



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 06:54 PM BST

PDB ID : 4V5D
Title : Structure of the *Thermus thermophilus* 70S ribosome in complex with mRNA, paromomycin, acylated A- and P-site tRNAs, and E-site tRNA.
Authors : Voorhees, R.M.; Weixlbaumer, A.; Loakes, D.; Kelley, A.C.; Ramakrishnan, V.
Deposited on : 2009-03-24
Resolution : 3.50 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>

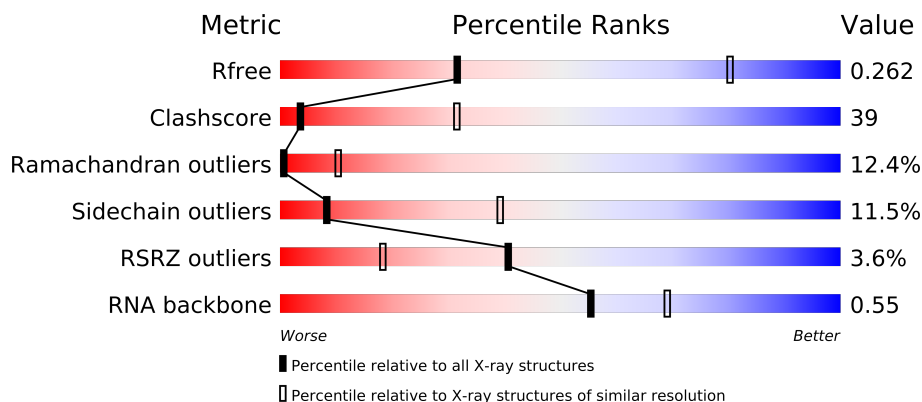
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.50 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	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)
RNA backbone	1838	1007 (4.22-2.76)

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	AY	77	
22	CV	77	
22	CY	77	
23	AW	76	
23	CW	76	
24	AX	11	
24	CX	11	
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	B9	37	
34	D9	37	
35	BA	2822	
35	DA	2822	
36	BB	122	
36	DB	122	
37	BC	229	
37	DC	229	
38	BD	276	
38	DD	276	
39	BE	206	
39	DE	206	
40	BF	210	
40	DF	210	
41	BG	182	
41	DG	182	
42	BH	180	
42	DH	180	
43	BI	148	
43	DI	148	
44	BN	140	
44	DN	140	
45	BO	122	
45	DO	122	
46	BP	150	
46	DP	150	
47	BQ	141	
47	DQ	141	

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

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 296042 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 AND A-SITE PHE-TRNA PHE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0	0
			1630	732	292	531	75			
22	AY	77	Total	C	N	O	P	0	0	0
			1630	732	292	531	75			
22	CV	77	Total	C	N	O	P	0	0	0
			1630	732	292	531	75			
22	CY	77	Total	C	N	O	P	0	0	0
			1630	732	292	531	75			

- Molecule 23 is a RNA chain called E-SITE TRNA PHE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
23	CW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			

- 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
			227	104	39	74	10			
24	CX	11	Total	C	N	O	P	0	0	0
			227	104	39	74	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
25	D0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			
26	D1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
27	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	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	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			
29	D4	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			
34	D9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

- Molecule 35 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BA	2807	Total	C	N	O	P	0	0	0
			60459	26907	11311	19435	2806			
35	DA	2807	Total	C	N	O	P	0	0	0
			60459	26907	11311	19435	2806			

- Molecule 36 is a RNA chain called 5S RIBOSOMAL RNA.

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

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	BC	191	Total	C	N	O	0	0	1
			1140	689	221	230			
37	DC	191	Total	C	N	O	0	0	1
			1142	691	221	230			

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

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

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

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

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.

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

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L9.

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

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L17.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L18.

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

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

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L24.

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

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L25.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BA	422	Total	Mg	0	0
			422	422		
57	CA	199	Total	Mg	0	0
			199	199		
57	DF	2	Total	Mg	0	0
			2	2		
57	CV	5	Total	Mg	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	D2	3	Total 3	Mg 3	0	0
57	BE	1	Total 1	Mg 1	0	0
57	AW	8	Total 8	Mg 8	0	0
57	B1	1	Total 1	Mg 1	0	0
57	AN	1	Total 1	Mg 1	0	0
57	AX	2	Total 2	Mg 2	0	0
57	CN	1	Total 1	Mg 1	0	0
57	DN	1	Total 1	Mg 1	0	0
57	DC	1	Total 1	Mg 1	0	0
57	DD	2	Total 2	Mg 2	0	0
57	B5	2	Total 2	Mg 2	0	0
57	BB	14	Total 14	Mg 14	0	0
57	DO	1	Total 1	Mg 1	0	0
57	AE	1	Total 1	Mg 1	0	0
57	BF	1	Total 1	Mg 1	0	0
57	AV	5	Total 5	Mg 5	0	0
57	BX	2	Total 2	Mg 2	0	0
57	B2	2	Total 2	Mg 2	0	0
57	AA	198	Total 198	Mg 198	0	0
57	D7	2	Total 2	Mg 2	0	0
57	CX	3	Total 3	Mg 3	0	0

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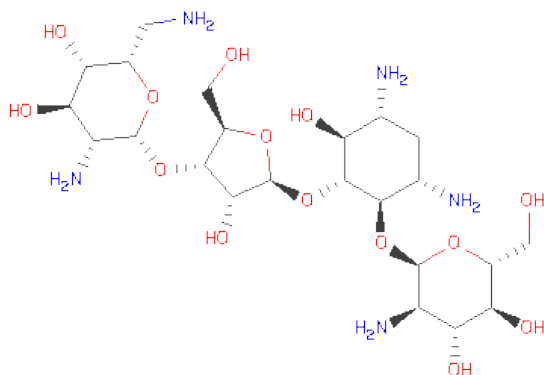
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DV	1	Total 1	Mg 1	0	0
57	BU	1	Total 1	Mg 1	0	0
57	AD	1	Total 1	Mg 1	0	0
57	BN	1	Total 1	Mg 1	0	0
57	AI	1	Total 1	Mg 1	0	0
57	DS	1	Total 1	Mg 1	0	0
57	DE	1	Total 1	Mg 1	0	0
57	DX	3	Total 3	Mg 3	0	0
57	DA	421	Total 421	Mg 421	0	0
57	B7	1	Total 1	Mg 1	0	0
57	AL	2	Total 2	Mg 2	0	0
57	BV	1	Total 1	Mg 1	0	0
57	AG	1	Total 1	Mg 1	0	0
57	BO	1	Total 1	Mg 1	0	0
57	D1	1	Total 1	Mg 1	0	0
57	CI	1	Total 1	Mg 1	0	0
57	CW	7	Total 7	Mg 7	0	0
57	D5	2	Total 2	Mg 2	0	0
57	BD	2	Total 2	Mg 2	0	0
57	B0	1	Total 1	Mg 1	0	0
57	CE	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CL	1	Total	Mg	0	0
			1	1		
57	DB	13	Total	Mg	0	0
			13	13		

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	CN	1	Total	Zn	0	0
			1	1		
59	AN	1	Total	Zn	0	0
			1	1		
59	B9	1	Total	Zn	0	0
			1	1		
59	D9	1	Total	Zn	0	0
			1	1		
59	CD	1	Total	Zn	0	0
			1	1		

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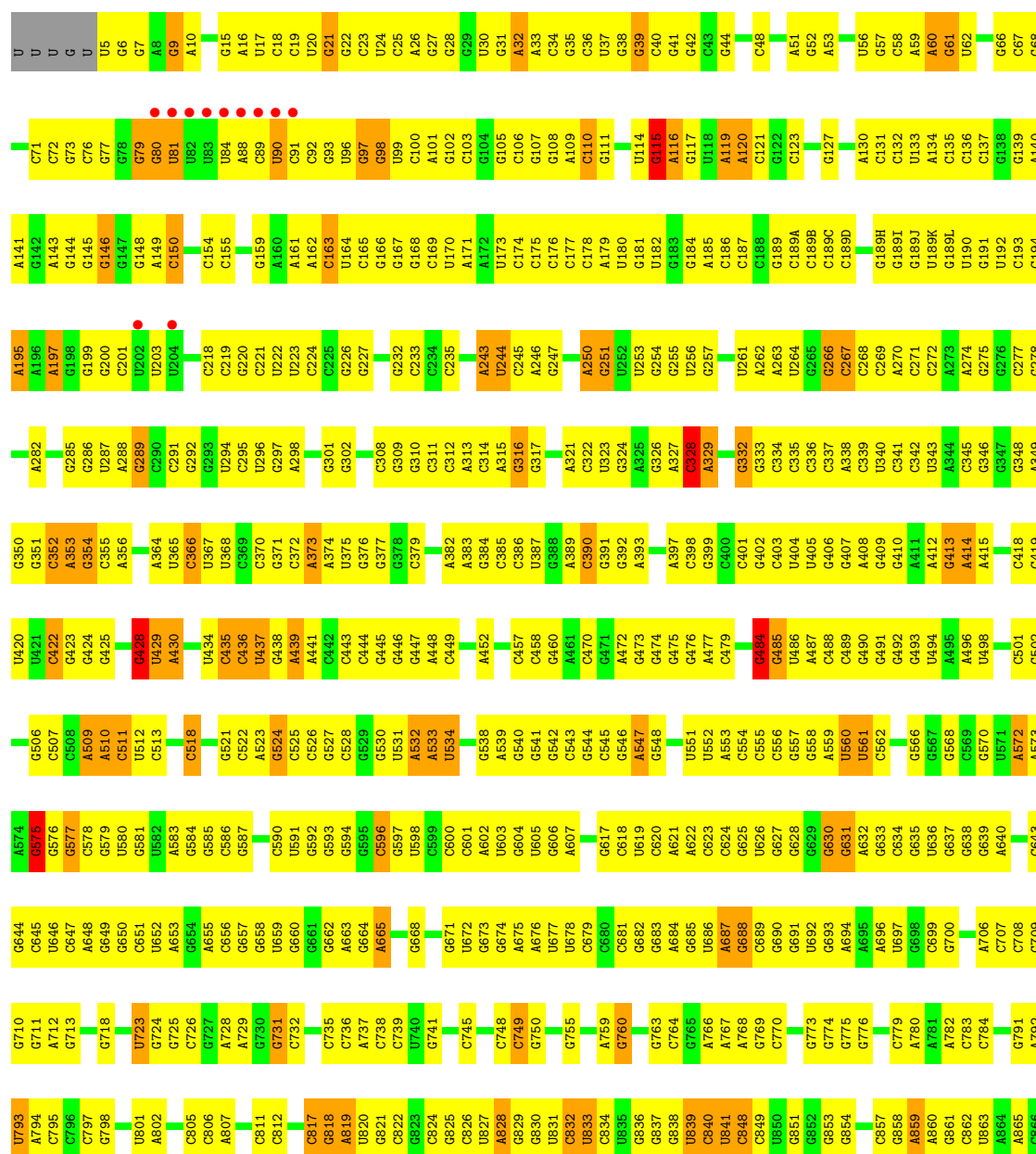
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AD	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

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

• Molecule 1: 16S RRNA

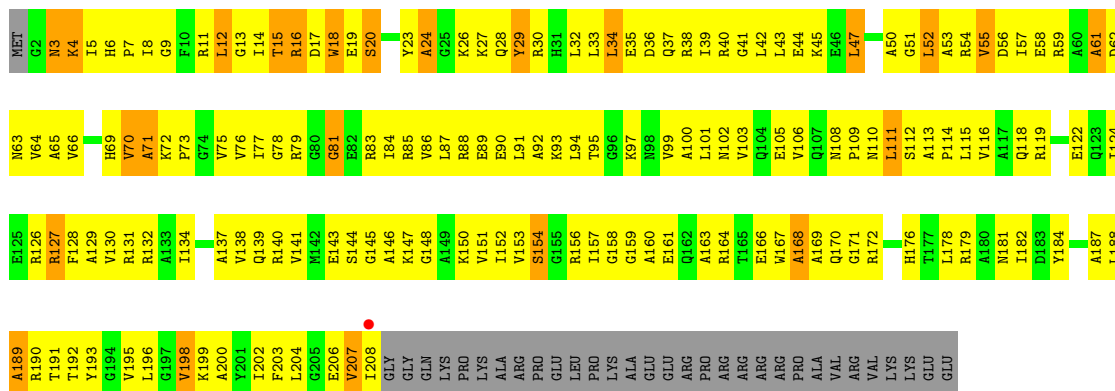
Chain AA: 





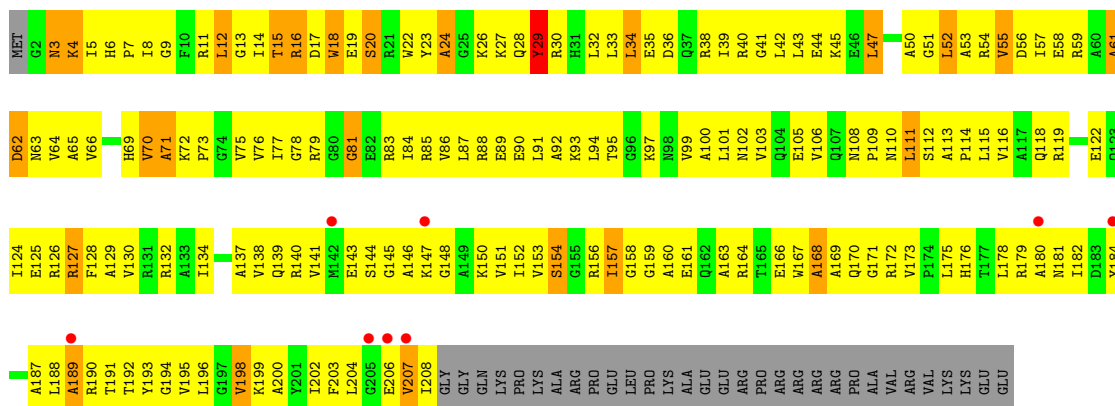
- Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain AC:



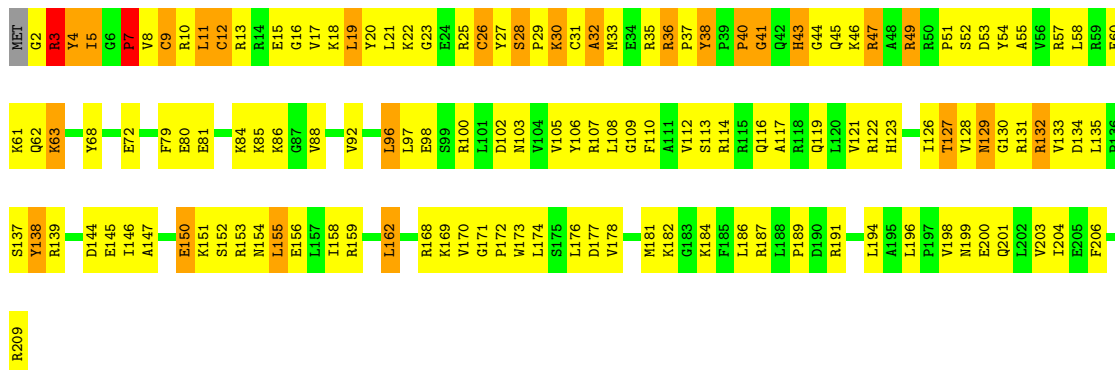
- Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain CC:



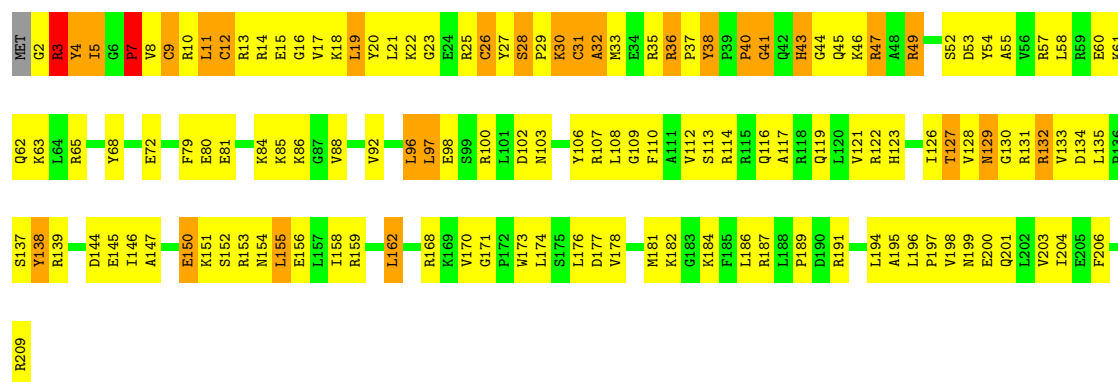
- Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AD:



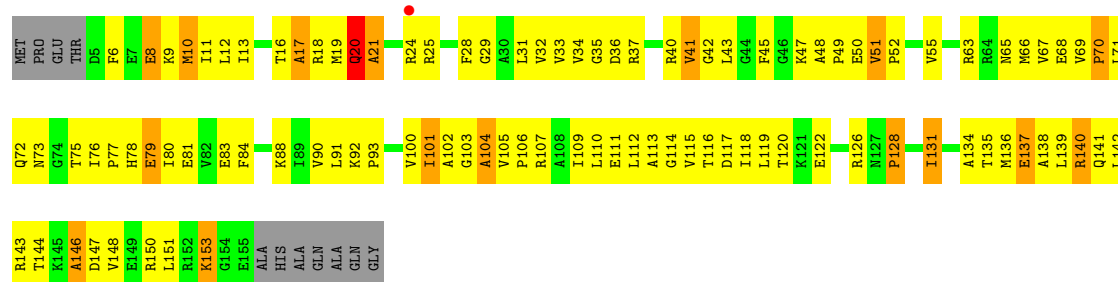
- Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain CD:



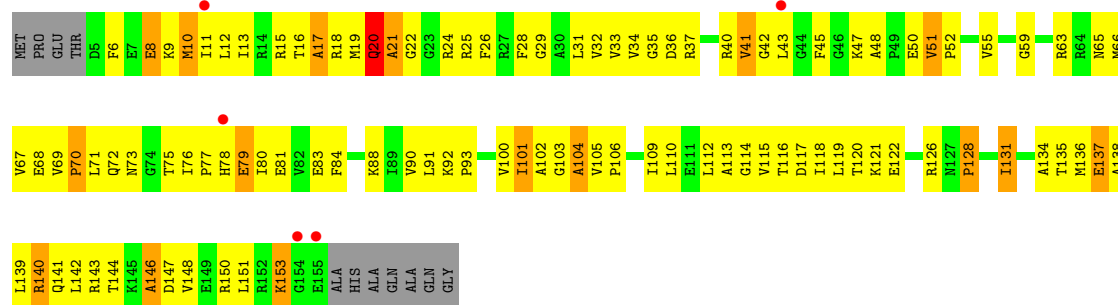
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain AE:



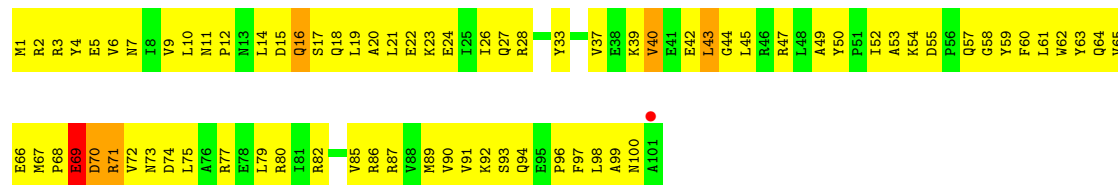
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain CE:



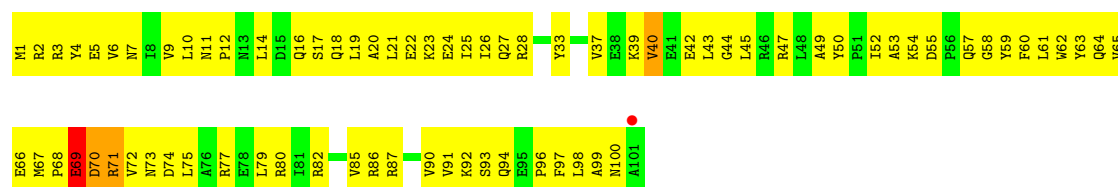
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AF:



• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain CF:



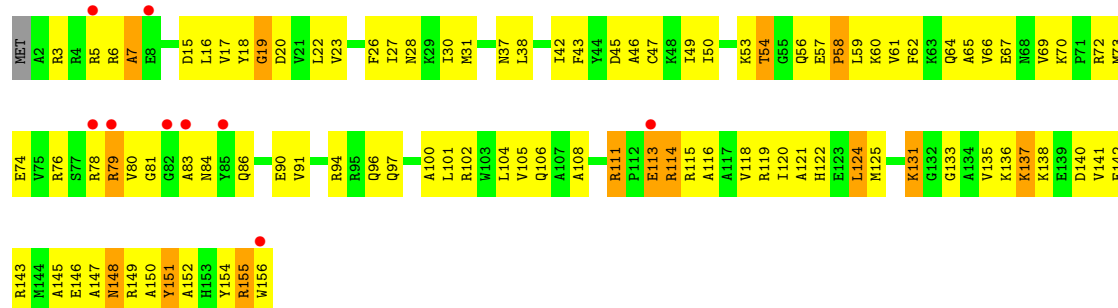
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AG:



• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain CG:



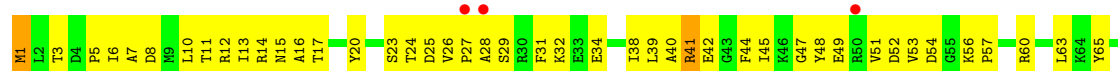
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

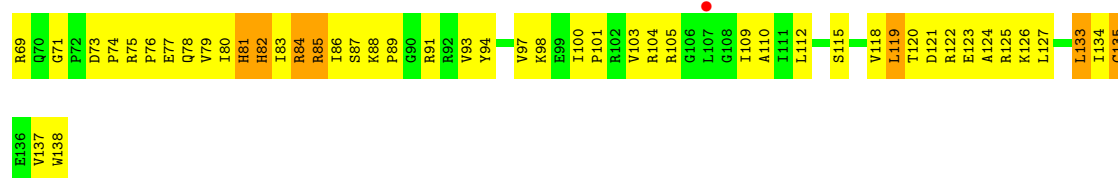
Chain AH:



• Molecule 8: 30S RIBOSOMAL PROTEIN S8

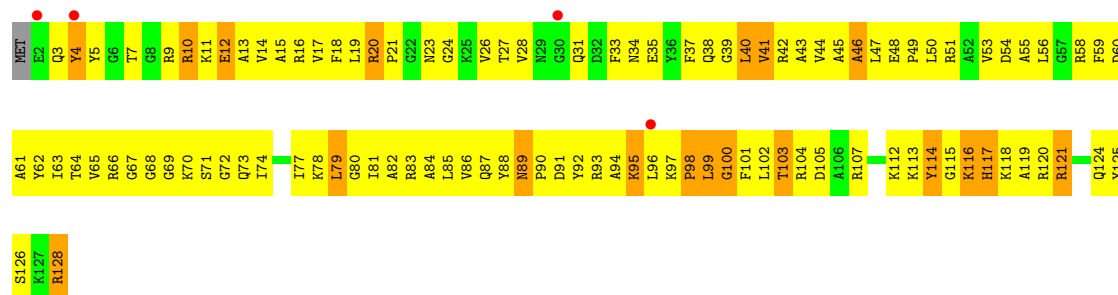
Chain CH:





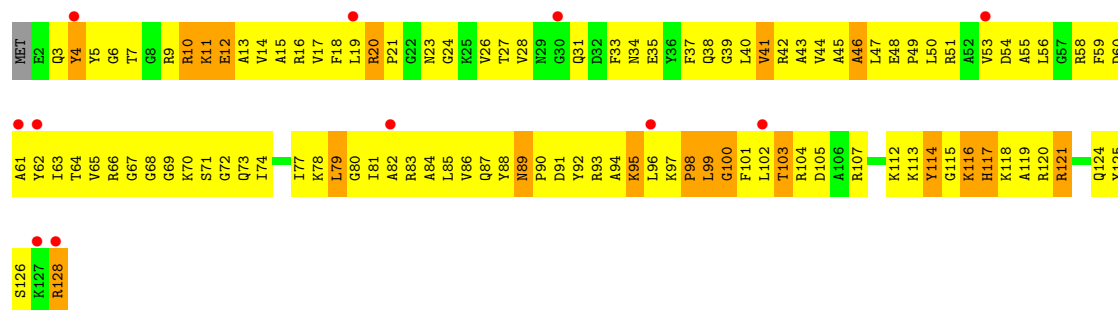
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AI:



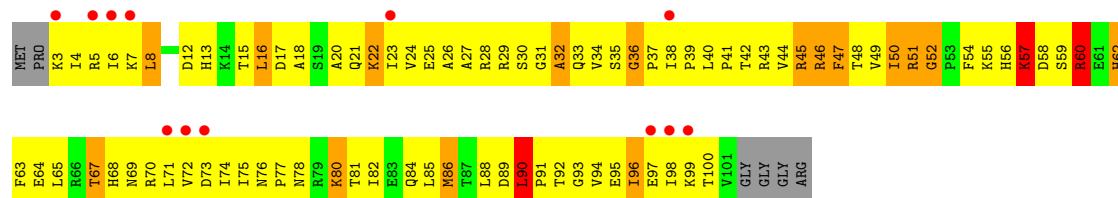
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CI:



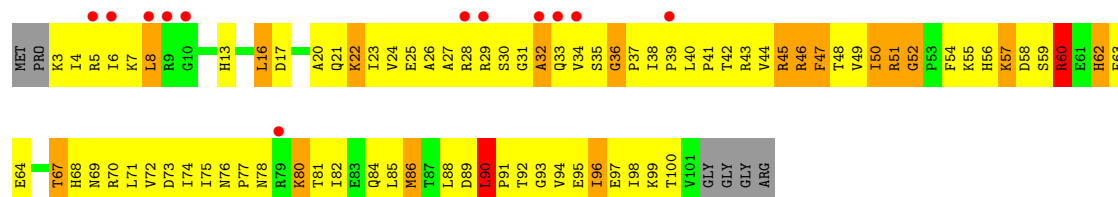
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AJ:



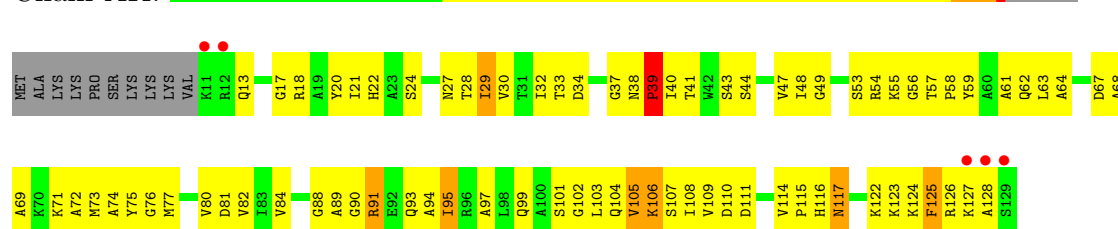
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain CJ:



- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AK:



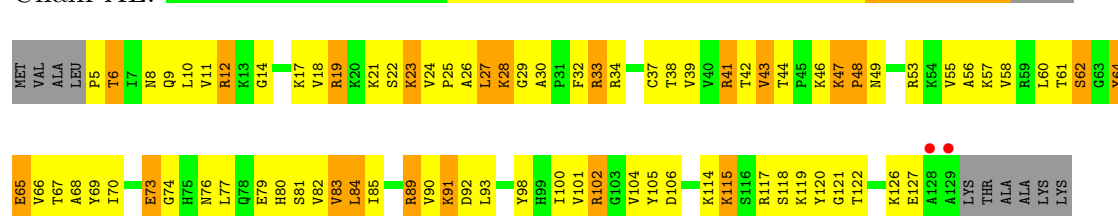
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain CK:



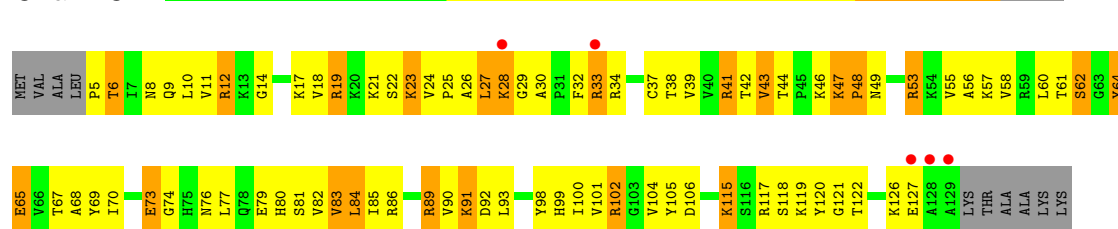
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AL:



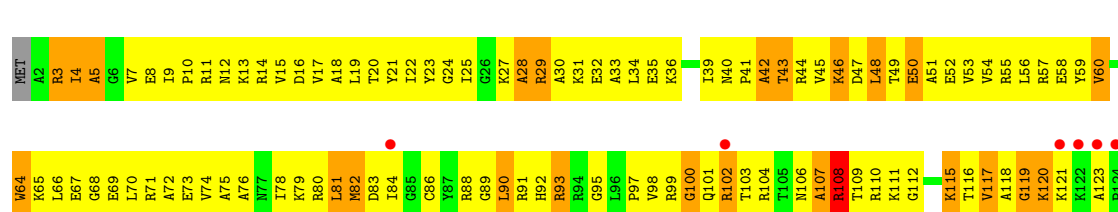
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain CL:



- Molecule 13: 30S RIBOSOMAL PROTEIN S13

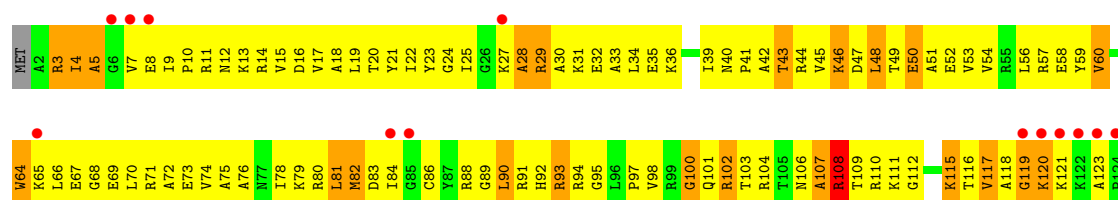
Chain AM:





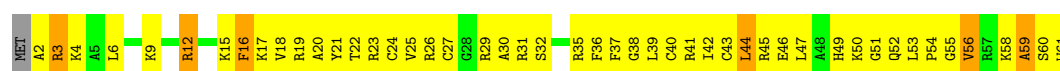
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain CM:



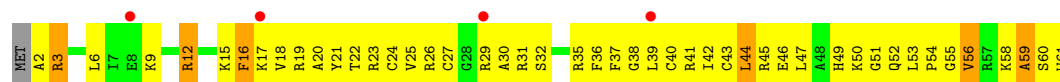
• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain AN:



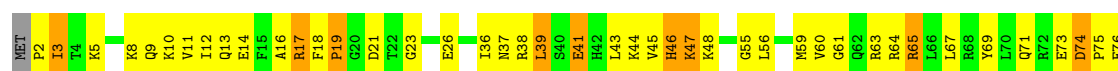
• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain CN:



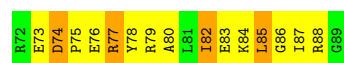
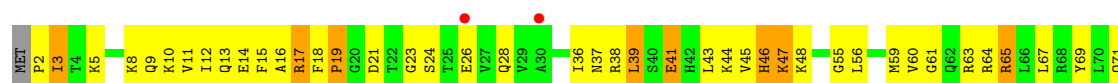
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO:



