	1/1	0.93	0.08	53,53,53,53	0
56	MG	BB	3009	1/1	0.93	0.12	49,49,49,49	0
56	MG	DA	3640	1/1	0.93	0.10	53,53,53,53	0
56	MG	DA	3395	1/1	0.93	0.07	40,40,40,40	0
56	MG	DA	3399	1/1	0.93	0.23	39,39,39,39	0
56	MG	DA	3400	1/1	0.93	0.16	42,42,42,42	0
56	MG	DA	3651	1/1	0.93	0.08	48,48,48,48	0
56	MG	AA	3130	1/1	0.93	0.19	55,55,55,55	0
56	MG	DA	3406	1/1	0.93	0.09	48,48,48,48	0
56	MG	DA	3409	1/1	0.93	0.07	54,54,54,54	0
56	MG	AA	3222	1/1	0.93	0.20	64,64,64,64	0
56	MG	BA	3100	1/1	0.93	0.15	42,42,42,42	0
56	MG	BA	3503	1/1	0.93	0.12	56,56,56,56	0
56	MG	DB	3007	1/1	0.93	0.24	45,45,45,45	0
56	MG	BA	3504	1/1	0.93	0.18	54,54,54,54	0
56	MG	DA	3132	1/1	0.93	0.20	47,47,47,47	0
56	MG	BA	3183	1/1	0.93	0.11	40,40,40,40	0
56	MG	DD	303	1/1	0.93	0.54	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DE	302	1/1	0.93	0.14	46,46,46,46	0
56	MG	BA	3141	1/1	0.93	0.27	43,43,43,43	0
56	MG	CE	3002	1/1	0.93	0.08	69,69,69,69	0
56	MG	BA	3250	1/1	0.93	0.29	61,61,61,61	0
56	MG	BA	3336	1/1	0.93	0.14	46,46,46,46	0
56	MG	BE	307	1/1	0.93	0.20	51,51,51,51	0
56	MG	BA	3518	1/1	0.93	0.09	52,52,52,52	0
56	MG	DA	3442	1/1	0.93	0.17	58,58,58,58	0
56	MG	DA	3002	1/1	0.93	0.19	47,47,47,47	0
56	MG	BA	3008	1/1	0.93	0.15	30,30,30,30	0
56	MG	DA	3156	1/1	0.93	0.32	38,38,38,38	0
56	MG	BA	3104	1/1	0.93	0.23	34,34,34,34	0
56	MG	AA	3146	1/1	0.93	0.08	55,55,55,55	0
56	MG	DV	203	1/1	0.93	0.18	41,41,41,41	0
56	MG	BA	3660	1/1	0.93	0.15	58,58,58,58	0
56	MG	DA	3014	1/1	0.93	0.08	38,38,38,38	0
56	MG	DA	3164	1/1	0.93	0.06	40,40,40,40	0
56	MG	BA	3254	1/1	0.93	0.10	40,40,40,40	0
58	ZN	B4	501	1/1	0.93	0.10	152,152,152,152	0
56	MG	BA	3189	1/1	0.93	0.05	39,39,39,39	0
56	MG	DA	3019	1/1	0.93	0.13	32,32,32,32	0
56	MG	BA	3664	1/1	0.93	0.17	63,63,63,63	0
56	MG	BA	3665	1/1	0.93	0.23	39,39,39,39	0
56	MG	BA	3268	1/1	0.94	0.19	29,29,29,29	0
56	MG	BW	3003	1/1	0.94	0.14	39,39,39,39	0
56	MG	DA	3434	1/1	0.94	0.10	51,51,51,51	0
56	MG	CA	3132	1/1	0.94	0.13	66,66,66,66	0
56	MG	CA	3134	1/1	0.94	0.11	92,92,92,92	0
56	MG	BA	3436	1/1	0.94	0.12	35,35,35,35	0
56	MG	DA	3438	1/1	0.94	0.19	50,50,50,50	0
56	MG	BW	3005	1/1	0.94	0.14	38,38,38,38	0
56	MG	BA	3444	1/1	0.94	0.14	29,29,29,29	0
56	MG	BA	3001	1/1	0.94	0.18	52,52,52,52	0
56	MG	DA	3129	1/1	0.94	0.08	45,45,45,45	0
56	MG	BA	3002	1/1	0.94	0.15	38,38,38,38	0
56	MG	B0	104	1/1	0.94	0.11	55,55,55,55	0
56	MG	BA	3274	1/1	0.94	0.21	54,54,54,54	0
56	MG	BA	3458	1/1	0.94	0.14	46,46,46,46	0
56	MG	DA	3137	1/1	0.94	0.27	62,62,62,62	0
56	MG	DA	3138	1/1	0.94	0.27	53,53,53,53	0
56	MG	DA	3140	1/1	0.94	0.26	55,55,55,55	0
56	MG	B1	3002	1/1	0.94	0.06	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	CA	3148	1/1	0.94	0.12	65,65,65,65	0
56	MG	AA	3153	1/1	0.94	0.14	46,46,46,46	0
56	MG	AA	3011	1/1	0.94	0.34	44,44,44,44	0
56	MG	AA	3210	1/1	0.94	0.08	48,48,48,48	0
56	MG	BA	3138	1/1	0.94	0.23	54,54,54,54	0
56	MG	BA	3074	1/1	0.94	0.06	38,38,38,38	0
56	MG	BA	3286	1/1	0.94	0.18	42,42,42,42	0
56	MG	DA	3473	1/1	0.94	0.14	50,50,50,50	0
56	MG	BA	3288	1/1	0.94	0.10	45,45,45,45	0
56	MG	AA	3155	1/1	0.94	0.13	54,54,54,54	0
56	MG	AA	3213	1/1	0.94	0.09	74,74,74,74	0
56	MG	DA	3482	1/1	0.94	0.06	45,45,45,45	0
56	MG	CA	3005	1/1	0.94	0.23	37,37,37,37	0
56	MG	AA	3122	1/1	0.94	0.34	40,40,40,40	0
56	MG	BA	3017	1/1	0.94	0.20	38,38,38,38	0
56	MG	DA	3167	1/1	0.94	0.19	46,46,46,46	0
56	MG	BA	3084	1/1	0.94	0.33	47,47,47,47	0
56	MG	BA	3205	1/1	0.94	0.19	38,38,38,38	0
56	MG	DA	3493	1/1	0.94	0.12	38,38,38,38	0
56	MG	BA	3482	1/1	0.94	0.11	59,59,59,59	0
56	MG	CA	3165	1/1	0.94	0.14	47,47,47,47	0
56	MG	DA	3173	1/1	0.94	0.12	50,50,50,50	0
56	MG	DA	3499	1/1	0.94	0.18	44,44,44,44	0
56	MG	CA	3167	1/1	0.94	0.06	68,68,68,68	0
56	MG	DA	3176	1/1	0.94	0.11	52,52,52,52	0
56	MG	DA	3503	1/1	0.94	0.07	41,41,41,41	0
56	MG	DA	3179	1/1	0.94	0.23	36,36,36,36	0
56	MG	BA	3207	1/1	0.94	0.20	44,44,44,44	0
56	MG	AA	3109	1/1	0.94	0.13	59,59,59,59	0
56	MG	DA	3187	1/1	0.94	0.18	52,52,52,52	0
56	MG	DA	3188	1/1	0.94	0.23	52,52,52,52	0
56	MG	BA	3498	1/1	0.94	0.07	81,81,81,81	0
56	MG	BA	3298	1/1	0.94	0.25	45,45,45,45	0
56	MG	DA	3516	1/1	0.94	0.21	54,54,54,54	0
56	MG	AA	3051	1/1	0.94	0.08	56,56,56,56	0
56	MG	DA	3518	1/1	0.94	0.07	40,40,40,40	0
56	MG	BA	3211	1/1	0.94	0.08	43,43,43,43	0
56	MG	AA	3041	1/1	0.94	0.08	41,41,41,41	0
56	MG	AA	3035	1/1	0.94	0.07	59,59,59,59	0
56	MG	CX	102	1/1	0.94	0.07	60,60,60,60	0
56	MG	BA	3677	1/1	0.94	0.13	47,47,47,47	0
56	MG	BA	3507	1/1	0.94	0.09	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	BA	3509	1/1	0.94	0.13	29,29,29,29	0
56	MG	DA	3206	1/1	0.94	0.24	36,36,36,36	0
56	MG	BA	3307	1/1	0.94	0.08	35,35,35,35	0
56	MG	BA	3685	1/1	0.94	0.20	58,58,58,58	0
56	MG	BA	3097	1/1	0.94	0.17	30,30,30,30	0
56	MG	DA	3216	1/1	0.94	0.10	47,47,47,47	0
56	MG	DA	3535	1/1	0.94	0.08	58,58,58,58	0
56	MG	BA	3513	1/1	0.94	0.20	51,51,51,51	0
56	MG	DA	3013	1/1	0.94	0.16	38,38,38,38	0
56	MG	BA	3215	1/1	0.94	0.08	32,32,32,32	0
56	MG	AA	3190	1/1	0.94	0.26	61,61,61,61	0
56	MG	DA	3017	1/1	0.94	0.07	51,51,51,51	0
56	MG	BA	3219	1/1	0.94	0.24	36,36,36,36	0
56	MG	DA	3227	1/1	0.94	0.08	40,40,40,40	0
56	MG	BA	3315	1/1	0.94	0.22	43,43,43,43	0
56	MG	BA	3221	1/1	0.94	0.27	55,55,55,55	0
56	MG	BA	3533	1/1	0.94	0.14	30,30,30,30	0
56	MG	CA	3040	1/1	0.94	0.21	47,47,47,47	0
56	MG	DA	3238	1/1	0.94	0.07	37,37,37,37	0
56	MG	DA	3027	1/1	0.94	0.21	49,49,49,49	0
56	MG	BA	3157	1/1	0.94	0.07	52,52,52,52	0
56	MG	AA	3054	1/1	0.94	0.13	46,46,46,46	0
56	MG	DA	3244	1/1	0.94	0.15	23,23,23,23	0
56	MG	DA	3565	1/1	0.94	0.13	48,48,48,48	0
56	MG	BA	3539	1/1	0.94	0.11	23,23,23,23	0
56	MG	DA	3248	1/1	0.94	0.15	30,30,30,30	0
56	MG	BA	3225	1/1	0.94	0.23	42,42,42,42	0
56	MG	CA	3045	1/1	0.94	0.22	60,60,60,60	0
