



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 07:10 PM BST

PDB ID : 4V5J
Title : Structure of the 70S ribosome bound to Release factor 2 and a substrate analog provides insights into catalysis of peptide release
Authors : Jin, H.; Kelley, A.C.; Loakes, D.; Ramakrishnan, V.
Deposited on : 2010-03-24
Resolution : 3.10 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>

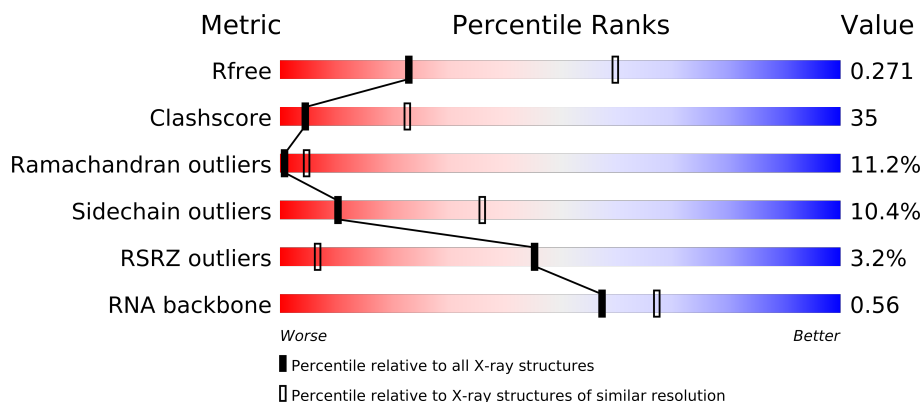
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.10 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	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)
RNA backbone	1838	1047 (3.60-2.60)

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	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	77	
22	AW	77	
22	CV	77	
22	CW	77	
23	AX	8	
23	CX	8	
24	AY	351	
24	CY	351	
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	2915	
35	DA	2915	
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	BJ	130	
44	DJ	130	
45	BK	147	
45	DK	147	
46	BN	140	
46	DN	140	
47	BO	122	
47	DO	122	

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Mol	Chain	Length	Quality of chain
48	BP	150	
48	DP	150	
49	BQ	141	
49	DQ	141	
50	BR	118	
50	DR	118	
51	BS	112	
51	DS	112	
52	BT	146	
52	DT	146	
53	BU	118	
53	DU	118	
54	BV	101	
54	DV	101	
55	BW	113	
55	DW	113	
56	BX	96	
56	DX	96	
57	BY	110	
57	DY	110	
58	BZ	206	
58	DZ	206	

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 305067 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 TYPE Z.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			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 E-SITE TRNA PHE OR P-SITE TRNA PHE (UNMODIFIED BASES).

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

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	8	Total	C	N	O	P	0	0	0
			165	76	29	53	7			
23	CX	8	Total	C	N	O	P	0	0	0
			165	76	29	53	7			

- Molecule 24 is a protein called PEPTIDE CHAIN RELEASE FACTOR 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	351	Total	C	N	O	S	0	0	0
			2801	1752	506	535	8			
24	CY	351	Total	C	N	O	S	0	0	0
			2801	1752	506	535	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	B0	83	Total	C	N	O	S	0	0	0
			657	407	139	110	1			
25	D0	83	Total	C	N	O	S	0	0	0
			657	407	139	110	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	2901	Total	C	N	O	P	0	0	0
			62474	27806	11681	20087	2900			
35	DA	2901	Total	C	N	O	P	0	0	0
			62474	27806	11681	20087	2900			

- 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	120	Total	C	N	O	S	0	0	0
			937	590	174	172	1			
37	DC	120	Total	C	N	O	S	0	0	0
			937	590	174	172	1			

- 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 L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BJ	130	Total	C	N	O		0	0	0
			651	390	130	131				
44	DJ	130	Total	C	N	O		0	0	0
			651	390	130	131				

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BK	141	Total	C	N	O	S	0	0	1
			1038	661	184	187	6			
45	DK	141	Total	C	N	O	S	0	0	1
			1038	661	184	187	6			

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

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

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L18.

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

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L19.

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

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L24.

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

- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BZ	185	Total 1468	C 936	N 262	O 268	S 2	0	0	1
58	DZ	185	Total 1468	C 936	N 262	O 268	S 2	0	0	1

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	BA	357	Total 357	Mg 357	0	0
59	CA	155	Total 155	Mg 155	0	0
59	DF	1	Total 1	Mg 1	0	0
59	CV	7	Total 7	Mg 7	0	0
59	AW	4	Total 4	Mg 4	0	0
59	B1	1	Total 1	Mg 1	0	0
59	CD	1	Total 1	Mg 1	0	0
59	AX	1	Total 1	Mg 1	0	0
59	AS	1	Total 1	Mg 1	0	0
59	B5	2	Total 2	Mg 2	0	0
59	BB	4	Total 4	Mg 4	0	0
59	BT	1	Total 1	Mg 1	0	0
59	DG	1	Total 1	Mg 1	0	0
59	BF	2	Total 2	Mg 2	0	0
59	AV	7	Total 7	Mg 7	0	0
59	BX	1	Total 1	Mg 1	0	0
59	AA	161	Total 161	Mg 161	0	0
59	CX	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	CN	1	Total 1	Mg 1	0	0
59	DD	1	Total 1	Mg 1	0	0
59	DH	1	Total 1	Mg 1	0	0
59	DS	1	Total 1	Mg 1	0	0
59	BG	1	Total 1	Mg 1	0	0
59	BY	1	Total 1	Mg 1	0	0
59	DX	1	Total 1	Mg 1	0	0
59	DA	359	Total 359	Mg 359	0	0
59	AL	1	Total 1	Mg 1	0	0
59	DE	1	Total 1	Mg 1	0	0
59	AY	1	Total 1	Mg 1	0	0
59	D1	1	Total 1	Mg 1	0	0
59	DP	1	Total 1	Mg 1	0	0
59	CW	4	Total 4	Mg 4	0	0
59	D5	2	Total 2	Mg 2	0	0
59	BD	2	Total 2	Mg 2	0	0
59	CS	1	Total 1	Mg 1	0	0
59	CL	2	Total 2	Mg 2	0	0
59	DB	4	Total 4	Mg 4	0	0

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 61 is water.

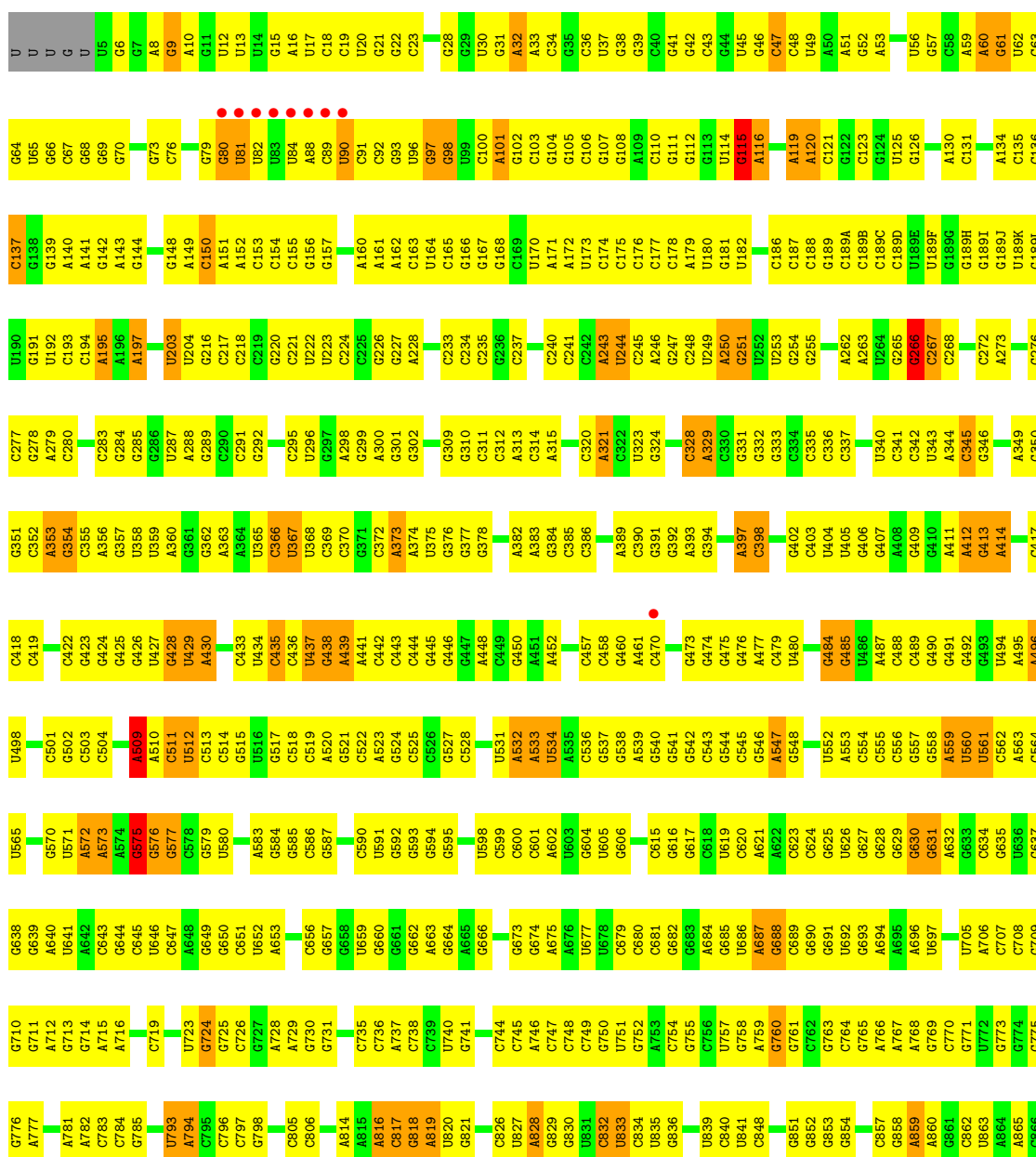
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AV	1	Total 1	O 1	0	0
61	AY	1	Total 1	O 1	0	0
61	BA	1	Total 1	O 1	0	0

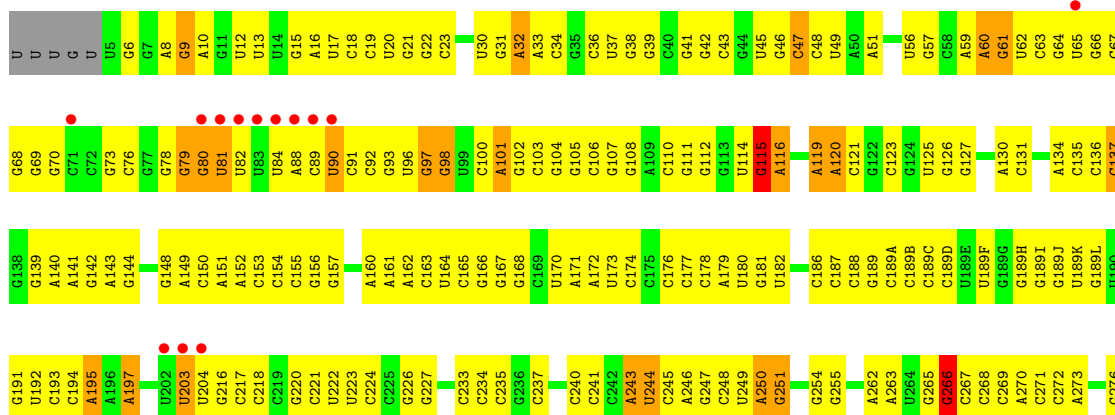
3 Residue-property plots

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

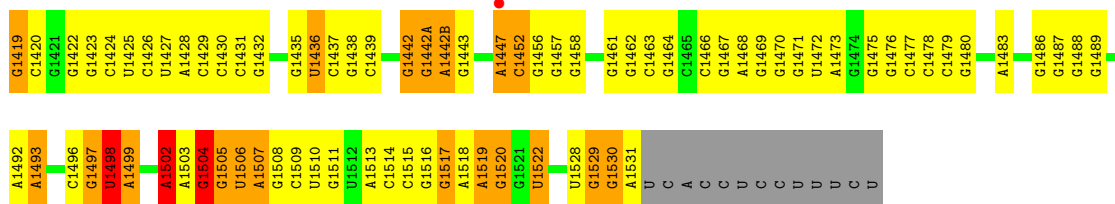
• Molecule 1: 16S RRNA

Chain AA: 



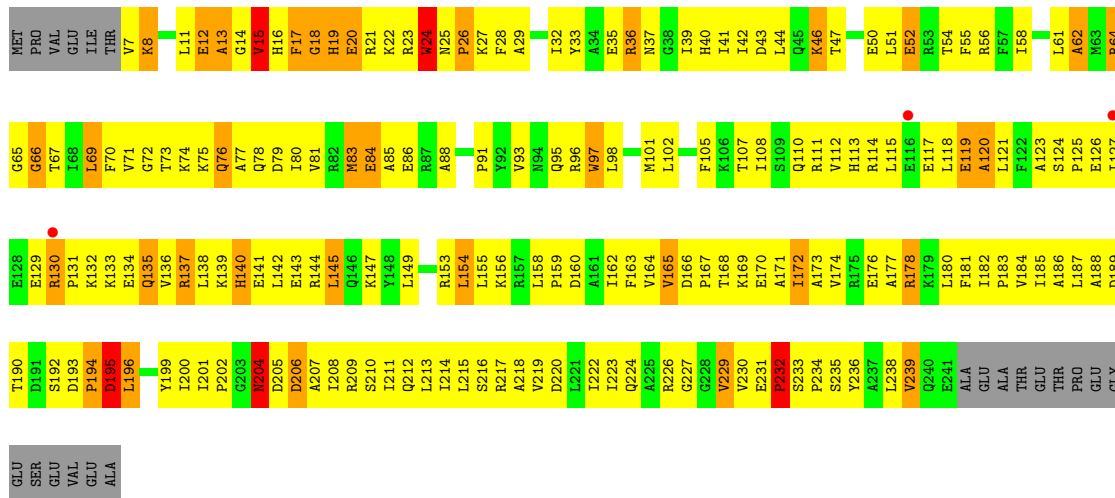


A1350	G1283	G1144	G1077	A1015	U952	G869	G785	A715	G643	G570	C501	U420	G354	C277
U1351	C1284	C1145	U1078	A1016	G953	U870	A790	A716	G644	U571	C502	U421	C355	G278
A1285	A1286	A1146	G1079	G1017	G954	G878			G645	A572	G503	C422	A356	A279
G1352	C1217	A1080	A1080	C1018	U955	C879	U793	C719	U646	A573	C504	C423	G357	C280
C1354	G1281	U1148	G1081	C1019	U956	C880	G794	U723	G647	A574		G424	U358	
G1355	U1219	U1149	G1082	U1020	U957	G881	C795	G724	G648	A575	A509	G425	U359	C283
G1356	G1220	U1150	U1083	G1021	A958	G882	C796	G725	G649	G576	A510	U426	A360	G284
A1357	G1221	A1151	U1084	U1025	A959	C883	C797	G726	G650	G577	A511	U427	G361	G285
U1358	G1222	A1152	U1085	G1026	U960	G884	C798	G727	G651	G578	A512	U428	G362	
C1359	G1223	C1153	U1086	C1027	U961	G885	G799	G728	U652	C579	U513	U429	A363	C289
G1360	G1224		G1087	G1028	G962	G886		G729	A653	A583	C513	A430	A364	C290
G1361	A1225	A1157	G1088	C1029	G963	G888	A802	G730	G656	G584	C514		U365	C291
G1362	A1226	U1158	G1089	C1030	A964	U894	G803	G731	G657	G585	C515	C433	U366	G292
C1363	A1227	U1159		G1031	A965	C806	A814		G658	G587	U516	U434	U367	
A1363A	A1228	G1160	G1094	G1030A	G966	C807	A815	C735	G659		G517	C435	U368	C295
U1364	A1229	C1161	U1095	G1030B	G967	C808	A816	C736	G660	C590	C518	C436	U369	U296
C1369	A1230	C1162	C1096	G1030C	A968	A817	A817	C737	G661	U591	C519	U437	C370	G297
G1370	G1234	C1163	C1097	A1030D	A969	A818	A818	C738	G662	U592	A520	G438	G371	A298
G1371	U1235	G1164	C1098	G1031	C970	A819	A819	C739	G663	G593	C521	A439	C372	G299
G1372	A1238	G1165		G1032	G971	U820	U820	C740	G664	G594	A522	A441	A373	A300
A1373	U1239	C1166	A1101	G1033	C972	G821	C741	C741	G665	G595	A523	C442	A374	A301
A1374	A1240	C1167	C1102	A1034	A973	A914	C742	C742	G666	C599	C524	C443	U375	G302
A1375	U1307	A1168	C1103	A1035	A974	A915	G743	G743	G667	U598	C525	C444	U376	
U1376	G1241	A1169	G1104	G1036	A975	A916	C744	C744	G668	C599	C526	G445	G377	G309
U1377	C1242	G1170	A1105	G1037	G976	A917	C745	C745	G669	C600	U531	G446	G378	G310
G1378	G1243	C1171	G1106	U1040	A977	A918	C746		G670	C601	A532	G447	A382	C321
G1379	C1246	G1172	C1107	A1041	A978	C826	C747		G671	C602	A533	C448	A383	C322
G1380	U1247	A1176	G1108	A1042	A979	A827	C748		G672	C615	A534	C449	A384	U323
U1381	A1248	C1177	C1109	C1043	U981	A828	C749		G673	C616	G540	G450	G390	C324
C1382	C1249	G1178	A1110		C984	A829	C750		G674	C617	G541	A461	G391	
U1383	A1250	A1179	C1112	G1047	C985	U831	C751		G675	C620	G542	C470	G392	C328
U1384	A1251	A1180	C1116	G1048	C986	C832	C752		G676	A621	C543	G473	A393	A329
G1385	A1252	G1181	C1117	U1049	A986	C833	C753		G677	A622	C544	G474	G394	C330
G1386	G1253	C1182	C1118	G1050	G987	U834	C754		G678	C621	C545	G475	A397	G331
G1387	C1254	G1183	C1119	G1051	C990	U835	C755		G679	C622	C546	G476	C398	G332
C1388	G1255	A1188	U1121	U1052	U991	U836	C756		G680	A623	C547	A477	G402	G333
U1389	A1256	C1189	U1122	G1053	U992	U837	C757		G681	A624	C548	C478	G403	C334
U1390	U1257	G1190	A1123	C1054	U993	U838	C758		G682	A625	C549	U480	G404	C335
G1391	C1258		U1124	U1055	G994	C840	C759		G683	C623	C550	G481	U405	C336
U1392	C1259	G1193	U1125	U1056	A994	U841	C760		G684	C624	C551	G482	U406	A338
C1393	C1260	U1194	U1126	G1057	U997	U842	C761		G685	C625	C552	A479	G407	C339
C1394	A1261	C1195	U1127	G1058	G998	U843	C762		G686	C626	C553	C480	G408	U340
C1395		U1196	C1128	C1059	C999	U844	C763		G687	C627	C554	U481	G409	C341
C1396	C1264	G1197	C1129	C1060	C999	U845	C764		G688	C628	C555	G483	G410	C342
C1397	G1265	U1198	U1130	G1061	U1000	U846	C765		G689	C629	C556	G484	U411	U343
C1398	U1266	C1199	U1131	U1062	A1001	U847	C766		G690	C630	C557	G485	G412	A344
C1399	A1269	U1200	U1132	C1063	G1001A	U848	C767		G691	C631	C558	U486	A413	C345
C1400	G1270	C1201	C1133	G1064	G1002	U849	C768		G692	A632	C559	A487	G414	
G1401	G1271	G1202	U1134	U1065	G1003	U850	C769		G693	A633	C560	C488	G415	A349
C1402		C1203	U1135	C1066	A1004	U851	C770		G694	C632	C561	C489	G416	G350
C1403	G1274	C1204	U1136	A1067	A1005	U852	C771		G695	C633	C562	C490	G417	G351
C1404	A1275	U1205	U1137	G1068	C1006	U853	C772		G696	C634	C563	G491	G418	C352
C1405	G1276	G1206	C1137	C1069	C1007	U854	C773		G697	C635	C564	G492	G419	A353
C1406	U1277	G1207	U1138	G1071	C1008	U855	C774		G698	C636	C565	G493		
C1407	A1278	C1208	C1140	G1072	G1009	U856	C775		G699	C637	C566	U494		
A1408	G1279	U1209	C1141	U1073	U1012	U857	C776		G700	C638	C567	U495		
C1409	A1280	U1210	U1142	G1074	C1013	U858	C777		G701	C639	C568	A496		
G1410	G1281	C1211	C1143	C1075	A1014	U859	C778		G702	C640	C569	A497		
C1411	U1282	C1212		C1076		U860	C779		G703	C641	C570	A498		
C1412	U1283	A1213		C1077		U861	C780		G704	C642	C571	A499		
A1413	C1284			C1078		U862	C781		G705	C643	C572	A500		
A1414				C1079		U863	C782		G706	C644	C573	A501		
A1415				C1080		U864	C783		G707	C645	C574	A502		
A1416				C1081		U865	C784		G708	C646	C575	A503		
A1417				C1082		U866	C785		G709	C647	C576	A504		
A1418				C1083		U867	C786		G710	C648	C577	A505		
A1419				C1084		U868	C787		G711	C649	C578	A506		
A1420				C1085		U869	C788		G712	C650	C579	A507		
A1421				C1086		U870	C789		G713	C651	C580	A508		
A1422				C1087		U871	C790		G714	C652	C581	A509		
A1423				C1088		U872	C791		G715	C653	C582	A510		
A1424				C1089		U873	C792		G716	C654	C583	A511		
A1425				C1090		U874	C793		G717	C655	C584	A512		
A1426				C1091		U875	C794		G718	C656	C585	A513		
A1427				C1092		U876	C795		G719	C657	C586	A514		
A1428				C1093		U877	C796		G720	C658	C587	A515		
A1429				C1094		U878	C797		G721	C659	C588	A516		
A1430				C1095		U879	C798		G722	C660	C589	A517		
A1431				C1096		U880	C799		G723	C661	C590	A518		
A1432				C1097		U881	C800		G724	C662	C591	A519		
A1433				C1098		U882	C801		G725	C663	C592	A520		
A1434				C1099		U883	C802		G726	C664	C593	A521		
A1435				C1100		U884	C803		G727	C665	C594	A522		
A1436				C1101		U885	C804		G728	C666	C595	A523		
A1437				C1102		U886	C805		G729	C667	C596	A524		
A1438				C1103		U887	C806		G730	C668	C597	A525		
A1439				C1104		U888	C807		G731	C669	C598	A526		
A1440				C1105		U889	C808		G732	C670	C599	A527		
A1441				C1106		U890	C809		G733	C671	C600	A528		
A1442				C1107		U891	C810		G734	C672	C601	A529		
A1443				C1108		U892	C811		G735	C673	C602	A530		
A1444				C1109		U893	C812		G736	C674	C603	A531		
A1445				C1110		U894	C813		G737	C675	C604	A532		
A1446				C1111		U895	C814		G738	C676	C605	A533		
A1447				C1112		U896	C815		G739	C677	C606	A534		
A1448				C1113		U897	C816		G740	C678	C607	A535		
A1449				C1114		U898	C817		G741	C679	C608	A536		
A1450				C1115		U899	C818		G742	C680	C609	A537		
A1451				C1116		U900	C819		G743	C681	C610	A538		
A1452				C1117		U901	C820		G744	C682	C611	A539		
A1453				C1118		U902	C821		G745	C683	C612	A540		
A1454				C1119		U903	C822		G746	C684	C613	A541		
A1455				C1120		U904	C823		G747	C685	C614	A542		
A1456				C1121		U905	C824		G748	C686	C615	A543		
A1457				C1122		U906	C825		G749	C687				



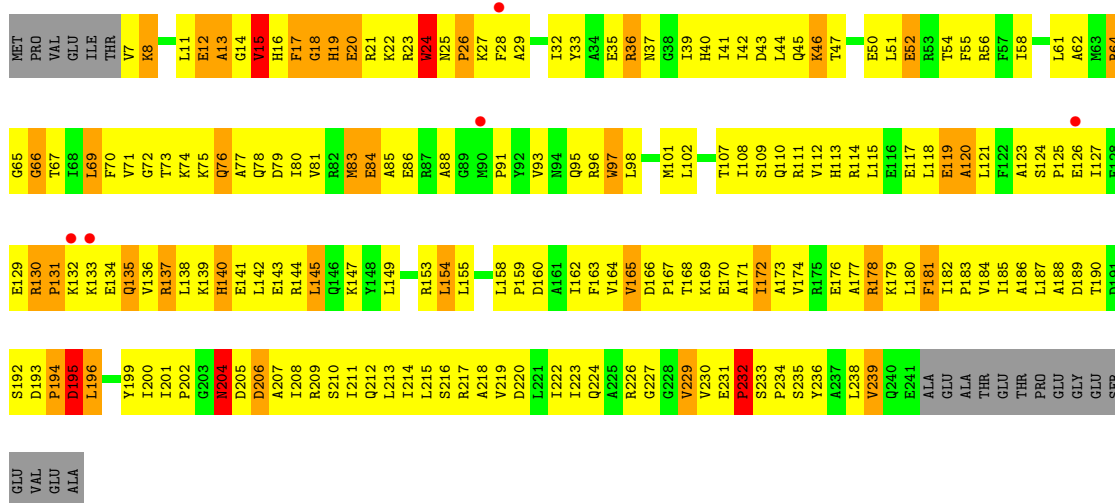
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain AB:



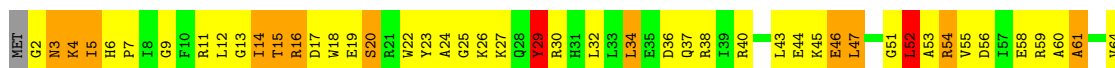
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

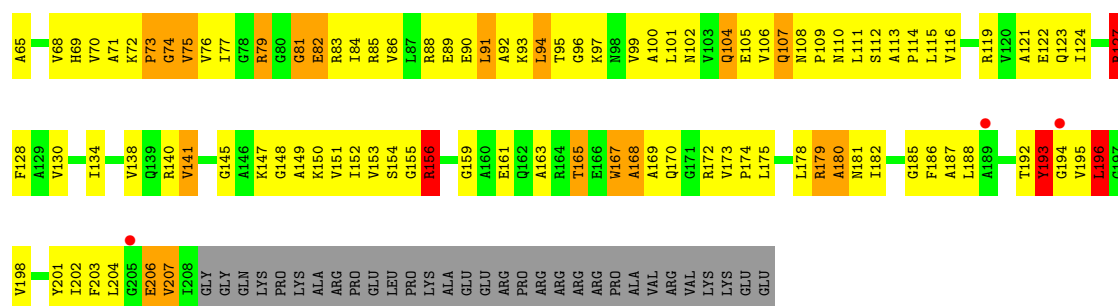
Chain CB:



• Molecule 3: 30S RIBOSOMAL PROTEIN S3

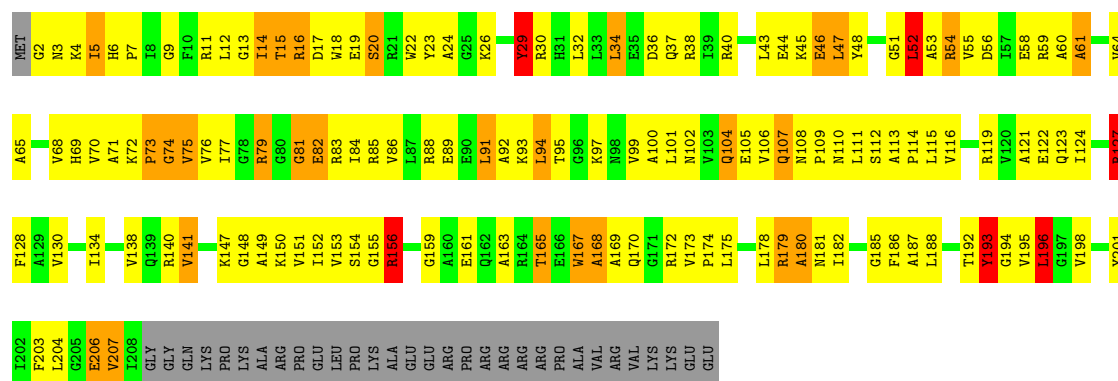
Chain AC:





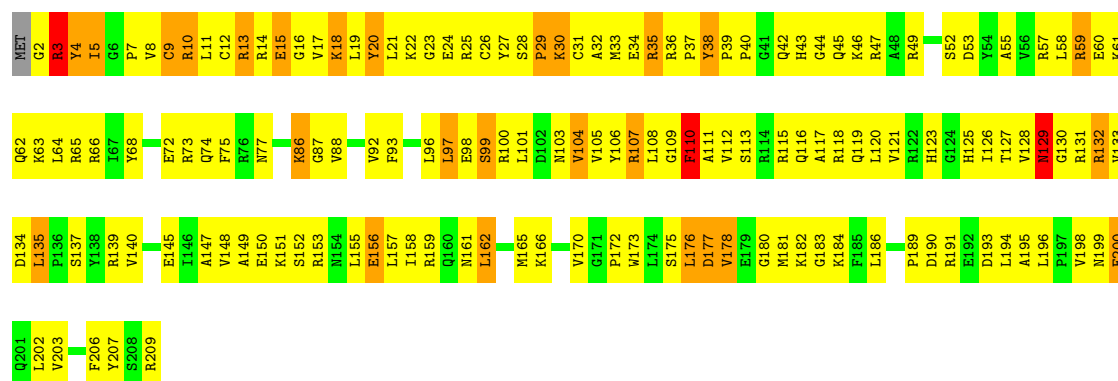
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain CC:



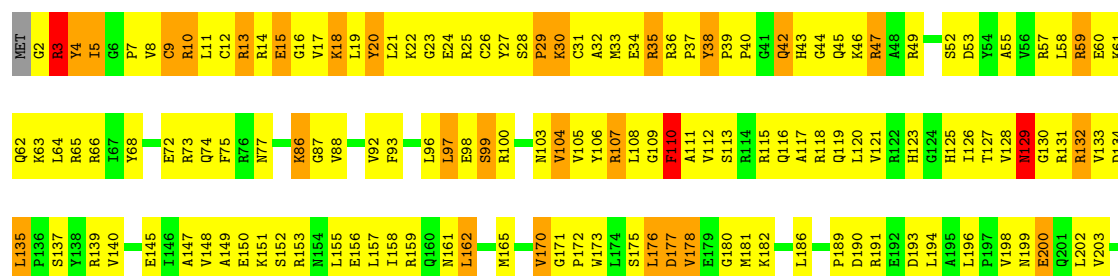
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AD:



• Molecule 4: 30S RIBOSOMAL PROTEIN S4

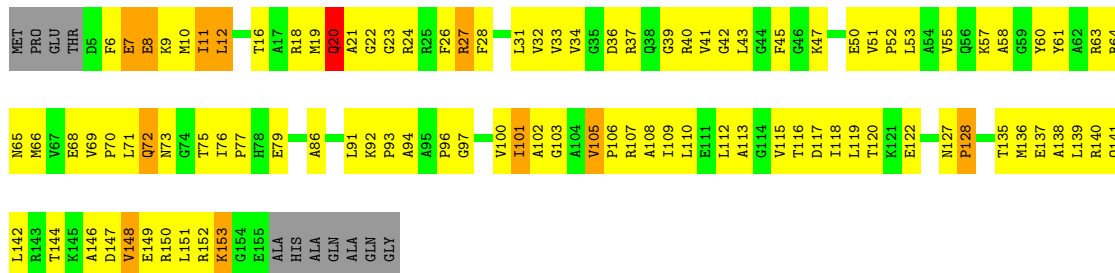
Chain CD:



F206
Y207
S208
R209

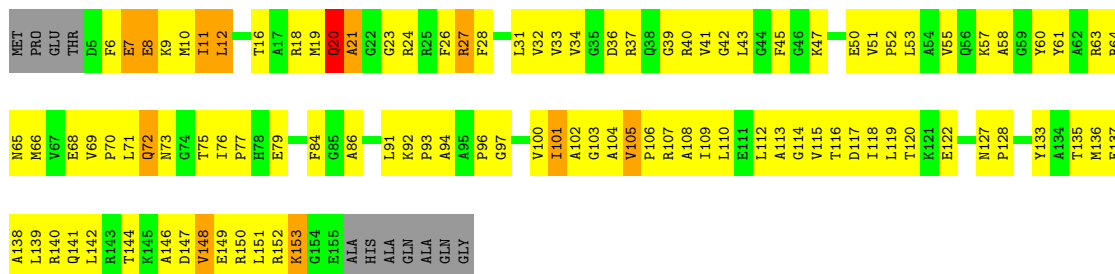
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain AE:



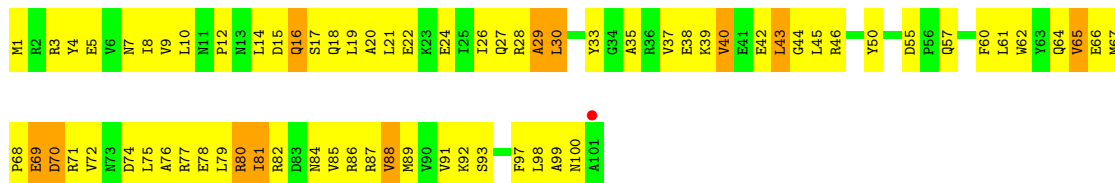
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain CE:



• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AF:



• Molecule 6: 30S RIBOSOMAL PROTEIN S6

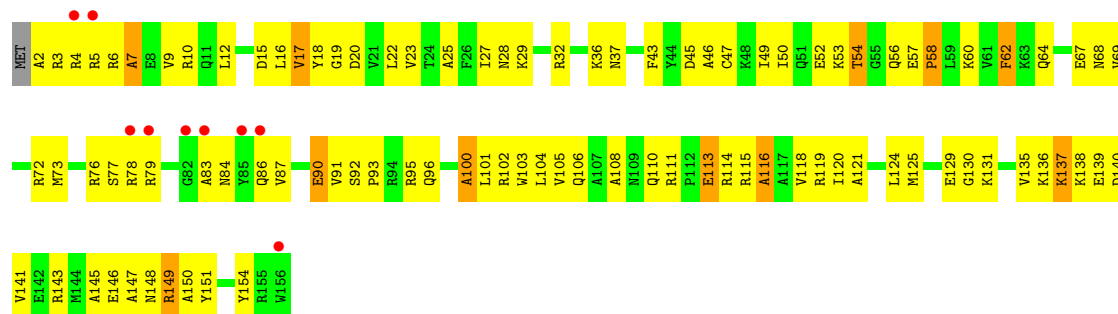
Chain CF:



• Molecule 7: 30S RIBOSOMAL PROTEIN S7

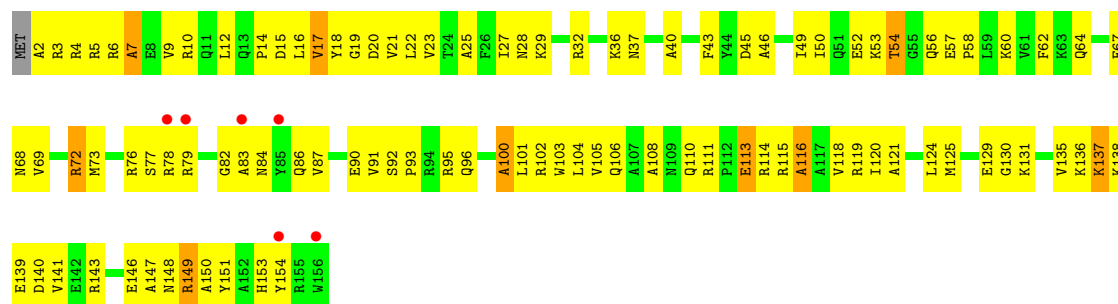
Chain AG:





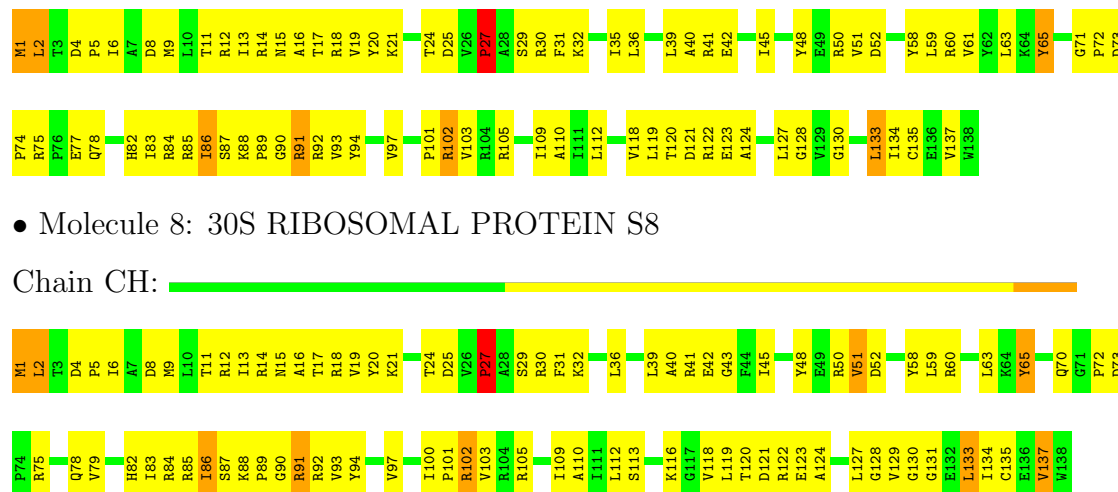
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain CG:



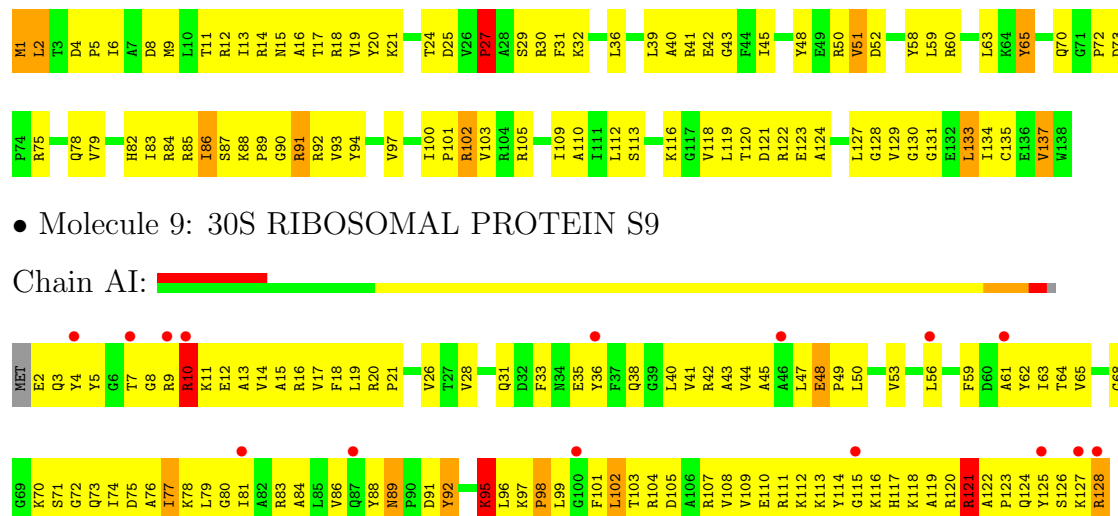
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AH:



• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain CH:

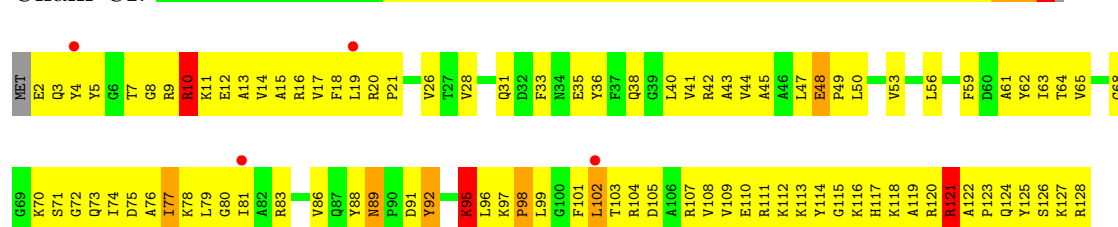


• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AI:

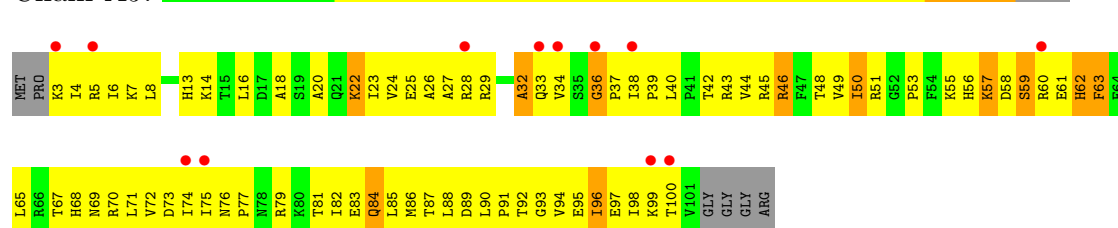
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CI:



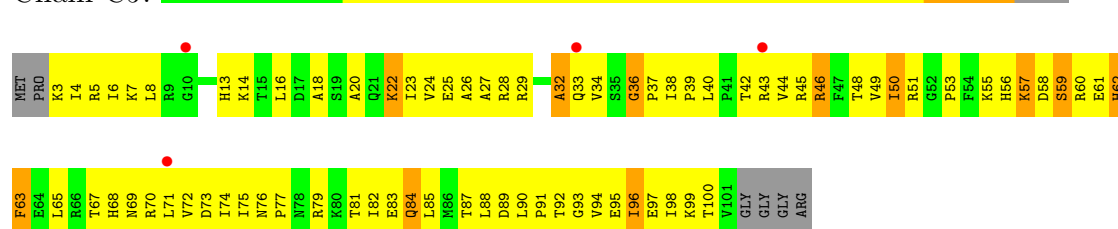
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AJ:



- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain CJ:



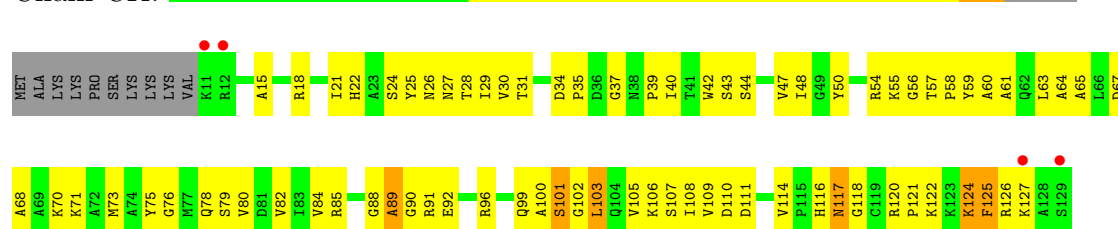
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AK:



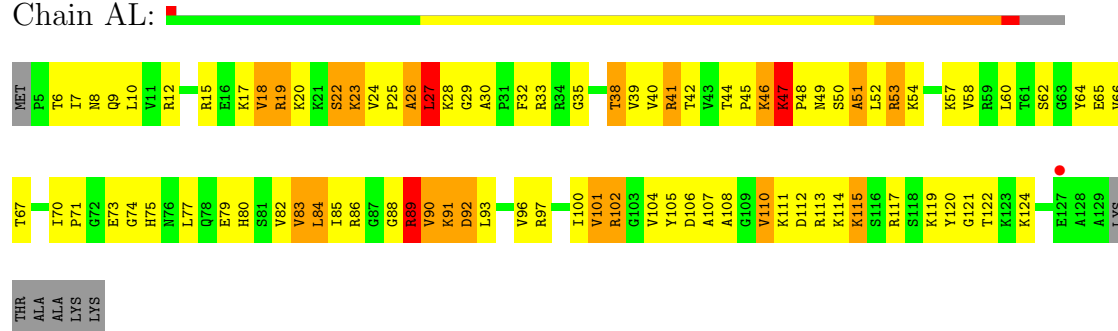
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain CK:



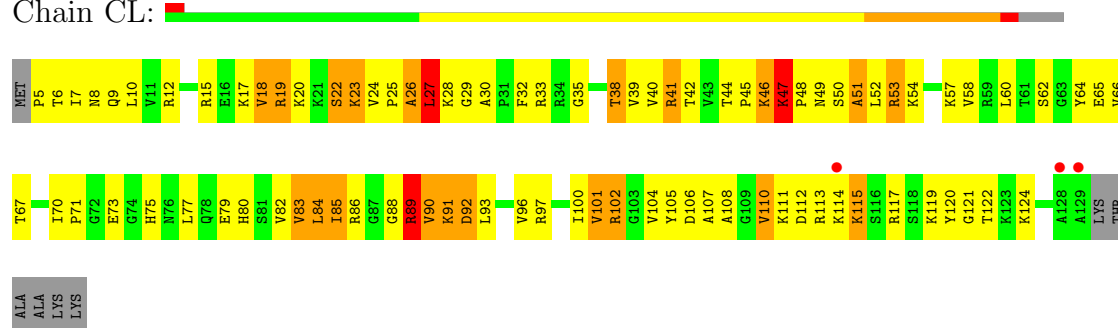
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AL:



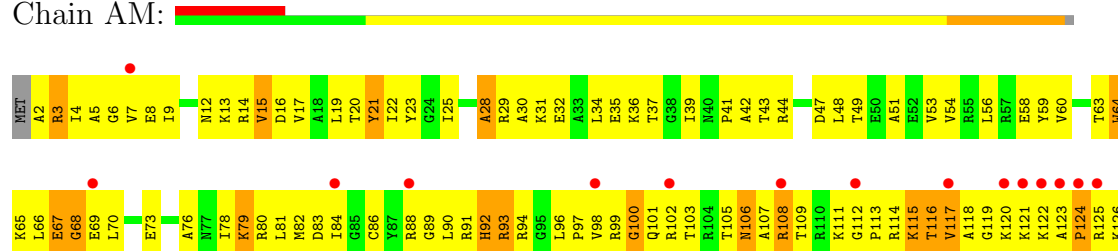
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain CL:



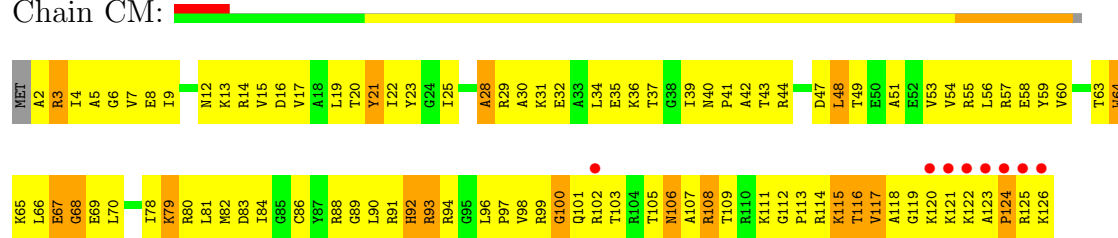
- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain AM:



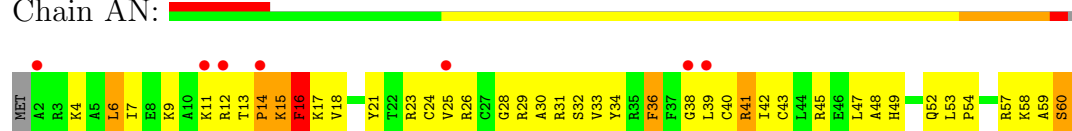
- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain CM:



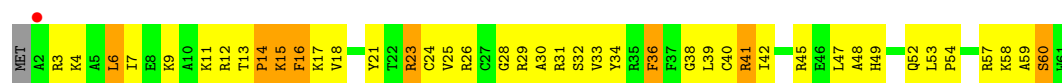
- Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain AN:



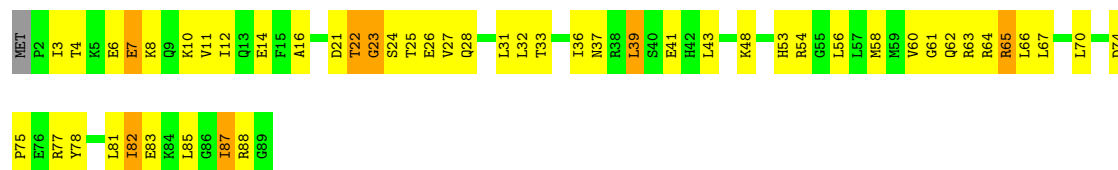
- Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain CN: 



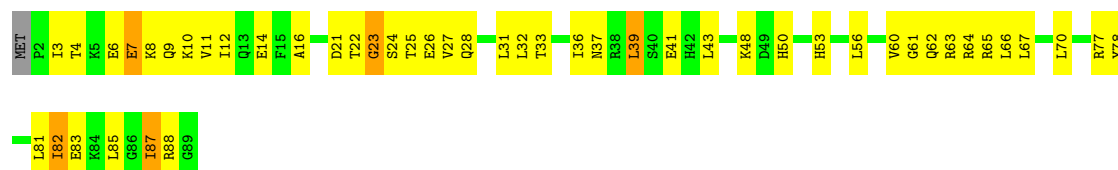
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO: 



• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CO: 



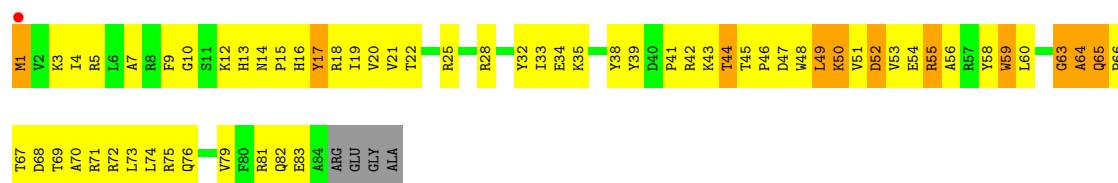
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP: 



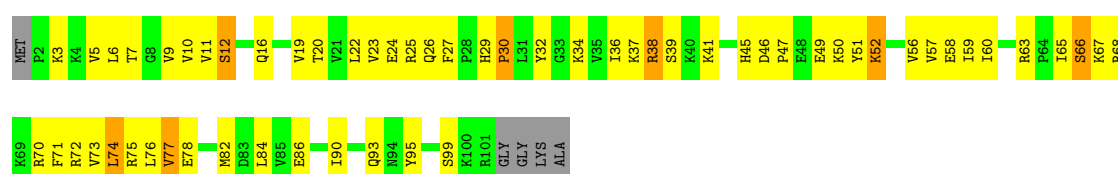
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CP: 



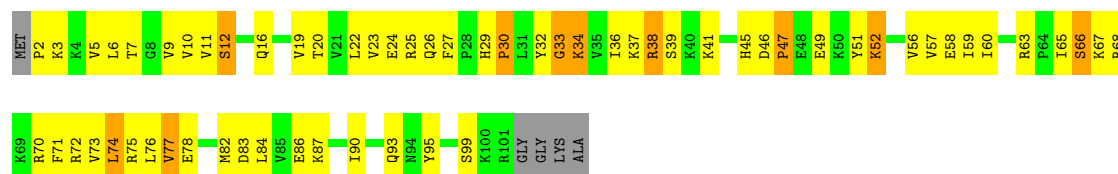
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ: 



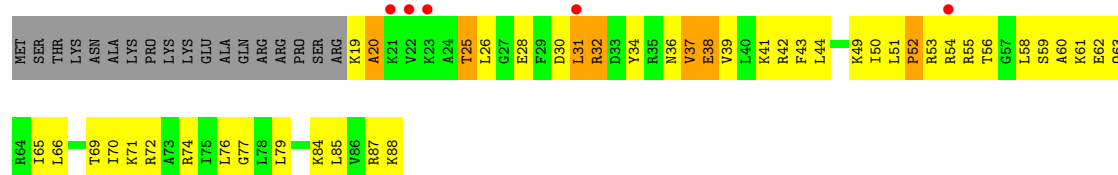
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CQ:



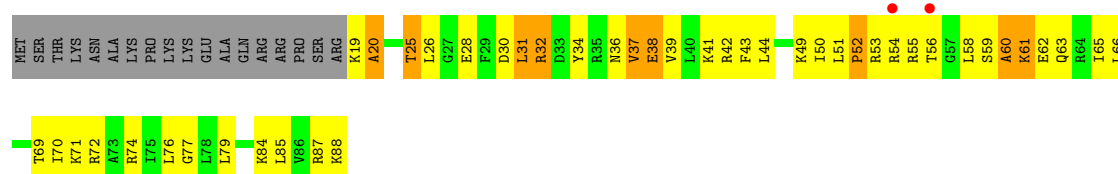
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR:



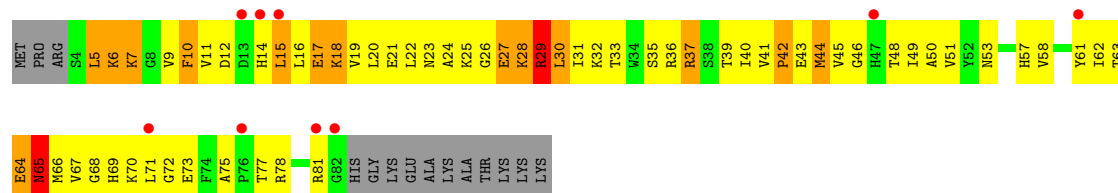
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain CR:



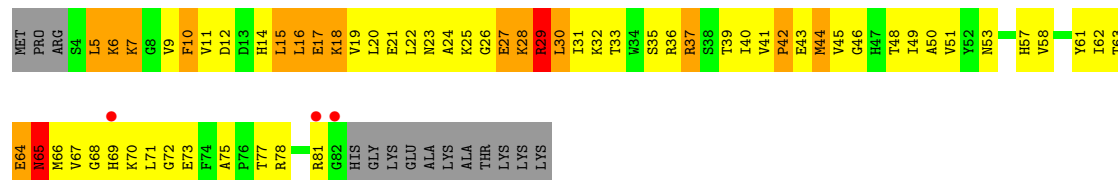
- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AS:



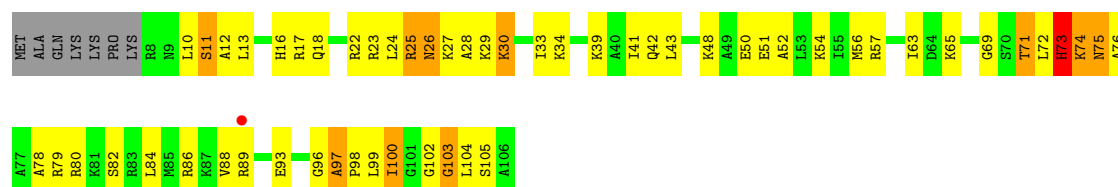
- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain CS:



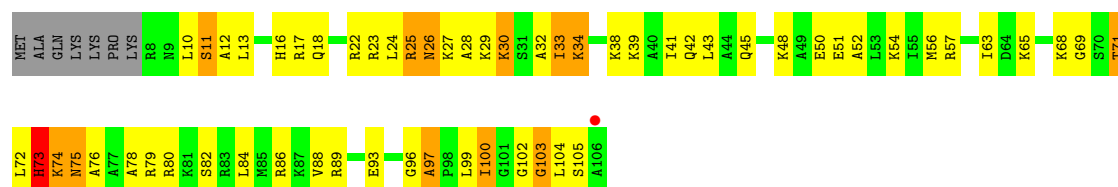
- Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain AT:



• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain CT:



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AU:



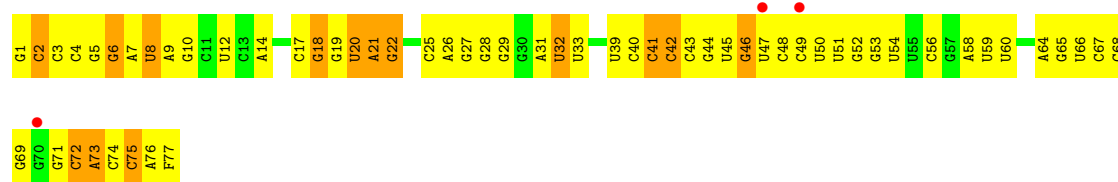
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CU:



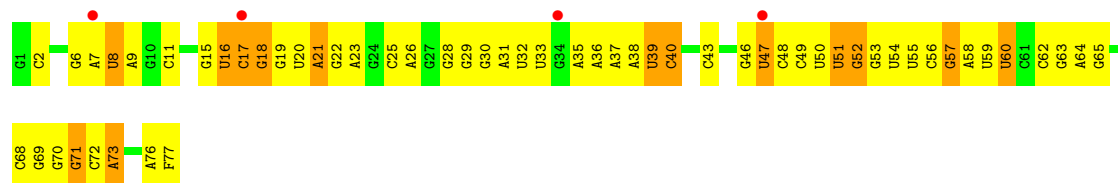
• Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE (UNMODIFIED BASES)

Chain AV:



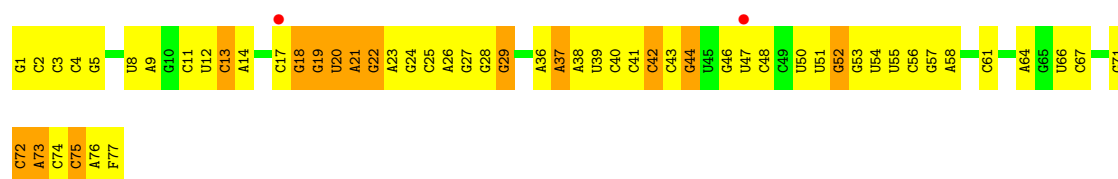
• Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE (UNMODIFIED BASES)

Chain AW:



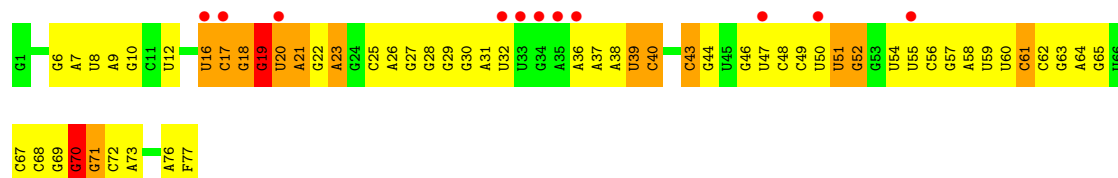
• Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE (UNMODIFIED BASES)

Chain CV:



- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE (UNMODIFIED BASES)

Chain CW:



- Molecule 23: MRNA

Chain AX:



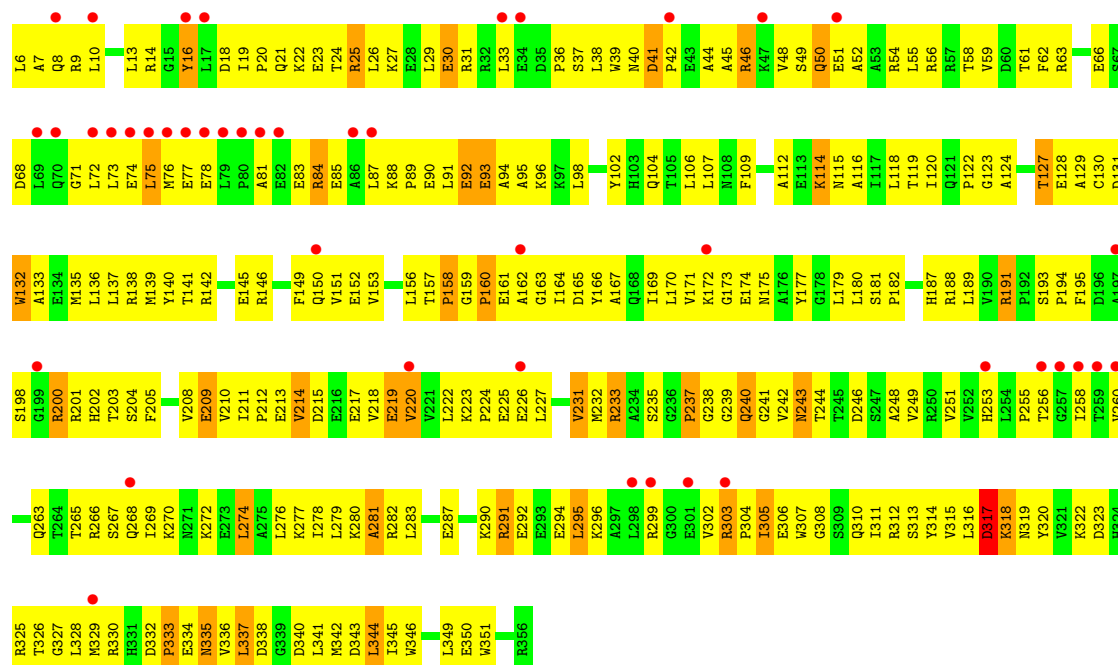
- Molecule 23: MRNA

Chain CX:



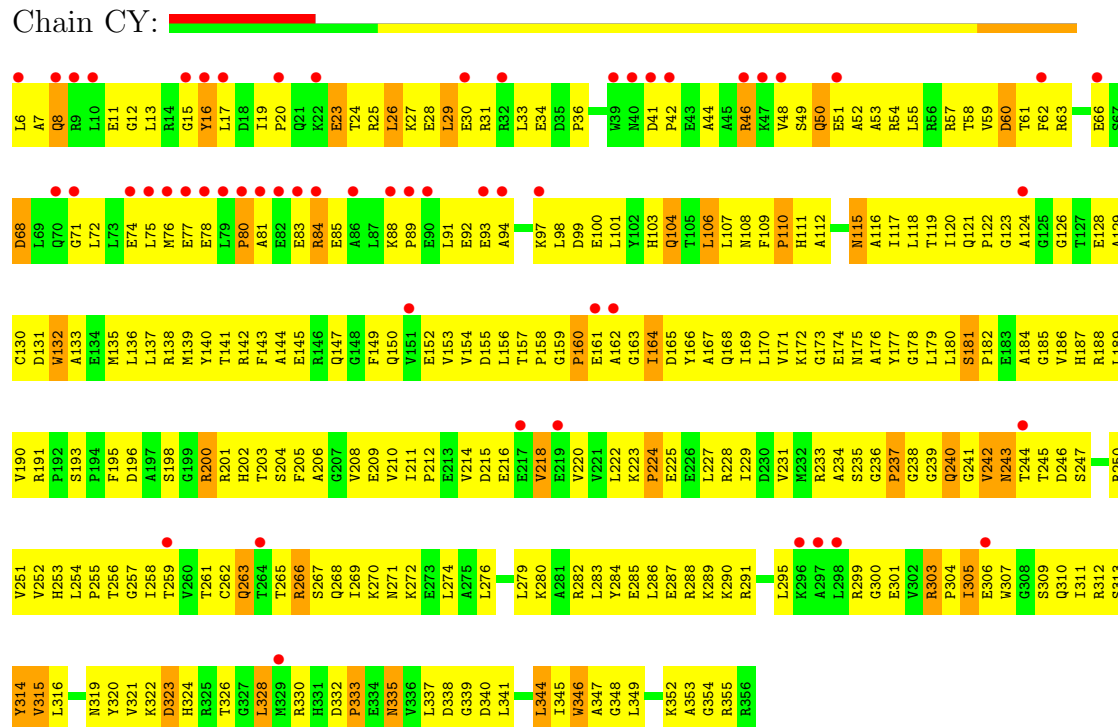
- Molecule 24: PEPTIDE CHAIN RELEASE FACTOR 2