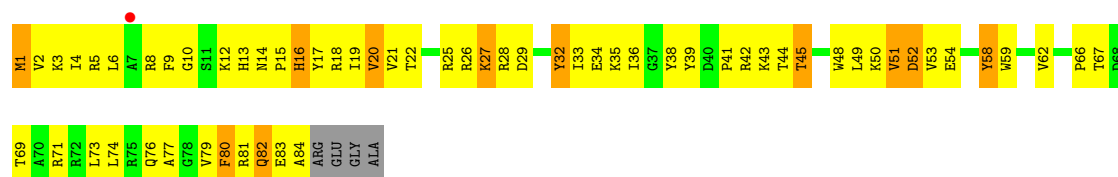
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CO:



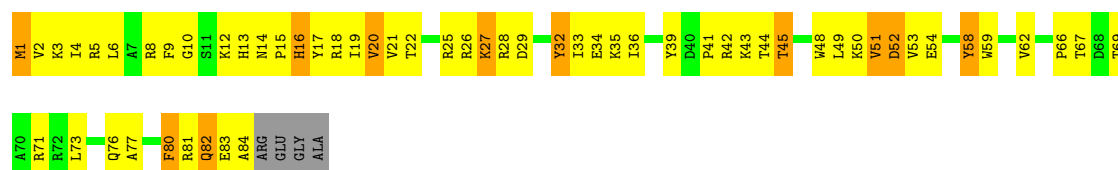
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP:



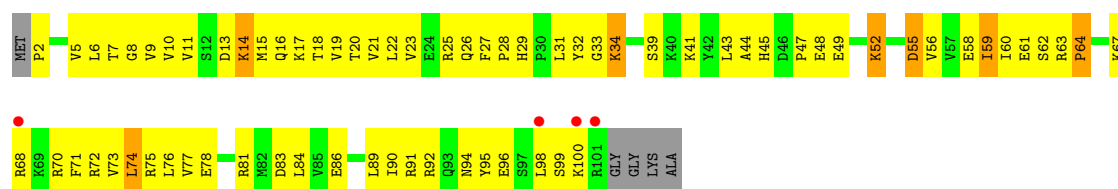
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CP:



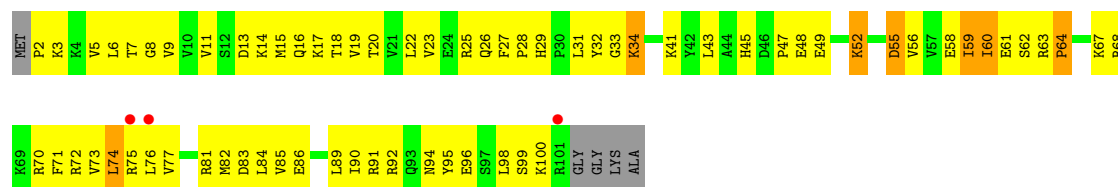
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ:



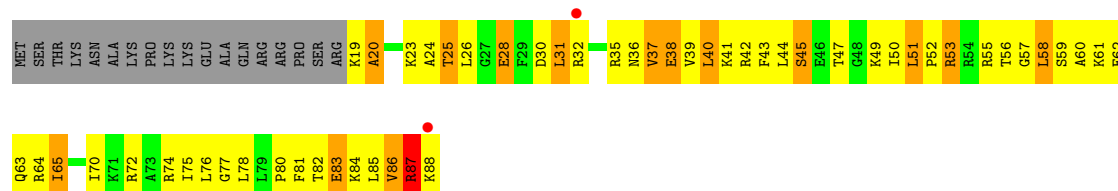
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CQ:



• Molecule 18: 30S RIBOSOMAL PROTEIN S18

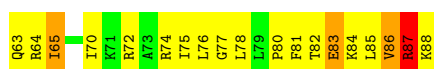
Chain AR:



• Molecule 18: 30S RIBOSOMAL PROTEIN S18

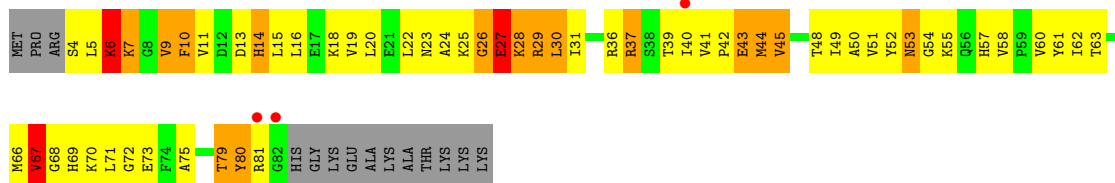
Chain CR:





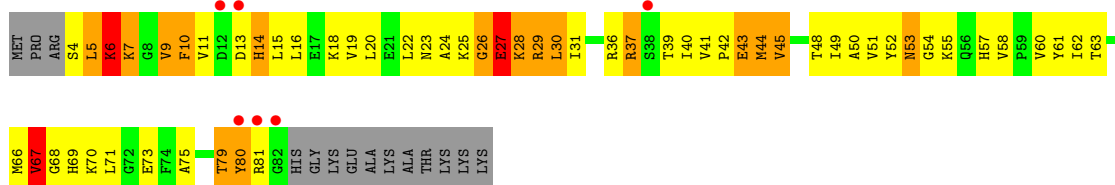
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AS:



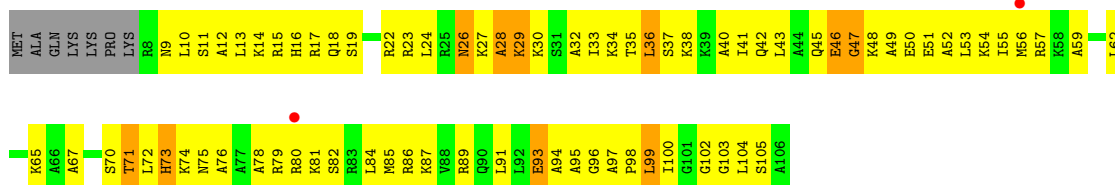
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain CS:



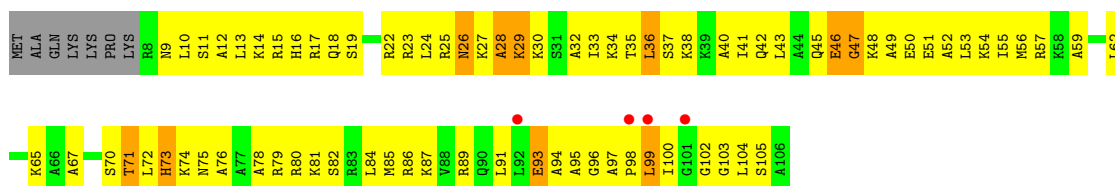
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain AT:



• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain CT:



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AU:



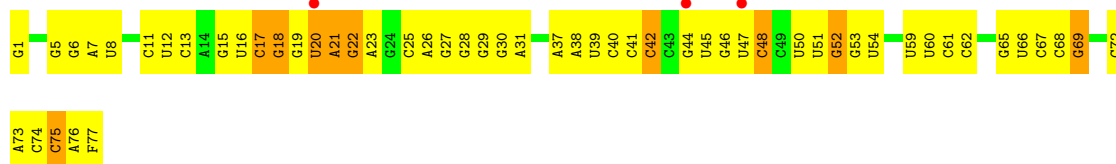
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CU:



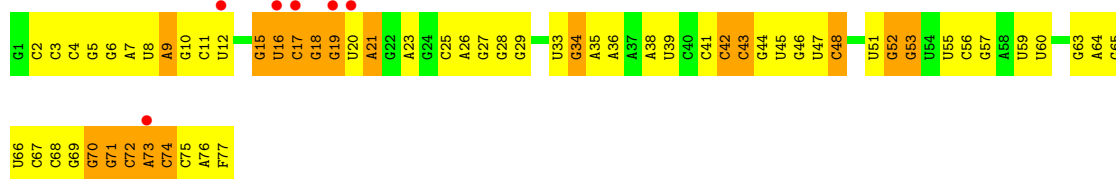
- Molecule 22: P AND A-SITE PHE-TRNA PHE

Chain AV:



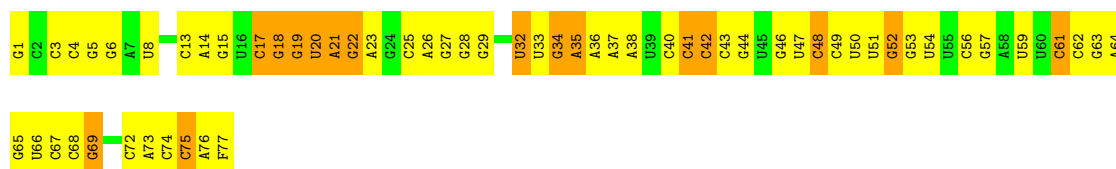
- Molecule 22: P AND A-SITE PHE-TRNA PHE

Chain AY:



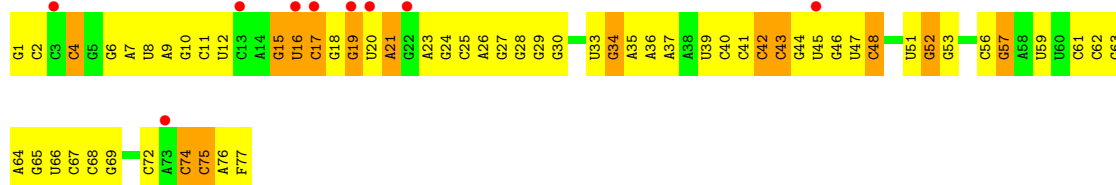
- Molecule 22: P AND A-SITE PHE-TRNA PHE

Chain CV:



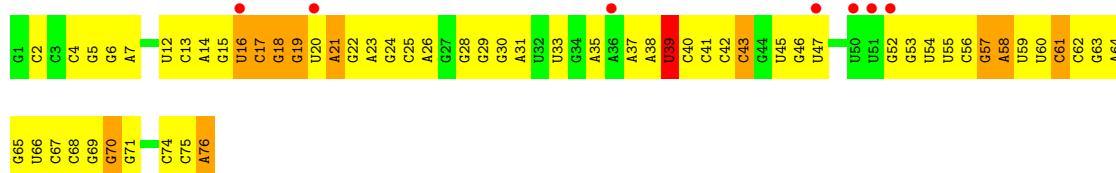
- Molecule 22: P AND A-SITE PHE-TRNA PHE

Chain CY:



- Molecule 23: E-SITE TRNA PHE

Chain AW:



- Molecule 23: E-SITE TRNA PHE

Chain CW:



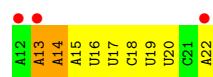
- Molecule 24: MRNA

Chain AX:



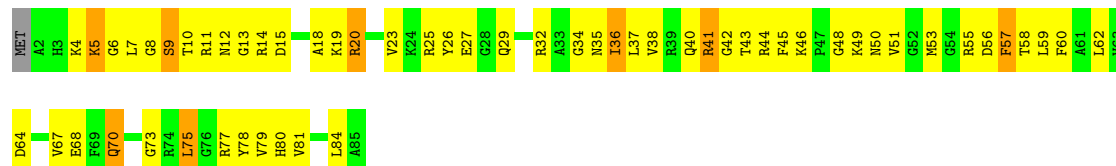
- Molecule 24: MRNA

Chain CX:



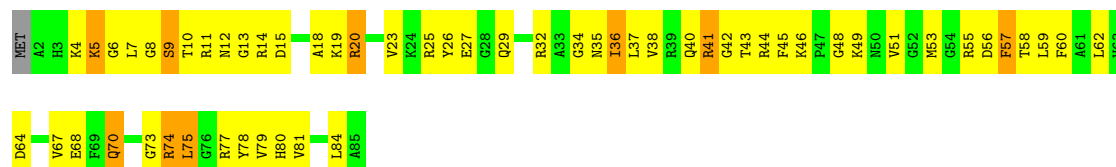
- Molecule 25: 50S RIBOSOMAL PROTEIN L27

Chain B0:



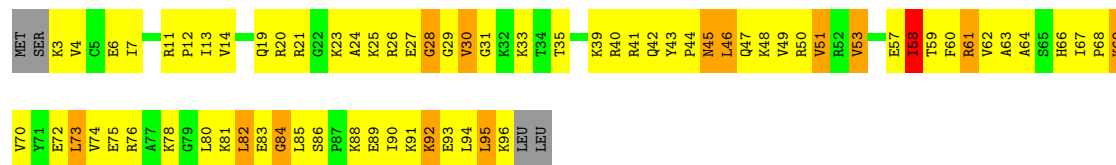
- Molecule 25: 50S RIBOSOMAL PROTEIN L27

Chain D0:



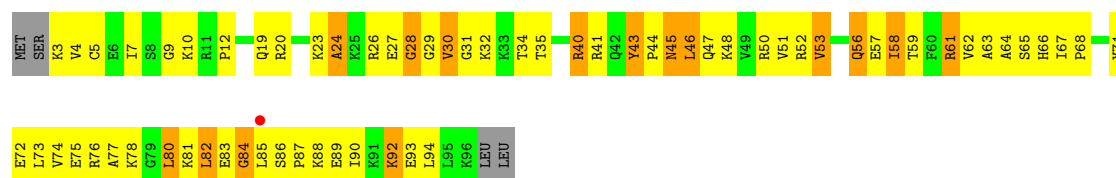
- Molecule 26: 50S RIBOSOMAL PROTEIN L28

Chain B1:



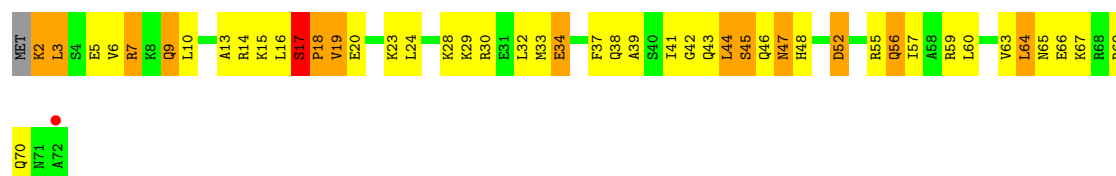
- Molecule 26: 50S RIBOSOMAL PROTEIN L28

Chain D1: 



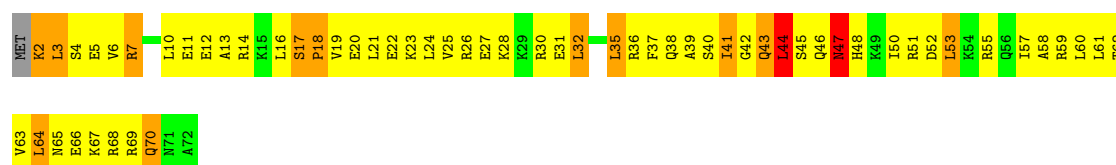
• Molecule 27: 50S RIBOSOMAL PROTEIN L29

Chain B2: 



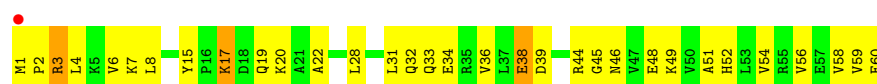
• Molecule 27: 50S RIBOSOMAL PROTEIN L29

Chain D2: 



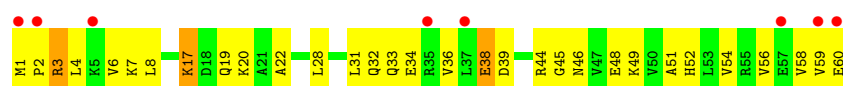
• Molecule 28: 50S RIBOSOMAL PROTEIN L30

Chain B3: 



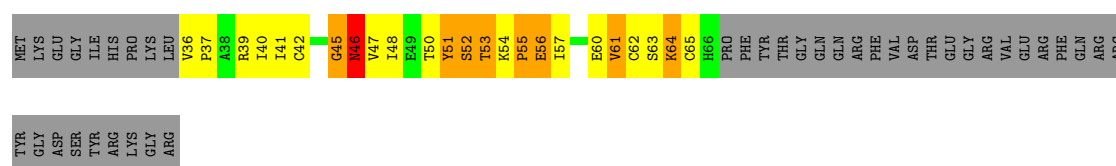
• Molecule 28: 50S RIBOSOMAL PROTEIN L30

Chain D3: 



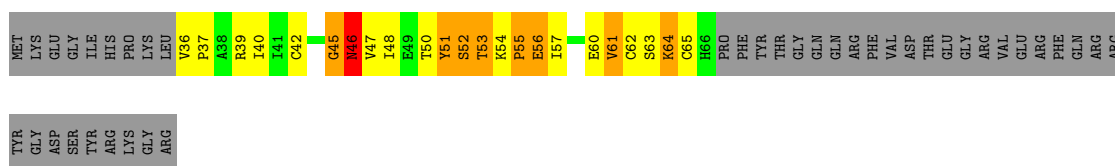
• Molecule 29: 50S RIBOSOMAL PROTEIN L31

Chain B4: 



• Molecule 29: 50S RIBOSOMAL PROTEIN L31

Chain D4: 



- Molecule 30: 50S RIBOSOMAL PROTEIN L32

Chain B5:

- Molecule 30: 50S RIBOSOMAL PROTEIN L32

Chain D5:

- Molecule 31: 50S RIBOSOMAL PROTEIN L33

Chain B6:

- Molecule 31: 50S RIBOSOMAL PROTEIN L33

Chain D6:

- Molecule 32: 50S RIBOSOMAL PROTEIN L34

Chain B7:

- Molecule 32: 50S RIBOSOMAL PROTEIN L34

Chain D7:

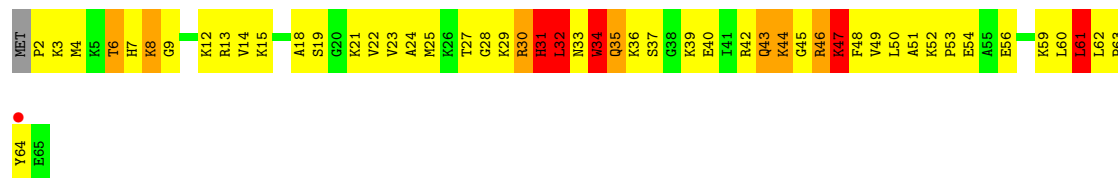
- Molecule 33: 50S RIBOSOMAL PROTEIN L35

Chain B8:



• Molecule 33: 50S RIBOSOMAL PROTEIN L35

Chain D8:



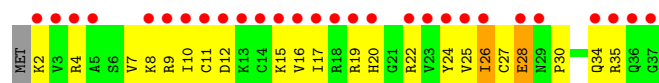
• Molecule 34: 50S RIBOSOMAL PROTEIN L36

Chain B9:



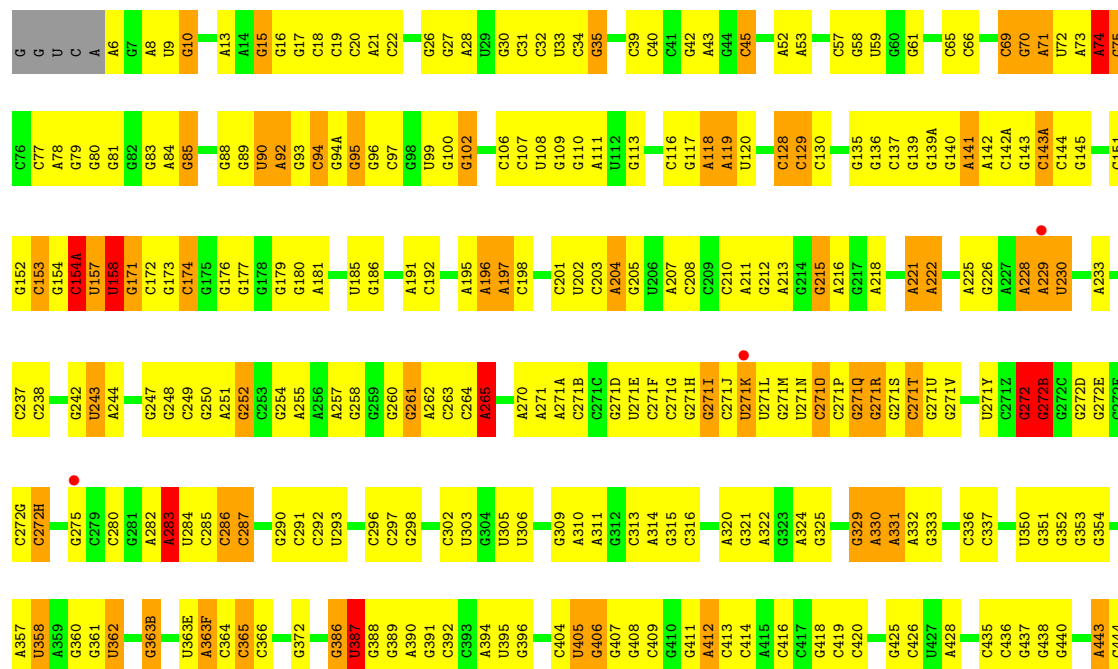
• Molecule 34: 50S RIBOSOMAL PROTEIN L36

Chain D9:



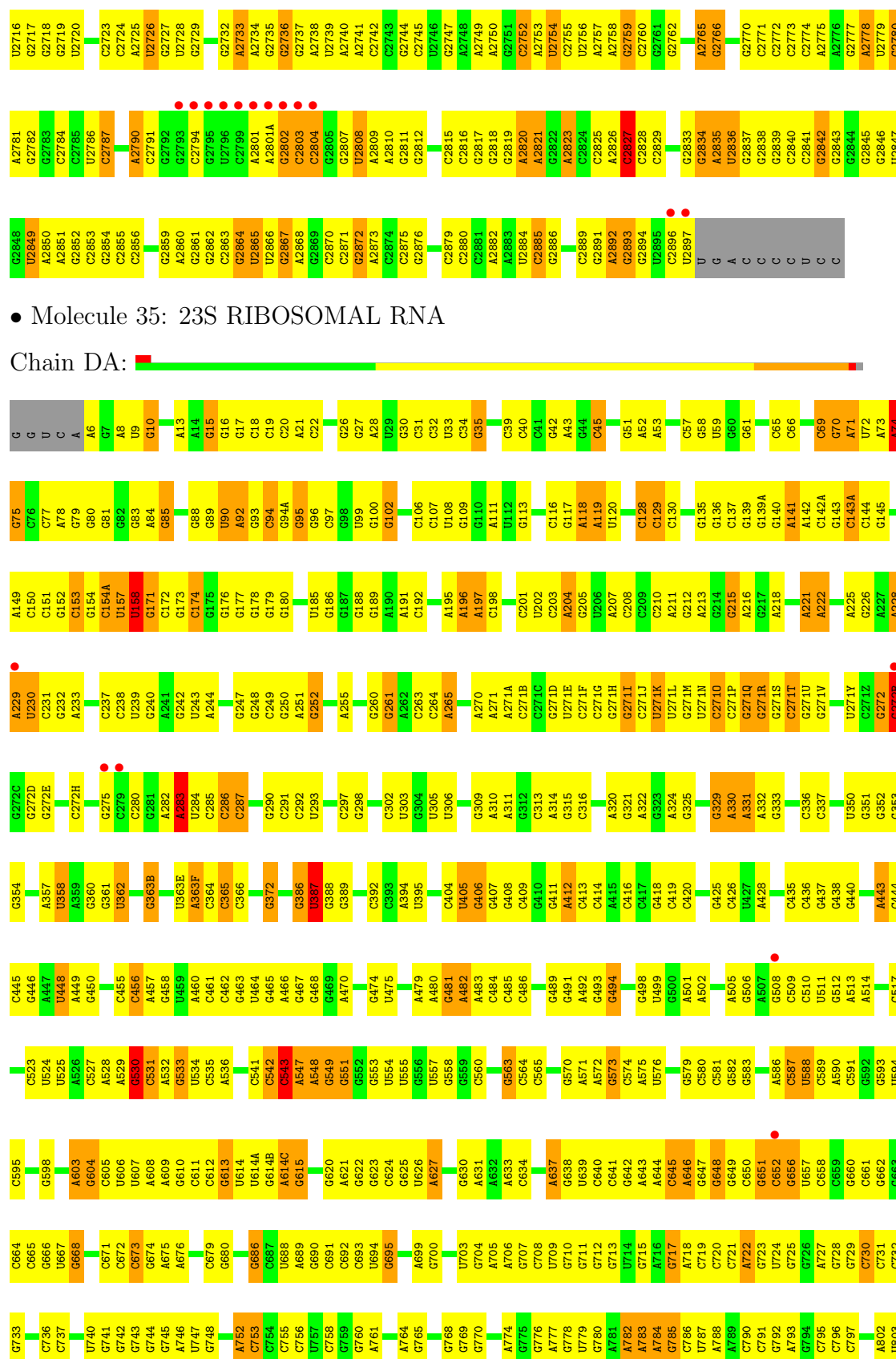
• Molecule 35: 23S RIBOSOMAL RNA

Chain BA:



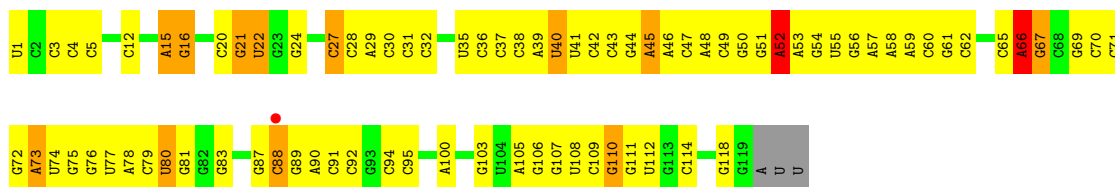


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G2645	C2567	C2499	G2350	U2203	C2143	G2070	U1993	A1919	C1844	G1776	G1687	A1608
G2646	C2568	G2351	G2283	C2205	U2144	A2071	G1994	C1920	G1845	U1777	U1688	A1609
U2647	G2569	G2352	C2285	G2206	C2145	G2072	C1996	G1921	A1846	U1778	A1689	A1610
G2648	G2570	G2353	A2286	G2207	G2146	G2073	G1997	G1922	A1847	U1779	A1690	C1611
U2649	C2571	G2354	A2287	A2208	G2147	C2073	G1998	U1923	A1848	A1780	C1691	G1612
C2652	A2572	U2506	A2288	U2218	G2148	A2082	C1999	C1924	U1851	C1781	U1692	G1613
	C2573	G2507	G2289	G2220	G2149	G2083	G2000	C1925	C1852	G1782	G1696	A1614
A2657	G2578	C2507	G2358	G2221	G2150	G2084	G2001	U1926	A1853	A1783	G1697	A1615
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A2662	G2581	G2513	G2366	G2225	G2153	G2088	U2011	G1929	A1856	A1786	G1699	C1618
G2663	G2582	U2514	A2298	C2226	G2154	U2089	G2012	G1930	G1856	A1787	A1700	A1619
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G2672	C2591	G2521	A2305	G2234	C2161	U2099	A2019	A1937	A1863	U1796	U1713	A1641
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G2686		U2531	C2314	U2243	A2170	G2110	A2031	U1955	A1881	C1881	A1741	A1656
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	C2610	C2538	A2320	U2249	C2177	G2116	G2037	U1964	A1887	A1813	G1748	C1662
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U2696	U2615	G2544	G2325	G2253	G2181	G2123	C2043	A1970	G1896	U1817	C1754	G1666
G2697	C2616		C2326	U2257	C2182	G2124	A2051	A1971	A1897	U1818	A1755	G1667
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U2702	G2619	G2550	G2329	C2260	C2185	G2127	G2054	C1974	A1902	G1824	G1758	U1671
C2703	C2620	C2551	G2330	C2261	G2186	G2128	G2055	A1975	C1902	A1825		
G2704	G2625	U2552	G2331	U2262	C2187	C2129	C2056	G1976	G1903	G1826		
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G2706		U2554	A2333	A2267	G2189	U2131	A2058	G1980	G1906	U1828	G1763	C1675
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C2710	A2632	U2558	G2337	G2271	G2193	G2135	A2062	G1984	C1910	U1834	C1767	U1679
A2711	G2633	G2559	G2338	U2272	C2194	A2136	C2063	G1985	G1911	U1835	U1768	
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A2714	U2636	U2562	G2345		A2198	G2139	C2066	C1988	C1914		G1772	G1682
G2715		A2564	A2346	G2279	A2199	C2140	G1989	G1990	U1915		A1773	
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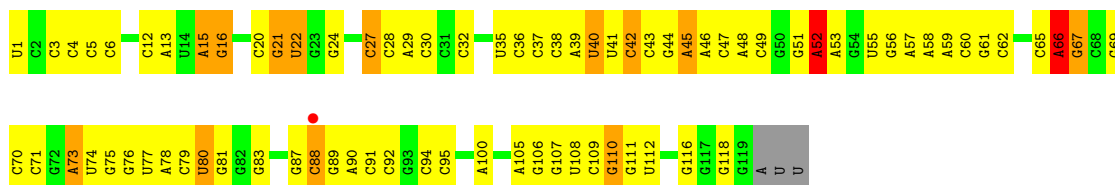
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C1909	G1764	G1765	G1674	C1509A	G1441	C1364	U1291	A1220	C1150	A1032	A957		C806
G1910	G1765	G1765	G1675	A1509B	G1442	A1365	U1292	C1221	C1151	U1033	G958	G882	U807
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A1912	G1837	U1768	A1677	C1511	A1445	G1369	C1295	G1223	C1153	U1035	G961	G885	G808
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C1914	G1839	C1771	U1679	U1518	C1446	A1373	G1299	G1227	A1155	G1037	U963	G887	U811
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G1935	G1860	C1790	C1549	C1549	A1469	C1403	G1328	G1252	A1175	G1108		A911	C840
A1937	G1861	U1629	C1550	C1550	G1470	A1404	U1329	C1253	G1176	C1109			
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C1958	G1883	U1722	G1651	A1569	A1486	G1418	U1341	A1265	C1190	G1126	C999	C925	G855
G1959	A1884	U1739	A1653	A1570	G1487	G1419		G1266	G1191	A1126	A1000	A926	C856
	C1885	G1740	G1653	A1571	G1488	U1420	G1344	U1267	C1192	A1127	A1001		C857
A1960	C1886	A1741	A1654	A1572	U1489	G1421	C1345	A1268	C1193	A1128	G1002	G932	U858
C1961	C1887	G1742	A1655	C1573	A1490	G1424	G1346	A1269	G1194		G1003		G859
U1963	A1889	C1743	G1656	C1574	G1491	G1425	G1347	C1270	G1195	G1131		A941	U860
G1964	A1890	C1744	C1657	U1578	C1493	G1426	A1349	A1271	C1201	U1133		G942	A861
		G1747	U1659	A1579	A1494	A1427	C1350	A1272	G1203	C1136		U943	G862
	G1896	G1747A	C1660	A1580	A1495	C1428	C1351		A1204	G1137		G944	A863
G1967	G1968	G1748	C1661	G1581	A1496	G1429	U1352	A1275	G1205	G1138	U1019	A945	C865
A1969	U1898		C1662	C1582	U1497	C1430	A1353	A1278	A1206	G1139	A1020	G946	A866
A1970	G1899		C1663	A1583	C1498	U1431	A1354	G1279	U1205	G1140	A1021	G947	
A1972	A1900	G1824	A1664	C1584			G1355	G1280	G1208	C1141	G1022	C949	G869
A1973	C1902	C1752	A1665	A1586	C1501	A1434	G1356	G1281	G1209	U1141	G1023	G950	
	G1903	G1753	G1666	A1587	C1502	G1435	U1357		A1210	U1142	G1024	C951	
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		G1756	A1668	C1589	C1504	C1437	A1359	A1287	G1212		U1026	A953	G875
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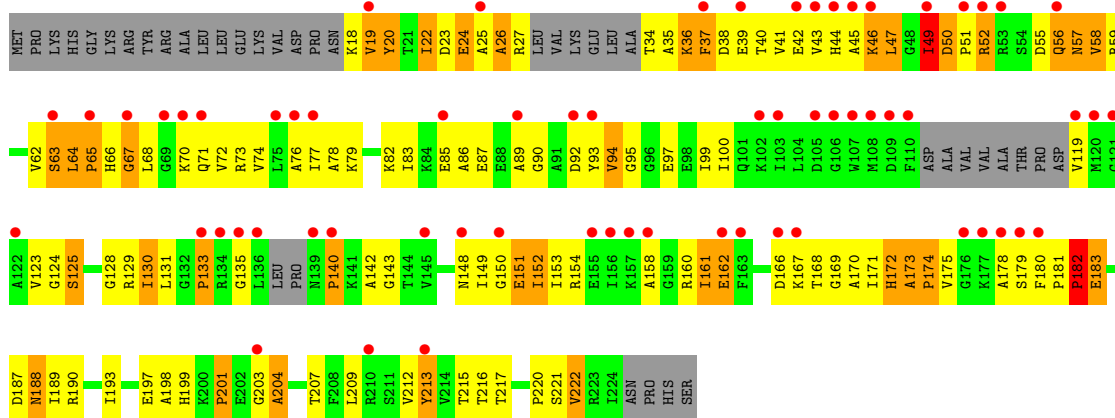
• Molecule 36: 5S RIBOSOMAL RNA

