wwPDB EM Validation Summary Report (i)

Jul 3, 2024 – 04:50 am BST

PDB ID	:	6GSN
EMDB ID	:	EMD-0058
Title	:	Structure of a partial yeast 48S preinitiation complex in closed conformation
Authors	:	Llacer, J.L.; Hussain, T.; Ramakrishnan, V.
Deposited on	:	2018-06-14
Resolution	:	5.75 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

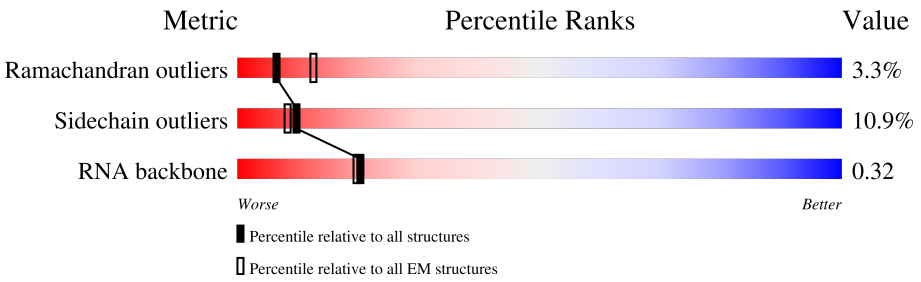
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 5.75 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)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	1798	53% 47%
2	C	217	85% 14% •
3	D	223	78% 22%
4	F	206	79% 19% •
5	K	96	77% 23%
6	M	118	12% 80% 19% ••
7	P	117	78% 20% •
8	Q	141	81% 19%

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Mol	Chain	Length	Quality of chain
9	R	130	82% 17%
10	S	145	6% 79% 21%
11	T	143	82% 18%
12	U	106	6% 85% 13%
13	Z	70	14% 81% 17%
14	c	62	87% 13%
15	f	69	6% 81% 17%
16	g	324	87% 11%
17	d	53	81% 19%
18	e	58	12% 84% 16%
19	h	25	40% 80% 20%
20	3	14	7% 43% 57%
21	i	111	9% 89% 11%
22	m	90	47% 90% 10%
23	o	567	80% 84% 8% 8%
24	q	699	92% 89% 8%
25	k	430	72% 89% 8%
26	l	144	58% 78% 9% 12%
27	j	263	39% 82% 12% 5%
28	1	75	9% 53% 47%
29	A	219	87% 12%
30	B	231	85% 11%
31	E	260	90% 10%
32	G	226	93% 7%
33	H	184	85% 15%

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Mol	Chain	Length	Quality of chain
34	I	200	82% 10% 6%
35	J	182	82% 18%
36	L	155	8% 81% 18%
37	N	150	87% 12%
38	O	127	86% 13%
39	V	87	89% 8%
40	W	129	90% 9%
41	Y	134	91% 9%
42	X	144	5% 84% 15%
43	a	98	91% 9%
44	b	81	89% 11%
45	p	666	36% 92% 6%
46	s	342	95% 96%
47	r	49	98% 100%

2 Entry composition (i)

There are 51 unique types of molecules in this entry. The entry contains 103798 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 18S rRNA (1798-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1798	38175	17061	6721	12595	1798	0	0

- Molecule 2 is a protein called KLLA0F09812p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	217	1629	1041	287	297	4	0	0

- Molecule 3 is a protein called KLLA0D08305p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	223	1744	1108	313	318	5	0	0

- Molecule 4 is a protein called KLLA0D10659p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	206	1609	1008	298	300	3	0	0

- Molecule 5 is a protein called KLLA0B08173p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	K	96	809	533	129	146	1	0	0

- Molecule 6 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	M	117	885	553	161	171	0	0

- Molecule 7 is a protein called KLLA0F07843p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	P	117	927	595	166	161	5	0	0

- Molecule 8 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	Q	141	1105	709	204	192	0	0

- Molecule 9 is a protein called KLLA0B01474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	R	130	1027	640	191	193	3	0	0

- Molecule 10 is a protein called KLLA0B01562p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	S	145	1193	741	240	210	2	0	0

- Molecule 11 is a protein called KLLA0A07194p.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	T	143	1110	693	210	207	0	0

- Molecule 12 is a protein called KLLA0F25542p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	U	106	845	540	152	152	1	0	0

- Molecule 13 is a protein called KLLA0B06182p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	Z	70	558	355	104	98	1	0	0

- Molecule 14 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	c	62	487	301	97	88	1	0	0

- Molecule 15 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	f	69	546	351	101	90	4	0	0

- Molecule 16 is a protein called KLLA0E12277p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	g	318	2466	1561	430	470	5	0	0

- Molecule 17 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	d	53	446	280	89	76	1	0	0

- Molecule 18 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	e	58	463	290	94	78	1	0	0

- Molecule 19 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	h	25	233	142	63	27	1	0	0

- Molecule 20 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
20	3	14	287	129	42	102	14	0	0

- Molecule 21 is a protein called Eukaryotic translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	i	111	884	542	170	167	5	0	0

- Molecule 22 is a protein called Eukaryotic translation initiation factor eIF-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	m	90	716	452	132	128	4	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	20	ALA	THR	conflict	UNP P32911
m	23	ALA	SER	conflict	UNP P32911

