



wwPDB X-ray Structure Validation Summary Report

Sep 11, 2014 – 04:49 AM EDT

PDB ID : 1VY7
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in the pre-attack state of peptide bond formation containing short substrate-mimic Cytidine-Cytidine-Puromycin in the A site and acylated tRNA in the P site.
Authors : Polikanov, Y.S.; Steitz, T.A.; Innis, C.A.
Deposited on : 2014-05-13
Resolution : 2.80 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>

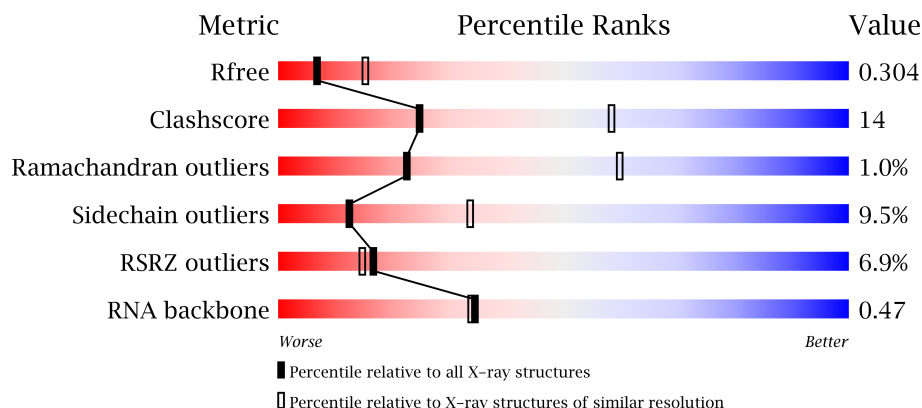
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.80 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	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)
RNA backbone	1838	1076 (3.30-2.30)

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	3	
23	CW	3	
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 290205 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			
			714	445	138	131	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
22	CV	6	Total	C	N	O	P	0	0	0
			129	58	24	41	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			
23	CW	3	Total	C	N	O	P	0	0	0
			74	40	13	19	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
			1633	730	296	529	76	2			
24	CX	76	Total	C	N	O	P	S	0	0	0
			1635	731	296	530	76	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AY	5	Total	C	N	O	P	0	0	0
			104	47	19	33	5			
25	CY	5	Total	C	N	O	P	0	0	0
			104	47	19	33	5			

- 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
			552	349	99	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	BA	720	Total	Mg	0	0
			720	720		
57	AK	1	Total	Mg	0	0
			1	1		
57	DQ	3	Total	Mg	0	0
			3	3		
57	D3	1	Total	Mg	0	0
			1	1		
57	DF	4	Total	Mg	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	B8	1	Total 1	Mg 1	0	0
57	BE	7	Total 7	Mg 7	0	0
57	AW	1	Total 1	Mg 1	0	0
57	DU	4	Total 4	Mg 4	0	0
57	B1	1	Total 1	Mg 1	0	0
57	AN	2	Total 2	Mg 2	0	0
57	BP	4	Total 4	Mg 4	0	0
57	AX	11	Total 11	Mg 11	0	0
57	DN	1	Total 1	Mg 1	0	0
57	AS	1	Total 1	Mg 1	0	0
57	CA	160	Total 160	Mg 160	0	0
57	B5	2	Total 2	Mg 2	0	0
57	BB	20	Total 20	Mg 20	0	0
57	AJ	1	Total 1	Mg 1	0	0
57	D8	2	Total 2	Mg 2	0	0
57	AE	2	Total 2	Mg 2	0	0
57	DG	1	Total 1	Mg 1	0	0
57	B9	1	Total 1	Mg 1	0	0
57	BF	10	Total 10	Mg 10	0	0
57	AV	1	Total 1	Mg 1	0	0
57	BX	1	Total 1	Mg 1	0	0

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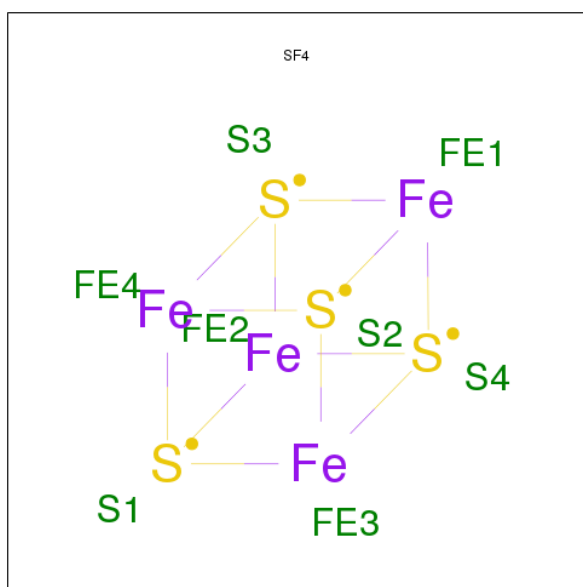
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	B2	1	Total 1	Mg 1	0	0
57	AA	207	Total 207	Mg 207	0	0
57	BQ	5	Total 5	Mg 5	0	0
57	CX	2	Total 2	Mg 2	0	0
57	DV	2	Total 2	Mg 2	0	0
57	AM	1	Total 1	Mg 1	0	0
57	BU	8	Total 8	Mg 8	0	0
57	DR	2	Total 2	Mg 2	0	0
57	AD	2	Total 2	Mg 2	0	0
57	BN	6	Total 6	Mg 6	0	0
57	CT	1	Total 1	Mg 1	0	0
57	BG	2	Total 2	Mg 2	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	3	Total 3	Mg 3	0	0
57	DA	629	Total 629	Mg 629	0	0
57	DP	2	Total 2	Mg 2	0	0
57	DW	2	Total 2	Mg 2	0	0
57	B7	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CF	1	Total 1	Mg 1	0	0
57	BV	4	Total 4	Mg 4	0	0
57	DO	1	Total 1	Mg 1	0	0
57	BO	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	D5	1	Total 1	Mg 1	0	0
57	BD	11	Total 11	Mg 11	0	0
57	B0	4	Total 4	Mg 4	0	0
57	CE	1	Total 1	Mg 1	0	0
57	BW	5	Total 5	Mg 5	0	0
57	DD	7	Total 7	Mg 7	0	0
57	CK	1	Total 1	Mg 1	0	0
57	AF	1	Total 1	Mg 1	0	0
57	DB	10	Total 10	Mg 10	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	170	Total 170	O 170	0	0
61	AL	2	Total 2	O 2	0	0
61	AO	1	Total 1	O 1	0	0
61	AU	1	Total 1	O 1	0	0
61	AV	2	Total 2	O 2	0	0
61	AW	3	Total 3	O 3	0	0
61	BA	1102	Total 1102	O 1102	0	0
61	BB	36	Total 36	O 36	0	0
61	BD	8	Total 8	O 8	0	0
61	BE	13	Total 13	O 13	0	0
61	BF	4	Total 4	O 4	0	0
61	BG	3	Total 3	O 3	0	0
61	BI	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	BP	15	Total 15	O 15	0	0
61	BQ	3	Total 3	O 3	0	0
61	BR	1	Total 1	O 1	0	0
61	BS	1	Total 1	O 1	0	0
61	BT	3	Total 3	O 3	0	0
61	BU	1	Total 1	O 1	0	0
61	BV	4	Total 4	O 4	0	0
61	BW	2	Total 2	O 2	0	0
61	BX	2	Total 2	O 2	0	0
61	B0	4	Total 4	O 4	0	0
61	B1	1	Total 1	O 1	0	0
61	B3	1	Total 1	O 1	0	0
61	B5	5	Total 5	O 5	0	0
61	B7	1	Total 1	O 1	0	0
61	B8	7	Total 7	O 7	0	0
61	CA	130	Total 130	O 130	0	0
61	CE	1	Total 1	O 1	0	0
61	CJ	2	Total 2	O 2	0	0
61	CN	1	Total 1	O 1	0	0
61	CT	1	Total 1	O 1	0	0
61	CV	1	Total 1	O 1	0	0

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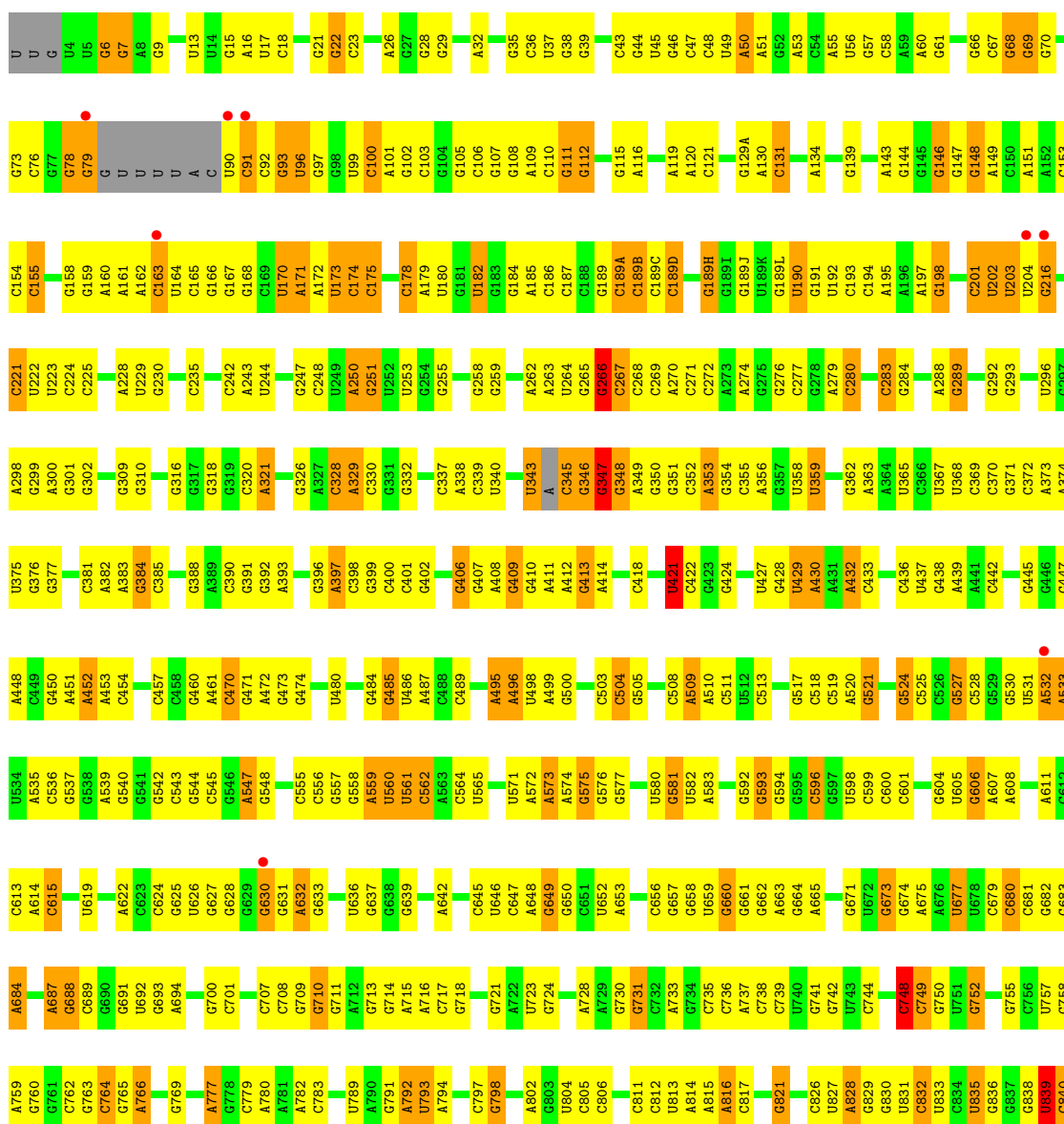
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	CW	1	Total 1	O 1	0	0
61	CX	1	Total 1	O 1	0	0
61	DA	767	Total 767	O 767	0	0
61	DB	9	Total 9	O 9	0	0
61	DD	9	Total 9	O 9	0	0
61	DE	5	Total 5	O 5	0	0
61	DF	6	Total 6	O 6	0	0
61	DN	2	Total 2	O 2	0	0
61	DP	12	Total 12	O 12	0	0
61	DR	2	Total 2	O 2	0	0
61	DT	1	Total 1	O 1	0	0
61	DU	2	Total 2	O 2	0	0
61	DV	1	Total 1	O 1	0	0
61	DX	2	Total 2	O 2	0	0
61	DY	1	Total 1	O 1	0	0
61	D0	5	Total 5	O 5	0	0
61	D1	1	Total 1	O 1	0	0
61	D3	2	Total 2	O 2	0	0
61	D7	1	Total 1	O 1	0	0
61	D8	4	Total 4	O 4	0	0

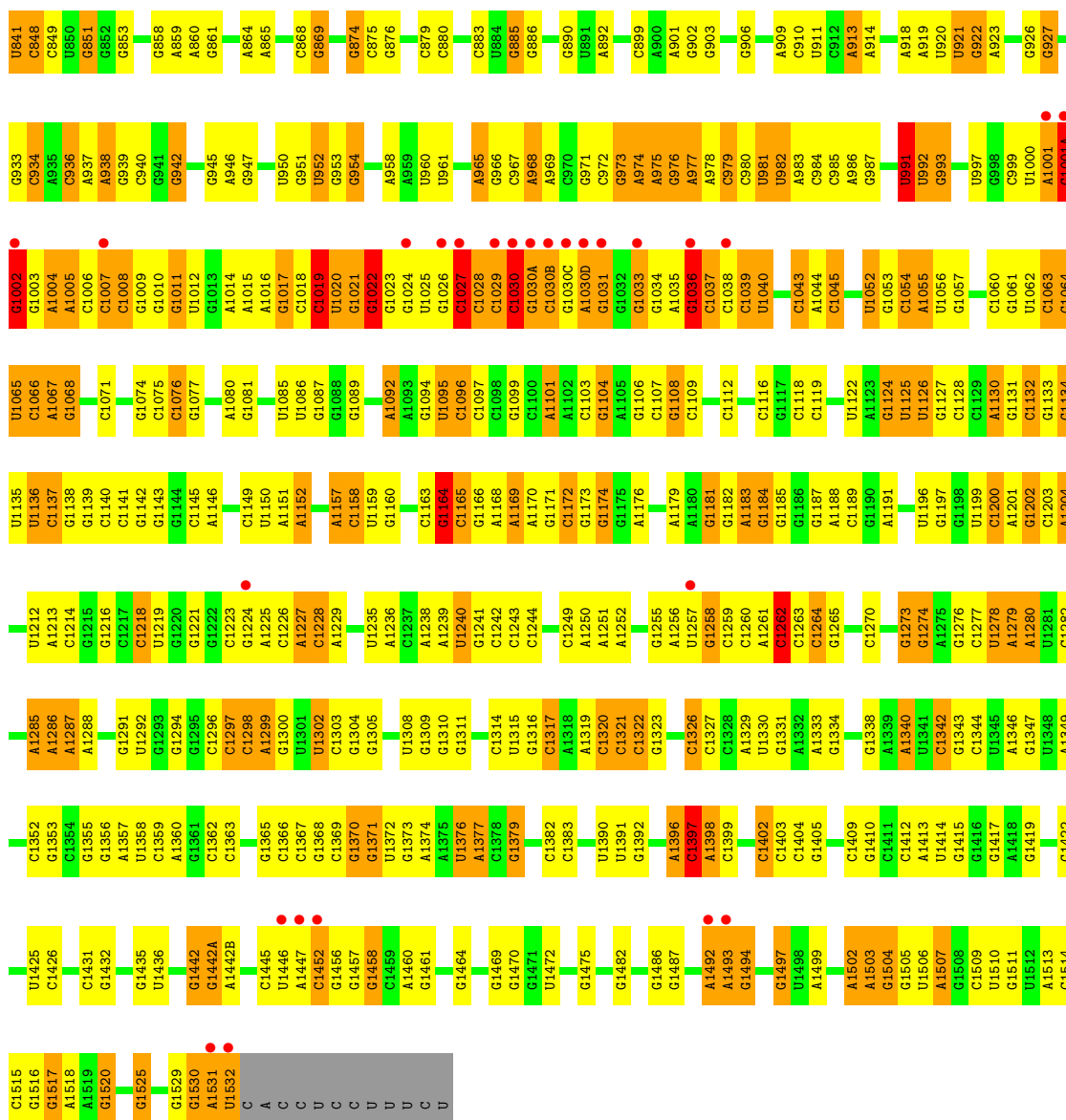
3 Residue-property plots

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

• Molecule 1: 16S Ribosomal RNA

Chain AA: 



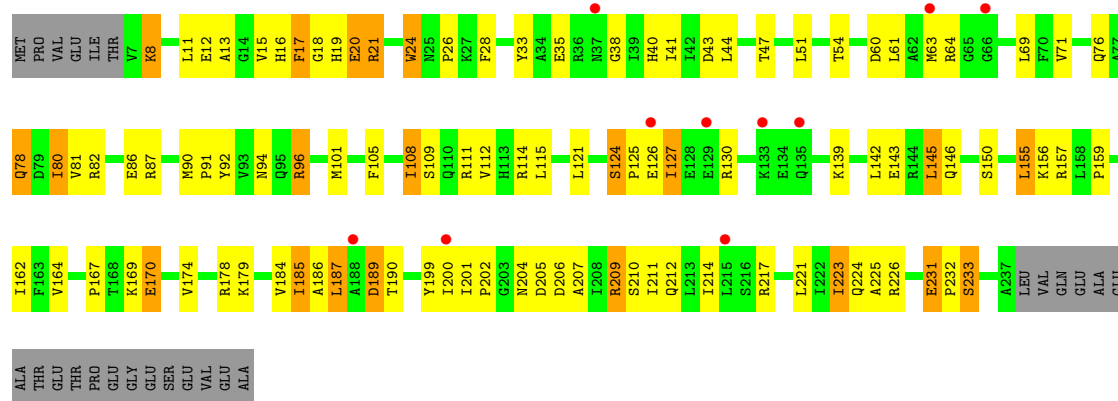






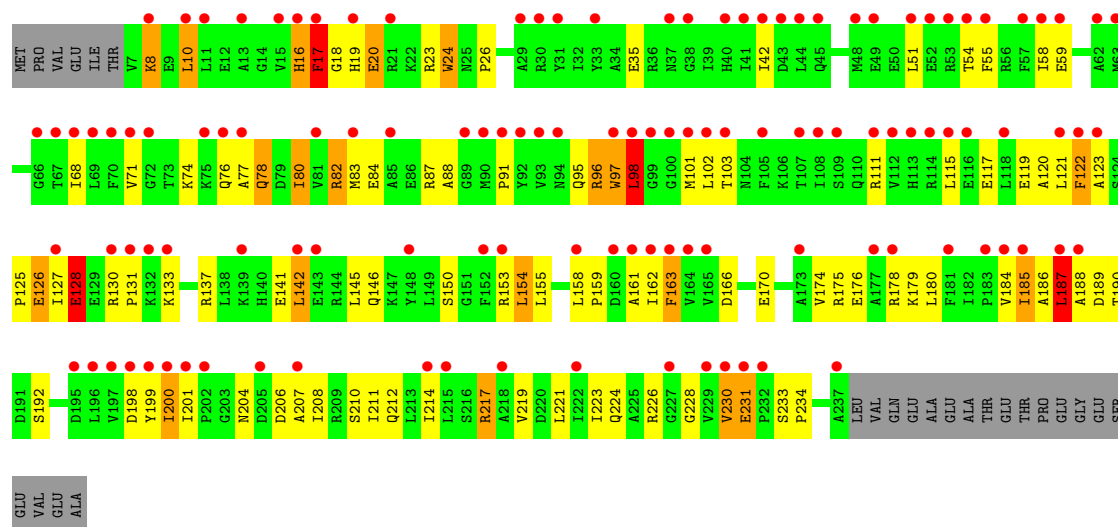
• Molecule 2: 30S ribosomal protein S2

Chain AB:



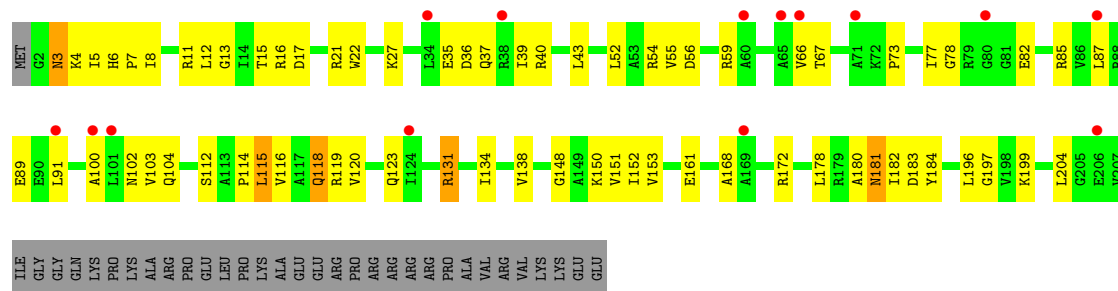
• Molecule 2: 30S ribosomal protein S2

Chain CB:



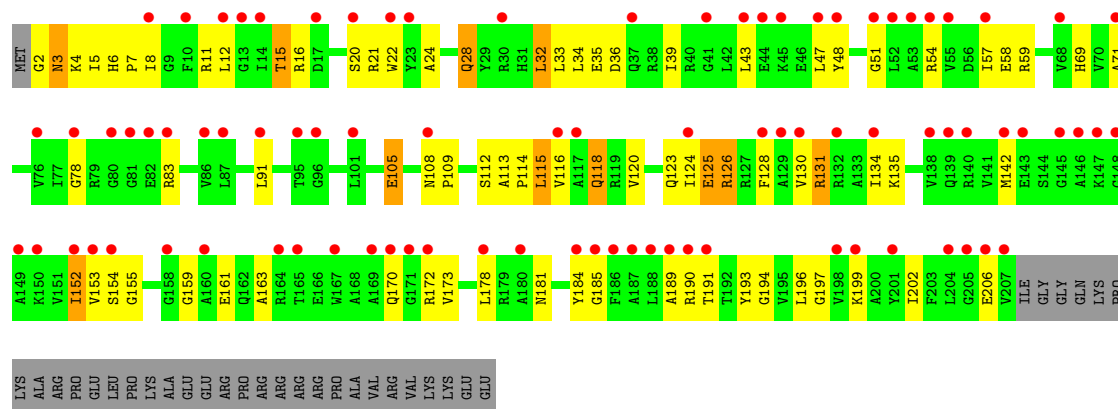
• Molecule 3: 30S ribosomal protein S3

Chain AC:



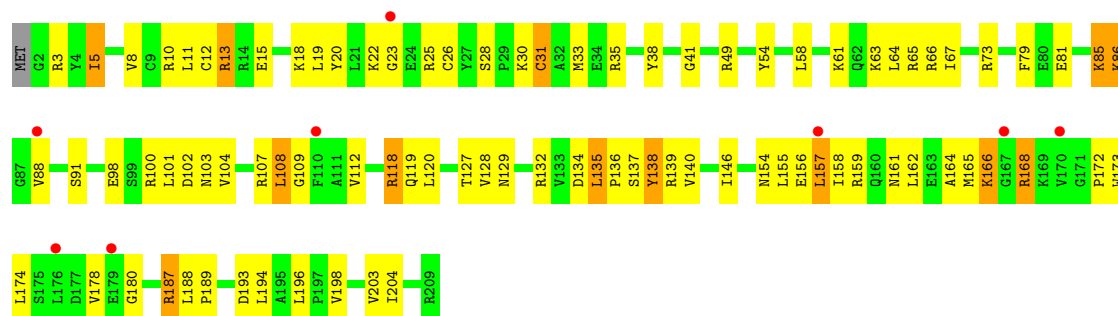
• Molecule 3: 30S ribosomal protein S3

Chain CC:



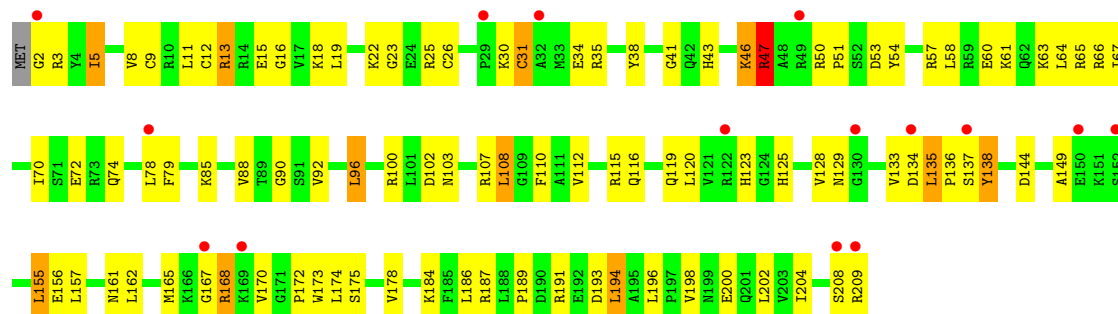
• Molecule 4: 30S ribosomal protein S4

Chain AD:



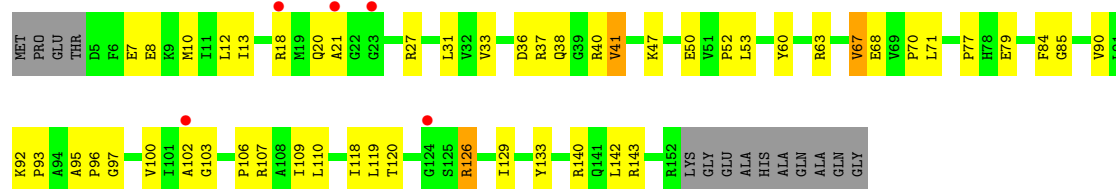
• Molecule 4: 30S ribosomal protein S4

Chain CD:



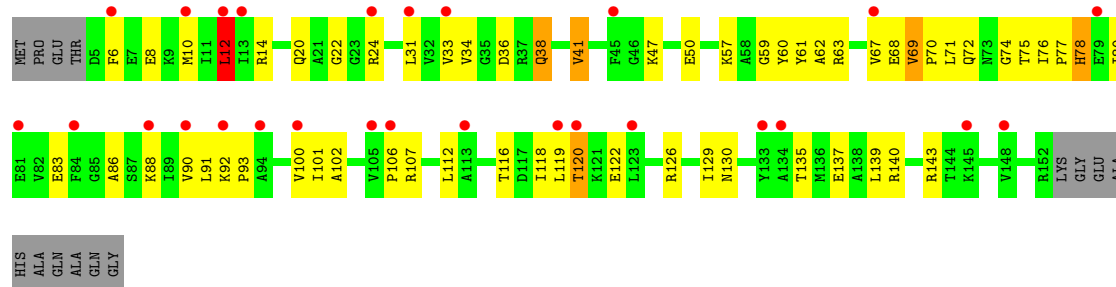
- Molecule 5: 30S ribosomal protein S5

Chain AE:



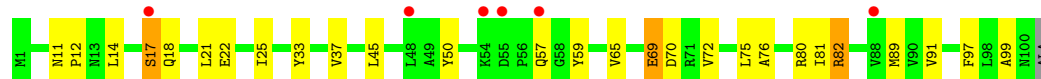
- Molecule 5: 30S ribosomal protein S5

Chain CE:



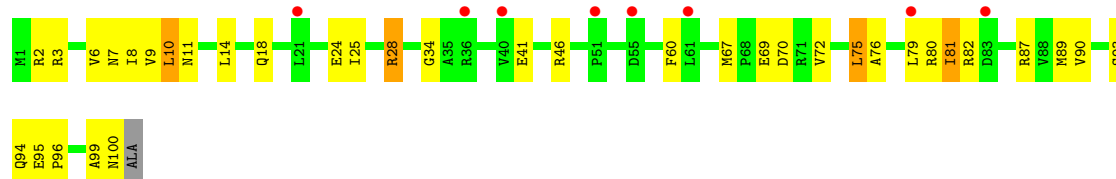
- Molecule 6: 30S ribosomal protein S6

Chain AF:



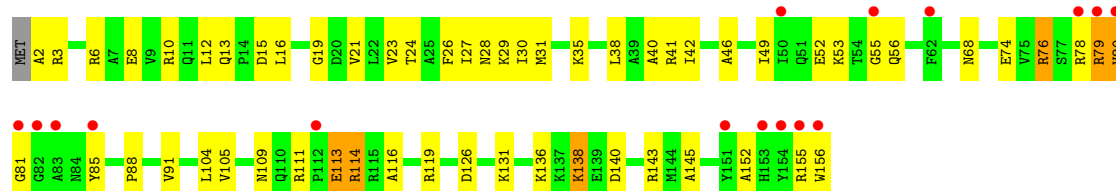
- Molecule 6: 30S ribosomal protein S6

Chain CF:



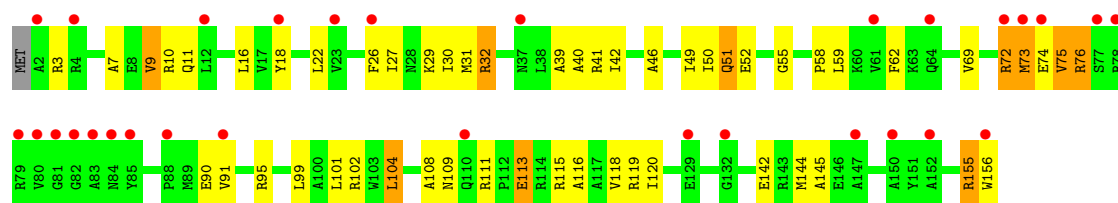
- Molecule 7: 30S ribosomal protein S7

Chain AG:



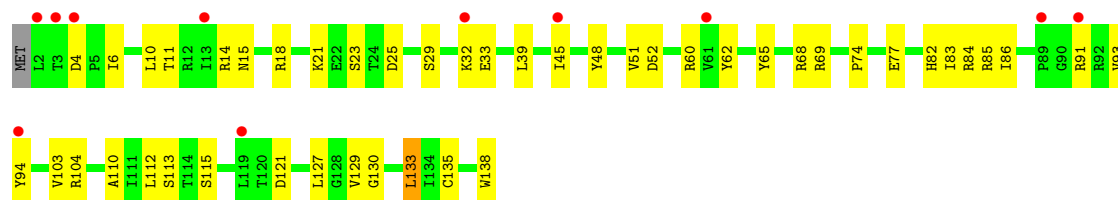
- Molecule 7: 30S ribosomal protein S7

Chain CG:



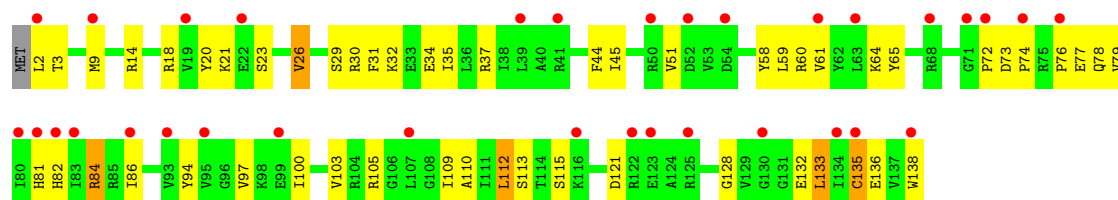
• Molecule 8: 30S ribosomal protein S8

Chain AH:



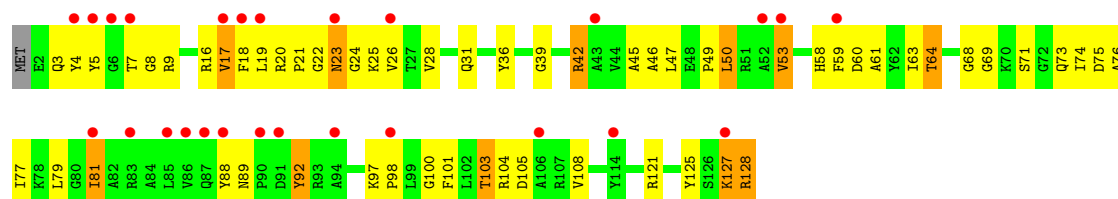
• Molecule 8: 30S ribosomal protein S8

Chain CH:



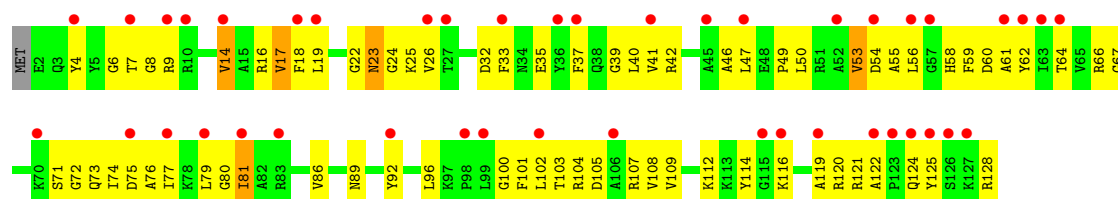
• Molecule 9: 30S ribosomal protein S9

Chain AI:



• Molecule 9: 30S ribosomal protein S9

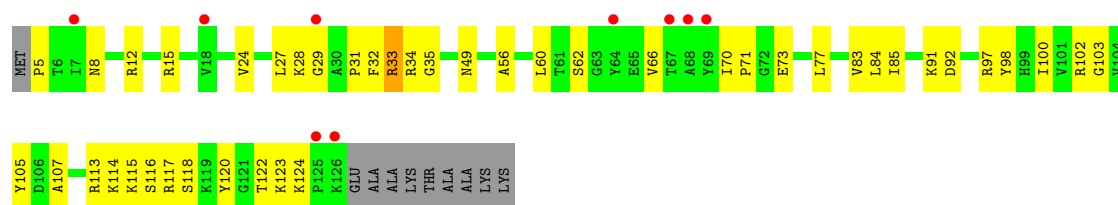
Chain CI:



