



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 08:52 am GMT

PDB ID : 4V5O
Title : CRYSTAL STRUCTURE OF THE EUKARYOTIC 40S RIBOSOMAL SUB-UNIT IN COMPLEX WITH INITIATION FACTOR 1.
Authors : Rabl, J.; Leibundgut, M.; Ataide, S.F.; Haag, A.; Ban, N.
Deposited on : 2010-11-26
Resolution : 3.93 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28972

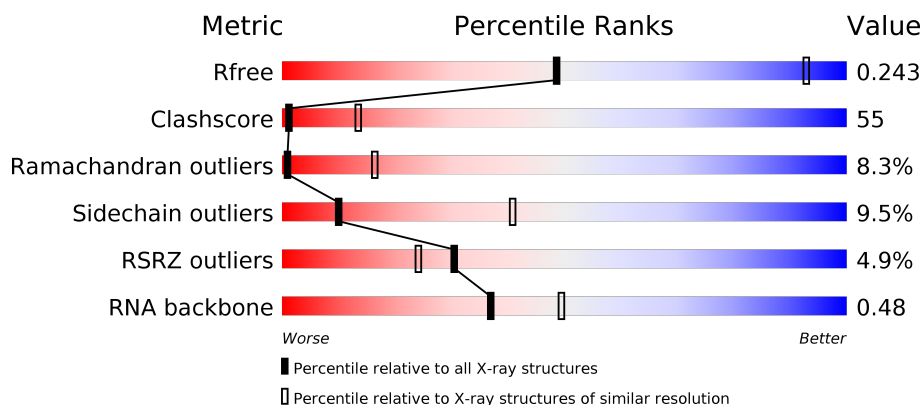
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.93 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}	100719	1021 (4.28-3.60)
Clashscore	112137	1117 (4.28-3.60)
Ramachandran outliers	110173	1076 (4.28-3.60)
Sidechain outliers	110143	1067 (4.28-3.60)
RSRZ outliers	101464	1034 (4.28-3.60)
RNA backbone	2435	1018 (4.84-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A1	68	<div> <div>8%</div> <div>31%</div> <div>51%</div> <div>16%</div> <div>.</div> </div>
1	B1	68	<div> <div>26%</div> <div>59%</div> <div>13%</div> <div>.</div> </div>
2	A2	208	<div> <div>28%</div> <div>20%</div> <div>66%</div> <div>13%</div> </div>
2	B2	208	<div> <div>8%</div> <div>19%</div> <div>67%</div> <div>13%</div> </div>

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Mol	Chain	Length	Quality of chain
3	A3	197	
3	B3	197	
4	A4	265	
4	B4	265	
5	A5	119	
5	B5	119	
6	A6	81	
6	B6	81	
7	A7	162	
7	B7	162	
8	A8	143	
8	B8	143	
9	A9	189	
9	B9	189	
10	AA	1753	
10	BA	1753	
11	AB	241	
11	BB	241	
12	AC	243	
12	BC	243	
13	AD	181	
13	BD	181	
14	AE	296	
14	BE	296	
15	AF	101	

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Mol	Chain	Length	Quality of chain
15	BF	101	
16	AG	200	
16	BG	200	
17	AH	130	
17	BH	130	
18	AI	145	
18	BI	145	
19	AJ	120	
19	BJ	120	
20	AK	151	
20	BK	151	
21	AL	142	
21	BL	142	
22	AM	155	
22	BM	155	
23	AN	55	
23	BN	55	
24	AO	153	
24	BO	153	
25	AP	149	
25	BP	149	
26	AQ	157	
26	BQ	157	
27	AR	343	
27	BR	343	

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Mol	Chain	Length	Quality of chain
28	AS	144	
28	BS	144	
29	AT	155	
29	BT	155	
30	AU	126	
30	BU	126	
31	AV	130	
31	BV	130	
32	AW	260	
32	BW	260	
33	AX	80	
33	BX	80	
34	AY	293	
34	BY	293	
35	AZ	97	
35	BZ	97	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	MG	AA	1815	-	-	-	X
36	MG	AA	1851	-	-	-	X
36	MG	AA	1856	-	-	-	X
36	MG	AA	1868	-	-	-	X
36	MG	AA	1874	-	-	-	X
36	MG	AA	1881	-	-	-	X
36	MG	AA	1889	-	-	-	X
36	MG	BA	1803	-	-	-	X
36	MG	BA	1810	-	-	-	X
36	MG	BA	1815	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	MG	BA	1873	-	-	-	X
36	MG	BA	1888	-	-	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 157632 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 protein called RIBOSOMAL PROTEIN S28E CONTAINING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A1	67	Total	C	N	O	S	0	0	0
			519	312	105	98	4			
1	B1	67	Total	C	N	O	S	0	0	0
			519	312	105	98	4			

- Molecule 2 is a protein called 40S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A2	207	Total	C	N	O	S	0	0	0
			1693	1057	336	296	4			
2	B2	207	Total	C	N	O	S	0	0	0
			1693	1057	336	296	4			

- Molecule 3 is a protein called RPS7E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A3	196	Total	C	N	O	S	0	0	0
			1629	1048	286	294	1			
3	B3	196	Total	C	N	O	S	0	0	0
			1629	1048	286	294	1			

- Molecule 4 is a protein called 40S RIBOSOMAL PROTEIN S3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A4	215	Total	C	N	O	S	0	0	0
			1724	1090	314	316	4			
4	B4	215	Total	C	N	O	S	0	0	0
			1724	1090	314	316	4			

- Molecule 5 is a protein called RIBOSOMAL PROTEIN S26E CONTAINING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A5	98	Total	C	N	O	S	0	0	0
			797	485	170	136	6			
5	B5	98	Total	C	N	O	S	0	0	0
			797	485	170	136	6			

- Molecule 6 is a protein called RPS27E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	A6	80	Total	C	N	O	S	0	0	0
			632	398	110	116	8			
6	B6	80	Total	C	N	O	S	0	0	0
			632	398	110	116	8			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B6	54	CYS	-	EXPRESSION TAG	UNP Q22CK0
B6	55	GLU	-	EXPRESSION TAG	UNP Q22CK0
B6	56	LYS	-	EXPRESSION TAG	UNP Q22CK0
B6	57	CYS	-	EXPRESSION TAG	UNP Q22CK0
B6	58	SER	-	EXPRESSION TAG	UNP Q22CK0
B6	59	ALA	-	EXPRESSION TAG	UNP Q22CK0
B6	60	ILE	-	EXPRESSION TAG	UNP Q22CK0
B6	61	LEU	-	EXPRESSION TAG	UNP Q22CK0
B6	62	CYS	-	EXPRESSION TAG	UNP Q22CK0
B6	63	LYS	-	EXPRESSION TAG	UNP Q22CK0
B6	64	PRO	-	EXPRESSION TAG	UNP Q22CK0
B6	65	THR	-	EXPRESSION TAG	UNP Q22CK0
B6	66	GLY	-	EXPRESSION TAG	UNP Q22CK0
B6	67	GLY	-	EXPRESSION TAG	UNP Q22CK0
B6	68	LYS	-	EXPRESSION TAG	UNP Q22CK0
B6	69	VAL	-	EXPRESSION TAG	UNP Q22CK0
B6	70	GLN	-	EXPRESSION TAG	UNP Q22CK0
B6	71	ILE	-	EXPRESSION TAG	UNP Q22CK0
B6	72	GLN	-	EXPRESSION TAG	UNP Q22CK0
B6	73	ALA	-	EXPRESSION TAG	UNP Q22CK0
B6	74	GLY	-	EXPRESSION TAG	UNP Q22CK0
B6	75	CYS	-	EXPRESSION TAG	UNP Q22CK0
B6	76	ALA	-	EXPRESSION TAG	UNP Q22CK0
B6	77	PHE	-	EXPRESSION TAG	UNP Q22CK0
B6	78	LYS	-	EXPRESSION TAG	UNP Q22CK0
B6	79	ILE	-	EXPRESSION TAG	UNP Q22CK0
B6	80	LYS	-	EXPRESSION TAG	UNP Q22CK0

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Chain	Residue	Modelled	Actual	Comment	Reference
B6	81	ASN	-	EXPRESSION TAG	UNP Q22CK0

- Molecule 7 is a protein called PLECTIN/S10 DOMAIN CONTAINING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	A7	104	Total	C	N	O	S	0	0	0
			859	560	142	155	2			
7	B7	104	Total	C	N	O	S	0	0	0
			859	560	142	155	2			

- Molecule 8 is a protein called RPS25E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	A8	93	Total	C	N	O	S	0	0	0
			725	460	135	128	2			
8	B8	93	Total	C	N	O	S	0	0	0
			725	460	135	128	2			

- Molecule 9 is a protein called RPS31E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	A9	98	Total	C	N	O	S	0	0	0
			742	479	139	119	5			
9	B9	98	Total	C	N	O	S	0	0	0
			742	479	139	119	5			

- Molecule 10 is a RNA chain called 18S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AA	1745	Total	C	N	O	P	0	0	0
			37231	16654	6651	12181	1745			
10	BA	1745	Total	C	N	O	P	0	0	0
			37231	16654	6651	12181	1745			

- Molecule 11 is a protein called RPS0E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AB	204	Total	C	N	O	S	0	0	0
			1642	1039	288	304	11			
11	BB	204	Total	C	N	O	S	0	0	0
			1642	1039	288	304	11			

- Molecule 12 is a protein called KH DOMAIN CONTAINING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AC	229	Total	C	N	O	S	0	0	0
			1820	1173	320	319	8			
12	BC	229	Total	C	N	O	S	0	0	0
			1820	1173	320	319	8			

- Molecule 13 is a protein called RIBOSOMAL PROTEIN S4 CONTAINING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AD	179	Total	C	N	O	S	0	0	0
			1475	931	286	252	6			
13	BD	179	Total	C	N	O	S	0	0	0
			1475	931	286	252	6			

- Molecule 14 is a protein called RIBOSOMAL PROTEIN S5 CONTAINING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AE	230	Total	C	N	O	S	0	0	0
			1827	1176	323	325	3			
14	BE	230	Total	C	N	O	S	0	0	0
			1827	1176	323	325	3			

- Molecule 15 is a protein called EIF1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AF	89	Total	C	N	O	S	0	0	0
			736	465	131	137	3			
15	BF	89	Total	C	N	O	S	0	0	0
			736	465	131	137	3			

- Molecule 16 is a protein called RIBOSOMAL PROTEIN S7 CONTAINING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AG	192	Total	C	N	O	S	0	0	0
			1520	961	281	270	8			
16	BG	192	Total	C	N	O	S	0	0	0
			1520	961	281	270	8			

- Molecule 17 is a protein called RIBOSOMAL PROTEIN S8 CONTAINING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AH	129	Total	C	N	O	S	0	0	0
			1040	671	184	180	5			
17	BH	129	Total	C	N	O	S	0	0	0
			1040	671	184	180	5			

- Molecule 18 is a protein called RPS16E, 40S RIBOSOMAL PROTEIN RPS16E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AI	143	Total	C	N	O	S	0	0	0
			1135	715	217	198	5			
18	BI	143	Total	C	N	O	S	0	0	0
			1135	715	217	198	5			

- Molecule 19 is a protein called RIBOSOMAL PROTEIN S10 CONTAINING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AJ	105	Total	C	N	O	S	0	0	0
			833	525	150	152	6			
19	BJ	105	Total	C	N	O	S	0	0	0
			833	525	150	152	6			

- Molecule 20 is a protein called RPS14E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AK	140	Total	C	N	O	S	0	0	0
			1063	654	206	197	6			
20	BK	140	Total	C	N	O	S	0	0	0
			1063	654	206	197	6			

- Molecule 21 is a protein called 40S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AL	141	Total	C	N	O	S	0	0	0
			1097	691	221	180	5			
21	BL	141	Total	C	N	O	S	0	0	0
			1097	691	221	180	5			

- Molecule 22 is a protein called RPS18E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AM	154	Total	C	N	O	S	0	0	0
			1239	780	237	216	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BM	154	Total	C	N	O	S	0	0	0
			1239	780	237	216	6			

- Molecule 23 is a protein called RPS29E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AN	53	Total	C	N	O	S	0	0	0
			447	278	91	72	6			
23	BN	53	Total	C	N	O	S	0	0	0
			447	278	91	72	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BN	54	TYR	-	EXPRESSION TAG	UNP Q22MB0
BN	55	ARG	-	EXPRESSION TAG	UNP Q22MB0

- Molecule 24 is a protein called RPS13E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AO	150	Total	C	N	O	S	0	0	0
			1214	782	228	200	4			
24	BO	150	Total	C	N	O	S	0	0	0
			1214	782	228	200	4			

- Molecule 25 is a protein called RPS24E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	AP	148	Total	C	N	O	0	0	0
			1197	763	221	213			
25	BP	148	Total	C	N	O	0	0	0
			1197	763	221	213			

- Molecule 26 is a protein called RIBOSOMAL PROTEIN S17 CONTAINING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	AQ	157	Total	C	N	O	S	0	0	0
			1275	818	235	217	5			
26	BQ	157	Total	C	N	O	S	0	0	0
			1275	818	235	217	5			

- Molecule 27 is a protein called RACK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	AR	338	Total	C	N	O	S	0	0	0
			2682	1711	462	501	8			
27	BR	338	Total	C	N	O	S	0	0	0
			2682	1711	462	501	8			

- Molecule 28 is a protein called RPS15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	AS	125	Total	C	N	O	S	0	0	0
			985	632	173	176	4			
28	BS	125	Total	C	N	O	S	0	0	0
			985	632	173	176	4			

- Molecule 29 is a protein called RPS19E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	AT	150	Total	C	N	O	S	0	0	0
			1211	769	227	213	2			
29	BT	150	Total	C	N	O	S	0	0	0
			1211	769	227	213	2			

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L7AE CONTAINING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	AU	124	Total	C	N	O	S	0	0	0
			952	599	166	182	5			
30	BU	124	Total	C	N	O	S	0	0	0
			952	599	166	182	5			

- Molecule 31 is a protein called RPS17E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	AV	121	Total	C	N	O	S	0	0	0
			979	619	182	176	2			
31	BV	121	Total	C	N	O	S	0	0	0
			979	619	182	176	2			

- Molecule 32 is a protein called 40S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	AW	259	Total	C	N	O	S	0	0	0
			2079	1322	383	370	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BW	259	Total	C	N	O	S	0	0	0
			2079	1322	383	370	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BW	1	MET	-	EXPRESSION TAG	UNP P0C233
BW	70	GLN	GLY	CONFLICT	UNP P0C233
BW	236	SER	LEU	CONFLICT	UNP P0C233
BW	237	TRP	TYR	CONFLICT	UNP P0C233

- Molecule 33 is a protein called RPS30E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	AX	68	Total	C	N	O	S	0	0	0
			554	350	113	90	1			
33	BX	68	Total	C	N	O	S	0	0	0
			554	350	113	90	1			

- Molecule 34 is a protein called RPS6E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	AY	235	Total	C	N	O	S	0	0	0
			1868	1184	347	326	11			
34	BY	235	Total	C	N	O	S	0	0	0
			1868	1184	347	326	11			

- Molecule 35 is a protein called RPS21E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	AZ	97	Total	C	N	O	S	0	0	0
			747	458	139	146	4			
35	BZ	97	Total	C	N	O	S	0	0	0
			747	458	139	146	4			

- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	AA	90	Total	Mg	0	0
			90	90		
36	B4	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	BA	89	Total 89	Mg 89	0	0
36	BD	1	Total 1	Mg 1	0	0
36	A4	1	Total 1	Mg 1	0	0
36	BW	1	Total 1	Mg 1	0	0
36	AL	1	Total 1	Mg 1	0	0

- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	B5	1	Total 1	Zn 1	0	0
37	BN	1	Total 1	Zn 1	0	0
37	B9	1	Total 1	Zn 1	0	0
37	A6	1	Total 1	Zn 1	0	0
37	AN	1	Total 1	Zn 1	0	0
37	A5	1	Total 1	Zn 1	0	0
37	A9	1	Total 1	Zn 1	0	0
37	B6	1	Total 1	Zn 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	A2	2	Total 2	O 2	0	0
38	A4	2	Total 2	O 2	0	0
38	A5	1	Total 1	O 1	0	0
38	AA	516	Total 516	O 516	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	AC	1	Total 1	O 1	0	0
38	AD	4	Total 4	O 4	0	0
38	AE	3	Total 3	O 3	0	0
38	AL	3	Total 3	O 3	0	0
38	AM	4	Total 4	O 4	0	0
38	AO	1	Total 1	O 1	0	0
38	AP	1	Total 1	O 1	0	0
38	AQ	2	Total 2	O 2	0	0
38	AT	4	Total 4	O 4	0	0
38	AW	4	Total 4	O 4	0	0
38	AY	4	Total 4	O 4	0	0
38	B2	2	Total 2	O 2	0	0
38	B4	2	Total 2	O 2	0	0
38	B5	1	Total 1	O 1	0	0
38	BA	512	Total 512	O 512	0	0
38	BC	2	Total 2	O 2	0	0
38	BD	2	Total 2	O 2	0	0
38	BE	5	Total 5	O 5	0	0
38	BK	1	Total 1	O 1	0	0
38	BL	2	Total 2	O 2	0	0
38	BM	6	Total 6	O 6	0	0

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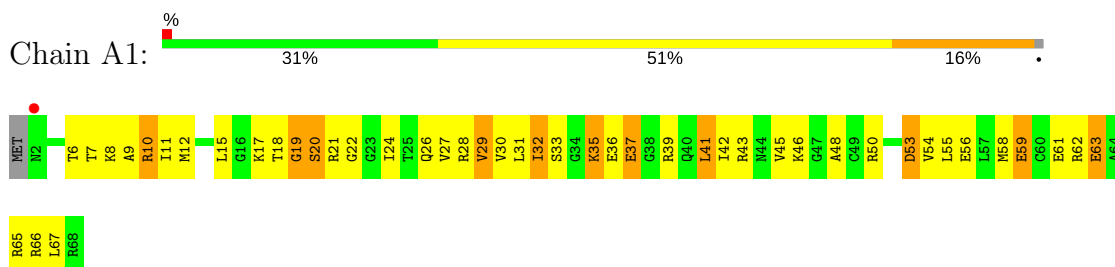
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	BO	1	Total 1	O 1	0	0
38	BP	1	Total 1	O 1	0	0
38	BQ	1	Total 1	O 1	0	0
38	BT	6	Total 6	O 6	0	0
38	BW	5	Total 5	O 5	0	0
38	BY	3	Total 3	O 3	0	0