- Molecule 23 is a protein called Eukaryotic translation initiation factor 3 subunit A,eIF3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	o	521	3996	2554	685	750	7	0	0

- Molecule 24 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	q	675	5179	3309	874	984	12	0	0

- Molecule 25 is a protein called Eukaryotic translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	k	414	3123	1985	560	562	16	0	0

- Molecule 26 is a protein called Eukaryotic translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	l	126	1016	646	183	180	7	0	0

- Molecule 27 is a protein called Eukaryotic translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	j	249	2006	1283	333	382	8	0	0

- Molecule 28 is a RNA chain called tRNAi (75-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
28	1	75	1607	716	296	520	75	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	31	U	G	conflict	GB 176433
1	39	A	C	conflict	GB 176433

- Molecule 29 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	A	219	1702	1085	299	316	2	0	0

- Molecule 30 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	B	222	1769	1117	324	325	3	0	0

- Molecule 31 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	E	260	2078	1322	393	359	4	0	0

- Molecule 32 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	G	226	1812	1134	348	326	4	0	0

- Molecule 33 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
33	H	184	1483	950	270	263	0	0

- Molecule 34 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	I	188	1489	923	300	265	1	0	0

- Molecule 35 is a protein called KLLA0E23673p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	J	182	1471	929	287	254	1	0	0

- Molecule 36 is a protein called KLLA0A10483p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	L	155	1248	798	237	210	3	0	0

- Molecule 37 is a protein called KLLA0F18040p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	N	150	1187	756	223	206	2	0	0

- Molecule 38 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	O	127	942	578	188	173	3	0	0

- Molecule 39 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	V	87	687	424	126	135	2	0	0

- Molecule 40 is a protein called 40S ribosomal protein S22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	W	129	1021	651	187	180	3	0	0

- Molecule 41 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
41	Y	134	1061	665	207	189	0	0

- Molecule 42 is a protein called RPS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	X	144	1119	708	218	191	2	0	0

- Molecule 43 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	a	98	779	480	165	129	5	0	0

- Molecule 44 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	b	81	609	379	112	113	5	0	0

- Molecule 45 is a protein called Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	p	658	5147	3295	889	945	18	0	0

- Molecule 46 is a protein called Eukaryotic translation initiation factor 3 subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	s	330	2606	1661	429	507	9	0	0

- Molecule 47 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
47	r	49	392	240	76	76	0	0

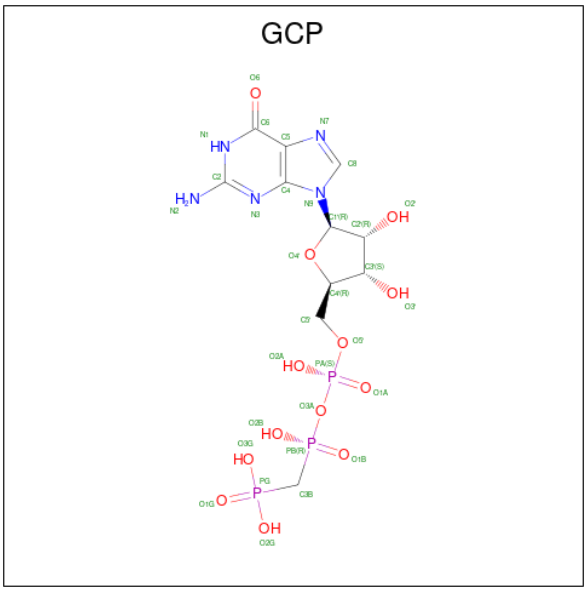
- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
48	2	76	76	76	0
48	C	1	1	1	0
48	h	1	1	1	0
48	k	1	1	1	0
48	B	1	1	1	0
48	a	1	1	1	0

- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

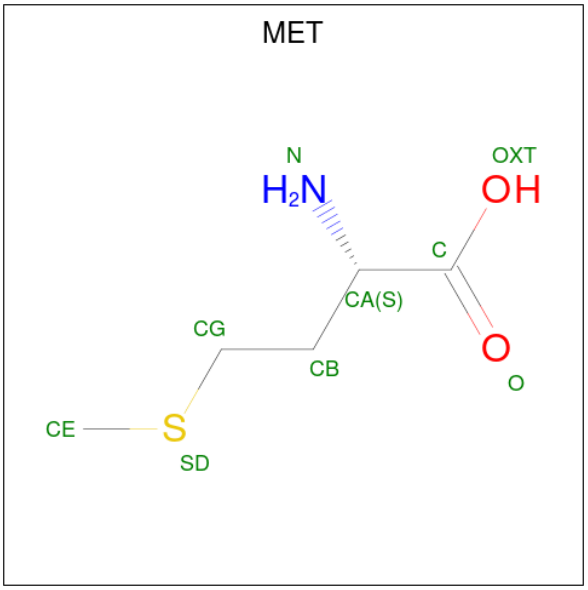
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
49	f	1	1	1	0
49	l	1	1	1	0
49	a	1	1	1	0
49	b	1	1	1	0

- Molecule 50 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
50	k	1	32	11	5	13	3	0

- Molecule 51 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).



