



# wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 10:05 PM BST

PDB ID : 4V9R  
Title : Crystal structure of antibiotic DITYROMYCIN bound to 70S ribosome  
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Deposited on : 2013-12-05  
Resolution : 3.00 Å(reported)

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

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

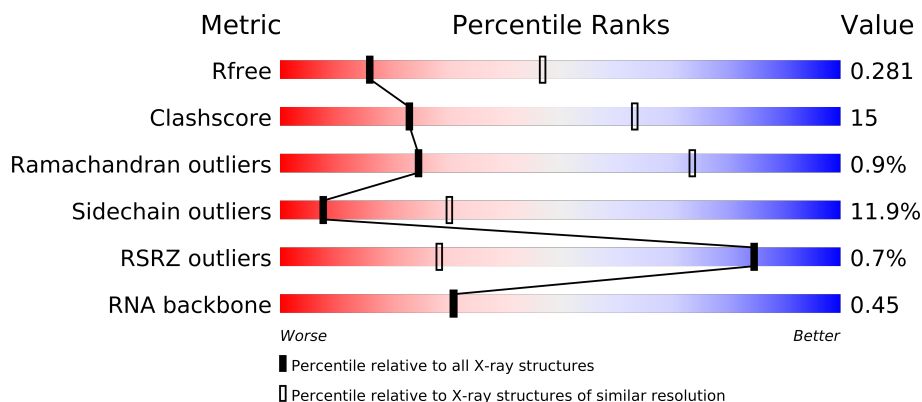
MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable23397  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline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



# 1 Overall quality at a glance

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

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  $\geq 3$ , 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 Dityromycin.

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

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

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

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

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

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

- Molecule 27 is a protein called 50S Ribosomal Protein L2.

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

- Molecule 28 is a protein called 50S Ribosomal Protein L3.

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

- Molecule 29 is a protein called 50S Ribosomal Protein L4.

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

- Molecule 30 is a protein called 50S Ribosomal Protein L5.

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

- Molecule 31 is a protein called 50S Ribosomal Protein L6.

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



- Molecule 32 is a protein called 50S Ribosomal Protein L9.

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

- Molecule 33 is a protein called 50S Ribosomal Protein L13.

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

- Molecule 34 is a protein called 50S Ribosomal Protein L14.

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

- Molecule 35 is a protein called 50S Ribosomal Protein L15.

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

- Molecule 36 is a protein called 50S Ribosomal Protein L16.

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

- Molecule 37 is a protein called 50S Ribosomal Protein L17.



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

- Molecule 38 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BS	110	Total	C	N	O	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	BA	739	Total	Mg	0	0
			739	739		
56	AK	1	Total	Mg	0	0
			1	1		
56	DQ	4	Total	Mg	0	0
			4	4		
56	D3	1	Total	Mg	0	0
			1	1		
56	DF	5	Total	Mg	0	0
			5	5		
56	B8	2	Total	Mg	0	0
			2	2		
56	BE	9	Total	Mg	0	0
			9	9		
56	DU	2	Total	Mg	0	0
			2	2		
56	B1	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AN	1	Total 1	Mg 1	0	0
56	BP	4	Total 4	Mg 4	0	0
56	AX	9	Total 9	Mg 9	0	0
56	CN	1	Total 1	Mg 1	0	0
56	DN	1	Total 1	Mg 1	0	0
56	AS	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	CF	1	Total 1	Mg 1	0	0
56	B9	1	Total 1	Mg 1	0	0
56	BF	6	Total 6	Mg 6	0	0
56	AV	1	Total 1	Mg 1	0	0
56	BX	2	Total 2	Mg 2	0	0
56	B2	1	Total 1	Mg 1	0	0
56	AA	222	Total 222	Mg 222	0	0
56	BQ	4	Total 4	Mg 4	0	0
56	CX	3	Total 3	Mg 3	0	0
56	DV	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AM	2	Total 2	Mg 2	0	0
56	BU	9	Total 9	Mg 9	0	0
56	DR	1	Total 1	Mg 1	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	BG	4	Total 4	Mg 4	0	0
56	DE	6	Total 6	Mg 6	0	0
56	B3	3	Total 3	Mg 3	0	0
56	BR	3	Total 3	Mg 3	0	0
56	DA	657	Total 657	Mg 657	0	0
56	DP	2	Total 2	Mg 2	0	0
56	DW	2	Total 2	Mg 2	0	0
56	B7	4	Total 4	Mg 4	0	0
56	AL	1	Total 1	Mg 1	0	0
56	BV	3	Total 3	Mg 3	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

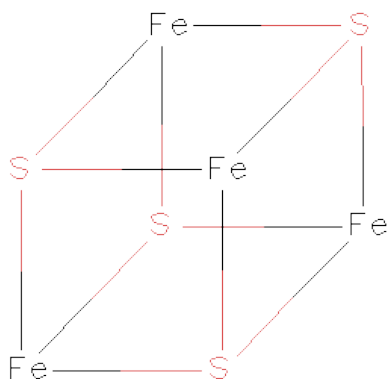
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BD	12	Total	Mg	0	0
			12	12		
56	B0	6	Total	Mg	0	0
			6	6		
56	CE	2	Total	Mg	0	0
			2	2		
56	BW	5	Total	Mg	0	0
			5	5		
56	DD	5	Total	Mg	0	0
			5	5		
56	AF	1	Total	Mg	0	0
			1	1		
56	DB	12	Total	Mg	0	0
			12	12		

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



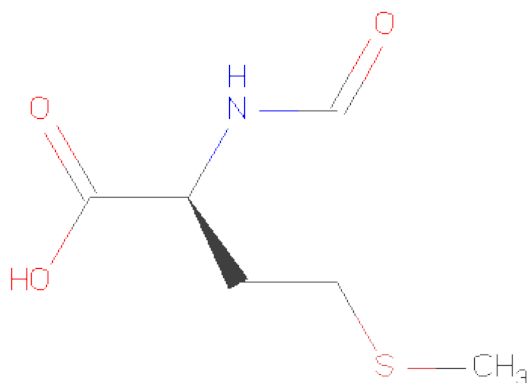
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	AD	1	Total	Fe	S	0	0
			8	4	4		
57	CD	1	Total	Fe	S	0	0
			8	4	4		

- 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		
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	147	Total	O	0	0
			147	147		
61	AD	1	Total	O	0	0
			1	1		
61	AE	2	Total	O	0	0
			2	2		
61	AJ	1	Total	O	0	0
			1	1		
61	AL	2	Total	O	0	0
			2	2		
61	AO	2	Total	O	0	0
			2	2		
61	AU	1	Total	O	0	0
			1	1		
61	AV	2	Total	O	0	0
			2	2		
61	AX	1	Total	O	0	0
			1	1		
61	BA	1086	Total	O	0	0
			1086	1086		
61	BB	26	Total	O	0	0
			26	26		
61	BD	6	Total	O	0	0
			6	6		
61	BE	13	Total	O	0	0
			13	13		
61	BF	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	BG	1	Total	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	2	Total	O	0	0
			2	2		
61	BU	5	Total	O	0	0
			5	5		
61	BV	2	Total	O	0	0
			2	2		
61	BW	4	Total	O	0	0
			4	4		
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	2	Total	O	0	0
			2	2		
61	B7	1	Total	O	0	0
			1	1		
61	B8	7	Total	O	0	0
			7	7		
61	CA	186	Total	O	0	0
			186	186		
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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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	DA	906	Total 906	O 906	0	0
61	DB	7	Total 7	O 7	0	0
61	DD	10	Total 10	O 10	0	0
61	DE	11	Total 11	O 11	0	0
61	DF	4	Total 4	O 4	0	0
61	DO	1	Total 1	O 1	0	0
61	DP	14	Total 14	O 14	0	0
61	DQ	3	Total 3	O 3	0	0
61	DR	1	Total 1	O 1	0	0
61	DU	4	Total 4	O 4	0	0
61	DV	1	Total 1	O 1	0	0
61	DX	2	Total 2	O 2	0	0
61	DY	1	Total 1	O 1	0	0
61	D0	3	Total 3	O 3	0	0
61	D1	1	Total 1	O 1	0	0
61	D3	1	Total 1	O 1	0	0
61	D7	1	Total 1	O 1	0	0
61	D8	4	Total 4	O 4	0	0





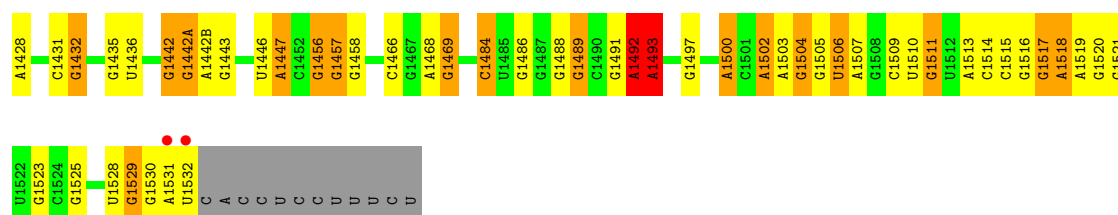






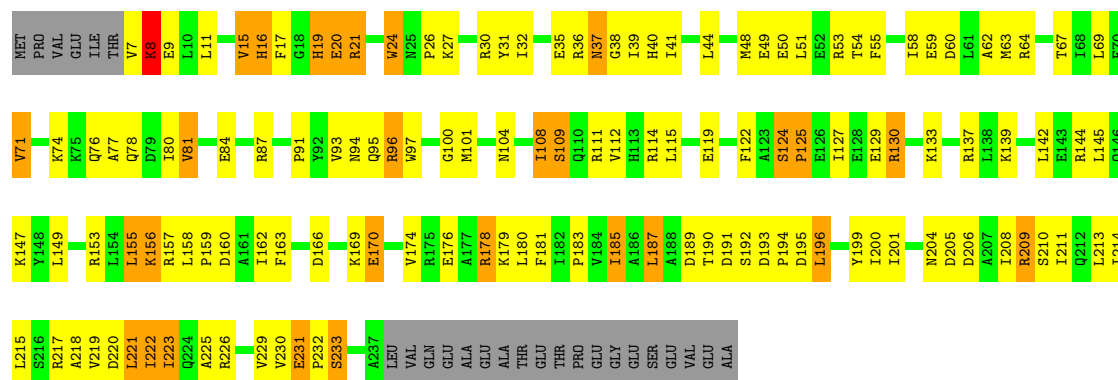
G1359	C1234	A1168	G1107	G1043	A986	U920	C840	A767	G689	C620	G546	G473	C401	A329
A1360	U1235	A1169	G1108	A1044	C990	U921	G841	A768	G690	A621	A547	G474	G402	C330
G1361	A1236	A1170	C1109	G1047	U991	G922	C848	G769	G691	A622	U552	G475	U403	G331
G1362	C1237	G1171	A1110	G1048	U992	A923	C849	C770	U692	C623	U553	G476	U404	G332
C1363	A1172	C1172	A1111	G1049	G993	G924	G850	U772	G693	C624	C554	A477	U405	G333
C1366	C1239	G1173	C1112	U1049	G993	G925	G851	U772	A694	C625	C555	C479	G406	C337
G1304	U1240	G1174	C1113	G1050	A984	G926	G852	G773	G700	U626	C556	U480	G407	C338
G1305	G1241	A1175	C1114	C1051	C995	G927	G853	G774		U627	C557		G410	C339
A1306	C1242	A1176	C1115	U1052	A996		G854	A777	A704	C628	C558		A411	U340
G1368	G1243	G1177	C1116	G1053	U997		G855			C629	C559	G484	A412	U341
G1369	C1244	G1178	G1117	C1054	G998		C856			U630	A560	G485	A413	C342
G1370	G1245	G1179	C1118	C1055	C999		G857	A780	C708		U561	U486	G414	U343
G1371	A1245	A1180	C1119	U1055	U1000		G858		G709	U633	C562	A487	A414	U344
U1372	C1246	G1181	G1120	G1057	A1001		A859	C783	G710		C563	C488	A415	A344
G1373		G1182	U1121	U1058	G1001A		A860	G784	G711	U639	A563	C489		C345
A1374	C1249	G1183	U1122		G1002		G861	G785	G712	A640	A564	C490	C418	C346
A1375	A1250	G1184	A1123	G1061	A938			G786	G713	U641	U565	C491	C419	G347
U1376	A1251	G1185	G1124	U1062	G939		A865	A787	G714	A642	G566	G492	U420	G348
A1377	A1252	G1186	U1125	C1063	C940		C866		A715	C643	G567		U421	A349
U1378	G1253	G1187	U1126	G1064	G941		C867	A790	A716		G568		C422	G350
G1379	C1254	A1188	G1127	U1065	G942		C868	G791		U646		A496	G423	G351
U1380	G1255	G1189	C1128	C1066	U943		G869	A792	C719	C647	U571	U498	G424	C352
	U1256	G1190	C1129	A1067	G944		U870	U793	C720	A648	A572	A499	G425	A353
	C1257	A1191	A1067	G1009	G944		U871	A794	G721	U649	A573		G426	G354
	G1258	C1192	A1130	G1010			C866		A722	G650		C501	U427	C355
	G1259	G1193	G1131	C1069	G1011		A872		U723	C651	G576	G502	G428	
	C1260		C1132	U1070	U1012		A873	G799	G724	U652	G577	C503	U429	U358
	A1261	U1196	G1133	C1071	C1013		C874	G800		A653	U580	C504	A430	U359
	G1262	G1197	G1134	U1072	A1014		C875	U801		G654	G581	C505	A431	
	C1263	G1198	U1135	U1073	A1015		G876	A802	G727	A655	G582	C506	A432	A364
	G1264	G1199	U1136	G1074	A1016		C877	G803	A728	G656	U583		C433	U365
	C1265	U1200	C1137	C1075	G1017		G878	U804	A729	G657	A509		U434	C366
	G1266	A1201	G1138	C1076	C1018		C879	C905	G730		A583		C435	U367
	C1267	G1202	C1139	U1077	C1019		C880	C906	G731	G658	A584		C436	
	A1268	G1203	C1140	G1077	U1020		G881		C732	U659	G585		U437	C372
	C1270	A1204	C1141	G1081	U1021			C911	A733	U660	C586		U438	A373
	G1271	U1205	G1142	U1082	G1022		G885	C912	G734	G661		C513	A439	
	C1272	G1206	G1143	U1083	G1023			U813	C735	G662	C589		A441	G376
	G1273	G1207	G1144	G1084	G1024		G890	A814	C736	A663	C590		C442	G377
	C1274	C1208	C1145	U1085	U1025			A815	A737	G664	U591		C443	
		C1209	A1146	U1086	G1026		C893	A816	C738	A665	G592		C444	G380
		G1210	C1147	G1087	C1027		G894	C917	C739	G666			C445	C381
		U1211	U1148	G1088	C1028			G818	U740	G667	C596		G446	A382
		U1212	C1149	U1089	G1029		C897	A819	G741		G597		G447	A383
	A1213	U1212	U1150	U1090	C1030			U820	G742	G671	U598		A448	G384
		G1216	A1151	U1091	G1030A		A900	G821		U672	C599		C449	
	C1217	G1217	A1152	A1092	C1030B		A901	C926	C745	G673	C600		U451	U387
	G1218	C1218	C1153	A1093	G1030C		G902	U827	G749	A675	A602		A452	G388
	C1219	U1219	G1154	U1095	A1030D		G906	A828		A676	A532		A453	A389
	U1220	G1220	G1155	C1096	G1031			G829	G752	U677	A533		A454	C390
	A1285	G1221	U1156	C1097	G1032		A909	G830	A753	U678	U605		C453	G391
	C1286	G1222	C1158	C1098	G1033		C910	U831	C607	G679	C606		C456	G392
	A1287	G1223	U1159	G1099	A1035			C932	A608	C680	A537		C457	A393
	C1288	G1224	G1160	C1100	G1036		A913	U833	A609		A539		C458	G394
	U1289	G1225	C1161	A1101	C1037		G980	C834	G610	G683	G610		C459	C395
	G1290	A1225	C1162	U1102	C1038		A914	U835	G757	A684	G541		C460	G396
	C1291	C1226	G1163	G1103	C1039		A915	G836	A759	G685	G542		C461	A397
	U1292	A1227	G1164	U1104	G1040		G917	G837	G760	U686	G616		C470	C398
	G1293	A1228	C1165	A1105	U1041		A918	G838	U687	A687	G617		G471	C399
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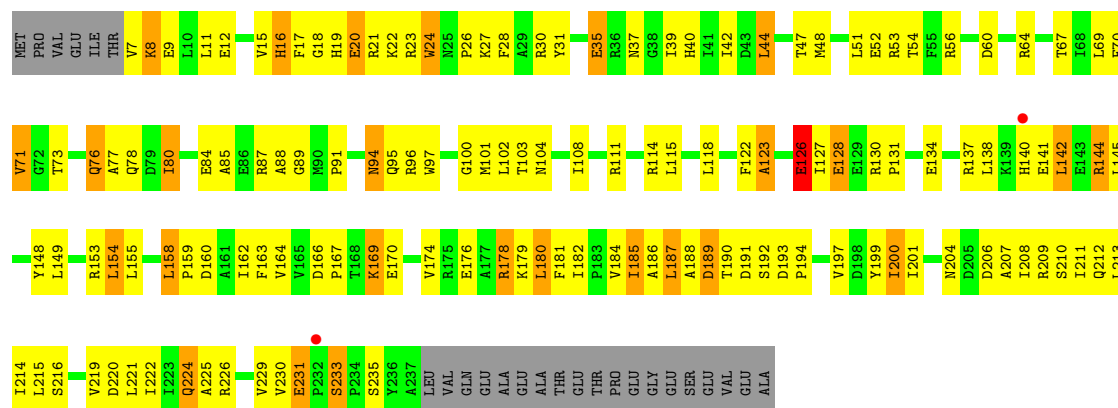
• Molecule 2: 30S Ribosomal Protein S2

Chain AB:



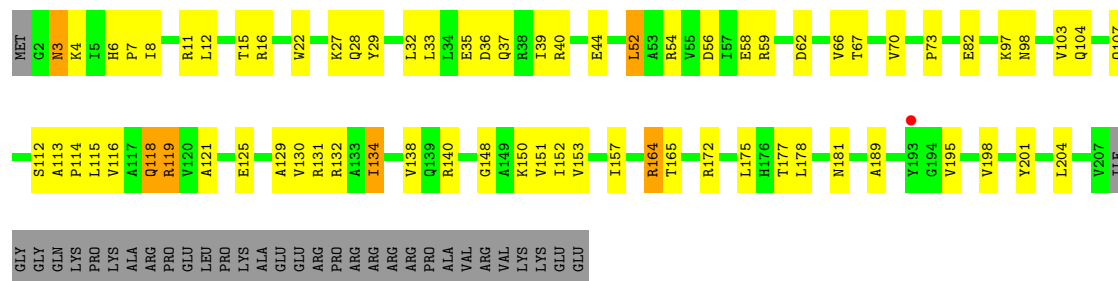
• Molecule 2: 30S Ribosomal Protein S2

Chain CB:



• Molecule 3: 30S Ribosomal Protein S3

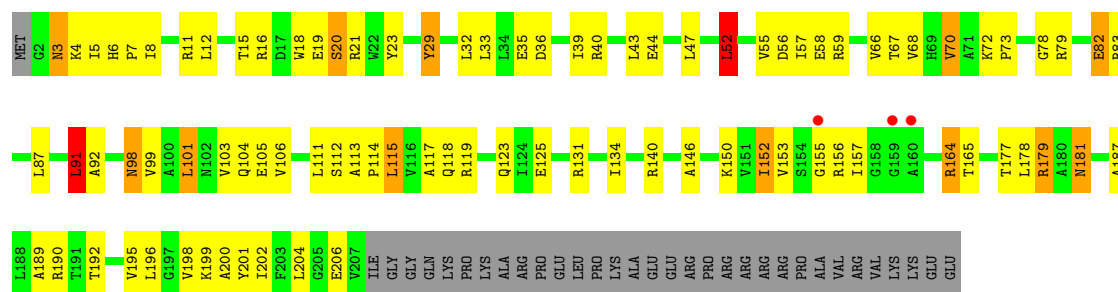
Chain AC:



• Molecule 3: 30S Ribosomal Protein S3

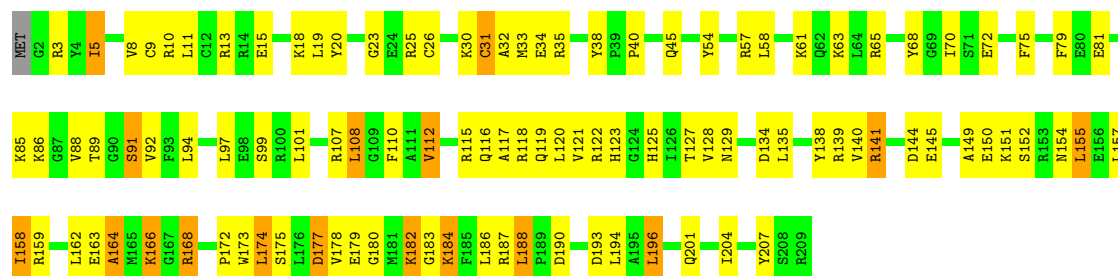


Chain CC:



- Molecule 4: 30S Ribosomal Protein S4

Chain AD:



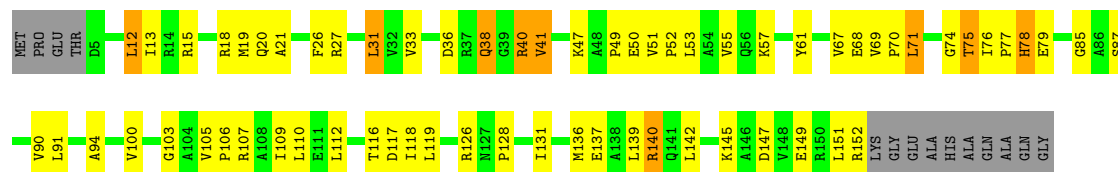
- Molecule 4: 30S Ribosomal Protein S4

Chain CD:



- Molecule 5: 30S Ribosomal Protein S5

Chain AE:



- Molecule 5: 30S Ribosomal Protein S5

Chain CE:

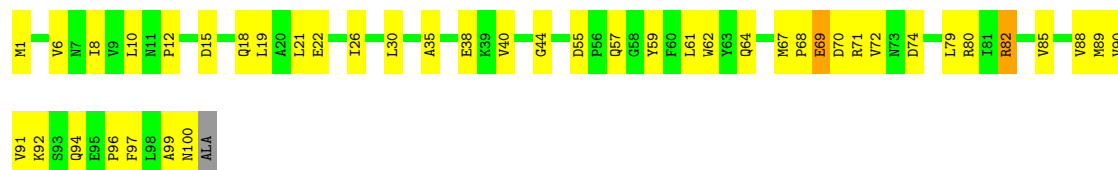






- Molecule 6: 30S Ribosomal Protein S6

Chain AF:



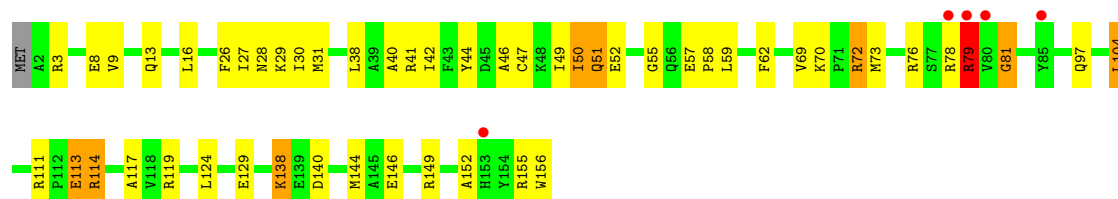
- Molecule 6: 30S Ribosomal Protein S6

Chain CF:



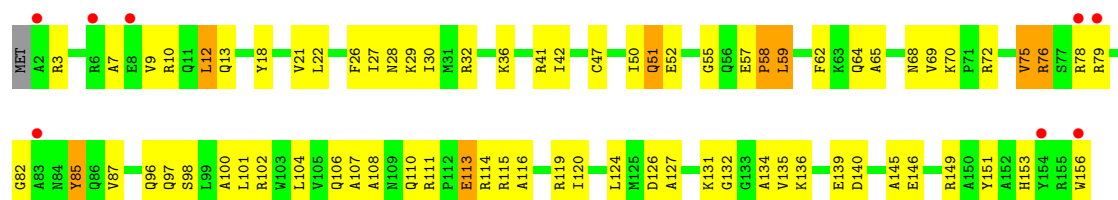
- Molecule 7: 30S Ribosomal Protein S7

Chain AG:



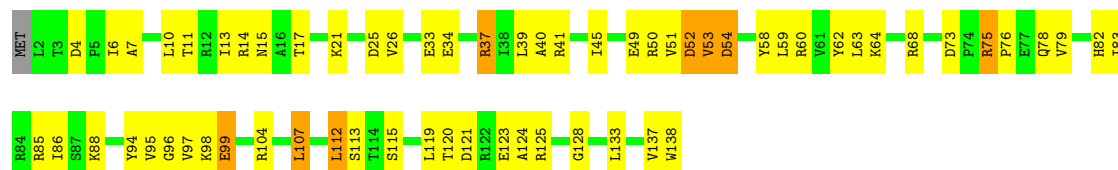
- Molecule 7: 30S Ribosomal Protein S7

Chain CG:



- Molecule 8: 30S Ribosomal Protein S8

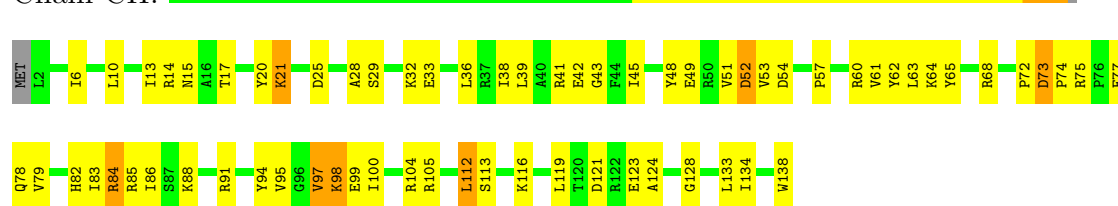
Chain AH:



- Molecule 8: 30S Ribosomal Protein S8

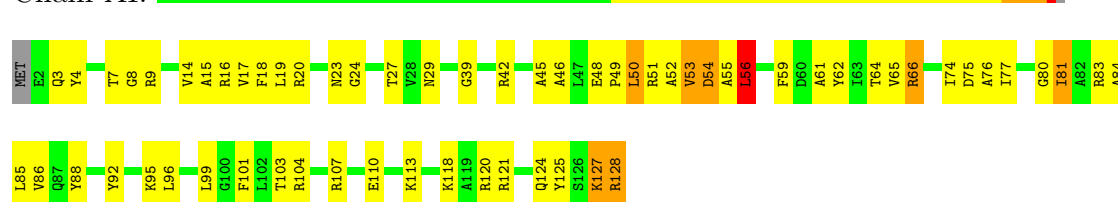


Chain CH:



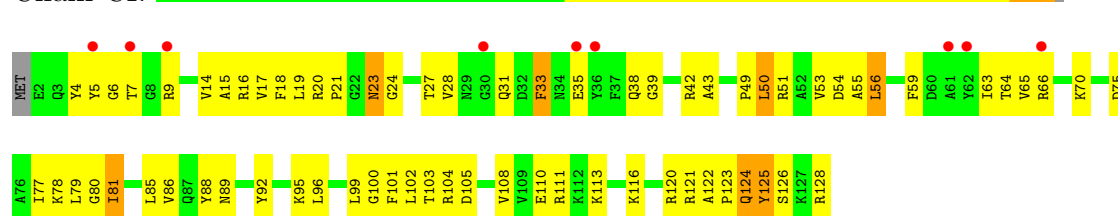
- Molecule 9: 30S Ribosomal Protein S9

Chain AI:



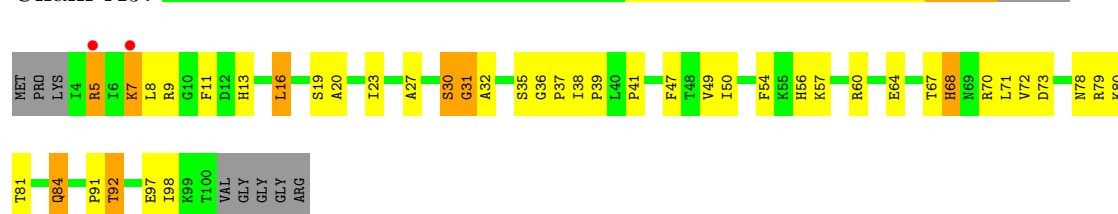
- Molecule 9: 30S Ribosomal Protein S9

Chain CI:



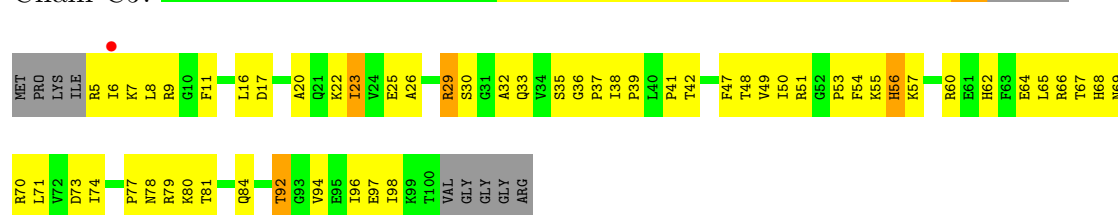
- Molecule 10: 30S Ribosomal Protein S10

Chain AJ:



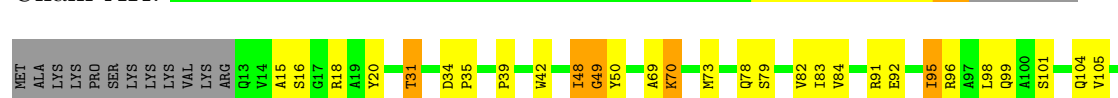
- Molecule 10: 30S Ribosomal Protein S10

Chain CJ:

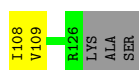


- Molecule 11: 30S Ribosomal Protein S11

Chain AK:







• Molecule 11: 30S Ribosomal Protein S11

Chain CK:



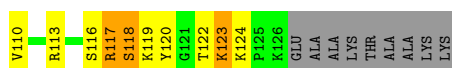
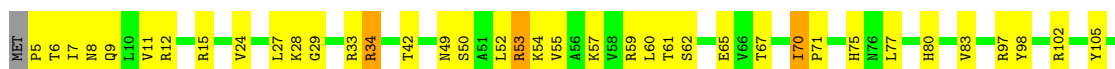
• Molecule 12: 30S Ribosomal Protein S12

Chain AL:



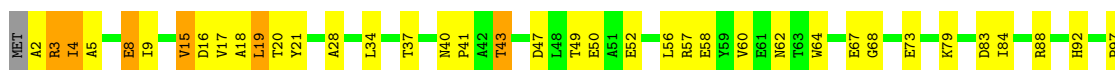
• Molecule 12: 30S Ribosomal Protein S12

Chain CL:



• Molecule 13: 30S Ribosomal Protein S13

Chain AM:



• Molecule 13: 30S Ribosomal Protein S13

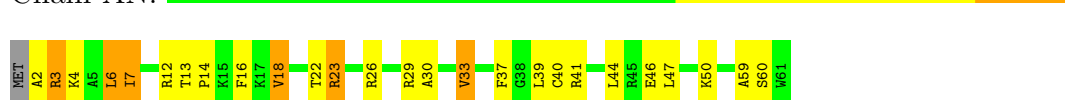
Chain CM:



• Molecule 14: 30S Ribosomal Protein S14



Chain AN:



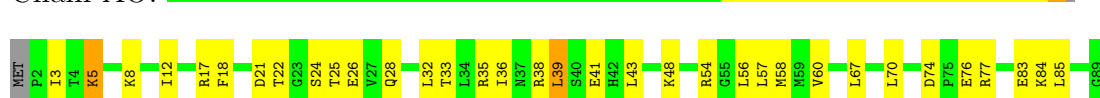
- Molecule 14: 30S Ribosomal Protein S14

Chain CN:



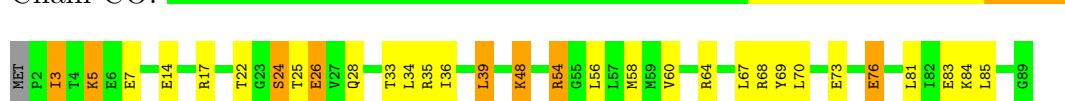
- Molecule 15: 30S Ribosomal Protein S15

Chain AO:



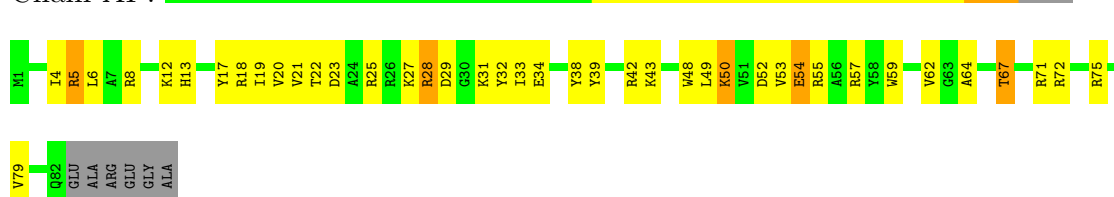
- Molecule 15: 30S Ribosomal Protein S15

Chain CO:



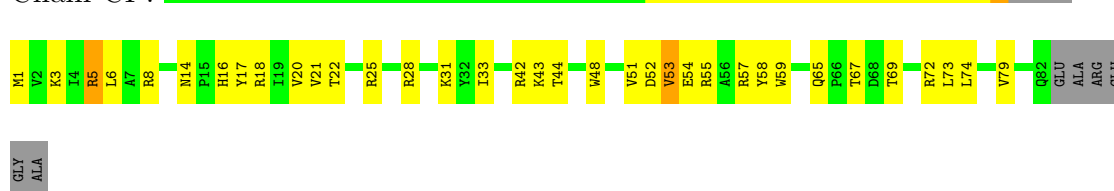
- Molecule 16: 30S Ribosomal Protein S16

Chain AP:



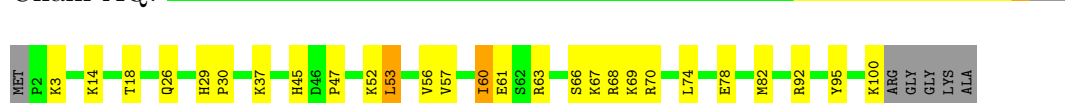
- Molecule 16: 30S Ribosomal Protein S16