Chain DB:



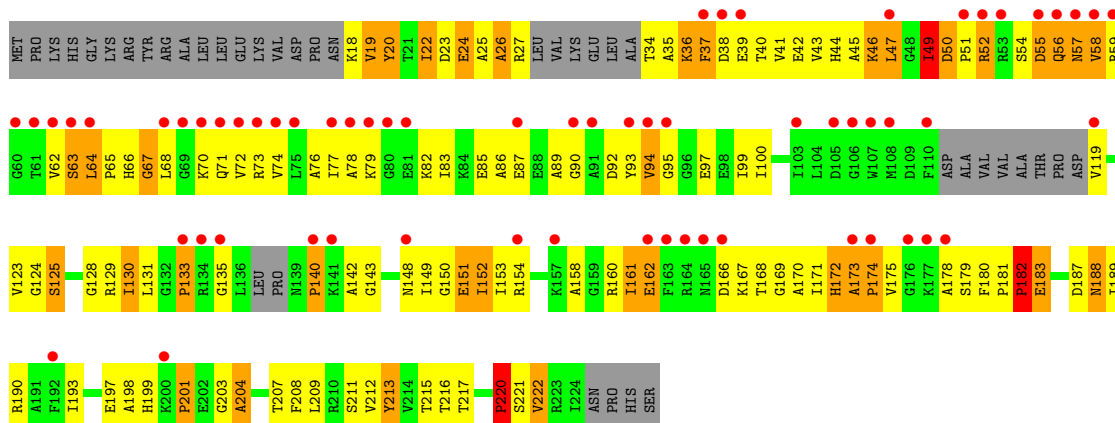
• Molecule 37: 50S RIBOSOMAL PROTEIN L1

Chain BC:



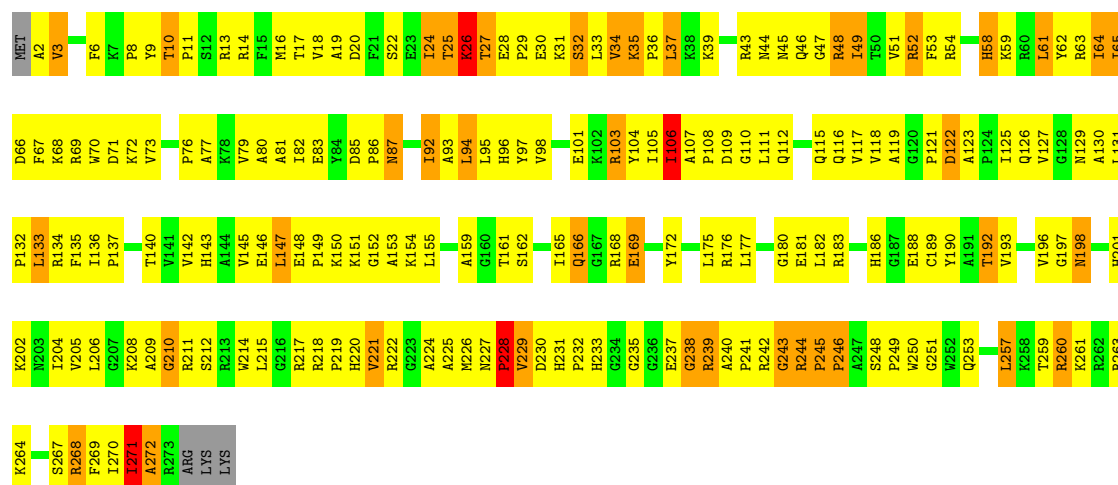
• Molecule 37: 50S RIBOSOMAL PROTEIN L1

Chain DC:



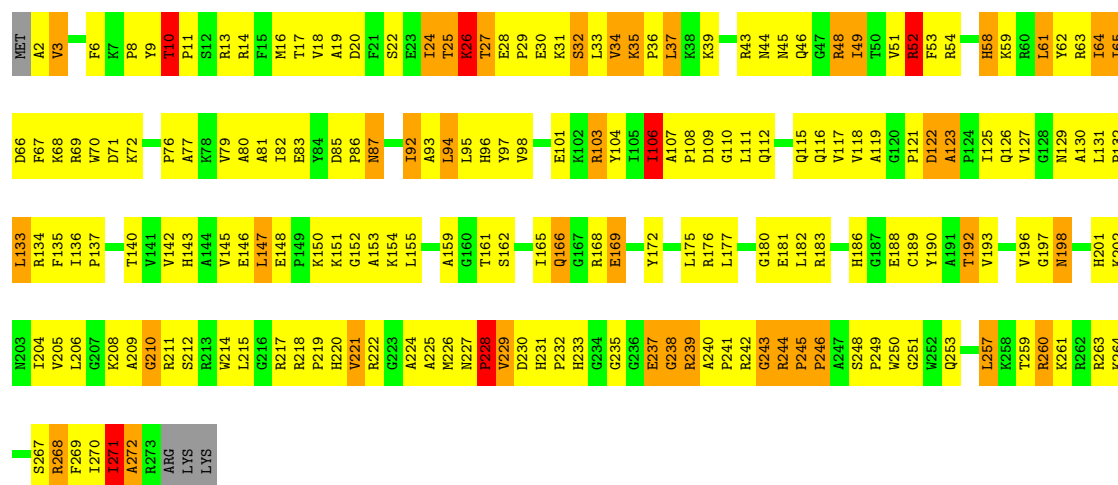
• Molecule 38: 50S RIBOSOMAL PROTEIN L2

Chain BD:



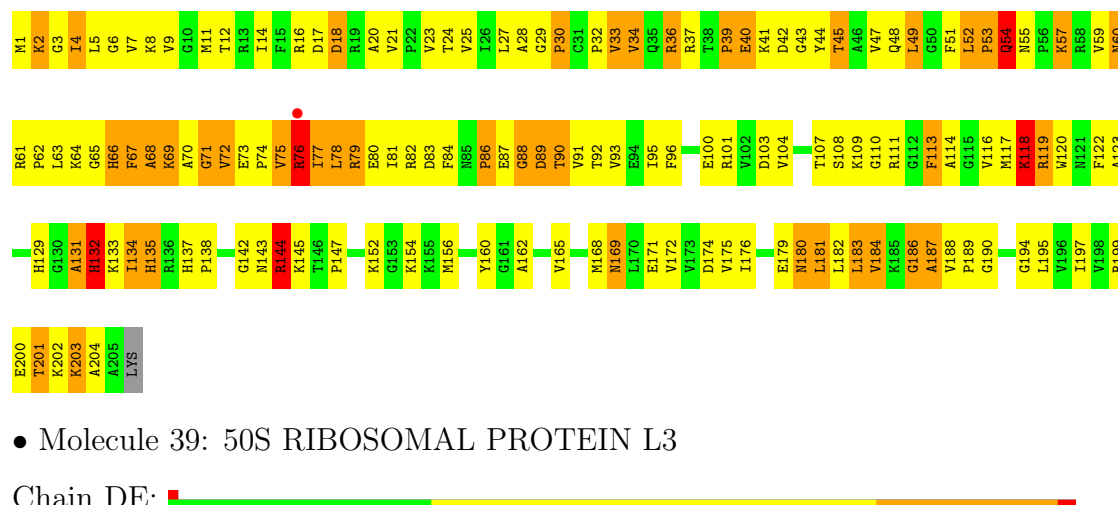
• Molecule 38: 50S RIBOSOMAL PROTEIN L2

Chain DD:



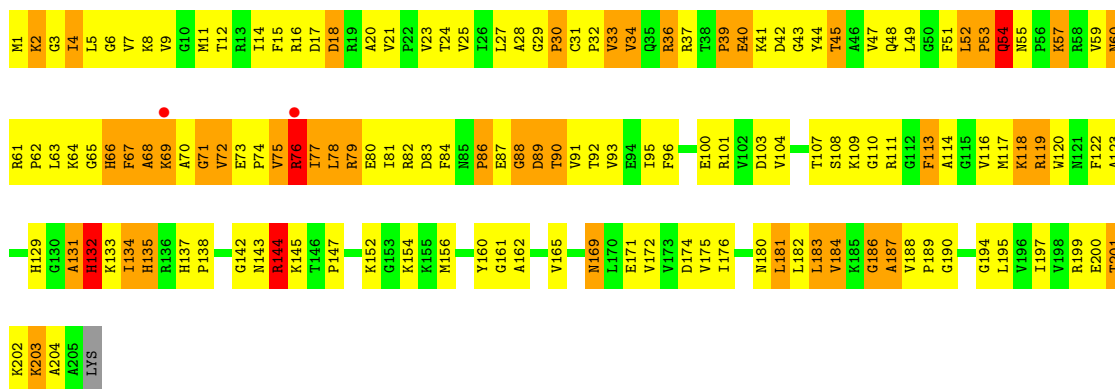
• Molecule 39: 50S RIBOSOMAL PROTEIN L3

Chain BE:



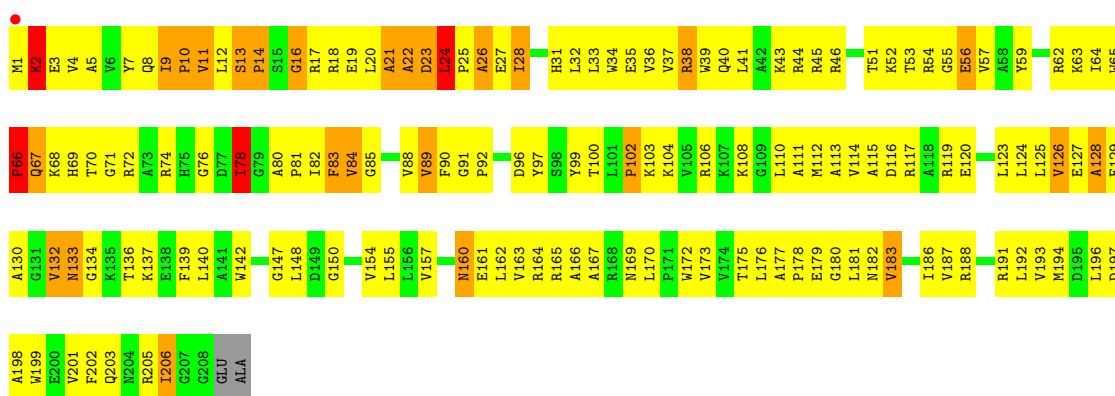
• Molecule 39: 50S RIBOSOMAL PROTEIN L3

Chain DE:



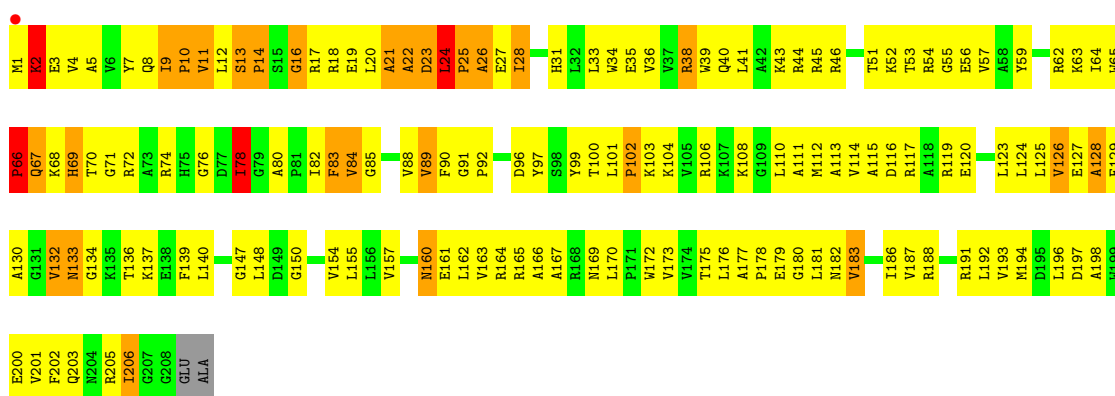
• Molecule 40: 50S RIBOSOMAL PROTEIN L4

Chain BF:



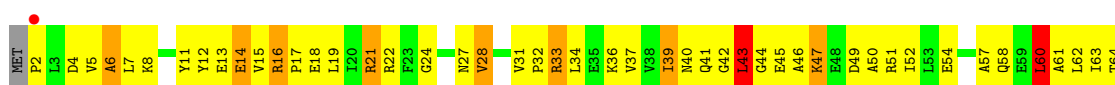
• Molecule 40: 50S RIBOSOMAL PROTEIN L4

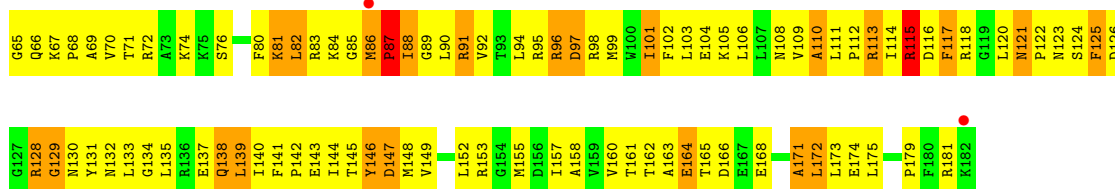
Chain DF:



• Molecule 41: 50S RIBOSOMAL PROTEIN L5

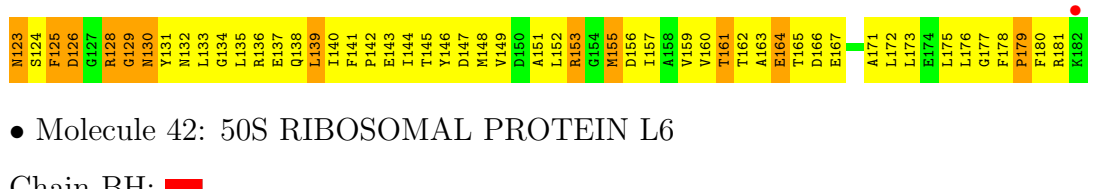
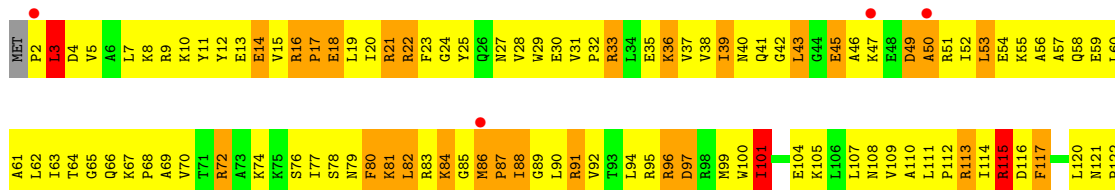
Chain BG:





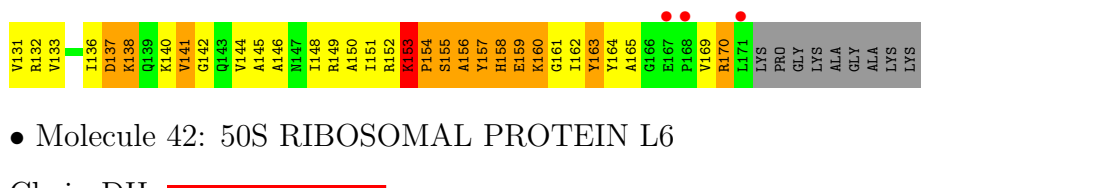
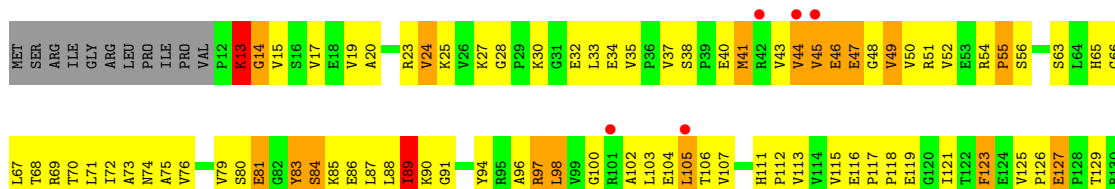
• Molecule 41: 50S RIBOSOMAL PROTEIN L5

Chain DG:



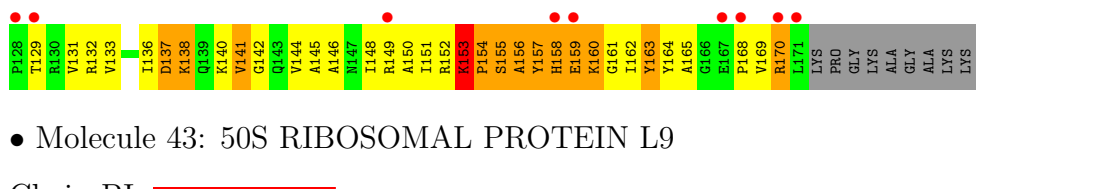
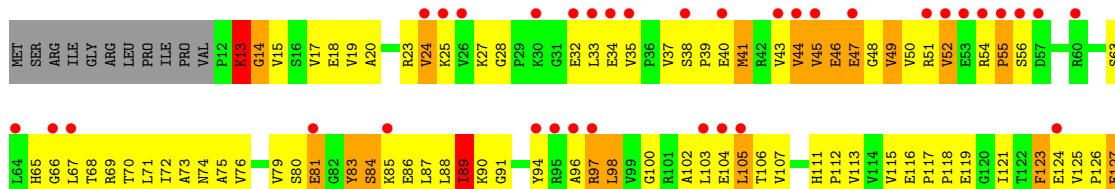
• Molecule 42: 50S RIBOSOMAL PROTEIN L6

Chain BH:



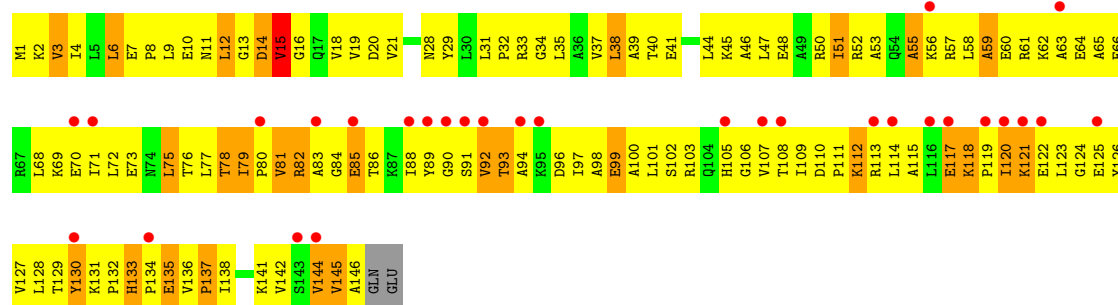
• Molecule 42: 50S RIBOSOMAL PROTEIN L6

Chain DH:



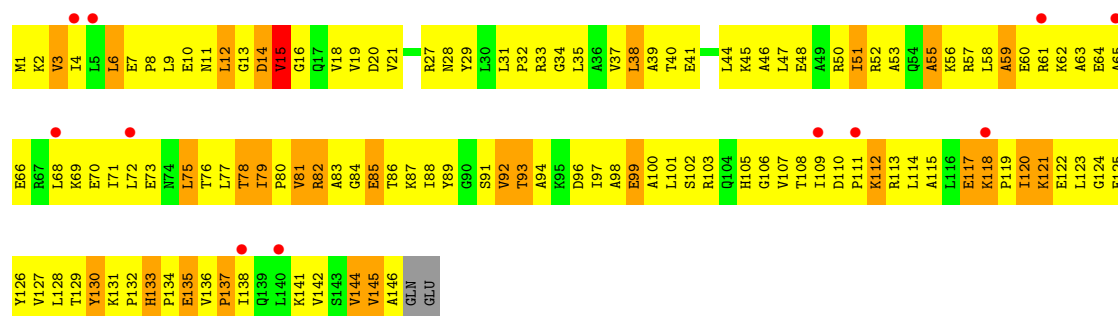
• Molecule 43: 50S RIBOSOMAL PROTEIN L9

Chain BI:



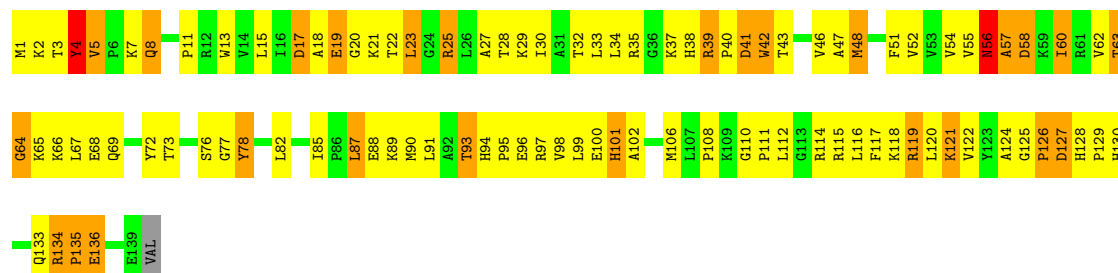
• Molecule 43: 50S RIBOSOMAL PROTEIN L9

Chain DI:



• Molecule 44: 50S RIBOSOMAL PROTEIN L13

Chain BN:



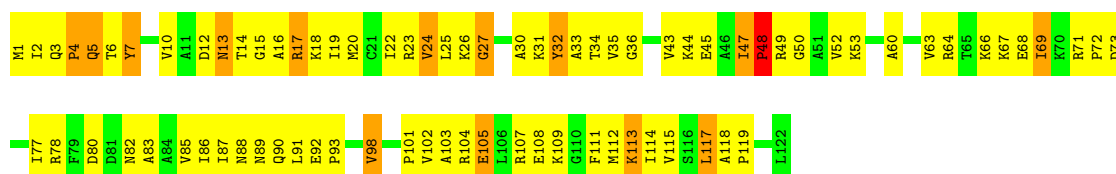
• Molecule 44: 50S RIBOSOMAL PROTEIN L13

Chain DN:



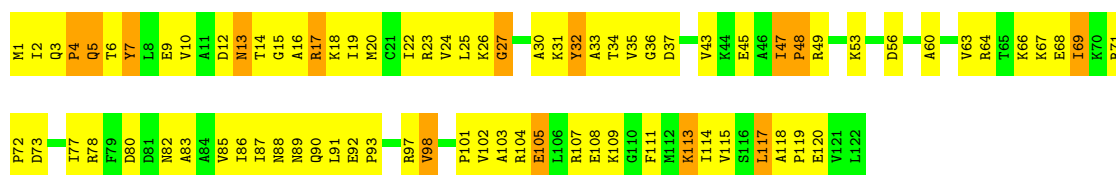
• Molecule 45: 50S RIBOSOMAL PROTEIN L14

Chain BO:



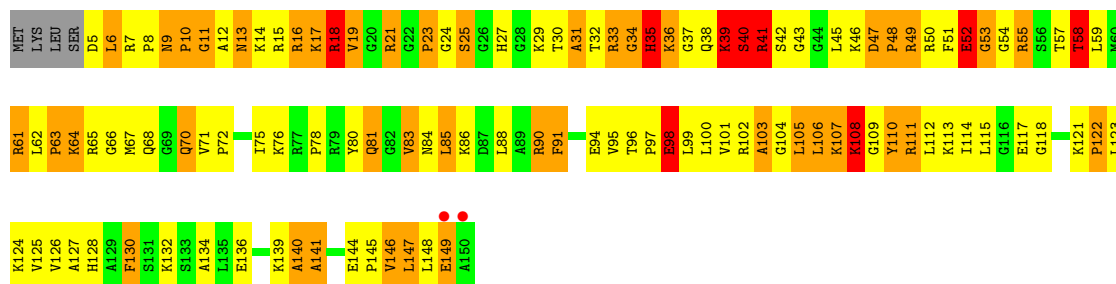
• Molecule 45: 50S RIBOSOMAL PROTEIN L14

Chain DO:



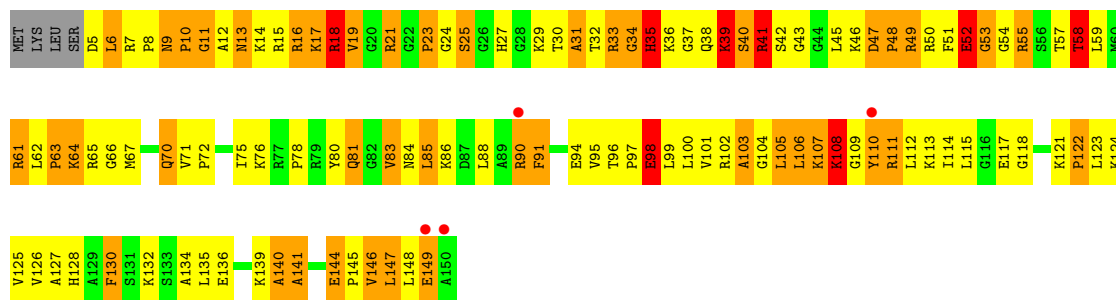
• Molecule 46: 50S RIBOSOMAL PROTEIN L15

Chain BP:



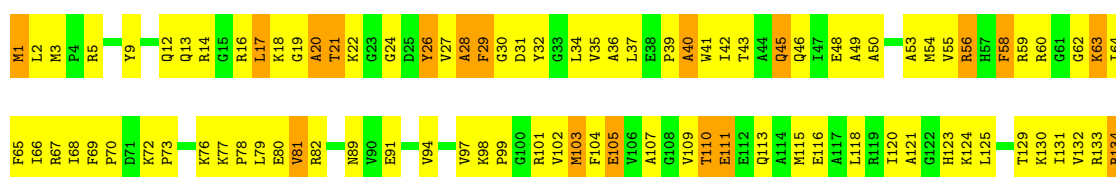
• Molecule 46: 50S RIBOSOMAL PROTEIN L15

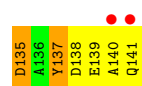
Chain DP:



• Molecule 47: 50S RIBOSOMAL PROTEIN L16

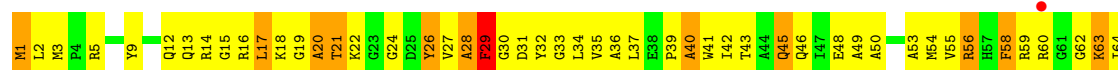
Chain BQ:





• Molecule 47: 50S RIBOSOMAL PROTEIN L16

Chain DQ:



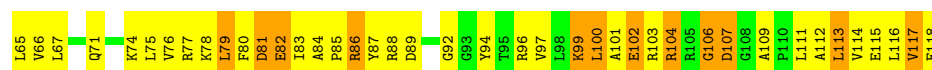
• Molecule 48: 50S RIBOSOMAL PROTEIN L17

Chain BR:



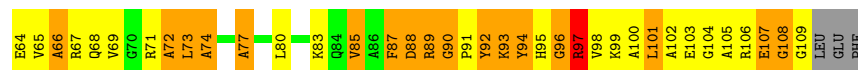
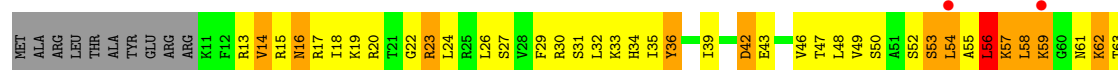
• Molecule 48: 50S RIBOSOMAL PROTEIN L17

Chain DR:



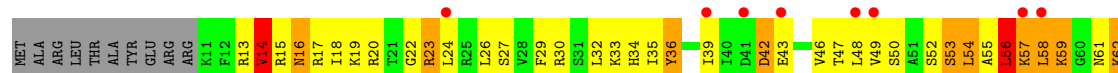
• Molecule 49: 50S RIBOSOMAL PROTEIN L18

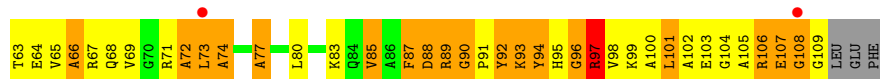
Chain BS:



• Molecule 49: 50S RIBOSOMAL PROTEIN L18

Chain DS:





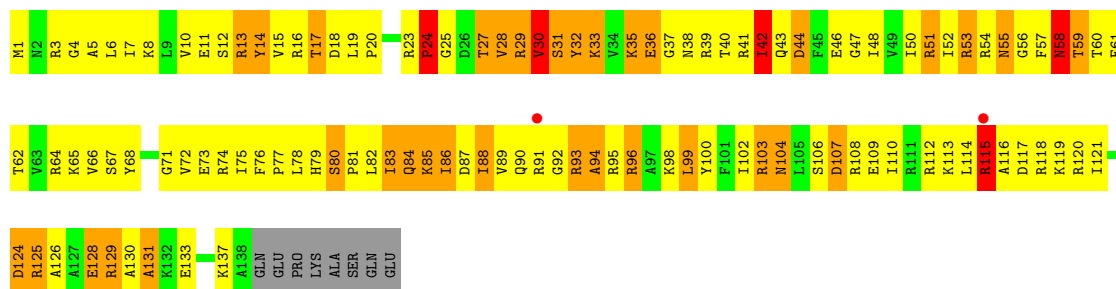
• Molecule 50: 50S RIBOSOMAL PROTEIN L19

Chain BT:



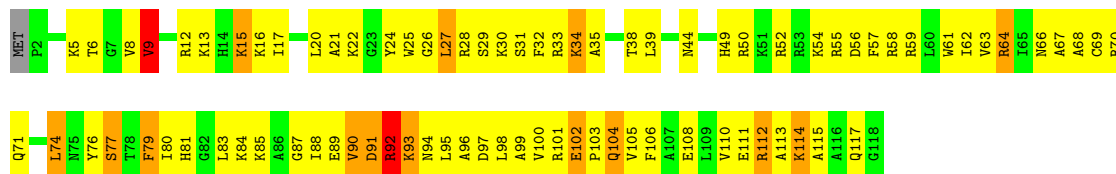
• Molecule 50: 50S RIBOSOMAL PROTEIN L19

Chain DT:



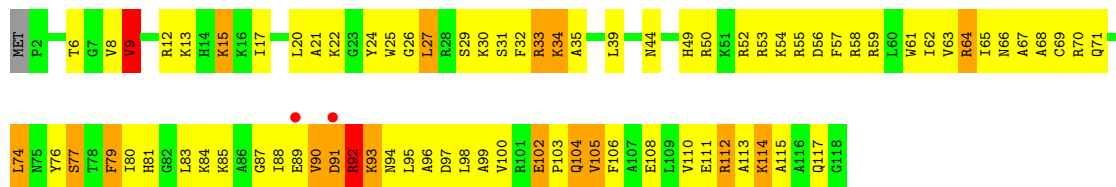
• Molecule 51: 50S RIBOSOMAL PROTEIN L20