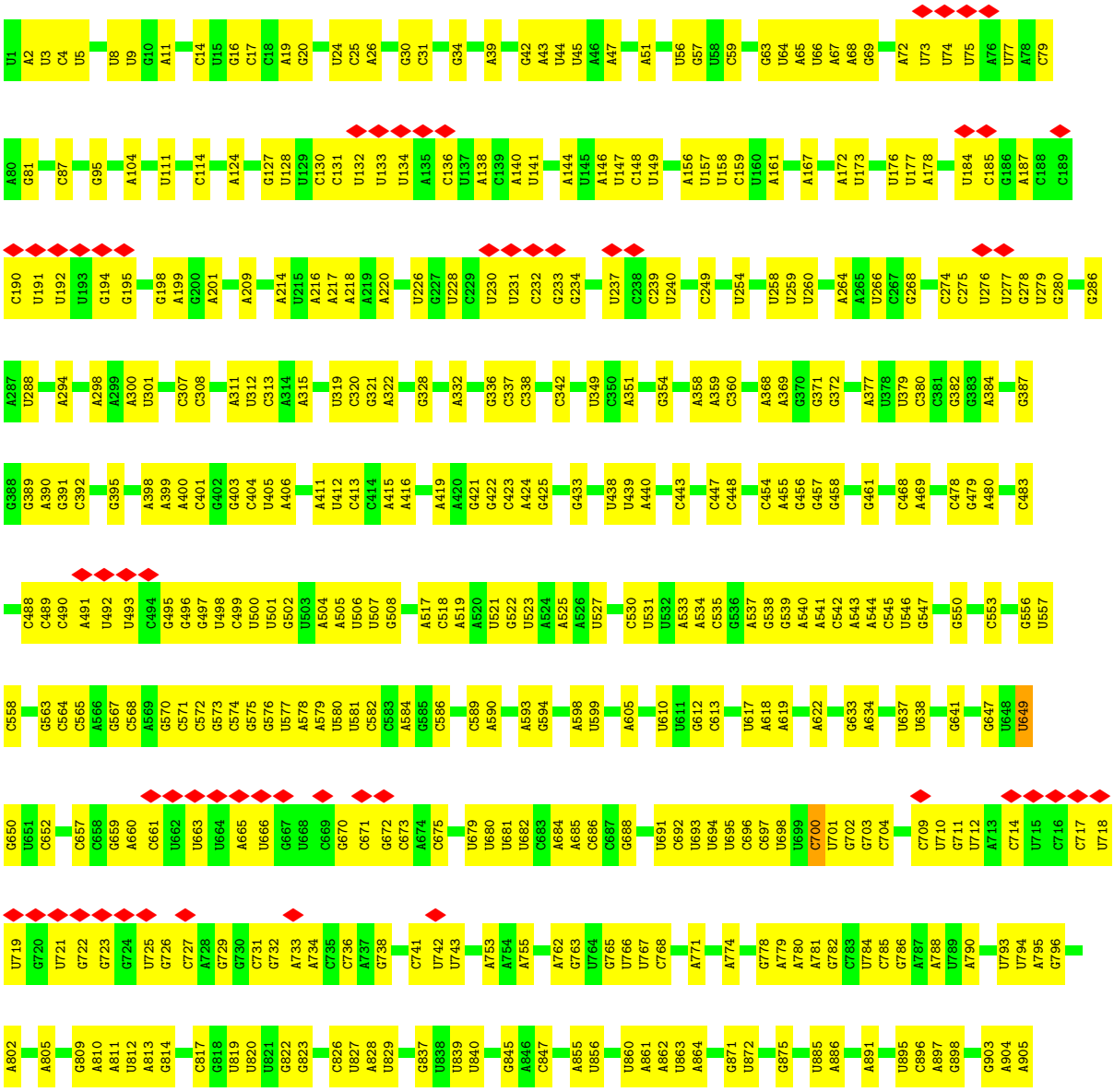
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
51	k	1	8	5	1	1	1	0