• Molecule 10: 30S ribosomal protein S10

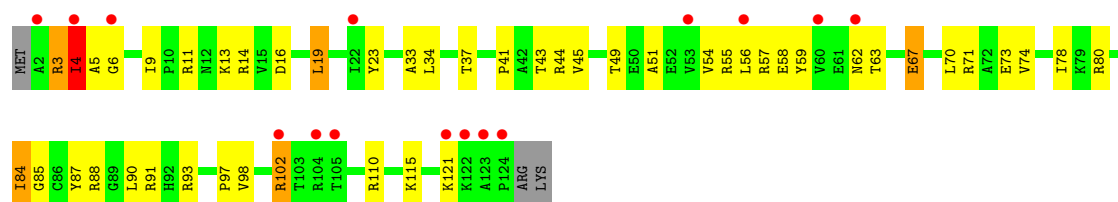
Chain AJ:





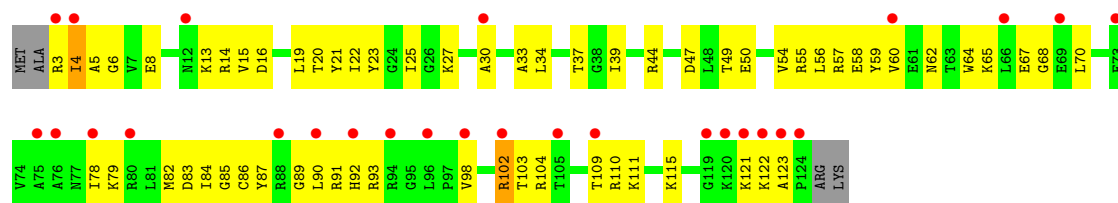
• Molecule 13: 30S ribosomal protein S13

Chain AM:



• Molecule 13: 30S ribosomal protein S13

Chain CM:



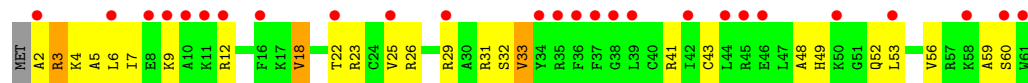
• Molecule 14: 30S ribosomal protein S14 type Z

Chain AN:



• Molecule 14: 30S ribosomal protein S14 type Z

Chain CN:



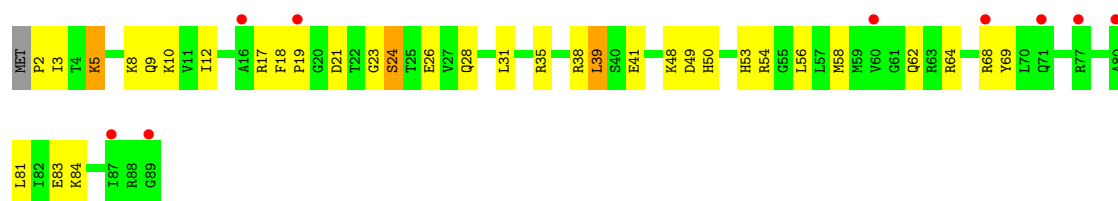
• Molecule 15: 30S ribosomal protein S15

Chain AO:



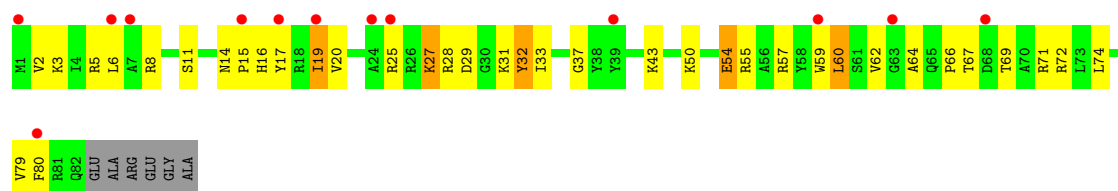
• Molecule 15: 30S ribosomal protein S15

Chain CO:



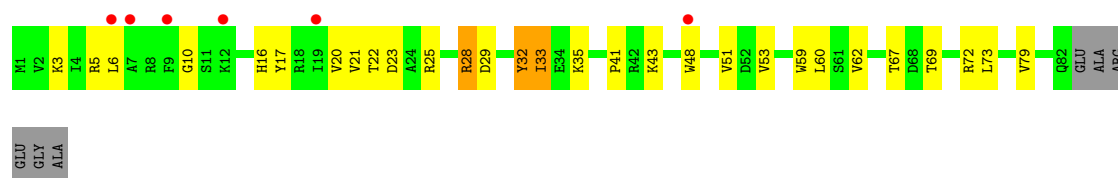
- Molecule 16: 30S ribosomal protein S16

Chain AP:



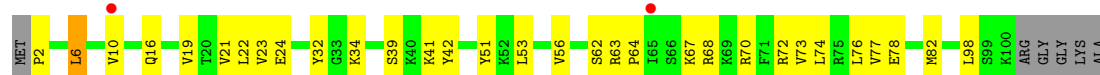
- Molecule 16: 30S ribosomal protein S16

Chain CP:



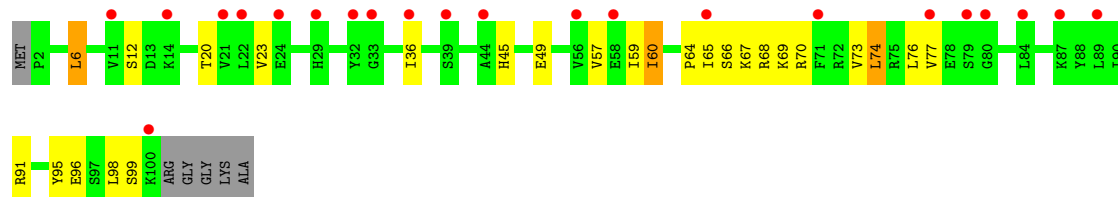
- Molecule 17: 30S ribosomal protein S17

Chain AQ:



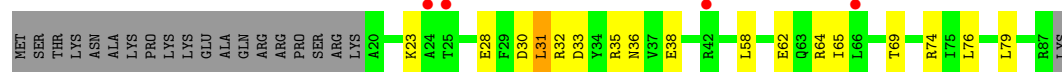
- Molecule 17: 30S ribosomal protein S17

Chain CQ:



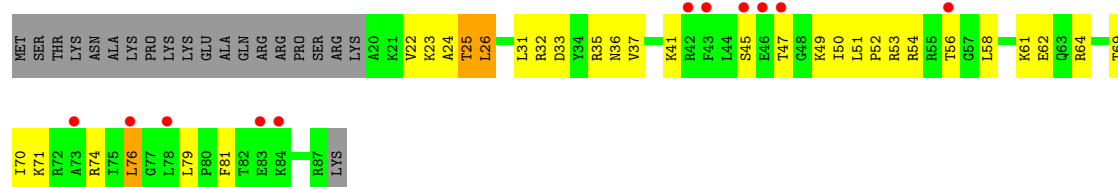
- Molecule 18: 30S ribosomal protein S18

Chain AR:



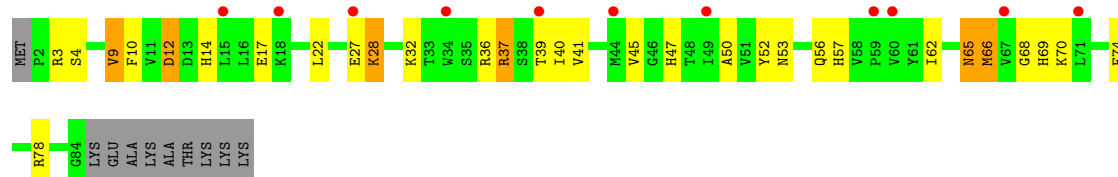
- Molecule 18: 30S ribosomal protein S18

Chain CR: 



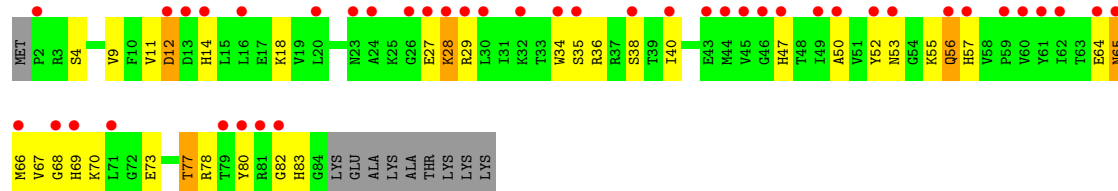
- Molecule 19: 30S ribosomal protein S19

Chain AS: 



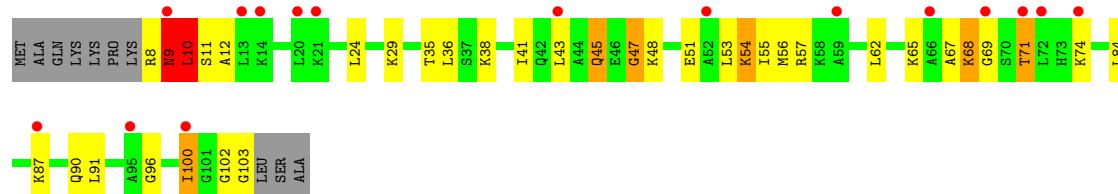
- Molecule 19: 30S ribosomal protein S19

Chain CS: 



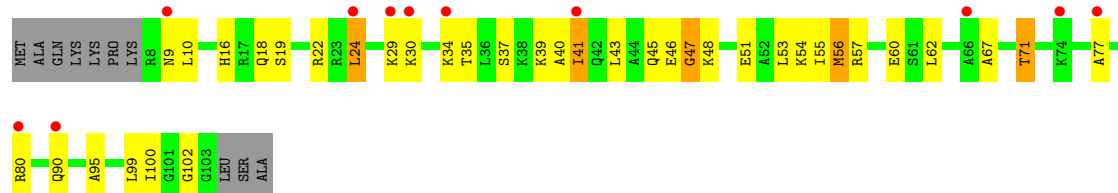
- Molecule 20: 30S ribosomal protein S20

Chain AT: 



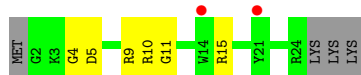
- Molecule 20: 30S ribosomal protein S20

Chain CT: 



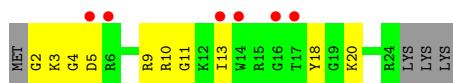
- Molecule 21: 30S ribosomal protein Thx

Chain AU: 



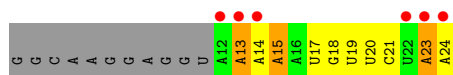
- Molecule 21: 30S ribosomal protein Thx

Chain CU:



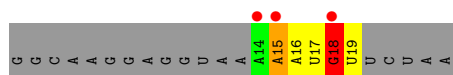
- Molecule 22: mRNA

Chain AV:



- Molecule 22: mRNA

Chain CV:



- Molecule 23: Cytidine-Puromycin

Chain AW:



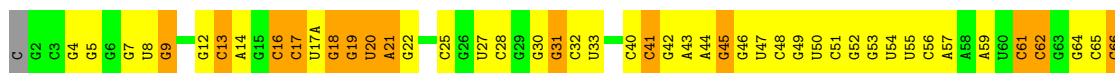
- Molecule 23: Cytidine-Puromycin

Chain CW:



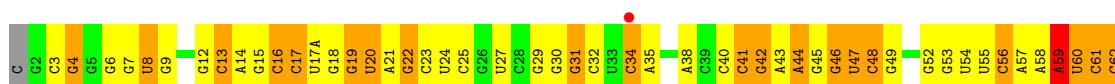
- Molecule 24: P-site tRNA

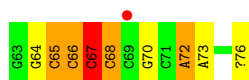
Chain AX:



- Molecule 24: P-site tRNA

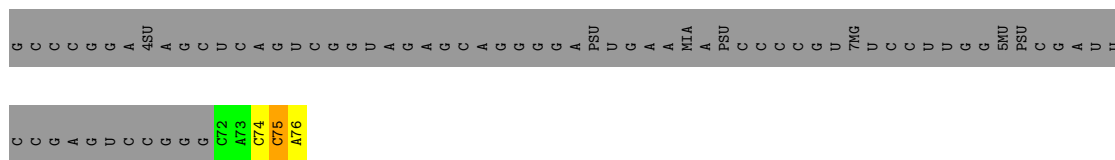
Chain CX:





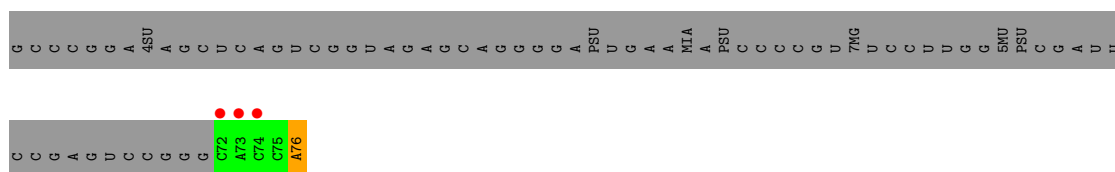
- Molecule 25: E-site tRNA

Chain AY:



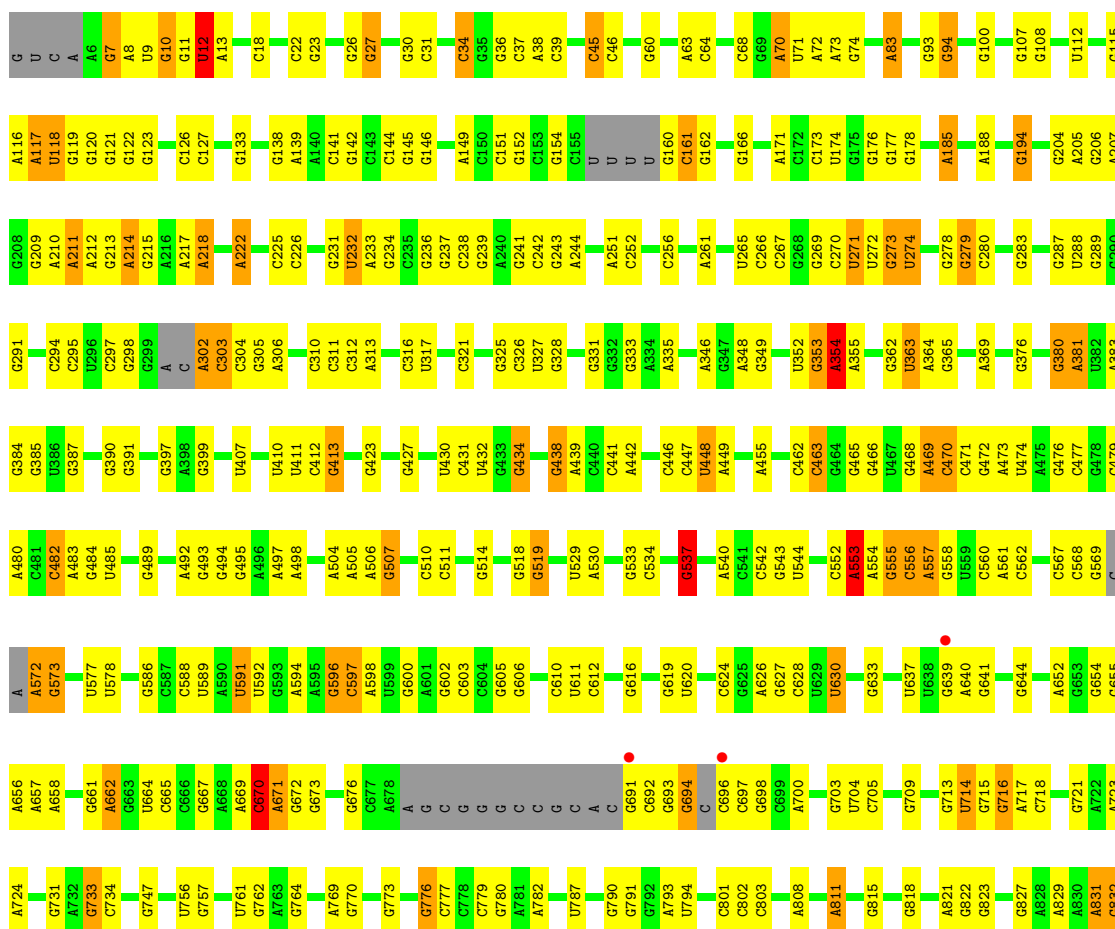
- Molecule 25: E-site tRNA

Chain CY:

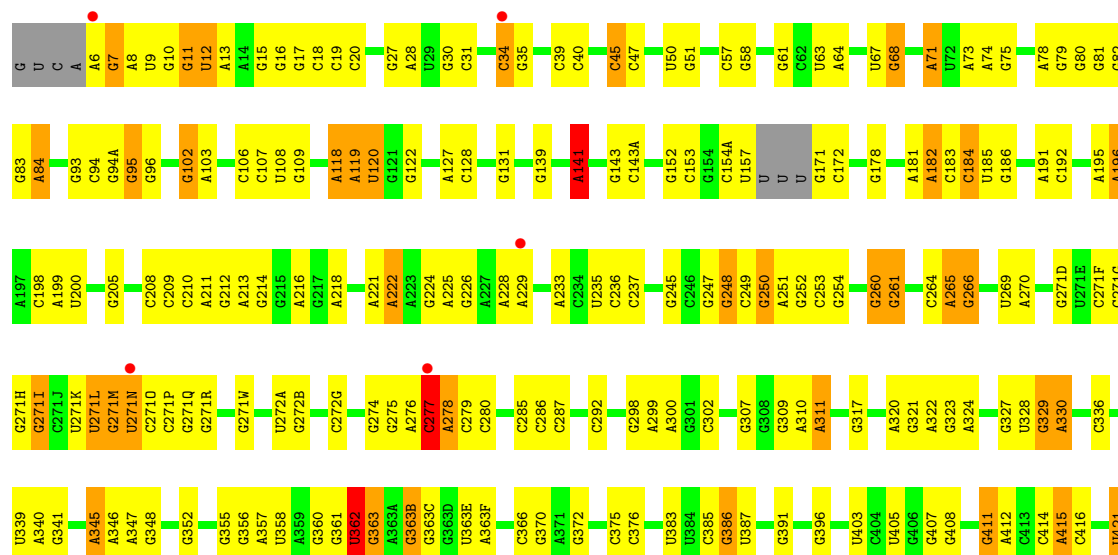


- Molecule 26: 23S Ribosomal RNA

Chain BA:

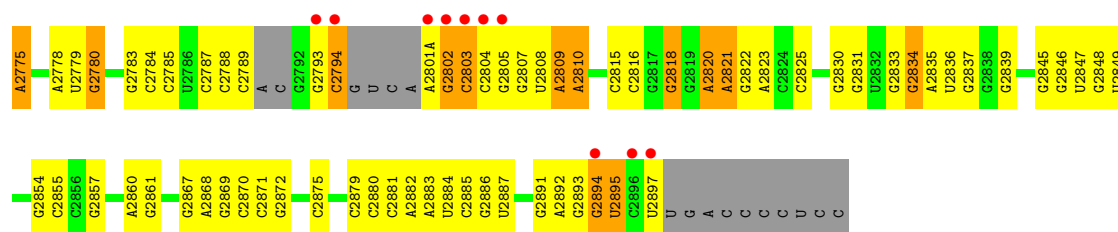






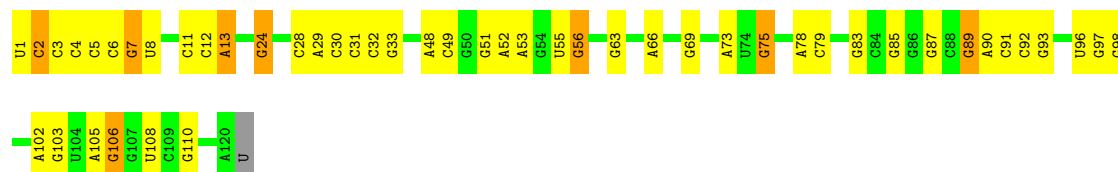


C2699	C2700	C2701	C2702	C2703	C2704	A2705	G2706	C2707	C2708	C2709	C2710	A2711	U2712	A2712A	A2713	C2714	C2715	U2716		A2721	G2722	C2723	C2724	A2725	U2726	C2727	U2728		G2732	A2733	A2734	G2735	G2736		A2741	C2742	U2746	G2747	A2748		G2751	C2752	A2753	U2756	A2757	A2758	G2759		G2763	A2764	A2765	G2766	C2767	C2768		C2773	C2774											
G2623	C2626	C2627	C2628	A2629	G2630	G2631	G2632	G2633	G2634	C2635	U2636	U2637	U2638	U2639	G2640	G2641		G2642	G2643	G2644	G2645	G2646	G2647	C2648	G2649	G2650	G2651	G2652	U2653	U2654	G2655	G2656	G2657	U2658	G2659	C2660	G2661	G2662	G2663	C2667	G2668	G2669	A2675		A2679	U2682	C2683	U2684	A2685	G2686	U2689	C2690	A2693	G2694	C2695	U2696	C2697	C2698	C2700	C2701								
A2542	G2543	G2544		U2547	G2548	G2549		U2552	G2553	U2554		G2557	C2558		U2562	U2563	U2564	A2565	A2566	G2567	C2568	A2569		A2572	C2573	G2574	C2575	C2576	C2577	G2578	C2579	U2580		G2583	U2584	U2585	C2586	A2587	G2588	A2589	A2590	C2591	G2592		A2602	G2603	U2604		G2608	U2609	C2610	U2611	C2612		U2615	C2616	C2617											
C2465	C2466	C2467	C2468	A2469	C2470	C2471	C2472	U2473		A2476	C2477	A2478	G2479	C2480	C2483	C2484	C2485	C2486	G2487	C2488	A2489	U2490	U2491	U2492	U2493	C2494	C2495	C2496	A2497	C2498	C2499	U2500	C2501	G2502	A2503	U2504	G2505	C2506	C2507	G2508		U2514	C2515	C2516	A2518		U2522	G2523			G2526		U2529		G2532		G2535	G2536										
C2389	U2390		C2394	C2395	G2396	G2397	U2398	C2399	G2400	U2401	C2402		G2405	U2406	C2407	U2408	C2409	G2410		C2416	C2417	A2418	U2419	C2420	G2421	A2422		A2425	A2426	C2427	G2428	G2429	A2430		A2435	G2436		A2439	C2440	C2441	C2442	C2443		G2444	G2445	G2446	U2448	A2449	A2450	A2451	C2452	A2453	G2454		U2457	G2458	A2459	U2460										
C2317	G2318	G2319	A2320	G2321		G2325	G2326	A2327	U2328	C2329	G2330	C2331	U2332	A2333	C2334	A2335	A2336	C2337		G2341	C2342	C2343	U2344		C2347	U2348	G2349		A2352	G2353	G2354		U2357	C2358	C2359	A2360	A2361	G2362	C2363	C2364	G2365	A2366	C2367		G2370	C2371	G2372	C2373		A2376	A2377	A2378	G2379		G2383	G2384	C2385		A2388									
U2243	U2244	U2245	U2246	G2246	A2247	C2248	U2249	G2250		G2253		G2259		U2262	C2263	C2264		A2268	A2269		U2273	C2274	C2275	G2276	G2277	A2278	G2279		C2282	C2283	C2284	G2285	A2286	A2287	A2288		U2291	C2292	C2293		U2296	G2297	A2298		C2301	G2302	C2303	G2304	A2305		G2308	A2309	A2310	U2311	U2312	C2313	C2314	G2315	C2316									
G2165	G2166	U2167	C2168	A2169	A2170	A2171	U2172	C2173	C2174	C2175	A2176	C2177	C2178	U2179	U2180	C2181	C2182	C2183	G2184	C2185	C2186	C2187	C2188	U2189	C2190	C2191	C2192	C2193	C2194	A2198	A2199	C2200		U2203	C2205	G2206	C2207	A2208	U2218	C2219	G2220	C2221	G2222	C2223	G2224	C2225	C2226	A2227		G2230	C2231	U2232	U2233	U2234		G2238	C2239	G2240										
C2105	G2106	C2107	C2108	G2109	U2110	C2111	G2112	U2113	A2114	G2115	C2116	A2117	U2118	A2119	C2120	C2121	U2122	G2123	G2124	C2125	A2126	C2127	C2128	C2129	U2130	C2131	U2132	C2133	A2134	A2135	C2136	C2137	C2138	C2139	C2140	C2141	C2142	C2143	U2144	C2145	G2146	G2147	C2148	G2149	G2150	G2151	G2152	C2153	G2154	G2155	G2156	C2157	A2158	C2159	U2160	C2161	C2162	C2163	C2164									
G1929	G1930	U1931	G1932	C1933	C1934	G1935	A1936	A1937	U1938	U1939	U1940		U1951	A1952	A1953	G1954	U1955		G1959	A1960		U1963	G1964	C1965	A1966	C1967	A1968	A1969	U1970	A1971	A1972	C1973	C1974	U1978	C1979		G1984		G1987	C1988		U1991	G1992	U1993		G1997		G2000	A2001	G2002	G2012	A2013	A2014	A2015	U2016	U2017												
C1838	G1839	U1840	U1841	G1842		A1847	A1848	G1849	G1850	U1851	C1852	A1853		G1857	G1858	A1859	G1860	G1861	G1862		C1866	A1867	A1868	G1869	C1870	A1871	A1872	A1873	A1874	A1875	A1876	C1877	A1878	A1879	U1794	C1795	U1796	C1797	U1798	G1799	C1800	A1801	A1802	A1803		G1811	G1812	G1813	A1814	A1815	G1816	U1817	U1818	A1819	U1820		G1826	G1827	G1828	A1829	C1830	A1831	C1832	U1833	U1834	C1835	U1836	C1837
A1570	A1571		U1578	A1579	C1580	G1581	C1582	A1583	C1584	U1585	A1586	C1587	C1588	C1589		C1592	G1593	G1594	G1595	A1596	A1597	C1598	C1599	C1600	G1601	U1602	A1603	C1604		C1607	A1608	A1609	A1610		G1613	A1614				G1619			G1622		G1626		C1631	A1631A	A1632		C1636	A1637	C1638	U1639	C1640	G1641	G1642		G1645	C1646	C1647	G1648	G1649					



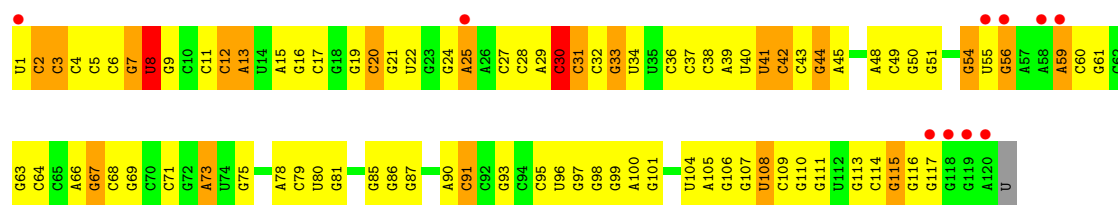
• Molecule 27: 5S Ribosomal RNA

Chain BB:



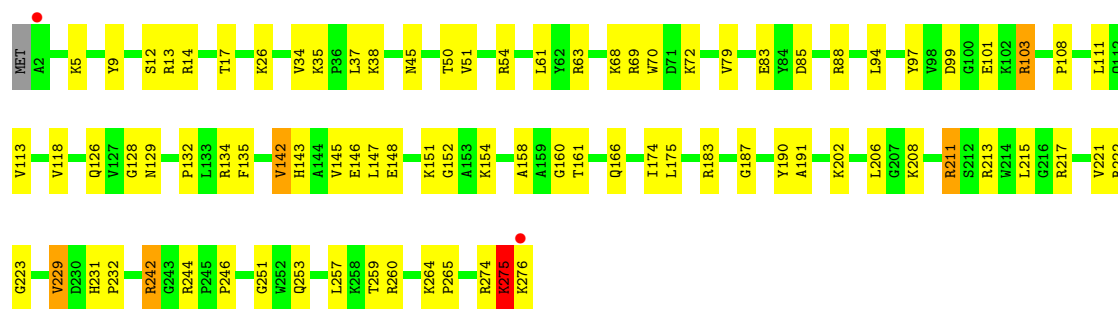
• Molecule 27: 5S Ribosomal RNA

Chain DB:



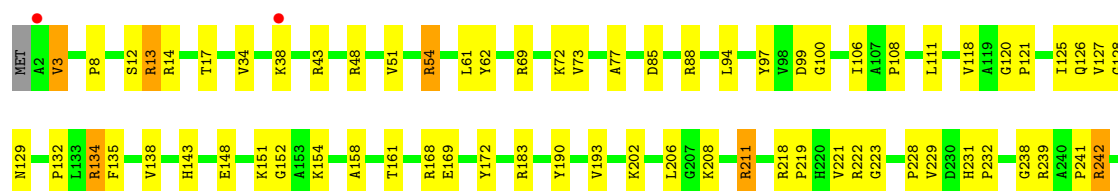
• Molecule 28: 50S ribosomal protein L2

Chain BD:



• Molecule 28: 50S ribosomal protein L2

Chain DD:





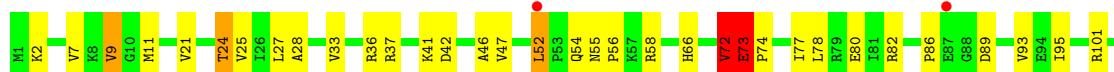
- Molecule 29: 50S ribosomal protein L3

Chain BE:



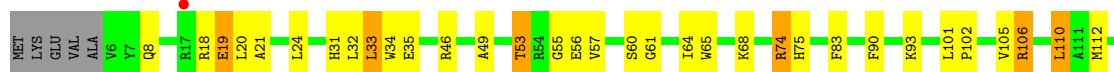
- Molecule 29: 50S ribosomal protein L3

Chain DE:



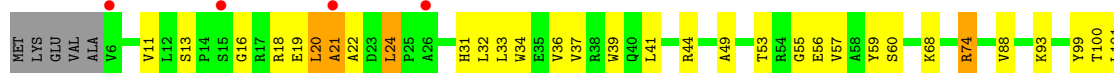
- Molecule 30: 50S ribosomal protein L4

Chain BF:



- Molecule 30: 50S ribosomal protein L4

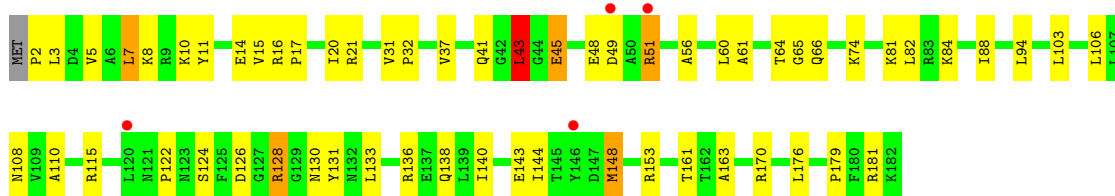
Chain DF:



- Molecule 31: 50S ribosomal protein L5

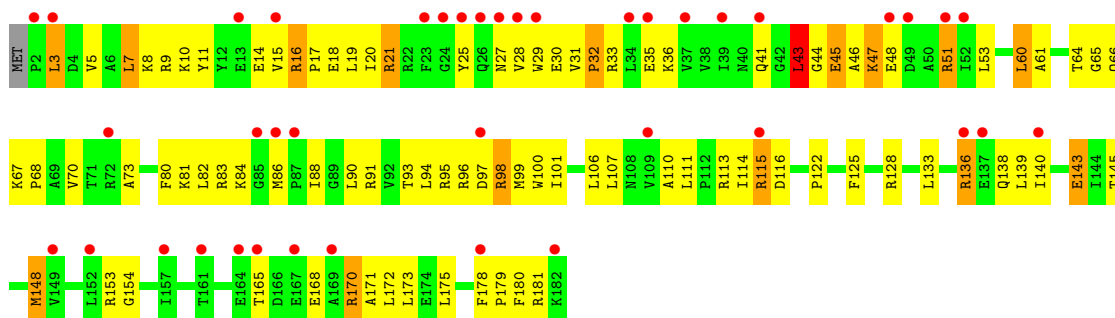
Chain BG:





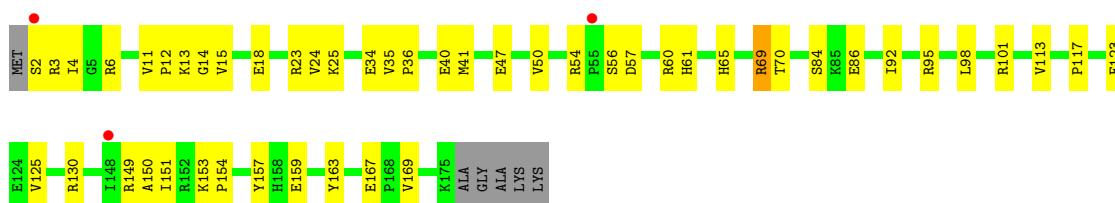
• Molecule 31: 50S ribosomal protein L5

Chain DG:



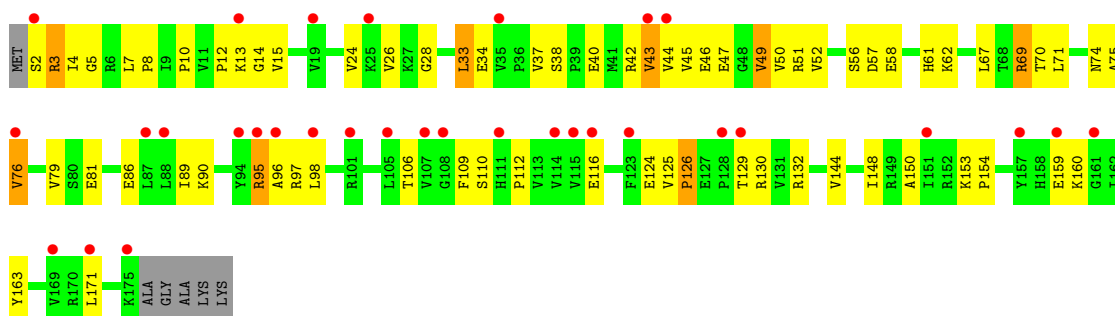
• Molecule 32: 50S ribosomal protein L6

Chain BH:



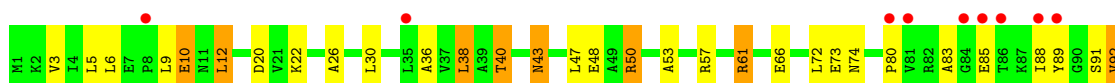
• Molecule 32: 50S ribosomal protein L6

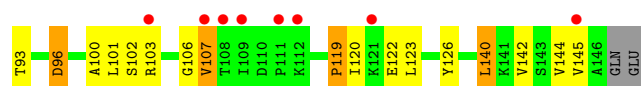
Chain DH:



• Molecule 33: 50S ribosomal protein L9

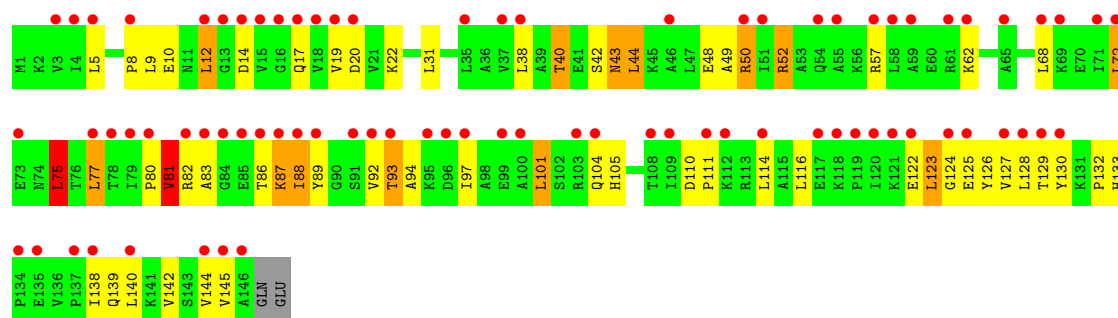
Chain BI:





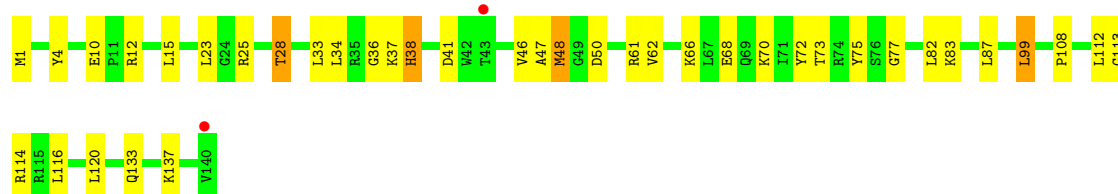
- Molecule 33: 50S ribosomal protein L9

Chain DI:



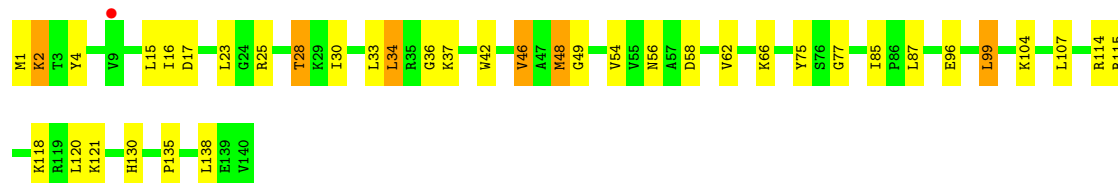
- Molecule 34: 50S ribosomal protein L13

Chain BN:



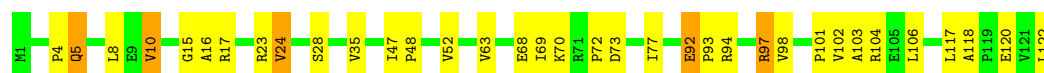
- Molecule 34: 50S ribosomal protein L13

Chain DN:



- Molecule 35: 50S ribosomal protein L14

Chain BO:



- Molecule 35: 50S ribosomal protein L14

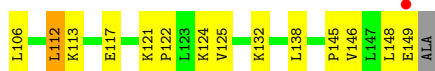
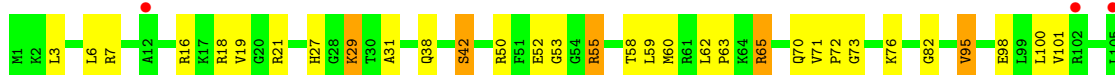
Chain DO:





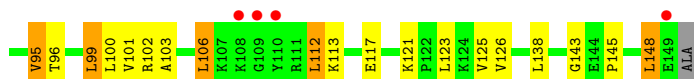
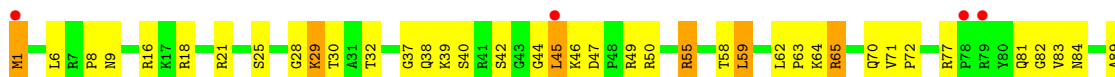
- Molecule 36: 50S ribosomal protein L15

Chain BP:



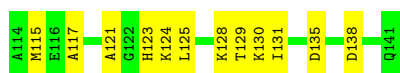
- Molecule 36: 50S ribosomal protein L15

Chain DP:



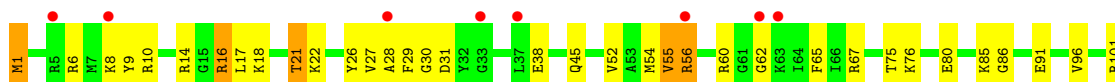
- Molecule 37: 50S ribosomal protein L16

Chain BQ:



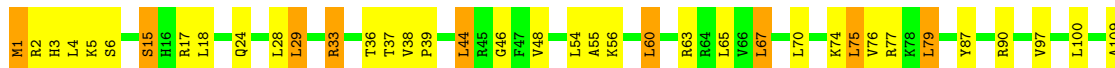
- Molecule 37: 50S ribosomal protein L16

Chain DQ:



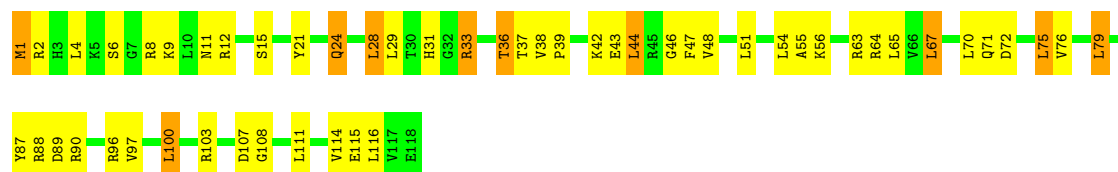
- Molecule 38: 50S ribosomal protein L17

Chain BR:



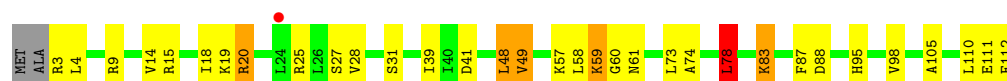
- Molecule 38: 50S ribosomal protein L17

Chain DR:



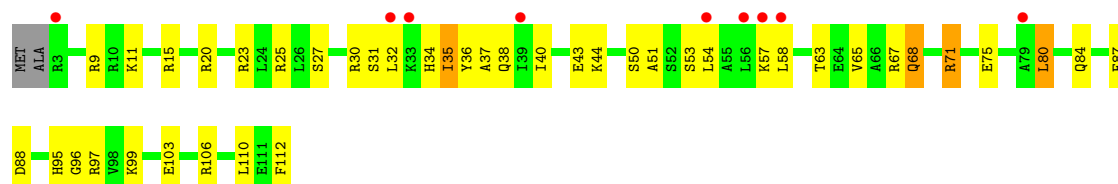
- Molecule 39: 50S ribosomal protein L18

Chain BS:



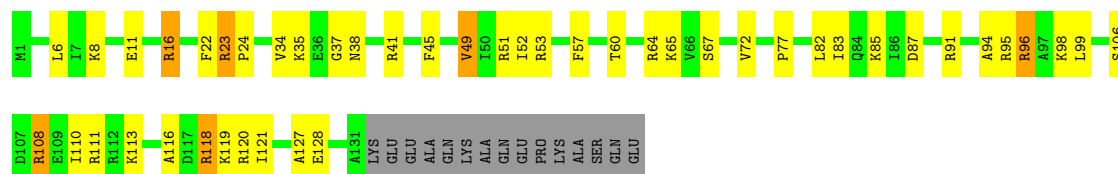
- Molecule 39: 50S ribosomal protein L18

Chain DS:



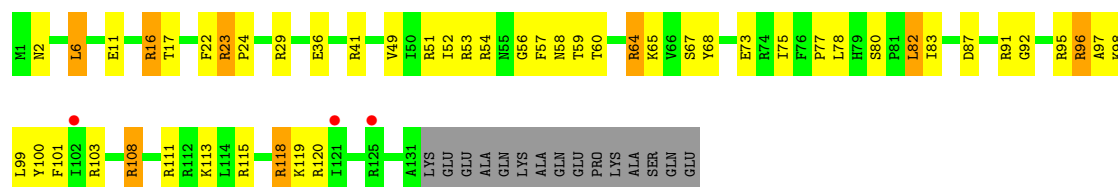
- Molecule 40: 50S ribosomal protein L19

Chain BT:



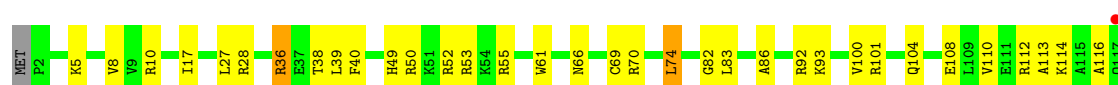
- Molecule 40: 50S ribosomal protein L19

Chain DT:



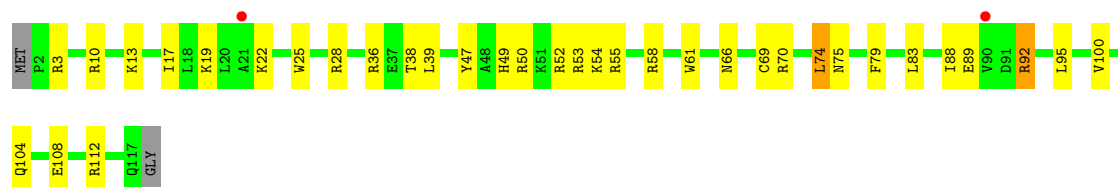
- Molecule 41: 50S ribosomal protein L20

Chain BU:

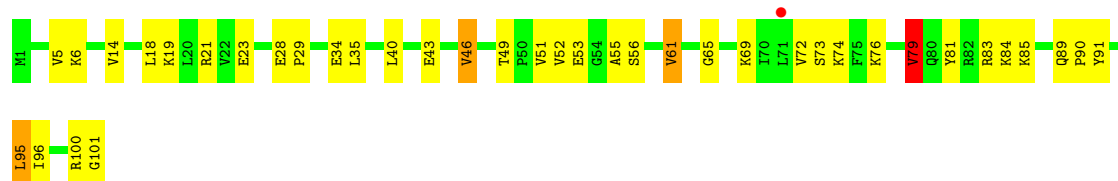


GLY

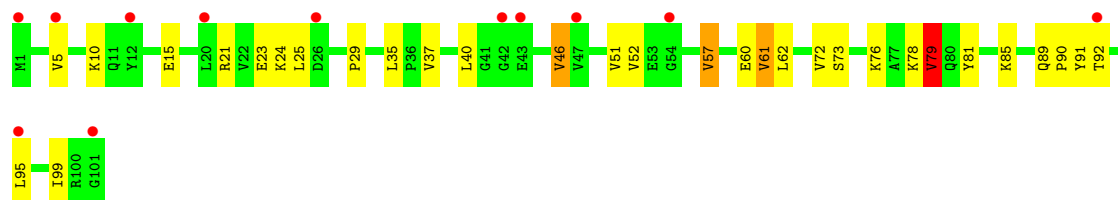
- Molecule 41: 50S ribosomal protein L20

Chain DU: 

- Molecule 42: 50S ribosomal protein L21

Chain BV: 

- Molecule 42: 50S ribosomal protein L21

Chain DV: 

- Molecule 43: 50S ribosomal protein L22

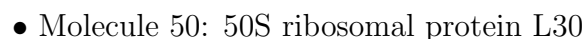
Chain BW: 

- Molecule 43: 50S ribosomal protein L22

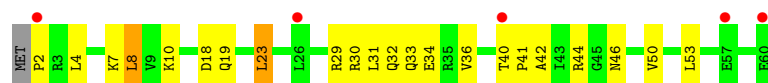
Chain DW: 

- Molecule 44: 50S ribosomal protein L23

Chain BX: 

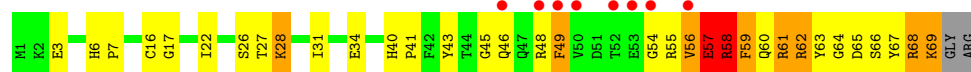


Chain D3:



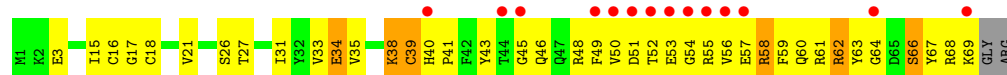
- Molecule 51: 50S ribosomal protein L31

Chain B4:



- Molecule 51: 50S ribosomal protein L31

Chain D4:



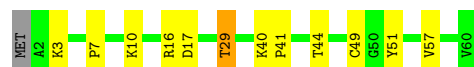
- Molecule 52: 50S ribosomal protein L32

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:



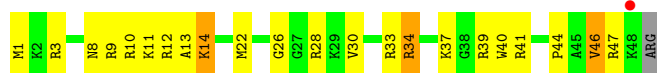
- Molecule 54: 50S ribosomal protein L34

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	207.56Å 444.23Å 613.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	150.38 – 2.80 150.38 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (150.38-2.80) 98.0 (150.38-2.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.82Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.234 , 0.280 0.255 , 0.304	Depositor DCC
R_{free} test set	36605 reflections (2.72%)	DCC
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 1345521 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	290205	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.41	4/36049 (0.0%)	0.98	71/56261 (0.1%)
1	CA	0.42	7/36170 (0.0%)	1.05	147/56452 (0.3%)
2	AB	0.29	0/1881	0.59	0/2542
2	CB	0.33	0/1860	0.68	3/2518 (0.1%)
3	AC	0.28	0/1576	0.52	0/2130
3	CC	0.30	0/1566	0.58	0/2119
4	AD	0.28	0/1689	0.55	0/2267
4	CD	0.30	0/1704	0.56	0/2284
5	AE	0.29	0/1145	0.52	0/1543
5	CE	0.30	0/1149	0.58	1/1548 (0.1%)
6	AF	0.29	0/819	0.50	0/1111
6	CF	0.30	0/829	0.49	0/1123
7	AG	0.27	0/1250	0.51	0/1679
7	CG	0.29	0/1254	0.53	0/1683
8	AH	0.27	0/1108	0.51	0/1494
8	CH	0.27	0/1108	0.55	0/1494
9	AI	0.28	0/1002	0.54	0/1346
9	CI	0.30	0/997	0.56	0/1343
10	AJ	0.27	0/722	0.60	0/982
10	CJ	0.30	0/727	0.57	0/988
11	AK	0.29	0/844	0.50	0/1145
11	CK	0.27	0/848	0.50	0/1149
12	AL	0.29	0/946	0.51	0/1274
12	CL	0.29	0/946	0.56	0/1274
13	AM	0.28	0/969	0.58	0/1302
13	CM	0.29	0/961	0.57	0/1291
14	AN	0.30	0/501	0.55	0/664
14	CN	0.32	0/501	0.55	0/664
15	AO	0.27	0/739	0.53	0/985
15	CO	0.30	0/739	0.54	0/985
16	AP	0.29	0/697	0.53	0/939
16	CP	0.28	0/693	0.54	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.29	0/836	0.55	0/1117
17	CQ	0.29	0/836	0.53	0/1117
18	AR	0.27	0/560	0.48	0/746
18	CR	0.28	0/560	0.52	0/746
19	AS	0.28	0/667	0.54	0/900
19	CS	0.30	0/661	0.68	0/893
20	AT	0.27	0/730	0.58	0/965
20	CT	0.27	0/729	0.52	0/965
21	AU	0.29	0/203	0.56	0/266
21	CU	0.32	0/203	0.48	0/266
22	AV	0.49	0/310	0.95	1/480 (0.2%)
22	CV	1.15	3/144 (2.1%)	3.12	11/222 (5.0%)
23	AW	0.45	0/40	1.07	0/60
23	CW	0.35	0/40	1.09	0/60
24	AX	0.53	2/1700 (0.1%)	1.24	23/2650 (0.9%)
24	CX	0.54	0/1700	1.36	19/2650 (0.7%)
25	AY	0.33	0/115	0.82	0/176
25	CY	0.29	0/115	0.95	0/176
26	BA	0.50	4/68013 (0.0%)	0.93	70/106165 (0.1%)
26	DA	0.42	0/67542	0.94	88/105428 (0.1%)
27	BB	0.41	0/2878	0.91	2/4490 (0.0%)
27	DB	0.41	0/2878	1.00	8/4490 (0.2%)
28	BD	0.37	0/2186	0.57	0/2944
28	DD	0.34	0/2186	0.56	0/2944
29	BE	0.36	0/1592	0.53	0/2149
29	DE	0.34	0/1592	0.59	1/2149 (0.0%)
30	BF	0.35	0/1619	0.53	0/2193
30	DF	0.33	0/1615	0.56	0/2188
31	BG	0.29	0/1450	0.54	0/1959
31	DG	0.32	0/1449	0.57	0/1958
32	BH	0.30	0/1356	0.51	0/1834
32	DH	0.29	0/1356	0.51	0/1834
33	BI	0.31	0/1100	0.59	0/1501
33	DI	0.37	0/1076	0.78	4/1471 (0.3%)
34	BN	0.34	0/1144	0.54	0/1543
34	DN	0.31	0/1144	0.52	0/1543
35	BO	0.34	0/943	0.56	0/1269
35	DO	0.33	0/943	0.55	1/1269 (0.1%)
36	BP	0.35	0/1152	0.57	0/1533
36	DP	0.32	0/1152	0.63	0/1533
37	BQ	0.35	0/1143	0.59	1/1527 (0.1%)
37	DQ	0.32	0/1143	0.54	0/1527
38	BR	0.36	0/982	0.57	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DR	0.29	0/982	0.55	0/1312
39	BS	0.32	0/887	0.57	1/1180 (0.1%)
39	DS	0.29	0/880	0.57	0/1172
40	BT	0.34	0/1105	0.61	0/1477
40	DT	0.30	0/1097	0.53	0/1468
41	BU	0.35	0/977	0.53	0/1301
41	DU	0.28	0/977	0.50	0/1301
42	BV	0.36	0/782	0.55	0/1049
42	DV	0.29	0/782	0.54	0/1049
43	BW	0.35	0/897	0.53	0/1205
43	DW	0.30	0/897	0.49	0/1205
44	BX	0.39	0/764	0.58	1/1025 (0.1%)
44	DX	0.32	0/764	0.53	1/1025 (0.1%)
45	BY	0.34	0/819	0.59	0/1095
45	DY	0.30	0/819	0.55	0/1095
46	BZ	0.32	0/1379	0.58	0/1873
46	DZ	0.29	0/1390	0.54	0/1890
47	B0	0.36	0/662	0.60	0/881
47	D0	0.30	0/662	0.50	0/881
48	B1	0.32	0/762	0.53	0/1014
48	D1	0.31	0/762	0.53	0/1014
49	B2	0.32	0/590	0.57	0/781
49	D2	0.26	0/590	0.49	0/781
50	B3	0.35	0/474	0.52	0/635
50	D3	0.31	0/469	0.54	0/630
51	B4	0.34	0/565	0.70	0/761
51	D4	0.32	0/545	0.67	0/737
52	B5	0.37	0/469	0.62	1/635 (0.2%)
52	D5	0.32	0/469	0.54	0/635
53	B6	0.36	0/460	0.53	0/613
53	D6	0.34	0/456	0.51	0/608
54	B7	0.36	0/426	0.56	0/561
54	D7	0.34	0/426	0.49	0/561
55	B8	0.37	0/519	0.54	0/684
55	D8	0.31	0/525	0.50	0/691
56	B9	0.43	0/310	0.65	0/407
56	D9	0.33	0/310	0.59	0/407
All	All	0.41	20/310421 (0.0%)	0.88	455/464361 (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	1
7	AG	0	1
20	AT	0	1
29	DE	0	1
33	DI	0	1
39	BS	0	1
46	BZ	0	1
51	B4	0	2
51	D4	0	1
All	All	0	10

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	1154	G	C6-N1	-12.37	1.30	1.39
1	AA	1172	C	N3-C4	-10.50	1.26	1.33
1	CA	1154	G	N1-C2	-10.41	1.29	1.37
1	AA	1172	C	C2-N3	-8.49	1.28	1.35
1	AA	1164	G	N1-C2	-6.91	1.32	1.37

The worst 5 of 455 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1172	C	N1-C2-O2	39.76	142.76	118.90
1	CA	1119	C	N1-C2-O2	26.84	135.00	118.90
1	AA	1172	C	N3-C2-O2	-25.31	104.18	121.90
1	CA	1154	G	C5-C6-O6	24.22	143.13	128.60
1	CA	1154	G	N1-C2-N2	-23.61	94.95	116.20

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	8	LYS	Peptide
7	AG	79	ARG	Peptide
20	AT	9	ASN	Peptide
39	BS	58	LEU	Peptide
46	BZ	158	PRO	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32205	0	16255	743	1
1	CA	32312	0	16307	964	1
2	AB	1846	0	1867	74	0
2	CB	1825	0	1828	76	0
3	AC	1552	0	1546	49	0
3	CC	1542	0	1517	58	0
4	AD	1659	0	1676	74	0
4	CD	1674	0	1714	83	0
5	AE	1129	0	1184	33	0
5	CE	1133	0	1191	39	0
6	AF	806	0	793	16	0
6	CF	816	0	808	23	0
7	AG	1231	0	1238	37	0
7	CG	1235	0	1249	38	0
8	AH	1088	0	1126	35	0
8	CH	1088	0	1126	40	0
9	AI	983	0	986	48	0
9	CI	978	0	966	53	0
10	AJ	709	0	650	35	0
10	CJ	714	0	672	38	0
11	AK	829	0	825	23	0
11	CK	833	0	836	20	0
12	AL	930	0	980	21	0
12	CL	930	0	980	33	0
13	AM	958	0	1002	37	0
13	CM	950	0	988	47	0
14	AN	492	0	529	27	0
14	CN	492	0	529	23	0
15	AO	728	0	760	22	0
15	CO	728	0	760	27	0
16	AP	681	0	697	27	0
16	CP	677	0	686	26	0
17	AQ	823	0	891	23	0
17	CQ	823	0	891	18	0
18	AR	555	0	618	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	CR	555	0	618	23	0
19	AS	652	0	662	29	0
19	CS	646	0	644	40	0
20	AT	728	0	798	27	0
20	CT	727	0	796	23	0
21	AU	199	0	208	5	0
21	CU	199	0	208	8	0
22	AV	277	0	140	7	0
22	CV	129	0	65	16	0
23	AW	74	0	51	5	0
23	CW	74	0	51	10	0
24	AX	1633	0	816	35	0
24	CX	1635	0	816	82	0
25	AY	104	0	56	3	0
25	CY	104	0	56	2	0
26	BA	60729	0	30620	950	0
26	DA	60311	0	30412	1223	1
27	BB	2573	0	1306	32	0
27	DB	2573	0	1306	87	0
28	BD	2136	0	2218	67	0
28	DD	2136	0	2218	74	0
29	BE	1559	0	1618	43	0
29	DE	1559	0	1618	56	0
30	BF	1584	0	1625	49	0
30	DF	1580	0	1619	55	0
31	BG	1425	0	1443	37	0
31	DG	1424	0	1434	73	0
32	BH	1330	0	1407	29	0
32	DH	1330	0	1407	44	0
33	BI	1085	0	1114	28	1
33	DI	1061	0	1080	50	0
34	BN	1117	0	1184	21	0
34	DN	1117	0	1184	29	0
35	BO	933	0	996	27	0
35	DO	933	0	996	38	0
36	BP	1135	0	1212	53	0
36	DP	1135	0	1212	61	0
37	BQ	1122	0	1179	38	0
37	DQ	1122	0	1179	33	0
38	BR	968	0	1033	26	1
38	DR	968	0	1033	36	0
39	BS	877	0	938	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	DS	870	0	923	29	0
40	BT	1091	0	1151	37	0
40	DT	1083	0	1136	39	0
41	BU	959	0	1019	24	0
41	DU	959	0	1018	29	0
42	BV	771	0	830	21	1
42	DV	771	0	830	24	0
43	BW	886	0	940	15	0
43	DW	886	0	940	20	0
44	BX	750	0	814	24	0
44	DX	750	0	814	19	0
45	BY	806	0	881	24	0
45	DY	806	0	881	19	0
46	BZ	1349	0	1355	38	0
46	DZ	1360	0	1363	47	0
47	B0	653	0	674	20	0
47	D0	653	0	674	19	0
48	B1	755	0	826	19	0
48	D1	755	0	826	20	0
49	B2	588	0	643	8	0
49	D2	588	0	643	9	0
50	B3	469	0	518	15	0
50	D3	464	0	514	15	0
51	B4	552	0	533	32	0
51	D4	532	0	503	28	0
52	B5	455	0	465	8	0
52	D5	455	0	465	10	0
53	B6	453	0	473	13	0
53	D6	449	0	469	6	0
54	B7	418	0	467	19	0
54	D7	418	0	467	15	0
55	B8	511	0	571	29	0
55	D8	517	0	582	14	0
56	B9	307	0	335	8	0
56	D9	307	0	335	10	0
57	AA	207	0	0	0	0
57	AD	2	0	0	0	0
57	AE	2	0	0	0	0
57	AF	1	0	0	0	0
57	AJ	1	0	0	0	0
57	AK	1	0	0	0	0
57	AM	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	AN	2	0	0	0	0
57	AS	1	0	0	0	0
57	AV	1	0	0	0	0
57	AW	1	0	0	0	0
57	AX	11	0	0	0	0
57	B0	4	0	0	0	0
57	B1	1	0	0	0	0
57	B2	1	0	0	0	0
57	B3	2	0	0	0	0
57	B5	2	0	0	0	0
57	B7	3	0	0	0	0
57	B8	1	0	0	0	0
57	B9	1	0	0	0	0
57	BA	720	0	0	0	0
57	BB	20	0	0	0	0
57	BD	11	0	0	0	0
57	BE	7	0	0	0	0
57	BF	10	0	0	0	0
57	BG	2	0	0	0	0
57	BN	6	0	0	0	0
57	BO	1	0	0	0	0
57	BP	4	0	0	0	0
57	BQ	5	0	0	0	0
57	BR	3	0	0	0	0
57	BU	8	0	0	0	0
57	BV	4	0	0	0	0
57	BW	5	0	0	0	0
57	BX	1	0	0	0	0
57	BY	1	0	0	0	0
57	BZ	1	0	0	0	0
57	CA	160	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	CW	1	0	0	0	0
57	CX	2	0	0	0	0
57	D3	1	0	0	0	0
57	D5	1	0	0	0	0
57	D8	2	0	0	0	0
57	DA	629	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	DB	10	0	0	0	0
57	DD	7	0	0	0	0
57	DE	4	0	0	0	0
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	3	0	0	0	0
57	DR	2	0	0	0	0
57	DU	4	0	0	0	0
57	DV	2	0	0	0	0
57	DW	2	0	0	0	0
57	DY	1	0	0	0	0
58	AD	8	0	0	1	0
58	CD	8	0	0	1	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	170	0	0	16	0
61	AL	2	0	0	1	0
61	AO	1	0	0	0	0
61	AU	1	0	0	1	0
61	AV	2	0	0	0	0
61	AW	3	0	0	0	0
61	B0	4	0	0	0	0
61	B1	1	0	0	0	0
61	B3	1	0	0	0	0
61	B5	5	0	0	0	0
61	B7	1	0	0	1	0
61	B8	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	BA	1102	0	0	59	0
61	BB	36	0	0	1	0
61	BD	8	0	0	1	0
61	BE	13	0	0	5	0
61	BF	4	0	0	0	0
61	BG	3	0	0	0	0
61	BI	1	0	0	0	0
61	BP	15	0	0	1	0
61	BQ	3	0	0	0	0
61	BR	1	0	0	1	0
61	BS	1	0	0	0	0
61	BT	3	0	0	0	0
61	BU	1	0	0	1	0
61	BV	4	0	0	0	0
61	BW	2	0	0	0	0
61	BX	2	0	0	0	0
61	CA	130	0	0	8	0
61	CE	1	0	0	0	0
61	CJ	2	0	0	0	0
61	CN	1	0	0	0	0
61	CT	1	0	0	0	0
61	CV	1	0	0	0	0
61	CW	1	0	0	0	0
61	CX	1	0	0	1	0
61	D0	5	0	0	1	0
61	D1	1	0	0	0	0
61	D3	2	0	0	0	0
61	D7	1	0	0	0	0
61	D8	4	0	0	0	0
61	DA	767	0	0	55	0
61	DB	9	0	0	0	0
61	DD	9	0	0	3	0
61	DE	5	0	0	0	0
61	DF	6	0	0	0	0
61	DN	2	0	0	0	0
61	DP	12	0	0	3	0
61	DR	2	0	0	1	0
61	DT	1	0	0	0	0
61	DU	2	0	0	0	0
61	DV	1	0	0	1	0
61	DX	2	0	0	0	0
61	DY	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	290205	0	193125	6241	3

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

The worst 5 of 6241 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:CA:1002:G:H1	1:CA:1038:C:N4	1.48	1.11
26:DA:2121:G:H1	26:DA:2177:C:N4	1.52	1.06
1:AA:1164:G:N2	1:AA:1165:C:C5	2.24	1.06
1:CA:72:C:N4	1:CA:97:G:N1	2.04	1.05
26:DA:2139:C:N4	26:DA:2152:G:H1	1.55	1.04

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:AA:1043:C:O2'	26:DA:2137:C:O2'[2_655]	2.08	0.12
33:BI:89:TYR:O	1:CA:357:G:O2'[3_654]	2.10	0.10
38:BR:33:ARG:NH2	42:BV:53:GLU:OE2[4_445]	2.19	0.01

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%)	204 (89%)	21 (9%)	4 (2%)	14	42
2	CB	229/256 (90%)	204 (89%)	14 (6%)	11 (5%)	4	10
3	AC	204/239 (85%)	189 (93%)	13 (6%)	2 (1%)	22	60
3	CC	204/239 (85%)	188 (92%)	15 (7%)	1 (0%)	38	76
4	AD	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	38	76
4	CD	206/209 (99%)	196 (95%)	7 (3%)	3 (2%)	15	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	AE	146/162 (90%)	136 (93%)	9 (6%)	1 (1%)	30	69
5	CE	146/162 (90%)	135 (92%)	10 (7%)	1 (1%)	30	69
6	AF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
6	CF	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
7	AG	153/156 (98%)	143 (94%)	7 (5%)	3 (2%)	11	35
7	CG	153/156 (98%)	143 (94%)	9 (6%)	1 (1%)	30	69
8	AH	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
8	CH	135/138 (98%)	130 (96%)	4 (3%)	1 (1%)	30	69
9	AI	125/128 (98%)	118 (94%)	7 (6%)	0	100	100
9	CI	125/128 (98%)	118 (94%)	6 (5%)	1 (1%)	27	65
10	AJ	95/105 (90%)	83 (87%)	5 (5%)	7 (7%)	2	3
10	CJ	94/105 (90%)	83 (88%)	6 (6%)	5 (5%)	3	9
11	AK	112/129 (87%)	106 (95%)	5 (4%)	1 (1%)	25	63
11	CK	112/129 (87%)	105 (94%)	6 (5%)	1 (1%)	25	63
12	AL	120/132 (91%)	116 (97%)	4 (3%)	0	100	100
12	CL	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
13	AM	121/126 (96%)	113 (93%)	6 (5%)	2 (2%)	14	42
13	CM	120/126 (95%)	110 (92%)	9 (8%)	1 (1%)	27	65
14	AN	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
14	CN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
15	AO	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
15	CO	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
16	AP	80/88 (91%)	75 (94%)	5 (6%)	0	100	100
16	CP	80/88 (91%)	76 (95%)	4 (5%)	0	100	100
17	AQ	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
17	CQ	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
18	AR	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
18	CR	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
19	AS	81/93 (87%)	70 (86%)	11 (14%)	0	100	100
19	CS	81/93 (87%)	71 (88%)	8 (10%)	2 (2%)	9	28
20	AT	94/106 (89%)	85 (90%)	3 (3%)	6 (6%)	2	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	CT	94/106 (89%)	84 (89%)	6 (6%)	4 (4%)	4	13
21	AU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
21	CU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
28	BD	273/276 (99%)	263 (96%)	9 (3%)	1 (0%)	43	80
28	DD	273/276 (99%)	261 (96%)	10 (4%)	2 (1%)	30	69
29	BE	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	38	76
29	DE	202/206 (98%)	193 (96%)	7 (4%)	2 (1%)	22	60
30	BF	201/210 (96%)	197 (98%)	3 (2%)	1 (0%)	38	76
30	DF	201/210 (96%)	197 (98%)	2 (1%)	2 (1%)	22	60
31	BG	179/182 (98%)	166 (93%)	9 (5%)	4 (2%)	10	32
31	DG	179/182 (98%)	166 (93%)	9 (5%)	4 (2%)	10	32
32	BH	172/180 (96%)	161 (94%)	9 (5%)	2 (1%)	19	54
32	DH	172/180 (96%)	163 (95%)	7 (4%)	2 (1%)	19	54
33	BI	144/148 (97%)	132 (92%)	9 (6%)	3 (2%)	11	33
33	DI	144/148 (97%)	130 (90%)	12 (8%)	2 (1%)	16	49
34	BN	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
34	DN	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	30	69
35	BO	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	27	65
35	DO	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	27	65
36	BP	147/150 (98%)	138 (94%)	8 (5%)	1 (1%)	30	69
36	DP	147/150 (98%)	133 (90%)	13 (9%)	1 (1%)	30	69
37	BQ	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
37	DQ	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
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%)	4 (4%)	0	100	100
39	DS	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	25	63
40	BT	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
40	DT	129/146 (88%)	125 (97%)	3 (2%)	1 (1%)	27	65
41	BU	114/118 (97%)	114 (100%)	0	0	100	100
41	DU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	BV	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	22	60
42	DV	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	22	60
43	BW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
43	DW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
44	BX	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
44	DX	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
45	BY	105/110 (96%)	95 (90%)	10 (10%)	0	100	100
45	DY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
46	BZ	169/206 (82%)	148 (88%)	19 (11%)	2 (1%)	19	54
46	DZ	172/206 (84%)	156 (91%)	14 (8%)	2 (1%)	19	54
47	B0	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
47	D0	81/85 (95%)	77 (95%)	4 (5%)	0	100	100
48	B1	95/98 (97%)	94 (99%)	0	1 (1%)	21	57
48	D1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	21	57
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%)	55 (96%)	2 (4%)	0	100	100
50	D3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
51	B4	67/71 (94%)	54 (81%)	8 (12%)	5 (8%)	2	3
51	D4	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	2	6
52	B5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
52	D5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
53	B6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
53	D6	51/54 (94%)	50 (98%)	1 (2%)	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	32
55	B8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
55	D8	62/65 (95%)	61 (98%)	1 (2%)	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%)	10783 (94%)	516 (4%)	110 (1%)	22	60

