



wwPDB X-ray Structure Validation Summary Report

Sep 10, 2014 – 11:09 PM EDT

PDB ID : 1VY5
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in the post-catalysis state of peptide bond formation containing dipeptidyl-tRNA in the A site and deacylated tRNA in the P site.
Authors : Polikanov, Y.S.; Steitz, T.A.; Innis, C.A.
Deposited on : 2014-05-13
Resolution : 2.55 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>

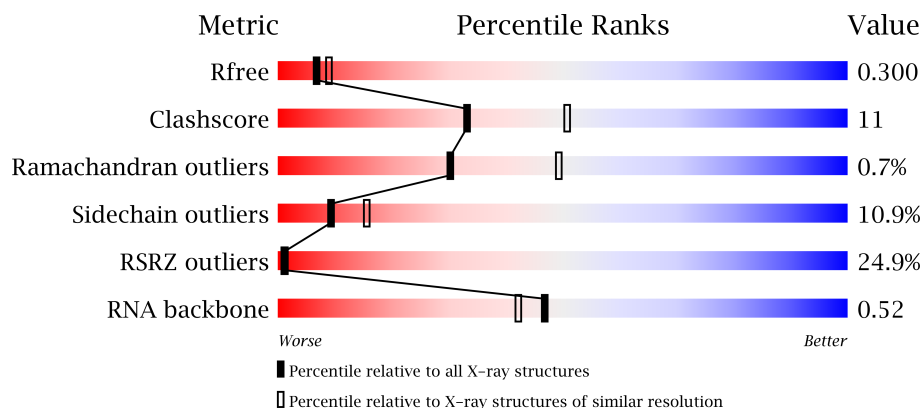
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.55 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	3413 (2.58-2.50)
Clashscore	79885	4284 (2.58-2.50)
Ramachandran outliers	78287	4193 (2.58-2.50)
Sidechain outliers	78261	4195 (2.58-2.50)
RSRZ outliers	66119	3414 (2.58-2.50)
RNA backbone	1838	1058 (3.10-1.98)

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	76	
23	CW	76	
24	AX	77	
24	CX	77	
25	AY	76	
25	CY	76	
26	BA	2915	
26	DA	2915	
27	BB	121	

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Mol	Chain	Length	Quality of chain
27	DB	121	
28	BD	276	
28	DD	276	
29	BE	206	
29	DE	206	
30	BF	210	
30	DF	210	
31	BG	182	
31	DG	182	
32	BH	180	
32	DH	180	
33	BI	148	
33	DI	148	
34	BN	140	
34	DN	140	
35	BO	122	
35	DO	122	
36	BP	150	
36	DP	150	
37	BQ	141	
37	DQ	141	
38	BR	118	
38	DR	118	
39	BS	112	
39	DS	112	
40	BT	146	
40	DT	146	
41	BU	118	
41	DU	118	
42	BV	101	
42	DV	101	
43	BW	113	
43	DW	113	
44	BX	96	
44	DX	96	
45	BY	110	
45	DY	110	
46	BZ	206	
46	DZ	206	
47	B0	85	
47	D0	85	
48	B1	98	

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Mol	Chain	Length	Quality of chain
48	D1	98	
49	B2	72	
49	D2	72	
50	B3	60	
50	D3	60	
51	B4	71	
51	D4	71	
52	B5	60	
52	D5	60	
53	B6	54	
53	D6	54	
54	B7	49	
54	D7	49	
55	B8	65	
55	D8	65	
56	B9	37	
56	D9	37	

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 297141 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
			1674	1050	333	284	7			

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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	0	0	0
			829	516	155	155	3			
11	CK	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

- 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	0	0	0
			930	585	185	159	1			
12	CL	122	Total	C	N	O	S	0	0	0
			930	585	185	159	1			

- 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	0	0	0
			958	592	198	166	2			
13	CM	122	Total	C	N	O	S	0	0	0
			950	586	197	165	2			

- 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	0	0	0
			492	312	104	72	4			
14	CN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- 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	0	0	0
			728	456	144	126	2			
15	CO	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- 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 A-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	AW	74	Total	C	N	O	P	S	0	0	0
			1607	727	288	516	73	3			
23	CW	72	Total	C	N	O	P	S	0	0	0
			1560	702	281	503	72	2			

- 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
			1625	725	294	529	76	1			
24	CX	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 25 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
25	AY	74	Total	C	N	O	P	S	0	0	0
			1581	707	285	515	73	1			
25	CY	73	Total	C	N	O	P	S	0	0	0
			1561	698	283	507	72	1			

- Molecule 26 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BA	2819	Total	C	N	O	P	0	0	0
			60729	27026	11370	19515	2818			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	DA	2800	Total	C	N	O	P	0	0	0
			60311	26840	11284	19388	2799			

- Molecule 27 is a RNA chain called 5S Ribosomal RNA.

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

- Molecule 28 is a protein called 50S ribosomal protein L2.

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

- Molecule 29 is a protein called 50S ribosomal protein L3.

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

- Molecule 30 is a protein called 50S ribosomal protein L4.

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

- Molecule 31 is a protein called 50S ribosomal protein L5.

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

- Molecule 32 is a protein called 50S ribosomal protein L6.

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

- Molecule 33 is a protein called 50S ribosomal protein L9.

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

- Molecule 34 is a protein called 50S ribosomal protein L13.

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

- Molecule 35 is a protein called 50S ribosomal protein L14.

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

- Molecule 36 is a protein called 50S ribosomal protein L15.

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

- Molecule 37 is a protein called 50S ribosomal protein L16.

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

- Molecule 38 is a protein called 50S ribosomal protein L17.

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

- Molecule 39 is a protein called 50S ribosomal protein L18.

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

- Molecule 40 is a protein called 50S ribosomal protein L19.

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

- Molecule 41 is a protein called 50S ribosomal protein L20.

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

- Molecule 42 is a protein called 50S ribosomal protein L21.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L22.

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

- Molecule 44 is a protein called 50S ribosomal protein L23.

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

- Molecule 45 is a protein called 50S ribosomal protein L24.

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

- Molecule 46 is a protein called 50S ribosomal protein L25.

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

- Molecule 47 is a protein called 50S ribosomal protein L27.

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

- Molecule 48 is a protein called 50S ribosomal protein L28.

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

- Molecule 49 is a protein called 50S ribosomal protein L29.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B4	69	Total	C	N	O	S	0	0	0
			558	352	102	99	5			
51	D4	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

- Molecule 52 is a protein called 50S ribosomal protein L32.

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

- Molecule 53 is a protein called 50S ribosomal protein L33.

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

- Molecule 54 is a protein called 50S ribosomal protein L34.

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

- Molecule 55 is a protein called 50S ribosomal protein L35.

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

- Molecule 56 is a protein called 50S ribosomal protein L36.

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

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	B4	1	Total	Mg	0	0
			1	1		
57	BA	812	Total	Mg	0	0
			812	812		
57	AK	1	Total	Mg	0	0
			1	1		
57	DQ	4	Total	Mg	0	0
			4	4		
57	D3	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DF	4	Total 4	Mg 4	0	0
57	CV	1	Total 1	Mg 1	0	0
57	B8	1	Total 1	Mg 1	0	0
57	BE	8	Total 8	Mg 8	0	0
57	AW	4	Total 4	Mg 4	0	0
57	DU	2	Total 2	Mg 2	0	0
57	B1	1	Total 1	Mg 1	0	0
57	AN	2	Total 2	Mg 2	0	0
57	BP	5	Total 5	Mg 5	0	0
57	AX	15	Total 15	Mg 15	0	0
57	DN	1	Total 1	Mg 1	0	0
57	CA	170	Total 170	Mg 170	0	0
57	B5	1	Total 1	Mg 1	0	0
57	BB	20	Total 20	Mg 20	0	0
57	D8	1	Total 1	Mg 1	0	0
57	AE	3	Total 3	Mg 3	0	0
57	DG	1	Total 1	Mg 1	0	0
57	B9	1	Total 1	Mg 1	0	0
57	BF	9	Total 9	Mg 9	0	0
57	BX	3	Total 3	Mg 3	0	0
57	B2	1	Total 1	Mg 1	0	0

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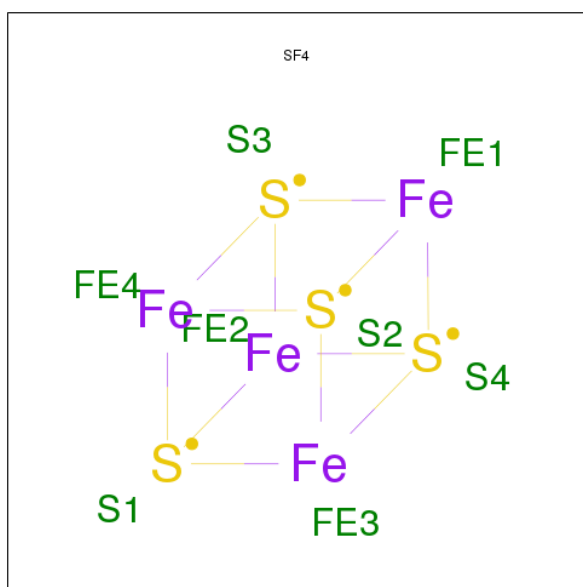
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	214	Total 214	Mg 214	0	0
57	BQ	5	Total 5	Mg 5	0	0
57	CX	3	Total 3	Mg 3	0	0
57	DV	3	Total 3	Mg 3	0	0
57	B6	2	Total 2	Mg 2	0	0
57	AM	1	Total 1	Mg 1	0	0
57	BU	8	Total 8	Mg 8	0	0
57	DR	1	Total 1	Mg 1	0	0
57	BN	6	Total 6	Mg 6	0	0
57	CT	1	Total 1	Mg 1	0	0
57	D0	1	Total 1	Mg 1	0	0
57	BG	3	Total 3	Mg 3	0	0
57	BY	1	Total 1	Mg 1	0	0
57	DE	4	Total 4	Mg 4	0	0
57	B3	2	Total 2	Mg 2	0	0
57	CJ	1	Total 1	Mg 1	0	0
57	BR	2	Total 2	Mg 2	0	0
57	DA	677	Total 677	Mg 677	0	0
57	DP	2	Total 2	Mg 2	0	0
57	DW	4	Total 4	Mg 4	0	0
57	B7	5	Total 5	Mg 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CF	1	Total 1	Mg 1	0	0
57	BV	5	Total 5	Mg 5	0	0
57	DO	1	Total 1	Mg 1	0	0
57	BO	2	Total 2	Mg 2	0	0
57	DX	1	Total 1	Mg 1	0	0
57	BZ	1	Total 1	Mg 1	0	0
57	DY	1	Total 1	Mg 1	0	0
57	CW	1	Total 1	Mg 1	0	0
57	CD	1	Total 1	Mg 1	0	0
57	BD	9	Total 9	Mg 9	0	0
57	B0	3	Total 3	Mg 3	0	0
57	CE	1	Total 1	Mg 1	0	0
57	BW	4	Total 4	Mg 4	0	0
57	AY	3	Total 3	Mg 3	0	0
57	DD	9	Total 9	Mg 9	0	0
57	CK	1	Total 1	Mg 1	0	0
57	AF	1	Total 1	Mg 1	0	0
57	DB	13	Total 13	Mg 13	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	D9	1	Total 1	Zn 1	0	0
59	B6	1	Total 1	Zn 1	0	0

- Molecule 60 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AX	1	Total 1	K 1	0	0
60	CX	1	Total 1	K 1	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AA	227	Total 227	O 227	0	0
61	AE	2	Total 2	O 2	0	0
61	AJ	1	Total 1	O 1	0	0
61	AL	1	Total 1	O 1	0	0
61	AM	1	Total 1	O 1	0	0
61	AU	1	Total 1	O 1	0	0
61	AV	3	Total 3	O 3	0	0
61	AW	3	Total 3	O 3	0	0
61	AX	6	Total 6	O 6	0	0
61	AY	1	Total 1	O 1	0	0
61	BA	1383	Total 1383	O 1383	0	0
61	BB	36	Total 36	O 36	0	0
61	BD	12	Total 12	O 12	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	BE	14	Total 14	O 14	0	0
61	BF	8	Total 8	O 8	0	0
61	BG	3	Total 3	O 3	0	0
61	BI	1	Total 1	O 1	0	0
61	BO	4	Total 4	O 4	0	0
61	BP	16	Total 16	O 16	0	0
61	BQ	4	Total 4	O 4	0	0
61	BR	2	Total 2	O 2	0	0
61	BT	2	Total 2	O 2	0	0
61	BU	3	Total 3	O 3	0	0
61	BV	2	Total 2	O 2	0	0
61	BW	1	Total 1	O 1	0	0
61	BX	4	Total 4	O 4	0	0
61	BZ	1	Total 1	O 1	0	0
61	B0	3	Total 3	O 3	0	0
61	B1	1	Total 1	O 1	0	0
61	B3	2	Total 2	O 2	0	0
61	B5	2	Total 2	O 2	0	0
61	B6	1	Total 1	O 1	0	0
61	B7	2	Total 2	O 2	0	0
61	B8	8	Total 8	O 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	CA	185	Total 185	O 185	0	0
61	CJ	2	Total 2	O 2	0	0
61	CL	1	Total 1	O 1	0	0
61	CT	1	Total 1	O 1	0	0
61	CV	1	Total 1	O 1	0	0
61	CW	2	Total 2	O 2	0	0
61	DA	1025	Total 1025	O 1025	0	0
61	DB	9	Total 9	O 9	0	0
61	DD	19	Total 19	O 19	0	0
61	DE	11	Total 11	O 11	0	0
61	DF	3	Total 3	O 3	0	0
61	DN	2	Total 2	O 2	0	0
61	DO	1	Total 1	O 1	0	0
61	DP	16	Total 16	O 16	0	0
61	DR	1	Total 1	O 1	0	0
61	DT	3	Total 3	O 3	0	0
61	DU	2	Total 2	O 2	0	0
61	DX	3	Total 3	O 3	0	0
61	DY	2	Total 2	O 2	0	0
61	D0	3	Total 3	O 3	0	0
61	D1	1	Total 1	O 1	0	0

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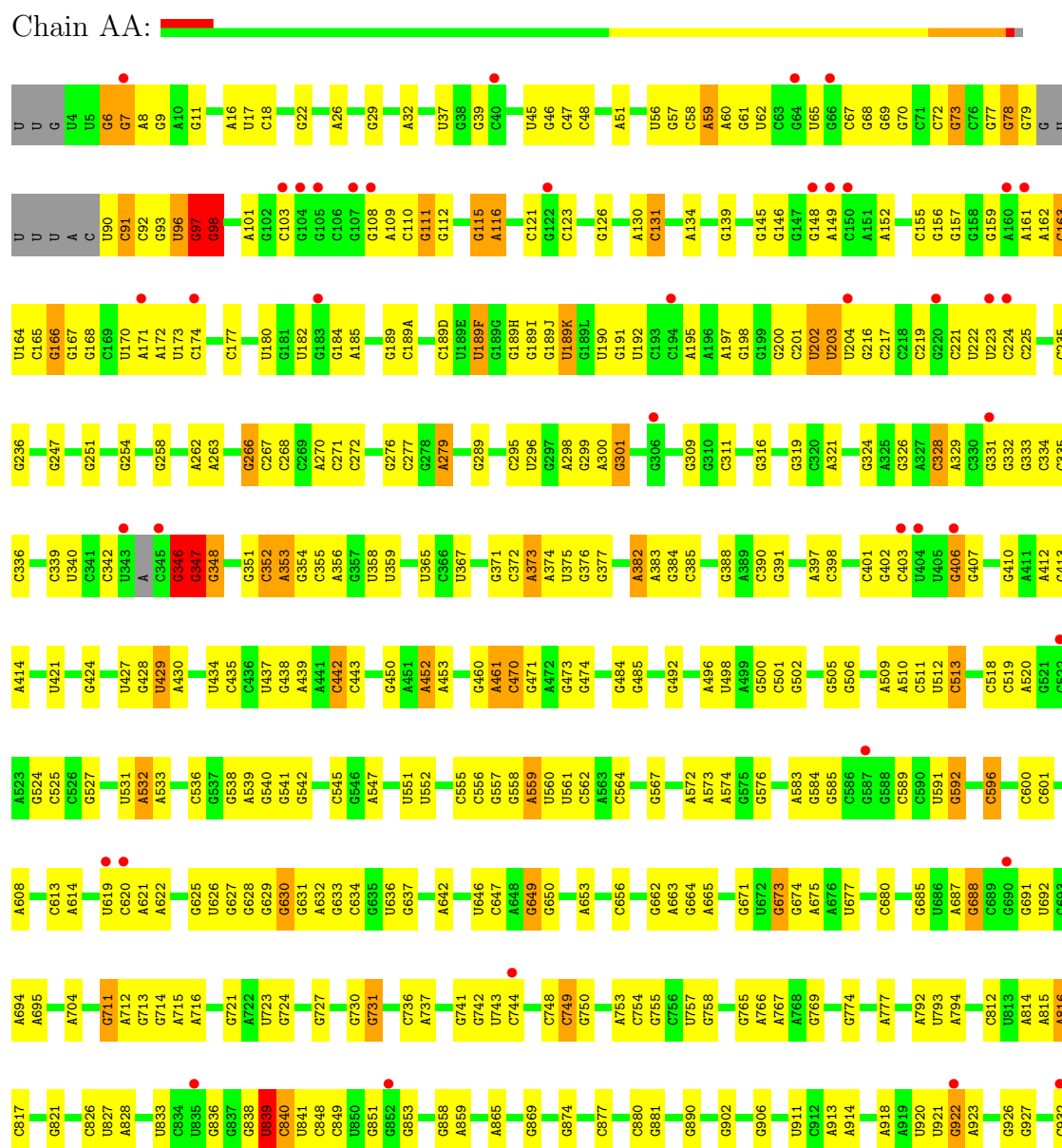
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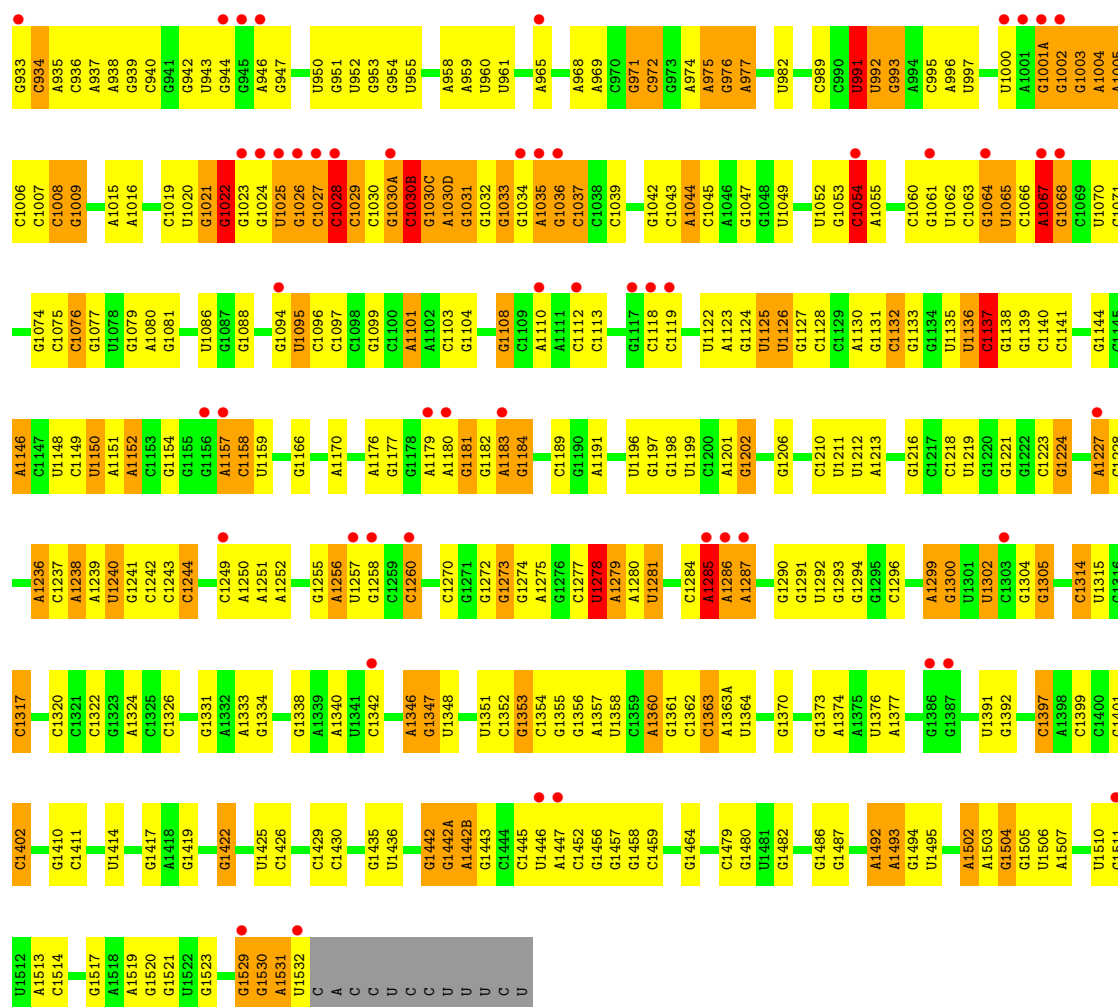
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	D3	1	Total	O	0	0
			1	1		
61	D7	3	Total	O	0	0
			3	3		
61	D8	4	Total	O	0	0
			4	4		

3 Residue-property plots

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

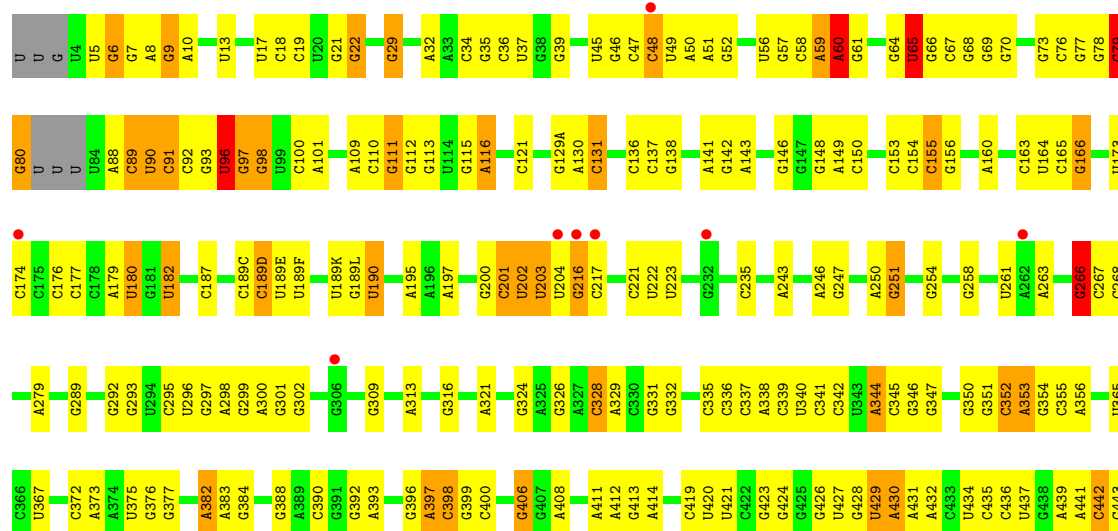
• Molecule 1: 16S Ribosomal RNA





• Molecule 1: 16S Ribosomal RNA

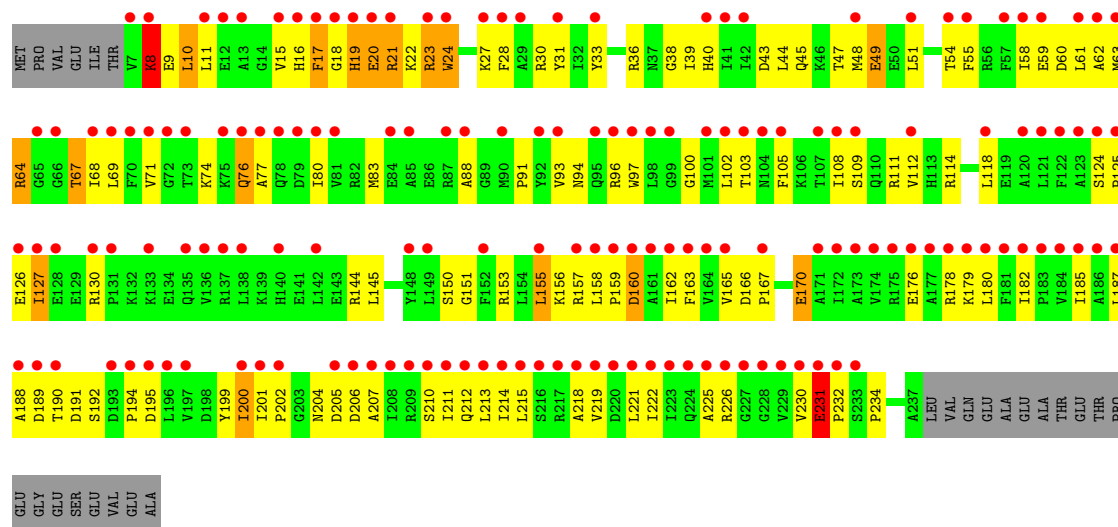
Chain CA:



C1366	C1367	C1368	C1369	C1370	C1371	C1372	C1373	C1374	C1375	C1376	C1377	C1378	C1379	C1383	C1386	C1387	C1388	C1391	C1392	C1397	C1398	C1399	C1402	C1410	C1411	C1412	C1413	C1414	C1419	C1422	C1423	C1424	C1429	C1430	C1435	C1436	C1441	C1442	C1442A	C1442B	C1446	C1447	C1452	C1456	C1457	C1469												
U1301	U1302	C1303	C1304	C1305	C1310	C1311	C1312	C1313	C1314	U1315	U1316	C1317	C1318	C1319	C1320	C1321	C1322	C1323	C1324	C1325	C1326	C1327	C1328	C1331	C1332	C1333	C1334	C1338	C1339	C1340	C1341	C1342	C1343	C1344	C1345	C1346	C1347	U1348	C1349	C1350	U1351	C1352	C1353	C1354	C1355	C1356	C1357	C1358	C1359	C1360	C1361	C1362	C1363	C1363A	C1364	C1365		
U1232	C1233	C1234	U1235	C1236	C1237	U1238	U1239	U1240	C1243	C1244	C1245	C1246	C1249	C1250	C1251	C1252	C1255	C1256	C1257	C1258	C1259	C1260	C1261	C1262	C1263	C1269	C1270	C1271	C1272	C1273	C1274	C1277	U1278	C1279	C1280	U1281	C1282	C1283	C1284	C1285	C1286	C1287	C1288	C1289	C1290	C1291	C1292	C1293	C1294	C1297	C1298	C1299	C1300					
U1162	C1163	C1164	C1165	C1169	C1170	C1171	C1172	C1173	C1174	C1175	C1176	C1177	C1178	C1179	C1180	C1181	C1182	C1183	C1184	C1185	C1186	C1190	C1191	C1192	U1196	C1197	C1198	C1199	C1200	C1201	C1202	C1203	C1204	C1205	C1206	C1211	C1212	C1213	C1214	C1215	C1216	C1217	C1218	C1219	C1220	C1221	C1222	C1223	C1224	C1225	C1226	C1227	C1228	C1231				
G1099	G1100	C1101	C1102	C1103	C1104	G1108	C1109	C1110	C1111	C1112	C1113	C1114	C1115	C1116	C1117	C1118	C1119	C1120	C1121	C1122	C1123	C1124	U1125	U1126	C1127	C1128	C1129	C1130	C1131	C1132	C1133	C1134	U1135	C1136	C1137	C1138	C1139	C1140	C1141	C1142	C1143	C1144	C1145	C1146	C1147	U1148	C1149	C1150	C1151	C1152	C1153	C1154	C1155	C1156	C1157	C1158	C1159	
C1037	C1038	C1039	U1040	U1041	C1042	C1043	C1044	C1047	C1048	U1049	C1050	C1051	U1052	C1053	C1054	C1055	U1056	C1057	C1058	C1059	C1060	C1061	U1062	C1063	C1064	C1065	C1066	C1067	C1068	C1069	U1070	C1071	C1072	C1073	C1074	C1075	C1076	C1079	C1080	C1081	C1082	C1083	C1084	U1085	U1086	C1087	C1088	C1089	U1090	U1091	C1092	C1093	C1094	U1095	C1096	C1097	C1098	
U982	A983	C984	C985	A986	C987	C988	C989	C990	U991	U992	C993	A994	C995	A996	U997	C998	C999	U1000	A1001	C1001A	C1002	C1003	A1004	A1005	C1006	C1007	C1008	C1009	C1010	C1011	U1012	C1013	C1014	C1015	C1016	C1017	C1018	C1019	U1020	C1021	C1022	C1023	C1024	U1025	C1026	C1027	C1028	C1029	C1030	C1030A	C1030B	C1030C	A1031	C1032	C1033	C1034	C1035	C1036
A914	U920	U921	C922	C923	C924	C925	C926	C927	C931	C932	C933	C934	A935	C936	A937	C938	A939	U940	C941	C942	C943	C944	C945	A946	U950	C951	U952	C953	C954	U955	U956	U957	A958	A959	U960	U961	C962	C963	A964	A965	C966	C967	A968	A969	C970	C971	C972	C973	A974	A975	A976	A977	A978	C979	C980	C981		
C811	A814	A815	A816	C817	C821	C825	U827	A828	U833	C838	U839	C840	U841	C848	C851	C852	C853	C857	C858	A859	C860	C861	C866	C867	C868	C869	C874	C875	C876	C879	C880	C883	U884	C885	C890	C895	A896	A897	A898	A899	A901	C902	A902	A903	A904	U1096	C1097	C1098										
C720	G721	A722	U723	G724	G727	A728	A729	G730	G731	C736	A737	G741	G742	C748	G749	G750	A753	C754	G755	C756	G757	G758	G765	A766	A767	A768	G769	C770	A771	U772	G773	G774	G775	G776	A777	G778	A780	A781	A782	C783	C784	G791	G792	A793	U794	G711	A712	G713	A802	G803	U804	C805						
U641	A642	C643	G644	U645	G646	C647	A648	G649	G650	A653	A654	C655	G656	A657	G658	G662	A663	A665	G673	G674	U677	C680	G683	A684	G685	U686	A687	G688	C689	G690	G691	G692	C596	A697	A698	A699	G610	C620	G625	U626	G627	G628	G629	U531	A532	A533	U534	C535										
C444	G445	G446	G447	C448	C449	G450	A451	A452	A453	G460	A461	C470	G471	A472	G473	G474	G484	G485	C488	G492	A496	U498	A499	G500	C501	G502	C503	C504	G505	A509	A510	C511	U512	C513	C514	C518	G521	A522	A523	C526	G527	G529	G530	U531	A532	A533	U534	C535										

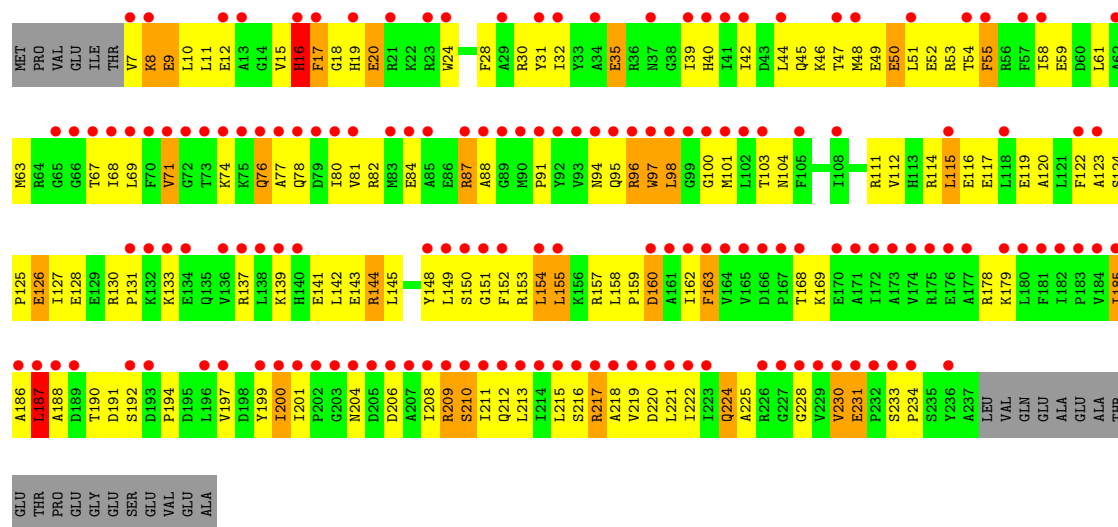
• Molecule 2: 30S ribosomal protein S2

Chain AB:



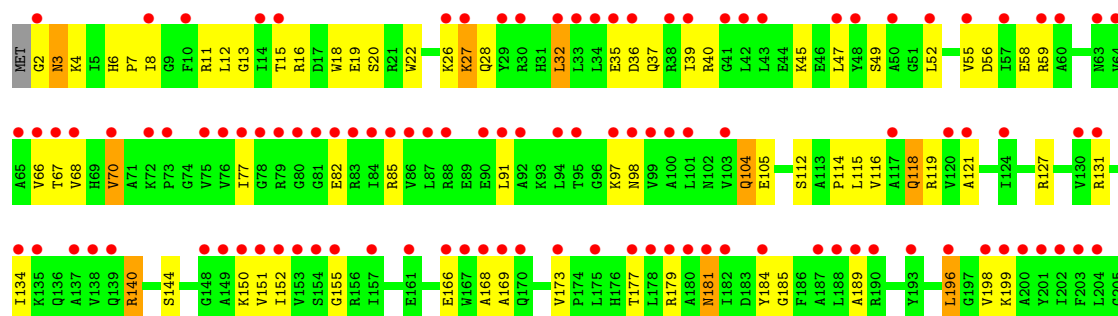
• Molecule 2: 30S ribosomal protein S2

Chain CB:

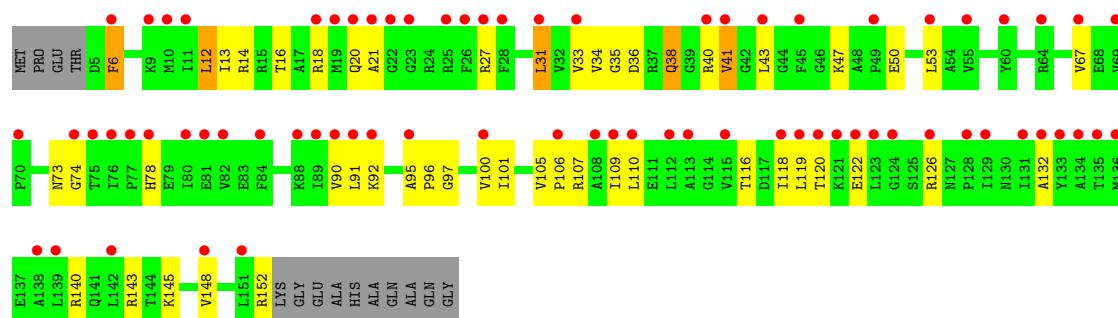


• Molecule 3: 30S ribosomal protein S3

Chain AC:

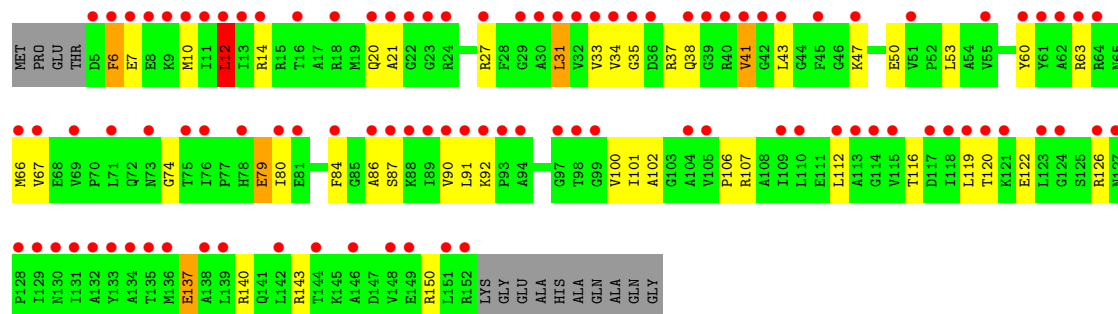






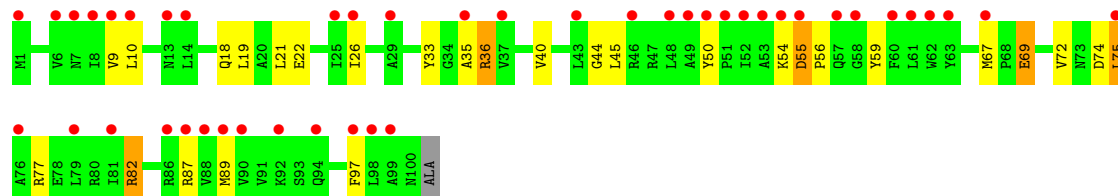
• Molecule 5: 30S ribosomal protein S5

Chain CE:



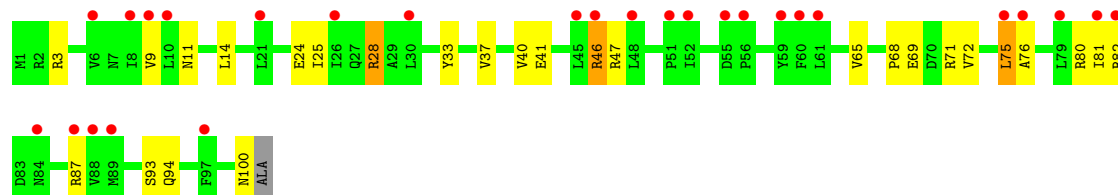
• Molecule 6: 30S ribosomal protein S6

Chain AF:



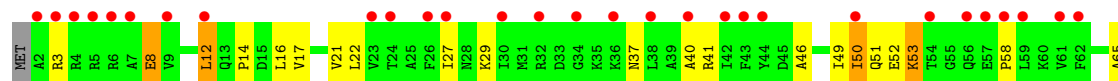
• Molecule 6: 30S ribosomal protein S6

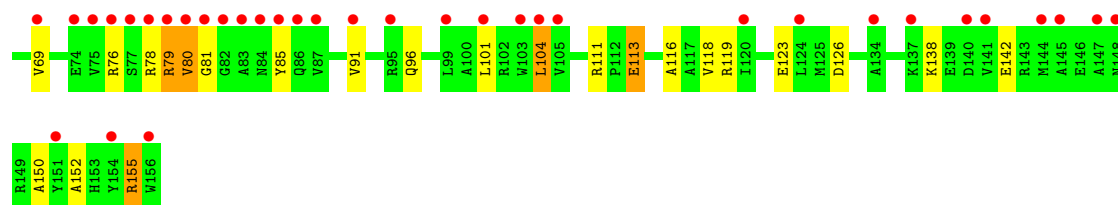
Chain CF:



• Molecule 7: 30S ribosomal protein S7

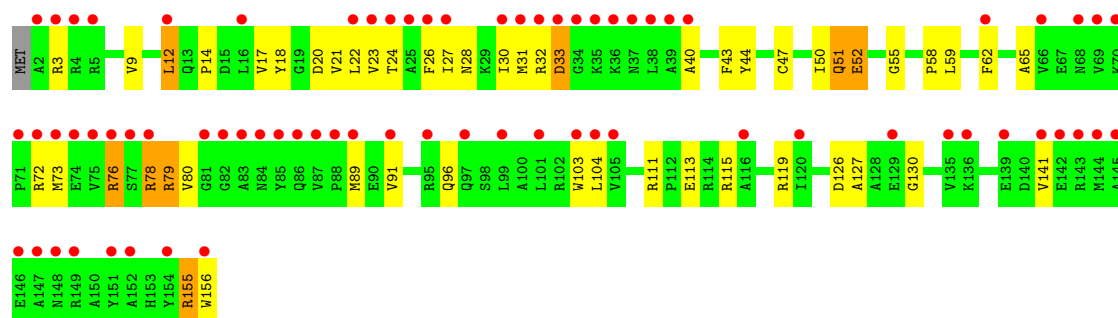
Chain AG:





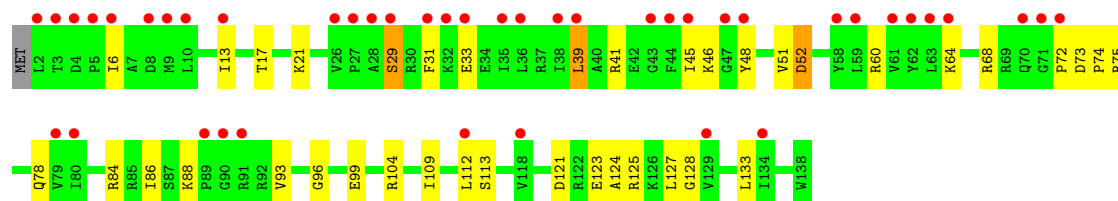
• Molecule 7: 30S ribosomal protein S7

Chain CG:



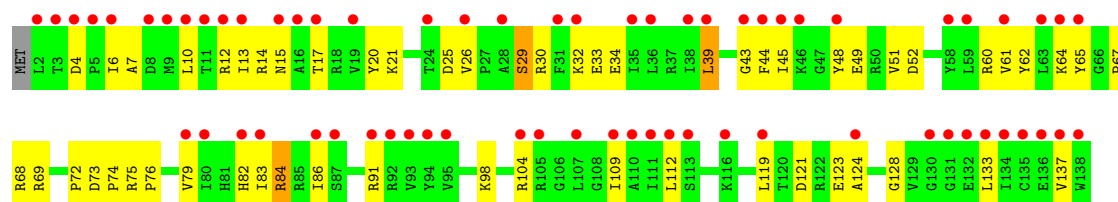
• Molecule 8: 30S ribosomal protein S8

Chain AH:



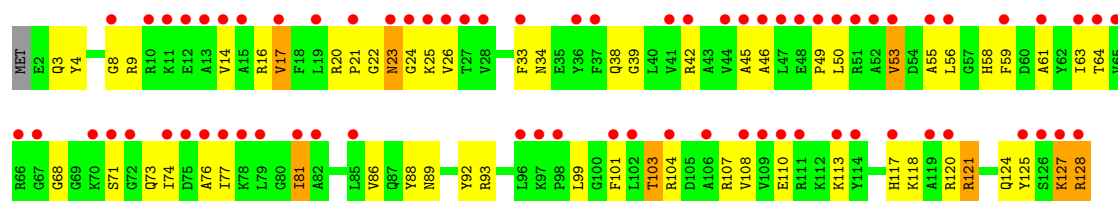
• Molecule 8: 30S ribosomal protein S8

Chain CH:



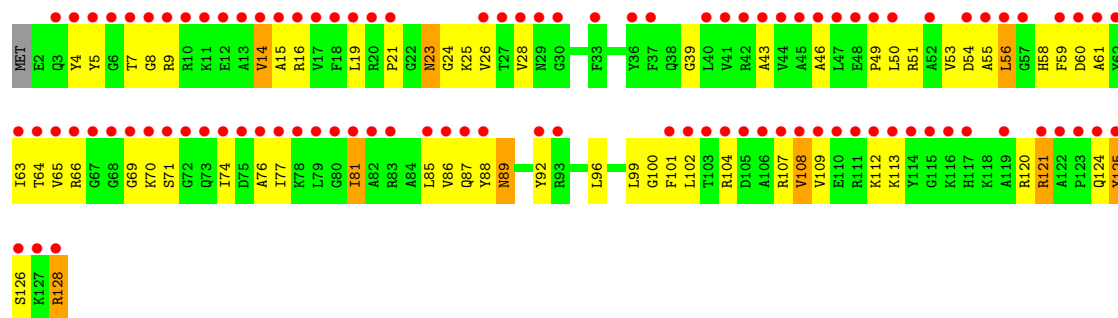
• Molecule 9: 30S ribosomal protein S9

Chain AI:



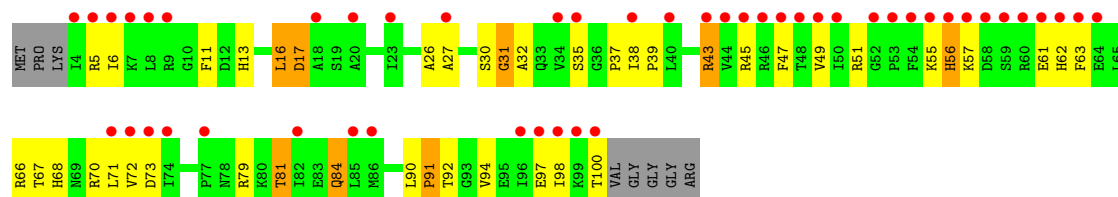
• Molecule 9: 30S ribosomal protein S9

Chain CI:



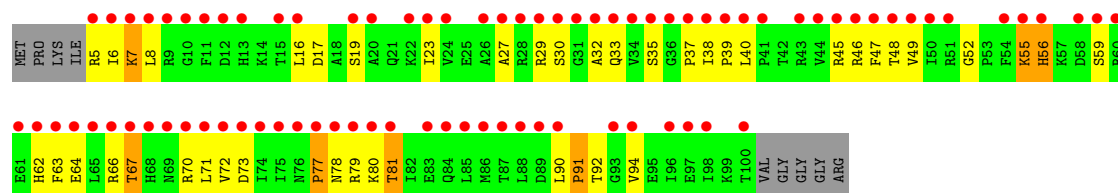
- Molecule 10: 30S ribosomal protein S10

Chain AJ:



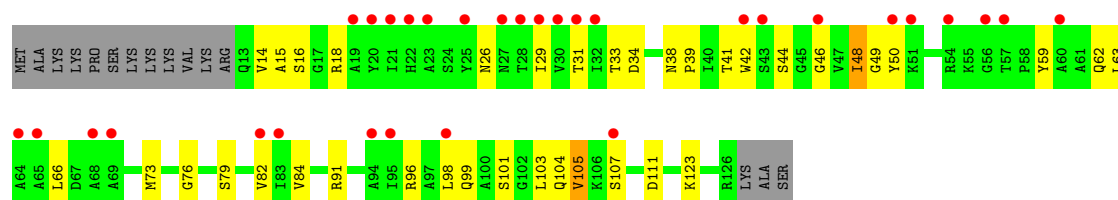
- Molecule 10: 30S ribosomal protein S10

Chain CJ:



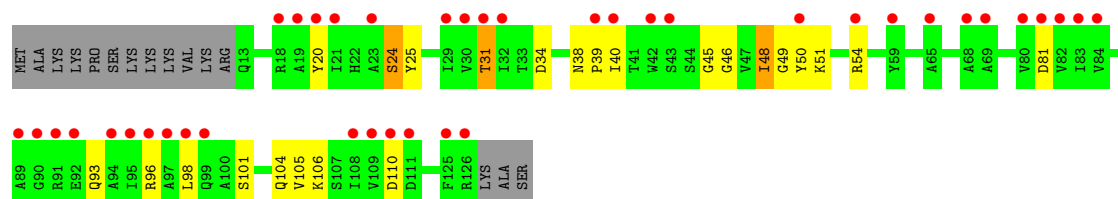
- Molecule 11: 30S ribosomal protein S11

Chain AK:



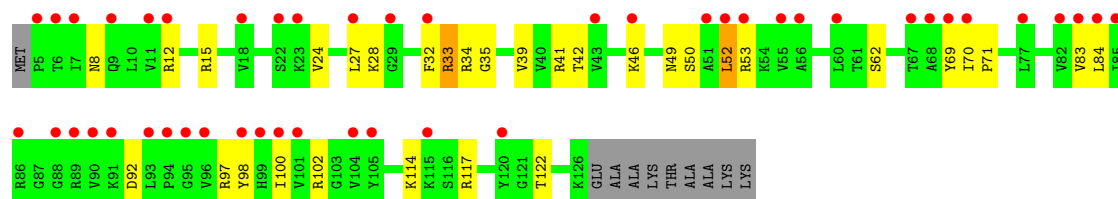
- Molecule 11: 30S ribosomal protein S11

Chain CK:



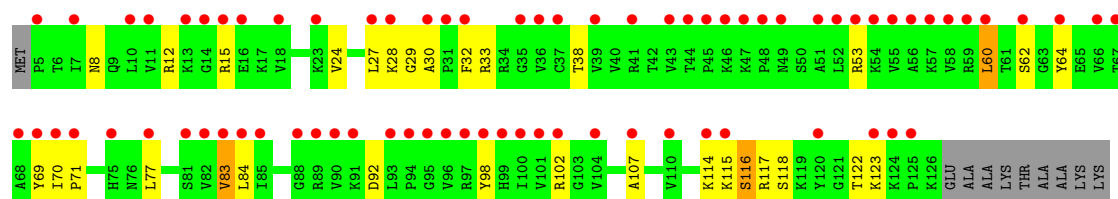
- Molecule 12: 30S ribosomal protein S12

Chain AL:



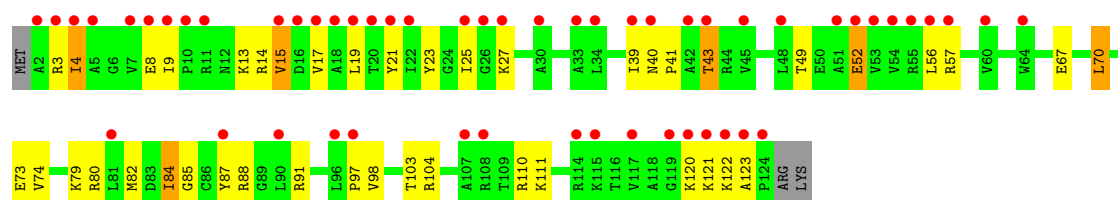
- Molecule 12: 30S ribosomal protein S12

Chain CL:



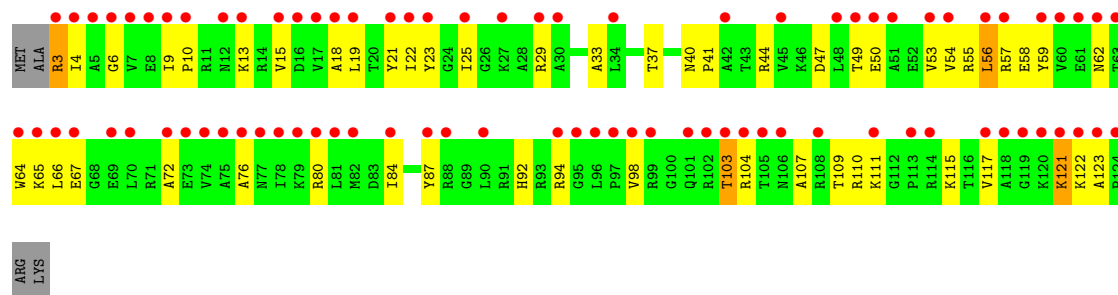
- Molecule 13: 30S ribosomal protein S13

Chain AM:



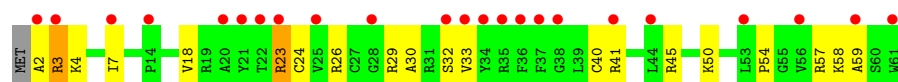
- Molecule 13: 30S ribosomal protein S13

Chain CM:

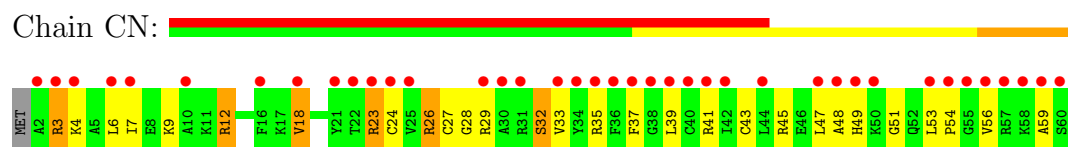


- Molecule 14: 30S ribosomal protein S14 type Z

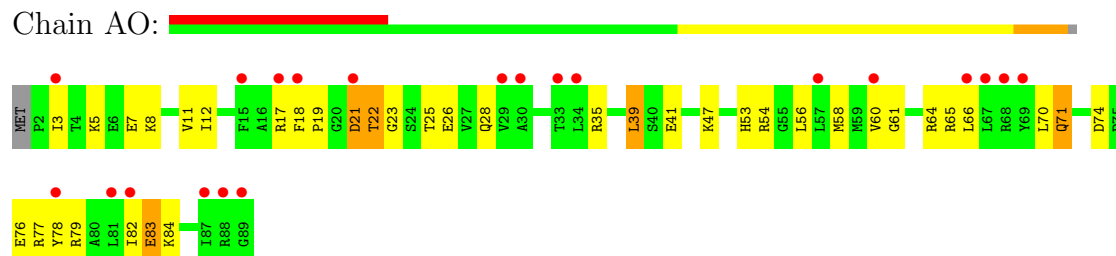
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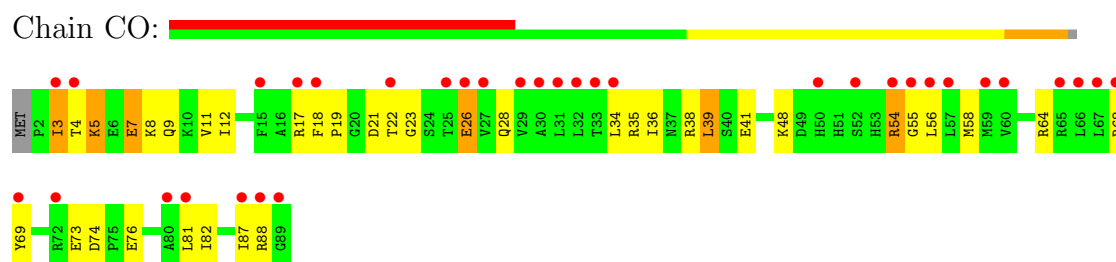
- Molecule 14: 30S ribosomal protein S14 type Z



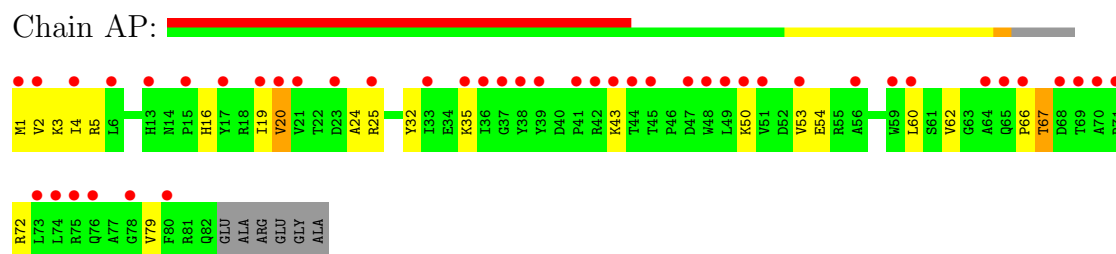
- Molecule 15: 30S ribosomal protein S15



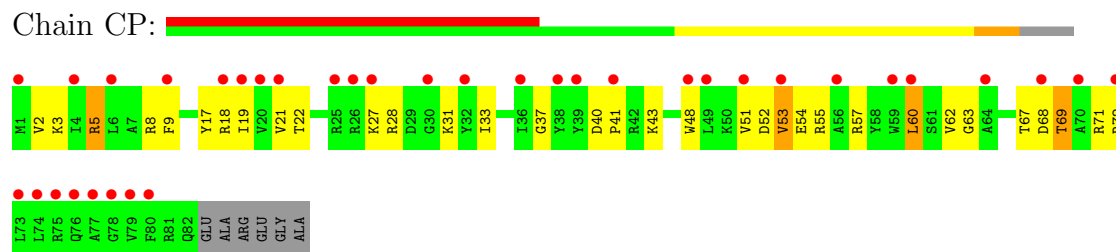
- Molecule 15: 30S ribosomal protein S15



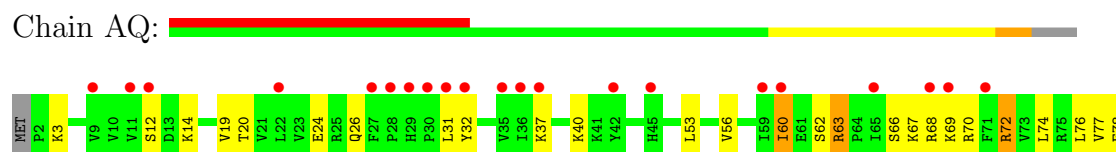
- Molecule 16: 30S ribosomal protein S16

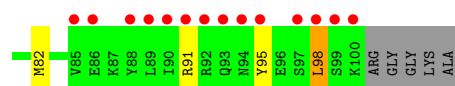


- Molecule 16: 30S ribosomal protein S16



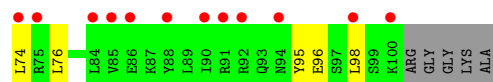
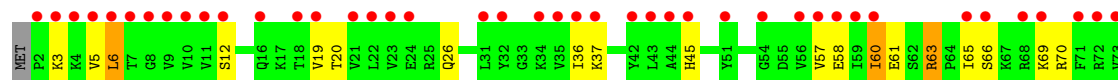
- Molecule 17: 30S ribosomal protein S17





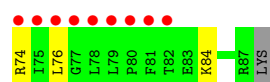
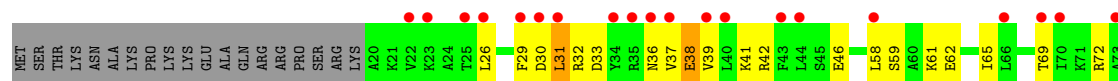
- Molecule 17: 30S ribosomal protein S17

Chain CQ:



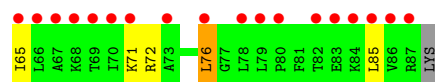
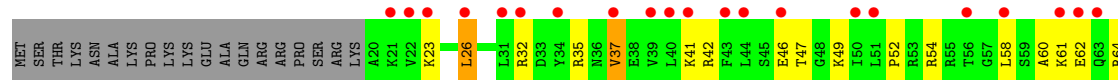
- Molecule 18: 30S ribosomal protein S18

Chain AR:



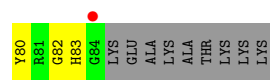
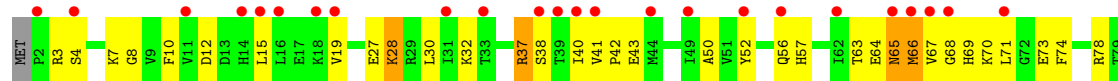
- Molecule 18: 30S ribosomal protein S18

Chain CR:



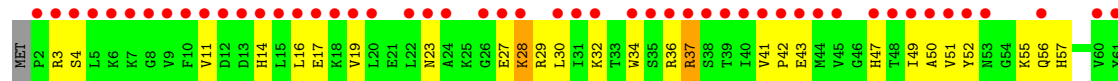
- Molecule 19: 30S ribosomal protein S19

Chain AS:

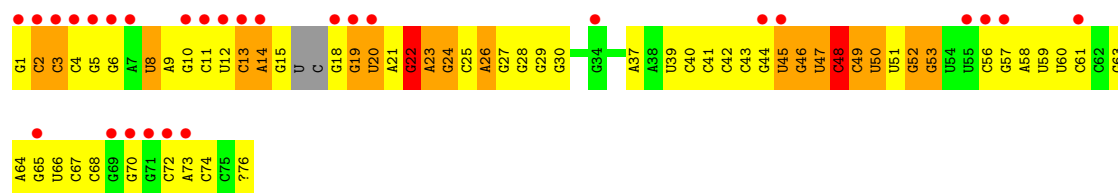


- Molecule 19: 30S ribosomal protein S19

Chain CS:

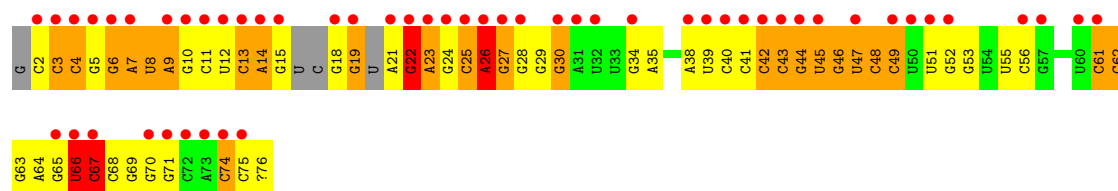


Chain AW:



• Molecule 23: A-site tRNA

Chain CW:



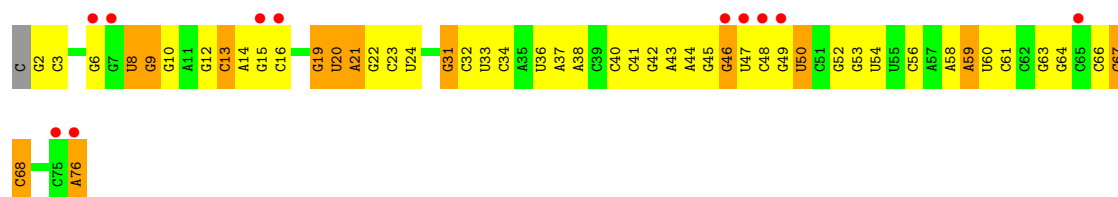
• Molecule 24: P-site tRNA

Chain AX:



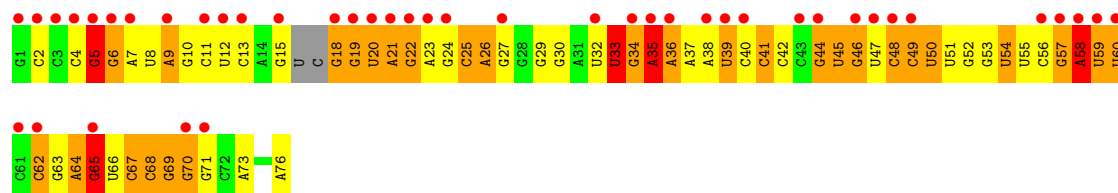
• Molecule 24: P-site tRNA

Chain CX:



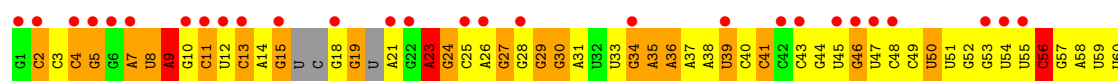
• Molecule 25: E-site tRNA

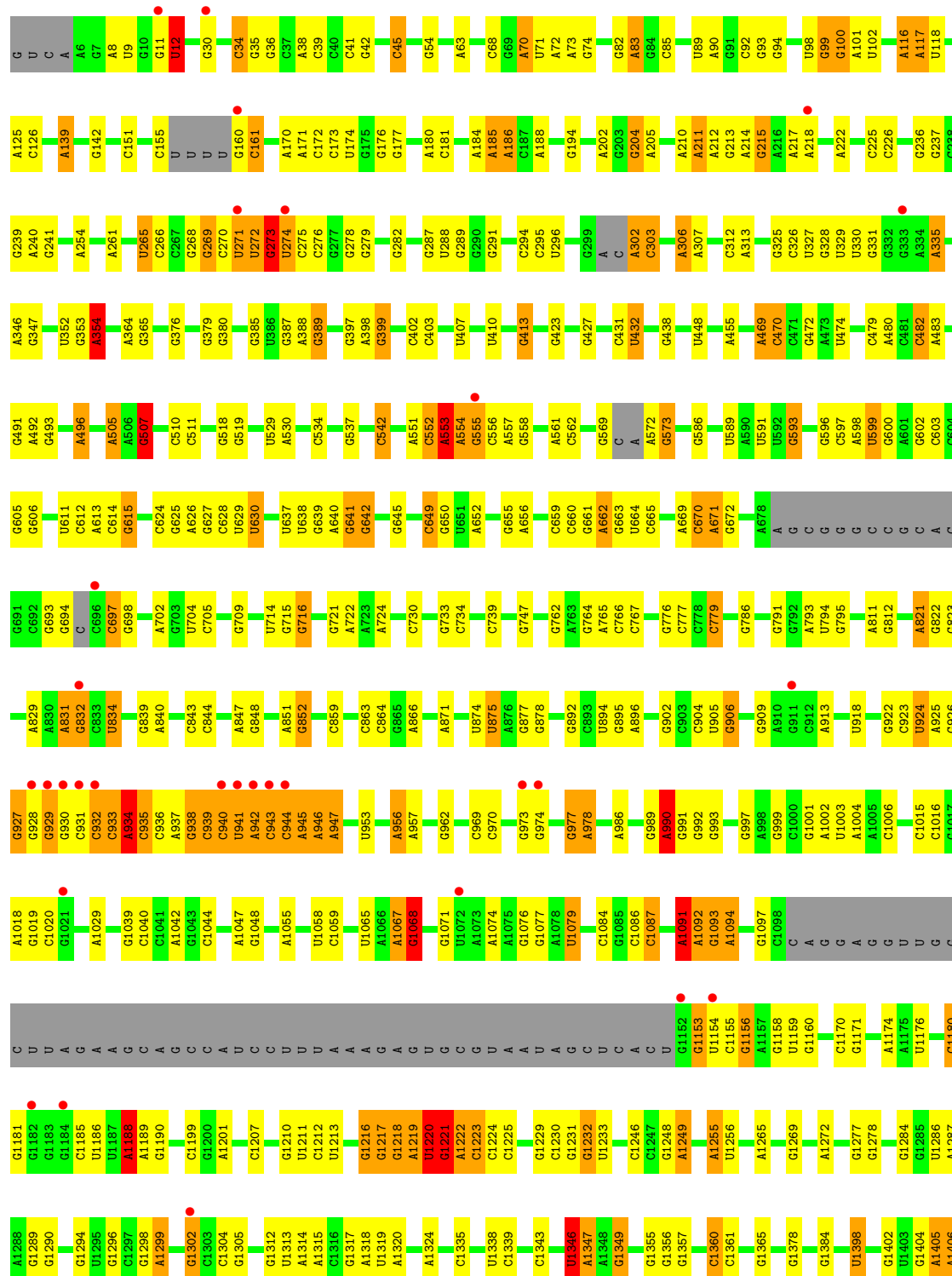
Chain AY:



• Molecule 25: E-site tRNA

Chain CY:

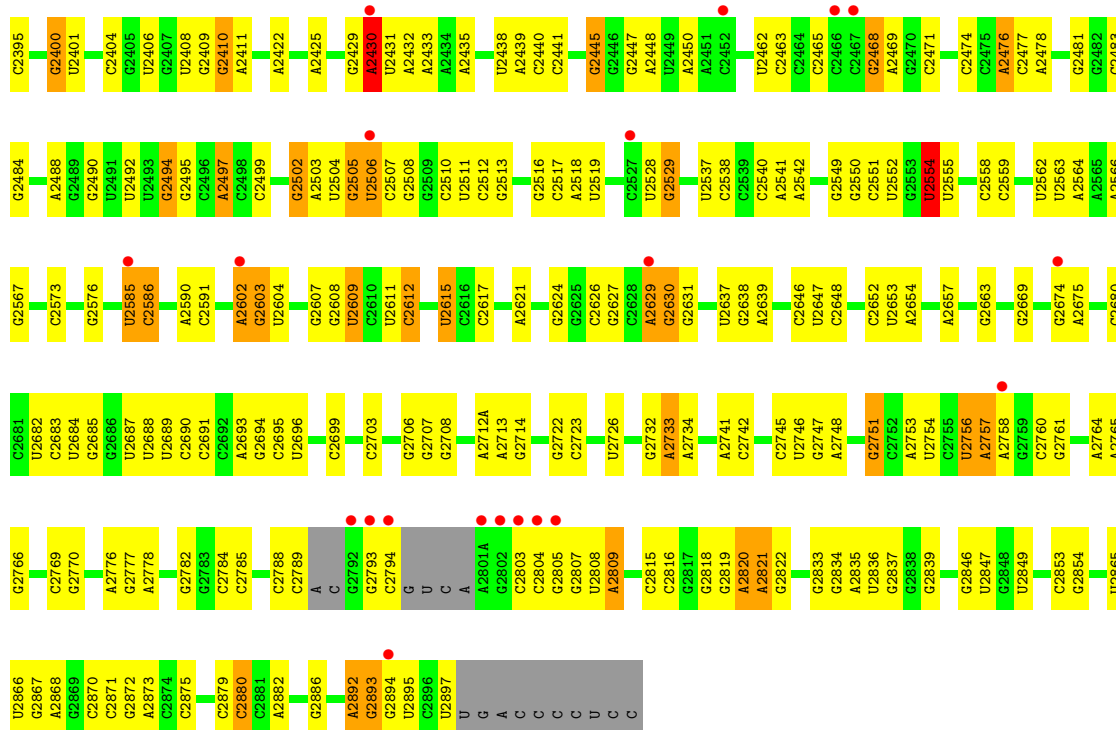




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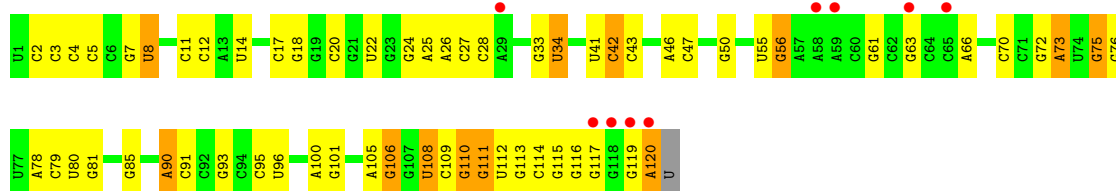
• Molecule 27: 5S Ribosomal RNA

Chain BB:



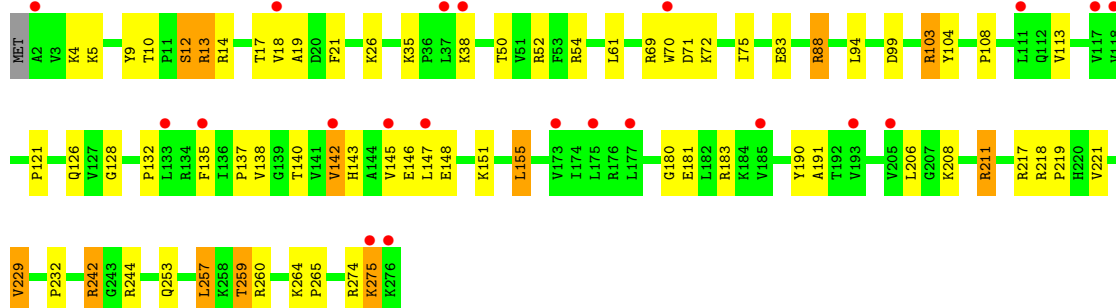
• Molecule 27: 5S Ribosomal RNA

Chain DB:

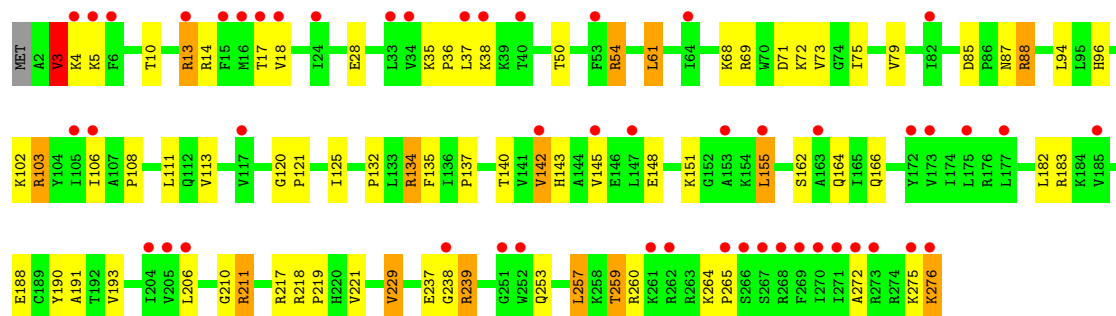


• Molecule 28: 50S ribosomal protein L2

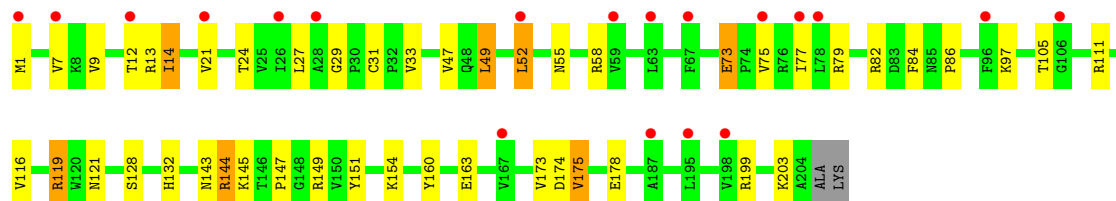
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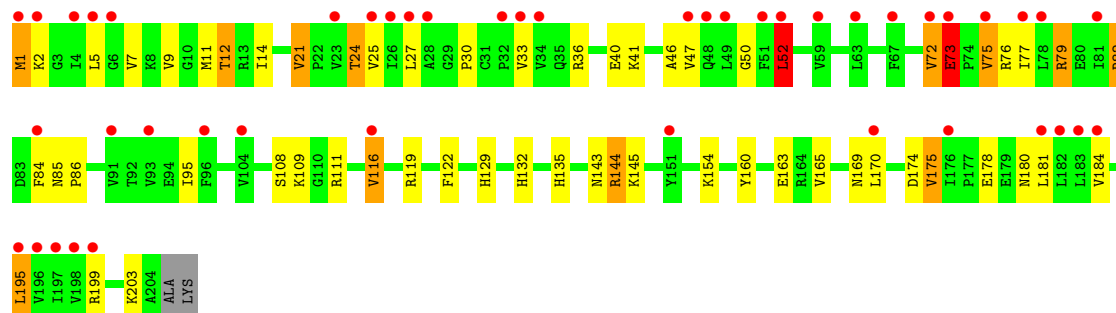
- Molecule 28: 50S ribosomal protein L2

Chain DD: 

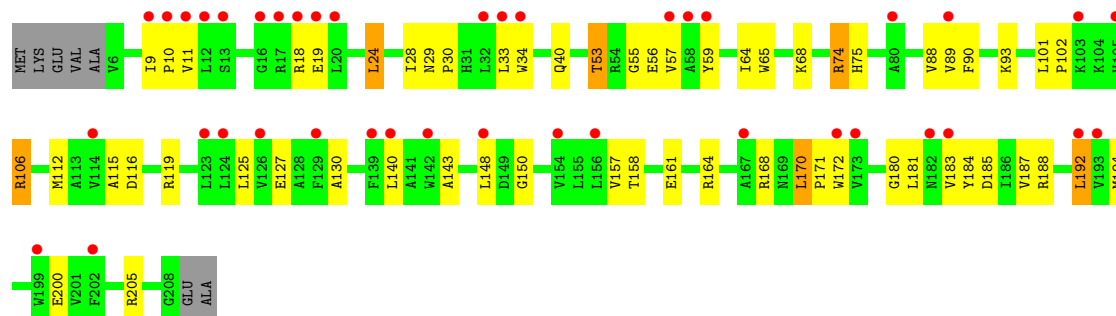
- Molecule 29: 50S ribosomal protein L3

Chain BE: 

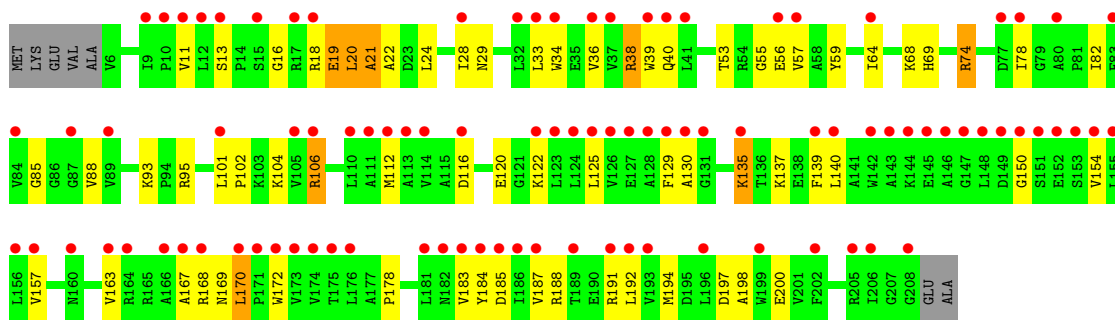
- Molecule 29: 50S ribosomal protein L3

Chain DE: 

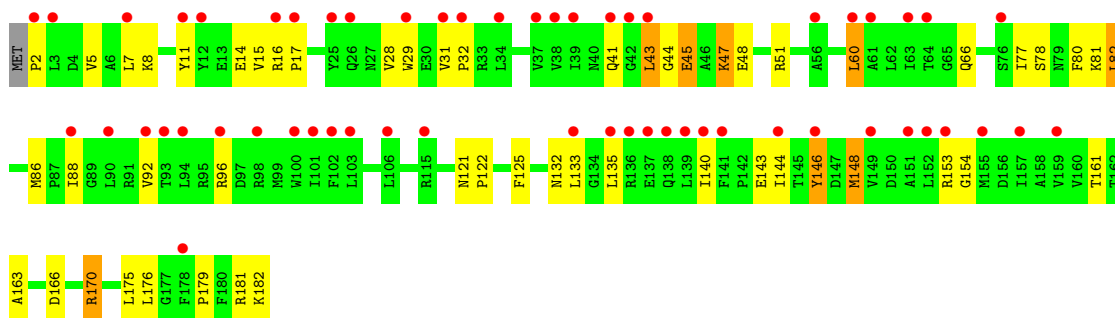
- Molecule 30: 50S ribosomal protein L4

Chain BF: 

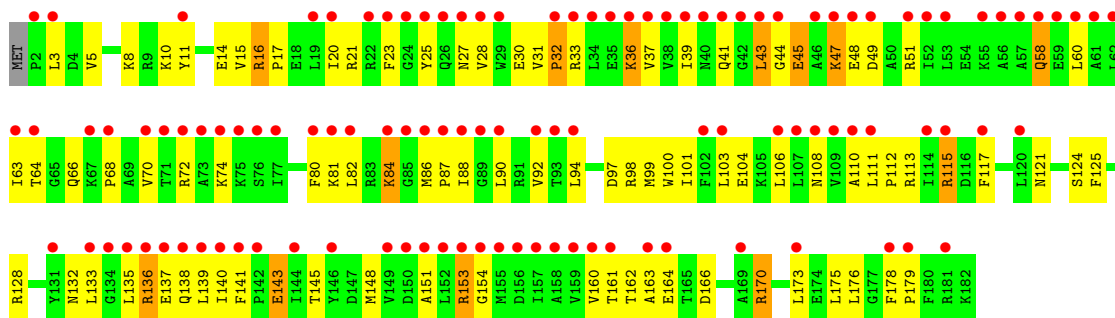
- Molecule 30: 50S ribosomal protein L4

Chain DF: 

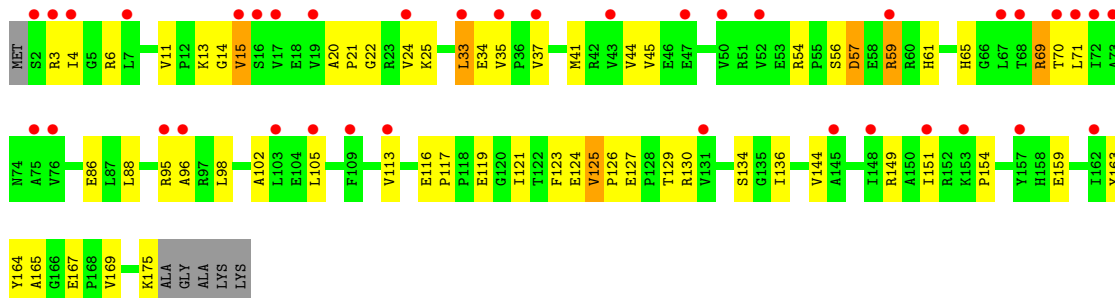
- Molecule 31: 50S ribosomal protein L5

Chain BG: 

