



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2025 – 04:45 AM EDT

PDB ID : 4V9S
Title : Crystal structure of antibiotic GE82832 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 : 3.10 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

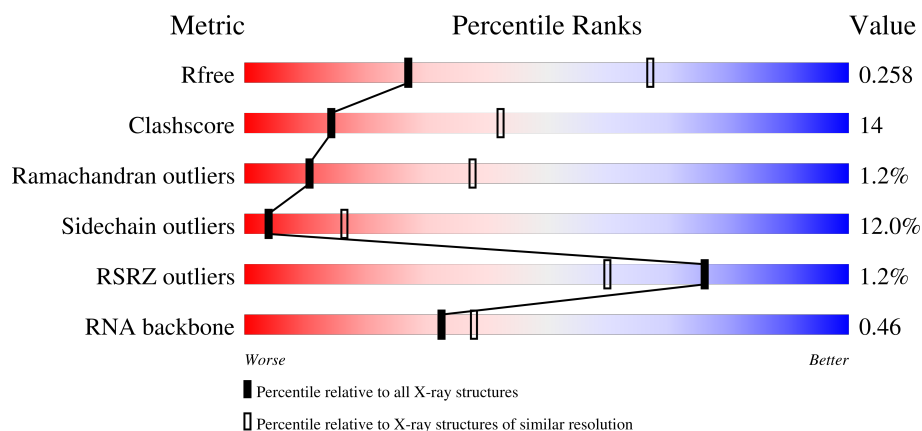
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)
RNA backbone	3690	1021 (3.36-2.84)

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	<div> <div>2%</div> <div>36% 43% 17% . .</div> </div>
1	CA	1522	<div> <div>34% 43% 18% . .</div> </div>
2	AB	256	<div> <div>2%</div> <div>38% 39% 11% . 10%</div> </div>
2	CB	256	<div> <div>2%</div> <div>36% 44% 10% 10%</div> </div>

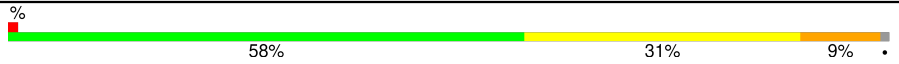

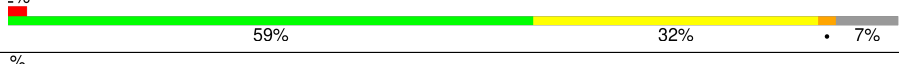



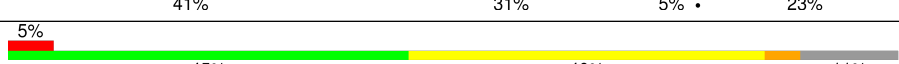
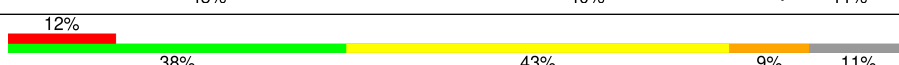
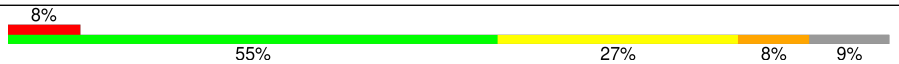





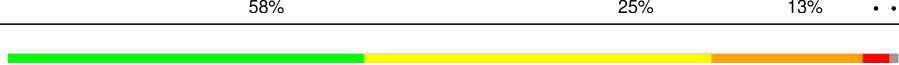



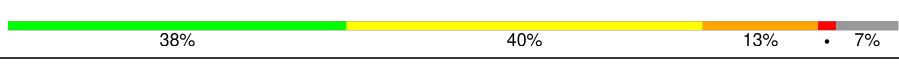
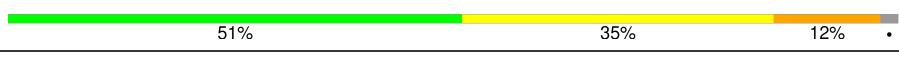





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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126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






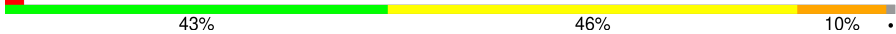



















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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	24	
22	CV	24	
23	AX	77	
23	CX	77	
24	AW	10	
24	CW	10	
25	BA	2915	
25	DA	2915	
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
24	2QY	CW	10	-	-	X	-
24	MVA	CW	9	-	-	X	-
56	MG	AA	3030	-	-	-	X
56	MG	AA	3084	-	-	-	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 GE82832.

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	S	0	0	0
			877	553	175	149				
38	DS	110	Total	C	N	O	S	0	0	0
			870	549	173	148				

- Molecule 39 is a protein called 50S Ribosomal Protein L19.

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

- Molecule 40 is a protein called 50S Ribosomal Protein L20.

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

- Molecule 41 is a protein called 50S Ribosomal Protein L21.

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

- Molecule 42 is a protein called 50S Ribosomal Protein L22.

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

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

- Molecule 43 is a protein called 50S Ribosomal Protein L23.

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

- Molecule 44 is a protein called 50S Ribosomal Protein L24.

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

- Molecule 45 is a protein called 50S Ribosomal Protein L25.

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

- Molecule 46 is a protein called 50S Ribosomal Protein L27.

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

- Molecule 47 is a protein called 50S Ribosomal Protein L28.

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

- Molecule 48 is a protein called 50S Ribosomal Protein L29.

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

- Molecule 49 is a protein called 50S Ribosomal Protein L30.

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

- Molecule 50 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B4	69	Total	C	N	O	S	0	0	0
			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 (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	221	Total	Mg	0	0
			221	221		
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	AM	1	Total	Mg	0	0
			1	1		
56	AN	2	Total	Mg	0	0
			2	2		
56	AV	1	Total	Mg	0	0
			1	1		
56	AX	9	Total	Mg	0	0
			9	9		
56	BA	738	Total	Mg	0	0
			738	738		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BB	18	Total 18	Mg 18	0	0
56	BD	12	Total 12	Mg 12	0	0
56	BE	10	Total 10	Mg 10	0	0
56	BF	8	Total 8	Mg 8	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	5	Total 5	Mg 5	0	0
56	BR	4	Total 4	Mg 4	0	0
56	BU	8	Total 8	Mg 8	0	0
56	BV	4	Total 4	Mg 4	0	0
56	BW	5	Total 5	Mg 5	0	0
56	BX	1	Total 1	Mg 1	0	0
56	BY	1	Total 1	Mg 1	0	0
56	BZ	1	Total 1	Mg 1	0	0
56	B0	4	Total 4	Mg 4	0	0
56	B1	1	Total 1	Mg 1	0	0
56	B2	1	Total 1	Mg 1	0	0
56	B3	3	Total 3	Mg 3	0	0
56	B4	1	Total 1	Mg 1	0	0

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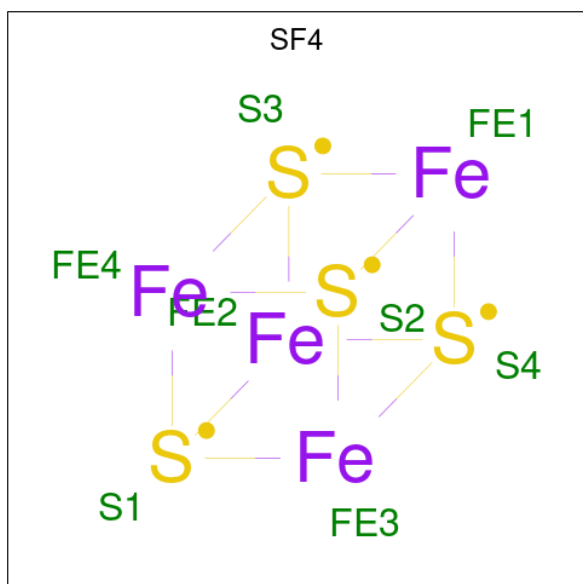
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B5	1	Total 1	Mg 1	0	0
56	B7	4	Total 4	Mg 4	0	0
56	B8	3	Total 3	Mg 3	0	0
56	B9	1	Total 1	Mg 1	0	0
56	CA	172	Total 172	Mg 172	0	0
56	CE	2	Total 2	Mg 2	0	0
56	CF	1	Total 1	Mg 1	0	0
56	CQ	1	Total 1	Mg 1	0	0
56	CT	1	Total 1	Mg 1	0	0
56	CX	3	Total 3	Mg 3	0	0
56	DA	653	Total 653	Mg 653	0	0
56	DB	12	Total 12	Mg 12	0	0
56	DD	8	Total 8	Mg 8	0	0
56	DE	6	Total 6	Mg 6	0	0
56	DF	6	Total 6	Mg 6	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	DQ	5	Total 5	Mg 5	0	0
56	DR	2	Total 2	Mg 2	0	0
56	DV	4	Total 4	Mg 4	0	0

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

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

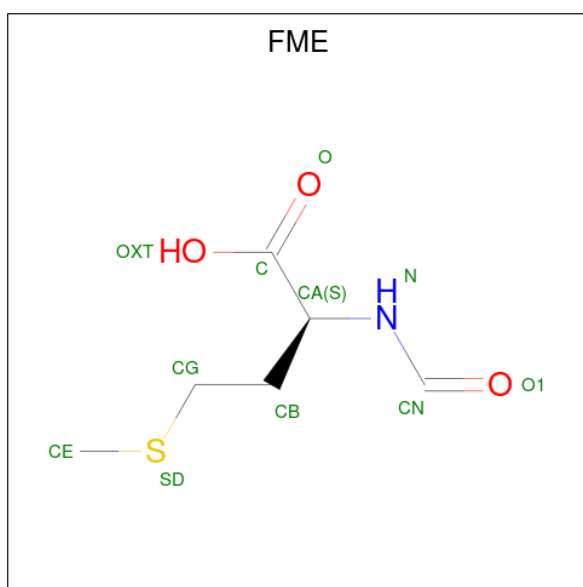
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AN	1	Total	Zn	0	0
			1	1		

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

- Molecule 59 is N-FORMYLMETHIONINE (three-letter code: 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 (three-letter code: 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	148	Total	O	0	0
			148	148		
61	AD	1	Total	O	0	0
			1	1		
61	AE	3	Total	O	0	0
			3	3		
61	AJ	1	Total	O	0	0
			1	1		
61	AL	1	Total	O	0	0
			1	1		
61	AP	1	Total	O	0	0
			1	1		
61	AU	1	Total	O	0	0
			1	1		
61	AV	1	Total	O	0	0
			1	1		
61	AX	1	Total	O	0	0
			1	1		
61	BA	1092	Total	O	0	0
			1092	1092		
61	BB	26	Total	O	0	0
			26	26		
61	BD	8	Total	O	0	0
			8	8		
61	BE	9	Total	O	0	0
			9	9		
61	BF	4	Total	O	0	0
			4	4		

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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	1	Total 1	O 1	0	0
61	BU	4	Total 4	O 4	0	0
61	BV	2	Total 2	O 2	0	0
61	BW	2	Total 2	O 2	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	3	Total 3	O 3	0	0
61	B7	1	Total 1	O 1	0	0
61	B8	8	Total 8	O 8	0	0
61	CA	187	Total 187	O 187	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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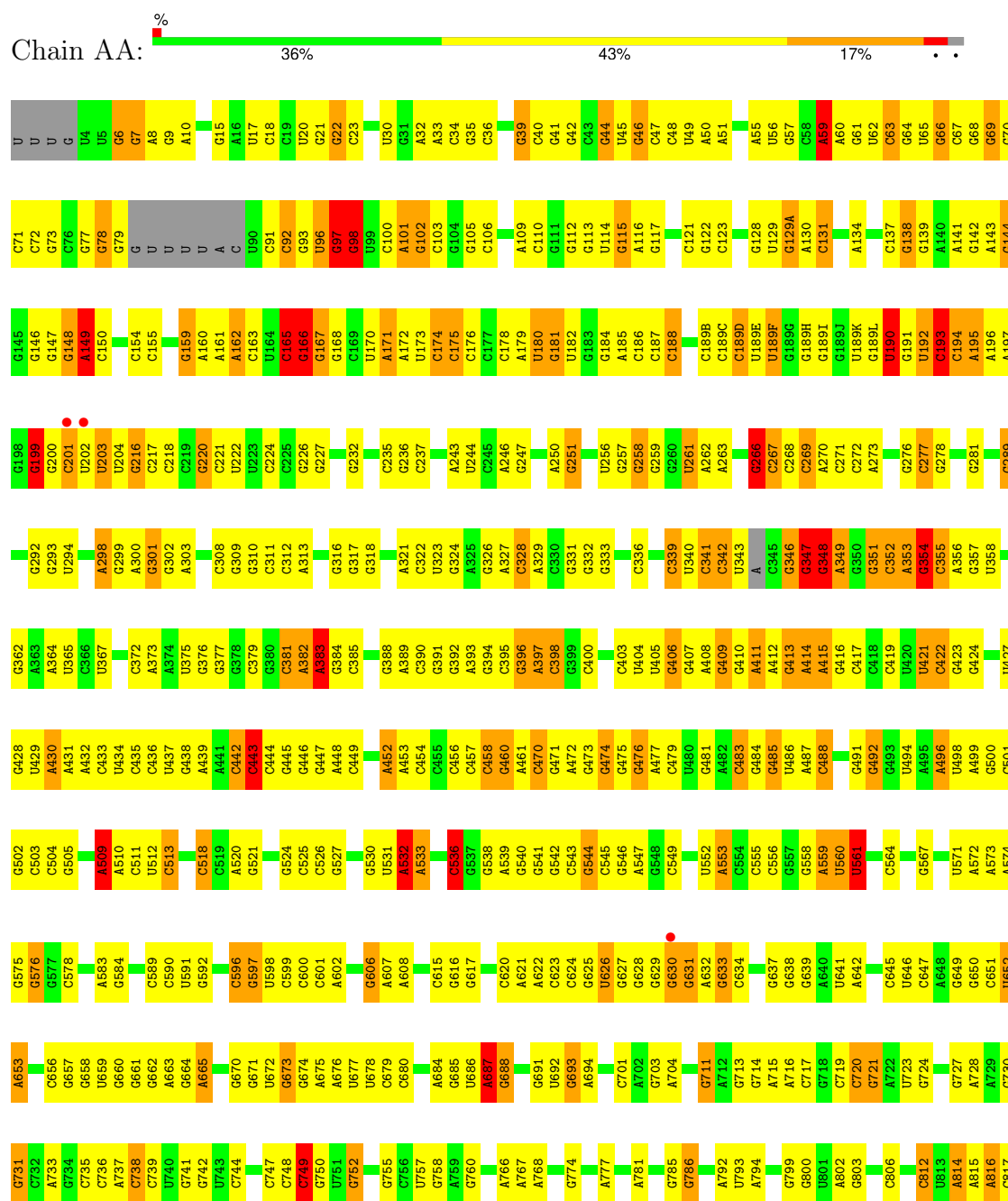
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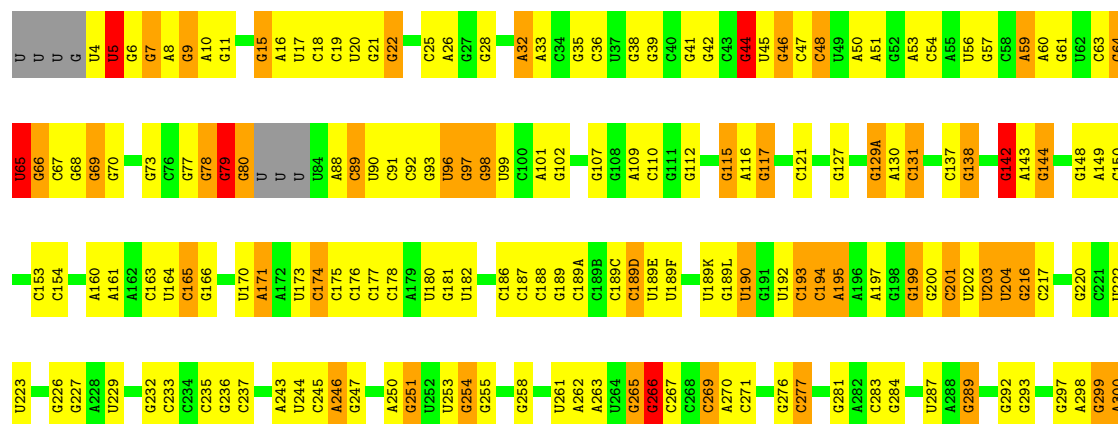
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	DA	902	Total 902	O 902	0	0
61	DB	7	Total 7	O 7	0	0
61	DD	8	Total 8	O 8	0	0
61	DE	13	Total 13	O 13	0	0
61	DF	5	Total 5	O 5	0	0
61	DO	1	Total 1	O 1	0	0
61	DP	14	Total 14	O 14	0	0
61	DQ	3	Total 3	O 3	0	0
61	DU	4	Total 4	O 4	0	0
61	DV	1	Total 1	O 1	0	0
61	DX	2	Total 2	O 2	0	0
61	DY	2	Total 2	O 2	0	0
61	D0	5	Total 5	O 5	0	0
61	D1	1	Total 1	O 1	0	0
61	D7	2	Total 2	O 2	0	0
61	D8	4	Total 4	O 4	0	0

3 Residue-property plots

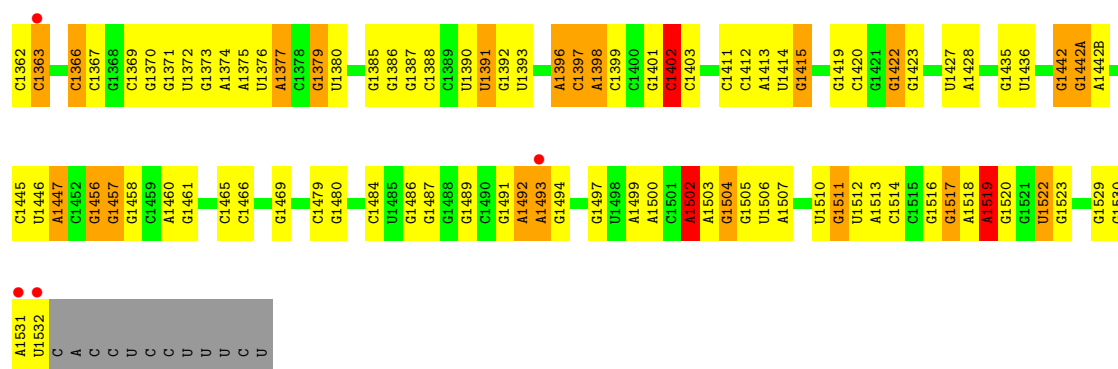
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

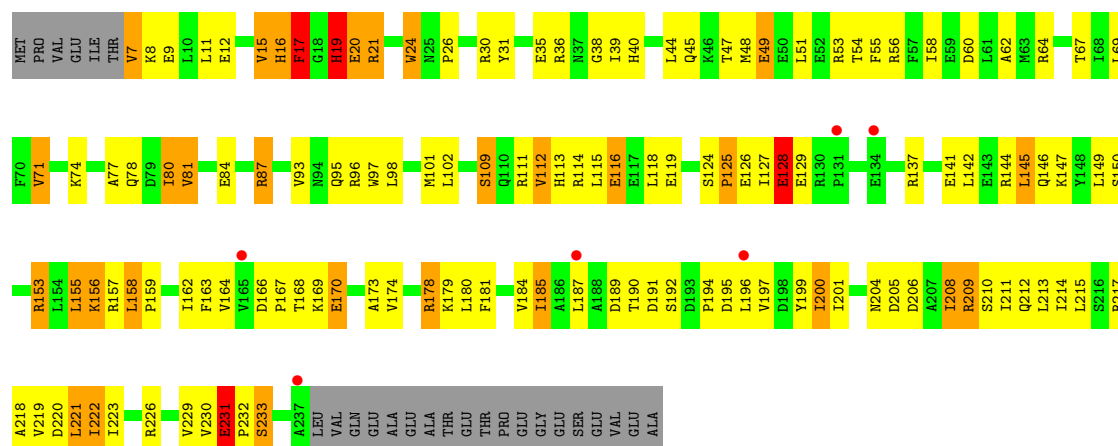
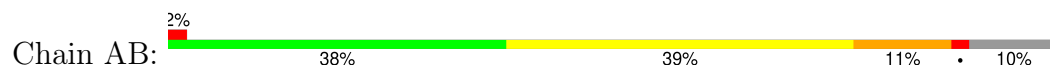




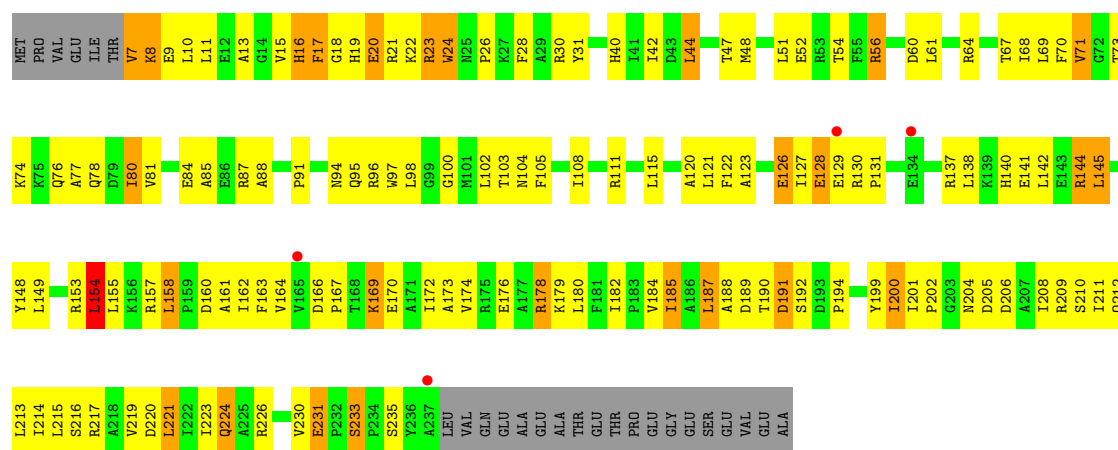
C1297	C1298	A1299	G1300	C1303	G1304	G1305	A1306	U1307	U1308	G1309	C1242	C1243	C1244	G1311	G1312	U1313	U1314	U1315	G1316	C1317	A1318	A1319	C1320	C1321	C1322	G1323	A1324	C1325	C1326	C1327	C1328	A1329	U1330	G1331	C1332	A1333	G1334	G1335	C1336	G1337	G1338	A1339	A1340	U1341	C1342	G1343	U1344	U1345	G1346	G1347	U1348	C1352	C1353	C1354	U1355	U1358	A1359	A1360	G1361																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
C1228	G1233	C1234	U1235	A1236	C1237	A1238	A1239	U1240	G1241	C1242	C1243	C1244	G1245	C1246	C1247	C1248	C1249	A1250	A1251	A1252	A1253	A1254	A1255	A1256	A1257	G1258	C1259	C1260	A1261	C1262	C1263	C1264	G1265	G1266	C1267	A1268	A1269	G1270	G1271	G1272	C1273	G1274	C1275	C1276	C1277	A1278	A1279	A1280	U1281	C1282	G1283	G1284	A1285	A1286	A1287	A1288	A1289	G1290	C1291	U1292	G1293	A1294																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
A1168	A1169	G1170	G1171	G1172	G1173	G1174	G1175	G1176	G1177	G1178	A1179	A1180	G1181	G1182	A1183	G1184	G1185	G1186	G1187	A1188	G1189	G1190	A1191	C1192	G1193	U1194	C1195	U1196	U1197	C1198	G1199	C1200	G1201	G1202	C1203	A1204	U1205	G1206	G1207	C1208	C1209	C1210	U1211	U1212	A1213	C1214	G1215	G1216	C1217	C1218	U1219	C1220	G1221	G1222	A1223	G1224	A1225	C1226	A1227																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
A1105	G1106	C1107	G1108	C1109	A1110	A1111	C1112	C1113	C1114	C1115	C1116	C1117	C1118	C1119	U1120	U1121	A1122	A1123	G1124	U1125	U1126	C1127	C1128	C1129	A1130	G1131	C1132	G1133	C1134	U1135	C1136	C1137	G1138	C1139	C1140	C1141	G1142	G1143	G1144	C1145	A1146	C1147	U1148	C1149	U1150	A1151	A1152	C1153	G1154	G1155	G1156	A1157	C1158	U1159	U1160	C1161	C1162	C1163	C1164	G1165																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
A1041	G1042	A1043	A1044	G1045	G1046	C1047	G1048	C1049	C1050	U1051	U1052	G1053	U1054	U1055	U1056	G1057	G1058	C1059	C1060	G1061	U1062	C1063	U1064	C1065	C1066	A1067	G1068	C1069	U1070	C1071	C1072	U1073	G1074	C1075	C1076	C1077	U1078	C1079	A1080	G1081	G1082	G1083	U1084	U1085	U1086	G1087	G1088	G1089	U1090	U1091	A1092	A1093	U1094	U1095	C1096	G1097	C1098	C1099	U1100	A1101	A1102	C1103	G1104																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
C985	A986	C987	C988	C989	U990	U991	U992	G993	A994	C995	A996	C997	C998	C999	U1000	A1001	C1002	G1003	A1004	C1005	C1006	C1007	C1008	G1009	G1010	G1011	U1012	G1013	A1014	G1015	U1016	C1017	C1018	U1019	U1020	G1021	G1022	G1023	U1024	U1025	G1026	C1027	C1028	G1029	C1030	U1031	C1032	G1033	A1034	C1035	G1036	C1037	C1038	C1039	U1040																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
A1041	G1042	A1043	A1044	G1045	G1046	C1047	G1048	C1049	C1050	U1051	U1052	G1053	U1054	U1055	U1056	G1057	G1058	C1059	C1060	G1061	U1062	C1063	U1064	C1065	C1066	A1067	G1068	C1069	U1070	C1071	C1072	U1073	G1074	C1075	C1076	C1077	U1078	C1079	A1080	G1081	G1082	G1083	U1084	U1085	U1086	G1087	G1088	G1089	U1090	U1091	A1092	A1093	U1094	U1095	C1096	G1097	C1098	C1099	U1100	A1101	A1102	C1103	G1104																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
A1105	G1106	C1107	G1108	C1109	A1110	A1111	C1112	C1113	C1114	C1115	C1116	C1117	C1118	C1119	U1120	U1121	A1122	A1123	G1124	U1125	U1126	C1127	C1128	C1129	A1130	G1131	C1132	G1133	C1134	U1135	C1136	C1137	G1138	C1139	C1140	C1141	G1142	G1143	G1144	C1145	A1146	C1147	U1148	C1149	U1150	A1151	A1152	C1153	G1154	G1155	G1156	A1157	C1158	U1159	U1160	C1161	C1162	C1163	C1164	G1165																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
A1168	A1169	G1170	G1171	G1172	G1173	G1174	G1175	G1176	G1177	G1178	A1179	A1180	G1181	G1182	A1183	G1184	G1185	G1186	G1187	A1188	G1189	G1190	A1191	C1192	G1193	U1194	C1195	U1196	U1197	C1198	G1199	C1200	G1201	G1202	C1203	A1204	U1205	G1206	G1207	C1208	C1209	C1210	U1211	U1212	A1213	C1214	G1215	G1216	C1217	C1218	U1219	C1220	G1221	G1222	A1223	G1224	A1225	C1226	A1227																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
C1228	G1233	C1234	U1235	A1236	C1237	A1238	A1239	U1240	G1241	C1242	C1243	C1244	G1245	C1246	C1247	C1248	C1249	A1250	A1251	A1252	A1253	A1254	A1255	A1256	A1257	G1258	C1259	C1260	A1261	C1262	C1263	C1264	G1265	G1266	C1267	A1268	A1269	G1270	G1271	G1272	C1273	G1274	C1275	C1276	C1277	A1278	A1279	A1280	U1281	C1282	G1283	G1284	A1285	A1286	A1287	A1288	A1289	G1290	C1291	U1292	G1293	A1294																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
C388	C389	C390	G316	G392	A393	C454	C455	C456	C457	C458	C460	A461	C470	C471	A472	C473	C474	C475	C485	C486	C487	C488	C489	C490	C491	C492	C493	C494	C495	C496	C497	C498	C499	C500	C501	C502	C503	C504	C505	C506	C507	C508	C509	C510	C511	C512	C513	C514	C515	C516	C517	C518	C519	C520	C521	C522	C523	C524	C525	C526	C527	C528	C529	C530	C531	C532	C533	C534	C535	C536	C537	C538	C539	C540	C541	C542	C543	C544	C545	C546	C547	C548	C549	C550	C551	C552	C553	C554	C555	C556	C557	C558	C559	C560	C561	C562	C563	C564	C565	C566	C567	C568	C569	C570	C571	C572	C573	C574	C575	C576	C577	C578	C579	C580	C581	C582	C583	C584	C585	C586	C587	C588	C589	C590	C591	C592	C593	C594	C595	C596	C597	C598	C599	C600	C601	C602	C603	C604	C605	C606	C607	C608	C609	C610	C611	C612	C613	C614	C615	C616	C617	C618	C619	C620	C621	C622	C623	C624	C625	C626	C627	C628	C629	C630	C631	C632	C633	C634	C635	C636	C637	C638	C639	C640	C641	C642	C643	C644	C645	C646	C647	C648	C649	C650	C651	C652	C653	C654	C655	C656	C657	C658	C659	C660	C661	C662	C663	C664	C665	C666	C667	C668	C669	C670	C671	C672	C673	C674	C675	C676	C677	C678	C679	C680	C681	C682	C683	C684	C685	C686	C687	C688	C689	C690	C691	C692	C693	C694	C695	C696	C697	C698	C699	C700	C701	C702	C703	C704	C705	C706	C707	C708	C709	C710	C711	C712	C713	C714	C715	C716	C717	C718	C719	C720	C721	C722	C723	C724	C725	C726	C727	C728	C729	C730	C731	C732	C733	C734	C735	C736	C737	C738	C739	C740	C741	C742	C743	C744	C745	C746	C747	C748	C749	C750	C751	C752	C753	C754	C755	C756	C757	C758	C759	C760	C761	C762	C763	C764	C765	C766	C767	C768	C769	C770	C771	C772	C773	C774	C775	C776	C777	C778	C779	C780	C781	C782	C783	C784	C785	C786	C787	C788	C789	C790	C791	C792	C793	C794	C795	C796	C797	C798	C799	C800	C801	C802	C803	C804	C805	C806	C807	C808	C809	C810	C811	C812	C813	C814	C815	C816	C817	C818	C819	C820	C821	C822	C823	C824	C825	C826	C827	C828	C829	C830	C831	C832	C833	C834	C835	C836	C837	C838	C839	C840	C841	C842	C843	C844	C845	C846	C847	C848	C849	C850	C851	C852	C853	C854	C855	C856	C857	C858	C859	C860	C861	C862	C863	C864	C865	C866	C867	C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	C1000	C1001	C1002	C1003	C1004	C1005	C1006	C1007	C1008	C1009	C1010	C1011	C1012	C1013	C1014	C1015	C1016	C1017	C1018	C1019	C1020	C1021	C1022	C1023	C1024	C1025	C1026	C1027	C1028	C1029	C1030	C1031	C1032	C1033	C1034	C1035	C1036	C1037	C1038	C1039	C1040	C1041	C1042	C1043	C1044	C1045	C1046	C1047	C1048	C1049	C1050	C1051	C1052	C1053	C1054	C1055	C1056	C1057	C1058	C1059	C1060	C1061	C1062	C1063	C1064	C1065	C1066	C1067	C1068	C1069	C1070	C1071	C1072	C1073	C1074	C1075	C1076	C1077	C1078	C1079	C1080	C1081	C1082	C1083	C1084	C1085	C1086	C1087	C1088	C1089	C1090	C1091	C1092	C1093	C1094	C1095	C1096	C1097	C1098	C1099	C1100	C1101	C1102	C1103	C1104	C1105	C1106	C1107	C1108	C1109	C1110	C1111	C1112	C1113	C1114	C1115	C1116	C1117	C1118	C1119	C1120	C1121	C1122	C1123	C1124	C1125	C1126	C1127	C1128	C1129	C1130	C1131	C1132	C1133	C1134	C1135	C1136	C1137	C1138	C1139	C1140	C1141	C1142	C1143	C1144	C1145	C1146	C1147	C1148	C1149	C1150	C1151	C1152	C1153	C1154	C1155	C1156	C1157	C1158	C1159	C1160	C1161	C1162	C1163	C1164	C1165	C1166	C1167	C1168	C1169	C1170	C1171	C1172	C1173	C1174	C1175	C1176	C1177	C1178	C1179	C1180	C1181	C1182	C1183	C1184	C1185	C1186	C1187	C1188	C1189	C1190	C1191	C1192	C1193	C1194	C1195	C1196	C1197	C1198	C1199	C1200	C1201	C1202	C1203	C1204	C1205	C1206	C1207	C1208	C1209	C1210	C1211	C1212	C1213	C1214	C1215	C1216	C1217	C1218	C1219	C1220	C1221	C1222	C1223	C1224	C1225	C1226	C1227	C1228	C1229	C1230	C1231	C1232	C1233	C1234	C1235	C1236	C1237	C1238	C1239	C1240	C1241	C1242	C1243	C1244	C1245	C1246	C1247	C1248	C1249	C1250	C1251	C1252	C1253	C1254	C1255	C1256	C1257	C1258	C1259	C1260	C1261	C1262	C1263	C1264	C1265	C1266	C1267	C1268	C1269	C1270	C1271	C1272	C1273	C1274