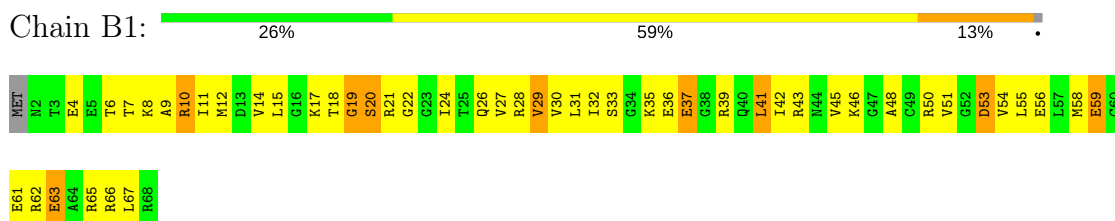
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

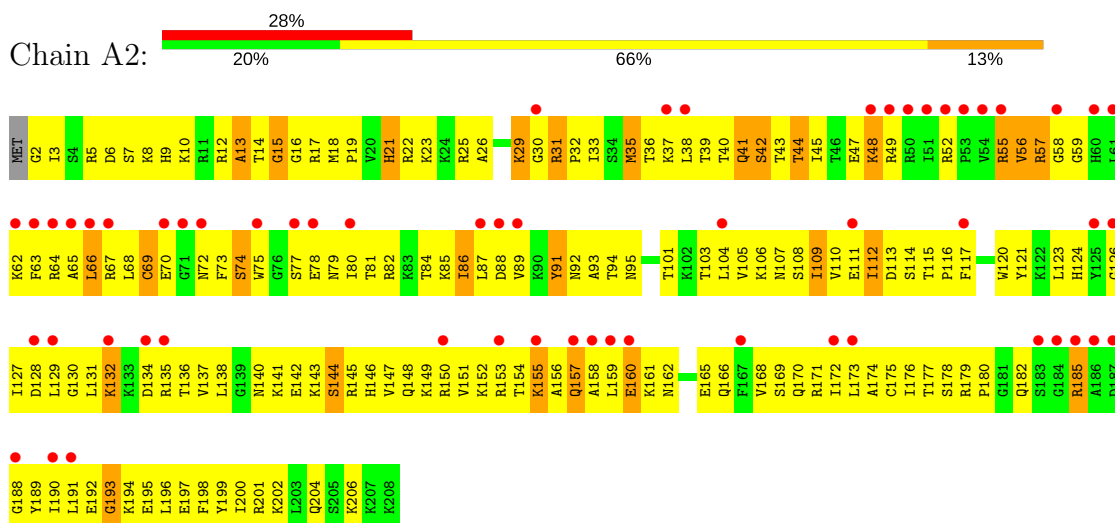
• Molecule 1: RIBOSOMAL PROTEIN S28E CONTAINING PROTEIN



• Molecule 1: RIBOSOMAL PROTEIN S28E CONTAINING PROTEIN

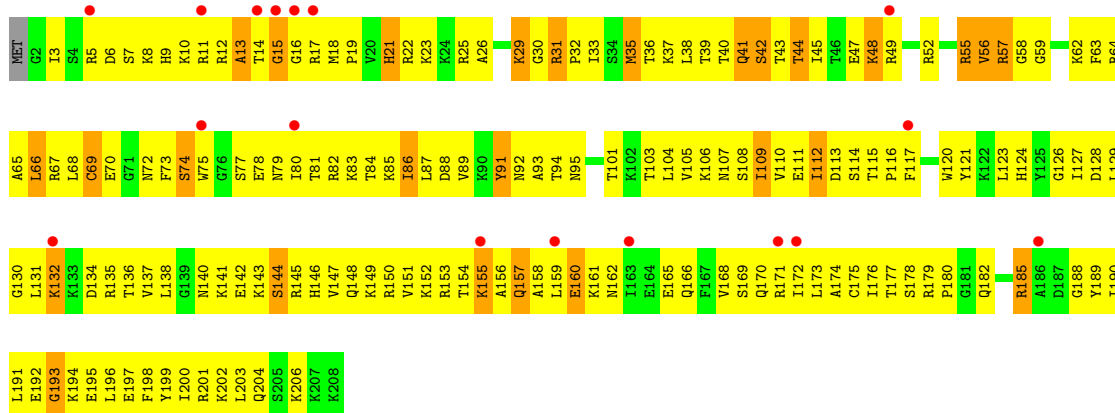


• Molecule 2: 40S RIBOSOMAL PROTEIN S8

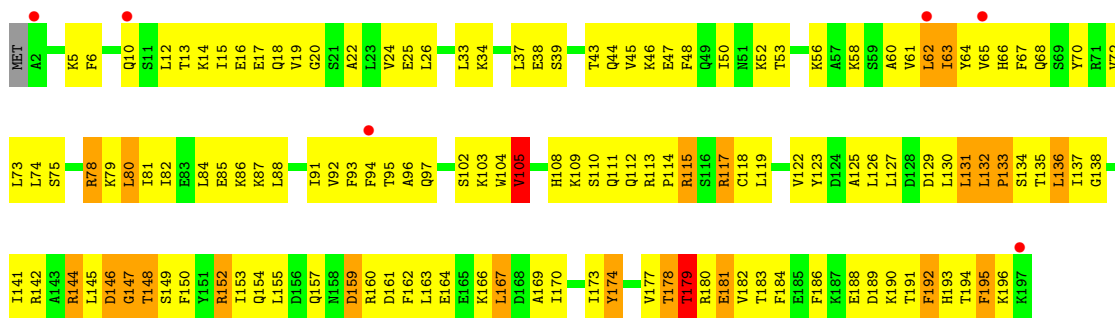


• Molecule 2: 40S RIBOSOMAL PROTEIN S8

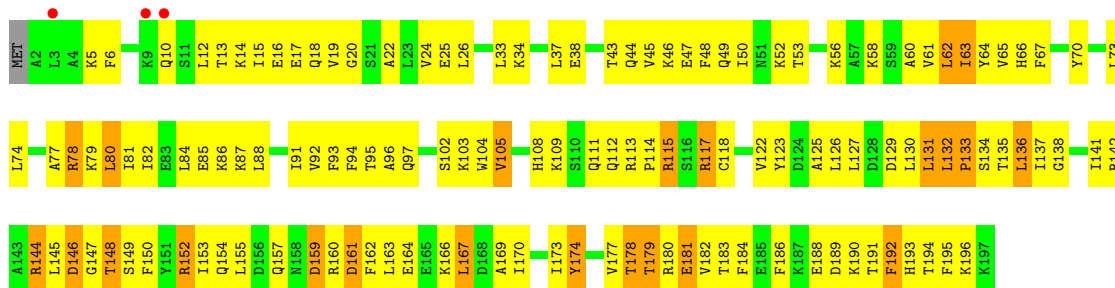




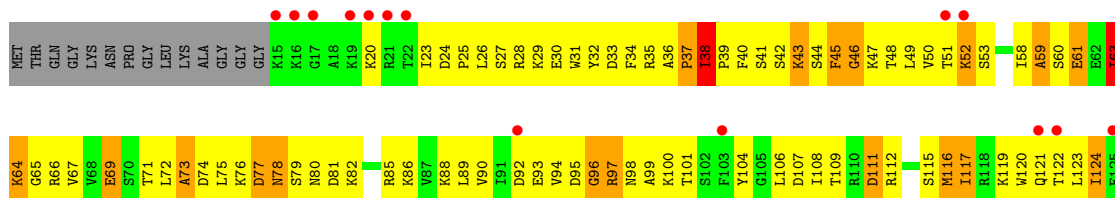
• Molecule 3: RPS7E

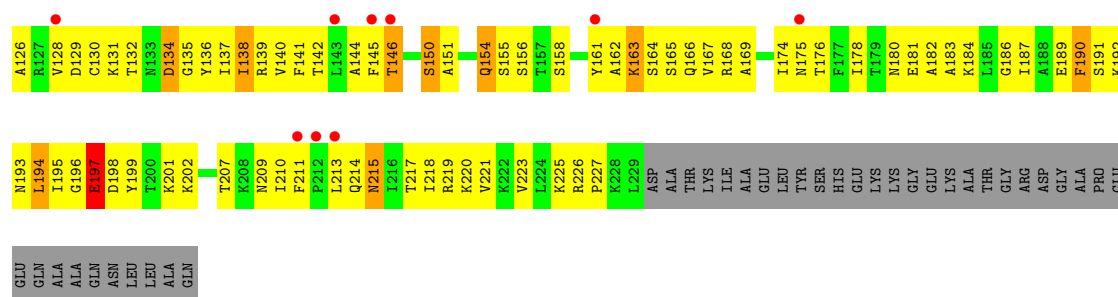


• Molecule 3: RPS7E

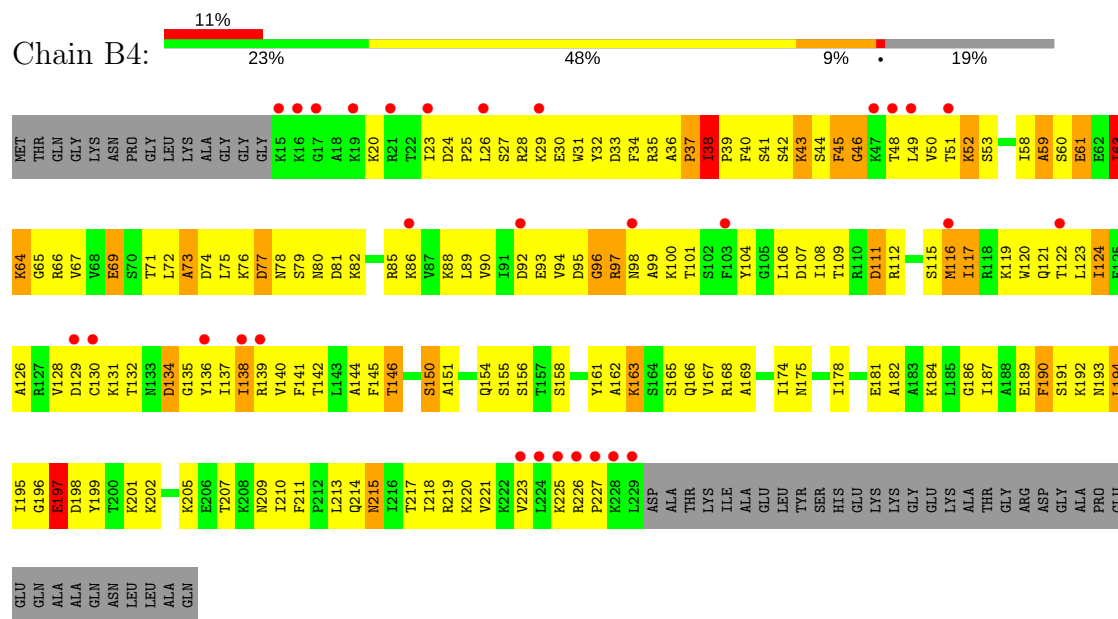


• Molecule 4: 40S RIBOSOMAL PROTEIN S3A

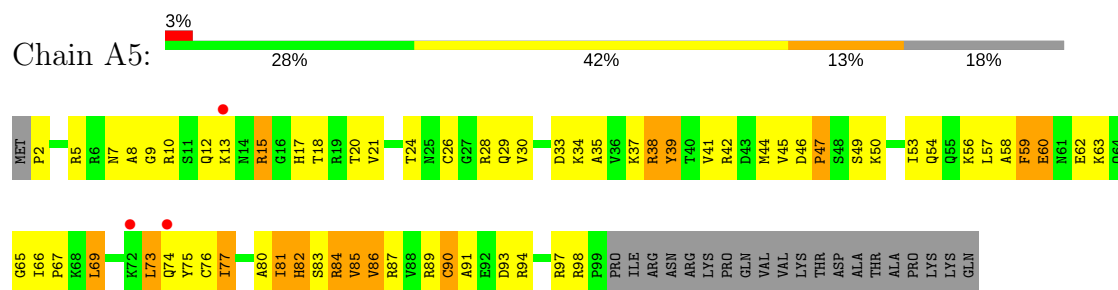




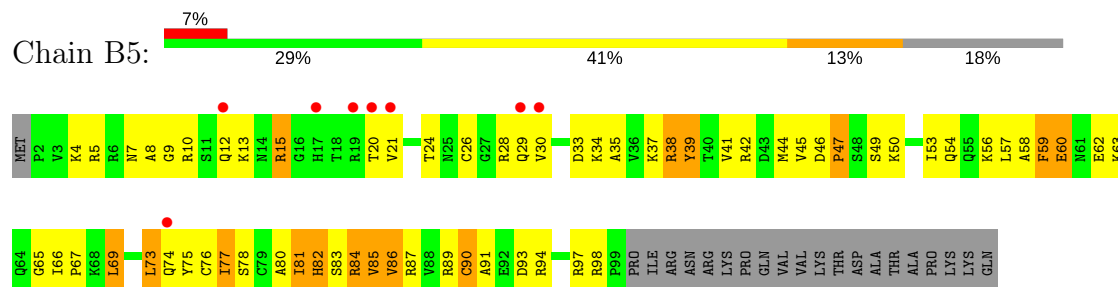
• Molecule 4: 40S RIBOSOMAL PROTEIN S3A



• Molecule 5: RIBOSOMAL PROTEIN S26E CONTAINING PROTEIN



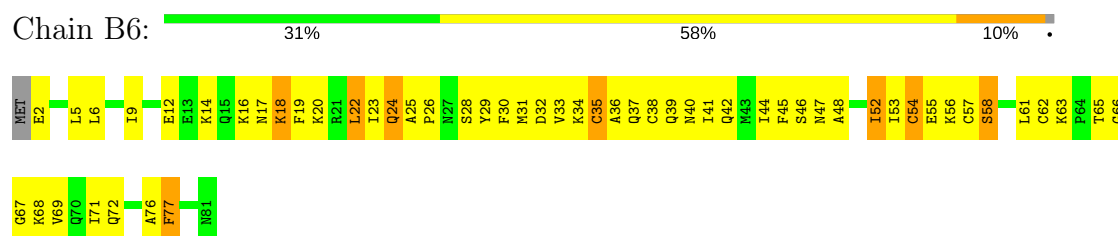
• Molecule 5: RIBOSOMAL PROTEIN S26E CONTAINING PROTEIN



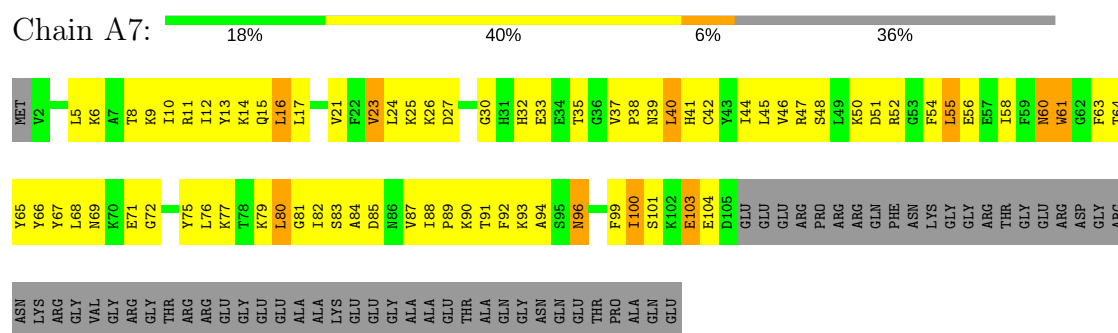
• Molecule 6: RPS27E



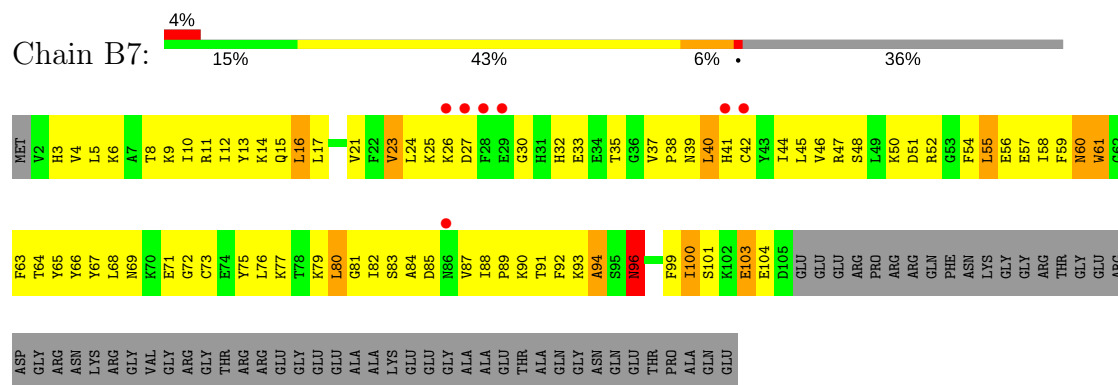
• Molecule 6: RPS27E



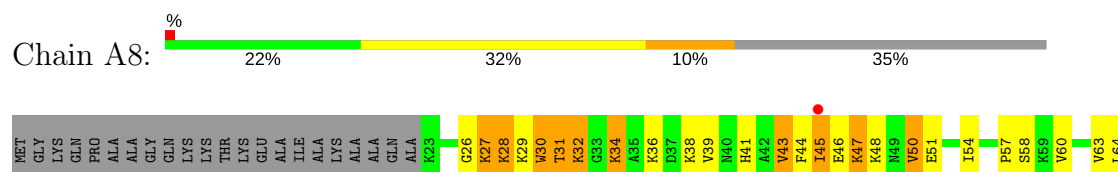
• Molecule 7: PLECTIN/S10 DOMAIN CONTAINING PROTEIN



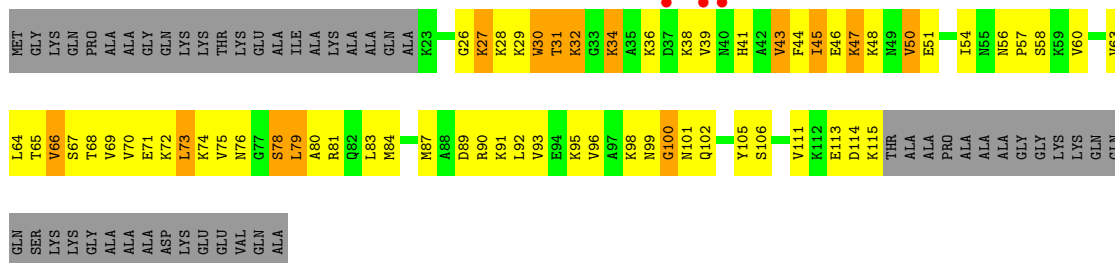
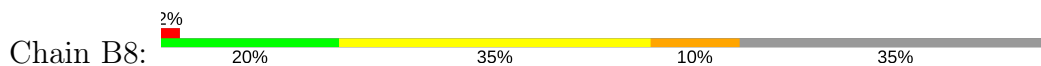
• Molecule 7: PLECTIN/S10 DOMAIN CONTAINING PROTEIN



