



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 06:59 PM BST

PDB ID : 4V51
Title : Structure of the *Thermus thermophilus* 70S ribosome complexed with mRNA, tRNA and paromomycin
Authors : Selmer, M.; Dunham, C.M.; Murphy, F.V.; Weixlbaumer, A.; Petry, S.; Weir, J.R.; Kelley, A.C.; Ramakrishnan, V.
Deposited on : 2006-07-31
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>

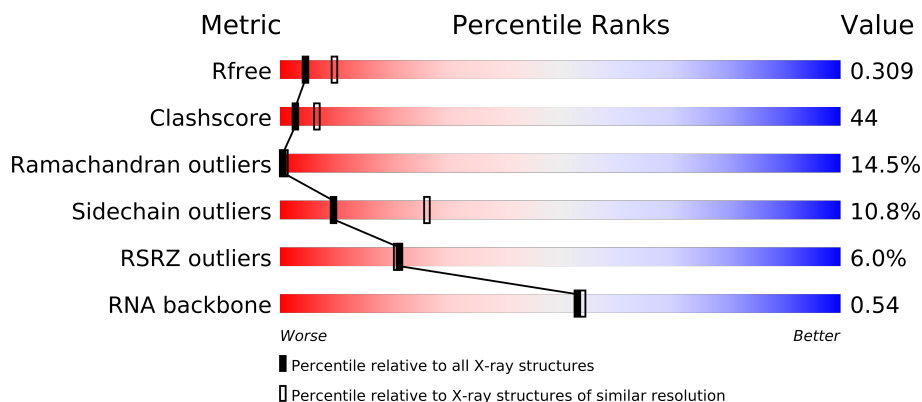
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 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	1522	
1	CA	1522	
2	AB	256	
2	CB	256	
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	

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Mol	Chain	Length	Quality of chain
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	135	
12	CL	135	
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	77	
22	CV	77	
23	AW	76	
23	AY	76	
23	CW	76	
23	CY	76	
24	AX	24	
24	CX	24	
25	B0	85	
25	D0	85	
26	B1	98	
26	D1	98	

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Mol	Chain	Length	Quality of chain
27	B2	72	
27	D2	72	
28	B3	60	
28	D3	60	
29	B4	71	
29	D4	71	
30	B5	60	
30	D5	60	
31	B6	54	
31	D6	54	
32	B7	49	
32	D7	49	
33	B8	65	
33	D8	65	
34	BA	2787	
34	DA	2787	
35	BB	122	
35	DB	122	
36	BC	229	
36	DC	229	
37	BD	276	
37	DD	276	
38	BE	206	
38	DE	206	
39	BF	210	
39	DF	210	
40	BG	182	
40	DG	182	
41	BH	180	
41	DH	180	
42	BI	148	
42	DI	148	
43	BN	140	
43	DN	140	
44	BO	122	
44	DO	122	
45	BP	150	
45	DP	150	
46	BQ	141	
46	DQ	141	
47	BR	118	
47	DR	118	

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Mol	Chain	Length	Quality of chain
48	BS	112	
48	DS	112	
49	BT	146	
49	DT	146	
50	BU	118	
50	DU	118	
51	BV	101	
51	DV	101	
52	BW	113	
52	DW	113	
53	BX	96	
53	DX	96	
54	BY	110	
54	DY	110	
55	BZ	206	
55	DZ	206	

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 291077 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 RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			
3	CC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	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
			1703	1066	339	291	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			
5	CE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	CF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	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
			1257	781	252	218	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	CH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- 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
			1011	639	198	174				
9	CI	127	Total	C	N	O		0	0	0
			1011	639	198	174				

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	CK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			
12	CL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			
13	CM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	CO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			
16	CP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			
17	CQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	CR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			
19	CS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	CT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	25	Total	C	N	O	0	0	1
			209	128	51	30			
21	CU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0	0
			1645	733	297	538	77			
22	CV	77	Total	C	N	O	P	0	0	0
			1645	733	297	538	77			

- Molecule 23 is a RNA chain called E-SITE TRNA PHE OR A-SITE TRNA PHE (UNMODIFIED BASES).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			
23	AY	19	Total	C	N	O	P	0	0	0
			407	183	78	128	18			
23	CW	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			
23	CY	19	Total	C	N	O	P	0	0	0
			407	183	78	128	18			

- Molecule 24 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	11	Total	C	N	O	P	0	0	0
			236	106	44	75	11			
24	CX	11	Total	C	N	O	P	0	0	0
			236	106	44	75	11			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	B0	85	Total	C	N	O	S	0	0	0
			650	401	137	111	1			
25	D0	85	Total	C	N	O	S	0	0	0
			650	401	137	111	1			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	B1	89	Total	C	N	O	0	0	1
			693	435	140	118			
26	D1	89	Total	C	N	O	0	0	1
			693	435	140	118			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B2	51	Total	C	N	O	S	0	0	1
			421	263	85	72	1			
27	D2	51	Total	C	N	O	S	0	0	1
			421	263	85	72	1			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			
28	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
29	B4	50	Total	C	N	O	0	0	1
			242	143	50	49			
29	D4	50	Total	C	N	O	0	0	1
			242	143	50	49			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
30	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			
31	D6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			
32	D7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			
33	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 34 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BA	2772	Total	C	N	O	P	0	0	0
			59708	26573	11171	19193	2771			
34	DA	2772	Total	C	N	O	P	0	0	0
			59708	26573	11171	19193	2771			

- Molecule 35 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
35	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 36 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	BC	191	Total	C	N	O	0	0	1
			1142	691	221	230			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	DC	191	Total	C	N	O	0	0	1
			1142	691	221	230			

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			
37	DD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			
38	DE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			
39	DF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
40	DG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			
41	DH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			
42	DI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			
43	DN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
45	DP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BQ	136	Total	C	N	O	S	0	0	0
			1080	688	204	183	5			
46	DQ	136	Total	C	N	O	S	0	0	0
			1080	688	204	183	5			

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	BR	117	Total	C	N	O	0	0	0
			960	599	202	159			
47	DR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	BS	99	Total	C	N	O	0	0	1
			771	486	155	130			
48	DS	99	Total	C	N	O	0	0	1
			771	486	155	130			

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			
49	DT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			
50	DU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
51	DV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	DW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BX	93	Total	C	N	O		0	0	1
			726	471	132	123				
53	DX	93	Total	C	N	O		0	0	1
			726	471	132	123				

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			
54	DY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			
55	DZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BA	454	Total	Mg	0	0
			454	454		
56	CA	189	Total	Mg	0	0
			189	189		
56	DF	1	Total	Mg	0	0
			1	1		
56	CV	4	Total	Mg	0	0
			4	4		
56	BE	1	Total	Mg	0	0
			1	1		
56	AW	22	Total	Mg	0	0
			22	22		

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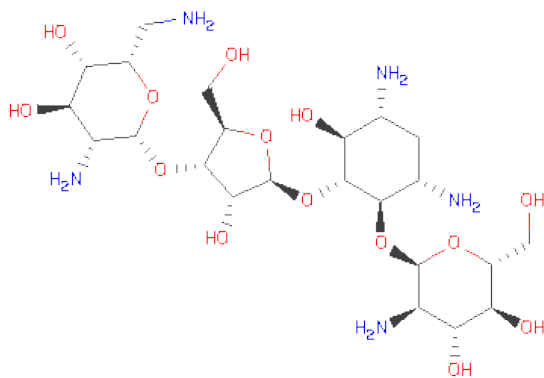
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DU	1	Total 1	Mg 1	0	0
56	B1	1	Total 1	Mg 1	0	0
56	DZ	1	Total 1	Mg 1	0	0
56	AX	4	Total 4	Mg 4	0	0
56	DD	2	Total 2	Mg 2	0	0
56	B5	2	Total 2	Mg 2	0	0
56	BB	19	Total 19	Mg 19	0	0
56	DO	1	Total 1	Mg 1	0	0
56	AE	1	Total 1	Mg 1	0	0
56	CU	1	Total 1	Mg 1	0	0
56	BF	2	Total 2	Mg 2	0	0
56	AV	7	Total 7	Mg 7	0	0
56	BX	1	Total 1	Mg 1	0	0
56	B2	5	Total 5	Mg 5	0	0
56	AA	215	Total 215	Mg 215	0	0
56	CX	6	Total 6	Mg 6	0	0
56	BN	1	Total 1	Mg 1	0	0
56	DH	1	Total 1	Mg 1	0	0
56	DS	1	Total 1	Mg 1	0	0
56	DE	1	Total 1	Mg 1	0	0
56	B3	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CJ	1	Total 1	Mg 1	0	0
56	DA	398	Total 398	Mg 398	0	0
56	B7	2	Total 2	Mg 2	0	0
56	CF	1	Total 1	Mg 1	0	0
56	BV	1	Total 1	Mg 1	0	0
56	CM	1	Total 1	Mg 1	0	0
56	BO	1	Total 1	Mg 1	0	0
56	CW	13	Total 13	Mg 13	0	0
56	D5	2	Total 2	Mg 2	0	0
56	DN	1	Total 1	Mg 1	0	0
56	AY	1	Total 1	Mg 1	0	0
56	DB	12	Total 12	Mg 12	0	0

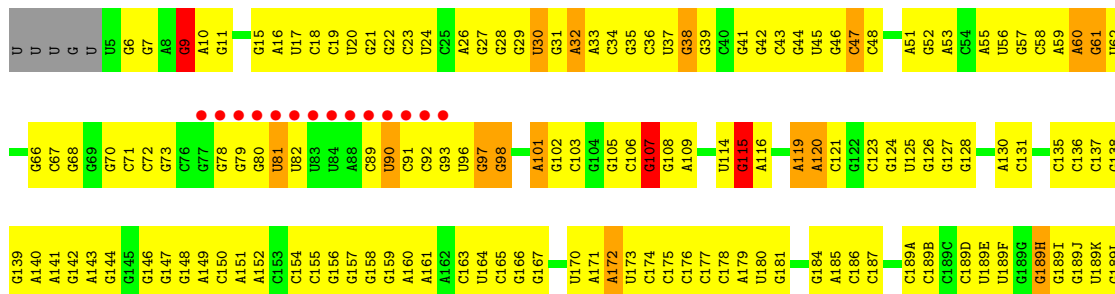
- Molecule 57 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



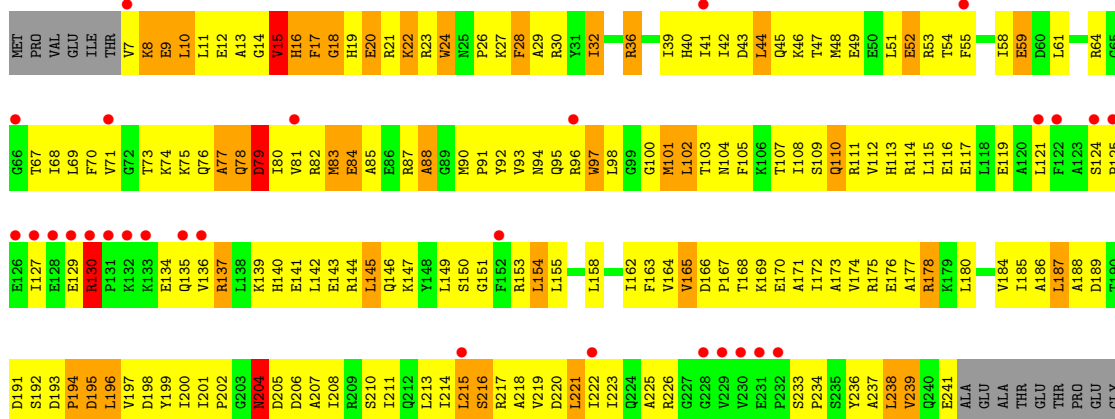
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	AA	1	Total	C	N	O	0	0
			42	23	5	14		
57	CA	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	CN	1	Total	Zn	0	0
			1	1		
58	AD	1	Total	Zn	0	0
			1	1		
58	CD	1	Total	Zn	0	0
			1	1		
58	AN	1	Total	Zn	0	0
			1	1		



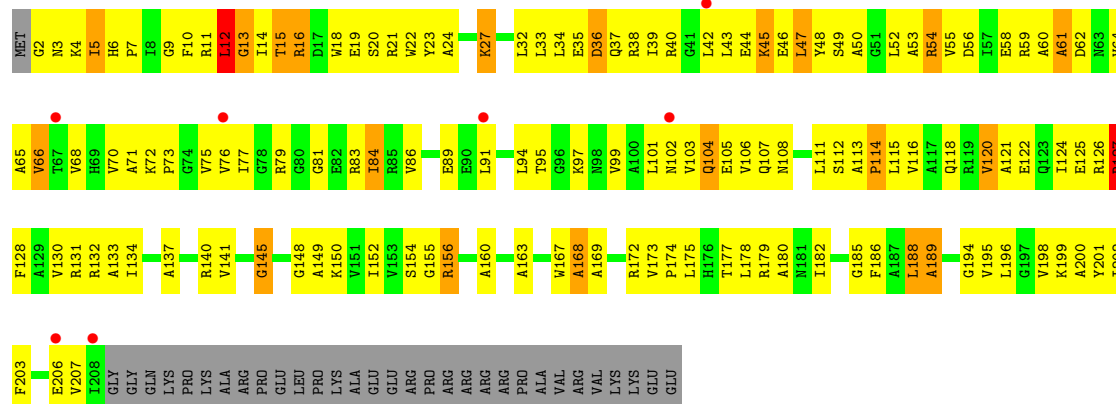
G1220	A1151	G1088	G1026	A959	G888	G618	A753	C680	G617	G546	G475	G399	C336	C268	U190
G1221	A1152	G1089	C1027	U960	U891	A819	C754	G683	C618	A547	G476	C403	C337	C269	G191
G1222	G1153	U1090	C1028	U961	G755	U820	C756	A684	U619	U551	A477	U404	A338	A270	U192
C1223	G1154	G1090	C1029	C962	C756	G821	G757	G685	C620	U552	C479	U405	C339	C271	C193
A1224	G1155	C893	C1030	G963	G758	C824	G758	U686	A621	A553	A482	U406	C341	A272	C194
G1225	A1225	A1092	G1030A	A964	G894	G825	A759	A687	G623	C554	C483	C409	C342	A273	A195
C1226	A1157	A1093	G1030B	A965	A900	G826	G760	G688	C624	C555	G484	G410	C345	A196	A197
A1227	C1158	G1094	G1030C	G966	A901	U827	G763	G689	G625	C556	G485	C411	C346	A198	G198
C1228	U1159	U1095	G1031	A968	A902	A828	C764	G690	U626	C557	U486	A412	G277	G199	G199
A1229	C1161	C1096	G1032	A969	G903	G829	G765	G691	G627	C558	A487	A413	G278	G200	G200
C1230	C1162	C1097	G1033	C970	G903	G830	A766	U692	G628	A559	C488	G414	G275	C201	C201
U1232	C1163	G1098	G1034	G971	A908	U831	A767	G693	G629	U560	G491	A414	A349	U202	U202
G1233	G1164	A1101	A1035	C972	A909	C832	A767	A694	G630	U561	G492	A415	G350	U203	U203
C1234	C1165	A1102	G1036	G973	C912	C833	A768	A695	G631	C562	G492	G416	G351	U204	U204
U1235	G1166	C1103	G1037	A974	C912	C834	G769	A696	A632	A563	C562	A417	C352	G216	G216
U1236	A1168	A1104	C1038	G975	A913	U835	C770	G696	G633	C564	A496	C418	A353	U287	C217
C1237	A1169	A1105	C1039	G976	A914	U836	C771	G771	G634	U565	U498	C419	A354	C218	C218
A1238	A1170	G1106	U1040	A977	G922	U850	U772	G713	G635	C566	C567	C422	C355	C219	C219
U1239	G1171	C1107	U1041	A978	A923	G851	C772	G714	A642	C567	C567	C423	A356	G220	G220
U1240	G1178	G1108	G1042	A979	G917	U839	G773	C708	A643	C568	G502	C424	A364	C221	C221
G1241	A1179	C1109	C1045	A980	A918	C940	G774	G709	G637	C568	G502	G425	A365	C291	C291
C1242	G1180	G1110	C1046	U981	A919	U841	G775	G710	G638	A572	C503	G426	C366	U222	U222
C1243	A1181	A1111	G1048	C984	U920	C948	G776	G711	G639	A573	C504	G427	C367	G293	G293
A1244	G1182	C1112	U1049	C985	U921	C949	G777	G712	A640	A574	G505	U427	C368	U294	U294
A1245	A1183	C1116	C1048	C986	A923	G852	C779	G713	A641	C575	C505	U428	C369	C295	C295
C1246	A1184	G1117	U1049	A986	A924	G853	G780	G714	A642	C576	A509	C428	C370	G226	G226
U1247	C1118	C1118	C1051	C989	G926	G854	A781	A715	G644	C577	C510	U429	C371	C297	C297
C1249	A1189	C1119	G1053	C990	G927	C854	A782	G716	G645	C578	C511	U430	C372	A298	A298
A1250	G1190	G1120	C1054	U991	G928	C855	G783	G717	U646	C579	C512	U431	C373	G299	G299
A1251	A1191	U1121	A1055	U992	C930	C857	G784	C719	G647	U580	C514	C433	C374	A300	A300
A1252	C1192	U1122	U1056	G993	C931	U859	G785	C720	A648	C581	G515	U434	C375	G301	G301
G1253	G1193	A1123	G1057	A994	C932	A859	G786	G724	G650	U582	C518	U435	C376	G302	G302
C1254	U1194	G1124	G1058	C995	G933	A860	A787	G725	G651	A583	C519	U437	C377	C308	C308
A1255	C1195	U1125	C1059	A996	C934	C862	A790	G726	U652	C585	A520	C438	C378	G310	G310
G1256	U1196	G1061	G1060	C999	C935	U863	G791	G727	A653	C586	G521	A439	A374	C311	C311
U1257	G1197	U1062	G1061	U1000	C936	A864	A792	A728	G658	C587	C522	A441	U375	C312	C312
G1258	C1198	C1063	U1062	A1001	A937	C865	A793	A729	U659	C588	G523	C442	G376	A313	A313
C1259	U1199	G1063	C1063	G1001A	A938	C866	C790	G730	U659	C589	G524	C443	G377	U243	U243
C1260	A1200	G1064	G1064	G1001A	G939	C867	C795	G731	G660	C590	C525	C444	C378	A244	A244
A1261	C1201	U1065	U1065	G1002	C940	C868	C796	G732	G661	C591	C526	U445	C379	A245	A245
C1262	G1202	C1066	C1066	G1003	G941	G869	C797	G733	G662	U591	G527	C446	G380	G247	G247
C1203	C1203	A1067	A1067	A1004	G942	U870	G798	G734	A663	G594	C528	C447	C381	G319	G319
A1204	A1204	G1068	G1068	A1005	U943	U871	C798	C735	A663	G595	C536	C454	C382	C320	C320
U1205	U1205	C1069	C1069	C1006	G944	C874	U801	C736	G664	C596	U531	A448	A382	A321	A321
G1206	G1206	U1070	U1070	G1006	G945	C875	A802	A737	A665	C597	C532	C449	A383	G251	G251
C1207	G1207	C1071	C1071	G1009	A946	C876	G803	C738	G666	U598	A533	C450	C384	U252	U252
G1208	G1208	G1072	G1072	G1010	G947	G876	U804	C739	G667	C599	U534	A452	C385	U253	U253
C1209	C1209	U1073	U1073	G1010	C948	C877	C805	U740	G668	C600	A535	A453	C386	G324	G324
C1210	C1210	G1074	G1074	A1014	A949	C878	C806	G741	U669	C601	C536	C454	U387	A395	A395
U1211	U1211	C1075	C1075	A1015	A950	G879	C807	G742	G670	A602	G537	C454	C388	G326	G326
U1212	U1212	G1076	G1076	A1016	U950	C880	A807	U743	A671	G603	G538	C458	C389	U257	U257
A1213	A1213	C1077	C1077	G1017	G951	C881	C808	G744	U672	U603	A539	C460	C390	C328	C328
U1214	U1214	U1078	U1078	C1018	U952	C882	G811	C745	G673	G604	G540	C461	C391	A329	A329
G1215	G1215	G1079	G1079	C1019	G954	C883	C747	A746	A674	G675	G541	C470	G392	C330	C330
A1216	A1216	U1080	U1080	C1019	G954	C884	C748	A747	A675	C612	G542	C471	A393	A263	A263
U1217	U1217	G1081	G1081	U1020	U955	U884	A814	C749	A676	C613	G543	A472	G394	G332	G332
C1218	C1218	U1081	U1081	G1024	U956	G885	A815	G750	U677	A614	C544	C473	A397	C333	C333
U1219	U1219	G1084	G1084	U1025	A958	G887	C817	G750	C679	C616	C545	C474	C398	G265	G265



GLU
SER
GLU
VAL
GLU
ALA

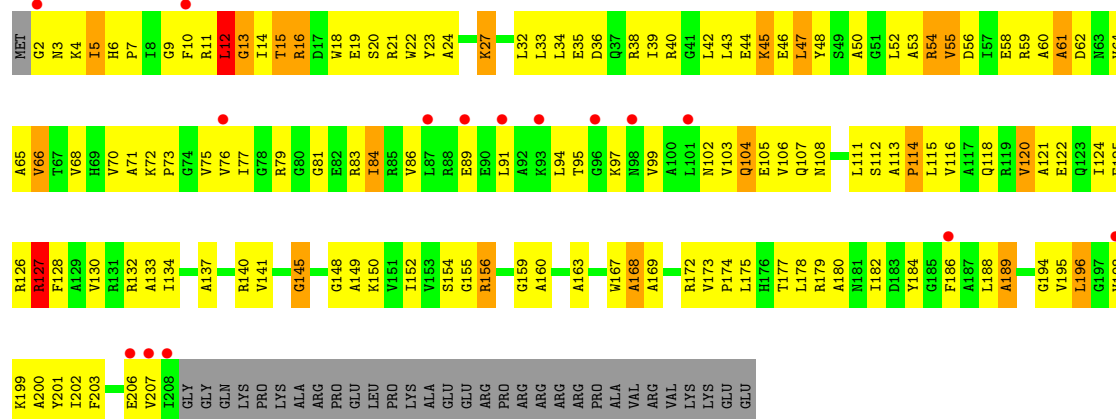
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain AC: 



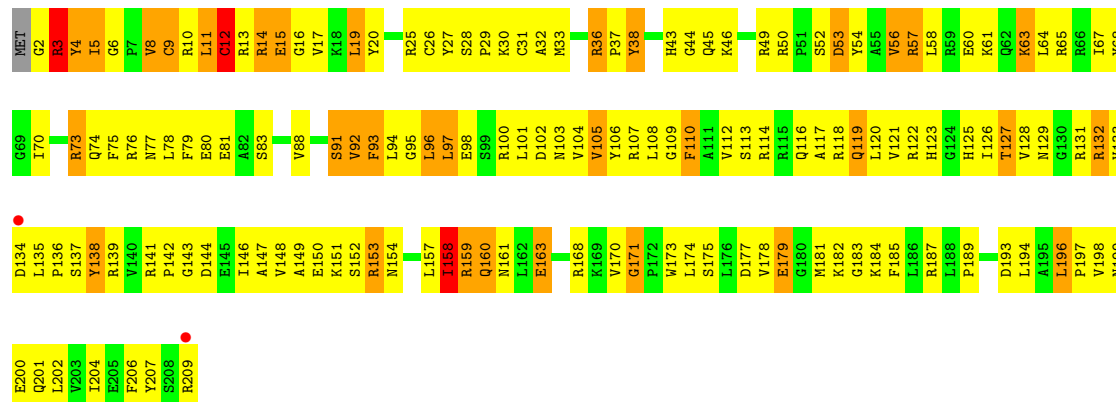
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain CC: 



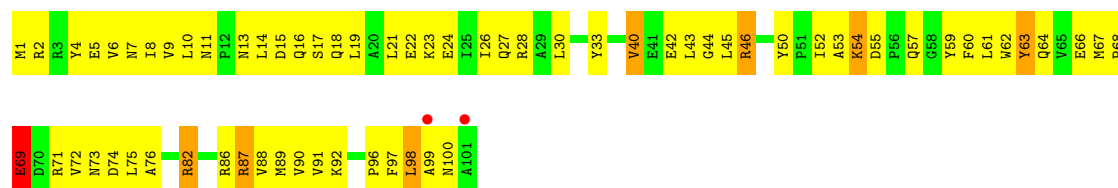
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AD: 



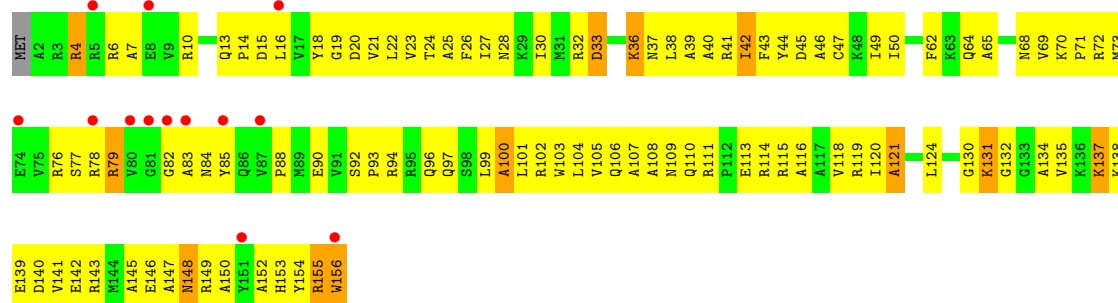
- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain CF:



- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AG:



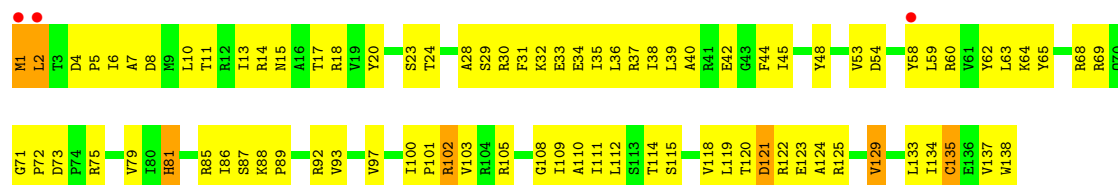
- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain CG:



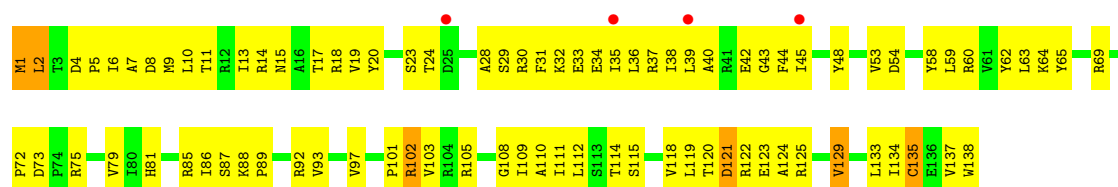
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AH:



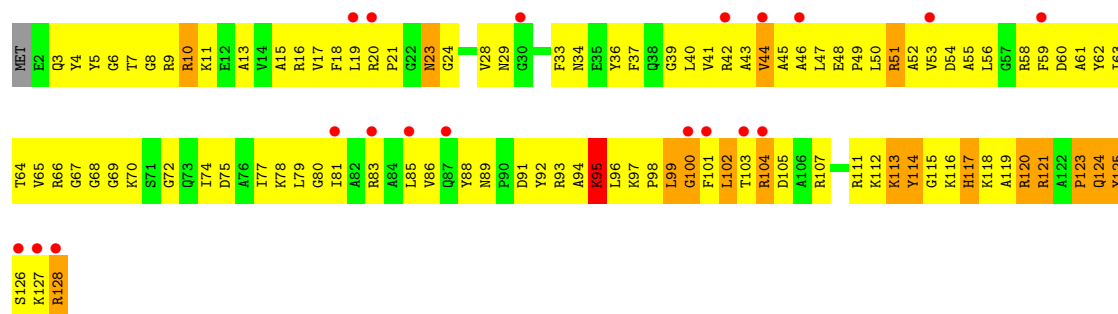
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain CH:



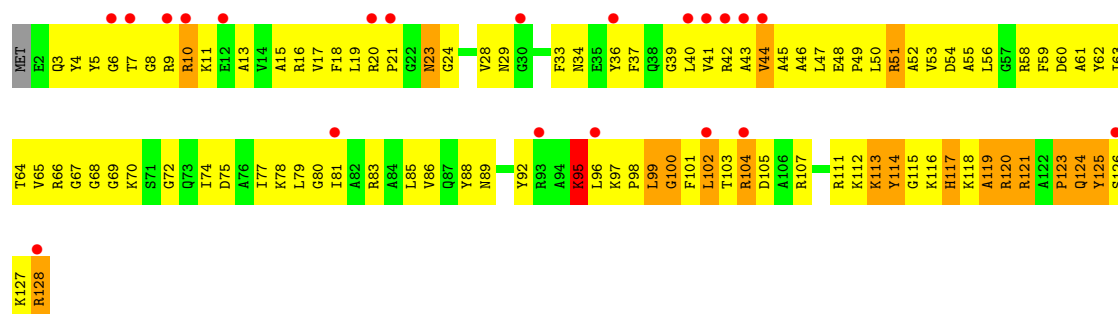
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AI:



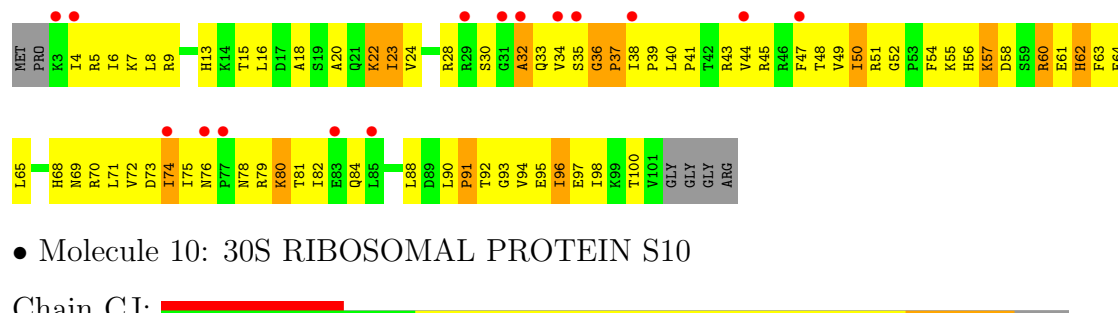
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CI:



