



wwPDB X-ray Structure Validation Summary Report

Sep 11, 2014 – 03:48 AM EDT

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

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

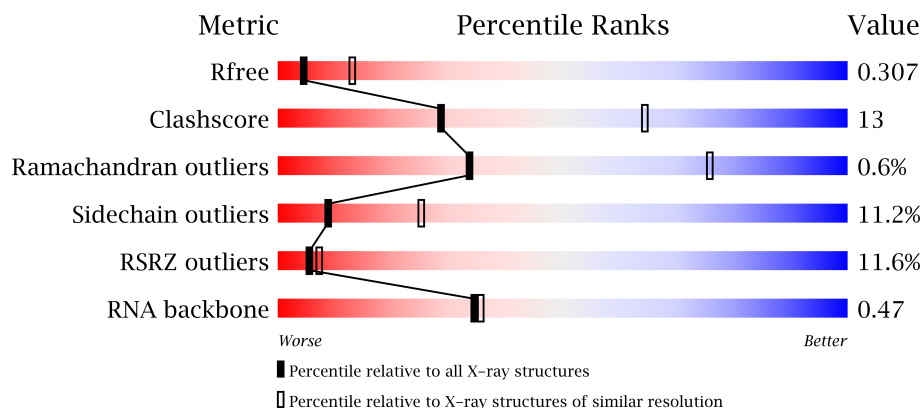
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
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) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)
RNA backbone	1838	1055 (3.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	1521	
1	CA	1521	
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	

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Mol	Chain	Length	Quality of chain
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	24	
22	CV	24	
23	AW	2	
23	CW	2	
24	AX	77	
24	CX	77	
25	BA	2915	
25	DA	2915	
26	BB	121	
26	DB	121	
27	BD	276	

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Mol	Chain	Length	Quality of chain
27	DD	276	
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	

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Mol	Chain	Length	Quality of chain
48	D2	72	
49	B3	60	
49	D3	60	
50	B4	71	
50	D4	71	
51	B5	60	
51	D5	60	
52	B6	54	
52	D6	54	
53	B7	49	
53	D7	49	
54	B8	65	
54	D8	65	
55	B9	37	
55	D9	37	

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 289646 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
			32205	14333	5970	10404	1498			
1	CA	1503	Total	C	N	O	P	0	0	0
			32312	14381	5990	10438	1503			

- Molecule 2 is a protein called 30S ribosomal protein S2.

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

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1659	1040	326	286	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1670	1047	332	284	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.

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

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

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

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

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

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

- Molecule 11 is a protein called 30S ribosomal protein S11.

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

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

- Molecule 13 is a protein called 30S ribosomal protein S13.

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

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S		
			492	312	104	72	4	0	0
14	CN	60	Total	C	N	O	S		
			492	312	104	72	4	0	0

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S		
			728	456	144	126	2	0	0
15	CO	88	Total	C	N	O	S		
			728	456	144	126	2	0	0

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
16	CP	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
17	CQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	68	Total	C	N	O	0	0	0
			555	355	108	92			
18	CR	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	83	Total	C	N	O	S	0	0	0
			652	417	120	113	2			
19	CS	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
20	CT	96	Total	C	N	O	S	0	0	0
			727	446	155	124	2			

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	23	Total	C	N	O	0	0	0
			199	122	48	29			
21	CU	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
22	CV	12	Total	C	N	O	P	0	0	0
			252	115	46	80	11			

- Molecule 23 is a RNA chain called Cytidine-Puromycin.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B4	1	Total	Mg	0	0
			1	1		
56	BA	675	Total	Mg	0	0
			675	675		
56	AK	1	Total	Mg	0	0
			1	1		
56	DQ	3	Total	Mg	0	0
			3	3		
56	D3	1	Total	Mg	0	0
			1	1		
56	DF	3	Total	Mg	0	0
			3	3		
56	B8	1	Total	Mg	0	0
			1	1		
56	BE	6	Total	Mg	0	0
			6	6		
56	DU	1	Total	Mg	0	0
			1	1		

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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	7	Total 7	Mg 7	0	0
56	DN	1	Total 1	Mg 1	0	0
56	CA	154	Total 154	Mg 154	0	0
56	B5	2	Total 2	Mg 2	0	0
56	BB	18	Total 18	Mg 18	0	0
56	AE	2	Total 2	Mg 2	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	5	Total 5	Mg 5	0	0
56	BX	3	Total 3	Mg 3	0	0
56	D8	2	Total 2	Mg 2	0	0
56	AA	187	Total 187	Mg 187	0	0
56	BQ	3	Total 3	Mg 3	0	0
56	D7	1	Total 1	Mg 1	0	0
56	CX	1	Total 1	Mg 1	0	0
56	DV	2	Total 2	Mg 2	0	0
56	AM	1	Total 1	Mg 1	0	0
56	BU	5	Total 5	Mg 5	0	0

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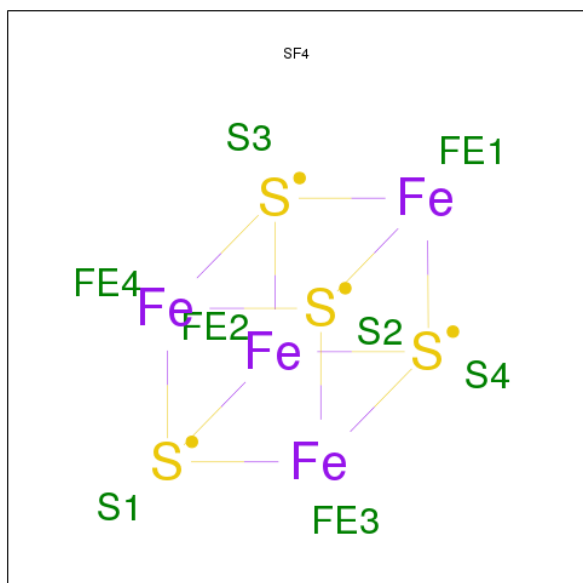
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DR	2	Total 2	Mg 2	0	0
56	AD	1	Total 1	Mg 1	0	0
56	BN	2	Total 2	Mg 2	0	0
56	CT	1	Total 1	Mg 1	0	0
56	D0	1	Total 1	Mg 1	0	0
56	BG	3	Total 3	Mg 3	0	0
56	BY	2	Total 2	Mg 2	0	0
56	DE	5	Total 5	Mg 5	0	0
56	B3	2	Total 2	Mg 2	0	0
56	CJ	1	Total 1	Mg 1	0	0
56	BR	3	Total 3	Mg 3	0	0
56	DA	595	Total 595	Mg 595	0	0
56	DP	1	Total 1	Mg 1	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	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	1	Total 1	Mg 1	0	0

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

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

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

- Molecule 58 is ZINC ION (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 POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 60 is water.

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

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

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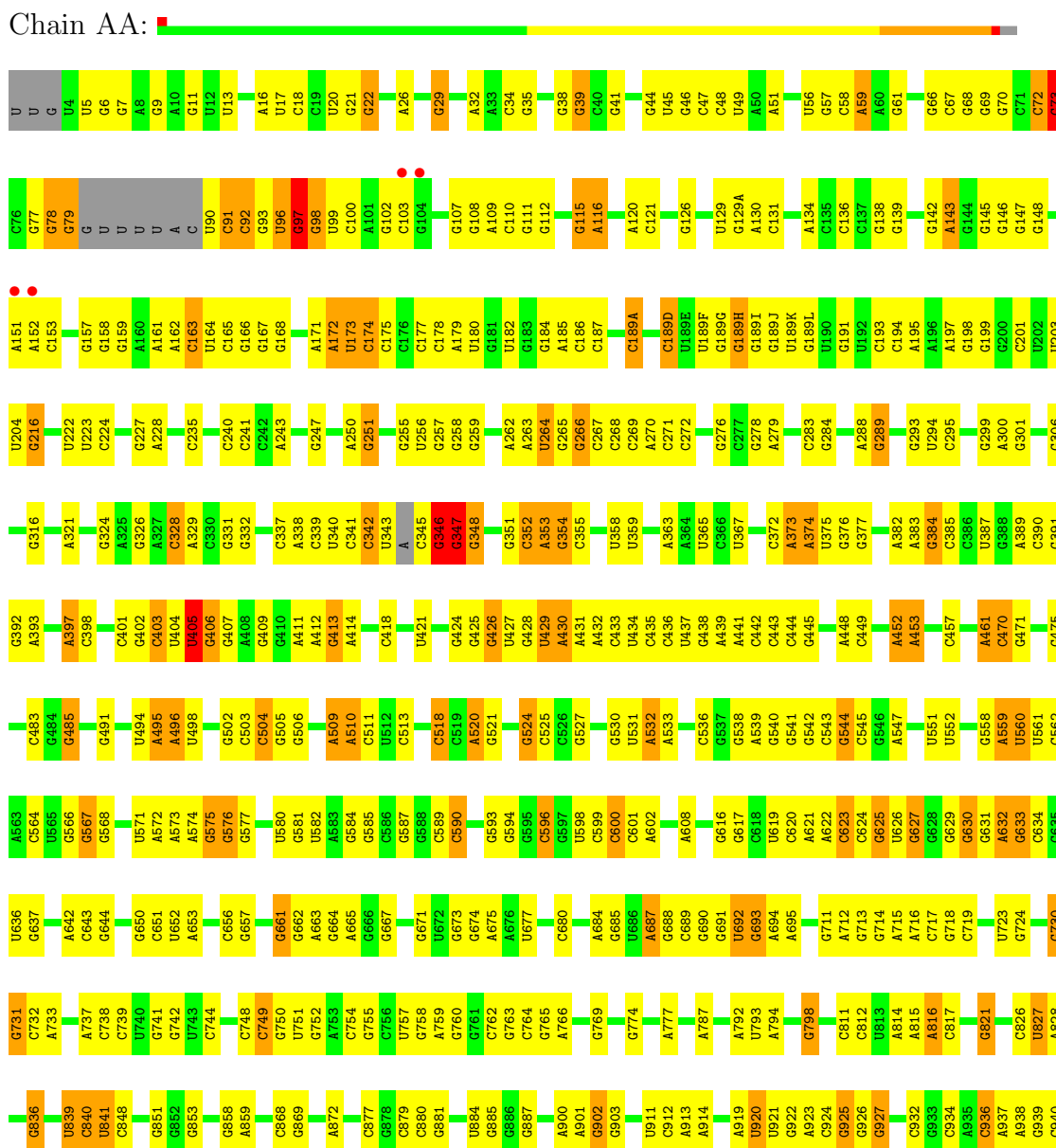
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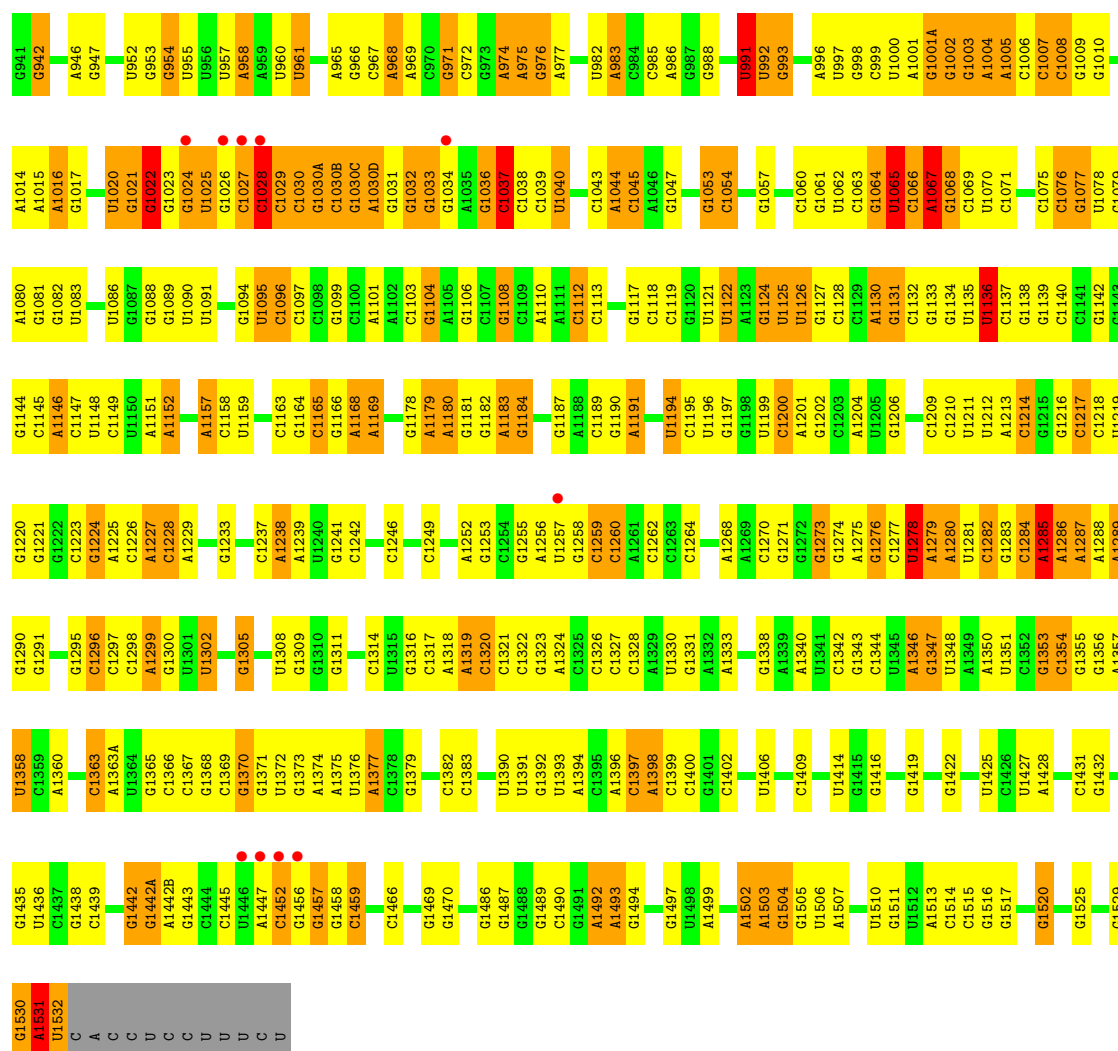
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	DF	6	Total 6	O 6	0	0
60	DO	1	Total 1	O 1	0	0
60	DP	6	Total 6	O 6	0	0
60	DU	3	Total 3	O 3	0	0
60	DV	1	Total 1	O 1	0	0
60	DW	1	Total 1	O 1	0	0
60	DX	3	Total 3	O 3	0	0
60	D0	5	Total 5	O 5	0	0
60	D1	1	Total 1	O 1	0	0
60	D3	1	Total 1	O 1	0	0
60	D8	3	Total 3	O 3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

3 Residue-property plots

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

• Molecule 1: 16S Ribosomal RNA

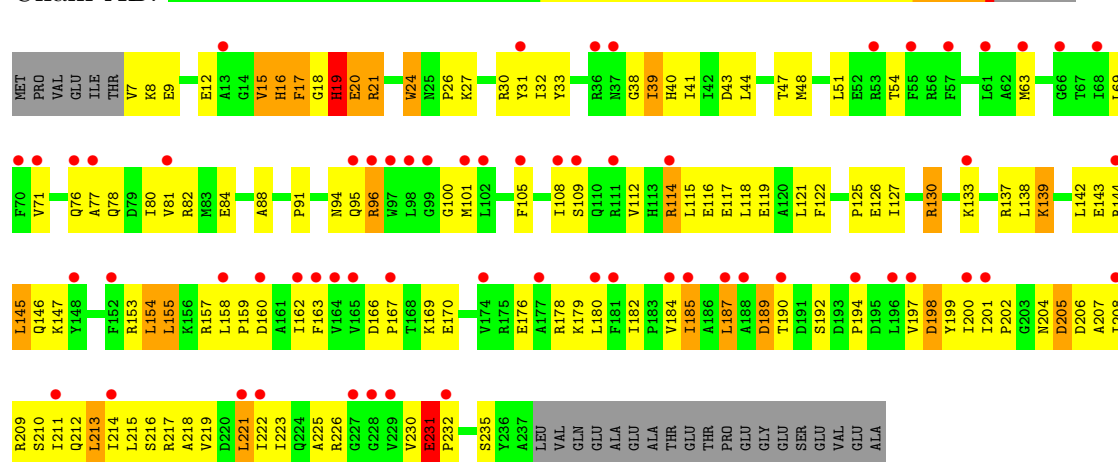




G1487	G1488	G1489	C1490	G1491	A1492	A1493	A1398	G1399	G1400	G1401	C1402	G1501	A1502	A1503	G1504	G1505	U1506	G1509	U1510	G1511	A1512	A1513	C1514	G1515	G1516	G1517	A1518	A1519	G1520	G1523	G1529	G1530	A1531	C	A	C	C	U	C	U	U	C	U																		
U1390	U1391	G1392	U1393	A1394	C1397	A1398	A1399	G1400	G1401	C1402	U1406	C1409	C1412	A1413	G1419	G1422	G1423	G1424	U1425	G1426	U1427	A1428	C1429	C1430	C1431	G1432	A1433	G1434	U1435	G1436	C1437	G1438	C1439	C	A	C	C	U	C	U	U	C	U																		
C1264	U1199	C1267	A1268	G1269	A1269	C1270	U1204	U1205	G1272	G1273	G1274	A1275	G1276	C1277	U1278	A1279	A1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	A1288	G1289	A1290	G1291	U1292	U1293	G1294	C1295	C1296	C1297	C1298	A1299	G1300	U1301	U1302	C1303	G1304	G1305	A1306	U1307	U1308	G1309	G1310	G1311	G1312	U1313	C1314	U1315	G1316	C1317	C1318	A1319	C1320	C1321	C1322	A1323	A1324
G1198	U1199	C1200	A1201	C1202	C1203	A1204	U1205	G1206	C1209	G1274	A1275	G1276	C1277	U1278	A1279	A1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	A1288	A1289	G1290	A1291	U1292	U1293	G1294	C1295	C1296	C1297	C1298	A1299	G1300	U1301	U1302	C1303	G1304	G1305	A1306	U1307	U1308	G1309	G1310	G1311	G1312	U1313	C1314	U1315	G1316	C1317	C1318	A1319	C1320	C1321	C1322	A1323	A1324	
G1133	G1134	U1135	U1136	C1137	G1138	C1139	G1140	C1141	G1142	G1143	C1144	C1145	A1146	C1147	U1148	C1149	U1150	A1151	A1152	C1153	G1154	G1155	G1156	A1157	C1158	U1159	C1162	C1163	G1164	C1165	G1166	A1168	A1169	A1170	G1171	C1172	G1173	G1174	A1179	A1180	G1181	G1182	A1183	G1184	G1185	G1186	G1187	A1188	G1189	G1190	A1191	U1192	C1193	G1194	U1195	A1196	G1197				
G1068	C1069	U1070	U1071	U1072	G1073	G1074	C1075	C1076	U1077	U1078	G1079	A1080	G1081	U1082	U1083	U1084	U1085	U1086	U1087	G1088	U1089	U1090	U1091	A1092	U1093	U1094	U1095	U1096	U1097	U1098	U1099	C1100	A1101	A1102	C1103	G1104	A1105	G1106	C1107	G1108	C1112	C1113	C1114	G1117	C1118	C1119	G1120	U1121	U1122	A1123	G1124	U1125	U1126	U1127	C1128	C1129	A1130	U1131	C1132		
G1009	G1010	U1011	U1012	G1013	A1014	A1015	U1016	G1017	C1018	C1019	U1020	G1021	G1022	G1023	U1024	U1025	U1026	C1027	C1028	C1029	C1030	C1031	G1032	A1033	G1034	U1035	G1036	C1037	C1038	C1039	U1040	A1041	G1042	C1043	C1044	C1045	A1046	G1047	G1048	G1053	C1054	A1055	U1056	G1057	G1058	C1059	G1060	U1061	U1062	G1063	A1064	U1065	A1066	C1067	A1068						
G945	A946	C947	C948	C949	G950	G951	U952	G953	U954	U955	A956	A957	U958	U959	U960	U961	A965	G966	C967	A968	C969	A970	C971	C972	C973	A974	A975	A976	A977	A978	U981	U982	A983	C984	C985	A986	C989	C990	U991	U992	C993	A994	C995	A996	U997	G998	C999	U1000	A1001	G1001A	G1002	U1003	A1004	A1005	C1006	C1007	C1008				
G853	G854	G855	C856	C857	G858	A859	A860	A861	C862	A863	G864	G865	A866	G867	C868	G869	U870	C875	C876	C877	C878	C879	C880	U884	A889	G890	U891	A900	A901	G902	G906	A913	A914	A915	A916	C917	C921	C922	A923	C924	G925	G926	G927	C932	G933	U934	A935	C936	A937	U938	A939	U941	C948	C949	U943	G944					
G758	A759	G760	U766	C764	G765	A766	A767	G768	G769	G774	A777	A781	A782	C783	C784	G785	G786	A787	U788	A789	A790	G791	A792	U793	A794	C797	G798	A802	A815	A816	C917	C921	C922	A923	C924	G925	G926	G927	C932	G933	U934	A935	C936	A937	U938	A939	U941	C948	C949	U943	G944										
G680	G685	C686	A687	C688	C689	C690	A691	G692	G693	A694	A695	A696	U697	C698	C699	G700	C701	A702	C707	C708	A712	C717	G718	C719	C720	C721	A722	U723	G724	A725	A726	A727	A728	A729	G730	C732	A733	G734	C738	G741	G742	A745	C748	C749	G750	U751	C754	G755	C756	U757											
A510	C511	U512	C513	C514	G515	C518	C519	A520	C521	C522	A523	G527	C531	A532	A533	C536	G537	G538	A539	G540	A541	G542	C543	G544	A547	A553	C554	A559	U560	U561	G567	G568	U571	A572	A573	A574	G575	G576	G577	U580	G581	U582	C586	G587	G588	C589	U591														
G426	U427	G428	U429	A430	C433	U434	C435	U436	U437	G438	A439	A441	C442	C443	C444	G445	G446	G447	A448	A452	A453	C454	C455	G460	A461	C470	G471	A472	G476	A481	A482	C483	G484	G485	U486	A487	C488	C489	G490	G491	G492	A495	A496	U498	C501	G502	C503	C504	G505	G506	A509										

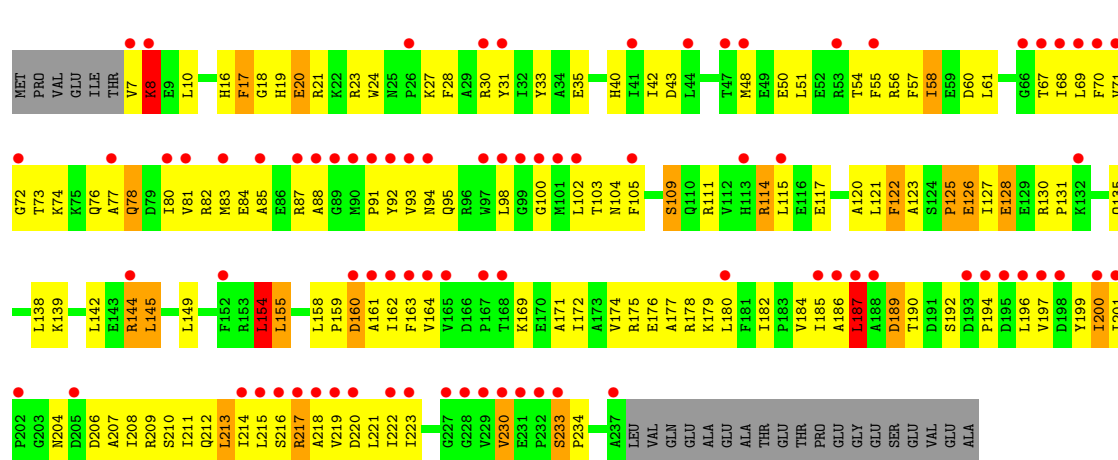
- Molecule 2: 30S ribosomal protein S2

Chain AB:



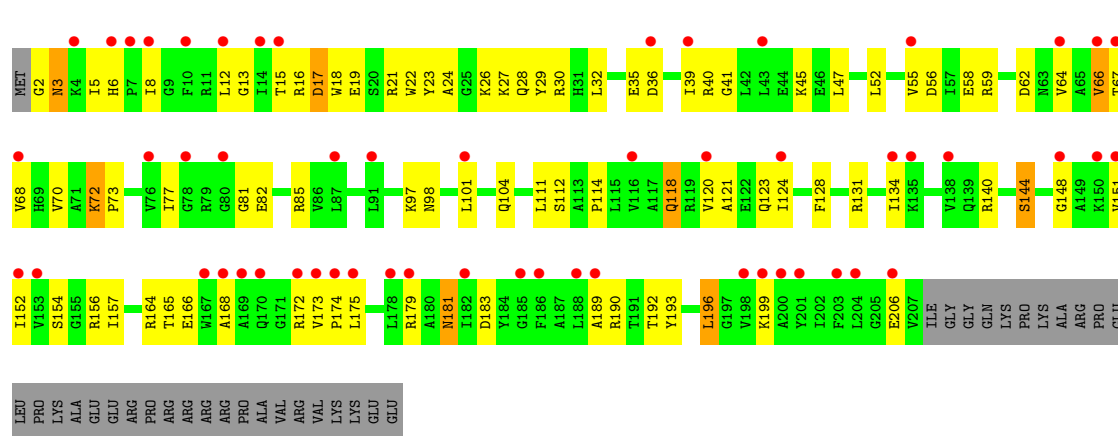
- Molecule 2: 30S ribosomal protein S2

Chain CB:



- Molecule 3: 30S ribosomal protein S3

Chain AC:



- Molecule 3: 30S ribosomal protein S3

LYS	V153	H69	WET
ALA	S154		G2
GLU	G155		R3
GLU	R156	K72	K4
ARG		P73	I5
PRO	G159		H6
ARG	A160	I77	P7
ARG			I8
ARG	R164	G80	G9
ARG	T165	G81	F10
PRO	E166	E32	R11
ALA	M167	R83	L12
VAL		I84	G13
ARG	Q170	R85	I14
VAL	G171	H86	T15
LYS	R172	L87	R16
LYS	V173		D17
GLU	P174	L91	M18
GLU	L175		E19
GLU	H176	L101	S20
	T177		R21
	L178	E105	W22
	R179		W23
	A180	M108	
	M181	P109	W29
	I182	M110	R30
	D183	L111	H31
	Y184		L32
	G185	V116	L33
	F186	A117	
		Q118	D36
	A189	R119	I37
	R190	W120	R38
	T191	A121	I39
		E122	R40
	L196	Q123	G41
	G197	I124	L42
	V198	E125	L43
	A199	R126	E44
	A200		K45
	Y201		E46
	T202	R131	L47
	F203		
	L204	I134	A50
	G205	A137	G51
	E206	V138	L52
	W207	Q139	A53
ILE		R140	R54
GLY		V141	V55
GLY		M142	D56
GLN		E143	I57
LYS		S144	E58
PRO		G145	R59
LYS		A146	A60
ALA		K147	A61
ARG		G148	D62
PRO		A149	N63
GLU		M150	V64
LEU		V151	A65
PRO		T152	H65

- Chain AD:

L162	L163	A164	M165	K166	G167	G168	K169	V170	G171	P172	W173	L174	S175	L176	D177	V178	G180	M181	K182	G183	L186	R187	L188	P189	D190	L194	E200	Q201	L202	V203	I204	S208	R209																					
L97	E98	S99	R100	L101	D102	N103	V104	Y105	Y106	L107	L108	G109	F110	A111	V112	R115	Q116	A117	R118	Q119	L120	V121	R122	H123	G124	H125	L126	T127	V128	N129	G130	R131	R132	V133	D134	L135	P136	S137	Y138	R139	V140	R141	D144	A147	V148	A149	E150	K151	S152	L155	E156	L157	I158	R159
MET	G2	R3	A4	Y5	V8	C9	L11	C12	R13	R14	G16	L19	Y20	L21	K22	C31	R35	R36	Y38	K46	R49	D53	R57	L58	R59	E60	K61	Q62	K63	L64	R65	Y68	G69	I70	S71	E72	N77	E80	E81	K85	K86	L94												

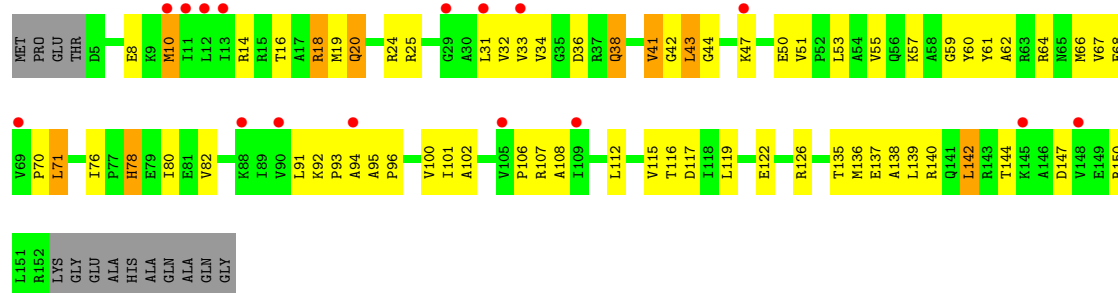
- Chain CD:

Gene	Chromosome	Start (kb)	End (kb)	Strand	Transcript	Exons	Introns	UTRs	Annotations
L157	1	100000	100050	+	L157	1	0	0	5' UTR, CDS, 3' UTR
L158	1	100050	100100	+	L158	1	0	0	5' UTR, CDS, 3' UTR
R159	1	100100	100150	-	R159	1	0	0	5' UTR, CDS, 3' UTR
Q160	1	100150	100200	+	Q160	1	0	0	5' UTR, CDS, 3' UTR
N161	1	100200	100250	-	N161	1	0	0	5' UTR, CDS, 3' UTR
L162	1	100250	100300	+	L162	1	0	0	5' UTR, CDS, 3' UTR
E163	1	100300	100350	-	E163	1	0	0	5' UTR, CDS, 3' UTR
A164	1	100350	100400	+	A164	1	0	0	5' UTR, CDS, 3' UTR
M165	1	100400	100450	-	M165	1	0	0	5' UTR, CDS, 3' UTR
K166	1	100450	100500	+	K166	1	0	0	5' UTR, CDS, 3' UTR
G167	1	100500	100550	-	G167	1	0	0	5' UTR, CDS, 3' UTR
R168	1	100550	100600	+	R168	1	0	0	5' UTR, CDS, 3' UTR
K169	1	100600	100650	-	K169	1	0	0	5' UTR, CDS, 3' UTR
V170	1	100650	100700	+	V170	1	0	0	5' UTR, CDS, 3' UTR
G171	1	100700	100750	-	G171	1	0	0	5' UTR, CDS, 3' UTR
P172	1	100750	100800	+	P172	1	0	0	5' UTR, CDS, 3' UTR
W173	1	100800	100850	-	W173	1	0	0	5' UTR, CDS, 3' UTR
L174	1	100850	100900	+	L174	1	0	0	5' UTR, CDS, 3' UTR
S175	1	100900	100950	-	S175	1	0	0	5' UTR, CDS, 3' UTR
L176	1	100950	101000	+	L176	1	0	0	5' UTR, CDS, 3' UTR
D177	1	101000	101050	-	D177	1	0	0	5' UTR, CDS, 3' UTR
V178	1	101050	101100	+	V178	1	0	0	5' UTR, CDS, 3' UTR
M181	1	101100	101150	-	M181	1	0	0	5' UTR, CDS, 3' UTR
K182	1	101150	101200	+	K182	1	0	0	5' UTR, CDS, 3' UTR
G183	1	101200	101250	-	G183	1	0	0	5' UTR, CDS, 3' UTR
K184	1	101250	101300	+	K184	1	0	0	5' UTR, CDS, 3' UTR
F185	1	101300	101350	-	F185	1	0	0	5' UTR, CDS, 3' UTR
L186	1	101350	101400	+	L186	1	0	0	5' UTR, CDS, 3' UTR
R187	1	101400	101450	-	R187	1	0	0	5' UTR, CDS, 3' UTR
L188	1	101450	101500	+	L188	1	0	0	5' UTR, CDS, 3' UTR
P189	1	101500	101550	-	P189	1	0	0	5' UTR, CDS, 3' UTR
D193	1	101550	101600	+	D193	1	0	0	5' UTR, CDS, 3' UTR
L194	1	101600	101650	-	L194	1	0	0	5' UTR, CDS, 3' UTR
P197	1	101650	101700	+	P197	1	0	0	5' UTR, CDS, 3' UTR
V198	1	101700	101750	-	V198	1	0	0	5' UTR, CDS, 3' UTR
N199	1	101750	101800	+	N199	1	0	0	5' UTR, CDS, 3' UTR
E200	1	101800	101850	-	E200	1	0	0	5' UTR, CDS, 3' UTR
Q201	1	101850	101900	+	Q201	1	0	0	5' UTR, CDS, 3' UTR
L202	1	101900	101950	-	L202	1	0	0	5' UTR, CDS, 3' UTR
T203</									

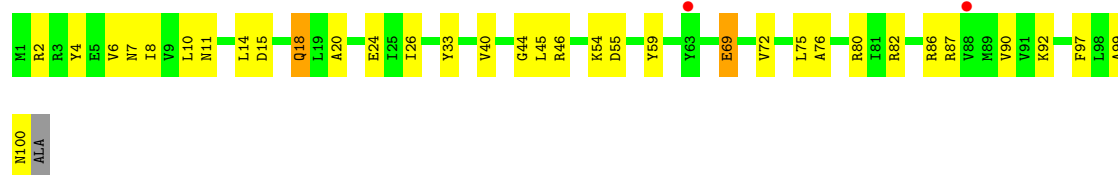
- Chain AE:

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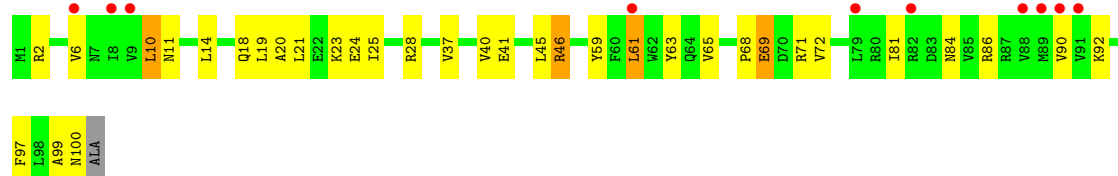
- Molecule 5: 30S ribosomal protein S5

Chain CE: 

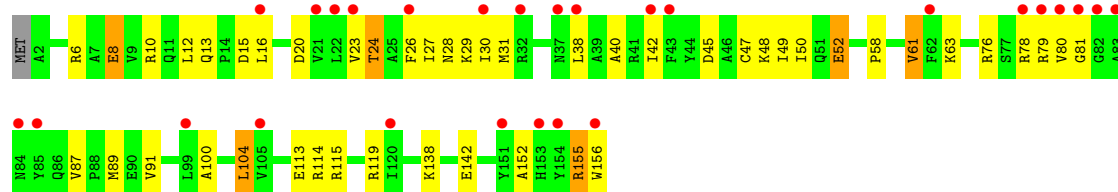
- Molecule 6: 30S ribosomal protein S6

Chain AF: 

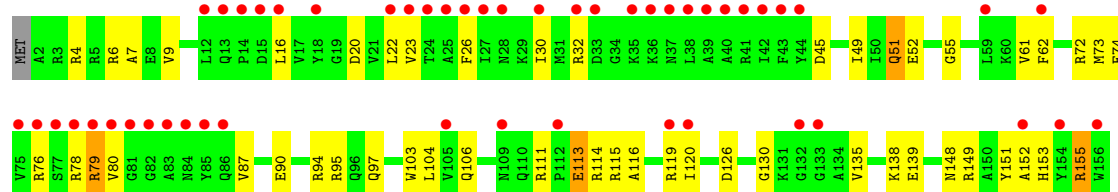
- Molecule 6: 30S ribosomal protein S6

Chain CF: 

- Molecule 7: 30S ribosomal protein S7

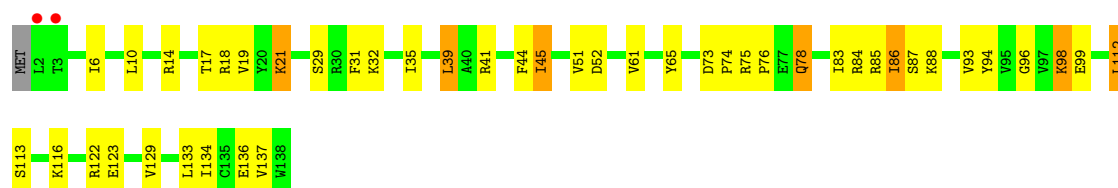
Chain AG: 

- Molecule 7: 30S ribosomal protein S7

Chain CG: 

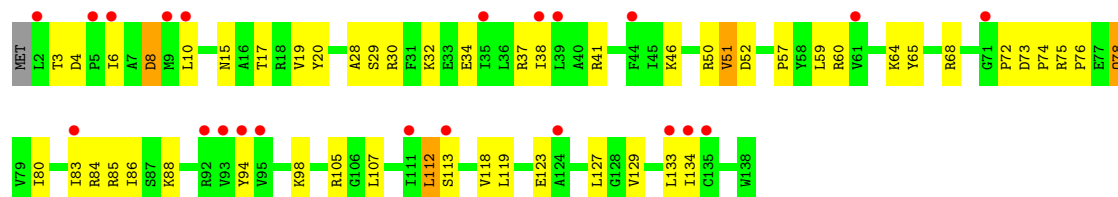
- Molecule 8: 30S ribosomal protein S8

Chain AH:



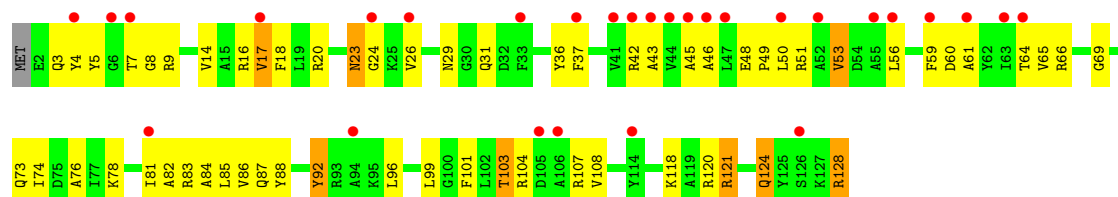
- Molecule 8: 30S ribosomal protein S8

Chain CH:



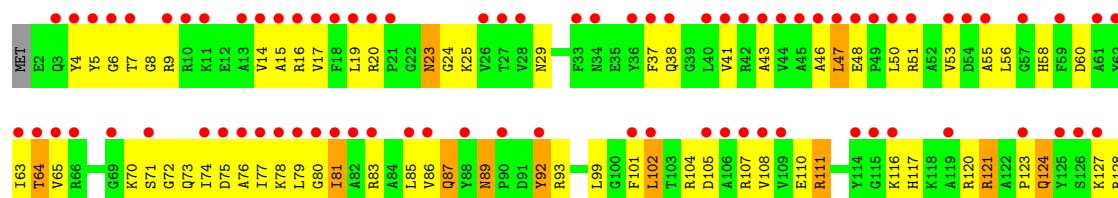
- Molecule 9: 30S ribosomal protein S9

Chain AI:



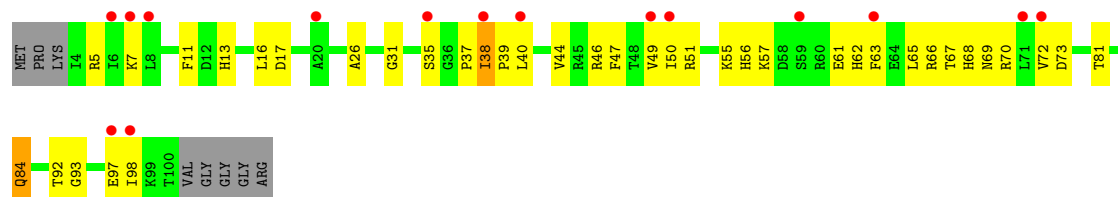
- Molecule 9: 30S ribosomal protein S9

Chain CI:



- Molecule 10: 30S ribosomal protein S10

Chain AJ:



- Molecule 10: 30S ribosomal protein S10

- Molecule 11: 30S ribosomal protein S11

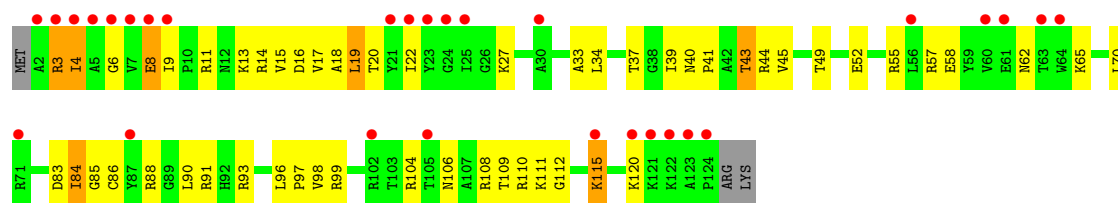
- Molecule 11: 30S ribosomal protein S11

- Molecule 12: 30S ribosomal protein S12

- Molecule 12: 30S ribosomal protein S12

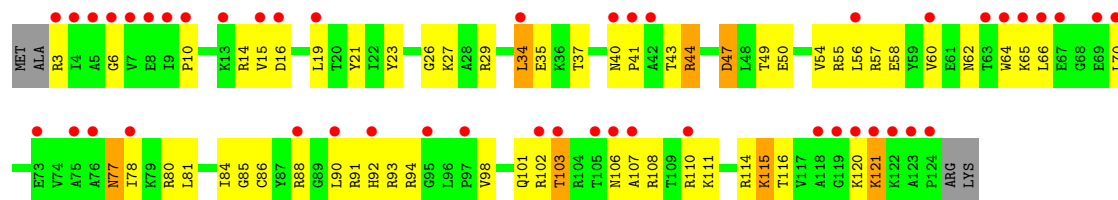
- Molecule 13: 30S ribosomal protein S13





• Molecule 13: 30S ribosomal protein S13

Chain CM:



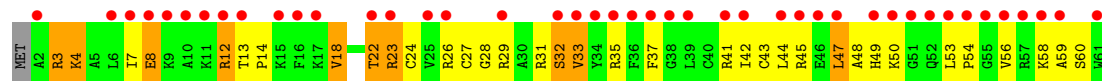
• Molecule 14: 30S ribosomal protein S14 type Z

Chain AN:



• Molecule 14: 30S ribosomal protein S14 type Z

Chain CN:



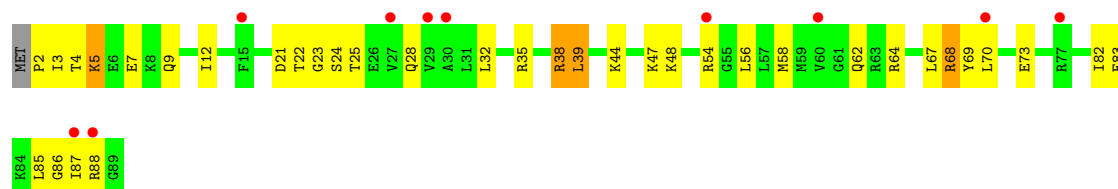
• Molecule 15: 30S ribosomal protein S15

Chain AO:



• Molecule 15: 30S ribosomal protein S15

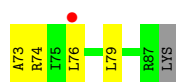
Chain CO:



• Molecule 16: 30S ribosomal protein S16

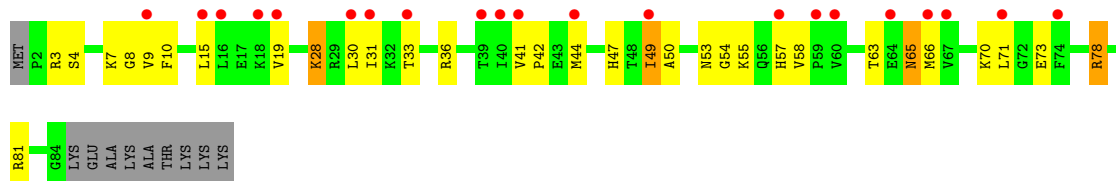
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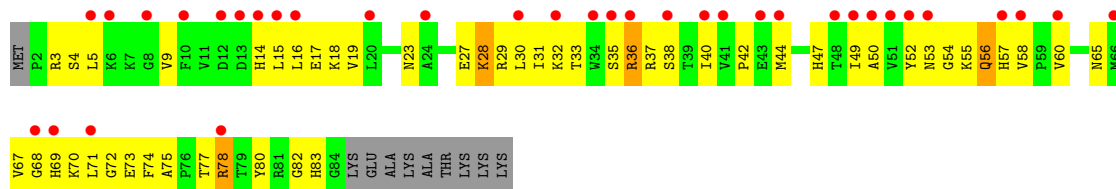
- Molecule 19: 30S ribosomal protein S19

Chain AS:



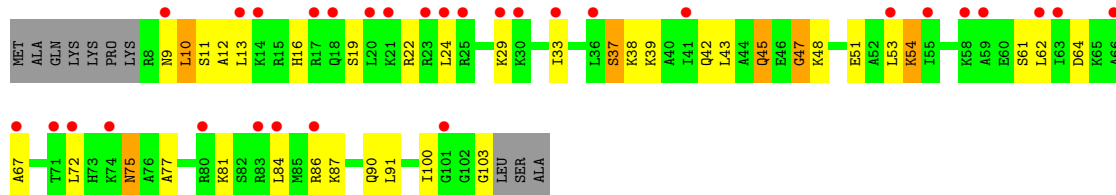
- Molecule 19: 30S ribosomal protein S19

Chain CS:



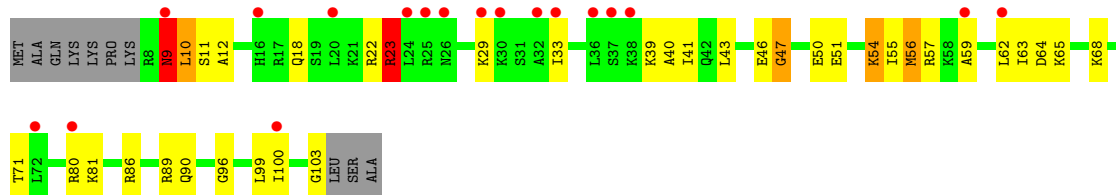
- Molecule 20: 30S ribosomal protein S20

Chain AT:



- Molecule 20: 30S ribosomal protein S20

Chain CT:



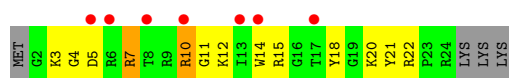
- Molecule 21: 30S ribosomal protein Thx

Chain AU:



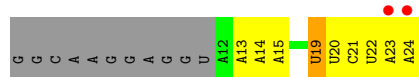
- Molecule 21: 30S ribosomal protein Thx

Chain CU:



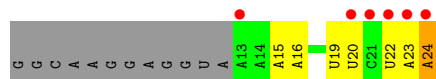
- Molecule 22: mRNA

Chain AV:



- Molecule 22: mRNA

Chain CV:



- Molecule 23: Cytidine-Puromycin

Chain AW:



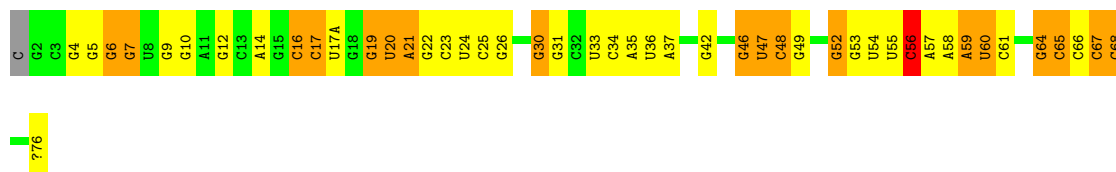
- Molecule 23: Cytidine-Puromycin

Chain CW:



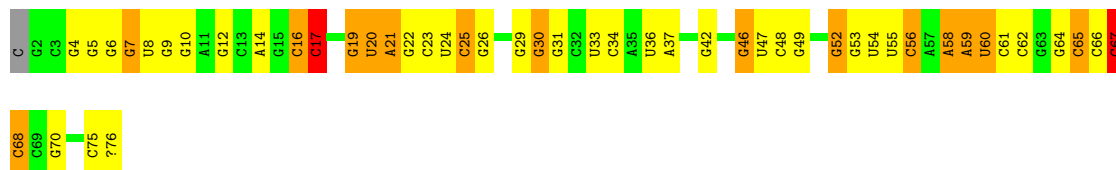
- Molecule 24: P-site tRNA

Chain AX:



- Molecule 24: P-site tRNA

Chain CX:



- Molecule 25: 23S Ribosomal RNA

Chain BA:

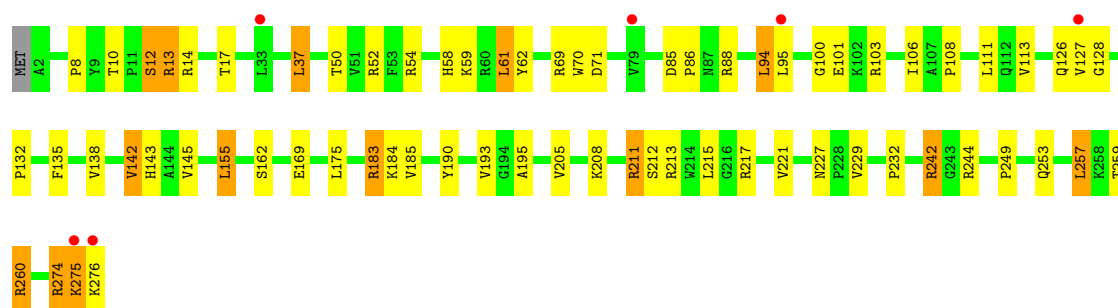
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		G1281	G	G	C1032	C931	C844	G715	G633		U448	G333	G234	C151	G35
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		G1285	U	U	C936	C936	G852		G639		G437	A347	C238	U	
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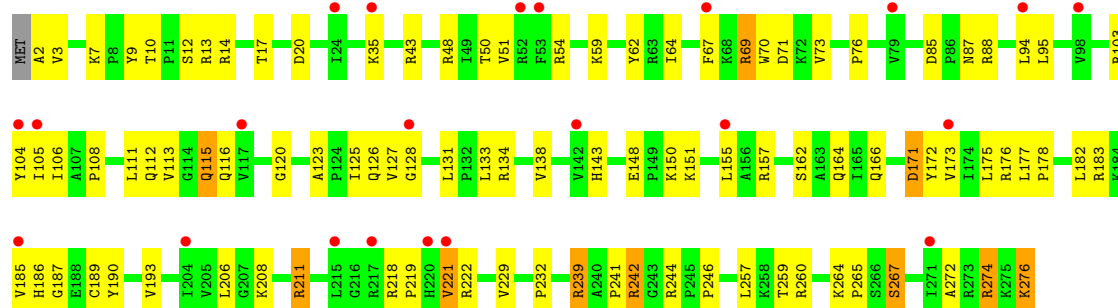
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G2290	C2195	G1980	G2064	G1980	A1876	U1779	A1666	A1597	G1531	C1464	A1367	G1271	C1122	C
U2291	C2196	A1981	G2067	G1981	G1878	U1780	C1670	C1598	C1532	G1465	A1368	A1272	C1123	C
C2292	U2197	C1982	U2068	C1982	G1879	G1781	G1674	C1599	U1540	G1466	G1369	U1273	C1124	C
C2293	A2198	C1983	G2069	C1984	C1880	G1782	A1675	C1600	G1533	C1467	C1370	A1274	G1125	C
C2294	A2199	G1985	C2070	G1985	C1881	A1783	A1676	G1601	U	C1468	U1371	A1275	A1204	C
C2295	U2203	G2141	A2071	A1986	C1882	A1784	A1677	C1602	A	C1469	A1379	G1276	U1206	C
U2296	C2205	G2142	G2072	G1992	A1889	A1785	A1678	C1603	G1537	C1469	A1380	A1277	G1207	C
G2297	G2206	C2143	C2073	U1993	A1890	A1786	A1679	C1604	G1538	G1469	A1384	G1278	C1207	C
A2298	G2207	U2144	U2074	G1993	A1890	A1787	A1680	C1605	U1542	C1470	A1384	A1279	G1216	C
G2299	C2208	C2145	U2075	G1997	C1894	C1788	G1682	C1606	G1543	G1473	A1386	U1288	G1219	C
G2302	U2213	C2146	C2078	U1997	C1894	A1789	G1685	C1607	G1544	U1547	A1386	U1289	G1216	C
G2303	G2224	G2147	U2079	G2000	C1895	C1790	C1686	A1608	G1539	C1467	A1384	C1289	G1216	C
G2304	G2304	G2148	U2079	A2001	G1896	A1791	G1687	A1609	G1537	C1468	A1384	C1290	G1216	C
A2305	G2225	G2149	G2080	A2001	G1899	G1792	G1687	C1610	G1538	C1469	A1384	C1291	G1216	C
C2306	C2226	U2150	C2081	G2002	G1900	C1793	G1688	C1611	G1539	C1469	A1384	C1291	G1216	C
G2308	G2230	G2151	U2086	G2012	A1901	U1794	A1689	C1615	G1544	C1470	A1384	C1291	G1216	C
G2312	U2312	G2152	G2087	A2013	C1902	C1795	A1689	A1616	A1544	G1470	A1384	C1291	G1216	C
C2313	U2232	G2154	G2087	A2014	G1906	U1796	U1692	C1617	A1545	A1471	A1384	C1291	G1216	C
C2314	G2314	G2155	U2092	A2014	G1907	U1798	C1694	G1619	C1547	G1473	A1386	U1292	G1219	C





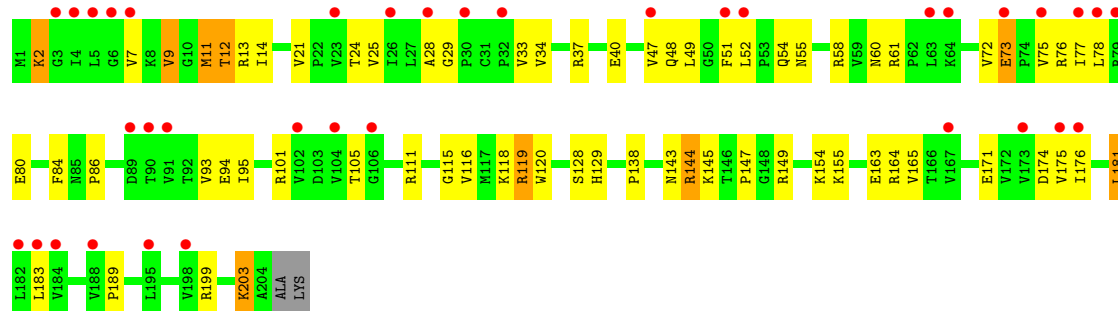
- Molecule 27: 50S ribosomal protein L2

Chain DD:



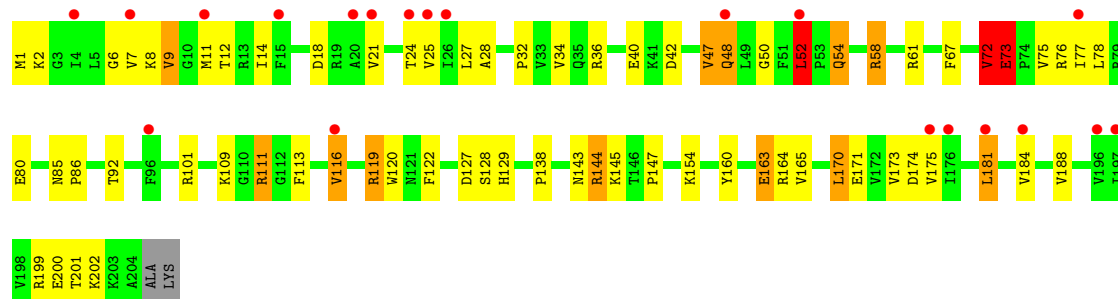
- Molecule 28: 50S ribosomal protein L3

Chain BE:



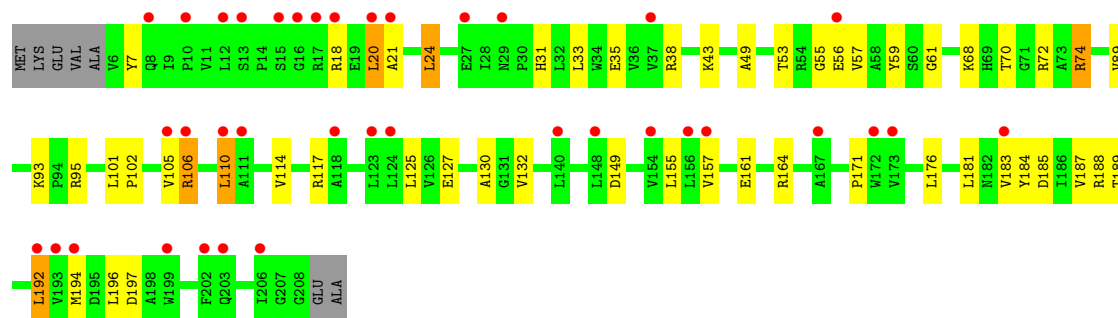
- Molecule 28: 50S ribosomal protein L3

Chain DE:



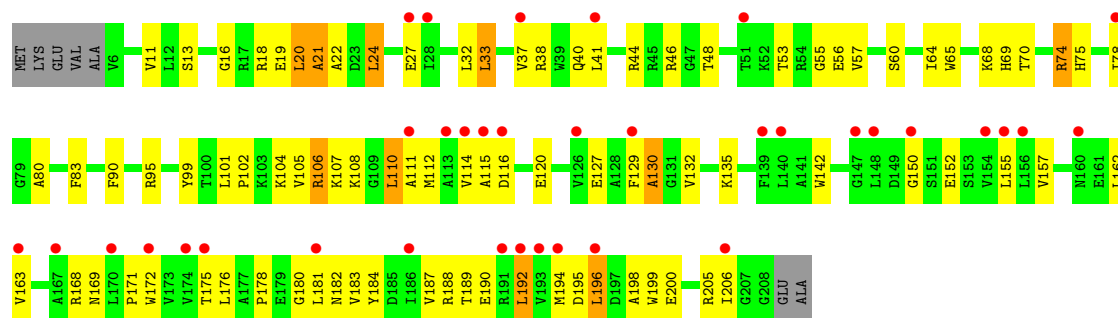
- Molecule 29: 50S ribosomal protein L4

Chain BF:



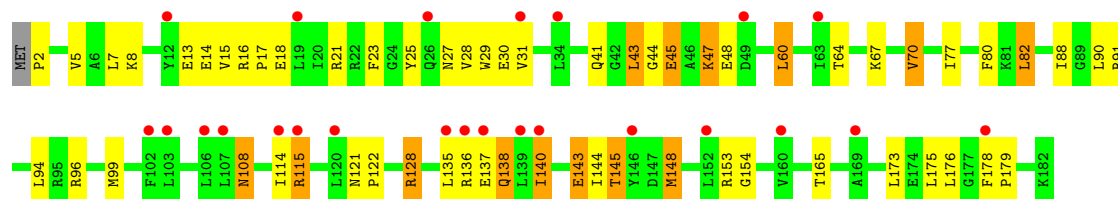
- Molecule 29: 50S ribosomal protein L4

Chain DF:



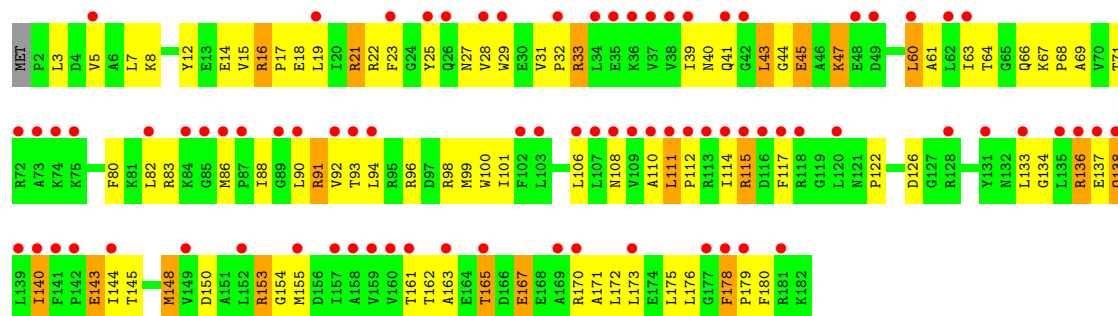
- Molecule 30: 50S ribosomal protein L5

Chain BG:



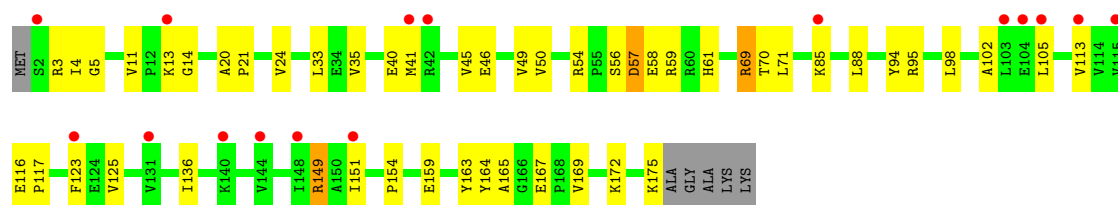
- Molecule 30: 50S ribosomal protein L5

Chain DG:



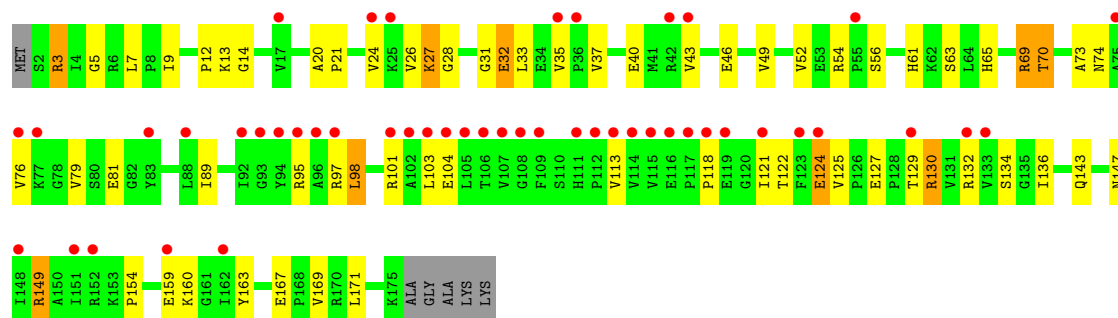
- Molecule 31: 50S ribosomal protein L6

Chain BH:



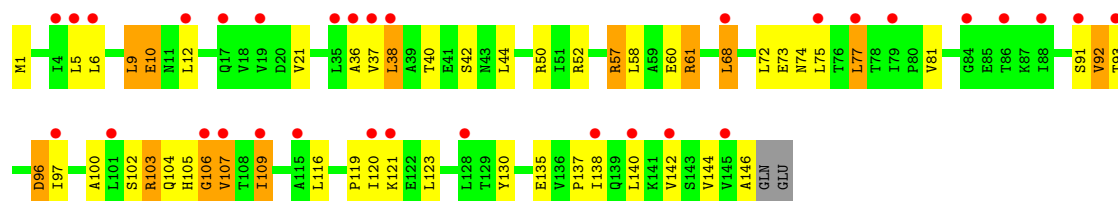
• Molecule 31: 50S ribosomal protein L6

Chain DH:



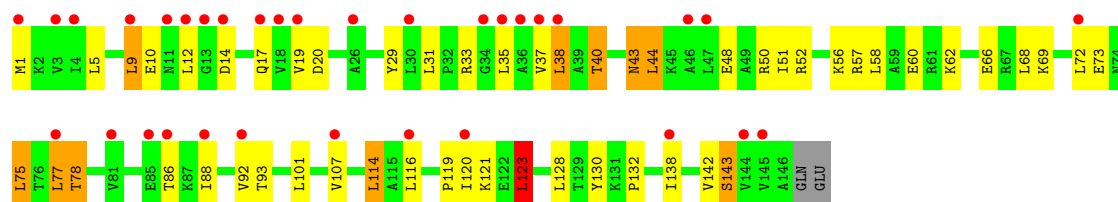
• Molecule 32: 50S ribosomal protein L9

Chain BI:



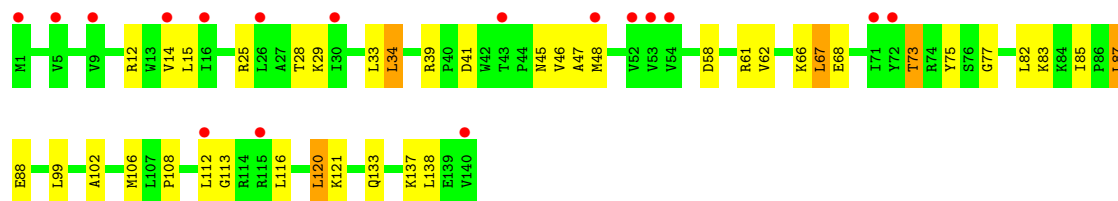
• Molecule 32: 50S ribosomal protein L9

Chain DI:



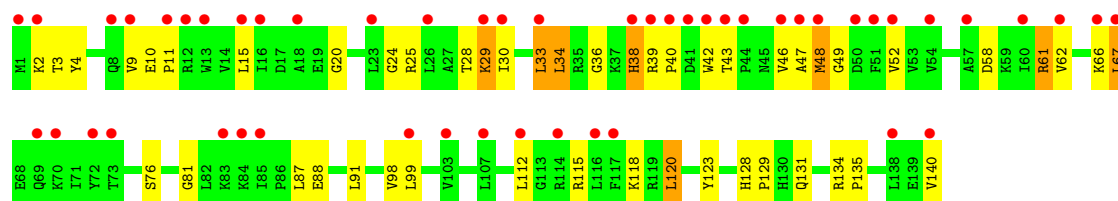
• Molecule 33: 50S ribosomal protein L13

Chain BN:



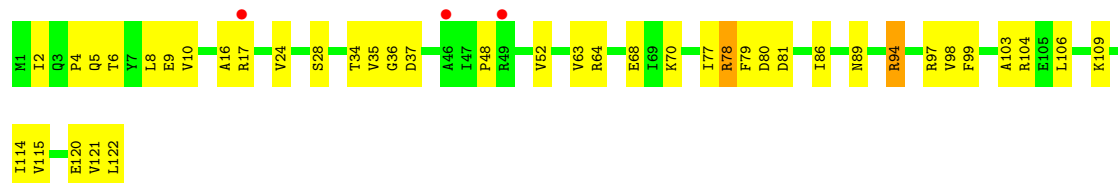
• Molecule 33: 50S ribosomal protein L13

Chain DN: 