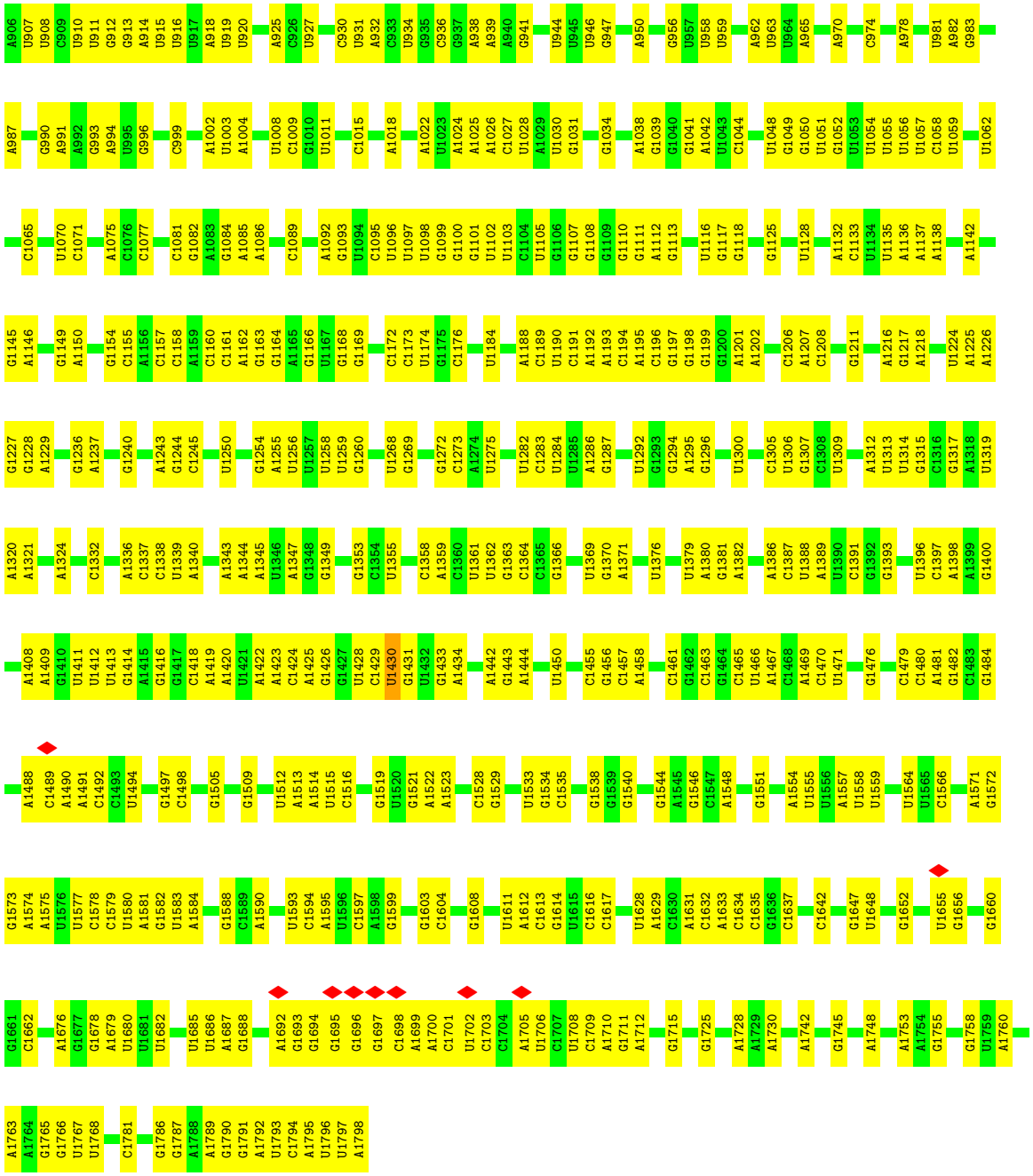
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: 18S rRNA (1798-MER)

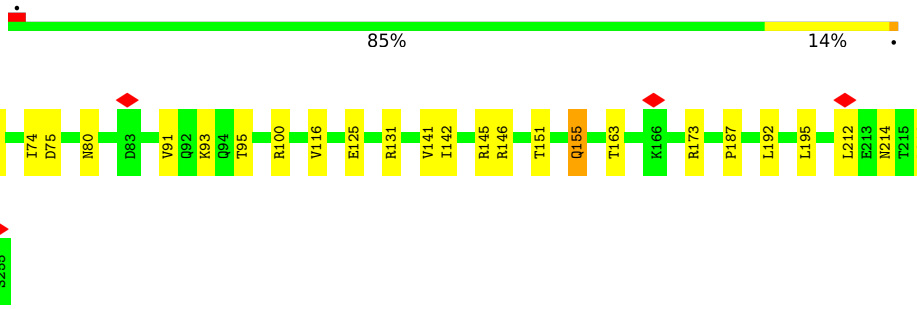
Chain 2:





- Molecule 2: KLLA0F09812p

Chain C:



- Molecule 3: KLLA0D08305p

Chain D: 78% 22%

A3 I4 I5 L11 E20 L21 N22 E28 L29 A30 E31 E47 R51 A52 T53 D57 V58 N62 G63 R64 R65 I66 N67 E68 L69 T70 L71 K75 R76 R81 D93 R94 Q101 M105 L113 R117 V122 K132 R143 A144 A145 R146

L157 P163 D166 F167 R173 T196 S197 G198 P199 K200 V206 K212 E215 P216 V217 L218 E219 P220 S221 V222 K223 D224 Y225

- Molecule 4: KLLA0D10659p

Chain F: 79% 19%

F22 V23 P24 T29 T30 I31 Q37 A38 Q39 I42 K43 L44 F45 S59 L60 I66 S67 V72 A73 K86 I91 G103 R104 K108 V116 Q133 V134 R150 V151 G154 G155 A156 A157 R158 R159 D163 V164 R169 I174 A175 L176 L177

E183 F186 R187 N188 E199 L200 T209 D217 E220 R221 K224 S225 N226 R227

- Molecule 5: KLLA0B08173p

Chain K: 77% 23%

M1 E6 K9 L21 V22 A23 T37 L40 K44 L49 F54 V55 Q58 F59 Y63 Y64 Y65 Y66 T67 L68 T69 E70 E71 G72 V73 V74 Y75 L80 N81 L92 A93 G94 Q95 S96

- Molecule 6: 40S ribosomal protein S12

Chain M: 12% 80% 19%

I17 E18 D19 A20 L21 V24 H31 D32 G33 L34 K43 L55 E61 L67 E74 ASN N76 V82 A83 D84 E90 W91 A92 G93 L94 G95 K96 I97 D98 R99 D100 A103 R104 K105 V106 S110 D120 T121 L128 E129 H130 Q133 Q134