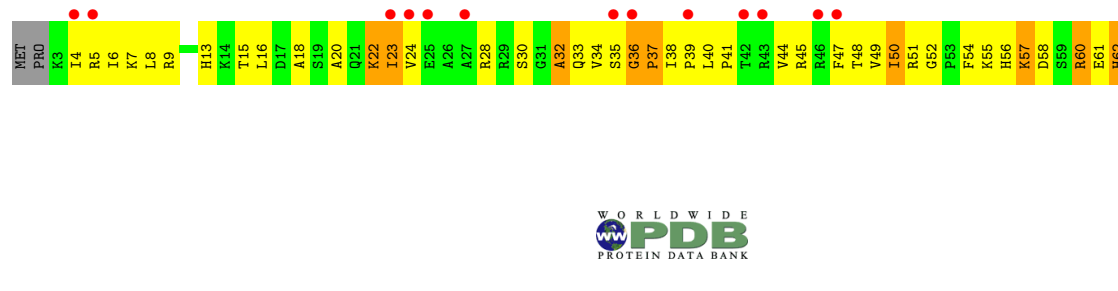
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AJ:



• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain CJ:





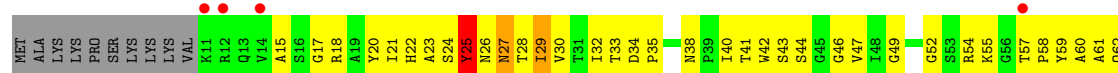
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AK:



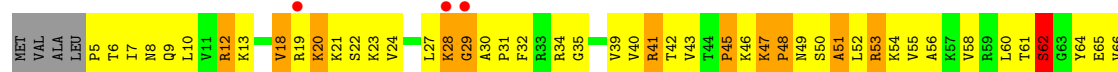
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain CK:



• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AL:



• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain CL:



• Molecule 13: 30S RIBOSOMAL PROTEIN S13

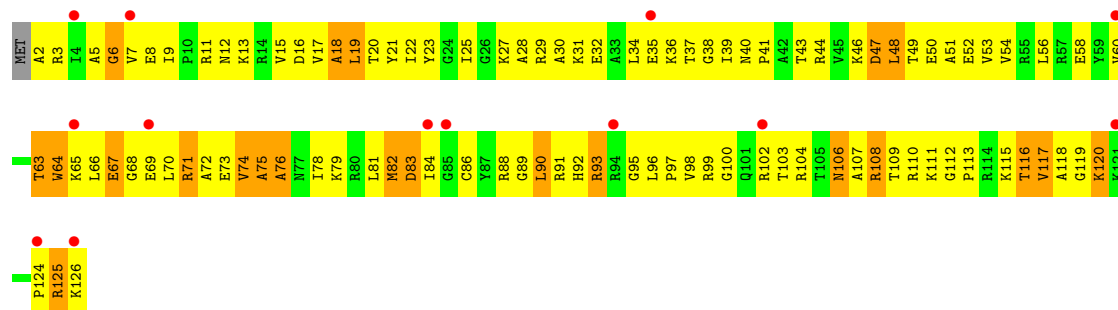
Chain AM:





• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain CM:



• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain AN:



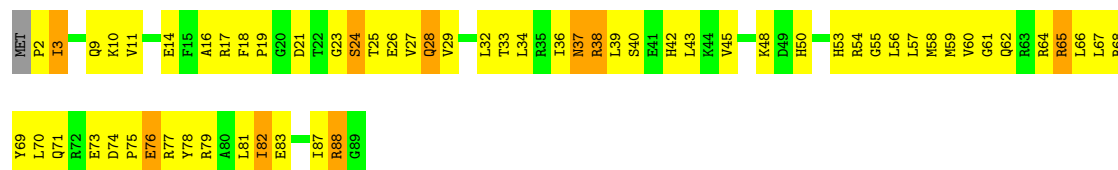
• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain CN:



• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO:



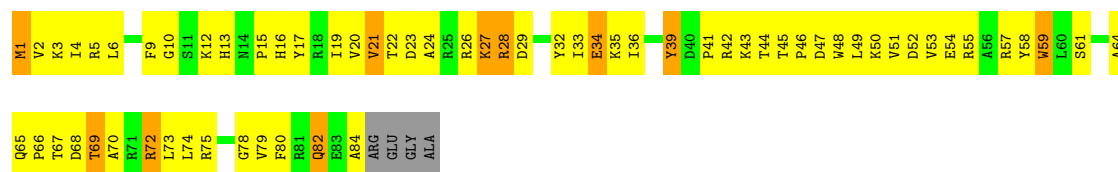
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CO:



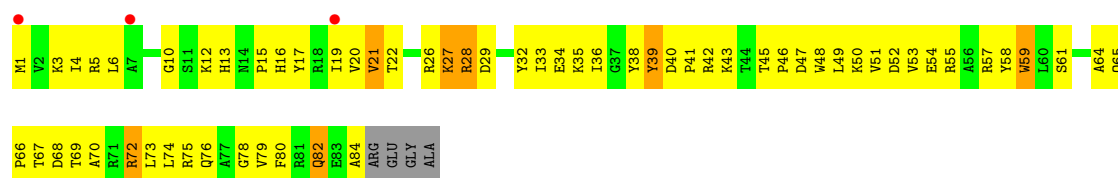
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP:



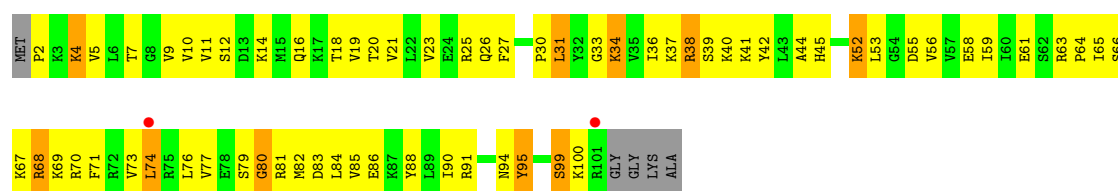
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CP:



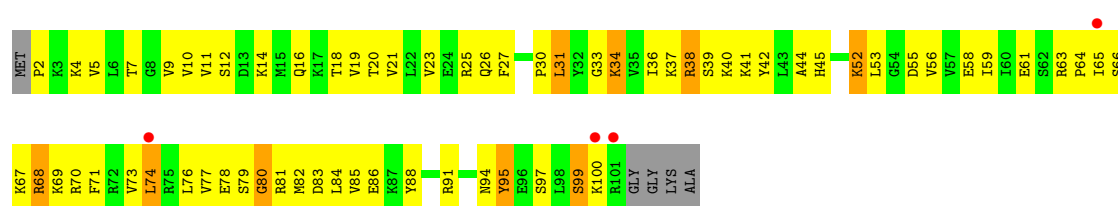
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ:



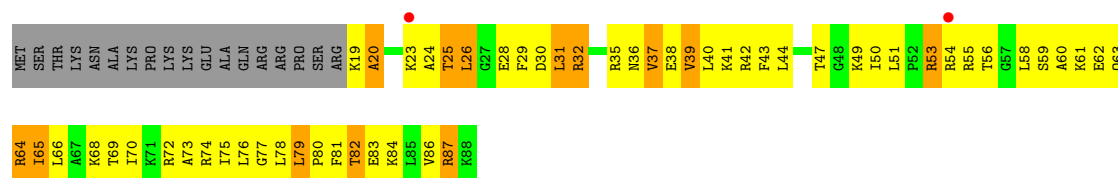
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CQ:



- Molecule 18: 30S RIBOSOMAL PROTEIN S18

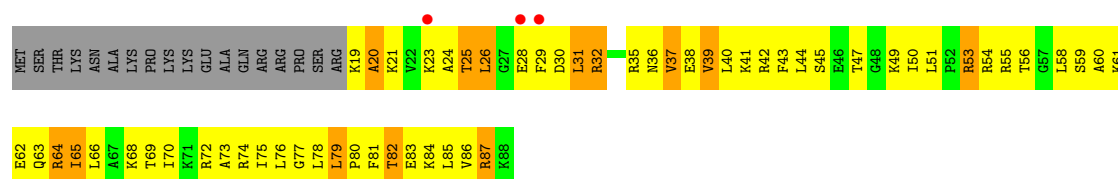
Chain AR:



- Molecule 18: 30S RIBOSOMAL PROTEIN S18

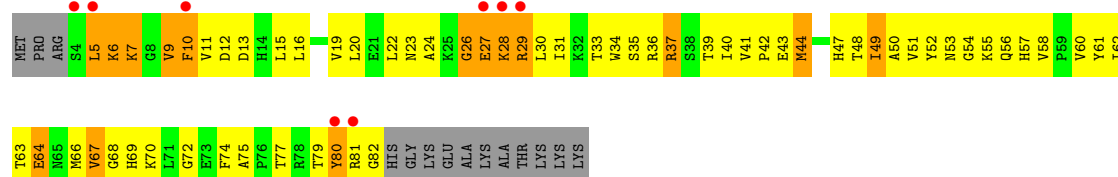
Chain CR:





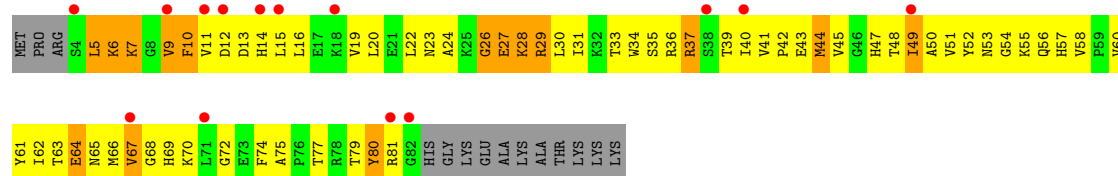
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AS:



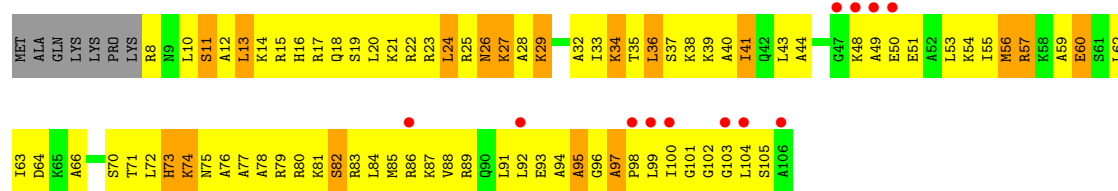
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain CS:



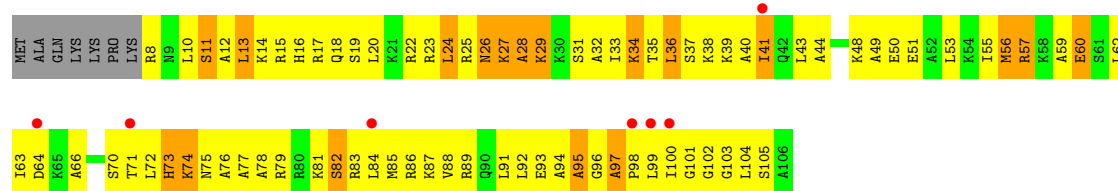
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain AT:



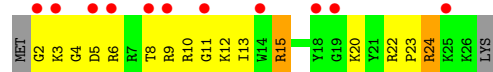
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain CT:



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AU:

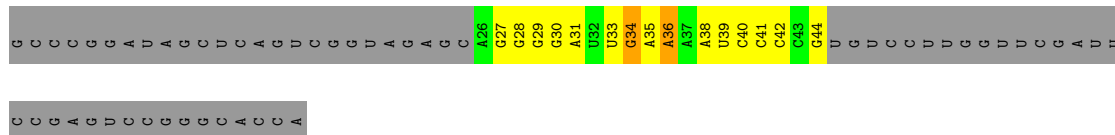


- [illegible]



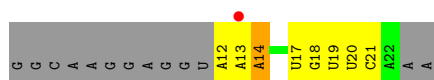
- Molecule 23: E-SITE TRNA PHE OR A-SITE TRNA PHE (UNMODIFIED BASES)

Chain CY:



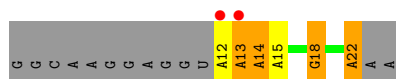
- Molecule 24: MRNA

Chain AX:



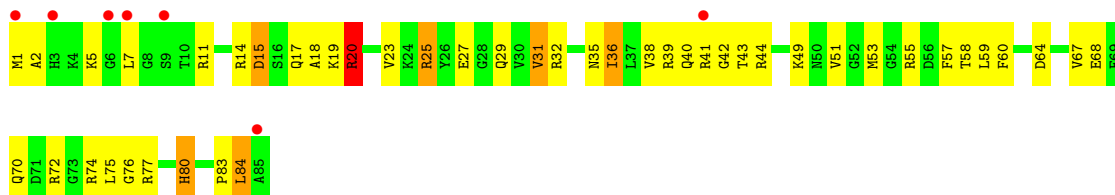
- Molecule 24: MRNA

Chain CX:



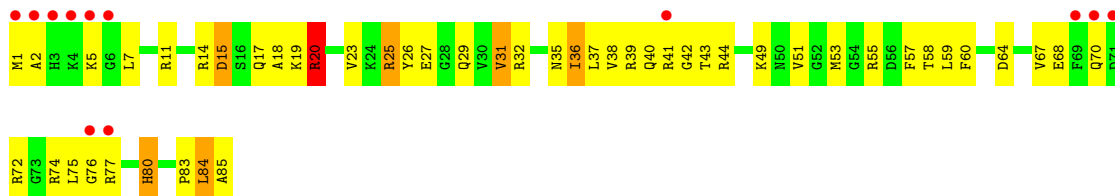
- Molecule 25: 50S RIBOSOMAL PROTEIN L27

Chain B0:



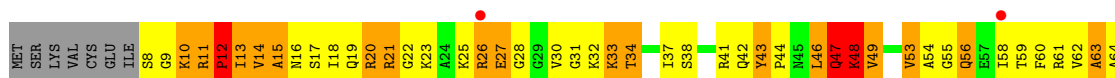
- Molecule 25: 50S RIBOSOMAL PROTEIN L27

Chain D0:



- Molecule 26: 50S RIBOSOMAL PROTEIN L28

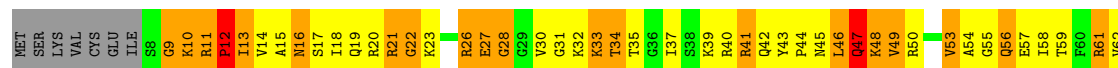
Chain B1:





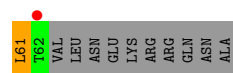
• Molecule 26: 50S RIBOSOMAL PROTEIN L28

Chain D1:



• Molecule 27: 50S RIBOSOMAL PROTEIN L29

Chain B2:



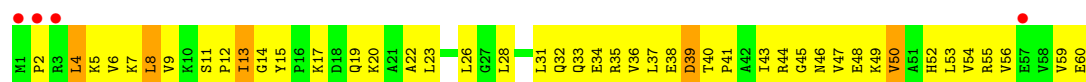
• Molecule 27: 50S RIBOSOMAL PROTEIN L29

Chain D2:



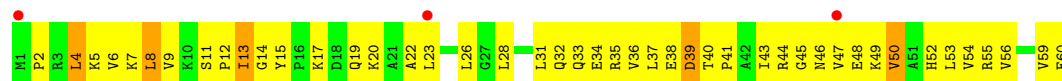
• Molecule 28: 50S RIBOSOMAL PROTEIN L30

Chain B3:



• Molecule 28: 50S RIBOSOMAL PROTEIN L30

Chain D3:



• Molecule 29: 50S RIBOSOMAL PROTEIN L31

Chain B4:



LYS
GLY
ARG

• Molecule 29: 50S RIBOSOMAL PROTEIN L31

Chain D4:

M1 K2 E3 G4 I5 H6 P7 K8 L9 V10 P11 A12 R13 R14 I15 C16 G19 N20 N21 T22 E23 T24 T27 K28 E29 E30 I31 V32 C36 S37 H40 P41 F42 Y43 T44 Q47 R48 F49 V50 ASP THR GLU GLY VAL ARG GLU ARG PHE GLN ARG TYR GLY ASP SER

TYR
ARG
LYS
GLY
ARG

• Molecule 30: 50S RIBOSOMAL PROTEIN L32

Chain B5:

MET A2 K3 H4 P5 V6 P7 K8 T11 S12 A13 K14 R15 R16 D17 A18 R19 R20 R21 S21 H22 H23 A24 L25 T26 T29 L30 V31 P32 C33 C34 E35 C36 K37 K38 A39 K40 P41 P42 H43 T44 V45 C46 P47 E48 C49 G50 Y51 Y52 A53 G54 R55 V57 L58 E59 V60

• Molecule 30: 50S RIBOSOMAL PROTEIN L32

Chain D5:

MET A2 K3 H4 P5 V6 P7 K8 S12 K13 A14 R15 R16 D17 A18 R19 R20 R21 S21 H22 H23 A24 L25 T26 T29 L30 V31 P32 C33 C34 E35 C36 K37 K38 A39 K40 P41 P42 H43 T44 V45 C46 P47 E48 C49 G50 Y51 Y52 A53 G54 R55 V57 L58 E59 V60

• Molecule 31: 50S RIBOSOMAL PROTEIN L33

Chain B6:

MET ALA SER GLU VAL ARG ILE LYS L9 L10 L11 E12 C13 T14 E15 C16 K17 R18 R19 N20 Y21 A22 T23 E24 K25 N26 K27 R28 N29 T30 T31 N32 K33 L34 L36 E35 L37 K38 Y39 C40 P41 W42 C43 R44 K45 H46 T47 V48 H49 R50 E51 V52 K53 ILE

• Molecule 31: 50S RIBOSOMAL PROTEIN L33

Chain D6:

MET ALA SER GLU VAL ARG ILE LYS L9 L10 L11 E12 C13 T14 E15 C16 K17 R18 R19 N20 Y21 A22 T23 E24 K25 N26 K27 R28 N29 T30 T31 N32 K33 L34 L36 E35 L37 K38 Y39 C40 P41 W42 C43 R44 K45 H46 T47 V48 H49 R50 E51 V52 K53 ILE

• Molecule 32: 50S RIBOSOMAL PROTEIN L34

Chain B7:

M1 K2 E3 T4 V5 Q6 P7 N8 R9 R10 R11 R12 H16 R19 T24 P25 G26 G27 V30 L31 K32 R33 R34 R35 Q36 K37 T43 P44 A45 V46 R47 K48 R49

• Molecule 32: 50S RIBOSOMAL PROTEIN L34

Chain D7:

M1 K2 E3 T4 V5 Q6 P7 N8 R9 R10 R11 R12 H16 R19 T24 P25 G26 G27 V30 L31 K32 R33 R34 R35 Q36 K37 R41 L42 T43 P44 A45 V46 R47 K48 R49

C1548	C1549	C1550	C1551	A1554	A1558	G1559	A1562	G1563	C1564	G1568	A1569	A1570	A1571	A1572	G1573	C1574	C1577	A1578	A1579	C1582	C1583	C1584	C1585	C1586	C1587	C1588	C1589	C1590	C1591	C1592	C1593	C1594	G1595	G1596	A1597	C1598	U1602	A1603	C1607	A1609	A1610	C1611	A1614	C1615	A1616	C1617	A1618	G1619	U1621											
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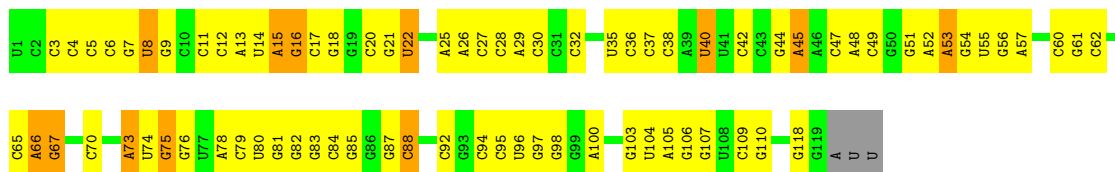




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G2907	G2842	U2593	U2593	G2523	G2450	U2383	G2320	G2252	G2176	U2016	U2016	G1936
G2908	G2843	U2594	U2594	G2524	G2451	U2384	G2321	G2253	G2177	G2083	G2017	A1937
G2909	G2844	U2595	U2595	G2525	G2452	U2385	G2322	G2254	G2178	G2084	G2018	A1938
G2910	G2845	U2596	U2596	G2526	G2453	U2386	G2323	G2255	G2179	G2085	G2019	G1939
G2911	G2846	U2597	U2597	G2527	G2454	U2387	G2324	G2256	G2180	G2086	A2020	U1940
G2912	G2847	U2598	U2598	G2528	G2455	U2388	G2325	G2257	G2181	G2087	G2021	U1941
G2913	G2848	U2599	U2599	G2529	G2456	U2389	G2326	G2258	G2182	G2088	U2022	U1942
G2914	G2849	U2600	U2600	G2530	G2457	U2390	G2327	G2259	G2183	U2089	G2023	C1946
G2915	G2850	U2601	U2601	G2531	G2458	U2391	G2328	G2260	G2184	G2090	G2024	C1947
G2916	G2851	U2602	U2602	G2532	G2459	U2392	G2329	G2261	G2185	U2091	G2025	G1948
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G2919	G2854	U2605	U2605	G2535	G2462	U2395	G2332	G2264	G2188	G2094	G2028	U1951
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G2922	G2857	U2608	U2608	G2538	G2465	U2398	G2335	G2267	G2191	G2097	G2031	U1954
G2923	G2858	U2609	U2609	G2539	G2466	U2399	G2336	G2268	G2192	G2098	G2032	U1955
G2924	G2859	U2610	U2610	G2540	G2467	U2400	G2337	G2269	G2193	G2099	G2033	U1956
G2925	G2860	U2611	U2611	G2541	G2468	U2401	G2338	G2270	G2194	G2100	U1957	U1957
G2926	G2861	U2612	U2612	G2542	G2469	U2402	G2339	G2271	G2195	G2101	U1958	U1958
G2927	G2862	U2613	U2613	G2543	G2470	U2403	G2340	G2272	G2196	G2102	U1959	U1959
G2928	G2863	U2614	U2614	G2544	G2471	U2404	G2341	G2273	G2197	G2103	U1960	U1960
G2929	G2864	U2615	U2615	G2545	G2472	U2405	G2342	G2274	G2198	G2104	U1961	U1961
G2930	G2865	U2616	U2616	G2546	G2473	U2406	G2343	G2275	G2199	G2105	U1962	U1962
G2931	G2866	U2617	U2617	G2547	G2474	U2407	G2344	G2276	G2200	G2036	U1963	U1963
G2932	G2867	U2618	U2618	G2548	G2475	U2408	G2345	G2277	G2201	G2037	U1964	U1964
G2933	G2868	U2619	U2619	G2549	G2476	U2409	G2346	G2278	G2202	G2038	U1965	U1965
G2934	G2869	U2620	U2620	G2550	G2477	U2410	G2347	G2279	G2203	G2039	U1966	U1966
G2935	G2870	U2621	U2621	G2551	G2478	U2411	G2348	G2280	G2204	U2040	U1967	U1967
G2936	G2871	U2622	U2622	G2552	G2479	G2412	G2349	G2281	G2205	U2041	C1968	A1885
G2937	G2872	U2623	U2623	G2553	G2480	G2413	G2350	G2282	G2206	U2042	C1969	C1886
G2938	G2873	U2624	U2624	G2554	G2481	G2414	G2351	G2283	G2207	C2043	A1970	C1887
G2939	G2874	U2625	U2625	G2555	G2482	G2415	G2352	G2284	G2208	G2044	A1971	G1888
G2940	G2875	U2626	U2626	G2556	G2483	G2416	G2353	G2285	G2209	C2045	A1972	G1889
G2941	G2876	U2627	U2627	G2557	G2484	G2417	G2354	G2286	G2210	A2050	G1980	G1890
G2942	G2877	U2628	U2628	G2558	G2485	G2418	G2355	G2287	G2211	G2052	G1981	A1900
G2943	G2878	U2629	U2629	G2559	G2486	G2419	G2356	G2288	G2212	A2054	C1982	C1902
G2944	G2879	U2630	U2630	G2560	G2487	G2420	G2357	G2289	G2213	G2055	G1983	C1903
G2945	G2880	U2631	U2631	G2561	G2488	G2421	G2358	G2290	G2214	G2056	G1984	G1904
G2946	G2881	U2632	U2632	G2562	G2489	G2422	G2359	G2291	G2215	G2057	G1985	G1905
G2947	G2882	U2633	U2633	G2563	G2490	G2423	G2360	G2292	G2216	G2058	C1986	C1906
G2948	G2883	U2634	U2634	G2564	G2491	G2424	G2361	G2293	G2217	G2059	C1987	G1907
G2949	G2884	U2635	U2635	G2565	G2492	G2425	G2362	G2294	G2218	G2060	C1988	G1908
G2950	G2885	U2636	U2636	G2566	G2493	G2426	G2363	G2295	G2219	A2062	C1989	C1909
G2951	G2886	U2637	U2637	G2567	G2494	G2427	G2364	G2296	G2220	G2063	C1990	C1910
G2952	G2887	U2638	U2638	G2568	G2495	G2428	G2365	G2297	G2221	C2064	U1991	G1910
G2953	G2888	U2639	U2639	G2569	G2496	G2429	G2366	G2298	G2222	G2065	U1992	U1911
G2954	G2889	U2640	U2640	G2570	G2497	G2430	G2367	G2299	G2223	G2066	U1993	A1912
G2955	G2890	U2641	U2641	G2571	G2498	G2431	G2368					

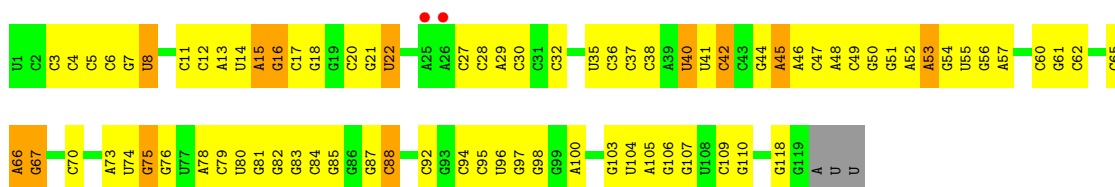
- Molecule 35: 5S RIBOSOMAL RNA

Chain BB:



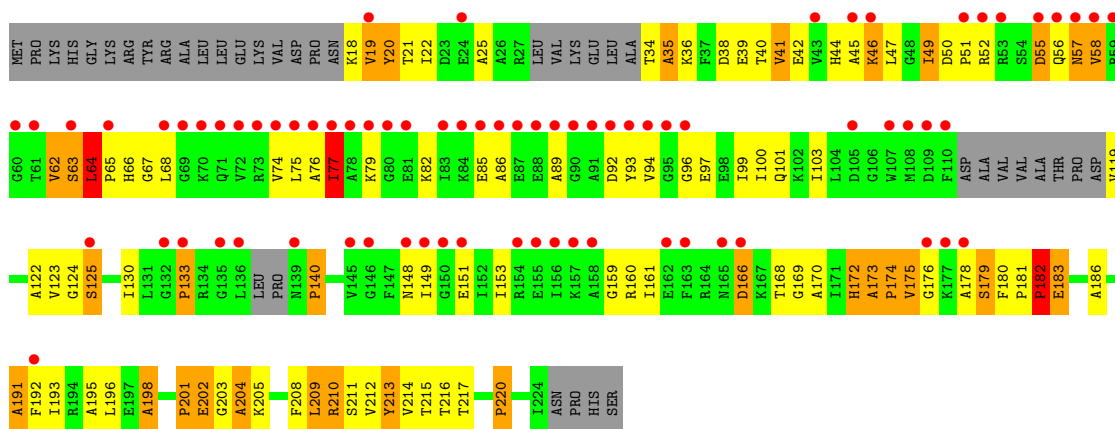
- Molecule 35: 5S RIBOSOMAL RNA

Chain DB:



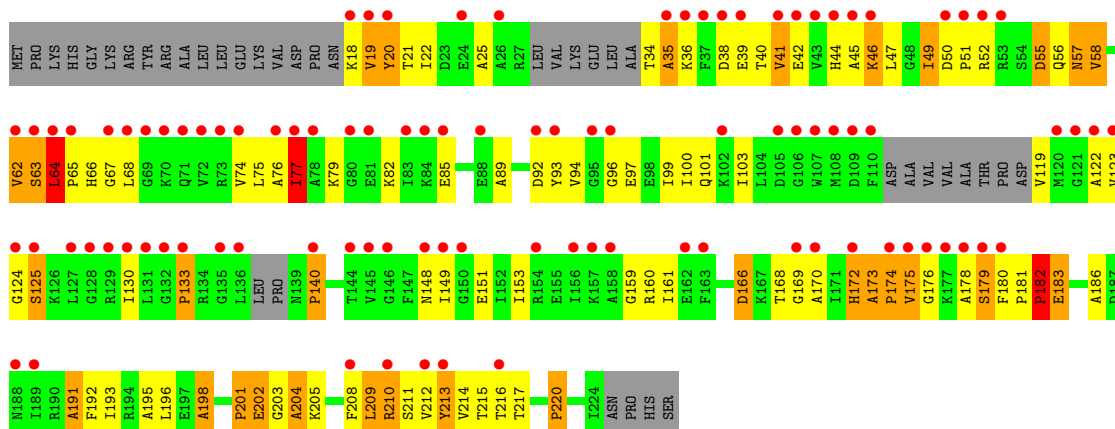
- Molecule 36: 50S RIBOSOMAL PROTEIN L1

Chain BC:



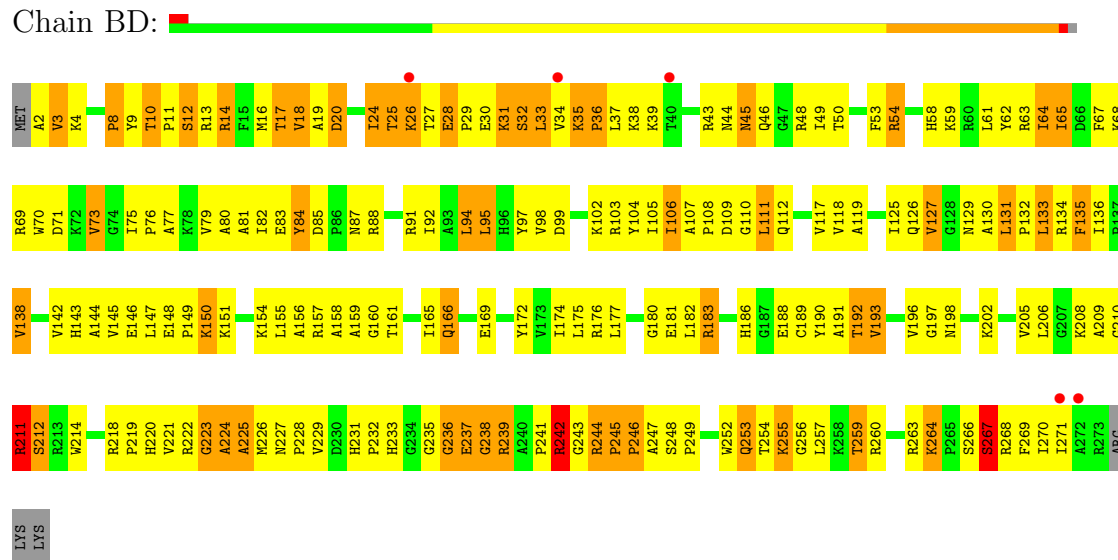
- Molecule 36: 50S RIBOSOMAL PROTEIN L1

Chain DC:



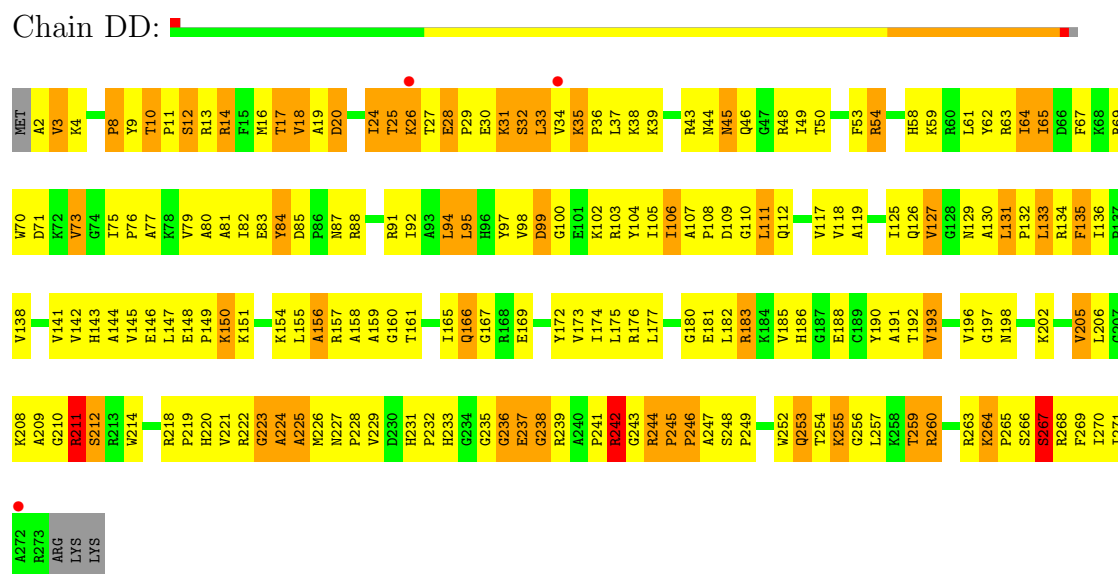
• Molecule 37: 50S RIBOSOMAL PROTEIN L2

Chain BD:



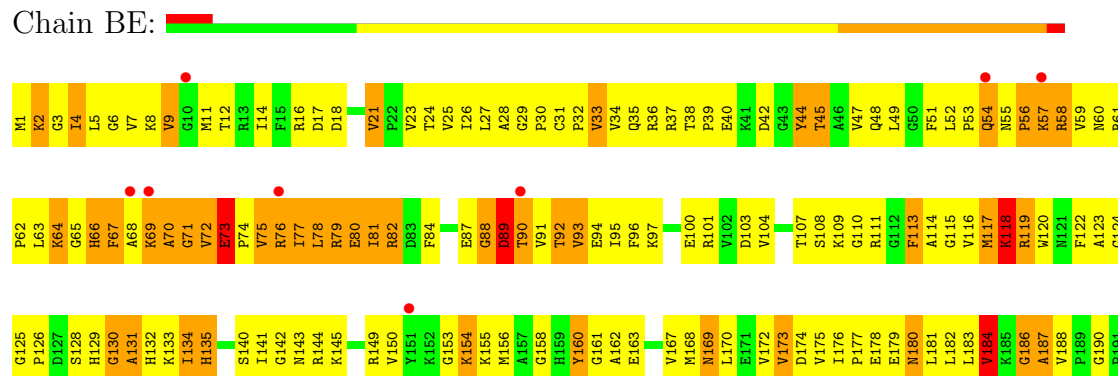
• Molecule 37: 50S RIBOSOMAL PROTEIN L2

Chain DD:



• Molecule 38: 50S RIBOSOMAL PROTEIN L3

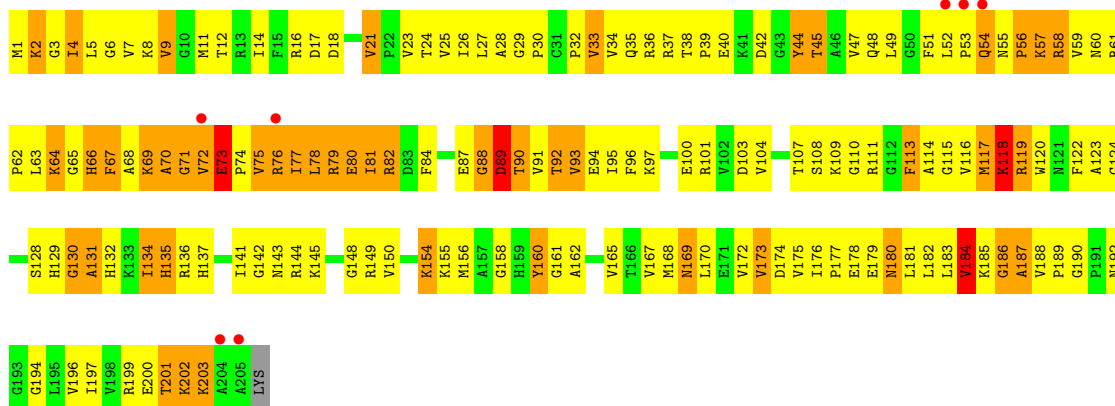
Chain BE:





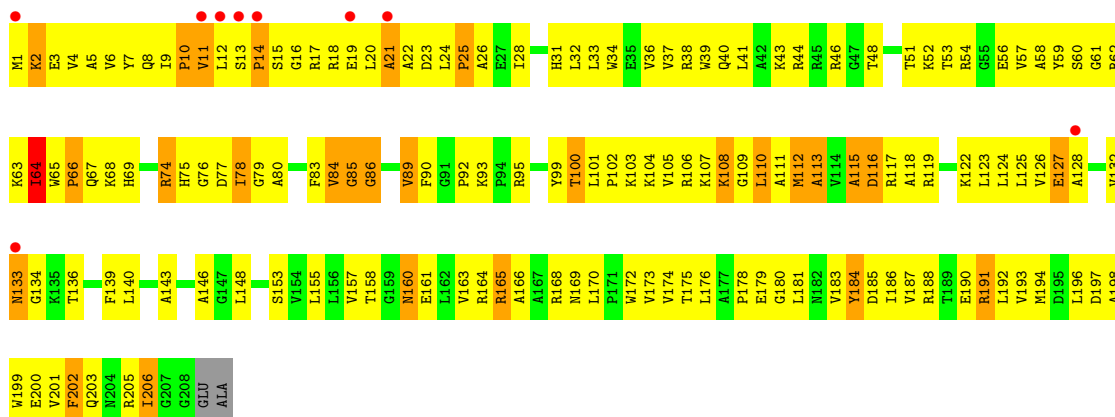
• Molecule 38: 50S RIBOSOMAL PROTEIN L3

Chain DE:



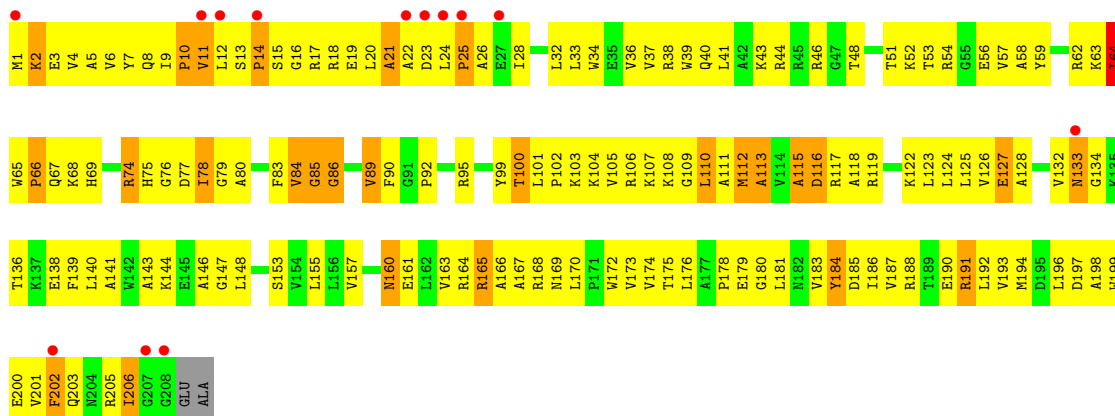
• Molecule 39: 50S RIBOSOMAL PROTEIN L4

Chain BF:



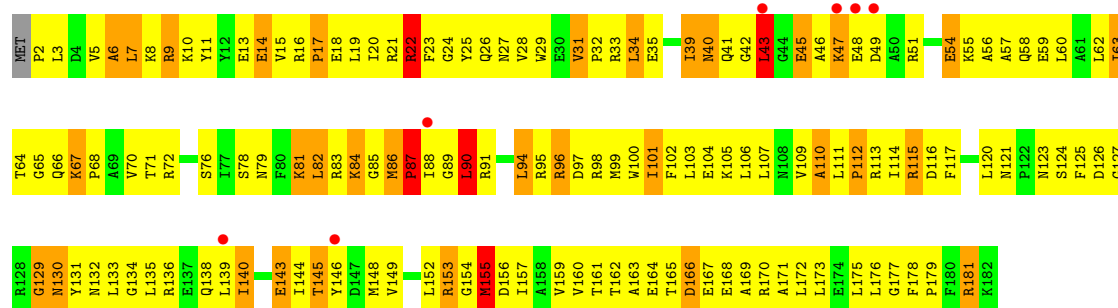
• Molecule 39: 50S RIBOSOMAL PROTEIN L4

Chain DF:



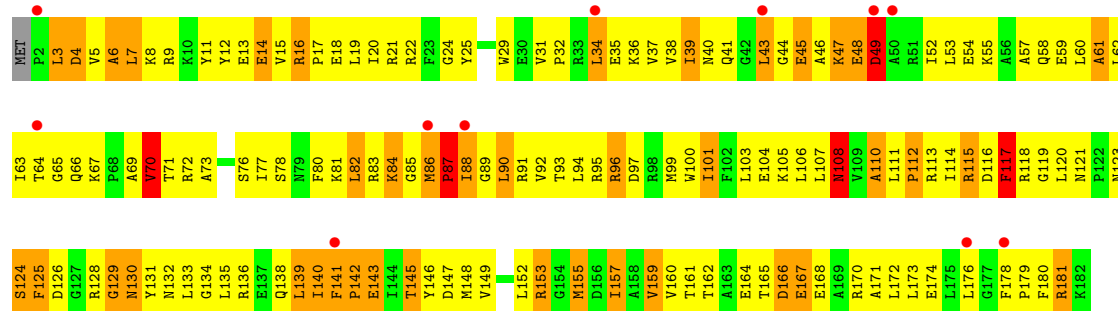
- Molecule 40: 50S RIBOSOMAL PROTEIN L5

Chain BG:



- Molecule 40: 50S RIBOSOMAL PROTEIN L5

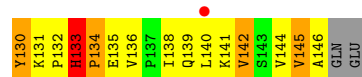
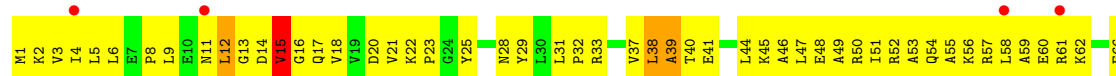
Chain DG:





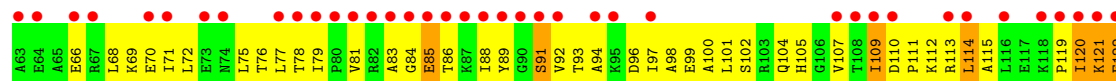
• Molecule 42: 50S RIBOSOMAL PROTEIN L9

Chain BI:



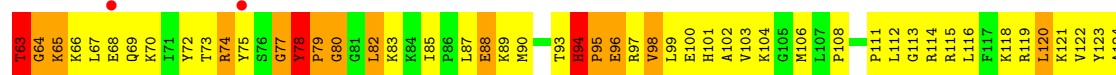
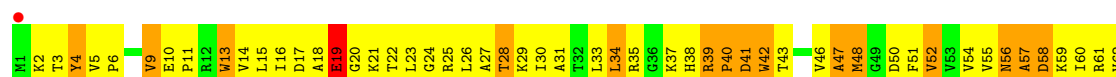
• Molecule 42: 50S RIBOSOMAL PROTEIN L9

Chain DI:



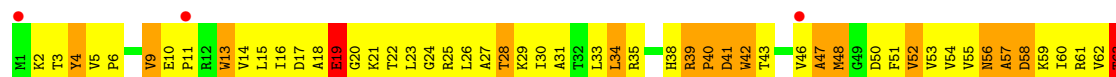
• Molecule 43: 50S RIBOSOMAL PROTEIN L13

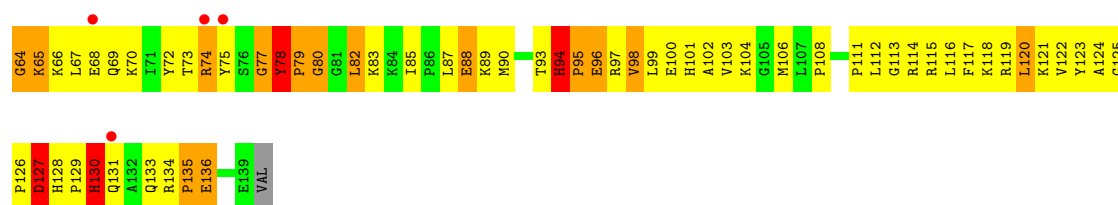
Chain BN:



• Molecule 43: 50S RIBOSOMAL PROTEIN L13

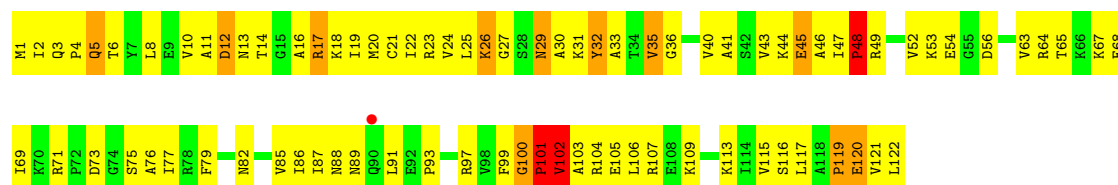
Chain DN:





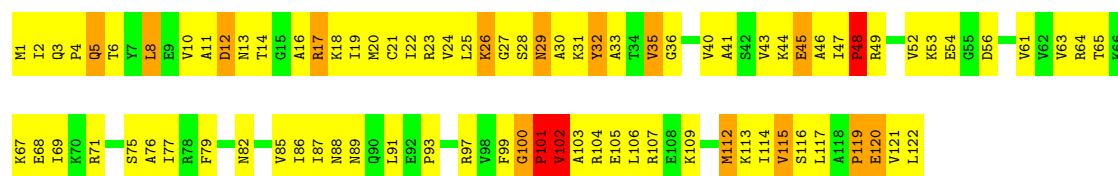
• Molecule 44: 50S RIBOSOMAL PROTEIN L14

Chain BO:



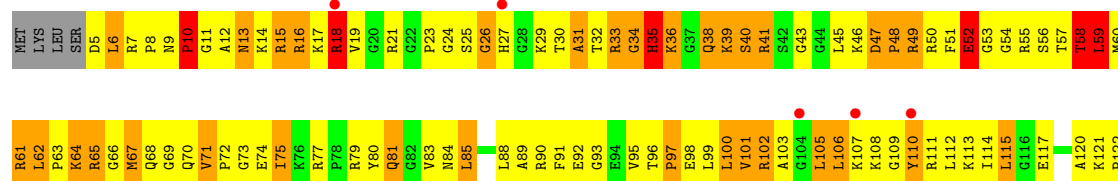
• Molecule 44: 50S RIBOSOMAL PROTEIN L14

Chain DO:



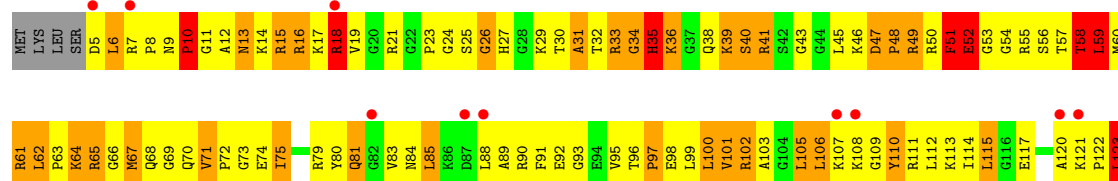
• Molecule 45: 50S RIBOSOMAL PROTEIN L15

Chain BP:



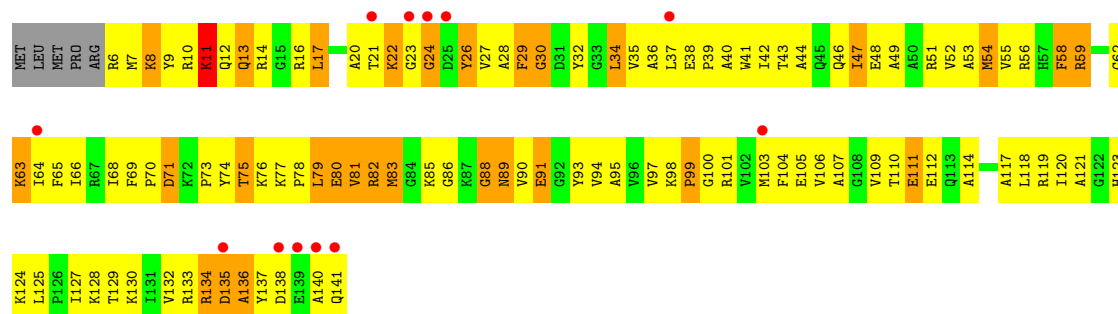
• Molecule 45: 50S RIBOSOMAL PROTEIN L15

Chain DP:



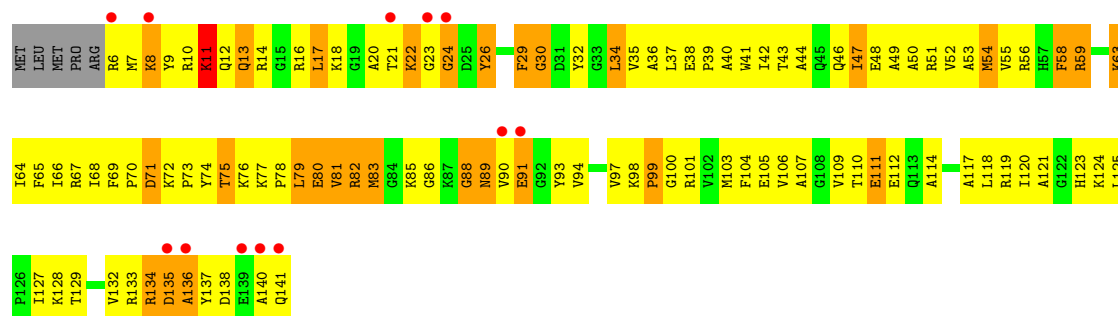
- Molecule 46: 50S RIBOSOMAL PROTEIN L16

Chain BQ:



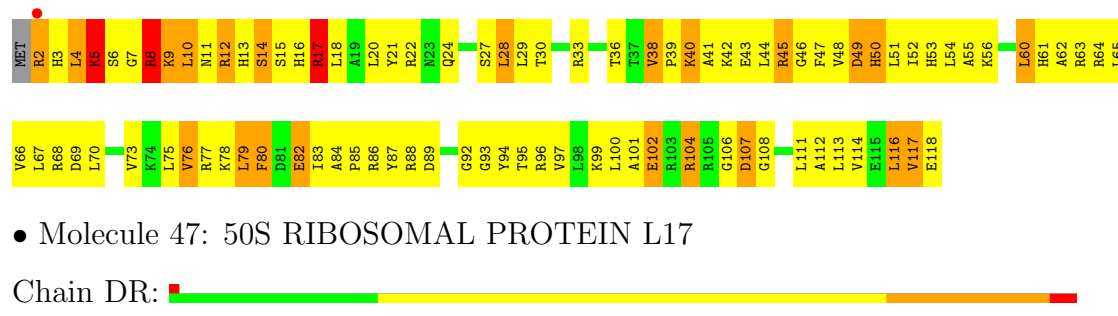
- Molecule 46: 50S RIBOSOMAL PROTEIN L16

Chain DQ:



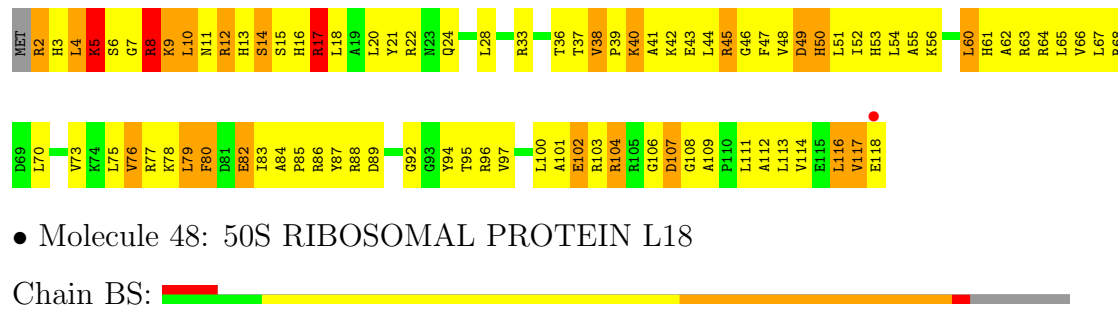
- Molecule 47: 50S RIBOSOMAL PROTEIN L17

Chain BR:



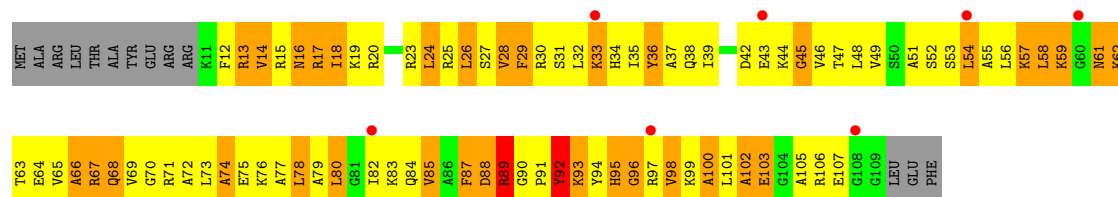
- Molecule 47: 50S RIBOSOMAL PROTEIN L17

Chain DR:



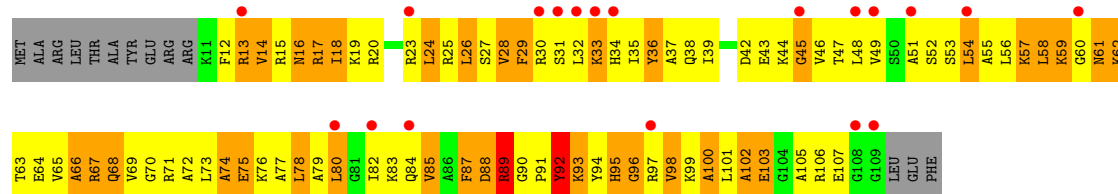
- Molecule 48: 50S RIBOSOMAL PROTEIN L18

Chain BS:



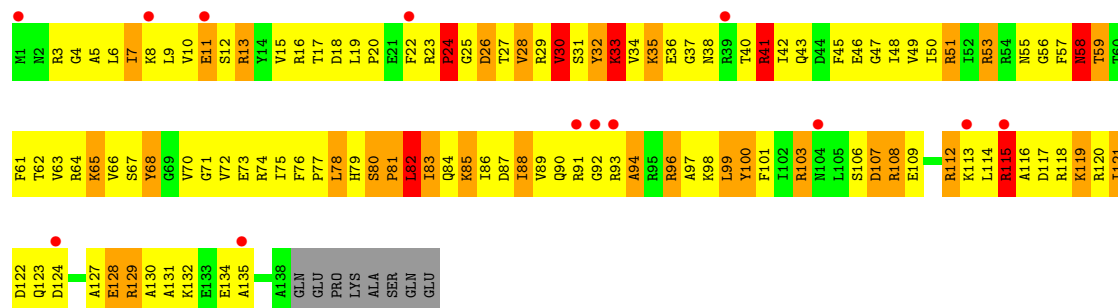
• Molecule 48: 50S RIBOSOMAL PROTEIN L18

Chain DS:



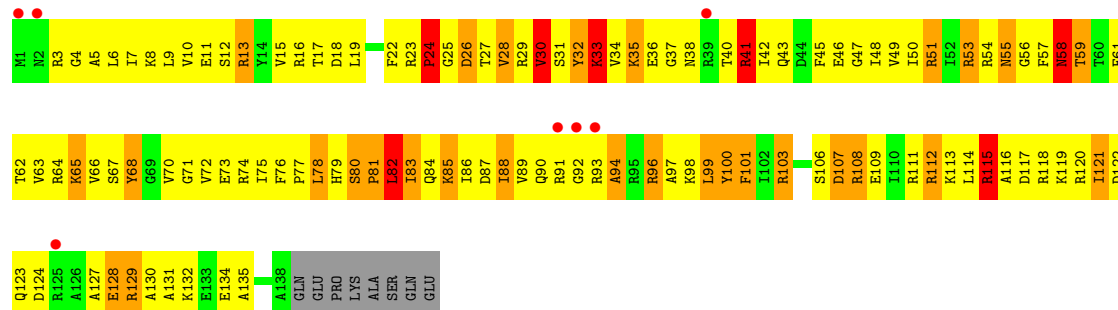
• Molecule 49: 50S RIBOSOMAL PROTEIN L19

Chain BT:



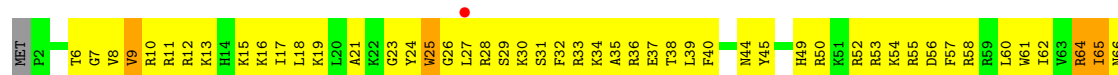
• Molecule 49: 50S RIBOSOMAL PROTEIN L19

Chain DT:



• Molecule 50: 50S RIBOSOMAL PROTEIN L20

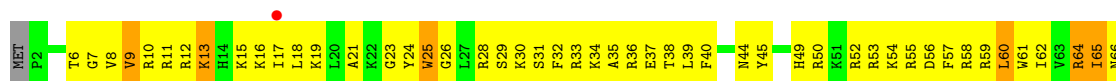
Chain BU:





• Molecule 50: 50S RIBOSOMAL PROTEIN L20

Chain DU:



• Molecule 51: 50S RIBOSOMAL PROTEIN L21

Chain BV:



• Molecule 51: 50S RIBOSOMAL PROTEIN L21

Chain DV:



• Molecule 52: 50S RIBOSOMAL PROTEIN L22

Chain BW:



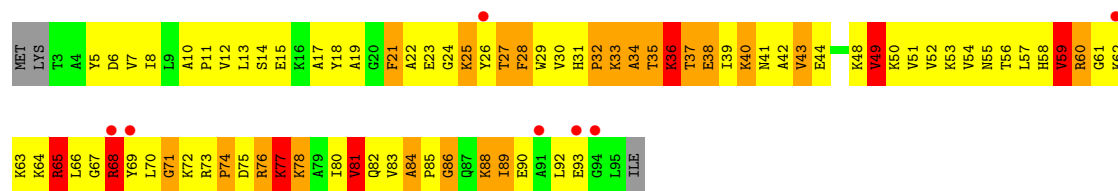
• Molecule 52: 50S RIBOSOMAL PROTEIN L22

Chain DW:



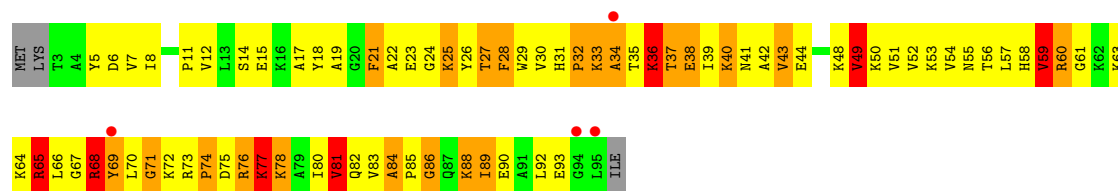
- Molecule 53: 50S RIBOSOMAL PROTEIN L23

Chain BX:



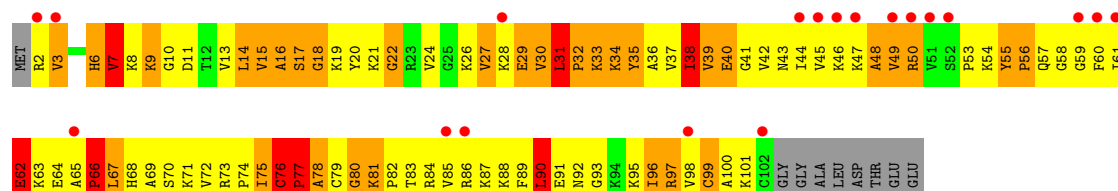
- Molecule 53: 50S RIBOSOMAL PROTEIN L23

Chain DX:



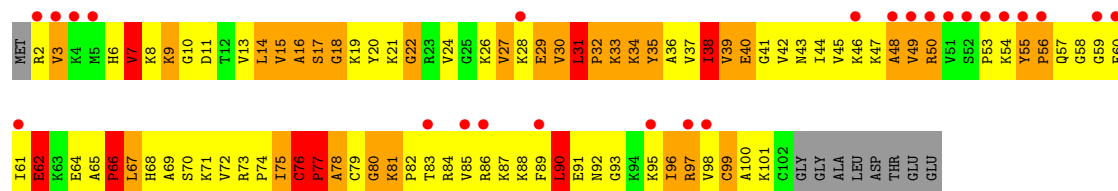
- Molecule 54: 50S RIBOSOMAL PROTEIN L24

Chain BY:



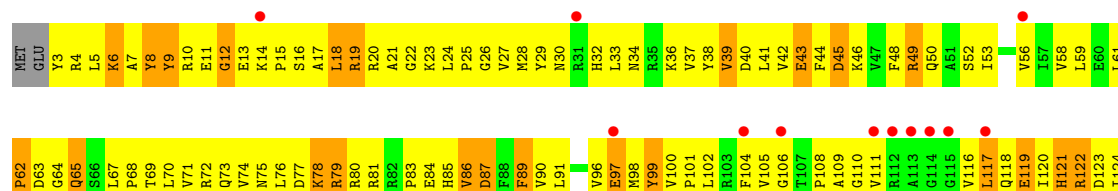
- Molecule 54: 50S RIBOSOMAL PROTEIN L24

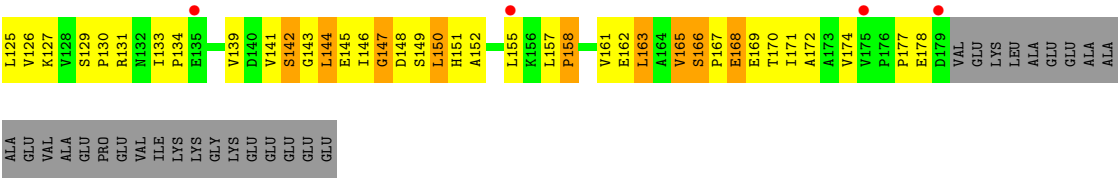
Chain DY:



- Molecule 55: 50S RIBOSOMAL PROTEIN L25

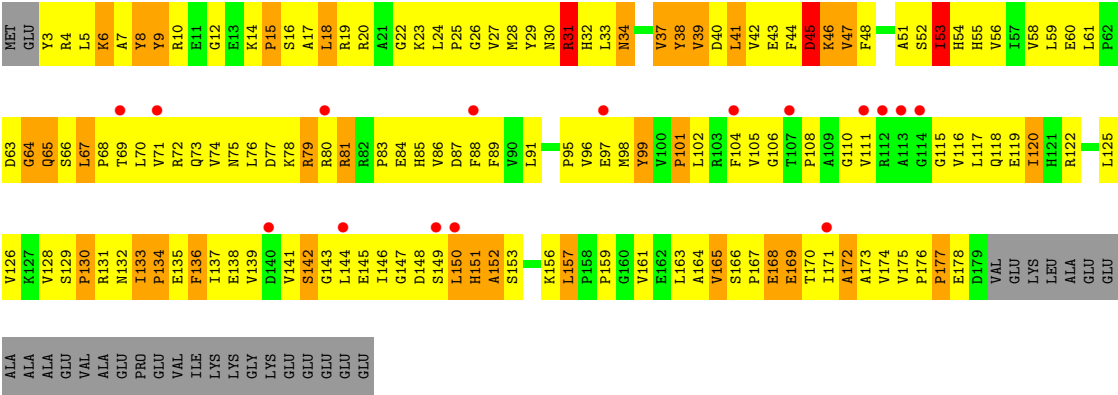
Chain BZ:





• Molecule 55: 50S RIBOSOMAL PROTEIN L25

Chain DZ:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	213.32Å 452.95Å 631.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 49.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	90.7 (50.00-2.80) 90.7 (49.96-2.80)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.272 , 0.313 0.268 , 0.309	Depositor DCC
R_{free} test set	64102 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 44.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.17$	Xtriage
Outliers	0 of 1342659 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	291077	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ZN, MG, PAR

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	0.50	0/36190	0.71	20/56486 (0.0%)
1	CA	0.47	0/36190	0.71	24/56486 (0.0%)
2	AB	0.33	0/1936	0.59	0/2611
2	CB	0.33	0/1936	0.59	0/2611
3	AC	0.35	0/1637	0.58	0/2207
3	CC	0.34	0/1637	0.58	0/2207
4	AD	0.42	0/1733	0.67	0/2318
4	CD	0.41	0/1733	0.66	0/2318
5	AE	0.41	0/1163	0.66	0/1566
5	CE	0.39	0/1163	0.65	0/1566
6	AF	0.37	0/856	0.64	0/1154
6	CF	0.38	0/856	0.65	0/1154
7	AG	0.34	0/1276	0.54	0/1709
7	CG	0.33	0/1276	0.54	0/1709
8	AH	0.35	0/1136	0.62	0/1527
8	CH	0.34	0/1136	0.62	0/1527
9	AI	0.32	0/1027	0.55	0/1372
9	CI	0.32	0/1027	0.55	0/1372
10	AJ	0.36	0/808	0.62	0/1087
10	CJ	0.34	0/808	0.62	0/1087
11	AK	0.38	0/900	0.64	0/1213
11	CK	0.35	0/900	0.63	0/1213
12	AL	0.42	0/987	0.71	0/1322
12	CL	0.43	0/987	0.73	0/1322
13	AM	0.34	0/994	0.62	0/1322
13	CM	0.32	0/994	0.61	0/1322
14	AN	0.39	0/501	0.66	0/664
14	CN	0.38	0/501	0.64	0/664
15	AO	0.38	0/745	0.63	0/992
15	CO	0.36	0/745	0.61	0/992
16	AP	0.43	0/717	0.69	0/965
16	CP	0.42	0/717	0.68	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.41	0/837	0.67	0/1119
17	CQ	0.38	0/837	0.66	0/1119
18	AR	0.39	0/579	0.70	0/768
18	CR	0.38	0/579	0.70	0/768
19	AS	0.37	0/643	0.61	0/867
19	CS	0.36	0/643	0.60	0/867
20	AT	0.33	0/765	0.59	0/1007
20	CT	0.32	0/765	0.59	0/1007
21	AU	0.45	0/213	0.56	0/279
21	CU	0.44	0/213	0.55	0/279
22	AV	0.51	1/1814 (0.1%)	0.72	0/2825
22	CV	0.50	1/1814 (0.1%)	0.72	0/2825
23	AW	0.43	1/1813 (0.1%)	0.77	6/2823 (0.2%)
23	AY	0.36	0/456	0.72	0/710
23	CW	0.45	1/1813 (0.1%)	0.76	2/2823 (0.1%)
23	CY	0.35	0/456	0.68	0/710
24	AX	0.73	1/264 (0.4%)	0.84	0/407
24	CX	0.73	1/264 (0.4%)	0.81	1/407 (0.2%)
25	B0	0.38	0/658	0.65	0/878
25	D0	0.39	0/658	0.65	0/878
26	B1	0.61	0/700	1.04	1/931 (0.1%)
26	D1	0.52	0/700	0.99	1/931 (0.1%)
27	B2	0.45	0/423	0.99	3/560 (0.5%)
27	D2	0.45	0/423	0.89	2/560 (0.4%)
28	B3	0.37	0/473	0.61	0/636
28	D3	0.39	0/473	0.61	0/636
29	B4	0.47	0/241	0.88	4/334 (1.2%)
29	D4	0.44	0/241	0.88	4/334 (1.2%)
30	B5	0.42	0/473	0.74	0/639
30	D5	0.40	0/473	0.73	0/639
31	B6	0.39	0/387	0.62	0/517
31	D6	0.39	0/387	0.62	0/517
32	B7	0.51	0/427	0.73	0/563
32	D7	0.53	0/427	0.70	0/563
33	B8	0.50	0/516	0.81	0/681
33	D8	0.48	0/516	0.80	0/681
34	BA	0.62	4/66876 (0.0%)	0.77	56/104407 (0.1%)
34	DA	0.62	5/66876 (0.0%)	0.77	53/104407 (0.1%)
35	BB	0.39	0/2853	0.70	0/4451
35	DB	0.38	0/2853	0.70	0/4451
36	BC	0.38	0/1145	0.68	7/1556 (0.4%)
36	DC	0.40	0/1145	0.68	7/1556 (0.4%)
37	BD	0.52	0/2155	0.87	3/2907 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DD	0.51	0/2155	0.86	3/2907 (0.1%)
38	BE	0.43	0/1597	0.76	0/2155
38	DE	0.45	0/1597	0.77	0/2155
39	BF	0.45	0/1659	0.70	0/2246
39	DF	0.44	0/1659	0.69	0/2246
40	BG	0.39	0/1498	0.72	1/2013 (0.0%)
40	DG	0.35	0/1498	0.73	0/2013
41	BH	0.33	0/1246	0.69	0/1684
41	DH	0.35	0/1246	0.69	0/1684
42	BI	0.35	0/1147	0.66	0/1553
42	DI	0.34	0/1147	0.66	0/1553
43	BN	0.40	0/1132	0.78	0/1527
43	DN	0.45	0/1132	0.79	0/1527
44	BO	0.48	0/943	0.74	0/1269
44	DO	0.49	0/943	0.75	0/1269
45	BP	0.42	0/1131	1.00	6/1504 (0.4%)
45	DP	0.41	0/1131	1.00	7/1504 (0.5%)
46	BQ	0.37	0/1100	0.72	1/1470 (0.1%)
46	DQ	0.37	0/1100	0.72	1/1470 (0.1%)
47	BR	0.40	0/974	0.74	1/1302 (0.1%)
47	DR	0.38	0/974	0.74	1/1302 (0.1%)
48	BS	0.40	0/779	0.73	0/1038
48	DS	0.39	0/779	0.73	0/1038
49	BT	0.42	0/1156	0.77	2/1544 (0.1%)
49	DT	0.42	0/1156	0.77	1/1544 (0.1%)
50	BU	0.37	0/975	0.68	0/1297
50	DU	0.40	0/975	0.69	0/1297
51	BV	0.38	0/789	0.73	0/1054
51	DV	0.40	0/789	0.73	0/1054
52	BW	0.43	0/907	0.72	0/1216
52	DW	0.45	0/907	0.72	0/1216
53	BX	0.53	0/740	0.89	3/995 (0.3%)
53	DX	0.50	0/740	0.89	3/995 (0.3%)
54	BY	0.41	0/789	0.78	0/1053
54	DY	0.43	0/789	0.78	0/1053
55	BZ	0.35	0/1436	0.64	0/1951
55	DZ	0.36	0/1436	0.62	0/1951
All	All	0.52	15/314630 (0.0%)	0.74	224/470502 (0.0%)

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
1	AA	2	37
1	CA	2	29
22	AV	0	2
22	CV	0	2
23	AW	3	1
23	CW	2	0
24	CX	0	1
26	B1	0	1
34	BA	30	81
34	DA	28	79
All	All	67	233

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CX	12	A	OP3-P	-7.28	1.52	1.61
23	CW	1	G	OP3-P	-7.25	1.52	1.61
23	AW	1	G	OP3-P	-7.19	1.52	1.61
22	CV	1	C	OP3-P	-7.12	1.52	1.61
24	AX	12	A	OP3-P	-7.08	1.52	1.61

The worst 5 of 224 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	CW	17	C	N1-C1'-C2'	10.99	128.28	114.00
34	DA	1962	C	N1-C1'-C2'	10.90	128.18	114.00
34	BA	1962	C	N1-C1'-C2'	10.48	127.62	114.00
34	BA	669	G	N9-C1'-C2'	10.36	127.47	114.00
34	DA	669	G	N9-C1'-C2'	10.24	127.32	114.00

5 of 67 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	410	G	C3'
1	AA	412	A	C1'
23	AW	17	C	C1'
23	AW	47	U	C1'
23	AW	70	G	C3'

5 of 233 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	107	G	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	253	U	Sidechain
1	AA	371	G	Sidechain
1	AA	38	G	Sidechain
1	AA	9	G	Sidechain

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	32329	0	16314	1351	0
1	CA	32329	0	16316	1334	0
2	AB	1901	0	1951	258	0
2	CB	1901	0	1951	256	0
3	AC	1613	0	1677	209	0
3	CC	1613	0	1677	203	0
4	AD	1703	0	1764	192	0
4	CD	1703	0	1766	191	0
5	AE	1147	0	1207	161	0
5	CE	1147	0	1206	159	0
6	AF	843	0	857	98	0
6	CF	843	0	857	101	0
7	AG	1257	0	1296	125	0
7	CG	1257	0	1296	122	0
8	AH	1116	0	1177	128	0
8	CH	1116	0	1177	130	0
9	AI	1011	0	1041	140	0
9	CI	1011	0	1041	140	0
10	AJ	795	0	840	147	0
10	CJ	795	0	840	144	0
11	AK	885	0	904	104	0
11	CK	885	0	904	96	0
12	AL	971	0	1057	122	0
12	CL	971	0	1057	120	0
13	AM	988	0	1055	156	0
13	CM	988	0	1055	151	0
14	AN	492	0	530	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	CN	492	0	529	61	0
15	AO	734	0	771	70	0
15	CO	734	0	771	76	0
16	AP	701	0	720	83	0
16	CP	701	0	720	75	0
17	AQ	824	0	891	91	0
17	CQ	824	0	891	90	0
18	AR	574	0	644	97	0
18	CR	574	0	644	94	0
19	AS	630	0	652	106	0
19	CS	630	0	652	106	0
20	AT	763	0	861	106	0
20	CT	763	0	861	102	0
21	AU	209	0	221	23	0
21	CU	209	0	221	22	0
22	AV	1645	0	838	62	0
22	CV	1645	0	838	51	0
23	AW	1623	0	821	83	0
23	AY	407	0	208	16	0
23	CW	1623	0	821	82	0
23	CY	407	0	208	13	0
24	AX	236	0	119	6	0
24	CX	236	0	119	5	0
25	B0	650	0	654	72	0
25	D0	650	0	654	78	0
26	B1	693	0	764	182	0
26	D1	693	0	764	197	0
27	B2	421	0	460	124	0
27	D2	421	0	461	125	0
28	B3	468	0	523	53	0
28	D3	468	0	523	52	0
29	B4	242	0	103	22	0
29	D4	242	0	103	23	0
30	B5	459	0	480	75	0
30	D5	459	0	480	70	0
31	B6	381	0	390	59	0
31	D6	381	0	390	56	0
32	B7	419	0	467	35	0
32	D7	419	0	467	35	0
33	B8	508	0	576	110	0
33	D8	508	0	576	114	0
34	BA	59708	0	30096	2498	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	DA	59708	0	30096	2502	0
35	BB	2551	0	1294	106	0
35	DB	2551	0	1294	100	0
36	BC	1142	0	865	109	0
36	DC	1142	0	865	106	0
37	BD	2105	0	2182	357	0
37	DD	2105	0	2182	362	0
38	BE	1564	0	1629	325	0
38	DE	1564	0	1629	323	0
39	BF	1624	0	1677	237	0
39	DF	1624	0	1677	235	0
40	BG	1474	0	1534	237	0
40	DG	1474	0	1534	242	0
41	BH	1223	0	1282	199	0
41	DH	1223	0	1282	211	0
42	BI	1132	0	1218	198	0
42	DI	1132	0	1218	200	0
43	BN	1105	0	1180	209	0
43	DN	1105	0	1180	215	0
44	BO	933	0	996	139	0
44	DO	933	0	996	139	0
45	BP	1114	0	1187	322	0
45	DP	1114	0	1187	322	0
46	BQ	1080	0	1127	224	0
46	DQ	1080	0	1127	214	0
47	BR	960	0	1021	171	0
47	DR	960	0	1021	170	0
48	BS	771	0	832	182	0
48	DS	771	0	831	186	0
49	BT	1142	0	1202	219	0
49	DT	1142	0	1202	231	0
50	BU	958	0	1015	183	0
50	DU	958	0	1014	186	0
51	BV	779	0	851	212	0
51	DV	779	0	851	216	0
52	BW	896	0	953	111	0
52	DW	896	0	953	110	0
53	BX	726	0	778	203	0
53	DX	726	0	778	200	0
54	BY	776	0	870	220	0
54	DY	776	0	870	216	0
55	BZ	1404	0	1432	219	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	DZ	1404	0	1432	241	0
56	AA	215	0	0	0	0
56	AE	1	0	0	0	0
56	AV	7	0	0	0	0
56	AW	22	0	0	0	0
56	AX	4	0	0	0	0
56	AY	1	0	0	0	0
56	B1	1	0	0	0	0
56	B2	5	0	0	0	0
56	B3	1	0	0	0	0
56	B5	2	0	0	0	0
56	B7	2	0	0	0	0
56	BA	454	0	0	0	0
56	BB	19	0	0	0	0
56	BE	1	0	0	0	0
56	BF	2	0	0	0	0
56	BN	1	0	0	0	0
56	BO	1	0	0	0	0
56	BV	1	0	0	0	0
56	BX	1	0	0	0	0
56	CA	189	0	0	0	0
56	CF	1	0	0	0	0
56	CJ	1	0	0	0	0
56	CM	1	0	0	0	0
56	CU	1	0	0	0	0
56	CV	4	0	0	0	0
56	CW	13	0	0	0	0
56	CX	6	0	0	0	0
56	D5	2	0	0	0	0
56	DA	398	0	0	0	0
56	DB	12	0	0	0	0
56	DD	2	0	0	0	0
56	DE	1	0	0	0	0
56	DF	1	0	0	0	0
56	DH	1	0	0	0	0
56	DN	1	0	0	0	0
56	DO	1	0	0	0	0
56	DS	1	0	0	0	0
56	DU	1	0	0	0	0
56	DZ	1	0	0	0	0
57	AA	42	0	45	3	0
57	CA	42	0	45	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	AD	1	0	0	0	0
58	AN	1	0	0	0	0
58	CD	1	0	0	0	0
58	CN	1	0	0	0	0
All	All	291077	0	196199	21272	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 44.

The worst 5 of 21272 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
51:DV:70:ILE:HB	51:DV:90:PRO:HB2	1.21	1.18
3:CC:20:SER:HB2	3:CC:40:ARG:HH22	1.00	1.17
42:BI:79:ILE:HG12	42:BI:140:LEU:HD11	1.21	1.17
37:DD:35:LYS:HD3	37:DD:63:ARG:HB3	1.24	1.17
34:DA:2491:U:H5'	34:DA:2570:G:H5''	1.26	1.16

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	147 (63%)	54 (23%)	32 (14%)	0	1
2	CB	233/256 (91%)	149 (64%)	52 (22%)	32 (14%)	0	1
3	AC	205/239 (86%)	130 (63%)	55 (27%)	20 (10%)	1	2
3	CC	205/239 (86%)	130 (63%)	57 (28%)	18 (9%)	1	2
4	AD	206/209 (99%)	130 (63%)	51 (25%)	25 (12%)	1	1
4	CD	206/209 (99%)	128 (62%)	54 (26%)	24 (12%)	1	1
5	AE	149/162 (92%)	108 (72%)	28 (19%)	13 (9%)	1	2
5	CE	149/162 (92%)	107 (72%)	30 (20%)	12 (8%)	1	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	AF	99/101 (98%)	72 (73%)	21 (21%)	6 (6%)	2	6
6	CF	99/101 (98%)	72 (73%)	22 (22%)	5 (5%)	3	9
7	AG	153/156 (98%)	100 (65%)	41 (27%)	12 (8%)	1	3
7	CG	153/156 (98%)	100 (65%)	42 (28%)	11 (7%)	2	4
8	AH	136/138 (99%)	103 (76%)	28 (21%)	5 (4%)	5	16
8	CH	136/138 (99%)	102 (75%)	29 (21%)	5 (4%)	5	16
9	AI	121/128 (94%)	80 (66%)	30 (25%)	11 (9%)	1	2
9	CI	121/128 (94%)	81 (67%)	28 (23%)	12 (10%)	1	2
10	AJ	97/105 (92%)	70 (72%)	18 (19%)	9 (9%)	1	2
10	CJ	97/105 (92%)	70 (72%)	18 (19%)	9 (9%)	1	2
11	AK	117/129 (91%)	87 (74%)	25 (21%)	5 (4%)	4	13
11	CK	117/129 (91%)	88 (75%)	24 (20%)	5 (4%)	4	13
12	AL	123/135 (91%)	83 (68%)	22 (18%)	18 (15%)	0	1
12	CL	123/135 (91%)	84 (68%)	20 (16%)	19 (15%)	0	1
13	AM	113/126 (90%)	68 (60%)	26 (23%)	19 (17%)	0	0
13	CM	113/126 (90%)	69 (61%)	23 (20%)	21 (19%)	0	0
14	AN	58/61 (95%)	35 (60%)	17 (29%)	6 (10%)	1	1
14	CN	58/61 (95%)	35 (60%)	17 (29%)	6 (10%)	1	1
15	AO	86/89 (97%)	48 (56%)	34 (40%)	4 (5%)	4	11
15	CO	86/89 (97%)	50 (58%)	31 (36%)	5 (6%)	3	7
16	AP	82/88 (93%)	53 (65%)	24 (29%)	5 (6%)	2	6
16	CP	82/88 (93%)	53 (65%)	25 (30%)	4 (5%)	3	10
17	AQ	98/105 (93%)	74 (76%)	15 (15%)	9 (9%)	1	2
17	CQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	3
18	AR	68/88 (77%)	38 (56%)	21 (31%)	9 (13%)	0	1
18	CR	68/88 (77%)	38 (56%)	21 (31%)	9 (13%)	0	1
19	AS	77/93 (83%)	52 (68%)	14 (18%)	11 (14%)	0	1
19	CS	77/93 (83%)	51 (66%)	15 (20%)	11 (14%)	0	1
20	AT	97/106 (92%)	54 (56%)	29 (30%)	14 (14%)	0	1
20	CT	97/106 (92%)	56 (58%)	27 (28%)	14 (14%)	0	1
21	AU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	4	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	CU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	4	13
25	B0	83/85 (98%)	62 (75%)	16 (19%)	5 (6%)	2	6
25	D0	83/85 (98%)	63 (76%)	15 (18%)	5 (6%)	2	6
26	B1	87/98 (89%)	43 (49%)	25 (29%)	19 (22%)	0	0
26	D1	87/98 (89%)	42 (48%)	21 (24%)	24 (28%)	0	0
27	B2	49/72 (68%)	16 (33%)	16 (33%)	17 (35%)	0	0
27	D2	49/72 (68%)	15 (31%)	15 (31%)	19 (39%)	0	0
28	B3	58/60 (97%)	42 (72%)	12 (21%)	4 (7%)	2	4
28	D3	58/60 (97%)	42 (72%)	12 (21%)	4 (7%)	2	4
29	B4	48/71 (68%)	14 (29%)	11 (23%)	23 (48%)	0	0
29	D4	48/71 (68%)	14 (29%)	11 (23%)	23 (48%)	0	0
30	B5	57/60 (95%)	37 (65%)	13 (23%)	7 (12%)	1	1
30	D5	57/60 (95%)	38 (67%)	12 (21%)	7 (12%)	1	1
31	B6	41/54 (76%)	18 (44%)	16 (39%)	7 (17%)	0	0
31	D6	41/54 (76%)	18 (44%)	16 (39%)	7 (17%)	0	0
32	B7	47/49 (96%)	36 (77%)	10 (21%)	1 (2%)	11	33
32	D7	47/49 (96%)	37 (79%)	8 (17%)	2 (4%)	4	13
33	B8	62/65 (95%)	38 (61%)	13 (21%)	11 (18%)	0	0
33	D8	62/65 (95%)	37 (60%)	14 (23%)	11 (18%)	0	0
36	BC	183/229 (80%)	88 (48%)	52 (28%)	43 (24%)	0	0
36	DC	183/229 (80%)	87 (48%)	53 (29%)	43 (24%)	0	0
37	BD	270/276 (98%)	193 (72%)	51 (19%)	26 (10%)	1	2
37	DD	270/276 (98%)	194 (72%)	50 (18%)	26 (10%)	1	2
38	BE	203/206 (98%)	116 (57%)	49 (24%)	38 (19%)	0	0
38	DE	203/206 (98%)	116 (57%)	49 (24%)	38 (19%)	0	0
39	BF	206/210 (98%)	142 (69%)	40 (19%)	24 (12%)	1	1
39	DF	206/210 (98%)	142 (69%)	41 (20%)	23 (11%)	1	1
40	BG	177/182 (97%)	93 (52%)	56 (32%)	28 (16%)	0	1
40	DG	177/182 (97%)	101 (57%)	45 (25%)	31 (18%)	0	0
41	BH	158/180 (88%)	100 (63%)	31 (20%)	27 (17%)	0	0
41	DH	158/180 (88%)	100 (63%)	31 (20%)	27 (17%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	BI	144/148 (97%)	98 (68%)	36 (25%)	10 (7%)	2	4
42	DI	144/148 (97%)	97 (67%)	36 (25%)	11 (8%)	2	3
43	BN	137/140 (98%)	75 (55%)	35 (26%)	27 (20%)	0	0
43	DN	137/140 (98%)	77 (56%)	33 (24%)	27 (20%)	0	0
44	BO	120/122 (98%)	92 (77%)	17 (14%)	11 (9%)	1	2
44	DO	120/122 (98%)	90 (75%)	18 (15%)	12 (10%)	1	2
45	BP	144/150 (96%)	72 (50%)	37 (26%)	35 (24%)	0	0
45	DP	144/150 (96%)	72 (50%)	38 (26%)	34 (24%)	0	0
46	BQ	134/141 (95%)	81 (60%)	34 (25%)	19 (14%)	0	1
46	DQ	134/141 (95%)	79 (59%)	35 (26%)	20 (15%)	0	1
47	BR	115/118 (98%)	74 (64%)	20 (17%)	21 (18%)	0	0
47	DR	115/118 (98%)	72 (63%)	23 (20%)	20 (17%)	0	0
48	BS	97/112 (87%)	49 (50%)	19 (20%)	29 (30%)	0	0
48	DS	97/112 (87%)	49 (50%)	18 (19%)	30 (31%)	0	0
49	BT	136/146 (93%)	77 (57%)	34 (25%)	25 (18%)	0	0
49	DT	136/146 (93%)	79 (58%)	33 (24%)	24 (18%)	0	0
50	BU	115/118 (98%)	61 (53%)	42 (36%)	12 (10%)	1	1
50	DU	115/118 (98%)	61 (53%)	40 (35%)	14 (12%)	1	1
51	BV	97/101 (96%)	47 (48%)	23 (24%)	27 (28%)	0	0
51	DV	97/101 (96%)	47 (48%)	23 (24%)	27 (28%)	0	0
52	BW	111/113 (98%)	74 (67%)	23 (21%)	14 (13%)	0	1
52	DW	111/113 (98%)	77 (69%)	19 (17%)	15 (14%)	0	1
53	BX	91/96 (95%)	45 (50%)	23 (25%)	23 (25%)	0	0
53	DX	91/96 (95%)	45 (50%)	23 (25%)	23 (25%)	0	0
54	BY	99/110 (90%)	41 (41%)	24 (24%)	34 (34%)	0	0
54	DY	99/110 (90%)	41 (41%)	24 (24%)	34 (34%)	0	0
55	BZ	175/206 (85%)	99 (57%)	48 (27%)	28 (16%)	0	1
55	DZ	175/206 (85%)	109 (62%)	33 (19%)	33 (19%)	0	0
All	All	11570/12518 (92%)	7170 (62%)	2726 (24%)	1674 (14%)	0	1