Chain CP:



- Molecule 17: 30S Ribosomal Protein S17

Chain AQ:



- Molecule 17: 30S Ribosomal Protein S17

Chain CQ:



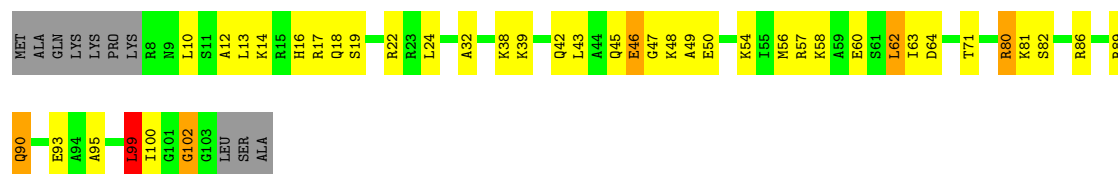






- Molecule 20: 30S Ribosomal Protein S20

Chain CT:



- Molecule 21: 30S Ribosomal Protein THX

Chain AU:



- Molecule 21: 30S Ribosomal Protein THX

Chain CU:



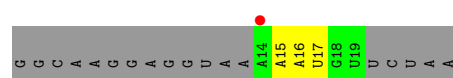
- Molecule 22: mRNA

Chain AV:



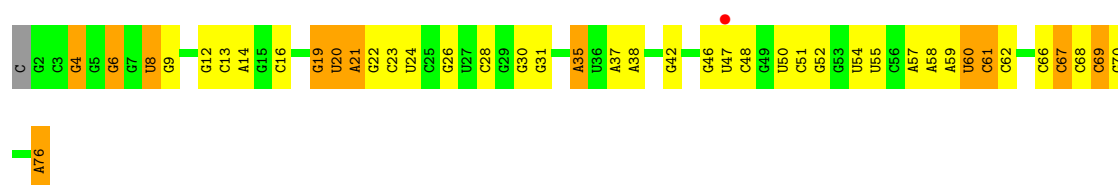
- Molecule 22: mRNA

Chain CV:



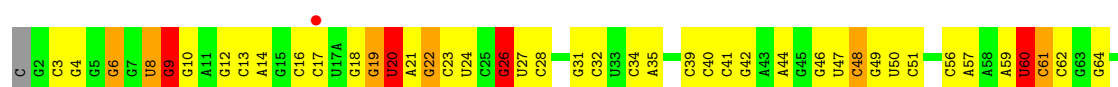
- Molecule 23: P-site tRNA

Chain AX:



- Molecule 23: P-site tRNA

Chain CX:



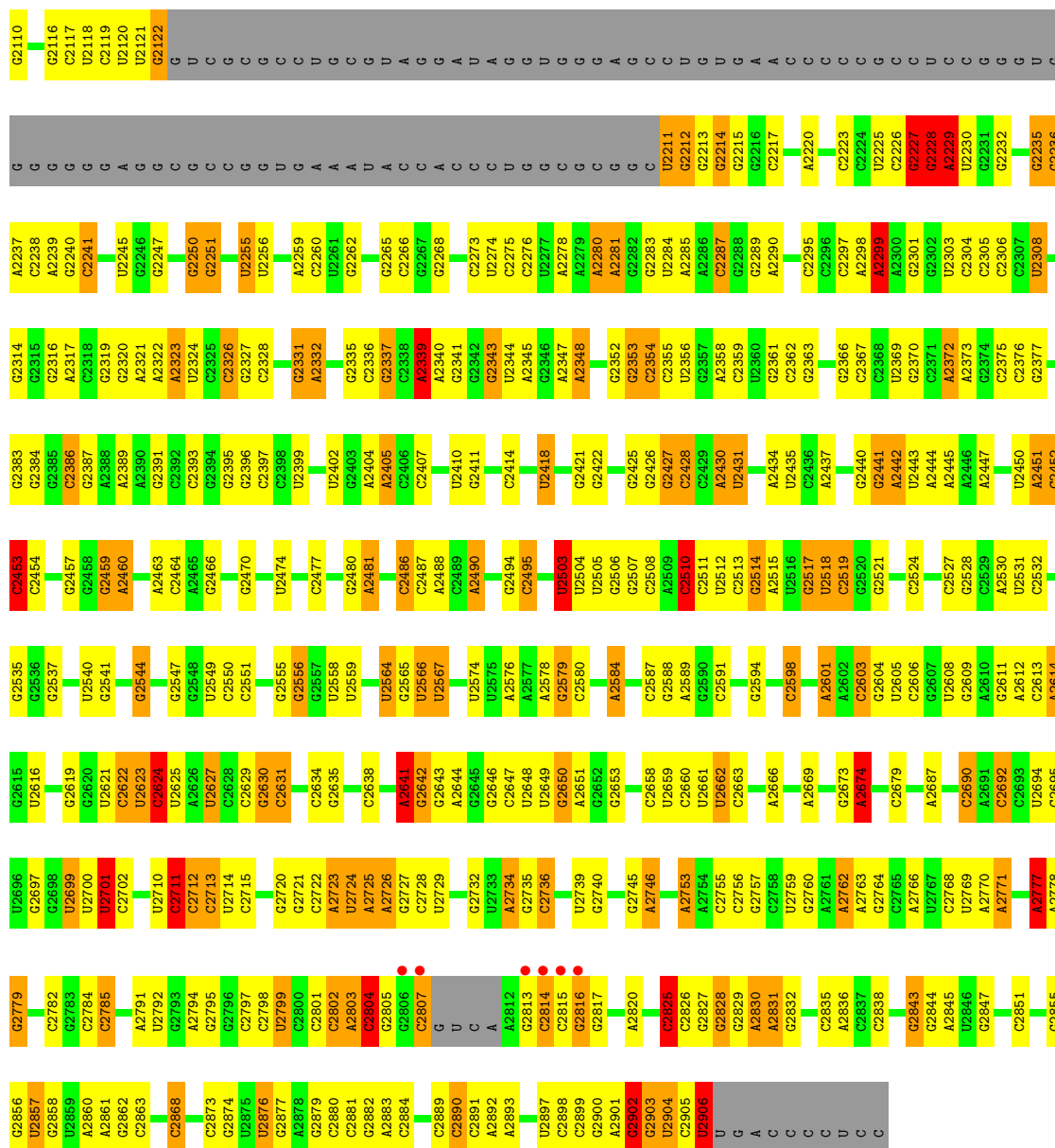






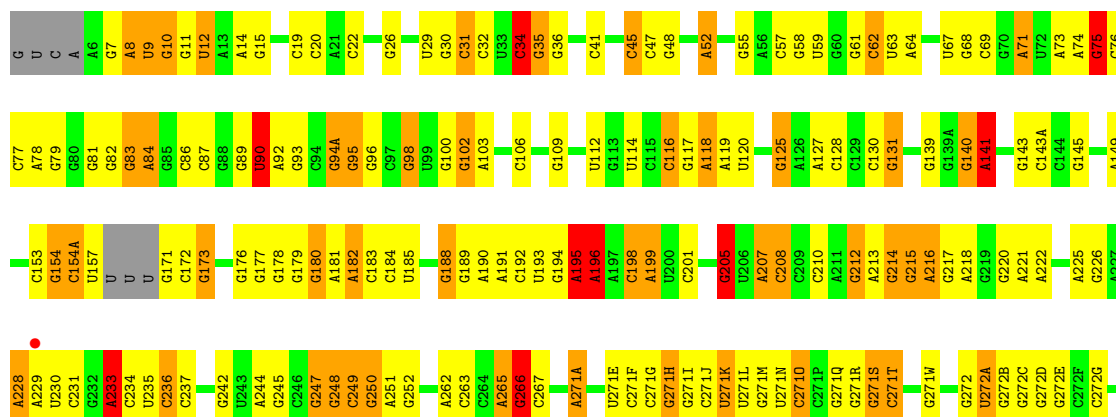
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A2036	C1936	G1857	C1787	C1702	A1613	G1530	C1452	C1361	G1263	G1182	A955
A2037	A1940	C1858	G1787	C1703	A1616	G1531	C1453	C1366	A1265	G1183	G962
U2038	A1941	G1859	A1790	G1707	A1617	A1532	C1454	C1367	G1269	G1184	C886
	C1942	A1860	A1791	G1708	A1618	G1533	U1461	A1368	C1270	C1185	C887
A2041	C1946	G1861	A1792	C1709	A1619	G1534	U1462	A1369	G1284	U1186	
A2042	A2043	G1862	C1792	C1710	A1620	U1535	C1463	G1370	G1285	U1187	G992
C2043	U2044	C1863	A1793	A1711	A1621	A1536	C1464	U1369	G1286	A1188	C893
G2045	G1951	U1864	G1794	A1712	C1624	G1537	U1465	U1370	U1286	A1189	G895
	G1952	C1865	G1795	G1713	U1625	G1538	U1466	G1371	A1287	G1190	A896
	U1953	G1867	C1796	G1714	U1626	G1539	C1467	U1372	U1288	U1188	
G2049	A1954	C1868		A1715	G1628	A1540	G1468	C1373	A1289	G1195	U982
U2050	G1955	C1869	A1804	A1716	C1629	A1541	G1469	C1376	G1290	C1199	G983
U2051	C1956	G1870	C1805	C1717	A1630	A1542	G1470	A1377	G1291	G984	C903
A2052	G1957	G1871	U1806	U1718	C1631	G1548	G1471	G1378	G1296	A1201	C904
A2053	A1958	C1872	G1807	C1719	A1632	U1549	C1472	U1378	A1202	A986	U905
G2054	A1959	U1873	U1808	U1720	A1633	C1550	C1473	A1382	C1297	G987	G906
A2055	C1960	A1878	U1809	G1721		C1551	C1474	U1386	G1298	U988	U907
		A1879	U1810	G1722	C1638	C1552	C1475	U1387	A1299	G889	A908
		G1880	A1811	A1723	C1639	C1553	C1476	U1388	G1302	A990	G909
C2058	C1964	C1881	C1812	A1724	G1640	A1554	U1477	U1389	G1306	U1071	A910
U2062	G1971	C1882	G1813	G1725		U1555	U1478	G1390	C1307	U1072	G911
U2063	U1972	C1883	A1814		G1647	A1556	U1479	C1391	U1308	A1073	
A2064		G1884	A1815	C1733		A1557	A1480		A1075	A1074	A817
C2065		A1890	A1816	C1734	C1650	A1558		C1397	G1006	U1075	U918
	U1977	A1891	C1817	U1735	C1651	A1559	C1483	U1398	G1007	G1076	
G2070	U1985	G1894	A1818	U1736	G1652	C1560	U1484	U1399	G1008	U1077	
C2071	G1986	C1895	C1819	A1737	C1653	U1561	A1485	A1405	U1009	A1078	G923
A2073	C1987	G1896	U1820	G1738	A1654	C1561	G1486	A1406	G1010	U1079	C922
C2074	A1988	C1897	C1821	U1739	A1655		G1487	G1402	A1005	A1080	
G2075	C1989	A1898	A1822	U1740	A1656	G1565	G1488	A1403	G1006	G1006	G826
A2076	G1990	U1899	G1823	C1741	C1657	U1566	G1489	G1404	U1007	G1007	G827
C2077	A1991	C1901	C1824	G1742	G1657	U1567	U1490	A1405	U1008	G1008	G828
G2078	C1992		U1825	G1743	G1658	U1568	A1491	A1406	U1009	C1009	G929
A2079	A1993	G1904	C1826	G1744	A1660	U1569		U1407	G1011	G1011	G930
A2080	C1994	G1905	U1827	A1745			G1494	G1410	G1012	C931	C931
			C1828	G1746	C1663	G1573	G1495	A1411	G1013	C932	C932
G2081	U1999	A1911	U1829	A1747	A1664	A1574	A1496	A1321	G1014	A934	
A2082	A2000	A1912	C1830	G1748	G1665	A1575	G1497	A1322	G1015	A935	
G2083	C2001	G1913	C1831	G1749		G1576		G1325	G1016	G936	
A2084		C1914	A1832	G1750	G1668	U1577	A1500	U1334	G1017	A937	
		G1915	A1833			C1578		C1385	G1018	G938	
C2087	C2004	C1916	A1834	C1755	A1679	C1579	C1506	U1418	G1019	C939	
C2088		U1835	C1835	U1756	G1680	G	A1507	A1419	G1020	C940	
G2091	A2008	G1919	C1837	C1757	C1683	U	C1511	C1421	C	U941	
G2092	U2013	U1920	G1838	G1765	U1686	C	G1512	C1422	G1024	A942	
A2093	G2014	G1921	U1839	A1767	C1687	G1582	G1513	U1423	G1025	A943	
G2094	U2015	A1922		U1768	G1688	G1585	C1514	G1243	A1026	C944	
			A1843	U1769	G1689	U1586	A1425	U1244	G	A945	
U2101	G2018	G1925	G1844	A1770	G1691	U1587	G1515	C1245	A	A946	
C2102	C2019	G1926	G1845	G1771	G1692	U1588	A1516	C1246	G	A947	
C2103	A1846	C1927	A1846	C1772	C1693	A1589	G1517	C1247	U	G1035	
A2104	A2023	G1928	G1847		G1694	U1590	A1518	A1430	U	A1036	
G2105	C2024	C1929	G1848	C1775	G1695	A1591		G1431	G	G1039	
		C1930	U1849	G1776	G1697	A1592	C1521	U1440	C	C1040	
U2108	C2028		A1850	G1777	G1698	A1593	U1522	A1441	U	U952	
G2109			U1933	G1778	A1699		U1522	U1442	A1175	U1042	





• Molecule 25: 23S Ribosomal RNA

Chain DA:



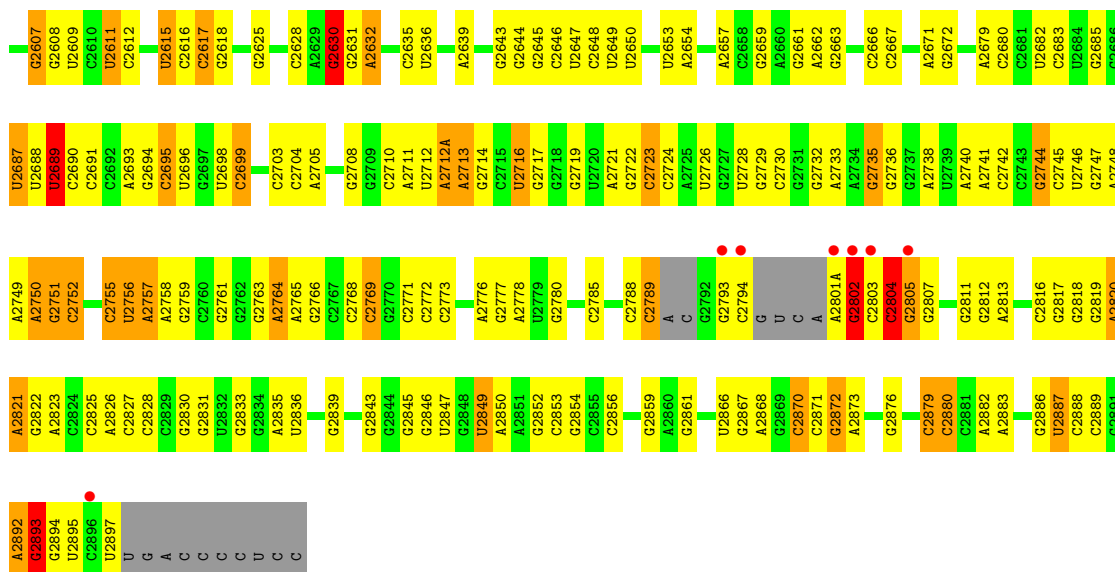


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C1320	U1249	U	A983	A917	C856	A777	U688	A643	C581	G508	C436	A345	C277
A1321	G1178	C	A984	A918	C857	A778	C692	A644	C582	C509	G437	A346	A278
G1322	C1179	G	C985	G919	U858	A782	C693	C845	G583	G512	G438	A347	C279
U1323	C1180	G	C986	G920	U859	A783	C698	C846	G584	G513	G440	G349	C280
G1324	C1181	C	G987	U922	A861	G785	C698	G547	C585	A514	G441	U350	U284
A1263	A1182	A	A990	C923	G862	G785	C698	G548	G586	G515	G442	G351	U285
U1265	G1183	C	C991	A926	A863	A788	G704	G549	U886	U519	G443	G352	C286
G1328	G1256	G	C994	G927	C864	A789	A705	A652B	C587	G520	G444	A357	C287
C1330	C1257	G	C995	G928	C865	C790	C708	G520C	U588	G521	G445	U358	C288
A1331	U1188	G	A996	G928	C867	C791	U709	C522	C589	G522	G446	A289	A289
G1332	U1189	U	G997	G932	U868	G792	G710	C523	G591	G523	A447	G290	G290
C1333	C1121	C	C998	A933	U870	A793	G710	G524	G592	U524	U448	C291	C291
U1334	G1122	G	U999	U922	A871	C795	G710	G	C595	A526	U449	U362	C292
G1335	G1123	G	U999	U922	A872	C796	G710	G	C596	G527	G450	G363	G295
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A1336	G1125	U	C1006	G938	G873	G798	G720	G	C598	A529	C455	G363B	C297
G1337	A1126	U	C1006	G938	G874	G799	G720	G	G600	A530	C456	G363C	G298
G1338	U1197	U	C1006	G938	G874	G799	G720	G	C601	A531	C456	C364	A299
C1339	U1198	G	C1007	G940	U875	A800	G723	A	G602	A532	A457	A300	A300
U1340	U1199	G	C1008	A941	C876	G801	U724	C	A603	G533	G458	G370	G301
U1341	C1201	A	A1009	G942	U877	A802	G725	G	G604	G533	U459	A371	C302
G1344	C1201	A	A1010	U943	A878	A802	G726	G	C605	A536	A460	C371	U303
C1345	A1132	G	G1011	G944	G879	G805	G726	G	C606	A537	C461	C375	G304
G1348	U1133	C	U1012	A945	C880	C906	C730	G	G607	G537	G462	C376	G307
A1349	C1135	A	C1013	U945	C881	U807	C731	G	U607	G538	G463	C376	G308
C1350	G1136	C	U1014	G947	C882	G808	G732	C	A608	G539	U464	U384	G309
C1351	U1137	C	G1015	G948	C883	G809	G733	C552T	A609	C540	G465	C385	A310
U1352	G1138	C	C1016	C949	C884	G812	A735	C552V	G610	C542	G466	G386	A310
U1353	U1139	A	G1017	C950	C885	C812	A735	C552V	U614	C542	G467	G386	A310
A1353	C1140	U	C1018	C951	C886	U913	C736	A533	U614A	C542	G468	A390	A311
C1354	U1141	C	U1019	G952	A887	C814	G737	A654	A614B	C	G469	A391	G312
G1358	U1142	U	A1020	A953	C888	C815	G738	G655	A614C	A	A471	G391	G315
A1359	A1143	U	G1022	C954	C889	C816	G739	G656	G615	G549	A472	C392	C316
C1360	A1143	U	G1022	C955	A890	C817	U740	G657	G615	G549	U475	U395	C319
A1360	G1144	U	U1023	C956	C892	G818	G741	C859	C616	G551	U478	G397	A320
C1363	A1148	A	G1024	A957	C893	A819	G742	G660	G619	G552	A479	G398	A322
G1364	U1149	A	G1025	U958	C894	A824	G743	G662	G620	G553	G480	G399	G323
A1365	C1150	G	U1026	A959	U895	C825	U747	G663	G623	G556	G481	U403	A324
U1372	G1153	A	A1027	C961	C897	C826	G748	C664	C524	U557	A482	U403	A324
G1368	G1154	U	A1028	C962	C898	U827	G748	C665	G625	G563	A483	C403	G327
G1369	U1159	G	G1030	U963	A899	U828	A752	C666	G626	C564	A484	U405	U328
C1370	U1160	C	A1031	C964	A900	A829	C753	U667	U627	C564	C485	U405	G329
G1371	G1160	G	U1033	G965	A901	G830	C754	U668	G628	U566	G489	C409	A330
U1372	C1161	U	U1034	G966	C902	G831	C755	G669	G629	A567	G489	C410	A331
U1300	G1162	A	U1035	C967	C903	C837	G760	A670	G630	U568	G491	G411	A332
A1301	U1163	U	G1036	U969	U905	C838	A761	C871	A631	U569	A492	A412	G333
C1305	G1164	U	C1037	C970	G906	U839	U762	G674	A632	U569	A493	C413	C334
G1309	U1165	A	C1038	C971	U907	C940	G763	C578	A633	A570	G494	C414	C335
U1340	C1166	G	G972	G972	C908	A947	A764	C579	C635	A572	G500	A415	G338
A1241	U1167	C	A973	A909	A910	U847	G765	C579	G636	C574	G500	C416	U339
U1240	G1168	U	C1040	G974	A911	A849	G770	G680	A637	A575	A503	A422	A340
A1242	U1169	C	G1042	C975	C912	A849	G770	G680	U639	U576	U504	A422	A340
G1243	G1170	C	C1043	G975A	U913	G852	U773	C583	G638	U576	A505	A422	G342
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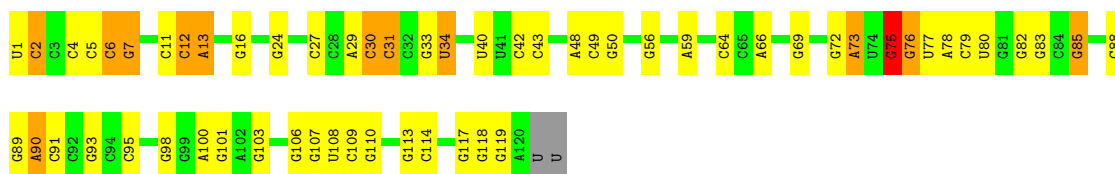
WORLDWIDE  
**PDB**  
PROTEIN DATA BANK





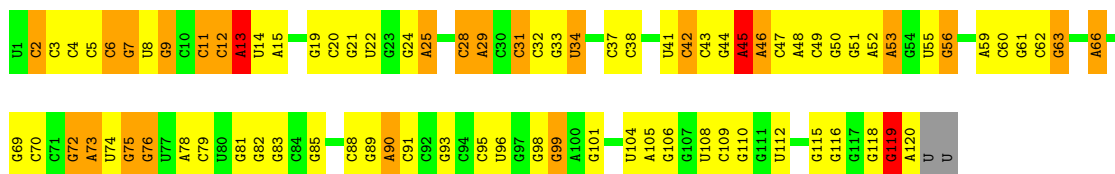
• Molecule 26: 5S Ribosomal RNA

Chain BB:



• Molecule 26: 5S Ribosomal RNA

Chain DB:



• Molecule 27: 50S Ribosomal Protein L2

Chain BD:

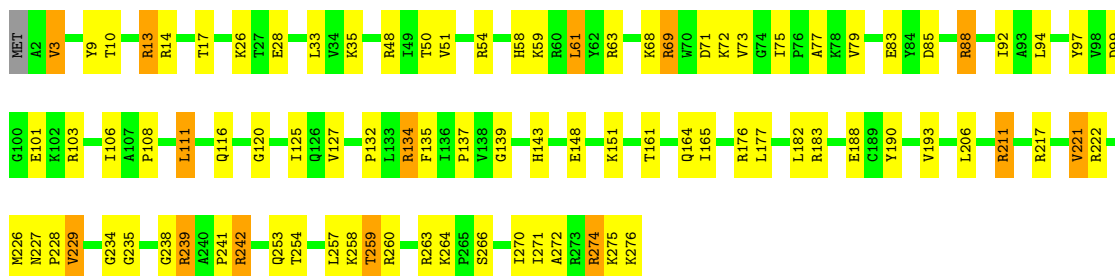


• Molecule 27: 50S Ribosomal Protein L2

Chain DD:

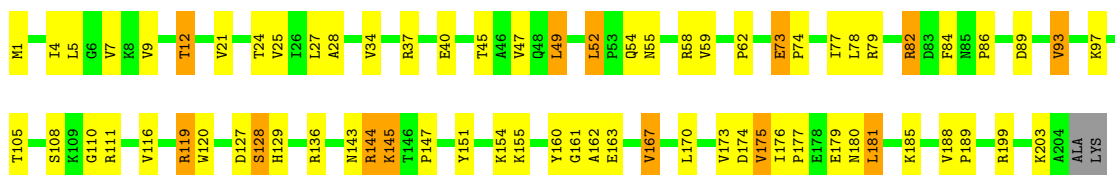






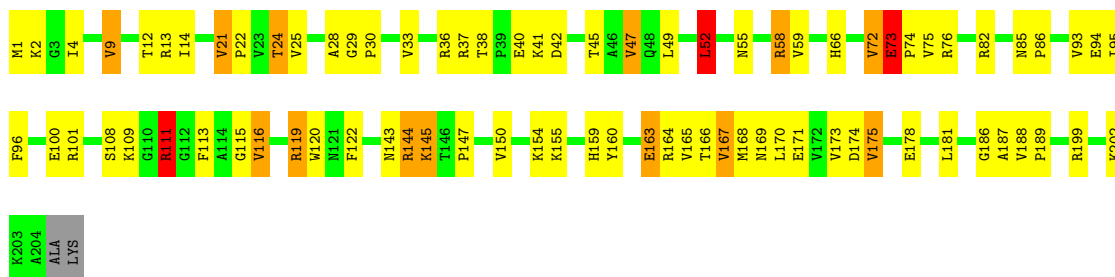
• Molecule 28: 50S Ribosomal Protein L3

Chain BE:



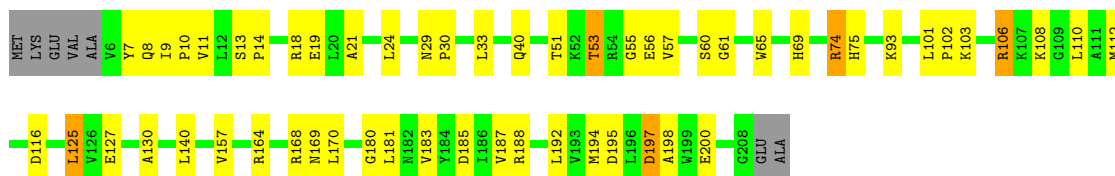
• Molecule 28: 50S Ribosomal Protein L3

Chain DE:



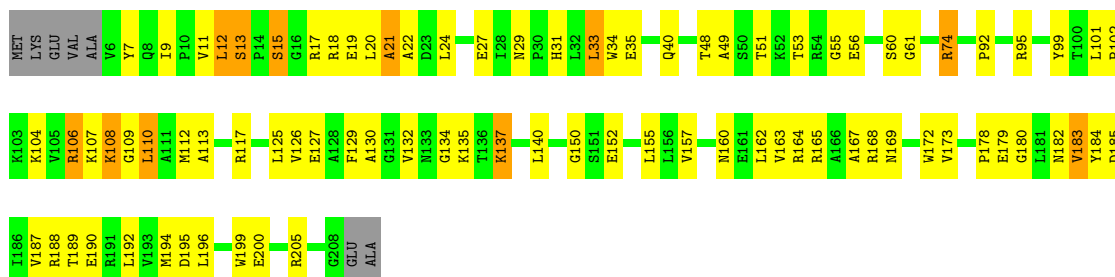
• Molecule 29: 50S Ribosomal Protein L4

Chain BF:



• Molecule 29: 50S Ribosomal Protein L4

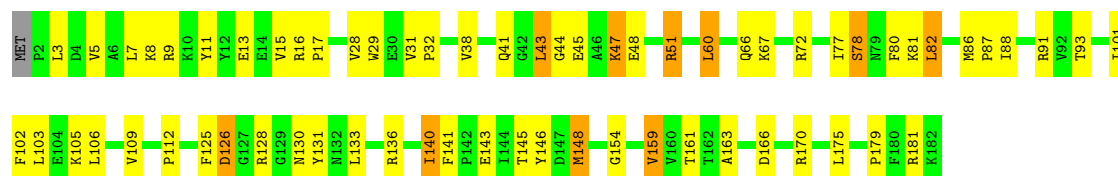
Chain DF:





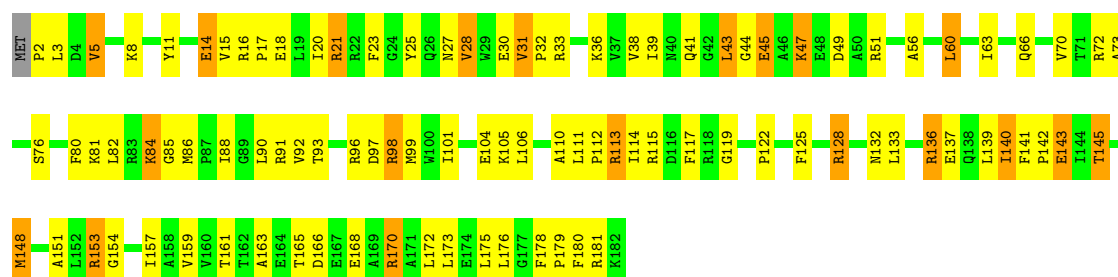
- Molecule 30: 50S Ribosomal Protein L5

Chain BG: 



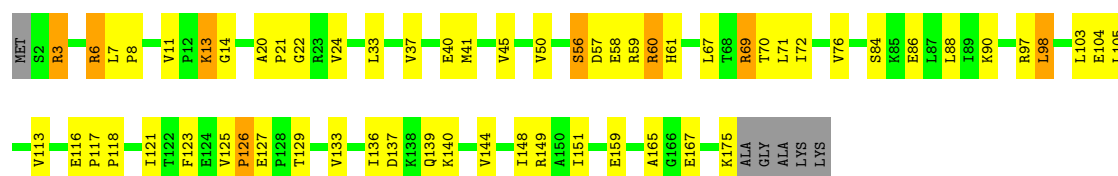
- Molecule 30: 50S Ribosomal Protein L5

Chain DG: 



- Molecule 31: 50S Ribosomal Protein L6

Chain BH: 



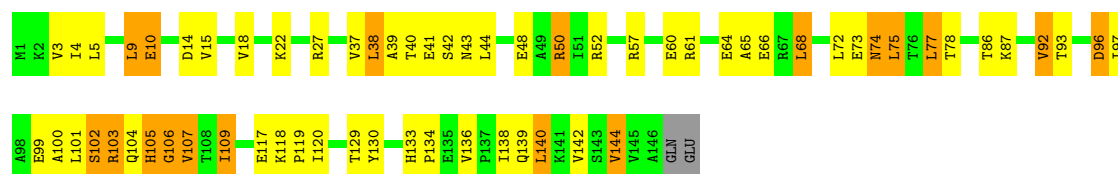
- Molecule 31: 50S Ribosomal Protein L6

Chain DH: 



- Molecule 32: 50S Ribosomal Protein L9

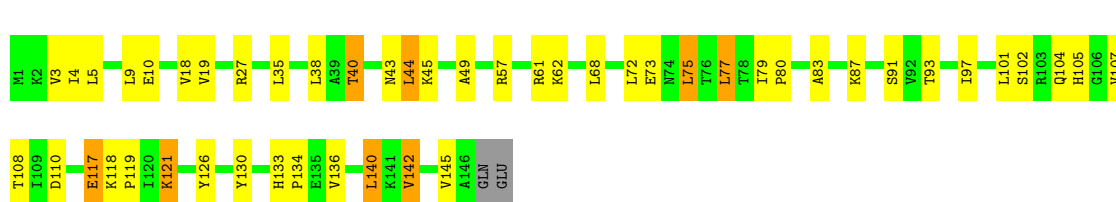
Chain BI: 





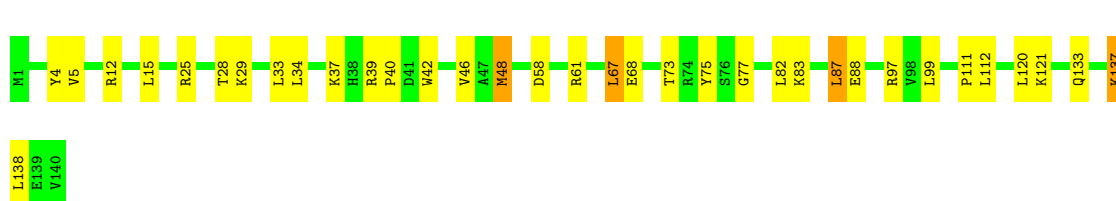
- Molecule 32: 50S Ribosomal Protein L9

Chain DI:



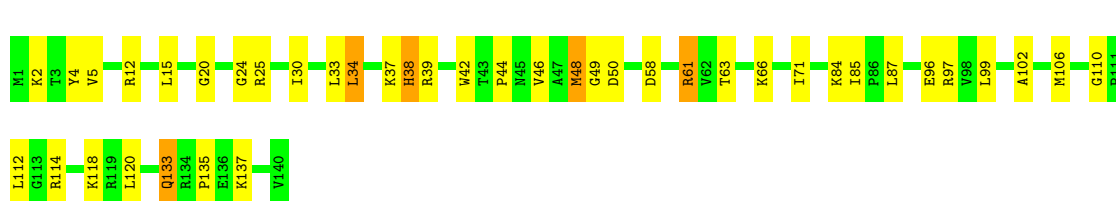
- Molecule 33: 50S Ribosomal Protein L13

Chain BN:



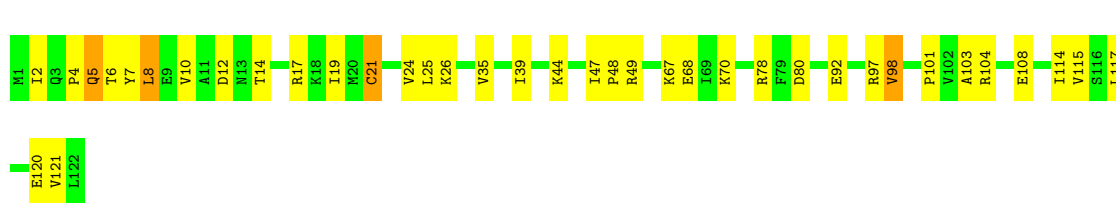
- Molecule 33: 50S Ribosomal Protein L13

Chain DN:



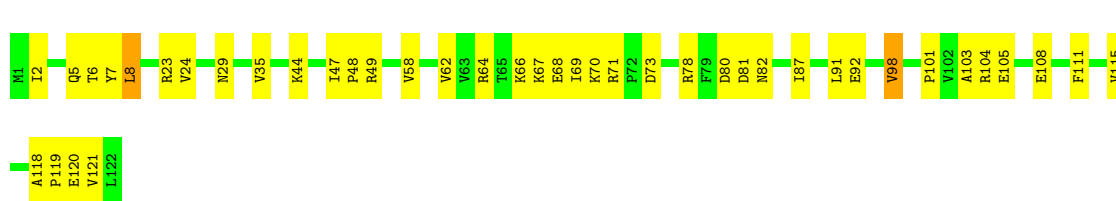
- Molecule 34: 50S Ribosomal Protein L14