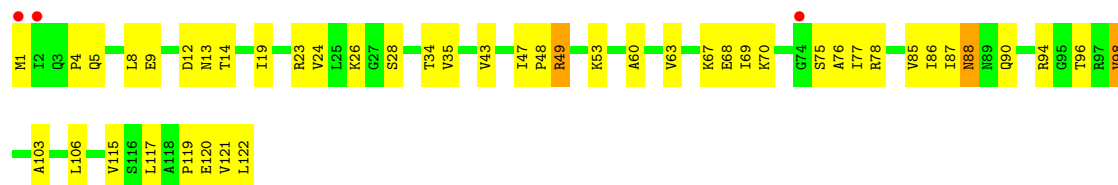
- Molecule 34: 50S ribosomal protein L14

Chain BO: 



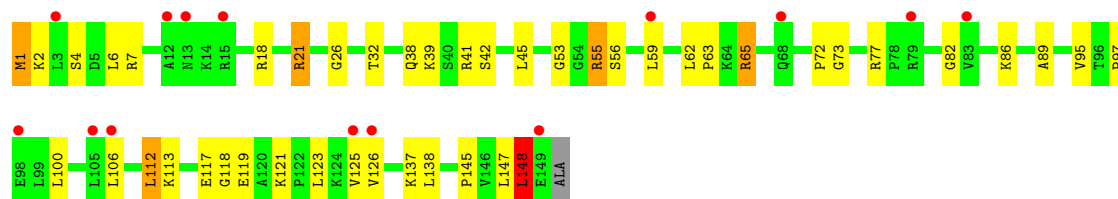
- Molecule 34: 50S ribosomal protein L14

Chain DO: 



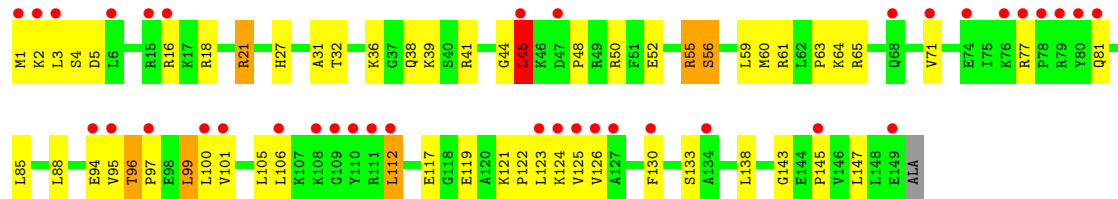
- Molecule 35: 50S ribosomal protein L15

Chain BP: 



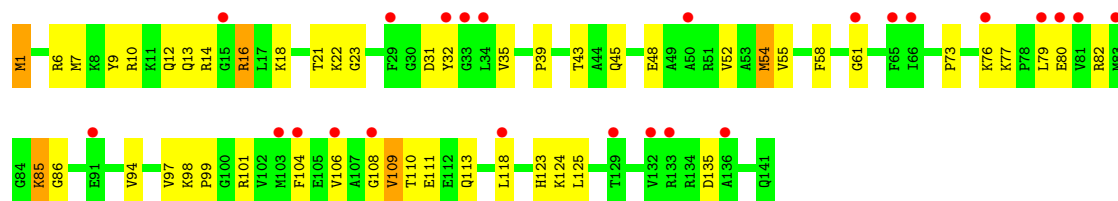
- Molecule 35: 50S ribosomal protein L15

Chain DP: 



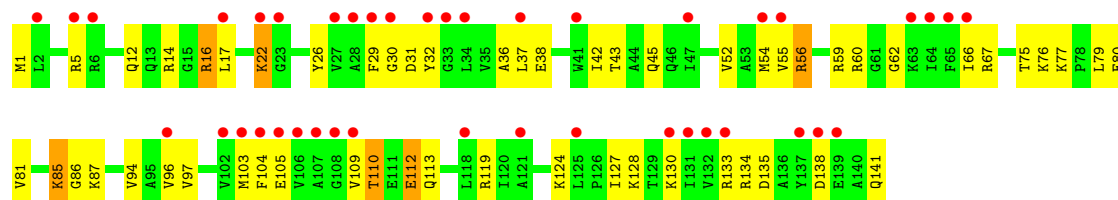
- Molecule 36: 50S ribosomal protein L16

Chain BQ: 



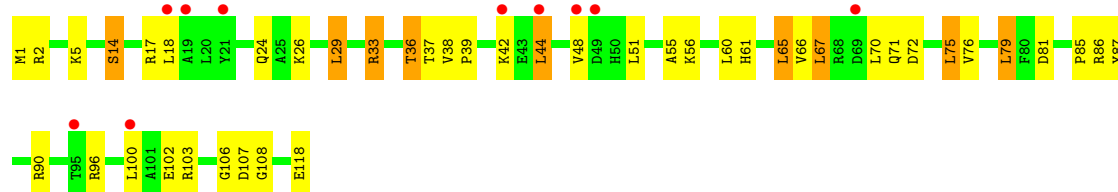
• Molecule 36: 50S ribosomal protein L16

Chain DQ:



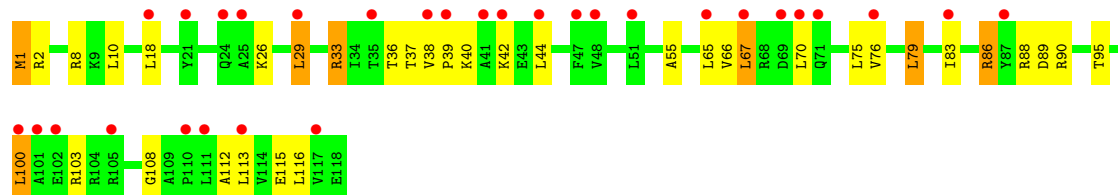
• Molecule 37: 50S ribosomal protein L17

Chain BR:



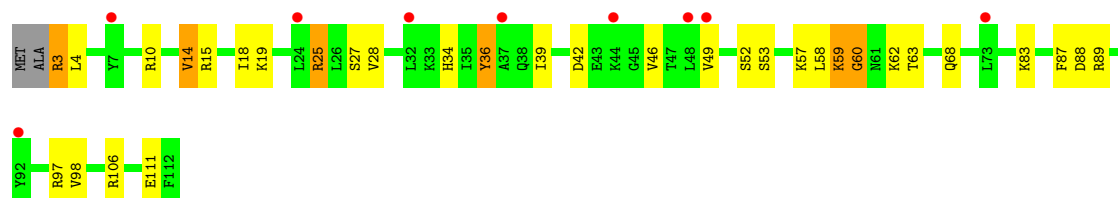
• Molecule 37: 50S ribosomal protein L17

Chain DR:



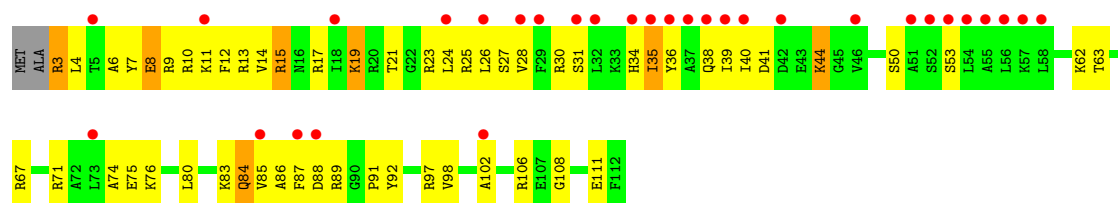
• Molecule 38: 50S ribosomal protein L18

Chain BS:



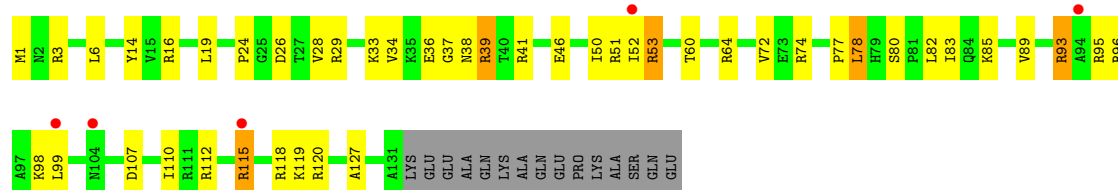
• Molecule 38: 50S ribosomal protein L18

Chain DS:



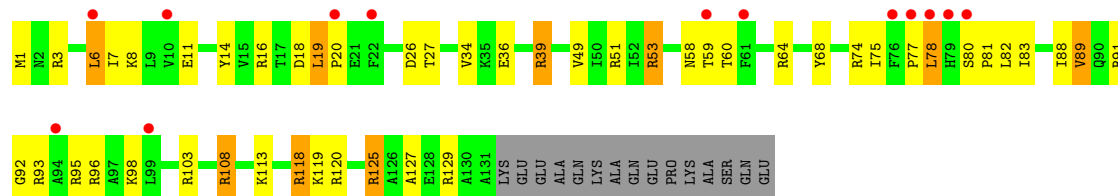
- Molecule 39: 50S ribosomal protein L19

Chain BT:



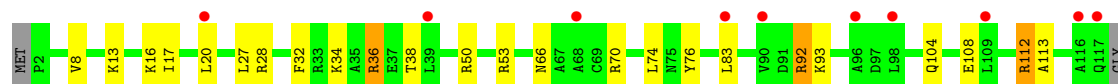
- Molecule 39: 50S ribosomal protein L19

Chain DT:



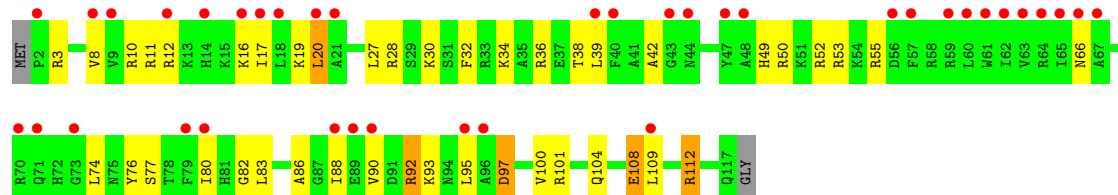
- Molecule 40: 50S ribosomal protein L20

Chain BU:



- Molecule 40: 50S ribosomal protein L20

Chain DU:



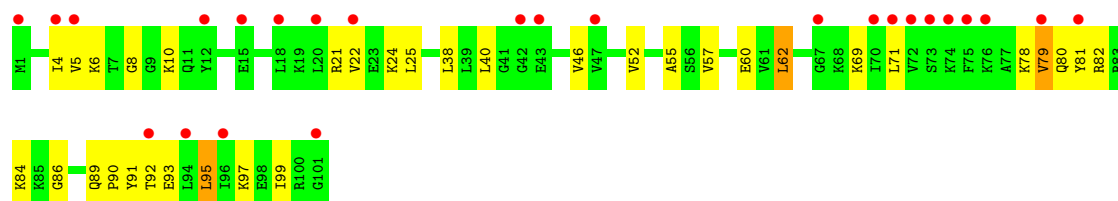
- Molecule 41: 50S ribosomal protein L21

Chain BV:



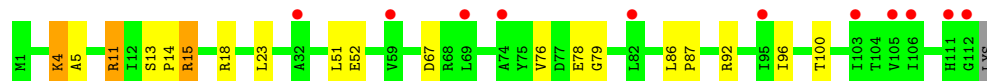
- Molecule 41: 50S ribosomal protein L21

Chain DV: 



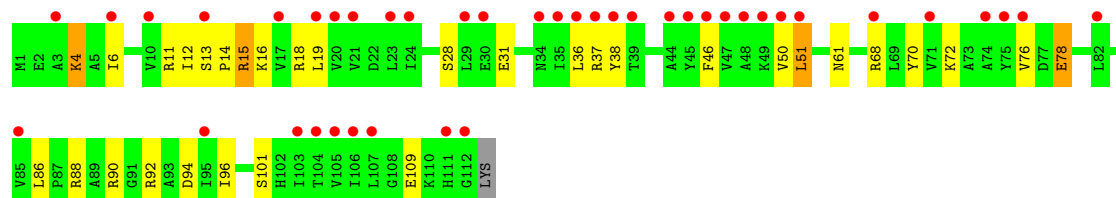
- Molecule 42: 50S ribosomal protein L22

Chain BW: 



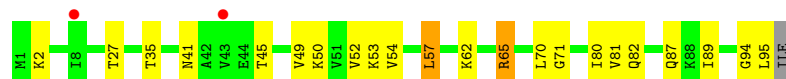
- Molecule 42: 50S ribosomal protein L22

Chain DW: 



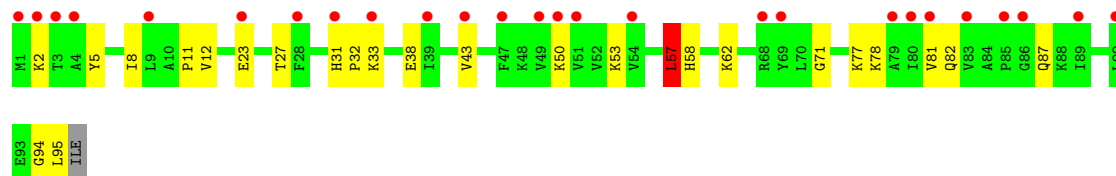
- Molecule 43: 50S ribosomal protein L23

Chain BX: 



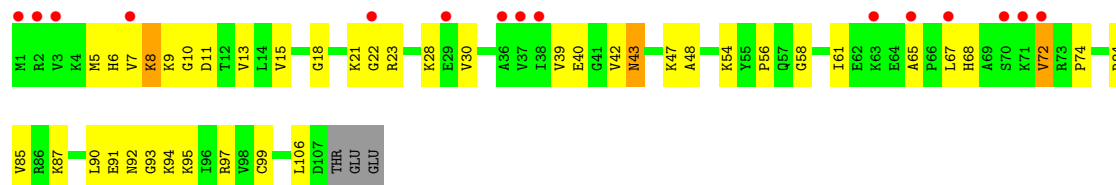
- Molecule 43: 50S ribosomal protein L23

Chain DX: 



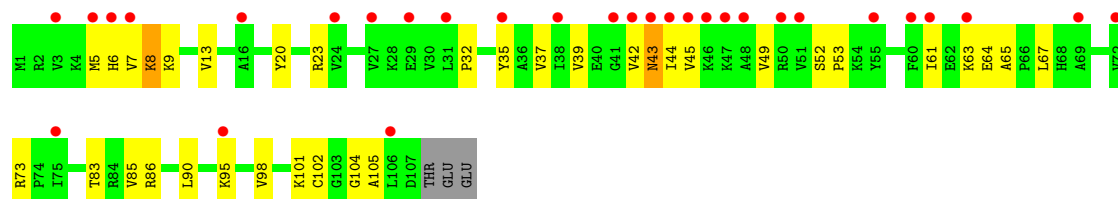
- Molecule 44: 50S ribosomal protein L24

Chain BY: 



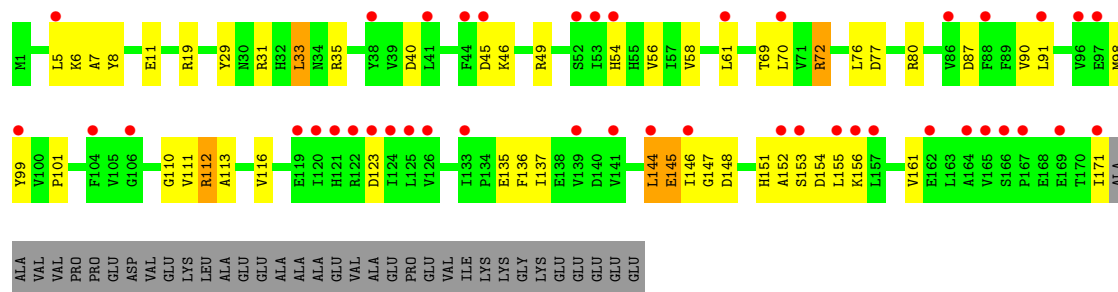
- Molecule 44: 50S ribosomal protein L24

Chain DY:



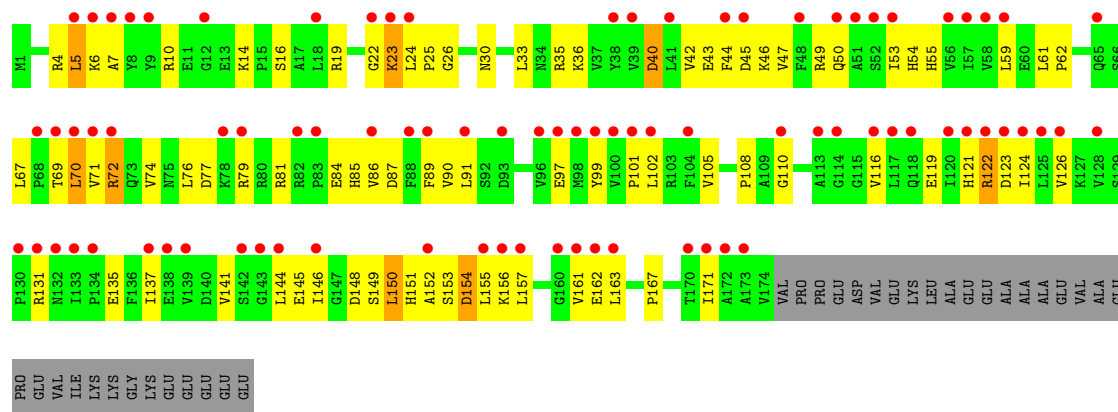
- Molecule 45: 50S ribosomal protein L25

Chain BZ:



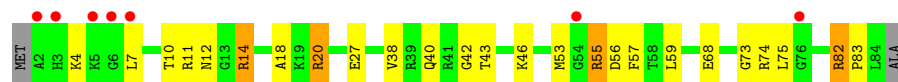
- Molecule 45: 50S ribosomal protein L25

Chain DZ:



- Molecule 46: 50S ribosomal protein L27

Chain B0:



- Molecule 46: 50S ribosomal protein L27

Chain D0:





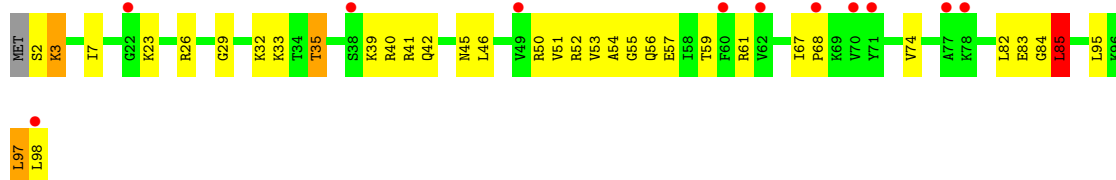
- Molecule 47: 50S ribosomal protein L28

Chain B1:



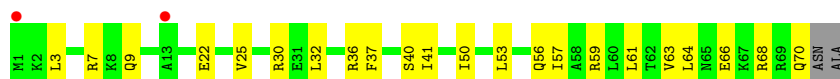
- Molecule 47: 50S ribosomal protein L28

Chain D1:



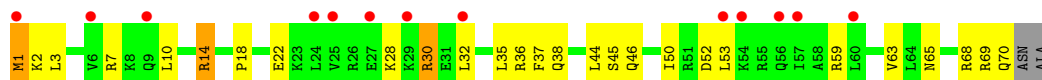
- Molecule 48: 50S ribosomal protein L29

Chain B2:



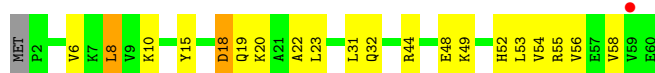
- Molecule 48: 50S ribosomal protein L29

Chain D2:



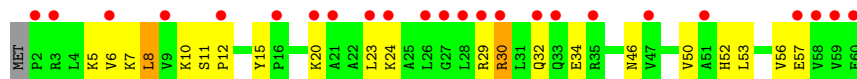
- Molecule 49: 50S ribosomal protein L30

Chain B3:



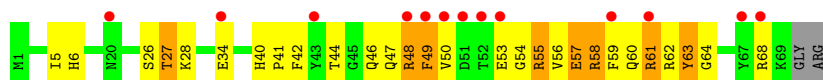
- Molecule 49: 50S ribosomal protein L30

Chain D3:



- Molecule 50: 50S ribosomal protein L31

Chain B4:



- Molecule 50: 50S ribosomal protein L31

Chain D4: 



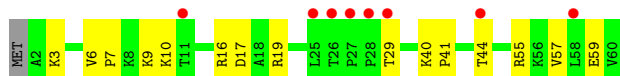
- Molecule 51: 50S ribosomal protein L32

Chain B5: 



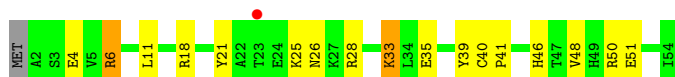
- Molecule 51: 50S ribosomal protein L32

Chain D5: 



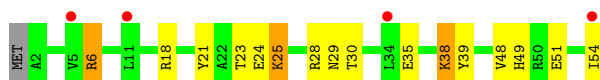
- Molecule 52: 50S ribosomal protein L33

Chain B6: 



- Molecule 52: 50S ribosomal protein L33

Chain D6: 



- Molecule 53: 50S ribosomal protein L34

Chain B7: 



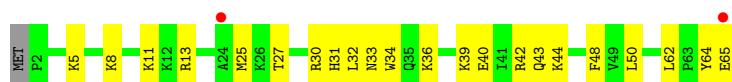
- Molecule 53: 50S ribosomal protein L34

Chain D7: 



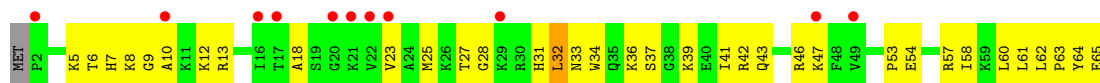
- Molecule 54: 50S ribosomal protein L35

Chain B8: 



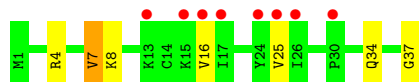
- Molecule 54: 50S ribosomal protein L35

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, α , β , γ	209.25Å 448.46Å 618.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	362.98 – 2.90 362.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.9 (362.98-2.90) 96.9 (362.98-2.90)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.231 , 0.286 0.248 , 0.307	Depositor DCC
R_{free} test set	33963 reflections (2.76%)	DCC
Wilson B-factor (Å ²)	54.8	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 40.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 1229139 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	289646	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, MG, PPU, K, ZN, 31H, 5MC, 4SU, SF4, PSU

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	0.39	0/36049	0.94	50/56261 (0.1%)
1	CA	0.41	6/36170 (0.0%)	1.02	84/56452 (0.1%)
2	AB	0.31	0/1881	0.63	0/2542
2	CB	0.32	0/1860	0.65	3/2518 (0.1%)
3	AC	0.30	0/1576	0.51	0/2130
3	CC	0.31	0/1566	0.61	2/2119 (0.1%)
4	AD	0.31	0/1689	0.59	1/2267 (0.0%)
4	CD	0.30	0/1700	0.54	0/2280
5	AE	0.29	0/1145	0.56	0/1543
5	CE	0.32	0/1149	0.59	0/1548
6	AF	0.30	0/819	0.51	0/1111
6	CF	0.30	0/829	0.50	0/1123
7	AG	0.28	0/1250	0.51	0/1679
7	CG	0.30	0/1254	0.54	0/1683
8	AH	0.29	0/1108	0.51	0/1494
8	CH	0.28	0/1108	0.55	0/1494
9	AI	0.31	0/1002	0.59	0/1346
9	CI	0.32	0/997	0.56	0/1343
10	AJ	0.28	0/722	0.57	0/982
10	CJ	0.30	0/727	0.56	0/988
11	AK	0.28	0/844	0.51	0/1145
11	CK	0.29	0/848	0.51	0/1149
12	AL	0.31	0/946	0.51	0/1274
12	CL	0.31	0/946	0.57	0/1274
13	AM	0.28	0/969	0.63	0/1302
13	CM	0.32	0/961	0.61	0/1291
14	AN	0.32	0/501	0.54	0/664
14	CN	0.31	0/501	0.60	0/664
15	AO	0.29	0/739	0.50	0/985
15	CO	0.28	0/739	0.52	0/985
16	AP	0.30	0/697	0.54	0/939
16	CP	0.29	0/693	0.52	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.30	0/836	0.54	0/1117
17	CQ	0.29	0/836	0.52	0/1117
18	AR	0.29	0/560	0.54	0/746
18	CR	0.29	0/560	0.57	1/746 (0.1%)
19	AS	0.28	0/667	0.53	0/900
19	CS	0.32	0/661	0.67	0/893
20	AT	0.31	0/730	0.60	0/965
20	CT	0.29	0/729	0.63	1/965 (0.1%)
21	AU	0.28	0/203	0.49	0/266
21	CU	0.33	0/203	0.47	0/266
22	AV	0.42	0/310	0.95	0/480
22	CV	0.45	0/282	0.97	0/437
23	AW	0.35	0/18	0.66	0/26
23	CW	0.27	0/18	0.91	0/26
24	AX	0.52	0/1700	1.21	18/2650 (0.7%)
24	CX	0.55	3/1700 (0.2%)	1.24	16/2650 (0.6%)
25	BA	0.48	1/68013 (0.0%)	0.94	53/106165 (0.0%)
25	DA	0.42	0/67542	0.95	80/105428 (0.1%)
26	BB	0.42	0/2878	0.93	0/4490
26	DB	0.45	0/2878	1.00	3/4490 (0.1%)
27	BD	0.37	0/2186	0.57	0/2944
27	DD	0.33	0/2186	0.56	0/2944
28	BE	0.35	0/1592	0.55	0/2149
28	DE	0.33	0/1592	0.58	1/2149 (0.0%)
29	BF	0.34	0/1619	0.54	0/2193
29	DF	0.32	0/1615	0.57	0/2188
30	BG	0.30	0/1450	0.57	0/1959
30	DG	0.35	0/1449	0.61	0/1958
31	BH	0.32	0/1356	0.53	0/1834
31	DH	0.29	0/1356	0.55	0/1834
32	BI	0.29	0/1100	0.58	0/1501
32	DI	0.30	0/1076	0.60	1/1471 (0.1%)
33	BN	0.32	0/1144	0.52	0/1543
33	DN	0.31	0/1144	0.54	0/1543
34	BO	0.37	0/943	0.59	0/1269
34	DO	0.33	0/943	0.55	0/1269
35	BP	0.34	0/1152	0.58	1/1533 (0.1%)
35	DP	0.32	0/1152	0.60	0/1533
36	BQ	0.35	0/1143	0.53	0/1527
36	DQ	0.33	0/1143	0.55	0/1527
37	BR	0.34	0/982	0.55	0/1312
37	DR	0.30	0/982	0.53	0/1312
38	BS	0.33	0/887	0.56	0/1180

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DS	0.30	0/880	0.59	0/1172
39	BT	0.33	0/1105	0.56	0/1477
39	DT	0.30	0/1097	0.54	0/1468
40	BU	0.36	0/977	0.53	0/1301
40	DU	0.31	0/977	0.55	0/1301
41	BV	0.36	0/782	0.54	0/1049
41	DV	0.32	0/782	0.57	0/1049
42	BW	0.35	0/897	0.54	0/1205
42	DW	0.31	0/897	0.52	0/1205
43	BX	0.38	0/764	0.58	1/1025 (0.1%)
43	DX	0.32	0/764	0.56	1/1025 (0.1%)
44	BY	0.35	0/819	0.56	0/1095
44	DY	0.31	0/819	0.56	0/1095
45	BZ	0.33	0/1379	0.61	0/1873
45	DZ	0.30	0/1390	0.55	0/1890
46	B0	0.35	0/662	0.59	0/881
46	D0	0.31	0/662	0.50	0/881
47	B1	0.34	0/762	0.56	0/1014
47	D1	0.33	0/762	0.57	1/1014 (0.1%)
48	B2	0.32	0/590	0.57	0/781
48	D2	0.30	0/590	0.49	0/781
49	B3	0.35	0/474	0.55	0/635
49	D3	0.30	0/469	0.53	0/630
50	B4	0.36	0/565	0.71	0/761
50	D4	0.35	0/545	0.69	0/737
51	B5	0.33	0/469	0.55	0/635
51	D5	0.32	0/469	0.54	0/635
52	B6	0.39	0/460	0.53	0/613
52	D6	0.33	0/456	0.53	0/608
53	B7	0.37	0/426	0.56	0/561
53	D7	0.34	0/426	0.48	0/561
54	B8	0.37	0/519	0.55	0/684
54	D8	0.31	0/525	0.52	0/691
55	B9	0.35	0/310	0.50	0/407
55	D9	0.34	0/310	0.54	0/407
All	All	0.40	10/310281 (0.0%)	0.87	318/464152 (0.1%)

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

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

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	1154	G	C6-N1	-12.01	1.31	1.39
1	CA	1154	G	N1-C2	-11.43	1.28	1.37
1	CA	1119	C	N3-C4	-10.12	1.26	1.33
1	CA	1154	G	N7-C5	-6.67	1.35	1.39
24	CX	14	A	N7-C5	-5.86	1.35	1.39

The worst 5 of 318 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1119	C	N1-C2-O2	29.84	136.81	118.90
1	CA	1154	G	C5-C6-O6	27.03	144.82	128.60
1	CA	1154	G	N3-C2-N2	25.60	137.82	119.90
1	CA	1154	G	N1-C2-N2	-23.27	95.25	116.20
1	CA	1119	C	C2-N3-C4	19.75	129.77	119.90

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

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

5.2 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	32205	0	16254	640	0
1	CA	32312	0	16307	729	0
2	AB	1846	0	1867	85	0
2	CB	1825	0	1828	97	0
3	AC	1552	0	1546	67	0
3	CC	1542	0	1517	73	0
4	AD	1659	0	1676	65	0
4	CD	1670	0	1703	68	0
5	AE	1129	0	1185	30	0
5	CE	1133	0	1191	53	0
6	AF	806	0	793	28	0
6	CF	816	0	808	22	0
7	AG	1231	0	1238	28	0
7	CG	1235	0	1249	30	0
8	AH	1088	0	1126	25	0
8	CH	1088	0	1126	38	0
9	AI	983	0	986	52	0
9	CI	978	0	966	55	0
10	AJ	709	0	650	34	0
10	CJ	714	0	672	35	0
11	AK	829	0	825	18	0
11	CK	833	0	836	23	0
12	AL	930	0	979	31	0
12	CL	930	0	980	33	0
13	AM	958	0	1002	39	0
13	CM	950	0	988	56	0
14	AN	492	0	529	25	0
14	CN	492	0	529	36	0
15	AO	728	0	760	22	0
15	CO	728	0	760	30	0
16	AP	681	0	697	31	0
16	CP	677	0	686	26	0
17	AQ	823	0	891	24	0
17	CQ	823	0	891	21	0
18	AR	555	0	618	13	0
18	CR	555	0	618	21	0
19	AS	652	0	662	28	0
19	CS	646	0	644	52	0
20	AT	728	0	798	26	0
20	CT	727	0	796	28	0
21	AU	199	0	208	8	0
21	CU	199	0	208	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	AV	277	0	140	6	0
22	CV	252	0	130	8	0
23	AW	54	0	40	5	0
23	CW	54	0	40	7	0
24	AX	1635	0	816	34	0
24	CX	1635	0	816	39	0
25	BA	60729	0	30621	813	0
25	DA	60311	0	30408	1066	0
26	BB	2573	0	1306	29	0
26	DB	2573	0	1306	91	0
27	BD	2136	0	2218	58	0
27	DD	2136	0	2217	68	0
28	BE	1559	0	1618	52	0
28	DE	1559	0	1618	56	0
29	BF	1584	0	1625	36	0
29	DF	1580	0	1619	68	0
30	BG	1425	0	1443	45	0
30	DG	1424	0	1434	77	0
31	BH	1330	0	1407	29	0
31	DH	1330	0	1407	42	0
32	BI	1085	0	1114	39	0
32	DI	1061	0	1080	34	0
33	BN	1117	0	1184	24	0
33	DN	1117	0	1184	33	0
34	BO	933	0	996	26	0
34	DO	933	0	996	34	0
35	BP	1135	0	1212	34	0
35	DP	1135	0	1211	50	0
36	BQ	1122	0	1179	35	0
36	DQ	1122	0	1179	43	0
37	BR	968	0	1033	28	0
37	DR	968	0	1033	27	0
38	BS	877	0	938	22	0
38	DS	870	0	923	53	0
39	BT	1091	0	1151	30	0
39	DT	1083	0	1136	37	0
40	BU	959	0	1019	18	0
40	DU	959	0	1019	33	0
41	BV	771	0	830	14	0
41	DV	771	0	830	26	0
42	BW	886	0	940	9	0
42	DW	886	0	940	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	BX	750	0	814	13	0
43	DX	750	0	814	17	0
44	BY	806	0	881	31	0
44	DY	806	0	881	26	0
45	BZ	1349	0	1355	30	0
45	DZ	1360	0	1363	64	0
46	B0	653	0	674	26	0
46	D0	653	0	674	24	0
47	B1	755	0	826	12	0
47	D1	755	0	826	26	0
48	B2	588	0	643	12	0
48	D2	588	0	643	17	0
49	B3	469	0	518	9	0
49	D3	464	0	514	17	0
50	B4	552	0	533	25	0
50	D4	532	0	503	30	0
51	B5	455	0	465	12	0
51	D5	455	0	465	13	0
52	B6	453	0	473	9	0
52	D6	449	0	469	13	0
53	B7	418	0	467	13	0
53	D7	418	0	467	14	0
54	B8	511	0	571	18	0
54	D8	517	0	582	33	0
55	B9	307	0	335	4	0
55	D9	307	0	335	13	0
56	AA	187	0	0	0	0
56	AD	1	0	0	0	0
56	AE	2	0	0	0	0
56	AF	1	0	0	0	0
56	AK	1	0	0	0	0
56	AL	1	0	0	0	0
56	AM	1	0	0	0	0
56	AN	1	0	0	0	0
56	AX	7	0	0	0	0
56	B0	5	0	0	0	0
56	B3	2	0	0	0	0
56	B4	1	0	0	0	0
56	B5	2	0	0	0	0
56	B7	4	0	0	0	0
56	B8	1	0	0	0	0
56	B9	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BA	675	0	0	0	0
56	BB	18	0	0	0	0
56	BD	8	0	0	0	0
56	BE	6	0	0	0	0
56	BF	5	0	0	0	0
56	BG	3	0	0	0	0
56	BH	1	0	0	0	0
56	BN	2	0	0	0	0
56	BO	1	0	0	0	0
56	BP	4	0	0	0	0
56	BQ	3	0	0	0	0
56	BR	3	0	0	0	0
56	BU	5	0	0	0	0
56	BV	3	0	0	0	0
56	BW	4	0	0	0	0
56	BX	3	0	0	0	0
56	BY	2	0	0	0	0
56	BZ	1	0	0	0	0
56	CA	154	0	0	0	0
56	CE	2	0	0	0	0
56	CF	1	0	0	0	0
56	CJ	1	0	0	0	0
56	CK	1	0	0	0	0
56	CT	1	0	0	0	0
56	CX	1	0	0	0	0
56	D0	1	0	0	0	0
56	D3	1	0	0	0	0
56	D5	1	0	0	0	0
56	D7	1	0	0	0	0
56	D8	2	0	0	0	0
56	DA	595	0	0	0	0
56	DB	12	0	0	0	0
56	DD	2	0	0	0	0
56	DE	5	0	0	0	0
56	DF	3	0	0	0	0
56	DG	1	0	0	0	0
56	DN	1	0	0	0	0
56	DP	1	0	0	0	0
56	DQ	3	0	0	0	0
56	DR	2	0	0	0	0
56	DT	1	0	0	0	0
56	DU	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DV	2	0	0	0	0
56	DW	2	0	0	0	0
56	DY	1	0	0	0	0
57	AD	8	0	0	0	0
57	CD	8	0	0	0	0
58	AN	1	0	0	0	0
58	B4	1	0	0	0	0
58	B5	1	0	0	0	0
58	B6	1	0	0	0	0
58	B9	1	0	0	0	0
58	BY	1	0	0	0	0
58	CN	1	0	0	0	0
58	D4	1	0	0	0	0
58	D5	1	0	0	0	0
58	D6	1	0	0	0	0
58	D9	1	0	0	0	0
58	DY	1	0	0	0	0
59	AX	1	0	0	0	0
59	DA	1	0	0	0	0
60	AA	165	0	0	12	0
60	AJ	1	0	0	0	0
60	AL	3	0	0	2	0
60	AP	1	0	0	0	0
60	AU	1	0	0	0	0
60	AV	2	0	0	0	0
60	AW	3	0	0	0	0
60	B0	4	0	0	0	0
60	B1	2	0	0	0	0
60	B2	1	0	0	0	0
60	B3	1	0	0	0	0
60	B5	2	0	0	0	0
60	B7	2	0	0	1	0
60	B8	8	0	0	2	0
60	BA	924	0	0	61	0
60	BB	27	0	0	0	0
60	BD	6	0	0	2	0
60	BE	8	0	0	0	0
60	BF	6	0	0	1	0
60	BG	1	0	0	0	0
60	BH	1	0	0	1	0
60	BN	3	0	0	0	0
60	BO	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	BP	14	0	0	2	0
60	BQ	2	0	0	0	0
60	BS	1	0	0	0	0
60	BT	4	0	0	1	0
60	BU	2	0	0	0	0
60	BV	5	0	0	0	0
60	BW	1	0	0	0	0
60	BX	2	0	0	0	0
60	BZ	1	0	0	0	0
60	CA	113	0	0	5	0
60	CE	2	0	0	0	0
60	CJ	2	0	0	1	0
60	CL	1	0	0	1	0
60	CO	1	0	0	0	0
60	CW	1	0	0	1	0
60	CX	1	0	0	1	0
60	D0	5	0	0	0	0
60	D1	1	0	0	0	0
60	D3	1	0	0	3	0
60	D8	3	0	0	0	0
60	DA	689	0	0	58	0
60	DB	9	0	0	0	0
60	DD	11	0	0	2	0
60	DE	5	0	0	1	0
60	DF	6	0	0	0	0
60	DO	1	0	0	0	0
60	DP	6	0	0	0	0
60	DU	3	0	0	0	0
60	DV	1	0	0	0	0
60	DW	1	0	0	0	0
60	DX	3	0	0	0	0
All	All	289646	0	193040	5715	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 13.