Chain BU:



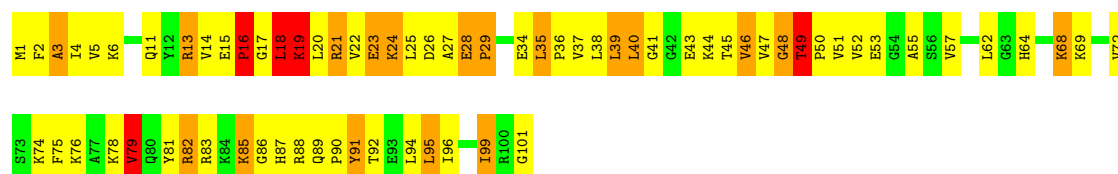
• Molecule 51: 50S RIBOSOMAL PROTEIN L20

Chain DU:



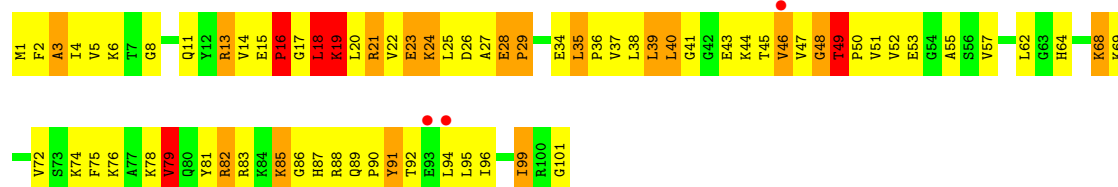
• Molecule 52: 50S RIBOSOMAL PROTEIN L21

Chain BV:



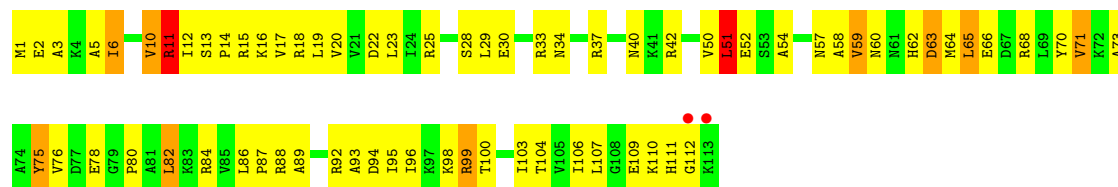
• Molecule 52: 50S RIBOSOMAL PROTEIN L21

Chain DV:



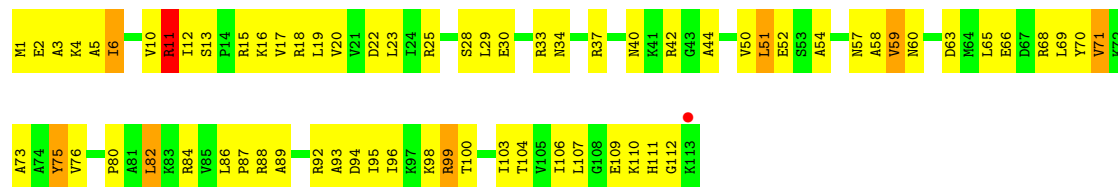
• Molecule 53: 50S RIBOSOMAL PROTEIN L22

Chain BW:



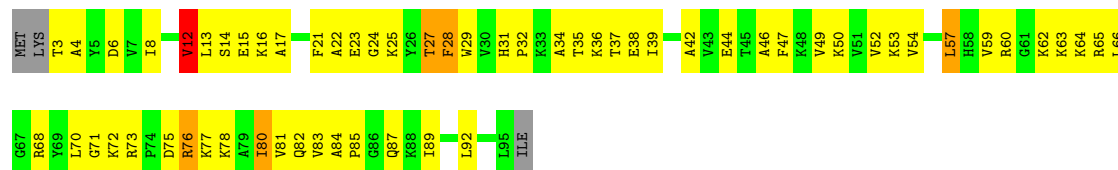
• Molecule 53: 50S RIBOSOMAL PROTEIN L22

Chain DW:



• Molecule 54: 50S RIBOSOMAL PROTEIN L23

Chain BX:



• Molecule 54: 50S RIBOSOMAL PROTEIN L23

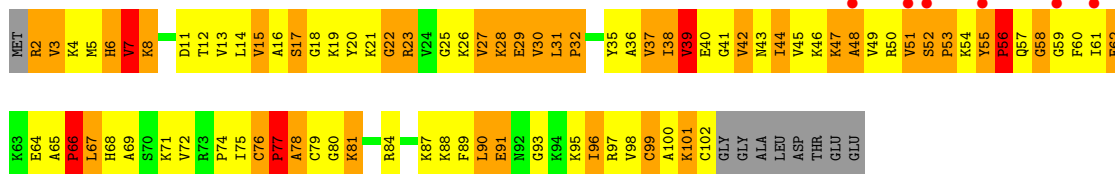
Chain DX:





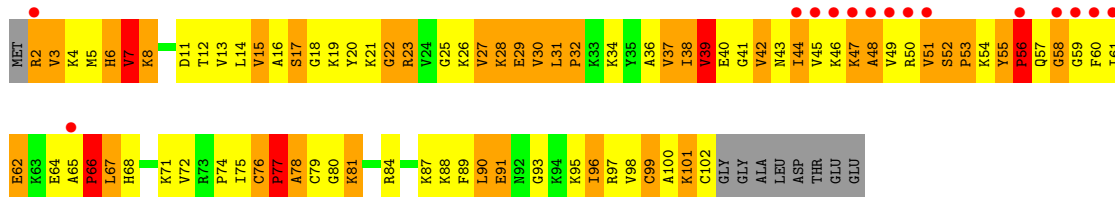
• Molecule 55: 50S RIBOSOMAL PROTEIN L24

Chain BY:



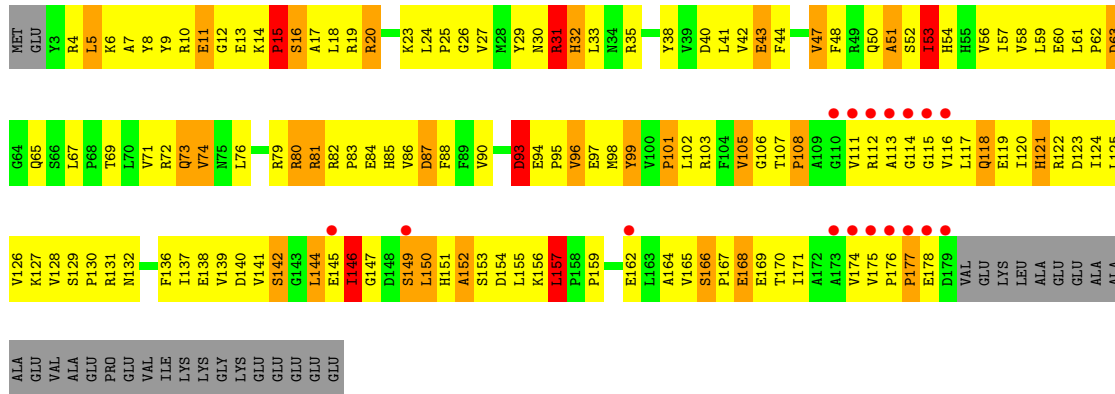
• Molecule 55: 50S RIBOSOMAL PROTEIN L24

Chain DY:



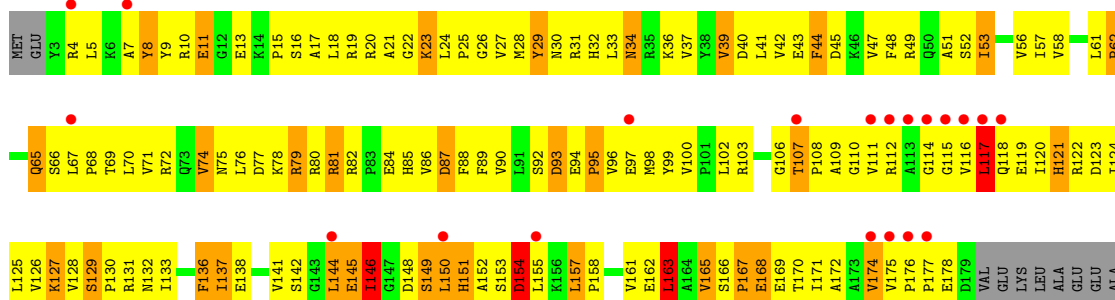
• Molecule 56: 50S RIBOSOMAL PROTEIN L25

Chain BZ:



• Molecule 56: 50S RIBOSOMAL PROTEIN L25

Chain DZ:



ALA
ALA
GLU
VAL
ALA
GLU
PRO
GLU
VAL
ILE
LYS
LYS
GLY
LYS
GLU
GLU
GLU
GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.86Å 450.46Å 628.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.50 49.74 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-3.50) 97.2 (49.74-3.40)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.40Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.208 , 0.256 0.217 , 0.262	Depositor DCC
R_{free} test set	36181 reflections (4.81%)	DCC
Wilson B-factor (Å ²)	83.7	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 56.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 789128 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	296042	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% 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: ZN, MG, PAR, 8AN, PHA

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	0.42	0/36190	0.70	16/56486 (0.0%)
1	CA	0.40	0/36190	0.69	14/56486 (0.0%)
2	AB	0.33	0/1936	0.60	0/2611
2	CB	0.32	0/1936	0.60	0/2611
3	AC	0.34	0/1637	0.60	0/2207
3	CC	0.33	0/1637	0.59	0/2207
4	AD	0.36	0/1733	0.64	0/2318
4	CD	0.36	0/1733	0.64	0/2318
5	AE	0.36	0/1163	0.64	0/1566
5	CE	0.35	0/1163	0.64	0/1566
6	AF	0.36	0/856	0.66	0/1154
6	CF	0.35	0/856	0.66	0/1154
7	AG	0.32	0/1276	0.57	0/1709
7	CG	0.31	0/1276	0.57	0/1709
8	AH	0.31	0/1136	0.63	0/1527
8	CH	0.30	0/1136	0.62	0/1527
9	AI	0.32	0/1027	0.59	0/1372
9	CI	0.32	0/1027	0.59	0/1372
10	AJ	0.36	0/808	0.66	0/1087
10	CJ	0.35	0/808	0.64	0/1087
11	AK	0.35	0/900	0.62	0/1213
11	CK	0.33	0/900	0.61	0/1213
12	AL	0.39	0/987	0.70	0/1322
12	CL	0.37	0/987	0.68	0/1322
13	AM	0.34	0/996	0.66	0/1329
13	CM	0.33	0/996	0.66	0/1329
14	AN	0.36	0/501	0.62	0/664
14	CN	0.33	0/501	0.61	0/664
15	AO	0.35	0/745	0.59	0/992
15	CO	0.33	0/745	0.58	0/992
16	AP	0.37	0/717	0.63	0/965
16	CP	0.37	0/717	0.63	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.36	0/837	0.61	0/1119
17	CQ	0.37	0/837	0.62	0/1119
18	AR	0.36	0/579	0.60	0/768
18	CR	0.36	0/579	0.60	0/768
19	AS	0.38	0/643	0.63	0/867
19	CS	0.36	0/643	0.62	0/867
20	AT	0.30	0/765	0.59	0/1007
20	CT	0.30	0/765	0.58	0/1007
21	AU	0.46	0/213	0.61	0/279
21	CU	0.45	0/213	0.60	0/279
22	AV	0.44	0/1784	0.75	0/2780
22	AY	0.47	0/1784	0.74	0/2780
22	CV	0.40	0/1784	0.71	0/2780
22	CY	0.41	0/1784	0.73	0/2780
23	AW	0.43	0/1809	0.71	0/2819
23	CW	0.42	0/1809	0.71	0/2819
24	AX	0.48	0/253	0.72	0/391
24	CX	0.42	0/253	0.73	1/391 (0.3%)
25	B0	0.44	0/671	0.71	0/892
25	D0	0.41	0/671	0.69	0/892
26	B1	0.48	0/739	0.85	0/983
26	D1	0.46	0/739	0.72	0/983
27	B2	0.43	0/600	0.73	0/793
27	D2	0.39	0/600	0.65	0/793
28	B3	0.43	0/473	0.68	0/636
28	D3	0.37	0/473	0.64	0/636
29	B4	0.46	0/229	0.68	0/311
29	D4	0.44	0/229	0.67	0/311
30	B5	0.62	0/473	0.96	0/639
30	D5	0.49	0/473	0.92	0/639
31	B6	0.57	0/387	0.76	0/517
31	D6	0.51	0/387	0.75	0/517
32	B7	0.52	0/427	0.67	0/563
32	D7	0.48	0/427	0.65	0/563
33	B8	0.59	0/516	0.89	2/681 (0.3%)
33	D8	0.51	0/516	0.88	2/681 (0.3%)
34	B9	0.33	0/302	0.54	0/397
34	D9	0.29	0/302	0.53	0/397
35	BA	0.59	5/67716 (0.0%)	0.76	38/105718 (0.0%)
35	DA	0.48	4/67716 (0.0%)	0.74	31/105718 (0.0%)
36	BB	0.50	0/2853	0.75	1/4451 (0.0%)
36	DB	0.42	0/2853	0.74	1/4451 (0.0%)
37	BC	0.37	0/1143	0.68	5/1552 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DC	0.37	0/1145	0.69	6/1556 (0.4%)
38	BD	0.51	0/2155	0.80	1/2907 (0.0%)
38	DD	0.47	0/2155	0.79	1/2907 (0.0%)
39	BE	0.47	0/1597	0.80	1/2155 (0.0%)
39	DE	0.41	0/1597	0.77	0/2155
40	BF	0.46	0/1659	0.71	0/2246
40	DF	0.42	0/1659	0.69	0/2246
41	BG	0.40	0/1498	0.77	2/2013 (0.1%)
41	DG	0.38	0/1498	0.71	1/2013 (0.0%)
42	BH	0.44	0/1246	0.77	0/1684
42	DH	0.37	0/1246	0.74	0/1684
43	BI	0.36	0/1147	0.65	0/1553
43	DI	0.35	0/1147	0.63	0/1553
44	BN	0.45	0/1132	0.75	0/1527
44	DN	0.38	0/1132	0.72	0/1527
45	BO	0.44	0/943	0.68	0/1269
45	DO	0.37	0/943	0.67	0/1269
46	BP	0.51	0/1131	1.01	5/1504 (0.3%)
46	DP	0.45	0/1131	0.98	5/1504 (0.3%)
47	BQ	0.45	0/1143	0.69	0/1527
47	DQ	0.40	0/1143	0.67	0/1527
48	BR	0.44	0/974	0.79	2/1302 (0.2%)
48	DR	0.39	0/974	0.76	1/1302 (0.1%)
49	BS	0.48	0/779	0.83	1/1038 (0.1%)
49	DS	0.42	0/779	0.79	2/1038 (0.2%)
50	BT	0.44	0/1156	0.79	1/1544 (0.1%)
50	DT	0.41	0/1156	0.78	1/1544 (0.1%)
51	BU	0.52	0/975	0.79	2/1297 (0.2%)
51	DU	0.42	0/975	0.74	2/1297 (0.2%)
52	BV	0.46	0/790	0.77	1/1057 (0.1%)
52	DV	0.38	0/790	0.74	1/1057 (0.1%)
53	BW	0.49	0/907	0.78	1/1216 (0.1%)
53	DW	0.42	0/907	0.75	0/1216
54	BX	0.48	0/740	0.73	1/995 (0.1%)
54	DX	0.44	0/740	0.71	1/995 (0.1%)
55	BY	0.56	0/789	0.85	0/1053
55	DY	0.49	0/789	0.83	0/1053
56	BZ	0.42	0/1436	0.72	0/1951
56	DZ	0.36	0/1436	0.65	0/1951
All	All	0.47	9/320004 (0.0%)	0.72	150/478610 (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	0	10
1	CA	0	8
23	AW	0	2
35	BA	4	39
35	DA	3	33
36	BB	0	3
36	DB	0	3
All	All	7	98

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BA	652	C	C3'-O3'	8.01	1.53	1.42
35	DA	652	C	C3'-O3'	7.44	1.52	1.42
35	BA	652	C	O3'-P	6.31	1.68	1.61
35	DA	652	C	O3'-P	5.91	1.68	1.61
35	BA	652	C	O5'-C5'	5.67	1.53	1.44

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	BP	52	GLU	N-CA-C	9.63	137.00	111.00
46	DP	52	GLU	N-CA-C	9.54	136.76	111.00
35	BA	283	A	C2'-C3'-O3'	9.40	130.18	109.50
35	BA	1799	G	C2'-C3'-O3'	9.35	130.07	109.50
35	DA	1799	G	C2'-C3'-O3'	9.28	129.91	109.50

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	BA	283	A	C3'
35	BA	1378	A	C3'
35	BA	1799	G	C3'
35	BA	1819	A	C3'
35	DA	283	A	C3'

5 of 98 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	21	G	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	484	G	Sidechain
1	AA	760	G	Sidechain
1	AA	832	C	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	16315	1281	0
1	CA	32329	0	16312	1277	0
2	AB	1901	0	1951	273	0
2	CB	1901	0	1951	273	0
3	AC	1613	0	1677	245	0
3	CC	1613	0	1677	250	0
4	AD	1703	0	1762	166	0
4	CD	1703	0	1763	166	0
5	AE	1147	0	1207	137	0
5	CE	1147	0	1207	134	0
6	AF	843	0	857	97	0
6	CF	843	0	857	91	0
7	AG	1257	0	1296	117	0
7	CG	1257	0	1296	113	0
8	AH	1116	0	1177	127	0
8	CH	1116	0	1177	127	0
9	AI	1011	0	1041	170	0
9	CI	1011	0	1041	167	0
10	AJ	795	0	840	175	0
10	CJ	795	0	840	177	0
11	AK	885	0	904	103	0
11	CK	885	0	904	98	0
12	AL	971	0	1057	130	0
12	CL	971	0	1057	126	0
13	AM	988	0	1056	173	0
13	CM	988	0	1056	168	0
14	AN	492	0	529	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	CN	492	0	529	75	0
15	AO	734	0	771	74	0
15	CO	734	0	771	77	0
16	AP	701	0	720	82	0
16	CP	701	0	720	78	0
17	AQ	824	0	891	92	0
17	CQ	824	0	891	88	0
18	AR	574	0	644	82	0
18	CR	574	0	644	86	0
19	AS	630	0	652	105	0
19	CS	630	0	652	96	0
20	AT	763	0	861	102	0
20	CT	763	0	861	102	0
21	AU	209	0	221	17	0
21	CU	209	0	221	19	0
22	AV	1630	0	831	66	0
22	AY	1630	0	831	84	0
22	CV	1630	0	831	78	0
22	CY	1630	0	831	71	0
23	AW	1619	0	822	93	0
23	CW	1619	0	821	94	0
24	AX	227	0	119	7	0
24	CX	227	0	118	10	0
25	B0	662	0	688	81	0
25	D0	662	0	688	81	0
26	B1	732	0	808	95	0
26	D1	732	0	808	88	0
27	B2	598	0	653	59	0
27	D2	598	0	653	86	0
28	B3	468	0	523	31	0
28	D3	468	0	523	30	0
29	B4	226	0	229	43	0
29	D4	226	0	229	35	0
30	B5	459	0	480	86	0
30	D5	459	0	480	86	0
31	B6	381	0	390	106	0
31	D6	381	0	390	105	0
32	B7	419	0	467	30	0
32	D7	419	0	467	30	0
33	B8	508	0	576	100	0
33	D8	508	0	576	98	0
34	B9	299	0	325	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	D9	299	0	325	31	0
35	BA	60459	0	30474	2058	0
35	DA	60459	0	30478	2069	0
36	BB	2551	0	1294	105	0
36	DB	2551	0	1294	89	0
37	BC	1140	0	863	123	0
37	DC	1142	0	865	126	0
38	BD	2105	0	2182	327	0
38	DD	2105	0	2182	319	0
39	BE	1564	0	1629	245	0
39	DE	1564	0	1629	245	0
40	BF	1624	0	1677	211	0
40	DF	1624	0	1677	207	0
41	BG	1474	0	1534	253	0
41	DG	1474	0	1534	269	0
42	BH	1223	0	1282	173	0
42	DH	1223	0	1282	173	0
43	BI	1132	0	1218	196	0
43	DI	1132	0	1218	198	0
44	BN	1105	0	1180	138	0
44	DN	1105	0	1180	138	0
45	BO	933	0	996	121	0
45	DO	933	0	996	123	0
46	BP	1114	0	1187	280	0
46	DP	1114	0	1187	278	0
47	BQ	1122	0	1179	169	0
47	DQ	1122	0	1179	166	0
48	BR	960	0	1021	139	0
48	DR	960	0	1021	140	0
49	BS	771	0	832	152	0
49	DS	771	0	832	143	0
50	BT	1142	0	1202	241	0
50	DT	1142	0	1202	228	0
51	BU	958	0	1015	156	0
51	DU	958	0	1015	154	0
52	BV	779	0	852	159	0
52	DV	779	0	852	162	0
53	BW	896	0	953	90	0
53	DW	896	0	953	85	0
54	BX	726	0	778	87	0
54	DX	726	0	778	86	0
55	BY	776	0	870	184	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	DY	776	0	870	193	0
56	BZ	1404	0	1432	232	0
56	DZ	1404	0	1432	232	0
57	AA	198	0	0	0	0
57	AD	1	0	0	0	0
57	AE	1	0	0	0	0
57	AG	1	0	0	0	0
57	AI	1	0	0	0	0
57	AL	2	0	0	0	0
57	AN	1	0	0	0	0
57	AV	5	0	0	0	0
57	AW	8	0	0	0	0
57	AX	2	0	0	0	0
57	B0	1	0	0	0	0
57	B1	1	0	0	0	0
57	B2	2	0	0	0	0
57	B5	2	0	0	0	0
57	B7	1	0	0	0	0
57	BA	422	0	0	0	0
57	BB	14	0	0	0	0
57	BD	2	0	0	0	0
57	BE	1	0	0	0	0
57	BF	1	0	0	0	0
57	BN	1	0	0	0	0
57	BO	1	0	0	0	0
57	BU	1	0	0	1	0
57	BV	1	0	0	0	0
57	BX	2	0	0	0	0
57	CA	199	0	0	0	0
57	CE	1	0	0	0	0
57	CI	1	0	0	0	0
57	CL	1	0	0	0	0
57	CN	1	0	0	0	0
57	CV	5	0	0	0	0
57	CW	7	0	0	0	0
57	CX	3	0	0	0	0
57	D1	1	0	0	0	0
57	D2	3	0	0	0	0
57	D5	2	0	0	0	0
57	D7	2	0	0	0	0
57	DA	421	0	0	0	0
57	DB	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	DC	1	0	0	0	0
57	DD	2	0	0	0	0
57	DE	1	0	0	0	0
57	DF	2	0	0	0	0
57	DN	1	0	0	0	0
57	DO	1	0	0	0	0
57	DS	1	0	0	0	0
57	DV	1	0	0	0	0
57	DX	3	0	0	0	0
58	AA	42	0	45	2	0
58	CA	42	0	45	2	0
59	AD	1	0	0	0	0
59	AN	1	0	0	0	0
59	B9	1	0	0	0	0
59	CD	1	0	0	0	0
59	CN	1	0	0	0	0
59	D9	1	0	0	0	0
All	All	296042	0	199734	19173	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 39.

The worst 5 of 19173 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
54:BX:63:LYS:HE3	54:BX:72:LYS:HE3	1.23	1.21
56:DZ:53:ILE:HG23	56:DZ:71:VAL:HG23	1.21	1.18
46:DP:59:LEU:HA	46:DP:61:ARG:CZ	1.73	1.18
53:BW:1:MET:HE2	53:BW:2:GLU:H	1.06	1.17
35:BA:2334:G:H21	49:BS:18:ILE:HD11	1.09	1.17

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%)	138 (59%)	63 (27%)	32 (14%)	0	8
2	CB	233/256 (91%)	138 (59%)	62 (27%)	33 (14%)	0	7
3	AC	205/239 (86%)	130 (63%)	55 (27%)	20 (10%)	1	16
3	CC	205/239 (86%)	128 (62%)	56 (27%)	21 (10%)	1	14
4	AD	206/209 (99%)	149 (72%)	39 (19%)	18 (9%)	1	19
4	CD	206/209 (99%)	150 (73%)	38 (18%)	18 (9%)	1	19
5	AE	149/162 (92%)	115 (77%)	23 (15%)	11 (7%)	2	24
5	CE	149/162 (92%)	115 (77%)	22 (15%)	12 (8%)	1	21
6	AF	99/101 (98%)	78 (79%)	16 (16%)	5 (5%)	3	36
6	CF	99/101 (98%)	79 (80%)	15 (15%)	5 (5%)	3	36
7	AG	153/156 (98%)	111 (72%)	36 (24%)	6 (4%)	5	45
7	CG	153/156 (98%)	111 (72%)	36 (24%)	6 (4%)	5	45
8	AH	136/138 (99%)	107 (79%)	25 (18%)	4 (3%)	7	54
8	CH	136/138 (99%)	108 (79%)	24 (18%)	4 (3%)	7	54
9	AI	121/128 (94%)	85 (70%)	23 (19%)	13 (11%)	1	13
9	CI	121/128 (94%)	83 (69%)	26 (22%)	12 (10%)	1	15
10	AJ	97/105 (92%)	62 (64%)	25 (26%)	10 (10%)	1	14
10	CJ	97/105 (92%)	63 (65%)	24 (25%)	10 (10%)	1	14
11	AK	117/129 (91%)	86 (74%)	26 (22%)	5 (4%)	4	42
11	CK	117/129 (91%)	88 (75%)	24 (20%)	5 (4%)	4	42
12	AL	123/135 (91%)	82 (67%)	27 (22%)	14 (11%)	1	12
12	CL	123/135 (91%)	83 (68%)	26 (21%)	14 (11%)	1	12
13	AM	117/126 (93%)	67 (57%)	30 (26%)	20 (17%)	0	4
13	CM	117/126 (93%)	67 (57%)	31 (26%)	19 (16%)	0	5
14	AN	58/61 (95%)	34 (59%)	16 (28%)	8 (14%)	0	8
14	CN	58/61 (95%)	34 (59%)	16 (28%)	8 (14%)	0	8
15	AO	86/89 (97%)	58 (67%)	20 (23%)	8 (9%)	1	18
15	CO	86/89 (97%)	57 (66%)	21 (24%)	8 (9%)	1	18
16	AP	82/88 (93%)	60 (73%)	20 (24%)	2 (2%)	9	59
16	CP	82/88 (93%)	59 (72%)	21 (26%)	2 (2%)	9	59
17	AQ	98/105 (93%)	74 (76%)	20 (20%)	4 (4%)	4	44
17	CQ	98/105 (93%)	76 (78%)	19 (19%)	3 (3%)	7	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AR	68/88 (77%)	41 (60%)	14 (21%)	13 (19%)	0	3
18	CR	68/88 (77%)	41 (60%)	13 (19%)	14 (21%)	0	2
19	AS	77/93 (83%)	49 (64%)	16 (21%)	12 (16%)	0	5
19	CS	77/93 (83%)	49 (64%)	15 (20%)	13 (17%)	0	4
20	AT	97/106 (92%)	69 (71%)	18 (19%)	10 (10%)	1	14
20	CT	97/106 (92%)	71 (73%)	16 (16%)	10 (10%)	1	14
21	AU	23/27 (85%)	13 (56%)	8 (35%)	2 (9%)	1	19
21	CU	23/27 (85%)	13 (56%)	8 (35%)	2 (9%)	1	19
25	B0	82/85 (96%)	65 (79%)	14 (17%)	3 (4%)	5	48
25	D0	82/85 (96%)	61 (74%)	17 (21%)	4 (5%)	3	37
26	B1	92/98 (94%)	65 (71%)	17 (18%)	10 (11%)	1	13
26	D1	92/98 (94%)	66 (72%)	18 (20%)	8 (9%)	1	19
27	B2	69/72 (96%)	43 (62%)	19 (28%)	7 (10%)	1	15
27	D2	69/72 (96%)	37 (54%)	23 (33%)	9 (13%)	0	10
28	B3	58/60 (97%)	48 (83%)	7 (12%)	3 (5%)	3	35
28	D3	58/60 (97%)	48 (83%)	7 (12%)	3 (5%)	3	35
29	B4	29/71 (41%)	16 (55%)	7 (24%)	6 (21%)	0	2
29	D4	29/71 (41%)	16 (55%)	7 (24%)	6 (21%)	0	2
30	B5	57/60 (95%)	38 (67%)	8 (14%)	11 (19%)	0	3
30	D5	57/60 (95%)	39 (68%)	6 (10%)	12 (21%)	0	2
31	B6	41/54 (76%)	17 (42%)	15 (37%)	9 (22%)	0	1
31	D6	41/54 (76%)	17 (42%)	15 (37%)	9 (22%)	0	1
32	B7	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
32	D7	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
33	B8	62/65 (95%)	44 (71%)	9 (14%)	9 (14%)	0	7
33	D8	62/65 (95%)	43 (69%)	10 (16%)	9 (14%)	0	7
34	B9	34/37 (92%)	29 (85%)	5 (15%)	0	100	100
34	D9	34/37 (92%)	29 (85%)	5 (15%)	0	100	100
37	BC	183/229 (80%)	81 (44%)	47 (26%)	55 (30%)	0	0
37	DC	183/229 (80%)	82 (45%)	47 (26%)	54 (30%)	0	0
38	BD	270/276 (98%)	208 (77%)	38 (14%)	24 (9%)	1	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	DD	270/276 (98%)	205 (76%)	38 (14%)	27 (10%)	1	15
39	BE	203/206 (98%)	130 (64%)	40 (20%)	33 (16%)	0	5
39	DE	203/206 (98%)	127 (63%)	44 (22%)	32 (16%)	0	5
40	BF	206/210 (98%)	142 (69%)	35 (17%)	29 (14%)	0	8
40	DF	206/210 (98%)	143 (69%)	35 (17%)	28 (14%)	0	8
41	BG	177/182 (97%)	107 (60%)	50 (28%)	20 (11%)	1	12
41	DG	177/182 (97%)	108 (61%)	45 (25%)	24 (14%)	0	8
42	BH	158/180 (88%)	99 (63%)	32 (20%)	27 (17%)	0	4
42	DH	158/180 (88%)	99 (63%)	32 (20%)	27 (17%)	0	4
43	BI	144/148 (97%)	87 (60%)	35 (24%)	22 (15%)	0	6
43	DI	144/148 (97%)	85 (59%)	37 (26%)	22 (15%)	0	6
44	BN	137/140 (98%)	90 (66%)	30 (22%)	17 (12%)	1	10
44	DN	137/140 (98%)	91 (66%)	29 (21%)	17 (12%)	1	10
45	BO	120/122 (98%)	91 (76%)	21 (18%)	8 (7%)	2	28
45	DO	120/122 (98%)	88 (73%)	24 (20%)	8 (7%)	2	28
46	BP	144/150 (96%)	73 (51%)	30 (21%)	41 (28%)	0	0
46	DP	144/150 (96%)	73 (51%)	30 (21%)	41 (28%)	0	0
47	BQ	139/141 (99%)	107 (77%)	24 (17%)	8 (6%)	3	32
47	DQ	139/141 (99%)	106 (76%)	23 (16%)	10 (7%)	2	25
48	BR	115/118 (98%)	83 (72%)	18 (16%)	14 (12%)	1	11
48	DR	115/118 (98%)	83 (72%)	18 (16%)	14 (12%)	1	11
49	BS	97/112 (87%)	47 (48%)	25 (26%)	25 (26%)	0	1
49	DS	97/112 (87%)	47 (48%)	25 (26%)	25 (26%)	0	1
50	BT	136/146 (93%)	82 (60%)	26 (19%)	28 (21%)	0	2
50	DT	136/146 (93%)	81 (60%)	27 (20%)	28 (21%)	0	2
51	BU	115/118 (98%)	86 (75%)	22 (19%)	7 (6%)	2	30
51	DU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	22
52	BV	99/101 (98%)	62 (63%)	22 (22%)	15 (15%)	0	6
52	DV	99/101 (98%)	63 (64%)	21 (21%)	15 (15%)	0	6
53	BW	111/113 (98%)	87 (78%)	15 (14%)	9 (8%)	1	21
53	DW	111/113 (98%)	88 (79%)	15 (14%)	8 (7%)	2	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	BX	91/96 (95%)	74 (81%)	14 (15%)	3 (3%)	6	51
54	DX	91/96 (95%)	74 (81%)	13 (14%)	4 (4%)	4	41
55	BY	99/110 (90%)	37 (37%)	30 (30%)	32 (32%)	0	0
55	DY	99/110 (90%)	35 (35%)	32 (32%)	32 (32%)	0	0
56	BZ	175/206 (85%)	113 (65%)	38 (22%)	24 (14%)	0	8
56	DZ	175/206 (85%)	103 (59%)	45 (26%)	27 (15%)	0	6
All	All	11670/12592 (93%)	7783 (67%)	2440 (21%)	1447 (12%)	1	10

