



# wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 06:27 PM BST

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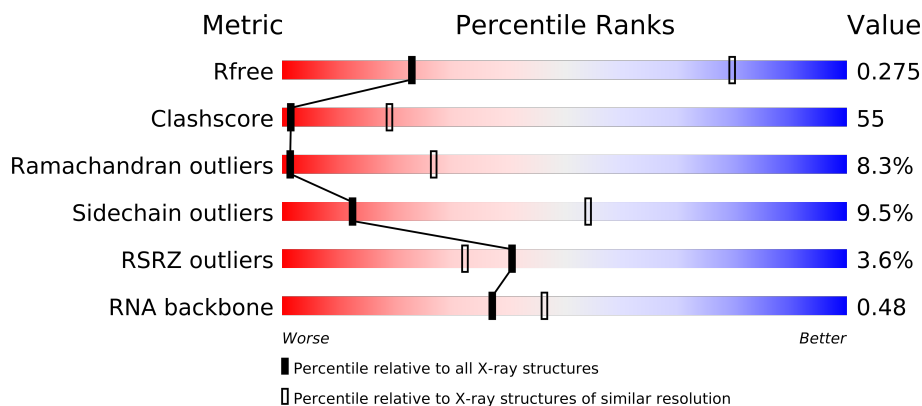
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.93 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))
$R_{free}$	66092	1009 (4.42-3.44)
Clashscore	79885	1184 (4.38-3.50)
Ramachandran outliers	78287	1128 (4.38-3.50)
Sidechain outliers	78261	1116 (4.38-3.50)
RSRZ outliers	66119	1009 (4.42-3.44)
RNA backbone	1838	1018 (5.00-2.80)

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	A1	68	
1	B1	68	
2	A2	208	
2	B2	208	
3	A3	197	
3	B3	197	
4	A4	265	
4	B4	265	
5	A5	119	
5	B5	119	
6	A6	81	

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Mol	Chain	Length	Quality of chain
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	
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	

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Mol	Chain	Length	Quality of chain
27	BR	343	
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 that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
36	MG	AA	1805	-	X
36	MG	AA	1827	-	X
36	MG	AA	1829	-	X
36	MG	AA	1845	-	X
36	MG	AA	1855	-	X
36	MG	AA	1856	-	X
36	MG	AA	1868	-	X
36	MG	AA	1873	-	X
36	MG	AA	1883	-	X
36	MG	AA	1884	-	X
36	MG	AA	1889	-	X
36	MG	BA	1807	-	X
36	MG	BA	1836	-	X
36	MG	BA	1838	-	X
36	MG	BA	1840	-	X
36	MG	BA	1845	-	X
36	MG	BA	1852	-	X
36	MG	BA	1855	-	X
36	MG	BA	1866	-	X
36	MG	BA	1873	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
36	MG	BA	1875	-	X
36	MG	BA	1882	-	X
36	MG	BA	1883	-	X
36	MG	BA	1886	-	X
36	MG	BA	1888	-	X
37	ZN	B6	500	-	X

## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 157632 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 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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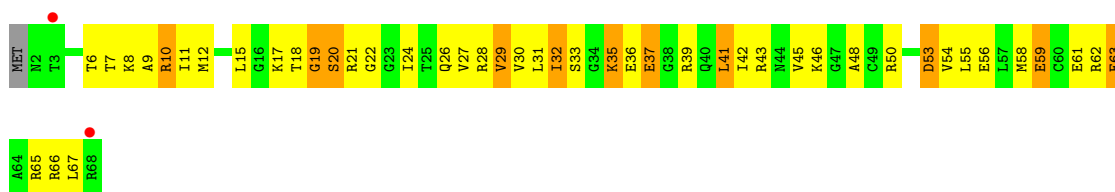
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	BO	1	Total 1	O 1	0	0
38	BP	1	Total 1	O 1	0	0
38	BQ	1	Total 1	O 1	0	0
38	BT	6	Total 6	O 6	0	0
38	BW	5	Total 5	O 5	0	0
38	BY	3	Total 3	O 3	0	0

### 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 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.

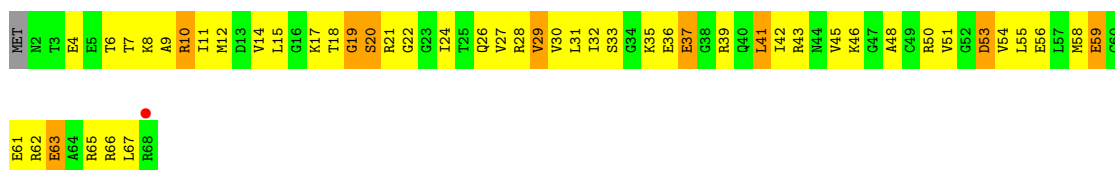
- Molecule 1: RIBOSOMAL PROTEIN S28E CONTAINING PROTEIN

Chain A1: 



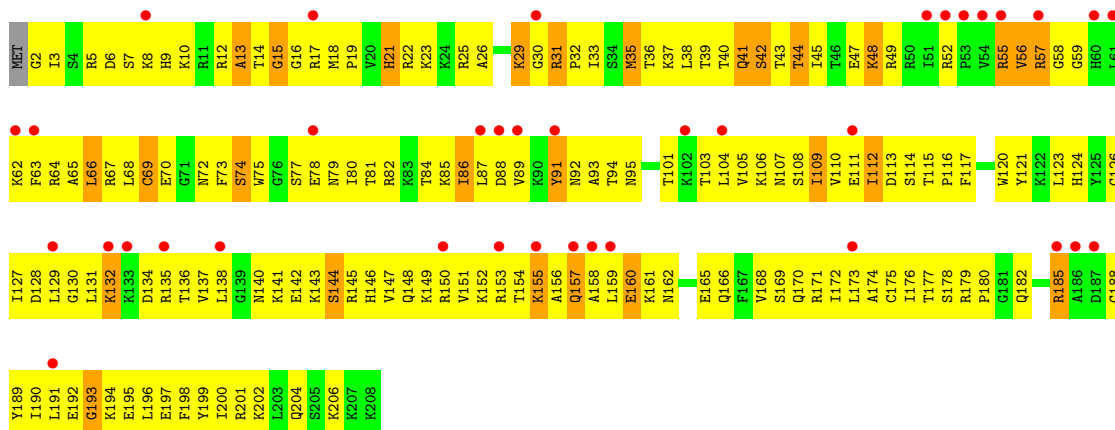
- Molecule 1: RIBOSOMAL PROTEIN S28E CONTAINING PROTEIN

Chain B1: 



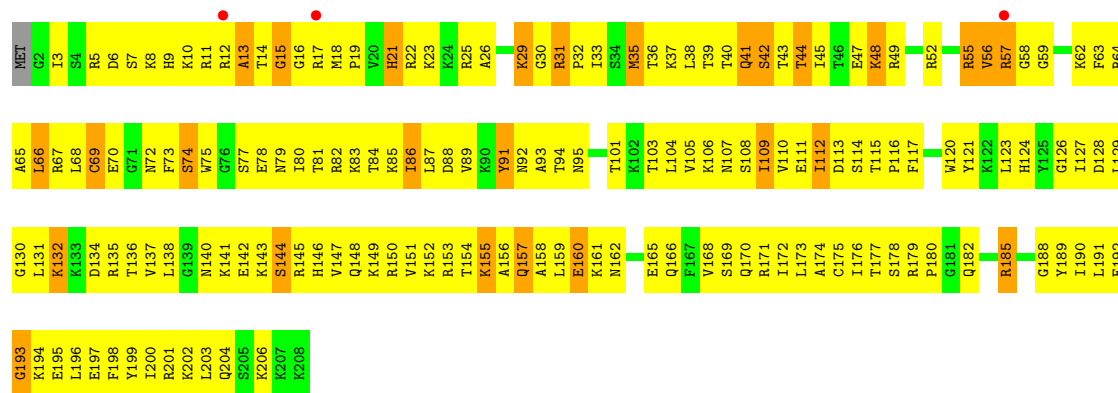
- Molecule 2: 40S RIBOSOMAL PROTEIN S8

Chain A2: 



- Molecule 2: 40S RIBOSOMAL PROTEIN S8

Chain B2: 



• Molecule 3: RPS7E

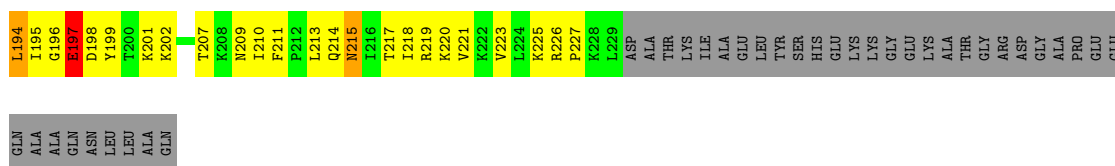
Chain A3:

• Molecule 3: RPS7E

Chain B3:

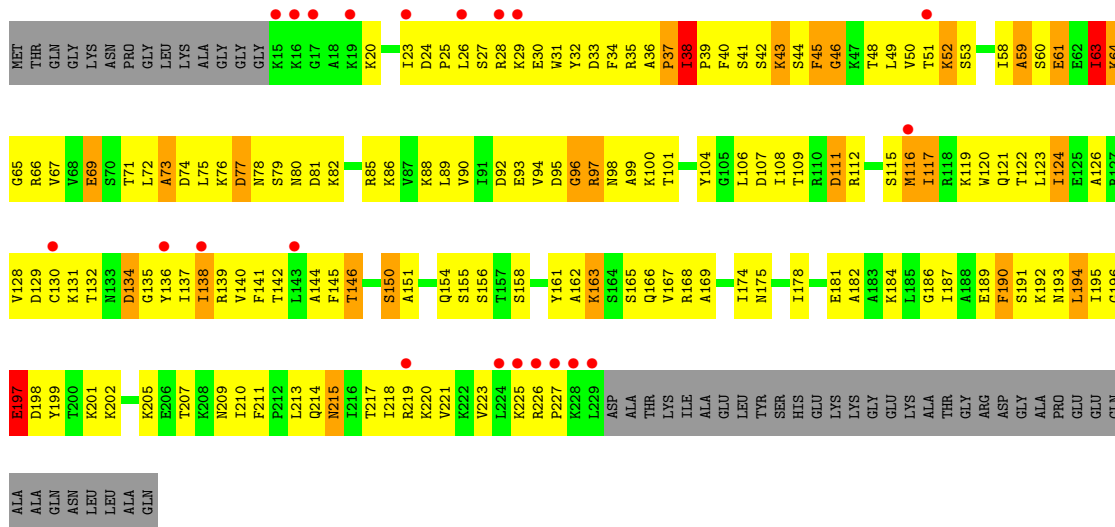
• Molecule 4: 40S RIBOSOMAL PROTEIN S3A

Chain A4:



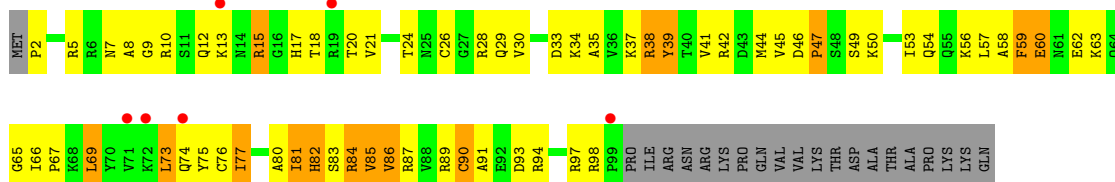
• Molecule 4: 40S RIBOSOMAL PROTEIN S3A

Chain B4:



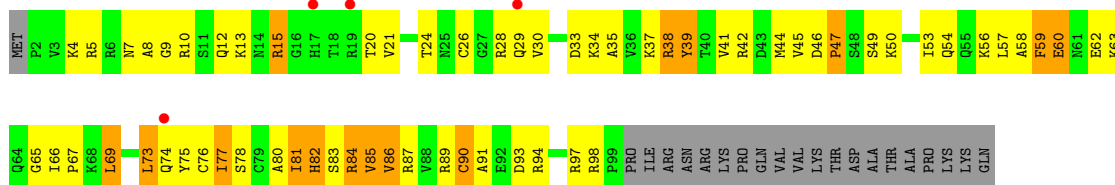
• Molecule 5: RIBOSOMAL PROTEIN S26E CONTAINING PROTEIN

Chain A5:



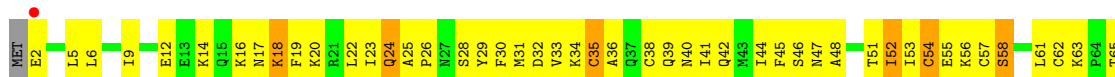
• Molecule 5: RIBOSOMAL PROTEIN S26E CONTAINING PROTEIN

Chain B5:

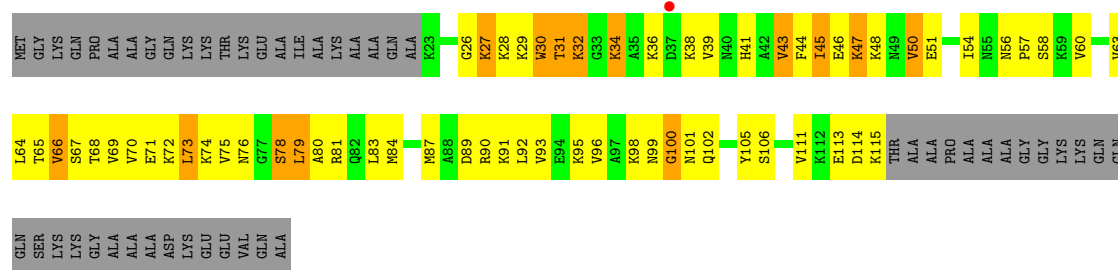


• Molecule 6: RPS27E

Chain A6:

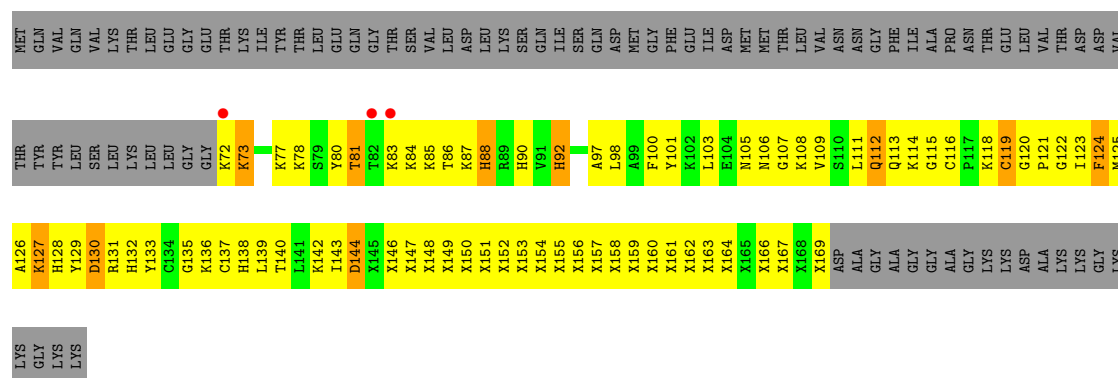






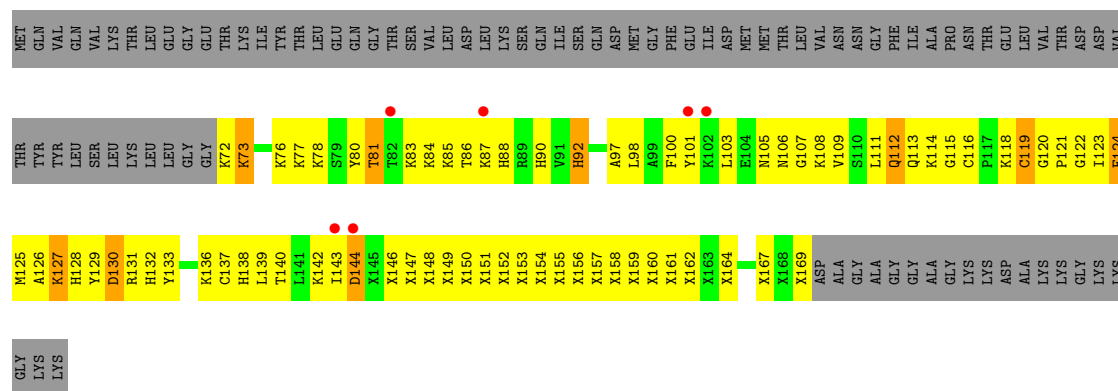
• Molecule 9: RPS31E

Chain A9:



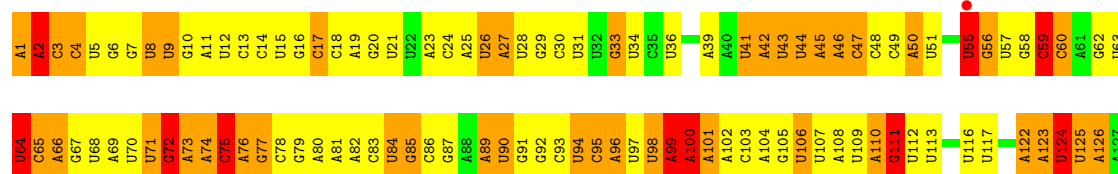
• Molecule 9: RPS31E

Chain B9:



• Molecule 10: 18S RRNA

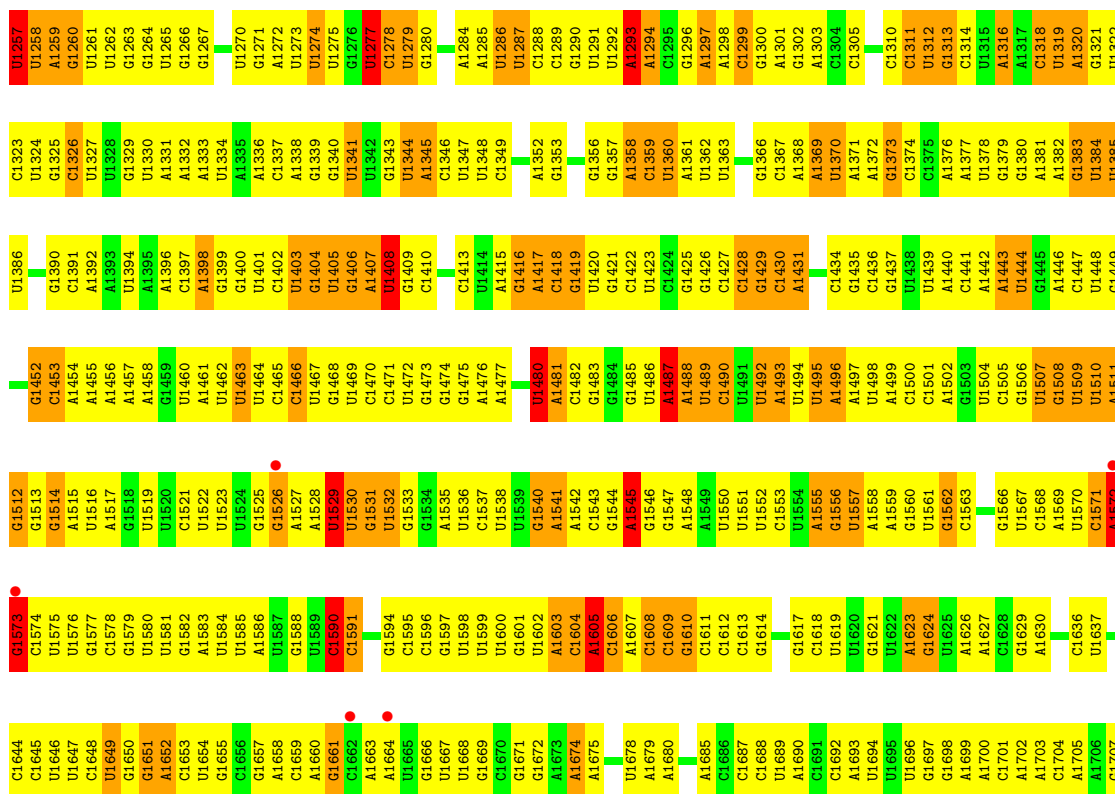
Chain AA:



G1062	A1063	A1064	A1065	G1066	C1067	U1068	U1070	U1071	G1072	G1073	G1074	U1075	U1076	G1077	U1078	G1079	G1080	G1081	G1082	A1085	G1086	U1087	A1088	U1089	G1090	G1091	U1092	A1093	G1094	G1095	G1096	A1097	A1098	G1099	U1100	C1101	U1102	G1103	A1106	C1107	U1108	U1109	A1110	A1111	A1112	G1113	G1114	A1115	A1116	U1117	U1118	G1119	G1122	A1123	A1124	A1125																																																																																																																																																																																																																																																																																																																																				
U936	U937	U938	U939	C940	A941	U942	U943	A944	U945	U946	C947	A948	A949	G950	G954	A955	A956	A957	G958	G962	G963	G964	G965	U966	U967	G968	A969	A970	A971	G972	A973	C974	G975	A976	U977	C978	A979	G980	A981	U982	A983	C984	C985	C986	U987	C988	U989	G991	G992	U993	C994	U995	U996	A997	U1000																																																																																																																																																																																																																																																																																																																																					
A1001	U1002	A1003	A1004	A1005	C1006	U1007	A1008	U1009	A1010	C1011	C1012	A1013	A1014	C1015	U1016	U1017	G1018	G1019	G1020	A1021	U1022	G1025	C1026	U1027	G1028	U1029	U1030	A1031	A1032	A1033	A1034	U1035	A1036	G1037	U1038	C1039	U1040	A1041	G1042	U1043	U1044	G1045	G1046	A1047	A1048	C1049	C1050	G1051	U1052	A1053	U1054	G1055	A1056	U1057	A1058	A1059	A1060	U1061																																																																																																																																																																																																																																																																																																																																		
G873	U874	C875	A876	A877	A878	G879	G880	U881	U881	G882	A883	A884	A885	U886	U887	C888	U889	U890	G891	G892	A893	U894	U895	U896	A897	U898	U899	A900	U901	G902	G903	A904	C905	U906	A907	A908	C909	U910	A911	A912	U913	G914	C915	A919	G920	C921	U922	U923	G926	C927	C928	A929	A930	A931	U932	A933	A934	C935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948	A949	A950	A951	A952	A953	A954	A955	A956	A957	A958	A959	A960	A961																																																																																																																																																																																																																																																																																																								
A803	A804	U805	U806	C807	U811	U812	U813	A814	U820	U821	C821	C822	U823	U824	A826	U827	U828	U829	G830	G831	U832	A833	A834	U835	A836	U837	U838	U839	A840	A841	U842	A843	U844	U845	U846	U847	U848	U849	U850	U851	G854	G855	U856	U857	U858	U859	A862	U863	U864	A865	U866	A867	U868	A869	U870	U871	A872	A873	A874	A875	A876	A877	A878	A879	A880	C881	U882	A883	A884	A885	A886	A887	A888	A889	A890	A891	A892	A893	A894	A895	A896	A897	A898	A899	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948	A949	A950	A951	A952	A953	A954	A955	A956	A957	A958	A959	A960	A961																																																																																																																																																																																																																																										
U742	U743	A744	G745	A746	G747	U748	G749	U750	U751	C752	C753	A754	G755	G756	C757	A758	G759	G760	U761	U762	U763	U764	U765	G766	C767	C768	C769	G770	A771	A772	U773	A774	C775	U776	U777	U778	U779	A780	C781	U782	U783	A784	G785	A786	A787	U788	A789	G792	G793	A794	U795	U796	A797	U798	U799	A800	C801	U802	A803	A804	A805	A806	A807	A808	A809	A810	A811	A812	A813	A814	A815	A816	A817	A818	A819	A820	A821	A822	A823	A824	A825	A826	A827	A828	A829	A830	A831	A832	A833	A834	A835	A836	A837	A838	A839	A840	A841	A842	A843	A844	A845	A846	A847	A848	A849	A850	U851	U852	U853	U854	U855	U856	U857	U858	U859	U860	U861	U862	U863	U864	A865	A866	A867	U868	A869	A870	A871	A872	A873	A874	A875	A876	A877	A878	A879	A880	A881	A882	A883	A884	A885	A886	A887	A888	A889	A890	A891	A892	A893	A894	A895	A896	A897	A898	A899	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948	A949	A950	A951	A952	A953	A954	A955	A956	A957	A958	A959	A960	A961																																																																																																																																																																			
U620	C621	A622	C623	A624	A625	C626	C627	C628	A629	C630	C631	U632	U633	A634	U635	U636	C637	U638	C639	A640	A641	U642	U643	U644	U645	U646	U647	U648	U649	C650	C651	A652	U653	U654	C655	C656	C657	U658	U659	U660	C661	U662	U663	A664	A665	A666	A667	U668	U669	A670	A671	C672	U673	A674	U675	U676	A677	A678	A679	A680	U681	U682	U683	U684	U685	U686	U687	U688	U689	U690	U691	U692	U693	U694	U695	U696	U697	U698	U699	U700	U701	U702	U703	U704	U705	U706	U707	U708	U709	U710	U711	U712	U713	U714	U715	U716	U717	U718	U719	U720	U721	U722	A723	A724	A725	U726	U727	U728	U729	A730	C731	U732	G733	U734	G735	A736	U737	A738	A739	U740	U741	U742	U743	U744	U745	U746	U747	U748	U749	U750	U751	U752	U753	U754	U755	U756	U757	U758	U759	U760	U761	U762	U763	U764	U765	U766	U767	U768	U769	U770	U771	U772	U773	U774	U775	U776	U777	U778	U779	U780	U781	U782	U783	U784	U785	U786	U787	U788	U789	U790	U791	U792	U793	U794	U795	U796	U797	U798	U799	U800	U801	U802	U803	U804	U805	U806	U807	U808	U809	U810	U811	U812	U813	U814	U815	U816	U817	U818	U819	U820	U821	U822	U823	U824	U825	U826	U827	U828	U829	U830	U831	U832	U833	U834	U835	U836	U837	U838	U839	U840	U841	U842	U843	U844	U845	U846	U847	U848	U849	U850	U851	U852	U853	U854	U855	U856	U857	U858	U859	U860	U861	U862	U863	U864	U865	U866	U867	U868	U869	U870	U871	U872	U873	U874	U875	U876	U877	U878	U879	U880	U881	U882	U883	U884	U885	U886	U887	U888	U889	U890	U891	U892	U893	U894	U895	U896	U897	U898	U899	U900	U901	U902	U903	U904	U905	U906	U907	U908	U909	U910	U911	U912	U913	U914	U915	U916	U917	U918	U919	U920	U921	U922	U923	U924	U925	U926	U927	U928	U929	U930	U931	U932	U933	U934	U935	U936	U937	U938	U939	U940	U941	U942	U943	U944	U945	U946	U947	U948	U949	U950	U951	U952	U953	U954	U955	U956	U957	U958	U959	U960	U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000
C435	A436	A437	C440	C441	U442	A443	A444	C445	U446	C447	A448	G449	G450	A451	A452	C453	C454	C455	A456	U457	U458	C459	A460	C461	A462	A463	G464	A465	A466	U467	U468	A469	G470	C471	U472	U473	C474	U475	C476	U477	U478	C479	U480	A481	A482	C483	U484	U485	U486	U487	U488	U489	U490	U491	A492	U493	U494	U495	U496	U497	U498	U499	U500	U501	U502	U503	U504	U505	U506	U507	U508	U509	U510	U511	U512	U513	U514	U515	U516	U517	U518	U519	U520	U521	U522	U523	U524	U525	U526	U527	U528	U529	U530	U531	U532	U533	U534	U535	U536	U537	U538	U539	U540	U541	U542	U543	U544	U545	U546	U547	U548	U549	U550	U551	U552	U553	U554	U555	U556	U557	U558	U559	U560	U561	U562	U563	U564	U565	U566	U567	U568	U569	U570	U571	U572	U573	U574	U575	U576	U577	U578	U579	U580	U581	U582	U583	U584	U585	U586	U587	U588	U589	U590	U591	U592	U593	U594	U595	U596	U597	U598	U599	U600	U601	U602	U603	U604	U605	U606	U607	U608	U609	U610	U611	U612	U613	U614	U615	U616	U617	U618	U619	U620	U621	U622	U623	U624	U625	U626	U627	U628	U629	U630	U631	U632	U633	U634	U635	U636	U637	U638	U639	U640	U641	U642	U643	U644	U645	U646	U647	U648	U649	U650	U651	U652	U653	U654	U655	U656	U657	U658	U659	U660	U661	U662	U663	U664	U665	U666	U667	U668	U669	U670	U671	U672	U673	U674	U675	U676	U677	U678	U679	U680	U681	U682	U683	U684	U685	U686	U687	U688	U689	U690	U691	U692																																																																																																																													

