



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 09:38 PM BST

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 validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

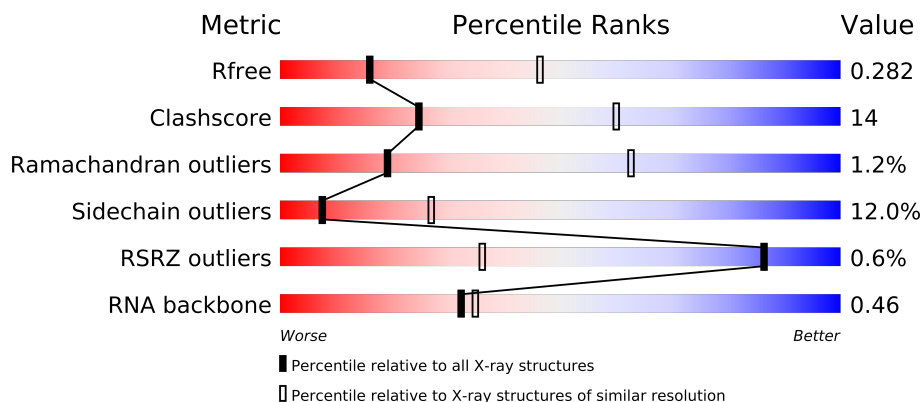
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : stable23397
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23397

1 Overall quality at a glance

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}	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)
RNA backbone	1838	1047 (3.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	1522	
1	CA	1522	
2	AB	256	
2	CB	256	
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	

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Mol	Chain	Length	Quality of chain
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	
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	
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	

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Mol	Chain	Length	Quality of chain
49	B3	60	
49	D3	60	
50	B4	71	
50	D4	71	
51	B5	60	
51	D5	60	
52	B6	54	
52	D6	54	
53	B7	49	
53	D7	49	
54	B8	65	
54	D8	65	
55	B9	37	
55	D9	37	

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 286321 atoms, of which 0 are hydrogen and 0 are deuterium.

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	B4	1	Total	Mg	0	0
			1	1		
56	BA	738	Total	Mg	0	0
			738	738		
56	AK	1	Total	Mg	0	0
			1	1		
56	DQ	5	Total	Mg	0	0
			5	5		
56	D3	1	Total	Mg	0	0
			1	1		
56	DF	6	Total	Mg	0	0
			6	6		
56	B8	3	Total	Mg	0	0
			3	3		
56	BE	10	Total	Mg	0	0
			10	10		
56	B1	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AN	2	Total 2	Mg 2	0	0
56	BP	4	Total 4	Mg 4	0	0
56	AX	9	Total 9	Mg 9	0	0
56	DN	1	Total 1	Mg 1	0	0
56	CA	172	Total 172	Mg 172	0	0
56	B5	1	Total 1	Mg 1	0	0
56	BB	18	Total 18	Mg 18	0	0
56	D8	1	Total 1	Mg 1	0	0
56	DG	1	Total 1	Mg 1	0	0
56	B9	1	Total 1	Mg 1	0	0
56	BF	8	Total 8	Mg 8	0	0
56	AV	1	Total 1	Mg 1	0	0
56	BX	1	Total 1	Mg 1	0	0
56	B2	1	Total 1	Mg 1	0	0
56	AA	221	Total 221	Mg 221	0	0
56	BQ	5	Total 5	Mg 5	0	0
56	CQ	1	Total 1	Mg 1	0	0
56	CX	3	Total 3	Mg 3	0	0
56	DV	4	Total 4	Mg 4	0	0
56	AM	1	Total 1	Mg 1	0	0
56	BU	8	Total 8	Mg 8	0	0

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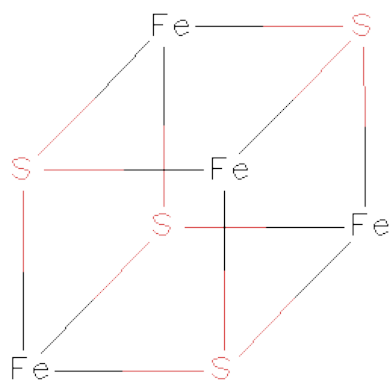
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DR	2	Total 2	Mg 2	0	0
56	AD	1	Total 1	Mg 1	0	0
56	BN	6	Total 6	Mg 6	0	0
56	CT	1	Total 1	Mg 1	0	0
56	D0	1	Total 1	Mg 1	0	0
56	BG	4	Total 4	Mg 4	0	0
56	BY	1	Total 1	Mg 1	0	0
56	DE	6	Total 6	Mg 6	0	0
56	B3	3	Total 3	Mg 3	0	0
56	BR	4	Total 4	Mg 4	0	0
56	DA	653	Total 653	Mg 653	0	0
56	DW	2	Total 2	Mg 2	0	0
56	B7	4	Total 4	Mg 4	0	0
56	CF	1	Total 1	Mg 1	0	0
56	BV	4	Total 4	Mg 4	0	0
56	DO	1	Total 1	Mg 1	0	0
56	BO	1	Total 1	Mg 1	0	0
56	BZ	1	Total 1	Mg 1	0	0
56	DY	1	Total 1	Mg 1	0	0
56	D5	2	Total 2	Mg 2	0	0
56	BD	12	Total 12	Mg 12	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B0	4	Total	Mg	0	0
			4	4		
56	CE	2	Total	Mg	0	0
			2	2		
56	BW	5	Total	Mg	0	0
			5	5		
56	DD	8	Total	Mg	0	0
			8	8		
56	AF	1	Total	Mg	0	0
			1	1		
56	DB	12	Total	Mg	0	0
			12	12		

- 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).

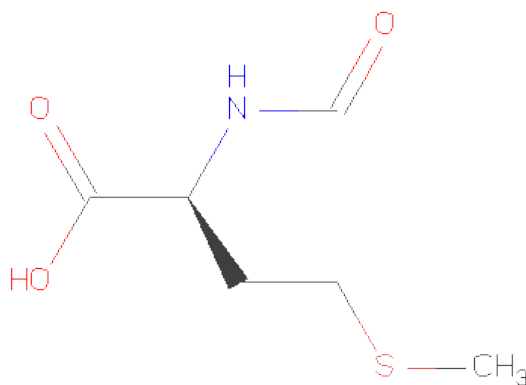
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	B5	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	B4	1	Total	Zn	0	0
			1	1		
58	CN	1	Total	Zn	0	0
			1	1		
58	BY	1	Total	Zn	0	0
			1	1		
58	B9	1	Total	Zn	0	0
			1	1		
58	DY	1	Total	Zn	0	0
			1	1		
58	D5	1	Total	Zn	0	0
			1	1		
58	D4	1	Total	Zn	0	0
			1	1		
58	AN	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		
58	B6	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	O	0	0
			1	1		
61	BN	3	Total	O	0	0
			3	3		
61	BO	2	Total	O	0	0
			2	2		
61	BP	15	Total	O	0	0
			15	15		
61	BQ	3	Total	O	0	0
			3	3		
61	BR	1	Total	O	0	0
			1	1		
61	BT	1	Total	O	0	0
			1	1		
61	BU	4	Total	O	0	0
			4	4		
61	BV	2	Total	O	0	0
			2	2		
61	BW	2	Total	O	0	0
			2	2		
61	BX	4	Total	O	0	0
			4	4		
61	B0	4	Total	O	0	0
			4	4		
61	B1	2	Total	O	0	0
			2	2		
61	B5	3	Total	O	0	0
			3	3		
61	B7	1	Total	O	0	0
			1	1		
61	B8	8	Total	O	0	0
			8	8		
61	CA	187	Total	O	0	0
			187	187		
61	CE	2	Total	O	0	0
			2	2		
61	CN	1	Total	O	0	0
			1	1		
61	CT	1	Total	O	0	0
			1	1		
61	CX	2	Total	O	0	0
			2	2		

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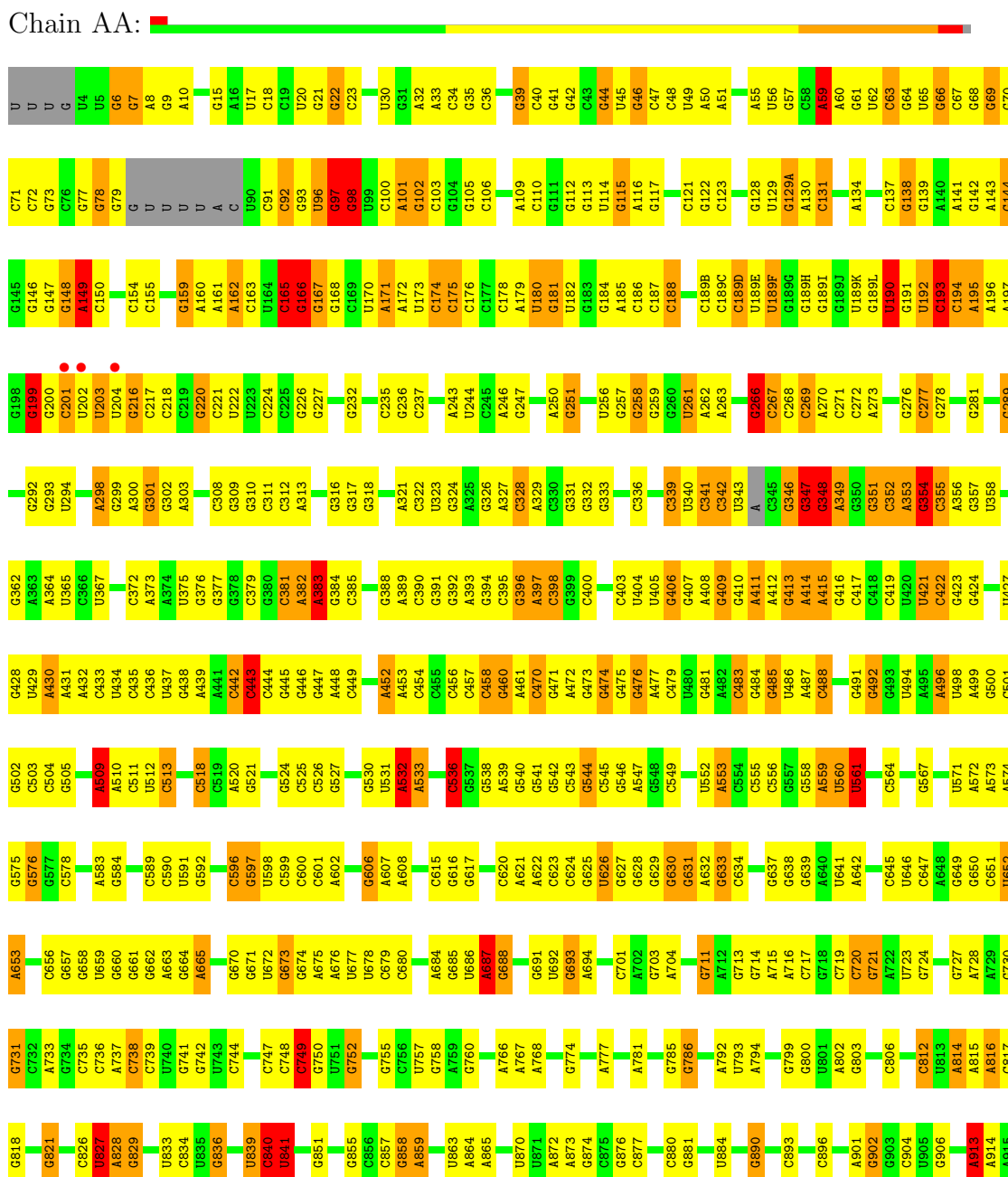
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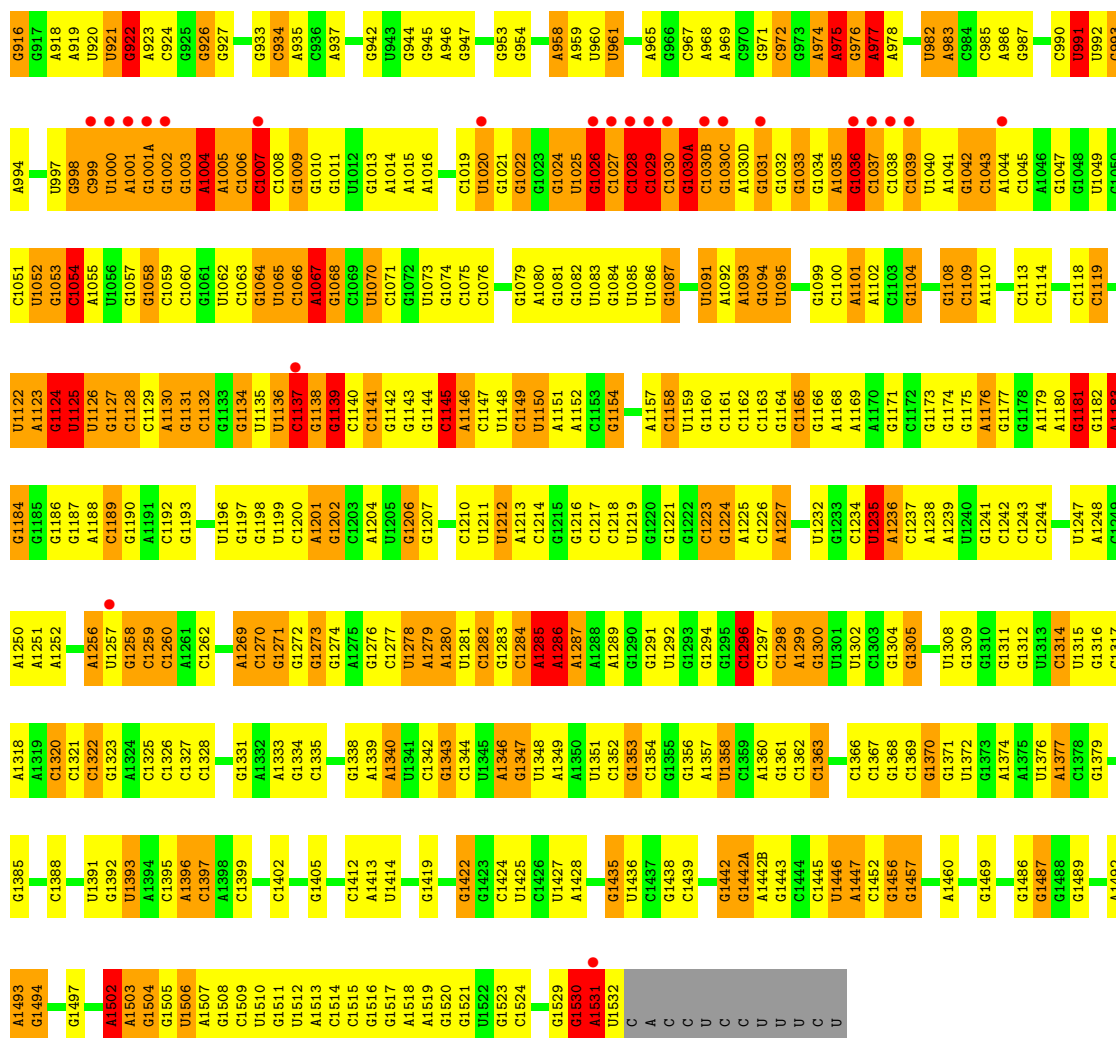
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	DA	902	Total 902	O 902	0	0
61	DB	7	Total 7	O 7	0	0
61	DD	8	Total 8	O 8	0	0
61	DE	13	Total 13	O 13	0	0
61	DF	5	Total 5	O 5	0	0
61	DO	1	Total 1	O 1	0	0
61	DP	14	Total 14	O 14	0	0
61	DQ	3	Total 3	O 3	0	0
61	DU	4	Total 4	O 4	0	0
61	DV	1	Total 1	O 1	0	0
61	DX	2	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 and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

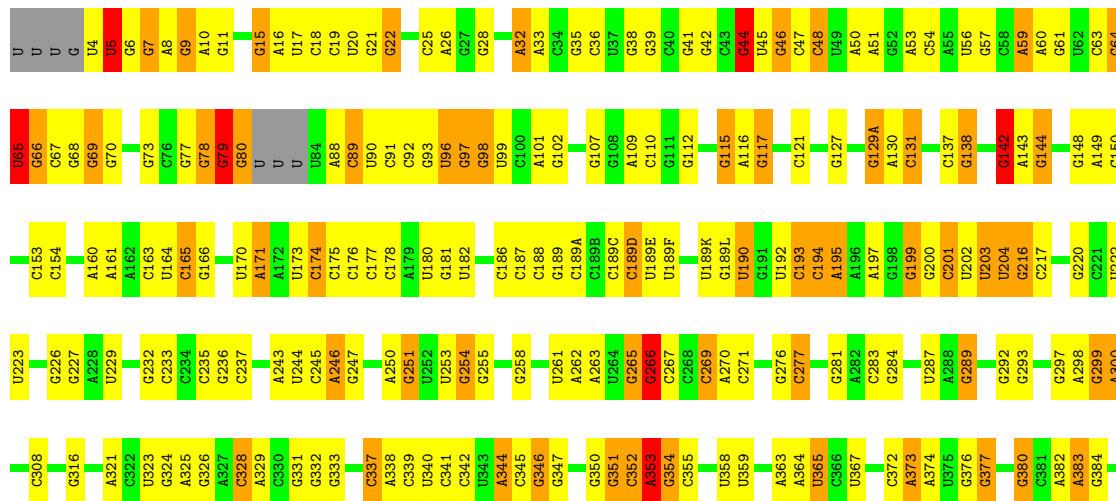
• Molecule 1: 16S Ribosomal RNA





• Molecule 1: 16S Ribosomal RNA

Chain CA:

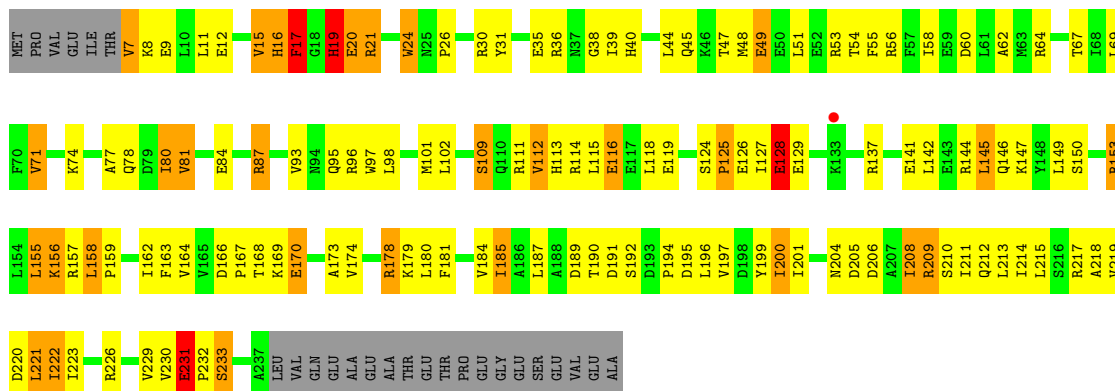


C1445	C1362	C1297	C1228	A1168	A1105	A1041	C985	A919	C934	G752	C680	A608	G538	C454	G388
U1446	C1363	C1298	G1233	A1169	G1106	G1042	A986	U920	U835	A753	C683	A609	A539	C455	A389
A1447	C1366	A1299	C1234	A1170	G1107	G1043	C989	U921	G836	G754	G684	G610	G540	C456	C390
G1452	C1367	G1300	G1171	G1171	G1108	A1044	C989	G922	G837	G755	A684	G611	G541	C457	G391
G1456	C1368	C1367	G1172	G1172	C1109	G1047	C991	G923	G838	G756	G685	G615	G542	C458	G392
G1457	C1369	C1304	G1173	G1173	A1110	G1048	U991	G924	U839	U757	U686	G616	C543	C460	A393
G1458	G1370	G1305	G1174	G1174	A1111	C1051	U992	G925	C940	G758	A687	A461	G544	A461	
C1459	A1239	A1306	G1175	G1175	C1112	G1056	G993	G926	U841	A759	G688	C470	C545	C471	G396
A1460	G1371	G1307	A1176	A1176	C1113	G1057	A994	G927	C948	G760	C689	A472	G546	A472	C397
G1461	U1372	U1307	G1177	G1177	C1116	G1058	A995	G928	C949	G761	C690	A473	G547	A473	C398
C1465	G1373	U1308	G1178	G1178	G1117	G1059	A996	C931	U850	A767	G691	A622		C474	C400
C1466	A1374	C1242	A1179	A1179	G1118	A1054	U997	C932	G851	A768	U692	C623	U551	C475	C401
C1467	A1375	C1243	A1180	A1180	C1119	U1055	C999	C933	G855	G769	G693	C624	U552	G402	
G1469	U1376	C1244	G1181	G1181	G1120	U1056	C999	G934		G774	A694	C625	A553	C403	
C1479	A1377	A1245	G1182	G1182	G1121	G1057	U1000	C935	G858	G775	C701	U626	C554	G494	
G1480	C1312	C1246	A1183	A1183	U1121	G1058	A1001	A935	A859	G776	A704	G627	C555	A496	
C1484	U1313	G1249	G1184	G1184	A1122	C1059	U1001A	C936	A860	A777	U705	G628	C556	U486	
U1485	U1315	A1250	G1185	G1185	A1123	G1060	G1003	A937	G861		A706	G629	G557	A487	G406
G1486	C1316	A1251	G1186	G1186	G1124	G1061	G1003	A938	G861	C783	U706	G630	G558	C488	G407
G1487	C1317	A1252	G1187	G1187	U1125	U1062	A1004	C939		C784	A707	G631	A559	C489	A408
C1488	C1318		G1188	G1188	U1126	C1063	A1005	C940	A865	G785	C707	A632	U560	G490	G409
G1489	C1319	A1256	C1189	C1189	G1127	U1064	C1006	G941	C968	G786	G708	G634	C562	G491	G410
C1490	U1320	U1257	G1190	G1190	C1128	U1065	C1007	G942	G869	G790	G710	G635	A563	G492	A411
G1491	C1321	A1191	A1192	A1192	U1129	C1066	G1008	G947		A791	G711	G638	C564	U494	A412
A1492	G1322	G1193	G1193	G1193	A1130	A1067	G1009	C948	A872	G791	A712	G639	C565	A495	A413
A1493	A1323	U1194	U1194	U1194	G1131	G1068	G1010		A873	A792	G713	A640	U565	A496	A414
G1494	C1324	C1195	C1195	C1195	C1132	C1069	G1011	G951	G874	A793	G714	U641	G568	U498	C418
C1497	C1325	G1196	G1196	G1196	G1133	C1071	U1012	U952	C980	G800	A715	A642	U571	A499	G500
U1498	C1326	U1197	U1197	U1197	G1134	G1071	C1013	G953	C981	U801	A716		A572	C501	C419
A1499	C1327	G1198	G1198	G1198	U1135	G1072	A1014	G954	G876	A802		U646	C578	G502	
C1500	C1328	G1199	G1199	G1199	C1136	U1073	G1015	U955	C877	G803	G719	U647	C579	A509	
C1501	C1329	U1200	U1200	U1200	C1137	G1074	A1016	U956	G878	U804	G720	C647	C580	A510	G428
A1502	U1330	A1201	G1200	G1200	G1138	C1075	G1017	U957	C980	G805	G721	A648	U582	C511	G429
A1503	C1331	G1202	G1202	G1202	C1139	U1076	C1018	A958	C982	C806	G722	G650	U583	C512	G430
G1504	A1400	C1203	C1203	C1203	G1140	G1077	U1020	U959	G885	C811	G723	C651	G584	C513	A431
C1505	C1401	A1204	A1204	A1204	C1141	U1078	G1021	U960		C812	G724	U652	G585	C514	
G1506	C1402	U1205	U1205	U1205	G1142	A1080	G1022	U961	G890	C813	G725	A653	C586	C515	A432
A1507	G1403	G1206	G1206	G1206	G1143	G1081	G1023	A964	U891	C814	G726	A654	C587	C516	A433
C1508	C1411	C1207	C1207	C1207	G1144	G1082	G1024	A965	U892	C815	G727	A655	G588	C517	A434
G1509	C1412	G1208	G1208	G1208	C1145	U1085	U1025	G966	U893	C816	G728	A656	C589	A520	C435
C1510	U1413	C1209	C1209	C1209	A1146	G1086	G1026	G967	C993	C817	G729	G662	C590	G521	C436
U1510	G1415	G1210	G1210	G1210	C1147	U1087	C1027	A968	G894	C818	G730	G663	C591	C522	C437
G1511	C1419	U1211	U1211	U1211	U1148	G1088	G1028	A969		C819	G731	G664	C592	C523	C438
U1512	C1420	U1212	U1212	U1212	U1150	G1089	C1029	A970	C999	C820	G732	G665	U591	C524	A439
A1513	G1421	A1213	A1213	A1213	A1151	U1090	G1030	A971	A900	A814	A733	G666	G592	C525	A441
C1514	G1422	U1281	C1214	C1214	A1152	G1091	G1030A	G972	A901	A815	G734	G667	C593	C526	C442
G1515	G1423	G1215	G1215	G1215	C1153	U1092	C1030B	C973	G902	A816	G735	G668	C594	C527	C443
C1516	G1427	G1283	G1216	G1216	G1154	A1092	G1030C	A974	G906	C817	G736	G669	C595	C528	C444
G1517	U1427	C1284	C1217	C1217	G1155	A1093	A1030D	A975	A907	C818	G737	G670	C596	C529	C445
A1518	A1428	A1285	U1218	U1218	G1156	G1094	G1031	A976	A908	C819	G738	G671	C597	C530	C446
G1519	G1435	A1286	G1219	G1219	A1157	U1095	G1032	A977	U826	C821	G739	U672	C598	C531	C447
C1520	U1436	A1287	G1220	G1220	C1158	G1096	G1033	A978	A909	C822	U740	G673	C599	C532	A448
U1522	C1354	A1288	G1221	G1221	U1159	C1097	G1034	C979	A813	C823	G741	G674	C600	C533	
G1523	C1355	A1289	G1222	G1222	G1160	C1100	A1035	C980	A915	A828	G742	G675	C601	C534	
C1524	U1388	G1290	C1223	C1223	C1161	C1101	G1036	U981	G916	G829	C745	U677	C602	C535	
G1529	C1359	G1291	G1224	G1224	C1162	A1101	C1037	U982	G917	G830		U678	C603	C536	
A1530	A1442A	U1292	A1225	A1225	C1163	A1102	C1038	A983	G918	U831	C749	G679	C604	C537	A452
	G1442B	U1293	C1226	C1226	C1164	C1103	U1040	C984	A918	C832	U751	C679	A507	G537	A453



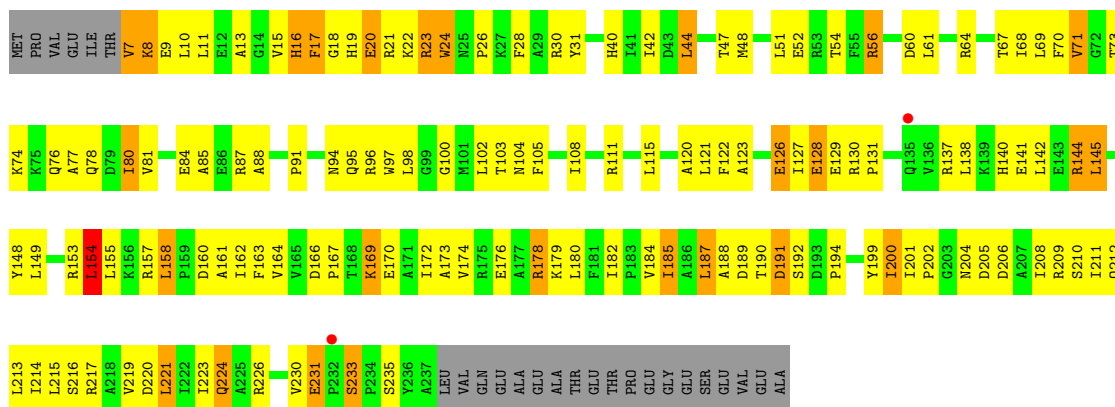
• Molecule 2: 30S Ribosomal Protein S2

Chain AB:



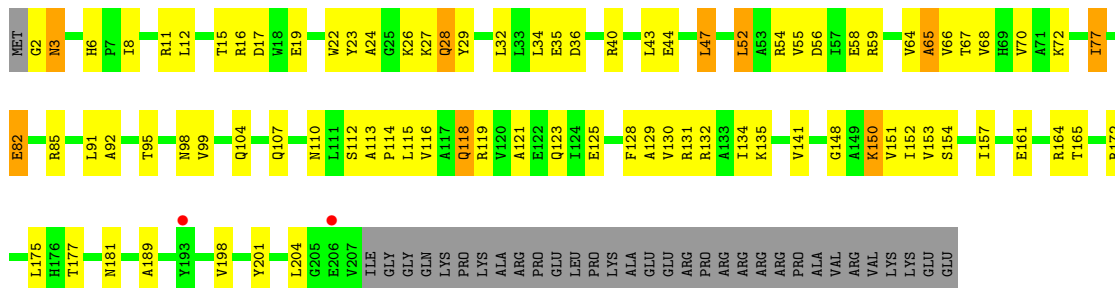
• Molecule 2: 30S Ribosomal Protein S2

Chain CB:



• Molecule 3: 30S Ribosomal Protein S3

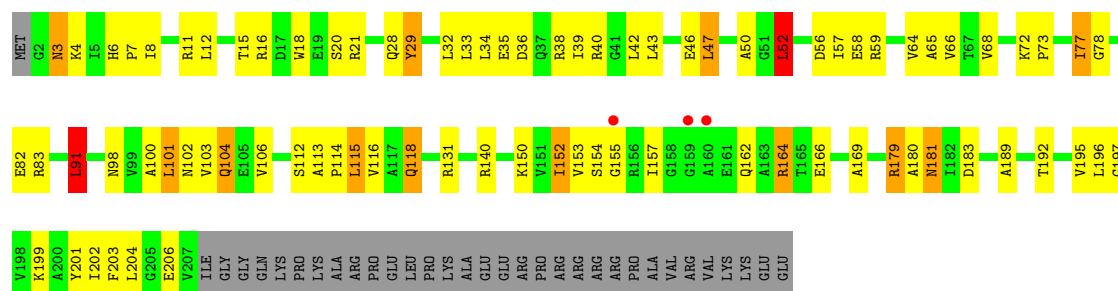
Chain AC:



• Molecule 3: 30S Ribosomal Protein S3

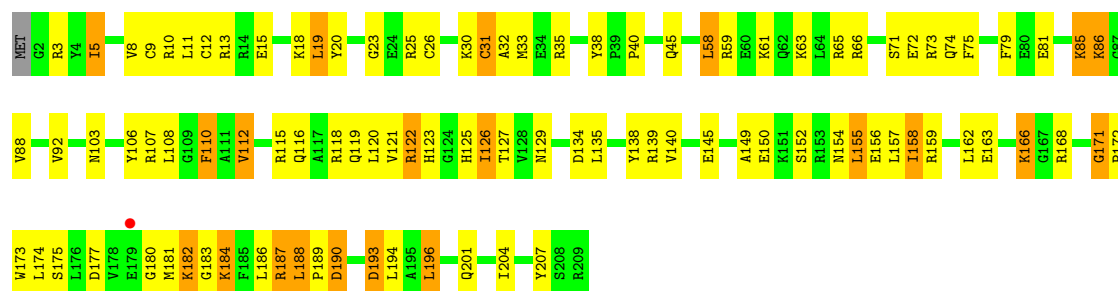
Chain CC:





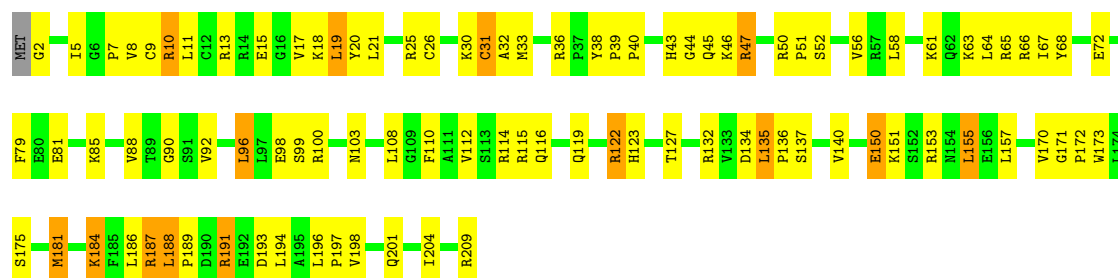
• Molecule 4: 30S Ribosomal Protein S4

Chain AD:



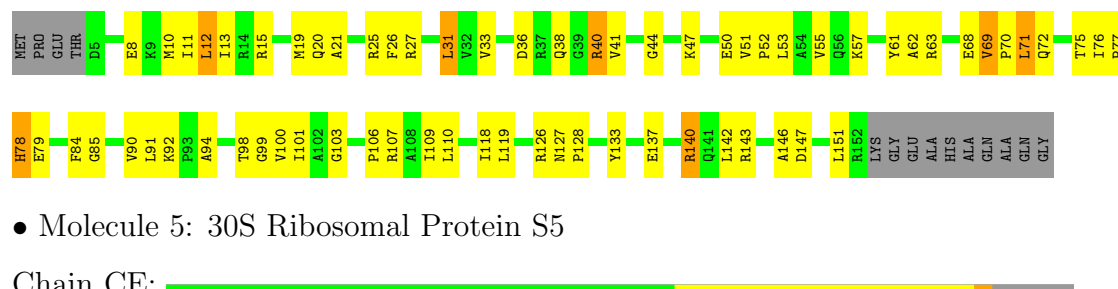
• Molecule 4: 30S Ribosomal Protein S4

Chain CD:



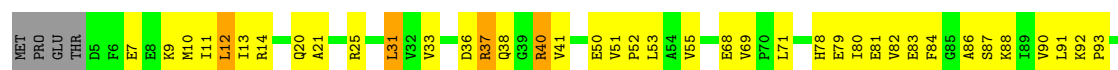
• Molecule 5: 30S Ribosomal Protein S5

Chain AE:



• Molecule 5: 30S Ribosomal Protein S5

Chain CE:





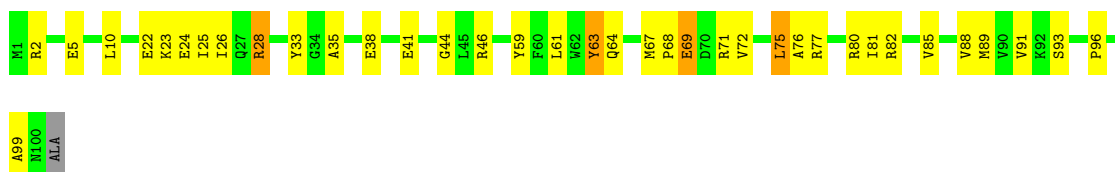
- Molecule 6: 30S Ribosomal Protein S6

Chain AF:



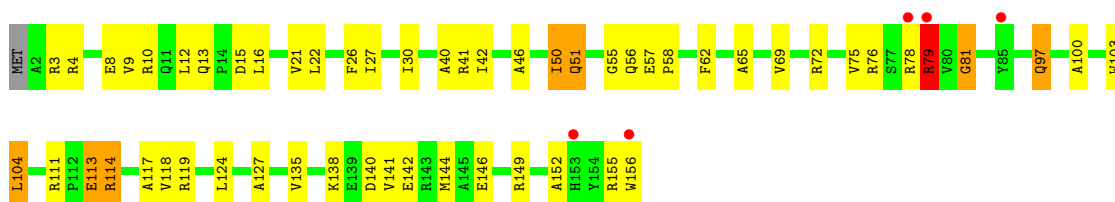
- Molecule 6: 30S Ribosomal Protein S6

Chain CF:



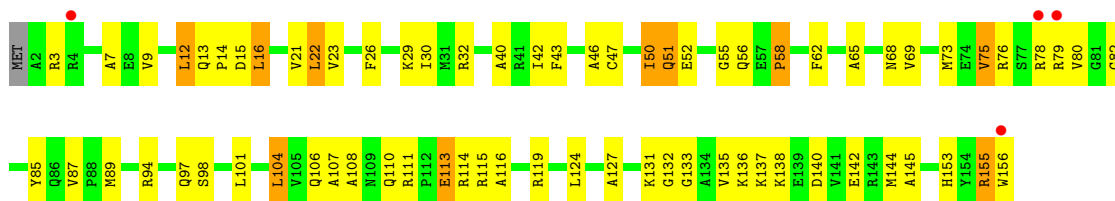
- Molecule 7: 30S Ribosomal Protein S7

Chain AG:



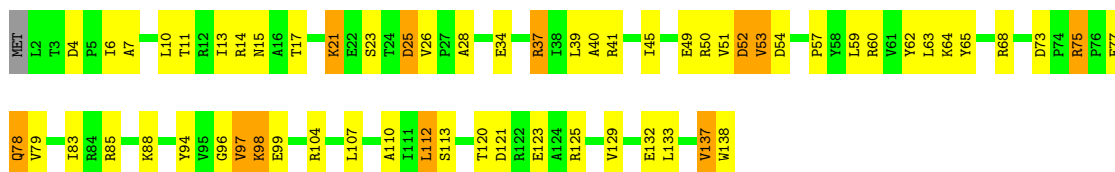
- Molecule 7: 30S Ribosomal Protein S7

Chain CG:



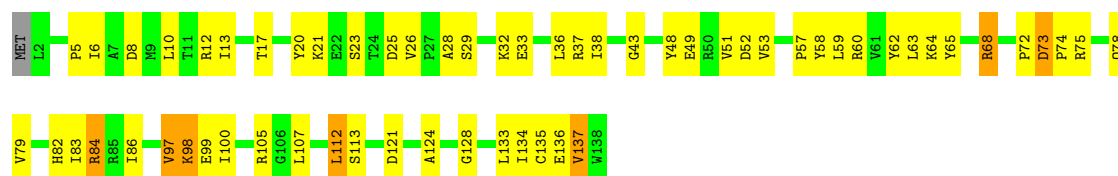
- Molecule 8: 30S Ribosomal Protein S8

Chain AH:



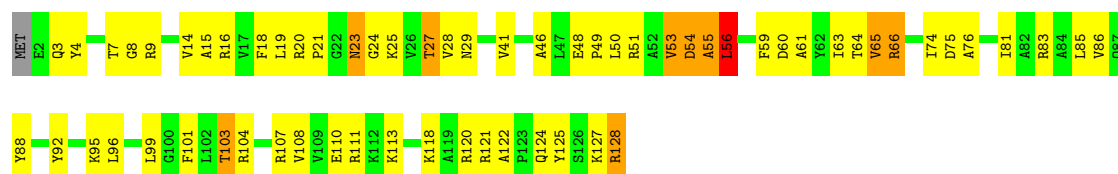
- Molecule 8: 30S Ribosomal Protein S8

Chain CH:



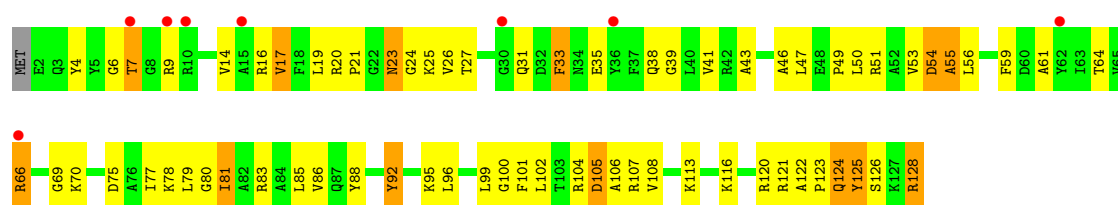
• Molecule 9: 30S Ribosomal Protein S9

Chain AI:



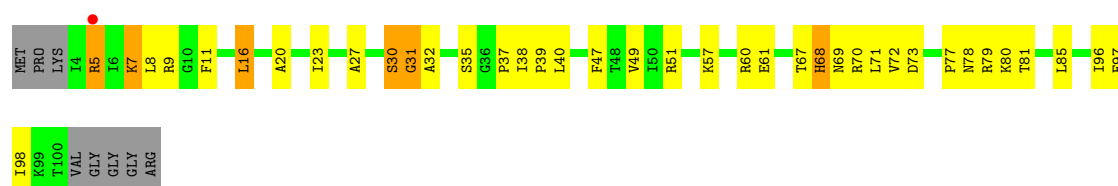
• Molecule 9: 30S Ribosomal Protein S9

Chain CI:



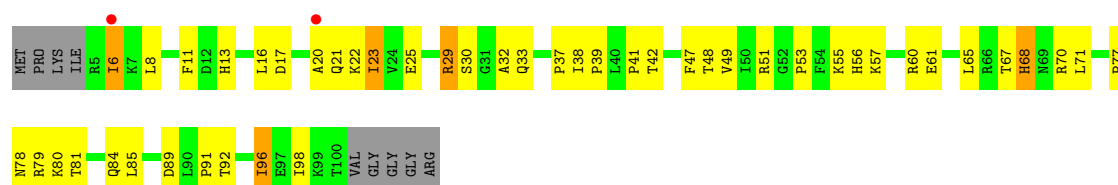
• Molecule 10: 30S Ribosomal Protein S10

Chain AJ:



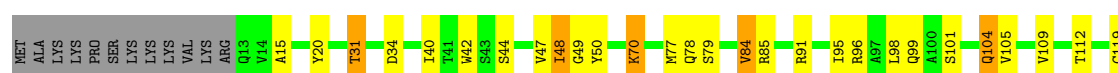
• Molecule 10: 30S Ribosomal Protein S10

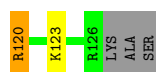
Chain CJ:



• Molecule 11: 30S Ribosomal Protein S11

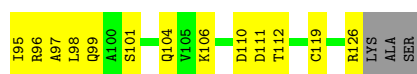
Chain AK:





• Molecule 11: 30S Ribosomal Protein S11

Chain CK:



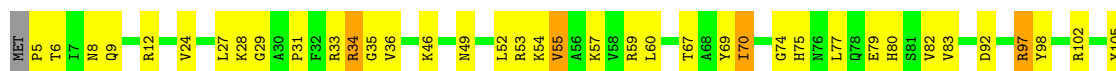
• Molecule 12: 30S Ribosomal Protein S12

Chain AL:



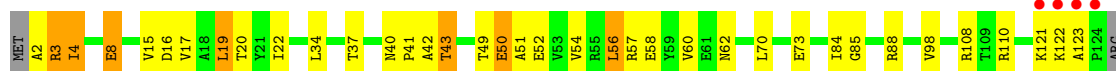
• Molecule 12: 30S Ribosomal Protein S12

Chain CL:



• Molecule 13: 30S Ribosomal Protein S13

Chain AM:



• Molecule 13: 30S Ribosomal Protein S13

Chain CM:



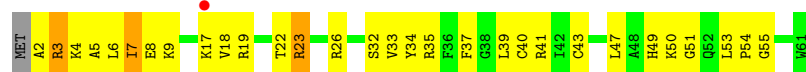
• Molecule 14: 30S Ribosomal Protein S14

Chain AN:



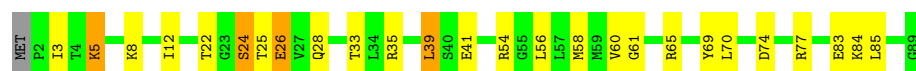
- Molecule 14: 30S Ribosomal Protein S14

Chain CN:



- Molecule 15: 30S Ribosomal Protein S15

Chain AO:



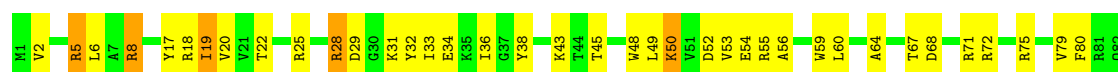
- Molecule 15: 30S Ribosomal Protein S15

Chain CO:



- Molecule 16: 30S Ribosomal Protein S16

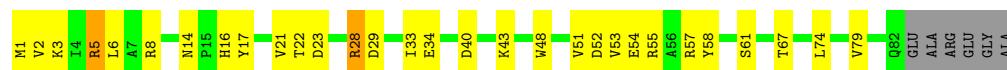
Chain AP:



GLU
ALA
ALA
ARG
GLU
GLY
ALA

- Molecule 16: 30S Ribosomal Protein S16

Chain CP:



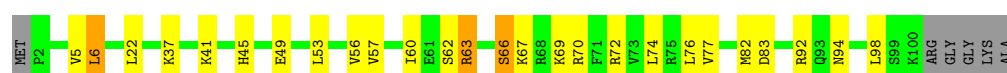
- Molecule 17: 30S Ribosomal Protein S17

Chain AQ:



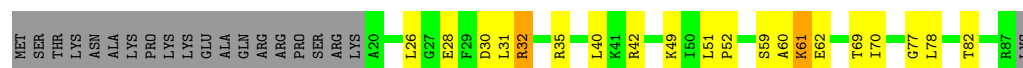
- Molecule 17: 30S Ribosomal Protein S17

Chain CQ:



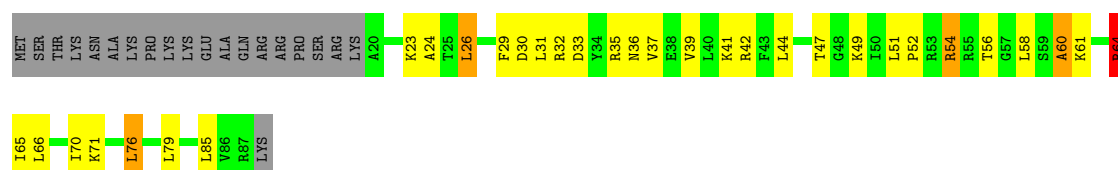
- Molecule 18: 30S Ribosomal Protein S18

Chain AR:



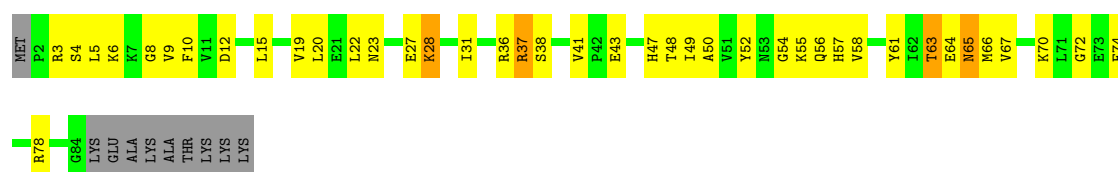
- Molecule 18: 30S Ribosomal Protein S18

Chain CR:



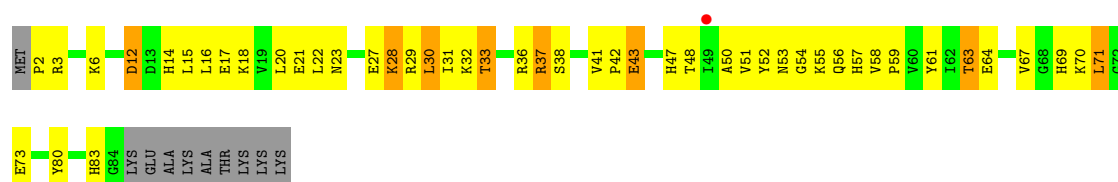
- Molecule 19: 30S Ribosomal Protein S19

Chain AS:



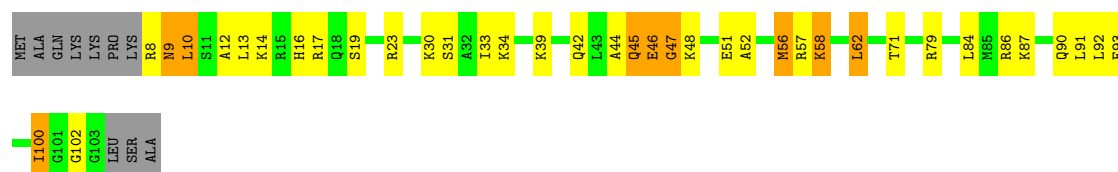
- Molecule 19: 30S Ribosomal Protein S19

Chain CS:



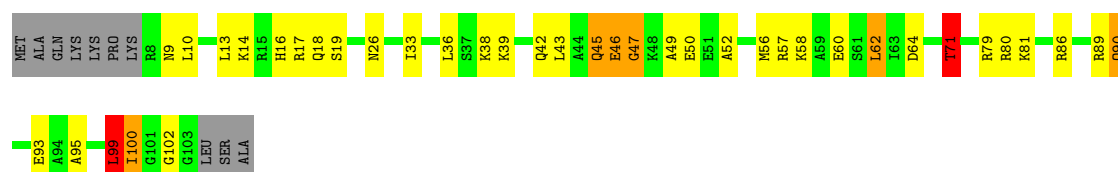
- Molecule 20: 30S Ribosomal Protein S20

Chain AT:



- Molecule 20: 30S Ribosomal Protein S20

Chain CT:



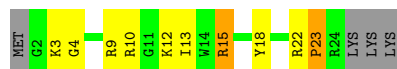
- Molecule 21: 30S Ribosomal Protein THX

Chain AU: 



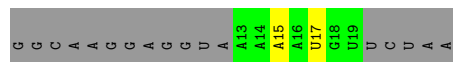
- Molecule 21: 30S Ribosomal Protein THX

Chain CU: 



- Molecule 22: mRNA

Chain AV: 



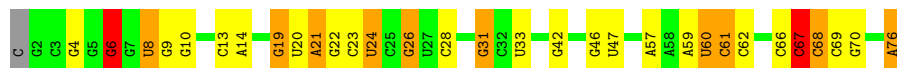
- Molecule 22: mRNA

Chain CV: 



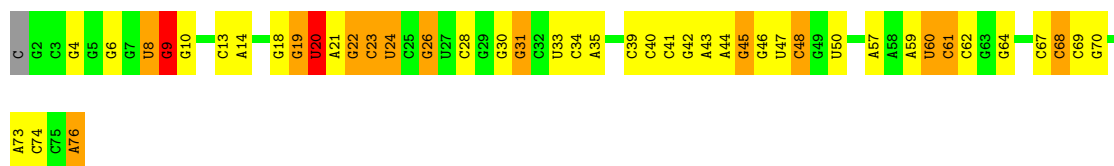
- Molecule 23: P-site tRNA

Chain AX: 



- Molecule 23: P-site tRNA

Chain CX: 



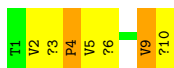
- Molecule 24: GE82832

Chain AW: 

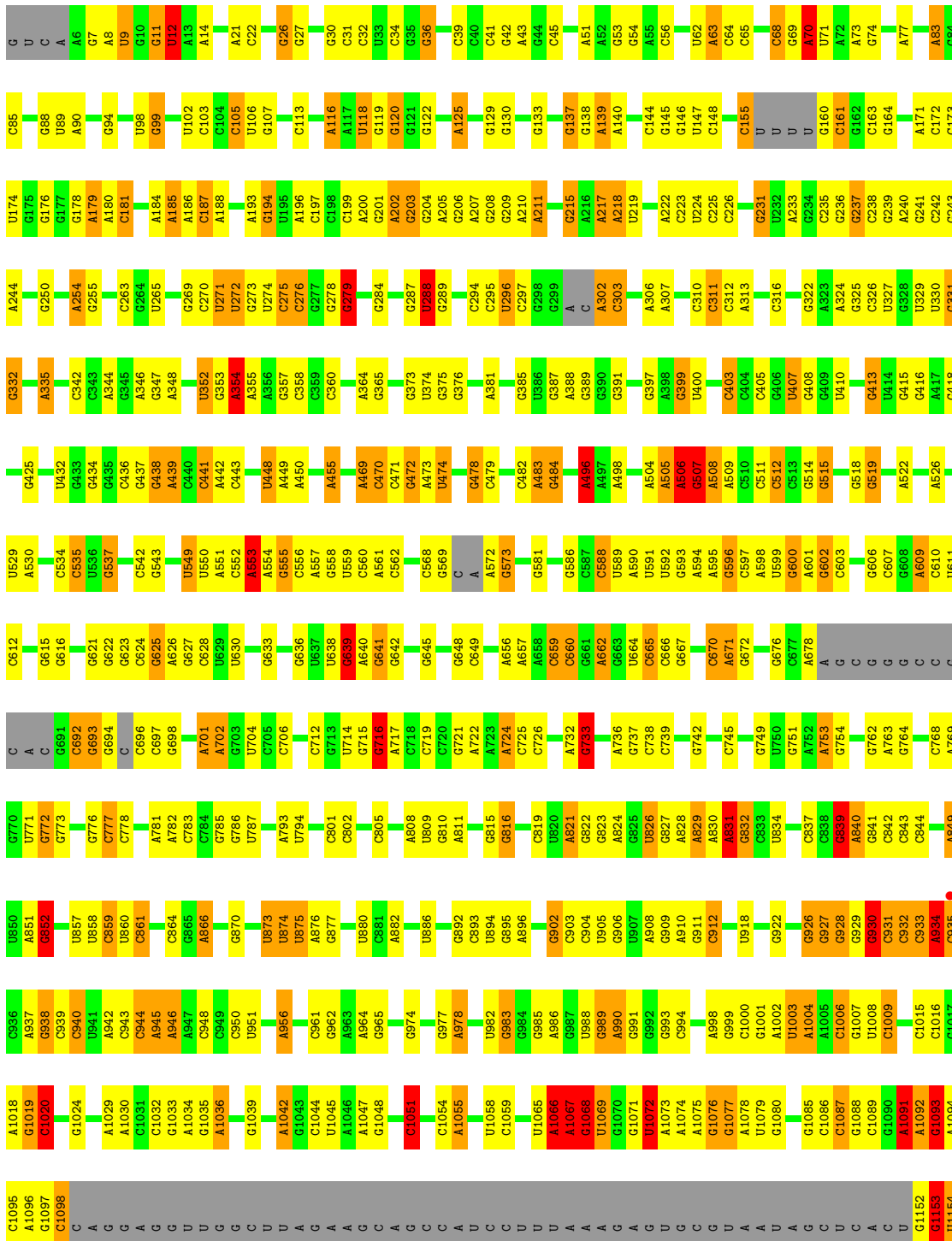


- Molecule 24: GE82832

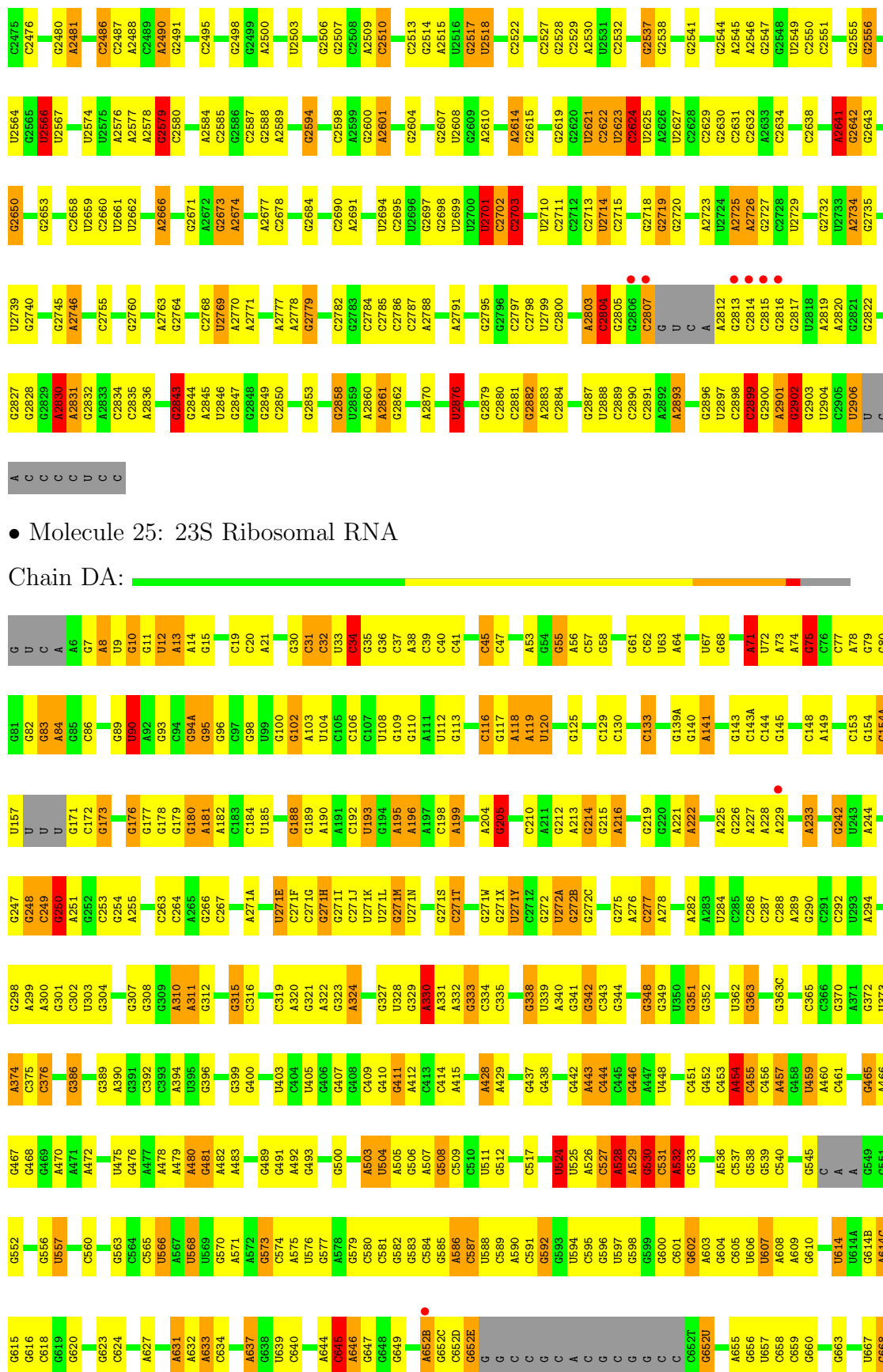
Chain CW: 



Chain BA:

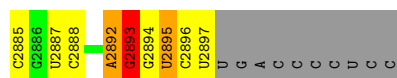


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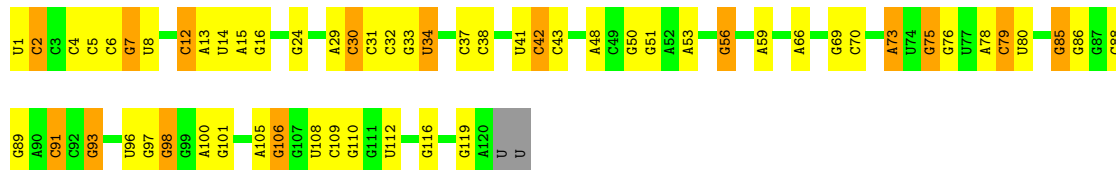
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G1764	A1665	C1509	A1434	A1360	U1288	G1136	A	A945	G874	A804	G733
C1765	G1666	A1509B	C1437	U1363	C1291	G1137	G	G946	G880	G805	A734
U1766	G1667	G1510	U1438	G1364	U1292	U1138	C	G947	G881	C806	A735
C1767	A1668	G1510	A1439	A1365	C1293	C1139	C	G948	U811	U807	C736
U1768	A1669	C1513	G1440	A1366	A1294	U1141	A	C949	G882	G808	C737
G1769	U1671	U1514	G1441	A1367	G1295	U1142	C	G950	G883	U813	U747
A1773	C1672	C1516	A1445	G1368	G1296	A142A	U	G951	C884	C814	U747
				G1369	G1297	A142A	C	G952	C885	C815	G746
						A143	C	G953	C886	C816	G745
						G1149	U	A953	C887	C817	C749
								G954	C888	G818	A752
									C889		

A	G2729	C2646	G2567	A2497	G2429	A2360	C2293	G2219	C	G2080	U2016	G1933	C1844	G1774
A2801A	G2729	U2647	G2567	C2498	A2430	A2361	C2294	G2219	U	C2081	U2017	C1934	G1845	U1775
C2803	G2732	C2648	G2570	C2499	U2431	C2364	U2295	A2225	C	A2082	G2018	G1935	G1846	G1776
C2804	A2733	U2650	G2571	U2500	A2432	C2365	U2296	C2226	C	G2083	A2019	A1936	A1847	U1777
C2805	A2734	G2735	C2574	G2501	A2433	G2366	C2297	A2227	G	C2084	A2021	A1937	A1848	U1778
C2807	G2735	A2684	C2575	G2502	A2434	G2367	A2298	G2228	G	C2085	C2021	A1938	G1849	U1779
			C2576	A2503	A2435	G2370	G2299	C2229	G	U2086	U2022	A1939	G1850	A1780
			A2577	U2504	G2436	G2371	G2299	C2230	U	G2087	G2023	C1942	U1851	C1781
			G2578	G2505	U2437	G2372	G2302	G2234	G	G2090	G2024	U1943		C1782
			G2579	U2506	A2438	G2373	G2303	G2235	G	G2091	C2025	U1944	A1854	A1783
			U2580	G2507	A2439	C2374	G2304	G2236	G	G2092	C2026	U1945	A1855	A1784
			G2581	C2508	C2440	G2375	A2305	G2237	G	G2093	G2027	C1947	G1856	A1785
			G2582	U2510	C2441	A2376	C2306	G2238	G	G2094	U2028		G1857	A1786
			G2583	U2511	C2442	A2377	G2307	G2239	G	C2097	G2029	G1954	G1858	A1787
			U2584	C2512	C2443	A2377	G2308	G2240	G	U2098	A2030	U1955	A1859	C1788
			U2585	G2516	G2444	A2377	G2309	G2242	A	U2099	A2031	U1956	G1860	A1789
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			A2587	U2518	G2446	A2377	G2311	U2245	C	G2101	U2034	A1960	A1876	A1791
			A2588	G2519	A2448	A2377	G2312	C2248	G			C1961	A1877	U1794
			U2589	U2520	A2451	A2377	G2313	U2249	C			C1962	G1878	U1795
			A2590	G2521	G2452	A2377	G2314	G2250	C			U1963	G1879	U1796
			G2591	G2522	G2453	A2377	G2315	G2251	C			G1964	C1880	C1797
			G2592	G2523	G2454	A2377	G2316	G2252	G			C1965	C1881	U1798
			G2595	G2524	G2455	A2377	G2317	G2253	G			C1966	C1882	G1799
				G2525	G2456	A2377	G2318	G2254	G			C1967	G1883	C1800
					G2457	A2377	G2319	U2257	A			G1968	A1884	G1801
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						A2377	G2330	G2270	U				G1903	G1816
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						A2377	G2334	A2274	C			G1996	C1908	G1823
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						A2377	G2427	G2367	C					
						A								



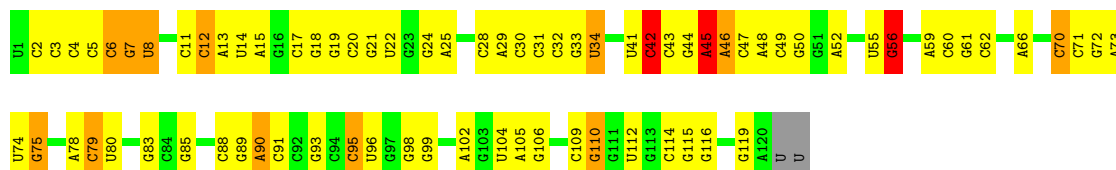
- Molecule 26: 5S Ribosomal RNA

Chain BB:



- Molecule 26: 5S Ribosomal RNA

Chain DB:



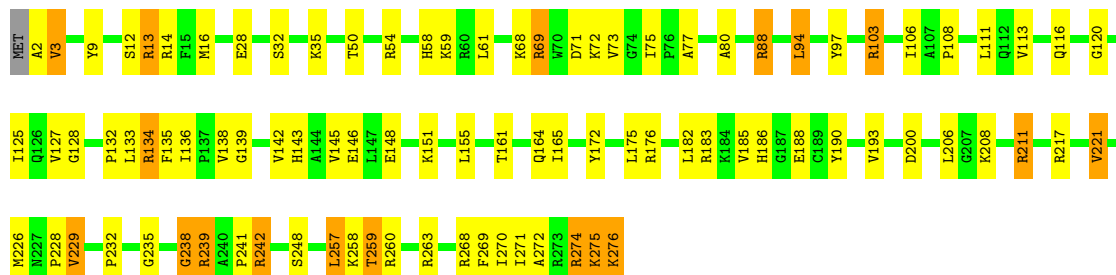
- Molecule 27: 50S Ribosomal Protein L2

Chain BD:



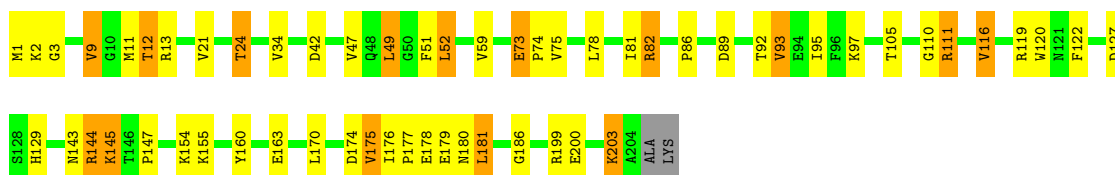
- Molecule 27: 50S Ribosomal Protein L2

Chain DD:



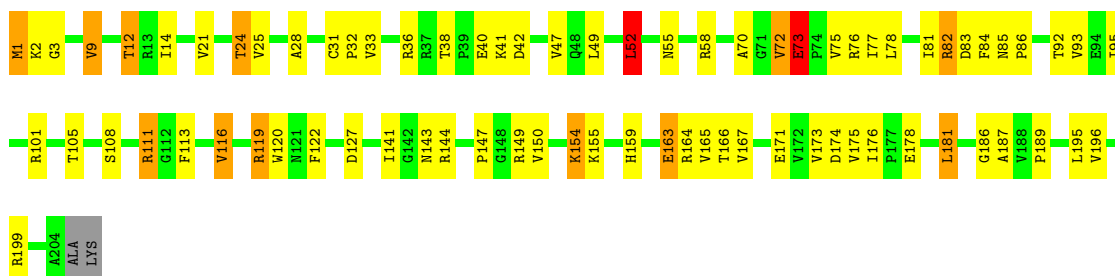
- Molecule 28: 50S Ribosomal Protein L3

Chain BE:



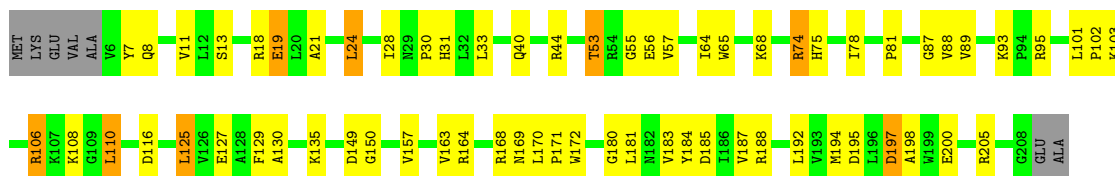
• Molecule 28: 50S Ribosomal Protein L3

Chain DE:



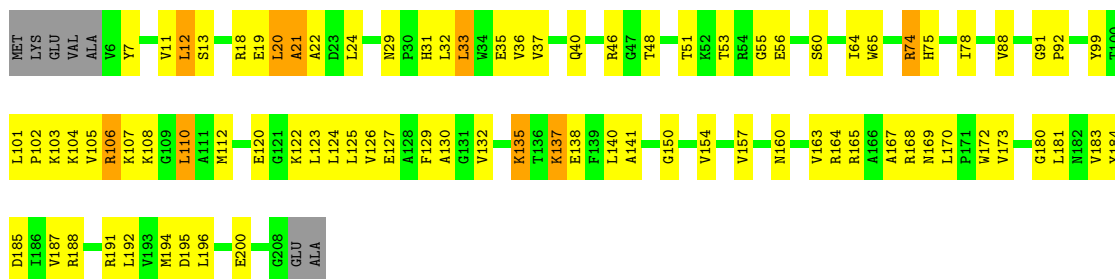
• Molecule 29: 50S Ribosomal Protein L4

Chain BF:



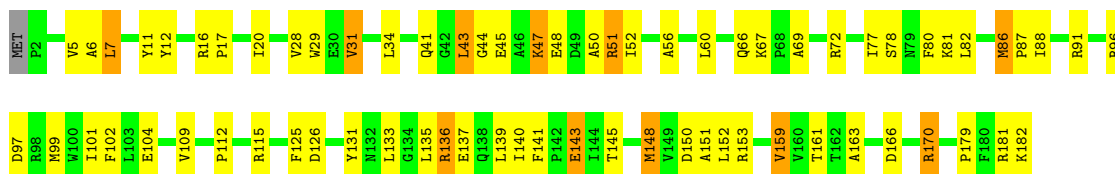
• Molecule 29: 50S Ribosomal Protein L4

Chain DF:



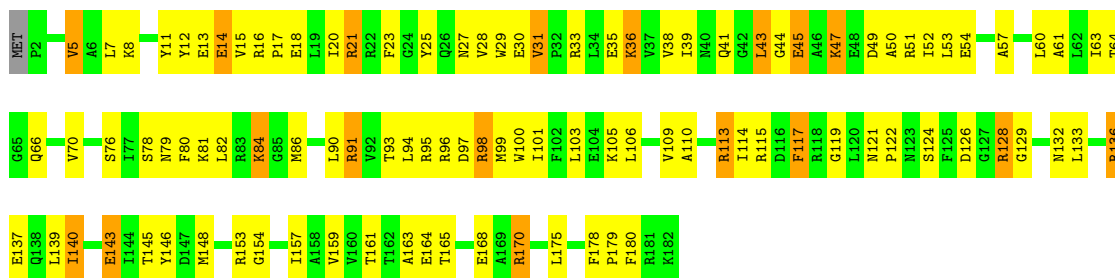
• Molecule 30: 50S Ribosomal Protein L5

Chain BG:



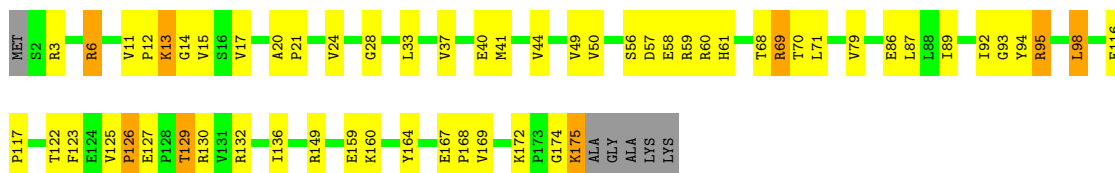
• Molecule 30: 50S Ribosomal Protein L5

Chain DG:



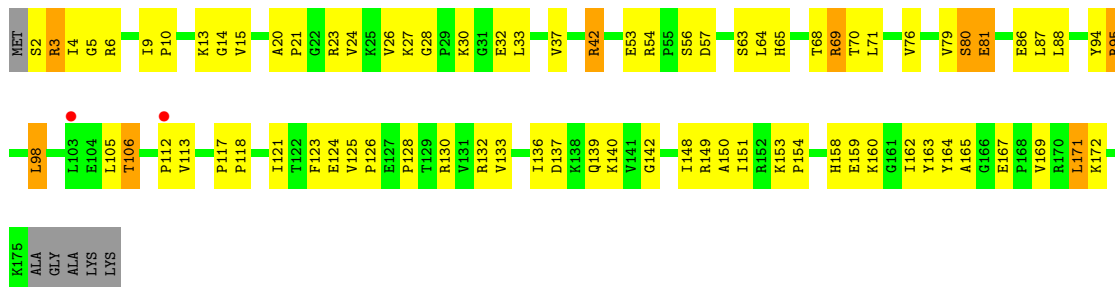
• Molecule 31: 50S Ribosomal Protein L6

Chain BH:



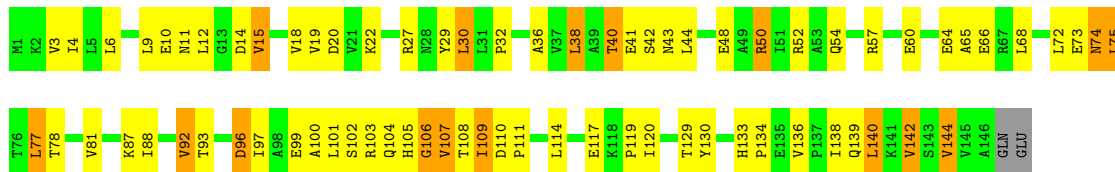
• Molecule 31: 50S Ribosomal Protein L6

Chain DH:



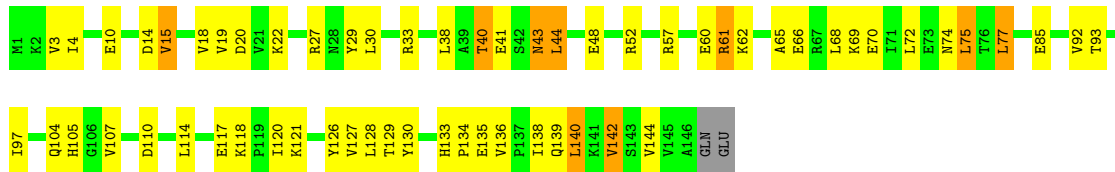
• Molecule 32: 50S Ribosomal Protein L9

Chain BI:



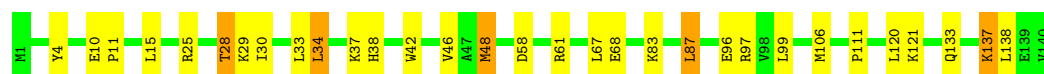
• Molecule 32: 50S Ribosomal Protein L9

Chain DI:



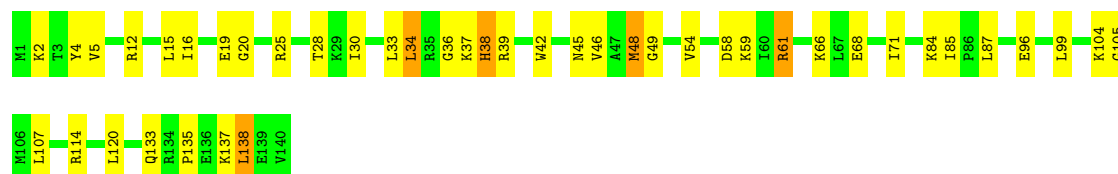
• Molecule 33: 50S Ribosomal Protein L13

Chain BN: 



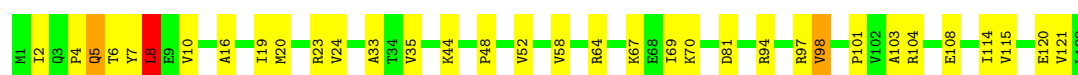
- Molecule 33: 50S Ribosomal Protein L13

Chain DN: 



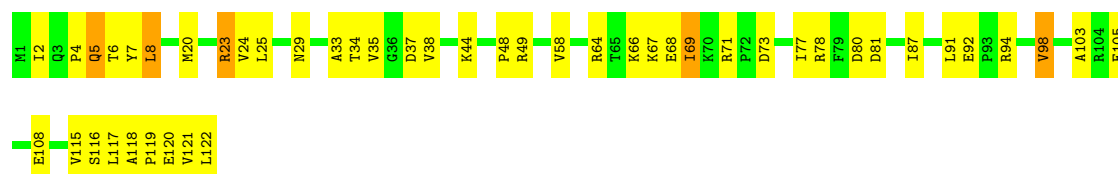
- Molecule 34: 50S Ribosomal Protein L14

Chain BO: 



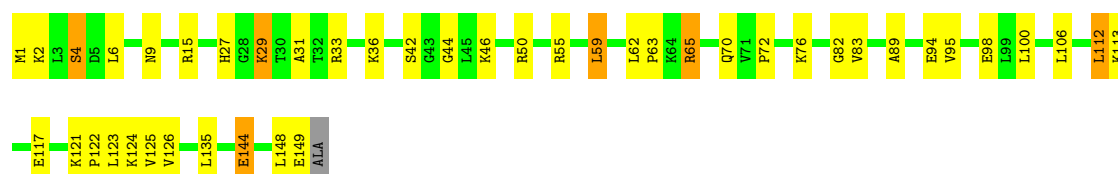
- Molecule 34: 50S Ribosomal Protein L14

Chain DO: 



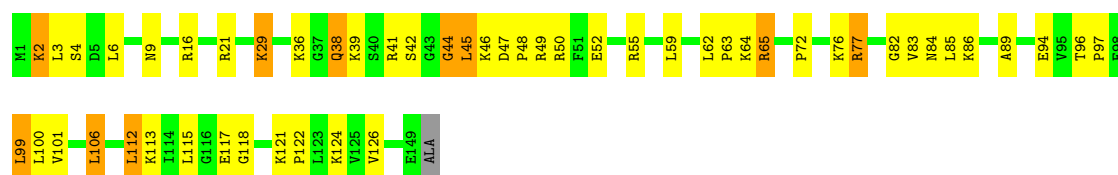
- Molecule 35: 50S Ribosomal Protein L15

Chain BP: 



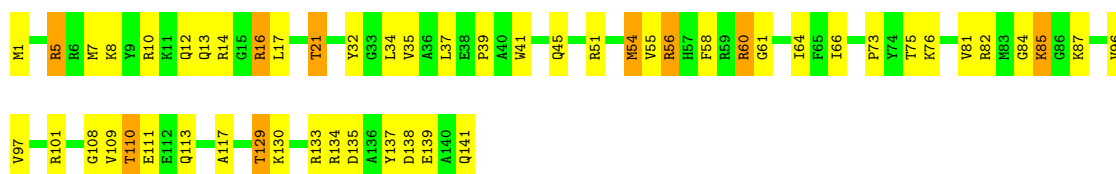
- Molecule 35: 50S Ribosomal Protein L15

Chain DP: 



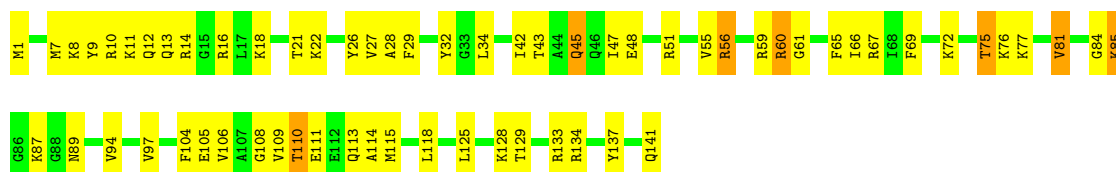
- Molecule 36: 50S Ribosomal Protein L16

Chain BQ: 



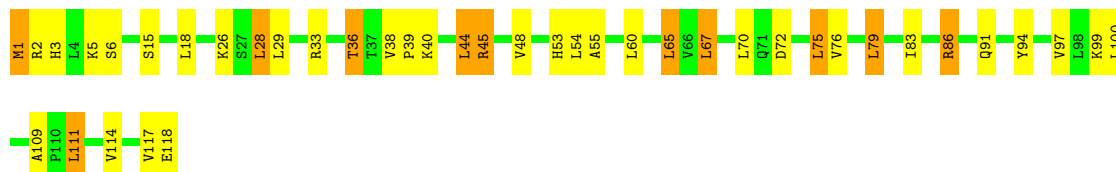
• Molecule 36: 50S Ribosomal Protein L16

Chain DQ:



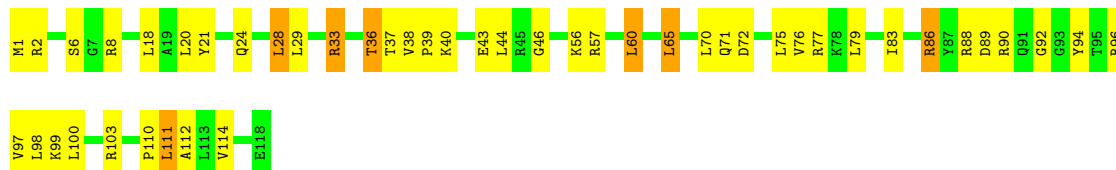
• Molecule 37: 50S Ribosomal Protein L17

Chain BR:



• Molecule 37: 50S Ribosomal Protein L17

Chain DR:



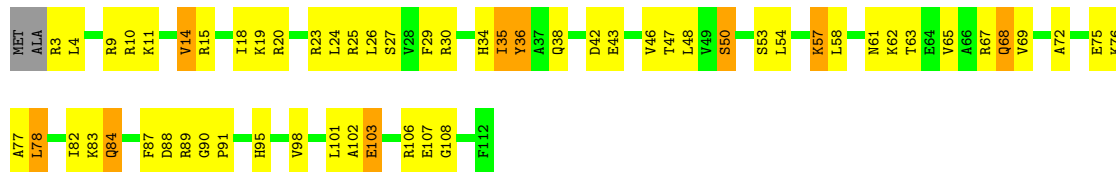
• Molecule 38: 50S Ribosomal Protein L18

Chain BS:



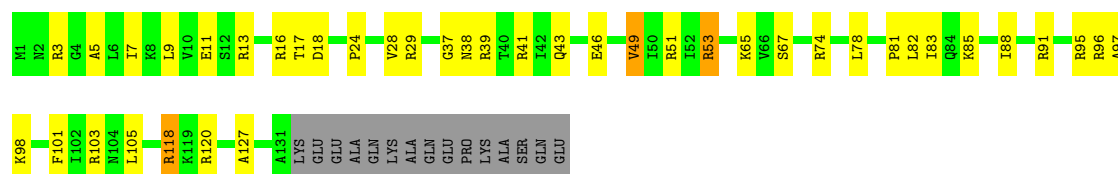
• Molecule 38: 50S Ribosomal Protein L18

Chain DS:



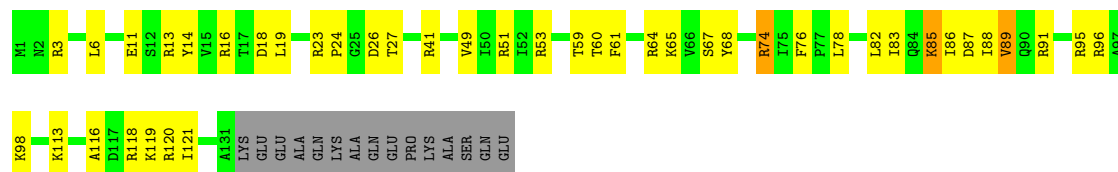
• Molecule 39: 50S Ribosomal Protein L19

Chain BT:



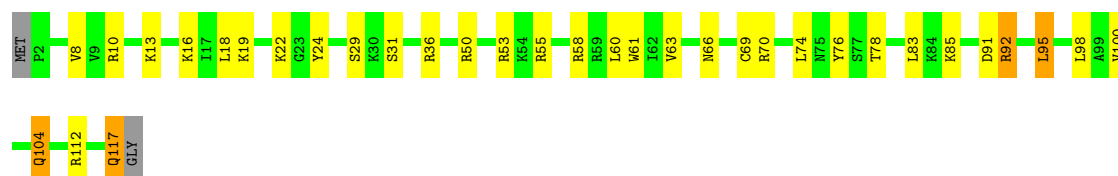
• Molecule 39: 50S Ribosomal Protein L19

Chain DT:



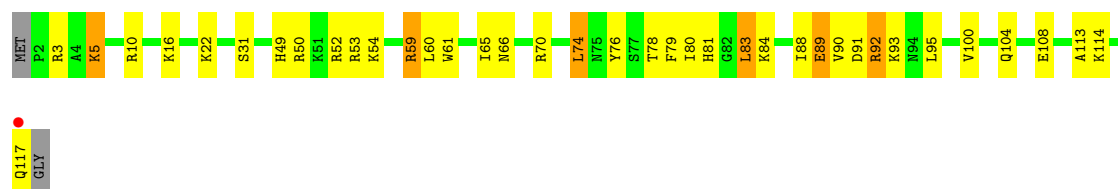
• Molecule 40: 50S Ribosomal Protein L20

Chain BU:



• Molecule 40: 50S Ribosomal Protein L20

Chain DU:



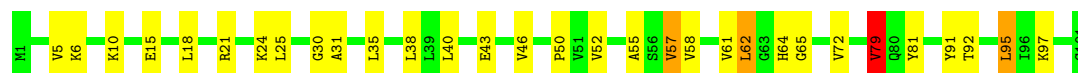
• Molecule 41: 50S Ribosomal Protein L21

Chain BV:



• Molecule 41: 50S Ribosomal Protein L21

Chain DV:



• Molecule 42: 50S Ribosomal Protein L22

Chain BW:



- Molecule 42: 50S Ribosomal Protein L22

Chain DW:



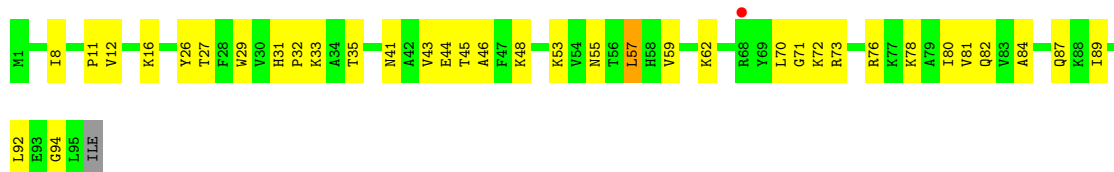
- Molecule 43: 50S Ribosomal Protein L23

Chain BX:



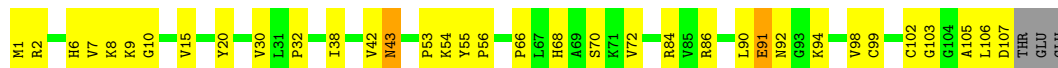
- Molecule 43: 50S Ribosomal Protein L23

Chain DX:



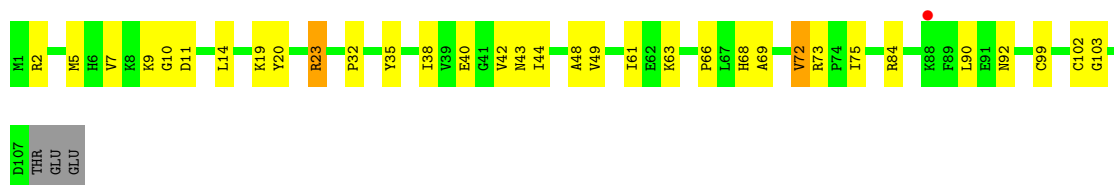
- Molecule 44: 50S Ribosomal Protein L24

Chain BY:



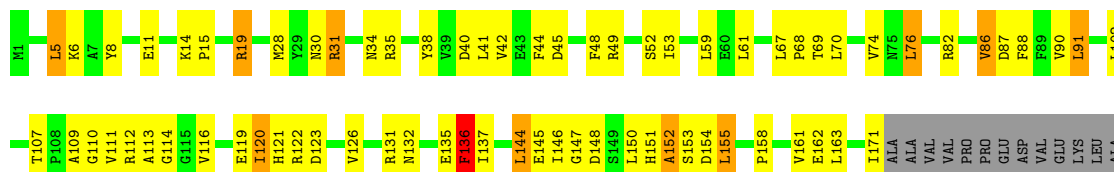
- Molecule 44: 50S Ribosomal Protein L24

Chain DY:



- Molecule 45: 50S Ribosomal Protein L25

Chain BZ:



GLU
GLU
ALA
ALA
ALA
GLU
VAL
ALA
GLU
PRO
GLU
VAL
ILE
LYS
LYS
GLY
LYS
GLU
GLU
GLU

• Molecule 45: 50S Ribosomal Protein L25

Chain DZ:

H1 L5 K6 A7 Y8 E11 G12 R19 R30 R31 R32 R33 Y38 V39 D40 L41 V42 E43 F44 D45 K46 V47 F48 R49 Q50 A51 S52 S53 S54 L61 P62 L67 P68 T69 L70 V165 V171 R72 Q73 V74 V75 L76 P83 V86 D87 V90 L91 S92 D93 E94 P95

V96 E97 P101 T107 P108 V116 H121 R122 D123 L124 L125 V128 S129 P130 R131 M132 I133 V141 L144 L150 H151 A152 S153 D154 L155 K156 L157 P158 V161 E162 L163 A164 V165 S166 P167 V174 VAL PRO PRO GLU ASP VAL VAL LYS LEU ALA GLU ALA ALA

ALA
GLU
VAL
GLU
PRO
GLU
VAL
ILE
LYS
LYS
GLY
GLU
GLU
GLU
GLU

• Molecule 46: 50S Ribosomal Protein L27

Chain B0:

MET A2 H3 K4 K5 G6 L7 G8 T10 R11 N12 G13 R14 K19 R20 V23 E27 V30 R39 Q40 T43 K46 K49 N50 M53 G54 R55 D56 F57 T58 L59 V66 V67 E68 F69 G73 R77 L84 ALA

• Molecule 46: 50S Ribosomal Protein L27

Chain D0:

MET A2 H3 K4 K5 G6 L7 G8 T10 R11 R14 B15 S16 K19 R20 V23 K24 R25 Y26 E27 R32 Q40 T43 M53 G54 R55 D56 F57 T58 L59 E68 F69 R72 L75 G76 R82 P83 L84 ALA

• Molecule 47: 50S Ribosomal Protein L28

Chain B1:

MET S2 K3 R11 R21 G22 K23 R26 G29 K33 T34 T35 R40 N45 R50 V51 R52 T59 F60 R61 A64 S65 H66 I67 Y71 Y74 L82 L85 S86 E89 I90 K91 L95 L98

• Molecule 47: 50S Ribosomal Protein L28

Chain D1:

MET S2 K3 I7 R21 G22 K23 A24 K25 R26 G29 V30 G31 T35 K39 R40 R50 V51 R52 E57 T59 F60 R61 A64 S65 H66 I67 Y71 Y74 L82 L85 S86 E89 I90 K91 L95 L98

• Molecule 48: 50S Ribosomal Protein L29

Chain B2:

M1 K2 L3 V6 L10 L16 S17 P18 L21 R26 E27 K28 K29 R30 E31 L32 R36 F37 S40 T41 L44 S45 Q46 M47 H48 K49 D52 L53 V54 R55 V63 L64 N65 E66 K67 R68 R69 Q70 ASN ALA

• 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

Chain B5:



- Molecule 51: 50S Ribosomal Protein L32

Chain D5:



- Molecule 52: 50S Ribosomal Protein L33

Chain B6:



- Molecule 52: 50S Ribosomal Protein L33

Chain D6:



- Molecule 53: 50S Ribosomal Protein L34

Chain B7:



- Molecule 53: 50S Ribosomal Protein L34

Chain D7:



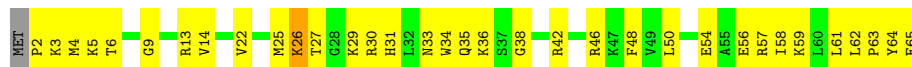
- Molecule 54: 50S Ribosomal Protein L35

Chain B8:



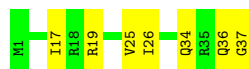
- Molecule 54: 50S Ribosomal Protein L35

Chain D8:



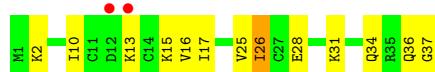
- Molecule 55: 50S Ribosomal Protein L36

Chain B9:



- Molecule 55: 50S Ribosomal Protein L36

Chain D9:



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) 98.2 (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 (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.203 , 0.260 0.231 , 0.282	Depositor DCC
R_{free} test set	41240 reflections (3.99%)	DCC
Wilson B-factor (Å ²)	71.0	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 1034786 reflections	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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, K, 2QZ, ZN, 2QY, MVA, 004, FME, 2R3, SF4, 2R1

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	CR	555	0	618	27	0
19	AS	652	0	662	36	0
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	51	6	0
24	CW	93	0	51	7	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	DT	1083	0	1136	36	0
40	BU	959	0	1019	26	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	B1	1	0	0	0	0
56	B2	1	0	0	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DO	1	0	0	0	0
56	DQ	5	0	0	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	BF	4	0	0	0	0
61	BG	1	0	0	0	0
61	BN	3	0	0	0	0
61	BO	2	0	0	0	0
61	BP	15	0	0	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	191060	6362	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

The worst 5 of 6362 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	229/256 (90%)	200 (87%)	23 (10%)	6 (3%)	8	41
2	CB	229/256 (90%)	201 (88%)	18 (8%)	10 (4%)	4	25
3	AC	204/239 (85%)	179 (88%)	22 (11%)	3 (2%)	15	57
3	CC	204/239 (85%)	178 (87%)	24 (12%)	2 (1%)	22	68
4	AD	206/209 (99%)	182 (88%)	22 (11%)	2 (1%)	22	68
4	CD	206/209 (99%)	185 (90%)	18 (9%)	3 (2%)	15	57
5	AE	146/162 (90%)	127 (87%)	15 (10%)	4 (3%)	8	39
5	CE	146/162 (90%)	133 (91%)	10 (7%)	3 (2%)	11	48
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%)	18	60
7	CG	153/156 (98%)	137 (90%)	15 (10%)	1 (1%)	30	76
8	AH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
8	CH	135/138 (98%)	129 (96%)	5 (4%)	1 (1%)	30	76
9	AI	125/128 (98%)	111 (89%)	10 (8%)	4 (3%)	6	35
9	CI	125/128 (98%)	112 (90%)	11 (9%)	2 (2%)	14	55
10	AJ	95/105 (90%)	85 (90%)	7 (7%)	3 (3%)	6	35
10	CJ	94/105 (90%)	86 (92%)	7 (7%)	1 (1%)	21	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	AK	112/129 (87%)	98 (88%)	13 (12%)	1 (1%)	25	71
11	CK	112/129 (87%)	99 (88%)	12 (11%)	1 (1%)	25	71
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%)	14	54
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%)	19	62
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%)	15	57
18	CR	66/88 (75%)	60 (91%)	5 (8%)	1 (2%)	15	57
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%)	3	21
20	CT	94/106 (89%)	85 (90%)	3 (3%)	6 (6%)	2	15
21	AU	21/27 (78%)	17 (81%)	4 (19%)	0	100	100
21	CU	21/27 (78%)	18 (86%)	1 (5%)	2 (10%)	1	7
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%)	43	84
27	DD	273/276 (99%)	257 (94%)	13 (5%)	3 (1%)	21	65
28	BE	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	38	81
28	DE	202/206 (98%)	194 (96%)	6 (3%)	2 (1%)	22	68
29	BF	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	38	81
29	DF	201/210 (96%)	189 (94%)	10 (5%)	2 (1%)	22	68
30	BG	179/182 (98%)	163 (91%)	13 (7%)	3 (2%)	14	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	DG	179/182 (98%)	160 (89%)	13 (7%)	6 (3%)	6	32
31	BH	172/180 (96%)	161 (94%)	10 (6%)	1 (1%)	33	78
31	DH	172/180 (96%)	159 (92%)	11 (6%)	2 (1%)	19	62
32	BI	144/148 (97%)	122 (85%)	17 (12%)	5 (4%)	6	32
32	DI	144/148 (97%)	123 (85%)	17 (12%)	4 (3%)	8	39
33	BN	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
33	DN	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	30	76
34	BO	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	27	74
34	DO	120/122 (98%)	117 (98%)	2 (2%)	1 (1%)	27	74
35	BP	147/150 (98%)	132 (90%)	14 (10%)	1 (1%)	30	76
35	DP	147/150 (98%)	133 (90%)	12 (8%)	2 (1%)	16	58
36	BQ	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	30	76
36	DQ	139/141 (99%)	129 (93%)	8 (6%)	2 (1%)	16	58
37	BR	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	25	71
37	DR	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
38	BS	108/112 (96%)	100 (93%)	7 (6%)	1 (1%)	25	71
38	DS	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	25	71
39	BT	129/146 (88%)	124 (96%)	4 (3%)	1 (1%)	27	74
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%)	22	68
41	DV	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	22	68
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%)	21	65
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%)	19	62
45	DZ	172/206 (84%)	157 (91%)	15 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	B0	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	19	62
46	D0	81/85 (95%)	76 (94%)	5 (6%)	0	100	100
47	B1	95/98 (97%)	93 (98%)	0	2 (2%)	11	48
47	D1	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	21	65
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%)	1	4
50	D4	67/71 (94%)	50 (75%)	8 (12%)	9 (13%)	0	2
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%)	10	46
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%)	19	62