5 of 1447 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	9	GLU
2	AB	15	VAL
2	AB	88	ALA
2	AB	154	LEU
2	AB	165	VAL

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%)	181 (90%)	21 (10%)	10	47
2	CB	202/220 (92%)	181 (90%)	21 (10%)	10	47
3	AC	160/188 (85%)	152 (95%)	8 (5%)	34	79
3	CC	160/188 (85%)	151 (94%)	9 (6%)	30	76
4	AD	180/181 (99%)	161 (89%)	19 (11%)	10	45
4	CD	180/181 (99%)	159 (88%)	21 (12%)	8	38
5	AE	115/123 (94%)	106 (92%)	9 (8%)	18	63
5	CE	115/123 (94%)	107 (93%)	8 (7%)	21	68
6	AF	90/90 (100%)	85 (94%)	5 (6%)	30	76
6	CF	90/90 (100%)	85 (94%)	5 (6%)	30	76
7	AG	126/127 (99%)	118 (94%)	8 (6%)	25	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	CG	126/127 (99%)	117 (93%)	9 (7%)	21	67
8	AH	119/119 (100%)	111 (93%)	8 (7%)	23	70
8	CH	119/119 (100%)	111 (93%)	8 (7%)	23	70
9	AI	98/99 (99%)	88 (90%)	10 (10%)	11	48
9	CI	98/99 (99%)	88 (90%)	10 (10%)	11	48
10	AJ	88/92 (96%)	76 (86%)	12 (14%)	5	30
10	CJ	88/92 (96%)	77 (88%)	11 (12%)	7	35
11	AK	90/99 (91%)	84 (93%)	6 (7%)	23	70
11	CK	90/99 (91%)	84 (93%)	6 (7%)	23	70
12	AL	104/111 (94%)	93 (89%)	11 (11%)	10	45
12	CL	104/111 (94%)	92 (88%)	12 (12%)	8	39
13	AM	99/101 (98%)	90 (91%)	9 (9%)	14	54
13	CM	99/101 (98%)	90 (91%)	9 (9%)	14	54
14	AN	49/50 (98%)	46 (94%)	3 (6%)	26	73
14	CN	49/50 (98%)	46 (94%)	3 (6%)	26	73
15	AO	79/80 (99%)	70 (89%)	9 (11%)	8	40
15	CO	79/80 (99%)	70 (89%)	9 (11%)	8	40
16	AP	72/74 (97%)	61 (85%)	11 (15%)	4	25
16	CP	72/74 (97%)	61 (85%)	11 (15%)	4	25
17	AQ	94/97 (97%)	89 (95%)	5 (5%)	32	78
17	CQ	94/97 (97%)	89 (95%)	5 (5%)	32	78
18	AR	61/77 (79%)	53 (87%)	8 (13%)	6	32
18	CR	61/77 (79%)	52 (85%)	9 (15%)	4	26
19	AS	69/80 (86%)	60 (87%)	9 (13%)	6	33
19	CS	69/80 (86%)	60 (87%)	9 (13%)	6	33
20	AT	76/82 (93%)	71 (93%)	5 (7%)	24	71
20	CT	76/82 (93%)	71 (93%)	5 (7%)	24	71
21	AU	19/22 (86%)	18 (95%)	1 (5%)	32	78
21	CU	19/22 (86%)	18 (95%)	1 (5%)	32	78
25	B0	66/67 (98%)	59 (89%)	7 (11%)	10	45
25	D0	66/67 (98%)	59 (89%)	7 (11%)	10	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	B1	78/83 (94%)	65 (83%)	13 (17%)	3	19
26	D1	78/83 (94%)	66 (85%)	12 (15%)	4	24
27	B2	66/67 (98%)	57 (86%)	9 (14%)	5	30
27	D2	66/67 (98%)	57 (86%)	9 (14%)	5	30
28	B3	51/52 (98%)	49 (96%)	2 (4%)	43	85
28	D3	51/52 (98%)	49 (96%)	2 (4%)	43	85
29	B4	27/63 (43%)	23 (85%)	4 (15%)	4	26
29	D4	27/63 (43%)	23 (85%)	4 (15%)	4	26
30	B5	51/52 (98%)	42 (82%)	9 (18%)	3	16
30	D5	51/52 (98%)	41 (80%)	10 (20%)	2	11
31	B6	43/52 (83%)	34 (79%)	9 (21%)	1	10
31	D6	43/52 (83%)	34 (79%)	9 (21%)	1	10
32	B7	41/42 (98%)	36 (88%)	5 (12%)	7	36
32	D7	41/42 (98%)	36 (88%)	5 (12%)	7	36
33	B8	53/55 (96%)	42 (79%)	11 (21%)	2	10
33	D8	53/55 (96%)	42 (79%)	11 (21%)	2	10
34	B9	33/34 (97%)	30 (91%)	3 (9%)	14	54
34	D9	33/34 (97%)	30 (91%)	3 (9%)	14	54
37	BC	61/181 (34%)	53 (87%)	8 (13%)	6	32
37	DC	61/181 (34%)	53 (87%)	8 (13%)	6	32
38	BD	213/218 (98%)	183 (86%)	30 (14%)	5	28
38	DD	213/218 (98%)	183 (86%)	30 (14%)	5	28
39	BE	165/166 (99%)	142 (86%)	23 (14%)	5	29
39	DE	165/166 (99%)	143 (87%)	22 (13%)	6	31
40	BF	165/166 (99%)	150 (91%)	15 (9%)	14	54
40	DF	165/166 (99%)	151 (92%)	14 (8%)	15	58
41	BG	155/156 (99%)	133 (86%)	22 (14%)	5	28
41	DG	155/156 (99%)	129 (83%)	26 (17%)	3	19
42	BH	132/148 (89%)	119 (90%)	13 (10%)	12	50
42	DH	132/148 (89%)	119 (90%)	13 (10%)	12	50
43	BI	122/124 (98%)	113 (93%)	9 (7%)	20	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	DI	122/124 (98%)	113 (93%)	9 (7%)	20	66
44	BN	117/119 (98%)	98 (84%)	19 (16%)	3	21
44	DN	117/119 (98%)	100 (86%)	17 (14%)	5	27
45	BO	100/100 (100%)	90 (90%)	10 (10%)	11	49
45	DO	100/100 (100%)	92 (92%)	8 (8%)	17	61
46	BP	112/116 (97%)	92 (82%)	20 (18%)	2	15
46	DP	112/116 (97%)	93 (83%)	19 (17%)	3	18
47	BQ	111/111 (100%)	94 (85%)	17 (15%)	4	25
47	DQ	111/111 (100%)	94 (85%)	17 (15%)	4	25
48	BR	100/101 (99%)	88 (88%)	12 (12%)	7	37
48	DR	100/101 (99%)	88 (88%)	12 (12%)	7	37
49	BS	77/88 (88%)	68 (88%)	9 (12%)	8	38
49	DS	77/88 (88%)	67 (87%)	10 (13%)	6	33
50	BT	120/127 (94%)	101 (84%)	19 (16%)	4	23
50	DT	120/127 (94%)	101 (84%)	19 (16%)	4	23
51	BU	92/94 (98%)	80 (87%)	12 (13%)	6	33
51	DU	92/94 (98%)	80 (87%)	12 (13%)	6	33
52	BV	82/82 (100%)	68 (83%)	14 (17%)	3	18
52	DV	82/82 (100%)	69 (84%)	13 (16%)	4	22
53	BW	91/92 (99%)	83 (91%)	8 (9%)	14	57
53	DW	91/92 (99%)	83 (91%)	8 (9%)	14	57
54	BX	74/78 (95%)	67 (90%)	7 (10%)	12	51
54	DX	74/78 (95%)	67 (90%)	7 (10%)	12	51
55	BY	84/91 (92%)	70 (83%)	14 (17%)	3	19
55	DY	84/91 (92%)	70 (83%)	14 (17%)	3	19
56	BZ	155/179 (87%)	133 (86%)	22 (14%)	5	28
56	DZ	155/179 (87%)	131 (84%)	24 (16%)	4	24
All	All	9654/10432 (92%)	8547 (88%)	1107 (12%)	8	39

5 of 1107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
52	BV	99	ILE

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Mol	Chain	Res	Type
7	CG	113	GLU
50	DT	99	LEU
54	BX	80	ILE
2	CB	94	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 306 such sidechains are listed below:

Mol	Chain	Res	Type
53	BW	62	HIS
6	CF	100	ASN
48	DR	53	HIS
54	BX	55	ASN
3	CC	37	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	215 (14%)	29 (1%)
1	CA	1503/1522 (98%)	216 (14%)	29 (1%)
22	AV	74/77 (96%)	15 (20%)	0
22	AY	74/77 (96%)	20 (27%)	1 (1%)
22	CV	74/77 (96%)	19 (25%)	1 (1%)
22	CY	74/77 (96%)	20 (27%)	1 (1%)
23	AW	75/76 (98%)	13 (17%)	0
23	CW	75/76 (98%)	15 (20%)	0
24	AX	10/11 (90%)	1 (10%)	0
24	CX	10/11 (90%)	2 (20%)	0
35	BA	2806/2822 (99%)	516 (18%)	55 (1%)
35	DA	2806/2822 (99%)	515 (18%)	53 (1%)
36	BB	118/122 (96%)	13 (11%)	1 (0%)
36	DB	118/122 (96%)	13 (11%)	1 (0%)
All	All	9320/9414 (99%)	1593 (17%)	171 (1%)

5 of 1593 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

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Mol	Chain	Res	Type
1	AA	48	C

5 of 171 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	BA	2481	G
1	CA	366	C
35	DA	2172	U
35	BA	2610	C
1	CA	30	U

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

8 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	8AN	AV	76	57,22	24,24,25	0.91	1 (4%)	34,35,38	1.09	3 (8%)
22	PHA	AV	77	22	11,11,11	0.81	0	13,13,13	0.69	0
22	8AN	AY	76	22	24,24,25	0.94	1 (4%)	34,35,38	1.08	3 (8%)
22	PHA	AY	77	22	11,11,11	1.02	1 (9%)	13,13,13	1.06	2 (15%)
22	8AN	CV	76	57,22	24,24,25	0.98	2 (8%)	34,35,38	1.23	4 (11%)
22	PHA	CV	77	22	11,11,11	0.83	0	13,13,13	0.67	0
22	8AN	CY	76	22	24,24,25	0.88	1 (4%)	34,35,38	0.93	2 (5%)
22	PHA	CY	77	22	11,11,11	1.64	1 (9%)	13,13,13	0.81	0

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	8AN	AV	76	57,22	-	0/9/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PHA	AV	77	22	-	0/5/6/6	0/1/1/1
22	8AN	AY	76	22	-	0/9/25/26	0/3/3/3
22	PHA	AY	77	22	-	0/5/6/6	0/1/1/1
22	8AN	CV	76	57,22	-	0/9/25/26	0/3/3/3
22	PHA	CV	77	22	-	1/5/6/6	0/1/1/1
22	8AN	CY	76	22	-	0/9/25/26	0/3/3/3
22	PHA	CY	77	22	-	0/5/6/6	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	CY	77	PHA	CA-C	4.18	1.53	1.49
22	AY	76	8AN	C3'-N3'	-3.46	1.41	1.47
22	AV	76	8AN	C3'-N3'	-3.41	1.41	1.47
22	CV	76	8AN	C3'-N3'	-3.25	1.42	1.47
22	AY	77	PHA	CA-C	2.68	1.52	1.49

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	CV	76	8AN	C4'-C3'-N3'	-3.47	106.97	114.04
22	CV	76	8AN	C5'-C4'-C3'	3.02	120.23	115.95
22	AY	76	8AN	C2'-C3'-N3'	-2.89	108.69	113.90
22	AY	76	8AN	C4'-C3'-N3'	-2.77	108.39	114.04
22	CV	76	8AN	C2'-C3'-N3'	-2.64	109.15	113.90

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	CV	77	PHA	O-C-CA-CB

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 1354 ligands modelled in this entry, 1352 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	PAR	AA	1799	-	45,45,45	1.91	14 (31%)	67,67,67	1.40	8 (11%)
58	PAR	CA	1800	-	45,45,45	1.68	10 (22%)	67,67,67	1.31	9 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PAR	AA	1799	-	-	0/18/94/94	0/4/4/4
58	PAR	CA	1800	-	-	0/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	AA	1799	PAR	C31-C21	4.77	1.60	1.53
58	AA	1799	PAR	C11-C21	4.26	1.60	1.52
58	CA	1800	PAR	O54-C14	3.59	1.51	1.41
58	AA	1799	PAR	C64-C54	3.31	1.60	1.51
58	AA	1799	PAR	C52-C42	3.14	1.58	1.52

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	AA	1799	PAR	O52-C13-C23	4.12	114.86	107.50
58	CA	1800	PAR	O52-C13-C23	4.01	114.65	107.50
58	AA	1799	PAR	O54-C54-C64	3.79	113.19	105.97
58	CA	1800	PAR	C14-O54-C54	3.75	120.99	113.73
58	CA	1800	PAR	O54-C54-C64	3.74	113.09	105.97

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	3
13	AM	3
9	AI	2
9	CI	2
41	DG	1
41	BG	1
31	D6	1
31	B6	1

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D6	46:HIS	C	47:THR	N	4.60
1	B6	46:HIS	C	47:THR	N	4.59
1	BG	112:PRO	C	113:ARG	N	3.80
1	DG	112:PRO	C	113:ARG	N	3.77
1	CM	69:GLU	C	70:LEU	N	3.15

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%)	-0.10	23 (1%) 70 36	47, 104, 183, 200	0
1	CA	1504/1522 (98%)	0.02	29 (1%) 64 32	69, 117, 189, 200	0
2	AB	235/256 (91%)	0.24	5 (2%) 60 29	73, 131, 181, 200	0
2	CB	235/256 (91%)	0.37	5 (2%) 60 29	85, 154, 189, 200	0
3	AC	207/239 (86%)	0.21	1 (0%) 88 64	71, 116, 160, 200	0
3	CC	207/239 (86%)	0.41	8 (3%) 37 16	87, 139, 180, 200	0
4	AD	208/209 (99%)	0.06	0 100 100	60, 110, 153, 185	0
4	CD	208/209 (99%)	-0.05	0 100 100	58, 101, 142, 181	0
5	AE	151/162 (93%)	0.08	1 (0%) 84 56	52, 101, 144, 174	0
5	CE	151/162 (93%)	0.39	5 (3%) 44 20	66, 119, 168, 200	0
6	AF	101/101 (100%)	-0.06	1 (0%) 79 47	56, 96, 142, 181	0
6	CF	101/101 (100%)	-0.01	1 (0%) 79 47	51, 107, 147, 196	0
7	AG	155/156 (99%)	0.35	10 (6%) 18 8	65, 117, 166, 200	0
7	CG	155/156 (99%)	0.41	9 (5%) 22 9	80, 129, 161, 182	0
8	AH	138/138 (100%)	0.18	1 (0%) 84 56	62, 106, 140, 174	0
8	CH	138/138 (100%)	0.46	4 (2%) 49 23	82, 122, 160, 195	0
9	AI	127/128 (99%)	0.42	4 (3%) 47 22	79, 136, 176, 200	0
9	CI	127/128 (99%)	0.70	11 (8%) 10 6	96, 145, 188, 200	0
10	AJ	99/105 (94%)	0.69	12 (12%) 5 3	65, 140, 184, 200	0
10	CJ	99/105 (94%)	0.89	12 (12%) 5 3	70, 153, 195, 200	0
11	AK	119/129 (92%)	0.22	5 (4%) 35 14	62, 99, 159, 198	0
11	CK	119/129 (92%)	0.13	4 (3%) 43 19	74, 111, 155, 184	0
12	AL	125/135 (92%)	0.10	2 (1%) 68 35	51, 91, 144, 190	0
12	CL	125/135 (92%)	0.46	5 (4%) 36 16	59, 113, 161, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	125/126 (99%)	0.37	7 (5%) 24 10	75, 120, 163, 200	0
13	CM	125/126 (99%)	0.74	15 (12%) 5 4	77, 137, 184, 200	0
14	AN	60/61 (98%)	-0.03	0 100 100	50, 109, 147, 200	0
14	CN	60/61 (98%)	0.71	4 (6%) 17 8	89, 135, 183, 200	0
15	AO	88/89 (98%)	0.10	1 (1%) 77 44	55, 100, 144, 162	0
15	CO	88/89 (98%)	0.25	2 (2%) 57 27	69, 108, 154, 182	0
16	AP	84/88 (95%)	0.51	1 (1%) 75 42	78, 107, 147, 184	0
16	CP	84/88 (95%)	0.42	0 100 100	61, 100, 150, 179	0
17	AQ	100/105 (95%)	0.30	4 (4%) 36 16	82, 109, 150, 181	0
17	CQ	100/105 (95%)	0.32	3 (3%) 48 22	71, 115, 153, 167	0
18	AR	70/88 (79%)	0.13	2 (2%) 49 23	59, 96, 139, 169	0
18	CR	70/88 (79%)	0.41	1 (1%) 72 38	66, 111, 152, 173	0
19	AS	79/93 (84%)	0.57	3 (3%) 38 17	82, 122, 176, 200	0
19	CS	79/93 (84%)	0.88	6 (7%) 14 7	91, 145, 188, 200	0
20	AT	99/106 (93%)	0.40	2 (2%) 62 30	77, 120, 170, 195	0
20	CT	99/106 (93%)	0.39	4 (4%) 36 16	67, 116, 174, 200	0
21	AU	25/27 (92%)	1.30	5 (20%) 2 2	80, 119, 154, 178	0
21	CU	25/27 (92%)	1.68	8 (32%) 1 1	79, 141, 171, 185	0
22	AV	77/77 (100%)	0.01	3 (3%) 37 16	55, 121, 158, 197	0
22	AY	77/77 (100%)	0.57	6 (7%) 13 7	45, 162, 196, 200	0
22	CV	77/77 (100%)	-0.20	0 100 100	62, 144, 178, 192	0
22	CY	77/77 (100%)	0.97	9 (11%) 5 4	46, 181, 199, 200	0
23	AW	76/76 (100%)	0.43	7 (9%) 9 5	99, 173, 199, 200	0
23	CW	76/76 (100%)	0.49	5 (6%) 18 8	117, 178, 200, 200	0
24	AX	11/11 (100%)	0.53	1 (9%) 9 5	68, 116, 146, 168	0
24	CX	11/11 (100%)	0.94	3 (27%) 1 2	87, 126, 158, 159	0
25	B0	84/85 (98%)	0.03	0 100 100	30, 62, 111, 143	0
25	D0	84/85 (98%)	0.40	0 100 100	58, 106, 148, 178	0
26	B1	94/98 (95%)	0.11	0 100 100	37, 68, 129, 162	0
26	D1	94/98 (95%)	0.21	1 (1%) 77 44	38, 79, 131, 166	0
27	B2	71/72 (98%)	0.08	1 (1%) 72 38	40, 80, 141, 188	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	D2	71/72 (98%)	0.10	0 100 100	62, 97, 150, 182	0
28	B3	60/60 (100%)	0.04	1 (1%) 67 34	31, 67, 112, 190	0
28	D3	60/60 (100%)	1.08	8 (13%) 4 3	65, 124, 163, 200	0
29	B4	31/71 (43%)	-0.00	0 100 100	67, 132, 172, 182	0
29	D4	31/71 (43%)	0.09	0 100 100	105, 142, 184, 197	0
30	B5	59/60 (98%)	-0.03	2 (3%) 43 19	37, 60, 164, 200	0
30	D5	59/60 (98%)	0.12	4 (6%) 17 8	52, 88, 175, 191	0
31	B6	45/54 (83%)	0.92	4 (8%) 10 6	57, 113, 166, 174	0
31	D6	45/54 (83%)	1.49	13 (28%) 1 1	92, 138, 175, 200	0
32	B7	49/49 (100%)	-0.00	0 100 100	25, 53, 112, 194	0
32	D7	49/49 (100%)	0.21	0 100 100	41, 67, 119, 181	0
33	B8	64/65 (98%)	0.22	1 (1%) 68 35	25, 69, 131, 198	0
33	D8	64/65 (98%)	0.34	1 (1%) 68 35	45, 92, 149, 183	0
34	B9	36/37 (97%)	1.67	10 (27%) 1 1	70, 99, 142, 153	0
34	D9	36/37 (97%)	3.27	28 (77%) 0 0	120, 159, 194, 200	0
35	BA	2807/2822 (99%)	-0.13	45 (1%) 68 35	35, 64, 176, 200	0
35	DA	2807/2822 (99%)	-0.05	56 (1%) 62 30	44, 93, 186, 200	0
36	BB	119/122 (97%)	-0.35	1 (0%) 83 53	57, 81, 135, 179	0
36	DB	119/122 (97%)	-0.11	1 (0%) 83 53	90, 129, 183, 197	0
37	BC	191/229 (83%)	1.78	64 (33%) 1 1	115, 175, 200, 200	0
37	DC	191/229 (83%)	1.53	63 (32%) 1 1	113, 172, 200, 200	0
38	BD	272/276 (98%)	-0.10	0 100 100	33, 62, 106, 186	0
38	DD	272/276 (98%)	0.01	0 100 100	40, 76, 114, 158	0
39	BE	205/206 (99%)	0.05	1 (0%) 88 64	28, 65, 151, 200	0
39	DE	205/206 (99%)	0.36	2 (0%) 79 47	53, 105, 162, 193	0
40	BF	208/210 (99%)	-0.12	1 (0%) 88 64	26, 65, 154, 194	0
40	DF	208/210 (99%)	0.07	1 (0%) 88 64	41, 91, 166, 200	0
41	BG	181/182 (99%)	0.11	3 (1%) 67 34	57, 99, 158, 197	0
41	DG	181/182 (99%)	0.36	5 (2%) 50 23	78, 120, 160, 182	0
42	BH	160/180 (88%)	0.27	8 (5%) 28 12	44, 94, 160, 199	0
42	DH	160/180 (88%)	1.35	44 (27%) 1 2	107, 169, 200, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BI	146/148 (98%)	1.05	30 (20%) 1 2	48, 154, 200, 200	0
43	DI	146/148 (98%)	0.61	11 (7%) 14 7	74, 126, 175, 200	0
44	BN	139/140 (99%)	-0.10	0 100 100	33, 68, 138, 187	0
44	DN	139/140 (99%)	0.56	5 (3%) 41 18	75, 116, 173, 200	0
45	BO	122/122 (100%)	-0.13	0 100 100	30, 69, 107, 139	0
45	DO	122/122 (100%)	0.13	0 100 100	59, 105, 137, 157	0
46	BP	146/150 (97%)	0.19	2 (1%) 72 38	25, 84, 158, 188	0
46	DP	146/150 (97%)	0.41	4 (2%) 52 24	51, 108, 169, 200	0
47	BQ	141/141 (100%)	-0.02	2 (1%) 72 38	41, 69, 130, 200	0
47	DQ	141/141 (100%)	0.28	3 (2%) 60 29	66, 115, 166, 200	0
48	BR	117/118 (99%)	-0.07	0 100 100	21, 62, 114, 165	0
48	DR	117/118 (99%)	0.18	0 100 100	37, 89, 131, 173	0
49	BS	99/112 (88%)	0.27	2 (2%) 62 30	43, 83, 138, 181	0
49	DS	99/112 (88%)	0.73	10 (10%) 7 5	80, 128, 179, 200	0
50	BT	138/146 (94%)	-0.01	1 (0%) 84 56	40, 86, 164, 195	0
50	DT	138/146 (94%)	0.20	2 (1%) 72 38	74, 116, 173, 200	0
51	BU	117/118 (99%)	-0.24	0 100 100	23, 55, 106, 158	0
51	DU	117/118 (99%)	0.12	2 (1%) 67 34	56, 101, 167, 200	0
52	BV	101/101 (100%)	-0.04	0 100 100	29, 76, 135, 200	0
52	DV	101/101 (100%)	0.59	3 (2%) 48 22	55, 135, 177, 200	0
53	BW	113/113 (100%)	-0.02	2 (1%) 65 33	26, 55, 122, 200	0
53	DW	113/113 (100%)	0.12	1 (0%) 81 51	50, 80, 140, 194	0
54	BX	93/96 (96%)	-0.18	0 100 100	41, 66, 106, 157	0
54	DX	93/96 (96%)	0.07	0 100 100	42, 86, 118, 150	0
55	BY	101/110 (91%)	0.41	6 (5%) 22 9	42, 88, 178, 200	0
55	DY	101/110 (91%)	0.88	15 (14%) 3 3	49, 107, 181, 200	0
56	BZ	177/206 (85%)	0.38	17 (9%) 8 5	40, 107, 185, 200	0
56	DZ	177/206 (85%)	0.87	20 (11%) 6 4	96, 152, 198, 200	0
All	All	21252/22006 (96%)	0.17	767 (3%) 41 18	21, 102, 183, 200	0

The worst 5 of 767 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CA	83	U	13.8
56	DZ	112	ARG	10.4
22	CY	17	C	10.1
22	AY	17	C	9.2
1	AA	89	C	9.2