5 of 1674 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	52	GLU
2	AB	77	ALA
2	AB	84	GLU
2	AB	154	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	202/220 (92%)	182 (90%)	20 (10%)	11	31
2	CB	202/220 (92%)	182 (90%)	20 (10%)	11	31
3	AC	160/188 (85%)	151 (94%)	9 (6%)	30	64
3	CC	160/188 (85%)	150 (94%)	10 (6%)	25	59
4	AD	180/181 (99%)	159 (88%)	21 (12%)	8	22
4	CD	180/181 (99%)	161 (89%)	19 (11%)	10	27
5	AE	115/123 (94%)	102 (89%)	13 (11%)	9	24
5	CE	115/123 (94%)	103 (90%)	12 (10%)	10	28
6	AF	90/90 (100%)	84 (93%)	6 (7%)	23	55
6	CF	90/90 (100%)	84 (93%)	6 (7%)	23	55
7	AG	126/127 (99%)	122 (97%)	4 (3%)	51	85
7	CG	126/127 (99%)	122 (97%)	4 (3%)	51	85
8	AH	119/119 (100%)	114 (96%)	5 (4%)	40	77
8	CH	119/119 (100%)	114 (96%)	5 (4%)	40	77
9	AI	98/99 (99%)	88 (90%)	10 (10%)	11	29
9	CI	98/99 (99%)	88 (90%)	10 (10%)	11	29
10	AJ	88/92 (96%)	82 (93%)	6 (7%)	22	54
10	CJ	88/92 (96%)	82 (93%)	6 (7%)	22	54
11	AK	90/99 (91%)	85 (94%)	5 (6%)	30	64
11	CK	90/99 (91%)	86 (96%)	4 (4%)	39	75
12	AL	104/111 (94%)	95 (91%)	9 (9%)	15	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	CL	104/111 (94%)	96 (92%)	8 (8%)	18	45
13	AM	99/101 (98%)	93 (94%)	6 (6%)	26	61
13	CM	99/101 (98%)	93 (94%)	6 (6%)	26	61
14	AN	49/50 (98%)	47 (96%)	2 (4%)	41	77
14	CN	49/50 (98%)	47 (96%)	2 (4%)	41	77
15	AO	79/80 (99%)	74 (94%)	5 (6%)	25	59
15	CO	79/80 (99%)	74 (94%)	5 (6%)	25	59
16	AP	72/74 (97%)	65 (90%)	7 (10%)	12	32
16	CP	72/74 (97%)	65 (90%)	7 (10%)	12	32
17	AQ	94/97 (97%)	92 (98%)	2 (2%)	66	93
17	CQ	94/97 (97%)	92 (98%)	2 (2%)	66	93
18	AR	61/77 (79%)	55 (90%)	6 (10%)	12	32
18	CR	61/77 (79%)	55 (90%)	6 (10%)	12	32
19	AS	69/80 (86%)	62 (90%)	7 (10%)	11	30
19	CS	69/80 (86%)	62 (90%)	7 (10%)	11	30
20	AT	76/82 (93%)	65 (86%)	11 (14%)	5	13
20	CT	76/82 (93%)	65 (86%)	11 (14%)	5	13
21	AU	19/22 (86%)	17 (90%)	2 (10%)	10	27
21	CU	19/22 (86%)	17 (90%)	2 (10%)	10	27
25	B0	61/67 (91%)	54 (88%)	7 (12%)	8	23
25	D0	61/67 (91%)	54 (88%)	7 (12%)	8	23
26	B1	73/83 (88%)	62 (85%)	11 (15%)	4	12
26	D1	73/83 (88%)	63 (86%)	10 (14%)	5	15
27	B2	46/67 (69%)	35 (76%)	11 (24%)	1	3
27	D2	46/67 (69%)	35 (76%)	11 (24%)	1	3
28	B3	51/52 (98%)	49 (96%)	2 (4%)	43	80
28	D3	51/52 (98%)	49 (96%)	2 (4%)	43	80
30	B5	51/52 (98%)	41 (80%)	10 (20%)	2	6
30	D5	51/52 (98%)	41 (80%)	10 (20%)	2	6
31	B6	43/52 (83%)	36 (84%)	7 (16%)	3	10
31	D6	43/52 (83%)	36 (84%)	7 (16%)	3	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	B7	41/42 (98%)	37 (90%)	4 (10%)	12	32
32	D7	41/42 (98%)	37 (90%)	4 (10%)	12	32
33	B8	53/55 (96%)	45 (85%)	8 (15%)	4	12
33	D8	53/55 (96%)	45 (85%)	8 (15%)	4	12
36	BC	61/181 (34%)	54 (88%)	7 (12%)	8	23
36	DC	61/181 (34%)	54 (88%)	7 (12%)	8	23
37	BD	213/218 (98%)	179 (84%)	34 (16%)	3	10
37	DD	213/218 (98%)	181 (85%)	32 (15%)	4	12
38	BE	165/166 (99%)	145 (88%)	20 (12%)	7	21
38	DE	165/166 (99%)	145 (88%)	20 (12%)	7	21
39	BF	165/166 (99%)	153 (93%)	12 (7%)	20	49
39	DF	165/166 (99%)	153 (93%)	12 (7%)	20	49
40	BG	155/156 (99%)	135 (87%)	20 (13%)	6	18
40	DG	155/156 (99%)	132 (85%)	23 (15%)	4	13
41	BH	132/148 (89%)	117 (89%)	15 (11%)	8	24
41	DH	132/148 (89%)	117 (89%)	15 (11%)	8	24
42	BI	122/124 (98%)	113 (93%)	9 (7%)	20	48
42	DI	122/124 (98%)	113 (93%)	9 (7%)	20	48
43	BN	117/119 (98%)	98 (84%)	19 (16%)	3	10
43	DN	117/119 (98%)	97 (83%)	20 (17%)	3	8
44	BO	100/100 (100%)	92 (92%)	8 (8%)	17	44
44	DO	100/100 (100%)	91 (91%)	9 (9%)	14	37
45	BP	112/116 (97%)	92 (82%)	20 (18%)	2	7
45	DP	112/116 (97%)	91 (81%)	21 (19%)	2	7
46	BQ	106/111 (96%)	93 (88%)	13 (12%)	7	20
46	DQ	106/111 (96%)	93 (88%)	13 (12%)	7	20
47	BR	100/101 (99%)	91 (91%)	9 (9%)	14	37
47	DR	100/101 (99%)	91 (91%)	9 (9%)	14	37
48	BS	77/88 (88%)	65 (84%)	12 (16%)	4	11
48	DS	77/88 (88%)	65 (84%)	12 (16%)	4	11
49	BT	120/127 (94%)	99 (82%)	21 (18%)	3	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	DT	120/127 (94%)	99 (82%)	21 (18%)	3	8
50	BU	92/94 (98%)	85 (92%)	7 (8%)	19	46
50	DU	92/94 (98%)	85 (92%)	7 (8%)	19	46
51	BV	82/82 (100%)	64 (78%)	18 (22%)	1	4
51	DV	82/82 (100%)	64 (78%)	18 (22%)	1	4
52	BW	91/92 (99%)	85 (93%)	6 (7%)	24	56
52	DW	91/92 (99%)	84 (92%)	7 (8%)	18	45
53	BX	74/78 (95%)	59 (80%)	15 (20%)	2	5
53	DX	74/78 (95%)	60 (81%)	14 (19%)	2	7
54	BY	84/91 (92%)	67 (80%)	17 (20%)	2	5
54	DY	84/91 (92%)	67 (80%)	17 (20%)	2	5
55	BZ	155/179 (87%)	144 (93%)	11 (7%)	21	51
55	DZ	155/179 (87%)	141 (91%)	14 (9%)	14	37
All	All	9464/10238 (92%)	8444 (89%)	1020 (11%)	9	26

5 of 1020 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
52	BW	25	ARG
6	CF	46	ARG
49	DT	128	GLU
53	BX	49	VAL
2	CB	59	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 275 such sidechains are listed below:

Mol	Chain	Res	Type
51	BV	89	GLN
6	CF	13	ASN
48	DS	84	GLN
52	BW	62	HIS
2	CB	78	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	200 (13%)	36 (2%)
1	CA	1503/1522 (98%)	204 (13%)	36 (2%)
22	AV	76/77 (98%)	18 (23%)	0
22	CV	76/77 (98%)	20 (26%)	0
23	AW	75/76 (98%)	15 (20%)	3 (4%)
23	AY	18/76 (23%)	2 (11%)	0
23	CW	75/76 (98%)	16 (21%)	3 (4%)
23	CY	18/76 (23%)	3 (16%)	0
24	AX	10/24 (41%)	2 (20%)	0
24	CX	10/24 (41%)	2 (20%)	0
34	BA	2771/2787 (99%)	563 (20%)	76 (2%)
34	DA	2771/2787 (99%)	560 (20%)	76 (2%)
35	BB	118/122 (96%)	14 (11%)	1 (0%)
35	DB	118/122 (96%)	14 (11%)	1 (0%)
All	All	9142/9368 (97%)	1633 (17%)	232 (2%)

5 of 1633 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G
1	AA	47	C

5 of 232 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	BA	2422	A
1	CA	429	U
34	DA	2031	A
34	BA	2662	A
1	CA	60	A

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

2 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	$\# Z > 2$
22	5MU	AV	54	22	20,22,23	1.03	2 (10%)	25,32,35	1.34	3 (12%)
22	5MU	CV	54	22	20,22,23	1.08	3 (15%)	25,32,35	1.28	3 (12%)

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
22	5MU	AV	54	22	-	0/6/25/26	0/2/2/2
22	5MU	CV	54	22	-	0/6/25/26	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	CV	54	5MU	C6-N1	2.38	1.38	1.34
22	AV	54	5MU	C6-N1	2.22	1.38	1.34
22	AV	54	5MU	C6-C5	-2.20	1.34	1.40
22	CV	54	5MU	C6-C5	-2.17	1.34	1.40
22	CV	54	5MU	C4-C5	2.11	1.45	1.40

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AV	54	5MU	C6-N1-C2	-4.66	121.08	122.41
22	CV	54	5MU	C6-N1-C2	-4.51	121.12	122.41
22	AV	54	5MU	C5M-C5-C4	-2.11	118.85	121.08
22	AV	54	5MU	C5M-C5-C6	2.07	122.92	118.61
22	CV	54	5MU	C5-C6-N1	2.02	123.83	122.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 1385 ligands modelled in this entry, 1383 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
57	PAR	AA	1816	-	45,45,45	1.44	8 (17%)	67,67,67	1.19	5 (7%)
57	PAR	CA	1790	-	45,45,45	1.43	10 (22%)	67,67,67	1.32	7 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PAR	AA	1816	-	-	0/18/94/94	0/4/4/4
57	PAR	CA	1790	-	-	0/18/94/94	0/4/4/4

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	CA	1790	PAR	C34-C24	4.06	1.59	1.53
57	AA	1816	PAR	C52-C42	3.19	1.58	1.52
57	AA	1816	PAR	C64-C54	2.89	1.59	1.51
57	AA	1816	PAR	O54-C14	2.82	1.49	1.41
57	AA	1816	PAR	C11-C21	2.60	1.57	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	AA	1816	PAR	O33-C14-C24	4.24	116.47	108.08
57	AA	1816	PAR	O52-C13-C23	4.14	114.89	107.50
57	CA	1790	PAR	O33-C14-C24	3.93	115.86	108.08
57	CA	1790	PAR	O54-C54-C64	3.78	113.18	105.97
57	CA	1790	PAR	O52-C13-C23	3.72	114.13	107.50

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	CM	5
13	AM	5
9	AI	2
9	CI	2
51	DV	1
40	DG	1
40	BG	1
51	BV	1
31	D6	1
31	B6	1

The worst 5 of 20 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B6	46:HIS	C	47:THR	N	4.89
1	D6	46:HIS	C	47:THR	N	4.87
1	AM	69:GLU	C	70:LEU	N	4.66
1	CM	69:GLU	C	70:LEU	N	4.66
1	CI	53:VAL	C	54:ASP	N	4.02

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	1504/1522 (98%)	-0.21	34 (2%) 57 58	2, 42, 165, 200	0
1	CA	1504/1522 (98%)	-0.11	39 (2%) 53 54	3, 50, 172, 200	0
2	AB	235/256 (91%)	0.25	27 (11%) 5 4	17, 94, 183, 200	0
2	CB	235/256 (91%)	0.49	29 (12%) 5 4	17, 104, 187, 200	0
3	AC	207/239 (86%)	-0.09	7 (3%) 43 44	17, 70, 156, 200	0
3	CC	207/239 (86%)	0.22	15 (7%) 15 14	19, 84, 149, 190	0
4	AD	208/209 (99%)	-0.38	2 (0%) 79 79	1, 43, 127, 198	0
4	CD	208/209 (99%)	-0.25	5 (2%) 56 57	4, 51, 133, 182	0
5	AE	151/162 (93%)	-0.36	2 (1%) 74 75	4, 51, 128, 177	0
5	CE	151/162 (93%)	-0.12	5 (3%) 44 45	3, 56, 140, 185	0
6	AF	101/101 (100%)	-0.35	3 (2%) 48 49	5, 48, 131, 156	0
6	CF	101/101 (100%)	-0.33	2 (1%) 62 63	2, 54, 130, 151	0
7	AG	155/156 (99%)	0.08	13 (8%) 11 9	8, 68, 151, 184	0
7	CG	155/156 (99%)	0.76	26 (16%) 2 2	15, 87, 155, 190	0
8	AH	138/138 (100%)	-0.20	3 (2%) 59 60	3, 52, 120, 173	0
8	CH	138/138 (100%)	-0.11	4 (2%) 49 50	16, 58, 138, 152	0
9	AI	127/128 (99%)	0.74	19 (14%) 3 2	26, 97, 171, 200	0
9	CI	127/128 (99%)	0.71	21 (16%) 2 2	28, 111, 175, 200	0
10	AJ	99/105 (94%)	0.62	15 (15%) 3 2	17, 105, 178, 200	0
10	CJ	99/105 (94%)	1.04	21 (21%) 1 1	34, 123, 176, 197	0
11	AK	119/129 (92%)	-0.27	4 (3%) 43 44	8, 46, 151, 192	0
11	CK	119/129 (92%)	0.08	7 (5%) 22 21	16, 61, 147, 200	0
12	AL	125/135 (92%)	-0.13	7 (5%) 24 23	5, 38, 133, 200	0
12	CL	125/135 (92%)	-0.04	5 (4%) 36 37	1, 38, 132, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	125/126 (99%)	0.47	15 (12%) 5 4	13, 74, 159, 196	0
13	CM	125/126 (99%)	0.37	13 (10%) 7 6	19, 91, 160, 191	0
14	AN	60/61 (98%)	0.67	11 (18%) 2 2	14, 66, 161, 184	0
14	CN	60/61 (98%)	0.35	4 (6%) 17 16	19, 73, 143, 182	0
15	AO	88/89 (98%)	-0.53	0 100 100	2, 42, 129, 141	0
15	CO	88/89 (98%)	-0.36	1 (1%) 77 78	2, 56, 124, 167	0
16	AP	84/88 (95%)	-0.22	0 100 100	6, 36, 104, 190	0
16	CP	84/88 (95%)	0.03	3 (3%) 41 41	6, 49, 121, 199	0
17	AQ	100/105 (95%)	-0.35	2 (2%) 62 63	1, 45, 110, 193	0
17	CQ	100/105 (95%)	0.27	4 (4%) 36 37	18, 60, 105, 194	0
18	AR	70/88 (79%)	-0.13	2 (2%) 49 50	10, 50, 140, 172	0
18	CR	70/88 (79%)	0.25	3 (4%) 34 34	7, 56, 144, 179	0
19	AS	79/93 (84%)	0.28	8 (10%) 7 6	22, 79, 186, 200	0
19	CS	79/93 (84%)	0.58	14 (17%) 2 2	25, 83, 175, 197	0
20	AT	99/106 (93%)	0.41	12 (12%) 5 4	5, 60, 152, 180	0
20	CT	99/106 (93%)	0.20	7 (7%) 16 14	17, 77, 141, 183	0
21	AU	25/27 (92%)	2.03	11 (44%) 1 0	27, 72, 128, 141	0
21	CU	25/27 (92%)	2.96	14 (56%) 0 0	40, 74, 127, 139	0
22	AV	77/77 (100%)	-0.44	0 100 100	14, 53, 143, 194	0
22	CV	77/77 (100%)	-0.31	1 (1%) 74 75	21, 55, 146, 198	0
23	AW	76/76 (100%)	0.08	6 (7%) 13 11	30, 103, 164, 199	0
23	AY	19/76 (25%)	0.06	1 (5%) 25 26	23, 72, 190, 196	0
23	CW	76/76 (100%)	0.23	7 (9%) 9 7	35, 116, 165, 196	0
23	CY	19/76 (25%)	-0.12	0 100 100	26, 76, 186, 196	0
24	AX	11/24 (45%)	0.21	1 (9%) 9 8	12, 33, 170, 185	0
24	CX	11/24 (45%)	0.58	2 (18%) 2 2	14, 39, 167, 192	0
25	B0	85/85 (100%)	0.38	7 (8%) 12 10	8, 43, 138, 196	0
25	D0	85/85 (100%)	0.74	12 (14%) 3 3	18, 57, 137, 179	0
26	B1	89/98 (90%)	0.08	5 (5%) 24 23	1, 35, 143, 157	0
26	D1	89/98 (90%)	-0.13	2 (2%) 59 60	1, 44, 145, 200	0
27	B2	51/72 (70%)	-0.03	4 (7%) 13 11	5, 66, 145, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	D2	51/72 (70%)	0.56	7 (13%) 4 3	13, 79, 154, 200	0
28	B3	60/60 (100%)	0.32	4 (6%) 17 16	5, 57, 140, 190	0
28	D3	60/60 (100%)	0.35	3 (5%) 28 28	5, 58, 146, 198	0
29	B4	50/71 (70%)	-0.46	1 (2%) 62 63	38, 90, 158, 173	0
29	D4	50/71 (70%)	0.28	7 (14%) 3 3	54, 117, 160, 198	0
30	B5	59/60 (98%)	0.87	13 (22%) 1 1	5, 51, 192, 200	0
30	D5	59/60 (98%)	0.48	7 (11%) 5 4	1, 65, 179, 200	0
31	B6	45/54 (83%)	1.90	21 (46%) 1 0	54, 103, 171, 180	0
31	D6	45/54 (83%)	2.81	27 (60%) 0 0	64, 139, 171, 189	0
32	B7	49/49 (100%)	-0.14	4 (8%) 12 10	1, 19, 115, 165	0
32	D7	49/49 (100%)	-0.03	4 (8%) 12 10	1, 19, 88, 174	0
33	B8	64/65 (98%)	0.55	6 (9%) 9 7	4, 44, 140, 195	0
33	D8	64/65 (98%)	0.32	6 (9%) 9 7	5, 52, 155, 192	0
34	BA	2772/2787 (99%)	-0.34	40 (1%) 72 72	1, 29, 145, 200	0
34	DA	2772/2787 (99%)	-0.30	49 (1%) 65 66	1, 30, 152, 200	0
35	BB	119/122 (97%)	-0.32	0 100 100	22, 64, 108, 197	0
35	DB	119/122 (97%)	-0.12	2 (1%) 67 68	34, 76, 127, 188	0
36	BC	191/229 (83%)	2.04	75 (39%) 1 0	51, 144, 186, 200	0
36	DC	191/229 (83%)	2.67	97 (50%) 0 0	61, 146, 186, 200	0
37	BD	272/276 (98%)	-0.51	5 (1%) 65 66	1, 19, 89, 196	0
37	DD	272/276 (98%)	-0.48	3 (1%) 77 78	1, 21, 89, 200	0
38	BE	205/206 (99%)	0.03	10 (4%) 28 29	1, 46, 141, 193	0
38	DE	205/206 (99%)	-0.13	7 (3%) 43 44	1, 43, 144, 199	0
39	BF	208/210 (99%)	-0.26	9 (4%) 34 34	1, 44, 155, 200	0
39	DF	208/210 (99%)	0.15	13 (6%) 19 18	1, 44, 160, 200	0
40	BG	181/182 (99%)	-0.16	7 (3%) 37 37	8, 65, 142, 188	0
40	DG	181/182 (99%)	0.16	11 (6%) 21 20	10, 82, 149, 195	0
41	BH	160/180 (88%)	1.04	35 (21%) 1 1	51, 124, 175, 200	0
41	DH	160/180 (88%)	0.79	28 (17%) 2 2	10, 102, 174, 194	0
42	BI	146/148 (98%)	0.33	12 (8%) 12 10	5, 78, 148, 187	0
42	DI	146/148 (98%)	2.64	57 (39%) 1 0	9, 124, 184, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
43	BN	139/140 (99%)	-0.09	4 (2%)	49	50	10, 68, 144, 163	0
43	DN	139/140 (99%)	0.10	7 (5%)	28	28	15, 63, 141, 165	0
44	BO	122/122 (100%)	-0.46	1 (0%)	83	83	3, 32, 103, 177	0
44	DO	122/122 (100%)	-0.48	0	100	100	1, 33, 102, 126	0
45	BP	146/150 (97%)	0.20	6 (4%)	35	36	1, 61, 159, 193	0
45	DP	146/150 (97%)	0.32	11 (7%)	14	12	2, 71, 165, 198	0
46	BQ	136/141 (96%)	0.48	12 (8%)	10	8	7, 58, 171, 200	0
46	DQ	136/141 (96%)	0.21	12 (8%)	10	8	7, 54, 164, 200	0
47	BR	117/118 (99%)	-0.19	1 (0%)	81	81	3, 32, 132, 146	0
47	DR	117/118 (99%)	-0.11	1 (0%)	81	81	3, 42, 126, 166	0
48	BS	99/112 (88%)	0.31	7 (7%)	16	14	21, 76, 134, 173	0
48	DS	99/112 (88%)	0.82	19 (19%)	2	1	24, 89, 143, 171	0
49	BT	138/146 (94%)	0.13	13 (9%)	9	7	3, 67, 169, 190	0
49	DT	138/146 (94%)	-0.02	7 (5%)	27	27	7, 65, 171, 200	0
50	BU	117/118 (99%)	-0.01	7 (5%)	21	21	5, 50, 142, 200	0
50	DU	117/118 (99%)	-0.12	3 (2%)	53	54	1, 46, 145, 190	0
51	BV	101/101 (100%)	0.46	8 (7%)	13	11	14, 96, 174, 192	0
51	DV	101/101 (100%)	0.16	5 (4%)	28	28	11, 93, 172, 193	0
52	BW	113/113 (100%)	-0.53	0	100	100	1, 26, 121, 161	0
52	DW	113/113 (100%)	-0.45	0	100	100	3, 28, 126, 200	0
53	BX	93/96 (96%)	-0.24	7 (7%)	14	12	1, 46, 137, 168	0
53	DX	93/96 (96%)	-0.01	4 (4%)	34	34	8, 54, 138, 157	0
54	BY	101/110 (91%)	0.95	19 (18%)	2	2	1, 79, 170, 195	0
54	DY	101/110 (91%)	1.44	25 (24%)	1	1	1, 79, 177, 196	0
55	BZ	177/206 (85%)	0.32	16 (9%)	10	8	19, 96, 177, 200	0
55	DZ	177/206 (85%)	0.40	16 (9%)	10	8	18, 98, 178, 198	0
All	All	20974/21886 (95%)	0.03	1268 (6%)	21	21	1, 51, 163, 200	0

The worst 5 of 1268 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
42	DI	84	GLY	36.6
46	BQ	140	ALA	25.2

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Mol	Chain	Res	Type	RSRZ
17	CQ	101	ARG	24.5
36	DC	145	VAL	22.3
42	DI	120	ILE	22.1