• Molecule 2: 30S Ribosomal Protein S2

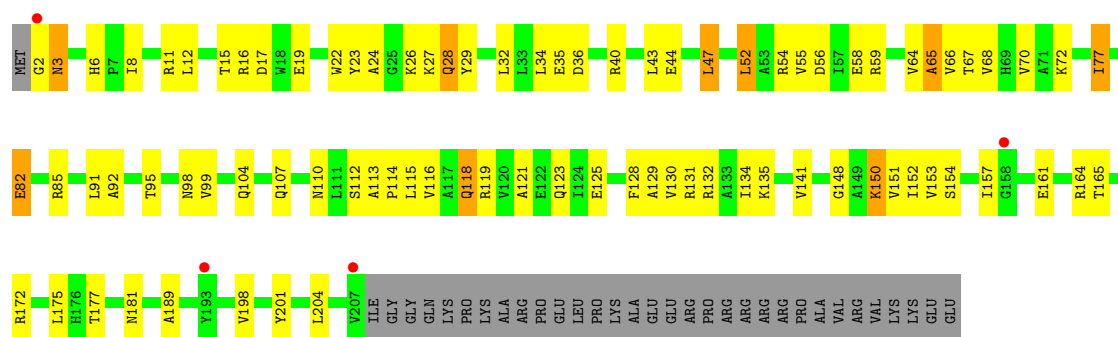


• Molecule 2: 30S Ribosomal Protein S2

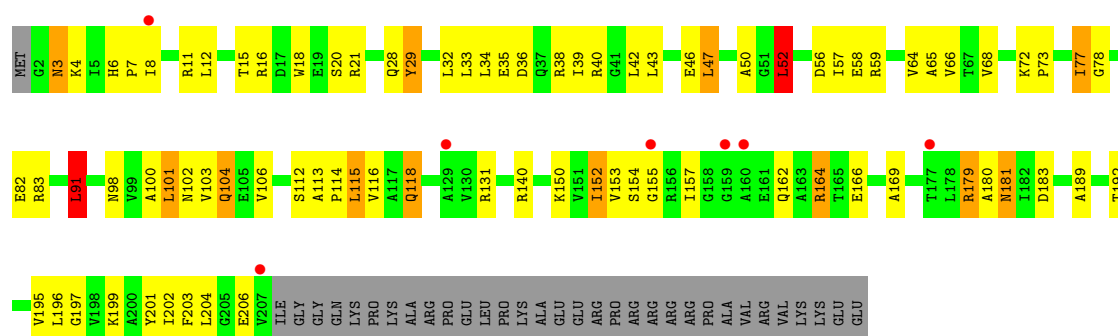


• Molecule 3: 30S Ribosomal Protein S3

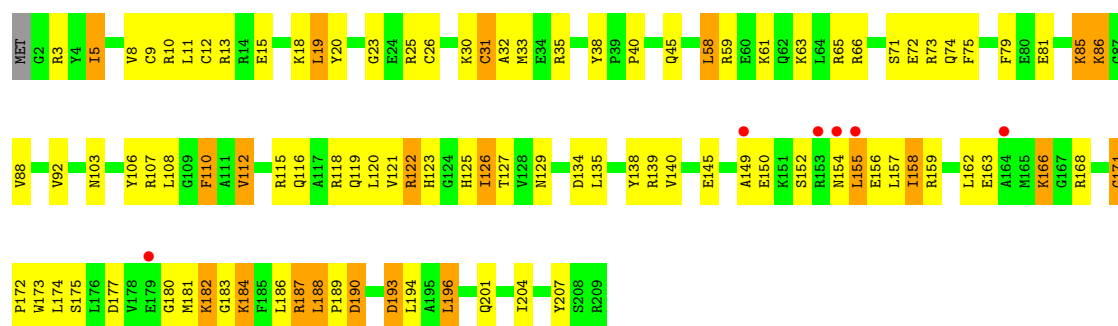




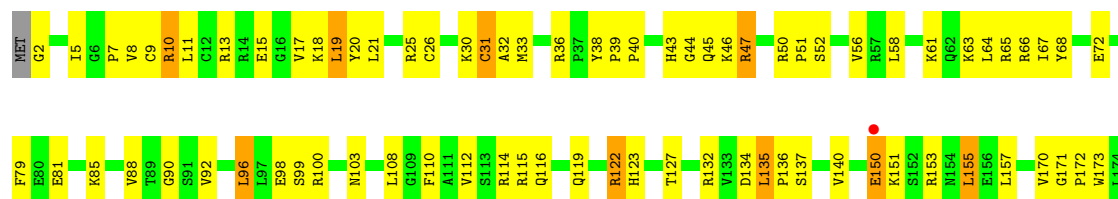
• Molecule 3: 30S Ribosomal Protein S3



• Molecule 4: 30S Ribosomal Protein S4

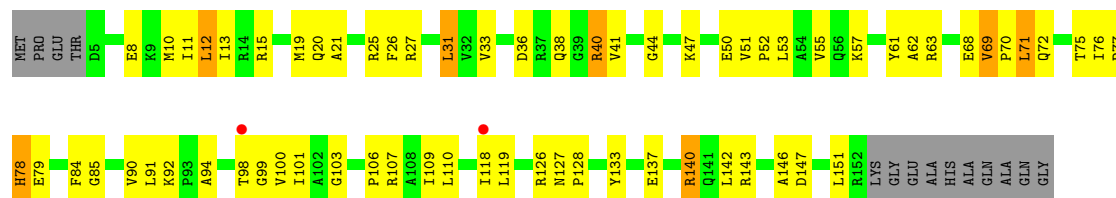


• Molecule 4: 30S Ribosomal Protein S4

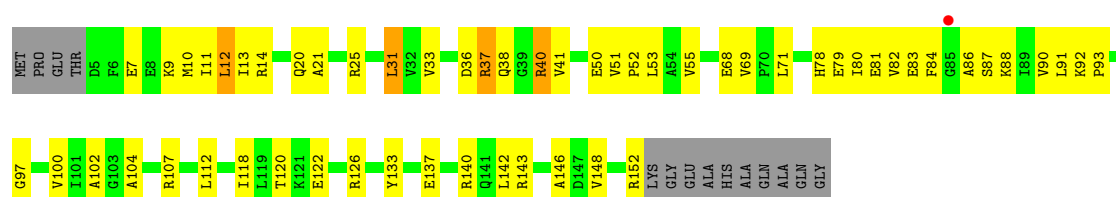




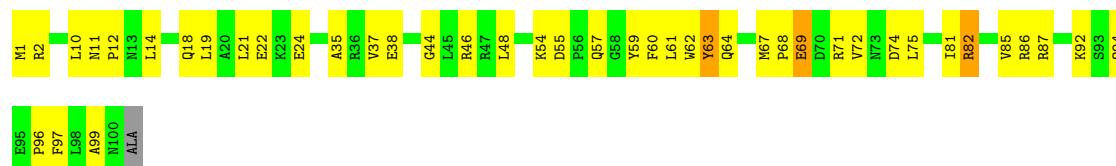
- Molecule 5: 30S Ribosomal Protein S5



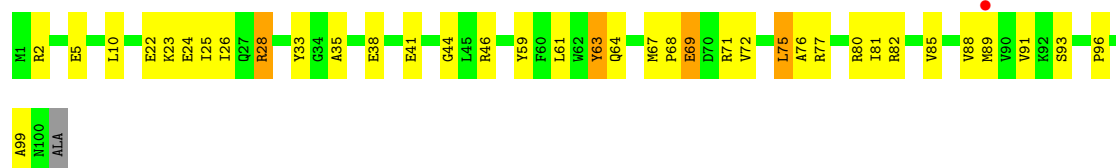
- Molecule 5: 30S Ribosomal Protein S5



- Molecule 6: 30S Ribosomal Protein S6

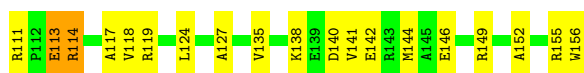


- Molecule 6: 30S Ribosomal Protein S6

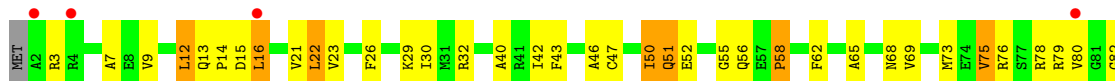


- Molecule 7: 30S Ribosomal Protein S7

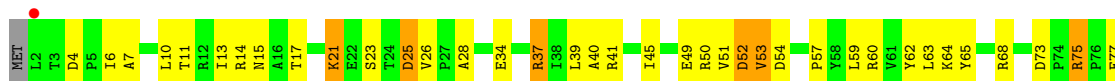




• Molecule 7: 30S Ribosomal Protein S7



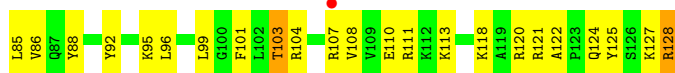
• Molecule 8: 30S Ribosomal Protein S8



• Molecule 8: 30S Ribosomal Protein S8

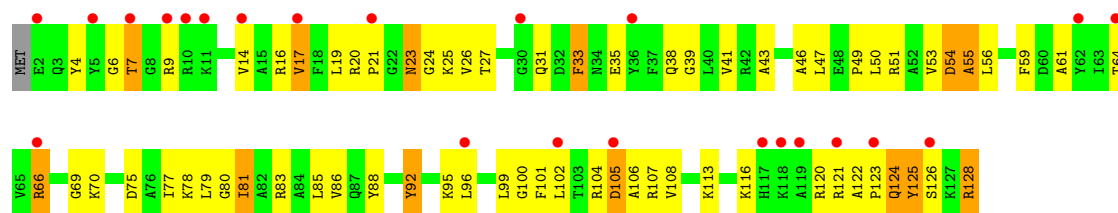


• Molecule 9: 30S Ribosomal Protein S9

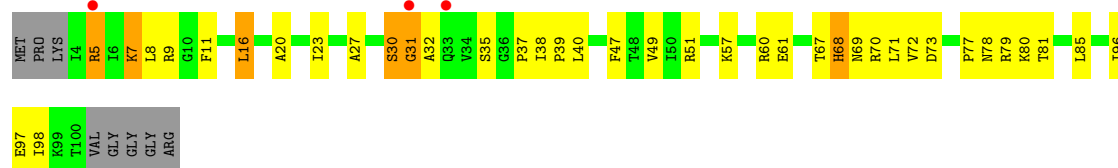


• Molecule 9: 30S Ribosomal Protein S9

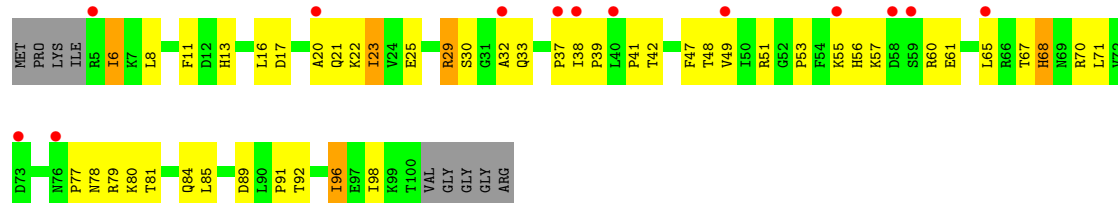




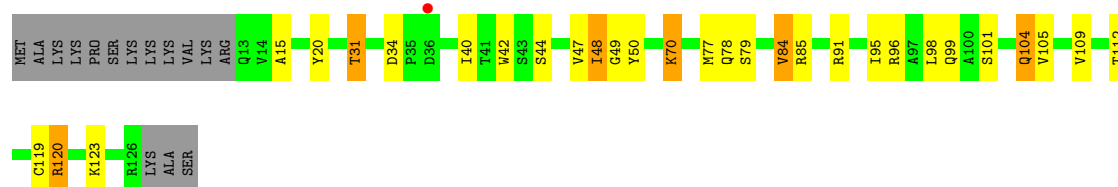
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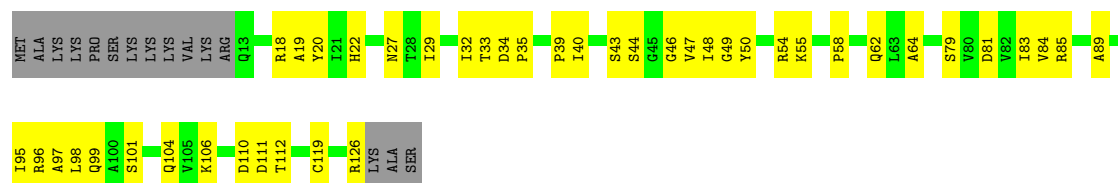
● Molecule 10: 30S Ribosomal Protein S10



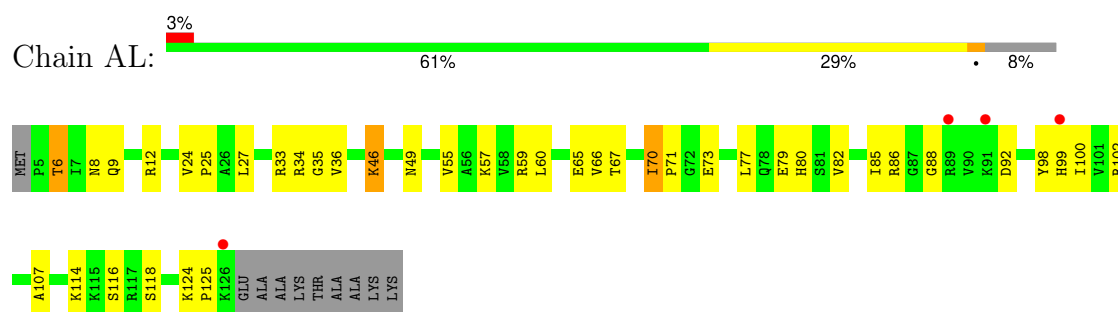
● Molecule 11: 30S Ribosomal Protein S11



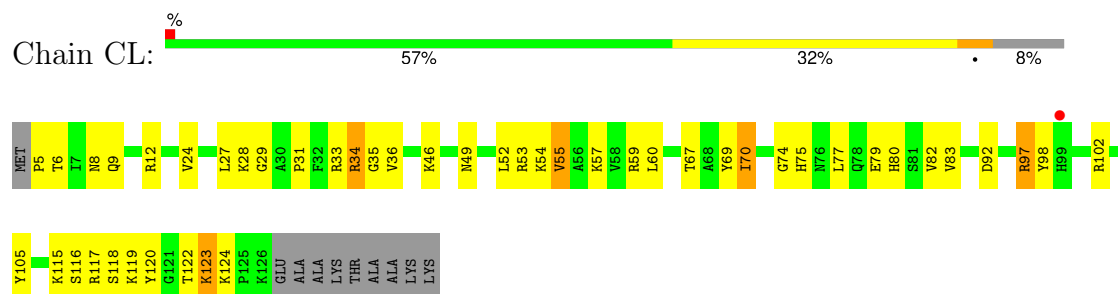
● Molecule 11: 30S Ribosomal Protein S11



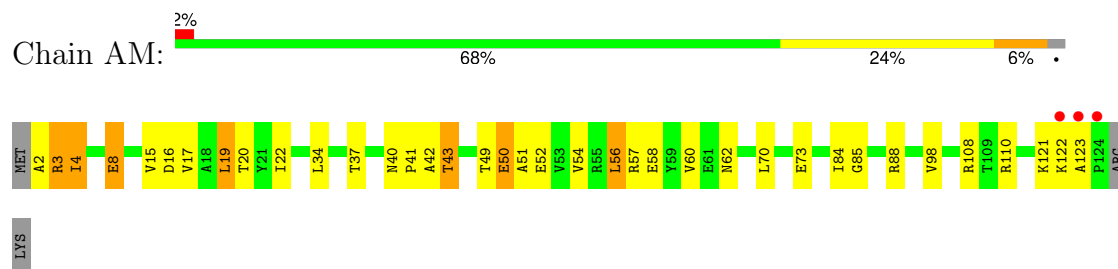
● Molecule 12: 30S Ribosomal Protein S12



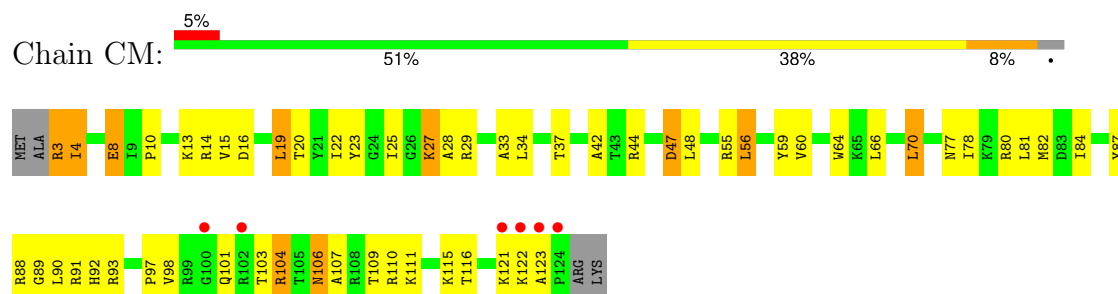
• Molecule 12: 30S Ribosomal Protein S12



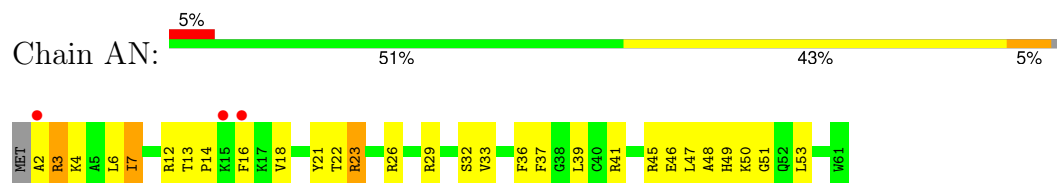
• Molecule 13: 30S Ribosomal Protein S13



• Molecule 13: 30S Ribosomal Protein S13

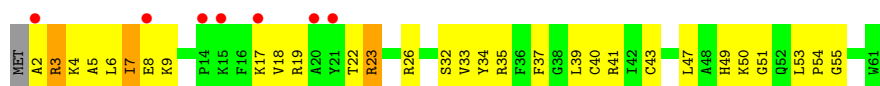


• Molecule 14: 30S Ribosomal Protein S14

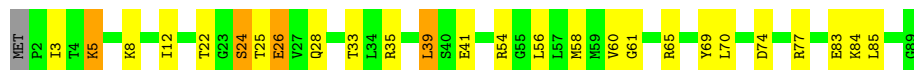


• Molecule 14: 30S Ribosomal Protein S14

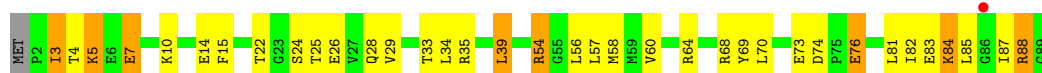




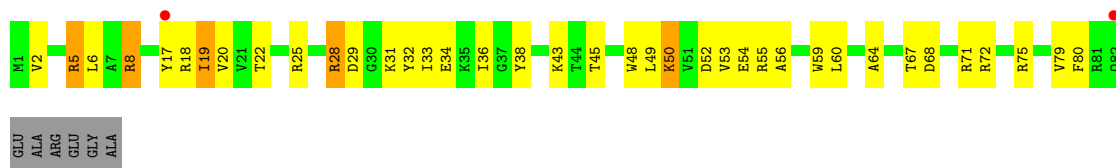
- Molecule 15: 30S Ribosomal Protein S15



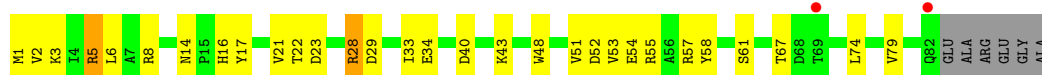
- Molecule 15: 30S Ribosomal Protein S15



- Molecule 16: 30S Ribosomal Protein S16



- Molecule 16: 30S Ribosomal Protein S16



- Molecule 17: 30S Ribosomal Protein S17

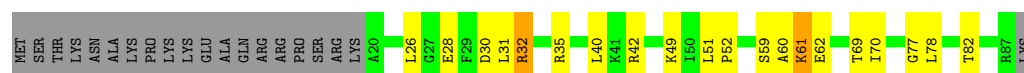


- Molecule 17: 30S Ribosomal Protein S17



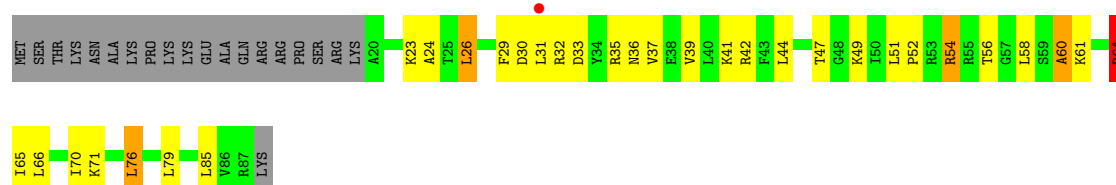
- Molecule 18: 30S Ribosomal Protein S18

Chain AR: 



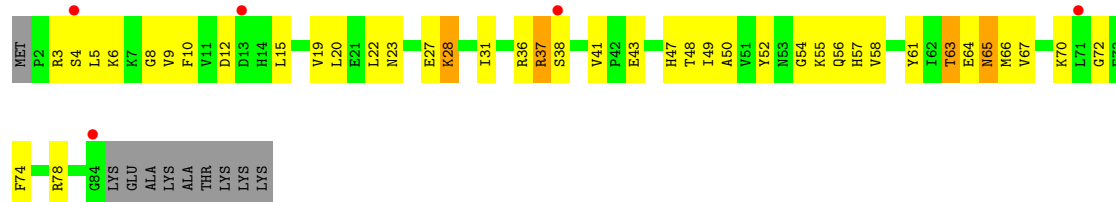
• Molecule 18: 30S Ribosomal Protein S18

Chain CR: 



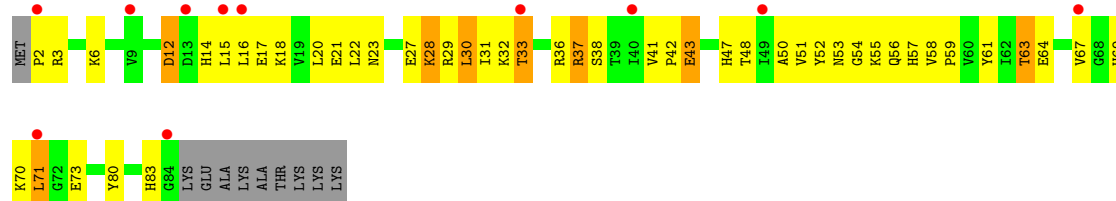
• Molecule 19: 30S Ribosomal Protein S19

Chain AS: 



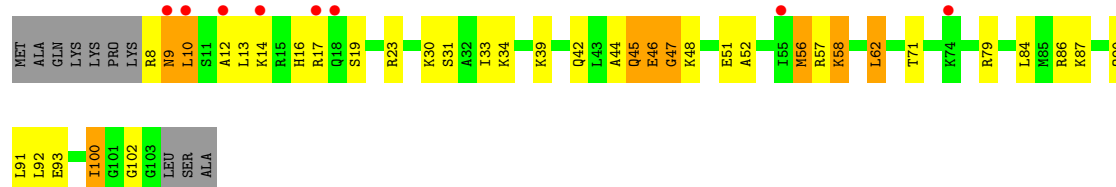
• Molecule 19: 30S Ribosomal Protein S19

Chain CS: 

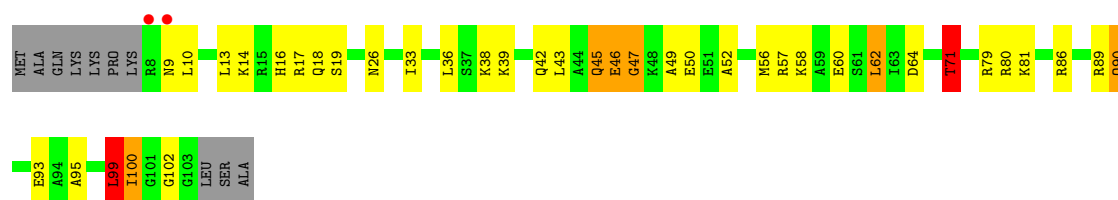


• Molecule 20: 30S Ribosomal Protein S20

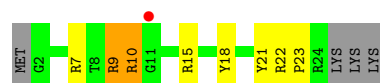
Chain AT: 



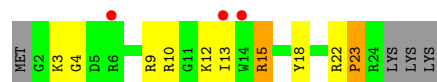
• Molecule 20: 30S Ribosomal Protein S20



• Molecule 21: 30S Ribosomal Protein THX



• Molecule 21: 30S Ribosomal Protein THX



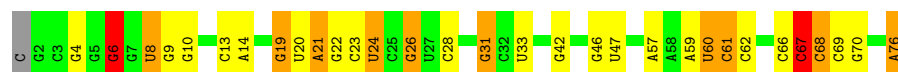
• Molecule 22: mRNA



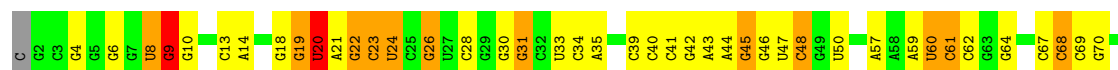
• Molecule 22: mRNA



• Molecule 23: P-site tRNA

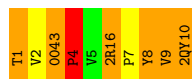


• Molecule 23: P-site tRNA

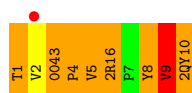




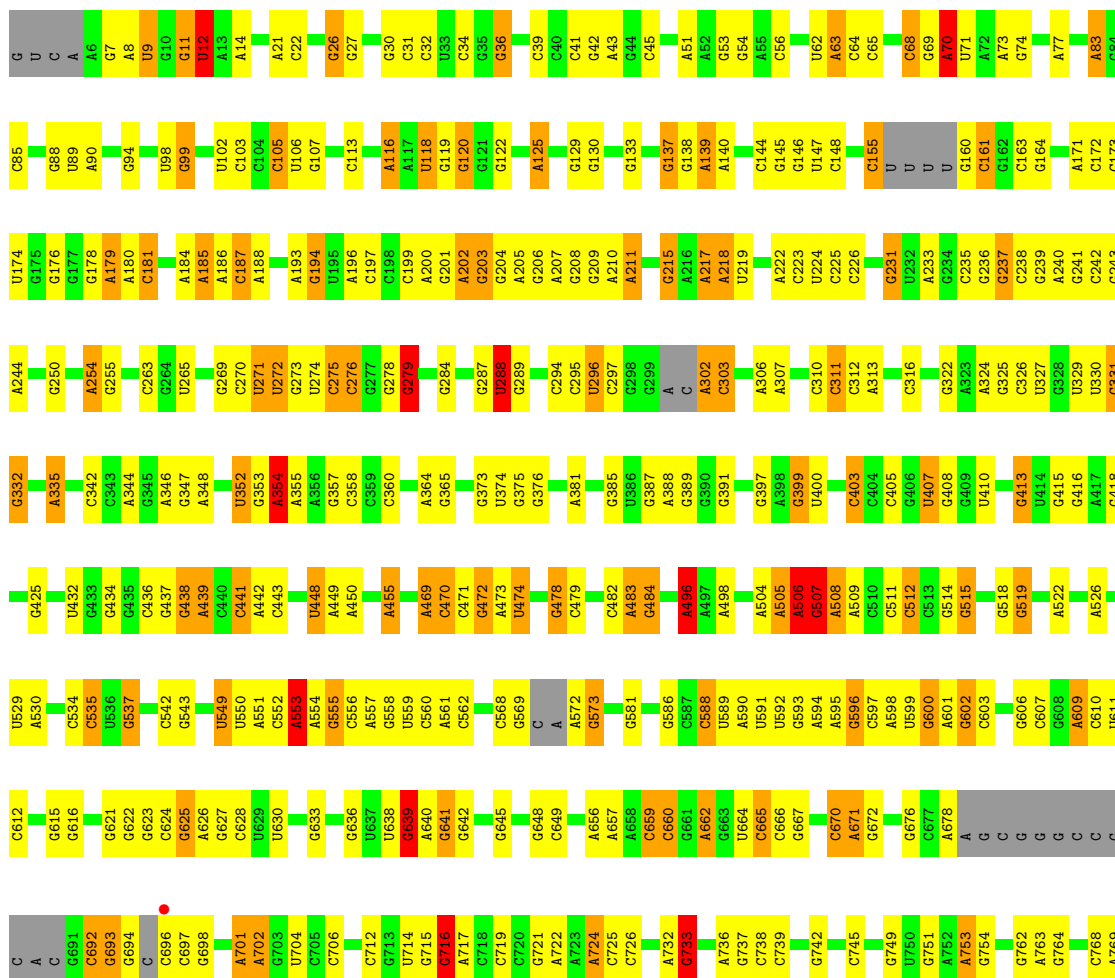
• Molecule 24: GE82832



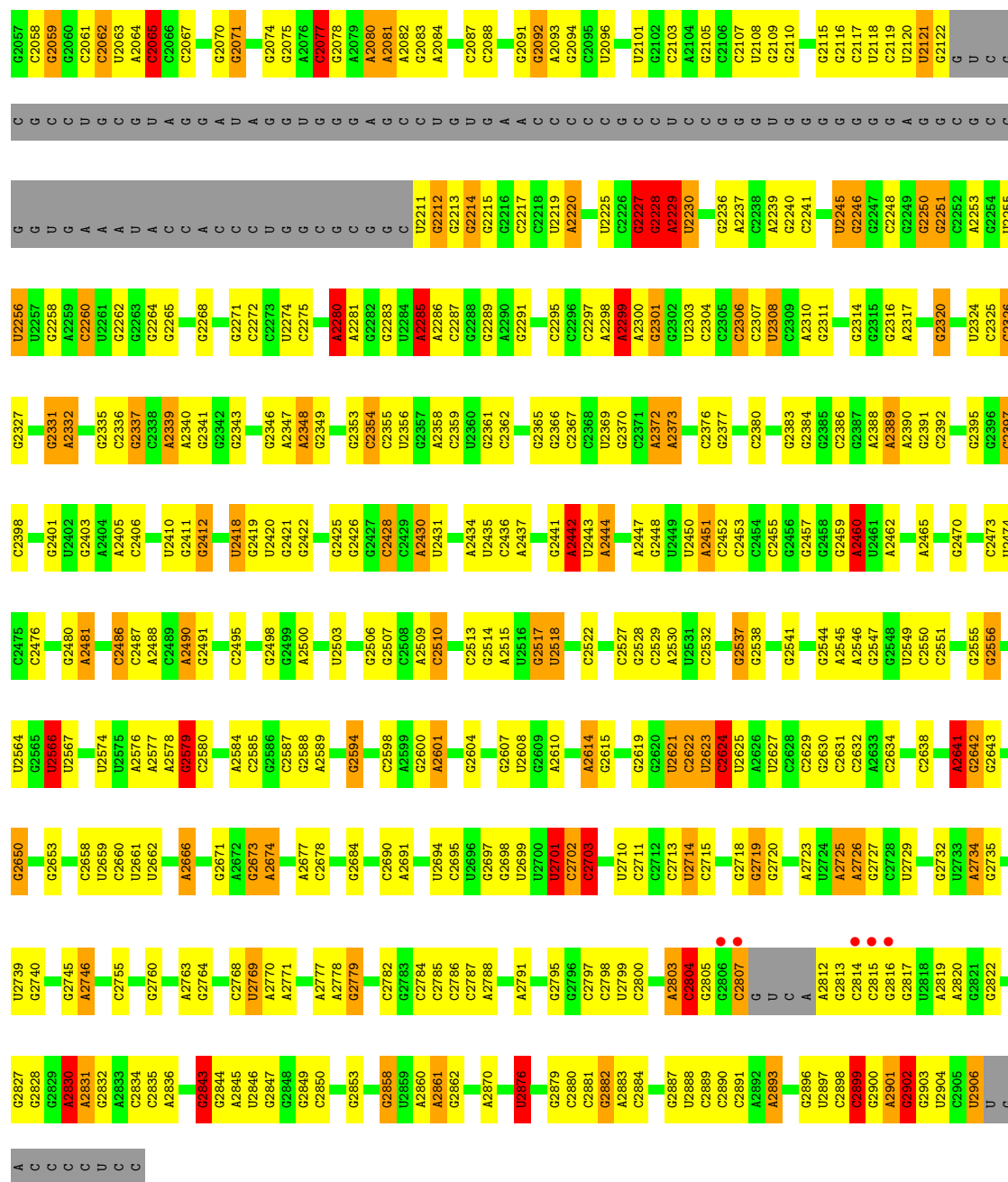
• Molecule 24: GE82832



• Molecule 25: 23S Ribosomal RNA

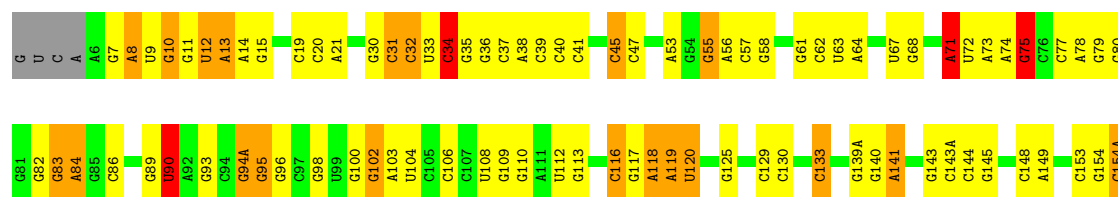


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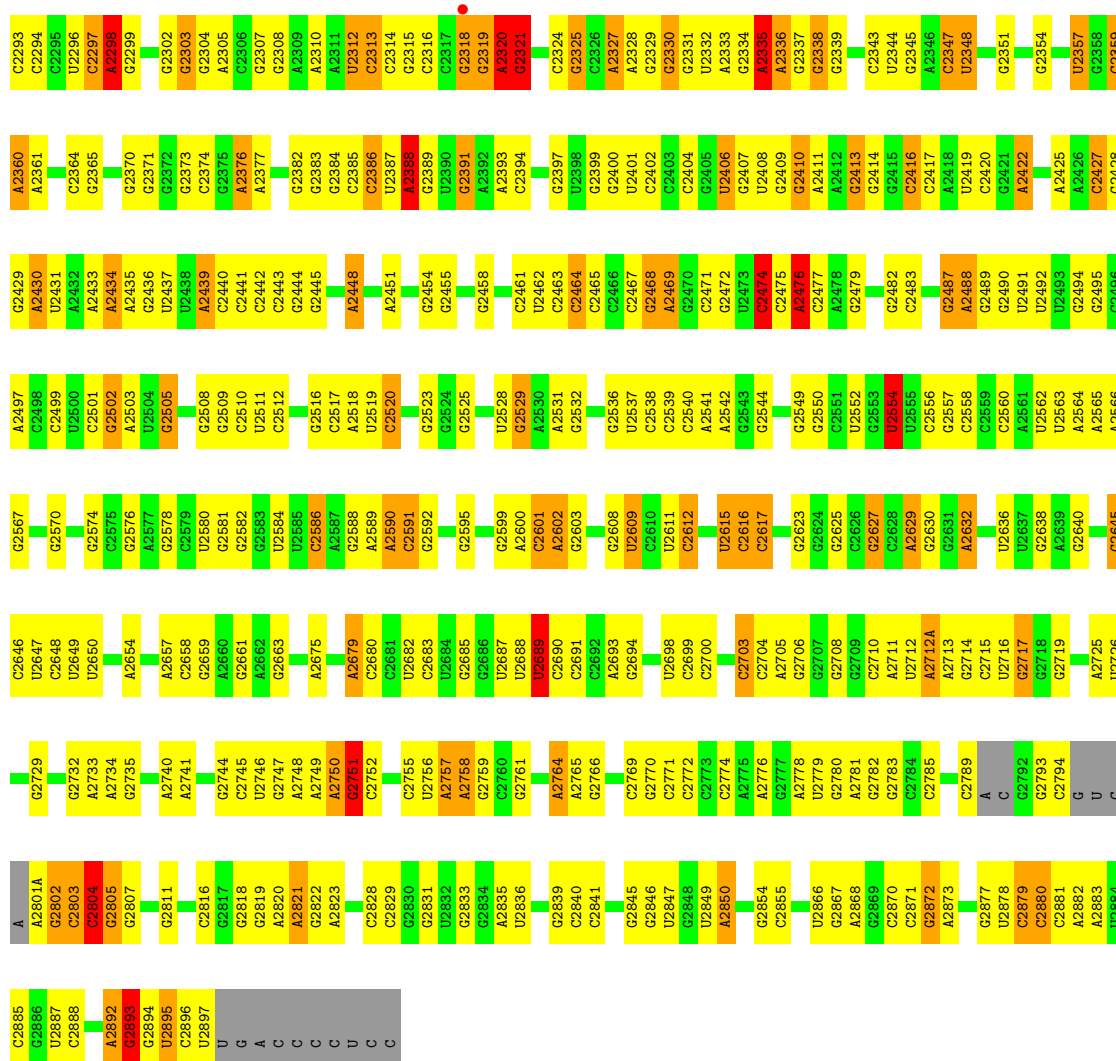
Molecule 25: 23S Ribosomal RNA

Chain DA: 38% 40% 13% 7%

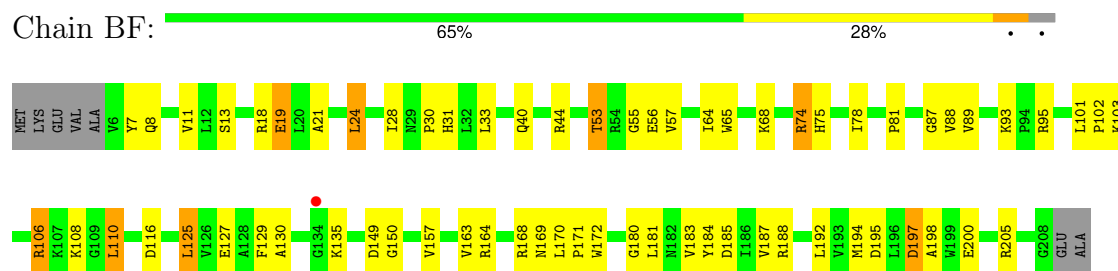


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G1415	G1416	G1417	G1418	G1419	G1420	G1421	G1422	G1423	G1424	G1425	G1426	G1427	G1428	G1429	G1430	G1431	G1432	G1433	G1434	G1435	G1436
G1437	G1438	G1439	G1440	G1441	G1442	G1443	G1444	G1445	G1446	G1447	G1448	G1449	G1450	G1451	G1452	G1453	G1454	G1455	G1456	G1457	G1458
G1459	G1460	G1461	G1462	G1463	G1464	G1465	G1466	G1467	G1468	G1469	G1470	G1471	G1472	G1473	G1474	G1475	G1476	G1477	G1478	G1479	G1480
G1481	G1482	G1483	G1484	G1485	G1486	G1487	G1488	G1489	G1490	G1491	G1492	G1493	G1494	G1495	G1496	G1497	G1498	G1499	G1500	G1501	G1502
G1503	G1504	G1505	G1506	G1507	G1508	G1509	G1510	G1511	G1512	G1513	G1514	G1515	G1516	G1517	G1518	G1519	G1520	G1521	G1522	G1523	G1524
G1525	G1526	G1527	G1528	G1529	G1530	G1531	G1532	G1533	G1534	G1535	G1536	G1537	G1538	G1539	G1540	G1541	G1542	G1543	G1544	G1545	G1546
G1547	G1548	G1549	G1550	G1551	G1552	G1553	G1554	G1555	G1556	G1557	G1558	G1559	G1560	G1561	G1562	G1563	G1564	G1565	G1566	G1567	G1568
G1569	G1570	G1571	G1572	G1573	G1574	G1575	G1576	G1577	G1578	G1579	G1580	G1581	G1582	G1583	G1584	G1585	G1586	G1587	G1588	G1589	G1590
G1591	G1592	G1593	G1594	G1595	G1596	G1597	G1598	G1599	G1600	G1601	G1602	G1603	G1604	G1605	G1606	G1607	G1608	G1609	G1610	G1611	G1612
G1613	G1614	G																			