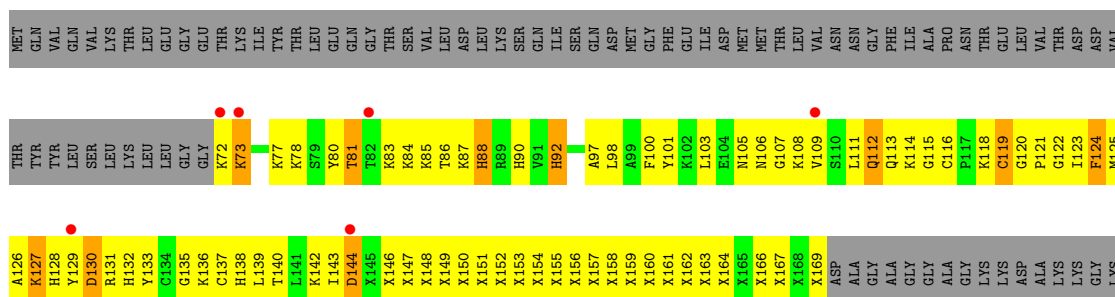
• Molecule 8: RPS25E



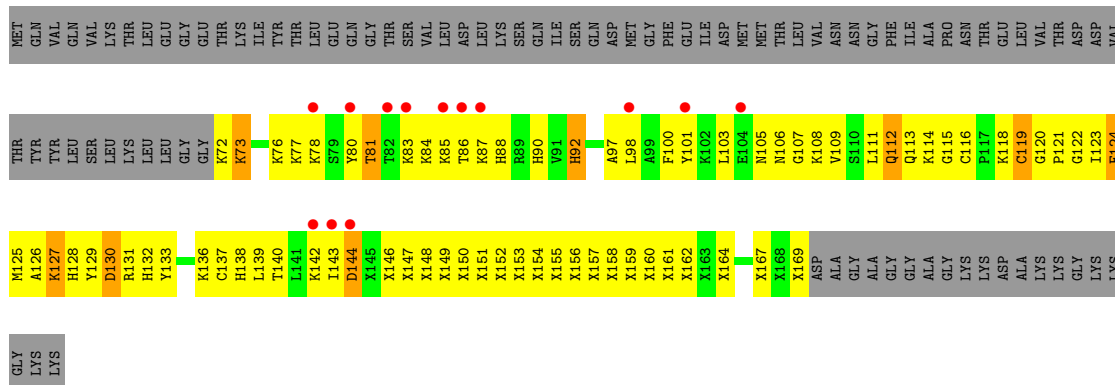
- Molecule 8: RPS25E



- Molecule 9: RPS31E

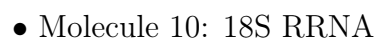


- Molecule 9: RPS31E

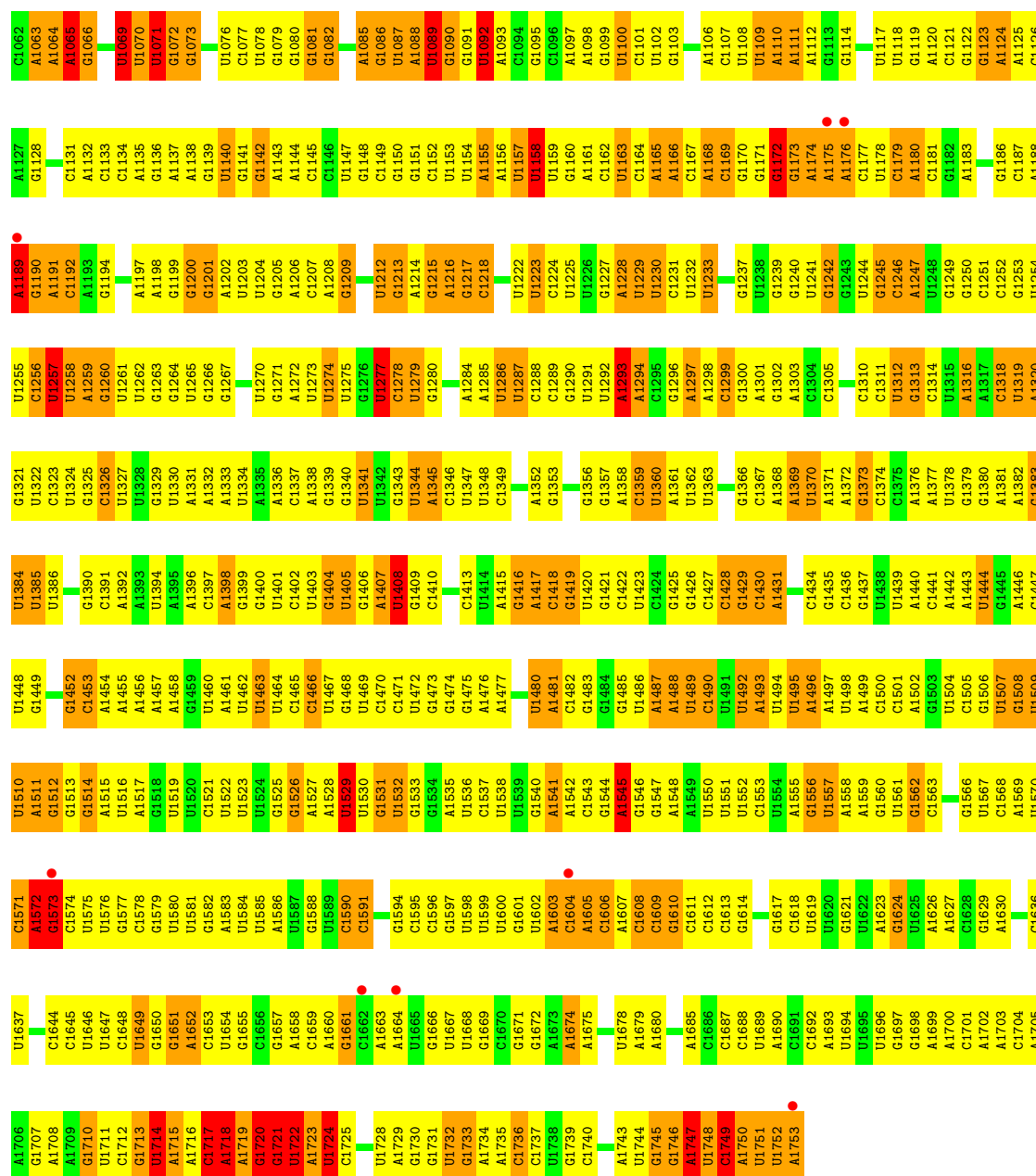


- Molecule 10: 18S rRNA



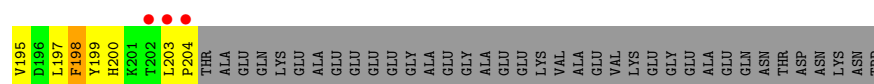


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A1001	U838	C873	A803	U680	U620	G497	C374	C310	A250	G190	A128	C65
U1002	U743	U874	A804	C681	C589	G498	G375	U311	G251	A191	G219	A67
A1003	C875	C876	G805	C682	C590	A499	A376	C312	U252	C192	A130	U66
A1004	U744	A744	G806	A683	A561	U500	C377	G313	A253	C193	U131	U68
A1005	G877	A746	C807	A684	C563	U501	A378	A314	A254	G194	U132	A69
C1006	G747	A747	G807	A685	A564	G502	A379	U315	C255	G195	A133	U70
U1007	U748	U748	U811	C886	C565	A503	G380	G316	U256	A196	C134	U71
A1008	G749	G749	U812	U687	C566	A504	G381	G317	G257	A197	A135	G72
U1009	U750	A688	A813	A688	C567	A505	A382	U318	A258	C198	U136	A73
A1010	U751	U751	A814	A689	C568	U506	A383	A319	U259	G199	G137	A74
	C752	C752	U820	C569	C569	G507	C384	G320	C260	U200	G138	C75
G1013	G753	A691	C821	A690	C570	A508	C385	U321	C261	A201	A139	A76
A1014	A754	U692	C822	C631	G571	G509	U386	G322	G262	U202	U140	G77
C1015	G755	C693	U822	U633	U572		G387	U323	A263	U203	A141	C78
U1016	G756	C694	A832	C634	A573		A388	A324	U264	U204	A142	G79
C1017	C757	G695	U827	U635	A574	G514	A389	U325	C265	A205	C143	A80
G1018	A758	C696	U828	U636	A575	U515	A390	U326	G266	U206	C144	A81
G1019	G759	C	U829	U637	U576	U516	A391	G327	A267	U207	G145	A82
A1020	U760	U	G830	U638	C577	U517	A392	G328	G268	A208	A146	C83
U1022	U761	U	G831	C839		U518	C393	A329	G269	G209	G147	U84
	U762	C	U832	A640	C580	A519	G394	C330	U270	A210	C148	C86
G1026	U763	A	U833	G641	C581	A520	G395	U331	U271	U211	U149	C86
C1027	U764	U	U834	G642	U582	A521	C396	A332	U272	A212	A150	C87
U1028	A765	C	A835	U643	C583	U522	U397	C333	A273	U213	A151	A88
G1029	G766	G	G836	U644	C584	C522	A398	C334	C274	U214	U152	A89
U1027	C767		A837	C645	A585	U523	C399	A335	C275	A215	U153	U90
A1030	C768		U838	A646	A586	G524	U400	U336	U276	G216	G154	G91
A1031	G769		U839	U647	U587	U525		G337	C277	A217	U155	G92
A1032	G770		A840	U648	A588	U526		G338	G278	C218	U156	C93
U1033	A771		U841	U649	G569	A527	A403	C339	A279	C219	G157	U94
A1034	A772		U842	C590	C590	G528	A407	A340	U280	A220	G158	C95
A1035	U773		A843	G591	G591	G529	C408	G341	A281	A221	G159	A96
U1036	A774		G844	A852	U592	A530	A409	U342	A282	C222	C160	U97
G1037	C775		G845	U653	A593	A531	G410	C343	C223	C223	U161	U98
U1038	A776		U846	U654	U594	G532	U411	A344	U284	G224	A162	A99
G975	U777		A847	C655	A595	G533	U412	C345	C285	C225	A163	A100
A976	U778		C848	G656	U596	A534	C413	G346	A286	A226	U164	A101
U977	A779		A849	U657	U597	A535	G414	G347	U287	G227	A165	A102
C978	G780		G850	C658	A598	C536	G415	G348	C288	C228	C166	C103
A979	C781		U851	G659	A599	A537	C416	U349	U289	A229	C167	A104
U1042	A782		U852	U660	A600	A538	A417	A350	A290	A230	U168	G105
G1043	U783		G853	G661	G601	U539	G418	A351	C291	U231	G169	U106
A1044	G784		G854	U662	U602	U540	C419	C352	C292	G232	C170	U107
G1045	G785		G855	G663	U603	G541	A420	G353	U293	U233	U171	A108
G1046	A786		G856	A664	G604	G542	G421		U294	G234	U172	A109
A1048	U787		G857	A665	U605	A543	A422	A357	U295	A235	A173	A110
C1049	U788		C858	A666	U606	G544	G423	A358	C296	U236	A174	G111
C1050	A789		A859	C667	G607	G545	A424	U359	U297	U237		
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U1052	G792		A862	G669	A609	C547	A426	A361	C299	A239	U178	U116
C927	G793		G863	G670	G610	A548	A427	G362	C300	G240	U179	U117
A929	U794		U864	A671	U611	A549	A428	G363	C301	A241	C180	
A930	A795		A865	C672	U612	G550	A429	G364	U302	U242	G181	A120
A931	U796		U866	A673	U613	U551	A430		U303	G243	U182	U121
C994	G797		U867	G674	A614	C552	U431		U304	A244	G183	A122
A933	U798		U868	A675	A615	A553	U432		C305	A245		A123
U934	G799		A869	C676	A616	U554	G433	U370	A306	U246	C186	U124
G935	A800		A870	G777	A617	G555	G434		G307	C247	U187	U125
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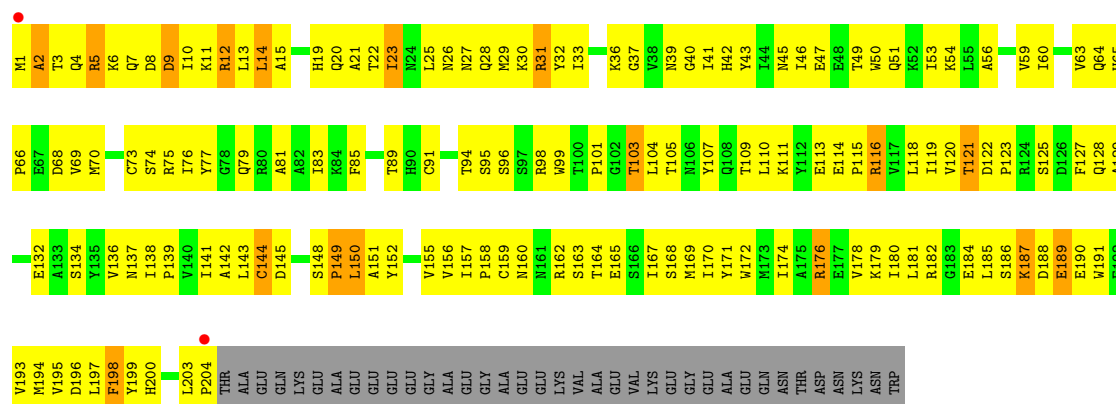


• Molecule 11: RPSOE

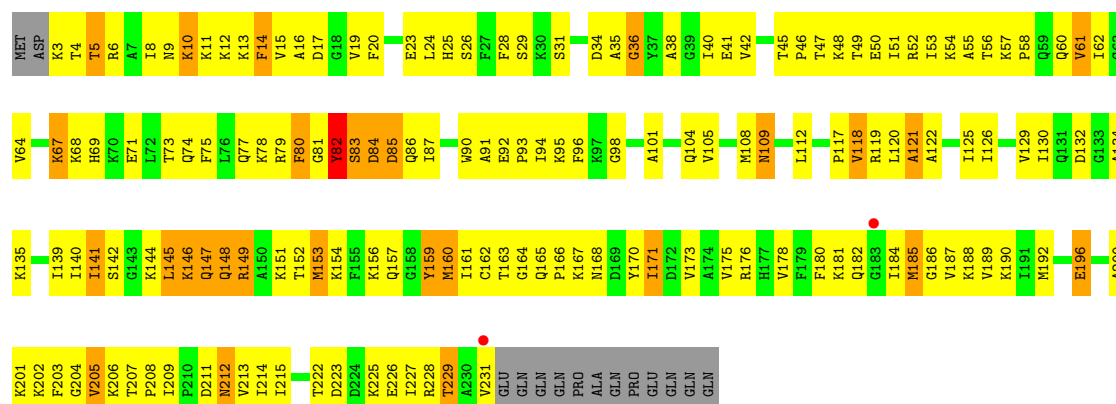




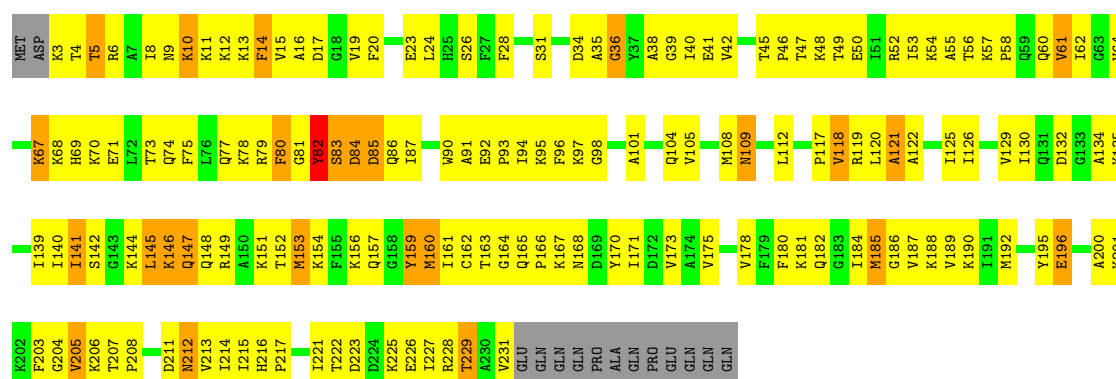
● Molecule 11: RPSOE



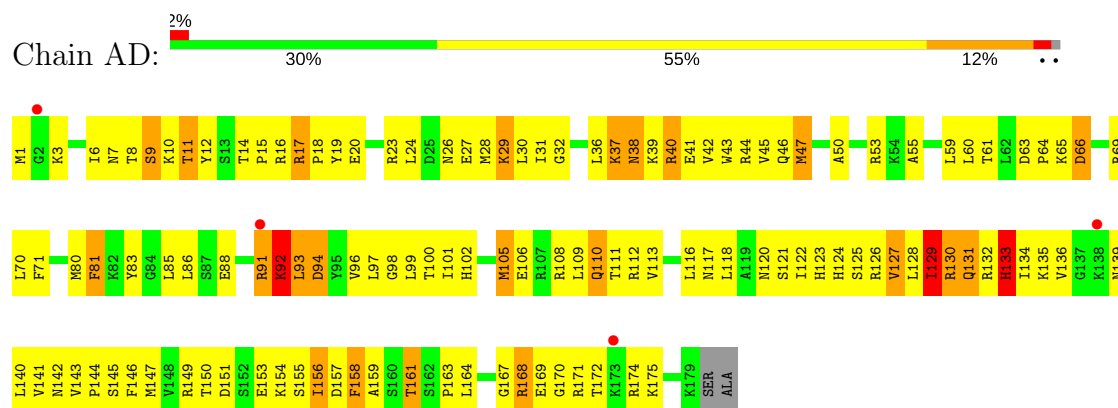
● Molecule 12: KH DOMAIN CONTAINING PROTEIN