56	MG	DA	3034	1/1	0.94	0.18	40,40,40,40	0
56	MG	BA	3325	1/1	0.94	0.10	39,39,39,39	0
56	MG	BA	3546	1/1	0.94	0.17	46,46,46,46	0
56	MG	DA	3578	1/1	0.94	0.21	68,68,68,68	0
56	MG	DA	3582	1/1	0.94	0.17	44,44,44,44	0
56	MG	DA	3038	1/1	0.94	0.06	37,37,37,37	0
56	MG	BA	3548	1/1	0.94	0.19	40,40,40,40	0
56	MG	BA	3227	1/1	0.94	0.14	67,67,67,67	0
56	MG	CA	3052	1/1	0.94	0.14	47,47,47,47	0
56	MG	BA	3550	1/1	0.94	0.11	32,32,32,32	0
56	MG	DA	3269	1/1	0.94	0.12	47,47,47,47	0
56	MG	DA	3044	1/1	0.94	0.23	45,45,45,45	0
56	MG	DA	3271	1/1	0.94	0.08	45,45,45,45	0
56	MG	DA	3597	1/1	0.94	0.11	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3161	1/1	0.94	0.12	50,50,50,50	0
56	MG	BA	3557	1/1	0.94	0.18	35,35,35,35	0
56	MG	AA	3170	1/1	0.94	0.16	83,83,83,83	0
56	MG	BA	3101	1/1	0.94	0.30	47,47,47,47	0
56	MG	BA	3725	1/1	0.94	0.06	29,29,29,29	0
56	MG	DA	3056	1/1	0.94	0.15	37,37,37,37	0
56	MG	BA	3234	1/1	0.94	0.19	48,48,48,48	0
56	MG	BA	3339	1/1	0.94	0.15	47,47,47,47	0
56	MG	BA	3030	1/1	0.94	0.27	26,26,26,26	0
56	MG	BA	3577	1/1	0.94	0.13	63,63,63,63	0
56	MG	DA	3290	1/1	0.94	0.13	59,59,59,59	0
56	MG	DA	3295	1/1	0.94	0.11	31,31,31,31	0
56	MG	DA	3614	1/1	0.94	0.10	46,46,46,46	0
56	MG	BA	3237	1/1	0.94	0.16	43,43,43,43	0
56	MG	DA	3298	1/1	0.94	0.20	45,45,45,45	0
56	MG	BA	3037	1/1	0.94	0.24	39,39,39,39	0
56	MG	CA	3068	1/1	0.94	0.15	47,47,47,47	0
56	MG	BA	3352	1/1	0.94	0.08	58,58,58,58	0
56	MG	DA	3067	1/1	0.94	0.19	35,35,35,35	0
56	MG	BA	3169	1/1	0.94	0.12	39,39,39,39	0
56	MG	DA	3623	1/1	0.94	0.08	63,63,63,63	0
56	MG	DA	3624	1/1	0.94	0.07	54,54,54,54	0
56	MG	DA	3626	1/1	0.94	0.08	63,63,63,63	0
56	MG	DA	3316	1/1	0.94	0.22	47,47,47,47	0
56	MG	DA	3317	1/1	0.94	0.13	34,34,34,34	0
56	MG	BA	3171	1/1	0.94	0.24	42,42,42,42	0
56	MG	DA	3320	1/1	0.94	0.17	50,50,50,50	0
56	MG	DA	3634	1/1	0.94	0.12	33,33,33,33	0
56	MG	BA	3595	1/1	0.94	0.10	37,37,37,37	0
56	MG	AM	3001	1/1	0.94	0.05	76,76,76,76	0
56	MG	AA	3012	1/1	0.94	0.13	58,58,58,58	0
56	MG	BA	3361	1/1	0.94	0.06	39,39,39,39	0
56	MG	BB	3011	1/1	0.94	0.12	45,45,45,45	0
56	MG	CA	3080	1/1	0.94	0.13	51,51,51,51	0
56	MG	DA	3644	1/1	0.94	0.19	50,50,50,50	0
56	MG	AA	3006	1/1	0.94	0.09	84,84,84,84	0
56	MG	AA	3059	1/1	0.94	0.17	49,49,49,49	0
56	MG	DA	3648	1/1	0.94	0.10	43,43,43,43	0
56	MG	BA	3602	1/1	0.94	0.08	44,44,44,44	0
56	MG	AA	3014	1/1	0.94	0.06	24,24,24,24	0
56	MG	BD	302	1/1	0.94	0.38	44,44,44,44	0
56	MG	BD	303	1/1	0.94	0.10	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3113	1/1	0.94	0.20	48,48,48,48	0
56	MG	AA	3201	1/1	0.94	0.12	76,76,76,76	0
56	MG	AA	3202	1/1	0.94	0.14	72,72,72,72	0
56	MG	DA	3364	1/1	0.94	0.11	40,40,40,40	0
56	MG	BA	3383	1/1	0.94	0.16	51,51,51,51	0
56	MG	DA	3369	1/1	0.94	0.09	53,53,53,53	0
56	MG	BA	3613	1/1	0.94	0.15	47,47,47,47	0
56	MG	BE	306	1/1	0.94	0.24	38,38,38,38	0
56	MG	DD	304	1/1	0.94	0.22	40,40,40,40	0
56	MG	BA	3384	1/1	0.94	0.16	47,47,47,47	0
56	MG	BA	3385	1/1	0.94	0.07	56,56,56,56	0
56	MG	DE	304	1/1	0.94	0.09	30,30,30,30	0
56	MG	BA	3051	1/1	0.94	0.18	34,34,34,34	0
56	MG	DA	3385	1/1	0.94	0.21	58,58,58,58	0
56	MG	BA	3619	1/1	0.94	0.16	42,42,42,42	0
56	MG	BA	3391	1/1	0.94	0.12	39,39,39,39	0
56	MG	BA	3256	1/1	0.94	0.21	60,60,60,60	0
56	MG	BA	3052	1/1	0.94	0.14	29,29,29,29	0
56	MG	DA	3103	1/1	0.94	0.11	52,52,52,52	0
56	MG	BN	3003	1/1	0.94	0.14	67,67,67,67	0
56	MG	BA	3056	1/1	0.94	0.23	39,39,39,39	0
56	MG	DR	5001	1/1	0.94	0.13	39,39,39,39	0
56	MG	BA	3404	1/1	0.94	0.05	42,42,42,42	0
56	MG	AA	3062	1/1	0.94	0.09	30,30,30,30	0
56	MG	AA	3151	1/1	0.94	0.07	49,49,49,49	0
56	MG	DA	3407	1/1	0.94	0.10	35,35,35,35	0
56	MG	BA	3428	1/1	0.94	0.17	36,36,36,36	0
56	MG	BA	3265	1/1	0.94	0.21	39,39,39,39	0
56	MG	AA	3206	1/1	0.94	0.15	79,79,79,79	0
56	MG	BA	3434	1/1	0.94	0.16	22,22,22,22	0
58	ZN	D4	501	1/1	0.94	0.10	155,155,155,155	0
56	MG	DA	3114	1/1	0.94	0.09	47,47,47,47	0
56	MG	DA	3422	1/1	0.94	0.19	45,45,45,45	0
56	MG	CA	3128	1/1	0.94	0.14	55,55,55,55	0
56	MG	BA	3635	1/1	0.94	0.07	52,52,52,52	0
56	MG	BA	3558	1/1	0.95	0.12	47,47,47,47	0
56	MG	CA	3011	1/1	0.95	0.19	27,27,27,27	0
56	MG	DA	3446	1/1	0.95	0.14	46,46,46,46	0
56	MG	CA	3012	1/1	0.95	0.04	50,50,50,50	0
56	MG	BA	3559	1/1	0.95	0.16	29,29,29,29	0
56	MG	BA	3396	1/1	0.95	0.13	41,41,41,41	0
56	MG	BA	3401	1/1	0.95	0.11	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3698	1/1	0.95	0.25	58,58,58,58	0
56	MG	CA	3166	1/1	0.95	0.09	71,71,71,71	0
56	MG	BA	3700	1/1	0.95	0.13	26,26,26,26	0
56	MG	BA	3165	1/1	0.95	0.29	44,44,44,44	0
56	MG	AA	3119	1/1	0.95	0.20	42,42,42,42	0
56	MG	DA	3459	1/1	0.95	0.09	43,43,43,43	0
56	MG	CA	3170	1/1	0.95	0.14	44,44,44,44	0
56	MG	BA	3406	1/1	0.95	0.19	54,54,54,54	0
56	MG	BA	3423	1/1	0.95	0.15	45,45,45,45	0
56	MG	DA	3463	1/1	0.95	0.07	32,32,32,32	0
56	MG	BA	3424	1/1	0.95	0.11	44,44,44,44	0
56	MG	AA	3042	1/1	0.95	0.17	50,50,50,50	0
56	MG	DA	3466	1/1	0.95	0.07	43,43,43,43	0
56	MG	CF	3001	1/1	0.95	0.09	56,56,56,56	0
56	MG	DA	3472	1/1	0.95	0.07	38,38,38,38	0
56	MG	BA	3020	1/1	0.95	0.28	43,43,43,43	0
56	MG	DA	3182	1/1	0.95	0.15	29,29,29,29	0
56	MG	AA	3058	1/1	0.95	0.25	59,59,59,59	0
56	MG	DA	3186	1/1	0.95	0.09	38,38,38,38	0
56	MG	DA	3480	1/1	0.95	0.09	42,42,42,42	0
56	MG	DA	3481	1/1	0.95	0.09	59,59,59,59	0
56	MG	BA	3712	1/1	0.95	0.10	47,47,47,47	0
56	MG	BA	3713	1/1	0.95	0.07	49,49,49,49	0
56	MG	CX	104	1/1	0.95	0.08	52,52,52,52	0
56	MG	BA	3430	1/1	0.95	0.11	47,47,47,47	0
56	MG	DA	3193	1/1	0.95	0.15	42,42,42,42	0
56	MG	BA	3594	1/1	0.95	0.16	55,55,55,55	0
56	MG	DA	3488	1/1	0.95	0.08	48,48,48,48	0
56	MG	BA	3073	1/1	0.95	0.05	43,43,43,43	0
56	MG	AA	3186	1/1	0.95	0.11	51,51,51,51	0
56	MG	DA	3197	1/1	0.95	0.22	43,43,43,43	0