5 of 110 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	231	GLU
4	AD	166	LYS
7	AG	80	VAL
10	AJ	55	LYS
20	AT	10	LEU

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%)	161 (84%)	31 (16%)	3	10
2	CB	187/220 (85%)	161 (86%)	26 (14%)	5	15
3	AC	143/188 (76%)	131 (92%)	12 (8%)	16	41
3	CC	140/188 (74%)	127 (91%)	13 (9%)	13	35
4	AD	170/181 (94%)	153 (90%)	17 (10%)	11	30
4	CD	173/181 (96%)	157 (91%)	16 (9%)	13	36
5	AE	113/123 (92%)	106 (94%)	7 (6%)	26	60
5	CE	114/123 (93%)	105 (92%)	9 (8%)	18	44
6	AF	83/90 (92%)	78 (94%)	5 (6%)	27	61
6	CF	85/90 (94%)	79 (93%)	6 (7%)	21	51
7	AG	119/127 (94%)	107 (90%)	12 (10%)	11	30
7	CG	120/127 (94%)	108 (90%)	12 (10%)	11	30
8	AH	114/119 (96%)	109 (96%)	5 (4%)	39	75
8	CH	114/119 (96%)	106 (93%)	8 (7%)	21	52
9	AI	90/99 (91%)	76 (84%)	14 (16%)	4	11
9	CI	89/99 (90%)	78 (88%)	11 (12%)	7	20
10	AJ	66/92 (72%)	60 (91%)	6 (9%)	14	37
10	CJ	69/92 (75%)	63 (91%)	6 (9%)	15	39
11	AK	82/99 (83%)	76 (93%)	6 (7%)	20	49
11	CK	83/99 (84%)	79 (95%)	4 (5%)	35	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	97/109 (89%)	91 (94%)	6 (6%)	26	60
12	CL	97/109 (89%)	94 (97%)	3 (3%)	52	86
13	AM	93/101 (92%)	82 (88%)	11 (12%)	8	22
13	CM	92/101 (91%)	81 (88%)	11 (12%)	7	21
14	AN	49/50 (98%)	43 (88%)	6 (12%)	7	20
14	CN	49/50 (98%)	43 (88%)	6 (12%)	7	20
15	AO	78/80 (98%)	66 (85%)	12 (15%)	4	12
15	CO	78/80 (98%)	70 (90%)	8 (10%)	10	28
16	AP	69/74 (93%)	60 (87%)	9 (13%)	6	17
16	CP	68/74 (92%)	62 (91%)	6 (9%)	14	38
17	AQ	94/97 (97%)	91 (97%)	3 (3%)	51	85
17	CQ	94/97 (97%)	87 (93%)	7 (7%)	20	48
18	AR	59/77 (77%)	54 (92%)	5 (8%)	15	41
18	CR	59/77 (77%)	54 (92%)	5 (8%)	15	41
19	AS	69/80 (86%)	61 (88%)	8 (12%)	8	23
19	CS	67/80 (84%)	62 (92%)	5 (8%)	19	47
20	AT	70/82 (85%)	60 (86%)	10 (14%)	5	14
20	CT	70/82 (85%)	63 (90%)	7 (10%)	11	30
21	AU	18/22 (82%)	16 (89%)	2 (11%)	9	25
21	CU	18/22 (82%)	17 (94%)	1 (6%)	30	64
28	BD	215/218 (99%)	201 (94%)	14 (6%)	24	57
28	DD	215/218 (99%)	200 (93%)	15 (7%)	21	52
29	BE	164/166 (99%)	144 (88%)	20 (12%)	7	20
29	DE	164/166 (99%)	147 (90%)	17 (10%)	10	28
30	BF	160/166 (96%)	145 (91%)	15 (9%)	13	34
30	DF	159/166 (96%)	146 (92%)	13 (8%)	17	43
31	BG	143/156 (92%)	128 (90%)	15 (10%)	10	27
31	DG	142/156 (91%)	122 (86%)	20 (14%)	5	14
32	BH	144/148 (97%)	138 (96%)	6 (4%)	40	77
32	DH	144/148 (97%)	132 (92%)	12 (8%)	16	42
33	BI	110/124 (89%)	90 (82%)	20 (18%)	2	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	DI	104/124 (84%)	87 (84%)	17 (16%)	3	10
34	BN	118/119 (99%)	103 (87%)	15 (13%)	6	19
34	DN	118/119 (99%)	108 (92%)	10 (8%)	15	41
35	BO	100/100 (100%)	94 (94%)	6 (6%)	27	61
35	DO	100/100 (100%)	96 (96%)	4 (4%)	42	79
36	BP	115/116 (99%)	105 (91%)	10 (9%)	15	39
36	DP	115/116 (99%)	103 (90%)	12 (10%)	10	28
37	BQ	111/111 (100%)	100 (90%)	11 (10%)	11	31
37	DQ	111/111 (100%)	100 (90%)	11 (10%)	11	31
38	BR	101/101 (100%)	82 (81%)	19 (19%)	2	7
38	DR	101/101 (100%)	84 (83%)	17 (17%)	3	9
39	BS	87/88 (99%)	79 (91%)	8 (9%)	13	36
39	DS	85/88 (97%)	75 (88%)	10 (12%)	8	22
40	BT	115/127 (91%)	106 (92%)	9 (8%)	18	45
40	DT	113/127 (89%)	103 (91%)	10 (9%)	14	38
41	BU	93/94 (99%)	86 (92%)	7 (8%)	19	47
41	DU	93/94 (99%)	88 (95%)	5 (5%)	31	66
42	BV	80/82 (98%)	68 (85%)	12 (15%)	4	12
42	DV	80/82 (98%)	72 (90%)	8 (10%)	11	30
43	BW	90/92 (98%)	84 (93%)	6 (7%)	23	55
43	DW	90/92 (98%)	82 (91%)	8 (9%)	14	38
44	BX	77/78 (99%)	74 (96%)	3 (4%)	43	80
44	DX	77/78 (99%)	72 (94%)	5 (6%)	24	57
45	BY	85/91 (93%)	77 (91%)	8 (9%)	13	34
45	DY	85/91 (93%)	78 (92%)	7 (8%)	17	43
46	BZ	145/179 (81%)	131 (90%)	14 (10%)	12	32
46	DZ	145/179 (81%)	127 (88%)	18 (12%)	7	20
47	B0	65/67 (97%)	62 (95%)	3 (5%)	37	73
47	D0	65/67 (97%)	62 (95%)	3 (5%)	37	73
48	B1	80/83 (96%)	72 (90%)	8 (10%)	11	30
48	D1	80/83 (96%)	73 (91%)	7 (9%)	14	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	B2	65/67 (97%)	56 (86%)	9 (14%)	5	15
49	D2	65/67 (97%)	59 (91%)	6 (9%)	13	36
50	B3	51/52 (98%)	45 (88%)	6 (12%)	8	22
50	D3	50/52 (96%)	47 (94%)	3 (6%)	27	61
51	B4	59/63 (94%)	47 (80%)	12 (20%)	2	5
51	D4	53/63 (84%)	46 (87%)	7 (13%)	6	16
52	B5	50/52 (96%)	48 (96%)	2 (4%)	42	79
52	D5	50/52 (96%)	48 (96%)	2 (4%)	42	79
53	B6	51/52 (98%)	44 (86%)	7 (14%)	5	15
53	D6	50/52 (96%)	48 (96%)	2 (4%)	42	79
54	B7	41/42 (98%)	38 (93%)	3 (7%)	20	49
54	D7	41/42 (98%)	38 (93%)	3 (7%)	20	49
55	B8	53/55 (96%)	49 (92%)	4 (8%)	19	47
55	D8	54/55 (98%)	53 (98%)	1 (2%)	69	94
56	B9	34/34 (100%)	31 (91%)	3 (9%)	14	38
56	D9	34/34 (100%)	33 (97%)	1 (3%)	55	88
All	All	9319/10066 (93%)	8433 (90%)	886 (10%)	12	33

5 of 886 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	BZ	136	PHE
3	CC	115	LEU
43	DW	51	LEU
48	B1	75	GLU
53	B6	28	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 129 such sidechains are listed below:

Mol	Chain	Res	Type
41	BU	117	GLN
2	CB	40	HIS
38	DR	71	GLN
45	BY	6	HIS
49	B2	48	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1495/1521 (98%)	407 (27%)	26 (1%)
1	CA	1501/1521 (98%)	413 (27%)	28 (1%)
22	AV	12/24 (50%)	7 (58%)	0
22	CV	5/24 (20%)	4 (80%)	0
23	AW	1/3 (33%)	0	0
23	CW	1/3 (33%)	0	0
24	AX	74/77 (96%)	26 (35%)	2 (2%)
24	CX	74/77 (96%)	31 (41%)	4 (5%)
25	AY	4/76 (5%)	1 (25%)	0
25	CY	4/76 (5%)	1 (25%)	0
26	BA	2811/2915 (96%)	529 (18%)	30 (1%)
26	DA	2791/2915 (95%)	595 (21%)	30 (1%)
27	BB	120/121 (99%)	16 (13%)	2 (1%)
27	DB	119/121 (98%)	31 (26%)	0
All	All	9012/9474 (95%)	2061 (22%)	122 (1%)

5 of 2061 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	7	G
1	AA	9	G
1	AA	15	G
1	AA	22	G

5 of 122 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	BA	2701	U
1	CA	509	A
26	DA	2104	G
26	BA	2769	U
1	CA	65	U

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PPU	AW	76	26,23	38,40,41	1.32	5 (13%)	54,57,60	2.32	15 (27%)
24	5MC	AX	32	24	20,22,23	1.68	4 (20%)	26,32,35	1.63	4 (15%)
24	5MU	AX	54	24	20,22,23	1.55	5 (25%)	25,32,35	2.35	4 (16%)
24	PSU	AX	55	24	19,21,22	1.85	4 (21%)	23,30,33	1.04	2 (8%)
24	31H	AX	76	24,57	30,32,35	1.15	3 (10%)	42,45,50	2.87	13 (30%)
24	4SU	AX	8	24	19,21,22	1.82	4 (21%)	23,30,33	34.02	2 (8%)
23	PPU	CW	76	26,23	38,40,41	1.26	5 (13%)	54,57,60	2.37	15 (27%)
24	5MC	CX	32	24	20,22,23	1.76	4 (20%)	26,32,35	1.46	4 (15%)
24	5MU	CX	54	24	20,22,23	1.54	4 (20%)	25,32,35	1.88	5 (20%)
24	PSU	CX	55	24	19,21,22	1.92	4 (21%)	23,30,33	1.07	3 (13%)
24	31H	CX	76	24,60,57	32,34,35	1.33	5 (15%)	44,47,50	2.56	10 (22%)
24	4SU	CX	8	24	19,21,22	1.87	4 (21%)	23,30,33	13.02	2 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PPU	AW	76	26,23	-	0/26/43/44	0/4/4/4
24	5MC	AX	32	24	-	0/6/25/26	0/2/2/2
24	5MU	AX	54	24	-	0/6/25/26	0/2/2/2
24	PSU	AX	55	24	-	0/8/25/26	0/2/2/2
24	31H	AX	76	24,57	-	0/20/37/41	0/3/3/3
24	4SU	AX	8	24	-	0/6/25/26	0/2/2/2
23	PPU	CW	76	26,23	-	0/26/43/44	0/4/4/4
24	5MC	CX	32	24	-	0/6/25/26	0/2/2/2
24	5MU	CX	54	24	-	0/6/25/26	0/2/2/2
24	PSU	CX	55	24	-	0/8/25/26	0/2/2/2
24	31H	CX	76	24,60,57	-	1/23/40/41	0/3/3/3
24	4SU	CX	8	24	-	0/6/25/26	0/2/2/2

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CX	32	5MC	C5-C4	4.62	1.48	1.41
24	CX	32	5MC	P-OP1	4.52	1.51	1.46
24	AX	32	5MC	C5-C4	4.47	1.48	1.41
24	CX	55	PSU	P-OP1	4.42	1.51	1.46
24	AX	55	PSU	P-OP1	4.36	1.51	1.46

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AX	8	4SU	C4-N3-C2	162.91	128.57	121.60
24	CX	8	4SU	C4-N3-C2	61.90	124.25	121.60
24	AX	76	31H	N3-C2-N1	-10.48	119.67	128.89
24	CX	76	31H	N3-C2-N1	-10.33	119.81	128.89
23	CW	76	PPU	C5-C4-N3	-8.77	117.43	125.98

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

5.5 Carbohydrates i

There are no carbohydrates in this entry.

5.6 Ligand geometry i

Of 1916 ligands modelled in this entry, 1914 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	302	4	12,12,12	21.81	12 (100%)	0,24,24	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	SF4	CD	501	4	12,12,12	21.37	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	302	4	-	0/0/48/48	0/6/5/5
58	SF4	CD	501	4	-	0/0/48/48	0/6/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	AD	302	SF4	S2-FE1	-22.57	2.18	2.33
58	CD	501	SF4	S3-FE1	-22.45	2.18	2.33
58	AD	302	SF4	S1-FE3	-22.26	2.18	2.33
58	AD	302	SF4	S2-FE4	-22.20	2.18	2.33
58	AD	302	SF4	S4-FE1	-22.09	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%)	0.45	34 (2%) 57 58	39, 73, 93, 105	0
1	CA	1503/1521 (98%)	0.42	60 (3%) 36 37	41, 75, 94, 106	0
2	AB	231/256 (90%)	0.29	10 (4%) 34 34	69, 82, 91, 101	0
2	CB	231/256 (90%)	2.37	120 (51%) 0 0	71, 84, 93, 101	0
3	AC	206/239 (86%)	0.57	14 (6%) 17 15	67, 79, 89, 95	0
3	CC	206/239 (86%)	2.05	86 (41%) 1 0	70, 81, 91, 95	0
4	AD	208/209 (99%)	0.44	8 (3%) 38 38	57, 74, 85, 91	0
4	CD	208/209 (99%)	0.62	15 (7%) 15 14	57, 75, 85, 92	0
5	AE	148/162 (91%)	0.43	5 (3%) 43 44	59, 71, 82, 90	0
5	CE	148/162 (91%)	0.95	27 (18%) 2 2	59, 73, 84, 91	0
6	AF	100/101 (99%)	0.55	6 (6%) 21 21	54, 69, 78, 83	0
6	CF	100/101 (99%)	0.36	8 (8%) 12 11	56, 71, 80, 83	0
7	AG	155/156 (99%)	0.49	16 (10%) 7 6	64, 76, 86, 92	0
7	CG	155/156 (99%)	1.13	30 (19%) 2 1	67, 78, 88, 92	0
8	AH	137/138 (99%)	0.52	11 (8%) 12 11	60, 72, 80, 85	0
8	CH	137/138 (99%)	1.29	33 (24%) 1 1	62, 74, 82, 85	0
9	AI	127/128 (99%)	1.06	26 (20%) 1 1	64, 83, 91, 96	0
9	CI	127/128 (99%)	1.60	43 (33%) 1 1	69, 84, 91, 98	0
10	AJ	97/105 (92%)	0.71	9 (9%) 9 7	66, 83, 92, 94	0
10	CJ	96/105 (91%)	1.87	45 (46%) 1 0	69, 85, 93, 94	0
11	AK	114/129 (88%)	0.67	10 (8%) 10 8	46, 70, 81, 85	0
11	CK	114/129 (88%)	0.33	6 (5%) 25 26	50, 71, 82, 85	0
12	AL	122/132 (92%)	0.44	3 (2%) 54 55	50, 64, 73, 81	0
12	CL	122/132 (92%)	0.55	9 (7%) 14 13	52, 65, 75, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)	Q<0.9
13	AM	123/126 (97%)	0.70	15 (12%) 5 4	58, 72, 83, 90	0
13	CM	122/126 (96%)	1.32	27 (22%) 1 1	72, 85, 93, 100	0
14	AN	60/61 (98%)	0.84	10 (16%) 2 2	65, 75, 81, 82	0
14	CN	60/61 (98%)	1.99	26 (43%) 1 0	69, 78, 83, 86	0
15	AO	88/89 (98%)	0.65	2 (2%) 57 58	54, 69, 81, 85	0
15	CO	88/89 (98%)	0.43	9 (10%) 7 6	53, 71, 82, 87	0
16	AP	82/88 (93%)	0.97	13 (15%) 3 2	59, 72, 82, 85	0
16	CP	82/88 (93%)	0.57	6 (7%) 15 13	57, 71, 81, 85	0
17	AQ	99/105 (94%)	0.58	2 (2%) 62 63	58, 71, 80, 83	0
17	CQ	99/105 (94%)	1.12	22 (22%) 1 1	56, 72, 81, 83	0
18	AR	68/88 (77%)	0.57	4 (5%) 22 21	59, 70, 80, 84	0
18	CR	68/88 (77%)	0.72	11 (16%) 2 2	60, 71, 82, 85	0
19	AS	83/93 (89%)	0.72	11 (13%) 4 3	72, 82, 89, 93	0
19	CS	83/93 (89%)	2.15	43 (51%) 0 0	73, 84, 91, 95	0
20	AT	96/106 (90%)	1.05	16 (16%) 2 2	60, 71, 83, 85	0
20	CT	96/106 (90%)	0.73	11 (11%) 5 4	56, 71, 83, 85	0
21	AU	23/27 (85%)	0.86	2 (8%) 10 9	69, 74, 79, 85	0
21	CU	23/27 (85%)	1.04	6 (26%) 1 1	71, 76, 84, 86	0
22	AV	13/24 (54%)	2.38	6 (46%) 1 0	56, 88, 93, 97	0
22	CV	6/24 (25%)	1.69	3 (50%) 0 0	59, 76, 95, 96	0
23	AW	3/3 (100%)	1.26	1 (33%) 1 1	28, 28, 30, 37	0
23	CW	3/3 (100%)	2.07	1 (33%) 1 1	42, 42, 50, 57	0
24	AX	75/77 (97%)	0.41	1 (1%) 74 75	27, 70, 84, 92	0
24	CX	75/77 (97%)	0.52	2 (2%) 52 52	30, 75, 86, 93	0
25	AY	5/76 (6%)	0.58	0 100 100	51, 76, 87, 94	0
25	CY	5/76 (6%)	2.05	3 (60%) 0 0	60, 79, 90, 91	0
26	BA	2819/2915 (96%)	0.43	55 (1%) 62 63	20, 42, 89, 107	0
26	DA	2800/2915 (96%)	0.15	79 (2%) 50 52	22, 46, 90, 107	0
27	BB	120/121 (99%)	0.33	0 100 100	37, 63, 77, 88	0
27	DB	120/121 (99%)	0.48	10 (8%) 11 10	42, 68, 80, 91	0
28	BD	275/276 (99%)	0.15	2 (0%) 84 85	21, 41, 58, 78	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DD	275/276 (99%)	-0.04	3 (1%) 77 78	23, 43, 61, 80	0
29	BE	204/206 (99%)	0.09	1 (0%) 88 90	21, 46, 65, 82	0
29	DE	204/206 (99%)	-0.17	2 (0%) 79 79	23, 48, 67, 84	0
30	BF	203/210 (96%)	0.14	2 (0%) 79 79	22, 51, 73, 87	0
30	DF	203/210 (96%)	0.03	5 (2%) 54 55	24, 54, 74, 86	0
31	BG	181/182 (99%)	0.15	4 (2%) 59 60	55, 70, 82, 93	0
31	DG	181/182 (99%)	1.16	40 (22%) 1 1	59, 74, 85, 93	0
32	BH	174/180 (96%)	0.14	3 (1%) 67 68	49, 65, 77, 81	0
32	DH	174/180 (96%)	1.03	32 (18%) 2 2	52, 70, 80, 84	0
33	BI	146/148 (98%)	0.75	17 (11%) 5 4	47, 81, 90, 95	0
33	DI	146/148 (98%)	3.02	79 (54%) 0 0	46, 84, 94, 99	0
34	BN	140/140 (100%)	0.22	2 (1%) 72 72	29, 49, 72, 82	0
34	DN	140/140 (100%)	-0.00	1 (0%) 84 85	33, 53, 74, 83	0
35	BO	122/122 (100%)	-0.04	0 100 100	26, 42, 61, 65	0
35	DO	122/122 (100%)	-0.01	1 (0%) 83 83	36, 57, 70, 79	0
36	BP	149/150 (99%)	0.39	4 (2%) 52 52	25, 52, 76, 85	0
36	DP	149/150 (99%)	0.41	8 (5%) 25 25	28, 54, 78, 86	0
37	BQ	141/141 (100%)	0.13	0 100 100	29, 51, 65, 78	0
37	DQ	141/141 (100%)	0.58	14 (9%) 8 6	31, 55, 69, 79	0
38	BR	118/118 (100%)	-0.11	0 100 100	23, 37, 56, 63	0
38	DR	118/118 (100%)	0.13	0 100 100	31, 50, 64, 71	0
39	BS	110/112 (98%)	0.01	1 (0%) 81 81	33, 51, 63, 76	0
39	DS	110/112 (98%)	0.58	9 (8%) 12 10	55, 76, 86, 89	0
40	BT	131/146 (89%)	-0.27	0 100 100	27, 44, 73, 86	0
40	DT	131/146 (89%)	0.13	3 (2%) 57 58	42, 59, 78, 86	0
41	BU	116/118 (98%)	-0.10	1 (0%) 81 81	18, 32, 52, 73	0
41	DU	116/118 (98%)	0.27	2 (1%) 67 68	37, 58, 75, 80	0
42	BV	101/101 (100%)	-0.10	1 (0%) 79 79	20, 43, 61, 76	0
42	DV	101/101 (100%)	0.79	12 (11%) 5 4	36, 67, 81, 87	0
43	BW	112/113 (99%)	-0.05	1 (0%) 81 81	20, 33, 51, 84	0
43	DW	112/113 (99%)	0.14	2 (1%) 65 66	32, 47, 65, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BX	95/96 (98%)	0.06	1 (1%) 77 78	22, 37, 57, 82	0
44	DX	95/96 (98%)	0.64	9 (9%) 8 7	39, 59, 73, 82	0
45	BY	107/110 (97%)	0.12	1 (0%) 81 81	32, 48, 70, 81	0
45	DY	107/110 (97%)	0.85	10 (9%) 9 7	48, 68, 78, 89	0
46	BZ	171/206 (83%)	0.39	3 (1%) 65 66	40, 63, 83, 88	0
46	DZ	174/206 (84%)	1.41	48 (27%) 1 1	64, 82, 94, 97	0
47	B0	83/85 (97%)	-0.03	0 100 100	23, 38, 52, 66	0
47	D0	83/85 (97%)	0.64	5 (6%) 21 21	36, 61, 72, 81	0
48	B1	97/98 (98%)	0.14	3 (3%) 47 47	21, 42, 65, 74	0
48	D1	97/98 (98%)	0.39	5 (5%) 26 26	30, 54, 76, 82	0
49	B2	70/72 (97%)	0.05	1 (1%) 72 72	32, 48, 63, 87	0
49	D2	70/72 (97%)	0.41	1 (1%) 72 72	50, 67, 78, 83	0
50	B3	59/60 (98%)	-0.17	1 (1%) 67 68	21, 37, 62, 81	0
50	D3	59/60 (98%)	0.85	5 (8%) 11 9	44, 60, 77, 87	0
51	B4	69/71 (97%)	0.40	8 (11%) 5 4	54, 76, 91, 98	0
51	D4	69/71 (97%)	0.97	14 (20%) 1 1	80, 90, 95, 99	0
52	B5	59/60 (98%)	-0.16	1 (1%) 67 68	19, 33, 53, 65	0
52	D5	59/60 (98%)	-0.08	0 100 100	28, 48, 69, 72	0
53	B6	53/54 (98%)	-0.24	0 100 100	28, 40, 60, 64	0
53	D6	53/54 (98%)	0.51	3 (5%) 23 23	43, 59, 72, 82	0
54	B7	48/49 (97%)	-0.08	2 (4%) 35 35	18, 25, 54, 63	0
54	D7	48/49 (97%)	-0.02	1 (2%) 60 61	29, 39, 63, 81	0
55	B8	64/65 (98%)	-0.06	1 (1%) 68 69	23, 32, 46, 61	0
55	D8	64/65 (98%)	0.56	2 (3%) 47 47	37, 55, 66, 70	0
56	B9	37/37 (100%)	0.49	1 (2%) 52 52	27, 49, 67, 71	0
56	D9	37/37 (100%)	1.08	6 (16%) 2 2	46, 54, 67, 74	0
All	All	20650/21602 (95%)	0.47	1415 (6%) 17 15	18, 63, 89, 107	0

The worst 5 of 1415 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
33	DI	65	ALA	12.8
33	DI	111	PRO	11.9

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Mol	Chain	Res	Type	RSRZ
33	DI	119	PRO	11.9
33	DI	146	ALA	11.8
13	CM	124	PRO	10.8