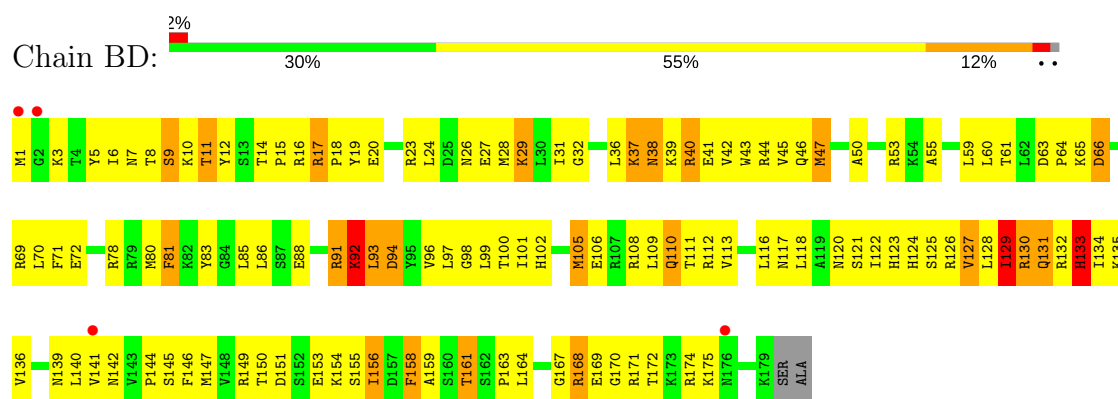
● Molecule 12: KH DOMAIN CONTAINING PROTEIN



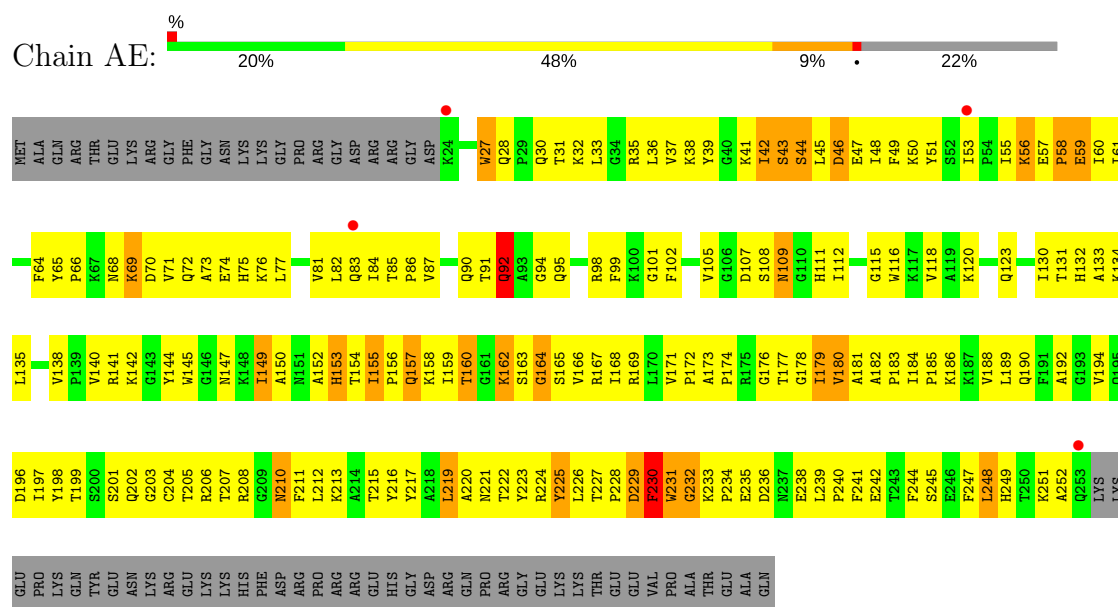
● Molecule 13: RIBOSOMAL PROTEIN S4 CONTAINING PROTEIN



● Molecule 13: RIBOSOMAL PROTEIN S4 CONTAINING PROTEIN

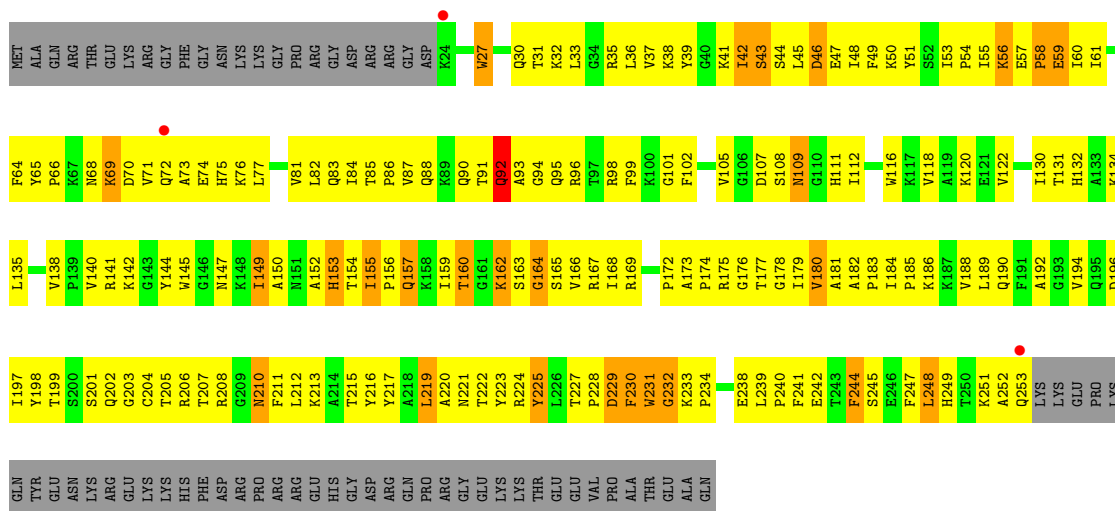


● Molecule 14: RIBOSOMAL PROTEIN S5 CONTAINING PROTEIN

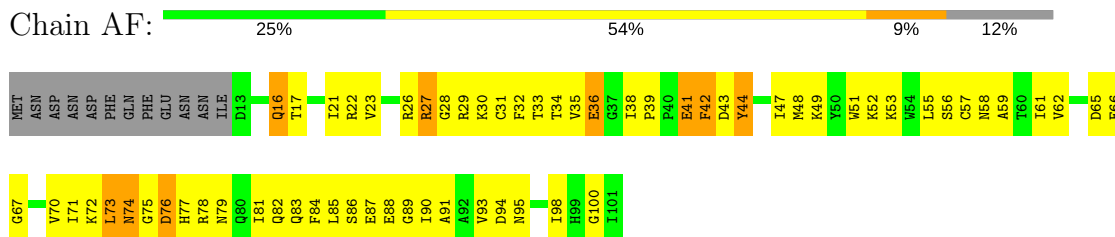


● Molecule 14: RIBOSOMAL PROTEIN S5 CONTAINING PROTEIN

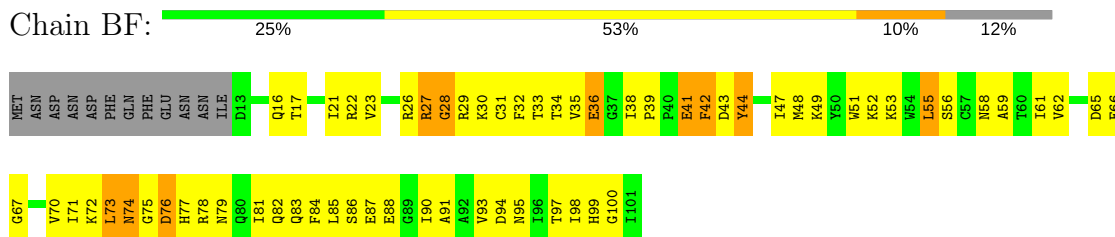




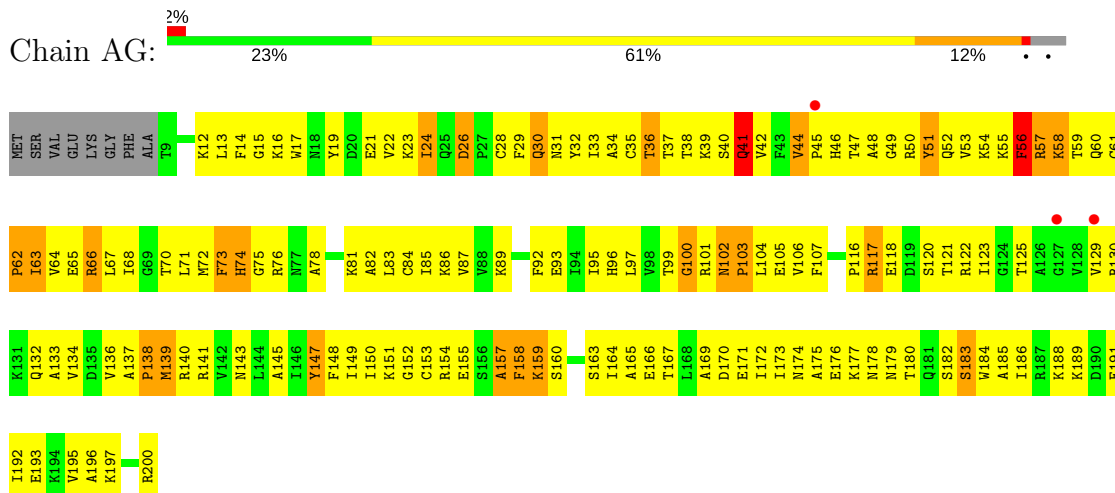
- Molecule 15: EIF1



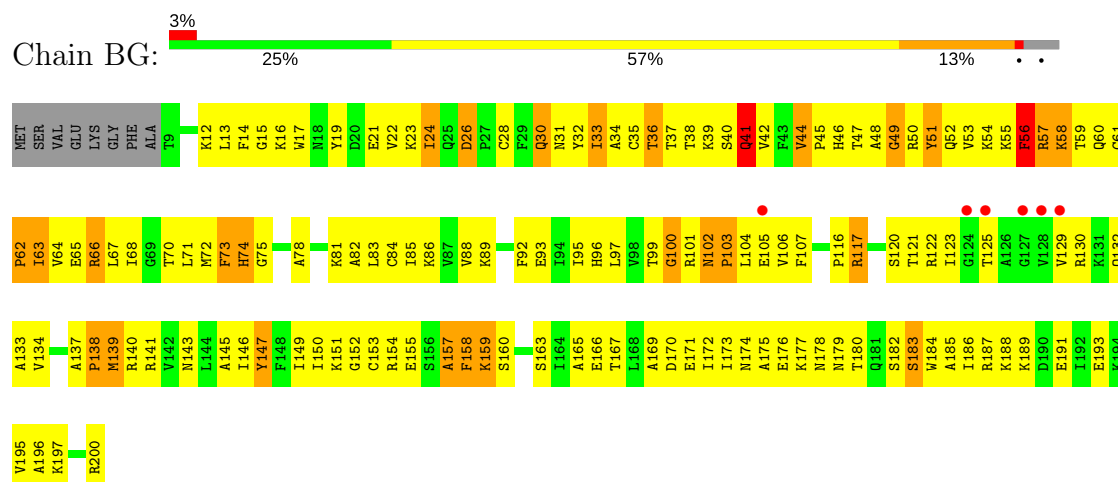
- Molecule 15: EIF1



- Molecule 16: RIBOSOMAL PROTEIN S7 CONTAINING PROTEIN

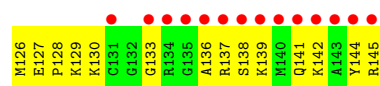


● Molecule 16: RIBOSOMAL PROTEIN S7 CONTAINING PROTEIN

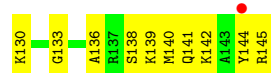
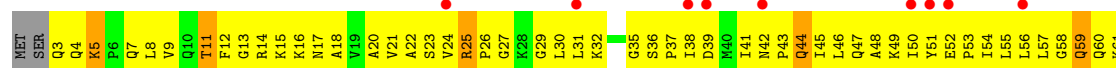


● Molecule 17: RIBOSOMAL PROTEIN S8 CONTAINING PROTEIN

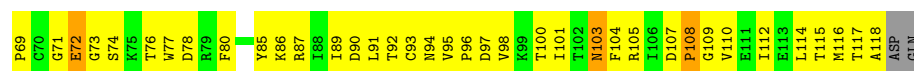




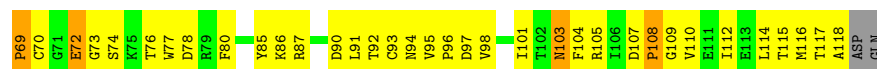
• Molecule 18: RPS16E, 40S RIBOSOMAL PROTEIN RPS16E



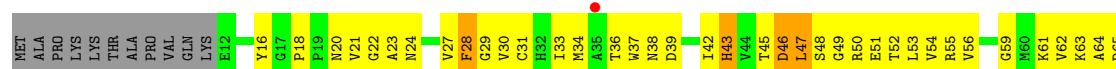
• Molecule 19: RIBOSOMAL PROTEIN S10 CONTAINING PROTEIN



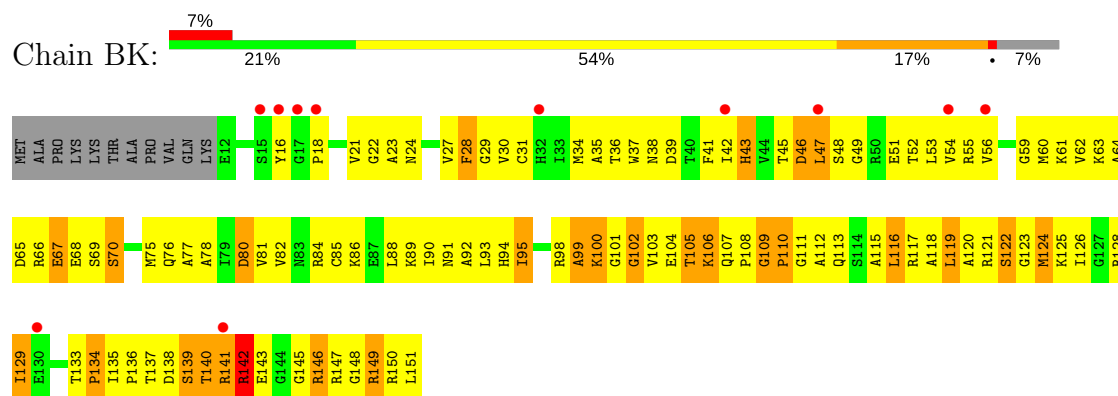
• Molecule 19: RIBOSOMAL PROTEIN S10 CONTAINING PROTEIN



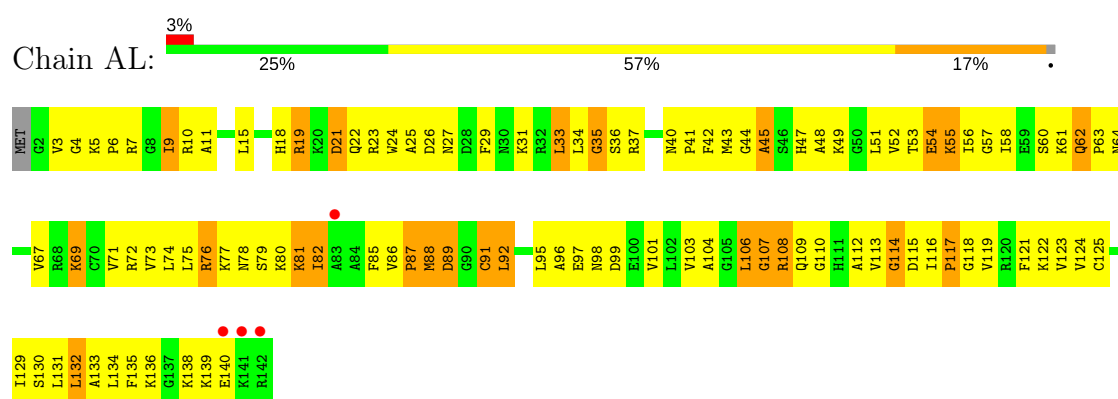
• Molecule 20: RPS14E



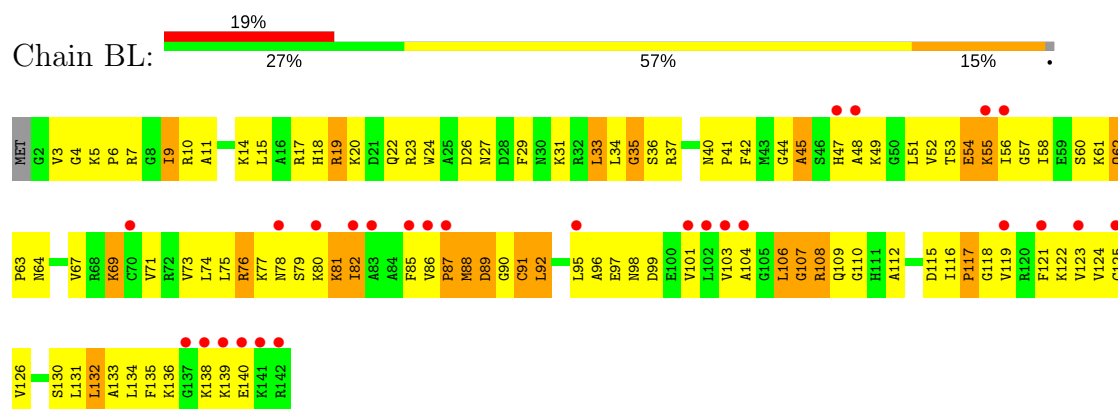
- Molecule 20: RPS14E



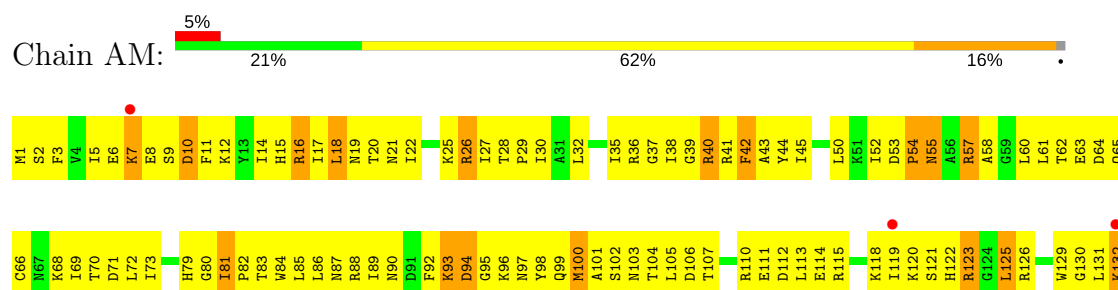
- Molecule 21: 40S RIBOSOMAL PROTEIN S12



- Molecule 21: 40S RIBOSOMAL PROTEIN S12

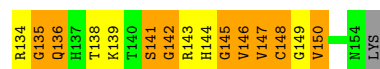
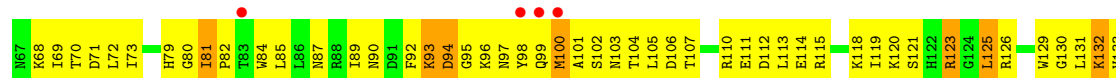