Chain BO:



- Molecule 34: 50S Ribosomal Protein L14

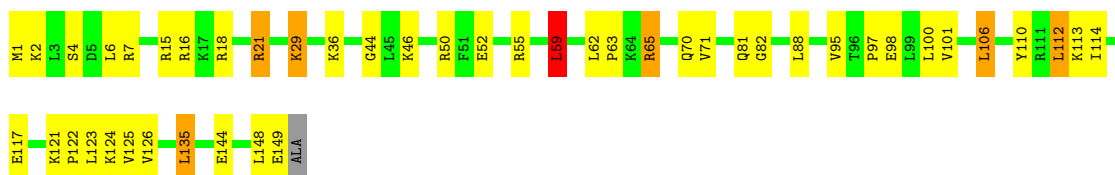
Chain DO:



- Molecule 35: 50S Ribosomal Protein L15

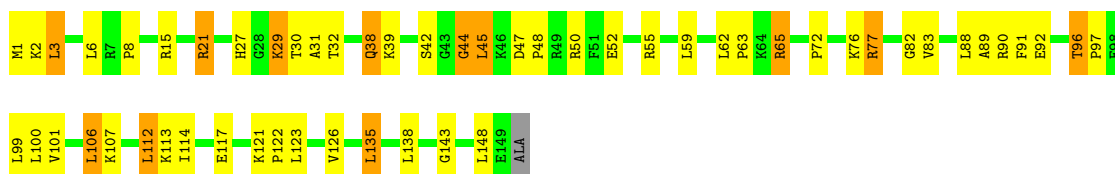
Chain BP:





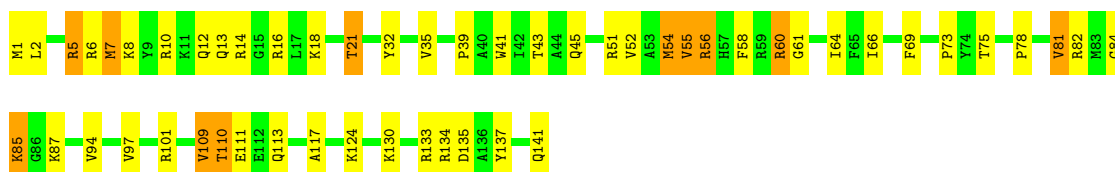
• Molecule 35: 50S Ribosomal Protein L15

Chain DP:



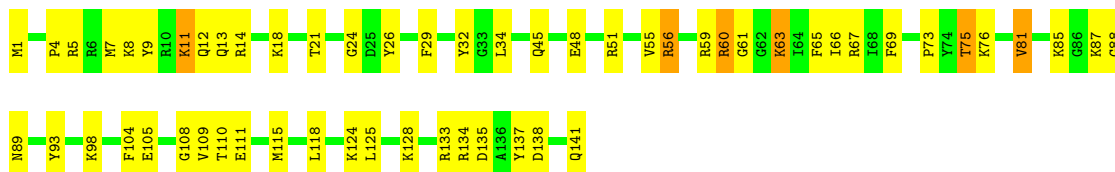
• Molecule 36: 50S Ribosomal Protein L16

Chain BQ:



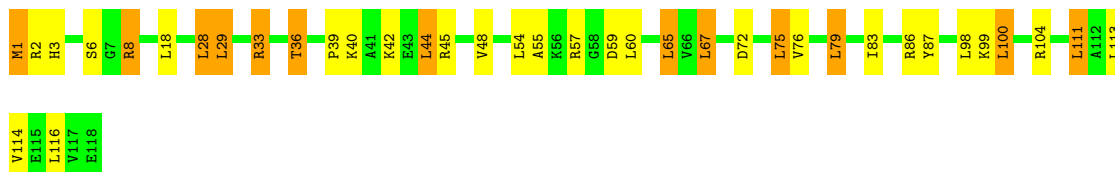
• Molecule 36: 50S Ribosomal Protein L16

Chain DQ:



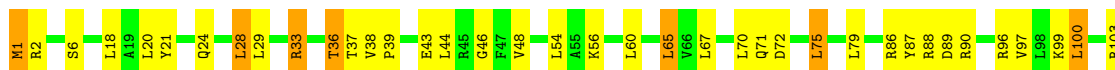
• Molecule 37: 50S Ribosomal Protein L17

Chain BR:

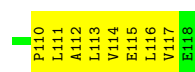


• Molecule 37: 50S Ribosomal Protein L17

Chain DR:

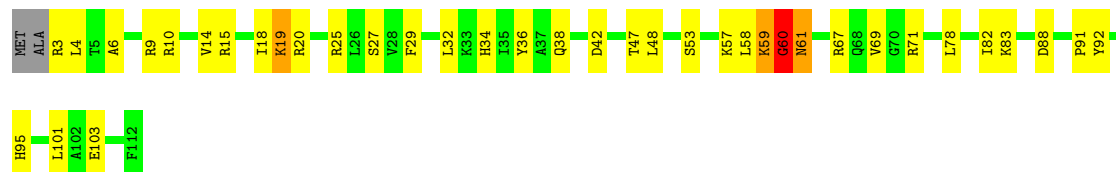






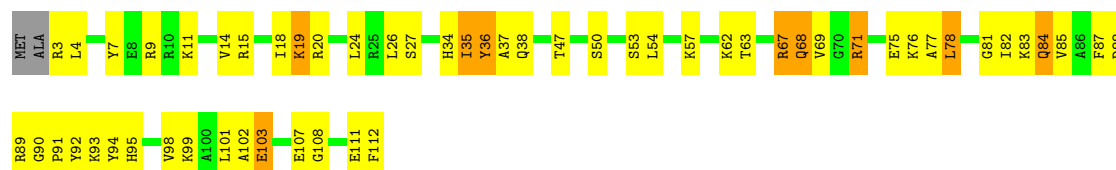
- Molecule 38: 50S Ribosomal Protein L18

Chain BS:



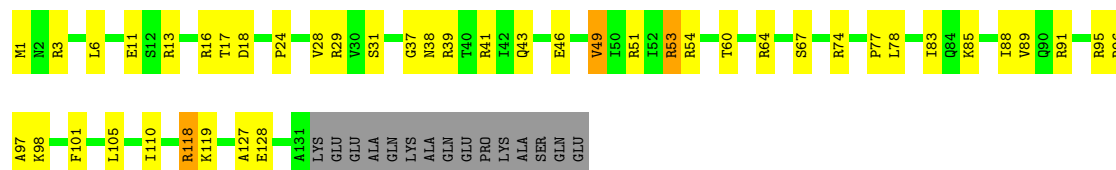
- Molecule 38: 50S Ribosomal Protein L18

Chain DS:



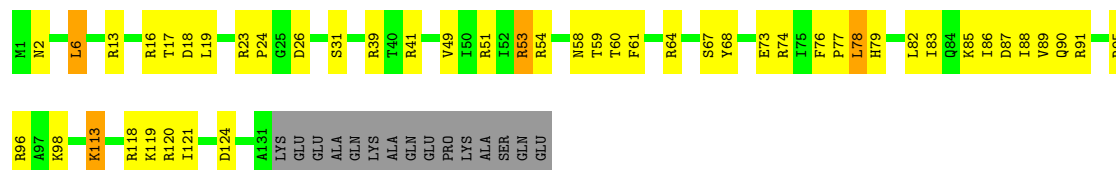
- Molecule 39: 50S Ribosomal Protein L19

Chain BT:



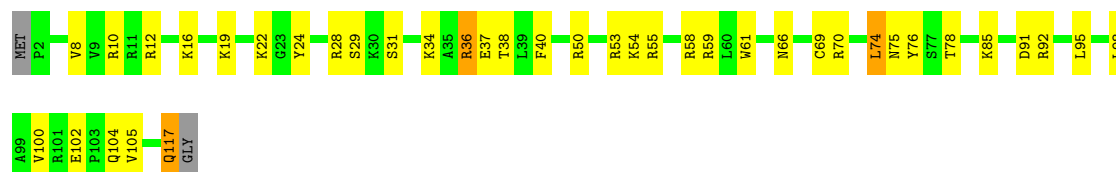
- Molecule 39: 50S Ribosomal Protein L19

Chain DT:



- Molecule 40: 50S Ribosomal Protein L20

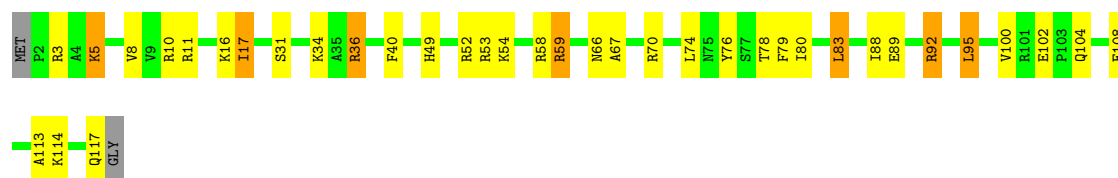
Chain BU:



- Molecule 40: 50S Ribosomal Protein L20



Chain DU: 



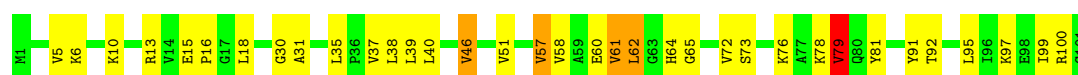
- Molecule 41: 50S Ribosomal Protein L21

Chain BV: 



- Molecule 41: 50S Ribosomal Protein L21

Chain DV: 



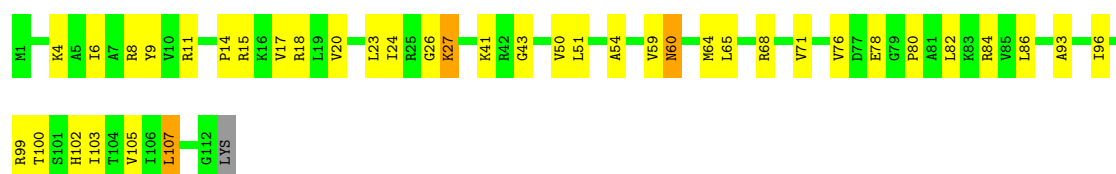
- Molecule 42: 50S Ribosomal Protein L22

Chain BW: 



- Molecule 42: 50S Ribosomal Protein L22

Chain DW: 



- Molecule 43: 50S Ribosomal Protein L23

Chain BX: 



- Molecule 43: 50S Ribosomal Protein L23

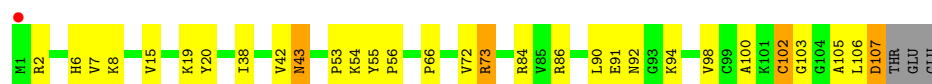
Chain DX: 



- Molecule 44: 50S Ribosomal Protein L24

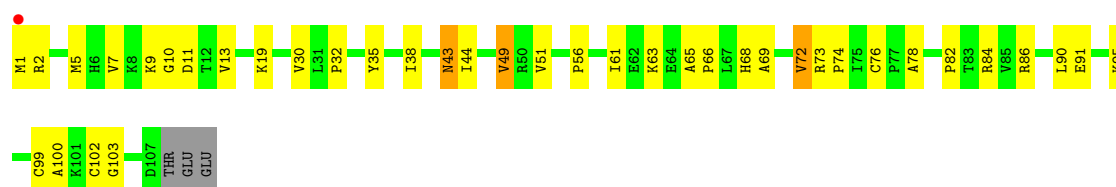
Chain BY: 





• Molecule 44: 50S Ribosomal Protein L24

Chain DY:



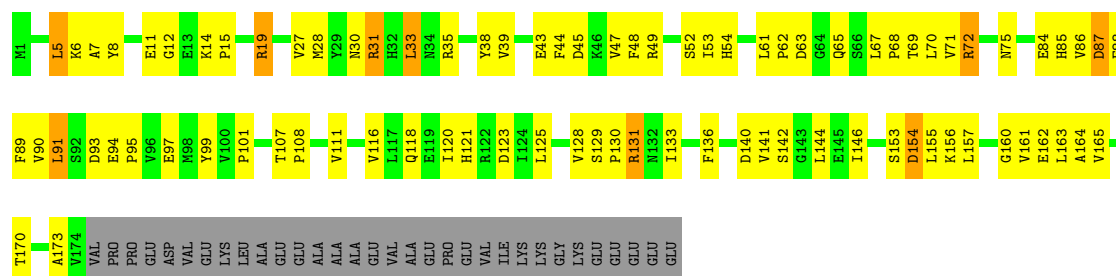
• Molecule 45: 50S Ribosomal Protein L25

Chain BZ:



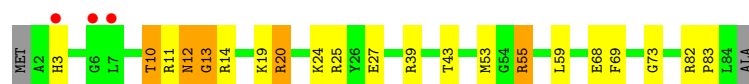
• Molecule 45: 50S Ribosomal Protein L25

Chain DZ:



• Molecule 46: 50S Ribosomal Protein L27

Chain B0:



• Molecule 46: 50S Ribosomal Protein L27

Chain D0:



• Molecule 47: 50S Ribosomal Protein L28



Chain B1:



- Molecule 47: 50S Ribosomal Protein L28

Chain D1:



- Molecule 48: 50S Ribosomal Protein L29

Chain B2:



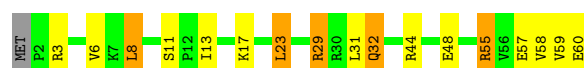
- Molecule 48: 50S Ribosomal Protein L29

Chain D2:



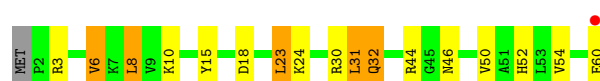
- Molecule 49: 50S Ribosomal Protein L30

Chain B3:



- Molecule 49: 50S Ribosomal Protein L30

Chain D3:



- Molecule 50: 50S Ribosomal Protein L31

Chain B4:



- Molecule 50: 50S Ribosomal Protein L31

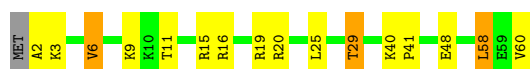
Chain D4:



- Molecule 51: 50S Ribosomal Protein L32

Chain B5:





- Molecule 51: 50S Ribosomal Protein L32

Chain D5:



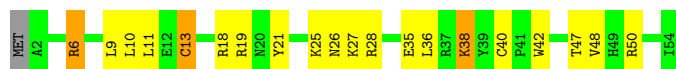
- Molecule 52: 50S Ribosomal Protein L33

Chain B6:



- Molecule 52: 50S Ribosomal Protein L33

Chain D6:



- Molecule 53: 50S Ribosomal Protein L34

Chain B7:



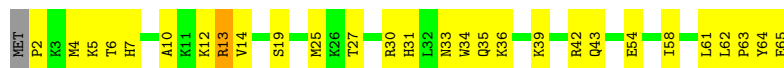
- Molecule 53: 50S Ribosomal Protein L34

Chain D7:



- Molecule 54: 50S Ribosomal Protein L35

Chain B8:



- Molecule 54: 50S Ribosomal Protein L35

Chain D8:



- Molecule 55: 50S Ribosomal Protein L36

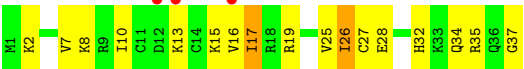
Chain B9:





● 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, $\alpha$ , $\beta$ , $\gamma$	210.08Å 449.83Å 619.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.74 – 3.00 49.75 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.74-3.00) 98.8 (49.75-3.00)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	0.24	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.203 , 0.259 0.229 , 0.281	Depositor DCC
$R_{free}$ test set	44205 reflections (3.87%)	DCC
Wilson B-factor (Å <sup>2</sup> )	66.8	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 36.8	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 1143007 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	286321	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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	0.77	7/36038 (0.0%)	1.39	355/56244 (0.6%)
1	CA	0.76	13/36170 (0.0%)	1.43	365/56452 (0.6%)
2	AB	0.49	0/1881	0.77	0/2542
2	CB	0.56	0/1860	0.81	2/2518 (0.1%)
3	AC	0.48	0/1576	0.64	0/2130
3	CC	0.50	0/1566	0.72	2/2119 (0.1%)
4	AD	0.49	0/1689	0.76	1/2267 (0.0%)
4	CD	0.50	0/1704	0.71	0/2284
5	AE	0.47	0/1145	0.71	0/1543
5	CE	0.50	0/1149	0.76	0/1548
6	AF	0.48	0/819	0.69	0/1111
6	CF	0.53	0/829	0.76	0/1123
7	AG	0.48	0/1250	0.66	1/1679 (0.1%)
7	CG	0.50	0/1254	0.72	1/1683 (0.1%)
8	AH	0.46	0/1108	0.69	0/1494
8	CH	0.47	0/1108	0.71	0/1494
9	AI	0.47	0/1002	0.73	1/1346 (0.1%)
9	CI	0.56	0/997	0.75	2/1343 (0.1%)
10	AJ	0.47	0/722	0.67	0/982
10	CJ	0.53	0/727	0.69	0/988
11	AK	0.44	0/844	0.65	1/1145 (0.1%)
11	CK	0.46	0/848	0.67	0/1149
12	AL	0.50	0/946	0.73	0/1274
12	CL	0.52	0/946	0.74	0/1274
13	AM	0.48	0/969	0.68	0/1302
13	CM	0.48	0/961	0.66	0/1291
14	AN	0.48	0/501	0.71	0/664
14	CN	0.55	0/501	0.71	0/664
15	AO	0.49	0/739	0.76	0/985
15	CO	0.47	0/739	0.70	0/985
16	AP	0.47	0/697	0.73	0/939
16	CP	0.49	0/693	0.70	0/935



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.51	0/836	0.68	0/1117
17	CQ	0.51	0/836	0.70	0/1117
18	AR	0.48	0/560	0.73	0/746
18	CR	0.50	0/560	0.75	1/746 (0.1%)
19	AS	0.47	0/667	0.66	0/900
19	CS	0.50	0/661	0.80	1/893 (0.1%)
20	AT	0.48	0/730	0.77	0/965
20	CT	0.43	0/729	0.68	0/965
21	AU	0.47	0/203	0.62	0/266
21	CU	0.51	0/203	0.64	0/266
22	AV	0.99	0/127	1.42	2/198 (1.0%)
22	CV	0.82	0/126	1.39	1/195 (0.5%)
23	AX	0.88	8/1813 (0.4%)	1.62	47/2825 (1.7%)
23	CX	0.94	6/1813 (0.3%)	1.87	57/2825 (2.0%)
24	AW	0.46	0/20	0.84	0/23
24	CW	0.34	0/20	0.64	0/23
25	BA	1.07	33/65892 (0.1%)	1.49	877/102850 (0.9%)
25	DA	0.82	13/65466 (0.0%)	1.46	741/102184 (0.7%)
26	BB	0.83	0/2878	1.31	13/4490 (0.3%)
26	DB	0.93	2/2878 (0.1%)	1.50	45/4490 (1.0%)
27	BD	0.71	2/2186 (0.1%)	0.82	0/2944
27	DD	0.63	2/2186 (0.1%)	0.77	0/2944
28	BE	0.72	0/1592	0.77	0/2149
28	DE	0.57	0/1592	0.79	2/2149 (0.1%)
29	BF	0.73	0/1619	0.75	0/2193
29	DF	0.53	0/1615	0.80	2/2188 (0.1%)
30	BG	0.46	0/1450	0.71	0/1959
30	DG	0.54	0/1449	0.76	0/1958
31	BH	0.61	0/1356	0.72	0/1834
31	DH	0.54	0/1356	0.71	1/1834 (0.1%)
32	BI	0.51	0/1100	0.70	0/1501
32	DI	0.51	0/1076	0.74	0/1471
33	BN	0.67	0/1144	0.75	0/1543
33	DN	0.54	0/1144	0.74	0/1543
34	BO	0.66	0/943	0.78	1/1269 (0.1%)
34	DO	0.56	0/943	0.78	1/1269 (0.1%)
35	BP	0.64	0/1152	0.82	1/1533 (0.1%)
35	DP	0.55	0/1152	0.83	2/1533 (0.1%)
36	BQ	0.69	0/1143	0.81	0/1527
36	DQ	0.59	0/1143	0.77	0/1527
37	BR	0.62	0/982	0.86	0/1312
37	DR	0.51	0/982	0.70	0/1312
38	BS	0.55	0/887	0.78	1/1180 (0.1%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DS	0.51	0/880	0.74	0/1172
39	BT	0.59	0/1105	0.79	0/1477
39	DT	0.53	0/1097	0.74	0/1468
40	BU	0.70	0/977	0.76	0/1301
40	DU	0.52	0/977	0.71	0/1301
41	BV	0.67	0/782	0.72	0/1049
41	DV	0.57	0/782	0.75	0/1049
42	BW	0.73	0/897	0.76	0/1205
42	DW	0.59	0/897	0.74	0/1205
43	BX	0.71	0/764	0.75	1/1025 (0.1%)
43	DX	0.56	0/764	0.80	2/1025 (0.2%)
44	BY	0.70	0/819	0.78	0/1095
44	DY	0.57	0/819	0.75	0/1095
45	BZ	0.55	0/1379	0.74	0/1873
45	DZ	0.54	0/1390	0.70	0/1890
46	B0	0.63	0/662	0.81	2/881 (0.2%)
46	D0	0.55	0/662	0.78	0/881
47	B1	0.66	0/762	0.81	3/1014 (0.3%)
47	D1	0.55	0/762	0.74	0/1014
48	B2	0.61	0/590	0.81	0/781
48	D2	0.47	0/590	0.67	0/781
49	B3	0.67	0/474	0.78	0/635
49	D3	0.50	0/469	0.70	0/630
50	B4	0.57	0/564	0.81	0/759
50	D4	0.59	0/544	0.89	1/735 (0.1%)
51	B5	0.72	0/469	0.84	1/635 (0.2%)
51	D5	0.59	0/469	0.73	1/635 (0.2%)
52	B6	0.66	0/460	0.66	0/613
52	D6	0.58	0/456	0.72	0/608
53	B7	0.74	0/426	0.82	0/561
53	D7	0.60	0/426	0.78	1/561 (0.2%)
54	B8	0.68	0/519	0.72	0/684
54	D8	0.58	0/525	0.73	0/691
55	B9	0.74	0/310	0.73	0/407
55	D9	0.61	0/310	0.80	0/407
All	All	0.81	86/305966 (0.0%)	1.30	2539/457396 (0.6%)

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



Mol	Chain	#Chirality outliers	#Planarity outliers
2	AB	0	3
4	CD	0	1
7	AG	0	1
9	AI	0	1
19	CS	0	1
23	CX	1	0
24	AW	0	1
24	CW	0	1
27	DD	0	1
38	BS	0	1
44	BY	0	1
45	BZ	0	1
50	B4	0	1
50	D4	0	1
All	All	1	15

The worst 5 of 86 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	1154	G	C6-N1	-13.21	1.30	1.39
1	CA	1119	C	N3-C4	-13.12	1.24	1.33
1	AA	343	U	C4-O4	12.79	1.33	1.23
1	CA	1154	G	N1-C2	-12.44	1.27	1.37
23	CX	76	A	N7-C5	-12.26	1.31	1.39

The worst 5 of 2539 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1119	C	N1-C2-O2	40.38	143.13	118.90
1	CA	1154	G	C5-C6-O6	34.47	149.28	128.60
23	CX	76	A	O4'-C1'-N9	33.86	135.29	108.20
1	CA	1154	G	N3-C2-N2	29.11	140.27	119.90
1	CA	1154	G	N1-C2-N2	-27.03	91.87	116.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	CX	76	A	C1'

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	231	GLU	Peptide

*Continued on next page...*



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

## 5.2 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	16250	907	0
1	CA	32312	0	16307	1000	0
2	AB	1846	0	1867	106	0
2	CB	1825	0	1828	118	0
3	AC	1552	0	1546	51	0
3	CC	1542	0	1517	81	0
4	AD	1659	0	1676	86	0
4	CD	1674	0	1714	83	0
5	AE	1129	0	1185	44	0
5	CE	1133	0	1191	57	0
6	AF	806	0	793	34	0
6	CF	816	0	808	24	0
7	AG	1231	0	1238	33	0
7	CG	1235	0	1249	53	0
8	AH	1088	0	1126	43	0
8	CH	1088	0	1126	56	0
9	AI	983	0	986	47	0
9	CI	978	0	966	55	0
10	AJ	709	0	650	41	0
10	CJ	714	0	672	58	0
11	AK	829	0	825	17	0
11	CK	833	0	836	27	0
12	AL	930	0	980	36	0
12	CL	930	0	980	40	0
13	AM	958	0	1002	35	0
13	CM	950	0	988	50	0
14	AN	492	0	529	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	CN	492	0	529	31	0
15	AO	728	0	760	23	0
15	CO	728	0	760	26	0
16	AP	681	0	697	35	0
16	CP	677	0	686	30	0
17	AQ	823	0	891	21	0
17	CQ	823	0	891	27	0
18	AR	555	0	618	24	0
18	CR	555	0	618	19	0
19	AS	652	0	662	42	0
19	CS	646	0	644	49	0
20	AT	728	0	798	36	0
20	CT	727	0	796	26	0
21	AU	199	0	208	6	0
21	CU	199	0	208	8	0
22	AV	114	0	54	1	0
22	CV	113	0	54	1	0
23	AX	1623	0	823	23	0
23	CX	1623	0	823	22	0
24	AW	93	0	51	7	0
24	CW	93	0	51	4	0
25	BA	58834	0	29666	828	0
25	DA	58458	0	29481	1163	0
26	BB	2573	0	1306	33	0
26	DB	2573	0	1306	65	0
27	BD	2136	0	2218	62	0
27	DD	2136	0	2218	74	0
28	BE	1559	0	1618	55	0
28	DE	1559	0	1618	65	0
29	BF	1584	0	1625	38	0
29	DF	1580	0	1619	65	0
30	BG	1425	0	1443	41	0
30	DG	1424	0	1434	89	0
31	BH	1330	0	1407	37	0
31	DH	1330	0	1407	50	0
32	BI	1085	0	1114	42	0
32	DI	1061	0	1080	27	0
33	BN	1117	0	1183	18	0
33	DN	1117	0	1184	25	0
34	BO	933	0	996	26	0
34	DO	933	0	996	30	0
35	BP	1135	0	1212	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	DP	1135	0	1212	52	0
36	BQ	1122	0	1179	38	0
36	DQ	1122	0	1179	38	0
37	BR	968	0	1033	24	0
37	DR	968	0	1032	28	0
38	BS	877	0	938	30	0
38	DS	870	0	923	45	0
39	BT	1091	0	1151	36	0
39	DT	1083	0	1136	38	0
40	BU	959	0	1019	28	0
40	DU	959	0	1019	26	0
41	BV	771	0	830	15	0
41	DV	771	0	830	23	0
42	BW	886	0	940	15	0
42	DW	886	0	940	25	0
43	BX	750	0	814	19	0
43	DX	750	0	814	22	0
44	BY	806	0	881	22	0
44	DY	806	0	881	27	0
45	BZ	1349	0	1355	44	0
45	DZ	1360	0	1363	55	0
46	B0	653	0	674	19	0
46	D0	653	0	674	31	0
47	B1	755	0	826	19	0
47	D1	755	0	826	20	0
48	B2	588	0	643	13	0
48	D2	588	0	643	18	0
49	B3	469	0	518	12	0
49	D3	464	0	514	10	0
50	B4	551	0	532	38	0
50	D4	531	0	502	38	0
51	B5	455	0	465	14	0
51	D5	455	0	465	8	0
52	B6	453	0	473	10	0
52	D6	449	0	469	13	0
53	B7	418	0	467	11	0
53	D7	418	0	467	8	0
54	B8	511	0	571	31	0
54	D8	517	0	582	24	0
55	B9	307	0	335	7	0
55	D9	307	0	335	14	0
56	AA	222	0	0	0	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DA	657	0	0	0	0
56	DB	12	0	0	0	0
56	DD	5	0	0	0	0
56	DE	6	0	0	0	0
56	DF	5	0	0	0	0
56	DG	1	0	0	0	0
56	DN	1	0	0	0	0
56	DO	1	0	0	0	0
56	DP	2	0	0	0	0
56	DQ	4	0	0	0	0
56	DR	1	0	0	0	0
56	DU	2	0	0	0	0
56	DV	3	0	0	0	0
56	DW	2	0	0	0	0
56	DY	1	0	0	0	0
57	AD	8	0	0	1	0
57	CD	8	0	0	1	0
58	AN	1	0	0	0	0
58	B4	1	0	0	0	0
58	B5	1	0	0	0	0
58	B6	1	0	0	0	0
58	B9	1	0	0	0	0
58	BY	1	0	0	0	0
58	CN	1	0	0	0	0
58	D4	1	0	0	0	0
58	D5	1	0	0	0	0
58	D6	1	0	0	0	0
58	D9	1	0	0	0	0
58	DY	1	0	0	0	0
59	AX	10	0	10	1	0
59	CX	10	0	10	2	0
60	BA	1	0	0	0	0
60	DA	1	0	0	0	0
61	AA	147	0	0	23	0
61	AD	1	0	0	0	0
61	AE	2	0	0	0	0
61	AJ	1	0	0	0	0
61	AL	2	0	0	0	0
61	AO	2	0	0	0	0
61	AU	1	0	0	1	0
61	AV	2	0	0	0	0
61	AX	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	B0	4	0	0	0	0
61	B1	2	0	0	0	0
61	B5	2	0	0	0	0
61	B7	1	0	0	1	0
61	B8	7	0	0	1	0
61	BA	1086	0	0	94	0
61	BB	26	0	0	2	0
61	BD	6	0	0	0	0
61	BE	13	0	0	3	0
61	BF	5	0	0	0	0
61	BG	1	0	0	0	0
61	BN	3	0	0	0	0
61	BO	2	0	0	0	0
61	BP	15	0	0	2	0
61	BQ	3	0	0	1	0
61	BR	1	0	0	0	0
61	BT	2	0	0	0	0
61	BU	5	0	0	0	0
61	BV	2	0	0	0	0
61	BW	4	0	0	0	0
61	BX	4	0	0	1	0
61	CA	186	0	0	24	0
61	CE	2	0	0	0	0
61	CN	1	0	0	0	0
61	CT	1	0	0	0	0
61	CX	2	0	0	0	0
61	D0	3	0	0	1	0
61	D1	1	0	0	0	0
61	D3	1	0	0	0	0
61	D7	1	0	0	0	0
61	D8	4	0	0	0	0
61	DA	906	0	0	116	0
61	DB	7	0	0	0	0
61	DD	10	0	0	0	0
61	DE	11	0	0	1	0
61	DF	4	0	0	0	0
61	DO	1	0	0	0	0
61	DP	14	0	0	2	0
61	DQ	3	0	0	1	0
61	DR	1	0	0	0	0
61	DU	4	0	0	0	0
61	DV	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	DX	2	0	0	1	0
61	DY	1	0	0	0	0
All	All	286321	0	191058	6675	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 15.

The worst 5 of 6675 close contacts within the same asymmetric unit are listed below.