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%)	1	5
2	CB	187/220 (85%)	152 (81%)	35 (19%)	2	9
3	AC	143/188 (76%)	125 (87%)	18 (13%)	7	24
3	CC	140/188 (74%)	122 (87%)	18 (13%)	6	24
4	AD	170/181 (94%)	145 (85%)	25 (15%)	4	18
4	CD	173/181 (96%)	152 (88%)	21 (12%)	7	27
5	AE	113/123 (92%)	104 (92%)	9 (8%)	17	55
5	CE	114/123 (93%)	107 (94%)	7 (6%)	26	67
6	AF	83/90 (92%)	76 (92%)	7 (8%)	16	52
6	CF	85/90 (94%)	79 (93%)	6 (7%)	21	61
7	AG	119/127 (94%)	100 (84%)	19 (16%)	3	13
7	CG	120/127 (94%)	102 (85%)	18 (15%)	4	17
8	AH	114/119 (96%)	98 (86%)	16 (14%)	5	21
8	CH	114/119 (96%)	102 (90%)	12 (10%)	10	35
9	AI	90/99 (91%)	76 (84%)	14 (16%)	4	14
9	CI	89/99 (90%)	75 (84%)	14 (16%)	4	14
10	AJ	66/92 (72%)	60 (91%)	6 (9%)	14	45
10	CJ	69/92 (75%)	64 (93%)	5 (7%)	21	60
11	AK	82/99 (83%)	73 (89%)	9 (11%)	9	34
11	CK	83/99 (84%)	77 (93%)	6 (7%)	21	60
12	AL	97/109 (89%)	90 (93%)	7 (7%)	21	60
12	CL	97/109 (89%)	87 (90%)	10 (10%)	10	36
13	AM	93/101 (92%)	82 (88%)	11 (12%)	8	29
13	CM	92/101 (91%)	80 (87%)	12 (13%)	6	23
14	AN	49/50 (98%)	41 (84%)	8 (16%)	3	12
14	CN	49/50 (98%)	42 (86%)	7 (14%)	5	19
15	AO	78/80 (98%)	69 (88%)	9 (12%)	8	31
15	CO	78/80 (98%)	66 (85%)	12 (15%)	4	15
16	AP	69/74 (93%)	60 (87%)	9 (13%)	6	23
16	CP	68/74 (92%)	63 (93%)	5 (7%)	20	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	AQ	94/97 (97%)	89 (95%)	5 (5%)	32	72
17	CQ	94/97 (97%)	87 (93%)	7 (7%)	20	59
18	AR	59/77 (77%)	55 (93%)	4 (7%)	22	62
18	CR	59/77 (77%)	52 (88%)	7 (12%)	8	27
19	AS	69/80 (86%)	63 (91%)	6 (9%)	15	49
19	CS	67/80 (84%)	57 (85%)	10 (15%)	4	17
20	AT	70/82 (85%)	61 (87%)	9 (13%)	6	24
20	CT	70/82 (85%)	60 (86%)	10 (14%)	5	19
21	AU	18/22 (82%)	14 (78%)	4 (22%)	1	6
21	CU	18/22 (82%)	16 (89%)	2 (11%)	9	33
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%)	18	55
27	DD	215/218 (99%)	190 (88%)	25 (12%)	8	30
28	BE	164/166 (99%)	142 (87%)	22 (13%)	6	22
28	DE	164/166 (99%)	144 (88%)	20 (12%)	7	26
29	BF	160/166 (96%)	143 (89%)	17 (11%)	10	35
29	DF	159/166 (96%)	145 (91%)	14 (9%)	14	49
30	BG	143/156 (92%)	123 (86%)	20 (14%)	5	21
30	DG	142/156 (91%)	116 (82%)	26 (18%)	2	10
31	BH	144/148 (97%)	129 (90%)	15 (10%)	10	36
31	DH	144/148 (97%)	131 (91%)	13 (9%)	14	47
32	BI	110/124 (89%)	82 (74%)	28 (26%)	1	2
32	DI	104/124 (84%)	86 (83%)	18 (17%)	3	11
33	BN	118/119 (99%)	103 (87%)	15 (13%)	6	24
33	DN	118/119 (99%)	102 (86%)	16 (14%)	5	21
34	BO	100/100 (100%)	94 (94%)	6 (6%)	27	67
34	DO	100/100 (100%)	91 (91%)	9 (9%)	14	47
35	BP	115/116 (99%)	102 (89%)	13 (11%)	9	32
35	DP	115/116 (99%)	104 (90%)	11 (10%)	12	42
36	BQ	111/111 (100%)	94 (85%)	17 (15%)	4	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	DQ	111/111 (100%)	96 (86%)	15 (14%)	6	22
37	BR	101/101 (100%)	83 (82%)	18 (18%)	2	10
37	DR	101/101 (100%)	85 (84%)	16 (16%)	4	14
38	BS	87/88 (99%)	77 (88%)	10 (12%)	8	31
38	DS	85/88 (97%)	70 (82%)	15 (18%)	3	10
39	BT	115/127 (91%)	104 (90%)	11 (10%)	12	42
39	DT	113/127 (89%)	105 (93%)	8 (7%)	21	61
40	BU	93/94 (99%)	83 (89%)	10 (11%)	9	34
40	DU	93/94 (99%)	82 (88%)	11 (12%)	8	29
41	BV	80/82 (98%)	69 (86%)	11 (14%)	5	21
41	DV	80/82 (98%)	71 (89%)	9 (11%)	9	32
42	BW	90/92 (98%)	79 (88%)	11 (12%)	7	26
42	DW	90/92 (98%)	80 (89%)	10 (11%)	9	33
43	BX	77/78 (99%)	73 (95%)	4 (5%)	32	73
43	DX	77/78 (99%)	74 (96%)	3 (4%)	43	83
44	BY	85/91 (93%)	79 (93%)	6 (7%)	21	61
44	DY	85/91 (93%)	79 (93%)	6 (7%)	21	61
45	BZ	145/179 (81%)	121 (83%)	24 (17%)	3	12
45	DZ	145/179 (81%)	126 (87%)	19 (13%)	6	23
46	B0	65/67 (97%)	61 (94%)	4 (6%)	26	66
46	D0	65/67 (97%)	59 (91%)	6 (9%)	13	45
47	B1	80/83 (96%)	72 (90%)	8 (10%)	11	38
47	D1	80/83 (96%)	73 (91%)	7 (9%)	14	49
48	B2	65/67 (97%)	56 (86%)	9 (14%)	5	21
48	D2	65/67 (97%)	57 (88%)	8 (12%)	7	26
49	B3	51/52 (98%)	44 (86%)	7 (14%)	5	21
49	D3	50/52 (96%)	43 (86%)	7 (14%)	5	21
50	B4	59/63 (94%)	48 (81%)	11 (19%)	2	9
50	D4	53/63 (84%)	45 (85%)	8 (15%)	4	16
51	B5	50/52 (96%)	45 (90%)	5 (10%)	11	38
51	D5	50/52 (96%)	45 (90%)	5 (10%)	11	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	B6	51/52 (98%)	45 (88%)	6 (12%)	8	29
52	D6	50/52 (96%)	46 (92%)	4 (8%)	17	55
53	B7	41/42 (98%)	37 (90%)	4 (10%)	12	40
53	D7	41/42 (98%)	39 (95%)	2 (5%)	35	76
54	B8	53/55 (96%)	49 (92%)	4 (8%)	19	58
54	D8	54/55 (98%)	50 (93%)	4 (7%)	20	59
55	B9	34/34 (100%)	33 (97%)	1 (3%)	55	88
55	D9	34/34 (100%)	33 (97%)	1 (3%)	55	88
All	All	9325/10072 (93%)	8209 (88%)	1116 (12%)	7	27

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

Mol	Chain	Res	Type
45	BZ	87	ASP
3	CC	154	SER
42	DW	51	LEU
46	B0	55	ARG
53	B7	1	MET

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

Mol	Chain	Res	Type
44	BY	43	ASN
3	CC	28	GLN
37	DR	71	GLN
45	BZ	32	HIS
49	B3	32	GLN

5.3.3 RNA ⓘ

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

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
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	BA	2623	U
1	CA	560	U
25	DA	1790	C
25	BA	2763	A
1	CA	97	G

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	2QZ	AW	1	24	8,8,9	6.07	2 (25%)	7,10,12	4.48	1 (14%)
24	2QY	AW	10	24	12,13,14	1.40	2 (16%)	13,16,18	2.74	4 (30%)
24	004	AW	3	24	10,10,11	6.58	3 (30%)	10,12,14	4.25	1 (10%)
24	MVA	AW	5	24	7,7,8	6.69	2 (28%)	5,8,10	1.83	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	2R1	AW	6	24	9,10,11	2.24	4 (44%)	10,13,15	42.20	3 (30%)
24	2R3	AW	8	24	14,14,15	5.64	1 (7%)	16,18,20	1.98	7 (43%)
24	MVA	AW	9	24	7,7,8	5.33	2 (28%)	5,8,10	1.19	1 (20%)
24	2QZ	CW	1	24	8,8,9	6.20	2 (25%)	7,10,12	3.96	2 (28%)
24	2QY	CW	10	24	12,13,14	1.42	3 (25%)	13,16,18	2.11	2 (15%)
24	004	CW	3	24	10,10,11	5.93	3 (30%)	10,12,14	2.35	1 (10%)
24	MVA	CW	5	24	7,7,8	6.83	3 (42%)	5,8,10	1.21	1 (20%)
24	2R1	CW	6	24	9,10,11	2.27	3 (33%)	10,13,15	25.54	3 (30%)
24	2R3	CW	8	24	14,14,15	5.57	1 (7%)	16,18,20	1.81	6 (37%)
24	MVA	CW	9	24	7,7,8	6.38	3 (42%)	5,8,10	1.71	2 (40%)

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AW	8	2R3	O-C	20.93	1.25	1.11
24	CW	8	2R3	O-C	20.69	1.25	1.11
24	AW	3	004	O-C	19.96	1.25	1.11
24	CW	5	MVA	O-C	17.69	1.23	1.11
24	AW	5	MVA	O-C	17.46	1.23	1.11

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AW	6	2R1	CG1-CB-CA	132.32	125.12	119.61
24	CW	6	2R1	CG1-CB-CA	79.57	122.92	119.61
24	AW	6	2R1	OD2-CG2-CB	-16.77	88.98	112.43
24	CW	6	2R1	OD2-CG2-CB	-13.56	93.46	112.43
24	AW	3	004	C-CA-N	-13.05	111.79	113.27

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AW	1	2QZ	C-CA-N-CN1
24	CW	1	2QZ	C-CA-N-CN1
24	AW	5	MVA	CB-CA-N-CN
24	AW	10	2QY	CB-CA-N-CN

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
57	SF4	AD	501	4	12,12,12	22.94	12 (100%)	0,24,24	0.00	-
59	FME	AX	101	23	9,9,10	6.44	3 (33%)	6,9,11	1.55	2 (33%)
57	SF4	CD	501	4	12,12,12	21.98	12 (100%)	0,24,24	0.00	-
59	FME	CX	101	23	9,9,10	6.95	3 (33%)	6,9,11	1.27	1 (16%)

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	-	0/0/48/48	0/6/5/5
59	FME	AX	101	23	-	1/7/9/11	0/0/0/0
57	SF4	CD	501	4	-	0/0/48/48	0/6/5/5
59	FME	CX	101	23	-	1/7/9/11	0/0/0/0

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	AD	501	SF4	S1-FE2	-24.75	2.16	2.33
57	AD	501	SF4	S3-FE4	-24.11	2.17	2.33
57	CD	501	SF4	S4-FE3	-24.04	2.17	2.33
57	CD	501	SF4	S2-FE1	-23.63	2.17	2.33
57	AD	501	SF4	S2-FE1	-23.62	2.17	2.33

All (3) 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	CX	101	FME	CA-N-CN	-2.17	119.49	122.82
59	AX	101	FME	CB-CA-N	2.10	114.90	111.26

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	AX	101	FME	O1-CN-N-CA
59	CX	101	FME	O1-CN-N-CA

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.25	26 (1%) 67 15	36, 80, 103, 123	0
1	CA	1503/1522 (98%)	-0.27	22 (1%) 70 16	38, 80, 103, 122	0
2	AB	231/256 (90%)	-0.10	1 (0%) 90 45	71, 88, 98, 107	0
2	CB	231/256 (90%)	0.09	2 (0%) 81 25	71, 89, 99, 108	0
3	AC	206/239 (86%)	0.04	2 (0%) 79 23	74, 87, 96, 108	0
3	CC	206/239 (86%)	0.19	3 (1%) 70 16	75, 89, 98, 106	0
4	AD	208/209 (99%)	-0.02	1 (0%) 88 39	62, 80, 92, 99	0
4	CD	208/209 (99%)	-0.14	0 100 100	61, 79, 92, 99	0
5	AE	148/162 (91%)	-0.23	0 100 100	53, 73, 83, 96	0
5	CE	148/162 (91%)	-0.19	0 100 100	54, 74, 85, 98	0
6	AF	100/101 (99%)	-0.17	0 100 100	60, 78, 89, 92	0
6	CF	100/101 (99%)	-0.22	0 100 100	62, 79, 89, 94	0
7	AG	155/156 (99%)	0.17	5 (3%) 45 7	74, 85, 97, 104	0
7	CG	155/156 (99%)	0.18	4 (2%) 53 8	76, 86, 99, 105	0
8	AH	137/138 (99%)	-0.09	0 100 100	60, 75, 83, 90	0
8	CH	137/138 (99%)	-0.08	0 100 100	61, 76, 83, 90	0
9	AI	127/128 (99%)	0.27	0 100 100	70, 92, 99, 103	0
9	CI	127/128 (99%)	0.72	8 (6%) 19 3	69, 93, 100, 105	0
10	AJ	97/105 (92%)	0.34	1 (1%) 79 23	71, 93, 101, 106	0
10	CJ	96/105 (91%)	0.34	2 (2%) 60 11	75, 95, 102, 107	0
11	AK	114/129 (88%)	-0.24	0 100 100	53, 74, 88, 93	0
11	CK	114/129 (88%)	-0.16	0 100 100	54, 76, 88, 93	0
12	AL	122/132 (92%)	-0.14	0 100 100	56, 68, 80, 86	0
12	CL	122/132 (92%)	-0.11	0 100 100	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%)	0.21	4 (3%)	44	6	67, 83, 95, 104	0
13	CM	122/126 (96%)	0.41	7 (5%)	23	3	77, 91, 101, 105	0
14	AN	60/61 (98%)	0.07	1 (1%)	67	15	74, 85, 95, 97	0
14	CN	60/61 (98%)	0.34	1 (1%)	67	15	77, 88, 95, 100	0
15	AO	88/89 (98%)	-0.20	0	100	100	59, 73, 87, 94	0
15	CO	88/89 (98%)	-0.05	0	100	100	58, 73, 87, 95	0
16	AP	82/88 (93%)	0.22	0	100	100	66, 77, 88, 95	0
16	CP	82/88 (93%)	-0.05	0	100	100	66, 76, 89, 93	0
17	AQ	99/105 (94%)	0.00	0	100	100	59, 73, 84, 87	0
17	CQ	99/105 (94%)	-0.06	0	100	100	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%)	0.26	0	100	100	67, 77, 87, 89	0
19	AS	83/93 (89%)	0.39	0	100	100	79, 91, 100, 105	0
19	CS	83/93 (89%)	0.53	1 (1%)	75	20	82, 92, 102, 106	0
20	AT	96/106 (90%)	0.07	0	100	100	62, 75, 88, 91	0
20	CT	96/106 (90%)	0.01	0	100	100	62, 75, 86, 94	0
21	AU	23/27 (85%)	0.82	1 (4%)	34	5	76, 87, 90, 91	0
21	CU	23/27 (85%)	0.65	0	100	100	77, 87, 91, 92	0
22	AV	7/24 (29%)	0.03	0	100	100	61, 73, 97, 100	0
22	CV	6/24 (25%)	0.52	0	100	100	64, 75, 94, 103	0
23	AX	76/77 (98%)	-0.15	0	100	100	48, 79, 96, 101	0
23	CX	76/77 (98%)	-0.06	0	100	100	47, 81, 98, 101	0
24	AW	6/10 (60%)	-0.24	0	100	100	78, 83, 93, 96	0
24	CW	6/10 (60%)	-0.14	0	100	100	67, 77, 87, 96	0
25	BA	2731/2915 (93%)	-0.35	9 (0%)	91	53	24, 44, 86, 114	0
25	DA	2714/2915 (93%)	-0.54	13 (0%)	88	39	27, 48, 87, 118	0
26	BB	120/122 (98%)	-0.46	0	100	100	41, 68, 81, 96	0
26	DB	120/122 (98%)	-0.36	0	100	100	47, 73, 86, 98	0
27	BD	275/276 (99%)	-0.32	0	100	100	24, 41, 62, 85	0
27	DD	275/276 (99%)	-0.31	0	100	100	25, 44, 63, 86	0
28	BE	204/206 (99%)	-0.27	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%)	-0.31	0	100	100	24, 47, 70, 90	0
29	BF	203/210 (96%)	-0.24	0	100	100	24, 53, 77, 97	0
29	DF	203/210 (96%)	-0.29	0	100	100	25, 56, 79, 96	0
30	BG	181/182 (99%)	-0.25	0	100	100	61, 76, 89, 100	0
30	DG	181/182 (99%)	-0.01	0	100	100	65, 79, 91, 100	0
31	BH	174/180 (96%)	-0.22	0	100	100	49, 67, 81, 85	0
31	DH	174/180 (96%)	0.27	2 (1%)	77	22	54, 72, 85, 89	0
32	BI	146/148 (98%)	-0.11	0	100	100	49, 77, 88, 94	0
32	DI	146/148 (98%)	0.01	0	100	100	49, 78, 88, 94	0
33	BN	140/140 (100%)	-0.29	0	100	100	33, 48, 71, 78	0
33	DN	140/140 (100%)	-0.32	0	100	100	35, 52, 73, 81	0
34	BO	122/122 (100%)	-0.33	0	100	100	23, 40, 61, 76	0
34	DO	122/122 (100%)	-0.31	0	100	100	37, 53, 71, 80	0
35	BP	149/150 (99%)	-0.25	0	100	100	25, 54, 77, 83	0
35	DP	149/150 (99%)	-0.07	0	100	100	27, 57, 81, 87	0
36	BQ	141/141 (100%)	-0.23	0	100	100	36, 52, 68, 79	0
36	DQ	141/141 (100%)	-0.32	0	100	100	38, 55, 71, 81	0
37	BR	118/118 (100%)	-0.34	0	100	100	20, 35, 52, 64	0
37	DR	118/118 (100%)	-0.27	0	100	100	36, 52, 68, 84	0
38	BS	110/112 (98%)	-0.32	0	100	100	35, 54, 71, 85	0
38	DS	110/112 (98%)	0.13	0	100	100	65, 81, 92, 95	0
39	BT	131/146 (89%)	-0.34	0	100	100	31, 45, 75, 92	0
39	DT	131/146 (89%)	-0.30	0	100	100	45, 59, 80, 90	0
40	BU	116/118 (98%)	-0.45	0	100	100	21, 31, 52, 63	0
40	DU	116/118 (98%)	-0.29	1 (0%)	81	25	36, 61, 78, 92	0
41	BV	101/101 (100%)	-0.33	0	100	100	27, 53, 73, 80	0
41	DV	101/101 (100%)	-0.20	0	100	100	29, 58, 78, 80	0
42	BW	112/113 (99%)	-0.33	0	100	100	27, 38, 62, 92	0
42	DW	112/113 (99%)	-0.19	0	100	100	30, 42, 64, 94	0
43	BX	95/96 (98%)	-0.30	0	100	100	29, 47, 72, 81	0
43	DX	95/96 (98%)	-0.19	1 (1%)	77	22	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%)	-0.10	0 100 100	39, 61, 80, 89	0
44	DY	107/110 (97%)	0.15	1 (0%) 81 25	43, 65, 82, 92	0
45	BZ	171/206 (83%)	-0.25	0 100 100	53, 71, 85, 96	0
45	DZ	174/206 (84%)	-0.08	0 100 100	58, 74, 87, 95	0
46	B0	83/85 (97%)	-0.07	6 (7%) 15 2	25, 39, 80, 108	0
46	D0	83/85 (97%)	0.20	4 (4%) 29 4	42, 66, 86, 104	0
47	B1	97/98 (98%)	-0.23	0 100 100	27, 44, 74, 83	0
47	D1	97/98 (98%)	-0.21	0 100 100	35, 58, 79, 86	0
48	B2	70/72 (97%)	-0.35	0 100 100	35, 48, 64, 90	0
48	D2	70/72 (97%)	-0.21	0 100 100	59, 74, 83, 92	0
49	B3	59/60 (98%)	-0.29	0 100 100	24, 38, 63, 85	0
49	D3	59/60 (98%)	0.19	0 100 100	45, 62, 80, 90	0
50	B4	69/71 (97%)	-0.13	0 100 100	60, 85, 103, 105	0
50	D4	69/71 (97%)	0.12	1 (1%) 72 17	82, 96, 106, 112	0
51	B5	59/60 (98%)	-0.42	0 100 100	14, 36, 59, 74	0
51	D5	59/60 (98%)	-0.37	0 100 100	31, 50, 72, 82	0
52	B6	53/54 (98%)	-0.27	0 100 100	43, 53, 68, 75	0
52	D6	53/54 (98%)	-0.22	0 100 100	45, 56, 69, 73	0
53	B7	48/49 (97%)	-0.19	0 100 100	24, 32, 62, 84	0
53	D7	48/49 (97%)	-0.18	1 (2%) 60 11	26, 35, 63, 86	0
54	B8	64/65 (98%)	-0.23	0 100 100	31, 42, 51, 64	0
54	D8	64/65 (98%)	-0.21	0 100 100	34, 46, 56, 66	0
55	B9	37/37 (100%)	0.08	0 100 100	43, 53, 71, 77	0
55	D9	37/37 (100%)	0.47	2 (5%) 25 4	46, 58, 73, 78	0
All	All	20468/21468 (95%)	-0.22	133 (0%) 86 36	14, 65, 95, 123	0

The worst 5 of 133 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	CM	124	PRO	8.7
13	CM	123	ALA	7.7
13	AM	123	ALA	6.0
13	AM	124	PRO	5.9
1	CA	1030(B)	C	5.9