- Molecule 22: RPS18E





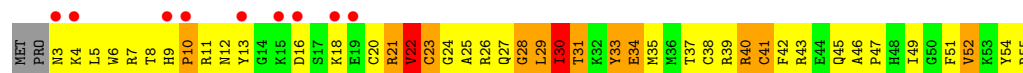
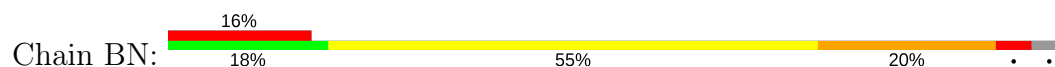
• Molecule 22: RPS18E



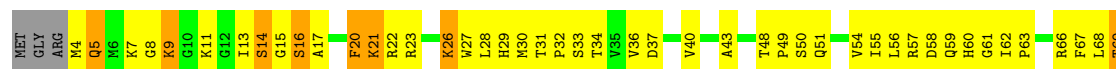
• Molecule 23: RPS29E



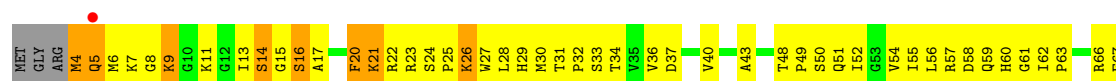
• Molecule 23: RPS29E



• Molecule 24: RPS13E

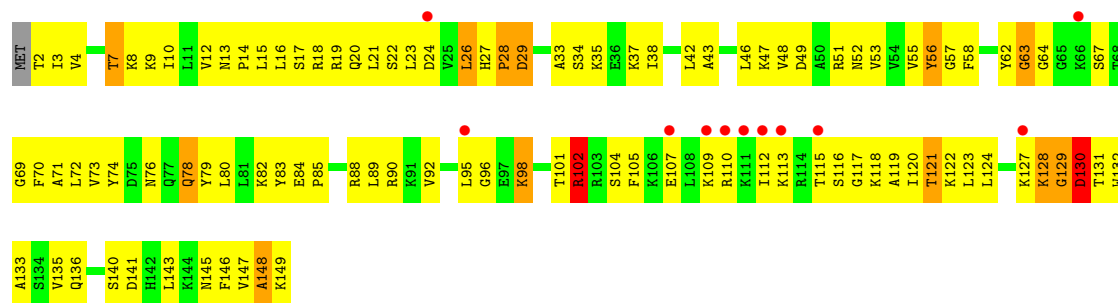


• Molecule 24: RPS13E

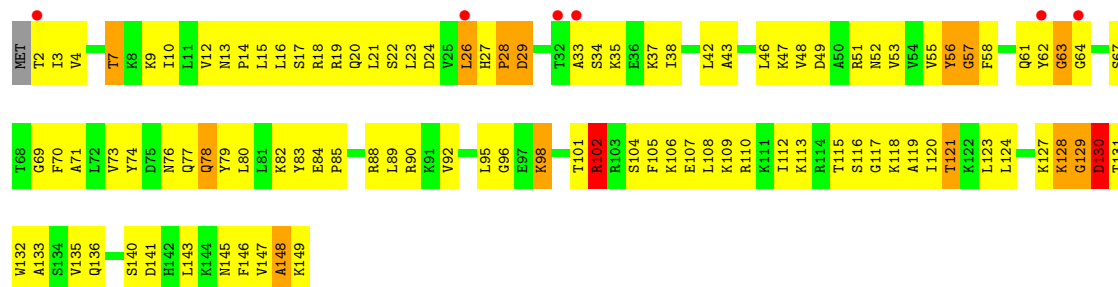




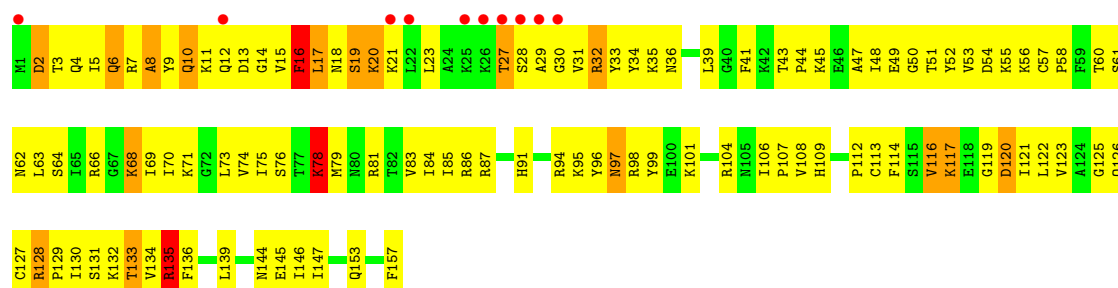
• Molecule 25: RPS24E



• Molecule 25: RPS24E

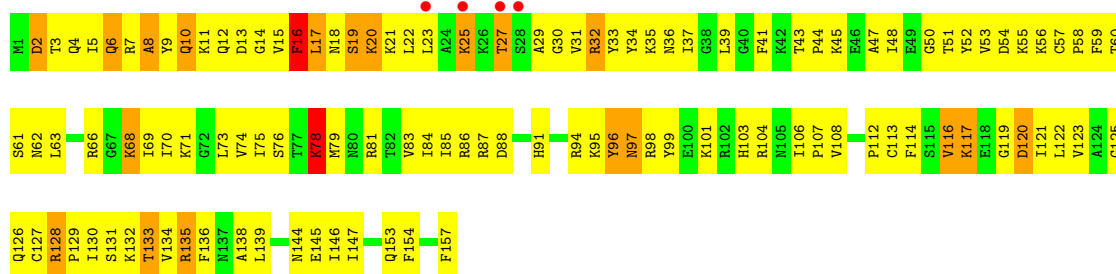


• Molecule 26: RIBOSOMAL PROTEIN S17 CONTAINING PROTEIN

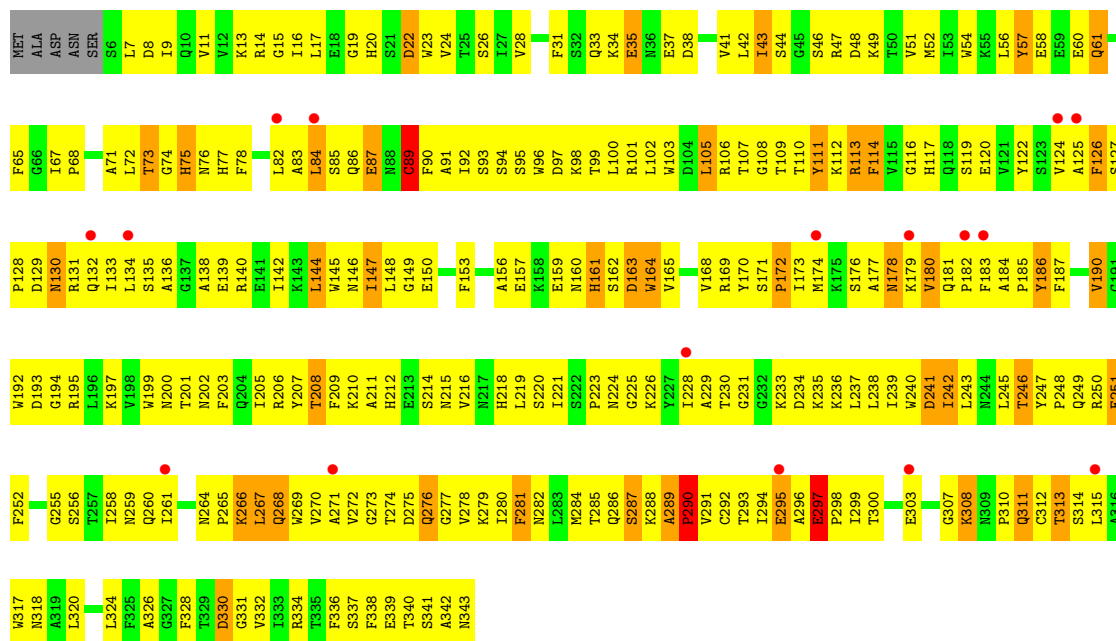


• Molecule 26: RIBOSOMAL PROTEIN S17 CONTAINING PROTEIN

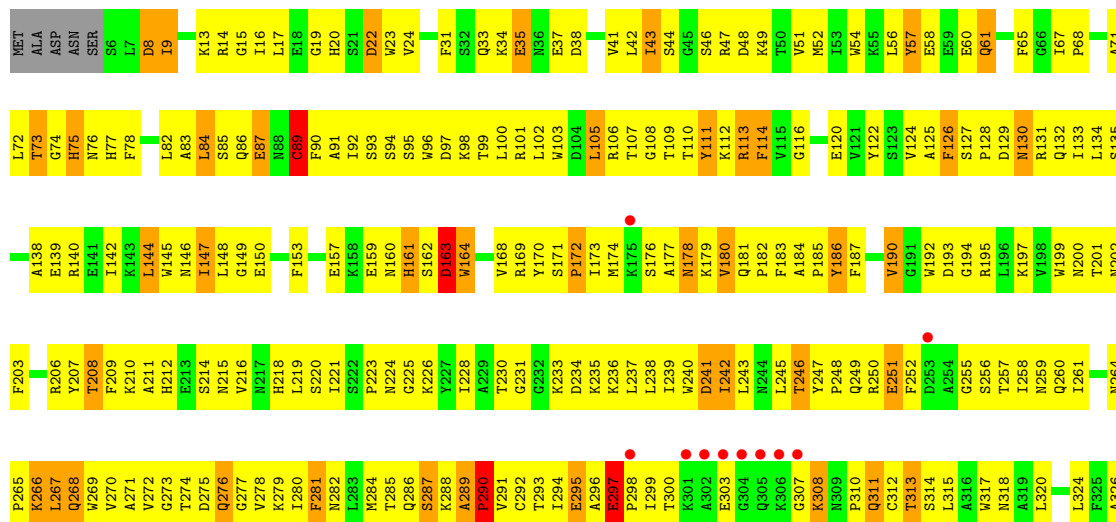




• Molecule 27: RACK1

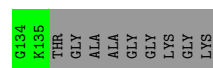
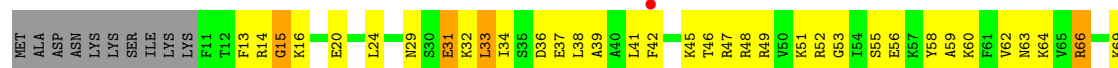


• Molecule 27: RACK1

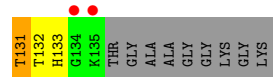
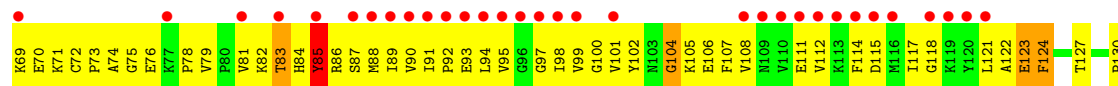
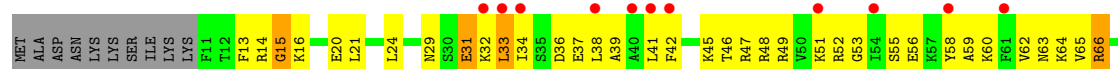




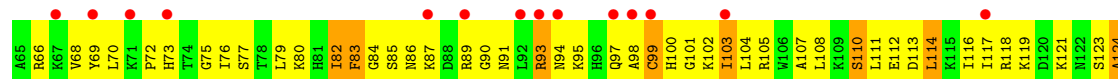
• Molecule 28: RPS15E



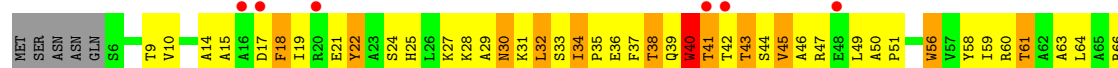
• Molecule 28: RPS15E

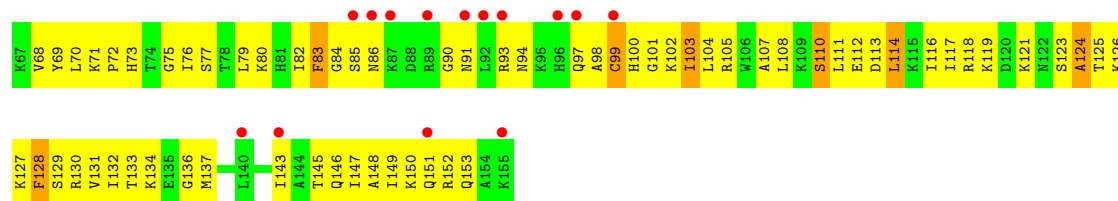


• Molecule 29: RPS19E

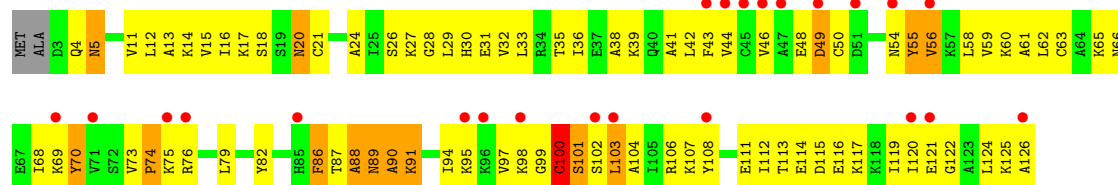


• Molecule 29: RPS19E

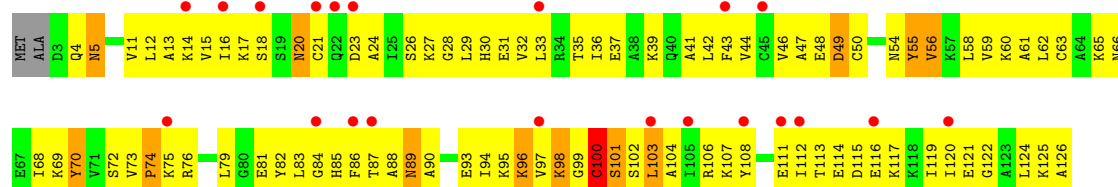




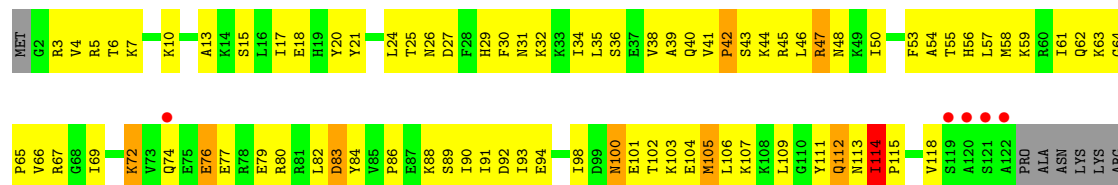
• Molecule 30: RIBOSOMAL PROTEIN L7AE CONTAINING PROTEIN