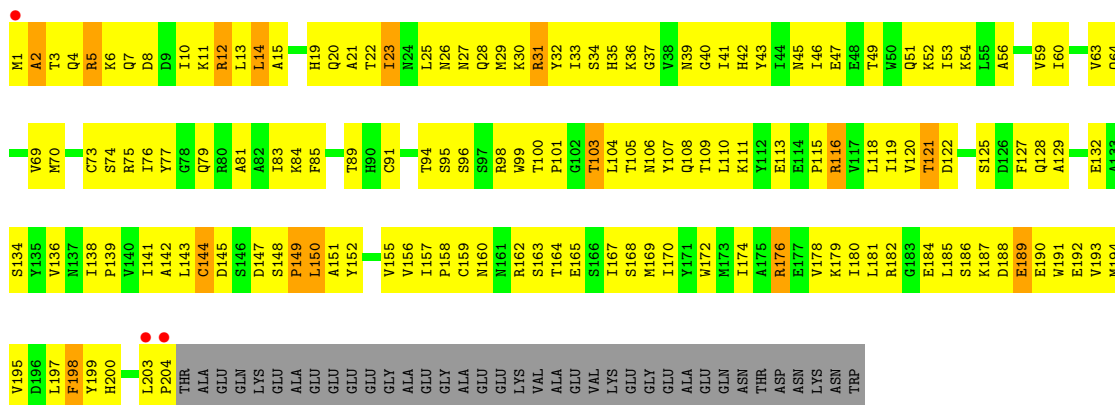






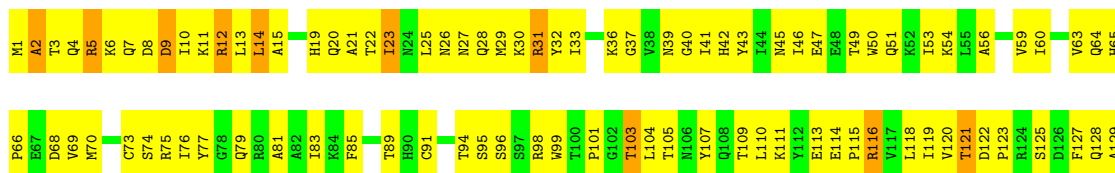
## • Molecule 11: RPSOE

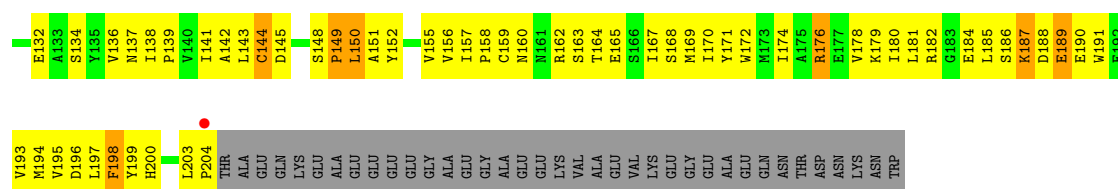
Chain AB:



## • Molecule 11: RPSOE

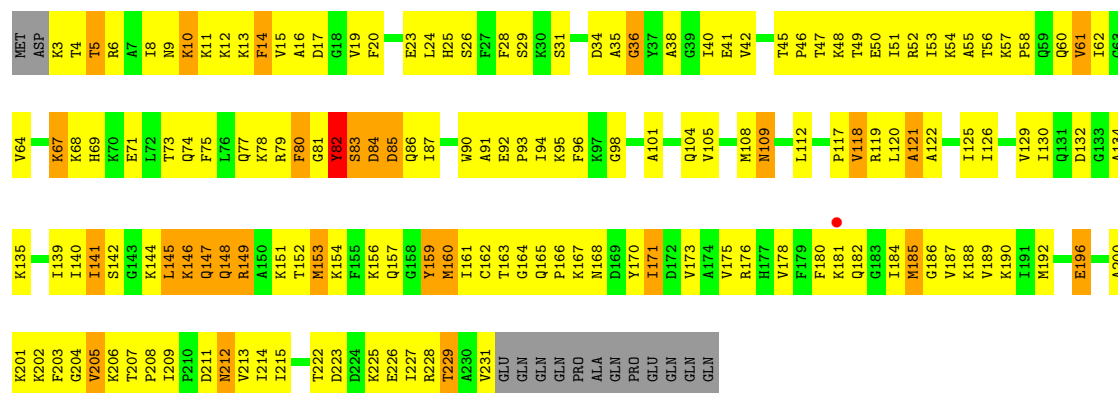
Chain BB:





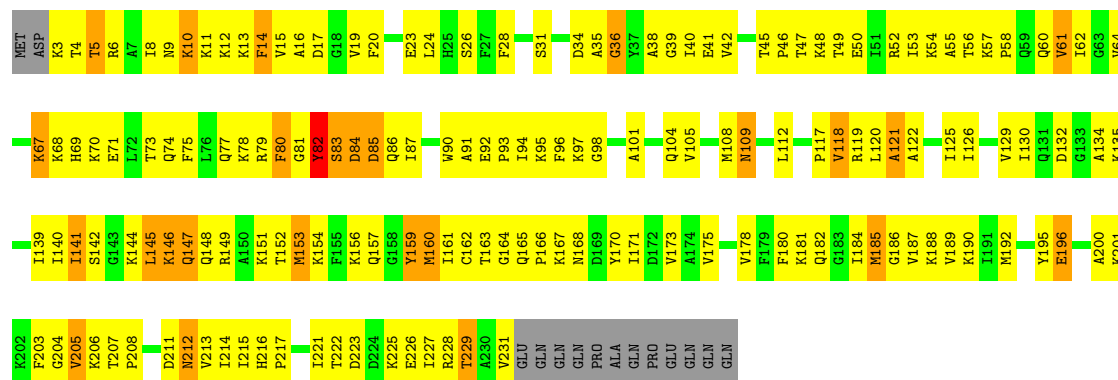
• Molecule 12: KH DOMAIN CONTAINING PROTEIN

Chain AC:



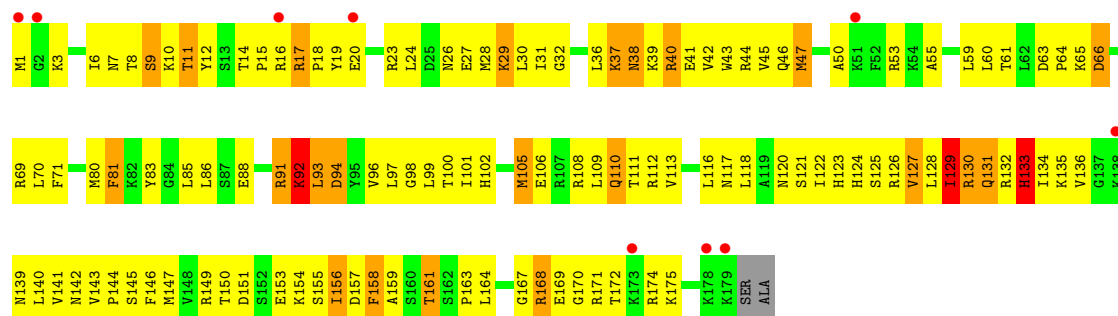
• Molecule 12: KH DOMAIN CONTAINING PROTEIN

Chain BC:



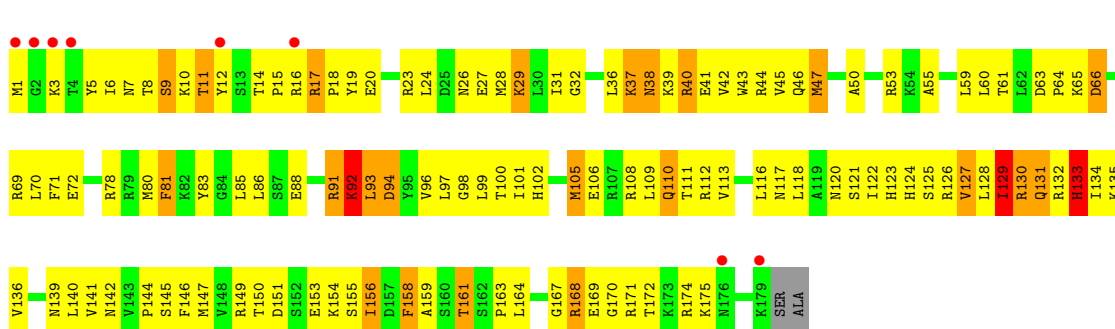
• Molecule 13: RIBOSOMAL PROTEIN S4 CONTAINING PROTEIN

Chain AD:



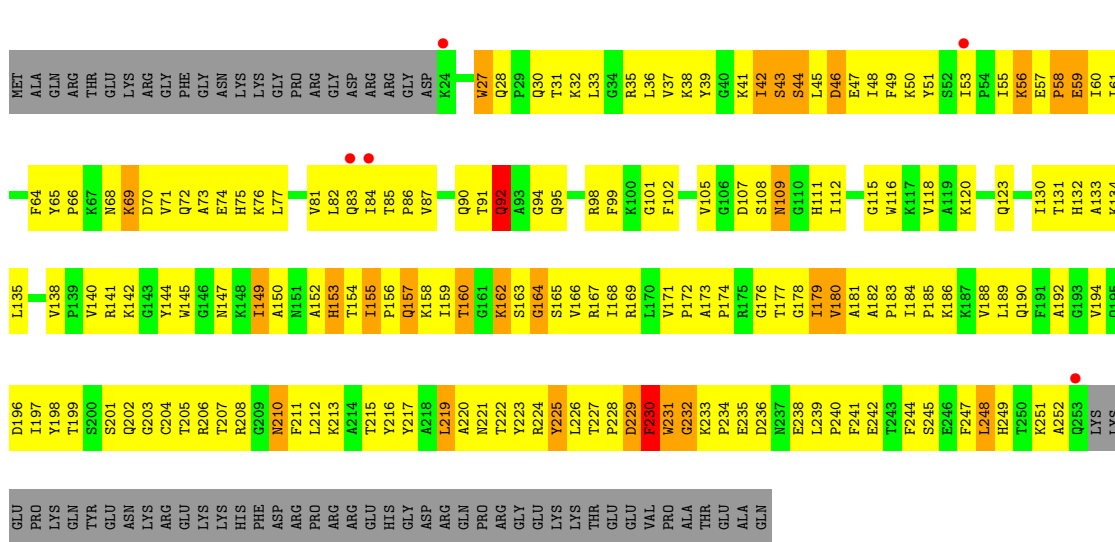
• Molecule 13: RIBOSOMAL PROTEIN S4 CONTAINING PROTEIN

Chain BD:



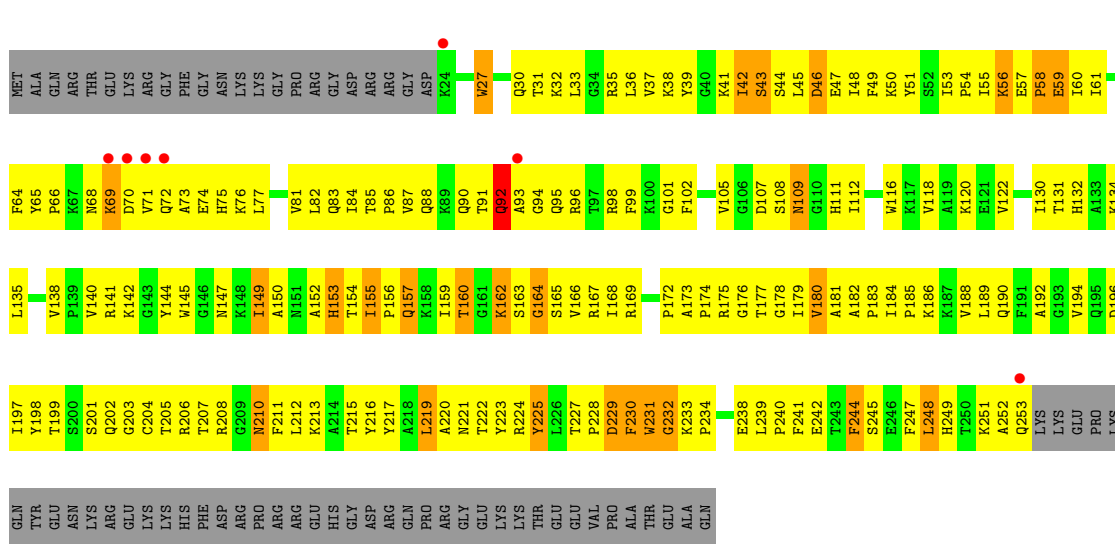
- Molecule 14: RIBOSOMAL PROTEIN S5 CONTAINING PROTEIN

Chain AE:



- Molecule 14: RIBOSOMAL PROTEIN S5 CONTAINING PROTEIN

Chain BE:



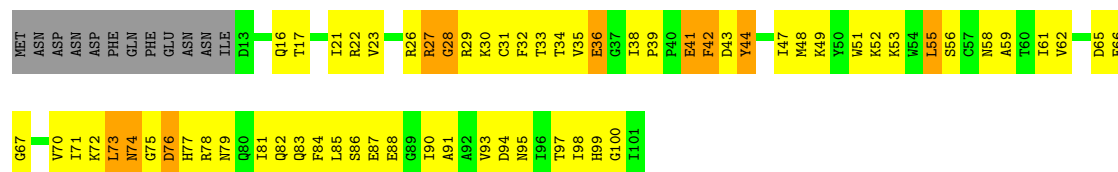
- Molecule 15: EIF1

Chain AF:



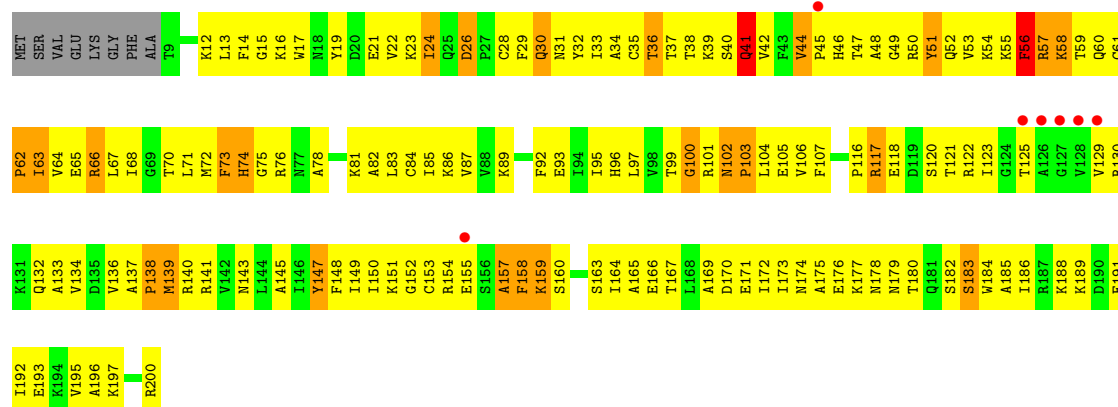
• Molecule 15: EIF1

Chain BF:



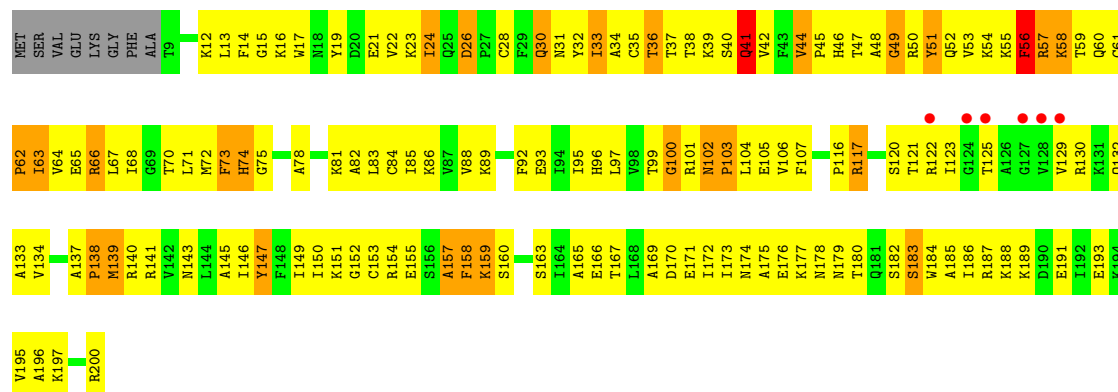
• Molecule 16: RIBOSOMAL PROTEIN S7 CONTAINING PROTEIN

