



# wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 06:37 PM BST

PDB ID : 4V5E  
Title : Insights into translational termination from the structure of RF2 bound to the ribosome  
Authors : Weixlbaumer, A.; Jin, H.; Neubauer, C.; Voorhees, R.M.; Petry, S.; Kelley, A.C.; Ramakrishnan, V.  
Deposited on : 2009-04-30  
Resolution : 3.45 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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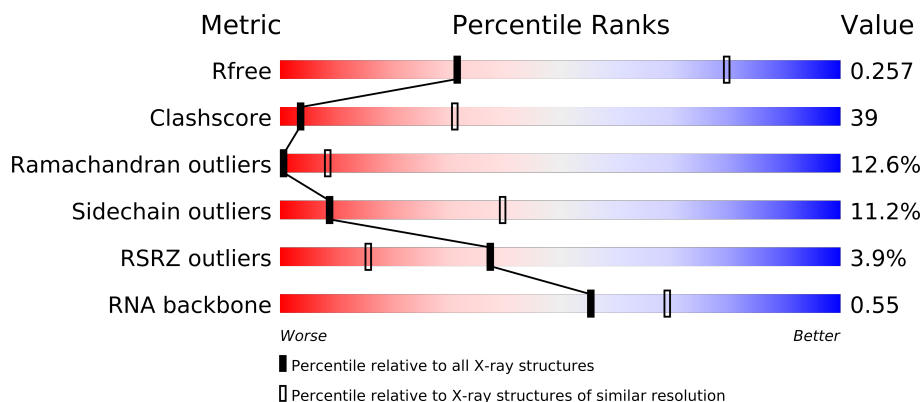
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.45 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	1149 (3.62-3.30)
Clashscore	79885	1012 (3.60-3.32)
Ramachandran outliers	78287	1401 (3.62-3.30)
Sidechain outliers	78261	1401 (3.62-3.30)
RSRZ outliers	66119	1149 (3.62-3.30)
RNA backbone	1838	1004 (4.10-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	76	
22	AW	76	
22	CV	76	
22	CW	76	
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	
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	2901	
35	DA	2901	
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	
44	BJ	130	
44	DJ	130	
45	BK	147	
45	DK	147	
46	BN	140	
46	DN	140	
47	BO	122	
47	DO	122	
48	BP	150	
48	DP	150	

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Mol	Chain	Length	Quality of chain
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	
59	D4	30	
60	DI	148	

## 2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 304505 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	126	Total	C	N	O	S	0	0	1
			976	614	197	164	1			
12	CL	126	Total	C	N	O	S	0	0	1
			976	614	197	164	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	121	Total	C	N	O	S	0	0	1
			956	591	198	165	2			
13	CM	121	Total	C	N	O	S	0	0	1
			956	591	198	165	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			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	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
22	AW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
22	CV	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
22	CW	76	Total	C	N	O	P	0	0	0
			1619	723	290	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
			166	76	29	54	7			
23	CX	8	Total	C	N	O	P	0	0	0
			166	76	29	54	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
			2799	1751	503	537	8			
24	CY	351	Total	C	N	O	S	0	0	0
			2799	1751	503	537	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	303	GLU	ARG	CONFLICT	UNP Q5SM01
CY	303	GLU	ARG	CONFLICT	UNP Q5SM01

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	B0	76	Total	C	N	O	S	0	0	0
			607	376	128	102	1			
25	D0	76	Total	C	N	O	S	0	0	0
			607	376	128	102	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			

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

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

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

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

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

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

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

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

- Molecule 34 is a 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	2886	Total	C	N	O	P	0	0	0
			62154	27663	11625	19981	2885			
35	DA	2886	Total	C	N	O	P	0	0	0
			62154	27663	11625	19981	2885			

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			

- 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			
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			

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

- Molecule 59 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	D4	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			

- Molecule 60 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	DI	146	Total	C	N	O	S	0	0	1
			1133	724	201	207	1			

- Molecule 61 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	BA	354	Total	Mg	0	0
			354	354		
61	CA	157	Total	Mg	0	0
			157	157		
61	DQ	1	Total	Mg	0	0
			1	1		
61	DF	3	Total	Mg	0	0
			3	3		
61	CV	7	Total	Mg	0	0
			7	7		
61	AW	5	Total	Mg	0	0
			5	5		
61	DU	1	Total	Mg	0	0
			1	1		
61	B1	1	Total	Mg	0	0
			1	1		
61	DY	1	Total	Mg	0	0
			1	1		
61	BP	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	DC	1	Total 1	Mg 1	0	0
61	CY	1	Total 1	Mg 1	0	0
61	B5	2	Total 2	Mg 2	0	0
61	BB	4	Total 4	Mg 4	0	0
61	AE	1	Total 1	Mg 1	0	0
61	DB	4	Total 4	Mg 4	0	0
61	D3	1	Total 1	Mg 1	0	0
61	BF	1	Total 1	Mg 1	0	0
61	AV	7	Total 7	Mg 7	0	0
61	DR	1	Total 1	Mg 1	0	0
61	AA	157	Total 157	Mg 157	0	0
61	BQ	1	Total 1	Mg 1	0	0
61	D7	1	Total 1	Mg 1	0	0
61	BC	1	Total 1	Mg 1	0	0
61	AM	1	Total 1	Mg 1	0	0
61	BU	1	Total 1	Mg 1	0	0
61	CN	1	Total 1	Mg 1	0	0
61	DD	2	Total 2	Mg 2	0	0
61	DH	1	Total 1	Mg 1	0	0
61	B3	1	Total 1	Mg 1	0	0
61	DX	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	DA	353	Total 353	Mg 353	0	0
61	B7	2	Total 2	Mg 2	0	0
61	AL	1	Total 1	Mg 1	0	0
61	D1	1	Total 1	Mg 1	0	0
61	BS	1	Total 1	Mg 1	0	0
61	CW	5	Total 5	Mg 5	0	0
61	D5	2	Total 2	Mg 2	0	0
61	BD	2	Total 2	Mg 2	0	0
61	AY	1	Total 1	Mg 1	0	0
61	CL	1	Total 1	Mg 1	0	0
61	BH	1	Total 1	Mg 1	0	0

- Molecule 62 is ZINC ION (three-letter code: ZN) (formula: Zn).

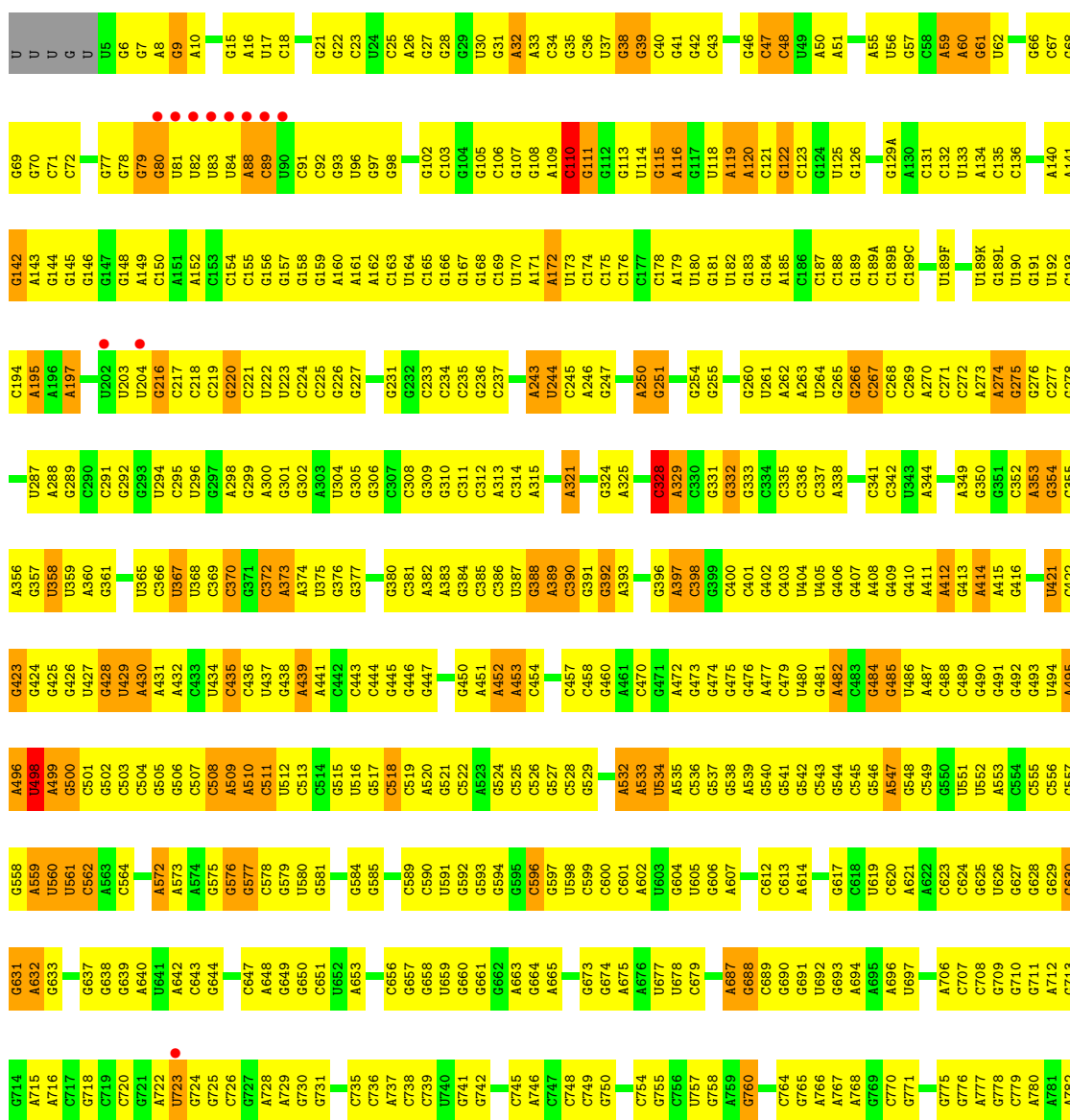
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	CN	1	Total 1	Zn 1	0	0
62	AN	1	Total 1	Zn 1	0	0
62	B9	1	Total 1	Zn 1	0	0
62	D9	1	Total 1	Zn 1	0	0
62	CD	1	Total 1	Zn 1	0	0
62	AD	1	Total 1	Zn 1	0	0

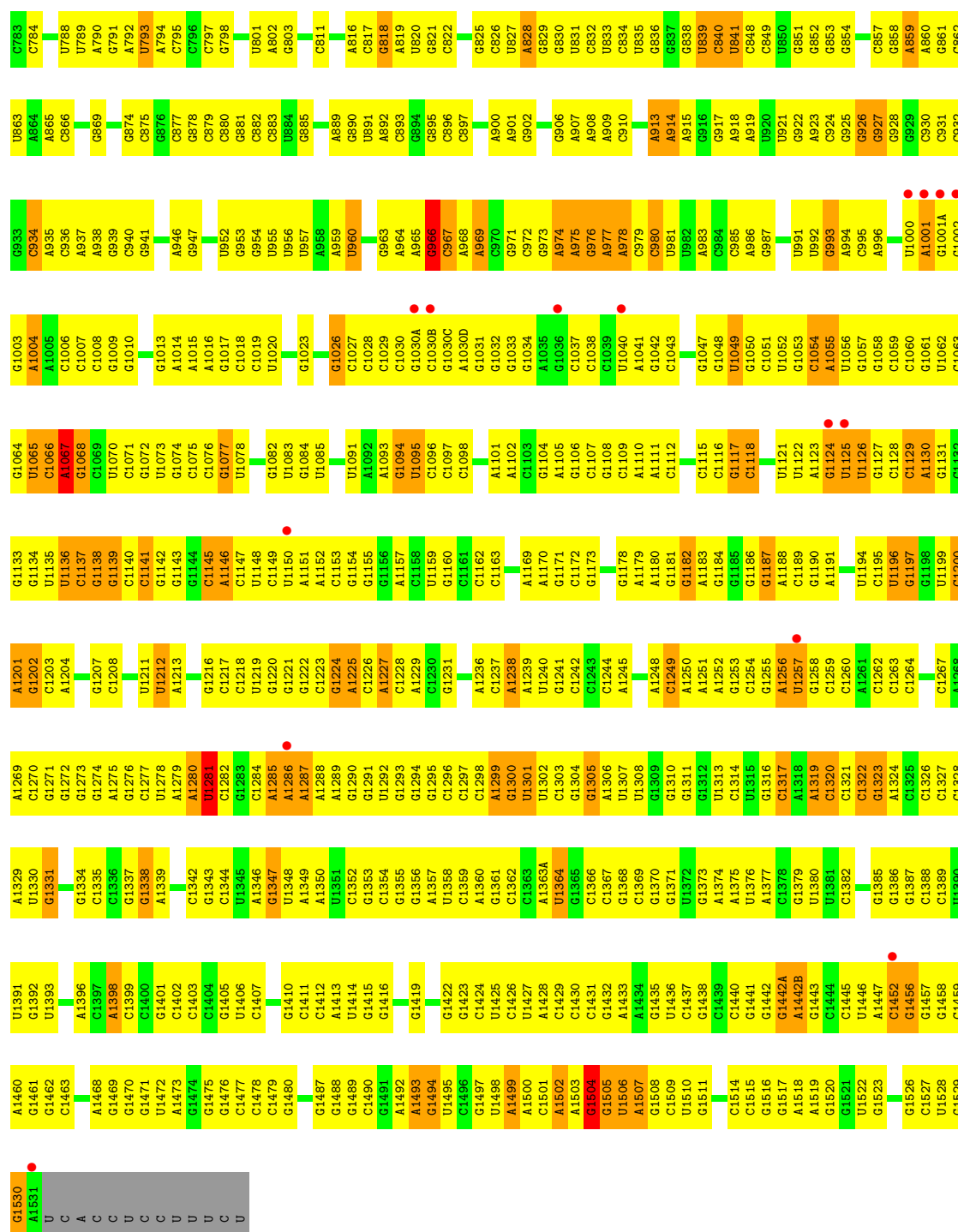
### 3 Residue-property plots

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

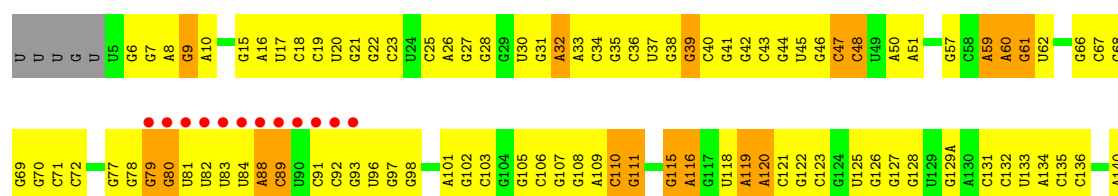
Chain AA: 



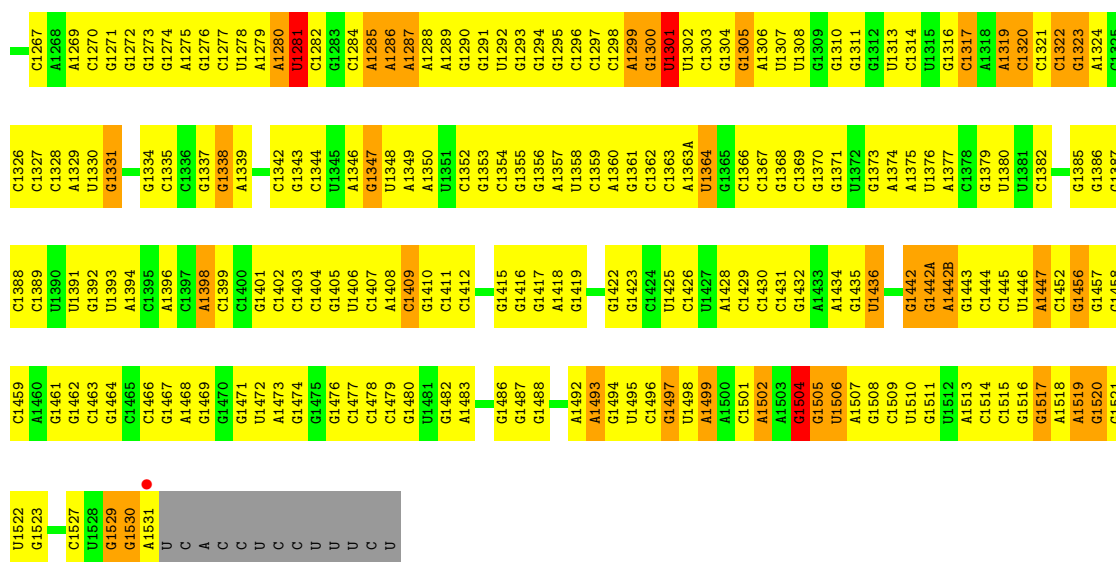


## • Molecule 1: 16S rRNA

Chain CA:

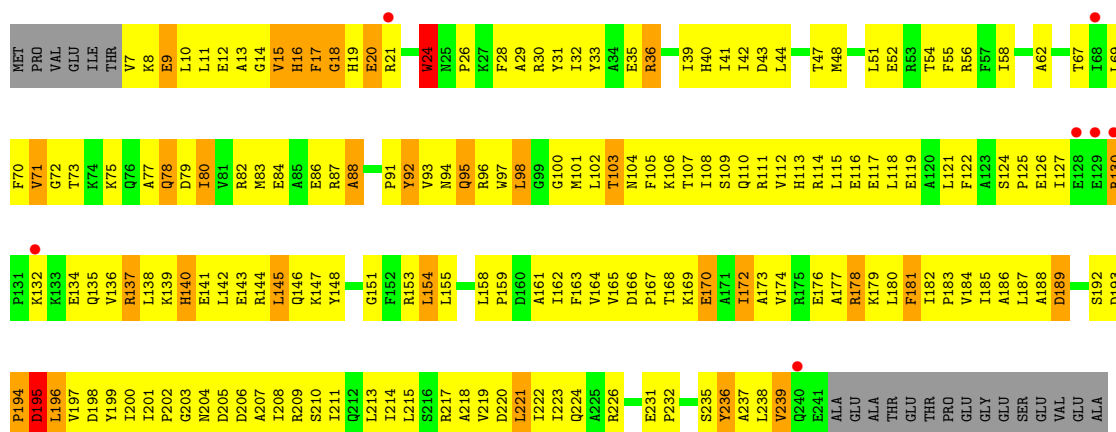






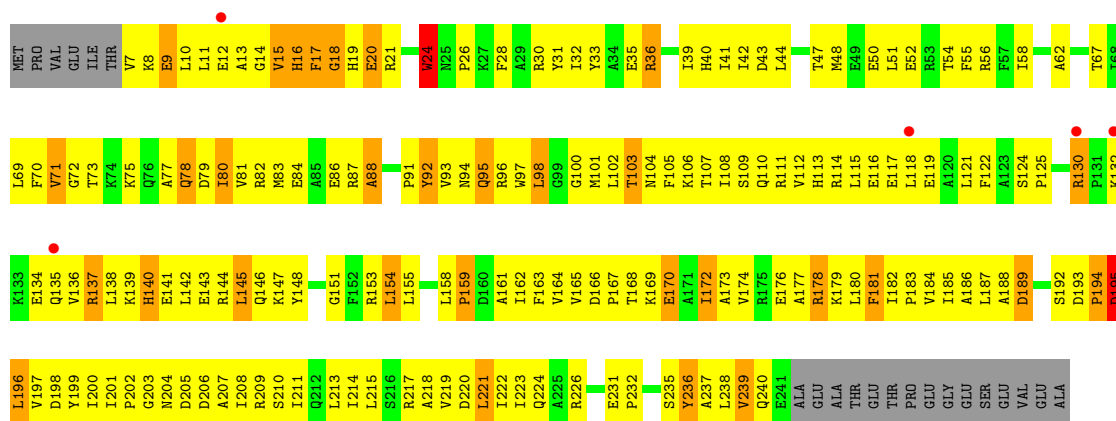
### • Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain AB:



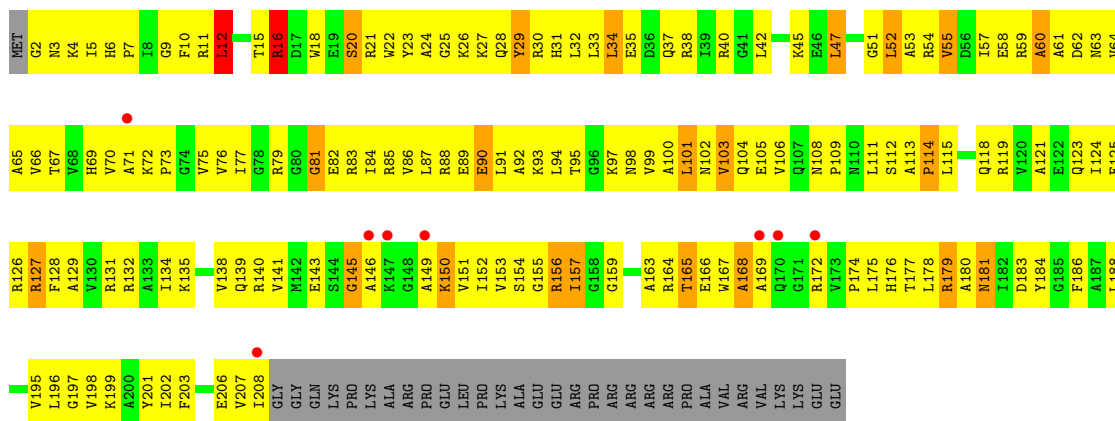
### • Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain CB:



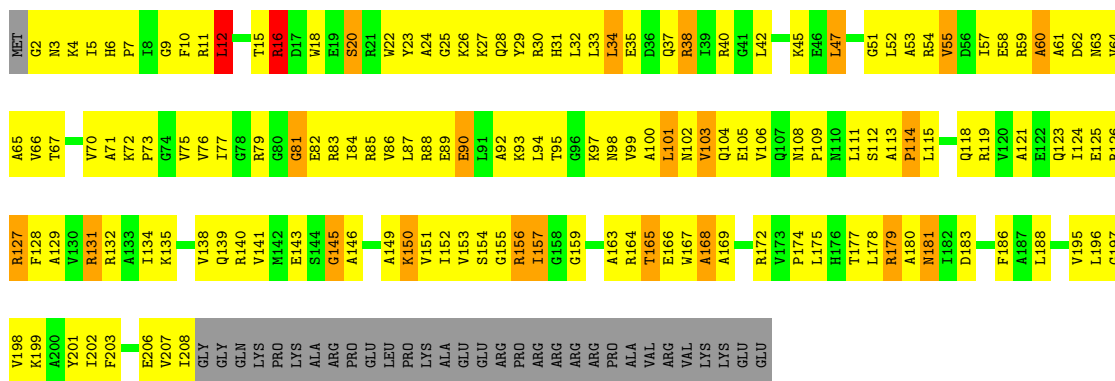
### • Molecule 3: 30S RIBOSOMAL PROTEIN S3

## Chain AC:



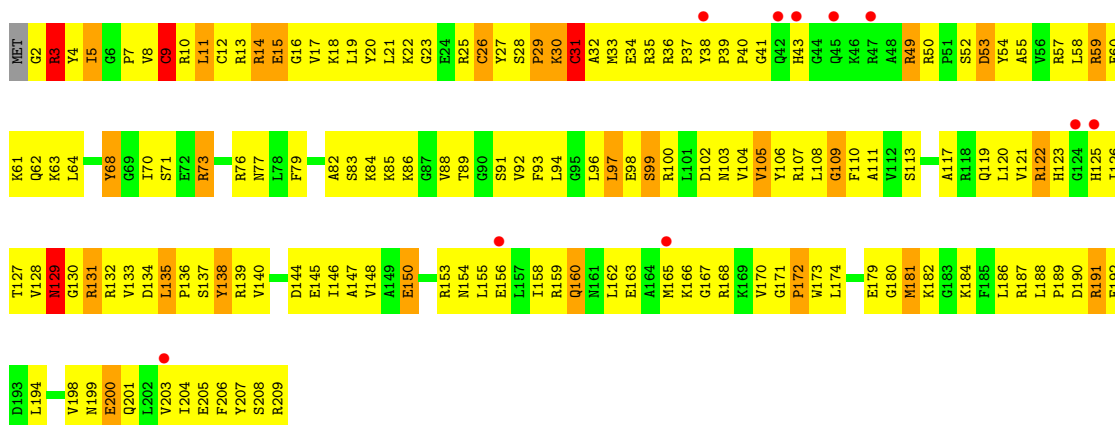
## • Molecule 3: 30S RIBOSOMAL PROTEIN S3

## Chain CC:



## • Molecule 4: 30S RIBOSOMAL PROTEIN S4

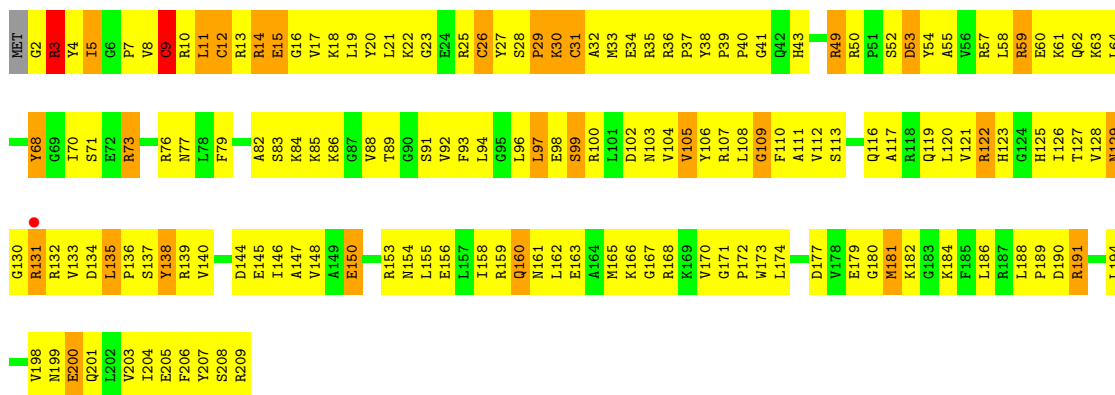
## Chain AD:



## • Molecule 4: 30S RIBOSOMAL PROTEIN S4

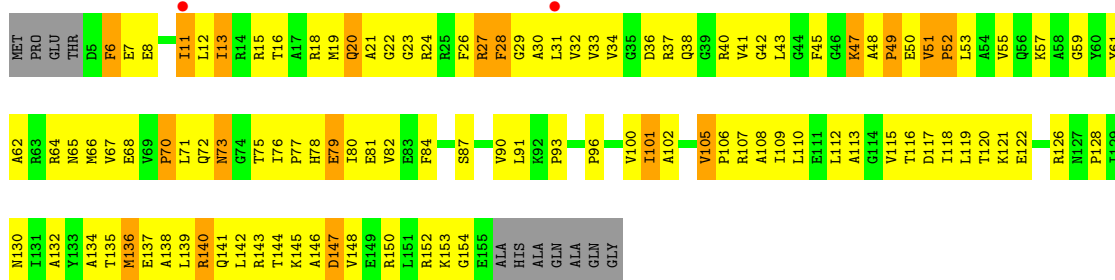
## Chain CD:





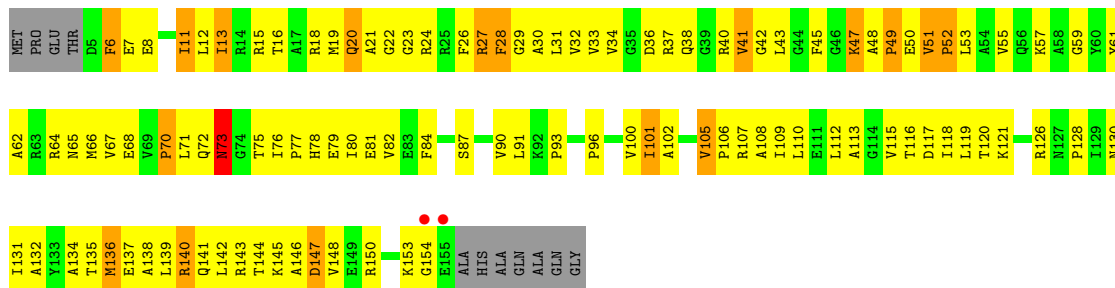
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain AE:



• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain CE:



• Molecule 6: 30S RIBOSOMAL PROTEIN S6

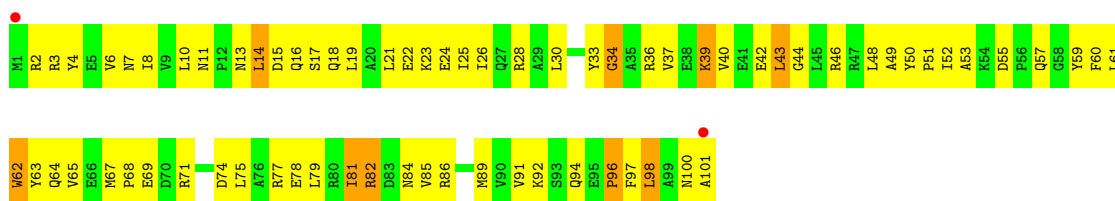
Chain AF:



• Molecule 6: 30S RIBOSOMAL PROTEIN S6

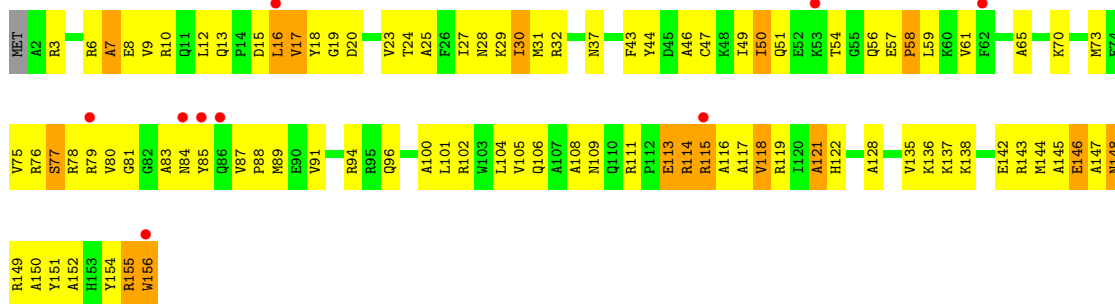
Chain CF:





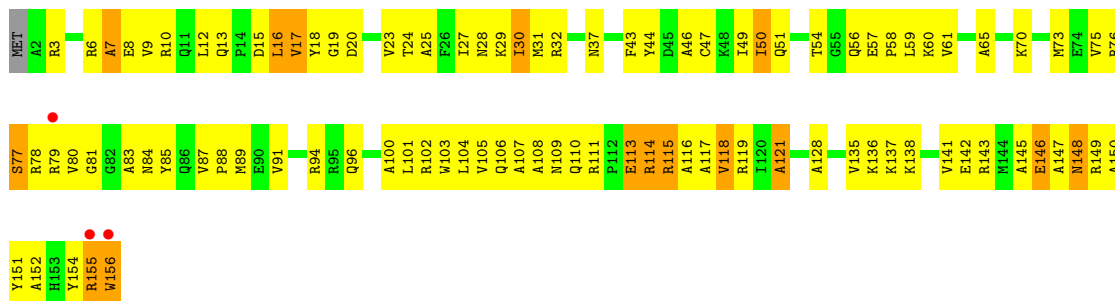
### • Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AG:



### • Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain CG:



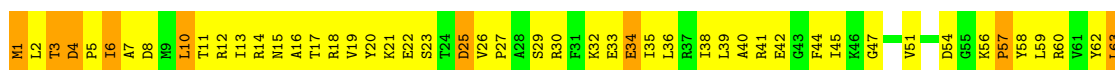
### • Molecule 8: 30S RIBOSOMAL PROTEIN S8

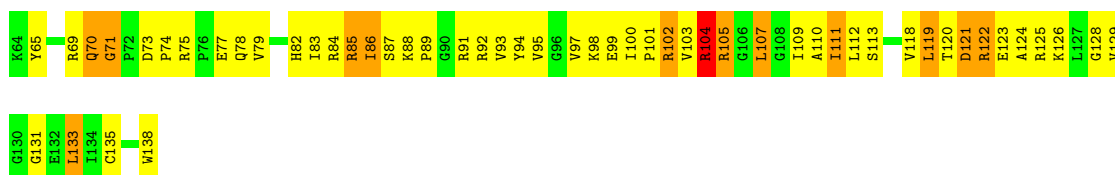
Chain AH:



### • Molecule 8: 30S RIBOSOMAL PROTEIN S8

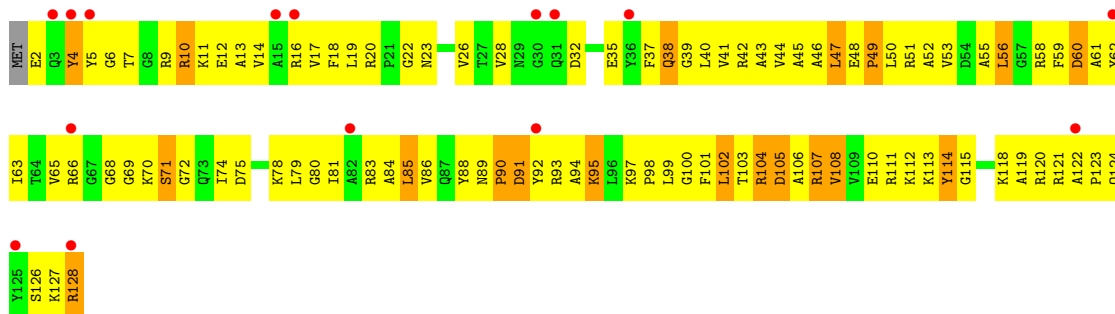
Chain CH:





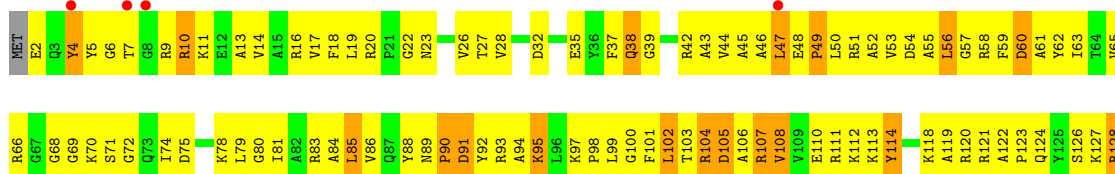
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AI:



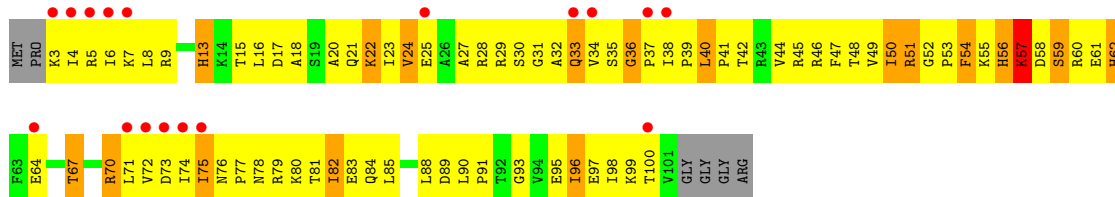
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CI:



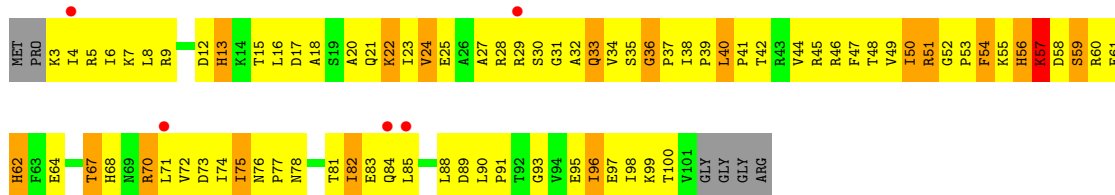
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AJ:



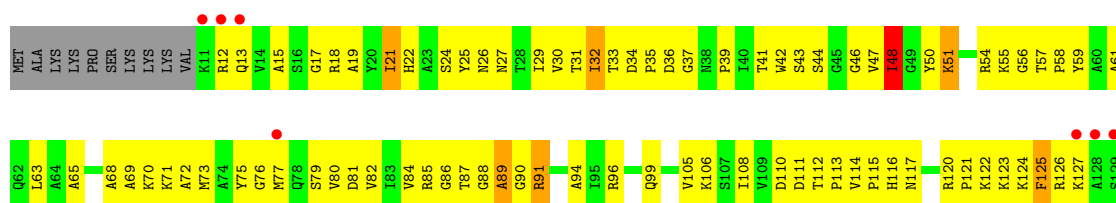
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain CJ:



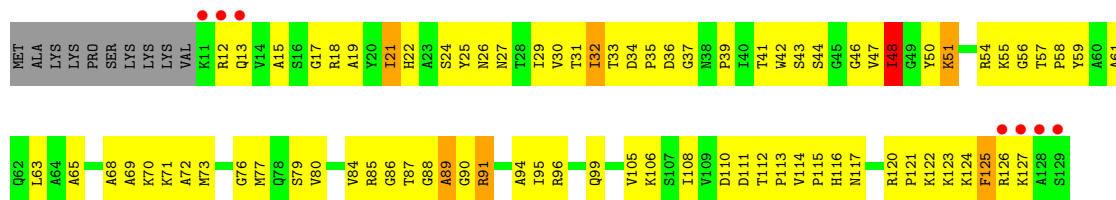
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AK:



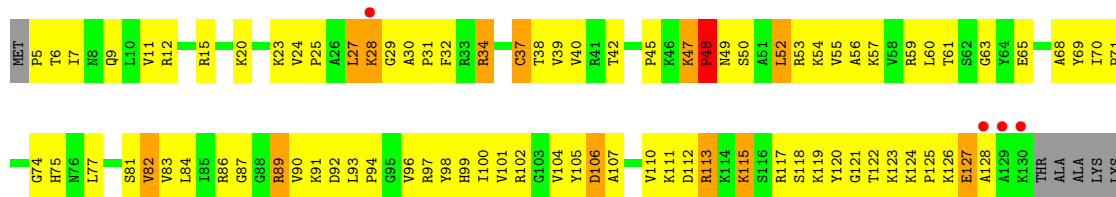
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain CK:



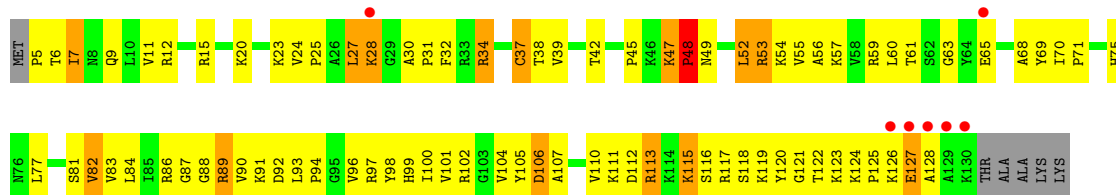
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AL:



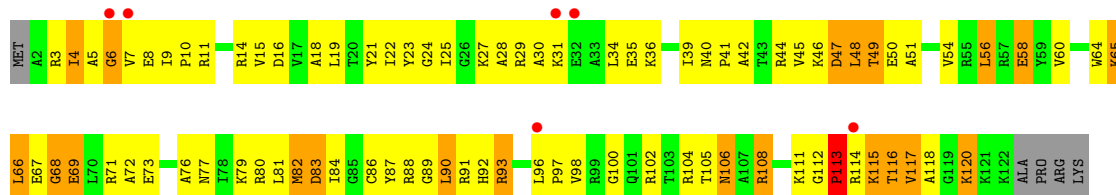
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

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:



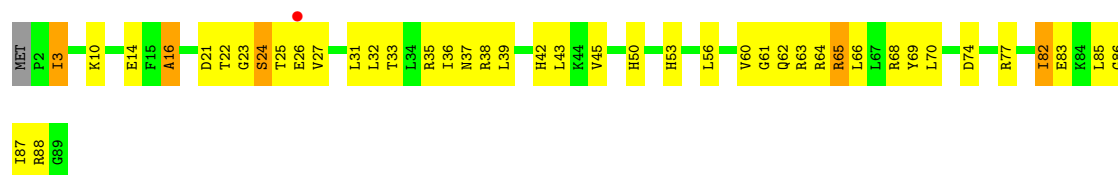
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain CN:



• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO:



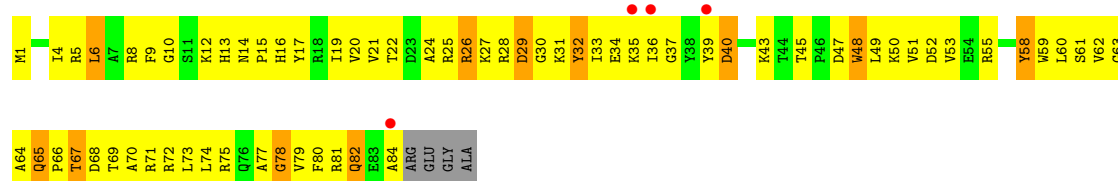
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CO:



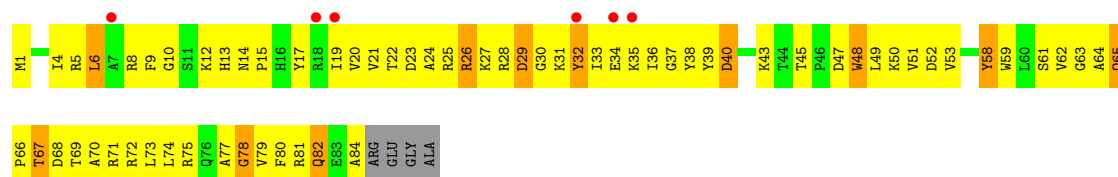
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP:



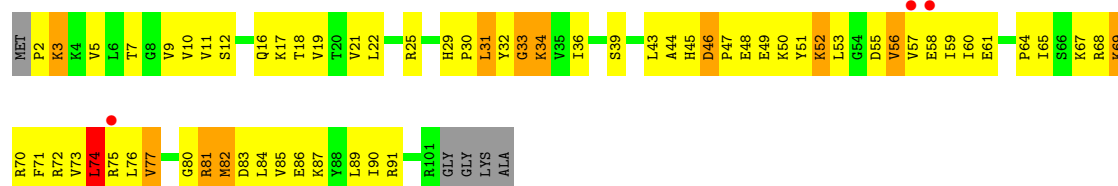
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CP:



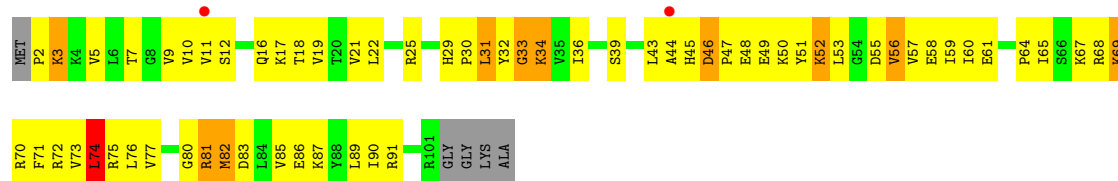
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ:



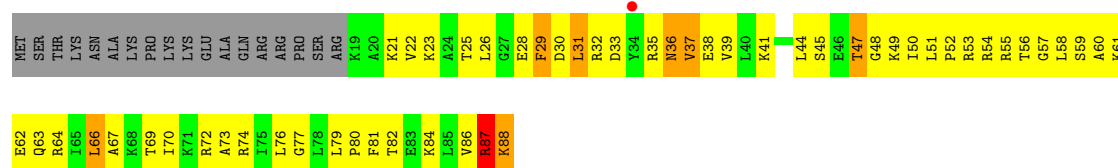
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CQ:



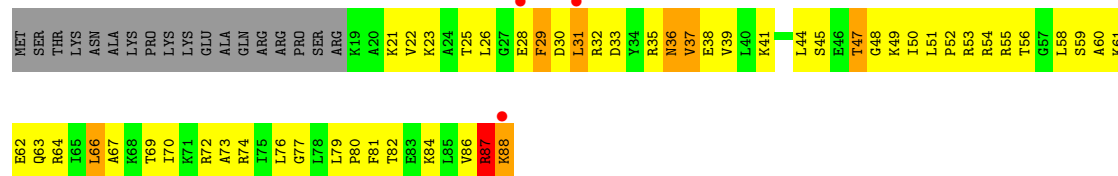
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR:



• Molecule 18: 30S RIBOSOMAL PROTEIN S18

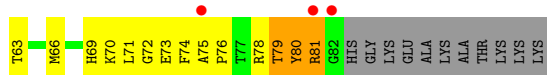
Chain CR:



• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AS:





• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain CS:



• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain AT:



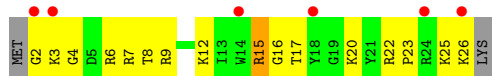
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain CT:



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AU:



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

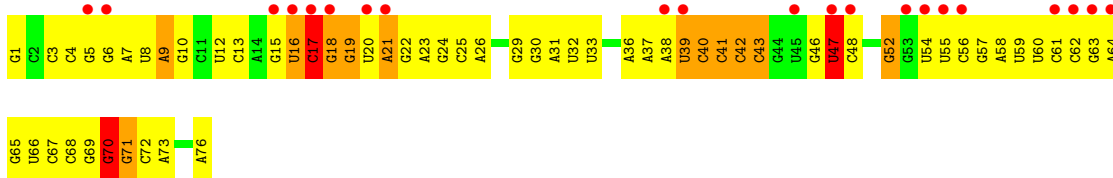
Chain CU:





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

Chain AW:



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

Chain CV:



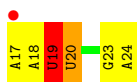
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE (UNMODIFIED BASES)

Chain CW:



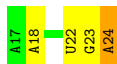
- Molecule 23: MRNA

Chain AX:



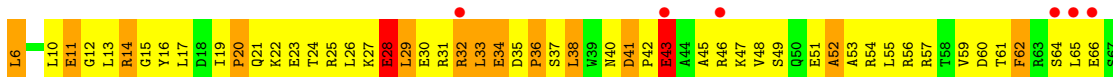
- Molecule 23: MRNA

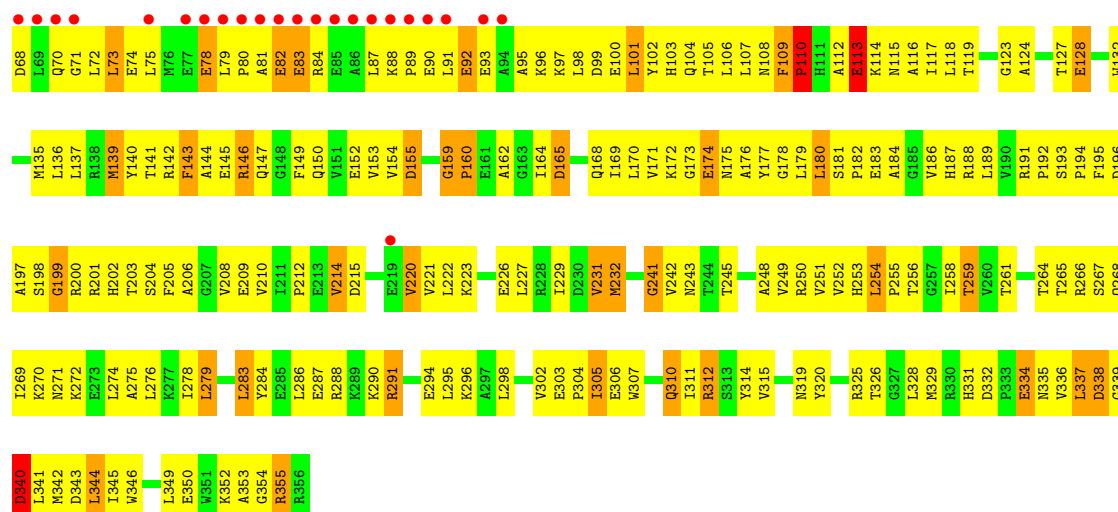
Chain CX:



- Molecule 24: PEPTIDE CHAIN RELEASE FACTOR 2

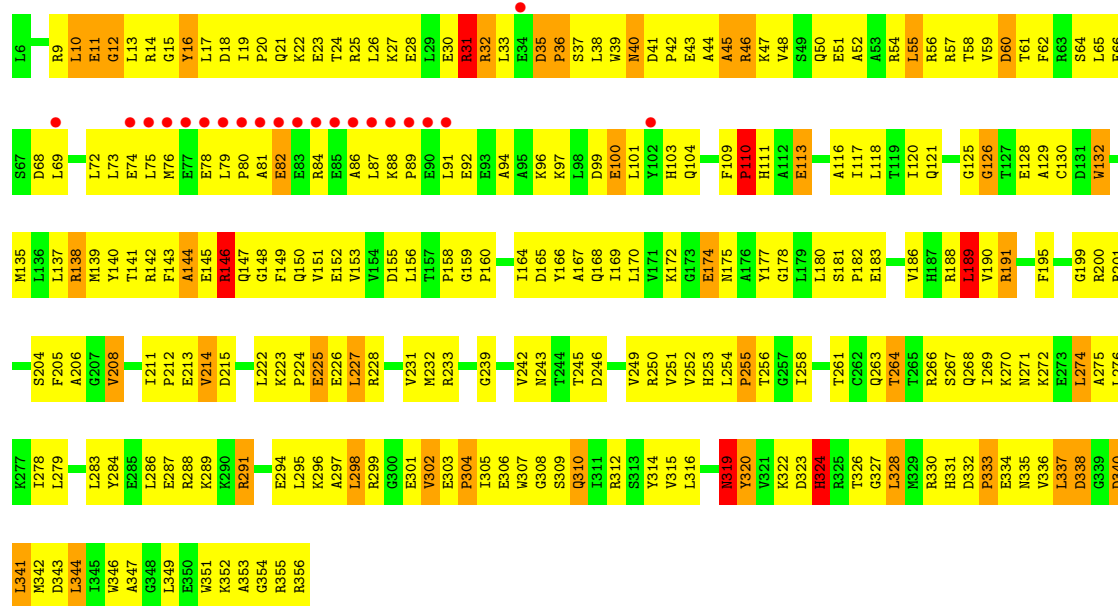
Chain AY:





### • Molecule 24: PEPTIDE CHAIN RELEASE FACTOR 2

Chain CY:



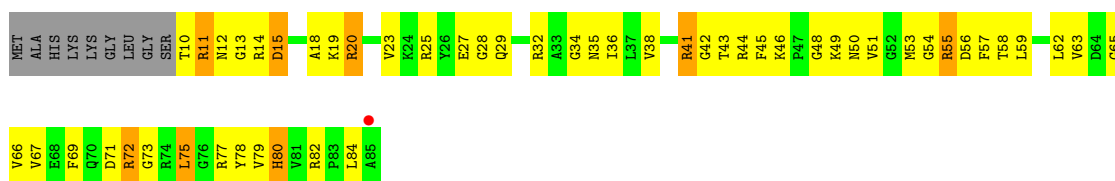
### • Molecule 25: 50S RIBOSOMAL PROTEIN L27

Chain B0:



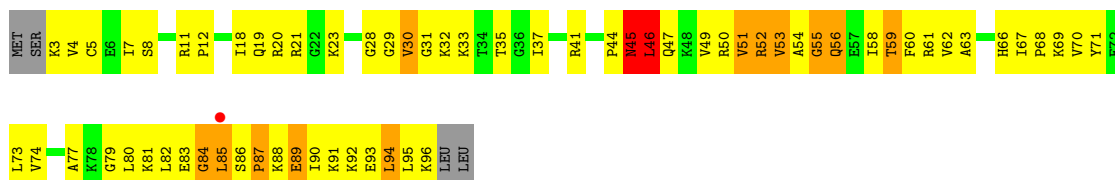
### • Molecule 25: 50S RIBOSOMAL PROTEIN L27

Chain D0:



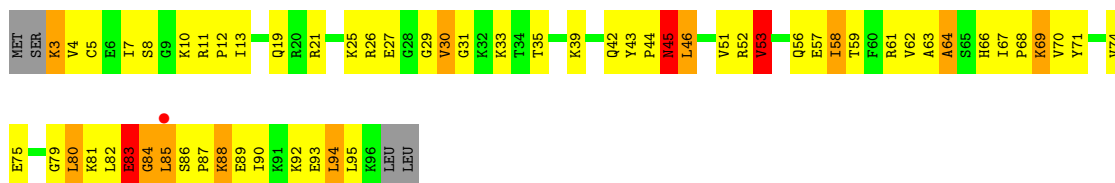
• Molecule 26: 50S RIBOSOMAL PROTEIN L28

Chain B1:



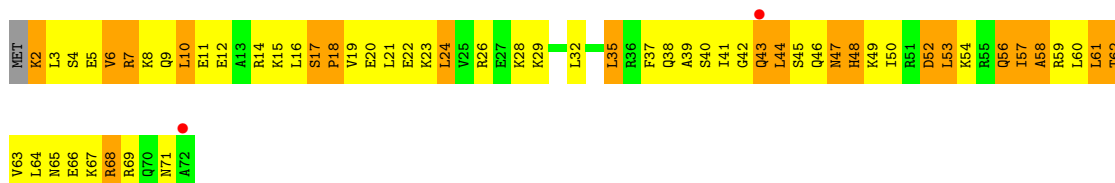
• Molecule 26: 50S RIBOSOMAL PROTEIN L28

Chain D1:



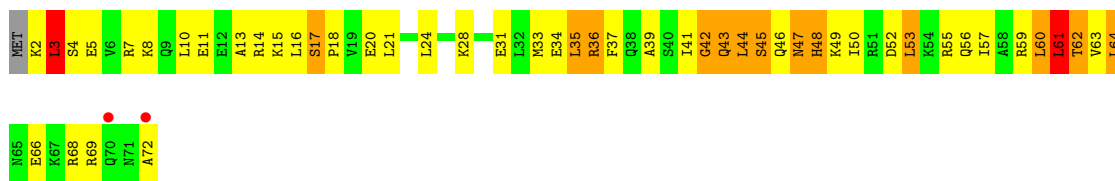
• Molecule 27: 50S RIBOSOMAL PROTEIN L29

Chain B2:



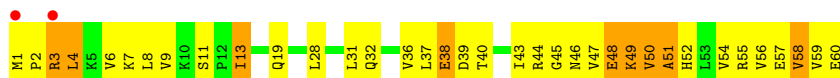
• Molecule 27: 50S RIBOSOMAL PROTEIN L29

Chain D2:



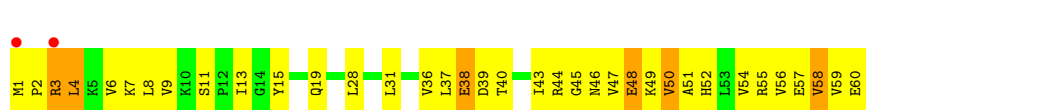
• Molecule 28: 50S RIBOSOMAL PROTEIN L30

Chain B3:



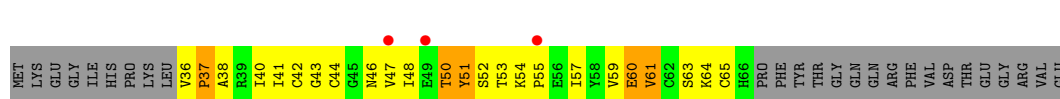
- Molecule 28: 50S RIBOSOMAL PROTEIN L30

Chain D3:



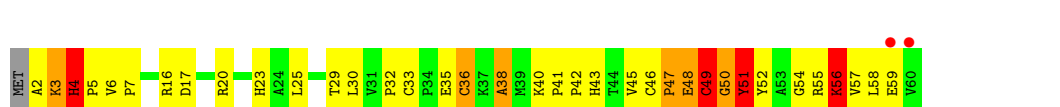
- Molecule 29: 50S RIBOSOMAL PROTEIN L31

Chain B4:



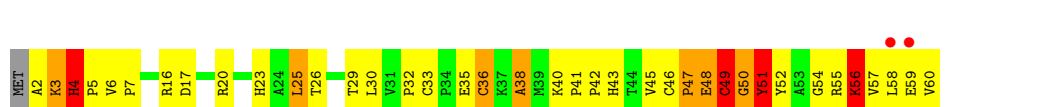
- Molecule 30: 50S RIBOSOMAL PROTEIN L32

Chain B5:



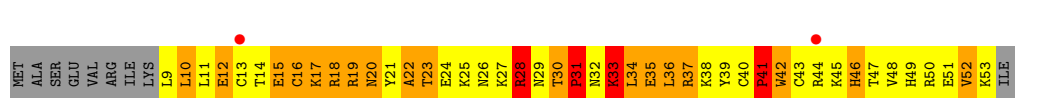
- Molecule 30: 50S RIBOSOMAL PROTEIN L32

Chain D5:



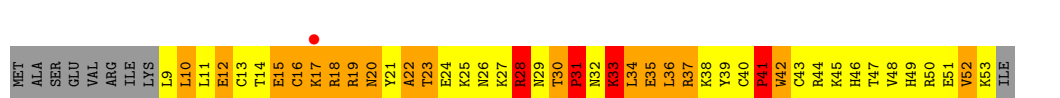
- Molecule 31: 50S RIBOSOMAL PROTEIN L33

Chain B6:



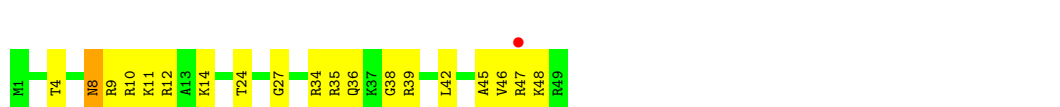
- Molecule 31: 50S RIBOSOMAL PROTEIN L33

Chain D6:



- Molecule 32: 50S RIBOSOMAL PROTEIN L34

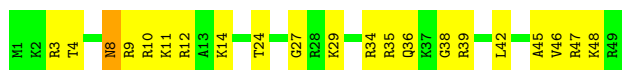
Chain B7:



- Molecule 32: 50S RIBOSOMAL PROTEIN L34

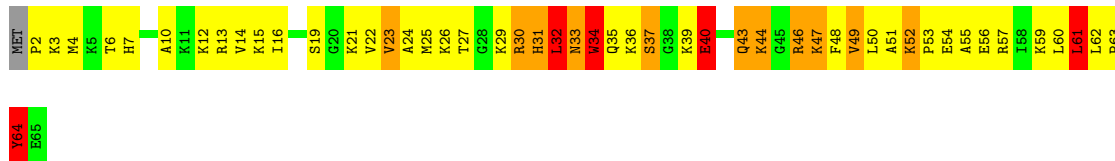
Chain D7:





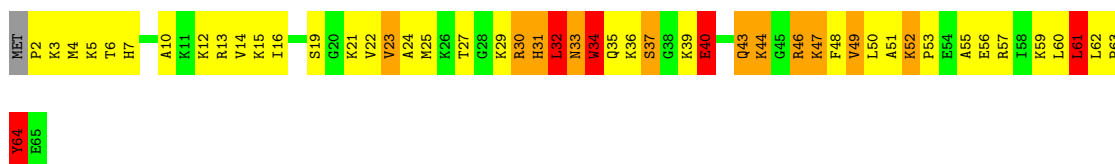
• Molecule 33: 50S RIBOSOMAL PROTEIN L35

Chain B8:



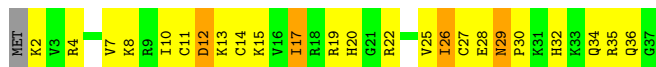
• Molecule 33: 50S RIBOSOMAL PROTEIN L35

Chain D8:



• Molecule 34: 50S RIBOSOMAL PROTEIN L36

Chain B9:



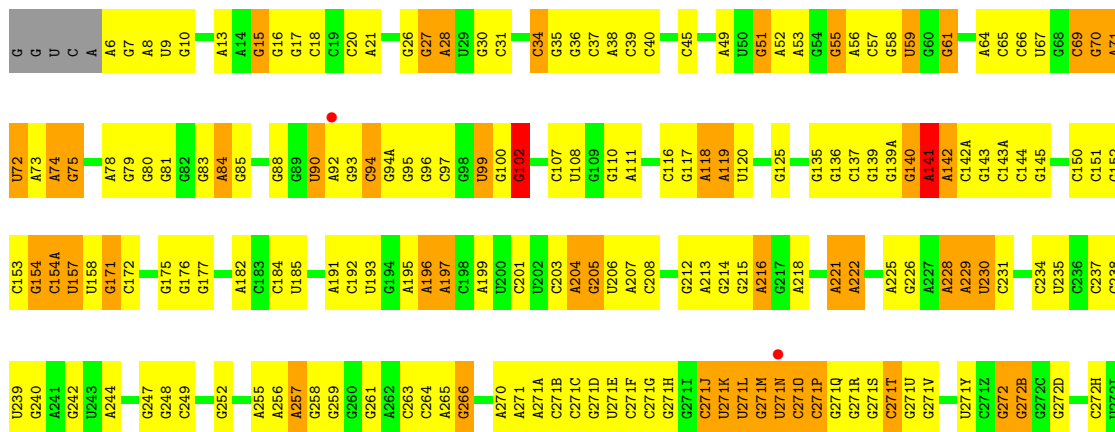
• Molecule 34: 50S RIBOSOMAL PROTEIN L36

Chain D9:



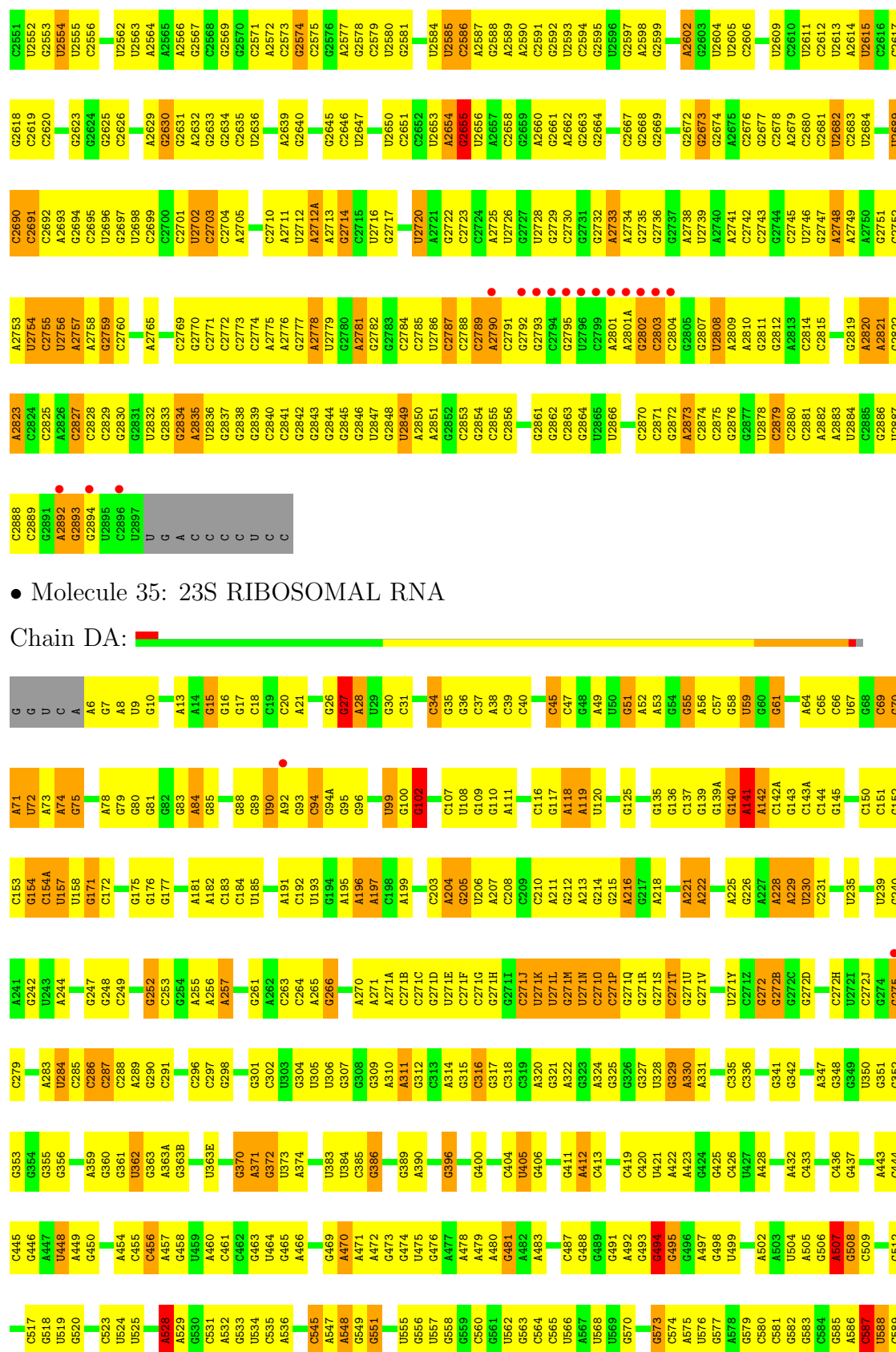
• Molecule 35: 23S RIBOSOMAL RNA

Chain BA:



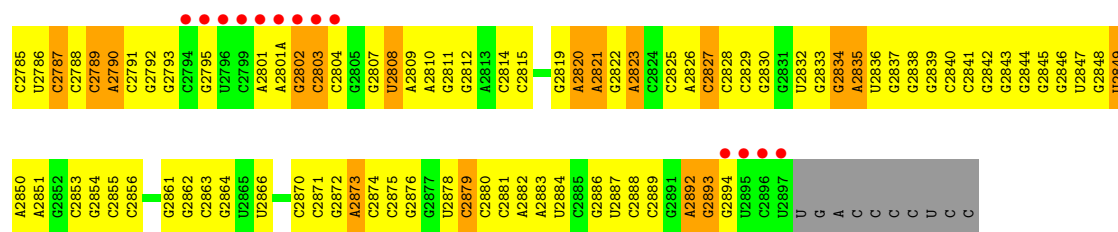
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A1127	A1128	A1129	U1130	U1061	G1063	C1064	U1065	U1066	U1067	G1068	A1069	A1070	G1071	C1072	C1075	C1076	A1077	U1078	C1079	C1080	U1081	U1082	C1153	G1154	A1155	A1156	G1157	C1158	U1159	G1160	C1161	G1162	G1163	A1164	U1165	C1166	U1167	G1168	G1169	G1170	C1101	U1101	C1102	A1103	C1104	G1105	G1106	C1107	U1108	A1179	C1180	C1181	G1110	A1111	G1112	C1116	C1117	C1118	G1125	A1126					
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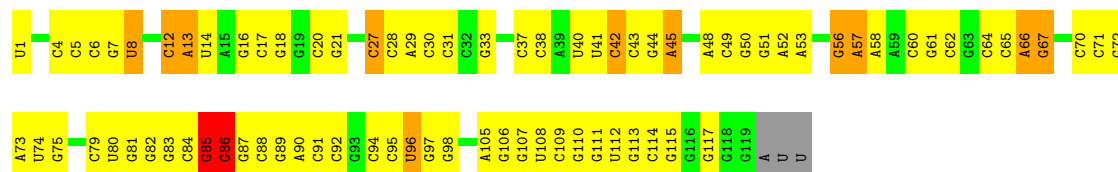
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C1506	C1505	G1508	U1438	G1369	C1289	G1192	A1128	G1063	C995	U922	G851	G785	C708	G654B	G592
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C1584	G1510	G1509B	C1446	C1376	C1298	G1203	G1136	U1069	A1001	G928	C857	G791	U714	G654H	G601
U1582	C1511	C1511	U1378	G1377	G1299	A1204	G1137	A1070	G1002	G929	G858	G792	A716	G654I	A603
A1587	U1512	U1512	A1378	A1301	U1300	U1205	U1141	G1071	C1006	A933	G862	A793	G717	G654J	G604
C1588	C1513	C1513	G1380	A1302	A1302	C1208	U1142	C1072			A863	G794	A718	G654K	G605
C1589	U1514	U1514	G1381			G1209	A1143	C1075	U1010	A941	G864	G795	C719	G654L	U606
U1590	G1515	G1515	G1382			U1210	C1144	U1077	U1012	G942	A865	G796	G720	G654M	U607
G1591	C1516	C1516	U1383			G1211	C1145	U1078	U1013	U943	A870	G797	A722	G654N	A608
G1595	U1517	U1517	G1384			G1212	C1146	C1079	U1014	G944	A871	G798	G723	G654O	G610
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A1597	G1519	G1519	G1386			A1220	A1148	U1081	G1016			G800	G725	G654Q	C612
C1598	G1520	G1520	U1387			C1221	C1149	U1082	U1017	C951	U877	A801	G729	G654R	G613
C1599	U1523	U1523	G1388			G1223	G1150	A1088	C1018	G952	A878	G802	C730	G654S	U614
G1600	G1524	G1524	G1389			U1226	C1151	A1088	U1019	A953	G879	G803	C731	A654V	G614B
G1601	G1525	G1525	U1390			G1227	C1152	U1088	U1020	G954	G880	G804	G732	A655	A614C
G1602	C1526	C1526	U1391			G1235	C1153	U1088	U1021	C955	G881	G805	G733	G656	G615
A1603	G1527	G1527	C1392			C1236	G1154	U1088	U1022	G956	G882	G806	G734	U657	
A1607	C1528	A1528A	A1321			U1240	A1155	U1088	U1023	G957	G883	G807	U740	C658	G620
A1609	G1529	G1529	G1393			C1250	A1156	U1090	U1024	A958	G884	G808	G741	G659	A621
A1610	C1530	C1530	C1394			G1257	G1157	U1091	G1025	U959	C885	G809	G742	G660	G622
A1614	C1531	C1531	U1395			U1234	C1158	U1092	U1026	A960	C886	G814	G743	G661	G623
A1615	G1532	G1532	U1396			G1235	U1159	U1093	U1027	C961	A887	G815	G744	G662	C624
A1616	C1533	C1533	U1397			U1240	G1160	U1094	U1028	G962	C888	G819	U747	G665	G625
A1618	G1534	G1534	U1398			C1242	C1161	U1095	U1029	A963	C889	A820	U626	G666	U626
G1624	C1535	C1535	U1399			A1242	G1162	U1097	G1030	C964	A890	A821	A752	C671	G630
G1625	U1536	U1536	U1335			G1248	G1165	U1098	G1034	C970	C893	G825	G753	G672	A631
G1626	A1537	A1537	A1336			U1249	C1166	C1100	U1035	C971	C894	U826	C754	G673	A632
A1637	C1538	C1538	G1337			C1251	U1167	U1101	G1036		U895	U827	C755	G674	A633
A1639	U1539	U1539	G1338			G1252	G1168	U1102	G1037	G974	A896	U828	C756	A675	C634
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G1644	U1543	U1543	G1342			C1257	U1172	U1106	C1043	G977	C902	G832	G765	G682	G638
G1647	C1544	C1544	U1343			U1271	U1173	U1107	G1044	G978	C903	U833	C766	G683	U639
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A1654	U1549	U1549	U1348			G1276	U1178	U1112	C1049	A983	A910	U839	U774	G697	A646
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A1658	G1551	G1551	C1350			G1279	G1183	U1114	G1051	C986	C912	A841	G775	G698	G648
A1659	C1552	C1552	U1351			U1280	G1184	U1115	C1052	U913	U913	G699	G776	G699	G649
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A1661	C1554	C1554	U1353			U1282	G1186	U1117	G1055	C989	G916	G845	U780	G701	C651
A1662	U1555	U1555	G1354			U1286	U1187	U1118	G1056	C991	A917	G846	A781	G703	G652
A1663	C1556	C1556	U1355			A1286	U1188	U1119	A1057	C992	A918	G847	A782	A705	A653
A1664	U1557	U1557	A1356				A1189	G1120	G1058		G919	G848			
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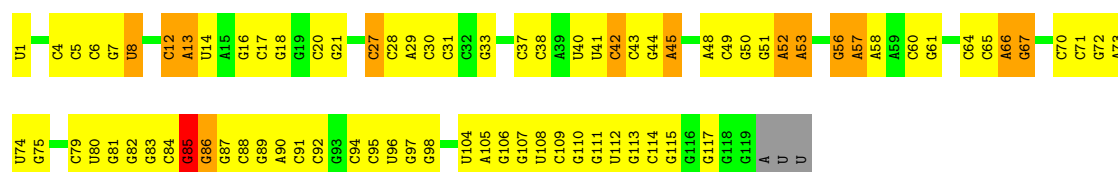
• Molecule 36: 5S RIBOSOMAL RNA

Chain BB:



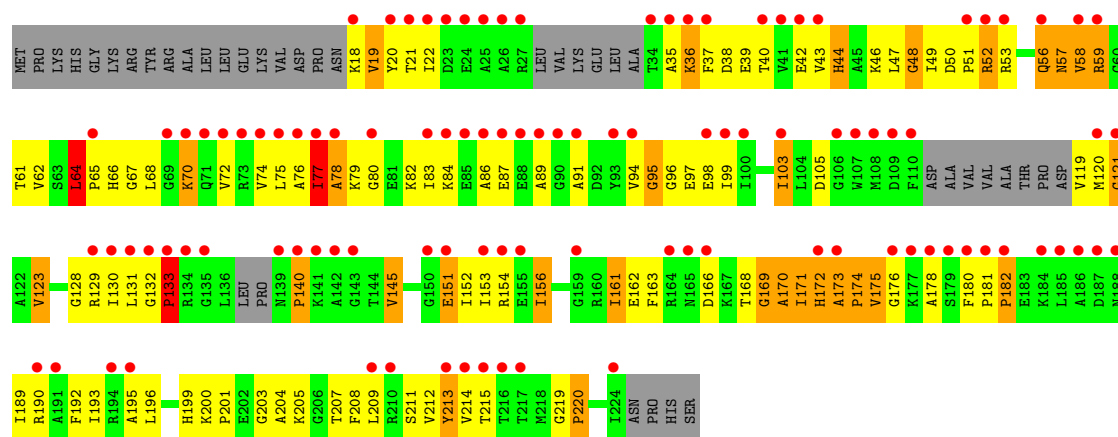
• Molecule 36: 5S RIBOSOMAL RNA

Chain DB:



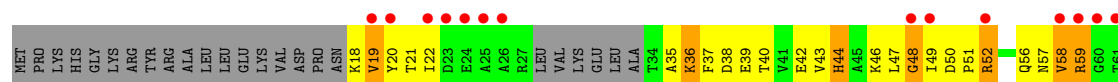
• Molecule 37: 50S RIBOSOMAL PROTEIN L1

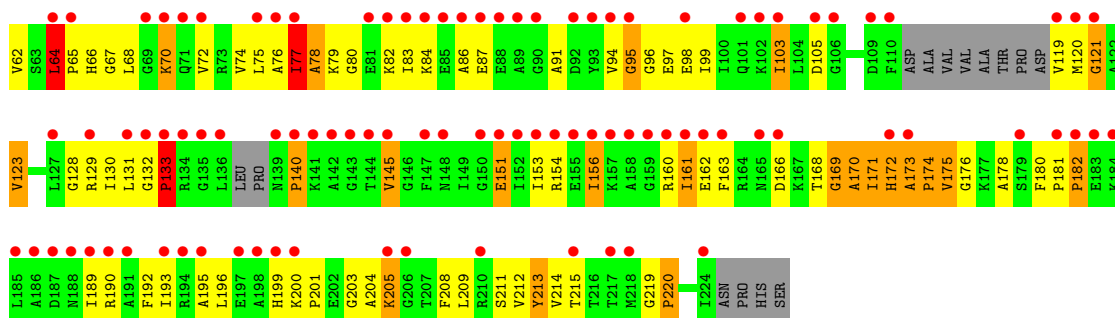
Chain BC:



• Molecule 37: 50S RIBOSOMAL PROTEIN L1

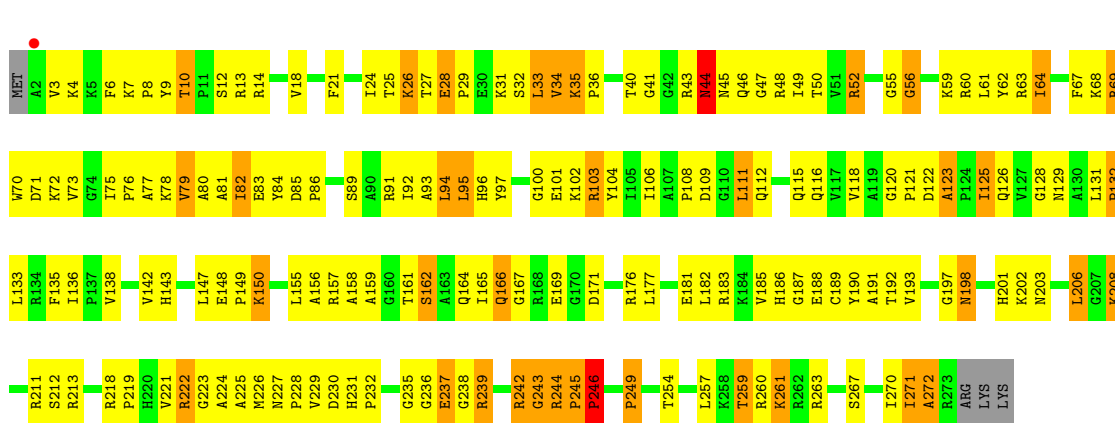
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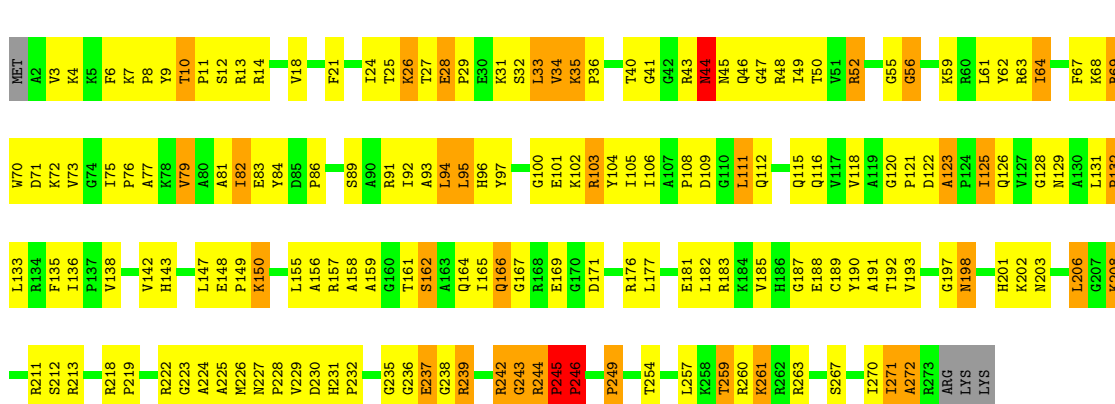
• Molecule 38: 50S RIBOSOMAL PROTEIN L2

Chain BD:



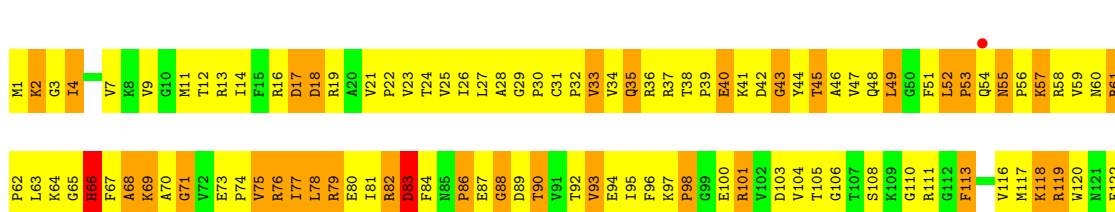
• Molecule 38: 50S RIBOSOMAL PROTEIN L2

Chain DD:

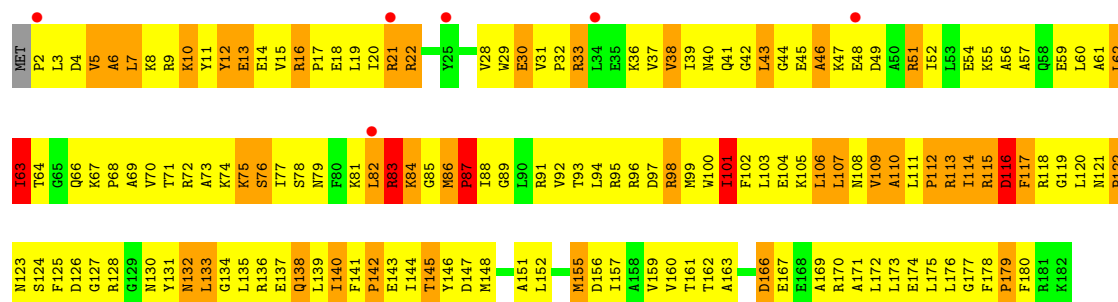


• Molecule 39: 50S RIBOSOMAL PROTEIN L3

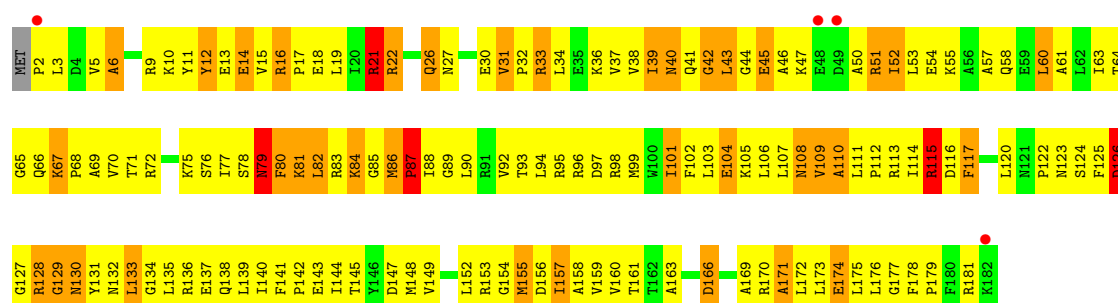
Chain BE:



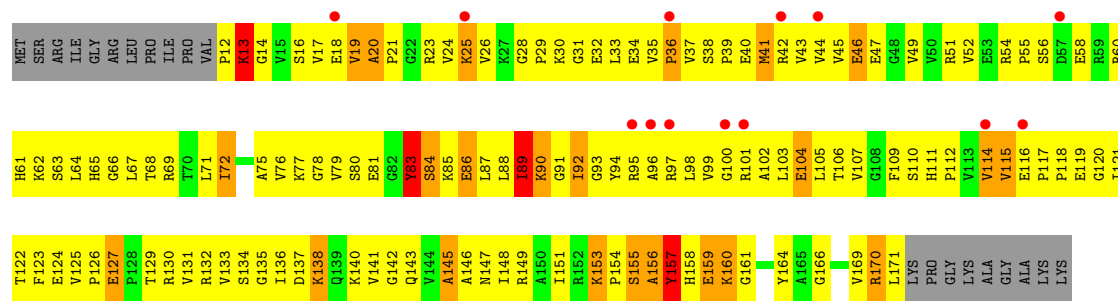


Chain BG: 

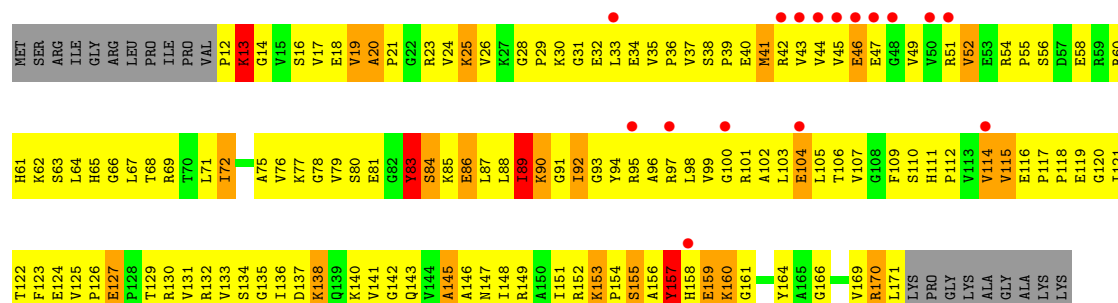
- Molecule 41: 50S RIBOSOMAL PROTEIN L5

Chain DG: 

- Molecule 42: 50S RIBOSOMAL PROTEIN L6

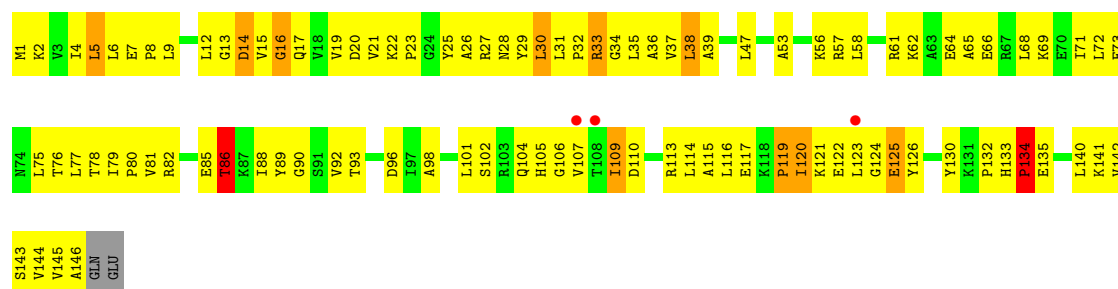
Chain BH: 

- Molecule 42: 50S RIBOSOMAL PROTEIN L6

Chain DH: 

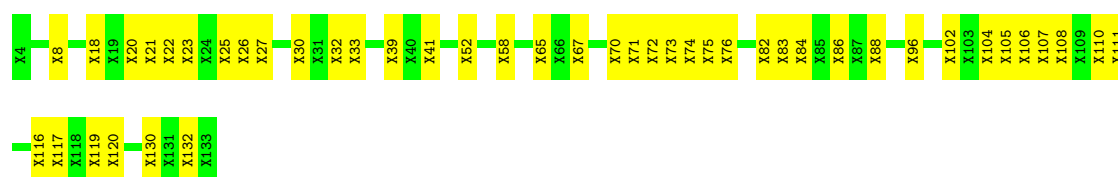
- Molecule 43: 50S RIBOSOMAL PROTEIN L9

Chain BI:



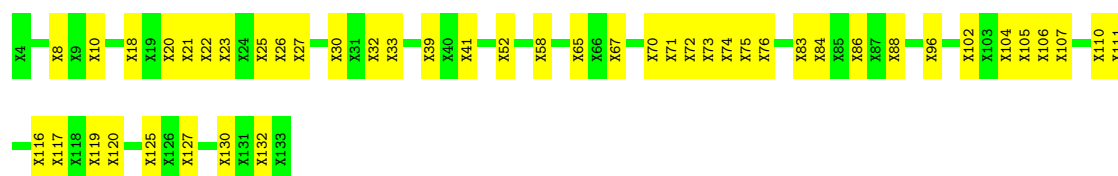
- Molecule 44: 50S RIBOSOMAL PROTEIN L10

Chain BJ:



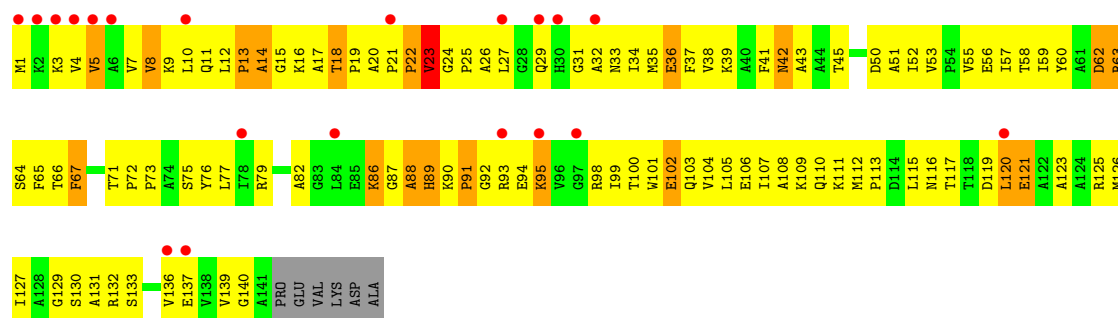
- Molecule 44: 50S RIBOSOMAL PROTEIN L10

Chain DJ:



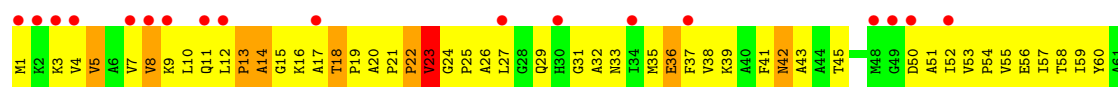
- Molecule 45: 50S RIBOSOMAL PROTEIN L11

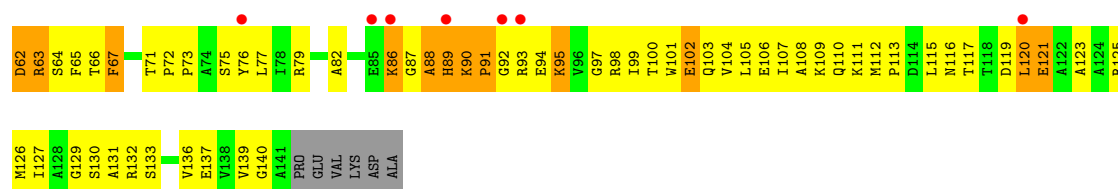
Chain BK:



- Molecule 45: 50S RIBOSOMAL PROTEIN L11

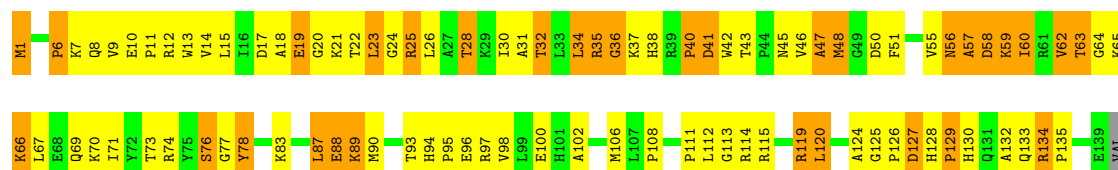
Chain DK:





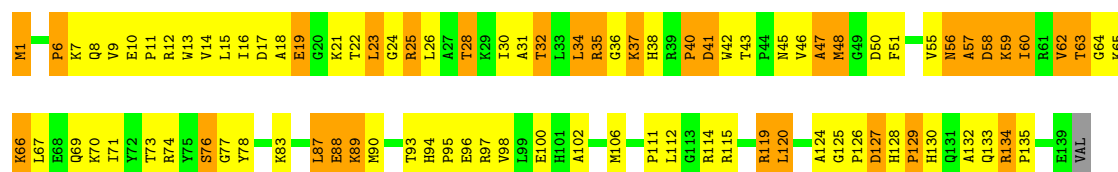
• Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain BN:



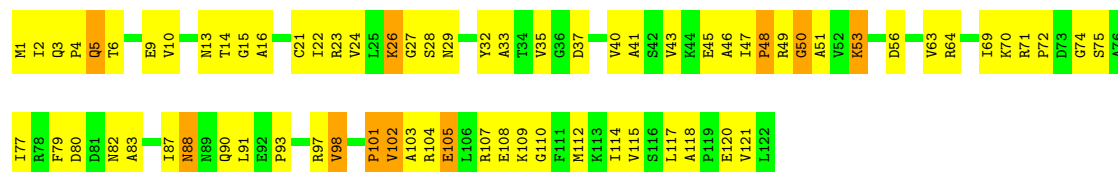
• Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain DN:



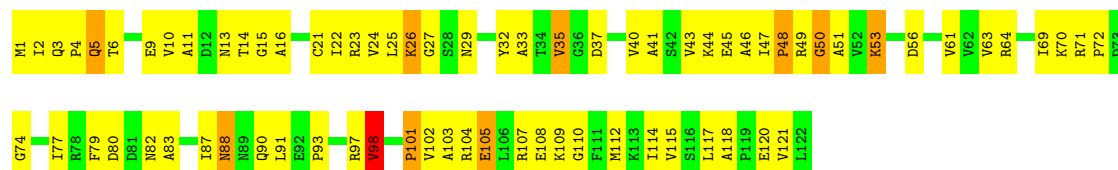
• Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain BO:



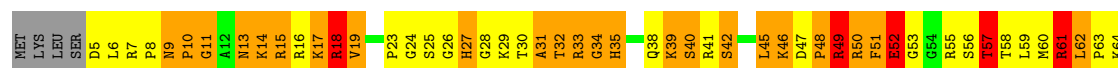
• Molecule 47: 50S RIBOSOMAL PROTEIN L14

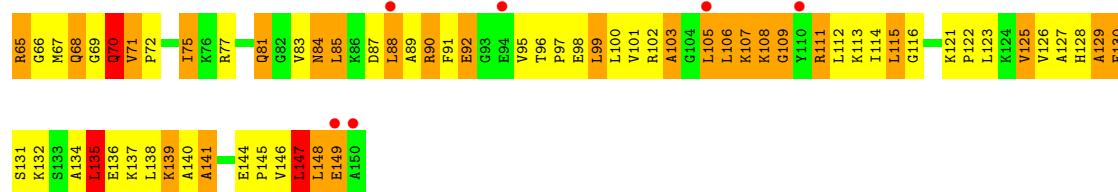
Chain DO:



• Molecule 48: 50S RIBOSOMAL PROTEIN L15

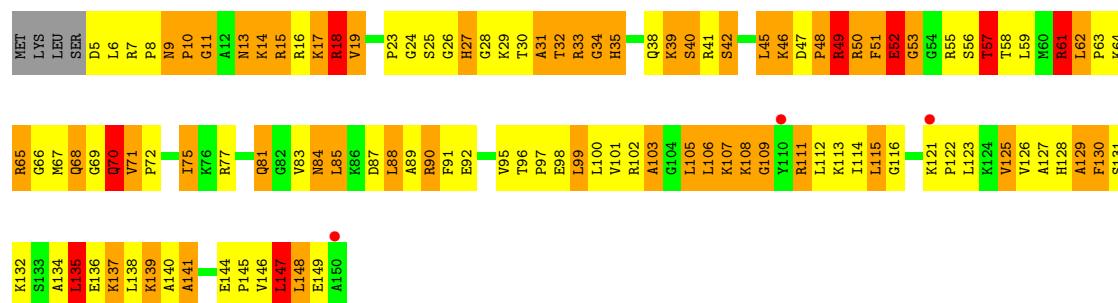
Chain BP:





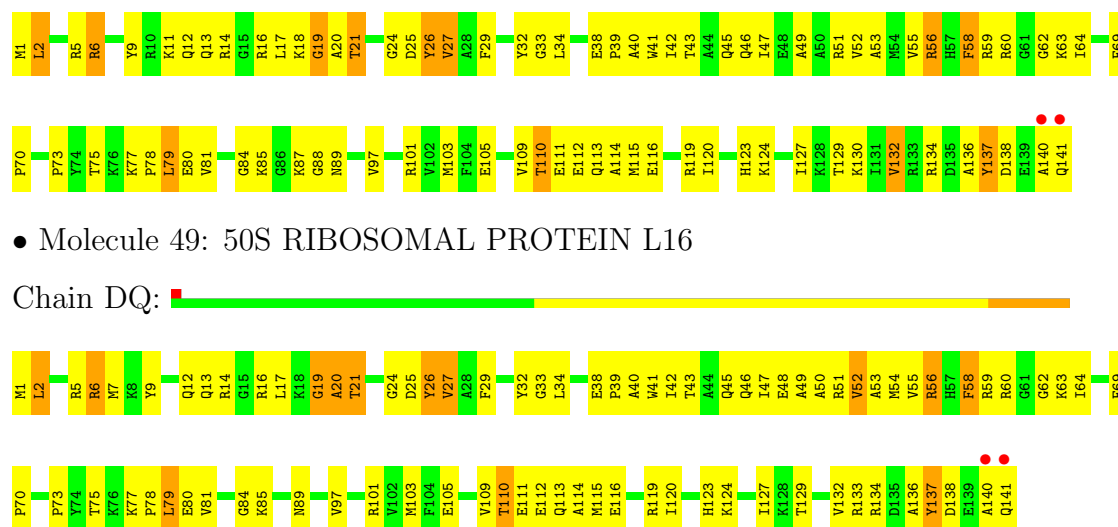
• Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain DP:



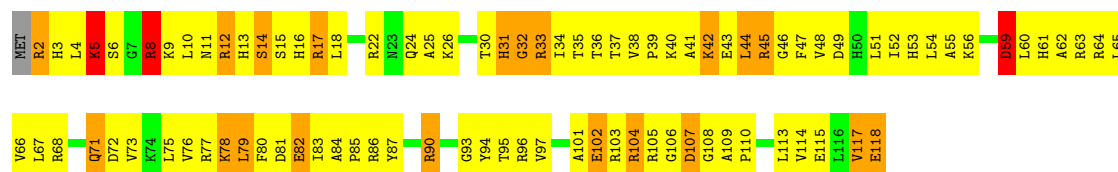
• Molecule 49: 50S RIBOSOMAL PROTEIN L16

Chain BQ:



• Molecule 50: 50S RIBOSOMAL PROTEIN L17

Chain BR:



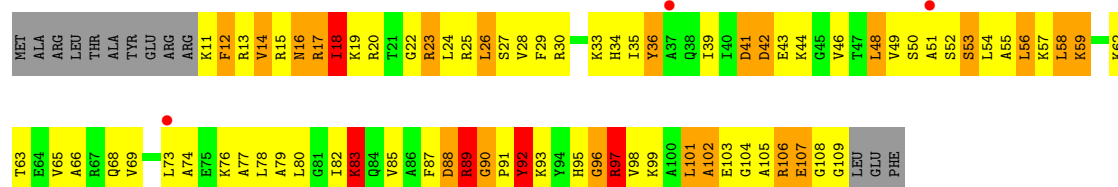
• Molecule 50: 50S RIBOSOMAL PROTEIN L17

Chain DR:



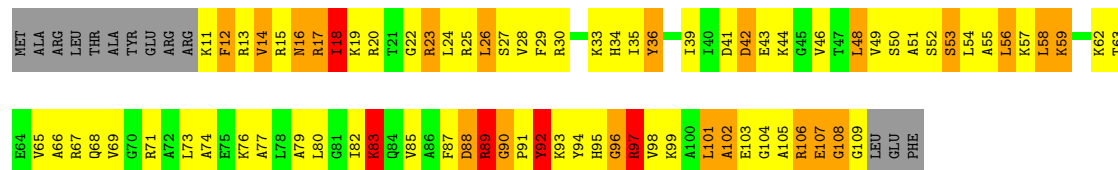
• Molecule 51: 50S RIBOSOMAL PROTEIN L18

Chain BS:



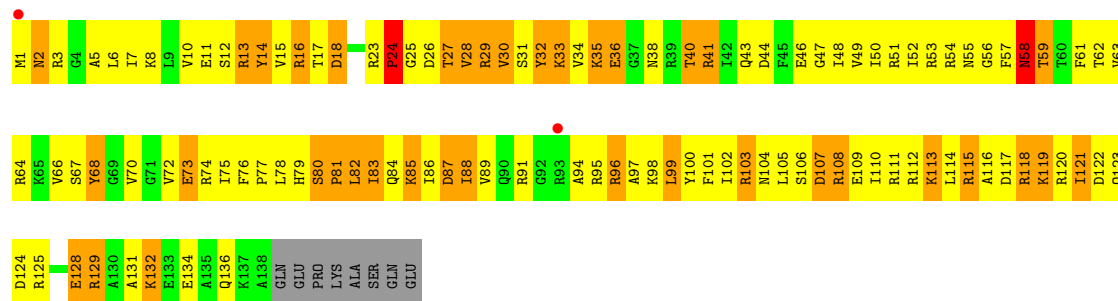
• Molecule 51: 50S RIBOSOMAL PROTEIN L18

Chain DS:



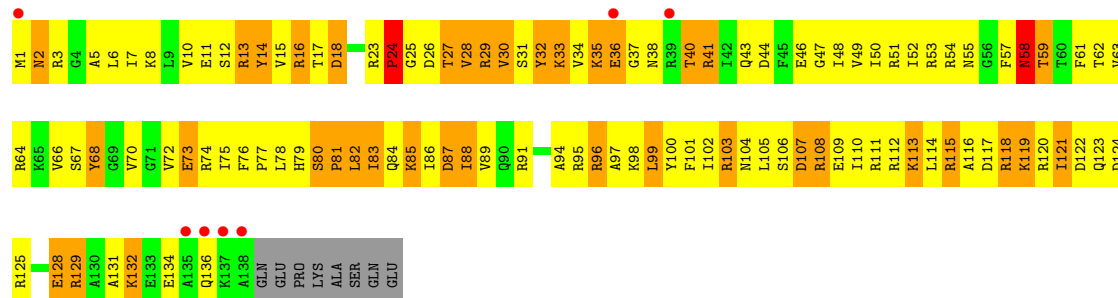
• Molecule 52: 50S RIBOSOMAL PROTEIN L19

Chain BT:



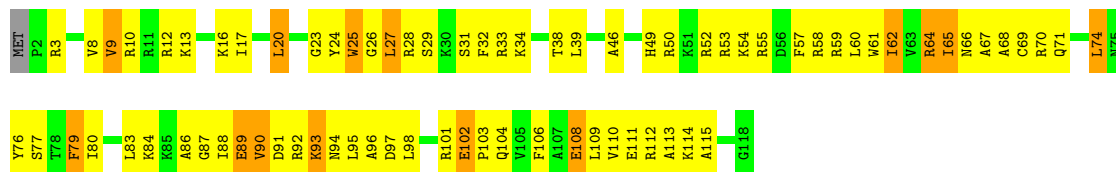
• Molecule 52: 50S RIBOSOMAL PROTEIN L19

Chain DT:



- Molecule 53: 50S RIBOSOMAL PROTEIN L20

Chain BU:



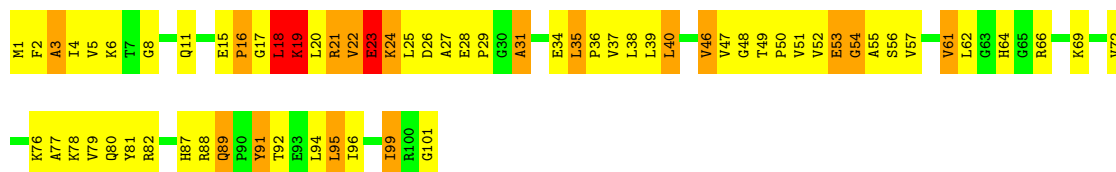
- Molecule 53: 50S RIBOSOMAL PROTEIN L20

Chain DU:



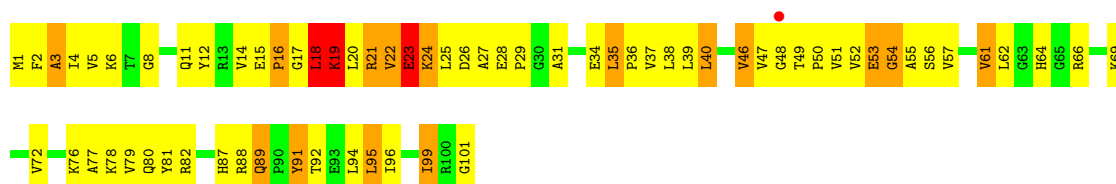
- Molecule 54: 50S RIBOSOMAL PROTEIN L21

Chain BV:



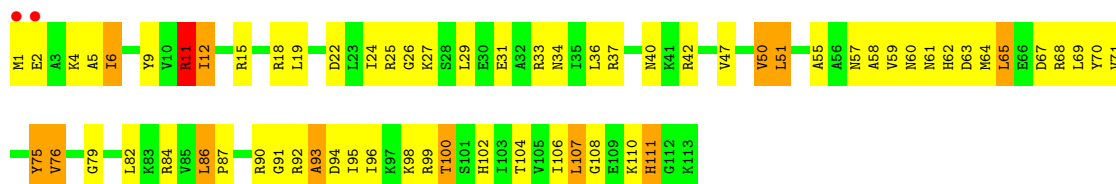
- Molecule 54: 50S RIBOSOMAL PROTEIN L21

Chain DV:



- Molecule 55: 50S RIBOSOMAL PROTEIN L22

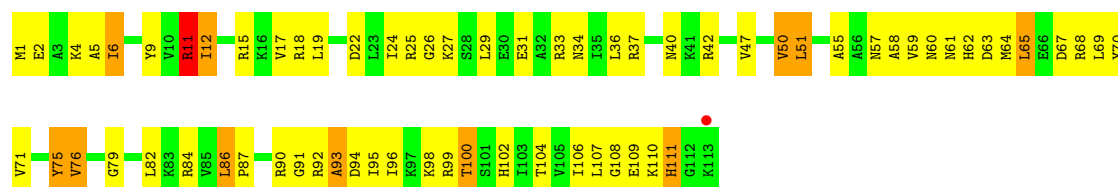
Chain BW:



- Molecule 55: 50S RIBOSOMAL PROTEIN L22

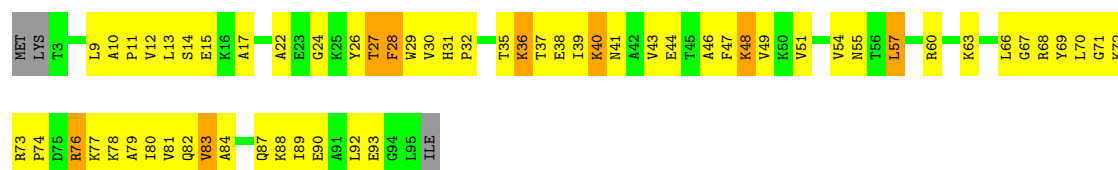
Chain DW:





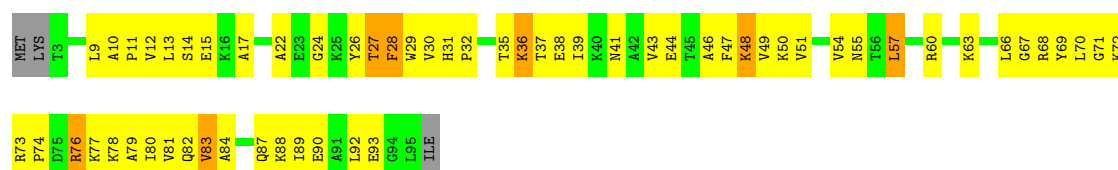
• Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain BX:



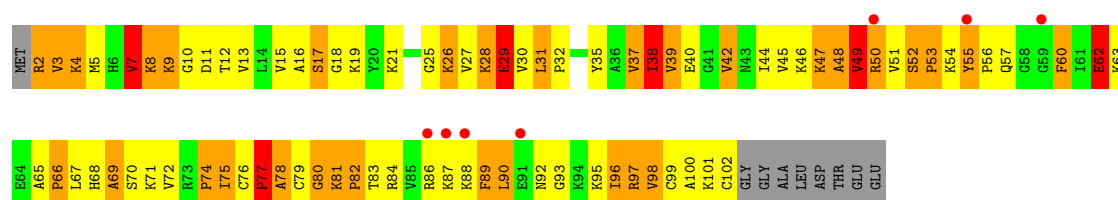
• Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain DX:



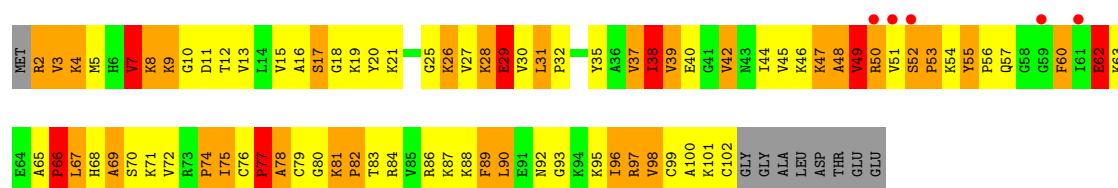
• Molecule 57: 50S RIBOSOMAL PROTEIN L24

Chain BY:



• Molecule 57: 50S RIBOSOMAL PROTEIN L24

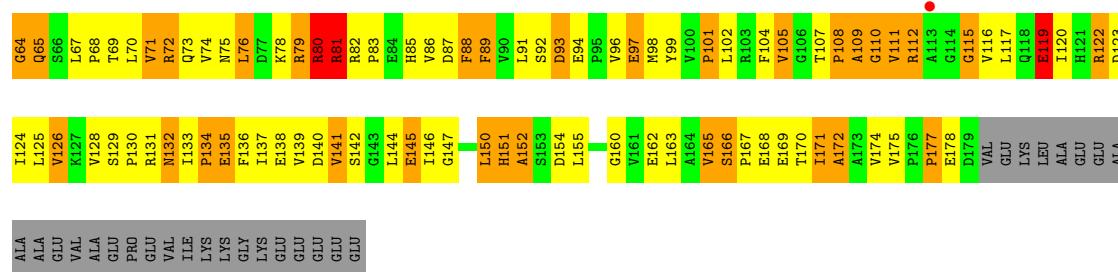
Chain DY:



• Molecule 58: 50S RIBOSOMAL PROTEIN L25

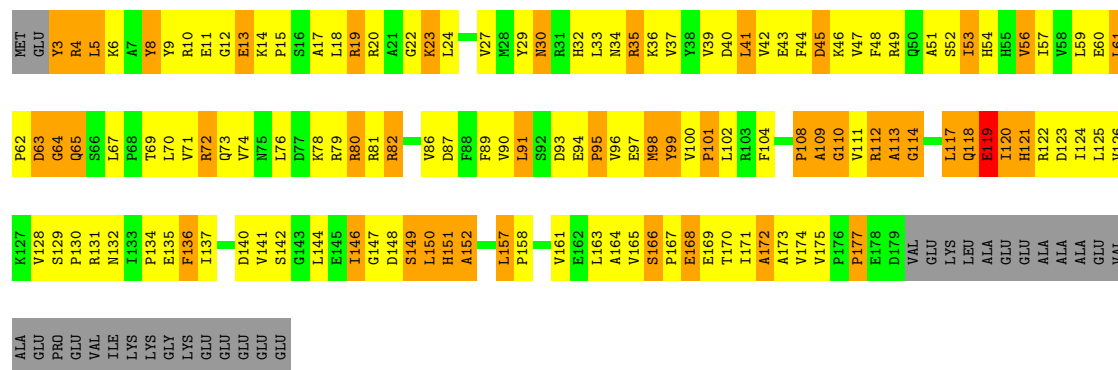
Chain BZ:





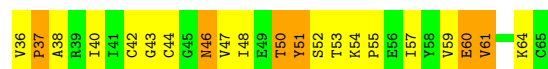
• Molecule 58: 50S RIBOSOMAL PROTEIN L25

Chain DZ:



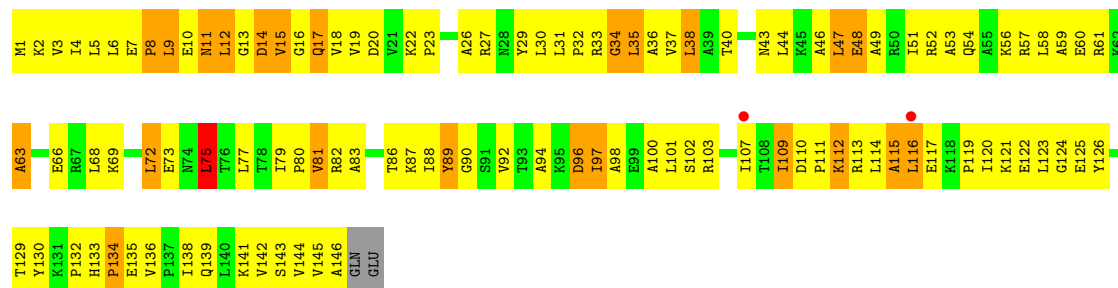
• Molecule 59: 50S RIBOSOMAL PROTEIN L31

Chain D4:



• Molecule 60: 50S RIBOSOMAL PROTEIN L9

Chain DI:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.34Å 450.91Å 614.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.57 – 3.45 49.57 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.57-3.45) 99.6 (49.57-3.45)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 3.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.210 , 0.257 0.211 , 0.257	Depositor DCC
$R_{free}$ test set	33081 reflections (4.55%)	DCC
Wilson B-factor (Å <sup>2</sup> )	76.9	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 44.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 759980 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	304505	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.39	0/36190	0.69	9/56486 (0.0%)
1	CA	0.41	0/36190	0.69	11/56486 (0.0%)
2	AB	0.32	0/1936	0.61	0/2611
2	CB	0.32	0/1936	0.61	0/2611
3	AC	0.32	0/1637	0.57	0/2207
3	CC	0.35	0/1637	0.57	0/2207
4	AD	0.34	0/1733	0.58	0/2318
4	CD	0.36	0/1733	0.59	0/2318
5	AE	0.36	0/1163	0.61	0/1566
5	CE	0.37	0/1163	0.62	0/1566
6	AF	0.29	0/856	0.58	0/1154
6	CF	0.29	0/856	0.58	0/1154
7	AG	0.30	0/1276	0.54	0/1709
7	CG	0.33	0/1276	0.56	0/1709
8	AH	0.32	0/1136	0.62	0/1527
8	CH	0.33	0/1136	0.63	0/1527
9	AI	0.31	0/1029	0.60	0/1378
9	CI	0.33	0/1029	0.61	0/1378
10	AJ	0.33	0/808	0.60	0/1087
10	CJ	0.34	0/808	0.61	0/1087
11	AK	0.32	0/900	0.60	0/1213
11	CK	0.33	0/900	0.60	0/1213
12	AL	0.40	0/992	0.74	0/1329
12	CL	0.40	0/992	0.75	0/1329
13	AM	0.32	0/966	0.65	0/1294
13	CM	0.34	0/966	0.66	0/1294
14	AN	0.35	0/501	0.58	0/664
14	CN	0.38	0/501	0.60	0/664
15	AO	0.31	0/745	0.54	0/992
15	CO	0.32	0/745	0.55	0/992
16	AP	0.37	0/717	0.63	0/965
16	CP	0.37	0/717	0.63	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.37	0/837	0.60	0/1119
17	CQ	0.37	0/837	0.60	0/1119
18	AR	0.32	0/579	0.61	0/768
18	CR	0.32	0/579	0.62	0/768
19	AS	0.37	0/643	0.60	0/867
19	CS	0.39	0/643	0.60	0/867
20	AT	0.29	0/765	0.55	0/1007
20	CT	0.29	0/765	0.56	0/1007
21	AU	0.44	0/213	0.53	0/279
21	CU	0.43	0/213	0.54	0/279
22	AV	0.52	0/1809	0.77	1/2819 (0.0%)
22	AW	0.42	0/1809	0.78	5/2819 (0.2%)
22	CV	0.53	0/1809	0.78	2/2819 (0.1%)
22	CW	0.39	0/1809	0.76	4/2819 (0.1%)
23	AX	0.53	0/185	0.79	1/286 (0.3%)
23	CX	0.56	0/185	0.71	0/286
24	AY	0.34	0/2847	0.66	0/3846
24	CY	0.36	0/2847	0.70	1/3846 (0.0%)
25	B0	0.42	0/615	0.72	0/819
25	D0	0.44	0/615	0.73	0/819
26	B1	0.44	0/739	0.79	1/983 (0.1%)
26	D1	0.49	0/739	0.77	0/983
27	B2	0.39	0/600	0.73	0/793
27	D2	0.44	0/600	0.75	1/793 (0.1%)
28	B3	0.44	0/473	0.74	0/636
28	D3	0.45	0/473	0.73	0/636
29	B4	0.38	0/229	0.53	0/311
30	B5	0.46	0/473	0.83	0/639
30	D5	0.45	0/473	0.85	0/639
31	B6	0.62	1/388 (0.3%)	0.97	0/520
31	D6	0.71	1/388 (0.3%)	1.00	0/520
32	B7	0.48	0/427	0.70	0/563
32	D7	0.48	0/427	0.69	0/563
33	B8	0.63	0/516	0.88	0/681
33	D8	0.67	0/516	0.91	0/681
34	B9	0.42	0/302	0.77	1/397 (0.3%)
34	D9	0.45	0/302	0.77	1/397 (0.3%)
35	BA	0.53	1/69614 (0.0%)	0.74	40/108679 (0.0%)
35	DA	0.56	3/69614 (0.0%)	0.75	40/108679 (0.0%)
36	BB	0.50	2/2853 (0.1%)	0.87	4/4451 (0.1%)
36	DB	0.52	1/2853 (0.0%)	0.84	3/4451 (0.1%)
37	BC	0.36	0/1145	0.65	7/1556 (0.4%)
37	DC	0.35	0/1145	0.66	7/1556 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	BD	0.45	0/2155	0.68	1/2907 (0.0%)
38	DD	0.47	0/2155	0.68	1/2907 (0.0%)
39	BE	0.43	0/1597	0.76	1/2155 (0.0%)
39	DE	0.44	0/1597	0.76	1/2155 (0.0%)
40	BF	0.48	0/1659	0.77	0/2246
40	DF	0.49	0/1659	0.77	0/2246
41	BG	0.37	0/1499	0.69	0/2016
41	DG	0.41	0/1499	0.76	1/2016 (0.0%)
42	BH	0.36	0/1246	0.69	1/1684 (0.1%)
42	DH	0.37	0/1246	0.69	1/1684 (0.1%)
43	BI	0.31	0/1147	0.60	0/1553
45	BK	0.31	0/1057	0.57	0/1432
45	DK	0.31	0/1057	0.57	0/1432
46	BN	0.38	0/1132	0.69	0/1527
46	DN	0.41	0/1132	0.70	0/1527
47	BO	0.42	0/943	0.71	0/1269
47	DO	0.40	0/943	0.71	0/1269
48	BP	0.41	0/1131	0.78	1/1504 (0.1%)
48	DP	0.44	0/1131	0.78	1/1504 (0.1%)
49	BQ	0.44	0/1143	0.71	0/1527
49	DQ	0.46	0/1143	0.72	0/1527
50	BR	0.36	0/974	0.71	1/1302 (0.1%)
50	DR	0.37	0/974	0.72	1/1302 (0.1%)
51	BS	0.45	0/779	0.85	1/1038 (0.1%)
51	DS	0.56	0/779	0.89	1/1038 (0.1%)
52	BT	0.40	0/1156	0.74	0/1544
52	DT	0.41	0/1156	0.75	0/1544
53	BU	0.47	0/975	0.77	1/1297 (0.1%)
53	DU	0.47	0/975	0.80	1/1297 (0.1%)
54	BV	0.42	0/790	0.73	0/1057
54	DV	0.46	0/790	0.76	0/1057
55	BW	0.39	0/907	0.67	0/1216
55	DW	0.41	0/907	0.69	0/1216
56	BX	0.43	0/740	0.71	0/995
56	DX	0.44	0/740	0.72	0/995
57	BY	0.50	0/789	0.80	0/1053
57	DY	0.49	0/789	0.81	0/1053
58	BZ	0.41	0/1436	0.72	0/1951
58	DZ	0.41	0/1436	0.77	0/1951
59	D4	0.32	0/229	0.53	0/309
60	DI	0.36	0/1148	0.73	0/1554
All	All	0.47	9/327803 (0.0%)	0.72	154/489221 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	9
1	CA	0	10
22	AW	3	0
22	CV	0	2
22	CW	3	0
23	AX	0	1
30	B5	0	1
30	D5	0	2
35	BA	2	40
35	DA	3	46
All	All	11	111

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	DB	86	G	P-OP1	-7.68	1.35	1.49
35	BA	568	U	C4-O4	7.25	1.29	1.23
36	BB	86	G	P-OP1	-7.23	1.36	1.49
36	BB	96	U	C2-O2	-6.42	1.16	1.22
31	D6	42	TRP	CB-CG	6.09	1.61	1.50

The worst 5 of 154 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BB	85	G	OP1-P-O3'	-22.67	55.33	105.20
36	DB	85	G	OP1-P-O3'	-19.05	63.30	105.20
36	BB	85	G	OP2-P-O3'	13.54	134.99	105.20
36	DB	85	G	OP2-P-O3'	12.71	133.15	105.20
36	DB	86	G	O5'-P-OP1	11.85	124.92	110.70