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	PPU	AW	76	37/38	0.18	-	12,29,37,42	0
24	5MC	CX	32	21/22	0.20	-	68,80,88,99	0
24	PSU	AX	55	20/21	0.15	-	58,70,77,82	0
24	PSU	CX	55	20/21	0.16	-	61,72,81,89	0
24	5MU	CX	54	21/22	0.14	-	71,79,92,107	0
24	5MC	AX	32	21/22	0.17	-	46,55,75,77	0
24	5MU	AX	54	21/22	0.16	-	57,67,82,96	0
24	4SU	AX	8	20/21	0.16	-	47,59,67,84	0
24	31H	AX	76	30/33	0.24	-	14,31,55,77	8
24	31H	CX	76	32/33	0.22	-	23,42,61,84	10
24	4SU	CX	8	20/21	0.17	-	61,80,93,118	0
23	PPU	CW	76	37/38	0.21	-	27,41,53,63	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	BA	3653	1/1	0.20	-	51,51,51,51	0
57	MG	BA	3534	1/1	0.27	-	23,23,23,23	0
57	MG	CA	3105	1/1	0.18	-	76,76,76,76	0
57	MG	BA	3007	1/1	0.10	-	39,39,39,39	0
57	MG	DA	3242	1/1	0.18	-	48,48,48,48	0
57	MG	BA	3556	1/1	0.16	-	52,52,52,52	0
57	MG	DA	3127	1/1	0.36	-	40,40,40,40	0
57	MG	BA	3606	1/1	0.16	-	39,39,39,39	0
57	MG	DA	3366	1/1	0.15	-	40,40,40,40	0
57	MG	DA	3074	1/1	0.17	-	38,38,38,38	0
57	MG	BU	201	1/1	0.10	-	36,36,36,36	0
57	MG	BA	3442	1/1	0.11	-	51,51,51,51	0
57	MG	DE	303	1/1	0.14	-	49,49,49,49	0
57	MG	DA	3247	1/1	0.11	-	43,43,43,43	0
57	MG	BQ	3004	1/1	0.24	-	35,35,35,35	0
57	MG	AA	3078	1/1	0.18	-	66,66,66,66	0
57	MG	B7	101	1/1	0.17	-	48,48,48,48	0
57	MG	BA	3364	1/1	0.19	-	37,37,37,37	0
57	MG	DA	3188	1/1	0.21	-	48,48,48,48	0
57	MG	DA	3202	1/1	0.38	-	41,41,41,41	0
57	MG	BA	3321	1/1	0.14	-	31,31,31,31	0
57	MG	AW	101	1/1	0.25	-	24,24,24,24	0
57	MG	DA	3563	1/1	0.10	-	55,55,55,55	0
59	ZN	B4	501	1/1	0.07	-	94,94,94,94	0
57	MG	CA	3098	1/1	0.07	-	76,76,76,76	0
57	MG	BA	3488	1/1	0.05	-	34,34,34,34	0
57	MG	BA	3420	1/1	0.11	-	23,23,23,23	0
57	MG	BA	3696	1/1	0.09	-	41,41,41,41	0
57	MG	DA	3156	1/1	0.14	-	46,46,46,46	0
57	MG	CA	3090	1/1	0.37	-	64,64,64,64	0
57	MG	BU	204	1/1	0.38	-	38,38,38,38	0
57	MG	BA	3657	1/1	0.11	-	55,55,55,55	0
57	MG	DA	3417	1/1	0.19	-	46,46,46,46	0
57	MG	DA	3621	1/1	0.38	-	61,61,61,61	0
57	MG	DA	3398	1/1	0.12	-	37,37,37,37	0
57	MG	CA	3003	1/1	0.12	-	74,74,74,74	0
57	MG	BF	309	1/1	0.42	-	61,61,61,61	0
57	MG	BA	3110	1/1	0.14	-	40,40,40,40	0
57	MG	DA	3322	1/1	0.17	-	51,51,51,51	0
57	MG	BA	3550	1/1	0.12	-	60,60,60,60	0
57	MG	BA	3313	1/1	0.15	-	30,30,30,30	0
57	MG	BA	3192	1/1	0.09	-	35,35,35,35	0
57	MG	BA	3602	1/1	0.34	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3382	1/1	0.22	-	20,20,20,20	0
57	MG	CA	3143	1/1	0.13	-	59,59,59,59	0
57	MG	DA	3338	1/1	0.12	-	36,36,36,36	0
57	MG	BA	3650	1/1	0.10	-	49,49,49,49	0
57	MG	BA	3059	1/1	0.21	-	50,50,50,50	0
57	MG	BA	3609	1/1	0.13	-	47,47,47,47	0
57	MG	DA	3261	1/1	0.22	-	38,38,38,38	0
57	MG	BD	308	1/1	0.28	-	41,41,41,41	0
57	MG	BA	3342	1/1	0.19	-	38,38,38,38	0
57	MG	BQ	3002	1/1	0.27	-	39,39,39,39	0
57	MG	AA	3029	1/1	0.06	-	42,42,42,42	0
57	MG	DA	3050	1/1	0.13	-	48,48,48,48	0
57	MG	AA	3049	1/1	0.17	-	43,43,43,43	0
57	MG	DA	3001	1/1	0.35	-	45,45,45,45	0
57	MG	BA	3572	1/1	0.19	-	27,27,27,27	0
57	MG	DA	3056	1/1	0.08	-	35,35,35,35	0
57	MG	BA	3642	1/1	0.17	-	50,50,50,50	0
57	MG	DA	3350	1/1	0.35	-	44,44,44,44	0
57	MG	BA	3438	1/1	0.14	-	19,19,19,19	0
57	MG	DA	3390	1/1	0.19	-	54,54,54,54	0
57	MG	BP	3002	1/1	0.25	-	32,32,32,32	0
57	MG	AA	3150	1/1	0.09	-	65,65,65,65	0
57	MG	DA	3118	1/1	0.11	-	46,46,46,46	0
57	MG	CA	3141	1/1	0.16	-	69,69,69,69	0
57	MG	DA	3133	1/1	0.10	-	52,52,52,52	0
57	MG	AA	3117	1/1	0.13	-	55,55,55,55	0
57	MG	DA	3267	1/1	0.25	-	45,45,45,45	0
57	MG	BE	3002	1/1	0.46	-	50,50,50,50	0
57	MG	BA	3227	1/1	0.16	-	39,39,39,39	0
57	MG	DA	3046	1/1	0.30	-	50,50,50,50	0
57	MG	DA	3405	1/1	0.06	-	45,45,45,45	0
57	MG	AA	3038	1/1	0.22	-	58,58,58,58	0
57	MG	DA	3274	1/1	0.21	-	45,45,45,45	0
57	MG	CA	3001	1/1	0.09	-	53,53,53,53	0
57	MG	BA	3400	1/1	0.20	-	33,33,33,33	0
57	MG	BA	3473	1/1	0.15	-	31,31,31,31	0
57	MG	DA	3558	1/1	0.08	-	45,45,45,45	0
57	MG	DA	3210	1/1	0.37	-	57,57,57,57	0
57	MG	DA	3250	1/1	0.15	-	41,41,41,41	0
57	MG	BE	3007	1/1	0.08	-	31,31,31,31	0
57	MG	BA	3132	1/1	0.17	-	52,52,52,52	0
57	MG	BA	3369	1/1	0.14	-	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	AA	3101	1/1	0.19	-	53,53,53,53	0
57	MG	BA	3510	1/1	0.23	-	20,20,20,20	0
57	MG	DA	3079	1/1	0.16	-	41,41,41,41	0
57	MG	BA	3112	1/1	0.23	-	58,58,58,58	0
57	MG	BA	3171	1/1	0.38	-	44,44,44,44	0
57	MG	BA	3168	1/1	0.16	-	32,32,32,32	0
57	MG	BA	3390	1/1	0.09	-	31,31,31,31	0
57	MG	DA	3280	1/1	0.18	-	49,49,49,49	0
57	MG	DA	3071	1/1	0.11	-	42,42,42,42	0
57	MG	DA	3302	1/1	0.17	-	30,30,30,30	0
57	MG	DA	3377	1/1	0.15	-	31,31,31,31	0
57	MG	CA	3072	1/1	0.25	-	38,38,38,38	0
57	MG	BA	3559	1/1	0.16	-	36,36,36,36	0
57	MG	DA	3301	1/1	0.10	-	54,54,54,54	0
57	MG	DE	304	1/1	0.11	-	47,47,47,47	0
57	MG	AA	3153	1/1	0.08	-	46,46,46,46	0
57	MG	DA	3422	1/1	0.25	-	40,40,40,40	0
57	MG	AX	3008	1/1	0.12	-	58,58,58,58	0
57	MG	BA	3081	1/1	0.12	-	26,26,26,26	0
57	MG	DA	3282	1/1	0.19	-	36,36,36,36	0
57	MG	DR	3001	1/1	1.33	-	66,66,66,66	0
57	MG	BA	3015	1/1	0.14	-	50,50,50,50	0
57	MG	BA	3700	1/1	0.18	-	69,69,69,69	0
57	MG	BA	3099	1/1	0.29	-	36,36,36,36	0
57	MG	AA	3170	1/1	0.15	-	70,70,70,70	0
57	MG	BA	3526	1/1	0.16	-	48,48,48,48	0
57	MG	BA	3506	1/1	0.12	-	39,39,39,39	0
57	MG	DA	3168	1/1	0.30	-	50,50,50,50	0
60	K	CX	3001	1/1	0.09	-	54,54,54,54	0
57	MG	DA	3317	1/1	0.19	-	42,42,42,42	0
57	MG	BA	3056	1/1	0.18	-	21,21,21,21	0
57	MG	BA	3065	1/1	0.23	-	43,43,43,43	0
57	MG	DA	3227	1/1	0.13	-	57,57,57,57	0
57	MG	DA	3506	1/1	0.19	-	38,38,38,38	0
57	MG	BA	3437	1/1	0.20	-	52,52,52,52	0
57	MG	DA	3311	1/1	0.19	-	42,42,42,42	0
57	MG	BA	3174	1/1	0.15	-	44,44,44,44	0
57	MG	BA	3547	1/1	0.18	-	33,33,33,33	0
57	MG	DA	3622	1/1	1.14	-	58,58,58,58	0
57	MG	BA	3360	1/1	0.17	-	60,60,60,60	0
57	MG	CA	3037	1/1	0.17	-	60,60,60,60	0
57	MG	AA	3041	1/1	0.20	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3049	1/1	0.23	-	53,53,53,53	0
57	MG	BA	3374	1/1	0.14	-	48,48,48,48	0
57	MG	DA	3096	1/1	0.22	-	52,52,52,52	0
57	MG	BA	3298	1/1	0.20	-	50,50,50,50	0
57	MG	AA	3172	1/1	0.25	-	54,54,54,54	0
57	MG	DA	3076	1/1	0.17	-	53,53,53,53	0
57	MG	BA	3604	1/1	0.10	-	62,62,62,62	0
57	MG	AA	3070	1/1	0.23	-	43,43,43,43	0
57	MG	BA	3493	1/1	0.12	-	39,39,39,39	0
57	MG	DA	3262	1/1	0.07	-	39,39,39,39	0
57	MG	B8	101	1/1	0.12	-	34,34,34,34	0
57	MG	BA	3291	1/1	0.15	-	44,44,44,44	0
57	MG	DA	3061	1/1	0.26	-	36,36,36,36	0
57	MG	DA	3514	1/1	0.19	-	34,34,34,34	0
57	MG	CA	3006	1/1	0.11	-	43,43,43,43	0
57	MG	CA	3122	1/1	0.09	-	50,50,50,50	0
57	MG	DA	3605	1/1	0.09	-	64,64,64,64	0
57	MG	BA	3521	1/1	0.27	-	32,32,32,32	0
57	MG	BA	3209	1/1	0.24	-	32,32,32,32	0
57	MG	BA	3119	1/1	0.21	-	41,41,41,41	0
57	MG	BA	3594	1/1	0.11	-	34,34,34,34	0
57	MG	BA	3317	1/1	0.14	-	49,49,49,49	0
57	MG	DA	3528	1/1	0.11	-	60,60,60,60	0
57	MG	BA	3410	1/1	0.17	-	40,40,40,40	0
57	MG	DA	3440	1/1	0.26	-	44,44,44,44	0
57	MG	DA	3197	1/1	0.13	-	35,35,35,35	0
57	MG	DA	3332	1/1	0.10	-	52,52,52,52	0
57	MG	CA	3032	1/1	0.40	-	58,58,58,58	0
57	MG	DA	3490	1/1	0.07	-	62,62,62,62	0
57	MG	DA	3208	1/1	0.16	-	50,50,50,50	0
57	MG	BA	3586	1/1	0.08	-	33,33,33,33	0
57	MG	BA	3164	1/1	0.22	-	44,44,44,44	0
57	MG	DA	3566	1/1	0.08	-	40,40,40,40	0
57	MG	DD	307	1/1	0.12	-	50,50,50,50	0
57	MG	DA	3434	1/1	0.09	-	48,48,48,48	0
57	MG	AA	3081	1/1	0.07	-	44,44,44,44	0
57	MG	CA	3114	1/1	0.23	-	96,96,96,96	0
57	MG	BA	3228	1/1	0.24	-	33,33,33,33	0
57	MG	CA	3139	1/1	0.10	-	82,82,82,82	0
57	MG	AA	3136	1/1	0.12	-	43,43,43,43	0
57	MG	BA	3117	1/1	0.14	-	24,24,24,24	0
57	MG	BA	3472	1/1	0.10	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3058	1/1	0.16	-	47,47,47,47	0
57	MG	BA	3098	1/1	0.57	-	50,50,50,50	0
57	MG	BA	3674	1/1	0.19	-	59,59,59,59	0
57	MG	BA	3661	1/1	0.18	-	56,56,56,56	0
57	MG	DA	3095	1/1	0.23	-	45,45,45,45	0
57	MG	DU	3003	1/1	0.18	-	60,60,60,60	0
57	MG	DA	3002	1/1	0.31	-	44,44,44,44	0
57	MG	AA	3182	1/1	0.13	-	40,40,40,40	0
57	MG	D8	101	1/1	0.17	-	60,60,60,60	0
57	MG	DA	3143	1/1	0.17	-	47,47,47,47	0
57	MG	DA	3077	1/1	0.17	-	58,58,58,58	0
57	MG	BA	3045	1/1	0.16	-	33,33,33,33	0
57	MG	DB	3004	1/1	0.12	-	38,38,38,38	0
57	MG	BA	3308	1/1	0.14	-	14,14,14,14	0
57	MG	DA	3152	1/1	0.19	-	38,38,38,38	0
57	MG	DA	3425	1/1	0.12	-	40,40,40,40	0
57	MG	BA	3019	1/1	0.12	-	30,30,30,30	0
57	MG	DA	3290	1/1	0.11	-	43,43,43,43	0
57	MG	DA	3629	1/1	0.27	-	40,40,40,40	0
57	MG	AX	3009	1/1	0.10	-	50,50,50,50	0
57	MG	AA	3096	1/1	0.05	-	57,57,57,57	0
57	MG	BA	3536	1/1	0.11	-	42,42,42,42	0
57	MG	DA	3333	1/1	0.09	-	41,41,41,41	0
57	MG	CA	3052	1/1	0.07	-	61,61,61,61	0
57	MG	BA	3412	1/1	0.37	-	44,44,44,44	0
57	MG	BA	3454	1/1	0.14	-	45,45,45,45	0
57	MG	DA	3044	1/1	0.16	-	38,38,38,38	0
57	MG	BA	3273	1/1	0.17	-	30,30,30,30	0
57	MG	CA	3091	1/1	0.18	-	75,75,75,75	0
57	MG	BA	3421	1/1	0.16	-	29,29,29,29	0
57	MG	DA	3120	1/1	0.25	-	55,55,55,55	0
57	MG	CA	3021	1/1	0.15	-	46,46,46,46	0
57	MG	DA	3124	1/1	0.21	-	30,30,30,30	0
57	MG	BA	3244	1/1	0.35	-	29,29,29,29	0
57	MG	BA	3134	1/1	0.23	-	43,43,43,43	0
57	MG	CA	3041	1/1	0.13	-	62,62,62,62	0
57	MG	BA	3675	1/1	0.11	-	41,41,41,41	0
57	MG	DA	3059	1/1	0.14	-	60,60,60,60	0
57	MG	BA	3302	1/1	0.13	-	50,50,50,50	0
57	MG	BA	3334	1/1	0.17	-	37,37,37,37	0
57	MG	BA	3618	1/1	0.11	-	64,64,64,64	0
57	MG	AA	3006	1/1	0.08	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3300	1/1	0.12	-	38,38,38,38	0
57	MG	BA	3250	1/1	0.15	-	47,47,47,47	0
57	MG	BA	3397	1/1	0.11	-	33,33,33,33	0
57	MG	AA	3185	1/1	0.13	-	50,50,50,50	0
57	MG	DA	3591	1/1	0.08	-	69,69,69,69	0
57	MG	BA	3596	1/1	0.12	-	56,56,56,56	0
57	MG	DA	3245	1/1	0.13	-	46,46,46,46	0
57	MG	BA	3565	1/1	0.11	-	50,50,50,50	0
57	MG	BA	3557	1/1	0.15	-	35,35,35,35	0
57	MG	DA	3099	1/1	0.13	-	40,40,40,40	0
57	MG	DA	3330	1/1	0.14	-	49,49,49,49	0
57	MG	BA	3038	1/1	0.08	-	38,38,38,38	0
57	MG	BA	3484	1/1	0.07	-	50,50,50,50	0
59	ZN	DY	501	1/1	0.10	-	88,88,88,88	0
57	MG	BB	3012	1/1	0.15	-	33,33,33,33	0
57	MG	BF	310	1/1	0.13	-	51,51,51,51	0
57	MG	BA	3142	1/1	0.17	-	35,35,35,35	0
57	MG	BD	302	1/1	0.22	-	38,38,38,38	0
57	MG	AA	3002	1/1	0.10	-	58,58,58,58	0
57	MG	CA	3124	1/1	0.18	-	57,57,57,57	0
57	MG	BA	3677	1/1	0.24	-	30,30,30,30	0
57	MG	BA	3451	1/1	0.17	-	59,59,59,59	0
57	MG	BQ	3003	1/1	0.60	-	68,68,68,68	0
57	MG	DA	3572	1/1	0.15	-	46,46,46,46	0
57	MG	BN	3002	1/1	0.26	-	46,46,46,46	0
57	MG	DA	3387	1/1	0.16	-	29,29,29,29	0
57	MG	BA	3293	1/1	0.14	-	43,43,43,43	0
57	MG	DA	3198	1/1	0.06	-	41,41,41,41	0
57	MG	BA	3341	1/1	0.08	-	52,52,52,52	0
57	MG	DA	3473	1/1	0.20	-	32,32,32,32	0
57	MG	DD	305	1/1	0.43	-	48,48,48,48	0
57	MG	BA	3431	1/1	0.20	-	25,25,25,25	0
57	MG	AA	3005	1/1	0.14	-	66,66,66,66	0
57	MG	BA	3079	1/1	0.24	-	55,55,55,55	0
57	MG	AX	3006	1/1	0.24	-	59,59,59,59	0
57	MG	BA	3491	1/1	0.16	-	33,33,33,33	0
57	MG	BA	3304	1/1	0.25	-	49,49,49,49	0
57	MG	DA	3540	1/1	0.07	-	43,43,43,43	0
57	MG	DA	3423	1/1	0.20	-	33,33,33,33	0
57	MG	BA	3085	1/1	0.14	-	18,18,18,18	0
57	MG	DA	3170	1/1	0.37	-	47,47,47,47	0
57	MG	CA	3062	1/1	0.09	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	3084	1/1	0.14	-	43,43,43,43	0
57	MG	DW	202	1/1	0.14	-	43,43,43,43	0
57	MG	AA	3175	1/1	0.31	-	61,61,61,61	0
57	MG	DA	3293	1/1	0.18	-	41,41,41,41	0
57	MG	DA	3511	1/1	0.13	-	40,40,40,40	0
57	MG	DA	3522	1/1	0.15	-	41,41,41,41	0
57	MG	DA	3515	1/1	0.16	-	53,53,53,53	0
57	MG	DA	3166	1/1	0.17	-	47,47,47,47	0
57	MG	BA	3071	1/1	0.19	-	48,48,48,48	0
57	MG	AA	3062	1/1	0.18	-	57,57,57,57	0
57	MG	BA	3562	1/1	0.15	-	47,47,47,47	0
57	MG	AA	3089	1/1	0.22	-	61,61,61,61	0
57	MG	BA	3579	1/1	0.31	-	44,44,44,44	0
57	MG	BV	202	1/1	0.20	-	29,29,29,29	0
57	MG	AA	3022	1/1	0.06	-	57,57,57,57	0
57	MG	DA	3005	1/1	0.17	-	29,29,29,29	0
57	MG	CA	3157	1/1	0.09	-	61,61,61,61	0
57	MG	BG	3001	1/1	0.19	-	44,44,44,44	0
57	MG	CA	3018	1/1	0.11	-	47,47,47,47	0
57	MG	DA	3237	1/1	0.27	-	41,41,41,41	0
57	MG	BA	3357	1/1	0.17	-	31,31,31,31	0
57	MG	DA	3268	1/1	0.10	-	35,35,35,35	0
57	MG	BA	3091	1/1	0.22	-	56,56,56,56	0
57	MG	AX	3003	1/1	0.34	-	66,66,66,66	0
57	MG	DA	3134	1/1	0.15	-	59,59,59,59	0
57	MG	BA	3057	1/1	0.17	-	21,21,21,21	0
57	MG	DA	3371	1/1	0.20	-	47,47,47,47	0
57	MG	DA	3608	1/1	0.12	-	61,61,61,61	0
57	MG	AA	3138	1/1	0.19	-	40,40,40,40	0
57	MG	DA	3243	1/1	0.26	-	41,41,41,41	0
57	MG	AA	3013	1/1	0.10	-	53,53,53,53	0
57	MG	BA	3666	1/1	0.17	-	79,79,79,79	0
57	MG	DA	3459	1/1	0.42	-	40,40,40,40	0
57	MG	AA	3093	1/1	0.17	-	56,56,56,56	0
57	MG	DA	3386	1/1	0.20	-	39,39,39,39	0
57	MG	DA	3173	1/1	0.32	-	42,42,42,42	0
57	MG	CA	3100	1/1	0.17	-	48,48,48,48	0
57	MG	BA	3447	1/1	0.12	-	44,44,44,44	0
57	MG	BA	3197	1/1	0.15	-	32,32,32,32	0
57	MG	DA	3344	1/1	0.12	-	42,42,42,42	0
57	MG	BA	3222	1/1	0.17	-	52,52,52,52	0
57	MG	DA	3414	1/1	0.12	-	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	3441	1/1	0.10	-	56,56,56,56	0
57	MG	AA	3173	1/1	0.14	-	53,53,53,53	0
57	MG	BA	3508	1/1	0.19	-	52,52,52,52	0
57	MG	DA	3579	1/1	0.21	-	58,58,58,58	0
59	ZN	CN	501	1/1	0.07	-	101,101,101,101	0
57	MG	CA	3107	1/1	0.22	-	89,89,89,89	0
57	MG	CA	3118	1/1	0.14	-	69,69,69,69	0
57	MG	BA	3223	1/1	0.14	-	38,38,38,38	0
57	MG	DA	3385	1/1	0.08	-	47,47,47,47	0
57	MG	BA	3348	1/1	0.11	-	17,17,17,17	0
57	MG	BA	3430	1/1	0.15	-	54,54,54,54	0
57	MG	BA	3564	1/1	0.13	-	44,44,44,44	0
57	MG	BA	3485	1/1	0.10	-	40,40,40,40	0
57	MG	DA	3614	1/1	0.40	-	56,56,56,56	0
57	MG	BA	3270	1/1	0.37	-	47,47,47,47	0
57	MG	BA	3563	1/1	0.10	-	38,38,38,38	0
57	MG	DA	3298	1/1	0.10	-	35,35,35,35	0
57	MG	BA	3141	1/1	0.17	-	38,38,38,38	0
57	MG	DA	3189	1/1	0.20	-	57,57,57,57	0
57	MG	CA	3127	1/1	0.29	-	76,76,76,76	0
57	MG	DA	3110	1/1	0.12	-	60,60,60,60	0
57	MG	DA	3509	1/1	0.29	-	42,42,42,42	0
57	MG	BA	3051	1/1	0.17	-	36,36,36,36	0
57	MG	BA	3624	1/1	0.09	-	26,26,26,26	0
57	MG	BA	3709	1/1	0.39	-	45,45,45,45	0
57	MG	BA	3494	1/1	0.21	-	30,30,30,30	0
57	MG	DA	3487	1/1	0.09	-	44,44,44,44	0
57	MG	DA	3543	1/1	0.15	-	61,61,61,61	0
57	MG	DA	3607	1/1	0.22	-	73,73,73,73	0
57	MG	BA	3414	1/1	0.19	-	59,59,59,59	0
57	MG	DA	3264	1/1	0.09	-	33,33,33,33	0
57	MG	CA	3138	1/1	0.15	-	66,66,66,66	0
57	MG	DA	3328	1/1	0.14	-	66,66,66,66	0
57	MG	CA	3017	1/1	0.30	-	69,69,69,69	0
57	MG	DA	3199	1/1	0.08	-	41,41,41,41	0
57	MG	DA	3620	1/1	0.14	-	47,47,47,47	0
57	MG	DA	3373	1/1	0.20	-	43,43,43,43	0
57	MG	DA	3451	1/1	0.20	-	39,39,39,39	0
57	MG	DA	3138	1/1	0.19	-	39,39,39,39	0
57	MG	DA	3383	1/1	0.14	-	45,45,45,45	0
57	MG	BA	3220	1/1	0.22	-	54,54,54,54	0
57	MG	BA	3509	1/1	0.31	-	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	3478	1/1	0.15	-	22,22,22,22	0
57	MG	DA	3445	1/1	0.10	-	59,59,59,59	0
57	MG	DA	3393	1/1	0.12	-	41,41,41,41	0
57	MG	CA	3094	1/1	0.10	-	80,80,80,80	0
57	MG	DA	3356	1/1	0.20	-	53,53,53,53	0
57	MG	AA	3073	1/1	0.14	-	59,59,59,59	0
57	MG	B2	3001	1/1	0.10	-	43,43,43,43	0
57	MG	CA	3075	1/1	0.14	-	48,48,48,48	0
57	MG	BA	3662	1/1	0.24	-	62,62,62,62	0
57	MG	DA	3438	1/1	0.13	-	42,42,42,42	0
57	MG	BA	3165	1/1	0.20	-	34,34,34,34	0
57	MG	CA	3020	1/1	0.14	-	51,51,51,51	0
57	MG	DA	3265	1/1	0.14	-	33,33,33,33	0
57	MG	DW	201	1/1	0.18	-	70,70,70,70	0
57	MG	BA	3585	1/1	0.15	-	45,45,45,45	0
57	MG	BA	3468	1/1	0.11	-	42,42,42,42	0
57	MG	DA	3027	1/1	0.20	-	42,42,42,42	0
57	MG	DA	3132	1/1	0.12	-	53,53,53,53	0
57	MG	DA	3450	1/1	0.16	-	34,34,34,34	0
57	MG	DA	3113	1/1	0.21	-	42,42,42,42	0
57	MG	BA	3009	1/1	0.08	-	34,34,34,34	0
57	MG	DA	3049	1/1	0.14	-	46,46,46,46	0
57	MG	AA	3127	1/1	0.28	-	73,73,73,73	0
57	MG	DA	3349	1/1	0.16	-	35,35,35,35	0
57	MG	BA	3131	1/1	0.38	-	31,31,31,31	0
57	MG	BA	3629	1/1	0.19	-	37,37,37,37	0
57	MG	BA	3318	1/1	0.15	-	39,39,39,39	0
57	MG	BA	3537	1/1	0.17	-	35,35,35,35	0
57	MG	CA	3040	1/1	0.19	-	67,67,67,67	0
57	MG	AA	3094	1/1	0.15	-	54,54,54,54	0
57	MG	DA	3618	1/1	0.15	-	46,46,46,46	0
57	MG	AA	3151	1/1	0.16	-	72,72,72,72	0
57	MG	BA	3282	1/1	0.08	-	44,44,44,44	0
57	MG	DA	3072	1/1	0.30	-	46,46,46,46	0
57	MG	BA	3530	1/1	0.25	-	20,20,20,20	0
57	MG	DA	3070	1/1	0.19	-	35,35,35,35	0
57	MG	BA	3416	1/1	0.13	-	73,73,73,73	0
57	MG	CA	3044	1/1	0.19	-	59,59,59,59	0
57	MG	AA	3035	1/1	0.32	-	52,52,52,52	0
57	MG	DA	3130	1/1	0.21	-	55,55,55,55	0
57	MG	DA	3200	1/1	0.14	-	38,38,38,38	0
57	MG	DA	3289	1/1	0.23	-	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	3291	1/1	0.21	-	56,56,56,56	0
57	MG	DA	3628	1/1	0.56	-	59,59,59,59	0
57	MG	BA	3047	1/1	0.20	-	44,44,44,44	0
57	MG	BA	3242	1/1	0.22	-	45,45,45,45	0
57	MG	BA	3492	1/1	0.18	-	30,30,30,30	0
57	MG	DA	3088	1/1	0.17	-	41,41,41,41	0
57	MG	DA	3533	1/1	0.56	-	47,47,47,47	0
57	MG	BA	3645	1/1	0.13	-	43,43,43,43	0
57	MG	DA	3553	1/1	0.37	-	75,75,75,75	0
57	MG	AA	3111	1/1	0.12	-	70,70,70,70	0
57	MG	AA	3120	1/1	0.08	-	53,53,53,53	0
57	MG	BA	3685	1/1	0.14	-	40,40,40,40	0
57	MG	BA	3542	1/1	0.12	-	40,40,40,40	0
57	MG	AA	3122	1/1	0.11	-	52,52,52,52	0
57	MG	CA	3045	1/1	0.11	-	53,53,53,53	0
57	MG	AA	3063	1/1	0.12	-	89,89,89,89	0
57	MG	DA	3400	1/1	0.12	-	33,33,33,33	0
57	MG	BA	3125	1/1	0.36	-	30,30,30,30	0
57	MG	BA	3358	1/1	0.07	-	35,35,35,35	0
57	MG	DA	3191	1/1	0.10	-	54,54,54,54	0
57	MG	CA	3147	1/1	0.12	-	56,56,56,56	0
57	MG	CT	3001	1/1	0.07	-	59,59,59,59	0
57	MG	CA	3129	1/1	0.21	-	83,83,83,83	0
57	MG	DA	3083	1/1	0.22	-	30,30,30,30	0
57	MG	BA	3225	1/1	0.08	-	45,45,45,45	0
57	MG	DA	3278	1/1	0.08	-	38,38,38,38	0
57	MG	BA	3654	1/1	0.14	-	42,42,42,42	0
57	MG	DA	3570	1/1	0.17	-	28,28,28,28	0
57	MG	BA	3424	1/1	0.20	-	29,29,29,29	0
57	MG	CA	3120	1/1	0.24	-	72,72,72,72	0
57	MG	DA	3430	1/1	0.21	-	26,26,26,26	0
57	MG	DA	3521	1/1	0.10	-	57,57,57,57	0
57	MG	BA	3383	1/1	0.12	-	37,37,37,37	0
57	MG	BA	3576	1/1	0.25	-	29,29,29,29	0
57	MG	DA	3180	1/1	0.31	-	41,41,41,41	0
57	MG	DA	3325	1/1	0.10	-	43,43,43,43	0
57	MG	DA	3310	1/1	0.18	-	43,43,43,43	0
57	MG	DO	5001	1/1	0.15	-	53,53,53,53	0
57	MG	DA	3391	1/1	0.16	-	39,39,39,39	0
57	MG	BA	3701	1/1	0.18	-	17,17,17,17	0
57	MG	B0	101	1/1	0.10	-	33,33,33,33	0
57	MG	BA	3311	1/1	0.06	-	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	CA	3081	1/1	0.12	-	67,67,67,67	0
57	MG	CA	3111	1/1	0.08	-	65,65,65,65	0
57	MG	DA	3097	1/1	0.13	-	50,50,50,50	0
57	MG	AA	3113	1/1	0.29	-	54,54,54,54	0
57	MG	CA	3068	1/1	0.07	-	53,53,53,53	0
57	MG	BA	3118	1/1	0.24	-	28,28,28,28	0
57	MG	CA	3155	1/1	0.14	-	66,66,66,66	0
57	MG	BN	3006	1/1	0.61	-	47,47,47,47	0
57	MG	BA	3356	1/1	0.11	-	36,36,36,36	0
57	MG	CA	3028	1/1	0.27	-	57,57,57,57	0
57	MG	BA	3102	1/1	0.21	-	43,43,43,43	0
57	MG	DD	302	1/1	0.15	-	50,50,50,50	0
57	MG	CA	3096	1/1	0.16	-	51,51,51,51	0
57	MG	DA	3335	1/1	0.11	-	48,48,48,48	0
57	MG	DA	3054	1/1	0.16	-	40,40,40,40	0
57	MG	CA	3026	1/1	0.11	-	59,59,59,59	0
57	MG	BA	3444	1/1	0.18	-	32,32,32,32	0
57	MG	BA	3215	1/1	0.10	-	53,53,53,53	0
57	MG	DA	3397	1/1	0.07	-	46,46,46,46	0
57	MG	DA	3252	1/1	0.11	-	63,63,63,63	0
57	MG	BA	3608	1/1	0.09	-	50,50,50,50	0
57	MG	DA	3559	1/1	0.21	-	31,31,31,31	0
57	MG	AA	3007	1/1	0.18	-	47,47,47,47	0
57	MG	AA	3050	1/1	0.20	-	49,49,49,49	0
57	MG	BA	3616	1/1	0.18	-	32,32,32,32	0
57	MG	BA	3173	1/1	0.24	-	28,28,28,28	0
57	MG	CA	3154	1/1	0.18	-	68,68,68,68	0
57	MG	DA	3259	1/1	0.13	-	39,39,39,39	0
57	MG	DA	3456	1/1	0.33	-	59,59,59,59	0
57	MG	BA	3108	1/1	0.13	-	36,36,36,36	0
57	MG	DA	3493	1/1	0.11	-	53,53,53,53	0
57	MG	AA	3075	1/1	0.14	-	57,57,57,57	0
57	MG	BA	3461	1/1	0.24	-	32,32,32,32	0
57	MG	BA	3669	1/1	0.27	-	34,34,34,34	0
57	MG	BA	3319	1/1	0.13	-	37,37,37,37	0
57	MG	CA	3035	1/1	0.20	-	63,63,63,63	0
57	MG	BA	3426	1/1	0.16	-	30,30,30,30	0
57	MG	CA	3076	1/1	0.16	-	59,59,59,59	0
57	MG	BE	3001	1/1	0.29	-	48,48,48,48	0
57	MG	BA	3268	1/1	0.15	-	45,45,45,45	0
57	MG	AA	3030	1/1	0.22	-	41,41,41,41	0
57	MG	AA	3164	1/1	0.12	-	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	BA	3136	1/1	0.28	-	56,56,56,56	0
57	MG	DA	3319	1/1	0.31	-	45,45,45,45	0
57	MG	BA	3613	1/1	0.07	-	74,74,74,74	0
57	MG	BA	3393	1/1	0.16	-	30,30,30,30	0
57	MG	BA	3399	1/1	0.14	-	26,26,26,26	0
57	MG	BA	3116	1/1	0.28	-	54,54,54,54	0