56	MG	DA	3007	1/1	0.95	0.15	43,43,43,43	0
56	MG	DA	3497	1/1	0.95	0.06	37,37,37,37	0
56	MG	AA	3008	1/1	0.95	0.11	61,61,61,61	0
56	MG	DA	3011	1/1	0.95	0.07	42,42,42,42	0
56	MG	BA	3720	1/1	0.95	0.06	51,51,51,51	0
56	MG	BA	3121	1/1	0.95	0.13	50,50,50,50	0
56	MG	BA	3438	1/1	0.95	0.13	30,30,30,30	0
56	MG	BA	3443	1/1	0.95	0.15	34,34,34,34	0
56	MG	DA	3210	1/1	0.95	0.14	46,46,46,46	0
56	MG	DA	3211	1/1	0.95	0.21	46,46,46,46	0
56	MG	BA	3726	1/1	0.95	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	3511	1/1	0.95	0.08	47,47,47,47	0
56	MG	BA	3729	1/1	0.95	0.07	54,54,54,54	0
56	MG	BA	3302	1/1	0.95	0.07	48,48,48,48	0
56	MG	DA	3217	1/1	0.95	0.17	33,33,33,33	0
56	MG	DA	3218	1/1	0.95	0.12	31,31,31,31	0
56	MG	DA	3021	1/1	0.95	0.18	43,43,43,43	0
56	MG	BA	3733	1/1	0.95	0.16	40,40,40,40	0
56	MG	DA	3519	1/1	0.95	0.07	39,39,39,39	0
56	MG	CA	3046	1/1	0.95	0.22	52,52,52,52	0
56	MG	AA	3110	1/1	0.95	0.11	41,41,41,41	0
56	MG	BA	3451	1/1	0.95	0.09	31,31,31,31	0
56	MG	BA	3606	1/1	0.95	0.06	44,44,44,44	0
56	MG	AX	107	1/1	0.95	0.06	82,82,82,82	0
56	MG	DA	3228	1/1	0.95	0.19	49,49,49,49	0
56	MG	DA	3229	1/1	0.95	0.13	44,44,44,44	0
56	MG	CA	3051	1/1	0.95	0.11	77,77,77,77	0
56	MG	BA	3308	1/1	0.95	0.13	33,33,33,33	0
56	MG	BA	3239	1/1	0.95	0.06	33,33,33,33	0
56	MG	BA	3459	1/1	0.95	0.08	51,51,51,51	0
56	MG	BA	3124	1/1	0.95	0.10	46,46,46,46	0
56	MG	BA	3615	1/1	0.95	0.16	55,55,55,55	0
56	MG	BA	3125	1/1	0.95	0.16	26,26,26,26	0
56	MG	DA	3242	1/1	0.95	0.11	31,31,31,31	0
56	MG	BA	3243	1/1	0.95	0.10	43,43,43,43	0
56	MG	BB	3008	1/1	0.95	0.14	49,49,49,49	0
56	MG	DA	3245	1/1	0.95	0.16	43,43,43,43	0
56	MG	AA	3105	1/1	0.95	0.24	54,54,54,54	0
56	MG	BA	3128	1/1	0.95	0.11	28,28,28,28	0
56	MG	BA	3031	1/1	0.95	0.14	44,44,44,44	0
56	MG	DA	3548	1/1	0.95	0.13	60,60,60,60	0
56	MG	BA	3249	1/1	0.95	0.13	46,46,46,46	0
56	MG	BA	3132	1/1	0.95	0.11	28,28,28,28	0
56	MG	DA	3050	1/1	0.95	0.09	30,30,30,30	0
56	MG	BA	3085	1/1	0.95	0.19	35,35,35,35	0
56	MG	BA	3326	1/1	0.95	0.17	15,15,15,15	0
56	MG	BA	3134	1/1	0.95	0.13	34,34,34,34	0
56	MG	BA	3086	1/1	0.95	0.06	50,50,50,50	0
56	MG	DA	3561	1/1	0.95	0.11	40,40,40,40	0
56	MG	DA	3562	1/1	0.95	0.09	41,41,41,41	0
56	MG	AX	109	1/1	0.95	0.13	56,56,56,56	0
56	MG	DA	3267	1/1	0.95	0.11	40,40,40,40	0
56	MG	BD	306	1/1	0.95	0.07	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	AX	110	1/1	0.95	0.10	45,45,45,45	0
56	MG	BD	310	1/1	0.95	0.12	48,48,48,48	0
56	MG	CA	3078	1/1	0.95	0.10	51,51,51,51	0
56	MG	BA	3089	1/1	0.95	0.13	50,50,50,50	0
56	MG	BA	3092	1/1	0.95	0.08	28,28,28,28	0
56	MG	BA	3259	1/1	0.95	0.14	59,59,59,59	0
56	MG	BA	3341	1/1	0.95	0.11	31,31,31,31	0
56	MG	CA	3085	1/1	0.95	0.18	58,58,58,58	0
56	MG	DA	3583	1/1	0.95	0.12	35,35,35,35	0
56	MG	BF	302	1/1	0.95	0.18	49,49,49,49	0
56	MG	CA	3087	1/1	0.95	0.09	40,40,40,40	0
56	MG	BA	3501	1/1	0.95	0.10	35,35,35,35	0
56	MG	DA	3588	1/1	0.95	0.11	47,47,47,47	0
56	MG	CA	3089	1/1	0.95	0.11	54,54,54,54	0
56	MG	BF	304	1/1	0.95	0.21	30,30,30,30	0
56	MG	DA	3592	1/1	0.95	0.09	49,49,49,49	0
56	MG	DA	3593	1/1	0.95	0.13	62,62,62,62	0
56	MG	BA	3142	1/1	0.95	0.13	57,57,57,57	0
56	MG	DA	3294	1/1	0.95	0.15	30,30,30,30	0
56	MG	CA	3092	1/1	0.95	0.12	56,56,56,56	0
56	MG	CA	3093	1/1	0.95	0.11	65,65,65,65	0
56	MG	CA	3095	1/1	0.95	0.11	35,35,35,35	0
56	MG	DA	3599	1/1	0.95	0.16	69,69,69,69	0
56	MG	DA	3080	1/1	0.95	0.15	43,43,43,43	0
56	MG	AA	3221	1/1	0.95	0.21	52,52,52,52	0
56	MG	DA	3305	1/1	0.95	0.12	33,33,33,33	0
56	MG	CA	3100	1/1	0.95	0.13	72,72,72,72	0
56	MG	BA	3350	1/1	0.95	0.10	36,36,36,36	0
56	MG	DA	3313	1/1	0.95	0.10	30,30,30,30	0
56	MG	BA	3040	1/1	0.95	0.09	40,40,40,40	0
56	MG	CA	3105	1/1	0.95	0.09	59,59,59,59	0
56	MG	DA	3609	1/1	0.95	0.13	49,49,49,49	0
56	MG	DA	3610	1/1	0.95	0.06	49,49,49,49	0
56	MG	BN	3001	1/1	0.95	0.11	65,65,65,65	0
56	MG	BA	3264	1/1	0.95	0.10	29,29,29,29	0
56	MG	AA	3179	1/1	0.95	0.14	34,34,34,34	0
56	MG	BN	3004	1/1	0.95	0.20	69,69,69,69	0
56	MG	BA	3147	1/1	0.95	0.13	42,42,42,42	0
56	MG	BA	3650	1/1	0.95	0.09	44,44,44,44	0
56	MG	BP	204	1/1	0.95	0.08	53,53,53,53	0
56	MG	BQ	3001	1/1	0.95	0.21	38,38,38,38	0
56	MG	AA	3205	1/1	0.95	0.12	66,66,66,66	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	0.95	0.20	46,46,46,46	0
56	MG	BA	3360	1/1	0.95	0.09	39,39,39,39	0
56	MG	DA	3339	1/1	0.95	0.15	35,35,35,35	0
56	MG	BA	3270	1/1	0.95	0.12	29,29,29,29	0
56	MG	DA	3625	1/1	0.95	0.07	48,48,48,48	0
56	MG	BU	201	1/1	0.95	0.34	33,33,33,33	0
56	MG	DA	3347	1/1	0.95	0.09	39,39,39,39	0
56	MG	BA	3516	1/1	0.95	0.09	64,64,64,64	0
56	MG	BA	3367	1/1	0.95	0.11	29,29,29,29	0
56	MG	BU	209	1/1	0.95	0.40	36,36,36,36	0
56	MG	DA	3358	1/1	0.95	0.09	38,38,38,38	0
56	MG	DA	3635	1/1	0.95	0.07	39,39,39,39	0
56	MG	DA	3107	1/1	0.95	0.12	50,50,50,50	0
56	MG	BV	3001	1/1	0.95	0.10	42,42,42,42	0
56	MG	BA	3659	1/1	0.95	0.06	42,42,42,42	0
56	MG	DA	3365	1/1	0.95	0.06	52,52,52,52	0
56	MG	DA	3366	1/1	0.95	0.06	43,43,43,43	0
56	MG	BA	3005	1/1	0.95	0.11	43,43,43,43	0
56	MG	AA	3044	1/1	0.95	0.15	60,60,60,60	0
56	MG	BA	3527	1/1	0.95	0.17	45,45,45,45	0
56	MG	DA	3371	1/1	0.95	0.07	37,37,37,37	0
56	MG	BA	3529	1/1	0.95	0.10	22,22,22,22	0
56	MG	DA	3377	1/1	0.95	0.13	32,32,32,32	0
56	MG	DA	3652	1/1	0.95	0.15	26,26,26,26	0
56	MG	DA	3654	1/1	0.95	0.07	50,50,50,50	0
56	MG	BA	3151	1/1	0.95	0.16	40,40,40,40	0
56	MG	DA	3657	1/1	0.95	0.07	55,55,55,55	0
56	MG	DA	3379	1/1	0.95	0.08	63,63,63,63	0
56	MG	AK	3001	1/1	0.95	0.10	48,48,48,48	0
56	MG	BA	3102	1/1	0.95	0.18	45,45,45,45	0
56	MG	BA	3668	1/1	0.95	0.11	42,42,42,42	0
56	MG	B0	105	1/1	0.95	0.23	44,44,44,44	0
56	MG	CA	3137	1/1	0.95	0.13	59,59,59,59	0
56	MG	CA	3138	1/1	0.95	0.14	59,59,59,59	0
56	MG	AL	3001	1/1	0.95	0.10	50,50,50,50	0