The worst 5 of 5715 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:DA:2121:G:H1	25:DA:2177:C:N4	1.35	1.23
19:CS:42:PRO:HG3	50:D4:61:ARG:HG2	1.39	1.04
1:AA:1028:C:N4	1:AA:1033:G:H1	1.56	1.01
25:DA:2128:C:H42	25:DA:2160:G:H1	1.08	1.00

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:DA:2137:C:H42	25:DA:2154:G:H1	1.05	0.99

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	229/256 (90%)	208 (91%)	18 (8%)	3 (1%)	18	54
2	CB	229/256 (90%)	206 (90%)	17 (7%)	6 (3%)	8	32
3	AC	204/239 (85%)	193 (95%)	10 (5%)	1 (0%)	38	79
3	CC	204/239 (85%)	187 (92%)	15 (7%)	2 (1%)	22	63
4	AD	206/209 (99%)	195 (95%)	9 (4%)	2 (1%)	22	63
4	CD	206/209 (99%)	194 (94%)	11 (5%)	1 (0%)	38	79
5	AE	146/162 (90%)	140 (96%)	4 (3%)	2 (1%)	16	52
5	CE	146/162 (90%)	142 (97%)	4 (3%)	0	100	100
6	AF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
6	CF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
7	AG	153/156 (98%)	148 (97%)	2 (1%)	3 (2%)	11	40
7	CG	153/156 (98%)	151 (99%)	1 (1%)	1 (1%)	30	72
8	AH	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
8	CH	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
9	AI	125/128 (98%)	118 (94%)	7 (6%)	0	100	100
9	CI	125/128 (98%)	120 (96%)	5 (4%)	0	100	100
10	AJ	95/105 (90%)	87 (92%)	7 (7%)	1 (1%)	21	60
10	CJ	94/105 (90%)	87 (93%)	5 (5%)	2 (2%)	11	39
11	AK	112/129 (87%)	104 (93%)	5 (4%)	3 (3%)	8	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	CK	112/129 (87%)	103 (92%)	7 (6%)	2 (2%)	13	44
12	AL	120/132 (91%)	115 (96%)	5 (4%)	0	100	100
12	CL	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
13	AM	121/126 (96%)	113 (93%)	8 (7%)	0	100	100
13	CM	120/126 (95%)	114 (95%)	5 (4%)	1 (1%)	27	68
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%)	83 (96%)	3 (4%)	0	100	100
15	CO	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	AP	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
16	CP	80/88 (91%)	77 (96%)	2 (2%)	1 (1%)	18	54
17	AQ	97/105 (92%)	92 (95%)	4 (4%)	1 (1%)	22	63
17	CQ	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
18	AR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
18	CR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
19	AS	81/93 (87%)	76 (94%)	5 (6%)	0	100	100
19	CS	81/93 (87%)	75 (93%)	6 (7%)	0	100	100
20	AT	94/106 (89%)	87 (93%)	6 (6%)	1 (1%)	21	60
20	CT	94/106 (89%)	86 (92%)	5 (5%)	3 (3%)	6	25
21	AU	21/27 (78%)	21 (100%)	0	0	100	100
21	CU	21/27 (78%)	21 (100%)	0	0	100	100
27	BD	273/276 (99%)	263 (96%)	9 (3%)	1 (0%)	43	82
27	DD	273/276 (99%)	262 (96%)	9 (3%)	2 (1%)	30	72
28	BE	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	38	79
28	DE	202/206 (98%)	193 (96%)	7 (4%)	2 (1%)	22	63
29	BF	201/210 (96%)	197 (98%)	3 (2%)	1 (0%)	38	79
29	DF	201/210 (96%)	197 (98%)	2 (1%)	2 (1%)	22	63
30	BG	179/182 (98%)	171 (96%)	7 (4%)	1 (1%)	33	76
30	DG	179/182 (98%)	167 (93%)	11 (6%)	1 (1%)	33	76
31	BH	172/180 (96%)	169 (98%)	3 (2%)	0	100	100
31	DH	172/180 (96%)	168 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	BI	144/148 (97%)	130 (90%)	10 (7%)	4 (3%)	8	29
32	DI	144/148 (97%)	137 (95%)	6 (4%)	1 (1%)	30	72
33	BN	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
33	DN	138/140 (99%)	135 (98%)	2 (1%)	1 (1%)	30	72
34	BO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
34	DO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
35	BP	147/150 (98%)	141 (96%)	6 (4%)	0	100	100
35	DP	147/150 (98%)	140 (95%)	5 (3%)	2 (1%)	16	52
36	BQ	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
36	DQ	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
37	BR	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
37	DR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
38	BS	108/112 (96%)	103 (95%)	4 (4%)	1 (1%)	25	66
38	DS	108/112 (96%)	105 (97%)	2 (2%)	1 (1%)	25	66
39	BT	129/146 (88%)	123 (95%)	4 (3%)	2 (2%)	14	47
39	DT	129/146 (88%)	125 (97%)	3 (2%)	1 (1%)	27	68
40	BU	114/118 (97%)	114 (100%)	0	0	100	100
40	DU	114/118 (97%)	114 (100%)	0	0	100	100
41	BV	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
41	DV	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
42	BW	110/113 (97%)	110 (100%)	0	0	100	100
42	DW	110/113 (97%)	110 (100%)	0	0	100	100
43	BX	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
43	DX	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
44	BY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
44	DY	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
45	BZ	169/206 (82%)	152 (90%)	16 (10%)	1 (1%)	33	76
45	DZ	172/206 (84%)	158 (92%)	14 (8%)	0	100	100
46	B0	81/85 (95%)	81 (100%)	0	0	100	100
46	D0	81/85 (95%)	79 (98%)	1 (1%)	1 (1%)	19	57
47	B1	95/98 (97%)	94 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	D1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	21	60
48	B2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
48	D2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
49	B3	57/60 (95%)	57 (100%)	0	0	100	100
49	D3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
50	B4	67/71 (94%)	56 (84%)	9 (13%)	2 (3%)	7	27
50	D4	67/71 (94%)	54 (81%)	8 (12%)	5 (8%)	2	4
51	B5	57/60 (95%)	57 (100%)	0	0	100	100
51	D5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
52	B6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
52	D6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
53	B7	46/49 (94%)	46 (100%)	0	0	100	100
53	D7	46/49 (94%)	45 (98%)	0	1 (2%)	10	37
54	B8	62/65 (95%)	62 (100%)	0	0	100	100
54	D8	62/65 (95%)	62 (100%)	0	0	100	100
55	B9	35/37 (95%)	35 (100%)	0	0	100	100
55	D9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11409/12128 (94%)	10906 (96%)	432 (4%)	71 (1%)	33	76

5 of 71 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	19	HIS
2	AB	231	GLU
4	AD	166	LYS
7	AG	80	VAL
27	BD	275	LYS

5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	192/220 (87%)	151 (79%)	41 (21%)	1	4
2	CB	187/220 (85%)	154 (82%)	33 (18%)	3	8
3	AC	143/188 (76%)	125 (87%)	18 (13%)	7	18
3	CC	140/188 (74%)	121 (86%)	19 (14%)	5	15
4	AD	170/181 (94%)	146 (86%)	24 (14%)	5	14
4	CD	172/181 (95%)	145 (84%)	27 (16%)	4	11
5	AE	113/123 (92%)	103 (91%)	10 (9%)	14	40
5	CE	114/123 (93%)	98 (86%)	16 (14%)	5	14
6	AF	83/90 (92%)	78 (94%)	5 (6%)	27	63
6	CF	85/90 (94%)	77 (91%)	8 (9%)	13	36
7	AG	119/127 (94%)	108 (91%)	11 (9%)	13	38
7	CG	120/127 (94%)	109 (91%)	11 (9%)	13	38
8	AH	114/119 (96%)	103 (90%)	11 (10%)	12	35
8	CH	114/119 (96%)	104 (91%)	10 (9%)	14	40
9	AI	90/99 (91%)	76 (84%)	14 (16%)	4	11
9	CI	89/99 (90%)	70 (79%)	19 (21%)	1	5
10	AJ	66/92 (72%)	63 (96%)	3 (4%)	38	77
10	CJ	69/92 (75%)	64 (93%)	5 (7%)	21	51
11	AK	82/99 (83%)	75 (92%)	7 (8%)	15	42
11	CK	83/99 (84%)	79 (95%)	4 (5%)	35	74
12	AL	97/109 (89%)	89 (92%)	8 (8%)	17	44
12	CL	97/109 (89%)	88 (91%)	9 (9%)	13	37
13	AM	93/101 (92%)	79 (85%)	14 (15%)	4	12
13	CM	92/101 (91%)	77 (84%)	15 (16%)	3	10
14	AN	49/50 (98%)	42 (86%)	7 (14%)	5	13
14	CN	49/50 (98%)	39 (80%)	10 (20%)	2	5
15	AO	78/80 (98%)	70 (90%)	8 (10%)	10	30
15	CO	78/80 (98%)	71 (91%)	7 (9%)	14	39
16	AP	69/74 (93%)	54 (78%)	15 (22%)	1	4
16	CP	68/74 (92%)	59 (87%)	9 (13%)	6	16
17	AQ	94/97 (97%)	87 (93%)	7 (7%)	20	50
17	CQ	94/97 (97%)	88 (94%)	6 (6%)	25	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AR	59/77 (77%)	52 (88%)	7 (12%)	8	21
18	CR	59/77 (77%)	52 (88%)	7 (12%)	8	21
19	AS	69/80 (86%)	63 (91%)	6 (9%)	15	41
19	CS	67/80 (84%)	59 (88%)	8 (12%)	8	21
20	AT	70/82 (85%)	61 (87%)	9 (13%)	6	17
20	CT	70/82 (85%)	59 (84%)	11 (16%)	4	11
21	AU	18/22 (82%)	15 (83%)	3 (17%)	3	9
21	CU	18/22 (82%)	15 (83%)	3 (17%)	3	9
27	BD	215/218 (99%)	196 (91%)	19 (9%)	14	40
27	DD	215/218 (99%)	194 (90%)	21 (10%)	12	34
28	BE	164/166 (99%)	144 (88%)	20 (12%)	7	20
28	DE	164/166 (99%)	143 (87%)	21 (13%)	6	18
29	BF	160/166 (96%)	146 (91%)	14 (9%)	14	40
29	DF	159/166 (96%)	144 (91%)	15 (9%)	13	36
30	BG	143/156 (92%)	123 (86%)	20 (14%)	5	14
30	DG	142/156 (91%)	118 (83%)	24 (17%)	3	9
31	BH	144/148 (97%)	136 (94%)	8 (6%)	30	66
31	DH	144/148 (97%)	131 (91%)	13 (9%)	14	39
32	BI	110/124 (89%)	93 (84%)	17 (16%)	4	11
32	DI	104/124 (84%)	87 (84%)	17 (16%)	3	10
33	BN	118/119 (99%)	104 (88%)	14 (12%)	8	21
33	DN	118/119 (99%)	104 (88%)	14 (12%)	8	21
34	BO	100/100 (100%)	92 (92%)	8 (8%)	17	45
34	DO	100/100 (100%)	90 (90%)	10 (10%)	11	32
35	BP	115/116 (99%)	102 (89%)	13 (11%)	9	25
35	DP	115/116 (99%)	103 (90%)	12 (10%)	10	29
36	BQ	111/111 (100%)	100 (90%)	11 (10%)	11	34
36	DQ	111/111 (100%)	98 (88%)	13 (12%)	8	22
37	BR	101/101 (100%)	86 (85%)	15 (15%)	4	12
37	DR	101/101 (100%)	90 (89%)	11 (11%)	9	26
38	BS	87/88 (99%)	80 (92%)	7 (8%)	17	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	DS	85/88 (97%)	76 (89%)	9 (11%)	10	28
39	BT	115/127 (91%)	104 (90%)	11 (10%)	12	35
39	DT	113/127 (89%)	98 (87%)	15 (13%)	6	16
40	BU	93/94 (99%)	85 (91%)	8 (9%)	15	41
40	DU	93/94 (99%)	85 (91%)	8 (9%)	15	41
41	BV	80/82 (98%)	72 (90%)	8 (10%)	11	32
41	DV	80/82 (98%)	75 (94%)	5 (6%)	25	60
42	BW	90/92 (98%)	82 (91%)	8 (9%)	14	40
42	DW	90/92 (98%)	84 (93%)	6 (7%)	23	56
43	BX	77/78 (99%)	73 (95%)	4 (5%)	32	71
43	DX	77/78 (99%)	75 (97%)	2 (3%)	59	90
44	BY	85/91 (93%)	77 (91%)	8 (9%)	13	36
44	DY	85/91 (93%)	81 (95%)	4 (5%)	36	75
45	BZ	145/179 (81%)	126 (87%)	19 (13%)	6	17
45	DZ	145/179 (81%)	128 (88%)	17 (12%)	8	22
46	B0	65/67 (97%)	61 (94%)	4 (6%)	26	61
46	D0	65/67 (97%)	61 (94%)	4 (6%)	26	61
47	B1	80/83 (96%)	75 (94%)	5 (6%)	25	60
47	D1	80/83 (96%)	73 (91%)	7 (9%)	14	40
48	B2	65/67 (97%)	61 (94%)	4 (6%)	26	61
48	D2	65/67 (97%)	57 (88%)	8 (12%)	7	20
49	B3	51/52 (98%)	45 (88%)	6 (12%)	8	22
49	D3	50/52 (96%)	46 (92%)	4 (8%)	17	45
50	B4	59/63 (94%)	50 (85%)	9 (15%)	4	12
50	D4	53/63 (84%)	40 (76%)	13 (24%)	1	3
51	B5	50/52 (96%)	44 (88%)	6 (12%)	7	21
51	D5	50/52 (96%)	46 (92%)	4 (8%)	17	45
52	B6	51/52 (98%)	45 (88%)	6 (12%)	8	22
52	D6	50/52 (96%)	45 (90%)	5 (10%)	11	32
53	B7	41/42 (98%)	37 (90%)	4 (10%)	12	34
53	D7	41/42 (98%)	37 (90%)	4 (10%)	12	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	B8	53/55 (96%)	49 (92%)	4 (8%)	19	49
54	D8	54/55 (98%)	50 (93%)	4 (7%)	20	50
55	B9	34/34 (100%)	32 (94%)	2 (6%)	28	64
55	D9	34/34 (100%)	30 (88%)	4 (12%)	8	22
All	All	9318/10066 (93%)	8277 (89%)	1041 (11%)	9	25

5 of 1041 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	B2	32	LEU
4	CD	170	VAL
43	DX	57	LEU
50	B4	58	ARG
2	CB	144	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 128 such sidechains are listed below:

Mol	Chain	Res	Type
49	B3	32	GLN
4	CD	77	ASN
39	DT	123	GLN
52	B6	20	ASN
2	CB	224	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1495/1521 (98%)	387 (25%)	22 (1%)
1	CA	1501/1521 (98%)	391 (26%)	24 (1%)
22	AV	12/24 (50%)	4 (33%)	0
22	CV	11/24 (45%)	4 (36%)	0
23	AW	0/2	-	-
23	CW	0/2	-	-
24	AX	74/77 (96%)	25 (33%)	1 (1%)
24	CX	74/77 (96%)	26 (35%)	1 (1%)
25	BA	2811/2915 (96%)	537 (19%)	24 (0%)
25	DA	2791/2915 (95%)	622 (22%)	29 (1%)
26	BB	120/121 (99%)	19 (15%)	3 (2%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	DB	119/121 (98%)	36 (30%)	0
All	All	9008/9320 (96%)	2051 (22%)	104 (1%)

5 of 2051 RNA backbone outliers are listed below:

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

5 of 104 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	BB	1	U
1	CA	560	U
25	DA	2169	A
26	BB	52	A
1	CA	65	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PPU	AW	76	25,23	38,40,41	1.33	5 (13%)	54,57,60	2.28	14 (25%)
24	5MC	AX	32	24	20,22,23	1.73	4 (20%)	26,32,35	1.55	4 (15%)
24	5MU	AX	54	24,56	20,22,23	1.55	5 (25%)	25,32,35	2.58	5 (20%)
24	PSU	AX	55	24	19,21,22	1.88	5 (26%)	23,30,33	1.28	2 (8%)
24	31H	AX	76	24,56	32,34,35	1.18	3 (9%)	44,47,50	2.59	11 (25%)
24	4SU	AX	8	24	19,21,22	1.78	4 (21%)	23,30,33	28.80	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PPU	CW	76	23	38,40,41	1.29	4 (10%)	54,57,60	2.19	12 (22%)
24	5MC	CX	32	24	20,22,23	1.72	4 (20%)	26,32,35	1.48	4 (15%)
24	5MU	CX	54	24	20,22,23	1.57	4 (20%)	25,32,35	2.01	4 (16%)
24	PSU	CX	55	24	19,21,22	1.91	4 (21%)	23,30,33	1.09	2 (8%)
24	31H	CX	76	24	32,34,35	1.20	4 (12%)	44,47,50	2.57	11 (25%)
24	4SU	CX	8	24	19,21,22	1.94	4 (21%)	23,30,33	33.33	2 (8%)

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
23	PPU	AW	76	25,23	-	0/26/43/44	0/4/4/4
24	5MC	AX	32	24	-	0/6/25/26	0/2/2/2
24	5MU	AX	54	24,56	-	0/6/25/26	0/2/2/2
24	PSU	AX	55	24	-	0/8/25/26	0/2/2/2
24	31H	AX	76	24,56	-	1/23/40/41	0/3/3/3
24	4SU	AX	8	24	-	0/6/25/26	0/2/2/2
23	PPU	CW	76	23	-	0/26/43/44	0/4/4/4
24	5MC	CX	32	24	-	0/6/25/26	0/2/2/2
24	5MU	CX	54	24	-	0/6/25/26	0/2/2/2
24	PSU	CX	55	24	-	0/8/25/26	0/2/2/2
24	31H	CX	76	24	-	1/23/40/41	0/3/3/3
24	4SU	CX	8	24	-	0/6/25/26	0/2/2/2

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CX	8	4SU	O2-C2	5.01	1.28	1.21
24	AX	32	5MC	C5-C4	4.72	1.48	1.41
24	CX	32	5MC	C5-C4	4.55	1.48	1.41
24	CX	55	PSU	C5-C1'	-4.50	1.48	1.52
24	AX	55	PSU	C5-C1'	-4.44	1.48	1.52

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	CX	8	4SU	C4-N3-C2	159.52	128.42	121.60
24	AX	8	4SU	C4-N3-C2	138.03	127.50	121.60
24	AX	76	31H	N3-C2-N1	-10.57	119.59	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	CX	76	31H	N3-C2-N1	-10.03	120.06	128.89
24	CX	8	4SU	C2-N1-C1'	9.45	124.14	118.21

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AX	76	31H	OCN-CN-N-CA
24	CX	76	31H	OCN-CN-N-CA

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 1780 ligands modelled in this entry, 1778 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
57	SF4	AD	501	4	12,12,12	21.76	12 (100%)	0,24,24	0.00	-
57	SF4	CD	501	4	12,12,12	20.96	12 (100%)	0,24,24	0.00	-

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	SF4	CD	501	4	-	0/0/48/48	0/6/5/5

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	AD	501	SF4	S1-FE3	-23.11	2.17	2.33
57	AD	501	SF4	S4-FE2	-22.99	2.17	2.33
57	AD	501	SF4	S4-FE3	-22.79	2.17	2.33
57	AD	501	SF4	S2-FE4	-22.65	2.18	2.33
57	AD	501	SF4	S2-FE1	-22.28	2.18	2.33

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1498/1521 (98%)	0.21	14 (0%) 81 88	39, 74, 94, 105	0
1	CA	1503/1521 (98%)	0.12	23 (1%) 70 79	41, 75, 94, 105	0
2	AB	231/256 (90%)	1.18	62 (26%) 1 1	65, 82, 90, 96	0
2	CB	231/256 (90%)	1.83	83 (35%) 1 1	67, 83, 92, 96	0
3	AC	206/239 (86%)	1.19	55 (26%) 1 1	67, 78, 86, 94	0
3	CC	206/239 (86%)	1.33	66 (32%) 1 1	69, 80, 87, 92	0
4	AD	208/209 (99%)	1.17	54 (25%) 1 1	57, 72, 82, 86	0
4	CD	208/209 (99%)	1.06	39 (18%) 2 2	57, 73, 82, 87	0
5	AE	148/162 (91%)	0.63	11 (7%) 14 17	55, 71, 81, 86	0
5	CE	148/162 (91%)	0.83	16 (10%) 6 8	58, 73, 82, 89	0
6	AF	100/101 (99%)	0.27	2 (2%) 62 71	55, 71, 80, 82	0
6	CF	100/101 (99%)	0.41	10 (10%) 8 10	58, 73, 80, 82	0
7	AG	155/156 (99%)	0.91	27 (17%) 2 3	67, 76, 85, 94	0
7	CG	155/156 (99%)	1.45	50 (32%) 1 1	68, 78, 86, 96	0
8	AH	137/138 (99%)	0.24	2 (1%) 70 79	62, 72, 78, 86	0
8	CH	137/138 (99%)	0.90	22 (16%) 2 3	62, 73, 80, 88	0
9	AI	127/128 (99%)	1.13	29 (22%) 1 2	64, 82, 87, 90	0
9	CI	127/128 (99%)	2.96	80 (62%) 0 0	67, 83, 89, 91	0
10	AJ	97/105 (92%)	0.69	15 (15%) 3 4	63, 80, 89, 95	0
10	CJ	96/105 (91%)	3.01	65 (67%) 0 0	70, 86, 93, 100	0
11	AK	114/129 (88%)	0.75	16 (14%) 3 5	54, 72, 81, 83	0
11	CK	114/129 (88%)	0.98	22 (19%) 2 2	56, 72, 80, 83	0
12	AL	122/132 (92%)	0.66	11 (9%) 10 12	55, 65, 75, 78	0
12	CL	122/132 (92%)	0.72	15 (12%) 5 6	57, 67, 75, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	123/126 (97%)	1.21	29 (23%) 1 2	64, 78, 86, 91	0
13	CM	122/126 (96%)	1.84	47 (38%) 1 0	68, 80, 88, 93	0
14	AN	60/61 (98%)	1.10	13 (21%) 1 2	65, 76, 83, 86	0
14	CN	60/61 (98%)	3.33	43 (71%) 0 0	69, 79, 84, 88	0
15	AO	88/89 (98%)	0.58	5 (5%) 23 28	56, 69, 80, 90	0
15	CO	88/89 (98%)	0.67	10 (11%) 6 7	56, 70, 80, 90	0
16	AP	82/88 (93%)	1.12	19 (23%) 1 2	58, 73, 83, 85	0
16	CP	82/88 (93%)	1.04	12 (14%) 3 5	58, 72, 82, 85	0
17	AQ	99/105 (94%)	1.10	19 (19%) 2 2	60, 70, 81, 85	0
17	CQ	99/105 (94%)	0.66	7 (7%) 16 19	57, 70, 80, 84	0
18	AR	68/88 (77%)	1.08	14 (20%) 1 2	60, 70, 81, 85	0
18	CR	68/88 (77%)	0.54	3 (4%) 33 40	61, 72, 82, 86	0
19	AS	83/93 (89%)	1.16	21 (25%) 1 2	67, 81, 88, 96	0
19	CS	83/93 (89%)	1.85	35 (42%) 1 0	71, 83, 91, 97	0
20	AT	96/106 (90%)	1.39	31 (32%) 1 1	58, 72, 82, 89	0
20	CT	96/106 (90%)	0.99	18 (18%) 2 2	59, 72, 82, 88	0
21	AU	23/27 (85%)	0.58	0 100 100	65, 75, 80, 86	0
21	CU	23/27 (85%)	1.62	7 (30%) 1 1	66, 76, 83, 87	0
22	AV	13/24 (54%)	1.42	2 (15%) 3 4	60, 92, 100, 100	0
22	CV	12/24 (50%)	2.52	6 (50%) 0 0	63, 93, 99, 99	0
23	AW	2/2 (100%)	2.87	1 (50%) 0 0	35, 35, 35, 42	0
23	CW	2/2 (100%)	3.99	1 (50%) 0 0	52, 52, 52, 59	0
24	AX	75/77 (97%)	0.10	0 100 100	37, 71, 84, 92	0
24	CX	75/77 (97%)	-0.05	0 100 100	39, 73, 86, 92	0
25	BA	2819/2915 (96%)	0.45	47 (1%) 67 76	23, 46, 89, 107	0
25	DA	2800/2915 (96%)	0.10	33 (1%) 75 83	26, 50, 90, 107	0
26	BB	120/121 (99%)	0.41	0 100 100	40, 65, 76, 91	0
26	DB	120/121 (99%)	0.16	4 (3%) 44 53	44, 70, 81, 93	0
27	BD	275/276 (99%)	0.36	6 (2%) 59 67	24, 45, 61, 77	0
27	DD	275/276 (99%)	0.73	22 (8%) 12 15	27, 47, 63, 78	0
28	BE	204/206 (99%)	0.92	36 (17%) 2 3	18, 44, 66, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DE	204/206 (99%)	0.61	20 (9%) 8 10	32, 57, 72, 86	0
29	BF	203/210 (96%)	1.04	37 (18%) 2 3	26, 55, 74, 84	0
29	DF	203/210 (96%)	0.98	36 (17%) 2 3	26, 58, 75, 85	0
30	BG	181/182 (99%)	0.89	24 (13%) 4 6	56, 70, 82, 91	0
30	DG	181/182 (99%)	2.17	80 (44%) 1 0	61, 73, 85, 91	0
31	BH	174/180 (96%)	0.90	16 (9%) 9 11	51, 66, 76, 82	0
31	DH	174/180 (96%)	1.60	48 (27%) 1 1	55, 69, 80, 85	0
32	BI	146/148 (98%)	1.06	32 (21%) 1 2	46, 74, 85, 87	0
32	DI	146/148 (98%)	1.05	33 (22%) 1 2	50, 75, 84, 87	0
33	BN	140/140 (100%)	1.07	17 (12%) 5 7	33, 53, 72, 80	0
33	DN	140/140 (100%)	1.66	50 (35%) 1 1	36, 56, 72, 81	0
34	BO	122/122 (100%)	0.27	3 (2%) 54 64	25, 43, 60, 76	0
34	DO	122/122 (100%)	0.21	3 (2%) 54 64	42, 59, 73, 77	0
35	BP	149/150 (99%)	0.88	14 (9%) 9 11	27, 57, 73, 87	0
35	DP	149/150 (99%)	1.14	37 (24%) 1 2	29, 59, 76, 86	0
36	BQ	141/141 (100%)	1.08	24 (17%) 2 3	35, 53, 64, 71	0
36	DQ	141/141 (100%)	1.47	41 (29%) 1 1	38, 56, 68, 76	0
37	BR	118/118 (100%)	0.58	10 (8%) 11 13	25, 37, 56, 66	0
37	DR	118/118 (100%)	1.28	30 (25%) 1 2	40, 54, 66, 76	0
38	BS	110/112 (98%)	0.67	9 (8%) 12 15	40, 52, 63, 68	0
38	DS	110/112 (98%)	1.46	31 (28%) 1 1	57, 76, 86, 92	0
39	BT	131/146 (89%)	0.32	5 (3%) 38 45	32, 50, 74, 86	0
39	DT	131/146 (89%)	0.73	13 (9%) 8 10	44, 60, 75, 85	0
40	BU	116/118 (98%)	0.81	10 (8%) 11 13	23, 35, 55, 76	0
40	DU	116/118 (98%)	1.54	38 (32%) 1 1	41, 61, 77, 87	0
41	BV	101/101 (100%)	0.68	7 (6%) 17 20	19, 43, 64, 76	0
41	DV	101/101 (100%)	1.31	25 (24%) 1 2	44, 71, 80, 88	0
42	BW	112/113 (99%)	0.98	11 (9%) 8 10	21, 38, 53, 75	0
42	DW	112/113 (99%)	1.65	41 (36%) 1 0	31, 51, 69, 85	0
43	BX	95/96 (98%)	0.55	2 (2%) 60 69	25, 43, 64, 82	0
43	DX	95/96 (98%)	1.45	26 (27%) 1 1	43, 62, 78, 91	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BY	107/110 (97%)	0.97	15 (14%) 3 5	36, 51, 69, 80	0
44	DY	107/110 (97%)	1.25	30 (28%) 1 1	55, 72, 81, 89	0
45	BZ	171/206 (83%)	1.18	43 (25%) 1 2	42, 63, 77, 92	0
45	DZ	174/206 (84%)	2.24	85 (48%) 1 0	61, 80, 90, 100	0
46	B0	83/85 (97%)	0.53	7 (8%) 11 14	16, 43, 56, 67	0
46	D0	83/85 (97%)	1.01	12 (14%) 3 5	44, 65, 74, 80	0
47	B1	97/98 (98%)	0.26	3 (3%) 47 55	27, 49, 70, 77	0
47	D1	97/98 (98%)	0.73	11 (11%) 6 7	38, 59, 75, 78	0
48	B2	70/72 (97%)	0.52	2 (2%) 49 58	37, 50, 66, 72	0
48	D2	70/72 (97%)	1.21	13 (18%) 2 2	58, 70, 79, 85	0
49	B3	59/60 (98%)	0.63	1 (1%) 67 76	26, 41, 61, 72	0
49	D3	59/60 (98%)	1.97	24 (40%) 1 0	44, 64, 77, 80	0
50	B4	69/71 (97%)	0.80	13 (18%) 2 2	57, 76, 91, 94	0
50	D4	69/71 (97%)	1.51	21 (30%) 1 1	77, 87, 97, 104	0
51	B5	59/60 (98%)	0.37	3 (5%) 27 33	19, 38, 57, 78	0
51	D5	59/60 (98%)	0.88	8 (13%) 4 5	31, 52, 69, 76	0
52	B6	53/54 (98%)	0.41	1 (1%) 64 72	29, 43, 60, 71	0
52	D6	53/54 (98%)	0.50	4 (7%) 14 17	50, 63, 75, 83	0
53	B7	48/49 (97%)	0.71	6 (12%) 5 6	20, 30, 53, 72	0
53	D7	48/49 (97%)	0.88	6 (12%) 5 6	35, 46, 71, 76	0
54	B8	64/65 (98%)	0.75	2 (3%) 47 55	27, 36, 47, 55	0
54	D8	64/65 (98%)	1.10	11 (17%) 2 3	44, 58, 67, 75	0
55	B9	37/37 (100%)	1.30	8 (21%) 1 2	31, 52, 64, 69	0
55	D9	37/37 (100%)	1.39	10 (27%) 1 1	44, 58, 67, 73	0
All	All	20644/21448 (96%)	0.70	2392 (11%) 5 7	16, 65, 87, 107	0