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
22	5MU	CV	54	21/22	0.14	-	64,75,79,79	0
22	5MU	AV	54	21/22	0.16	-	75,83,108,108	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
56	MG	CA	1745	1/1	0.36	-	77,77,77,77	0
56	MG	DA	3105	1/1	0.18	-	6,6,6,6	0
56	MG	AA	1704	1/1	0.07	-	0,0,0,0	0
56	MG	DA	3385	1/1	0.07	-	29,29,29,29	0
56	MG	DA	3028	1/1	0.14	-	0,0,0,0	0
56	MG	DA	3277	1/1	0.22	-	55,55,55,55	0
56	MG	CA	1687	1/1	0.07	-	0,0,0,0	0
56	MG	BA	3427	1/1	0.06	-	12,12,12,12	0
56	MG	DA	3357	1/1	0.15	-	26,26,26,26	0
56	MG	BA	3153	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
56	MG	BA	3330	1/1	0.07	-	33,33,33,33	0
56	MG	BA	3304	1/1	0.13	-	35,35,35,35	0
56	MG	AW	118	1/1	0.16	-	46,46,46,46	0
56	MG	BA	3241	1/1	0.17	-	43,43,43,43	0
56	MG	BA	3302	1/1	0.15	-	14,14,14,14	0
56	MG	BA	3406	1/1	0.15	-	18,18,18,18	0
56	MG	BA	3381	1/1	0.10	-	21,21,21,21	0
56	MG	AA	1758	1/1	0.12	-	62,62,62,62	0
56	MG	BA	3442	1/1	0.10	-	29,29,29,29	0
56	MG	DA	3061	1/1	0.24	-	0,0,0,0	0
56	MG	AA	1682	1/1	0.18	-	17,17,17,17	0
56	MG	DA	3175	1/1	0.23	-	30,30,30,30	0
56	MG	AA	1632	1/1	0.10	-	24,24,24,24	0
56	MG	DA	3262	1/1	0.32	-	72,72,72,72	0
56	MG	CA	1770	1/1	0.11	-	14,14,14,14	0
56	MG	AA	1775	1/1	0.11	-	29,29,29,29	0
56	MG	DA	3110	1/1	0.18	-	1,1,1,1	0
56	MG	DA	3129	1/1	0.15	-	6,6,6,6	0
56	MG	DA	3361	1/1	0.25	-	5,5,5,5	0
56	MG	BA	3135	1/1	0.14	-	18,18,18,18	0
56	MG	DA	3317	1/1	0.06	-	11,11,11,11	1
56	MG	CA	1777	1/1	0.16	-	0,0,0,0	0
56	MG	DA	3042	1/1	0.55	-	58,58,58,58	0
56	MG	BA	3129	1/1	0.14	-	21,21,21,21	0
56	MG	CX	105	1/1	0.11	-	41,41,41,41	0
56	MG	CA	1623	1/1	0.10	-	9,9,9,9	0
56	MG	DA	3132	1/1	0.08	-	13,13,13,13	0
56	MG	CA	1643	1/1	0.43	-	48,48,48,48	0
56	MG	BA	3361	1/1	0.21	-	53,53,53,53	0
56	MG	DA	3134	1/1	0.20	-	4,4,4,4	0
56	MG	BA	3084	1/1	0.20	-	0,0,0,0	0
56	MG	DA	3377	1/1	0.12	-	6,6,6,6	1
56	MG	AA	1674	1/1	0.22	-	33,33,33,33	0
56	MG	DA	3185	1/1	0.13	-	8,8,8,8	1
56	MG	DA	3051	1/1	0.16	-	0,0,0,0	0
56	MG	BA	3428	1/1	0.69	-	72,72,72,72	1
56	MG	CA	1751	1/1	0.21	-	81,81,81,81	0
56	MG	CA	1746	1/1	0.25	-	18,18,18,18	0
56	MG	BA	3106	1/1	0.18	-	0,0,0,0	0
56	MG	BA	3223	1/1	0.13	-	8,8,8,8	0
56	MG	AA	1712	1/1	0.05	-	22,22,22,22	0
56	MG	BA	3398	1/1	0.07	-	9,9,9,9	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	1767	1/1	0.17	-	48,48,48,48	0
56	MG	DA	3235	1/1	0.06	-	39,39,39,39	0
56	MG	BA	3355	1/1	0.10	-	20,20,20,20	0
56	MG	AA	1664	1/1	0.09	-	0,0,0,0	0
56	MG	BA	3298	1/1	0.31	-	25,25,25,25	0
56	MG	BA	3103	1/1	0.17	-	55,55,55,55	0
56	MG	CA	1603	1/1	0.10	-	25,25,25,25	0
56	MG	DA	3102	1/1	0.12	-	0,0,0,0	0
56	MG	BA	3122	1/1	0.13	-	8,8,8,8	0
56	MG	DA	3398	1/1	0.16	-	7,7,7,7	0
56	MG	BA	3375	1/1	0.27	-	42,42,42,42	1
56	MG	BA	3431	1/1	0.12	-	51,51,51,51	0
56	MG	DA	3118	1/1	0.08	-	6,6,6,6	0
56	MG	BA	3230	1/1	0.18	-	36,36,36,36	0
56	MG	CA	1701	1/1	0.09	-	16,16,16,16	0
56	MG	DA	3390	1/1	0.11	-	73,73,73,73	0
56	MG	BA	3157	1/1	0.26	-	39,39,39,39	0
56	MG	B5	101	1/1	0.15	-	6,6,6,6	0
56	MG	AA	1811	1/1	0.11	-	16,16,16,16	0
56	MG	DA	3079	1/1	0.14	-	13,13,13,13	0
56	MG	AA	1748	1/1	0.24	-	59,59,59,59	0
56	MG	DA	3223	1/1	0.32	-	11,11,11,11	0
56	MG	DA	3086	1/1	0.20	-	0,0,0,0	0
56	MG	CA	1658	1/1	0.09	-	40,40,40,40	0
56	MG	DA	3298	1/1	0.13	-	5,5,5,5	0
56	MG	DA	3123	1/1	0.10	-	20,20,20,20	0
56	MG	AA	1680	1/1	0.15	-	30,30,30,30	0
56	MG	AA	1641	1/1	0.07	-	0,0,0,0	0
56	MG	AA	1739	1/1	0.15	-	23,23,23,23	0
56	MG	DA	3328	1/1	0.10	-	27,27,27,27	0
56	MG	CA	1682	1/1	0.13	-	32,32,32,32	0
56	MG	CA	1726	1/1	0.12	-	29,29,29,29	0
56	MG	DA	3217	1/1	0.14	-	62,62,62,62	0
56	MG	AA	1666	1/1	0.18	-	1,1,1,1	0
56	MG	DA	3305	1/1	0.12	-	28,28,28,28	0
56	MG	DA	3092	1/1	0.10	-	4,4,4,4	0
56	MG	DA	3127	1/1	0.10	-	0,0,0,0	0
56	MG	DA	3252	1/1	0.07	-	0,0,0,0	1
56	MG	BA	3104	1/1	0.18	-	12,12,12,12	0
56	MG	DA	3023	1/1	0.27	-	0,0,0,0	0
56	MG	AA	1719	1/1	0.06	-	65,65,65,65	0
56	MG	DA	3066	1/1	0.24	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	B7	102	1/1	0.07	-	11,11,11,11	1
56	MG	AA	1714	1/1	0.26	-	28,28,28,28	0
56	MG	AA	1677	1/1	0.13	-	41,41,41,41	0
56	MG	AA	1809	1/1	0.17	-	40,40,40,40	1
56	MG	DA	3043	1/1	0.14	-	2,2,2,2	0
56	MG	BA	3452	1/1	0.13	-	39,39,39,39	0
56	MG	BA	3040	1/1	0.07	-	22,22,22,22	0
56	MG	BA	3092	1/1	0.17	-	0,0,0,0	0
56	MG	DA	3008	1/1	0.16	-	23,23,23,23	0
56	MG	AW	104	1/1	0.05	-	28,28,28,28	0
56	MG	DA	3108	1/1	0.24	-	0,0,0,0	0
56	MG	DB	207	1/1	0.20	-	52,52,52,52	1
56	MG	CA	1740	1/1	0.05	-	19,19,19,19	0
56	MG	AA	1780	1/1	0.10	-	60,60,60,60	0
56	MG	DA	3347	1/1	0.08	-	34,34,34,34	0
56	MG	BA	3226	1/1	0.09	-	20,20,20,20	0
56	MG	DA	3281	1/1	0.20	-	14,14,14,14	1
56	MG	DA	3331	1/1	0.19	-	42,42,42,42	0
56	MG	DA	3238	1/1	0.26	-	54,54,54,54	0
56	MG	DA	3099	1/1	0.11	-	10,10,10,10	0
56	MG	BA	3364	1/1	0.13	-	35,35,35,35	0
56	MG	AA	1699	1/1	0.14	-	0,0,0,0	0
56	MG	DA	3254	1/1	0.10	-	1,1,1,1	0
56	MG	AA	1754	1/1	0.10	-	16,16,16,16	0
56	MG	BA	3208	1/1	0.11	-	8,8,8,8	0
56	MG	BA	3423	1/1	0.16	-	21,21,21,21	0
56	MG	DA	3002	1/1	0.24	-	38,38,38,38	0
56	MG	BA	3120	1/1	0.06	-	23,23,23,23	0
56	MG	DA	3368	1/1	0.75	-	71,71,71,71	0
56	MG	AA	1631	1/1	0.30	-	21,21,21,21	0
56	MG	BA	3444	1/1	0.09	-	7,7,7,7	0
56	MG	BA	3169	1/1	0.08	-	8,8,8,8	0
56	MG	DA	3321	1/1	0.08	-	45,45,45,45	1
56	MG	BA	3419	1/1	0.27	-	39,39,39,39	0
56	MG	DA	3164	1/1	0.06	-	8,8,8,8	0
56	MG	BA	3306	1/1	0.23	-	20,20,20,20	0
56	MG	AA	1769	1/1	0.20	-	61,61,61,61	0
56	MG	BB	203	1/1	0.14	-	52,52,52,52	0
56	MG	BA	3449	1/1	0.13	-	27,27,27,27	0
56	MG	BA	3163	1/1	0.13	-	17,17,17,17	0
56	MG	BA	3397	1/1	0.08	-	32,32,32,32	0
56	MG	BA	3115	1/1	0.08	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3171	1/1	0.18	-	37,37,37,37	0
56	MG	BA	3218	1/1	0.08	-	56,56,56,56	0
56	MG	BA	3128	1/1	0.18	-	18,18,18,18	0
56	MG	CA	1691	1/1	0.23	-	56,56,56,56	0
56	MG	DA	3226	1/1	0.09	-	5,5,5,5	0
56	MG	CA	1604	1/1	0.19	-	45,45,45,45	0
56	MG	DA	3276	1/1	0.36	-	45,45,45,45	0
56	MG	CW	105	1/1	0.04	-	30,30,30,30	0
56	MG	CA	1715	1/1	0.07	-	55,55,55,55	0
56	MG	BA	3312	1/1	0.20	-	0,0,0,0	0
56	MG	AA	1779	1/1	0.19	-	46,46,46,46	0
56	MG	AV	102	1/1	0.05	-	28,28,28,28	0
56	MG	DA	3264	1/1	0.10	-	11,11,11,11	0
56	MG	AA	1798	1/1	0.12	-	36,36,36,36	0
56	MG	CA	1627	1/1	0.14	-	34,34,34,34	0
56	MG	AE	201	1/1	0.10	-	47,47,47,47	0
56	MG	DA	3342	1/1	0.21	-	49,49,49,49	0
56	MG	DA	3022	1/1	0.16	-	37,37,37,37	0
56	MG	BA	3186	1/1	0.14	-	25,25,25,25	0
56	MG	DB	211	1/1	0.06	-	45,45,45,45	0
56	MG	AA	1737	1/1	0.13	-	60,60,60,60	0
56	MG	BA	3184	1/1	0.15	-	1,1,1,1	0
56	MG	BA	3388	1/1	0.23	-	22,22,22,22	0
56	MG	CA	1681	1/1	0.07	-	40,40,40,40	0
56	MG	DA	3009	1/1	0.19	-	3,3,3,3	0
56	MG	BA	3023	1/1	0.26	-	0,0,0,0	0
56	MG	AA	1651	1/1	0.20	-	35,35,35,35	0
56	MG	CA	1743	1/1	0.18	-	1,1,1,1	0
56	MG	AX	104	1/1	0.12	-	44,44,44,44	0
56	MG	CA	1636	1/1	0.15	-	36,36,36,36	0
56	MG	DA	3015	1/1	0.11	-	0,0,0,0	0
56	MG	DA	3351	1/1	0.15	-	16,16,16,16	0
56	MG	DA	3282	1/1	0.15	-	41,41,41,41	0
56	MG	DA	3081	1/1	0.20	-	4,4,4,4	0
56	MG	BA	3097	1/1	0.07	-	2,2,2,2	0
56	MG	DA	3364	1/1	0.09	-	57,57,57,57	0
56	MG	DA	3215	1/1	0.04	-	31,31,31,31	0
56	MG	AA	1727	1/1	0.18	-	40,40,40,40	0
56	MG	DA	3039	1/1	0.18	-	10,10,10,10	0
56	MG	CA	1752	1/1	0.54	-	83,83,83,83	0
56	MG	BA	3170	1/1	0.15	-	0,0,0,0	0
56	MG	CA	1700	1/1	0.13	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3232	1/1	0.13	-	13,13,13,13	0
56	MG	DA	3203	1/1	0.08	-	58,58,58,58	0
56	MG	BA	3042	1/1	0.06	-	13,13,13,13	0
56	MG	DA	3312	1/1	0.12	-	44,44,44,44	0
56	MG	BA	3450	1/1	0.10	-	55,55,55,55	0
56	MG	BA	3439	1/1	0.27	-	31,31,31,31	0
56	MG	BA	3214	1/1	0.39	-	44,44,44,44	0
56	MG	AA	1725	1/1	0.12	-	53,53,53,53	0
56	MG	CJ	201	1/1	0.12	-	44,44,44,44	0
56	MG	BA	3243	1/1	0.16	-	18,18,18,18	0
56	MG	BA	3066	1/1	0.08	-	0,0,0,0	0
56	MG	BA	3392	1/1	0.10	-	8,8,8,8	0
56	MG	BA	3061	1/1	0.17	-	0,0,0,0	0
56	MG	AA	1740	1/1	0.13	-	40,40,40,40	0
56	MG	DA	3244	1/1	0.28	-	0,0,0,0	0
58	ZN	CD	301	1/1	0.18	-	24,24,24,24	0
56	MG	DA	3141	1/1	0.07	-	0,0,0,0	0
56	MG	AA	1654	1/1	0.23	-	50,50,50,50	0
56	MG	AV	105	1/1	0.10	-	12,12,12,12	0
56	MG	DA	3191	1/1	0.20	-	25,25,25,25	0
56	MG	DA	3340	1/1	0.11	-	30,30,30,30	0
56	MG	CA	1724	1/1	0.08	-	38,38,38,38	0
56	MG	DA	3249	1/1	0.48	-	57,57,57,57	0
56	MG	AA	1609	1/1	0.16	-	44,44,44,44	0
56	MG	DA	3056	1/1	0.14	-	9,9,9,9	0
56	MG	BA	3334	1/1	0.12	-	40,40,40,40	0
56	MG	DA	3396	1/1	0.18	-	27,27,27,27	1
56	MG	DA	3338	1/1	0.09	-	53,53,53,53	0
56	MG	DA	3220	1/1	0.09	-	3,3,3,3	0
56	MG	CA	1660	1/1	0.19	-	22,22,22,22	0
56	MG	BA	3386	1/1	0.07	-	85,85,85,85	0
56	MG	CA	1614	1/1	0.10	-	20,20,20,20	0
56	MG	DA	3005	1/1	0.07	-	13,13,13,13	0
56	MG	BA	3225	1/1	0.16	-	0,0,0,0	0
56	MG	CA	1694	1/1	0.18	-	33,33,33,33	0
56	MG	DA	3324	1/1	0.18	-	56,56,56,56	0
56	MG	DA	3365	1/1	0.09	-	29,29,29,29	0
56	MG	DA	3150	1/1	0.16	-	40,40,40,40	0
56	MG	BB	219	1/1	0.09	-	24,24,24,24	0
56	MG	BA	3260	1/1	0.10	-	23,23,23,23	0
56	MG	AA	1702	1/1	0.20	-	23,23,23,23	0
56	MG	AA	1672	1/1	0.14	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3250	1/1	0.07	-	57,57,57,57	0
56	MG	AW	115	1/1	0.12	-	42,42,42,42	0
56	MG	AA	1688	1/1	0.28	-	39,39,39,39	0
56	MG	BA	3148	1/1	0.14	-	37,37,37,37	0
56	MG	DA	3366	1/1	0.13	-	3,3,3,3	0
56	MG	DA	3256	1/1	0.08	-	22,22,22,22	0
56	MG	DA	3346	1/1	0.09	-	29,29,29,29	0
56	MG	BO	201	1/1	0.17	-	13,13,13,13	0
56	MG	CA	1703	1/1	0.07	-	19,19,19,19	0
56	MG	BA	3051	1/1	0.18	-	56,56,56,56	0
56	MG	AA	1770	1/1	0.12	-	16,16,16,16	0
56	MG	DA	3057	1/1	0.26	-	35,35,35,35	0
56	MG	BA	3090	1/1	0.16	-	0,0,0,0	0
56	MG	AA	1637	1/1	0.14	-	0,0,0,0	0
56	MG	BA	3054	1/1	0.11	-	0,0,0,0	0
56	MG	AW	116	1/1	0.14	-	58,58,58,58	0
56	MG	DA	3348	1/1	0.14	-	46,46,46,46	0
56	MG	BA	3111	1/1	0.15	-	27,27,27,27	0
56	MG	BA	3357	1/1	0.07	-	19,19,19,19	0
56	MG	AA	1724	1/1	0.06	-	0,0,0,0	0
56	MG	DA	3394	1/1	0.19	-	66,66,66,66	0
56	MG	AA	1705	1/1	0.06	-	21,21,21,21	0
56	MG	BA	3130	1/1	0.04	-	4,4,4,4	0
56	MG	DA	3275	1/1	0.42	-	75,75,75,75	0
56	MG	DA	3360	1/1	0.25	-	39,39,39,39	0
56	MG	AW	114	1/1	0.13	-	25,25,25,25	1
56	MG	BA	3343	1/1	0.30	-	34,34,34,34	0
56	MG	BA	3048	1/1	0.19	-	0,0,0,0	0
56	MG	DA	3374	1/1	0.14	-	50,50,50,50	0
56	MG	AA	1787	1/1	0.08	-	15,15,15,15	0
56	MG	DA	3139	1/1	0.10	-	28,28,28,28	0
56	MG	DA	3111	1/1	0.25	-	1,1,1,1	0
56	MG	DA	3001	1/1	0.17	-	20,20,20,20	0
56	MG	BA	3204	1/1	0.10	-	0,0,0,0	0
56	MG	BA	3282	1/1	0.33	-	49,49,49,49	0
56	MG	BA	3443	1/1	0.04	-	20,20,20,20	0
56	MG	AA	1736	1/1	0.12	-	19,19,19,19	0
56	MG	DA	3213	1/1	0.37	-	84,84,84,84	0
56	MG	AA	1621	1/1	0.09	-	14,14,14,14	0
56	MG	CA	1721	1/1	0.30	-	57,57,57,57	0
56	MG	BA	3030	1/1	0.13	-	0,0,0,0	0
56	MG	BA	3200	1/1	0.06	-	5,5,5,5	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	1686	1/1	0.10	-	57,57,57,57	0
56	MG	DA	3050	1/1	0.32	-	0,0,0,0	0
56	MG	CA	1778	1/1	0.11	-	3,3,3,3	0
56	MG	DB	208	1/1	0.16	-	9,9,9,9	0
56	MG	CW	108	1/1	0.08	-	10,10,10,10	1
56	MG	AA	1692	1/1	0.17	-	0,0,0,0	0
56	MG	BA	3038	1/1	0.19	-	10,10,10,10	0
56	MG	DA	3018	1/1	0.08	-	3,3,3,3	0
56	MG	AW	102	1/1	0.23	-	51,51,51,51	0
56	MG	AA	1650	1/1	0.12	-	31,31,31,31	0
56	MG	BA	3365	1/1	0.14	-	60,60,60,60	0
56	MG	CA	1693	1/1	0.17	-	18,18,18,18	1
56	MG	CA	1667	1/1	0.18	-	41,41,41,41	0
56	MG	BA	3216	1/1	0.20	-	50,50,50,50	0
56	MG	BA	3213	1/1	0.17	-	19,19,19,19	0
56	MG	DA	3011	1/1	0.18	-	11,11,11,11	0
56	MG	CA	1648	1/1	0.12	-	34,34,34,34	0
56	MG	BA	3171	1/1	0.09	-	0,0,0,0	1
56	MG	CA	1733	1/1	0.11	-	31,31,31,31	0
56	MG	DA	3052	1/1	0.17	-	0,0,0,0	0
56	MG	DA	3192	1/1	0.12	-	17,17,17,17	0
56	MG	BA	3314	1/1	0.41	-	47,47,47,47	1
56	MG	DA	3199	1/1	0.10	-	26,26,26,26	0
56	MG	DA	3308	1/1	0.09	-	20,20,20,20	0
56	MG	DA	3314	1/1	0.12	-	16,16,16,16	0
56	MG	AA	1763	1/1	0.30	-	58,58,58,58	1
56	MG	BA	3301	1/1	0.17	-	19,19,19,19	0
56	MG	BA	3083	1/1	0.14	-	20,20,20,20	0
56	MG	BA	3114	1/1	0.18	-	0,0,0,0	0
56	MG	CA	1659	1/1	0.06	-	9,9,9,9	0
56	MG	CA	1699	1/1	0.09	-	0,0,0,0	0
56	MG	AA	1695	1/1	0.16	-	13,13,13,13	1
56	MG	BA	3076	1/1	0.16	-	4,4,4,4	0
56	MG	DA	3309	1/1	0.11	-	6,6,6,6	0
56	MG	BA	3385	1/1	0.07	-	12,12,12,12	0
56	MG	AA	1697	1/1	0.41	-	88,88,88,88	0
56	MG	DA	3126	1/1	0.08	-	29,29,29,29	0
56	MG	DA	3020	1/1	0.27	-	1,1,1,1	0
56	MG	AA	1801	1/1	0.21	-	34,34,34,34	0
56	MG	BA	3384	1/1	0.11	-	36,36,36,36	0
56	MG	CA	1622	1/1	1.02	-	123,123,123,123	0
56	MG	DA	3300	1/1	0.15	-	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CW	107	1/1	0.24	-	63,63,63,63	1
56	MG	CA	1773	1/1	0.08	-	13,13,13,13	0
56	MG	BA	3283	1/1	0.05	-	36,36,36,36	0
56	MG	BA	3376	1/1	0.21	-	47,47,47,47	0
56	MG	BA	3403	1/1	0.46	-	78,78,78,78	0
56	MG	AA	1629	1/1	0.12	-	29,29,29,29	0
56	MG	BA	3440	1/1	0.13	-	33,33,33,33	0
56	MG	BE	301	1/1	0.16	-	8,8,8,8	0
56	MG	DA	3197	1/1	0.17	-	13,13,13,13	0
56	MG	CA	1606	1/1	0.17	-	16,16,16,16	0
56	MG	DA	3323	1/1	0.19	-	31,31,31,31	0
56	MG	CW	103	1/1	0.06	-	45,45,45,45	0
56	MG	BA	3333	1/1	0.14	-	41,41,41,41	0
56	MG	CV	101	1/1	0.13	-	32,32,32,32	0
56	MG	BA	3160	1/1	0.11	-	17,17,17,17	0
56	MG	DA	3376	1/1	0.09	-	25,25,25,25	0
56	MG	AA	1771	1/1	0.06	-	6,6,6,6	0
56	MG	DA	3334	1/1	0.09	-	34,34,34,34	1
56	MG	DA	3257	1/1	0.21	-	27,27,27,27	0
56	MG	BA	3414	1/1	0.34	-	44,44,44,44	0
56	MG	BA	3352	1/1	0.09	-	30,30,30,30	1
56	MG	DA	3332	1/1	0.05	-	45,45,45,45	0
56	MG	BA	3277	1/1	0.21	-	38,38,38,38	0
56	MG	CA	1647	1/1	0.45	-	57,57,57,57	0
56	MG	BA	3143	1/1	0.26	-	21,21,21,21	0
56	MG	DA	3182	1/1	0.08	-	5,5,5,5	0
56	MG	CW	111	1/1	0.19	-	77,77,77,77	0
56	MG	DA	3136	1/1	0.22	-	3,3,3,3	0
56	MG	AW	121	1/1	0.07	-	36,36,36,36	0
56	MG	DA	3370	1/1	0.11	-	22,22,22,22	0
56	MG	CA	1664	1/1	0.17	-	28,28,28,28	0
56	MG	BA	3309	1/1	0.14	-	14,14,14,14	0
56	MG	DA	3071	1/1	0.10	-	18,18,18,18	0
56	MG	BA	3041	1/1	0.15	-	0,0,0,0	0
56	MG	AA	1667	1/1	0.15	-	50,50,50,50	0
56	MG	BB	204	1/1	0.14	-	42,42,42,42	0
56	MG	DA	3040	1/1	0.04	-	45,45,45,45	0
56	MG	BA	3188	1/1	0.19	-	13,13,13,13	0
56	MG	DA	3290	1/1	0.08	-	0,0,0,0	0
56	MG	DA	3344	1/1	0.32	-	32,32,32,32	0
56	MG	BA	3404	1/1	0.25	-	17,17,17,17	0
56	MG	CA	1742	1/1	0.15	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	1655	1/1	0.15	-	32,32,32,32	0
56	MG	B1	101	1/1	0.15	-	0,0,0,0	0
56	MG	DA	3229	1/1	0.20	-	1,1,1,1	0
56	MG	BA	3105	1/1	0.19	-	13,13,13,13	0
56	MG	BA	3288	1/1	0.20	-	32,32,32,32	1
56	MG	DD	302	1/1	0.10	-	7,7,7,7	0
56	MG	AA	1728	1/1	0.07	-	2,2,2,2	0
56	MG	CA	1689	1/1	0.08	-	0,0,0,0	0
56	MG	CA	1736	1/1	0.14	-	30,30,30,30	0
56	MG	BA	3140	1/1	0.11	-	10,10,10,10	0
56	MG	BA	3033	1/1	0.19	-	30,30,30,30	0
56	MG	BA	3003	1/1	0.15	-	28,28,28,28	0
56	MG	DA	3168	1/1	0.36	-	56,56,56,56	0
56	MG	DA	3174	1/1	0.24	-	26,26,26,26	0
56	MG	B5	102	1/1	0.30	-	24,24,24,24	0
56	MG	BA	3378	1/1	0.04	-	54,54,54,54	1
56	MG	CA	1631	1/1	0.46	-	48,48,48,48	0
56	MG	AA	1802	1/1	0.11	-	44,44,44,44	0
56	MG	DA	3302	1/1	0.10	-	11,11,11,11	0
56	MG	BA	3296	1/1	0.34	-	75,75,75,75	0
56	MG	AA	1616	1/1	0.12	-	18,18,18,18	0
56	MG	BA	3009	1/1	0.20	-	20,20,20,20	0
56	MG	BA	3127	1/1	0.10	-	8,8,8,8	0
56	MG	BA	3441	1/1	0.08	-	33,33,33,33	0
56	MG	AA	1661	1/1	0.30	-	60,60,60,60	0
56	MG	BA	3254	1/1	0.15	-	48,48,48,48	0
56	MG	DA	3292	1/1	0.07	-	5,5,5,5	0
56	MG	BA	3034	1/1	0.09	-	0,0,0,0	0
56	MG	DA	3316	1/1	0.13	-	7,7,7,7	0
56	MG	CA	1735	1/1	0.16	-	17,17,17,17	0
56	MG	DA	3033	1/1	0.25	-	17,17,17,17	1
56	MG	BA	3116	1/1	0.26	-	12,12,12,12	0
56	MG	CA	1772	1/1	0.17	-	37,37,37,37	0
56	MG	BA	3178	1/1	0.13	-	54,54,54,54	0
56	MG	AX	103	1/1	0.08	-	29,29,29,29	0
56	MG	AA	1747	1/1	0.16	-	37,37,37,37	0
56	MG	BA	3420	1/1	0.26	-	59,59,59,59	1
56	MG	DA	3121	1/1	0.12	-	12,12,12,12	0
56	MG	AA	1610	1/1	0.16	-	0,0,0,0	0
56	MG	DA	3093	1/1	0.09	-	16,16,16,16	0
56	MG	DA	3388	1/1	0.16	-	15,15,15,15	0
56	MG	CA	1671	1/1	0.28	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	1804	1/1	0.15	-	31,31,31,31	0
56	MG	CA	1677	1/1	0.12	-	28,28,28,28	0
56	MG	B2	101	1/1	0.11	-	36,36,36,36	0
56	MG	DA	3318	1/1	0.31	-	45,45,45,45	0
56	MG	CA	1759	1/1	0.19	-	68,68,68,68	0
56	MG	DA	3112	1/1	0.08	-	0,0,0,0	0
56	MG	BA	3063	1/1	0.26	-	0,0,0,0	0
56	MG	BA	3453	1/1	0.16	-	49,49,49,49	0
56	MG	BA	3006	1/1	0.27	-	24,24,24,24	0
58	ZN	CN	101	1/1	0.10	-	53,53,53,53	0
56	MG	BA	3299	1/1	0.20	-	22,22,22,22	0
56	MG	BA	3281	1/1	0.10	-	0,0,0,0	0
56	MG	AA	1665	1/1	0.20	-	27,27,27,27	0
56	MG	BA	3138	1/1	0.18	-	12,12,12,12	0
56	MG	BA	3032	1/1	0.08	-	17,17,17,17	0
56	MG	CA	1714	1/1	0.15	-	81,81,81,81	0
56	MG	BA	3152	1/1	0.16	-	45,45,45,45	0
56	MG	DA	3122	1/1	0.16	-	43,43,43,43	0
56	MG	DA	3341	1/1	0.09	-	26,26,26,26	0
56	MG	BA	3257	1/1	0.14	-	55,55,55,55	0
56	MG	DA	3124	1/1	0.14	-	0,0,0,0	0
56	MG	DA	3179	1/1	0.05	-	10,10,10,10	0
56	MG	CA	1787	1/1	0.28	-	39,39,39,39	1
56	MG	CA	1610	1/1	0.24	-	15,15,15,15	0
56	MG	DA	3006	1/1	0.17	-	41,41,41,41	0
56	MG	AA	1796	1/1	0.08	-	10,10,10,10	1
56	MG	BB	201	1/1	0.42	-	54,54,54,54	1
56	MG	CA	1766	1/1	0.22	-	18,18,18,18	0
56	MG	BA	3065	1/1	0.10	-	1,1,1,1	0
56	MG	BA	3317	1/1	0.17	-	50,50,50,50	0
56	MG	BA	3358	1/1	0.13	-	42,42,42,42	0
56	MG	CA	1776	1/1	0.20	-	44,44,44,44	0
56	MG	DA	3297	1/1	0.14	-	23,23,23,23	0
56	MG	BA	3018	1/1	0.23	-	22,22,22,22	0
56	MG	CV	102	1/1	0.08	-	56,56,56,56	0
56	MG	CA	1711	1/1	0.20	-	63,63,63,63	0
56	MG	DA	3327	1/1	0.10	-	6,6,6,6	0
56	MG	DA	3143	1/1	0.17	-	36,36,36,36	0
56	MG	DA	3059	1/1	0.21	-	0,0,0,0	0
56	MG	CA	1638	1/1	0.12	-	42,42,42,42	0
56	MG	DA	3345	1/1	0.24	-	17,17,17,17	0
56	MG	CA	1781	1/1	0.15	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	1806	1/1	0.24	-	24,24,24,24	0
56	MG	BA	3022	1/1	0.13	-	25,25,25,25	0
56	MG	BA	3323	1/1	0.11	-	79,79,79,79	0
56	MG	DA	3085	1/1	0.20	-	0,0,0,0	0
56	MG	BA	3438	1/1	0.11	-	25,25,25,25	0
56	MG	BA	3012	1/1	0.12	-	20,20,20,20	0
56	MG	BA	3325	1/1	0.08	-	28,28,28,28	0
56	MG	BA	3371	1/1	0.09	-	15,15,15,15	0
56	MG	CA	1619	1/1	0.19	-	55,55,55,55	0
56	MG	BA	3246	1/1	0.14	-	15,15,15,15	0
56	MG	BA	3354	1/1	0.09	-	35,35,35,35	0
56	MG	BB	213	1/1	0.69	-	71,71,71,71	0
56	MG	CV	103	1/1	0.15	-	56,56,56,56	0
56	MG	BA	3207	1/1	0.12	-	0,0,0,0	0
56	MG	AA	1797	1/1	0.08	-	26,26,26,26	0
56	MG	DA	3135	1/1	0.20	-	7,7,7,7	0
56	MG	AA	1700	1/1	0.19	-	31,31,31,31	0
56	MG	BB	212	1/1	0.14	-	18,18,18,18	1
56	MG	DA	3363	1/1	0.12	-	30,30,30,30	0
56	MG	DZ	301	1/1	0.10	-	27,27,27,27	0
56	MG	AA	1706	1/1	0.07	-	10,10,10,10	0
56	MG	AA	1749	1/1	0.14	-	38,38,38,38	0
56	MG	DA	3243	1/1	0.09	-	3,3,3,3	0
56	MG	DA	3246	1/1	0.15	-	38,38,38,38	0
56	MG	AA	1788	1/1	0.07	-	16,16,16,16	0
56	MG	DA	3383	1/1	0.08	-	32,32,32,32	0
56	MG	DA	3073	1/1	0.09	-	0,0,0,0	0
56	MG	BA	3369	1/1	0.10	-	30,30,30,30	0