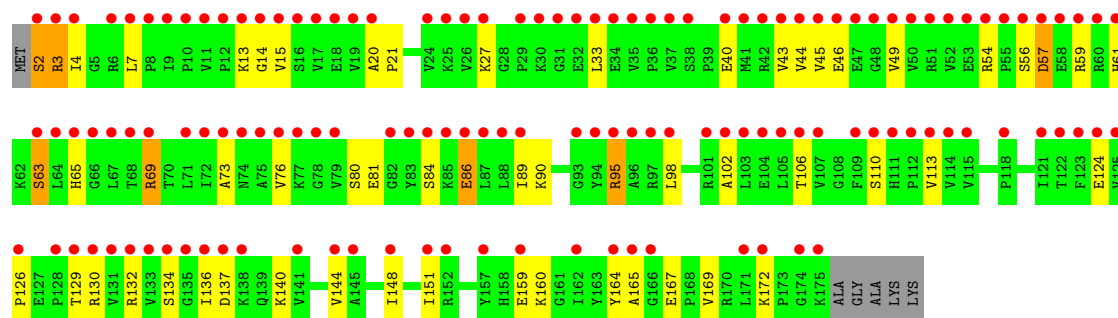
- Molecule 31: 50S ribosomal protein L5

Chain DG: 

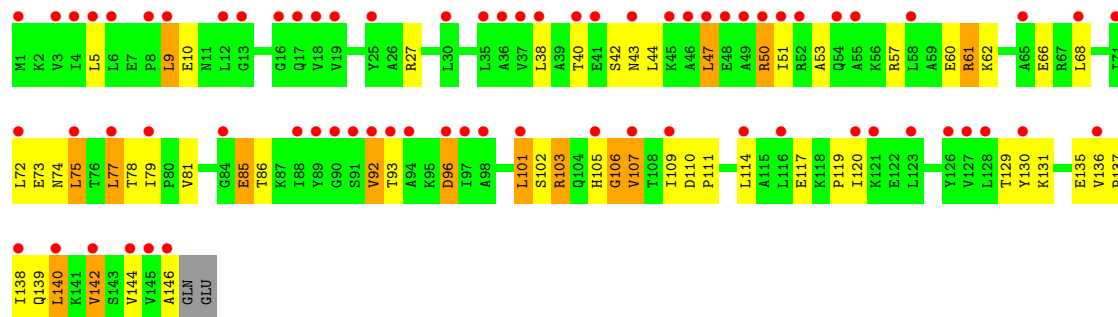
- Molecule 32: 50S ribosomal protein L6

Chain BH: 

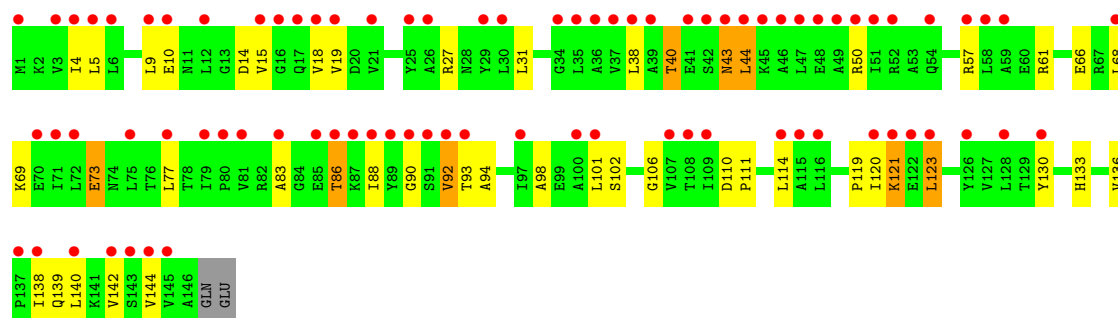
- Molecule 32: 50S ribosomal protein L6

Chain DH: 

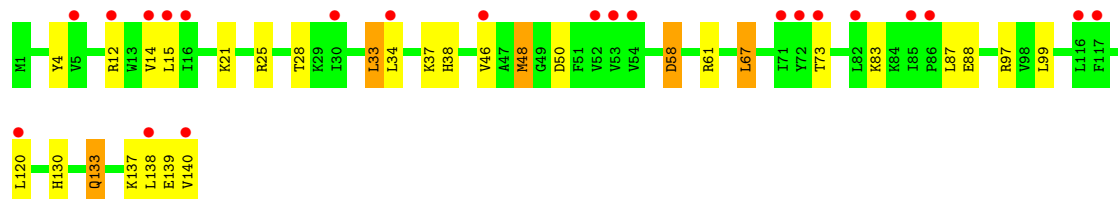
- Molecule 33: 50S ribosomal protein L9

Chain BI: 

- Molecule 33: 50S ribosomal protein L9

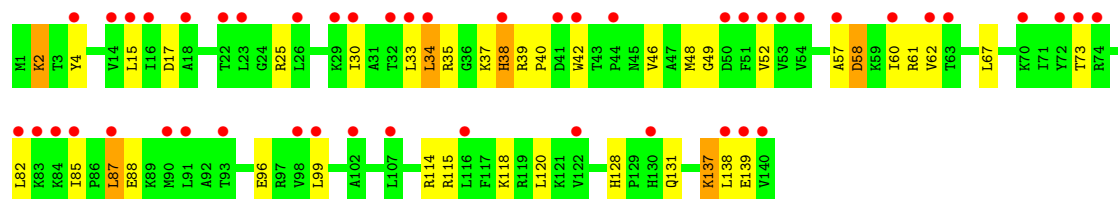
Chain DI: 

- Molecule 34: 50S ribosomal protein L13

Chain BN: 

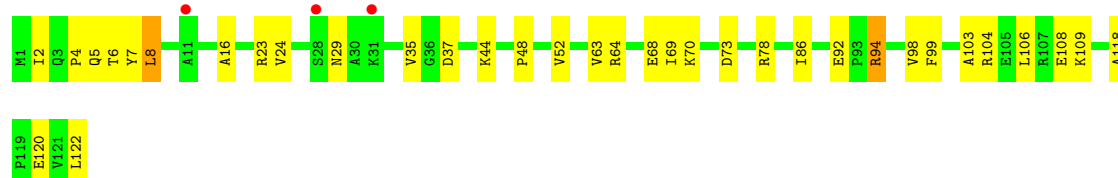
- Molecule 34: 50S ribosomal protein L13

Chain DN: 



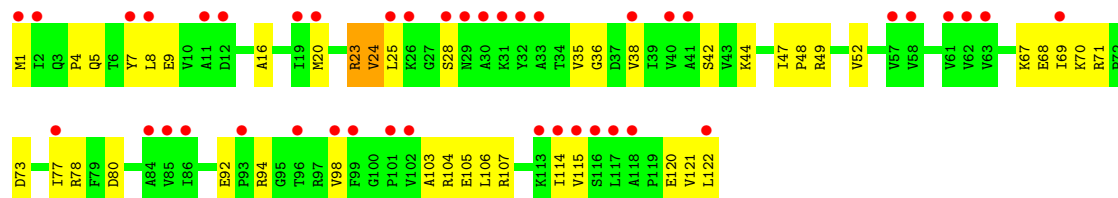
- Molecule 35: 50S ribosomal protein L14

Chain BO: 



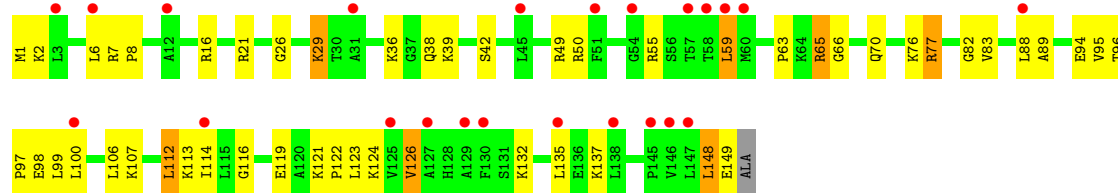
- Molecule 35: 50S ribosomal protein L14

Chain DO: 



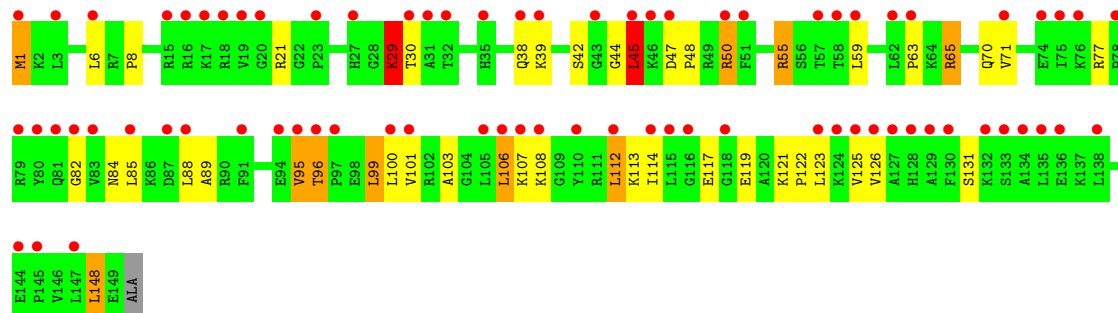
- Molecule 36: 50S ribosomal protein L15

Chain BP: 

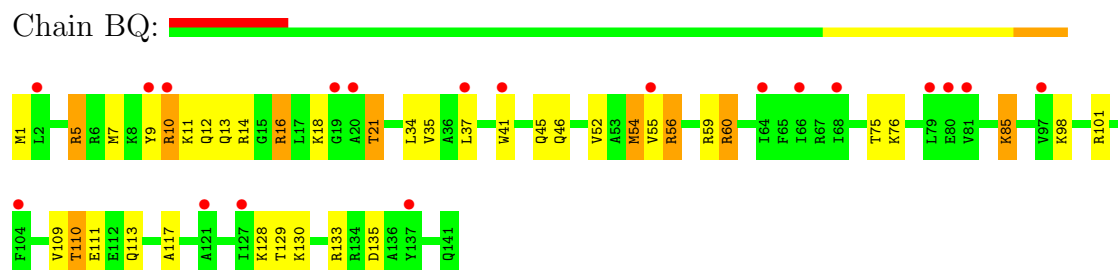


- Molecule 36: 50S ribosomal protein L15

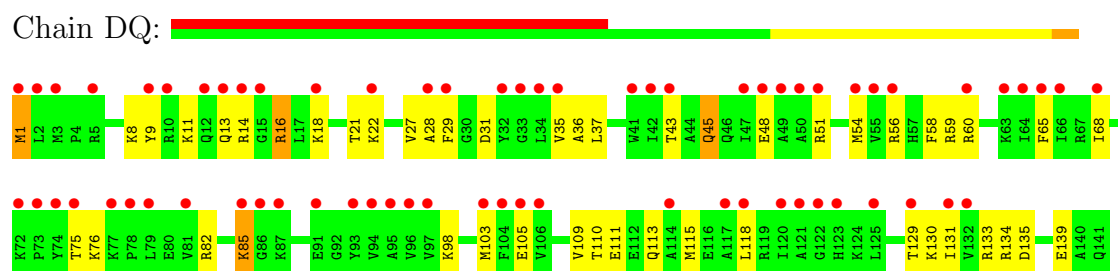
Chain DP: 



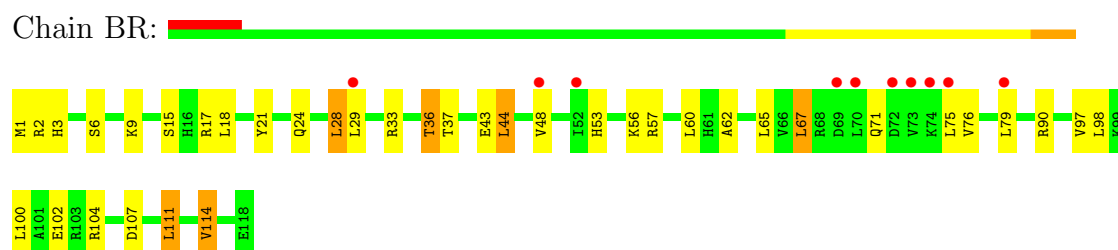
- Molecule 37: 50S ribosomal protein L16



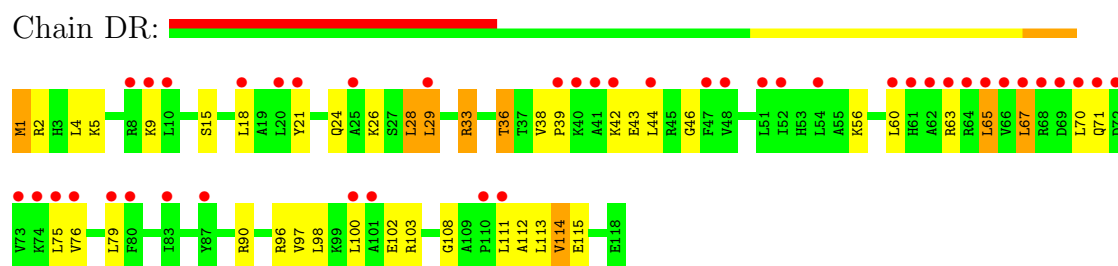
- Molecule 37: 50S ribosomal protein L16



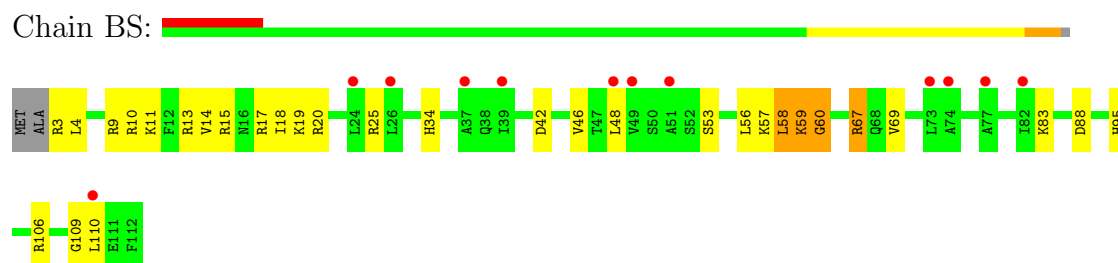
- Molecule 38: 50S ribosomal protein L17



- Molecule 38: 50S ribosomal protein L17

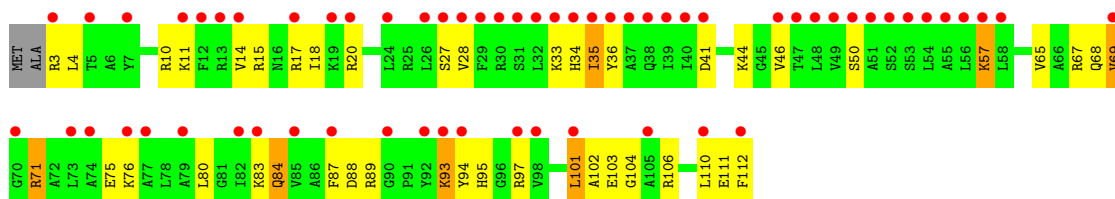


- Molecule 39: 50S ribosomal protein L18



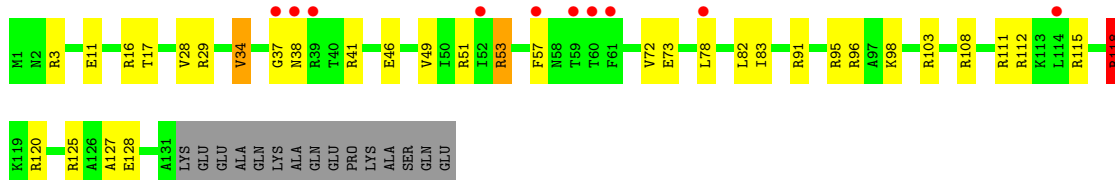
- Molecule 39: 50S ribosomal protein L18

Chain DS: 



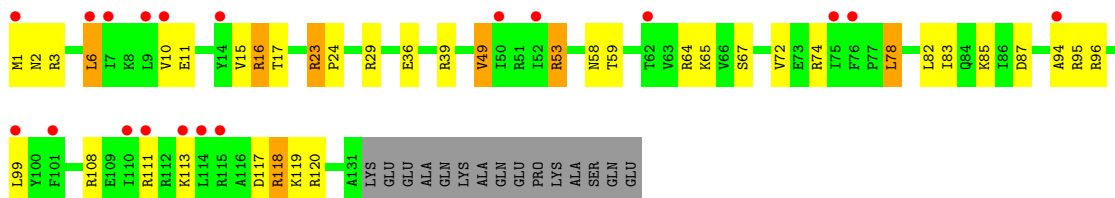
- Molecule 40: 50S ribosomal protein L19

Chain BT: 



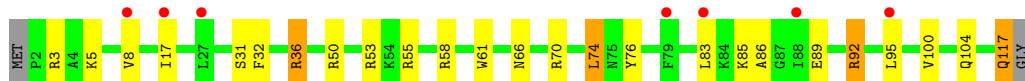
- Molecule 40: 50S ribosomal protein L19

Chain DT: 



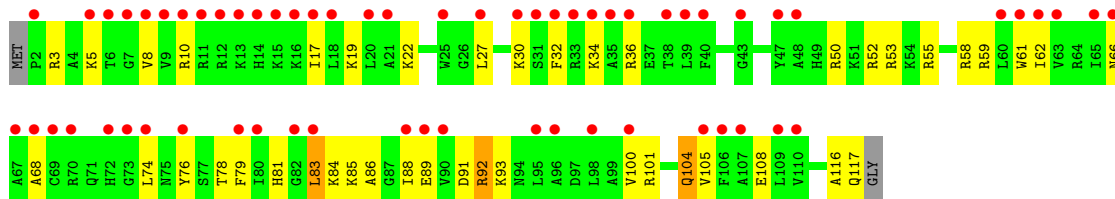
- Molecule 41: 50S ribosomal protein L20

Chain BU: 



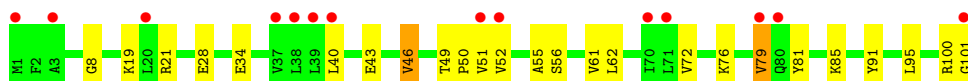
- Molecule 41: 50S ribosomal protein L20

Chain DU: 

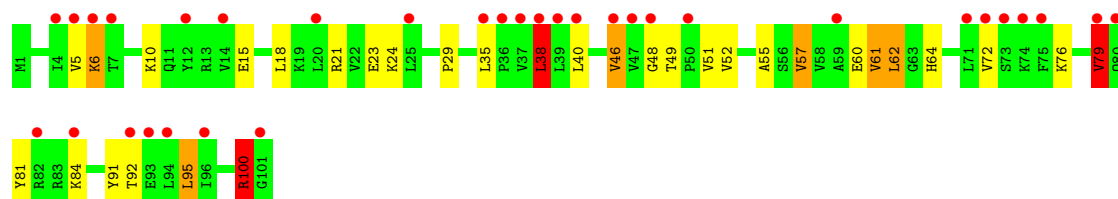


- Molecule 42: 50S ribosomal protein L21

Chain BV: 



- Molecule 42: 50S ribosomal protein L21

Chain DV: 

- Molecule 43: 50S ribosomal protein L22

Chain BW: 

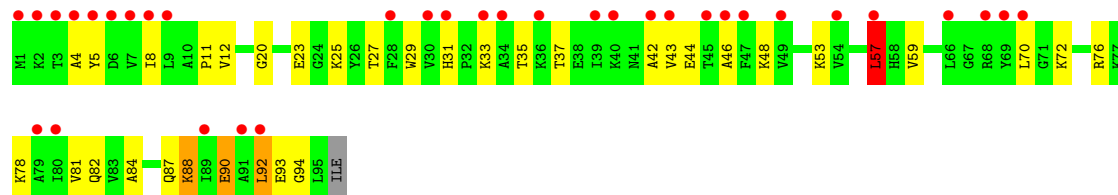
- Molecule 43: 50S ribosomal protein L22

Chain DW: 

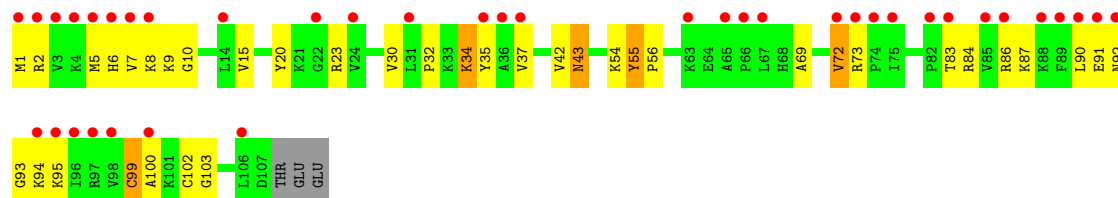
- Molecule 44: 50S ribosomal protein L23

Chain BX: 

- Molecule 44: 50S ribosomal protein L23

Chain DX: 

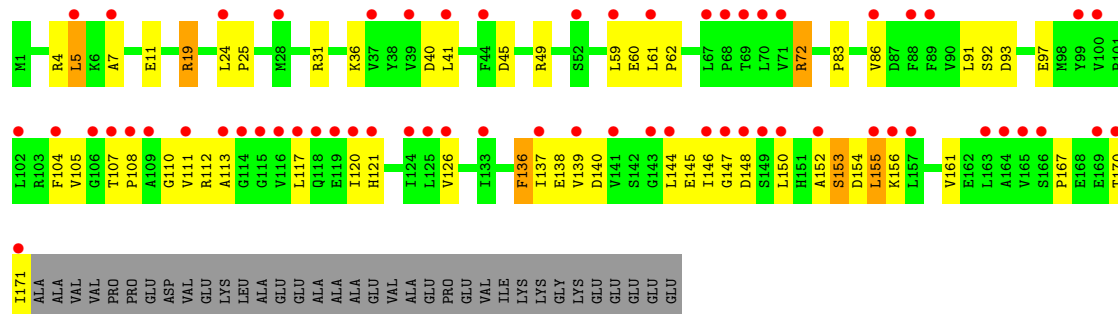
- Molecule 45: 50S ribosomal protein L24

Chain BY: 

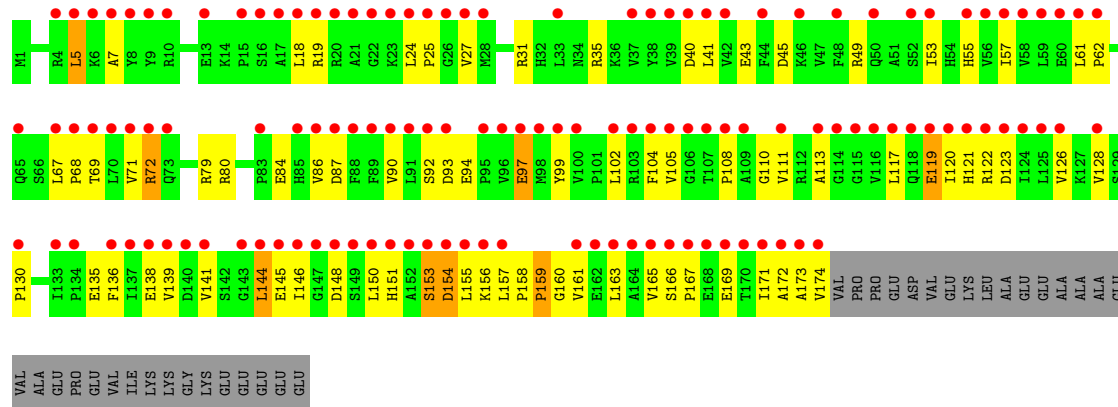
- Molecule 45: 50S ribosomal protein L24

The chart displays the distribution of 100 amino acids across 10 categories. The categories are represented by colored blocks: R73 (red), P74 (orange), I75 (yellow), G80 (green), K81 (dark green), P82 (dark orange), T83 (light green), R84 (dark red), V85 (dark green), R86 (dark red), K87 (dark green), F89 (dark orange), L90 (light green), E91 (yellow), K95 (dark green), I96 (yellow), R97 (dark red), V98 (dark green), C99 (orange), A100 (yellow), L106 (light green), D107 (yellow), THR (grey), and GLU (grey). The chart shows the relative frequency of each amino acid across these categories.

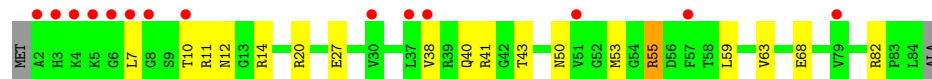
- Chain BZ:



- Chain DZ:

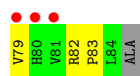


- Chain B0:



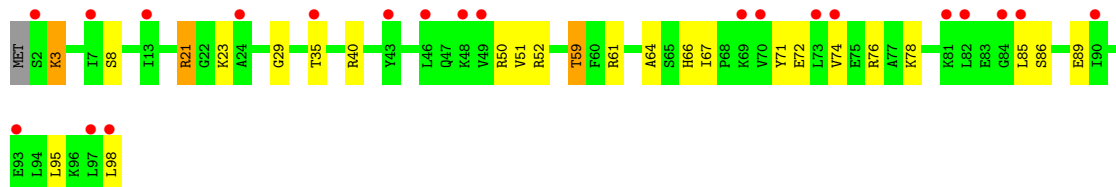
- Chain D0:





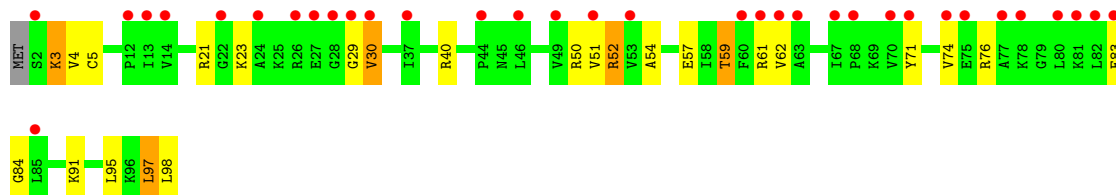
- Molecule 48: 50S ribosomal protein L28

Chain B1:



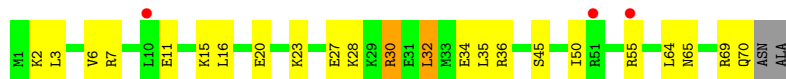
- Molecule 48: 50S ribosomal protein L28

Chain D1:



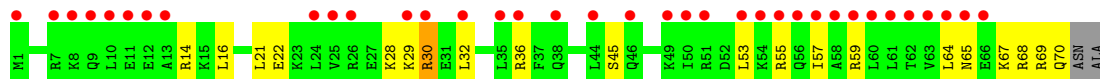
- Molecule 49: 50S ribosomal protein L29

Chain B2:



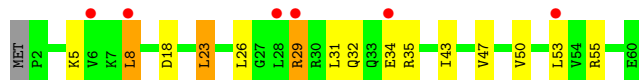
- Molecule 49: 50S ribosomal protein L29

Chain D2:



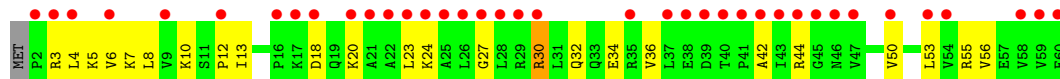
- Molecule 50: 50S ribosomal protein L30

Chain B3:



- Molecule 50: 50S ribosomal protein L30

Chain D3:



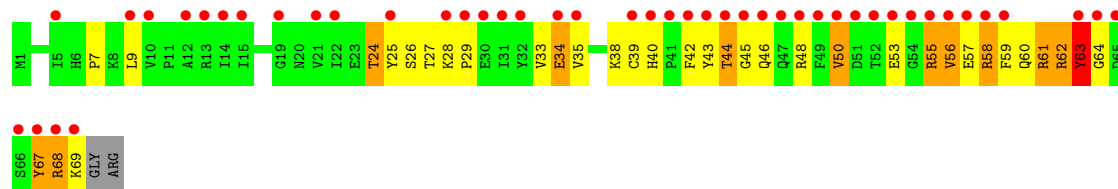
- Molecule 51: 50S ribosomal protein L31

Chain B4:



- Molecule 51: 50S ribosomal protein L31

Chain D4:



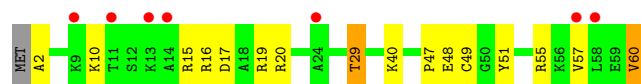
- Molecule 52: 50S ribosomal protein L32

Chain B5:



- Molecule 52: 50S ribosomal protein L32

Chain D5:



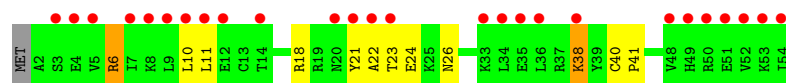
- Molecule 53: 50S ribosomal protein L33

Chain B6:



- Molecule 53: 50S ribosomal protein L33

Chain D6:



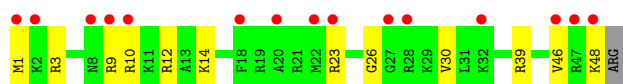
- Molecule 54: 50S ribosomal protein L34

Chain B7:



- Molecule 54: 50S ribosomal protein L34

Chain D7:



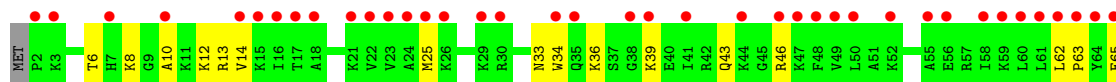
- Molecule 55: 50S ribosomal protein L35

Chain B8:



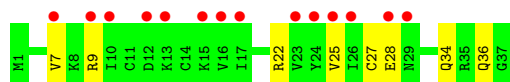
- Molecule 55: 50S ribosomal protein L35

Chain D8:



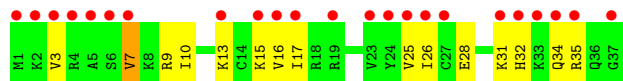
- Molecule 56: 50S ribosomal protein L36

Chain B9:



- Molecule 56: 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	209.32Å 450.06Å 622.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.51 – 2.55 255.92 – 2.55	Depositor EDS
% Data completeness (in resolution range)	95.8 (152.51-2.55) 95.8 (255.92-2.55)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.55Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.233 , 0.280 0.253 , 0.300	Depositor DCC
R_{free} test set	43781 reflections (2.43%)	DCC
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 1802139 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	297141	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 1.64% 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, ZN, 31M, MIA, SF4, MG, 5MC, 4SU, 7MG, K, 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	0.37	0/36049	0.91	42/56261 (0.1%)
1	CA	0.40	6/36170 (0.0%)	1.00	88/56452 (0.2%)
2	AB	0.31	0/1881	0.60	0/2542
2	CB	0.33	0/1860	0.65	1/2518 (0.0%)
3	AC	0.28	0/1576	0.52	0/2130
3	CC	0.32	0/1566	0.61	0/2119
4	AD	0.29	0/1689	0.58	2/2267 (0.1%)
4	CD	0.30	0/1704	0.54	0/2284
5	AE	0.30	0/1145	0.55	0/1543
5	CE	0.31	0/1149	0.62	1/1548 (0.1%)
6	AF	0.28	0/819	0.49	0/1111
6	CF	0.31	0/829	0.52	0/1123
7	AG	0.27	0/1250	0.51	0/1679
7	CG	0.28	0/1254	0.53	0/1683
8	AH	0.27	0/1108	0.50	0/1494
8	CH	0.27	0/1108	0.52	0/1494
9	AI	0.30	0/1002	0.59	0/1346
9	CI	0.30	0/997	0.57	0/1343
10	AJ	0.28	0/722	0.59	0/982
10	CJ	0.31	0/727	0.59	0/988
11	AK	0.28	0/844	0.60	1/1145 (0.1%)
11	CK	0.28	0/848	0.53	0/1149
12	AL	0.30	0/946	0.52	0/1274
12	CL	0.30	0/946	0.55	0/1274
13	AM	0.28	0/969	0.61	0/1302
13	CM	0.29	0/961	0.57	0/1291
14	AN	0.30	0/501	0.50	0/664
14	CN	0.33	0/501	0.57	0/664
15	AO	0.28	0/739	0.55	0/985
15	CO	0.30	0/739	0.54	0/985
16	AP	0.28	0/697	0.52	0/939
16	CP	0.31	0/693	0.51	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.28	0/836	0.53	0/1117
17	CQ	0.29	0/836	0.50	0/1117
18	AR	0.27	0/560	0.56	0/746
18	CR	0.28	0/560	0.56	0/746
19	AS	0.29	0/667	0.58	0/900
19	CS	0.32	0/661	0.67	0/893
20	AT	0.28	0/730	0.58	0/965
20	CT	0.28	0/729	0.52	0/965
21	AU	0.26	0/203	0.52	0/266
21	CU	0.35	0/203	0.52	0/266
22	AV	0.41	0/310	0.94	0/480
22	CV	0.45	0/282	1.06	1/437 (0.2%)
23	AW	0.47	0/1577	1.18	6/2454 (0.2%)
23	CW	0.59	0/1531	1.46	25/2379 (1.1%)
24	AX	0.51	0/1725	1.17	14/2689 (0.5%)
24	CX	0.44	0/1725	1.12	10/2689 (0.4%)
25	AY	0.62	0/1602	1.43	22/2493 (0.9%)
25	CY	0.64	0/1579	1.46	32/2455 (1.3%)
26	BA	0.48	2/68013 (0.0%)	0.95	84/106165 (0.1%)
26	DA	0.42	1/67542 (0.0%)	0.94	72/105428 (0.1%)
27	BB	0.41	0/2878	0.88	0/4490
27	DB	0.44	0/2878	0.94	0/4490
28	BD	0.37	0/2186	0.59	0/2944
28	DD	0.33	0/2186	0.55	0/2944
29	BE	0.36	0/1592	0.57	0/2149
29	DE	0.34	0/1592	0.60	1/2149 (0.0%)
30	BF	0.35	0/1619	0.55	0/2193
30	DF	0.32	0/1615	0.58	0/2188
31	BG	0.31	0/1450	0.54	0/1959
31	DG	0.33	0/1449	0.57	0/1958
32	BH	0.33	0/1356	0.54	0/1834
32	DH	0.30	0/1356	0.52	0/1834
33	BI	0.29	0/1100	0.60	0/1501
33	DI	0.28	0/1076	0.57	0/1471
34	BN	0.32	0/1144	0.53	0/1543
34	DN	0.31	0/1144	0.54	0/1543
35	BO	0.34	0/943	0.58	1/1269 (0.1%)
35	DO	0.31	0/943	0.51	0/1269
36	BP	0.34	0/1152	0.58	0/1533
36	DP	0.31	0/1152	0.59	0/1533
37	BQ	0.34	0/1143	0.53	0/1527
37	DQ	0.31	0/1143	0.52	0/1527
38	BR	0.35	0/982	0.58	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DR	0.29	0/982	0.52	0/1312
39	BS	0.31	0/887	0.63	2/1180 (0.2%)
39	DS	0.29	0/880	0.61	0/1172
40	BT	0.33	0/1105	0.59	1/1477 (0.1%)
40	DT	0.29	0/1097	0.56	0/1468
41	BU	0.37	0/977	0.56	0/1301
41	DU	0.31	0/977	0.50	0/1301
42	BV	0.39	0/782	0.58	0/1049
42	DV	0.32	0/782	0.64	2/1049 (0.2%)
43	BW	0.38	0/897	0.57	0/1205
43	DW	0.31	0/897	0.52	0/1205
44	BX	0.39	0/764	0.59	1/1025 (0.1%)
44	DX	0.32	0/764	0.56	1/1025 (0.1%)
45	BY	0.34	0/819	0.57	0/1095
45	DY	0.31	0/819	0.55	0/1095
46	BZ	0.31	0/1379	0.61	0/1873
46	DZ	0.29	0/1390	0.57	0/1890
47	B0	0.35	0/662	0.57	0/881
47	D0	0.29	0/662	0.49	0/881
48	B1	0.34	0/762	0.56	0/1014
48	D1	0.32	0/762	0.54	0/1014
49	B2	0.32	0/590	0.56	0/781
49	D2	0.27	0/590	0.46	0/781
50	B3	0.36	0/474	0.58	0/635
50	D3	0.27	0/469	0.50	0/630
51	B4	0.35	0/571	0.71	0/768
51	D4	0.34	0/545	0.70	0/737
52	B5	0.38	0/469	0.60	0/635
52	D5	0.33	0/469	0.52	0/635
53	B6	0.36	0/460	0.51	0/613
53	D6	0.30	0/456	0.48	0/608
54	B7	0.39	0/426	0.55	0/561
54	D7	0.33	0/426	0.59	0/561
55	B8	0.36	0/519	0.58	0/684
55	D8	0.32	0/525	0.52	0/691
56	B9	0.35	0/310	0.51	0/407
56	D9	0.31	0/310	0.56	0/407
All	All	0.40	9/316594 (0.0%)	0.88	410/473970 (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	4
7	AG	0	2
7	CG	0	1
20	CT	0	1
28	BD	0	1
39	BS	0	1
51	B4	0	2
51	D4	0	1
All	All	0	13

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	1154	G	N1-C2	-11.01	1.28	1.37
1	CA	1154	G	C6-N1	-10.68	1.32	1.39
1	CA	1119	C	N3-C4	-9.86	1.27	1.33
1	CA	1154	G	N7-C5	-7.17	1.34	1.39
26	BA	354	A	N9-C4	-6.79	1.33	1.37

The worst 5 of 410 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1119	C	N1-C2-O2	32.18	138.21	118.90
1	CA	1154	G	N3-C2-N2	24.48	137.03	119.90
1	CA	1154	G	C5-C6-O6	24.01	143.00	128.60
1	CA	1154	G	N1-C2-N2	-21.95	96.45	116.20
1	CA	1119	C	N3-C2-O2	-20.26	107.72	121.90