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
24	2R3	CW	8	14/15	0.11	-	47,70,74,79	0
24	MVA	CW	5	8/9	0.19	-	51,78,86,88	0
24	MVA	AW	9	8/9	0.24	-	65,78,87,91	0
24	2QZ	AW	1	9/10	0.23	-	58,64,81,82	0
24	MVA	CW	9	8/9	0.20	-	61,72,80,84	0
24	2QY	AW	10	13/14	0.13	-	55,67,75,79	0
24	2R1	AW	6	10/11	0.12	-	68,82,98,104	0
24	2R3	AW	8	14/15	0.13	-	54,79,87,90	0
24	MVA	AW	5	8/9	0.19	-	66,87,90,90	0
24	2QZ	CW	1	9/10	0.22	-	57,72,81,93	0
24	004	CW	3	10/11	0.14	-	60,76,84,86	0
24	2R1	CW	6	10/11	0.11	-	79,86,90,94	0
24	2QY	CW	10	13/14	0.14	-	55,69,84,94	0
24	004	AW	3	10/11	0.13	-	71,89,99,106	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
56	MG	CA	3155	1/1	0.14	-	71,71,71,71	0
56	MG	DB	3002	1/1	0.27	-	56,56,56,56	0
56	MG	DA	3246	1/1	0.17	-	24,24,24,24	0
56	MG	AA	3074	1/1	0.38	-	47,47,47,47	0
56	MG	BA	3041	1/1	0.37	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	3151	1/1	0.07	-	41,41,41,41	0
56	MG	BA	3001	1/1	0.16	-	69,69,69,69	0
56	MG	DA	3304	1/1	0.10	-	35,35,35,35	0
56	MG	DA	3499	1/1	0.14	-	46,46,46,46	0
56	MG	BA	3249	1/1	0.22	-	40,40,40,40	0
56	MG	BA	3251	1/1	0.21	-	61,61,61,61	0
56	MG	BA	3481	1/1	0.22	-	38,38,38,38	0
56	MG	DA	3369	1/1	0.14	-	47,47,47,47	0
56	MG	BA	3643	1/1	0.27	-	43,43,43,43	0
56	MG	BA	3404	1/1	0.15	-	35,35,35,35	0
56	MG	BA	3106	1/1	0.12	-	48,48,48,48	0
56	MG	BA	3004	1/1	0.12	-	24,24,24,24	0
56	MG	BA	3194	1/1	0.18	-	55,55,55,55	0
56	MG	AA	3023	1/1	0.17	-	65,65,65,65	0
56	MG	DA	3082	1/1	0.10	-	19,19,19,19	0
56	MG	BA	3586	1/1	0.19	-	29,29,29,29	0
56	MG	CA	3099	1/1	0.32	-	65,65,65,65	0
56	MG	DA	3089	1/1	0.38	-	57,57,57,57	0
56	MG	AA	3202	1/1	0.23	-	76,76,76,76	0
56	MG	DA	3190	1/1	0.12	-	37,37,37,37	0
56	MG	BA	3712	1/1	0.10	-	58,58,58,58	0
56	MG	BA	3162	1/1	0.19	-	23,23,23,23	0
56	MG	DF	303	1/1	0.34	-	43,43,43,43	0
56	MG	BA	3299	1/1	0.23	-	9,9,9,9	0
56	MG	BA	3241	1/1	0.38	-	63,63,63,63	0
56	MG	DA	3523	1/1	0.07	-	55,55,55,55	0
56	MG	DA	3595	1/1	0.18	-	72,72,72,72	0
56	MG	DA	3511	1/1	0.07	-	65,65,65,65	0
56	MG	BA	3053	1/1	0.34	-	39,39,39,39	0
56	MG	DA	3549	1/1	0.26	-	52,52,52,52	0
56	MG	AX	110	1/1	0.19	-	42,42,42,42	0
56	MG	BE	309	1/1	0.26	-	25,25,25,25	0
56	MG	DB	3004	1/1	0.15	-	68,68,68,68	0
56	MG	BA	3018	1/1	0.40	-	40,40,40,40	0
56	MG	BA	3113	1/1	0.08	-	32,32,32,32	0
56	MG	BA	3574	1/1	0.07	-	54,54,54,54	0
56	MG	DA	3612	1/1	0.14	-	39,39,39,39	0
56	MG	BA	3208	1/1	0.24	-	41,41,41,41	0
56	MG	CA	3150	1/1	0.10	-	59,59,59,59	0
56	MG	DA	3323	1/1	0.18	-	30,30,30,30	0
56	MG	BA	3223	1/1	0.60	-	47,47,47,47	0
56	MG	CA	3015	1/1	0.35	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3246	1/1	0.22	-	46,46,46,46	0
56	MG	DA	3481	1/1	0.28	-	47,47,47,47	0
56	MG	BA	3050	1/1	0.16	-	21,21,21,21	0
56	MG	BA	3312	1/1	0.09	-	58,58,58,58	0
56	MG	DA	3351	1/1	0.40	-	35,35,35,35	0
56	MG	BA	3242	1/1	0.33	-	48,48,48,48	0
58	ZN	DY	501	1/1	0.05	-	83,83,83,83	0
56	MG	AA	3021	1/1	0.23	-	76,76,76,76	0
56	MG	BE	306	1/1	0.44	-	46,46,46,46	0
56	MG	BA	3178	1/1	0.25	-	48,48,48,48	0
56	MG	BA	3119	1/1	0.25	-	58,58,58,58	0
56	MG	AA	3177	1/1	0.16	-	80,80,80,80	0
56	MG	BB	3006	1/1	0.24	-	39,39,39,39	0
56	MG	DA	3070	1/1	0.25	-	44,44,44,44	0
56	MG	BA	3459	1/1	0.21	-	31,31,31,31	0
56	MG	AA	3131	1/1	0.48	-	56,56,56,56	0
56	MG	BA	3294	1/1	0.29	-	37,37,37,37	0
56	MG	BA	3713	1/1	0.12	-	66,66,66,66	0
56	MG	BA	3135	1/1	0.16	-	42,42,42,42	0
56	MG	DA	3027	1/1	0.42	-	39,39,39,39	0
56	MG	AA	3087	1/1	0.43	-	72,72,72,72	0
56	MG	DA	3149	1/1	0.06	-	47,47,47,47	0
56	MG	DA	3017	1/1	0.18	-	46,46,46,46	0
56	MG	BA	3075	1/1	0.23	-	45,45,45,45	0
56	MG	BA	3719	1/1	0.24	-	25,25,25,25	0
56	MG	DA	3111	1/1	0.20	-	53,53,53,53	0
56	MG	DA	3495	1/1	0.23	-	39,39,39,39	0
56	MG	BA	3490	1/1	0.23	-	38,38,38,38	0
56	MG	BA	3056	1/1	0.41	-	44,44,44,44	0
56	MG	DA	3610	1/1	0.25	-	54,54,54,54	0
56	MG	BA	3128	1/1	0.30	-	40,40,40,40	0
56	MG	BA	3327	1/1	0.17	-	38,38,38,38	0
56	MG	BA	3254	1/1	0.16	-	59,59,59,59	0
56	MG	D5	101	1/1	0.44	-	53,53,53,53	0
56	MG	AA	3123	1/1	0.46	-	39,39,39,39	0
56	MG	DA	3095	1/1	0.24	-	61,61,61,61	0
59	FME	CX	101	10/11	0.58	-	71,82,97,105	0
56	MG	BA	3594	1/1	0.32	-	42,42,42,42	0
56	MG	BA	3040	1/1	0.34	-	51,51,51,51	0
56	MG	AA	3103	1/1	0.20	-	38,38,38,38	0
56	MG	BA	3027	1/1	0.16	-	45,45,45,45	0
56	MG	BD	305	1/1	0.24	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3505	1/1	0.06	-	65,65,65,65	0
56	MG	DA	3164	1/1	0.27	-	48,48,48,48	0
56	MG	BB	3016	1/1	0.12	-	21,21,21,21	0
56	MG	DA	3454	1/1	0.29	-	55,55,55,55	0
56	MG	BA	3191	1/1	0.18	-	52,52,52,52	0
56	MG	BA	3715	1/1	0.13	-	47,47,47,47	0
56	MG	DA	3456	1/1	0.13	-	47,47,47,47	0
56	MG	AA	3133	1/1	0.36	-	63,63,63,63	0
56	MG	AX	106	1/1	0.15	-	73,73,73,73	0
56	MG	BA	3686	1/1	0.13	-	25,25,25,25	0
56	MG	AA	3160	1/1	0.29	-	52,52,52,52	0
56	MG	BA	3700	1/1	0.12	-	67,67,67,67	0
56	MG	BA	3470	1/1	0.20	-	54,54,54,54	0
56	MG	BA	3488	1/1	0.34	-	35,35,35,35	0
56	MG	BA	3569	1/1	0.18	-	19,19,19,19	0
56	MG	DA	3036	1/1	0.30	-	35,35,35,35	0
56	MG	AA	3092	1/1	0.47	-	50,50,50,50	0
56	MG	BA	3396	1/1	0.18	-	22,22,22,22	0
56	MG	B7	103	1/1	0.92	-	48,48,48,48	0
56	MG	DA	3541	1/1	0.26	-	35,35,35,35	0
56	MG	BA	3533	1/1	0.15	-	32,32,32,32	0
56	MG	CA	3004	1/1	0.24	-	96,96,96,96	0
56	MG	DA	3566	1/1	0.15	-	71,71,71,71	0
56	MG	BA	3193	1/1	0.70	-	52,52,52,52	0
56	MG	AA	3053	1/1	0.34	-	49,49,49,49	0
56	MG	DA	3401	1/1	0.28	-	58,58,58,58	0
56	MG	AA	3128	1/1	0.21	-	68,68,68,68	0
56	MG	DV	202	1/1	0.80	-	63,63,63,63	0
56	MG	BA	3253	1/1	0.17	-	51,51,51,51	0
56	MG	DQ	204	1/1	0.16	-	43,43,43,43	0
56	MG	CA	3152	1/1	0.39	-	55,55,55,55	0
56	MG	DA	3178	1/1	0.36	-	43,43,43,43	0
56	MG	DD	308	1/1	0.16	-	55,55,55,55	0
56	MG	BA	3402	1/1	0.24	-	71,71,71,71	0
56	MG	CA	3112	1/1	0.23	-	59,59,59,59	0
56	MG	BW	203	1/1	0.28	-	45,45,45,45	0
56	MG	CA	3140	1/1	0.16	-	73,73,73,73	0
56	MG	DA	3065	1/1	0.22	-	38,38,38,38	0
56	MG	BA	3130	1/1	0.45	-	43,43,43,43	0
56	MG	DA	3441	1/1	0.34	-	53,53,53,53	0
56	MG	BA	3549	1/1	0.21	-	27,27,27,27	0
56	MG	DA	3144	1/1	0.40	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	3034	1/1	0.17	-	48,48,48,48	0
56	MG	CE	3002	1/1	0.07	-	55,55,55,55	0
56	MG	DA	3421	1/1	0.21	-	34,34,34,34	0
56	MG	AA	3204	1/1	0.13	-	54,54,54,54	0
56	MG	AA	3024	1/1	0.17	-	53,53,53,53	0
56	MG	BA	3644	1/1	0.15	-	43,43,43,43	0
56	MG	BA	3116	1/1	0.19	-	31,31,31,31	0
56	MG	B5	502	1/1	0.11	-	54,54,54,54	0
56	MG	DA	3121	1/1	0.26	-	48,48,48,48	0
56	MG	BA	3167	1/1	0.33	-	39,39,39,39	0
56	MG	BA	3124	1/1	0.17	-	39,39,39,39	0
56	MG	DA	3571	1/1	0.13	-	46,46,46,46	0
56	MG	BP	203	1/1	0.68	-	29,29,29,29	0
56	MG	BA	3333	1/1	0.12	-	49,49,49,49	0
58	ZN	B9	501	1/1	0.10	-	48,48,48,48	0
56	MG	BA	3104	1/1	0.32	-	45,45,45,45	0
56	MG	DA	3615	1/1	0.40	-	60,60,60,60	0
56	MG	BA	3540	1/1	0.24	-	34,34,34,34	0
56	MG	BA	3391	1/1	0.14	-	48,48,48,48	0
56	MG	BA	3081	1/1	0.10	-	14,14,14,14	0
56	MG	DA	3232	1/1	0.23	-	50,50,50,50	0
56	MG	BA	3638	1/1	0.25	-	37,37,37,37	0
56	MG	BA	3301	1/1	0.13	-	56,56,56,56	0
56	MG	DA	3363	1/1	0.09	-	57,57,57,57	0
56	MG	BA	3716	1/1	0.11	-	27,27,27,27	0
56	MG	BA	3252	1/1	0.17	-	55,55,55,55	0
56	MG	DA	3476	1/1	0.20	-	45,45,45,45	0
56	MG	DA	3606	1/1	0.12	-	58,58,58,58	0
56	MG	BA	3108	1/1	0.14	-	55,55,55,55	0
56	MG	DA	3334	1/1	0.17	-	49,49,49,49	0
56	MG	BA	3090	1/1	0.18	-	46,46,46,46	0
56	MG	BA	3118	1/1	0.18	-	39,39,39,39	0
56	MG	AA	3088	1/1	0.33	-	63,63,63,63	0
56	MG	AX	109	1/1	0.08	-	43,43,43,43	0
60	K	DA	3231	1/1	0.29	-	96,96,96,96	0
56	MG	BA	3140	1/1	0.18	-	64,64,64,64	0
56	MG	BA	3679	1/1	0.38	-	27,27,27,27	0
56	MG	BA	3697	1/1	0.14	-	78,78,78,78	0
56	MG	DA	3107	1/1	0.29	-	55,55,55,55	0
56	MG	CA	3169	1/1	0.17	-	57,57,57,57	0
56	MG	BA	3274	1/1	0.15	-	52,52,52,52	0
56	MG	BA	3534	1/1	0.12	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	3081	1/1	0.24	-	41,41,41,41	0
56	MG	BA	3581	1/1	0.10	-	51,51,51,51	0
56	MG	DA	3546	1/1	0.12	-	44,44,44,44	0
56	MG	AA	3216	1/1	0.14	-	58,58,58,58	0
56	MG	DA	3025	1/1	0.34	-	44,44,44,44	0
56	MG	BA	3381	1/1	0.10	-	37,37,37,37	0
56	MG	BA	3248	1/1	0.27	-	43,43,43,43	0
56	MG	DA	3151	1/1	0.29	-	60,60,60,60	0
56	MG	AA	3162	1/1	0.24	-	74,74,74,74	0
56	MG	DA	3594	1/1	0.34	-	47,47,47,47	0
56	MG	BA	3288	1/1	0.24	-	61,61,61,61	0
56	MG	BA	3365	1/1	0.14	-	20,20,20,20	0
56	MG	DA	3411	1/1	0.16	-	21,21,21,21	0
56	MG	DA	3307	1/1	0.28	-	37,37,37,37	0
56	MG	BA	3087	1/1	0.51	-	61,61,61,61	0
56	MG	AA	3112	1/1	0.17	-	51,51,51,51	0
56	MG	AA	3082	1/1	0.27	-	39,39,39,39	0
56	MG	CA	3063	1/1	0.11	-	61,61,61,61	0
56	MG	DA	3236	1/1	0.20	-	46,46,46,46	0
56	MG	BW	204	1/1	0.37	-	35,35,35,35	0
56	MG	DA	3413	1/1	0.23	-	53,53,53,53	0
56	MG	CA	3032	1/1	0.18	-	42,42,42,42	0
56	MG	CA	3028	1/1	0.40	-	43,43,43,43	0
56	MG	DA	3455	1/1	0.19	-	60,60,60,60	0
56	MG	AA	3069	1/1	0.12	-	84,84,84,84	0
56	MG	CA	3055	1/1	0.27	-	62,62,62,62	0
56	MG	BA	3065	1/1	0.41	-	50,50,50,50	0
56	MG	DA	3352	1/1	0.41	-	47,47,47,47	0
56	MG	CA	3057	1/1	0.24	-	49,49,49,49	0
56	MG	DA	3423	1/1	0.14	-	29,29,29,29	0
56	MG	BB	3002	1/1	0.20	-	59,59,59,59	0
56	MG	BA	3006	1/1	0.26	-	42,42,42,42	0
56	MG	AA	3039	1/1	0.20	-	60,60,60,60	0
56	MG	CA	3127	1/1	0.25	-	79,79,79,79	0
56	MG	BA	3061	1/1	0.47	-	51,51,51,51	0
56	MG	DA	3459	1/1	0.11	-	33,33,33,33	0
56	MG	DA	3488	1/1	0.05	-	46,46,46,46	0
56	MG	BA	3080	1/1	0.46	-	45,45,45,45	0
56	MG	BA	3447	1/1	0.13	-	37,37,37,37	0
56	MG	BA	3625	1/1	0.13	-	51,51,51,51	0
56	MG	CA	3041	1/1	0.68	-	75,75,75,75	0
56	MG	BA	3455	1/1	0.13	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3191	1/1	0.49	-	47,47,47,47	0
56	MG	BA	3539	1/1	0.16	-	35,35,35,35	0
56	MG	DA	3258	1/1	0.17	-	32,32,32,32	0
56	MG	AX	107	1/1	0.24	-	66,66,66,66	0
56	MG	BA	3261	1/1	0.28	-	34,34,34,34	0
56	MG	BD	307	1/1	0.19	-	43,43,43,43	0
56	MG	DA	3326	1/1	0.20	-	33,33,33,33	0
56	MG	BE	302	1/1	0.21	-	33,33,33,33	0
56	MG	AA	3209	1/1	0.31	-	70,70,70,70	0
56	MG	CA	3110	1/1	0.19	-	97,97,97,97	0
56	MG	BB	3014	1/1	0.12	-	69,69,69,69	0
56	MG	DA	3467	1/1	0.08	-	35,35,35,35	0
56	MG	CA	3019	1/1	0.07	-	49,49,49,49	0
56	MG	DA	3196	1/1	0.32	-	44,44,44,44	0
56	MG	AA	3015	1/1	0.13	-	73,73,73,73	0
56	MG	DA	3001	1/1	0.32	-	78,78,78,78	0
56	MG	DE	305	1/1	0.74	-	65,65,65,65	0
56	MG	DA	3439	1/1	0.18	-	28,28,28,28	0
56	MG	BU	208	1/1	0.93	-	56,56,56,56	0
56	MG	AA	3001	1/1	0.21	-	68,68,68,68	0
56	MG	BA	3409	1/1	0.21	-	27,27,27,27	0
56	MG	DA	3632	1/1	0.19	-	71,71,71,71	0
56	MG	BA	3271	1/1	0.14	-	36,36,36,36	0
56	MG	CA	3105	1/1	0.08	-	79,79,79,79	0
56	MG	DA	3184	1/1	0.33	-	45,45,45,45	0
56	MG	AA	3026	1/1	0.18	-	41,41,41,41	0
56	MG	BA	3629	1/1	0.14	-	47,47,47,47	0
56	MG	DA	3277	1/1	0.25	-	49,49,49,49	0
56	MG	BA	3069	1/1	0.41	-	41,41,41,41	0
56	MG	BA	3400	1/1	0.18	-	24,24,24,24	0
56	MG	DA	3212	1/1	0.09	-	48,48,48,48	0
56	MG	AA	3173	1/1	0.23	-	32,32,32,32	0
56	MG	BA	3278	1/1	0.17	-	34,34,34,34	0
56	MG	DA	3465	1/1	0.17	-	49,49,49,49	0
56	MG	DA	3135	1/1	0.21	-	50,50,50,50	0
56	MG	DA	3031	1/1	0.28	-	55,55,55,55	0
56	MG	BA	3688	1/1	0.10	-	54,54,54,54	0
56	MG	BA	3179	1/1	0.21	-	43,43,43,43	0
56	MG	DA	3104	1/1	0.27	-	62,62,62,62	0
56	MG	B4	3001	1/1	0.24	-	100,100,100,100	0
56	MG	DA	3309	1/1	0.18	-	33,33,33,33	0
56	MG	BA	3567	1/1	0.22	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3685	1/1	0.09	-	67,67,67,67	0
56	MG	AA	3156	1/1	0.19	-	62,62,62,62	0
56	MG	BA	3472	1/1	0.08	-	30,30,30,30	0
56	MG	BQ	201	1/1	0.51	-	61,61,61,61	0
56	MG	BA	3528	1/1	0.22	-	33,33,33,33	0
56	MG	BA	3012	1/1	0.16	-	40,40,40,40	0
56	MG	BA	3491	1/1	0.18	-	23,23,23,23	0
56	MG	CA	3091	1/1	0.15	-	72,72,72,72	0
56	MG	BA	3503	1/1	0.29	-	31,31,31,31	0
56	MG	BA	3291	1/1	0.17	-	41,41,41,41	0
56	MG	BQ	203	1/1	0.22	-	58,58,58,58	0
56	MG	AD	502	1/1	0.39	-	43,43,43,43	0
56	MG	AA	3067	1/1	0.40	-	87,87,87,87	0
56	MG	CA	3097	1/1	0.13	-	48,48,48,48	0
56	MG	B7	102	1/1	0.25	-	40,40,40,40	0
56	MG	DA	3448	1/1	0.07	-	57,57,57,57	0
56	MG	BA	3489	1/1	0.14	-	43,43,43,43	0
56	MG	DA	3186	1/1	0.45	-	53,53,53,53	0
56	MG	BA	3036	1/1	0.17	-	38,38,38,38	0
56	MG	DO	5001	1/1	0.12	-	35,35,35,35	0
56	MG	CA	3023	1/1	0.13	-	37,37,37,37	0
56	MG	BA	3667	1/1	0.09	-	63,63,63,63	0
56	MG	BA	3660	1/1	0.34	-	71,71,71,71	0
56	MG	CA	3133	1/1	0.06	-	49,49,49,49	0
56	MG	BA	3133	1/1	0.23	-	32,32,32,32	0
56	MG	DA	3366	1/1	0.37	-	36,36,36,36	0
56	MG	DA	3327	1/1	0.18	-	29,29,29,29	0
56	MG	BA	3550	1/1	0.24	-	45,45,45,45	0
56	MG	AA	3071	1/1	0.34	-	60,60,60,60	0
56	MG	BA	3627	1/1	0.20	-	50,50,50,50	0
56	MG	BV	204	1/1	0.19	-	20,20,20,20	0
56	MG	CA	3134	1/1	0.12	-	82,82,82,82	0
56	MG	BA	3484	1/1	0.16	-	54,54,54,54	0
56	MG	CA	3088	1/1	0.24	-	43,43,43,43	0
56	MG	BA	3026	1/1	0.43	-	36,36,36,36	0
56	MG	DA	3648	1/1	0.14	-	52,52,52,52	0
56	MG	BA	3462	1/1	0.10	-	52,52,52,52	0
56	MG	BA	3597	1/1	0.34	-	60,60,60,60	0
56	MG	DA	3240	1/1	0.23	-	51,51,51,51	0
56	MG	BA	3482	1/1	0.17	-	72,72,72,72	0
56	MG	DA	3553	1/1	0.34	-	70,70,70,70	0
56	MG	BN	3001	1/1	0.74	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DB	3011	1/1	0.34	-	55,55,55,55	0
56	MG	AA	3076	1/1	0.31	-	66,66,66,66	0
56	MG	DA	3324	1/1	0.26	-	40,40,40,40	0
56	MG	BD	312	1/1	0.84	-	80,80,80,80	0
56	MG	BA	3446	1/1	0.12	-	49,49,49,49	0
56	MG	BA	3474	1/1	0.22	-	42,42,42,42	0
56	MG	BD	302	1/1	0.34	-	58,58,58,58	0
56	MG	CA	3102	1/1	0.09	-	41,41,41,41	0
56	MG	DA	3285	1/1	0.21	-	55,55,55,55	0
56	MG	BA	3738	1/1	0.29	-	59,59,59,59	0
56	MG	BA	3100	1/1	0.23	-	48,48,48,48	0
56	MG	AA	3002	1/1	0.19	-	57,57,57,57	0
56	MG	AA	3022	1/1	0.25	-	48,48,48,48	0
56	MG	DA	3078	1/1	0.20	-	44,44,44,44	0
56	MG	B7	104	1/1	0.13	-	51,51,51,51	0
56	MG	DA	3640	1/1	0.68	-	56,56,56,56	0
56	MG	CA	3080	1/1	0.15	-	55,55,55,55	0
56	MG	CA	3126	1/1	0.23	-	61,61,61,61	0
56	MG	BA	3367	1/1	0.09	-	50,50,50,50	0
56	MG	CA	3039	1/1	0.35	-	72,72,72,72	0
56	MG	DA	3302	1/1	0.17	-	22,22,22,22	0
56	MG	DA	3564	1/1	0.74	-	61,61,61,61	0
56	MG	DA	3464	1/1	0.61	-	50,50,50,50	0
56	MG	BA	3202	1/1	0.27	-	41,41,41,41	0
56	MG	CA	3136	1/1	0.20	-	45,45,45,45	0
56	MG	AA	3014	1/1	0.19	-	28,28,28,28	0
56	MG	DA	3247	1/1	0.09	-	31,31,31,31	0
56	MG	BE	301	1/1	0.50	-	43,43,43,43	0
56	MG	BA	3717	1/1	0.21	-	57,57,57,57	0
56	MG	DA	3555	1/1	0.13	-	41,41,41,41	0
56	MG	BA	3226	1/1	0.29	-	32,32,32,32	0
56	MG	DA	3322	1/1	0.14	-	55,55,55,55	0
56	MG	DA	3313	1/1	0.13	-	52,52,52,52	0
56	MG	BA	3126	1/1	0.21	-	24,24,24,24	0
56	MG	CA	3090	1/1	0.16	-	73,73,73,73	0
56	MG	AA	3064	1/1	0.17	-	79,79,79,79	0
56	MG	AA	3179	1/1	0.27	-	34,34,34,34	0
56	MG	DA	3311	1/1	0.10	-	32,32,32,32	0
56	MG	BA	3515	1/1	0.06	-	56,56,56,56	0
56	MG	CA	3144	1/1	0.56	-	63,63,63,63	0
56	MG	BA	3681	1/1	0.14	-	40,40,40,40	0
56	MG	BA	3354	1/1	0.14	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	3104	1/1	0.17	-	37,37,37,37	0
56	MG	AA	3099	1/1	0.44	-	60,60,60,60	0
56	MG	DA	3122	1/1	0.14	-	62,62,62,62	0
56	MG	DA	3561	1/1	0.16	-	45,45,45,45	0
56	MG	AA	3150	1/1	0.27	-	46,46,46,46	0
56	MG	BB	3012	1/1	0.17	-	56,56,56,56	0
56	MG	BA	3541	1/1	0.22	-	30,30,30,30	0
56	MG	BN	3006	1/1	0.13	-	24,24,24,24	0
56	MG	DA	3654	1/1	0.19	-	52,52,52,52	0
56	MG	DA	3254	1/1	0.23	-	30,30,30,30	0
56	MG	DA	3368	1/1	0.11	-	39,39,39,39	0
56	MG	DA	3046	1/1	0.20	-	56,56,56,56	0
56	MG	BA	3458	1/1	0.12	-	29,29,29,29	0
56	MG	DA	3028	1/1	0.06	-	35,35,35,35	0
56	MG	BA	3382	1/1	0.13	-	51,51,51,51	0
56	MG	DA	3219	1/1	0.16	-	60,60,60,60	0
56	MG	AA	3142	1/1	0.26	-	38,38,38,38	0
56	MG	DA	3417	1/1	0.15	-	34,34,34,34	0
56	MG	DA	3043	1/1	0.45	-	54,54,54,54	0
56	MG	BA	3476	1/1	0.13	-	40,40,40,40	0
56	MG	DA	3379	1/1	0.22	-	28,28,28,28	0
56	MG	BR	203	1/1	0.20	-	15,15,15,15	0
56	MG	BA	3532	1/1	0.19	-	34,34,34,34	0
56	MG	BA	3257	1/1	0.33	-	38,38,38,38	0
56	MG	BA	3495	1/1	0.36	-	84,84,84,84	0
56	MG	DA	3494	1/1	0.09	-	78,78,78,78	0
56	MG	BA	3587	1/1	0.20	-	23,23,23,23	0
56	MG	DA	3038	1/1	0.15	-	39,39,39,39	0
56	MG	DA	3280	1/1	0.20	-	57,57,57,57	0
56	MG	BA	3115	1/1	0.29	-	36,36,36,36	0
56	MG	BA	3184	1/1	0.40	-	49,49,49,49	0
56	MG	BA	3255	1/1	0.18	-	41,41,41,41	0
56	MG	BA	3353	1/1	0.30	-	57,57,57,57	0
56	MG	BA	3121	1/1	0.27	-	57,57,57,57	0
56	MG	DA	3106	1/1	0.17	-	41,41,41,41	0
56	MG	BA	3282	1/1	0.41	-	49,49,49,49	0
56	MG	BA	3595	1/1	0.19	-	41,41,41,41	0
56	MG	AA	3080	1/1	0.17	-	53,53,53,53	0
56	MG	BA	3624	1/1	0.24	-	52,52,52,52	0
56	MG	BA	3334	1/1	0.28	-	73,73,73,73	0
56	MG	DA	3428	1/1	0.27	-	51,51,51,51	0
56	MG	BA	3330	1/1	0.18	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	3073	1/1	0.31	-	55,55,55,55	0
56	MG	BA	3170	1/1	0.61	-	48,48,48,48	0
56	MG	CA	3131	1/1	0.11	-	55,55,55,55	0
56	MG	BA	3316	1/1	0.16	-	28,28,28,28	0
56	MG	DA	3158	1/1	0.37	-	57,57,57,57	0
56	MG	DA	3373	1/1	0.24	-	29,29,29,29	0
56	MG	DA	3550	1/1	0.16	-	53,53,53,53	0
56	MG	CA	3156	1/1	0.16	-	70,70,70,70	0
56	MG	DA	3453	1/1	0.39	-	61,61,61,61	0
56	MG	DA	3129	1/1	0.13	-	43,43,43,43	0
56	MG	DA	3582	1/1	0.10	-	52,52,52,52	0
56	MG	DA	3222	1/1	0.13	-	71,71,71,71	0
56	MG	BA	3572	1/1	0.20	-	36,36,36,36	0
56	MG	CA	3067	1/1	0.30	-	80,80,80,80	0
56	MG	DA	3482	1/1	0.14	-	55,55,55,55	0
56	MG	BA	3201	1/1	0.31	-	36,36,36,36	0
56	MG	AA	3168	1/1	0.34	-	68,68,68,68	0
56	MG	BA	3479	1/1	0.11	-	56,56,56,56	0
56	MG	CA	3165	1/1	0.09	-	40,40,40,40	0
56	MG	AA	3038	1/1	0.33	-	66,66,66,66	0
56	MG	DA	3355	1/1	0.26	-	18,18,18,18	0
56	MG	DA	3256	1/1	0.18	-	63,63,63,63	0
56	MG	CA	3011	1/1	0.30	-	42,42,42,42	0
56	MG	AA	3097	1/1	0.23	-	43,43,43,43	0
56	MG	BA	3297	1/1	1.47	-	53,53,53,53	0
56	MG	B2	101	1/1	0.40	-	40,40,40,40	0
56	MG	CA	3035	1/1	0.23	-	52,52,52,52	0
56	MG	DA	3591	1/1	0.23	-	58,58,58,58	0
56	MG	BA	3439	1/1	0.15	-	34,34,34,34	0
56	MG	DA	3493	1/1	0.14	-	29,29,29,29	0
56	MG	DA	3003	1/1	0.36	-	56,56,56,56	0
56	MG	BA	3062	1/1	0.34	-	42,42,42,42	0
56	MG	CA	3093	1/1	0.06	-	53,53,53,53	0
56	MG	CA	3016	1/1	0.48	-	76,76,76,76	0
56	MG	DA	3384	1/1	0.12	-	23,23,23,23	0
56	MG	DA	3475	1/1	0.10	-	36,36,36,36	0
59	FME	AX	101	10/11	0.44	-	48,75,97,113	0
56	MG	DA	3187	1/1	0.49	-	59,59,59,59	0
56	MG	DA	3444	1/1	0.14	-	43,43,43,43	0
56	MG	BU	205	1/1	0.32	-	42,42,42,42	0
56	MG	DA	3442	1/1	0.16	-	40,40,40,40	0
56	MG	BA	3142	1/1	0.72	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3452	1/1	0.17	-	56,56,56,56	0
56	MG	DA	3156	1/1	0.57	-	29,29,29,29	0
56	MG	DA	3405	1/1	0.10	-	47,47,47,47	0
58	ZN	AN	102	1/1	0.11	-	90,90,90,90	0
56	MG	BA	3487	1/1	0.13	-	31,31,31,31	0
56	MG	DW	201	1/1	0.32	-	46,46,46,46	0
56	MG	BA	3412	1/1	0.18	-	26,26,26,26	0
56	MG	DA	3625	1/1	0.10	-	35,35,35,35	0
56	MG	BA	3077	1/1	0.20	-	39,39,39,39	0
56	MG	BA	3247	1/1	0.81	-	68,68,68,68	0
56	MG	DA	3193	1/1	0.21	-	65,65,65,65	0
56	MG	BA	3259	1/1	0.49	-	27,27,27,27	0
56	MG	CA	3162	1/1	0.22	-	46,46,46,46	0
56	MG	BA	3032	1/1	0.19	-	49,49,49,49	0
56	MG	CA	3074	1/1	0.20	-	54,54,54,54	0
56	MG	AA	3186	1/1	0.06	-	49,49,49,49	0
56	MG	DA	3055	1/1	0.24	-	48,48,48,48	0
56	MG	CA	3002	1/1	0.06	-	62,62,62,62	0
56	MG	CA	3151	1/1	0.24	-	80,80,80,80	0
56	MG	CA	3095	1/1	0.12	-	39,39,39,39	0
56	MG	BA	3044	1/1	0.29	-	42,42,42,42	0
56	MG	BA	3702	1/1	0.13	-	56,56,56,56	0
56	MG	DA	3593	1/1	0.25	-	73,73,73,73	0
56	MG	BA	3157	1/1	0.45	-	63,63,63,63	0
56	MG	AA	3107	1/1	0.26	-	44,44,44,44	0
56	MG	DA	3468	1/1	0.14	-	48,48,48,48	0
56	MG	DA	3039	1/1	0.35	-	59,59,59,59	0
56	MG	CA	3060	1/1	0.37	-	43,43,43,43	0
56	MG	DA	3367	1/1	0.24	-	42,42,42,42	0
56	MG	BA	3655	1/1	0.18	-	52,52,52,52	0
56	MG	BA	3600	1/1	0.18	-	47,47,47,47	0
56	MG	BA	3302	1/1	0.14	-	27,27,27,27	0
56	MG	BA	3375	1/1	0.22	-	31,31,31,31	0
56	MG	BA	3730	1/1	0.67	-	45,45,45,45	0
56	MG	BA	3307	1/1	0.23	-	33,33,33,33	0
56	MG	DF	305	1/1	0.78	-	39,39,39,39	0
56	MG	DY	502	1/1	0.09	-	60,60,60,60	0
56	MG	AA	3050	1/1	0.48	-	63,63,63,63	0
56	MG	DA	3252	1/1	0.12	-	45,45,45,45	0
56	MG	DA	3002	1/1	0.20	-	55,55,55,55	0
56	MG	DA	3643	1/1	0.68	-	53,53,53,53	0
56	MG	DA	3614	1/1	0.21	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3019	1/1	0.18	-	39,39,39,39	0
56	MG	DA	3331	1/1	0.10	-	34,34,34,34	0
56	MG	AA	3056	1/1	0.19	-	39,39,39,39	0
56	MG	DA	3177	1/1	0.07	-	33,33,33,33	0
56	MG	BA	3153	1/1	0.33	-	35,35,35,35	0
56	MG	CA	3086	1/1	0.22	-	80,80,80,80	0
56	MG	DA	3040	1/1	0.11	-	42,42,42,42	0
56	MG	BA	3608	1/1	0.16	-	68,68,68,68	0
56	MG	BA	3310	1/1	0.16	-	13,13,13,13	0
56	MG	BA	3692	1/1	0.37	-	36,36,36,36	0
56	MG	DA	3221	1/1	0.19	-	49,49,49,49	0
56	MG	BA	3410	1/1	0.13	-	27,27,27,27	0
56	MG	BA	3438	1/1	0.21	-	30,30,30,30	0
56	MG	CA	3062	1/1	0.23	-	57,57,57,57	0
56	MG	BA	3147	1/1	0.23	-	46,46,46,46	0
56	MG	DA	3601	1/1	0.12	-	77,77,77,77	0
56	MG	BB	3001	1/1	0.17	-	54,54,54,54	0
56	MG	BO	201	1/1	0.15	-	70,70,70,70	0
56	MG	DA	3068	1/1	0.30	-	55,55,55,55	0