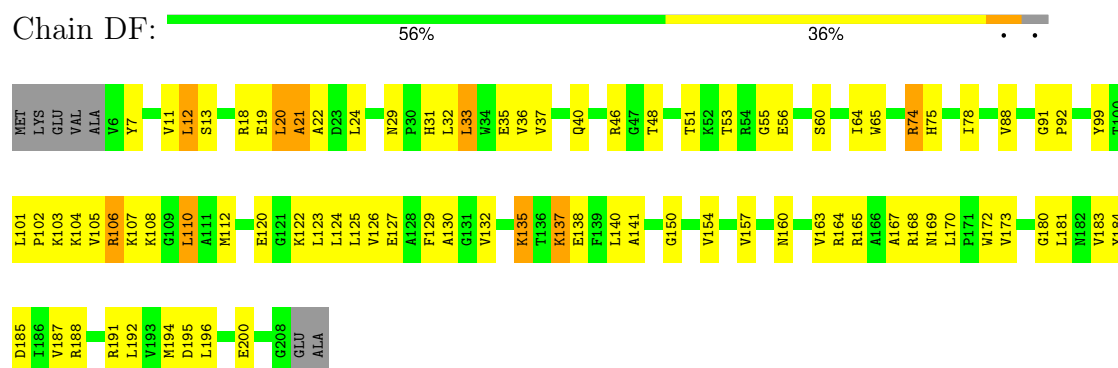




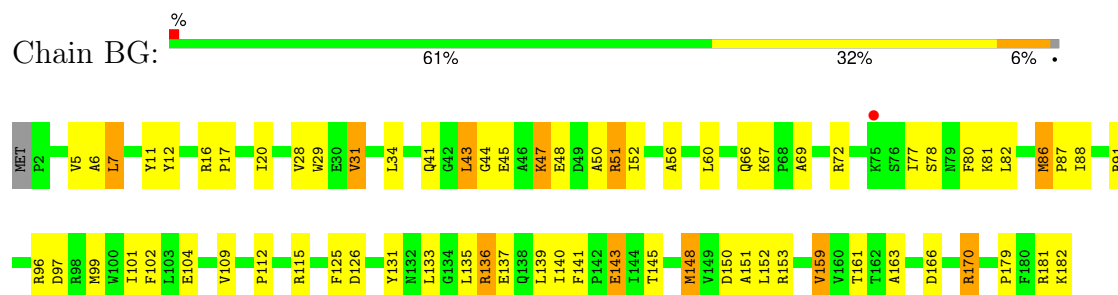
- Molecule 29: 50S Ribosomal Protein L4



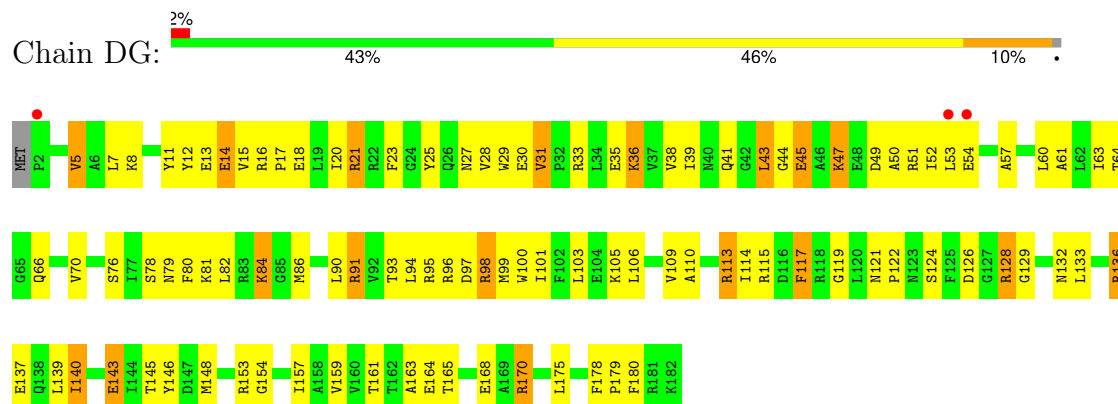
- Molecule 29: 50S Ribosomal Protein L4



- Molecule 30: 50S Ribosomal Protein L5



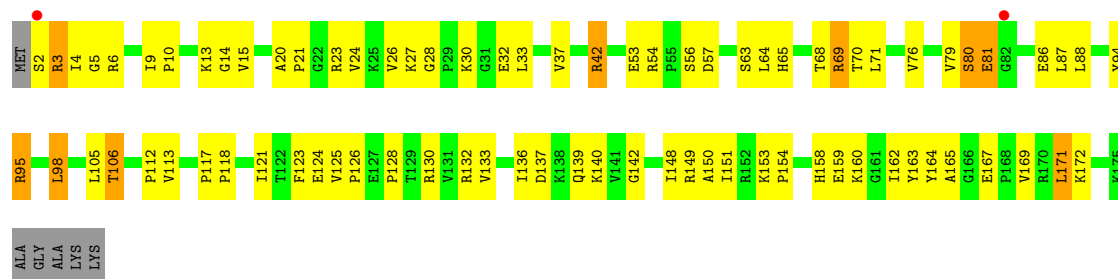
- Molecule 30: 50S Ribosomal Protein L5



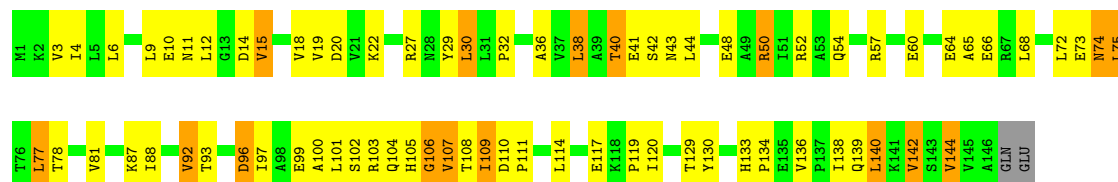
- Molecule 31: 50S Ribosomal Protein L6



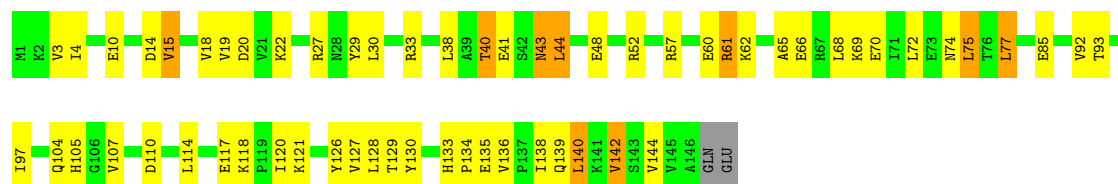
- Molecule 31: 50S Ribosomal Protein L6



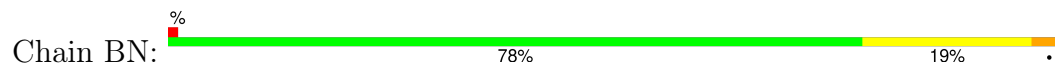
- Molecule 32: 50S Ribosomal Protein L9



- Molecule 32: 50S Ribosomal Protein L9

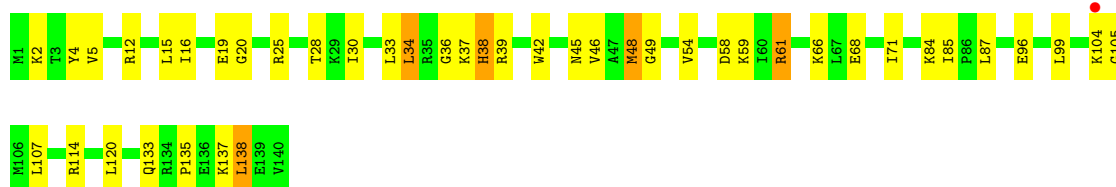


- Molecule 33: 50S Ribosomal Protein L13



- Molecule 33: 50S Ribosomal Protein L13





- Molecule 34: 50S Ribosomal Protein L14

Chain BO: 72% 25% ..



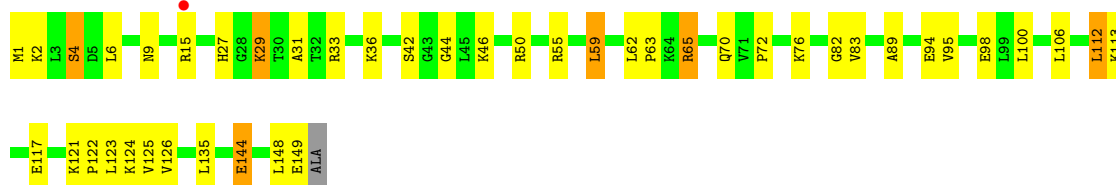
- Molecule 34: 50S Ribosomal Protein L14

Chain DO: 61% 34% .



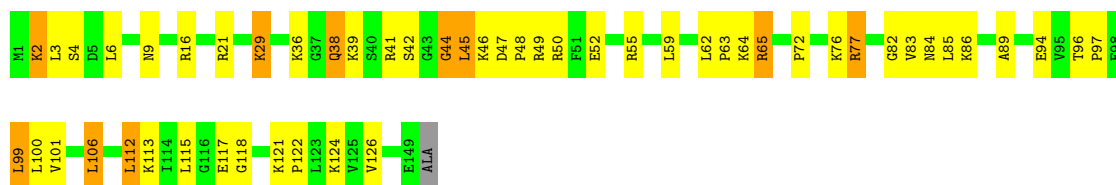
- Molecule 35: 50S Ribosomal Protein L15

Chain BP: 70% 25% ..



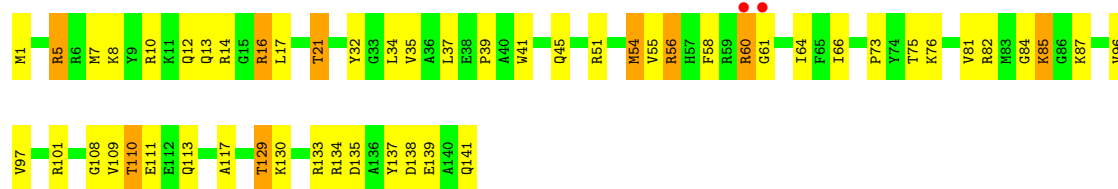
- Molecule 35: 50S Ribosomal Protein L15

Chain DP: 65% 28% 7% .

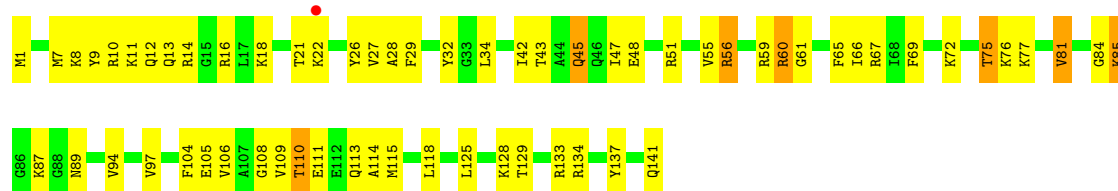


- Molecule 36: 50S Ribosomal Protein L16

Chain BQ: 62% 31% 6%



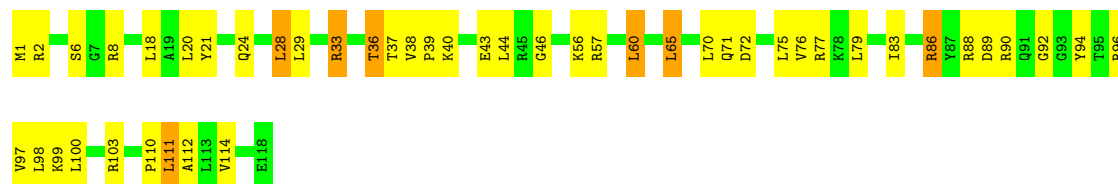
• Molecule 36: 50S Ribosomal Protein L16



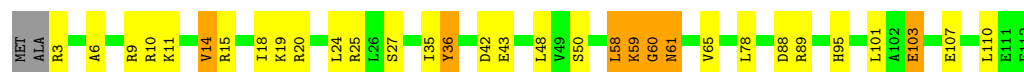
• Molecule 37: 50S Ribosomal Protein L17



• Molecule 37: 50S Ribosomal Protein L17

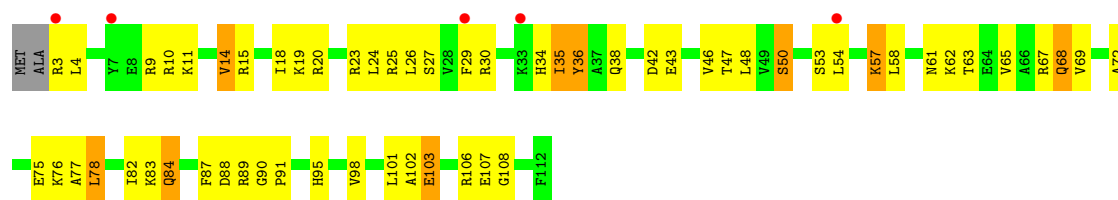


• Molecule 38: 50S Ribosomal Protein L18

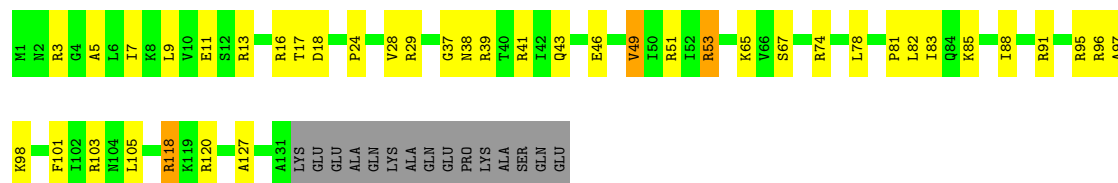


• Molecule 38: 50S Ribosomal Protein L18

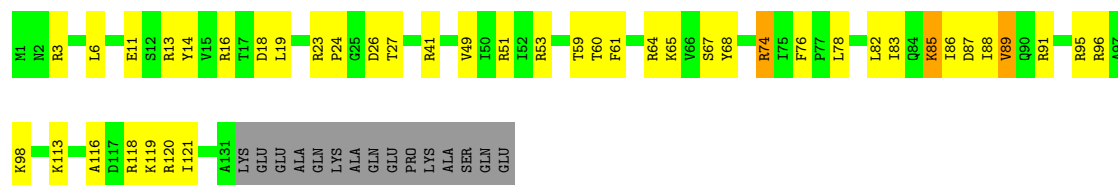




• Molecule 39: 50S Ribosomal Protein L19



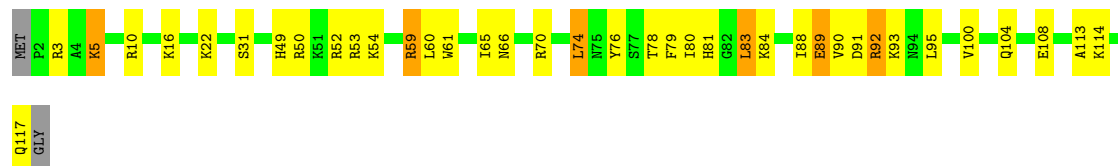
• Molecule 39: 50S Ribosomal Protein L19



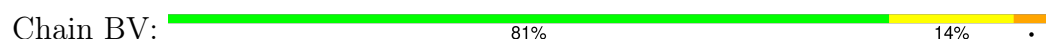
• Molecule 40: 50S Ribosomal Protein L20



• Molecule 40: 50S Ribosomal Protein L20



• Molecule 41: 50S Ribosomal Protein L21





- Molecule 41: 50S Ribosomal Protein L21

Chain DV: 69% 27% ..



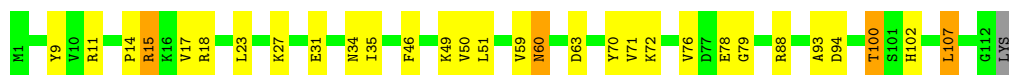
- Molecule 42: 50S Ribosomal Protein L22

Chain BW: 79% 17% ..



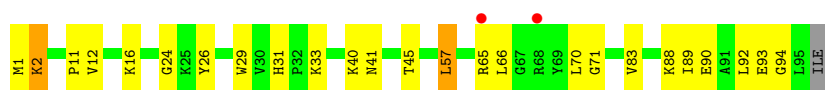
- Molecule 42: 50S Ribosomal Protein L22

Chain DW: 73% 23% ..



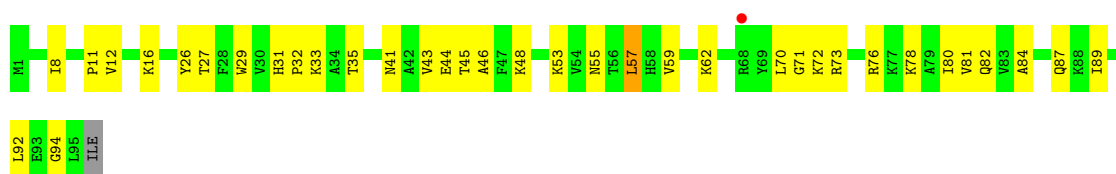
- Molecule 43: 50S Ribosomal Protein L23

Chain BX: 2% 73% 24% ..



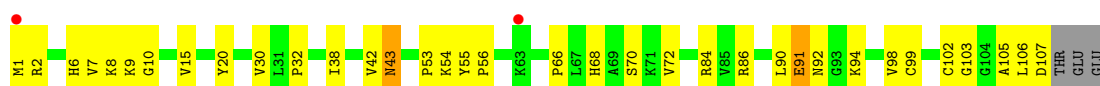
- Molecule 43: 50S Ribosomal Protein L23

Chain DX: 61% 36% ..

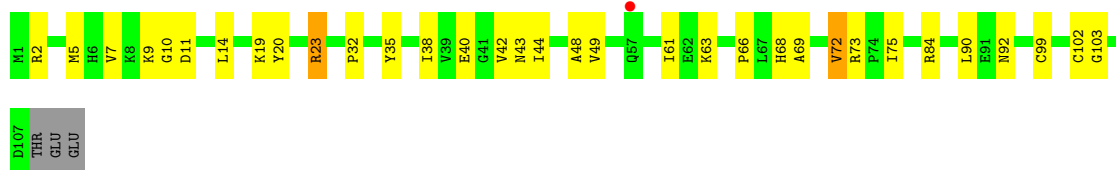


- Molecule 44: 50S Ribosomal Protein L24

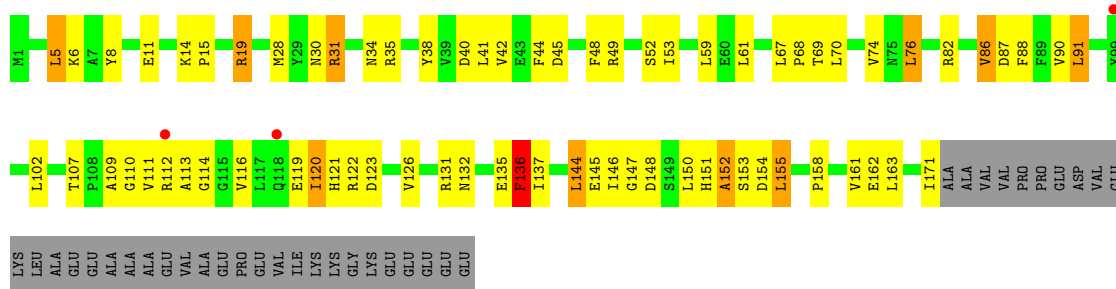
Chain BY: 2% 65% 30% ..



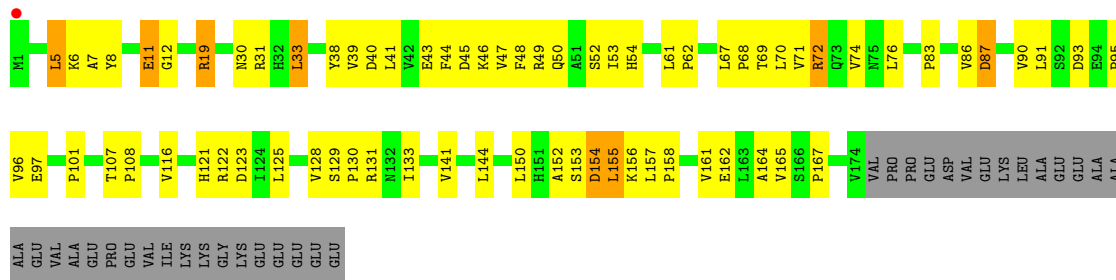
- Molecule 44: 50S Ribosomal Protein L24



• Molecule 45: 50S Ribosomal Protein L25



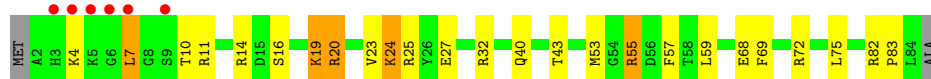
• Molecule 45: 50S Ribosomal Protein L25



• Molecule 46: 50S Ribosomal Protein L27

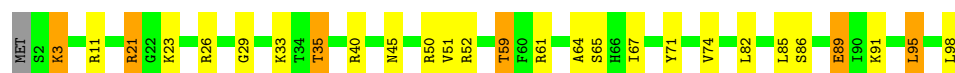


• Molecule 46: 50S Ribosomal Protein L27



• Molecule 47: 50S Ribosomal Protein L28

Chain B1: 



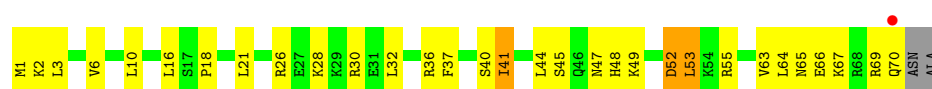
• Molecule 47: 50S Ribosomal Protein L28

Chain D1: 



• Molecule 48: 50S Ribosomal Protein L29

Chain B2: 



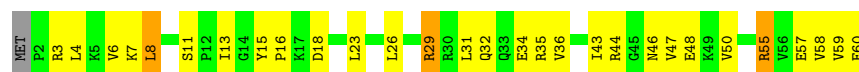
• Molecule 48: 50S Ribosomal Protein L29

Chain D2: 



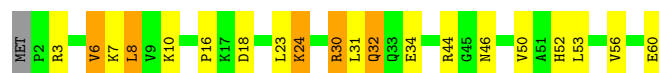
• Molecule 49: 50S Ribosomal Protein L30

Chain B3: 



• Molecule 49: 50S Ribosomal Protein L30

Chain D3: 



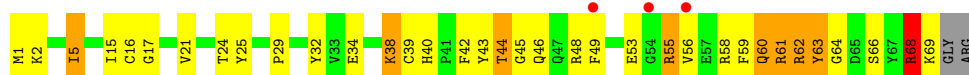
• Molecule 50: 50S Ribosomal Protein L31

Chain B4: 



• Molecule 50: 50S Ribosomal Protein L31

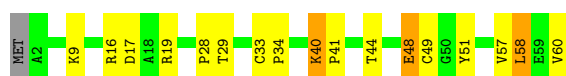
Chain D4: 



- Molecule 51: 50S Ribosomal Protein L32



- Molecule 51: 50S Ribosomal Protein L32



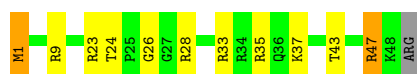
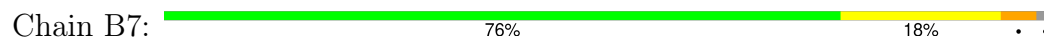
- Molecule 52: 50S Ribosomal Protein L33



- Molecule 52: 50S Ribosomal Protein L33



- Molecule 53: 50S Ribosomal Protein L34



- Molecule 53: 50S Ribosomal Protein L34

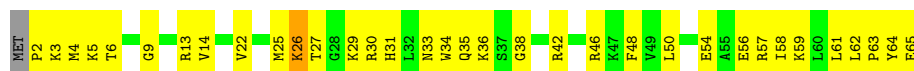


- Molecule 54: 50S Ribosomal Protein L35

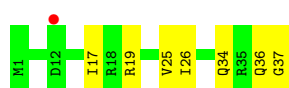
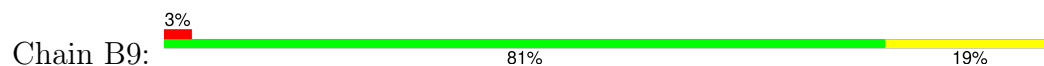




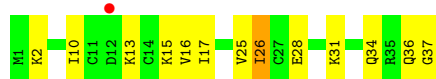
- Molecule 54: 50S Ribosomal Protein L35



- 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	209.68Å 450.64Å 622.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.68 – 3.10 49.68 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.68-3.10) 98.1 (49.68-3.10)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.25	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.203 , 0.260 0.203 , 0.258	Depositor DCC
R_{free} test set	51894 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	71.0	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 55.6	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 1.83% 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: ZN, 2R3, 2QZ, SF4, MVA, 2QY, 004, FME, 2R1, K, 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	0.75	2/36038 (0.0%)	1.31	240/56244 (0.4%)
1	CA	0.75	10/36170 (0.0%)	1.36	314/56452 (0.6%)
2	AB	0.49	0/1881	0.77	1/2542 (0.0%)
2	CB	0.54	0/1860	0.79	1/2518 (0.0%)
3	AC	0.47	0/1576	0.65	0/2130
3	CC	0.51	0/1566	0.71	2/2119 (0.1%)
4	AD	0.49	0/1689	0.73	0/2267
4	CD	0.49	0/1704	0.70	1/2284 (0.0%)
5	AE	0.47	0/1145	0.70	0/1543
5	CE	0.50	0/1149	0.71	0/1548
6	AF	0.47	0/819	0.69	0/1111
6	CF	0.52	0/829	0.74	1/1123 (0.1%)
7	AG	0.48	0/1250	0.67	1/1679 (0.1%)
7	CG	0.50	0/1254	0.71	1/1683 (0.1%)
8	AH	0.45	0/1108	0.66	0/1494
8	CH	0.48	0/1108	0.69	0/1494
9	AI	0.46	0/1002	0.72	0/1346
9	CI	0.56	0/997	0.75	1/1343 (0.1%)
10	AJ	0.47	0/722	0.68	0/982
10	CJ	0.51	0/727	0.68	0/988
11	AK	0.44	0/844	0.62	0/1145
11	CK	0.46	0/848	0.66	0/1149
12	AL	0.52	0/946	0.69	0/1274
12	CL	0.51	0/946	0.73	0/1274
13	AM	0.46	0/969	0.69	0/1302
13	CM	0.49	0/961	0.66	0/1291
14	AN	0.51	0/501	0.67	0/664
14	CN	0.54	0/501	0.68	0/664
15	AO	0.47	0/739	0.72	0/985
15	CO	0.46	0/739	0.73	0/985
16	AP	0.45	0/697	0.71	0/939
16	CP	0.47	0/693	0.65	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.48	0/836	0.66	0/1117
17	CQ	0.49	0/836	0.68	0/1117
18	AR	0.49	0/560	0.72	0/746
18	CR	0.51	0/560	0.75	1/746 (0.1%)
19	AS	0.47	0/667	0.68	0/900
19	CS	0.54	0/661	0.82	2/893 (0.2%)
20	AT	0.51	0/730	0.76	0/965
20	CT	0.44	0/729	0.68	0/965
21	AU	0.45	0/203	0.65	0/266
21	CU	0.51	0/203	0.68	0/266
22	AV	0.94	0/127	1.36	2/198 (1.0%)
22	CV	0.86	0/126	1.29	0/195
23	AX	0.85	5/1813 (0.3%)	1.59	36/2825 (1.3%)
23	CX	0.88	4/1813 (0.2%)	1.81	40/2825 (1.4%)
24	AW	0.50	0/20	0.80	0/23
24	CW	0.43	0/20	0.70	0/23
25	BA	1.06	33/65892 (0.1%)	1.42	649/102850 (0.6%)
25	DA	0.79	9/65466 (0.0%)	1.39	590/102184 (0.6%)
26	BB	0.82	0/2878	1.26	11/4490 (0.2%)
26	DB	0.89	0/2878	1.39	18/4490 (0.4%)
27	BD	0.67	1/2186 (0.0%)	0.78	1/2944 (0.0%)
27	DD	0.61	2/2186 (0.1%)	0.77	1/2944 (0.0%)
28	BE	0.69	0/1592	0.75	0/2149
28	DE	0.55	0/1592	0.77	1/2149 (0.0%)
29	BF	0.69	0/1619	0.76	0/2193
29	DF	0.53	0/1615	0.77	1/2188 (0.0%)
30	BG	0.46	0/1450	0.70	0/1959
30	DG	0.55	0/1449	0.74	0/1958
31	BH	0.60	0/1356	0.70	0/1834
31	DH	0.56	0/1356	0.70	0/1834
32	BI	0.49	0/1100	0.74	1/1501 (0.1%)
32	DI	0.48	0/1076	0.77	0/1471
33	BN	0.65	0/1144	0.73	0/1543
33	DN	0.50	0/1144	0.72	0/1543
34	BO	0.65	0/943	0.73	1/1269 (0.1%)
34	DO	0.54	0/943	0.73	1/1269 (0.1%)
35	BP	0.62	0/1152	0.77	0/1533
35	DP	0.53	0/1152	0.80	1/1533 (0.1%)
36	BQ	0.64	0/1143	0.76	0/1527
36	DQ	0.60	0/1143	0.79	0/1527
37	BR	0.59	0/982	0.78	0/1312
37	DR	0.49	0/982	0.71	0/1312
38	BS	0.54	0/887	0.77	0/1180

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DS	0.47	0/880	0.72	0/1172
39	BT	0.59	0/1105	0.79	1/1477 (0.1%)
39	DT	0.50	0/1097	0.72	0/1468
40	BU	0.71	1/977 (0.1%)	0.73	0/1301
40	DU	0.54	0/977	0.71	1/1301 (0.1%)
41	BV	0.68	0/782	0.74	1/1049 (0.1%)
41	DV	0.55	0/782	0.71	0/1049
42	BW	0.74	0/897	0.74	0/1205
42	DW	0.56	0/897	0.72	0/1205
43	BX	0.66	0/764	0.96	3/1025 (0.3%)
43	DX	0.55	0/764	0.75	1/1025 (0.1%)
44	BY	0.64	0/819	0.78	0/1095
44	DY	0.54	0/819	0.74	0/1095
45	BZ	0.56	0/1379	0.75	0/1873
45	DZ	0.53	0/1390	0.71	0/1890
46	B0	0.63	0/662	0.81	2/881 (0.2%)
46	D0	0.54	0/662	0.73	0/881
47	B1	0.61	0/762	0.74	0/1014
47	D1	0.51	0/762	0.75	1/1014 (0.1%)
48	B2	0.61	0/590	0.79	0/781
48	D2	0.48	0/590	0.66	0/781
49	B3	0.70	0/474	0.76	0/635
49	D3	0.45	0/469	0.67	0/630
50	B4	0.58	0/564	0.79	0/759
50	D4	0.59	0/544	0.86	1/735 (0.1%)
51	B5	0.66	0/469	0.78	0/635
51	D5	0.53	0/469	0.74	1/635 (0.2%)
52	B6	0.67	0/460	0.64	0/613
52	D6	0.53	0/456	0.70	0/608
53	B7	0.79	0/426	0.78	0/561
53	D7	0.62	0/426	0.76	1/561 (0.2%)
54	B8	0.70	0/519	0.71	0/684
54	D8	0.55	0/525	0.75	0/691
55	B9	0.69	0/310	0.76	0/407
55	D9	0.60	0/310	0.79	0/407
All	All	0.79	67/305966 (0.0%)	1.24	1933/457396 (0.4%)

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
23	CX	1	0
24	AW	0	1
24	CW	0	1
27	DD	0	1
38	BS	0	1
45	BZ	0	1
50	B4	0	1
All	All	1	11

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AX	76	A	N7-C5	-11.16	1.32	1.39
1	CA	1154	G	C6-N1	-11.02	1.31	1.39
1	CA	1154	G	N1-C2	-10.69	1.29	1.37
25	BA	1188	A	N9-C4	-10.29	1.31	1.37
1	CA	1119	C	N3-C4	-10.20	1.26	1.33

The worst 5 of 1933 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	CX	76	A	O4'-C1'-N9	38.71	139.17	108.20
1	CA	1119	C	N1-C2-O2	32.56	138.44	118.90
1	CA	1154	G	C5-C6-O6	28.63	145.78	128.60
1	CA	1154	G	N3-C2-N2	25.05	137.43	119.90
1	CA	1154	G	N1-C2-N2	-22.71	95.76	116.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	CX	76	A	C1'

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	231	GLU	Peptide
2	AB	8	LYS	Peptide
2	AB	9	GLU	Peptide
7	AG	79	ARG	Peptide
24	AW	4	PRO	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	16251	809	0
1	CA	32312	0	16307	915	0
2	AB	1846	0	1867	109	0
2	CB	1825	0	1828	119	0
3	AC	1552	0	1546	59	0
3	CC	1542	0	1517	66	0
4	AD	1659	0	1676	99	0
4	CD	1674	0	1714	78	0
5	AE	1129	0	1185	50	0
5	CE	1133	0	1191	45	0
6	AF	806	0	793	33	0
6	CF	816	0	808	27	0
7	AG	1231	0	1238	35	0
7	CG	1235	0	1249	56	0
8	AH	1088	0	1126	48	0
8	CH	1088	0	1126	46	0
9	AI	983	0	986	54	0
9	CI	978	0	966	57	0
10	AJ	709	0	650	35	0
10	CJ	714	0	672	47	0
11	AK	829	0	825	19	0
11	CK	833	0	836	29	0
12	AL	930	0	980	28	0
12	CL	930	0	980	34	0
13	AM	958	0	1002	25	0
13	CM	950	0	988	56	0
14	AN	492	0	529	26	0
14	CN	492	0	529	29	0
15	AO	728	0	760	16	0
15	CO	728	0	760	27	0
16	AP	681	0	697	29	0
16	CP	677	0	686	28	0
17	AQ	823	0	891	21	0
17	CQ	823	0	891	19	0
18	AR	555	0	618	17	0
18	CR	555	0	618	27	0
19	AS	652	0	662	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	CS	646	0	644	56	0
20	AT	728	0	798	30	0
20	CT	727	0	796	28	0
21	AU	199	0	208	5	0
21	CU	199	0	208	7	0
22	AV	114	0	54	0	0
22	CV	113	0	54	0	0
23	AX	1623	0	823	18	0
23	CX	1623	0	824	24	0
24	AW	93	0	84	9	0
24	CW	93	0	84	14	0
25	BA	58834	0	29667	785	0
25	DA	58458	0	29482	1100	0
26	BB	2573	0	1306	38	0
26	DB	2573	0	1306	54	0
27	BD	2136	0	2218	64	0
27	DD	2136	0	2218	74	0
28	BE	1559	0	1618	38	0
28	DE	1559	0	1618	60	0
29	BF	1584	0	1625	46	0
29	DF	1580	0	1619	69	0
30	BG	1425	0	1443	45	0
30	DG	1424	0	1434	82	0
31	BH	1330	0	1407	33	0
31	DH	1330	0	1407	52	0
32	BI	1085	0	1114	42	0
32	DI	1061	0	1080	31	0
33	BN	1117	0	1183	17	0
33	DN	1117	0	1184	26	0
34	BO	933	0	996	24	0
34	DO	933	0	996	36	0
35	BP	1135	0	1212	37	0
35	DP	1135	0	1211	46	0
36	BQ	1122	0	1179	38	0
36	DQ	1122	0	1179	47	0
37	BR	968	0	1033	24	0
37	DR	968	0	1032	30	0
38	BS	877	0	938	25	0
38	DS	870	0	923	47	0
39	BT	1091	0	1151	28	0
39	DT	1083	0	1136	36	0
40	BU	959	0	1019	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	DU	959	0	1019	37	0
41	BV	771	0	830	11	0
41	DV	771	0	830	23	0
42	BW	886	0	940	9	0
42	DW	886	0	940	17	0
43	BX	750	0	814	20	0
43	DX	750	0	814	25	0
44	BY	806	0	881	25	0
44	DY	806	0	881	21	0
45	BZ	1349	0	1355	47	0
45	DZ	1360	0	1363	48	0
46	B0	653	0	674	25	0
46	D0	653	0	674	23	0
47	B1	755	0	826	19	0
47	D1	755	0	826	26	0
48	B2	588	0	643	18	0
48	D2	588	0	643	20	0
49	B3	469	0	518	17	0
49	D3	464	0	514	12	0
50	B4	551	0	532	38	0
50	D4	531	0	502	32	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	10	0
53	B7	418	0	466	9	0
53	D7	418	0	467	9	0
54	B8	511	0	571	27	0
54	D8	517	0	582	27	0
55	B9	307	0	335	5	0
55	D9	307	0	335	10	0
56	AA	221	0	0	0	0
56	AD	1	0	0	0	0
56	AF	1	0	0	0	0
56	AK	1	0	0	0	0
56	AM	1	0	0	0	0
56	AN	2	0	0	0	0
56	AV	1	0	0	0	0
56	AX	9	0	0	0	0
56	B0	4	0	0	0	0
56	B1	1	0	0	0	0
56	B2	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	B3	3	0	0	0	0
56	B4	1	0	0	0	0
56	B5	1	0	0	0	0
56	B7	4	0	0	0	0
56	B8	3	0	0	0	0
56	B9	1	0	0	0	0
56	BA	738	0	0	0	0
56	BB	18	0	0	0	0
56	BD	12	0	0	0	0
56	BE	10	0	0	0	0
56	BF	8	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	5	0	0	0	0
56	BR	4	0	0	0	0
56	BU	8	0	0	0	0
56	BV	4	0	0	0	0
56	BW	5	0	0	0	0
56	BX	1	0	0	0	0
56	BY	1	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	CQ	1	0	0	0	0
56	CT	1	0	0	0	0
56	CX	3	0	0	0	0
56	D0	1	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	653	0	0	0	0
56	DB	12	0	0	0	0
56	DD	8	0	0	0	0
56	DE	6	0	0	0	0
56	DF	6	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	DQ	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DR	2	0	0	0	0
56	DV	4	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	0	0
59	CX	10	0	10	2	0
60	BA	1	0	0	0	0
60	DA	1	0	0	0	0
61	AA	148	0	0	27	0
61	AD	1	0	0	0	0
61	AE	3	0	0	0	0
61	AJ	1	0	0	0	0
61	AL	1	0	0	0	0
61	AP	1	0	0	0	0
61	AU	1	0	0	0	0
61	AV	1	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
61	B5	3	0	0	1	0
61	B7	1	0	0	1	0
61	B8	8	0	0	1	0
61	BA	1092	0	0	113	0
61	BB	26	0	0	0	0
61	BD	8	0	0	1	0
61	BE	9	0	0	4	0
61	BF	4	0	0	0	0
61	BG	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	BN	3	0	0	0	0
61	BO	2	0	0	0	0
61	BP	15	0	0	3	0
61	BQ	3	0	0	1	0
61	BR	1	0	0	0	0
61	BT	1	0	0	0	0
61	BU	4	0	0	0	0
61	BV	2	0	0	0	0
61	BW	2	0	0	0	0
61	BX	4	0	0	1	0
61	CA	187	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	5	0	0	1	0
61	D1	1	0	0	0	0
61	D7	2	0	0	0	0
61	D8	4	0	0	0	0
61	DA	902	0	0	120	0
61	DB	7	0	0	0	0
61	DD	8	0	0	0	0
61	DE	13	0	0	1	0
61	DF	5	0	0	0	0
61	DO	1	0	0	0	0
61	DP	14	0	0	0	0
61	DQ	3	0	0	1	0
61	DU	4	0	0	0	0
61	DV	1	0	0	0	0
61	DX	2	0	0	0	0
61	DY	2	0	0	0	0
All	All	286321	0	191126	6372	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 14.