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	18	GLY	Peptide
2	AB	231	GLU	Peptide
2	AB	8	LYS	Peptide
2	AB	9	GLU	Peptide
7	AG	78	ARG	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	495	0
1	CA	32312	0	16307	663	0
2	AB	1846	0	1867	92	0
2	CB	1825	0	1828	102	0
3	AC	1552	0	1546	53	0
3	CC	1542	0	1517	81	0
4	AD	1659	0	1676	73	0
4	CD	1674	0	1714	61	0
5	AE	1129	0	1185	34	0
5	CE	1133	0	1191	33	0
6	AF	806	0	793	24	0
6	CF	816	0	808	18	0
7	AG	1231	0	1238	28	0
7	CG	1235	0	1249	37	0
8	AH	1088	0	1126	26	0
8	CH	1088	0	1126	42	0
9	AI	983	0	986	47	0
9	CI	978	0	966	47	0
10	AJ	709	0	650	35	0
10	CJ	714	0	672	36	0
11	AK	829	0	825	20	0
11	CK	833	0	836	14	0
12	AL	930	0	980	24	0
12	CL	930	0	980	27	0
13	AM	958	0	1002	31	0
13	CM	950	0	988	39	0
14	AN	492	0	529	16	0
14	CN	492	0	529	33	0
15	AO	728	0	760	20	0
15	CO	728	0	760	31	0
16	AP	681	0	697	12	0
16	CP	677	0	686	23	0
17	AQ	823	0	891	22	0
17	CQ	823	0	891	15	0
18	AR	555	0	618	17	0
18	CR	555	0	618	16	0
19	AS	652	0	662	31	0
19	CS	646	0	644	42	0
20	AT	728	0	798	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	CT	727	0	796	25	0
21	AU	199	0	208	8	0
21	CU	199	0	208	10	0
22	AV	277	0	140	2	0
22	CV	252	0	130	7	0
23	AW	1607	0	808	52	0
23	CW	1560	0	772	52	0
24	AX	1625	0	828	34	0
24	CX	1625	0	828	32	0
25	AY	1581	0	805	96	0
25	CY	1561	0	796	79	0
26	BA	60729	0	30621	667	0
26	DA	60311	0	30409	875	0
27	BB	2573	0	1306	19	0
27	DB	2573	0	1306	50	0
28	BD	2136	0	2218	51	0
28	DD	2136	0	2218	61	0
29	BE	1559	0	1618	30	0
29	DE	1559	0	1618	45	0
30	BF	1584	0	1625	47	0
30	DF	1580	0	1619	50	0
31	BG	1425	0	1443	38	0
31	DG	1424	0	1434	66	0
32	BH	1330	0	1407	28	0
32	DH	1330	0	1407	30	0
33	BI	1085	0	1114	41	0
33	DI	1061	0	1080	25	0
34	BN	1117	0	1183	17	0
34	DN	1117	0	1184	27	0
35	BO	933	0	996	20	0
35	DO	933	0	996	29	0
36	BP	1135	0	1212	38	0
36	DP	1135	0	1212	43	0
37	BQ	1122	0	1179	31	0
37	DQ	1122	0	1179	35	0
38	BR	968	0	1033	18	0
38	DR	968	0	1033	28	0
39	BS	877	0	938	23	0
39	DS	870	0	923	34	0
40	BT	1091	0	1151	27	0
40	DT	1083	0	1136	31	0
41	BU	959	0	1019	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	DU	959	0	1019	38	0
42	BV	771	0	830	13	0
42	DV	771	0	830	25	0
43	BW	886	0	939	12	0
43	DW	886	0	940	9	0
44	BX	750	0	814	16	0
44	DX	750	0	814	23	0
45	BY	806	0	881	23	0
45	DY	806	0	881	26	0
46	BZ	1349	0	1355	44	0
46	DZ	1360	0	1363	61	0
47	B0	653	0	674	14	0
47	D0	653	0	674	20	0
48	B1	755	0	826	18	0
48	D1	755	0	826	18	0
49	B2	588	0	643	11	0
49	D2	588	0	643	12	0
50	B3	469	0	518	9	0
50	D3	464	0	514	12	0
51	B4	558	0	544	22	0
51	D4	532	0	503	31	0
52	B5	455	0	465	11	0
52	D5	455	0	465	12	0
53	B6	453	0	473	13	0
53	D6	449	0	469	9	0
54	B7	418	0	467	9	0
54	D7	418	0	467	10	0
55	B8	511	0	571	21	0
55	D8	517	0	582	10	0
56	B9	307	0	335	7	0
56	D9	307	0	335	13	0
57	AA	214	0	0	0	0
57	AE	3	0	0	0	0
57	AF	1	0	0	0	0
57	AK	1	0	0	0	0
57	AM	1	0	0	0	0
57	AN	2	0	0	0	0
57	AW	4	0	0	0	0
57	AX	15	0	0	0	0
57	AY	3	0	0	0	0
57	B0	3	0	0	0	0
57	B1	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	B2	1	0	0	0	0
57	B3	2	0	0	0	0
57	B4	1	0	0	0	0
57	B5	1	0	0	0	0
57	B6	2	0	0	0	0
57	B7	5	0	0	0	0
57	B8	1	0	0	0	0
57	B9	1	0	0	0	0
57	BA	812	0	0	0	0
57	BB	20	0	0	0	0
57	BD	9	0	0	0	0
57	BE	8	0	0	0	0
57	BF	9	0	0	0	0
57	BG	3	0	0	0	0
57	BN	6	0	0	0	0
57	BO	2	0	0	0	0
57	BP	5	0	0	0	0
57	BQ	5	0	0	0	0
57	BR	2	0	0	0	0
57	BU	8	0	0	0	0
57	BV	5	0	0	0	0
57	BW	4	0	0	0	0
57	BX	3	0	0	0	0
57	BY	1	0	0	0	0
57	BZ	1	0	0	0	0
57	CA	170	0	0	0	0
57	CD	1	0	0	0	0
57	CE	1	0	0	0	0
57	CF	1	0	0	0	0
57	CJ	1	0	0	0	0
57	CK	1	0	0	0	0
57	CT	1	0	0	0	0
57	CV	1	0	0	0	0
57	CW	1	0	0	0	0
57	CX	3	0	0	1	0
57	D0	1	0	0	0	0
57	D3	1	0	0	0	0
57	D8	1	0	0	0	0
57	DA	677	0	0	0	0
57	DB	13	0	0	0	0
57	DD	9	0	0	0	0
57	DE	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	DF	4	0	0	0	0
57	DG	1	0	0	0	0
57	DN	1	0	0	0	0
57	DO	1	0	0	0	0
57	DP	2	0	0	0	0
57	DQ	4	0	0	0	0
57	DR	1	0	0	0	0
57	DU	2	0	0	0	0
57	DV	3	0	0	0	0
57	DW	4	0	0	0	0
57	DX	1	0	0	0	0
57	DY	1	0	0	0	0
58	AD	8	0	0	0	0
58	CD	8	0	0	0	0
59	AN	1	0	0	0	0
59	B4	1	0	0	0	0
59	B5	1	0	0	0	0
59	B6	1	0	0	0	0
59	B9	1	0	0	0	0
59	BY	1	0	0	0	0
59	CN	1	0	0	0	0
59	D4	1	0	0	0	0
59	D5	1	0	0	0	0
59	D6	1	0	0	0	0
59	D9	1	0	0	0	0
59	DY	1	0	0	0	0
60	AX	1	0	0	0	0
60	CX	1	0	0	0	0
61	AA	227	0	0	17	0
61	AE	2	0	0	0	0
61	AJ	1	0	0	0	0
61	AL	1	0	0	1	0
61	AM	1	0	0	0	0
61	AU	1	0	0	1	0
61	AV	3	0	0	0	0
61	AW	3	0	0	0	0
61	AX	6	0	0	2	0
61	AY	1	0	0	0	0
61	B0	3	0	0	0	0
61	B1	1	0	0	0	0
61	B3	2	0	0	0	0
61	B5	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	B6	1	0	0	0	0
61	B7	2	0	0	0	0
61	B8	8	0	0	1	0
61	BA	1383	0	0	61	0
61	BB	36	0	0	1	0
61	BD	12	0	0	1	0
61	BE	14	0	0	4	0
61	BF	8	0	0	0	0
61	BG	3	0	0	0	0
61	BI	1	0	0	0	0
61	BO	4	0	0	0	0
61	BP	16	0	0	3	0
61	BQ	4	0	0	0	0
61	BR	2	0	0	0	0
61	BT	2	0	0	0	0
61	BU	3	0	0	0	0
61	BV	2	0	0	0	0
61	BW	1	0	0	0	0
61	BX	4	0	0	0	0
61	BZ	1	0	0	0	0
61	CA	185	0	0	17	0
61	CJ	2	0	0	1	0
61	CL	1	0	0	0	0
61	CT	1	0	0	0	0
61	CV	1	0	0	0	0
61	CW	2	0	0	0	0
61	D0	3	0	0	0	0
61	D1	1	0	0	0	0
61	D3	1	0	0	1	0
61	D7	3	0	0	0	0
61	D8	4	0	0	0	0
61	DA	1025	0	0	79	0
61	DB	9	0	0	0	0
61	DD	19	0	0	4	0
61	DE	11	0	0	0	0
61	DF	3	0	0	0	0
61	DN	2	0	0	1	0
61	DO	1	0	0	0	0
61	DP	16	0	0	2	0
61	DR	1	0	0	0	0
61	DT	3	0	0	0	0
61	DU	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	DX	3	0	0	0	0
61	DY	2	0	0	0	0
All	All	297141	0	196189	5222	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 11.

The worst 5 of 5222 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:CY:7:A:N6	25:CY:66:U:H3	1.37	1.21
25:AY:49:C:N4	25:AY:65:G:H1	1.44	1.16
26:DA:2139:C:N4	26:DA:2152:G:H1	1.42	1.16
1:CA:1000:U:H3	1:CA:1041:A:N6	1.44	1.15
1:CA:1002:G:H1	1:CA:1038:C:N4	1.48	1.12

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%)	14 (6%)	7 (3%)	7	8
2	CB	229/256 (90%)	206 (90%)	16 (7%)	7 (3%)	7	8
3	AC	204/239 (85%)	195 (96%)	8 (4%)	1 (0%)	38	60
3	CC	204/239 (85%)	189 (93%)	15 (7%)	0	100	100
4	AD	206/209 (99%)	197 (96%)	7 (3%)	2 (1%)	22	37
4	CD	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	38	60
5	AE	146/162 (90%)	142 (97%)	4 (3%)	0	100	100
5	CE	146/162 (90%)	140 (96%)	6 (4%)	0	100	100
6	AF	98/101 (97%)	97 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	CF	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
7	AG	153/156 (98%)	144 (94%)	5 (3%)	4 (3%)	8	11
7	CG	153/156 (98%)	144 (94%)	8 (5%)	1 (1%)	30	49
8	AH	135/138 (98%)	134 (99%)	1 (1%)	0	100	100
8	CH	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
9	AI	125/128 (98%)	117 (94%)	8 (6%)	0	100	100
9	CI	125/128 (98%)	119 (95%)	5 (4%)	1 (1%)	27	45
10	AJ	95/105 (90%)	85 (90%)	6 (6%)	4 (4%)	4	4
10	CJ	94/105 (90%)	85 (90%)	4 (4%)	5 (5%)	3	2
11	AK	112/129 (87%)	104 (93%)	6 (5%)	2 (2%)	13	20
11	CK	112/129 (87%)	103 (92%)	7 (6%)	2 (2%)	13	20
12	AL	120/132 (91%)	117 (98%)	3 (2%)	0	100	100
12	CL	120/132 (91%)	118 (98%)	2 (2%)	0	100	100
13	AM	121/126 (96%)	116 (96%)	5 (4%)	0	100	100
13	CM	120/126 (95%)	113 (94%)	7 (6%)	0	100	100
14	AN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
14	CN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
15	AO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
15	CO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	AP	80/88 (91%)	79 (99%)	1 (1%)	0	100	100
16	CP	80/88 (91%)	78 (98%)	1 (1%)	1 (1%)	18	29
17	AQ	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
17	CQ	97/105 (92%)	93 (96%)	4 (4%)	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%)	73 (90%)	7 (9%)	1 (1%)	19	31
19	CS	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
20	AT	94/106 (89%)	87 (93%)	3 (3%)	4 (4%)	4	4
20	CT	94/106 (89%)	88 (94%)	3 (3%)	3 (3%)	6	7
21	AU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
21	CU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	BD	273/276 (99%)	264 (97%)	8 (3%)	1 (0%)	43	66
28	DD	273/276 (99%)	263 (96%)	8 (3%)	2 (1%)	30	49
29	BE	202/206 (98%)	196 (97%)	5 (2%)	1 (0%)	38	60
29	DE	202/206 (98%)	196 (97%)	4 (2%)	2 (1%)	22	37
30	BF	201/210 (96%)	200 (100%)	0	1 (0%)	38	60
30	DF	201/210 (96%)	199 (99%)	0	2 (1%)	22	37
31	BG	179/182 (98%)	170 (95%)	8 (4%)	1 (1%)	33	54
31	DG	179/182 (98%)	171 (96%)	5 (3%)	3 (2%)	14	21
32	BH	172/180 (96%)	168 (98%)	3 (2%)	1 (1%)	33	54
32	DH	172/180 (96%)	166 (96%)	5 (3%)	1 (1%)	33	54
33	BI	144/148 (97%)	130 (90%)	11 (8%)	3 (2%)	11	16
33	DI	144/148 (97%)	133 (92%)	10 (7%)	1 (1%)	30	49
34	BN	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
34	DN	138/140 (99%)	135 (98%)	2 (1%)	1 (1%)	30	49
35	BO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
35	DO	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
36	BP	147/150 (98%)	140 (95%)	6 (4%)	1 (1%)	30	49
36	DP	147/150 (98%)	138 (94%)	7 (5%)	2 (1%)	16	27
37	BQ	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
37	DQ	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	30	49
38	BR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
38	DR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
39	BS	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	25	41
39	DS	108/112 (96%)	105 (97%)	2 (2%)	1 (1%)	25	41
40	BT	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
40	DT	129/146 (88%)	127 (98%)	2 (2%)	0	100	100
41	BU	114/118 (97%)	114 (100%)	0	0	100	100
41	DU	114/118 (97%)	114 (100%)	0	0	100	100
42	BV	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
42	DV	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	22	37
43	BW	110/113 (97%)	110 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	DW	110/113 (97%)	110 (100%)	0	0	100	100
44	BX	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
44	DX	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
45	BY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
45	DY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
46	BZ	169/206 (82%)	153 (90%)	15 (9%)	1 (1%)	33	54
46	DZ	172/206 (84%)	161 (94%)	11 (6%)	0	100	100
47	B0	81/85 (95%)	81 (100%)	0	0	100	100
47	D0	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
48	B1	95/98 (97%)	94 (99%)	0	1 (1%)	21	34
48	D1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	21	34
49	B2	68/72 (94%)	68 (100%)	0	0	100	100
49	D2	68/72 (94%)	68 (100%)	0	0	100	100
50	B3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
50	D3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
51	B4	67/71 (94%)	53 (79%)	11 (16%)	3 (4%)	4	4
51	D4	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	2	1
52	B5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
52	D5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
53	B6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
53	D6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
54	B7	46/49 (94%)	46 (100%)	0	0	100	100
54	D7	46/49 (94%)	45 (98%)	0	1 (2%)	10	15
55	B8	62/65 (95%)	62 (100%)	0	0	100	100
55	D8	62/65 (95%)	62 (100%)	0	0	100	100
56	B9	35/37 (95%)	35 (100%)	0	0	100	100
56	D9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11409/12128 (94%)	10908 (96%)	416 (4%)	85 (1%)	30	49

5 of 85 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	126	GLU

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Mol	Chain	Res	Type
7	AG	80	VAL
20	AT	10	LEU
20	AT	96	GLY
28	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%)	163 (85%)	29 (15%)	4	7
2	CB	187/220 (85%)	149 (80%)	38 (20%)	2	3
3	AC	143/188 (76%)	121 (85%)	22 (15%)	4	6
3	CC	140/188 (74%)	124 (89%)	16 (11%)	8	14
4	AD	170/181 (94%)	152 (89%)	18 (11%)	10	17
4	CD	173/181 (96%)	152 (88%)	21 (12%)	7	12
5	AE	113/123 (92%)	105 (93%)	8 (7%)	21	36
5	CE	114/123 (93%)	101 (89%)	13 (11%)	8	14
6	AF	83/90 (92%)	76 (92%)	7 (8%)	16	27
6	CF	85/90 (94%)	80 (94%)	5 (6%)	28	46
7	AG	119/127 (94%)	108 (91%)	11 (9%)	13	23
7	CG	120/127 (94%)	109 (91%)	11 (9%)	13	23
8	AH	114/119 (96%)	105 (92%)	9 (8%)	18	30
8	CH	114/119 (96%)	107 (94%)	7 (6%)	26	44
9	AI	90/99 (91%)	76 (84%)	14 (16%)	4	6
9	CI	89/99 (90%)	76 (85%)	13 (15%)	5	7
10	AJ	66/92 (72%)	58 (88%)	8 (12%)	7	12
10	CJ	69/92 (75%)	63 (91%)	6 (9%)	15	26
11	AK	82/99 (83%)	77 (94%)	5 (6%)	26	44
11	CK	83/99 (84%)	76 (92%)	7 (8%)	16	27
12	AL	97/109 (89%)	93 (96%)	4 (4%)	41	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	CL	97/109 (89%)	93 (96%)	4 (4%)	41	66
13	AM	93/101 (92%)	82 (88%)	11 (12%)	8	13
13	CM	92/101 (91%)	80 (87%)	12 (13%)	6	10
14	AN	49/50 (98%)	42 (86%)	7 (14%)	5	8
14	CN	49/50 (98%)	41 (84%)	8 (16%)	3	5
15	AO	78/80 (98%)	64 (82%)	14 (18%)	2	4
15	CO	78/80 (98%)	69 (88%)	9 (12%)	8	14
16	AP	69/74 (93%)	60 (87%)	9 (13%)	6	10
16	CP	68/74 (92%)	61 (90%)	7 (10%)	10	18
17	AQ	94/97 (97%)	85 (90%)	9 (10%)	12	21
17	CQ	94/97 (97%)	87 (93%)	7 (7%)	20	34
18	AR	59/77 (77%)	54 (92%)	5 (8%)	15	27
18	CR	59/77 (77%)	52 (88%)	7 (12%)	8	13
19	AS	69/80 (86%)	64 (93%)	5 (7%)	21	35
19	CS	67/80 (84%)	63 (94%)	4 (6%)	27	45
20	AT	70/82 (85%)	62 (89%)	8 (11%)	8	14
20	CT	70/82 (85%)	62 (89%)	8 (11%)	8	14
21	AU	18/22 (82%)	15 (83%)	3 (17%)	3	5
21	CU	18/22 (82%)	17 (94%)	1 (6%)	30	49
28	BD	215/218 (99%)	195 (91%)	20 (9%)	13	22
28	DD	215/218 (99%)	193 (90%)	22 (10%)	11	18
29	BE	164/166 (99%)	146 (89%)	18 (11%)	9	15
29	DE	164/166 (99%)	145 (88%)	19 (12%)	8	13
30	BF	160/166 (96%)	149 (93%)	11 (7%)	22	37
30	DF	159/166 (96%)	144 (91%)	15 (9%)	13	22
31	BG	143/156 (92%)	128 (90%)	15 (10%)	10	17
31	DG	142/156 (91%)	122 (86%)	20 (14%)	5	8
32	BH	144/148 (97%)	126 (88%)	18 (12%)	7	11
32	DH	144/148 (97%)	126 (88%)	18 (12%)	7	11
33	BI	110/124 (89%)	86 (78%)	24 (22%)	1	2
33	DI	104/124 (84%)	88 (85%)	16 (15%)	4	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	BN	118/119 (99%)	103 (87%)	15 (13%)	6	11
34	DN	118/119 (99%)	106 (90%)	12 (10%)	11	18
35	BO	100/100 (100%)	93 (93%)	7 (7%)	21	37
35	DO	100/100 (100%)	93 (93%)	7 (7%)	21	37
36	BP	115/116 (99%)	98 (85%)	17 (15%)	4	7
36	DP	115/116 (99%)	100 (87%)	15 (13%)	6	10
37	BQ	111/111 (100%)	95 (86%)	16 (14%)	5	8
37	DQ	111/111 (100%)	99 (89%)	12 (11%)	9	16
38	BR	101/101 (100%)	82 (81%)	19 (19%)	2	3
38	DR	101/101 (100%)	83 (82%)	18 (18%)	2	4
39	BS	87/88 (99%)	81 (93%)	6 (7%)	22	37
39	DS	85/88 (97%)	75 (88%)	10 (12%)	8	13
40	BT	115/127 (91%)	106 (92%)	9 (8%)	18	31
40	DT	113/127 (89%)	103 (91%)	10 (9%)	14	25
41	BU	93/94 (99%)	84 (90%)	9 (10%)	12	20
41	DU	93/94 (99%)	85 (91%)	8 (9%)	15	26
42	BV	80/82 (98%)	68 (85%)	12 (15%)	4	7
42	DV	80/82 (98%)	67 (84%)	13 (16%)	3	5
43	BW	90/92 (98%)	83 (92%)	7 (8%)	18	31
43	DW	90/92 (98%)	83 (92%)	7 (8%)	18	31
44	BX	77/78 (99%)	71 (92%)	6 (8%)	18	31
44	DX	77/78 (99%)	71 (92%)	6 (8%)	18	31
45	BY	85/91 (93%)	75 (88%)	10 (12%)	8	13
45	DY	85/91 (93%)	79 (93%)	6 (7%)	21	36
46	BZ	145/179 (81%)	133 (92%)	12 (8%)	16	28
46	DZ	145/179 (81%)	129 (89%)	16 (11%)	9	15
47	B0	65/67 (97%)	62 (95%)	3 (5%)	37	60
47	D0	65/67 (97%)	60 (92%)	5 (8%)	18	32
48	B1	80/83 (96%)	73 (91%)	7 (9%)	14	25
48	D1	80/83 (96%)	71 (89%)	9 (11%)	9	14
49	B2	65/67 (97%)	57 (88%)	8 (12%)	7	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	D2	65/67 (97%)	59 (91%)	6 (9%)	13	23
50	B3	51/52 (98%)	46 (90%)	5 (10%)	12	20
50	D3	50/52 (96%)	44 (88%)	6 (12%)	7	12
51	B4	60/63 (95%)	47 (78%)	13 (22%)	1	2
51	D4	53/63 (84%)	43 (81%)	10 (19%)	2	3
52	B5	50/52 (96%)	45 (90%)	5 (10%)	11	19
52	D5	50/52 (96%)	46 (92%)	4 (8%)	17	30
53	B6	51/52 (98%)	44 (86%)	7 (14%)	5	9
53	D6	50/52 (96%)	48 (96%)	2 (4%)	42	67
54	B7	41/42 (98%)	38 (93%)	3 (7%)	20	35
54	D7	41/42 (98%)	38 (93%)	3 (7%)	20	35
55	B8	53/55 (96%)	49 (92%)	4 (8%)	19	33
55	D8	54/55 (98%)	51 (94%)	3 (6%)	30	49
56	B9	34/34 (100%)	34 (100%)	0	100	100
56	D9	34/34 (100%)	32 (94%)	2 (6%)	28	46
All	All	9320/10066 (93%)	8304 (89%)	1016 (11%)	9	15

5 of 1016 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	B0	82	ARG
4	CD	31	CYS
44	DX	57	LEU
49	B2	64	LEU
2	CB	24	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 130 such sidechains are listed below:

Mol	Chain	Res	Type
40	BT	123	GLN
3	CC	28	GLN
40	DT	123	GLN
44	BX	31	HIS
51	B4	46	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1495/1521 (98%)	304 (20%)	25 (1%)
1	CA	1501/1521 (98%)	316 (21%)	28 (1%)
22	AV	12/24 (50%)	3 (25%)	0
22	CV	11/24 (45%)	2 (18%)	0
23	AW	70/76 (92%)	30 (42%)	2 (2%)
23	CW	67/76 (88%)	32 (47%)	2 (2%)
24	AX	75/77 (97%)	16 (21%)	0
24	CX	75/77 (97%)	21 (28%)	0
25	AY	71/76 (93%)	35 (49%)	4 (5%)
25	CY	69/76 (90%)	32 (46%)	1 (1%)
26	BA	2811/2915 (96%)	450 (16%)	34 (1%)
26	DA	2791/2915 (95%)	552 (19%)	30 (1%)
27	BB	119/121 (98%)	14 (11%)	0
27	DB	119/121 (98%)	17 (14%)	0
All	All	9286/9620 (96%)	1824 (19%)	126 (1%)

5 of 1824 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	7	G
1	AA	9	G
1	AA	22	G
1	AA	29	G

5 of 126 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	BA	2148	A
1	CA	509	A
26	DA	1992	G
26	BA	2205	C
26	BA	2769	U

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

38 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	PSU	AW	32	23	19,21,22	1.79	4 (21%)	23,30,33	1.25	2 (8%)
23	MIA	AW	37	23	29,31,32	1.83	5 (17%)	41,44,47	1.87	9 (21%)
23	PSU	AW	39	23	19,21,22	1.96	5 (26%)	23,30,33	1.05	1 (4%)
23	7MG	AW	46	23	24,26,27	2.02	7 (29%)	34,39,42	2.55	10 (29%)
23	5MU	AW	54	23	20,22,23	1.64	4 (20%)	25,32,35	2.01	3 (12%)
23	PSU	AW	55	23	19,21,22	1.84	4 (21%)	23,30,33	1.35	2 (8%)
23	31M	AW	76	23	42,44,45	1.40	5 (11%)	58,61,64	1.99	11 (18%)
23	4SU	AW	8	23	19,21,22	1.78	4 (21%)	23,30,33	1.81	4 (17%)
24	5MC	AX	32	24	20,22,23	1.77	4 (20%)	26,32,35	1.58	4 (15%)
24	5MU	AX	54	24,57	20,22,23	1.69	5 (25%)	25,32,35	2.17	5 (20%)
24	PSU	AX	55	24,57	19,21,22	1.93	4 (21%)	23,30,33	1.11	3 (13%)
24	4SU	AX	8	24	19,21,22	1.75	4 (21%)	23,30,33	34.05	2 (8%)
25	PSU	AY	32	25	19,21,22	1.77	4 (21%)	23,30,33	1.26	3 (13%)
25	MIA	AY	37	25	20,24,32	1.77	5 (25%)	27,35,47	1.92	5 (18%)
25	PSU	AY	39	25	19,21,22	1.82	6 (31%)	23,30,33	1.55	1 (4%)
25	7MG	AY	46	25	24,26,27	2.00	7 (29%)	34,39,42	2.47	10 (29%)
25	5MU	AY	54	25	20,22,23	1.92	5 (25%)	25,32,35	2.00	5 (20%)
25	PSU	AY	55	25	19,21,22	2.03	5 (26%)	23,30,33	1.26	4 (17%)
25	4SU	AY	8	25	19,21,22	1.77	4 (21%)	23,30,33	2.51	4 (17%)
23	PSU	CW	32	23	19,21,22	1.87	4 (21%)	23,30,33	0.91	2 (8%)
23	MIA	CW	37	23	20,24,32	1.73	5 (25%)	27,35,47	1.99	4 (14%)
23	PSU	CW	39	23	19,21,22	1.97	4 (21%)	23,30,33	1.25	2 (8%)
23	7MG	CW	46	23	24,26,27	2.00	8 (33%)	34,39,42	2.24	9 (26%)
23	5MU	CW	54	23	20,22,23	1.68	4 (20%)	25,32,35	2.05	4 (16%)
23	PSU	CW	55	23	19,21,22	1.78	4 (21%)	23,30,33	1.29	2 (8%)
23	31M	CW	76	23	42,44,45	1.39	5 (11%)	58,61,64	1.93	9 (15%)
23	4SU	CW	8	23	19,21,22	1.69	4 (21%)	23,30,33	7.12	4 (17%)
24	5MC	CX	32	24	20,22,23	1.75	4 (20%)	26,32,35	1.53	4 (15%)
24	5MU	CX	54	24	20,22,23	1.57	5 (25%)	25,32,35	2.72	4 (16%)
24	PSU	CX	55	24	19,21,22	1.83	4 (21%)	23,30,33	1.01	3 (13%)
24	4SU	CX	8	24	19,21,22	1.86	4 (21%)	23,30,33	23.29	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PSU	CY	32	25	19,21,22	1.79	4 (21%)	23,30,33	1.06	3 (13%)
25	MIA	CY	37	25	20,24,32	1.81	5 (25%)	27,35,47	2.02	5 (18%)
25	PSU	CY	39	25	19,21,22	1.86	4 (21%)	23,30,33	1.22	2 (8%)
25	7MG	CY	46	25	24,26,27	2.04	7 (29%)	34,39,42	2.48	10 (29%)
25	5MU	CY	54	25	20,22,23	1.67	5 (25%)	25,32,35	1.63	4 (16%)
25	PSU	CY	55	25	19,21,22	1.74	5 (26%)	23,30,33	2.17	3 (13%)
25	4SU	CY	8	25	19,21,22	1.80	4 (21%)	23,30,33	14.01	4 (17%)

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	PSU	AW	32	23	-	0/8/25/26	0/2/2/2
23	MIA	AW	37	23	-	0/16/33/34	0/3/3/3
23	PSU	AW	39	23	-	0/8/25/26	0/2/2/2
23	7MG	AW	46	23	-	1/8/37/38	0/3/3/3
23	5MU	AW	54	23	-	0/6/25/26	0/2/2/2
23	PSU	AW	55	23	-	0/8/25/26	0/2/2/2
23	31M	AW	76	23	-	0/32/49/50	0/4/4/4
23	4SU	AW	8	23	-	0/6/25/26	0/2/2/2
24	5MC	AX	32	24	-	0/6/25/26	0/2/2/2
24	5MU	AX	54	24,57	-	0/6/25/26	0/2/2/2
24	PSU	AX	55	24,57	-	0/8/25/26	0/2/2/2
24	4SU	AX	8	24	-	0/6/25/26	0/2/2/2
25	PSU	AY	32	25	-	0/8/25/26	0/2/2/2
25	MIA	AY	37	25	-	0/8/25/34	0/3/3/3
25	PSU	AY	39	25	-	0/8/25/26	0/2/2/2
25	7MG	AY	46	25	-	1/8/37/38	0/3/3/3
25	5MU	AY	54	25	-	1/6/25/26	0/2/2/2
25	PSU	AY	55	25	-	0/8/25/26	0/2/2/2
25	4SU	AY	8	25	-	0/6/25/26	0/2/2/2
23	PSU	CW	32	23	-	0/8/25/26	0/2/2/2
23	MIA	CW	37	23	-	0/8/25/34	0/3/3/3
23	PSU	CW	39	23	-	0/8/25/26	0/2/2/2
23	7MG	CW	46	23	-	1/8/37/38	0/3/3/3
23	5MU	CW	54	23	-	0/6/25/26	0/2/2/2
23	PSU	CW	55	23	-	0/8/25/26	0/2/2/2
23	31M	CW	76	23	-	0/32/49/50	0/4/4/4
23	4SU	CW	8	23	-	0/6/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	4SU	CX	8	24	-	0/6/25/26	0/2/2/2
25	PSU	CY	32	25	-	0/8/25/26	0/2/2/2
25	MIA	CY	37	25	-	0/8/25/34	0/3/3/3
25	PSU	CY	39	25	-	0/8/25/26	0/2/2/2
25	7MG	CY	46	25	-	0/8/37/38	0/3/3/3
25	5MU	CY	54	25	-	0/6/25/26	0/2/2/2
25	PSU	CY	55	25	-	0/8/25/26	0/2/2/2
25	4SU	CY	8	25	-	1/6/25/26	0/2/2/2

The worst 5 of 180 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	37	MIA	C2-S10	-6.34	1.70	1.75
25	CY	46	7MG	C6-C5	5.92	1.48	1.41
25	AY	55	PSU	C5-C1'	-5.64	1.47	1.52
23	CW	46	7MG	C6-C5	5.55	1.48	1.41
23	AW	46	7MG	C6-C5	5.10	1.47	1.41

The worst 5 of 168 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AX	8	4SU	C4-N3-C2	163.15	128.58	121.60
24	CX	8	4SU	C4-N3-C2	111.39	126.36	121.60
25	CY	8	4SU	C4-N3-C2	-66.72	118.75	121.60
23	CW	8	4SU	C4-N3-C2	-33.23	120.18	121.60
23	AW	76	31M	N3-C2-N1	-10.00	120.09	128.89

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	CY	8	4SU	OP2-P-O5'-C5'
23	CW	46	7MG	OP2-P-O5'-C5'
25	AY	46	7MG	OP2-P-O5'-C5'
25	AY	54	5MU	OP2-P-O5'-C5'
23	AW	46	7MG	OP2-P-O5'-C5'

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2093 ligands modelled in this entry, 2091 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	$\# Z > 2$
58	SF4	AD	501	4	12,12,12	22.07	12 (100%)	0,24,24	0.00	-
58	SF4	CD	302	4	12,12,12	21.92	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
58	SF4	AD	501	4	-	0/0/48/48	0/6/5/5
58	SF4	CD	302	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)
58	CD	302	SF4	S4-FE2	-23.18	2.17	2.33
58	AD	501	SF4	S3-FE2	-22.89	2.17	2.33
58	CD	302	SF4	S1-FE2	-22.79	2.17	2.33
58	CD	302	SF4	S4-FE1	-22.67	2.18	2.33
58	AD	501	SF4	S2-FE1	-22.60	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%)	0.84	92 (6%) 21 21	42, 72, 93, 108	0
1	CA	1503/1521 (98%)	0.86	178 (11%) 5 5	44, 74, 94, 109	0
2	AB	231/256 (90%)	3.78	158 (68%) 0 0	72, 82, 90, 94	0
2	CB	231/256 (90%)	4.30	154 (66%) 0 0	73, 84, 90, 95	0
3	AC	206/239 (86%)	2.65	111 (53%) 0 0	68, 79, 87, 94	0
3	CC	206/239 (86%)	3.23	129 (62%) 0 0	71, 81, 89, 94	0
4	AD	208/209 (99%)	2.74	121 (58%) 0 0	57, 72, 81, 90	0
4	CD	208/209 (99%)	2.17	92 (44%) 1 0	58, 71, 80, 91	0
5	AE	148/162 (91%)	2.21	72 (48%) 1 0	58, 71, 80, 85	0
5	CE	148/162 (91%)	3.17	99 (66%) 0 0	60, 73, 81, 86	0
6	AF	100/101 (99%)	2.02	44 (44%) 1 0	56, 69, 78, 82	0
6	CF	100/101 (99%)	1.58	27 (27%) 1 1	57, 70, 78, 82	0
7	AG	155/156 (99%)	2.07	64 (41%) 1 0	65, 75, 83, 91	0
7	CG	155/156 (99%)	2.09	72 (46%) 1 0	66, 76, 84, 92	0
8	AH	137/138 (99%)	1.80	43 (31%) 1 1	62, 72, 79, 87	0
8	CH	137/138 (99%)	2.82	66 (48%) 1 0	64, 74, 80, 87	0
9	AI	127/128 (99%)	2.82	72 (56%) 0 0	65, 80, 86, 89	0
9	CI	127/128 (99%)	4.52	100 (78%) 0 0	68, 82, 88, 91	0
10	AJ	97/105 (92%)	2.12	48 (49%) 1 0	64, 82, 90, 93	0
10	CJ	96/105 (91%)	4.62	82 (85%) 0 0	67, 84, 91, 93	0
11	AK	114/129 (88%)	1.57	31 (27%) 1 1	48, 70, 79, 84	0
11	CK	114/129 (88%)	1.94	40 (35%) 1 1	51, 71, 79, 84	0
12	AL	122/132 (92%)	1.84	46 (37%) 1 0	50, 65, 73, 78	0
12	CL	122/132 (92%)	2.81	75 (61%) 0 0	53, 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%)	2.40	54 (43%)	1	0	55, 70, 81, 89	0
13	CM	122/126 (96%)	3.96	83 (68%)	0	0	70, 84, 91, 99	0
14	AN	60/61 (98%)	1.83	23 (38%)	1	0	67, 74, 83, 84	0
14	CN	60/61 (98%)	4.29	40 (66%)	0	0	69, 77, 84, 88	0
15	AO	88/89 (98%)	1.46	21 (23%)	1	1	56, 67, 80, 81	0
15	CO	88/89 (98%)	1.92	34 (38%)	1	0	59, 69, 80, 83	0
16	AP	82/88 (93%)	2.78	45 (54%)	0	0	57, 71, 80, 84	0
16	CP	82/88 (93%)	2.32	36 (43%)	1	0	58, 70, 80, 84	0
17	AQ	99/105 (94%)	1.73	35 (35%)	1	1	59, 71, 80, 84	0
17	CQ	99/105 (94%)	2.71	54 (54%)	0	0	61, 71, 81, 85	0
18	AR	68/88 (77%)	2.27	29 (42%)	1	0	59, 68, 81, 83	0
18	CR	68/88 (77%)	2.67	39 (57%)	0	0	61, 70, 80, 84	0
19	AS	83/93 (89%)	1.54	25 (30%)	1	1	71, 80, 86, 95	0
19	CS	83/93 (89%)	5.55	72 (86%)	0	0	74, 82, 89, 96	0
20	AT	96/106 (90%)	2.82	52 (54%)	0	0	57, 71, 81, 85	0
20	CT	96/106 (90%)	2.06	45 (46%)	1	0	58, 70, 82, 85	0
21	AU	23/27 (85%)	2.65	10 (43%)	1	0	67, 74, 77, 81	0
21	CU	23/27 (85%)	4.10	18 (78%)	0	0	71, 75, 80, 84	0
22	AV	13/24 (54%)	1.45	4 (30%)	1	1	58, 81, 96, 99	0
22	CV	12/24 (50%)	2.45	6 (50%)	0	0	63, 84, 93, 94	0
23	AW	72/76 (94%)	2.08	28 (38%)	1	0	68, 96, 103, 105	0
23	CW	70/76 (92%)	3.82	53 (75%)	0	0	73, 97, 103, 106	0
24	AX	76/77 (98%)	0.82	7 (9%)	9	9	39, 68, 87, 91	0
24	CX	76/77 (98%)	0.78	11 (14%)	3	3	53, 82, 93, 97	0
25	AY	73/76 (96%)	2.94	43 (58%)	0	0	44, 97, 102, 105	0
25	CY	72/76 (94%)	2.15	36 (50%)	0	0	47, 98, 103, 105	0
26	BA	2819/2915 (96%)	1.10	88 (3%)	47	49	26, 45, 89, 104	0
26	DA	2800/2915 (96%)	0.55	104 (3%)	39	42	30, 49, 90, 108	0
27	BB	120/121 (99%)	1.07	2 (1%)	67	70	40, 64, 73, 86	0
27	DB	120/121 (99%)	0.48	9 (7%)	14	14	46, 69, 76, 90	0
28	BD	275/276 (99%)	0.94	21 (7%)	14	14	27, 43, 58, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DD	275/276 (99%)	1.26	50 (18%) 2 2	29, 45, 61, 81	0
29	BE	204/206 (99%)	1.00	19 (9%) 9 8	25, 48, 66, 80	0
29	DE	204/206 (99%)	1.13	45 (22%) 1 1	29, 52, 67, 81	0
30	BF	203/210 (96%)	1.20	40 (19%) 2 1	26, 53, 76, 87	0
30	DF	203/210 (96%)	2.40	95 (46%) 1 0	30, 58, 77, 87	0
31	BG	181/182 (99%)	1.63	56 (30%) 1 1	51, 69, 81, 88	0
31	DG	181/182 (99%)	3.42	111 (61%) 0 0	56, 73, 82, 90	0
32	BH	174/180 (96%)	1.27	38 (21%) 1 1	51, 65, 75, 88	0
32	DH	174/180 (96%)	4.13	132 (75%) 0 0	55, 70, 78, 88	0
33	BI	146/148 (98%)	2.22	71 (48%) 1 0	50, 74, 82, 87	0
33	DI	146/148 (98%)	2.77	82 (56%) 0 0	52, 75, 82, 86	0
34	BN	140/140 (100%)	1.23	22 (15%) 3 2	32, 50, 67, 76	0
34	DN	140/140 (100%)	1.67	48 (34%) 1 1	36, 55, 70, 77	0
35	BO	122/122 (100%)	0.71	3 (2%) 54 58	30, 43, 59, 70	0
35	DO	122/122 (100%)	1.58	42 (34%) 1 1	45, 59, 73, 78	0
36	BP	149/150 (99%)	1.11	23 (15%) 3 2	26, 55, 75, 83	0
36	DP	149/150 (99%)	2.27	75 (50%) 0 0	30, 59, 77, 85	0
37	BQ	141/141 (100%)	1.17	19 (13%) 4 3	36, 52, 67, 80	0
37	DQ	141/141 (100%)	2.10	67 (47%) 1 0	41, 57, 70, 82	0
38	BR	118/118 (100%)	0.80	10 (8%) 11 10	25, 36, 54, 59	0
38	DR	118/118 (100%)	1.62	43 (36%) 1 0	41, 54, 65, 72	0
39	BS	110/112 (98%)	0.91	12 (10%) 6 6	38, 51, 65, 72	0
39	DS	110/112 (98%)	2.99	61 (55%) 0 0	63, 77, 84, 92	0
40	BT	131/146 (89%)	0.70	10 (7%) 14 14	32, 47, 69, 82	0
40	DT	131/146 (89%)	0.90	19 (14%) 3 3	48, 63, 79, 85	0
41	BU	116/118 (98%)	0.92	7 (6%) 21 22	18, 33, 49, 59	0
41	DU	116/118 (98%)	2.33	62 (53%) 0 0	42, 61, 78, 84	0
42	BV	101/101 (100%)	0.89	14 (13%) 4 3	21, 41, 58, 67	0
42	DV	101/101 (100%)	1.57	33 (32%) 1 1	41, 71, 83, 91	0
43	BW	112/113 (99%)	0.73	3 (2%) 52 55	23, 34, 54, 79	0
43	DW	112/113 (99%)	1.29	22 (19%) 2 1	39, 50, 67, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BX	95/96 (98%)	0.65	3 (3%) 45 48	23, 38, 61, 84	0
44	DX	95/96 (98%)	1.80	34 (35%) 1 1	43, 60, 76, 79	0
45	BY	107/110 (97%)	1.62	39 (36%) 1 0	32, 50, 69, 83	0
45	DY	107/110 (97%)	2.78	58 (54%) 0 0	57, 71, 81, 88	0
46	BZ	171/206 (83%)	2.00	62 (36%) 1 0	39, 64, 91, 95	0
46	DZ	174/206 (84%)	4.56	129 (74%) 0 0	66, 84, 94, 101	0
47	B0	83/85 (97%)	1.25	14 (16%) 2 2	27, 39, 61, 73	0
47	D0	83/85 (97%)	2.41	42 (50%) 0 0	47, 66, 75, 82	0
48	B1	97/98 (98%)	1.33	21 (21%) 1 1	30, 48, 70, 76	0
48	D1	97/98 (98%)	1.64	34 (35%) 1 1	38, 58, 74, 83	0
49	B2	70/72 (97%)	0.74	3 (4%) 34 36	34, 50, 64, 79	0
49	D2	70/72 (97%)	2.57	36 (51%) 0 0	56, 70, 80, 86	0
50	B3	59/60 (98%)	0.85	6 (10%) 7 7	24, 37, 63, 71	0
50	D3	59/60 (98%)	3.29	38 (64%) 0 0	49, 64, 79, 85	0
51	B4	69/71 (97%)	0.91	9 (13%) 4 4	54, 73, 87, 92	0
51	D4	69/71 (97%)	3.53	46 (66%) 0 0	74, 88, 94, 99	0
52	B5	59/60 (98%)	0.70	5 (8%) 11 10	20, 33, 54, 67	0
52	D5	59/60 (98%)	0.97	7 (11%) 5 5	36, 51, 67, 73	0
53	B6	53/54 (98%)	1.24	9 (16%) 2 2	31, 44, 61, 68	0
53	D6	53/54 (98%)	2.39	26 (49%) 1 0	52, 63, 76, 79	0
54	B7	48/49 (97%)	1.18	7 (14%) 3 3	21, 30, 62, 76	0
54	D7	48/49 (97%)	1.81	15 (31%) 1 1	33, 42, 61, 70	0
55	B8	64/65 (98%)	0.97	6 (9%) 9 8	25, 36, 45, 60	0
55	D8	64/65 (98%)	2.39	39 (60%) 0 0	46, 58, 66, 72	0
56	B9	37/37 (100%)	2.15	14 (37%) 1 0	31, 49, 73, 74	0
56	D9	37/37 (100%)	3.19	23 (62%) 0 0	46, 57, 73, 76	0
All	All	20929/21748 (96%)	1.58	5202 (24%) 1 1	18, 64, 89, 109	0