Chain AG:



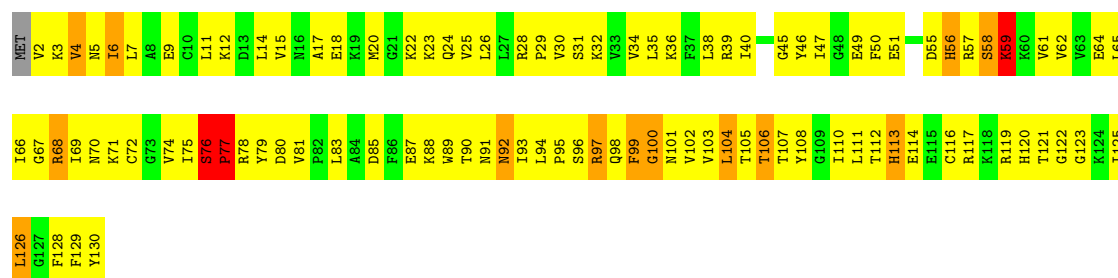
• Molecule 16: RIBOSOMAL PROTEIN S7 CONTAINING PROTEIN

Chain BG:



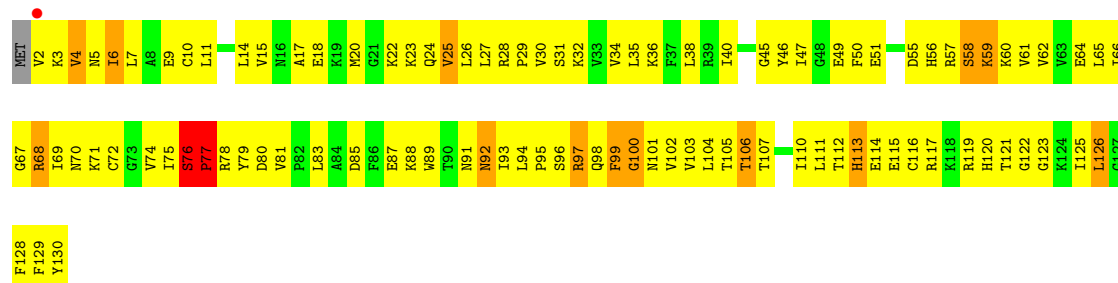
• Molecule 17: RIBOSOMAL PROTEIN S8 CONTAINING PROTEIN

Chain AH:



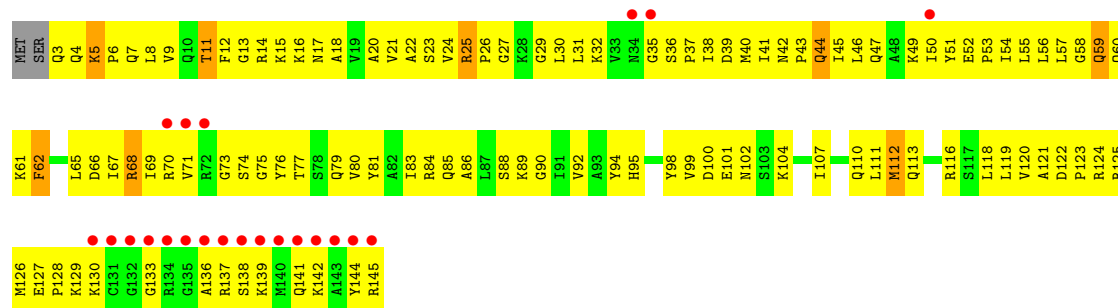
• Molecule 17: RIBOSOMAL PROTEIN S8 CONTAINING PROTEIN

Chain BH:



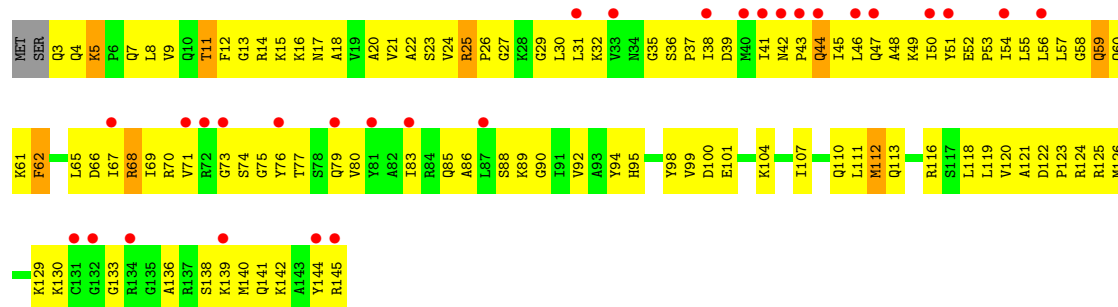
• Molecule 18: RPS16E, 40S RIBOSOMAL PROTEIN RPS16E

Chain AI:



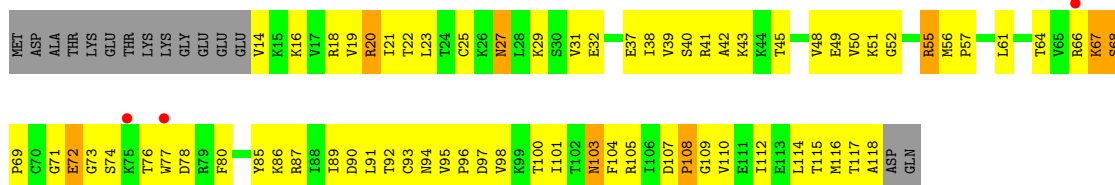
• Molecule 18: RPS16E, 40S RIBOSOMAL PROTEIN RPS16E

Chain BI:



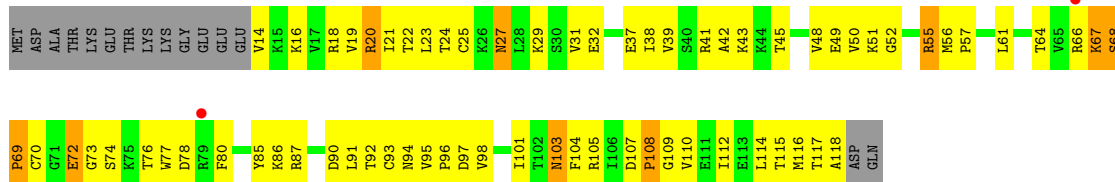
• Molecule 19: RIBOSOMAL PROTEIN S10 CONTAINING PROTEIN

Chain AJ:



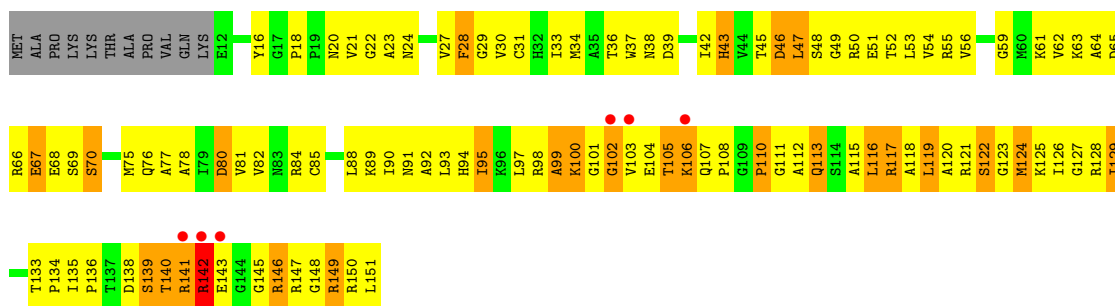
• Molecule 19: RIBOSOMAL PROTEIN S10 CONTAINING PROTEIN

Chain BJ:



• Molecule 20: RPS14E

Chain AK:



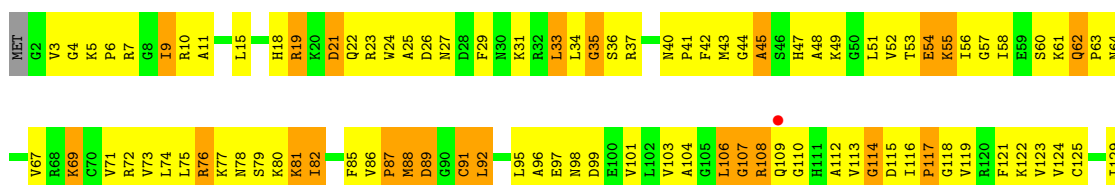
• Molecule 20: RPS14E

Chain BK:



• Molecule 21: 40S RIBOSOMAL PROTEIN S12

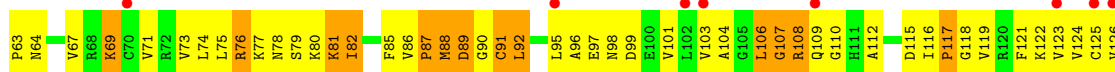
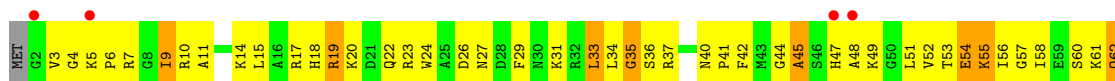
Chain AL:





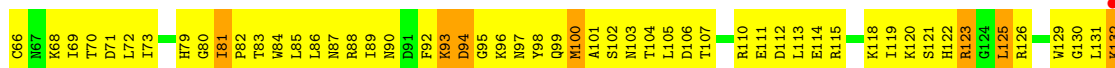
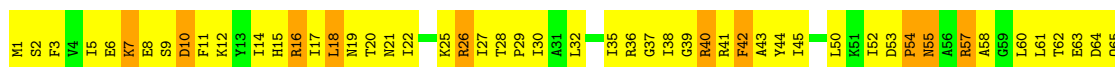
• Molecule 21: 40S RIBOSOMAL PROTEIN S12

Chain BL:



• Molecule 22: RPS18E

Chain AM:



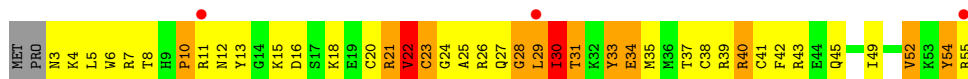
• Molecule 22: RPS18E

Chain BM:



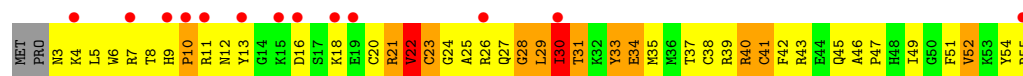
• Molecule 23: RPS29E

Chain AN:



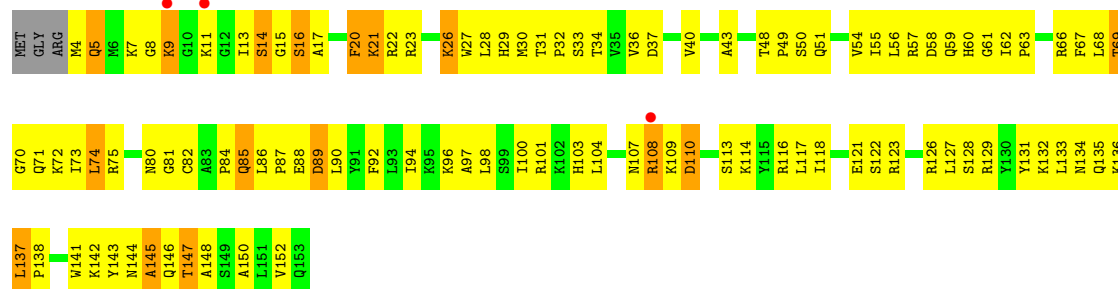
• Molecule 23: RPS29E

Chain BN: 



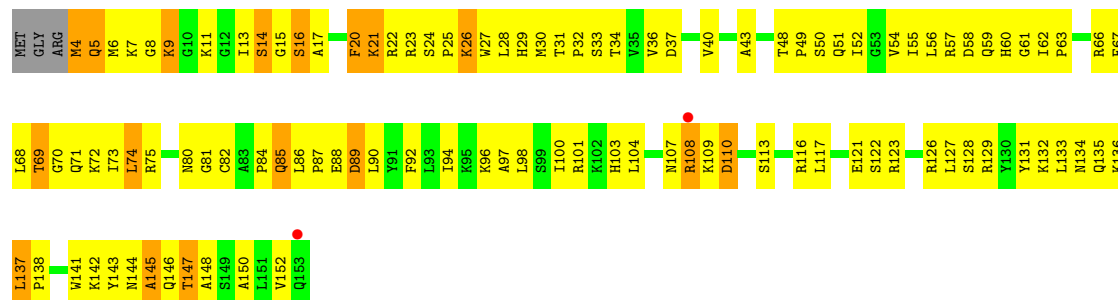
• Molecule 24: RPS13E

Chain AO: 



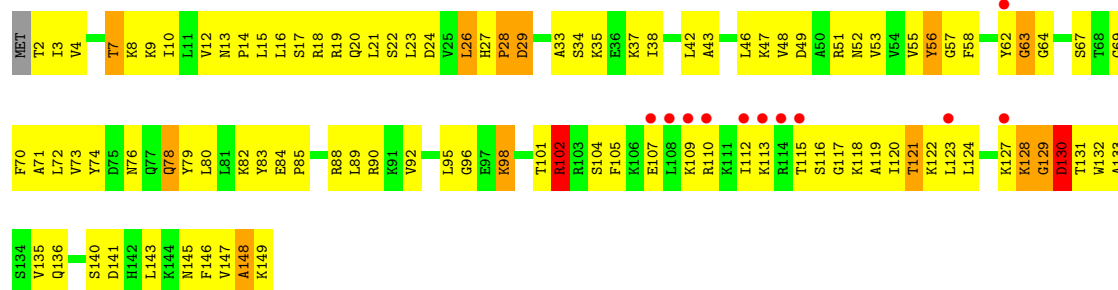
• Molecule 24: RPS13E

Chain BO: 



• Molecule 25: RPS24E

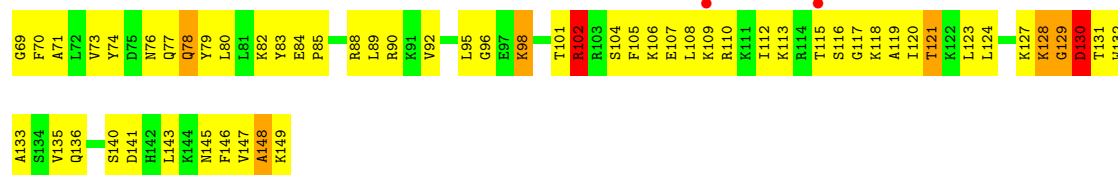
Chain AP: 