Chain AY:



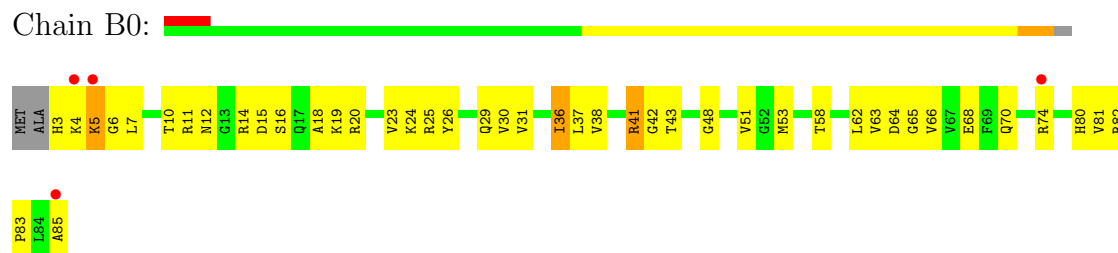
● Molecule 24: PEPTIDE CHAIN RELEASE FACTOR 2

Chain CY:



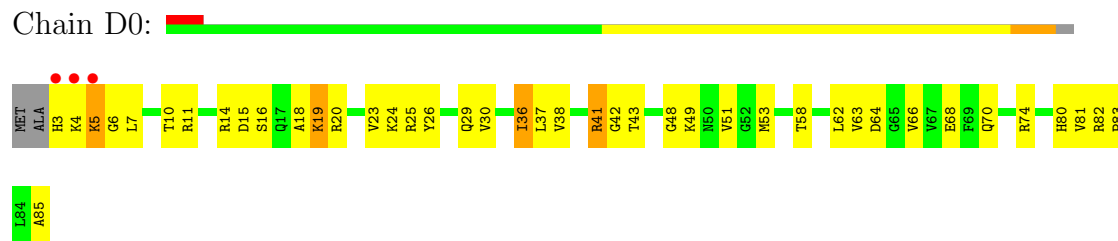
● Molecule 25: 50S RIBOSOMAL PROTEIN L27

Chain B0:



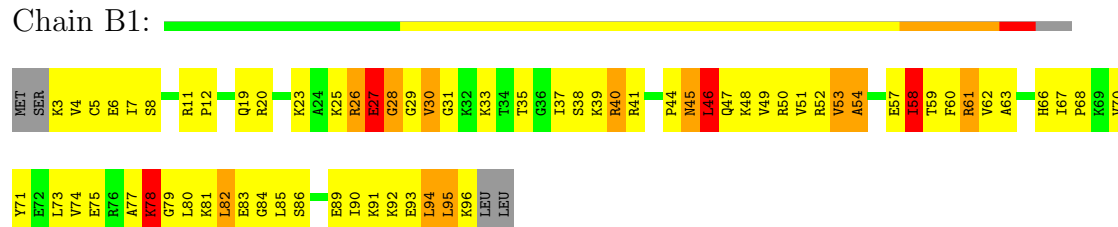
● Molecule 25: 50S RIBOSOMAL PROTEIN L27

Chain D0:



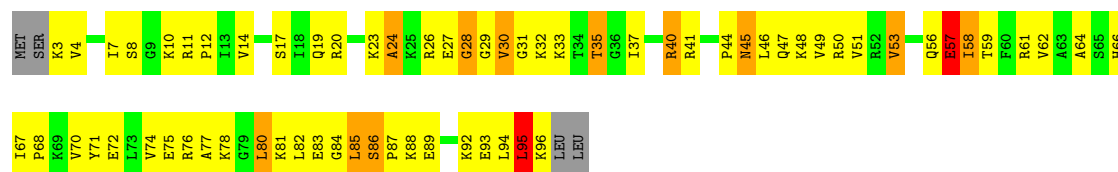
● Molecule 26: 50S RIBOSOMAL PROTEIN L28

Chain B1:



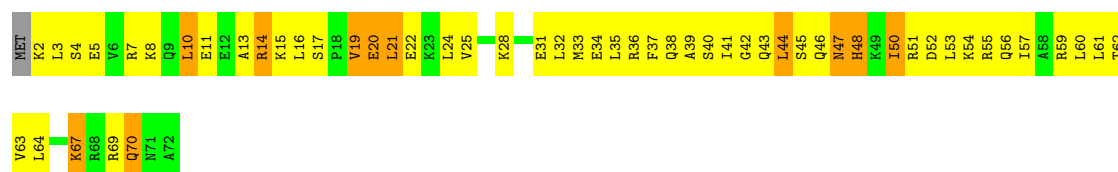
- Molecule 26: 50S RIBOSOMAL PROTEIN L28

Chain D1:



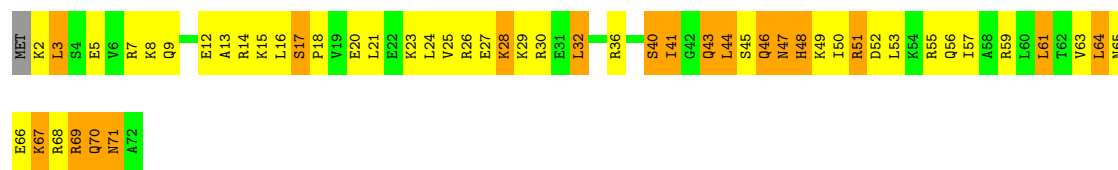
- Molecule 27: 50S RIBOSOMAL PROTEIN L29

Chain B2:



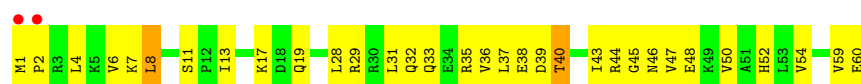
- Molecule 27: 50S RIBOSOMAL PROTEIN L29

Chain D2:



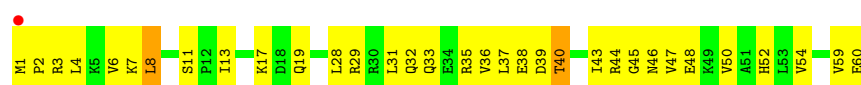
- Molecule 28: 50S RIBOSOMAL PROTEIN L30

Chain B3:



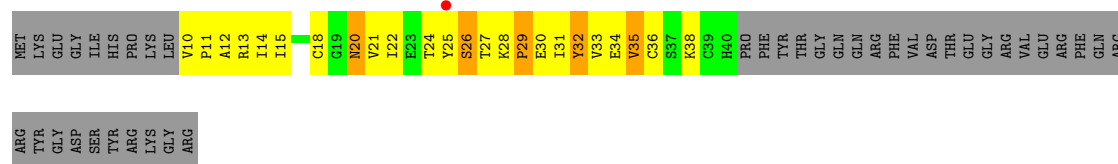
- Molecule 28: 50S RIBOSOMAL PROTEIN L30

Chain D3:



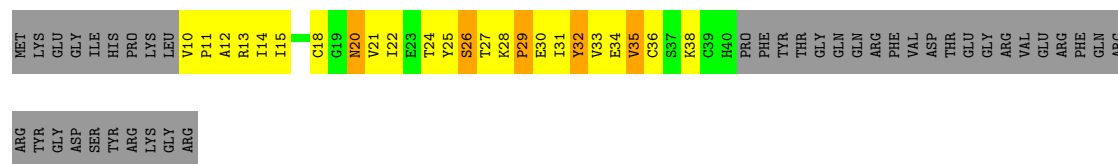
- Molecule 29: 50S RIBOSOMAL PROTEIN L31

Chain B4:



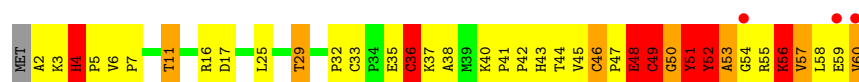
- Molecule 29: 50S RIBOSOMAL PROTEIN L31

Chain D4:



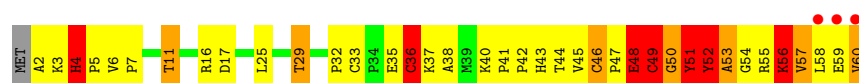
- Molecule 30: 50S RIBOSOMAL PROTEIN L32

Chain B5:



- Molecule 30: 50S RIBOSOMAL PROTEIN L32

Chain D5:



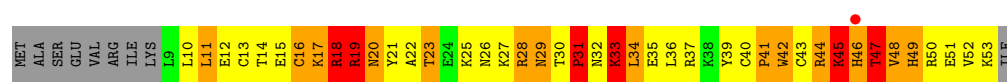
- Molecule 31: 50S RIBOSOMAL PROTEIN L33

Chain B6:



- Molecule 31: 50S RIBOSOMAL PROTEIN L33

Chain D6:



- Molecule 32: 50S RIBOSOMAL PROTEIN L34

Chain B7:



- Molecule 32: 50S RIBOSOMAL PROTEIN L34

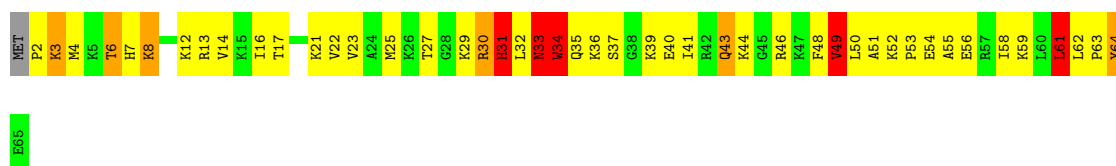
Chain D7:



- Molecule 33: 50S RIBOSOMAL PROTEIN L35

Chain B8:





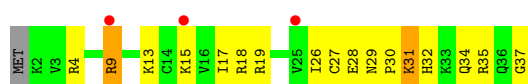
- Molecule 33: 50S RIBOSOMAL PROTEIN L35

Chain D8:



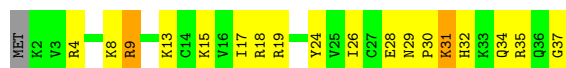
- Molecule 34: 50S RIBOSOMAL PROTEIN L36

Chain B9:



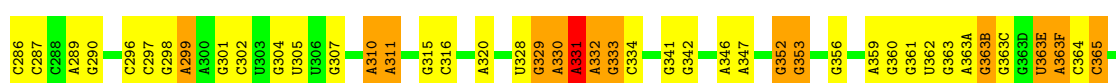
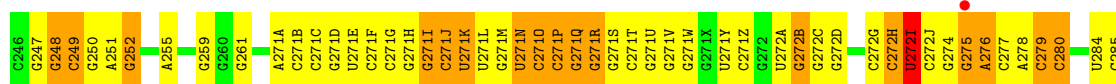
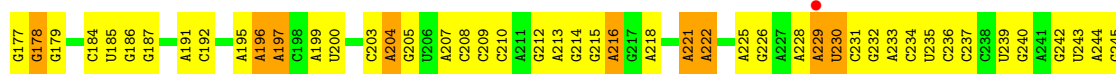
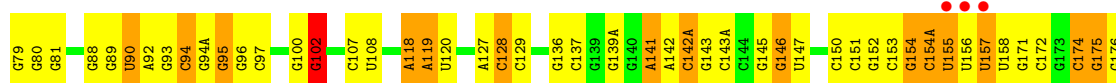
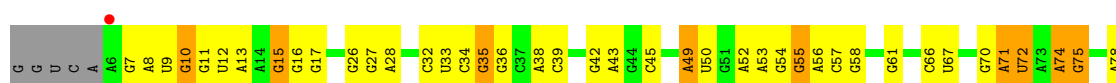
- Molecule 34: 50S RIBOSOMAL PROTEIN L36

Chain D9:



- Molecule 35: 23S RIBOSOMAL RNA

Chain BA:



U1590	G1510	G1441	U1357	G1270	C1178	G1106	A1045	C964	C893	C914	G733	U657	A614C	A547
G1591	G1515	G1442	G1358	G1271	C1179	G1107	A1046	C965	C894	C915	G738	C858	G615	A548
C1592	C1516	A1445	A1359	A1272	C1180	U1108	G1047	U969	U895	C916	G739	C859	G620	G549
G1595	U1517	C1445A	C1362	U1273	C1181	C1109	A1048	C970	A896	C917	G739	G660	A621	G553
C1598	G1519	G1447	G1364	A1274	A1182	A1111	C1049	G974	C897	G818	G743	G661	G622	U654
G1601	G1520	G1448	A1365	A1275	G1186	G1112	G1051	C975	C898	G819	G744	G663	G623	G558
U1602	G1525	A1449	A1366	A1276	G1187	U1113	C1052	C976	A899	U827	U747	C864	G624	G559
A1603	G1526	G1450	A1367	A1277	U1188	G1114	C1053	C977	C902	U828	G748	G625	G625	G562
C1527	G1527	U1453	U1372	G1280	G1192	C1116	G1054	A980	C903	G830	A751	U626	A627	U662
U1528	A1528	C1464	A1373	G1281	G1193	G1117	A1056	A983	U905	G831	A752	U627	G628	G563
A1528A	A1528A	A1460	G1374	U1282	A1194	G1122	A1057	G1058	U907	G832	C672	G628	G629	C564
A1609	G1529	G1461	C1375	A1283	G1195	U1115	G1059	C986	C908	G833	C673	G630	G630	C565
A1610	C1530	U1461	U1378	G1284	G1196	G1116	U1060	C987	A909	G834	C674	A631	A632	U666
C1531	C1531	C1464	A1378	A1285	G1201	G1117	A1061	U989	A910	C940	A676	A633	A633	G570
U1532	G1532	G1465	A1379	G1285	C1202	G1125	A1062	A1000	A911	C943	A764	A634	G634	A571
G1533	G1533	G1466	G1380	C1291	G1203	U1129	G1063	C991	C912	G843	G768	C635	C635	A572
U1534	A1535	C1467	A1384	U1292	A1204	G1131	G1064	C992	U913	C944	G769	G636	G636	G573
A1536	G1536	G1468	G1385	U1293	U1205	A1132	U1065	G993	C914	G845	G770	A637	A637	G574
G1537	G1537	G1470	C1386	U1294	U1206	U1133	A1067	A996	C915	G846	G771	A685	A685	A575
G1538	G1538	A1471	C1387	U1300	G1209	C1135	A1067	G997	G916	U847	U773	G686	G686	U576
G1539	G1539	A1472	U1301	A1301	A1210	G1136	G1068	C998	A917	G848	A774	G687	G687	G577
U1540	U1540	G1473	A1302	A1302	G1212	G1138	A1069	U999	A918	C850	G775	G642	G642	A578
G1541	C1474	C1474	C1403	A1307	G1215	U1141	G1076	A1010	U922	C851	G776	A644	A644	G579
A1542	A1542	G1475	C1404	A1308	G1216	U1142	A1077	G1011	C923	U851	A777	A646	A646	C580
C1543	C1543	G1478	G1405	G1309	C1217	A1142A	A1073	U1012	C924	G852	G778	G647	G647	C581
A1544	A1544	G1478	U1406	G1310	G1218	A1143	C1075	C1013	U960	G853	U779	G648	G648	G582
C1547	C1547	G1480	C1407	G1311	G1218	A1144	C1076	A1009	G927	C856	G780	G649	G649	G583
C1548	C1548	U1481	C1408	U1313	C1221	G1145	A1076	A1010	U928	C857	A781	G650	G650	C584
G1549	G1549	G1482	C1409	C1314	C1221A	C1146	U1078	G1011	G932	U858	A782	G651	G651	G585
C1550	G1484	G1484	G1410	G1315	G1232	C1147	C1079	U1012	U943	C859	A783	C652	C652	C587
C1551	G1485	G1485	C1411	U1316	G1227	A1148	C1080	C935	C936	A861	G785	A654	A654	C589
A1554	A1554	G1488	A1412	A1317	G1230	C1150	U1081	U1015	U937	G862	G786	G654A	G654A	A590
C1557	C1557	U1489	G1413	C1318	G1231	G1151	U1082	G1016	G938	A863	U787	G654B	G654B	C591
A1558	A1558	A1490	G1416	A1321	G1232	C1152	U1083	U1019	A941	A866	A788	G654C	G654C	G592
G1559	G1559	G1491	C1417	A1322	C1233	C1153	A1085	A1020	U942	G869	G799	G654D	G654D	G593
G1568	G1568	G1492	G1418	U1323	U1234	G1154	A1086	A1021	C942	G870	G712	G654E	G654E	U697
A1569	A1569	C1493	A1419	U1324	G1235	A1155	G1087	G1022	U943	G871	G713	G654F	G654F	U697
A1570	A1570	A1494	U1420	G1324	G1235	C1155	A1088	U1023	G944	A870	G714	G654G	G654G	G598
A1571	A1571	A1496	G1421	G1328	G1239	C1158	G1089	G1024	A945	G874	G715	G654H	G654H	C601
A1572	A1572	U1497	G1425	U1329	A1240	U1159	G1090	G1025	G946	G875	A716	C654I	C654I	G602
G1573	G1573	C1498	G1426	C1330	U1241	G1160	G1091	U1026	U958	C976	G717	A654J	A654J	A603
C1574	C1574	A1427	A1427	A1331	A1242	C1161	C1092	U1027	C951	G877	G718	G654K	G654K	G604
C1577	C1577	C1428	C1428	G1332	G1243	U1165	G1093	A1028	G952	U877	G719	G654L	G654L	C605
U1578	U1578	G1500	G1429	A1336	C1251	C1166	U1094	U1033	A953	G879	C720	G654M	G654M	U606
A1579	A1579	C1430	C1430	C1345	G1252	C1169	U1097	G1034	C954	G880	C721	G654N	G654N	U607
A1580	A1580	U1431	U1431	U1345	A1253	G1169	A1098	G1034	C955	G881	A722	G654O	G654O	U608
C1584	C1584	A1434	A1434	G1349	G1256	G1170	G1099	C1038	A957	G882	G723	C654P	C654P	A609
A1586	A1586	U1437	C1437	A1349	U1263	G1171	C1100	G1039	U959	G883	A727	G654Q	G654Q	G610
A1587	A1587	U1438	U1438	A1352	A1264	G1173	U1101	G1039	A957	U807	G728	G654R	G654R	C611
A1588	A1588	A1439	A1439	U1352	G1265	A1174	C1102	C1040	A960	G887	G729	G654S	G654S	C612
C1589	C1589	A1509A	A1509A	A1353	A1265	U1175	A1103	G1042	C961	U811	G730	A654T	A654T	G613
G1668	G1668	A1509B	G1440	U1353	G1266	A1176	C1104	C1043	G962	C812	C731	A654U	A654U	U614
A1689	A1689					A1177	U1105	G1044	U963	G892	C732	G656	G656	G614B

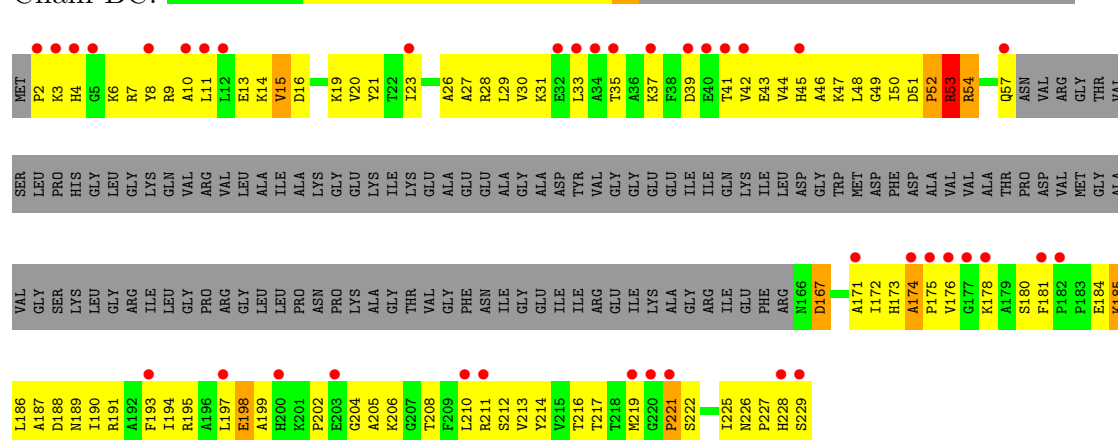






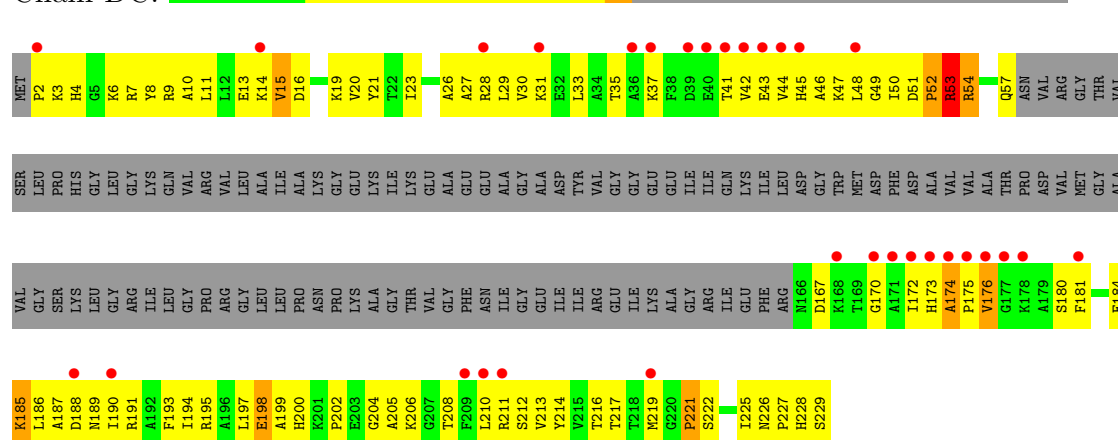
● Molecule 37: 50S RIBOSOMAL PROTEIN L1

Chain BC:



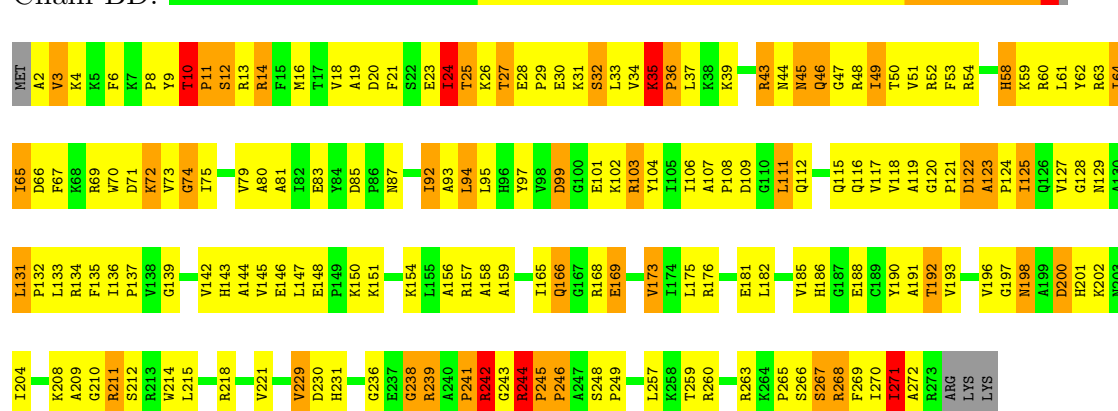
● Molecule 37: 50S RIBOSOMAL PROTEIN L1

Chain DC:



● Molecule 38: 50S RIBOSOMAL PROTEIN L2

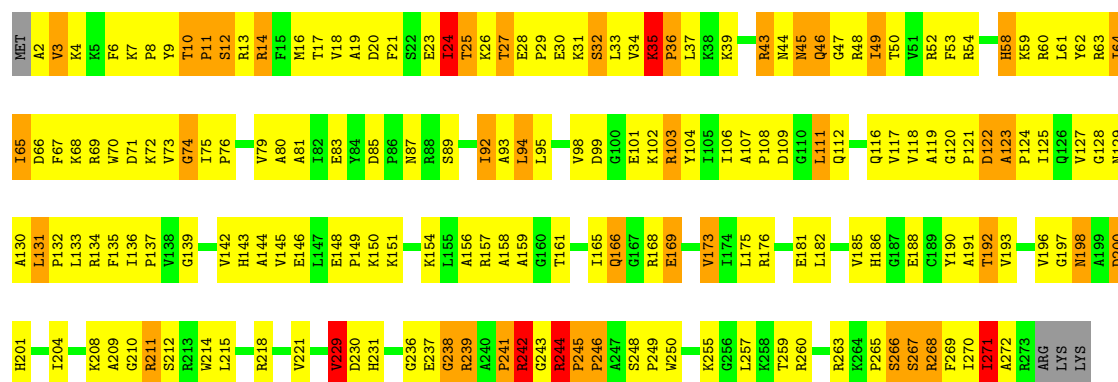
Chain BD:



● Molecule 38: 50S RIBOSOMAL PROTEIN L2

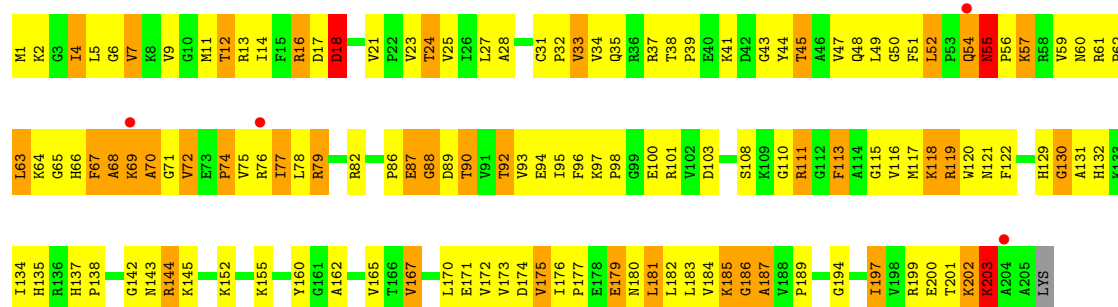
Chain DD:





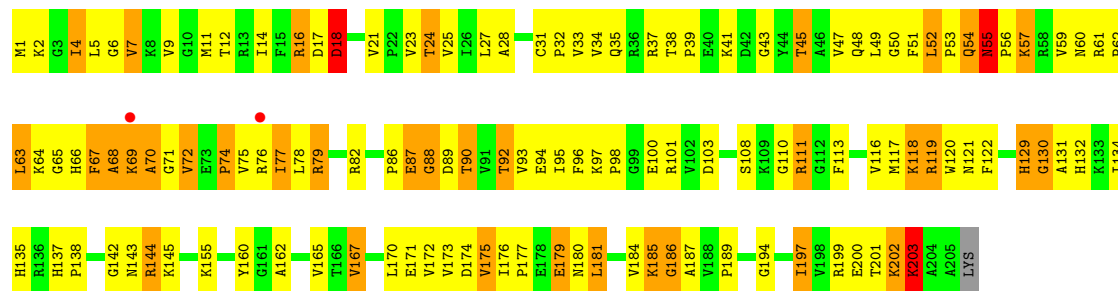
• Molecule 39: 50S RIBOSOMAL PROTEIN L3

Chain BE:



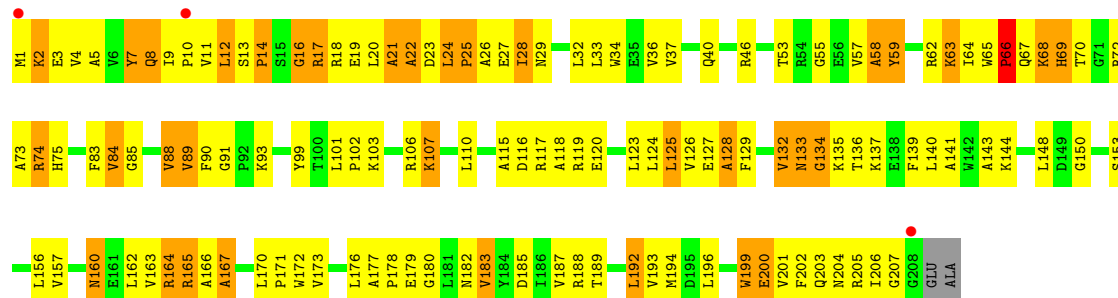
• Molecule 39: 50S RIBOSOMAL PROTEIN L3

Chain DE:



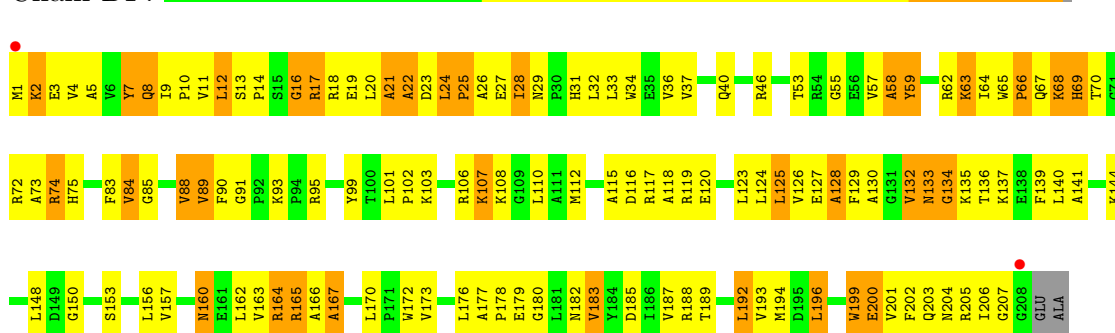
• Molecule 40: 50S RIBOSOMAL PROTEIN L4

Chain BF:



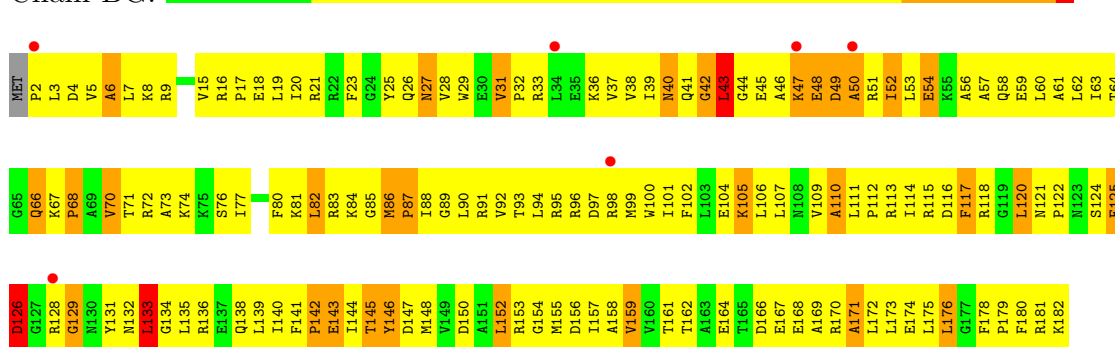
● Molecule 40: 50S RIBOSOMAL PROTEIN L4

Chain DF:



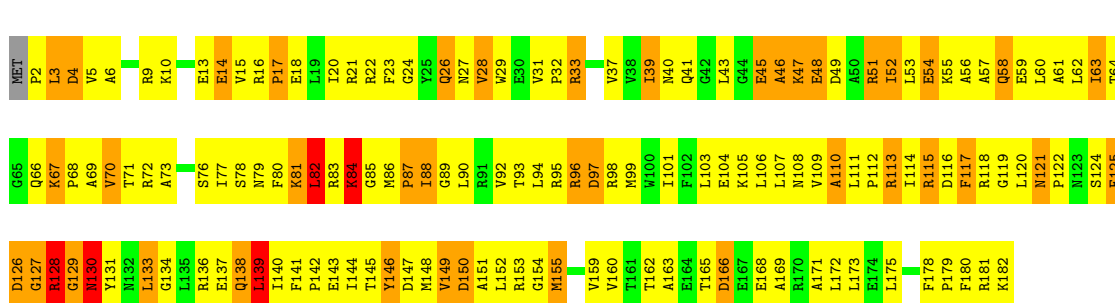
● Molecule 41: 50S RIBOSOMAL PROTEIN L5

Chain BG:



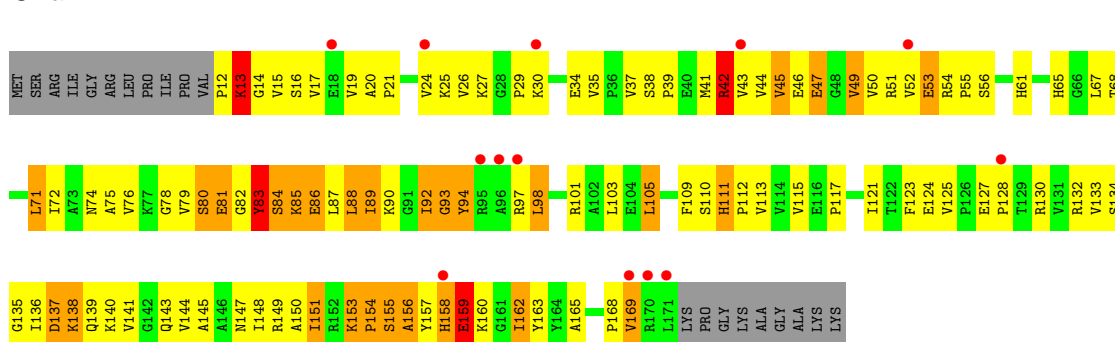
● Molecule 41: 50S RIBOSOMAL PROTEIN L5

Chain DG:



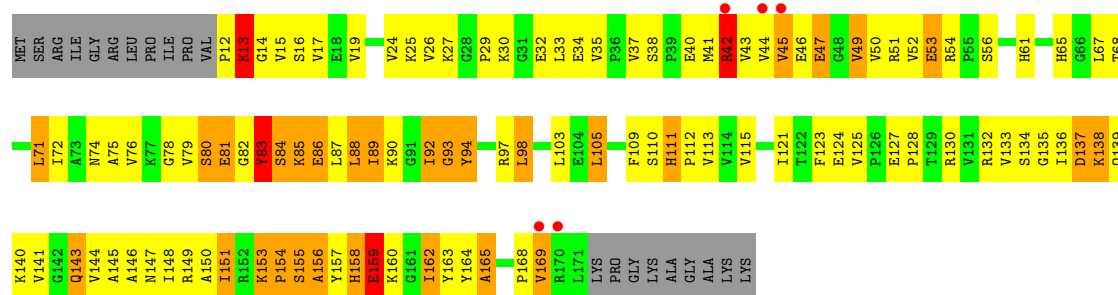
● Molecule 42: 50S RIBOSOMAL PROTEIN L6

Chain BH:



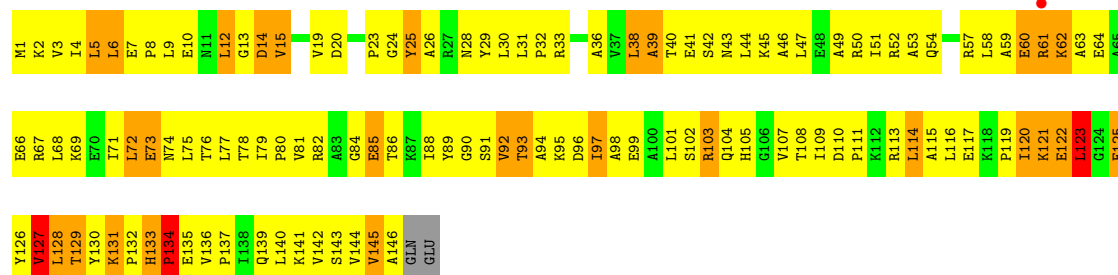
• Molecule 42: 50S RIBOSOMAL PROTEIN L6

Chain DH:



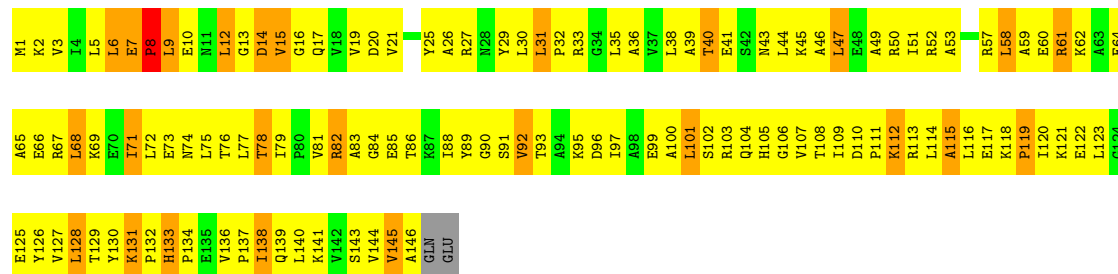
• Molecule 43: 50S RIBOSOMAL PROTEIN L9

Chain BI:



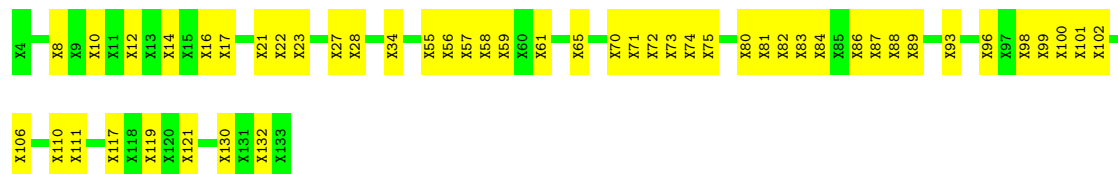
• Molecule 43: 50S RIBOSOMAL PROTEIN L9

Chain DI:



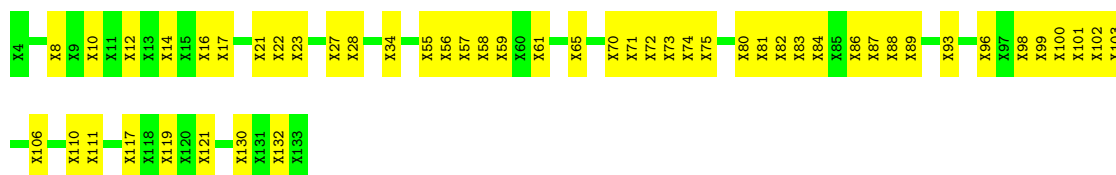
• Molecule 44: 50S RIBOSOMAL PROTEIN L10

Chain BJ:



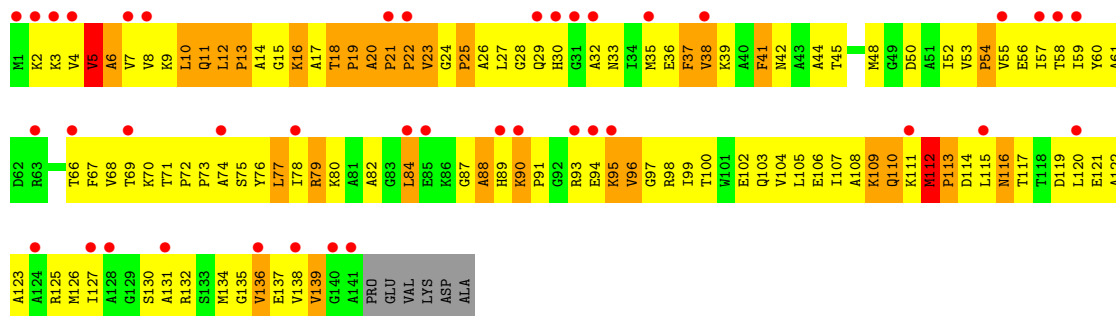
• Molecule 44: 50S RIBOSOMAL PROTEIN L10

Chain DJ:



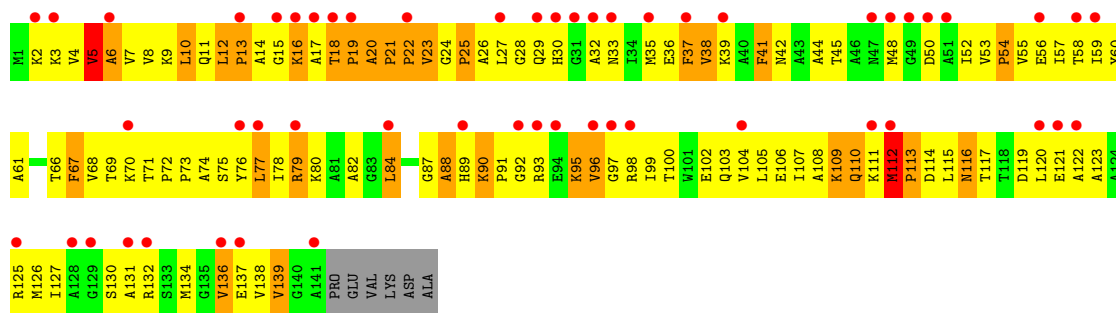
• Molecule 45: 50S RIBOSOMAL PROTEIN L11

Chain BK:



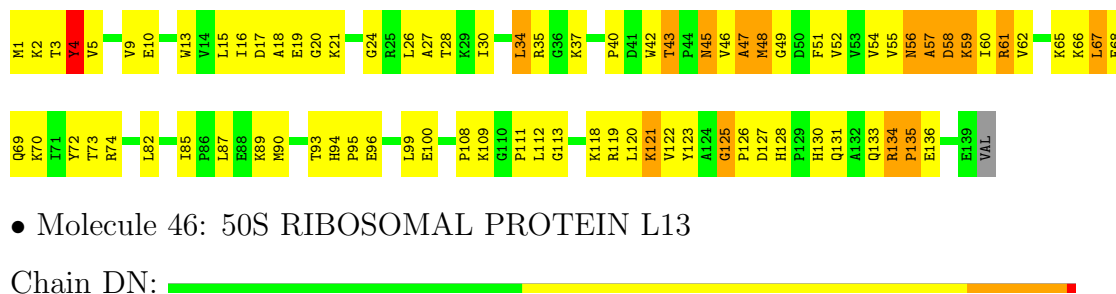
• Molecule 45: 50S RIBOSOMAL PROTEIN L11

Chain DK:



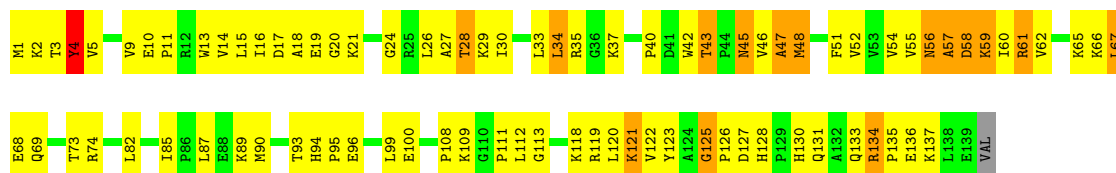
• Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain BN:

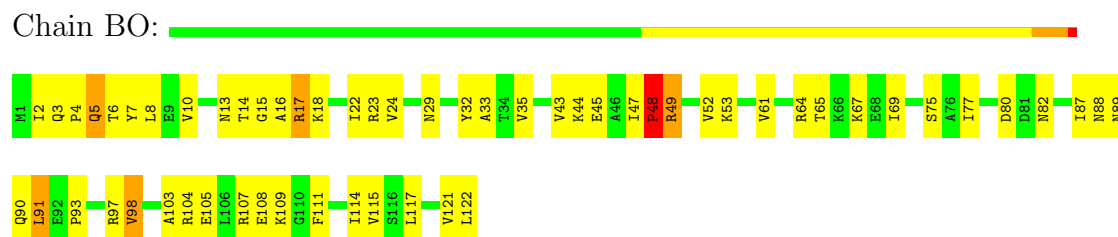


• Molecule 46: 50S RIBOSOMAL PROTEIN L13

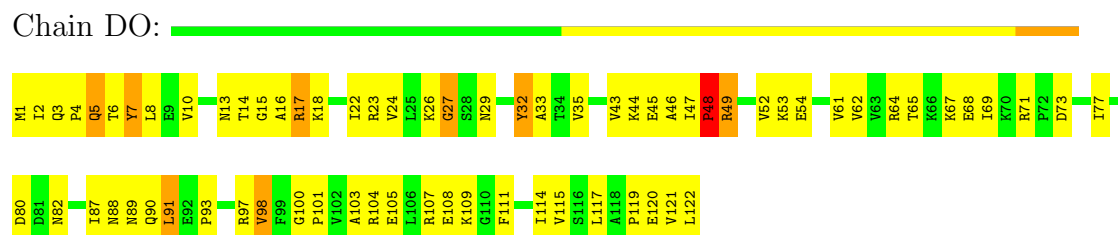
Chain DN:



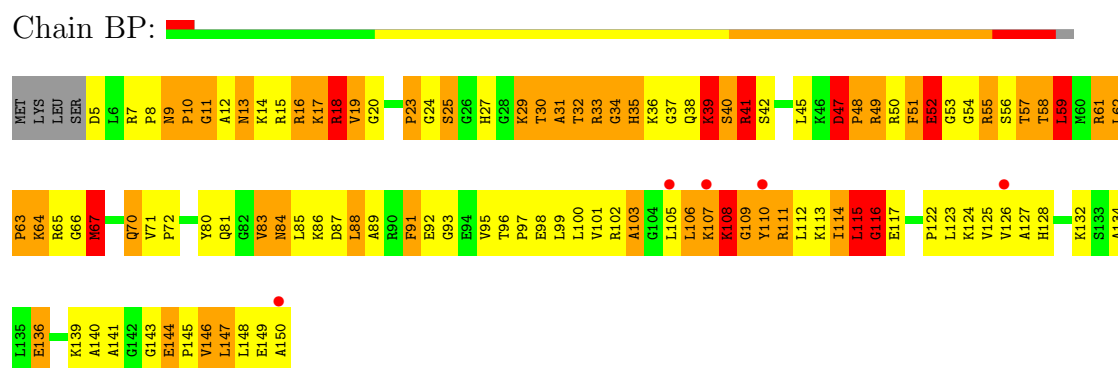
- Molecule 47: 50S RIBOSOMAL PROTEIN L14



- Molecule 47: 50S RIBOSOMAL PROTEIN L14



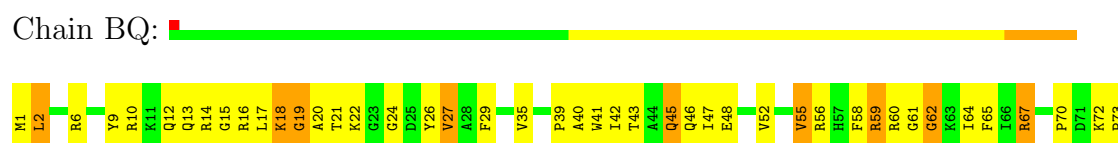
- Molecule 48: 50S RIBOSOMAL PROTEIN L15



- Molecule 48: 50S RIBOSOMAL PROTEIN L15



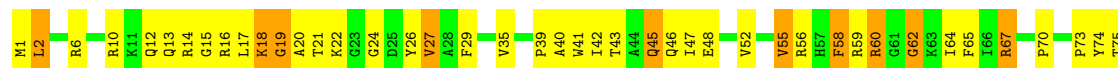
- Molecule 49: 50S RIBOSOMAL PROTEIN L16





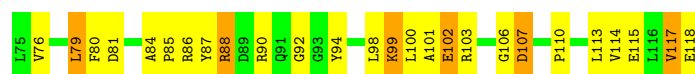
• Molecule 49: 50S RIBOSOMAL PROTEIN L16

Chain DQ:



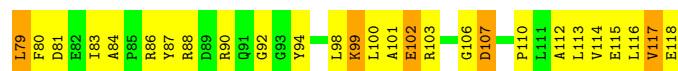
• Molecule 50: 50S RIBOSOMAL PROTEIN L17

Chain BR:



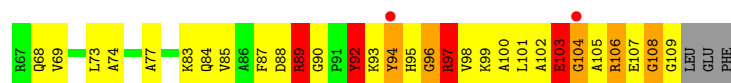
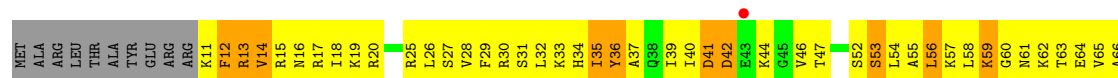
• Molecule 50: 50S RIBOSOMAL PROTEIN L17

Chain DR:



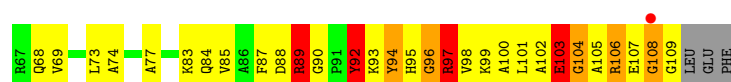
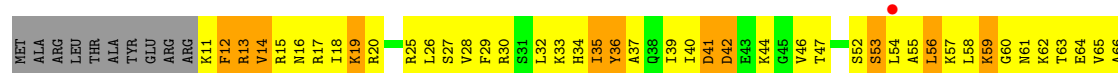
• Molecule 51: 50S RIBOSOMAL PROTEIN L18

Chain BS:



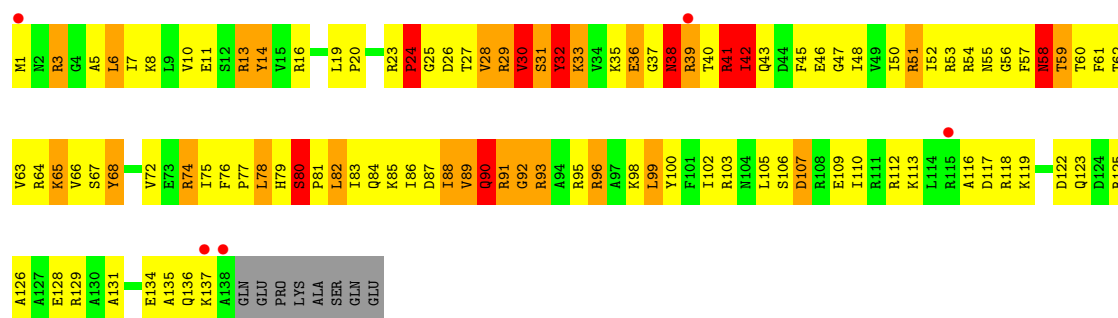
• Molecule 51: 50S RIBOSOMAL PROTEIN L18

Chain DS:



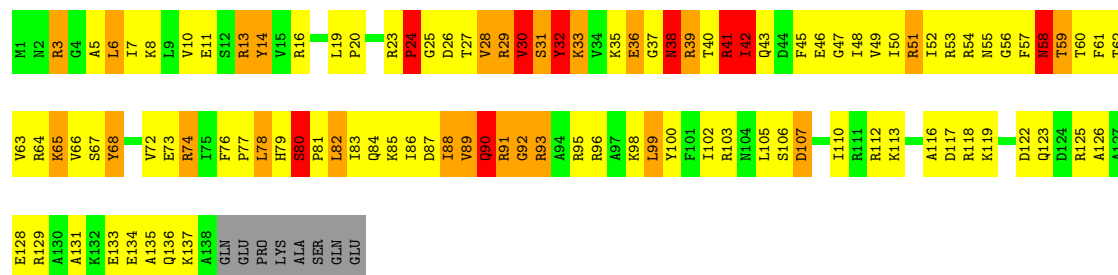
- Molecule 52: 50S RIBOSOMAL PROTEIN L19

Chain BT:



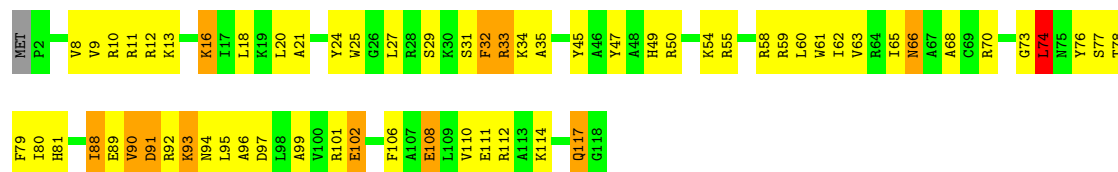
- Molecule 52: 50S RIBOSOMAL PROTEIN L19

Chain DT:



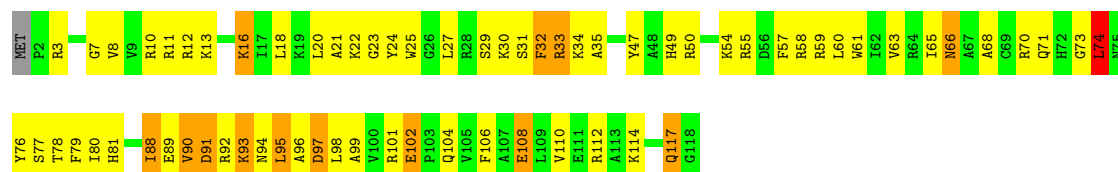
- Molecule 53: 50S RIBOSOMAL PROTEIN L20

Chain BU:



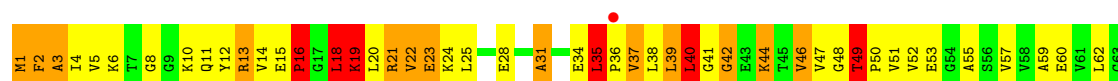
- Molecule 53: 50S RIBOSOMAL PROTEIN L20

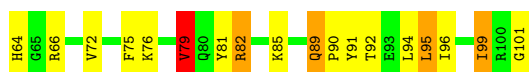
Chain DU:



- Molecule 54: 50S RIBOSOMAL PROTEIN L21

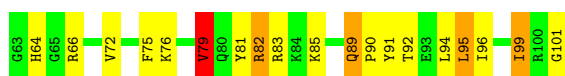
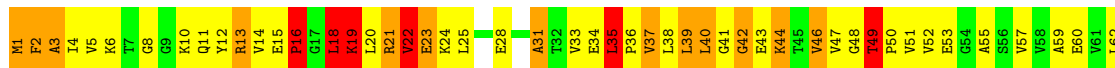
Chain BV:





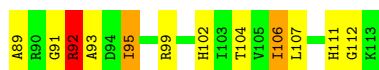
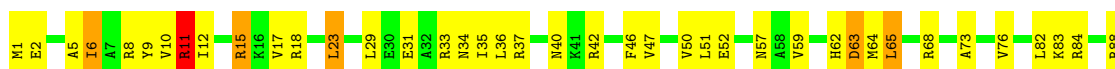
• Molecule 54: 50S RIBOSOMAL PROTEIN L21

Chain DV:



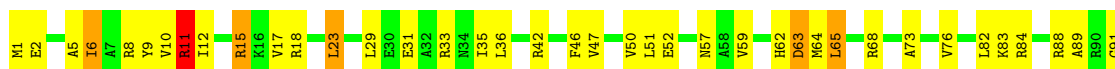
• Molecule 55: 50S RIBOSOMAL PROTEIN L22

Chain BW:



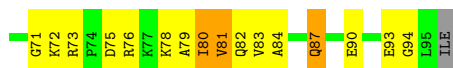
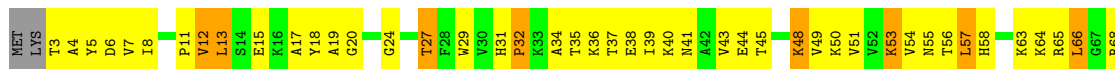
• Molecule 55: 50S RIBOSOMAL PROTEIN L22

Chain DW:



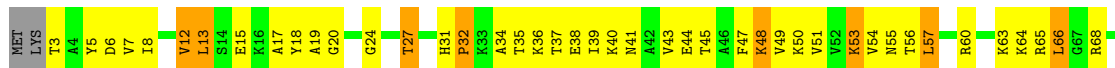
• Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain BX:



• Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain DX:



• Molecule 57: 50S RIBOSOMAL PROTEIN L24

MET	R2	V3	K4	M5	H6	V7	K8	G9	K10		V13	L14	V15	A16	S17	G18	K19	V20	K21	G22	R23		K26	V27	K28	E29	V30	L31	P32	K33	K34	V35	A36	V37	T38	V39	E40	G41	V42	N43	I44	V45	K46	K47	A48	V49	R50	V51	S52	P53	K54	V55	P56	Q57	G58	G59	F60	I61	F62
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K63	E64	A65	P66	L67	H68	A69	S70	K71	V72	R73	P74	I75	C76	P77	A78	C79	G80	K81	P82		R86	K87	K88	F89	L90	E91	N92	G93	K94	K95	I96	R97	V98	C99	A100	C101	C102	GLY	GLY	ALA	LEU	ASP	THR	GLU	GLU
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	--	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----

- Chain DY: 

K63	E64	A65	P66	L67	H68	A69	S70	K71	V72	R73	P74	I75	C76	P77	A78	C79	G80	K81	P82	G86	K87	K88	F89	L90	E91	N92	G93	K94	K95	R96	K97	K98	R99	R26	V27	K28	E29	V30	P31	P32	K33	K34	P35	A36	V37	V38	V39	E40	G41	V42	N43	I44	A45	K46	K47	A48	V49	R50	V51	S52	P53	K54	V55	P56	G57	G58	G59	F60	L61	F62
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- Chain BZ:

GLU	P130	L67	MET
PRO	N131	P68	GLU
GLU	N132	T69	Y3
VAL	I133	L70	R4
ILE	P134	V71	L5
LYS	E135	R72	K6
LYS	P136	Q73	A7
GLY	I137	V74	Y8
LYS	E138	W75	Y9
GLU	V139	D77	R10
GLU	D140	K78	O11
GLU	V141	R79	E11
GLU	L144	R80	K14
GLU	E145	R81	P15
	I146	R82	S16
	G147	P83	A17
	D148	E84	L18
	S149	H85	R19
	L150	V86	R20
	H151	D87	
	A152	F88	K23
	S153	F89	L24
	D154	V90	P25
	L155	L91	G26
	K156	S92	V27
	L157	P95	M28
	P158	V96	Y29
		E97	N30
	V161	K98	N34
	E162	Y99	R35
	L163	V100	K36
	A164	P101	V37
	V165	L102	Y38
	S166	R103	V39
	P167	F104	D40
	E168		L41
	E169	T107	V42
	T170	P108	E43
	I171	A109	F44
	A172	G110	D45
	A173	V111	K46
	V174	R112	
	V175	A113	R49
	P176	G114	Q50
	P177	G115	A51
	E178	V116	S52
	D179	L117	I53
	V190	Q118	
		E119	V56
	L183	T120	I57
	A184	H121	V58
	E185	R122	L59
	E186	D123	E60
	A187	L124	L61
	ALA	I125	P62
	ALA	L126	D63
	GLU	K127	G64
	VAL	V128	Q65
	A129	S129	S66

- Chain DZ:

VAL	P134	Q65	MET
ILE	E135		GLU
LVS	F136	T69	Y3
LVS	I137	L70	R4
GLY	E138	W71	L5
LVS	V139	R72	K6
GLU	D140	Q73	A7
GLU	V141	V74	Y8
GLU	S142		Y9
GLU	G143	D77	R10
GLU	L144	K78	E11
GLU	E145	R79	
	L146	R80	K14
	G147	R81	P15
	D148		S16
	S149	E84	A17
	L150	R85	L18
	H151	V86	R19
	A152	D87	R20
	S153	F88	A21
	D154	F89	G22
	L155	V90	K23
	K156	L91	L24
	L157	S92	P25
	P158	D93	G26
	P159	E94	V27
	L160	E95	M28
	V161	V96	Y29
	E162	E97	N30
	L163	H98	R31
	A164	Y99	
	V165	R103	N34
	R166	F104	R35
	E168	V105	K36
	E169		V37
	T170	P108	T38
	I171	A109	V39
		G110	D40
	V174	V111	L41
	V175	R112	V42
	P176	A113	E43
	P177	G114	F44
	E178	G115	D45
	D179	V116	K46
	A180		V47
		E119	F48
	L183	L120	R49
	A184	H121	Q56
	E185	R122	A51
	E186		S52
	A187	L125	I53
ALA	ALA	V126	V56
ALA	ALA	K127	I57
GLU	GLU	V128	V58
VAL	VAL	S129	L59
ALA	ALA	P130	E60
GLU	GLU	R131	
PRO	PRO	N132	D63
GLU	GLU	L133	G64

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.42Å 452.50Å 625.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.86 – 3.10 49.71 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.86-3.10) 99.6 (49.71-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.223 , 0.264 0.232 , 0.271	Depositor DCC
R_{free} test set	52374 reflections (4.65%)	DCC
Wilson B-factor (Å ²)	55.0	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 45.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 1179114 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	305067	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% 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: MG, ZN, 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	0.37	0/36190	0.69	14/56486 (0.0%)
1	CA	0.39	0/36190	0.69	11/56486 (0.0%)
2	AB	0.31	0/1936	0.58	0/2611
2	CB	0.33	0/1936	0.58	0/2611
3	AC	0.32	0/1637	0.54	0/2207
3	CC	0.32	0/1637	0.54	0/2207
4	AD	0.33	0/1733	0.63	0/2318
4	CD	0.33	0/1733	0.62	0/2318
5	AE	0.34	0/1163	0.61	0/1566
5	CE	0.35	0/1163	0.62	0/1566
6	AF	0.32	0/856	0.63	0/1154
6	CF	0.34	0/856	0.64	0/1154
7	AG	0.30	0/1276	0.56	0/1709
7	CG	0.31	0/1276	0.56	0/1709
8	AH	0.32	0/1136	0.61	0/1527
8	CH	0.32	0/1136	0.62	0/1527
9	AI	0.31	0/1027	0.58	0/1372
9	CI	0.32	0/1027	0.58	0/1372
10	AJ	0.32	0/808	0.56	0/1087
10	CJ	0.33	0/808	0.56	0/1087
11	AK	0.32	0/900	0.58	0/1213
11	CK	0.36	0/900	0.59	0/1213
12	AL	0.36	0/987	0.67	0/1322
12	CL	0.36	0/987	0.67	0/1322
13	AM	0.30	0/994	0.56	0/1322
13	CM	0.32	0/994	0.56	0/1322
14	AN	0.31	0/501	0.53	0/664
14	CN	0.33	0/501	0.55	0/664
15	AO	0.32	0/745	0.57	0/992
15	CO	0.33	0/745	0.58	0/992
16	AP	0.36	0/717	0.58	0/965
16	CP	0.34	0/717	0.58	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.33	0/837	0.61	0/1119
17	CQ	0.35	0/837	0.61	0/1119
18	AR	0.33	0/579	0.60	0/768
18	CR	0.34	0/579	0.60	0/768
19	AS	0.34	0/643	0.56	0/867
19	CS	0.34	0/643	0.57	0/867
20	AT	0.29	0/765	0.58	0/1007
20	CT	0.29	0/765	0.58	0/1007
21	AU	0.41	0/213	0.49	0/279
21	CU	0.42	0/213	0.50	0/279
22	AV	0.38	0/1784	0.70	0/2780
22	AW	0.35	0/1784	0.71	0/2780
22	CV	0.44	0/1784	0.69	0/2780
22	CW	0.36	0/1784	0.70	0/2780
23	AX	0.39	0/184	0.74	0/284
23	CX	0.45	0/184	0.76	0/284
24	AY	0.31	0/2849	0.60	0/3848
24	CY	0.33	0/2849	0.66	0/3848
25	B0	0.36	0/666	0.63	0/885
25	D0	0.42	0/666	0.67	0/885
26	B1	0.41	0/739	0.73	1/983 (0.1%)
26	D1	0.50	0/739	0.79	0/983
27	B2	0.36	0/600	0.60	0/793
27	D2	0.46	0/600	0.79	0/793
28	B3	0.34	0/473	0.61	0/636
28	D3	0.43	0/473	0.65	0/636
29	B4	0.38	0/229	0.61	0/311
29	D4	0.40	0/229	0.62	0/311
30	B5	0.49	0/473	0.94	2/639 (0.3%)
30	D5	0.71	2/473 (0.4%)	1.01	2/639 (0.3%)
31	B6	0.48	0/387	0.79	0/517
31	D6	0.54	0/388	0.77	0/520
32	B7	0.46	0/427	0.67	0/563
32	D7	0.53	0/427	0.70	0/563
33	B8	0.50	0/516	0.78	0/681
33	D8	0.59	0/516	0.81	0/681
34	B9	0.33	0/302	0.63	0/397
34	D9	0.44	0/302	0.68	0/397
35	BA	0.46	1/69972 (0.0%)	0.74	51/109237 (0.0%)
35	DA	0.60	1/69972 (0.0%)	0.76	63/109237 (0.1%)
36	BB	0.37	0/2853	0.73	0/4451
36	DB	0.50	0/2853	0.74	0/4451
37	BC	0.27	0/956	0.51	0/1288