56	MG	BA	3009	1/1	0.95	0.12	36,36,36,36	0
56	MG	DD	302	1/1	0.95	0.29	48,48,48,48	0
56	MG	DA	3394	1/1	0.95	0.07	46,46,46,46	0
56	MG	DA	3125	1/1	0.95	0.09	55,55,55,55	0
56	MG	DD	305	1/1	0.95	0.11	73,73,73,73	0
56	MG	DE	301	1/1	0.95	0.18	51,51,51,51	0
56	MG	BA	3011	1/1	0.95	0.11	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	3127	1/1	0.95	0.06	44,44,44,44	0
56	MG	BA	3543	1/1	0.95	0.11	24,24,24,24	0
56	MG	BA	3285	1/1	0.95	0.14	44,44,44,44	0
56	MG	DF	301	1/1	0.95	0.16	40,40,40,40	0
56	MG	DA	3130	1/1	0.95	0.06	34,34,34,34	0
56	MG	DF	305	1/1	0.95	0.22	55,55,55,55	0
56	MG	DA	3408	1/1	0.95	0.09	35,35,35,35	0
56	MG	BA	3545	1/1	0.95	0.11	20,20,20,20	0
56	MG	DA	3413	1/1	0.95	0.10	44,44,44,44	0
56	MG	BA	3387	1/1	0.95	0.09	49,49,49,49	0
56	MG	DQ	3001	1/1	0.95	0.16	40,40,40,40	0
56	MG	AA	3193	1/1	0.95	0.15	65,65,65,65	0
56	MG	DA	3417	1/1	0.95	0.12	54,54,54,54	0
56	MG	AA	3142	1/1	0.95	0.16	60,60,60,60	0
56	MG	BA	3162	1/1	0.95	0.08	43,43,43,43	0
56	MG	CA	3002	1/1	0.95	0.05	74,74,74,74	0
56	MG	DA	3139	1/1	0.95	0.11	47,47,47,47	0
56	MG	BA	3016	1/1	0.95	0.12	50,50,50,50	0
56	MG	DA	3428	1/1	0.95	0.09	30,30,30,30	0
56	MG	BA	3683	1/1	0.95	0.19	37,37,37,37	0
56	MG	DA	3143	1/1	0.95	0.09	53,53,53,53	0
56	MG	D5	101	1/1	0.95	0.14	44,44,44,44	0
56	MG	DA	3144	1/1	0.95	0.21	37,37,37,37	0
56	MG	DA	3145	1/1	0.95	0.11	52,52,52,52	0
56	MG	CA	3154	1/1	0.95	0.16	54,54,54,54	0
56	MG	BA	3553	1/1	0.95	0.18	46,46,46,46	0
56	MG	BA	3554	1/1	0.95	0.16	25,25,25,25	0
56	MG	AA	3195	1/1	0.95	0.21	58,58,58,58	0
56	MG	BA	3690	1/1	0.95	0.16	55,55,55,55	0
56	MG	BA	3623	1/1	0.96	0.12	43,43,43,43	0
56	MG	BB	3015	1/1	0.96	0.08	35,35,35,35	0
56	MG	DA	3469	1/1	0.96	0.14	52,52,52,52	0
56	MG	DA	3470	1/1	0.96	0.15	45,45,45,45	0
56	MG	BA	3484	1/1	0.96	0.08	40,40,40,40	0
56	MG	BA	3269	1/1	0.96	0.15	32,32,32,32	0
56	MG	BA	3486	1/1	0.96	0.12	55,55,55,55	0
56	MG	CA	3066	1/1	0.96	0.06	47,47,47,47	0
56	MG	DA	3213	1/1	0.96	0.15	48,48,48,48	0
56	MG	BA	3628	1/1	0.96	0.09	39,39,39,39	0
56	MG	DA	3215	1/1	0.96	0.25	43,43,43,43	0
56	MG	DA	3037	1/1	0.96	0.19	37,37,37,37	0
56	MG	AA	3161	1/1	0.96	0.06	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3630	1/1	0.96	0.12	48,48,48,48	0
56	MG	BA	3493	1/1	0.96	0.08	51,51,51,51	0
56	MG	BA	3496	1/1	0.96	0.20	21,21,21,21	0
56	MG	AA	3010	1/1	0.96	0.05	71,71,71,71	0
56	MG	AA	3050	1/1	0.96	0.08	50,50,50,50	0
56	MG	DA	3046	1/1	0.96	0.10	48,48,48,48	0
56	MG	DA	3047	1/1	0.96	0.09	36,36,36,36	0
56	MG	DA	3226	1/1	0.96	0.21	47,47,47,47	0
56	MG	BA	3048	1/1	0.96	0.20	33,33,33,33	0
56	MG	BA	3050	1/1	0.96	0.12	33,33,33,33	0
56	MG	CA	3076	1/1	0.96	0.14	48,48,48,48	0
56	MG	DA	3051	1/1	0.96	0.08	39,39,39,39	0
56	MG	BE	302	1/1	0.96	0.12	29,29,29,29	0
56	MG	DA	3501	1/1	0.96	0.16	67,67,67,67	0
56	MG	DA	3232	1/1	0.96	0.05	39,39,39,39	0
56	MG	BE	305	1/1	0.96	0.21	44,44,44,44	0
56	MG	BA	3090	1/1	0.96	0.07	42,42,42,42	0
56	MG	BA	3218	1/1	0.96	0.09	58,58,58,58	0
56	MG	DA	3239	1/1	0.96	0.13	54,54,54,54	0
56	MG	BF	301	1/1	0.96	0.10	46,46,46,46	0
56	MG	BA	3281	1/1	0.96	0.07	45,45,45,45	0
56	MG	DA	3059	1/1	0.96	0.07	42,42,42,42	0
56	MG	BA	3506	1/1	0.96	0.10	33,33,33,33	0
56	MG	BA	3282	1/1	0.96	0.10	34,34,34,34	0
56	MG	BA	3372	1/1	0.96	0.08	42,42,42,42	0
56	MG	BA	3645	1/1	0.96	0.21	63,63,63,63	0
56	MG	DA	3247	1/1	0.96	0.17	34,34,34,34	0
56	MG	BA	3646	1/1	0.96	0.12	39,39,39,39	0
56	MG	BA	3170	1/1	0.96	0.21	34,34,34,34	0
56	MG	BA	3511	1/1	0.96	0.17	40,40,40,40	0
56	MG	AA	3104	1/1	0.96	0.10	35,35,35,35	0
56	MG	BA	3129	1/1	0.96	0.28	44,44,44,44	0
56	MG	BA	3130	1/1	0.96	0.38	51,51,51,51	0
56	MG	BA	3652	1/1	0.96	0.18	54,54,54,54	0
56	MG	DA	3072	1/1	0.96	0.14	40,40,40,40	0
56	MG	BO	201	1/1	0.96	0.07	63,63,63,63	0
56	MG	DA	3261	1/1	0.96	0.13	44,44,44,44	0
56	MG	DA	3262	1/1	0.96	0.18	60,60,60,60	0
56	MG	AA	3167	1/1	0.96	0.16	78,78,78,78	0
56	MG	DA	3533	1/1	0.96	0.12	59,59,59,59	0
56	MG	DA	3264	1/1	0.96	0.07	38,38,38,38	0
56	MG	BP	203	1/1	0.96	0.55	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	3076	1/1	0.96	0.24	38,38,38,38	0
56	MG	BA	3517	1/1	0.96	0.11	52,52,52,52	0
56	MG	DA	3538	1/1	0.96	0.13	37,37,37,37	0
56	MG	BA	3226	1/1	0.96	0.23	31,31,31,31	0
56	MG	BA	3290	1/1	0.96	0.07	35,35,35,35	0
56	MG	DA	3272	1/1	0.96	0.13	36,36,36,36	0
56	MG	BA	3388	1/1	0.96	0.07	30,30,30,30	0
56	MG	DA	3274	1/1	0.96	0.22	49,49,49,49	0
56	MG	DA	3546	1/1	0.96	0.14	38,38,38,38	0
56	MG	BA	3525	1/1	0.96	0.09	31,31,31,31	0
56	MG	DA	3277	1/1	0.96	0.05	46,46,46,46	0
56	MG	DA	3083	1/1	0.96	0.05	44,44,44,44	0
56	MG	DA	3279	1/1	0.96	0.12	32,32,32,32	0
56	MG	DA	3280	1/1	0.96	0.11	46,46,46,46	0
56	MG	BA	3526	1/1	0.96	0.12	49,49,49,49	0
56	MG	BA	3175	1/1	0.96	0.17	40,40,40,40	0
56	MG	DA	3283	1/1	0.96	0.07	47,47,47,47	0
56	MG	BA	3055	1/1	0.96	0.21	44,44,44,44	0
56	MG	BU	207	1/1	0.96	0.13	38,38,38,38	0
56	MG	CA	3115	1/1	0.96	0.06	81,81,81,81	0
56	MG	BA	3095	1/1	0.96	0.21	55,55,55,55	0
56	MG	BA	3532	1/1	0.96	0.15	42,42,42,42	0
56	MG	CA	3118	1/1	0.96	0.08	39,39,39,39	0
56	MG	BA	3096	1/1	0.96	0.23	35,35,35,35	0
56	MG	BA	3232	1/1	0.96	0.15	32,32,32,32	0
56	MG	BA	3025	1/1	0.96	0.09	48,48,48,48	0
56	MG	BW	3002	1/1	0.96	0.16	34,34,34,34	0
56	MG	BA	3400	1/1	0.96	0.06	29,29,29,29	0
56	MG	BA	3136	1/1	0.96	0.09	47,47,47,47	0
56	MG	DA	3576	1/1	0.96	0.09	57,57,57,57	0
56	MG	BA	3402	1/1	0.96	0.13	23,23,23,23	0
56	MG	DA	3580	1/1	0.96	0.08	35,35,35,35	0
56	MG	DA	3581	1/1	0.96	0.10	41,41,41,41	0
56	MG	BA	3059	1/1	0.96	0.21	35,35,35,35	0
56	MG	AA	3138	1/1	0.96	0.21	38,38,38,38	0
56	MG	DA	3312	1/1	0.96	0.09	24,24,24,24	0
56	MG	AA	3212	1/1	0.96	0.10	36,36,36,36	0
56	MG	B0	103	1/1	0.96	0.07	46,46,46,46	0