• Molecule 25: RPS24E

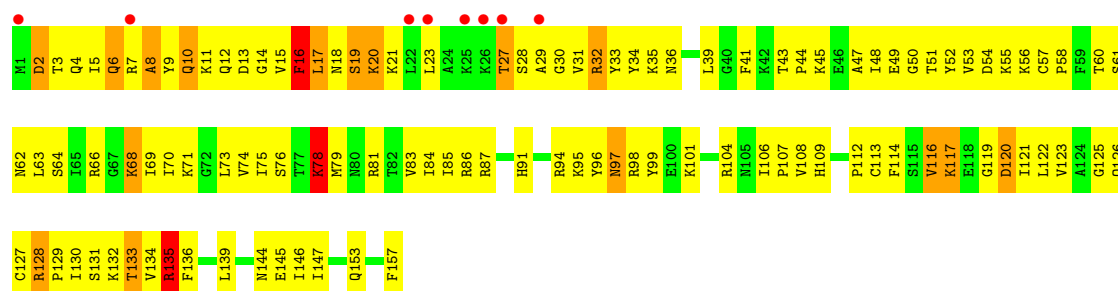
Chain BP: 





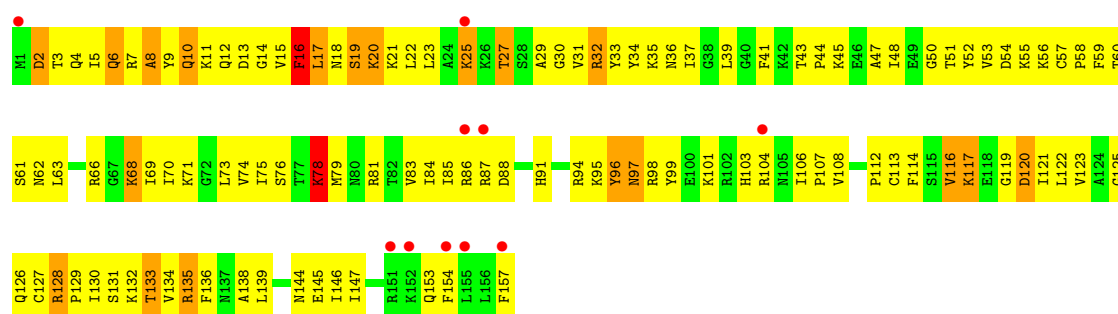
• Molecule 26: RIBOSOMAL PROTEIN S17 CONTAINING PROTEIN

Chain AQ:



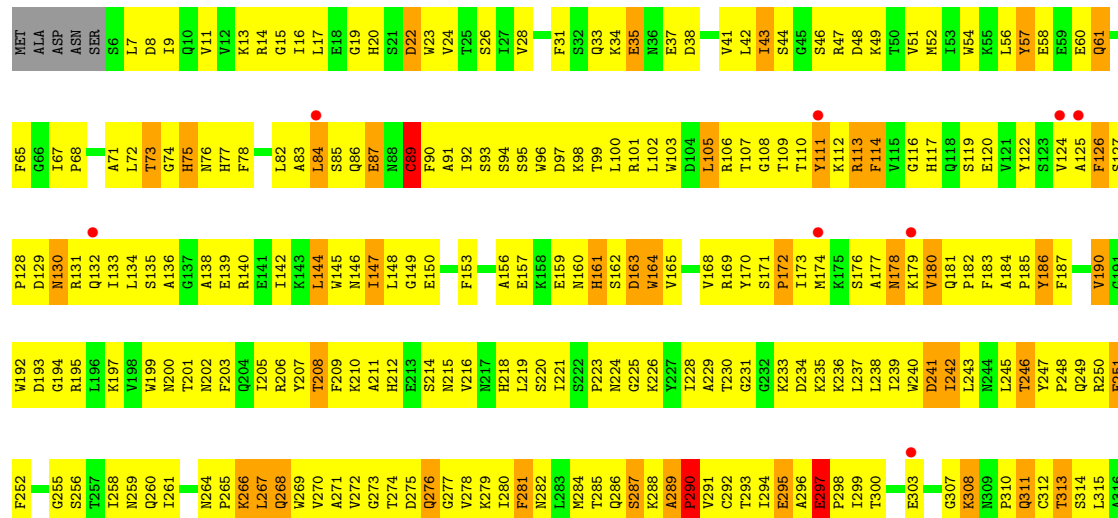
• Molecule 26: RIBOSOMAL PROTEIN S17 CONTAINING PROTEIN

Chain BQ:



• Molecule 27: RACK1

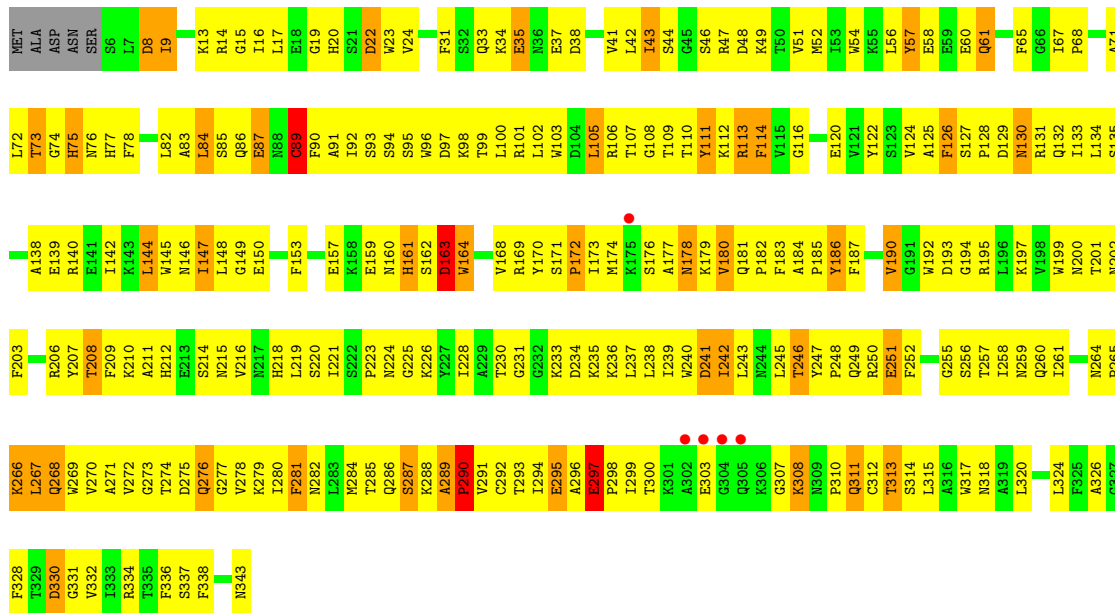
Chain AR:





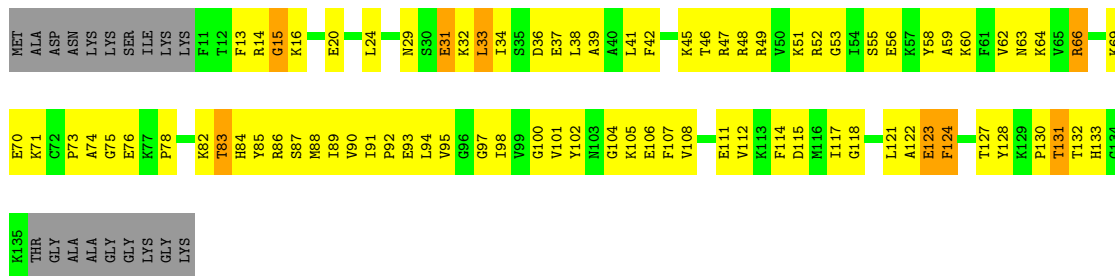
• Molecule 27: RACK1

Chain BR:



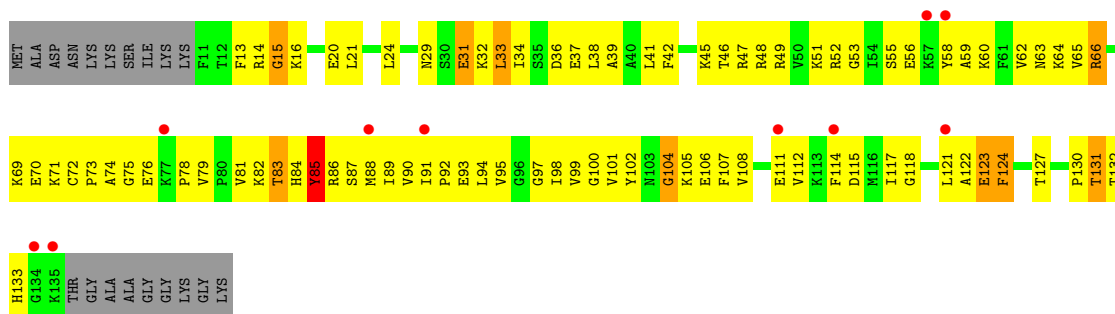
• Molecule 28: RPS15E

Chain AS:



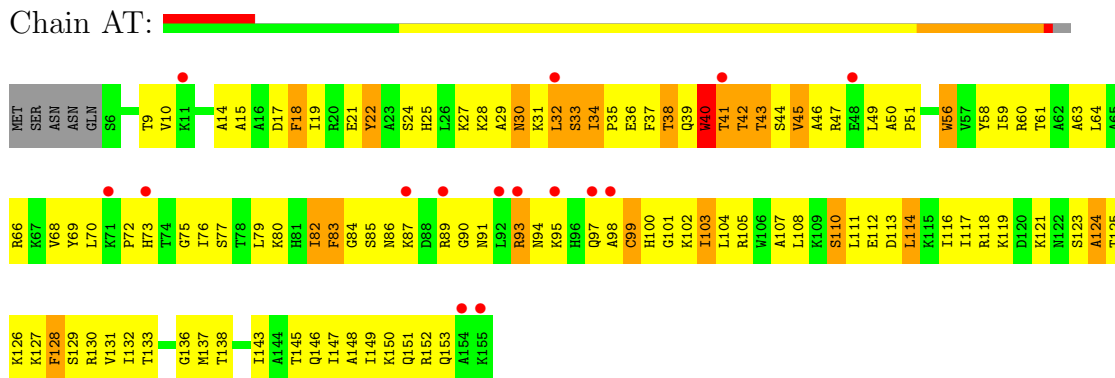
• Molecule 28: RPS15E

Chain BS:



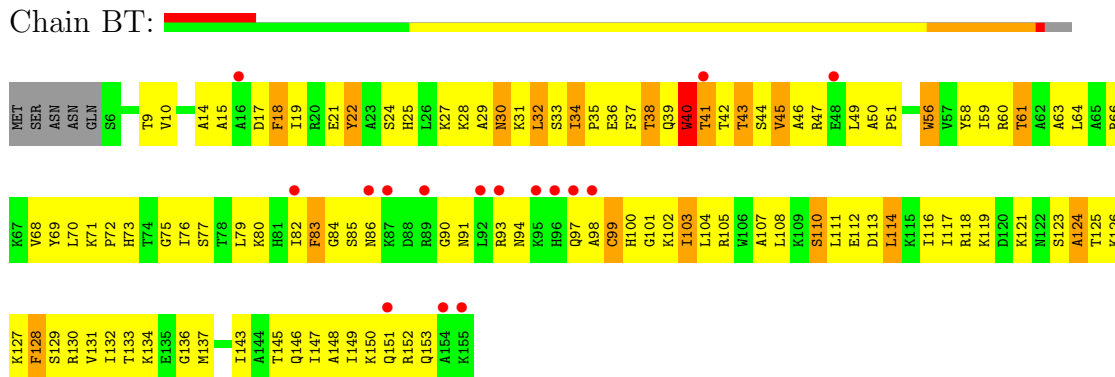
• Molecule 29: RPS19E

Chain AT:



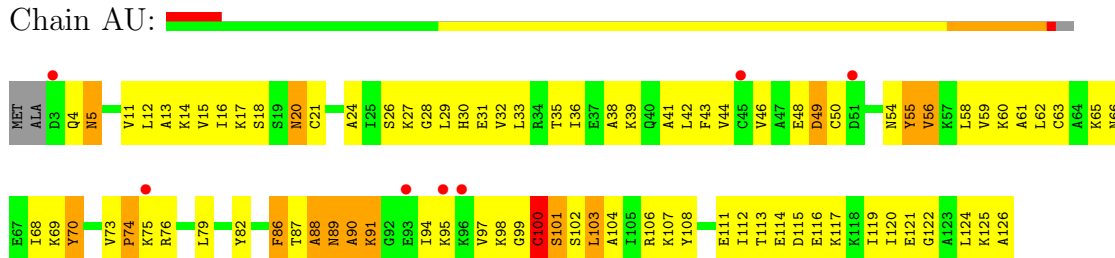
- Molecule 29: RPS19E

Chain BT:



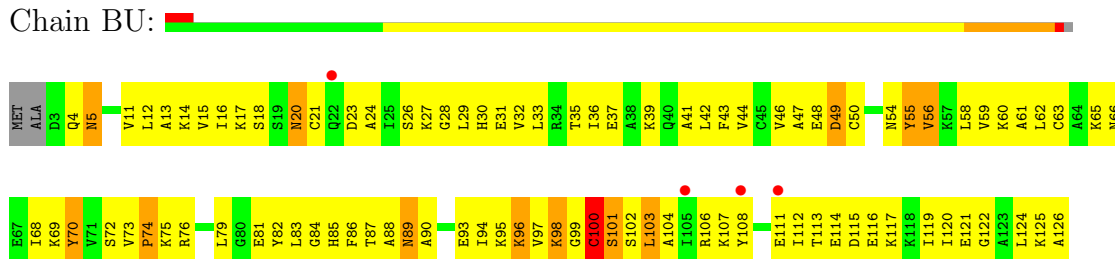
- Molecule 30: RIBOSOMAL PROTEIN L7AE CONTAINING PROTEIN

Chain AU:



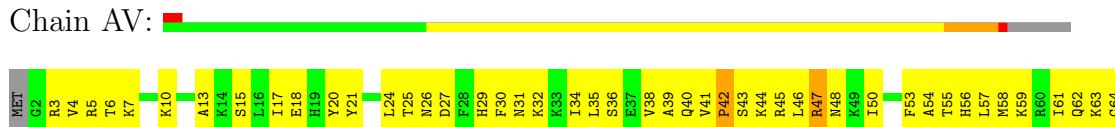
- Molecule 30: RIBOSOMAL PROTEIN L7AE CONTAINING PROTEIN

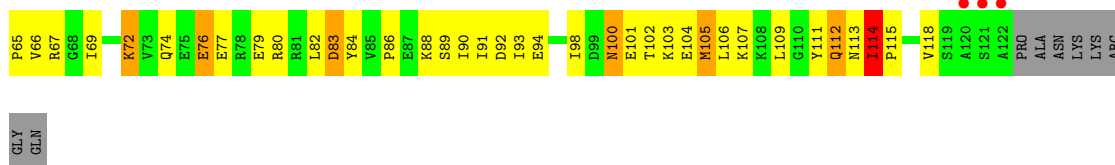
Chain BU:



- Molecule 31: RPS17E

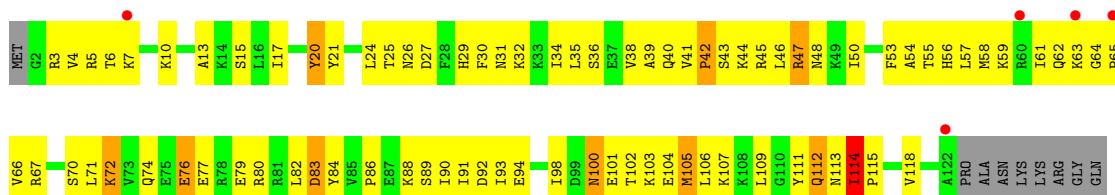
Chain AV:





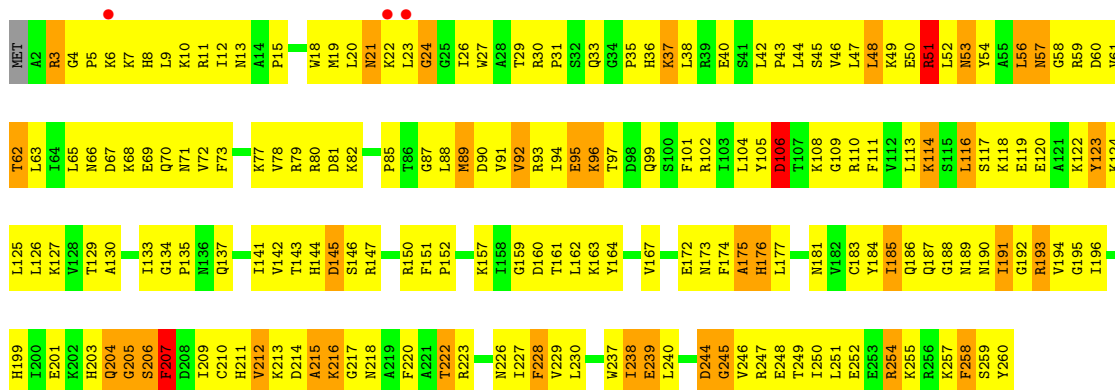
• Molecule 31: RPS17E

Chain BV:



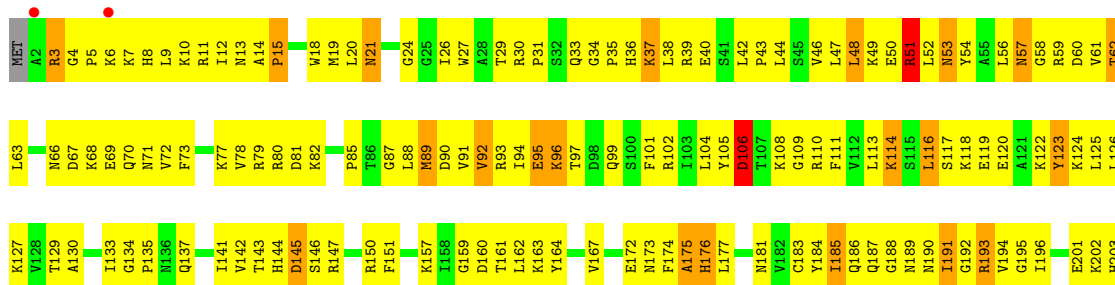
• Molecule 32: 40S RIBOSOMAL PROTEIN S4

Chain AW:



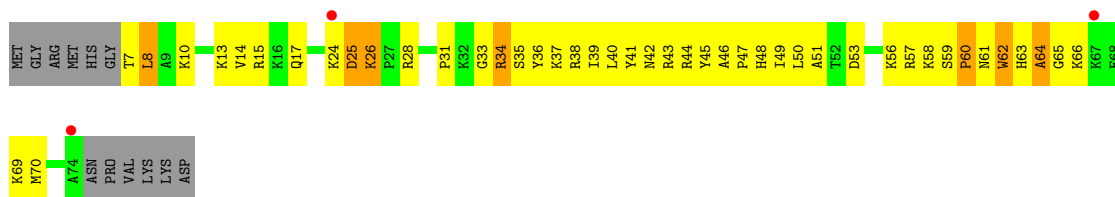
• Molecule 32: 40S RIBOSOMAL PROTEIN S4

Chain BW:



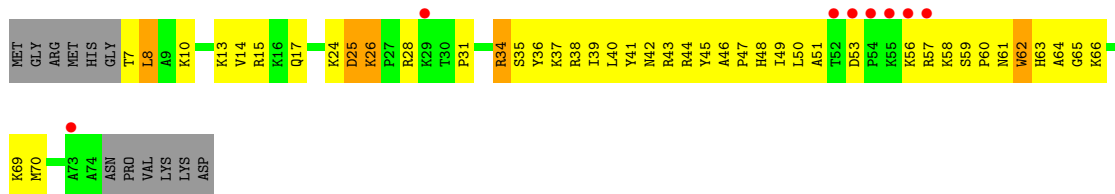
• Molecule 33: RPS30E

Chain AX:



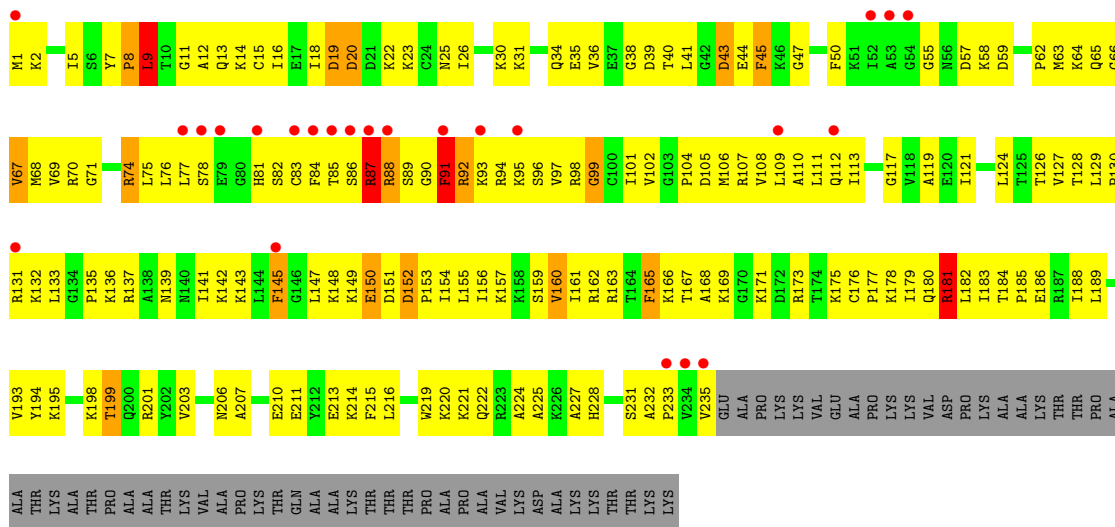
• Molecule 33: RPS30E

Chain BX:



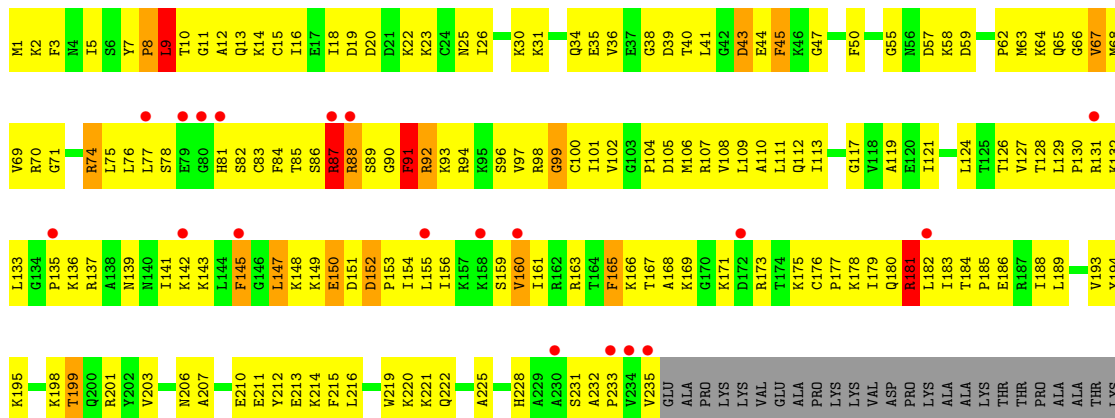
• Molecule 34: RPS6E

Chain AY:



• Molecule 34: RPS6E

Chain BY:



ALA	THR	PRO	ALA	ALA	THR	LYS	VAL	ALA	PRO	LYS	THR	GLN	ALA	ALA	LYS	THR	THR	PRO	ALA	PRO	ALA	VAL	LYS	ASP	ALA	LYS	LYS	THR	THR	LYS	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

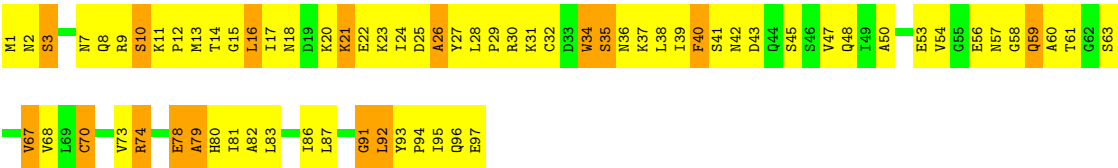
● Molecule 35: RPS21E

Chain AZ:



● Molecule 35: RPS21E

Chain BZ:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 3.89Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.206 , 0.243 0.248 , 0.275	Depositor DCC
$R_{free}$ test set	6661 reflections (2.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	126.5	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 96.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 364650 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	157632	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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	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 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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	BI	1135	0	1204	146	0
19	AJ	833	0	903	82	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	A5	1	0	0	0	0
37	A6	1	0	0	0	0
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

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 55.

The worst 5 of 15283 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

### 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	
1	A1	65/68 (96%)	45 (69%)	11 (17%)	9 (14%)	0	11
1	B1	65/68 (96%)	44 (68%)	12 (18%)	9 (14%)	0	11
2	A2	205/208 (99%)	147 (72%)	38 (18%)	20 (10%)	1	21
2	B2	205/208 (99%)	146 (71%)	39 (19%)	20 (10%)	1	21
3	A3	194/197 (98%)	159 (82%)	25 (13%)	10 (5%)	3	42
3	B3	194/197 (98%)	159 (82%)	24 (12%)	11 (6%)	3	39
4	A4	213/265 (80%)	161 (76%)	33 (16%)	19 (9%)	1	25
4	B4	213/265 (80%)	161 (76%)	34 (16%)	18 (8%)	1	26
5	A5	96/119 (81%)	66 (69%)	20 (21%)	10 (10%)	1	18
5	B5	96/119 (81%)	65 (68%)	21 (22%)	10 (10%)	1	18
6	A6	78/81 (96%)	57 (73%)	15 (19%)	6 (8%)	1	29
6	B6	78/81 (96%)	57 (73%)	15 (19%)	6 (8%)	1	29
7	A7	102/162 (63%)	78 (76%)	17 (17%)	7 (7%)	2	33
7	B7	102/162 (63%)	78 (76%)	17 (17%)	7 (7%)	2	33
8	A8	91/143 (64%)	71 (78%)	13 (14%)	7 (8%)	1	29
8	B8	91/143 (64%)	71 (78%)	13 (14%)	7 (8%)	1	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	A9	72/189 (38%)	50 (69%)	17 (24%)	5 (7%)	2	33
9	B9	72/189 (38%)	50 (69%)	17 (24%)	5 (7%)	2	33
11	AB	202/241 (84%)	168 (83%)	28 (14%)	6 (3%)	7	59
11	BB	202/241 (84%)	167 (83%)	28 (14%)	7 (4%)	6	55
12	AC	227/243 (93%)	177 (78%)	31 (14%)	19 (8%)	1	26
12	BC	227/243 (93%)	176 (78%)	32 (14%)	19 (8%)	1	26
13	AD	177/181 (98%)	132 (75%)	36 (20%)	9 (5%)	3	42
13	BD	177/181 (98%)	130 (73%)	38 (22%)	9 (5%)	3	42
14	AE	228/296 (77%)	170 (75%)	40 (18%)	18 (8%)	1	28
14	BE	228/296 (77%)	172 (75%)	39 (17%)	17 (8%)	2	30
15	AF	87/101 (86%)	70 (80%)	12 (14%)	5 (6%)	3	39
15	BF	87/101 (86%)	70 (80%)	12 (14%)	5 (6%)	3	39
16	AG	190/200 (95%)	141 (74%)	33 (17%)	16 (8%)	1	26
16	BG	190/200 (95%)	142 (75%)	31 (16%)	17 (9%)	1	25
17	AH	127/130 (98%)	98 (77%)	24 (19%)	5 (4%)	5	51
17	BH	127/130 (98%)	98 (77%)	26 (20%)	3 (2%)	9	63
18	AI	141/145 (97%)	111 (79%)	25 (18%)	5 (4%)	6	55
18	BI	141/145 (97%)	110 (78%)	26 (18%)	5 (4%)	6	55
19	AJ	103/120 (86%)	89 (86%)	6 (6%)	8 (8%)	1	29
19	BJ	103/120 (86%)	89 (86%)	6 (6%)	8 (8%)	1	29
20	AK	138/151 (91%)	96 (70%)	28 (20%)	14 (10%)	1	20
20	BK	138/151 (91%)	95 (69%)	27 (20%)	16 (12%)	1	15
21	AL	139/142 (98%)	106 (76%)	17 (12%)	16 (12%)	1	15
21	BL	139/142 (98%)	106 (76%)	18 (13%)	15 (11%)	1	17
22	AM	152/155 (98%)	109 (72%)	22 (14%)	21 (14%)	0	11
22	BM	152/155 (98%)	110 (72%)	21 (14%)	21 (14%)	0	11
23	AN	51/55 (93%)	30 (59%)	11 (22%)	10 (20%)	0	4
23	BN	51/55 (93%)	31 (61%)	11 (22%)	9 (18%)	0	5
24	AO	148/153 (97%)	112 (76%)	20 (14%)	16 (11%)	1	17
24	BO	148/153 (97%)	113 (76%)	19 (13%)	16 (11%)	1	17
25	AP	146/149 (98%)	115 (79%)	20 (14%)	11 (8%)	2	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	BP	146/149 (98%)	115 (79%)	20 (14%)	11 (8%)	2	30
26	AQ	155/157 (99%)	115 (74%)	26 (17%)	14 (9%)	1	24
26	BQ	155/157 (99%)	112 (72%)	27 (17%)	16 (10%)	1	19
27	AR	336/343 (98%)	255 (76%)	48 (14%)	33 (10%)	1	21
27	BR	336/343 (98%)	256 (76%)	48 (14%)	32 (10%)	1	22
28	AS	123/144 (85%)	91 (74%)	25 (20%)	7 (6%)	3	39
28	BS	123/144 (85%)	90 (73%)	25 (20%)	8 (6%)	2	36
29	AT	148/155 (96%)	114 (77%)	17 (12%)	17 (12%)	1	15
29	BT	148/155 (96%)	113 (76%)	20 (14%)	15 (10%)	1	20
30	AU	122/126 (97%)	91 (75%)	20 (16%)	11 (9%)	1	24
30	BU	122/126 (97%)	89 (73%)	22 (18%)	11 (9%)	1	24
31	AV	119/130 (92%)	94 (79%)	16 (13%)	9 (8%)	2	29
31	BV	119/130 (92%)	96 (81%)	14 (12%)	9 (8%)	2	29
32	AW	257/260 (99%)	193 (75%)	40 (16%)	24 (9%)	1	23
32	BW	257/260 (99%)	195 (76%)	38 (15%)	24 (9%)	1	23
33	AX	66/80 (82%)	48 (73%)	12 (18%)	6 (9%)	1	24
33	BX	66/80 (82%)	48 (73%)	12 (18%)	6 (9%)	1	24
34	AY	233/293 (80%)	188 (81%)	31 (13%)	14 (6%)	2	38
34	BY	233/293 (80%)	187 (80%)	32 (14%)	14 (6%)	2	38
35	AZ	95/97 (98%)	70 (74%)	13 (14%)	12 (13%)	0	13
35	BZ	95/97 (98%)	69 (73%)	14 (15%)	12 (13%)	0	13
All	All	10052/11358 (88%)	7627 (76%)	1588 (16%)	837 (8%)	1	27