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	PHA	CY	77	11/11	0.38	-	42,44,48,152	0
22	8AN	AY	76	22/23	0.22	-	29,48,67,71	0
22	8AN	CV	76	22/23	0.17	-	12,58,100,116	0
22	8AN	AV	76	22/23	0.20	-	12,58,100,116	0
22	PHA	AV	77	11/11	0.34	-	121,125,131,132	0
22	PHA	CV	77	11/11	0.27	-	121,125,131,132	0
22	8AN	CY	76	22/23	0.23	-	29,48,67,71	0
22	PHA	AY	77	11/11	0.36	-	42,44,47,48	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
57	MG	BA	3182	1/1	0.21	-	62,62,62,62	0
57	MG	AA	1766	1/1	0.21	-	67,67,67,67	0
57	MG	BA	3154	1/1	0.34	-	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3421	1/1	0.16	-	110,110,110,110	1
57	MG	BA	3377	1/1	0.17	-	126,126,126,126	0
57	MG	DA	3246	1/1	0.48	-	97,97,97,97	0
57	MG	DA	3394	1/1	0.15	-	103,103,103,103	0
57	MG	DA	3120	1/1	0.17	-	39,39,39,39	0
57	MG	BA	3351	1/1	0.29	-	135,135,135,135	0
57	MG	DA	3210	1/1	0.54	-	96,96,96,96	0
57	MG	BA	3189	1/1	0.14	-	8,8,8,8	0
57	MG	BA	3303	1/1	0.15	-	49,49,49,49	1
57	MG	DA	3313	1/1	0.31	-	80,80,80,80	0
57	MG	BA	3118	1/1	0.25	-	68,68,68,68	0
57	MG	DA	3233	1/1	0.47	-	36,36,36,36	0
57	MG	BA	3300	1/1	0.32	-	3,3,3,3	0
57	MG	DA	3194	1/1	0.14	-	59,59,59,59	0
57	MG	DA	3278	1/1	0.28	-	54,54,54,54	0
57	MG	AA	1702	1/1	0.93	-	126,126,126,126	0
57	MG	AA	1794	1/1	0.17	-	126,126,126,126	0
57	MG	DA	3023	1/1	0.34	-	20,20,20,20	0
57	MG	BA	3065	1/1	0.24	-	1,1,1,1	0
57	MG	DA	3175	1/1	0.17	-	63,63,63,63	0
57	MG	AA	1608	1/1	0.18	-	46,46,46,46	0
57	MG	CX	103	1/1	0.25	-	108,108,108,108	0
57	MG	CA	1638	1/1	0.27	-	42,42,42,42	0
57	MG	AA	1669	1/1	0.27	-	57,57,57,57	0
57	MG	DA	3410	1/1	0.28	-	87,87,87,87	1
57	MG	BA	3057	1/1	0.47	-	85,85,85,85	0
57	MG	AA	1617	1/1	0.68	-	51,51,51,51	0
57	MG	BB	208	1/1	1.04	-	61,61,61,61	1
57	MG	BA	3008	1/1	0.26	-	3,3,3,3	0
57	MG	DA	3052	1/1	0.11	-	30,30,30,30	0
57	MG	BA	3417	1/1	0.12	-	72,72,72,72	0
57	MG	CV	105	1/1	0.15	-	65,65,65,65	0
57	MG	AA	1638	1/1	0.21	-	36,36,36,36	0
57	MG	AA	1636	1/1	0.45	-	74,74,74,74	0
57	MG	DF	302	1/1	0.55	-	91,91,91,91	0
57	MG	BA	3224	1/1	0.31	-	91,91,91,91	0
57	MG	BA	3358	1/1	0.24	-	24,24,24,24	0
57	MG	CA	1705	1/1	0.47	-	150,150,150,150	0
57	MG	DA	3102	1/1	0.46	-	129,129,129,129	1
57	MG	AA	1770	1/1	0.43	-	163,163,163,163	0
57	MG	D2	601	1/1	0.32	-	35,35,35,35	1
57	MG	AA	1725	1/1	0.17	-	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	1656	1/1	0.75	-	97,97,97,97	0
57	MG	BA	3389	1/1	0.34	-	62,62,62,62	0
57	MG	BA	3106	1/1	0.27	-	20,20,20,20	0
57	MG	DA	3384	1/1	0.22	-	115,115,115,115	0
57	MG	AA	1634	1/1	0.85	-	73,73,73,73	0
57	MG	BA	3144	1/1	0.21	-	58,58,58,58	0
57	MG	BA	3244	1/1	0.32	-	88,88,88,88	0
59	ZN	AN	102	1/1	0.18	-	109,109,109,109	0
57	MG	CA	1614	1/1	1.00	-	89,89,89,89	0
57	MG	DA	3186	1/1	0.23	-	48,48,48,48	0
57	MG	CA	1629	1/1	0.21	-	59,59,59,59	0
57	MG	BF	301	1/1	0.19	-	41,41,41,41	0
57	MG	CA	1715	1/1	0.11	-	66,66,66,66	0
57	MG	BB	206	1/1	0.14	-	105,105,105,105	0
57	MG	BA	3028	1/1	0.20	-	12,12,12,12	0
57	MG	CA	1648	1/1	0.53	-	83,83,83,83	0
57	MG	DA	3018	1/1	0.31	-	31,31,31,31	0
57	MG	BA	3376	1/1	0.46	-	81,81,81,81	0
57	MG	DA	3248	1/1	0.24	-	90,90,90,90	0
57	MG	CA	1748	1/1	0.23	-	63,63,63,63	0
57	MG	BA	3274	1/1	0.70	-	85,85,85,85	0
57	MG	DA	3051	1/1	0.25	-	75,75,75,75	0
57	MG	DA	3360	1/1	0.09	-	83,83,83,83	0
57	MG	BA	3095	1/1	0.31	-	27,27,27,27	0
57	MG	DA	3092	1/1	0.36	-	46,46,46,46	0
57	MG	BA	3107	1/1	0.45	-	44,44,44,44	0
57	MG	BA	3344	1/1	0.14	-	57,57,57,57	0
57	MG	BA	3149	1/1	0.33	-	13,13,13,13	1
57	MG	AA	1709	1/1	0.07	-	49,49,49,49	0
57	MG	AG	201	1/1	0.45	-	80,80,80,80	0
57	MG	BA	3230	1/1	0.46	-	97,97,97,97	0
57	MG	DA	3048	1/1	0.64	-	61,61,61,61	0
57	MG	BA	3250	1/1	0.27	-	76,76,76,76	0
57	MG	CA	1650	1/1	0.11	-	89,89,89,89	1
57	MG	DA	3045	1/1	0.29	-	35,35,35,35	0
57	MG	BA	3388	1/1	0.36	-	12,12,12,12	0
57	MG	DA	3335	1/1	0.24	-	80,80,80,80	0
57	MG	DA	3318	1/1	0.19	-	138,138,138,138	0
57	MG	AA	1643	1/1	0.30	-	84,84,84,84	0
59	ZN	CD	301	1/1	0.22	-	55,55,55,55	0
57	MG	CA	1633	1/1	0.14	-	42,42,42,42	0
57	MG	AA	1640	1/1	0.28	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3020	1/1	0.30	-	59,59,59,59	0
57	MG	CA	1608	1/1	0.17	-	39,39,39,39	0
57	MG	CA	1631	1/1	0.27	-	65,65,65,65	0
57	MG	CW	104	1/1	0.14	-	130,130,130,130	1
57	MG	BA	3366	1/1	0.42	-	112,112,112,112	0
57	MG	DA	3010	1/1	0.32	-	18,18,18,18	0
57	MG	DA	3196	1/1	0.31	-	96,96,96,96	0
57	MG	DA	3269	1/1	0.35	-	47,47,47,47	0
57	MG	BA	3074	1/1	0.18	-	24,24,24,24	0
57	MG	AA	1658	1/1	0.17	-	25,25,25,25	0
57	MG	BA	3359	1/1	0.17	-	86,86,86,86	1
57	MG	BA	3217	1/1	0.31	-	78,78,78,78	0
57	MG	DA	3009	1/1	0.14	-	45,45,45,45	0
57	MG	BA	3346	1/1	0.38	-	67,67,67,67	0
57	MG	AA	1760	1/1	0.40	-	90,90,90,90	0
57	MG	BA	3098	1/1	0.19	-	6,6,6,6	0
57	MG	BA	3336	1/1	0.08	-	105,105,105,105	1
57	MG	BA	3284	1/1	0.65	-	53,53,53,53	0
57	MG	BA	3047	1/1	0.79	-	72,72,72,72	0
57	MG	DA	3070	1/1	0.74	-	94,94,94,94	0
57	MG	CA	1692	1/1	0.20	-	59,59,59,59	0
58	PAR	AA	1799	42/42	0.23	-	60,65,83,87	0
57	MG	BA	3331	1/1	0.40	-	65,65,65,65	1
57	MG	BA	3056	1/1	0.32	-	17,17,17,17	0
57	MG	BA	3187	1/1	0.39	-	108,108,108,108	0
57	MG	BA	3003	1/1	0.84	-	85,85,85,85	0
57	MG	CA	1697	1/1	0.16	-	72,72,72,72	0
57	MG	BA	3179	1/1	1.50	-	117,117,117,117	0
57	MG	BA	3318	1/1	0.35	-	70,70,70,70	1
57	MG	DA	3298	1/1	0.19	-	56,56,56,56	0
57	MG	BA	3079	1/1	0.19	-	31,31,31,31	0
57	MG	CA	1703	1/1	0.35	-	87,87,87,87	0
57	MG	BA	3117	1/1	0.54	-	59,59,59,59	0
57	MG	DA	3095	1/1	0.10	-	37,37,37,37	0
57	MG	DA	3114	1/1	0.27	-	29,29,29,29	0
57	MG	DA	3191	1/1	0.19	-	41,41,41,41	0
57	MG	DA	3379	1/1	0.60	-	105,105,105,105	0
57	MG	CA	1731	1/1	0.28	-	85,85,85,85	0
57	MG	CA	1698	1/1	0.12	-	86,86,86,86	0
57	MG	DA	3249	1/1	0.41	-	60,60,60,60	0
57	MG	AA	1716	1/1	0.18	-	86,86,86,86	0
57	MG	BA	3233	1/1	0.40	-	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3411	1/1	0.13	-	51,51,51,51	1
57	MG	AA	1758	1/1	0.26	-	97,97,97,97	0
57	MG	DA	3337	1/1	0.11	-	76,76,76,76	0
57	MG	BA	3324	1/1	0.43	-	39,39,39,39	1
57	MG	BA	3222	1/1	0.15	-	84,84,84,84	0
57	MG	AA	1700	1/1	0.50	-	79,79,79,79	0
57	MG	DA	3243	1/1	0.71	-	76,76,76,76	0
57	MG	BA	3019	1/1	0.28	-	28,28,28,28	0
57	MG	BA	3030	1/1	0.22	-	18,18,18,18	0
57	MG	DA	3370	1/1	0.47	-	92,92,92,92	0
57	MG	DA	3307	1/1	0.41	-	51,51,51,51	0
57	MG	BA	3297	1/1	0.70	-	77,77,77,77	0
57	MG	DA	3363	1/1	0.13	-	68,68,68,68	0
57	MG	DA	3049	1/1	0.79	-	71,71,71,71	0
57	MG	BA	3082	1/1	0.30	-	37,37,37,37	0
57	MG	BA	3322	1/1	0.64	-	42,42,42,42	1
57	MG	DA	3183	1/1	0.29	-	96,96,96,96	0
57	MG	CE	201	1/1	0.15	-	90,90,90,90	0
57	MG	BA	3267	1/1	0.42	-	56,56,56,56	0
57	MG	BV	201	1/1	0.24	-	64,64,64,64	0
57	MG	CA	1636	1/1	0.45	-	50,50,50,50	0
57	MG	BB	213	1/1	0.29	-	87,87,87,87	0
57	MG	BA	3040	1/1	0.32	-	20,20,20,20	0
57	MG	AA	1727	1/1	0.41	-	54,54,54,54	1
57	MG	DA	3141	1/1	0.39	-	67,67,67,67	0
57	MG	BA	3362	1/1	0.19	-	85,85,85,85	0
57	MG	BA	3104	1/1	0.28	-	20,20,20,20	0
57	MG	CA	1679	1/1	0.13	-	86,86,86,86	0
57	MG	DD	301	1/1	0.24	-	38,38,38,38	0
57	MG	DA	3008	1/1	0.27	-	36,36,36,36	0
57	MG	CA	1753	1/1	0.30	-	130,130,130,130	1
57	MG	DA	3281	1/1	0.21	-	52,52,52,52	0
57	MG	AA	1625	1/1	0.45	-	65,65,65,65	0
57	MG	AA	1710	1/1	0.25	-	71,71,71,71	0
57	MG	AW	108	1/1	0.24	-	82,82,82,82	1
57	MG	CA	1793	1/1	0.34	-	100,100,100,100	1
57	MG	DA	3326	1/1	0.14	-	78,78,78,78	1
57	MG	BA	3127	1/1	0.34	-	44,44,44,44	1
57	MG	BA	3262	1/1	0.13	-	100,100,100,100	0
57	MG	CA	1701	1/1	0.95	-	93,93,93,93	0
57	MG	DA	3347	1/1	0.24	-	53,53,53,53	0
57	MG	CA	1671	1/1	0.33	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3173	1/1	0.13	-	50,50,50,50	0
57	MG	DA	3126	1/1	0.13	-	59,59,59,59	0
57	MG	DA	3057	1/1	0.25	-	31,31,31,31	0
57	MG	BA	3393	1/1	0.36	-	74,74,74,74	0
57	MG	BA	3157	1/1	0.36	-	74,74,74,74	0
57	MG	CX	101	1/1	0.50	-	123,123,123,123	0
57	MG	DA	3400	1/1	0.34	-	77,77,77,77	0
57	MG	BA	3163	1/1	0.13	-	42,42,42,42	0
57	MG	DA	3350	1/1	0.13	-	89,89,89,89	1
57	MG	DA	3056	1/1	0.33	-	49,49,49,49	0
57	MG	AA	1697	1/1	0.21	-	78,78,78,78	0
57	MG	AA	1665	1/1	0.45	-	53,53,53,53	0
57	MG	DA	3291	1/1	0.26	-	58,58,58,58	0
57	MG	BA	3350	1/1	0.18	-	81,81,81,81	1
57	MG	AA	1741	1/1	0.74	-	124,124,124,124	0
57	MG	CA	1784	1/1	0.17	-	68,68,68,68	1
57	MG	DA	3200	1/1	0.19	-	59,59,59,59	0
57	MG	AA	1745	1/1	0.49	-	62,62,62,62	0
57	MG	BA	3198	1/1	0.18	-	51,51,51,51	0
57	MG	DA	3190	1/1	0.23	-	67,67,67,67	0
57	MG	DB	205	1/1	0.12	-	55,55,55,55	0
57	MG	BA	3146	1/1	0.20	-	57,57,57,57	0
57	MG	DA	3359	1/1	0.07	-	62,62,62,62	1
57	MG	AA	1644	1/1	0.33	-	110,110,110,110	0
57	MG	D2	603	1/1	0.28	-	95,95,95,95	0
57	MG	BA	3228	1/1	0.43	-	51,51,51,51	0
57	MG	BA	3092	1/1	0.24	-	28,28,28,28	0
57	MG	BA	3321	1/1	0.12	-	80,80,80,80	0
57	MG	BA	3014	1/1	0.26	-	61,61,61,61	0
57	MG	DA	3112	1/1	0.34	-	39,39,39,39	0
57	MG	DA	3262	1/1	0.47	-	73,73,73,73	0
57	MG	BA	3004	1/1	0.29	-	42,42,42,42	0
57	MG	DA	3040	1/1	0.21	-	25,25,25,25	0
57	MG	DA	3189	1/1	0.28	-	69,69,69,69	0
57	MG	DA	3258	1/1	0.38	-	37,37,37,37	0
57	MG	DA	3406	1/1	0.17	-	51,51,51,51	0
57	MG	AA	1641	1/1	0.68	-	83,83,83,83	0
57	MG	DA	3275	1/1	0.12	-	98,98,98,98	0
57	MG	DA	3403	1/1	0.17	-	55,55,55,55	0
57	MG	BA	3176	1/1	0.41	-	97,97,97,97	0
57	MG	AA	1736	1/1	0.22	-	87,87,87,87	0
57	MG	AA	1731	1/1	0.47	-	73,73,73,73	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	1753	1/1	0.19	-	103,103,103,103	0
57	MG	BA	3283	1/1	0.23	-	33,33,33,33	0
57	MG	BA	3363	1/1	0.14	-	73,73,73,73	0
57	MG	DA	3261	1/1	0.28	-	95,95,95,95	0
57	MG	DA	3287	1/1	0.25	-	148,148,148,148	0
57	MG	DA	3185	1/1	0.29	-	33,33,33,33	0
57	MG	BA	3208	1/1	0.44	-	61,61,61,61	0
57	MG	DA	3085	1/1	0.14	-	32,32,32,32	0
57	MG	DA	3004	1/1	0.67	-	86,86,86,86	0
57	MG	BA	3113	1/1	0.23	-	3,3,3,3	0
57	MG	BA	3235	1/1	0.59	-	156,156,156,156	0
57	MG	BA	3087	1/1	0.21	-	10,10,10,10	0
57	MG	DA	3015	1/1	0.46	-	79,79,79,79	0
57	MG	DA	3066	1/1	0.44	-	43,43,43,43	0
57	MG	BA	3305	1/1	1.31	-	101,101,101,101	0
57	MG	DA	3176	1/1	0.39	-	69,69,69,69	0
57	MG	CA	1708	1/1	0.12	-	89,89,89,89	0
57	MG	DA	3036	1/1	0.30	-	32,32,32,32	0
57	MG	DB	209	1/1	0.54	-	7,7,7,7	1
57	MG	BA	3407	1/1	0.22	-	52,52,52,52	0
57	MG	DC	301	1/1	0.26	-	91,91,91,91	1
57	MG	BA	3190	1/1	0.27	-	51,51,51,51	0
57	MG	DA	3197	1/1	0.62	-	106,106,106,106	0
57	MG	BA	3237	1/1	0.53	-	74,74,74,74	0
57	MG	CA	1624	1/1	0.26	-	55,55,55,55	0
57	MG	CA	1728	1/1	0.67	-	101,101,101,101	0
57	MG	AA	1759	1/1	0.32	-	96,96,96,96	0
57	MG	AA	1673	1/1	1.40	-	76,76,76,76	1
57	MG	BA	3053	1/1	0.40	-	64,64,64,64	0
57	MG	CA	1765	1/1	0.23	-	60,60,60,60	0
57	MG	CA	1745	1/1	0.92	-	115,115,115,115	0
57	MG	DA	3290	1/1	1.12	-	73,73,73,73	0
57	MG	AA	1797	1/1	0.54	-	53,53,53,53	0
57	MG	DA	3315	1/1	0.31	-	85,85,85,85	1
57	MG	CA	1612	1/1	0.16	-	91,91,91,91	0
57	MG	D7	102	1/1	0.86	-	62,62,62,62	1
57	MG	BA	3419	1/1	1.23	-	90,90,90,90	1
57	MG	DA	3345	1/1	0.41	-	43,43,43,43	1
57	MG	DA	3229	1/1	0.65	-	92,92,92,92	0
57	MG	CA	1611	1/1	0.38	-	110,110,110,110	0
57	MG	BA	3330	1/1	0.23	-	85,85,85,85	1
57	MG	CA	1644	1/1	0.41	-	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	1740	1/1	0.32	-	87,87,87,87	0
57	MG	DA	3361	1/1	0.13	-	64,64,64,64	0
57	MG	DA	3205	1/1	0.26	-	37,37,37,37	0
57	MG	DA	3115	1/1	0.25	-	22,22,22,22	0
57	MG	DA	3078	1/1	0.19	-	20,20,20,20	0
57	MG	BA	3131	1/1	0.27	-	31,31,31,31	0
57	MG	DA	3286	1/1	0.78	-	75,75,75,75	0
57	MG	AA	1713	1/1	0.15	-	53,53,53,53	0
57	MG	DA	3090	1/1	0.81	-	77,77,77,77	0
57	MG	DD	302	1/1	0.26	-	46,46,46,46	0
57	MG	DA	3017	1/1	0.46	-	31,31,31,31	0
57	MG	BA	3309	1/1	0.13	-	112,112,112,112	1
57	MG	AA	1767	1/1	0.30	-	44,44,44,44	0
57	MG	BA	3160	1/1	0.46	-	74,74,74,74	0
57	MG	CA	1741	1/1	0.18	-	53,53,53,53	0
57	MG	CA	1758	1/1	0.28	-	64,64,64,64	1
57	MG	CV	101	1/1	0.21	-	20,20,20,20	0
57	MG	AA	1763	1/1	0.18	-	62,62,62,62	0
57	MG	CA	1704	1/1	0.27	-	114,114,114,114	0
57	MG	DA	3177	1/1	0.46	-	77,77,77,77	0
57	MG	DA	3152	1/1	0.81	-	82,82,82,82	0
57	MG	DA	3171	1/1	0.24	-	43,43,43,43	0
57	MG	AA	1687	1/1	0.12	-	9,9,9,9	1
57	MG	AA	1730	1/1	0.31	-	107,107,107,107	0
57	MG	BA	3205	1/1	0.28	-	17,17,17,17	0
57	MG	DA	3178	1/1	0.26	-	88,88,88,88	0
57	MG	CA	1667	1/1	0.49	-	55,55,55,55	0
57	MG	BA	3277	1/1	0.77	-	35,35,35,35	1
57	MG	DA	3080	1/1	0.14	-	63,63,63,63	0
57	MG	DA	3232	1/1	0.28	-	93,93,93,93	0
57	MG	CA	1647	1/1	0.51	-	68,68,68,68	0
57	MG	DA	3074	1/1	0.27	-	26,26,26,26	0
57	MG	BA	3328	1/1	0.17	-	168,168,168,168	0
57	MG	CA	1798	1/1	0.21	-	55,55,55,55	0
57	MG	DA	3257	1/1	0.14	-	52,52,52,52	0
57	MG	BA	3323	1/1	0.35	-	86,86,86,86	1
57	MG	DA	3158	1/1	0.55	-	48,48,48,48	0
57	MG	BA	3002	1/1	0.16	-	139,139,139,139	0
57	MG	BA	3252	1/1	0.26	-	79,79,79,79	0
57	MG	DA	3082	1/1	0.29	-	59,59,59,59	0
57	MG	BA	3333	1/1	0.19	-	40,40,40,40	0
57	MG	CA	1720	1/1	0.23	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3298	1/1	0.54	-	69,69,69,69	0
57	MG	DA	3273	1/1	0.19	-	59,59,59,59	0
57	MG	DA	3353	1/1	0.59	-	107,107,107,107	0
57	MG	CA	1652	1/1	0.72	-	52,52,52,52	0
57	MG	CA	1681	1/1	0.50	-	49,49,49,49	0
57	MG	DA	3169	1/1	0.52	-	43,43,43,43	1
57	MG	BA	3413	1/1	0.59	-	33,33,33,33	0
57	MG	BA	3258	1/1	0.32	-	32,32,32,32	0
57	MG	CA	1764	1/1	0.21	-	68,68,68,68	1
57	MG	BA	3050	1/1	0.28	-	30,30,30,30	0
57	MG	CA	1682	1/1	0.72	-	90,90,90,90	0
57	MG	AA	1764	1/1	0.35	-	64,64,64,64	0
57	MG	D1	101	1/1	0.20	-	29,29,29,29	1
57	MG	AA	1689	1/1	0.51	-	118,118,118,118	0
57	MG	AA	1774	1/1	0.31	-	88,88,88,88	0
57	MG	DA	3260	1/1	0.92	-	81,81,81,81	0
57	MG	AA	1723	1/1	0.66	-	79,79,79,79	1
57	MG	DA	3227	1/1	1.32	-	136,136,136,136	0
57	MG	DA	3113	1/1	0.37	-	27,27,27,27	0
57	MG	DA	3131	1/1	0.21	-	23,23,23,23	0
57	MG	BA	3295	1/1	0.43	-	64,64,64,64	0
57	MG	BU	201	1/1	0.40	-	166,166,166,166	1
57	MG	BA	3374	1/1	0.06	-	92,92,92,92	0
57	MG	BA	3128	1/1	0.16	-	27,27,27,27	0
57	MG	BA	3174	1/1	0.20	-	55,55,55,55	0
57	MG	DA	3151	1/1	0.45	-	57,57,57,57	1
57	MG	DA	3268	1/1	0.09	-	41,41,41,41	0
58	PAR	CA	1800	42/42	0.25	-	86,91,109,113	0
57	MG	BA	3381	1/1	0.40	-	29,29,29,29	0
57	MG	DA	3391	1/1	0.09	-	120,120,120,120	0
57	MG	DA	3222	1/1	0.55	-	95,95,95,95	0
57	MG	BA	3099	1/1	0.21	-	37,37,37,37	0
57	MG	BA	3251	1/1	0.44	-	136,136,136,136	1
57	MG	DB	204	1/1	0.16	-	90,90,90,90	0
57	MG	BA	3365	1/1	0.18	-	1,1,1,1	0
57	MG	BA	3090	1/1	0.35	-	29,29,29,29	0
57	MG	AA	1639	1/1	0.29	-	99,99,99,99	0
57	MG	AA	1705	1/1	0.54	-	63,63,63,63	0
57	MG	AA	1732	1/1	0.52	-	61,61,61,61	0
57	MG	DA	3297	1/1	0.41	-	71,71,71,71	0
57	MG	AA	1789	1/1	0.28	-	81,81,81,81	1
57	MG	CA	1786	1/1	0.10	-	71,71,71,71	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3227	1/1	0.31	-	74,74,74,74	0
57	MG	CA	1693	1/1	0.14	-	87,87,87,87	0
57	MG	DA	3264	1/1	0.16	-	96,96,96,96	0
57	MG	AA	1630	1/1	0.23	-	55,55,55,55	0
57	MG	DA	3106	1/1	0.42	-	78,78,78,78	0
57	MG	BA	3185	1/1	0.21	-	1,1,1,1	0
57	MG	BA	3126	1/1	0.25	-	39,39,39,39	0
57	MG	BA	3352	1/1	0.73	-	23,23,23,23	1
57	MG	BA	3264	1/1	0.29	-	58,58,58,58	0
57	MG	DA	3304	1/1	0.41	-	49,49,49,49	0
57	MG	CA	1792	1/1	0.10	-	95,95,95,95	0
57	MG	DA	3140	1/1	0.24	-	90,90,90,90	0
57	MG	DA	3300	1/1	0.30	-	95,95,95,95	0
57	MG	AA	1751	1/1	0.41	-	72,72,72,72	1
57	MG	BA	3409	1/1	0.34	-	20,20,20,20	0
57	MG	CA	1641	1/1	0.41	-	64,64,64,64	0
57	MG	AA	1719	1/1	0.53	-	52,52,52,52	0
57	MG	CW	101	1/1	0.38	-	144,144,144,144	0
57	MG	AA	1667	1/1	0.47	-	72,72,72,72	0
57	MG	BA	3197	1/1	0.28	-	46,46,46,46	0
57	MG	BA	3011	1/1	0.31	-	32,32,32,32	0
57	MG	BA	3111	1/1	0.38	-	23,23,23,23	0
57	MG	DA	3314	1/1	0.20	-	141,141,141,141	0
57	MG	AA	1660	1/1	0.37	-	43,43,43,43	0
57	MG	DA	3378	1/1	0.34	-	72,72,72,72	0
57	MG	BA	3243	1/1	0.16	-	65,65,65,65	0
57	MG	DA	3028	1/1	0.41	-	47,47,47,47	0
57	MG	DA	3164	1/1	0.22	-	84,84,84,84	0
57	MG	CA	1743	1/1	0.52	-	65,65,65,65	0
57	MG	DB	210	1/1	0.26	-	74,74,74,74	0
57	MG	BA	3173	1/1	0.20	-	33,33,33,33	0
57	MG	CA	1621	1/1	0.13	-	58,58,58,58	0
57	MG	DA	3330	1/1	0.14	-	51,51,51,51	1
57	MG	AA	1748	1/1	0.32	-	144,144,144,144	1
57	MG	DB	213	1/1	0.49	-	93,93,93,93	0
57	MG	BB	207	1/1	0.50	-	29,29,29,29	1
57	MG	BA	3060	1/1	0.36	-	1,1,1,1	0
57	MG	DA	3156	1/1	0.48	-	38,38,38,38	0
57	MG	DA	3338	1/1	0.29	-	74,74,74,74	0
57	MG	BA	3139	1/1	0.17	-	85,85,85,85	0
57	MG	BA	3271	1/1	0.49	-	43,43,43,43	0
57	MG	DA	3238	1/1	0.29	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3014	1/1	0.16	-	31,31,31,31	0
57	MG	CA	1722	1/1	0.53	-	121,121,121,121	0
57	MG	AA	1609	1/1	0.19	-	36,36,36,36	0
57	MG	BA	3204	1/1	0.26	-	33,33,33,33	0
57	MG	BA	3368	1/1	0.22	-	61,61,61,61	0
57	MG	AA	1649	1/1	0.14	-	56,56,56,56	1
57	MG	DA	3146	1/1	0.31	-	55,55,55,55	0
57	MG	CA	1759	1/1	0.69	-	67,67,67,67	1
57	MG	BA	3066	1/1	0.34	-	26,26,26,26	0
57	MG	BA	3232	1/1	0.21	-	27,27,27,27	0
57	MG	BA	3281	1/1	0.40	-	53,53,53,53	0
57	MG	DA	3310	1/1	0.45	-	54,54,54,54	1
57	MG	AA	1787	1/1	0.10	-	41,41,41,41	1
57	MG	DA	3283	1/1	0.21	-	77,77,77,77	0
57	MG	DA	3206	1/1	0.21	-	33,33,33,33	0
57	MG	DA	3316	1/1	0.10	-	88,88,88,88	0
57	MG	BA	3076	1/1	0.19	-	25,25,25,25	0
57	MG	DA	3289	1/1	1.15	-	74,74,74,74	0
57	MG	AA	1712	1/1	0.30	-	61,61,61,61	0
57	MG	CA	1775	1/1	0.19	-	79,79,79,79	0
57	MG	AA	1674	1/1	0.15	-	42,42,42,42	0
57	MG	DA	3374	1/1	0.15	-	37,37,37,37	1
57	MG	DA	3059	1/1	0.36	-	46,46,46,46	0
57	MG	BA	3102	1/1	0.40	-	13,13,13,13	0
57	MG	DA	3019	1/1	0.48	-	29,29,29,29	0
57	MG	CA	1740	1/1	0.42	-	61,61,61,61	1
57	MG	BA	3348	1/1	0.19	-	79,79,79,79	0
57	MG	CA	1761	1/1	0.63	-	74,74,74,74	0
57	MG	BA	3372	1/1	0.41	-	57,57,57,57	1
57	MG	DA	3239	1/1	1.04	-	79,79,79,79	0
57	MG	DA	3182	1/1	0.58	-	60,60,60,60	0
57	MG	DA	3303	1/1	0.28	-	30,30,30,30	0
57	MG	CA	1711	1/1	0.15	-	74,74,74,74	0
57	MG	CA	1795	1/1	0.60	-	78,78,78,78	0
57	MG	AA	1776	1/1	0.27	-	103,103,103,103	0
57	MG	AA	1642	1/1	0.23	-	45,45,45,45	0
57	MG	BA	3161	1/1	0.24	-	86,86,86,86	0
57	MG	CA	1716	1/1	0.69	-	68,68,68,68	1
57	MG	BA	3073	1/1	0.15	-	5,5,5,5	0
57	MG	D2	602	1/1	0.30	-	99,99,99,99	0
57	MG	AN	101	1/1	0.24	-	50,50,50,50	0
57	MG	AV	104	1/1	0.48	-	127,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3334	1/1	0.30	-	79,79,79,79	0
57	MG	AA	1686	1/1	0.54	-	104,104,104,104	0
57	MG	BA	3353	1/1	0.45	-	79,79,79,79	0
57	MG	BA	3276	1/1	0.29	-	49,49,49,49	0
57	MG	CA	1610	1/1	0.12	-	88,88,88,88	0
57	MG	DA	3225	1/1	0.57	-	71,71,71,71	0
57	MG	BA	3125	1/1	0.25	-	62,62,62,62	0
57	MG	DA	3309	1/1	0.22	-	47,47,47,47	0
57	MG	CA	1603	1/1	0.24	-	68,68,68,68	0
57	MG	CA	1664	1/1	0.51	-	53,53,53,53	0
57	MG	AA	1698	1/1	0.13	-	42,42,42,42	0
57	MG	DA	3168	1/1	0.23	-	36,36,36,36	0
57	MG	BA	3100	1/1	0.48	-	49,49,49,49	0
57	MG	BA	3169	1/1	0.22	-	18,18,18,18	0
57	MG	CA	1778	1/1	0.35	-	66,66,66,66	0
57	MG	BA	3130	1/1	0.19	-	8,8,8,8	0
57	MG	DA	3043	1/1	0.21	-	51,51,51,51	0
57	MG	DA	3091	1/1	0.30	-	39,39,39,39	0
57	MG	DA	3333	1/1	0.14	-	108,108,108,108	0
57	MG	BA	3038	1/1	0.14	-	41,41,41,41	0
57	MG	BA	3137	1/1	0.17	-	33,33,33,33	0
57	MG	CA	1797	1/1	0.10	-	120,120,120,120	0