• Molecule 30: RIBOSOMAL PROTEIN L7AE CONTAINING PROTEIN



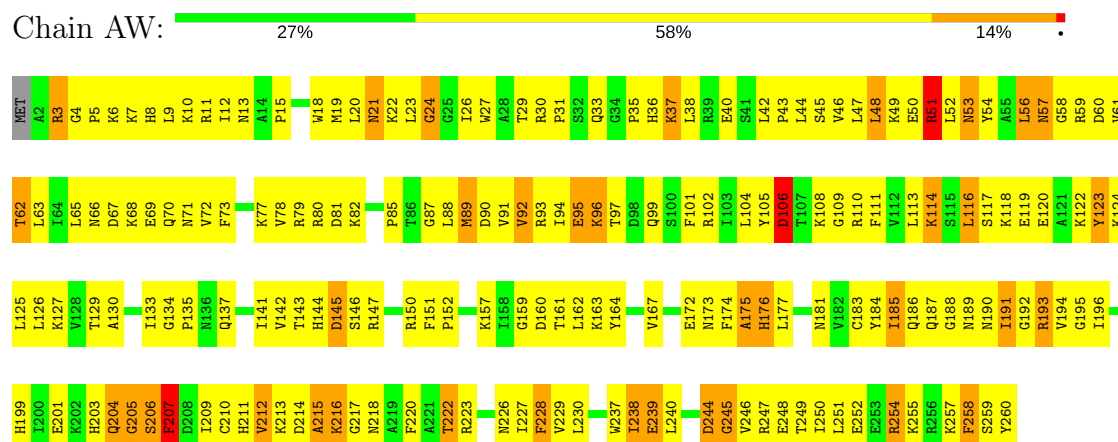
• Molecule 31: RPS17E



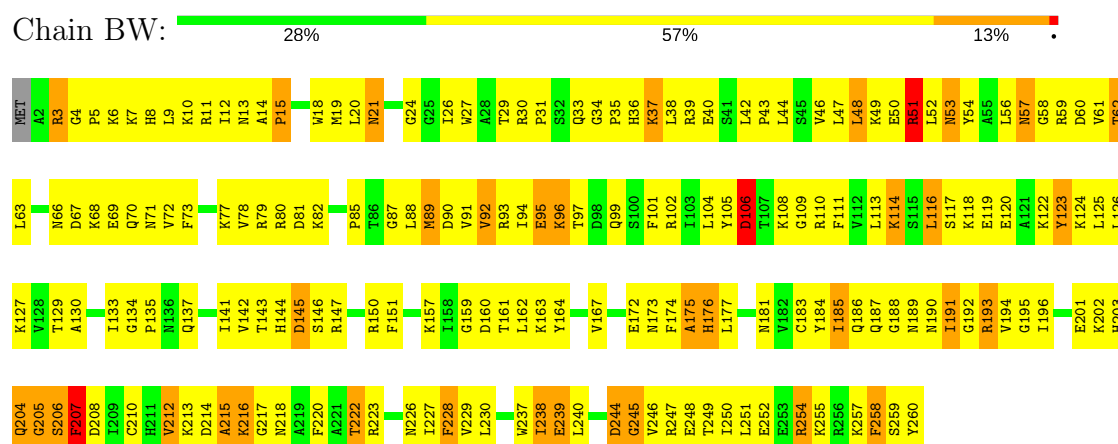
• Molecule 31: RPS17E



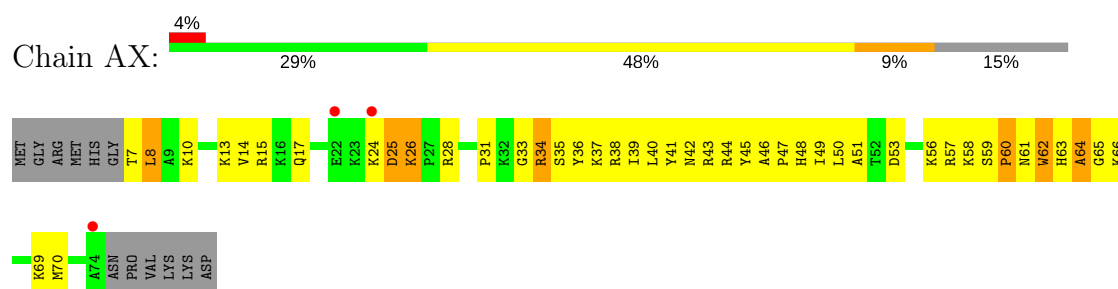
• Molecule 32: 40S RIBOSOMAL PROTEIN S4



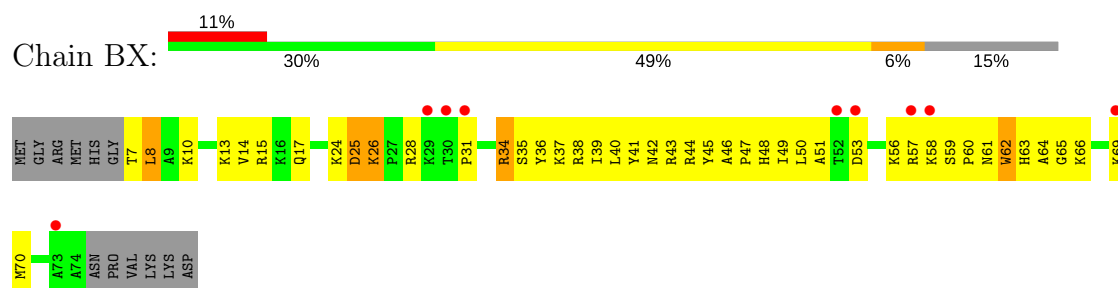
• Molecule 32: 40S RIBOSOMAL PROTEIN S4



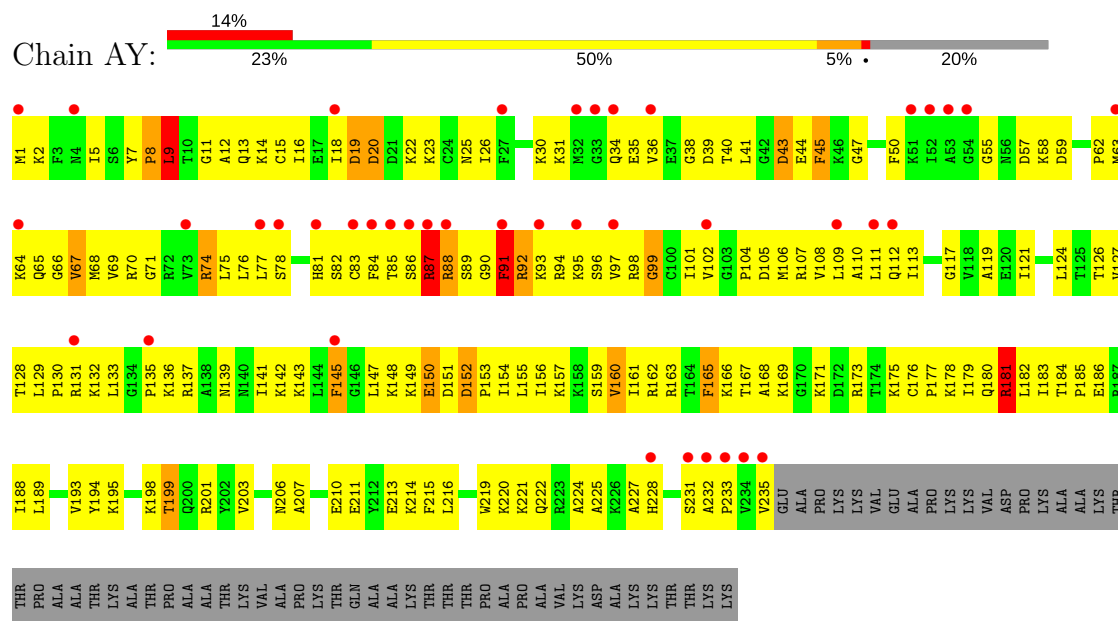
• Molecule 33: RPS30E



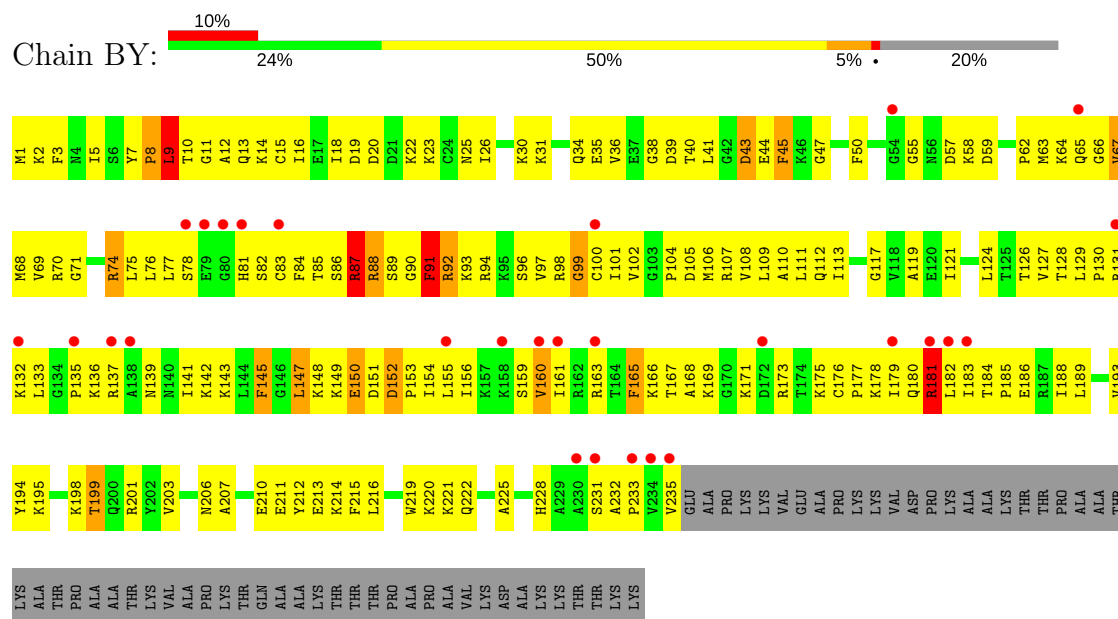
• Molecule 33: RPS30E



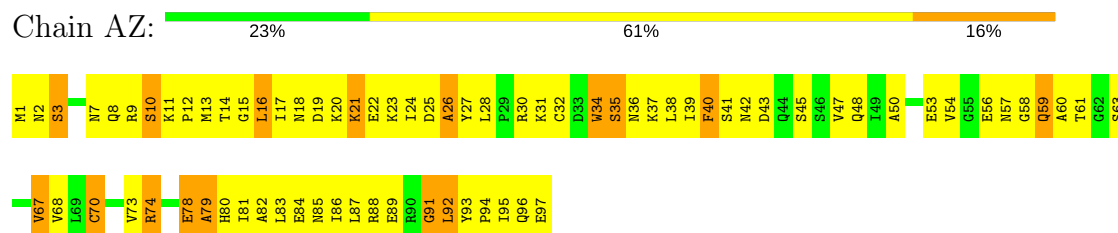
- Molecule 34: RPS6E



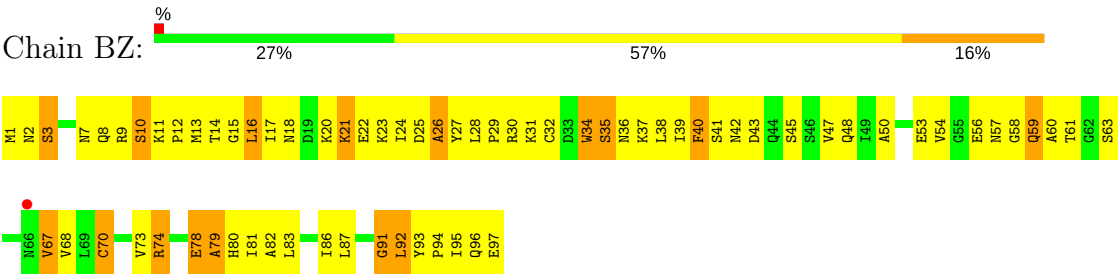
- Molecule 34: RPS6E



- Molecule 35: RPS21E



- Molecule 35: RPS21E



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	320.52Å 362.21Å 412.11Å 90.00° 109.61° 90.00°	Depositor
Resolution (Å)	25.00 – 3.93 97.05 – 3.93	Depositor EDS
% Data completeness (in resolution range)	85.1 (25.00-3.93) 85.1 (97.05-3.93)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 3.89Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.206 , 0.243 0.209 , 0.243	Depositor DCC
R_{free} test set	6686 reflections (2.00%)	DCC
Wilson B-factor (Å ²)	126.5	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 99.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	157632	wwPDB-VP
Average B, all atoms (Å ²)	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	A1	0.38	0/518	0.74	0/688
1	B1	0.37	0/518	0.73	0/688
2	A2	0.38	0/1717	0.70	1/2288 (0.0%)
2	B2	0.39	0/1717	0.71	1/2288 (0.0%)
3	A3	0.41	0/1656	0.70	0/2223
3	B3	0.42	0/1656	0.71	0/2223
4	A4	0.40	0/1748	0.71	1/2340 (0.0%)
4	B4	0.40	0/1748	0.71	1/2340 (0.0%)
5	A5	0.42	0/807	0.77	0/1077
5	B5	0.43	0/807	0.77	0/1077
6	A6	0.46	0/640	0.71	0/855
6	B6	0.48	0/640	0.71	0/855
7	A7	0.40	0/879	0.73	0/1183
7	B7	0.43	0/879	0.73	0/1183
8	A8	0.38	0/732	0.66	0/974
8	B8	0.37	0/732	0.65	0/974
9	A9	0.39	0/605	0.69	0/799
9	B9	0.39	0/605	0.69	0/799
10	AA	0.59	6/41668 (0.0%)	0.86	69/64931 (0.1%)
10	BA	0.58	6/41668 (0.0%)	0.86	70/64931 (0.1%)
11	AB	0.41	0/1676	0.66	0/2273
11	BB	0.40	0/1676	0.66	0/2273
12	AC	0.43	0/1855	0.71	0/2490
12	BC	0.42	0/1855	0.71	0/2490
13	AD	0.43	0/1498	0.69	0/1998
13	BD	0.41	0/1498	0.68	0/1998
14	AE	0.47	0/1873	0.75	1/2533 (0.0%)
14	BE	0.46	0/1873	0.74	1/2533 (0.0%)
15	AF	0.43	0/751	0.68	0/1010
15	BF	0.44	0/751	0.68	0/1010
16	AG	0.45	0/1546	0.71	0/2079
16	BG	0.45	0/1546	0.71	0/2079

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AH	0.48	0/1058	0.83	0/1421
17	BH	0.49	0/1058	0.85	1/1421 (0.1%)
18	AI	0.42	0/1151	0.68	0/1540
18	BI	0.41	0/1151	0.68	0/1540
19	AJ	0.38	0/842	0.77	0/1133
19	BJ	0.39	0/842	0.77	0/1133
20	AK	0.42	0/1078	0.73	0/1452
20	BK	0.41	0/1078	0.73	0/1452
21	AL	0.41	0/1114	0.73	0/1485
21	BL	0.43	0/1114	0.74	0/1485
22	AM	0.37	0/1260	0.67	0/1690
22	BM	0.39	0/1260	0.67	0/1690
23	AN	0.46	0/457	0.74	0/608
23	BN	0.49	0/457	0.75	0/608
24	AO	0.43	0/1238	0.74	1/1658 (0.1%)
24	BO	0.41	0/1238	0.73	1/1658 (0.1%)
25	AP	0.41	0/1215	0.70	0/1626
25	BP	0.41	0/1215	0.69	0/1626
26	AQ	0.46	0/1298	0.74	0/1741
26	BQ	0.44	0/1298	0.74	0/1741
27	AR	0.38	0/2750	0.69	0/3726
27	BR	0.38	0/2750	0.69	0/3726
28	AS	0.37	0/1003	0.65	1/1342 (0.1%)
28	BS	0.39	0/1003	0.66	1/1342 (0.1%)
29	AT	0.43	0/1233	0.66	0/1656
29	BT	0.42	0/1233	0.66	0/1656
30	AU	0.35	0/961	0.63	0/1288
30	BU	0.35	0/961	0.62	0/1288
31	AV	0.40	0/992	0.69	0/1326
31	BV	0.42	0/992	0.68	0/1326
32	AW	0.42	0/2119	0.74	0/2849
32	BW	0.42	0/2119	0.73	0/2849
33	AX	0.36	0/566	0.70	0/753
33	BX	0.36	0/566	0.71	0/753
34	AY	0.38	0/1895	0.67	0/2523
34	BY	0.38	0/1895	0.67	0/2523
35	AZ	0.42	0/755	0.75	0/1013
35	BZ	0.42	0/755	0.76	0/1013
All	All	0.51	12/166308 (0.0%)	0.79	150/241142 (0.1%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	A5	0	1
5	B5	0	1
10	AA	1	70
10	BA	1	74
26	BQ	0	1
27	AR	0	1
27	BR	0	1
All	All	2	149

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	AA	1109	U	O3'-P	7.44	1.70	1.61
10	BA	1	A	OP3-P	-7.12	1.52	1.61
10	AA	1	A	OP3-P	-6.89	1.52	1.61
10	BA	1109	U	O3'-P	-6.87	1.52	1.61
10	AA	1721	G	O3'-P	6.41	1.68	1.61

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	AA	1718	A	N9-C1'-C2'	11.64	129.13	114.00
10	BA	1718	A	N9-C1'-C2'	11.45	128.89	114.00
10	BA	1749	C	N1-C1'-C2'	10.71	127.93	114.00
10	BA	391	A	N9-C1'-C2'	10.52	127.67	114.00
10	AA	391	A	N9-C1'-C2'	10.36	127.47	114.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	AA	1718	A	C1'
10	BA	1718	A	C1'

5 of 149 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A5	39	TYR	Sidechain
10	AA	43	U	Sidechain
10	AA	55	U	Sidechain
10	AA	59	C	Sidechain
10	AA	64	U	Sidechain

5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	519	0	550	78	0
1	B1	519	0	550	80	0
2	A2	1693	0	1795	257	0
2	B2	1693	0	1795	265	0
3	A3	1629	0	1708	185	0
3	B3	1629	0	1708	178	0
4	A4	1724	0	1822	197	0
4	B4	1724	0	1822	191	0
5	A5	797	0	836	121	0
5	B5	797	0	837	108	0
6	A6	632	0	646	88	0
6	B6	632	0	646	97	0
7	A7	859	0	860	123	0
7	B7	859	0	860	129	0
8	A8	725	0	795	134	0
8	B8	725	0	795	124	0
9	A9	742	0	785	148	0
9	B9	742	0	787	134	0
10	AA	37231	0	18715	3075	0
10	BA	37231	0	18715	3021	0
11	AB	1642	0	1653	207	0
11	BB	1642	0	1653	216	0
12	AC	1820	0	1920	241	0
12	BC	1820	0	1920	236	0
13	AD	1475	0	1571	213	0
13	BD	1475	0	1571	211	0
14	AE	1827	0	1861	287	0
14	BE	1827	0	1861	282	0
15	AF	736	0	722	78	0
15	BF	736	0	722	88	0
16	AG	1520	0	1572	231	0
16	BG	1520	0	1572	231	0
17	AH	1040	0	1096	166	0
17	BH	1040	0	1096	170	0
18	AI	1135	0	1204	159	0
18	BI	1135	0	1204	146	0
19	AJ	833	0	903	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	BJ	833	0	903	81	0
20	AK	1063	0	1088	184	0
20	BK	1063	0	1088	178	0
21	AL	1097	0	1169	138	0
21	BL	1097	0	1169	135	0
22	AM	1239	0	1288	192	0
22	BM	1239	0	1288	192	0
23	AN	447	0	446	74	0
23	BN	447	0	446	81	0
24	AO	1214	0	1322	131	0
24	BO	1214	0	1322	131	0
25	AP	1197	0	1285	152	0
25	BP	1197	0	1285	142	0
26	AQ	1275	0	1354	213	0
26	BQ	1275	0	1354	199	0
27	AR	2682	0	2629	355	0
27	BR	2682	0	2629	327	0
28	AS	985	0	1026	114	0
28	BS	985	0	1026	122	0
29	AT	1211	0	1265	159	0
29	BT	1211	0	1265	162	0
30	AU	952	0	993	107	0
30	BU	952	0	993	124	0
31	AV	979	0	1041	136	0
31	BV	979	0	1041	141	0
32	AW	2079	0	2151	286	0
32	BW	2079	0	2151	293	0
33	AX	554	0	604	64	0
33	BX	554	0	604	72	0
34	AY	1868	0	1999	256	0
34	BY	1868	0	1999	242	0
35	AZ	747	0	758	107	0
35	BZ	747	0	758	109	0
36	A4	1	0	0	0	0
36	AA	90	0	0	0	0
36	AL	1	0	0	0	0
36	B4	1	0	0	0	0
36	BA	89	0	0	0	0
36	BD	1	0	0	0	0
36	BW	1	0	0	0	0
37	A5	1	0	0	0	0
37	A6	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	A9	1	0	0	0	0
37	AN	1	0	0	0	0
37	B5	1	0	0	0	0
37	B6	1	0	0	0	0
37	B9	1	0	0	0	0
37	BN	1	0	0	0	0
38	A2	2	0	0	0	0
38	A4	2	0	0	0	0
38	A5	1	0	0	0	0
38	AA	516	0	0	14	0
38	AC	1	0	0	0	0
38	AD	4	0	0	0	0
38	AE	3	0	0	0	0
38	AL	3	0	0	0	0
38	AM	4	0	0	1	0
38	AO	1	0	0	0	0
38	AP	1	0	0	0	0
38	AQ	2	0	0	0	0
38	AT	4	0	0	0	0
38	AW	4	0	0	0	0
38	AY	4	0	0	0	0
38	B2	2	0	0	0	0
38	B4	2	0	0	0	0
38	B5	1	0	0	0	0
38	BA	512	0	0	5	0
38	BC	2	0	0	0	0
38	BD	2	0	0	0	0
38	BE	5	0	0	0	0
38	BK	1	0	0	0	0
38	BL	2	0	0	0	0
38	BM	6	0	0	0	0
38	BO	1	0	0	0	0
38	BP	1	0	0	0	0
38	BQ	1	0	0	0	0
38	BT	6	0	0	0	0
38	BW	5	0	0	0	0
38	BY	3	0	0	0	0
All	All	157632	0	122867	15283	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 55.