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DC	0.27	0/956	0.51	0/1288
38	BD	0.42	0/2155	0.77	1/2907 (0.0%)
38	DD	0.49	0/2155	0.80	2/2907 (0.1%)
39	BE	0.42	0/1597	0.77	0/2155
39	DE	0.52	0/1597	0.80	0/2155
40	BF	0.41	0/1659	0.72	1/2246 (0.0%)
40	DF	0.49	0/1659	0.76	1/2246 (0.0%)
41	BG	0.32	0/1498	0.62	0/2013
41	DG	0.39	0/1499	0.75	2/2016 (0.1%)
42	BH	0.35	0/1246	0.70	0/1684
42	DH	0.43	0/1246	0.73	0/1684
43	BI	0.36	0/1147	0.68	0/1553
43	DI	0.35	0/1147	0.74	0/1553
45	BK	0.33	0/1057	0.58	0/1432
45	DK	0.34	0/1057	0.58	0/1432
46	BN	0.37	0/1132	0.76	1/1527 (0.1%)
46	DN	0.47	0/1132	0.80	1/1527 (0.1%)
47	BO	0.42	0/943	0.69	0/1269
47	DO	0.47	0/943	0.71	0/1269
48	BP	0.44	0/1131	0.99	7/1504 (0.5%)
48	DP	0.55	0/1131	1.04	7/1504 (0.5%)
49	BQ	0.37	0/1143	0.66	0/1527
49	DQ	0.46	0/1143	0.69	0/1527
50	BR	0.39	0/974	0.73	2/1302 (0.2%)
50	DR	0.48	0/974	0.77	2/1302 (0.2%)
51	BS	0.39	0/779	0.70	0/1038
51	DS	0.48	0/779	0.73	0/1038
52	BT	0.43	0/1156	0.81	3/1544 (0.2%)
52	DT	0.48	0/1156	0.83	3/1544 (0.2%)
53	BU	0.41	0/975	0.68	1/1297 (0.1%)
53	DU	0.54	0/975	0.75	2/1297 (0.2%)
54	BV	0.38	0/790	0.73	0/1057
54	DV	0.48	0/790	0.79	0/1057
55	BW	0.39	0/907	0.70	0/1216
55	DW	0.48	0/907	0.74	0/1216
56	BX	0.41	0/740	0.70	0/995
56	DX	0.49	0/740	0.73	0/995
57	BY	0.44	0/789	0.75	0/1053
57	DY	0.52	0/789	0.77	1/1053 (0.1%)
58	BZ	0.36	0/1500	0.65	0/2037
58	DZ	0.42	0/1500	0.71	0/2037
All	All	0.46	4/328312 (0.0%)	0.72	181/489974 (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	1	15
1	CA	1	17
22	AW	0	1
22	CV	0	1
22	CW	0	3
30	B5	0	2
30	D5	0	2
35	BA	5	59
35	DA	6	77
36	BB	0	2
36	DB	0	3
All	All	13	182

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	D5	49	CYS	CB-SG	5.59	1.91	1.82
35	DA	2685	G	C6-O6	5.54	1.29	1.24
35	BA	1899	G	C2-N2	-5.53	1.29	1.34
30	D5	51	TYR	CD1-CE1	5.27	1.47	1.39

The worst 5 of 181 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BA	1992	G	C2'-C3'-O3'	10.98	133.66	109.50
35	DA	1992	G	C2'-C3'-O3'	10.73	133.11	109.50
35	DA	331	A	C2'-C3'-O3'	9.84	131.14	109.50
35	BA	331	A	C2'-C3'-O3'	9.40	130.19	109.50
35	DA	1653	G	C2'-C3'-O3'	9.16	129.65	109.50

5 of 13 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	1504	G	C3'
35	BA	587	C	C3'
35	BA	1300	U	C3'
35	BA	1799	G	C3'
35	BA	1819	A	C3'

5 of 182 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	21	G	Sidechain
1	AA	575	G	Sidechain
1	AA	587	G	Sidechain
1	AA	760	G	Sidechain
1	AA	832	C	Sidechain

5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16314	1205	0
1	CA	32329	0	16316	1221	0
2	AB	1901	0	1951	258	0
2	CB	1901	0	1951	259	0
3	AC	1613	0	1677	199	0
3	CC	1613	0	1677	196	0
4	AD	1703	0	1763	219	0
4	CD	1703	0	1763	207	0
5	AE	1147	0	1207	125	0
5	CE	1147	0	1207	125	0
6	AF	843	0	857	88	0
6	CF	843	0	857	95	0
7	AG	1257	0	1296	113	0
7	CG	1257	0	1296	121	0
8	AH	1116	0	1177	118	0
8	CH	1116	0	1177	113	0
9	AI	1011	0	1041	126	0
9	CI	1011	0	1041	129	0
10	AJ	795	0	840	146	0
10	CJ	795	0	840	144	0
11	AK	885	0	904	74	0
11	CK	885	0	904	77	0
12	AL	971	0	1057	122	0
12	CL	971	0	1057	124	0
13	AM	988	0	1055	161	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	CM	988	0	1055	153	0
14	AN	492	0	530	66	0
14	CN	492	0	529	65	0
15	AO	734	0	771	55	0
15	CO	734	0	771	52	0
16	AP	701	0	720	81	0
16	CP	701	0	720	87	0
17	AQ	824	0	891	62	0
17	CQ	824	0	891	63	0
18	AR	574	0	644	59	0
18	CR	574	0	644	59	0
19	AS	630	0	651	98	0
19	CS	630	0	651	100	0
20	AT	763	0	861	73	0
20	CT	763	0	861	78	0
21	AU	209	0	221	24	0
21	CU	209	0	221	26	0
22	AV	1630	0	831	77	0
22	AW	1630	0	831	101	0
22	CV	1630	0	831	65	0
22	CW	1630	0	832	109	0
23	AX	165	0	87	11	0
23	CX	165	0	87	17	0
24	AY	2801	0	2816	377	0
24	CY	2801	0	2816	430	0
25	B0	657	0	683	58	0
25	D0	657	0	683	55	0
26	B1	732	0	808	88	0
26	D1	732	0	808	80	0
27	B2	598	0	653	81	0
27	D2	598	0	653	77	0
28	B3	468	0	523	40	0
28	D3	468	0	523	42	0
29	B4	226	0	229	46	0
29	D4	226	0	229	45	0
30	B5	459	0	480	74	0
30	D5	459	0	480	74	0
31	B6	381	0	390	73	0
31	D6	381	0	389	149	0
32	B7	419	0	467	19	0
32	D7	419	0	467	22	0
33	B8	508	0	576	103	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	D8	508	0	576	103	0
34	B9	299	0	323	24	0
34	D9	299	0	323	24	0
35	BA	62474	0	31492	1876	0
35	DA	62474	0	31493	1854	0
36	BB	2551	0	1295	80	0
36	DB	2551	0	1295	70	0
37	BC	937	0	957	106	0
37	DC	937	0	957	108	0
38	BD	2105	0	2182	248	0
38	DD	2105	0	2182	254	0
39	BE	1564	0	1629	191	0
39	DE	1564	0	1629	192	0
40	BF	1624	0	1677	189	0
40	DF	1624	0	1677	188	0
41	BG	1474	0	1534	286	0
41	DG	1474	0	1535	240	0
42	BH	1223	0	1282	139	0
42	DH	1223	0	1282	145	0
43	BI	1132	0	1218	179	0
43	DI	1132	0	1218	181	0
44	BJ	651	0	151	34	0
44	DJ	651	0	151	34	0
45	BK	1038	0	1089	196	0
45	DK	1038	0	1089	192	0
46	BN	1105	0	1180	127	0
46	DN	1105	0	1180	134	0
47	BO	933	0	996	84	0
47	DO	933	0	996	93	0
48	BP	1114	0	1187	268	0
48	DP	1114	0	1187	263	0
49	BQ	1122	0	1179	127	0
49	DQ	1122	0	1179	110	0
50	BR	960	0	1021	93	0
50	DR	960	0	1021	94	0
51	BS	771	0	832	126	0
51	DS	771	0	832	121	0
52	BT	1142	0	1202	223	0
52	DT	1142	0	1202	228	0
53	BU	958	0	1015	103	0
53	DU	958	0	1015	109	0
54	BV	779	0	852	132	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	DV	779	0	852	133	0
55	BW	896	0	953	50	0
55	DW	896	0	953	50	0
56	BX	726	0	778	73	0
56	DX	726	0	778	70	0
57	BY	776	0	870	178	0
57	DY	776	0	870	190	0
58	BZ	1468	0	1492	228	0
58	DZ	1468	0	1492	188	0
59	AA	161	0	0	0	0
59	AL	1	0	0	0	0
59	AS	1	0	0	0	0
59	AV	7	0	0	0	0
59	AW	4	0	0	0	0
59	AX	1	0	0	0	0
59	AY	1	0	0	0	0
59	B1	1	0	0	0	0
59	B5	2	0	0	0	0
59	BA	357	0	0	0	0
59	BB	4	0	0	0	0
59	BD	2	0	0	0	0
59	BF	2	0	0	0	0
59	BG	1	0	0	0	0
59	BT	1	0	0	0	0
59	BX	1	0	0	0	0
59	BY	1	0	0	0	0
59	CA	155	0	0	0	0
59	CD	1	0	0	0	0
59	CL	2	0	0	0	0
59	CN	1	0	0	0	0
59	CS	1	0	0	0	0
59	CV	7	0	0	0	0
59	CW	4	0	0	0	0
59	CX	1	0	0	0	0
59	D1	1	0	0	0	0
59	D5	2	0	0	0	0
59	DA	359	0	0	0	0
59	DB	4	0	0	0	0
59	DD	1	0	0	0	0
59	DE	1	0	0	0	0
59	DF	1	0	0	0	0
59	DG	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	DH	1	0	0	0	0
59	DP	1	0	0	0	0
59	DS	1	0	0	0	0
59	DX	1	0	0	0	0
60	AD	1	0	0	0	0
60	AN	1	0	0	0	0
60	B9	1	0	0	0	0
60	CD	1	0	0	0	0
60	CN	1	0	0	0	0
60	D9	1	0	0	0	0
61	AV	1	0	0	0	0
61	AY	1	0	0	0	0
61	BA	1	0	0	1	0
All	All	305067	0	208379	18089	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 35.

The worst 5 of 18089 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:CY:303:ARG:HH22	35:DA:1914:C:C1'	1.34	1.39
24:CY:303:ARG:NH2	35:DA:1914:C:H1'	1.33	1.39
31:D6:41:PRO:HD3	31:D6:46:HIS:CB	1.55	1.36
31:D6:46:HIS:CA	31:D6:47:THR:HG23	1.58	1.33
35:DA:1899:G:N2	35:DA:1902:C:H41	1.26	1.32

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%)	127 (54%)	71 (30%)	35 (15%)	0 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	CB	233/256 (91%)	128 (55%)	70 (30%)	35 (15%)	0	1
3	AC	205/239 (86%)	129 (63%)	40 (20%)	36 (18%)	0	0
3	CC	205/239 (86%)	129 (63%)	42 (20%)	34 (17%)	0	0
4	AD	206/209 (99%)	139 (68%)	45 (22%)	22 (11%)	1	5
4	CD	206/209 (99%)	139 (68%)	44 (21%)	23 (11%)	1	5
5	AE	149/162 (92%)	115 (77%)	23 (15%)	11 (7%)	2	11
5	CE	149/162 (92%)	114 (76%)	24 (16%)	11 (7%)	2	11
6	AF	99/101 (98%)	70 (71%)	21 (21%)	8 (8%)	1	10
6	CF	99/101 (98%)	73 (74%)	18 (18%)	8 (8%)	1	10
7	AG	153/156 (98%)	117 (76%)	26 (17%)	10 (6%)	2	15
7	CG	153/156 (98%)	117 (76%)	27 (18%)	9 (6%)	2	17
8	AH	136/138 (99%)	106 (78%)	23 (17%)	7 (5%)	3	22
8	CH	136/138 (99%)	104 (76%)	24 (18%)	8 (6%)	2	17
9	AI	121/128 (94%)	86 (71%)	24 (20%)	11 (9%)	1	8
9	CI	121/128 (94%)	86 (71%)	24 (20%)	11 (9%)	1	8
10	AJ	97/105 (92%)	70 (72%)	22 (23%)	5 (5%)	3	21
10	CJ	97/105 (92%)	71 (73%)	21 (22%)	5 (5%)	3	21
11	AK	117/129 (91%)	86 (74%)	27 (23%)	4 (3%)	6	32
11	CK	117/129 (91%)	87 (74%)	26 (22%)	4 (3%)	6	32
12	AL	123/132 (93%)	84 (68%)	21 (17%)	18 (15%)	0	2
12	CL	123/132 (93%)	84 (68%)	21 (17%)	18 (15%)	0	2
13	AM	113/126 (90%)	71 (63%)	25 (22%)	17 (15%)	0	1
13	CM	113/126 (90%)	70 (62%)	26 (23%)	17 (15%)	0	1
14	AN	58/61 (95%)	40 (69%)	13 (22%)	5 (9%)	1	9
14	CN	58/61 (95%)	40 (69%)	12 (21%)	6 (10%)	1	6
15	AO	86/89 (97%)	66 (77%)	18 (21%)	2 (2%)	10	45
15	CO	86/89 (97%)	66 (77%)	18 (21%)	2 (2%)	10	45
16	AP	82/88 (93%)	58 (71%)	17 (21%)	7 (8%)	1	9
16	CP	82/88 (93%)	58 (71%)	16 (20%)	8 (10%)	1	6
17	AQ	98/105 (93%)	76 (78%)	13 (13%)	9 (9%)	1	7
17	CQ	98/105 (93%)	76 (78%)	12 (12%)	10 (10%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AR	68/88 (77%)	45 (66%)	16 (24%)	7 (10%)	1	6
18	CR	68/88 (77%)	45 (66%)	15 (22%)	8 (12%)	1	4
19	AS	77/93 (83%)	44 (57%)	22 (29%)	11 (14%)	0	2
19	CS	77/93 (83%)	44 (57%)	22 (29%)	11 (14%)	0	2
20	AT	97/106 (92%)	63 (65%)	26 (27%)	8 (8%)	1	10
20	CT	97/106 (92%)	63 (65%)	24 (25%)	10 (10%)	1	6
21	AU	23/27 (85%)	16 (70%)	5 (22%)	2 (9%)	1	9
21	CU	23/27 (85%)	16 (70%)	5 (22%)	2 (9%)	1	9
24	AY	349/351 (99%)	263 (75%)	65 (19%)	21 (6%)	2	17
24	CY	349/351 (99%)	272 (78%)	55 (16%)	22 (6%)	2	16
25	B0	81/85 (95%)	69 (85%)	11 (14%)	1 (1%)	19	62
25	D0	81/85 (95%)	69 (85%)	11 (14%)	1 (1%)	19	62
26	B1	92/98 (94%)	64 (70%)	16 (17%)	12 (13%)	0	3
26	D1	92/98 (94%)	72 (78%)	12 (13%)	8 (9%)	1	9
27	B2	69/72 (96%)	46 (67%)	12 (17%)	11 (16%)	0	1
27	D2	69/72 (96%)	42 (61%)	16 (23%)	11 (16%)	0	1
28	B3	58/60 (97%)	52 (90%)	6 (10%)	0	100	100
28	D3	58/60 (97%)	52 (90%)	6 (10%)	0	100	100
29	B4	29/71 (41%)	16 (55%)	10 (34%)	3 (10%)	1	6
29	D4	29/71 (41%)	16 (55%)	10 (34%)	3 (10%)	1	6
30	B5	57/60 (95%)	41 (72%)	5 (9%)	11 (19%)	0	0
30	D5	57/60 (95%)	41 (72%)	5 (9%)	11 (19%)	0	0
31	B6	41/54 (76%)	18 (44%)	7 (17%)	16 (39%)	0	0
31	D6	43/54 (80%)	17 (40%)	9 (21%)	17 (40%)	0	0
32	B7	47/49 (96%)	47 (100%)	0	0	100	100
32	D7	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
33	B8	62/65 (95%)	43 (69%)	11 (18%)	8 (13%)	0	3
33	D8	62/65 (95%)	44 (71%)	9 (14%)	9 (14%)	0	2
34	B9	34/37 (92%)	31 (91%)	2 (6%)	1 (3%)	7	38
34	D9	34/37 (92%)	31 (91%)	2 (6%)	1 (3%)	7	38
37	BC	116/229 (51%)	88 (76%)	19 (16%)	9 (8%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	DC	116/229 (51%)	88 (76%)	19 (16%)	9 (8%)	1	11
38	BD	270/276 (98%)	203 (75%)	37 (14%)	30 (11%)	1	5
38	DD	270/276 (98%)	205 (76%)	37 (14%)	28 (10%)	1	5
39	BE	203/206 (98%)	146 (72%)	34 (17%)	23 (11%)	1	4
39	DE	203/206 (98%)	149 (73%)	32 (16%)	22 (11%)	1	5
40	BF	206/210 (98%)	149 (72%)	33 (16%)	24 (12%)	1	4
40	DF	206/210 (98%)	149 (72%)	34 (16%)	23 (11%)	1	5
41	BG	177/182 (97%)	98 (55%)	50 (28%)	29 (16%)	0	0
41	DG	179/182 (98%)	123 (69%)	26 (14%)	30 (17%)	0	0
42	BH	158/180 (88%)	105 (66%)	27 (17%)	26 (16%)	0	0
42	DH	158/180 (88%)	105 (66%)	28 (18%)	25 (16%)	0	1
43	BI	144/148 (97%)	86 (60%)	34 (24%)	24 (17%)	0	0
43	DI	144/148 (97%)	90 (62%)	40 (28%)	14 (10%)	1	6
45	BK	139/147 (95%)	78 (56%)	37 (27%)	24 (17%)	0	0
45	DK	139/147 (95%)	78 (56%)	37 (27%)	24 (17%)	0	0
46	BN	137/140 (98%)	105 (77%)	24 (18%)	8 (6%)	3	18
46	DN	137/140 (98%)	103 (75%)	26 (19%)	8 (6%)	3	18
47	BO	120/122 (98%)	101 (84%)	14 (12%)	5 (4%)	4	27
47	DO	120/122 (98%)	102 (85%)	12 (10%)	6 (5%)	3	22
48	BP	144/150 (96%)	71 (49%)	32 (22%)	41 (28%)	0	0
48	DP	144/150 (96%)	71 (49%)	33 (23%)	40 (28%)	0	0
49	BQ	139/141 (99%)	108 (78%)	25 (18%)	6 (4%)	4	26
49	DQ	139/141 (99%)	109 (78%)	23 (16%)	7 (5%)	3	22
50	BR	115/118 (98%)	92 (80%)	15 (13%)	8 (7%)	2	13
50	DR	115/118 (98%)	93 (81%)	14 (12%)	8 (7%)	2	13
51	BS	97/112 (87%)	51 (53%)	29 (30%)	17 (18%)	0	0
51	DS	97/112 (87%)	51 (53%)	28 (29%)	18 (19%)	0	0
52	BT	136/146 (93%)	84 (62%)	33 (24%)	19 (14%)	0	2
52	DT	136/146 (93%)	85 (62%)	32 (24%)	19 (14%)	0	2
53	BU	115/118 (98%)	97 (84%)	11 (10%)	7 (6%)	2	16
53	DU	115/118 (98%)	98 (85%)	9 (8%)	8 (7%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	BV	99/101 (98%)	72 (73%)	12 (12%)	15 (15%)	0	1
54	DV	99/101 (98%)	72 (73%)	11 (11%)	16 (16%)	0	0
55	BW	111/113 (98%)	93 (84%)	10 (9%)	8 (7%)	2	12
55	DW	111/113 (98%)	93 (84%)	10 (9%)	8 (7%)	2	12
56	BX	91/96 (95%)	73 (80%)	10 (11%)	8 (9%)	1	8
56	DX	91/96 (95%)	73 (80%)	10 (11%)	8 (9%)	1	8
57	BY	99/110 (90%)	55 (56%)	17 (17%)	27 (27%)	0	0
57	DY	99/110 (90%)	54 (54%)	18 (18%)	27 (27%)	0	0
58	BZ	183/206 (89%)	107 (58%)	45 (25%)	31 (17%)	0	0
58	DZ	183/206 (89%)	127 (69%)	38 (21%)	18 (10%)	1	6
All	All	12522/13582 (92%)	8790 (70%)	2335 (19%)	1397 (11%)	1	5

5 of 1397 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	12	GLU
2	AB	15	VAL
2	AB	19	HIS
2	AB	20	GLU
2	AB	64	ARG

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%)	185 (92%)	17 (8%)	16	52
2	CB	202/220 (92%)	185 (92%)	17 (8%)	16	52
3	AC	160/188 (85%)	146 (91%)	14 (9%)	14	49
3	CC	160/188 (85%)	146 (91%)	14 (9%)	14	49
4	AD	180/181 (99%)	160 (89%)	20 (11%)	9	33
4	CD	180/181 (99%)	159 (88%)	21 (12%)	8	29
5	AE	115/123 (94%)	110 (96%)	5 (4%)	40	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	CE	115/123 (94%)	110 (96%)	5 (4%)	40	80
6	AF	90/90 (100%)	87 (97%)	3 (3%)	50	86
6	CF	90/90 (100%)	87 (97%)	3 (3%)	50	86
7	AG	126/127 (99%)	121 (96%)	5 (4%)	42	82
7	CG	126/127 (99%)	121 (96%)	5 (4%)	42	82
8	AH	119/119 (100%)	115 (97%)	4 (3%)	49	86
8	CH	119/119 (100%)	114 (96%)	5 (4%)	40	81
9	AI	98/99 (99%)	89 (91%)	9 (9%)	13	45
9	CI	98/99 (99%)	89 (91%)	9 (9%)	13	45
10	AJ	88/92 (96%)	82 (93%)	6 (7%)	22	62
10	CJ	88/92 (96%)	82 (93%)	6 (7%)	22	62
11	AK	90/99 (91%)	86 (96%)	4 (4%)	39	79
11	CK	90/99 (91%)	86 (96%)	4 (4%)	39	79
12	AL	104/109 (95%)	90 (86%)	14 (14%)	6	22
12	CL	104/109 (95%)	90 (86%)	14 (14%)	6	22
13	AM	99/101 (98%)	92 (93%)	7 (7%)	21	61
13	CM	99/101 (98%)	91 (92%)	8 (8%)	17	53
14	AN	49/50 (98%)	45 (92%)	4 (8%)	17	53
14	CN	49/50 (98%)	45 (92%)	4 (8%)	17	53
15	AO	79/80 (99%)	73 (92%)	6 (8%)	19	58
15	CO	79/80 (99%)	73 (92%)	6 (8%)	19	58
16	AP	72/74 (97%)	68 (94%)	4 (6%)	30	70
16	CP	72/74 (97%)	68 (94%)	4 (6%)	30	70
17	AQ	94/97 (97%)	92 (98%)	2 (2%)	66	92
17	CQ	94/97 (97%)	92 (98%)	2 (2%)	66	92
18	AR	61/77 (79%)	59 (97%)	2 (3%)	50	86
18	CR	61/77 (79%)	59 (97%)	2 (3%)	50	86
19	AS	69/80 (86%)	60 (87%)	9 (13%)	6	23
19	CS	69/80 (86%)	59 (86%)	10 (14%)	5	18
20	AT	76/82 (93%)	70 (92%)	6 (8%)	18	55
20	CT	76/82 (93%)	69 (91%)	7 (9%)	13	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	AU	19/22 (86%)	17 (90%)	2 (10%)	10	35
21	CU	19/22 (86%)	17 (90%)	2 (10%)	10	35
24	AY	298/298 (100%)	267 (90%)	31 (10%)	10	36
24	CY	298/298 (100%)	265 (89%)	33 (11%)	9	33
25	B0	66/67 (98%)	61 (92%)	5 (8%)	19	58
25	D0	66/67 (98%)	61 (92%)	5 (8%)	19	58
26	B1	78/83 (94%)	69 (88%)	9 (12%)	8	31
26	D1	78/83 (94%)	68 (87%)	10 (13%)	6	24
27	B2	66/67 (98%)	64 (97%)	2 (3%)	53	87
27	D2	66/67 (98%)	56 (85%)	10 (15%)	4	16
28	B3	51/52 (98%)	49 (96%)	2 (4%)	43	83
28	D3	51/52 (98%)	49 (96%)	2 (4%)	43	83
29	B4	27/63 (43%)	25 (93%)	2 (7%)	20	59
29	D4	27/63 (43%)	25 (93%)	2 (7%)	20	59
30	B5	51/52 (98%)	43 (84%)	8 (16%)	4	14
30	D5	51/52 (98%)	43 (84%)	8 (16%)	4	14
31	B6	43/52 (83%)	34 (79%)	9 (21%)	1	7
31	D6	43/52 (83%)	33 (77%)	10 (23%)	1	5
32	B7	41/42 (98%)	39 (95%)	2 (5%)	35	76
32	D7	41/42 (98%)	39 (95%)	2 (5%)	35	76
33	B8	53/55 (96%)	43 (81%)	10 (19%)	2	9
33	D8	53/55 (96%)	43 (81%)	10 (19%)	2	9
34	B9	33/34 (97%)	32 (97%)	1 (3%)	53	87
34	D9	33/34 (97%)	32 (97%)	1 (3%)	53	87
37	BC	99/181 (55%)	96 (97%)	3 (3%)	53	87
37	DC	99/181 (55%)	96 (97%)	3 (3%)	53	87
38	BD	213/218 (98%)	183 (86%)	30 (14%)	5	20
38	DD	213/218 (98%)	184 (86%)	29 (14%)	5	21
39	BE	165/166 (99%)	140 (85%)	25 (15%)	4	16
39	DE	165/166 (99%)	141 (86%)	24 (14%)	5	18
40	BF	165/166 (99%)	149 (90%)	16 (10%)	12	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	DF	165/166 (99%)	149 (90%)	16 (10%)	12	41
41	BG	155/156 (99%)	138 (89%)	17 (11%)	9	34
41	DG	155/156 (99%)	133 (86%)	22 (14%)	5	20
42	BH	132/148 (89%)	116 (88%)	16 (12%)	7	27
42	DH	132/148 (89%)	116 (88%)	16 (12%)	7	27
43	BI	122/124 (98%)	112 (92%)	10 (8%)	17	53
43	DI	122/124 (98%)	101 (83%)	21 (17%)	3	11
45	BK	106/111 (96%)	91 (86%)	15 (14%)	5	20
45	DK	106/111 (96%)	92 (87%)	14 (13%)	6	23
46	BN	117/119 (98%)	107 (92%)	10 (8%)	15	51
46	DN	117/119 (98%)	107 (92%)	10 (8%)	15	51
47	BO	100/100 (100%)	94 (94%)	6 (6%)	27	67
47	DO	100/100 (100%)	94 (94%)	6 (6%)	27	67
48	BP	112/116 (97%)	89 (80%)	23 (20%)	2	8
48	DP	112/116 (97%)	89 (80%)	23 (20%)	2	8
49	BQ	111/111 (100%)	101 (91%)	10 (9%)	14	47
49	DQ	111/111 (100%)	100 (90%)	11 (10%)	11	39
50	BR	100/101 (99%)	84 (84%)	16 (16%)	3	13
50	DR	100/101 (99%)	84 (84%)	16 (16%)	3	13
51	BS	77/88 (88%)	66 (86%)	11 (14%)	5	19
51	DS	77/88 (88%)	66 (86%)	11 (14%)	5	19
52	BT	120/127 (94%)	97 (81%)	23 (19%)	2	9
52	DT	120/127 (94%)	98 (82%)	22 (18%)	2	10
53	BU	92/94 (98%)	84 (91%)	8 (9%)	15	49
53	DU	92/94 (98%)	84 (91%)	8 (9%)	15	49
54	BV	82/82 (100%)	64 (78%)	18 (22%)	1	6
54	DV	82/82 (100%)	64 (78%)	18 (22%)	1	6
55	BW	91/92 (99%)	81 (89%)	10 (11%)	9	34
55	DW	91/92 (99%)	81 (89%)	10 (11%)	9	34
56	BX	74/78 (95%)	63 (85%)	11 (15%)	4	17
56	DX	74/78 (95%)	63 (85%)	11 (15%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	BY	84/91 (92%)	70 (83%)	14 (17%)	3	11
57	DY	84/91 (92%)	70 (83%)	14 (17%)	3	11
58	BZ	162/179 (90%)	152 (94%)	10 (6%)	26	66
58	DZ	162/179 (90%)	140 (86%)	22 (14%)	5	21
All	All	10552/11246 (94%)	9458 (90%)	1094 (10%)	10	36

5 of 1094 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
56	BX	53	LYS
11	CK	117	ASN
53	DU	16	LYS
57	BY	40	GLU
3	CC	193	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 365 such sidechains are listed below:

Mol	Chain	Res	Type
55	BW	34	ASN
6	CF	27	GLN
50	DR	23	ASN
55	BW	62	HIS
2	CB	204	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	203 (13%)	32 (2%)
1	CA	1503/1522 (98%)	207 (13%)	31 (2%)
22	AV	74/77 (96%)	18 (24%)	0
22	AW	74/77 (96%)	17 (22%)	0
22	CV	74/77 (96%)	19 (25%)	0
22	CW	74/77 (96%)	17 (22%)	1 (1%)
23	AX	7/8 (87%)	3 (42%)	0
23	CX	7/8 (87%)	2 (28%)	1 (14%)
35	BA	2900/2915 (99%)	503 (17%)	54 (1%)
35	DA	2900/2915 (99%)	509 (17%)	56 (1%)
36	BB	118/122 (96%)	13 (11%)	1 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
36	DB	118/122 (96%)	13 (11%)	1 (0%)
All	All	9352/9442 (99%)	1524 (16%)	177 (1%)

5 of 1524 RNA backbone outliers are listed below:

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

5 of 177 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	BA	2464	C
1	CA	484	G
35	DA	2126	A
35	BA	2611	U
1	CA	115	G

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	59,22	24,24,25	0.69	1 (4%)	34,35,38	1.27	3 (8%)
22	PHA	AV	77	22	11,11,11	1.79	1 (9%)	13,13,13	1.19	1 (7%)
22	8AN	AW	76	22	24,24,25	0.81	1 (4%)	34,35,38	1.11	3 (8%)
22	PHA	AW	77	22	11,11,11	2.03	1 (9%)	13,13,13	0.80	1 (7%)
22	8AN	CV	76	59,22	24,24,25	0.69	1 (4%)	34,35,38	1.08	4 (11%)
22	PHA	CV	77	22	11,11,11	1.88	1 (9%)	13,13,13	1.24	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	8AN	CW	76	22	24,24,25	0.65	0	34,35,38	1.15	2 (5%)
22	PHA	CW	77	22	11,11,11	2.23	1 (9%)	13,13,13	0.81	1 (7%)