The worst 5 of 6372 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1002:G:H1	1:CA:1038:C:N4	1.42	1.16
1:AA:348:G:H2'	1:AA:349:A:H5'	1.36	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1125:U:N3	1:AA:1127:G:N7	2.06	1.03
39:BT:16:ARG:NH2	39:BT:83:ILE:O	1.92	1.02
2:CB:185:ILE:HG22	2:CB:199:TYR:HB2	1.40	1.02

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%)	200 (87%)	23 (10%)	6 (3%)	4	21
2	CB	229/256 (90%)	201 (88%)	18 (8%)	10 (4%)	2	12
3	AC	204/239 (85%)	179 (88%)	22 (11%)	3 (2%)	8	33
3	CC	204/239 (85%)	178 (87%)	24 (12%)	2 (1%)	13	42
4	AD	206/209 (99%)	182 (88%)	22 (11%)	2 (1%)	13	42
4	CD	206/209 (99%)	185 (90%)	18 (9%)	3 (2%)	8	33
5	AE	146/162 (90%)	127 (87%)	15 (10%)	4 (3%)	4	21
5	CE	146/162 (90%)	133 (91%)	10 (7%)	3 (2%)	5	25
6	AF	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
6	CF	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
7	AG	153/156 (98%)	137 (90%)	14 (9%)	2 (1%)	10	36
7	CG	153/156 (98%)	137 (90%)	15 (10%)	1 (1%)	19	51
8	AH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
8	CH	135/138 (98%)	129 (96%)	5 (4%)	1 (1%)	19	51
9	AI	125/128 (98%)	111 (89%)	10 (8%)	4 (3%)	3	18
9	CI	125/128 (98%)	112 (90%)	11 (9%)	2 (2%)	8	31
10	AJ	95/105 (90%)	85 (90%)	7 (7%)	3 (3%)	3	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	CJ	94/105 (90%)	86 (92%)	7 (7%)	1 (1%)	12	39
11	AK	112/129 (87%)	98 (88%)	13 (12%)	1 (1%)	14	45
11	CK	112/129 (87%)	99 (88%)	12 (11%)	1 (1%)	14	45
12	AL	120/132 (91%)	116 (97%)	4 (3%)	0	100	100
12	CL	120/132 (91%)	112 (93%)	8 (7%)	0	100	100
13	AM	121/126 (96%)	106 (88%)	15 (12%)	0	100	100
13	CM	120/126 (95%)	104 (87%)	14 (12%)	2 (2%)	7	30
14	AN	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
14	CN	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
15	AO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
15	CO	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	11	38
16	AP	80/88 (91%)	69 (86%)	11 (14%)	0	100	100
16	CP	80/88 (91%)	70 (88%)	10 (12%)	0	100	100
17	AQ	97/105 (92%)	91 (94%)	6 (6%)	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	33
18	CR	66/88 (75%)	60 (91%)	5 (8%)	1 (2%)	8	33
19	AS	81/93 (87%)	74 (91%)	7 (9%)	0	100	100
19	CS	81/93 (87%)	69 (85%)	12 (15%)	0	100	100
20	AT	94/106 (89%)	84 (89%)	5 (5%)	5 (5%)	1	10
20	CT	94/106 (89%)	85 (90%)	3 (3%)	6 (6%)	1	6
21	AU	21/27 (78%)	17 (81%)	4 (19%)	0	100	100
21	CU	21/27 (78%)	18 (86%)	1 (5%)	2 (10%)	0	3
24	AW	3/10 (30%)	1 (33%)	0	2 (67%)	0	0
24	CW	3/10 (30%)	1 (33%)	1 (33%)	1 (33%)	0	0
27	BD	273/276 (99%)	259 (95%)	13 (5%)	1 (0%)	30	63
27	DD	273/276 (99%)	257 (94%)	13 (5%)	3 (1%)	12	39
28	BE	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	25	58
28	DE	202/206 (98%)	194 (96%)	6 (3%)	2 (1%)	13	42
29	BF	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	25	58
29	DF	201/210 (96%)	189 (94%)	10 (5%)	2 (1%)	13	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	BG	179/182 (98%)	163 (91%)	13 (7%)	3 (2%)	7	30
30	DG	179/182 (98%)	160 (89%)	13 (7%)	6 (3%)	3	17
31	BH	172/180 (96%)	161 (94%)	10 (6%)	1 (1%)	22	53
31	DH	172/180 (96%)	159 (92%)	11 (6%)	2 (1%)	11	38
32	BI	144/148 (97%)	122 (85%)	17 (12%)	5 (4%)	3	16
32	DI	144/148 (97%)	123 (85%)	17 (12%)	4 (3%)	4	20
33	BN	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
33	DN	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	19	51
34	BO	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	16	48
34	DO	120/122 (98%)	117 (98%)	2 (2%)	1 (1%)	16	48
35	BP	147/150 (98%)	132 (90%)	14 (10%)	1 (1%)	19	51
35	DP	147/150 (98%)	133 (90%)	12 (8%)	2 (1%)	9	34
36	BQ	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	19	51
36	DQ	139/141 (99%)	129 (93%)	8 (6%)	2 (1%)	9	34
37	BR	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	14	45
37	DR	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
38	BS	108/112 (96%)	100 (93%)	7 (6%)	1 (1%)	14	45
38	DS	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	14	45
39	BT	129/146 (88%)	124 (96%)	4 (3%)	1 (1%)	16	48
39	DT	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
40	BU	114/118 (97%)	114 (100%)	0	0	100	100
40	DU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
41	BV	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	13	42
41	DV	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	13	42
42	BW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
42	DW	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
43	BX	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	12	39
43	DX	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
44	BY	105/110 (96%)	95 (90%)	10 (10%)	0	100	100
44	DY	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
45	BZ	169/206 (82%)	150 (89%)	17 (10%)	2 (1%)	11	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	DZ	172/206 (84%)	157 (91%)	15 (9%)	0	100	100
46	B0	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	11	38
46	D0	81/85 (95%)	76 (94%)	5 (6%)	0	100	100
47	B1	95/98 (97%)	93 (98%)	0	2 (2%)	5	25
47	D1	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	12	39
48	B2	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
48	D2	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
49	B3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
49	D3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
50	B4	67/71 (94%)	50 (75%)	9 (13%)	8 (12%)	0	1
50	D4	67/71 (94%)	50 (75%)	8 (12%)	9 (13%)	0	1
51	B5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
51	D5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
52	B6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
52	D6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
53	B7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
53	D7	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	5	24
54	B8	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
54	D8	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
55	B9	35/37 (95%)	35 (100%)	0	0	100	100
55	D9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11415/12148 (94%)	10525 (92%)	749 (7%)	141 (1%)	11	38

5 of 141 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	17	PHE
2	AB	125	PRO
3	AC	65	ALA
3	AC	107	GLN
4	AD	166	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	192/220 (87%)	147 (77%)	45 (23%)	0	2
2	CB	187/220 (85%)	152 (81%)	35 (19%)	1	5
3	AC	143/188 (76%)	125 (87%)	18 (13%)	3	15
3	CC	140/188 (74%)	122 (87%)	18 (13%)	3	15
4	AD	170/181 (94%)	145 (85%)	25 (15%)	2	11
4	CD	173/181 (96%)	152 (88%)	21 (12%)	4	16
5	AE	113/123 (92%)	104 (92%)	9 (8%)	10	34
5	CE	114/123 (93%)	107 (94%)	7 (6%)	15	43
6	AF	83/90 (92%)	76 (92%)	7 (8%)	9	32
6	CF	85/90 (94%)	79 (93%)	6 (7%)	12	39
7	AG	119/127 (94%)	100 (84%)	19 (16%)	2	9
7	CG	120/127 (94%)	102 (85%)	18 (15%)	2	10
8	AH	114/119 (96%)	98 (86%)	16 (14%)	3	12
8	CH	114/119 (96%)	102 (90%)	12 (10%)	5	22
9	AI	90/99 (91%)	76 (84%)	14 (16%)	2	9
9	CI	89/99 (90%)	75 (84%)	14 (16%)	2	9
10	AJ	66/92 (72%)	60 (91%)	6 (9%)	7	28
10	CJ	69/92 (75%)	64 (93%)	5 (7%)	12	38
11	AK	82/99 (83%)	73 (89%)	9 (11%)	5	21
11	CK	83/99 (84%)	77 (93%)	6 (7%)	12	38
12	AL	97/109 (89%)	90 (93%)	7 (7%)	12	38
12	CL	97/109 (89%)	87 (90%)	10 (10%)	6	22
13	AM	93/101 (92%)	82 (88%)	11 (12%)	4	17
13	CM	92/101 (91%)	80 (87%)	12 (13%)	3	14
14	AN	49/50 (98%)	41 (84%)	8 (16%)	2	8
14	CN	49/50 (98%)	42 (86%)	7 (14%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	AO	78/80 (98%)	69 (88%)	9 (12%)	4	19
15	CO	78/80 (98%)	66 (85%)	12 (15%)	2	9
16	AP	69/74 (93%)	60 (87%)	9 (13%)	3	14
16	CP	68/74 (92%)	63 (93%)	5 (7%)	11	36
17	AQ	94/97 (97%)	89 (95%)	5 (5%)	19	48
17	CQ	94/97 (97%)	87 (93%)	7 (7%)	11	36
18	AR	59/77 (77%)	55 (93%)	4 (7%)	13	40
18	CR	59/77 (77%)	52 (88%)	7 (12%)	4	17
19	AS	69/80 (86%)	63 (91%)	6 (9%)	8	31
19	CS	67/80 (84%)	57 (85%)	10 (15%)	2	10
20	AT	70/82 (85%)	61 (87%)	9 (13%)	3	15
20	CT	70/82 (85%)	60 (86%)	10 (14%)	2	11
21	AU	18/22 (82%)	14 (78%)	4 (22%)	1	3
21	CU	18/22 (82%)	16 (89%)	2 (11%)	5	20
24	AW	3/3 (100%)	2 (67%)	1 (33%)	0	0
24	CW	3/3 (100%)	2 (67%)	1 (33%)	0	0
27	BD	215/218 (99%)	198 (92%)	17 (8%)	10	34
27	DD	215/218 (99%)	190 (88%)	25 (12%)	4	18
28	BE	164/166 (99%)	142 (87%)	22 (13%)	3	13
28	DE	164/166 (99%)	144 (88%)	20 (12%)	4	16
29	BF	160/166 (96%)	143 (89%)	17 (11%)	5	21
29	DF	159/166 (96%)	145 (91%)	14 (9%)	8	30
30	BG	143/156 (92%)	123 (86%)	20 (14%)	3	12
30	DG	142/156 (91%)	116 (82%)	26 (18%)	1	6
31	BH	144/148 (97%)	129 (90%)	15 (10%)	5	22
31	DH	144/148 (97%)	131 (91%)	13 (9%)	8	29
32	BI	110/124 (89%)	82 (74%)	28 (26%)	0	1
32	DI	104/124 (84%)	86 (83%)	18 (17%)	1	7
33	BN	118/119 (99%)	103 (87%)	15 (13%)	3	15
33	DN	118/119 (99%)	102 (86%)	16 (14%)	3	13
34	BO	100/100 (100%)	94 (94%)	6 (6%)	16	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	DO	100/100 (100%)	91 (91%)	9 (9%)	8	29
35	BP	115/116 (99%)	102 (89%)	13 (11%)	4	20
35	DP	115/116 (99%)	104 (90%)	11 (10%)	7	26
36	BQ	111/111 (100%)	94 (85%)	17 (15%)	2	10
36	DQ	111/111 (100%)	96 (86%)	15 (14%)	3	13
37	BR	101/101 (100%)	83 (82%)	18 (18%)	1	6
37	DR	101/101 (100%)	85 (84%)	16 (16%)	2	9
38	BS	87/88 (99%)	77 (88%)	10 (12%)	4	19
38	DS	85/88 (97%)	70 (82%)	15 (18%)	1	7
39	BT	115/127 (91%)	104 (90%)	11 (10%)	7	26
39	DT	113/127 (89%)	105 (93%)	8 (7%)	12	39
40	BU	93/94 (99%)	83 (89%)	10 (11%)	5	21
40	DU	93/94 (99%)	82 (88%)	11 (12%)	4	17
41	BV	80/82 (98%)	69 (86%)	11 (14%)	3	13
41	DV	80/82 (98%)	71 (89%)	9 (11%)	4	20
42	BW	90/92 (98%)	79 (88%)	11 (12%)	4	16
42	DW	90/92 (98%)	80 (89%)	10 (11%)	5	20
43	BX	77/78 (99%)	73 (95%)	4 (5%)	19	48
43	DX	77/78 (99%)	74 (96%)	3 (4%)	27	58
44	BY	85/91 (93%)	79 (93%)	6 (7%)	12	39
44	DY	85/91 (93%)	79 (93%)	6 (7%)	12	39
45	BZ	145/179 (81%)	121 (83%)	24 (17%)	2	8
45	DZ	145/179 (81%)	126 (87%)	19 (13%)	3	14
46	B0	65/67 (97%)	61 (94%)	4 (6%)	15	43
46	D0	65/67 (97%)	59 (91%)	6 (9%)	7	28
47	B1	80/83 (96%)	72 (90%)	8 (10%)	6	24
47	D1	80/83 (96%)	73 (91%)	7 (9%)	8	30
48	B2	65/67 (97%)	56 (86%)	9 (14%)	3	13
48	D2	65/67 (97%)	57 (88%)	8 (12%)	4	16
49	B3	51/52 (98%)	44 (86%)	7 (14%)	3	13
49	D3	50/52 (96%)	43 (86%)	7 (14%)	3	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	B4	59/63 (94%)	48 (81%)	11 (19%)	1	6
50	D4	53/63 (84%)	45 (85%)	8 (15%)	2	10
51	B5	50/52 (96%)	45 (90%)	5 (10%)	6	24
51	D5	50/52 (96%)	45 (90%)	5 (10%)	6	24
52	B6	51/52 (98%)	45 (88%)	6 (12%)	4	17
52	D6	50/52 (96%)	46 (92%)	4 (8%)	10	34
53	B7	41/42 (98%)	37 (90%)	4 (10%)	6	25
53	D7	41/42 (98%)	39 (95%)	2 (5%)	21	51
54	B8	53/55 (96%)	49 (92%)	4 (8%)	11	36
54	D8	54/55 (98%)	50 (93%)	4 (7%)	11	36
55	B9	34/34 (100%)	33 (97%)	1 (3%)	37	65
55	D9	34/34 (100%)	33 (97%)	1 (3%)	37	65
All	All	9325/10072 (93%)	8209 (88%)	1116 (12%)	4	16

5 of 1116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	DN	87	LEU
36	DQ	7	MET
33	DN	85	ILE
44	DY	11	ASP
35	BP	98	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 113 such sidechains are listed below:

Mol	Chain	Res	Type
49	B3	32	GLN
46	D0	3	HIS
4	CD	125	HIS
44	DY	43	ASN
31	DH	158	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1495/1522 (98%)	393 (26%)	25 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	CA	1502/1522 (98%)	388 (25%)	31 (2%)
22	AV	4/24 (16%)	1 (25%)	0
22	CV	4/24 (16%)	1 (25%)	0
23	AX	75/77 (97%)	16 (21%)	0
23	CX	75/77 (97%)	16 (21%)	0
25	BA	2722/2915 (93%)	508 (18%)	40 (1%)
25	DA	2704/2915 (92%)	535 (19%)	37 (1%)
26	BB	119/122 (97%)	18 (15%)	0
26	DB	119/122 (97%)	24 (20%)	1 (0%)
All	All	8819/9320 (94%)	1900 (21%)	134 (1%)

5 of 1900 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	9	G
1	AA	15	G
1	AA	22	G
1	AA	32	A

5 of 134 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	DA	1420	U
25	DA	1558	A
25	DA	2689	U
25	BA	1507	A
25	BA	1466	U

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	AW	9	24	6,7,8	0.45	0	6,8,10	1.08	1 (16%)
24	004	CW	3	24	9,10,11	1.34	2 (22%)	9,12,14	1.05	0
24	2R3	AW	8	24	12,14,15	0.82	0	16,18,20	1.74	5 (31%)
24	2QZ	CW	1	24	7,8,9	0.63	0	7,10,12	3.86	1 (14%)
24	2R3	CW	8	24	12,14,15	0.68	0	16,18,20	1.65	4 (25%)
24	004	AW	3	24	9,10,11	1.11	1 (11%)	9,12,14	1.54	3 (33%)
24	2R1	AW	6	24	10,10,11	2.21	3 (30%)	8,13,15	4.70	3 (37%)
24	2QZ	AW	1	24	7,8,9	0.40	0	7,10,12	4.39	1 (14%)
24	MVA	CW	9	24	6,7,8	0.98	1 (16%)	6,8,10	1.63	2 (33%)
24	MVA	CW	5	24	6,7,8	0.70	0	6,8,10	1.55	1 (16%)
24	2QY	CW	10	24	12,13,14	2.05	2 (16%)	14,16,18	3.33	3 (21%)
24	2R1	CW	6	24	10,10,11	1.94	2 (20%)	8,13,15	3.97	3 (37%)
24	2QY	AW	10	24	12,13,14	1.82	2 (16%)	14,16,18	3.99	5 (35%)
24	MVA	AW	5	24	6,7,8	0.38	0	6,8,10	0.96	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	AW	9	24	-	4/6/8/10	-
24	004	CW	3	24	-	0/4/6/8	0/1/1/1
24	2R3	AW	8	24	-	4/11/12/14	0/1/1/1
24	2QZ	CW	1	24	-	1/8/10/12	-
24	2R3	CW	8	24	-	7/11/12/14	0/1/1/1
24	004	AW	3	24	-	0/4/6/8	0/1/1/1
24	2R1	AW	6	24	-	1/2/14/16	0/1/1/1
24	2QZ	AW	1	24	-	3/8/10/12	-
24	MVA	CW	9	24	-	5/6/8/10	-
24	MVA	CW	5	24	-	5/6/8/10	-
24	2QY	CW	10	24	-	2/5/8/10	0/1/1/1
24	2R1	CW	6	24	-	0/2/14/16	0/1/1/1
24	2QY	AW	10	24	-	3/5/8/10	0/1/1/1
24	MVA	AW	5	24	-	3/6/8/10	-

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	5.98	1.53	1.43
24	AW	10	2QY	C-CA	5.42	1.52	1.43
24	AW	6	2R1	OD1-CG1	4.56	1.55	1.42
24	CW	6	2R1	CA-N	4.04	1.46	1.36
24	AW	6	2R1	CA-N	3.71	1.45	1.36

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AW	6	2R1	OD2-CG2-CB	-12.41	88.98	111.99
24	AW	1	2QZ	OG1-CB-CG2	11.13	142.97	109.68
24	AW	10	2QY	CN-N-CA	-10.64	107.83	123.98
24	CW	6	2R1	OD2-CG2-CB	-9.99	93.46	111.99
24	CW	10	2QY	CN-N-CA	-9.73	109.22	123.98

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AW	1	2QZ	N-CA-CB-OG1
24	AW	1	2QZ	C-CA-CB-OG1
24	AW	5	MVA	CB-CA-N-CN
24	AW	5	MVA	C-CA-CB-CG1
24	AW	5	MVA	C-CA-CB-CG2

There are no ring outliers.

13 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AW	9	MVA	3	0
24	CW	3	004	1	0
24	AW	8	2R3	1	0
24	CW	1	2QZ	2	0
24	CW	8	2R3	2	0
24	AW	3	004	1	0
24	AW	6	2R1	1	0
24	AW	1	2QZ	2	0
24	CW	9	MVA	6	0
24	CW	5	MVA	2	0
24	CW	10	2QY	9	0
24	CW	6	2R1	1	0
24	AW	10	2QY	5	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	$\# Z > 2$
59	FME	CX	101	23	8,9,10	0.99	0	8,9,11	1.45	3 (37%)
57	SF4	AD	501	4	0,12,12	-	-	-		
59	FME	AX	101	23	8,9,10	0.87	0	8,9,11	1.63	2 (25%)
57	SF4	CD	501	4	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	SF4	AD	501	4	-	-	0/6/5/5
59	FME	AX	101	23	-	3/7/9/11	-
59	FME	CX	101	23	-	3/7/9/11	-
57	SF4	CD	501	4	-	-	0/6/5/5

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	AX	101	FME	CA-N-CN	-2.85	118.44	122.82
59	AX	101	FME	CB-CA-N	2.41	114.90	110.52
59	CX	101	FME	CA-N-CN	-2.17	119.49	122.82
59	CX	101	FME	CB-CA-N	2.17	114.47	110.52
59	CX	101	FME	C-CA-N	2.08	113.52	109.50

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	CX	101	FME	2	0
57	AD	501	SF4	1	0
57	CD	501	SF4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1498/1522 (98%)	-0.15	15 (1%) 79 64	36, 80, 103, 123	0
1	CA	1503/1522 (98%)	-0.11	19 (1%) 74 58	38, 80, 103, 122	0
2	AB	231/256 (90%)	0.24	6 (2%) 57 38	71, 88, 98, 107	0
2	CB	231/256 (90%)	0.35	4 (1%) 69 50	71, 89, 99, 108	0
3	AC	206/239 (86%)	0.20	4 (1%) 66 47	74, 87, 96, 108	0
3	CC	206/239 (86%)	0.42	7 (3%) 48 28	75, 89, 98, 106	0
4	AD	208/209 (99%)	0.36	6 (2%) 54 34	62, 80, 92, 99	0
4	CD	208/209 (99%)	0.18	1 (0%) 87 75	61, 79, 92, 99	0
5	AE	148/162 (91%)	-0.13	2 (1%) 73 56	53, 73, 83, 96	0
5	CE	148/162 (91%)	-0.01	1 (0%) 84 70	54, 74, 85, 98	0
6	AF	100/101 (99%)	0.01	0 100 100	60, 78, 89, 92	0
6	CF	100/101 (99%)	0.02	1 (1%) 79 64	62, 79, 89, 94	0
7	AG	155/156 (99%)	0.05	2 (1%) 74 58	74, 85, 97, 104	0
7	CG	155/156 (99%)	0.18	5 (3%) 50 31	76, 86, 99, 105	0
8	AH	137/138 (99%)	0.01	1 (0%) 84 70	60, 75, 83, 90	0
8	CH	137/138 (99%)	0.02	0 100 100	61, 76, 83, 90	0
9	AI	127/128 (99%)	0.63	8 (6%) 27 16	70, 92, 99, 103	0
9	CI	127/128 (99%)	1.13	23 (18%) 4 2	69, 93, 100, 105	0
10	AJ	97/105 (92%)	0.66	3 (3%) 51 32	71, 93, 101, 106	0
10	CJ	96/105 (91%)	1.05	13 (13%) 8 5	75, 95, 102, 107	0
11	AK	114/129 (88%)	-0.22	1 (0%) 81 66	53, 74, 88, 93	0
11	CK	114/129 (88%)	-0.14	0 100 100	54, 76, 88, 93	0
12	AL	122/132 (92%)	0.12	4 (3%) 49 30	56, 68, 80, 86	0
12	CL	122/132 (92%)	0.05	1 (0%) 82 68	55, 68, 79, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	123/126 (97%)	0.13	3 (2%) 59 41	67, 83, 95, 104	0
13	CM	122/126 (96%)	0.68	6 (4%) 36 21	77, 91, 101, 105	0
14	AN	60/61 (98%)	0.61	3 (5%) 35 21	74, 85, 95, 97	0
14	CN	60/61 (98%)	1.04	7 (11%) 10 7	77, 88, 95, 100	0
15	AO	88/89 (98%)	-0.11	0 100 100	59, 73, 87, 94	0
15	CO	88/89 (98%)	-0.02	1 (1%) 77 61	58, 73, 87, 95	0
16	AP	82/88 (93%)	0.42	2 (2%) 59 41	66, 77, 88, 95	0
16	CP	82/88 (93%)	0.39	2 (2%) 59 41	66, 76, 88, 93	0
17	AQ	99/105 (94%)	0.12	1 (1%) 79 64	59, 73, 84, 87	0
17	CQ	99/105 (94%)	0.02	1 (1%) 79 64	60, 73, 84, 85	0
18	AR	68/88 (77%)	-0.13	0 100 100	66, 76, 86, 90	0
18	CR	68/88 (77%)	0.06	1 (1%) 71 54	67, 77, 87, 89	0
19	AS	83/93 (89%)	0.55	5 (6%) 29 17	79, 91, 100, 105	0
19	CS	83/93 (89%)	0.88	11 (13%) 8 5	82, 92, 102, 106	0
20	AT	96/106 (90%)	0.39	8 (8%) 19 10	62, 75, 88, 91	0
20	CT	96/106 (90%)	0.19	2 (2%) 63 44	62, 75, 86, 94	0
21	AU	23/27 (85%)	1.12	1 (4%) 40 24	76, 87, 90, 91	0
21	CU	23/27 (85%)	1.23	3 (13%) 9 5	77, 87, 91, 92	0
22	AV	7/24 (29%)	0.13	0 100 100	61, 73, 97, 100	0
22	CV	6/24 (25%)	0.09	0 100 100	64, 75, 94, 103	0
23	AX	76/77 (98%)	-0.54	0 100 100	48, 79, 96, 101	0
23	CX	76/77 (98%)	-0.32	0 100 100	47, 81, 98, 101	0
24	AW	3/10 (30%)	0.64	0 100 100	78, 78, 93, 96	0
24	CW	3/10 (30%)	0.53	1 (33%) 1 0	67, 67, 87, 96	0
25	BA	2731/2915 (93%)	-0.71	8 (0%) 90 81	24, 44, 86, 114	0
25	DA	2714/2915 (93%)	-0.73	7 (0%) 90 81	27, 48, 87, 118	0
26	BB	120/122 (98%)	-0.40	0 100 100	41, 68, 81, 96	0
26	DB	120/122 (98%)	0.02	0 100 100	47, 73, 86, 98	0
27	BD	275/276 (99%)	-0.56	0 100 100	24, 41, 62, 85	0
27	DD	275/276 (99%)	-0.48	0 100 100	25, 44, 63, 86	0
28	BE	204/206 (99%)	-0.54	0 100 100	22, 45, 68, 90	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DE	204/206 (99%)	-0.53	1 (0%) 87 75	24, 47, 70, 90	0
29	BF	203/210 (96%)	-0.25	1 (0%) 87 75	24, 52, 77, 97	0
29	DF	203/210 (96%)	-0.32	0 100 100	25, 56, 79, 96	0
30	BG	181/182 (99%)	0.03	1 (0%) 85 72	61, 76, 89, 100	0
30	DG	181/182 (99%)	0.35	3 (1%) 69 50	65, 79, 91, 100	0
31	BH	174/180 (96%)	-0.03	1 (0%) 85 72	49, 67, 81, 85	0
31	DH	174/180 (96%)	0.22	2 (1%) 77 61	54, 72, 85, 89	0
32	BI	146/148 (98%)	-0.07	0 100 100	49, 77, 88, 94	0
32	DI	146/148 (98%)	-0.02	0 100 100	49, 78, 88, 94	0
33	BN	140/140 (100%)	-0.37	1 (0%) 84 70	33, 48, 71, 78	0
33	DN	140/140 (100%)	-0.33	1 (0%) 84 70	35, 52, 73, 81	0
34	BO	122/122 (100%)	-0.68	0 100 100	23, 40, 61, 76	0
34	DO	122/122 (100%)	-0.51	0 100 100	37, 53, 71, 80	0
35	BP	149/150 (99%)	-0.27	1 (0%) 84 70	25, 54, 77, 83	0
35	DP	149/150 (99%)	-0.20	0 100 100	27, 57, 81, 87	0
36	BQ	141/141 (100%)	-0.22	2 (1%) 73 56	36, 52, 68, 79	0
36	DQ	141/141 (100%)	-0.22	1 (0%) 84 70	38, 55, 71, 81	0
37	BR	118/118 (100%)	-0.68	0 100 100	20, 35, 52, 64	0
37	DR	118/118 (100%)	-0.39	0 100 100	36, 52, 68, 84	0
38	BS	110/112 (98%)	-0.57	0 100 100	35, 54, 71, 85	0
38	DS	110/112 (98%)	0.39	5 (4%) 39 23	65, 81, 92, 95	0
39	BT	131/146 (89%)	-0.50	0 100 100	31, 45, 75, 92	0
39	DT	131/146 (89%)	-0.32	0 100 100	45, 59, 80, 90	0
40	BU	116/118 (98%)	-0.81	0 100 100	21, 31, 52, 63	0
40	DU	116/118 (98%)	-0.25	0 100 100	36, 61, 78, 92	0
41	BV	101/101 (100%)	-0.43	0 100 100	27, 53, 73, 80	0
41	DV	101/101 (100%)	-0.40	0 100 100	29, 58, 78, 80	0
42	BW	112/113 (99%)	-0.63	0 100 100	27, 38, 62, 92	0
42	DW	112/113 (99%)	-0.55	0 100 100	30, 42, 64, 94	0
43	BX	95/96 (98%)	-0.29	2 (2%) 63 44	29, 47, 72, 81	0
43	DX	95/96 (98%)	-0.17	1 (1%) 77 61	33, 51, 73, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BY	107/110 (97%)	-0.04	2 (1%) 66 47	39, 61, 80, 89	0
44	DY	107/110 (97%)	0.05	1 (0%) 81 66	43, 65, 82, 92	0
45	BZ	171/206 (83%)	-0.03	3 (1%) 67 49	53, 71, 85, 96	0
45	DZ	174/206 (84%)	0.12	1 (0%) 85 72	58, 74, 87, 95	0
46	B0	83/85 (97%)	-0.25	7 (8%) 18 10	25, 39, 80, 108	0
46	D0	83/85 (97%)	0.25	6 (7%) 23 13	42, 66, 86, 104	0
47	B1	97/98 (98%)	-0.51	0 100 100	27, 44, 74, 83	0
47	D1	97/98 (98%)	-0.24	1 (1%) 79 64	35, 58, 79, 86	0
48	B2	70/72 (97%)	-0.40	1 (1%) 73 56	35, 48, 64, 90	0
48	D2	70/72 (97%)	-0.12	0 100 100	59, 74, 83, 92	0
49	B3	59/60 (98%)	-0.60	0 100 100	24, 38, 63, 85	0
49	D3	59/60 (98%)	-0.33	0 100 100	45, 62, 80, 90	0
50	B4	69/71 (97%)	0.04	0 100 100	60, 85, 103, 105	0
50	D4	69/71 (97%)	0.55	3 (4%) 40 24	82, 96, 106, 112	0
51	B5	59/60 (98%)	-0.82	0 100 100	14, 36, 59, 74	0
51	D5	59/60 (98%)	-0.51	0 100 100	31, 50, 72, 82	0
52	B6	53/54 (98%)	-0.59	0 100 100	43, 53, 68, 75	0
52	D6	53/54 (98%)	-0.30	0 100 100	45, 56, 69, 73	0
53	B7	48/49 (97%)	-0.47	0 100 100	24, 32, 62, 84	0
53	D7	48/49 (97%)	-0.38	1 (2%) 63 44	26, 35, 63, 86	0
54	B8	64/65 (98%)	-0.42	0 100 100	31, 42, 51, 64	0
54	D8	64/65 (98%)	-0.29	0 100 100	34, 46, 56, 66	0
55	B9	37/37 (100%)	-0.13	1 (2%) 56 36	43, 53, 71, 77	0
55	D9	37/37 (100%)	0.16	1 (2%) 56 36	46, 58, 73, 78	0
All	All	20462/21468 (95%)	-0.24	251 (1%) 76 60	14, 65, 95, 123	0

The worst 5 of 251 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	CM	124	PRO	7.0
13	CM	123	ALA	5.9
14	CN	2	ALA	5.7
13	AM	123	ALA	5.6
9	CI	105	ASP	5.5