57	MG	AX	3004	1/1	0.11	-	45,45,45,45	0
57	MG	AA	3107	1/1	0.14	-	50,50,50,50	0
57	MG	DA	3577	1/1	0.17	-	25,25,25,25	0
57	MG	BA	3622	1/1	0.09	-	24,24,24,24	0
57	MG	DA	3157	1/1	0.16	-	44,44,44,44	0
57	MG	DA	3021	1/1	0.12	-	50,50,50,50	0
57	MG	BF	301	1/1	0.15	-	30,30,30,30	0
57	MG	BA	3247	1/1	0.14	-	37,37,37,37	0
57	MG	DA	3060	1/1	0.11	-	50,50,50,50	0
57	MG	DA	3216	1/1	0.30	-	43,43,43,43	0
57	MG	DA	3427	1/1	0.19	-	26,26,26,26	0
57	MG	DA	3599	1/1	0.20	-	36,36,36,36	0
57	MG	BA	3433	1/1	0.11	-	32,32,32,32	0
57	MG	AX	3012	1/1	0.20	-	15,15,15,15	0
57	MG	BA	3384	1/1	0.27	-	19,19,19,19	0
57	MG	BA	3264	1/1	0.09	-	47,47,47,47	0
57	MG	CA	3047	1/1	0.21	-	50,50,50,50	0
57	MG	DA	3211	1/1	0.13	-	43,43,43,43	0
57	MG	BA	3702	1/1	0.12	-	41,41,41,41	0
57	MG	DA	3612	1/1	0.11	-	64,64,64,64	0
57	MG	BA	3694	1/1	0.16	-	11,11,11,11	0
57	MG	BA	3386	1/1	0.25	-	30,30,30,30	0
57	MG	BA	3205	1/1	0.14	-	52,52,52,52	0
57	MG	DA	3483	1/1	0.31	-	41,41,41,41	0
57	MG	BA	3021	1/1	0.20	-	35,35,35,35	0
57	MG	DA	3586	1/1	0.11	-	21,21,21,21	0
57	MG	AA	3033	1/1	0.18	-	43,43,43,43	0
57	MG	BA	3289	1/1	0.12	-	41,41,41,41	0
57	MG	BA	3655	1/1	0.07	-	68,68,68,68	0
57	MG	DA	3294	1/1	0.19	-	18,18,18,18	0
57	MG	BA	3349	1/1	0.18	-	55,55,55,55	0
57	MG	AA	3163	1/1	0.13	-	70,70,70,70	0
57	MG	DA	3453	1/1	0.23	-	44,44,44,44	0
57	MG	BA	3275	1/1	0.09	-	38,38,38,38	0
57	MG	CA	3121	1/1	0.13	-	51,51,51,51	0
57	MG	AA	3183	1/1	0.16	-	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	3263	1/1	0.12	-	47,47,47,47	0
57	MG	BA	3157	1/1	0.12	-	42,42,42,42	0
57	MG	DA	3066	1/1	0.08	-	55,55,55,55	0
57	MG	AA	3130	1/1	0.15	-	52,52,52,52	0
57	MG	BA	3716	1/1	0.17	-	53,53,53,53	0
57	MG	DA	3562	1/1	0.07	-	58,58,58,58	0
57	MG	CA	3016	1/1	0.04	-	52,52,52,52	0
57	MG	CA	3110	1/1	0.18	-	56,56,56,56	0
57	MG	BN	3003	1/1	0.33	-	61,61,61,61	0
57	MG	BA	3710	1/1	0.10	-	21,21,21,21	0
57	MG	BA	3656	1/1	0.14	-	57,57,57,57	0
57	MG	DA	3443	1/1	0.17	-	27,27,27,27	0
57	MG	BA	3591	1/1	0.09	-	42,42,42,42	0
57	MG	BA	3248	1/1	0.21	-	32,32,32,32	0
57	MG	AX	3005	1/1	0.30	-	57,57,57,57	0
57	MG	DA	3100	1/1	0.15	-	38,38,38,38	0
57	MG	DA	3203	1/1	0.14	-	46,46,46,46	0
57	MG	DB	3008	1/1	0.09	-	59,59,59,59	0
57	MG	BA	3002	1/1	0.13	-	45,45,45,45	0
57	MG	BA	3423	1/1	0.26	-	26,26,26,26	0
57	MG	DA	3285	1/1	0.12	-	50,50,50,50	0
57	MG	BA	3398	1/1	0.21	-	36,36,36,36	0
57	MG	BA	3022	1/1	0.16	-	47,47,47,47	0
57	MG	BA	3041	1/1	0.24	-	39,39,39,39	0
57	MG	BB	3002	1/1	0.19	-	44,44,44,44	0
57	MG	BA	3630	1/1	0.15	-	72,72,72,72	0
57	MG	DA	3436	1/1	0.12	-	61,61,61,61	0
57	MG	DA	3304	1/1	0.13	-	44,44,44,44	0
57	MG	BA	3589	1/1	0.12	-	35,35,35,35	0
57	MG	AA	3205	1/1	0.24	-	48,48,48,48	0
57	MG	AA	3025	1/1	0.15	-	46,46,46,46	0
57	MG	CA	3007	1/1	0.12	-	55,55,55,55	0
57	MG	CA	3019	1/1	0.14	-	57,57,57,57	0
57	MG	BA	3486	1/1	0.13	-	32,32,32,32	0
57	MG	AA	3156	1/1	0.13	-	86,86,86,86	0
57	MG	DA	3037	1/1	0.15	-	41,41,41,41	0
57	MG	AA	3027	1/1	0.17	-	55,55,55,55	0
57	MG	BA	3665	1/1	0.13	-	50,50,50,50	0
57	MG	BA	3528	1/1	0.17	-	37,37,37,37	0
57	MG	BF	303	1/1	0.24	-	35,35,35,35	0
57	MG	DB	3006	1/1	0.11	-	44,44,44,44	0
57	MG	BA	3269	1/1	0.22	-	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	3009	1/1	0.07	-	40,40,40,40	0
57	MG	AA	3109	1/1	0.20	-	75,75,75,75	0
57	MG	DA	3318	1/1	0.15	-	39,39,39,39	0
57	MG	DA	3111	1/1	0.22	-	54,54,54,54	0
57	MG	BF	305	1/1	0.14	-	33,33,33,33	0
57	MG	BA	3254	1/1	0.18	-	30,30,30,30	0
57	MG	DA	3222	1/1	0.20	-	38,38,38,38	0
57	MG	DA	3536	1/1	0.12	-	48,48,48,48	0
57	MG	DA	3560	1/1	0.16	-	48,48,48,48	0
57	MG	BA	3240	1/1	0.29	-	52,52,52,52	0
57	MG	BA	3560	1/1	0.14	-	54,54,54,54	0
57	MG	BA	3034	1/1	0.11	-	21,21,21,21	0
57	MG	DA	3239	1/1	0.29	-	51,51,51,51	0
57	MG	BA	3292	1/1	0.16	-	26,26,26,26	0
57	MG	DA	3260	1/1	0.21	-	43,43,43,43	0
57	MG	BA	3219	1/1	0.38	-	42,42,42,42	0
57	MG	AX	3010	1/1	0.17	-	61,61,61,61	0
57	MG	BA	3167	1/1	0.20	-	51,51,51,51	0
57	MG	BA	3651	1/1	0.25	-	62,62,62,62	0
57	MG	BA	3427	1/1	0.14	-	23,23,23,23	0
57	MG	BA	3648	1/1	0.12	-	50,50,50,50	0
57	MG	DA	3063	1/1	0.09	-	40,40,40,40	0
57	MG	CA	3071	1/1	0.39	-	49,49,49,49	0
57	MG	DA	3164	1/1	0.06	-	44,44,44,44	0
57	MG	CA	3113	1/1	0.18	-	75,75,75,75	0
57	MG	DA	3578	1/1	0.20	-	63,63,63,63	0
57	MG	CA	3043	1/1	0.13	-	68,68,68,68	0
57	MG	DA	3031	1/1	0.10	-	36,36,36,36	0
57	MG	AA	3192	1/1	0.12	-	72,72,72,72	0
57	MG	DA	3489	1/1	0.14	-	38,38,38,38	0
57	MG	DA	3201	1/1	0.21	-	42,42,42,42	0
57	MG	DA	3465	1/1	0.10	-	45,45,45,45	0
57	MG	BA	3330	1/1	0.16	-	14,14,14,14	0
57	MG	DA	3023	1/1	0.18	-	35,35,35,35	0
57	MG	BA	3720	1/1	0.21	-	48,48,48,48	0
57	MG	BA	3063	1/1	0.11	-	39,39,39,39	0
57	MG	BA	3084	1/1	0.14	-	37,37,37,37	0
57	MG	BA	3229	1/1	0.41	-	52,52,52,52	0
57	MG	DA	3339	1/1	0.16	-	23,23,23,23	0
57	MG	BB	3015	1/1	0.10	-	42,42,42,42	0
57	MG	CA	3053	1/1	0.13	-	59,59,59,59	0
57	MG	BA	3092	1/1	0.15	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3217	1/1	0.30	-	57,57,57,57	0
57	MG	AA	3099	1/1	0.12	-	59,59,59,59	0
57	MG	BA	3152	1/1	0.23	-	45,45,45,45	0
57	MG	CA	3027	1/1	0.07	-	62,62,62,62	0
57	MG	DA	3575	1/1	0.20	-	19,19,19,19	0
57	MG	DA	3221	1/1	0.11	-	49,49,49,49	0
57	MG	BA	3290	1/1	0.14	-	43,43,43,43	0
57	MG	BA	3107	1/1	0.23	-	49,49,49,49	0
57	MG	DA	3057	1/1	0.22	-	22,22,22,22	0
57	MG	DA	3544	1/1	0.05	-	59,59,59,59	0
57	MG	B7	103	1/1	0.19	-	51,51,51,51	0
57	MG	AA	3011	1/1	0.15	-	67,67,67,67	0
57	MG	DA	3380	1/1	0.14	-	65,65,65,65	0
57	MG	BA	3511	1/1	0.17	-	41,41,41,41	0
57	MG	AA	3134	1/1	0.12	-	59,59,59,59	0
57	MG	BA	3670	1/1	0.09	-	25,25,25,25	0
57	MG	DA	3015	1/1	0.30	-	41,41,41,41	0
57	MG	BA	3150	1/1	0.15	-	40,40,40,40	0
57	MG	DA	3360	1/1	0.09	-	54,54,54,54	0
57	MG	DA	3526	1/1	0.13	-	41,41,41,41	0
57	MG	BA	3600	1/1	0.21	-	59,59,59,59	0
57	MG	BA	3445	1/1	0.22	-	35,35,35,35	0
57	MG	DA	3258	1/1	0.24	-	32,32,32,32	0
57	MG	AA	3001	1/1	0.14	-	72,72,72,72	0
57	MG	BA	3040	1/1	0.12	-	28,28,28,28	0
57	MG	DA	3581	1/1	0.14	-	53,53,53,53	0
57	MG	CF	3001	1/1	0.15	-	51,51,51,51	0
57	MG	CW	101	1/1	0.19	-	43,43,43,43	0
57	MG	BA	3519	1/1	0.15	-	26,26,26,26	0
57	MG	DA	3408	1/1	0.10	-	44,44,44,44	0
57	MG	DA	3114	1/1	0.11	-	51,51,51,51	0
57	MG	DA	3611	1/1	0.17	-	58,58,58,58	0
57	MG	CA	3039	1/1	0.09	-	52,52,52,52	0
57	MG	DA	3454	1/1	0.25	-	28,28,28,28	0
57	MG	BE	3006	1/1	0.34	-	72,72,72,72	0
57	MG	DA	3036	1/1	0.14	-	48,48,48,48	0
57	MG	BA	3558	1/1	0.17	-	63,63,63,63	0
57	MG	BW	205	1/1	0.12	-	30,30,30,30	0
59	ZN	D9	501	1/1	0.07	-	75,75,75,75	0
57	MG	DA	3492	1/1	0.09	-	45,45,45,45	0
57	MG	BA	3200	1/1	0.21	-	39,39,39,39	0
57	MG	BA	3176	1/1	0.20	-	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	BA	3139	1/1	0.33	-	45,45,45,45	0
57	MG	BA	3114	1/1	0.20	-	41,41,41,41	0
57	MG	BA	3546	1/1	0.24	-	27,27,27,27	0
57	MG	BA	3080	1/1	0.16	-	51,51,51,51	0
57	MG	DA	3004	1/1	0.29	-	32,32,32,32	0
57	MG	CA	3099	1/1	0.22	-	50,50,50,50	0
57	MG	DA	3106	1/1	0.17	-	52,52,52,52	0
57	MG	DA	3277	1/1	0.40	-	50,50,50,50	0
57	MG	AA	3142	1/1	0.26	-	53,53,53,53	0
57	MG	BA	3481	1/1	0.18	-	35,35,35,35	0
57	MG	BR	202	1/1	0.17	-	49,49,49,49	0
57	MG	BA	3714	1/1	0.10	-	42,42,42,42	0
57	MG	BA	3471	1/1	0.08	-	42,42,42,42	0
57	MG	AA	3058	1/1	0.14	-	48,48,48,48	0
57	MG	AA	3123	1/1	0.09	-	59,59,59,59	0
57	MG	DA	3413	1/1	0.23	-	30,30,30,30	0
57	MG	DA	3175	1/1	0.18	-	42,42,42,42	0
57	MG	DA	3326	1/1	0.11	-	40,40,40,40	0
57	MG	DA	3508	1/1	0.10	-	58,58,58,58	0
57	MG	CA	3159	1/1	0.11	-	46,46,46,46	0
57	MG	BU	206	1/1	0.35	-	39,39,39,39	0
57	MG	BA	3183	1/1	0.25	-	50,50,50,50	0
57	MG	AD	303	1/1	0.19	-	60,60,60,60	0
57	MG	BA	3543	1/1	0.10	-	69,69,69,69	0
57	MG	AA	3044	1/1	0.11	-	46,46,46,46	0
57	MG	CA	3136	1/1	0.12	-	68,68,68,68	0
57	MG	BA	3705	1/1	0.30	-	32,32,32,32	0
57	MG	DA	3012	1/1	0.06	-	42,42,42,42	0
57	MG	BA	3039	1/1	0.14	-	27,27,27,27	0
57	MG	BA	3189	1/1	0.18	-	33,33,33,33	0
57	MG	DA	3295	1/1	0.07	-	58,58,58,58	0
57	MG	DA	3341	1/1	0.14	-	32,32,32,32	0
57	MG	DA	3407	1/1	0.23	-	67,67,67,67	0
57	MG	BQ	3005	1/1	0.17	-	39,39,39,39	0
57	MG	CA	3109	1/1	0.19	-	61,61,61,61	0
57	MG	BA	3148	1/1	0.18	-	44,44,44,44	0
57	MG	BA	3699	1/1	0.09	-	33,33,33,33	0
57	MG	DA	3461	1/1	0.13	-	55,55,55,55	0
57	MG	DA	3219	1/1	0.18	-	54,54,54,54	0
57	MG	DA	3283	1/1	0.14	-	40,40,40,40	0
57	MG	BA	3113	1/1	0.22	-	57,57,57,57	0
57	MG	B7	102	1/1	0.36	-	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	DA	3476	1/1	0.12	-	49,49,49,49	0
57	MG	DB	3003	1/1	0.07	-	76,76,76,76	0
57	MG	BA	3032	1/1	0.21	-	30,30,30,30	0
57	MG	CA	3066	1/1	0.22	-	69,69,69,69	0
57	MG	DA	3550	1/1	0.25	-	63,63,63,63	0
57	MG	AA	3068	1/1	0.12	-	64,64,64,64	0
57	MG	DA	3503	1/1	0.19	-	51,51,51,51	0
57	MG	DA	3270	1/1	0.14	-	57,57,57,57	0
57	MG	BA	3499	1/1	0.23	-	51,51,51,51	0
57	MG	DB	3001	1/1	0.06	-	50,50,50,50	0
57	MG	AA	3140	1/1	0.09	-	56,56,56,56	0
57	MG	DA	3343	1/1	0.15	-	37,37,37,37	0
57	MG	BA	3514	1/1	0.35	-	36,36,36,36	0
57	MG	BA	3314	1/1	0.23	-	42,42,42,42	0
57	MG	BA	3688	1/1	0.32	-	46,46,46,46	0
57	MG	DA	3094	1/1	0.18	-	38,38,38,38	0
57	MG	DA	3098	1/1	0.17	-	32,32,32,32	0
57	MG	AA	3167	1/1	0.10	-	65,65,65,65	0
57	MG	DA	3616	1/1	0.14	-	28,28,28,28	0
57	MG	BA	3503	1/1	0.10	-	50,50,50,50	0
57	MG	BA	3587	1/1	0.17	-	51,51,51,51	0
57	MG	BA	3224	1/1	0.41	-	48,48,48,48	0
57	MG	BA	3678	1/1	0.14	-	49,49,49,49	0
57	MG	DA	3601	1/1	0.12	-	43,43,43,43	0
57	MG	BA	3036	1/1	0.63	-	42,42,42,42	0
57	MG	DA	3530	1/1	0.12	-	43,43,43,43	0
57	MG	DA	3207	1/1	0.22	-	39,39,39,39	0
57	MG	DA	3573	1/1	0.09	-	49,49,49,49	0
57	MG	DA	3007	1/1	0.09	-	48,48,48,48	0
57	MG	AA	3100	1/1	0.17	-	69,69,69,69	0
57	MG	AA	3004	1/1	0.20	-	61,61,61,61	0
57	MG	BA	3054	1/1	0.20	-	44,44,44,44	0
57	MG	DA	3108	1/1	0.14	-	50,50,50,50	0
57	MG	DA	3532	1/1	0.07	-	43,43,43,43	0
57	MG	BA	3090	1/1	0.20	-	50,50,50,50	0
57	MG	BD	310	1/1	0.50	-	34,34,34,34	0
57	MG	DA	3172	1/1	0.07	-	32,32,32,32	0
57	MG	AA	3155	1/1	0.18	-	65,65,65,65	0
57	MG	CA	3079	1/1	0.13	-	42,42,42,42	0
57	MG	CA	3151	1/1	0.13	-	58,58,58,58	0
57	MG	AA	3125	1/1	0.11	-	60,60,60,60	0
57	MG	BA	3031	1/1	0.11	-	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	AA	3045	1/1	0.12	-	44,44,44,44	0
57	MG	BA	3692	1/1	0.14	-	64,64,64,64	0
57	MG	AA	3086	1/1	0.12	-	45,45,45,45	0
57	MG	BA	3474	1/1	0.17	-	64,64,64,64	0
57	MG	BA	3668	1/1	0.15	-	39,39,39,39	0
57	MG	BA	3052	1/1	0.21	-	44,44,44,44	0
57	MG	BA	3599	1/1	0.14	-	43,43,43,43	0
57	MG	DD	306	1/1	0.37	-	44,44,44,44	0
57	MG	DA	3085	1/1	0.12	-	27,27,27,27	0
57	MG	AA	3083	1/1	0.28	-	38,38,38,38	0
57	MG	DE	302	1/1	0.59	-	51,51,51,51	0
57	MG	CJ	5001	1/1	0.10	-	51,51,51,51	0
57	MG	BA	3066	1/1	0.16	-	53,53,53,53	0
57	MG	DY	502	1/1	0.10	-	56,56,56,56	0
57	MG	AA	3121	1/1	0.09	-	66,66,66,66	0
57	MG	DA	3008	1/1	0.18	-	26,26,26,26	0
57	MG	DA	3321	1/1	0.13	-	40,40,40,40	0
57	MG	CA	3102	1/1	0.11	-	56,56,56,56	0
57	MG	DA	3171	1/1	0.21	-	38,38,38,38	0
57	MG	BA	3016	1/1	0.13	-	35,35,35,35	0
57	MG	BA	3235	1/1	0.18	-	52,52,52,52	0
57	MG	DA	3030	1/1	0.29	-	32,32,32,32	0
57	MG	DA	3055	1/1	0.08	-	35,35,35,35	0
57	MG	BA	3552	1/1	0.10	-	59,59,59,59	0
57	MG	BA	3355	1/1	0.11	-	30,30,30,30	0
57	MG	BA	3204	1/1	0.14	-	61,61,61,61	0
57	MG	DA	3420	1/1	0.09	-	41,41,41,41	0
57	MG	BA	3625	1/1	0.11	-	46,46,46,46	0
57	MG	DA	3174	1/1	0.20	-	38,38,38,38	0
57	MG	DA	3494	1/1	0.17	-	56,56,56,56	0
57	MG	CA	3009	1/1	0.06	-	44,44,44,44	0
57	MG	AA	3187	1/1	0.14	-	47,47,47,47	0
57	MG	BA	3707	1/1	0.40	-	34,34,34,34	0
57	MG	AA	3160	1/1	0.23	-	58,58,58,58	0
57	MG	CA	3022	1/1	0.24	-	55,55,55,55	0
57	MG	D5	101	1/1	0.15	-	42,42,42,42	0
57	MG	CX	3003	1/1	0.13	-	53,53,53,53	0
57	MG	DA	3627	1/1	0.24	-	56,56,56,56	0
57	MG	AA	3195	1/1	0.09	-	58,58,58,58	0
57	MG	BA	3501	1/1	0.08	-	67,67,67,67	0
57	MG	BA	3479	1/1	0.12	-	22,22,22,22	0
57	MG	DA	3358	1/1	0.51	-	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	BD	301	1/1	0.35	-	37,37,37,37	0
57	MG	DA	3497	1/1	0.17	-	61,61,61,61	0
57	MG	AA	3088	1/1	0.19	-	40,40,40,40	0
57	MG	DA	3345	1/1	0.17	-	28,28,28,28	0
57	MG	DA	3439	1/1	0.17	-	44,44,44,44	0
57	MG	BA	3046	1/1	0.17	-	30,30,30,30	0
57	MG	BA	3135	1/1	0.16	-	48,48,48,48	0
57	MG	DA	3093	1/1	0.11	-	45,45,45,45	0
57	MG	DA	3240	1/1	0.22	-	36,36,36,36	0
57	MG	DA	3053	1/1	0.23	-	50,50,50,50	0
60	K	AX	3001	1/1	0.09	-	39,39,39,39	0
57	MG	DA	3091	1/1	0.22	-	37,37,37,37	0
57	MG	BA	3372	1/1	0.09	-	58,58,58,58	0
57	MG	DA	3549	1/1	0.18	-	47,47,47,47	0
57	MG	BA	3120	1/1	0.28	-	52,52,52,52	0
57	MG	BA	3408	1/1	0.18	-	42,42,42,42	0
57	MG	DA	3223	1/1	0.08	-	56,56,56,56	0
57	MG	BA	3389	1/1	0.12	-	57,57,57,57	0
57	MG	AF	3001	1/1	0.21	-	58,58,58,58	0
57	MG	AA	3178	1/1	0.16	-	67,67,67,67	0
57	MG	DA	3395	1/1	0.10	-	31,31,31,31	0
57	MG	BA	3315	1/1	0.10	-	42,42,42,42	0
57	MG	DA	3220	1/1	0.16	-	54,54,54,54	0
57	MG	AA	3003	1/1	0.10	-	53,53,53,53	0
57	MG	BA	3436	1/1	0.20	-	21,21,21,21	0
57	MG	BA	3658	1/1	0.19	-	16,16,16,16	0
57	MG	AA	3161	1/1	0.19	-	28,28,28,28	0
57	MG	BA	3671	1/1	0.16	-	55,55,55,55	0
57	MG	BA	3695	1/1	0.16	-	19,19,19,19	0
57	MG	BA	3407	1/1	0.16	-	29,29,29,29	0
57	MG	BU	202	1/1	0.10	-	45,45,45,45	0
57	MG	BA	3115	1/1	0.40	-	49,49,49,49	0
57	MG	CA	3056	1/1	0.10	-	56,56,56,56	0
57	MG	CA	3106	1/1	0.14	-	65,65,65,65	0
57	MG	BA	3332	1/1	0.20	-	29,29,29,29	0
57	MG	AA	3141	1/1	0.10	-	54,54,54,54	0
57	MG	BA	3381	1/1	0.18	-	30,30,30,30	0
57	MG	BA	3301	1/1	0.20	-	43,43,43,43	0
57	MG	DA	3122	1/1	0.12	-	58,58,58,58	0
57	MG	DA	3531	1/1	0.05	-	40,40,40,40	0
57	MG	BA	3367	1/1	0.05	-	42,42,42,42	0
57	MG	AA	3026	1/1	0.09	-	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	3308	1/1	0.14	-	52,52,52,52	0
57	MG	DA	3296	1/1	0.16	-	46,46,46,46	0
57	MG	BA	3365	1/1	0.14	-	40,40,40,40	0
57	MG	DA	3089	1/1	0.15	-	36,36,36,36	0
57	MG	DA	3551	1/1	0.08	-	57,57,57,57	0
57	MG	BW	202	1/1	0.51	-	41,41,41,41	0
57	MG	DA	3067	1/1	0.10	-	54,54,54,54	0
57	MG	CA	3117	1/1	0.12	-	100,100,100,100	0
57	MG	BE	3003	1/1	0.16	-	25,25,25,25	0
57	MG	BA	3402	1/1	0.20	-	39,39,39,39	0
57	MG	DA	3478	1/1	0.14	-	57,57,57,57	0
57	MG	BA	3411	1/1	0.20	-	24,24,24,24	0
57	MG	AA	3190	1/1	0.11	-	75,75,75,75	0
57	MG	BA	3531	1/1	0.27	-	20,20,20,20	0
57	MG	BF	308	1/1	0.20	-	46,46,46,46	0
57	MG	BB	3003	1/1	0.17	-	40,40,40,40	0
57	MG	AA	3196	1/1	0.12	-	60,60,60,60	0
57	MG	DA	3187	1/1	0.20	-	39,39,39,39	0
57	MG	DA	3190	1/1	0.32	-	52,52,52,52	0
57	MG	BO	5001	1/1	0.13	-	49,49,49,49	0
57	MG	DA	3101	1/1	0.43	-	45,45,45,45	0
59	ZN	AN	501	1/1	0.12	-	71,71,71,71	0
57	MG	BA	3096	1/1	0.16	-	39,39,39,39	0
59	ZN	BY	202	1/1	0.11	-	70,70,70,70	0
57	MG	DQ	3001	1/1	0.10	-	58,58,58,58	0
57	MG	BA	3109	1/1	0.12	-	53,53,53,53	0
57	MG	BA	3070	1/1	0.24	-	44,44,44,44	0
57	MG	DA	3303	1/1	0.19	-	57,57,57,57	0
57	MG	DA	3090	1/1	0.17	-	52,52,52,52	0
57	MG	DA	3472	1/1	0.17	-	24,24,24,24	0
57	MG	DA	3051	1/1	0.08	-	54,54,54,54	0
57	MG	DA	3115	1/1	0.12	-	58,58,58,58	0
57	MG	DA	3590	1/1	0.08	-	58,58,58,58	0
57	MG	DA	3014	1/1	0.12	-	45,45,45,45	0
57	MG	CA	3070	1/1	0.27	-	42,42,42,42	0
57	MG	DA	3507	1/1	0.20	-	33,33,33,33	0
57	MG	DD	304	1/1	0.13	-	40,40,40,40	0
57	MG	DD	301	1/1	0.17	-	31,31,31,31	0
57	MG	BA	3262	1/1	0.24	-	38,38,38,38	0
57	MG	BA	3147	1/1	0.21	-	34,34,34,34	0
57	MG	DA	3460	1/1	0.10	-	57,57,57,57	0
57	MG	BA	3551	1/1	0.22	-	17,17,17,17	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	0.24	-	57,57,57,57	0
57	MG	BA	3163	1/1	0.25	-	43,43,43,43	0
57	MG	BA	3713	1/1	0.15	-	63,63,63,63	0
57	MG	DA	3363	1/1	0.18	-	35,35,35,35	0
57	MG	BU	207	1/1	0.15	-	23,23,23,23	0
58	SF4	CD	501	8/8	0.12	-	59,71,83,91	0
57	MG	DA	3589	1/1	0.10	-	52,52,52,52	0
57	MG	DV	202	1/1	0.63	-	75,75,75,75	0
57	MG	BA	3077	1/1	0.12	-	33,33,33,33	0
57	MG	BA	3690	1/1	0.12	-	49,49,49,49	0
57	MG	DA	3226	1/1	0.16	-	54,54,54,54	0
57	MG	BA	3075	1/1	0.28	-	45,45,45,45	0
57	MG	DA	3043	1/1	0.14	-	44,44,44,44	0
57	MG	BA	3284	1/1	0.10	-	41,41,41,41	0
57	MG	BA	3614	1/1	0.10	-	64,64,64,64	0
57	MG	BA	3017	1/1	0.22	-	48,48,48,48	0
57	MG	BA	3409	1/1	0.25	-	27,27,27,27	0
57	MG	DA	3026	1/1	0.09	-	41,41,41,41	0
57	MG	DA	3372	1/1	0.09	-	49,49,49,49	0
57	MG	BA	3340	1/1	0.15	-	59,59,59,59	0
57	MG	DA	3582	1/1	0.15	-	24,24,24,24	0
57	MG	DA	3241	1/1	0.15	-	40,40,40,40	0
57	MG	AA	3072	1/1	0.10	-	65,65,65,65	0
57	MG	BA	3636	1/1	0.28	-	45,45,45,45	0
57	MG	DR	3002	1/1	0.12	-	51,51,51,51	0
57	MG	DA	3442	1/1	0.24	-	34,34,34,34	0
57	MG	BA	3529	1/1	0.29	-	29,29,29,29	0
57	MG	DA	3346	1/1	0.10	-	39,39,39,39	0
57	MG	AA	3112	1/1	0.13	-	44,44,44,44	0
57	MG	BA	3515	1/1	0.15	-	44,44,44,44	0
57	MG	DA	3561	1/1	0.16	-	51,51,51,51	0
57	MG	BA	3380	1/1	0.17	-	55,55,55,55	0
57	MG	AA	3201	1/1	0.06	-	68,68,68,68	0
57	MG	DA	3541	1/1	0.09	-	40,40,40,40	0
57	MG	BA	3058	1/1	0.19	-	24,24,24,24	0
57	MG	DA	3102	1/1	0.13	-	64,64,64,64	0
57	MG	AK	3001	1/1	0.12	-	55,55,55,55	0
57	MG	BA	3687	1/1	0.13	-	30,30,30,30	0
57	MG	CA	3063	1/1	0.10	-	59,59,59,59	0
57	MG	DA	3103	1/1	0.47	-	55,55,55,55	0
57	MG	CA	3077	1/1	0.14	-	63,63,63,63	0
57	MG	AA	3180	1/1	0.21	-	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	BA	3368	1/1	0.32	-	26,26,26,26	0
57	MG	CA	3104	1/1	0.17	-	37,37,37,37	0
57	MG	DA	3504	1/1	0.19	-	46,46,46,46	0
57	MG	AA	3206	1/1	0.06	-	62,62,62,62	0
57	MG	AA	3056	1/1	0.24	-	66,66,66,66	0
57	MG	AA	3157	1/1	0.12	-	38,38,38,38	0
57	MG	BA	3230	1/1	0.31	-	45,45,45,45	0
57	MG	DA	3235	1/1	0.26	-	48,48,48,48	0
57	MG	BA	3104	1/1	0.18	-	54,54,54,54	0
57	MG	DA	3410	1/1	0.22	-	37,37,37,37	0
57	MG	DN	5001	1/1	0.06	-	53,53,53,53	0
57	MG	DA	3512	1/1	0.10	-	24,24,24,24	0
57	MG	DA	3137	1/1	0.21	-	48,48,48,48	0
57	MG	DB	3009	1/1	0.20	-	55,55,55,55	0
57	MG	DA	3162	1/1	0.46	-	58,58,58,58	0
57	MG	BA	3181	1/1	0.23	-	49,49,49,49	0
57	MG	BA	3206	1/1	0.11	-	37,37,37,37	0
57	MG	BA	3064	1/1	0.12	-	38,38,38,38	0
57	MG	BA	3567	1/1	0.17	-	55,55,55,55	0
57	MG	DA	3019	1/1	0.16	-	54,54,54,54	0
57	MG	AN	502	1/1	0.15	-	61,61,61,61	0
57	MG	DA	3433	1/1	0.19	-	27,27,27,27	0
57	MG	DA	3585	1/1	0.22	-	45,45,45,45	0
57	MG	BF	307	1/1	0.35	-	25,25,25,25	0
57	MG	AA	3119	1/1	0.10	-	50,50,50,50	0
57	MG	DA	3481	1/1	0.11	-	69,69,69,69	0
57	MG	DA	3353	1/1	0.12	-	42,42,42,42	0
57	MG	CA	3146	1/1	0.16	-	74,74,74,74	0
57	MG	BA	3033	1/1	0.15	-	39,39,39,39	0
57	MG	BA	3548	1/1	0.18	-	54,54,54,54	0
57	MG	BA	3245	1/1	0.28	-	37,37,37,37	0
57	MG	DA	3217	1/1	0.32	-	50,50,50,50	0
57	MG	CA	3015	1/1	0.10	-	61,61,61,61	0
57	MG	BA	3194	1/1	0.18	-	42,42,42,42	0
57	MG	DA	3092	1/1	0.08	-	29,29,29,29	0
57	MG	BA	3598	1/1	0.23	-	54,54,54,54	0
57	MG	DA	3449	1/1	0.08	-	52,52,52,52	0
57	MG	BA	3283	1/1	0.21	-	22,22,22,22	0
57	MG	AA	3065	1/1	0.09	-	48,48,48,48	0
57	MG	AA	3090	1/1	0.15	-	70,70,70,70	0
57	MG	AA	3066	1/1	0.09	-	66,66,66,66	0
57	MG	CA	3048	1/1	0.15	-	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	DA	3253	1/1	0.20	-	34,34,34,34	0
57	MG	CA	3023	1/1	0.13	-	88,88,88,88	0
57	MG	AA	3019	1/1	0.13	-	52,52,52,52	0
57	MG	BP	3003	1/1	0.15	-	42,42,42,42	0
57	MG	BA	3190	1/1	0.20	-	24,24,24,24	0
57	MG	BA	3568	1/1	0.21	-	43,43,43,43	0
57	MG	DA	3148	1/1	0.17	-	45,45,45,45	0
57	MG	DA	3491	1/1	0.17	-	43,43,43,43	0
57	MG	BA	3638	1/1	0.08	-	41,41,41,41	0
57	MG	DA	3020	1/1	0.16	-	32,32,32,32	0
57	MG	DA	3606	1/1	0.18	-	54,54,54,54	0
57	MG	AA	3051	1/1	0.25	-	51,51,51,51	0
57	MG	DA	3028	1/1	0.12	-	52,52,52,52	0
57	MG	DA	3081	1/1	0.25	-	45,45,45,45	0
57	MG	BA	3641	1/1	0.14	-	33,33,33,33	0
57	MG	BA	3246	1/1	0.24	-	46,46,46,46	0
57	MG	BA	3184	1/1	0.26	-	42,42,42,42	0
57	MG	CA	3010	1/1	0.16	-	56,56,56,56	0
57	MG	DA	3045	1/1	0.11	-	39,39,39,39	0
57	MG	AA	3053	1/1	0.16	-	54,54,54,54	0
57	MG	AA	3193	1/1	0.30	-	77,77,77,77	0
57	MG	BA	3628	1/1	0.18	-	60,60,60,60	0
57	MG	AA	3115	1/1	0.30	-	38,38,38,38	0
57	MG	DA	3404	1/1	0.07	-	48,48,48,48	0
57	MG	BA	3689	1/1	0.13	-	46,46,46,46	0
57	MG	DA	3176	1/1	0.15	-	42,42,42,42	0
57	MG	CA	3050	1/1	0.11	-	56,56,56,56	0