The worst 5 of 2392 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	CM	124	PRO	14.4
10	CJ	71	LEU	11.6
10	CJ	6	ILE	10.8
2	CB	70	PHE	10.5
14	CN	25	VAL	10.4

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
24	PSU	CX	55	20/21	0.12	-	59,68,84,85	0
24	5MC	CX	32	21/22	0.13	-	52,69,78,83	0
23	PPU	CW	76	37/38	0.26	-	31,50,63,70	0
24	5MU	CX	54	21/22	0.18	-	66,78,87,98	0
24	4SU	AX	8	20/21	0.16	-	50,63,78,79	0
24	5MU	AX	54	21/22	0.14	-	55,69,75,82	0
24	4SU	CX	8	20/21	0.14	-	65,84,90,94	0
24	5MC	AX	32	21/22	0.15	-	46,61,70,75	0
24	31H	AX	76	32/33	0.26	-	27,44,76,98	0
23	PPU	AW	76	37/38	0.22	-	25,33,43,45	0
24	PSU	AX	55	20/21	0.14	-	57,66,78,79	0
24	31H	CX	76	32/33	0.26	-	33,54,78,89	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
56	MG	DA	3590	1/1	0.31	-	38,38,38,38	0
56	MG	BA	3293	1/1	0.12	-	17,17,17,17	0
56	MG	CA	3057	1/1	0.13	-	41,41,41,41	0
56	MG	BA	3185	1/1	0.16	-	43,43,43,43	0
56	MG	DA	3528	1/1	0.05	-	37,37,37,37	0
56	MG	DA	3339	1/1	0.12	-	32,32,32,32	0
56	MG	BA	3436	1/1	0.10	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BG	3002	1/1	0.09	-	27,27,27,27	0
56	MG	DA	3455	1/1	0.17	-	45,45,45,45	0
56	MG	DA	3084	1/1	0.21	-	39,39,39,39	0
56	MG	DA	3351	1/1	0.11	-	46,46,46,46	0
56	MG	CA	3052	1/1	0.10	-	39,39,39,39	0
56	MG	DA	3320	1/1	0.07	-	46,46,46,46	0
56	MG	BA	3551	1/1	0.09	-	48,48,48,48	0
56	MG	DA	3553	1/1	0.11	-	46,46,46,46	0
56	MG	AA	3186	1/1	0.11	-	55,55,55,55	0
56	MG	DA	3244	1/1	0.13	-	48,48,48,48	0
56	MG	BA	3188	1/1	0.14	-	39,39,39,39	0
56	MG	CA	3017	1/1	0.11	-	41,41,41,41	0
56	MG	BA	3553	1/1	0.67	-	48,48,48,48	0
56	MG	DA	3238	1/1	0.15	-	42,42,42,42	0
56	MG	DA	3293	1/1	0.15	-	34,34,34,34	0
56	MG	DA	3178	1/1	0.25	-	46,46,46,46	0
56	MG	BA	3113	1/1	0.14	-	41,41,41,41	0
56	MG	BA	3351	1/1	0.09	-	33,33,33,33	0
56	MG	B7	3003	1/1	0.23	-	28,28,28,28	0
56	MG	BA	3447	1/1	0.14	-	55,55,55,55	0
56	MG	CA	3092	1/1	0.12	-	54,54,54,54	0
56	MG	BA	3361	1/1	0.09	-	45,45,45,45	0
56	MG	DA	3379	1/1	0.08	-	26,26,26,26	0
56	MG	BA	3332	1/1	0.10	-	61,61,61,61	0
56	MG	BA	3423	1/1	0.12	-	47,47,47,47	0
56	MG	DA	3059	1/1	0.12	-	33,33,33,33	0
56	MG	BA	3217	1/1	0.23	-	29,29,29,29	0
56	MG	BA	3424	1/1	0.16	-	38,38,38,38	0
56	MG	CA	3154	1/1	0.14	-	62,62,62,62	0
56	MG	BB	3014	1/1	0.17	-	35,35,35,35	0
56	MG	CA	3005	1/1	0.10	-	42,42,42,42	0
56	MG	DA	3436	1/1	0.09	-	27,27,27,27	0
56	MG	BA	3474	1/1	0.16	-	53,53,53,53	0
56	MG	DA	3542	1/1	0.12	-	30,30,30,30	0
56	MG	CA	3125	1/1	0.23	-	71,71,71,71	0
56	MG	AF	3001	1/1	0.13	-	52,52,52,52	0
56	MG	CA	3114	1/1	0.06	-	80,80,80,80	0
56	MG	DA	3002	1/1	0.11	-	33,33,33,33	0
56	MG	DA	3425	1/1	0.13	-	37,37,37,37	0
56	MG	CA	3006	1/1	0.30	-	37,37,37,37	0
56	MG	DA	3415	1/1	0.18	-	40,40,40,40	0
56	MG	DA	3394	1/1	0.16	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3240	1/1	0.26	-	43,43,43,43	0
56	MG	DA	3111	1/1	0.18	-	39,39,39,39	0
56	MG	DA	3120	1/1	0.20	-	33,33,33,33	0
56	MG	BA	3247	1/1	0.18	-	48,48,48,48	0
56	MG	DA	3108	1/1	0.09	-	46,46,46,46	0
56	MG	DA	3058	1/1	0.25	-	45,45,45,45	0
56	MG	BA	3357	1/1	0.11	-	30,30,30,30	0
56	MG	BA	3629	1/1	0.17	-	60,60,60,60	0
56	MG	BA	3318	1/1	0.10	-	44,44,44,44	0
56	MG	BA	3655	1/1	0.12	-	18,18,18,18	0
56	MG	BA	3239	1/1	0.12	-	52,52,52,52	0
56	MG	BA	3146	1/1	0.16	-	31,31,31,31	0
56	MG	BA	3360	1/1	0.14	-	21,21,21,21	0
56	MG	CA	3103	1/1	0.12	-	52,52,52,52	0
56	MG	AA	3151	1/1	0.18	-	45,45,45,45	0
56	MG	DA	3540	1/1	0.11	-	46,46,46,46	0
56	MG	BB	3010	1/1	0.15	-	77,77,77,77	0
56	MG	DA	3044	1/1	0.11	-	47,47,47,47	0
56	MG	BA	3440	1/1	0.05	-	38,38,38,38	0
56	MG	DA	3081	1/1	0.11	-	44,44,44,44	0
56	MG	AA	3008	1/1	0.52	-	55,55,55,55	0
56	MG	AA	3034	1/1	0.18	-	54,54,54,54	0
56	MG	BA	3513	1/1	0.12	-	60,60,60,60	0
56	MG	BB	3015	1/1	0.15	-	48,48,48,48	0
56	MG	BA	3057	1/1	0.12	-	38,38,38,38	0
56	MG	CA	3112	1/1	0.11	-	55,55,55,55	0
56	MG	DA	3007	1/1	0.08	-	39,39,39,39	0
56	MG	DA	3290	1/1	0.09	-	36,36,36,36	0
56	MG	DA	3032	1/1	0.11	-	42,42,42,42	0
56	MG	DA	3441	1/1	0.12	-	45,45,45,45	0
56	MG	BA	3316	1/1	0.08	-	61,61,61,61	0
56	MG	BA	3523	1/1	0.08	-	50,50,50,50	0
56	MG	BA	3618	1/1	0.19	-	54,54,54,54	0
56	MG	DA	3532	1/1	0.06	-	51,51,51,51	0
56	MG	AA	3041	1/1	0.16	-	52,52,52,52	0
56	MG	DA	3266	1/1	0.11	-	46,46,46,46	0
56	MG	AA	3022	1/1	0.07	-	39,39,39,39	0
56	MG	CA	3123	1/1	0.15	-	66,66,66,66	0
56	MG	B0	105	1/1	0.10	-	43,43,43,43	0
56	MG	DA	3573	1/1	0.14	-	45,45,45,45	0
56	MG	AA	3125	1/1	0.19	-	41,41,41,41	0
56	MG	DA	3062	1/1	0.19	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BP	204	1/1	0.28	-	31,31,31,31	0
56	MG	BX	102	1/1	0.37	-	38,38,38,38	0
56	MG	AA	3137	1/1	0.09	-	79,79,79,79	0
56	MG	BE	302	1/1	0.71	-	36,36,36,36	0
56	MG	BA	3366	1/1	0.06	-	34,34,34,34	0
56	MG	AA	3039	1/1	0.09	-	45,45,45,45	0
56	MG	DA	3074	1/1	0.12	-	29,29,29,29	0
56	MG	DA	3153	1/1	0.13	-	42,42,42,42	0
56	MG	BA	3104	1/1	0.20	-	42,42,42,42	0
56	MG	BA	3174	1/1	0.09	-	29,29,29,29	0
56	MG	DA	3443	1/1	0.08	-	49,49,49,49	0
56	MG	BA	3646	1/1	0.10	-	23,23,23,23	0
56	MG	BA	3092	1/1	0.21	-	44,44,44,44	0
56	MG	DA	3110	1/1	0.14	-	42,42,42,42	0
56	MG	DA	3519	1/1	0.06	-	42,42,42,42	0
56	MG	BA	3624	1/1	0.28	-	49,49,49,49	0
56	MG	DA	3145	1/1	0.12	-	31,31,31,31	0
56	MG	DA	3413	1/1	0.15	-	24,24,24,24	0
56	MG	BR	3002	1/1	0.18	-	23,23,23,23	0
56	MG	CA	3108	1/1	0.14	-	59,59,59,59	0
56	MG	DA	3303	1/1	0.06	-	43,43,43,43	0
56	MG	BA	3526	1/1	0.22	-	25,25,25,25	0
56	MG	DA	3071	1/1	0.26	-	36,36,36,36	0
56	MG	DA	3240	1/1	0.13	-	54,54,54,54	0
56	MG	DA	3232	1/1	0.10	-	38,38,38,38	0
56	MG	AA	3178	1/1	0.27	-	62,62,62,62	0
56	MG	DA	3254	1/1	0.06	-	46,46,46,46	0
56	MG	AM	3001	1/1	0.13	-	54,54,54,54	0
56	MG	DA	3182	1/1	0.11	-	38,38,38,38	0
56	MG	BA	3065	1/1	0.16	-	29,29,29,29	0
56	MG	DA	3515	1/1	0.12	-	64,64,64,64	0
56	MG	DA	3336	1/1	0.17	-	22,22,22,22	0
56	MG	DA	3593	1/1	0.27	-	51,51,51,51	0
56	MG	DA	3435	1/1	0.18	-	33,33,33,33	0
56	MG	BA	3205	1/1	0.10	-	40,40,40,40	0
56	MG	BA	3005	1/1	0.15	-	29,29,29,29	0
56	MG	BA	3495	1/1	0.33	-	48,48,48,48	0
56	MG	DA	3410	1/1	0.13	-	64,64,64,64	0
56	MG	DA	3008	1/1	0.12	-	38,38,38,38	0
56	MG	DA	3547	1/1	0.16	-	41,41,41,41	0
56	MG	DA	3311	1/1	0.10	-	43,43,43,43	0
56	MG	DA	3304	1/1	0.14	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3173	1/1	0.12	-	45,45,45,45	0
56	MG	DA	3205	1/1	0.14	-	32,32,32,32	0
56	MG	AX	3004	1/1	0.20	-	39,39,39,39	0
56	MG	AA	3176	1/1	0.14	-	60,60,60,60	0
56	MG	BA	3078	1/1	0.14	-	53,53,53,53	0
56	MG	AX	3006	1/1	0.12	-	54,54,54,54	0
56	MG	BG	3003	1/1	0.10	-	41,41,41,41	0
56	MG	DA	3557	1/1	0.11	-	62,62,62,62	0
56	MG	BA	3583	1/1	0.10	-	37,37,37,37	0
56	MG	BB	3002	1/1	0.25	-	41,41,41,41	0
56	MG	AA	3109	1/1	0.27	-	44,44,44,44	0
56	MG	BA	3614	1/1	0.05	-	55,55,55,55	0
56	MG	AA	3053	1/1	0.07	-	50,50,50,50	0
56	MG	BB	3016	1/1	0.09	-	24,24,24,24	0
56	MG	BA	3630	1/1	0.07	-	47,47,47,47	0
56	MG	DA	3377	1/1	0.14	-	37,37,37,37	0
56	MG	BA	3623	1/1	0.10	-	48,48,48,48	0
56	MG	BA	3410	1/1	0.10	-	43,43,43,43	0
56	MG	BA	3275	1/1	0.15	-	39,39,39,39	0
56	MG	BA	3602	1/1	0.20	-	31,31,31,31	0
56	MG	DA	3270	1/1	0.07	-	37,37,37,37	0
56	MG	BA	3154	1/1	0.22	-	40,40,40,40	0
56	MG	DA	3235	1/1	0.21	-	42,42,42,42	0
56	MG	AA	3032	1/1	0.14	-	42,42,42,42	0
56	MG	BA	3365	1/1	0.11	-	41,41,41,41	0
56	MG	DA	3287	1/1	0.10	-	38,38,38,38	0
56	MG	AA	3012	1/1	0.09	-	64,64,64,64	0
56	MG	DA	3196	1/1	0.13	-	33,33,33,33	0
56	MG	AA	3054	1/1	0.14	-	65,65,65,65	0
56	MG	BA	3027	1/1	0.17	-	28,28,28,28	0
56	MG	BA	3109	1/1	0.10	-	36,36,36,36	0
56	MG	DA	3215	1/1	0.13	-	31,31,31,31	0
56	MG	AA	3169	1/1	0.12	-	71,71,71,71	0
56	MG	CA	3070	1/1	0.06	-	39,39,39,39	0
56	MG	DA	3325	1/1	0.14	-	54,54,54,54	0
56	MG	DA	3299	1/1	0.10	-	50,50,50,50	0
56	MG	BA	3207	1/1	0.12	-	36,36,36,36	0
56	MG	BA	3196	1/1	0.17	-	17,17,17,17	0
56	MG	BA	3401	1/1	0.14	-	32,32,32,32	0
56	MG	CA	3023	1/1	0.10	-	38,38,38,38	0
56	MG	DA	3551	1/1	0.14	-	52,52,52,52	0
56	MG	BQ	202	1/1	0.12	-	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3578	1/1	0.17	-	47,47,47,47	0
56	MG	AA	3027	1/1	0.19	-	71,71,71,71	0
56	MG	BA	3050	1/1	0.14	-	44,44,44,44	0
56	MG	DA	3020	1/1	0.36	-	50,50,50,50	0
56	MG	BA	3329	1/1	0.11	-	30,30,30,30	0
56	MG	DB	3009	1/1	0.12	-	60,60,60,60	0
56	MG	CA	3101	1/1	0.12	-	53,53,53,53	0
56	MG	AA	3115	1/1	0.06	-	35,35,35,35	0
56	MG	BA	3672	1/1	0.10	-	46,46,46,46	0
56	MG	CA	3036	1/1	0.10	-	56,56,56,56	0
56	MG	BA	3308	1/1	0.17	-	52,52,52,52	0
56	MG	BA	3449	1/1	0.06	-	47,47,47,47	0
56	MG	BA	3644	1/1	0.07	-	41,41,41,41	0
56	MG	DA	3364	1/1	0.05	-	37,37,37,37	0
56	MG	BA	3416	1/1	0.16	-	64,64,64,64	0
56	MG	DA	3506	1/1	0.12	-	65,65,65,65	0
56	MG	DA	3500	1/1	0.16	-	46,46,46,46	0
56	MG	BA	3274	1/1	0.20	-	47,47,47,47	0
56	MG	DA	3088	1/1	0.11	-	39,39,39,39	0
56	MG	BA	3179	1/1	0.11	-	27,27,27,27	0
56	MG	BU	204	1/1	0.20	-	29,29,29,29	0
56	MG	AA	3181	1/1	0.19	-	53,53,53,53	0
56	MG	DA	3370	1/1	0.12	-	44,44,44,44	0
56	MG	BA	3199	1/1	0.15	-	32,32,32,32	0
56	MG	DA	3512	1/1	0.11	-	36,36,36,36	0
56	MG	CA	3050	1/1	0.13	-	67,67,67,67	0
56	MG	BA	3162	1/1	0.16	-	39,39,39,39	0
56	MG	BA	3036	1/1	0.09	-	56,56,56,56	0
56	MG	BA	3411	1/1	0.15	-	25,25,25,25	0
56	MG	DE	3003	1/1	0.12	-	40,40,40,40	0
56	MG	AA	3102	1/1	0.15	-	60,60,60,60	0
56	MG	DA	3451	1/1	0.08	-	30,30,30,30	0
56	MG	BA	3397	1/1	0.10	-	30,30,30,30	0
56	MG	AA	3105	1/1	0.14	-	44,44,44,44	0
56	MG	DA	3345	1/1	0.15	-	33,33,33,33	0
56	MG	BA	3341	1/1	0.10	-	32,32,32,32	0
56	MG	DA	3439	1/1	0.11	-	28,28,28,28	0
56	MG	DA	3331	1/1	0.08	-	41,41,41,41	0
56	MG	CA	3093	1/1	0.12	-	72,72,72,72	0
56	MG	BA	3060	1/1	0.12	-	42,42,42,42	0
56	MG	BA	3586	1/1	0.18	-	45,45,45,45	0
56	MG	DN	5001	1/1	0.16	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	3081	1/1	0.23	-	56,56,56,56	0
56	MG	BA	3434	1/1	0.12	-	43,43,43,43	0
56	MG	DA	3317	1/1	0.11	-	53,53,53,53	0
56	MG	BA	3276	1/1	0.13	-	42,42,42,42	0
56	MG	DA	3038	1/1	0.10	-	30,30,30,30	0
56	MG	DA	3510	1/1	0.10	-	53,53,53,53	0
56	MG	BA	3007	1/1	0.13	-	32,32,32,32	0
56	MG	DA	3305	1/1	0.15	-	30,30,30,30	0
56	MG	BA	3047	1/1	0.20	-	41,41,41,41	0
56	MG	CA	3094	1/1	0.13	-	67,67,67,67	0
56	MG	AA	3051	1/1	0.11	-	49,49,49,49	0
56	MG	BA	3389	1/1	0.19	-	35,35,35,35	0
58	ZN	CN	501	1/1	0.10	-	82,82,82,82	0
56	MG	BA	3379	1/1	0.16	-	31,31,31,31	0
56	MG	BA	3529	1/1	0.18	-	33,33,33,33	0
56	MG	BA	3230	1/1	0.15	-	40,40,40,40	0
56	MG	BU	202	1/1	0.11	-	40,40,40,40	0
56	MG	BA	3022	1/1	0.12	-	26,26,26,26	0
56	MG	BN	3001	1/1	0.16	-	57,57,57,57	0
56	MG	BA	3304	1/1	0.06	-	43,43,43,43	0
56	MG	DA	3558	1/1	0.08	-	39,39,39,39	0
56	MG	BA	3651	1/1	0.12	-	42,42,42,42	0
56	MG	BA	3202	1/1	0.12	-	30,30,30,30	0
56	MG	BA	3539	1/1	0.15	-	58,58,58,58	0
56	MG	DA	3286	1/1	0.07	-	35,35,35,35	0
56	MG	BA	3161	1/1	0.11	-	39,39,39,39	0
56	MG	BA	3534	1/1	0.14	-	20,20,20,20	0
56	MG	CA	3133	1/1	0.15	-	68,68,68,68	0
56	MG	BA	3609	1/1	0.12	-	44,44,44,44	0
56	MG	CA	3020	1/1	0.24	-	46,46,46,46	0
56	MG	DA	3480	1/1	0.10	-	32,32,32,32	0
56	MG	DA	3177	1/1	0.11	-	52,52,52,52	0
56	MG	AA	3078	1/1	0.15	-	34,34,34,34	0
56	MG	DA	3395	1/1	0.09	-	41,41,41,41	0
56	MG	AA	3146	1/1	0.13	-	41,41,41,41	0
56	MG	BA	3283	1/1	0.10	-	57,57,57,57	0
56	MG	BA	3466	1/1	0.23	-	49,49,49,49	0
56	MG	BA	3031	1/1	0.45	-	46,46,46,46	0
56	MG	DA	3060	1/1	0.10	-	45,45,45,45	0
56	MG	AA	3112	1/1	0.18	-	94,94,94,94	0
56	MG	DA	3033	1/1	0.17	-	37,37,37,37	0
56	MG	DA	3475	1/1	0.24	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3169	1/1	0.09	-	38,38,38,38	0
56	MG	DA	3045	1/1	0.09	-	48,48,48,48	0
56	MG	AA	3067	1/1	0.12	-	42,42,42,42	0
56	MG	BA	3235	1/1	0.34	-	51,51,51,51	0
56	MG	DA	3456	1/1	0.13	-	34,34,34,34	0
56	MG	BA	3045	1/1	0.13	-	34,34,34,34	0
56	MG	AA	3021	1/1	0.11	-	41,41,41,41	0
56	MG	CA	3056	1/1	0.20	-	40,40,40,40	0
56	MG	DA	3494	1/1	0.22	-	49,49,49,49	0
56	MG	BA	3485	1/1	0.11	-	64,64,64,64	0
56	MG	AA	3164	1/1	0.18	-	61,61,61,61	0
56	MG	DA	3384	1/1	0.14	-	52,52,52,52	0
56	MG	DA	3571	1/1	0.15	-	48,48,48,48	0
56	MG	AA	3046	1/1	0.10	-	42,42,42,42	0
56	MG	DA	3383	1/1	0.08	-	47,47,47,47	0
56	MG	AA	3101	1/1	0.10	-	53,53,53,53	0
56	MG	DA	3453	1/1	0.10	-	31,31,31,31	0
56	MG	BA	3395	1/1	0.14	-	54,54,54,54	0
56	MG	AA	3131	1/1	0.21	-	55,55,55,55	0
56	MG	AX	3002	1/1	0.16	-	56,56,56,56	0
56	MG	DA	3308	1/1	0.13	-	29,29,29,29	0
56	MG	BB	3004	1/1	0.09	-	49,49,49,49	0
56	MG	BA	3604	1/1	0.10	-	28,28,28,28	0
56	MG	BA	3037	1/1	0.11	-	24,24,24,24	0
56	MG	BA	3668	1/1	0.16	-	26,26,26,26	0
56	MG	BA	3058	1/1	0.13	-	43,43,43,43	0
56	MG	BW	3001	1/1	0.12	-	25,25,25,25	0
56	MG	BA	3671	1/1	0.27	-	48,48,48,48	0
56	MG	BA	3030	1/1	0.60	-	43,43,43,43	0
56	MG	BA	3600	1/1	0.11	-	68,68,68,68	0
56	MG	DA	3423	1/1	0.14	-	40,40,40,40	0
56	MG	BA	3556	1/1	0.05	-	41,41,41,41	0
56	MG	DA	3314	1/1	0.11	-	54,54,54,54	0
56	MG	BA	3435	1/1	0.18	-	36,36,36,36	0
56	MG	DA	3454	1/1	0.08	-	64,64,64,64	0
56	MG	BA	3422	1/1	0.08	-	46,46,46,46	0
56	MG	DA	3216	1/1	0.12	-	37,37,37,37	0
56	MG	DA	3517	1/1	0.21	-	47,47,47,47	0
56	MG	DA	3013	1/1	0.19	-	37,37,37,37	0
56	MG	DA	3525	1/1	0.05	-	44,44,44,44	0
56	MG	DA	3457	1/1	0.14	-	38,38,38,38	0
56	MG	BN	3002	1/1	0.14	-	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3173	1/1	0.13	-	54,54,54,54	0
56	MG	AA	3065	1/1	0.08	-	48,48,48,48	0
56	MG	BA	3577	1/1	0.07	-	57,57,57,57	0
56	MG	AK	3001	1/1	0.15	-	43,43,43,43	0
56	MG	DA	3005	1/1	0.08	-	26,26,26,26	0
56	MG	BA	3364	1/1	0.16	-	29,29,29,29	0
56	MG	CA	3153	1/1	0.13	-	37,37,37,37	0
56	MG	DA	3162	1/1	0.09	-	57,57,57,57	0
56	MG	BA	3356	1/1	0.09	-	46,46,46,46	0
56	MG	BA	3165	1/1	0.22	-	43,43,43,43	0
56	MG	DA	3426	1/1	0.20	-	35,35,35,35	0
56	MG	BA	3616	1/1	0.13	-	34,34,34,34	0
56	MG	DA	3407	1/1	0.04	-	40,40,40,40	0
56	MG	DA	3294	1/1	0.12	-	37,37,37,37	0
56	MG	DA	3042	1/1	0.09	-	32,32,32,32	0
56	MG	AA	3043	1/1	0.07	-	53,53,53,53	0
56	MG	DA	3230	1/1	0.11	-	41,41,41,41	0
56	MG	DA	3154	1/1	0.12	-	24,24,24,24	0
56	MG	CA	3116	1/1	0.14	-	59,59,59,59	0
56	MG	BP	203	1/1	0.12	-	47,47,47,47	0
56	MG	AA	3045	1/1	0.14	-	60,60,60,60	0
56	MG	DA	3388	1/1	0.05	-	35,35,35,35	0
56	MG	AA	3074	1/1	0.12	-	38,38,38,38	0
56	MG	BA	3100	1/1	0.14	-	29,29,29,29	0
56	MG	BG	3001	1/1	0.10	-	71,71,71,71	0
56	MG	DA	3581	1/1	0.17	-	53,53,53,53	0
56	MG	DA	3065	1/1	0.13	-	49,49,49,49	0
56	MG	B7	3004	1/1	0.09	-	34,34,34,34	0
56	MG	D8	5002	1/1	0.24	-	64,64,64,64	0
56	MG	DA	3431	1/1	0.10	-	61,61,61,61	0
56	MG	CA	3035	1/1	0.13	-	66,66,66,66	0
56	MG	CA	3030	1/1	0.10	-	41,41,41,41	0
56	MG	CA	3029	1/1	0.17	-	48,48,48,48	0
56	MG	CA	3145	1/1	0.12	-	59,59,59,59	0
56	MG	DA	3432	1/1	0.14	-	33,33,33,33	0
56	MG	DA	3501	1/1	0.08	-	55,55,55,55	0
56	MG	DA	3197	1/1	0.11	-	38,38,38,38	0
56	MG	BA	3455	1/1	0.12	-	21,21,21,21	0
56	MG	BA	3070	1/1	0.12	-	30,30,30,30	0
56	MG	BA	3482	1/1	0.07	-	23,23,23,23	0
56	MG	DA	3037	1/1	0.08	-	40,40,40,40	0
56	MG	DA	3118	1/1	0.19	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3472	1/1	0.16	-	53,53,53,53	0
56	MG	BA	3580	1/1	0.10	-	62,62,62,62	0
56	MG	DF	303	1/1	0.09	-	57,57,57,57	0
56	MG	B7	3002	1/1	0.28	-	35,35,35,35	0
56	MG	DA	3126	1/1	0.19	-	42,42,42,42	0
56	MG	DA	3116	1/1	0.16	-	29,29,29,29	0
56	MG	DA	3505	1/1	0.09	-	44,44,44,44	0
56	MG	BA	3370	1/1	0.12	-	29,29,29,29	0
56	MG	BA	3448	1/1	0.09	-	42,42,42,42	0
58	ZN	B5	501	1/1	0.14	-	42,42,42,42	0
56	MG	BA	3611	1/1	0.38	-	59,59,59,59	0
56	MG	CA	3022	1/1	0.13	-	34,34,34,34	0
56	MG	DA	3362	1/1	0.08	-	43,43,43,43	0
56	MG	BA	3396	1/1	0.18	-	38,38,38,38	0
56	MG	DA	3239	1/1	0.17	-	56,56,56,56	0
56	MG	DA	3445	1/1	0.11	-	48,48,48,48	0
56	MG	DA	3052	1/1	0.12	-	49,49,49,49	0
56	MG	DA	3567	1/1	0.14	-	41,41,41,41	0
56	MG	BA	3342	1/1	0.12	-	35,35,35,35	0
56	MG	DA	3504	1/1	0.13	-	49,49,49,49	0
56	MG	BA	3467	1/1	0.17	-	20,20,20,20	0
56	MG	BA	3427	1/1	0.19	-	49,49,49,49	0
56	MG	AA	3087	1/1	0.17	-	62,62,62,62	0
56	MG	AA	3145	1/1	0.13	-	35,35,35,35	0
56	MG	BA	3169	1/1	0.12	-	39,39,39,39	0
56	MG	DA	3210	1/1	0.09	-	37,37,37,37	0
56	MG	AA	3133	1/1	0.08	-	38,38,38,38	0
56	MG	DA	3138	1/1	0.08	-	33,33,33,33	0
56	MG	DB	3008	1/1	0.12	-	35,35,35,35	0
56	MG	DA	3412	1/1	0.20	-	53,53,53,53	0
56	MG	DA	3424	1/1	0.17	-	30,30,30,30	0
56	MG	D8	5001	1/1	0.07	-	50,50,50,50	0
56	MG	BA	3576	1/1	0.16	-	48,48,48,48	0
56	MG	BA	3143	1/1	0.47	-	36,36,36,36	0
56	MG	DA	3115	1/1	0.16	-	36,36,36,36	0
56	MG	DA	3277	1/1	0.06	-	48,48,48,48	0
56	MG	AA	3075	1/1	0.16	-	39,39,39,39	0
56	MG	DA	3589	1/1	0.15	-	33,33,33,33	0
56	MG	DA	3313	1/1	0.09	-	40,40,40,40	0
56	MG	DA	3533	1/1	0.07	-	60,60,60,60	0
56	MG	DA	3146	1/1	0.11	-	34,34,34,34	0
56	MG	DA	3171	1/1	0.17	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3483	1/1	0.08	-	54,54,54,54	0
56	MG	DA	3082	1/1	0.16	-	58,58,58,58	0
56	MG	DA	3131	1/1	0.11	-	46,46,46,46	0
56	MG	DA	3167	1/1	0.08	-	51,51,51,51	0
56	MG	BA	3048	1/1	0.17	-	47,47,47,47	0
56	MG	BA	3079	1/1	0.11	-	46,46,46,46	0
56	MG	AA	3015	1/1	0.13	-	56,56,56,56	0
56	MG	DA	3024	1/1	0.23	-	36,36,36,36	0
56	MG	DA	3458	1/1	0.12	-	34,34,34,34	0
56	MG	BA	3333	1/1	0.16	-	35,35,35,35	0
56	MG	DA	3550	1/1	0.11	-	46,46,46,46	0
56	MG	BA	3101	1/1	0.14	-	30,30,30,30	0
56	MG	DA	3261	1/1	0.13	-	49,49,49,49	0
56	MG	CA	3119	1/1	0.08	-	48,48,48,48	0
56	MG	BA	3452	1/1	0.14	-	38,38,38,38	0
56	MG	BA	3083	1/1	0.14	-	34,34,34,34	0
56	MG	DA	3570	1/1	0.29	-	52,52,52,52	0
56	MG	BA	3481	1/1	0.10	-	31,31,31,31	0
56	MG	CA	3069	1/1	0.12	-	34,34,34,34	0
56	MG	CA	3091	1/1	0.13	-	66,66,66,66	0
56	MG	BA	3320	1/1	0.12	-	44,44,44,44	0
56	MG	DA	3003	1/1	0.17	-	47,47,47,47	0
56	MG	BA	3521	1/1	0.14	-	54,54,54,54	0
56	MG	CA	3062	1/1	0.09	-	57,57,57,57	0
56	MG	DA	3490	1/1	0.12	-	34,34,34,34	0
56	MG	DA	3056	1/1	0.08	-	36,36,36,36	0
56	MG	DA	3057	1/1	0.11	-	30,30,30,30	0
56	MG	DA	3536	1/1	0.10	-	56,56,56,56	0
56	MG	BA	3667	1/1	0.53	-	38,38,38,38	0
56	MG	BW	3003	1/1	0.16	-	27,27,27,27	0
56	MG	DA	3249	1/1	0.07	-	34,34,34,34	0
56	MG	AA	3144	1/1	0.16	-	42,42,42,42	0
56	MG	BA	3090	1/1	0.21	-	44,44,44,44	0
56	MG	DA	3419	1/1	0.23	-	59,59,59,59	0
56	MG	AA	3028	1/1	0.20	-	39,39,39,39	0
56	MG	BA	3450	1/1	0.15	-	45,45,45,45	0
56	MG	AA	3142	1/1	0.17	-	60,60,60,60	0
56	MG	DA	3143	1/1	0.17	-	27,27,27,27	0
56	MG	BA	3327	1/1	0.10	-	44,44,44,44	0
59	K	DA	3001	1/1	0.09	-	48,48,48,48	0
56	MG	AA	3096	1/1	0.20	-	53,53,53,53	0
56	MG	BA	3399	1/1	0.11	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3539	1/1	0.13	-	52,52,52,52	0
56	MG	BA	3493	1/1	0.12	-	40,40,40,40	0
56	MG	CA	3124	1/1	0.09	-	52,52,52,52	0
56	MG	CA	3075	1/1	0.18	-	53,53,53,53	0