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	0.73	0.14	68,82,98,104	0
24	004	AW	3	10/11	0.76	0.17	71,89,99,106	0
24	2R1	CW	6	10/11	0.76	0.12	79,86,90,94	0
24	MVA	AW	5	8/9	0.81	0.15	66,87,90,90	0
24	2QY	CW	10	13/14	0.87	0.11	55,69,84,94	0
24	2R3	AW	8	14/15	0.89	0.09	54,79,87,90	0
24	004	CW	3	10/11	0.90	0.10	60,76,84,86	0
24	MVA	CW	5	8/9	0.90	0.08	51,78,86,88	0
24	MVA	CW	9	8/9	0.91	0.14	61,72,80,84	0
24	MVA	AW	9	8/9	0.91	0.14	65,78,87,91	0
24	2R3	CW	8	14/15	0.93	0.07	47,70,74,79	0
24	2QZ	CW	1	9/10	0.94	0.12	57,72,81,93	0
24	2QY	AW	10	13/14	0.95	0.06	55,67,75,79	0
24	2QZ	AW	1	9/10	0.95	0.10	58,64,81,82	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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	BZ	3001	1/1	0.39	0.27	61,61,61,61	0
56	MG	B4	3001	1/1	0.47	0.20	100,100,100,100	0
56	MG	CA	3025	1/1	0.49	0.25	94,94,94,94	0
56	MG	CA	3139	1/1	0.50	0.21	75,75,75,75	0
56	MG	DB	3001	1/1	0.53	0.17	68,68,68,68	0
56	MG	CA	3114	1/1	0.54	0.19	82,82,82,82	0
56	MG	CA	3042	1/1	0.56	0.35	85,85,85,85	0
56	MG	AA	3129	1/1	0.58	0.27	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3087	1/1	0.59	0.19	72,72,72,72	0
56	MG	BA	3579	1/1	0.60	0.23	63,63,63,63	0
56	MG	AA	3093	1/1	0.61	0.38	88,88,88,88	0
56	MG	AA	3132	1/1	0.64	0.33	76,76,76,76	0
56	MG	AA	3120	1/1	0.64	0.35	71,71,71,71	0
56	MG	CA	3110	1/1	0.64	0.22	97,97,97,97	0
56	MG	CA	3067	1/1	0.65	0.26	80,80,80,80	0
56	MG	AA	3164	1/1	0.66	0.19	69,69,69,69	0
56	MG	CA	3127	1/1	0.66	0.22	79,79,79,79	0
56	MG	CA	3109	1/1	0.67	0.17	83,83,83,83	0
56	MG	AA	3147	1/1	0.67	0.17	61,61,61,61	0
56	MG	AA	3061	1/1	0.67	0.14	82,82,82,82	0
56	MG	BA	3622	1/1	0.68	0.23	77,77,77,77	0
56	MG	CA	3147	1/1	0.68	0.18	66,66,66,66	0
56	MG	AA	3030	1/1	0.68	0.42	69,69,69,69	0
56	MG	AA	3067	1/1	0.69	0.34	87,87,87,87	0
56	MG	DA	3093	1/1	0.69	0.11	53,53,53,53	0
56	MG	DA	3460	1/1	0.69	0.14	50,50,50,50	0
56	MG	DA	3615	1/1	0.69	0.16	60,60,60,60	0
56	MG	BA	3140	1/1	0.69	0.24	64,64,64,64	0
56	MG	BA	3658	1/1	0.70	0.18	79,79,79,79	0
56	MG	BA	3247	1/1	0.70	0.18	68,68,68,68	0
56	MG	BA	3088	1/1	0.70	0.16	56,56,56,56	0
56	MG	AA	3013	1/1	0.70	0.11	78,78,78,78	0
56	MG	DA	3284	1/1	0.71	0.13	68,68,68,68	0
56	MG	CA	3081	1/1	0.71	0.15	72,72,72,72	0
56	MG	BA	3023	1/1	0.72	0.21	66,66,66,66	0
56	MG	BA	3353	1/1	0.72	0.15	57,57,57,57	0
56	MG	CA	3070	1/1	0.72	0.16	55,55,55,55	0
56	MG	AA	3084	1/1	0.72	0.42	78,78,78,78	0
56	MG	AA	3180	1/1	0.72	0.22	66,66,66,66	0
56	MG	DA	3162	1/1	0.73	0.29	71,71,71,71	0
56	MG	DA	3256	1/1	0.73	0.16	63,63,63,63	0
56	MG	DA	3638	1/1	0.73	0.23	62,62,62,62	0
56	MG	CA	3030	1/1	0.73	0.32	73,73,73,73	0
56	MG	CQ	201	1/1	0.75	0.14	56,56,56,56	0
56	MG	DA	3062	1/1	0.75	0.17	55,55,55,55	0
56	MG	CA	3038	1/1	0.75	0.19	70,70,70,70	0
56	MG	AA	3218	1/1	0.75	0.35	65,65,65,65	0
56	MG	CA	3053	1/1	0.75	0.46	73,73,73,73	0
56	MG	CA	3125	1/1	0.75	0.13	72,72,72,72	0
56	MG	DA	3438	1/1	0.75	0.20	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3044	1/1	0.75	0.17	66,66,66,66	0
56	MG	DA	3464	1/1	0.75	0.22	50,50,50,50	0
56	MG	DA	3492	1/1	0.75	0.15	68,68,68,68	0
56	MG	DA	3553	1/1	0.75	0.15	70,70,70,70	0
56	MG	CA	3135	1/1	0.75	0.27	76,76,76,76	0
56	MG	DA	3635	1/1	0.75	0.20	58,58,58,58	0
56	MG	AA	3131	1/1	0.75	0.24	56,56,56,56	0
56	MG	BA	3669	1/1	0.75	0.17	75,75,75,75	0
56	MG	AA	3022	1/1	0.76	0.18	48,48,48,48	0
56	MG	BA	3370	1/1	0.76	0.11	54,54,54,54	0
56	MG	DA	3427	1/1	0.76	0.20	60,60,60,60	0
56	MG	BA	3495	1/1	0.76	0.16	84,84,84,84	0
56	MG	DA	3134	1/1	0.76	0.15	46,46,46,46	0
56	MG	CA	3003	1/1	0.76	0.14	66,66,66,66	0
59	FME	CX	101	10/11	0.76	0.32	71,82,97,105	0
56	MG	BB	3014	1/1	0.77	0.19	69,69,69,69	0
56	MG	DA	3482	1/1	0.77	0.14	55,55,55,55	0
56	MG	BN	3002	1/1	0.77	0.11	56,56,56,56	0
56	MG	BA	3297	1/1	0.77	0.36	53,53,53,53	0
56	MG	DA	3598	1/1	0.77	0.14	66,66,66,66	0
56	MG	CA	3161	1/1	0.77	0.12	54,54,54,54	0
56	MG	DA	3401	1/1	0.77	0.26	58,58,58,58	0
56	MG	BA	3157	1/1	0.77	0.19	63,63,63,63	0
56	MG	BA	3354	1/1	0.77	0.12	74,74,74,74	0
56	MG	BB	3005	1/1	0.77	0.24	61,61,61,61	0
56	MG	DA	3124	1/1	0.78	0.14	67,67,67,67	0
56	MG	BA	3288	1/1	0.78	0.26	61,61,61,61	0
56	MG	CA	3041	1/1	0.78	0.30	75,75,75,75	0
56	MG	DA	3195	1/1	0.78	0.20	50,50,50,50	0
56	MG	DA	3503	1/1	0.78	0.19	71,71,71,71	0
56	MG	DA	3228	1/1	0.78	0.11	45,45,45,45	0
56	MG	BA	3158	1/1	0.78	0.37	64,64,64,64	0
56	MG	DA	3001	1/1	0.78	0.30	78,78,78,78	0
56	MG	CA	3047	1/1	0.78	0.18	63,63,63,63	0
56	MG	BA	3089	1/1	0.78	0.13	61,61,61,61	0
56	MG	DA	3122	1/1	0.78	0.20	62,62,62,62	0
56	MG	DB	3011	1/1	0.78	0.20	55,55,55,55	0
56	MG	DA	3456	1/1	0.78	0.18	47,47,47,47	0
56	MG	AA	3071	1/1	0.79	0.28	60,60,60,60	0
56	MG	BA	3183	1/1	0.79	0.26	48,48,48,48	0
56	MG	DA	3410	1/1	0.79	0.30	69,69,69,69	0
56	MG	BA	3215	1/1	0.79	0.20	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3153	1/1	0.79	0.14	83,83,83,83	0
56	MG	AA	3200	1/1	0.79	0.21	68,68,68,68	0
56	MG	CA	3048	1/1	0.79	0.28	62,62,62,62	0
56	MG	BA	3718	1/1	0.79	0.14	57,57,57,57	0
56	MG	AA	3046	1/1	0.79	0.24	73,73,73,73	0
56	MG	DA	3484	1/1	0.79	0.12	51,51,51,51	0
56	MG	AA	3085	1/1	0.79	0.23	69,69,69,69	0
56	MG	CA	3073	1/1	0.79	0.21	55,55,55,55	0
56	MG	BA	3331	1/1	0.79	0.18	47,47,47,47	0
56	MG	AA	3021	1/1	0.79	0.14	76,76,76,76	0
56	MG	AA	3019	1/1	0.79	0.11	74,74,74,74	0
56	MG	DA	3623	1/1	0.79	0.16	53,53,53,53	0
56	MG	DA	3624	1/1	0.79	0.23	51,51,51,51	0
56	MG	DA	3185	1/1	0.79	0.21	52,52,52,52	0
56	MG	AA	3162	1/1	0.79	0.21	74,74,74,74	0
56	MG	BA	3462	1/1	0.79	0.15	52,52,52,52	0
56	MG	DA	3240	1/1	0.79	0.14	51,51,51,51	0
56	MG	AA	3109	1/1	0.79	0.19	65,65,65,65	0
56	MG	DA	3099	1/1	0.80	0.19	44,44,44,44	0
56	MG	DA	3314	1/1	0.80	0.19	64,64,64,64	0
56	MG	DA	3526	1/1	0.80	0.13	54,54,54,54	0
56	MG	DA	3361	1/1	0.80	0.12	61,61,61,61	0
56	MG	DA	3563	1/1	0.80	0.15	64,64,64,64	0
56	MG	BA	3189	1/1	0.80	0.14	54,54,54,54	0
56	MG	DA	3613	1/1	0.80	0.10	54,54,54,54	0
56	MG	BA	3094	1/1	0.80	0.32	61,61,61,61	0
56	MG	BA	3136	1/1	0.80	0.15	58,58,58,58	0
56	MG	AA	3039	1/1	0.80	0.15	60,60,60,60	0
56	MG	BA	3067	1/1	0.80	0.19	53,53,53,53	0
56	MG	AA	3007	1/1	0.80	0.22	82,82,82,82	0
56	MG	BA	3168	1/1	0.80	0.18	42,42,42,42	0
56	MG	DB	3010	1/1	0.80	0.20	73,73,73,73	0
56	MG	DA	3084	1/1	0.80	0.17	70,70,70,70	0
56	MG	DF	302	1/1	0.80	0.10	43,43,43,43	0
56	MG	AA	3076	1/1	0.80	0.26	66,66,66,66	0
56	MG	AA	3128	1/1	0.81	0.18	68,68,68,68	0
56	MG	DA	3491	1/1	0.81	0.10	56,56,56,56	0
56	MG	BA	3289	1/1	0.81	0.28	60,60,60,60	0
56	MG	DA	3248	1/1	0.81	0.24	51,51,51,51	0
56	MG	DA	3515	1/1	0.81	0.12	48,48,48,48	0
56	MG	DA	3061	1/1	0.81	0.26	52,52,52,52	0
56	MG	DA	3279	1/1	0.81	0.19	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3032	1/1	0.81	0.18	42,42,42,42	0
56	MG	AA	3206	1/1	0.81	0.12	70,70,70,70	0
56	MG	DA	3609	1/1	0.81	0.24	64,64,64,64	0
56	MG	DA	3340	1/1	0.81	0.09	47,47,47,47	0
56	MG	AA	3009	1/1	0.81	0.23	79,79,79,79	0
56	MG	DA	3621	1/1	0.81	0.10	54,54,54,54	0
56	MG	AA	3113	1/1	0.81	0.21	68,68,68,68	0
56	MG	AA	3094	1/1	0.81	0.12	68,68,68,68	0
56	MG	BA	3193	1/1	0.81	0.18	52,52,52,52	0
56	MG	BA	3144	1/1	0.81	0.30	74,74,74,74	0
56	MG	DA	3161	1/1	0.81	0.17	60,60,60,60	0
56	MG	CA	3057	1/1	0.81	0.20	49,49,49,49	0
56	MG	BA	3234	1/1	0.81	0.19	55,55,55,55	0
56	MG	DA	3481	1/1	0.81	0.10	47,47,47,47	0
56	MG	DG	3001	1/1	0.81	0.13	63,63,63,63	0
56	MG	BA	3156	1/1	0.81	0.32	56,56,56,56	0
60	K	DA	3231	1/1	0.81	0.24	96,96,96,96	0
56	MG	BA	3712	1/1	0.82	0.16	58,58,58,58	0
56	MG	AA	3024	1/1	0.82	0.14	53,53,53,53	0
56	MG	DA	3267	1/1	0.82	0.13	61,61,61,61	0
56	MG	CA	3146	1/1	0.82	0.15	69,69,69,69	0
56	MG	BA	3099	1/1	0.82	0.20	44,44,44,44	0
56	MG	DA	3487	1/1	0.82	0.19	57,57,57,57	0
56	MG	BA	3507	1/1	0.82	0.24	68,68,68,68	0
56	MG	CA	3157	1/1	0.82	0.12	54,54,54,54	0
56	MG	AA	3112	1/1	0.82	0.23	51,51,51,51	0
56	MG	DA	3511	1/1	0.82	0.16	65,65,65,65	0
56	MG	CE	3001	1/1	0.82	0.33	68,68,68,68	0
56	MG	AA	3212	1/1	0.82	0.11	79,79,79,79	0
56	MG	BA	3180	1/1	0.82	0.42	43,43,43,43	0
56	MG	AA	3072	1/1	0.82	0.24	79,79,79,79	0
56	MG	BA	3683	1/1	0.82	0.23	60,60,60,60	0
56	MG	BA	3263	1/1	0.83	0.28	79,79,79,79	0
56	MG	CA	3035	1/1	0.83	0.19	52,52,52,52	0
56	MG	BA	3027	1/1	0.83	0.14	45,45,45,45	0
56	MG	BA	3029	1/1	0.83	0.35	53,53,53,53	0
56	MG	DA	3499	1/1	0.83	0.12	46,46,46,46	0
56	MG	DA	3500	1/1	0.83	0.13	50,50,50,50	0
56	MG	BA	3040	1/1	0.83	0.27	51,51,51,51	0
56	MG	DA	3510	1/1	0.83	0.16	63,63,63,63	0
56	MG	DA	3212	1/1	0.83	0.11	48,48,48,48	0
56	MG	BA	3693	1/1	0.83	0.16	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3118	1/1	0.83	0.33	52,52,52,52	0
56	MG	CA	3159	1/1	0.83	0.32	91,91,91,91	0
56	MG	AA	3088	1/1	0.83	0.46	63,63,63,63	0
56	MG	CA	3170	1/1	0.83	0.22	50,50,50,50	0
56	MG	AA	3023	1/1	0.83	0.25	65,65,65,65	0
56	MG	AA	3065	1/1	0.83	0.24	60,60,60,60	0
56	MG	AA	3059	1/1	0.83	0.28	54,54,54,54	0
56	MG	DA	3003	1/1	0.83	0.12	56,56,56,56	0
56	MG	DA	3060	1/1	0.83	0.16	55,55,55,55	0
56	MG	AA	3069	1/1	0.83	0.10	84,84,84,84	0
56	MG	B2	101	1/1	0.83	0.14	40,40,40,40	0
56	MG	CA	3086	1/1	0.83	0.27	80,80,80,80	0
56	MG	AA	3136	1/1	0.83	0.16	62,62,62,62	0
56	MG	AA	3060	1/1	0.83	0.38	60,60,60,60	0
56	MG	DA	3115	1/1	0.83	0.13	63,63,63,63	0
56	MG	BA	3611	1/1	0.83	0.13	52,52,52,52	0
56	MG	DA	3465	1/1	0.83	0.11	49,49,49,49	0
56	MG	DQ	205	1/1	0.83	0.17	55,55,55,55	0
56	MG	DW	202	1/1	0.83	0.15	58,58,58,58	0
59	FME	AX	101	10/11	0.83	0.22	48,75,97,113	0
56	MG	BA	3613	1/1	0.83	0.16	76,76,76,76	0
56	MG	DA	3131	1/1	0.83	0.09	54,54,54,54	0
56	MG	BA	3700	1/1	0.84	0.11	67,67,67,67	0
56	MG	AA	3047	1/1	0.84	0.16	61,61,61,61	0
56	MG	AA	3209	1/1	0.84	0.14	70,70,70,70	0
56	MG	BA	3739	1/1	0.84	0.22	50,50,50,50	0
56	MG	DA	3117	1/1	0.84	0.12	53,53,53,53	0
56	MG	BA	3372	1/1	0.84	0.14	38,38,38,38	0
56	MG	BA	3430	1/1	0.84	0.30	49,49,49,49	0
56	MG	AA	3045	1/1	0.84	0.30	61,61,61,61	0
56	MG	BW	205	1/1	0.84	0.21	41,41,41,41	0
56	MG	AA	3089	1/1	0.84	0.32	78,78,78,78	0
56	MG	B0	103	1/1	0.84	0.32	59,59,59,59	0
56	MG	DA	3170	1/1	0.84	0.19	57,57,57,57	0
56	MG	BA	3496	1/1	0.84	0.27	57,57,57,57	0
56	MG	AX	106	1/1	0.84	0.11	73,73,73,73	0
56	MG	DA	3545	1/1	0.84	0.18	75,75,75,75	0
56	MG	BA	3123	1/1	0.84	0.23	69,69,69,69	0
56	MG	DA	3223	1/1	0.84	0.31	66,66,66,66	0
56	MG	DA	3581	1/1	0.84	0.31	73,73,73,73	0
56	MG	DA	3224	1/1	0.84	0.17	47,47,47,47	0
56	MG	CA	3008	1/1	0.84	0.27	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3018	1/1	0.84	0.12	54,54,54,54	0
56	MG	BA	3580	1/1	0.84	0.14	58,58,58,58	0
56	MG	DA	3620	1/1	0.84	0.13	71,71,71,71	0
56	MG	CA	3158	1/1	0.84	0.15	76,76,76,76	0
56	MG	BA	3020	1/1	0.84	0.20	45,45,45,45	0
56	MG	AA	3090	1/1	0.84	0.17	68,68,68,68	0
56	MG	BA	3617	1/1	0.84	0.19	62,62,62,62	0
56	MG	AA	3017	1/1	0.84	0.24	55,55,55,55	0
56	MG	BA	3628	1/1	0.84	0.21	41,41,41,41	0
56	MG	BA	3645	1/1	0.84	0.13	56,56,56,56	0
56	MG	AA	3195	1/1	0.84	0.24	71,71,71,71	0
56	MG	DA	3402	1/1	0.84	0.13	61,61,61,61	0
56	MG	DA	3023	1/1	0.84	0.19	52,52,52,52	0
56	MG	DA	3054	1/1	0.84	0.21	51,51,51,51	0
56	MG	AA	3134	1/1	0.84	0.34	70,70,70,70	0
56	MG	BA	3061	1/1	0.84	0.28	51,51,51,51	0
56	MG	BA	3065	1/1	0.84	0.13	50,50,50,50	0
56	MG	DA	3071	1/1	0.84	0.22	46,46,46,46	0
56	MG	CA	3027	1/1	0.85	0.18	57,57,57,57	0
56	MG	BA	3402	1/1	0.85	0.18	71,71,71,71	0
56	MG	BA	3426	1/1	0.85	0.26	51,51,51,51	0
56	MG	DA	3169	1/1	0.85	0.25	57,57,57,57	0
56	MG	AA	3026	1/1	0.85	0.17	41,41,41,41	0
56	MG	DA	3494	1/1	0.85	0.14	78,78,78,78	0
56	MG	BA	3221	1/1	0.85	0.20	44,44,44,44	0
56	MG	BA	3482	1/1	0.85	0.12	72,72,72,72	0
56	MG	DA	3207	1/1	0.85	0.14	58,58,58,58	0
56	MG	AA	3102	1/1	0.85	0.19	64,64,64,64	0
56	MG	BA	3736	1/1	0.85	0.11	48,48,48,48	0
56	MG	AA	3051	1/1	0.85	0.14	73,73,73,73	0
56	MG	AX	103	1/1	0.85	0.14	66,66,66,66	0
56	MG	DA	3537	1/1	0.85	0.15	65,65,65,65	0
56	MG	DA	3238	1/1	0.85	0.07	61,61,61,61	0
56	MG	CX	103	1/1	0.85	0.16	60,60,60,60	0
56	MG	DA	3557	1/1	0.85	0.17	45,45,45,45	0
56	MG	BB	3009	1/1	0.85	0.13	48,48,48,48	0
56	MG	DA	3252	1/1	0.85	0.15	45,45,45,45	0
56	MG	DA	3590	1/1	0.85	0.19	80,80,80,80	0
56	MG	CA	3061	1/1	0.85	0.21	46,46,46,46	0
56	MG	DA	3265	1/1	0.85	0.15	51,51,51,51	0
56	MG	BA	3562	1/1	0.85	0.13	73,73,73,73	0
56	MG	AA	3006	1/1	0.85	0.12	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3071	1/1	0.85	0.15	63,63,63,63	0
56	MG	DA	3303	1/1	0.85	0.09	47,47,47,47	0
56	MG	AA	3189	1/1	0.85	0.11	77,77,77,77	0
56	MG	BA	3598	1/1	0.85	0.14	56,56,56,56	0
56	MG	DA	3632	1/1	0.85	0.13	71,71,71,71	0
56	MG	DA	3357	1/1	0.85	0.12	56,56,56,56	0
56	MG	DA	3069	1/1	0.85	0.10	51,51,51,51	0
56	MG	DA	3654	1/1	0.85	0.30	52,52,52,52	0
56	MG	AA	3068	1/1	0.85	0.15	66,66,66,66	0
56	MG	AA	3117	1/1	0.85	0.12	71,71,71,71	0
56	MG	DA	3092	1/1	0.85	0.27	39,39,39,39	0
56	MG	BA	3334	1/1	0.85	0.24	73,73,73,73	0
56	MG	BA	3103	1/1	0.85	0.17	53,53,53,53	0
56	MG	AA	3002	1/1	0.85	0.10	57,57,57,57	0
56	MG	BA	3135	1/1	0.85	0.18	42,42,42,42	0
56	MG	CA	3021	1/1	0.85	0.17	53,53,53,53	0
56	MG	BA	3205	1/1	0.85	0.10	40,40,40,40	0
60	K	BA	3300	1/1	0.85	0.20	100,100,100,100	0
56	MG	CA	3141	1/1	0.85	0.29	70,70,70,70	0
56	MG	DA	3458	1/1	0.86	0.12	71,71,71,71	0
56	MG	BA	3293	1/1	0.86	0.09	45,45,45,45	0
56	MG	CA	3119	1/1	0.86	0.16	64,64,64,64	0
56	MG	CA	3014	1/1	0.86	0.29	50,50,50,50	0
56	MG	BA	3196	1/1	0.86	0.34	56,56,56,56	0
56	MG	DA	3123	1/1	0.86	0.28	59,59,59,59	0
56	MG	BA	3309	1/1	0.86	0.12	46,46,46,46	0
56	MG	AA	3035	1/1	0.86	0.15	71,71,71,71	0
56	MG	BA	3543	1/1	0.86	0.17	52,52,52,52	0
56	MG	DA	3135	1/1	0.86	0.15	50,50,50,50	0
56	MG	CA	3142	1/1	0.86	0.09	59,59,59,59	0
56	MG	BA	3714	1/1	0.86	0.10	58,58,58,58	0
56	MG	DA	3164	1/1	0.86	0.15	48,48,48,48	0
56	MG	BA	3206	1/1	0.86	0.16	57,57,57,57	0
56	MG	AA	3096	1/1	0.86	0.18	44,44,44,44	0
56	MG	AA	3170	1/1	0.86	0.29	101,101,101,101	0
56	MG	BB	3003	1/1	0.86	0.14	43,43,43,43	0
56	MG	BA	3593	1/1	0.86	0.08	74,74,74,74	0
56	MG	DA	3527	1/1	0.86	0.09	46,46,46,46	0
56	MG	BA	3075	1/1	0.86	0.10	45,45,45,45	0
56	MG	CA	3164	1/1	0.86	0.17	49,49,49,49	0
56	MG	AN	103	1/1	0.86	0.18	60,60,60,60	0
56	MG	CA	3171	1/1	0.86	0.18	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3049	1/1	0.86	0.28	53,53,53,53	0
56	MG	DA	3564	1/1	0.86	0.18	61,61,61,61	0
56	MG	DA	3565	1/1	0.86	0.10	57,57,57,57	0
56	MG	BG	3004	1/1	0.86	0.14	62,62,62,62	0
56	MG	CT	3001	1/1	0.86	0.26	57,57,57,57	0
56	MG	CA	3054	1/1	0.86	0.20	48,48,48,48	0
56	MG	AA	3110	1/1	0.86	0.14	48,48,48,48	0
56	MG	BQ	203	1/1	0.86	0.14	58,58,58,58	0
56	MG	CA	3065	1/1	0.86	0.15	75,75,75,75	0
56	MG	DA	3024	1/1	0.86	0.20	65,65,65,65	0
56	MG	DA	3030	1/1	0.86	0.18	51,51,51,51	0
56	MG	DA	3293	1/1	0.86	0.14	53,53,53,53	0
56	MG	DA	3039	1/1	0.86	0.23	59,59,59,59	0
56	MG	BA	3405	1/1	0.86	0.10	34,34,34,34	0
56	MG	DA	3318	1/1	0.86	0.12	45,45,45,45	0
56	MG	DA	3322	1/1	0.86	0.15	55,55,55,55	0
56	MG	DA	3647	1/1	0.86	0.24	66,66,66,66	0
56	MG	BA	3276	1/1	0.86	0.19	40,40,40,40	0
56	MG	AX	105	1/1	0.86	0.10	56,56,56,56	0
56	MG	BA	3444	1/1	0.86	0.08	74,74,74,74	0
56	MG	BA	3146	1/1	0.86	0.15	52,52,52,52	0
56	MG	B7	103	1/1	0.86	0.17	48,48,48,48	0
56	MG	DA	3074	1/1	0.86	0.18	54,54,54,54	0
56	MG	DA	3415	1/1	0.86	0.12	56,56,56,56	0
56	MG	CA	3103	1/1	0.86	0.17	83,83,83,83	0
56	MG	BA	3661	1/1	0.86	0.11	68,68,68,68	0
56	MG	DA	3445	1/1	0.86	0.20	39,39,39,39	0
56	MG	DA	3454	1/1	0.86	0.10	55,55,55,55	0
56	MG	CA	3007	1/1	0.86	0.14	68,68,68,68	0
56	MG	DA	3154	1/1	0.87	0.36	45,45,45,45	0
56	MG	DA	3478	1/1	0.87	0.12	46,46,46,46	0
56	MG	AA	3033	1/1	0.87	0.25	64,64,64,64	0
56	MG	BA	3198	1/1	0.87	0.17	52,52,52,52	0
56	MG	BA	3134	1/1	0.87	0.21	47,47,47,47	0
56	MG	AA	3196	1/1	0.87	0.23	65,65,65,65	0
56	MG	BA	3619	1/1	0.87	0.21	40,40,40,40	0
56	MG	CA	3172	1/1	0.87	0.11	51,51,51,51	0
56	MG	DA	3186	1/1	0.87	0.15	53,53,53,53	0
56	MG	BV	203	1/1	0.87	0.30	46,46,46,46	0
56	MG	CA	3063	1/1	0.87	0.12	61,61,61,61	0
56	MG	DA	3502	1/1	0.87	0.07	65,65,65,65	0
56	MG	AA	3029	1/1	0.87	0.25	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3221	1/1	0.87	0.25	49,49,49,49	0
56	MG	DA	3222	1/1	0.87	0.18	71,71,71,71	0
56	MG	BA	3216	1/1	0.87	0.17	41,41,41,41	0
56	MG	BA	3644	1/1	0.87	0.09	43,43,43,43	0
56	MG	AA	3138	1/1	0.87	0.23	37,37,37,37	0
56	MG	DA	3013	1/1	0.87	0.19	47,47,47,47	0
56	MG	DA	3015	1/1	0.87	0.24	49,49,49,49	0
56	MG	DA	3243	1/1	0.87	0.16	67,67,67,67	0
56	MG	DA	3554	1/1	0.87	0.27	70,70,70,70	0
56	MG	BA	3059	1/1	0.87	0.33	45,45,45,45	0
56	MG	AA	3099	1/1	0.87	0.20	60,60,60,60	0
56	MG	BA	3664	1/1	0.87	0.21	68,68,68,68	0
56	MG	AA	3155	1/1	0.87	0.17	70,70,70,70	0
56	MG	DA	3566	1/1	0.87	0.30	71,71,71,71	0
56	MG	BA	3673	1/1	0.87	0.09	53,53,53,53	0
56	MG	AA	3037	1/1	0.87	0.19	61,61,61,61	0
56	MG	DA	3591	1/1	0.87	0.15	58,58,58,58	0
56	MG	BA	3282	1/1	0.87	0.22	49,49,49,49	0
56	MG	DA	3286	1/1	0.87	0.15	62,62,62,62	0
56	MG	AA	3079	1/1	0.87	0.42	74,74,74,74	0
56	MG	BA	3165	1/1	0.87	0.20	53,53,53,53	0
56	MG	BA	3713	1/1	0.87	0.12	66,66,66,66	0
56	MG	AA	3083	1/1	0.87	0.13	65,65,65,65	0
56	MG	DA	3080	1/1	0.87	0.16	44,44,44,44	0
56	MG	CA	3138	1/1	0.87	0.17	72,72,72,72	0
56	MG	DA	3631	1/1	0.87	0.10	56,56,56,56	0
56	MG	DA	3352	1/1	0.87	0.13	47,47,47,47	0
56	MG	BA	3560	1/1	0.87	0.25	61,61,61,61	0
56	MG	CA	3034	1/1	0.87	0.20	65,65,65,65	0
56	MG	DA	3363	1/1	0.87	0.18	57,57,57,57	0
56	MG	BA	3735	1/1	0.87	0.11	45,45,45,45	0
56	MG	DA	3107	1/1	0.87	0.09	55,55,55,55	0
56	MG	DA	3112	1/1	0.87	0.26	54,54,54,54	0
56	MG	AX	104	1/1	0.87	0.27	76,76,76,76	0
56	MG	DE	303	1/1	0.87	0.15	41,41,41,41	0
56	MG	AA	3111	1/1	0.87	0.11	95,95,95,95	0
56	MG	CA	3148	1/1	0.87	0.17	68,68,68,68	0
56	MG	CA	3149	1/1	0.87	0.11	74,74,74,74	0
56	MG	CA	3150	1/1	0.87	0.08	59,59,59,59	0
56	MG	D5	101	1/1	0.87	0.35	53,53,53,53	0
56	MG	DA	3127	1/1	0.87	0.10	48,48,48,48	0
56	MG	AA	3063	1/1	0.87	0.33	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3044	1/1	0.87	0.20	63,63,63,63	0
56	MG	AA	3190	1/1	0.87	0.21	67,67,67,67	0
56	MG	DA	3466	1/1	0.88	0.18	56,56,56,56	0
56	MG	AA	3012	1/1	0.88	0.08	56,56,56,56	0
56	MG	DA	3479	1/1	0.88	0.21	57,57,57,57	0
56	MG	CA	3016	1/1	0.88	0.15	76,76,76,76	0
56	MG	BA	3071	1/1	0.88	0.16	55,55,55,55	0
56	MG	DA	3483	1/1	0.88	0.11	49,49,49,49	0
56	MG	BA	3440	1/1	0.88	0.15	38,38,38,38	0
56	MG	CA	3022	1/1	0.88	0.10	70,70,70,70	0
56	MG	AA	3048	1/1	0.88	0.15	57,57,57,57	0
56	MG	CA	3156	1/1	0.88	0.15	70,70,70,70	0
56	MG	BA	3456	1/1	0.88	0.10	52,52,52,52	0
56	MG	BA	3147	1/1	0.88	0.23	46,46,46,46	0
56	MG	DA	3172	1/1	0.88	0.21	51,51,51,51	0
56	MG	BA	3479	1/1	0.88	0.13	56,56,56,56	0
56	MG	BA	3244	1/1	0.88	0.26	65,65,65,65	0
56	MG	BA	3703	1/1	0.88	0.10	31,31,31,31	0
56	MG	BA	3083	1/1	0.88	0.26	63,63,63,63	0
56	MG	BA	3086	1/1	0.88	0.26	49,49,49,49	0
56	MG	BA	3502	1/1	0.88	0.13	43,43,43,43	0
56	MG	AX	108	1/1	0.88	0.18	61,61,61,61	0
56	MG	CA	3046	1/1	0.88	0.32	53,53,53,53	0
56	MG	DA	3543	1/1	0.88	0.12	42,42,42,42	0
56	MG	BA	3724	1/1	0.88	0.12	58,58,58,58	0
56	MG	BA	3727	1/1	0.88	0.24	68,68,68,68	0
56	MG	BA	3511	1/1	0.88	0.11	39,39,39,39	0
56	MG	BA	3160	1/1	0.88	0.28	53,53,53,53	0
56	MG	DA	3005	1/1	0.88	0.09	42,42,42,42	0
56	MG	BA	3546	1/1	0.88	0.22	48,48,48,48	0
56	MG	BA	3164	1/1	0.88	0.23	56,56,56,56	0
56	MG	DA	3018	1/1	0.88	0.19	48,48,48,48	0
56	MG	AA	3133	1/1	0.88	0.33	63,63,63,63	0
56	MG	CA	3062	1/1	0.88	0.28	57,57,57,57	0
56	MG	AA	3119	1/1	0.88	0.28	63,63,63,63	0
56	MG	DA	3592	1/1	0.88	0.19	65,65,65,65	0
56	MG	DA	3593	1/1	0.88	0.20	73,73,73,73	0
56	MG	DA	3032	1/1	0.88	0.12	46,46,46,46	0
56	MG	BA	3295	1/1	0.88	0.32	75,75,75,75	0
56	MG	DA	3041	1/1	0.88	0.29	57,57,57,57	0
56	MG	BB	3017	1/1	0.88	0.15	64,64,64,64	0
56	MG	BA	3173	1/1	0.88	0.30	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BN	3001	1/1	0.88	0.24	54,54,54,54	0
56	MG	AA	3004	1/1	0.88	0.20	55,55,55,55	0
56	MG	AA	3095	1/1	0.88	0.31	58,58,58,58	0
56	MG	DA	3626	1/1	0.88	0.07	68,68,68,68	0
56	MG	DA	3627	1/1	0.88	0.15	43,43,43,43	0
56	MG	DA	3350	1/1	0.88	0.07	32,32,32,32	0
56	MG	BU	204	1/1	0.88	0.22	44,44,44,44	0
56	MG	BA	3104	1/1	0.88	0.28	45,45,45,45	0
56	MG	DA	3078	1/1	0.88	0.11	44,44,44,44	0
56	MG	DA	3640	1/1	0.88	0.41	56,56,56,56	0
56	MG	DA	3643	1/1	0.88	0.25	53,53,53,53	0
56	MG	CA	3105	1/1	0.88	0.10	79,79,79,79	0
56	MG	BA	3111	1/1	0.88	0.15	53,53,53,53	0
56	MG	BA	3618	1/1	0.88	0.10	46,46,46,46	0
56	MG	AA	3219	1/1	0.88	0.19	57,57,57,57	0
56	MG	DA	3096	1/1	0.88	0.11	60,60,60,60	0
56	MG	AA	3141	1/1	0.88	0.20	48,48,48,48	0
56	MG	CA	3123	1/1	0.88	0.12	77,77,77,77	0
56	MG	AA	3194	1/1	0.88	0.16	54,54,54,54	0
56	MG	DA	3450	1/1	0.88	0.09	43,43,43,43	0
56	MG	BA	3632	1/1	0.88	0.18	57,57,57,57	0
56	MG	D3	101	1/1	0.88	0.10	63,63,63,63	0
56	MG	AA	3114	1/1	0.88	0.30	66,66,66,66	0
56	MG	CA	3004	1/1	0.88	0.10	96,96,96,96	0
56	MG	CA	3005	1/1	0.88	0.19	54,54,54,54	0
56	MG	BA	3209	1/1	0.88	0.18	40,40,40,40	0
56	MG	BA	3649	1/1	0.88	0.19	66,66,66,66	0
56	MG	BA	3464	1/1	0.89	0.07	43,43,43,43	0
56	MG	AA	3127	1/1	0.89	0.22	62,62,62,62	0
56	MG	AA	3038	1/1	0.89	0.32	66,66,66,66	0
56	MG	AA	3135	1/1	0.89	0.14	41,41,41,41	0
56	MG	AA	3106	1/1	0.89	0.21	56,56,56,56	0
56	MG	BA	3192	1/1	0.89	0.13	58,58,58,58	0
56	MG	DA	3497	1/1	0.89	0.15	60,60,60,60	0
56	MG	DA	3008	1/1	0.89	0.14	51,51,51,51	0
56	MG	DA	3218	1/1	0.89	0.09	62,62,62,62	0
56	MG	AA	3203	1/1	0.89	0.13	63,63,63,63	0
56	MG	CA	3079	1/1	0.89	0.13	48,48,48,48	0
56	MG	BA	3674	1/1	0.89	0.15	55,55,55,55	0
56	MG	BA	3085	1/1	0.89	0.32	48,48,48,48	0
56	MG	CA	3099	1/1	0.89	0.17	65,65,65,65	0
56	MG	DA	3519	1/1	0.89	0.09	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3525	1/1	0.89	0.41	70,70,70,70	0
56	MG	DA	3029	1/1	0.89	0.16	61,61,61,61	0
56	MG	BA	3197	1/1	0.89	0.13	39,39,39,39	0
56	MG	DA	3528	1/1	0.89	0.09	56,56,56,56	0
56	MG	DA	3536	1/1	0.89	0.13	80,80,80,80	0
56	MG	AA	3137	1/1	0.89	0.13	42,42,42,42	0
56	MG	DA	3034	1/1	0.89	0.10	40,40,40,40	0
56	MG	DA	3544	1/1	0.89	0.14	51,51,51,51	0
56	MG	BA	3201	1/1	0.89	0.20	36,36,36,36	0
56	MG	CA	3013	1/1	0.89	0.07	51,51,51,51	0
56	MG	DA	3053	1/1	0.89	0.12	42,42,42,42	0
56	MG	CA	3111	1/1	0.89	0.16	64,64,64,64	0
56	MG	DA	3562	1/1	0.89	0.16	61,61,61,61	0
56	MG	DA	3268	1/1	0.89	0.08	40,40,40,40	0
56	MG	BA	3706	1/1	0.89	0.28	63,63,63,63	0