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%)	31	78
1	B1	56/57 (98%)	53 (95%)	3 (5%)	31	78
2	A2	184/185 (100%)	171 (93%)	13 (7%)	21	68
2	B2	184/185 (100%)	171 (93%)	13 (7%)	21	68
3	A3	182/183 (100%)	164 (90%)	18 (10%)	11	52
3	B3	182/183 (100%)	165 (91%)	17 (9%)	13	55
4	A4	191/225 (85%)	166 (87%)	25 (13%)	6	37
4	B4	191/225 (85%)	166 (87%)	25 (13%)	6	37
5	A5	88/107 (82%)	80 (91%)	8 (9%)	14	57
5	B5	88/107 (82%)	80 (91%)	8 (9%)	14	57
6	A6	71/72 (99%)	67 (94%)	4 (6%)	30	77
6	B6	71/72 (99%)	67 (94%)	4 (6%)	30	77
7	A7	94/136 (69%)	84 (89%)	10 (11%)	10	48
7	B7	94/136 (69%)	84 (89%)	10 (11%)	10	48
8	A8	80/109 (73%)	68 (85%)	12 (15%)	4	30
8	B8	80/109 (73%)	68 (85%)	12 (15%)	4	30
9	A9	64/138 (46%)	56 (88%)	8 (12%)	7	40
9	B9	64/138 (46%)	56 (88%)	8 (12%)	7	40
11	AB	183/211 (87%)	167 (91%)	16 (9%)	15	59
11	BB	183/211 (87%)	167 (91%)	16 (9%)	15	59
12	AC	197/210 (94%)	178 (90%)	19 (10%)	12	54
12	BC	197/210 (94%)	179 (91%)	18 (9%)	14	57
13	AD	161/162 (99%)	137 (85%)	24 (15%)	4	31
13	BD	161/162 (99%)	137 (85%)	24 (15%)	4	31
14	AE	194/250 (78%)	171 (88%)	23 (12%)	8	42
14	BE	194/250 (78%)	171 (88%)	23 (12%)	8	42
15	AF	80/92 (87%)	72 (90%)	8 (10%)	11	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	BF	80/92 (87%)	71 (89%)	9 (11%)	9	44
16	AG	163/169 (96%)	147 (90%)	16 (10%)	12	53
16	BG	163/169 (96%)	146 (90%)	17 (10%)	10	50
17	AH	116/117 (99%)	101 (87%)	15 (13%)	6	38
17	BH	116/117 (99%)	102 (88%)	14 (12%)	7	41
18	AI	120/122 (98%)	115 (96%)	5 (4%)	40	84
18	BI	120/122 (98%)	115 (96%)	5 (4%)	40	84
19	AJ	98/111 (88%)	93 (95%)	5 (5%)	33	79
19	BJ	98/111 (88%)	93 (95%)	5 (5%)	33	79
20	AK	112/121 (93%)	96 (86%)	16 (14%)	5	33
20	BK	112/121 (93%)	96 (86%)	16 (14%)	5	33
21	AL	113/114 (99%)	101 (89%)	12 (11%)	10	48
21	BL	113/114 (99%)	102 (90%)	11 (10%)	12	53
22	AM	134/135 (99%)	121 (90%)	13 (10%)	12	53
22	BM	134/135 (99%)	121 (90%)	13 (10%)	12	53
23	AN	47/49 (96%)	41 (87%)	6 (13%)	6	38
23	BN	47/49 (96%)	41 (87%)	6 (13%)	6	38
24	AO	134/136 (98%)	127 (95%)	7 (5%)	32	79
24	BO	134/136 (98%)	127 (95%)	7 (5%)	32	79
25	AP	133/134 (99%)	124 (93%)	9 (7%)	22	70
25	BP	133/134 (99%)	124 (93%)	9 (7%)	22	70
26	AQ	141/141 (100%)	125 (89%)	16 (11%)	9	44
26	BQ	141/141 (100%)	126 (89%)	15 (11%)	10	48
27	AR	291/295 (99%)	261 (90%)	30 (10%)	10	50
27	BR	291/295 (99%)	260 (89%)	31 (11%)	10	48
28	AS	105/117 (90%)	102 (97%)	3 (3%)	55	89
28	BS	105/117 (90%)	101 (96%)	4 (4%)	44	85
29	AT	129/134 (96%)	117 (91%)	12 (9%)	13	55
29	BT	129/134 (96%)	116 (90%)	13 (10%)	11	51
30	AU	103/104 (99%)	97 (94%)	6 (6%)	28	75
30	BU	103/104 (99%)	99 (96%)	4 (4%)	43	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	AV	108/115 (94%)	100 (93%)	8 (7%)	20	66
31	BV	108/115 (94%)	99 (92%)	9 (8%)	16	62
32	AW	226/227 (100%)	196 (87%)	30 (13%)	6	37
32	BW	226/227 (100%)	197 (87%)	29 (13%)	6	38
33	AX	57/67 (85%)	55 (96%)	2 (4%)	48	87
33	BX	57/67 (85%)	55 (96%)	2 (4%)	48	87
34	AY	201/244 (82%)	187 (93%)	14 (7%)	21	69
34	BY	201/244 (82%)	187 (93%)	14 (7%)	21	69
35	AZ	82/82 (100%)	76 (93%)	6 (7%)	20	67
35	BZ	82/82 (100%)	76 (93%)	6 (7%)	20	67
All	All	8876/9742 (91%)	8034 (90%)	842 (10%)	12	54

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%)	194 (11%)
10	BA	1743/1753 (99%)	453 (25%)	194 (11%)
All	All	3486/3506 (99%)	905 (25%)	388 (11%)

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

5 of 388 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	AA	1555	A
10	BA	164	U
10	BA	1443	A
10	AA	1605	A
10	BA	41	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 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.

## 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	A1	67/68 (98%)	-0.13	2 (2%) 48 36	99, 157, 220, 262	0
1	B1	67/68 (98%)	-0.23	1 (1%) 70 54	99, 157, 220, 262	0
2	A2	207/208 (99%)	1.07	37 (17%) 2 4	96, 144, 194, 231	0
2	B2	207/208 (99%)	0.17	3 (1%) 72 56	98, 145, 194, 231	0
3	A3	196/197 (99%)	0.07	1 (0%) 88 77	82, 138, 187, 267	0
3	B3	196/197 (99%)	0.16	5 (2%) 53 40	75, 138, 186, 266	0
4	A4	215/265 (81%)	0.43	9 (4%) 35 27	80, 146, 201, 228	0
4	B4	215/265 (81%)	0.76	21 (9%) 8 10	77, 145, 202, 229	0
5	A5	98/119 (82%)	0.51	6 (6%) 21 19	71, 124, 201, 246	0
5	B5	98/119 (82%)	0.54	4 (4%) 35 28	68, 124, 201, 246	0
6	A6	80/81 (98%)	0.43	1 (1%) 74 58	86, 130, 172, 187	0
6	B6	80/81 (98%)	0.14	0 100 100	86, 128, 172, 186	0
7	A7	104/162 (64%)	0.22	0 100 100	100, 150, 201, 249	0
7	B7	104/162 (64%)	0.33	6 (5%) 22 20	104, 151, 199, 249	0
8	A8	93/143 (65%)	0.17	6 (6%) 18 18	112, 159, 219, 255	0
8	B8	93/143 (65%)	-0.08	1 (1%) 77 61	110, 159, 219, 256	0
9	A9	73/189 (38%)	0.16	3 (4%) 35 28	146, 185, 238, 253	0
9	B9	73/189 (38%)	0.30	6 (8%) 12 12	148, 186, 238, 254	0
10	AA	1745/1753 (99%)	0.04	33 (1%) 64 48	80, 134, 291, 454	0
10	BA	1745/1753 (99%)	-0.08	24 (1%) 72 56	80, 134, 291, 454	0
11	AB	204/241 (84%)	0.05	3 (1%) 70 54	82, 136, 177, 225	0
11	BB	204/241 (84%)	0.10	1 (0%) 88 77	78, 136, 177, 224	0
12	AC	229/243 (94%)	0.02	1 (0%) 90 82	89, 131, 194, 244	0
12	BC	229/243 (94%)	-0.12	0 100 100	87, 132, 195, 246	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
13	AD	179/181 (98%)	0.54	9 (5%)	28	23	77, 122, 182, 214	0
13	BD	179/181 (98%)	0.12	8 (4%)	32	26	82, 125, 184, 215	0
14	AE	230/296 (77%)	0.32	5 (2%)	59	44	62, 114, 194, 243	0
14	BE	230/296 (77%)	0.23	7 (3%)	48	36	65, 116, 194, 244	0
15	AF	89/101 (88%)	-0.20	0	100	100	87, 136, 190, 230	0
15	BF	89/101 (88%)	-0.21	0	100	100	86, 137, 190, 229	0
16	AG	192/200 (96%)	0.25	7 (3%)	41	32	86, 140, 191, 286	0
16	BG	192/200 (96%)	0.13	6 (3%)	47	36	86, 140, 191, 287	0
17	AH	129/130 (99%)	0.10	0	100	100	65, 105, 154, 194	0
17	BH	129/130 (99%)	0.27	1 (0%)	83	69	62, 106, 154, 193	0
18	AI	143/145 (98%)	1.15	22 (15%)	3	5	87, 135, 188, 222	0
18	BI	143/145 (98%)	1.06	29 (20%)	1	3	87, 135, 189, 221	0
19	AJ	105/120 (87%)	0.13	3 (2%)	49	38	84, 132, 199, 218	0
19	BJ	105/120 (87%)	0.08	2 (1%)	64	48	86, 133, 198, 218	0
20	AK	140/151 (92%)	0.27	6 (4%)	34	27	93, 144, 191, 223	0
20	BK	140/151 (92%)	0.34	2 (1%)	72	56	90, 144, 192, 224	0
21	AL	141/142 (99%)	0.37	2 (1%)	72	56	71, 126, 169, 213	0
21	BL	141/142 (99%)	0.69	15 (10%)	7	9	74, 128, 169, 212	0
22	AM	154/155 (99%)	0.17	2 (1%)	74	58	94, 154, 204, 233	0
22	BM	154/155 (99%)	0.17	2 (1%)	74	58	95, 155, 205, 233	0
23	AN	53/55 (96%)	0.70	3 (5%)	23	20	83, 124, 156, 193	0
23	BN	53/55 (96%)	1.45	13 (24%)	1	3	83, 126, 157, 192	0
24	AO	150/153 (98%)	0.09	3 (2%)	62	46	73, 124, 223, 287	0
24	BO	150/153 (98%)	0.24	2 (1%)	74	58	71, 124, 222, 288	0
25	AP	148/149 (99%)	0.33	11 (7%)	14	14	92, 141, 168, 200	0
25	BP	148/149 (99%)	0.04	2 (1%)	72	56	94, 141, 170, 200	0
26	AQ	157/157 (100%)	0.36	8 (5%)	27	23	69, 129, 214, 227	0
26	BQ	157/157 (100%)	0.39	10 (6%)	19	18	65, 128, 208, 258	0
27	AR	338/343 (98%)	0.20	8 (2%)	56	42	93, 146, 218, 268	0
27	BR	338/343 (98%)	0.03	5 (1%)	70	54	94, 145, 209, 245	0
28	AS	125/144 (86%)	-0.03	0	100	100	117, 165, 222, 245	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	BS	125/144 (86%)	0.70	10 (8%) 12 13	119, 165, 222, 245	0
29	AT	150/155 (96%)	0.78	15 (10%) 8 10	80, 152, 191, 230	0
29	BT	150/155 (96%)	0.59	16 (10%) 6 9	79, 151, 192, 229	0
30	AU	124/126 (98%)	0.37	7 (5%) 24 20	117, 177, 213, 227	0
30	BU	124/126 (98%)	0.19	4 (3%) 45 35	136, 185, 221, 250	0
31	AV	121/130 (93%)	-0.00	3 (2%) 54 41	78, 143, 206, 254	0
31	BV	121/130 (93%)	0.41	5 (4%) 35 28	76, 142, 206, 253	0
32	AW	259/260 (99%)	0.10	3 (1%) 75 60	84, 125, 166, 200	0
32	BW	259/260 (99%)	-0.17	2 (0%) 83 69	87, 126, 167, 199	0
33	AX	68/80 (85%)	0.42	3 (4%) 33 27	106, 155, 242, 271	0
33	BX	68/80 (85%)	0.58	8 (11%) 5 7	107, 158, 243, 271	0
34	AY	235/293 (80%)	0.54	24 (10%) 7 9	108, 159, 237, 316	0
34	BY	235/293 (80%)	0.31	19 (8%) 12 13	110, 159, 237, 315	0
35	AZ	97/97 (100%)	0.13	0 100 100	74, 129, 185, 209	0
35	BZ	97/97 (100%)	-0.05	0 100 100	77, 129, 184, 210	0
All	All	13676/14864 (92%)	0.20	486 (3%) 41 32	62, 139, 215, 454	0

The worst 5 of 486 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	AI	140	MET	10.8
18	AI	141	GLN	10.6
10	AA	696	C	10.2
26	AQ	1	MET	10.1
4	B4	15	LYS	10.0