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	59,22	-	0/9/25/26	0/3/3/3
22	PHA	AV	77	22	-	1/5/6/6	0/1/1/1
22	8AN	AW	76	22	-	0/9/25/26	0/3/3/3
22	PHA	AW	77	22	-	0/5/6/6	0/1/1/1
22	8AN	CV	76	59,22	-	0/9/25/26	0/3/3/3
22	PHA	CV	77	22	-	0/5/6/6	0/1/1/1
22	8AN	CW	76	22	-	0/9/25/26	0/3/3/3
22	PHA	CW	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	CW	77	PHA	CA-C	6.71	1.56	1.49
22	AW	77	PHA	CA-C	5.71	1.55	1.49
22	CV	77	PHA	CA-C	5.51	1.55	1.49
22	AV	77	PHA	CA-C	5.00	1.54	1.49
22	AV	76	8AN	C3'-N3'	-2.14	1.43	1.47

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AV	76	8AN	C4'-C3'-N3'	-4.43	105.02	114.04
22	CV	77	PHA	C-CA-N	3.63	117.11	109.91
22	AV	77	PHA	C-CA-N	3.57	117.00	109.91
22	CW	76	8AN	C2'-C1'-N9	3.29	122.30	113.35
22	AW	76	8AN	C2'-C1'-N9	2.74	120.82	113.35

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	AV	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 1100 ligands modelled in this entry, 1100 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	CM	5
13	AM	5
9	AI	2
9	CI	2
41	BG	1
31	B6	1

The worst 5 of 16 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B6	46:HIS	C	47:THR	N	7.42
1	AI	104:ARG	C	105:ASP	N	4.76
1	CI	104:ARG	C	105:ASP	N	4.74
1	AM	112:GLY	C	113:PRO	N	4.66
1	CM	112:GLY	C	113:PRO	N	4.66

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%)	-0.05	31 (2%) 60 11	44, 101, 185, 201	0
1	CA	1504/1522 (98%)	-0.11	33 (2%) 59 11	34, 96, 178, 201	0
2	AB	235/256 (91%)	0.34	3 (1%) 74 19	81, 138, 188, 201	0
2	CB	235/256 (91%)	0.17	5 (2%) 60 11	34, 118, 174, 201	0
3	AC	207/239 (86%)	0.37	3 (1%) 72 17	73, 133, 173, 201	0
3	CC	207/239 (86%)	0.04	0 100 100	62, 113, 157, 198	0
4	AD	208/209 (99%)	-0.08	0 100 100	50, 93, 140, 190	0
4	CD	208/209 (99%)	0.06	0 100 100	63, 108, 157, 201	0
5	AE	151/162 (93%)	0.06	0 100 100	51, 97, 147, 177	0
5	CE	151/162 (93%)	-0.06	0 100 100	52, 84, 132, 163	0
6	AF	101/101 (100%)	-0.04	1 (0%) 79 23	63, 105, 149, 201	0
6	CF	101/101 (100%)	-0.13	0 100 100	51, 88, 141, 168	0
7	AG	155/156 (99%)	0.39	9 (5%) 22 3	65, 130, 177, 191	0
7	CG	155/156 (99%)	0.18	6 (3%) 37 5	60, 106, 163, 201	0
8	AH	138/138 (100%)	0.05	0 100 100	53, 105, 151, 172	0
8	CH	138/138 (100%)	-0.03	0 100 100	48, 83, 125, 157	0
9	AI	127/128 (99%)	0.88	15 (11%) 5 1	82, 148, 193, 201	0
9	CI	127/128 (99%)	0.44	4 (3%) 47 7	57, 123, 185, 200	0
10	AJ	99/105 (94%)	0.84	12 (12%) 5 1	62, 148, 189, 201	0
10	CJ	99/105 (94%)	0.65	4 (4%) 36 5	66, 133, 186, 201	0
11	AK	119/129 (92%)	0.21	4 (3%) 43 6	50, 109, 158, 185	0
11	CK	119/129 (92%)	-0.04	4 (3%) 43 6	38, 81, 138, 181	0
12	AL	125/132 (94%)	0.05	1 (0%) 83 28	46, 86, 126, 188	0
12	CL	125/132 (94%)	0.14	3 (2%) 56 9	40, 90, 142, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	125/126 (99%)	0.81	15 (12%) 5 1	83, 152, 196, 201	0
13	CM	125/126 (99%)	0.35	8 (6%) 19 3	40, 112, 176, 201	0
14	AN	60/61 (98%)	0.67	7 (11%) 5 1	72, 143, 178, 201	0
14	CN	60/61 (98%)	0.07	1 (1%) 67 15	63, 102, 144, 167	0
15	AO	88/89 (98%)	0.09	0 100 100	59, 101, 135, 182	0
15	CO	88/89 (98%)	-0.07	0 100 100	45, 82, 126, 162	0
16	AP	84/88 (95%)	0.02	0 100 100	45, 83, 143, 196	0
16	CP	84/88 (95%)	0.27	1 (1%) 75 20	63, 105, 145, 168	0
17	AQ	100/105 (95%)	-0.05	0 100 100	43, 89, 133, 153	0
17	CQ	100/105 (95%)	0.04	0 100 100	49, 86, 121, 161	0
18	AR	70/88 (79%)	0.55	5 (7%) 16 3	74, 104, 159, 191	0
18	CR	70/88 (79%)	0.13	2 (2%) 49 7	61, 85, 129, 150	0
19	AS	79/93 (84%)	0.93	9 (11%) 6 1	102, 156, 194, 200	0
19	CS	79/93 (84%)	0.55	3 (3%) 38 5	69, 126, 187, 201	0
20	AT	99/106 (93%)	0.26	1 (1%) 79 23	54, 96, 158, 201	0
20	CT	99/106 (93%)	0.17	1 (1%) 79 23	49, 101, 152, 192	0
21	AU	25/27 (92%)	1.99	12 (48%) 1 0	92, 133, 184, 200	0
21	CU	25/27 (92%)	0.89	2 (8%) 12 2	77, 106, 145, 200	0
22	AV	77/77 (100%)	0.18	3 (3%) 37 5	64, 131, 176, 185	0
22	AW	77/77 (100%)	0.37	4 (5%) 26 4	77, 175, 200, 201	0
22	CV	77/77 (100%)	0.12	2 (2%) 53 8	61, 106, 152, 192	0
22	CW	77/77 (100%)	0.49	11 (14%) 3 1	64, 163, 200, 201	0
23	AX	8/8 (100%)	0.05	0 100 100	77, 106, 136, 153	0
23	CX	8/8 (100%)	0.33	1 (12%) 5 1	46, 77, 146, 167	0
24	AY	351/351 (100%)	0.82	43 (12%) 5 1	68, 137, 194, 201	0
24	CY	351/351 (100%)	0.95	55 (15%) 3 1	66, 142, 191, 201	0
25	B0	83/85 (97%)	0.30	4 (4%) 29 4	55, 90, 160, 185	0
25	D0	83/85 (97%)	-0.13	3 (3%) 41 6	17, 43, 119, 176	0
26	B1	94/98 (95%)	-0.11	0 100 100	32, 69, 121, 148	0
26	D1	94/98 (95%)	-0.24	0 100 100	18, 50, 99, 171	0
27	B2	71/72 (98%)	0.12	0 100 100	53, 93, 147, 185	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	D2	71/72 (98%)	-0.28	0 100 100	23, 48, 119, 154	0
28	B3	60/60 (100%)	0.43	2 (3%) 44 6	53, 82, 125, 183	0
28	D3	60/60 (100%)	-0.30	1 (1%) 67 15	13, 40, 82, 179	0
29	B4	31/71 (43%)	0.45	1 (3%) 45 7	86, 154, 187, 200	0
29	D4	31/71 (43%)	-0.01	0 100 100	77, 111, 160, 187	0
30	B5	59/60 (98%)	0.12	3 (5%) 27 4	30, 69, 181, 201	0
30	D5	59/60 (98%)	-0.07	3 (5%) 27 4	10, 35, 157, 163	0
31	B6	45/54 (83%)	1.08	8 (17%) 2 0	71, 128, 178, 200	0
31	D6	45/54 (83%)	0.49	1 (2%) 59 11	40, 83, 144, 186	0
32	B7	49/49 (100%)	0.04	1 (2%) 62 12	25, 52, 117, 184	0
32	D7	49/49 (100%)	-0.16	1 (2%) 62 12	12, 26, 103, 200	0
33	B8	64/65 (98%)	0.19	0 100 100	38, 78, 141, 201	0
33	D8	64/65 (98%)	-0.21	0 100 100	14, 45, 102, 180	0
34	B9	36/37 (97%)	0.93	3 (8%) 11 2	61, 94, 137, 149	0
34	D9	36/37 (97%)	0.03	0 100 100	29, 48, 106, 125	0
35	BA	2901/2915 (99%)	-0.17	73 (2%) 54 9	31, 70, 183, 201	0
35	DA	2901/2915 (99%)	-0.33	52 (1%) 65 14	10, 41, 178, 201	0
36	BB	119/122 (97%)	0.14	0 100 100	76, 144, 190, 200	0
36	DB	119/122 (97%)	-0.43	0 100 100	29, 59, 101, 171	0
37	BC	120/229 (52%)	1.56	39 (32%) 1 0	107, 177, 201, 201	0
37	DC	120/229 (52%)	1.51	31 (25%) 1 0	91, 170, 200, 201	0
38	BD	272/276 (98%)	-0.18	0 100 100	24, 63, 111, 158	0
38	DD	272/276 (98%)	-0.34	0 100 100	15, 40, 84, 154	0
39	BE	205/206 (99%)	0.00	4 (1%) 62 12	29, 67, 136, 201	0
39	DE	205/206 (99%)	-0.20	2 (0%) 79 23	10, 41, 138, 200	0
40	BF	208/210 (99%)	-0.08	3 (1%) 72 17	33, 77, 161, 201	0
40	DF	208/210 (99%)	-0.25	2 (0%) 79 23	9, 44, 158, 196	0
41	BG	181/182 (99%)	0.36	6 (3%) 44 6	67, 137, 182, 201	0
41	DG	181/182 (99%)	-0.09	0 100 100	34, 79, 147, 181	0
42	BH	160/180 (88%)	0.72	13 (8%) 12 2	70, 132, 180, 201	0
42	DH	160/180 (88%)	-0.03	5 (3%) 47 7	29, 69, 139, 201	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BI	146/148 (98%)	0.24	1 (0%) 84 32	53, 112, 152, 186	0
43	DI	146/148 (98%)	0.08	0 100 100	36, 94, 142, 187	0
44	BJ	0/130	-	-	-	-
44	DJ	0/130	-	-	-	-
45	BK	141/147 (95%)	1.69	41 (29%) 1 0	122, 170, 201, 201	0
45	DK	141/147 (95%)	1.81	53 (37%) 1 0	117, 178, 201, 201	0
46	BN	139/140 (99%)	0.05	0 100 100	43, 85, 141, 201	0
46	DN	139/140 (99%)	-0.34	0 100 100	18, 42, 104, 201	0
47	BO	122/122 (100%)	-0.31	0 100 100	36, 62, 91, 112	0
47	DO	122/122 (100%)	-0.37	0 100 100	20, 43, 81, 130	0
48	BP	146/150 (97%)	0.31	5 (3%) 43 6	37, 100, 161, 198	0
48	DP	146/150 (97%)	0.00	1 (0%) 84 32	16, 58, 135, 188	0
49	BQ	141/141 (100%)	0.12	1 (0%) 84 32	46, 91, 143, 179	0
49	DQ	141/141 (100%)	-0.28	1 (0%) 84 32	21, 46, 101, 181	0
50	BR	117/118 (99%)	-0.09	0 100 100	36, 66, 109, 152	0
50	DR	117/118 (99%)	-0.31	0 100 100	14, 39, 82, 142	0
51	BS	99/112 (88%)	0.59	3 (3%) 48 7	64, 131, 182, 191	0
51	DS	99/112 (88%)	0.02	2 (2%) 62 12	31, 67, 128, 181	0
52	BT	138/146 (94%)	0.12	5 (3%) 41 6	40, 81, 169, 201	0
52	DT	138/146 (94%)	-0.17	0 100 100	22, 61, 150, 201	0
53	BU	117/118 (99%)	-0.13	0 100 100	33, 73, 134, 191	0
53	DU	117/118 (99%)	-0.39	0 100 100	11, 32, 85, 147	0
54	BV	101/101 (100%)	0.08	1 (0%) 79 23	33, 96, 143, 201	0
54	DV	101/101 (100%)	-0.33	0 100 100	7, 45, 101, 201	0
55	BW	113/113 (100%)	-0.16	0 100 100	31, 62, 117, 193	0
55	DW	113/113 (100%)	-0.36	1 (0%) 81 25	9, 32, 68, 201	0
56	BX	93/96 (96%)	-0.08	0 100 100	45, 79, 118, 158	0
56	DX	93/96 (96%)	-0.34	0 100 100	12, 43, 80, 121	0
57	BY	101/110 (91%)	0.51	7 (6%) 17 3	52, 102, 172, 201	0
57	DY	101/110 (91%)	0.09	2 (1%) 62 12	18, 73, 156, 191	0
58	BZ	185/206 (89%)	0.28	2 (1%) 77 22	64, 120, 168, 201	0
58	DZ	185/206 (89%)	-0.13	3 (1%) 68 15	36, 75, 154, 201	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	22138/23284 (95%)	0.04	714 (3%) 45 7	7, 85, 180, 201	0

The worst 5 of 714 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AA	82	U	12.4
45	BK	3	LYS	11.2
1	CA	89	C	9.0
13	CM	126	LYS	8.6
1	AA	89	C	8.6