56	MG	BA	3232	1/1	0.19	-	41,41,41,41	0
56	MG	DA	3397	1/1	0.16	-	18,18,18,18	0
56	MG	DA	3104	1/1	0.13	-	35,35,35,35	0
56	MG	DA	3367	1/1	0.13	-	47,47,47,47	0
56	MG	AA	3183	1/1	0.20	-	55,55,55,55	0
56	MG	BA	3059	1/1	0.08	-	27,27,27,27	0
56	MG	BA	3549	1/1	0.09	-	57,57,57,57	0
56	MG	DA	3338	1/1	0.15	-	36,36,36,36	0
56	MG	BA	3430	1/1	0.09	-	29,29,29,29	0
56	MG	AA	3006	1/1	0.14	-	67,67,67,67	0
56	MG	BA	3081	1/1	0.24	-	42,42,42,42	0
56	MG	BB	3003	1/1	0.13	-	61,61,61,61	0
56	MG	BA	3052	1/1	0.12	-	27,27,27,27	0
56	MG	DA	3469	1/1	0.17	-	33,33,33,33	0
56	MG	DA	3470	1/1	0.14	-	52,52,52,52	0
56	MG	BA	3215	1/1	0.14	-	32,32,32,32	0
56	MG	AA	3040	1/1	0.14	-	27,27,27,27	0
56	MG	BA	3398	1/1	0.15	-	41,41,41,41	0
56	MG	BA	3665	1/1	0.09	-	30,30,30,30	0
56	MG	DA	3265	1/1	0.28	-	51,51,51,51	0
56	MG	BA	3354	1/1	0.12	-	42,42,42,42	0
56	MG	BA	3594	1/1	0.14	-	37,37,37,37	0
56	MG	DA	3521	1/1	0.20	-	51,51,51,51	0
56	MG	BA	3201	1/1	0.10	-	41,41,41,41	0
56	MG	BQ	201	1/1	0.07	-	52,52,52,52	0
56	MG	CA	3015	1/1	0.13	-	43,43,43,43	0
56	MG	DA	3079	1/1	0.10	-	54,54,54,54	0
56	MG	BA	3066	1/1	0.15	-	48,48,48,48	0
56	MG	BA	3610	1/1	0.16	-	47,47,47,47	0
56	MG	AA	3158	1/1	0.09	-	54,54,54,54	0
56	MG	BA	3160	1/1	0.16	-	29,29,29,29	0
56	MG	CA	3027	1/1	0.19	-	64,64,64,64	0
56	MG	BA	3390	1/1	0.10	-	47,47,47,47	0
56	MG	BA	3238	1/1	0.22	-	47,47,47,47	0
56	MG	BA	3574	1/1	0.13	-	55,55,55,55	0
56	MG	BA	3533	1/1	0.13	-	45,45,45,45	0
56	MG	BA	3674	1/1	0.17	-	54,54,54,54	0
56	MG	DA	3312	1/1	0.03	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3358	1/1	0.12	-	39,39,39,39	0
56	MG	BF	301	1/1	0.25	-	56,56,56,56	0
56	MG	CA	3060	1/1	0.16	-	50,50,50,50	0
56	MG	BE	303	1/1	0.14	-	41,41,41,41	0
56	MG	BA	3628	1/1	0.14	-	38,38,38,38	0
56	MG	BA	3262	1/1	0.18	-	24,24,24,24	0
56	MG	BF	303	1/1	0.28	-	20,20,20,20	0
56	MG	BA	3498	1/1	0.18	-	37,37,37,37	0
56	MG	AA	3091	1/1	0.10	-	36,36,36,36	0
56	MG	BA	3233	1/1	0.12	-	41,41,41,41	0
56	MG	BA	3376	1/1	0.13	-	39,39,39,39	0
56	MG	BA	3528	1/1	0.19	-	38,38,38,38	0
56	MG	CA	3045	1/1	0.18	-	52,52,52,52	0
56	MG	BA	3296	1/1	0.11	-	25,25,25,25	0
56	MG	DA	3150	1/1	0.75	-	55,55,55,55	0
56	MG	AA	3009	1/1	0.13	-	54,54,54,54	0
56	MG	AA	3077	1/1	0.13	-	39,39,39,39	0
56	MG	DA	3072	1/1	0.09	-	33,33,33,33	0
56	MG	CA	3010	1/1	0.18	-	53,53,53,53	0
56	MG	DA	3283	1/1	0.14	-	38,38,38,38	0
56	MG	BA	3186	1/1	0.13	-	39,39,39,39	0
56	MG	DA	3264	1/1	0.23	-	47,47,47,47	0
56	MG	BA	3546	1/1	0.12	-	57,57,57,57	0
56	MG	BA	3626	1/1	0.15	-	50,50,50,50	0
56	MG	BA	3505	1/1	0.20	-	46,46,46,46	0
56	MG	AA	3180	1/1	0.11	-	56,56,56,56	0
56	MG	AA	3141	1/1	0.05	-	47,47,47,47	0
56	MG	DA	3284	1/1	0.07	-	23,23,23,23	0
56	MG	DA	3546	1/1	0.05	-	40,40,40,40	0
56	MG	BA	3642	1/1	0.16	-	47,47,47,47	0
56	MG	DA	3468	1/1	0.17	-	55,55,55,55	0
56	MG	CA	3066	1/1	0.21	-	43,43,43,43	0
56	MG	DA	3376	1/1	0.06	-	38,38,38,38	0
56	MG	DA	3296	1/1	0.06	-	28,28,28,28	0
56	MG	AA	3058	1/1	0.10	-	62,62,62,62	0
56	MG	DA	3374	1/1	0.12	-	35,35,35,35	0
56	MG	DA	3474	1/1	0.10	-	62,62,62,62	0
56	MG	DA	3396	1/1	0.10	-	45,45,45,45	0
56	MG	BB	3018	1/1	0.15	-	30,30,30,30	0
56	MG	AA	3134	1/1	0.24	-	52,52,52,52	0
56	MG	BA	3008	1/1	0.08	-	27,27,27,27	0
56	MG	AA	3099	1/1	0.26	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3033	1/1	0.16	-	33,33,33,33	0
56	MG	BA	3567	1/1	0.16	-	53,53,53,53	0
56	MG	AA	3182	1/1	0.14	-	57,57,57,57	0
56	MG	BA	3006	1/1	0.38	-	36,36,36,36	0
56	MG	AA	3118	1/1	0.16	-	36,36,36,36	0
56	MG	DA	3591	1/1	0.07	-	42,42,42,42	0
56	MG	AA	3055	1/1	0.15	-	72,72,72,72	0
56	MG	BA	3660	1/1	0.07	-	49,49,49,49	0
56	MG	DA	3464	1/1	0.09	-	46,46,46,46	0
56	MG	B4	502	1/1	0.35	-	61,61,61,61	0
56	MG	BA	3558	1/1	0.12	-	59,59,59,59	0
56	MG	BA	3581	1/1	0.11	-	34,34,34,34	0
56	MG	AA	3147	1/1	0.09	-	67,67,67,67	0
56	MG	AA	3106	1/1	0.16	-	50,50,50,50	0
56	MG	BA	3647	1/1	0.12	-	30,30,30,30	0
56	MG	BA	3544	1/1	0.17	-	25,25,25,25	0
56	MG	AA	3080	1/1	0.26	-	39,39,39,39	0
56	MG	BW	3002	1/1	0.23	-	57,57,57,57	0
56	MG	B3	102	1/1	0.24	-	22,22,22,22	0
56	MG	BA	3381	1/1	0.19	-	31,31,31,31	0
56	MG	DE	3002	1/1	0.26	-	35,35,35,35	0
56	MG	BA	3261	1/1	0.11	-	53,53,53,53	0
56	MG	BA	3158	1/1	0.12	-	33,33,33,33	0
56	MG	BA	3475	1/1	0.11	-	45,45,45,45	0
56	MG	AE	3001	1/1	0.08	-	71,71,71,71	0
56	MG	DA	3498	1/1	0.12	-	48,48,48,48	0
56	MG	BV	203	1/1	0.07	-	24,24,24,24	0
56	MG	BA	3307	1/1	0.07	-	63,63,63,63	0
56	MG	DA	3237	1/1	0.46	-	39,39,39,39	0
56	MG	BA	3107	1/1	0.14	-	21,21,21,21	0
56	MG	BA	3190	1/1	0.28	-	31,31,31,31	0
56	MG	BA	3294	1/1	0.10	-	32,32,32,32	0
56	MG	CA	3115	1/1	0.08	-	62,62,62,62	0
56	MG	BA	3168	1/1	0.19	-	47,47,47,47	0
56	MG	CA	3090	1/1	0.19	-	66,66,66,66	0
56	MG	AA	3172	1/1	0.08	-	69,69,69,69	0
56	MG	DA	3430	1/1	0.22	-	30,30,30,30	0
56	MG	BX	103	1/1	0.23	-	25,25,25,25	0
56	MG	DA	3473	1/1	0.05	-	50,50,50,50	0
56	MG	BA	3194	1/1	0.11	-	23,23,23,23	0
56	MG	AA	3170	1/1	0.15	-	54,54,54,54	0
56	MG	BA	3251	1/1	0.19	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3152	1/1	0.24	-	39,39,39,39	0
56	MG	BA	3652	1/1	0.07	-	49,49,49,49	0
56	MG	AA	3062	1/1	0.18	-	58,58,58,58	0
56	MG	BA	3004	1/1	0.08	-	23,23,23,23	0
56	MG	BA	3313	1/1	0.11	-	17,17,17,17	0
56	MG	BA	3019	1/1	0.25	-	49,49,49,49	0
56	MG	DA	3228	1/1	0.07	-	51,51,51,51	0
58	ZN	BY	501	1/1	0.13	-	51,51,51,51	0
56	MG	BA	3373	1/1	0.17	-	41,41,41,41	0
56	MG	DB	3003	1/1	0.10	-	29,29,29,29	0
56	MG	DA	3399	1/1	0.14	-	40,40,40,40	0
56	MG	BA	3615	1/1	0.11	-	42,42,42,42	0
56	MG	BA	3111	1/1	0.12	-	27,27,27,27	0
56	MG	DA	3267	1/1	0.04	-	47,47,47,47	0
56	MG	BA	3271	1/1	0.15	-	49,49,49,49	0
56	MG	CA	3134	1/1	0.17	-	53,53,53,53	0
56	MG	CA	3131	1/1	0.07	-	65,65,65,65	0
56	MG	CA	3151	1/1	0.14	-	50,50,50,50	0
56	MG	DA	3355	1/1	0.06	-	36,36,36,36	0
56	MG	DA	3484	1/1	0.13	-	34,34,34,34	0
56	MG	BD	308	1/1	0.15	-	35,35,35,35	0
56	MG	B9	502	1/1	0.34	-	41,41,41,41	0
56	MG	BA	3253	1/1	0.50	-	47,47,47,47	0
56	MG	CA	3063	1/1	0.16	-	53,53,53,53	0
56	MG	DW	3001	1/1	0.20	-	38,38,38,38	0
56	MG	AA	3103	1/1	0.12	-	51,51,51,51	0
56	MG	BA	3557	1/1	0.16	-	42,42,42,42	0
56	MG	DA	3417	1/1	0.14	-	40,40,40,40	0
56	MG	B0	103	1/1	0.10	-	33,33,33,33	0
56	MG	AE	3002	1/1	0.11	-	38,38,38,38	0
56	MG	BA	3432	1/1	0.12	-	37,37,37,37	0
56	MG	BA	3648	1/1	0.09	-	28,28,28,28	0
56	MG	AA	3044	1/1	0.20	-	50,50,50,50	0
56	MG	CA	3080	1/1	0.10	-	41,41,41,41	0
56	MG	BA	3363	1/1	0.20	-	29,29,29,29	0
56	MG	AA	3025	1/1	0.14	-	37,37,37,37	0
56	MG	AA	3153	1/1	0.16	-	50,50,50,50	0
56	MG	BA	3289	1/1	0.12	-	28,28,28,28	0
56	MG	BA	3391	1/1	0.09	-	37,37,37,37	0
56	MG	DA	3568	1/1	0.14	-	60,60,60,60	0
56	MG	DA	3029	1/1	0.09	-	40,40,40,40	0
56	MG	DA	3017	1/1	0.19	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3051	1/1	0.08	-	50,50,50,50	0
56	MG	BA	3650	1/1	0.11	-	31,31,31,31	0
56	MG	AA	3081	1/1	0.09	-	44,44,44,44	0
56	MG	BA	3524	1/1	0.10	-	57,57,57,57	0
56	MG	DE	3004	1/1	0.18	-	48,48,48,48	0
56	MG	BA	3181	1/1	0.12	-	37,37,37,37	0
56	MG	BA	3639	1/1	0.18	-	64,64,64,64	0
56	MG	BA	3451	1/1	0.07	-	48,48,48,48	0
56	MG	BA	3541	1/1	0.10	-	26,26,26,26	0
56	MG	BA	3041	1/1	0.11	-	42,42,42,42	0
56	MG	AA	3063	1/1	0.25	-	39,39,39,39	0
56	MG	BA	3659	1/1	0.13	-	28,28,28,28	0
56	MG	CA	3058	1/1	0.12	-	56,56,56,56	0
56	MG	CA	3043	1/1	0.17	-	60,60,60,60	0
56	MG	BA	3559	1/1	0.12	-	52,52,52,52	0
56	MG	BA	3198	1/1	0.09	-	34,34,34,34	0
56	MG	BD	304	1/1	0.17	-	28,28,28,28	0
56	MG	BA	3164	1/1	0.10	-	37,37,37,37	0
56	MG	BA	3472	1/1	0.11	-	34,34,34,34	0
56	MG	BA	3428	1/1	0.07	-	58,58,58,58	0
56	MG	DA	3580	1/1	0.14	-	58,58,58,58	0
56	MG	AA	3135	1/1	0.11	-	46,46,46,46	0
56	MG	BA	3139	1/1	0.14	-	31,31,31,31	0
56	MG	BA	3470	1/1	0.14	-	48,48,48,48	0
56	MG	B5	503	1/1	0.16	-	47,47,47,47	0
56	MG	DA	3085	1/1	0.10	-	40,40,40,40	0
58	ZN	D6	501	1/1	0.18	-	68,68,68,68	0
56	MG	B8	5001	1/1	0.12	-	36,36,36,36	0
56	MG	DA	3117	1/1	0.17	-	43,43,43,43	0
56	MG	BA	3506	1/1	0.08	-	39,39,39,39	0
56	MG	BA	3536	1/1	0.19	-	53,53,53,53	0
56	MG	BO	5001	1/1	0.12	-	62,62,62,62	0
56	MG	BA	3224	1/1	0.22	-	45,45,45,45	0
56	MG	BA	3669	1/1	0.20	-	29,29,29,29	0
56	MG	DA	3450	1/1	0.11	-	37,37,37,37	0
56	MG	CA	3098	1/1	0.17	-	42,42,42,42	0
56	MG	BA	3612	1/1	0.18	-	51,51,51,51	0
56	MG	CA	3026	1/1	0.16	-	44,44,44,44	0
56	MG	BA	3142	1/1	0.09	-	40,40,40,40	0
56	MG	CA	3140	1/1	0.21	-	61,61,61,61	0
56	MG	BA	3148	1/1	0.19	-	25,25,25,25	0
56	MG	DA	3408	1/1	0.13	-	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3036	1/1	0.07	-	38,38,38,38	0
56	MG	BA	3218	1/1	0.17	-	38,38,38,38	0
56	MG	DA	3492	1/1	0.09	-	44,44,44,44	0
56	MG	BA	3021	1/1	0.08	-	37,37,37,37	0
56	MG	CA	3016	1/1	0.14	-	68,68,68,68	0
56	MG	BA	3105	1/1	0.14	-	32,32,32,32	0
56	MG	AA	3173	1/1	0.12	-	32,32,32,32	0
56	MG	BE	304	1/1	0.14	-	13,13,13,13	0
56	MG	BA	3561	1/1	0.09	-	55,55,55,55	0
56	MG	DA	3307	1/1	0.17	-	53,53,53,53	0
56	MG	DA	3569	1/1	0.21	-	55,55,55,55	0
56	MG	DA	3046	1/1	0.23	-	34,34,34,34	0
56	MG	DA	3234	1/1	0.13	-	45,45,45,45	0
56	MG	AA	3016	1/1	0.21	-	49,49,49,49	0
56	MG	BA	3265	1/1	0.31	-	47,47,47,47	0
56	MG	DB	3006	1/1	0.12	-	55,55,55,55	0
56	MG	AA	3149	1/1	0.12	-	68,68,68,68	0
56	MG	BA	3331	1/1	0.18	-	59,59,59,59	0
56	MG	DA	3070	1/1	0.14	-	49,49,49,49	0
56	MG	BA	3279	1/1	0.09	-	38,38,38,38	0
56	MG	BA	3299	1/1	0.12	-	36,36,36,36	0
56	MG	DA	3096	1/1	0.10	-	29,29,29,29	0
56	MG	BA	3312	1/1	0.09	-	18,18,18,18	0
56	MG	BA	3565	1/1	0.12	-	51,51,51,51	0
56	MG	BA	3144	1/1	0.33	-	44,44,44,44	0
56	MG	AA	3047	1/1	0.12	-	45,45,45,45	0
56	MG	B0	101	1/1	0.13	-	71,71,71,71	0
56	MG	DA	3018	1/1	0.10	-	39,39,39,39	0
56	MG	CA	3002	1/1	0.09	-	43,43,43,43	0
56	MG	BA	3471	1/1	0.16	-	35,35,35,35	0
56	MG	BA	3183	1/1	0.26	-	35,35,35,35	0
56	MG	BA	3155	1/1	0.30	-	27,27,27,27	0
56	MG	BA	3562	1/1	0.09	-	46,46,46,46	0
56	MG	DA	3301	1/1	0.10	-	56,56,56,56	0
56	MG	AA	3030	1/1	0.08	-	47,47,47,47	0
56	MG	BA	3213	1/1	0.23	-	21,21,21,21	0
56	MG	DA	3582	1/1	0.16	-	38,38,38,38	0
56	MG	DA	3136	1/1	0.14	-	36,36,36,36	0
56	MG	DA	3552	1/1	0.18	-	49,49,49,49	0
56	MG	CA	3121	1/1	0.13	-	61,61,61,61	0
56	MG	D0	5001	1/1	0.05	-	39,39,39,39	0
56	MG	BA	3445	1/1	0.07	-	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3206	1/1	0.13	-	50,50,50,50	0
56	MG	DA	3080	1/1	0.17	-	29,29,29,29	0
56	MG	BA	3254	1/1	0.17	-	45,45,45,45	0
56	MG	DA	3555	1/1	0.12	-	51,51,51,51	0
56	MG	CA	3095	1/1	0.09	-	56,56,56,56	0
56	MG	DA	3243	1/1	0.09	-	50,50,50,50	0
56	MG	BA	3334	1/1	0.09	-	32,32,32,32	0
56	MG	AA	3014	1/1	0.10	-	49,49,49,49	0
56	MG	BA	3026	1/1	0.19	-	46,46,46,46	0
56	MG	BA	3061	1/1	0.24	-	44,44,44,44	0
56	MG	BA	3054	1/1	0.12	-	42,42,42,42	0
56	MG	DA	3123	1/1	0.11	-	51,51,51,51	0
56	MG	CA	3147	1/1	0.14	-	52,52,52,52	0
56	MG	BA	3490	1/1	0.10	-	38,38,38,38	0
56	MG	BA	3484	1/1	0.11	-	46,46,46,46	0
56	MG	DA	3273	1/1	0.18	-	31,31,31,31	0
56	MG	BA	3548	1/1	0.08	-	30,30,30,30	0
56	MG	BA	3496	1/1	0.17	-	31,31,31,31	0
56	MG	AA	3108	1/1	0.12	-	54,54,54,54	0
56	MG	AA	3166	1/1	0.13	-	53,53,53,53	0
56	MG	DA	3565	1/1	0.10	-	51,51,51,51	0
56	MG	DA	3328	1/1	0.17	-	48,48,48,48	0
56	MG	BA	3400	1/1	0.41	-	45,45,45,45	0
56	MG	DA	3135	1/1	0.16	-	47,47,47,47	0
56	MG	DA	3572	1/1	0.07	-	51,51,51,51	0
56	MG	BB	3008	1/1	0.17	-	21,21,21,21	0
56	MG	CA	3130	1/1	0.13	-	57,57,57,57	0
56	MG	DA	3156	1/1	0.08	-	38,38,38,38	0
56	MG	CA	3079	1/1	0.15	-	55,55,55,55	0
56	MG	BX	101	1/1	0.18	-	46,46,46,46	0
56	MG	BA	3056	1/1	0.13	-	46,46,46,46	0
56	MG	BA	3252	1/1	0.26	-	51,51,51,51	0
56	MG	BA	3017	1/1	0.14	-	40,40,40,40	0
56	MG	BA	3593	1/1	0.24	-	39,39,39,39	0
56	MG	CA	3061	1/1	0.10	-	45,45,45,45	0
56	MG	DA	3337	1/1	0.08	-	42,42,42,42	0
56	MG	DA	3140	1/1	0.08	-	37,37,37,37	0
56	MG	DA	3548	1/1	0.17	-	40,40,40,40	0
56	MG	DA	3462	1/1	0.11	-	35,35,35,35	0
56	MG	BA	3637	1/1	0.17	-	24,24,24,24	0
56	MG	DA	3348	1/1	0.12	-	25,25,25,25	0
56	MG	CA	3055	1/1	0.17	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3142	1/1	0.14	-	37,37,37,37	0
56	MG	CA	3032	1/1	0.12	-	68,68,68,68	0
56	MG	DA	3252	1/1	0.22	-	53,53,53,53	0
56	MG	DA	3092	1/1	0.19	-	45,45,45,45	0
56	MG	DA	3163	1/1	0.25	-	31,31,31,31	0
56	MG	DD	301	1/1	0.13	-	43,43,43,43	0
56	MG	DA	3574	1/1	0.11	-	56,56,56,56	0
56	MG	AX	3007	1/1	0.14	-	60,60,60,60	0
56	MG	DA	3440	1/1	0.14	-	52,52,52,52	0
56	MG	DB	3011	1/1	0.07	-	29,29,29,29	0
56	MG	BA	3039	1/1	0.09	-	31,31,31,31	0
56	MG	DA	3587	1/1	0.09	-	53,53,53,53	0
56	MG	BA	3270	1/1	0.13	-	21,21,21,21	0
56	MG	BA	3214	1/1	0.23	-	28,28,28,28	0
58	ZN	AN	501	1/1	0.14	-	67,67,67,67	0
56	MG	BA	3517	1/1	0.12	-	40,40,40,40	0
56	MG	AA	3126	1/1	0.08	-	54,54,54,54	0
56	MG	AA	3156	1/1	0.09	-	61,61,61,61	0
56	MG	BR	3003	1/1	0.12	-	39,39,39,39	0
56	MG	AA	3011	1/1	0.07	-	24,24,24,24	0
56	MG	BA	3631	1/1	0.12	-	41,41,41,41	0
56	MG	BA	3343	1/1	0.16	-	27,27,27,27	0
56	MG	DA	3158	1/1	0.17	-	36,36,36,36	0
56	MG	DA	3164	1/1	0.19	-	36,36,36,36	0
56	MG	DA	3055	1/1	0.09	-	34,34,34,34	0
56	MG	BA	3645	1/1	0.12	-	66,66,66,66	0
56	MG	CA	3087	1/1	0.11	-	33,33,33,33	0
56	MG	DA	3247	1/1	0.13	-	49,49,49,49	0
56	MG	AA	3116	1/1	0.15	-	51,51,51,51	0
56	MG	D5	502	1/1	0.44	-	36,36,36,36	0
56	MG	BA	3125	1/1	0.18	-	51,51,51,51	0
56	MG	CA	3025	1/1	0.09	-	48,48,48,48	0
56	MG	DA	3245	1/1	0.12	-	46,46,46,46	0
56	MG	BA	3016	1/1	0.12	-	50,50,50,50	0
56	MG	BA	3080	1/1	0.14	-	29,29,29,29	0
56	MG	BA	3491	1/1	0.10	-	39,39,39,39	0
56	MG	BA	3622	1/1	0.12	-	45,45,45,45	0
56	MG	BA	3387	1/1	0.24	-	49,49,49,49	0
56	MG	DA	3174	1/1	0.11	-	44,44,44,44	0
56	MG	CA	3152	1/1	0.16	-	75,75,75,75	0
56	MG	BA	3554	1/1	0.06	-	47,47,47,47	0
56	MG	DA	3109	1/1	0.13	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3137	1/1	0.10	-	37,37,37,37	0
56	MG	CA	3044	1/1	0.14	-	56,56,56,56	0
56	MG	BA	3067	1/1	0.12	-	34,34,34,34	0
56	MG	BA	3393	1/1	0.14	-	49,49,49,49	0
56	MG	AA	3056	1/1	0.14	-	69,69,69,69	0
56	MG	AA	3003	1/1	0.16	-	57,57,57,57	0
56	MG	BA	3458	1/1	0.06	-	60,60,60,60	0
56	MG	DA	3381	1/1	0.26	-	56,56,56,56	0
56	MG	AA	3037	1/1	0.12	-	51,51,51,51	0
56	MG	BA	3123	1/1	0.16	-	36,36,36,36	0
56	MG	DA	3409	1/1	0.19	-	53,53,53,53	0
56	MG	DA	3181	1/1	0.10	-	40,40,40,40	0
56	MG	AA	3117	1/1	0.08	-	47,47,47,47	0
56	MG	BA	3140	1/1	0.14	-	33,33,33,33	0
56	MG	BA	3282	1/1	0.22	-	31,31,31,31	0
56	MG	DA	3496	1/1	0.07	-	46,46,46,46	0
56	MG	CA	3014	1/1	0.12	-	39,39,39,39	0
56	MG	BA	3446	1/1	0.13	-	61,61,61,61	0
56	MG	BA	3330	1/1	0.24	-	44,44,44,44	0
56	MG	BA	3236	1/1	0.26	-	42,42,42,42	0
56	MG	DA	3358	1/1	0.21	-	45,45,45,45	0
56	MG	AL	201	1/1	0.08	-	63,63,63,63	0
56	MG	DA	3097	1/1	0.09	-	46,46,46,46	0
56	MG	AA	3138	1/1	0.10	-	50,50,50,50	0
59	K	AX	3001	1/1	0.06	-	48,48,48,48	0
56	MG	BA	3537	1/1	0.13	-	58,58,58,58	0
56	MG	BD	306	1/1	0.18	-	36,36,36,36	0
56	MG	DA	3404	1/1	0.10	-	46,46,46,46	0
56	MG	DA	3048	1/1	0.23	-	41,41,41,41	0
56	MG	CA	3128	1/1	0.08	-	39,39,39,39	0
56	MG	DA	3391	1/1	0.06	-	42,42,42,42	0
56	MG	DA	3291	1/1	0.07	-	38,38,38,38	0
56	MG	BA	3285	1/1	0.09	-	48,48,48,48	0
56	MG	BA	3204	1/1	0.18	-	35,35,35,35	0
56	MG	AA	3013	1/1	0.08	-	58,58,58,58	0
56	MG	BA	3211	1/1	0.27	-	29,29,29,29	0
56	MG	AA	3143	1/1	0.08	-	32,32,32,32	0
56	MG	BA	3114	1/1	0.19	-	34,34,34,34	0
56	MG	AA	3175	1/1	0.10	-	53,53,53,53	0
56	MG	BA	3599	1/1	0.13	-	46,46,46,46	0
56	MG	BA	3287	1/1	0.13	-	46,46,46,46	0
56	MG	CA	3106	1/1	0.19	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3076	1/1	0.10	-	43,43,43,43	0
56	MG	CA	3089	1/1	0.13	-	40,40,40,40	0
56	MG	CK	3001	1/1	0.13	-	50,50,50,50	0
56	MG	BA	3195	1/1	0.13	-	47,47,47,47	0
56	MG	CA	3054	1/1	0.09	-	44,44,44,44	0
56	MG	DA	3289	1/1	0.14	-	26,26,26,26	0
56	MG	DA	3011	1/1	0.13	-	38,38,38,38	0
56	MG	AA	3184	1/1	0.16	-	74,74,74,74	0
56	MG	CA	3137	1/1	0.13	-	66,66,66,66	0
56	MG	DA	3165	1/1	0.10	-	34,34,34,34	0
56	MG	DA	3401	1/1	0.06	-	55,55,55,55	0
56	MG	CA	3019	1/1	0.22	-	71,71,71,71	0
56	MG	DB	3007	1/1	0.17	-	38,38,38,38	0
56	MG	AA	3136	1/1	0.17	-	56,56,56,56	0
56	MG	AA	3036	1/1	0.07	-	41,41,41,41	0
56	MG	DA	3102	1/1	0.16	-	51,51,51,51	0
56	MG	DA	3280	1/1	0.12	-	50,50,50,50	0
56	MG	AA	3129	1/1	0.10	-	35,35,35,35	0
56	MG	BA	3571	1/1	0.15	-	50,50,50,50	0
56	MG	CA	3047	1/1	0.19	-	51,51,51,51	0
56	MG	CA	3046	1/1	0.07	-	41,41,41,41	0
56	MG	BA	3512	1/1	0.12	-	45,45,45,45	0
56	MG	BA	3267	1/1	0.15	-	40,40,40,40	0
56	MG	BA	3492	1/1	0.15	-	42,42,42,42	0
56	MG	BA	3029	1/1	0.13	-	12,12,12,12	0
56	MG	DA	3026	1/1	0.08	-	34,34,34,34	0
56	MG	AA	3035	1/1	0.17	-	65,65,65,65	0
56	MG	DA	3329	1/1	0.08	-	48,48,48,48	0
56	MG	BA	3382	1/1	0.13	-	27,27,27,27	0
56	MG	CA	3149	1/1	0.15	-	66,66,66,66	0
56	MG	BA	3305	1/1	0.16	-	28,28,28,28	0
56	MG	BA	3014	1/1	0.34	-	35,35,35,35	0
56	MG	AA	3121	1/1	0.09	-	40,40,40,40	0
56	MG	AA	3174	1/1	0.10	-	55,55,55,55	0
56	MG	DA	3272	1/1	0.09	-	57,57,57,57	0
56	MG	BA	3034	1/1	0.19	-	24,24,24,24	0
56	MG	DA	3334	1/1	0.11	-	24,24,24,24	0
56	MG	DA	3019	1/1	0.10	-	40,40,40,40	0
56	MG	BA	3510	1/1	0.20	-	25,25,25,25	0
56	MG	AA	3154	1/1	0.20	-	51,51,51,51	0
56	MG	AA	3020	1/1	0.16	-	49,49,49,49	0
56	MG	DA	3523	1/1	0.08	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3560	1/1	0.18	-	55,55,55,55	0
56	MG	BA	3585	1/1	0.16	-	50,50,50,50	0
56	MG	BA	3643	1/1	0.09	-	42,42,42,42	0
56	MG	AA	3111	1/1	0.22	-	45,45,45,45	0
56	MG	DV	3002	1/1	0.14	-	43,43,43,43	0
56	MG	BA	3141	1/1	0.10	-	45,45,45,45	0
56	MG	DA	3365	1/1	0.10	-	29,29,29,29	0
56	MG	DA	3579	1/1	0.07	-	54,54,54,54	0
56	MG	BA	3552	1/1	0.09	-	31,31,31,31	0
56	MG	AA	3060	1/1	0.16	-	55,55,55,55	0
56	MG	BA	3494	1/1	0.14	-	34,34,34,34	0
56	MG	BA	3335	1/1	0.10	-	40,40,40,40	0
56	MG	DF	302	1/1	0.34	-	41,41,41,41	0
56	MG	DA	3549	1/1	0.09	-	41,41,41,41	0
56	MG	BY	503	1/1	0.12	-	42,42,42,42	0
56	MG	BA	3157	1/1	0.16	-	34,34,34,34	0
56	MG	DA	3114	1/1	0.07	-	37,37,37,37	0
56	MG	BA	3241	1/1	0.29	-	26,26,26,26	0
56	MG	BA	3071	1/1	0.12	-	32,32,32,32	0
56	MG	BA	3461	1/1	0.38	-	52,52,52,52	0
56	MG	CA	3150	1/1	0.12	-	62,62,62,62	0
56	MG	DA	3356	1/1	0.07	-	31,31,31,31	0
56	MG	BA	3468	1/1	0.15	-	32,32,32,32	0
56	MG	CA	3059	1/1	0.13	-	58,58,58,58	0
56	MG	BA	3462	1/1	0.05	-	44,44,44,44	0
56	MG	DA	3466	1/1	0.10	-	38,38,38,38	0
56	MG	CA	3068	1/1	0.08	-	74,74,74,74	0
56	MG	AA	3132	1/1	0.21	-	50,50,50,50	0
56	MG	BA	3540	1/1	0.13	-	46,46,46,46	0
56	MG	DA	3350	1/1	0.12	-	36,36,36,36	0
56	MG	DA	3187	1/1	0.12	-	46,46,46,46	0
56	MG	BA	3606	1/1	0.12	-	32,32,32,32	0
56	MG	DA	3566	1/1	0.12	-	61,61,61,61	0
56	MG	BE	306	1/1	0.07	-	32,32,32,32	0
56	MG	CA	3031	1/1	0.13	-	52,52,52,52	0