The worst 5 of 5202 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	CB	165	VAL	29.5
51	D4	49	PHE	22.0

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Mol	Chain	Res	Type	RSRZ
2	CB	163	PHE	19.2
10	CJ	85	LEU	18.9
46	DZ	155	LEU	18.9

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

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
23	5MU	CW	54	21/22	0.21	-	74,88,99,101	0
24	5MC	AX	32	21/22	0.18	-	43,53,62,78	0
23	MIA	AW	37	29/30	0.20	-	59,71,81,86	0
25	PSU	CY	55	20/21	0.34	-	94,102,110,124	0
23	4SU	AW	8	20/21	0.22	-	86,95,112,128	0
23	PSU	CW	39	20/21	0.36	-	78,84,97,98	0
25	MIA	CY	37	22/30	0.24	-	72,95,113,138	0
24	5MC	CX	32	21/22	0.17	-	63,76,86,88	0
23	PSU	AW	32	20/21	0.23	-	77,83,92,98	0
23	PSU	CW	32	20/21	0.51	-	81,87,94,103	0
25	7MG	CY	46	24/25	0.38	-	86,105,111,137	0
23	31M	CW	76	41/42	0.65	-	50,63,73,88	20
25	4SU	AY	8	20/21	0.24	-	82,96,103,118	0
23	PSU	AW	55	20/21	0.29	-	77,90,98,104	0
24	PSU	AX	55	20/21	0.18	-	50,63,73,83	0
25	PSU	AY	55	20/21	0.24	-	93,101,108,122	0
25	PSU	CY	32	20/21	0.14	-	80,92,101,107	0
23	PSU	CW	55	20/21	0.21	-	79,89,99,104	0
24	5MU	CX	54	21/22	0.16	-	70,81,89,99	0
24	4SU	CX	8	20/21	0.38	-	77,87,95,97	0
25	PSU	AY	32	20/21	0.29	-	78,93,100,106	0
24	4SU	AX	8	20/21	0.20	-	54,66,82,89	0
23	MIA	CW	37	22/30	0.19	-	75,85,92,100	0
23	5MU	AW	54	21/22	0.21	-	65,82,91,93	0
23	7MG	AW	46	24/25	0.24	-	84,99,117,133	0
24	PSU	CX	55	20/21	0.12	-	70,80,91,96	0
23	7MG	CW	46	24/25	0.31	-	79,96,109,133	0
25	PSU	CY	39	20/21	0.26	-	79,90,116,130	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	PSU	AW	39	20/21	0.15	-	73,82,95,97	0
25	MIA	AY	37	22/30	0.35	-	77,90,111,119	0
23	31M	AW	76	41/42	0.43	-	37,54,66,83	9
25	5MU	AY	54	21/22	0.17	-	80,96,105,131	0
25	4SU	CY	8	20/21	0.27	-	93,103,113,128	0
25	5MU	CY	54	21/22	0.40	-	78,94,109,140	0
25	PSU	AY	39	20/21	0.49	-	78,90,117,123	0
25	7MG	AY	46	24/25	0.50	-	75,101,111,123	0
24	5MU	AX	54	21/22	0.17	-	49,68,79,84	0
23	4SU	CW	8	20/21	0.34	-	81,98,120,127	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(\AA^2)	Q<0.9
57	MG	DA	3266	1/1	0.06	-	57,57,57,57	0
57	MG	AA	3124	1/1	0.08	-	47,47,47,47	0
57	MG	B3	3002	1/1	0.09	-	66,66,66,66	0
57	MG	CA	3161	1/1	0.09	-	56,56,56,56	0
57	MG	DA	3335	1/1	0.12	-	47,47,47,47	0
57	MG	DA	3543	1/1	0.09	-	53,53,53,53	0
57	MG	BA	3674	1/1	0.12	-	63,63,63,63	0
57	MG	BA	3095	1/1	0.19	-	51,51,51,51	0
57	MG	BA	3480	1/1	0.19	-	35,35,35,35	0
57	MG	DA	3425	1/1	0.11	-	61,61,61,61	0
57	MG	CA	3061	1/1	0.19	-	66,66,66,66	0
57	MG	DA	3393	1/1	0.06	-	50,50,50,50	0
57	MG	BA	3569	1/1	0.18	-	49,49,49,49	0
57	MG	DA	3034	1/1	0.10	-	38,38,38,38	0
57	MG	BA	3340	1/1	0.10	-	39,39,39,39	0
57	MG	BA	3594	1/1	0.14	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	3130	1/1	0.09	-	57,57,57,57	0
57	MG	CA	3045	1/1	0.19	-	54,54,54,54	0
57	MG	BA	3316	1/1	0.12	-	66,66,66,66	0
57	MG	DA	3314	1/1	0.14	-	43,43,43,43	0
57	MG	AA	3198	1/1	0.09	-	61,61,61,61	0
57	MG	BA	3491	1/1	0.12	-	45,45,45,45	0
57	MG	AA	3100	1/1	0.10	-	65,65,65,65	0
57	MG	BA	3496	1/1	0.19	-	41,41,41,41	0
57	MG	BA	3671	1/1	0.20	-	63,63,63,63	0
57	MG	BA	3604	1/1	0.12	-	36,36,36,36	0
57	MG	AA	3096	1/1	0.20	-	63,63,63,63	0
57	MG	DA	3434	1/1	0.12	-	39,39,39,39	0
57	MG	BA	3656	1/1	0.23	-	53,53,53,53	0
57	MG	BA	3038	1/1	0.18	-	35,35,35,35	0
57	MG	CA	3144	1/1	0.22	-	71,71,71,71	0
57	MG	BA	3250	1/1	0.61	-	42,42,42,42	0
57	MG	AA	3065	1/1	0.19	-	63,63,63,63	0
57	MG	DA	3609	1/1	0.10	-	46,46,46,46	0
57	MG	DA	3070	1/1	0.14	-	58,58,58,58	0
57	MG	BA	3217	1/1	0.12	-	37,37,37,37	0
57	MG	BA	3328	1/1	0.22	-	40,40,40,40	0
57	MG	DA	3313	1/1	0.18	-	47,47,47,47	0
57	MG	CA	3037	1/1	0.10	-	73,73,73,73	0
57	MG	DA	3327	1/1	0.20	-	57,57,57,57	0
57	MG	DA	3511	1/1	0.14	-	49,49,49,49	0
57	MG	BA	3366	1/1	0.11	-	57,57,57,57	0
57	MG	CW	3001	1/1	0.19	-	67,67,67,67	0
57	MG	DA	3595	1/1	0.17	-	59,59,59,59	0
57	MG	CA	3030	1/1	0.08	-	57,57,57,57	0
57	MG	DA	3247	1/1	0.15	-	45,45,45,45	0
57	MG	DA	3550	1/1	0.13	-	57,57,57,57	0
57	MG	DA	3317	1/1	0.12	-	44,44,44,44	0
57	MG	AA	3043	1/1	0.22	-	51,51,51,51	0
57	MG	DA	3494	1/1	0.20	-	47,47,47,47	0
57	MG	AA	3195	1/1	0.14	-	57,57,57,57	0
57	MG	BA	3522	1/1	0.10	-	52,52,52,52	0
57	MG	DA	3192	1/1	0.15	-	60,60,60,60	0
57	MG	BA	3764	1/1	0.16	-	51,51,51,51	0
57	MG	DA	3563	1/1	0.26	-	74,74,74,74	0
57	MG	DA	3265	1/1	0.12	-	30,30,30,30	0
57	MG	DA	3618	1/1	0.10	-	53,53,53,53	0
57	MG	DA	3517	1/1	0.12	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BB	209	1/1	0.21	-	65,65,65,65	0
57	MG	BA	3104	1/1	0.27	-	42,42,42,42	0
57	MG	BA	3450	1/1	0.15	-	48,48,48,48	0
57	MG	DA	3048	1/1	0.07	-	53,53,53,53	0
57	MG	DA	3506	1/1	0.08	-	42,42,42,42	0
57	MG	AY	3001	1/1	0.30	-	65,65,65,65	0
57	MG	CA	3141	1/1	0.05	-	92,92,92,92	0
57	MG	DA	3339	1/1	0.16	-	61,61,61,61	0
57	MG	DA	3603	1/1	0.07	-	41,41,41,41	0
57	MG	DA	3280	1/1	0.19	-	33,33,33,33	0
57	MG	DW	3001	1/1	0.58	-	54,54,54,54	0
57	MG	BA	3738	1/1	0.12	-	43,43,43,43	0
57	MG	BA	3549	1/1	0.14	-	39,39,39,39	0
57	MG	BA	3025	1/1	0.11	-	27,27,27,27	0
57	MG	CA	3133	1/1	0.16	-	59,59,59,59	0
57	MG	B7	104	1/1	0.35	-	48,48,48,48	0
57	MG	CA	3075	1/1	0.14	-	59,59,59,59	0
57	MG	BA	3040	1/1	0.39	-	35,35,35,35	0
57	MG	CA	3016	1/1	0.12	-	57,57,57,57	0
57	MG	BA	3358	1/1	0.23	-	49,49,49,49	0
57	MG	BA	3468	1/1	0.07	-	62,62,62,62	0
57	MG	AA	3076	1/1	0.26	-	77,77,77,77	0
57	MG	BA	3051	1/1	0.16	-	43,43,43,43	0
57	MG	CX	3002	1/1	0.17	-	70,70,70,70	0
57	MG	DA	3193	1/1	0.06	-	57,57,57,57	0
57	MG	BA	3162	1/1	0.11	-	38,38,38,38	0
59	ZN	DY	501	1/1	0.14	-	96,96,96,96	0
57	MG	DA	3347	1/1	0.23	-	27,27,27,27	0
57	MG	DA	3363	1/1	0.16	-	29,29,29,29	0
57	MG	DA	3612	1/1	0.09	-	62,62,62,62	0
57	MG	BA	3767	1/1	0.11	-	73,73,73,73	0
57	MG	CA	3100	1/1	0.11	-	52,52,52,52	0
57	MG	DA	3644	1/1	0.05	-	55,55,55,55	0
57	MG	BA	3690	1/1	0.15	-	58,58,58,58	0
57	MG	DA	3269	1/1	0.05	-	49,49,49,49	0
57	MG	AA	3121	1/1	0.11	-	70,70,70,70	0
57	MG	BA	3658	1/1	0.29	-	61,61,61,61	0
57	MG	DA	3646	1/1	0.12	-	59,59,59,59	0
57	MG	BA	3627	1/1	0.16	-	56,56,56,56	0
57	MG	AA	3196	1/1	0.39	-	74,74,74,74	0
57	MG	DA	3372	1/1	0.04	-	56,56,56,56	0
57	MG	BA	3686	1/1	0.13	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3401	1/1	0.07	-	38,38,38,38	0
57	MG	DB	3007	1/1	0.20	-	58,58,58,58	0
57	MG	DA	3001	1/1	0.21	-	60,60,60,60	0
57	MG	BA	3538	1/1	0.14	-	40,40,40,40	0
57	MG	BA	3003	1/1	0.19	-	60,60,60,60	0
57	MG	BA	3282	1/1	0.15	-	39,39,39,39	0
57	MG	DA	3325	1/1	0.12	-	35,35,35,35	0
57	MG	BA	3528	1/1	0.20	-	56,56,56,56	0
57	MG	DA	3007	1/1	0.11	-	50,50,50,50	0
57	MG	CA	3070	1/1	0.17	-	63,63,63,63	0
57	MG	DA	3306	1/1	0.13	-	55,55,55,55	0
59	ZN	AN	501	1/1	0.19	-	69,69,69,69	0
57	MG	BA	3176	1/1	0.11	-	45,45,45,45	0
57	MG	CV	101	1/1	0.09	-	72,72,72,72	0
57	MG	DA	3555	1/1	0.23	-	53,53,53,53	0
57	MG	DA	3282	1/1	0.07	-	52,52,52,52	0
57	MG	BA	3796	1/1	0.19	-	45,45,45,45	0
57	MG	AA	3068	1/1	0.15	-	69,69,69,69	0
57	MG	BU	202	1/1	0.48	-	40,40,40,40	0
57	MG	BA	3343	1/1	0.14	-	53,53,53,53	0
57	MG	BA	3625	1/1	0.14	-	39,39,39,39	0
57	MG	BA	3375	1/1	0.25	-	68,68,68,68	0
57	MG	AX	3012	1/1	0.16	-	59,59,59,59	0
57	MG	CA	3038	1/1	0.13	-	58,58,58,58	0
57	MG	DA	3349	1/1	0.04	-	52,52,52,52	0
57	MG	AA	3004	1/1	0.12	-	67,67,67,67	0
57	MG	BA	3407	1/1	0.15	-	47,47,47,47	0
57	MG	BA	3732	1/1	0.37	-	51,51,51,51	0
57	MG	BA	3759	1/1	0.18	-	33,33,33,33	0
57	MG	DA	3156	1/1	0.07	-	51,51,51,51	0
57	MG	DA	3395	1/1	0.10	-	47,47,47,47	0
57	MG	DA	3263	1/1	0.16	-	41,41,41,41	0
57	MG	BA	3427	1/1	0.22	-	61,61,61,61	0
57	MG	AA	3024	1/1	0.09	-	54,54,54,54	0
57	MG	BV	203	1/1	0.19	-	38,38,38,38	0
57	MG	BA	3184	1/1	0.24	-	43,43,43,43	0
57	MG	DA	3049	1/1	0.11	-	52,52,52,52	0
57	MG	DA	3223	1/1	0.10	-	50,50,50,50	0
57	MG	BA	3349	1/1	0.10	-	56,56,56,56	0
57	MG	DA	3613	1/1	0.09	-	54,54,54,54	0
57	MG	DA	3285	1/1	0.10	-	32,32,32,32	0
57	MG	BA	3798	1/1	0.17	-	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DD	306	1/1	0.35	-	39,39,39,39	0
57	MG	DA	3259	1/1	0.26	-	43,43,43,43	0
57	MG	DQ	3004	1/1	0.41	-	54,54,54,54	0
57	MG	BA	3506	1/1	0.21	-	58,58,58,58	0
57	MG	BA	3295	1/1	0.19	-	38,38,38,38	0
57	MG	BA	3545	1/1	0.14	-	65,65,65,65	0
57	MG	BA	3317	1/1	0.20	-	53,53,53,53	0
57	MG	BA	3310	1/1	0.15	-	58,58,58,58	0
57	MG	BA	3012	1/1	0.19	-	39,39,39,39	0
57	MG	BA	3560	1/1	0.11	-	56,56,56,56	0
57	MG	CA	3085	1/1	0.10	-	54,54,54,54	0
57	MG	CA	3002	1/1	0.12	-	63,63,63,63	0
57	MG	BA	3464	1/1	0.13	-	45,45,45,45	0
57	MG	DA	3218	1/1	0.21	-	59,59,59,59	0
57	MG	DA	3440	1/1	0.12	-	61,61,61,61	0
57	MG	DA	3354	1/1	0.16	-	44,44,44,44	0
57	MG	DA	3043	1/1	0.11	-	38,38,38,38	0
57	MG	BA	3661	1/1	0.10	-	44,44,44,44	0
57	MG	BA	3356	1/1	0.15	-	37,37,37,37	0
57	MG	DA	3406	1/1	0.12	-	51,51,51,51	0
57	MG	DA	3257	1/1	0.19	-	50,50,50,50	0
57	MG	BA	3195	1/1	0.10	-	46,46,46,46	0
57	MG	DA	3518	1/1	0.21	-	54,54,54,54	0
57	MG	BA	3441	1/1	0.13	-	35,35,35,35	0
57	MG	BA	3599	1/1	0.19	-	43,43,43,43	0
57	MG	AA	3188	1/1	0.08	-	69,69,69,69	0
57	MG	BA	3654	1/1	0.14	-	57,57,57,57	0
57	MG	DA	3159	1/1	0.18	-	58,58,58,58	0
57	MG	CA	3029	1/1	0.14	-	63,63,63,63	0
57	MG	CA	3079	1/1	0.15	-	66,66,66,66	0
57	MG	BA	3109	1/1	0.15	-	51,51,51,51	0
57	MG	BA	3411	1/1	0.18	-	33,33,33,33	0
57	MG	DA	3439	1/1	0.15	-	42,42,42,42	0
57	MG	BA	3234	1/1	0.14	-	38,38,38,38	0
57	MG	DA	3482	1/1	0.06	-	50,50,50,50	0
57	MG	BA	3149	1/1	0.13	-	40,40,40,40	0
57	MG	BA	3208	1/1	0.13	-	44,44,44,44	0
57	MG	AA	3095	1/1	0.22	-	60,60,60,60	0
57	MG	BA	3187	1/1	0.20	-	29,29,29,29	0
57	MG	DA	3624	1/1	0.15	-	56,56,56,56	0
57	MG	DA	3539	1/1	0.10	-	53,53,53,53	0
57	MG	BA	3478	1/1	0.13	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3611	1/1	0.13	-	48,48,48,48	0
57	MG	CA	3064	1/1	0.12	-	60,60,60,60	0
57	MG	CA	3101	1/1	0.06	-	49,49,49,49	0
57	MG	DA	3510	1/1	0.20	-	49,49,49,49	0
57	MG	DA	3362	1/1	0.17	-	44,44,44,44	0
57	MG	CA	3116	1/1	0.21	-	68,68,68,68	0
57	MG	BA	3171	1/1	0.36	-	31,31,31,31	0
57	MG	DA	3342	1/1	0.12	-	42,42,42,42	0
57	MG	BA	3459	1/1	0.21	-	48,48,48,48	0
57	MG	BU	208	1/1	0.19	-	40,40,40,40	0
57	MG	BA	3544	1/1	0.16	-	44,44,44,44	0
57	MG	BA	3525	1/1	0.16	-	34,34,34,34	0
57	MG	DA	3301	1/1	0.18	-	52,52,52,52	0
57	MG	DA	3413	1/1	0.24	-	48,48,48,48	0
57	MG	DD	309	1/1	0.34	-	59,59,59,59	0
57	MG	AA	3080	1/1	0.18	-	58,58,58,58	0
57	MG	DA	3385	1/1	0.10	-	52,52,52,52	0
57	MG	BA	3303	1/1	0.21	-	36,36,36,36	0
57	MG	AA	3101	1/1	0.12	-	43,43,43,43	0
57	MG	DA	3544	1/1	0.17	-	65,65,65,65	0
57	MG	BA	3786	1/1	0.12	-	35,35,35,35	0
57	MG	AA	3177	1/1	0.08	-	66,66,66,66	0
57	MG	DA	3540	1/1	0.15	-	42,42,42,42	0
57	MG	CA	3049	1/1	0.26	-	63,63,63,63	0
57	MG	DA	3308	1/1	0.19	-	61,61,61,61	0
57	MG	BA	3315	1/1	0.21	-	31,31,31,31	0
57	MG	DA	3226	1/1	0.35	-	45,45,45,45	0
57	MG	DA	3429	1/1	0.17	-	41,41,41,41	0
57	MG	DA	3029	1/1	0.51	-	49,49,49,49	0
57	MG	BA	3446	1/1	0.17	-	40,40,40,40	0
57	MG	DA	3645	1/1	0.11	-	45,45,45,45	0
57	MG	BA	3369	1/1	0.10	-	44,44,44,44	0
57	MG	DA	3186	1/1	0.16	-	54,54,54,54	0
57	MG	DA	3112	1/1	0.10	-	59,59,59,59	0
57	MG	CA	3011	1/1	0.23	-	61,61,61,61	0
57	MG	DA	3577	1/1	0.10	-	58,58,58,58	0
57	MG	DA	3153	1/1	0.16	-	47,47,47,47	0
57	MG	AA	3071	1/1	0.28	-	53,53,53,53	0
57	MG	BA	3159	1/1	0.33	-	50,50,50,50	0
57	MG	BA	3117	1/1	0.19	-	59,59,59,59	0
57	MG	DA	3649	1/1	0.12	-	58,58,58,58	0
57	MG	BW	201	1/1	0.24	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3157	1/1	0.15	-	45,45,45,45	0
57	MG	BA	3547	1/1	0.23	-	39,39,39,39	0
57	MG	DA	3260	1/1	0.09	-	55,55,55,55	0
57	MG	BA	3150	1/1	0.21	-	55,55,55,55	0
57	MG	CA	3149	1/1	0.13	-	52,52,52,52	0
57	MG	BA	3059	1/1	0.15	-	26,26,26,26	0
57	MG	DA	3598	1/1	0.09	-	61,61,61,61	0
57	MG	BA	3219	1/1	0.13	-	36,36,36,36	0
57	MG	AA	3189	1/1	0.11	-	65,65,65,65	0
57	MG	AA	3119	1/1	0.09	-	51,51,51,51	0
57	MG	BO	202	1/1	0.10	-	65,65,65,65	0
57	MG	DF	3001	1/1	0.28	-	44,44,44,44	0
57	MG	AK	3001	1/1	0.13	-	44,44,44,44	0
57	MG	BA	3384	1/1	0.17	-	41,41,41,41	0
57	MG	DA	3326	1/1	0.15	-	43,43,43,43	0
57	MG	BA	3412	1/1	0.21	-	40,40,40,40	0
57	MG	DA	3408	1/1	0.07	-	58,58,58,58	0
57	MG	DA	3012	1/1	0.09	-	33,33,33,33	0
57	MG	BA	3011	1/1	0.15	-	35,35,35,35	0
57	MG	CA	3159	1/1	0.21	-	70,70,70,70	0
57	MG	AA	3169	1/1	0.12	-	62,62,62,62	0
57	MG	DA	3442	1/1	0.13	-	39,39,39,39	0
57	MG	BA	3377	1/1	0.17	-	44,44,44,44	0
57	MG	AA	3058	1/1	0.22	-	59,59,59,59	0
57	MG	BA	3337	1/1	0.12	-	58,58,58,58	0
57	MG	CA	3151	1/1	0.26	-	59,59,59,59	0
57	MG	DA	3397	1/1	0.08	-	57,57,57,57	0
57	MG	BA	3136	1/1	0.11	-	30,30,30,30	0
57	MG	BA	3681	1/1	0.08	-	66,66,66,66	0
57	MG	DA	3249	1/1	0.11	-	45,45,45,45	0
57	MG	DA	3351	1/1	0.16	-	48,48,48,48	0
57	MG	BA	3057	1/1	0.17	-	34,34,34,34	0
57	MG	BA	3622	1/1	0.15	-	48,48,48,48	0
57	MG	BA	3233	1/1	0.11	-	56,56,56,56	0
57	MG	DA	3065	1/1	0.13	-	43,43,43,43	0
57	MG	BA	3616	1/1	0.19	-	65,65,65,65	0
57	MG	BN	3002	1/1	0.12	-	39,39,39,39	0
57	MG	BA	3200	1/1	0.17	-	67,67,67,67	0
57	MG	DA	3590	1/1	0.08	-	51,51,51,51	0
57	MG	BA	3359	1/1	0.28	-	62,62,62,62	0
57	MG	DA	3166	1/1	0.11	-	55,55,55,55	0
57	MG	DA	3224	1/1	0.17	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	3087	1/1	0.08	-	41,41,41,41	0
57	MG	BA	3719	1/1	0.13	-	53,53,53,53	0
57	MG	BA	3791	1/1	0.16	-	28,28,28,28	0
57	MG	BA	3017	1/1	0.23	-	48,48,48,48	0
57	MG	DA	3144	1/1	0.10	-	38,38,38,38	0
57	MG	CA	3051	1/1	0.25	-	81,81,81,81	0
57	MG	BA	3186	1/1	0.53	-	45,45,45,45	0
57	MG	DA	3028	1/1	0.27	-	52,52,52,52	0
57	MG	DA	3654	1/1	0.11	-	56,56,56,56	0
57	MG	DA	3107	1/1	0.09	-	51,51,51,51	0
57	MG	BG	203	1/1	0.14	-	42,42,42,42	0
57	MG	DA	3126	1/1	0.08	-	55,55,55,55	0
57	MG	BA	3403	1/1	0.13	-	54,54,54,54	0
57	MG	DA	3564	1/1	0.13	-	61,61,61,61	0
57	MG	BA	3433	1/1	0.20	-	32,32,32,32	0
57	MG	DA	3593	1/1	0.14	-	40,40,40,40	0
57	MG	BA	3154	1/1	0.19	-	47,47,47,47	0
57	MG	BA	3696	1/1	0.16	-	33,33,33,33	0
57	MG	BX	3001	1/1	0.89	-	48,48,48,48	0
57	MG	AX	3014	1/1	0.20	-	72,72,72,72	0
57	MG	BA	3286	1/1	0.16	-	34,34,34,34	0
59	ZN	B6	103	1/1	0.20	-	49,49,49,49	0
57	MG	BA	3122	1/1	0.10	-	41,41,41,41	0
57	MG	BA	3624	1/1	0.07	-	68,68,68,68	0
57	MG	AA	3181	1/1	0.17	-	51,51,51,51	0
57	MG	BA	3720	1/1	0.14	-	65,65,65,65	0
57	MG	BA	3114	1/1	0.14	-	53,53,53,53	0
57	MG	BA	3474	1/1	0.18	-	55,55,55,55	0
57	MG	CT	3001	1/1	0.09	-	56,56,56,56	0
57	MG	DA	3233	1/1	0.28	-	53,53,53,53	0
57	MG	BW	204	1/1	0.34	-	42,42,42,42	0
57	MG	BA	3245	1/1	0.25	-	34,34,34,34	0
57	MG	DA	3222	1/1	0.12	-	57,57,57,57	0
57	MG	BA	3774	1/1	0.31	-	46,46,46,46	0
57	MG	CA	3156	1/1	0.06	-	73,73,73,73	0
57	MG	BA	3629	1/1	0.18	-	43,43,43,43	0
57	MG	DA	3452	1/1	0.13	-	51,51,51,51	0
57	MG	BA	3470	1/1	0.13	-	62,62,62,62	0
57	MG	AA	3194	1/1	0.12	-	56,56,56,56	0
57	MG	DA	3082	1/1	0.12	-	47,47,47,47	0
57	MG	DA	3322	1/1	0.18	-	51,51,51,51	0
57	MG	AA	3118	1/1	0.18	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3527	1/1	0.15	-	54,54,54,54	0
57	MG	BA	3074	1/1	0.17	-	46,46,46,46	0
57	MG	BA	3248	1/1	0.18	-	42,42,42,42	0
57	MG	BA	3490	1/1	0.08	-	54,54,54,54	0
57	MG	DA	3450	1/1	0.10	-	40,40,40,40	0
57	MG	BF	305	1/1	0.11	-	49,49,49,49	0
57	MG	CA	3008	1/1	0.23	-	51,51,51,51	0
57	MG	DA	3675	1/1	0.10	-	52,52,52,52	0
57	MG	BA	3334	1/1	0.11	-	37,37,37,37	0
57	MG	AA	3182	1/1	0.09	-	49,49,49,49	0
57	MG	BA	3784	1/1	0.16	-	33,33,33,33	0
58	SF4	CD	302	8/8	0.18	-	60,68,83,86	0
57	MG	BA	3745	1/1	0.24	-	75,75,75,75	0
57	MG	DA	3036	1/1	0.13	-	48,48,48,48	0
57	MG	BA	3731	1/1	0.27	-	37,37,37,37	0
57	MG	AA	3157	1/1	0.15	-	45,45,45,45	0
57	MG	DA	3146	1/1	0.12	-	55,55,55,55	0
57	MG	AA	3163	1/1	0.17	-	56,56,56,56	0
57	MG	BA	3189	1/1	0.09	-	39,39,39,39	0
57	MG	AA	3147	1/1	0.13	-	70,70,70,70	0
57	MG	BA	3275	1/1	0.22	-	58,58,58,58	0
57	MG	BA	3501	1/1	0.17	-	71,71,71,71	0
57	MG	BA	3212	1/1	0.24	-	54,54,54,54	0
57	MG	AA	3180	1/1	0.14	-	73,73,73,73	0
57	MG	DA	3113	1/1	0.11	-	60,60,60,60	0
57	MG	DA	3087	1/1	0.10	-	58,58,58,58	0
57	MG	BA	3015	1/1	0.15	-	32,32,32,32	0
57	MG	BA	3466	1/1	0.14	-	49,49,49,49	0
57	MG	BA	3254	1/1	0.18	-	25,25,25,25	0
57	MG	BB	211	1/1	0.09	-	51,51,51,51	0
57	MG	CA	3137	1/1	0.12	-	56,56,56,56	0
57	MG	BA	3269	1/1	0.24	-	53,53,53,53	0
57	MG	DA	3358	1/1	0.13	-	45,45,45,45	0
57	MG	DB	3012	1/1	0.23	-	61,61,61,61	0
57	MG	DA	3318	1/1	0.07	-	40,40,40,40	0
57	MG	DA	3639	1/1	0.75	-	59,59,59,59	0
57	MG	AA	3023	1/1	0.14	-	74,74,74,74	0
57	MG	AA	3150	1/1	0.19	-	57,57,57,57	0
57	MG	DA	3435	1/1	0.15	-	50,50,50,50	0
57	MG	CA	3107	1/1	0.30	-	80,80,80,80	0
57	MG	BA	3734	1/1	0.12	-	52,52,52,52	0
57	MG	DA	3207	1/1	0.47	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3531	1/1	0.31	-	61,61,61,61	0
57	MG	CA	3003	1/1	0.14	-	57,57,57,57	0
57	MG	DA	3514	1/1	0.12	-	42,42,42,42	0
57	MG	AA	3156	1/1	0.14	-	63,63,63,63	0
57	MG	AA	3176	1/1	0.11	-	67,67,67,67	0
57	MG	CA	3158	1/1	0.08	-	67,67,67,67	0
57	MG	BA	3808	1/1	0.28	-	42,42,42,42	0
57	MG	AA	3159	1/1	0.11	-	66,66,66,66	0
57	MG	BA	3668	1/1	0.14	-	53,53,53,53	0
57	MG	DA	3448	1/1	0.21	-	70,70,70,70	0
57	MG	AE	202	1/1	0.14	-	80,80,80,80	0
57	MG	BA	3274	1/1	0.10	-	49,49,49,49	0
57	MG	AA	3149	1/1	0.09	-	46,46,46,46	0
57	MG	BA	3080	1/1	0.15	-	60,60,60,60	0
57	MG	CA	3092	1/1	0.10	-	50,50,50,50	0
57	MG	BA	3472	1/1	0.12	-	20,20,20,20	0
57	MG	DA	3169	1/1	0.51	-	47,47,47,47	0
57	MG	BA	3401	1/1	0.17	-	35,35,35,35	0
57	MG	BA	3082	1/1	0.21	-	39,39,39,39	0
57	MG	BN	3006	1/1	0.30	-	49,49,49,49	0
57	MG	DA	3258	1/1	0.11	-	48,48,48,48	0
57	MG	BA	3177	1/1	0.20	-	46,46,46,46	0
57	MG	BA	3765	1/1	0.21	-	48,48,48,48	0
57	MG	BA	3434	1/1	0.13	-	55,55,55,55	0
57	MG	BA	3134	1/1	0.13	-	48,48,48,48	0
57	MG	BA	3131	1/1	0.15	-	58,58,58,58	0
57	MG	BA	3688	1/1	0.14	-	46,46,46,46	0
57	MG	CK	3001	1/1	0.16	-	45,45,45,45	0
57	MG	DA	3099	1/1	0.13	-	32,32,32,32	0
57	MG	BA	3489	1/1	0.07	-	59,59,59,59	0
57	MG	BB	204	1/1	0.15	-	41,41,41,41	0
57	MG	DA	3090	1/1	0.09	-	52,52,52,52	0
57	MG	BA	3461	1/1	0.13	-	62,62,62,62	0
57	MG	BA	3479	1/1	0.05	-	50,50,50,50	0
57	MG	CA	3065	1/1	0.15	-	49,49,49,49	0
57	MG	BA	3703	1/1	0.20	-	64,64,64,64	0
57	MG	DA	3663	1/1	0.13	-	60,60,60,60	0
57	MG	DA	3320	1/1	0.16	-	55,55,55,55	0
57	MG	DA	3264	1/1	0.14	-	40,40,40,40	0
57	MG	DA	3467	1/1	0.26	-	40,40,40,40	0
57	MG	AX	3015	1/1	0.19	-	42,42,42,42	0
57	MG	DA	3463	1/1	0.13	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3555	1/1	0.15	-	29,29,29,29	0
57	MG	B7	103	1/1	0.17	-	42,42,42,42	0
57	MG	BA	3595	1/1	0.10	-	51,51,51,51	0
57	MG	AA	3044	1/1	0.26	-	60,60,60,60	0
57	MG	BA	3535	1/1	0.20	-	31,31,31,31	0
57	MG	BA	3148	1/1	0.30	-	44,44,44,44	0
57	MG	DA	3243	1/1	0.19	-	55,55,55,55	0
57	MG	BA	3706	1/1	0.13	-	53,53,53,53	0
57	MG	DA	3489	1/1	0.12	-	51,51,51,51	0
57	MG	AX	3005	1/1	0.10	-	47,47,47,47	0
57	MG	AA	3191	1/1	0.12	-	47,47,47,47	0
57	MG	DA	3643	1/1	0.11	-	61,61,61,61	0
57	MG	DA	3271	1/1	0.15	-	48,48,48,48	0
57	MG	BB	219	1/1	0.10	-	67,67,67,67	0
57	MG	BA	3659	1/1	0.20	-	61,61,61,61	0
57	MG	BA	3617	1/1	0.12	-	51,51,51,51	0
57	MG	BA	3167	1/1	0.11	-	41,41,41,41	0
57	MG	BA	3495	1/1	0.10	-	37,37,37,37	0
57	MG	AA	3112	1/1	0.07	-	63,63,63,63	0
57	MG	DA	3066	1/1	0.11	-	42,42,42,42	0
57	MG	DA	3232	1/1	0.06	-	62,62,62,62	0
57	MG	BA	3694	1/1	0.08	-	51,51,51,51	0
57	MG	DA	3102	1/1	0.25	-	40,40,40,40	0
57	MG	BA	3019	1/1	0.11	-	42,42,42,42	0
57	MG	CF	3001	1/1	0.09	-	46,46,46,46	0
57	MG	DA	3570	1/1	0.11	-	31,31,31,31	0
57	MG	DA	3045	1/1	0.23	-	51,51,51,51	0
57	MG	CA	3081	1/1	0.07	-	46,46,46,46	0
57	MG	BA	3043	1/1	0.12	-	48,48,48,48	0
57	MG	BA	3418	1/1	0.13	-	30,30,30,30	0
57	MG	AA	3104	1/1	0.24	-	59,59,59,59	0
57	MG	BA	3795	1/1	0.15	-	35,35,35,35	0
57	MG	B6	102	1/1	0.15	-	68,68,68,68	0
57	MG	DA	3183	1/1	0.16	-	38,38,38,38	0
57	MG	CA	3154	1/1	0.19	-	56,56,56,56	0
57	MG	BA	3419	1/1	0.24	-	37,37,37,37	0
57	MG	BA	3518	1/1	0.18	-	44,44,44,44	0
57	MG	BA	3740	1/1	0.16	-	28,28,28,28	0
57	MG	DA	3423	1/1	0.11	-	49,49,49,49	0
57	MG	CA	3027	1/1	0.21	-	64,64,64,64	0
57	MG	DA	3629	1/1	0.18	-	62,62,62,62	0
57	MG	BA	3327	1/1	0.14	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3006	1/1	0.07	-	38,38,38,38	0
57	MG	DA	3052	1/1	0.15	-	61,61,61,61	0
57	MG	DA	3486	1/1	0.08	-	47,47,47,47	0
57	MG	DA	3658	1/1	0.10	-	62,62,62,62	0
57	MG	AA	3089	1/1	0.14	-	60,60,60,60	0
57	MG	AW	3002	1/1	0.17	-	53,53,53,53	0
57	MG	BA	3642	1/1	0.11	-	48,48,48,48	0
57	MG	BA	3285	1/1	0.21	-	50,50,50,50	0
57	MG	BA	3023	1/1	0.18	-	36,36,36,36	0
57	MG	AA	3037	1/1	0.14	-	55,55,55,55	0
57	MG	DA	3161	1/1	0.14	-	38,38,38,38	0
57	MG	DA	3515	1/1	0.14	-	45,45,45,45	0
57	MG	DA	3420	1/1	0.24	-	60,60,60,60	0
57	MG	DA	3642	1/1	0.47	-	54,54,54,54	0
57	MG	BA	3708	1/1	0.28	-	50,50,50,50	0
57	MG	CA	3050	1/1	0.08	-	61,61,61,61	0
57	MG	BU	206	1/1	0.68	-	35,35,35,35	0
57	MG	BA	3648	1/1	0.11	-	65,65,65,65	0
57	MG	BA	3742	1/1	0.22	-	65,65,65,65	0
57	MG	CJ	5001	1/1	0.18	-	73,73,73,73	0
57	MG	AA	3170	1/1	0.13	-	75,75,75,75	0
57	MG	BA	3573	1/1	0.13	-	51,51,51,51	0
57	MG	AA	3099	1/1	0.14	-	51,51,51,51	0
57	MG	BA	3437	1/1	0.16	-	36,36,36,36	0
57	MG	DA	3312	1/1	0.11	-	54,54,54,54	0
57	MG	DA	3078	1/1	0.15	-	57,57,57,57	0
57	MG	CA	3077	1/1	0.07	-	66,66,66,66	0
57	MG	BA	3272	1/1	0.45	-	48,48,48,48	0
57	MG	BA	3737	1/1	0.26	-	43,43,43,43	0
57	MG	DA	3044	1/1	0.43	-	62,62,62,62	0
57	MG	DA	3472	1/1	0.15	-	44,44,44,44	0
57	MG	BA	3374	1/1	0.23	-	40,40,40,40	0
57	MG	DA	3220	1/1	0.18	-	46,46,46,46	0
57	MG	BA	3801	1/1	0.35	-	50,50,50,50	0
57	MG	AA	3094	1/1	0.11	-	59,59,59,59	0
57	MG	BA	3319	1/1	0.16	-	46,46,46,46	0
57	MG	DA	3261	1/1	0.12	-	49,49,49,49	0
57	MG	BN	3003	1/1	0.18	-	48,48,48,48	0
57	MG	BA	3583	1/1	0.21	-	45,45,45,45	0
57	MG	DA	3067	1/1	0.19	-	57,57,57,57	0
57	MG	DA	3370	1/1	0.09	-	51,51,51,51	0
57	MG	AA	3106	1/1	0.07	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3273	1/1	0.11	-	47,47,47,47	0
57	MG	BA	3050	1/1	0.14	-	38,38,38,38	0
57	MG	DA	3061	1/1	0.10	-	48,48,48,48	0
57	MG	BA	3689	1/1	0.21	-	42,42,42,42	0
57	MG	BB	201	1/1	0.14	-	55,55,55,55	0
57	MG	BA	3633	1/1	0.09	-	49,49,49,49	0
57	MG	DW	3003	1/1	0.24	-	72,72,72,72	0