56	MG	BA	3407	1/1	0.96	0.17	35,35,35,35	0
56	MG	BA	3408	1/1	0.96	0.08	28,28,28,28	0
56	MG	DA	3590	1/1	0.96	0.07	39,39,39,39	0
56	MG	BA	3678	1/1	0.96	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	BA	3412	1/1	0.96	0.16	29,29,29,29	0
56	MG	BA	3551	1/1	0.96	0.13	31,31,31,31	0
56	MG	BA	3419	1/1	0.96	0.30	36,36,36,36	0
56	MG	BA	3140	1/1	0.96	0.18	50,50,50,50	0
56	MG	BA	3241	1/1	0.96	0.23	41,41,41,41	0
56	MG	DA	3329	1/1	0.96	0.07	40,40,40,40	0
56	MG	DA	3330	1/1	0.96	0.06	30,30,30,30	0
56	MG	CA	3140	1/1	0.96	0.14	75,75,75,75	0
56	MG	BA	3556	1/1	0.96	0.07	25,25,25,25	0
56	MG	DA	3334	1/1	0.96	0.11	37,37,37,37	0
56	MG	AA	3183	1/1	0.96	0.12	56,56,56,56	0
56	MG	CA	3143	1/1	0.96	0.11	91,91,91,91	0
56	MG	DA	3118	1/1	0.96	0.07	44,44,44,44	0
56	MG	BA	3688	1/1	0.96	0.07	58,58,58,58	0
56	MG	DA	3345	1/1	0.96	0.06	16,16,16,16	0
56	MG	DA	3120	1/1	0.96	0.39	50,50,50,50	0
56	MG	BA	3689	1/1	0.96	0.09	25,25,25,25	0
56	MG	CA	3001	1/1	0.96	0.06	48,48,48,48	0
56	MG	BA	3029	1/1	0.96	0.29	53,53,53,53	0
56	MG	DA	3354	1/1	0.96	0.05	39,39,39,39	0
56	MG	DA	3355	1/1	0.96	0.17	39,39,39,39	0
56	MG	BA	3692	1/1	0.96	0.16	36,36,36,36	0
56	MG	BA	3244	1/1	0.96	0.22	46,46,46,46	0
56	MG	BA	3245	1/1	0.96	0.13	45,45,45,45	0
56	MG	BA	3695	1/1	0.96	0.23	34,34,34,34	0
56	MG	BA	3067	1/1	0.96	0.28	55,55,55,55	0
56	MG	AA	3060	1/1	0.96	0.28	52,52,52,52	0
56	MG	BA	3069	1/1	0.96	0.12	33,33,33,33	0
56	MG	BA	3568	1/1	0.96	0.07	68,68,68,68	0
56	MG	BA	3106	1/1	0.96	0.22	52,52,52,52	0
56	MG	CA	3013	1/1	0.96	0.05	46,46,46,46	0
56	MG	BA	3576	1/1	0.96	0.06	45,45,45,45	0
56	MG	BA	3703	1/1	0.96	0.09	44,44,44,44	0
56	MG	BA	3194	1/1	0.96	0.25	43,43,43,43	0
56	MG	CA	3017	1/1	0.96	0.17	54,54,54,54	0
56	MG	BA	3581	1/1	0.96	0.17	54,54,54,54	0
56	MG	AA	3199	1/1	0.96	0.08	62,62,62,62	0
56	MG	DA	3632	1/1	0.96	0.16	60,60,60,60	0
56	MG	BA	3033	1/1	0.96	0.24	54,54,54,54	0
56	MG	BA	3588	1/1	0.96	0.07	41,41,41,41	0
56	MG	BA	3446	1/1	0.96	0.11	25,25,25,25	0
56	MG	BA	3197	1/1	0.96	0.21	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	3147	1/1	0.96	0.15	46,46,46,46	0
56	MG	DA	3148	1/1	0.96	0.09	41,41,41,41	0
56	MG	BA	3450	1/1	0.96	0.07	40,40,40,40	0
56	MG	DA	3151	1/1	0.96	0.30	48,48,48,48	0
56	MG	BA	3110	1/1	0.96	0.10	43,43,43,43	0
56	MG	DA	3398	1/1	0.96	0.07	50,50,50,50	0
56	MG	BA	3715	1/1	0.96	0.13	44,44,44,44	0
56	MG	DA	3647	1/1	0.96	0.13	45,45,45,45	0
56	MG	BA	3452	1/1	0.96	0.07	16,16,16,16	0
56	MG	DA	3402	1/1	0.96	0.14	33,33,33,33	0
56	MG	DA	3404	1/1	0.96	0.09	57,57,57,57	0
56	MG	BA	3036	1/1	0.96	0.13	25,25,25,25	0
56	MG	BA	3200	1/1	0.96	0.09	32,32,32,32	0
56	MG	DA	3656	1/1	0.96	0.08	62,62,62,62	0
56	MG	BA	3598	1/1	0.96	0.09	32,32,32,32	0
56	MG	DA	3658	1/1	0.96	0.26	50,50,50,50	0
56	MG	DA	3158	1/1	0.96	0.28	47,47,47,47	0
56	MG	BA	3010	1/1	0.96	0.05	35,35,35,35	0
56	MG	BA	3332	1/1	0.96	0.13	52,52,52,52	0
56	MG	BA	3258	1/1	0.96	0.05	35,35,35,35	0
56	MG	DB	3005	1/1	0.96	0.14	41,41,41,41	0
56	MG	BA	3723	1/1	0.96	0.08	25,25,25,25	0
56	MG	DA	3165	1/1	0.96	0.28	48,48,48,48	0
56	MG	BA	3461	1/1	0.96	0.07	33,33,33,33	0
56	MG	BA	3462	1/1	0.96	0.13	30,30,30,30	0
56	MG	DA	3168	1/1	0.96	0.34	46,46,46,46	0
56	MG	DA	3423	1/1	0.96	0.07	29,29,29,29	0
56	MG	BA	3728	1/1	0.96	0.10	56,56,56,56	0
56	MG	BA	3464	1/1	0.96	0.09	40,40,40,40	0
56	MG	AA	3066	1/1	0.96	0.17	41,41,41,41	0
56	MG	DA	3004	1/1	0.96	0.06	24,24,24,24	0
56	MG	BA	3260	1/1	0.96	0.11	47,47,47,47	0
56	MG	DA	3433	1/1	0.96	0.19	39,39,39,39	0
56	MG	DA	3174	1/1	0.96	0.22	26,26,26,26	0
56	MG	BA	3608	1/1	0.96	0.13	51,51,51,51	0
56	MG	BA	3609	1/1	0.96	0.16	29,29,29,29	0
56	MG	DF	303	1/1	0.96	0.10	42,42,42,42	0
56	MG	DA	3009	1/1	0.96	0.04	33,33,33,33	0
56	MG	DA	3010	1/1	0.96	0.07	42,42,42,42	0
56	MG	DA	3439	1/1	0.96	0.13	45,45,45,45	0
56	MG	DA	3181	1/1	0.96	0.30	55,55,55,55	0
56	MG	AA	3091	1/1	0.96	0.12	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3443	1/1	0.96	0.13	30,30,30,30	0
56	MG	DA	3183	1/1	0.96	0.11	42,42,42,42	0
56	MG	BA	3738	1/1	0.96	0.17	58,58,58,58	0
56	MG	DA	3185	1/1	0.96	0.15	42,42,42,42	0
56	MG	BA	3611	1/1	0.96	0.07	61,61,61,61	0
56	MG	BA	3076	1/1	0.96	0.13	40,40,40,40	0
56	MG	AA	3024	1/1	0.96	0.12	49,49,49,49	0
56	MG	DU	3002	1/1	0.96	0.23	52,52,52,52	0
56	MG	DV	201	1/1	0.96	0.07	56,56,56,56	0
56	MG	DA	3016	1/1	0.96	0.10	33,33,33,33	0
56	MG	BA	3041	1/1	0.96	0.24	45,45,45,45	0
56	MG	DW	201	1/1	0.96	0.08	45,45,45,45	0
56	MG	DA	3192	1/1	0.96	0.15	48,48,48,48	0
56	MG	AA	3034	1/1	0.96	0.14	46,46,46,46	0
56	MG	BA	3344	1/1	0.96	0.06	65,65,65,65	0
56	MG	DA	3020	1/1	0.96	0.14	45,45,45,45	0
56	MG	D5	102	1/1	0.96	0.23	44,44,44,44	0
56	MG	BA	3346	1/1	0.96	0.07	33,33,33,33	0
56	MG	CA	3055	1/1	0.96	0.26	61,61,61,61	0
56	MG	BA	3349	1/1	0.96	0.07	31,31,31,31	0
56	MG	AA	3160	1/1	0.96	0.19	52,52,52,52	0
56	MG	BA	3210	1/1	0.96	0.20	39,39,39,39	0
56	MG	DA	3202	1/1	0.96	0.08	39,39,39,39	0
56	MG	BA	3355	1/1	0.96	0.07	39,39,39,39	0
56	MG	AA	3208	1/1	0.97	0.13	38,38,38,38	0
56	MG	DA	3311	1/1	0.97	0.06	33,33,33,33	0
56	MG	BA	3699	1/1	0.97	0.08	23,23,23,23	0
56	MG	AA	3144	1/1	0.97	0.08	56,56,56,56	0
56	MG	AA	3103	1/1	0.97	0.15	43,43,43,43	0
56	MG	DA	3522	1/1	0.97	0.07	46,46,46,46	0
56	MG	DA	3315	1/1	0.97	0.10	39,39,39,39	0
56	MG	BA	3023	1/1	0.97	0.18	34,34,34,34	0
56	MG	BV	3003	1/1	0.97	0.14	27,27,27,27	0
56	MG	DA	3159	1/1	0.97	0.06	50,50,50,50	0
56	MG	DA	3160	1/1	0.97	0.08	47,47,47,47	0
56	MG	BA	3508	1/1	0.97	0.08	46,46,46,46	0
56	MG	BA	3216	1/1	0.97	0.09	46,46,46,46	0
56	MG	BA	3024	1/1	0.97	0.06	31,31,31,31	0
56	MG	DA	3327	1/1	0.97	0.05	45,45,45,45	0
56	MG	BA	3706	1/1	0.97	0.11	38,38,38,38	0
56	MG	BA	3707	1/1	0.97	0.06	57,57,57,57	0