56	MG	AA	3178	1/1	0.89	0.20	65,65,65,65	0
56	MG	AA	3005	1/1	0.89	0.44	66,66,66,66	0
56	MG	CA	3019	1/1	0.89	0.15	49,49,49,49	0
56	MG	AA	3217	1/1	0.89	0.35	67,67,67,67	0
56	MG	AA	3139	1/1	0.89	0.20	56,56,56,56	0
56	MG	BA	3597	1/1	0.89	0.20	60,60,60,60	0
56	MG	BA	3159	1/1	0.89	0.06	48,48,48,48	0
56	MG	CA	3140	1/1	0.89	0.19	73,73,73,73	0
56	MG	BA	3604	1/1	0.89	0.18	72,72,72,72	0
56	MG	BA	3608	1/1	0.89	0.07	68,68,68,68	0
56	MG	BA	3102	1/1	0.89	0.23	52,52,52,52	0
56	MG	BA	3225	1/1	0.89	0.30	62,62,62,62	0
56	MG	BA	3615	1/1	0.89	0.15	36,36,36,36	0
56	MG	DA	3365	1/1	0.89	0.12	40,40,40,40	0
56	MG	DA	3387	1/1	0.89	0.08	56,56,56,56	0
56	MG	DA	3110	1/1	0.89	0.12	49,49,49,49	0
56	MG	CA	3039	1/1	0.89	0.27	72,72,72,72	0
56	MG	BA	3422	1/1	0.89	0.17	42,42,42,42	0
56	MG	DA	3412	1/1	0.89	0.19	30,30,30,30	0
56	MG	DA	3414	1/1	0.89	0.10	49,49,49,49	0
56	MG	CA	3151	1/1	0.89	0.12	80,80,80,80	0
56	MG	DA	3119	1/1	0.89	0.14	44,44,44,44	0
56	MG	BA	3230	1/1	0.89	0.15	46,46,46,46	0
56	MG	DA	3440	1/1	0.89	0.21	33,33,33,33	0
56	MG	DA	3652	1/1	0.89	0.14	60,60,60,60	0
56	MG	AA	3052	1/1	0.89	0.26	60,60,60,60	0
56	MG	BD	306	1/1	0.89	0.08	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DB	3003	1/1	0.89	0.13	63,63,63,63	0
56	MG	DA	3453	1/1	0.89	0.15	61,61,61,61	0
56	MG	BF	308	1/1	0.89	0.10	28,28,28,28	0
56	MG	DA	3455	1/1	0.89	0.13	60,60,60,60	0
56	MG	BA	3241	1/1	0.89	0.17	63,63,63,63	0
56	MG	AA	3221	1/1	0.89	0.23	64,64,64,64	0
56	MG	AN	101	1/1	0.89	0.10	63,63,63,63	0
56	MG	DA	3141	1/1	0.89	0.16	62,62,62,62	0
56	MG	CA	3166	1/1	0.89	0.12	59,59,59,59	0
56	MG	DA	3158	1/1	0.89	0.23	57,57,57,57	0
56	MG	BA	3641	1/1	0.89	0.17	45,45,45,45	0
56	MG	CA	3056	1/1	0.89	0.27	64,64,64,64	0
56	MG	BU	201	1/1	0.89	0.36	39,39,39,39	0
56	MG	BA	3262	1/1	0.89	0.26	56,56,56,56	0
56	MG	BA	3601	1/1	0.90	0.26	64,64,64,64	0
56	MG	AA	3054	1/1	0.90	0.15	45,45,45,45	0
56	MG	DA	3139	1/1	0.90	0.12	40,40,40,40	0
56	MG	BA	3391	1/1	0.90	0.21	48,48,48,48	0
56	MG	DA	3153	1/1	0.90	0.13	38,38,38,38	0
56	MG	BA	3394	1/1	0.90	0.09	49,49,49,49	0
56	MG	DA	3157	1/1	0.90	0.38	62,62,62,62	0
56	MG	AA	3098	1/1	0.90	0.21	72,72,72,72	0
56	MG	BA	3107	1/1	0.90	0.19	40,40,40,40	0
56	MG	BD	305	1/1	0.90	0.23	48,48,48,48	0
56	MG	BA	3108	1/1	0.90	0.15	55,55,55,55	0
56	MG	DA	3167	1/1	0.90	0.19	48,48,48,48	0
56	MG	AA	3074	1/1	0.90	0.25	47,47,47,47	0
56	MG	BG	3003	1/1	0.90	0.10	42,42,42,42	0
56	MG	DA	3495	1/1	0.90	0.19	39,39,39,39	0
56	MG	BA	3119	1/1	0.90	0.20	58,58,58,58	0
56	MG	BA	3620	1/1	0.90	0.15	47,47,47,47	0
56	MG	BA	3245	1/1	0.90	0.10	47,47,47,47	0
56	MG	AA	3216	1/1	0.90	0.21	58,58,58,58	0
56	MG	BQ	205	1/1	0.90	0.14	49,49,49,49	0
56	MG	BA	3186	1/1	0.90	0.10	53,53,53,53	0
56	MG	DA	3216	1/1	0.90	0.15	31,31,31,31	0
56	MG	BA	3068	1/1	0.90	0.34	54,54,54,54	0
56	MG	BV	201	1/1	0.90	0.17	53,53,53,53	0
56	MG	DA	3022	1/1	0.90	0.10	45,45,45,45	0
56	MG	BA	3643	1/1	0.90	0.14	43,43,43,43	0
56	MG	BA	3463	1/1	0.90	0.12	55,55,55,55	0
56	MG	AA	3100	1/1	0.90	0.18	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B0	102	1/1	0.90	0.15	40,40,40,40	0
56	MG	BA	3466	1/1	0.90	0.15	61,61,61,61	0
56	MG	BA	3005	1/1	0.90	0.14	36,36,36,36	0
56	MG	DA	3036	1/1	0.90	0.11	35,35,35,35	0
56	MG	BA	3287	1/1	0.90	0.21	53,53,53,53	0
56	MG	DA	3040	1/1	0.90	0.09	42,42,42,42	0
56	MG	BA	3008	1/1	0.90	0.10	50,50,50,50	0
56	MG	DA	3048	1/1	0.90	0.21	37,37,37,37	0
56	MG	B9	502	1/1	0.90	0.20	49,49,49,49	0
56	MG	DA	3278	1/1	0.90	0.11	47,47,47,47	0
56	MG	BA	3142	1/1	0.90	0.42	46,46,46,46	0
56	MG	DA	3058	1/1	0.90	0.12	47,47,47,47	0
56	MG	AA	3070	1/1	0.90	0.11	75,75,75,75	0
56	MG	DA	3578	1/1	0.90	0.17	49,49,49,49	0
56	MG	DA	3288	1/1	0.90	0.17	47,47,47,47	0
56	MG	AA	3168	1/1	0.90	0.13	68,68,68,68	0
56	MG	DA	3296	1/1	0.90	0.08	31,31,31,31	0
56	MG	CA	3006	1/1	0.90	0.11	77,77,77,77	0
56	MG	DA	3068	1/1	0.90	0.11	55,55,55,55	0
56	MG	BA	3675	1/1	0.90	0.18	49,49,49,49	0
56	MG	DA	3602	1/1	0.90	0.16	52,52,52,52	0
56	MG	DA	3603	1/1	0.90	0.14	55,55,55,55	0
56	MG	DA	3607	1/1	0.90	0.09	45,45,45,45	0
56	MG	DA	3321	1/1	0.90	0.15	41,41,41,41	0
56	MG	BA	3510	1/1	0.90	0.18	40,40,40,40	0
56	MG	CA	3126	1/1	0.90	0.11	61,61,61,61	0
56	MG	DA	3342	1/1	0.90	0.09	52,52,52,52	0
56	MG	DA	3077	1/1	0.90	0.15	50,50,50,50	0
56	MG	AA	3041	1/1	0.90	0.18	49,49,49,49	0
56	MG	DA	3353	1/1	0.90	0.10	62,62,62,62	0
56	MG	BA	3306	1/1	0.90	0.15	48,48,48,48	0
56	MG	BA	3545	1/1	0.90	0.21	47,47,47,47	0
56	MG	DA	3089	1/1	0.90	0.10	57,57,57,57	0
56	MG	AA	3202	1/1	0.90	0.15	76,76,76,76	0
56	MG	BA	3709	1/1	0.90	0.19	86,86,86,86	0
56	MG	DA	3388	1/1	0.90	0.09	54,54,54,54	0
56	MG	DA	3390	1/1	0.90	0.09	42,42,42,42	0
56	MG	DA	3641	1/1	0.90	0.25	61,61,61,61	0
56	MG	DA	3398	1/1	0.90	0.15	35,35,35,35	0
56	MG	DA	3400	1/1	0.90	0.12	42,42,42,42	0
56	MG	BA	3312	1/1	0.90	0.12	58,58,58,58	0
56	MG	BA	3039	1/1	0.90	0.14	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3106	1/1	0.90	0.08	41,41,41,41	0
56	MG	BA	3210	1/1	0.90	0.13	34,34,34,34	0
56	MG	DB	3009	1/1	0.90	0.27	40,40,40,40	0
56	MG	BA	3717	1/1	0.90	0.21	57,57,57,57	0
56	MG	CA	3029	1/1	0.90	0.17	59,59,59,59	0
56	MG	DD	306	1/1	0.90	0.85	44,44,44,44	0
56	MG	BA	3340	1/1	0.90	0.08	57,57,57,57	0
56	MG	BA	3588	1/1	0.90	0.12	48,48,48,48	0
56	MG	DF	305	1/1	0.90	0.17	39,39,39,39	0
56	MG	CA	3033	1/1	0.90	0.16	68,68,68,68	0
56	MG	CA	3152	1/1	0.90	0.20	55,55,55,55	0
56	MG	DW	201	1/1	0.90	0.09	46,46,46,46	0
56	MG	BA	3214	1/1	0.90	0.21	53,53,53,53	0
56	MG	D0	101	1/1	0.90	0.13	63,63,63,63	0
56	MG	DA	3452	1/1	0.90	0.10	56,56,56,56	0
56	MG	AA	3081	1/1	0.90	0.24	41,41,41,41	0
56	MG	DA	3125	1/1	0.90	0.15	48,48,48,48	0
56	MG	DA	3126	1/1	0.90	0.19	43,43,43,43	0
56	MG	CA	3036	1/1	0.90	0.08	68,68,68,68	0
56	MG	BA	3043	1/1	0.90	0.17	52,52,52,52	0
56	MG	BA	3692	1/1	0.91	0.19	36,36,36,36	0
56	MG	BA	3072	1/1	0.91	0.25	45,45,45,45	0
56	MG	BA	3296	1/1	0.91	0.23	46,46,46,46	0
56	MG	BA	3535	1/1	0.91	0.11	37,37,37,37	0
56	MG	BA	3203	1/1	0.91	0.22	32,32,32,32	0
56	MG	BA	3304	1/1	0.91	0.14	49,49,49,49	0
56	MG	CA	3028	1/1	0.91	0.26	43,43,43,43	0
56	MG	AA	3016	1/1	0.91	0.10	63,63,63,63	0
56	MG	BA	3549	1/1	0.91	0.15	27,27,27,27	0
56	MG	CA	3160	1/1	0.91	0.17	59,59,59,59	0
56	MG	BA	3559	1/1	0.91	0.13	48,48,48,48	0
56	MG	DA	3145	1/1	0.91	0.15	65,65,65,65	0
56	MG	DA	3147	1/1	0.91	0.11	53,53,53,53	0
56	MG	DA	3150	1/1	0.91	0.08	64,64,64,64	0
56	MG	DA	3471	1/1	0.91	0.13	37,37,37,37	0
56	MG	DA	3152	1/1	0.91	0.13	50,50,50,50	0
56	MG	BA	3082	1/1	0.91	0.17	41,41,41,41	0
56	MG	AA	3210	1/1	0.91	0.09	40,40,40,40	0
56	MG	DA	3156	1/1	0.91	0.25	29,29,29,29	0
56	MG	CA	3168	1/1	0.91	0.22	77,77,77,77	0
56	MG	BA	3719	1/1	0.91	0.08	25,25,25,25	0
56	MG	DA	3159	1/1	0.91	0.08	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3077	1/1	0.91	0.30	65,65,65,65	0
56	MG	BA	3151	1/1	0.91	0.12	52,52,52,52	0
56	MG	BA	3731	1/1	0.91	0.11	55,55,55,55	0
56	MG	BA	3336	1/1	0.91	0.21	54,54,54,54	0
56	MG	DA	3496	1/1	0.91	0.23	53,53,53,53	0
56	MG	AA	3025	1/1	0.91	0.07	69,69,69,69	0
56	MG	BA	3594	1/1	0.91	0.14	42,42,42,42	0
56	MG	DA	3171	1/1	0.91	0.16	39,39,39,39	0
56	MG	BB	3001	1/1	0.91	0.16	54,54,54,54	0
56	MG	DA	3176	1/1	0.91	0.19	39,39,39,39	0
56	MG	DA	3178	1/1	0.91	0.40	43,43,43,43	0
56	MG	BB	3002	1/1	0.91	0.16	59,59,59,59	0
56	MG	DA	3512	1/1	0.91	0.33	61,61,61,61	0
56	MG	AA	3058	1/1	0.91	0.18	50,50,50,50	0
56	MG	DA	3517	1/1	0.91	0.12	50,50,50,50	0
56	MG	AA	3140	1/1	0.91	0.08	70,70,70,70	0
56	MG	DA	3522	1/1	0.91	0.11	61,61,61,61	0
56	MG	BA	3356	1/1	0.91	0.15	56,56,56,56	0
56	MG	DA	3208	1/1	0.91	0.18	43,43,43,43	0
56	MG	DA	3210	1/1	0.91	0.23	40,40,40,40	0
56	MG	DA	3211	1/1	0.91	0.20	51,51,51,51	0
56	MG	AA	3032	1/1	0.91	0.24	57,57,57,57	0
56	MG	AA	3001	1/1	0.91	0.11	68,68,68,68	0
56	MG	BB	3018	1/1	0.91	0.17	60,60,60,60	0
56	MG	BA	3373	1/1	0.91	0.16	36,36,36,36	0
56	MG	BA	3384	1/1	0.91	0.17	60,60,60,60	0
56	MG	BA	3233	1/1	0.91	0.23	47,47,47,47	0
56	MG	AF	3001	1/1	0.91	0.17	61,61,61,61	0
56	MG	DA	3226	1/1	0.91	0.23	50,50,50,50	0
56	MG	AA	3097	1/1	0.91	0.21	43,43,43,43	0
56	MG	BA	3047	1/1	0.91	0.12	47,47,47,47	0
56	MG	BA	3105	1/1	0.91	0.43	34,34,34,34	0
56	MG	BA	3621	1/1	0.91	0.14	74,74,74,74	0
56	MG	CA	3074	1/1	0.91	0.22	54,54,54,54	0
56	MG	DA	3567	1/1	0.91	0.19	62,62,62,62	0
56	MG	DA	3249	1/1	0.91	0.18	28,28,28,28	0
56	MG	CA	3077	1/1	0.91	0.23	53,53,53,53	0
56	MG	DA	3043	1/1	0.91	0.28	54,54,54,54	0
56	MG	DA	3260	1/1	0.91	0.11	40,40,40,40	0
56	MG	DA	3044	1/1	0.91	0.16	46,46,46,46	0
56	MG	CA	3078	1/1	0.91	0.13	46,46,46,46	0
56	MG	BA	3048	1/1	0.91	0.16	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3274	1/1	0.91	0.10	52,52,52,52	0
56	MG	BA	3248	1/1	0.91	0.16	43,43,43,43	0
56	MG	DA	3604	1/1	0.91	0.13	54,54,54,54	0
56	MG	DA	3606	1/1	0.91	0.09	58,58,58,58	0
56	MG	DA	3056	1/1	0.91	0.22	43,43,43,43	0
56	MG	DA	3280	1/1	0.91	0.10	57,57,57,57	0
56	MG	BA	3259	1/1	0.91	0.31	27,27,27,27	0
56	MG	BA	3050	1/1	0.91	0.12	21,21,21,21	0
56	MG	DA	3617	1/1	0.91	0.19	58,58,58,58	0
56	MG	AA	3050	1/1	0.91	0.15	63,63,63,63	0
56	MG	BA	3269	1/1	0.91	0.29	34,34,34,34	0
56	MG	AX	102	1/1	0.91	0.20	74,74,74,74	0
56	MG	BA	3646	1/1	0.91	0.23	52,52,52,52	0
56	MG	DA	3307	1/1	0.91	0.22	37,37,37,37	0
56	MG	BA	3648	1/1	0.91	0.21	49,49,49,49	0
56	MG	DA	3630	1/1	0.91	0.13	40,40,40,40	0
56	MG	BA	3277	1/1	0.91	0.18	45,45,45,45	0
56	MG	BA	3650	1/1	0.91	0.20	45,45,45,45	0
56	MG	BA	3653	1/1	0.91	0.12	69,69,69,69	0
56	MG	DA	3329	1/1	0.91	0.07	53,53,53,53	0
56	MG	CA	3124	1/1	0.91	0.12	61,61,61,61	0
56	MG	BA	3654	1/1	0.91	0.13	25,25,25,25	0
56	MG	DA	3086	1/1	0.91	0.19	43,43,43,43	0
56	MG	DA	3087	1/1	0.91	0.15	49,49,49,49	0
56	MG	CA	3002	1/1	0.91	0.12	62,62,62,62	0
56	MG	AA	3201	1/1	0.91	0.14	67,67,67,67	0
56	MG	DA	3359	1/1	0.91	0.14	46,46,46,46	0
56	MG	CA	3132	1/1	0.91	0.15	70,70,70,70	0
56	MG	DB	3004	1/1	0.91	0.13	68,68,68,68	0
56	MG	DA	3095	1/1	0.91	0.19	61,61,61,61	0
56	MG	BA	3467	1/1	0.91	0.14	40,40,40,40	0
56	MG	DA	3374	1/1	0.91	0.06	37,37,37,37	0
56	MG	DD	302	1/1	0.91	0.16	46,46,46,46	0
56	MG	DA	3377	1/1	0.91	0.15	59,59,59,59	0
56	MG	DA	3383	1/1	0.91	0.10	56,56,56,56	0
56	MG	DA	3386	1/1	0.91	0.10	56,56,56,56	0
56	MG	DA	3098	1/1	0.91	0.61	43,43,43,43	0
56	MG	BA	3284	1/1	0.91	0.12	54,54,54,54	0
56	MG	DN	5001	1/1	0.91	0.09	75,75,75,75	0
56	MG	DA	3100	1/1	0.91	0.25	56,56,56,56	0
56	MG	DV	202	1/1	0.91	0.23	63,63,63,63	0
56	MG	DA	3105	1/1	0.91	0.13	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3132	1/1	0.91	0.09	35,35,35,35	0
56	MG	BA	3671	1/1	0.91	0.14	57,57,57,57	0
56	MG	AA	3027	1/1	0.91	0.07	55,55,55,55	0
56	MG	CA	3009	1/1	0.91	0.08	47,47,47,47	0
56	MG	AA	3064	1/1	0.91	0.08	79,79,79,79	0
56	MG	BA	3291	1/1	0.91	0.11	41,41,41,41	0
56	MG	DA	3118	1/1	0.91	0.06	39,39,39,39	0
56	MG	AA	3169	1/1	0.91	0.11	76,76,76,76	0
56	MG	DA	3140	1/1	0.92	0.22	54,54,54,54	0
56	MG	AA	3181	1/1	0.92	0.17	57,57,57,57	0
56	MG	BA	3101	1/1	0.92	0.12	35,35,35,35	0
56	MG	BA	3294	1/1	0.92	0.22	37,37,37,37	0
56	MG	CA	3010	1/1	0.92	0.10	32,32,32,32	0
56	MG	CA	3011	1/1	0.92	0.27	42,42,42,42	0
56	MG	DA	3459	1/1	0.92	0.09	33,33,33,33	0
56	MG	BA	3678	1/1	0.92	0.24	53,53,53,53	0
56	MG	AA	3184	1/1	0.92	0.07	72,72,72,72	0
56	MG	BA	3690	1/1	0.92	0.15	53,53,53,53	0
56	MG	CA	3163	1/1	0.92	0.08	65,65,65,65	0
56	MG	BA	3691	1/1	0.92	0.15	49,49,49,49	0
56	MG	BA	3211	1/1	0.92	0.15	38,38,38,38	0
56	MG	BA	3066	1/1	0.92	0.18	44,44,44,44	0
56	MG	BA	3694	1/1	0.92	0.32	56,56,56,56	0
56	MG	BA	3697	1/1	0.92	0.13	78,78,78,78	0
56	MG	BA	3537	1/1	0.92	0.23	31,31,31,31	0
56	MG	DA	3168	1/1	0.92	0.26	48,48,48,48	0
56	MG	BA	3298	1/1	0.92	0.09	49,49,49,49	0
56	MG	AA	3126	1/1	0.92	0.24	54,54,54,54	0
56	MG	AA	3086	1/1	0.92	0.08	51,51,51,51	0
56	MG	CX	102	1/1	0.92	0.11	61,61,61,61	0
56	MG	CA	3031	1/1	0.92	0.26	53,53,53,53	0
56	MG	BA	3307	1/1	0.92	0.21	33,33,33,33	0
56	MG	DA	3181	1/1	0.92	0.18	36,36,36,36	0
56	MG	BA	3554	1/1	0.92	0.16	31,31,31,31	0
56	MG	BA	3031	1/1	0.92	0.59	41,41,41,41	0
56	MG	BA	3311	1/1	0.92	0.13	42,42,42,42	0
56	MG	DA	3012	1/1	0.92	0.16	57,57,57,57	0
56	MG	DA	3504	1/1	0.92	0.07	44,44,44,44	0
56	MG	DA	3509	1/1	0.92	0.14	55,55,55,55	0
56	MG	AA	3020	1/1	0.92	0.07	77,77,77,77	0
56	MG	BA	3313	1/1	0.92	0.15	36,36,36,36	0
56	MG	DA	3016	1/1	0.92	0.23	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3110	1/1	0.92	0.29	55,55,55,55	0
56	MG	DA	3215	1/1	0.92	0.24	29,29,29,29	0
56	MG	BA	3231	1/1	0.92	0.24	38,38,38,38	0
56	MG	DA	3521	1/1	0.92	0.12	62,62,62,62	0
56	MG	AA	3082	1/1	0.92	0.21	39,39,39,39	0
56	MG	DA	3524	1/1	0.92	0.09	28,28,28,28	0
56	MG	BA	3112	1/1	0.92	0.11	38,38,38,38	0
56	MG	BA	3238	1/1	0.92	0.28	51,51,51,51	0
56	MG	BA	3080	1/1	0.92	0.21	45,45,45,45	0
56	MG	BA	3599	1/1	0.92	0.12	46,46,46,46	0
56	MG	AA	3108	1/1	0.92	0.15	67,67,67,67	0
56	MG	CA	3052	1/1	0.92	0.13	39,39,39,39	0
56	MG	DA	3538	1/1	0.92	0.08	44,44,44,44	0
56	MG	BA	3368	1/1	0.92	0.15	35,35,35,35	0
56	MG	DA	3239	1/1	0.92	0.15	39,39,39,39	0
56	MG	BB	3004	1/1	0.92	0.18	54,54,54,54	0
56	MG	BA	3182	1/1	0.92	0.31	51,51,51,51	0
56	MG	BA	3246	1/1	0.92	0.14	46,46,46,46	0
56	MG	BA	3127	1/1	0.92	0.16	50,50,50,50	0
56	MG	BA	3376	1/1	0.92	0.08	48,48,48,48	0
56	MG	DA	3254	1/1	0.92	0.13	30,30,30,30	0
56	MG	BA	3129	1/1	0.92	0.14	36,36,36,36	0
56	MG	BA	3387	1/1	0.92	0.11	48,48,48,48	0
56	MG	BA	3252	1/1	0.92	0.08	55,55,55,55	0
56	MG	DA	3266	1/1	0.92	0.14	43,43,43,43	0
56	MG	DA	3057	1/1	0.92	0.14	52,52,52,52	0
56	MG	BD	312	1/1	0.92	0.24	80,80,80,80	0
56	MG	DA	3582	1/1	0.92	0.07	52,52,52,52	0
56	MG	DA	3269	1/1	0.92	0.13	48,48,48,48	0
56	MG	DA	3059	1/1	0.92	0.11	46,46,46,46	0
56	MG	BE	301	1/1	0.92	0.21	43,43,43,43	0
56	MG	CA	3072	1/1	0.92	0.18	38,38,38,38	0
56	MG	BE	308	1/1	0.92	0.18	52,52,52,52	0
56	MG	DA	3599	1/1	0.92	0.11	72,72,72,72	0
56	MG	DA	3064	1/1	0.92	0.14	50,50,50,50	0
56	MG	DA	3285	1/1	0.92	0.10	55,55,55,55	0
56	MG	BF	302	1/1	0.92	0.16	46,46,46,46	0
56	MG	BF	304	1/1	0.92	0.16	35,35,35,35	0
56	MG	DA	3291	1/1	0.92	0.15	35,35,35,35	0
56	MG	DA	3608	1/1	0.92	0.14	57,57,57,57	0
56	MG	DA	3070	1/1	0.92	0.26	44,44,44,44	0
56	MG	DA	3610	1/1	0.92	0.09	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3257	1/1	0.92	0.26	38,38,38,38	0
56	MG	BA	3187	1/1	0.92	0.15	50,50,50,50	0
56	MG	BA	3044	1/1	0.92	0.20	42,42,42,42	0
56	MG	CA	3085	1/1	0.92	0.17	43,43,43,43	0
56	MG	BA	3133	1/1	0.92	0.16	32,32,32,32	0
56	MG	BA	3631	1/1	0.92	0.11	78,78,78,78	0
56	MG	BA	3264	1/1	0.92	0.19	30,30,30,30	0
56	MG	DA	3325	1/1	0.92	0.11	36,36,36,36	0
56	MG	BA	3639	1/1	0.92	0.09	50,50,50,50	0
56	MG	CA	3108	1/1	0.92	0.14	52,52,52,52	0
56	MG	BR	201	1/1	0.92	0.20	51,51,51,51	0
56	MG	AA	3043	1/1	0.92	0.31	74,74,74,74	0
56	MG	BA	3275	1/1	0.92	0.17	46,46,46,46	0
56	MG	DA	3636	1/1	0.92	0.13	61,61,61,61	0
56	MG	CA	3113	1/1	0.92	0.12	77,77,77,77	0
56	MG	DA	3097	1/1	0.92	0.20	61,61,61,61	0
56	MG	AA	3055	1/1	0.92	0.17	50,50,50,50	0
56	MG	DA	3360	1/1	0.92	0.11	41,41,41,41	0
56	MG	AA	3034	1/1	0.92	0.14	48,48,48,48	0
56	MG	BW	204	1/1	0.92	0.15	35,35,35,35	0
56	MG	DA	3653	1/1	0.92	0.09	60,60,60,60	0
56	MG	DA	3102	1/1	0.92	0.10	41,41,41,41	0
56	MG	BA	3457	1/1	0.92	0.10	57,57,57,57	0
56	MG	DB	3002	1/1	0.92	0.17	56,56,56,56	0
56	MG	DA	3376	1/1	0.92	0.08	31,31,31,31	0
56	MG	BA	3280	1/1	0.92	0.37	69,69,69,69	0
56	MG	DB	3008	1/1	0.92	0.16	45,45,45,45	0
56	MG	BA	3281	1/1	0.92	0.21	52,52,52,52	0
56	MG	BA	3052	1/1	0.92	0.14	29,29,29,29	0
56	MG	B0	104	1/1	0.92	0.08	43,43,43,43	0
56	MG	DB	3012	1/1	0.92	0.24	59,59,59,59	0
56	MG	DA	3113	1/1	0.92	0.18	43,43,43,43	0
56	MG	DA	3389	1/1	0.92	0.18	27,27,27,27	0
56	MG	CA	3133	1/1	0.92	0.15	49,49,49,49	0
56	MG	B1	3001	1/1	0.92	0.32	54,54,54,54	0
56	MG	AD	502	1/1	0.92	0.22	43,43,43,43	0
56	MG	B3	102	1/1	0.92	0.11	59,59,59,59	0
56	MG	BA	3098	1/1	0.92	0.16	35,35,35,35	0
56	MG	DA	3404	1/1	0.92	0.14	47,47,47,47	0
56	MG	DR	201	1/1	0.92	0.24	65,65,65,65	0
56	MG	B7	101	1/1	0.92	0.12	43,43,43,43	0
56	MG	DV	203	1/1	0.92	0.23	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DV	204	1/1	0.92	0.11	41,41,41,41	0
56	MG	BA	3204	1/1	0.92	0.24	25,25,25,25	0
56	MG	CA	3143	1/1	0.92	0.10	87,87,87,87	0
56	MG	BA	3145	1/1	0.92	0.28	38,38,38,38	0
56	MG	DA	3420	1/1	0.92	0.10	51,51,51,51	0
56	MG	BA	3484	1/1	0.92	0.16	54,54,54,54	0
56	MG	BA	3666	1/1	0.92	0.16	61,61,61,61	0
56	MG	BA	3668	1/1	0.92	0.11	38,38,38,38	0
56	MG	BA	3488	1/1	0.92	0.14	35,35,35,35	0
56	MG	BA	3290	1/1	0.92	0.13	49,49,49,49	0
56	MG	BA	3634	1/1	0.93	0.64	63,63,63,63	0
56	MG	BN	3003	1/1	0.93	0.12	59,59,59,59	0
56	MG	BN	3005	1/1	0.93	0.23	52,52,52,52	0
56	MG	DA	3435	1/1	0.93	0.13	46,46,46,46	0
56	MG	BQ	202	1/1	0.93	0.19	28,28,28,28	0
56	MG	BA	3637	1/1	0.93	0.19	33,33,33,33	0
56	MG	BA	3446	1/1	0.93	0.09	49,49,49,49	0
56	MG	DA	3447	1/1	0.93	0.06	56,56,56,56	0
56	MG	BA	3640	1/1	0.93	0.10	60,60,60,60	0
56	MG	BA	3450	1/1	0.93	0.18	46,46,46,46	0
56	MG	AA	3080	1/1	0.93	0.13	53,53,53,53	0
56	MG	CA	3136	1/1	0.93	0.16	45,45,45,45	0
56	MG	BU	208	1/1	0.93	0.62	56,56,56,56	0
56	MG	AA	3148	1/1	0.93	0.09	66,66,66,66	0
56	MG	DA	3457	1/1	0.93	0.14	37,37,37,37	0
56	MG	BA	3003	1/1	0.93	0.15	43,43,43,43	0
56	MG	BW	201	1/1	0.93	0.21	53,53,53,53	0
56	MG	BA	3199	1/1	0.93	0.22	36,36,36,36	0
56	MG	DA	3461	1/1	0.93	0.07	41,41,41,41	0
56	MG	DA	3148	1/1	0.93	0.17	47,47,47,47	0
56	MG	AA	3211	1/1	0.93	0.16	36,36,36,36	0
56	MG	DA	3151	1/1	0.93	0.41	60,60,60,60	0
56	MG	CA	3145	1/1	0.93	0.05	43,43,43,43	0
56	MG	AA	3101	1/1	0.93	0.11	56,56,56,56	0
56	MG	BA	3009	1/1	0.93	0.10	25,25,25,25	0
56	MG	DA	3155	1/1	0.93	0.21	50,50,50,50	0
56	MG	BA	3651	1/1	0.93	0.20	45,45,45,45	0
56	MG	BA	3475	1/1	0.93	0.19	36,36,36,36	0
56	MG	BA	3074	1/1	0.93	0.11	42,42,42,42	0
56	MG	BA	3657	1/1	0.93	0.18	56,56,56,56	0
56	MG	DA	3489	1/1	0.93	0.06	36,36,36,36	0
56	MG	BA	3481	1/1	0.93	0.10	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	B3	103	1/1	0.93	0.23	41,41,41,41	0
56	MG	BA	3660	1/1	0.93	0.20	71,71,71,71	0
56	MG	BA	3292	1/1	0.93	0.08	63,63,63,63	0
56	MG	BA	3663	1/1	0.93	0.24	56,56,56,56	0
56	MG	BA	3011	1/1	0.93	0.06	37,37,37,37	0
56	MG	BA	3207	1/1	0.93	0.17	35,35,35,35	0
56	MG	BA	3017	1/1	0.93	0.14	44,44,44,44	0
56	MG	BA	3141	1/1	0.93	0.16	43,43,43,43	0
56	MG	DA	3173	1/1	0.93	0.31	39,39,39,39	0
56	MG	BA	3498	1/1	0.93	0.09	39,39,39,39	0
56	MG	BA	3672	1/1	0.93	0.23	48,48,48,48	0
56	MG	CA	3167	1/1	0.93	0.05	78,78,78,78	0
56	MG	DA	3182	1/1	0.93	0.15	32,32,32,32	0
56	MG	DA	3183	1/1	0.93	0.13	54,54,54,54	0
56	MG	DA	3514	1/1	0.93	0.10	39,39,39,39	0
56	MG	DA	3184	1/1	0.93	0.18	45,45,45,45	0
56	MG	BA	3499	1/1	0.93	0.12	55,55,55,55	0
56	MG	CA	3169	1/1	0.93	0.15	57,57,57,57	0
56	MG	DA	3189	1/1	0.93	0.07	55,55,55,55	0
56	MG	DA	3191	1/1	0.93	0.14	47,47,47,47	0
56	MG	AA	3159	1/1	0.93	0.18	57,57,57,57	0
56	MG	DA	3196	1/1	0.93	0.22	44,44,44,44	0
56	MG	DA	3197	1/1	0.93	0.27	36,36,36,36	0
56	MG	BA	3021	1/1	0.93	0.29	42,42,42,42	0
56	MG	BA	3509	1/1	0.93	0.09	27,27,27,27	0
56	MG	DA	3534	1/1	0.93	0.15	45,45,45,45	0
56	MG	DA	3535	1/1	0.93	0.14	33,33,33,33	0
56	MG	BA	3680	1/1	0.93	0.19	37,37,37,37	0
56	MG	CA	3012	1/1	0.93	0.06	49,49,49,49	0
56	MG	AA	3053	1/1	0.93	0.15	49,49,49,49	0
56	MG	DA	3539	1/1	0.93	0.12	53,53,53,53	0
56	MG	DA	3213	1/1	0.93	0.18	44,44,44,44	0
56	MG	BA	3684	1/1	0.93	0.15	58,58,58,58	0
56	MG	BA	3686	1/1	0.93	0.08	25,25,25,25	0
56	MG	DA	3547	1/1	0.93	0.09	41,41,41,41	0
56	MG	DA	3550	1/1	0.93	0.05	53,53,53,53	0
56	MG	BA	3689	1/1	0.93	0.17	39,39,39,39	0
56	MG	DA	3002	1/1	0.93	0.26	55,55,55,55	0
56	MG	DA	3555	1/1	0.93	0.11	41,41,41,41	0
56	MG	AA	3036	1/1	0.93	0.13	71,71,71,71	0
56	MG	CA	3020	1/1	0.93	0.14	47,47,47,47	0
56	MG	BA	3515	1/1	0.93	0.09	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3115	1/1	0.93	0.16	48,48,48,48	0
56	MG	AA	3040	1/1	0.93	0.11	55,55,55,55	0
56	MG	BA	3541	1/1	0.93	0.13	30,30,30,30	0
56	MG	BA	3153	1/1	0.93	0.19	35,35,35,35	0
56	MG	BA	3699	1/1	0.93	0.12	56,56,56,56	0
56	MG	AA	3197	1/1	0.93	0.08	69,69,69,69	0
56	MG	BA	3097	1/1	0.93	0.20	33,33,33,33	0
56	MG	DA	3587	1/1	0.93	0.07	64,64,64,64	0
56	MG	BA	3705	1/1	0.93	0.12	39,39,39,39	0
56	MG	DA	3251	1/1	0.93	0.11	54,54,54,54	0
56	MG	BA	3547	1/1	0.93	0.11	31,31,31,31	0
56	MG	BA	3708	1/1	0.93	0.08	40,40,40,40	0
56	MG	DA	3594	1/1	0.93	0.10	47,47,47,47	0
56	MG	DA	3597	1/1	0.93	0.12	47,47,47,47	0
56	MG	BA	3320	1/1	0.93	0.16	57,57,57,57	0
56	MG	BA	3551	1/1	0.93	0.18	25,25,25,25	0
56	MG	CA	3037	1/1	0.93	0.21	67,67,67,67	0
56	MG	AA	3014	1/1	0.93	0.10	28,28,28,28	0
56	MG	BA	3558	1/1	0.93	0.10	35,35,35,35	0
56	MG	BA	3332	1/1	0.93	0.16	39,39,39,39	0
56	MG	BA	3235	1/1	0.93	0.07	47,47,47,47	0
56	MG	AK	3001	1/1	0.93	0.17	45,45,45,45	0
56	MG	DA	3046	1/1	0.93	0.17	56,56,56,56	0
56	MG	BA	3573	1/1	0.93	0.14	56,56,56,56	0
56	MG	DA	3051	1/1	0.93	0.08	46,46,46,46	0
56	MG	AM	3001	1/1	0.93	0.05	65,65,65,65	0
56	MG	DA	3616	1/1	0.93	0.14	62,62,62,62	0
56	MG	BA	3242	1/1	0.93	0.23	48,48,48,48	0
56	MG	AA	3173	1/1	0.93	0.08	32,32,32,32	0
56	MG	DA	3287	1/1	0.93	0.17	53,53,53,53	0
56	MG	AA	3175	1/1	0.93	0.13	76,76,76,76	0
56	MG	BA	3737	1/1	0.93	0.18	60,60,60,60	0
56	MG	BA	3738	1/1	0.93	0.07	59,59,59,59	0
56	MG	DA	3294	1/1	0.93	0.11	47,47,47,47	0
56	MG	CA	3055	1/1	0.93	0.28	62,62,62,62	0
56	MG	BA	3366	1/1	0.93	0.15	63,63,63,63	0
56	MG	BA	3166	1/1	0.93	0.21	59,59,59,59	0
56	MG	BA	3049	1/1	0.93	0.25	35,35,35,35	0
56	MG	DA	3067	1/1	0.93	0.25	43,43,43,43	0
56	MG	DA	3319	1/1	0.93	0.06	53,53,53,53	0
56	MG	BA	3169	1/1	0.93	0.53	46,46,46,46	0
56	MG	AA	3176	1/1	0.93	0.10	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3253	1/1	0.93	0.15	51,51,51,51	0
56	MG	DA	3644	1/1	0.93	0.10	42,42,42,42	0
56	MG	BB	3006	1/1	0.93	0.17	39,39,39,39	0
56	MG	DA	3648	1/1	0.93	0.15	52,52,52,52	0
56	MG	CA	3068	1/1	0.93	0.14	41,41,41,41	0
56	MG	DA	3075	1/1	0.93	0.08	44,44,44,44	0
56	MG	BB	3008	1/1	0.93	0.08	35,35,35,35	0
56	MG	BA	3256	1/1	0.93	0.10	58,58,58,58	0
56	MG	BA	3609	1/1	0.93	0.13	46,46,46,46	0
56	MG	AA	3204	1/1	0.93	0.15	54,54,54,54	0
56	MG	BA	3181	1/1	0.93	0.16	38,38,38,38	0
56	MG	DB	3007	1/1	0.93	0.24	45,45,45,45	0
56	MG	CA	3075	1/1	0.93	0.26	76,76,76,76	0