5 of 11 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	AW	17	C	C1'
22	AW	47	U	C1'
22	AW	70	G	C3'
35	BA	1784	A	C3'
35	BA	1799	G	C3'

5 of 111 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	110	C	Sidechain
1	AA	324	G	Sidechain
1	AA	38	G	Sidechain
1	AA	388	G	Sidechain
1	AA	498	U	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	16318	1300	0
1	CA	32329	0	16318	1291	0
2	AB	1901	0	1951	253	0
2	CB	1901	0	1951	256	0
3	AC	1613	0	1677	193	0
3	CC	1613	0	1677	190	0
4	AD	1703	0	1763	215	0
4	CD	1703	0	1763	213	0
5	AE	1147	0	1207	140	0
5	CE	1147	0	1207	134	0
6	AF	843	0	857	93	0
6	CF	843	0	857	98	0
7	AG	1257	0	1296	112	0
7	CG	1257	0	1296	112	0
8	AH	1116	0	1177	160	0
8	CH	1116	0	1177	152	0
9	AI	1011	0	1043	164	0
9	CI	1011	0	1043	172	0
10	AJ	795	0	840	170	0
10	CJ	795	0	840	165	0
11	AK	885	0	904	101	0
11	CK	885	0	904	104	0
12	AL	976	0	1062	99	0
12	CL	976	0	1062	93	0
13	AM	956	0	1021	104	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	CM	956	0	1021	106	0
14	AN	492	0	529	59	0
14	CN	492	0	529	57	0
15	AO	734	0	771	52	0
15	CO	734	0	771	48	0
16	AP	701	0	720	100	0
16	CP	701	0	720	106	0
17	AQ	824	0	891	69	0
17	CQ	824	0	891	70	0
18	AR	574	0	644	78	0
18	CR	574	0	644	78	0
19	AS	630	0	652	97	0
19	CS	630	0	652	97	0
20	AT	763	0	861	112	0
20	CT	763	0	861	110	0
21	AU	209	0	221	18	0
21	CU	209	0	221	18	0
22	AV	1619	0	822	76	0
22	AW	1619	0	822	98	0
22	CV	1619	0	822	83	0
22	CW	1619	0	822	92	0
23	AX	166	0	87	17	0
23	CX	166	0	87	7	0
24	AY	2799	0	2809	362	0
24	CY	2799	0	2809	344	0
25	B0	607	0	628	82	0
25	D0	607	0	628	82	0
26	B1	732	0	808	113	0
26	D1	732	0	808	108	0
27	B2	598	0	653	85	0
27	D2	598	0	653	78	0
28	B3	468	0	523	59	3
28	D3	468	0	523	60	0
29	B4	226	0	229	33	0
30	B5	459	0	480	64	0
30	D5	459	0	480	72	0
31	B6	381	0	391	117	0
31	D6	381	0	391	123	0
32	B7	419	0	467	25	0
32	D7	419	0	467	29	0
33	B8	508	0	576	122	0
33	D8	508	0	576	130	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	B9	299	0	324	33	0
34	D9	299	0	324	31	0
35	BA	62154	0	31337	2154	0
35	DA	62154	0	31337	2170	9
36	BB	2551	0	1295	103	6
36	DB	2551	0	1295	103	0
37	BC	1142	0	865	110	0
37	DC	1142	0	865	103	0
38	BD	2105	0	2182	255	0
38	DD	2105	0	2182	246	0
39	BE	1564	0	1629	245	0
39	DE	1564	0	1629	252	0
40	BF	1624	0	1677	227	0
40	DF	1624	0	1677	226	0
41	BG	1474	0	1535	288	0
41	DG	1474	0	1535	249	0
42	BH	1223	0	1282	214	0
42	DH	1223	0	1282	212	0
43	BI	1132	0	1218	120	0
44	BJ	651	0	146	35	0
44	DJ	651	0	146	36	0
45	BK	1038	0	1089	157	0
45	DK	1038	0	1089	184	0
46	BN	1105	0	1180	129	0
46	DN	1105	0	1180	122	0
47	BO	933	0	996	92	0
47	DO	933	0	996	94	0
48	BP	1114	0	1187	261	0
48	DP	1114	0	1187	259	0
49	BQ	1122	0	1179	121	0
49	DQ	1122	0	1179	123	0
50	BR	960	0	1021	134	0
50	DR	960	0	1020	134	0
51	BS	771	0	832	147	0
51	DS	771	0	832	149	0
52	BT	1142	0	1202	231	0
52	DT	1142	0	1202	231	0
53	BU	958	0	1015	134	0
53	DU	958	0	1015	139	0
54	BV	779	0	852	144	0
54	DV	779	0	852	149	0
55	BW	896	0	953	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	DW	896	0	953	77	0
56	BX	726	0	778	67	0
56	DX	726	0	778	65	0
57	BY	776	0	870	181	0
57	DY	776	0	870	182	0
58	BZ	1404	0	1432	232	0
58	DZ	1404	0	1432	245	0
59	D4	226	0	229	36	0
60	DI	1133	0	1220	185	0
61	AA	157	0	0	0	0
61	AE	1	0	0	0	0
61	AL	1	0	0	0	0
61	AM	1	0	0	0	0
61	AV	7	0	0	0	0
61	AW	5	0	0	0	0
61	AY	1	0	0	0	0
61	B1	1	0	0	0	0
61	B3	1	0	0	0	0
61	B5	2	0	0	0	0
61	B7	2	0	0	0	0
61	BA	354	0	0	0	0
61	BB	4	0	0	0	0
61	BC	1	0	0	0	0
61	BD	2	0	0	0	0
61	BF	1	0	0	0	0
61	BH	1	0	0	0	0
61	BP	1	0	0	0	0
61	BQ	1	0	0	0	0
61	BS	1	0	0	0	0
61	BU	1	0	0	0	0
61	CA	157	0	0	0	0
61	CL	1	0	0	0	0
61	CN	1	0	0	0	0
61	CV	7	0	0	0	0
61	CW	5	0	0	0	0
61	CY	1	0	0	0	0
61	D1	1	0	0	0	0
61	D3	1	0	0	0	0
61	D5	2	0	0	0	0
61	D7	1	0	0	0	0
61	DA	353	0	0	0	0
61	DB	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	DC	1	0	0	0	0
61	DD	2	0	0	0	0
61	DF	3	0	0	0	0
61	DH	1	0	0	0	0
61	DQ	1	0	0	0	0
61	DR	1	0	0	0	0
61	DU	1	0	0	0	0
61	DX	1	0	0	0	0
61	DY	1	0	0	0	0
62	AD	1	0	0	0	0
62	AN	1	0	0	0	0
62	B9	1	0	0	0	0
62	CD	1	0	0	0	0
62	CN	1	0	0	0	0
62	D9	1	0	0	0	0
All	All	304505	0	207553	19772	9

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 39.

The worst 5 of 19772 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
26:D1:81:LYS:CE	35:DA:271(H):G:H5'	1.21	1.60
26:B1:81:LYS:HE2	35:BA:271(H):G:C5'	1.23	1.59
26:D1:81:LYS:HE2	35:DA:271(H):G:C5'	1.31	1.54
26:B1:81:LYS:CE	35:BA:271(H):G:H5'	1.10	1.53
51:DS:97:ARG:NH2	51:DS:98:VAL:HA	1.57	1.18

The worst 5 of 9 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
28:B3:48:GLU:O	35:DA:654(L):G:OP2[3_455]	1.99	0.21
36:BB:97:G:N7	35:DA:654(J):A:OP1[3_455]	2.05	0.15
36:BB:97:G:OP2	35:DA:654(I):C:O2'[3_455]	2.06	0.14
36:BB:96:U:C3'	35:DA:654(I):C:O2'[3_455]	2.09	0.11
36:BB:96:U:O2	35:DA:654(K):C:OP1[3_455]	2.10	0.10

## 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%)	155 (66%)	58 (25%)	20 (9%)	1	17
2	CB	233/256 (91%)	156 (67%)	56 (24%)	21 (9%)	1	16
3	AC	205/239 (86%)	125 (61%)	57 (28%)	23 (11%)	1	10
3	CC	205/239 (86%)	128 (62%)	55 (27%)	22 (11%)	1	11
4	AD	206/209 (99%)	134 (65%)	49 (24%)	23 (11%)	1	10
4	CD	206/209 (99%)	135 (66%)	49 (24%)	22 (11%)	1	11
5	AE	149/162 (92%)	98 (66%)	36 (24%)	15 (10%)	1	13
5	CE	149/162 (92%)	100 (67%)	34 (23%)	15 (10%)	1	13
6	AF	99/101 (98%)	75 (76%)	17 (17%)	7 (7%)	2	24
6	CF	99/101 (98%)	75 (76%)	17 (17%)	7 (7%)	2	24
7	AG	153/156 (98%)	108 (71%)	34 (22%)	11 (7%)	2	24
7	CG	153/156 (98%)	108 (71%)	34 (22%)	11 (7%)	2	24
8	AH	136/138 (99%)	92 (68%)	32 (24%)	12 (9%)	1	17
8	CH	136/138 (99%)	92 (68%)	32 (24%)	12 (9%)	1	17
9	AI	125/128 (98%)	83 (66%)	30 (24%)	12 (10%)	1	14
9	CI	125/128 (98%)	82 (66%)	31 (25%)	12 (10%)	1	14
10	AJ	97/105 (92%)	64 (66%)	21 (22%)	12 (12%)	1	9
10	CJ	97/105 (92%)	64 (66%)	21 (22%)	12 (12%)	1	9
11	AK	117/129 (91%)	89 (76%)	24 (20%)	4 (3%)	6	49
11	CK	117/129 (91%)	89 (76%)	24 (20%)	4 (3%)	6	49
12	AL	124/132 (94%)	89 (72%)	26 (21%)	9 (7%)	2	23
12	CL	124/132 (94%)	90 (73%)	25 (20%)	9 (7%)	2	23
13	AM	119/126 (94%)	82 (69%)	23 (19%)	14 (12%)	1	10
13	CM	119/126 (94%)	84 (71%)	21 (18%)	14 (12%)	1	10
14	AN	58/61 (95%)	39 (67%)	12 (21%)	7 (12%)	1	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	CN	58/61 (95%)	38 (66%)	12 (21%)	8 (14%)	0	6
15	AO	86/89 (97%)	59 (69%)	23 (27%)	4 (5%)	4	37
15	CO	86/89 (97%)	57 (66%)	25 (29%)	4 (5%)	4	37
16	AP	82/88 (93%)	51 (62%)	22 (27%)	9 (11%)	1	11
16	CP	82/88 (93%)	53 (65%)	20 (24%)	9 (11%)	1	11
17	AQ	98/105 (93%)	68 (69%)	17 (17%)	13 (13%)	0	7
17	CQ	98/105 (93%)	69 (70%)	17 (17%)	12 (12%)	1	9
18	AR	68/88 (77%)	45 (66%)	16 (24%)	7 (10%)	1	12
18	CR	68/88 (77%)	45 (66%)	16 (24%)	7 (10%)	1	12
19	AS	77/93 (83%)	36 (47%)	30 (39%)	11 (14%)	0	6
19	CS	77/93 (83%)	36 (47%)	30 (39%)	11 (14%)	0	6
20	AT	97/106 (92%)	68 (70%)	18 (19%)	11 (11%)	1	10
20	CT	97/106 (92%)	68 (70%)	18 (19%)	11 (11%)	1	10
21	AU	23/27 (85%)	18 (78%)	3 (13%)	2 (9%)	1	17
21	CU	23/27 (85%)	18 (78%)	3 (13%)	2 (9%)	1	17
24	AY	349/351 (99%)	246 (70%)	70 (20%)	33 (10%)	1	15
24	CY	349/351 (99%)	256 (73%)	61 (18%)	32 (9%)	1	15
25	B0	74/85 (87%)	58 (78%)	10 (14%)	6 (8%)	1	19
25	D0	74/85 (87%)	58 (78%)	10 (14%)	6 (8%)	1	19
26	B1	92/98 (94%)	65 (71%)	15 (16%)	12 (13%)	0	8
26	D1	92/98 (94%)	72 (78%)	12 (13%)	8 (9%)	1	17
27	B2	69/72 (96%)	40 (58%)	17 (25%)	12 (17%)	0	3
27	D2	69/72 (96%)	39 (56%)	20 (29%)	10 (14%)	0	5
28	B3	58/60 (97%)	43 (74%)	9 (16%)	6 (10%)	1	12
28	D3	58/60 (97%)	43 (74%)	9 (16%)	6 (10%)	1	12
29	B4	29/71 (41%)	14 (48%)	11 (38%)	4 (14%)	0	6
30	B5	57/60 (95%)	40 (70%)	7 (12%)	10 (18%)	0	3
30	D5	57/60 (95%)	40 (70%)	7 (12%)	10 (18%)	0	3
31	B6	43/54 (80%)	17 (40%)	12 (28%)	14 (33%)	0	0
31	D6	43/54 (80%)	17 (40%)	13 (30%)	13 (30%)	0	0
32	B7	47/49 (96%)	44 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	D7	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
33	B8	62/65 (95%)	38 (61%)	15 (24%)	9 (14%)	0	5
33	D8	62/65 (95%)	38 (61%)	15 (24%)	9 (14%)	0	5
34	B9	34/37 (92%)	23 (68%)	11 (32%)	0	100	100
34	D9	34/37 (92%)	24 (71%)	10 (29%)	0	100	100
37	BC	183/229 (80%)	64 (35%)	71 (39%)	48 (26%)	0	1
37	DC	183/229 (80%)	65 (36%)	72 (39%)	46 (25%)	0	1
38	BD	270/276 (98%)	199 (74%)	39 (14%)	32 (12%)	1	9
38	DD	270/276 (98%)	198 (73%)	40 (15%)	32 (12%)	1	9
39	BE	203/206 (98%)	124 (61%)	45 (22%)	34 (17%)	0	4
39	DE	203/206 (98%)	123 (61%)	44 (22%)	36 (18%)	0	3
40	BF	206/210 (98%)	149 (72%)	33 (16%)	24 (12%)	1	10
40	DF	206/210 (98%)	149 (72%)	33 (16%)	24 (12%)	1	10
41	BG	179/182 (98%)	92 (51%)	54 (30%)	33 (18%)	0	3
41	DG	179/182 (98%)	107 (60%)	46 (26%)	26 (14%)	0	5
42	BH	158/180 (88%)	90 (57%)	38 (24%)	30 (19%)	0	2
42	DH	158/180 (88%)	91 (58%)	36 (23%)	31 (20%)	0	2
43	BI	144/148 (97%)	100 (69%)	28 (19%)	16 (11%)	1	11
45	BK	139/147 (95%)	88 (63%)	33 (24%)	18 (13%)	0	8
45	DK	139/147 (95%)	87 (63%)	34 (24%)	18 (13%)	0	8
46	BN	137/140 (98%)	97 (71%)	20 (15%)	20 (15%)	0	5
46	DN	137/140 (98%)	99 (72%)	18 (13%)	20 (15%)	0	5
47	BO	120/122 (98%)	97 (81%)	17 (14%)	6 (5%)	3	35
47	DO	120/122 (98%)	98 (82%)	14 (12%)	8 (7%)	2	26
48	BP	144/150 (96%)	68 (47%)	36 (25%)	40 (28%)	0	0
48	DP	144/150 (96%)	68 (47%)	36 (25%)	40 (28%)	0	0
49	BQ	139/141 (99%)	111 (80%)	19 (14%)	9 (6%)	2	27
49	DQ	139/141 (99%)	114 (82%)	16 (12%)	9 (6%)	2	27
50	BR	115/118 (98%)	72 (63%)	29 (25%)	14 (12%)	1	9
50	DR	115/118 (98%)	70 (61%)	31 (27%)	14 (12%)	1	9
51	BS	97/112 (87%)	55 (57%)	22 (23%)	20 (21%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	DS	97/112 (87%)	54 (56%)	22 (23%)	21 (22%)	0	1
52	BT	136/146 (93%)	84 (62%)	23 (17%)	29 (21%)	0	2
52	DT	136/146 (93%)	85 (62%)	22 (16%)	29 (21%)	0	2
53	BU	115/118 (98%)	78 (68%)	27 (24%)	10 (9%)	1	17
53	DU	115/118 (98%)	77 (67%)	28 (24%)	10 (9%)	1	17
54	BV	99/101 (98%)	72 (73%)	13 (13%)	14 (14%)	0	6
54	DV	99/101 (98%)	72 (73%)	14 (14%)	13 (13%)	0	8
55	BW	111/113 (98%)	83 (75%)	22 (20%)	6 (5%)	3	33
55	DW	111/113 (98%)	83 (75%)	22 (20%)	6 (5%)	3	33
56	BX	91/96 (95%)	75 (82%)	14 (15%)	2 (2%)	10	60
56	DX	91/96 (95%)	74 (81%)	16 (18%)	1 (1%)	21	76
57	BY	99/110 (90%)	46 (46%)	20 (20%)	33 (33%)	0	0
57	DY	99/110 (90%)	47 (48%)	20 (20%)	32 (32%)	0	0
58	BZ	175/206 (85%)	102 (58%)	41 (23%)	32 (18%)	0	3
58	DZ	175/206 (85%)	110 (63%)	36 (21%)	29 (17%)	0	4
59	D4	28/30 (93%)	14 (50%)	11 (39%)	3 (11%)	1	11
60	DI	144/148 (97%)	81 (56%)	42 (29%)	21 (15%)	0	5
All	All	12651/13541 (93%)	8336 (66%)	2725 (22%)	1590 (13%)	0	8

5 of 1590 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	20	GLU
2	AB	88	ALA
2	AB	95	GLN
2	AB	195	ASP

### 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%)	184 (91%)	18 (9%)	14	54
2	CB	202/220 (92%)	184 (91%)	18 (9%)	14	54
3	AC	160/188 (85%)	149 (93%)	11 (7%)	22	68
3	CC	160/188 (85%)	150 (94%)	10 (6%)	25	72
4	AD	180/181 (99%)	159 (88%)	21 (12%)	8	37
4	CD	180/181 (99%)	159 (88%)	21 (12%)	8	37
5	AE	115/123 (94%)	103 (90%)	12 (10%)	10	45
5	CE	115/123 (94%)	101 (88%)	14 (12%)	7	35
6	AF	90/90 (100%)	86 (96%)	4 (4%)	39	83
6	CF	90/90 (100%)	86 (96%)	4 (4%)	39	83
7	AG	126/127 (99%)	117 (93%)	9 (7%)	21	66
7	CG	126/127 (99%)	118 (94%)	8 (6%)	25	72
8	AH	119/119 (100%)	105 (88%)	14 (12%)	8	37
8	CH	119/119 (100%)	105 (88%)	14 (12%)	8	37
9	AI	98/99 (99%)	88 (90%)	10 (10%)	11	46
9	CI	98/99 (99%)	88 (90%)	10 (10%)	11	46
10	AJ	88/92 (96%)	78 (89%)	10 (11%)	8	38
10	CJ	88/92 (96%)	78 (89%)	10 (11%)	8	38
11	AK	90/99 (91%)	84 (93%)	6 (7%)	23	69
11	CK	90/99 (91%)	84 (93%)	6 (7%)	23	69
12	AL	104/109 (95%)	98 (94%)	6 (6%)	28	74
12	CL	104/109 (95%)	96 (92%)	8 (8%)	18	63
13	AM	96/101 (95%)	83 (86%)	13 (14%)	6	30
13	CM	96/101 (95%)	83 (86%)	13 (14%)	6	30
14	AN	49/50 (98%)	46 (94%)	3 (6%)	26	73
14	CN	49/50 (98%)	46 (94%)	3 (6%)	26	73
15	AO	79/80 (99%)	76 (96%)	3 (4%)	44	85
15	CO	79/80 (99%)	76 (96%)	3 (4%)	44	85
16	AP	72/74 (97%)	64 (89%)	8 (11%)	9	41
16	CP	72/74 (97%)	64 (89%)	8 (11%)	9	41
17	AQ	94/97 (97%)	92 (98%)	2 (2%)	66	93
17	CQ	94/97 (97%)	92 (98%)	2 (2%)	66	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AR	61/77 (79%)	57 (93%)	4 (7%)	24	70
18	CR	61/77 (79%)	57 (93%)	4 (7%)	24	70
19	AS	69/80 (86%)	61 (88%)	8 (12%)	8	38
19	CS	69/80 (86%)	61 (88%)	8 (12%)	8	38
20	AT	76/82 (93%)	70 (92%)	6 (8%)	18	61
20	CT	76/82 (93%)	70 (92%)	6 (8%)	18	61
21	AU	19/22 (86%)	18 (95%)	1 (5%)	32	77
21	CU	19/22 (86%)	19 (100%)	0	100	100
24	AY	298/298 (100%)	264 (89%)	34 (11%)	8	38
24	CY	298/298 (100%)	264 (89%)	34 (11%)	8	38
25	B0	61/67 (91%)	58 (95%)	3 (5%)	35	79
25	D0	61/67 (91%)	58 (95%)	3 (5%)	35	79
26	B1	78/83 (94%)	70 (90%)	8 (10%)	10	45
26	D1	78/83 (94%)	66 (85%)	12 (15%)	4	23
27	B2	66/67 (98%)	55 (83%)	11 (17%)	3	19
27	D2	66/67 (98%)	59 (89%)	7 (11%)	10	43
28	B3	51/52 (98%)	47 (92%)	4 (8%)	18	62
28	D3	51/52 (98%)	48 (94%)	3 (6%)	28	74
29	B4	27/63 (43%)	25 (93%)	2 (7%)	20	64
30	B5	51/52 (98%)	45 (88%)	6 (12%)	8	37
30	D5	51/52 (98%)	44 (86%)	7 (14%)	5	29
31	B6	43/52 (83%)	32 (74%)	11 (26%)	1	5
31	D6	43/52 (83%)	32 (74%)	11 (26%)	1	5
32	B7	41/42 (98%)	39 (95%)	2 (5%)	35	79
32	D7	41/42 (98%)	39 (95%)	2 (5%)	35	79
33	B8	53/55 (96%)	41 (77%)	12 (23%)	1	7
33	D8	53/55 (96%)	41 (77%)	12 (23%)	1	7
34	B9	33/34 (97%)	28 (85%)	5 (15%)	4	24
34	D9	33/34 (97%)	28 (85%)	5 (15%)	4	24
37	BC	61/181 (34%)	55 (90%)	6 (10%)	12	48
37	DC	61/181 (34%)	55 (90%)	6 (10%)	12	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BD	213/218 (98%)	192 (90%)	21 (10%)	11	47
38	DD	213/218 (98%)	191 (90%)	22 (10%)	10	45
39	BE	165/166 (99%)	137 (83%)	28 (17%)	3	18
39	DE	165/166 (99%)	136 (82%)	29 (18%)	3	15
40	BF	165/166 (99%)	144 (87%)	21 (13%)	6	33
40	DF	165/166 (99%)	146 (88%)	19 (12%)	8	38
41	BG	155/156 (99%)	131 (84%)	24 (16%)	4	23
41	DG	155/156 (99%)	129 (83%)	26 (17%)	3	18
42	BH	132/148 (89%)	122 (92%)	10 (8%)	19	64
42	DH	132/148 (89%)	122 (92%)	10 (8%)	19	64
43	BI	122/124 (98%)	116 (95%)	6 (5%)	35	79
45	BK	106/111 (96%)	97 (92%)	9 (8%)	15	57
45	DK	106/111 (96%)	97 (92%)	9 (8%)	15	57
46	BN	117/119 (98%)	101 (86%)	16 (14%)	5	29
46	DN	117/119 (98%)	101 (86%)	16 (14%)	5	29
47	BO	100/100 (100%)	94 (94%)	6 (6%)	27	73
47	DO	100/100 (100%)	95 (95%)	5 (5%)	34	79
48	BP	112/116 (97%)	84 (75%)	28 (25%)	1	5
48	DP	112/116 (97%)	84 (75%)	28 (25%)	1	5
49	BQ	111/111 (100%)	97 (87%)	14 (13%)	7	33
49	DQ	111/111 (100%)	96 (86%)	15 (14%)	6	30
50	BR	100/101 (99%)	88 (88%)	12 (12%)	7	36
50	DR	100/101 (99%)	88 (88%)	12 (12%)	7	36
51	BS	77/88 (88%)	61 (79%)	16 (21%)	2	9
51	DS	77/88 (88%)	61 (79%)	16 (21%)	2	9
52	BT	120/127 (94%)	102 (85%)	18 (15%)	4	25
52	DT	120/127 (94%)	102 (85%)	18 (15%)	4	25
53	BU	92/94 (98%)	85 (92%)	7 (8%)	19	64
53	DU	92/94 (98%)	85 (92%)	7 (8%)	19	64
54	BV	82/82 (100%)	73 (89%)	9 (11%)	9	41
54	DV	82/82 (100%)	72 (88%)	10 (12%)	7	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	BW	91/92 (99%)	79 (87%)	12 (13%)	6	31
55	DW	91/92 (99%)	80 (88%)	11 (12%)	7	35
56	BX	74/78 (95%)	65 (88%)	9 (12%)	7	35
56	DX	74/78 (95%)	65 (88%)	9 (12%)	7	35
57	BY	84/91 (92%)	67 (80%)	17 (20%)	2	10
57	DY	84/91 (92%)	67 (80%)	17 (20%)	2	10
58	BZ	155/179 (87%)	128 (83%)	27 (17%)	3	16
58	DZ	155/179 (87%)	129 (83%)	26 (17%)	3	18
59	D4	27/27 (100%)	24 (89%)	3 (11%)	9	41
60	DI	122/124 (98%)	118 (97%)	4 (3%)	50	88
All	All	10446/11210 (93%)	9279 (89%)	1167 (11%)	9	40

5 of 1167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
55	BW	86	LEU
7	CG	114	ARG
52	DT	87	ASP
57	BY	15	VAL
2	CB	137	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 327 such sidechains are listed below:

Mol	Chain	Res	Type
51	BS	68	GLN
4	CD	74	GLN
49	DQ	123	HIS
53	BU	71	GLN
58	BZ	75	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	222 (14%)	34 (2%)
1	CA	1503/1522 (98%)	217 (14%)	34 (2%)
22	AV	75/76 (98%)	17 (22%)	1 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	AW	75/76 (98%)	15 (20%)	3 (4%)
22	CV	75/76 (98%)	18 (24%)	0
22	CW	75/76 (98%)	16 (21%)	4 (5%)
23	AX	7/8 (87%)	1 (14%)	1 (14%)
23	CX	7/8 (87%)	1 (14%)	0
35	BA	2885/2901 (99%)	515 (17%)	58 (2%)
35	DA	2885/2901 (99%)	516 (17%)	57 (1%)
36	BB	118/122 (96%)	15 (12%)	3 (2%)
36	DB	118/122 (96%)	14 (11%)	3 (2%)
All	All	9326/9410 (99%)	1567 (16%)	198 (2%)