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

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 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%)	201 (88%)	23 (10%)	5 (2%)	10	45
2	CB	229/256 (90%)	201 (88%)	21 (9%)	7 (3%)	7	34
3	AC	204/239 (85%)	182 (89%)	20 (10%)	2 (1%)	22	70
3	CC	204/239 (85%)	181 (89%)	21 (10%)	2 (1%)	22	70
4	AD	206/209 (99%)	184 (89%)	20 (10%)	2 (1%)	22	70
4	CD	206/209 (99%)	185 (90%)	18 (9%)	3 (2%)	15	58
5	AE	146/162 (90%)	136 (93%)	8 (6%)	2 (1%)	16	60
5	CE	146/162 (90%)	134 (92%)	12 (8%)	0	100	100
6	AF	98/101 (97%)	94 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	CF	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
7	AG	153/156 (98%)	137 (90%)	15 (10%)	1 (1%)	30	78
7	CG	153/156 (98%)	139 (91%)	13 (8%)	1 (1%)	30	78
8	AH	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
8	CH	135/138 (98%)	131 (97%)	3 (2%)	1 (1%)	30	78
9	AI	125/128 (98%)	112 (90%)	10 (8%)	3 (2%)	9	42
9	CI	125/128 (98%)	115 (92%)	8 (6%)	2 (2%)	14	56
10	AJ	95/105 (90%)	84 (88%)	8 (8%)	3 (3%)	6	33
10	CJ	94/105 (90%)	84 (89%)	8 (8%)	2 (2%)	11	47
11	AK	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	25	73
11	CK	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	25	73
12	AL	120/132 (91%)	117 (98%)	3 (2%)	0	100	100
12	CL	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
13	AM	121/126 (96%)	113 (93%)	7 (6%)	1 (1%)	27	76
13	CM	120/126 (95%)	113 (94%)	6 (5%)	1 (1%)	27	76
14	AN	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
14	CN	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
15	AO	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
15	CO	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	AP	80/88 (91%)	74 (92%)	6 (8%)	0	100	100
16	CP	80/88 (91%)	73 (91%)	6 (8%)	1 (1%)	18	62
17	AQ	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
17	CQ	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
18	AR	66/88 (75%)	60 (91%)	5 (8%)	1 (2%)	15	58
18	CR	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
19	AS	81/93 (87%)	76 (94%)	5 (6%)	0	100	100
19	CS	81/93 (87%)	74 (91%)	7 (9%)	0	100	100
20	AT	94/106 (89%)	84 (89%)	9 (10%)	1 (1%)	21	67
20	CT	94/106 (89%)	86 (92%)	5 (5%)	3 (3%)	6	33
21	AU	21/27 (78%)	17 (81%)	4 (19%)	0	100	100
21	CU	21/27 (78%)	18 (86%)	3 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	AW	3/10 (30%)	0	2 (67%)	1 (33%)	0	0
24	CW	3/10 (30%)	1 (33%)	1 (33%)	1 (33%)	0	0
27	BD	273/276 (99%)	260 (95%)	12 (4%)	1 (0%)	43	87
27	DD	273/276 (99%)	258 (94%)	13 (5%)	2 (1%)	30	78
28	BE	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	38	84
28	DE	202/206 (98%)	195 (96%)	4 (2%)	3 (2%)	15	58
29	BF	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	38	84
29	DF	201/210 (96%)	195 (97%)	4 (2%)	2 (1%)	22	70
30	BG	179/182 (98%)	167 (93%)	9 (5%)	3 (2%)	14	54
30	DG	179/182 (98%)	161 (90%)	14 (8%)	4 (2%)	10	45
31	BH	172/180 (96%)	165 (96%)	6 (4%)	1 (1%)	33	81
31	DH	172/180 (96%)	164 (95%)	7 (4%)	1 (1%)	33	81
32	BI	144/148 (97%)	124 (86%)	14 (10%)	6 (4%)	4	24
32	DI	144/148 (97%)	124 (86%)	17 (12%)	3 (2%)	11	47
33	BN	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
33	DN	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	30	78
34	BO	120/122 (98%)	116 (97%)	3 (2%)	1 (1%)	27	76
34	DO	120/122 (98%)	117 (98%)	2 (2%)	1 (1%)	27	76
35	BP	147/150 (98%)	138 (94%)	8 (5%)	1 (1%)	30	78
35	DP	147/150 (98%)	135 (92%)	9 (6%)	3 (2%)	11	48
36	BQ	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	30	78
36	DQ	139/141 (99%)	129 (93%)	9 (6%)	1 (1%)	30	78
37	BR	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	25	73
37	DR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
38	BS	108/112 (96%)	103 (95%)	4 (4%)	1 (1%)	25	73
38	DS	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	25	73
39	BT	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
39	DT	129/146 (88%)	127 (98%)	2 (2%)	0	100	100
40	BU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
40	DU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
41	BV	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	22	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	DV	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	22	70
42	BW	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
42	DW	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
43	BX	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
43	DX	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
44	BY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
44	DY	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
45	BZ	169/206 (82%)	150 (89%)	18 (11%)	1 (1%)	33	81
45	DZ	172/206 (84%)	162 (94%)	10 (6%)	0	100	100
46	B0	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	19	64
46	D0	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	19	64
47	B1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	21	67
47	D1	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	21	67
48	B2	68/72 (94%)	68 (100%)	0	0	100	100
48	D2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
49	B3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
49	D3	57/60 (95%)	57 (100%)	0	0	100	100
50	B4	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	2	8
50	D4	67/71 (94%)	52 (78%)	8 (12%)	7 (10%)	1	4
51	B5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
51	D5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
52	B6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
52	D6	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
53	B7	46/49 (94%)	46 (100%)	0	0	100	100
53	D7	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	10	45
54	B8	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
54	D8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
55	B9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
55	D9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
All	All	11415/12148 (94%)	10659 (93%)	648 (6%)	108 (1%)	25	73

5 of 108 Ramachandran outliers are listed below:



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

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	192/220 (87%)	154 (80%)	38 (20%)	2	11
2	CB	187/220 (85%)	155 (83%)	32 (17%)	3	15
3	AC	143/188 (76%)	128 (90%)	15 (10%)	10	37
3	CC	140/188 (74%)	123 (88%)	17 (12%)	7	29
4	AD	170/181 (94%)	146 (86%)	24 (14%)	5	23
4	CD	173/181 (96%)	152 (88%)	21 (12%)	7	29
5	AE	113/123 (92%)	102 (90%)	11 (10%)	12	42
5	CE	114/123 (93%)	104 (91%)	10 (9%)	14	48
6	AF	83/90 (92%)	76 (92%)	7 (8%)	16	51
6	CF	85/90 (94%)	79 (93%)	6 (7%)	21	61
7	AG	119/127 (94%)	100 (84%)	19 (16%)	3	17
7	CG	120/127 (94%)	102 (85%)	18 (15%)	4	20
8	AH	114/119 (96%)	97 (85%)	17 (15%)	4	20
8	CH	114/119 (96%)	102 (90%)	12 (10%)	10	37
9	AI	90/99 (91%)	78 (87%)	12 (13%)	6	25
9	CI	89/99 (90%)	75 (84%)	14 (16%)	4	18
10	AJ	66/92 (72%)	59 (89%)	7 (11%)	10	36
10	CJ	69/92 (75%)	65 (94%)	4 (6%)	28	71
11	AK	82/99 (83%)	75 (92%)	7 (8%)	15	51
11	CK	83/99 (84%)	77 (93%)	6 (7%)	21	59
12	AL	97/109 (89%)	87 (90%)	10 (10%)	10	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	CL	97/109 (89%)	83 (86%)	14 (14%)	5	22
13	AM	93/101 (92%)	81 (87%)	12 (13%)	6	26
13	CM	92/101 (91%)	78 (85%)	14 (15%)	4	20
14	AN	49/50 (98%)	41 (84%)	8 (16%)	3	17
14	CN	49/50 (98%)	41 (84%)	8 (16%)	3	17
15	AO	78/80 (98%)	68 (87%)	10 (13%)	6	27
15	CO	78/80 (98%)	66 (85%)	12 (15%)	4	19
16	AP	69/74 (93%)	61 (88%)	8 (12%)	8	31
16	CP	68/74 (92%)	64 (94%)	4 (6%)	28	70
17	AQ	94/97 (97%)	88 (94%)	6 (6%)	25	66
17	CQ	94/97 (97%)	86 (92%)	8 (8%)	15	51
18	AR	59/77 (77%)	56 (95%)	3 (5%)	33	76
18	CR	59/77 (77%)	53 (90%)	6 (10%)	11	38
19	AS	69/80 (86%)	63 (91%)	6 (9%)	15	49
19	CS	67/80 (84%)	59 (88%)	8 (12%)	8	30
20	AT	70/82 (85%)	60 (86%)	10 (14%)	5	22
20	CT	70/82 (85%)	61 (87%)	9 (13%)	6	26
21	AU	18/22 (82%)	15 (83%)	3 (17%)	3	16
21	CU	18/22 (82%)	16 (89%)	2 (11%)	9	34
24	AW	3/3 (100%)	2 (67%)	1 (33%)	0	2
24	CW	3/3 (100%)	2 (67%)	1 (33%)	0	2
27	BD	215/218 (99%)	193 (90%)	22 (10%)	11	38
27	DD	215/218 (99%)	195 (91%)	20 (9%)	13	45
28	BE	164/166 (99%)	140 (85%)	24 (15%)	5	21
28	DE	164/166 (99%)	140 (85%)	24 (15%)	5	21
29	BF	160/166 (96%)	145 (91%)	15 (9%)	13	44
29	DF	159/166 (96%)	142 (89%)	17 (11%)	10	35
30	BG	143/156 (92%)	124 (87%)	19 (13%)	6	25
30	DG	142/156 (91%)	117 (82%)	25 (18%)	3	14
31	BH	144/148 (97%)	128 (89%)	16 (11%)	9	34
31	DH	144/148 (97%)	131 (91%)	13 (9%)	14	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	BI	110/124 (89%)	85 (77%)	25 (23%)	1	6
32	DI	104/124 (84%)	90 (86%)	14 (14%)	6	24
33	BN	118/119 (99%)	100 (85%)	18 (15%)	4	19
33	DN	118/119 (99%)	102 (86%)	16 (14%)	5	24
34	BO	100/100 (100%)	95 (95%)	5 (5%)	34	77
34	DO	100/100 (100%)	92 (92%)	8 (8%)	17	53
35	BP	115/116 (99%)	103 (90%)	12 (10%)	10	37
35	DP	115/116 (99%)	102 (89%)	13 (11%)	9	33
36	BQ	111/111 (100%)	96 (86%)	15 (14%)	6	24
36	DQ	111/111 (100%)	97 (87%)	14 (13%)	7	27
37	BR	101/101 (100%)	83 (82%)	18 (18%)	2	14
37	DR	101/101 (100%)	84 (83%)	17 (17%)	3	15
38	BS	87/88 (99%)	78 (90%)	9 (10%)	10	38
38	DS	85/88 (97%)	73 (86%)	12 (14%)	5	23
39	BT	115/127 (91%)	103 (90%)	12 (10%)	10	37
39	DT	113/127 (89%)	103 (91%)	10 (9%)	14	48
40	BU	93/94 (99%)	85 (91%)	8 (9%)	15	50
40	DU	93/94 (99%)	79 (85%)	14 (15%)	4	20
41	BV	80/82 (98%)	68 (85%)	12 (15%)	4	20
41	DV	80/82 (98%)	70 (88%)	10 (12%)	7	28
42	BW	90/92 (98%)	83 (92%)	7 (8%)	18	55
42	DW	90/92 (98%)	82 (91%)	8 (9%)	14	48
43	BX	77/78 (99%)	74 (96%)	3 (4%)	43	85
43	DX	77/78 (99%)	73 (95%)	4 (5%)	32	75
44	BY	85/91 (93%)	76 (89%)	9 (11%)	10	36
44	DY	85/91 (93%)	77 (91%)	8 (9%)	13	44
45	BZ	145/179 (81%)	127 (88%)	18 (12%)	7	28
45	DZ	145/179 (81%)	128 (88%)	17 (12%)	8	31
46	B0	65/67 (97%)	62 (95%)	3 (5%)	37	80
46	D0	65/67 (97%)	60 (92%)	5 (8%)	18	56
47	B1	80/83 (96%)	70 (88%)	10 (12%)	7	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	D1	80/83 (96%)	69 (86%)	11 (14%)	5	24
48	B2	65/67 (97%)	56 (86%)	9 (14%)	5	24
48	D2	65/67 (97%)	57 (88%)	8 (12%)	7	28
49	B3	51/52 (98%)	44 (86%)	7 (14%)	5	24
49	D3	50/52 (96%)	42 (84%)	8 (16%)	3	17
50	B4	59/63 (94%)	47 (80%)	12 (20%)	2	9
50	D4	53/63 (84%)	44 (83%)	9 (17%)	3	15
51	B5	50/52 (96%)	45 (90%)	5 (10%)	11	39
51	D5	50/52 (96%)	45 (90%)	5 (10%)	11	39
52	B6	51/52 (98%)	47 (92%)	4 (8%)	18	55
52	D6	50/52 (96%)	43 (86%)	7 (14%)	5	23
53	B7	41/42 (98%)	39 (95%)	2 (5%)	35	78
53	D7	41/42 (98%)	38 (93%)	3 (7%)	20	59
54	B8	53/55 (96%)	50 (94%)	3 (6%)	29	71
54	D8	54/55 (98%)	52 (96%)	2 (4%)	45	86
55	B9	34/34 (100%)	33 (97%)	1 (3%)	55	90
55	D9	34/34 (100%)	31 (91%)	3 (9%)	14	48
All	All	9325/10072 (93%)	8217 (88%)	1108 (12%)	8	30

5 of 1108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	B0	10	THR
4	CD	170	VAL
44	DY	43	ASN
48	B2	30	ARG
2	CB	67	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
45	BZ	32	HIS
3	CC	123	GLN
39	DT	58	ASN
45	BZ	151	HIS

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Mol	Chain	Res	Type
2	CB	224	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1495/1522 (98%)	421 (28%)	24 (1%)
1	CA	1501/1522 (98%)	421 (28%)	30 (1%)
22	AV	4/24 (16%)	1 (25%)	0
22	CV	4/24 (16%)	1 (25%)	0
23	AX	75/77 (97%)	18 (24%)	0
23	CX	75/77 (97%)	19 (25%)	0
25	BA	2722/2915 (93%)	527 (19%)	41 (1%)
25	DA	2704/2915 (92%)	526 (19%)	35 (1%)
26	BB	119/122 (97%)	21 (17%)	0
26	DB	119/122 (97%)	23 (19%)	1 (0%)
All	All	8818/9320 (94%)	1978 (22%)	131 (1%)

5 of 1978 RNA backbone outliers are listed below:

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

5 of 131 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	2459	G
1	CA	429	U
25	DA	1992	G
25	BA	2701	U
1	CA	60	A

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

14 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and



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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	2QZ	AW	1	24	8,8,9	6.11	2 (25%)	7,10,12	2.52	1 (14%)
24	2QY	AW	10	24	12,13,14	1.43	3 (25%)	13,16,18	2.58	5 (38%)
24	004	AW	3	24	10,10,11	6.47	3 (30%)	10,12,14	5.74	1 (10%)
24	MVA	AW	5	24	7,7,8	6.71	2 (28%)	5,8,10	2.10	1 (20%)
24	2R1	AW	6	24	9,10,11	2.55	5 (55%)	10,13,15	54.55	3 (30%)
24	2R3	AW	8	24	14,14,15	5.87	1 (7%)	16,18,20	2.48	9 (56%)
24	MVA	AW	9	24	7,7,8	5.79	2 (28%)	5,8,10	1.05	1 (20%)
24	2QZ	CW	1	24	8,8,9	6.33	3 (37%)	7,10,12	3.80	2 (28%)
24	2QY	CW	10	24	12,13,14	1.41	3 (25%)	13,16,18	2.30	2 (15%)
24	004	CW	3	24	10,10,11	6.07	3 (30%)	10,12,14	9.22	1 (10%)
24	MVA	CW	5	24	7,7,8	6.99	3 (42%)	5,8,10	1.00	0
24	2R1	CW	6	24	9,10,11	2.31	3 (33%)	10,13,15	13.39	2 (20%)
24	2R3	CW	8	24	14,14,15	5.39	1 (7%)	16,18,20	2.75	7 (43%)
24	MVA	CW	9	24	7,7,8	6.86	3 (42%)	5,8,10	1.53	1 (20%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	MVA	CW	9	24	-	0/6/8/10	0/0/0/0

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AW	8	2R3	O-C	21.83	1.26	1.11
24	CW	8	2R3	O-C	20.03	1.25	1.11
24	AW	3	004	O-C	19.40	1.24	1.11
24	CW	5	MVA	O-C	18.00	1.23	1.11
24	CW	3	004	O-C	17.75	1.23	1.11

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AW	6	2R1	CG1-CB-CA	171.85	126.77	119.61
24	CW	6	2R1	CG1-CB-CA	40.48	121.30	119.61
24	CW	3	004	C-CA-N	-29.06	109.98	113.27
24	AW	3	004	C-CA-N	-17.91	111.24	113.27
24	AW	6	2R1	OD2-CG2-CB	-14.50	92.15	112.43

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	22.61	12 (100%)	0,24,24	0.00	-
59	FME	AX	101	23	9,9,10	6.14	3 (33%)	6,9,11	1.39	1 (16%)
57	SF4	CD	501	4	12,12,12	21.29	12 (100%)	0,24,24	0.00	-
59	FME	CX	101	23	9,9,10	6.72	3 (33%)	6,9,11	1.21	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	-23.92	2.17	2.33
57	AD	501	SF4	S2-FE1	-23.56	2.17	2.33
57	AD	501	SF4	S4-FE1	-23.55	2.17	2.33
57	AD	501	SF4	S4-FE3	-23.55	2.17	2.33
57	CD	501	SF4	S3-FE1	-23.54	2.17	2.33

All (2) bond angle outliers are listed below:

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AA	1498/1522 (98%)	-0.20	32 (2%)	60	12	39, 80, 103, 118	0
1	CA	1503/1522 (98%)	-0.23	28 (1%)	64	13	41, 80, 103, 119	0
2	AB	231/256 (90%)	-0.08	0	100	100	69, 86, 97, 105	0
2	CB	231/256 (90%)	0.09	2 (0%)	81	24	70, 88, 98, 107	0
3	AC	206/239 (86%)	0.08	1 (0%)	88	36	73, 87, 95, 104	0
3	CC	206/239 (86%)	0.22	3 (1%)	70	16	72, 89, 97, 104	0
4	AD	208/209 (99%)	-0.07	0	100	100	61, 80, 90, 97	0
4	CD	208/209 (99%)	-0.17	0	100	100	61, 79, 89, 97	0
5	AE	148/162 (91%)	-0.30	0	100	100	51, 73, 82, 93	0
5	CE	148/162 (91%)	-0.24	0	100	100	53, 75, 84, 96	0
6	AF	100/101 (99%)	-0.22	0	100	100	63, 77, 87, 94	0
6	CF	100/101 (99%)	-0.25	0	100	100	62, 78, 87, 95	0
7	AG	155/156 (99%)	0.24	5 (3%)	45	9	74, 86, 99, 106	0
7	CG	155/156 (99%)	0.25	8 (5%)	26	6	75, 86, 99, 105	0
8	AH	137/138 (99%)	-0.09	0	100	100	60, 74, 82, 89	0
8	CH	137/138 (99%)	-0.10	0	100	100	62, 75, 83, 89	0
9	AI	127/128 (99%)	0.26	0	100	100	73, 91, 99, 101	0
9	CI	127/128 (99%)	0.78	9 (7%)	16	4	72, 93, 100, 102	0
10	AJ	97/105 (92%)	0.40	2 (2%)	60	12	73, 91, 100, 105	0
10	CJ	96/105 (91%)	0.55	1 (1%)	79	22	77, 93, 100, 104	0
11	AK	114/129 (88%)	-0.24	0	100	100	53, 74, 87, 91	0
11	CK	114/129 (88%)	-0.09	0	100	100	55, 76, 87, 92	0
12	AL	122/132 (92%)	-0.21	0	100	100	53, 68, 80, 87	0
12	CL	122/132 (92%)	-0.16	0	100	100	53, 69, 80, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	123/126 (97%)	0.25	4 (3%)	44	8	67, 85, 95, 105	0
13	CM	122/126 (96%)	0.36	6 (4%)	28	6	77, 92, 100, 109	0
14	AN	60/61 (98%)	0.06	0	100	100	75, 87, 94, 103	0
14	CN	60/61 (98%)	0.52	2 (3%)	44	8	77, 89, 94, 100	0
15	AO	88/89 (98%)	-0.13	0	100	100	55, 72, 85, 90	0
15	CO	88/89 (98%)	-0.14	0	100	100	55, 72, 85, 91	0
16	AP	82/88 (93%)	0.26	0	100	100	67, 78, 89, 94	0
16	CP	82/88 (93%)	0.02	0	100	100	66, 76, 88, 94	0
17	AQ	99/105 (94%)	-0.15	0	100	100	59, 72, 83, 90	0
17	CQ	99/105 (94%)	-0.12	0	100	100	58, 72, 83, 89	0
18	AR	68/88 (77%)	0.16	0	100	100	65, 73, 87, 91	0
18	CR	68/88 (77%)	0.15	0	100	100	64, 75, 87, 91	0
19	AS	83/93 (89%)	0.50	2 (2%)	56	11	77, 92, 99, 106	0
19	CS	83/93 (89%)	0.54	1 (1%)	75	20	79, 92, 101, 106	0
20	AT	96/106 (90%)	0.11	0	100	100	62, 76, 86, 90	0
20	CT	96/106 (90%)	0.07	0	100	100	62, 74, 86, 92	0
21	AU	23/27 (85%)	0.95	1 (4%)	34	7	73, 88, 93, 94	0
21	CU	23/27 (85%)	0.91	0	100	100	73, 89, 92, 94	0
22	AV	7/24 (29%)	0.58	0	100	100	65, 77, 102, 104	0
22	CV	6/24 (25%)	0.84	1 (16%)	2	1	67, 78, 103, 103	0
23	AX	76/77 (98%)	0.24	1 (1%)	74	19	52, 80, 97, 105	0
23	CX	76/77 (98%)	0.20	1 (1%)	74	19	52, 82, 100, 106	0
24	AW	6/10 (60%)	-0.23	1 (16%)	2	1	67, 81, 87, 98	0
24	CW	6/10 (60%)	-0.06	0	100	100	67, 78, 82, 87	0
25	BA	2731/2915 (93%)	-0.36	11 (0%)	90	41	23, 44, 85, 111	0
25	DA	2714/2915 (93%)	-0.54	11 (0%)	90	41	26, 47, 85, 118	0
26	BB	120/122 (98%)	-0.46	0	100	100	42, 68, 80, 95	0
26	DB	120/122 (98%)	-0.37	0	100	100	48, 74, 84, 97	0
27	BD	275/276 (99%)	-0.34	0	100	100	22, 42, 58, 77	0
27	DD	275/276 (99%)	-0.36	0	100	100	23, 44, 60, 79	0
28	BE	204/206 (99%)	-0.29	0	100	100	23, 45, 67, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DE	204/206 (99%)	-0.31	0 100 100	24, 47, 70, 88	0
29	BF	203/210 (96%)	-0.26	0 100 100	20, 51, 77, 94	0
29	DF	203/210 (96%)	-0.32	0 100 100	22, 54, 78, 93	0
30	BG	181/182 (99%)	-0.26	0 100 100	59, 77, 90, 103	0
30	DG	181/182 (99%)	0.01	0 100 100	63, 80, 92, 102	0
31	BH	174/180 (96%)	-0.25	0 100 100	50, 66, 78, 84	0
31	DH	174/180 (96%)	0.15	0 100 100	54, 71, 82, 87	0
32	BI	146/148 (98%)	-0.25	0 100 100	45, 75, 87, 92	0
32	DI	146/148 (98%)	0.01	0 100 100	48, 76, 86, 91	0
33	BN	140/140 (100%)	-0.33	0 100 100	32, 49, 68, 80	0
33	DN	140/140 (100%)	-0.35	0 100 100	34, 53, 72, 81	0
34	BO	122/122 (100%)	-0.34	0 100 100	25, 39, 60, 78	0
34	DO	122/122 (100%)	-0.32	0 100 100	34, 52, 68, 79	0
35	BP	149/150 (99%)	-0.27	0 100 100	26, 54, 76, 84	0
35	DP	149/150 (99%)	-0.13	0 100 100	30, 57, 79, 86	0
36	BQ	141/141 (100%)	-0.26	0 100 100	33, 51, 65, 79	0
36	DQ	141/141 (100%)	-0.31	0 100 100	35, 54, 70, 80	0
37	BR	118/118 (100%)	-0.38	0 100 100	22, 35, 51, 64	0
37	DR	118/118 (100%)	-0.30	0 100 100	36, 50, 64, 81	0
38	BS	110/112 (98%)	-0.23	0 100 100	38, 55, 69, 81	0
38	DS	110/112 (98%)	0.13	0 100 100	66, 78, 90, 100	0
39	BT	131/146 (89%)	-0.33	0 100 100	33, 45, 75, 91	0
39	DT	131/146 (89%)	-0.36	0 100 100	44, 56, 80, 86	0
40	BU	116/118 (98%)	-0.45	0 100 100	19, 30, 50, 63	0
40	DU	116/118 (98%)	-0.29	0 100 100	39, 61, 79, 88	0
41	BV	101/101 (100%)	-0.31	0 100 100	29, 52, 70, 77	0
41	DV	101/101 (100%)	-0.19	0 100 100	32, 58, 74, 79	0
42	BW	112/113 (99%)	-0.36	0 100 100	27, 37, 61, 94	0
42	DW	112/113 (99%)	-0.28	0 100 100	31, 40, 63, 94	0
43	BX	95/96 (98%)	-0.31	0 100 100	32, 46, 69, 82	0
43	DX	95/96 (98%)	-0.22	0 100 100	38, 50, 72, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BY	107/110 (97%)	-0.18	1 (0%) 81 24	44, 59, 77, 82	0
44	DY	107/110 (97%)	0.17	1 (0%) 81 24	46, 63, 80, 85	0
45	BZ	171/206 (83%)	-0.30	0 100 100	52, 71, 85, 93	0
45	DZ	174/206 (84%)	-0.14	0 100 100	56, 74, 87, 95	0
46	B0	83/85 (97%)	-0.11	3 (3%) 41 8	22, 40, 75, 104	0
46	D0	83/85 (97%)	0.10	2 (2%) 56 11	45, 66, 87, 98	0
47	B1	97/98 (98%)	-0.21	0 100 100	25, 42, 71, 77	0
47	D1	97/98 (98%)	-0.21	0 100 100	35, 56, 79, 85	0
48	B2	70/72 (97%)	-0.33	0 100 100	31, 48, 64, 77	0
48	D2	70/72 (97%)	-0.24	0 100 100	56, 73, 84, 86	0
49	B3	59/60 (98%)	-0.21	0 100 100	26, 38, 63, 86	0
49	D3	59/60 (98%)	0.07	1 (1%) 67 15	49, 62, 80, 93	0
50	B4	69/71 (97%)	-0.03	0 100 100	64, 87, 101, 104	0
50	D4	69/71 (97%)	0.19	2 (2%) 49 9	85, 95, 104, 107	0
51	B5	59/60 (98%)	-0.43	0 100 100	14, 35, 55, 71	0
51	D5	59/60 (98%)	-0.39	0 100 100	29, 51, 70, 77	0
52	B6	53/54 (98%)	-0.32	0 100 100	40, 54, 68, 74	0
52	D6	53/54 (98%)	-0.28	0 100 100	42, 58, 68, 74	0
53	B7	48/49 (97%)	-0.20	0 100 100	26, 32, 67, 78	0
53	D7	48/49 (97%)	-0.18	1 (2%) 60 12	27, 34, 66, 79	0
54	B8	64/65 (98%)	-0.26	0 100 100	33, 43, 51, 57	0
54	D8	64/65 (98%)	-0.21	0 100 100	34, 46, 56, 60	0
55	B9	37/37 (100%)	0.07	0 100 100	43, 52, 68, 77	0
55	D9	37/37 (100%)	0.65	3 (8%) 12 3	48, 57, 72, 78	0
All	All	20468/21468 (95%)	-0.21	147 (0%) 84 28	14, 65, 95, 119	0

The worst 5 of 147 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	CM	124	PRO	8.9
13	CM	123	ALA	6.8
13	AM	123	ALA	5.8
7	CG	78	ARG	5.5
1	CA	1030(B)	C	5.4