56	MG	CA	3076	1/1	0.93	0.19	40,40,40,40	0
56	MG	BD	302	1/1	0.93	0.22	58,58,58,58	0
56	MG	BD	304	1/1	0.93	0.20	58,58,58,58	0
56	MG	DA	3367	1/1	0.93	0.07	42,42,42,42	0
56	MG	BA	3392	1/1	0.93	0.23	56,56,56,56	0
56	MG	BA	3053	1/1	0.93	0.23	39,39,39,39	0
56	MG	DE	301	1/1	0.93	0.34	51,51,51,51	0
56	MG	CA	3084	1/1	0.93	0.17	64,64,64,64	0
56	MG	DF	301	1/1	0.93	0.25	32,32,32,32	0
56	MG	DA	3378	1/1	0.93	0.07	45,45,45,45	0
56	MG	BA	3058	1/1	0.93	0.18	38,38,38,38	0
56	MG	AA	3011	1/1	0.93	0.36	55,55,55,55	0
56	MG	CA	3096	1/1	0.93	0.09	60,60,60,60	0
56	MG	DQ	203	1/1	0.93	0.09	57,57,57,57	0
56	MG	BE	305	1/1	0.93	0.23	42,42,42,42	0
56	MG	BA	3060	1/1	0.93	0.28	40,40,40,40	0
56	MG	CA	3104	1/1	0.93	0.17	62,62,62,62	0
56	MG	DA	3391	1/1	0.93	0.07	41,41,41,41	0
56	MG	DA	3395	1/1	0.93	0.20	34,34,34,34	0
56	MG	BA	3188	1/1	0.93	0.13	37,37,37,37	0
56	MG	DA	3109	1/1	0.93	0.11	66,66,66,66	0
56	MG	BA	3114	1/1	0.93	0.27	51,51,51,51	0
56	MG	BF	307	1/1	0.93	0.07	47,47,47,47	0
56	MG	BA	3624	1/1	0.93	0.19	52,52,52,52	0
56	MG	DA	3409	1/1	0.93	0.09	32,32,32,32	0
56	MG	BA	3432	1/1	0.93	0.12	60,60,60,60	0
56	MG	BA	3115	1/1	0.93	0.30	36,36,36,36	0
56	MG	AA	3207	1/1	0.93	0.16	45,45,45,45	0
56	MG	DA	3433	1/1	0.94	0.15	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3434	1/1	0.94	0.23	49,49,49,49	0
56	MG	AA	3062	1/1	0.94	0.10	32,32,32,32	0
56	MG	DA	3436	1/1	0.94	0.09	62,62,62,62	0
56	MG	DA	3437	1/1	0.94	0.06	49,49,49,49	0
56	MG	BA	3603	1/1	0.94	0.05	39,39,39,39	0
56	MG	BA	3278	1/1	0.94	0.14	34,34,34,34	0
56	MG	DA	3441	1/1	0.94	0.25	53,53,53,53	0
56	MG	DA	3442	1/1	0.94	0.15	40,40,40,40	0
56	MG	BA	3607	1/1	0.94	0.34	53,53,53,53	0
56	MG	BA	3279	1/1	0.94	0.21	48,48,48,48	0
56	MG	AA	3031	1/1	0.94	0.15	41,41,41,41	0
56	MG	CA	3024	1/1	0.94	0.23	65,65,65,65	0
56	MG	BA	3728	1/1	0.94	0.23	32,32,32,32	0
56	MG	BA	3610	1/1	0.94	0.13	40,40,40,40	0
56	MG	BA	3028	1/1	0.94	0.10	48,48,48,48	0
56	MG	DA	3163	1/1	0.94	0.11	39,39,39,39	0
56	MG	BA	3062	1/1	0.94	0.24	42,42,42,42	0
56	MG	BA	3152	1/1	0.94	0.20	46,46,46,46	0
56	MG	BA	3616	1/1	0.94	0.13	33,33,33,33	0
56	MG	BA	3448	1/1	0.94	0.11	29,29,29,29	0
56	MG	AA	3028	1/1	0.94	0.21	60,60,60,60	0
56	MG	DA	3462	1/1	0.94	0.09	55,55,55,55	0
56	MG	BA	3155	1/1	0.94	0.18	57,57,57,57	0
56	MG	BA	3030	1/1	0.94	0.24	51,51,51,51	0
56	MG	BA	3461	1/1	0.94	0.10	36,36,36,36	0
56	MG	DA	3174	1/1	0.94	0.14	41,41,41,41	0
56	MG	BA	3212	1/1	0.94	0.21	43,43,43,43	0
56	MG	AA	3003	1/1	0.94	0.09	63,63,63,63	0
56	MG	DA	3480	1/1	0.94	0.10	52,52,52,52	0
56	MG	DA	3180	1/1	0.94	0.29	46,46,46,46	0
56	MG	BA	3625	1/1	0.94	0.17	51,51,51,51	0
56	MG	BA	3626	1/1	0.94	0.07	43,43,43,43	0
56	MG	BA	3034	1/1	0.94	0.26	52,52,52,52	0
56	MG	DA	3007	1/1	0.94	0.15	30,30,30,30	0
56	MG	CA	3043	1/1	0.94	0.15	49,49,49,49	0
56	MG	BA	3630	1/1	0.94	0.20	52,52,52,52	0
56	MG	CA	3045	1/1	0.94	0.14	54,54,54,54	0
56	MG	AA	3158	1/1	0.94	0.12	44,44,44,44	0
56	MG	DA	3193	1/1	0.94	0.14	65,65,65,65	0
56	MG	BA	3218	1/1	0.94	0.10	62,62,62,62	0
56	MG	BD	303	1/1	0.94	0.13	42,42,42,42	0
56	MG	DA	3498	1/1	0.94	0.07	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3470	1/1	0.94	0.15	54,54,54,54	0
56	MG	DA	3202	1/1	0.94	0.14	42,42,42,42	0
56	MG	DA	3206	1/1	0.94	0.20	42,42,42,42	0
56	MG	AA	3073	1/1	0.94	0.09	46,46,46,46	0
56	MG	BA	3163	1/1	0.94	0.10	50,50,50,50	0
56	MG	DA	3027	1/1	0.94	0.17	39,39,39,39	0
56	MG	BA	3228	1/1	0.94	0.15	63,63,63,63	0
56	MG	BA	3041	1/1	0.94	0.23	32,32,32,32	0
56	MG	BE	304	1/1	0.94	0.08	49,49,49,49	0
56	MG	DA	3033	1/1	0.94	0.11	39,39,39,39	0
56	MG	AA	3066	1/1	0.94	0.21	38,38,38,38	0
56	MG	CA	3060	1/1	0.94	0.27	43,43,43,43	0
56	MG	DA	3219	1/1	0.94	0.19	60,60,60,60	0
56	MG	DA	3220	1/1	0.94	0.10	37,37,37,37	0
56	MG	BA	3076	1/1	0.94	0.15	41,41,41,41	0
56	MG	BA	3116	1/1	0.94	0.20	31,31,31,31	0
56	MG	BA	3078	1/1	0.94	0.08	17,17,17,17	0
56	MG	DA	3042	1/1	0.94	0.22	36,36,36,36	0
56	MG	CA	3064	1/1	0.94	0.08	58,58,58,58	0
56	MG	DA	3227	1/1	0.94	0.17	53,53,53,53	0
56	MG	BA	3647	1/1	0.94	0.09	34,34,34,34	0
56	MG	DA	3232	1/1	0.94	0.20	50,50,50,50	0
56	MG	DA	3233	1/1	0.94	0.08	42,42,42,42	0
56	MG	DA	3045	1/1	0.94	0.22	41,41,41,41	0
56	MG	BA	3122	1/1	0.94	0.12	52,52,52,52	0
56	MG	BG	3001	1/1	0.94	0.07	64,64,64,64	0
56	MG	DA	3241	1/1	0.94	0.12	15,15,15,15	0
56	MG	BA	3177	1/1	0.94	0.08	62,62,62,62	0
56	MG	DA	3246	1/1	0.94	0.10	24,24,24,24	0
56	MG	DA	3247	1/1	0.94	0.06	31,31,31,31	0
56	MG	DA	3052	1/1	0.94	0.08	23,23,23,23	0
56	MG	DA	3551	1/1	0.94	0.12	52,52,52,52	0
56	MG	BA	3501	1/1	0.94	0.14	59,59,59,59	0
56	MG	AA	3103	1/1	0.94	0.21	38,38,38,38	0
56	MG	BA	3045	1/1	0.94	0.17	34,34,34,34	0
56	MG	BA	3328	1/1	0.94	0.10	42,42,42,42	0
56	MG	DA	3559	1/1	0.94	0.13	46,46,46,46	0
56	MG	BN	3004	1/1	0.94	0.18	66,66,66,66	0
56	MG	AA	3116	1/1	0.94	0.18	52,52,52,52	0
56	MG	DA	3264	1/1	0.94	0.13	49,49,49,49	0
56	MG	BO	201	1/1	0.94	0.09	70,70,70,70	0
56	MG	BA	3130	1/1	0.94	0.18	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3514	1/1	0.94	0.15	37,37,37,37	0
56	MG	DA	3572	1/1	0.94	0.10	53,53,53,53	0
56	MG	DA	3575	1/1	0.94	0.10	43,43,43,43	0
56	MG	DA	3577	1/1	0.94	0.11	44,44,44,44	0
56	MG	CA	3080	1/1	0.94	0.15	55,55,55,55	0
56	MG	DA	3580	1/1	0.94	0.18	46,46,46,46	0
56	MG	BA	3184	1/1	0.94	0.13	49,49,49,49	0
56	MG	DA	3273	1/1	0.94	0.06	30,30,30,30	0
56	MG	DA	3584	1/1	0.94	0.14	61,61,61,61	0
56	MG	DA	3585	1/1	0.94	0.09	62,62,62,62	0
56	MG	BA	3523	1/1	0.94	0.13	48,48,48,48	0
56	MG	DA	3275	1/1	0.94	0.08	38,38,38,38	0
56	MG	BR	202	1/1	0.94	0.08	27,27,27,27	0
56	MG	BR	204	1/1	0.94	0.17	43,43,43,43	0
56	MG	CA	3088	1/1	0.94	0.09	43,43,43,43	0
56	MG	DA	3281	1/1	0.94	0.13	42,42,42,42	0
56	MG	DA	3073	1/1	0.94	0.11	44,44,44,44	0
56	MG	CA	3089	1/1	0.94	0.12	52,52,52,52	0
56	MG	CA	3092	1/1	0.94	0.11	47,47,47,47	0
56	MG	CA	3093	1/1	0.94	0.07	53,53,53,53	0
56	MG	CA	3094	1/1	0.94	0.22	43,43,43,43	0
56	MG	DA	3079	1/1	0.94	0.06	37,37,37,37	0
56	MG	DA	3292	1/1	0.94	0.08	37,37,37,37	0
56	MG	BA	3185	1/1	0.94	0.20	47,47,47,47	0
56	MG	DA	3082	1/1	0.94	0.05	19,19,19,19	0
56	MG	BA	3339	1/1	0.94	0.07	43,43,43,43	0
56	MG	DA	3299	1/1	0.94	0.12	40,40,40,40	0
56	MG	BU	206	1/1	0.94	0.14	60,60,60,60	0
56	MG	BA	3251	1/1	0.94	0.15	61,61,61,61	0
56	MG	DA	3309	1/1	0.94	0.11	33,33,33,33	0
56	MG	DA	3310	1/1	0.94	0.12	53,53,53,53	0
56	MG	DA	3618	1/1	0.94	0.08	39,39,39,39	0
56	MG	DA	3312	1/1	0.94	0.27	43,43,43,43	0
56	MG	DA	3313	1/1	0.94	0.16	52,52,52,52	0
56	MG	DA	3622	1/1	0.94	0.08	55,55,55,55	0
56	MG	AA	3105	1/1	0.94	0.15	46,46,46,46	0
56	MG	CA	3107	1/1	0.94	0.12	60,60,60,60	0
56	MG	BA	3670	1/1	0.94	0.15	59,59,59,59	0
56	MG	AA	3042	1/1	0.94	0.14	44,44,44,44	0
56	MG	DA	3628	1/1	0.94	0.15	63,63,63,63	0
56	MG	BA	3254	1/1	0.94	0.15	59,59,59,59	0
56	MG	BA	3357	1/1	0.94	0.08	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3326	1/1	0.94	0.11	33,33,33,33	0
56	MG	BA	3548	1/1	0.94	0.20	50,50,50,50	0
56	MG	DA	3330	1/1	0.94	0.11	37,37,37,37	0
56	MG	B0	101	1/1	0.94	0.10	36,36,36,36	0
56	MG	CA	3118	1/1	0.94	0.07	37,37,37,37	0
56	MG	DA	3343	1/1	0.94	0.09	41,41,41,41	0
56	MG	BA	3255	1/1	0.94	0.11	41,41,41,41	0
56	MG	DA	3103	1/1	0.94	0.20	48,48,48,48	0
56	MG	DA	3645	1/1	0.94	0.07	30,30,30,30	0
56	MG	BA	3676	1/1	0.94	0.12	51,51,51,51	0
56	MG	BA	3677	1/1	0.94	0.15	67,67,67,67	0
56	MG	DA	3650	1/1	0.94	0.22	48,48,48,48	0
56	MG	BA	3550	1/1	0.94	0.19	45,45,45,45	0
56	MG	DA	3108	1/1	0.94	0.18	37,37,37,37	0
56	MG	BA	3087	1/1	0.94	0.07	61,61,61,61	0
56	MG	DA	3362	1/1	0.94	0.08	41,41,41,41	0
56	MG	AA	3107	1/1	0.94	0.18	44,44,44,44	0
56	MG	CA	3129	1/1	0.94	0.14	45,45,45,45	0
56	MG	DA	3366	1/1	0.94	0.20	36,36,36,36	0
56	MG	DB	3006	1/1	0.94	0.07	42,42,42,42	0
56	MG	CA	3131	1/1	0.94	0.08	55,55,55,55	0
56	MG	DA	3369	1/1	0.94	0.09	47,47,47,47	0
56	MG	BA	3555	1/1	0.94	0.12	53,53,53,53	0
56	MG	AA	3008	1/1	0.94	0.16	54,54,54,54	0
56	MG	B5	502	1/1	0.94	0.11	54,54,54,54	0
56	MG	BA	3260	1/1	0.94	0.12	22,22,22,22	0
56	MG	BA	3374	1/1	0.94	0.06	44,44,44,44	0
56	MG	B8	102	1/1	0.94	0.07	60,60,60,60	0
56	MG	BA	3138	1/1	0.94	0.18	46,46,46,46	0
56	MG	DE	302	1/1	0.94	0.14	44,44,44,44	0
56	MG	BA	3563	1/1	0.94	0.09	37,37,37,37	0
56	MG	DE	304	1/1	0.94	0.13	41,41,41,41	0
56	MG	BA	3568	1/1	0.94	0.14	47,47,47,47	0
56	MG	BA	3377	1/1	0.94	0.12	32,32,32,32	0
56	MG	DF	303	1/1	0.94	0.07	43,43,43,43	0
56	MG	DF	304	1/1	0.94	0.14	44,44,44,44	0
56	MG	DA	3128	1/1	0.94	0.12	52,52,52,52	0
56	MG	BA	3578	1/1	0.94	0.22	54,54,54,54	0
56	MG	BA	3139	1/1	0.94	0.18	51,51,51,51	0
56	MG	DQ	201	1/1	0.94	0.11	48,48,48,48	0
56	MG	DA	3399	1/1	0.94	0.08	41,41,41,41	0
56	MG	BA	3386	1/1	0.94	0.13	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3091	1/1	0.94	0.27	45,45,45,45	0
56	MG	DR	202	1/1	0.94	0.12	37,37,37,37	0
56	MG	BA	3591	1/1	0.94	0.16	48,48,48,48	0
56	MG	BA	3268	1/1	0.94	0.24	46,46,46,46	0
56	MG	AA	3121	1/1	0.94	0.17	51,51,51,51	0
56	MG	DA	3146	1/1	0.94	0.17	34,34,34,34	0
56	MG	BA	3274	1/1	0.94	0.20	52,52,52,52	0
56	MG	BA	3056	1/1	0.94	0.26	44,44,44,44	0
56	MG	DA	3149	1/1	0.94	0.06	47,47,47,47	0
56	MG	CA	3155	1/1	0.94	0.08	71,71,71,71	0
58	ZN	B4	3002	1/1	0.94	0.09	165,165,165,165	0
56	MG	DA	3423	1/1	0.94	0.08	29,29,29,29	0
56	MG	AA	3125	1/1	0.94	0.07	47,47,47,47	0
56	MG	DA	3430	1/1	0.94	0.16	55,55,55,55	0
56	MG	DA	3431	1/1	0.94	0.08	41,41,41,41	0
56	MG	BA	3721	1/1	0.95	0.07	25,25,25,25	0
56	MG	BA	3227	1/1	0.95	0.23	32,32,32,32	0
56	MG	BA	3120	1/1	0.95	0.13	51,51,51,51	0
56	MG	BA	3079	1/1	0.95	0.10	42,42,42,42	0
56	MG	DA	3443	1/1	0.95	0.09	53,53,53,53	0
56	MG	DA	3444	1/1	0.95	0.13	43,43,43,43	0
56	MG	DA	3165	1/1	0.95	0.16	44,44,44,44	0
56	MG	DA	3446	1/1	0.95	0.07	52,52,52,52	0
56	MG	BA	3729	1/1	0.95	0.22	46,46,46,46	0
56	MG	DA	3449	1/1	0.95	0.08	43,43,43,43	0
56	MG	BA	3730	1/1	0.95	0.34	45,45,45,45	0
56	MG	CA	3026	1/1	0.95	0.11	52,52,52,52	0
56	MG	BA	3452	1/1	0.95	0.13	47,47,47,47	0
56	MG	BA	3732	1/1	0.95	0.11	61,61,61,61	0
56	MG	BA	3170	1/1	0.95	0.52	48,48,48,48	0
56	MG	CF	3001	1/1	0.95	0.12	55,55,55,55	0
56	MG	BA	3232	1/1	0.95	0.07	29,29,29,29	0
56	MG	DA	3175	1/1	0.95	0.15	40,40,40,40	0
56	MG	BA	3171	1/1	0.95	0.12	40,40,40,40	0
56	MG	BA	3046	1/1	0.95	0.09	29,29,29,29	0
56	MG	DA	3179	1/1	0.95	0.22	46,46,46,46	0
56	MG	BA	3174	1/1	0.95	0.12	48,48,48,48	0
56	MG	CX	104	1/1	0.95	0.10	40,40,40,40	0
56	MG	BA	3301	1/1	0.95	0.08	56,56,56,56	0
56	MG	BA	3236	1/1	0.95	0.11	36,36,36,36	0
56	MG	DA	3469	1/1	0.95	0.11	47,47,47,47	0
56	MG	BA	3237	1/1	0.95	0.46	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3476	1/1	0.95	0.13	45,45,45,45	0
56	MG	DA	3004	1/1	0.95	0.05	29,29,29,29	0
56	MG	BA	3468	1/1	0.95	0.10	30,30,30,30	0
56	MG	DA	3188	1/1	0.95	0.14	47,47,47,47	0
56	MG	DA	3006	1/1	0.95	0.08	42,42,42,42	0
56	MG	BA	3175	1/1	0.95	0.10	48,48,48,48	0
56	MG	DA	3192	1/1	0.95	0.13	47,47,47,47	0
56	MG	BA	3176	1/1	0.95	0.10	38,38,38,38	0
56	MG	DA	3194	1/1	0.95	0.09	48,48,48,48	0
56	MG	DA	3488	1/1	0.95	0.06	46,46,46,46	0
56	MG	DA	3009	1/1	0.95	0.05	31,31,31,31	0
56	MG	BA	3476	1/1	0.95	0.09	40,40,40,40	0
56	MG	BA	3124	1/1	0.95	0.06	39,39,39,39	0
56	MG	DA	3199	1/1	0.95	0.04	42,42,42,42	0
56	MG	DA	3014	1/1	0.95	0.07	34,34,34,34	0
56	MG	BB	3010	1/1	0.95	0.12	40,40,40,40	0
56	MG	AA	3191	1/1	0.95	0.08	71,71,71,71	0
56	MG	BB	3015	1/1	0.95	0.08	37,37,37,37	0
56	MG	DA	3209	1/1	0.95	0.18	41,41,41,41	0
56	MG	DA	3020	1/1	0.95	0.19	52,52,52,52	0
56	MG	DA	3021	1/1	0.95	0.20	35,35,35,35	0
56	MG	BB	3016	1/1	0.95	0.14	21,21,21,21	0
56	MG	BA	3627	1/1	0.95	0.07	50,50,50,50	0
56	MG	DA	3505	1/1	0.95	0.06	65,65,65,65	0
56	MG	BA	3016	1/1	0.95	0.20	33,33,33,33	0
56	MG	BD	301	1/1	0.95	0.11	28,28,28,28	0
56	MG	BA	3084	1/1	0.95	0.12	33,33,33,33	0
56	MG	BA	3486	1/1	0.95	0.08	38,38,38,38	0
56	MG	DA	3513	1/1	0.95	0.09	49,49,49,49	0
56	MG	BA	3324	1/1	0.95	0.18	36,36,36,36	0
56	MG	BA	3633	1/1	0.95	0.08	58,58,58,58	0
56	MG	BA	3490	1/1	0.95	0.07	38,38,38,38	0
56	MG	DA	3035	1/1	0.95	0.09	56,56,56,56	0
56	MG	BD	310	1/1	0.95	0.11	48,48,48,48	0
56	MG	DA	3225	1/1	0.95	0.15	45,45,45,45	0
56	MG	DA	3523	1/1	0.95	0.11	55,55,55,55	0
56	MG	CA	3058	1/1	0.95	0.08	40,40,40,40	0
56	MG	CA	3059	1/1	0.95	0.16	51,51,51,51	0
56	MG	BD	311	1/1	0.95	0.13	45,45,45,45	0
56	MG	BA	3327	1/1	0.95	0.10	38,38,38,38	0
56	MG	AA	3104	1/1	0.95	0.09	37,37,37,37	0
56	MG	DA	3530	1/1	0.95	0.13	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3532	1/1	0.95	0.05	57,57,57,57	0
56	MG	DA	3533	1/1	0.95	0.11	68,68,68,68	0
56	MG	DA	3237	1/1	0.95	0.12	45,45,45,45	0
56	MG	BE	302	1/1	0.95	0.18	33,33,33,33	0
56	MG	BE	303	1/1	0.95	0.11	29,29,29,29	0
56	MG	BA	3497	1/1	0.95	0.14	62,62,62,62	0
56	MG	CA	3066	1/1	0.95	0.10	55,55,55,55	0
56	MG	DA	3242	1/1	0.95	0.18	35,35,35,35	0
56	MG	DA	3541	1/1	0.95	0.14	35,35,35,35	0
56	MG	DA	3049	1/1	0.95	0.14	58,58,58,58	0
56	MG	BA	3018	1/1	0.95	0.23	40,40,40,40	0
56	MG	BA	3642	1/1	0.95	0.19	51,51,51,51	0
56	MG	CA	3069	1/1	0.95	0.22	69,69,69,69	0
56	MG	DA	3549	1/1	0.95	0.19	52,52,52,52	0
56	MG	BA	3249	1/1	0.95	0.19	40,40,40,40	0
56	MG	BF	303	1/1	0.95	0.14	36,36,36,36	0
56	MG	BA	3500	1/1	0.95	0.07	37,37,37,37	0
56	MG	AA	3161	1/1	0.95	0.11	72,72,72,72	0
56	MG	AA	3177	1/1	0.95	0.08	80,80,80,80	0
56	MG	BA	3505	1/1	0.95	0.11	59,59,59,59	0
56	MG	BA	3338	1/1	0.95	0.15	50,50,50,50	0
56	MG	BA	3508	1/1	0.95	0.18	34,34,34,34	0
56	MG	BA	3054	1/1	0.95	0.23	46,46,46,46	0
56	MG	DA	3065	1/1	0.95	0.13	38,38,38,38	0
56	MG	DA	3066	1/1	0.95	0.33	53,53,53,53	0
56	MG	BA	3055	1/1	0.95	0.09	44,44,44,44	0
56	MG	BA	3351	1/1	0.95	0.06	30,30,30,30	0
56	MG	DA	3571	1/1	0.95	0.12	46,46,46,46	0
56	MG	BA	3352	1/1	0.95	0.10	34,34,34,34	0
56	MG	BA	3093	1/1	0.95	0.06	25,25,25,25	0
56	MG	BN	3006	1/1	0.95	0.04	24,24,24,24	0
56	MG	DA	3072	1/1	0.95	0.15	41,41,41,41	0
56	MG	BA	3522	1/1	0.95	0.09	49,49,49,49	0
56	MG	CA	3087	1/1	0.95	0.11	41,41,41,41	0
56	MG	BQ	201	1/1	0.95	0.23	61,61,61,61	0
56	MG	DA	3583	1/1	0.95	0.15	48,48,48,48	0
56	MG	DA	3076	1/1	0.95	0.27	44,44,44,44	0
56	MG	BA	3022	1/1	0.95	0.17	52,52,52,52	0
56	MG	CA	3091	1/1	0.95	0.05	72,72,72,72	0
56	MG	BA	3530	1/1	0.95	0.14	31,31,31,31	0
56	MG	DA	3290	1/1	0.95	0.06	42,42,42,42	0
56	MG	BA	3662	1/1	0.95	0.18	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3081	1/1	0.95	0.15	48,48,48,48	0
56	MG	BA	3355	1/1	0.95	0.12	64,64,64,64	0
56	MG	DA	3596	1/1	0.95	0.12	67,67,67,67	0
56	MG	CA	3095	1/1	0.95	0.10	39,39,39,39	0
56	MG	DA	3085	1/1	0.95	0.09	36,36,36,36	0
56	MG	DA	3297	1/1	0.95	0.10	57,57,57,57	0
56	MG	DA	3601	1/1	0.95	0.10	77,77,77,77	0
56	MG	AA	3213	1/1	0.95	0.10	29,29,29,29	0
56	MG	CA	3097	1/1	0.95	0.12	48,48,48,48	0
56	MG	BA	3540	1/1	0.95	0.14	34,34,34,34	0
56	MG	DA	3091	1/1	0.95	0.29	44,44,44,44	0
56	MG	CA	3100	1/1	0.95	0.08	60,60,60,60	0
56	MG	BA	3667	1/1	0.95	0.10	63,63,63,63	0
56	MG	DA	3094	1/1	0.95	0.09	26,26,26,26	0
56	MG	AA	3015	1/1	0.95	0.06	73,73,73,73	0
56	MG	DA	3611	1/1	0.95	0.05	42,42,42,42	0
56	MG	DA	3316	1/1	0.95	0.16	58,58,58,58	0
56	MG	DA	3614	1/1	0.95	0.07	48,48,48,48	0
56	MG	BA	3360	1/1	0.95	0.09	38,38,38,38	0
56	MG	BA	3361	1/1	0.95	0.12	34,34,34,34	0
56	MG	BA	3365	1/1	0.95	0.10	20,20,20,20	0
56	MG	BV	202	1/1	0.95	0.16	56,56,56,56	0
56	MG	DA	3619	1/1	0.95	0.06	48,48,48,48	0
56	MG	BA	3143	1/1	0.95	0.13	40,40,40,40	0
56	MG	AA	3123	1/1	0.95	0.29	39,39,39,39	0
56	MG	DA	3327	1/1	0.95	0.07	29,29,29,29	0
56	MG	DA	3328	1/1	0.95	0.09	28,28,28,28	0
56	MG	BW	203	1/1	0.95	0.17	45,45,45,45	0
56	MG	DA	3104	1/1	0.95	0.16	62,62,62,62	0
56	MG	DA	3332	1/1	0.95	0.11	33,33,33,33	0
56	MG	DA	3333	1/1	0.95	0.13	58,58,58,58	0
56	MG	DA	3334	1/1	0.95	0.14	49,49,49,49	0
56	MG	DA	3335	1/1	0.95	0.15	38,38,38,38	0
56	MG	BA	3100	1/1	0.95	0.31	48,48,48,48	0
56	MG	DA	3634	1/1	0.95	0.09	51,51,51,51	0
56	MG	CA	3116	1/1	0.95	0.14	76,76,76,76	0
56	MG	AA	3124	1/1	0.95	0.17	57,57,57,57	0
56	MG	DA	3637	1/1	0.95	0.15	48,48,48,48	0
56	MG	DA	3348	1/1	0.95	0.13	37,37,37,37	0
56	MG	DA	3349	1/1	0.95	0.16	54,54,54,54	0
56	MG	BX	3001	1/1	0.95	0.13	55,55,55,55	0
56	MG	CA	3121	1/1	0.95	0.25	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BY	201	1/1	0.95	0.28	58,58,58,58	0
56	MG	DA	3111	1/1	0.95	0.16	53,53,53,53	0
56	MG	DA	3646	1/1	0.95	0.07	38,38,38,38	0
56	MG	DA	3358	1/1	0.95	0.16	46,46,46,46	0
56	MG	BA	3202	1/1	0.95	0.08	41,41,41,41	0
56	MG	DA	3649	1/1	0.95	0.15	24,24,24,24	0
56	MG	AA	3150	1/1	0.95	0.18	46,46,46,46	0
56	MG	DA	3651	1/1	0.95	0.10	52,52,52,52	0
56	MG	DA	3114	1/1	0.95	0.06	37,37,37,37	0
56	MG	BA	3270	1/1	0.95	0.20	50,50,50,50	0
56	MG	DA	3116	1/1	0.95	0.14	39,39,39,39	0
56	MG	BA	3679	1/1	0.95	0.19	27,27,27,27	0
56	MG	BA	3273	1/1	0.95	0.26	42,42,42,42	0
56	MG	BA	3380	1/1	0.95	0.12	53,53,53,53	0
56	MG	DA	3120	1/1	0.95	0.30	51,51,51,51	0
56	MG	DA	3372	1/1	0.95	0.10	45,45,45,45	0
56	MG	DA	3373	1/1	0.95	0.13	29,29,29,29	0
56	MG	BA	3382	1/1	0.95	0.08	51,51,51,51	0
56	MG	BA	3383	1/1	0.95	0.11	38,38,38,38	0
56	MG	BA	3001	1/1	0.95	0.10	69,69,69,69	0
56	MG	BA	3564	1/1	0.95	0.05	52,52,52,52	0
56	MG	BA	3002	1/1	0.95	0.24	54,54,54,54	0
56	MG	BA	3036	1/1	0.95	0.12	38,38,38,38	0
56	MG	BA	3577	1/1	0.95	0.08	52,52,52,52	0
56	MG	DA	3129	1/1	0.95	0.06	43,43,43,43	0
56	MG	BA	3038	1/1	0.95	0.26	51,51,51,51	0
56	MG	DA	3133	1/1	0.95	0.17	33,33,33,33	0
56	MG	BA	3069	1/1	0.95	0.20	41,41,41,41	0
56	MG	DE	305	1/1	0.95	0.23	65,65,65,65	0
56	MG	AA	3186	1/1	0.95	0.06	49,49,49,49	0
56	MG	DA	3396	1/1	0.95	0.11	35,35,35,35	0
56	MG	DA	3136	1/1	0.95	0.06	49,49,49,49	0
56	MG	DA	3137	1/1	0.95	0.22	56,56,56,56	0
56	MG	CA	3144	1/1	0.95	0.20	63,63,63,63	0
56	MG	BA	3584	1/1	0.95	0.12	22,22,22,22	0
56	MG	BA	3004	1/1	0.95	0.08	24,24,24,24	0
56	MG	DA	3143	1/1	0.95	0.09	46,46,46,46	0
56	MG	DA	3405	1/1	0.95	0.11	47,47,47,47	0
56	MG	BA	3704	1/1	0.95	0.09	85,85,85,85	0
56	MG	BA	3590	1/1	0.95	0.10	64,64,64,64	0
56	MG	BA	3073	1/1	0.95	0.27	41,41,41,41	0
56	MG	AA	3188	1/1	0.95	0.15	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3007	1/1	0.95	0.05	35,35,35,35	0
56	MG	BA	3711	1/1	0.95	0.10	86,86,86,86	0
56	MG	AA	3018	1/1	0.95	0.15	38,38,38,38	0
56	MG	BA	3117	1/1	0.95	0.25	25,25,25,25	0
56	MG	AA	3049	1/1	0.95	0.20	51,51,51,51	0
56	MG	BA	3167	1/1	0.95	0.20	39,39,39,39	0
56	MG	DA	3432	1/1	0.95	0.11	66,66,66,66	0
56	MG	D8	5001	1/1	0.95	0.18	47,47,47,47	0
56	MG	CA	3015	1/1	0.95	0.12	51,51,51,51	0
56	MG	BA	3602	1/1	0.95	0.07	35,35,35,35	0
56	MG	CA	3017	1/1	0.95	0.15	42,42,42,42	0
56	MG	BA	3445	1/1	0.95	0.11	25,25,25,25	0
56	MG	CA	3162	1/1	0.95	0.13	46,46,46,46	0
56	MG	DA	3144	1/1	0.96	0.19	36,36,36,36	0
56	MG	AA	3214	1/1	0.96	0.14	75,75,75,75	0
56	MG	DA	3516	1/1	0.96	0.05	40,40,40,40	0
56	MG	AA	3199	1/1	0.96	0.09	88,88,88,88	0
56	MG	BA	3687	1/1	0.96	0.16	38,38,38,38	0
56	MG	DA	3520	1/1	0.96	0.07	51,51,51,51	0
56	MG	BA	3688	1/1	0.96	0.12	54,54,54,54	0
56	MG	BA	3261	1/1	0.96	0.25	34,34,34,34	0
56	MG	AA	3167	1/1	0.96	0.09	67,67,67,67	0
56	MG	AA	3153	1/1	0.96	0.14	45,45,45,45	0
56	MG	BA	3592	1/1	0.96	0.09	28,28,28,28	0
56	MG	BA	3335	1/1	0.96	0.09	35,35,35,35	0
56	MG	DA	3028	1/1	0.96	0.04	35,35,35,35	0
56	MG	CA	3082	1/1	0.96	0.06	47,47,47,47	0
56	MG	BA	3213	1/1	0.96	0.08	41,41,41,41	0
56	MG	DA	3531	1/1	0.96	0.10	57,57,57,57	0
56	MG	BA	3266	1/1	0.96	0.19	46,46,46,46	0
56	MG	BA	3698	1/1	0.96	0.06	41,41,41,41	0
56	MG	AA	3142	1/1	0.96	0.11	38,38,38,38	0
56	MG	BA	3106	1/1	0.96	0.18	48,48,48,48	0
56	MG	BA	3600	1/1	0.96	0.07	47,47,47,47	0
56	MG	DA	3038	1/1	0.96	0.10	39,39,39,39	0
56	MG	BA	3474	1/1	0.96	0.12	42,42,42,42	0
56	MG	BA	3345	1/1	0.96	0.09	33,33,33,33	0
56	MG	BA	3346	1/1	0.96	0.09	37,37,37,37	0
56	MG	DA	3542	1/1	0.96	0.11	32,32,32,32	0
56	MG	BA	3707	1/1	0.96	0.09	36,36,36,36	0
56	MG	AA	3143	1/1	0.96	0.10	45,45,45,45	0
56	MG	BA	3271	1/1	0.96	0.22	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3546	1/1	0.96	0.13	44,44,44,44	0
56	MG	DA	3344	1/1	0.96	0.07	26,26,26,26	0
56	MG	BA	3272	1/1	0.96	0.17	7,7,7,7	0
56	MG	AA	3171	1/1	0.96	0.14	72,72,72,72	0
56	MG	AA	3092	1/1	0.96	0.28	50,50,50,50	0
56	MG	DA	3351	1/1	0.96	0.15	35,35,35,35	0
56	MG	BA	3006	1/1	0.96	0.06	42,42,42,42	0
56	MG	DA	3050	1/1	0.96	0.12	31,31,31,31	0
56	MG	BA	3715	1/1	0.96	0.07	47,47,47,47	0
56	MG	DA	3558	1/1	0.96	0.08	37,37,37,37	0
56	MG	BA	3489	1/1	0.96	0.09	43,43,43,43	0
56	MG	DA	3560	1/1	0.96	0.05	34,34,34,34	0
56	MG	CA	3106	1/1	0.96	0.17	64,64,64,64	0
56	MG	BA	3226	1/1	0.96	0.20	32,32,32,32	0
56	MG	DA	3055	1/1	0.96	0.15	48,48,48,48	0
56	MG	BA	3494	1/1	0.96	0.16	18,18,18,18	0
56	MG	BA	3358	1/1	0.96	0.06	33,33,33,33	0
56	MG	B8	101	1/1	0.96	0.28	49,49,49,49	0
56	MG	DA	3569	1/1	0.96	0.14	37,37,37,37	0
56	MG	BA	3057	1/1	0.96	0.18	35,35,35,35	0
56	MG	CA	3112	1/1	0.96	0.10	59,59,59,59	0
56	MG	DA	3187	1/1	0.96	0.31	59,59,59,59	0
56	MG	BA	3726	1/1	0.96	0.21	47,47,47,47	0
56	MG	BA	3113	1/1	0.96	0.14	32,32,32,32	0
56	MG	DA	3579	1/1	0.96	0.09	23,23,23,23	0
56	MG	DA	3063	1/1	0.96	0.05	52,52,52,52	0
56	MG	AA	3160	1/1	0.96	0.17	52,52,52,52	0
56	MG	CA	3117	1/1	0.96	0.12	68,68,68,68	0
56	MG	BA	3035	1/1	0.96	0.04	37,37,37,37	0
56	MG	DA	3381	1/1	0.96	0.15	47,47,47,47	0
56	MG	BA	3150	1/1	0.96	0.20	34,34,34,34	0
56	MG	CA	3120	1/1	0.96	0.10	58,58,58,58	0
56	MG	DA	3588	1/1	0.96	0.07	40,40,40,40	0
56	MG	DA	3589	1/1	0.96	0.11	59,59,59,59	0
56	MG	BA	3623	1/1	0.96	0.09	47,47,47,47	0
56	MG	DA	3198	1/1	0.96	0.15	48,48,48,48	0
56	MG	AA	3208	1/1	0.96	0.15	46,46,46,46	0
56	MG	DA	3200	1/1	0.96	0.12	42,42,42,42	0
56	MG	DA	3201	1/1	0.96	0.06	48,48,48,48	0
56	MG	DA	3595	1/1	0.96	0.09	72,72,72,72	0
56	MG	BA	3734	1/1	0.96	0.22	45,45,45,45	0
56	MG	DA	3204	1/1	0.96	0.22	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3037	1/1	0.96	0.15	31,31,31,31	0
56	MG	BA	3503	1/1	0.96	0.12	31,31,31,31	0
56	MG	BA	3504	1/1	0.96	0.17	41,41,41,41	0
56	MG	BA	3285	1/1	0.96	0.13	32,32,32,32	0
56	MG	BA	3629	1/1	0.96	0.12	47,47,47,47	0
56	MG	BA	3506	1/1	0.96	0.09	30,30,30,30	0
56	MG	AA	3193	1/1	0.96	0.10	60,60,60,60	0
56	MG	BA	3154	1/1	0.96	0.10	61,61,61,61	0
56	MG	BA	3191	1/1	0.96	0.06	52,52,52,52	0
56	MG	BA	3379	1/1	0.96	0.13	22,22,22,22	0
56	MG	DA	3217	1/1	0.96	0.24	54,54,54,54	0