5 of 1567 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 198 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	BA	2439	A
1	CA	372	C
35	DA	2225	A
35	BA	2542	A
1	CA	30	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 1098 ligands modelled in this entry, 1098 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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AA	1504/1522 (98%)	-0.00	26 (1%) 67 32	43, 106, 183, 201	0
1	CA	1504/1522 (98%)	-0.09	41 (2%) 52 23	35, 87, 183, 201	0
2	AB	235/256 (91%)	0.38	7 (2%) 48 21	76, 137, 191, 201	0
2	CB	235/256 (91%)	0.14	5 (2%) 60 28	51, 117, 180, 201	0
3	AC	207/239 (86%)	0.45	8 (3%) 37 16	71, 130, 177, 201	0
3	CC	207/239 (86%)	-0.00	0 100 100	48, 96, 159, 200	0
4	AD	208/209 (99%)	0.40	10 (4%) 29 12	53, 116, 168, 199	0
4	CD	208/209 (99%)	0.07	1 (0%) 88 63	41, 95, 158, 183	0
5	AE	151/162 (93%)	0.17	2 (1%) 74 39	48, 102, 156, 179	0
5	CE	151/162 (93%)	-0.04	2 (1%) 74 39	29, 86, 145, 193	0
6	AF	101/101 (100%)	0.50	1 (0%) 79 46	75, 120, 170, 189	0
6	CF	101/101 (100%)	0.20	2 (1%) 62 29	60, 116, 162, 184	0
7	AG	155/156 (99%)	0.56	9 (5%) 22 9	64, 137, 182, 201	0
7	CG	155/156 (99%)	0.07	3 (1%) 64 30	42, 89, 143, 193	0
8	AH	138/138 (100%)	0.25	4 (2%) 49 22	50, 101, 152, 201	0
8	CH	138/138 (100%)	0.05	0 100 100	50, 97, 148, 188	0
9	AI	127/128 (99%)	0.91	15 (11%) 5 4	66, 148, 192, 201	0
9	CI	127/128 (99%)	0.37	4 (3%) 47 21	43, 97, 148, 183	0
10	AJ	99/105 (94%)	1.04	17 (17%) 2 2	64, 154, 198, 201	0
10	CJ	99/105 (94%)	0.57	5 (5%) 27 11	44, 122, 197, 201	0
11	AK	119/129 (92%)	0.50	7 (5%) 22 9	52, 100, 155, 172	0
11	CK	119/129 (92%)	0.17	7 (5%) 22 9	49, 89, 165, 183	0
12	AL	126/132 (95%)	0.25	4 (3%) 45 19	42, 81, 146, 193	0
12	CL	126/132 (95%)	0.24	7 (5%) 24 10	37, 75, 148, 201	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
13	AM	121/126 (96%)	0.54	6 (4%)	28	11	69, 133, 191, 201	0
13	CM	121/126 (96%)	0.12	2 (1%)	67	32	26, 96, 156, 189	0
14	AN	60/61 (98%)	0.45	1 (1%)	67	32	76, 124, 173, 187	0
14	CN	60/61 (98%)	-0.05	0	100	100	40, 82, 118, 155	0
15	AO	88/89 (98%)	0.28	1 (1%)	77	42	43, 100, 153, 177	0
15	CO	88/89 (98%)	0.25	1 (1%)	77	42	55, 92, 138, 155	0
16	AP	84/88 (95%)	0.47	4 (4%)	29	12	59, 104, 142, 201	0
16	CP	84/88 (95%)	0.68	6 (7%)	16	7	56, 106, 157, 201	0
17	AQ	100/105 (95%)	0.32	3 (3%)	48	21	54, 96, 137, 165	0
17	CQ	100/105 (95%)	0.22	2 (2%)	62	29	53, 99, 152, 162	0
18	AR	70/88 (79%)	0.35	1 (1%)	72	37	62, 116, 160, 183	0
18	CR	70/88 (79%)	0.44	3 (4%)	34	14	51, 101, 157, 183	0
19	AS	79/93 (84%)	0.62	4 (5%)	27	11	91, 140, 191, 201	0
19	CS	79/93 (84%)	0.50	5 (6%)	19	8	51, 103, 193, 201	0
20	AT	99/106 (93%)	0.53	3 (3%)	48	21	55, 112, 165, 201	0
20	CT	99/106 (93%)	0.65	5 (5%)	27	11	68, 115, 177, 201	0
21	AU	25/27 (92%)	1.25	6 (24%)	1	2	78, 131, 167, 178	0
21	CU	25/27 (92%)	0.42	0	100	100	58, 85, 117, 123	0
22	AV	76/76 (100%)	-0.13	0	100	100	42, 85, 152, 176	0
22	AW	76/76 (100%)	1.37	21 (27%)	1	2	48, 184, 201, 201	0
22	CV	76/76 (100%)	-0.38	1 (1%)	74	39	35, 65, 135, 185	0
22	CW	76/76 (100%)	0.83	9 (11%)	5	4	30, 166, 198, 201	0
23	AX	8/8 (100%)	0.34	1 (12%)	5	3	67, 76, 160, 166	0
23	CX	8/8 (100%)	0.05	0	100	100	46, 62, 153, 170	0
24	AY	351/351 (100%)	0.40	29 (8%)	11	6	31, 109, 190, 201	0
24	CY	351/351 (100%)	0.32	21 (5%)	21	9	25, 95, 188, 201	0
25	B0	76/85 (89%)	0.09	0	100	100	25, 64, 105, 177	0
25	D0	76/85 (89%)	0.09	1 (1%)	74	39	10, 43, 103, 179	0
26	B1	94/98 (95%)	0.02	1 (1%)	77	42	23, 61, 123, 173	0
26	D1	94/98 (95%)	-0.11	1 (1%)	77	42	18, 52, 109, 155	0
27	B2	71/72 (98%)	0.24	2 (2%)	50	22	36, 85, 156, 201	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
27	D2	71/72 (98%)	0.02	2 (2%)	50	22	27, 76, 144, 186	0
28	B3	60/60 (100%)	0.30	2 (3%)	44	19	19, 56, 131, 197	0
28	D3	60/60 (100%)	0.23	2 (3%)	44	19	20, 51, 112, 201	0
29	B4	31/71 (43%)	0.73	3 (9%)	8	5	99, 184, 201, 201	0
30	B5	59/60 (98%)	-0.05	2 (3%)	43	18	22, 74, 170, 190	0
30	D5	59/60 (98%)	0.11	2 (3%)	43	18	7, 55, 183, 201	0
31	B6	45/54 (83%)	0.67	2 (4%)	33	13	39, 85, 140, 198	0
31	D6	45/54 (83%)	0.25	1 (2%)	59	26	24, 65, 117, 183	0
32	B7	49/49 (100%)	0.14	1 (2%)	62	29	7, 48, 129, 165	0
32	D7	49/49 (100%)	0.08	0	100	100	7, 37, 113, 189	0
33	B8	64/65 (98%)	0.03	0	100	100	17, 51, 125, 160	0
33	D8	64/65 (98%)	-0.15	0	100	100	8, 40, 120, 162	0
34	B9	36/37 (97%)	0.43	0	100	100	45, 69, 127, 147	0
34	D9	36/37 (97%)	0.54	2 (5%)	24	10	40, 74, 133, 162	0
35	BA	2886/2901 (99%)	-0.19	79 (2%)	52	23	16, 58, 179, 201	0
35	DA	2886/2901 (99%)	-0.13	88 (3%)	48	21	14, 51, 181, 201	0
36	BB	119/122 (97%)	-0.16	0	100	100	46, 105, 160, 186	0
36	DB	119/122 (97%)	-0.32	0	100	100	34, 65, 99, 129	0
37	BC	191/229 (83%)	2.73	104 (54%)	0	1	91, 174, 201, 201	0
37	DC	191/229 (83%)	2.61	109 (57%)	0	1	104, 177, 201, 201	0
38	BD	272/276 (98%)	0.06	1 (0%)	90	70	27, 71, 122, 165	0
38	DD	272/276 (98%)	-0.03	0	100	100	25, 66, 108, 168	0
39	BE	205/206 (99%)	0.00	2 (0%)	79	46	22, 69, 152, 201	0
39	DE	205/206 (99%)	0.11	4 (1%)	62	29	16, 67, 144, 197	0
40	BF	208/210 (99%)	-0.16	2 (0%)	79	46	9, 52, 134, 194	0
40	DF	208/210 (99%)	-0.09	5 (2%)	56	25	9, 48, 140, 179	0
41	BG	181/182 (99%)	0.44	6 (3%)	44	19	64, 118, 173, 200	0
41	DG	181/182 (99%)	0.02	4 (2%)	59	26	30, 76, 137, 201	0
42	BH	160/180 (88%)	0.57	13 (8%)	12	6	50, 123, 181, 201	0
42	DH	160/180 (88%)	0.71	16 (10%)	8	5	63, 137, 186, 201	0
43	BI	146/148 (98%)	0.35	3 (2%)	60	28	41, 138, 187, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BJ	0/130	-	-	-	-
44	DJ	0/130	-	-	-	-
45	BK	141/147 (95%)	1.13	20 (14%) 3 3	85, 158, 195, 201	0
45	DK	141/147 (95%)	1.20	25 (17%) 2 2	99, 158, 197, 201	0
46	BN	139/140 (99%)	-0.04	0 100 100	30, 70, 129, 164	0
46	DN	139/140 (99%)	-0.07	0 100 100	24, 62, 122, 186	0
47	BO	122/122 (100%)	-0.17	0 100 100	28, 64, 101, 158	0
47	DO	122/122 (100%)	-0.13	0 100 100	25, 68, 101, 120	0
48	BP	146/150 (97%)	0.47	6 (4%) 35 15	27, 89, 163, 200	0
48	DP	146/150 (97%)	0.13	3 (2%) 60 28	25, 72, 147, 201	0
49	BQ	141/141 (100%)	-0.00	2 (1%) 72 37	23, 65, 127, 198	0
49	DQ	141/141 (100%)	-0.16	2 (1%) 72 37	14, 53, 105, 196	0
50	BR	117/118 (99%)	-0.04	0 100 100	33, 72, 126, 156	0
50	DR	117/118 (99%)	0.06	0 100 100	26, 68, 122, 150	0
51	BS	99/112 (88%)	0.48	3 (3%) 48 21	60, 104, 165, 188	0
51	DS	99/112 (88%)	-0.14	0 100 100	25, 61, 120, 171	0
52	BT	138/146 (94%)	0.16	2 (1%) 72 37	44, 87, 164, 201	0
52	DT	138/146 (94%)	0.20	7 (5%) 27 11	39, 87, 172, 199	0
53	BU	117/118 (99%)	-0.18	0 100 100	18, 55, 112, 140	0
53	DU	117/118 (99%)	-0.27	1 (0%) 81 49	12, 45, 111, 190	0
54	BV	101/101 (100%)	0.12	0 100 100	34, 79, 137, 185	0
54	DV	101/101 (100%)	-0.01	1 (0%) 79 46	25, 66, 141, 201	0
55	BW	113/113 (100%)	-0.10	2 (1%) 65 31	25, 57, 114, 201	0
55	DW	113/113 (100%)	-0.16	1 (0%) 81 49	16, 47, 115, 170	0
56	BX	93/96 (96%)	0.05	0 100 100	31, 74, 129, 155	0
56	DX	93/96 (96%)	-0.04	0 100 100	33, 67, 114, 160	0
57	BY	101/110 (91%)	0.57	7 (6%) 17 7	27, 84, 157, 201	0
57	DY	101/110 (91%)	0.40	5 (4%) 28 11	25, 81, 162, 201	0
58	BZ	177/206 (85%)	0.23	4 (2%) 57 26	36, 98, 156, 201	0
58	DZ	177/206 (85%)	-0.05	0 100 100	30, 83, 130, 192	0
59	D4	30/30 (100%)	0.14	0 100 100	80, 143, 184, 200	0
60	DI	146/148 (98%)	0.33	2 (1%) 72 37	28, 109, 155, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
All	All	22209/23211 (95%)	0.13	875 (3%)	37	16	7, 84, 181, 201	0

The worst 5 of 875 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
35	DA	654(A)	G	14.1
35	DA	2142	C	11.3
35	DA	2143	C	10.9
35	DA	2144	U	10.9
1	CA	89	C	10.6