## 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
36	MG	BA	1838	1/1	0.33	39.70	172,172,172,172	0
36	MG	BA	1888	1/1	0.90	30.72	227,227,227,227	0
36	MG	AA	1873	1/1	0.44	25.30	196,196,196,196	0
36	MG	BA	1883	1/1	0.42	19.95	187,187,187,187	0
36	MG	AA	1827	1/1	0.32	18.17	178,178,178,178	0
36	MG	BA	1873	1/1	0.37	16.96	218,218,218,218	0
36	MG	BA	1855	1/1	0.42	11.56	275,275,275,275	0
36	MG	BA	1807	1/1	0.18	9.00	210,210,210,210	0
36	MG	AA	1855	1/1	0.41	8.20	214,214,214,214	0
36	MG	AA	1884	1/1	0.47	7.78	190,190,190,190	0
36	MG	AA	1829	1/1	0.16	7.00	160,160,160,160	0
36	MG	AA	1883	1/1	0.51	6.69	209,209,209,209	0
36	MG	BA	1836	1/1	0.29	5.67	175,175,175,175	0
36	MG	AA	1805	1/1	0.37	5.46	175,175,175,175	0
36	MG	BA	1852	1/1	0.22	5.07	170,170,170,170	0
36	MG	BA	1845	1/1	0.27	4.11	225,225,225,225	0
36	MG	BA	1882	1/1	0.31	3.76	196,196,196,196	0
36	MG	BA	1875	1/1	0.29	3.76	193,193,193,193	0
36	MG	AA	1889	1/1	0.25	3.28	200,200,200,200	0
36	MG	BA	1886	1/1	0.18	3.00	214,214,214,214	0
36	MG	BA	1866	1/1	0.18	2.78	186,186,186,186	0
37	ZN	B6	500	1/1	0.24	2.69	108,108,108,108	0
36	MG	AA	1845	1/1	0.27	2.51	193,193,193,193	0
36	MG	BA	1840	1/1	0.18	2.04	128,128,128,128	0
36	MG	BA	1815	1/1	0.31	1.81	155,155,155,155	0
36	MG	BA	1872	1/1	0.33	1.31	200,200,200,200	0
36	MG	AA	1868	1/1	0.57	1.22	197,197,197,197	0
36	MG	BA	1842	1/1	0.19	1.01	210,210,210,210	0
36	MG	AA	1870	1/1	0.27	1.00	195,195,195,195	0
36	MG	BA	1811	1/1	0.38	0.98	170,170,170,170	0
36	MG	BD	201	1/1	0.29	0.93	233,233,233,233	0
36	MG	BA	1879	1/1	0.21	0.48	221,221,221,221	0
36	MG	AA	1853	1/1	0.18	0.45	177,177,177,177	0
36	MG	BA	1810	1/1	0.26	0.42	188,188,188,188	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
37	ZN	A9	500	1/1	0.19	0.40	169,169,169,169	0
36	MG	BA	1803	1/1	0.27	0.34	169,169,169,169	0
36	MG	BA	1812	1/1	0.37	0.27	166,166,166,166	0
36	MG	BA	1868	1/1	0.30	0.25	208,208,208,208	0
36	MG	BA	1850	1/1	0.14	0.24	221,221,221,221	0
36	MG	AA	1856	1/1	0.56	0.21	182,182,182,182	0
36	MG	AA	1869	1/1	0.32	0.20	209,209,209,209	0
36	MG	BA	1832	1/1	0.13	-0.10	194,194,194,194	0
36	MG	AA	1871	1/1	0.19	-0.10	201,201,201,201	0
36	MG	AA	1879	1/1	0.18	-0.11	193,193,193,193	0
36	MG	AA	1812	1/1	0.27	-0.12	173,173,173,173	0
36	MG	AA	1874	1/1	0.17	-0.34	194,194,194,194	0
36	MG	AA	1808	1/1	0.33	-0.38	136,136,136,136	0
37	ZN	B5	500	1/1	0.21	-0.50	87,87,87,87	0
36	MG	AA	1839	1/1	0.16	-0.57	143,143,143,143	0
37	ZN	A6	500	1/1	0.17	-0.59	118,118,118,118	0
36	MG	AA	1809	1/1	0.19	-0.68	193,193,193,193	0
36	MG	AA	1872	1/1	0.16	-0.69	196,196,196,196	0
36	MG	BA	1856	1/1	0.08	-0.72	173,173,173,173	0
37	ZN	B9	500	1/1	0.11	-0.80	247,247,247,247	0
37	ZN	AN	500	1/1	0.17	-0.84	105,105,105,105	0
36	MG	BA	1848	1/1	0.14	-0.86	206,206,206,206	0
36	MG	BA	1808	1/1	0.18	-0.90	140,140,140,140	0
36	MG	BA	1831	1/1	0.16	-0.92	115,115,115,115	0
36	MG	BA	1802	1/1	0.12	-0.94	169,169,169,169	0
36	MG	AA	1815	1/1	0.20	-0.95	144,144,144,144	0
36	MG	AA	1875	1/1	0.22	-0.98	152,152,152,152	0
36	MG	AA	1821	1/1	0.18	-1.03	144,144,144,144	0
36	MG	AA	1882	1/1	0.20	-1.05	181,181,181,181	0
36	MG	AA	1851	1/1	0.19	-1.19	187,187,187,187	0
36	MG	BA	1821	1/1	0.17	-1.26	160,160,160,160	0
36	MG	AA	1802	1/1	0.09	-1.27	175,175,175,175	0
37	ZN	BN	500	1/1	0.13	-1.33	113,113,113,113	0
37	ZN	A5	500	1/1	0.15	-1.41	95,95,95,95	0
36	MG	AA	1820	1/1	0.15	-1.49	157,157,157,157	0
36	MG	AA	1810	1/1	0.15	-1.61	175,175,175,175	0
36	MG	BA	1887	1/1	0.22	-1.75	206,206,206,206	0
36	MG	BA	1881	1/1	0.09	-1.79	149,149,149,149	0
36	MG	AA	1844	1/1	0.11	-1.81	166,166,166,166	0
36	MG	BA	1876	1/1	0.15	-1.89	184,184,184,184	0
36	MG	AA	1831	1/1	0.15	-1.90	111,111,111,111	0
36	MG	A4	301	1/1	0.08	-1.91	174,174,174,174	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	MG	AA	1822	1/1	0.11	-1.92	139,139,139,139	0
36	MG	AA	1819	1/1	0.14	-1.93	136,136,136,136	0
36	MG	BA	1816	1/1	0.14	-1.98	127,127,127,127	0
36	MG	AA	1887	1/1	0.13	-2.06	198,198,198,198	0
36	MG	BA	1860	1/1	0.09	-2.09	177,177,177,177	0
36	MG	BA	1844	1/1	0.07	-2.10	157,157,157,157	0
36	MG	AA	1860	1/1	0.10	-2.13	176,176,176,176	0
36	MG	BA	1889	1/1	0.13	-2.18	209,209,209,209	0
36	MG	BA	1828	1/1	0.09	-2.19	145,145,145,145	0
36	MG	AA	1888	1/1	0.16	-2.26	205,205,205,205	0
36	MG	AA	1846	1/1	0.16	-2.27	161,161,161,161	0
36	MG	AA	1823	1/1	0.14	-2.49	130,130,130,130	0
36	MG	AA	1852	1/1	0.09	-2.55	173,173,173,173	0
36	MG	B4	301	1/1	0.10	-2.55	165,165,165,165	0
36	MG	BA	1820	1/1	0.14	-2.62	170,170,170,170	0
36	MG	AL	201	1/1	0.13	-2.65	182,182,182,182	0
36	MG	BA	1853	1/1	0.10	-2.72	194,194,194,194	0
36	MG	BA	1826	1/1	0.10	-2.78	185,185,185,185	0
36	MG	AA	1804	1/1	0.14	-2.78	150,150,150,150	0
36	MG	AA	1806	1/1	0.09	-2.79	151,151,151,151	0
36	MG	BA	1806	1/1	0.08	-2.82	168,168,168,168	0
36	MG	BA	1827	1/1	0.12	-2.83	199,199,199,199	0
36	MG	BA	1819	1/1	0.09	-2.95	122,122,122,122	0
36	MG	AA	1886	1/1	0.10	-2.99	148,148,148,148	0
36	MG	AA	1828	1/1	0.12	-3.06	133,133,133,133	0
36	MG	BA	1859	1/1	0.07	-3.07	194,194,194,194	0
36	MG	BA	1839	1/1	0.07	-3.10	140,140,140,140	0
36	MG	AA	1862	1/1	0.08	-3.10	191,191,191,191	0
36	MG	AA	1816	1/1	0.10	-3.10	96,96,96,96	0
36	MG	AA	1835	1/1	0.09	-3.15	159,159,159,159	0
36	MG	AA	1833	1/1	0.09	-3.18	135,135,135,135	0
36	MG	AA	1866	1/1	0.16	-3.20	197,197,197,197	0
36	MG	BA	1824	1/1	0.12	-3.34	172,172,172,172	0
36	MG	BA	1822	1/1	0.13	-3.48	151,151,151,151	0
36	MG	BA	1867	1/1	0.10	-3.55	180,180,180,180	0
36	MG	AA	1843	1/1	0.07	-3.60	182,182,182,182	0
36	MG	BW	301	1/1	0.06	-3.62	166,166,166,166	0
36	MG	AA	1826	1/1	0.12	-3.65	155,155,155,155	0
36	MG	AA	1885	1/1	0.10	-3.72	223,223,223,223	0
36	MG	AA	1836	1/1	0.14	-3.73	166,166,166,166	0
36	MG	BA	1878	1/1	0.10	-3.80	177,177,177,177	0
36	MG	BA	1851	1/1	0.09	-3.94	169,169,169,169	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	MG	AA	1838	1/1	0.12	-3.99	144,144,144,144	0
36	MG	BA	1834	1/1	0.11	-4.05	138,138,138,138	0
36	MG	BA	1846	1/1	0.10	-4.12	147,147,147,147	0
36	MG	BA	1858	1/1	0.10	-4.23	163,163,163,163	0
36	MG	AA	1818	1/1	0.09	-4.26	121,121,121,121	0
36	MG	BA	1854	1/1	0.07	-4.37	189,189,189,189	0
36	MG	BA	1814	1/1	0.05	-4.39	214,214,214,214	0
36	MG	AA	1859	1/1	0.11	-4.42	193,193,193,193	0
36	MG	BA	1833	1/1	0.11	-4.49	172,172,172,172	0
36	MG	AA	1876	1/1	0.12	-4.60	180,180,180,180	0
36	MG	AA	1864	1/1	0.10	-4.66	176,176,176,176	0
36	MG	BA	1818	1/1	0.12	-4.70	111,111,111,111	0
36	MG	AA	1840	1/1	0.10	-4.72	124,124,124,124	0
36	MG	BA	1817	1/1	0.08	-4.84	134,134,134,134	0
36	MG	BA	1804	1/1	0.05	-4.91	191,191,191,191	0
36	MG	BA	1874	1/1	0.12	-4.92	164,164,164,164	0
36	MG	AA	1878	1/1	0.13	-4.92	160,160,160,160	0
36	MG	AA	1847	1/1	0.11	-4.98	186,186,186,186	0
36	MG	BA	1864	1/1	0.08	-5.16	182,182,182,182	0
36	MG	AA	1881	1/1	0.09	-5.17	198,198,198,198	0
36	MG	BA	1837	1/1	0.12	-5.24	178,178,178,178	0
36	MG	BA	1884	1/1	0.06	-5.28	219,219,219,219	0
36	MG	BA	1863	1/1	0.06	-5.46	166,166,166,166	0
36	MG	BA	1830	1/1	0.06	-5.48	204,204,204,204	0
36	MG	BA	1841	1/1	0.08	-5.57	129,129,129,129	0
36	MG	BA	1801	1/1	0.03	-5.64	186,186,186,186	0
36	MG	AA	1814	1/1	0.09	-5.85	197,197,197,197	0
36	MG	AA	1813	1/1	0.06	-5.99	191,191,191,191	0
36	MG	AA	1803	1/1	0.06	-6.03	147,147,147,147	0
36	MG	AA	1837	1/1	0.13	-6.15	149,149,149,149	0
36	MG	AA	1849	1/1	0.13	-6.30	159,159,159,159	0
36	MG	BA	1865	1/1	0.06	-6.33	183,183,183,183	0
36	MG	BA	1849	1/1	0.07	-6.45	198,198,198,198	0
36	MG	AA	1867	1/1	0.05	-6.67	193,193,193,193	0
36	MG	AA	1880	1/1	0.07	-6.68	193,193,193,193	0
36	MG	BA	1885	1/1	0.10	-6.73	161,161,161,161	0
36	MG	AA	1848	1/1	0.09	-7.00	183,183,183,183	0
36	MG	AA	1865	1/1	0.06	-7.07	184,184,184,184	0
36	MG	AA	1877	1/1	0.17	-7.07	170,170,170,170	0
36	MG	AA	1861	1/1	0.12	-7.10	204,204,204,204	0
36	MG	AA	1857	1/1	0.10	-7.37	140,140,140,140	0
36	MG	AA	1858	1/1	0.10	-7.40	162,162,162,162	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	MG	BA	1861	1/1	0.12	-7.55	181,181,181,181	0
36	MG	AA	1824	1/1	0.08	-7.56	148,148,148,148	0
36	MG	BA	1825	1/1	0.09	-7.75	153,153,153,153	0
36	MG	BA	1869	1/1	0.19	-7.80	188,188,188,188	0
36	MG	AA	1825	1/1	0.06	-7.91	115,115,115,115	0
36	MG	AA	1832	1/1	0.10	-8.00	189,189,189,189	0
36	MG	BA	1857	1/1	0.09	-8.04	130,130,130,130	0
36	MG	BA	1835	1/1	0.08	-8.29	187,187,187,187	0
36	MG	AA	1890	1/1	0.12	-8.53	218,218,218,218	0
36	MG	BA	1813	1/1	0.10	-8.83	187,187,187,187	0
36	MG	BA	1880	1/1	0.06	-8.85	193,193,193,193	0
36	MG	AA	1801	1/1	0.06	-9.39	160,160,160,160	0
36	MG	BA	1823	1/1	0.10	-9.42	123,123,123,123	0
36	MG	AA	1863	1/1	0.07	-9.57	183,183,183,183	0
36	MG	AA	1850	1/1	0.07	-10.93	185,185,185,185	0
36	MG	BA	1862	1/1	0.08	-11.36	177,177,177,177	0
36	MG	AA	1834	1/1	0.10	-11.55	182,182,182,182	0
36	MG	BA	1870	1/1	0.05	-12.51	205,205,205,205	0
36	MG	AA	1811	1/1	0.15	-13.24	154,154,154,154	0
36	MG	AA	1817	1/1	0.08	-13.35	126,126,126,126	0
36	MG	BA	1847	1/1	0.09	-14.33	204,204,204,204	0
36	MG	AA	1842	1/1	0.04	-15.67	175,175,175,175	0
36	MG	AA	1841	1/1	0.13	-16.11	170,170,170,170	0
36	MG	AA	1854	1/1	0.09	-16.91	158,158,158,158	0
36	MG	BA	1877	1/1	0.11	-24.22	177,177,177,177	0
36	MG	BA	1843	1/1	0.12	-25.00	196,196,196,196	0
36	MG	AA	1807	1/1	0.10	-32.33	194,194,194,194	0
36	MG	BA	1829	1/1	0.05	-43.50	163,163,163,163	0
36	MG	BA	1809	1/1	0.07	-120.00	172,172,172,172	0
36	MG	BA	1871	1/1	0.14	-	209,209,209,209	0
36	MG	AA	1830	1/1	0.09	-	183,183,183,183	0
36	MG	BA	1805	1/1	0.21	-	150,150,150,150	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.