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	8AN	AW	76	22/23	0.16	-	71,74,82,82	0
22	PHA	CV	77	11/11	0.48	-	70,70,72,73	0
22	8AN	AV	76	22/23	0.20	-	59,59,59,104	0
22	8AN	CV	76	22/23	0.26	-	59,59,59,104	0
22	PHA	CW	77	11/11	0.55	-	77,77,79,80	0
22	PHA	AV	77	11/11	0.43	-	70,70,72,73	0
22	8AN	CW	76	22/23	0.21	-	71,74,82,82	0
22	PHA	AW	77	11/11	0.79	-	77,77,79,80	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
59	MG	DA	3119	1/1	0.54	-	40,40,40,40	0
59	MG	DA	3243	1/1	0.27	-	54,54,54,54	1
59	MG	DA	3242	1/1	0.17	-	11,11,11,11	1
59	MG	BA	3337	1/1	0.25	-	55,55,55,55	0
59	MG	CA	1722	1/1	0.29	-	74,74,74,74	1
59	MG	CA	1700	1/1	0.31	-	58,58,58,58	0
59	MG	AA	1740	1/1	0.52	-	75,75,75,75	0
59	MG	DP	201	1/1	1.10	-	1,1,1,1	1
59	MG	DA	3311	1/1	0.17	-	75,75,75,75	0
59	MG	BA	3182	1/1	0.23	-	70,70,70,70	0
59	MG	DA	3192	1/1	0.10	-	35,35,35,35	0
59	MG	BA	3061	1/1	0.42	-	21,21,21,21	0
59	MG	DA	3349	1/1	0.32	-	18,18,18,18	1
59	MG	CA	1646	1/1	0.19	-	37,37,37,37	0
59	MG	DA	3100	1/1	0.32	-	3,3,3,3	0
59	MG	BA	3177	1/1	0.24	-	77,77,77,77	0
59	MG	DA	3159	1/1	0.32	-	68,68,68,68	0
59	MG	DA	3102	1/1	0.09	-	1,1,1,1	0
59	MG	BA	3173	1/1	0.38	-	51,51,51,51	0
59	MG	AA	1735	1/1	0.35	-	74,74,74,74	0
59	MG	DA	3270	1/1	0.22	-	30,30,30,30	0
59	MG	AW	102	1/1	0.15	-	25,25,25,25	1
59	MG	BA	3119	1/1	0.53	-	39,39,39,39	0
59	MG	AA	1609	1/1	0.13	-	38,38,38,38	1
59	MG	CA	1610	1/1	0.15	-	60,60,60,60	0
59	MG	DA	3350	1/1	0.34	-	37,37,37,37	0
59	MG	CA	1668	1/1	0.39	-	50,50,50,50	0
59	MG	DA	3058	1/1	0.35	-	23,23,23,23	0
59	MG	AA	1642	1/1	0.29	-	55,55,55,55	0
59	MG	DA	3342	1/1	0.49	-	61,61,61,61	0
59	MG	BA	3058	1/1	0.33	-	30,30,30,30	0
59	MG	DA	3331	1/1	0.14	-	30,30,30,30	0
59	MG	DA	3292	1/1	0.23	-	40,40,40,40	0
59	MG	AA	1706	1/1	0.33	-	69,69,69,69	0
59	MG	BA	3199	1/1	0.29	-	60,60,60,60	0
59	MG	AA	1708	1/1	0.11	-	76,76,76,76	1
59	MG	AA	1676	1/1	0.12	-	21,21,21,21	1
59	MG	DA	3271	1/1	0.43	-	58,58,58,58	0
59	MG	AA	1630	1/1	0.41	-	72,72,72,72	0
59	MG	DA	3067	1/1	0.10	-	13,13,13,13	0
59	MG	BA	3073	1/1	0.36	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	1628	1/1	0.21	-	50,50,50,50	0
59	MG	AA	1643	1/1	0.23	-	93,93,93,93	0
59	MG	DA	3001	1/1	0.20	-	29,29,29,29	1
59	MG	DA	3039	1/1	0.34	-	97,97,97,97	0
59	MG	D1	101	1/1	0.15	-	22,22,22,22	1
59	MG	BA	3032	1/1	0.13	-	49,49,49,49	0
59	MG	AX	101	1/1	0.36	-	27,27,27,27	1
59	MG	AA	1753	1/1	0.34	-	16,16,16,16	1
59	MG	DA	3084	1/1	0.25	-	13,13,13,13	0
59	MG	BA	3314	1/1	0.43	-	45,45,45,45	0
59	MG	BA	3121	1/1	0.72	-	92,92,92,92	0
59	MG	CA	1675	1/1	0.40	-	64,64,64,64	0
59	MG	DA	3164	1/1	0.43	-	44,44,44,44	0
59	MG	BA	3190	1/1	0.16	-	47,47,47,47	0
59	MG	BA	3296	1/1	0.25	-	83,83,83,83	0
59	MG	BA	3234	1/1	0.33	-	26,26,26,26	0
59	MG	DA	3183	1/1	0.14	-	45,45,45,45	0
59	MG	AV	107	1/1	0.20	-	65,65,65,65	1
59	MG	DA	3337	1/1	0.36	-	102,102,102,102	0
59	MG	DA	3040	1/1	0.23	-	27,27,27,27	0
59	MG	BA	3089	1/1	0.26	-	28,28,28,28	0
59	MG	BA	3049	1/1	0.51	-	46,46,46,46	0
59	MG	BA	3213	1/1	0.22	-	80,80,80,80	1
59	MG	AA	1637	1/1	0.18	-	63,63,63,63	0
59	MG	DA	3034	1/1	0.32	-	32,32,32,32	0
59	MG	AA	1761	1/1	0.16	-	88,88,88,88	0
59	MG	AA	1698	1/1	0.27	-	25,25,25,25	1
59	MG	AA	1693	1/1	0.20	-	41,41,41,41	0
59	MG	BA	3033	1/1	0.27	-	35,35,35,35	0
59	MG	BA	3236	1/1	0.23	-	54,54,54,54	0
59	MG	AA	1616	1/1	0.19	-	36,36,36,36	1
59	MG	CA	1637	1/1	0.43	-	65,65,65,65	0
59	MG	DA	3020	1/1	0.26	-	11,11,11,11	0
59	MG	DA	3172	1/1	0.18	-	3,3,3,3	0
59	MG	DB	203	1/1	0.24	-	20,20,20,20	0
59	MG	AA	1615	1/1	0.47	-	50,50,50,50	0
59	MG	DA	3141	1/1	0.26	-	56,56,56,56	0
59	MG	BA	3176	1/1	0.16	-	59,59,59,59	0
59	MG	BA	3224	1/1	0.09	-	37,37,37,37	0
59	MG	AA	1653	1/1	0.34	-	44,44,44,44	0
59	MG	CA	1745	1/1	0.29	-	37,37,37,37	0
59	MG	DA	3265	1/1	0.09	-	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	DA	3228	1/1	0.34	-	41,41,41,41	0
59	MG	BA	3009	1/1	0.32	-	21,21,21,21	0
59	MG	BA	3062	1/1	0.34	-	16,16,16,16	0
59	MG	AA	1720	1/1	0.48	-	55,55,55,55	0
59	MG	BA	3322	1/1	0.29	-	52,52,52,52	0
59	MG	DA	3217	1/1	0.16	-	7,7,7,7	0
59	MG	CA	1743	1/1	0.27	-	61,61,61,61	0
59	MG	BA	3050	1/1	0.20	-	36,36,36,36	0
59	MG	DA	3258	1/1	0.40	-	58,58,58,58	0
59	MG	BA	3187	1/1	0.36	-	18,18,18,18	0
59	MG	BA	3170	1/1	0.29	-	38,38,38,38	0
59	MG	DA	3194	1/1	0.25	-	32,32,32,32	0
59	MG	DA	3259	1/1	0.31	-	31,31,31,31	0
59	MG	BA	3350	1/1	0.69	-	69,69,69,69	0
59	MG	BA	3153	1/1	0.23	-	48,48,48,48	0
59	MG	DA	3092	1/1	0.28	-	18,18,18,18	0
59	MG	DA	3310	1/1	0.21	-	51,51,51,51	0
59	MG	BA	3133	1/1	0.27	-	118,118,118,118	0
59	MG	BA	3080	1/1	0.26	-	42,42,42,42	0
59	MG	CA	1655	1/1	0.31	-	37,37,37,37	0
59	MG	DA	3045	1/1	0.42	-	34,34,34,34	0
59	MG	CA	1711	1/1	0.23	-	40,40,40,40	0
59	MG	AA	1650	1/1	0.22	-	40,40,40,40	0
59	MG	DA	3068	1/1	0.20	-	6,6,6,6	0
59	MG	AA	1631	1/1	0.05	-	45,45,45,45	0
59	MG	AA	1602	1/1	0.17	-	53,53,53,53	1
59	MG	BA	3022	1/1	0.38	-	22,22,22,22	0
59	MG	BA	3249	1/1	0.47	-	103,103,103,103	0
59	MG	DA	3107	1/1	0.26	-	31,31,31,31	0
59	MG	BA	3014	1/1	0.29	-	45,45,45,45	0
59	MG	CA	1713	1/1	0.28	-	94,94,94,94	0
59	MG	BA	3340	1/1	0.08	-	73,73,73,73	0
59	MG	AA	1670	1/1	0.17	-	34,34,34,34	0
59	MG	AA	1737	1/1	0.18	-	42,42,42,42	0
59	MG	DA	3199	1/1	0.39	-	14,14,14,14	0
59	MG	DA	3326	1/1	0.53	-	35,35,35,35	0
59	MG	CA	1653	1/1	0.07	-	44,44,44,44	0
59	MG	CA	1746	1/1	0.11	-	10,10,10,10	1
59	MG	BA	3346	1/1	0.19	-	69,69,69,69	0
59	MG	DA	3052	1/1	0.25	-	25,25,25,25	0
59	MG	CA	1724	1/1	0.30	-	58,58,58,58	0
59	MG	AA	1687	1/1	0.27	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3145	1/1	0.11	-	60,60,60,60	0
59	MG	BA	3276	1/1	0.39	-	60,60,60,60	0
59	MG	DA	3138	1/1	0.31	-	58,58,58,58	0
59	MG	AA	1619	1/1	0.29	-	39,39,39,39	0
59	MG	BA	3196	1/1	0.29	-	52,52,52,52	0
59	MG	CA	1651	1/1	0.32	-	40,40,40,40	0
59	MG	DA	3122	1/1	0.61	-	73,73,73,73	0
59	MG	BG	201	1/1	0.41	-	1,1,1,1	1
59	MG	BA	3323	1/1	0.28	-	49,49,49,49	1
59	MG	AA	1679	1/1	0.24	-	82,82,82,82	0
59	MG	DA	3106	1/1	0.37	-	23,23,23,23	0
59	MG	BA	3090	1/1	0.26	-	33,33,33,33	0
59	MG	CA	1751	1/1	0.12	-	62,62,62,62	0
59	MG	DA	3081	1/1	0.23	-	16,16,16,16	0
59	MG	AA	1604	1/1	0.15	-	57,57,57,57	0
59	MG	BA	3309	1/1	0.18	-	51,51,51,51	0
59	MG	BA	3215	1/1	0.08	-	26,26,26,26	0
59	MG	DA	3182	1/1	0.23	-	42,42,42,42	0
59	MG	AA	1729	1/1	0.33	-	88,88,88,88	0
59	MG	DA	3090	1/1	0.23	-	20,20,20,20	0
59	MG	BA	3128	1/1	0.18	-	60,60,60,60	0
59	MG	BA	3242	1/1	0.15	-	106,106,106,106	0
59	MG	DA	3237	1/1	0.37	-	39,39,39,39	0
59	MG	CA	1623	1/1	0.26	-	51,51,51,51	0
59	MG	AA	1663	1/1	0.15	-	50,50,50,50	0
59	MG	AV	104	1/1	0.08	-	109,109,109,109	0
59	MG	DA	3171	1/1	0.14	-	3,3,3,3	0
59	MG	BA	3291	1/1	0.12	-	42,42,42,42	0
59	MG	DA	3304	1/1	0.22	-	18,18,18,18	1
59	MG	BA	3286	1/1	0.39	-	71,71,71,71	0
59	MG	BA	3353	1/1	0.28	-	61,61,61,61	0
59	MG	CA	1666	1/1	0.42	-	59,59,59,59	0
59	MG	BA	3202	1/1	0.17	-	42,42,42,42	0
59	MG	CA	1742	1/1	0.22	-	32,32,32,32	1
59	MG	CA	1662	1/1	0.11	-	49,49,49,49	0
59	MG	DA	3290	1/1	0.43	-	1,1,1,1	1
59	MG	AA	1611	1/1	0.47	-	74,74,74,74	0
59	MG	DA	3005	1/1	0.33	-	21,21,21,21	0
59	MG	DA	3130	1/1	0.36	-	45,45,45,45	0
59	MG	DA	3303	1/1	0.26	-	25,25,25,25	0
59	MG	DA	3025	1/1	0.27	-	29,29,29,29	0
59	MG	DA	3224	1/1	0.47	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3189	1/1	0.17	-	41,41,41,41	0
59	MG	BA	3294	1/1	0.33	-	32,32,32,32	0
59	MG	BD	301	1/1	0.23	-	22,22,22,22	0
59	MG	AA	1625	1/1	0.30	-	53,53,53,53	0
59	MG	BB	204	1/1	0.25	-	22,22,22,22	1
59	MG	DA	3220	1/1	0.54	-	51,51,51,51	0
59	MG	CA	1707	1/1	0.18	-	65,65,65,65	0
59	MG	BA	3077	1/1	0.23	-	74,74,74,74	0
59	MG	AA	1701	1/1	0.20	-	61,61,61,61	0
59	MG	BA	3330	1/1	0.41	-	49,49,49,49	0
59	MG	DA	3154	1/1	0.21	-	31,31,31,31	0
59	MG	CA	1721	1/1	0.16	-	74,74,74,74	0
59	MG	BA	3301	1/1	0.21	-	36,36,36,36	0
59	MG	BA	3001	1/1	0.20	-	62,62,62,62	0
59	MG	DA	3144	1/1	0.19	-	56,56,56,56	0
59	MG	BA	3120	1/1	0.20	-	25,25,25,25	0
59	MG	AA	1656	1/1	0.07	-	30,30,30,30	0
59	MG	DA	3302	1/1	0.11	-	1,1,1,1	0
59	MG	DA	3017	1/1	0.20	-	22,22,22,22	0
59	MG	BA	3137	1/1	0.14	-	38,38,38,38	0
59	MG	DA	3260	1/1	0.33	-	43,43,43,43	0
59	MG	DA	3347	1/1	0.34	-	24,24,24,24	1
59	MG	BA	3095	1/1	0.31	-	73,73,73,73	0
59	MG	BA	3043	1/1	0.25	-	22,22,22,22	0
59	MG	CA	1755	1/1	0.19	-	97,97,97,97	1
59	MG	BA	3126	1/1	0.09	-	21,21,21,21	0
59	MG	DA	3283	1/1	0.10	-	35,35,35,35	0
59	MG	AA	1739	1/1	0.12	-	54,54,54,54	0
60	ZN	CD	302	1/1	0.23	-	80,80,80,80	0
59	MG	AA	1721	1/1	0.42	-	87,87,87,87	0
59	MG	AA	1669	1/1	0.28	-	34,34,34,34	0
59	MG	DA	3030	1/1	0.32	-	34,34,34,34	0
59	MG	DA	3015	1/1	0.23	-	9,9,9,9	0
59	MG	AA	1741	1/1	0.30	-	44,44,44,44	0
59	MG	DA	3094	1/1	0.28	-	9,9,9,9	0
59	MG	DA	3208	1/1	0.13	-	26,26,26,26	0
59	MG	BA	3162	1/1	0.30	-	96,96,96,96	0
59	MG	BA	3270	1/1	0.26	-	49,49,49,49	0
59	MG	DA	3026	1/1	0.19	-	21,21,21,21	0
59	MG	DA	3273	1/1	0.28	-	1,1,1,1	1
59	MG	AV	101	1/1	0.18	-	72,72,72,72	0
59	MG	DA	3177	1/1	0.21	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	1649	1/1	0.19	-	22,22,22,22	0
59	MG	DA	3082	1/1	0.22	-	56,56,56,56	0
59	MG	AA	1746	1/1	0.40	-	54,54,54,54	0
59	MG	BA	3127	1/1	0.53	-	75,75,75,75	0
59	MG	CA	1678	1/1	0.18	-	101,101,101,101	0
59	MG	DA	3049	1/1	0.28	-	15,15,15,15	0
59	MG	CA	1667	1/1	0.15	-	57,57,57,57	0
59	MG	DA	3078	1/1	0.22	-	33,33,33,33	0
59	MG	BA	3351	1/1	0.39	-	82,82,82,82	0
59	MG	DD	301	1/1	0.26	-	37,37,37,37	0
59	MG	BA	3115	1/1	0.45	-	43,43,43,43	0
59	MG	AA	1607	1/1	0.28	-	57,57,57,57	0
59	MG	BT	201	1/1	0.19	-	49,49,49,49	0
59	MG	CA	1616	1/1	0.48	-	65,65,65,65	0
59	MG	AA	1743	1/1	0.08	-	49,49,49,49	1
59	MG	DA	3150	1/1	0.25	-	48,48,48,48	0
59	MG	CA	1703	1/1	0.09	-	62,62,62,62	0
59	MG	DA	3113	1/1	0.20	-	16,16,16,16	0
59	MG	DA	3210	1/1	0.54	-	95,95,95,95	0
59	MG	BA	3228	1/1	0.10	-	48,48,48,48	1
59	MG	BA	3313	1/1	0.40	-	86,86,86,86	0
59	MG	DA	3024	1/1	0.33	-	10,10,10,10	0
59	MG	DA	3095	1/1	0.80	-	111,111,111,111	0
59	MG	DA	3230	1/1	0.18	-	42,42,42,42	0
59	MG	CA	1705	1/1	0.20	-	47,47,47,47	0
59	MG	BA	3312	1/1	0.12	-	93,93,93,93	0
59	MG	DA	3299	1/1	0.39	-	49,49,49,49	0
59	MG	BA	3355	1/1	0.18	-	9,9,9,9	1
59	MG	DA	3163	1/1	0.14	-	27,27,27,27	0
59	MG	AA	1707	1/1	0.15	-	58,58,58,58	0
59	MG	BA	3076	1/1	0.17	-	28,28,28,28	0
59	MG	AA	1684	1/1	0.30	-	59,59,59,59	0
60	ZN	D9	101	1/1	0.10	-	59,59,59,59	0
59	MG	BA	3201	1/1	0.15	-	37,37,37,37	0
59	MG	CA	1681	1/1	0.10	-	58,58,58,58	0
59	MG	DA	3355	1/1	0.37	-	68,68,68,68	0
59	MG	CA	1712	1/1	0.42	-	67,67,67,67	0
59	MG	BA	3347	1/1	0.18	-	30,30,30,30	0
59	MG	AA	1635	1/1	0.08	-	50,50,50,50	0
59	MG	BA	3293	1/1	0.56	-	83,83,83,83	0
59	MG	DA	3148	1/1	0.26	-	7,7,7,7	0
59	MG	AA	1688	1/1	0.26	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3099	1/1	0.21	-	43,43,43,43	0
59	MG	DA	3324	1/1	0.29	-	25,25,25,25	1
59	MG	BA	3071	1/1	0.10	-	28,28,28,28	0
59	MG	CA	1704	1/1	0.43	-	75,75,75,75	0
59	MG	AA	1632	1/1	0.57	-	56,56,56,56	0
59	MG	BA	3151	1/1	0.15	-	52,52,52,52	0
59	MG	AA	1682	1/1	0.68	-	77,77,77,77	0
59	MG	BA	3109	1/1	0.26	-	37,37,37,37	1
59	MG	DA	3057	1/1	0.34	-	10,10,10,10	0
59	MG	CX	101	1/1	0.39	-	79,79,79,79	0
59	MG	BA	3034	1/1	0.17	-	39,39,39,39	0
59	MG	DA	3135	1/1	0.15	-	33,33,33,33	0
59	MG	CA	1694	1/1	0.12	-	37,37,37,37	1
59	MG	CA	1691	1/1	0.32	-	33,33,33,33	0
59	MG	CA	1648	1/1	0.38	-	72,72,72,72	0
59	MG	BA	3093	1/1	0.25	-	38,38,38,38	0
59	MG	DA	3340	1/1	0.14	-	25,25,25,25	0
59	MG	DA	3035	1/1	0.24	-	19,19,19,19	0
59	MG	BA	3078	1/1	0.26	-	58,58,58,58	0
59	MG	BA	3222	1/1	0.40	-	29,29,29,29	0
59	MG	AV	106	1/1	0.08	-	77,77,77,77	0
59	MG	DA	3044	1/1	0.67	-	62,62,62,62	0
59	MG	AA	1760	1/1	0.24	-	27,27,27,27	1
59	MG	BA	3259	1/1	0.17	-	80,80,80,80	0
59	MG	BA	3143	1/1	0.35	-	90,90,90,90	0
59	MG	AA	1732	1/1	0.47	-	72,72,72,72	0
59	MG	BA	3031	1/1	0.28	-	37,37,37,37	0
59	MG	AA	1705	1/1	0.14	-	43,43,43,43	0
59	MG	DA	3143	1/1	0.24	-	48,48,48,48	0
59	MG	AA	1675	1/1	0.13	-	35,35,35,35	0
59	MG	DA	3229	1/1	0.21	-	56,56,56,56	0
59	MG	BA	3021	1/1	0.20	-	32,32,32,32	0
59	MG	BA	3181	1/1	0.29	-	60,60,60,60	0
59	MG	BA	3036	1/1	0.13	-	44,44,44,44	0
59	MG	BA	3004	1/1	0.36	-	118,118,118,118	1
59	MG	CA	1676	1/1	0.16	-	46,46,46,46	1
59	MG	DA	3251	1/1	0.19	-	18,18,18,18	1
59	MG	DA	3133	1/1	0.18	-	13,13,13,13	1
59	MG	DA	3023	1/1	0.44	-	20,20,20,20	0
59	MG	CV	107	1/1	0.13	-	51,51,51,51	0
59	MG	BA	3214	1/1	0.15	-	55,55,55,55	0
59	MG	DA	3021	1/1	0.22	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	1625	1/1	0.17	-	36,36,36,36	0
59	MG	DA	3308	1/1	0.19	-	41,41,41,41	0
59	MG	BA	3250	1/1	0.25	-	50,50,50,50	1
59	MG	CA	1640	1/1	0.28	-	37,37,37,37	0
59	MG	BA	3284	1/1	0.18	-	31,31,31,31	0
59	MG	BA	3135	1/1	0.41	-	53,53,53,53	0
59	MG	BA	3283	1/1	0.16	-	49,49,49,49	0
59	MG	DA	3286	1/1	0.33	-	41,41,41,41	0
59	MG	AA	1754	1/1	0.10	-	51,51,51,51	0
59	MG	CA	1673	1/1	0.08	-	15,15,15,15	0
59	MG	BA	3103	1/1	0.42	-	28,28,28,28	0
59	MG	BA	3186	1/1	0.30	-	28,28,28,28	0
59	MG	DA	3245	1/1	0.17	-	38,38,38,38	0
59	MG	CA	1606	1/1	0.39	-	58,58,58,58	0
59	MG	DA	3007	1/1	0.23	-	4,4,4,4	0
59	MG	DA	3041	1/1	0.29	-	17,17,17,17	0
59	MG	BA	3321	1/1	0.14	-	73,73,73,73	0
59	MG	DA	3223	1/1	0.39	-	32,32,32,32	0
59	MG	DH	201	1/1	0.18	-	44,44,44,44	0
59	MG	DA	3261	1/1	0.16	-	33,33,33,33	0
59	MG	CA	1687	1/1	0.13	-	64,64,64,64	0
59	MG	CA	1739	1/1	0.20	-	94,94,94,94	1
59	MG	BY	201	1/1	0.11	-	42,42,42,42	0
59	MG	CA	1749	1/1	0.22	-	65,65,65,65	0
59	MG	BA	3295	1/1	0.18	-	81,81,81,81	1
59	MG	BA	3352	1/1	0.40	-	62,62,62,62	0
59	MG	DA	3128	1/1	0.33	-	56,56,56,56	0
59	MG	DA	3155	1/1	0.21	-	50,50,50,50	0
59	MG	BA	3194	1/1	0.43	-	70,70,70,70	0
59	MG	DA	3029	1/1	0.28	-	49,49,49,49	0
59	MG	AA	1606	1/1	0.42	-	65,65,65,65	0
59	MG	BA	3165	1/1	0.41	-	40,40,40,40	0
59	MG	CA	1639	1/1	0.27	-	51,51,51,51	0
59	MG	BF	302	1/1	0.31	-	63,63,63,63	0
59	MG	DA	3250	1/1	0.43	-	68,68,68,68	0
59	MG	BA	3045	1/1	0.55	-	44,44,44,44	0
59	MG	BA	3204	1/1	0.37	-	35,35,35,35	1
59	MG	BA	3065	1/1	0.34	-	67,67,67,67	0
59	MG	BA	3320	1/1	0.28	-	57,57,57,57	0
59	MG	DA	3240	1/1	0.35	-	50,50,50,50	1
59	MG	AA	1665	1/1	0.25	-	61,61,61,61	0
59	MG	DA	3132	1/1	0.15	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	1742	1/1	0.78	-	72,72,72,72	0
59	MG	CA	1608	1/1	0.15	-	35,35,35,35	0
59	MG	DA	3062	1/1	0.24	-	1,1,1,1	0
59	MG	BA	3348	1/1	0.52	-	48,48,48,48	1
59	MG	DA	3080	1/1	0.30	-	32,32,32,32	0
59	MG	BA	3010	1/1	0.60	-	63,63,63,63	0
59	MG	DA	3202	1/1	0.31	-	35,35,35,35	0
59	MG	BA	3303	1/1	0.34	-	57,57,57,57	0
59	MG	DA	3254	1/1	0.16	-	50,50,50,50	1
59	MG	BA	3114	1/1	0.28	-	37,37,37,37	0
59	MG	AA	1695	1/1	0.18	-	56,56,56,56	0
59	MG	DA	3293	1/1	0.76	-	63,63,63,63	0
59	MG	BA	3232	1/1	0.49	-	59,59,59,59	0
59	MG	BA	3113	1/1	0.30	-	33,33,33,33	0
59	MG	AA	1700	1/1	0.36	-	77,77,77,77	0
59	MG	DA	3236	1/1	0.29	-	43,43,43,43	0
59	MG	DA	3356	1/1	0.62	-	74,74,74,74	0
59	MG	DA	3089	1/1	0.28	-	5,5,5,5	0
59	MG	AA	1757	1/1	0.15	-	49,49,49,49	0
59	MG	BA	3319	1/1	0.57	-	77,77,77,77	0
59	MG	DA	3008	1/1	0.23	-	10,10,10,10	0
59	MG	BA	3052	1/1	0.13	-	28,28,28,28	0
59	MG	BA	3335	1/1	0.21	-	173,173,173,173	0
59	MG	BA	3148	1/1	0.08	-	44,44,44,44	0
59	MG	BA	3125	1/1	0.30	-	19,19,19,19	0
59	MG	DA	3246	1/1	0.22	-	45,45,45,45	0
59	MG	BA	3203	1/1	0.27	-	43,43,43,43	0
59	MG	DA	3201	1/1	0.39	-	29,29,29,29	0
59	MG	AA	1726	1/1	0.19	-	2,2,2,2	1
59	MG	DA	3219	1/1	0.15	-	32,32,32,32	0
59	MG	CA	1615	1/1	0.33	-	26,26,26,26	0
59	MG	AA	1751	1/1	0.23	-	11,11,11,11	1
59	MG	BA	3046	1/1	0.24	-	22,22,22,22	0
59	MG	BA	3105	1/1	0.14	-	9,9,9,9	0
59	MG	BA	3272	1/1	0.48	-	44,44,44,44	0
59	MG	AA	1724	1/1	0.42	-	1,1,1,1	1
59	MG	BA	3238	1/1	0.09	-	17,17,17,17	0
59	MG	CA	1669	1/1	0.27	-	33,33,33,33	0
59	MG	CA	1627	1/1	0.08	-	51,51,51,51	0
59	MG	BA	3094	1/1	0.22	-	36,36,36,36	0
59	MG	BA	3174	1/1	0.27	-	29,29,29,29	0
59	MG	DS	201	1/1	0.24	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3357	1/1	0.45	-	68,68,68,68	1
59	MG	CA	1698	1/1	0.40	-	20,20,20,20	1
59	MG	DA	3112	1/1	0.13	-	42,42,42,42	0
59	MG	BA	3207	1/1	0.18	-	68,68,68,68	0
59	MG	CA	1752	1/1	0.09	-	84,84,84,84	0
59	MG	CA	1715	1/1	0.38	-	50,50,50,50	1
59	MG	DA	3233	1/1	0.33	-	37,37,37,37	0
59	MG	DA	3274	1/1	0.38	-	69,69,69,69	0
59	MG	DA	3284	1/1	0.21	-	1,1,1,1	0
59	MG	BA	3068	1/1	0.25	-	30,30,30,30	0
59	MG	CA	1617	1/1	0.32	-	61,61,61,61	0
59	MG	BA	3235	1/1	0.20	-	42,42,42,42	0
59	MG	CA	1604	1/1	0.16	-	51,51,51,51	0
59	MG	DA	3345	1/1	0.23	-	46,46,46,46	0
59	MG	BA	3263	1/1	0.33	-	54,54,54,54	0
59	MG	BF	301	1/1	0.13	-	33,33,33,33	0
59	MG	DA	3013	1/1	0.17	-	16,16,16,16	0
59	MG	CA	1660	1/1	0.25	-	69,69,69,69	0
59	MG	BA	3179	1/1	0.47	-	43,43,43,43	0
59	MG	BA	3083	1/1	0.23	-	25,25,25,25	0
59	MG	CA	1702	1/1	0.26	-	57,57,57,57	0
59	MG	BA	3271	1/1	0.35	-	55,55,55,55	0
59	MG	DA	3002	1/1	0.18	-	39,39,39,39	1
59	MG	CA	1692	1/1	0.59	-	73,73,73,73	0
59	MG	DA	3134	1/1	0.16	-	28,28,28,28	0
59	MG	BA	3051	1/1	0.20	-	25,25,25,25	0
59	MG	AS	101	1/1	0.08	-	115,115,115,115	0
59	MG	CA	1744	1/1	0.29	-	38,38,38,38	0
59	MG	DA	3234	1/1	0.39	-	69,69,69,69	0
59	MG	DA	3140	1/1	0.22	-	57,57,57,57	0
59	MG	BA	3048	1/1	0.24	-	32,32,32,32	0
59	MG	DF	301	1/1	0.10	-	9,9,9,9	0
59	MG	DA	3114	1/1	0.18	-	15,15,15,15	0
59	MG	CA	1638	1/1	0.62	-	77,77,77,77	0
59	MG	BA	3274	1/1	0.11	-	57,57,57,57	0
59	MG	DA	3323	1/1	0.39	-	45,45,45,45	0
59	MG	AA	1617	1/1	0.09	-	44,44,44,44	0
59	MG	BA	3037	1/1	0.23	-	23,23,23,23	0
59	MG	DA	3248	1/1	0.12	-	2,2,2,2	1
59	MG	DA	3279	1/1	0.23	-	16,16,16,16	0
59	MG	BA	3258	1/1	0.31	-	48,48,48,48	0
59	MG	BA	3265	1/1	0.07	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3247	1/1	0.13	-	66,66,66,66	0
59	MG	DA	3247	1/1	0.13	-	44,44,44,44	0
59	MG	DA	3263	1/1	0.43	-	53,53,53,53	0
59	MG	CA	1663	1/1	0.23	-	57,57,57,57	0
59	MG	BA	3130	1/1	0.08	-	29,29,29,29	0
59	MG	BA	3070	1/1	0.21	-	37,37,37,37	0
59	MG	DA	3256	1/1	0.19	-	49,49,49,49	0
59	MG	CA	1664	1/1	0.16	-	28,28,28,28	0
59	MG	BA	3349	1/1	0.34	-	45,45,45,45	0
59	MG	AA	1651	1/1	0.30	-	49,49,49,49	0
59	MG	AA	1749	1/1	0.26	-	48,48,48,48	0
59	MG	DA	3162	1/1	0.18	-	1,1,1,1	0
59	MG	BA	3229	1/1	0.12	-	37,37,37,37	0
59	MG	DA	3093	1/1	0.25	-	11,11,11,11	0
59	MG	CA	1632	1/1	0.71	-	88,88,88,88	0
59	MG	DA	3165	1/1	0.32	-	45,45,45,45	0
59	MG	AA	1672	1/1	0.06	-	55,55,55,55	0
59	MG	BA	3219	1/1	0.32	-	46,46,46,46	0
59	MG	BA	3279	1/1	0.27	-	39,39,39,39	0
59	MG	DA	3294	1/1	0.31	-	33,33,33,33	0
59	MG	BA	3123	1/1	0.63	-	72,72,72,72	0
59	MG	BA	3209	1/1	0.69	-	66,66,66,66	0
59	MG	CA	1630	1/1	0.32	-	68,68,68,68	0
59	MG	DA	3169	1/1	0.16	-	47,47,47,47	0
59	MG	DA	3309	1/1	0.11	-	61,61,61,61	0
59	MG	DA	3010	1/1	0.30	-	54,54,54,54	0
59	MG	BA	3053	1/1	0.12	-	45,45,45,45	1
59	MG	DA	3048	1/1	0.27	-	22,22,22,22	0
59	MG	DA	3088	1/1	0.40	-	8,8,8,8	0
59	MG	BA	3331	1/1	0.30	-	47,47,47,47	0
59	MG	BA	3040	1/1	0.23	-	36,36,36,36	0
59	MG	CA	1710	1/1	0.10	-	120,120,120,120	0
59	MG	DA	3318	1/1	0.36	-	49,49,49,49	0
59	MG	BA	3160	1/1	0.10	-	36,36,36,36	0
59	MG	BA	3211	1/1	0.22	-	44,44,44,44	0
59	MG	DA	3043	1/1	0.26	-	2,2,2,2	0
59	MG	DG	201	1/1	0.48	-	1,1,1,1	1
59	MG	BA	3267	1/1	0.21	-	25,25,25,25	0
59	MG	CA	1629	1/1	0.48	-	55,55,55,55	0
59	MG	BA	3225	1/1	0.48	-	73,73,73,73	0
59	MG	DA	3187	1/1	0.51	-	44,44,44,44	0
59	MG	BA	3042	1/1	0.43	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	DA	3051	1/1	0.34	-	23,23,23,23	0
59	MG	BA	3005	1/1	0.35	-	27,27,27,27	0
59	MG	DA	3033	1/1	0.22	-	16,16,16,16	0
59	MG	DA	3117	1/1	0.13	-	16,16,16,16	0
59	MG	DA	3149	1/1	0.16	-	43,43,43,43	0
59	MG	DA	3343	1/1	0.30	-	48,48,48,48	0
59	MG	BA	3311	1/1	0.20	-	75,75,75,75	0
59	MG	DA	3036	1/1	0.14	-	39,39,39,39	0
59	MG	DA	3330	1/1	0.20	-	23,23,23,23	0
59	MG	DA	3238	1/1	0.36	-	47,47,47,47	0
59	MG	DA	3296	1/1	0.06	-	34,34,34,34	0
59	MG	BA	3002	1/1	0.39	-	80,80,80,80	0
59	MG	DA	3099	1/1	0.25	-	12,12,12,12	0
59	MG	DA	3338	1/1	0.32	-	58,58,58,58	0
59	MG	AA	1712	1/1	0.20	-	47,47,47,47	0
59	MG	AA	1661	1/1	0.14	-	52,52,52,52	0
59	MG	AA	1718	1/1	0.26	-	71,71,71,71	0
59	MG	BA	3112	1/1	0.15	-	44,44,44,44	0
59	MG	DA	3327	1/1	0.23	-	38,38,38,38	0
59	MG	AA	1756	1/1	0.10	-	64,64,64,64	0
59	MG	BA	3124	1/1	0.37	-	65,65,65,65	0
59	MG	BA	3088	1/1	0.46	-	38,38,38,38	0
59	MG	BA	3184	1/1	0.30	-	27,27,27,27	0
59	MG	BA	3141	1/1	0.27	-	42,42,42,42	0
59	MG	DA	3166	1/1	0.14	-	29,29,29,29	0
59	MG	AA	1681	1/1	0.20	-	60,60,60,60	0
59	MG	BA	3007	1/1	0.29	-	39,39,39,39	0
59	MG	BA	3057	1/1	0.28	-	21,21,21,21	0
59	MG	BA	3168	1/1	0.11	-	37,37,37,37	0
59	MG	DA	3061	1/1	0.23	-	10,10,10,10	0
59	MG	DA	3285	1/1	0.30	-	48,48,48,48	0
59	MG	DA	3332	1/1	0.24	-	26,26,26,26	1
59	MG	DA	3086	1/1	0.23	-	18,18,18,18	0
59	MG	CA	1731	1/1	0.18	-	69,69,69,69	0
59	MG	BA	3171	1/1	0.17	-	30,30,30,30	0
59	MG	CA	1737	1/1	0.53	-	59,59,59,59	0
59	MG	BA	3156	1/1	0.13	-	58,58,58,58	0
59	MG	AA	1752	1/1	0.64	-	57,57,57,57	1
59	MG	DA	3063	1/1	0.18	-	17,17,17,17	0
59	MG	DA	3212	1/1	0.19	-	59,59,59,59	0
59	MG	CA	1728	1/1	0.29	-	53,53,53,53	0
59	MG	DA	3156	1/1	0.24	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CL	201	1/1	0.12	-	8,8,8,8	1
59	MG	CV	106	1/1	0.17	-	96,96,96,96	0
59	MG	AA	1601	1/1	0.34	-	58,58,58,58	1
59	MG	CA	1642	1/1	0.29	-	67,67,67,67	1
59	MG	DA	3353	1/1	0.20	-	43,43,43,43	0
59	MG	BA	3206	1/1	0.14	-	85,85,85,85	0
59	MG	CA	1671	1/1	0.14	-	44,44,44,44	0
59	MG	AA	1654	1/1	0.14	-	78,78,78,78	0
59	MG	AA	1725	1/1	0.09	-	94,94,94,94	0
59	MG	BA	3205	1/1	0.20	-	75,75,75,75	0
59	MG	BA	3067	1/1	0.11	-	30,30,30,30	0
59	MG	BA	3111	1/1	0.40	-	65,65,65,65	0
59	MG	BA	3025	1/1	0.22	-	40,40,40,40	0
59	MG	AA	1638	1/1	0.11	-	43,43,43,43	0
59	MG	CA	1665	1/1	0.44	-	46,46,46,46	0
59	MG	DA	3321	1/1	0.47	-	85,85,85,85	0
59	MG	DA	3137	1/1	0.27	-	11,11,11,11	0
59	MG	CA	1654	1/1	0.35	-	48,48,48,48	0
59	MG	CA	1633	1/1	0.22	-	69,69,69,69	0
59	MG	BA	3107	1/1	0.21	-	25,25,25,25	1
59	MG	DA	3038	1/1	0.23	-	20,20,20,20	0
59	MG	DA	3069	1/1	0.23	-	19,19,19,19	0
59	MG	DA	3322	1/1	0.15	-	38,38,38,38	0
59	MG	CA	1657	1/1	0.18	-	52,52,52,52	0
59	MG	CA	1618	1/1	0.13	-	38,38,38,38	0
59	MG	BA	3023	1/1	0.41	-	52,52,52,52	0
59	MG	DA	3315	1/1	0.16	-	15,15,15,15	0
59	MG	AA	1717	1/1	0.57	-	110,110,110,110	0
59	MG	BA	3305	1/1	0.35	-	54,54,54,54	0
59	MG	AA	1689	1/1	0.17	-	37,37,37,37	0
59	MG	BA	3028	1/1	0.26	-	40,40,40,40	0
59	MG	DA	3125	1/1	0.38	-	18,18,18,18	0
59	MG	CA	1754	1/1	0.45	-	68,68,68,68	1
59	MG	BA	3019	1/1	0.34	-	26,26,26,26	0
59	MG	AA	1747	1/1	0.30	-	81,81,81,81	0
59	MG	BA	3261	1/1	0.26	-	60,60,60,60	0
59	MG	BA	3329	1/1	0.48	-	58,58,58,58	0
59	MG	DA	3317	1/1	0.27	-	63,63,63,63	0
59	MG	BA	3064	1/1	0.60	-	61,61,61,61	0
59	MG	BA	3087	1/1	0.20	-	13,13,13,13	0
59	MG	DA	3064	1/1	0.28	-	18,18,18,18	0
59	MG	DA	3075	1/1	0.28	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	1622	1/1	0.14	-	53,53,53,53	0