- Molecule 7: KLLA0F07843p

Chain P: 78% 20%

K13 T14 L25 L26 E27 D32 R43 R47 S50 E51 A54 G55 L56 E71 K72 T78 H79 L80 R81 N82 M83 I84 I85 M89 I90 V93 E106 I107 R108 P109 E110 M111 T122 V126 R127 H128 G129

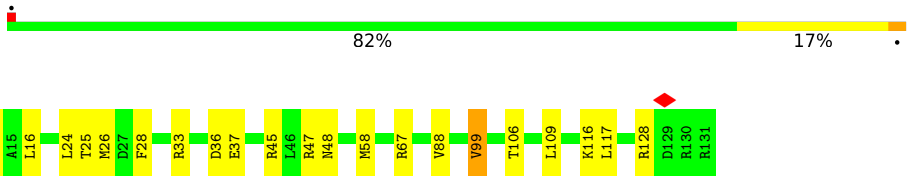
- Molecule 8: 40S ribosomal protein S16

Chain Q: 81% 19%

T3 K14 G27 L28 N32 I36 T37 L38 V39 Q40 R45 F46 K47 L54 R82 Q83 V97 D98 E99 Q100 T115 L116 L117 S121 R122 R123 R132 R137 F138 Q139 R143

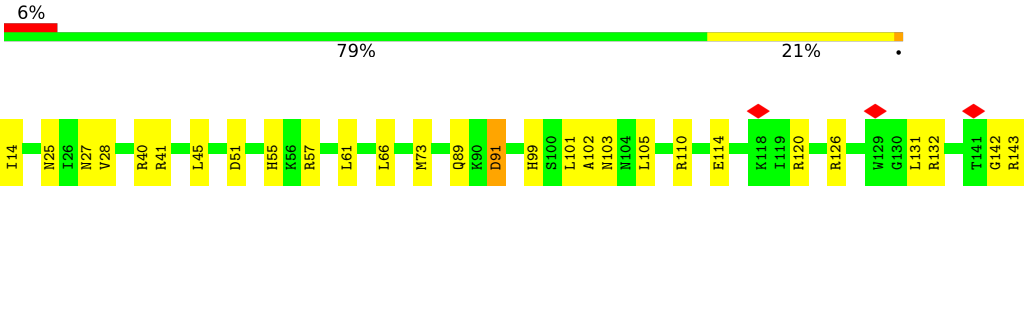
- Molecule 9: KLLA0B01474p

Chain R:



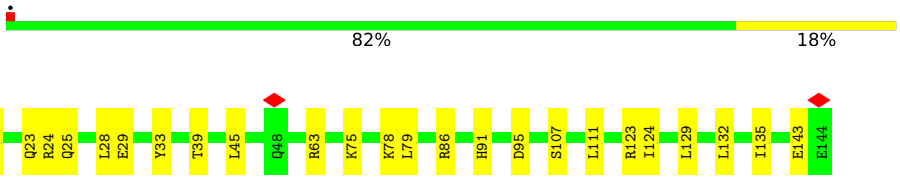
- Molecule 10: KLLA0B01562p

Chain S:



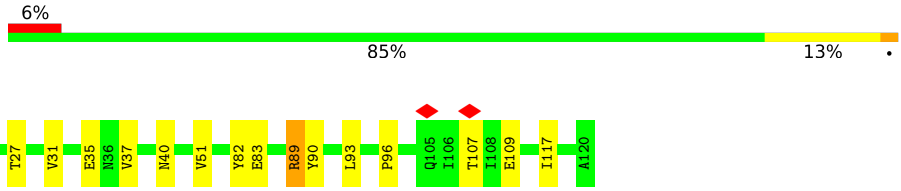
- Molecule 11: KLLA0A07194p

Chain T:



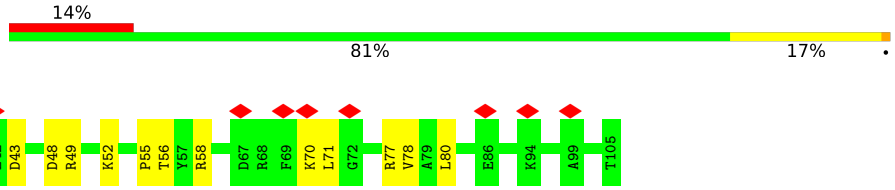
- Molecule 12: KLLA0F25542p

Chain U:



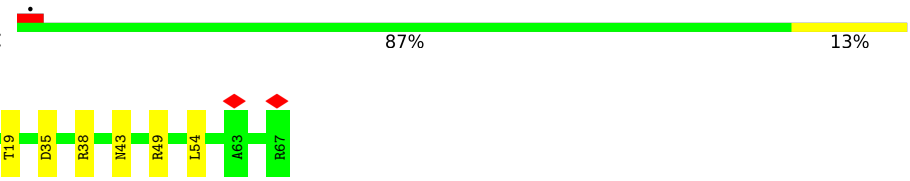
- Molecule 13: KLLA0B06182p

Chain Z:



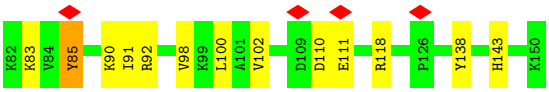
- Molecule 14: 40S ribosomal protein S28

Chain c:



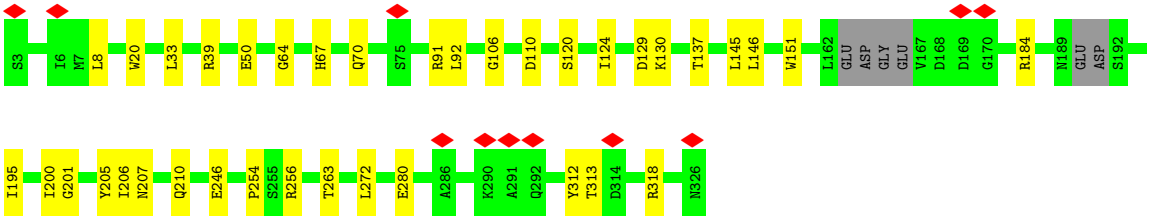
- Molecule 15: Ubiquitin-40S ribosomal protein S27a

Chain f: 6% 81% 17%



• Molecule 16: KLLA0E12277p

Chain g: 87% 11%

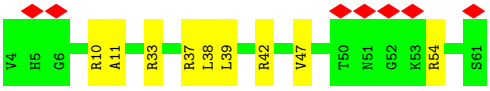


• Molecule 17: 40S ribosomal protein S29

Chain d: 81% 19%

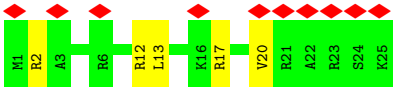
• Molecule 18: 40S ribosomal protein S30

Chain e: 12% 84% 16%



• Molecule 19: 60S ribosomal protein L41-A

Chain h: 40% 80% 20%



• Molecule 20: mRNA

Chain 3: 7% 43% 57%

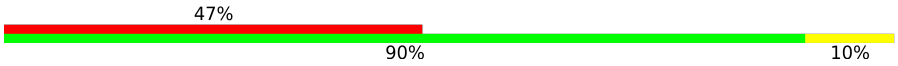
• Molecule 21: Eukaryotic translation initiation factor 1A

Chain i: 9% 89% 11%

N5 T6 G12 R13 N17 D20 R24 E30 E31 G32 Q33 E34 Q37 L42 R57 M58 R62 K68 R82 D86 D87 K94 E111 I115

- Molecule 22: Eukaryotic translation initiation factor eIF-1

Chain m:



E19 A20 A21 T22 A23 N24 Y25 R29 I30 R33 N34 G35 R36 K37 T38 P46 E47 E48 Y49 D50 I54 L55 K60 C64 N65 G66 N67 I68 V69 E73 I77 I78 Q79 L80 Q81 G82 D83 Q84 R85 A86 F91 N92 I93 L96 K100 I103 K104 I105

H106 G107 F108

- Molecule 23: Eukaryotic translation initiation factor 3 subunit A,eIF3a

Chain o:

P5 F6 R7 P8 E9 N10 A11 I12 K13 R14 A15 D16 E17 L18 I19 S20 V21 G22 E23 K24 Q25 A26 A27 L28 Q29 S30 L31 H32 D33 F34 I35 T36 A37 R38 R39 I40 R41 W42 A43 T44 P45 S46 T47 V48 E49 P50 V51 V52 F53 K54 F55 L56 E57 I58 G59 V60 E61 L62 K63 K64

G65 K66 L67 L68 K69 D70 G71 L72 H73 Q74 Y75 K76 K77 L78 I79 Q80 G81 S82 T83 E84 G85 L86 V87 S88 V89 G90 A91 V92 A93 R94 K95 F96 I97 D98 L99 V100 E101 S102 K103 I104 A105 S106 E107 Q108 T109 R110 A111 ASP GLU LEU LEU GLN LYS GLN GLU ILE ASP ASP ASP LEU GLU

GLY GLY VAL THR PRO GLU ASN LEU LEU ILE SER VAL TYR GLU SER ASP GLN SER VAL ALA GLY PHE ASN ASP GLU ALA I151 T152 S153 W154 L155 R156 F157 T158 W159 E160 S161 Y162 R163 A164 V165 L166 D167 L168 L169 R170 N171 N172 A173 L174 L175 E176 I177 T178 Y179 S180 G181 V182 V183 K184

K185 T186 M187 H188 F189 C190 L191 K192 Y193 Q194 R195 K196 N197 E198 F199 K200 R201 L202 A203 E204 M205 L206 R207 Q208 H209 L210 D211 A212 A213 N214 TYR GLN GLN SER LYS SER GLY N222 N223 L224 V225 D226 L227 S228 D229 A230 D231 T232 L233 Q234 R235 Y236 L237 D238 Q239 R240 F241 Q242 Q243 V244

D245 V246 S247 V248 K249 L250 E251 L252 W253 H254 E255 A256 Y257 R258 S259 I260 E261 D262 V263 F264 H265 L266 M267 K268 I269 S270 K271 R272 A273 P274 K275 P276 S277 T278 L279 A280 N281 Y282 Y283 E284 N285 L286 V287 K288 V289 F290 F291 V292 S293 G294 D295 P296 L297 L298 H299 T300 T301 A302 W303 K304

K305 F306 Y307 K308 L309 Y310 S311 T312 N313 P314 R315 A316 T317 E318 E319 E320 F321 K322 T323 Y324 S325 S326 T327 I328 F329 L330 S331 A332 I333 S334 T335 Q336 L337 D338 E339 I340 P341 S342 I343 G344 Y345 D346 P347 H348 L349 R350 M351 Y352 R353 L354 L355 N356 L357 D358 A359 K360 P361 T362 R363 K364