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
24	2QZ	AW	1	9/10	0.26	-	50,71,82,83	0
24	MVA	AW	5	8/9	0.20	-	69,82,86,91	0
24	2R3	AW	8	14/15	0.22	-	70,78,86,87	0
24	2R3	CW	8	14/15	0.13	-	62,69,77,78	0
24	2QY	CW	10	13/14	0.15	-	60,72,80,86	0
24	MVA	CW	5	8/9	0.23	-	76,88,91,99	0
24	2QZ	CW	1	9/10	0.27	-	63,71,80,101	0
24	2R1	CW	6	10/11	0.13	-	68,82,90,91	0
24	MVA	CW	9	8/9	0.23	-	70,73,84,91	0
24	004	CW	3	10/11	0.15	-	69,78,82,83	0
24	2QY	AW	10	13/14	0.13	-	49,70,87,100	0
24	2R1	AW	6	10/11	0.14	-	66,72,84,91	0
24	004	AW	3	10/11	0.12	-	67,87,95,97	0
24	MVA	AW	9	8/9	0.27	-	63,74,87,88	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
56	MG	BA	3054	1/1	0.18	-	39,39,39,39	0
56	MG	AA	3126	1/1	0.18	-	54,54,54,54	0
56	MG	DA	3292	1/1	0.17	-	34,34,34,34	0
56	MG	BA	3004	1/1	0.21	-	45,45,45,45	0
56	MG	BA	3337	1/1	0.10	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3385	1/1	0.34	-	58,58,58,58	0
56	MG	BA	3087	1/1	0.42	-	48,48,48,48	0
56	MG	BA	3456	1/1	0.21	-	24,24,24,24	0
56	MG	CA	3057	1/1	0.21	-	40,40,40,40	0
56	MG	DA	3532	1/1	0.10	-	60,60,60,60	0
56	MG	BA	3493	1/1	0.12	-	51,51,51,51	0
56	MG	DA	3369	1/1	0.05	-	53,53,53,53	0
56	MG	DA	3032	1/1	0.13	-	36,36,36,36	0
56	MG	DA	3613	1/1	0.30	-	64,64,64,64	0
56	MG	DA	3603	1/1	0.21	-	66,66,66,66	0
56	MG	AA	3016	1/1	0.11	-	70,70,70,70	0
56	MG	BA	3383	1/1	0.15	-	51,51,51,51	0
56	MG	DA	3263	1/1	0.15	-	48,48,48,48	0
56	MG	DA	3220	1/1	0.35	-	61,61,61,61	0
56	MG	DA	3615	1/1	0.09	-	57,57,57,57	0
56	MG	BA	3375	1/1	0.18	-	44,44,44,44	0
56	MG	DA	3268	1/1	0.15	-	42,42,42,42	0
56	MG	DA	3314	1/1	0.17	-	56,56,56,56	0
56	MG	BA	3263	1/1	0.58	-	35,35,35,35	0
56	MG	DA	3566	1/1	0.13	-	55,55,55,55	0
56	MG	BA	3393	1/1	0.18	-	27,27,27,27	0
56	MG	DA	3136	1/1	0.07	-	39,39,39,39	0
58	ZN	B6	501	1/1	0.12	-	51,51,51,51	0
56	MG	DA	3394	1/1	0.07	-	46,46,46,46	0
56	MG	DA	3393	1/1	0.24	-	35,35,35,35	0
56	MG	BA	3155	1/1	0.46	-	56,56,56,56	0
56	MG	DA	3299	1/1	0.12	-	35,35,35,35	0
56	MG	DA	3165	1/1	0.28	-	48,48,48,48	0
56	MG	DA	3347	1/1	0.20	-	39,39,39,39	0
56	MG	BA	3301	1/1	0.56	-	44,44,44,44	0
56	MG	BA	3062	1/1	0.40	-	46,46,46,46	0
56	MG	BA	3532	1/1	0.22	-	42,42,42,42	0
56	MG	BA	3606	1/1	0.09	-	44,44,44,44	0
56	MG	BA	3575	1/1	0.14	-	26,26,26,26	0
56	MG	BA	3648	1/1	0.18	-	54,54,54,54	0
56	MG	DA	3162	1/1	0.11	-	69,69,69,69	0
56	MG	CA	3025	1/1	0.13	-	102,102,102,102	0
56	MG	AA	3007	1/1	0.14	-	68,68,68,68	0
56	MG	BF	306	1/1	0.42	-	52,52,52,52	0
56	MG	AA	3019	1/1	0.48	-	64,64,64,64	0
56	MG	CA	3156	1/1	0.26	-	80,80,80,80	0
56	MG	CA	3027	1/1	0.34	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3158	1/1	0.43	-	47,47,47,47	0
56	MG	B3	3402	1/1	0.09	-	49,49,49,49	0
56	MG	CA	3009	1/1	0.12	-	55,55,55,55	0
56	MG	BA	3472	1/1	0.12	-	53,53,53,53	0
56	MG	BA	3505	1/1	0.27	-	45,45,45,45	0
56	MG	BA	3705	1/1	0.22	-	64,64,64,64	0
56	MG	BA	3354	1/1	0.27	-	45,45,45,45	0
56	MG	BA	3469	1/1	0.13	-	60,60,60,60	0
56	MG	BA	3594	1/1	0.35	-	55,55,55,55	0
56	MG	DA	3618	1/1	0.26	-	61,61,61,61	0
56	MG	DA	3517	1/1	0.27	-	47,47,47,47	0
56	MG	CA	3163	1/1	0.24	-	60,60,60,60	0
56	MG	BD	301	1/1	0.38	-	35,35,35,35	0
56	MG	BA	3218	1/1	0.11	-	58,58,58,58	0
56	MG	BA	3068	1/1	0.44	-	43,43,43,43	0
56	MG	DA	3021	1/1	0.10	-	43,43,43,43	0
56	MG	DA	3377	1/1	0.19	-	32,32,32,32	0
56	MG	BA	3576	1/1	0.10	-	45,45,45,45	0
56	MG	BA	3082	1/1	0.17	-	54,54,54,54	0
56	MG	BA	3293	1/1	0.30	-	69,69,69,69	0
56	MG	BA	3515	1/1	0.23	-	46,46,46,46	0
56	MG	BA	3715	1/1	0.29	-	44,44,44,44	0
56	MG	BA	3453	1/1	0.29	-	54,54,54,54	0
56	MG	BA	3553	1/1	0.17	-	46,46,46,46	0
56	MG	DA	3275	1/1	0.25	-	34,34,34,34	0
56	MG	AA	3057	1/1	0.15	-	45,45,45,45	0
56	MG	AA	3071	1/1	0.30	-	60,60,60,60	0
56	MG	AM	3001	1/1	0.08	-	76,76,76,76	0
56	MG	DA	3647	1/1	0.56	-	45,45,45,45	0
56	MG	CA	3037	1/1	0.24	-	45,45,45,45	0
56	MG	DA	3041	1/1	0.37	-	54,54,54,54	0
56	MG	BA	3036	1/1	0.17	-	25,25,25,25	0
56	MG	BA	3332	1/1	0.12	-	52,52,52,52	0
56	MG	BA	3443	1/1	0.31	-	34,34,34,34	0
56	MG	BA	3708	1/1	0.28	-	38,38,38,38	0
56	MG	DA	3248	1/1	0.20	-	30,30,30,30	0
56	MG	DA	3321	1/1	0.11	-	31,31,31,31	0
56	MG	DA	3214	1/1	0.09	-	48,48,48,48	0
56	MG	DA	3280	1/1	0.22	-	46,46,46,46	0
56	MG	BA	3307	1/1	0.16	-	35,35,35,35	0
56	MG	BA	3459	1/1	0.12	-	51,51,51,51	0
56	MG	AA	3183	1/1	0.10	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3123	1/1	0.37	-	38,38,38,38	0
56	MG	DA	3398	1/1	0.14	-	50,50,50,50	0
56	MG	DA	3022	1/1	0.17	-	41,41,41,41	0
56	MG	AA	3206	1/1	0.15	-	79,79,79,79	0
56	MG	DD	305	1/1	0.16	-	73,73,73,73	0
56	MG	CA	3061	1/1	0.49	-	68,68,68,68	0
56	MG	CA	3099	1/1	0.39	-	64,64,64,64	0
56	MG	AA	3027	1/1	0.30	-	67,67,67,67	0
56	MG	DA	3195	1/1	0.21	-	51,51,51,51	0
56	MG	DA	3522	1/1	0.22	-	46,46,46,46	0
56	MG	BA	3310	1/1	0.12	-	59,59,59,59	0
56	MG	BA	3410	1/1	0.17	-	21,21,21,21	0
58	ZN	DY	501	1/1	0.04	-	90,90,90,90	0
56	MG	DF	303	1/1	0.25	-	42,42,42,42	0
56	MG	DA	3403	1/1	0.21	-	42,42,42,42	0
56	MG	AA	3054	1/1	0.21	-	46,46,46,46	0
56	MG	CA	3011	1/1	0.26	-	27,27,27,27	0
56	MG	DA	3563	1/1	0.13	-	49,49,49,49	0
56	MG	BA	3152	1/1	0.07	-	52,52,52,52	0
56	MG	BA	3298	1/1	0.37	-	45,45,45,45	0
56	MG	DF	305	1/1	0.51	-	55,55,55,55	0
56	MG	DA	3642	1/1	0.19	-	67,67,67,67	0
56	MG	AA	3219	1/1	0.17	-	54,54,54,54	0
56	MG	BA	3222	1/1	0.50	-	56,56,56,56	0
56	MG	DA	3232	1/1	0.13	-	39,39,39,39	0
56	MG	BA	3356	1/1	0.13	-	33,33,33,33	0
56	MG	BA	3500	1/1	0.12	-	43,43,43,43	0
56	MG	BA	3671	1/1	0.14	-	44,44,44,44	0
56	MG	BA	3401	1/1	0.16	-	49,49,49,49	0
56	MG	BA	3193	1/1	0.46	-	53,53,53,53	0
56	MG	DA	3243	1/1	0.40	-	49,49,49,49	0
56	MG	DA	3600	1/1	0.14	-	73,73,73,73	0
56	MG	BA	3335	1/1	0.14	-	51,51,51,51	0
56	MG	BA	3581	1/1	0.33	-	54,54,54,54	0
56	MG	CA	3001	1/1	0.18	-	48,48,48,48	0
56	MG	BR	202	1/1	0.25	-	25,25,25,25	0
56	MG	DA	3361	1/1	0.15	-	58,58,58,58	0
56	MG	DA	3400	1/1	0.20	-	42,42,42,42	0
56	MG	AA	3049	1/1	0.36	-	46,46,46,46	0
56	MG	BA	3259	1/1	0.21	-	59,59,59,59	0
56	MG	BA	3199	1/1	0.33	-	31,31,31,31	0
56	MG	DA	3301	1/1	0.28	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	K	DA	3234	1/1	0.24	-	102,102,102,102	0
56	MG	AF	3001	1/1	0.16	-	62,62,62,62	0
56	MG	AA	3061	1/1	0.14	-	57,57,57,57	0
56	MG	BA	3518	1/1	0.09	-	52,52,52,52	0
56	MG	BA	3630	1/1	0.13	-	48,48,48,48	0
56	MG	DA	3555	1/1	0.14	-	43,43,43,43	0
56	MG	BA	3286	1/1	0.25	-	42,42,42,42	0
56	MG	AA	3134	1/1	0.29	-	70,70,70,70	0
56	MG	BA	3270	1/1	0.29	-	29,29,29,29	0
56	MG	BA	3642	1/1	0.14	-	52,52,52,52	0
56	MG	DB	3009	1/1	0.37	-	41,41,41,41	0
56	MG	BA	3092	1/1	0.24	-	28,28,28,28	0
56	MG	BA	3071	1/1	0.24	-	55,55,55,55	0
56	MG	BA	3067	1/1	0.42	-	55,55,55,55	0
56	MG	AA	3042	1/1	0.26	-	50,50,50,50	0
56	MG	DA	3656	1/1	0.11	-	62,62,62,62	0
56	MG	DA	3186	1/1	0.33	-	38,38,38,38	0
56	MG	CA	3040	1/1	0.38	-	47,47,47,47	0
56	MG	BA	3445	1/1	0.16	-	16,16,16,16	0
56	MG	BB	3007	1/1	0.12	-	49,49,49,49	0
56	MG	AA	3191	1/1	0.12	-	56,56,56,56	0
56	MG	BA	3623	1/1	0.16	-	43,43,43,43	0
56	MG	BV	3002	1/1	0.63	-	42,42,42,42	0
56	MG	BA	3462	1/1	0.22	-	30,30,30,30	0
56	MG	BA	3190	1/1	0.33	-	42,42,42,42	0
56	MG	DA	3439	1/1	0.22	-	45,45,45,45	0
56	MG	BA	3265	1/1	0.24	-	39,39,39,39	0
56	MG	DA	3096	1/1	0.33	-	68,68,68,68	0
56	MG	CA	3142	1/1	0.23	-	80,80,80,80	0
56	MG	DA	3097	1/1	0.18	-	58,58,58,58	0
56	MG	BA	3387	1/1	0.28	-	49,49,49,49	0
56	MG	BA	3334	1/1	0.14	-	41,41,41,41	0
56	MG	CA	3032	1/1	0.21	-	44,44,44,44	0
56	MG	BA	3548	1/1	0.29	-	40,40,40,40	0
56	MG	DA	3611	1/1	0.15	-	51,51,51,51	0
56	MG	BA	3446	1/1	0.20	-	25,25,25,25	0
56	MG	BA	3069	1/1	0.11	-	33,33,33,33	0
56	MG	DA	3178	1/1	0.18	-	43,43,43,43	0
56	MG	AA	3159	1/1	0.28	-	57,57,57,57	0
56	MG	CA	3114	1/1	0.21	-	67,67,67,67	0
56	MG	BB	3014	1/1	0.09	-	68,68,68,68	0
56	MG	BA	3524	1/1	0.13	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3045	1/1	0.15	-	27,27,27,27	0
56	MG	AA	3034	1/1	0.23	-	46,46,46,46	0
56	MG	BA	3225	1/1	0.39	-	42,42,42,42	0
56	MG	BA	3271	1/1	0.32	-	40,40,40,40	0
56	MG	DA	3052	1/1	0.12	-	20,20,20,20	0
56	MG	BA	3070	1/1	0.26	-	46,46,46,46	0
56	MG	BD	306	1/1	0.59	-	47,47,47,47	0
56	MG	BA	3289	1/1	0.12	-	53,53,53,53	0
56	MG	BA	3291	1/1	0.16	-	44,44,44,44	0
56	MG	AA	3109	1/1	0.22	-	59,59,59,59	0
56	MG	DA	3255	1/1	0.16	-	46,46,46,46	0
56	MG	DA	3520	1/1	0.10	-	38,38,38,38	0
56	MG	DA	3040	1/1	0.21	-	45,45,45,45	0
56	MG	AA	3119	1/1	0.32	-	42,42,42,42	0
56	MG	BA	3699	1/1	0.15	-	23,23,23,23	0
56	MG	BA	3415	1/1	0.14	-	28,28,28,28	0
56	MG	BA	3230	1/1	1.00	-	70,70,70,70	0
56	MG	DA	3371	1/1	0.24	-	37,37,37,37	0
56	MG	BA	3129	1/1	0.63	-	44,44,44,44	0
56	MG	BA	3114	1/1	0.28	-	46,46,46,46	0
56	MG	BA	3562	1/1	0.14	-	42,42,42,42	0
56	MG	CA	3140	1/1	0.15	-	75,75,75,75	0
56	MG	D8	5001	1/1	0.22	-	53,53,53,53	0
56	MG	DA	3326	1/1	0.10	-	61,61,61,61	0
56	MG	BA	3640	1/1	0.20	-	31,31,31,31	0
56	MG	DA	3558	1/1	0.20	-	77,77,77,77	0
56	MG	CA	3047	1/1	0.17	-	56,56,56,56	0
56	MG	BA	3073	1/1	0.17	-	43,43,43,43	0
56	MG	BA	3083	1/1	0.13	-	33,33,33,33	0
56	MG	BG	3004	1/1	0.06	-	53,53,53,53	0
56	MG	DA	3420	1/1	0.05	-	43,43,43,43	0
56	MG	DA	3429	1/1	0.08	-	30,30,30,30	0
56	MG	DA	3583	1/1	0.24	-	35,35,35,35	0
56	MG	DA	3472	1/1	0.19	-	38,38,38,38	0
56	MG	BA	3386	1/1	0.13	-	29,29,29,29	0
56	MG	BA	3584	1/1	0.09	-	43,43,43,43	0
56	MG	BA	3228	1/1	0.32	-	23,23,23,23	0
56	MG	AA	3211	1/1	0.12	-	58,58,58,58	0
56	MG	BA	3013	1/1	0.43	-	36,36,36,36	0
56	MG	DA	3387	1/1	0.14	-	50,50,50,50	0
56	MG	DA	3375	1/1	0.09	-	40,40,40,40	0
56	MG	DA	3307	1/1	0.11	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3193	1/1	0.19	-	42,42,42,42	0
56	MG	DA	3481	1/1	0.09	-	59,59,59,59	0
56	MG	CA	3100	1/1	0.17	-	72,72,72,72	0
56	MG	CA	3004	1/1	0.32	-	88,88,88,88	0
56	MG	DA	3210	1/1	0.33	-	46,46,46,46	0
56	MG	DV	202	1/1	0.69	-	45,45,45,45	0
56	MG	CA	3155	1/1	0.15	-	71,71,71,71	0
56	MG	AA	3079	1/1	0.86	-	65,65,65,65	0
56	MG	BA	3707	1/1	0.16	-	57,57,57,57	0
56	MG	DA	3281	1/1	0.14	-	33,33,33,33	0
56	MG	DA	3372	1/1	0.10	-	37,37,37,37	0
56	MG	BA	3512	1/1	0.18	-	42,42,42,42	0
56	MG	AA	3155	1/1	0.18	-	54,54,54,54	0
56	MG	CA	3086	1/1	0.14	-	70,70,70,70	0
58	ZN	D9	501	1/1	0.05	-	63,63,63,63	0
56	MG	CA	3118	1/1	0.07	-	39,39,39,39	0
56	MG	BE	308	1/1	0.26	-	27,27,27,27	0
56	MG	BA	3637	1/1	0.79	-	52,52,52,52	0
56	MG	DA	3039	1/1	0.55	-	46,46,46,46	0
56	MG	CA	3083	1/1	0.10	-	30,30,30,30	0
56	MG	AA	3194	1/1	0.16	-	50,50,50,50	0
56	MG	AA	3069	1/1	0.07	-	77,77,77,77	0
56	MG	DA	3649	1/1	0.10	-	39,39,39,39	0
56	MG	BA	3219	1/1	0.39	-	36,36,36,36	0
56	MG	BA	3046	1/1	0.41	-	52,52,52,52	0
56	MG	AA	3102	1/1	0.05	-	68,68,68,68	0
56	MG	DA	3033	1/1	0.21	-	41,41,41,41	0
56	MG	CA	3126	1/1	0.24	-	56,56,56,56	0
56	MG	BW	3005	1/1	0.42	-	38,38,38,38	0
56	MG	DA	3592	1/1	0.14	-	49,49,49,49	0
56	MG	BA	3368	1/1	0.16	-	22,22,22,22	0
56	MG	AA	3199	1/1	0.12	-	62,62,62,62	0
56	MG	BA	3312	1/1	0.10	-	43,43,43,43	0
56	MG	DA	3457	1/1	0.14	-	44,44,44,44	0
56	MG	DA	3153	1/1	0.31	-	51,51,51,51	0
56	MG	AA	3204	1/1	0.15	-	70,70,70,70	0
56	MG	BU	203	1/1	0.28	-	26,26,26,26	0
56	MG	AX	109	1/1	0.10	-	56,56,56,56	0
56	MG	BA	3714	1/1	0.14	-	72,72,72,72	0
56	MG	DA	3168	1/1	0.62	-	46,46,46,46	0
56	MG	AA	3133	1/1	0.76	-	71,71,71,71	0
56	MG	B7	103	1/1	0.45	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3036	1/1	0.19	-	69,69,69,69	0
56	MG	BA	3084	1/1	0.52	-	47,47,47,47	0
56	MG	BA	3608	1/1	0.15	-	51,51,51,51	0
56	MG	AA	3022	1/1	0.24	-	56,56,56,56	0
56	MG	BA	3327	1/1	0.16	-	21,21,21,21	0
56	MG	BA	3571	1/1	0.22	-	48,48,48,48	0
56	MG	BA	3616	1/1	0.28	-	73,73,73,73	0
56	MG	DA	3144	1/1	0.34	-	37,37,37,37	0
56	MG	CA	3165	1/1	0.18	-	47,47,47,47	0
56	MG	DA	3297	1/1	0.15	-	36,36,36,36	0
56	MG	DA	3422	1/1	0.21	-	45,45,45,45	0
56	MG	CA	3088	1/1	0.20	-	49,49,49,49	0
56	MG	DA	3217	1/1	0.27	-	33,33,33,33	0
56	MG	BA	3052	1/1	0.25	-	29,29,29,29	0
56	MG	DA	3318	1/1	0.19	-	47,47,47,47	0
56	MG	DA	3114	1/1	0.16	-	47,47,47,47	0
56	MG	DA	3629	1/1	0.13	-	30,30,30,30	0
56	MG	BD	312	1/1	0.94	-	72,72,72,72	0
56	MG	DA	3290	1/1	0.19	-	59,59,59,59	0
56	MG	BA	3049	1/1	0.18	-	17,17,17,17	0
56	MG	DA	3070	1/1	0.31	-	51,51,51,51	0
56	MG	AA	3009	1/1	0.25	-	71,71,71,71	0
56	MG	BA	3680	1/1	0.24	-	62,62,62,62	0
56	MG	D5	102	1/1	0.54	-	44,44,44,44	0
56	MG	BA	3314	1/1	0.13	-	22,22,22,22	0
56	MG	DB	3011	1/1	0.34	-	49,49,49,49	0
56	MG	CA	3129	1/1	0.23	-	54,54,54,54	0
56	MG	BA	3123	1/1	0.22	-	47,47,47,47	0
56	MG	BA	3380	1/1	0.07	-	32,32,32,32	0
56	MG	BA	3017	1/1	0.33	-	38,38,38,38	0
56	MG	BA	3421	1/1	0.14	-	28,28,28,28	0
56	MG	DA	3173	1/1	0.26	-	50,50,50,50	0
56	MG	DA	3282	1/1	0.30	-	58,58,58,58	0
56	MG	CF	3001	1/1	0.19	-	56,56,56,56	0
56	MG	AA	3212	1/1	0.16	-	36,36,36,36	0
56	MG	DA	3304	1/1	0.19	-	44,44,44,44	0
56	MG	DA	3386	1/1	0.18	-	18,18,18,18	0
56	MG	CA	3162	1/1	0.26	-	60,60,60,60	0
56	MG	BA	3540	1/1	0.33	-	29,29,29,29	0
56	MG	DA	3395	1/1	0.14	-	40,40,40,40	0
56	MG	BA	3423	1/1	0.36	-	45,45,45,45	0
56	MG	BA	3205	1/1	0.31	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3668	1/1	0.21	-	42,42,42,42	0
56	MG	CA	3031	1/1	0.32	-	55,55,55,55	0
56	MG	CA	3003	1/1	0.14	-	69,69,69,69	0
56	MG	BA	3130	1/1	0.38	-	51,51,51,51	0
56	MG	BA	3085	1/1	0.36	-	35,35,35,35	0
56	MG	DA	3445	1/1	0.47	-	60,60,60,60	0
56	MG	BA	3626	1/1	0.13	-	50,50,50,50	0
56	MG	AA	3218	1/1	0.24	-	73,73,73,73	0
56	MG	AA	3106	1/1	0.26	-	68,68,68,68	0
56	MG	CA	3141	1/1	0.32	-	85,85,85,85	0
56	MG	AX	106	1/1	0.09	-	64,64,64,64	0
56	MG	BA	3266	1/1	0.22	-	47,47,47,47	0
58	ZN	B4	501	1/1	0.08	-	152,152,152,152	0
56	MG	DA	3174	1/1	0.42	-	26,26,26,26	0
56	MG	BA	3055	1/1	0.26	-	44,44,44,44	0
56	MG	DA	3121	1/1	0.27	-	46,46,46,46	0
56	MG	CA	3026	1/1	0.13	-	52,52,52,52	0
56	MG	DA	3519	1/1	0.13	-	39,39,39,39	0
56	MG	BA	3537	1/1	0.17	-	45,45,45,45	0
56	MG	DA	3123	1/1	0.17	-	61,61,61,61	0
56	MG	BA	3722	1/1	0.27	-	49,49,49,49	0
56	MG	BA	3636	1/1	0.11	-	54,54,54,54	0
56	MG	BA	3095	1/1	0.73	-	55,55,55,55	0
56	MG	DA	3654	1/1	0.29	-	50,50,50,50	0
56	MG	BA	3371	1/1	0.19	-	38,38,38,38	0
56	MG	B7	104	1/1	0.19	-	55,55,55,55	0
56	MG	DA	3417	1/1	0.21	-	54,54,54,54	0
56	MG	BA	3713	1/1	0.22	-	49,49,49,49	0
56	MG	DA	3228	1/1	0.18	-	49,49,49,49	0
56	MG	DA	3362	1/1	0.33	-	42,42,42,42	0
56	MG	BA	3248	1/1	0.39	-	68,68,68,68	0
56	MG	DA	3590	1/1	0.18	-	39,39,39,39	0
56	MG	DA	3657	1/1	0.39	-	55,55,55,55	0
56	MG	DA	3501	1/1	0.09	-	67,67,67,67	0
56	MG	DA	3570	1/1	0.12	-	67,67,67,67	0
56	MG	B0	101	1/1	0.21	-	57,57,57,57	0
56	MG	BA	3351	1/1	0.24	-	21,21,21,21	0
56	MG	DD	301	1/1	0.24	-	23,23,23,23	0
56	MG	AA	3201	1/1	0.12	-	76,76,76,76	0
56	MG	DA	3313	1/1	0.18	-	30,30,30,30	0
56	MG	BA	3437	1/1	0.14	-	37,37,37,37	0
56	MG	BA	3104	1/1	0.37	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BW	3004	1/1	0.66	-	46,46,46,46	0
56	MG	BA	3234	1/1	0.36	-	48,48,48,48	0
56	MG	BA	3549	1/1	0.30	-	49,49,49,49	0
56	MG	CA	3132	1/1	0.08	-	66,66,66,66	0
56	MG	BA	3316	1/1	0.13	-	51,51,51,51	0
56	MG	BA	3001	1/1	0.29	-	52,52,52,52	0
56	MG	BA	3223	1/1	0.44	-	49,49,49,49	0
56	MG	DA	3020	1/1	0.27	-	45,45,45,45	0
56	MG	BA	3331	1/1	0.17	-	61,61,61,61	0
56	MG	AA	3070	1/1	0.23	-	68,68,68,68	0
56	MG	BA	3110	1/1	0.26	-	43,43,43,43	0
56	MG	DA	3390	1/1	0.18	-	58,58,58,58	0
56	MG	BA	3012	1/1	0.10	-	34,34,34,34	0
56	MG	BA	3064	1/1	0.37	-	49,49,49,49	0
56	MG	DA	3315	1/1	0.11	-	39,39,39,39	0
56	MG	DA	3064	1/1	0.38	-	55,55,55,55	0
56	MG	BA	3333	1/1	0.15	-	27,27,27,27	0
56	MG	DA	3454	1/1	0.12	-	52,52,52,52	0
56	MG	BA	3239	1/1	0.21	-	33,33,33,33	0
56	MG	BA	3044	1/1	0.36	-	32,32,32,32	0
56	MG	AA	3128	1/1	0.16	-	64,64,64,64	0
56	MG	BA	3481	1/1	0.19	-	41,41,41,41	0
56	MG	AA	3125	1/1	0.14	-	56,56,56,56	0
56	MG	BB	3002	1/1	0.20	-	49,49,49,49	0
56	MG	DA	3215	1/1	0.32	-	43,43,43,43	0
56	MG	DA	3421	1/1	0.17	-	43,43,43,43	0
56	MG	BA	3252	1/1	0.55	-	65,65,65,65	0
56	MG	BA	3256	1/1	0.12	-	60,60,60,60	0
56	MG	DA	3616	1/1	0.17	-	41,41,41,41	0
56	MG	DA	3221	1/1	0.29	-	56,56,56,56	0
56	MG	BA	3593	1/1	0.12	-	51,51,51,51	0
56	MG	BA	3210	1/1	0.29	-	39,39,39,39	0
56	MG	BA	3660	1/1	0.14	-	58,58,58,58	0
56	MG	BA	3476	1/1	0.08	-	47,47,47,47	0
56	MG	DA	3117	1/1	0.16	-	46,46,46,46	0
56	MG	BA	3079	1/1	0.26	-	50,50,50,50	0
56	MG	BA	3094	1/1	0.40	-	62,62,62,62	0
56	MG	DA	3111	1/1	0.20	-	67,67,67,67	0
56	MG	BA	3681	1/1	0.17	-	54,54,54,54	0
56	MG	CA	3072	1/1	0.24	-	57,57,57,57	0
56	MG	BA	3409	1/1	0.17	-	40,40,40,40	0
56	MG	B1	3002	1/1	0.13	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BN	3004	1/1	0.46	-	69,69,69,69	0
56	MG	CA	3043	1/1	0.34	-	62,62,62,62	0
56	MG	BA	3377	1/1	0.14	-	27,27,27,27	0
56	MG	DA	3402	1/1	0.17	-	33,33,33,33	0
56	MG	BA	3484	1/1	0.16	-	40,40,40,40	0
56	MG	BA	3319	1/1	0.13	-	34,34,34,34	0
56	MG	DA	3559	1/1	0.11	-	47,47,47,47	0
56	MG	AA	3130	1/1	0.17	-	55,55,55,55	0
56	MG	BA	3565	1/1	0.15	-	75,75,75,75	0
56	MG	BA	3602	1/1	0.15	-	44,44,44,44	0
56	MG	BA	3187	1/1	0.22	-	53,53,53,53	0
56	MG	DA	3166	1/1	0.10	-	37,37,37,37	0
56	MG	CA	3052	1/1	0.16	-	47,47,47,47	0
56	MG	B2	101	1/1	0.28	-	34,34,34,34	0
56	MG	BA	3157	1/1	0.34	-	52,52,52,52	0
56	MG	BA	3672	1/1	0.28	-	63,63,63,63	0
56	MG	DA	3303	1/1	0.15	-	37,37,37,37	0
56	MG	DA	3451	1/1	0.08	-	68,68,68,68	0
56	MG	DA	3638	1/1	0.10	-	53,53,53,53	0
56	MG	CA	3048	1/1	0.23	-	70,70,70,70	0
56	MG	AA	3077	1/1	0.39	-	67,67,67,67	0
56	MG	DA	3099	1/1	0.36	-	39,39,39,39	0
56	MG	AA	3104	1/1	0.19	-	35,35,35,35	0
56	MG	BA	3450	1/1	0.14	-	40,40,40,40	0
56	MG	BA	3113	1/1	0.22	-	48,48,48,48	0
56	MG	BA	3605	1/1	0.10	-	35,35,35,35	0
56	MG	BA	3349	1/1	0.18	-	31,31,31,31	0
56	MG	DF	304	1/1	0.59	-	39,39,39,39	0
56	MG	BA	3374	1/1	0.29	-	26,26,26,26	0
56	MG	AA	3058	1/1	0.36	-	59,59,59,59	0
56	MG	DA	3079	1/1	0.25	-	44,44,44,44	0
56	MG	BA	3192	1/1	0.38	-	48,48,48,48	0
56	MG	AA	3135	1/1	0.31	-	49,49,49,49	0
56	MG	BA	3734	1/1	0.36	-	42,42,42,42	0
56	MG	DA	3448	1/1	0.38	-	67,67,67,67	0
56	MG	DA	3049	1/1	0.21	-	56,56,56,56	0
56	MG	AA	3051	1/1	0.17	-	56,56,56,56	0
56	MG	CN	502	1/1	0.30	-	70,70,70,70	0
56	MG	BA	3076	1/1	0.23	-	40,40,40,40	0
56	MG	BA	3008	1/1	0.14	-	30,30,30,30	0
56	MG	DA	3047	1/1	0.12	-	36,36,36,36	0
56	MG	DA	3007	1/1	0.27	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3135	1/1	0.39	-	61,61,61,61	0
56	MG	DA	3539	1/1	0.22	-	35,35,35,35	0
56	MG	AA	3146	1/1	0.24	-	55,55,55,55	0
56	MG	DE	306	1/1	0.12	-	44,44,44,44	0
56	MG	DA	3370	1/1	0.22	-	40,40,40,40	0
56	MG	DA	3349	1/1	0.09	-	27,27,27,27	0
56	MG	DA	3235	1/1	0.38	-	46,46,46,46	0
56	MG	DA	3645	1/1	0.35	-	57,57,57,57	0
56	MG	BA	3323	1/1	0.16	-	25,25,25,25	0
56	MG	BA	3247	1/1	0.22	-	58,58,58,58	0
56	MG	DA	3355	1/1	0.40	-	39,39,39,39	0
56	MG	DA	3116	1/1	0.40	-	43,43,43,43	0
56	MG	DA	3364	1/1	0.17	-	40,40,40,40	0
56	MG	B7	101	1/1	0.18	-	45,45,45,45	0
56	MG	DA	3591	1/1	0.14	-	67,67,67,67	0
56	MG	AA	3015	1/1	0.25	-	74,74,74,74	0
56	MG	AA	3008	1/1	0.23	-	61,61,61,61	0
56	MG	CA	3137	1/1	0.14	-	59,59,59,59	0
56	MG	BB	3017	1/1	0.23	-	80,80,80,80	0
56	MG	CX	102	1/1	0.07	-	60,60,60,60	0
56	MG	BA	3429	1/1	0.16	-	55,55,55,55	0
56	MG	BA	3434	1/1	0.30	-	22,22,22,22	0
56	MG	CA	3090	1/1	0.17	-	63,63,63,63	0
56	MG	CA	3158	1/1	0.11	-	64,64,64,64	0
56	MG	DA	3098	1/1	1.07	-	45,45,45,45	0
56	MG	AA	3023	1/1	0.12	-	56,56,56,56	0
56	MG	CA	3019	1/1	0.15	-	62,62,62,62	0
56	MG	BA	3300	1/1	0.25	-	48,48,48,48	0
56	MG	DA	3484	1/1	0.06	-	47,47,47,47	0
56	MG	DB	3002	1/1	0.23	-	72,72,72,72	0
56	MG	DA	3594	1/1	0.21	-	63,63,63,63	0
56	MG	DA	3447	1/1	0.17	-	56,56,56,56	0
56	MG	BA	3666	1/1	0.37	-	54,54,54,54	0
56	MG	BA	3102	1/1	0.07	-	45,45,45,45	0
56	MG	AA	3171	1/1	0.33	-	77,77,77,77	0
56	MG	BA	3737	1/1	0.26	-	39,39,39,39	0
56	MG	DA	3489	1/1	0.08	-	36,36,36,36	0
56	MG	BA	3470	1/1	0.05	-	44,44,44,44	0
56	MG	BA	3521	1/1	0.14	-	38,38,38,38	0
56	MG	BA	3555	1/1	0.23	-	31,31,31,31	0
56	MG	DA	3383	1/1	0.18	-	27,27,27,27	0
56	MG	BB	3004	1/1	0.29	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3569	1/1	0.07	-	55,55,55,55	0
56	MG	DA	3198	1/1	0.33	-	34,34,34,34	0
56	MG	AA	3116	1/1	0.47	-	62,62,62,62	0
56	MG	DA	3026	1/1	0.20	-	36,36,36,36	0
56	MG	BA	3704	1/1	0.38	-	58,58,58,58	0
56	MG	BA	3552	1/1	0.25	-	30,30,30,30	0
56	MG	AA	3010	1/1	0.13	-	71,71,71,71	0
56	MG	DA	3019	1/1	0.21	-	32,32,32,32	0
56	MG	CA	3069	1/1	0.22	-	63,63,63,63	0
56	MG	BA	3509	1/1	0.20	-	29,29,29,29	0
56	MG	BA	3709	1/1	0.16	-	77,77,77,77	0
56	MG	BA	3254	1/1	0.28	-	40,40,40,40	0
56	MG	DA	3567	1/1	0.10	-	68,68,68,68	0
56	MG	CA	3046	1/1	0.17	-	52,52,52,52	0
56	MG	BA	3433	1/1	0.28	-	46,46,46,46	0
56	MG	BA	3649	1/1	0.27	-	43,43,43,43	0
56	MG	DA	3273	1/1	0.24	-	32,32,32,32	0
56	MG	BA	3582	1/1	0.21	-	52,52,52,52	0