56	MG	BA	3426	1/1	0.97	0.07	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3427	1/1	0.97	0.07	20,20,20,20	0
56	MG	CA	3096	1/1	0.97	0.06	54,54,54,54	0
56	MG	CA	3097	1/1	0.97	0.09	60,60,60,60	0
56	MG	DA	3539	1/1	0.97	0.09	35,35,35,35	0
56	MG	DA	3335	1/1	0.97	0.09	36,36,36,36	0
56	MG	AA	3049	1/1	0.97	0.18	46,46,46,46	0
56	MG	B0	102	1/1	0.97	0.06	50,50,50,50	0
56	MG	DA	3042	1/1	0.97	0.14	38,38,38,38	0
56	MG	DA	3342	1/1	0.97	0.09	31,31,31,31	0
56	MG	DA	3545	1/1	0.97	0.14	35,35,35,35	0
56	MG	BA	3617	1/1	0.97	0.16	30,30,30,30	0
56	MG	BA	3347	1/1	0.97	0.10	44,44,44,44	0
56	MG	BA	3045	1/1	0.97	0.08	27,27,27,27	0
56	MG	BA	3220	1/1	0.97	0.18	27,27,27,27	0
56	MG	DA	3550	1/1	0.97	0.09	54,54,54,54	0
56	MG	DA	3350	1/1	0.97	0.11	21,21,21,21	0
56	MG	DA	3553	1/1	0.97	0.12	58,58,58,58	0
56	MG	DA	3177	1/1	0.97	0.13	30,30,30,30	0
56	MG	DA	3178	1/1	0.97	0.07	43,43,43,43	0
56	MG	DA	3556	1/1	0.97	0.07	35,35,35,35	0
56	MG	AA	3165	1/1	0.97	0.09	24,24,24,24	0
56	MG	BA	3354	1/1	0.97	0.05	45,45,45,45	0
56	MG	BA	3521	1/1	0.97	0.10	38,38,38,38	0
56	MG	DA	3357	1/1	0.97	0.06	50,50,50,50	0
56	MG	B3	3401	1/1	0.97	0.10	24,24,24,24	0
56	MG	DA	3052	1/1	0.97	0.05	20,20,20,20	0
56	MG	B3	3402	1/1	0.97	0.07	49,49,49,49	0
56	MG	BA	3522	1/1	0.97	0.12	42,42,42,42	0
56	MG	BA	3222	1/1	0.97	0.23	56,56,56,56	0
56	MG	B7	102	1/1	0.97	0.06	29,29,29,29	0
56	MG	AA	3031	1/1	0.97	0.19	41,41,41,41	0
56	MG	BA	3439	1/1	0.97	0.05	35,35,35,35	0
56	MG	AA	3214	1/1	0.97	0.17	42,42,42,42	0
56	MG	DA	3574	1/1	0.97	0.11	22,22,22,22	0
56	MG	B8	5002	1/1	0.97	0.10	48,48,48,48	0
56	MG	BA	3160	1/1	0.97	0.15	24,24,24,24	0
56	MG	DA	3577	1/1	0.97	0.09	44,44,44,44	0
56	MG	DA	3374	1/1	0.97	0.10	40,40,40,40	0
56	MG	DA	3579	1/1	0.97	0.11	38,38,38,38	0
56	MG	DA	3376	1/1	0.97	0.08	42,42,42,42	0
56	MG	CA	3120	1/1	0.97	0.12	59,59,59,59	0
56	MG	DA	3063	1/1	0.97	0.07	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	AA	3158	1/1	0.97	0.12	47,47,47,47	0
56	MG	BA	3531	1/1	0.97	0.11	28,28,28,28	0
56	MG	BA	3078	1/1	0.97	0.10	44,44,44,44	0
56	MG	DA	3383	1/1	0.97	0.08	27,27,27,27	0
56	MG	DA	3199	1/1	0.97	0.15	46,46,46,46	0
56	MG	BA	3449	1/1	0.97	0.10	59,59,59,59	0
56	MG	BA	3730	1/1	0.97	0.06	43,43,43,43	0
56	MG	CA	3006	1/1	0.97	0.07	72,72,72,72	0
56	MG	BA	3731	1/1	0.97	0.11	52,52,52,52	0
56	MG	DA	3204	1/1	0.97	0.23	44,44,44,44	0
56	MG	BA	3013	1/1	0.97	0.16	36,36,36,36	0
56	MG	BA	3364	1/1	0.97	0.08	30,30,30,30	0
56	MG	DA	3397	1/1	0.97	0.11	40,40,40,40	0
56	MG	DA	3207	1/1	0.97	0.12	41,41,41,41	0
56	MG	BA	3303	1/1	0.97	0.11	11,11,11,11	0
56	MG	AA	3177	1/1	0.97	0.05	58,58,58,58	0
56	MG	BA	3542	1/1	0.97	0.11	37,37,37,37	0
56	MG	DA	3403	1/1	0.97	0.06	42,42,42,42	0
56	MG	CA	3133	1/1	0.97	0.04	45,45,45,45	0
56	MG	BA	3108	1/1	0.97	0.09	32,32,32,32	0
56	MG	BA	3642	1/1	0.97	0.08	52,52,52,52	0
56	MG	BA	3456	1/1	0.97	0.08	24,24,24,24	0
56	MG	BA	3457	1/1	0.97	0.06	25,25,25,25	0
56	MG	BA	3266	1/1	0.97	0.21	47,47,47,47	0
56	MG	DA	3410	1/1	0.97	0.05	40,40,40,40	0
56	MG	BA	3053	1/1	0.97	0.11	52,52,52,52	0
56	MG	DA	3219	1/1	0.97	0.20	49,49,49,49	0
56	MG	BA	3233	1/1	0.97	0.12	49,49,49,49	0
56	MG	DA	3085	1/1	0.97	0.07	35,35,35,35	0
56	MG	CA	3020	1/1	0.97	0.12	45,45,45,45	0
56	MG	BA	3054	1/1	0.97	0.07	39,39,39,39	0
56	MG	DA	3421	1/1	0.97	0.11	43,43,43,43	0
56	MG	DA	3088	1/1	0.97	0.06	47,47,47,47	0
56	MG	BA	3168	1/1	0.97	0.28	52,52,52,52	0
56	MG	CA	3023	1/1	0.97	0.14	37,37,37,37	0
56	MG	BB	3007	1/1	0.97	0.04	49,49,49,49	0
56	MG	DA	3426	1/1	0.97	0.09	41,41,41,41	0
56	MG	BA	3377	1/1	0.97	0.04	27,27,27,27	0
56	MG	DA	3429	1/1	0.97	0.05	30,30,30,30	0
56	MG	CA	3026	1/1	0.97	0.04	52,52,52,52	0
56	MG	BA	3380	1/1	0.97	0.10	32,32,32,32	0
56	MG	BA	3381	1/1	0.97	0.04	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3382	1/1	0.97	0.12	21,21,21,21	0
56	MG	DA	3629	1/1	0.97	0.09	30,30,30,30	0
56	MG	DA	3233	1/1	0.97	0.08	58,58,58,58	0
56	MG	BA	3271	1/1	0.97	0.16	40,40,40,40	0
56	MG	BA	3655	1/1	0.97	0.11	44,44,44,44	0
56	MG	DA	3237	1/1	0.97	0.15	37,37,37,37	0
56	MG	AA	3149	1/1	0.97	0.05	49,49,49,49	0
56	MG	DA	3440	1/1	0.97	0.05	48,48,48,48	0
56	MG	BA	3034	1/1	0.97	0.05	37,37,37,37	0
56	MG	DA	3101	1/1	0.97	0.13	59,59,59,59	0
56	MG	BA	3560	1/1	0.97	0.14	24,24,24,24	0
56	MG	BA	3471	1/1	0.97	0.05	28,28,28,28	0
56	MG	DA	3641	1/1	0.97	0.12	47,47,47,47	0
56	MG	BA	3562	1/1	0.97	0.11	42,42,42,42	0
56	MG	BA	3472	1/1	0.97	0.07	53,53,53,53	0
56	MG	BA	3662	1/1	0.97	0.08	46,46,46,46	0
56	MG	BD	308	1/1	0.97	0.15	21,21,21,21	0
56	MG	BA	3386	1/1	0.97	0.07	29,29,29,29	0
56	MG	DA	3451	1/1	0.97	0.03	68,68,68,68	0
56	MG	DA	3649	1/1	0.97	0.05	39,39,39,39	0
56	MG	BA	3566	1/1	0.97	0.12	43,43,43,43	0
56	MG	DA	3453	1/1	0.97	0.09	44,44,44,44	0
56	MG	DA	3653	1/1	0.97	0.06	52,52,52,52	0
56	MG	BA	3474	1/1	0.97	0.09	43,43,43,43	0
56	MG	BA	3058	1/1	0.97	0.20	41,41,41,41	0
56	MG	BA	3569	1/1	0.97	0.09	55,55,55,55	0
56	MG	BE	304	1/1	0.97	0.15	45,45,45,45	0
56	MG	BA	3321	1/1	0.97	0.14	47,47,47,47	0
56	MG	BA	3573	1/1	0.97	0.06	53,53,53,53	0
56	MG	BA	3670	1/1	0.97	0.08	55,55,55,55	0
56	MG	DA	3258	1/1	0.97	0.14	39,39,39,39	0
56	MG	BE	308	1/1	0.97	0.14	27,27,27,27	0
56	MG	BE	309	1/1	0.97	0.06	37,37,37,37	0
56	MG	BA	3389	1/1	0.97	0.15	52,52,52,52	0
56	MG	BA	3276	1/1	0.97	0.15	9,9,9,9	0
56	MG	DB	3008	1/1	0.97	0.09	36,36,36,36	0
56	MG	DB	3009	1/1	0.97	0.27	41,41,41,41	0
56	MG	BA	3580	1/1	0.97	0.10	58,58,58,58	0
56	MG	DA	3467	1/1	0.97	0.12	48,48,48,48	0
56	MG	DA	3265	1/1	0.97	0.13	44,44,44,44	0
56	MG	DD	301	1/1	0.97	0.08	23,23,23,23	0
56	MG	BA	3035	1/1	0.97	0.06	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BF	305	1/1	0.97	0.15	38,38,38,38	0
56	MG	DA	3471	1/1	0.97	0.09	32,32,32,32	0
56	MG	BA	3278	1/1	0.97	0.19	53,53,53,53	0