56	MG	BA	3426	1/1	0.10	-	3,3,3,3	0
56	MG	BA	3391	1/1	0.06	-	26,26,26,26	0
56	MG	AA	1731	1/1	0.16	-	56,56,56,56	0
56	MG	DA	3224	1/1	0.27	-	2,2,2,2	0
56	MG	CA	1628	1/1	0.13	-	35,35,35,35	0
56	MG	DA	3266	1/1	0.06	-	11,11,11,11	0
56	MG	BA	3201	1/1	0.18	-	21,21,21,21	0
56	MG	AX	102	1/1	0.10	-	32,32,32,32	0
56	MG	BA	3228	1/1	0.12	-	46,46,46,46	0
56	MG	BA	3102	1/1	0.11	-	15,15,15,15	0
56	MG	CA	1786	1/1	0.18	-	29,29,29,29	0
56	MG	AA	1721	1/1	0.08	-	28,28,28,28	0
56	MG	DA	3152	1/1	0.07	-	17,17,17,17	0
56	MG	CA	1634	1/1	0.11	-	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3024	1/1	0.12	-	0,0,0,0	0
56	MG	AA	1772	1/1	0.22	-	73,73,73,73	0
56	MG	D5	102	1/1	0.10	-	6,6,6,6	1
56	MG	CA	1683	1/1	0.11	-	2,2,2,2	0
56	MG	BA	3175	1/1	0.09	-	0,0,0,0	0
56	MG	BA	3172	1/1	0.19	-	22,22,22,22	0
56	MG	DA	3068	1/1	0.14	-	14,14,14,14	0
56	MG	BA	3192	1/1	0.10	-	0,0,0,0	0
56	MG	DA	3107	1/1	0.23	-	12,12,12,12	0
56	MG	AA	1686	1/1	0.19	-	52,52,52,52	0
56	MG	CA	1673	1/1	0.25	-	80,80,80,80	1
56	MG	AA	1696	1/1	0.09	-	0,0,0,0	0
56	MG	BA	3267	1/1	0.10	-	43,43,43,43	0
56	MG	BA	3027	1/1	0.08	-	8,8,8,8	0
56	MG	AA	1620	1/1	0.15	-	28,28,28,28	0
56	MG	CA	1755	1/1	0.23	-	26,26,26,26	1
56	MG	AA	1670	1/1	0.14	-	52,52,52,52	0
56	MG	BA	3141	1/1	0.10	-	20,20,20,20	0
56	MG	AA	1742	1/1	0.36	-	45,45,45,45	0
56	MG	CA	1769	1/1	0.10	-	18,18,18,18	0
56	MG	AA	1720	1/1	0.17	-	29,29,29,29	0
56	MG	BA	3380	1/1	0.37	-	77,77,77,77	0
56	MG	BA	3432	1/1	0.08	-	15,15,15,15	0
56	MG	DA	3188	1/1	0.25	-	42,42,42,42	0
56	MG	BA	3134	1/1	0.12	-	1,1,1,1	0
56	MG	BA	3011	1/1	0.20	-	0,0,0,0	0
56	MG	DA	3094	1/1	0.06	-	10,10,10,10	0
56	MG	DA	3329	1/1	0.16	-	45,45,45,45	0
56	MG	BA	3407	1/1	0.09	-	40,40,40,40	0
56	MG	BA	3069	1/1	0.14	-	36,36,36,36	0
56	MG	BB	206	1/1	0.36	-	78,78,78,78	0
56	MG	DA	3019	1/1	0.25	-	0,0,0,0	0
56	MG	DB	202	1/1	0.21	-	57,57,57,57	0
56	MG	DA	3017	1/1	0.09	-	6,6,6,6	0
56	MG	AA	1723	1/1	0.07	-	9,9,9,9	0
56	MG	DA	3010	1/1	0.12	-	44,44,44,44	0
56	MG	CA	1719	1/1	1.12	-	99,99,99,99	0
56	MG	DA	3320	1/1	0.18	-	70,70,70,70	0
56	MG	BA	3082	1/1	0.08	-	22,22,22,22	0
56	MG	CU	101	1/1	0.11	-	38,38,38,38	0
56	MG	BA	3307	1/1	0.05	-	7,7,7,7	0
56	MG	BA	3237	1/1	0.31	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3272	1/1	0.42	-	49,49,49,49	0
56	MG	DA	3151	1/1	0.23	-	46,46,46,46	0
56	MG	BB	207	1/1	0.10	-	23,23,23,23	0
56	MG	AV	103	1/1	0.08	-	28,28,28,28	0
56	MG	CA	1764	1/1	0.11	-	15,15,15,15	0
56	MG	BA	3044	1/1	0.17	-	5,5,5,5	0
56	MG	AA	1690	1/1	0.09	-	48,48,48,48	0
56	MG	AA	1622	1/1	0.08	-	8,8,8,8	0
56	MG	AA	1752	1/1	0.21	-	25,25,25,25	0
56	MG	CA	1656	1/1	0.08	-	14,14,14,14	0
56	MG	BA	3126	1/1	0.09	-	1,1,1,1	0
56	MG	BA	3320	1/1	0.09	-	37,37,37,37	0
56	MG	BA	3405	1/1	0.09	-	11,11,11,11	0
56	MG	BA	3424	1/1	0.09	-	38,38,38,38	0
56	MG	DA	3310	1/1	0.28	-	50,50,50,50	0
56	MG	BA	3270	1/1	0.06	-	0,0,0,0	0
56	MG	BA	3067	1/1	0.16	-	5,5,5,5	0
56	MG	AA	1694	1/1	0.42	-	58,58,58,58	0
56	MG	AA	1815	1/1	0.13	-	36,36,36,36	0
56	MG	BA	3279	1/1	0.18	-	55,55,55,55	0
56	MG	CA	1780	1/1	0.16	-	38,38,38,38	0
56	MG	DA	3137	1/1	0.14	-	62,62,62,62	0
56	MG	BA	3402	1/1	0.19	-	19,19,19,19	0
56	MG	DA	3325	1/1	0.09	-	35,35,35,35	0
56	MG	DA	3157	1/1	0.24	-	34,34,34,34	0
56	MG	CA	1661	1/1	0.17	-	13,13,13,13	0
56	MG	CA	1645	1/1	0.12	-	74,74,74,74	0
56	MG	BA	3379	1/1	0.12	-	39,39,39,39	0
56	MG	BF	302	1/1	0.25	-	46,46,46,46	0
56	MG	CX	103	1/1	0.27	-	40,40,40,40	0
56	MG	DA	3313	1/1	0.12	-	35,35,35,35	1
56	MG	DA	3278	1/1	0.22	-	38,38,38,38	0
56	MG	DA	3115	1/1	0.12	-	16,16,16,16	0
56	MG	DA	3014	1/1	0.20	-	4,4,4,4	0
57	PAR	AA	1816	42/42	0.16	-	15,20,38,42	0
56	MG	BA	3177	1/1	0.10	-	7,7,7,7	0
56	MG	DA	3247	1/1	0.20	-	18,18,18,18	0
56	MG	BA	3064	1/1	0.19	-	30,30,30,30	0
56	MG	BA	3205	1/1	0.11	-	0,0,0,0	0
56	MG	BA	3189	1/1	0.09	-	3,3,3,3	0
56	MG	BA	3446	1/1	0.14	-	43,43,43,43	0
56	MG	BA	3203	1/1	0.21	-	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3131	1/1	0.17	-	0,0,0,0	0
56	MG	CA	1602	1/1	0.13	-	14,14,14,14	0
56	MG	AA	1755	1/1	0.19	-	47,47,47,47	0
56	MG	BA	3448	1/1	0.06	-	35,35,35,35	0
56	MG	AA	1657	1/1	0.17	-	50,50,50,50	0
56	MG	CA	1744	1/1	0.14	-	64,64,64,64	0
56	MG	DA	3372	1/1	0.06	-	12,12,12,12	0
56	MG	AA	1685	1/1	0.07	-	38,38,38,38	0
56	MG	AA	1602	1/1	0.13	-	39,39,39,39	0
56	MG	DA	3076	1/1	0.13	-	0,0,0,0	0
56	MG	BA	3445	1/1	0.11	-	52,52,52,52	0
56	MG	AA	1627	1/1	0.47	-	39,39,39,39	0
56	MG	CA	1739	1/1	0.13	-	66,66,66,66	0
56	MG	BA	3197	1/1	0.12	-	18,18,18,18	0
56	MG	BA	3238	1/1	0.20	-	0,0,0,0	0
56	MG	AA	1658	1/1	0.18	-	37,37,37,37	0
56	MG	AA	1611	1/1	0.16	-	18,18,18,18	0
56	MG	BA	3271	1/1	0.11	-	33,33,33,33	0
56	MG	BA	3158	1/1	0.21	-	44,44,44,44	0
56	MG	BA	3400	1/1	0.15	-	46,46,46,46	0
56	MG	DA	3047	1/1	0.19	-	0,0,0,0	0
56	MG	DA	3261	1/1	0.85	-	94,94,94,94	0
56	MG	DA	3088	1/1	0.20	-	4,4,4,4	0
56	MG	BA	3250	1/1	0.19	-	22,22,22,22	1
56	MG	CA	1705	1/1	0.14	-	22,22,22,22	0
56	MG	BA	3447	1/1	0.08	-	37,37,37,37	0
56	MG	DA	3155	1/1	0.07	-	50,50,50,50	0
56	MG	AW	122	1/1	0.12	-	37,37,37,37	0
56	MG	AA	1808	1/1	0.07	-	33,33,33,33	0
56	MG	BA	3182	1/1	0.07	-	16,16,16,16	0
56	MG	CA	1646	1/1	0.41	-	62,62,62,62	0
56	MG	BA	3107	1/1	0.18	-	53,53,53,53	0
56	MG	BA	3149	1/1	0.11	-	10,10,10,10	0
56	MG	CA	1635	1/1	0.20	-	19,19,19,19	0
56	MG	BA	3072	1/1	0.18	-	13,13,13,13	0
56	MG	AA	1773	1/1	0.08	-	41,41,41,41	0
56	MG	BA	3293	1/1	0.19	-	51,51,51,51	0
56	MG	DA	3212	1/1	0.22	-	61,61,61,61	0
56	MG	BA	3179	1/1	0.09	-	28,28,28,28	0
56	MG	AA	1762	1/1	0.14	-	18,18,18,18	0
56	MG	DA	3133	1/1	0.12	-	39,39,39,39	0
56	MG	CA	1620	1/1	0.14	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3233	1/1	0.28	-	77,77,77,77	0
56	MG	BA	3222	1/1	0.20	-	41,41,41,41	0
56	MG	CA	1765	1/1	0.07	-	38,38,38,38	0
56	MG	AA	1791	1/1	0.31	-	22,22,22,22	1
56	MG	AW	101	1/1	0.26	-	35,35,35,35	0
56	MG	BA	3308	1/1	0.19	-	25,25,25,25	0
56	MG	BA	3313	1/1	0.10	-	21,21,21,21	0
56	MG	AA	1761	1/1	0.14	-	16,16,16,16	0
56	MG	AA	1743	1/1	0.10	-	44,44,44,44	0
56	MG	BA	3359	1/1	0.06	-	75,75,75,75	0
56	MG	CA	1674	1/1	0.09	-	58,58,58,58	0
56	MG	DA	3380	1/1	0.32	-	55,55,55,55	0
56	MG	BA	3319	1/1	0.07	-	0,0,0,0	0
56	MG	BA	3324	1/1	0.11	-	18,18,18,18	1
56	MG	BA	3389	1/1	0.09	-	0,0,0,0	0
56	MG	AA	1760	1/1	0.10	-	48,48,48,48	0
56	MG	BB	218	1/1	0.10	-	36,36,36,36	1
56	MG	CA	1680	1/1	0.18	-	51,51,51,51	0
56	MG	AA	1729	1/1	0.12	-	45,45,45,45	0
56	MG	DA	3116	1/1	0.10	-	10,10,10,10	0
56	MG	CW	102	1/1	0.05	-	52,52,52,52	0
56	MG	AA	1656	1/1	0.15	-	12,12,12,12	0
56	MG	DA	3395	1/1	0.16	-	45,45,45,45	0
56	MG	AA	1615	1/1	0.14	-	33,33,33,33	0
56	MG	DA	3117	1/1	0.05	-	1,1,1,1	0
56	MG	DA	3159	1/1	0.17	-	57,57,57,57	0
56	MG	BA	3351	1/1	0.30	-	78,78,78,78	0
56	MG	DA	3240	1/1	0.11	-	43,43,43,43	0
56	MG	DA	3306	1/1	0.18	-	6,6,6,6	0
56	MG	AA	1792	1/1	0.20	-	74,74,74,74	0
56	MG	BA	3252	1/1	0.16	-	25,25,25,25	0
56	MG	AA	1662	1/1	0.13	-	31,31,31,31	0
56	MG	CA	1669	1/1	0.06	-	0,0,0,0	0
56	MG	CA	1629	1/1	0.11	-	10,10,10,10	0
56	MG	BA	3155	1/1	0.47	-	66,66,66,66	0
56	MG	AA	1707	1/1	0.07	-	2,2,2,2	0
56	MG	BA	3264	1/1	0.23	-	0,0,0,0	0
56	MG	CA	1756	1/1	0.15	-	41,41,41,41	0
56	MG	DA	3100	1/1	0.22	-	21,21,21,21	0
56	MG	BA	3202	1/1	0.06	-	0,0,0,0	0
56	MG	DA	3307	1/1	0.09	-	34,34,34,34	1
56	MG	DA	3287	1/1	0.23	-	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	1614	1/1	0.07	-	19,19,19,19	0
56	MG	AA	1649	1/1	0.19	-	0,0,0,0	0
56	MG	DA	3145	1/1	0.12	-	27,27,27,27	0
56	MG	DA	3041	1/1	0.20	-	8,8,8,8	0
56	MG	DA	3339	1/1	0.07	-	17,17,17,17	0
56	MG	BA	3387	1/1	0.12	-	38,38,38,38	0
56	MG	AA	1726	1/1	0.10	-	12,12,12,12	0
56	MG	DA	3271	1/1	0.32	-	7,7,7,7	0
56	MG	DA	3221	1/1	0.10	-	11,11,11,11	0
56	MG	DA	3358	1/1	0.33	-	54,54,54,54	0
56	MG	CA	1613	1/1	0.22	-	4,4,4,4	0
56	MG	DA	3062	1/1	0.28	-	13,13,13,13	0
56	MG	AA	1698	1/1	0.16	-	38,38,38,38	0
56	MG	BA	3345	1/1	0.17	-	59,59,59,59	0
56	MG	CA	1655	1/1	0.11	-	0,0,0,0	0
56	MG	BA	3073	1/1	0.11	-	4,4,4,4	0
56	MG	BA	3335	1/1	0.12	-	45,45,45,45	0
56	MG	CA	1649	1/1	0.12	-	37,37,37,37	0
56	MG	CA	1741	1/1	0.26	-	40,40,40,40	0
56	MG	DA	3311	1/1	0.20	-	53,53,53,53	0
56	MG	CA	1729	1/1	0.44	-	71,71,71,71	0
56	MG	BA	3176	1/1	0.08	-	11,11,11,11	0
56	MG	DA	3183	1/1	0.05	-	0,0,0,0	0
56	MG	BA	3433	1/1	0.17	-	74,74,74,74	0
56	MG	DA	3211	1/1	0.10	-	1,1,1,1	0
56	MG	CA	1697	1/1	0.15	-	49,49,49,49	0
56	MG	DA	3326	1/1	0.31	-	25,25,25,25	0
56	MG	AA	1708	1/1	0.19	-	41,41,41,41	0
56	MG	BA	3366	1/1	0.16	-	27,27,27,27	0
56	MG	BA	3109	1/1	0.27	-	34,34,34,34	0
56	MG	AA	1783	1/1	0.34	-	46,46,46,46	0
56	MG	BV	201	1/1	0.13	-	23,23,23,23	0
56	MG	DA	3096	1/1	0.22	-	21,21,21,21	0
56	MG	AA	1636	1/1	0.15	-	27,27,27,27	1
56	MG	CA	1747	1/1	0.09	-	28,28,28,28	0
56	MG	BA	3144	1/1	0.13	-	8,8,8,8	0
56	MG	DA	3080	1/1	0.17	-	0,0,0,0	0
56	MG	BA	3060	1/1	0.21	-	0,0,0,0	0
56	MG	BA	3353	1/1	0.38	-	42,42,42,42	1
56	MG	DA	3333	1/1	0.26	-	67,67,67,67	0
56	MG	DA	3242	1/1	0.14	-	9,9,9,9	0
56	MG	CA	1725	1/1	0.24	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3039	1/1	0.28	-	31,31,31,31	0
56	MG	BA	3124	1/1	0.20	-	17,17,17,17	0
56	MG	DB	201	1/1	0.06	-	19,19,19,19	0
56	MG	CW	104	1/1	0.09	-	46,46,46,46	0
56	MG	DA	3201	1/1	0.19	-	7,7,7,7	0
56	MG	AW	103	1/1	0.18	-	51,51,51,51	0
56	MG	AW	106	1/1	0.06	-	26,26,26,26	0
56	MG	BA	3337	1/1	0.05	-	57,57,57,57	0
56	MG	B2	104	1/1	0.09	-	34,34,34,34	0
56	MG	DA	3209	1/1	0.35	-	31,31,31,31	0
56	MG	DA	3216	1/1	0.09	-	34,34,34,34	0
56	MG	BA	3211	1/1	0.13	-	42,42,42,42	0
56	MG	DA	3146	1/1	0.14	-	22,22,22,22	0
56	MG	BA	3263	1/1	0.09	-	4,4,4,4	0
56	MG	DA	3381	1/1	0.21	-	77,77,77,77	0
56	MG	AA	1812	1/1	0.10	-	50,50,50,50	0
56	MG	AA	1735	1/1	0.20	-	84,84,84,84	0
56	MG	CW	106	1/1	0.07	-	50,50,50,50	1
56	MG	CA	1605	1/1	0.09	-	10,10,10,10	0
56	MG	DA	3083	1/1	0.23	-	13,13,13,13	0
56	MG	BA	3344	1/1	0.11	-	17,17,17,17	0
56	MG	DA	3163	1/1	0.17	-	51,51,51,51	0
56	MG	BA	3101	1/1	0.11	-	3,3,3,3	0
56	MG	BA	3004	1/1	0.38	-	77,77,77,77	0
56	MG	DA	3184	1/1	0.09	-	10,10,10,10	0
56	MG	DA	3299	1/1	0.11	-	0,0,0,0	0
56	MG	BA	3434	1/1	0.08	-	28,28,28,28	0
56	MG	BA	3028	1/1	0.35	-	36,36,36,36	0
56	MG	CA	1784	1/1	0.08	-	15,15,15,15	0
56	MG	AA	1691	1/1	0.07	-	11,11,11,11	0
56	MG	CA	1730	1/1	0.12	-	56,56,56,56	0
56	MG	CA	1692	1/1	0.08	-	19,19,19,19	0
56	MG	BA	3183	1/1	0.07	-	18,18,18,18	0
56	MG	DA	3384	1/1	0.08	-	25,25,25,25	0
56	MG	AA	1803	1/1	0.20	-	48,48,48,48	0
56	MG	DA	3030	1/1	0.09	-	0,0,0,0	0
56	MG	DA	3210	1/1	0.10	-	0,0,0,0	0
56	MG	DA	3095	1/1	0.20	-	0,0,0,0	0
56	MG	BA	3374	1/1	0.28	-	48,48,48,48	0
56	MG	DA	3202	1/1	0.21	-	37,37,37,37	0
56	MG	DA	3149	1/1	0.50	-	84,84,84,84	0
56	MG	BA	3043	1/1	0.30	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	1728	1/1	0.15	-	42,42,42,42	0
56	MG	BA	3362	1/1	0.16	-	58,58,58,58	0
56	MG	BA	3251	1/1	0.15	-	11,11,11,11	0
56	MG	DA	3198	1/1	0.08	-	10,10,10,10	0
56	MG	CA	1608	1/1	0.11	-	0,0,0,0	0
56	MG	BA	3253	1/1	0.10	-	38,38,38,38	0
56	MG	AW	105	1/1	0.12	-	64,64,64,64	0
56	MG	DA	3097	1/1	0.12	-	12,12,12,12	0
56	MG	BA	3377	1/1	0.20	-	43,43,43,43	0
56	MG	CA	1698	1/1	0.36	-	42,42,42,42	0
56	MG	CA	1789	1/1	0.19	-	33,33,33,33	0
56	MG	AA	1663	1/1	0.11	-	24,24,24,24	0
56	MG	BA	3013	1/1	0.12	-	0,0,0,0	0
56	MG	BA	3147	1/1	0.20	-	20,20,20,20	0
56	MG	CA	1637	1/1	0.45	-	81,81,81,81	0
56	MG	BA	3332	1/1	0.19	-	53,53,53,53	1
56	MG	BB	202	1/1	0.10	-	14,14,14,14	0
56	MG	AV	106	1/1	0.07	-	40,40,40,40	0
56	MG	DA	3025	1/1	0.14	-	6,6,6,6	0
56	MG	BA	3133	1/1	0.06	-	11,11,11,11	0
56	MG	DA	3153	1/1	0.30	-	40,40,40,40	0
56	MG	BA	3278	1/1	0.42	-	90,90,90,90	0
56	MG	DA	3013	1/1	0.10	-	1,1,1,1	0
56	MG	BA	3303	1/1	0.17	-	15,15,15,15	0
56	MG	DD	301	1/1	0.11	-	1,1,1,1	0
56	MG	AA	1671	1/1	0.13	-	19,19,19,19	0
56	MG	BA	3305	1/1	0.23	-	30,30,30,30	0
56	MG	BA	3417	1/1	0.26	-	29,29,29,29	0
56	MG	CA	1771	1/1	0.14	-	28,28,28,28	0
56	MG	DA	3274	1/1	0.12	-	53,53,53,53	0
56	MG	DA	3170	1/1	0.10	-	54,54,54,54	0
56	MG	AA	1789	1/1	0.13	-	18,18,18,18	0
56	MG	BB	214	1/1	0.17	-	46,46,46,46	0
56	MG	DA	3355	1/1	0.06	-	7,7,7,7	0
56	MG	DA	3230	1/1	0.20	-	20,20,20,20	0
56	MG	DA	3176	1/1	0.19	-	13,13,13,13	0
56	MG	CA	1732	1/1	0.21	-	43,43,43,43	0
56	MG	AA	1630	1/1	0.10	-	13,13,13,13	0
56	MG	AA	1669	1/1	0.40	-	38,38,38,38	0
56	MG	AA	1612	1/1	0.11	-	31,31,31,31	0
56	MG	BA	3161	1/1	0.08	-	11,11,11,11	0
56	MG	BA	3247	1/1	0.15	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3024	1/1	0.19	-	20,20,20,20	0
56	MG	DA	3089	1/1	0.10	-	4,4,4,4	0
56	MG	BA	3367	1/1	0.23	-	50,50,50,50	0
56	MG	BA	3131	1/1	0.17	-	0,0,0,0	0
56	MG	BA	3110	1/1	0.11	-	0,0,0,0	0
56	MG	BA	3287	1/1	0.12	-	46,46,46,46	0
56	MG	DA	3268	1/1	0.20	-	51,51,51,51	0
56	MG	DA	3353	1/1	0.31	-	42,42,42,42	0
56	MG	DA	3144	1/1	0.15	-	31,31,31,31	0
56	MG	BA	3329	1/1	0.10	-	34,34,34,34	0
56	MG	DA	3064	1/1	0.20	-	0,0,0,0	0
56	MG	DA	3016	1/1	0.12	-	52,52,52,52	0
56	MG	D5	101	1/1	0.09	-	7,7,7,7	0
56	MG	AA	1710	1/1	0.20	-	29,29,29,29	0
56	MG	AA	1618	1/1	0.38	-	66,66,66,66	0
56	MG	BA	3221	1/1	0.14	-	49,49,49,49	0
56	MG	CA	1632	1/1	0.07	-	11,11,11,11	0
56	MG	AA	1668	1/1	0.07	-	23,23,23,23	0
56	MG	DA	3228	1/1	0.16	-	19,19,19,19	0
56	MG	AA	1626	1/1	0.28	-	50,50,50,50	0
56	MG	BA	3136	1/1	0.20	-	8,8,8,8	0
56	MG	DF	301	1/1	0.15	-	29,29,29,29	0
56	MG	BA	3190	1/1	0.23	-	49,49,49,49	0
56	MG	BA	3289	1/1	0.17	-	41,41,41,41	0
56	MG	BA	3075	1/1	0.20	-	0,0,0,0	0
56	MG	BA	3268	1/1	0.16	-	24,24,24,24	0
56	MG	AA	1750	1/1	0.13	-	57,57,57,57	0
56	MG	BA	3274	1/1	0.07	-	0,0,0,0	0
56	MG	BA	3435	1/1	0.09	-	52,52,52,52	1
56	MG	AA	1777	1/1	0.13	-	55,55,55,55	0
56	MG	DA	3037	1/1	0.11	-	4,4,4,4	0
56	MG	AV	107	1/1	0.08	-	25,25,25,25	0
56	MG	CA	1713	1/1	0.23	-	93,93,93,93	0
56	MG	DA	3169	1/1	0.26	-	27,27,27,27	0
56	MG	BA	3194	1/1	0.20	-	30,30,30,30	0
56	MG	CA	1761	1/1	0.26	-	26,26,26,26	0
56	MG	DA	3294	1/1	0.17	-	0,0,0,0	0
56	MG	BA	3002	1/1	0.14	-	21,21,21,21	0
56	MG	DA	3048	1/1	0.26	-	53,53,53,53	0
56	MG	CA	1641	1/1	0.16	-	13,13,13,13	0
56	MG	BA	3401	1/1	0.24	-	48,48,48,48	0
56	MG	BA	3156	1/1	0.06	-	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3292	1/1	0.11	-	14,14,14,14	0
56	MG	BA	3008	1/1	0.34	-	22,22,22,22	0
56	MG	DA	3078	1/1	0.18	-	2,2,2,2	0
56	MG	AA	1790	1/1	0.07	-	65,65,65,65	0
56	MG	BA	3165	1/1	0.15	-	0,0,0,0	0
56	MG	AY	101	1/1	0.17	-	56,56,56,56	0
56	MG	CA	1758	1/1	0.15	-	44,44,44,44	0
56	MG	BA	3074	1/1	0.21	-	10,10,10,10	0
56	MG	BA	3015	1/1	0.17	-	0,0,0,0	0
56	MG	BA	3275	1/1	0.18	-	19,19,19,19	0
56	MG	DA	3245	1/1	0.14	-	38,38,38,38	0
56	MG	AA	1813	1/1	0.14	-	25,25,25,25	0
56	MG	DA	3147	1/1	0.12	-	19,19,19,19	0
56	MG	DA	3113	1/1	0.08	-	11,11,11,11	0
56	MG	CA	1708	1/1	0.31	-	43,43,43,43	0
56	MG	DA	3065	1/1	0.24	-	0,0,0,0	0
56	MG	DA	3349	1/1	0.12	-	27,27,27,27	0
56	MG	CA	1663	1/1	0.17	-	32,32,32,32	0
56	MG	AA	1805	1/1	0.17	-	0,0,0,0	0
56	MG	BA	3016	1/1	0.19	-	37,37,37,37	0
56	MG	CA	1712	1/1	0.17	-	19,19,19,19	0
56	MG	DA	3233	1/1	0.11	-	0,0,0,0	0
56	MG	DA	3293	1/1	0.09	-	2,2,2,2	0
56	MG	BA	3300	1/1	0.10	-	6,6,6,6	0
56	MG	CA	1612	1/1	0.10	-	17,17,17,17	0
56	MG	DA	3218	1/1	0.05	-	27,27,27,27	0
56	MG	DA	3103	1/1	0.14	-	9,9,9,9	0
56	MG	BA	3021	1/1	0.24	-	17,17,17,17	0
56	MG	AA	1608	1/1	0.11	-	47,47,47,47	0
56	MG	AA	1733	1/1	0.41	-	63,63,63,63	0
56	MG	BA	3348	1/1	0.14	-	26,26,26,26	0
56	MG	BA	3235	1/1	0.06	-	7,7,7,7	0
56	MG	BA	3276	1/1	0.08	-	6,6,6,6	0
56	MG	BA	3341	1/1	0.15	-	21,21,21,21	0
56	MG	BA	3259	1/1	0.07	-	32,32,32,32	0
56	MG	BA	3244	1/1	0.16	-	19,19,19,19	0
56	MG	AA	1757	1/1	0.06	-	0,0,0,0	0
56	MG	BA	3232	1/1	0.11	-	23,23,23,23	0
56	MG	DN	201	1/1	0.09	-	16,16,16,16	0
56	MG	BA	3173	1/1	0.16	-	14,14,14,14	0
56	MG	DA	3356	1/1	0.06	-	12,12,12,12	0
56	MG	AA	1766	1/1	0.10	-	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3338	1/1	0.07	-	22,22,22,22	1
56	MG	CA	1710	1/1	0.10	-	22,22,22,22	0
56	MG	AA	1635	1/1	0.09	-	16,16,16,16	0
56	MG	BA	3081	1/1	0.14	-	10,10,10,10	0
56	MG	BA	3418	1/1	0.12	-	64,64,64,64	0
56	MG	DA	3035	1/1	0.09	-	0,0,0,0	0
56	MG	BA	3079	1/1	0.14	-	0,0,0,0	0
56	MG	DA	3077	1/1	0.15	-	0,0,0,0	0
56	MG	DE	301	1/1	0.20	-	18,18,18,18	0
56	MG	BA	3290	1/1	0.07	-	2,2,2,2	0
56	MG	BA	3255	1/1	0.14	-	28,28,28,28	0
56	MG	AA	1605	1/1	0.10	-	16,16,16,16	0
56	MG	DA	3173	1/1	0.12	-	41,41,41,41	0
56	MG	BA	3019	1/1	0.32	-	0,0,0,0	0
56	MG	CA	1615	1/1	0.28	-	61,61,61,61	0
56	MG	CA	1618	1/1	0.12	-	25,25,25,25	0
56	MG	DA	3044	1/1	0.12	-	15,15,15,15	0
56	MG	BA	3224	1/1	0.24	-	2,2,2,2	0
56	MG	BA	3151	1/1	0.07	-	2,2,2,2	0
56	MG	BA	3220	1/1	0.07	-	29,29,29,29	0
56	MG	AA	1647	1/1	0.21	-	71,71,71,71	0
56	MG	BB	209	1/1	0.10	-	49,49,49,49	0
56	MG	DA	3027	1/1	0.27	-	39,39,39,39	0
56	MG	DA	3101	1/1	0.14	-	38,38,38,38	0
56	MG	DA	3253	1/1	0.16	-	71,71,71,71	0
56	MG	BA	3036	1/1	0.11	-	25,25,25,25	0
56	MG	BA	3026	1/1	0.23	-	0,0,0,0	0
56	MG	CA	1679	1/1	0.05	-	4,4,4,4	0
56	MG	BA	3068	1/1	0.20	-	0,0,0,0	0
56	MG	BA	3098	1/1	0.05	-	5,5,5,5	0
56	MG	BA	3346	1/1	0.20	-	60,60,60,60	0
56	MG	BA	3370	1/1	0.20	-	28,28,28,28	1
56	MG	BA	3311	1/1	0.07	-	2,2,2,2	0
56	MG	CA	1657	1/1	0.14	-	24,24,24,24	0
56	MG	BA	3236	1/1	0.10	-	3,3,3,3	0
56	MG	CA	1763	1/1	0.18	-	32,32,32,32	0
56	MG	BA	3245	1/1	0.11	-	9,9,9,9	0
56	MG	AA	1745	1/1	0.22	-	56,56,56,56	0
56	MG	BA	3408	1/1	0.17	-	46,46,46,46	0
56	MG	DA	3350	1/1	0.17	-	37,37,37,37	0
56	MG	BA	3421	1/1	0.06	-	44,44,44,44	0
56	MG	BA	3045	1/1	0.11	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3123	1/1	0.09	-	6,6,6,6	0
56	MG	BA	3121	1/1	0.12	-	2,2,2,2	0
56	MG	CA	1678	1/1	0.15	-	0,0,0,0	0
56	MG	BA	3258	1/1	0.12	-	70,70,70,70	0
56	MG	BA	3099	1/1	0.20	-	1,1,1,1	0
56	MG	DA	3067	1/1	0.12	-	26,26,26,26	0
56	MG	BA	3295	1/1	0.15	-	16,16,16,16	0
56	MG	DA	3391	1/1	0.21	-	62,62,62,62	1
56	MG	DA	3208	1/1	0.20	-	40,40,40,40	0
56	MG	AA	1715	1/1	0.08	-	24,24,24,24	0
56	MG	CA	1672	1/1	0.14	-	32,32,32,32	0
56	MG	DA	3104	1/1	0.12	-	9,9,9,9	0
56	MG	BA	3080	1/1	0.11	-	0,0,0,0	0
56	MG	BA	3001	1/1	0.19	-	38,38,38,38	0
56	MG	AA	1678	1/1	0.10	-	43,43,43,43	0
56	MG	DA	3196	1/1	0.24	-	18,18,18,18	0
56	MG	BA	3395	1/1	0.19	-	54,54,54,54	1
56	MG	DA	3205	1/1	0.08	-	19,19,19,19	0
56	MG	AA	1810	1/1	0.27	-	47,47,47,47	0
56	MG	CA	1609	1/1	0.10	-	33,33,33,33	0
56	MG	BA	3321	1/1	0.19	-	4,4,4,4	0
56	MG	AA	1732	1/1	0.06	-	3,3,3,3	0
56	MG	DA	3054	1/1	0.13	-	5,5,5,5	0
56	MG	DA	3142	1/1	0.09	-	52,52,52,52	0
56	MG	BA	3415	1/1	0.26	-	38,38,38,38	0
56	MG	BA	3413	1/1	0.53	-	63,63,63,63	0
56	MG	AA	1774	1/1	0.08	-	9,9,9,9	0
56	MG	BA	3242	1/1	0.08	-	4,4,4,4	0
56	MG	CA	1684	1/1	0.21	-	30,30,30,30	0
56	MG	DA	3336	1/1	0.12	-	3,3,3,3	1