56	MG	BA	3184	1/1	0.65	-	51,51,51,51	0
56	MG	DA	3167	1/1	0.26	-	46,46,46,46	0
56	MG	BA	3041	1/1	0.35	-	45,45,45,45	0
56	MG	BA	3274	1/1	0.19	-	54,54,54,54	0
56	MG	DA	3182	1/1	0.20	-	29,29,29,29	0
56	MG	DA	3427	1/1	0.16	-	29,29,29,29	0
56	MG	DA	3302	1/1	0.25	-	42,42,42,42	0
56	MG	BB	3003	1/1	0.24	-	40,40,40,40	0
56	MG	CA	3171	1/1	0.16	-	61,61,61,61	0
56	MG	DA	3261	1/1	0.24	-	44,44,44,44	0
56	MG	CA	3084	1/1	0.18	-	80,80,80,80	0
56	MG	DA	3461	1/1	0.08	-	40,40,40,40	0
56	MG	DA	3336	1/1	0.14	-	36,36,36,36	0
56	MG	AX	107	1/1	0.41	-	82,82,82,82	0
56	MG	DA	3078	1/1	0.17	-	49,49,49,49	0
56	MG	BA	3343	1/1	0.19	-	37,37,37,37	0
56	MG	BA	3246	1/1	0.32	-	38,38,38,38	0
56	MG	DA	3627	1/1	0.23	-	52,52,52,52	0
56	MG	BA	3647	1/1	0.25	-	40,40,40,40	0
56	MG	BA	3489	1/1	0.11	-	50,50,50,50	0
56	MG	DA	3258	1/1	0.25	-	39,39,39,39	0
56	MG	BA	3449	1/1	0.10	-	59,59,59,59	0
56	MG	AA	3012	1/1	0.15	-	58,58,58,58	0
56	MG	BA	3023	1/1	0.42	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3602	1/1	0.17	-	63,63,63,63	0
56	MG	CA	3095	1/1	0.17	-	35,35,35,35	0
56	MG	CA	3148	1/1	0.19	-	65,65,65,65	0
56	MG	DA	3503	1/1	0.06	-	41,41,41,41	0
56	MG	DA	3084	1/1	0.18	-	55,55,55,55	0
56	MG	AA	3004	1/1	0.14	-	50,50,50,50	0
56	MG	BA	3224	1/1	0.35	-	48,48,48,48	0
56	MG	AA	3168	1/1	0.31	-	80,80,80,80	0
56	MG	BA	3435	1/1	0.24	-	59,59,59,59	0
56	MG	BA	3132	1/1	0.20	-	28,28,28,28	0
56	MG	AX	110	1/1	0.16	-	45,45,45,45	0
56	MG	DA	3154	1/1	0.48	-	45,45,45,45	0
56	MG	BA	3198	1/1	0.34	-	29,29,29,29	0
56	MG	DA	3526	1/1	0.14	-	49,49,49,49	0
56	MG	BB	3010	1/1	0.20	-	44,44,44,44	0
56	MG	AX	108	1/1	0.13	-	66,66,66,66	0
56	MG	D5	101	1/1	0.59	-	44,44,44,44	0
56	MG	DA	3027	1/1	0.61	-	49,49,49,49	0
56	MG	DA	3379	1/1	0.14	-	63,63,63,63	0
56	MG	DA	3595	1/1	0.19	-	53,53,53,53	0
56	MG	DA	3156	1/1	0.60	-	38,38,38,38	0
56	MG	DA	3105	1/1	0.15	-	56,56,56,56	0
56	MG	DA	3246	1/1	0.17	-	55,55,55,55	0
56	MG	DA	3065	1/1	0.18	-	40,40,40,40	0
56	MG	DA	3511	1/1	0.10	-	47,47,47,47	0
56	MG	BA	3613	1/1	0.18	-	47,47,47,47	0
56	MG	BA	3665	1/1	0.21	-	39,39,39,39	0
56	MG	DA	3463	1/1	0.07	-	32,32,32,32	0
56	MG	AA	3040	1/1	0.07	-	46,46,46,46	0
56	MG	CA	3117	1/1	0.17	-	58,58,58,58	0
56	MG	DA	3259	1/1	0.23	-	45,45,45,45	0
56	MG	BA	3458	1/1	0.23	-	46,46,46,46	0
56	MG	DA	3170	1/1	0.27	-	45,45,45,45	0
56	MG	BA	3522	1/1	0.16	-	42,42,42,42	0
56	MG	CA	3038	1/1	0.27	-	54,54,54,54	0
56	MG	CA	3082	1/1	0.10	-	46,46,46,46	0
56	MG	DA	3163	1/1	0.20	-	52,52,52,52	0
56	MG	DA	3339	1/1	0.27	-	35,35,35,35	0
56	MG	BA	3634	1/1	0.09	-	77,77,77,77	0
56	MG	DA	3253	1/1	0.13	-	35,35,35,35	0
56	MG	BA	3188	1/1	0.29	-	49,49,49,49	0
56	MG	BA	3065	1/1	0.27	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3523	1/1	0.12	-	47,47,47,47	0
56	MG	B1	3001	1/1	0.77	-	63,63,63,63	0
56	MG	DA	3091	1/1	0.48	-	50,50,50,50	0
56	MG	DA	3432	1/1	0.23	-	37,37,37,37	0
56	MG	AA	3148	1/1	0.21	-	72,72,72,72	0
56	MG	DA	3358	1/1	0.15	-	38,38,38,38	0
56	MG	AA	3082	1/1	0.24	-	52,52,52,52	0
56	MG	BU	209	1/1	1.04	-	36,36,36,36	0
56	MG	AA	3029	1/1	1.03	-	60,60,60,60	0
56	MG	DA	3346	1/1	0.21	-	64,64,64,64	0
56	MG	BO	201	1/1	0.11	-	63,63,63,63	0
56	MG	BA	3619	1/1	0.17	-	42,42,42,42	0
56	MG	BA	3100	1/1	0.18	-	42,42,42,42	0
56	MG	DA	3634	1/1	0.18	-	33,33,33,33	0
56	MG	CA	3017	1/1	0.20	-	54,54,54,54	0
56	MG	DA	3515	1/1	0.07	-	57,57,57,57	0
56	MG	DA	3632	1/1	0.16	-	60,60,60,60	0
56	MG	CA	3144	1/1	0.78	-	84,84,84,84	0
56	MG	DA	3584	1/1	0.14	-	47,47,47,47	0
56	MG	BA	3621	1/1	0.22	-	57,57,57,57	0
56	MG	AA	3043	1/1	0.38	-	63,63,63,63	0
56	MG	BA	3479	1/1	0.16	-	44,44,44,44	0
56	MG	DA	3149	1/1	0.07	-	47,47,47,47	0
56	MG	DA	3115	1/1	0.09	-	64,64,64,64	0
56	MG	AA	3144	1/1	0.12	-	56,56,56,56	0
56	MG	DA	3628	1/1	0.14	-	38,38,38,38	0
56	MG	BA	3679	1/1	0.12	-	39,39,39,39	0
56	MG	CA	3079	1/1	0.09	-	37,37,37,37	0
56	MG	B0	106	1/1	0.09	-	43,43,43,43	0
56	MG	BA	3005	1/1	0.14	-	43,43,43,43	0
56	MG	BA	3413	1/1	0.07	-	19,19,19,19	0
56	MG	DA	3230	1/1	0.17	-	61,61,61,61	0
56	MG	DA	3104	1/1	0.15	-	46,46,46,46	0
56	MG	DA	3564	1/1	0.11	-	29,29,29,29	0
56	MG	AA	3099	1/1	0.51	-	49,49,49,49	0
56	MG	BA	3050	1/1	0.17	-	33,33,33,33	0
59	FME	AX	101	10/11	0.47	-	55,74,92,107	0
56	MG	DA	3112	1/1	0.31	-	49,49,49,49	0
56	MG	DA	3146	1/1	0.18	-	34,34,34,34	0
56	MG	BA	3112	1/1	0.12	-	46,46,46,46	0
56	MG	DA	3287	1/1	0.06	-	53,53,53,53	0
56	MG	BA	3010	1/1	0.08	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3572	1/1	0.10	-	39,39,39,39	0
56	MG	BA	3056	1/1	0.26	-	39,39,39,39	0
56	MG	BX	102	1/1	0.22	-	60,60,60,60	0
56	MG	DA	3605	1/1	0.07	-	58,58,58,58	0
56	MG	AA	3002	1/1	0.20	-	74,74,74,74	0
56	MG	AA	3037	1/1	0.29	-	53,53,53,53	0
56	MG	DA	3536	1/1	0.14	-	57,57,57,57	0
56	MG	CA	3041	1/1	0.38	-	71,71,71,71	0
56	MG	DA	3037	1/1	0.37	-	37,37,37,37	0
56	MG	AA	3167	1/1	0.15	-	78,78,78,78	0
56	MG	BA	3019	1/1	0.10	-	42,42,42,42	0
56	MG	DA	3179	1/1	0.41	-	36,36,36,36	0
56	MG	BA	3167	1/1	0.39	-	50,50,50,50	0
56	MG	BA	3607	1/1	0.18	-	74,74,74,74	0
56	MG	DA	3376	1/1	0.18	-	42,42,42,42	0
56	MG	DA	3322	1/1	0.07	-	41,41,41,41	0
56	MG	DA	3407	1/1	0.14	-	35,35,35,35	0
56	MG	BA	3461	1/1	0.13	-	33,33,33,33	0
56	MG	CA	3087	1/1	0.14	-	40,40,40,40	0
56	MG	BA	3120	1/1	0.30	-	56,56,56,56	0
56	MG	BU	207	1/1	0.37	-	38,38,38,38	0
56	MG	BA	3720	1/1	0.19	-	51,51,51,51	0
56	MG	DA	3381	1/1	0.27	-	68,68,68,68	0
56	MG	DA	3207	1/1	0.12	-	41,41,41,41	0
56	MG	AA	3122	1/1	0.40	-	40,40,40,40	0
56	MG	BA	3384	1/1	0.29	-	47,47,47,47	0
56	MG	BA	3620	1/1	0.24	-	57,57,57,57	0
56	MG	BA	3373	1/1	0.10	-	48,48,48,48	0
56	MG	DA	3211	1/1	0.19	-	46,46,46,46	0
56	MG	BA	3145	1/1	0.33	-	40,40,40,40	0
56	MG	BA	3138	1/1	0.14	-	54,54,54,54	0
56	MG	DA	3426	1/1	0.13	-	41,41,41,41	0
56	MG	BA	3612	1/1	0.16	-	41,41,41,41	0
56	MG	DA	3194	1/1	0.60	-	65,65,65,65	0
56	MG	DA	3466	1/1	0.09	-	43,43,43,43	0
56	MG	BA	3529	1/1	0.21	-	22,22,22,22	0
56	MG	AA	3032	1/1	0.33	-	65,65,65,65	0
56	MG	CA	3138	1/1	0.12	-	59,59,59,59	0
56	MG	DA	3086	1/1	0.28	-	43,43,43,43	0
56	MG	B9	502	1/1	0.26	-	49,49,49,49	0
56	MG	BA	3402	1/1	0.21	-	23,23,23,23	0
56	MG	DA	3640	1/1	0.19	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3114	1/1	0.21	-	73,73,73,73	0
56	MG	AA	3139	1/1	0.20	-	58,58,58,58	0
56	MG	CA	3136	1/1	0.29	-	70,70,70,70	0
56	MG	BA	3204	1/1	0.19	-	48,48,48,48	0
56	MG	BA	3740	1/1	1.11	-	57,57,57,57	0
56	MG	DA	3224	1/1	0.11	-	53,53,53,53	0
56	MG	BA	3731	1/1	0.27	-	52,52,52,52	0
56	MG	AA	3164	1/1	0.22	-	61,61,61,61	0
56	MG	DA	3267	1/1	0.28	-	40,40,40,40	0
56	MG	DO	5001	1/1	0.09	-	33,33,33,33	0
56	MG	BA	3279	1/1	0.17	-	60,60,60,60	0
56	MG	BA	3025	1/1	0.19	-	48,48,48,48	0
56	MG	BA	3573	1/1	0.16	-	53,53,53,53	0
56	MG	DA	3015	1/1	0.31	-	54,54,54,54	0
56	MG	DQ	3003	1/1	0.23	-	58,58,58,58	0
56	MG	CA	3023	1/1	0.21	-	37,37,37,37	0
56	MG	B8	5002	1/1	0.22	-	48,48,48,48	0
56	MG	BA	3572	1/1	0.19	-	23,23,23,23	0
56	MG	DA	3341	1/1	0.06	-	40,40,40,40	0
56	MG	DE	302	1/1	0.29	-	46,46,46,46	0
56	MG	BA	3028	1/1	0.31	-	59,59,59,59	0
56	MG	DE	305	1/1	0.63	-	68,68,68,68	0
56	MG	DA	3658	1/1	0.30	-	50,50,50,50	0
56	MG	BD	305	1/1	0.27	-	41,41,41,41	0
56	MG	AA	3013	1/1	0.22	-	75,75,75,75	0
56	MG	DA	3343	1/1	0.12	-	37,37,37,37	0
56	MG	BA	3457	1/1	0.10	-	25,25,25,25	0
56	MG	DA	3072	1/1	0.15	-	40,40,40,40	0
56	MG	BA	3227	1/1	0.18	-	67,67,67,67	0
56	MG	BA	3658	1/1	0.21	-	62,62,62,62	0
56	MG	BA	3622	1/1	0.24	-	32,32,32,32	0
56	MG	BA	3262	1/1	0.33	-	44,44,44,44	0
56	MG	BA	3215	1/1	0.09	-	32,32,32,32	0
56	MG	DB	3010	1/1	0.21	-	66,66,66,66	0
56	MG	DA	3271	1/1	0.08	-	45,45,45,45	0
56	MG	CA	3166	1/1	0.07	-	71,71,71,71	0
56	MG	AA	3052	1/1	0.23	-	58,58,58,58	0
56	MG	BA	3040	1/1	0.24	-	40,40,40,40	0
56	MG	DA	3551	1/1	0.08	-	43,43,43,43	0
56	MG	DA	3418	1/1	0.27	-	57,57,57,57	0
56	MG	BA	3035	1/1	0.14	-	32,32,32,32	0
56	MG	DA	3502	1/1	0.17	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3321	1/1	0.20	-	47,47,47,47	0
56	MG	DA	3442	1/1	0.28	-	58,58,58,58	0
56	MG	BA	3533	1/1	0.29	-	30,30,30,30	0
56	MG	BA	3598	1/1	0.23	-	32,32,32,32	0
56	MG	DA	3480	1/1	0.17	-	42,42,42,42	0
56	MG	DQ	3004	1/1	0.22	-	52,52,52,52	0
56	MG	BA	3089	1/1	0.23	-	50,50,50,50	0
56	MG	BA	3213	1/1	0.19	-	63,63,63,63	0
56	MG	DA	3317	1/1	0.20	-	34,34,34,34	0
56	MG	BA	3528	1/1	0.20	-	44,44,44,44	0
56	MG	DA	3017	1/1	0.22	-	51,51,51,51	0
56	MG	BA	3717	1/1	0.13	-	51,51,51,51	0
56	MG	BA	3440	1/1	0.11	-	40,40,40,40	0
56	MG	BB	3011	1/1	0.17	-	45,45,45,45	0
56	MG	BA	3272	1/1	0.07	-	49,49,49,49	0
56	MG	DA	3187	1/1	0.59	-	52,52,52,52	0
56	MG	BA	3287	1/1	0.15	-	11,11,11,11	0
56	MG	BA	3676	1/1	0.14	-	63,63,63,63	0
56	MG	BA	3191	1/1	0.21	-	56,56,56,56	0
56	MG	BA	3243	1/1	0.09	-	43,43,43,43	0
56	MG	DA	3067	1/1	0.28	-	35,35,35,35	0
56	MG	BA	3693	1/1	0.26	-	57,57,57,57	0
56	MG	DA	3325	1/1	0.23	-	31,31,31,31	0
56	MG	DA	3610	1/1	0.13	-	49,49,49,49	0
56	MG	BA	3488	1/1	0.29	-	43,43,43,43	0
56	MG	CT	3001	1/1	0.20	-	57,57,57,57	0
56	MG	BE	305	1/1	0.66	-	44,44,44,44	0
56	MG	CA	3169	1/1	0.18	-	52,52,52,52	0
56	MG	AA	3124	1/1	0.20	-	61,61,61,61	0
56	MG	DA	3554	1/1	0.26	-	62,62,62,62	0
56	MG	DA	3373	1/1	0.25	-	52,52,52,52	0
56	MG	CA	3028	1/1	0.48	-	62,62,62,62	0
56	MG	BA	3128	1/1	0.14	-	28,28,28,28	0
56	MG	DA	3059	1/1	0.05	-	42,42,42,42	0
56	MG	DA	3471	1/1	0.13	-	32,32,32,32	0
56	MG	DA	3024	1/1	0.61	-	59,59,59,59	0
56	MG	BA	3180	1/1	0.33	-	48,48,48,48	0
56	MG	DA	3342	1/1	0.15	-	31,31,31,31	0
56	MG	AA	3152	1/1	0.12	-	29,29,29,29	0
56	MG	DA	3574	1/1	0.20	-	22,22,22,22	0
56	MG	DA	3311	1/1	0.35	-	33,33,33,33	0
56	MG	DA	3409	1/1	0.10	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3499	1/1	0.20	-	50,50,50,50	0
56	MG	BA	3137	1/1	0.22	-	59,59,59,59	0
56	MG	DA	3464	1/1	0.20	-	51,51,51,51	0
56	MG	AA	3196	1/1	0.28	-	78,78,78,78	0
56	MG	BA	3395	1/1	0.38	-	56,56,56,56	0
56	MG	DA	3637	1/1	0.22	-	59,59,59,59	0
56	MG	DA	3051	1/1	0.14	-	39,39,39,39	0
56	MG	BA	3305	1/1	0.12	-	48,48,48,48	0
56	MG	AA	3193	1/1	0.17	-	65,65,65,65	0
56	MG	AA	3062	1/1	0.15	-	30,30,30,30	0
56	MG	BA	3341	1/1	0.17	-	31,31,31,31	0
56	MG	BA	3651	1/1	0.35	-	52,52,52,52	0
56	MG	BA	3452	1/1	0.12	-	16,16,16,16	0
56	MG	CA	3012	1/1	0.12	-	50,50,50,50	0
56	MG	BA	3567	1/1	0.09	-	54,54,54,54	0
56	MG	DA	3219	1/1	0.35	-	49,49,49,49	0
56	MG	DA	3227	1/1	0.15	-	40,40,40,40	0
56	MG	BA	3216	1/1	0.27	-	46,46,46,46	0
56	MG	DA	3295	1/1	0.22	-	31,31,31,31	0
56	MG	AA	3097	1/1	0.42	-	53,53,53,53	0
56	MG	DV	203	1/1	0.33	-	41,41,41,41	0
56	MG	BA	3175	1/1	0.46	-	40,40,40,40	0
56	MG	DA	3134	1/1	0.19	-	37,37,37,37	0
56	MG	CA	3062	1/1	0.34	-	67,67,67,67	0
56	MG	BA	3257	1/1	0.25	-	56,56,56,56	0
56	MG	BA	3006	1/1	0.26	-	46,46,46,46	0
56	MG	BA	3585	1/1	0.21	-	25,25,25,25	0
56	MG	BA	3352	1/1	0.16	-	58,58,58,58	0
56	MG	DA	3060	1/1	0.38	-	51,51,51,51	0
56	MG	DA	3510	1/1	0.10	-	67,67,67,67	0
58	ZN	BY	501	1/1	0.08	-	67,67,67,67	0
56	MG	DA	3338	1/1	0.18	-	58,58,58,58	0
56	MG	DA	3512	1/1	0.09	-	37,37,37,37	0
56	MG	BA	3471	1/1	0.09	-	28,28,28,28	0
56	MG	BA	3183	1/1	0.24	-	40,40,40,40	0
56	MG	BA	3447	1/1	0.09	-	76,76,76,76	0
56	MG	DA	3565	1/1	0.20	-	48,48,48,48	0
56	MG	B0	103	1/1	0.18	-	46,46,46,46	0
56	MG	BA	3244	1/1	0.17	-	46,46,46,46	0
56	MG	BP	202	1/1	0.39	-	47,47,47,47	0
56	MG	DA	3038	1/1	0.26	-	37,37,37,37	0
56	MG	BA	3465	1/1	0.08	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3153	1/1	0.37	-	47,47,47,47	0
56	MG	DA	3063	1/1	0.14	-	55,55,55,55	0
56	MG	CA	3146	1/1	0.16	-	61,61,61,61	0
56	MG	AA	3149	1/1	0.10	-	49,49,49,49	0
56	MG	AA	3085	1/1	0.42	-	57,57,57,57	0
56	MG	DA	3399	1/1	0.21	-	39,39,39,39	0
56	MG	BA	3736	1/1	0.13	-	40,40,40,40	0
56	MG	BA	3267	1/1	0.20	-	56,56,56,56	0
56	MG	AN	101	1/1	0.14	-	64,64,64,64	0
56	MG	BA	3588	1/1	0.20	-	41,41,41,41	0
56	MG	BA	3601	1/1	0.18	-	61,61,61,61	0
56	MG	BA	3116	1/1	0.28	-	30,30,30,30	0
56	MG	DA	3081	1/1	0.21	-	56,56,56,56	0
56	MG	DA	3568	1/1	0.40	-	58,58,58,58	0
56	MG	DA	3538	1/1	0.16	-	37,37,37,37	0
56	MG	AA	3198	1/1	0.17	-	73,73,73,73	0
56	MG	BA	3236	1/1	0.28	-	37,37,37,37	0
56	MG	BR	203	1/1	0.59	-	48,48,48,48	0
56	MG	BA	3427	1/1	0.19	-	20,20,20,20	0
56	MG	BA	3284	1/1	0.74	-	76,76,76,76	0
56	MG	AA	3118	1/1	0.44	-	39,39,39,39	0
56	MG	BA	3196	1/1	0.20	-	45,45,45,45	0
56	MG	DA	3337	1/1	0.14	-	50,50,50,50	0
56	MG	DA	3575	1/1	0.12	-	51,51,51,51	0
56	MG	BA	3703	1/1	0.12	-	44,44,44,44	0
56	MG	BA	3194	1/1	0.51	-	43,43,43,43	0
56	MG	DA	3113	1/1	1.15	-	61,61,61,61	0
56	MG	DA	3056	1/1	0.34	-	37,37,37,37	0
56	MG	BE	301	1/1	0.21	-	28,28,28,28	0
56	MG	CA	3077	1/1	0.29	-	51,51,51,51	0
56	MG	D3	101	1/1	0.51	-	54,54,54,54	0
56	MG	DA	3547	1/1	0.13	-	47,47,47,47	0
56	MG	DA	3460	1/1	0.11	-	47,47,47,47	0
56	MG	AA	3127	1/1	0.21	-	50,50,50,50	0
56	MG	BA	3507	1/1	0.22	-	37,37,37,37	0
56	MG	CA	3149	1/1	0.17	-	81,81,81,81	0
56	MG	BA	3694	1/1	0.26	-	48,48,48,48	0
56	MG	DA	3374	1/1	0.15	-	40,40,40,40	0
56	MG	BA	3396	1/1	0.20	-	41,41,41,41	0
56	MG	BA	3258	1/1	0.15	-	35,35,35,35	0
56	MG	BA	3159	1/1	0.27	-	47,47,47,47	0
56	MG	DP	201	1/1	0.37	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3138	1/1	0.37	-	38,38,38,38	0
56	MG	DA	3291	1/1	0.20	-	42,42,42,42	0
56	MG	BB	3018	1/1	0.27	-	54,54,54,54	0
56	MG	DA	3016	1/1	0.21	-	33,33,33,33	0
56	MG	BA	3697	1/1	0.20	-	63,63,63,63	0
56	MG	DA	3562	1/1	0.19	-	41,41,41,41	0
56	MG	DA	3470	1/1	0.15	-	45,45,45,45	0
56	MG	DA	3521	1/1	0.18	-	46,46,46,46	0
56	MG	DA	3209	1/1	0.10	-	44,44,44,44	0
56	MG	DA	3157	1/1	0.50	-	56,56,56,56	0
56	MG	DA	3542	1/1	0.17	-	44,44,44,44	0
56	MG	BA	3043	1/1	0.36	-	33,33,33,33	0
56	MG	AA	3221	1/1	0.10	-	52,52,52,52	0
56	MG	BA	3212	1/1	0.17	-	47,47,47,47	0
56	MG	BA	3568	1/1	0.20	-	68,68,68,68	0
56	MG	BA	3400	1/1	0.18	-	29,29,29,29	0
56	MG	AL	3001	1/1	0.15	-	50,50,50,50	0
56	MG	DA	3434	1/1	0.19	-	51,51,51,51	0
56	MG	AA	3101	1/1	0.14	-	61,61,61,61	0
56	MG	BA	3566	1/1	0.23	-	43,43,43,43	0
56	MG	DA	3203	1/1	0.13	-	48,48,48,48	0
56	MG	BA	3002	1/1	0.17	-	38,38,38,38	0
56	MG	AA	3080	1/1	0.26	-	58,58,58,58	0
56	MG	B3	3401	1/1	0.19	-	24,24,24,24	0
56	MG	AA	3086	1/1	0.64	-	65,65,65,65	0
56	MG	BA	3732	1/1	0.41	-	56,56,56,56	0
56	MG	BN	3005	1/1	0.94	-	63,63,63,63	0
56	MG	DA	3058	1/1	0.21	-	56,56,56,56	0
56	MG	BA	3564	1/1	0.15	-	26,26,26,26	0
56	MG	BA	3022	1/1	0.17	-	66,66,66,66	0
56	MG	BA	3583	1/1	0.20	-	57,57,57,57	0
56	MG	DA	3424	1/1	0.18	-	58,58,58,58	0
56	MG	BA	3164	1/1	0.47	-	57,57,57,57	0
56	MG	DA	3508	1/1	0.04	-	30,30,30,30	0
56	MG	BA	3275	1/1	0.20	-	28,28,28,28	0
56	MG	DA	3419	1/1	0.09	-	53,53,53,53	0
56	MG	BA	3504	1/1	0.17	-	54,54,54,54	0
56	MG	CA	3106	1/1	0.34	-	72,72,72,72	0
56	MG	CA	3127	1/1	0.20	-	72,72,72,72	0
56	MG	BA	3325	1/1	0.18	-	39,39,39,39	0
56	MG	BQ	3002	1/1	0.26	-	51,51,51,51	0
56	MG	BA	3195	1/1	0.11	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3358	1/1	0.17	-	78,78,78,78	0
56	MG	BA	3467	1/1	0.15	-	44,44,44,44	0
56	MG	CA	3104	1/1	0.12	-	60,60,60,60	0
56	MG	DA	3331	1/1	0.18	-	27,27,27,27	0
56	MG	BA	3691	1/1	0.10	-	40,40,40,40	0
56	MG	DA	3270	1/1	0.24	-	55,55,55,55	0
56	MG	BN	3006	1/1	0.07	-	33,33,33,33	0
56	MG	DA	3120	1/1	0.63	-	50,50,50,50	0
56	MG	BA	3260	1/1	0.12	-	47,47,47,47	0
56	MG	AA	3041	1/1	0.12	-	41,41,41,41	0
56	MG	DA	3277	1/1	0.09	-	46,46,46,46	0
56	MG	BA	3189	1/1	0.21	-	39,39,39,39	0
56	MG	DA	3540	1/1	0.13	-	76,76,76,76	0
56	MG	BE	304	1/1	0.58	-	45,45,45,45	0
56	MG	AA	3214	1/1	0.31	-	42,42,42,42	0
56	MG	DA	3240	1/1	0.22	-	58,58,58,58	0
56	MG	DA	3102	1/1	0.28	-	49,49,49,49	0
56	MG	BN	3002	1/1	0.26	-	52,52,52,52	0
56	MG	CA	3035	1/1	0.26	-	49,49,49,49	0
56	MG	DA	3249	1/1	0.21	-	25,25,25,25	0
56	MG	BA	3407	1/1	0.22	-	35,35,35,35	0
56	MG	DA	3444	1/1	0.26	-	43,43,43,43	0
56	MG	DA	3598	1/1	0.18	-	45,45,45,45	0
56	MG	DA	3414	1/1	0.23	-	59,59,59,59	0
56	MG	BA	3719	1/1	0.08	-	63,63,63,63	0
56	MG	BA	3131	1/1	0.12	-	31,31,31,31	0
56	MG	BA	3600	1/1	0.33	-	54,54,54,54	0
56	MG	DA	3651	1/1	0.12	-	48,48,48,48	0
56	MG	DA	3332	1/1	0.12	-	29,29,29,29	0
56	MG	DA	3633	1/1	0.23	-	25,25,25,25	0
56	MG	CA	3111	1/1	0.10	-	69,69,69,69	0
56	MG	CA	3120	1/1	0.18	-	59,59,59,59	0
56	MG	DA	3128	1/1	0.35	-	54,54,54,54	0
56	MG	CA	3122	1/1	0.22	-	70,70,70,70	0
56	MG	BA	3296	1/1	0.64	-	69,69,69,69	0
56	MG	BA	3093	1/1	0.45	-	52,52,52,52	0
56	MG	CA	3063	1/1	0.10	-	57,57,57,57	0
56	MG	BA	3105	1/1	0.19	-	54,54,54,54	0
56	MG	CA	3154	1/1	0.18	-	54,54,54,54	0
56	MG	BA	3176	1/1	0.21	-	50,50,50,50	0
56	MG	BA	3527	1/1	0.22	-	45,45,45,45	0
56	MG	BA	3245	1/1	0.23	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3363	1/1	0.17	-	56,56,56,56	0
56	MG	DA	3046	1/1	0.09	-	48,48,48,48	0
56	MG	DA	3478	1/1	0.09	-	58,58,58,58	0
56	MG	DN	5001	1/1	0.13	-	71,71,71,71	0
56	MG	CA	3139	1/1	0.26	-	76,76,76,76	0
56	MG	DA	3411	1/1	0.21	-	33,33,33,33	0
56	MG	AA	3129	1/1	0.23	-	77,77,77,77	0
56	MG	BA	3253	1/1	0.27	-	63,63,63,63	0
56	MG	BU	208	1/1	0.21	-	42,42,42,42	0
56	MG	AA	3177	1/1	0.14	-	58,58,58,58	0
56	MG	BE	309	1/1	0.18	-	37,37,37,37	0
56	MG	DA	3101	1/1	0.30	-	59,59,59,59	0
56	MG	CA	3024	1/1	0.36	-	57,57,57,57	0
56	MG	DA	3639	1/1	0.14	-	55,55,55,55	0
56	MG	DA	3092	1/1	0.28	-	48,48,48,48	0
56	MG	DA	3622	1/1	0.15	-	40,40,40,40	0
56	MG	BA	3021	1/1	0.36	-	62,62,62,62	0
56	MG	DA	3507	1/1	0.22	-	53,53,53,53	0
56	MG	BA	3148	1/1	0.63	-	49,49,49,49	0
56	MG	AA	3120	1/1	0.46	-	53,53,53,53	0
56	MG	DA	3054	1/1	0.10	-	34,34,34,34	0
56	MG	BA	3020	1/1	0.28	-	43,43,43,43	0
56	MG	DA	3293	1/1	0.10	-	34,34,34,34	0
56	MG	DA	3175	1/1	0.31	-	52,52,52,52	0
56	MG	BD	309	1/1	0.18	-	43,43,43,43	0
56	MG	DA	3469	1/1	0.18	-	52,52,52,52	0
56	MG	BA	3057	1/1	0.40	-	36,36,36,36	0
56	MG	BA	3168	1/1	0.44	-	52,52,52,52	0
56	MG	DA	3431	1/1	0.36	-	56,56,56,56	0
56	MG	BA	3115	1/1	0.16	-	28,28,28,28	0
56	MG	AA	3111	1/1	0.15	-	70,70,70,70	0
56	MG	AA	3166	1/1	0.22	-	55,55,55,55	0
56	MG	CA	3113	1/1	0.28	-	84,84,84,84	0
56	MG	AA	3068	1/1	0.11	-	67,67,67,67	0
58	ZN	AN	102	1/1	0.11	-	88,88,88,88	0
56	MG	BA	3360	1/1	0.20	-	39,39,39,39	0
56	MG	CA	3010	1/1	0.16	-	34,34,34,34	0
56	MG	DA	3491	1/1	0.27	-	55,55,55,55	0
56	MG	DA	3127	1/1	0.11	-	44,44,44,44	0
56	MG	DA	3076	1/1	0.44	-	38,38,38,38	0
56	MG	BA	3127	1/1	0.34	-	42,42,42,42	0
56	MG	CA	3147	1/1	0.36	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3088	1/1	0.18	-	55,55,55,55	0
56	MG	BA	3061	1/1	0.35	-	44,44,44,44	0
56	MG	CA	3050	1/1	0.20	-	54,54,54,54	0
56	MG	DA	3527	1/1	0.12	-	58,58,58,58	0
56	MG	AA	3005	1/1	0.27	-	66,66,66,66	0
56	MG	BA	3363	1/1	0.17	-	29,29,29,29	0
56	MG	CA	3044	1/1	0.12	-	52,52,52,52	0
56	MG	BA	3554	1/1	0.20	-	25,25,25,25	0
56	MG	BA	3226	1/1	0.33	-	31,31,31,31	0
56	MG	BA	3739	1/1	0.31	-	50,50,50,50	0
56	MG	AA	3035	1/1	0.29	-	59,59,59,59	0
56	MG	BA	3177	1/1	0.48	-	35,35,35,35	0
56	MG	DA	3505	1/1	0.16	-	24,24,24,24	0
56	MG	AX	104	1/1	0.23	-	62,62,62,62	0
56	MG	BA	3485	1/1	0.20	-	67,67,67,67	0
56	MG	BA	3197	1/1	0.44	-	39,39,39,39	0
56	MG	AA	3209	1/1	0.25	-	66,66,66,66	0
56	MG	DA	3125	1/1	0.41	-	55,55,55,55	0
56	MG	BA	3171	1/1	0.38	-	42,42,42,42	0
58	ZN	B9	501	1/1	0.10	-	49,49,49,49	0
56	MG	CA	3030	1/1	0.35	-	74,74,74,74	0
56	MG	DA	3449	1/1	0.29	-	46,46,46,46	0
56	MG	BA	3615	1/1	0.20	-	55,55,55,55	0
56	MG	BA	3034	1/1	0.15	-	37,37,37,37	0
56	MG	DD	303	1/1	0.60	-	48,48,48,48	0
56	MG	DA	3002	1/1	0.24	-	47,47,47,47	0
56	MG	BW	3002	1/1	0.20	-	34,34,34,34	0
56	MG	DA	3535	1/1	0.18	-	58,58,58,58	0
56	MG	BW	3001	1/1	0.29	-	55,55,55,55	0
56	MG	BA	3673	1/1	0.17	-	60,60,60,60	0
56	MG	DA	3029	1/1	0.13	-	62,62,62,62	0
56	MG	BA	3058	1/1	0.38	-	41,41,41,41	0
56	MG	BA	3726	1/1	0.30	-	29,29,29,29	0
56	MG	DA	3042	1/1	0.34	-	38,38,38,38	0
56	MG	DA	3533	1/1	0.12	-	59,59,59,59	0
56	MG	BA	3632	1/1	0.18	-	55,55,55,55	0
56	MG	BA	3099	1/1	0.30	-	55,55,55,55	0
56	MG	BA	3238	1/1	0.18	-	48,48,48,48	0
56	MG	BP	201	1/1	0.61	-	37,37,37,37	0
56	MG	DA	3441	1/1	0.18	-	46,46,46,46	0
56	MG	BA	3103	1/1	0.34	-	58,58,58,58	0
56	MG	BA	3233	1/1	0.19	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BU	206	1/1	0.23	-	41,41,41,41	0
56	MG	DA	3284	1/1	0.20	-	45,45,45,45	0
56	MG	DA	3576	1/1	0.17	-	57,57,57,57	0
56	MG	DA	3348	1/1	0.10	-	39,39,39,39	0
56	MG	DA	3430	1/1	0.18	-	75,75,75,75	0
56	MG	AA	3205	1/1	0.19	-	66,66,66,66	0
56	MG	BA	3670	1/1	0.11	-	55,55,55,55	0
56	MG	BA	3597	1/1	0.30	-	46,46,46,46	0
56	MG	AA	3047	1/1	0.45	-	59,59,59,59	0
56	MG	BA	3669	1/1	0.21	-	61,61,61,61	0
56	MG	CE	3002	1/1	0.06	-	69,69,69,69	0
56	MG	BA	3702	1/1	0.24	-	56,56,56,56	0
56	MG	BA	3290	1/1	0.16	-	35,35,35,35	0
56	MG	AA	3083	1/1	0.09	-	56,56,56,56	0
56	MG	BA	3560	1/1	0.27	-	24,24,24,24	0
56	MG	DD	304	1/1	0.55	-	40,40,40,40	0
56	MG	BA	3133	1/1	0.48	-	53,53,53,53	0