57	MG	AA	1737	1/1	1.75	-	136,136,136,136	0
57	MG	DA	3373	1/1	0.17	-	98,98,98,98	0
57	MG	CA	1666	1/1	0.69	-	87,87,87,87	0
57	MG	BA	3183	1/1	0.33	-	20,20,20,20	0
57	MG	CA	1677	1/1	0.14	-	48,48,48,48	0
57	MG	BA	3039	1/1	0.27	-	14,14,14,14	0
57	MG	CA	1619	1/1	0.16	-	80,80,80,80	0
57	MG	BA	3240	1/1	0.12	-	11,11,11,11	0
57	MG	DA	3252	1/1	0.12	-	95,95,95,95	0
57	MG	DA	3192	1/1	0.63	-	74,74,74,74	0
57	MG	AA	1788	1/1	0.21	-	73,73,73,73	0
57	MG	BA	3367	1/1	0.36	-	1,1,1,1	1
57	MG	BA	3212	1/1	0.35	-	88,88,88,88	0
57	MG	DA	3420	1/1	0.10	-	137,137,137,137	1
57	MG	DB	207	1/1	0.30	-	49,49,49,49	1
57	MG	CA	1785	1/1	0.31	-	95,95,95,95	0
57	MG	BA	3088	1/1	0.22	-	21,21,21,21	0
57	MG	AA	1618	1/1	0.30	-	38,38,38,38	0
57	MG	DA	3407	1/1	0.20	-	45,45,45,45	0
57	MG	AA	1685	1/1	0.25	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3237	1/1	0.17	-	156,156,156,156	0
57	MG	BA	3246	1/1	0.23	-	74,74,74,74	0
57	MG	CA	1721	1/1	0.46	-	97,97,97,97	0
57	MG	BA	3006	1/1	0.86	-	66,66,66,66	0
57	MG	BA	3191	1/1	0.17	-	14,14,14,14	0
57	MG	BA	3308	1/1	0.20	-	114,114,114,114	1
57	MG	BA	3052	1/1	0.32	-	13,13,13,13	0
57	MG	CA	1767	1/1	0.18	-	97,97,97,97	0
57	MG	DA	3037	1/1	0.20	-	45,45,45,45	0
57	MG	DA	3255	1/1	0.27	-	61,61,61,61	0
57	MG	AA	1728	1/1	0.30	-	67,67,67,67	0
57	MG	CA	1672	1/1	0.23	-	59,59,59,59	0
57	MG	BA	3196	1/1	0.68	-	130,130,130,130	1
57	MG	DA	3138	1/1	0.26	-	68,68,68,68	0
57	MG	DA	3389	1/1	1.08	-	113,113,113,113	0
57	MG	BA	3299	1/1	0.26	-	46,46,46,46	1
57	MG	BA	3214	1/1	0.51	-	83,83,83,83	0
57	MG	CN	101	1/1	0.15	-	57,57,57,57	0
57	MG	CA	1781	1/1	0.08	-	58,58,58,58	0
57	MG	CW	102	1/1	0.07	-	112,112,112,112	0
57	MG	DA	3320	1/1	0.29	-	34,34,34,34	1
57	MG	CA	1661	1/1	0.62	-	56,56,56,56	0
57	MG	AA	1790	1/1	0.11	-	63,63,63,63	0
57	MG	BA	3188	1/1	0.24	-	64,64,64,64	0
57	MG	CA	1713	1/1	0.17	-	73,73,73,73	0
57	MG	AA	1652	1/1	0.33	-	82,82,82,82	0
57	MG	DE	301	1/1	0.25	-	39,39,39,39	0
57	MG	AA	1690	1/1	0.30	-	81,81,81,81	0
57	MG	DA	3024	1/1	0.24	-	49,49,49,49	0
57	MG	DA	3062	1/1	0.32	-	33,33,33,33	0
57	MG	BA	3216	1/1	0.34	-	80,80,80,80	0
57	MG	BA	3138	1/1	1.02	-	124,124,124,124	0
57	MG	DA	3154	1/1	0.33	-	60,60,60,60	0
57	MG	AA	1747	1/1	0.15	-	135,135,135,135	0
57	MG	DA	3367	1/1	0.54	-	108,108,108,108	0
57	MG	DA	3174	1/1	0.11	-	53,53,53,53	0
57	MG	DA	3231	1/1	0.34	-	31,31,31,31	0
57	MG	DA	3098	1/1	0.61	-	38,38,38,38	0
57	MG	DA	3385	1/1	0.25	-	79,79,79,79	0
57	MG	CA	1727	1/1	0.88	-	139,139,139,139	0
57	MG	BB	214	1/1	0.57	-	75,75,75,75	1
57	MG	DA	3365	1/1	0.25	-	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3398	1/1	0.65	-	86,86,86,86	0
57	MG	DA	3132	1/1	0.33	-	41,41,41,41	0
57	MG	CA	1736	1/1	0.54	-	73,73,73,73	0
57	MG	AA	1795	1/1	0.49	-	128,128,128,128	0
57	MG	CA	1788	1/1	0.26	-	75,75,75,75	0
57	MG	BA	3059	1/1	0.22	-	9,9,9,9	0
57	MG	AA	1668	1/1	0.31	-	51,51,51,51	0
57	MG	BA	3416	1/1	0.31	-	93,93,93,93	0
57	MG	DA	3221	1/1	0.51	-	50,50,50,50	0
57	MG	DA	3096	1/1	0.21	-	24,24,24,24	0
57	MG	DX	103	1/1	0.51	-	102,102,102,102	0
57	MG	DA	3033	1/1	0.39	-	70,70,70,70	0
57	MG	BA	3345	1/1	0.41	-	69,69,69,69	1
57	MG	CA	1762	1/1	0.39	-	84,84,84,84	0
57	MG	DA	3217	1/1	0.28	-	62,62,62,62	0
57	MG	AV	105	1/1	0.87	-	89,89,89,89	0
57	MG	DA	3108	1/1	0.79	-	83,83,83,83	0
57	MG	BB	211	1/1	0.15	-	119,119,119,119	0
57	MG	BA	3396	1/1	0.27	-	11,11,11,11	0
57	MG	AA	1729	1/1	0.39	-	69,69,69,69	0
57	MG	CA	1699	1/1	0.16	-	50,50,50,50	0
57	MG	BA	3312	1/1	0.35	-	102,102,102,102	0
57	MG	CA	1752	1/1	0.23	-	112,112,112,112	1
57	MG	AA	1621	1/1	0.29	-	50,50,50,50	0
57	MG	DA	3342	1/1	0.26	-	90,90,90,90	0
57	MG	CA	1769	1/1	0.30	-	27,27,27,27	0
57	MG	BA	3078	1/1	0.18	-	13,13,13,13	0
57	MG	DA	3016	1/1	0.27	-	51,51,51,51	0
57	MG	BA	3380	1/1	0.60	-	54,54,54,54	0
57	MG	AA	1744	1/1	0.57	-	84,84,84,84	0
57	MG	CA	1772	1/1	0.24	-	77,77,77,77	0
57	MG	BA	3114	1/1	0.43	-	3,3,3,3	0
57	MG	DA	3272	1/1	0.42	-	108,108,108,108	0
57	MG	CA	1646	1/1	0.22	-	81,81,81,81	0
57	MG	AA	1743	1/1	0.60	-	86,86,86,86	0
57	MG	BA	3044	1/1	0.28	-	1,1,1,1	0
57	MG	CA	1676	1/1	0.44	-	71,71,71,71	0
57	MG	DA	3380	1/1	0.42	-	52,52,52,52	0
57	MG	CA	1729	1/1	0.22	-	70,70,70,70	1
57	MG	DA	3123	1/1	0.39	-	89,89,89,89	0
57	MG	DA	3026	1/1	0.26	-	19,19,19,19	0
57	MG	CA	1702	1/1	0.43	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3101	1/1	0.34	-	67,67,67,67	0
57	MG	BB	203	1/1	0.47	-	14,14,14,14	1
57	MG	DA	3328	1/1	0.58	-	50,50,50,50	0
57	MG	CA	1717	1/1	0.12	-	82,82,82,82	0
57	MG	CA	1626	1/1	0.24	-	34,34,34,34	0
57	MG	BA	3220	1/1	0.45	-	95,95,95,95	0
57	MG	DA	3021	1/1	0.16	-	35,35,35,35	0
57	MG	BA	3143	1/1	0.27	-	49,49,49,49	1
57	MG	CA	1687	1/1	0.40	-	84,84,84,84	0
57	MG	DA	3404	1/1	0.08	-	97,97,97,97	1
57	MG	BA	3025	1/1	0.49	-	9,9,9,9	0
57	MG	BA	3261	1/1	0.55	-	23,23,23,23	0
57	MG	AE	201	1/1	0.11	-	101,101,101,101	0
57	MG	BA	3067	1/1	0.70	-	53,53,53,53	0
57	MG	AA	1683	1/1	0.25	-	101,101,101,101	0
57	MG	DA	3167	1/1	0.12	-	37,37,37,37	0
57	MG	CA	1618	1/1	0.28	-	53,53,53,53	0
57	MG	BA	3273	1/1	0.09	-	75,75,75,75	0
57	MG	AA	1671	1/1	0.30	-	73,73,73,73	0
57	MG	BA	3398	1/1	0.33	-	84,84,84,84	0
57	MG	DA	3162	1/1	0.31	-	77,77,77,77	0
57	MG	BA	3108	1/1	0.20	-	4,4,4,4	0
57	MG	CA	1723	1/1	0.33	-	86,86,86,86	0
57	MG	BA	3061	1/1	0.30	-	10,10,10,10	0
57	MG	BA	3294	1/1	0.39	-	33,33,33,33	0
57	MG	BA	3211	1/1	0.17	-	40,40,40,40	0
57	MG	BN	201	1/1	0.59	-	64,64,64,64	0
57	MG	DA	3411	1/1	0.07	-	46,46,46,46	0
57	MG	CA	1602	1/1	0.77	-	101,101,101,101	0
57	MG	AA	1629	1/1	0.29	-	62,62,62,62	0
57	MG	DA	3109	1/1	0.21	-	29,29,29,29	0
57	MG	DA	3111	1/1	1.63	-	111,111,111,111	0
57	MG	BA	3024	1/1	0.42	-	11,11,11,11	0
57	MG	DA	3265	1/1	0.31	-	71,71,71,71	0
57	MG	BA	3186	1/1	0.28	-	144,144,144,144	0
57	MG	BA	3399	1/1	0.60	-	64,64,64,64	0
57	MG	BA	3384	1/1	0.32	-	53,53,53,53	0
57	MG	CA	1678	1/1	0.43	-	94,94,94,94	0
57	MG	DA	3064	1/1	0.16	-	32,32,32,32	0
57	MG	BA	3152	1/1	0.50	-	93,93,93,93	0
57	MG	DA	3250	1/1	0.41	-	63,63,63,63	1
57	MG	BA	3378	1/1	0.39	-	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3164	1/1	0.16	-	56,56,56,56	0
57	MG	DA	3204	1/1	0.41	-	39,39,39,39	0
57	MG	DA	3245	1/1	0.25	-	69,69,69,69	0
57	MG	AA	1678	1/1	0.12	-	166,166,166,166	0
57	MG	AA	1606	1/1	0.11	-	34,34,34,34	0
57	MG	BA	3136	1/1	0.23	-	16,16,16,16	0
57	MG	BA	3009	1/1	0.32	-	17,17,17,17	0
57	MG	BA	3077	1/1	0.15	-	1,1,1,1	0
57	MG	BA	3241	1/1	0.49	-	70,70,70,70	0
57	MG	DA	3421	1/1	0.19	-	168,168,168,168	0
57	MG	DA	3084	1/1	0.41	-	44,44,44,44	0
57	MG	BA	3405	1/1	0.36	-	164,164,164,164	1
57	MG	DA	3215	1/1	0.07	-	68,68,68,68	1
57	MG	CA	1689	1/1	0.14	-	40,40,40,40	0
57	MG	CA	1724	1/1	0.19	-	80,80,80,80	0
57	MG	DA	3284	1/1	0.41	-	74,74,74,74	0
57	MG	DA	3213	1/1	0.40	-	89,89,89,89	0
57	MG	DA	3081	1/1	0.32	-	38,38,38,38	0
57	MG	DA	3038	1/1	0.21	-	49,49,49,49	0
57	MG	DA	3267	1/1	0.17	-	71,71,71,71	0
57	MG	AX	101	1/1	0.08	-	118,118,118,118	0
57	MG	DA	3263	1/1	0.86	-	69,69,69,69	0
57	MG	DA	3296	1/1	0.64	-	138,138,138,138	0
57	MG	BA	3338	1/1	0.37	-	52,52,52,52	0
57	MG	CA	1662	1/1	0.62	-	80,80,80,80	0
57	MG	BA	3203	1/1	0.13	-	30,30,30,30	0
57	MG	CA	1616	1/1	0.39	-	43,43,43,43	0
57	MG	DA	3364	1/1	0.22	-	52,52,52,52	0
57	MG	DO	201	1/1	0.37	-	85,85,85,85	0
57	MG	BA	3410	1/1	0.40	-	120,120,120,120	0
57	MG	BA	3202	1/1	0.42	-	16,16,16,16	0
57	MG	CA	1714	1/1	0.11	-	62,62,62,62	0
57	MG	BA	3245	1/1	0.12	-	42,42,42,42	0
57	MG	DA	3122	1/1	0.56	-	77,77,77,77	0
57	MG	CA	1620	1/1	0.25	-	59,59,59,59	0
57	MG	AA	1765	1/1	0.19	-	94,94,94,94	0
57	MG	DA	3118	1/1	0.60	-	62,62,62,62	0
57	MG	BB	202	1/1	0.43	-	92,92,92,92	0
57	MG	AA	1651	1/1	0.69	-	70,70,70,70	0
57	MG	AA	1784	1/1	0.05	-	81,81,81,81	1
57	MG	DA	3029	1/1	0.41	-	40,40,40,40	0
57	MG	DA	3417	1/1	0.07	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	1715	1/1	0.66	-	39,39,39,39	1
57	MG	BA	3035	1/1	0.23	-	2,2,2,2	0
57	MG	CA	1780	1/1	0.56	-	32,32,32,32	1
57	MG	CA	1755	1/1	0.17	-	107,107,107,107	0
57	MG	BA	3168	1/1	0.49	-	87,87,87,87	0
57	MG	CA	1783	1/1	0.35	-	105,105,105,105	0
57	MG	AA	1768	1/1	0.42	-	71,71,71,71	0
57	MG	BA	3135	1/1	0.62	-	36,36,36,36	0
57	MG	CW	105	1/1	0.34	-	70,70,70,70	1
57	MG	BB	205	1/1	0.21	-	25,25,25,25	0
57	MG	AA	1742	1/1	0.40	-	100,100,100,100	0
57	MG	CA	1760	1/1	0.23	-	145,145,145,145	0
57	MG	DA	3324	1/1	0.38	-	64,64,64,64	1
59	ZN	AD	302	1/1	0.23	-	55,55,55,55	0
57	MG	CA	1750	1/1	0.25	-	77,77,77,77	1
57	MG	AA	1657	1/1	0.56	-	121,121,121,121	0
57	MG	BA	3042	1/1	0.15	-	36,36,36,36	0
57	MG	BO	201	1/1	0.23	-	29,29,29,29	0
57	MG	DA	3161	1/1	0.32	-	65,65,65,65	0
57	MG	AA	1720	1/1	0.28	-	137,137,137,137	0
57	MG	AA	1603	1/1	0.72	-	84,84,84,84	0
57	MG	AA	1757	1/1	0.84	-	87,87,87,87	1
57	MG	BA	3253	1/1	0.37	-	87,87,87,87	0
57	MG	BA	3256	1/1	0.34	-	11,11,11,11	0
57	MG	DA	3073	1/1	0.18	-	36,36,36,36	0
57	MG	DA	3271	1/1	0.35	-	47,47,47,47	0
57	MG	BA	3219	1/1	0.57	-	30,30,30,30	0
57	MG	DA	3302	1/1	0.19	-	43,43,43,43	1
57	MG	BA	3332	1/1	0.50	-	29,29,29,29	0
57	MG	D7	101	1/1	0.42	-	73,73,73,73	0
57	MG	BA	3097	1/1	0.30	-	7,7,7,7	0
57	MG	BA	3170	1/1	0.36	-	61,61,61,61	0
57	MG	BA	3083	1/1	0.36	-	30,30,30,30	0
57	MG	DA	3413	1/1	0.24	-	84,84,84,84	0
57	MG	DA	3343	1/1	0.20	-	71,71,71,71	0
57	MG	CA	1770	1/1	0.48	-	94,94,94,94	0
57	MG	AA	1696	1/1	0.10	-	47,47,47,47	0
57	MG	DA	3293	1/1	0.23	-	74,74,74,74	0
57	MG	CA	1799	1/1	0.28	-	75,75,75,75	0
57	MG	CA	1622	1/1	0.36	-	117,117,117,117	0
57	MG	CA	1790	1/1	0.19	-	48,48,48,48	0
57	MG	BA	3266	1/1	0.29	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3351	1/1	0.53	-	94,94,94,94	0
57	MG	BA	3005	1/1	0.42	-	7,7,7,7	0
57	MG	CA	1690	1/1	0.85	-	110,110,110,110	0
57	MG	DA	3193	1/1	0.28	-	48,48,48,48	0
57	MG	CA	1737	1/1	0.25	-	87,87,87,87	0
57	MG	BA	3020	1/1	0.25	-	28,28,28,28	0
57	MG	DB	202	1/1	0.26	-	113,113,113,113	0
57	MG	BA	3302	1/1	0.24	-	26,26,26,26	0
57	MG	DA	3163	1/1	0.33	-	52,52,52,52	0
57	MG	BA	3231	1/1	0.64	-	38,38,38,38	0
57	MG	DA	3274	1/1	0.25	-	60,60,60,60	0
57	MG	AA	1735	1/1	0.30	-	108,108,108,108	0
57	MG	DA	3133	1/1	0.24	-	35,35,35,35	0
57	MG	DA	3022	1/1	0.32	-	34,34,34,34	0
57	MG	CA	1613	1/1	0.53	-	51,51,51,51	0
57	MG	AA	1793	1/1	0.33	-	91,91,91,91	0
57	MG	AA	1662	1/1	0.08	-	95,95,95,95	0
57	MG	BA	3055	1/1	0.30	-	18,18,18,18	0
57	MG	DA	3395	1/1	0.34	-	49,49,49,49	0
57	MG	DA	3063	1/1	0.49	-	32,32,32,32	0
57	MG	AA	1666	1/1	0.43	-	93,93,93,93	0
59	ZN	B9	101	1/1	0.04	-	94,94,94,94	0
57	MG	DA	3050	1/1	0.14	-	69,69,69,69	1
57	MG	DA	3088	1/1	0.39	-	37,37,37,37	0
57	MG	BA	3404	1/1	0.18	-	56,56,56,56	0
57	MG	AA	1754	1/1	0.31	-	64,64,64,64	0
57	MG	CA	1645	1/1	0.71	-	66,66,66,66	0
57	MG	BA	3394	1/1	0.46	-	81,81,81,81	1
57	MG	DA	3226	1/1	0.40	-	88,88,88,88	0
57	MG	DA	3046	1/1	0.56	-	30,30,30,30	0
57	MG	BA	3089	1/1	0.59	-	43,43,43,43	0
57	MG	CA	1739	1/1	0.47	-	128,128,128,128	0
57	MG	BA	3018	1/1	0.47	-	9,9,9,9	0
57	MG	BA	3291	1/1	0.34	-	42,42,42,42	0
57	MG	BA	3234	1/1	0.50	-	56,56,56,56	0
57	MG	BA	3048	1/1	0.66	-	33,33,33,33	0
57	MG	DA	3208	1/1	0.19	-	32,32,32,32	0
57	MG	DA	3060	1/1	0.30	-	30,30,30,30	0
57	MG	DA	3416	1/1	0.12	-	81,81,81,81	0
57	MG	AA	1703	1/1	0.12	-	38,38,38,38	0
57	MG	BA	3116	1/1	0.12	-	4,4,4,4	0
57	MG	CA	1771	1/1	0.71	-	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3147	1/1	0.30	-	59,59,59,59	0
57	MG	DA	3005	1/1	0.27	-	52,52,52,52	0
57	MG	AA	1782	1/1	0.18	-	96,96,96,96	1
57	MG	BA	3238	1/1	0.32	-	51,51,51,51	0
57	MG	DA	3340	1/1	0.58	-	98,98,98,98	1
57	MG	DB	201	1/1	0.18	-	74,74,74,74	0
57	MG	BA	3272	1/1	0.24	-	46,46,46,46	0
57	MG	BA	3033	1/1	0.37	-	33,33,33,33	0
57	MG	DA	3075	1/1	0.21	-	37,37,37,37	0
57	MG	DA	3331	1/1	0.31	-	155,155,155,155	1
57	MG	CW	103	1/1	0.20	-	87,87,87,87	0
57	MG	AA	1739	1/1	0.31	-	115,115,115,115	0
57	MG	BA	3016	1/1	0.47	-	28,28,28,28	0
57	MG	DA	3251	1/1	0.16	-	96,96,96,96	0
57	MG	CA	1751	1/1	0.16	-	66,66,66,66	1
57	MG	DA	3368	1/1	0.31	-	45,45,45,45	1
57	MG	AA	1675	1/1	0.60	-	63,63,63,63	0
57	MG	BA	3142	1/1	0.47	-	20,20,20,20	0
57	MG	DA	3352	1/1	0.51	-	20,20,20,20	1
57	MG	CA	1725	1/1	0.37	-	116,116,116,116	1
57	MG	DA	3025	1/1	0.47	-	13,13,13,13	0
57	MG	BA	3383	1/1	0.91	-	101,101,101,101	0
57	MG	AA	1778	1/1	0.61	-	65,65,65,65	1
57	MG	BA	3239	1/1	0.31	-	20,20,20,20	0
57	MG	DA	3415	1/1	0.33	-	96,96,96,96	0
57	MG	BA	3096	1/1	0.14	-	1,1,1,1	0
57	MG	CA	1663	1/1	0.06	-	53,53,53,53	0
57	MG	CA	1749	1/1	0.15	-	98,98,98,98	0
57	MG	BA	3314	1/1	0.45	-	92,92,92,92	1
57	MG	BA	3122	1/1	0.49	-	94,94,94,94	0
57	MG	DA	3285	1/1	0.22	-	71,71,71,71	0
57	MG	DA	3067	1/1	0.57	-	46,46,46,46	0
57	MG	AA	1726	1/1	0.45	-	71,71,71,71	0
57	MG	CA	1709	1/1	0.27	-	73,73,73,73	0
57	MG	BA	3343	1/1	0.12	-	37,37,37,37	0
57	MG	B2	601	1/1	0.22	-	55,55,55,55	1
57	MG	AA	1721	1/1	0.51	-	90,90,90,90	0
57	MG	DA	3266	1/1	0.26	-	84,84,84,84	0
57	MG	DA	3149	1/1	0.29	-	57,57,57,57	0
57	MG	AA	1663	1/1	0.57	-	47,47,47,47	0
57	MG	BA	3132	1/1	0.20	-	14,14,14,14	0
57	MG	DA	3198	1/1	0.41	-	58,58,58,58	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	1785	1/1	0.20	-	105,105,105,105	0
57	MG	DA	3311	1/1	0.16	-	65,65,65,65	1
57	MG	DA	3130	1/1	0.30	-	41,41,41,41	0
57	MG	BA	3080	1/1	0.29	-	26,26,26,26	0
57	MG	CA	1685	1/1	0.19	-	62,62,62,62	0
57	MG	DA	3031	1/1	0.33	-	41,41,41,41	0
57	MG	AA	1707	1/1	0.34	-	116,116,116,116	0
57	MG	BA	3364	1/1	0.14	-	35,35,35,35	0
57	MG	DA	3288	1/1	0.67	-	37,37,37,37	0
57	MG	BA	3172	1/1	0.21	-	52,52,52,52	0
57	MG	BA	3418	1/1	0.08	-	59,59,59,59	0
57	MG	AA	1691	1/1	0.11	-	27,27,27,27	0
57	MG	AX	102	1/1	0.34	-	83,83,83,83	0
57	MG	BA	3403	1/1	0.23	-	65,65,65,65	0
57	MG	DA	3301	1/1	0.82	-	84,84,84,84	0
57	MG	DA	3230	1/1	0.67	-	71,71,71,71	0
57	MG	CA	1627	1/1	0.39	-	78,78,78,78	0
57	MG	BA	3379	1/1	0.22	-	36,36,36,36	0
57	MG	AA	1701	1/1	0.75	-	92,92,92,92	0
57	MG	AA	1733	1/1	0.92	-	141,141,141,141	0
57	MG	AA	1604	1/1	0.14	-	55,55,55,55	0
57	MG	BA	3209	1/1	0.40	-	14,14,14,14	0
57	MG	BA	3151	1/1	0.43	-	45,45,45,45	1
57	MG	DA	3357	1/1	0.14	-	111,111,111,111	0
57	MG	CA	1630	1/1	0.34	-	84,84,84,84	0
57	MG	BA	3249	1/1	0.42	-	114,114,114,114	0
57	MG	CA	1791	1/1	0.10	-	85,85,85,85	1
57	MG	BA	3225	1/1	0.64	-	128,128,128,128	0
57	MG	DA	3306	1/1	0.18	-	51,51,51,51	0
57	MG	AW	107	1/1	0.39	-	101,101,101,101	0
57	MG	BA	3062	1/1	0.55	-	31,31,31,31	0
57	MG	BA	3320	1/1	0.24	-	141,141,141,141	0
57	MG	BA	3313	1/1	0.31	-	162,162,162,162	0
57	MG	CA	1605	1/1	0.12	-	47,47,47,47	0
57	MG	DA	3207	1/1	0.25	-	67,67,67,67	0
57	MG	DA	3386	1/1	0.71	-	115,115,115,115	0
57	MG	DA	3181	1/1	0.23	-	100,100,100,100	0
57	MG	CL	201	1/1	0.84	-	91,91,91,91	0
57	MG	DA	3032	1/1	0.51	-	66,66,66,66	0
57	MG	DA	3376	1/1	0.46	-	110,110,110,110	0
57	MG	AA	1628	1/1	0.09	-	37,37,37,37	0
57	MG	DA	3055	1/1	0.14	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3327	1/1	0.89	-	67,67,67,67	0
57	MG	DS	201	1/1	0.31	-	74,74,74,74	1
57	MG	DA	3366	1/1	0.07	-	29,29,29,29	1
57	MG	CA	1607	1/1	0.16	-	30,30,30,30	0
57	MG	BA	3412	1/1	0.09	-	30,30,30,30	0
57	MG	BA	3110	1/1	0.19	-	44,44,44,44	0
57	MG	DA	3065	1/1	0.16	-	17,17,17,17	0
57	MG	BB	209	1/1	0.53	-	1,1,1,1	1
57	MG	DA	3387	1/1	0.52	-	66,66,66,66	0
57	MG	CA	1763	1/1	0.28	-	98,98,98,98	0
57	MG	BA	3247	1/1	0.33	-	49,49,49,49	0
57	MG	AA	1637	1/1	0.11	-	58,58,58,58	0
57	MG	D5	101	1/1	0.22	-	51,51,51,51	0
57	MG	AW	101	1/1	0.27	-	157,157,157,157	0
57	MG	BA	3165	1/1	0.13	-	38,38,38,38	0
57	MG	AA	1798	1/1	0.57	-	90,90,90,90	0
57	MG	DA	3399	1/1	0.28	-	119,119,119,119	0
57	MG	BA	3392	1/1	0.12	-	139,139,139,139	0
57	MG	BA	3414	1/1	0.10	-	60,60,60,60	0
57	MG	CW	106	1/1	0.18	-	86,86,86,86	1
57	MG	DA	3279	1/1	0.94	-	49,49,49,49	1
57	MG	BA	3155	1/1	0.91	-	116,116,116,116	0
57	MG	AA	1631	1/1	0.36	-	54,54,54,54	0
57	MG	AA	1724	1/1	0.33	-	68,68,68,68	1
57	MG	CA	1637	1/1	0.11	-	83,83,83,83	0
57	MG	CA	1766	1/1	0.15	-	96,96,96,96	0
57	MG	CA	1670	1/1	0.13	-	69,69,69,69	0
57	MG	AA	1750	1/1	0.33	-	62,62,62,62	1
57	MG	CA	1651	1/1	0.18	-	85,85,85,85	0
57	MG	CA	1746	1/1	0.46	-	91,91,91,91	0
57	MG	BA	3119	1/1	0.23	-	35,35,35,35	0
57	MG	BA	3071	1/1	0.29	-	52,52,52,52	0
57	MG	B5	102	1/1	0.48	-	58,58,58,58	1
57	MG	BA	3192	1/1	0.17	-	21,21,21,21	0
57	MG	DA	3199	1/1	0.92	-	101,101,101,101	0
57	MG	BA	3279	1/1	0.30	-	53,53,53,53	0
57	MG	BA	3317	1/1	0.15	-	167,167,167,167	0
57	MG	BA	3255	1/1	0.39	-	37,37,37,37	0
57	MG	AA	1626	1/1	0.17	-	37,37,37,37	0
57	MG	BA	3150	1/1	0.41	-	64,64,64,64	0
57	MG	DA	3134	1/1	0.20	-	57,57,57,57	0
57	MG	DA	3042	1/1	0.30	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3010	1/1	0.41	-	41,41,41,41	0
57	MG	AA	1752	1/1	0.35	-	120,120,120,120	1
57	MG	DA	3372	1/1	0.40	-	120,120,120,120	1
57	MG	DA	3148	1/1	0.37	-	46,46,46,46	0
57	MG	BA	3265	1/1	0.15	-	30,30,30,30	0
57	MG	BA	3103	1/1	0.20	-	31,31,31,31	0
57	MG	BA	3162	1/1	0.12	-	79,79,79,79	0
57	MG	DA	3327	1/1	1.02	-	64,64,64,64	1
57	MG	AA	1672	1/1	0.94	-	125,125,125,125	1
57	MG	DA	3003	1/1	0.21	-	91,91,91,91	0
57	MG	AA	1779	1/1	0.13	-	90,90,90,90	0
57	MG	DA	3325	1/1	0.28	-	83,83,83,83	1
57	MG	DA	3219	1/1	0.35	-	99,99,99,99	0
57	MG	DA	3165	1/1	0.17	-	78,78,78,78	0
57	MG	CA	1655	1/1	0.59	-	94,94,94,94	1
57	MG	BA	3158	1/1	0.71	-	55,55,55,55	0
57	MG	AD	301	1/1	0.46	-	155,155,155,155	0
57	MG	DA	3371	1/1	0.10	-	61,61,61,61	1
57	MG	BA	3329	1/1	0.16	-	126,126,126,126	0
57	MG	BA	3357	1/1	0.16	-	84,84,84,84	0
57	MG	BA	3270	1/1	0.43	-	76,76,76,76	0
57	MG	AA	1614	1/1	0.41	-	14,14,14,14	0
57	MG	BA	3420	1/1	0.11	-	78,78,78,78	0
57	MG	BB	204	1/1	0.24	-	106,106,106,106	0
57	MG	BA	3268	1/1	0.28	-	34,34,34,34	0
57	MG	DA	3388	1/1	0.24	-	68,68,68,68	0
57	MG	DA	3093	1/1	0.21	-	36,36,36,36	0
57	MG	AA	1684	1/1	0.17	-	74,74,74,74	0
57	MG	AA	1677	1/1	0.29	-	89,89,89,89	0
57	MG	DA	3007	1/1	0.65	-	59,59,59,59	0
57	MG	DA	3077	1/1	0.14	-	29,29,29,29	0
57	MG	BA	3339	1/1	0.78	-	125,125,125,125	1
57	MG	DA	3072	1/1	0.51	-	94,94,94,94	0
57	MG	DA	3087	1/1	0.37	-	84,84,84,84	0
57	MG	AA	1773	1/1	0.37	-	72,72,72,72	0
57	MG	BA	3199	1/1	0.65	-	116,116,116,116	0
57	MG	DA	3143	1/1	0.37	-	18,18,18,18	0
57	MG	BA	3280	1/1	0.12	-	28,28,28,28	0
57	MG	DA	3124	1/1	0.61	-	28,28,28,28	0
57	MG	DA	3013	1/1	0.35	-	31,31,31,31	0
57	MG	CA	1789	1/1	0.52	-	64,64,64,64	1
57	MG	BA	3175	1/1	0.35	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3064	1/1	0.31	-	20,20,20,20	0
57	MG	DA	3153	1/1	0.42	-	60,60,60,60	1
57	MG	AA	1796	1/1	0.54	-	121,121,121,121	0
57	MG	AA	1771	1/1	0.51	-	40,40,40,40	0
57	MG	DA	3299	1/1	0.50	-	93,93,93,93	0
57	MG	AA	1738	1/1	0.34	-	55,55,55,55	1
57	MG	DA	3027	1/1	0.42	-	37,37,37,37	0
57	MG	BA	3248	1/1	0.25	-	50,50,50,50	1
57	MG	DB	206	1/1	0.10	-	75,75,75,75	0
57	MG	AA	1605	1/1	0.10	-	120,120,120,120	0
57	MG	BA	3221	1/1	0.54	-	80,80,80,80	1
57	MG	DA	3053	1/1	0.16	-	26,26,26,26	0
57	MG	AA	1619	1/1	0.43	-	65,65,65,65	0
57	MG	AA	1780	1/1	0.33	-	115,115,115,115	0
57	MG	BA	3386	1/1	0.09	-	76,76,76,76	0