56	MG	AA	1717	1/1	0.08	-	21,21,21,21	0
56	MG	DA	3046	1/1	0.28	-	0,0,0,0	0
56	MG	AA	1734	1/1	0.21	-	48,48,48,48	1
56	MG	DA	3190	1/1	0.07	-	2,2,2,2	0
56	MG	DA	3120	1/1	0.10	-	25,25,25,25	0
56	MG	DA	3393	1/1	0.12	-	80,80,80,80	0
56	MG	AA	1673	1/1	0.12	-	26,26,26,26	0
56	MG	BA	3266	1/1	0.25	-	28,28,28,28	0
56	MG	DA	3158	1/1	0.08	-	5,5,5,5	0
56	MG	BA	3316	1/1	0.20	-	49,49,49,49	0
56	MG	DB	206	1/1	0.09	-	0,0,0,0	1
56	MG	CA	1723	1/1	0.36	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3078	1/1	0.20	-	11,11,11,11	0
56	MG	AA	1681	1/1	0.15	-	21,21,21,21	0
56	MG	DA	3359	1/1	0.18	-	15,15,15,15	0
56	MG	DA	3343	1/1	0.11	-	4,4,4,4	0
56	MG	CA	1665	1/1	0.45	-	71,71,71,71	0
56	MG	BA	3014	1/1	0.26	-	7,7,7,7	0
56	MG	AA	1603	1/1	0.11	-	47,47,47,47	0
56	MG	BA	3191	1/1	0.25	-	23,23,23,23	0
56	MG	CA	1633	1/1	0.21	-	19,19,19,19	0
56	MG	DA	3082	1/1	0.20	-	10,10,10,10	0
56	MG	BA	3113	1/1	0.23	-	14,14,14,14	0
56	MG	BA	3429	1/1	0.22	-	41,41,41,41	0
56	MG	DA	3177	1/1	0.20	-	22,22,22,22	0
56	MG	CA	1750	1/1	0.10	-	50,50,50,50	0
56	MG	DA	3106	1/1	0.15	-	15,15,15,15	0
56	MG	CA	1626	1/1	0.12	-	11,11,11,11	0
56	MG	AA	1676	1/1	0.07	-	7,7,7,7	0
56	MG	DA	3389	1/1	0.11	-	22,22,22,22	0
56	MG	AA	1644	1/1	0.15	-	17,17,17,17	0
56	MG	BA	3142	1/1	0.28	-	66,66,66,66	0
56	MG	BA	3347	1/1	0.16	-	22,22,22,22	1
56	MG	DA	3260	1/1	0.42	-	44,44,44,44	0
56	MG	BA	3088	1/1	0.29	-	35,35,35,35	0
56	MG	BA	3100	1/1	0.20	-	3,3,3,3	0
56	MG	DA	3091	1/1	0.13	-	0,0,0,0	0
56	MG	AA	1617	1/1	0.29	-	24,24,24,24	0
56	MG	AA	1716	1/1	0.42	-	73,73,73,73	0
56	MG	CA	1702	1/1	0.12	-	36,36,36,36	0
56	MG	CA	1639	1/1	0.24	-	71,71,71,71	0
56	MG	DB	209	1/1	0.13	-	20,20,20,20	0
56	MG	AA	1785	1/1	0.13	-	32,32,32,32	0
56	MG	DA	3207	1/1	0.10	-	8,8,8,8	0
56	MG	DA	3166	1/1	0.07	-	0,0,0,0	0
56	MG	BA	3284	1/1	0.21	-	14,14,14,14	0
56	MG	BA	3046	1/1	0.26	-	0,0,0,0	0
56	MG	DA	3239	1/1	0.13	-	39,39,39,39	0
56	MG	CA	1748	1/1	0.07	-	7,7,7,7	0
56	MG	AA	1718	1/1	0.14	-	0,0,0,0	0
56	MG	CA	1650	1/1	0.16	-	68,68,68,68	0
56	MG	AA	1623	1/1	0.08	-	32,32,32,32	0
56	MG	BA	3193	1/1	0.20	-	8,8,8,8	0
56	MG	DA	3038	1/1	0.12	-	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3059	1/1	0.11	-	16,16,16,16	0
56	MG	BA	3219	1/1	0.07	-	45,45,45,45	0
56	MG	AA	1625	1/1	0.07	-	3,3,3,3	0
56	MG	DA	3114	1/1	0.08	-	8,8,8,8	0
56	MG	CX	104	1/1	0.16	-	31,31,31,31	1
56	MG	CA	1617	1/1	0.10	-	25,25,25,25	0
56	MG	AA	1613	1/1	0.23	-	2,2,2,2	0
56	MG	DA	3032	1/1	0.19	-	59,59,59,59	0
56	MG	DA	3140	1/1	0.13	-	22,22,22,22	0
56	MG	BA	3273	1/1	0.14	-	20,20,20,20	0
56	MG	DA	3026	1/1	0.26	-	0,0,0,0	0
56	MG	CA	1718	1/1	0.19	-	47,47,47,47	0
56	MG	CA	1779	1/1	0.18	-	31,31,31,31	0
56	MG	BA	3315	1/1	0.10	-	43,43,43,43	0
56	MG	DA	3148	1/1	0.12	-	5,5,5,5	0
56	MG	DA	3156	1/1	0.14	-	36,36,36,36	0
56	MG	DA	3367	1/1	0.10	-	19,19,19,19	0
56	MG	BA	3328	1/1	0.08	-	30,30,30,30	0
56	MG	AA	1659	1/1	0.13	-	14,14,14,14	1
56	MG	CA	1685	1/1	0.46	-	82,82,82,82	0
56	MG	DA	3189	1/1	0.29	-	34,34,34,34	0
56	MG	DA	3161	1/1	0.12	-	39,39,39,39	0
56	MG	BB	208	1/1	0.06	-	27,27,27,27	0
56	MG	DA	3098	1/1	0.10	-	19,19,19,19	0
56	MG	AA	1645	1/1	0.17	-	25,25,25,25	0
56	MG	DA	3258	1/1	0.49	-	80,80,80,80	0
56	MG	BA	3394	1/1	0.09	-	26,26,26,26	0
56	MG	AA	1643	1/1	0.18	-	22,22,22,22	0
56	MG	CA	1762	1/1	0.19	-	39,39,39,39	0
56	MG	AA	1684	1/1	0.13	-	17,17,17,17	0
56	MG	AA	1793	1/1	0.13	-	71,71,71,71	0
56	MG	CA	1621	1/1	0.19	-	0,0,0,0	0
56	MG	BA	3168	1/1	0.12	-	22,22,22,22	0
56	MG	CA	1688	1/1	0.08	-	46,46,46,46	0
56	MG	DA	3003	1/1	0.07	-	26,26,26,26	0
56	MG	CA	1738	1/1	0.11	-	23,23,23,23	0
56	MG	BA	3240	1/1	0.22	-	15,15,15,15	0
56	MG	DA	3263	1/1	0.17	-	30,30,30,30	0
56	MG	CV	104	1/1	0.20	-	36,36,36,36	0
56	MG	CA	1676	1/1	0.39	-	46,46,46,46	0
56	MG	DA	3075	1/1	0.21	-	0,0,0,0	0
56	MG	DA	3301	1/1	0.09	-	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3047	1/1	0.27	-	0,0,0,0	0
56	MG	BF	301	1/1	0.15	-	17,17,17,17	0
56	MG	BA	3162	1/1	0.18	-	12,12,12,12	0
56	MG	DA	3248	1/1	0.90	-	82,82,82,82	0
56	MG	CA	1731	1/1	0.08	-	32,32,32,32	0
56	MG	BA	3181	1/1	0.07	-	36,36,36,36	0
56	MG	BA	3416	1/1	0.11	-	16,16,16,16	0
56	MG	DB	203	1/1	0.12	-	33,33,33,33	0
56	MG	DA	3241	1/1	0.10	-	12,12,12,12	0
56	MG	BA	3196	1/1	0.07	-	0,0,0,0	0
56	MG	BA	3159	1/1	0.18	-	12,12,12,12	0
56	MG	AA	1601	1/1	0.10	-	35,35,35,35	0
56	MG	BA	3050	1/1	0.14	-	0,0,0,0	0
56	MG	AA	1713	1/1	0.15	-	7,7,7,7	0
56	MG	AA	1687	1/1	0.12	-	10,10,10,10	0
56	MG	DB	205	1/1	0.23	-	51,51,51,51	0
56	MG	AA	1738	1/1	0.18	-	49,49,49,49	0
56	MG	DA	3195	1/1	0.09	-	0,0,0,0	1
56	MG	AA	1786	1/1	0.13	-	31,31,31,31	0
56	MG	BA	3112	1/1	0.13	-	31,31,31,31	0
56	MG	BA	3071	1/1	0.23	-	20,20,20,20	0
56	MG	BB	211	1/1	0.09	-	40,40,40,40	1
56	MG	BA	3396	1/1	0.14	-	15,15,15,15	0
56	MG	CA	1670	1/1	0.14	-	23,23,23,23	0
56	MG	DA	3295	1/1	0.06	-	6,6,6,6	0
56	MG	CA	1607	1/1	0.19	-	15,15,15,15	0
56	MG	DA	3021	1/1	0.22	-	0,0,0,0	0
56	MG	DA	3265	1/1	0.06	-	0,0,0,0	0
56	MG	DA	3060	1/1	0.29	-	0,0,0,0	0
56	MG	DA	3058	1/1	0.18	-	6,6,6,6	0
56	MG	DB	210	1/1	0.05	-	15,15,15,15	0
56	MG	CA	1690	1/1	0.08	-	19,19,19,19	0
56	MG	AW	111	1/1	0.26	-	32,32,32,32	1
56	MG	AA	1652	1/1	0.09	-	7,7,7,7	0
56	MG	DA	3227	1/1	0.06	-	8,8,8,8	0
56	MG	BA	3326	1/1	0.08	-	49,49,49,49	0
56	MG	BA	3108	1/1	0.11	-	0,0,0,0	0
56	MG	BA	3339	1/1	0.08	-	0,0,0,0	1
56	MG	BA	3117	1/1	0.25	-	3,3,3,3	0
56	MG	BA	3212	1/1	0.16	-	47,47,47,47	0
56	MG	BB	216	1/1	0.20	-	11,11,11,11	1
56	MG	BA	3383	1/1	0.06	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3138	1/1	0.26	-	40,40,40,40	0
56	MG	DA	3193	1/1	0.23	-	35,35,35,35	0
56	MG	AA	1778	1/1	0.14	-	0,0,0,0	0
56	MG	AA	1640	1/1	0.24	-	18,18,18,18	0
56	MG	AA	1794	1/1	0.20	-	56,56,56,56	0
56	MG	BA	3086	1/1	0.12	-	2,2,2,2	0
56	MG	DO	201	1/1	0.16	-	67,67,67,67	0
56	MG	DA	3070	1/1	0.15	-	0,0,0,0	0
56	MG	DA	3289	1/1	0.09	-	18,18,18,18	0
56	MG	DA	3204	1/1	0.11	-	8,8,8,8	0
56	MG	DA	3055	1/1	0.19	-	0,0,0,0	0
56	MG	DA	3206	1/1	0.08	-	47,47,47,47	0
56	MG	BA	3368	1/1	0.06	-	32,32,32,32	0
56	MG	BA	3093	1/1	0.16	-	15,15,15,15	0
56	MG	CA	1666	1/1	0.05	-	41,41,41,41	0
56	MG	BA	3167	1/1	0.15	-	33,33,33,33	0
56	MG	BA	3053	1/1	0.15	-	0,0,0,0	0
56	MG	DA	3231	1/1	0.49	-	72,72,72,72	0
56	MG	BA	3017	1/1	0.11	-	19,19,19,19	0
56	MG	AA	1730	1/1	0.52	-	82,82,82,82	0
56	MG	BA	3393	1/1	0.52	-	60,60,60,60	0
56	MG	DA	3304	1/1	0.07	-	9,9,9,9	0
56	MG	BX	101	1/1	0.11	-	26,26,26,26	0
56	MG	AA	1646	1/1	0.15	-	3,3,3,3	0
56	MG	BA	3231	1/1	0.41	-	45,45,45,45	0
56	MG	DA	3352	1/1	0.11	-	9,9,9,9	0
56	MG	AA	1753	1/1	0.09	-	26,26,26,26	0
56	MG	AA	1768	1/1	0.15	-	14,14,14,14	1
56	MG	DA	3267	1/1	0.11	-	13,13,13,13	0
58	ZN	AD	301	1/1	0.17	-	21,21,21,21	0
56	MG	DA	3354	1/1	0.05	-	2,2,2,2	0
56	MG	DA	3284	1/1	0.11	-	12,12,12,12	0
56	MG	CA	1783	1/1	0.16	-	13,13,13,13	0
56	MG	DA	3012	1/1	0.15	-	27,27,27,27	0
56	MG	BA	3239	1/1	0.26	-	12,12,12,12	0
56	MG	DA	3369	1/1	0.15	-	46,46,46,46	0
56	MG	BA	3399	1/1	0.21	-	27,27,27,27	0
56	MG	BA	3174	1/1	0.10	-	0,0,0,0	0
56	MG	BA	3035	1/1	0.29	-	10,10,10,10	0
56	MG	AA	1741	1/1	0.06	-	38,38,38,38	0
56	MG	CA	1757	1/1	0.15	-	56,56,56,56	0
56	MG	BA	3409	1/1	0.18	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3262	1/1	0.06	-	20,20,20,20	0
56	MG	AX	101	1/1	0.05	-	0,0,0,0	0
58	ZN	AN	101	1/1	0.05	-	50,50,50,50	0
56	MG	BA	3451	1/1	0.09	-	43,43,43,43	0
57	PAR	CA	1790	42/42	0.18	-	7,11,29,33	0
56	MG	BA	3119	1/1	0.26	-	16,16,16,16	0
56	MG	BA	3154	1/1	0.14	-	28,28,28,28	1
56	MG	AA	1756	1/1	0.21	-	15,15,15,15	0
56	MG	BB	215	1/1	0.10	-	40,40,40,40	0
56	MG	CA	1717	1/1	0.07	-	16,16,16,16	0
56	MG	DA	3379	1/1	0.16	-	31,31,31,31	0
56	MG	DA	3371	1/1	0.12	-	40,40,40,40	0
56	MG	DA	3063	1/1	0.12	-	0,0,0,0	0
56	MG	BA	3234	1/1	0.28	-	29,29,29,29	0
56	MG	BA	3422	1/1	0.24	-	39,39,39,39	0
56	MG	BA	3055	1/1	0.08	-	0,0,0,0	0
56	MG	CA	1704	1/1	0.10	-	5,5,5,5	0
56	MG	DA	3069	1/1	0.23	-	45,45,45,45	0
56	MG	BA	3412	1/1	0.23	-	48,48,48,48	0
56	MG	BA	3294	1/1	0.10	-	6,6,6,6	0
56	MG	BA	3166	1/1	0.06	-	39,39,39,39	0
56	MG	CA	1760	1/1	0.14	-	33,33,33,33	0
56	MG	AW	109	1/1	0.06	-	34,34,34,34	1
56	MG	AA	1638	1/1	0.26	-	24,24,24,24	0
56	MG	AA	1807	1/1	0.10	-	19,19,19,19	1
56	MG	B2	105	1/1	0.12	-	0,0,0,0	0
56	MG	BA	3199	1/1	0.11	-	9,9,9,9	0
56	MG	AA	1764	1/1	0.10	-	6,6,6,6	0
56	MG	DA	3397	1/1	0.14	-	31,31,31,31	0
56	MG	DA	3225	1/1	0.23	-	22,22,22,22	0
56	MG	BA	3215	1/1	0.17	-	30,30,30,30	0
56	MG	BA	3269	1/1	0.33	-	43,43,43,43	0
56	MG	DA	3087	1/1	0.28	-	23,23,23,23	0
56	MG	CX	101	1/1	0.14	-	3,3,3,3	0
56	MG	AW	107	1/1	0.06	-	28,28,28,28	0
56	MG	CA	1601	1/1	0.14	-	26,26,26,26	0
56	MG	AW	117	1/1	0.20	-	24,24,24,24	0
56	MG	BA	3331	1/1	0.09	-	45,45,45,45	0
56	MG	CA	1696	1/1	0.23	-	51,51,51,51	0
56	MG	BA	3372	1/1	0.22	-	43,43,43,43	1
56	MG	AA	1683	1/1	0.11	-	17,17,17,17	0
56	MG	BA	3373	1/1	0.04	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	1774	1/1	0.18	-	21,21,21,21	0
56	MG	CA	1734	1/1	0.14	-	59,59,59,59	0
56	MG	AV	104	1/1	0.16	-	27,27,27,27	0
56	MG	DA	3337	1/1	0.06	-	4,4,4,4	0
56	MG	DA	3386	1/1	0.28	-	0,0,0,0	0
56	MG	DA	3125	1/1	0.14	-	0,0,0,0	0
56	MG	AA	1701	1/1	0.11	-	18,18,18,18	0
56	MG	BA	3322	1/1	0.14	-	35,35,35,35	0
56	MG	CA	1707	1/1	0.18	-	6,6,6,6	0
56	MG	CA	1753	1/1	0.25	-	33,33,33,33	0
56	MG	BB	210	1/1	0.09	-	33,33,33,33	1
56	MG	DA	3273	1/1	0.56	-	59,59,59,59	0
56	MG	CA	1616	1/1	0.27	-	24,24,24,24	0
56	MG	BA	3410	1/1	0.12	-	41,41,41,41	0
56	MG	BA	3005	1/1	0.13	-	26,26,26,26	0
56	MG	AA	1639	1/1	0.15	-	30,30,30,30	0
56	MG	DA	3237	1/1	0.06	-	15,15,15,15	0
56	MG	CF	201	1/1	0.09	-	44,44,44,44	0
56	MG	DA	3128	1/1	0.10	-	0,0,0,0	0
56	MG	BA	3145	1/1	0.13	-	0,0,0,0	0
56	MG	AA	1660	1/1	0.23	-	61,61,61,61	0
56	MG	BA	3029	1/1	0.21	-	30,30,30,30	0
56	MG	AA	1633	1/1	0.51	-	90,90,90,90	0
56	MG	DA	3234	1/1	0.09	-	33,33,33,33	0
56	MG	DA	3072	1/1	0.06	-	0,0,0,0	0
56	MG	BA	3118	1/1	0.12	-	0,0,0,0	0
56	MG	BA	3437	1/1	0.08	-	4,4,4,4	0
56	MG	CA	1720	1/1	0.14	-	69,69,69,69	0
56	MG	BA	3095	1/1	0.12	-	0,0,0,0	0
56	MG	DA	3162	1/1	0.20	-	35,35,35,35	0
56	MG	BA	3336	1/1	0.09	-	45,45,45,45	0
56	MG	CA	1675	1/1	0.26	-	57,57,57,57	0
56	MG	BA	3349	1/1	0.14	-	28,28,28,28	1
56	MG	CA	1611	1/1	0.20	-	67,67,67,67	0
56	MG	AA	1795	1/1	0.20	-	30,30,30,30	0
56	MG	DA	3392	1/1	0.15	-	47,47,47,47	0
56	MG	BA	3077	1/1	0.22	-	6,6,6,6	0
56	MG	BA	3280	1/1	0.12	-	10,10,10,10	0
56	MG	DA	3180	1/1	0.24	-	0,0,0,0	0
56	MG	DA	3119	1/1	0.12	-	7,7,7,7	0
56	MG	DA	3194	1/1	0.09	-	0,0,0,0	1
56	MG	AA	1648	1/1	0.18	-	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AW	120	1/1	0.10	-	52,52,52,52	0
56	MG	BA	3056	1/1	0.16	-	0,0,0,0	0
56	MG	AA	1628	1/1	0.12	-	2,2,2,2	0
56	MG	CA	1767	1/1	0.27	-	67,67,67,67	0
56	MG	AA	1776	1/1	0.09	-	30,30,30,30	0
56	MG	DA	3373	1/1	0.09	-	28,28,28,28	0
56	MG	BA	3091	1/1	0.17	-	20,20,20,20	0
56	MG	BA	3411	1/1	0.19	-	62,62,62,62	0
56	MG	AW	119	1/1	0.07	-	19,19,19,19	0
56	MG	BA	3037	1/1	0.18	-	0,0,0,0	0
56	MG	CW	110	1/1	0.18	-	38,38,38,38	0
56	MG	AA	1782	1/1	0.28	-	68,68,68,68	0
56	MG	BA	3164	1/1	0.06	-	9,9,9,9	0
56	MG	BA	3430	1/1	0.20	-	30,30,30,30	0
56	MG	BA	3217	1/1	0.14	-	37,37,37,37	0
56	MG	AA	1634	1/1	0.25	-	34,34,34,34	0
56	MG	CA	1640	1/1	0.08	-	43,43,43,43	0
56	MG	DH	201	1/1	0.19	-	36,36,36,36	0
56	MG	AA	1759	1/1	0.07	-	5,5,5,5	1
56	MG	BA	3096	1/1	0.07	-	0,0,0,0	0
56	MG	BA	3010	1/1	0.07	-	30,30,30,30	0
56	MG	BA	3256	1/1	0.08	-	22,22,22,22	0
56	MG	BA	3187	1/1	0.16	-	2,2,2,2	0
56	MG	DA	3335	1/1	0.04	-	10,10,10,10	0
56	MG	DA	3200	1/1	0.16	-	26,26,26,26	0
56	MG	DA	3178	1/1	0.07	-	19,19,19,19	0
56	MG	AV	101	1/1	0.05	-	5,5,5,5	0
56	MG	BA	3049	1/1	0.28	-	36,36,36,36	0
56	MG	DA	3160	1/1	0.16	-	37,37,37,37	0
56	MG	AA	1607	1/1	0.07	-	12,12,12,12	0
56	MG	BA	3195	1/1	0.22	-	16,16,16,16	0
56	MG	DA	3036	1/1	0.19	-	43,43,43,43	0
56	MG	CW	112	1/1	0.11	-	53,53,53,53	0
56	MG	DU	201	1/1	0.10	-	45,45,45,45	0
56	MG	CA	1775	1/1	0.25	-	35,35,35,35	0
56	MG	CA	1785	1/1	0.12	-	44,44,44,44	0
56	MG	DA	3084	1/1	0.10	-	29,29,29,29	0
56	MG	DA	3270	1/1	0.10	-	47,47,47,47	0
56	MG	CW	109	1/1	0.18	-	81,81,81,81	0
56	MG	BA	3087	1/1	0.17	-	16,16,16,16	0
56	MG	AA	1693	1/1	0.40	-	43,43,43,43	0
56	MG	CA	1654	1/1	0.07	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3187	1/1	0.34	-	86,86,86,86	0
56	MG	BA	3261	1/1	0.10	-	24,24,24,24	0
56	MG	AA	1709	1/1	0.14	-	33,33,33,33	0
56	MG	BA	3206	1/1	0.17	-	25,25,25,25	0
56	MG	DA	3167	1/1	0.11	-	101,101,101,101	0
56	MG	BA	3229	1/1	0.17	-	36,36,36,36	0
56	MG	BA	3310	1/1	0.16	-	22,22,22,22	0
56	MG	AA	1781	1/1	0.20	-	27,27,27,27	0
56	MG	CA	1706	1/1	0.18	-	54,54,54,54	0
56	MG	DA	3214	1/1	0.10	-	32,32,32,32	0
56	MG	BA	3436	1/1	0.12	-	39,39,39,39	1
56	MG	DA	3291	1/1	0.11	-	0,0,0,0	0
56	MG	AA	1604	1/1	0.15	-	52,52,52,52	0
56	MG	DA	3283	1/1	0.19	-	35,35,35,35	0
56	MG	CX	106	1/1	0.35	-	47,47,47,47	0
56	MG	AA	1799	1/1	0.09	-	71,71,71,71	0
56	MG	CM	201	1/1	0.05	-	21,21,21,21	0
56	MG	DA	3222	1/1	0.20	-	24,24,24,24	0
56	MG	BA	3137	1/1	0.14	-	6,6,6,6	0
56	MG	DB	204	1/1	0.13	-	48,48,48,48	0
56	MG	BA	3125	1/1	0.30	-	18,18,18,18	0
56	MG	DA	3181	1/1	0.08	-	17,17,17,17	0
56	MG	B2	103	1/1	0.27	-	46,46,46,46	0
56	MG	DA	3186	1/1	0.25	-	24,24,24,24	0
56	MG	CA	1651	1/1	0.18	-	31,31,31,31	0
56	MG	BA	3360	1/1	0.07	-	25,25,25,25	0
56	MG	BN	201	1/1	0.31	-	25,25,25,25	0
56	MG	CA	1737	1/1	0.15	-	35,35,35,35	0
56	MG	DA	3315	1/1	0.07	-	4,4,4,4	0
56	MG	AA	1619	1/1	0.36	-	41,41,41,41	0
56	MG	DA	3330	1/1	0.44	-	81,81,81,81	0
56	MG	CA	1716	1/1	0.32	-	67,67,67,67	0
56	MG	CA	1630	1/1	0.09	-	0,0,0,0	0
56	MG	BA	3180	1/1	0.09	-	33,33,33,33	0
56	MG	BB	205	1/1	0.36	-	35,35,35,35	1
56	MG	DA	3382	1/1	0.11	-	6,6,6,6	0
56	MG	CA	1749	1/1	0.08	-	7,7,7,7	0
56	MG	CW	113	1/1	0.05	-	24,24,24,24	0
56	MG	DA	3165	1/1	0.17	-	38,38,38,38	0
56	MG	CA	1695	1/1	0.13	-	70,70,70,70	0
56	MG	BB	217	1/1	0.10	-	34,34,34,34	0
56	MG	CA	1709	1/1	0.07	-	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	1800	1/1	0.11	-	36,36,36,36	0
56	MG	CA	1625	1/1	0.20	-	19,19,19,19	0
56	MG	DA	3269	1/1	0.35	-	33,33,33,33	0
56	MG	DA	3172	1/1	0.21	-	25,25,25,25	0
56	MG	BA	3265	1/1	0.20	-	37,37,37,37	0
56	MG	DA	3286	1/1	0.12	-	0,0,0,0	0
56	MG	BA	3382	1/1	0.11	-	63,63,63,63	0
56	MG	AA	1784	1/1	0.33	-	41,41,41,41	0
56	MG	DA	3280	1/1	0.07	-	16,16,16,16	0
56	MG	CX	102	1/1	0.32	-	75,75,75,75	0
56	MG	DA	3251	1/1	0.16	-	20,20,20,20	0
56	MG	AA	1765	1/1	0.04	-	43,43,43,43	0
56	MG	BA	3089	1/1	0.15	-	6,6,6,6	0
56	MG	AW	110	1/1	0.21	-	46,46,46,46	0
56	MG	BA	3139	1/1	0.11	-	9,9,9,9	0
56	MG	BA	3031	1/1	0.21	-	11,11,11,11	0
56	MG	BA	3249	1/1	0.07	-	11,11,11,11	0
56	MG	DA	3255	1/1	0.45	-	92,92,92,92	0
56	MG	BA	3070	1/1	0.22	-	24,24,24,24	0
56	MG	BA	3363	1/1	0.09	-	8,8,8,8	0
56	MG	AA	1689	1/1	0.06	-	50,50,50,50	0
56	MG	BA	3150	1/1	0.13	-	35,35,35,35	0
56	MG	DA	3279	1/1	0.20	-	15,15,15,15	0
56	MG	AA	1703	1/1	0.14	-	23,23,23,23	0
56	MG	AW	108	1/1	0.09	-	35,35,35,35	0
56	MG	BA	3007	1/1	0.24	-	0,0,0,0	0
56	MG	DA	3378	1/1	0.10	-	8,8,8,8	0
56	MG	DA	3034	1/1	0.07	-	7,7,7,7	0
56	MG	DA	3031	1/1	0.09	-	0,0,0,0	0
56	MG	B7	101	1/1	0.08	-	7,7,7,7	0
56	MG	DA	3322	1/1	0.09	-	27,27,27,27	0
56	MG	CA	1662	1/1	0.09	-	18,18,18,18	0
56	MG	DA	3272	1/1	0.40	-	47,47,47,47	0
56	MG	BA	3025	1/1	0.14	-	0,0,0,0	0
56	MG	DA	3236	1/1	0.10	-	54,54,54,54	0
56	MG	BA	3052	1/1	0.26	-	0,0,0,0	0
56	MG	DA	3029	1/1	0.16	-	36,36,36,36	0
56	MG	CA	1668	1/1	0.10	-	42,42,42,42	0
56	MG	DA	3387	1/1	0.10	-	11,11,11,11	0
56	MG	BA	3020	1/1	0.22	-	1,1,1,1	0
56	MG	AA	1744	1/1	0.31	-	18,18,18,18	0
56	MG	DA	3045	1/1	0.14	-	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	3185	1/1	0.04	-	9,9,9,9	0
56	MG	AA	1642	1/1	0.12	-	8,8,8,8	0
56	MG	DA	3154	1/1	0.17	-	31,31,31,31	0
56	MG	BA	3132	1/1	0.14	-	2,2,2,2	0
56	MG	CA	1788	1/1	0.18	-	42,42,42,42	1
56	MG	BA	3248	1/1	0.27	-	33,33,33,33	0
56	MG	BA	3454	1/1	0.12	-	44,44,44,44	0
56	MG	DA	3074	1/1	0.22	-	11,11,11,11	0
56	MG	AW	113	1/1	0.35	-	46,46,46,46	1
56	MG	BA	3318	1/1	0.19	-	30,30,30,30	0
56	MG	CA	1652	1/1	0.15	-	52,52,52,52	0
56	MG	AW	112	1/1	0.15	-	29,29,29,29	0
56	MG	DA	3219	1/1	0.58	-	75,75,75,75	0
56	MG	DA	3296	1/1	0.11	-	59,59,59,59	0
56	MG	DA	3259	1/1	0.14	-	14,14,14,14	0
56	MG	BA	3390	1/1	0.09	-	20,20,20,20	1
56	MG	BA	3356	1/1	0.07	-	37,37,37,37	0
56	MG	B3	101	1/1	0.28	-	48,48,48,48	1
56	MG	BA	3291	1/1	0.05	-	12,12,12,12	0
56	MG	BA	3227	1/1	0.22	-	49,49,49,49	0
56	MG	DA	3303	1/1	0.10	-	11,11,11,11	0
56	MG	BA	3297	1/1	0.24	-	7,7,7,7	0
56	MG	AA	1653	1/1	0.14	-	39,39,39,39	0
56	MG	AA	1722	1/1	0.13	-	20,20,20,20	0
56	MG	DA	3109	1/1	0.14	-	0,0,0,0	0
56	MG	DA	3007	1/1	0.32	-	39,39,39,39	0
56	MG	DA	3375	1/1	0.10	-	42,42,42,42	1
56	MG	BA	3210	1/1	0.16	-	11,11,11,11	0
56	MG	AA	1814	1/1	0.15	-	25,25,25,25	0
56	MG	BA	3340	1/1	0.09	-	28,28,28,28	0
56	MG	DA	3090	1/1	0.10	-	0,0,0,0	0
56	MG	BA	3425	1/1	0.19	-	61,61,61,61	0
56	MG	CA	1768	1/1	0.15	-	37,37,37,37	0
56	MG	DA	3053	1/1	0.15	-	24,24,24,24	0
56	MG	BA	3094	1/1	0.20	-	0,0,0,0	0
56	MG	AA	1751	1/1	0.06	-	19,19,19,19	0
56	MG	BA	3062	1/1	0.27	-	0,0,0,0	0
56	MG	DA	3319	1/1	0.21	-	52,52,52,52	0
56	MG	AA	1711	1/1	0.05	-	8,8,8,8	0
56	MG	DB	212	1/1	0.07	-	27,27,27,27	0
56	MG	BA	3057	1/1	0.24	-	17,17,17,17	0
56	MG	CA	1722	1/1	0.29	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	1606	1/1	0.33	-	53,53,53,53	0
56	MG	CA	1642	1/1	0.13	-	56,56,56,56	0
56	MG	CA	1782	1/1	0.07	-	29,29,29,29	0
56	MG	AA	1675	1/1	0.20	-	4,4,4,4	0
56	MG	DA	3049	1/1	0.20	-	0,0,0,0	0
56	MG	BA	3285	1/1	0.47	-	74,74,74,74	0
56	MG	AA	1746	1/1	0.09	-	11,11,11,11	0
56	MG	BA	3085	1/1	0.16	-	0,0,0,0	0
56	MG	BA	3209	1/1	0.18	-	15,15,15,15	0
56	MG	BA	3327	1/1	0.09	-	30,30,30,30	0
56	MG	DA	3004	1/1	0.41	-	90,90,90,90	0
56	MG	DA	3130	1/1	0.13	-	14,14,14,14	0
56	MG	AA	1679	1/1	0.08	-	5,5,5,5	1
56	MG	B2	102	1/1	0.17	-	44,44,44,44	0
56	MG	CA	1727	1/1	0.23	-	37,37,37,37	0
56	MG	BA	3058	1/1	0.20	-	0,0,0,0	0
56	MG	DA	3362	1/1	0.14	-	10,10,10,10	1
56	MG	AA	1624	1/1	0.10	-	33,33,33,33	0
56	MG	BA	3198	1/1	0.09	-	0,0,0,0	0
56	MG	BA	3342	1/1	0.28	-	52,52,52,52	1
56	MG	BA	3350	1/1	0.16	-	32,32,32,32	0
56	MG	CA	1653	1/1	0.05	-	60,60,60,60	0
56	MG	BA	3286	1/1	0.20	-	38,38,38,38	0
56	MG	DA	3288	1/1	0.08	-	25,25,25,25	1
56	MG	CA	1754	1/1	0.11	-	6,6,6,6	0
56	MG	CA	1624	1/1	0.08	-	16,16,16,16	0
56	MG	DS	201	1/1	0.39	-	14,14,14,14	1
56	MG	DA	3285	1/1	0.22	-	15,15,15,15	0
56	MG	CA	1644	1/1	0.17	-	59,59,59,59	0
56	MG	BA	3146	1/1	0.23	-	0,0,0,0	0
56	MG	CW	101	1/1	0.07	-	36,36,36,36	0

6.5 Other polymers ⓘ

There are no such residues in this entry.