57	MG	BA	3082	1/1	0.15	-	57,57,57,57	0
57	MG	BA	3539	1/1	0.20	-	18,18,18,18	0
57	MG	BA	3259	1/1	0.26	-	40,40,40,40	0
57	MG	BZ	3001	1/1	0.23	-	56,56,56,56	0
57	MG	DA	3161	1/1	0.18	-	35,35,35,35	0
57	MG	BU	205	1/1	0.14	-	32,32,32,32	0
57	MG	AA	3108	1/1	0.21	-	54,54,54,54	0
57	MG	DA	3362	1/1	0.24	-	48,48,48,48	0
57	MG	BA	3504	1/1	0.23	-	33,33,33,33	0
57	MG	BA	3339	1/1	0.35	-	52,52,52,52	0
57	MG	BA	3382	1/1	0.17	-	31,31,31,31	0
59	ZN	D4	501	1/1	0.14	-	154,154,154,154	0
57	MG	DA	3276	1/1	0.13	-	56,56,56,56	0
57	MG	AA	3171	1/1	0.19	-	45,45,45,45	0
57	MG	BA	3121	1/1	0.22	-	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	3216	1/1	0.16	-	35,35,35,35	0
57	MG	DA	3537	1/1	0.20	-	45,45,45,45	0
57	MG	BA	3123	1/1	0.15	-	56,56,56,56	0
57	MG	DA	3109	1/1	0.36	-	45,45,45,45	0
57	MG	DA	3144	1/1	0.08	-	48,48,48,48	0
57	MG	BE	3005	1/1	0.15	-	15,15,15,15	0
57	MG	BA	3048	1/1	0.12	-	44,44,44,44	0
57	MG	BA	3378	1/1	0.17	-	45,45,45,45	0
57	MG	BA	3088	1/1	0.40	-	59,59,59,59	0
57	MG	BA	3452	1/1	0.15	-	15,15,15,15	0
57	MG	CA	3012	1/1	0.32	-	45,45,45,45	0
57	MG	DA	3034	1/1	0.22	-	46,46,46,46	0
57	MG	DA	3169	1/1	0.16	-	45,45,45,45	0
57	MG	AA	3124	1/1	0.17	-	58,58,58,58	0
57	MG	AA	3036	1/1	0.11	-	51,51,51,51	0
57	MG	AA	3095	1/1	0.11	-	44,44,44,44	0
57	MG	AA	3148	1/1	0.13	-	61,61,61,61	0
57	MG	DA	3185	1/1	0.24	-	57,57,57,57	0
57	MG	BA	3535	1/1	0.23	-	29,29,29,29	0
57	MG	CA	3004	1/1	0.22	-	70,70,70,70	0
57	MG	DA	3367	1/1	0.14	-	24,24,24,24	0
57	MG	AA	3067	1/1	0.11	-	47,47,47,47	0
57	MG	BA	3584	1/1	0.09	-	59,59,59,59	0
57	MG	BA	3061	1/1	0.09	-	58,58,58,58	0
57	MG	DA	3013	1/1	0.16	-	43,43,43,43	0
57	MG	BA	3375	1/1	0.20	-	46,46,46,46	0
57	MG	DA	3340	1/1	0.16	-	38,38,38,38	0
57	MG	BA	3149	1/1	0.16	-	40,40,40,40	0
57	MG	DA	3539	1/1	0.20	-	52,52,52,52	0
57	MG	DA	3571	1/1	0.18	-	54,54,54,54	0
57	MG	BA	3373	1/1	0.20	-	46,46,46,46	0
57	MG	DA	3437	1/1	0.16	-	48,48,48,48	0
57	MG	BA	3391	1/1	0.23	-	30,30,30,30	0
57	MG	BA	3419	1/1	0.21	-	58,58,58,58	0
57	MG	BA	3352	1/1	0.14	-	29,29,29,29	0
57	MG	B0	103	1/1	0.11	-	38,38,38,38	0
57	MG	BA	3111	1/1	0.26	-	51,51,51,51	0
57	MG	BA	3350	1/1	0.14	-	43,43,43,43	0
57	MG	DA	3496	1/1	0.17	-	63,63,63,63	0
57	MG	BA	3440	1/1	0.20	-	40,40,40,40	0
57	MG	BA	3146	1/1	0.17	-	47,47,47,47	0
57	MG	BA	3252	1/1	0.20	-	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	CA	3115	1/1	0.12	-	59,59,59,59	0
57	MG	DA	3463	1/1	0.09	-	54,54,54,54	0
57	MG	BA	3637	1/1	0.11	-	40,40,40,40	0
57	MG	DA	3254	1/1	0.25	-	42,42,42,42	0
57	MG	BA	3719	1/1	0.07	-	53,53,53,53	0
57	MG	BA	3682	1/1	0.19	-	30,30,30,30	0
57	MG	DA	3039	1/1	0.36	-	48,48,48,48	0
57	MG	BA	3322	1/1	0.16	-	40,40,40,40	0
57	MG	BA	3453	1/1	0.11	-	47,47,47,47	0
57	MG	DA	3516	1/1	0.05	-	43,43,43,43	0
57	MG	AA	3082	1/1	0.13	-	55,55,55,55	0
57	MG	DB	3005	1/1	0.18	-	54,54,54,54	0
57	MG	DA	3257	1/1	0.32	-	46,46,46,46	0
57	MG	BA	3459	1/1	0.25	-	44,44,44,44	0
57	MG	AA	3176	1/1	0.08	-	43,43,43,43	0
57	MG	BW	204	1/1	0.23	-	27,27,27,27	0
57	MG	BA	3512	1/1	0.10	-	32,32,32,32	0
57	MG	B9	502	1/1	0.10	-	31,31,31,31	0
57	MG	BA	3078	1/1	0.15	-	55,55,55,55	0
57	MG	BA	3003	1/1	0.15	-	44,44,44,44	0
57	MG	BA	3577	1/1	0.23	-	35,35,35,35	0
57	MG	DA	3529	1/1	0.09	-	43,43,43,43	0
57	MG	DA	3178	1/1	0.17	-	39,39,39,39	0
57	MG	DA	3535	1/1	0.22	-	21,21,21,21	0
57	MG	CA	3148	1/1	0.16	-	81,81,81,81	0
57	MG	CA	3082	1/1	0.15	-	71,71,71,71	0
57	MG	CA	3029	1/1	0.14	-	48,48,48,48	0
57	MG	BA	3023	1/1	0.14	-	25,25,25,25	0
57	MG	BV	204	1/1	0.08	-	36,36,36,36	0
57	MG	CA	3064	1/1	0.15	-	64,64,64,64	0
57	MG	BA	3083	1/1	0.17	-	33,33,33,33	0
57	MG	DA	3153	1/1	0.14	-	34,34,34,34	0
57	MG	AA	3017	1/1	0.16	-	63,63,63,63	0
57	MG	BA	3256	1/1	0.08	-	36,36,36,36	0
57	MG	DA	3155	1/1	0.16	-	34,34,34,34	0
57	MG	AA	3034	1/1	0.06	-	47,47,47,47	0
57	MG	AA	3144	1/1	0.24	-	44,44,44,44	0
57	MG	BA	3187	1/1	0.13	-	35,35,35,35	0
57	MG	CA	3144	1/1	0.16	-	58,58,58,58	0
57	MG	CA	3055	1/1	0.12	-	66,66,66,66	0
57	MG	BA	3455	1/1	0.16	-	44,44,44,44	0
57	MG	CA	3031	1/1	0.09	-	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	DA	3306	1/1	0.09	-	31,31,31,31	0
57	MG	AA	3079	1/1	0.05	-	62,62,62,62	0
57	MG	DA	3587	1/1	0.19	-	35,35,35,35	0
57	MG	BA	3237	1/1	0.16	-	36,36,36,36	0
57	MG	BA	3469	1/1	0.17	-	42,42,42,42	0
57	MG	BF	304	1/1	0.25	-	35,35,35,35	0
57	MG	DA	3003	1/1	0.15	-	56,56,56,56	0
57	MG	BA	3312	1/1	0.17	-	44,44,44,44	0
57	MG	DA	3369	1/1	0.25	-	36,36,36,36	0
57	MG	DA	3251	1/1	0.27	-	34,34,34,34	0
57	MG	DA	3625	1/1	0.24	-	57,57,57,57	0
57	MG	DA	3505	1/1	0.07	-	41,41,41,41	0
57	MG	DA	3324	1/1	0.21	-	42,42,42,42	0
57	MG	DA	3469	1/1	0.28	-	41,41,41,41	0
57	MG	DA	3192	1/1	0.20	-	31,31,31,31	0
57	MG	DA	3617	1/1	0.16	-	40,40,40,40	0
57	MG	BN	3001	1/1	0.52	-	46,46,46,46	0
57	MG	BA	3062	1/1	0.22	-	52,52,52,52	0
57	MG	CA	3002	1/1	0.13	-	66,66,66,66	0
57	MG	BA	3706	1/1	0.27	-	27,27,27,27	0
57	MG	BA	3271	1/1	0.31	-	45,45,45,45	0
57	MG	BA	3320	1/1	0.11	-	56,56,56,56	0
57	MG	DA	3547	1/1	0.21	-	68,68,68,68	0
57	MG	DA	3163	1/1	0.19	-	43,43,43,43	0
57	MG	AA	3204	1/1	0.21	-	64,64,64,64	0
57	MG	BA	3035	1/1	0.20	-	28,28,28,28	0
57	MG	AA	3179	1/1	0.06	-	56,56,56,56	0
57	MG	DA	3119	1/1	0.17	-	52,52,52,52	0
57	MG	AA	3064	1/1	0.14	-	65,65,65,65	0
57	MG	BA	3621	1/1	0.14	-	18,18,18,18	0
57	MG	DA	3209	1/1	0.16	-	53,53,53,53	0
57	MG	DA	3215	1/1	0.15	-	35,35,35,35	0
57	MG	DA	3513	1/1	0.13	-	49,49,49,49	0
57	MG	AA	3197	1/1	0.14	-	50,50,50,50	0
57	MG	BA	3288	1/1	0.16	-	37,37,37,37	0
57	MG	BA	3607	1/1	0.19	-	41,41,41,41	0
57	MG	BA	3523	1/1	0.13	-	31,31,31,31	0
57	MG	DA	3281	1/1	0.12	-	37,37,37,37	0
57	MG	BA	3505	1/1	0.19	-	16,16,16,16	0
57	MG	DA	3574	1/1	0.13	-	59,59,59,59	0
57	MG	BA	3432	1/1	0.25	-	35,35,35,35	0
57	MG	BA	3703	1/1	0.08	-	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	3089	1/1	0.12	-	30,30,30,30	0
57	MG	BA	3346	1/1	0.20	-	29,29,29,29	0
57	MG	DA	3603	1/1	0.09	-	40,40,40,40	0
57	MG	BA	3698	1/1	0.32	-	51,51,51,51	0
57	MG	DA	3525	1/1	0.09	-	40,40,40,40	0
57	MG	AA	3128	1/1	0.20	-	53,53,53,53	0
57	MG	BA	3191	1/1	0.06	-	22,22,22,22	0
57	MG	BA	3643	1/1	0.16	-	47,47,47,47	0
57	MG	BA	3541	1/1	0.17	-	43,43,43,43	0
57	MG	BA	3632	1/1	0.10	-	43,43,43,43	0
57	MG	BA	3042	1/1	0.14	-	34,34,34,34	0
57	MG	DA	3022	1/1	0.09	-	27,27,27,27	0
57	MG	DA	3619	1/1	0.47	-	63,63,63,63	0
57	MG	AA	3177	1/1	0.15	-	66,66,66,66	0
57	MG	AA	3023	1/1	0.07	-	60,60,60,60	0
57	MG	BA	3456	1/1	0.11	-	44,44,44,44	0
57	MG	DA	3342	1/1	0.15	-	49,49,49,49	0
57	MG	BA	3006	1/1	0.18	-	38,38,38,38	0
57	MG	BA	3401	1/1	0.26	-	31,31,31,31	0
57	MG	BA	3024	1/1	0.17	-	42,42,42,42	0
57	MG	BA	3074	1/1	0.12	-	43,43,43,43	0
57	MG	DA	3495	1/1	0.11	-	48,48,48,48	0
57	MG	CA	3013	1/1	0.17	-	45,45,45,45	0
57	MG	BA	3026	1/1	0.23	-	36,36,36,36	0
57	MG	BB	3020	1/1	0.15	-	55,55,55,55	0
57	MG	BA	3137	1/1	0.17	-	57,57,57,57	0
57	MG	BD	309	1/1	0.26	-	33,33,33,33	0
57	MG	DA	3316	1/1	0.12	-	39,39,39,39	0
57	MG	DA	3010	1/1	0.18	-	51,51,51,51	0
57	MG	BA	3180	1/1	0.24	-	32,32,32,32	0
57	MG	BA	3392	1/1	0.17	-	27,27,27,27	0
57	MG	BA	3069	1/1	0.18	-	48,48,48,48	0
57	MG	DA	3087	1/1	0.14	-	65,65,65,65	0
57	MG	DE	301	1/1	0.09	-	52,52,52,52	0
57	MG	AA	3166	1/1	0.19	-	70,70,70,70	0
57	MG	DA	3464	1/1	0.13	-	51,51,51,51	0
57	MG	BD	304	1/1	0.15	-	36,36,36,36	0
57	MG	BA	3376	1/1	0.18	-	21,21,21,21	0
57	MG	DA	3160	1/1	0.11	-	65,65,65,65	0
57	MG	BA	3672	1/1	0.11	-	28,28,28,28	0
57	MG	DA	3352	1/1	0.23	-	25,25,25,25	0
57	MG	DA	3184	1/1	0.09	-	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	3044	1/1	0.12	-	40,40,40,40	0
57	MG	BA	3588	1/1	0.16	-	19,19,19,19	0
57	MG	BA	3477	1/1	0.11	-	19,19,19,19	0
57	MG	BA	3207	1/1	0.15	-	55,55,55,55	0
57	MG	DA	3368	1/1	0.09	-	58,58,58,58	0
57	MG	DA	3006	1/1	0.10	-	40,40,40,40	0
57	MG	BA	3633	1/1	0.11	-	54,54,54,54	0
57	MG	AX	3011	1/1	0.32	-	73,73,73,73	0
57	MG	BA	3211	1/1	0.13	-	50,50,50,50	0
57	MG	BA	3261	1/1	0.18	-	52,52,52,52	0
57	MG	BA	3693	1/1	0.14	-	48,48,48,48	0
57	MG	BA	3338	1/1	0.08	-	50,50,50,50	0
57	MG	BA	3691	1/1	0.28	-	54,54,54,54	0
57	MG	BA	3151	1/1	0.12	-	42,42,42,42	0
57	MG	BD	306	1/1	0.27	-	30,30,30,30	0
57	MG	BB	3009	1/1	0.15	-	63,63,63,63	0
57	MG	DA	3409	1/1	0.06	-	70,70,70,70	0
57	MG	BA	3043	1/1	0.16	-	44,44,44,44	0
57	MG	DV	201	1/1	0.32	-	49,49,49,49	0
57	MG	BA	3258	1/1	0.21	-	35,35,35,35	0
57	MG	BA	3144	1/1	0.18	-	42,42,42,42	0
57	MG	BA	3715	1/1	0.12	-	33,33,33,33	0
57	MG	AA	3039	1/1	0.25	-	62,62,62,62	0
57	MG	DA	3351	1/1	0.32	-	45,45,45,45	0
57	MG	DA	3379	1/1	0.12	-	37,37,37,37	0
57	MG	AA	3169	1/1	0.14	-	48,48,48,48	0
57	MG	DA	3025	1/1	0.19	-	35,35,35,35	0
57	MG	AA	3194	1/1	0.19	-	41,41,41,41	0
57	MG	BA	3518	1/1	0.20	-	48,48,48,48	0
57	MG	BA	3030	1/1	0.11	-	44,44,44,44	0
57	MG	AA	3028	1/1	0.13	-	58,58,58,58	0
57	MG	BA	3544	1/1	0.16	-	52,52,52,52	0
57	MG	CA	3060	1/1	0.15	-	78,78,78,78	0
57	MG	BA	3415	1/1	0.19	-	61,61,61,61	0
57	MG	BA	3154	1/1	0.20	-	36,36,36,36	0
57	MG	B1	101	1/1	0.44	-	37,37,37,37	0
57	MG	DA	3231	1/1	0.25	-	33,33,33,33	0
57	MG	BA	3027	1/1	1.05	-	36,36,36,36	0
57	MG	BA	3202	1/1	0.17	-	42,42,42,42	0
57	MG	CA	3152	1/1	0.15	-	66,66,66,66	0
57	MG	BA	3156	1/1	0.16	-	43,43,43,43	0
57	MG	BB	3011	1/1	0.09	-	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	3194	1/1	0.25	-	43,43,43,43	0
57	MG	BA	3072	1/1	0.10	-	32,32,32,32	0
57	MG	BA	3635	1/1	0.10	-	59,59,59,59	0
57	MG	BA	3170	1/1	0.22	-	41,41,41,41	0
57	MG	BA	3103	1/1	0.38	-	62,62,62,62	0
57	MG	DA	3594	1/1	0.13	-	51,51,51,51	0
57	MG	BA	3428	1/1	0.15	-	54,54,54,54	0
57	MG	BA	3218	1/1	0.54	-	52,52,52,52	0
57	MG	DA	3545	1/1	0.16	-	70,70,70,70	0
57	MG	DA	3229	1/1	0.17	-	39,39,39,39	0
57	MG	DA	3150	1/1	0.29	-	41,41,41,41	0
57	MG	BA	3186	1/1	0.19	-	42,42,42,42	0
57	MG	AA	3012	1/1	0.20	-	61,61,61,61	0
57	MG	BA	3076	1/1	0.23	-	34,34,34,34	0
57	MG	DA	3255	1/1	0.28	-	34,34,34,34	0
57	MG	DA	3458	1/1	0.09	-	44,44,44,44	0
57	MG	DU	3002	1/1	0.37	-	67,67,67,67	0
57	MG	BA	3601	1/1	0.18	-	69,69,69,69	0
57	MG	BA	3178	1/1	0.20	-	52,52,52,52	0
57	MG	BA	3470	1/1	0.13	-	69,69,69,69	0
57	MG	BA	3143	1/1	0.16	-	41,41,41,41	0
57	MG	BF	306	1/1	0.07	-	43,43,43,43	0
57	MG	BA	3253	1/1	0.22	-	28,28,28,28	0
57	MG	DA	3129	1/1	0.11	-	41,41,41,41	0
57	MG	BA	3513	1/1	0.09	-	55,55,55,55	0
57	MG	BA	3251	1/1	0.24	-	48,48,48,48	0
57	MG	BA	3597	1/1	0.27	-	56,56,56,56	0
57	MG	BA	3106	1/1	0.22	-	24,24,24,24	0
57	MG	DA	3272	1/1	0.07	-	29,29,29,29	0
57	MG	BA	3663	1/1	0.17	-	36,36,36,36	0
57	MG	BA	3417	1/1	0.15	-	49,49,49,49	0
57	MG	DP	202	1/1	0.35	-	48,48,48,48	0
57	MG	DA	3596	1/1	0.27	-	71,71,71,71	0
57	MG	CA	3046	1/1	0.20	-	53,53,53,53	0
57	MG	BA	3140	1/1	0.17	-	26,26,26,26	0
57	MG	AA	3146	1/1	0.13	-	81,81,81,81	0
57	MG	CA	3149	1/1	0.10	-	49,49,49,49	0
57	MG	BB	3007	1/1	0.09	-	51,51,51,51	0
57	MG	CA	3085	1/1	0.30	-	71,71,71,71	0
57	MG	DA	3149	1/1	0.16	-	42,42,42,42	0
57	MG	DA	3510	1/1	0.13	-	52,52,52,52	0
57	MG	DA	3486	1/1	0.20	-	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	3610	1/1	0.22	-	60,60,60,60	0
57	MG	BA	3300	1/1	0.11	-	55,55,55,55	0
57	MG	BA	3533	1/1	0.27	-	45,45,45,45	0
57	MG	AA	3202	1/1	0.05	-	60,60,60,60	0
57	MG	DA	3501	1/1	0.20	-	47,47,47,47	0
57	MG	DA	3432	1/1	0.11	-	33,33,33,33	0
57	MG	CA	3067	1/1	0.13	-	45,45,45,45	0
57	MG	BA	3467	1/1	0.23	-	51,51,51,51	0
57	MG	DA	3470	1/1	0.13	-	34,34,34,34	0
57	MG	DA	3104	1/1	0.25	-	47,47,47,47	0
57	MG	DA	3604	1/1	0.15	-	61,61,61,61	0
57	MG	DQ	3002	1/1	0.14	-	45,45,45,45	0
57	MG	DA	3195	1/1	0.20	-	42,42,42,42	0
57	MG	AA	3199	1/1	0.14	-	58,58,58,58	0
57	MG	BA	3498	1/1	0.25	-	45,45,45,45	0
57	MG	AA	3189	1/1	0.12	-	69,69,69,69	0
57	MG	BA	3177	1/1	0.20	-	39,39,39,39	0
57	MG	BQ	3001	1/1	0.33	-	51,51,51,51	0
57	MG	BA	3331	1/1	0.24	-	39,39,39,39	0
57	MG	AA	3077	1/1	0.20	-	52,52,52,52	0
57	MG	BA	3126	1/1	0.24	-	34,34,34,34	0
57	MG	DA	3466	1/1	0.21	-	41,41,41,41	0
57	MG	AA	3149	1/1	0.14	-	48,48,48,48	0
57	MG	DA	3064	1/1	0.24	-	52,52,52,52	0
57	MG	CA	3038	1/1	0.13	-	68,68,68,68	0
57	MG	BA	3581	1/1	0.08	-	55,55,55,55	0
57	MG	BA	3005	1/1	0.24	-	44,44,44,44	0
57	MG	BA	3037	1/1	0.14	-	38,38,38,38	0
57	MG	DA	3107	1/1	0.19	-	39,39,39,39	0
57	MG	BA	3160	1/1	0.20	-	23,23,23,23	0
57	MG	DA	3205	1/1	0.11	-	52,52,52,52	0
57	MG	DA	3567	1/1	0.10	-	49,49,49,49	0
57	MG	DA	3376	1/1	0.25	-	40,40,40,40	0
57	MG	AA	3139	1/1	0.12	-	51,51,51,51	0
57	MG	DA	3419	1/1	0.18	-	37,37,37,37	0
57	MG	DF	3004	1/1	0.25	-	56,56,56,56	0
57	MG	DA	3041	1/1	0.17	-	36,36,36,36	0
57	MG	BA	3595	1/1	0.20	-	52,52,52,52	0
57	MG	AA	3054	1/1	0.19	-	62,62,62,62	0
57	MG	BR	201	1/1	0.23	-	30,30,30,30	0
57	MG	BA	3060	1/1	0.24	-	59,59,59,59	0
57	MG	B0	104	1/1	0.05	-	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	BA	3457	1/1	0.08	-	41,41,41,41	0
57	MG	AA	3133	1/1	0.16	-	59,59,59,59	0
57	MG	DA	3518	1/1	0.07	-	42,42,42,42	0
57	MG	BA	3351	1/1	0.10	-	62,62,62,62	0
57	MG	DA	3286	1/1	0.26	-	45,45,45,45	0
57	MG	AA	3131	1/1	0.17	-	56,56,56,56	0
57	MG	BA	3549	1/1	0.15	-	55,55,55,55	0
57	MG	BA	3287	1/1	0.23	-	42,42,42,42	0
57	MG	DA	3105	1/1	0.23	-	37,37,37,37	0
57	MG	BA	3466	1/1	0.23	-	57,57,57,57	0
57	MG	AA	3059	1/1	0.30	-	61,61,61,61	0
57	MG	DA	3527	1/1	0.26	-	52,52,52,52	0
57	MG	BA	3571	1/1	0.18	-	24,24,24,24	0
57	MG	CA	3101	1/1	0.13	-	41,41,41,41	0
57	MG	BA	3497	1/1	0.17	-	41,41,41,41	0
57	MG	DA	3018	1/1	0.27	-	51,51,51,51	0
57	MG	DA	3165	1/1	0.14	-	54,54,54,54	0
57	MG	CA	3080	1/1	0.15	-	61,61,61,61	0
57	MG	AA	3116	1/1	0.20	-	41,41,41,41	0
57	MG	BA	3631	1/1	0.09	-	53,53,53,53	0
57	MG	D8	102	1/1	0.19	-	63,63,63,63	0
57	MG	DF	3001	1/1	0.12	-	36,36,36,36	0
57	MG	CA	3086	1/1	0.13	-	56,56,56,56	0
57	MG	DA	3602	1/1	0.27	-	50,50,50,50	0
57	MG	AA	3110	1/1	0.20	-	52,52,52,52	0
57	MG	BA	3155	1/1	0.17	-	44,44,44,44	0
57	MG	BA	3233	1/1	0.31	-	55,55,55,55	0
57	MG	BA	3538	1/1	0.15	-	25,25,25,25	0
57	MG	BA	3507	1/1	0.17	-	48,48,48,48	0
57	MG	BA	3097	1/1	0.21	-	44,44,44,44	0
57	MG	BA	3199	1/1	0.22	-	60,60,60,60	0
57	MG	BA	3718	1/1	0.17	-	36,36,36,36	0
57	MG	DA	3519	1/1	0.16	-	60,60,60,60	0
57	MG	BA	3162	1/1	0.24	-	39,39,39,39	0
57	MG	AA	3106	1/1	0.07	-	53,53,53,53	0
57	MG	DA	3320	1/1	0.10	-	19,19,19,19	0
57	MG	DB	3010	1/1	0.17	-	55,55,55,55	0
57	MG	AA	3060	1/1	0.27	-	49,49,49,49	0
57	MG	DA	3177	1/1	0.31	-	29,29,29,29	0
57	MG	DA	3374	1/1	0.15	-	42,42,42,42	0
57	MG	DA	3314	1/1	0.12	-	56,56,56,56	0
57	MG	AA	3104	1/1	0.14	-	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	DA	3069	1/1	0.45	-	59,59,59,59	0
57	MG	DA	3457	1/1	0.20	-	45,45,45,45	0
57	MG	BA	3490	1/1	0.28	-	17,17,17,17	0
57	MG	BA	3366	1/1	0.20	-	38,38,38,38	0
57	MG	BF	302	1/1	0.15	-	59,59,59,59	0
57	MG	DA	3412	1/1	0.09	-	60,60,60,60	0
57	MG	CA	3131	1/1	0.14	-	57,57,57,57	0
57	MG	BA	3517	1/1	0.12	-	20,20,20,20	0
57	MG	BB	3010	1/1	0.14	-	28,28,28,28	0
57	MG	DA	3179	1/1	0.20	-	50,50,50,50	0
57	MG	BA	3446	1/1	0.08	-	49,49,49,49	0
57	MG	BA	3377	1/1	0.23	-	58,58,58,58	0
57	MG	DA	3520	1/1	0.21	-	51,51,51,51	0
57	MG	BA	3068	1/1	0.13	-	46,46,46,46	0
57	MG	DA	3448	1/1	0.23	-	36,36,36,36	0
57	MG	BY	201	1/1	0.18	-	51,51,51,51	0
57	MG	CA	3065	1/1	0.07	-	60,60,60,60	0
57	MG	DA	3542	1/1	0.07	-	44,44,44,44	0
57	MG	BA	3482	1/1	0.13	-	56,56,56,56	0
57	MG	AA	3203	1/1	0.09	-	42,42,42,42	0
57	MG	CA	3112	1/1	0.09	-	31,31,31,31	0
57	MG	CA	3059	1/1	0.13	-	60,60,60,60	0
57	MG	DA	3154	1/1	0.17	-	40,40,40,40	0
57	MG	DA	3357	1/1	0.18	-	29,29,29,29	0
57	MG	BR	203	1/1	0.31	-	31,31,31,31	0
57	MG	BN	3004	1/1	0.61	-	49,49,49,49	0
57	MG	BB	3004	1/1	0.10	-	43,43,43,43	0
57	MG	AA	3043	1/1	0.25	-	59,59,59,59	0
57	MG	AA	3154	1/1	0.20	-	46,46,46,46	0
57	MG	BA	3053	1/1	0.22	-	33,33,33,33	0
57	MG	BA	3434	1/1	0.19	-	27,27,27,27	0
57	MG	BA	3296	1/1	0.23	-	31,31,31,31	0
57	MG	BE	3004	1/1	0.09	-	49,49,49,49	0
57	MG	BB	3005	1/1	0.17	-	42,42,42,42	0
57	MG	BA	3203	1/1	0.22	-	56,56,56,56	0
57	MG	DA	3429	1/1	0.15	-	38,38,38,38	0
57	MG	BD	303	1/1	0.29	-	42,42,42,42	0
57	MG	DA	3042	1/1	0.27	-	37,37,37,37	0
57	MG	BX	101	1/1	0.26	-	36,36,36,36	0
57	MG	CA	3137	1/1	0.16	-	81,81,81,81	0
57	MG	DA	3073	1/1	0.17	-	49,49,49,49	0
57	MG	AA	3055	1/1	0.31	-	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	AA	3042	1/1	0.13	-	52,52,52,52	0
57	MG	BA	3325	1/1	0.10	-	38,38,38,38	0
57	MG	AA	3024	1/1	0.22	-	49,49,49,49	0
57	MG	BA	3387	1/1	0.15	-	29,29,29,29	0
57	MG	DA	3479	1/1	0.16	-	45,45,45,45	0
57	MG	BA	3681	1/1	0.16	-	42,42,42,42	0
57	MG	DA	3141	1/1	0.18	-	37,37,37,37	0
57	MG	DA	3181	1/1	0.18	-	36,36,36,36	0
57	MG	BA	3159	1/1	0.23	-	43,43,43,43	0
57	MG	DA	3233	1/1	0.24	-	41,41,41,41	0
57	MG	DA	3275	1/1	0.16	-	36,36,36,36	0
57	MG	DU	3004	1/1	0.17	-	69,69,69,69	0
57	MG	BA	3195	1/1	0.24	-	46,46,46,46	0
57	MG	DA	3288	1/1	0.22	-	32,32,32,32	0
57	MG	BV	203	1/1	0.10	-	31,31,31,31	0
57	MG	BA	3425	1/1	0.20	-	28,28,28,28	0
57	MG	DA	3355	1/1	0.19	-	48,48,48,48	0
57	MG	BA	3522	1/1	0.08	-	34,34,34,34	0
57	MG	BA	3580	1/1	0.26	-	13,13,13,13	0
57	MG	CA	3030	1/1	0.08	-	75,75,75,75	0
57	MG	DA	3597	1/1	0.07	-	42,42,42,42	0
57	MG	BA	3574	1/1	0.11	-	41,41,41,41	0
57	MG	B3	3001	1/1	0.10	-	43,43,43,43	0
57	MG	DQ	3003	1/1	0.24	-	59,59,59,59	0
57	MG	DA	3502	1/1	0.12	-	51,51,51,51	0
57	MG	BA	3646	1/1	0.08	-	43,43,43,43	0
57	MG	DA	3331	1/1	0.26	-	54,54,54,54	0
57	MG	BA	3464	1/1	0.20	-	26,26,26,26	0
57	MG	BA	3232	1/1	0.16	-	31,31,31,31	0
57	MG	BA	3540	1/1	0.19	-	24,24,24,24	0
57	MG	AA	3010	1/1	0.04	-	54,54,54,54	0
57	MG	DA	3401	1/1	0.11	-	36,36,36,36	0
57	MG	AX	3007	1/1	0.25	-	54,54,54,54	0
57	MG	DA	3075	1/1	0.15	-	40,40,40,40	0
57	MG	DA	3167	1/1	0.16	-	26,26,26,26	0
57	MG	BA	3305	1/1	0.15	-	45,45,45,45	0
57	MG	DA	3292	1/1	0.12	-	29,29,29,29	0
57	MG	DA	3354	1/1	0.23	-	25,25,25,25	0
57	MG	BA	3361	1/1	0.06	-	38,38,38,38	0
57	MG	BA	3133	1/1	0.19	-	29,29,29,29	0
57	MG	AA	3147	1/1	0.06	-	51,51,51,51	0
57	MG	DA	3613	1/1	0.34	-	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	DA	3256	1/1	0.11	-	52,52,52,52	0
57	MG	BW	201	1/1	0.15	-	48,48,48,48	0
57	MG	B0	102	1/1	0.12	-	53,53,53,53	0
57	MG	CA	3005	1/1	0.13	-	81,81,81,81	0
57	MG	DA	3610	1/1	0.15	-	42,42,42,42	0
57	MG	DA	3556	1/1	0.12	-	49,49,49,49	0
57	MG	DF	3002	1/1	0.11	-	51,51,51,51	0
57	MG	DA	3384	1/1	0.08	-	41,41,41,41	0
57	MG	BA	3406	1/1	0.21	-	24,24,24,24	0
57	MG	AA	3186	1/1	0.06	-	43,43,43,43	0
57	MG	DA	3011	1/1	0.10	-	36,36,36,36	0
57	MG	DA	3146	1/1	0.10	-	44,44,44,44	0
57	MG	BA	3087	1/1	0.19	-	44,44,44,44	0
57	MG	BA	3336	1/1	0.09	-	47,47,47,47	0
57	MG	BA	3704	1/1	0.10	-	31,31,31,31	0
57	MG	BA	3263	1/1	0.31	-	50,50,50,50	0
57	MG	DA	3183	1/1	0.17	-	31,31,31,31	0
57	MG	DA	3580	1/1	0.11	-	47,47,47,47	0
57	MG	BA	3363	1/1	0.18	-	31,31,31,31	0
57	MG	DA	3084	1/1	0.15	-	42,42,42,42	0
57	MG	AA	3174	1/1	0.15	-	64,64,64,64	0
57	MG	DA	3402	1/1	0.15	-	47,47,47,47	0
57	MG	BA	3566	1/1	0.17	-	31,31,31,31	0
57	MG	BA	3094	1/1	0.15	-	46,46,46,46	0
57	MG	DA	3484	1/1	0.09	-	41,41,41,41	0
57	MG	BA	3011	1/1	0.16	-	32,32,32,32	0
57	MG	BA	3272	1/1	0.20	-	38,38,38,38	0
57	MG	BA	3018	1/1	0.18	-	58,58,58,58	0
57	MG	BA	3012	1/1	0.14	-	38,38,38,38	0
57	MG	DA	3232	1/1	0.08	-	48,48,48,48	0
57	MG	BA	3274	1/1	0.16	-	44,44,44,44	0
57	MG	BA	3101	1/1	0.27	-	29,29,29,29	0
57	MG	DA	3116	1/1	0.20	-	36,36,36,36	0
57	MG	BA	3660	1/1	0.11	-	62,62,62,62	0
57	MG	DA	3062	1/1	0.30	-	49,49,49,49	0
57	MG	DA	3388	1/1	0.17	-	33,33,33,33	0
57	MG	BA	3213	1/1	0.15	-	48,48,48,48	0
57	MG	CA	3095	1/1	0.24	-	52,52,52,52	0
57	MG	CA	3132	1/1	0.12	-	51,51,51,51	0
57	MG	DA	3475	1/1	0.18	-	35,35,35,35	0
57	MG	BA	3620	1/1	0.12	-	35,35,35,35	0
57	MG	BA	3182	1/1	0.18	-	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	BA	3266	1/1	0.17	-	53,53,53,53	0
57	MG	BA	3483	1/1	0.12	-	36,36,36,36	0
57	MG	DA	3196	1/1	0.17	-	46,46,46,46	0
57	MG	BA	3337	1/1	0.14	-	51,51,51,51	0
57	MG	BA	3554	1/1	0.10	-	44,44,44,44	0