57	MG	DA	3024	1/1	0.12	-	59,59,59,59	0
57	MG	DA	3384	1/1	0.07	-	49,49,49,49	0
57	MG	CA	3099	1/1	0.14	-	44,44,44,44	0
57	MG	AA	3035	1/1	0.20	-	56,56,56,56	0
57	MG	CA	3015	1/1	0.15	-	56,56,56,56	0
57	MG	DA	3130	1/1	0.14	-	52,52,52,52	0
57	MG	DA	3009	1/1	0.22	-	48,48,48,48	0
57	MG	BA	3421	1/1	0.17	-	32,32,32,32	0
57	MG	BA	3408	1/1	0.19	-	36,36,36,36	0
57	MG	DA	3605	1/1	0.14	-	58,58,58,58	0
57	MG	BA	3267	1/1	0.15	-	65,65,65,65	0
57	MG	DA	3038	1/1	0.10	-	47,47,47,47	0
57	MG	BA	3030	1/1	0.16	-	46,46,46,46	0
57	MG	BA	3161	1/1	0.12	-	52,52,52,52	0
57	MG	DA	3245	1/1	0.08	-	54,54,54,54	0
57	MG	DA	3137	1/1	0.14	-	54,54,54,54	0
57	MG	DA	3500	1/1	0.35	-	49,49,49,49	0
57	MG	BA	3094	1/1	0.16	-	36,36,36,36	0
57	MG	BA	3486	1/1	0.14	-	57,57,57,57	0
57	MG	DA	3665	1/1	0.09	-	42,42,42,42	0
57	MG	DA	3135	1/1	0.10	-	38,38,38,38	0
57	MG	BA	3415	1/1	0.15	-	28,28,28,28	0
57	MG	CA	3020	1/1	0.16	-	56,56,56,56	0
57	MG	BA	3169	1/1	0.18	-	45,45,45,45	0
57	MG	BB	215	1/1	0.18	-	73,73,73,73	0
57	MG	DA	3507	1/1	0.10	-	43,43,43,43	0
57	MG	BA	3736	1/1	0.24	-	42,42,42,42	0
57	MG	DA	3498	1/1	0.08	-	51,51,51,51	0
57	MG	DA	3042	1/1	0.20	-	38,38,38,38	0
57	MG	BQ	3001	1/1	0.17	-	45,45,45,45	0
57	MG	DA	3248	1/1	0.12	-	56,56,56,56	0
57	MG	DA	3039	1/1	0.13	-	43,43,43,43	0
57	MG	DA	3369	1/1	0.13	-	28,28,28,28	0
57	MG	CA	3022	1/1	0.13	-	78,78,78,78	0
57	MG	DA	3559	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
57	MG	DA	3461	1/1	0.14	-	62,62,62,62	0
57	MG	DA	3443	1/1	0.12	-	54,54,54,54	0
57	MG	DA	3172	1/1	0.12	-	62,62,62,62	0
57	MG	DA	3361	1/1	0.14	-	44,44,44,44	0
57	MG	BA	3313	1/1	0.06	-	53,53,53,53	0
57	MG	AA	3052	1/1	0.22	-	65,65,65,65	0
57	MG	BA	3193	1/1	0.16	-	48,48,48,48	0
57	MG	DA	3389	1/1	0.12	-	46,46,46,46	0
57	MG	BB	202	1/1	0.25	-	59,59,59,59	0
59	ZN	D9	501	1/1	0.10	-	68,68,68,68	0
57	MG	BA	3020	1/1	0.19	-	53,53,53,53	0
57	MG	DA	3055	1/1	0.15	-	49,49,49,49	0
57	MG	DA	3520	1/1	0.14	-	57,57,57,57	0
57	MG	DA	3537	1/1	0.05	-	44,44,44,44	0
57	MG	CA	3106	1/1	0.07	-	56,56,56,56	0
57	MG	BA	3634	1/1	0.18	-	62,62,62,62	0
57	MG	BA	3277	1/1	0.66	-	47,47,47,47	0
57	MG	DA	3089	1/1	0.42	-	52,52,52,52	0
57	MG	DA	3291	1/1	0.18	-	44,44,44,44	0
57	MG	BR	201	1/1	0.19	-	57,57,57,57	0
57	MG	DA	3662	1/1	0.10	-	62,62,62,62	0
57	MG	CA	3122	1/1	0.22	-	64,64,64,64	0
57	MG	BA	3628	1/1	0.17	-	49,49,49,49	0
57	MG	BA	3667	1/1	0.12	-	61,61,61,61	0
57	MG	AA	3162	1/1	0.06	-	66,66,66,66	0
57	MG	BA	3413	1/1	0.13	-	47,47,47,47	0
57	MG	DA	3473	1/1	0.08	-	50,50,50,50	0
57	MG	DU	3001	1/1	0.37	-	55,55,55,55	0
57	MG	DA	3484	1/1	0.12	-	62,62,62,62	0
57	MG	DA	3109	1/1	0.33	-	40,40,40,40	0
57	MG	AA	3214	1/1	0.15	-	73,73,73,73	0
57	MG	DA	3383	1/1	0.15	-	54,54,54,54	0
57	MG	AA	3200	1/1	0.09	-	73,73,73,73	0
57	MG	DA	3239	1/1	0.11	-	56,56,56,56	0
57	MG	DA	3436	1/1	0.09	-	54,54,54,54	0
57	MG	DA	3096	1/1	0.24	-	42,42,42,42	0
57	MG	BA	3028	1/1	0.13	-	51,51,51,51	0
57	MG	BA	3341	1/1	0.11	-	51,51,51,51	0
57	MG	CA	3164	1/1	0.16	-	60,60,60,60	0
57	MG	AA	3103	1/1	0.18	-	73,73,73,73	0
57	MG	BA	3198	1/1	0.47	-	37,37,37,37	0
57	MG	DA	3522	1/1	0.13	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3170	1/1	0.16	-	38,38,38,38	0
57	MG	CA	3098	1/1	0.10	-	65,65,65,65	0
57	MG	BA	3773	1/1	0.19	-	52,52,52,52	0
57	MG	BA	3257	1/1	0.22	-	53,53,53,53	0
57	MG	BA	3699	1/1	0.19	-	35,35,35,35	0
57	MG	DA	3403	1/1	0.13	-	57,57,57,57	0
57	MG	DA	3201	1/1	0.13	-	61,61,61,61	0
57	MG	BA	3775	1/1	0.21	-	33,33,33,33	0
57	MG	BA	3753	1/1	0.16	-	33,33,33,33	0
57	MG	DA	3209	1/1	0.15	-	53,53,53,53	0
57	MG	DA	3631	1/1	0.10	-	57,57,57,57	0
57	MG	DA	3677	1/1	0.68	-	52,52,52,52	0
57	MG	DA	3225	1/1	0.14	-	49,49,49,49	0
57	MG	DA	3062	1/1	0.34	-	63,63,63,63	0
57	MG	DA	3121	1/1	0.10	-	44,44,44,44	0
57	MG	BA	3762	1/1	0.14	-	46,46,46,46	0
57	MG	CA	3058	1/1	0.12	-	68,68,68,68	0
57	MG	BA	3032	1/1	0.19	-	47,47,47,47	0
57	MG	B5	101	1/1	0.51	-	51,51,51,51	0
57	MG	BA	3034	1/1	0.13	-	56,56,56,56	0
57	MG	CA	3135	1/1	0.14	-	63,63,63,63	0
57	MG	DA	3462	1/1	0.25	-	42,42,42,42	0
57	MG	DA	3155	1/1	0.18	-	48,48,48,48	0
57	MG	BA	3718	1/1	0.14	-	71,71,71,71	0
57	MG	BU	204	1/1	0.28	-	35,35,35,35	0
57	MG	BA	3550	1/1	0.17	-	36,36,36,36	0
57	MG	BA	3693	1/1	0.13	-	56,56,56,56	0
57	MG	BP	205	1/1	0.23	-	65,65,65,65	0
57	MG	BA	3782	1/1	0.12	-	65,65,65,65	0
57	MG	DA	3512	1/1	0.10	-	47,47,47,47	0
57	MG	DA	3568	1/1	0.07	-	52,52,52,52	0
57	MG	DA	3150	1/1	0.07	-	56,56,56,56	0
57	MG	AF	3001	1/1	0.16	-	44,44,44,44	0
57	MG	DA	3010	1/1	0.07	-	47,47,47,47	0
57	MG	BA	3350	1/1	0.18	-	28,28,28,28	0
57	MG	AA	3130	1/1	0.09	-	56,56,56,56	0
57	MG	AA	3201	1/1	0.08	-	52,52,52,52	0
57	MG	DA	3158	1/1	0.11	-	60,60,60,60	0
57	MG	AY	3003	1/1	0.39	-	53,53,53,53	0
57	MG	DA	3270	1/1	0.10	-	46,46,46,46	0
57	MG	AA	3107	1/1	0.16	-	64,64,64,64	0
57	MG	AA	3213	1/1	0.21	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3651	1/1	0.70	-	75,75,75,75	0
57	MG	BA	3680	1/1	0.09	-	68,68,68,68	0
57	MG	AA	3049	1/1	0.17	-	64,64,64,64	0
57	MG	AA	3123	1/1	0.20	-	51,51,51,51	0
57	MG	BA	3143	1/1	0.22	-	45,45,45,45	0
57	MG	CA	3125	1/1	0.06	-	63,63,63,63	0
57	MG	AA	3033	1/1	0.11	-	59,59,59,59	0
57	MG	BA	3013	1/1	0.16	-	32,32,32,32	0
57	MG	BA	3727	1/1	0.12	-	51,51,51,51	0
57	MG	DA	3064	1/1	0.35	-	49,49,49,49	0
57	MG	BA	3153	1/1	0.23	-	47,47,47,47	0
57	MG	DV	3002	1/1	0.61	-	49,49,49,49	0
57	MG	DA	3221	1/1	0.31	-	52,52,52,52	0
57	MG	DF	3004	1/1	0.41	-	44,44,44,44	0
57	MG	BA	3605	1/1	0.14	-	43,43,43,43	0
57	MG	DA	3184	1/1	0.12	-	47,47,47,47	0
57	MG	DA	3388	1/1	0.12	-	53,53,53,53	0
57	MG	BA	3781	1/1	0.18	-	41,41,41,41	0
57	MG	BA	3181	1/1	0.16	-	43,43,43,43	0
57	MG	BA	3576	1/1	0.07	-	57,57,57,57	0
57	MG	DA	3046	1/1	0.14	-	47,47,47,47	0
57	MG	BA	3251	1/1	0.13	-	44,44,44,44	0
57	MG	BA	3516	1/1	0.17	-	52,52,52,52	0
57	MG	CA	3166	1/1	0.15	-	66,66,66,66	0
57	MG	AA	3057	1/1	0.23	-	64,64,64,64	0
57	MG	DA	3023	1/1	0.24	-	40,40,40,40	0
57	MG	BA	3044	1/1	0.26	-	20,20,20,20	0
57	MG	BE	303	1/1	0.13	-	51,51,51,51	0
57	MG	BD	304	1/1	0.15	-	32,32,32,32	0
57	MG	AA	3207	1/1	0.07	-	65,65,65,65	0
57	MG	BD	306	1/1	0.21	-	38,38,38,38	0
57	MG	AA	3171	1/1	0.09	-	51,51,51,51	0
57	MG	BA	3785	1/1	0.23	-	59,59,59,59	0
57	MG	BA	3142	1/1	0.30	-	49,49,49,49	0
57	MG	DA	3141	1/1	0.28	-	61,61,61,61	0
57	MG	BA	3380	1/1	0.08	-	48,48,48,48	0
57	MG	BA	3333	1/1	0.18	-	38,38,38,38	0
57	MG	AA	3142	1/1	0.11	-	41,41,41,41	0
57	MG	AA	3120	1/1	0.14	-	45,45,45,45	0
57	MG	DA	3093	1/1	0.10	-	62,62,62,62	0
57	MG	BA	3812	1/1	0.48	-	47,47,47,47	0
57	MG	BA	3236	1/1	0.17	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3072	1/1	0.14	-	47,47,47,47	0
57	MG	BA	3465	1/1	0.15	-	43,43,43,43	0
57	MG	BA	3346	1/1	0.08	-	27,27,27,27	0
57	MG	BA	3663	1/1	0.15	-	41,41,41,41	0
57	MG	DA	3446	1/1	0.11	-	45,45,45,45	0
57	MG	BA	3409	1/1	0.16	-	30,30,30,30	0
57	MG	BA	3314	1/1	0.16	-	58,58,58,58	0
57	MG	BA	3508	1/1	0.18	-	51,51,51,51	0
57	MG	AA	3132	1/1	0.17	-	55,55,55,55	0
59	ZN	B5	102	1/1	0.21	-	48,48,48,48	0
57	MG	BA	3022	1/1	0.13	-	60,60,60,60	0
57	MG	BA	3156	1/1	0.33	-	41,41,41,41	0
57	MG	AA	3075	1/1	0.09	-	49,49,49,49	0
57	MG	BA	3542	1/1	0.16	-	45,45,45,45	0
57	MG	DA	3496	1/1	0.09	-	53,53,53,53	0
57	MG	DA	3254	1/1	0.06	-	52,52,52,52	0
57	MG	DA	3278	1/1	0.07	-	43,43,43,43	0
57	MG	AA	3168	1/1	0.10	-	59,59,59,59	0
57	MG	BA	3484	1/1	0.10	-	54,54,54,54	0
57	MG	BA	3067	1/1	0.10	-	41,41,41,41	0
57	MG	AA	3088	1/1	0.23	-	65,65,65,65	0
57	MG	AA	3064	1/1	0.20	-	60,60,60,60	0
57	MG	BA	3083	1/1	0.10	-	56,56,56,56	0
57	MG	DA	3017	1/1	0.07	-	55,55,55,55	0
57	MG	DA	3340	1/1	0.15	-	58,58,58,58	0
57	MG	DA	3585	1/1	0.10	-	43,43,43,43	0
57	MG	BA	3106	1/1	0.17	-	42,42,42,42	0
57	MG	AA	3066	1/1	0.25	-	60,60,60,60	0
57	MG	BA	3270	1/1	0.19	-	48,48,48,48	0
57	MG	DA	3534	1/1	0.15	-	55,55,55,55	0
57	MG	DA	3068	1/1	0.13	-	58,58,58,58	0
57	MG	DA	3177	1/1	0.15	-	42,42,42,42	0
57	MG	DA	3382	1/1	0.05	-	48,48,48,48	0
57	MG	DA	3289	1/1	0.07	-	53,53,53,53	0
57	MG	AA	3114	1/1	0.10	-	59,59,59,59	0
57	MG	CA	3072	1/1	0.07	-	54,54,54,54	0
59	ZN	BY	501	1/1	0.13	-	58,58,58,58	0
57	MG	AA	3179	1/1	0.14	-	69,69,69,69	0
57	MG	AW	3004	1/1	0.12	-	49,49,49,49	0
57	MG	BF	304	1/1	0.28	-	45,45,45,45	0
57	MG	DA	3293	1/1	0.11	-	54,54,54,54	0
57	MG	B0	101	1/1	0.27	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DN	5001	1/1	0.10	-	66,66,66,66	0
57	MG	DA	3140	1/1	0.15	-	58,58,58,58	0
57	MG	CA	3143	1/1	0.16	-	64,64,64,64	0
57	MG	BA	3590	1/1	0.15	-	50,50,50,50	0
57	MG	BA	3725	1/1	0.14	-	44,44,44,44	0
57	MG	BA	3163	1/1	0.10	-	55,55,55,55	0
57	MG	BA	3453	1/1	0.35	-	45,45,45,45	0
57	MG	DA	3566	1/1	0.16	-	69,69,69,69	0
57	MG	BA	3710	1/1	0.19	-	57,57,57,57	0
57	MG	CA	3124	1/1	0.13	-	59,59,59,59	0
57	MG	DA	3567	1/1	0.61	-	62,62,62,62	0
57	MG	BA	3417	1/1	0.18	-	38,38,38,38	0
57	MG	AA	3204	1/1	0.16	-	53,53,53,53	0
57	MG	AA	3093	1/1	0.17	-	66,66,66,66	0
57	MG	DB	3011	1/1	0.09	-	72,72,72,72	0
57	MG	BA	3602	1/1	0.17	-	53,53,53,53	0
57	MG	BA	3526	1/1	0.10	-	44,44,44,44	0
57	MG	BA	3692	1/1	0.10	-	40,40,40,40	0
57	MG	BA	3600	1/1	0.23	-	44,44,44,44	0
57	MG	DA	3424	1/1	0.09	-	61,61,61,61	0
57	MG	BA	3673	1/1	0.20	-	55,55,55,55	0
57	MG	AA	3152	1/1	0.10	-	62,62,62,62	0
57	MG	BA	3173	1/1	0.13	-	48,48,48,48	0
57	MG	BA	3750	1/1	0.17	-	27,27,27,27	0
57	MG	AX	3004	1/1	0.16	-	64,64,64,64	0
57	MG	BA	3640	1/1	0.20	-	53,53,53,53	0
57	MG	DA	3069	1/1	0.12	-	57,57,57,57	0
57	MG	BA	3462	1/1	0.13	-	36,36,36,36	0
57	MG	BX	3003	1/1	0.15	-	35,35,35,35	0
57	MG	BA	3568	1/1	0.09	-	59,59,59,59	0
57	MG	BA	3770	1/1	0.16	-	45,45,45,45	0
57	MG	BA	3021	1/1	0.12	-	49,49,49,49	0
57	MG	BA	3289	1/1	0.15	-	56,56,56,56	0
57	MG	BA	3091	1/1	0.36	-	56,56,56,56	0
57	MG	DA	3210	1/1	0.08	-	53,53,53,53	0
57	MG	BA	3216	1/1	0.24	-	37,37,37,37	0
57	MG	BA	3062	1/1	0.24	-	42,42,42,42	0
57	MG	BA	3385	1/1	0.13	-	59,59,59,59	0
57	MG	CA	3142	1/1	0.11	-	69,69,69,69	0
57	MG	CA	3086	1/1	0.12	-	64,64,64,64	0
57	MG	AA	3158	1/1	0.15	-	45,45,45,45	0
57	MG	BD	305	1/1	0.13	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DR	5001	1/1	0.37	-	70,70,70,70	0
57	MG	DA	3398	1/1	0.11	-	45,45,45,45	0
57	MG	AA	3039	1/1	0.17	-	56,56,56,56	0
57	MG	BA	3536	1/1	0.27	-	49,49,49,49	0
57	MG	DA	3215	1/1	0.13	-	59,59,59,59	0
57	MG	BA	3454	1/1	0.24	-	27,27,27,27	0
57	MG	DA	3535	1/1	0.20	-	56,56,56,56	0
57	MG	CA	3090	1/1	0.10	-	67,67,67,67	0
57	MG	BA	3712	1/1	0.18	-	53,53,53,53	0
57	MG	BA	3598	1/1	0.19	-	63,63,63,63	0
57	MG	BA	3488	1/1	0.14	-	60,60,60,60	0
57	MG	DA	3599	1/1	0.16	-	36,36,36,36	0
57	MG	DA	3163	1/1	0.09	-	49,49,49,49	0
57	MG	DD	307	1/1	0.45	-	43,43,43,43	0
57	MG	BA	3205	1/1	0.28	-	50,50,50,50	0
57	MG	BD	309	1/1	0.27	-	57,57,57,57	0
57	MG	BA	3705	1/1	0.10	-	62,62,62,62	0
57	MG	BA	3630	1/1	0.13	-	58,58,58,58	0
57	MG	DA	3476	1/1	0.16	-	62,62,62,62	0
57	MG	DA	3346	1/1	0.11	-	48,48,48,48	0
57	MG	AA	3059	1/1	0.11	-	78,78,78,78	0
57	MG	DA	3653	1/1	0.10	-	52,52,52,52	0
57	MG	DA	3336	1/1	0.16	-	40,40,40,40	0
57	MG	AA	3148	1/1	0.20	-	57,57,57,57	0
57	MG	BA	3416	1/1	0.22	-	21,21,21,21	0
57	MG	AA	3072	1/1	0.09	-	66,66,66,66	0
57	MG	DA	3178	1/1	0.20	-	50,50,50,50	0
57	MG	DB	3003	1/1	0.13	-	57,57,57,57	0
57	MG	DA	3129	1/1	0.10	-	46,46,46,46	0
57	MG	BA	3651	1/1	0.13	-	45,45,45,45	0
57	MG	BA	3514	1/1	0.21	-	48,48,48,48	0
57	MG	BA	3164	1/1	0.27	-	48,48,48,48	0
57	MG	BA	3556	1/1	0.22	-	36,36,36,36	0
57	MG	DA	3202	1/1	0.18	-	57,57,57,57	0
57	MG	CA	3140	1/1	0.12	-	67,67,67,67	0
57	MG	DA	3311	1/1	0.18	-	54,54,54,54	0
57	MG	DA	3602	1/1	0.06	-	65,65,65,65	0
57	MG	DA	3134	1/1	0.24	-	41,41,41,41	0
57	MG	BA	3554	1/1	0.10	-	51,51,51,51	0
57	MG	DA	3180	1/1	0.16	-	42,42,42,42	0
57	MG	BA	3139	1/1	0.37	-	40,40,40,40	0
57	MG	BA	3761	1/1	0.16	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3323	1/1	0.23	-	30,30,30,30	0
57	MG	BA	3601	1/1	0.08	-	55,55,55,55	0
57	MG	BA	3312	1/1	0.20	-	32,32,32,32	0
57	MG	BA	3180	1/1	0.16	-	47,47,47,47	0
57	MG	BA	3371	1/1	0.10	-	35,35,35,35	0
57	MG	BY	502	1/1	0.15	-	40,40,40,40	0
57	MG	BA	3645	1/1	0.17	-	33,33,33,33	0
57	MG	DA	3123	1/1	0.14	-	56,56,56,56	0
57	MG	DA	3418	1/1	0.13	-	52,52,52,52	0
57	MG	DA	3672	1/1	0.29	-	71,71,71,71	0
57	MG	DA	3353	1/1	0.13	-	42,42,42,42	0
57	MG	BP	203	1/1	0.13	-	33,33,33,33	0
57	MG	AA	3029	1/1	0.20	-	53,53,53,53	0
57	MG	DA	3027	1/1	0.36	-	51,51,51,51	0
57	MG	BA	3084	1/1	0.20	-	38,38,38,38	0
57	MG	DA	3617	1/1	0.13	-	56,56,56,56	0
57	MG	BA	3228	1/1	0.14	-	59,59,59,59	0
57	MG	DA	3356	1/1	0.10	-	36,36,36,36	0
57	MG	DA	3421	1/1	0.12	-	50,50,50,50	0
57	MG	DA	3206	1/1	0.09	-	50,50,50,50	0
57	MG	DA	3572	1/1	0.08	-	62,62,62,62	0
57	MG	BA	3799	1/1	0.06	-	49,49,49,49	0
57	MG	BA	3593	1/1	0.19	-	38,38,38,38	0
57	MG	DA	3300	1/1	0.19	-	45,45,45,45	0
57	MG	DA	3108	1/1	0.07	-	52,52,52,52	0
57	MG	DA	3647	1/1	0.14	-	54,54,54,54	0
57	MG	BA	3221	1/1	0.12	-	37,37,37,37	0
57	MG	DB	3009	1/1	0.14	-	59,59,59,59	0
57	MG	DA	3058	1/1	0.09	-	29,29,29,29	0
57	MG	BA	3141	1/1	0.50	-	42,42,42,42	0
57	MG	CA	3053	1/1	0.14	-	41,41,41,41	0
57	MG	BA	3060	1/1	0.18	-	30,30,30,30	0
57	MG	BA	3422	1/1	0.21	-	33,33,33,33	0
57	MG	BA	3355	1/1	0.18	-	61,61,61,61	0
57	MG	BA	3432	1/1	0.18	-	58,58,58,58	0
57	MG	DA	3244	1/1	0.09	-	71,71,71,71	0
57	MG	CA	3087	1/1	0.14	-	67,67,67,67	0
57	MG	BA	3424	1/1	0.23	-	39,39,39,39	0
57	MG	DA	3438	1/1	0.16	-	47,47,47,47	0
57	MG	DU	3002	1/1	0.99	-	55,55,55,55	0
57	MG	BA	3637	1/1	0.10	-	39,39,39,39	0
57	MG	BA	3360	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
57	MG	DB	3002	1/1	0.19	-	65,65,65,65	0
57	MG	AA	3174	1/1	0.07	-	50,50,50,50	0
57	MG	DA	3471	1/1	0.39	-	50,50,50,50	0
57	MG	DA	3250	1/1	0.28	-	69,69,69,69	0
57	MG	DA	3625	1/1	0.06	-	69,69,69,69	0
57	MG	DA	3431	1/1	0.25	-	50,50,50,50	0
57	MG	DA	3626	1/1	0.14	-	67,67,67,67	0
57	MG	BA	3196	1/1	0.43	-	38,38,38,38	0
57	MG	AA	3062	1/1	0.28	-	51,51,51,51	0
57	MG	BA	3125	1/1	0.14	-	47,47,47,47	0
57	MG	DA	3284	1/1	0.11	-	47,47,47,47	0
57	MG	DA	3047	1/1	0.10	-	49,49,49,49	0
57	MG	BO	201	1/1	0.18	-	50,50,50,50	0
57	MG	CA	3063	1/1	0.11	-	58,58,58,58	0
57	MG	DA	3187	1/1	0.11	-	42,42,42,42	0
57	MG	DA	3168	1/1	0.21	-	45,45,45,45	0
57	MG	DA	3488	1/1	0.08	-	41,41,41,41	0
57	MG	DA	3079	1/1	0.17	-	55,55,55,55	0
57	MG	DA	3454	1/1	0.14	-	56,56,56,56	0
57	MG	DD	304	1/1	0.27	-	52,52,52,52	0
57	MG	BA	3191	1/1	0.14	-	43,43,43,43	0
57	MG	DA	3164	1/1	0.09	-	51,51,51,51	0
57	MG	BA	3768	1/1	0.10	-	47,47,47,47	0
57	MG	BA	3511	1/1	0.12	-	30,30,30,30	0
57	MG	BA	3066	1/1	0.29	-	49,49,49,49	0
57	MG	DA	3392	1/1	0.14	-	70,70,70,70	0
57	MG	BA	3410	1/1	0.17	-	27,27,27,27	0
57	MG	DA	3297	1/1	0.08	-	39,39,39,39	0
57	MG	BN	3001	1/1	0.48	-	53,53,53,53	0
57	MG	BR	202	1/1	0.10	-	31,31,31,31	0
57	MG	BA	3183	1/1	0.19	-	42,42,42,42	0
57	MG	BA	3780	1/1	0.11	-	62,62,62,62	0
57	MG	DA	3267	1/1	0.10	-	49,49,49,49	0
57	MG	DA	3552	1/1	0.07	-	54,54,54,54	0
57	MG	DA	3030	1/1	0.10	-	39,39,39,39	0
57	MG	DA	3104	1/1	0.27	-	53,53,53,53	0
57	MG	DA	3527	1/1	0.10	-	60,60,60,60	0
57	MG	BA	3636	1/1	0.12	-	64,64,64,64	0
57	MG	DA	3262	1/1	0.11	-	65,65,65,65	0
57	MG	AW	3001	1/1	0.09	-	60,60,60,60	0
57	MG	DA	3157	1/1	0.24	-	47,47,47,47	0
57	MG	DA	3162	1/1	0.32	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3360	1/1	0.15	-	46,46,46,46	0
57	MG	BA	3677	1/1	0.15	-	60,60,60,60	0
57	MG	BA	3103	1/1	0.14	-	38,38,38,38	0
57	MG	BA	3735	1/1	0.62	-	57,57,57,57	0
57	MG	BA	3229	1/1	0.14	-	54,54,54,54	0
57	MG	BA	3713	1/1	0.14	-	33,33,33,33	0
57	MG	CA	3025	1/1	0.13	-	51,51,51,51	0
57	MG	DA	3228	1/1	0.40	-	38,38,38,38	0
57	MG	DA	3546	1/1	0.11	-	71,71,71,71	0
57	MG	BZ	3001	1/1	0.21	-	55,55,55,55	0
57	MG	BA	3557	1/1	0.15	-	33,33,33,33	0
57	MG	AA	3205	1/1	0.19	-	51,51,51,51	0
57	MG	AA	3083	1/1	0.35	-	57,57,57,57	0
57	MG	DA	3536	1/1	0.08	-	48,48,48,48	0
57	MG	DA	3208	1/1	0.40	-	58,58,58,58	0
57	MG	BA	3085	1/1	0.20	-	35,35,35,35	0
57	MG	BA	3537	1/1	0.18	-	45,45,45,45	0
57	MG	CA	3028	1/1	0.11	-	41,41,41,41	0
57	MG	BA	3423	1/1	0.18	-	44,44,44,44	0
57	MG	DA	3407	1/1	0.04	-	66,66,66,66	0
57	MG	DA	3573	1/1	0.07	-	43,43,43,43	0
57	MG	BU	207	1/1	0.33	-	38,38,38,38	0
57	MG	BA	3290	1/1	0.24	-	40,40,40,40	0
57	MG	BA	3024	1/1	0.17	-	49,49,49,49	0
57	MG	CA	3129	1/1	0.07	-	43,43,43,43	0
57	MG	BA	3039	1/1	0.13	-	32,32,32,32	0
57	MG	BA	3123	1/1	0.27	-	32,32,32,32	0
57	MG	BA	3115	1/1	0.24	-	59,59,59,59	0
57	MG	BA	3729	1/1	0.14	-	47,47,47,47	0
57	MG	BA	3090	1/1	0.15	-	53,53,53,53	0
57	MG	DA	3571	1/1	0.18	-	56,56,56,56	0
57	MG	DA	3483	1/1	0.46	-	55,55,55,55	0
57	MG	DV	3001	1/1	0.10	-	70,70,70,70	0
57	MG	AA	3082	1/1	0.19	-	46,46,46,46	0
57	MG	DA	3551	1/1	0.06	-	55,55,55,55	0
57	MG	DA	3277	1/1	0.13	-	55,55,55,55	0
57	MG	BA	3232	1/1	0.14	-	52,52,52,52	0
57	MG	CA	3019	1/1	0.07	-	65,65,65,65	0
57	MG	BA	3578	1/1	0.13	-	46,46,46,46	0
57	MG	DA	3323	1/1	0.11	-	50,50,50,50	0
57	MG	DA	3410	1/1	0.12	-	53,53,53,53	0
57	MG	DA	3252	1/1	0.07	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3321	1/1	0.07	-	48,48,48,48	0
57	MG	BA	3120	1/1	0.17	-	55,55,55,55	0
59	ZN	D5	501	1/1	0.18	-	58,58,58,58	0
57	MG	CA	3108	1/1	0.10	-	68,68,68,68	0
57	MG	AA	3092	1/1	0.11	-	63,63,63,63	0
57	MG	BA	3108	1/1	0.25	-	44,44,44,44	0
57	MG	BA	3683	1/1	0.10	-	73,73,73,73	0
57	MG	BA	3018	1/1	0.53	-	56,56,56,56	0
57	MG	CA	3111	1/1	0.15	-	64,64,64,64	0
57	MG	BA	3529	1/1	0.14	-	56,56,56,56	0
57	MG	BA	3088	1/1	0.35	-	48,48,48,48	0
57	MG	DA	3128	1/1	0.16	-	58,58,58,58	0
57	MG	DA	3174	1/1	0.09	-	44,44,44,44	0
57	MG	DA	3485	1/1	0.09	-	52,52,52,52	0
57	MG	BA	3402	1/1	0.11	-	40,40,40,40	0
57	MG	BA	3288	1/1	0.27	-	56,56,56,56	0
57	MG	BA	3771	1/1	0.29	-	50,50,50,50	0
57	MG	BA	3297	1/1	0.16	-	43,43,43,43	0
57	MG	BA	3447	1/1	0.08	-	72,72,72,72	0
57	MG	AA	3051	1/1	0.31	-	73,73,73,73	0
57	MG	DA	3185	1/1	0.47	-	68,68,68,68	0
57	MG	BA	3304	1/1	0.15	-	67,67,67,67	0
57	MG	DA	3674	1/1	0.25	-	37,37,37,37	0
57	MG	CD	301	1/1	0.12	-	56,56,56,56	0
57	MG	BA	3300	1/1	0.21	-	57,57,57,57	0
57	MG	DA	3151	1/1	0.07	-	55,55,55,55	0
57	MG	CA	3084	1/1	0.10	-	60,60,60,60	0
57	MG	CA	3132	1/1	0.28	-	66,66,66,66	0
57	MG	DA	3197	1/1	0.11	-	55,55,55,55	0
57	MG	BA	3672	1/1	0.21	-	43,43,43,43	0
57	MG	DA	3041	1/1	0.07	-	38,38,38,38	0
57	MG	BB	213	1/1	0.15	-	60,60,60,60	0
57	MG	BA	3746	1/1	0.13	-	51,51,51,51	0
57	MG	DA	3060	1/1	0.10	-	64,64,64,64	0
57	MG	BD	303	1/1	0.20	-	39,39,39,39	0
57	MG	DA	3432	1/1	0.14	-	37,37,37,37	0
57	MG	BA	3222	1/1	0.17	-	37,37,37,37	0
59	ZN	D6	501	1/1	0.17	-	71,71,71,71	0
57	MG	DA	3035	1/1	0.53	-	52,52,52,52	0
57	MG	DA	3281	1/1	0.14	-	53,53,53,53	0
57	MG	DA	3470	1/1	0.21	-	45,45,45,45	0
57	MG	BA	3500	1/1	0.16	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3433	1/1	0.20	-	46,46,46,46	0
57	MG	DA	3348	1/1	0.12	-	34,34,34,34	0
57	MG	CA	3117	1/1	0.14	-	71,71,71,71	0
57	MG	AX	3008	1/1	0.17	-	70,70,70,70	0
57	MG	BA	3691	1/1	0.18	-	55,55,55,55	0
57	MG	CA	3024	1/1	0.12	-	74,74,74,74	0
57	MG	DA	3466	1/1	0.16	-	41,41,41,41	0
57	MG	AA	3137	1/1	0.12	-	51,51,51,51	0
57	MG	DA	3635	1/1	0.11	-	38,38,38,38	0
57	MG	BA	3336	1/1	0.12	-	64,64,64,64	0
59	ZN	B9	501	1/1	0.14	-	38,38,38,38	0
57	MG	BA	3353	1/1	0.17	-	50,50,50,50	0
57	MG	DA	3666	1/1	0.12	-	35,35,35,35	0
57	MG	BA	3321	1/1	0.21	-	55,55,55,55	0
57	MG	DA	3303	1/1	0.07	-	48,48,48,48	0
57	MG	DA	3212	1/1	0.11	-	45,45,45,45	0
57	MG	BA	3420	1/1	0.15	-	40,40,40,40	0
57	MG	DA	3632	1/1	0.12	-	36,36,36,36	0
57	MG	BA	3763	1/1	0.17	-	24,24,24,24	0
57	MG	DA	3584	1/1	0.18	-	53,53,53,53	0
57	MG	DA	3191	1/1	0.14	-	37,37,37,37	0
57	MG	BA	3179	1/1	0.16	-	50,50,50,50	0
57	MG	DA	3526	1/1	0.11	-	48,48,48,48	0
57	MG	AA	3031	1/1	0.16	-	70,70,70,70	0
57	MG	DA	3367	1/1	0.17	-	61,61,61,61	0
57	MG	BA	3728	1/1	0.33	-	48,48,48,48	0
57	MG	DA	3655	1/1	0.13	-	64,64,64,64	0
57	MG	BA	3287	1/1	0.10	-	42,42,42,42	0
57	MG	BD	302	1/1	0.33	-	50,50,50,50	0
57	MG	DE	302	1/1	0.10	-	33,33,33,33	0
57	MG	BA	3098	1/1	0.21	-	40,40,40,40	0
57	MG	B4	502	1/1	0.14	-	71,71,71,71	0
57	MG	BA	3394	1/1	0.19	-	40,40,40,40	0
57	MG	AA	3125	1/1	0.22	-	37,37,37,37	0
57	MG	BA	3026	1/1	0.12	-	41,41,41,41	0
57	MG	BA	3101	1/1	0.33	-	53,53,53,53	0
57	MG	BA	3140	1/1	0.14	-	47,47,47,47	0
57	MG	CA	3148	1/1	0.13	-	70,70,70,70	0
57	MG	BA	3036	1/1	0.13	-	40,40,40,40	0
57	MG	BA	3096	1/1	0.39	-	54,54,54,54	0
57	MG	BG	202	1/1	0.15	-	41,41,41,41	0
57	MG	BA	3749	1/1	0.11	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BU	203	1/1	0.31	-	47,47,47,47	0
57	MG	DA	3447	1/1	0.17	-	58,58,58,58	0
57	MG	AX	3011	1/1	0.23	-	78,78,78,78	0
57	MG	BA	3016	1/1	0.13	-	38,38,38,38	0
57	MG	DA	3114	1/1	0.18	-	55,55,55,55	0
57	MG	AA	3084	1/1	0.23	-	51,51,51,51	0
57	MG	BA	3007	1/1	0.18	-	55,55,55,55	0
57	MG	DA	3501	1/1	0.24	-	37,37,37,37	0
57	MG	BA	3064	1/1	0.28	-	43,43,43,43	0
57	MG	DA	3143	1/1	0.15	-	38,38,38,38	0
57	MG	BA	3172	1/1	0.20	-	46,46,46,46	0
57	MG	BA	3426	1/1	0.20	-	37,37,37,37	0
57	MG	BA	3223	1/1	0.10	-	41,41,41,41	0
57	MG	AA	3161	1/1	0.12	-	65,65,65,65	0
57	MG	DA	3641	1/1	0.36	-	69,69,69,69	0
57	MG	BA	3225	1/1	0.17	-	61,61,61,61	0
57	MG	CA	3009	1/1	0.10	-	64,64,64,64	0
57	MG	CA	3036	1/1	0.12	-	66,66,66,66	0
57	MG	AX	3016	1/1	0.18	-	56,56,56,56	0
57	MG	B2	3001	1/1	0.34	-	56,56,56,56	0
57	MG	CA	3127	1/1	0.12	-	62,62,62,62	0
57	MG	BA	3318	1/1	0.13	-	41,41,41,41	0
57	MG	BA	3265	1/1	0.17	-	54,54,54,54	0
57	MG	BQ	3002	1/1	0.13	-	43,43,43,43	0
57	MG	DA	3152	1/1	0.18	-	51,51,51,51	0
57	MG	BA	3611	1/1	0.14	-	46,46,46,46	0
57	MG	BA	3618	1/1	0.13	-	65,65,65,65	0
57	MG	BA	3612	1/1	0.14	-	21,21,21,21	0
57	MG	BA	3794	1/1	0.25	-	51,51,51,51	0
57	MG	BA	3695	1/1	0.19	-	67,67,67,67	0
57	MG	BA	3320	1/1	0.17	-	48,48,48,48	0
57	MG	AA	3175	1/1	0.19	-	63,63,63,63	0
57	MG	BA	3256	1/1	0.14	-	40,40,40,40	0
57	MG	BA	3523	1/1	0.10	-	48,48,48,48	0
57	MG	BA	3363	1/1	0.12	-	22,22,22,22	0
57	MG	DA	3338	1/1	0.13	-	61,61,61,61	0
57	MG	AA	3027	1/1	0.21	-	50,50,50,50	0
59	ZN	D4	501	1/1	0.06	-	144,144,144,144	0
57	MG	BA	3476	1/1	0.23	-	55,55,55,55	0
57	MG	BB	216	1/1	0.25	-	51,51,51,51	0