56	MG	DA	3638	1/1	0.30	-	62,62,62,62	0
56	MG	DA	3018	1/1	0.51	-	48,48,48,48	0
56	MG	DA	3650	1/1	0.60	-	48,48,48,48	0
56	MG	BA	3721	1/1	0.08	-	25,25,25,25	0
56	MG	BA	3204	1/1	0.39	-	25,25,25,25	0
56	MG	DA	3119	1/1	0.15	-	44,44,44,44	0
56	MG	DF	306	1/1	0.28	-	50,50,50,50	0
56	MG	DA	3317	1/1	0.11	-	32,32,32,32	0
56	MG	DA	3472	1/1	0.15	-	36,36,36,36	0
56	MG	DA	3103	1/1	0.87	-	48,48,48,48	0
56	MG	BA	3699	1/1	0.54	-	56,56,56,56	0
56	MG	DA	3338	1/1	0.13	-	29,29,29,29	0
56	MG	BA	3622	1/1	0.53	-	77,77,77,77	0
56	MG	BA	3139	1/1	0.28	-	51,51,51,51	0
56	MG	DA	3312	1/1	0.28	-	43,43,43,43	0
56	MG	BA	3029	1/1	0.40	-	53,53,53,53	0
56	MG	DA	3080	1/1	0.12	-	44,44,44,44	0
56	MG	BE	307	1/1	0.26	-	39,39,39,39	0
56	MG	DA	3227	1/1	0.13	-	53,53,53,53	0
56	MG	BA	3163	1/1	0.18	-	50,50,50,50	0
56	MG	AA	3046	1/1	0.14	-	73,73,73,73	0
56	MG	AA	3148	1/1	0.20	-	66,66,66,66	0
56	MG	AA	3200	1/1	0.26	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3530	1/1	0.16	-	49,49,49,49	0
56	MG	DA	3054	1/1	0.11	-	51,51,51,51	0
56	MG	DA	3604	1/1	0.18	-	54,54,54,54	0
56	MG	BA	3519	1/1	0.15	-	39,39,39,39	0
56	MG	BA	3422	1/1	0.22	-	42,42,42,42	0
56	MG	AA	3143	1/1	0.10	-	45,45,45,45	0
56	MG	DA	3424	1/1	0.22	-	30,30,30,30	0
56	MG	BA	3607	1/1	0.47	-	53,53,53,53	0
56	MG	DA	3297	1/1	0.14	-	57,57,57,57	0
56	MG	AA	3054	1/1	0.24	-	45,45,45,45	0
56	MG	BA	3669	1/1	0.26	-	75,75,75,75	0
56	MG	DA	3265	1/1	0.25	-	51,51,51,51	0
56	MG	BA	3656	1/1	0.12	-	33,33,33,33	0
56	MG	DA	3596	1/1	0.08	-	67,67,67,67	0
56	MG	AA	3221	1/1	0.10	-	64,64,64,64	0
56	MG	BA	3535	1/1	0.18	-	37,37,37,37	0
56	MG	BA	3093	1/1	0.21	-	25,25,25,25	0
56	MG	BA	3394	1/1	0.13	-	49,49,49,49	0
56	MG	DA	3161	1/1	0.30	-	60,60,60,60	0
56	MG	BA	3529	1/1	0.21	-	35,35,35,35	0
56	MG	DA	3199	1/1	0.12	-	42,42,42,42	0
56	MG	AA	3164	1/1	0.38	-	69,69,69,69	0
56	MG	BQ	202	1/1	0.29	-	28,28,28,28	0
56	MG	BA	3445	1/1	0.21	-	25,25,25,25	0
56	MG	AA	3012	1/1	0.15	-	56,56,56,56	0
56	MG	BA	3374	1/1	0.21	-	44,44,44,44	0
56	MG	DA	3274	1/1	0.11	-	52,52,52,52	0
56	MG	DA	3132	1/1	0.75	-	54,54,54,54	0
56	MG	BA	3078	1/1	0.28	-	17,17,17,17	0
56	MG	BA	3185	1/1	0.21	-	47,47,47,47	0
56	MG	DA	3004	1/1	0.20	-	29,29,29,29	0
56	MG	DA	3173	1/1	0.43	-	39,39,39,39	0
56	MG	BA	3348	1/1	0.20	-	64,64,64,64	0
56	MG	CA	3026	1/1	0.08	-	52,52,52,52	0
56	MG	DA	3079	1/1	0.21	-	37,37,37,37	0
56	MG	BA	3578	1/1	0.31	-	54,54,54,54	0
56	MG	BA	3514	1/1	0.14	-	37,37,37,37	0
56	MG	AA	3055	1/1	0.20	-	50,50,50,50	0
56	MG	DA	3407	1/1	0.23	-	21,21,21,21	0
56	MG	BA	3573	1/1	0.14	-	56,56,56,56	0
56	MG	AA	3145	1/1	0.26	-	63,63,63,63	0
56	MG	BA	3161	1/1	0.69	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AN	101	1/1	0.20	-	63,63,63,63	0
56	MG	DA	3275	1/1	0.10	-	38,38,38,38	0
56	MG	BA	3361	1/1	0.25	-	34,34,34,34	0
56	MG	BE	308	1/1	0.17	-	52,52,52,52	0
56	MG	DA	3162	1/1	0.17	-	71,71,71,71	0
56	MG	DD	302	1/1	0.22	-	46,46,46,46	0
56	MG	CA	3111	1/1	0.12	-	64,64,64,64	0
56	MG	DA	3629	1/1	0.16	-	19,19,19,19	0
56	MG	CA	3034	1/1	0.23	-	65,65,65,65	0
56	MG	BF	303	1/1	0.21	-	36,36,36,36	0
56	MG	DA	3134	1/1	0.23	-	46,46,46,46	0
56	MG	CA	3164	1/1	0.39	-	49,49,49,49	0
56	MG	BA	3691	1/1	0.37	-	49,49,49,49	0
56	MG	AA	3083	1/1	0.08	-	65,65,65,65	0
56	MG	DA	3592	1/1	0.18	-	65,65,65,65	0
56	MG	AA	3049	1/1	0.50	-	51,51,51,51	0
58	ZN	CN	501	1/1	0.11	-	108,108,108,108	0
56	MG	BF	306	1/1	0.19	-	37,37,37,37	0
56	MG	DA	3030	1/1	0.33	-	51,51,51,51	0
56	MG	BA	3726	1/1	0.42	-	47,47,47,47	0
56	MG	AA	3100	1/1	0.69	-	40,40,40,40	0
56	MG	DA	3139	1/1	0.17	-	40,40,40,40	0
56	MG	BA	3114	1/1	0.34	-	51,51,51,51	0
56	MG	AA	3161	1/1	0.13	-	72,72,72,72	0
56	MG	BA	3565	1/1	0.10	-	55,55,55,55	0
56	MG	BP	204	1/1	0.19	-	55,55,55,55	0
56	MG	BA	3451	1/1	0.29	-	28,28,28,28	0
56	MG	AA	3201	1/1	0.12	-	67,67,67,67	0
56	MG	BA	3633	1/1	0.10	-	58,58,58,58	0
56	MG	DA	3225	1/1	0.15	-	45,45,45,45	0
56	MG	BA	3398	1/1	0.12	-	41,41,41,41	0
56	MG	AX	108	1/1	0.22	-	61,61,61,61	0
56	MG	BA	3457	1/1	0.10	-	57,57,57,57	0
56	MG	BA	3345	1/1	0.21	-	33,33,33,33	0
56	MG	BA	3509	1/1	0.16	-	27,27,27,27	0
56	MG	CA	3147	1/1	0.27	-	66,66,66,66	0
56	MG	BA	3362	1/1	0.09	-	43,43,43,43	0
56	MG	DA	3042	1/1	0.26	-	36,36,36,36	0
56	MG	BA	3435	1/1	0.21	-	24,24,24,24	0
56	MG	DA	3608	1/1	0.28	-	57,57,57,57	0
56	MG	BA	3433	1/1	0.22	-	39,39,39,39	0
56	MG	DA	3215	1/1	0.31	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3192	1/1	0.12	-	47,47,47,47	0
56	MG	BA	3144	1/1	0.28	-	74,74,74,74	0
56	MG	BA	3319	1/1	0.17	-	25,25,25,25	0
56	MG	BA	3105	1/1	0.45	-	34,34,34,34	0
56	MG	BA	3709	1/1	0.12	-	86,86,86,86	0
56	MG	DA	3558	1/1	0.19	-	37,37,37,37	0
56	MG	DA	3627	1/1	0.20	-	43,43,43,43	0
56	MG	DA	3374	1/1	0.05	-	37,37,37,37	0
56	MG	DB	3008	1/1	0.08	-	45,45,45,45	0
56	MG	DA	3589	1/1	0.18	-	59,59,59,59	0
56	MG	DA	3182	1/1	0.15	-	32,32,32,32	0
56	MG	BA	3366	1/1	0.09	-	63,63,63,63	0
56	MG	AA	3170	1/1	0.19	-	101,101,101,101	0
56	MG	CA	3113	1/1	0.26	-	77,77,77,77	0
56	MG	CA	3047	1/1	0.14	-	63,63,63,63	0
56	MG	DA	3230	1/1	0.14	-	62,62,62,62	0
56	MG	BF	301	1/1	0.59	-	45,45,45,45	0
56	MG	CA	3121	1/1	0.29	-	53,53,53,53	0
56	MG	DA	3242	1/1	0.23	-	35,35,35,35	0
56	MG	BQ	204	1/1	0.17	-	12,12,12,12	0
56	MG	DA	3321	1/1	0.23	-	41,41,41,41	0
56	MG	BA	3063	1/1	0.25	-	43,43,43,43	0
56	MG	BA	3718	1/1	0.38	-	57,57,57,57	0
56	MG	AA	3098	1/1	0.31	-	72,72,72,72	0
56	MG	DA	3244	1/1	0.30	-	29,29,29,29	0
56	MG	BA	3125	1/1	0.20	-	39,39,39,39	0
56	MG	BA	3584	1/1	0.18	-	22,22,22,22	0
56	MG	AA	3198	1/1	0.12	-	87,87,87,87	0
56	MG	DA	3484	1/1	0.25	-	51,51,51,51	0
56	MG	DA	3176	1/1	0.28	-	39,39,39,39	0
56	MG	BA	3338	1/1	0.20	-	50,50,50,50	0
56	MG	BF	308	1/1	0.25	-	28,28,28,28	0
56	MG	DA	3517	1/1	0.20	-	50,50,50,50	0
56	MG	AA	3091	1/1	0.13	-	75,75,75,75	0
56	MG	AA	3190	1/1	0.32	-	67,67,67,67	0
56	MG	BA	3486	1/1	0.06	-	38,38,38,38	0
56	MG	CA	3014	1/1	0.18	-	50,50,50,50	0
56	MG	DA	3419	1/1	0.17	-	31,31,31,31	0
56	MG	BA	3373	1/1	0.28	-	36,36,36,36	0
56	MG	DB	3012	1/1	0.29	-	59,59,59,59	0
56	MG	BA	3507	1/1	0.08	-	68,68,68,68	0
56	MG	AA	3155	1/1	0.15	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	3208	1/1	0.35	-	46,46,46,46	0
56	MG	AA	3206	1/1	0.07	-	70,70,70,70	0
56	MG	DA	3519	1/1	0.14	-	44,44,44,44	0
56	MG	BA	3710	1/1	0.20	-	48,48,48,48	0
56	MG	DD	305	1/1	0.66	-	49,49,49,49	0
56	MG	DA	3479	1/1	0.23	-	57,57,57,57	0
56	MG	CA	3107	1/1	0.12	-	60,60,60,60	0
56	MG	BA	3623	1/1	0.24	-	47,47,47,47	0
56	MG	CA	3027	1/1	0.16	-	57,57,57,57	0
56	MG	DA	3399	1/1	0.18	-	41,41,41,41	0
56	MG	DA	3283	1/1	0.16	-	33,33,33,33	0
56	MG	CA	3005	1/1	0.29	-	54,54,54,54	0
56	MG	BA	3552	1/1	0.23	-	29,29,29,29	0
56	MG	BA	3020	1/1	0.11	-	45,45,45,45	0
56	MG	BA	3545	1/1	0.24	-	47,47,47,47	0
56	MG	AA	3172	1/1	0.07	-	53,53,53,53	0
56	MG	DA	3267	1/1	0.16	-	61,61,61,61	0
56	MG	DA	3229	1/1	0.14	-	40,40,40,40	0
56	MG	BA	3152	1/1	0.34	-	46,46,46,46	0
56	MG	DA	3200	1/1	0.18	-	42,42,42,42	0
56	MG	DA	3616	1/1	0.21	-	62,62,62,62	0
56	MG	BA	3576	1/1	0.26	-	23,23,23,23	0
56	MG	DB	3009	1/1	0.36	-	40,40,40,40	0
56	MG	BA	3428	1/1	0.12	-	45,45,45,45	0
56	MG	DA	3072	1/1	0.14	-	41,41,41,41	0
56	MG	DA	3233	1/1	0.19	-	42,42,42,42	0
56	MG	DA	3086	1/1	0.29	-	43,43,43,43	0
56	MG	DA	3291	1/1	0.26	-	35,35,35,35	0
56	MG	BA	3303	1/1	0.17	-	35,35,35,35	0
56	MG	DQ	201	1/1	0.35	-	48,48,48,48	0
56	MG	BA	3442	1/1	0.15	-	12,12,12,12	0
56	MG	B1	3001	1/1	0.86	-	54,54,54,54	0
56	MG	CA	3154	1/1	0.16	-	49,49,49,49	0
56	MG	AA	3063	1/1	0.31	-	61,61,61,61	0
56	MG	DA	3090	1/1	0.29	-	47,47,47,47	0
56	MG	BA	3092	1/1	0.26	-	51,51,51,51	0
56	MG	CA	3072	1/1	0.23	-	38,38,38,38	0
56	MG	DA	3114	1/1	0.18	-	37,37,37,37	0
56	MG	DA	3387	1/1	0.13	-	56,56,56,56	0
56	MG	DA	3118	1/1	0.09	-	39,39,39,39	0
56	MG	CA	3141	1/1	0.25	-	70,70,70,70	0
56	MG	BA	3230	1/1	0.50	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3536	1/1	0.13	-	27,27,27,27	0
56	MG	BA	3143	1/1	0.32	-	40,40,40,40	0
56	MG	DA	3370	1/1	0.17	-	38,38,38,38	0
56	MG	BU	207	1/1	0.19	-	40,40,40,40	0
56	MG	DA	3133	1/1	0.16	-	33,33,33,33	0
56	MG	BD	303	1/1	0.24	-	42,42,42,42	0
56	MG	DA	3460	1/1	0.35	-	50,50,50,50	0
56	MG	DA	3600	1/1	0.07	-	45,45,45,45	0
56	MG	BA	3122	1/1	0.25	-	52,52,52,52	0
56	MG	DA	3102	1/1	0.26	-	41,41,41,41	0
56	MG	AA	3030	1/1	0.30	-	69,69,69,69	0
56	MG	AA	3078	1/1	0.28	-	42,42,42,42	0
56	MG	BA	3494	1/1	0.32	-	18,18,18,18	0
56	MG	BA	3324	1/1	0.17	-	36,36,36,36	0
56	MG	BA	3668	1/1	0.13	-	38,38,38,38	0
56	MG	BA	3030	1/1	0.42	-	51,51,51,51	0
56	MG	BA	3222	1/1	0.30	-	25,25,25,25	0
56	MG	DA	3611	1/1	0.08	-	42,42,42,42	0
56	MG	CA	3132	1/1	0.11	-	70,70,70,70	0
56	MG	BA	3577	1/1	0.10	-	52,52,52,52	0
56	MG	BA	3048	1/1	0.23	-	31,31,31,31	0
56	MG	BD	310	1/1	0.31	-	48,48,48,48	0
56	MG	DA	3535	1/1	0.19	-	33,33,33,33	0
56	MG	BA	3173	1/1	0.61	-	37,37,37,37	0
56	MG	BA	3452	1/1	0.25	-	47,47,47,47	0
56	MG	DA	3398	1/1	0.15	-	35,35,35,35	0
56	MG	BA	3192	1/1	0.53	-	58,58,58,58	0
56	MG	DA	3310	1/1	0.20	-	53,53,53,53	0
56	MG	DA	3015	1/1	0.23	-	49,49,49,49	0
56	MG	DA	3409	1/1	0.13	-	32,32,32,32	0
56	MG	DE	301	1/1	0.61	-	51,51,51,51	0
56	MG	DA	3058	1/1	0.43	-	47,47,47,47	0
56	MG	DA	3463	1/1	0.34	-	43,43,43,43	0
56	MG	DA	3051	1/1	0.12	-	46,46,46,46	0
56	MG	CA	3100	1/1	0.13	-	60,60,60,60	0
56	MG	BA	3187	1/1	0.66	-	50,50,50,50	0
56	MG	BA	3296	1/1	0.23	-	46,46,46,46	0
56	MG	DA	3362	1/1	0.12	-	41,41,41,41	0
56	MG	BA	3520	1/1	0.15	-	34,34,34,34	0
56	MG	DA	3120	1/1	0.78	-	51,51,51,51	0
56	MG	CA	3089	1/1	0.17	-	52,52,52,52	0
56	MG	AA	3192	1/1	0.09	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3244	1/1	0.47	-	65,65,65,65	0
56	MG	AA	3035	1/1	0.40	-	71,71,71,71	0
56	MG	B7	101	1/1	0.18	-	43,43,43,43	0
56	MG	BA	3357	1/1	0.15	-	49,49,49,49	0
56	MG	BA	3277	1/1	0.35	-	45,45,45,45	0
56	MG	BA	3551	1/1	0.21	-	25,25,25,25	0
56	MG	BA	3197	1/1	0.27	-	39,39,39,39	0
56	MG	BA	3372	1/1	0.17	-	38,38,38,38	0
56	MG	DA	3578	1/1	0.40	-	49,49,49,49	0
56	MG	AA	3108	1/1	0.34	-	67,67,67,67	0
56	MG	CX	102	1/1	0.06	-	61,61,61,61	0
56	MG	BA	3054	1/1	0.25	-	46,46,46,46	0
56	MG	DA	3635	1/1	0.31	-	58,58,58,58	0
56	MG	BA	3195	1/1	0.32	-	47,47,47,47	0
56	MG	AA	3084	1/1	0.33	-	78,78,78,78	0
56	MG	BU	202	1/1	0.35	-	32,32,32,32	0
56	MG	BA	3571	1/1	0.08	-	65,65,65,65	0
56	MG	DA	3576	1/1	0.14	-	38,38,38,38	0
56	MG	AA	3093	1/1	0.60	-	88,88,88,88	0
56	MG	DA	3525	1/1	0.58	-	70,70,70,70	0
56	MG	BA	3436	1/1	0.09	-	37,37,37,37	0
56	MG	BA	3145	1/1	0.37	-	38,38,38,38	0
56	MG	BA	3735	1/1	0.20	-	45,45,45,45	0
56	MG	DA	3573	1/1	0.28	-	40,40,40,40	0
56	MG	DB	3010	1/1	0.20	-	73,73,73,73	0
56	MG	DA	3432	1/1	0.24	-	66,66,66,66	0
56	MG	DA	3091	1/1	0.39	-	44,44,44,44	0
56	MG	CA	3149	1/1	0.17	-	74,74,74,74	0
56	MG	DA	3357	1/1	0.22	-	56,56,56,56	0
56	MG	BA	3599	1/1	0.29	-	46,46,46,46	0
56	MG	BA	3298	1/1	0.36	-	49,49,49,49	0
56	MG	BA	3671	1/1	0.27	-	57,57,57,57	0
56	MG	DA	3238	1/1	0.10	-	61,61,61,61	0
56	MG	BA	3648	1/1	0.30	-	49,49,49,49	0
56	MG	DA	3380	1/1	0.15	-	26,26,26,26	0
56	MG	DA	3547	1/1	0.09	-	41,41,41,41	0
56	MG	AA	3073	1/1	0.06	-	46,46,46,46	0
56	MG	DA	3197	1/1	0.43	-	36,36,36,36	0
56	MG	DA	3457	1/1	0.12	-	37,37,37,37	0
56	MG	AA	3013	1/1	0.24	-	78,78,78,78	0
56	MG	BA	3215	1/1	0.18	-	69,69,69,69	0
56	MG	BA	3331	1/1	0.18	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BR	204	1/1	0.64	-	43,43,43,43	0
56	MG	BA	3238	1/1	0.16	-	51,51,51,51	0
56	MG	BA	3180	1/1	0.87	-	43,43,43,43	0
56	MG	CA	3081	1/1	0.10	-	72,72,72,72	0
56	MG	BA	3557	1/1	0.26	-	31,31,31,31	0
56	MG	AA	3048	1/1	0.20	-	57,57,57,57	0
56	MG	BA	3311	1/1	0.27	-	42,42,42,42	0
56	MG	DA	3062	1/1	0.32	-	55,55,55,55	0
56	MG	BA	3049	1/1	0.36	-	35,35,35,35	0
56	MG	DA	3056	1/1	0.38	-	43,43,43,43	0
56	MG	BA	3290	1/1	0.25	-	49,49,49,49	0
56	MG	DA	3316	1/1	0.16	-	58,58,58,58	0
56	MG	DA	3165	1/1	0.23	-	44,44,44,44	0
56	MG	AA	3020	1/1	0.12	-	77,77,77,77	0
56	MG	BA	3183	1/1	0.24	-	48,48,48,48	0
56	MG	BA	3342	1/1	0.16	-	31,31,31,31	0
56	MG	AA	3027	1/1	0.06	-	55,55,55,55	0
56	MG	CA	3012	1/1	0.10	-	49,49,49,49	0
56	MG	BA	3067	1/1	0.34	-	53,53,53,53	0
56	MG	DG	3001	1/1	0.14	-	63,63,63,63	0
56	MG	DA	3260	1/1	0.10	-	40,40,40,40	0
56	MG	BA	3465	1/1	0.13	-	40,40,40,40	0
56	MG	BA	3548	1/1	0.21	-	50,50,50,50	0
56	MG	BA	3262	1/1	0.23	-	56,56,56,56	0
56	MG	CA	3161	1/1	0.13	-	54,54,54,54	0
56	MG	DA	3538	1/1	0.17	-	44,44,44,44	0
56	MG	BA	3684	1/1	0.16	-	58,58,58,58	0
56	MG	CA	3049	1/1	0.25	-	53,53,53,53	0
56	MG	DA	3415	1/1	0.21	-	56,56,56,56	0
56	MG	DA	3644	1/1	0.07	-	42,42,42,42	0
56	MG	DA	3016	1/1	0.26	-	37,37,37,37	0
56	MG	DA	3211	1/1	0.09	-	51,51,51,51	0
56	MG	CA	3160	1/1	0.14	-	59,59,59,59	0
56	MG	AA	3047	1/1	0.29	-	61,61,61,61	0
56	MG	BA	3003	1/1	0.15	-	43,43,43,43	0
56	MG	BA	3385	1/1	0.22	-	26,26,26,26	0
56	MG	BA	3198	1/1	0.16	-	52,52,52,52	0
56	MG	BA	3405	1/1	0.13	-	34,34,34,34	0
56	MG	DA	3587	1/1	0.14	-	64,64,64,64	0
56	MG	B8	103	1/1	0.17	-	24,24,24,24	0
56	MG	BA	3363	1/1	0.13	-	39,39,39,39	0
56	MG	BA	3388	1/1	0.15	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3527	1/1	0.17	-	64,64,64,64	0
56	MG	DA	3526	1/1	0.20	-	54,54,54,54	0
56	MG	DA	3064	1/1	0.40	-	50,50,50,50	0
56	MG	DA	3617	1/1	0.18	-	58,58,58,58	0
56	MG	AA	3077	1/1	0.44	-	65,65,65,65	0
56	MG	BA	3524	1/1	0.25	-	55,55,55,55	0
56	MG	BA	3408	1/1	0.15	-	24,24,24,24	0
56	MG	DA	3208	1/1	0.99	-	43,43,43,43	0
56	MG	DA	3301	1/1	0.14	-	45,45,45,45	0
56	MG	AA	3163	1/1	0.17	-	28,28,28,28	0
56	MG	AA	3210	1/1	0.05	-	40,40,40,40	0
56	MG	BA	3615	1/1	0.20	-	36,36,36,36	0
56	MG	DA	3140	1/1	0.34	-	54,54,54,54	0
56	MG	BA	3698	1/1	0.21	-	41,41,41,41	0
56	MG	BA	3651	1/1	0.14	-	45,45,45,45	0
56	MG	DA	3101	1/1	0.37	-	48,48,48,48	0
56	MG	AA	3004	1/1	0.11	-	55,55,55,55	0
56	MG	AA	3144	1/1	0.08	-	48,48,48,48	0
56	MG	CA	3163	1/1	0.23	-	65,65,65,65	0
56	MG	DA	3568	1/1	0.09	-	42,42,42,42	0
56	MG	AA	3139	1/1	0.33	-	56,56,56,56	0
56	MG	CA	3048	1/1	0.20	-	62,62,62,62	0
56	MG	BA	3172	1/1	0.92	-	48,48,48,48	0
56	MG	BA	3555	1/1	0.18	-	53,53,53,53	0
56	MG	BA	3411	1/1	0.14	-	38,38,38,38	0
56	MG	CA	3051	1/1	0.10	-	63,63,63,63	0
56	MG	BA	3390	1/1	0.20	-	30,30,30,30	0
56	MG	BA	3635	1/1	0.09	-	78,78,78,78	0
56	MG	CA	3153	1/1	0.12	-	83,83,83,83	0
56	MG	DA	3356	1/1	0.12	-	27,27,27,27	0
56	MG	DA	3350	1/1	0.04	-	32,32,32,32	0
56	MG	DA	3404	1/1	0.13	-	47,47,47,47	0
56	MG	DA	3185	1/1	0.61	-	52,52,52,52	0
56	MG	BA	3347	1/1	0.27	-	25,25,25,25	0
56	MG	DA	3203	1/1	0.14	-	41,41,41,41	0
56	MG	DA	3014	1/1	0.20	-	34,34,34,34	0
56	MG	BA	3463	1/1	0.18	-	55,55,55,55	0
56	MG	BA	3341	1/1	0.09	-	33,33,33,33	0
56	MG	DQ	202	1/1	0.23	-	34,34,34,34	0
56	MG	DA	3137	1/1	0.26	-	56,56,56,56	0
56	MG	BA	3196	1/1	0.76	-	56,56,56,56	0
56	MG	DA	3354	1/1	0.15	-	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3296	1/1	0.09	-	31,31,31,31	0
56	MG	AA	3214	1/1	0.29	-	75,75,75,75	0
56	MG	BA	3546	1/1	0.29	-	48,48,48,48	0
56	MG	BA	3621	1/1	0.33	-	74,74,74,74	0
56	MG	AA	3068	1/1	0.08	-	66,66,66,66	0
56	MG	BB	3013	1/1	0.11	-	39,39,39,39	0
56	MG	BA	3662	1/1	0.14	-	39,39,39,39	0
56	MG	BA	3613	1/1	0.28	-	76,76,76,76	0
56	MG	DV	201	1/1	0.32	-	55,55,55,55	0
56	MG	CA	3075	1/1	0.20	-	76,76,76,76	0
56	MG	DA	3605	1/1	0.13	-	44,44,44,44	0
56	MG	BA	3034	1/1	0.41	-	52,52,52,52	0
56	MG	BA	3232	1/1	0.11	-	29,29,29,29	0
56	MG	BA	3460	1/1	0.13	-	33,33,33,33	0
56	MG	CA	3170	1/1	0.45	-	50,50,50,50	0
56	MG	BA	3647	1/1	0.11	-	34,34,34,34	0
56	MG	AA	3041	1/1	0.17	-	49,49,49,49	0
56	MG	BA	3522	1/1	0.13	-	49,49,49,49	0
56	MG	DA	3477	1/1	0.10	-	49,49,49,49	0
56	MG	AA	3199	1/1	0.13	-	88,88,88,88	0
56	MG	DA	3033	1/1	0.26	-	39,39,39,39	0
56	MG	AA	3101	1/1	0.16	-	56,56,56,56	0
56	MG	AA	3115	1/1	0.10	-	48,48,48,48	0
56	MG	BA	3304	1/1	0.19	-	49,49,49,49	0
56	MG	BA	3134	1/1	0.34	-	47,47,47,47	0
56	MG	CA	3066	1/1	0.11	-	55,55,55,55	0
56	MG	DA	3210	1/1	0.16	-	40,40,40,40	0
56	MG	AA	3122	1/1	0.54	-	44,44,44,44	0
56	MG	BA	3654	1/1	0.17	-	25,25,25,25	0
56	MG	DA	3391	1/1	0.14	-	41,41,41,41	0
56	MG	BA	3305	1/1	0.13	-	44,44,44,44	0
56	MG	CA	3013	1/1	0.11	-	51,51,51,51	0
56	MG	BA	3015	1/1	0.34	-	44,44,44,44	0
56	MG	AA	3042	1/1	0.33	-	44,44,44,44	0
56	MG	DA	3537	1/1	0.20	-	65,65,65,65	0
56	MG	BA	3371	1/1	0.17	-	15,15,15,15	0
56	MG	BA	3432	1/1	0.17	-	60,60,60,60	0
56	MG	DA	3063	1/1	0.13	-	52,52,52,52	0
56	MG	DA	3469	1/1	0.17	-	47,47,47,47	0
56	MG	CA	3003	1/1	0.14	-	66,66,66,66	0
56	MG	CA	3109	1/1	0.14	-	83,83,83,83	0
56	MG	DA	3022	1/1	0.22	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3116	1/1	0.30	-	39,39,39,39	0
56	MG	DA	3047	1/1	0.08	-	34,34,34,34	0
56	MG	BA	3216	1/1	0.26	-	41,41,41,41	0
56	MG	BA	3002	1/1	0.20	-	54,54,54,54	0
56	MG	BA	3694	1/1	0.36	-	56,56,56,56	0
56	MG	DA	3057	1/1	0.19	-	52,52,52,52	0
56	MG	AA	3135	1/1	0.20	-	41,41,41,41	0
56	MG	BA	3295	1/1	0.54	-	75,75,75,75	0
56	MG	BA	3559	1/1	0.14	-	48,48,48,48	0
56	MG	BQ	205	1/1	0.42	-	49,49,49,49	0
56	MG	BA	3160	1/1	0.66	-	53,53,53,53	0
56	MG	DA	3249	1/1	0.21	-	28,28,28,28	0
56	MG	CA	3166	1/1	0.17	-	59,59,59,59	0
56	MG	DA	3575	1/1	0.19	-	43,43,43,43	0
56	MG	BA	3335	1/1	0.18	-	35,35,35,35	0
56	MG	DA	3206	1/1	0.28	-	42,42,42,42	0
56	MG	BA	3508	1/1	0.16	-	34,34,34,34	0
56	MG	BA	3306	1/1	0.14	-	48,48,48,48	0
56	MG	BB	3009	1/1	0.14	-	48,48,48,48	0
56	MG	DA	3359	1/1	0.22	-	46,46,46,46	0
56	MG	BD	306	1/1	0.53	-	46,46,46,46	0
56	MG	AA	3118	1/1	0.35	-	52,52,52,52	0
56	MG	DA	3383	1/1	0.08	-	56,56,56,56	0
56	MG	DA	3438	1/1	0.52	-	70,70,70,70	0
56	MG	BA	3355	1/1	0.19	-	64,64,64,64	0
56	MG	DA	3008	1/1	0.28	-	51,51,51,51	0
56	MG	BA	3427	1/1	0.10	-	48,48,48,48	0
56	MG	DA	3295	1/1	0.23	-	39,39,39,39	0
56	MG	DA	3514	1/1	0.11	-	39,39,39,39	0
56	MG	DA	3294	1/1	0.08	-	47,47,47,47	0
56	MG	AA	3106	1/1	0.26	-	56,56,56,56	0
56	MG	AA	3075	1/1	0.11	-	52,52,52,52	0
56	MG	BA	3156	1/1	0.35	-	56,56,56,56	0
56	MG	DA	3544	1/1	0.11	-	51,51,51,51	0
56	MG	BV	202	1/1	0.48	-	56,56,56,56	0
56	MG	CA	3078	1/1	0.31	-	46,46,46,46	0
56	MG	DA	3245	1/1	0.14	-	37,37,37,37	0
56	MG	DA	3406	1/1	0.09	-	40,40,40,40	0
56	MG	BA	3630	1/1	0.26	-	52,52,52,52	0
56	MG	BA	3064	1/1	0.22	-	39,39,39,39	0
56	MG	DA	3349	1/1	0.14	-	54,54,54,54	0
56	MG	BA	3563	1/1	0.22	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3136	1/1	0.12	-	49,49,49,49	0
56	MG	CA	3007	1/1	0.58	-	68,68,68,68	0
56	MG	DA	3270	1/1	0.22	-	36,36,36,36	0
56	MG	DA	3532	1/1	0.09	-	57,57,57,57	0
56	MG	AA	3194	1/1	0.16	-	54,54,54,54	0
56	MG	CA	3142	1/1	0.19	-	59,59,59,59	0
58	ZN	D4	501	1/1	0.08	-	153,153,153,153	0
56	MG	DA	3466	1/1	0.14	-	56,56,56,56	0
56	MG	DA	3400	1/1	0.19	-	42,42,42,42	0
56	MG	BA	3512	1/1	0.21	-	40,40,40,40	0
56	MG	AN	103	1/1	0.41	-	60,60,60,60	0
56	MG	BA	3448	1/1	0.10	-	29,29,29,29	0
56	MG	BA	3110	1/1	0.31	-	55,55,55,55	0
56	MG	AA	3165	1/1	0.16	-	23,23,23,23	0
56	MG	AA	3220	1/1	0.12	-	40,40,40,40	0
58	ZN	D5	103	1/1	0.06	-	70,70,70,70	0
56	MG	BA	3729	1/1	0.46	-	46,46,46,46	0
56	MG	DA	3207	1/1	0.12	-	58,58,58,58	0
56	MG	DF	302	1/1	0.25	-	43,43,43,43	0
56	MG	BA	3091	1/1	0.59	-	45,45,45,45	0
56	MG	BA	3628	1/1	0.18	-	41,41,41,41	0
56	MG	BA	3537	1/1	0.36	-	31,31,31,31	0
56	MG	BA	3420	1/1	0.30	-	33,33,33,33	0
56	MG	BA	3217	1/1	0.08	-	28,28,28,28	0
56	MG	DA	3141	1/1	0.14	-	62,62,62,62	0
56	MG	DA	3451	1/1	0.08	-	49,49,49,49	0
56	MG	BA	3211	1/1	0.30	-	38,38,38,38	0
56	MG	BA	3045	1/1	0.30	-	34,34,34,34	0
56	MG	CA	3020	1/1	0.18	-	47,47,47,47	0
56	MG	BA	3325	1/1	0.17	-	58,58,58,58	0
56	MG	BB	3010	1/1	0.25	-	40,40,40,40	0
56	MG	DA	3098	1/1	1.35	-	43,43,43,43	0
56	MG	DA	3223	1/1	0.24	-	66,66,66,66	0
56	MG	DA	3364	1/1	0.20	-	32,32,32,32	0
56	MG	BA	3076	1/1	0.21	-	41,41,41,41	0
56	MG	AA	3011	1/1	1.09	-	55,55,55,55	0
56	MG	DE	306	1/1	0.14	-	32,32,32,32	0
56	MG	BA	3352	1/1	0.11	-	34,34,34,34	0
56	MG	DA	3109	1/1	0.53	-	66,66,66,66	0
56	MG	BA	3332	1/1	0.19	-	39,39,39,39	0
56	MG	DA	3041	1/1	0.47	-	57,57,57,57	0
56	MG	DF	304	1/1	0.28	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3359	1/1	0.20	-	23,23,23,23	0
56	MG	DA	3006	1/1	0.15	-	42,42,42,42	0
56	MG	BA	3506	1/1	0.14	-	30,30,30,30	0
56	MG	BA	3141	1/1	0.28	-	43,43,43,43	0
56	MG	DA	3298	1/1	0.32	-	37,37,37,37	0
56	MG	DA	3049	1/1	0.32	-	58,58,58,58	0
56	MG	BA	3631	1/1	0.12	-	78,78,78,78	0
56	MG	DA	3443	1/1	0.15	-	53,53,53,53	0
56	MG	BA	3349	1/1	0.25	-	43,43,43,43	0
56	MG	BA	3609	1/1	0.12	-	46,46,46,46	0
56	MG	BA	3728	1/1	0.48	-	32,32,32,32	0
56	MG	DA	3377	1/1	0.28	-	59,59,59,59	0
56	MG	DA	3201	1/1	0.13	-	48,48,48,48	0
56	MG	DA	3024	1/1	0.48	-	65,65,65,65	0
56	MG	DA	3393	1/1	0.20	-	41,41,41,41	0
56	MG	BA	3344	1/1	0.10	-	30,30,30,30	0
56	MG	BA	3419	1/1	0.13	-	24,24,24,24	0