The worst 5 of 15283 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AA:604:G:H1	10:AA:1080:G:N2	1.23	1.36
4:A4:207:THR:HG21	4:A4:213:LEU:HG	1.21	1.21
10:BA:604:G:H1	10:BA:1080:G:N2	1.40	1.19
21:AL:9:ILE:HD12	21:AL:9:ILE:H	1.02	1.18
10:AA:534:A:H3'	10:AA:535:A:H5'	1.18	1.18

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	
1	A1	65/68 (96%)	45 (69%)	11 (17%)	9 (14%)	0	5
1	B1	65/68 (96%)	44 (68%)	12 (18%)	9 (14%)	0	5
2	A2	205/208 (99%)	147 (72%)	38 (18%)	20 (10%)	1	13
2	B2	205/208 (99%)	146 (71%)	39 (19%)	20 (10%)	1	13
3	A3	194/197 (98%)	159 (82%)	25 (13%)	10 (5%)	2	28
3	B3	194/197 (98%)	159 (82%)	24 (12%)	11 (6%)	2	26
4	A4	213/265 (80%)	161 (76%)	33 (16%)	19 (9%)	1	15
4	B4	213/265 (80%)	161 (76%)	34 (16%)	18 (8%)	1	16
5	A5	96/119 (81%)	66 (69%)	20 (21%)	10 (10%)	0	11
5	B5	96/119 (81%)	65 (68%)	21 (22%)	10 (10%)	0	11
6	A6	78/81 (96%)	57 (73%)	15 (19%)	6 (8%)	1	18
6	B6	78/81 (96%)	57 (73%)	15 (19%)	6 (8%)	1	18
7	A7	102/162 (63%)	78 (76%)	17 (17%)	7 (7%)	1	22
7	B7	102/162 (63%)	78 (76%)	17 (17%)	7 (7%)	1	22
8	A8	91/143 (64%)	71 (78%)	13 (14%)	7 (8%)	1	18
8	B8	91/143 (64%)	71 (78%)	13 (14%)	7 (8%)	1	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	A9	72/189 (38%)	50 (69%)	17 (24%)	5 (7%)	1	22
9	B9	72/189 (38%)	50 (69%)	17 (24%)	5 (7%)	1	22
11	AB	202/241 (84%)	168 (83%)	28 (14%)	6 (3%)	5	41
11	BB	202/241 (84%)	167 (83%)	28 (14%)	7 (4%)	4	38
12	AC	227/243 (93%)	177 (78%)	31 (14%)	19 (8%)	1	16
12	BC	227/243 (93%)	176 (78%)	32 (14%)	19 (8%)	1	16
13	AD	177/181 (98%)	132 (75%)	36 (20%)	9 (5%)	2	28
13	BD	177/181 (98%)	130 (73%)	38 (22%)	9 (5%)	2	28
14	AE	228/296 (77%)	170 (75%)	40 (18%)	18 (8%)	1	18
14	BE	228/296 (77%)	172 (75%)	39 (17%)	17 (8%)	1	19
15	AF	87/101 (86%)	70 (80%)	12 (14%)	5 (6%)	2	26
15	BF	87/101 (86%)	70 (80%)	12 (14%)	5 (6%)	2	26
16	AG	190/200 (95%)	141 (74%)	33 (17%)	16 (8%)	1	16
16	BG	190/200 (95%)	142 (75%)	31 (16%)	17 (9%)	1	15
17	AH	127/130 (98%)	98 (77%)	24 (19%)	5 (4%)	3	34
17	BH	127/130 (98%)	98 (77%)	26 (20%)	3 (2%)	7	45
18	AI	141/145 (97%)	111 (79%)	25 (18%)	5 (4%)	4	38
18	BI	141/145 (97%)	110 (78%)	26 (18%)	5 (4%)	4	38
19	AJ	103/120 (86%)	89 (86%)	6 (6%)	8 (8%)	1	18
19	BJ	103/120 (86%)	89 (86%)	6 (6%)	8 (8%)	1	18
20	AK	138/151 (91%)	96 (70%)	28 (20%)	14 (10%)	1	12
20	BK	138/151 (91%)	95 (69%)	27 (20%)	16 (12%)	0	8
21	AL	139/142 (98%)	106 (76%)	17 (12%)	16 (12%)	0	8
21	BL	139/142 (98%)	106 (76%)	18 (13%)	15 (11%)	0	10
22	AM	152/155 (98%)	109 (72%)	22 (14%)	21 (14%)	0	5
22	BM	152/155 (98%)	110 (72%)	21 (14%)	21 (14%)	0	5
23	AN	51/55 (93%)	30 (59%)	11 (22%)	10 (20%)	0	2
23	BN	51/55 (93%)	31 (61%)	11 (22%)	9 (18%)	0	3
24	AO	148/153 (97%)	112 (76%)	20 (14%)	16 (11%)	0	10
24	BO	148/153 (97%)	113 (76%)	19 (13%)	16 (11%)	0	10
25	AP	146/149 (98%)	115 (79%)	20 (14%)	11 (8%)	1	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	BP	146/149 (98%)	115 (79%)	20 (14%)	11 (8%)	1	19
26	AQ	155/157 (99%)	115 (74%)	26 (17%)	14 (9%)	1	15
26	BQ	155/157 (99%)	112 (72%)	27 (17%)	16 (10%)	0	11
27	AR	336/343 (98%)	255 (76%)	48 (14%)	33 (10%)	1	13
27	BR	336/343 (98%)	256 (76%)	48 (14%)	32 (10%)	1	14
28	AS	123/144 (85%)	91 (74%)	25 (20%)	7 (6%)	2	26
28	BS	123/144 (85%)	90 (73%)	25 (20%)	8 (6%)	1	24
29	AT	148/155 (96%)	114 (77%)	17 (12%)	17 (12%)	0	8
29	BT	148/155 (96%)	113 (76%)	20 (14%)	15 (10%)	1	12
30	AU	122/126 (97%)	91 (75%)	20 (16%)	11 (9%)	1	15
30	BU	122/126 (97%)	89 (73%)	22 (18%)	11 (9%)	1	15
31	AV	119/130 (92%)	94 (79%)	16 (13%)	9 (8%)	1	19
31	BV	119/130 (92%)	96 (81%)	14 (12%)	9 (8%)	1	19
32	AW	257/260 (99%)	193 (75%)	40 (16%)	24 (9%)	1	14
32	BW	257/260 (99%)	195 (76%)	38 (15%)	24 (9%)	1	14
33	AX	66/80 (82%)	48 (73%)	12 (18%)	6 (9%)	1	15
33	BX	66/80 (82%)	48 (73%)	12 (18%)	6 (9%)	1	15
34	AY	233/293 (80%)	188 (81%)	31 (13%)	14 (6%)	2	25
34	BY	233/293 (80%)	187 (80%)	32 (14%)	14 (6%)	2	25
35	AZ	95/97 (98%)	70 (74%)	13 (14%)	12 (13%)	0	7
35	BZ	95/97 (98%)	69 (73%)	14 (15%)	12 (13%)	0	7
All	All	10052/11358 (88%)	7627 (76%)	1588 (16%)	837 (8%)	1	16

5 of 837 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A1	20	SER
1	A1	35	LYS
1	A1	37	GLU
1	A1	59	GLU
1	A1	63	GLU

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	
1	A1	56/57 (98%)	53 (95%)	3 (5%)	26	62
1	B1	56/57 (98%)	53 (95%)	3 (5%)	26	62
2	A2	184/185 (100%)	171 (93%)	13 (7%)	17	54
2	B2	184/185 (100%)	171 (93%)	13 (7%)	17	54
3	A3	182/183 (100%)	164 (90%)	18 (10%)	9	39
3	B3	182/183 (100%)	165 (91%)	17 (9%)	10	42
4	A4	191/225 (85%)	166 (87%)	25 (13%)	5	28
4	B4	191/225 (85%)	166 (87%)	25 (13%)	5	28
5	A5	88/107 (82%)	80 (91%)	8 (9%)	11	43
5	B5	88/107 (82%)	80 (91%)	8 (9%)	11	43
6	A6	71/72 (99%)	67 (94%)	4 (6%)	25	61
6	B6	71/72 (99%)	67 (94%)	4 (6%)	25	61
7	A7	94/136 (69%)	84 (89%)	10 (11%)	8	36
7	B7	94/136 (69%)	84 (89%)	10 (11%)	8	36
8	A8	80/109 (73%)	68 (85%)	12 (15%)	3	23
8	B8	80/109 (73%)	68 (85%)	12 (15%)	3	23
9	A9	64/138 (46%)	56 (88%)	8 (12%)	5	29
9	B9	64/138 (46%)	56 (88%)	8 (12%)	5	29
11	AB	183/211 (87%)	167 (91%)	16 (9%)	12	45
11	BB	183/211 (87%)	167 (91%)	16 (9%)	12	45
12	AC	197/210 (94%)	178 (90%)	19 (10%)	10	40
12	BC	197/210 (94%)	179 (91%)	18 (9%)	11	43
13	AD	161/162 (99%)	137 (85%)	24 (15%)	3	24
13	BD	161/162 (99%)	137 (85%)	24 (15%)	3	24
14	AE	194/250 (78%)	171 (88%)	23 (12%)	6	32
14	BE	194/250 (78%)	171 (88%)	23 (12%)	6	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	AF	80/92 (87%)	72 (90%)	8 (10%)	9	38
15	BF	80/92 (87%)	71 (89%)	9 (11%)	7	34
16	AG	163/169 (96%)	147 (90%)	16 (10%)	9	39
16	BG	163/169 (96%)	146 (90%)	17 (10%)	8	37
17	AH	116/117 (99%)	101 (87%)	15 (13%)	5	29
17	BH	116/117 (99%)	102 (88%)	14 (12%)	6	31
18	AI	120/122 (98%)	115 (96%)	5 (4%)	34	68
18	BI	120/122 (98%)	115 (96%)	5 (4%)	34	68
19	AJ	98/111 (88%)	93 (95%)	5 (5%)	28	63
19	BJ	98/111 (88%)	93 (95%)	5 (5%)	28	63
20	AK	112/121 (93%)	96 (86%)	16 (14%)	4	26
20	BK	112/121 (93%)	96 (86%)	16 (14%)	4	26
21	AL	113/114 (99%)	101 (89%)	12 (11%)	8	36
21	BL	113/114 (99%)	102 (90%)	11 (10%)	9	40
22	AM	134/135 (99%)	121 (90%)	13 (10%)	9	40
22	BM	134/135 (99%)	121 (90%)	13 (10%)	9	40
23	AN	47/49 (96%)	41 (87%)	6 (13%)	5	29
23	BN	47/49 (96%)	41 (87%)	6 (13%)	5	29
24	AO	134/136 (98%)	127 (95%)	7 (5%)	27	63
24	BO	134/136 (98%)	127 (95%)	7 (5%)	27	63
25	AP	133/134 (99%)	124 (93%)	9 (7%)	18	55
25	BP	133/134 (99%)	124 (93%)	9 (7%)	18	55
26	AQ	141/141 (100%)	125 (89%)	16 (11%)	7	34
26	BQ	141/141 (100%)	126 (89%)	15 (11%)	8	36
27	AR	291/295 (99%)	261 (90%)	30 (10%)	8	37
27	BR	291/295 (99%)	260 (89%)	31 (11%)	8	36
28	AS	105/117 (90%)	102 (97%)	3 (3%)	48	75
28	BS	105/117 (90%)	101 (96%)	4 (4%)	38	70
29	AT	129/134 (96%)	117 (91%)	12 (9%)	10	42
29	BT	129/134 (96%)	116 (90%)	13 (10%)	9	38
30	AU	103/104 (99%)	97 (94%)	6 (6%)	23	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	BU	103/104 (99%)	99 (96%)	4 (4%)	37	69
31	AV	108/115 (94%)	100 (93%)	8 (7%)	16	52
31	BV	108/115 (94%)	99 (92%)	9 (8%)	13	47
32	AW	226/227 (100%)	196 (87%)	30 (13%)	4	28
32	BW	226/227 (100%)	197 (87%)	29 (13%)	5	29
33	AX	57/67 (85%)	55 (96%)	2 (4%)	41	72
33	BX	57/67 (85%)	55 (96%)	2 (4%)	41	72
34	AY	201/244 (82%)	187 (93%)	14 (7%)	18	54
34	BY	201/244 (82%)	187 (93%)	14 (7%)	18	54
35	AZ	82/82 (100%)	76 (93%)	6 (7%)	16	53
35	BZ	82/82 (100%)	76 (93%)	6 (7%)	16	53
All	All	8876/9742 (91%)	8034 (90%)	842 (10%)	10	41

5 of 842 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	AW	106	ASP
4	B4	134	ASP
30	BU	20	ASN
32	AW	212	VAL
2	B2	35	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 276 such sidechains are listed below:

Mol	Chain	Res	Type
31	AV	48	ASN
4	B4	175	ASN
30	BU	7	GLN
32	AW	53	ASN
34	AY	206	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	AA	1743/1753 (99%)	452 (25%)	0
10	BA	1743/1753 (99%)	453 (25%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	3486/3506 (99%)	905 (25%)	0

5 of 905 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	AA	2	A
10	AA	3	C
10	AA	4	C
10	AA	9	U
10	AA	17	C

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 192 ligands modelled in this entry, 192 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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A1	67/68 (98%)	-0.28	1 (1%) 74 64	99, 157, 220, 262	0
1	B1	67/68 (98%)	-0.53	0 100 100	99, 157, 220, 262	0
2	A2	207/208 (99%)	1.21	58 (28%) 1 1	96, 144, 194, 231	0
2	B2	207/208 (99%)	0.60	17 (8%) 12 10	98, 145, 194, 231	0
3	A3	196/197 (99%)	-0.00	6 (3%) 49 39	82, 138, 187, 267	0
3	B3	196/197 (99%)	-0.09	3 (1%) 74 64	75, 138, 186, 266	0
4	A4	215/265 (81%)	0.62	23 (10%) 7 6	80, 146, 201, 228	0
4	B4	215/265 (81%)	0.76	30 (13%) 3 4	77, 145, 202, 229	0
5	A5	98/119 (82%)	0.11	3 (3%) 49 39	71, 124, 201, 246	0
5	B5	98/119 (82%)	0.53	8 (8%) 12 10	68, 124, 201, 246	0
6	A6	80/81 (98%)	0.09	0 100 100	86, 130, 172, 187	0
6	B6	80/81 (98%)	-0.25	0 100 100	86, 128, 172, 186	0
7	A7	104/162 (64%)	-0.13	0 100 100	100, 150, 201, 249	0
7	B7	104/162 (64%)	0.19	7 (6%) 19 14	104, 151, 199, 249	0
8	A8	93/143 (65%)	0.08	1 (1%) 80 72	112, 159, 219, 255	0
8	B8	93/143 (65%)	0.10	3 (3%) 48 38	110, 159, 219, 256	0
9	A9	73/189 (38%)	0.26	6 (8%) 12 10	146, 185, 238, 253	0
9	B9	73/189 (38%)	0.62	13 (17%) 2 2	148, 186, 238, 254	0
10	AA	1745/1753 (99%)	0.05	33 (1%) 67 58	80, 134, 291, 454	0
10	BA	1745/1753 (99%)	0.04	33 (1%) 67 58	80, 134, 291, 454	0
11	AB	204/241 (84%)	-0.30	3 (1%) 74 64	82, 136, 177, 225	0
11	BB	204/241 (84%)	-0.05	2 (0%) 82 74	78, 136, 177, 224	0
12	AC	229/243 (94%)	-0.21	2 (0%) 84 76	89, 131, 194, 244	0
12	BC	229/243 (94%)	-0.34	0 100 100	87, 132, 195, 246	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AD	179/181 (98%)	0.17	4 (2%) 62 53	77, 122, 182, 214	0
13	BD	179/181 (98%)	-0.03	4 (2%) 62 53	82, 125, 184, 215	0
14	AE	230/296 (77%)	-0.01	4 (1%) 70 61	62, 114, 194, 243	0
14	BE	230/296 (77%)	-0.17	3 (1%) 77 68	65, 116, 194, 244	0
15	AF	89/101 (88%)	-0.30	0 100 100	87, 136, 190, 230	0
15	BF	89/101 (88%)	-0.36	0 100 100	86, 137, 190, 229	0
16	AG	192/200 (96%)	0.03	3 (1%) 72 62	86, 140, 191, 286	0
16	BG	192/200 (96%)	-0.13	6 (3%) 49 39	86, 140, 191, 287	0
17	AH	129/130 (99%)	-0.22	0 100 100	65, 105, 154, 194	0
17	BH	129/130 (99%)	-0.10	0 100 100	62, 106, 154, 193	0
18	AI	143/145 (98%)	0.56	17 (11%) 5 6	87, 135, 188, 222	0
18	BI	143/145 (98%)	0.66	14 (9%) 8 7	87, 135, 189, 221	0
19	AJ	105/120 (87%)	-0.14	1 (0%) 82 74	84, 132, 199, 218	0
19	BJ	105/120 (87%)	-0.07	0 100 100	86, 133, 198, 218	0
20	AK	140/151 (92%)	0.05	3 (2%) 64 54	93, 144, 191, 223	0
20	BK	140/151 (92%)	0.48	11 (7%) 13 11	90, 144, 192, 224	0
21	AL	141/142 (99%)	0.18	4 (2%) 53 43	71, 126, 169, 213	0
21	BL	141/142 (99%)	0.93	27 (19%) 1 2	74, 128, 169, 212	0
22	AM	154/155 (99%)	0.43	7 (4%) 34 27	94, 154, 204, 233	0
22	BM	154/155 (99%)	0.32	6 (3%) 40 31	95, 155, 205, 233	0
23	AN	53/55 (96%)	0.21	0 100 100	83, 124, 156, 193	0
23	BN	53/55 (96%)	0.78	9 (16%) 2 3	83, 126, 157, 192	0
24	AO	150/153 (98%)	-0.17	1 (0%) 87 81	73, 124, 223, 287	0
24	BO	150/153 (98%)	0.03	2 (1%) 77 68	71, 124, 222, 288	0
25	AP	148/149 (99%)	0.31	11 (7%) 15 12	92, 141, 168, 200	0
25	BP	148/149 (99%)	0.05	6 (4%) 38 30	94, 141, 170, 200	0
26	AQ	157/157 (100%)	0.12	10 (6%) 20 14	69, 129, 214, 227	0
26	BQ	157/157 (100%)	0.20	4 (2%) 58 47	65, 128, 208, 258	0
27	AR	338/343 (98%)	0.17	16 (4%) 32 25	93, 146, 218, 268	0
27	BR	338/343 (98%)	-0.05	10 (2%) 51 40	94, 145, 209, 245	0
28	AS	125/144 (86%)	0.07	5 (4%) 39 30	117, 165, 222, 245	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	BS	125/144 (86%)	1.59	45 (36%) 0 1	119, 165, 222, 245	0
29	AT	150/155 (96%)	1.02	25 (16%) 2 3	80, 152, 191, 230	0
29	BT	150/155 (96%)	0.70	20 (13%) 4 4	79, 151, 192, 229	0
30	AU	124/126 (98%)	0.67	23 (18%) 1 2	117, 177, 213, 227	0
30	BU	124/126 (98%)	0.96	21 (16%) 2 3	136, 185, 221, 250	0
31	AV	121/130 (93%)	-0.18	5 (4%) 38 30	78, 143, 206, 254	0
31	BV	121/130 (93%)	0.18	3 (2%) 58 47	76, 142, 206, 253	0
32	AW	259/260 (99%)	-0.22	0 100 100	84, 125, 166, 200	0
32	BW	259/260 (99%)	-0.45	0 100 100	87, 126, 167, 199	0
33	AX	68/80 (85%)	0.39	3 (4%) 35 27	106, 155, 242, 271	0
33	BX	68/80 (85%)	0.72	9 (13%) 4 4	107, 158, 243, 271	0
34	AY	235/293 (80%)	0.81	41 (17%) 2 2	108, 159, 237, 316	0
34	BY	235/293 (80%)	0.47	28 (11%) 5 6	110, 159, 237, 315	0
35	AZ	97/97 (100%)	-0.23	0 100 100	74, 129, 185, 209	0
35	BZ	97/97 (100%)	-0.39	1 (1%) 82 74	77, 129, 184, 210	0
All	All	13676/14864 (92%)	0.15	664 (4%) 30 24	62, 139, 215, 454	0