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
61	MG	BA	3277	1/1	0.73	-	57,57,57,57	0
61	MG	BA	3159	1/1	0.32	-	55,55,55,55	0
61	MG	DA	3022	1/1	0.23	-	47,47,47,47	0
61	MG	BA	3291	1/1	0.38	-	54,54,54,54	0
61	MG	AA	1754	1/1	0.22	-	55,55,55,55	0
61	MG	DA	3048	1/1	0.27	-	47,47,47,47	0
61	MG	BA	3057	1/1	0.51	-	47,47,47,47	0
61	MG	BA	3308	1/1	0.54	-	55,55,55,55	0
61	MG	BA	3184	1/1	0.46	-	47,47,47,47	0
61	MG	BA	3102	1/1	0.73	-	47,47,47,47	0
61	MG	BB	201	1/1	0.57	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
61	MG	BA	3330	1/1	0.22	-	55,55,55,55	0
61	MG	BA	3115	1/1	0.54	-	50,50,50,50	0
61	MG	AA	1737	1/1	0.60	-	55,55,55,55	0
61	MG	AA	1675	1/1	0.16	-	48,48,48,48	0
61	MG	AA	1621	1/1	0.23	-	56,56,56,56	0
61	MG	CA	1707	1/1	0.55	-	51,51,51,51	0
61	MG	BA	3130	1/1	0.12	-	48,48,48,48	0
61	MG	BA	3068	1/1	0.50	-	47,47,47,47	0
61	MG	CA	1630	1/1	0.27	-	47,47,47,47	0
61	MG	BA	3163	1/1	0.35	-	53,53,53,53	0
61	MG	DA	3320	1/1	0.19	-	55,55,55,55	0
62	ZN	CD	301	1/1	0.27	-	52,52,52,52	0
61	MG	BA	3351	1/1	0.49	-	55,55,55,55	0
61	MG	CA	1644	1/1	0.14	-	57,57,57,57	0
61	MG	BA	3005	1/1	0.75	-	47,47,47,47	0
61	MG	BA	3107	1/1	0.34	-	51,51,51,51	0
61	MG	AA	1753	1/1	0.51	-	55,55,55,55	1
61	MG	AA	1724	1/1	0.53	-	59,59,59,59	0
61	MG	BA	3193	1/1	0.28	-	53,53,53,53	0
61	MG	BA	3091	1/1	0.37	-	51,51,51,51	0
61	MG	BA	3229	1/1	0.16	-	49,49,49,49	0
61	MG	DA	3192	1/1	0.19	-	61,61,61,61	1
61	MG	DA	3106	1/1	0.38	-	47,47,47,47	0
61	MG	DA	3063	1/1	0.54	-	47,47,47,47	0
61	MG	DA	3201	1/1	0.44	-	60,60,60,60	0
61	MG	AA	1605	1/1	0.11	-	50,50,50,50	0
61	MG	AA	1747	1/1	0.37	-	55,55,55,55	1
61	MG	BA	3149	1/1	0.49	-	54,54,54,54	0
61	MG	BA	3249	1/1	0.43	-	56,56,56,56	0
61	MG	DA	3274	1/1	0.48	-	63,63,63,63	0
61	MG	DA	3341	1/1	0.47	-	55,55,55,55	0
61	MG	BA	3025	1/1	0.46	-	55,55,55,55	0
61	MG	DA	3124	1/1	0.48	-	53,53,53,53	0
61	MG	CA	1750	1/1	0.21	-	55,55,55,55	0
61	MG	BA	3279	1/1	0.18	-	55,55,55,55	0
61	MG	CA	1714	1/1	0.47	-	64,64,64,64	0
61	MG	DA	3280	1/1	0.59	-	57,57,57,57	0
61	MG	AA	1728	1/1	0.15	-	55,55,55,55	0
61	MG	CA	1628	1/1	0.31	-	56,56,56,56	0
61	MG	BA	3098	1/1	0.25	-	54,54,54,54	0
61	MG	AV	105	1/1	0.21	-	50,50,50,50	1
61	MG	DA	3094	1/1	0.45	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
61	MG	BA	3349	1/1	0.47	-	55,55,55,55	0
61	MG	BA	3144	1/1	0.47	-	49,49,49,49	0
61	MG	AA	1743	1/1	0.53	-	55,55,55,55	0
62	ZN	B9	101	1/1	0.06	-	55,55,55,55	0
61	MG	BA	3240	1/1	0.67	-	58,58,58,58	1
61	MG	CA	1738	1/1	0.92	-	55,55,55,55	0
61	MG	DA	3282	1/1	0.34	-	57,57,57,57	0
61	MG	BA	3287	1/1	0.38	-	51,51,51,51	0
61	MG	DA	3131	1/1	0.20	-	48,48,48,48	0
61	MG	DA	3088	1/1	0.41	-	49,49,49,49	0
61	MG	DA	3115	1/1	0.24	-	48,48,48,48	0
61	MG	DA	3163	1/1	0.67	-	50,50,50,50	0
61	MG	AA	1646	1/1	0.74	-	50,50,50,50	0
61	MG	DA	3172	1/1	0.50	-	50,50,50,50	0
61	MG	CA	1657	1/1	0.31	-	54,54,54,54	0
61	MG	BA	3200	1/1	0.29	-	60,60,60,60	0
61	MG	DA	3014	1/1	0.33	-	47,47,47,47	0
61	MG	AA	1677	1/1	0.27	-	55,55,55,55	1
61	MG	BA	3079	1/1	0.44	-	49,49,49,49	0
61	MG	BA	3353	1/1	0.51	-	55,55,55,55	0
61	MG	DA	3344	1/1	0.49	-	55,55,55,55	0
61	MG	CA	1621	1/1	0.19	-	48,48,48,48	0
61	MG	DH	201	1/1	0.13	-	50,50,50,50	0
61	MG	DA	3179	1/1	0.90	-	47,47,47,47	0
61	MG	BA	3095	1/1	0.59	-	60,60,60,60	0
61	MG	BA	3289	1/1	0.38	-	54,54,54,54	0
61	MG	AA	1610	1/1	0.32	-	55,55,55,55	0
61	MG	AA	1653	1/1	0.92	-	60,60,60,60	0
61	MG	DA	3217	1/1	0.15	-	49,49,49,49	0
61	MG	CA	1730	1/1	0.33	-	55,55,55,55	0
61	MG	BA	3350	1/1	0.32	-	55,55,55,55	0
61	MG	BA	3165	1/1	0.72	-	47,47,47,47	0
61	MG	AA	1680	1/1	0.42	-	49,49,49,49	0
61	MG	BA	3093	1/1	0.42	-	51,51,51,51	0
61	MG	DA	3092	1/1	0.48	-	51,51,51,51	1
61	MG	DA	3216	1/1	0.54	-	60,60,60,60	0
61	MG	BA	3315	1/1	0.41	-	55,55,55,55	1
61	MG	BA	3074	1/1	0.41	-	47,47,47,47	0
61	MG	DA	3194	1/1	0.46	-	53,53,53,53	0
61	MG	BA	3033	1/1	0.53	-	47,47,47,47	0
61	MG	BA	3276	1/1	0.48	-	58,58,58,58	0
61	MG	DA	3155	1/1	0.44	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
61	MG	AA	1670	1/1	0.32	-	69,69,69,69	0
61	MG	CV	107	1/1	0.28	-	54,54,54,54	0
61	MG	BD	301	1/1	0.47	-	47,47,47,47	0
61	MG	BA	3203	1/1	0.38	-	52,52,52,52	0
61	MG	AA	1748	1/1	0.39	-	55,55,55,55	0
61	MG	DA	3073	1/1	0.63	-	53,53,53,53	0
61	MG	AA	1710	1/1	0.12	-	55,55,55,55	0
61	MG	CN	101	1/1	0.37	-	55,55,55,55	0
61	MG	DA	3305	1/1	0.23	-	55,55,55,55	0
61	MG	CA	1680	1/1	0.33	-	49,49,49,49	0
61	MG	BA	3040	1/1	0.63	-	47,47,47,47	0
61	MG	BA	3014	1/1	0.55	-	53,53,53,53	0
61	MG	BA	3313	1/1	0.19	-	55,55,55,55	0
61	MG	DA	3054	1/1	0.34	-	51,51,51,51	0
61	MG	BA	3120	1/1	0.64	-	50,50,50,50	0
61	MG	DA	3139	1/1	0.66	-	50,50,50,50	0
61	MG	CA	1633	1/1	0.91	-	52,52,52,52	0
61	MG	BA	3123	1/1	0.66	-	53,53,53,53	0
61	MG	BA	3046	1/1	0.44	-	47,47,47,47	0
61	MG	DA	3316	1/1	0.49	-	55,55,55,55	0
61	MG	DA	3348	1/1	0.33	-	55,55,55,55	0
61	MG	CA	1670	1/1	0.83	-	69,69,69,69	0
61	MG	DA	3099	1/1	0.35	-	54,54,54,54	0
61	MG	BA	3322	1/1	0.37	-	55,55,55,55	0
61	MG	BA	3250	1/1	0.44	-	52,52,52,52	0
61	MG	DA	3089	1/1	0.61	-	48,48,48,48	0
61	MG	BA	3212	1/1	0.50	-	55,55,55,55	0
61	MG	AA	1617	1/1	0.16	-	54,54,54,54	0
61	MG	DA	3039	1/1	0.38	-	51,51,51,51	0
61	MG	AA	1604	1/1	0.35	-	61,61,61,61	0
61	MG	BA	3109	1/1	0.36	-	48,48,48,48	0
61	MG	BA	3226	1/1	0.46	-	56,56,56,56	0
61	MG	AW	104	1/1	0.13	-	56,56,56,56	0
61	MG	DA	3247	1/1	0.32	-	55,55,55,55	1
61	MG	AA	1691	1/1	0.48	-	59,59,59,59	0
61	MG	DA	3278	1/1	0.64	-	51,51,51,51	0
61	MG	DA	3245	1/1	0.55	-	53,53,53,53	0
61	MG	BA	3142	1/1	0.40	-	47,47,47,47	0
61	MG	CA	1675	1/1	0.19	-	48,48,48,48	1
61	MG	DA	3196	1/1	0.38	-	52,52,52,52	0
61	MG	B5	102	1/1	0.58	-	53,53,53,53	0
61	MG	DA	3312	1/1	0.18	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
61	MG	AA	1707	1/1	0.48	-	49,49,49,49	0
61	MG	DA	3347	1/1	0.25	-	55,55,55,55	0
61	MG	CA	1606	1/1	0.31	-	58,58,58,58	0
61	MG	DA	3288	1/1	0.20	-	66,66,66,66	0
61	MG	DA	3260	1/1	0.51	-	59,59,59,59	0
61	MG	BA	3230	1/1	0.77	-	54,54,54,54	0
61	MG	CA	1735	1/1	0.13	-	55,55,55,55	1
61	MG	AV	104	1/1	0.11	-	54,54,54,54	0
61	MG	DA	3240	1/1	0.79	-	55,55,55,55	1
61	MG	AA	1642	1/1	0.32	-	55,55,55,55	0
61	MG	BA	3056	1/1	0.67	-	47,47,47,47	0
61	MG	BA	3267	1/1	0.25	-	54,54,54,54	0
61	MG	BA	3060	1/1	0.58	-	47,47,47,47	0
61	MG	CY	401	1/1	0.55	-	55,55,55,55	0
61	MG	BA	3195	1/1	0.42	-	52,52,52,52	0
61	MG	DA	3145	1/1	0.39	-	49,49,49,49	0
61	MG	AA	1671	1/1	0.34	-	47,47,47,47	0
61	MG	AA	1726	1/1	0.24	-	56,56,56,56	0
61	MG	DA	3044	1/1	0.53	-	47,47,47,47	0
61	MG	CA	1663	1/1	0.24	-	51,51,51,51	0
61	MG	BA	3302	1/1	0.65	-	55,55,55,55	0
61	MG	DA	3040	1/1	0.33	-	68,68,68,68	0
61	MG	BA	3087	1/1	0.31	-	49,49,49,49	0
61	MG	BA	3225	1/1	0.36	-	51,51,51,51	0
61	MG	BA	3019	1/1	0.54	-	47,47,47,47	0
61	MG	BA	3157	1/1	0.15	-	53,53,53,53	0
61	MG	DA	3161	1/1	0.34	-	47,47,47,47	0
61	MG	BA	3222	1/1	0.28	-	49,49,49,49	0
61	MG	CA	1643	1/1	0.59	-	49,49,49,49	0
61	MG	DA	3125	1/1	0.23	-	49,49,49,49	0
61	MG	DA	3269	1/1	0.51	-	52,52,52,52	0
61	MG	BA	3009	1/1	0.64	-	47,47,47,47	0
61	MG	AA	1656	1/1	0.67	-	47,47,47,47	0
61	MG	CA	1614	1/1	0.82	-	53,53,53,53	0
61	MG	DA	3083	1/1	0.30	-	51,51,51,51	0
61	MG	CA	1696	1/1	0.13	-	62,62,62,62	0
61	MG	BA	3072	1/1	0.73	-	53,53,53,53	0
61	MG	DA	3006	1/1	0.81	-	47,47,47,47	0
61	MG	AA	1633	1/1	0.13	-	55,55,55,55	0
61	MG	BA	3312	1/1	0.74	-	55,55,55,55	0
61	MG	DA	3034	1/1	0.54	-	47,47,47,47	0
61	MG	CA	1722	1/1	0.38	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
61	MG	BA	3205	1/1	0.17	-	50,50,50,50	0
61	MG	BA	3032	1/1	0.19	-	53,53,53,53	0
61	MG	BA	3238	1/1	0.10	-	55,55,55,55	1
61	MG	BD	302	1/1	0.58	-	47,47,47,47	0
61	MG	AA	1732	1/1	0.51	-	55,55,55,55	0
61	MG	AA	1607	1/1	0.47	-	58,58,58,58	0
61	MG	BA	3343	1/1	0.53	-	55,55,55,55	0
61	MG	CL	201	1/1	0.56	-	51,51,51,51	1
61	MG	CA	1683	1/1	0.28	-	47,47,47,47	0
61	MG	BA	3331	1/1	0.26	-	55,55,55,55	0
61	MG	AA	1676	1/1	0.32	-	58,58,58,58	0
61	MG	BA	3306	1/1	0.19	-	55,55,55,55	0
61	MG	DA	3221	1/1	0.56	-	54,54,54,54	0
61	MG	AA	1660	1/1	0.12	-	58,58,58,58	0
61	MG	DA	3228	1/1	0.38	-	55,55,55,55	0
61	MG	CA	1639	1/1	0.29	-	48,48,48,48	0
61	MG	AA	1622	1/1	0.24	-	48,48,48,48	0
61	MG	AA	1740	1/1	0.32	-	55,55,55,55	0
61	MG	AA	1719	1/1	0.15	-	56,56,56,56	0
61	MG	CA	1692	1/1	0.48	-	59,59,59,59	0
61	MG	DA	3010	1/1	0.65	-	47,47,47,47	0
61	MG	BA	3171	1/1	0.18	-	58,58,58,58	0
61	MG	DA	3338	1/1	0.71	-	55,55,55,55	0
61	MG	AA	1729	1/1	0.25	-	55,55,55,55	0
61	MG	DA	3154	1/1	0.26	-	53,53,53,53	0
61	MG	CA	1648	1/1	0.30	-	53,53,53,53	1
61	MG	AA	1751	1/1	0.09	-	55,55,55,55	0
61	MG	CA	1753	1/1	1.00	-	55,55,55,55	1
61	MG	AA	1648	1/1	0.13	-	62,62,62,62	0
61	MG	BA	3332	1/1	0.09	-	55,55,55,55	0
61	MG	CV	102	1/1	0.38	-	54,54,54,54	0
61	MG	BA	3036	1/1	0.23	-	53,53,53,53	0
61	MG	CA	1646	1/1	0.39	-	62,62,62,62	0
61	MG	AL	201	1/1	0.28	-	51,51,51,51	1
61	MG	DA	3009	1/1	0.57	-	55,55,55,55	0
61	MG	BA	3006	1/1	0.84	-	53,53,53,53	0
61	MG	DA	3129	1/1	0.19	-	50,50,50,50	0
61	MG	BA	3280	1/1	0.44	-	57,57,57,57	0
61	MG	BA	3156	1/1	0.51	-	48,48,48,48	0
61	MG	DA	3193	1/1	0.40	-	65,65,65,65	0
61	MG	AV	102	1/1	0.27	-	54,54,54,54	0
61	MG	DA	3195	1/1	0.26	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
61	MG	DA	3128	1/1	0.30	-	56,56,56,56	0
61	MG	B7	101	1/1	0.49	-	49,49,49,49	0
61	MG	CA	1754	1/1	0.24	-	55,55,55,55	0
61	MG	CW	103	1/1	0.34	-	54,54,54,54	1
61	MG	CA	1659	1/1	0.25	-	57,57,57,57	0
61	MG	CA	1705	1/1	0.47	-	49,49,49,49	1
61	MG	BA	3208	1/1	0.43	-	51,51,51,51	0
61	MG	DA	3103	1/1	0.47	-	47,47,47,47	0
61	MG	BA	3253	1/1	0.50	-	54,54,54,54	0
61	MG	DA	3058	1/1	0.65	-	47,47,47,47	0
61	MG	CW	104	1/1	0.33	-	56,56,56,56	0
61	MG	DA	3169	1/1	0.41	-	47,47,47,47	0
61	MG	CA	1661	1/1	0.57	-	52,52,52,52	0
61	MG	BA	3047	1/1	0.30	-	47,47,47,47	0
61	MG	DA	3119	1/1	0.52	-	49,49,49,49	0
61	MG	BA	3164	1/1	0.24	-	47,47,47,47	0
61	MG	CV	106	1/1	0.15	-	57,57,57,57	1
61	MG	AA	1609	1/1	0.28	-	52,52,52,52	0
61	MG	CA	1634	1/1	0.19	-	47,47,47,47	0
61	MG	BA	3295	1/1	0.18	-	49,49,49,49	0
61	MG	DA	3104	1/1	0.41	-	50,50,50,50	0
61	MG	BA	3223	1/1	0.36	-	52,52,52,52	0
61	MG	BA	3255	1/1	0.22	-	55,55,55,55	0
61	MG	DA	3175	1/1	0.45	-	56,56,56,56	0
61	MG	AA	1745	1/1	0.63	-	55,55,55,55	0
61	MG	BA	3293	1/1	0.46	-	55,55,55,55	1
61	MG	DA	3001	1/1	0.34	-	57,57,57,57	0
61	MG	AA	1650	1/1	0.48	-	47,47,47,47	0
61	MG	BA	3298	1/1	0.44	-	55,55,55,55	0
61	MG	DC	301	1/1	0.65	-	52,52,52,52	1
61	MG	DA	3126	1/1	0.77	-	47,47,47,47	0
61	MG	BA	3125	1/1	0.66	-	47,47,47,47	0
61	MG	BA	3070	1/1	0.41	-	50,50,50,50	0
61	MG	DA	3110	1/1	0.28	-	48,48,48,48	0
61	MG	CA	1651	1/1	0.39	-	47,47,47,47	0
61	MG	DA	3186	1/1	0.53	-	50,50,50,50	0
61	MG	CA	1629	1/1	0.49	-	51,51,51,51	0
61	MG	BA	3094	1/1	0.60	-	47,47,47,47	0
61	MG	DA	3329	1/1	0.31	-	55,55,55,55	0
61	MG	BA	3317	1/1	0.58	-	55,55,55,55	0
61	MG	DF	302	1/1	0.23	-	53,53,53,53	0
61	MG	BA	3214	1/1	0.30	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
61	MG	CA	1743	1/1	0.20	-	55,55,55,55	0
61	MG	D7	101	1/1	0.39	-	54,54,54,54	0
61	MG	AA	1735	1/1	0.60	-	55,55,55,55	0
61	MG	DA	3162	1/1	0.33	-	47,47,47,47	0
61	MG	AA	1713	1/1	0.16	-	64,64,64,64	0
61	MG	DA	3225	1/1	0.89	-	51,51,51,51	0
61	MG	CA	1708	1/1	0.25	-	49,49,49,49	0
61	MG	DB	201	1/1	0.95	-	67,67,67,67	0
61	MG	BA	3188	1/1	0.39	-	57,57,57,57	0
61	MG	DA	3137	1/1	0.64	-	50,50,50,50	0
61	MG	DA	3276	1/1	0.79	-	58,58,58,58	0
61	MG	BA	3269	1/1	0.53	-	52,52,52,52	0
61	MG	DA	3302	1/1	0.49	-	55,55,55,55	0
61	MG	BA	3143	1/1	0.29	-	57,57,57,57	0
61	MG	CA	1620	1/1	0.21	-	56,56,56,56	0
61	MG	DA	3349	1/1	0.56	-	55,55,55,55	0
61	MG	CA	1740	1/1	0.32	-	55,55,55,55	0
61	MG	DA	3160	1/1	0.32	-	55,55,55,55	0
61	MG	CA	1728	1/1	0.51	-	55,55,55,55	0
61	MG	AA	1665	1/1	0.68	-	50,50,50,50	0
61	MG	DA	3230	1/1	0.10	-	49,49,49,49	0
61	MG	DA	3353	1/1	0.63	-	55,55,55,55	0
61	MG	DA	3350	1/1	0.42	-	55,55,55,55	0
61	MG	AA	1699	1/1	0.52	-	54,54,54,54	1
61	MG	DA	3237	1/1	0.81	-	60,60,60,60	0
61	MG	CA	1686	1/1	0.39	-	57,57,57,57	0
61	MG	DA	3076	1/1	0.37	-	47,47,47,47	0
61	MG	BA	3077	1/1	0.53	-	51,51,51,51	0
61	MG	AA	1681	1/1	0.26	-	66,66,66,66	0
61	MG	BA	3352	1/1	0.33	-	55,55,55,55	0
61	MG	CA	1610	1/1	0.59	-	48,48,48,48	0
61	MG	DA	3166	1/1	0.67	-	47,47,47,47	0
61	MG	AV	107	1/1	0.64	-	54,54,54,54	1
61	MG	BA	3310	1/1	0.23	-	55,55,55,55	0
61	MG	DA	3198	1/1	0.53	-	58,58,58,58	0
61	MG	DA	3265	1/1	0.60	-	53,53,53,53	0
61	MG	DA	3272	1/1	0.41	-	59,59,59,59	1
61	MG	AA	1643	1/1	0.18	-	56,56,56,56	0
61	MG	BA	3134	1/1	0.25	-	54,54,54,54	0
61	MG	DA	3012	1/1	0.30	-	47,47,47,47	0
61	MG	DA	3017	1/1	0.67	-	47,47,47,47	0
61	MG	BB	202	1/1	0.44	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
61	MG	DA	3147	1/1	0.40	-	47,47,47,47	0
61	MG	AA	1683	1/1	0.48	-	47,47,47,47	0
61	MG	CA	1632	1/1	0.12	-	55,55,55,55	0
61	MG	BA	3209	1/1	0.51	-	66,66,66,66	0
61	MG	DA	3239	1/1	0.22	-	67,67,67,67	1
61	MG	DA	3168	1/1	0.18	-	53,53,53,53	0
61	MG	DA	3263	1/1	0.43	-	63,63,63,63	0
61	MG	AA	1688	1/1	0.47	-	63,63,63,63	1
62	ZN	AD	301	1/1	0.21	-	52,52,52,52	0
61	MG	AA	1632	1/1	0.58	-	53,53,53,53	0
61	MG	BA	3168	1/1	0.37	-	47,47,47,47	0
61	MG	DA	3109	1/1	0.38	-	52,52,52,52	0
61	MG	BA	3172	1/1	0.34	-	52,52,52,52	0
61	MG	BA	3320	1/1	0.42	-	55,55,55,55	0
61	MG	DA	3016	1/1	0.55	-	47,47,47,47	0
61	MG	AW	102	1/1	0.13	-	60,60,60,60	1
61	MG	DA	3187	1/1	0.53	-	51,51,51,51	0
61	MG	BA	3345	1/1	0.24	-	55,55,55,55	0
61	MG	BA	3261	1/1	0.51	-	52,52,52,52	0
61	MG	DA	3208	1/1	0.24	-	60,60,60,60	0
61	MG	DA	3120	1/1	0.88	-	49,49,49,49	0
61	MG	DA	3215	1/1	0.47	-	48,48,48,48	0
61	MG	DA	3146	1/1	0.44	-	47,47,47,47	0
61	MG	D1	101	1/1	0.35	-	55,55,55,55	0
61	MG	DA	3273	1/1	0.29	-	58,58,58,58	0
61	MG	DA	3050	1/1	0.53	-	47,47,47,47	0
61	MG	BA	3236	1/1	0.12	-	47,47,47,47	0
61	MG	BA	3007	1/1	0.48	-	52,52,52,52	0
61	MG	BA	3177	1/1	0.85	-	47,47,47,47	0
61	MG	BA	3086	1/1	0.48	-	48,48,48,48	0
61	MG	BC	301	1/1	0.49	-	52,52,52,52	1
61	MG	AA	1612	1/1	0.12	-	52,52,52,52	0
61	MG	BA	3339	1/1	0.24	-	55,55,55,55	0
61	MG	DA	3255	1/1	0.44	-	60,60,60,60	0
61	MG	DA	3059	1/1	0.77	-	55,55,55,55	0
61	MG	CA	1622	1/1	0.85	-	57,57,57,57	0
61	MG	AA	1654	1/1	0.16	-	53,53,53,53	0
61	MG	BA	3128	1/1	0.23	-	50,50,50,50	0
61	MG	AA	1694	1/1	0.21	-	56,56,56,56	0
61	MG	BA	3081	1/1	0.36	-	47,47,47,47	0
61	MG	DA	3135	1/1	0.52	-	54,54,54,54	0
61	MG	DB	204	1/1	0.27	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
61	MG	BA	3246	1/1	0.40	-	55,55,55,55	0
61	MG	AA	1725	1/1	1.03	-	54,54,54,54	0
61	MG	DA	3286	1/1	0.23	-	60,60,60,60	0
61	MG	DA	3295	1/1	0.74	-	55,55,55,55	0
61	MG	BA	3035	1/1	0.34	-	55,55,55,55	0
61	MG	DA	3085	1/1	0.43	-	47,47,47,47	0
61	MG	DA	3299	1/1	0.36	-	55,55,55,55	0
61	MG	BA	3034	1/1	0.37	-	50,50,50,50	0
61	MG	DA	3308	1/1	0.14	-	55,55,55,55	0
61	MG	DA	3123	1/1	0.23	-	64,64,64,64	1
61	MG	AV	101	1/1	0.40	-	49,49,49,49	0
61	MG	AA	1673	1/1	0.12	-	52,52,52,52	0
61	MG	AA	1734	1/1	0.16	-	55,55,55,55	0
61	MG	DA	3020	1/1	0.58	-	47,47,47,47	0
61	MG	CA	1625	1/1	0.60	-	53,53,53,53	0
61	MG	BA	3266	1/1	0.56	-	59,59,59,59	0
61	MG	BA	3085	1/1	0.18	-	47,47,47,47	0
61	MG	CW	102	1/1	0.18	-	60,60,60,60	0
61	MG	DA	3084	1/1	0.35	-	47,47,47,47	0
61	MG	DA	3256	1/1	0.55	-	55,55,55,55	0
61	MG	DA	3148	1/1	0.36	-	51,51,51,51	0
61	MG	DA	3136	1/1	0.91	-	58,58,58,58	0
61	MG	BA	3160	1/1	0.32	-	47,47,47,47	0
61	MG	BA	3305	1/1	0.73	-	55,55,55,55	0
61	MG	BA	3354	1/1	0.24	-	55,55,55,55	0
61	MG	DA	3070	1/1	0.34	-	48,48,48,48	0
61	MG	BA	3282	1/1	0.46	-	57,57,57,57	0
61	MG	CA	1712	1/1	0.53	-	47,47,47,47	0
61	MG	AA	1742	1/1	0.31	-	55,55,55,55	0
61	MG	DY	201	1/1	0.29	-	55,55,55,55	0
61	MG	DA	3108	1/1	0.19	-	51,51,51,51	0
61	MG	CA	1605	1/1	0.61	-	59,59,59,59	0
61	MG	DA	3055	1/1	0.64	-	47,47,47,47	0
61	MG	BA	3183	1/1	0.58	-	56,56,56,56	0
61	MG	BA	3294	1/1	0.12	-	52,52,52,52	0
61	MG	BA	3219	1/1	0.87	-	49,49,49,49	0
61	MG	AA	1718	1/1	0.24	-	55,55,55,55	0
61	MG	BA	3262	1/1	0.18	-	63,63,63,63	1
61	MG	AA	1666	1/1	0.71	-	57,57,57,57	0
61	MG	CA	1637	1/1	0.27	-	52,52,52,52	0
61	MG	BA	3066	1/1	0.94	-	50,50,50,50	0
61	MG	AA	1625	1/1	0.35	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
61	MG	BA	3185	1/1	0.62	-	50,50,50,50	0
61	MG	DA	3205	1/1	0.55	-	57,57,57,57	0
61	MG	BF	301	1/1	0.22	-	47,47,47,47	0
61	MG	DA	3035	1/1	0.42	-	50,50,50,50	0
61	MG	DA	3281	1/1	0.37	-	57,57,57,57	0
61	MG	BA	3316	1/1	0.51	-	55,55,55,55	0
61	MG	BA	3135	1/1	0.70	-	58,58,58,58	0
61	MG	DA	3015	1/1	0.54	-	53,53,53,53	0
61	MG	AA	1644	1/1	0.38	-	49,49,49,49	0
61	MG	CA	1752	1/1	0.16	-	55,55,55,55	1
61	MG	DA	3173	1/1	0.26	-	58,58,58,58	0
61	MG	CA	1756	1/1	0.36	-	55,55,55,55	1
61	MG	DB	202	1/1	0.74	-	55,55,55,55	0
61	MG	DA	3102	1/1	0.75	-	47,47,47,47	0
61	MG	BA	3192	1/1	0.31	-	65,65,65,65	0
61	MG	AA	1620	1/1	0.31	-	55,55,55,55	0
61	MG	AV	103	1/1	0.20	-	54,54,54,54	1
61	MG	BA	3062	1/1	0.53	-	47,47,47,47	0
61	MG	BA	3054	1/1	0.77	-	47,47,47,47	0
61	MG	BA	3096	1/1	0.44	-	56,56,56,56	0
61	MG	BA	3348	1/1	0.62	-	55,55,55,55	0
61	MG	DA	3165	1/1	0.29	-	47,47,47,47	0
61	MG	AA	1652	1/1	0.35	-	47,47,47,47	0
61	MG	AA	1613	1/1	0.29	-	56,56,56,56	0
61	MG	AA	1669	1/1	0.27	-	47,47,47,47	0
61	MG	DA	3149	1/1	0.23	-	47,47,47,47	0
61	MG	BA	3010	1/1	0.55	-	52,52,52,52	0
61	MG	BA	3112	1/1	0.35	-	48,48,48,48	0
61	MG	AA	1628	1/1	0.37	-	70,70,70,70	0
61	MG	CA	1748	1/1	0.64	-	55,55,55,55	1
61	MG	CA	1703	1/1	0.31	-	47,47,47,47	0
61	MG	BA	3116	1/1	0.38	-	47,47,47,47	0
61	MG	CA	1727	1/1	0.27	-	56,56,56,56	0
61	MG	AA	1702	1/1	0.34	-	47,47,47,47	0
61	MG	CA	1624	1/1	0.42	-	51,51,51,51	0
61	MG	BA	3075	1/1	0.41	-	47,47,47,47	0
61	MG	BA	3083	1/1	0.52	-	47,47,47,47	0
61	MG	DA	3327	1/1	0.50	-	55,55,55,55	0
61	MG	AA	1739	1/1	0.21	-	55,55,55,55	1
61	MG	BA	3119	1/1	0.75	-	49,49,49,49	0
61	MG	DA	3105	1/1	0.83	-	48,48,48,48	0
61	MG	DA	3130	1/1	0.24	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
61	MG	DA	3203	1/1	0.45	-	47,47,47,47	0
61	MG	AA	1655	1/1	0.40	-	52,52,52,52	0
61	MG	BA	3049	1/1	0.56	-	47,47,47,47	0
61	MG	BA	3202	1/1	0.33	-	47,47,47,47	0
61	MG	DD	302	1/1	0.45	-	47,47,47,47	0
61	MG	CA	1734	1/1	0.24	-	55,55,55,55	1
61	MG	DA	3008	1/1	0.35	-	52,52,52,52	0
61	MG	AA	1638	1/1	0.26	-	52,52,52,52	0
61	MG	CV	105	1/1	0.26	-	50,50,50,50	0
61	MG	AA	1685	1/1	0.30	-	57,57,57,57	0
61	MG	BA	3170	1/1	0.43	-	50,50,50,50	0
61	MG	CA	1666	1/1	0.47	-	57,57,57,57	0
61	MG	AA	1649	1/1	0.17	-	53,53,53,53	0
61	MG	DA	3319	1/1	0.48	-	55,55,55,55	0
61	MG	BA	3028	1/1	0.46	-	52,52,52,52	0
61	MG	CA	1676	1/1	0.52	-	58,58,58,58	0
61	MG	CA	1631	1/1	0.82	-	53,53,53,53	0
61	MG	CA	1717	1/1	0.43	-	52,52,52,52	0
61	MG	DA	3262	1/1	0.32	-	52,52,52,52	0
61	MG	DA	3250	1/1	0.43	-	56,56,56,56	0
61	MG	DA	3087	1/1	0.57	-	48,48,48,48	0
61	MG	DA	3007	1/1	0.72	-	53,53,53,53	0
61	MG	BA	3340	1/1	0.55	-	55,55,55,55	0
61	MG	BA	3146	1/1	0.65	-	47,47,47,47	0
61	MG	BA	3136	1/1	0.75	-	50,50,50,50	0
61	MG	BA	3105	1/1	0.48	-	47,47,47,47	0
61	MG	DA	3326	1/1	0.53	-	55,55,55,55	0
61	MG	DA	3264	1/1	0.12	-	56,56,56,56	0
61	MG	CA	1619	1/1	0.21	-	55,55,55,55	0
61	MG	BA	3299	1/1	0.39	-	55,55,55,55	0
61	MG	DA	3180	1/1	0.21	-	52,52,52,52	0
61	MG	CA	1656	1/1	0.78	-	47,47,47,47	0
61	MG	CA	1693	1/1	0.76	-	59,59,59,59	0
61	MG	CA	1623	1/1	0.43	-	48,48,48,48	0
61	MG	BA	3342	1/1	0.29	-	55,55,55,55	0
61	MG	DA	3095	1/1	0.76	-	47,47,47,47	0
61	MG	BA	3029	1/1	0.36	-	55,55,55,55	0
61	MG	DA	3224	1/1	0.48	-	52,52,52,52	0
61	MG	BA	3020	1/1	0.59	-	47,47,47,47	0
61	MG	DA	3033	1/1	0.26	-	53,53,53,53	0
61	MG	DX	101	1/1	0.27	-	55,55,55,55	0
61	MG	DA	3258	1/1	0.74	-	51,51,51,51	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
61	MG	BA	3002	1/1	0.28	-	67,67,67,67	0
61	MG	AA	1696	1/1	0.32	-	62,62,62,62	0
61	MG	BA	3187	1/1	0.39	-	48,48,48,48	0
61	MG	DA	3223	1/1	0.32	-	49,49,49,49	0
61	MG	DB	203	1/1	0.74	-	55,55,55,55	0
61	MG	DA	3078	1/1	0.89	-	51,51,51,51	0
61	MG	BA	3232	1/1	0.48	-	53,53,53,53	0
61	MG	DA	3298	1/1	0.29	-	55,55,55,55	0
61	MG	BA	3113	1/1	0.52	-	47,47,47,47	0
61	MG	BA	3004	1/1	0.26	-	53,53,53,53	0
61	MG	BA	3173	1/1	0.36	-	56,56,56,56	0
61	MG	CA	1723	1/1	0.10	-	55,55,55,55	0
61	MG	BA	3216	1/1	0.29	-	49,49,49,49	0
61	MG	AA	1658	1/1	0.28	-	49,49,49,49	0
61	MG	AA	1722	1/1	0.27	-	55,55,55,55	0
61	MG	BA	3179	1/1	0.38	-	59,59,59,59	0
61	MG	BA	3323	1/1	0.86	-	55,55,55,55	0
61	MG	DA	3226	1/1	0.44	-	51,51,51,51	0
61	MG	AA	1640	1/1	0.43	-	48,48,48,48	0
61	MG	AA	1602	1/1	0.41	-	52,52,52,52	0
61	MG	CA	1685	1/1	0.34	-	47,47,47,47	0
61	MG	AA	1756	1/1	0.14	-	55,55,55,55	1
61	MG	AA	1647	1/1	0.40	-	62,62,62,62	0
61	MG	AA	1657	1/1	0.27	-	54,54,54,54	0
61	MG	AV	106	1/1	0.05	-	57,57,57,57	0
61	MG	CA	1615	1/1	0.66	-	64,64,64,64	0
61	MG	DA	3064	1/1	0.41	-	56,56,56,56	0
61	MG	DA	3003	1/1	0.42	-	67,67,67,67	0
61	MG	BA	3248	1/1	0.26	-	56,56,56,56	1
61	MG	BA	3337	1/1	0.15	-	55,55,55,55	0
61	MG	CA	1690	1/1	0.20	-	59,59,59,59	0
61	MG	DA	3049	1/1	0.44	-	47,47,47,47	0
61	MG	DA	3159	1/1	0.82	-	49,49,49,49	0
61	MG	DA	3345	1/1	0.34	-	55,55,55,55	0
61	MG	DA	3206	1/1	0.33	-	50,50,50,50	0
61	MG	AA	1738	1/1	0.08	-	55,55,55,55	0
61	MG	DA	3303	1/1	0.77	-	55,55,55,55	0
61	MG	DA	3279	1/1	0.29	-	55,55,55,55	0
61	MG	DA	3199	1/1	0.52	-	53,53,53,53	0
61	MG	BA	3038	1/1	0.47	-	51,51,51,51	0
61	MG	BA	3346	1/1	0.44	-	55,55,55,55	0
61	MG	BA	3263	1/1	0.12	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
61	MG	BA	3082	1/1	0.68	-	51,51,51,51	0
61	MG	BA	3207	1/1	0.56	-	60,60,60,60	0
61	MG	DA	3185	1/1	0.53	-	56,56,56,56	0
61	MG	DA	3134	1/1	0.66	-	64,64,64,64	0
61	MG	BA	3260	1/1	0.16	-	57,57,57,57	0
61	MG	BA	3138	1/1	0.40	-	50,50,50,50	0
61	MG	AA	1661	1/1	0.46	-	52,52,52,52	0
61	MG	AA	1717	1/1	0.24	-	66,66,66,66	0
61	MG	DA	3342	1/1	0.24	-	55,55,55,55	0
61	MG	CA	1711	1/1	0.15	-	55,55,55,55	0
61	MG	AA	1690	1/1	0.64	-	52,52,52,52	0
61	MG	DA	3182	1/1	0.30	-	56,56,56,56	0
61	MG	DA	3121	1/1	0.42	-	50,50,50,50	0
61	MG	DA	3072	1/1	0.24	-	47,47,47,47	0
61	MG	DA	3200	1/1	1.00	-	58,58,58,58	0
61	MG	AA	1615	1/1	0.81	-	53,53,53,53	0
61	MG	AA	1711	1/1	0.28	-	47,47,47,47	0
61	MG	BA	3273	1/1	0.47	-	58,58,58,58	0
61	MG	DA	3069	1/1	0.34	-	47,47,47,47	0
61	MG	DA	3141	1/1	0.36	-	56,56,56,56	0
61	MG	AA	1697	1/1	0.36	-	52,52,52,52	0
61	MG	DA	3335	1/1	0.49	-	55,55,55,55	0
61	MG	CA	1749	1/1	0.37	-	55,55,55,55	0
61	MG	CA	1609	1/1	0.34	-	55,55,55,55	0
61	MG	DA	3249	1/1	0.18	-	56,56,56,56	0
61	MG	BA	3080	1/1	0.67	-	52,52,52,52	0
61	MG	DA	3332	1/1	0.52	-	55,55,55,55	0
61	MG	DA	3218	1/1	0.54	-	51,51,51,51	0
61	MG	DA	3024	1/1	0.98	-	49,49,49,49	0
61	MG	CA	1617	1/1	0.34	-	51,51,51,51	0
61	MG	AA	1608	1/1	0.25	-	47,47,47,47	0
61	MG	BA	3271	1/1	0.56	-	51,51,51,51	0
61	MG	D3	101	1/1	0.47	-	58,58,58,58	0
61	MG	DA	3041	1/1	0.36	-	47,47,47,47	0