56	MG	BA	3039	1/1	0.31	-	44,44,44,44	0
56	MG	CA	3033	1/1	0.20	-	64,64,64,64	0
56	MG	BA	3695	1/1	0.25	-	34,34,34,34	0
56	MG	AA	3174	1/1	0.21	-	49,49,49,49	0
56	MG	BA	3419	1/1	0.30	-	36,36,36,36	0
56	MG	AA	3025	1/1	0.13	-	78,78,78,78	0
56	MG	BA	3610	1/1	1.07	-	49,49,49,49	0
56	MG	BA	3125	1/1	0.28	-	26,26,26,26	0
56	MG	CA	3008	1/1	1.06	-	59,59,59,59	0
56	MG	CA	3018	1/1	0.30	-	55,55,55,55	0
56	MG	AA	3121	1/1	0.48	-	52,52,52,52	0
56	MG	BA	3718	1/1	0.17	-	52,52,52,52	0
56	MG	CA	3076	1/1	0.25	-	48,48,48,48	0
56	MG	DA	3351	1/1	0.22	-	58,58,58,58	0
56	MG	AA	3145	1/1	0.24	-	63,63,63,63	0
56	MG	CA	3130	1/1	0.10	-	59,59,59,59	0
56	MG	BA	3491	1/1	0.21	-	38,38,38,38	0
56	MG	CA	3074	1/1	0.24	-	56,56,56,56	0
56	MG	DA	3549	1/1	0.35	-	73,73,73,73	0
56	MG	AA	3110	1/1	0.13	-	41,41,41,41	0
56	MG	BV	3001	1/1	0.32	-	42,42,42,42	0
56	MG	DW	202	1/1	0.38	-	53,53,53,53	0
56	MG	CA	3097	1/1	0.13	-	60,60,60,60	0
56	MG	BA	3033	1/1	0.47	-	54,54,54,54	0
56	MG	AX	103	1/1	0.07	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3411	1/1	0.19	-	21,21,21,21	0
56	MG	BA	3018	1/1	0.33	-	54,54,54,54	0
56	MG	DA	3531	1/1	0.11	-	44,44,44,44	0
56	MG	B3	3403	1/1	0.34	-	37,37,37,37	0
56	MG	DA	3018	1/1	0.32	-	41,41,41,41	0
56	MG	DB	3003	1/1	0.20	-	70,70,70,70	0
56	MG	DA	3500	1/1	0.24	-	66,66,66,66	0
56	MG	DB	3012	1/1	0.21	-	50,50,50,50	0
56	MG	DA	3176	1/1	0.10	-	52,52,52,52	0
56	MG	BA	3232	1/1	0.20	-	32,32,32,32	0
56	MG	CA	3015	1/1	0.29	-	53,53,53,53	0
56	MG	DA	3233	1/1	0.29	-	58,58,58,58	0
56	MG	DD	302	1/1	0.73	-	48,48,48,48	0
56	MG	DA	3488	1/1	0.16	-	48,48,48,48	0
56	MG	BA	3108	1/1	0.16	-	32,32,32,32	0
56	MG	BA	3480	1/1	0.11	-	22,22,22,22	0
56	MG	BA	3172	1/1	0.12	-	54,54,54,54	0
56	MG	DA	3009	1/1	0.10	-	33,33,33,33	0
56	MG	BA	3416	1/1	0.17	-	25,25,25,25	0
56	MG	BA	3231	1/1	0.20	-	50,50,50,50	0
56	MG	DA	3476	1/1	0.11	-	35,35,35,35	0
56	MG	AA	3046	1/1	0.16	-	60,60,60,60	0
56	MG	BA	3081	1/1	0.29	-	44,44,44,44	0
58	ZN	B5	501	1/1	0.10	-	49,49,49,49	0
59	FME	CX	101	10/11	0.46	-	59,80,100,106	0
56	MG	BA	3735	1/1	0.26	-	47,47,47,47	0
56	MG	BF	304	1/1	0.57	-	30,30,30,30	0
56	MG	AA	3208	1/1	0.32	-	38,38,38,38	0
56	MG	BA	3251	1/1	0.28	-	45,45,45,45	0
56	MG	AA	3215	1/1	0.91	-	77,77,77,77	0
56	MG	BA	3086	1/1	0.34	-	50,50,50,50	0
56	MG	BA	3412	1/1	0.26	-	29,29,29,29	0
56	MG	BA	3506	1/1	0.26	-	33,33,33,33	0
56	MG	AA	3074	1/1	0.23	-	40,40,40,40	0
56	MG	DA	3530	1/1	0.16	-	57,57,57,57	0
56	MG	BA	3015	1/1	0.27	-	30,30,30,30	0
56	MG	BA	3098	1/1	0.28	-	42,42,42,42	0
56	MG	BA	3309	1/1	0.14	-	43,43,43,43	0
56	MG	BA	3689	1/1	0.16	-	25,25,25,25	0
56	MG	DA	3309	1/1	0.16	-	25,25,25,25	0
56	MG	BA	3186	1/1	0.16	-	50,50,50,50	0
56	MG	DA	3446	1/1	0.14	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3388	1/1	0.13	-	25,25,25,25	0
56	MG	DA	3298	1/1	0.26	-	45,45,45,45	0
56	MG	BA	3202	1/1	0.46	-	29,29,29,29	0
56	MG	DA	3208	1/1	0.24	-	46,46,46,46	0
56	MG	AA	3192	1/1	0.07	-	73,73,73,73	0
56	MG	DA	3231	1/1	0.10	-	45,45,45,45	0
56	MG	DA	3504	1/1	0.16	-	46,46,46,46	0
56	MG	DE	304	1/1	0.17	-	30,30,30,30	0
56	MG	BA	3589	1/1	0.22	-	34,34,34,34	0
56	MG	BU	205	1/1	0.38	-	39,39,39,39	0
56	MG	DA	3265	1/1	0.30	-	44,44,44,44	0
56	MG	BA	3534	1/1	0.23	-	36,36,36,36	0
56	MG	AA	3178	1/1	0.18	-	63,63,63,63	0
56	MG	BA	3420	1/1	0.17	-	13,13,13,13	0
56	MG	BA	3174	1/1	0.20	-	52,52,52,52	0
56	MG	AA	3095	1/1	0.20	-	54,54,54,54	0
56	MG	AA	3113	1/1	0.15	-	56,56,56,56	0
56	MG	DA	3614	1/1	0.11	-	46,46,46,46	0
56	MG	BA	3237	1/1	0.19	-	43,43,43,43	0
56	MG	BA	3574	1/1	0.09	-	52,52,52,52	0
56	MG	DA	3612	1/1	0.33	-	46,46,46,46	0
56	MG	DA	3561	1/1	0.14	-	40,40,40,40	0
56	MG	DA	3048	1/1	0.38	-	29,29,29,29	0
56	MG	DA	3200	1/1	0.67	-	48,48,48,48	0
56	MG	DA	3164	1/1	0.18	-	40,40,40,40	0
56	MG	BA	3038	1/1	0.14	-	51,51,51,51	0
56	MG	DY	502	1/1	0.07	-	66,66,66,66	0
56	MG	DA	3529	1/1	0.40	-	72,72,72,72	0
56	MG	AA	3011	1/1	0.60	-	44,44,44,44	0
56	MG	DA	3140	1/1	0.34	-	55,55,55,55	0
56	MG	DA	3080	1/1	0.10	-	43,43,43,43	0
56	MG	DA	3225	1/1	0.10	-	64,64,64,64	0
56	MG	AV	101	1/1	0.26	-	51,51,51,51	0
56	MG	BA	3510	1/1	0.16	-	66,66,66,66	0
56	MG	DA	3013	1/1	0.11	-	38,38,38,38	0
56	MG	DA	3095	1/1	0.25	-	53,53,53,53	0
56	MG	AA	3053	1/1	0.38	-	56,56,56,56	0
56	MG	BA	3141	1/1	0.53	-	43,43,43,43	0
56	MG	BA	3344	1/1	0.16	-	65,65,65,65	0
56	MG	DA	3354	1/1	0.18	-	39,39,39,39	0
56	MG	BA	3439	1/1	0.08	-	35,35,35,35	0
56	MG	BA	3143	1/1	0.76	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3368	1/1	0.17	-	34,34,34,34	0
56	MG	AA	3108	1/1	0.26	-	72,72,72,72	0
56	MG	BA	3016	1/1	0.50	-	50,50,50,50	0
56	MG	DA	3599	1/1	0.27	-	69,69,69,69	0
56	MG	DA	3486	1/1	0.07	-	52,52,52,52	0
56	MG	BF	305	1/1	0.32	-	38,38,38,38	0
56	MG	BA	3391	1/1	0.18	-	39,39,39,39	0
56	MG	BA	3614	1/1	0.18	-	48,48,48,48	0
56	MG	BD	308	1/1	0.34	-	21,21,21,21	0
56	MG	DA	3252	1/1	0.22	-	36,36,36,36	0
56	MG	DA	3171	1/1	0.87	-	58,58,58,58	0
56	MG	BE	306	1/1	0.44	-	38,38,38,38	0
56	MG	AA	3014	1/1	0.13	-	24,24,24,24	0
56	MG	BA	3097	1/1	0.17	-	30,30,30,30	0
56	MG	BA	3403	1/1	0.21	-	28,28,28,28	0
56	MG	CA	3016	1/1	0.39	-	72,72,72,72	0
56	MG	CA	3134	1/1	0.19	-	92,92,92,92	0
56	MG	DA	3543	1/1	0.19	-	52,52,52,52	0
56	MG	AA	3073	1/1	0.11	-	63,63,63,63	0
56	MG	BA	3536	1/1	0.16	-	37,37,37,37	0
56	MG	DA	3356	1/1	0.42	-	57,57,57,57	0
56	MG	BA	3729	1/1	0.14	-	54,54,54,54	0
56	MG	BA	3543	1/1	0.22	-	24,24,24,24	0
56	MG	BA	3667	1/1	0.18	-	72,72,72,72	0
56	MG	BA	3361	1/1	0.11	-	39,39,39,39	0
56	MG	BW	3003	1/1	0.23	-	39,39,39,39	0
56	MG	BA	3653	1/1	0.15	-	46,46,46,46	0
56	MG	BA	3182	1/1	0.37	-	43,43,43,43	0
56	MG	CA	3159	1/1	0.61	-	76,76,76,76	0
56	MG	BA	3556	1/1	0.18	-	25,25,25,25	0
56	MG	DA	3236	1/1	0.15	-	38,38,38,38	0
56	MG	AA	3087	1/1	0.25	-	87,87,87,87	0
56	MG	BA	3158	1/1	0.45	-	43,43,43,43	0
56	MG	BA	3586	1/1	0.24	-	26,26,26,26	0
56	MG	BA	3531	1/1	0.21	-	28,28,28,28	0
56	MG	BA	3451	1/1	0.09	-	31,31,31,31	0
56	MG	CA	3105	1/1	0.07	-	59,59,59,59	0
56	MG	BA	3503	1/1	0.20	-	56,56,56,56	0
56	MG	CA	3080	1/1	0.13	-	51,51,51,51	0
56	MG	AA	3039	1/1	0.19	-	62,62,62,62	0
56	MG	BA	3178	1/1	0.50	-	51,51,51,51	0
56	MG	BA	3032	1/1	0.31	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3514	1/1	0.20	-	60,60,60,60	0
56	MG	CA	3152	1/1	0.33	-	45,45,45,45	0
56	MG	AA	3150	1/1	0.29	-	67,67,67,67	0
56	MG	DA	3188	1/1	0.54	-	52,52,52,52	0
56	MG	DA	3330	1/1	0.13	-	30,30,30,30	0
56	MG	BA	3595	1/1	0.15	-	37,37,37,37	0
56	MG	DA	3124	1/1	0.14	-	66,66,66,66	0
56	MG	BA	3538	1/1	0.20	-	29,29,29,29	0
56	MG	BA	3121	1/1	0.24	-	50,50,50,50	0
56	MG	BA	3303	1/1	0.21	-	11,11,11,11	0
56	MG	BA	3438	1/1	0.20	-	30,30,30,30	0
56	MG	AA	3103	1/1	0.13	-	43,43,43,43	0
56	MG	BA	3422	1/1	0.12	-	23,23,23,23	0
56	MG	BA	3101	1/1	0.40	-	47,47,47,47	0
56	MG	DP	202	1/1	0.20	-	54,54,54,54	0
56	MG	CA	3091	1/1	0.16	-	95,95,95,95	0
56	MG	BA	3080	1/1	0.10	-	12,12,12,12	0
56	MG	BA	3706	1/1	0.13	-	38,38,38,38	0
56	MG	DA	3152	1/1	0.26	-	43,43,43,43	0
56	MG	DA	3544	1/1	0.37	-	42,42,42,42	0
56	MG	BA	3221	1/1	0.64	-	55,55,55,55	0
56	MG	CA	3058	1/1	0.19	-	36,36,36,36	0
56	MG	CA	3143	1/1	0.08	-	91,91,91,91	0
56	MG	CA	3123	1/1	0.11	-	75,75,75,75	0
56	MG	AX	102	1/1	0.15	-	66,66,66,66	0
56	MG	CA	3049	1/1	0.17	-	51,51,51,51	0
56	MG	DA	3206	1/1	0.43	-	36,36,36,36	0
56	MG	DF	302	1/1	0.27	-	47,47,47,47	0
56	MG	DA	3103	1/1	0.42	-	52,52,52,52	0
56	MG	BA	3269	1/1	0.12	-	32,32,32,32	0
56	MG	AA	3136	1/1	0.11	-	68,68,68,68	0
56	MG	DA	3085	1/1	0.10	-	35,35,35,35	0
56	MG	DA	3262	1/1	0.25	-	60,60,60,60	0
56	MG	DA	3359	1/1	0.21	-	21,21,21,21	0
56	MG	BA	3179	1/1	0.32	-	53,53,53,53	0
56	MG	BA	3483	1/1	0.21	-	18,18,18,18	0
56	MG	BA	3404	1/1	0.10	-	42,42,42,42	0
56	MG	BA	3520	1/1	0.11	-	69,69,69,69	0
56	MG	BA	3628	1/1	0.09	-	39,39,39,39	0
56	MG	BA	3418	1/1	0.27	-	20,20,20,20	0
56	MG	BA	3448	1/1	0.21	-	23,23,23,23	0
56	MG	DA	3289	1/1	0.18	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3119	1/1	0.12	-	56,56,56,56	0
56	MG	BA	3692	1/1	0.19	-	36,36,36,36	0
56	MG	DA	3329	1/1	0.14	-	40,40,40,40	0
56	MG	BA	3696	1/1	0.26	-	36,36,36,36	0
56	MG	BA	3513	1/1	0.29	-	51,51,51,51	0
56	MG	BA	3701	1/1	0.10	-	69,69,69,69	0
56	MG	BA	3140	1/1	0.32	-	50,50,50,50	0
56	MG	AA	3142	1/1	0.41	-	60,60,60,60	0
56	MG	DA	3626	1/1	0.18	-	63,63,63,63	0
56	MG	AA	3066	1/1	0.19	-	41,41,41,41	0
56	MG	CA	3068	1/1	0.13	-	47,47,47,47	0
56	MG	DA	3617	1/1	0.08	-	51,51,51,51	0
56	MG	BA	3656	1/1	0.23	-	70,70,70,70	0
56	MG	BA	3611	1/1	0.10	-	61,61,61,61	0
56	MG	DA	3118	1/1	0.08	-	44,44,44,44	0
56	MG	DA	3257	1/1	0.19	-	25,25,25,25	0
56	MG	BA	3639	1/1	0.10	-	35,35,35,35	0
56	MG	BA	3357	1/1	0.19	-	45,45,45,45	0
56	MG	AA	3157	1/1	0.05	-	26,26,26,26	0
56	MG	AA	3165	1/1	0.14	-	24,24,24,24	0
56	MG	DA	3525	1/1	0.09	-	56,56,56,56	0
56	MG	DA	3139	1/1	0.22	-	47,47,47,47	0
56	MG	AA	3217	1/1	0.41	-	64,64,64,64	0
56	MG	DA	3423	1/1	0.18	-	29,29,29,29	0
56	MG	DA	3185	1/1	0.34	-	42,42,42,42	0
56	MG	DA	3278	1/1	0.08	-	39,39,39,39	0
56	MG	BA	3541	1/1	0.13	-	37,37,37,37	0
56	MG	BA	3398	1/1	0.14	-	36,36,36,36	0
56	MG	BA	3106	1/1	0.29	-	52,52,52,52	0
56	MG	AA	3084	1/1	0.31	-	71,71,71,71	0
56	MG	DA	3222	1/1	0.21	-	45,45,45,45	0
56	MG	BA	3635	1/1	0.16	-	52,52,52,52	0
56	MG	DA	3159	1/1	0.14	-	50,50,50,50	0
56	MG	AA	3045	1/1	0.28	-	71,71,71,71	0
56	MG	AA	3170	1/1	0.21	-	83,83,83,83	0
56	MG	BA	3659	1/1	0.11	-	42,42,42,42	0
56	MG	BD	311	1/1	0.90	-	53,53,53,53	0
60	K	BA	3304	1/1	0.39	-	93,93,93,93	0
56	MG	DA	3580	1/1	0.16	-	35,35,35,35	0
56	MG	DA	3528	1/1	0.15	-	33,33,33,33	0
56	MG	BA	3091	1/1	0.32	-	55,55,55,55	0
56	MG	CA	3125	1/1	0.21	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3045	1/1	0.08	-	60,60,60,60	0
56	MG	DA	3646	1/1	0.20	-	42,42,42,42	0
56	MG	BB	3009	1/1	0.11	-	49,49,49,49	0
56	MG	BA	3009	1/1	0.23	-	36,36,36,36	0
56	MG	DA	3438	1/1	0.27	-	50,50,50,50	0
56	MG	BA	3738	1/1	0.20	-	58,58,58,58	0
56	MG	CA	3102	1/1	0.05	-	55,55,55,55	0
56	MG	BA	3624	1/1	0.15	-	73,73,73,73	0
56	MG	BA	3135	1/1	0.23	-	57,57,57,57	0
56	MG	DA	3436	1/1	0.25	-	61,61,61,61	0
56	MG	BA	3487	1/1	0.19	-	47,47,47,47	0
56	MG	DA	3212	1/1	0.08	-	48,48,48,48	0
56	MG	DA	3145	1/1	0.32	-	52,52,52,52	0
56	MG	DA	3148	1/1	0.15	-	41,41,41,41	0
56	MG	CA	3121	1/1	0.44	-	59,59,59,59	0
56	MG	BA	3678	1/1	0.09	-	47,47,47,47	0
56	MG	DA	3477	1/1	0.43	-	35,35,35,35	0
56	MG	AA	3185	1/1	0.27	-	47,47,47,47	0
56	MG	BA	3250	1/1	0.32	-	61,61,61,61	0
56	MG	AA	3210	1/1	0.06	-	48,48,48,48	0
56	MG	DA	3623	1/1	0.13	-	63,63,63,63	0
56	MG	DA	3245	1/1	0.26	-	43,43,43,43	0
56	MG	BA	3725	1/1	0.11	-	29,29,29,29	0
56	MG	DA	3397	1/1	0.19	-	40,40,40,40	0
56	MG	DA	3499	1/1	0.20	-	44,44,44,44	0
56	MG	BA	3207	1/1	0.39	-	44,44,44,44	0
56	MG	BA	3641	1/1	0.12	-	33,33,33,33	0
56	MG	CA	3020	1/1	0.23	-	45,45,45,45	0
56	MG	AA	3173	1/1	0.11	-	37,37,37,37	0
56	MG	BA	3431	1/1	0.27	-	54,54,54,54	0
56	MG	DA	3003	1/1	0.17	-	43,43,43,43	0
56	MG	BA	3723	1/1	0.17	-	25,25,25,25	0
56	MG	DA	3189	1/1	0.27	-	55,55,55,55	0
56	MG	BA	3151	1/1	0.23	-	40,40,40,40	0
56	MG	DA	3083	1/1	0.14	-	44,44,44,44	0
56	MG	BA	3136	1/1	0.18	-	47,47,47,47	0
56	MG	BA	3478	1/1	0.21	-	36,36,36,36	0
56	MG	DA	3462	1/1	0.23	-	71,71,71,71	0
56	MG	AA	3213	1/1	0.10	-	74,74,74,74	0
56	MG	DA	3011	1/1	0.36	-	42,42,42,42	0
56	MG	DA	3465	1/1	0.20	-	41,41,41,41	0
56	MG	CA	3167	1/1	0.08	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3145	1/1	0.10	-	67,67,67,67	0
56	MG	BA	3339	1/1	0.15	-	47,47,47,47	0
56	MG	DA	3435	1/1	0.17	-	56,56,56,56	0
56	MG	BA	3379	1/1	0.09	-	43,43,43,43	0
56	MG	BA	3007	1/1	0.25	-	55,55,55,55	0
56	MG	BA	3359	1/1	0.15	-	63,63,63,63	0
56	MG	BA	3060	1/1	0.57	-	64,64,64,64	0
56	MG	BA	3027	1/1	0.23	-	53,53,53,53	0
56	MG	DA	3323	1/1	0.18	-	60,60,60,60	0
56	MG	BA	3320	1/1	0.22	-	41,41,41,41	0
56	MG	DA	3109	1/1	0.23	-	55,55,55,55	0
56	MG	BA	3599	1/1	0.11	-	56,56,56,56	0
56	MG	AA	3162	1/1	0.14	-	79,79,79,79	0
56	MG	BA	3490	1/1	0.10	-	40,40,40,40	0
56	MG	BA	3090	1/1	0.20	-	42,42,42,42	0
56	MG	AA	3089	1/1	0.34	-	80,80,80,80	0
56	MG	DA	3641	1/1	0.22	-	47,47,47,47	0
56	MG	AA	3160	1/1	0.28	-	52,52,52,52	0
56	MG	BA	3618	1/1	0.21	-	37,37,37,37	0
56	MG	DA	3031	1/1	0.17	-	60,60,60,60	0
56	MG	BA	3029	1/1	0.66	-	53,53,53,53	0
56	MG	DA	3366	1/1	0.09	-	43,43,43,43	0
56	MG	BA	3324	1/1	0.26	-	54,54,54,54	0
56	MG	BA	3014	1/1	0.37	-	48,48,48,48	0
56	MG	DA	3345	1/1	0.12	-	16,16,16,16	0
56	MG	CA	3071	1/1	0.15	-	64,64,64,64	0
56	MG	BA	3229	1/1	0.36	-	50,50,50,50	0
56	MG	BA	3638	1/1	0.09	-	73,73,73,73	0
56	MG	CA	3168	1/1	0.46	-	79,79,79,79	0
56	MG	DA	3573	1/1	0.16	-	32,32,32,32	0
56	MG	BA	3024	1/1	0.14	-	31,31,31,31	0
56	MG	DA	3652	1/1	0.25	-	26,26,26,26	0
56	MG	BA	3161	1/1	0.13	-	50,50,50,50	0
56	MG	BA	3362	1/1	0.16	-	23,23,23,23	0
56	MG	AA	3056	1/1	0.20	-	61,61,61,61	0
56	MG	BA	3294	1/1	0.15	-	59,59,59,59	0
56	MG	DA	3621	1/1	0.16	-	46,46,46,46	0
56	MG	BA	3643	1/1	0.18	-	59,59,59,59	0
56	MG	CA	3092	1/1	0.07	-	56,56,56,56	0
56	MG	CA	3014	1/1	0.21	-	56,56,56,56	0
56	MG	BA	3066	1/1	0.23	-	49,49,49,49	0
56	MG	DA	3450	1/1	0.18	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DB	3004	1/1	0.14	-	56,56,56,56	0
56	MG	DA	3075	1/1	0.20	-	45,45,45,45	0
56	MG	B7	102	1/1	0.26	-	29,29,29,29	0
56	MG	BA	3109	1/1	0.25	-	62,62,62,62	0
56	MG	CA	3103	1/1	0.44	-	101,101,101,101	0
56	MG	BA	3026	1/1	0.14	-	36,36,36,36	0
56	MG	BA	3686	1/1	0.30	-	65,65,65,65	0
56	MG	DA	3340	1/1	0.12	-	29,29,29,29	0
56	MG	BU	201	1/1	0.69	-	33,33,33,33	0
56	MG	CA	3108	1/1	0.14	-	45,45,45,45	0
56	MG	BA	3724	1/1	0.21	-	22,22,22,22	0
56	MG	DA	3636	1/1	0.11	-	64,64,64,64	0
56	MG	DA	3296	1/1	0.56	-	65,65,65,65	0
56	MG	BA	3684	1/1	0.16	-	44,44,44,44	0
56	MG	AA	3117	1/1	0.14	-	64,64,64,64	0
56	MG	DA	3191	1/1	0.17	-	31,31,31,31	0
56	MG	BA	3498	1/1	0.32	-	81,81,81,81	0
56	MG	DA	3541	1/1	0.13	-	55,55,55,55	0
56	MG	DA	3276	1/1	0.11	-	26,26,26,26	0
56	MG	BA	3185	1/1	0.22	-	40,40,40,40	0
56	MG	BA	3561	1/1	0.25	-	39,39,39,39	0
56	MG	BZ	3001	1/1	0.21	-	47,47,47,47	0
56	MG	AA	3176	1/1	0.14	-	60,60,60,60	0
56	MG	AD	502	1/1	0.58	-	56,56,56,56	0
56	MG	BA	3367	1/1	0.18	-	29,29,29,29	0
56	MG	BA	3285	1/1	0.18	-	44,44,44,44	0
56	MG	BA	3674	1/1	0.30	-	67,67,67,67	0
56	MG	DA	3479	1/1	0.17	-	35,35,35,35	0
56	MG	DA	3328	1/1	0.28	-	33,33,33,33	0
58	ZN	CN	501	1/1	0.10	-	104,104,104,104	0
56	MG	BA	3539	1/1	0.19	-	23,23,23,23	0
56	MG	DA	3456	1/1	0.20	-	58,58,58,58	0
56	MG	DA	3006	1/1	0.08	-	41,41,41,41	0
56	MG	DA	3650	1/1	0.04	-	35,35,35,35	0
56	MG	DA	3135	1/1	0.27	-	58,58,58,58	0
56	MG	AA	3161	1/1	0.10	-	61,61,61,61	0
56	MG	BA	3326	1/1	0.25	-	15,15,15,15	0
56	MG	BA	3496	1/1	0.45	-	21,21,21,21	0
56	MG	AM	3002	1/1	0.50	-	60,60,60,60	0
56	MG	BA	3220	1/1	0.28	-	27,27,27,27	0
56	MG	BA	3502	1/1	0.23	-	59,59,59,59	0
56	MG	BA	3716	1/1	0.24	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3389	1/1	0.20	-	32,32,32,32	0
56	MG	AA	3179	1/1	0.24	-	34,34,34,34	0
56	MG	BA	3399	1/1	0.23	-	22,22,22,22	0
56	MG	AA	3203	1/1	0.15	-	76,76,76,76	0
56	MG	DA	3581	1/1	0.23	-	41,41,41,41	0
56	MG	BA	3609	1/1	0.25	-	29,29,29,29	0
56	MG	BF	303	1/1	0.10	-	42,42,42,42	0
56	MG	BA	3464	1/1	0.18	-	40,40,40,40	0
56	MG	BA	3118	1/1	0.25	-	53,53,53,53	0
56	MG	DA	3596	1/1	0.15	-	68,68,68,68	0
56	MG	DA	3196	1/1	0.11	-	54,54,54,54	0
56	MG	BA	3698	1/1	0.35	-	58,58,58,58	0
56	MG	DB	3001	1/1	0.19	-	80,80,80,80	0
56	MG	DA	3516	1/1	0.19	-	54,54,54,54	0
56	MG	BA	3444	1/1	0.26	-	29,29,29,29	0
56	MG	DA	3335	1/1	0.21	-	36,36,36,36	0
56	MG	BA	3559	1/1	0.40	-	29,29,29,29	0
56	MG	DW	201	1/1	0.33	-	45,45,45,45	0
56	MG	BA	3495	1/1	0.28	-	27,27,27,27	0
56	MG	DA	3548	1/1	0.17	-	60,60,60,60	0
57	SF4	AD	501	8/8	0.12	-	62,75,82,88	0
56	MG	BA	3441	1/1	0.25	-	29,29,29,29	0
56	MG	DA	3132	1/1	0.65	-	47,47,47,47	0
56	MG	BA	3063	1/1	0.12	-	34,34,34,34	0
56	MG	BA	3273	1/1	0.59	-	35,35,35,35	0
56	MG	BA	3170	1/1	0.43	-	34,34,34,34	0
56	MG	BA	3011	1/1	0.17	-	39,39,39,39	0
56	MG	BA	3146	1/1	0.36	-	56,56,56,56	0
56	MG	DA	3130	1/1	0.09	-	34,34,34,34	0
56	MG	DA	3025	1/1	0.46	-	38,38,38,38	0
56	MG	AA	3186	1/1	0.13	-	51,51,51,51	0
56	MG	DA	3310	1/1	0.27	-	30,30,30,30	0
56	MG	DA	3004	1/1	0.16	-	24,24,24,24	0
56	MG	AA	3153	1/1	0.14	-	46,46,46,46	0
56	MG	DA	3556	1/1	0.10	-	35,35,35,35	0
56	MG	DA	3497	1/1	0.06	-	37,37,37,37	0
56	MG	BA	3297	1/1	0.33	-	43,43,43,43	0
56	MG	DA	3283	1/1	0.17	-	47,47,47,47	0
56	MG	CA	3112	1/1	0.27	-	69,69,69,69	0
56	MG	DA	3256	1/1	0.13	-	41,41,41,41	0
56	MG	BA	3688	1/1	0.06	-	58,58,58,58	0
56	MG	AK	3001	1/1	0.19	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3394	1/1	0.24	-	45,45,45,45	0
56	MG	DA	3155	1/1	0.27	-	50,50,50,50	0
56	MG	BA	3201	1/1	0.28	-	36,36,36,36	0
56	MG	BA	3675	1/1	0.25	-	68,68,68,68	0
56	MG	BA	3577	1/1	0.11	-	63,63,63,63	0
56	MG	DA	3655	1/1	0.12	-	62,62,62,62	0
56	MG	DA	3518	1/1	0.10	-	40,40,40,40	0
56	MG	DA	3260	1/1	0.07	-	32,32,32,32	0
56	MG	AA	3158	1/1	0.23	-	47,47,47,47	0
56	MG	AA	3063	1/1	0.12	-	57,57,57,57	0
56	MG	BA	3166	1/1	0.21	-	41,41,41,41	0
56	MG	BA	3519	1/1	0.06	-	57,57,57,57	0
56	MG	BA	3727	1/1	0.18	-	27,27,27,27	0
56	MG	CA	3056	1/1	0.17	-	63,63,63,63	0
56	MG	BN	3001	1/1	0.38	-	65,65,65,65	0
56	MG	BA	3299	1/1	0.33	-	56,56,56,56	0
56	MG	BA	3473	1/1	0.13	-	55,55,55,55	0
56	MG	CA	3098	1/1	0.20	-	37,37,37,37	0
56	MG	BA	3590	1/1	0.17	-	23,23,23,23	0
56	MG	BA	3072	1/1	0.68	-	45,45,45,45	0
56	MG	AA	3093	1/1	0.34	-	90,90,90,90	0
56	MG	DA	3218	1/1	0.10	-	31,31,31,31	0
56	MG	BA	3117	1/1	0.26	-	37,37,37,37	0
56	MG	BA	3147	1/1	0.61	-	42,42,42,42	0
56	MG	CA	3021	1/1	0.28	-	54,54,54,54	0
56	MG	DA	3147	1/1	0.19	-	46,46,46,46	0
56	MG	DA	3320	1/1	0.21	-	50,50,50,50	0
56	MG	BA	3547	1/1	0.20	-	30,30,30,30	0
56	MG	BA	3336	1/1	0.16	-	46,46,46,46	0
56	MG	DA	3205	1/1	0.25	-	41,41,41,41	0
56	MG	BA	3163	1/1	0.35	-	50,50,50,50	0
56	MG	DA	3066	1/1	0.33	-	59,59,59,59	0
56	MG	CA	3119	1/1	0.42	-	73,73,73,73	0
56	MG	BA	3047	1/1	0.34	-	30,30,30,30	0
56	MG	BA	3242	1/1	0.20	-	45,45,45,45	0
56	MG	DA	3010	1/1	0.32	-	42,42,42,42	0
56	MG	BA	3417	1/1	0.19	-	21,21,21,21	0
56	MG	DA	3601	1/1	0.21	-	50,50,50,50	0
56	MG	BA	3604	1/1	0.37	-	64,64,64,64	0
56	MG	DU	3002	1/1	0.62	-	52,52,52,52	0
56	MG	BG	3002	1/1	0.10	-	51,51,51,51	0
56	MG	BA	3364	1/1	0.21	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3443	1/1	0.21	-	30,30,30,30	0
56	MG	BA	3162	1/1	0.24	-	43,43,43,43	0
56	MG	BA	3721	1/1	0.31	-	56,56,56,56	0
56	MG	AA	3187	1/1	0.06	-	72,72,72,72	0
56	MG	DA	3410	1/1	0.08	-	40,40,40,40	0
56	MG	AA	3163	1/1	0.24	-	23,23,23,23	0
56	MG	BA	3134	1/1	0.13	-	34,34,34,34	0
56	MG	B8	5001	1/1	0.17	-	62,62,62,62	0
56	MG	AA	3181	1/1	0.18	-	46,46,46,46	0
56	MG	DA	3100	1/1	0.59	-	55,55,55,55	0
56	MG	DA	3378	1/1	0.10	-	38,38,38,38	0
56	MG	BA	3603	1/1	0.29	-	40,40,40,40	0
56	MG	DA	3088	1/1	0.18	-	47,47,47,47	0
56	MG	CE	3001	1/1	0.21	-	66,66,66,66	0
56	MG	CA	3065	1/1	0.36	-	81,81,81,81	0
56	MG	BA	3264	1/1	0.18	-	29,29,29,29	0
56	MG	CA	3066	1/1	0.09	-	47,47,47,47	0
56	MG	BA	3149	1/1	0.04	-	58,58,58,58	0
56	MG	AA	3048	1/1	0.09	-	52,52,52,52	0
56	MG	DA	3119	1/1	0.16	-	44,44,44,44	0
56	MG	BA	3486	1/1	0.27	-	55,55,55,55	0
56	MG	DA	3624	1/1	0.12	-	54,54,54,54	0
56	MG	DA	3475	1/1	0.12	-	35,35,35,35	0
56	MG	AA	3078	1/1	0.31	-	55,55,55,55	0
56	MG	DA	3129	1/1	0.34	-	45,45,45,45	0
56	MG	BA	3315	1/1	0.35	-	43,43,43,43	0
56	MG	AA	3140	1/1	0.11	-	65,65,65,65	0
56	MG	BA	3579	1/1	0.31	-	21,21,21,21	0
56	MG	DA	3172	1/1	0.33	-	46,46,46,46	0
56	MG	BA	3288	1/1	0.11	-	45,45,45,45	0
56	MG	AA	3024	1/1	0.09	-	49,49,49,49	0
56	MG	DA	3333	1/1	0.11	-	61,61,61,61	0
56	MG	BN	3003	1/1	0.38	-	67,67,67,67	0
56	MG	CA	3051	1/1	0.13	-	77,77,77,77	0
56	MG	BA	3240	1/1	0.28	-	54,54,54,54	0
56	MG	DA	3055	1/1	0.23	-	55,55,55,55	0
56	MG	DA	3440	1/1	0.07	-	48,48,48,48	0
56	MG	BA	3365	1/1	0.05	-	63,63,63,63	0
56	MG	BQ	3003	1/1	0.18	-	15,15,15,15	0
56	MG	BA	3425	1/1	0.22	-	42,42,42,42	0
56	MG	AA	3088	1/1	0.33	-	53,53,53,53	0
56	MG	DA	3392	1/1	0.14	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3053	1/1	1.84	-	87,87,87,87	0
56	MG	BA	3466	1/1	0.13	-	53,53,53,53	0
56	MG	BA	3463	1/1	0.11	-	32,32,32,32	0
56	MG	BA	3475	1/1	0.07	-	42,42,42,42	0
56	MG	CA	3115	1/1	0.07	-	81,81,81,81	0
56	MG	DA	3324	1/1	0.18	-	24,24,24,24	0
56	MG	BA	3523	1/1	0.16	-	32,32,32,32	0
56	MG	AA	3156	1/1	0.13	-	31,31,31,31	0
56	MG	DA	3305	1/1	0.19	-	33,33,33,33	0
56	MG	AA	3105	1/1	0.31	-	54,54,54,54	0
56	MG	AA	3050	1/1	0.28	-	50,50,50,50	0
56	MG	BA	3292	1/1	0.25	-	59,59,59,59	0
56	MG	BA	3682	1/1	0.35	-	50,50,50,50	0
56	MG	DA	3453	1/1	0.12	-	44,44,44,44	0
56	MG	AA	3090	1/1	0.19	-	64,64,64,64	0