57	MG	DP	202	1/1	0.11	-	53,53,53,53	0
57	MG	CA	3112	1/1	0.10	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3332	1/1	0.14	-	53,53,53,53	0
57	MG	BA	3118	1/1	0.14	-	48,48,48,48	0
57	MG	BA	3503	1/1	0.12	-	49,49,49,49	0
57	MG	BA	3797	1/1	0.14	-	53,53,53,53	0
57	MG	CA	3155	1/1	0.12	-	53,53,53,53	0
57	MG	AA	3040	1/1	0.08	-	60,60,60,60	0
57	MG	DG	3001	1/1	0.08	-	55,55,55,55	0
57	MG	DA	3582	1/1	0.07	-	56,56,56,56	0
57	MG	CA	3093	1/1	0.09	-	55,55,55,55	0
57	MG	BA	3580	1/1	0.12	-	55,55,55,55	0
57	MG	BA	3722	1/1	0.18	-	47,47,47,47	0
57	MG	AA	3164	1/1	0.11	-	61,61,61,61	0
57	MG	BA	3754	1/1	0.17	-	48,48,48,48	0
57	MG	BA	3609	1/1	0.13	-	39,39,39,39	0
57	MG	BA	3400	1/1	0.26	-	33,33,33,33	0
57	MG	BA	3405	1/1	0.21	-	63,63,63,63	0
57	MG	DA	3575	1/1	0.12	-	64,64,64,64	0
57	MG	BB	214	1/1	0.16	-	49,49,49,49	0
57	MG	BA	3302	1/1	0.11	-	69,69,69,69	0
60	K	AX	3001	1/1	0.12	-	65,65,65,65	0
57	MG	DA	3097	1/1	0.15	-	33,33,33,33	0
57	MG	DA	3083	1/1	0.37	-	40,40,40,40	0
57	MG	DA	3676	1/1	0.36	-	67,67,67,67	0
57	MG	DA	3586	1/1	0.13	-	60,60,60,60	0
57	MG	BA	3133	1/1	0.12	-	45,45,45,45	0
57	MG	BA	3670	1/1	0.21	-	61,61,61,61	0
57	MG	DA	3328	1/1	0.10	-	47,47,47,47	0
57	MG	BA	3769	1/1	0.13	-	52,52,52,52	0
57	MG	BA	3113	1/1	0.14	-	53,53,53,53	0
57	MG	DA	3581	1/1	0.21	-	57,57,57,57	0
59	ZN	CN	501	1/1	0.09	-	93,93,93,93	0
57	MG	CA	3031	1/1	0.19	-	68,68,68,68	0
57	MG	AA	3081	1/1	0.18	-	48,48,48,48	0
57	MG	BA	3231	1/1	0.30	-	63,63,63,63	0
57	MG	CA	3026	1/1	0.15	-	63,63,63,63	0
57	MG	DA	3018	1/1	0.25	-	62,62,62,62	0
57	MG	BA	3240	1/1	0.59	-	47,47,47,47	0
57	MG	BA	3452	1/1	0.13	-	55,55,55,55	0
57	MG	BA	3626	1/1	0.20	-	44,44,44,44	0
57	MG	BA	3777	1/1	0.13	-	40,40,40,40	0
57	MG	DA	3116	1/1	0.46	-	52,52,52,52	0
57	MG	BA	3147	1/1	0.17	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3551	1/1	0.16	-	36,36,36,36	0
57	MG	BA	3505	1/1	0.13	-	55,55,55,55	0
57	MG	DA	3238	1/1	0.18	-	44,44,44,44	0
57	MG	CA	3150	1/1	0.18	-	56,56,56,56	0
57	MG	DA	3444	1/1	0.06	-	44,44,44,44	0
57	MG	AA	3034	1/1	0.12	-	47,47,47,47	0
57	MG	DA	3051	1/1	0.11	-	48,48,48,48	0
57	MG	AA	3166	1/1	0.08	-	69,69,69,69	0
57	MG	DA	3031	1/1	0.41	-	43,43,43,43	0
57	MG	BB	207	1/1	0.17	-	54,54,54,54	0
57	MG	BA	3266	1/1	0.16	-	39,39,39,39	0
57	MG	DA	3650	1/1	0.14	-	67,67,67,67	0
57	MG	DA	3648	1/1	0.20	-	57,57,57,57	0
57	MG	BA	3613	1/1	0.47	-	42,42,42,42	0
57	MG	DA	3080	1/1	0.11	-	55,55,55,55	0
57	MG	DA	3404	1/1	0.09	-	48,48,48,48	0
57	MG	CA	3017	1/1	0.19	-	53,53,53,53	0
57	MG	DA	3286	1/1	0.12	-	42,42,42,42	0
57	MG	BA	3041	1/1	0.14	-	40,40,40,40	0
57	MG	BA	3061	1/1	0.23	-	29,29,29,29	0
57	MG	BA	3226	1/1	0.18	-	47,47,47,47	0
57	MG	CA	3054	1/1	0.26	-	69,69,69,69	0
57	MG	BA	3376	1/1	0.17	-	48,48,48,48	0
57	MG	BA	3055	1/1	0.17	-	45,45,45,45	0
57	MG	BQ	3003	1/1	0.22	-	49,49,49,49	0
57	MG	BA	3246	1/1	0.25	-	39,39,39,39	0
57	MG	DA	3458	1/1	0.09	-	52,52,52,52	0
57	MG	CA	3056	1/1	0.17	-	64,64,64,64	0
57	MG	DA	3110	1/1	0.24	-	58,58,58,58	0
57	MG	DB	3013	1/1	0.13	-	64,64,64,64	0
57	MG	DA	3464	1/1	0.11	-	46,46,46,46	0
57	MG	BA	3326	1/1	0.12	-	20,20,20,20	0
57	MG	BA	3442	1/1	0.15	-	44,44,44,44	0
57	MG	DA	3620	1/1	0.08	-	68,68,68,68	0
57	MG	DA	3553	1/1	0.10	-	49,49,49,49	0
57	MG	DA	3419	1/1	0.10	-	32,32,32,32	0
57	MG	AA	3116	1/1	0.11	-	55,55,55,55	0
57	MG	DA	3279	1/1	0.11	-	56,56,56,56	0
57	MG	BA	3406	1/1	0.10	-	50,50,50,50	0
57	MG	BA	3042	1/1	0.13	-	43,43,43,43	0
57	MG	AA	3151	1/1	0.14	-	45,45,45,45	0
57	MG	BF	302	1/1	0.15	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	3046	1/1	0.07	-	69,69,69,69	0
57	MG	BA	3587	1/1	0.21	-	36,36,36,36	0
57	MG	AX	3009	1/1	0.18	-	64,64,64,64	0
57	MG	DA	3357	1/1	0.08	-	50,50,50,50	0
57	MG	BA	3519	1/1	0.08	-	55,55,55,55	0
57	MG	DA	3469	1/1	0.28	-	44,44,44,44	0
57	MG	BA	3539	1/1	0.19	-	52,52,52,52	0
57	MG	DA	3377	1/1	0.08	-	38,38,38,38	0
57	MG	BA	3087	1/1	0.22	-	42,42,42,42	0
57	MG	DA	3199	1/1	0.22	-	47,47,47,47	0
57	MG	BA	3679	1/1	0.14	-	62,62,62,62	0
57	MG	BA	3211	1/1	0.58	-	55,55,55,55	0
57	MG	BA	3621	1/1	0.15	-	53,53,53,53	0
57	MG	DA	3453	1/1	0.18	-	60,60,60,60	0
57	MG	DA	3175	1/1	0.14	-	41,41,41,41	0
57	MG	BA	3220	1/1	0.19	-	29,29,29,29	0
57	MG	BA	3811	1/1	0.13	-	65,65,65,65	0
57	MG	AA	3145	1/1	0.20	-	66,66,66,66	0
57	MG	BA	3329	1/1	0.35	-	60,60,60,60	0
57	MG	CA	3165	1/1	0.09	-	45,45,45,45	0
57	MG	BA	3065	1/1	0.25	-	60,60,60,60	0
57	MG	BA	3053	1/1	0.15	-	54,54,54,54	0
57	MG	BA	3507	1/1	0.16	-	49,49,49,49	0
57	MG	CA	3080	1/1	0.09	-	49,49,49,49	0
57	MG	BA	3553	1/1	0.08	-	59,59,59,59	0
57	MG	BA	3704	1/1	0.09	-	77,77,77,77	0
57	MG	BA	3585	1/1	0.06	-	46,46,46,46	0
57	MG	CA	3153	1/1	0.12	-	70,70,70,70	0
57	MG	BA	3152	1/1	0.26	-	43,43,43,43	0
57	MG	DA	3459	1/1	0.16	-	47,47,47,47	0
57	MG	BA	3235	1/1	0.24	-	42,42,42,42	0
57	MG	BA	3009	1/1	0.08	-	28,28,28,28	0
57	MG	AA	3135	1/1	0.20	-	65,65,65,65	0
57	MG	DA	3026	1/1	0.50	-	59,59,59,59	0
57	MG	DA	3614	1/1	0.09	-	65,65,65,65	0
58	SF4	AD	501	8/8	0.17	-	62,68,73,86	0
57	MG	BA	3591	1/1	0.17	-	35,35,35,35	0
57	MG	DA	3402	1/1	0.10	-	66,66,66,66	0
57	MG	BB	205	1/1	0.11	-	60,60,60,60	0
57	MG	DA	3063	1/1	0.32	-	54,54,54,54	0
57	MG	BA	3716	1/1	0.15	-	65,65,65,65	0
57	MG	AA	3115	1/1	0.12	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3160	1/1	0.13	-	56,56,56,56	0
57	MG	B3	3001	1/1	0.10	-	34,34,34,34	0
57	MG	DA	3292	1/1	0.12	-	30,30,30,30	0
57	MG	CA	3067	1/1	0.29	-	61,61,61,61	0
57	MG	CA	3018	1/1	0.16	-	69,69,69,69	0
57	MG	BE	304	1/1	0.24	-	42,42,42,42	0
57	MG	BA	3589	1/1	0.23	-	27,27,27,27	0
57	MG	AN	502	1/1	0.27	-	63,63,63,63	0
57	MG	CA	3094	1/1	0.16	-	70,70,70,70	0
57	MG	BA	3097	1/1	0.20	-	44,44,44,44	0
57	MG	BA	3678	1/1	0.07	-	65,65,65,65	0
57	MG	DA	3054	1/1	0.25	-	48,48,48,48	0
57	MG	BA	3809	1/1	0.16	-	63,63,63,63	0
57	MG	BA	3383	1/1	0.10	-	53,53,53,53	0
57	MG	BA	3035	1/1	0.24	-	39,39,39,39	0
57	MG	DA	3094	1/1	0.16	-	50,50,50,50	0
57	MG	DA	3315	1/1	0.06	-	42,42,42,42	0
57	MG	DA	3033	1/1	0.08	-	42,42,42,42	0
57	MG	DA	3608	1/1	0.12	-	68,68,68,68	0
57	MG	BA	3209	1/1	0.19	-	54,54,54,54	0
57	MG	CA	3068	1/1	0.11	-	48,48,48,48	0
57	MG	BA	3168	1/1	0.14	-	47,47,47,47	0
57	MG	DA	3213	1/1	0.84	-	63,63,63,63	0
57	MG	BA	3244	1/1	0.23	-	53,53,53,53	0
57	MG	BA	3339	1/1	0.18	-	23,23,23,23	0
57	MG	DA	3657	1/1	0.08	-	63,63,63,63	0
57	MG	BA	3281	1/1	0.14	-	60,60,60,60	0
57	MG	CA	3147	1/1	0.12	-	64,64,64,64	0
57	MG	BB	218	1/1	0.13	-	77,77,77,77	0
57	MG	BA	3213	1/1	0.23	-	40,40,40,40	0
57	MG	DA	3304	1/1	0.07	-	48,48,48,48	0
57	MG	CA	3044	1/1	0.20	-	62,62,62,62	0
57	MG	AA	3013	1/1	0.11	-	69,69,69,69	0
57	MG	BA	3330	1/1	0.25	-	37,37,37,37	0
57	MG	BA	3077	1/1	0.12	-	49,49,49,49	0
57	MG	BA	3165	1/1	0.28	-	45,45,45,45	0
57	MG	DA	3115	1/1	0.13	-	40,40,40,40	0
57	MG	DA	3630	1/1	0.11	-	61,61,61,61	0
57	MG	DA	3205	1/1	0.11	-	56,56,56,56	0
57	MG	BA	3610	1/1	0.13	-	61,61,61,61	0
57	MG	DA	3391	1/1	0.09	-	45,45,45,45	0
57	MG	BQ	3004	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
57	MG	BA	3279	1/1	0.23	-	43,43,43,43	0
57	MG	DA	3503	1/1	0.14	-	52,52,52,52	0
57	MG	AA	3019	1/1	0.14	-	66,66,66,66	0
57	MG	AA	3056	1/1	0.19	-	61,61,61,61	0
57	MG	BA	3414	1/1	0.16	-	41,41,41,41	0
57	MG	DA	3560	1/1	0.06	-	40,40,40,40	0
57	MG	BA	3214	1/1	0.12	-	41,41,41,41	0
57	MG	DA	3181	1/1	0.09	-	50,50,50,50	0
57	MG	DA	3422	1/1	0.09	-	46,46,46,46	0
57	MG	AA	3202	1/1	0.17	-	57,57,57,57	0
57	MG	BA	3582	1/1	0.22	-	74,74,74,74	0
57	MG	DA	3532	1/1	0.20	-	69,69,69,69	0
57	MG	CA	3114	1/1	0.10	-	57,57,57,57	0
57	MG	DA	3556	1/1	0.18	-	67,67,67,67	0
57	MG	DA	3147	1/1	0.09	-	56,56,56,56	0
57	MG	BA	3089	1/1	0.15	-	19,19,19,19	0
57	MG	AA	3032	1/1	0.23	-	67,67,67,67	0
57	MG	BA	3469	1/1	0.13	-	49,49,49,49	0
57	MG	DA	3621	1/1	0.07	-	44,44,44,44	0
57	MG	AE	203	1/1	0.18	-	63,63,63,63	0
57	MG	AA	3086	1/1	0.11	-	57,57,57,57	0
57	MG	BA	3110	1/1	0.14	-	41,41,41,41	0
57	MG	BA	3054	1/1	0.23	-	36,36,36,36	0
57	MG	BA	3399	1/1	0.20	-	45,45,45,45	0
57	MG	BA	3249	1/1	0.32	-	49,49,49,49	0
57	MG	DA	3194	1/1	0.22	-	56,56,56,56	0
57	MG	CA	3169	1/1	0.14	-	51,51,51,51	0
57	MG	BA	3702	1/1	0.18	-	51,51,51,51	0
57	MG	BA	3107	1/1	0.14	-	53,53,53,53	0
57	MG	AA	3042	1/1	0.06	-	57,57,57,57	0
57	MG	BA	3562	1/1	0.13	-	37,37,37,37	0
57	MG	AX	3006	1/1	0.09	-	65,65,65,65	0
57	MG	B0	102	1/1	0.14	-	48,48,48,48	0
57	MG	DA	3105	1/1	0.15	-	48,48,48,48	0
57	MG	DA	3022	1/1	0.17	-	51,51,51,51	0
57	MG	DA	3525	1/1	0.16	-	59,59,59,59	0
57	MG	CA	3095	1/1	0.10	-	64,64,64,64	0
57	MG	DA	3558	1/1	0.15	-	61,61,61,61	0
57	MG	AA	3010	1/1	0.09	-	52,52,52,52	0
57	MG	DA	3451	1/1	0.13	-	55,55,55,55	0
57	MG	DA	3122	1/1	0.10	-	49,49,49,49	0
57	MG	DA	3493	1/1	0.20	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3348	1/1	0.18	-	36,36,36,36	0
57	MG	BA	3620	1/1	0.11	-	40,40,40,40	0
57	MG	DA	3333	1/1	0.13	-	41,41,41,41	0
57	MG	DA	3371	1/1	0.11	-	58,58,58,58	0
57	MG	CA	3160	1/1	0.17	-	62,62,62,62	0
57	MG	BA	3175	1/1	0.19	-	20,20,20,20	0
57	MG	CA	3048	1/1	0.33	-	67,67,67,67	0
57	MG	CA	3096	1/1	0.06	-	44,44,44,44	0
57	MG	CA	3170	1/1	0.12	-	58,58,58,58	0
57	MG	DB	3006	1/1	0.12	-	57,57,57,57	0
57	MG	BA	3682	1/1	0.18	-	53,53,53,53	0
57	MG	BA	3701	1/1	0.16	-	43,43,43,43	0
57	MG	AA	3167	1/1	0.15	-	57,57,57,57	0
59	ZN	B4	501	1/1	0.13	-	89,89,89,89	0
57	MG	CA	3014	1/1	0.10	-	58,58,58,58	0
57	MG	BA	3571	1/1	0.18	-	58,58,58,58	0
57	MG	AA	3212	1/1	0.12	-	42,42,42,42	0
57	MG	BA	3078	1/1	0.16	-	51,51,51,51	0
57	MG	BA	3510	1/1	0.14	-	46,46,46,46	0
57	MG	BA	3631	1/1	0.23	-	42,42,42,42	0
57	MG	AA	3126	1/1	0.06	-	49,49,49,49	0
57	MG	DA	3437	1/1	0.14	-	52,52,52,52	0
57	MG	DA	3050	1/1	0.13	-	59,59,59,59	0
57	MG	BD	308	1/1	0.36	-	46,46,46,46	0
57	MG	DA	3229	1/1	0.15	-	50,50,50,50	0
57	MG	BA	3430	1/1	0.15	-	37,37,37,37	0
57	MG	CA	3139	1/1	0.13	-	62,62,62,62	0
57	MG	DA	3310	1/1	0.15	-	38,38,38,38	0
57	MG	DA	3380	1/1	0.10	-	55,55,55,55	0
57	MG	AA	3060	1/1	0.22	-	46,46,46,46	0
57	MG	DA	3275	1/1	0.17	-	42,42,42,42	0
57	MG	D3	3001	1/1	0.30	-	57,57,57,57	0
57	MG	DA	3487	1/1	0.25	-	62,62,62,62	0
57	MG	BA	3111	1/1	0.13	-	54,54,54,54	0
57	MG	AA	3178	1/1	0.15	-	59,59,59,59	0
57	MG	BA	3739	1/1	0.23	-	40,40,40,40	0
57	MG	DA	3145	1/1	0.24	-	43,43,43,43	0
57	MG	CA	3157	1/1	0.11	-	58,58,58,58	0
57	MG	DA	3211	1/1	0.09	-	48,48,48,48	0
57	MG	CA	3035	1/1	0.10	-	59,59,59,59	0
57	MG	DA	3364	1/1	0.17	-	40,40,40,40	0
57	MG	DA	3379	1/1	0.10	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3756	1/1	0.17	-	48,48,48,48	0
57	MG	BP	202	1/1	0.22	-	36,36,36,36	0
57	MG	DA	3529	1/1	0.09	-	38,38,38,38	0
57	MG	BA	3352	1/1	0.23	-	53,53,53,53	0
57	MG	BA	3068	1/1	0.13	-	43,43,43,43	0
57	MG	DA	3288	1/1	0.15	-	52,52,52,52	0
57	MG	BA	3124	1/1	0.18	-	19,19,19,19	0
57	MG	BA	3075	1/1	0.19	-	45,45,45,45	0
57	MG	DA	3591	1/1	0.12	-	55,55,55,55	0
57	MG	BB	208	1/1	0.12	-	45,45,45,45	0
57	MG	AA	3193	1/1	0.09	-	72,72,72,72	0
57	MG	DA	3179	1/1	0.09	-	52,52,52,52	0
57	MG	AA	3050	1/1	0.19	-	33,33,33,33	0
57	MG	BA	3596	1/1	0.13	-	64,64,64,64	0
57	MG	BA	3513	1/1	0.10	-	59,59,59,59	0
57	MG	BA	3247	1/1	0.31	-	25,25,25,25	0
57	MG	BA	3293	1/1	0.22	-	50,50,50,50	0
57	MG	AX	3003	1/1	0.10	-	71,71,71,71	0
57	MG	DA	3399	1/1	0.14	-	59,59,59,59	0
57	MG	BA	3643	1/1	0.17	-	46,46,46,46	0
57	MG	BQ	3005	1/1	0.11	-	49,49,49,49	0
57	MG	AA	3002	1/1	0.13	-	71,71,71,71	0
57	MG	DA	3387	1/1	0.08	-	42,42,42,42	0
57	MG	BA	3440	1/1	0.08	-	42,42,42,42	0
57	MG	DA	3015	1/1	0.32	-	52,52,52,52	0
57	MG	BA	3639	1/1	0.36	-	48,48,48,48	0
57	MG	DA	3481	1/1	0.60	-	55,55,55,55	0
57	MG	DA	3428	1/1	0.17	-	37,37,37,37	0
57	MG	BP	204	1/1	0.09	-	46,46,46,46	0
57	MG	CA	3074	1/1	0.23	-	64,64,64,64	0
57	MG	DA	3368	1/1	0.23	-	50,50,50,50	0
57	MG	DA	3668	1/1	0.22	-	60,60,60,60	0
57	MG	DA	3148	1/1	0.14	-	54,54,54,54	0
57	MG	AE	201	1/1	0.16	-	59,59,59,59	0
57	MG	BA	3723	1/1	0.08	-	47,47,47,47	0
57	MG	AM	201	1/1	0.12	-	51,51,51,51	0
57	MG	BA	3757	1/1	0.19	-	76,76,76,76	0
57	MG	CA	3088	1/1	0.17	-	74,74,74,74	0
57	MG	DA	3219	1/1	0.15	-	53,53,53,53	0
57	MG	BA	3253	1/1	0.26	-	55,55,55,55	0
57	MG	DA	3670	1/1	0.29	-	60,60,60,60	0
57	MG	DA	3495	1/1	0.10	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3102	1/1	0.11	-	44,44,44,44	0
57	MG	DA	3189	1/1	0.21	-	41,41,41,41	0
57	MG	DW	3002	1/1	0.20	-	45,45,45,45	0
57	MG	BA	3572	1/1	0.19	-	61,61,61,61	0
57	MG	BA	3463	1/1	0.24	-	48,48,48,48	0
57	MG	BA	3194	1/1	0.15	-	47,47,47,47	0
57	MG	BA	3278	1/1	0.14	-	34,34,34,34	0
57	MG	BA	3776	1/1	0.16	-	43,43,43,43	0
57	MG	BD	307	1/1	0.30	-	40,40,40,40	0
57	MG	BA	3301	1/1	0.11	-	60,60,60,60	0
57	MG	DA	3057	1/1	0.16	-	42,42,42,42	0
57	MG	DA	3465	1/1	0.13	-	46,46,46,46	0
57	MG	DA	3008	1/1	0.08	-	36,36,36,36	0
57	MG	BA	3052	1/1	0.15	-	56,56,56,56	0
57	MG	BA	3037	1/1	0.18	-	34,34,34,34	0
57	MG	DA	3492	1/1	0.10	-	55,55,55,55	0
57	MG	AA	3005	1/1	0.14	-	62,62,62,62	0
57	MG	BA	3810	1/1	0.26	-	41,41,41,41	0
57	MG	BA	3492	1/1	0.14	-	46,46,46,46	0
57	MG	BF	307	1/1	0.34	-	37,37,37,37	0
57	MG	AA	3007	1/1	0.15	-	57,57,57,57	0
57	MG	CA	3113	1/1	0.08	-	67,67,67,67	0
57	MG	BA	3308	1/1	0.15	-	43,43,43,43	0
57	MG	DA	3381	1/1	0.11	-	56,56,56,56	0
57	MG	BA	3456	1/1	0.19	-	49,49,49,49	0
57	MG	CA	3032	1/1	0.18	-	62,62,62,62	0
57	MG	DA	3095	1/1	0.25	-	58,58,58,58	0
57	MG	BA	3092	1/1	0.14	-	37,37,37,37	0
57	MG	BA	3744	1/1	0.10	-	39,39,39,39	0
57	MG	BA	3354	1/1	0.08	-	48,48,48,48	0
57	MG	DA	3673	1/1	0.13	-	69,69,69,69	0
57	MG	BA	3473	1/1	0.24	-	56,56,56,56	0
57	MG	DA	3583	1/1	0.16	-	51,51,51,51	0
57	MG	BA	3045	1/1	0.23	-	36,36,36,36	0
60	K	CX	3001	1/1	0.33	-	82,82,82,82	0
57	MG	BA	3714	1/1	0.21	-	57,57,57,57	0
57	MG	BA	3584	1/1	0.24	-	63,63,63,63	0
57	MG	BA	3448	1/1	0.23	-	32,32,32,32	0
57	MG	CX	3004	1/1	0.15	-	63,63,63,63	0
57	MG	BE	302	1/1	0.29	-	39,39,39,39	0
57	MG	DA	3636	1/1	0.15	-	63,63,63,63	0
57	MG	DA	3217	1/1	0.11	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3378	1/1	0.12	-	57,57,57,57	0
57	MG	DA	3098	1/1	0.16	-	53,53,53,53	0
57	MG	BA	3652	1/1	0.10	-	67,67,67,67	0
57	MG	AA	3038	1/1	0.25	-	68,68,68,68	0
57	MG	DW	3004	1/1	0.28	-	52,52,52,52	0
57	MG	BA	3807	1/1	0.13	-	47,47,47,47	0
57	MG	BA	3298	1/1	0.11	-	51,51,51,51	0
57	MG	DA	3117	1/1	0.52	-	52,52,52,52	0
57	MG	AA	3074	1/1	0.13	-	50,50,50,50	0
57	MG	DF	3002	1/1	0.08	-	48,48,48,48	0
57	MG	DA	3412	1/1	0.14	-	50,50,50,50	0
57	MG	BA	3031	1/1	0.14	-	52,52,52,52	0
57	MG	CA	3073	1/1	0.15	-	57,57,57,57	0
57	MG	DA	3324	1/1	0.11	-	33,33,33,33	0
57	MG	AA	3197	1/1	0.29	-	70,70,70,70	0
57	MG	BA	3370	1/1	0.21	-	39,39,39,39	0
57	MG	BA	3579	1/1	0.10	-	49,49,49,49	0
57	MG	BA	3606	1/1	0.13	-	61,61,61,61	0
57	MG	BA	3243	1/1	0.11	-	53,53,53,53	0
57	MG	DA	3597	1/1	0.05	-	51,51,51,51	0
57	MG	DA	3592	1/1	0.10	-	51,51,51,51	0
57	MG	AA	3053	1/1	0.15	-	61,61,61,61	0
57	MG	BU	201	1/1	0.24	-	43,43,43,43	0
57	MG	BA	3561	1/1	0.11	-	45,45,45,45	0
57	MG	DA	3519	1/1	0.09	-	63,63,63,63	0
57	MG	AA	3067	1/1	0.24	-	57,57,57,57	0
57	MG	CA	3163	1/1	0.08	-	63,63,63,63	0
57	MG	DA	3365	1/1	0.07	-	36,36,36,36	0
57	MG	CA	3033	1/1	0.17	-	71,71,71,71	0
57	MG	CA	3146	1/1	0.17	-	66,66,66,66	0
57	MG	CA	3006	1/1	0.08	-	64,64,64,64	0
57	MG	DA	3165	1/1	0.14	-	57,57,57,57	0
57	MG	DA	3521	1/1	0.13	-	58,58,58,58	0
57	MG	B0	103	1/1	0.12	-	53,53,53,53	0
57	MG	BA	3190	1/1	0.15	-	52,52,52,52	0
57	MG	DA	3628	1/1	0.18	-	76,76,76,76	0
57	MG	AA	3008	1/1	0.15	-	73,73,73,73	0
57	MG	DA	3092	1/1	0.13	-	45,45,45,45	0
57	MG	DA	3414	1/1	0.13	-	43,43,43,43	0
57	MG	CA	3097	1/1	0.11	-	69,69,69,69	0
57	MG	BA	3664	1/1	0.13	-	55,55,55,55	0
57	MG	DA	3173	1/1	0.27	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	3057	1/1	0.17	-	76,76,76,76	0
57	MG	DA	3337	1/1	0.15	-	41,41,41,41	0
57	MG	DA	3283	1/1	0.09	-	51,51,51,51	0
57	MG	BA	3112	1/1	0.22	-	30,30,30,30	0
57	MG	BA	3261	1/1	0.12	-	61,61,61,61	0
57	MG	BA	3185	1/1	0.13	-	57,57,57,57	0
57	MG	BA	3666	1/1	0.18	-	50,50,50,50	0
57	MG	BA	3806	1/1	0.12	-	30,30,30,30	0
57	MG	DA	3235	1/1	0.12	-	45,45,45,45	0
57	MG	BA	3603	1/1	0.11	-	53,53,53,53	0
57	MG	BA	3509	1/1	0.20	-	31,31,31,31	0
57	MG	AA	3143	1/1	0.09	-	60,60,60,60	0
57	MG	DA	3190	1/1	0.22	-	54,54,54,54	0
57	MG	DA	3237	1/1	0.10	-	56,56,56,56	0
57	MG	BA	3482	1/1	0.12	-	51,51,51,51	0
57	MG	BA	3178	1/1	0.13	-	46,46,46,46	0
57	MG	DA	3053	1/1	0.08	-	47,47,47,47	0
57	MG	DA	3574	1/1	0.11	-	53,53,53,53	0
57	MG	B7	102	1/1	0.18	-	47,47,47,47	0
57	MG	DD	305	1/1	0.13	-	36,36,36,36	0
57	MG	CA	3168	1/1	0.09	-	56,56,56,56	0
57	MG	DA	3490	1/1	0.10	-	47,47,47,47	0
57	MG	BA	3793	1/1	0.21	-	40,40,40,40	0
57	MG	DA	3139	1/1	0.13	-	53,53,53,53	0
57	MG	DA	3524	1/1	0.12	-	61,61,61,61	0
57	MG	BA	3743	1/1	0.19	-	44,44,44,44	0
57	MG	DA	3071	1/1	0.15	-	59,59,59,59	0
57	MG	CA	3004	1/1	0.13	-	66,66,66,66	0
57	MG	DA	3604	1/1	0.26	-	59,59,59,59	0
57	MG	BA	3614	1/1	0.09	-	63,63,63,63	0
57	MG	CE	3001	1/1	0.09	-	79,79,79,79	0
57	MG	DA	3002	1/1	0.07	-	48,48,48,48	0
57	MG	DA	3606	1/1	0.13	-	71,71,71,71	0
57	MG	DA	3298	1/1	0.12	-	59,59,59,59	0
57	MG	BA	3273	1/1	0.17	-	54,54,54,54	0
57	MG	DA	3561	1/1	0.07	-	57,57,57,57	0
57	MG	BA	3174	1/1	0.20	-	37,37,37,37	0
57	MG	BA	3033	1/1	0.30	-	53,53,53,53	0
57	MG	DA	3557	1/1	0.17	-	51,51,51,51	0
57	MG	AA	3117	1/1	0.12	-	79,79,79,79	0
57	MG	DQ	3003	1/1	0.18	-	51,51,51,51	0
57	MG	AA	3192	1/1	0.11	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3032	1/1	0.12	-	48,48,48,48	0
57	MG	DF	3003	1/1	0.36	-	43,43,43,43	0
57	MG	DA	3396	1/1	0.10	-	40,40,40,40	0
57	MG	DA	3251	1/1	0.14	-	62,62,62,62	0
57	MG	BA	3570	1/1	0.14	-	42,42,42,42	0
57	MG	DA	3227	1/1	0.17	-	41,41,41,41	0
57	MG	BA	3436	1/1	0.15	-	40,40,40,40	0
57	MG	BA	3264	1/1	0.14	-	58,58,58,58	0
57	MG	DA	3528	1/1	0.11	-	62,62,62,62	0
57	MG	BA	3335	1/1	0.18	-	52,52,52,52	0
57	MG	DE	304	1/1	0.14	-	43,43,43,43	0
57	MG	DA	3508	1/1	0.33	-	44,44,44,44	0
57	MG	DA	3637	1/1	0.85	-	58,58,58,58	0
57	MG	CA	3102	1/1	0.12	-	68,68,68,68	0
57	MG	BA	3322	1/1	0.15	-	52,52,52,52	0
57	MG	B7	105	1/1	0.13	-	56,56,56,56	0
57	MG	CA	3062	1/1	0.15	-	64,64,64,64	0
57	MG	BA	3309	1/1	0.14	-	41,41,41,41	0
57	MG	BA	3224	1/1	0.22	-	65,65,65,65	0
57	MG	BA	3238	1/1	0.14	-	62,62,62,62	0
57	MG	BA	3014	1/1	0.64	-	42,42,42,42	0
57	MG	AA	3134	1/1	0.44	-	66,66,66,66	0
57	MG	BA	3760	1/1	0.17	-	44,44,44,44	0
57	MG	CA	3128	1/1	0.09	-	65,65,65,65	0
57	MG	DA	3076	1/1	0.11	-	58,58,58,58	0
57	MG	BA	3351	1/1	0.15	-	30,30,30,30	0
57	MG	BA	3392	1/1	0.16	-	53,53,53,53	0
57	MG	BA	3202	1/1	0.17	-	60,60,60,60	0
57	MG	CA	3110	1/1	0.09	-	65,65,65,65	0
57	MG	DA	3479	1/1	0.19	-	43,43,43,43	0
57	MG	BA	3305	1/1	0.09	-	62,62,62,62	0
57	MG	BA	3564	1/1	0.15	-	44,44,44,44	0
57	MG	CA	3041	1/1	0.15	-	59,59,59,59	0
57	MG	AA	3021	1/1	0.13	-	63,63,63,63	0
57	MG	BA	3515	1/1	0.27	-	53,53,53,53	0
57	MG	CA	3023	1/1	0.12	-	44,44,44,44	0
57	MG	BF	301	1/1	0.13	-	35,35,35,35	0
57	MG	BA	3291	1/1	0.18	-	33,33,33,33	0
57	MG	BA	3792	1/1	0.15	-	54,54,54,54	0
57	MG	DA	3562	1/1	0.10	-	64,64,64,64	0
57	MG	CA	3001	1/1	0.15	-	75,75,75,75	0
57	MG	DA	3652	1/1	0.57	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	3054	1/1	0.14	-	53,53,53,53	0
57	MG	BA	3373	1/1	0.16	-	48,48,48,48	0
57	MG	CA	3091	1/1	0.10	-	55,55,55,55	0
57	MG	BA	3451	1/1	0.19	-	31,31,31,31	0
57	MG	BA	3192	1/1	0.19	-	46,46,46,46	0
57	MG	BA	3460	1/1	0.13	-	62,62,62,62	0
57	MG	AA	3105	1/1	0.22	-	69,69,69,69	0
57	MG	DA	3246	1/1	0.14	-	43,43,43,43	0
57	MG	DA	3359	1/1	0.12	-	47,47,47,47	0
57	MG	DE	303	1/1	0.13	-	54,54,54,54	0
57	MG	AA	3061	1/1	0.30	-	55,55,55,55	0
57	MG	DA	3616	1/1	0.11	-	71,71,71,71	0
57	MG	DA	3196	1/1	0.19	-	49,49,49,49	0
57	MG	DA	3299	1/1	0.18	-	55,55,55,55	0
57	MG	DA	3214	1/1	0.18	-	59,59,59,59	0
57	MG	AA	3047	1/1	0.12	-	63,63,63,63	0
57	MG	AA	3012	1/1	0.17	-	46,46,46,46	0
57	MG	BA	3546	1/1	0.23	-	40,40,40,40	0
57	MG	BA	3804	1/1	0.50	-	53,53,53,53	0
57	MG	AA	3155	1/1	0.21	-	48,48,48,48	0
57	MG	CA	3115	1/1	0.12	-	63,63,63,63	0
57	MG	BA	3779	1/1	0.19	-	66,66,66,66	0
57	MG	AX	3007	1/1	0.18	-	67,67,67,67	0
57	MG	DA	3430	1/1	0.10	-	37,37,37,37	0
57	MG	BA	3367	1/1	0.16	-	29,29,29,29	0
57	MG	AA	3077	1/1	0.18	-	56,56,56,56	0
57	MG	BA	3073	1/1	0.15	-	61,61,61,61	0
57	MG	AA	3136	1/1	0.15	-	70,70,70,70	0
57	MG	DA	3073	1/1	0.10	-	42,42,42,42	0
57	MG	BA	3669	1/1	0.08	-	62,62,62,62	0
57	MG	AA	3079	1/1	0.12	-	68,68,68,68	0
57	MG	DA	3477	1/1	0.08	-	43,43,43,43	0
57	MG	DA	3334	1/1	0.12	-	52,52,52,52	0
57	MG	BA	3715	1/1	0.16	-	63,63,63,63	0
57	MG	BA	3342	1/1	0.10	-	46,46,46,46	0
57	MG	DA	3171	1/1	0.13	-	31,31,31,31	0
57	MG	DA	3132	1/1	0.21	-	52,52,52,52	0
57	MG	BA	3530	1/1	0.23	-	49,49,49,49	0
57	MG	BA	3477	1/1	0.15	-	61,61,61,61	0
57	MG	CA	3105	1/1	0.15	-	52,52,52,52	0
57	MG	BA	3565	1/1	0.18	-	40,40,40,40	0
57	MG	BA	3581	1/1	0.19	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	3108	1/1	0.25	-	67,67,67,67	0
57	MG	DA	3549	1/1	0.11	-	57,57,57,57	0
57	MG	DA	3125	1/1	0.20	-	70,70,70,70	0
57	MG	B1	101	1/1	0.59	-	51,51,51,51	0
57	MG	DA	3671	1/1	0.25	-	74,74,74,74	0
57	MG	BD	301	1/1	0.22	-	40,40,40,40	0
57	MG	BA	3623	1/1	0.28	-	55,55,55,55	0
57	MG	BA	3332	1/1	0.13	-	38,38,38,38	0
57	MG	DA	3100	1/1	0.13	-	43,43,43,43	0
57	MG	DA	3513	1/1	0.15	-	52,52,52,52	0
57	MG	DA	3124	1/1	0.08	-	57,57,57,57	0
57	MG	BA	3207	1/1	0.23	-	54,54,54,54	0
57	MG	BV	202	1/1	0.13	-	50,50,50,50	0
57	MG	BA	3201	1/1	0.10	-	62,62,62,62	0
57	MG	BA	3788	1/1	0.14	-	51,51,51,51	0
57	MG	BA	3093	1/1	0.16	-	56,56,56,56	0
57	MG	CA	3060	1/1	0.08	-	65,65,65,65	0
57	MG	DA	3405	1/1	0.15	-	46,46,46,46	0
57	MG	BA	3081	1/1	0.15	-	46,46,46,46	0
57	MG	BA	3296	1/1	0.12	-	53,53,53,53	0
57	MG	BA	3364	1/1	0.21	-	60,60,60,60	0
57	MG	BA	3747	1/1	0.14	-	52,52,52,52	0
57	MG	BA	3324	1/1	0.20	-	45,45,45,45	0
57	MG	DD	308	1/1	0.52	-	48,48,48,48	0
57	MG	AA	3131	1/1	0.06	-	71,71,71,71	0
57	MG	BA	3002	1/1	0.12	-	50,50,50,50	0
57	MG	DA	3475	1/1	0.28	-	51,51,51,51	0
57	MG	BA	3372	1/1	0.19	-	28,28,28,28	0
57	MG	CA	3136	1/1	0.15	-	72,72,72,72	0
57	MG	AA	3111	1/1	0.21	-	79,79,79,79	0