The worst 5 of 664 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	BA	213	U	12.8
10	BA	211	U	12.1
34	AY	235	VAL	10.0
4	B4	229	LEU	9.8
4	B4	15	LYS	9.6

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
36	MG	BA	1888	1/1	0.84	2.06	31.49	227,227,227,227	0
36	MG	BA	1873	1/1	0.76	0.59	17.23	218,218,218,218	0
36	MG	AA	1889	1/1	0.90	0.72	16.22	200,200,200,200	0
36	MG	AA	1851	1/1	0.95	0.31	10.11	187,187,187,187	0
36	MG	AA	1874	1/1	0.82	0.30	5.97	194,194,194,194	0
36	MG	AA	1815	1/1	0.96	0.39	5.29	144,144,144,144	0
36	MG	BA	1815	1/1	0.98	0.33	4.81	155,155,155,155	0
36	MG	BA	1810	1/1	0.93	0.42	4.14	188,188,188,188	0
36	MG	AA	1868	1/1	0.82	1.01	3.01	197,197,197,197	0
36	MG	AA	1881	1/1	0.95	0.29	2.78	198,198,198,198	0
36	MG	BA	1803	1/1	0.94	0.40	2.62	169,169,169,169	0
36	MG	AA	1856	1/1	0.91	0.74	1.92	182,182,182,182	0
36	MG	BA	1859	1/1	0.86	0.26	1.10	194,194,194,194	0
36	MG	AA	1810	1/1	0.97	0.28	0.61	175,175,175,175	0
36	MG	BA	1865	1/1	0.87	0.20	0.57	183,183,183,183	0
36	MG	BA	1868	1/1	0.92	0.20	-0.29	208,208,208,208	0
36	MG	BA	1851	1/1	0.85	0.17	-0.53	169,169,169,169	0
36	MG	AA	1802	1/1	0.90	0.19	-0.55	175,175,175,175	0
36	MG	BA	1825	1/1	0.84	0.13	-0.57	153,153,153,153	0
37	ZN	B6	500	1/1	0.99	0.13	-0.61	108,108,108,108	0
37	ZN	B5	500	1/1	0.99	0.16	-0.91	87,87,87,87	0
36	MG	BA	1802	1/1	0.92	0.11	-0.96	169,169,169,169	0
37	ZN	A6	500	1/1	0.99	0.11	-1.16	118,118,118,118	0
37	ZN	AN	500	1/1	0.99	0.12	-1.40	105,105,105,105	0
37	ZN	B9	500	1/1	0.95	0.06	-1.43	247,247,247,247	0
37	ZN	BN	500	1/1	0.98	0.11	-1.43	113,113,113,113	0
36	MG	BA	1814	1/1	0.91	0.11	-1.50	214,214,214,214	0
37	ZN	A5	500	1/1	0.99	0.11	-1.56	95,95,95,95	0
37	ZN	A9	500	1/1	0.99	0.10	-1.77	169,169,169,169	0
36	MG	BA	1833	1/1	0.93	0.13	-2.08	172,172,172,172	0
36	MG	BA	1884	1/1	0.82	0.13	-2.14	219,219,219,219	0
36	MG	AA	1818	1/1	0.96	0.14	-2.19	121,121,121,121	0
36	MG	BA	1831	1/1	0.97	0.13	-2.48	115,115,115,115	0
36	MG	AA	1819	1/1	0.98	0.12	-2.52	136,136,136,136	0
36	MG	AA	1803	1/1	0.95	0.08	-2.71	147,147,147,147	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	MG	AA	1831	1/1	0.96	0.19	-3.11	111,111,111,111	0
36	MG	AA	1865	1/1	0.93	0.11	-3.33	184,184,184,184	0
36	MG	AA	1814	1/1	0.88	0.07	-3.48	197,197,197,197	0
36	MG	BA	1818	1/1	0.98	0.07	-4.05	111,111,111,111	0
36	MG	AA	1816	1/1	0.98	0.09	-4.28	96,96,96,96	0
36	MG	AA	1887	1/1	0.91	0.08	-4.64	198,198,198,198	0
36	MG	BA	1880	1/1	0.87	0.09	-5.06	193,193,193,193	0
36	MG	BA	1819	1/1	0.97	0.11	-5.85	122,122,122,122	0
36	MG	B4	301	1/1	0.88	0.07	-	165,165,165,165	0
36	MG	AA	1882	1/1	0.77	0.43	-	181,181,181,181	0
36	MG	AA	1834	1/1	0.82	0.24	-	182,182,182,182	0
36	MG	AA	1822	1/1	0.95	0.13	-	139,139,139,139	0
36	MG	BA	1813	1/1	0.97	0.07	-	187,187,187,187	0
36	MG	BA	1863	1/1	0.97	0.12	-	166,166,166,166	0
36	MG	BA	1842	1/1	0.63	0.49	-	210,210,210,210	0
36	MG	AA	1817	1/1	0.98	0.19	-	126,126,126,126	0
36	MG	AA	1846	1/1	0.93	0.14	-	161,161,161,161	0
36	MG	BA	1882	1/1	0.93	0.59	-	196,196,196,196	0
36	MG	BA	1849	1/1	0.64	0.23	-	198,198,198,198	0
36	MG	AA	1806	1/1	0.89	0.14	-	151,151,151,151	0
36	MG	BA	1885	1/1	0.95	0.24	-	161,161,161,161	0
36	MG	BA	1845	1/1	0.68	0.23	-	225,225,225,225	0
36	MG	AA	1811	1/1	0.93	0.11	-	154,154,154,154	0
36	MG	AA	1835	1/1	0.90	0.15	-	159,159,159,159	0
36	MG	BA	1821	1/1	0.91	0.11	-	160,160,160,160	0
36	MG	BW	301	1/1	0.81	0.12	-	166,166,166,166	0
36	MG	BA	1857	1/1	0.95	0.18	-	130,130,130,130	0
36	MG	BA	1840	1/1	0.95	0.13	-	128,128,128,128	0
36	MG	AA	1832	1/1	0.90	0.07	-	189,189,189,189	0
36	MG	AA	1858	1/1	0.83	0.08	-	162,162,162,162	0
36	MG	AA	1880	1/1	0.94	0.09	-	193,193,193,193	0
36	MG	A4	301	1/1	0.96	0.16	-	174,174,174,174	0
36	MG	AA	1862	1/1	0.97	0.06	-	191,191,191,191	0
36	MG	BA	1841	1/1	0.96	0.11	-	129,129,129,129	0
36	MG	AA	1852	1/1	0.79	0.10	-	173,173,173,173	0
36	MG	AA	1857	1/1	0.94	0.09	-	140,140,140,140	0
36	MG	AA	1878	1/1	0.91	0.10	-	160,160,160,160	0
36	MG	BA	1878	1/1	0.79	0.17	-	177,177,177,177	0
36	MG	BA	1877	1/1	0.91	0.13	-	177,177,177,177	0
36	MG	AA	1833	1/1	0.97	0.10	-	135,135,135,135	0
36	MG	BA	1827	1/1	0.89	0.23	-	199,199,199,199	0
36	MG	BA	1828	1/1	0.95	0.18	-	145,145,145,145	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	MG	AA	1888	1/1	0.74	0.30	-	205,205,205,205	0
36	MG	AA	1805	1/1	0.94	0.49	-	175,175,175,175	0
36	MG	AA	1886	1/1	0.88	0.22	-	148,148,148,148	0
36	MG	BA	1854	1/1	0.77	0.26	-	189,189,189,189	0
36	MG	BA	1808	1/1	0.97	0.49	-	140,140,140,140	0
36	MG	AA	1807	1/1	0.88	0.07	-	194,194,194,194	0
36	MG	BA	1887	1/1	0.78	0.36	-	206,206,206,206	0
36	MG	AA	1869	1/1	0.84	0.32	-	209,209,209,209	0
36	MG	BA	1838	1/1	0.79	0.47	-	172,172,172,172	0
36	MG	BA	1836	1/1	0.81	0.37	-	175,175,175,175	0
36	MG	BA	1806	1/1	0.90	0.22	-	168,168,168,168	0
36	MG	AA	1844	1/1	0.92	0.36	-	166,166,166,166	0
36	MG	BA	1835	1/1	0.87	0.25	-	187,187,187,187	0
36	MG	AA	1873	1/1	0.89	0.56	-	196,196,196,196	0
36	MG	BA	1860	1/1	0.92	0.07	-	177,177,177,177	0
36	MG	AA	1809	1/1	0.80	0.40	-	193,193,193,193	0
36	MG	AA	1837	1/1	0.92	0.12	-	149,149,149,149	0
36	MG	BA	1811	1/1	0.89	0.22	-	170,170,170,170	0
36	MG	AA	1871	1/1	0.82	0.38	-	201,201,201,201	0
36	MG	BA	1867	1/1	0.66	0.14	-	180,180,180,180	0
36	MG	BA	1832	1/1	0.95	0.03	-	194,194,194,194	0
36	MG	AA	1876	1/1	0.79	0.14	-	180,180,180,180	0
36	MG	BA	1847	1/1	0.75	0.27	-	204,204,204,204	0
36	MG	BA	1817	1/1	0.94	0.07	-	134,134,134,134	0
36	MG	BA	1843	1/1	0.79	0.22	-	196,196,196,196	0
36	MG	BA	1829	1/1	0.82	0.12	-	163,163,163,163	0
36	MG	AA	1860	1/1	0.91	0.12	-	176,176,176,176	0
36	MG	BA	1883	1/1	0.77	0.61	-	187,187,187,187	0
36	MG	AA	1829	1/1	0.97	0.05	-	160,160,160,160	0
36	MG	AA	1848	1/1	0.84	0.13	-	183,183,183,183	0
36	MG	AA	1839	1/1	0.92	0.11	-	143,143,143,143	0
36	MG	BA	1820	1/1	0.81	0.15	-	170,170,170,170	0
36	MG	BA	1834	1/1	0.90	0.14	-	138,138,138,138	0
36	MG	AA	1804	1/1	0.95	0.11	-	150,150,150,150	0
36	MG	AA	1864	1/1	0.92	0.17	-	176,176,176,176	0
36	MG	AA	1825	1/1	0.98	0.13	-	115,115,115,115	0
36	MG	AA	1867	1/1	0.98	0.06	-	193,193,193,193	0
36	MG	BA	1872	1/1	0.76	0.62	-	200,200,200,200	0
36	MG	BD	201	1/1	0.92	0.61	-	233,233,233,233	0
36	MG	BA	1816	1/1	0.94	0.14	-	127,127,127,127	0
36	MG	BA	1871	1/1	0.78	0.19	-	209,209,209,209	0
36	MG	AA	1859	1/1	0.79	0.10	-	193,193,193,193	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	MG	AA	1855	1/1	0.80	0.61	-	214,214,214,214	0
36	MG	BA	1856	1/1	0.93	0.11	-	173,173,173,173	0
36	MG	AA	1870	1/1	0.73	0.42	-	195,195,195,195	0
36	MG	AA	1861	1/1	0.84	0.21	-	204,204,204,204	0
36	MG	AA	1885	1/1	0.93	0.19	-	223,223,223,223	0
36	MG	BA	1848	1/1	0.87	0.36	-	206,206,206,206	0
36	MG	BA	1822	1/1	0.91	0.13	-	151,151,151,151	0
36	MG	AA	1824	1/1	0.90	0.06	-	148,148,148,148	0
36	MG	AA	1821	1/1	0.96	0.18	-	144,144,144,144	0
36	MG	BA	1839	1/1	0.95	0.11	-	140,140,140,140	0
36	MG	AA	1879	1/1	0.87	0.21	-	193,193,193,193	0
36	MG	AA	1828	1/1	0.97	0.14	-	133,133,133,133	0
36	MG	BA	1875	1/1	0.18	0.45	-	193,193,193,193	0
36	MG	AA	1820	1/1	0.91	0.14	-	157,157,157,157	0
36	MG	BA	1852	1/1	0.90	0.21	-	170,170,170,170	0
36	MG	AA	1866	1/1	0.77	0.17	-	197,197,197,197	0
36	MG	AA	1826	1/1	0.89	0.11	-	155,155,155,155	0
36	MG	BA	1824	1/1	0.84	0.08	-	172,172,172,172	0
36	MG	BA	1855	1/1	0.56	0.81	-	275,275,275,275	0
36	MG	AA	1890	1/1	0.84	0.11	-	218,218,218,218	0
36	MG	AA	1850	1/1	0.88	0.17	-	185,185,185,185	0
36	MG	AA	1863	1/1	0.88	0.12	-	183,183,183,183	0
36	MG	BA	1804	1/1	0.94	0.10	-	191,191,191,191	0
36	MG	BA	1812	1/1	0.96	0.66	-	166,166,166,166	0
36	MG	BA	1805	1/1	0.98	0.10	-	150,150,150,150	0
36	MG	BA	1866	1/1	0.84	0.31	-	186,186,186,186	0
36	MG	BA	1809	1/1	0.95	0.19	-	172,172,172,172	0
36	MG	AA	1823	1/1	0.91	0.20	-	130,130,130,130	0
36	MG	AL	201	1/1	0.86	0.16	-	182,182,182,182	0
36	MG	BA	1837	1/1	0.76	0.25	-	178,178,178,178	0
36	MG	BA	1864	1/1	0.90	0.16	-	182,182,182,182	0
36	MG	AA	1883	1/1	0.79	0.40	-	209,209,209,209	0
36	MG	BA	1889	1/1	0.87	0.13	-	209,209,209,209	0
36	MG	AA	1812	1/1	0.89	0.55	-	173,173,173,173	0
36	MG	BA	1858	1/1	0.93	0.06	-	163,163,163,163	0
36	MG	BA	1876	1/1	0.75	0.24	-	184,184,184,184	0
36	MG	AA	1813	1/1	0.79	0.12	-	191,191,191,191	0
36	MG	AA	1854	1/1	0.88	0.14	-	158,158,158,158	0
36	MG	BA	1826	1/1	0.91	0.08	-	185,185,185,185	0
36	MG	BA	1861	1/1	0.91	0.18	-	181,181,181,181	0
36	MG	AA	1841	1/1	0.82	0.21	-	170,170,170,170	0
36	MG	AA	1838	1/1	0.90	0.12	-	144,144,144,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	MG	BA	1862	1/1	0.88	0.07	-	177,177,177,177	0
36	MG	BA	1879	1/1	0.88	0.43	-	221,221,221,221	0
36	MG	AA	1875	1/1	0.89	0.28	-	152,152,152,152	0
36	MG	BA	1869	1/1	0.89	0.15	-	188,188,188,188	0
36	MG	AA	1853	1/1	0.97	0.08	-	177,177,177,177	0
36	MG	BA	1846	1/1	0.95	0.07	-	147,147,147,147	0
36	MG	AA	1843	1/1	0.93	0.09	-	182,182,182,182	0
36	MG	BA	1801	1/1	0.85	0.13	-	186,186,186,186	0
36	MG	BA	1823	1/1	0.94	0.14	-	123,123,123,123	0
36	MG	BA	1830	1/1	0.91	0.34	-	204,204,204,204	0
36	MG	BA	1886	1/1	0.76	0.22	-	214,214,214,214	0
36	MG	AA	1845	1/1	0.84	0.21	-	193,193,193,193	0
36	MG	AA	1849	1/1	0.97	0.21	-	159,159,159,159	0
36	MG	BA	1870	1/1	0.90	0.10	-	205,205,205,205	0
36	MG	AA	1801	1/1	0.96	0.06	-	160,160,160,160	0
36	MG	BA	1807	1/1	0.70	0.39	-	210,210,210,210	0
36	MG	BA	1874	1/1	0.97	0.39	-	164,164,164,164	0
36	MG	AA	1830	1/1	0.87	0.17	-	183,183,183,183	0
36	MG	AA	1872	1/1	0.91	0.32	-	196,196,196,196	0
36	MG	BA	1881	1/1	0.83	0.09	-	149,149,149,149	0
36	MG	BA	1850	1/1	0.89	0.49	-	221,221,221,221	0
36	MG	BA	1844	1/1	0.97	0.08	-	157,157,157,157	0
36	MG	AA	1842	1/1	0.93	0.13	-	175,175,175,175	0
36	MG	AA	1847	1/1	0.93	0.27	-	186,186,186,186	0
36	MG	AA	1884	1/1	0.91	0.47	-	190,190,190,190	0
36	MG	BA	1853	1/1	0.86	0.09	-	194,194,194,194	0
36	MG	AA	1827	1/1	0.94	0.43	-	178,178,178,178	0
36	MG	AA	1836	1/1	0.85	0.17	-	166,166,166,166	0
36	MG	AA	1840	1/1	0.98	0.09	-	124,124,124,124	0
36	MG	AA	1808	1/1	0.96	0.36	-	136,136,136,136	0
36	MG	AA	1877	1/1	0.98	0.19	-	170,170,170,170	0

6.5 Other polymers [i](#)

There are no such residues in this entry.