56	MG	BA	3635	1/1	0.96	0.08	78,78,78,78	0
56	MG	DA	3416	1/1	0.96	0.05	44,44,44,44	0
56	MG	DA	3419	1/1	0.96	0.07	31,31,31,31	0
56	MG	BA	3090	1/1	0.96	0.14	46,46,46,46	0
56	MG	DA	3422	1/1	0.96	0.07	38,38,38,38	0
56	MG	BA	3638	1/1	0.96	0.09	37,37,37,37	0
56	MG	BA	3513	1/1	0.96	0.06	45,45,45,45	0
56	MG	DA	3428	1/1	0.96	0.18	51,51,51,51	0
56	MG	DA	3429	1/1	0.96	0.17	44,44,44,44	0
56	MG	BA	3240	1/1	0.96	0.17	28,28,28,28	0
56	MG	DA	3088	1/1	0.96	0.05	46,46,46,46	0
56	MG	BA	3121	1/1	0.96	0.21	57,57,57,57	0
56	MG	BA	3521	1/1	0.96	0.09	49,49,49,49	0
56	MG	BA	3194	1/1	0.96	0.07	55,55,55,55	0
56	MG	BA	3243	1/1	0.96	0.18	48,48,48,48	0
56	MG	BA	3527	1/1	0.96	0.10	64,64,64,64	0
56	MG	DA	3229	1/1	0.96	0.04	40,40,40,40	0
56	MG	DA	3230	1/1	0.96	0.13	62,62,62,62	0
56	MG	BA	3010	1/1	0.96	0.14	32,32,32,32	0
56	MG	BA	3533	1/1	0.96	0.08	32,32,32,32	0
56	MG	DA	3235	1/1	0.96	0.09	50,50,50,50	0
56	MG	DA	3236	1/1	0.96	0.15	46,46,46,46	0
56	MG	BA	3389	1/1	0.96	0.06	48,48,48,48	0
56	MG	BA	3536	1/1	0.96	0.09	27,27,27,27	0
56	MG	AA	3057	1/1	0.96	0.04	37,37,37,37	0
56	MG	BD	307	1/1	0.96	0.08	43,43,43,43	0
56	MG	DA	3448	1/1	0.96	0.15	57,57,57,57	0
56	MG	BD	308	1/1	0.96	0.17	23,23,23,23	0
56	MG	BD	309	1/1	0.96	0.13	42,42,42,42	0
56	MG	BA	3013	1/1	0.96	0.07	40,40,40,40	0
56	MG	BA	3125	1/1	0.96	0.10	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3542	1/1	0.96	0.16	19,19,19,19	0
56	MG	BA	3398	1/1	0.96	0.08	41,41,41,41	0
56	MG	BA	3401	1/1	0.96	0.06	42,42,42,42	0
56	MG	BA	3659	1/1	0.96	0.16	46,46,46,46	0
56	MG	BA	3200	1/1	0.96	0.14	25,25,25,25	0
56	MG	DA	3253	1/1	0.96	0.10	42,42,42,42	0
56	MG	CA	3165	1/1	0.96	0.08	40,40,40,40	0
56	MG	BA	3404	1/1	0.96	0.12	35,35,35,35	0
56	MG	BE	306	1/1	0.96	0.16	46,46,46,46	0
56	MG	BA	3303	1/1	0.96	0.08	35,35,35,35	0
56	MG	BA	3409	1/1	0.96	0.13	27,27,27,27	0
56	MG	CA	3051	1/1	0.96	0.10	63,63,63,63	0
56	MG	DA	3468	1/1	0.96	0.07	48,48,48,48	0
56	MG	BA	3415	1/1	0.96	0.14	27,27,27,27	0
56	MG	DA	3470	1/1	0.96	0.12	52,52,52,52	0
56	MG	BA	3419	1/1	0.96	0.08	24,24,24,24	0
56	MG	DA	3473	1/1	0.96	0.20	32,32,32,32	0
56	MG	BA	3161	1/1	0.96	0.21	49,49,49,49	0
56	MG	DA	3270	1/1	0.96	0.14	36,36,36,36	0
56	MG	DD	304	1/1	0.96	0.17	35,35,35,35	0
56	MG	DA	3272	1/1	0.96	0.12	27,27,27,27	0
56	MG	DD	307	1/1	0.96	0.09	38,38,38,38	0
56	MG	DD	308	1/1	0.96	0.06	55,55,55,55	0
56	MG	BA	3250	1/1	0.96	0.11	45,45,45,45	0
56	MG	BA	3557	1/1	0.96	0.17	31,31,31,31	0
56	MG	BG	3002	1/1	0.96	0.15	42,42,42,42	0
56	MG	DA	3276	1/1	0.96	0.08	36,36,36,36	0
56	MG	BA	3162	1/1	0.96	0.15	23,23,23,23	0
56	MG	DA	3485	1/1	0.96	0.05	38,38,38,38	0
56	MG	BA	3126	1/1	0.96	0.13	24,24,24,24	0
56	MG	BA	3435	1/1	0.96	0.13	24,24,24,24	0
56	MG	BA	3438	1/1	0.96	0.12	30,30,30,30	0
56	MG	DA	3490	1/1	0.96	0.08	39,39,39,39	0
56	MG	DA	3282	1/1	0.96	0.07	36,36,36,36	0
56	MG	DA	3283	1/1	0.96	0.06	33,33,33,33	0
56	MG	DO	5001	1/1	0.96	0.08	35,35,35,35	0
56	MG	BA	3014	1/1	0.96	0.28	34,34,34,34	0
56	MG	AA	3149	1/1	0.96	0.09	50,50,50,50	0
56	MG	BA	3566	1/1	0.96	0.07	53,53,53,53	0
56	MG	AA	3122	1/1	0.96	0.34	44,44,44,44	0
56	MG	BA	3314	1/1	0.96	0.11	24,24,24,24	0
56	MG	BP	201	1/1	0.96	0.30	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BP	202	1/1	0.96	0.09	40,40,40,40	0
56	MG	DA	3501	1/1	0.96	0.12	23,23,23,23	0
56	MG	BP	203	1/1	0.96	0.41	29,29,29,29	0
56	MG	DA	3138	1/1	0.96	0.15	42,42,42,42	0
56	MG	DY	502	1/1	0.96	0.09	60,60,60,60	0
56	MG	DA	3011	1/1	0.96	0.10	45,45,45,45	0
56	MG	DA	3295	1/1	0.96	0.19	39,39,39,39	0
56	MG	DA	3507	1/1	0.96	0.13	54,54,54,54	0
56	MG	D5	102	1/1	0.96	0.17	55,55,55,55	0
56	MG	DA	3508	1/1	0.96	0.11	38,38,38,38	0
56	MG	AA	3166	1/1	0.96	0.10	48,48,48,48	0
58	ZN	D4	501	1/1	0.96	0.11	153,153,153,153	0
56	MG	BA	3322	1/1	0.96	0.14	22,22,22,22	0
56	MG	DA	3298	1/1	0.96	0.13	37,37,37,37	0
56	MG	BA	3208	1/1	0.96	0.11	41,41,41,41	0
56	MG	DA	3302	1/1	0.96	0.09	22,22,22,22	0
56	MG	BA	3308	1/1	0.97	0.06	44,44,44,44	0
56	MG	BA	3397	1/1	0.97	0.07	28,28,28,28	0
56	MG	CE	3002	1/1	0.97	0.06	55,55,55,55	0
56	MG	AA	3078	1/1	0.97	0.23	42,42,42,42	0
56	MG	BA	3636	1/1	0.97	0.06	36,36,36,36	0
56	MG	DA	3305	1/1	0.97	0.06	33,33,33,33	0
56	MG	BA	3517	1/1	0.97	0.10	49,49,49,49	0
56	MG	DA	3308	1/1	0.97	0.06	30,30,30,30	0
56	MG	DA	3142	1/1	0.97	0.24	33,33,33,33	0
56	MG	BA	3518	1/1	0.97	0.08	41,41,41,41	0
56	MG	DA	3311	1/1	0.97	0.08	32,32,32,32	0
56	MG	BA	3258	1/1	0.97	0.24	40,40,40,40	0
56	MG	AA	3157	1/1	0.97	0.05	35,35,35,35	0
56	MG	BA	3178	1/1	0.97	0.11	48,48,48,48	0
56	MG	BA	3524	1/1	0.97	0.22	55,55,55,55	0
56	MG	BA	3525	1/1	0.97	0.13	43,43,43,43	0
56	MG	BA	3526	1/1	0.97	0.08	19,19,19,19	0
56	MG	BA	3032	1/1	0.97	0.13	49,49,49,49	0
56	MG	CA	3050	1/1	0.97	0.10	43,43,43,43	0
56	MG	DA	3529	1/1	0.97	0.12	63,63,63,63	0
56	MG	DA	3323	1/1	0.97	0.06	30,30,30,30	0
56	MG	DA	3324	1/1	0.97	0.18	40,40,40,40	0
56	MG	BA	3528	1/1	0.97	0.13	33,33,33,33	0
56	MG	BA	3408	1/1	0.97	0.07	24,24,24,24	0
56	MG	AA	3130	1/1	0.97	0.17	46,46,46,46	0
56	MG	DA	3010	1/1	0.97	0.09	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3220	1/1	0.97	0.09	57,57,57,57	0
56	MG	BA	3416	1/1	0.97	0.25	42,42,42,42	0
56	MG	AA	3075	1/1	0.97	0.09	52,52,52,52	0
56	MG	BA	3652	1/1	0.97	0.14	64,64,64,64	0
56	MG	DA	3160	1/1	0.97	0.10	44,44,44,44	0
56	MG	BA	3538	1/1	0.97	0.08	36,36,36,36	0
56	MG	DA	3339	1/1	0.97	0.07	37,37,37,37	0
56	MG	BA	3539	1/1	0.97	0.09	35,35,35,35	0
56	MG	DA	3017	1/1	0.97	0.07	46,46,46,46	0
56	MG	BE	307	1/1	0.97	0.17	39,39,39,39	0
56	MG	BA	3655	1/1	0.97	0.11	52,52,52,52	0
56	MG	DA	3346	1/1	0.97	0.11	29,29,29,29	0
56	MG	DA	3166	1/1	0.97	0.06	32,32,32,32	0
56	MG	BE	310	1/1	0.97	0.08	50,50,50,50	0
56	MG	DA	3552	1/1	0.97	0.07	34,34,34,34	0
56	MG	BA	3326	1/1	0.97	0.13	41,41,41,41	0
56	MG	BA	3265	1/1	0.97	0.13	20,20,20,20	0
56	MG	BA	3222	1/1	0.97	0.19	25,25,25,25	0
56	MG	DA	3025	1/1	0.97	0.27	44,44,44,44	0
56	MG	BF	305	1/1	0.97	0.09	35,35,35,35	0
56	MG	BF	306	1/1	0.97	0.09	37,37,37,37	0
56	MG	BA	3330	1/1	0.97	0.09	39,39,39,39	0
56	MG	BA	3544	1/1	0.97	0.13	27,27,27,27	0
56	MG	DA	3031	1/1	0.97	0.11	55,55,55,55	0
56	MG	DA	3177	1/1	0.97	0.06	33,33,33,33	0
56	MG	BA	3433	1/1	0.97	0.14	39,39,39,39	0
56	MG	DA	3364	1/1	0.97	0.07	32,32,32,32	0
56	MG	BA	3267	1/1	0.97	0.15	41,41,41,41	0
56	MG	BA	3223	1/1	0.97	0.23	47,47,47,47	0
56	MG	DA	3570	1/1	0.97	0.14	28,28,28,28	0
56	MG	BA	3665	1/1	0.97	0.11	39,39,39,39	0
56	MG	BA	3439	1/1	0.97	0.07	34,34,34,34	0
56	MG	DA	3573	1/1	0.97	0.11	40,40,40,40	0
56	MG	DA	3574	1/1	0.97	0.09	56,56,56,56	0
56	MG	DA	3370	1/1	0.97	0.12	38,38,38,38	0
56	MG	DA	3576	1/1	0.97	0.08	38,38,38,38	0
56	MG	DA	3371	1/1	0.97	0.05	44,44,44,44	0
56	MG	BA	3333	1/1	0.97	0.16	49,49,49,49	0
56	MG	BA	3441	1/1	0.97	0.14	25,25,25,25	0
56	MG	BA	3443	1/1	0.97	0.09	26,26,26,26	0
56	MG	DA	3375	1/1	0.97	0.08	60,60,60,60	0
56	MG	BA	3224	1/1	0.97	0.25	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3148	1/1	0.97	0.25	52,52,52,52	0
56	MG	BA	3556	1/1	0.97	0.14	27,27,27,27	0
56	MG	BA	3149	1/1	0.97	0.12	40,40,40,40	0
56	MG	AA	3198	1/1	0.97	0.06	87,87,87,87	0
56	MG	CA	3083	1/1	0.97	0.07	39,39,39,39	0
56	MG	BA	3449	1/1	0.97	0.06	21,21,21,21	0
56	MG	BP	204	1/1	0.97	0.07	55,55,55,55	0
56	MG	BA	3118	1/1	0.97	0.12	39,39,39,39	0
56	MG	BA	3229	1/1	0.97	0.14	22,22,22,22	0
56	MG	BA	3453	1/1	0.97	0.09	18,18,18,18	0
56	MG	DA	3393	1/1	0.97	0.10	41,41,41,41	0
56	MG	BA	3454	1/1	0.97	0.06	22,22,22,22	0
56	MG	BA	3455	1/1	0.97	0.10	47,47,47,47	0
56	MG	DA	3397	1/1	0.97	0.11	41,41,41,41	0
56	MG	BA	3682	1/1	0.97	0.11	38,38,38,38	0
56	MG	BA	3341	1/1	0.97	0.04	33,33,33,33	0
56	MG	BA	3571	1/1	0.97	0.06	65,65,65,65	0
56	MG	DA	3203	1/1	0.97	0.08	41,41,41,41	0
56	MG	BU	202	1/1	0.97	0.23	32,32,32,32	0
56	MG	DA	3403	1/1	0.97	0.08	28,28,28,28	0
56	MG	DA	3205	1/1	0.97	0.09	38,38,38,38	0
56	MG	BU	203	1/1	0.97	0.07	33,33,33,33	0
56	MG	DA	3408	1/1	0.97	0.19	37,37,37,37	0
56	MG	BA	3685	1/1	0.97	0.07	67,67,67,67	0
56	MG	AA	3183	1/1	0.97	0.09	42,42,42,42	0
56	MG	DA	3411	1/1	0.97	0.06	21,21,21,21	0
56	MG	BU	207	1/1	0.97	0.11	40,40,40,40	0
56	MG	CA	3101	1/1	0.97	0.07	70,70,70,70	0
56	MG	CA	3102	1/1	0.97	0.06	41,41,41,41	0
56	MG	BA	3574	1/1	0.97	0.07	54,54,54,54	0
56	MG	BA	3576	1/1	0.97	0.13	23,23,23,23	0
56	MG	DA	3214	1/1	0.97	0.10	64,64,64,64	0
56	MG	DA	3421	1/1	0.97	0.16	34,34,34,34	0
56	MG	BA	3458	1/1	0.97	0.07	29,29,29,29	0
56	MG	AA	3215	1/1	0.97	0.09	53,53,53,53	0
56	MG	DA	3424	1/1	0.97	0.07	30,30,30,30	0
56	MG	DA	3426	1/1	0.97	0.15	74,74,74,74	0
56	MG	BV	204	1/1	0.97	0.12	20,20,20,20	0
56	MG	BA	3347	1/1	0.97	0.08	25,25,25,25	0
56	MG	BA	3349	1/1	0.97	0.12	43,43,43,43	0
56	MG	BA	3582	1/1	0.97	0.12	25,25,25,25	0
56	MG	AA	3145	1/1	0.97	0.11	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3585	1/1	0.97	0.06	51,51,51,51	0
56	MG	BA	3587	1/1	0.97	0.12	23,23,23,23	0
56	MG	DA	3633	1/1	0.97	0.14	54,54,54,54	0
56	MG	BA	3465	1/1	0.97	0.08	40,40,40,40	0
56	MG	BA	3589	1/1	0.97	0.09	51,51,51,51	0
56	MG	BA	3701	1/1	0.97	0.09	32,32,32,32	0
56	MG	BA	3702	1/1	0.97	0.07	56,56,56,56	0
56	MG	BA	3190	1/1	0.97	0.08	42,42,42,42	0
56	MG	AX	107	1/1	0.97	0.05	66,66,66,66	0
56	MG	AA	3185	1/1	0.97	0.15	46,46,46,46	0
56	MG	DA	3642	1/1	0.97	0.06	35,35,35,35	0
56	MG	CA	3122	1/1	0.97	0.14	47,47,47,47	0
56	MG	BA	3095	1/1	0.97	0.15	55,55,55,55	0
56	MG	BA	3471	1/1	0.97	0.18	51,51,51,51	0
56	MG	BA	3596	1/1	0.97	0.06	51,51,51,51	0
56	MG	BA	3473	1/1	0.97	0.06	51,51,51,51	0
56	MG	BA	3710	1/1	0.97	0.13	48,48,48,48	0
56	MG	DA	3090	1/1	0.97	0.10	47,47,47,47	0
56	MG	B7	102	1/1	0.97	0.07	40,40,40,40	0
56	MG	BA	3042	1/1	0.97	0.41	47,47,47,47	0
56	MG	B7	104	1/1	0.97	0.07	51,51,51,51	0
56	MG	BA	3283	1/1	0.97	0.08	17,17,17,17	0
56	MG	DA	3244	1/1	0.97	0.18	29,29,29,29	0
56	MG	CA	3134	1/1	0.97	0.06	82,82,82,82	0
56	MG	BA	3195	1/1	0.97	0.10	47,47,47,47	0
56	MG	BA	3239	1/1	0.97	0.11	33,33,33,33	0
56	MG	CA	3137	1/1	0.97	0.08	48,48,48,48	0
56	MG	DB	3005	1/1	0.97	0.20	43,43,43,43	0
56	MG	BA	3286	1/1	0.97	0.14	32,32,32,32	0
56	MG	BA	3364	1/1	0.97	0.08	29,29,29,29	0
56	MG	BA	3019	1/1	0.97	0.09	39,39,39,39	0
56	MG	BA	3605	1/1	0.97	0.13	59,59,59,59	0
56	MG	DA	3463	1/1	0.97	0.11	43,43,43,43	0
56	MG	DA	3255	1/1	0.97	0.12	40,40,40,40	0
56	MG	BA	3720	1/1	0.97	0.11	33,33,33,33	0
56	MG	DD	301	1/1	0.97	0.08	46,46,46,46	0
56	MG	DA	3257	1/1	0.97	0.05	48,48,48,48	0
56	MG	DD	303	1/1	0.97	0.08	19,19,19,19	0
56	MG	DA	3467	1/1	0.97	0.04	35,35,35,35	0
56	MG	DA	3258	1/1	0.97	0.11	32,32,32,32	0
56	MG	DA	3259	1/1	0.97	0.16	47,47,47,47	0
56	MG	BA	3606	1/1	0.97	0.15	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3261	1/1	0.97	0.10	35,35,35,35	0
56	MG	DA	3472	1/1	0.97	0.07	36,36,36,36	0
56	MG	BA	3485	1/1	0.97	0.13	44,44,44,44	0
56	MG	DA	3474	1/1	0.97	0.05	61,61,61,61	0
56	MG	BA	3070	1/1	0.97	0.13	35,35,35,35	0
56	MG	DA	3477	1/1	0.97	0.06	49,49,49,49	0
56	MG	BA	3367	1/1	0.97	0.04	50,50,50,50	0
56	MG	AX	110	1/1	0.97	0.15	42,42,42,42	0
56	MG	AA	3151	1/1	0.97	0.05	41,41,41,41	0
56	MG	BA	3131	1/1	0.97	0.40	54,54,54,54	0
56	MG	DF	306	1/1	0.97	0.12	50,50,50,50	0
56	MG	AA	3172	1/1	0.97	0.09	53,53,53,53	0
56	MG	AA	3146	1/1	0.97	0.09	48,48,48,48	0
56	MG	BA	3733	1/1	0.97	0.08	27,27,27,27	0
56	MG	BA	3375	1/1	0.97	0.14	31,31,31,31	0
56	MG	DQ	202	1/1	0.97	0.15	34,34,34,34	0
56	MG	BA	3024	1/1	0.97	0.19	35,35,35,35	0
56	MG	DQ	204	1/1	0.97	0.13	43,43,43,43	0
56	MG	BA	3025	1/1	0.97	0.08	28,28,28,28	0
56	MG	BA	3077	1/1	0.97	0.10	39,39,39,39	0
56	MG	BA	3137	1/1	0.97	0.13	42,42,42,42	0
56	MG	DV	201	1/1	0.97	0.08	55,55,55,55	0
56	MG	BA	3026	1/1	0.97	0.09	36,36,36,36	0
56	MG	DA	3121	1/1	0.97	0.07	48,48,48,48	0
56	MG	DA	3493	1/1	0.97	0.08	29,29,29,29	0
56	MG	BA	3299	1/1	0.97	0.11	9,9,9,9	0
56	MG	AA	3174	1/1	0.97	0.10	33,33,33,33	0
56	MG	BA	3385	1/1	0.97	0.07	26,26,26,26	0
56	MG	BA	3172	1/1	0.97	0.44	48,48,48,48	0
56	MG	BA	3109	1/1	0.97	0.05	36,36,36,36	0
56	MG	BA	3388	1/1	0.97	0.12	34,34,34,34	0
56	MG	BA	3305	1/1	0.97	0.11	44,44,44,44	0
56	MG	AA	3163	1/1	0.97	0.08	28,28,28,28	0
56	MG	DA	3130	1/1	0.97	0.10	32,32,32,32	0
58	ZN	CN	501	1/1	0.97	0.04	108,108,108,108	0
56	MG	AA	3154	1/1	0.97	0.09	63,63,63,63	0
56	MG	DA	3132	1/1	0.97	0.22	54,54,54,54	0
56	MG	BB	3012	1/1	0.97	0.09	56,56,56,56	0
56	MG	BB	3013	1/1	0.97	0.06	39,39,39,39	0
56	MG	BA	3512	1/1	0.97	0.12	40,40,40,40	0
56	MG	BA	3410	1/1	0.98	0.05	27,27,27,27	0
56	MG	CA	3098	1/1	0.98	0.14	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3329	1/1	0.98	0.10	29,29,29,29	0
56	MG	BE	309	1/1	0.98	0.12	25,25,25,25	0
56	MG	AA	3205	1/1	0.98	0.10	61,61,61,61	0
56	MG	DA	3315	1/1	0.98	0.04	31,31,31,31	0
56	MG	BF	301	1/1	0.98	0.17	45,45,45,45	0
56	MG	BA	3483	1/1	0.98	0.07	53,53,53,53	0
56	MG	BA	3417	1/1	0.98	0.11	18,18,18,18	0
56	MG	DA	3586	1/1	0.98	0.04	29,29,29,29	0
56	MG	DA	3451	1/1	0.98	0.05	49,49,49,49	0
56	MG	DA	3320	1/1	0.98	0.13	30,30,30,30	0
56	MG	BA	3552	1/1	0.98	0.17	29,29,29,29	0
56	MG	AA	3091	1/1	0.98	0.06	75,75,75,75	0
56	MG	BA	3421	1/1	0.98	0.09	36,36,36,36	0
56	MG	DA	3019	1/1	0.98	0.05	30,30,30,30	0
56	MG	BA	3063	1/1	0.98	0.18	43,43,43,43	0
56	MG	BA	3425	1/1	0.98	0.14	36,36,36,36	0
56	MG	CA	3023	1/1	0.98	0.06	37,37,37,37	0
56	MG	BA	3369	1/1	0.98	0.06	45,45,45,45	0
56	MG	BA	3491	1/1	0.98	0.08	23,23,23,23	0
56	MG	BA	3492	1/1	0.98	0.12	23,23,23,23	0
56	MG	DA	3331	1/1	0.98	0.08	34,34,34,34	0
56	MG	DA	3026	1/1	0.98	0.06	37,37,37,37	0
56	MG	BA	3427	1/1	0.98	0.10	48,48,48,48	0
56	MG	BA	3428	1/1	0.98	0.08	45,45,45,45	0
56	MG	BA	3064	1/1	0.98	0.08	39,39,39,39	0
56	MG	DA	3605	1/1	0.98	0.05	44,44,44,44	0
56	MG	DA	3336	1/1	0.98	0.06	27,27,27,27	0
56	MG	DA	3337	1/1	0.98	0.06	27,27,27,27	0
56	MG	DA	3338	1/1	0.98	0.07	29,29,29,29	0
56	MG	BA	3565	1/1	0.98	0.04	55,55,55,55	0
56	MG	BA	3431	1/1	0.98	0.12	17,17,17,17	0
56	MG	DA	3341	1/1	0.98	0.08	23,23,23,23	0
56	MG	BA	3567	1/1	0.98	0.13	37,37,37,37	0
56	MG	DA	3475	1/1	0.98	0.10	36,36,36,36	0
56	MG	BA	3371	1/1	0.98	0.06	15,15,15,15	0
56	MG	BA	3569	1/1	0.98	0.13	19,19,19,19	0
56	MG	BA	3570	1/1	0.98	0.09	61,61,61,61	0
56	MG	DA	3347	1/1	0.98	0.11	62,62,62,62	0
56	MG	AV	101	1/1	0.98	0.09	36,36,36,36	0
56	MG	DA	3037	1/1	0.98	0.19	35,35,35,35	0
56	MG	BA	3722	1/1	0.98	0.08	32,32,32,32	0
56	MG	BA	3723	1/1	0.98	0.07	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3234	1/1	0.98	0.10	33,33,33,33	0
56	MG	BA	3572	1/1	0.98	0.13	36,36,36,36	0
56	MG	DA	3625	1/1	0.98	0.09	35,35,35,35	0
56	MG	DA	3354	1/1	0.98	0.05	27,27,27,27	0
56	MG	DA	3355	1/1	0.98	0.10	18,18,18,18	0
56	MG	CA	3128	1/1	0.98	0.09	41,41,41,41	0
56	MG	CA	3040	1/1	0.98	0.19	42,42,42,42	0
56	MG	CA	3130	1/1	0.98	0.06	65,65,65,65	0
56	MG	BA	3725	1/1	0.98	0.10	49,49,49,49	0
56	MG	BA	3033	1/1	0.98	0.17	35,35,35,35	0
56	MG	BQ	204	1/1	0.98	0.04	12,12,12,12	0
56	MG	DA	3047	1/1	0.98	0.06	34,34,34,34	0
56	MG	BA	3436	1/1	0.98	0.04	37,37,37,37	0
56	MG	BA	3437	1/1	0.98	0.06	42,42,42,42	0
56	MG	DA	3245	1/1	0.98	0.09	37,37,37,37	0
56	MG	AA	3187	1/1	0.98	0.04	62,62,62,62	0
56	MG	BR	203	1/1	0.98	0.06	15,15,15,15	0
56	MG	BA	3337	1/1	0.98	0.07	23,23,23,23	0
56	MG	AA	3179	1/1	0.98	0.18	34,34,34,34	0
56	MG	DA	3250	1/1	0.98	0.05	31,31,31,31	0
56	MG	BA	3051	1/1	0.98	0.09	20,20,20,20	0
56	MG	BA	3581	1/1	0.98	0.04	51,51,51,51	0
56	MG	AA	3156	1/1	0.98	0.11	62,62,62,62	0
56	MG	AA	3220	1/1	0.98	0.05	40,40,40,40	0
56	MG	AA	3010	1/1	0.98	0.10	70,70,70,70	0
56	MG	BA	3092	1/1	0.98	0.11	51,51,51,51	0
56	MG	DA	3379	1/1	0.98	0.08	28,28,28,28	0
56	MG	AA	3182	1/1	0.98	0.05	49,49,49,49	0
56	MG	DA	3382	1/1	0.98	0.05	25,25,25,25	0
56	MG	BA	3348	1/1	0.98	0.06	64,64,64,64	0
56	MG	DA	3384	1/1	0.98	0.06	23,23,23,23	0
56	MG	DA	3385	1/1	0.98	0.08	35,35,35,35	0
56	MG	BA	3217	1/1	0.98	0.07	28,28,28,28	0
56	MG	BA	3451	1/1	0.98	0.11	28,28,28,28	0
56	MG	AA	3144	1/1	0.98	0.07	48,48,48,48	0
56	MG	DA	3262	1/1	0.98	0.08	44,44,44,44	0
56	MG	BW	202	1/1	0.98	0.15	34,34,34,34	0
56	MG	BA	3219	1/1	0.98	0.07	65,65,65,65	0
56	MG	DA	3392	1/1	0.98	0.08	35,35,35,35	0
56	MG	BA	3315	1/1	0.98	0.08	37,37,37,37	0
56	MG	DA	3394	1/1	0.98	0.06	47,47,47,47	0
56	MG	CA	3154	1/1	0.98	0.11	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3595	1/1	0.98	0.11	41,41,41,41	0
56	MG	BB	3007	1/1	0.98	0.05	47,47,47,47	0
56	MG	BA	3519	1/1	0.98	0.10	39,39,39,39	0
56	MG	BA	3390	1/1	0.98	0.10	30,30,30,30	0
56	MG	BA	3316	1/1	0.98	0.05	28,28,28,28	0
56	MG	BA	3012	1/1	0.98	0.12	40,40,40,40	0
56	MG	BA	3393	1/1	0.98	0.06	38,38,38,38	0
56	MG	BA	3459	1/1	0.98	0.12	31,31,31,31	0
56	MG	DA	3277	1/1	0.98	0.14	49,49,49,49	0
56	MG	BA	3096	1/1	0.98	0.16	62,62,62,62	0
56	MG	DA	3406	1/1	0.98	0.06	40,40,40,40	0
56	MG	BA	3395	1/1	0.98	0.09	25,25,25,25	0
56	MG	DE	306	1/1	0.98	0.07	32,32,32,32	0
56	MG	DA	3540	1/1	0.98	0.21	54,54,54,54	0
56	MG	B3	101	1/1	0.98	0.10	28,28,28,28	0
56	MG	AA	3056	1/1	0.98	0.07	39,39,39,39	0
56	MG	BA	3529	1/1	0.98	0.13	35,35,35,35	0
56	MG	BA	3325	1/1	0.98	0.12	58,58,58,58	0
56	MG	DA	3413	1/1	0.98	0.08	53,53,53,53	0
56	MG	DA	3083	1/1	0.98	0.05	41,41,41,41	0
56	MG	BA	3532	1/1	0.98	0.13	34,34,34,34	0
56	MG	BA	3399	1/1	0.98	0.14	18,18,18,18	0
56	MG	DA	3417	1/1	0.98	0.11	34,34,34,34	0
56	MG	BA	3400	1/1	0.98	0.06	24,24,24,24	0
56	MG	BA	3359	1/1	0.98	0.05	23,23,23,23	0
56	MG	BA	3179	1/1	0.98	0.11	43,43,43,43	0
56	MG	BA	3612	1/1	0.98	0.07	37,37,37,37	0
56	MG	BA	3469	1/1	0.98	0.05	38,38,38,38	0
56	MG	BA	3614	1/1	0.98	0.17	30,30,30,30	0
56	MG	DA	3425	1/1	0.98	0.05	27,27,27,27	0
56	MG	CA	3001	1/1	0.98	0.11	55,55,55,55	0
56	MG	BA	3403	1/1	0.98	0.11	41,41,41,41	0
56	MG	DA	3561	1/1	0.98	0.07	45,45,45,45	0
56	MG	AA	3165	1/1	0.98	0.09	23,23,23,23	0
56	MG	BA	3362	1/1	0.98	0.07	43,43,43,43	0
56	MG	CA	3090	1/1	0.98	0.08	73,73,73,73	0
56	MG	BA	3406	1/1	0.98	0.05	28,28,28,28	0
56	MG	DA	3301	1/1	0.98	0.14	45,45,45,45	0
56	MG	BA	3363	1/1	0.98	0.07	39,39,39,39	0
56	MG	DA	3568	1/1	0.98	0.05	42,42,42,42	0
56	MG	BA	3015	1/1	0.98	0.26	44,44,44,44	0
57	SF4	CD	501	8/8	0.98	0.04	64,75,91,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	ZN	AN	102	1/1	0.98	0.03	90,90,90,90	0
56	MG	DA	3304	1/1	0.98	0.07	35,35,35,35	0
56	MG	BA	3477	1/1	0.98	0.04	25,25,25,25	0
58	ZN	DY	501	1/1	0.98	0.03	83,83,83,83	0
56	MG	DA	3306	1/1	0.98	0.09	33,33,33,33	0
58	ZN	D9	501	1/1	0.98	0.04	66,66,66,66	0
56	MG	DA	3101	1/1	0.98	0.09	48,48,48,48	0
56	MG	DA	3439	1/1	0.98	0.10	28,28,28,28	0
56	MG	BA	3696	1/1	0.98	0.10	39,39,39,39	0
56	MG	BA	3478	1/1	0.98	0.11	29,29,29,29	0
56	MG	BU	205	1/1	0.99	0.09	42,42,42,42	0
56	MG	DA	3289	1/1	0.99	0.03	26,26,26,26	0
56	MG	DA	3345	1/1	0.99	0.03	31,31,31,31	0
56	MG	BA	3442	1/1	0.99	0.09	12,12,12,12	0
56	MG	CA	3115	1/1	0.99	0.03	55,55,55,55	0
56	MG	BA	3413	1/1	0.99	0.05	20,20,20,20	0
56	MG	DA	3407	1/1	0.99	0.09	21,21,21,21	0
56	MG	BA	3414	1/1	0.99	0.09	19,19,19,19	0
56	MG	BA	3317	1/1	0.99	0.10	40,40,40,40	0
56	MG	BA	3342	1/1	0.99	0.06	31,31,31,31	0
56	MG	DA	3190	1/1	0.99	0.03	37,37,37,37	0
56	MG	BA	3681	1/1	0.99	0.12	40,40,40,40	0
56	MG	BA	3553	1/1	0.99	0.03	31,31,31,31	0
56	MG	BA	3447	1/1	0.99	0.06	37,37,37,37	0
56	MG	DA	3300	1/1	0.99	0.06	37,37,37,37	0
56	MG	DA	3600	1/1	0.99	0.03	45,45,45,45	0
56	MG	BA	3480	1/1	0.99	0.09	17,17,17,17	0
56	MG	BA	3516	1/1	0.99	0.03	47,47,47,47	0
56	MG	DA	3418	1/1	0.99	0.12	29,29,29,29	0
56	MG	DD	305	1/1	0.99	0.20	49,49,49,49	0
56	MG	BA	3343	1/1	0.99	0.08	40,40,40,40	0
56	MG	BA	3418	1/1	0.99	0.08	27,27,27,27	0
56	MG	BA	3344	1/1	0.99	0.05	30,30,30,30	0
56	MG	BA	3420	1/1	0.99	0.10	33,33,33,33	0
56	MG	BA	3561	1/1	0.99	0.08	24,24,24,24	0
56	MG	BA	3318	1/1	0.99	0.04	33,33,33,33	0
56	MG	BA	3396	1/1	0.99	0.08	22,22,22,22	0
56	MG	BA	3487	1/1	0.99	0.07	31,31,31,31	0
56	MG	DA	3612	1/1	0.99	0.03	39,39,39,39	0
56	MG	DA	3548	1/1	0.99	0.04	37,37,37,37	0
56	MG	DA	3368	1/1	0.99	0.04	39,39,39,39	0
56	MG	BA	3423	1/1	0.99	0.08	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3695	1/1	0.99	0.10	15,15,15,15	0
56	MG	BA	3424	1/1	0.99	0.07	15,15,15,15	0
56	MG	BA	3378	1/1	0.99	0.02	20,20,20,20	0
56	MG	BA	3319	1/1	0.99	0.07	25,25,25,25	0
56	MG	BA	3310	1/1	0.99	0.09	13,13,13,13	0
56	MG	DA	3556	1/1	0.99	0.03	56,56,56,56	0
56	MG	BA	3493	1/1	0.99	0.11	15,15,15,15	0
56	MG	BA	3656	1/1	0.99	0.04	33,33,33,33	0
56	MG	BA	3531	1/1	0.99	0.16	38,38,38,38	0
56	MG	BA	3381	1/1	0.99	0.05	37,37,37,37	0
56	MG	BB	3011	1/1	0.99	0.08	37,37,37,37	0
56	MG	DA	3380	1/1	0.99	0.04	26,26,26,26	0
56	MG	BA	3460	1/1	0.99	0.05	33,33,33,33	0
56	MG	DA	3629	1/1	0.99	0.06	19,19,19,19	0
56	MG	BA	3534	1/1	0.99	0.04	41,41,41,41	0
56	MG	BA	3575	1/1	0.99	0.09	51,51,51,51	0
56	MG	DA	3271	1/1	0.99	0.11	37,37,37,37	0
56	MG	B8	103	1/1	0.99	0.06	24,24,24,24	0
56	MG	BA	3321	1/1	0.99	0.09	29,29,29,29	0
56	MG	DA	3506	1/1	0.99	0.05	59,59,59,59	0
56	MG	AA	3152	1/1	0.99	0.04	19,19,19,19	0
56	MG	BA	3350	1/1	0.99	0.04	47,47,47,47	0
56	MG	BA	3323	1/1	0.99	0.06	23,23,23,23	0
56	MG	DA	3639	1/1	0.99	0.13	15,15,15,15	0
56	MG	BA	3434	1/1	0.99	0.04	32,32,32,32	0
57	SF4	AD	501	8/8	0.99	0.04	59,72,92,96	0
56	MG	BA	3128	1/1	0.99	0.08	40,40,40,40	0
56	MG	AX	109	1/1	0.99	0.08	43,43,43,43	0
58	ZN	BY	202	1/1	0.99	0.02	71,71,71,71	0
56	MG	BA	3081	1/1	0.99	0.03	14,14,14,14	0
58	ZN	B5	501	1/1	0.99	0.02	54,54,54,54	0
56	MG	BA	3302	1/1	0.99	0.06	27,27,27,27	0
56	MG	BA	3716	1/1	0.99	0.05	27,27,27,27	0
56	MG	BA	3586	1/1	0.99	0.08	29,29,29,29	0
58	ZN	D5	103	1/1	0.99	0.02	70,70,70,70	0
58	ZN	D6	501	1/1	0.99	0.04	61,61,61,61	0
56	MG	AA	3192	1/1	0.99	0.07	57,57,57,57	0
56	MG	DA	3518	1/1	0.99	0.03	40,40,40,40	0
56	MG	BA	3411	1/1	0.99	0.08	38,38,38,38	0
56	MG	BA	3472	1/1	0.99	0.07	30,30,30,30	0
56	MG	BA	3412	1/1	0.99	0.08	26,26,26,26	0
56	MG	BA	3520	1/1	1.00	0.07	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3407	1/1	1.00	0.06	15,15,15,15	0
56	MG	BA	3429	1/1	1.00	0.05	20,20,20,20	0
56	MG	DA	3486	1/1	1.00	0.03	38,38,38,38	0
56	MG	DA	3317	1/1	1.00	0.03	32,32,32,32	0
56	MG	BA	3583	1/1	1.00	0.07	27,27,27,27	0
56	MG	DA	3263	1/1	1.00	0.05	31,31,31,31	0
56	MG	DA	3356	1/1	1.00	0.02	27,27,27,27	0
58	ZN	B6	501	1/1	1.00	0.04	49,49,49,49	0
58	ZN	B9	501	1/1	1.00	0.03	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.