56	MG	BA	3383	1/1	0.10	-	33,33,33,33	0
56	MG	CA	3135	1/1	0.09	-	62,62,62,62	0
56	MG	DA	3061	1/1	0.07	-	35,35,35,35	0
56	MG	AA	3179	1/1	0.15	-	63,63,63,63	0
56	MG	DA	3366	1/1	0.14	-	43,43,43,43	0
56	MG	BA	3638	1/1	0.08	-	32,32,32,32	0
56	MG	CA	3100	1/1	0.09	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3502	1/1	0.15	-	33,33,33,33	0
56	MG	BA	3309	1/1	0.13	-	32,32,32,32	0
56	MG	BA	3479	1/1	0.17	-	45,45,45,45	0
56	MG	BA	3151	1/1	0.09	-	34,34,34,34	0
56	MG	BA	3088	1/1	0.07	-	42,42,42,42	0
56	MG	AA	3127	1/1	0.04	-	68,68,68,68	0
56	MG	DA	3128	1/1	0.35	-	42,42,42,42	0
56	MG	DA	3422	1/1	0.09	-	63,63,63,63	0
56	MG	DA	3330	1/1	0.11	-	42,42,42,42	0
56	MG	BA	3126	1/1	0.10	-	45,45,45,45	0
56	MG	DA	3101	1/1	0.07	-	46,46,46,46	0
56	MG	DA	3281	1/1	0.14	-	56,56,56,56	0
56	MG	DA	3122	1/1	0.17	-	45,45,45,45	0
56	MG	DA	3463	1/1	0.14	-	28,28,28,28	0
56	MG	BA	3246	1/1	0.16	-	56,56,56,56	0
56	MG	AA	3114	1/1	0.14	-	56,56,56,56	0
56	MG	BA	3192	1/1	0.12	-	58,58,58,58	0
56	MG	BA	3153	1/1	0.20	-	39,39,39,39	0
56	MG	DA	3170	1/1	0.10	-	38,38,38,38	0
56	MG	DA	3049	1/1	0.10	-	40,40,40,40	0
56	MG	BA	3268	1/1	0.25	-	39,39,39,39	0
56	MG	BA	3457	1/1	0.13	-	29,29,29,29	0
56	MG	DA	3489	1/1	0.15	-	49,49,49,49	0
56	MG	DA	3322	1/1	0.16	-	23,23,23,23	0
56	MG	BA	3051	1/1	0.26	-	41,41,41,41	0
56	MG	BB	3005	1/1	0.24	-	30,30,30,30	0
56	MG	DG	3001	1/1	0.36	-	81,81,81,81	0
56	MG	DA	3258	1/1	0.17	-	49,49,49,49	0
56	MG	DA	3476	1/1	0.06	-	32,32,32,32	0
56	MG	DA	3352	1/1	0.10	-	45,45,45,45	0
56	MG	DA	3471	1/1	0.16	-	50,50,50,50	0
56	MG	DA	3389	1/1	0.11	-	42,42,42,42	0
56	MG	DA	3545	1/1	0.08	-	58,58,58,58	0
56	MG	BA	3654	1/1	0.16	-	64,64,64,64	0
56	MG	BA	3463	1/1	0.13	-	43,43,43,43	0
56	MG	BV	201	1/1	0.51	-	36,36,36,36	0
56	MG	DA	3421	1/1	0.14	-	52,52,52,52	0
56	MG	DA	3255	1/1	0.21	-	32,32,32,32	0
56	MG	BA	3621	1/1	0.13	-	30,30,30,30	0
56	MG	DA	3253	1/1	0.12	-	26,26,26,26	0
56	MG	BA	3120	1/1	0.20	-	44,44,44,44	0
56	MG	BA	3191	1/1	0.14	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BE	305	1/1	0.44	-	51,51,51,51	0
56	MG	BA	3322	1/1	0.11	-	40,40,40,40	0
56	MG	BA	3138	1/1	0.12	-	35,35,35,35	0
56	MG	DA	3113	1/1	0.09	-	41,41,41,41	0
56	MG	BA	3345	1/1	0.15	-	41,41,41,41	0
56	MG	BA	3197	1/1	0.13	-	19,19,19,19	0
56	MG	BH	3001	1/1	0.16	-	56,56,56,56	0
56	MG	BA	3569	1/1	0.18	-	55,55,55,55	0
56	MG	BA	3156	1/1	0.16	-	48,48,48,48	0
56	MG	DA	3444	1/1	0.16	-	53,53,53,53	0
56	MG	BP	202	1/1	0.47	-	31,31,31,31	0
56	MG	DA	3372	1/1	0.08	-	21,21,21,21	0
56	MG	BA	3405	1/1	0.14	-	26,26,26,26	0
56	MG	DA	3353	1/1	0.12	-	32,32,32,32	0
56	MG	DA	3148	1/1	0.26	-	47,47,47,47	0
56	MG	AA	3128	1/1	0.12	-	57,57,57,57	0
56	MG	DA	3319	1/1	0.18	-	38,38,38,38	0
56	MG	AA	3083	1/1	0.09	-	59,59,59,59	0
56	MG	DA	3428	1/1	0.18	-	33,33,33,33	0
56	MG	DA	3269	1/1	0.19	-	43,43,43,43	0
56	MG	DA	3359	1/1	0.13	-	43,43,43,43	0
56	MG	BA	3419	1/1	0.13	-	20,20,20,20	0
56	MG	BA	3131	1/1	0.24	-	36,36,36,36	0
56	MG	DA	3285	1/1	0.13	-	52,52,52,52	0
56	MG	DA	3229	1/1	0.16	-	38,38,38,38	0
56	MG	BA	3598	1/1	0.12	-	48,48,48,48	0
56	MG	CA	3037	1/1	0.07	-	45,45,45,45	0
56	MG	DR	202	1/1	0.15	-	32,32,32,32	0
56	MG	AA	3163	1/1	0.11	-	49,49,49,49	0
56	MG	BA	3097	1/1	0.10	-	53,53,53,53	0
56	MG	DA	3157	1/1	0.11	-	40,40,40,40	0
56	MG	DA	3560	1/1	0.16	-	51,51,51,51	0
56	MG	DA	3030	1/1	0.15	-	30,30,30,30	0
56	MG	DA	3208	1/1	0.08	-	43,43,43,43	0
56	MG	BA	3608	1/1	0.10	-	45,45,45,45	0
56	MG	AA	3139	1/1	0.09	-	36,36,36,36	0
56	MG	DA	3147	1/1	0.20	-	47,47,47,47	0
56	MG	BA	3368	1/1	0.08	-	42,42,42,42	0
56	MG	BA	3297	1/1	0.11	-	39,39,39,39	0
56	MG	D3	3001	1/1	0.75	-	70,70,70,70	0
56	MG	AA	3107	1/1	0.21	-	36,36,36,36	0
56	MG	CA	3072	1/1	0.21	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3185	1/1	0.16	-	32,32,32,32	0
56	MG	AA	3124	1/1	0.21	-	30,30,30,30	0
56	MG	BA	3129	1/1	0.14	-	42,42,42,42	0
56	MG	CA	3039	1/1	0.23	-	50,50,50,50	0
56	MG	BA	3627	1/1	0.10	-	54,54,54,54	0
56	MG	DB	3002	1/1	0.14	-	50,50,50,50	0
56	MG	AA	3140	1/1	0.11	-	31,31,31,31	0
56	MG	BA	3438	1/1	0.10	-	33,33,33,33	0
56	MG	BA	3588	1/1	0.11	-	51,51,51,51	0
56	MG	DA	3144	1/1	0.12	-	38,38,38,38	0
56	MG	DA	3537	1/1	0.10	-	47,47,47,47	0
56	MG	DA	3342	1/1	0.20	-	37,37,37,37	0
56	MG	DA	3538	1/1	0.11	-	39,39,39,39	0
56	MG	B0	102	1/1	0.29	-	42,42,42,42	0
56	MG	AA	3159	1/1	0.07	-	56,56,56,56	0
56	MG	AA	3031	1/1	0.07	-	60,60,60,60	0
56	MG	BA	3374	1/1	0.10	-	29,29,29,29	0
56	MG	CA	3082	1/1	0.13	-	62,62,62,62	0
56	MG	CA	3120	1/1	0.14	-	51,51,51,51	0
56	MG	BA	3108	1/1	0.12	-	38,38,38,38	0
56	MG	DA	3562	1/1	0.10	-	42,42,42,42	0
56	MG	DA	3095	1/1	0.31	-	47,47,47,47	0
56	MG	DA	3418	1/1	0.12	-	29,29,29,29	0
56	MG	BV	202	1/1	0.26	-	36,36,36,36	0
56	MG	BA	3453	1/1	0.07	-	27,27,27,27	0
56	MG	DA	3195	1/1	0.10	-	38,38,38,38	0
56	MG	DA	3543	1/1	0.06	-	63,63,63,63	0
56	MG	DA	3535	1/1	0.14	-	22,22,22,22	0
56	MG	AA	3071	1/1	0.14	-	36,36,36,36	0
56	MG	BA	3670	1/1	0.32	-	34,34,34,34	0
56	MG	DA	3224	1/1	0.16	-	22,22,22,22	0
56	MG	BA	3167	1/1	0.10	-	46,46,46,46	0
56	MG	BA	3442	1/1	0.12	-	20,20,20,20	0
56	MG	AD	502	1/1	0.17	-	55,55,55,55	0
56	MG	BA	3566	1/1	0.15	-	46,46,46,46	0
56	MG	BA	3460	1/1	0.11	-	57,57,57,57	0
56	MG	BA	3590	1/1	0.11	-	55,55,55,55	0
56	MG	BD	301	1/1	0.14	-	30,30,30,30	0
56	MG	BA	3132	1/1	0.14	-	25,25,25,25	0
56	MG	BA	3633	1/1	0.14	-	57,57,57,57	0
56	MG	DA	3213	1/1	0.08	-	34,34,34,34	0
56	MG	CA	3148	1/1	0.10	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	3029	1/1	0.10	-	52,52,52,52	0
56	MG	DA	3586	1/1	0.09	-	47,47,47,47	0
56	MG	BA	3062	1/1	0.17	-	46,46,46,46	0
56	MG	DA	3559	1/1	0.12	-	55,55,55,55	0
56	MG	DA	3083	1/1	0.07	-	48,48,48,48	0
56	MG	DA	3368	1/1	0.08	-	25,25,25,25	0
56	MG	AA	3064	1/1	0.15	-	45,45,45,45	0
56	MG	BA	3171	1/1	0.13	-	44,44,44,44	0
56	MG	BB	3001	1/1	0.12	-	36,36,36,36	0
56	MG	BA	3619	1/1	0.16	-	30,30,30,30	0
56	MG	BA	3404	1/1	0.16	-	38,38,38,38	0
56	MG	BA	3042	1/1	0.16	-	33,33,33,33	0
56	MG	AA	3113	1/1	0.18	-	53,53,53,53	0
56	MG	BA	3355	1/1	0.07	-	31,31,31,31	0
56	MG	BA	3219	1/1	0.10	-	20,20,20,20	0
56	MG	DA	3487	1/1	0.10	-	50,50,50,50	0
56	MG	AA	3152	1/1	0.13	-	57,57,57,57	0
56	MG	DA	3333	1/1	0.15	-	38,38,38,38	0
56	MG	BA	3303	1/1	0.11	-	31,31,31,31	0
56	MG	BA	3542	1/1	0.04	-	51,51,51,51	0
56	MG	BA	3110	1/1	0.21	-	31,31,31,31	0
56	MG	DA	3129	1/1	0.13	-	54,54,54,54	0
56	MG	DA	3556	1/1	0.15	-	36,36,36,36	0
56	MG	CA	3127	1/1	0.08	-	49,49,49,49	0
56	MG	DA	3227	1/1	0.15	-	49,49,49,49	0
56	MG	DA	3176	1/1	0.11	-	29,29,29,29	0
56	MG	BA	3023	1/1	0.13	-	40,40,40,40	0
56	MG	BA	3663	1/1	0.10	-	20,20,20,20	0
56	MG	DU	201	1/1	0.41	-	41,41,41,41	0
56	MG	DD	302	1/1	0.41	-	39,39,39,39	0
56	MG	CA	3048	1/1	0.28	-	52,52,52,52	0
56	MG	BA	3091	1/1	0.10	-	19,19,19,19	0
56	MG	BA	3292	1/1	0.10	-	43,43,43,43	0
56	MG	BA	3417	1/1	0.15	-	24,24,24,24	0
56	MG	BA	3286	1/1	0.11	-	32,32,32,32	0
56	MG	AA	3002	1/1	0.14	-	43,43,43,43	0
56	MG	DA	3023	1/1	0.12	-	37,37,37,37	0
56	MG	CA	3138	1/1	0.17	-	58,58,58,58	0
56	MG	DA	3160	1/1	0.18	-	44,44,44,44	0
56	MG	BA	3068	1/1	0.09	-	39,39,39,39	0
56	MG	BA	3115	1/1	0.12	-	34,34,34,34	0
56	MG	DA	3192	1/1	0.09	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3260	1/1	0.23	-	49,49,49,49	0
56	MG	BA	3040	1/1	0.12	-	43,43,43,43	0
56	MG	CA	3132	1/1	0.22	-	73,73,73,73	0
56	MG	BA	3367	1/1	0.18	-	49,49,49,49	0
56	MG	DA	3256	1/1	0.14	-	45,45,45,45	0
56	MG	DA	3075	1/1	0.17	-	41,41,41,41	0
56	MG	BA	3273	1/1	0.11	-	29,29,29,29	0
56	MG	CA	3076	1/1	0.25	-	48,48,48,48	0
56	MG	BA	3486	1/1	0.15	-	21,21,21,21	0
56	MG	BB	3006	1/1	0.15	-	49,49,49,49	0
56	MG	BA	3545	1/1	0.08	-	54,54,54,54	0
56	MG	CA	3007	1/1	0.09	-	50,50,50,50	0
56	MG	AA	3048	1/1	0.19	-	42,42,42,42	0
56	MG	BA	3212	1/1	0.17	-	28,28,28,28	0
56	MG	DA	3202	1/1	0.19	-	24,24,24,24	0
56	MG	BA	3664	1/1	0.14	-	30,30,30,30	0
56	MG	BA	3210	1/1	0.21	-	24,24,24,24	0
56	MG	DE	3001	1/1	0.18	-	43,43,43,43	0
56	MG	DA	3112	1/1	0.12	-	24,24,24,24	0
56	MG	AA	3066	1/1	0.17	-	46,46,46,46	0
56	MG	DA	3053	1/1	0.09	-	41,41,41,41	0
56	MG	BA	3209	1/1	0.14	-	26,26,26,26	0
56	MG	BA	3009	1/1	0.10	-	34,34,34,34	0
58	ZN	D5	501	1/1	0.14	-	67,67,67,67	0
56	MG	AA	3095	1/1	0.16	-	55,55,55,55	0
56	MG	BA	3127	1/1	0.15	-	45,45,45,45	0
56	MG	BA	3242	1/1	0.29	-	46,46,46,46	0
56	MG	AA	3122	1/1	0.13	-	58,58,58,58	0
56	MG	BA	3641	1/1	0.18	-	33,33,33,33	0
56	MG	BA	3099	1/1	0.24	-	32,32,32,32	0
56	MG	BA	3656	1/1	0.07	-	12,12,12,12	0
56	MG	BA	3500	1/1	0.12	-	35,35,35,35	0
56	MG	DA	3346	1/1	0.12	-	33,33,33,33	0
56	MG	AA	3161	1/1	0.10	-	66,66,66,66	0
56	MG	BA	3015	1/1	0.11	-	27,27,27,27	0
56	MG	BA	3394	1/1	0.18	-	35,35,35,35	0
56	MG	DA	3390	1/1	0.07	-	41,41,41,41	0
56	MG	DB	3010	1/1	0.15	-	60,60,60,60	0
56	MG	CA	3049	1/1	0.14	-	51,51,51,51	0
56	MG	DA	3461	1/1	0.17	-	33,33,33,33	0
56	MG	BA	3362	1/1	0.14	-	30,30,30,30	0
56	MG	BA	3563	1/1	0.17	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	3129	1/1	0.11	-	55,55,55,55	0
56	MG	DA	3159	1/1	0.17	-	31,31,31,31	0
56	MG	DA	3105	1/1	0.09	-	36,36,36,36	0
56	MG	BA	3020	1/1	0.12	-	33,33,33,33	0
56	MG	AA	3052	1/1	0.26	-	60,60,60,60	0
56	MG	BA	3280	1/1	0.12	-	48,48,48,48	0
56	MG	DA	3089	1/1	0.30	-	33,33,33,33	0
56	MG	DT	5001	1/1	0.06	-	42,42,42,42	0
56	MG	BA	3189	1/1	0.22	-	26,26,26,26	0
56	MG	BA	3522	1/1	0.09	-	52,52,52,52	0
56	MG	BA	3010	1/1	0.12	-	33,33,33,33	0
56	MG	BA	3501	1/1	0.11	-	44,44,44,44	0
56	MG	BA	3385	1/1	0.11	-	20,20,20,20	0
56	MG	BA	3180	1/1	0.20	-	33,33,33,33	0
56	MG	BA	3592	1/1	0.13	-	52,52,52,52	0
56	MG	AA	3157	1/1	0.07	-	55,55,55,55	0
56	MG	BA	3284	1/1	0.13	-	41,41,41,41	0
56	MG	BA	3613	1/1	0.17	-	45,45,45,45	0
56	MG	AA	3171	1/1	0.10	-	62,62,62,62	0
56	MG	BA	3344	1/1	0.12	-	35,35,35,35	0
56	MG	BA	3509	1/1	0.17	-	23,23,23,23	0
56	MG	AA	3092	1/1	0.18	-	61,61,61,61	0
56	MG	DA	3349	1/1	0.21	-	46,46,46,46	0
56	MG	DA	3271	1/1	0.09	-	55,55,55,55	0
56	MG	DA	3373	1/1	0.12	-	42,42,42,42	0
56	MG	CT	3001	1/1	0.09	-	50,50,50,50	0
56	MG	BA	3369	1/1	0.18	-	33,33,33,33	0
56	MG	BA	3420	1/1	0.09	-	24,24,24,24	0
57	SF4	CD	501	8/8	0.14	-	58,71,82,82	0
56	MG	DA	3133	1/1	0.10	-	53,53,53,53	0
56	MG	DA	3371	1/1	0.13	-	46,46,46,46	0
56	MG	DA	3106	1/1	0.05	-	43,43,43,43	0
56	MG	BA	3130	1/1	0.21	-	40,40,40,40	0
56	MG	BA	3245	1/1	0.17	-	27,27,27,27	0
56	MG	BA	3375	1/1	0.25	-	51,51,51,51	0
56	MG	DA	3378	1/1	0.15	-	31,31,31,31	0
56	MG	BA	3444	1/1	0.11	-	34,34,34,34	0
56	MG	CA	3028	1/1	0.11	-	52,52,52,52	0
56	MG	DA	3507	1/1	0.11	-	54,54,54,54	0
56	MG	DA	3478	1/1	0.12	-	53,53,53,53	0
56	MG	BA	3538	1/1	0.14	-	55,55,55,55	0
56	MG	DA	3518	1/1	0.21	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3524	1/1	0.12	-	51,51,51,51	0
56	MG	DA	3344	1/1	0.15	-	31,31,31,31	0
56	MG	BA	3386	1/1	0.21	-	32,32,32,32	0
56	MG	DA	3119	1/1	0.17	-	37,37,37,37	0
56	MG	BA	3098	1/1	0.14	-	56,56,56,56	0
56	MG	BA	3378	1/1	0.16	-	16,16,16,16	0
56	MG	CA	3038	1/1	0.09	-	44,44,44,44	0
56	MG	BA	3531	1/1	0.10	-	41,41,41,41	0
56	MG	DA	3121	1/1	0.47	-	50,50,50,50	0
56	MG	BA	3584	1/1	0.24	-	44,44,44,44	0
56	MG	BD	307	1/1	0.26	-	27,27,27,27	0
56	MG	CA	3041	1/1	0.12	-	67,67,67,67	0
56	MG	DA	3493	1/1	0.07	-	45,45,45,45	0
56	MG	DA	3323	1/1	0.12	-	35,35,35,35	0
56	MG	AA	3094	1/1	0.15	-	49,49,49,49	0
56	MG	BA	3353	1/1	0.09	-	39,39,39,39	0
56	MG	BA	3525	1/1	0.11	-	46,46,46,46	0
56	MG	AA	3093	1/1	0.20	-	45,45,45,45	0
56	MG	DA	3497	1/1	0.07	-	45,45,45,45	0
56	MG	BA	3337	1/1	0.12	-	37,37,37,37	0
56	MG	BA	3476	1/1	0.07	-	51,51,51,51	0
56	MG	BA	3259	1/1	0.15	-	35,35,35,35	0
56	MG	DA	3460	1/1	0.11	-	50,50,50,50	0
56	MG	AN	502	1/1	0.20	-	53,53,53,53	0
56	MG	DA	3477	1/1	0.11	-	42,42,42,42	0
56	MG	BA	3291	1/1	0.13	-	14,14,14,14	0
56	MG	BA	3564	1/1	0.15	-	29,29,29,29	0
56	MG	DA	3398	1/1	0.12	-	51,51,51,51	0
56	MG	AA	3123	1/1	0.16	-	38,38,38,38	0
56	MG	BA	3244	1/1	0.47	-	46,46,46,46	0
56	MG	CA	3042	1/1	0.19	-	56,56,56,56	0
56	MG	BA	3306	1/1	0.11	-	54,54,54,54	0
56	MG	AA	3005	1/1	0.17	-	37,37,37,37	0
56	MG	BA	3046	1/1	0.19	-	29,29,29,29	0
56	MG	BA	3338	1/1	0.12	-	48,48,48,48	0
56	MG	BA	3543	1/1	0.11	-	47,47,47,47	0
56	MG	CA	3104	1/1	0.16	-	74,74,74,74	0
56	MG	BA	3372	1/1	0.17	-	29,29,29,29	0
56	MG	AA	3057	1/1	0.29	-	67,67,67,67	0
56	MG	DV	3001	1/1	0.57	-	45,45,45,45	0
56	MG	BA	3314	1/1	0.20	-	36,36,36,36	0
56	MG	CA	3143	1/1	0.17	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3582	1/1	0.08	-	31,31,31,31	0
56	MG	CA	3013	1/1	0.13	-	53,53,53,53	0
56	MG	DA	3009	1/1	0.09	-	42,42,42,42	0
56	MG	DA	3149	1/1	0.29	-	41,41,41,41	0
56	MG	BA	3075	1/1	0.32	-	58,58,58,58	0
56	MG	CA	3040	1/1	0.27	-	52,52,52,52	0
56	MG	BA	3473	1/1	0.10	-	37,37,37,37	0
56	MG	DA	3485	1/1	0.12	-	60,60,60,60	0
56	MG	DA	3361	1/1	0.16	-	38,38,38,38	0
56	MG	BA	3443	1/1	0.10	-	44,44,44,44	0
56	MG	CA	3099	1/1	0.12	-	57,57,57,57	0
58	ZN	B9	501	1/1	0.14	-	45,45,45,45	0
56	MG	DQ	3002	1/1	0.15	-	38,38,38,38	0
56	MG	DA	3217	1/1	0.09	-	39,39,39,39	0
56	MG	CA	3009	1/1	0.17	-	55,55,55,55	0
56	MG	BF	304	1/1	0.19	-	37,37,37,37	0
56	MG	BA	3089	1/1	0.12	-	37,37,37,37	0
56	MG	DA	3103	1/1	0.08	-	56,56,56,56	0
56	MG	DA	3021	1/1	0.19	-	55,55,55,55	0
56	MG	DA	3010	1/1	0.13	-	36,36,36,36	0
56	MG	DA	3219	1/1	0.09	-	33,33,33,33	0
56	MG	DF	301	1/1	0.28	-	44,44,44,44	0
56	MG	BA	3076	1/1	0.07	-	29,29,29,29	0
56	MG	CA	3142	1/1	0.12	-	42,42,42,42	0
56	MG	BA	3464	1/1	0.08	-	41,41,41,41	0
56	MG	DA	3495	1/1	0.33	-	45,45,45,45	0
56	MG	BA	3163	1/1	0.11	-	31,31,31,31	0
56	MG	DR	201	1/1	0.16	-	36,36,36,36	0
56	MG	DA	3360	1/1	0.09	-	39,39,39,39	0
56	MG	DA	3161	1/1	0.13	-	24,24,24,24	0
56	MG	DA	3459	1/1	0.26	-	38,38,38,38	0
56	MG	BA	3441	1/1	0.12	-	44,44,44,44	0
56	MG	CA	3003	1/1	0.11	-	65,65,65,65	0
56	MG	DA	3246	1/1	0.37	-	38,38,38,38	0
56	MG	DA	3047	1/1	0.11	-	41,41,41,41	0
56	MG	DA	3194	1/1	0.11	-	47,47,47,47	0
56	MG	AA	3082	1/1	0.09	-	57,57,57,57	0
56	MG	DA	3073	1/1	0.12	-	51,51,51,51	0
56	MG	BA	3223	1/1	0.15	-	51,51,51,51	0
56	MG	DB	3005	1/1	0.21	-	56,56,56,56	0
56	MG	BA	3182	1/1	0.27	-	30,30,30,30	0
56	MG	BA	3187	1/1	0.13	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3369	1/1	0.11	-	45,45,45,45	0
56	MG	DA	3067	1/1	0.14	-	53,53,53,53	0
56	MG	AA	3119	1/1	0.12	-	57,57,57,57	0
56	MG	BA	3044	1/1	0.14	-	30,30,30,30	0
56	MG	CA	3077	1/1	0.11	-	44,44,44,44	0
56	MG	DA	3257	1/1	0.18	-	55,55,55,55	0
56	MG	DA	3482	1/1	0.09	-	46,46,46,46	0
56	MG	BW	3004	1/1	0.30	-	30,30,30,30	0
56	MG	BA	3415	1/1	0.22	-	54,54,54,54	0
56	MG	BA	3038	1/1	0.12	-	30,30,30,30	0
56	MG	BA	3480	1/1	0.21	-	43,43,43,43	0
56	MG	DA	3099	1/1	0.17	-	37,37,37,37	0
56	MG	DA	3347	1/1	0.13	-	41,41,41,41	0
56	MG	DA	3326	1/1	0.12	-	41,41,41,41	0
56	MG	CA	3067	1/1	0.07	-	63,63,63,63	0
56	MG	BA	3587	1/1	0.07	-	42,42,42,42	0
56	MG	CA	3083	1/1	0.19	-	66,66,66,66	0
56	MG	BA	3514	1/1	0.09	-	32,32,32,32	0
56	MG	DA	3594	1/1	0.12	-	48,48,48,48	0
56	MG	BA	3508	1/1	0.12	-	25,25,25,25	0
56	MG	BA	3336	1/1	0.09	-	43,43,43,43	0
56	MG	DA	3180	1/1	0.18	-	30,30,30,30	0
56	MG	CF	3001	1/1	0.09	-	45,45,45,45	0
56	MG	DA	3300	1/1	0.20	-	58,58,58,58	0
56	MG	BA	3555	1/1	0.14	-	42,42,42,42	0
56	MG	BQ	203	1/1	0.46	-	33,33,33,33	0
56	MG	BA	3002	1/1	0.14	-	39,39,39,39	0
56	MG	BE	301	1/1	0.07	-	45,45,45,45	0
56	MG	CA	3107	1/1	0.17	-	56,56,56,56	0
56	MG	BA	3225	1/1	0.09	-	31,31,31,31	0
56	MG	BA	3119	1/1	0.08	-	29,29,29,29	0
56	MG	BA	3326	1/1	0.17	-	28,28,28,28	0
56	MG	AA	3072	1/1	0.10	-	39,39,39,39	0
56	MG	BA	3359	1/1	0.13	-	54,54,54,54	0
56	MG	BA	3206	1/1	0.17	-	41,41,41,41	0
56	MG	DA	3207	1/1	0.11	-	39,39,39,39	0
56	MG	DA	3078	1/1	0.08	-	46,46,46,46	0
56	MG	BA	3134	1/1	0.28	-	40,40,40,40	0
56	MG	BA	3321	1/1	0.06	-	53,53,53,53	0
56	MG	AX	3003	1/1	0.28	-	50,50,50,50	0
56	MG	BA	3170	1/1	0.09	-	34,34,34,34	0
56	MG	CA	3109	1/1	0.12	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3583	1/1	0.08	-	43,43,43,43	0
56	MG	AA	3042	1/1	0.14	-	54,54,54,54	0
56	MG	DA	3225	1/1	0.16	-	33,33,33,33	0
56	MG	DA	3585	1/1	0.06	-	37,37,37,37	0
56	MG	AA	3167	1/1	0.16	-	73,73,73,73	0
56	MG	CA	3078	1/1	0.08	-	66,66,66,66	0
56	MG	CE	202	1/1	0.10	-	68,68,68,68	0
56	MG	DA	3068	1/1	0.13	-	35,35,35,35	0
56	MG	BA	3231	1/1	0.25	-	41,41,41,41	0
56	MG	DA	3199	1/1	0.09	-	52,52,52,52	0
56	MG	BA	3431	1/1	0.09	-	44,44,44,44	0
56	MG	BU	203	1/1	0.42	-	32,32,32,32	0
56	MG	DA	3124	1/1	0.12	-	29,29,29,29	0
56	MG	CA	3021	1/1	0.16	-	52,52,52,52	0
56	MG	DA	3241	1/1	0.14	-	36,36,36,36	0
56	MG	BA	3145	1/1	0.23	-	30,30,30,30	0
56	MG	AA	3185	1/1	0.05	-	64,64,64,64	0
56	MG	DA	3479	1/1	0.13	-	63,63,63,63	0
56	MG	DA	3502	1/1	0.12	-	39,39,39,39	0
56	MG	BA	3049	1/1	0.12	-	43,43,43,43	0
56	MG	BA	3573	1/1	0.18	-	44,44,44,44	0
56	MG	DA	3168	1/1	0.11	-	39,39,39,39	0
56	MG	DA	3544	1/1	0.15	-	51,51,51,51	0
56	MG	BA	3288	1/1	0.26	-	48,48,48,48	0
56	MG	CA	3144	1/1	0.13	-	56,56,56,56	0
56	MG	BA	3607	1/1	0.14	-	51,51,51,51	0
56	MG	BP	201	1/1	0.40	-	36,36,36,36	0
56	MG	BA	3086	1/1	0.16	-	39,39,39,39	0
56	MG	BF	302	1/1	0.06	-	45,45,45,45	0
56	MG	AA	3033	1/1	0.31	-	48,48,48,48	0
56	MG	DA	3400	1/1	0.16	-	38,38,38,38	0
56	MG	AA	3177	1/1	0.11	-	32,32,32,32	0
56	MG	BA	3519	1/1	0.13	-	53,53,53,53	0
56	MG	DA	3448	1/1	0.20	-	29,29,29,29	0
56	MG	BA	3035	1/1	0.19	-	21,21,21,21	0
56	MG	BA	3403	1/1	0.10	-	18,18,18,18	0
56	MG	BA	3489	1/1	0.26	-	41,41,41,41	0
56	MG	DA	3298	1/1	0.12	-	32,32,32,32	0
56	MG	DA	3526	1/1	0.07	-	64,64,64,64	0
56	MG	BA	3012	1/1	0.15	-	39,39,39,39	0
56	MG	BA	3673	1/1	0.08	-	37,37,37,37	0
56	MG	BA	3620	1/1	0.14	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3675	1/1	0.39	-	33,33,33,33	0
56	MG	BA	3346	1/1	0.08	-	43,43,43,43	0
56	MG	DA	3054	1/1	0.25	-	45,45,45,45	0
56	MG	CA	3086	1/1	0.11	-	68,68,68,68	0
56	MG	BB	3013	1/1	0.14	-	57,57,57,57	0
56	MG	BA	3352	1/1	0.11	-	32,32,32,32	0
56	MG	DA	3186	1/1	0.14	-	41,41,41,41	0
56	MG	BA	3220	1/1	0.13	-	31,31,31,31	0
56	MG	DA	3465	1/1	0.12	-	38,38,38,38	0
58	ZN	DY	501	1/1	0.11	-	92,92,92,92	0
56	MG	DA	3295	1/1	0.17	-	61,61,61,61	0
56	MG	AA	3084	1/1	0.07	-	43,43,43,43	0
56	MG	BA	3176	1/1	0.10	-	47,47,47,47	0
56	MG	DW	3002	1/1	0.35	-	60,60,60,60	0
56	MG	DA	3503	1/1	0.08	-	38,38,38,38	0
56	MG	BA	3074	1/1	0.11	-	45,45,45,45	0
56	MG	BA	3425	1/1	0.25	-	53,53,53,53	0
56	MG	DA	3592	1/1	0.64	-	52,52,52,52	0
56	MG	BA	3013	1/1	0.12	-	35,35,35,35	0
56	MG	CA	3084	1/1	0.11	-	72,72,72,72	0
56	MG	DA	3288	1/1	0.14	-	64,64,64,64	0
56	MG	CA	3136	1/1	0.13	-	53,53,53,53	0
56	MG	BA	3208	1/1	0.22	-	25,25,25,25	0