56	MG	DA	3490	1/1	0.15	-	46,46,46,46	0
56	MG	DA	3244	1/1	0.21	-	23,23,23,23	0
56	MG	BA	3328	1/1	0.19	-	41,41,41,41	0
56	MG	DA	3044	1/1	0.23	-	45,45,45,45	0
56	MG	DA	3588	1/1	0.10	-	47,47,47,47	0
56	MG	BA	3283	1/1	0.18	-	61,61,61,61	0
56	MG	BA	3122	1/1	0.64	-	68,68,68,68	0
56	MG	BA	3687	1/1	0.15	-	59,59,59,59	0
56	MG	DA	3334	1/1	0.17	-	37,37,37,37	0
56	MG	CA	3078	1/1	0.28	-	51,51,51,51	0
56	MG	DA	3367	1/1	0.05	-	55,55,55,55	0
56	MG	BA	3217	1/1	0.32	-	59,59,59,59	0
56	MG	DA	3122	1/1	0.13	-	60,60,60,60	0
56	MG	BA	3308	1/1	0.19	-	33,33,33,33	0
56	MG	BB	3001	1/1	0.15	-	56,56,56,56	0
56	MG	DA	3050	1/1	0.46	-	30,30,30,30	0
56	MG	DA	3365	1/1	0.07	-	52,52,52,52	0
56	MG	B5	502	1/1	0.10	-	56,56,56,56	0
56	MG	BA	3591	1/1	0.23	-	38,38,38,38	0
56	MG	DA	3557	1/1	0.25	-	74,74,74,74	0
56	MG	AA	3098	1/1	0.46	-	76,76,76,76	0
56	MG	CA	3124	1/1	0.15	-	64,64,64,64	0
56	MG	CA	3036	1/1	0.25	-	56,56,56,56	0
56	MG	BA	3261	1/1	0.30	-	45,45,45,45	0
56	MG	DA	3272	1/1	0.12	-	36,36,36,36	0
56	MG	DA	3631	1/1	0.18	-	49,49,49,49	0
56	MG	BA	3677	1/1	0.19	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3067	1/1	0.28	-	66,66,66,66	0
56	MG	DA	3142	1/1	0.21	-	33,33,33,33	0
56	MG	AA	3003	1/1	0.28	-	70,70,70,70	0
56	MG	DA	3036	1/1	0.30	-	35,35,35,35	0
56	MG	BA	3306	1/1	0.15	-	19,19,19,19	0
56	MG	BA	3587	1/1	0.22	-	23,23,23,23	0
56	MG	DA	3030	1/1	0.28	-	49,49,49,49	0
56	MG	DA	3455	1/1	0.20	-	53,53,53,53	0
56	MG	AA	3143	1/1	0.20	-	67,67,67,67	0
56	MG	DA	3090	1/1	0.27	-	59,59,59,59	0
56	MG	DA	3415	1/1	0.08	-	22,22,22,22	0
56	MG	AA	3182	1/1	0.13	-	48,48,48,48	0
57	SF4	CD	501	8/8	0.11	-	63,76,87,96	0
56	MG	DA	3483	1/1	0.16	-	55,55,55,55	0
56	MG	DA	3237	1/1	0.33	-	37,37,37,37	0
56	MG	DA	3107	1/1	0.13	-	50,50,50,50	0
56	MG	CA	3029	1/1	0.23	-	54,54,54,54	0
56	MG	BB	3012	1/1	0.17	-	42,42,42,42	0
56	MG	BA	3317	1/1	0.23	-	40,40,40,40	0
56	MG	BA	3211	1/1	0.08	-	43,43,43,43	0
56	MG	DA	3458	1/1	0.23	-	47,47,47,47	0
56	MG	DA	3487	1/1	0.06	-	44,44,44,44	0
56	MG	DA	3437	1/1	0.18	-	46,46,46,46	0
56	MG	BA	3311	1/1	0.28	-	52,52,52,52	0
56	MG	AA	3115	1/1	0.19	-	67,67,67,67	0
56	MG	BA	3650	1/1	0.15	-	44,44,44,44	0
56	MG	DA	3396	1/1	0.14	-	37,37,37,37	0
56	MG	BE	303	1/1	0.08	-	39,39,39,39	0
56	MG	DA	3474	1/1	0.10	-	49,49,49,49	0
56	MG	BA	3545	1/1	0.18	-	20,20,20,20	0
56	MG	CA	3150	1/1	0.22	-	63,63,63,63	0
56	MG	BA	3428	1/1	0.41	-	36,36,36,36	0
56	MG	CX	104	1/1	0.11	-	52,52,52,52	0
56	MG	BA	3460	1/1	0.18	-	66,66,66,66	0
56	MG	DA	3404	1/1	0.19	-	57,57,57,57	0
56	MG	BA	3655	1/1	0.11	-	44,44,44,44	0
56	MG	AA	3141	1/1	0.22	-	51,51,51,51	0
56	MG	DA	3093	1/1	0.13	-	51,51,51,51	0
56	MG	DA	3184	1/1	0.18	-	54,54,54,54	0
56	MG	DA	3181	1/1	0.27	-	55,55,55,55	0
56	MG	AS	3001	1/1	0.15	-	79,79,79,79	0
56	MG	BA	3511	1/1	0.15	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3008	1/1	0.25	-	56,56,56,56	0
56	MG	AA	3001	1/1	0.24	-	74,74,74,74	0
56	MG	DA	3593	1/1	0.22	-	62,62,62,62	0
56	MG	DA	3382	1/1	0.06	-	44,44,44,44	0
56	MG	BA	3154	1/1	0.41	-	55,55,55,55	0
56	MG	BA	3348	1/1	0.09	-	29,29,29,29	0
56	MG	DB	3008	1/1	0.12	-	36,36,36,36	0
56	MG	DA	3077	1/1	0.32	-	48,48,48,48	0
56	MG	CA	3101	1/1	0.11	-	58,58,58,58	0
56	MG	AA	3184	1/1	0.13	-	81,81,81,81	0
56	MG	BA	3592	1/1	0.16	-	43,43,43,43	0
56	MG	DA	3251	1/1	0.27	-	50,50,50,50	0
56	MG	DA	3495	1/1	0.09	-	53,53,53,53	0
56	MG	DA	3053	1/1	0.20	-	47,47,47,47	0
56	MG	BR	201	1/1	0.41	-	44,44,44,44	0
56	MG	BA	3208	1/1	0.13	-	50,50,50,50	0
56	MG	AA	3064	1/1	0.14	-	65,65,65,65	0
56	MG	BD	307	1/1	0.26	-	36,36,36,36	0
56	MG	BA	3042	1/1	0.14	-	50,50,50,50	0
56	MG	AA	3072	1/1	0.25	-	69,69,69,69	0
56	MG	DA	3226	1/1	0.19	-	47,47,47,47	0
56	MG	BA	3627	1/1	0.29	-	50,50,50,50	0
56	MG	DA	3546	1/1	0.22	-	38,38,38,38	0
56	MG	BA	3378	1/1	0.18	-	24,24,24,24	0
56	MG	CA	3034	1/1	0.28	-	66,66,66,66	0
56	MG	BA	3173	1/1	0.23	-	41,41,41,41	0
56	MG	DA	3300	1/1	0.15	-	47,47,47,47	0
56	MG	BA	3278	1/1	0.16	-	53,53,53,53	0
56	MG	CA	3153	1/1	0.10	-	85,85,85,85	0
56	MG	BA	3570	1/1	0.21	-	33,33,33,33	0
56	MG	BA	3432	1/1	0.14	-	27,27,27,27	0
56	MG	AA	3055	1/1	0.28	-	56,56,56,56	0
56	MG	DA	3550	1/1	0.09	-	54,54,54,54	0
56	MG	AA	3031	1/1	0.25	-	41,41,41,41	0
56	MG	BA	3345	1/1	0.04	-	37,37,37,37	0
56	MG	DA	3391	1/1	0.14	-	54,54,54,54	0
56	MG	BQ	3004	1/1	0.32	-	41,41,41,41	0
56	MG	CA	3170	1/1	0.37	-	44,44,44,44	0
56	MG	BA	3644	1/1	0.11	-	38,38,38,38	0
56	MG	DA	3425	1/1	0.19	-	51,51,51,51	0
56	MG	BB	3013	1/1	0.17	-	31,31,31,31	0
56	MG	AX	105	1/1	0.41	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3111	1/1	0.19	-	43,43,43,43	0
56	MG	DA	3138	1/1	0.40	-	53,53,53,53	0
56	MG	BV	3003	1/1	0.24	-	27,27,27,27	0
56	MG	DA	3141	1/1	0.18	-	63,63,63,63	0
56	MG	DA	3126	1/1	0.17	-	61,61,61,61	0
56	MG	DA	3069	1/1	0.16	-	49,49,49,49	0
58	ZN	D6	501	1/1	0.11	-	65,65,65,65	0
56	MG	AA	3169	1/1	0.20	-	62,62,62,62	0
56	MG	DB	3006	1/1	0.20	-	54,54,54,54	0
56	MG	AA	3151	1/1	0.07	-	49,49,49,49	0
56	MG	BA	3392	1/1	0.13	-	53,53,53,53	0
56	MG	CA	3172	1/1	0.21	-	65,65,65,65	0
56	MG	BA	3107	1/1	0.17	-	60,60,60,60	0
56	MG	DA	3492	1/1	0.08	-	44,44,44,44	0
56	MG	AA	3092	1/1	0.47	-	59,59,59,59	0
56	MG	BG	3003	1/1	0.22	-	53,53,53,53	0
56	MG	DA	3607	1/1	0.19	-	68,68,68,68	0
56	MG	CA	3070	1/1	0.39	-	59,59,59,59	0
56	MG	BA	3376	1/1	0.32	-	35,35,35,35	0
56	MG	CA	3064	1/1	0.15	-	74,74,74,74	0
56	MG	BA	3124	1/1	0.22	-	46,46,46,46	0
56	MG	DA	3043	1/1	0.49	-	56,56,56,56	0
56	MG	AA	3172	1/1	0.08	-	36,36,36,36	0
56	MG	DA	3028	1/1	0.07	-	34,34,34,34	0
56	MG	AA	3220	1/1	0.10	-	42,42,42,42	0
56	MG	AA	3006	1/1	0.09	-	84,84,84,84	0
56	MG	DR	5001	1/1	0.16	-	39,39,39,39	0
56	MG	CA	3160	1/1	0.14	-	49,49,49,49	0
56	MG	DA	3087	1/1	0.26	-	43,43,43,43	0
56	MG	AA	3190	1/1	0.30	-	61,61,61,61	0
56	MG	DA	3644	1/1	0.68	-	50,50,50,50	0
56	MG	DA	3509	1/1	0.08	-	57,57,57,57	0
56	MG	DA	3577	1/1	0.23	-	44,44,44,44	0
56	MG	BA	3280	1/1	0.31	-	44,44,44,44	0
56	MG	AA	3188	1/1	0.26	-	52,52,52,52	0
56	MG	DA	3023	1/1	0.41	-	64,64,64,64	0
56	MG	CA	3128	1/1	0.25	-	55,55,55,55	0
56	MG	BA	3497	1/1	0.44	-	28,28,28,28	0
56	MG	CA	3081	1/1	0.08	-	72,72,72,72	0
56	MG	DA	3327	1/1	0.12	-	45,45,45,45	0
56	MG	BA	3645	1/1	0.20	-	63,63,63,63	0
56	MG	DA	3485	1/1	0.20	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3294	1/1	0.20	-	30,30,30,30	0
56	MG	DA	3405	1/1	0.33	-	53,53,53,53	0
56	MG	DA	3585	1/1	0.22	-	62,62,62,62	0
56	MG	DE	303	1/1	0.14	-	36,36,36,36	0
56	MG	DA	3582	1/1	0.37	-	44,44,44,44	0
56	MG	BA	3662	1/1	0.13	-	46,46,46,46	0
56	MG	DA	3620	1/1	0.19	-	66,66,66,66	0
56	MG	DA	3553	1/1	0.15	-	58,58,58,58	0
56	MG	DA	3161	1/1	0.17	-	51,51,51,51	0
56	MG	DA	3493	1/1	0.25	-	38,38,38,38	0
56	MG	DA	3014	1/1	0.29	-	38,38,38,38	0
56	MG	DA	3131	1/1	0.21	-	60,60,60,60	0
56	MG	BA	3381	1/1	0.07	-	25,25,25,25	0
56	MG	DA	3201	1/1	0.21	-	43,43,43,43	0
56	MG	DA	3312	1/1	0.23	-	24,24,24,24	0
56	MG	BA	3051	1/1	0.30	-	34,34,34,34	0
56	MG	DA	3635	1/1	0.12	-	39,39,39,39	0
56	MG	DA	3286	1/1	0.18	-	26,26,26,26	0
56	MG	BF	302	1/1	0.25	-	49,49,49,49	0
56	MG	BA	3617	1/1	0.34	-	30,30,30,30	0
56	MG	CA	3096	1/1	0.12	-	54,54,54,54	0
56	MG	BA	3517	1/1	0.12	-	52,52,52,52	0
56	MG	DA	3183	1/1	0.13	-	42,42,42,42	0
56	MG	AA	3189	1/1	0.14	-	74,74,74,74	0
56	MG	DA	3416	1/1	0.39	-	34,34,34,34	0
56	MG	BA	3329	1/1	0.06	-	49,49,49,49	0
56	MG	B0	104	1/1	0.38	-	55,55,55,55	0
56	MG	DA	3534	1/1	0.14	-	62,62,62,62	0
56	MG	DA	3035	1/1	0.52	-	58,58,58,58	0
56	MG	AA	3091	1/1	0.25	-	75,75,75,75	0
56	MG	BD	303	1/1	0.29	-	35,35,35,35	0
56	MG	BA	3255	1/1	0.20	-	53,53,53,53	0
56	MG	DA	3606	1/1	0.19	-	58,58,58,58	0
56	MG	BA	3048	1/1	0.33	-	33,33,33,33	0
56	MG	BA	3728	1/1	0.25	-	56,56,56,56	0
56	MG	AA	3021	1/1	0.16	-	76,76,76,76	0
56	MG	DA	3180	1/1	0.21	-	47,47,47,47	0
56	MG	DA	3071	1/1	0.52	-	46,46,46,46	0
56	MG	BA	3514	1/1	0.21	-	49,49,49,49	0
56	MG	BA	3030	1/1	0.34	-	26,26,26,26	0
56	MG	AA	3200	1/1	0.28	-	79,79,79,79	0
56	MG	CA	3006	1/1	0.09	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3216	1/1	0.17	-	47,47,47,47	0
56	MG	DA	3513	1/1	0.11	-	58,58,58,58	0
56	MG	BA	3281	1/1	0.21	-	45,45,45,45	0
56	MG	DA	3357	1/1	0.12	-	50,50,50,50	0
56	MG	DE	301	1/1	0.83	-	51,51,51,51	0
56	MG	DA	3545	1/1	0.26	-	35,35,35,35	0
56	MG	DA	3106	1/1	0.54	-	45,45,45,45	0
56	MG	DA	3057	1/1	0.27	-	57,57,57,57	0
56	MG	BA	3685	1/1	0.21	-	58,58,58,58	0
56	MG	BA	3442	1/1	0.18	-	33,33,33,33	0
56	MG	DA	3452	1/1	0.20	-	64,64,64,64	0
56	MG	BA	3563	1/1	0.38	-	66,66,66,66	0
56	MG	BA	3346	1/1	0.17	-	33,33,33,33	0
56	MG	DA	3643	1/1	0.28	-	18,18,18,18	0
56	MG	BA	3156	1/1	0.42	-	61,61,61,61	0
56	MG	BA	3200	1/1	0.28	-	32,32,32,32	0
56	MG	DA	3061	1/1	0.27	-	47,47,47,47	0
56	MG	DA	3625	1/1	0.16	-	48,48,48,48	0
56	MG	CA	3039	1/1	0.56	-	82,82,82,82	0
56	MG	CA	3002	1/1	0.07	-	74,74,74,74	0
56	MG	BA	3414	1/1	0.22	-	51,51,51,51	0
56	MG	DA	3192	1/1	0.54	-	48,48,48,48	0
56	MG	BX	101	1/1	0.08	-	38,38,38,38	0
56	MG	BA	3382	1/1	0.23	-	21,21,21,21	0
56	MG	AA	3060	1/1	0.41	-	52,52,52,52	0
56	MG	BA	3430	1/1	0.10	-	47,47,47,47	0
56	MG	BA	3077	1/1	0.18	-	20,20,20,20	0
56	MG	BA	3338	1/1	0.20	-	62,62,62,62	0
56	MG	DA	3352	1/1	0.27	-	24,24,24,24	0
56	MG	DA	3578	1/1	0.14	-	68,68,68,68	0
56	MG	DA	3401	1/1	0.14	-	41,41,41,41	0
56	MG	BA	3477	1/1	0.16	-	52,52,52,52	0
56	MG	BA	3235	1/1	0.33	-	44,44,44,44	0
56	MG	BA	3268	1/1	0.20	-	29,29,29,29	0
56	MG	CA	3042	1/1	0.29	-	69,69,69,69	0
56	MG	BA	3037	1/1	0.52	-	39,39,39,39	0
56	MG	DQ	3002	1/1	0.31	-	51,51,51,51	0
56	MG	DA	3350	1/1	0.23	-	21,21,21,21	0
56	MG	DA	3137	1/1	0.32	-	62,62,62,62	0
56	MG	CA	3005	1/1	0.37	-	37,37,37,37	0
56	MG	DA	3308	1/1	0.10	-	32,32,32,32	0
56	MG	BA	3318	1/1	0.14	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3712	1/1	0.25	-	47,47,47,47	0
56	MG	BA	3424	1/1	0.17	-	44,44,44,44	0
56	MG	BA	3390	1/1	0.09	-	40,40,40,40	0
56	MG	BA	3126	1/1	0.33	-	47,47,47,47	0
56	MG	DA	3412	1/1	0.16	-	34,34,34,34	0
56	MG	BA	3075	1/1	0.23	-	36,36,36,36	0
56	MG	BA	3664	1/1	0.18	-	63,63,63,63	0
56	MG	DA	3160	1/1	0.23	-	47,47,47,47	0
56	MG	BA	3160	1/1	0.16	-	24,24,24,24	0
56	MG	DA	3133	1/1	0.13	-	31,31,31,31	0
56	MG	BA	3405	1/1	0.23	-	57,57,57,57	0
56	MG	BA	3214	1/1	0.28	-	37,37,37,37	0
56	MG	BA	3142	1/1	0.30	-	57,57,57,57	0
56	MG	DA	3597	1/1	0.14	-	66,66,66,66	0
56	MG	BA	3558	1/1	0.19	-	47,47,47,47	0
56	MG	CA	3089	1/1	0.16	-	54,54,54,54	0
56	MG	DA	3279	1/1	0.27	-	32,32,32,32	0
56	MG	BA	3059	1/1	0.37	-	35,35,35,35	0
56	MG	BA	3663	1/1	0.32	-	73,73,73,73	0
56	MG	DA	3406	1/1	0.06	-	48,48,48,48	0
56	MG	CA	3022	1/1	0.05	-	67,67,67,67	0
56	MG	DA	3459	1/1	0.13	-	43,43,43,43	0
56	MG	DA	3250	1/1	0.09	-	42,42,42,42	0
56	MG	BD	304	1/1	0.39	-	41,41,41,41	0
56	MG	AA	3018	1/1	0.25	-	51,51,51,51	0
56	MG	BA	3578	1/1	0.18	-	47,47,47,47	0
56	MG	DA	3151	1/1	0.34	-	48,48,48,48	0
56	MG	AA	3222	1/1	0.14	-	64,64,64,64	0
56	MG	BA	3551	1/1	0.16	-	31,31,31,31	0
56	MG	BA	3031	1/1	0.58	-	44,44,44,44	0
56	MG	BA	3733	1/1	0.38	-	40,40,40,40	0
56	MG	BA	3206	1/1	0.26	-	32,32,32,32	0
56	MG	BA	3710	1/1	0.06	-	57,57,57,57	0
56	MG	BA	3683	1/1	0.28	-	37,37,37,37	0
56	MG	DA	3094	1/1	0.27	-	26,26,26,26	0
56	MG	CA	3013	1/1	0.09	-	46,46,46,46	0
56	MG	DA	3012	1/1	0.40	-	52,52,52,52	0
56	MG	CA	3093	1/1	0.10	-	65,65,65,65	0
56	MG	DA	3587	1/1	0.16	-	57,57,57,57	0
56	MG	AA	3100	1/1	0.58	-	43,43,43,43	0
56	MG	DA	3274	1/1	0.39	-	49,49,49,49	0
56	MG	BA	3347	1/1	0.15	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3241	1/1	0.10	-	74,74,74,74	0
56	MG	BA	3530	1/1	0.22	-	72,72,72,72	0
56	MG	AA	3067	1/1	0.36	-	76,76,76,76	0
56	MG	DF	301	1/1	0.36	-	40,40,40,40	0
56	MG	DA	3247	1/1	0.34	-	34,34,34,34	0
56	MG	DA	3199	1/1	0.16	-	46,46,46,46	0
56	MG	BG	3001	1/1	0.10	-	65,65,65,65	0
56	MG	AA	3107	1/1	0.29	-	44,44,44,44	0
56	MG	DA	3266	1/1	0.19	-	32,32,32,32	0
56	MG	DA	3239	1/1	0.14	-	54,54,54,54	0
56	MG	DA	3384	1/1	0.12	-	24,24,24,24	0
56	MG	DA	3264	1/1	0.19	-	38,38,38,38	0
58	ZN	D4	501	1/1	0.07	-	155,155,155,155	0
56	MG	DA	3537	1/1	0.18	-	74,74,74,74	0
56	MG	DA	3285	1/1	0.10	-	41,41,41,41	0
56	MG	BE	302	1/1	0.17	-	29,29,29,29	0
56	MG	DA	3062	1/1	0.40	-	58,58,58,58	0
56	MG	DA	3360	1/1	0.12	-	36,36,36,36	0
56	MG	BA	3468	1/1	0.17	-	45,45,45,45	0
56	MG	BU	202	1/1	0.75	-	41,41,41,41	0
56	MG	AA	3038	1/1	0.45	-	64,64,64,64	0
56	MG	DA	3202	1/1	0.21	-	39,39,39,39	0
56	MG	BA	3096	1/1	0.23	-	35,35,35,35	0
56	MG	DA	3001	1/1	0.28	-	76,76,76,76	0
56	MG	DA	3604	1/1	0.08	-	50,50,50,50	0
56	MG	BA	3557	1/1	0.26	-	35,35,35,35	0
56	MG	DA	3068	1/1	0.18	-	52,52,52,52	0
56	MG	BA	3652	1/1	0.22	-	54,54,54,54	0
56	MG	BP	203	1/1	0.75	-	39,39,39,39	0
56	MG	AA	3195	1/1	0.18	-	58,58,58,58	0
56	MG	BA	3366	1/1	0.13	-	30,30,30,30	0
56	MG	BA	3074	1/1	0.16	-	38,38,38,38	0
56	MG	BA	3139	1/1	0.78	-	50,50,50,50	0
56	MG	CA	3054	1/1	0.42	-	74,74,74,74	0
56	MG	AA	3017	1/1	0.28	-	57,57,57,57	0
56	MG	DA	3579	1/1	0.17	-	38,38,38,38	0
56	MG	B0	102	1/1	0.15	-	50,50,50,50	0
56	MG	BA	3690	1/1	0.22	-	55,55,55,55	0
56	MG	DA	3143	1/1	0.21	-	53,53,53,53	0
56	MG	DA	3288	1/1	0.21	-	68,68,68,68	0
56	MG	DA	3552	1/1	0.13	-	42,42,42,42	0
56	MG	CA	3133	1/1	0.14	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3455	1/1	0.39	-	47,47,47,47	0
56	MG	BA	3408	1/1	0.12	-	28,28,28,28	0
56	MG	BA	3282	1/1	0.15	-	34,34,34,34	0
56	MG	CA	3131	1/1	0.12	-	48,48,48,48	0
56	MG	CA	3059	1/1	0.17	-	51,51,51,51	0
56	MG	BA	3241	1/1	0.42	-	41,41,41,41	0
56	MG	DA	3089	1/1	0.27	-	51,51,51,51	0
56	MG	BA	3302	1/1	0.25	-	48,48,48,48	0
56	MG	BA	3482	1/1	0.11	-	59,59,59,59	0
56	MG	DB	3005	1/1	0.25	-	41,41,41,41	0
56	MG	DA	3619	1/1	0.17	-	67,67,67,67	0
56	MG	BA	3596	1/1	0.25	-	79,79,79,79	0
56	MG	BA	3169	1/1	0.21	-	39,39,39,39	0
56	MG	BA	3546	1/1	0.27	-	46,46,46,46	0
56	MG	AA	3094	1/1	0.24	-	78,78,78,78	0
56	MG	BB	3008	1/1	0.19	-	49,49,49,49	0
56	MG	AA	3175	1/1	0.15	-	70,70,70,70	0
56	MG	CA	3073	1/1	0.45	-	74,74,74,74	0
56	MG	CA	3116	1/1	0.20	-	76,76,76,76	0
56	MG	AA	3075	1/1	0.11	-	50,50,50,50	0
56	MG	BA	3661	1/1	0.25	-	69,69,69,69	0
56	MG	CA	3110	1/1	0.13	-	93,93,93,93	0
56	MG	AA	3020	1/1	0.20	-	80,80,80,80	0
56	MG	DA	3353	1/1	0.17	-	54,54,54,54	0
56	MG	BA	3340	1/1	0.20	-	57,57,57,57	0
56	MG	BA	3277	1/1	0.46	-	45,45,45,45	0
56	MG	BA	3436	1/1	0.27	-	35,35,35,35	0
56	MG	DA	3110	1/1	0.15	-	46,46,46,46	0
56	MG	DA	3467	1/1	0.30	-	48,48,48,48	0
56	MG	DA	3589	1/1	0.11	-	65,65,65,65	0
56	MG	DV	201	1/1	0.25	-	56,56,56,56	0
56	MG	BA	3633	1/1	0.34	-	54,54,54,54	0
56	MG	CA	3060	1/1	0.41	-	59,59,59,59	0
56	MG	DA	3074	1/1	0.27	-	60,60,60,60	0
56	MG	BA	3053	1/1	0.18	-	52,52,52,52	0
56	MG	BA	3508	1/1	0.17	-	46,46,46,46	0
56	MG	BA	3631	1/1	0.14	-	41,41,41,41	0
56	MG	BB	3006	1/1	0.30	-	34,34,34,34	0
56	MG	DA	3269	1/1	0.16	-	47,47,47,47	0
56	MG	BD	310	1/1	0.41	-	48,48,48,48	0
56	MG	CA	3094	1/1	0.21	-	37,37,37,37	0
56	MG	CA	3151	1/1	0.14	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3496	1/1	0.34	-	76,76,76,76	0
56	MG	AA	3131	1/1	0.37	-	65,65,65,65	0
56	MG	DA	3254	1/1	0.14	-	52,52,52,52	0
56	MG	CA	3161	1/1	0.18	-	71,71,71,71	0
56	MG	DA	3229	1/1	0.15	-	44,44,44,44	0
56	MG	DA	3494	1/1	0.12	-	50,50,50,50	0
56	MG	DA	3569	1/1	0.08	-	54,54,54,54	0
56	MG	BB	3015	1/1	0.08	-	35,35,35,35	0
56	MG	DA	3560	1/1	0.07	-	57,57,57,57	0
56	MG	BD	302	1/1	0.56	-	44,44,44,44	0
56	MG	DA	3034	1/1	0.20	-	40,40,40,40	0
56	MG	DA	3408	1/1	0.18	-	35,35,35,35	0
56	MG	BA	3700	1/1	0.24	-	26,26,26,26	0
56	MG	DA	3306	1/1	0.17	-	51,51,51,51	0
56	MG	BA	3492	1/1	0.19	-	48,48,48,48	0
56	MG	AA	3065	1/1	0.28	-	50,50,50,50	0
56	MG	BA	3397	1/1	0.10	-	44,44,44,44	0
56	MG	BA	3516	1/1	0.18	-	64,64,64,64	0
56	MG	DA	3608	1/1	0.28	-	63,63,63,63	0
56	MG	BA	3654	1/1	0.13	-	49,49,49,49	0
56	MG	BB	3005	1/1	0.18	-	62,62,62,62	0
56	MG	DA	3473	1/1	0.19	-	50,50,50,50	0
56	MG	AA	3112	1/1	0.12	-	53,53,53,53	0
56	MG	AA	3059	1/1	0.62	-	49,49,49,49	0
56	MG	DA	3108	1/1	0.54	-	50,50,50,50	0
56	MG	B0	105	1/1	0.27	-	44,44,44,44	0
56	MG	DA	3648	1/1	0.22	-	43,43,43,43	0
56	MG	DA	3319	1/1	0.12	-	31,31,31,31	0
56	MG	BA	3550	1/1	0.19	-	32,32,32,32	0
56	MG	AA	3180	1/1	0.45	-	75,75,75,75	0
56	MG	BE	307	1/1	0.28	-	51,51,51,51	0
56	MG	AA	3044	1/1	0.14	-	60,60,60,60	0
56	MG	BA	3535	1/1	0.19	-	42,42,42,42	0
56	MG	DA	3204	1/1	0.28	-	44,44,44,44	0
56	MG	DA	3571	1/1	0.10	-	57,57,57,57	0
56	MG	AA	3147	1/1	0.44	-	51,51,51,51	0
56	MG	BA	3203	1/1	0.20	-	45,45,45,45	0
56	MG	BA	3330	1/1	0.10	-	35,35,35,35	0
56	MG	AA	3137	1/1	0.16	-	40,40,40,40	0
56	MG	BA	3350	1/1	0.26	-	36,36,36,36	0
56	MG	CA	3085	1/1	0.28	-	58,58,58,58	0
56	MG	CA	3055	1/1	0.27	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BB	3016	1/1	0.14	-	24,24,24,24	0
56	MG	DA	3190	1/1	0.11	-	54,54,54,54	0
56	MG	BA	3388	1/1	0.23	-	30,30,30,30	0
56	MG	DA	3468	1/1	0.29	-	47,47,47,47	0
56	MG	DA	3213	1/1	0.07	-	48,48,48,48	0
56	MG	BA	3389	1/1	0.14	-	52,52,52,52	0
56	MG	BA	3165	1/1	0.42	-	44,44,44,44	0
56	MG	BQ	3001	1/1	0.33	-	38,38,38,38	0
56	MG	BA	3406	1/1	0.21	-	54,54,54,54	0
56	MG	DA	3177	1/1	0.23	-	30,30,30,30	0
56	MG	DA	3433	1/1	0.24	-	39,39,39,39	0
56	MG	DA	3506	1/1	0.09	-	61,61,61,61	0
56	MG	BA	3003	1/1	0.09	-	24,24,24,24	0
56	MG	BA	3544	1/1	0.21	-	35,35,35,35	0
56	MG	AA	3030	1/1	0.65	-	66,66,66,66	0
56	MG	BA	3711	1/1	0.45	-	64,64,64,64	0
56	MG	BA	3369	1/1	0.13	-	49,49,49,49	0
56	MG	DA	3524	1/1	0.23	-	51,51,51,51	0
56	MG	CA	3109	1/1	0.13	-	79,79,79,79	0
56	MG	BA	3625	1/1	0.47	-	80,80,80,80	0
56	MG	AA	3081	1/1	0.41	-	46,46,46,46	0
56	MG	DA	3428	1/1	0.29	-	30,30,30,30	0
56	MG	BA	3580	1/1	0.17	-	58,58,58,58	0
56	MG	BA	3150	1/1	0.35	-	42,42,42,42	0
56	MG	DA	3316	1/1	0.27	-	47,47,47,47	0
56	MG	DA	3150	1/1	0.10	-	57,57,57,57	0
56	MG	BA	3526	1/1	0.12	-	49,49,49,49	0
56	MG	CX	103	1/1	0.21	-	57,57,57,57	0
56	MG	AA	3028	1/1	0.56	-	72,72,72,72	0
56	MG	AA	3096	1/1	0.28	-	52,52,52,52	0
56	MG	BP	204	1/1	0.08	-	53,53,53,53	0
56	MG	AA	3197	1/1	0.12	-	64,64,64,64	0
56	MG	AA	3216	1/1	0.22	-	60,60,60,60	0
56	MG	BA	3313	1/1	0.12	-	56,56,56,56	0
56	MG	AA	3026	1/1	0.18	-	52,52,52,52	0
56	MG	DA	3242	1/1	0.24	-	31,31,31,31	0
56	MG	DA	3082	1/1	0.07	-	7,7,7,7	0
56	MG	BA	3542	1/1	0.18	-	37,37,37,37	0
56	MG	DA	3482	1/1	0.17	-	45,45,45,45	0
56	MG	CA	3007	1/1	0.33	-	63,63,63,63	0
56	MG	DA	3498	1/1	0.13	-	75,75,75,75	0
56	MG	AA	3154	1/1	0.09	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3276	1/1	0.27	-	9,9,9,9	0
56	MG	DG	3001	1/1	0.10	-	68,68,68,68	0
56	MG	CA	3075	1/1	0.36	-	76,76,76,76	0
56	MG	BA	3646	1/1	0.20	-	39,39,39,39	0
56	MG	AA	3202	1/1	0.21	-	72,72,72,72	0
56	MG	AA	3076	1/1	0.35	-	74,74,74,74	0
56	MG	BA	3454	1/1	0.23	-	20,20,20,20	0
56	MG	BA	3372	1/1	0.15	-	42,42,42,42	0
56	MG	DA	3238	1/1	0.12	-	37,37,37,37	0
56	MG	BA	3144	1/1	0.12	-	52,52,52,52	0
56	MG	BA	3209	1/1	0.42	-	39,39,39,39	0
56	MG	BA	3078	1/1	0.32	-	44,44,44,44	0
56	MG	DA	3586	1/1	0.10	-	57,57,57,57	0
56	MG	BF	301	1/1	0.60	-	46,46,46,46	0
56	MG	CA	3164	1/1	0.36	-	43,43,43,43	0
56	MG	BA	3370	1/1	0.06	-	39,39,39,39	0
56	MG	BA	3525	1/1	0.16	-	31,31,31,31	0
56	MG	DA	3073	1/1	0.17	-	50,50,50,50	0
56	MG	BA	3657	1/1	0.18	-	29,29,29,29	0
56	MG	DA	3169	1/1	0.27	-	58,58,58,58	0
56	MG	BA	3355	1/1	0.07	-	39,39,39,39	0
56	MG	DB	3007	1/1	0.29	-	45,45,45,45	0
56	MG	DA	3380	1/1	0.09	-	40,40,40,40	0
56	MG	BA	3353	1/1	0.26	-	31,31,31,31	0
56	MG	BA	3474	1/1	0.25	-	43,43,43,43	0
56	MG	DA	3413	1/1	0.16	-	44,44,44,44	0
58	ZN	D5	103	1/1	0.07	-	61,61,61,61	0
56	MG	BA	3501	1/1	0.17	-	35,35,35,35	0
56	MG	CA	3107	1/1	0.09	-	71,71,71,71	0
56	MG	BA	3730	1/1	0.16	-	43,43,43,43	0
56	MG	DA	3197	1/1	0.31	-	43,43,43,43	0
56	MG	BU	204	1/1	0.39	-	49,49,49,49	0
56	MG	DA	3630	1/1	0.09	-	67,67,67,67	0
56	MG	BA	3181	1/1	0.11	-	37,37,37,37	0
56	MG	BA	3322	1/1	0.13	-	46,46,46,46	0
56	MG	AA	3132	1/1	0.20	-	59,59,59,59	0
56	MG	DA	3653	1/1	0.12	-	52,52,52,52	0
56	MG	BA	3342	1/1	0.22	-	46,46,46,46	0
56	MG	DA	3045	1/1	0.25	-	49,49,49,49	0
56	MG	AA	3207	1/1	0.17	-	51,51,51,51	0
56	MG	DA	3609	1/1	0.20	-	49,49,49,49	0
56	MG	BA	3494	1/1	0.25	-	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3223	1/1	0.13	-	41,41,41,41	0
56	MG	BA	3385	1/1	0.06	-	56,56,56,56	0
56	MG	CA	3157	1/1	0.19	-	56,56,56,56	0
56	MG	DQ	3001	1/1	0.26	-	40,40,40,40	0
56	MG	AA	3033	1/1	0.48	-	68,68,68,68	0
56	MG	BA	3426	1/1	0.08	-	34,34,34,34	0
56	MG	BA	3629	1/1	0.14	-	51,51,51,51	0
56	MG	DU	3001	1/1	1.07	-	61,61,61,61	0
56	MG	BA	3249	1/1	0.37	-	46,46,46,46	0
56	MG	DA	3005	1/1	0.40	-	50,50,50,50	0
56	MG	DA	3344	1/1	0.12	-	48,48,48,48	0
56	MG	BA	3295	1/1	0.13	-	30,30,30,30	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.