56	MG	DA	3218	1/1	0.18	-	62,62,62,62	0
56	MG	AA	3146	1/1	0.22	-	48,48,48,48	0
56	MG	BB	3003	1/1	0.24	-	43,43,43,43	0
56	MG	BA	3203	1/1	0.27	-	32,32,32,32	0
56	MG	BB	3017	1/1	0.20	-	64,64,64,64	0
56	MG	DA	3340	1/1	0.14	-	47,47,47,47	0
56	MG	DA	3358	1/1	0.17	-	46,46,46,46	0
56	MG	BA	3235	1/1	0.29	-	47,47,47,47	0
56	MG	BA	3328	1/1	0.24	-	42,42,42,42	0
56	MG	BA	3616	1/1	0.12	-	33,33,33,33	0
56	MG	BA	3526	1/1	0.18	-	19,19,19,19	0
56	MG	BA	3560	1/1	0.20	-	61,61,61,61	0
56	MG	DA	3271	1/1	0.20	-	37,37,37,37	0
56	MG	CA	3025	1/1	0.20	-	94,94,94,94	0
56	MG	DA	3143	1/1	0.22	-	46,46,46,46	0
58	ZN	D6	501	1/1	0.12	-	61,61,61,61	0
58	ZN	B6	501	1/1	0.13	-	49,49,49,49	0
56	MG	DA	3586	1/1	0.09	-	29,29,29,29	0
56	MG	D8	5001	1/1	0.32	-	47,47,47,47	0
56	MG	BA	3500	1/1	0.17	-	37,37,37,37	0
56	MG	DA	3626	1/1	0.07	-	68,68,68,68	0
56	MG	DA	3598	1/1	0.30	-	66,66,66,66	0
56	MG	BA	3270	1/1	0.31	-	50,50,50,50	0
56	MG	DA	3584	1/1	0.11	-	61,61,61,61	0
56	MG	BD	304	1/1	0.50	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3322	1/1	0.25	-	22,22,22,22	0
56	MG	BA	3499	1/1	0.17	-	55,55,55,55	0
56	MG	BA	3009	1/1	0.17	-	25,25,25,25	0
56	MG	DE	302	1/1	0.36	-	44,44,44,44	0
56	MG	AA	3124	1/1	0.10	-	57,57,57,57	0
56	MG	BA	3568	1/1	0.22	-	47,47,47,47	0
56	MG	AA	3090	1/1	0.17	-	68,68,68,68	0
56	MG	DA	3378	1/1	0.14	-	45,45,45,45	0
56	MG	CA	3050	1/1	0.13	-	43,43,43,43	0
56	MG	BD	301	1/1	0.25	-	28,28,28,28	0
56	MG	DA	3458	1/1	0.15	-	71,71,71,71	0
56	MG	BA	3358	1/1	0.07	-	33,33,33,33	0
56	MG	AA	3176	1/1	0.12	-	63,63,63,63	0
56	MG	DA	3220	1/1	0.11	-	37,37,37,37	0
56	MG	DA	3094	1/1	0.18	-	26,26,26,26	0
56	MG	DA	3123	1/1	0.23	-	59,59,59,59	0
56	MG	DA	3152	1/1	0.23	-	50,50,50,50	0
56	MG	BB	3011	1/1	0.18	-	37,37,37,37	0
56	MG	BA	3393	1/1	0.19	-	38,38,38,38	0
56	MG	DA	3551	1/1	0.10	-	52,52,52,52	0
56	MG	BA	3150	1/1	0.48	-	34,34,34,34	0
56	MG	AA	3154	1/1	0.07	-	63,63,63,63	0
56	MG	BA	3610	1/1	0.22	-	40,40,40,40	0
56	MG	DA	3255	1/1	0.19	-	40,40,40,40	0
56	MG	AA	3180	1/1	0.37	-	66,66,66,66	0
56	MG	BA	3212	1/1	0.30	-	43,43,43,43	0
56	MG	DA	3093	1/1	0.20	-	53,53,53,53	0
56	MG	DA	3235	1/1	0.20	-	50,50,50,50	0
56	MG	DA	3613	1/1	0.15	-	54,54,54,54	0
56	MG	DA	3412	1/1	0.29	-	30,30,30,30	0
56	MG	BA	3732	1/1	0.47	-	61,61,61,61	0
56	MG	DA	3498	1/1	0.14	-	56,56,56,56	0
56	MG	BA	3483	1/1	0.25	-	53,53,53,53	0
56	MG	BA	3337	1/1	0.17	-	23,23,23,23	0
56	MG	BP	202	1/1	0.12	-	40,40,40,40	0
56	MG	DA	3490	1/1	0.10	-	39,39,39,39	0
56	MG	BA	3575	1/1	0.19	-	51,51,51,51	0
56	MG	DA	3287	1/1	0.26	-	53,53,53,53	0
56	MG	AA	3010	1/1	0.38	-	70,70,70,70	0
56	MG	AA	3196	1/1	0.32	-	65,65,65,65	0
56	MG	BA	3010	1/1	0.18	-	32,32,32,32	0
56	MG	BA	3096	1/1	0.38	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3071	1/1	0.30	-	55,55,55,55	0
56	MG	CA	3098	1/1	0.25	-	46,46,46,46	0
56	MG	DA	3382	1/1	0.13	-	25,25,25,25	0
56	MG	DA	3131	1/1	0.20	-	54,54,54,54	0
56	MG	DA	3179	1/1	0.23	-	46,46,46,46	0
56	MG	BA	3510	1/1	0.23	-	40,40,40,40	0
56	MG	DA	3372	1/1	0.11	-	45,45,45,45	0
56	MG	DA	3343	1/1	0.19	-	41,41,41,41	0
56	MG	BA	3088	1/1	0.34	-	56,56,56,56	0
56	MG	BA	3658	1/1	0.27	-	79,79,79,79	0
56	MG	BA	3498	1/1	0.14	-	39,39,39,39	0
56	MG	BA	3734	1/1	0.24	-	45,45,45,45	0
56	MG	BA	3205	1/1	0.18	-	40,40,40,40	0
56	MG	AA	3211	1/1	0.22	-	36,36,36,36	0
56	MG	DA	3572	1/1	0.09	-	53,53,53,53	0
56	MG	BA	3072	1/1	0.30	-	45,45,45,45	0
56	MG	DA	3146	1/1	0.16	-	34,34,34,34	0
56	MG	DA	3060	1/1	0.28	-	55,55,55,55	0
56	MG	BA	3705	1/1	0.05	-	39,39,39,39	0
56	MG	BA	3505	1/1	0.19	-	59,59,59,59	0
56	MG	DA	3394	1/1	0.17	-	47,47,47,47	0
56	MG	BA	3492	1/1	0.27	-	23,23,23,23	0
56	MG	DA	3084	1/1	0.28	-	70,70,70,70	0
56	MG	BA	3225	1/1	0.33	-	62,62,62,62	0
56	MG	BA	3553	1/1	0.12	-	31,31,31,31	0
56	MG	BA	3739	1/1	0.80	-	50,50,50,50	0
56	MG	BA	3214	1/1	0.09	-	53,53,53,53	0
56	MG	DA	3414	1/1	0.20	-	49,49,49,49	0
56	MG	CA	3104	1/1	0.20	-	62,62,62,62	0
56	MG	BA	3580	1/1	0.10	-	58,58,58,58	0
56	MG	AA	3219	1/1	0.18	-	57,57,57,57	0
56	MG	BA	3329	1/1	0.13	-	29,29,29,29	0
56	MG	DA	3649	1/1	0.23	-	24,24,24,24	0
56	MG	DA	3336	1/1	0.12	-	27,27,27,27	0
56	MG	B0	101	1/1	0.18	-	36,36,36,36	0
56	MG	BA	3619	1/1	0.28	-	40,40,40,40	0
56	MG	DA	3205	1/1	0.09	-	38,38,38,38	0
56	MG	DA	3261	1/1	0.22	-	35,35,35,35	0
56	MG	BA	3395	1/1	0.20	-	25,25,25,25	0
56	MG	AA	3134	1/1	0.35	-	70,70,70,70	0
56	MG	DA	3365	1/1	0.05	-	40,40,40,40	0
56	MG	CA	3071	1/1	0.09	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3042	1/1	0.62	-	47,47,47,47	0
56	MG	DA	3250	1/1	0.13	-	31,31,31,31	0
56	MG	DB	3003	1/1	0.13	-	63,63,63,63	0
56	MG	BA	3708	1/1	0.22	-	40,40,40,40	0
56	MG	DA	3125	1/1	0.50	-	48,48,48,48	0
56	MG	BA	3350	1/1	0.24	-	47,47,47,47	0
56	MG	DA	3284	1/1	0.12	-	68,68,68,68	0
56	MG	DA	3473	1/1	0.29	-	32,32,32,32	0
56	MG	DA	3486	1/1	0.12	-	38,38,38,38	0
56	MG	BA	3579	1/1	0.23	-	63,63,63,63	0
56	MG	BA	3240	1/1	0.18	-	28,28,28,28	0
56	MG	DA	3521	1/1	0.12	-	62,62,62,62	0
56	MG	AX	104	1/1	0.14	-	76,76,76,76	0
56	MG	CA	3021	1/1	0.22	-	53,53,53,53	0
56	MG	DA	3607	1/1	0.10	-	45,45,45,45	0
56	MG	BA	3074	1/1	0.08	-	42,42,42,42	0
56	MG	AA	3121	1/1	0.56	-	51,51,51,51	0
56	MG	DA	3385	1/1	0.15	-	35,35,35,35	0
56	MG	CA	3101	1/1	0.15	-	70,70,70,70	0
56	MG	DA	3228	1/1	0.27	-	45,45,45,45	0
56	MG	BA	3676	1/1	0.21	-	51,51,51,51	0
56	MG	BA	3673	1/1	0.19	-	53,53,53,53	0
56	MG	DA	3497	1/1	0.22	-	60,60,60,60	0
56	MG	BA	3227	1/1	0.32	-	32,32,32,32	0
56	MG	BA	3653	1/1	0.13	-	69,69,69,69	0
56	MG	DA	3543	1/1	0.16	-	42,42,42,42	0
56	MG	BA	3562	1/1	0.10	-	73,73,73,73	0
56	MG	DA	3390	1/1	0.11	-	42,42,42,42	0
56	MG	DA	3071	1/1	0.48	-	46,46,46,46	0
56	MG	DA	3430	1/1	0.26	-	55,55,55,55	0
56	MG	BA	3406	1/1	0.15	-	28,28,28,28	0
56	MG	DA	3345	1/1	0.09	-	31,31,31,31	0
56	MG	CA	3085	1/1	0.30	-	43,43,43,43	0
56	MG	BA	3137	1/1	0.29	-	42,42,42,42	0
56	MG	BA	3286	1/1	0.22	-	32,32,32,32	0
56	MG	BA	3340	1/1	0.14	-	57,57,57,57	0
56	MG	BA	3220	1/1	0.13	-	57,57,57,57	0
56	MG	BA	3129	1/1	0.23	-	36,36,36,36	0
56	MG	BF	307	1/1	0.44	-	47,47,47,47	0
56	MG	BA	3218	1/1	0.22	-	62,62,62,62	0
56	MG	DA	3554	1/1	0.18	-	70,70,70,70	0
56	MG	BA	3323	1/1	0.14	-	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3637	1/1	0.27	-	48,48,48,48	0
56	MG	DA	3332	1/1	0.12	-	33,33,33,33	0
56	MG	AA	3040	1/1	0.12	-	55,55,55,55	0
56	MG	DA	3478	1/1	0.25	-	46,46,46,46	0
56	MG	BA	3585	1/1	0.17	-	51,51,51,51	0
56	MG	BA	3229	1/1	0.14	-	22,22,22,22	0
56	MG	DA	3303	1/1	0.18	-	47,47,47,47	0
56	MG	DA	3641	1/1	0.36	-	61,61,61,61	0
56	MG	DA	3318	1/1	0.10	-	45,45,45,45	0
56	MG	AA	3189	1/1	0.09	-	77,77,77,77	0
56	MG	CA	3069	1/1	0.10	-	69,69,69,69	0
56	MG	BD	309	1/1	0.14	-	42,42,42,42	0
56	MG	DA	3167	1/1	0.24	-	48,48,48,48	0
56	MG	DA	3166	1/1	0.11	-	32,32,32,32	0
56	MG	BA	3703	1/1	0.21	-	31,31,31,31	0
56	MG	BA	3723	1/1	0.13	-	49,49,49,49	0
56	MG	BA	3530	1/1	0.29	-	31,31,31,31	0
56	MG	D5	102	1/1	0.57	-	55,55,55,55	0
56	MG	BA	3086	1/1	0.42	-	49,49,49,49	0
56	MG	CA	3108	1/1	0.24	-	52,52,52,52	0
56	MG	BA	3683	1/1	0.22	-	60,60,60,60	0
56	MG	DA	3032	1/1	0.15	-	46,46,46,46	0
56	MG	CA	3146	1/1	0.18	-	69,69,69,69	0
56	MG	BG	3003	1/1	0.17	-	42,42,42,42	0
56	MG	CA	3070	1/1	0.34	-	55,55,55,55	0
56	MG	BA	3733	1/1	0.10	-	27,27,27,27	0
56	MG	DA	3619	1/1	0.25	-	48,48,48,48	0
56	MG	DA	3308	1/1	0.34	-	30,30,30,30	0
56	MG	DA	3264	1/1	0.32	-	49,49,49,49	0
56	MG	DA	3083	1/1	0.23	-	41,41,41,41	0
56	MG	BA	3219	1/1	0.20	-	65,65,65,65	0
56	MG	BA	3714	1/1	0.25	-	58,58,58,58	0
56	MG	BA	3267	1/1	0.16	-	41,41,41,41	0
56	MG	BA	3693	1/1	0.15	-	64,64,64,64	0
56	MG	BA	3207	1/1	0.21	-	35,35,35,35	0
56	MG	BA	3642	1/1	0.27	-	51,51,51,51	0
56	MG	AA	3051	1/1	0.45	-	73,73,73,73	0
56	MG	BA	3028	1/1	0.20	-	48,48,48,48	0
56	MG	CA	3037	1/1	0.31	-	67,67,67,67	0
56	MG	AV	101	1/1	0.19	-	36,36,36,36	0
56	MG	BA	3561	1/1	0.19	-	24,24,24,24	0
56	MG	AA	3009	1/1	0.28	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BN	3004	1/1	0.37	-	66,66,66,66	0
56	MG	BA	3068	1/1	0.40	-	54,54,54,54	0
56	MG	BA	3521	1/1	0.12	-	49,49,49,49	0
56	MG	BA	3525	1/1	0.23	-	43,43,43,43	0
56	MG	DA	3539	1/1	0.18	-	53,53,53,53	0
56	MG	DA	3226	1/1	0.22	-	50,50,50,50	0
56	MG	BA	3283	1/1	0.17	-	17,17,17,17	0
56	MG	BA	3245	1/1	0.36	-	47,47,47,47	0
56	MG	BA	3051	1/1	0.15	-	20,20,20,20	0
56	MG	DA	3621	1/1	0.13	-	54,54,54,54	0
56	MG	BZ	3001	1/1	0.29	-	61,61,61,61	0
56	MG	BA	3423	1/1	0.07	-	26,26,26,26	0
56	MG	DA	3059	1/1	0.10	-	46,46,46,46	0
56	MG	DA	3435	1/1	0.23	-	46,46,46,46	0
56	MG	CA	3024	1/1	0.46	-	65,65,65,65	0
56	MG	DA	3181	1/1	0.30	-	36,36,36,36	0
56	MG	BA	3265	1/1	0.10	-	20,20,20,20	0
56	MG	DA	3567	1/1	0.17	-	62,62,62,62	0
56	MG	DA	3630	1/1	0.19	-	40,40,40,40	0
56	MG	DA	3510	1/1	0.23	-	63,63,63,63	0
56	MG	BA	3603	1/1	0.08	-	39,39,39,39	0
56	MG	BA	3617	1/1	0.23	-	62,62,62,62	0
56	MG	DA	3282	1/1	0.10	-	36,36,36,36	0
56	MG	AA	3167	1/1	0.18	-	67,67,67,67	0
56	MG	DA	3346	1/1	0.24	-	29,29,29,29	0
56	MG	AA	3174	1/1	0.23	-	33,33,33,33	0
56	MG	BA	3101	1/1	0.14	-	35,35,35,35	0
56	MG	CA	3042	1/1	0.55	-	85,85,85,85	0
56	MG	BA	3626	1/1	0.12	-	43,43,43,43	0
56	MG	BA	3107	1/1	0.20	-	40,40,40,40	0
56	MG	BA	3544	1/1	0.22	-	27,27,27,27	0
56	MG	CA	3167	1/1	0.08	-	78,78,78,78	0
56	MG	BA	3464	1/1	0.09	-	43,43,43,43	0
56	MG	DA	3528	1/1	0.09	-	56,56,56,56	0
56	MG	DA	3044	1/1	0.12	-	46,46,46,46	0
56	MG	BA	3016	1/1	0.24	-	33,33,33,33	0
56	MG	BA	3343	1/1	0.18	-	40,40,40,40	0
58	ZN	D9	501	1/1	0.04	-	66,66,66,66	0
56	MG	BA	3356	1/1	0.26	-	56,56,56,56	0
56	MG	BA	3711	1/1	0.17	-	86,86,86,86	0
56	MG	BN	3002	1/1	0.32	-	56,56,56,56	0
56	MG	AA	3185	1/1	0.28	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3014	1/1	0.69	-	34,34,34,34	0
56	MG	DB	3001	1/1	0.25	-	68,68,68,68	0
56	MG	DA	3508	1/1	0.21	-	38,38,38,38	0
56	MG	DA	3534	1/1	0.16	-	45,45,45,45	0
56	MG	BU	204	1/1	0.39	-	44,44,44,44	0
56	MG	DA	3371	1/1	0.07	-	44,44,44,44	0
56	MG	AA	3062	1/1	0.10	-	32,32,32,32	0
56	MG	AA	3019	1/1	0.44	-	74,74,74,74	0
56	MG	DD	307	1/1	0.54	-	38,38,38,38	0
56	MG	DA	3628	1/1	0.20	-	63,63,63,63	0
56	MG	BA	3639	1/1	0.15	-	50,50,50,50	0
56	MG	BA	3421	1/1	0.11	-	36,36,36,36	0
56	MG	BA	3046	1/1	0.14	-	29,29,29,29	0
56	MG	CA	3129	1/1	0.16	-	45,45,45,45	0
56	MG	BA	3637	1/1	0.36	-	33,33,33,33	0
56	MG	BA	3592	1/1	0.16	-	28,28,28,28	0
56	MG	AA	3217	1/1	0.70	-	67,67,67,67	0
56	MG	DF	301	1/1	0.47	-	32,32,32,32	0
56	MG	BA	3070	1/1	0.14	-	35,35,35,35	0
56	MG	BA	3132	1/1	0.23	-	35,35,35,35	0
56	MG	DA	3189	1/1	0.14	-	55,55,55,55	0
56	MG	BA	3123	1/1	0.34	-	69,69,69,69	0
56	MG	BA	3136	1/1	0.23	-	58,58,58,58	0
56	MG	DA	3503	1/1	0.19	-	71,71,71,71	0
56	MG	BA	3604	1/1	0.10	-	72,72,72,72	0
56	MG	DA	3504	1/1	0.06	-	44,44,44,44	0
56	MG	DA	3470	1/1	0.28	-	52,52,52,52	0
56	MG	BA	3336	1/1	0.21	-	54,54,54,54	0
56	MG	BA	3426	1/1	0.24	-	51,51,51,51	0
56	MG	BA	3281	1/1	0.19	-	52,52,52,52	0
56	MG	BA	3399	1/1	0.20	-	18,18,18,18	0
56	MG	BA	3645	1/1	0.09	-	56,56,56,56	0
56	MG	BA	3146	1/1	0.28	-	52,52,52,52	0
56	MG	DA	3422	1/1	0.12	-	38,38,38,38	0
56	MG	DA	3007	1/1	0.24	-	30,30,30,30	0
56	MG	DA	3652	1/1	0.40	-	60,60,60,60	0
56	MG	DA	3099	1/1	0.29	-	44,44,44,44	0
56	MG	BA	3517	1/1	0.09	-	49,49,49,49	0
56	MG	DA	3262	1/1	0.22	-	44,44,44,44	0
56	MG	AA	3094	1/1	0.19	-	68,68,68,68	0
56	MG	DA	3075	1/1	0.30	-	44,44,44,44	0
56	MG	BA	3318	1/1	0.12	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3379	1/1	0.24	-	22,22,22,22	0
56	MG	AA	3138	1/1	0.54	-	37,37,37,37	0
56	MG	AA	3184	1/1	0.09	-	72,72,72,72	0
56	MG	DA	3112	1/1	0.41	-	54,54,54,54	0
56	MG	AA	3178	1/1	0.20	-	65,65,65,65	0
56	MG	CA	3040	1/1	0.33	-	42,42,42,42	0
56	MG	BA	3672	1/1	0.28	-	48,48,48,48	0
56	MG	BA	3634	1/1	0.67	-	63,63,63,63	0
56	MG	DA	3204	1/1	0.41	-	34,34,34,34	0
56	MG	BA	3233	1/1	0.22	-	47,47,47,47	0
56	MG	BA	3263	1/1	0.24	-	79,79,79,79	0
56	MG	BA	3111	1/1	0.41	-	53,53,53,53	0
56	MG	DA	3293	1/1	0.27	-	53,53,53,53	0
56	MG	BB	3004	1/1	0.25	-	54,54,54,54	0
57	SF4	CD	501	8/8	0.13	-	64,75,91,95	0
56	MG	BA	3031	1/1	0.78	-	41,41,41,41	0
56	MG	AA	3110	1/1	0.24	-	48,48,48,48	0
56	MG	AA	3187	1/1	0.04	-	62,62,62,62	0
56	MG	BA	3159	1/1	0.33	-	48,48,48,48	0
56	MG	AA	3018	1/1	0.30	-	38,38,38,38	0
56	MG	BA	3602	1/1	0.09	-	35,35,35,35	0
56	MG	DA	3315	1/1	0.08	-	31,31,31,31	0
56	MG	DA	3188	1/1	0.38	-	47,47,47,47	0
56	MG	BA	3287	1/1	0.19	-	53,53,53,53	0
56	MG	AA	3052	1/1	0.24	-	60,60,60,60	0
56	MG	BA	3605	1/1	0.32	-	59,59,59,59	0
56	MG	BA	3035	1/1	0.10	-	37,37,37,37	0
56	MG	DA	3286	1/1	0.18	-	62,62,62,62	0
56	MG	AA	3169	1/1	0.13	-	76,76,76,76	0
56	MG	DA	3581	1/1	0.73	-	73,73,73,73	0
56	MG	DA	3599	1/1	0.23	-	72,72,72,72	0
56	MG	DA	3171	1/1	0.24	-	39,39,39,39	0
56	MG	BA	3538	1/1	0.15	-	36,36,36,36	0
56	MG	BA	3293	1/1	0.18	-	45,45,45,45	0
56	MG	DA	3126	1/1	0.37	-	43,43,43,43	0
56	MG	BA	3516	1/1	0.09	-	47,47,47,47	0
56	MG	CA	3145	1/1	0.07	-	43,43,43,43	0
56	MG	DA	3273	1/1	0.13	-	30,30,30,30	0
56	MG	BN	3003	1/1	0.40	-	59,59,59,59	0
56	MG	DA	3290	1/1	0.07	-	42,42,42,42	0
56	MG	BA	3166	1/1	0.54	-	59,59,59,59	0
56	MG	CA	3018	1/1	0.28	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	3136	1/1	0.09	-	62,62,62,62	0
56	MG	DA	3020	1/1	0.29	-	52,52,52,52	0
56	MG	BA	3424	1/1	0.17	-	15,15,15,15	0
56	MG	DA	3420	1/1	0.15	-	51,51,51,51	0
56	MG	BA	3234	1/1	0.30	-	55,55,55,55	0
56	MG	AA	3058	1/1	0.18	-	50,50,50,50	0
56	MG	BA	3017	1/1	0.56	-	44,44,44,44	0
56	MG	BA	3117	1/1	0.25	-	25,25,25,25	0
56	MG	DA	3563	1/1	0.17	-	64,64,64,64	0
56	MG	DA	3403	1/1	0.13	-	28,28,28,28	0
56	MG	CA	3096	1/1	0.09	-	60,60,60,60	0
56	MG	AA	3181	1/1	0.29	-	57,57,57,57	0
56	MG	CA	3128	1/1	0.26	-	41,41,41,41	0
56	MG	DA	3292	1/1	0.21	-	37,37,37,37	0
56	MG	CA	3119	1/1	0.20	-	64,64,64,64	0
56	MG	DA	3272	1/1	0.29	-	27,27,27,27	0
56	MG	BA	3501	1/1	0.24	-	59,59,59,59	0
56	MG	CA	3123	1/1	0.14	-	77,77,77,77	0
56	MG	DA	3281	1/1	0.25	-	42,42,42,42	0
56	MG	BA	3437	1/1	0.15	-	42,42,42,42	0
56	MG	AA	3070	1/1	0.11	-	75,75,75,75	0
56	MG	BA	3650	1/1	0.16	-	45,45,45,45	0
56	MG	AK	3001	1/1	0.22	-	45,45,45,45	0
56	MG	DA	3569	1/1	0.19	-	37,37,37,37	0
56	MG	BF	302	1/1	0.30	-	46,46,46,46	0
56	MG	DA	3474	1/1	0.09	-	61,61,61,61	0
56	MG	AA	3195	1/1	0.17	-	71,71,71,71	0
56	MG	BA	3339	1/1	0.22	-	43,43,43,43	0
56	MG	BA	3564	1/1	0.07	-	52,52,52,52	0
56	MG	BA	3418	1/1	0.14	-	27,27,27,27	0
56	MG	DA	3153	1/1	0.25	-	38,38,38,38	0
56	MG	CA	3076	1/1	0.32	-	40,40,40,40	0
56	MG	BG	3002	1/1	0.11	-	42,42,42,42	0
56	MG	CE	3001	1/1	0.33	-	68,68,68,68	0
56	MG	BA	3737	1/1	0.25	-	60,60,60,60	0
56	MG	BA	3272	1/1	0.33	-	7,7,7,7	0
56	MG	DA	3209	1/1	0.14	-	41,41,41,41	0
56	MG	DA	3248	1/1	0.27	-	51,51,51,51	0
56	MG	DB	3007	1/1	0.25	-	45,45,45,45	0
56	MG	BA	3228	1/1	0.26	-	63,63,63,63	0
56	MG	DN	5001	1/1	0.14	-	75,75,75,75	0
56	MG	DA	3446	1/1	0.12	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	3212	1/1	0.14	-	79,79,79,79	0
56	MG	AA	3025	1/1	0.13	-	69,69,69,69	0
56	MG	B3	101	1/1	0.15	-	28,28,28,28	0
56	MG	BA	3511	1/1	0.17	-	39,39,39,39	0
56	MG	DA	3172	1/1	0.45	-	51,51,51,51	0
56	MG	DA	3381	1/1	0.27	-	47,47,47,47	0
56	MG	AA	3117	1/1	0.23	-	71,71,71,71	0
56	MG	DA	3408	1/1	0.23	-	37,37,37,37	0
56	MG	BA	3037	1/1	0.20	-	31,31,31,31	0
56	MG	DA	3077	1/1	0.27	-	50,50,50,50	0
56	MG	BA	3055	1/1	0.20	-	44,44,44,44	0
56	MG	BA	3531	1/1	0.28	-	38,38,38,38	0
56	MG	BA	3558	1/1	0.21	-	35,35,35,35	0
56	MG	AA	3158	1/1	0.24	-	44,44,44,44	0
56	MG	CA	3135	1/1	0.52	-	76,76,76,76	0
56	MG	BA	3102	1/1	0.28	-	52,52,52,52	0
56	MG	CA	3125	1/1	0.15	-	72,72,72,72	0
56	MG	DA	3529	1/1	0.08	-	63,63,63,63	0
56	MG	DA	3557	1/1	0.11	-	45,45,45,45	0
56	MG	BA	3485	1/1	0.29	-	44,44,44,44	0
56	MG	BA	3513	1/1	0.11	-	45,45,45,45	0
56	MG	BA	3590	1/1	0.13	-	64,64,64,64	0
56	MG	BA	3058	1/1	0.41	-	38,38,38,38	0
57	SF4	AD	501	8/8	0.14	-	59,72,92,96	0
56	MG	BD	311	1/1	0.53	-	45,45,45,45	0
56	MG	BA	3084	1/1	0.17	-	33,33,33,33	0
56	MG	DA	3397	1/1	0.18	-	41,41,41,41	0
56	MG	DA	3288	1/1	0.18	-	47,47,47,47	0
56	MG	AA	3045	1/1	0.32	-	61,61,61,61	0
56	MG	CA	3043	1/1	0.32	-	49,49,49,49	0
56	MG	DA	3342	1/1	0.12	-	52,52,52,52	0
56	MG	BA	3441	1/1	0.24	-	25,25,25,25	0
56	MG	AA	3017	1/1	0.28	-	55,55,55,55	0
56	MG	BA	3079	1/1	0.27	-	42,42,42,42	0
56	MG	DQ	203	1/1	0.31	-	57,57,57,57	0
56	MG	CX	103	1/1	0.27	-	60,60,60,60	0
56	MG	BA	3112	1/1	0.09	-	38,38,38,38	0
56	MG	BA	3095	1/1	0.39	-	55,55,55,55	0
56	MG	CA	3158	1/1	0.23	-	76,76,76,76	0
56	MG	AX	105	1/1	0.66	-	56,56,56,56	0
56	MG	BA	3210	1/1	0.09	-	34,34,34,34	0
56	MG	BA	3308	1/1	0.08	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3097	1/1	0.19	-	33,33,33,33	0
56	MG	DA	3500	1/1	0.19	-	50,50,50,50	0
56	MG	DA	3314	1/1	0.20	-	64,64,64,64	0
56	MG	DW	202	1/1	0.44	-	58,58,58,58	0
56	MG	CA	3143	1/1	0.09	-	87,87,87,87	0
56	MG	DA	3634	1/1	0.15	-	51,51,51,51	0
56	MG	CA	3115	1/1	0.11	-	55,55,55,55	0
56	MG	BA	3675	1/1	0.12	-	49,49,49,49	0
56	MG	BA	3260	1/1	0.18	-	22,22,22,22	0
56	MG	DA	3023	1/1	0.33	-	52,52,52,52	0
56	MG	AA	3003	1/1	0.30	-	63,63,63,63	0
56	MG	BA	3570	1/1	0.12	-	61,61,61,61	0
56	MG	DA	3559	1/1	0.19	-	46,46,46,46	0
56	MG	DA	3524	1/1	0.11	-	28,28,28,28	0
56	MG	CA	3138	1/1	0.25	-	72,72,72,72	0
56	MG	DA	3097	1/1	0.27	-	61,61,61,61	0
56	MG	DA	3392	1/1	0.18	-	35,35,35,35	0
56	MG	DA	3081	1/1	0.20	-	48,48,48,48	0
56	MG	DA	3168	1/1	0.39	-	48,48,48,48	0
56	MG	DE	303	1/1	0.11	-	41,41,41,41	0
56	MG	BA	3120	1/1	0.07	-	51,51,51,51	0
56	MG	DA	3145	1/1	0.42	-	65,65,65,65	0
56	MG	DA	3590	1/1	0.18	-	80,80,80,80	0
56	MG	BW	202	1/1	0.17	-	34,34,34,34	0
56	MG	BA	3313	1/1	0.26	-	36,36,36,36	0
56	MG	BA	3680	1/1	0.38	-	37,37,37,37	0
56	MG	DA	3533	1/1	0.09	-	68,68,68,68	0
56	MG	AA	3197	1/1	0.40	-	69,69,69,69	0
56	MG	DA	3127	1/1	0.07	-	48,48,48,48	0
56	MG	BA	3724	1/1	0.18	-	58,58,58,58	0
56	MG	BA	3158	1/1	0.60	-	64,64,64,64	0
56	MG	DA	3183	1/1	0.12	-	54,54,54,54	0
56	MG	BA	3275	1/1	0.22	-	46,46,46,46	0
56	MG	BA	3598	1/1	0.11	-	56,56,56,56	0
56	MG	AA	3153	1/1	0.14	-	45,45,45,45	0
56	MG	BA	3736	1/1	0.23	-	48,48,48,48	0
56	MG	BA	3066	1/1	0.23	-	44,44,44,44	0
56	MG	AA	3215	1/1	0.10	-	53,53,53,53	0
56	MG	BA	3250	1/1	0.17	-	45,45,45,45	0
56	MG	BA	3566	1/1	0.10	-	53,53,53,53	0
56	MG	BA	3155	1/1	0.39	-	57,57,57,57	0
56	MG	BA	3186	1/1	0.15	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3105	1/1	0.34	-	48,48,48,48	0
56	MG	DA	3050	1/1	0.58	-	31,31,31,31	0
56	MG	AA	3191	1/1	0.13	-	71,71,71,71	0
56	MG	BA	3401	1/1	0.11	-	42,42,42,42	0
56	MG	DA	3234	1/1	0.22	-	33,33,33,33	0
56	MG	BA	3073	1/1	0.89	-	41,41,41,41	0
56	MG	CA	3017	1/1	0.23	-	42,42,42,42	0
56	MG	BA	3556	1/1	0.33	-	27,27,27,27	0
56	MG	CA	3009	1/1	0.13	-	47,47,47,47	0
56	MG	CA	3106	1/1	0.31	-	64,64,64,64	0
56	MG	BA	3175	1/1	0.27	-	48,48,48,48	0
56	MG	DA	3108	1/1	0.52	-	37,37,37,37	0
56	MG	DA	3325	1/1	0.16	-	36,36,36,36	0
56	MG	BA	3417	1/1	0.17	-	18,18,18,18	0
56	MG	DA	3214	1/1	0.27	-	64,64,64,64	0
56	MG	BA	3190	1/1	0.20	-	42,42,42,42	0
56	MG	DA	3213	1/1	0.23	-	44,44,44,44	0
56	MG	BA	3285	1/1	0.14	-	32,32,32,32	0
56	MG	DA	3347	1/1	0.16	-	62,62,62,62	0
56	MG	DA	3501	1/1	0.20	-	23,23,23,23	0
56	MG	AA	3028	1/1	0.47	-	60,60,60,60	0
56	MG	AA	3060	1/1	0.54	-	60,60,60,60	0
56	MG	BY	201	1/1	0.33	-	58,58,58,58	0
56	MG	DA	3507	1/1	0.15	-	54,54,54,54	0
56	MG	BA	3236	1/1	0.20	-	36,36,36,36	0
56	MG	BA	3103	1/1	0.12	-	53,53,53,53	0
56	MG	AA	3119	1/1	0.37	-	63,63,63,63	0
56	MG	CA	3010	1/1	0.10	-	32,32,32,32	0
56	MG	DA	3269	1/1	0.12	-	48,48,48,48	0
56	MG	DA	3276	1/1	0.22	-	36,36,36,36	0
56	MG	AA	3203	1/1	0.14	-	63,63,63,63	0
56	MG	BA	3652	1/1	0.21	-	64,64,64,64	0
56	MG	DA	3319	1/1	0.17	-	53,53,53,53	0
56	MG	DA	3515	1/1	0.27	-	48,48,48,48	0
56	MG	DA	3169	1/1	0.42	-	57,57,57,57	0
56	MG	BA	3392	1/1	0.24	-	56,56,56,56	0
56	MG	DA	3259	1/1	0.16	-	47,47,47,47	0
56	MG	AA	3137	1/1	0.21	-	42,42,42,42	0
56	MG	DQ	205	1/1	0.44	-	55,55,55,55	0
56	MG	DA	3329	1/1	0.16	-	53,53,53,53	0
56	MG	BA	3475	1/1	0.20	-	36,36,36,36	0
56	MG	DA	3623	1/1	0.16	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	3084	1/1	0.14	-	64,64,64,64	0
56	MG	DA	3066	1/1	0.40	-	53,53,53,53	0
56	MG	DA	3548	1/1	0.14	-	37,37,37,37	0
56	MG	BA	3440	1/1	0.37	-	38,38,38,38	0
56	MG	AA	3043	1/1	0.52	-	74,74,74,74	0
56	MG	DA	3348	1/1	0.30	-	37,37,37,37	0
56	MG	DA	3052	1/1	0.21	-	23,23,23,23	0
56	MG	BA	3677	1/1	0.25	-	67,67,67,67	0
56	MG	DA	3516	1/1	0.15	-	40,40,40,40	0
56	MG	DA	3061	1/1	0.41	-	52,52,52,52	0
56	MG	DA	3646	1/1	0.07	-	38,38,38,38	0
56	MG	DA	3202	1/1	0.31	-	42,42,42,42	0
56	MG	CA	3052	1/1	0.13	-	39,39,39,39	0
56	MG	AA	3066	1/1	0.27	-	38,38,38,38	0
56	MG	BA	3273	1/1	0.40	-	42,42,42,42	0