57	MG	BA	3575	1/1	0.15	-	30,30,30,30	0
57	MG	BA	3524	1/1	0.10	-	39,39,39,39	0
57	MG	AA	3048	1/1	0.16	-	42,42,42,42	0
57	MG	CA	3033	1/1	0.15	-	67,67,67,67	0
57	MG	DF	3003	1/1	0.21	-	36,36,36,36	0
57	MG	DA	3086	1/1	0.11	-	41,41,41,41	0
57	MG	AE	3002	1/1	0.15	-	61,61,61,61	0
57	MG	BA	3286	1/1	0.12	-	33,33,33,33	0
57	MG	AA	3198	1/1	0.14	-	66,66,66,66	0
59	ZN	D5	102	1/1	0.16	-	58,58,58,58	0
59	ZN	B5	102	1/1	0.15	-	41,41,41,41	0
57	MG	BA	3396	1/1	0.23	-	20,20,20,20	0
59	ZN	B6	501	1/1	0.14	-	43,43,43,43	0
57	MG	CA	3083	1/1	0.32	-	71,71,71,71	0
57	MG	AA	3184	1/1	0.09	-	56,56,56,56	0
57	MG	DA	3218	1/1	0.10	-	36,36,36,36	0
57	MG	BA	3309	1/1	0.08	-	31,31,31,31	0
57	MG	BA	3388	1/1	0.16	-	31,31,31,31	0
57	MG	DA	3136	1/1	0.14	-	62,62,62,62	0
57	MG	BA	3093	1/1	0.14	-	23,23,23,23	0
57	MG	DA	3313	1/1	0.05	-	51,51,51,51	0
57	MG	CA	3126	1/1	0.27	-	73,73,73,73	0
57	MG	DA	3047	1/1	0.17	-	44,44,44,44	0
57	MG	BA	3520	1/1	0.17	-	46,46,46,46	0
57	MG	DD	303	1/1	0.38	-	42,42,42,42	0
57	MG	CA	3025	1/1	0.17	-	66,66,66,66	0
57	MG	BB	3019	1/1	0.15	-	62,62,62,62	0
57	MG	BA	3527	1/1	0.19	-	37,37,37,37	0
57	MG	AA	3008	1/1	0.12	-	65,65,65,65	0
57	MG	DA	3323	1/1	0.07	-	39,39,39,39	0
57	MG	AA	3057	1/1	0.10	-	38,38,38,38	0
57	MG	AA	3018	1/1	0.16	-	62,62,62,62	0
57	MG	DA	3348	1/1	0.18	-	33,33,33,33	0
57	MG	AA	3076	1/1	0.20	-	62,62,62,62	0
57	MG	BA	3371	1/1	0.13	-	53,53,53,53	0
57	MG	DA	3554	1/1	0.20	-	46,46,46,46	0
57	MG	BA	3626	1/1	0.22	-	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	CA	3145	1/1	0.08	-	49,49,49,49	0
57	MG	BU	208	1/1	0.51	-	39,39,39,39	0
57	MG	BA	3489	1/1	0.22	-	36,36,36,36	0
57	MG	AA	3074	1/1	0.26	-	38,38,38,38	0
57	MG	BA	3647	1/1	0.10	-	41,41,41,41	0
57	MG	BA	3545	1/1	0.25	-	34,34,34,34	0
57	MG	BA	3238	1/1	0.25	-	26,26,26,26	0
57	MG	AA	3097	1/1	0.16	-	45,45,45,45	0
57	MG	BA	3561	1/1	0.16	-	37,37,37,37	0
57	MG	BA	3100	1/1	0.17	-	40,40,40,40	0
57	MG	BA	3449	1/1	0.14	-	31,31,31,31	0
57	MG	DA	3546	1/1	0.16	-	41,41,41,41	0
57	MG	BA	3073	1/1	0.25	-	39,39,39,39	0
57	MG	AV	3001	1/1	0.17	-	59,59,59,59	0
57	MG	BA	3169	1/1	0.13	-	40,40,40,40	0
57	MG	BA	3276	1/1	0.14	-	19,19,19,19	0
57	MG	DA	3186	1/1	0.07	-	33,33,33,33	0
57	MG	DA	3474	1/1	0.20	-	52,52,52,52	0
57	MG	DA	3488	1/1	0.11	-	47,47,47,47	0
57	MG	BA	3013	1/1	0.27	-	36,36,36,36	0
57	MG	AA	3015	1/1	0.11	-	28,28,28,28	0
57	MG	BA	3328	1/1	0.09	-	55,55,55,55	0
57	MG	BA	3095	1/1	0.22	-	29,29,29,29	0
57	MG	BD	305	1/1	0.14	-	41,41,41,41	0
57	MG	BA	3673	1/1	0.10	-	55,55,55,55	0
57	MG	BA	3193	1/1	0.18	-	30,30,30,30	0
57	MG	CA	3097	1/1	0.22	-	43,43,43,43	0
57	MG	BA	3210	1/1	0.14	-	42,42,42,42	0
57	MG	DA	3128	1/1	0.18	-	45,45,45,45	0
57	MG	DA	3477	1/1	0.10	-	37,37,37,37	0
57	MG	AA	3165	1/1	0.16	-	47,47,47,47	0
57	MG	BA	3055	1/1	0.24	-	43,43,43,43	0
57	MG	BA	3281	1/1	0.32	-	46,46,46,46	0
57	MG	DA	3552	1/1	0.17	-	43,43,43,43	0
57	MG	BA	3403	1/1	0.23	-	22,22,22,22	0
57	MG	AA	3162	1/1	0.09	-	40,40,40,40	0
57	MG	DA	3234	1/1	0.29	-	34,34,34,34	0
57	MG	DA	3112	1/1	0.15	-	63,63,63,63	0
57	MG	DA	3204	1/1	0.17	-	39,39,39,39	0
57	MG	BA	3138	1/1	0.24	-	57,57,57,57	0
57	MG	BA	3496	1/1	0.27	-	33,33,33,33	0
57	MG	CA	3074	1/1	0.21	-	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	BA	3277	1/1	0.26	-	34,34,34,34	0
57	MG	DA	3249	1/1	0.18	-	48,48,48,48	0
57	MG	AM	201	1/1	0.05	-	43,43,43,43	0
57	MG	BA	3569	1/1	0.22	-	46,46,46,46	0
57	MG	BA	3344	1/1	0.18	-	48,48,48,48	0
57	MG	BA	3249	1/1	0.18	-	44,44,44,44	0
57	MG	BA	3212	1/1	0.28	-	24,24,24,24	0
57	MG	DA	3444	1/1	0.23	-	37,37,37,37	0
57	MG	BA	3335	1/1	0.07	-	26,26,26,26	0
57	MG	DA	3600	1/1	0.09	-	45,45,45,45	0
57	MG	AA	3181	1/1	0.07	-	82,82,82,82	0
57	MG	DA	3182	1/1	0.32	-	52,52,52,52	0
57	MG	DA	3593	1/1	0.18	-	49,49,49,49	0
57	MG	BA	3532	1/1	0.23	-	39,39,39,39	0
57	MG	DA	3441	1/1	0.25	-	43,43,43,43	0
57	MG	BA	3676	1/1	0.18	-	44,44,44,44	0
57	MG	BA	3623	1/1	0.14	-	42,42,42,42	0
57	MG	CA	3057	1/1	0.13	-	48,48,48,48	0
57	MG	BA	3128	1/1	0.14	-	33,33,33,33	0
57	MG	BA	3605	1/1	0.21	-	44,44,44,44	0
57	MG	DA	3009	1/1	0.10	-	39,39,39,39	0
57	MG	BA	3603	1/1	0.18	-	42,42,42,42	0
57	MG	BA	3644	1/1	0.18	-	48,48,48,48	0
57	MG	BA	3050	1/1	0.09	-	44,44,44,44	0
57	MG	BA	3711	1/1	0.15	-	46,46,46,46	0
57	MG	DA	3471	1/1	0.22	-	23,23,23,23	0
57	MG	AA	3037	1/1	0.09	-	48,48,48,48	0
57	MG	BA	3717	1/1	0.46	-	40,40,40,40	0
57	MG	DA	3033	1/1	0.15	-	46,46,46,46	0
57	MG	DA	3327	1/1	0.12	-	49,49,49,49	0
57	MG	BP	3004	1/1	0.11	-	41,41,41,41	0
57	MG	DA	3297	1/1	0.13	-	48,48,48,48	0
57	MG	CA	3011	1/1	0.25	-	39,39,39,39	0
57	MG	BA	3327	1/1	0.16	-	32,32,32,32	0
57	MG	DA	3623	1/1	0.14	-	31,31,31,31	0
57	MG	DA	3538	1/1	0.21	-	77,77,77,77	0
57	MG	BA	3234	1/1	0.37	-	39,39,39,39	0
57	MG	BA	3297	1/1	0.22	-	36,36,36,36	0
57	MG	CA	3123	1/1	0.08	-	53,53,53,53	0
57	MG	BA	3347	1/1	0.21	-	32,32,32,32	0
57	MG	BA	3267	1/1	0.34	-	33,33,33,33	0
57	MG	AA	3061	1/1	0.09	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	3108	1/1	0.12	-	51,51,51,51	0
57	MG	DA	3548	1/1	0.15	-	58,58,58,58	0
57	MG	BA	3592	1/1	0.14	-	14,14,14,14	0
57	MG	DA	3416	1/1	0.06	-	46,46,46,46	0
57	MG	AX	3002	1/1	0.17	-	67,67,67,67	0
57	MG	DA	3446	1/1	0.18	-	37,37,37,37	0
57	MG	CA	3054	1/1	0.34	-	53,53,53,53	0
57	MG	DA	3029	1/1	0.15	-	44,44,44,44	0
57	MG	BA	3458	1/1	0.13	-	40,40,40,40	0
57	MG	CA	3014	1/1	0.11	-	58,58,58,58	0
57	MG	DA	3524	1/1	0.10	-	40,40,40,40	0
57	MG	AA	3016	1/1	0.13	-	52,52,52,52	0
57	MG	CA	3073	1/1	0.05	-	57,57,57,57	0
57	MG	DA	3117	1/1	0.14	-	40,40,40,40	0
57	MG	DA	3309	1/1	0.11	-	34,34,34,34	0
57	MG	BU	203	1/1	0.23	-	35,35,35,35	0
57	MG	DA	3396	1/1	0.08	-	43,43,43,43	0
57	MG	DA	3024	1/1	0.13	-	29,29,29,29	0
57	MG	DA	3557	1/1	0.07	-	54,54,54,54	0
57	MG	DA	3159	1/1	0.12	-	32,32,32,32	0
57	MG	BA	3418	1/1	0.21	-	26,26,26,26	0
57	MG	BA	3495	1/1	0.24	-	47,47,47,47	0
57	MG	BA	3127	1/1	0.25	-	41,41,41,41	0
57	MG	BA	3010	1/1	0.17	-	45,45,45,45	0
57	MG	BA	3329	1/1	0.15	-	21,21,21,21	0
57	MG	BA	3684	1/1	0.09	-	47,47,47,47	0
57	MG	BA	3231	1/1	0.15	-	42,42,42,42	0
57	MG	AA	3159	1/1	0.10	-	31,31,31,31	0
57	MG	BA	3480	1/1	0.23	-	50,50,50,50	0
57	MG	CA	3087	1/1	0.11	-	50,50,50,50	0
57	MG	CA	3061	1/1	0.11	-	87,87,87,87	0
57	MG	AA	3105	1/1	0.20	-	59,59,59,59	0
57	MG	BA	3450	1/1	0.08	-	45,45,45,45	0
57	MG	CA	3134	1/1	0.19	-	72,72,72,72	0
57	MG	AA	3080	1/1	0.15	-	82,82,82,82	0
57	MG	BA	3172	1/1	0.16	-	27,27,27,27	0
57	MG	BA	3198	1/1	0.19	-	45,45,45,45	0
57	MG	BA	3708	1/1	0.19	-	38,38,38,38	0
57	MG	BA	3257	1/1	0.30	-	40,40,40,40	0
57	MG	DA	3078	1/1	0.05	-	49,49,49,49	0
57	MG	CA	3042	1/1	0.15	-	68,68,68,68	0
57	MG	DA	3370	1/1	0.12	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	3040	1/1	0.18	-	67,67,67,67	0
57	MG	DA	3615	1/1	0.15	-	36,36,36,36	0
57	MG	BA	3362	1/1	0.10	-	43,43,43,43	0
57	MG	BA	3583	1/1	0.10	-	54,54,54,54	0
57	MG	BA	3413	1/1	0.09	-	50,50,50,50	0
57	MG	BA	3593	1/1	0.16	-	36,36,36,36	0
57	MG	CA	3103	1/1	0.15	-	71,71,71,71	0
57	MG	BA	3475	1/1	0.07	-	31,31,31,31	0
57	MG	DA	3564	1/1	0.15	-	48,48,48,48	0
57	MG	BB	3014	1/1	0.07	-	41,41,41,41	0
57	MG	AA	3091	1/1	0.23	-	35,35,35,35	0
57	MG	BA	3307	1/1	0.27	-	31,31,31,31	0
57	MG	BB	3013	1/1	0.18	-	43,43,43,43	0
57	MG	BA	3129	1/1	0.12	-	30,30,30,30	0
57	MG	BA	3354	1/1	0.10	-	31,31,31,31	0
57	MG	BV	201	1/1	0.21	-	33,33,33,33	0
57	MG	BD	307	1/1	0.20	-	40,40,40,40	0
57	MG	AA	3032	1/1	0.11	-	80,80,80,80	0
57	MG	DA	3016	1/1	0.11	-	34,34,34,34	0
57	MG	BA	3578	1/1	0.13	-	43,43,43,43	0
57	MG	AA	3143	1/1	0.14	-	32,32,32,32	0
57	MG	DA	3467	1/1	0.14	-	28,28,28,28	0
57	MG	BA	3686	1/1	0.26	-	36,36,36,36	0
57	MG	DA	3365	1/1	0.10	-	54,54,54,54	0
57	MG	AA	3114	1/1	0.29	-	57,57,57,57	0
57	MG	DA	3426	1/1	0.33	-	38,38,38,38	0
57	MG	DA	3403	1/1	0.11	-	31,31,31,31	0
57	MG	BN	3005	1/1	0.20	-	31,31,31,31	0
57	MG	CA	3034	1/1	0.23	-	49,49,49,49	0
57	MG	DA	3399	1/1	0.10	-	26,26,26,26	0
57	MG	AA	3188	1/1	0.08	-	62,62,62,62	0
57	MG	DA	3523	1/1	0.11	-	45,45,45,45	0
57	MG	DA	3452	1/1	0.16	-	40,40,40,40	0
57	MG	BB	3001	1/1	0.15	-	44,44,44,44	0
57	MG	BA	3516	1/1	0.15	-	32,32,32,32	0
57	MG	BG	3002	1/1	0.12	-	65,65,65,65	0
57	MG	CA	3119	1/1	0.10	-	74,74,74,74	0
57	MG	BA	3285	1/1	0.17	-	21,21,21,21	0
57	MG	BA	3236	1/1	0.15	-	39,39,39,39	0
57	MG	DA	3584	1/1	0.14	-	63,63,63,63	0
57	MG	CA	3142	1/1	0.19	-	55,55,55,55	0
57	MG	DA	3145	1/1	0.20	-	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	BA	3712	1/1	0.10	-	30,30,30,30	0
57	MG	BA	3404	1/1	0.20	-	30,30,30,30	0
57	MG	DA	3375	1/1	0.22	-	30,30,30,30	0
57	MG	AA	3047	1/1	0.22	-	59,59,59,59	0
57	MG	BA	3208	1/1	0.09	-	33,33,33,33	0
57	MG	BA	3175	1/1	0.16	-	55,55,55,55	0
59	ZN	D6	501	1/1	0.15	-	64,64,64,64	0
57	MG	BA	3394	1/1	0.15	-	22,22,22,22	0
57	MG	BA	3465	1/1	0.17	-	44,44,44,44	0
57	MG	BA	3500	1/1	0.09	-	54,54,54,54	0
57	MG	DA	3121	1/1	0.11	-	39,39,39,39	0
57	MG	DA	3394	1/1	0.10	-	48,48,48,48	0
57	MG	BA	3166	1/1	0.24	-	45,45,45,45	0
57	MG	DA	3224	1/1	0.24	-	60,60,60,60	0
57	MG	DA	3347	1/1	0.18	-	32,32,32,32	0
57	MG	DA	3279	1/1	0.27	-	50,50,50,50	0
57	MG	CA	3084	1/1	0.14	-	58,58,58,58	0
57	MG	DA	3334	1/1	0.09	-	31,31,31,31	0
57	MG	DG	3001	1/1	0.10	-	49,49,49,49	0
57	MG	BA	3611	1/1	0.13	-	61,61,61,61	0
57	MG	DA	3499	1/1	0.12	-	47,47,47,47	0
57	MG	BA	3405	1/1	0.19	-	31,31,31,31	0
57	MG	BA	3476	1/1	0.12	-	37,37,37,37	0
57	MG	BA	3487	1/1	0.11	-	70,70,70,70	0
57	MG	BA	3460	1/1	0.15	-	43,43,43,43	0
57	MG	AA	3118	1/1	0.15	-	50,50,50,50	0
57	MG	AD	301	1/1	0.12	-	47,47,47,47	0
57	MG	BA	3395	1/1	0.16	-	19,19,19,19	0
57	MG	DA	3147	1/1	0.15	-	42,42,42,42	0
57	MG	AA	3102	1/1	0.20	-	52,52,52,52	0
57	MG	BA	3359	1/1	0.12	-	56,56,56,56	0
57	MG	BA	3573	1/1	0.13	-	29,29,29,29	0
57	MG	CA	3008	1/1	0.12	-	67,67,67,67	0
57	MG	DA	3336	1/1	0.16	-	38,38,38,38	0
57	MG	BA	3683	1/1	0.25	-	44,44,44,44	0
57	MG	DA	3626	1/1	0.19	-	38,38,38,38	0
57	MG	BA	3652	1/1	0.15	-	65,65,65,65	0
57	MG	DA	3418	1/1	0.19	-	41,41,41,41	0
57	MG	CA	3069	1/1	0.36	-	56,56,56,56	0
57	MG	DA	3035	1/1	0.15	-	45,45,45,45	0
57	MG	BA	3188	1/1	0.19	-	48,48,48,48	0
57	MG	DA	3048	1/1	0.14	-	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	BA	3370	1/1	0.17	-	32,32,32,32	0
57	MG	AA	3126	1/1	0.15	-	52,52,52,52	0
57	MG	DA	3415	1/1	0.31	-	55,55,55,55	0
57	MG	BA	3679	1/1	0.18	-	38,38,38,38	0
57	MG	DA	3140	1/1	0.14	-	38,38,38,38	0
57	MG	BA	3443	1/1	0.23	-	38,38,38,38	0
57	MG	BA	3265	1/1	0.13	-	30,30,30,30	0
57	MG	DA	3534	1/1	0.12	-	30,30,30,30	0
58	SF4	AD	302	8/8	0.15	-	59,71,78,78	0
57	MG	DA	3455	1/1	0.32	-	34,34,34,34	0
57	MG	BA	3185	1/1	0.47	-	34,34,34,34	0
57	MG	DA	3065	1/1	0.09	-	38,38,38,38	0
57	MG	BA	3617	1/1	0.12	-	59,59,59,59	0
57	MG	DA	3592	1/1	0.14	-	62,62,62,62	0
57	MG	AA	3020	1/1	0.17	-	62,62,62,62	0
57	MG	DA	3485	1/1	0.17	-	41,41,41,41	0
57	MG	CA	3133	1/1	0.15	-	69,69,69,69	0
57	MG	DA	3212	1/1	0.07	-	47,47,47,47	0
57	MG	CA	3036	1/1	0.08	-	47,47,47,47	0
57	MG	DA	3206	1/1	0.19	-	37,37,37,37	0
57	MG	BA	3525	1/1	0.15	-	49,49,49,49	0
57	MG	BA	3067	1/1	0.21	-	26,26,26,26	0
57	MG	BA	3429	1/1	0.14	-	37,37,37,37	0
57	MG	DA	3378	1/1	0.13	-	33,33,33,33	0
57	MG	AA	3145	1/1	0.21	-	71,71,71,71	0
57	MG	BB	3016	1/1	0.06	-	39,39,39,39	0
57	MG	BA	3659	1/1	0.14	-	47,47,47,47	0
57	MG	AS	101	1/1	0.09	-	55,55,55,55	0
57	MG	BA	3570	1/1	0.11	-	48,48,48,48	0
57	MG	DA	3315	1/1	0.16	-	57,57,57,57	0
57	MG	DA	3555	1/1	0.14	-	70,70,70,70	0
57	MG	CA	3089	1/1	0.12	-	65,65,65,65	0
57	MG	DA	3569	1/1	0.15	-	42,42,42,42	0
57	MG	BA	3639	1/1	0.14	-	46,46,46,46	0
57	MG	AA	3129	1/1	0.15	-	37,37,37,37	0
57	MG	CA	3160	1/1	0.35	-	49,49,49,49	0
57	MG	CA	3049	1/1	0.11	-	42,42,42,42	0
57	MG	BA	3020	1/1	0.27	-	55,55,55,55	0
57	MG	CX	3002	1/1	0.27	-	75,75,75,75	0
57	MG	AA	3071	1/1	0.38	-	41,41,41,41	0
59	ZN	B9	501	1/1	0.12	-	59,59,59,59	0
57	MG	DA	3126	1/1	0.12	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	3031	1/1	0.11	-	41,41,41,41	0
57	MG	AA	3168	1/1	0.12	-	56,56,56,56	0
57	MG	DA	3193	1/1	0.17	-	43,43,43,43	0
57	MG	BA	3243	1/1	0.19	-	46,46,46,46	0
57	MG	AA	3158	1/1	0.09	-	72,72,72,72	0
57	MG	DA	3214	1/1	0.13	-	43,43,43,43	0
57	MG	B3	3002	1/1	0.15	-	58,58,58,58	0
57	MG	BA	3306	1/1	0.21	-	32,32,32,32	0
57	MG	DA	3266	1/1	0.12	-	45,45,45,45	0
57	MG	DB	3002	1/1	0.07	-	75,75,75,75	0
57	MG	DA	3361	1/1	0.16	-	32,32,32,32	0
57	MG	AA	3085	1/1	0.18	-	69,69,69,69	0
57	MG	DA	3337	1/1	0.21	-	46,46,46,46	0
57	MG	BA	3295	1/1	0.14	-	56,56,56,56	0
57	MG	DA	3142	1/1	0.18	-	50,50,50,50	0
57	MG	BA	3028	1/1	0.14	-	31,31,31,31	0
57	MG	DA	3125	1/1	0.10	-	48,48,48,48	0
57	MG	AA	3092	1/1	0.14	-	36,36,36,36	0
57	MG	AA	3014	1/1	0.08	-	73,73,73,73	0
57	MG	DA	3312	1/1	0.19	-	30,30,30,30	0
57	MG	BA	3555	1/1	0.07	-	62,62,62,62	0
57	MG	BA	3130	1/1	0.42	-	39,39,39,39	0
57	MG	AA	3103	1/1	0.17	-	42,42,42,42	0
57	MG	DA	3246	1/1	0.30	-	57,57,57,57	0
57	MG	BA	3025	1/1	0.18	-	12,12,12,12	0
57	MG	BA	3615	1/1	0.10	-	60,60,60,60	0
57	MG	BA	3627	1/1	0.08	-	28,28,28,28	0
57	MG	BA	3310	1/1	0.18	-	43,43,43,43	0
57	MG	BA	3697	1/1	0.15	-	23,23,23,23	0
57	MG	DA	3151	1/1	0.15	-	48,48,48,48	0
57	MG	D3	3001	1/1	0.15	-	54,54,54,54	0
57	MG	DU	3001	1/1	0.62	-	56,56,56,56	0
57	MG	DA	3244	1/1	0.19	-	43,43,43,43	0
57	MG	BA	3640	1/1	0.13	-	53,53,53,53	0
57	MG	DA	3411	1/1	0.10	-	51,51,51,51	0
57	MG	DB	3007	1/1	0.08	-	55,55,55,55	0
57	MG	CA	3092	1/1	0.14	-	76,76,76,76	0
57	MG	DA	3595	1/1	0.14	-	65,65,65,65	0
57	MG	BA	3124	1/1	0.11	-	31,31,31,31	0
57	MG	BA	3299	1/1	0.21	-	27,27,27,27	0
57	MG	BA	3422	1/1	0.17	-	39,39,39,39	0
57	MG	DA	3588	1/1	0.13	-	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3435	1/1	0.21	-	31,31,31,31	0
57	MG	BA	3582	1/1	0.15	-	23,23,23,23	0
57	MG	BA	3303	1/1	0.23	-	39,39,39,39	0
57	MG	BA	3260	1/1	0.25	-	45,45,45,45	0
57	MG	AN	503	1/1	0.14	-	61,61,61,61	0
57	MG	DA	3305	1/1	0.07	-	48,48,48,48	0
57	MG	AJ	201	1/1	0.07	-	67,67,67,67	0
57	MG	BB	3018	1/1	0.11	-	43,43,43,43	0
57	MG	BA	3553	1/1	0.19	-	41,41,41,41	0
57	MG	DA	3480	1/1	0.11	-	28,28,28,28	0
57	MG	BA	3179	1/1	0.16	-	49,49,49,49	0
57	MG	BA	3239	1/1	0.16	-	42,42,42,42	0
57	MG	BA	3014	1/1	0.09	-	46,46,46,46	0
57	MG	DA	3135	1/1	0.17	-	61,61,61,61	0
57	MG	DA	3299	1/1	0.12	-	32,32,32,32	0
57	MG	BA	3379	1/1	0.09	-	69,69,69,69	0
57	MG	DA	3359	1/1	0.13	-	42,42,42,42	0
57	MG	CE	3001	1/1	0.18	-	80,80,80,80	0
57	MG	DA	3609	1/1	0.25	-	55,55,55,55	0
57	MG	BA	3105	1/1	0.21	-	45,45,45,45	0
57	MG	DA	3123	1/1	0.17	-	45,45,45,45	0
57	MG	DA	3017	1/1	0.17	-	58,58,58,58	0
57	MG	AA	3132	1/1	0.21	-	67,67,67,67	0
57	MG	BA	3345	1/1	0.11	-	36,36,36,36	0
57	MG	DA	3468	1/1	0.23	-	64,64,64,64	0
57	MG	BA	3316	1/1	0.16	-	49,49,49,49	0
57	MG	DA	3225	1/1	0.12	-	42,42,42,42	0
57	MG	DA	3517	1/1	0.17	-	36,36,36,36	0
57	MG	DA	3082	1/1	0.14	-	47,47,47,47	0
57	MG	BA	3001	1/1	0.18	-	48,48,48,48	0
57	MG	BP	3001	1/1	0.40	-	49,49,49,49	0
57	MG	DA	3576	1/1	0.22	-	46,46,46,46	0
57	MG	CA	3128	1/1	0.11	-	43,43,43,43	0
57	MG	BA	3255	1/1	0.06	-	37,37,37,37	0
57	MG	CA	3125	1/1	0.14	-	64,64,64,64	0
57	MG	BA	3008	1/1	0.09	-	22,22,22,22	0
57	MG	DA	3139	1/1	0.18	-	49,49,49,49	0
57	MG	DA	3598	1/1	0.10	-	48,48,48,48	0
57	MG	BA	3612	1/1	0.20	-	58,58,58,58	0
57	MG	DA	3364	1/1	0.18	-	49,49,49,49	0
57	MG	DA	3230	1/1	0.21	-	46,46,46,46	0
57	MG	BB	3008	1/1	0.09	-	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	3213	1/1	0.28	-	51,51,51,51	0
57	MG	BW	203	1/1	0.14	-	39,39,39,39	0
57	MG	AA	3152	1/1	0.08	-	64,64,64,64	0
57	MG	BA	3326	1/1	0.13	-	40,40,40,40	0
57	MG	DA	3080	1/1	0.09	-	64,64,64,64	0
57	MG	DA	3568	1/1	0.12	-	45,45,45,45	0
57	MG	DA	3287	1/1	0.24	-	58,58,58,58	0
57	MG	DA	3482	1/1	0.21	-	31,31,31,31	0
57	MG	CA	3153	1/1	0.13	-	57,57,57,57	0
57	MG	BA	3214	1/1	0.18	-	48,48,48,48	0
57	MG	DA	3038	1/1	0.07	-	39,39,39,39	0
57	MG	BA	3619	1/1	0.14	-	54,54,54,54	0
57	MG	BA	3280	1/1	0.17	-	46,46,46,46	0
57	MG	B5	103	1/1	0.09	-	50,50,50,50	0
57	MG	BA	3634	1/1	0.24	-	58,58,58,58	0
57	MG	BA	3226	1/1	0.37	-	36,36,36,36	0
57	MG	DA	3248	1/1	0.26	-	59,59,59,59	0
57	MG	CA	3130	1/1	0.16	-	88,88,88,88	0
57	MG	CA	3150	1/1	0.07	-	66,66,66,66	0
57	MG	BA	3029	1/1	0.18	-	53,53,53,53	0
57	MG	BA	3201	1/1	0.11	-	44,44,44,44	0
57	MG	BA	3278	1/1	0.05	-	38,38,38,38	0
57	MG	CK	3001	1/1	0.20	-	57,57,57,57	0
57	MG	DA	3228	1/1	0.26	-	49,49,49,49	0
57	MG	BA	3353	1/1	0.07	-	46,46,46,46	0
57	MG	AA	3052	1/1	0.15	-	53,53,53,53	0
57	MG	DA	3238	1/1	0.40	-	31,31,31,31	0
57	MG	DP	201	1/1	0.35	-	61,61,61,61	0
57	MG	CA	3158	1/1	0.16	-	66,66,66,66	0
57	MG	DA	3498	1/1	0.07	-	66,66,66,66	0
57	MG	BA	3333	1/1	0.09	-	58,58,58,58	0
57	MG	AA	3098	1/1	0.19	-	42,42,42,42	0
57	MG	CA	3058	1/1	0.34	-	70,70,70,70	0
57	MG	BD	311	1/1	0.40	-	60,60,60,60	0
57	MG	AA	3191	1/1	0.19	-	56,56,56,56	0
57	MG	CA	3093	1/1	0.15	-	69,69,69,69	0
57	MG	CA	3135	1/1	0.12	-	85,85,85,85	0
57	MG	DA	3424	1/1	0.09	-	56,56,56,56	0
57	MG	DA	3500	1/1	0.13	-	32,32,32,32	0
57	MG	BB	3006	1/1	0.18	-	42,42,42,42	0
57	MG	AA	3021	1/1	0.15	-	58,58,58,58	0
57	MG	BA	3664	1/1	0.11	-	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	DA	3624	1/1	0.29	-	66,66,66,66	0
57	MG	DA	3392	1/1	0.19	-	40,40,40,40	0
57	MG	BA	3324	1/1	0.16	-	61,61,61,61	0
57	MG	DA	3307	1/1	0.16	-	51,51,51,51	0
57	MG	CA	3051	1/1	0.27	-	57,57,57,57	0
57	MG	BA	3196	1/1	0.25	-	51,51,51,51	0
57	MG	AA	3087	1/1	0.14	-	57,57,57,57	0
57	MG	BA	3145	1/1	0.13	-	41,41,41,41	0
57	MG	AA	3135	1/1	0.06	-	52,52,52,52	0
57	MG	BA	3649	1/1	0.10	-	65,65,65,65	0
57	MG	DA	3131	1/1	0.12	-	34,34,34,34	0
57	MG	AA	3207	1/1	0.08	-	57,57,57,57	0
57	MG	BA	3385	1/1	0.26	-	34,34,34,34	0
57	MG	BA	3221	1/1	0.21	-	59,59,59,59	0
57	MG	DA	3269	1/1	0.14	-	40,40,40,40	0
57	MG	BA	3279	1/1	0.23	-	48,48,48,48	0
57	MG	DA	3158	1/1	0.13	-	52,52,52,52	0
57	MG	BA	3153	1/1	0.07	-	53,53,53,53	0
57	MG	DA	3273	1/1	0.14	-	41,41,41,41	0
57	MG	BA	3122	1/1	0.25	-	39,39,39,39	0
57	MG	BA	3590	1/1	0.24	-	62,62,62,62	0
57	MG	DA	3431	1/1	0.15	-	56,56,56,56	0
57	MG	DA	3447	1/1	0.11	-	48,48,48,48	0
57	MG	DA	3032	1/1	0.16	-	34,34,34,34	0
57	MG	AA	3137	1/1	0.26	-	66,66,66,66	0
57	MG	BB	3017	1/1	0.08	-	28,28,28,28	0
57	MG	BA	3004	1/1	0.14	-	26,26,26,26	0
57	MG	AA	3200	1/1	0.11	-	58,58,58,58	0
57	MG	BA	3086	1/1	0.21	-	15,15,15,15	0
57	MG	AE	3001	1/1	0.31	-	85,85,85,85	0
57	MG	BA	3462	1/1	0.19	-	51,51,51,51	0
57	MG	DA	3565	1/1	0.20	-	49,49,49,49	0
57	MG	DA	3462	1/1	0.27	-	35,35,35,35	0
57	MG	BA	3294	1/1	0.22	-	37,37,37,37	0
57	MG	BA	3439	1/1	0.15	-	12,12,12,12	0
57	MG	DA	3435	1/1	0.13	-	59,59,59,59	0
57	MG	BA	3241	1/1	0.29	-	53,53,53,53	0
57	MG	DA	3583	1/1	0.12	-	44,44,44,44	0
57	MG	CA	3078	1/1	0.17	-	63,63,63,63	0
57	MG	BA	3667	1/1	0.17	-	31,31,31,31	0
57	MG	DA	3052	1/1	0.10	-	33,33,33,33	0
57	MG	CA	3140	1/1	0.06	-	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	DA	3389	1/1	0.14	-	31,31,31,31	0
57	MG	DA	3236	1/1	0.09	-	45,45,45,45	0
57	MG	BA	3161	1/1	0.25	-	54,54,54,54	0
57	MG	DA	3406	1/1	0.14	-	62,62,62,62	0
57	MG	BA	3323	1/1	0.09	-	59,59,59,59	0
57	MG	DA	3284	1/1	0.20	-	51,51,51,51	0
57	MG	CA	3024	1/1	0.06	-	58,58,58,58	0
57	MG	B5	101	1/1	0.20	-	30,30,30,30	0
57	MG	DA	3381	1/1	0.24	-	55,55,55,55	0
57	MG	BA	3158	1/1	0.36	-	48,48,48,48	0
57	MG	CA	3116	1/1	0.34	-	74,74,74,74	0
57	MG	BA	3343	1/1	0.17	-	18,18,18,18	0
57	MG	DA	3421	1/1	0.07	-	31,31,31,31	0
57	MG	CA	3088	1/1	0.11	-	61,61,61,61	0
57	MG	AA	3069	1/1	0.12	-	75,75,75,75	0
57	MG	AA	3046	1/1	0.24	-	72,72,72,72	0
57	MG	BA	3463	1/1	0.10	-	43,43,43,43	0
57	MG	DA	3271	1/1	0.16	-	47,47,47,47	0
57	MG	DA	3068	1/1	0.16	-	48,48,48,48	0
57	MG	BA	3448	1/1	0.08	-	42,42,42,42	0
57	MG	BA	3680	1/1	0.13	-	46,46,46,46	0
57	MG	DA	3428	1/1	0.20	-	46,46,46,46	0
57	MG	DA	3329	1/1	0.20	-	54,54,54,54	0
57	MG	CA	3156	1/1	0.04	-	57,57,57,57	0
57	MG	DA	3040	1/1	0.38	-	48,48,48,48	0

6.5 Other polymers ⓘ

There are no such residues in this entry.