57	MG	BA	3443	1/1	0.25	-	37,37,37,37	0
57	MG	DA	3468	1/1	0.54	-	66,66,66,66	0
57	MG	BA	3721	1/1	0.27	-	82,82,82,82	0
57	MG	BA	3563	1/1	0.16	-	36,36,36,36	0
57	MG	DA	3456	1/1	0.05	-	50,50,50,50	0
57	MG	DB	3001	1/1	0.19	-	64,64,64,64	0
57	MG	DA	3131	1/1	0.19	-	46,46,46,46	0
57	MG	BA	3497	1/1	0.17	-	28,28,28,28	0
57	MG	CA	3010	1/1	0.11	-	56,56,56,56	0
57	MG	DA	3253	1/1	0.05	-	45,45,45,45	0
57	MG	DA	3256	1/1	0.16	-	62,62,62,62	0
57	MG	DA	3240	1/1	0.12	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3121	1/1	0.15	-	64,64,64,64	0
57	MG	AA	3073	1/1	0.12	-	56,56,56,56	0
57	MG	DA	3329	1/1	0.13	-	54,54,54,54	0
57	MG	DA	3005	1/1	0.07	-	57,57,57,57	0
57	MG	DA	3020	1/1	0.20	-	55,55,55,55	0
57	MG	DA	3231	1/1	0.13	-	62,62,62,62	0
57	MG	BA	3649	1/1	0.08	-	40,40,40,40	0
57	MG	AA	3022	1/1	0.11	-	71,71,71,71	0
57	MG	BA	3389	1/1	0.11	-	55,55,55,55	0
57	MG	BA	3395	1/1	0.14	-	38,38,38,38	0
57	MG	BA	3575	1/1	0.09	-	48,48,48,48	0
57	MG	AA	3173	1/1	0.14	-	54,54,54,54	0
57	MG	DD	303	1/1	0.52	-	87,87,87,87	0
57	MG	DA	3623	1/1	0.10	-	66,66,66,66	0
57	MG	DA	3394	1/1	0.10	-	65,65,65,65	0
57	MG	DA	3234	1/1	0.12	-	63,63,63,63	0
57	MG	AA	3055	1/1	0.21	-	57,57,57,57	0
57	MG	BA	3532	1/1	0.21	-	52,52,52,52	0
57	MG	BA	3588	1/1	0.22	-	31,31,31,31	0
57	MG	BA	3644	1/1	0.11	-	35,35,35,35	0
57	MG	DA	3309	1/1	0.12	-	51,51,51,51	0
57	MG	DA	3660	1/1	0.17	-	61,61,61,61	0
57	MG	AA	3009	1/1	0.11	-	57,57,57,57	0
57	MG	DA	3272	1/1	0.07	-	41,41,41,41	0
57	MG	AA	3046	1/1	0.17	-	55,55,55,55	0
57	MG	AX	3002	1/1	0.16	-	58,58,58,58	0
57	MG	DA	3016	1/1	0.42	-	50,50,50,50	0
57	MG	DB	3004	1/1	0.12	-	55,55,55,55	0
57	MG	BA	3783	1/1	0.12	-	56,56,56,56	0
57	MG	BA	3368	1/1	0.13	-	40,40,40,40	0
57	MG	DP	201	1/1	0.50	-	70,70,70,70	0
57	MG	DA	3142	1/1	0.26	-	47,47,47,47	0
57	MG	BA	3517	1/1	0.13	-	45,45,45,45	0
57	MG	AA	3133	1/1	0.11	-	56,56,56,56	0
57	MG	BA	3056	1/1	0.18	-	40,40,40,40	0
57	MG	BA	3381	1/1	0.12	-	46,46,46,46	0
57	MG	BA	3331	1/1	0.14	-	49,49,49,49	0
57	MG	AA	3185	1/1	0.13	-	82,82,82,82	0
57	MG	BN	3004	1/1	0.09	-	60,60,60,60	0
57	MG	DA	3343	1/1	0.18	-	50,50,50,50	0
57	MG	BA	3512	1/1	0.15	-	52,52,52,52	0
57	MG	BA	3790	1/1	0.15	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3502	1/1	0.12	-	56,56,56,56	0
57	MG	BA	3130	1/1	0.08	-	44,44,44,44	0
57	MG	BA	3079	1/1	0.17	-	39,39,39,39	0
57	MG	BA	3558	1/1	0.14	-	32,32,32,32	0
57	MG	BB	220	1/1	0.12	-	57,57,57,57	0
57	MG	BU	205	1/1	0.34	-	47,47,47,47	0
57	MG	BA	3230	1/1	0.14	-	53,53,53,53	0
57	MG	BA	3687	1/1	0.22	-	22,22,22,22	0
57	MG	BA	3001	1/1	0.13	-	53,53,53,53	0
57	MG	AX	3013	1/1	0.12	-	58,58,58,58	0
57	MG	DQ	3002	1/1	0.27	-	51,51,51,51	0
57	MG	BA	3386	1/1	0.24	-	53,53,53,53	0
57	MG	AA	3018	1/1	0.25	-	56,56,56,56	0
57	MG	AA	3006	1/1	0.14	-	52,52,52,52	0
57	MG	AA	3110	1/1	0.11	-	48,48,48,48	0
57	MG	BA	3632	1/1	0.08	-	50,50,50,50	0
57	MG	BA	3534	1/1	0.16	-	44,44,44,44	0
57	MG	BA	3307	1/1	0.16	-	29,29,29,29	0
57	MG	BA	3635	1/1	0.09	-	58,58,58,58	0
57	MG	BA	3206	1/1	0.15	-	49,49,49,49	0
57	MG	BA	3382	1/1	0.06	-	63,63,63,63	0
57	MG	BA	3493	1/1	0.12	-	58,58,58,58	0
57	MG	BA	3071	1/1	0.23	-	59,59,59,59	0
57	MG	DA	3119	1/1	0.18	-	39,39,39,39	0
57	MG	BE	307	1/1	0.35	-	62,62,62,62	0
57	MG	AA	3128	1/1	0.07	-	57,57,57,57	0
57	MG	BA	3199	1/1	0.12	-	46,46,46,46	0
57	MG	DA	3255	1/1	0.08	-	51,51,51,51	0
57	MG	CA	3039	1/1	0.09	-	68,68,68,68	0
57	MG	BA	3435	1/1	0.22	-	45,45,45,45	0
57	MG	DA	3103	1/1	0.10	-	58,58,58,58	0
57	MG	BA	3268	1/1	0.53	-	55,55,55,55	0
57	MG	DB	3010	1/1	0.14	-	57,57,57,57	0
57	MG	DA	3417	1/1	0.11	-	52,52,52,52	0
57	MG	DA	3268	1/1	0.21	-	51,51,51,51	0
57	MG	BA	3487	1/1	0.17	-	50,50,50,50	0
57	MG	BA	3741	1/1	0.60	-	64,64,64,64	0
57	MG	BA	3398	1/1	0.22	-	32,32,32,32	0
57	MG	CX	3003	1/1	0.20	-	54,54,54,54	0
57	MG	DA	3319	1/1	0.09	-	41,41,41,41	0
57	MG	AA	3045	1/1	0.09	-	58,58,58,58	0
57	MG	AA	3209	1/1	0.10	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3299	1/1	0.14	-	25,25,25,25	0
57	MG	BB	206	1/1	0.24	-	47,47,47,47	0
57	MG	BA	3752	1/1	0.18	-	32,32,32,32	0
57	MG	DA	3548	1/1	0.07	-	60,60,60,60	0
57	MG	DA	3386	1/1	0.12	-	35,35,35,35	0
57	MG	BA	3390	1/1	0.23	-	38,38,38,38	0
57	MG	DA	3091	1/1	0.09	-	48,48,48,48	0
57	MG	BA	3126	1/1	0.13	-	54,54,54,54	0
57	MG	BA	3099	1/1	0.19	-	41,41,41,41	0
57	MG	DA	3081	1/1	0.22	-	55,55,55,55	0
57	MG	BF	308	1/1	0.28	-	46,46,46,46	0
57	MG	DA	3021	1/1	0.07	-	31,31,31,31	0
57	MG	BA	3428	1/1	0.20	-	46,46,46,46	0
57	MG	AA	3129	1/1	0.12	-	47,47,47,47	0
57	MG	BA	3524	1/1	0.14	-	42,42,42,42	0
57	MG	AA	3165	1/1	0.21	-	54,54,54,54	0
57	MG	CA	3043	1/1	0.17	-	47,47,47,47	0
57	MG	BA	3592	1/1	0.21	-	28,28,28,28	0
57	MG	CA	3089	1/1	0.11	-	47,47,47,47	0
57	MG	BA	3567	1/1	0.14	-	34,34,34,34	0
57	MG	DA	3075	1/1	0.15	-	59,59,59,59	0
57	MG	DB	3008	1/1	0.17	-	67,67,67,67	0
57	MG	BA	3379	1/1	0.18	-	31,31,31,31	0
57	MG	BA	3227	1/1	0.21	-	57,57,57,57	0
57	MG	B6	101	1/1	0.28	-	48,48,48,48	0
57	MG	DA	3138	1/1	0.09	-	55,55,55,55	0
57	MG	DA	3565	1/1	0.07	-	59,59,59,59	0
57	MG	AA	3127	1/1	0.16	-	65,65,65,65	0
57	MG	BA	3697	1/1	0.11	-	61,61,61,61	0
57	MG	BA	3615	1/1	0.16	-	68,68,68,68	0
57	MG	BA	3494	1/1	0.09	-	49,49,49,49	0
57	MG	CA	3123	1/1	0.14	-	58,58,58,58	0
57	MG	AA	3078	1/1	0.26	-	66,66,66,66	0
57	MG	BA	3294	1/1	0.30	-	61,61,61,61	0
57	MG	AA	3140	1/1	0.14	-	53,53,53,53	0
57	MG	DA	3580	1/1	0.15	-	36,36,36,36	0
57	MG	DA	3316	1/1	0.13	-	45,45,45,45	0
57	MG	BA	3029	1/1	0.61	-	37,37,37,37	0
57	MG	BA	3252	1/1	0.32	-	60,60,60,60	0
57	MG	DA	3627	1/1	0.15	-	63,63,63,63	0
57	MG	BA	3145	1/1	0.08	-	44,44,44,44	0
57	MG	AN	503	1/1	0.15	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	3190	1/1	0.09	-	58,58,58,58	0
57	MG	AA	3160	1/1	0.17	-	59,59,59,59	0
57	MG	DQ	3001	1/1	0.14	-	47,47,47,47	0
57	MG	BA	3748	1/1	0.11	-	29,29,29,29	0
57	MG	AA	3090	1/1	0.24	-	66,66,66,66	0
57	MG	BA	3204	1/1	0.18	-	36,36,36,36	0
57	MG	BA	3263	1/1	0.47	-	49,49,49,49	0
57	MG	BA	3676	1/1	0.22	-	33,33,33,33	0
57	MG	BA	3467	1/1	0.23	-	50,50,50,50	0
57	MG	DA	3415	1/1	0.12	-	68,68,68,68	0
57	MG	BA	3772	1/1	0.14	-	33,33,33,33	0
57	MG	BW	203	1/1	0.15	-	44,44,44,44	0
57	MG	AA	3199	1/1	0.19	-	73,73,73,73	0
57	MG	BA	3787	1/1	0.29	-	45,45,45,45	0
57	MG	AA	3211	1/1	0.12	-	47,47,47,47	0
57	MG	AA	3098	1/1	0.23	-	55,55,55,55	0
57	MG	CA	3121	1/1	0.07	-	63,63,63,63	0
57	MG	BA	3397	1/1	0.16	-	30,30,30,30	0
57	MG	BA	3531	1/1	0.21	-	26,26,26,26	0
57	MG	BA	3344	1/1	0.19	-	66,66,66,66	0
57	MG	D8	5001	1/1	0.21	-	66,66,66,66	0
57	MG	DA	3059	1/1	0.28	-	43,43,43,43	0
57	MG	BA	3439	1/1	0.10	-	33,33,33,33	0
57	MG	BA	3128	1/1	0.22	-	69,69,69,69	0
57	MG	DA	3596	1/1	0.09	-	56,56,56,56	0
57	MG	AA	3003	1/1	0.14	-	72,72,72,72	0
57	MG	DA	3416	1/1	0.12	-	50,50,50,50	0
57	MG	BB	210	1/1	0.10	-	61,61,61,61	0
57	MG	AA	3030	1/1	0.14	-	60,60,60,60	0
57	MG	DA	3607	1/1	0.14	-	65,65,65,65	0
57	MG	DA	3640	1/1	0.25	-	43,43,43,43	0
57	MG	BA	3116	1/1	0.30	-	50,50,50,50	0
57	MG	DA	3345	1/1	0.08	-	44,44,44,44	0
57	MG	DA	3355	1/1	0.09	-	58,58,58,58	0
57	MG	CA	3076	1/1	0.13	-	57,57,57,57	0
57	MG	DA	3638	1/1	0.10	-	51,51,51,51	0
57	MG	BE	308	1/1	0.14	-	40,40,40,40	0
57	MG	BA	3218	1/1	0.16	-	47,47,47,47	0
57	MG	BA	3766	1/1	0.12	-	28,28,28,28	0
57	MG	DX	101	1/1	0.11	-	51,51,51,51	0
57	MG	DA	3341	1/1	0.14	-	51,51,51,51	0
57	MG	DA	3307	1/1	0.10	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3137	1/1	0.23	-	39,39,39,39	0
57	MG	DA	3344	1/1	0.13	-	31,31,31,31	0
57	MG	CA	3134	1/1	0.12	-	69,69,69,69	0
57	MG	AA	3070	1/1	0.13	-	52,52,52,52	0
57	MG	DA	3610	1/1	0.34	-	64,64,64,64	0
57	MG	CA	3119	1/1	0.09	-	64,64,64,64	0
57	MG	DA	3204	1/1	0.19	-	46,46,46,46	0
57	MG	DA	3390	1/1	0.12	-	43,43,43,43	0
57	MG	BA	3255	1/1	0.21	-	47,47,47,47	0
57	MG	AA	3139	1/1	0.15	-	59,59,59,59	0
57	MG	BA	3362	1/1	0.19	-	41,41,41,41	0
57	MG	BA	3404	1/1	0.18	-	59,59,59,59	0
57	MG	BA	3008	1/1	0.12	-	47,47,47,47	0
57	MG	AA	3183	1/1	0.14	-	65,65,65,65	0
57	MG	DA	3120	1/1	0.07	-	49,49,49,49	0
57	MG	BA	3047	1/1	0.09	-	60,60,60,60	0
57	MG	BB	212	1/1	0.11	-	55,55,55,55	0
57	MG	CA	3052	1/1	0.17	-	72,72,72,72	0
57	MG	BA	3046	1/1	0.23	-	41,41,41,41	0
57	MG	BA	3396	1/1	0.12	-	50,50,50,50	0
57	MG	BB	203	1/1	0.25	-	43,43,43,43	0
57	MG	DA	3086	1/1	0.16	-	43,43,43,43	0
57	MG	BA	3711	1/1	0.15	-	54,54,54,54	0
57	MG	CA	3103	1/1	0.12	-	46,46,46,46	0
57	MG	BE	306	1/1	0.16	-	26,26,26,26	0
57	MG	DA	3084	1/1	0.08	-	39,39,39,39	0
57	MG	BA	3619	1/1	0.25	-	58,58,58,58	0
57	MG	AA	3097	1/1	0.34	-	56,56,56,56	0
57	MG	CA	3152	1/1	0.18	-	76,76,76,76	0
57	MG	CA	3034	1/1	0.12	-	59,59,59,59	0
57	MG	DA	3195	1/1	0.08	-	43,43,43,43	0
57	MG	BA	3574	1/1	0.18	-	66,66,66,66	0
57	MG	AA	3206	1/1	0.17	-	64,64,64,64	0
57	MG	BA	3657	1/1	0.27	-	47,47,47,47	0
57	MG	BA	3119	1/1	0.13	-	45,45,45,45	0
57	MG	BA	3276	1/1	0.31	-	54,54,54,54	0
57	MG	BA	3241	1/1	0.11	-	36,36,36,36	0
57	MG	BA	3388	1/1	0.16	-	48,48,48,48	0
57	MG	CA	3145	1/1	0.12	-	66,66,66,66	0
57	MG	CA	3083	1/1	0.11	-	79,79,79,79	0
57	MG	BA	3188	1/1	0.25	-	49,49,49,49	0
57	MG	BA	3520	1/1	0.18	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3460	1/1	0.10	-	41,41,41,41	0
57	MG	BA	3345	1/1	0.11	-	38,38,38,38	0
57	MG	BA	3069	1/1	0.20	-	22,22,22,22	0
57	MG	BA	3475	1/1	0.15	-	42,42,42,42	0
57	MG	DA	3287	1/1	0.07	-	41,41,41,41	0
57	MG	BA	3504	1/1	0.12	-	56,56,56,56	0
57	MG	BA	3144	1/1	0.14	-	41,41,41,41	0
57	MG	DA	3013	1/1	0.07	-	40,40,40,40	0
57	MG	D0	101	1/1	0.11	-	71,71,71,71	0
57	MG	DA	3074	1/1	0.10	-	37,37,37,37	0
57	MG	BA	3755	1/1	0.13	-	55,55,55,55	0
57	MG	BA	3284	1/1	0.34	-	43,43,43,43	0
57	MG	DA	3622	1/1	0.13	-	61,61,61,61	0
57	MG	DD	301	1/1	0.14	-	47,47,47,47	0
57	MG	BA	3499	1/1	0.11	-	58,58,58,58	0
57	MG	BA	3655	1/1	0.09	-	50,50,50,50	0
57	MG	BA	3707	1/1	0.28	-	44,44,44,44	0
57	MG	DA	3236	1/1	0.19	-	47,47,47,47	0
57	MG	DA	3533	1/1	0.10	-	43,43,43,43	0
57	MG	AA	3011	1/1	0.28	-	57,57,57,57	0
57	MG	AA	3138	1/1	0.18	-	71,71,71,71	0
57	MG	DA	3576	1/1	0.09	-	53,53,53,53	0
57	MG	CA	3071	1/1	0.13	-	68,68,68,68	0
57	MG	DA	3296	1/1	0.11	-	28,28,28,28	0
57	MG	CA	3012	1/1	0.15	-	60,60,60,60	0
57	MG	DA	3167	1/1	0.11	-	41,41,41,41	0
57	MG	BA	3805	1/1	0.12	-	44,44,44,44	0
57	MG	DA	3545	1/1	0.11	-	35,35,35,35	0
57	MG	DA	3290	1/1	0.16	-	59,59,59,59	0
57	MG	AY	3002	1/1	0.18	-	56,56,56,56	0
57	MG	AA	3141	1/1	0.24	-	61,61,61,61	0
57	MG	BV	205	1/1	0.12	-	38,38,38,38	0
57	MG	BA	3155	1/1	0.62	-	44,44,44,44	0
57	MG	BA	3259	1/1	0.22	-	25,25,25,25	0
57	MG	BA	3449	1/1	0.17	-	35,35,35,35	0
57	MG	BA	3292	1/1	0.11	-	48,48,48,48	0
57	MG	AA	3203	1/1	0.11	-	59,59,59,59	0
57	MG	BA	3086	1/1	0.15	-	22,22,22,22	0
57	MG	BA	3638	1/1	0.13	-	63,63,63,63	0
57	MG	CA	3059	1/1	0.17	-	72,72,72,72	0
57	MG	BA	3004	1/1	0.17	-	33,33,33,33	0
57	MG	DA	3331	1/1	0.16	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3543	1/1	0.23	-	37,37,37,37	0
57	MG	BA	3438	1/1	0.15	-	60,60,60,60	0
57	MG	AA	3113	1/1	0.12	-	58,58,58,58	0
57	MG	AA	3026	1/1	0.13	-	70,70,70,70	0
57	MG	DA	3242	1/1	0.13	-	52,52,52,52	0
57	MG	DA	3085	1/1	0.10	-	53,53,53,53	0
57	MG	DO	5001	1/1	0.12	-	59,59,59,59	0
57	MG	BA	3135	1/1	0.17	-	43,43,43,43	0
57	MG	DA	3101	1/1	0.13	-	49,49,49,49	0
57	MG	DA	3373	1/1	0.10	-	44,44,44,44	0
57	MG	DA	3659	1/1	0.11	-	48,48,48,48	0
57	MG	DV	3003	1/1	0.09	-	65,65,65,65	0
57	MG	BA	3100	1/1	0.14	-	39,39,39,39	0
57	MG	BA	3586	1/1	0.06	-	53,53,53,53	0
57	MG	BA	3800	1/1	0.18	-	38,38,38,38	0
57	MG	DA	3457	1/1	0.09	-	54,54,54,54	0
57	MG	CA	3013	1/1	0.12	-	69,69,69,69	0
57	MG	DA	3600	1/1	0.39	-	70,70,70,70	0
57	MG	DA	3400	1/1	0.12	-	54,54,54,54	0
57	MG	AW	3003	1/1	0.14	-	72,72,72,72	0
57	MG	BA	3541	1/1	0.18	-	38,38,38,38	0
57	MG	DA	3516	1/1	0.10	-	67,67,67,67	0
57	MG	BA	3105	1/1	0.11	-	37,37,37,37	0
57	MG	DA	3182	1/1	0.25	-	51,51,51,51	0
57	MG	DA	3154	1/1	0.12	-	48,48,48,48	0
57	MG	AA	3036	1/1	0.14	-	61,61,61,61	0
57	MG	CA	3066	1/1	0.08	-	66,66,66,66	0
57	MG	CA	3126	1/1	0.10	-	67,67,67,67	0
57	MG	BX	3002	1/1	0.30	-	46,46,46,46	0
57	MG	DA	3118	1/1	0.40	-	77,77,77,77	0
57	MG	BA	3027	1/1	0.09	-	26,26,26,26	0
57	MG	BA	3548	1/1	0.17	-	40,40,40,40	0
57	MG	BA	3306	1/1	0.14	-	37,37,37,37	0
57	MG	BA	3552	1/1	0.22	-	29,29,29,29	0
57	MG	BA	3271	1/1	0.14	-	58,58,58,58	0
57	MG	AA	3208	1/1	0.13	-	60,60,60,60	0
57	MG	DA	3106	1/1	0.13	-	52,52,52,52	0
57	MG	BA	3325	1/1	0.12	-	48,48,48,48	0
57	MG	AA	3025	1/1	0.09	-	62,62,62,62	0
57	MG	DA	3504	1/1	0.21	-	47,47,47,47	0
57	MG	BA	3700	1/1	0.14	-	61,61,61,61	0
57	MG	DA	3274	1/1	0.17	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	3069	1/1	0.45	-	68,68,68,68	0
57	MG	DA	3578	1/1	0.18	-	59,59,59,59	0
57	MG	BF	306	1/1	0.22	-	31,31,31,31	0
57	MG	DA	3149	1/1	0.07	-	56,56,56,56	0
57	MG	DA	3230	1/1	0.54	-	73,73,73,73	0
57	MG	DA	3656	1/1	0.11	-	58,58,58,58	0
57	MG	BA	3709	1/1	0.20	-	62,62,62,62	0
57	MG	AA	3109	1/1	0.08	-	62,62,62,62	0
57	MG	BA	3717	1/1	0.13	-	50,50,50,50	0
57	MG	BA	3365	1/1	0.13	-	62,62,62,62	0
57	MG	BA	3005	1/1	0.13	-	30,30,30,30	0
57	MG	BA	3010	1/1	0.14	-	39,39,39,39	0
57	MG	BA	3311	1/1	0.20	-	48,48,48,48	0
57	MG	BG	201	1/1	0.16	-	58,58,58,58	0
57	MG	DA	3411	1/1	0.18	-	53,53,53,53	0
57	MG	BA	3215	1/1	0.28	-	36,36,36,36	0
57	MG	BA	3566	1/1	0.20	-	67,67,67,67	0
57	MG	DA	3056	1/1	0.08	-	51,51,51,51	0
57	MG	DA	3003	1/1	0.13	-	27,27,27,27	0
57	MG	CA	3120	1/1	0.18	-	64,64,64,64	0
57	MG	BA	3653	1/1	0.13	-	39,39,39,39	0
57	MG	DA	3170	1/1	0.14	-	53,53,53,53	0
57	MG	BA	3533	1/1	0.12	-	59,59,59,59	0
57	MG	DA	3530	1/1	0.11	-	74,74,74,74	0
57	MG	CA	3138	1/1	0.20	-	80,80,80,80	0
57	MG	AA	3016	1/1	0.07	-	63,63,63,63	0
57	MG	BA	3006	1/1	0.35	-	48,48,48,48	0
57	MG	DA	3661	1/1	0.10	-	62,62,62,62	0
57	MG	BA	3481	1/1	0.18	-	41,41,41,41	0
57	MG	BA	3444	1/1	0.19	-	29,29,29,29	0
57	MG	DA	3366	1/1	0.14	-	42,42,42,42	0
57	MG	BA	3458	1/1	0.15	-	18,18,18,18	0
57	MG	AA	3014	1/1	0.16	-	32,32,32,32	0
57	MG	DA	3019	1/1	0.30	-	37,37,37,37	0
57	MG	BA	3726	1/1	0.14	-	63,63,63,63	0
57	MG	BA	3429	1/1	0.09	-	65,65,65,65	0
57	MG	BV	204	1/1	0.15	-	49,49,49,49	0
57	MG	BA	3724	1/1	0.19	-	62,62,62,62	0
57	MG	BA	3357	1/1	0.21	-	25,25,25,25	0
57	MG	DA	3542	1/1	0.14	-	24,24,24,24	0
57	MG	DA	3499	1/1	0.12	-	53,53,53,53	0
57	MG	DA	3136	1/1	0.09	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3347	1/1	0.18	-	44,44,44,44	0
57	MG	DA	3502	1/1	0.09	-	55,55,55,55	0
57	MG	DA	3615	1/1	0.13	-	65,65,65,65	0
57	MG	DA	3077	1/1	0.19	-	61,61,61,61	0
57	MG	CA	3118	1/1	0.10	-	68,68,68,68	0
57	MG	DA	3350	1/1	0.11	-	51,51,51,51	0
57	MG	BA	3540	1/1	0.22	-	37,37,37,37	0
57	MG	DA	3241	1/1	0.11	-	45,45,45,45	0
57	MG	AA	3122	1/1	0.10	-	56,56,56,56	0
57	MG	BA	3498	1/1	0.17	-	36,36,36,36	0
57	MG	DA	3541	1/1	0.11	-	44,44,44,44	0
57	MG	DA	3014	1/1	0.16	-	46,46,46,46	0
57	MG	DA	3004	1/1	0.19	-	40,40,40,40	0
57	MG	DA	3587	1/1	0.09	-	56,56,56,56	0
57	MG	BA	3258	1/1	0.14	-	44,44,44,44	0
57	MG	DA	3176	1/1	0.16	-	41,41,41,41	0
57	MG	DA	3426	1/1	0.24	-	49,49,49,49	0
57	MG	DD	302	1/1	0.20	-	42,42,42,42	0
57	MG	BA	3577	1/1	0.15	-	51,51,51,51	0
57	MG	BA	3425	1/1	0.13	-	40,40,40,40	0
57	MG	DA	3601	1/1	0.08	-	44,44,44,44	0
57	MG	DA	3588	1/1	0.32	-	65,65,65,65	0
57	MG	DA	3474	1/1	0.09	-	51,51,51,51	0
57	MG	DA	3305	1/1	0.19	-	50,50,50,50	0
57	MG	AA	3210	1/1	0.25	-	59,59,59,59	0
57	MG	BA	3197	1/1	0.43	-	41,41,41,41	0
57	MG	BA	3483	1/1	0.12	-	28,28,28,28	0
57	MG	BA	3260	1/1	0.24	-	39,39,39,39	0
57	MG	AA	3041	1/1	0.17	-	46,46,46,46	0
57	MG	BA	3072	1/1	0.27	-	47,47,47,47	0
57	MG	DE	301	1/1	0.36	-	46,46,46,46	0
57	MG	DA	3669	1/1	0.22	-	55,55,55,55	0
57	MG	DA	3040	1/1	0.08	-	31,31,31,31	0
57	MG	AA	3020	1/1	0.13	-	76,76,76,76	0
57	MG	BA	3361	1/1	0.09	-	49,49,49,49	0
57	MG	AA	3102	1/1	0.21	-	59,59,59,59	0
57	MG	BA	3646	1/1	0.13	-	42,42,42,42	0
57	MG	DA	3478	1/1	0.23	-	59,59,59,59	0
57	MG	AA	3184	1/1	0.12	-	60,60,60,60	0
57	MG	DA	3523	1/1	0.08	-	59,59,59,59	0
57	MG	BA	3203	1/1	0.42	-	40,40,40,40	0
57	MG	DA	3449	1/1	0.08	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3203	1/1	0.40	-	50,50,50,50	0
57	MG	DA	3374	1/1	0.14	-	56,56,56,56	0
57	MG	BA	3166	1/1	0.11	-	38,38,38,38	0
57	MG	CA	3104	1/1	0.10	-	68,68,68,68	0
57	MG	DB	3005	1/1	0.06	-	59,59,59,59	0
57	MG	BA	3471	1/1	0.21	-	53,53,53,53	0
57	MG	AA	3015	1/1	0.12	-	65,65,65,65	0
57	MG	BA	3242	1/1	0.18	-	55,55,55,55	0
57	MG	BA	3158	1/1	0.18	-	41,41,41,41	0
57	MG	AA	3146	1/1	0.12	-	66,66,66,66	0
57	MG	BA	3685	1/1	0.16	-	53,53,53,53	0
57	MG	AA	3085	1/1	0.13	-	48,48,48,48	0
57	MG	DA	3667	1/1	0.14	-	50,50,50,50	0
57	MG	DA	3547	1/1	0.11	-	54,54,54,54	0
57	MG	BA	3778	1/1	0.09	-	48,48,48,48	0
57	MG	BA	3665	1/1	0.11	-	49,49,49,49	0
57	MG	AA	3091	1/1	0.18	-	60,60,60,60	0
57	MG	BA	3393	1/1	0.15	-	51,51,51,51	0
57	MG	BA	3280	1/1	0.10	-	37,37,37,37	0
57	MG	DA	3295	1/1	0.18	-	44,44,44,44	0
57	MG	BA	3151	1/1	0.25	-	52,52,52,52	0
57	MG	DA	3127	1/1	0.12	-	35,35,35,35	0
57	MG	DA	3594	1/1	0.31	-	54,54,54,54	0
57	MG	BA	3391	1/1	0.24	-	63,63,63,63	0
57	MG	CA	3167	1/1	0.10	-	60,60,60,60	0
57	MG	BA	3521	1/1	0.22	-	39,39,39,39	0
57	MG	BA	3431	1/1	0.15	-	59,59,59,59	0
57	MG	DA	3302	1/1	0.14	-	70,70,70,70	0
57	MG	BA	3063	1/1	0.09	-	59,59,59,59	0
57	MG	DA	3409	1/1	0.18	-	57,57,57,57	0
57	MG	DA	3664	1/1	0.36	-	48,48,48,48	0
57	MG	BA	3675	1/1	0.20	-	67,67,67,67	0
57	MG	DA	3011	1/1	0.08	-	48,48,48,48	0
57	MG	DA	3111	1/1	0.10	-	61,61,61,61	0
57	MG	DA	3491	1/1	0.12	-	51,51,51,51	0
57	MG	BA	3378	1/1	0.07	-	28,28,28,28	0
57	MG	BA	3698	1/1	0.23	-	31,31,31,31	0
57	MG	DA	3505	1/1	0.13	-	56,56,56,56	0
57	MG	BA	3338	1/1	0.11	-	40,40,40,40	0
57	MG	CA	3078	1/1	0.13	-	44,44,44,44	0
57	MG	CA	3042	1/1	0.07	-	59,59,59,59	0
57	MG	BA	3146	1/1	0.18	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3330	1/1	0.17	-	45,45,45,45	0
57	MG	BA	3210	1/1	0.20	-	49,49,49,49	0
57	MG	DA	3480	1/1	0.06	-	40,40,40,40	0
57	MG	DA	3579	1/1	0.09	-	48,48,48,48	0
57	MG	BF	303	1/1	0.51	-	49,49,49,49	0
57	MG	AA	3001	1/1	0.19	-	61,61,61,61	0
57	MG	BA	3650	1/1	0.14	-	52,52,52,52	0
57	MG	BA	3239	1/1	0.23	-	48,48,48,48	0
57	MG	BA	3182	1/1	0.16	-	55,55,55,55	0
57	MG	AA	3154	1/1	0.10	-	69,69,69,69	0
57	MG	BE	305	1/1	0.20	-	43,43,43,43	0
57	MG	DA	3509	1/1	0.12	-	59,59,59,59	0
57	MG	BA	3127	1/1	0.17	-	57,57,57,57	0
57	MG	DA	3375	1/1	0.15	-	39,39,39,39	0
57	MG	DA	3276	1/1	0.11	-	49,49,49,49	0
57	MG	CA	3055	1/1	0.08	-	69,69,69,69	0
57	MG	BA	3608	1/1	0.27	-	62,62,62,62	0
57	MG	BA	3058	1/1	0.09	-	49,49,49,49	0
57	MG	DA	3619	1/1	0.18	-	69,69,69,69	0
57	MG	AA	3187	1/1	0.21	-	62,62,62,62	0
57	MG	DA	3198	1/1	0.10	-	40,40,40,40	0
57	MG	AA	3186	1/1	0.07	-	42,42,42,42	0
57	MG	AA	3028	1/1	0.22	-	76,76,76,76	0
57	MG	BA	3048	1/1	0.08	-	47,47,47,47	0
57	MG	BA	3283	1/1	0.12	-	35,35,35,35	0
57	MG	BA	3789	1/1	0.14	-	12,12,12,12	0
57	MG	AX	3010	1/1	0.12	-	59,59,59,59	0
57	MG	AA	3063	1/1	0.07	-	35,35,35,35	0
57	MG	DA	3088	1/1	0.13	-	47,47,47,47	0
57	MG	DA	3376	1/1	0.23	-	61,61,61,61	0
57	MG	BA	3237	1/1	0.13	-	45,45,45,45	0
57	MG	CA	3109	1/1	0.17	-	67,67,67,67	0
57	MG	BA	3070	1/1	0.31	-	59,59,59,59	0
57	MG	BA	3138	1/1	0.37	-	42,42,42,42	0
57	MG	BA	3684	1/1	0.30	-	68,68,68,68	0
57	MG	B9	502	1/1	0.14	-	48,48,48,48	0
57	MG	CA	3131	1/1	0.06	-	55,55,55,55	0
57	MG	BA	3641	1/1	0.20	-	68,68,68,68	0
57	MG	BW	202	1/1	0.07	-	54,54,54,54	0
57	MG	BN	3005	1/1	0.14	-	36,36,36,36	0
57	MG	DA	3188	1/1	0.12	-	48,48,48,48	0
57	MG	DA	3216	1/1	0.14	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3441	1/1	0.11	-	45,45,45,45	0
57	MG	BA	3733	1/1	0.10	-	58,58,58,58	0
57	MG	CA	3069	1/1	0.21	-	60,60,60,60	0
57	MG	CA	3040	1/1	0.10	-	51,51,51,51	0
57	MG	BA	3132	1/1	0.20	-	40,40,40,40	0
57	MG	DA	3352	1/1	0.17	-	63,63,63,63	0
57	MG	BA	3662	1/1	0.10	-	61,61,61,61	0
57	MG	AA	3048	1/1	0.13	-	57,57,57,57	0
57	MG	BA	3076	1/1	0.19	-	43,43,43,43	0
57	MG	DA	3445	1/1	0.08	-	32,32,32,32	0
57	MG	BA	3387	1/1	0.15	-	54,54,54,54	0
57	MG	DA	3633	1/1	0.25	-	58,58,58,58	0
57	MG	CA	3021	1/1	0.12	-	61,61,61,61	0
57	MG	BA	3730	1/1	0.20	-	71,71,71,71	0
57	MG	BA	3445	1/1	0.14	-	63,63,63,63	0
57	MG	BP	201	1/1	0.27	-	41,41,41,41	0
57	MG	BA	3457	1/1	0.21	-	32,32,32,32	0
57	MG	DA	3025	1/1	0.13	-	54,54,54,54	0
57	MG	BB	217	1/1	0.16	-	29,29,29,29	0
57	MG	DA	3427	1/1	0.12	-	45,45,45,45	0
57	MG	AA	3017	1/1	0.26	-	71,71,71,71	0
57	MG	BF	309	1/1	0.19	-	53,53,53,53	0
57	MG	BA	3660	1/1	0.09	-	61,61,61,61	0
57	MG	DA	3294	1/1	0.11	-	43,43,43,43	0
57	MG	CA	3162	1/1	0.06	-	66,66,66,66	0
57	MG	DA	3634	1/1	0.22	-	60,60,60,60	0
57	MG	DA	3538	1/1	0.09	-	58,58,58,58	0
57	MG	CA	3082	1/1	0.18	-	79,79,79,79	0
57	MG	DA	3200	1/1	0.14	-	66,66,66,66	0
57	MG	BA	3802	1/1	0.76	-	54,54,54,54	0
57	MG	BA	3758	1/1	0.10	-	45,45,45,45	0
57	MG	BA	3262	1/1	0.13	-	41,41,41,41	0
57	MG	BA	3751	1/1	0.15	-	26,26,26,26	0
57	MG	BA	3485	1/1	0.07	-	42,42,42,42	0
57	MG	BE	301	1/1	0.14	-	35,35,35,35	0
57	MG	BA	3049	1/1	0.25	-	36,36,36,36	0
57	MG	BA	3559	1/1	0.08	-	47,47,47,47	0
57	MG	DA	3554	1/1	0.09	-	62,62,62,62	0
57	MG	DA	3497	1/1	0.21	-	55,55,55,55	0
57	MG	BA	3160	1/1	0.28	-	55,55,55,55	0
57	MG	AA	3144	1/1	0.15	-	46,46,46,46	0
57	MG	DY	502	1/1	0.11	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3133	1/1	0.14	-	50,50,50,50	0
57	MG	BA	3129	1/1	0.22	-	58,58,58,58	0
57	MG	CA	3007	1/1	0.08	-	57,57,57,57	0
57	MG	CA	3047	1/1	0.16	-	53,53,53,53	0
57	MG	AA	3172	1/1	0.12	-	72,72,72,72	0
57	MG	AA	3153	1/1	0.15	-	74,74,74,74	0
57	MG	BV	201	1/1	0.37	-	33,33,33,33	0
57	MG	B8	101	1/1	0.17	-	44,44,44,44	0
57	MG	BA	3597	1/1	0.16	-	25,25,25,25	0
57	MG	DA	3455	1/1	0.11	-	47,47,47,47	0
57	MG	DA	3589	1/1	0.08	-	68,68,68,68	0
57	MG	CA	3005	1/1	0.10	-	62,62,62,62	0
57	MG	BA	3803	1/1	0.22	-	44,44,44,44	0
57	MG	DA	3037	1/1	0.15	-	43,43,43,43	0
57	MG	BA	3647	1/1	0.06	-	56,56,56,56	0
57	MG	BA	3455	1/1	0.11	-	64,64,64,64	0
57	MG	B7	101	1/1	0.25	-	39,39,39,39	0
57	MG	BA	3607	1/1	0.19	-	38,38,38,38	0
57	MG	DA	3569	1/1	0.21	-	49,49,49,49	0

6.5 Other polymers ⓘ

There are no such residues in this entry.