56	MG	BA	3115	1/1	0.97	0.14	28,28,28,28	0
56	MG	BA	3587	1/1	0.97	0.12	23,23,23,23	0
56	MG	CA	3059	1/1	0.97	0.18	51,51,51,51	0
56	MG	BA	3329	1/1	0.97	0.07	49,49,49,49	0
56	MG	DA	3479	1/1	0.97	0.11	35,35,35,35	0
56	MG	BA	3330	1/1	0.97	0.07	35,35,35,35	0
56	MG	DF	302	1/1	0.97	0.07	47,47,47,47	0
56	MG	AA	3057	1/1	0.97	0.05	45,45,45,45	0
56	MG	BA	3489	1/1	0.97	0.06	50,50,50,50	0
56	MG	BA	3490	1/1	0.97	0.07	40,40,40,40	0
56	MG	DA	3133	1/1	0.97	0.12	31,31,31,31	0
56	MG	DA	3006	1/1	0.97	0.10	41,41,41,41	0
56	MG	BA	3492	1/1	0.97	0.12	48,48,48,48	0
56	MG	BN	3006	1/1	0.97	0.04	33,33,33,33	0
56	MG	BA	3003	1/1	0.97	0.08	24,24,24,24	0
56	MG	BP	201	1/1	0.97	0.23	37,37,37,37	0
56	MG	DA	3492	1/1	0.97	0.05	44,44,44,44	0
56	MG	BA	3494	1/1	0.97	0.09	28,28,28,28	0
56	MG	DA	3494	1/1	0.97	0.07	50,50,50,50	0
56	MG	DA	3286	1/1	0.97	0.05	26,26,26,26	0
56	MG	BA	3334	1/1	0.97	0.08	41,41,41,41	0
56	MG	DA	3142	1/1	0.97	0.19	33,33,33,33	0
56	MG	BA	3497	1/1	0.97	0.21	28,28,28,28	0
56	MG	BA	3403	1/1	0.97	0.07	28,28,28,28	0
56	MG	DA	3292	1/1	0.97	0.06	34,34,34,34	0
56	MG	AV	101	1/1	0.97	0.15	51,51,51,51	0
56	MG	BA	3500	1/1	0.97	0.07	43,43,43,43	0
56	MG	BA	3603	1/1	0.97	0.11	40,40,40,40	0
56	MG	DA	3297	1/1	0.97	0.09	36,36,36,36	0
56	MG	BA	3146	1/1	0.97	0.23	56,56,56,56	0
56	MG	CA	3077	1/1	0.97	0.24	51,51,51,51	0
56	MG	DA	3300	1/1	0.97	0.07	47,47,47,47	0
56	MG	DA	3301	1/1	0.97	0.12	30,30,30,30	0
56	MG	DA	3150	1/1	0.97	0.05	57,57,57,57	0
56	MG	BA	3337	1/1	0.97	0.12	48,48,48,48	0
56	MG	BA	3065	1/1	0.97	0.15	31,31,31,31	0
56	MG	DA	3309	1/1	0.97	0.08	25,25,25,25	0
56	MG	DA	3308	1/1	0.98	0.05	32,32,32,32	0
56	MG	AA	3172	1/1	0.98	0.04	36,36,36,36	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	43,43,43,43	0
56	MG	BA	3584	1/1	0.98	0.07	43,43,43,43	0
56	MG	BA	3585	1/1	0.98	0.10	25,25,25,25	0
56	MG	DA	3208	1/1	0.98	0.16	46,46,46,46	0
56	MG	DA	3025	1/1	0.98	0.21	38,38,38,38	0
56	MG	DA	3026	1/1	0.98	0.08	36,36,36,36	0
56	MG	DA	3584	1/1	0.98	0.07	47,47,47,47	0
56	MG	BA	3409	1/1	0.98	0.07	40,40,40,40	0
56	MG	DA	3028	1/1	0.98	0.06	34,34,34,34	0
56	MG	DA	3450	1/1	0.98	0.06	47,47,47,47	0
56	MG	BA	3519	1/1	0.98	0.04	57,57,57,57	0
56	MG	DA	3319	1/1	0.98	0.05	31,31,31,31	0
56	MG	BA	3589	1/1	0.98	0.12	34,34,34,34	0
56	MG	DA	3322	1/1	0.98	0.09	41,41,41,41	0
56	MG	BA	3032	1/1	0.98	0.15	36,36,36,36	0
56	MG	DA	3324	1/1	0.98	0.09	24,24,24,24	0
56	MG	BA	3724	1/1	0.98	0.11	22,22,22,22	0
56	MG	BA	3413	1/1	0.98	0.05	19,19,19,19	0
56	MG	BQ	3003	1/1	0.98	0.07	15,15,15,15	0
56	MG	BA	3592	1/1	0.98	0.08	43,43,43,43	0
56	MG	BA	3727	1/1	0.98	0.10	27,27,27,27	0
56	MG	BR	202	1/1	0.98	0.09	25,25,25,25	0
56	MG	BA	3416	1/1	0.98	0.08	25,25,25,25	0
56	MG	DA	3332	1/1	0.98	0.06	29,29,29,29	0
56	MG	BA	3418	1/1	0.98	0.14	20,20,20,20	0
56	MG	BA	3077	1/1	0.98	0.03	20,20,20,20	0
56	MG	BU	203	1/1	0.98	0.10	26,26,26,26	0
56	MG	DA	3605	1/1	0.98	0.04	58,58,58,58	0
56	MG	BU	204	1/1	0.98	0.10	49,49,49,49	0
56	MG	BU	205	1/1	0.98	0.09	39,39,39,39	0
56	MG	BU	206	1/1	0.98	0.15	41,41,41,41	0
56	MG	DA	3341	1/1	0.98	0.03	40,40,40,40	0
56	MG	DA	3136	1/1	0.98	0.05	39,39,39,39	0
56	MG	DA	3343	1/1	0.98	0.07	37,37,37,37	0
56	MG	DA	3474	1/1	0.98	0.05	49,49,49,49	0
56	MG	BA	3422	1/1	0.98	0.08	23,23,23,23	0
56	MG	DA	3476	1/1	0.98	0.05	35,35,35,35	0
56	MG	BA	3236	1/1	0.98	0.11	37,37,37,37	0
56	MG	BA	3528	1/1	0.98	0.09	44,44,44,44	0
56	MG	AA	3137	1/1	0.98	0.14	40,40,40,40	0
56	MG	DA	3348	1/1	0.98	0.05	39,39,39,39	0
56	MG	BA	3475	1/1	0.98	0.05	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	3736	1/1	0.98	0.09	40,40,40,40	0
56	MG	DA	3352	1/1	0.98	0.06	24,24,24,24	0
56	MG	BA	3378	1/1	0.98	0.09	24,24,24,24	0
56	MG	BA	3379	1/1	0.98	0.07	43,43,43,43	0
56	MG	BA	3345	1/1	0.98	0.03	37,37,37,37	0
56	MG	BA	3534	1/1	0.98	0.11	36,36,36,36	0
56	MG	BA	3188	1/1	0.98	0.05	49,49,49,49	0
56	MG	DA	3489	1/1	0.98	0.04	36,36,36,36	0
56	MG	DA	3490	1/1	0.98	0.04	46,46,46,46	0
56	MG	BA	3536	1/1	0.98	0.07	37,37,37,37	0
56	MG	BA	3320	1/1	0.98	0.07	41,41,41,41	0
56	MG	DA	3362	1/1	0.98	0.19	42,42,42,42	0
56	MG	BA	3275	1/1	0.98	0.20	28,28,28,28	0
56	MG	BA	3483	1/1	0.98	0.09	18,18,18,18	0
56	MG	BA	3541	1/1	0.98	0.07	37,37,37,37	0
56	MG	BA	3431	1/1	0.98	0.18	54,54,54,54	0
56	MG	BA	3432	1/1	0.98	0.05	27,27,27,27	0
56	MG	DA	3368	1/1	0.98	0.06	34,34,34,34	0
56	MG	BA	3323	1/1	0.98	0.06	25,25,25,25	0
56	MG	BB	3010	1/1	0.98	0.10	44,44,44,44	0
56	MG	BA	3679	1/1	0.98	0.05	39,39,39,39	0
56	MG	DA	3643	1/1	0.98	0.13	18,18,18,18	0
56	MG	BB	3012	1/1	0.98	0.08	42,42,42,42	0
56	MG	DA	3253	1/1	0.98	0.04	35,35,35,35	0
56	MG	DA	3375	1/1	0.98	0.07	40,40,40,40	0
56	MG	BA	3351	1/1	0.98	0.10	21,21,21,21	0
56	MG	BA	3079	1/1	0.98	0.10	50,50,50,50	0
56	MG	DA	3510	1/1	0.98	0.05	67,67,67,67	0
56	MG	BA	3353	1/1	0.98	0.11	31,31,31,31	0
56	MG	DA	3512	1/1	0.98	0.08	37,37,37,37	0
56	MG	B5	502	1/1	0.98	0.05	56,56,56,56	0
56	MG	BA	3491	1/1	0.98	0.08	38,38,38,38	0
56	MG	DA	3260	1/1	0.98	0.03	32,32,32,32	0
56	MG	DA	3382	1/1	0.98	0.07	44,44,44,44	0
56	MG	BA	3206	1/1	0.98	0.09	32,32,32,32	0
56	MG	DA	3384	1/1	0.98	0.05	24,24,24,24	0
56	MG	BD	301	1/1	0.98	0.14	35,35,35,35	0
56	MG	DA	3386	1/1	0.98	0.06	18,18,18,18	0
56	MG	BA	3091	1/1	0.98	0.15	55,55,55,55	0
56	MG	DA	3388	1/1	0.98	0.07	25,25,25,25	0
56	MG	BA	3440	1/1	0.98	0.05	40,40,40,40	0
56	MG	BA	3495	1/1	0.98	0.14	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3266	1/1	0.98	0.08	32,32,32,32	0
56	MG	DA	3526	1/1	0.98	0.05	49,49,49,49	0
56	MG	BA	3442	1/1	0.98	0.12	33,33,33,33	0
56	MG	CA	3082	1/1	0.98	0.05	46,46,46,46	0
56	MG	BA	3555	1/1	0.98	0.17	31,31,31,31	0
56	MG	BD	307	1/1	0.98	0.05	36,36,36,36	0