59	MG	BA	3316	1/1	0.25	-	74,74,74,74	0
59	MG	BA	3216	1/1	0.21	-	59,59,59,59	0
59	MG	DA	3065	1/1	0.58	-	65,65,65,65	0
59	MG	CW	104	1/1	0.14	-	37,37,37,37	1
59	MG	DA	3003	1/1	0.30	-	35,35,35,35	0
59	MG	DA	3316	1/1	0.15	-	33,33,33,33	1
59	MG	AA	1702	1/1	0.20	-	51,51,51,51	0
59	MG	CA	1693	1/1	0.45	-	56,56,56,56	0
59	MG	AA	1678	1/1	0.34	-	56,56,56,56	0
59	MG	DA	3083	1/1	0.24	-	11,11,11,11	0
59	MG	DA	3277	1/1	0.29	-	37,37,37,37	0
59	MG	BA	3281	1/1	0.34	-	51,51,51,51	1
59	MG	DA	3344	1/1	0.13	-	43,43,43,43	0
59	MG	BA	3285	1/1	0.25	-	37,37,37,37	1
59	MG	DA	3146	1/1	0.10	-	27,27,27,27	0
59	MG	DA	3205	1/1	0.28	-	46,46,46,46	0
59	MG	DA	3115	1/1	0.26	-	44,44,44,44	0
59	MG	DA	3074	1/1	0.25	-	24,24,24,24	0
59	MG	DA	3180	1/1	0.30	-	11,11,11,11	0
59	MG	BA	3075	1/1	0.30	-	32,32,32,32	0
59	MG	BA	3333	1/1	0.38	-	23,23,23,23	1
59	MG	BA	3185	1/1	0.27	-	46,46,46,46	0
59	MG	CA	1680	1/1	0.60	-	67,67,67,67	0
59	MG	BA	3345	1/1	0.35	-	63,63,63,63	0
59	MG	DA	3160	1/1	0.33	-	18,18,18,18	0
59	MG	DA	3196	1/1	0.18	-	41,41,41,41	0
59	MG	DA	3198	1/1	0.38	-	52,52,52,52	0
59	MG	AA	1734	1/1	0.27	-	51,51,51,51	0
59	MG	BA	3132	1/1	0.18	-	80,80,80,80	0
59	MG	CA	1732	1/1	0.41	-	70,70,70,70	0
59	MG	CA	1748	1/1	1.04	-	1,1,1,1	1
59	MG	BA	3255	1/1	0.27	-	73,73,73,73	0
59	MG	DA	3221	1/1	0.26	-	63,63,63,63	0
59	MG	DA	3011	1/1	0.22	-	10,10,10,10	0
59	MG	AA	1666	1/1	0.73	-	70,70,70,70	0
59	MG	BA	3245	1/1	0.21	-	43,43,43,43	0
59	MG	DA	3319	1/1	0.36	-	71,71,71,71	0
59	MG	DA	3006	1/1	0.60	-	52,52,52,52	0
59	MG	CA	1641	1/1	0.46	-	43,43,43,43	0
59	MG	DA	3213	1/1	0.23	-	17,17,17,17	0
60	ZN	CN	102	1/1	0.12	-	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	1601	1/1	0.27	-	59,59,59,59	0
59	MG	AA	1748	1/1	0.58	-	81,81,81,81	0
59	MG	BA	3253	1/1	0.09	-	65,65,65,65	1
59	MG	BA	3047	1/1	0.17	-	18,18,18,18	0
59	MG	BA	3266	1/1	0.35	-	35,35,35,35	0
59	MG	DA	3066	1/1	0.36	-	14,14,14,14	0
59	MG	BA	3164	1/1	0.38	-	52,52,52,52	0
59	MG	DA	3118	1/1	0.24	-	15,15,15,15	0
59	MG	BA	3218	1/1	0.52	-	89,89,89,89	0
59	MG	CD	301	1/1	0.13	-	84,84,84,84	0
59	MG	CN	101	1/1	0.09	-	69,69,69,69	0
59	MG	BA	3012	1/1	0.21	-	25,25,25,25	0
59	MG	DA	3262	1/1	0.10	-	32,32,32,32	0
59	MG	AA	1634	1/1	0.45	-	39,39,39,39	0
59	MG	DA	3325	1/1	0.25	-	48,48,48,48	0
59	MG	DA	3193	1/1	0.18	-	61,61,61,61	0
59	MG	AA	1620	1/1	0.22	-	54,54,54,54	0
59	MG	AA	1667	1/1	0.31	-	85,85,85,85	0
59	MG	DA	3227	1/1	0.23	-	22,22,22,22	0
59	MG	DA	3314	1/1	0.52	-	31,31,31,31	0
60	ZN	B9	101	1/1	0.05	-	77,77,77,77	1
59	MG	BA	3356	1/1	0.23	-	68,68,68,68	0
59	MG	BA	3244	1/1	0.22	-	51,51,51,51	0
59	MG	DA	3231	1/1	0.21	-	27,27,27,27	0
59	MG	BA	3108	1/1	0.37	-	15,15,15,15	0
59	MG	AA	1618	1/1	0.09	-	30,30,30,30	1
59	MG	DA	3028	1/1	0.25	-	24,24,24,24	0
59	MG	DA	3098	1/1	0.14	-	6,6,6,6	0
59	MG	BA	3327	1/1	0.19	-	52,52,52,52	0
59	MG	DA	3077	1/1	0.29	-	9,9,9,9	0
59	MG	BA	3006	1/1	0.45	-	73,73,73,73	0
59	MG	DA	3354	1/1	0.19	-	21,21,21,21	0
59	MG	BA	3017	1/1	0.28	-	45,45,45,45	0
59	MG	BA	3280	1/1	0.14	-	56,56,56,56	0
59	MG	BA	3230	1/1	0.18	-	40,40,40,40	0
59	MG	BA	3116	1/1	0.28	-	45,45,45,45	0
59	MG	BA	3157	1/1	0.21	-	36,36,36,36	1
59	MG	DA	3157	1/1	0.23	-	26,26,26,26	0
59	MG	AA	1719	1/1	0.20	-	63,63,63,63	0
59	MG	CA	1690	1/1	0.27	-	54,54,54,54	0
59	MG	BA	3188	1/1	0.32	-	14,14,14,14	0
59	MG	DA	3170	1/1	0.18	-	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CV	101	1/1	0.16	-	29,29,29,29	0
59	MG	DA	3336	1/1	0.36	-	48,48,48,48	0
59	MG	DA	3244	1/1	0.56	-	1,1,1,1	1
59	MG	CA	1679	1/1	0.28	-	60,60,60,60	0
59	MG	BA	3310	1/1	0.27	-	68,68,68,68	0
59	MG	AA	1639	1/1	0.34	-	73,73,73,73	0
59	MG	CA	1688	1/1	0.10	-	56,56,56,56	0
59	MG	DA	3209	1/1	0.21	-	47,47,47,47	0
59	MG	BA	3054	1/1	0.30	-	19,19,19,19	0
59	MG	DA	3073	1/1	0.26	-	15,15,15,15	0
59	MG	DA	3127	1/1	0.10	-	6,6,6,6	0
59	MG	AA	1736	1/1	0.15	-	43,43,43,43	1
59	MG	AA	1704	1/1	0.29	-	56,56,56,56	0
59	MG	BA	3096	1/1	0.32	-	59,59,59,59	0
59	MG	BA	3055	1/1	0.31	-	25,25,25,25	0
59	MG	AA	1710	1/1	0.26	-	61,61,61,61	0
59	MG	CA	1683	1/1	0.14	-	35,35,35,35	0
59	MG	AA	1657	1/1	0.44	-	46,46,46,46	0
59	MG	CA	1734	1/1	0.30	-	72,72,72,72	1
59	MG	AA	1697	1/1	0.17	-	60,60,60,60	0
59	MG	BA	3217	1/1	0.46	-	54,54,54,54	0
59	MG	AA	1677	1/1	0.49	-	68,68,68,68	0
59	MG	BA	3306	1/1	0.34	-	29,29,29,29	0
59	MG	DA	3278	1/1	0.41	-	40,40,40,40	0
59	MG	BA	3154	1/1	0.22	-	44,44,44,44	0
59	MG	CV	103	1/1	0.08	-	57,57,57,57	0
59	MG	AA	1608	1/1	0.15	-	48,48,48,48	0
59	MG	CA	1685	1/1	0.39	-	53,53,53,53	0
59	MG	DA	3288	1/1	0.23	-	61,61,61,61	0
59	MG	DA	3186	1/1	0.28	-	17,17,17,17	0
59	MG	DA	3357	1/1	0.36	-	55,55,55,55	0
59	MG	BA	3343	1/1	0.12	-	75,75,75,75	0
59	MG	CA	1659	1/1	0.27	-	69,69,69,69	0
59	MG	DA	3298	1/1	0.30	-	78,78,78,78	0
59	MG	BA	3192	1/1	0.29	-	65,65,65,65	0
59	MG	BA	3134	1/1	0.17	-	52,52,52,52	0
59	MG	DA	3181	1/1	0.29	-	26,26,26,26	0
59	MG	AA	1699	1/1	0.28	-	83,83,83,83	0
59	MG	AA	1685	1/1	0.12	-	57,57,57,57	0
59	MG	AA	1709	1/1	0.22	-	50,50,50,50	0
59	MG	BA	3024	1/1	0.35	-	36,36,36,36	0
59	MG	BA	3300	1/1	0.25	-	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3169	1/1	0.22	-	45,45,45,45	0
59	MG	AA	1686	1/1	0.30	-	64,64,64,64	0
59	MG	AA	1722	1/1	0.15	-	46,46,46,46	1
59	MG	CA	1740	1/1	0.47	-	56,56,56,56	0
59	MG	DA	3329	1/1	0.51	-	47,47,47,47	0
59	MG	DB	204	1/1	0.22	-	1,1,1,1	1
59	MG	BA	3273	1/1	0.63	-	12,12,12,12	1
59	MG	BA	3140	1/1	0.30	-	77,77,77,77	0
59	MG	DA	3352	1/1	0.19	-	46,46,46,46	0
59	MG	DA	3126	1/1	0.28	-	6,6,6,6	0
59	MG	BA	3302	1/1	0.21	-	20,20,20,20	0
59	MG	AA	1750	1/1	0.32	-	54,54,54,54	0
59	MG	AA	1664	1/1	0.30	-	65,65,65,65	0
59	MG	DA	3348	1/1	0.16	-	18,18,18,18	0
59	MG	B5	101	1/1	0.25	-	38,38,38,38	0
59	MG	DA	3050	1/1	0.14	-	13,13,13,13	0
59	MG	DA	3123	1/1	0.53	-	76,76,76,76	0
59	MG	DA	3312	1/1	0.14	-	65,65,65,65	0
59	MG	DA	3104	1/1	0.32	-	35,35,35,35	0
59	MG	DA	3188	1/1	0.24	-	7,7,7,7	0
59	MG	DA	3071	1/1	0.19	-	18,18,18,18	0
59	MG	CA	1736	1/1	0.38	-	55,55,55,55	0
59	MG	AA	1694	1/1	0.33	-	54,54,54,54	0
59	MG	BA	3035	1/1	0.17	-	21,21,21,21	0
59	MG	DA	3203	1/1	0.22	-	37,37,37,37	0
59	MG	BA	3102	1/1	0.12	-	20,20,20,20	0
59	MG	CA	1747	1/1	0.17	-	21,21,21,21	1
59	MG	CA	1634	1/1	0.40	-	35,35,35,35	0
59	MG	BA	3163	1/1	0.32	-	67,67,67,67	0
59	MG	AA	1621	1/1	0.17	-	93,93,93,93	0
59	MG	BA	3079	1/1	0.30	-	36,36,36,36	0
59	MG	DA	3108	1/1	0.36	-	16,16,16,16	0
59	MG	DA	3116	1/1	0.14	-	7,7,7,7	0
59	MG	BA	3339	1/1	0.08	-	21,21,21,21	1
59	MG	CA	1706	1/1	0.20	-	53,53,53,53	0
59	MG	DA	3009	1/1	0.28	-	15,15,15,15	0
59	MG	CA	1719	1/1	0.23	-	98,98,98,98	0
59	MG	BA	3328	1/1	0.21	-	32,32,32,32	0
59	MG	DA	3178	1/1	0.16	-	51,51,51,51	0
59	MG	AA	1649	1/1	0.27	-	67,67,67,67	0
59	MG	DA	3351	1/1	0.65	-	70,70,70,70	0
59	MG	AA	1633	1/1	0.27	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3336	1/1	0.34	-	40,40,40,40	0
59	MG	BA	3200	1/1	0.30	-	36,36,36,36	0
59	MG	D5	101	1/1	0.25	-	25,25,25,25	0
59	MG	BA	3139	1/1	0.73	-	84,84,84,84	0
59	MG	BA	3231	1/1	0.23	-	25,25,25,25	1
59	MG	DA	3218	1/1	0.30	-	29,29,29,29	0
59	MG	BA	3166	1/1	0.12	-	42,42,42,42	0
59	MG	DA	3131	1/1	0.13	-	18,18,18,18	0
59	MG	DA	3300	1/1	0.17	-	10,10,10,10	0
59	MG	DA	3359	1/1	0.17	-	1,1,1,1	1
59	MG	BA	3288	1/1	0.17	-	52,52,52,52	0
59	MG	DA	3191	1/1	0.24	-	34,34,34,34	0
59	MG	DA	3266	1/1	0.21	-	27,27,27,27	0
59	MG	CA	1652	1/1	0.47	-	71,71,71,71	0
59	MG	BA	3298	1/1	0.23	-	68,68,68,68	0
59	MG	DA	3241	1/1	0.11	-	69,69,69,69	0
59	MG	DA	3272	1/1	0.24	-	19,19,19,19	0
59	MG	BA	3197	1/1	0.32	-	12,12,12,12	0
59	MG	AA	1629	1/1	0.20	-	61,61,61,61	0
59	MG	BA	3252	1/1	0.21	-	32,32,32,32	1
59	MG	BA	3152	1/1	0.20	-	104,104,104,104	0
59	MG	AA	1696	1/1	0.10	-	57,57,57,57	1
59	MG	AA	1711	1/1	0.19	-	63,63,63,63	0
59	MG	AA	1673	1/1	0.23	-	72,72,72,72	0
59	MG	AA	1727	1/1	0.82	-	20,20,20,20	1
59	MG	CW	103	1/1	0.33	-	15,15,15,15	1
59	MG	DA	3101	1/1	0.37	-	16,16,16,16	0
59	MG	BX	101	1/1	0.28	-	47,47,47,47	0
59	MG	CA	1636	1/1	0.30	-	52,52,52,52	0
59	MG	BA	3254	1/1	0.28	-	62,62,62,62	0
59	MG	BA	3029	1/1	0.53	-	66,66,66,66	0
59	MG	BA	3082	1/1	0.23	-	60,60,60,60	0
59	MG	DA	3249	1/1	0.13	-	27,27,27,27	1
59	MG	BA	3299	1/1	0.26	-	55,55,55,55	0
59	MG	DA	3053	1/1	0.27	-	50,50,50,50	0
59	MG	BA	3290	1/1	0.50	-	11,11,11,11	1
59	MG	DA	3012	1/1	0.34	-	19,19,19,19	0
59	MG	BA	3146	1/1	0.19	-	58,58,58,58	0
59	MG	BA	3269	1/1	0.38	-	34,34,34,34	0
59	MG	DA	3145	1/1	0.22	-	43,43,43,43	0
59	MG	DA	3129	1/1	0.19	-	46,46,46,46	0
59	MG	DA	3281	1/1	0.33	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	B1	101	1/1	0.27	-	6,6,6,6	1
59	MG	CA	1647	1/1	0.30	-	44,44,44,44	0
59	MG	DA	3346	1/1	0.20	-	42,42,42,42	0
59	MG	CA	1725	1/1	0.17	-	72,72,72,72	0
59	MG	AY	401	1/1	0.25	-	74,74,74,74	0
59	MG	CA	1644	1/1	0.09	-	64,64,64,64	0
59	MG	DA	3004	1/1	0.22	-	25,25,25,25	0
59	MG	CA	1611	1/1	0.36	-	51,51,51,51	0
59	MG	DA	3109	1/1	0.19	-	6,6,6,6	1
59	MG	DA	3287	1/1	0.15	-	28,28,28,28	0
59	MG	BA	3013	1/1	0.19	-	54,54,54,54	0
59	MG	CA	1682	1/1	0.20	-	60,60,60,60	0
59	MG	DA	3136	1/1	0.29	-	38,38,38,38	0
59	MG	AA	1614	1/1	0.18	-	68,68,68,68	0
59	MG	BA	3227	1/1	0.30	-	56,56,56,56	0
59	MG	DA	3328	1/1	0.15	-	32,32,32,32	0
59	MG	D5	102	1/1	0.42	-	28,28,28,28	0
59	MG	DA	3179	1/1	0.22	-	49,49,49,49	0
59	MG	AA	1692	1/1	0.33	-	50,50,50,50	0
59	MG	BA	3317	1/1	0.23	-	1,1,1,1	1
59	MG	DA	3046	1/1	0.28	-	11,11,11,11	0
59	MG	BA	3183	1/1	0.22	-	59,59,59,59	1
59	MG	DA	3214	1/1	0.38	-	117,117,117,117	0
59	MG	B5	102	1/1	0.45	-	78,78,78,78	0
59	MG	BA	3178	1/1	0.34	-	22,22,22,22	0
59	MG	CA	1733	1/1	0.20	-	50,50,50,50	0
59	MG	BA	3104	1/1	0.36	-	57,57,57,57	0
59	MG	AA	1627	1/1	0.13	-	40,40,40,40	0
59	MG	DA	3215	1/1	0.48	-	129,129,129,129	0
59	MG	CA	1686	1/1	0.14	-	21,21,21,21	0
59	MG	BA	3118	1/1	0.44	-	38,38,38,38	0
59	MG	DA	3197	1/1	0.40	-	94,94,94,94	0
59	MG	CL	202	1/1	0.54	-	80,80,80,80	0
59	MG	BA	3129	1/1	0.41	-	59,59,59,59	0
59	MG	BA	3289	1/1	0.21	-	59,59,59,59	0
59	MG	DA	3111	1/1	0.29	-	33,33,33,33	0
59	MG	DX	101	1/1	0.62	-	58,58,58,58	0
59	MG	BB	203	1/1	0.15	-	69,69,69,69	0
59	MG	CA	1612	1/1	0.20	-	65,65,65,65	0
59	MG	CS	101	1/1	0.17	-	52,52,52,52	1
59	MG	BA	3059	1/1	0.20	-	30,30,30,30	0
59	MG	CA	1718	1/1	0.14	-	44,44,44,44	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3161	1/1	0.20	-	54,54,54,54	0
59	MG	DA	3121	1/1	0.33	-	14,14,14,14	1
59	MG	DA	3335	1/1	0.34	-	88,88,88,88	0
59	MG	BB	201	1/1	0.46	-	38,38,38,38	1
59	MG	BA	3097	1/1	0.11	-	45,45,45,45	0
59	MG	DA	3253	1/1	0.51	-	18,18,18,18	1
59	MG	DA	3124	1/1	0.34	-	20,20,20,20	1
59	MG	BA	3191	1/1	0.16	-	84,84,84,84	0
59	MG	BA	3138	1/1	0.11	-	31,31,31,31	0
59	MG	AA	1655	1/1	0.16	-	57,57,57,57	0
59	MG	BA	3149	1/1	0.78	-	75,75,75,75	0
59	MG	BA	3341	1/1	0.35	-	61,61,61,61	0
59	MG	BA	3237	1/1	0.35	-	64,64,64,64	0
59	MG	AA	1605	1/1	0.10	-	58,58,58,58	0
59	MG	CA	1603	1/1	0.97	-	130,130,130,130	0
59	MG	BA	3243	1/1	0.22	-	10,10,10,10	1
59	MG	CA	1720	1/1	0.32	-	93,93,93,93	1
59	MG	BA	3066	1/1	0.49	-	25,25,25,25	0
59	MG	BA	3063	1/1	0.15	-	56,56,56,56	0
59	MG	BA	3264	1/1	0.17	-	64,64,64,64	0
59	MG	AA	1680	1/1	0.17	-	91,91,91,91	0
59	MG	DA	3027	1/1	0.16	-	1,1,1,1	0
59	MG	BA	3003	1/1	0.21	-	56,56,56,56	0
59	MG	BA	3287	1/1	0.16	-	65,65,65,65	0
59	MG	BA	3110	1/1	0.17	-	51,51,51,51	0
59	MG	DA	3019	1/1	0.31	-	17,17,17,17	0
59	MG	AA	1731	1/1	0.25	-	68,68,68,68	0
59	MG	CA	1714	1/1	0.52	-	62,62,62,62	0
59	MG	DA	3055	1/1	0.29	-	23,23,23,23	0
59	MG	AA	1738	1/1	0.11	-	85,85,85,85	0
59	MG	BA	3275	1/1	0.35	-	27,27,27,27	1
59	MG	DA	3320	1/1	0.30	-	56,56,56,56	0
59	MG	BA	3246	1/1	0.35	-	60,60,60,60	0
59	MG	DA	3195	1/1	0.15	-	102,102,102,102	0
59	MG	AA	1658	1/1	0.30	-	66,66,66,66	0
59	MG	DA	3269	1/1	0.19	-	7,7,7,7	0
59	MG	DA	3275	1/1	0.31	-	28,28,28,28	1
59	MG	BA	3131	1/1	0.61	-	67,67,67,67	0
59	MG	CW	102	1/1	0.31	-	51,51,51,51	1
59	MG	DA	3189	1/1	0.49	-	21,21,21,21	0
59	MG	BA	3241	1/1	0.19	-	1,1,1,1	1
59	MG	DB	201	1/1	0.38	-	27,27,27,27	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3081	1/1	0.27	-	21,21,21,21	0
59	MG	DA	3056	1/1	0.39	-	26,26,26,26	0
59	MG	BA	3044	1/1	0.41	-	49,49,49,49	0
59	MG	CA	1661	1/1	0.48	-	83,83,83,83	0
59	MG	DA	3037	1/1	0.24	-	7,7,7,7	0
59	MG	BA	3039	1/1	0.47	-	111,111,111,111	0
59	MG	DA	3313	1/1	0.22	-	74,74,74,74	0
59	MG	CA	1614	1/1	0.12	-	44,44,44,44	0
59	MG	BA	3122	1/1	0.64	-	62,62,62,62	0
59	MG	CA	1750	1/1	0.16	-	76,76,76,76	0
59	MG	DA	3085	1/1	0.13	-	5,5,5,5	0
59	MG	BA	3172	1/1	0.21	-	58,58,58,58	0
59	MG	CA	1709	1/1	0.08	-	40,40,40,40	1
59	MG	AA	1671	1/1	0.32	-	66,66,66,66	0
59	MG	CV	105	1/1	0.30	-	66,66,66,66	0
59	MG	BA	3175	1/1	0.11	-	65,65,65,65	0
59	MG	DA	3079	1/1	0.30	-	10,10,10,10	0
59	MG	BA	3041	1/1	0.31	-	17,17,17,17	0
59	MG	DA	3341	1/1	0.24	-	36,36,36,36	1
59	MG	CA	1624	1/1	0.33	-	52,52,52,52	0
59	MG	BA	3334	1/1	0.11	-	55,55,55,55	0
59	MG	BA	3098	1/1	0.09	-	15,15,15,15	0
59	MG	DA	3042	1/1	0.27	-	12,12,12,12	0
59	MG	AA	1622	1/1	0.27	-	81,81,81,81	0
59	MG	CA	1631	1/1	0.13	-	24,24,24,24	0
59	MG	AA	1683	1/1	0.09	-	63,63,63,63	0
59	MG	BA	3324	1/1	0.36	-	19,19,19,19	1
59	MG	BA	3092	1/1	0.29	-	40,40,40,40	0
59	MG	DA	3153	1/1	0.46	-	94,94,94,94	0
59	MG	BA	3354	1/1	0.74	-	91,91,91,91	0
59	MG	CA	1729	1/1	0.28	-	33,33,33,33	1
59	MG	BA	3072	1/1	0.42	-	41,41,41,41	0
59	MG	BA	3167	1/1	0.28	-	70,70,70,70	0
59	MG	BA	3008	1/1	0.29	-	58,58,58,58	0
59	MG	DA	3267	1/1	0.21	-	13,13,13,13	0
59	MG	DA	3139	1/1	0.28	-	23,23,23,23	0
59	MG	BA	3297	1/1	0.38	-	75,75,75,75	1
59	MG	DA	3096	1/1	0.33	-	50,50,50,50	0
59	MG	BA	3325	1/1	0.08	-	62,62,62,62	0
59	MG	AA	1662	1/1	0.31	-	56,56,56,56	0
59	MG	DA	3059	1/1	0.23	-	13,13,13,13	0
59	MG	DA	3110	1/1	0.29	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	1677	1/1	0.12	-	46,46,46,46	1
59	MG	DA	3307	1/1	0.30	-	14,14,14,14	0
59	MG	CA	1697	1/1	0.11	-	58,58,58,58	0
59	MG	BA	3262	1/1	0.08	-	49,49,49,49	0
59	MG	BA	3056	1/1	0.40	-	33,33,33,33	0
59	MG	BA	3084	1/1	0.17	-	27,27,27,27	0
59	MG	CA	1605	1/1	0.12	-	44,44,44,44	0
59	MG	DA	3334	1/1	0.12	-	63,63,63,63	0
59	MG	CA	1602	1/1	0.27	-	16,16,16,16	1
59	MG	DA	3257	1/1	0.10	-	35,35,35,35	0
59	MG	AA	1640	1/1	0.25	-	47,47,47,47	0
59	MG	CA	1723	1/1	0.34	-	45,45,45,45	1
60	ZN	AD	301	1/1	0.21	-	67,67,67,67	0
59	MG	AV	103	1/1	0.10	-	74,74,74,74	0
59	MG	CA	1645	1/1	0.19	-	45,45,45,45	1
59	MG	DA	3301	1/1	0.20	-	21,21,21,21	0
59	MG	CA	1717	1/1	0.19	-	63,63,63,63	1
59	MG	CA	1650	1/1	0.24	-	46,46,46,46	0
59	MG	AA	1647	1/1	0.16	-	66,66,66,66	0
59	MG	AA	1660	1/1	0.11	-	69,69,69,69	0
59	MG	BA	3268	1/1	0.32	-	66,66,66,66	0
59	MG	CA	1620	1/1	0.18	-	48,48,48,48	0
59	MG	BA	3226	1/1	0.53	-	58,58,58,58	0
59	MG	DA	3161	1/1	0.28	-	44,44,44,44	0
59	MG	DA	3339	1/1	0.60	-	89,89,89,89	0
59	MG	DA	3032	1/1	0.15	-	32,32,32,32	0
59	MG	AA	1691	1/1	0.16	-	69,69,69,69	0
59	MG	AA	1612	1/1	0.10	-	47,47,47,47	0
59	MG	BA	3221	1/1	0.42	-	53,53,53,53	0
59	MG	DA	3232	1/1	0.26	-	37,37,37,37	1
59	MG	CV	104	1/1	0.07	-	2,2,2,2	1
59	MG	DA	3190	1/1	0.26	-	16,16,16,16	0
59	MG	BA	3027	1/1	0.20	-	19,19,19,19	0
59	MG	BA	3198	1/1	0.24	-	38,38,38,38	0
59	MG	CA	1626	1/1	0.18	-	75,75,75,75	0
59	MG	AA	1690	1/1	0.08	-	64,64,64,64	0
59	MG	CA	1727	1/1	0.25	-	44,44,44,44	0
59	MG	DA	3291	1/1	0.11	-	49,49,49,49	0
59	MG	AA	1624	1/1	0.33	-	62,62,62,62	0
59	MG	DA	3268	1/1	0.16	-	30,30,30,30	0
59	MG	DA	3207	1/1	0.17	-	40,40,40,40	0
59	MG	BA	3257	1/1	0.16	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	1741	1/1	0.34	-	34,34,34,34	0
59	MG	DA	3175	1/1	0.29	-	59,59,59,59	0
59	MG	AA	1728	1/1	0.30	-	69,69,69,69	0
59	MG	AA	1613	1/1	0.15	-	60,60,60,60	0
59	MG	DA	3070	1/1	0.21	-	11,11,11,11	0
59	MG	DA	3358	1/1	0.43	-	50,50,50,50	0
59	MG	AL	201	1/1	0.09	-	15,15,15,15	1
59	MG	CA	1674	1/1	0.11	-	35,35,35,35	1
59	MG	BA	3144	1/1	0.17	-	46,46,46,46	0
59	MG	DA	3239	1/1	0.14	-	29,29,29,29	0
59	MG	BA	3106	1/1	0.22	-	34,34,34,34	0
59	MG	BA	3332	1/1	0.19	-	54,54,54,54	0
59	MG	CA	1730	1/1	0.26	-	72,72,72,72	0
59	MG	BA	3282	1/1	0.08	-	68,68,68,68	0
59	MG	DA	3333	1/1	0.16	-	55,55,55,55	0
59	MG	CA	1708	1/1	0.36	-	104,104,104,104	0
59	MG	CA	1684	1/1	0.50	-	50,50,50,50	0
59	MG	AA	1641	1/1	0.13	-	38,38,38,38	0
59	MG	BA	3278	1/1	0.25	-	59,59,59,59	0
59	MG	DA	3280	1/1	0.39	-	54,54,54,54	0
59	MG	DA	3060	1/1	0.21	-	17,17,17,17	0
59	MG	BA	3069	1/1	0.26	-	32,32,32,32	0
59	MG	DA	3235	1/1	0.29	-	18,18,18,18	0
59	MG	BA	3100	1/1	0.25	-	29,29,29,29	0
59	MG	DA	3255	1/1	0.17	-	13,13,13,13	0
59	MG	AA	1713	1/1	0.21	-	49,49,49,49	1
59	MG	DA	3142	1/1	0.41	-	17,17,17,17	0
59	MG	CA	1607	1/1	0.28	-	32,32,32,32	0
59	MG	BA	3180	1/1	0.31	-	46,46,46,46	1
59	MG	CA	1753	1/1	0.12	-	67,67,67,67	0
59	MG	CA	1658	1/1	0.21	-	53,53,53,53	0
59	MG	DA	3103	1/1	0.26	-	12,12,12,12	0
59	MG	BA	3326	1/1	0.31	-	42,42,42,42	0
59	MG	BA	3015	1/1	0.25	-	28,28,28,28	0
59	MG	DA	3204	1/1	0.28	-	59,59,59,59	0
59	MG	DA	3185	1/1	0.11	-	39,39,39,39	0
59	MG	CA	1619	1/1	0.26	-	41,41,41,41	0
59	MG	BA	3147	1/1	0.24	-	35,35,35,35	0
59	MG	AV	102	1/1	0.11	-	61,61,61,61	0
59	MG	DA	3158	1/1	0.29	-	37,37,37,37	0
59	MG	BA	3060	1/1	0.25	-	14,14,14,14	0
59	MG	CA	1701	1/1	0.49	-	55,55,55,55	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	DA	3147	1/1	0.18	-	52,52,52,52	0
59	MG	AA	1626	1/1	0.54	-	61,61,61,61	0
59	MG	CA	1689	1/1	0.14	-	57,57,57,57	0
59	MG	DA	3120	1/1	0.26	-	9,9,9,9	0
59	MG	BA	3074	1/1	0.28	-	37,37,37,37	0
59	MG	BA	3344	1/1	0.51	-	63,63,63,63	0
59	MG	AW	101	1/1	0.14	-	58,58,58,58	1
59	MG	AA	1733	1/1	0.38	-	79,79,79,79	0
59	MG	DA	3276	1/1	0.47	-	57,57,57,57	0
59	MG	DA	3226	1/1	0.57	-	64,64,64,64	0
59	MG	DA	3176	1/1	0.27	-	7,7,7,7	0
59	MG	DA	3097	1/1	0.13	-	15,15,15,15	0
59	MG	BA	3142	1/1	0.27	-	97,97,97,97	0
59	MG	BA	3240	1/1	0.14	-	73,73,73,73	0
59	MG	DA	3054	1/1	0.40	-	22,22,22,22	0
59	MG	BA	3030	1/1	0.31	-	59,59,59,59	0
59	MG	BA	3304	1/1	0.74	-	64,64,64,64	0
59	MG	AA	1645	1/1	0.35	-	88,88,88,88	0
59	MG	DA	3151	1/1	0.27	-	25,25,25,25	0
59	MG	DA	3018	1/1	0.23	-	16,16,16,16	0
59	MG	BA	3338	1/1	0.42	-	54,54,54,54	0
59	MG	AA	1674	1/1	0.15	-	69,69,69,69	0
59	MG	DA	3076	1/1	0.22	-	11,11,11,11	0
59	MG	CA	1613	1/1	0.31	-	58,58,58,58	0
59	MG	DA	3222	1/1	0.28	-	15,15,15,15	0
59	MG	BA	3155	1/1	0.18	-	53,53,53,53	0
59	MG	BA	3020	1/1	0.42	-	37,37,37,37	0
59	MG	DA	3047	1/1	0.20	-	20,20,20,20	0
59	MG	CA	1735	1/1	0.10	-	21,21,21,21	0
59	MG	DE	301	1/1	0.20	-	41,41,41,41	0
59	MG	DA	3297	1/1	0.38	-	42,42,42,42	1
59	MG	BA	3136	1/1	0.22	-	42,42,42,42	0
59	MG	AA	1716	1/1	0.20	-	66,66,66,66	1
59	MG	BA	3018	1/1	0.21	-	35,35,35,35	0
59	MG	BA	3251	1/1	0.28	-	55,55,55,55	0
59	MG	AA	1745	1/1	0.32	-	62,62,62,62	0
59	MG	DA	3225	1/1	0.11	-	34,34,34,34	0
59	MG	BA	3318	1/1	0.21	-	42,42,42,42	0
59	MG	AA	1610	1/1	0.13	-	80,80,80,80	1
59	MG	BA	3085	1/1	0.17	-	38,38,38,38	0
59	MG	CA	1726	1/1	0.73	-	48,48,48,48	0
59	MG	CA	1672	1/1	0.17	-	52,52,52,52	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3292	1/1	0.24	-	55,55,55,55	0
59	MG	DA	3022	1/1	0.40	-	16,16,16,16	0
59	MG	AA	1668	1/1	0.24	-	40,40,40,40	0
59	MG	DA	3200	1/1	0.31	-	18,18,18,18	0
59	MG	BA	3091	1/1	0.17	-	58,58,58,58	0
59	MG	DA	3206	1/1	0.18	-	57,57,57,57	0
59	MG	BA	3117	1/1	0.23	-	30,30,30,30	0
59	MG	CA	1716	1/1	0.31	-	50,50,50,50	0
59	MG	DA	3211	1/1	0.36	-	69,69,69,69	0
59	MG	CA	1670	1/1	0.32	-	77,77,77,77	0
59	MG	AA	1703	1/1	0.33	-	71,71,71,71	0
59	MG	AA	1744	1/1	0.23	-	1,1,1,1	1
59	MG	DA	3184	1/1	0.20	-	46,46,46,46	0
59	MG	BA	3248	1/1	0.07	-	62,62,62,62	0
59	MG	BA	3308	1/1	0.12	-	39,39,39,39	0
59	MG	DA	3105	1/1	0.09	-	1,1,1,1	0
59	MG	DA	3216	1/1	0.13	-	11,11,11,11	1
59	MG	BA	3208	1/1	0.53	-	100,100,100,100	0
59	MG	CW	101	1/1	0.20	-	46,46,46,46	1
59	MG	AA	1715	1/1	0.27	-	59,59,59,59	0
59	MG	DA	3174	1/1	0.13	-	46,46,46,46	0
59	MG	BA	3233	1/1	0.21	-	50,50,50,50	0
59	MG	BA	3220	1/1	0.20	-	79,79,79,79	0
59	MG	AA	1730	1/1	0.92	-	78,78,78,78	0
59	MG	BA	3086	1/1	0.32	-	25,25,25,25	0
59	MG	BA	3256	1/1	0.04	-	25,25,25,25	0
59	MG	AW	104	1/1	0.23	-	67,67,67,67	1
59	MG	CA	1609	1/1	0.24	-	58,58,58,58	0
59	MG	DA	3168	1/1	0.07	-	18,18,18,18	0
59	MG	BA	3277	1/1	0.61	-	68,68,68,68	0
59	MG	DA	3167	1/1	0.45	-	46,46,46,46	0
59	MG	BB	202	1/1	0.23	-	51,51,51,51	0
59	MG	DB	202	1/1	0.26	-	23,23,23,23	0
59	MG	BA	3011	1/1	0.37	-	43,43,43,43	0
59	MG	AA	1659	1/1	0.18	-	78,78,78,78	0
59	MG	DA	3173	1/1	0.22	-	12,12,12,12	0
59	MG	DA	3014	1/1	0.27	-	20,20,20,20	0
59	MG	BA	3159	1/1	0.37	-	55,55,55,55	0
59	MG	CA	1643	1/1	0.14	-	10,10,10,10	1
59	MG	BA	3016	1/1	0.37	-	18,18,18,18	0
59	MG	AA	1758	1/1	0.21	-	99,99,99,99	0
59	MG	AA	1623	1/1	0.29	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3342	1/1	0.36	-	64,64,64,64	0
59	MG	DA	3091	1/1	0.29	-	21,21,21,21	1
59	MG	BA	3193	1/1	0.44	-	5,5,5,5	1
59	MG	BA	3158	1/1	0.43	-	23,23,23,23	0
59	MG	AA	1652	1/1	0.39	-	50,50,50,50	0
59	MG	BD	302	1/1	0.17	-	29,29,29,29	0
59	MG	BA	3315	1/1	0.08	-	45,45,45,45	0
59	MG	AV	105	1/1	0.51	-	88,88,88,88	0
59	MG	CA	1699	1/1	0.57	-	84,84,84,84	0
59	MG	DA	3264	1/1	0.24	-	58,58,58,58	1
59	MG	AW	103	1/1	0.16	-	84,84,84,84	0
59	MG	BA	3038	1/1	0.24	-	44,44,44,44	0
59	MG	DA	3087	1/1	0.19	-	1,1,1,1	0
59	MG	AA	1755	1/1	0.05	-	51,51,51,51	0
59	MG	DA	3305	1/1	0.15	-	39,39,39,39	0
59	MG	AA	1644	1/1	0.15	-	54,54,54,54	0
59	MG	BA	3150	1/1	0.12	-	44,44,44,44	0
59	MG	BA	3101	1/1	0.36	-	27,27,27,27	0
59	MG	DA	3072	1/1	0.22	-	20,20,20,20	0
59	MG	DA	3306	1/1	0.38	-	15,15,15,15	0
59	MG	BA	3026	1/1	0.20	-	8,8,8,8	0
59	MG	CA	1695	1/1	0.38	-	46,46,46,46	1
59	MG	BA	3223	1/1	0.33	-	38,38,38,38	0
59	MG	AA	1603	1/1	0.13	-	60,60,60,60	0
59	MG	AA	1648	1/1	0.10	-	69,69,69,69	0
59	MG	BA	3307	1/1	0.28	-	14,14,14,14	0
59	MG	BA	3239	1/1	0.28	-	4,4,4,4	1
59	MG	DA	3031	1/1	0.24	-	52,52,52,52	0
59	MG	CV	102	1/1	0.11	-	43,43,43,43	0
59	MG	DA	3016	1/1	0.45	-	16,16,16,16	0
59	MG	BA	3260	1/1	0.33	-	53,53,53,53	0
60	ZN	AN	101	1/1	0.11	-	104,104,104,104	0
59	MG	DA	3289	1/1	0.12	-	17,17,17,17	0
59	MG	BA	3212	1/1	0.41	-	74,74,74,74	0
59	MG	AA	1759	1/1	0.10	-	139,139,139,139	0
59	MG	CA	1635	1/1	0.09	-	31,31,31,31	0
59	MG	CA	1656	1/1	0.42	-	29,29,29,29	0
59	MG	AA	1646	1/1	0.35	-	48,48,48,48	0
59	MG	DA	3282	1/1	0.16	-	41,41,41,41	0
59	MG	AA	1714	1/1	0.18	-	21,21,21,21	1
59	MG	DA	3295	1/1	0.18	-	13,13,13,13	1
59	MG	BA	3195	1/1	0.12	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3210	1/1	0.51	-	70,70,70,70	0
59	MG	AA	1636	1/1	0.12	-	21,21,21,21	0
59	MG	CA	1621	1/1	0.14	-	77,77,77,77	0
59	MG	AA	1723	1/1	0.25	-	54,54,54,54	1
59	MG	CA	1696	1/1	0.47	-	17,17,17,17	1
59	MG	CA	1738	1/1	0.22	-	15,15,15,15	1
59	MG	CA	1628	1/1	0.24	-	49,49,49,49	0
59	MG	DA	3252	1/1	0.30	-	51,51,51,51	0
59	MG	DA	3152	1/1	0.23	-	38,38,38,38	0

6.5 Other polymers ⓘ

There are no such residues in this entry.