61	MG	DA	3241	1/1	0.08	-	55,55,55,55	0
61	MG	CA	1660	1/1	0.20	-	58,58,58,58	0
61	MG	BU	201	1/1	0.40	-	48,48,48,48	0
61	MG	BA	3141	1/1	0.56	-	49,49,49,49	0
61	MG	CA	1671	1/1	0.20	-	47,47,47,47	0
61	MG	BA	3008	1/1	0.42	-	55,55,55,55	0
61	MG	AA	1672	1/1	0.22	-	53,53,53,53	0
61	MG	B5	101	1/1	0.34	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
61	MG	DA	3143	1/1	0.48	-	47,47,47,47	1
61	MG	DA	3052	1/1	0.55	-	51,51,51,51	0
61	MG	CA	1668	1/1	0.83	-	58,58,58,58	0
61	MG	CV	101	1/1	0.57	-	49,49,49,49	0
61	MG	DA	3046	1/1	0.79	-	47,47,47,47	0
61	MG	BA	3227	1/1	0.64	-	55,55,55,55	0
61	MG	AA	1626	1/1	0.28	-	53,53,53,53	0
61	MG	DA	3235	1/1	0.31	-	49,49,49,49	0
61	MG	BA	3058	1/1	0.72	-	55,55,55,55	0
61	MG	DA	3231	1/1	0.52	-	54,54,54,54	1
61	MG	BA	3090	1/1	0.46	-	48,48,48,48	0
61	MG	CA	1658	1/1	0.28	-	49,49,49,49	0
61	MG	CA	1721	1/1	0.28	-	58,58,58,58	0
61	MG	BA	3301	1/1	0.45	-	55,55,55,55	0
61	MG	BA	3012	1/1	0.55	-	49,49,49,49	0
61	MG	DA	3100	1/1	0.74	-	55,55,55,55	0
61	MG	DA	3026	1/1	0.45	-	55,55,55,55	0
61	MG	BA	3084	1/1	0.37	-	47,47,47,47	0
61	MG	BA	3015	1/1	0.49	-	47,47,47,47	0
61	MG	CA	1641	1/1	0.38	-	55,55,55,55	0
61	MG	AA	1659	1/1	0.30	-	57,57,57,57	0
61	MG	BA	3239	1/1	0.28	-	55,55,55,55	0
61	MG	BA	3045	1/1	0.83	-	47,47,47,47	0
61	MG	DR	201	1/1	0.33	-	47,47,47,47	0
61	MG	DA	3296	1/1	0.64	-	55,55,55,55	0
61	MG	DA	3090	1/1	0.66	-	48,48,48,48	0
61	MG	BP	201	1/1	0.20	-	49,49,49,49	0
61	MG	AA	1606	1/1	0.38	-	59,59,59,59	0
61	MG	DA	3238	1/1	0.24	-	47,47,47,47	0
61	MG	CA	1745	1/1	0.22	-	55,55,55,55	0
61	MG	DA	3004	1/1	0.40	-	61,61,61,61	0
61	MG	AA	1637	1/1	0.45	-	53,53,53,53	0
61	MG	BA	3235	1/1	0.24	-	60,60,60,60	0
61	MG	AA	1749	1/1	0.37	-	55,55,55,55	0
61	MG	AA	1700	1/1	0.31	-	51,51,51,51	0
61	MG	AA	1667	1/1	0.27	-	47,47,47,47	0
61	MG	CA	1647	1/1	0.23	-	62,62,62,62	0
61	MG	BA	3347	1/1	0.28	-	55,55,55,55	0
61	MG	DA	3315	1/1	0.25	-	55,55,55,55	0
61	MG	AA	1720	1/1	0.48	-	58,58,58,58	1
61	MG	BA	3186	1/1	0.90	-	51,51,51,51	0
61	MG	CA	1667	1/1	0.39	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
61	MG	DA	3176	1/1	0.41	-	58,58,58,58	0
62	ZN	AN	101	1/1	0.09	-	60,60,60,60	1
61	MG	DA	3306	1/1	0.10	-	55,55,55,55	0
61	MG	CA	1700	1/1	0.25	-	54,54,54,54	0
61	MG	BA	3027	1/1	0.30	-	50,50,50,50	0
61	MG	DA	3323	1/1	0.43	-	55,55,55,55	0
61	MG	BA	3234	1/1	0.79	-	52,52,52,52	0
61	MG	DA	3013	1/1	0.56	-	49,49,49,49	0
61	MG	BA	3272	1/1	0.27	-	59,59,59,59	1
61	MG	BA	3103	1/1	0.58	-	50,50,50,50	0
61	MG	BA	3319	1/1	0.27	-	55,55,55,55	0
61	MG	BB	204	1/1	0.23	-	55,55,55,55	0
61	MG	BA	3037	1/1	0.40	-	47,47,47,47	0
61	MG	AA	1701	1/1	0.28	-	51,51,51,51	0
61	MG	CA	1636	1/1	0.53	-	53,53,53,53	0
61	MG	DA	3174	1/1	0.31	-	52,52,52,52	0
61	MG	DA	3081	1/1	0.55	-	52,52,52,52	0
61	MG	CA	1684	1/1	0.16	-	49,49,49,49	0
61	MG	DA	3227	1/1	0.31	-	56,56,56,56	0
61	MG	DA	3082	1/1	0.78	-	47,47,47,47	0
61	MG	CA	1673	1/1	0.38	-	52,52,52,52	1
61	MG	DA	3234	1/1	0.54	-	47,47,47,47	0
61	MG	DA	3284	1/1	0.89	-	57,57,57,57	0
61	MG	AA	1679	1/1	0.21	-	53,53,53,53	0
61	MG	AA	1630	1/1	0.66	-	51,51,51,51	0
61	MG	BA	3321	1/1	0.18	-	55,55,55,55	0
61	MG	BA	3286	1/1	0.23	-	60,60,60,60	0
61	MG	AA	1687	1/1	0.21	-	48,48,48,48	0
61	MG	DA	3057	1/1	0.67	-	47,47,47,47	0
61	MG	DA	3011	1/1	0.52	-	52,52,52,52	0
61	MG	AA	1619	1/1	0.59	-	49,49,49,49	0
61	MG	DA	3244	1/1	0.50	-	47,47,47,47	0
61	MG	DA	3213	1/1	0.32	-	55,55,55,55	0
61	MG	BA	3076	1/1	0.26	-	48,48,48,48	0
61	MG	DA	3246	1/1	0.22	-	60,60,60,60	0
61	MG	DA	3351	1/1	0.65	-	55,55,55,55	0
61	MG	BA	3297	1/1	0.53	-	55,55,55,55	0
61	MG	CA	1718	1/1	0.42	-	66,66,66,66	0
61	MG	CA	1755	1/1	0.48	-	55,55,55,55	0
61	MG	DA	3337	1/1	0.24	-	55,55,55,55	0
61	MG	DA	3065	1/1	0.56	-	53,53,53,53	0
61	MG	BA	3204	1/1	0.41	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
61	MG	DA	3066	1/1	0.54	-	52,52,52,52	0
61	MG	CA	1626	1/1	0.17	-	53,53,53,53	0
61	MG	BA	3244	1/1	0.23	-	60,60,60,60	0
61	MG	BA	3140	1/1	0.48	-	56,56,56,56	0
61	MG	BA	3228	1/1	0.74	-	52,52,52,52	0
61	MG	CA	1709	1/1	0.39	-	65,65,65,65	0
61	MG	DA	3267	1/1	0.39	-	54,54,54,54	0
61	MG	AA	1629	1/1	0.23	-	56,56,56,56	0
61	MG	BA	3336	1/1	0.62	-	55,55,55,55	0
61	MG	DA	3188	1/1	0.43	-	48,48,48,48	0
61	MG	BA	3169	1/1	0.56	-	51,51,51,51	0
61	MG	CW	105	1/1	0.48	-	53,53,53,53	0
61	MG	BA	3329	1/1	0.39	-	55,55,55,55	1
61	MG	CA	1688	1/1	0.15	-	48,48,48,48	0
61	MG	BA	3100	1/1	0.82	-	51,51,51,51	0
61	MG	BA	3043	1/1	0.79	-	47,47,47,47	0
61	MG	DA	3031	1/1	0.73	-	47,47,47,47	0
61	MG	CA	1724	1/1	0.18	-	57,57,57,57	1
61	MG	AA	1645	1/1	0.18	-	57,57,57,57	0
61	MG	CA	1731	1/1	0.31	-	55,55,55,55	0
61	MG	AE	201	1/1	0.76	-	57,57,57,57	0
61	MG	CA	1638	1/1	0.60	-	53,53,53,53	0
61	MG	BA	3092	1/1	0.63	-	50,50,50,50	0
61	MG	BA	3252	1/1	0.33	-	49,49,49,49	0
61	MG	AA	1716	1/1	1.03	-	52,52,52,52	0
61	MG	BA	3003	1/1	0.31	-	61,61,61,61	0
61	MG	BA	3311	1/1	0.39	-	55,55,55,55	0
61	MG	BA	3251	1/1	0.34	-	61,61,61,61	0
61	MG	DD	301	1/1	0.58	-	47,47,47,47	0
61	MG	AA	1662	1/1	0.15	-	52,52,52,52	0
61	MG	BA	3158	1/1	0.85	-	49,49,49,49	0
61	MG	CA	1669	1/1	0.30	-	47,47,47,47	0
61	MG	DA	3171	1/1	0.66	-	51,51,51,51	0
61	MG	AA	1755	1/1	0.64	-	55,55,55,55	0
61	MG	BA	3122	1/1	0.43	-	64,64,64,64	1
61	MG	BA	3217	1/1	0.70	-	51,51,51,51	0
61	MG	DA	3328	1/1	0.38	-	55,55,55,55	1
61	MG	DA	3346	1/1	0.88	-	55,55,55,55	0
61	MG	BA	3237	1/1	0.26	-	67,67,67,67	0
61	MG	AA	1682	1/1	0.15	-	53,53,53,53	0
61	MG	BA	3114	1/1	0.29	-	48,48,48,48	0
61	MG	BA	3175	1/1	0.32	-	49,49,49,49	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
61	MG	CA	1618	1/1	0.30	-	49,49,49,49	0
61	MG	DA	3314	1/1	0.24	-	55,55,55,55	1
61	MG	DA	3300	1/1	0.37	-	55,55,55,55	0
61	MG	DA	3032	1/1	0.25	-	50,50,50,50	0
61	MG	AA	1678	1/1	0.05	-	49,49,49,49	0
61	MG	BA	3274	1/1	0.66	-	63,63,63,63	0
61	MG	BA	3258	1/1	0.38	-	58,58,58,58	0
61	MG	DA	3331	1/1	0.09	-	55,55,55,55	1
61	MG	BA	3247	1/1	0.18	-	59,59,59,59	0
61	MG	AA	1698	1/1	0.35	-	53,53,53,53	1
61	MG	AA	1750	1/1	0.24	-	55,55,55,55	0
61	MG	DA	3077	1/1	0.36	-	48,48,48,48	0
61	MG	AA	1651	1/1	0.70	-	54,54,54,54	0
61	MG	DA	3047	1/1	0.36	-	47,47,47,47	0
61	MG	BA	3268	1/1	0.71	-	59,59,59,59	0
61	MG	AW	103	1/1	0.07	-	54,54,54,54	0
61	MG	DA	3229	1/1	0.37	-	52,52,52,52	0
61	MG	DA	3037	1/1	0.39	-	53,53,53,53	0
61	MG	CW	101	1/1	0.72	-	56,56,56,56	1
61	MG	DA	3142	1/1	0.53	-	49,49,49,49	0
61	MG	DA	3028	1/1	0.39	-	50,50,50,50	0
61	MG	BA	3155	1/1	0.33	-	51,51,51,51	0
61	MG	BA	3051	1/1	0.35	-	51,51,51,51	0
61	MG	CA	1732	1/1	0.17	-	55,55,55,55	0
61	MG	DA	3086	1/1	0.15	-	47,47,47,47	0
61	MG	AA	1746	1/1	0.26	-	55,55,55,55	1
61	MG	BA	3117	1/1	0.44	-	52,52,52,52	0
61	MG	DA	3023	1/1	0.82	-	47,47,47,47	0
61	MG	DA	3343	1/1	0.47	-	55,55,55,55	0
61	MG	BA	3265	1/1	0.45	-	47,47,47,47	0
61	MG	DA	3324	1/1	0.51	-	55,55,55,55	0
61	MG	BA	3110	1/1	0.41	-	49,49,49,49	0
61	MG	DA	3133	1/1	0.34	-	57,57,57,57	0
61	MG	DA	3257	1/1	0.61	-	55,55,55,55	0
61	MG	D5	102	1/1	0.39	-	53,53,53,53	0
61	MG	BA	3290	1/1	0.35	-	57,57,57,57	0
61	MG	AA	1668	1/1	0.59	-	58,58,58,58	0
61	MG	AA	1603	1/1	0.28	-	57,57,57,57	0
61	MG	BA	3304	1/1	0.65	-	55,55,55,55	0
61	MG	BA	3194	1/1	0.27	-	53,53,53,53	0
61	MG	DA	3097	1/1	0.46	-	56,56,56,56	0
61	MG	BA	3181	1/1	0.28	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
61	MG	DA	3062	1/1	0.44	-	48,48,48,48	0
61	MG	BA	3071	1/1	0.41	-	47,47,47,47	0
61	MG	BA	3069	1/1	0.37	-	48,48,48,48	0
61	MG	DA	3112	1/1	0.33	-	52,52,52,52	0
61	MG	AA	1623	1/1	0.61	-	57,57,57,57	0
61	MG	AA	1664	1/1	0.33	-	60,60,60,60	0
61	MG	BA	3303	1/1	0.76	-	55,55,55,55	0
61	MG	CA	1742	1/1	0.69	-	55,55,55,55	0
61	MG	CA	1616	1/1	0.39	-	54,54,54,54	0
61	MG	BA	3309	1/1	0.23	-	55,55,55,55	0
61	MG	BA	3245	1/1	0.39	-	53,53,53,53	0
61	MG	BA	3106	1/1	0.73	-	51,51,51,51	0
61	MG	AA	1635	1/1	0.14	-	47,47,47,47	0
61	MG	BA	3022	1/1	1.00	-	47,47,47,47	0
61	MG	DA	3322	1/1	0.76	-	55,55,55,55	0
61	MG	CA	1645	1/1	0.65	-	50,50,50,50	0
61	MG	DA	3019	1/1	0.58	-	54,54,54,54	0
61	MG	BA	3256	1/1	0.64	-	55,55,55,55	0
61	MG	CA	1744	1/1	0.42	-	55,55,55,55	0
61	MG	DF	303	1/1	0.66	-	59,59,59,59	0
61	MG	BA	3338	1/1	0.32	-	55,55,55,55	0
61	MG	DA	3294	1/1	0.53	-	49,49,49,49	1
61	MG	BA	3104	1/1	0.76	-	48,48,48,48	0
61	MG	BA	3189	1/1	0.37	-	59,59,59,59	0
61	MG	DA	3113	1/1	0.31	-	48,48,48,48	0
61	MG	DA	3317	1/1	0.35	-	55,55,55,55	0
61	MG	BA	3211	1/1	0.26	-	59,59,59,59	1
61	MG	DA	3340	1/1	0.34	-	55,55,55,55	0
61	MG	DA	3214	1/1	0.35	-	58,58,58,58	0
61	MG	CA	1681	1/1	0.60	-	66,66,66,66	0
61	MG	BA	3324	1/1	0.36	-	55,55,55,55	0
61	MG	CA	1607	1/1	0.32	-	47,47,47,47	0
61	MG	AA	1611	1/1	0.52	-	48,48,48,48	0
61	MG	CA	1699	1/1	0.19	-	53,53,53,53	1
61	MG	DA	3029	1/1	0.32	-	52,52,52,52	0
61	MG	CA	1687	1/1	0.41	-	58,58,58,58	0
61	MG	DA	3219	1/1	0.40	-	66,66,66,66	0
61	MG	DA	3045	1/1	0.43	-	56,56,56,56	0
61	MG	DA	3266	1/1	0.51	-	47,47,47,47	0
61	MG	BA	3126	1/1	0.30	-	52,52,52,52	0
61	MG	CA	1654	1/1	0.72	-	57,57,57,57	0
61	MG	BA	3335	1/1	0.54	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
61	MG	CA	1601	1/1	0.30	-	56,56,56,56	0
61	MG	CV	103	1/1	0.26	-	54,54,54,54	0
61	MG	CA	1702	1/1	0.34	-	51,51,51,51	0
61	MG	BA	3333	1/1	0.71	-	55,55,55,55	0
61	MG	DA	3002	1/1	0.92	-	54,54,54,54	1
61	MG	BA	3241	1/1	0.25	-	61,61,61,61	1
61	MG	BA	3190	1/1	0.45	-	54,54,54,54	0
61	MG	BA	3078	1/1	0.67	-	56,56,56,56	0
61	MG	BA	3133	1/1	0.34	-	64,64,64,64	0
61	MG	BA	3176	1/1	0.58	-	48,48,48,48	0
61	MG	BA	3264	1/1	0.57	-	53,53,53,53	0
61	MG	DA	3071	1/1	0.31	-	50,50,50,50	0
61	MG	CA	1640	1/1	0.77	-	47,47,47,47	0
61	MG	BA	3196	1/1	0.44	-	47,47,47,47	0
61	MG	CA	1713	1/1	0.37	-	54,54,54,54	0
61	MG	DA	3254	1/1	0.28	-	54,54,54,54	0
61	MG	BA	3283	1/1	0.38	-	65,65,65,65	0
61	MG	BA	3131	1/1	0.40	-	59,59,59,59	0
61	MG	DA	3091	1/1	0.39	-	48,48,48,48	0
61	MG	DA	3313	1/1	0.78	-	55,55,55,55	0
61	MG	BA	3121	1/1	0.25	-	50,50,50,50	0
61	MG	CA	1664	1/1	0.43	-	60,60,60,60	0
61	MG	CA	1613	1/1	0.26	-	52,52,52,52	0
61	MG	BA	3059	1/1	0.27	-	48,48,48,48	0
61	MG	BA	3307	1/1	0.38	-	55,55,55,55	0
61	MG	BA	3099	1/1	0.76	-	55,55,55,55	0
61	MG	AA	1618	1/1	0.21	-	51,51,51,51	1
61	MG	BA	3318	1/1	0.29	-	55,55,55,55	0
61	MG	BA	3296	1/1	0.60	-	55,55,55,55	0
61	MG	CA	1649	1/1	0.42	-	47,47,47,47	0
61	MG	CA	1611	1/1	0.25	-	52,52,52,52	0
61	MG	BA	3167	1/1	0.30	-	53,53,53,53	0
61	MG	BA	3197	1/1	0.46	-	58,58,58,58	0
61	MG	BA	3111	1/1	0.31	-	52,52,52,52	0
61	MG	B1	101	1/1	0.47	-	55,55,55,55	0
61	MG	DF	301	1/1	0.26	-	47,47,47,47	0
61	MG	BA	3206	1/1	0.28	-	47,47,47,47	0
61	MG	BA	3041	1/1	0.64	-	47,47,47,47	0
61	MG	BA	3127	1/1	0.25	-	56,56,56,56	0
61	MG	DA	3283	1/1	0.46	-	65,65,65,65	0
61	MG	AY	401	1/1	0.52	-	55,55,55,55	0
61	MG	DA	3252	1/1	0.45	-	61,61,61,61	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
61	MG	BA	3161	1/1	0.34	-	47,47,47,47	0
61	MG	AA	1731	1/1	0.23	-	55,55,55,55	0
61	MG	DA	3291	1/1	0.68	-	54,54,54,54	0
61	MG	AA	1706	1/1	0.23	-	51,51,51,51	0
61	MG	DA	3056	1/1	0.45	-	47,47,47,47	0
61	MG	CV	104	1/1	0.08	-	54,54,54,54	0
61	MG	BA	3001	1/1	0.34	-	54,54,54,54	0
61	MG	DA	3334	1/1	0.32	-	55,55,55,55	0
61	MG	BA	3257	1/1	0.27	-	51,51,51,51	0
61	MG	DA	3222	1/1	0.70	-	53,53,53,53	0
61	MG	DA	3233	1/1	0.61	-	53,53,53,53	0
61	MG	BA	3139	1/1	0.49	-	50,50,50,50	0
61	MG	CA	1715	1/1	0.60	-	59,59,59,59	0
61	MG	AA	1733	1/1	0.25	-	55,55,55,55	0
61	MG	DA	3261	1/1	0.24	-	57,57,57,57	0
61	MG	DA	3067	1/1	0.62	-	50,50,50,50	0
61	MG	BA	3097	1/1	0.33	-	47,47,47,47	0
61	MG	AA	1703	1/1	0.24	-	62,62,62,62	0
61	MG	DA	3093	1/1	0.73	-	50,50,50,50	0
61	MG	AA	1624	1/1	0.29	-	48,48,48,48	0
61	MG	BA	3118	1/1	0.50	-	49,49,49,49	0
61	MG	AA	1693	1/1	0.52	-	61,61,61,61	0
61	MG	BA	3030	1/1	0.62	-	47,47,47,47	0
61	MG	CA	1627	1/1	0.24	-	70,70,70,70	0
61	MG	AA	1704	1/1	0.25	-	49,49,49,49	1
61	MG	DA	3117	1/1	0.27	-	47,47,47,47	0
61	MG	DA	3098	1/1	0.26	-	47,47,47,47	0
61	MG	AA	1757	1/1	0.35	-	55,55,55,55	0
61	MG	BA	3344	1/1	0.89	-	55,55,55,55	0
61	MG	BA	3259	1/1	0.28	-	59,59,59,59	0
61	MG	CA	1739	1/1	0.16	-	55,55,55,55	0
61	MG	BA	3017	1/1	0.54	-	52,52,52,52	0
61	MG	BA	3275	1/1	0.38	-	59,59,59,59	0
61	MG	BA	3013	1/1	0.41	-	47,47,47,47	0
61	MG	CA	1674	1/1	0.21	-	50,50,50,50	0
61	MG	AA	1601	1/1	0.22	-	56,56,56,56	0
61	MG	DA	3043	1/1	1.00	-	47,47,47,47	0
61	MG	DA	3318	1/1	0.18	-	55,55,55,55	0
61	MG	DA	3292	1/1	0.52	-	55,55,55,55	0
61	MG	AA	1631	1/1	0.24	-	47,47,47,47	0
61	MG	AA	1709	1/1	0.54	-	50,50,50,50	0
61	MG	CA	1691	1/1	0.65	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
61	MG	DA	3339	1/1	0.33	-	55,55,55,55	0
61	MG	BA	3039	1/1	0.25	-	68,68,68,68	0
61	MG	BA	3341	1/1	0.54	-	55,55,55,55	0
61	MG	DA	3289	1/1	0.47	-	54,54,54,54	0
61	MG	CA	1729	1/1	0.30	-	55,55,55,55	1
61	MG	BA	3288	1/1	0.23	-	66,66,66,66	0
61	MG	BA	3325	1/1	0.34	-	55,55,55,55	0
61	MG	CA	1719	1/1	0.35	-	55,55,55,55	1
61	MG	BA	3182	1/1	0.39	-	49,49,49,49	0
61	MG	DA	3021	1/1	0.52	-	47,47,47,47	0
61	MG	BA	3137	1/1	0.59	-	52,52,52,52	0
61	MG	CA	1672	1/1	0.40	-	53,53,53,53	0
61	MG	DA	3157	1/1	0.35	-	48,48,48,48	0
61	MG	BA	3254	1/1	0.63	-	60,60,60,60	0
61	MG	AM	201	1/1	0.50	-	47,47,47,47	0
61	MG	CA	1662	1/1	0.29	-	52,52,52,52	0
61	MG	BA	3053	1/1	0.18	-	51,51,51,51	0
61	MG	BA	3180	1/1	0.43	-	56,56,56,56	0
61	MG	AA	1634	1/1	0.67	-	52,52,52,52	0
61	MG	BS	201	1/1	0.42	-	55,55,55,55	0
61	MG	DA	3107	1/1	0.63	-	51,51,51,51	0
61	MG	DA	3184	1/1	0.53	-	49,49,49,49	0
61	MG	DA	3297	1/1	0.43	-	55,55,55,55	0
61	MG	DA	3151	1/1	0.51	-	51,51,51,51	0
61	MG	BA	3101	1/1	0.71	-	47,47,47,47	0
61	MG	BA	3065	1/1	0.27	-	52,52,52,52	0
61	MG	BA	3073	1/1	0.41	-	52,52,52,52	0
61	MG	CA	1710	1/1	0.33	-	50,50,50,50	0
61	MG	BA	3026	1/1	0.42	-	47,47,47,47	0
61	MG	DA	3309	1/1	0.46	-	55,55,55,55	1
61	MG	AA	1616	1/1	0.51	-	64,64,64,64	0
61	MG	BA	3199	1/1	0.64	-	58,58,58,58	0
61	MG	BA	3284	1/1	0.68	-	57,57,57,57	0
61	MG	CA	1679	1/1	0.36	-	53,53,53,53	1
61	MG	DA	3290	1/1	0.42	-	57,57,57,57	0
61	MG	DA	3190	1/1	0.27	-	59,59,59,59	0
61	MG	BA	3231	1/1	0.38	-	51,51,51,51	0
61	MG	AA	1639	1/1	0.24	-	53,53,53,53	0
61	MG	BA	3328	1/1	0.59	-	55,55,55,55	0
61	MG	BA	3153	1/1	0.46	-	53,53,53,53	0
61	MG	BA	3052	1/1	0.54	-	47,47,47,47	0
61	MG	AA	1663	1/1	0.26	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
61	MG	DA	3232	1/1	0.14	-	51,51,51,51	0
61	MG	AA	1614	1/1	0.09	-	52,52,52,52	0
61	MG	CA	1603	1/1	0.33	-	61,61,61,61	0
61	MG	AA	1730	1/1	0.43	-	55,55,55,55	0
61	MG	AW	105	1/1	0.17	-	53,53,53,53	0
61	MG	AA	1692	1/1	0.68	-	59,59,59,59	0
61	MG	DA	3243	1/1	0.12	-	61,61,61,61	1
61	MG	BA	3281	1/1	0.47	-	57,57,57,57	0
61	MG	BA	3016	1/1	0.88	-	47,47,47,47	0
61	MG	BH	201	1/1	0.14	-	50,50,50,50	0
61	MG	DA	3127	1/1	0.33	-	52,52,52,52	0
61	MG	CA	1665	1/1	0.46	-	50,50,50,50	0
61	MG	DA	3321	1/1	0.23	-	55,55,55,55	0
61	MG	AA	1641	1/1	0.44	-	47,47,47,47	0
61	MG	DA	3061	1/1	0.48	-	47,47,47,47	0
61	MG	DA	3068	1/1	0.44	-	50,50,50,50	0
61	MG	AA	1674	1/1	0.19	-	50,50,50,50	0
61	MG	DA	3038	1/1	0.60	-	47,47,47,47	0
61	MG	DA	3268	1/1	0.90	-	59,59,59,59	0
61	MG	BA	3233	1/1	0.58	-	47,47,47,47	0
61	MG	DA	3333	1/1	0.38	-	55,55,55,55	0
61	MG	DA	3189	1/1	0.17	-	57,57,57,57	0
61	MG	CA	1655	1/1	0.68	-	52,52,52,52	0
61	MG	BA	3031	1/1	0.22	-	50,50,50,50	0
61	MG	DA	3079	1/1	0.54	-	56,56,56,56	0
61	MG	BA	3242	1/1	0.40	-	47,47,47,47	0
61	MG	CA	1652	1/1	0.88	-	60,60,60,60	0
61	MG	AA	1752	1/1	0.17	-	55,55,55,55	0
61	MG	AA	1708	1/1	0.31	-	65,65,65,65	0
61	MG	DA	3096	1/1	0.54	-	60,60,60,60	0
61	MG	AA	1715	1/1	0.23	-	55,55,55,55	0
61	MG	BA	3243	1/1	0.45	-	53,53,53,53	0
61	MG	DA	3270	1/1	0.61	-	67,67,67,67	0
61	MG	DA	3251	1/1	0.19	-	52,52,52,52	0
61	MG	AA	1727	1/1	0.64	-	55,55,55,55	0
61	MG	DA	3287	1/1	0.44	-	51,51,51,51	0
61	MG	DA	3211	1/1	0.54	-	57,57,57,57	0
61	MG	CA	1747	1/1	0.29	-	55,55,55,55	1
61	MG	AA	1686	1/1	0.52	-	58,58,58,58	1
61	MG	BA	3154	1/1	0.37	-	48,48,48,48	0
61	MG	CA	1694	1/1	0.56	-	61,61,61,61	0
61	MG	CA	1733	1/1	0.51	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
61	MG	DA	3277	1/1	0.76	-	57,57,57,57	0
61	MG	BA	3327	1/1	0.48	-	55,55,55,55	0
61	MG	BB	203	1/1	0.70	-	55,55,55,55	0
61	MG	DA	3330	1/1	0.21	-	55,55,55,55	0
61	MG	DA	3060	1/1	0.42	-	48,48,48,48	0
61	MG	BA	3292	1/1	0.67	-	55,55,55,55	0
61	MG	CA	1678	1/1	0.13	-	49,49,49,49	0
61	MG	BA	3213	1/1	0.35	-	58,58,58,58	0
61	MG	AA	1684	1/1	0.17	-	49,49,49,49	0
61	MG	BA	3174	1/1	0.36	-	58,58,58,58	0
61	MG	BA	3089	1/1	0.56	-	48,48,48,48	0
61	MG	B3	101	1/1	0.54	-	58,58,58,58	0
61	MG	DA	3027	1/1	0.49	-	47,47,47,47	0
61	MG	DA	3236	1/1	0.89	-	52,52,52,52	0
61	MG	DA	3207	1/1	0.48	-	47,47,47,47	0
61	MG	BA	3166	1/1	0.11	-	47,47,47,47	0
61	MG	BA	3108	1/1	0.70	-	52,52,52,52	0
61	MG	BA	3150	1/1	0.49	-	51,51,51,51	0
61	MG	DA	3204	1/1	0.30	-	52,52,52,52	0
61	MG	DA	3075	1/1	0.50	-	47,47,47,47	0
61	MG	CA	1720	1/1	0.16	-	56,56,56,56	0
61	MG	CA	1602	1/1	0.23	-	52,52,52,52	0
61	MG	DA	3030	1/1	0.49	-	55,55,55,55	0
61	MG	DA	3242	1/1	0.21	-	58,58,58,58	1
61	MG	DA	3177	1/1	0.57	-	49,49,49,49	0
62	ZN	D9	101	1/1	0.10	-	55,55,55,55	1
61	MG	CA	1716	1/1	0.30	-	55,55,55,55	0
61	MG	DA	3164	1/1	0.70	-	53,53,53,53	0
61	MG	DA	3293	1/1	0.22	-	52,52,52,52	0
61	MG	BA	3064	1/1	0.53	-	53,53,53,53	0
61	MG	DA	3285	1/1	0.27	-	55,55,55,55	0
61	MG	BA	3191	1/1	0.22	-	61,61,61,61	0
61	MG	BA	3210	1/1	0.43	-	57,57,57,57	0
61	MG	DA	3132	1/1	0.27	-	59,59,59,59	0
61	MG	AA	1736	1/1	0.26	-	55,55,55,55	0
61	MG	BA	3198	1/1	0.63	-	53,53,53,53	0
61	MG	DA	3212	1/1	0.23	-	59,59,59,59	0
61	MG	DA	3158	1/1	0.47	-	53,53,53,53	0
61	MG	DA	3140	1/1	0.36	-	50,50,50,50	1
61	MG	DA	3101	1/1	0.52	-	51,51,51,51	0
61	MG	DA	3275	1/1	0.65	-	59,59,59,59	0
61	MG	BA	3044	1/1	0.87	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
61	MG	CA	1608	1/1	0.36	-	52,52,52,52	0
61	MG	CA	1704	1/1	0.64	-	62,62,62,62	0
61	MG	AA	1627	1/1	0.30	-	53,53,53,53	0
61	MG	BA	3326	1/1	0.85	-	55,55,55,55	0
61	MG	BA	3048	1/1	0.57	-	47,47,47,47	0
61	MG	BA	3021	1/1	0.37	-	47,47,47,47	0
61	MG	DA	3191	1/1	0.28	-	54,54,54,54	0
61	MG	BA	3215	1/1	0.71	-	60,60,60,60	0
61	MG	DA	3080	1/1	0.52	-	49,49,49,49	0
61	MG	AA	1705	1/1	0.22	-	51,51,51,51	0
61	MG	BA	3220	1/1	0.65	-	54,54,54,54	0
61	MG	DA	3310	1/1	0.27	-	55,55,55,55	0
61	MG	BA	3224	1/1	0.38	-	51,51,51,51	0
61	MG	DA	3311	1/1	0.64	-	55,55,55,55	0
61	MG	AA	1636	1/1	0.18	-	49,49,49,49	0
61	MG	DA	3352	1/1	0.55	-	55,55,55,55	0
61	MG	DA	3183	1/1	0.22	-	53,53,53,53	0
61	MG	BA	3162	1/1	0.84	-	50,50,50,50	0
61	MG	DA	3336	1/1	0.24	-	55,55,55,55	1
61	MG	AA	1695	1/1	0.28	-	62,62,62,62	0
61	MG	BA	3024	1/1	0.66	-	56,56,56,56	0
61	MG	AA	1712	1/1	0.44	-	54,54,54,54	0
61	MG	BA	3132	1/1	0.31	-	57,57,57,57	0
61	MG	DA	3051	1/1	0.18	-	47,47,47,47	0
61	MG	BA	3334	1/1	0.30	-	55,55,55,55	0
61	MG	AA	1721	1/1	0.44	-	55,55,55,55	1
61	MG	CA	1698	1/1	0.35	-	52,52,52,52	0
61	MG	BA	3278	1/1	0.33	-	51,51,51,51	0
61	MG	BA	3218	1/1	0.51	-	66,66,66,66	0
61	MG	CA	1741	1/1	0.51	-	55,55,55,55	0
61	MG	CA	1736	1/1	0.60	-	55,55,55,55	0
61	MG	CA	1725	1/1	0.37	-	59,59,59,59	0
61	MG	CA	1726	1/1	0.79	-	54,54,54,54	0
61	MG	DA	3150	1/1	0.63	-	54,54,54,54	0
61	MG	DA	3122	1/1	0.40	-	50,50,50,50	0
61	MG	AA	1744	1/1	0.28	-	55,55,55,55	0
61	MG	DA	3210	1/1	0.50	-	66,66,66,66	0
61	MG	BA	3148	1/1	0.18	-	47,47,47,47	0
61	MG	DA	3118	1/1	0.38	-	52,52,52,52	0
61	MG	BA	3270	1/1	0.71	-	67,67,67,67	0
61	MG	DA	3167	1/1	0.27	-	47,47,47,47	0
61	MG	DA	3156	1/1	0.35	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
61	MG	DA	3018	1/1	0.48	-	52,52,52,52	0
61	MG	CA	1751	1/1	0.28	-	55,55,55,55	0
61	MG	DA	3116	1/1	0.40	-	50,50,50,50	0
61	MG	BA	3067	1/1	0.32	-	50,50,50,50	0
61	MG	DA	3325	1/1	0.91	-	55,55,55,55	0
61	MG	CA	1635	1/1	0.39	-	49,49,49,49	0
61	MG	DA	3304	1/1	0.71	-	55,55,55,55	0
61	MG	D5	101	1/1	0.16	-	49,49,49,49	0
61	MG	DA	3025	1/1	0.77	-	56,56,56,56	0
61	MG	DA	3259	1/1	0.31	-	58,58,58,58	0
61	MG	CA	1677	1/1	0.25	-	55,55,55,55	1
61	MG	DA	3138	1/1	0.51	-	52,52,52,52	0
61	MG	DA	3111	1/1	0.25	-	49,49,49,49	0
61	MG	BA	3300	1/1	0.36	-	55,55,55,55	0
61	MG	AW	101	1/1	0.70	-	56,56,56,56	1
61	MG	CA	1653	1/1	0.07	-	53,53,53,53	0
61	MG	BA	3221	1/1	0.67	-	53,53,53,53	0
61	MG	BA	3285	1/1	0.27	-	55,55,55,55	0
61	MG	CA	1746	1/1	0.21	-	55,55,55,55	0
61	MG	CA	1701	1/1	0.49	-	51,51,51,51	0
61	MG	DQ	201	1/1	0.69	-	55,55,55,55	0
61	MG	CA	1697	1/1	0.14	-	62,62,62,62	0
61	MG	BA	3178	1/1	0.29	-	52,52,52,52	0
61	MG	BA	3124	1/1	0.31	-	49,49,49,49	0
61	MG	CA	1612	1/1	0.29	-	56,56,56,56	0
61	MG	DA	3170	1/1	0.49	-	49,49,49,49	1
61	MG	DA	3114	1/1	0.40	-	47,47,47,47	0
61	MG	DA	3153	1/1	0.14	-	50,50,50,50	0
61	MG	DA	3220	1/1	0.83	-	49,49,49,49	0
61	MG	DA	3042	1/1	0.75	-	47,47,47,47	0
61	MG	BA	3042	1/1	0.99	-	47,47,47,47	0
61	MG	DA	3197	1/1	0.56	-	47,47,47,47	0
61	MG	DA	3005	1/1	0.46	-	53,53,53,53	0
61	MG	BA	3314	1/1	0.26	-	55,55,55,55	0
61	MG	BA	3201	1/1	0.46	-	52,52,52,52	0
61	MG	DA	3271	1/1	0.47	-	51,51,51,51	0
61	MG	BA	3063	1/1	0.24	-	56,56,56,56	0
61	MG	CA	1642	1/1	0.58	-	56,56,56,56	0
61	MG	CA	1706	1/1	0.19	-	51,51,51,51	0
61	MG	DA	3178	1/1	0.51	-	48,48,48,48	0
61	MG	DA	3301	1/1	0.62	-	55,55,55,55	0
61	MG	DA	3053	1/1	0.60	-	47,47,47,47	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
61	MG	CA	1737	1/1	0.35	-	55,55,55,55	1
61	MG	BA	3151	1/1	0.29	-	47,47,47,47	0
61	MG	BA	3088	1/1	0.58	-	48,48,48,48	0
61	MG	DA	3074	1/1	0.43	-	52,52,52,52	0
61	MG	BA	3023	1/1	0.78	-	49,49,49,49	0
61	MG	BA	3152	1/1	0.12	-	50,50,50,50	0
61	MG	AA	1714	1/1	0.52	-	59,59,59,59	0
61	MG	CA	1650	1/1	0.68	-	54,54,54,54	0
61	MG	DA	3144	1/1	0.31	-	57,57,57,57	0
61	MG	DU	201	1/1	0.48	-	48,48,48,48	0
61	MG	BA	3018	1/1	0.57	-	54,54,54,54	0
61	MG	AA	1689	1/1	0.84	-	59,59,59,59	1
61	MG	BQ	201	1/1	0.72	-	55,55,55,55	0
61	MG	DA	3253	1/1	0.34	-	49,49,49,49	0
61	MG	DA	3209	1/1	0.47	-	51,51,51,51	0
61	MG	DA	3307	1/1	0.26	-	55,55,55,55	0
61	MG	DA	3248	1/1	0.14	-	59,59,59,59	1
61	MG	CA	1689	1/1	0.25	-	63,63,63,63	1
61	MG	AA	1741	1/1	0.50	-	55,55,55,55	0
61	MG	BA	3145	1/1	0.33	-	47,47,47,47	0
61	MG	B7	102	1/1	0.33	-	54,54,54,54	0
61	MG	BA	3055	1/1	0.65	-	47,47,47,47	0
61	MG	CA	1757	1/1	0.17	-	55,55,55,55	0
61	MG	DA	3152	1/1	0.41	-	47,47,47,47	0
61	MG	BA	3129	1/1	0.33	-	56,56,56,56	0
61	MG	CA	1682	1/1	0.11	-	53,53,53,53	0
61	MG	DA	3202	1/1	0.67	-	52,52,52,52	1
61	MG	AA	1723	1/1	0.28	-	57,57,57,57	0
61	MG	BA	3011	1/1	0.26	-	47,47,47,47	0
61	MG	CA	1604	1/1	0.21	-	50,50,50,50	0
61	MG	BA	3147	1/1	0.41	-	51,51,51,51	0
62	ZN	CN	102	1/1	0.12	-	60,60,60,60	0
61	MG	CA	1695	1/1	0.36	-	56,56,56,56	0
61	MG	BA	3061	1/1	0.54	-	48,48,48,48	0
61	MG	DA	3181	1/1	0.61	-	59,59,59,59	0
61	MG	DA	3036	1/1	0.43	-	55,55,55,55	0
61	MG	BA	3050	1/1	0.33	-	47,47,47,47	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.