56	MG	DA	3248	1/1	0.27	-	52,52,52,52	0
56	MG	AA	3010	1/1	0.15	-	60,60,60,60	0
56	MG	DA	3151	1/1	0.12	-	34,34,34,34	0
56	MG	DA	3315	1/1	0.15	-	43,43,43,43	0
56	MG	BA	3166	1/1	0.10	-	35,35,35,35	0
56	MG	CA	3102	1/1	0.18	-	30,30,30,30	0
56	MG	BA	3172	1/1	0.12	-	54,54,54,54	0
56	MG	DA	3263	1/1	0.11	-	39,39,39,39	0
56	MG	BA	3175	1/1	0.13	-	33,33,33,33	0
56	MG	DA	3341	1/1	0.14	-	25,25,25,25	0
56	MG	BA	3406	1/1	0.19	-	39,39,39,39	0
56	MG	CA	3141	1/1	0.17	-	54,54,54,54	0
56	MG	BA	3632	1/1	0.14	-	54,54,54,54	0
56	MG	BA	3662	1/1	0.19	-	36,36,36,36	0
56	MG	BA	3250	1/1	0.32	-	33,33,33,33	0
56	MG	BA	3053	1/1	0.18	-	31,31,31,31	0
56	MG	DA	3251	1/1	0.16	-	62,62,62,62	0
56	MG	DA	3429	1/1	0.13	-	35,35,35,35	0
56	MG	DA	3387	1/1	0.05	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3130	1/1	0.25	-	47,47,47,47	0
56	MG	BA	3657	1/1	0.12	-	24,24,24,24	0
56	MG	BB	3012	1/1	0.12	-	44,44,44,44	0
56	MG	BA	3087	1/1	0.17	-	36,36,36,36	0
56	MG	AA	3061	1/1	0.13	-	62,62,62,62	0
56	MG	BA	3032	1/1	0.21	-	40,40,40,40	0
56	MG	BA	3597	1/1	0.09	-	43,43,43,43	0
56	MG	BA	3281	1/1	0.21	-	51,51,51,51	0
56	MG	BB	3017	1/1	0.07	-	40,40,40,40	0
56	MG	AA	3026	1/1	0.12	-	40,40,40,40	0
56	MG	AA	3162	1/1	0.11	-	40,40,40,40	0
56	MG	DA	3166	1/1	0.14	-	35,35,35,35	0
56	MG	BA	3413	1/1	0.15	-	26,26,26,26	0
56	MG	DA	3193	1/1	0.15	-	49,49,49,49	0
56	MG	BY	502	1/1	0.17	-	35,35,35,35	0
56	MG	BA	3272	1/1	0.07	-	37,37,37,37	0
56	MG	CA	3122	1/1	0.24	-	54,54,54,54	0
56	MG	BA	3063	1/1	0.09	-	47,47,47,47	0
56	MG	AX	3005	1/1	0.22	-	42,42,42,42	0
56	MG	DA	3405	1/1	0.14	-	45,45,45,45	0
56	MG	DA	3276	1/1	0.15	-	50,50,50,50	0
56	MG	BA	3547	1/1	0.04	-	60,60,60,60	0
56	MG	DQ	3001	1/1	0.17	-	48,48,48,48	0
56	MG	AA	3085	1/1	0.13	-	63,63,63,63	0
56	MG	BA	3488	1/1	0.28	-	36,36,36,36	0
56	MG	BA	3634	1/1	0.34	-	41,41,41,41	0
56	MG	DA	3274	1/1	0.10	-	56,56,56,56	0
56	MG	BA	3073	1/1	0.16	-	14,14,14,14	0
56	MG	DA	3433	1/1	0.17	-	33,33,33,33	0
56	MG	BA	3384	1/1	0.12	-	28,28,28,28	0
56	MG	BA	3421	1/1	0.11	-	36,36,36,36	0
56	MG	DA	3090	1/1	0.08	-	54,54,54,54	0
56	MG	BA	3347	1/1	0.09	-	53,53,53,53	0
56	MG	CA	3074	1/1	0.17	-	48,48,48,48	0
56	MG	DA	3385	1/1	0.07	-	45,45,45,45	0
56	MG	BA	3499	1/1	0.13	-	35,35,35,35	0
56	MG	DA	3132	1/1	0.12	-	35,35,35,35	0
56	MG	BB	3007	1/1	0.14	-	35,35,35,35	0
56	MG	BA	3591	1/1	0.07	-	36,36,36,36	0
56	MG	AA	3090	1/1	0.18	-	28,28,28,28	0
56	MG	DA	3514	1/1	0.04	-	40,40,40,40	0
56	MG	BA	3483	1/1	0.13	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3203	1/1	0.12	-	35,35,35,35	0
56	MG	BA	3118	1/1	0.23	-	45,45,45,45	0
56	MG	CX	101	1/1	0.23	-	48,48,48,48	0
56	MG	BA	3298	1/1	0.11	-	28,28,28,28	0
56	MG	BA	3025	1/1	0.11	-	37,37,37,37	0
56	MG	AA	3089	1/1	0.13	-	36,36,36,36	0
56	MG	DA	3139	1/1	0.19	-	39,39,39,39	0
56	MG	BA	3277	1/1	0.20	-	32,32,32,32	0
56	MG	BA	3257	1/1	0.08	-	29,29,29,29	0
56	MG	AA	3017	1/1	0.17	-	63,63,63,63	0
56	MG	CA	3085	1/1	0.10	-	52,52,52,52	0
56	MG	BA	3504	1/1	0.17	-	39,39,39,39	0
56	MG	BA	3028	1/1	0.15	-	41,41,41,41	0
56	MG	DB	3012	1/1	0.12	-	53,53,53,53	0
56	MG	BA	3371	1/1	0.16	-	25,25,25,25	0
56	MG	DA	3335	1/1	0.15	-	36,36,36,36	0
56	MG	DA	3420	1/1	0.14	-	46,46,46,46	0
56	MG	DA	3214	1/1	0.18	-	30,30,30,30	0
56	MG	DA	3282	1/1	0.11	-	30,30,30,30	0
56	MG	DA	3200	1/1	0.08	-	28,28,28,28	0
56	MG	BA	3137	1/1	0.27	-	30,30,30,30	0
56	MG	CA	3024	1/1	0.08	-	64,64,64,64	0
56	MG	DB	3001	1/1	0.18	-	40,40,40,40	0
56	MG	DA	3306	1/1	0.14	-	38,38,38,38	0
56	MG	BA	3003	1/1	0.08	-	49,49,49,49	0
56	MG	DA	3310	1/1	0.08	-	41,41,41,41	0
56	MG	BA	3301	1/1	0.13	-	46,46,46,46	0
56	MG	AA	3130	1/1	0.10	-	50,50,50,50	0
56	MG	BA	3535	1/1	0.08	-	47,47,47,47	0
56	MG	AA	3038	1/1	0.11	-	53,53,53,53	0
56	MG	BA	3465	1/1	0.09	-	37,37,37,37	0
56	MG	AA	3187	1/1	0.11	-	33,33,33,33	0
56	MG	BA	3426	1/1	0.11	-	43,43,43,43	0
56	MG	AA	3079	1/1	0.32	-	49,49,49,49	0
56	MG	DA	3093	1/1	0.17	-	46,46,46,46	0
56	MG	BA	3234	1/1	0.14	-	57,57,57,57	0
56	MG	BA	3392	1/1	0.15	-	41,41,41,41	0
56	MG	DA	3006	1/1	0.12	-	33,33,33,33	0
56	MG	DA	3541	1/1	0.11	-	57,57,57,57	0
56	MG	BA	3311	1/1	0.15	-	39,39,39,39	0
56	MG	BA	3402	1/1	0.23	-	28,28,28,28	0
56	MG	DA	3279	1/1	0.11	-	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3260	1/1	0.20	-	36,36,36,36	0
56	MG	DA	3031	1/1	0.09	-	21,21,21,21	0
56	MG	BA	3636	1/1	0.08	-	32,32,32,32	0
56	MG	AA	3165	1/1	0.10	-	43,43,43,43	0
56	MG	BA	3348	1/1	0.13	-	31,31,31,31	0
56	MG	DA	3486	1/1	0.19	-	37,37,37,37	0
56	MG	CA	3088	1/1	0.10	-	41,41,41,41	0
56	MG	BA	3184	1/1	0.08	-	37,37,37,37	0
56	MG	AX	3008	1/1	0.15	-	23,23,23,23	0
56	MG	BA	3617	1/1	0.18	-	66,66,66,66	0
56	MG	DA	3125	1/1	0.12	-	47,47,47,47	0
56	MG	DA	3563	1/1	0.12	-	60,60,60,60	0
56	MG	BA	3323	1/1	0.06	-	61,61,61,61	0
56	MG	BA	3258	1/1	0.20	-	30,30,30,30	0
56	MG	DY	502	1/1	0.11	-	51,51,51,51	0
56	MG	BA	3412	1/1	0.17	-	48,48,48,48	0
56	MG	DA	3107	1/1	0.15	-	46,46,46,46	0
56	MG	DA	3467	1/1	0.10	-	47,47,47,47	0
56	MG	BA	3300	1/1	0.17	-	39,39,39,39	0
56	MG	AA	3004	1/1	0.15	-	67,67,67,67	0
58	ZN	D4	501	1/1	0.05	-	141,141,141,141	0
56	MG	DA	3039	1/1	0.25	-	51,51,51,51	0
56	MG	BA	3226	1/1	0.61	-	32,32,32,32	0
56	MG	BA	3520	1/1	0.12	-	24,24,24,24	0
56	MG	DA	3209	1/1	0.16	-	38,38,38,38	0
56	MG	DA	3340	1/1	0.09	-	47,47,47,47	0
56	MG	DA	3343	1/1	0.17	-	56,56,56,56	0
56	MG	CA	3146	1/1	0.07	-	42,42,42,42	0
56	MG	BA	3128	1/1	0.20	-	29,29,29,29	0
56	MG	AA	3024	1/1	0.16	-	60,60,60,60	0
56	MG	DA	3324	1/1	0.14	-	52,52,52,52	0
56	MG	DA	3297	1/1	0.14	-	38,38,38,38	0
56	MG	BA	3117	1/1	0.44	-	40,40,40,40	0
56	MG	CJ	5001	1/1	0.19	-	60,60,60,60	0
56	MG	BA	3518	1/1	0.15	-	41,41,41,41	0
56	MG	DA	3554	1/1	0.06	-	68,68,68,68	0
56	MG	BA	3228	1/1	0.12	-	40,40,40,40	0
56	MG	BA	3024	1/1	0.26	-	32,32,32,32	0
56	MG	BA	3328	1/1	0.13	-	39,39,39,39	0
56	MG	BD	303	1/1	0.41	-	37,37,37,37	0
56	MG	BA	3603	1/1	0.04	-	49,49,49,49	0
56	MG	DA	3141	1/1	0.08	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3184	1/1	0.20	-	30,30,30,30	0
56	MG	BU	201	1/1	0.30	-	32,32,32,32	0
56	MG	BA	3429	1/1	0.18	-	41,41,41,41	0
56	MG	BA	3256	1/1	0.23	-	41,41,41,41	0
56	MG	DA	3513	1/1	0.11	-	32,32,32,32	0
56	MG	DA	3427	1/1	0.14	-	25,25,25,25	0
56	MG	DA	3302	1/1	0.11	-	43,43,43,43	0
56	MG	BA	3579	1/1	0.15	-	46,46,46,46	0
56	MG	DA	3212	1/1	0.15	-	39,39,39,39	0
56	MG	DA	3190	1/1	0.17	-	34,34,34,34	0
56	MG	AA	3050	1/1	0.10	-	24,24,24,24	0
56	MG	DA	3262	1/1	0.10	-	39,39,39,39	0
56	MG	BA	3469	1/1	0.15	-	28,28,28,28	0
56	MG	BA	3302	1/1	0.11	-	55,55,55,55	0
56	MG	BA	3069	1/1	0.10	-	47,47,47,47	0
56	MG	BA	3243	1/1	0.15	-	45,45,45,45	0
56	MG	DA	3406	1/1	0.11	-	50,50,50,50	0
56	MG	CA	3073	1/1	0.10	-	57,57,57,57	0
56	MG	DA	3481	1/1	0.09	-	41,41,41,41	0
56	MG	CA	3033	1/1	0.09	-	52,52,52,52	0
56	MG	DA	3357	1/1	0.10	-	33,33,33,33	0
56	MG	CA	3096	1/1	0.14	-	61,61,61,61	0
56	MG	BA	3653	1/1	0.13	-	33,33,33,33	0
56	MG	DB	3004	1/1	0.16	-	36,36,36,36	0
56	MG	DA	3004	1/1	0.17	-	51,51,51,51	0
56	MG	DA	3022	1/1	0.12	-	39,39,39,39	0
56	MG	BA	3605	1/1	0.18	-	46,46,46,46	0
56	MG	BD	305	1/1	0.12	-	38,38,38,38	0
56	MG	BA	3388	1/1	0.06	-	54,54,54,54	0
56	MG	DA	3488	1/1	0.18	-	41,41,41,41	0
56	MG	DA	3012	1/1	0.10	-	30,30,30,30	0
56	MG	BA	3077	1/1	0.14	-	37,37,37,37	0
56	MG	CA	3018	1/1	0.12	-	43,43,43,43	0
56	MG	DA	3064	1/1	0.10	-	48,48,48,48	0
56	MG	BA	3248	1/1	0.20	-	21,21,21,21	0
56	MG	CA	3064	1/1	0.11	-	60,60,60,60	0
56	MG	BA	3503	1/1	0.14	-	30,30,30,30	0
56	MG	D7	101	1/1	0.66	-	51,51,51,51	0
56	MG	BA	3407	1/1	0.13	-	43,43,43,43	0
56	MG	DA	3534	1/1	0.12	-	54,54,54,54	0
56	MG	DA	3577	1/1	0.14	-	35,35,35,35	0
56	MG	DA	3332	1/1	0.08	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3595	1/1	0.10	-	47,47,47,47	0
56	MG	DA	3034	1/1	0.12	-	46,46,46,46	0
56	MG	AA	3076	1/1	0.17	-	52,52,52,52	0
56	MG	DA	3226	1/1	0.10	-	27,27,27,27	0
56	MG	BD	302	1/1	0.41	-	45,45,45,45	0
56	MG	BA	3082	1/1	0.28	-	47,47,47,47	0
56	MG	BA	3527	1/1	0.12	-	40,40,40,40	0
56	MG	DA	3179	1/1	0.13	-	20,20,20,20	0
56	MG	DA	3442	1/1	0.21	-	42,42,42,42	0
56	MG	DA	3127	1/1	0.19	-	41,41,41,41	0
56	MG	DA	3588	1/1	0.14	-	21,21,21,21	0
56	MG	AA	3100	1/1	0.10	-	35,35,35,35	0
56	MG	DA	3516	1/1	0.09	-	61,61,61,61	0
56	MG	DA	3183	1/1	0.07	-	37,37,37,37	0
56	MG	BA	3635	1/1	0.14	-	63,63,63,63	0
56	MG	BA	3112	1/1	0.19	-	40,40,40,40	0
56	MG	DA	3188	1/1	0.12	-	25,25,25,25	0
56	MG	DA	3204	1/1	0.06	-	37,37,37,37	0
56	MG	CA	3118	1/1	0.09	-	78,78,78,78	0
56	MG	DA	3531	1/1	0.11	-	69,69,69,69	0
56	MG	DA	3393	1/1	0.09	-	48,48,48,48	0
56	MG	DA	3411	1/1	0.07	-	36,36,36,36	0
56	MG	AA	3086	1/1	0.23	-	61,61,61,61	0
56	MG	BA	3578	1/1	0.15	-	59,59,59,59	0
56	MG	BA	3269	1/1	0.08	-	34,34,34,34	0
56	MG	BA	3136	1/1	0.18	-	44,44,44,44	0
56	MG	DA	3014	1/1	0.08	-	33,33,33,33	0
56	MG	DA	3511	1/1	0.06	-	53,53,53,53	0
56	MG	BB	3011	1/1	0.07	-	45,45,45,45	0
56	MG	DA	3318	1/1	0.10	-	43,43,43,43	0
56	MG	BA	3093	1/1	0.18	-	40,40,40,40	0
56	MG	BZ	3001	1/1	0.31	-	58,58,58,58	0
56	MG	DA	3043	1/1	0.11	-	30,30,30,30	0
56	MG	DA	3382	1/1	0.13	-	50,50,50,50	0
56	MG	AA	3155	1/1	0.07	-	61,61,61,61	0
56	MG	BA	3263	1/1	0.22	-	64,64,64,64	0
56	MG	BA	3625	1/1	0.14	-	25,25,25,25	0
56	MG	AA	3069	1/1	0.11	-	50,50,50,50	0
56	MG	DA	3077	1/1	0.09	-	34,34,34,34	0
56	MG	DP	3001	1/1	0.23	-	44,44,44,44	0
56	MG	DA	3402	1/1	0.09	-	63,63,63,63	0
56	MG	AA	3150	1/1	0.18	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	3059	1/1	0.08	-	54,54,54,54	0
58	ZN	D9	501	1/1	0.07	-	54,54,54,54	0
56	MG	BA	3658	1/1	0.09	-	27,27,27,27	0
56	MG	DA	3250	1/1	0.10	-	37,37,37,37	0
56	MG	CA	3113	1/1	0.14	-	57,57,57,57	0
56	MG	BA	3106	1/1	0.11	-	40,40,40,40	0
56	MG	BA	3278	1/1	0.11	-	50,50,50,50	0
56	MG	DA	3416	1/1	0.14	-	44,44,44,44	0
56	MG	BA	3122	1/1	0.39	-	39,39,39,39	0
56	MG	DQ	3003	1/1	0.17	-	50,50,50,50	0
56	MG	DA	3414	1/1	0.04	-	42,42,42,42	0
56	MG	BA	3290	1/1	0.13	-	36,36,36,36	0
56	MG	BA	3150	1/1	0.12	-	32,32,32,32	0
58	ZN	B6	501	1/1	0.14	-	45,45,45,45	0
56	MG	DA	3447	1/1	0.07	-	33,33,33,33	0
56	MG	DA	3527	1/1	0.12	-	43,43,43,43	0
56	MG	BA	3221	1/1	0.25	-	41,41,41,41	0
56	MG	DA	3452	1/1	0.13	-	56,56,56,56	0
56	MG	BA	3666	1/1	0.36	-	35,35,35,35	0
56	MG	DA	3278	1/1	0.14	-	50,50,50,50	0
56	MG	BA	3085	1/1	0.17	-	27,27,27,27	0
56	MG	BA	3516	1/1	0.13	-	43,43,43,43	0
56	MG	DA	3041	1/1	0.08	-	35,35,35,35	0
56	MG	BA	3177	1/1	0.13	-	44,44,44,44	0
56	MG	DA	3189	1/1	0.26	-	31,31,31,31	0
56	MG	DA	3175	1/1	0.14	-	47,47,47,47	0
56	MG	BA	3589	1/1	0.13	-	27,27,27,27	0
56	MG	BA	3325	1/1	0.14	-	42,42,42,42	0
56	MG	AA	3023	1/1	0.20	-	71,71,71,71	0
56	MG	DA	3050	1/1	0.09	-	41,41,41,41	0
56	MG	DA	3203	1/1	0.15	-	21,21,21,21	0
56	MG	CA	3001	1/1	0.06	-	72,72,72,72	0
56	MG	BA	3414	1/1	0.15	-	31,31,31,31	0
56	MG	DA	3172	1/1	0.10	-	35,35,35,35	0
56	MG	DA	3221	1/1	0.10	-	33,33,33,33	0
56	MG	BA	3102	1/1	0.09	-	49,49,49,49	0
56	MG	BA	3437	1/1	0.13	-	58,58,58,58	0
56	MG	DA	3015	1/1	0.30	-	41,41,41,41	0
56	MG	AA	3120	1/1	0.14	-	47,47,47,47	0
56	MG	DA	3223	1/1	0.13	-	47,47,47,47	0
58	ZN	B4	501	1/1	0.06	-	106,106,106,106	0
56	MG	BA	3264	1/1	0.15	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3354	1/1	0.17	-	51,51,51,51	0
56	MG	DA	3508	1/1	0.09	-	38,38,38,38	0
56	MG	BA	3550	1/1	0.19	-	44,44,44,44	0
56	MG	DA	3091	1/1	0.19	-	45,45,45,45	0
56	MG	CA	3034	1/1	0.12	-	67,67,67,67	0
56	MG	BA	3135	1/1	0.12	-	36,36,36,36	0
56	MG	DA	3236	1/1	0.10	-	47,47,47,47	0
56	MG	DA	3386	1/1	0.08	-	48,48,48,48	0
56	MG	CA	3071	1/1	0.24	-	51,51,51,51	0
56	MG	DA	3363	1/1	0.07	-	36,36,36,36	0
56	MG	DA	3509	1/1	0.08	-	36,36,36,36	0
56	MG	DA	3564	1/1	0.07	-	36,36,36,36	0
56	MG	BA	3001	1/1	0.13	-	35,35,35,35	0
56	MG	DA	3596	1/1	0.31	-	54,54,54,54	0
56	MG	DA	3576	1/1	0.14	-	36,36,36,36	0
56	MG	DA	3392	1/1	0.12	-	54,54,54,54	0
56	MG	DA	3268	1/1	0.17	-	38,38,38,38	0
56	MG	BA	3454	1/1	0.15	-	21,21,21,21	0
56	MG	DA	3275	1/1	0.12	-	45,45,45,45	0
56	MG	DA	3087	1/1	0.17	-	35,35,35,35	0
56	MG	DA	3233	1/1	0.27	-	36,36,36,36	0
56	MG	DA	3499	1/1	0.10	-	45,45,45,45	0
56	MG	BA	3649	1/1	0.13	-	50,50,50,50	0
56	MG	BA	3456	1/1	0.13	-	33,33,33,33	0
56	MG	BA	3497	1/1	0.13	-	34,34,34,34	0
56	MG	DA	3446	1/1	0.09	-	46,46,46,46	0
56	MG	CA	3065	1/1	0.07	-	55,55,55,55	0
56	MG	CA	3053	1/1	0.15	-	44,44,44,44	0
56	MG	BA	3216	1/1	0.27	-	33,33,33,33	0
56	MG	DA	3069	1/1	0.11	-	35,35,35,35	0
56	MG	CA	3126	1/1	0.20	-	73,73,73,73	0
56	MG	BB	3009	1/1	0.11	-	67,67,67,67	0
56	MG	CA	3051	1/1	0.14	-	66,66,66,66	0
56	MG	DA	3198	1/1	0.15	-	54,54,54,54	0
56	MG	BA	3043	1/1	0.15	-	36,36,36,36	0
56	MG	DA	3100	1/1	0.13	-	34,34,34,34	0
56	MG	AA	3088	1/1	0.22	-	62,62,62,62	0
56	MG	DA	3530	1/1	0.09	-	60,60,60,60	0
56	MG	BA	3018	1/1	0.23	-	47,47,47,47	0
56	MG	BU	205	1/1	0.40	-	53,53,53,53	0
56	MG	AA	3168	1/1	0.08	-	56,56,56,56	0
56	MG	BA	3511	1/1	0.13	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3028	1/1	0.36	-	47,47,47,47	0
56	MG	BA	3094	1/1	0.24	-	45,45,45,45	0
56	MG	CA	3097	1/1	0.18	-	67,67,67,67	0
56	MG	DA	3522	1/1	0.11	-	44,44,44,44	0
56	MG	BA	3193	1/1	0.21	-	48,48,48,48	0
56	MG	BA	3601	1/1	0.13	-	50,50,50,50	0
56	MG	DA	3222	1/1	0.12	-	36,36,36,36	0
56	MG	DA	3259	1/1	0.18	-	42,42,42,42	0
56	MG	AA	3110	1/1	0.12	-	60,60,60,60	0
56	MG	BA	3350	1/1	0.21	-	59,59,59,59	0
56	MG	DA	3152	1/1	0.16	-	34,34,34,34	0
56	MG	BA	3349	1/1	0.11	-	46,46,46,46	0
56	MG	DA	3155	1/1	0.24	-	45,45,45,45	0
56	MG	BA	3147	1/1	0.24	-	35,35,35,35	0
56	MG	DA	3380	1/1	0.09	-	33,33,33,33	0
56	MG	DA	3231	1/1	0.12	-	37,37,37,37	0
56	MG	AA	3104	1/1	0.07	-	56,56,56,56	0
56	MG	DA	3098	1/1	0.11	-	46,46,46,46	0
56	MG	BA	3295	1/1	0.22	-	61,61,61,61	0
56	MG	BR	3001	1/1	0.18	-	31,31,31,31	0
56	MG	BA	3487	1/1	0.14	-	17,17,17,17	0
56	MG	BA	3121	1/1	0.53	-	43,43,43,43	0
56	MG	AA	3049	1/1	0.23	-	47,47,47,47	0
56	MG	DA	3375	1/1	0.18	-	49,49,49,49	0
56	MG	DA	3316	1/1	0.13	-	57,57,57,57	0
56	MG	DE	3005	1/1	0.11	-	20,20,20,20	0
56	MG	DA	3321	1/1	0.10	-	45,45,45,45	0
56	MG	DA	3201	1/1	0.09	-	51,51,51,51	0
56	MG	BA	3324	1/1	0.10	-	53,53,53,53	0
56	MG	BA	3340	1/1	0.13	-	42,42,42,42	0
56	MG	BA	3530	1/1	0.12	-	36,36,36,36	0
56	MG	BA	3159	1/1	0.16	-	27,27,27,27	0
56	MG	DA	3309	1/1	0.12	-	60,60,60,60	0
56	MG	BA	3310	1/1	0.17	-	35,35,35,35	0
56	MG	DA	3094	1/1	0.24	-	35,35,35,35	0
56	MG	BA	3439	1/1	0.19	-	30,30,30,30	0
56	MG	CA	3110	1/1	0.14	-	64,64,64,64	0
56	MG	BA	3084	1/1	0.17	-	34,34,34,34	0
56	MG	BF	305	1/1	0.33	-	61,61,61,61	0
56	MG	CA	3012	1/1	0.12	-	52,52,52,52	0
56	MG	DA	3520	1/1	0.10	-	34,34,34,34	0
56	MG	B0	104	1/1	0.51	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3072	1/1	0.15	-	24,24,24,24	0
56	MG	DA	3595	1/1	0.08	-	43,43,43,43	0
56	MG	DA	3035	1/1	0.14	-	46,46,46,46	0
56	MG	DA	3584	1/1	0.10	-	61,61,61,61	0
56	MG	BA	3222	1/1	0.18	-	45,45,45,45	0
56	MG	BA	3095	1/1	0.08	-	33,33,33,33	0
56	MG	DA	3529	1/1	0.19	-	41,41,41,41	0
56	MG	BA	3478	1/1	0.12	-	47,47,47,47	0
56	MG	CA	3008	1/1	0.28	-	31,31,31,31	0
56	MG	BA	3200	1/1	0.21	-	25,25,25,25	0
56	MG	AA	3160	1/1	0.12	-	71,71,71,71	0
56	MG	DA	3027	1/1	0.10	-	30,30,30,30	0
56	MG	BA	3124	1/1	0.19	-	58,58,58,58	0
56	MG	BA	3266	1/1	0.19	-	29,29,29,29	0
56	MG	BA	3661	1/1	0.20	-	38,38,38,38	0
56	MG	DA	3561	1/1	0.16	-	63,63,63,63	0
56	MG	BA	3575	1/1	0.09	-	55,55,55,55	0
56	MG	BA	3380	1/1	0.13	-	17,17,17,17	0
56	MG	BA	3096	1/1	0.09	-	44,44,44,44	0
56	MG	BA	3103	1/1	0.20	-	42,42,42,42	0
56	MG	BA	3237	1/1	0.15	-	57,57,57,57	0
56	MG	DA	3040	1/1	0.19	-	34,34,34,34	0
56	MG	AA	3001	1/1	0.15	-	57,57,57,57	0
56	MG	BA	3640	1/1	0.19	-	33,33,33,33	0
56	MG	DA	3242	1/1	0.16	-	60,60,60,60	0
56	MG	DA	3292	1/1	0.18	-	45,45,45,45	0
56	MG	AA	3007	1/1	0.09	-	30,30,30,30	0
56	MG	AA	3148	1/1	0.07	-	56,56,56,56	0
56	MG	BA	3227	1/1	0.15	-	32,32,32,32	0
56	MG	BA	3064	1/1	0.17	-	30,30,30,30	0
56	MG	BA	3116	1/1	0.23	-	50,50,50,50	0
56	MG	B7	3001	1/1	0.20	-	45,45,45,45	0
56	MG	AA	3097	1/1	0.15	-	49,49,49,49	0
56	MG	DA	3218	1/1	0.12	-	33,33,33,33	0
56	MG	DA	3211	1/1	0.17	-	35,35,35,35	0
56	MG	BA	3459	1/1	0.10	-	42,42,42,42	0
56	MG	BA	3249	1/1	0.11	-	48,48,48,48	0
56	MG	AA	3018	1/1	0.10	-	50,50,50,50	0
56	MG	BA	3339	1/1	0.13	-	34,34,34,34	0
56	MG	BA	3011	1/1	0.09	-	30,30,30,30	0
56	MG	DA	3191	1/1	0.09	-	53,53,53,53	0
56	MG	BA	3409	1/1	0.15	-	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	3111	1/1	0.17	-	43,43,43,43	0
56	MG	DA	3066	1/1	0.17	-	49,49,49,49	0
56	MG	DA	3025	1/1	0.08	-	41,41,41,41	0
56	MG	DA	3086	1/1	0.06	-	41,41,41,41	0
56	MG	DA	3438	1/1	0.10	-	38,38,38,38	0
56	MG	DA	3220	1/1	0.13	-	43,43,43,43	0
56	MG	AA	3068	1/1	0.17	-	31,31,31,31	0
56	MG	CE	201	1/1	0.11	-	52,52,52,52	0
57	SF4	AD	501	8/8	0.17	-	50,63,78,83	0
56	MG	B3	101	1/1	0.35	-	35,35,35,35	0
56	MG	CA	3117	1/1	0.23	-	42,42,42,42	0
56	MG	BA	3319	1/1	0.24	-	39,39,39,39	0
56	MG	BA	3055	1/1	0.14	-	13,13,13,13	0
56	MG	BA	3568	1/1	0.11	-	42,42,42,42	0
56	MG	BA	3255	1/1	0.18	-	32,32,32,32	0
56	MG	BA	3178	1/1	0.24	-	26,26,26,26	0
56	MG	DA	3434	1/1	0.12	-	41,41,41,41	0
56	MG	BA	3149	1/1	0.09	-	50,50,50,50	0
56	MG	BA	3507	1/1	0.12	-	53,53,53,53	0
56	MG	DA	3437	1/1	0.29	-	48,48,48,48	0
56	MG	AA	3073	1/1	0.18	-	50,50,50,50	0
56	MG	BA	3433	1/1	0.09	-	33,33,33,33	0
56	MG	DA	3403	1/1	0.07	-	39,39,39,39	0
56	MG	BA	3532	1/1	0.04	-	53,53,53,53	0
56	MG	BA	3229	1/1	0.20	-	54,54,54,54	0
56	MG	AA	3098	1/1	0.18	-	48,48,48,48	0
56	MG	DA	3491	1/1	0.12	-	40,40,40,40	0
56	MG	BA	3515	1/1	0.16	-	25,25,25,25	0
56	MG	BA	3315	1/1	0.20	-	31,31,31,31	0
56	MG	DA	3575	1/1	0.09	-	49,49,49,49	0
56	MG	CA	3004	1/1	0.15	-	51,51,51,51	0
56	MG	BA	3133	1/1	0.10	-	33,33,33,33	0
56	MG	BA	3418	1/1	0.12	-	46,46,46,46	0
56	MG	CA	3139	1/1	0.08	-	67,67,67,67	0
56	MG	CA	3011	1/1	0.17	-	66,66,66,66	0
56	MG	DA	3063	1/1	0.11	-	31,31,31,31	0
56	MG	DA	3327	1/1	0.19	-	34,34,34,34	0
56	MG	DA	3016	1/1	0.18	-	31,31,31,31	0
56	MG	BA	3408	1/1	0.10	-	56,56,56,56	0
56	MG	DA	3449	1/1	0.14	-	29,29,29,29	0
56	MG	BA	3572	1/1	0.11	-	59,59,59,59	0
56	MG	BA	3377	1/1	0.16	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	3070	1/1	0.16	-	33,33,33,33	0
56	MG	AA	3019	1/1	0.20	-	62,62,62,62	0
56	MG	B5	502	1/1	0.33	-	34,34,34,34	0
56	MG	BA	3596	1/1	0.14	-	56,56,56,56	0
56	MG	DA	3134	1/1	0.24	-	33,33,33,33	0
56	MG	BA	3570	1/1	0.05	-	36,36,36,36	0
56	MG	BA	3317	1/1	0.14	-	35,35,35,35	0
56	MG	BA	3477	1/1	0.10	-	50,50,50,50	0
56	MG	CA	3105	1/1	0.06	-	84,84,84,84	0

6.5 Other polymers ⓘ

There are no such residues in this entry.