56	MG	AX	102	1/1	0.23	-	74,74,74,74	0
56	MG	BA	3461	1/1	0.24	-	36,36,36,36	0
56	MG	AA	3125	1/1	0.16	-	47,47,47,47	0
56	MG	B8	102	1/1	0.10	-	60,60,60,60	0
56	MG	BA	3690	1/1	0.17	-	53,53,53,53	0
56	MG	DA	3631	1/1	0.16	-	56,56,56,56	0
56	MG	DA	3026	1/1	0.21	-	37,37,37,37	0
56	MG	BE	305	1/1	0.69	-	42,42,42,42	0
56	MG	BA	3687	1/1	0.22	-	38,38,38,38	0
56	MG	DA	3096	1/1	0.16	-	60,60,60,60	0
56	MG	BA	3039	1/1	0.14	-	42,42,42,42	0
56	MG	DA	3011	1/1	0.42	-	45,45,45,45	0
56	MG	CA	3045	1/1	0.09	-	54,54,54,54	0
56	MG	CA	3077	1/1	0.21	-	53,53,53,53	0
56	MG	BA	3403	1/1	0.21	-	41,41,41,41	0
56	MG	AA	3089	1/1	0.43	-	78,78,78,78	0
56	MG	BA	3209	1/1	0.39	-	40,40,40,40	0
56	MG	AA	3057	1/1	0.08	-	37,37,37,37	0
56	MG	BA	3380	1/1	0.13	-	53,53,53,53	0
56	MG	AA	3044	1/1	0.22	-	66,66,66,66	0
56	MG	BD	308	1/1	0.34	-	23,23,23,23	0
56	MG	DA	3588	1/1	0.18	-	40,40,40,40	0
56	MG	BA	3177	1/1	0.22	-	62,62,62,62	0
56	MG	CA	3082	1/1	0.08	-	47,47,47,47	0
56	MG	DA	3574	1/1	0.17	-	56,56,56,56	0
56	MG	BA	3456	1/1	0.08	-	52,52,52,52	0
56	MG	BA	3664	1/1	0.28	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BU	203	1/1	0.30	-	33,33,33,33	0
56	MG	BA	3011	1/1	0.08	-	37,37,37,37	0
56	MG	D0	101	1/1	0.13	-	63,63,63,63	0
56	MG	BA	3008	1/1	0.15	-	50,50,50,50	0
56	MG	AA	3175	1/1	0.14	-	76,76,76,76	0
56	MG	DD	304	1/1	0.23	-	35,35,35,35	0
56	MG	BA	3416	1/1	0.25	-	42,42,42,42	0
56	MG	BA	3450	1/1	0.26	-	46,46,46,46	0
56	MG	BA	3360	1/1	0.18	-	38,38,38,38	0
56	MG	BF	304	1/1	0.07	-	35,35,35,35	0
56	MG	BA	3098	1/1	0.15	-	35,35,35,35	0
56	MG	AA	3036	1/1	0.25	-	71,71,71,71	0
56	MG	DA	3150	1/1	0.19	-	64,64,64,64	0
56	MG	BA	3430	1/1	0.29	-	49,49,49,49	0
56	MG	BA	3547	1/1	0.19	-	31,31,31,31	0
56	MG	B8	101	1/1	0.52	-	49,49,49,49	0
56	MG	BA	3082	1/1	0.28	-	41,41,41,41	0
56	MG	DA	3485	1/1	0.09	-	38,38,38,38	0
56	MG	BA	3266	1/1	0.32	-	46,46,46,46	0
56	MG	DA	3037	1/1	0.33	-	35,35,35,35	0
56	MG	AA	3188	1/1	0.25	-	53,53,53,53	0
56	MG	CA	3120	1/1	0.19	-	58,58,58,58	0
56	MG	BA	3151	1/1	0.07	-	52,52,52,52	0
56	MG	DA	3620	1/1	0.20	-	71,71,71,71	0
56	MG	BA	3280	1/1	0.66	-	69,69,69,69	0
56	MG	DA	3216	1/1	0.17	-	31,31,31,31	0
56	MG	BA	3386	1/1	0.15	-	58,58,58,58	0
56	MG	BA	3477	1/1	0.11	-	25,25,25,25	0
56	MG	BA	3171	1/1	0.33	-	40,40,40,40	0
58	ZN	B4	3002	1/1	0.06	-	165,165,165,165	0
56	MG	AA	3061	1/1	0.21	-	82,82,82,82	0
56	MG	DA	3170	1/1	0.74	-	57,57,57,57	0
56	MG	BA	3636	1/1	0.10	-	36,36,36,36	0
56	MG	BA	3471	1/1	0.17	-	51,51,51,51	0
56	MG	AA	3105	1/1	0.21	-	46,46,46,46	0
56	MG	DA	3433	1/1	0.19	-	48,48,48,48	0
56	MG	DA	3330	1/1	0.18	-	37,37,37,37	0
56	MG	BA	3666	1/1	0.30	-	61,61,61,61	0
56	MG	AM	3001	1/1	0.08	-	65,65,65,65	0
56	MG	DA	3579	1/1	0.17	-	23,23,23,23	0
56	MG	BA	3731	1/1	0.37	-	55,55,55,55	0
56	MG	BA	3606	1/1	0.21	-	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3436	1/1	0.08	-	62,62,62,62	0
56	MG	DA	3622	1/1	0.09	-	55,55,55,55	0
56	MG	DA	3009	1/1	0.12	-	31,31,31,31	0
56	MG	DA	3536	1/1	0.18	-	80,80,80,80	0
56	MG	CA	3029	1/1	0.21	-	59,59,59,59	0
56	MG	AA	3037	1/1	0.41	-	61,61,61,61	0
56	MG	DA	3019	1/1	0.12	-	30,30,30,30	0
56	MG	DA	3092	1/1	0.52	-	39,39,39,39	0
56	MG	DA	3487	1/1	0.18	-	57,57,57,57	0
56	MG	AA	3029	1/1	0.62	-	52,52,52,52	0
56	MG	CA	3033	1/1	0.18	-	68,68,68,68	0
56	MG	CA	3087	1/1	0.18	-	41,41,41,41	0
56	MG	DA	3128	1/1	0.21	-	52,52,52,52	0
56	MG	AA	3205	1/1	0.17	-	61,61,61,61	0
56	MG	B0	102	1/1	0.57	-	40,40,40,40	0
56	MG	DA	3239	1/1	0.23	-	39,39,39,39	0
56	MG	DA	3556	1/1	0.07	-	56,56,56,56	0
56	MG	DA	3502	1/1	0.10	-	65,65,65,65	0
56	MG	BA	3518	1/1	0.12	-	41,41,41,41	0
56	MG	AX	103	1/1	0.08	-	66,66,66,66	0
56	MG	DA	3160	1/1	0.15	-	44,44,44,44	0
56	MG	BA	3284	1/1	0.11	-	54,54,54,54	0
56	MG	BV	203	1/1	1.06	-	46,46,46,46	0
56	MG	BA	3013	1/1	0.08	-	40,40,40,40	0
56	MG	BA	3466	1/1	0.14	-	61,61,61,61	0
56	MG	BE	304	1/1	0.09	-	49,49,49,49	0
56	MG	DA	3386	1/1	0.16	-	56,56,56,56	0
56	MG	DA	3100	1/1	0.47	-	56,56,56,56	0
56	MG	DA	3496	1/1	0.14	-	53,53,53,53	0
56	MG	DA	3449	1/1	0.10	-	43,43,43,43	0
56	MG	BA	3047	1/1	0.47	-	47,47,47,47	0
56	MG	CA	3038	1/1	0.43	-	70,70,70,70	0
56	MG	BA	3583	1/1	0.21	-	27,27,27,27	0
56	MG	AA	3086	1/1	0.28	-	51,51,51,51	0
56	MG	BA	3213	1/1	0.05	-	41,41,41,41	0
56	MG	CA	3114	1/1	0.24	-	82,82,82,82	0
56	MG	DA	3651	1/1	0.60	-	52,52,52,52	0
56	MG	DA	3257	1/1	0.11	-	48,48,48,48	0
56	MG	CA	3031	1/1	0.40	-	53,53,53,53	0
56	MG	AA	3031	1/1	0.23	-	41,41,41,41	0
56	MG	BA	3268	1/1	0.18	-	46,46,46,46	0
56	MG	AA	3079	1/1	1.09	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3427	1/1	0.57	-	60,60,60,60	0
56	MG	BW	205	1/1	0.38	-	41,41,41,41	0
56	MG	CA	3172	1/1	0.14	-	51,51,51,51	0
56	MG	BA	3620	1/1	0.12	-	47,47,47,47	0
56	MG	DA	3396	1/1	0.22	-	35,35,35,35	0
56	MG	BA	3243	1/1	0.16	-	48,48,48,48	0
56	MG	AA	3126	1/1	0.15	-	54,54,54,54	0
58	ZN	BY	202	1/1	0.08	-	71,71,71,71	0
56	MG	BA	3231	1/1	0.49	-	38,38,38,38	0
56	MG	AA	3182	1/1	0.12	-	49,49,49,49	0
56	MG	BA	3493	1/1	0.36	-	15,15,15,15	0
56	MG	BA	3384	1/1	0.35	-	60,60,60,60	0
56	MG	BA	3060	1/1	0.39	-	40,40,40,40	0
56	MG	BA	3237	1/1	0.54	-	51,51,51,51	0
56	MG	BA	3189	1/1	0.17	-	54,54,54,54	0
56	MG	BA	3149	1/1	0.58	-	40,40,40,40	0
56	MG	AA	3102	1/1	0.06	-	64,64,64,64	0
56	MG	BA	3127	1/1	0.38	-	50,50,50,50	0
56	MG	DA	3636	1/1	0.14	-	61,61,61,61	0
56	MG	DA	3522	1/1	0.17	-	61,61,61,61	0
56	MG	BA	3364	1/1	0.23	-	29,29,29,29	0
56	MG	BA	3449	1/1	0.12	-	21,21,21,21	0
56	MG	DA	3045	1/1	0.36	-	41,41,41,41	0
56	MG	BA	3174	1/1	0.08	-	48,48,48,48	0
56	MG	AA	3152	1/1	0.09	-	19,19,19,19	0
56	MG	DA	3580	1/1	0.14	-	46,46,46,46	0
56	MG	BB	3007	1/1	0.08	-	47,47,47,47	0
56	MG	BA	3083	1/1	0.23	-	63,63,63,63	0
56	MG	AA	3132	1/1	0.32	-	76,76,76,76	0
56	MG	BA	3468	1/1	0.18	-	30,30,30,30	0
56	MG	CA	3094	1/1	0.18	-	43,43,43,43	0
56	MG	AA	3005	1/1	0.15	-	66,66,66,66	0
56	MG	BA	3443	1/1	0.16	-	26,26,26,26	0
56	MG	DA	3480	1/1	0.09	-	52,52,52,52	0
56	MG	DA	3299	1/1	0.20	-	40,40,40,40	0
56	MG	DA	3450	1/1	0.13	-	43,43,43,43	0
56	MG	DA	3531	1/1	0.10	-	57,57,57,57	0
56	MG	DA	3175	1/1	0.19	-	40,40,40,40	0
56	MG	DA	3266	1/1	0.24	-	43,43,43,43	0
56	MG	DA	3570	1/1	0.24	-	28,28,28,28	0
56	MG	CA	3124	1/1	0.15	-	61,61,61,61	0
56	MG	DA	3224	1/1	0.17	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	3044	1/1	0.23	-	63,63,63,63	0
56	MG	BA	3351	1/1	0.06	-	30,30,30,30	0
56	MG	BA	3663	1/1	0.27	-	56,56,56,56	0
56	MG	DA	3012	1/1	0.22	-	57,57,57,57	0
56	MG	BA	3618	1/1	0.28	-	46,46,46,46	0
56	MG	DA	3110	1/1	0.13	-	49,49,49,49	0
56	MG	AA	3147	1/1	0.41	-	61,61,61,61	0
56	MG	BE	310	1/1	0.27	-	50,50,50,50	0
56	MG	CA	3064	1/1	0.13	-	58,58,58,58	0
56	MG	BN	3005	1/1	0.85	-	52,52,52,52	0
56	MG	DA	3540	1/1	0.23	-	54,54,54,54	0
56	MG	CA	3103	1/1	0.18	-	83,83,83,83	0
56	MG	BA	3279	1/1	0.22	-	48,48,48,48	0
56	MG	BA	3022	1/1	0.33	-	52,52,52,52	0
56	MG	BA	3582	1/1	0.21	-	25,25,25,25	0
56	MG	BA	3292	1/1	0.21	-	63,63,63,63	0
56	MG	BA	3043	1/1	0.20	-	52,52,52,52	0
56	MG	DA	3124	1/1	0.13	-	67,67,67,67	0
56	MG	BA	3407	1/1	0.18	-	15,15,15,15	0
56	MG	DA	3426	1/1	0.15	-	74,74,74,74	0
56	MG	DA	3489	1/1	0.18	-	36,36,36,36	0
56	MG	AA	3072	1/1	0.29	-	79,79,79,79	0
56	MG	BA	3165	1/1	0.34	-	53,53,53,53	0
56	MG	DV	204	1/1	0.22	-	41,41,41,41	0
56	MG	BA	3425	1/1	0.34	-	36,36,36,36	0
56	MG	AA	3032	1/1	0.35	-	57,57,57,57	0
56	MG	BA	3264	1/1	0.17	-	30,30,30,30	0
56	MG	BA	3454	1/1	0.10	-	22,22,22,22	0
56	MG	BR	202	1/1	0.27	-	27,27,27,27	0
56	MG	AA	3218	1/1	0.54	-	65,65,65,65	0
56	MG	DA	3115	1/1	0.10	-	63,63,63,63	0
56	MG	DA	3447	1/1	0.06	-	56,56,56,56	0
56	MG	DA	3376	1/1	0.07	-	31,31,31,31	0
56	MG	DA	3142	1/1	0.24	-	33,33,33,33	0
56	MG	DA	3483	1/1	0.19	-	49,49,49,49	0
56	MG	CA	3159	1/1	0.58	-	91,91,91,91	0
56	MG	DA	3243	1/1	0.21	-	67,67,67,67	0
56	MG	BA	3434	1/1	0.12	-	32,32,32,32	0
56	MG	AA	3006	1/1	0.08	-	78,78,78,78	0
56	MG	CA	3022	1/1	0.04	-	70,70,70,70	0
56	MG	DA	3048	1/1	0.40	-	37,37,37,37	0
56	MG	AA	3149	1/1	0.09	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3339	1/1	0.09	-	37,37,37,37	0
56	MG	DA	3337	1/1	0.09	-	27,27,27,27	0
56	MG	BA	3670	1/1	0.15	-	59,59,59,59	0
56	MG	CA	3148	1/1	0.23	-	68,68,68,68	0
56	MG	BA	3038	1/1	0.53	-	51,51,51,51	0
56	MG	BA	3138	1/1	0.16	-	46,46,46,46	0
56	MG	BA	3309	1/1	0.14	-	46,46,46,46	0
56	MG	DA	3194	1/1	0.14	-	48,48,48,48	0
56	MG	DA	3279	1/1	0.29	-	63,63,63,63	0
56	MG	AA	3171	1/1	0.25	-	72,72,72,72	0
56	MG	DA	3069	1/1	0.11	-	51,51,51,51	0
56	MG	DA	3148	1/1	0.25	-	47,47,47,47	0
56	MG	AA	3085	1/1	0.30	-	69,69,69,69	0
56	MG	BA	3321	1/1	0.16	-	29,29,29,29	0
56	MG	CF	3001	1/1	0.24	-	55,55,55,55	0
56	MG	DD	301	1/1	0.46	-	46,46,46,46	0
56	MG	D3	101	1/1	0.43	-	63,63,63,63	0
56	MG	CA	3006	1/1	0.15	-	77,77,77,77	0
56	MG	BA	3596	1/1	0.11	-	51,51,51,51	0
56	MG	DA	3013	1/1	0.09	-	47,47,47,47	0
56	MG	BA	3727	1/1	0.57	-	68,68,68,68	0
56	MG	DA	3159	1/1	0.24	-	51,51,51,51	0
56	MG	BA	3199	1/1	0.48	-	36,36,36,36	0
56	MG	BA	3496	1/1	0.43	-	57,57,57,57	0
56	MG	DA	3353	1/1	0.11	-	62,62,62,62	0
56	MG	BA	3413	1/1	0.13	-	20,20,20,20	0
56	MG	AA	3016	1/1	0.06	-	63,63,63,63	0
56	MG	BA	3289	1/1	0.34	-	60,60,60,60	0
56	MG	AA	3157	1/1	0.08	-	35,35,35,35	0
56	MG	BA	3181	1/1	0.35	-	38,38,38,38	0
56	MG	DA	3603	1/1	0.17	-	55,55,55,55	0
56	MG	DV	203	1/1	0.78	-	54,54,54,54	0
56	MG	DA	3237	1/1	0.18	-	45,45,45,45	0
56	MG	BA	3387	1/1	0.08	-	48,48,48,48	0
56	MG	CA	3059	1/1	0.28	-	51,51,51,51	0
56	MG	BG	3004	1/1	0.04	-	62,62,62,62	0
56	MG	AA	3130	1/1	0.22	-	46,46,46,46	0
56	MG	DA	3653	1/1	0.34	-	60,60,60,60	0
56	MG	DA	3113	1/1	0.63	-	43,43,43,43	0
56	MG	BA	3317	1/1	0.15	-	40,40,40,40	0
56	MG	DA	3416	1/1	0.08	-	44,44,44,44	0
56	MG	DA	3217	1/1	0.47	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3326	1/1	0.09	-	41,41,41,41	0
56	MG	DA	3361	1/1	0.11	-	61,61,61,61	0
56	MG	BA	3701	1/1	0.13	-	32,32,32,32	0
56	MG	CA	3054	1/1	0.34	-	48,48,48,48	0
56	MG	DA	3445	1/1	0.24	-	39,39,39,39	0
56	MG	BA	3478	1/1	0.13	-	29,29,29,29	0
56	MG	BA	3444	1/1	0.12	-	74,74,74,74	0
56	MG	BA	3661	1/1	0.15	-	68,68,68,68	0
56	MG	DA	3647	1/1	0.40	-	66,66,66,66	0
56	MG	DA	3520	1/1	0.20	-	51,51,51,51	0
56	MG	AA	3096	1/1	0.28	-	44,44,44,44	0
56	MG	CT	3001	1/1	0.40	-	57,57,57,57	0
56	MG	BA	3397	1/1	0.19	-	28,28,28,28	0
56	MG	CA	3068	1/1	0.11	-	41,41,41,41	0
56	MG	CA	3061	1/1	0.26	-	46,46,46,46	0
56	MG	BB	3005	1/1	0.27	-	61,61,61,61	0
56	MG	DA	3147	1/1	0.13	-	53,53,53,53	0
56	MG	DA	3029	1/1	0.13	-	61,61,61,61	0
56	MG	DA	3609	1/1	0.34	-	64,64,64,64	0
56	MG	BA	3725	1/1	0.11	-	49,49,49,49	0
56	MG	BA	3612	1/1	0.13	-	37,37,37,37	0
56	MG	BA	3480	1/1	0.20	-	17,17,17,17	0
56	MG	BA	3368	1/1	0.20	-	35,35,35,35	0
56	MG	BA	3258	1/1	0.23	-	40,40,40,40	0
56	MG	BA	3378	1/1	0.12	-	20,20,20,20	0
56	MG	CX	104	1/1	0.12	-	40,40,40,40	0
56	MG	AA	3007	1/1	0.16	-	82,82,82,82	0
56	MG	BB	3015	1/1	0.11	-	37,37,37,37	0
56	MG	BA	3320	1/1	0.28	-	57,57,57,57	0
56	MG	DA	3602	1/1	0.18	-	52,52,52,52	0
56	MG	AA	3127	1/1	0.17	-	62,62,62,62	0
56	MG	BA	3414	1/1	0.21	-	19,19,19,19	0
56	MG	CA	3118	1/1	0.09	-	37,37,37,37	0
56	MG	DA	3395	1/1	0.22	-	34,34,34,34	0
56	MG	DA	3157	1/1	1.06	-	62,62,62,62	0
56	MG	AA	3113	1/1	0.34	-	68,68,68,68	0
56	MG	BA	3649	1/1	0.20	-	66,66,66,66	0
56	MG	DA	3251	1/1	0.12	-	54,54,54,54	0
56	MG	BA	3148	1/1	0.32	-	52,52,52,52	0
58	ZN	B5	501	1/1	0.10	-	54,54,54,54	0
56	MG	B9	502	1/1	0.25	-	49,49,49,49	0
56	MG	AA	3114	1/1	0.49	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3154	1/1	0.16	-	61,61,61,61	0
56	MG	BA	3221	1/1	0.29	-	44,44,44,44	0
56	MG	BA	3588	1/1	0.21	-	48,48,48,48	0
56	MG	DA	3471	1/1	0.12	-	37,37,37,37	0
56	MG	BA	3094	1/1	0.85	-	61,61,61,61	0
56	MG	BA	3057	1/1	0.28	-	35,35,35,35	0
56	MG	BA	3085	1/1	0.49	-	48,48,48,48	0
56	MG	BA	3176	1/1	0.18	-	38,38,38,38	0
56	MG	DA	3087	1/1	0.18	-	49,49,49,49	0
56	MG	CA	3130	1/1	0.08	-	65,65,65,65	0
56	MG	BA	3589	1/1	0.15	-	51,51,51,51	0
56	MG	BA	3377	1/1	0.12	-	32,32,32,32	0
56	MG	B3	102	1/1	0.13	-	59,59,59,59	0
56	MG	BA	3168	1/1	0.27	-	42,42,42,42	0
56	MG	DA	3085	1/1	0.13	-	36,36,36,36	0
56	MG	AA	3141	1/1	0.21	-	48,48,48,48	0
56	MG	DA	3138	1/1	0.20	-	42,42,42,42	0
56	MG	BA	3383	1/1	0.17	-	38,38,38,38	0
56	MG	DA	3341	1/1	0.19	-	23,23,23,23	0
56	MG	BA	3182	1/1	0.29	-	51,51,51,51	0
56	MG	BA	3665	1/1	0.20	-	39,39,39,39	0
56	MG	DA	3335	1/1	0.27	-	38,38,38,38	0
56	MG	AA	3193	1/1	0.12	-	60,60,60,60	0
56	MG	BA	3021	1/1	0.25	-	42,42,42,42	0
56	MG	BA	3502	1/1	0.23	-	43,43,43,43	0
56	MG	DA	3305	1/1	0.10	-	33,33,33,33	0
56	MG	BA	3542	1/1	0.22	-	19,19,19,19	0
56	MG	DA	3429	1/1	0.19	-	44,44,44,44	0
56	MG	AA	3095	1/1	0.24	-	58,58,58,58	0
56	MG	DA	3344	1/1	0.10	-	26,26,26,26	0
56	MG	CA	3058	1/1	0.09	-	40,40,40,40	0
56	MG	DA	3642	1/1	0.12	-	35,35,35,35	0
56	MG	DA	3440	1/1	0.28	-	33,33,33,33	0
56	MG	BA	3188	1/1	0.15	-	37,37,37,37	0
56	MG	DA	3431	1/1	0.11	-	41,41,41,41	0
56	MG	CA	3053	1/1	1.40	-	73,73,73,73	0
56	MG	BA	3689	1/1	0.23	-	39,39,39,39	0
56	MG	CA	3116	1/1	0.21	-	76,76,76,76	0
56	MG	AA	3116	1/1	0.56	-	52,52,52,52	0
56	MG	DA	3306	1/1	0.18	-	33,33,33,33	0
56	MG	AA	3120	1/1	0.67	-	71,71,71,71	0
56	MG	BA	3720	1/1	0.19	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DD	306	1/1	1.12	-	44,44,44,44	0
56	MG	BA	3523	1/1	0.14	-	48,48,48,48	0
56	MG	AA	3008	1/1	0.34	-	54,54,54,54	0
56	MG	AA	3033	1/1	0.37	-	64,64,64,64	0
56	MG	BA	3641	1/1	0.11	-	45,45,45,45	0
56	MG	BA	3591	1/1	0.38	-	48,48,48,48	0
56	MG	DA	3010	1/1	0.16	-	39,39,39,39	0
56	MG	CA	3008	1/1	0.75	-	53,53,53,53	0
56	MG	BA	3005	1/1	0.17	-	36,36,36,36	0
56	MG	DA	3117	1/1	0.18	-	53,53,53,53	0
56	MG	DA	3053	1/1	0.17	-	42,42,42,42	0
56	MG	DA	3542	1/1	0.18	-	32,32,32,32	0
56	MG	CA	3083	1/1	0.09	-	39,39,39,39	0
56	MG	DA	3268	1/1	0.15	-	40,40,40,40	0
56	MG	BA	3369	1/1	0.21	-	45,45,45,45	0
56	MG	BA	3007	1/1	0.21	-	35,35,35,35	0
56	MG	BA	3659	1/1	0.18	-	46,46,46,46	0
56	MG	AF	3001	1/1	0.16	-	61,61,61,61	0
56	MG	AA	3159	1/1	0.29	-	57,57,57,57	0
56	MG	DA	3289	1/1	0.13	-	26,26,26,26	0
56	MG	DA	3583	1/1	0.20	-	48,48,48,48	0
56	MG	DA	3491	1/1	0.16	-	56,56,56,56	0
56	MG	DA	3597	1/1	0.21	-	47,47,47,47	0
56	MG	DA	3512	1/1	0.24	-	61,61,61,61	0
56	MG	BU	201	1/1	0.71	-	39,39,39,39	0
56	MG	BW	201	1/1	0.77	-	53,53,53,53	0
56	MG	CA	3046	1/1	0.33	-	53,53,53,53	0
56	MG	BX	3001	1/1	0.32	-	55,55,55,55	0
60	K	BA	3300	1/1	0.31	-	100,100,100,100	0
56	MG	DB	3006	1/1	0.15	-	42,42,42,42	0
56	MG	BA	3706	1/1	0.44	-	63,63,63,63	0
56	MG	DA	3195	1/1	0.10	-	50,50,50,50	0
56	MG	DA	3562	1/1	0.10	-	61,61,61,61	0
56	MG	BA	3640	1/1	0.20	-	60,60,60,60	0
56	MG	BB	3008	1/1	0.22	-	35,35,35,35	0
56	MG	CA	3137	1/1	0.14	-	48,48,48,48	0
56	MG	DA	3241	1/1	0.21	-	15,15,15,15	0
56	MG	CA	3079	1/1	0.14	-	48,48,48,48	0
56	MG	DA	3035	1/1	0.18	-	56,56,56,56	0
56	MG	AA	3213	1/1	0.17	-	29,29,29,29	0
56	MG	DA	3088	1/1	0.14	-	46,46,46,46	0
56	MG	DA	3300	1/1	0.15	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3174	1/1	0.24	-	41,41,41,41	0
56	MG	BA	3682	1/1	0.16	-	38,38,38,38	0
56	MG	DA	3180	1/1	0.18	-	46,46,46,46	0
56	MG	DA	3418	1/1	0.17	-	29,29,29,29	0
56	MG	BA	3109	1/1	0.08	-	36,36,36,36	0
56	MG	B0	103	1/1	0.84	-	59,59,59,59	0
56	MG	DA	3410	1/1	0.23	-	69,69,69,69	0
56	MG	DA	3360	1/1	0.23	-	41,41,41,41	0
56	MG	BA	3099	1/1	0.19	-	44,44,44,44	0
56	MG	DA	3074	1/1	0.18	-	54,54,54,54	0
56	MG	DE	304	1/1	0.20	-	41,41,41,41	0
56	MG	BA	3611	1/1	0.26	-	52,52,52,52	0
56	MG	DA	3545	1/1	0.59	-	75,75,75,75	0
56	MG	DA	3461	1/1	0.22	-	41,41,41,41	0
56	MG	DA	3198	1/1	0.28	-	48,48,48,48	0
56	MG	DA	3527	1/1	0.09	-	46,46,46,46	0
56	MG	DA	3437	1/1	0.14	-	49,49,49,49	0
56	MG	BE	303	1/1	0.15	-	29,29,29,29	0
56	MG	DR	202	1/1	0.16	-	37,37,37,37	0
56	MG	BA	3453	1/1	0.19	-	18,18,18,18	0
56	MG	DD	303	1/1	0.20	-	19,19,19,19	0
56	MG	AA	3111	1/1	0.18	-	95,95,95,95	0
56	MG	BA	3389	1/1	0.12	-	48,48,48,48	0
56	MG	BA	3722	1/1	0.17	-	32,32,32,32	0
56	MG	CA	3056	1/1	0.12	-	64,64,64,64	0
56	MG	DA	3506	1/1	0.06	-	59,59,59,59	0
56	MG	CA	3168	1/1	0.36	-	77,77,77,77	0
56	MG	DA	3154	1/1	0.62	-	45,45,45,45	0
56	MG	BA	3200	1/1	0.26	-	25,25,25,25	0
56	MG	BA	3554	1/1	0.19	-	31,31,31,31	0
56	MG	BA	3269	1/1	0.63	-	34,34,34,34	0
56	MG	BA	3169	1/1	0.56	-	46,46,46,46	0
56	MG	BA	3224	1/1	0.74	-	64,64,64,64	0
56	MG	BA	3415	1/1	0.23	-	27,27,27,27	0
56	MG	DA	3333	1/1	0.25	-	58,58,58,58	0
56	MG	DA	3253	1/1	0.17	-	42,42,42,42	0
56	MG	BF	305	1/1	0.34	-	35,35,35,35	0
56	MG	DA	3624	1/1	0.34	-	51,51,51,51	0
56	MG	DA	3155	1/1	0.17	-	50,50,50,50	0
56	MG	BA	3256	1/1	0.20	-	58,58,58,58	0
56	MG	AA	3183	1/1	0.09	-	42,42,42,42	0
56	MG	DA	3618	1/1	0.09	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3497	1/1	0.13	-	62,62,62,62	0
56	MG	DA	3560	1/1	0.12	-	34,34,34,34	0
56	MG	BA	3024	1/1	0.41	-	35,35,35,35	0
56	MG	BA	3467	1/1	0.05	-	40,40,40,40	0
56	MG	BA	3707	1/1	0.20	-	36,36,36,36	0
56	MG	DA	3639	1/1	0.29	-	15,15,15,15	0
56	MG	DA	3513	1/1	0.21	-	49,49,49,49	0
56	MG	DA	3163	1/1	0.18	-	39,39,39,39	0
56	MG	BA	3370	1/1	0.20	-	54,54,54,54	0
56	MG	BA	3614	1/1	0.41	-	30,30,30,30	0
56	MG	BA	3593	1/1	0.14	-	74,74,74,74	0
56	MG	B0	104	1/1	0.11	-	43,43,43,43	0
56	MG	BA	3315	1/1	0.10	-	37,37,37,37	0
56	MG	BB	3018	1/1	0.18	-	60,60,60,60	0
56	MG	DA	3389	1/1	0.25	-	27,27,27,27	0
56	MG	BA	3632	1/1	0.25	-	57,57,57,57	0
56	MG	BA	3704	1/1	0.17	-	85,85,85,85	0
56	MG	DA	3005	1/1	0.22	-	42,42,42,42	0
56	MG	CA	3171	1/1	0.31	-	67,67,67,67	0
56	MG	BG	3001	1/1	0.15	-	64,64,64,64	0
56	MG	BR	201	1/1	0.54	-	51,51,51,51	0
56	MG	DA	3375	1/1	0.15	-	60,60,60,60	0
56	MG	BA	3543	1/1	0.30	-	52,52,52,52	0
56	MG	AA	3166	1/1	0.17	-	48,48,48,48	0
56	MG	CA	3122	1/1	0.05	-	47,47,47,47	0
56	MG	BA	3131	1/1	0.77	-	54,54,54,54	0
56	MG	DR	201	1/1	0.56	-	65,65,65,65	0
56	MG	B3	103	1/1	0.59	-	41,41,41,41	0
56	MG	BA	3276	1/1	0.28	-	40,40,40,40	0
56	MG	AA	3207	1/1	0.28	-	45,45,45,45	0
56	MG	DA	3034	1/1	0.15	-	40,40,40,40	0
56	MG	BA	3346	1/1	0.22	-	37,37,37,37	0
56	MG	BU	206	1/1	0.38	-	60,60,60,60	0
56	MG	DA	3278	1/1	0.19	-	47,47,47,47	0
56	MG	DA	3462	1/1	0.10	-	55,55,55,55	0
56	MG	BA	3678	1/1	0.16	-	53,53,53,53	0
56	MG	CQ	201	1/1	0.18	-	56,56,56,56	0
56	MG	CA	3001	1/1	0.13	-	55,55,55,55	0
56	MG	AA	3065	1/1	0.27	-	60,60,60,60	0
56	MG	BA	3695	1/1	0.16	-	15,15,15,15	0
56	MG	BA	3601	1/1	0.29	-	64,64,64,64	0
56	MG	DA	3509	1/1	0.18	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3577	1/1	0.24	-	44,44,44,44	0
56	MG	BA	3473	1/1	0.12	-	51,51,51,51	0
56	MG	AA	3129	1/1	0.31	-	77,77,77,77	0
56	MG	DA	3263	1/1	0.18	-	31,31,31,31	0
56	MG	DA	3552	1/1	0.12	-	34,34,34,34	0
56	MG	DA	3633	1/1	0.20	-	54,54,54,54	0
56	MG	BA	3646	1/1	0.24	-	52,52,52,52	0
56	MG	BA	3025	1/1	0.23	-	28,28,28,28	0
56	MG	CA	3030	1/1	0.48	-	73,73,73,73	0
56	MG	DA	3067	1/1	0.52	-	43,43,43,43	0
56	MG	DA	3585	1/1	0.15	-	62,62,62,62	0
56	MG	DA	3425	1/1	0.10	-	27,27,27,27	0
56	MG	DA	3492	1/1	0.35	-	68,68,68,68	0
56	MG	DA	3518	1/1	0.16	-	40,40,40,40	0
56	MG	CA	3139	1/1	0.29	-	75,75,75,75	0
56	MG	BA	3696	1/1	0.25	-	39,39,39,39	0
56	MG	DA	3130	1/1	0.14	-	32,32,32,32	0
56	MG	DB	3005	1/1	0.24	-	43,43,43,43	0
56	MG	DA	3434	1/1	0.26	-	49,49,49,49	0
56	MG	DA	3565	1/1	0.09	-	57,57,57,57	0
56	MG	BA	3164	1/1	0.74	-	56,56,56,56	0
56	MG	BA	3239	1/1	0.09	-	33,33,33,33	0
56	MG	BA	3314	1/1	0.17	-	24,24,24,24	0
56	MG	CA	3092	1/1	0.12	-	47,47,47,47	0
56	MG	CA	3117	1/1	0.12	-	68,68,68,68	0
56	MG	BA	3657	1/1	0.16	-	56,56,56,56	0
56	MG	BA	3429	1/1	0.13	-	20,20,20,20	0
56	MG	BA	3059	1/1	0.61	-	45,45,45,45	0
56	MG	BA	3504	1/1	0.28	-	41,41,41,41	0
56	MG	BA	3431	1/1	0.22	-	17,17,17,17	0
56	MG	AA	3109	1/1	0.35	-	65,65,65,65	0
56	MG	AA	3059	1/1	1.09	-	54,54,54,54	0
56	MG	BA	3033	1/1	0.40	-	35,35,35,35	0
56	MG	AA	3140	1/1	0.12	-	70,70,70,70	0
56	MG	DA	3328	1/1	0.15	-	28,28,28,28	0
56	MG	BA	3052	1/1	0.25	-	29,29,29,29	0
56	MG	BA	3469	1/1	0.09	-	38,38,38,38	0
56	MG	CA	3157	1/1	0.13	-	54,54,54,54	0
56	MG	BA	3089	1/1	0.44	-	61,61,61,61	0
56	MG	DA	3320	1/1	0.18	-	30,30,30,30	0
56	MG	BV	201	1/1	0.38	-	53,53,53,53	0
56	MG	CA	3065	1/1	0.23	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BP	201	1/1	0.69	-	40,40,40,40	0
56	MG	DA	3645	1/1	0.09	-	30,30,30,30	0
56	MG	BA	3023	1/1	0.14	-	66,66,66,66	0
56	MG	BA	3376	1/1	0.07	-	48,48,48,48	0
56	MG	DA	3402	1/1	0.09	-	61,61,61,61	0
56	MG	BA	3206	1/1	0.34	-	57,57,57,57	0
56	MG	CA	3036	1/1	0.65	-	68,68,68,68	0
56	MG	DA	3076	1/1	0.53	-	44,44,44,44	0
56	MG	DA	3073	1/1	0.16	-	44,44,44,44	0
56	MG	BA	3674	1/1	0.16	-	55,55,55,55	0
56	MG	DA	3388	1/1	0.15	-	54,54,54,54	0
56	MG	DA	3021	1/1	0.14	-	35,35,35,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.