57	MG	DA	3390	1/1	0.18	-	48,48,48,48	0
57	MG	DA	3408	1/1	0.38	-	44,44,44,44	0
57	MG	BA	3091	1/1	0.46	-	41,41,41,41	0
57	MG	BA	3335	1/1	0.10	-	62,62,62,62	0
57	MG	DA	3099	1/1	0.28	-	40,40,40,40	0
57	MG	BA	3081	1/1	0.20	-	7,7,7,7	0
57	MG	DA	3308	1/1	0.15	-	53,53,53,53	0
57	MG	BA	3109	1/1	0.18	-	39,39,39,39	0
57	MG	BA	3184	1/1	0.35	-	38,38,38,38	0
57	MG	B1	101	1/1	0.10	-	41,41,41,41	1
57	MG	BA	3021	1/1	0.35	-	30,30,30,30	0
57	MG	BA	3193	1/1	0.17	-	40,40,40,40	0
57	MG	DA	3071	1/1	0.52	-	23,23,23,23	0
57	MG	DA	3170	1/1	0.67	-	60,60,60,60	0
57	MG	DA	3235	1/1	0.30	-	30,30,30,30	0
57	MG	DA	3160	1/1	0.41	-	67,67,67,67	0
57	MG	BE	301	1/1	0.19	-	30,30,30,30	0
57	MG	BA	3201	1/1	0.12	-	35,35,35,35	0
57	MG	CA	1688	1/1	0.61	-	15,15,15,15	1
57	MG	DA	3418	1/1	0.58	-	47,47,47,47	1
57	MG	DA	3242	1/1	0.18	-	18,18,18,18	0
57	MG	AV	101	1/1	0.14	-	36,36,36,36	0
57	MG	AA	1633	1/1	0.15	-	40,40,40,40	0
57	MG	BA	3026	1/1	0.32	-	8,8,8,8	0
57	MG	BA	3046	1/1	0.26	-	4,4,4,4	0
57	MG	BA	3347	1/1	0.28	-	42,42,42,42	0
57	MG	BA	3402	1/1	0.10	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3355	1/1	0.18	-	95,95,95,95	0
57	MG	B2	602	1/1	0.53	-	55,55,55,55	0
57	MG	CA	1668	1/1	0.98	-	99,99,99,99	0
57	MG	BA	3207	1/1	0.17	-	45,45,45,45	0
57	MG	BA	3063	1/1	0.14	-	1,1,1,1	0
57	MG	AW	103	1/1	0.08	-	106,106,106,106	0
57	MG	AA	1694	1/1	0.46	-	84,84,84,84	0
57	MG	DA	3319	1/1	0.61	-	102,102,102,102	1
57	MG	AA	1654	1/1	0.30	-	52,52,52,52	1
57	MG	CA	1643	1/1	0.18	-	157,157,157,157	0
57	MG	BA	3023	1/1	0.33	-	23,23,23,23	0
57	MG	DA	3044	1/1	0.19	-	40,40,40,40	0
57	MG	CA	1734	1/1	0.68	-	67,67,67,67	0
57	MG	BA	3075	1/1	0.33	-	31,31,31,31	0
57	MG	CA	1691	1/1	0.24	-	110,110,110,110	0
57	MG	CA	1779	1/1	0.28	-	115,115,115,115	0
57	MG	BA	3292	1/1	0.17	-	23,23,23,23	0
57	MG	AA	1688	1/1	0.25	-	35,35,35,35	0
57	MG	BA	3072	1/1	0.11	-	3,3,3,3	0
57	MG	CA	1695	1/1	0.38	-	54,54,54,54	0
57	MG	BA	3269	1/1	0.32	-	38,38,38,38	0
57	MG	DA	3419	1/1	0.09	-	115,115,115,115	0
57	MG	CA	1732	1/1	0.08	-	82,82,82,82	0
57	MG	AA	1762	1/1	0.44	-	80,80,80,80	1
57	MG	AA	1648	1/1	0.35	-	87,87,87,87	0
57	MG	BA	3178	1/1	0.26	-	24,24,24,24	0
57	MG	DA	3079	1/1	0.14	-	37,37,37,37	0
57	MG	DA	3097	1/1	0.08	-	25,25,25,25	0
57	MG	DA	3294	1/1	0.26	-	54,54,54,54	0
57	MG	DN	201	1/1	2.48	-	129,129,129,129	0
57	MG	DA	3142	1/1	0.43	-	65,65,65,65	0
57	MG	BA	3141	1/1	0.26	-	56,56,56,56	0
57	MG	DA	3356	1/1	0.17	-	57,57,57,57	0
57	MG	CA	1756	1/1	0.35	-	53,53,53,53	0
57	MG	BA	3054	1/1	0.14	-	1,1,1,1	0
57	MG	CA	1653	1/1	0.14	-	83,83,83,83	0
57	MG	DA	3104	1/1	0.48	-	37,37,37,37	0
57	MG	CA	1649	1/1	0.42	-	95,95,95,95	0
57	MG	DA	3317	1/1	0.39	-	55,55,55,55	1
57	MG	BA	3316	1/1	0.21	-	55,55,55,55	1
57	MG	DA	3254	1/1	0.11	-	99,99,99,99	0
57	MG	AA	1681	1/1	0.99	-	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	1606	1/1	0.33	-	78,78,78,78	0
57	MG	BA	3415	1/1	0.39	-	77,77,77,77	0
57	MG	BA	3094	1/1	0.17	-	24,24,24,24	0
57	MG	AA	1670	1/1	0.38	-	49,49,49,49	0
57	MG	BA	3315	1/1	0.06	-	83,83,83,83	0
57	MG	BA	3120	1/1	0.31	-	90,90,90,90	0
57	MG	DB	212	1/1	0.44	-	99,99,99,99	1
57	MG	BA	3401	1/1	0.32	-	81,81,81,81	0
57	MG	CA	1673	1/1	0.63	-	128,128,128,128	1
57	MG	DA	3312	1/1	0.20	-	56,56,56,56	1
57	MG	BA	3001	1/1	0.22	-	33,33,33,33	0
57	MG	DA	3145	1/1	0.35	-	90,90,90,90	0
57	MG	CA	1733	1/1	0.49	-	81,81,81,81	1
57	MG	BA	3093	1/1	0.06	-	7,7,7,7	0
57	MG	CA	1754	1/1	0.50	-	105,105,105,105	1
57	MG	BA	3213	1/1	0.07	-	93,93,93,93	1
57	MG	AA	1772	1/1	0.31	-	85,85,85,85	0
57	MG	BA	3325	1/1	0.15	-	88,88,88,88	1
57	MG	DA	3339	1/1	0.30	-	57,57,57,57	1
57	MG	AA	1692	1/1	0.13	-	72,72,72,72	0
57	MG	DA	3236	1/1	0.32	-	47,47,47,47	0
57	MG	DA	3341	1/1	0.29	-	54,54,54,54	0
57	MG	BA	3210	1/1	1.04	-	84,84,84,84	0
57	MG	AA	1711	1/1	0.12	-	73,73,73,73	0
57	MG	BA	3007	1/1	0.26	-	22,22,22,22	0
57	MG	BA	3306	1/1	0.11	-	18,18,18,18	0
57	MG	CA	1694	1/1	0.39	-	116,116,116,116	0
57	MG	DA	3346	1/1	0.24	-	54,54,54,54	0
57	MG	DA	3100	1/1	0.19	-	63,63,63,63	0
57	MG	CA	1683	1/1	0.53	-	110,110,110,110	0
57	MG	AA	1722	1/1	0.15	-	75,75,75,75	0
57	MG	AA	1659	1/1	0.36	-	42,42,42,42	0
57	MG	BA	3167	1/1	0.38	-	32,32,32,32	1
57	MG	B5	101	1/1	0.16	-	42,42,42,42	0
57	MG	DA	3409	1/1	0.51	-	121,121,121,121	0
57	MG	BA	3282	1/1	0.48	-	23,23,23,23	0
57	MG	AA	1679	1/1	0.47	-	56,56,56,56	0
57	MG	DA	3334	1/1	0.25	-	72,72,72,72	0
57	MG	AA	1664	1/1	0.35	-	47,47,47,47	0
57	MG	BA	3134	1/1	0.18	-	10,10,10,10	0
57	MG	BA	3304	1/1	0.17	-	81,81,81,81	0
57	MG	CA	1777	1/1	1.28	-	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	1706	1/1	0.40	-	108,108,108,108	0
57	MG	CA	1744	1/1	0.62	-	63,63,63,63	0
57	MG	BA	3123	1/1	0.55	-	29,29,29,29	0
57	MG	DB	203	1/1	0.87	-	33,33,33,33	1
57	MG	DA	3322	1/1	0.21	-	62,62,62,62	0
57	MG	BA	3286	1/1	0.67	-	16,16,16,16	0
57	MG	BB	210	1/1	0.32	-	27,27,27,27	0
57	MG	DA	3172	1/1	0.27	-	58,58,58,58	0
57	MG	CA	1730	1/1	0.24	-	43,43,43,43	0
57	MG	BA	3206	1/1	0.24	-	22,22,22,22	0
57	MG	DA	3397	1/1	0.72	-	101,101,101,101	0
57	MG	AA	1791	1/1	0.18	-	26,26,26,26	1
57	MG	BA	3115	1/1	0.31	-	27,27,27,27	0
57	MG	DA	3375	1/1	0.17	-	83,83,83,83	0
57	MG	DA	3240	1/1	0.42	-	56,56,56,56	0
57	MG	AA	1627	1/1	0.27	-	54,54,54,54	0
57	MG	DA	3344	1/1	0.43	-	64,64,64,64	0
57	MG	DA	3041	1/1	0.23	-	46,46,46,46	0
57	MG	DA	3223	1/1	0.61	-	46,46,46,46	1
57	MG	DA	3076	1/1	0.30	-	45,45,45,45	0
57	MG	BA	3349	1/1	0.78	-	94,94,94,94	1
57	MG	CV	104	1/1	0.41	-	163,163,163,163	0
57	MG	CA	1625	1/1	0.42	-	96,96,96,96	0
57	MG	BA	3254	1/1	0.17	-	44,44,44,44	0
57	MG	AA	1746	1/1	0.34	-	95,95,95,95	0
57	MG	BA	3156	1/1	0.13	-	20,20,20,20	0
57	MG	BA	3391	1/1	0.20	-	37,37,37,37	0
57	MG	BA	3278	1/1	0.09	-	127,127,127,127	0
57	MG	BA	3395	1/1	0.20	-	113,113,113,113	0
57	MG	DA	3414	1/1	0.40	-	84,84,84,84	0
57	MG	AW	102	1/1	0.17	-	135,135,135,135	0
57	MG	CA	1768	1/1	0.38	-	72,72,72,72	0
57	MG	DA	3128	1/1	0.90	-	73,73,73,73	1
57	MG	DA	3218	1/1	0.42	-	94,94,94,94	0
57	MG	CV	103	1/1	0.60	-	74,74,74,74	0
57	MG	CA	1615	1/1	1.50	-	70,70,70,70	0
57	MG	DA	3125	1/1	0.20	-	53,53,53,53	0
57	MG	DA	3184	1/1	0.28	-	36,36,36,36	0
57	MG	AI	201	1/1	0.20	-	109,109,109,109	0
57	MG	BB	201	1/1	0.38	-	87,87,87,87	0
57	MG	BA	3223	1/1	0.49	-	64,64,64,64	0
57	MG	DA	3349	1/1	0.40	-	41,41,41,41	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3244	1/1	0.37	-	62,62,62,62	0
57	MG	DA	3220	1/1	0.39	-	26,26,26,26	0
57	MG	DA	3129	1/1	0.12	-	22,22,22,22	0
57	MG	DA	3094	1/1	0.13	-	22,22,22,22	0
57	MG	BA	3034	1/1	0.16	-	40,40,40,40	0
57	MG	BA	3285	1/1	0.45	-	89,89,89,89	0
57	MG	BA	3181	1/1	0.31	-	49,49,49,49	0
57	MG	DA	3202	1/1	1.01	-	73,73,73,73	0
57	MG	DA	3277	1/1	0.62	-	63,63,63,63	0
57	MG	BA	3422	1/1	0.29	-	120,120,120,120	0
57	MG	DA	3083	1/1	0.27	-	33,33,33,33	0
57	MG	CA	1634	1/1	0.60	-	53,53,53,53	0
57	MG	BA	3017	1/1	0.18	-	9,9,9,9	0
57	MG	DA	3116	1/1	0.79	-	50,50,50,50	0
57	MG	CA	1712	1/1	0.12	-	81,81,81,81	0
57	MG	BA	3259	1/1	0.17	-	24,24,24,24	0
57	MG	BA	3147	1/1	0.17	-	26,26,26,26	0
57	MG	BA	3340	1/1	0.58	-	90,90,90,90	1
57	MG	CV	102	1/1	0.20	-	46,46,46,46	1
57	MG	BA	3355	1/1	0.19	-	92,92,92,92	0
57	MG	DA	3089	1/1	0.26	-	26,26,26,26	0
57	MG	AA	1781	1/1	0.26	-	63,63,63,63	0
57	MG	AL	201	1/1	0.40	-	81,81,81,81	0
57	MG	DA	3295	1/1	0.09	-	78,78,78,78	0
57	MG	DA	3270	1/1	0.27	-	87,87,87,87	0
57	MG	AA	1676	1/1	0.14	-	48,48,48,48	0
57	MG	AA	1714	1/1	0.10	-	29,29,29,29	0
57	MG	DA	3110	1/1	0.19	-	41,41,41,41	0
57	MG	DA	3054	1/1	0.41	-	90,90,90,90	0
57	MG	BA	3068	1/1	0.17	-	38,38,38,38	0
57	MG	BA	3177	1/1	0.40	-	112,112,112,112	0
57	MG	BA	3382	1/1	0.24	-	31,31,31,31	0
57	MG	AA	1632	1/1	0.39	-	34,34,34,34	1
57	MG	DA	3012	1/1	0.27	-	45,45,45,45	0
57	MG	BA	3041	1/1	0.26	-	96,96,96,96	0
57	MG	BA	3194	1/1	0.27	-	42,42,42,42	0
57	MG	BA	3289	1/1	0.27	-	79,79,79,79	0
57	MG	DA	3214	1/1	0.28	-	129,129,129,129	0
57	MG	BX	101	1/1	0.35	-	58,58,58,58	0
57	MG	CA	1707	1/1	0.36	-	119,119,119,119	0
57	MG	BA	3341	1/1	0.22	-	40,40,40,40	0
57	MG	BA	3307	1/1	0.31	-	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	1776	1/1	0.17	-	46,46,46,46	0
57	MG	DA	3280	1/1	0.23	-	109,109,109,109	0
57	MG	BA	3360	1/1	0.40	-	140,140,140,140	0
57	MG	DA	3137	1/1	0.16	-	21,21,21,21	0
57	MG	DA	3002	1/1	0.23	-	69,69,69,69	0
57	MG	BA	3354	1/1	0.15	-	129,129,129,129	0
57	MG	CW	107	1/1	0.20	-	113,113,113,113	1
57	MG	AV	102	1/1	0.16	-	93,93,93,93	1
57	MG	DA	3001	1/1	0.18	-	42,42,42,42	0
57	MG	DA	3392	1/1	0.60	-	107,107,107,107	0
57	MG	BA	3105	1/1	0.41	-	50,50,50,50	0
57	MG	BA	3293	1/1	0.10	-	87,87,87,87	0
57	MG	BA	3022	1/1	0.38	-	20,20,20,20	0
57	MG	DA	3329	1/1	0.46	-	140,140,140,140	0
57	MG	DA	3103	1/1	0.42	-	34,34,34,34	0
57	MG	AA	1615	1/1	0.62	-	65,65,65,65	0
57	MG	BA	3390	1/1	0.24	-	37,37,37,37	0
57	MG	BA	3406	1/1	0.26	-	38,38,38,38	1
57	MG	DV	201	1/1	0.25	-	70,70,70,70	0
57	MG	DX	101	1/1	0.28	-	45,45,45,45	0
57	MG	BA	3140	1/1	0.34	-	66,66,66,66	0
57	MG	CA	1669	1/1	0.40	-	81,81,81,81	0
57	MG	DA	3362	1/1	0.31	-	112,112,112,112	0
57	MG	BA	3257	1/1	0.53	-	61,61,61,61	0
57	MG	DA	3369	1/1	0.35	-	112,112,112,112	0
57	MG	DA	3195	1/1	0.15	-	89,89,89,89	0
57	MG	CA	1782	1/1	0.34	-	77,77,77,77	0
57	MG	AA	1612	1/1	0.30	-	67,67,67,67	0
57	MG	BA	3200	1/1	0.24	-	52,52,52,52	0
57	MG	DA	3405	1/1	0.62	-	53,53,53,53	1
57	MG	BX	102	1/1	0.33	-	104,104,104,104	0
57	MG	DA	3393	1/1	0.55	-	109,109,109,109	1
57	MG	CA	1657	1/1	0.35	-	86,86,86,86	0
57	MG	AA	1647	1/1	0.21	-	74,74,74,74	0
57	MG	DA	3348	1/1	0.09	-	64,64,64,64	0
57	MG	D5	102	1/1	0.27	-	39,39,39,39	1
57	MG	CA	1623	1/1	0.50	-	71,71,71,71	0
57	MG	DA	3006	1/1	0.43	-	23,23,23,23	0
57	MG	BA	3371	1/1	0.68	-	101,101,101,101	0
57	MG	BA	3037	1/1	0.23	-	23,23,23,23	0
57	MG	AA	1682	1/1	0.42	-	131,131,131,131	0
57	MG	BA	3171	1/1	0.10	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3396	1/1	0.20	-	145,145,145,145	0
57	MG	AA	1749	1/1	0.37	-	100,100,100,100	1
57	MG	DA	3381	1/1	0.14	-	45,45,45,45	0
57	MG	CA	1680	1/1	1.11	-	94,94,94,94	0
57	MG	CA	1654	1/1	0.46	-	69,69,69,69	0
57	MG	DA	3354	1/1	0.12	-	84,84,84,84	0
57	MG	BA	3159	1/1	0.30	-	37,37,37,37	0
57	MG	AA	1616	1/1	0.90	-	70,70,70,70	0
57	MG	DA	3058	1/1	0.38	-	88,88,88,88	0
57	MG	BA	3086	1/1	0.38	-	32,32,32,32	0
57	MG	AA	1646	1/1	0.69	-	82,82,82,82	0
57	MG	BA	3043	1/1	0.19	-	20,20,20,20	0
57	MG	BA	3051	1/1	0.17	-	5,5,5,5	0
57	MG	CA	1640	1/1	1.07	-	121,121,121,121	0
57	MG	BA	3031	1/1	0.42	-	44,44,44,44	0
57	MG	DA	3234	1/1	0.15	-	22,22,22,22	0
57	MG	CA	1674	1/1	0.41	-	63,63,63,63	1
57	MG	CA	1635	1/1	0.21	-	74,74,74,74	0
57	MG	BA	3070	1/1	0.43	-	2,2,2,2	0
57	MG	BA	3084	1/1	0.17	-	12,12,12,12	0
57	MG	DA	3323	1/1	0.62	-	53,53,53,53	1
57	MG	DA	3256	1/1	0.26	-	79,79,79,79	0
57	MG	AA	1661	1/1	0.56	-	84,84,84,84	0
57	MG	AA	1650	1/1	0.21	-	99,99,99,99	0
57	MG	DA	3035	1/1	0.12	-	55,55,55,55	0
57	MG	CA	1686	1/1	0.32	-	43,43,43,43	0
57	MG	CA	1742	1/1	0.24	-	70,70,70,70	0
57	MG	DA	3187	1/1	0.18	-	55,55,55,55	0
57	MG	AA	1653	1/1	0.74	-	82,82,82,82	0
57	MG	CA	1601	1/1	0.25	-	140,140,140,140	0
57	MG	AA	1607	1/1	0.31	-	64,64,64,64	0
57	MG	CA	1628	1/1	0.09	-	81,81,81,81	0
57	MG	DA	3030	1/1	0.22	-	47,47,47,47	0
57	MG	CA	1642	1/1	0.28	-	74,74,74,74	0
57	MG	AA	1695	1/1	0.16	-	52,52,52,52	0
57	MG	CA	1710	1/1	0.07	-	54,54,54,54	0
57	MG	CA	1684	1/1	0.11	-	94,94,94,94	0
57	MG	BA	3373	1/1	0.59	-	83,83,83,83	1
57	MG	BA	3342	1/1	0.29	-	84,84,84,84	0
57	MG	CA	1665	1/1	0.32	-	68,68,68,68	0
57	MG	DA	3203	1/1	0.08	-	56,56,56,56	0
57	MG	CA	1675	1/1	0.21	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	1755	1/1	0.34	-	84,84,84,84	0
57	MG	BA	3069	1/1	0.54	-	63,63,63,63	0
57	MG	CA	1735	1/1	0.47	-	90,90,90,90	0
57	MG	DA	3321	1/1	0.55	-	126,126,126,126	0
57	MG	DA	3224	1/1	0.17	-	85,85,85,85	0
57	MG	BA	3301	1/1	0.35	-	57,57,57,57	0
57	MG	BA	3195	1/1	1.13	-	79,79,79,79	0
57	MG	BA	3263	1/1	0.63	-	77,77,77,77	0
57	MG	DA	3282	1/1	0.21	-	50,50,50,50	0
57	MG	DA	3119	1/1	0.34	-	86,86,86,86	0
57	MG	DA	3253	1/1	0.43	-	86,86,86,86	1
57	MG	DA	3276	1/1	0.80	-	115,115,115,115	0
57	MG	BA	3049	1/1	0.28	-	84,84,84,84	1
57	MG	DA	3305	1/1	0.38	-	100,100,100,100	1
57	MG	AA	1704	1/1	0.31	-	103,103,103,103	0
57	MG	AA	1792	1/1	0.48	-	58,58,58,58	0
57	MG	AV	103	1/1	0.45	-	81,81,81,81	0
57	MG	AA	1775	1/1	0.52	-	92,92,92,92	0
57	MG	DX	102	1/1	1.08	-	126,126,126,126	0
57	MG	BA	3385	1/1	0.12	-	87,87,87,87	0
57	MG	DA	3188	1/1	1.86	-	111,111,111,111	0
57	MG	CA	1706	1/1	0.73	-	80,80,80,80	0
57	MG	BA	3218	1/1	0.34	-	6,6,6,6	0
57	MG	DA	3127	1/1	0.46	-	67,67,67,67	0
57	MG	AA	1699	1/1	0.13	-	78,78,78,78	0
57	MG	DA	3069	1/1	0.31	-	75,75,75,75	0
57	MG	DA	3179	1/1	0.18	-	80,80,80,80	0
57	MG	BA	3375	1/1	0.21	-	21,21,21,21	1
57	MG	BA	3229	1/1	0.34	-	20,20,20,20	0
57	MG	AA	1756	1/1	0.29	-	47,47,47,47	1
57	MG	BA	3287	1/1	0.54	-	31,31,31,31	0
57	MG	AA	1610	1/1	0.62	-	49,49,49,49	0
57	MG	AA	1783	1/1	0.35	-	105,105,105,105	0
57	MG	CA	1718	1/1	0.15	-	67,67,67,67	0
57	MG	CA	1609	1/1	0.69	-	61,61,61,61	0
57	MG	BA	3226	1/1	0.17	-	58,58,58,58	0
57	MG	DA	3144	1/1	0.38	-	63,63,63,63	1
57	MG	BA	3310	1/1	0.18	-	102,102,102,102	1
57	MG	BA	3370	1/1	0.42	-	113,113,113,113	0
57	MG	DA	3402	1/1	0.31	-	125,125,125,125	0
57	MG	BA	3029	1/1	0.12	-	40,40,40,40	0
57	MG	CA	1794	1/1	0.59	-	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DF	301	1/1	0.11	-	56,56,56,56	0
57	MG	AA	1620	1/1	0.17	-	54,54,54,54	0
57	MG	BA	3013	1/1	0.14	-	7,7,7,7	0
57	MG	DA	3039	1/1	0.05	-	70,70,70,70	0
57	MG	B0	101	1/1	0.30	-	50,50,50,50	0
57	MG	BA	3112	1/1	0.37	-	15,15,15,15	0
57	MG	AA	1635	1/1	0.27	-	92,92,92,92	0
57	MG	BA	3275	1/1	0.47	-	98,98,98,98	0
57	MG	AA	1602	1/1	0.27	-	97,97,97,97	0
57	MG	BA	3215	1/1	0.29	-	33,33,33,33	0
57	MG	DA	3216	1/1	0.48	-	74,74,74,74	0
57	MG	DA	3336	1/1	0.16	-	77,77,77,77	1
57	MG	CI	201	1/1	0.24	-	75,75,75,75	0
57	MG	BA	3153	1/1	0.37	-	20,20,20,20	1
57	MG	AL	202	1/1	0.34	-	165,165,165,165	0
57	MG	BD	301	1/1	0.20	-	16,16,16,16	0
57	MG	AA	1645	1/1	0.55	-	41,41,41,41	0
57	MG	CA	1639	1/1	0.16	-	62,62,62,62	0
57	MG	DA	3383	1/1	0.32	-	67,67,67,67	0
57	MG	CA	1604	1/1	0.16	-	63,63,63,63	0
57	MG	BA	3145	1/1	0.20	-	27,27,27,27	0
57	MG	DA	3159	1/1	0.55	-	70,70,70,70	0
57	MG	CA	1738	1/1	0.26	-	62,62,62,62	0
57	MG	BA	3236	1/1	0.20	-	44,44,44,44	0
57	MG	AA	1777	1/1	0.28	-	141,141,141,141	0
57	MG	DA	3117	1/1	0.09	-	16,16,16,16	0
57	MG	BA	3166	1/1	0.07	-	31,31,31,31	0
57	MG	AW	104	1/1	0.10	-	60,60,60,60	1
57	MG	BA	3133	1/1	0.21	-	19,19,19,19	0
57	MG	DA	3201	1/1	1.28	-	88,88,88,88	0
57	MG	DA	3211	1/1	0.29	-	45,45,45,45	0
57	MG	DA	3247	1/1	0.21	-	61,61,61,61	0
57	MG	AA	1734	1/1	0.78	-	102,102,102,102	0
57	MG	DA	3209	1/1	0.16	-	73,73,73,73	0
57	MG	DA	3157	1/1	0.60	-	79,79,79,79	0
57	MG	DA	3332	1/1	0.43	-	33,33,33,33	0
57	MG	CA	1747	1/1	0.49	-	62,62,62,62	0
57	MG	AA	1693	1/1	0.19	-	54,54,54,54	0
57	MG	DA	3150	1/1	0.28	-	65,65,65,65	1
57	MG	AA	1761	1/1	0.88	-	122,122,122,122	0
57	MG	BA	3260	1/1	0.46	-	30,30,30,30	0
57	MG	CA	1696	1/1	0.53	-	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3296	1/1	0.22	-	66,66,66,66	0
57	MG	AA	1601	1/1	0.26	-	90,90,90,90	0
57	MG	CX	102	1/1	0.10	-	110,110,110,110	0
57	MG	AA	1786	1/1	0.27	-	108,108,108,108	0
57	MG	BA	3101	1/1	0.74	-	72,72,72,72	1
59	ZN	CN	102	1/1	0.11	-	120,120,120,120	0
57	MG	AA	1718	1/1	0.19	-	72,72,72,72	0
57	MG	DA	3068	1/1	0.29	-	98,98,98,98	0
57	MG	BA	3290	1/1	0.50	-	78,78,78,78	1
57	MG	BA	3288	1/1	0.76	-	59,59,59,59	0
57	MG	BA	3036	1/1	0.20	-	29,29,29,29	0
57	MG	DA	3401	1/1	0.14	-	57,57,57,57	0
57	MG	BA	3337	1/1	0.15	-	162,162,162,162	0
57	MG	BB	212	1/1	0.19	-	31,31,31,31	1
57	MG	DA	3212	1/1	0.91	-	91,91,91,91	0
57	MG	DB	208	1/1	1.26	-	76,76,76,76	1
57	MG	BA	3129	1/1	0.26	-	10,10,10,10	0
57	MG	DB	211	1/1	0.23	-	119,119,119,119	0
57	MG	DA	3155	1/1	0.40	-	21,21,21,21	1
57	MG	BD	302	1/1	0.19	-	22,22,22,22	0
57	MG	AA	1624	1/1	0.35	-	52,52,52,52	0
57	MG	CA	1660	1/1	0.33	-	59,59,59,59	0
57	MG	BA	3045	1/1	0.40	-	1,1,1,1	0
57	MG	DA	3259	1/1	0.27	-	56,56,56,56	0
57	MG	DA	3061	1/1	0.26	-	30,30,30,30	0
57	MG	DA	3292	1/1	0.77	-	51,51,51,51	1
57	MG	CA	1632	1/1	0.32	-	54,54,54,54	1
57	MG	CA	1659	1/1	0.18	-	42,42,42,42	0
57	MG	BA	3311	1/1	0.25	-	74,74,74,74	1
57	MG	BA	3326	1/1	0.27	-	46,46,46,46	1
57	MG	DA	3086	1/1	0.27	-	56,56,56,56	0
57	MG	AA	1622	1/1	0.60	-	135,135,135,135	0
57	MG	CA	1700	1/1	0.09	-	101,101,101,101	0
57	MG	DA	3121	1/1	0.39	-	83,83,83,83	0
57	MG	BA	3319	1/1	0.24	-	3,3,3,3	1
57	MG	BA	3400	1/1	0.16	-	47,47,47,47	0
57	MG	BA	3032	1/1	0.24	-	45,45,45,45	0
57	MG	BA	3408	1/1	0.19	-	43,43,43,43	0
57	MG	BA	3180	1/1	0.40	-	50,50,50,50	0
57	MG	DA	3382	1/1	0.12	-	74,74,74,74	0
57	MG	BA	3012	1/1	0.30	-	16,16,16,16	0
57	MG	DA	3139	1/1	1.46	-	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3011	1/1	0.46	-	52,52,52,52	0
57	MG	DA	3241	1/1	0.35	-	32,32,32,32	0
57	MG	DA	3412	1/1	0.37	-	74,74,74,74	0
57	MG	CA	1787	1/1	0.12	-	66,66,66,66	0
57	MG	CA	1617	1/1	0.54	-	81,81,81,81	0
57	MG	BA	3242	1/1	0.50	-	60,60,60,60	0
57	MG	BA	3369	1/1	0.30	-	53,53,53,53	1
57	MG	AA	1611	1/1	0.21	-	63,63,63,63	0
57	MG	BA	3085	1/1	0.22	-	21,21,21,21	0
57	MG	CA	1774	1/1	0.17	-	121,121,121,121	0
57	MG	BA	3387	1/1	0.48	-	119,119,119,119	0
57	MG	CA	1757	1/1	0.46	-	128,128,128,128	0
57	MG	DA	3135	1/1	0.28	-	39,39,39,39	0
57	MG	DA	3047	1/1	0.34	-	28,28,28,28	0
57	MG	DA	3180	1/1	0.17	-	35,35,35,35	0
57	MG	AA	1717	1/1	0.35	-	61,61,61,61	0
57	MG	DA	3107	1/1	0.08	-	32,32,32,32	0
57	MG	BA	3015	1/1	0.35	-	33,33,33,33	0
57	MG	AA	1623	1/1	0.59	-	70,70,70,70	0
57	MG	CA	1719	1/1	0.67	-	93,93,93,93	0
57	MG	CA	1773	1/1	0.75	-	55,55,55,55	0
57	MG	AA	1680	1/1	0.63	-	53,53,53,53	0
57	MG	AW	106	1/1	0.26	-	102,102,102,102	1
57	MG	AW	105	1/1	0.40	-	154,154,154,154	1
57	MG	CA	1726	1/1	0.62	-	104,104,104,104	1
57	MG	DA	3377	1/1	0.34	-	24,24,24,24	0
57	MG	BA	3148	1/1	0.24	-	57,57,57,57	0
57	MG	CA	1658	1/1	0.32	-	78,78,78,78	0
57	MG	BA	3058	1/1	0.38	-	19,19,19,19	0
57	MG	DA	3228	1/1	0.29	-	83,83,83,83	0
57	MG	AA	1613	1/1	0.21	-	81,81,81,81	0
57	MG	BA	3121	1/1	0.32	-	40,40,40,40	0
57	MG	BA	3124	1/1	0.26	-	46,46,46,46	0
57	MG	CA	1656	1/1	0.63	-	120,120,120,120	0
57	MG	AA	1655	1/1	0.38	-	74,74,74,74	0
57	MG	B7	101	1/1	0.26	-	45,45,45,45	1
57	MG	BA	3027	1/1	0.18	-	30,30,30,30	0
57	MG	BA	3361	1/1	0.12	-	28,28,28,28	0
57	MG	BA	3397	1/1	0.10	-	73,73,73,73	0
57	MG	AA	1769	1/1	0.46	-	80,80,80,80	0
57	MG	DA	3358	1/1	0.78	-	94,94,94,94	0
57	MG	CA	1796	1/1	0.24	-	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	1708	1/1	0.44	-	72,72,72,72	0
57	MG	DA	3034	1/1	0.52	-	52,52,52,52	0
59	ZN	D9	101	1/1	0.12	-	136,136,136,136	0
57	MG	DA	3136	1/1	0.89	-	63,63,63,63	0
57	MG	DA	3105	1/1	0.27	-	54,54,54,54	0
57	MG	DA	3166	1/1	0.43	-	75,75,75,75	0
57	MG	BA	3356	1/1	0.20	-	41,41,41,41	0

6.5 Other polymers ⓘ

There are no such residues in this entry.