E365 M366 L367 Q368 S369 I370 I371 E372 D373 E374 S375 I376 Y377 G378 K379 V380 D381 E382 E383 L384 K385 E386 L387 Y388 D389 I390 I391 E392 V393 N394 F395 D396 V397 D398 T399 V400 K401 Q402 Q403 L404 E405 N406 L407 L408 V409 K410 L411 S412 S413 K414 T415 Y416 F417 S418 Q419 Y420 I421 A422 P423 L424

R425 D426 V427 I428 M429 R430 R431 V432 F433 V434 A435 A436 S437 Q438 K439 F440 T441 T442 V443 S444 Q445 S446 E447 L448 Y449 K450 L451 A452 T453 L454 P455 A456 P457 L458 D459 L460 S461 A462 W463 D464 I465 E466 K467 S468 L469 L470 Q471 A472 A473 V474 E475 D476 Y477 V478 S479 I480 T481 I482 D483 H484

E485 S486 A487 K488 V489 T490 F491 A492 X693 X694 X695 X696 X697 X701 X702 X703 X704 X726 X727 X733 X740 X771

• Molecule 24: Eukaryotic translation initiation factor 3 subunit C

Chain q: 92% 89% 8%

Y96 D97 S98 S99 D100 E101 E102 S103 D104 E105 E106 D107 G108 K109 K110 V111 V112 K113 S114 A115 K116 E117 K118 L119 L120 D121 E122 M123 Q124 D125 V126 Y127 N128 S131 Q132 A133 E134 N135 S136 D137 ASP W139 L140 T141 I142 S143 N144 E145 F146 D147 L148 I149 S150 R151 L152 L153 V154 R155 A156

Q157 Q158 Q159 N160 W161 G162 T163 P164 N165 I166 F167 I168 K169 V170 V171 A172 Q173 V174 E175 D176 A177 V178 N179 N180 T181 Q182 L186 LYS ASN K189 A190 V191 Y195 T198 K199 Q200 R201 V202 K203 K204 V205 S206 R207 E208 N209 E210 D211 S212 M213 A214 K215 F216 R217 N218 D219 P220 E221

S222 F223 D224 K225 E226 P227 T228 A229 ASP LEU ASP ILE SER ALA ASN GLY PHE THR ILE SER SER SER GLN GLY ASN ASP GLN ALA VAL Q251 E252 D253 F254 F255 T256 R257 L258 Q259 T260 I261 I262 D263 S264 R265 G266 K267 K268 T269 V270 N271 Q272 Q273 S274 L275 I276 S277 T278 L279 E280 E281

L282 L283 T284 V285 A286 E287 K288 P289 Y290 E291 F292 I293 M294 A295 Y296 L297 T298 L299 I300 P301 S302 R303 F304 D305 A306 S307 A308 N309 L310 S311 Y312 Q313 P314 I315 D316 Q317 W318 K319 S320 S321 F322 N323 D324 I325 S326 K327 L328 L329 S330 I331 L332 D333 Q334 T335 I336 D337 T338 Y339 Q340 V341

N342 E343 F344 A345 D346 P347 I348 D349 F350 I351 E352 D353 E354 P355 K356 E357 D358 S359 D360 G361 V362 K363 R364 I365 L366 G367 S368 I369 F370 S371 F372 V373 E374 R375 L376 D377 D378 E379 F380 M381 K382 S383 L384 L385 N386 I387 D388 P389 H390 S391 S392 D393 Y394 L395 I396 R397 L398 R399 D400 E401

Q402 S403 I404 Y405 N406 L407 I408 L409 R410 T411 Q412 L413 Y414 F415 E416 A417 T418 L419 K420 D421 E422 H423 D424 L425 E426 R427 A428 L429 T430 R431 P432 F433 V434 K435 R436 L437 D438 H439 I440 Y441 Y442 K443 S444 E445 N446 L447 I448 K449 I450 M451 E452 T453 A454 A455 W456 N457 I458 I459 P460 A461

Q462 F463 K464 S465 K466 F467 T468 S469 K470 D471 Q472 L473 D474 S475 A476 D477 Y478 V479 D480 M481 L482 I483 D484 G485 L486 S487 T488 I489 L490 S491 K492 Q493 N494 M495 I496 A497 V498 Q499 K500 R501 A502 I503 L504 Y505 N506 I507 Y508 Y509 T510 A511 L512 N513 K514 D515 F516 Q517 T518 A519 K520 D521

M522 L523 L524 T525 S526 Q527 V528 Q529 T530 N531 I532 N533 Q534 F535 D536 S537 S538 L539 Q540 I541 L542 F543 N544 R545 V546 V547 V548 Q549 L550 G551 L552 S553 A554 F555 K556 L557 C558 L559 I560 E561 E562 C563 H564 Q565 I566 L567 N568 D569 L570 L571 S572 S573 S574 H575 L576 R577 E578 I579 L580 G581