56	MG	DA	3082	1/1	0.98	0.04	7,7,7,7	0
56	MG	BA	3176	1/1	0.98	0.10	50,50,50,50	0
56	MG	BA	3062	1/1	0.98	0.28	46,46,46,46	0
56	MG	BA	3626	1/1	0.98	0.05	50,50,50,50	0
56	MG	DA	3275	1/1	0.98	0.12	34,34,34,34	0
56	MG	BA	3445	1/1	0.98	0.10	16,16,16,16	0
56	MG	BA	3063	1/1	0.98	0.08	34,34,34,34	0
56	MG	BA	3393	1/1	0.98	0.07	27,27,27,27	0
56	MG	BA	3127	1/1	0.98	0.12	42,42,42,42	0
56	MG	BA	3228	1/1	0.98	0.05	23,23,23,23	0
56	MG	DE	306	1/1	0.98	0.07	44,44,44,44	0
56	MG	CA	3094	1/1	0.98	0.19	37,37,37,37	0
56	MG	BA	3049	1/1	0.98	0.15	17,17,17,17	0
56	MG	DA	3411	1/1	0.98	0.10	33,33,33,33	0
56	MG	DA	3412	1/1	0.98	0.12	34,34,34,34	0
56	MG	BA	3564	1/1	0.98	0.09	26,26,26,26	0
56	MG	BA	3397	1/1	0.98	0.04	44,44,44,44	0
56	MG	DA	3415	1/1	0.98	0.04	22,22,22,22	0
56	MG	DO	5001	1/1	0.98	0.05	33,33,33,33	0
56	MG	CA	3098	1/1	0.98	0.12	37,37,37,37	0
56	MG	BA	3398	1/1	0.98	0.07	36,36,36,36	0
56	MG	BA	3399	1/1	0.98	0.09	22,22,22,22	0
56	MG	CA	3101	1/1	0.98	0.07	58,58,58,58	0
56	MG	DA	3420	1/1	0.98	0.04	43,43,43,43	0
56	MG	CA	3102	1/1	0.98	0.04	55,55,55,55	0
56	MG	DA	3191	1/1	0.98	0.07	31,31,31,31	0
56	MG	DA	3291	1/1	0.98	0.11	42,42,42,42	0
56	MG	BA	3363	1/1	0.98	0.06	29,29,29,29	0
56	MG	BA	3153	1/1	0.98	0.08	47,47,47,47	0
56	MG	BA	3639	1/1	0.98	0.05	35,35,35,35	0
56	MG	DA	3560	1/1	0.98	0.05	57,57,57,57	0
56	MG	DA	3427	1/1	0.98	0.04	29,29,29,29	0
56	MG	BA	3365	1/1	0.98	0.05	63,63,63,63	0
56	MG	AA	3156	1/1	0.98	0.07	31,31,31,31	0
56	MG	DA	3564	1/1	0.98	0.03	29,29,29,29	0
56	MG	BG	3001	1/1	0.98	0.07	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3574	1/1	0.98	0.05	52,52,52,52	0
56	MG	BA	3287	1/1	0.98	0.07	11,11,11,11	0
57	SF4	CD	501	8/8	0.98	0.03	63,76,87,96	0
56	MG	AA	3040	1/1	0.98	0.05	46,46,46,46	0
58	ZN	CN	501	1/1	0.98	0.04	104,104,104,104	0
58	ZN	DY	501	1/1	0.98	0.04	90,90,90,90	0
56	MG	BA	3579	1/1	0.98	0.12	21,21,21,21	0
56	MG	DA	3303	1/1	0.98	0.06	37,37,37,37	0
56	MG	BA	3370	1/1	0.98	0.03	39,39,39,39	0
56	MG	BA	3515	1/1	0.98	0.12	46,46,46,46	0
56	MG	DA	3307	1/1	0.98	0.08	40,40,40,40	0
56	MG	BA	3572	1/1	0.99	0.09	23,23,23,23	0
56	MG	DA	3650	1/1	0.99	0.04	35,35,35,35	0
56	MG	BA	3192	1/1	0.99	0.04	48,48,48,48	0
56	MG	BA	3333	1/1	0.99	0.10	27,27,27,27	0
56	MG	BA	3575	1/1	0.99	0.07	26,26,26,26	0
56	MG	DA	3337	1/1	0.99	0.08	50,50,50,50	0
56	MG	DA	3396	1/1	0.99	0.06	37,37,37,37	0
56	MG	BA	3537	1/1	0.99	0.07	45,45,45,45	0
56	MG	CA	3083	1/1	0.99	0.05	30,30,30,30	0
56	MG	DA	3340	1/1	0.99	0.04	29,29,29,29	0
56	MG	DA	3045	1/1	0.99	0.12	49,49,49,49	0
56	MG	DA	3401	1/1	0.99	0.11	41,41,41,41	0
56	MG	BA	3437	1/1	0.99	0.06	37,37,37,37	0
56	MG	BA	3578	1/1	0.99	0.09	47,47,47,47	0
56	MG	BA	3410	1/1	0.99	0.05	21,21,21,21	0
56	MG	BA	3411	1/1	0.99	0.09	21,21,21,21	0
56	MG	BA	3080	1/1	0.99	0.03	12,12,12,12	0
56	MG	DA	3293	1/1	0.99	0.04	34,34,34,34	0
56	MG	BA	3441	1/1	0.99	0.09	29,29,29,29	0
56	MG	DA	3349	1/1	0.99	0.04	27,27,27,27	0
56	MG	AA	3157	1/1	0.99	0.03	26,26,26,26	0
56	MG	BA	3414	1/1	0.99	0.12	51,51,51,51	0
56	MG	BB	3013	1/1	0.99	0.07	31,31,31,31	0
56	MG	BA	3415	1/1	0.99	0.06	28,28,28,28	0
56	MG	BA	3586	1/1	0.99	0.08	26,26,26,26	0
56	MG	BA	3319	1/1	0.99	0.09	34,34,34,34	0
56	MG	BA	3547	1/1	0.99	0.10	30,30,30,30	0
56	MG	BA	3417	1/1	0.99	0.07	21,21,21,21	0
56	MG	BA	3306	1/1	0.99	0.05	19,19,19,19	0
56	MG	DA	3359	1/1	0.99	0.07	21,21,21,21	0
56	MG	DA	3360	1/1	0.99	0.02	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3304	1/1	0.99	0.04	44,44,44,44	0
56	MG	BA	3448	1/1	0.99	0.10	23,23,23,23	0
56	MG	BA	3374	1/1	0.99	0.11	26,26,26,26	0
56	MG	BA	3420	1/1	0.99	0.10	13,13,13,13	0
56	MG	DA	3257	1/1	0.99	0.08	25,25,25,25	0
56	MG	DA	3616	1/1	0.99	0.04	41,41,41,41	0
56	MG	BA	3421	1/1	0.99	0.07	28,28,28,28	0
56	MG	BA	3057	1/1	0.99	0.16	36,36,36,36	0
56	MG	DA	3552	1/1	0.99	0.05	42,42,42,42	0
56	MG	BA	3322	1/1	0.99	0.05	46,46,46,46	0
56	MG	BA	3454	1/1	0.99	0.07	20,20,20,20	0
56	MG	DA	3430	1/1	0.99	0.11	75,75,75,75	0
56	MG	BA	3488	1/1	0.99	0.14	43,43,43,43	0
56	MG	BA	3015	1/1	0.99	0.12	30,30,30,30	0
56	MG	DA	3372	1/1	0.99	0.03	37,37,37,37	0
56	MG	BA	3523	1/1	0.99	0.09	32,32,32,32	0
56	MG	AA	3145	1/1	0.99	0.10	63,63,63,63	0
56	MG	BE	301	1/1	0.99	0.14	28,28,28,28	0
56	MG	BA	3684	1/1	0.99	0.12	44,44,44,44	0
56	MG	BE	303	1/1	0.99	0.04	39,39,39,39	0
56	MG	AA	3220	1/1	0.99	0.06	42,42,42,42	0
56	MG	AA	3152	1/1	0.99	0.07	29,29,29,29	0
56	MG	DA	3633	1/1	0.99	0.09	25,25,25,25	0
56	MG	BA	3159	1/1	0.99	0.10	47,47,47,47	0
56	MG	BA	3362	1/1	0.99	0.05	23,23,23,23	0
56	MG	AA	3163	1/1	0.99	0.10	23,23,23,23	0
56	MG	DA	3505	1/1	0.99	0.06	24,24,24,24	0
56	MG	BA	3314	1/1	0.99	0.06	22,22,22,22	0
56	MG	BA	3691	1/1	0.99	0.10	40,40,40,40	0
57	SF4	AD	501	8/8	0.99	0.04	62,75,82,88	0
56	MG	DA	3572	1/1	0.99	0.05	39,39,39,39	0
58	ZN	AN	102	1/1	0.99	0.02	88,88,88,88	0
58	ZN	BY	501	1/1	0.99	0.03	67,67,67,67	0
56	MG	DA	3573	1/1	0.99	0.10	32,32,32,32	0
58	ZN	B5	501	1/1	0.99	0.02	49,49,49,49	0
56	MG	DA	3508	1/1	0.99	0.05	30,30,30,30	0
56	MG	BA	3463	1/1	0.99	0.05	32,32,32,32	0
56	MG	AA	3192	1/1	0.99	0.08	73,73,73,73	0
58	ZN	D5	103	1/1	0.99	0.02	61,61,61,61	0
58	ZN	D6	501	1/1	0.99	0.03	65,65,65,65	0
58	ZN	D9	501	1/1	0.99	0.04	63,63,63,63	0
56	MG	BA	3366	1/1	0.99	0.06	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	BA	3570	1/1	0.99	0.10	33,33,33,33	0
56	MG	DA	3389	1/1	0.99	0.07	32,32,32,32	0
56	MG	BA	3348	1/1	0.99	0.06	29,29,29,29	0
58	ZN	B6	501	1/1	1.00	0.03	51,51,51,51	0
58	ZN	B9	501	1/1	1.00	0.02	49,49,49,49	0
56	MG	BA	3327	1/1	1.00	0.05	21,21,21,21	0
56	MG	BA	3480	1/1	1.00	0.03	22,22,22,22	0
56	MG	DA	3321	1/1	1.00	0.03	31,31,31,31	0
56	MG	BX	101	1/1	1.00	0.04	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.