Q582 Q583 S584 L585 H586 R587 I588 S589 L590 N591 S592 S593 N594 N595 A596 S597 A598 D599 E600 R601 A602 R603 Q604 C605 L606 P607 Y608 H609 Q610 H611 I612 N613 L614 D615 L616 I617 D618 V619 V620 F621 L622 T623 C624 S625 L626 L627 I628 E629 I630 P631 R632 M633 T634 A635 F636 Y637 S638 G639 I640 K641

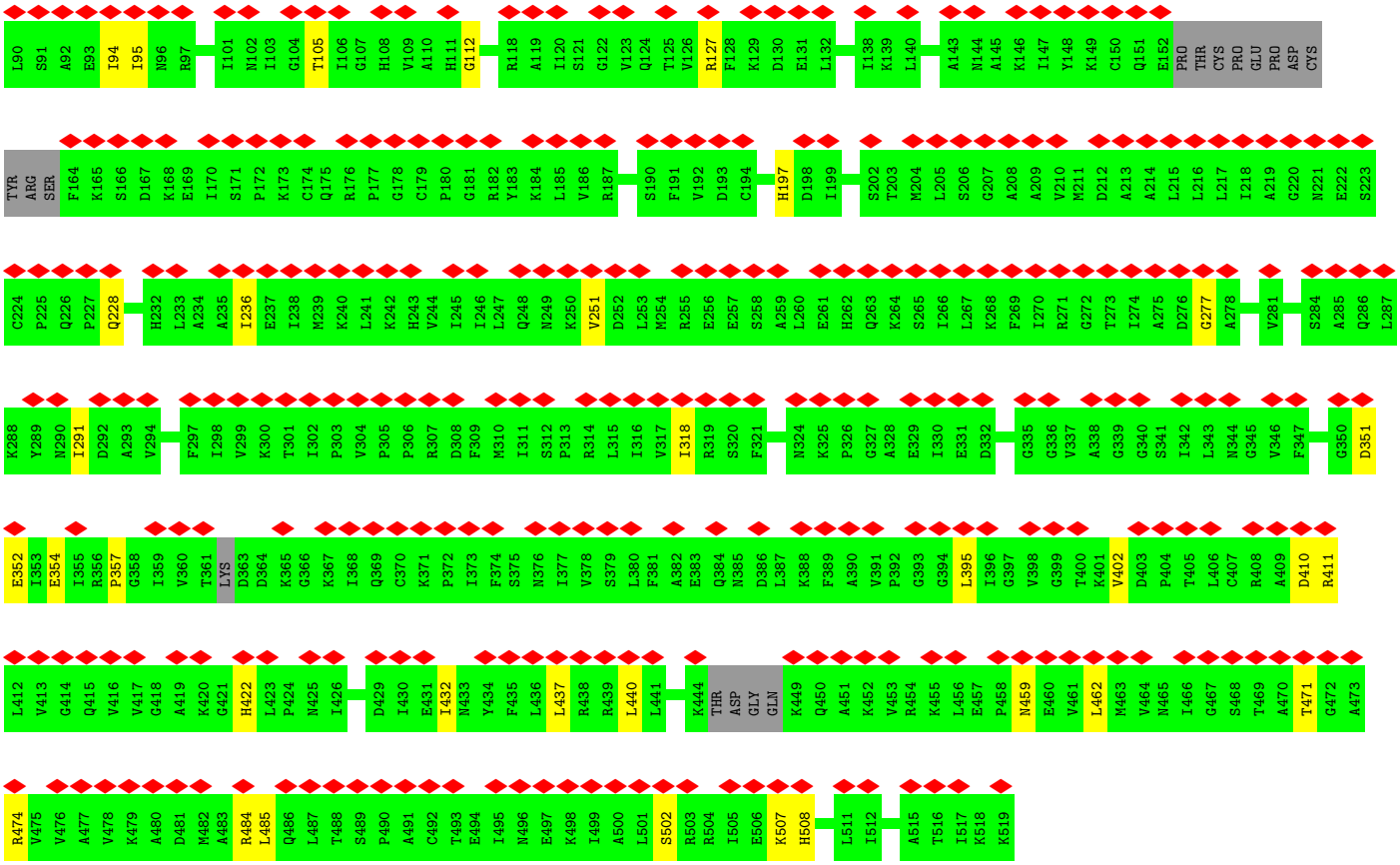
V642 K643 R644 I645 P646 Y647 S648 P649 K650 S651 I652 R653 R654 S655 L656 E657 H658 Y659 D660 K661 L662 S663 F664 Q665 G666 P667 P668 E669 T670 L671 R672 D673 Y674 V675 L676 F677 A678 A679 K680 S681 M682 Q683 K684 G685 N686 W687 R688 D689 S690 V691 R692 Y693 L694 R695 E696 I697 K698 S699 W700 A701

L702 L703 P704 N705 M706 E707 T708 V709 L710 N711 S712 L713 T714 E715 R716 V717 Q718 V719 E720 S721 L722 K723 T724 Y725 F726 F727 S728 F729 K730 R731 F732 Y733 S734 S735 F736 S737 V738 A739 K740 L741 A742 E743 L744 F745 D746 L747 P748 E749 N750 K751 R752 V753 E754 V755 L756 Q757 S758 V759 I760 A761

E762 L763 E764 I765 P766 A767 K768 L769 N770 D771 E772 K773 T774 I775 F776 V777 V778 E779 K780 G781 D782 E783 I784 T785 K786 L787 E788 E789 A790 M791 V792 K793 L794

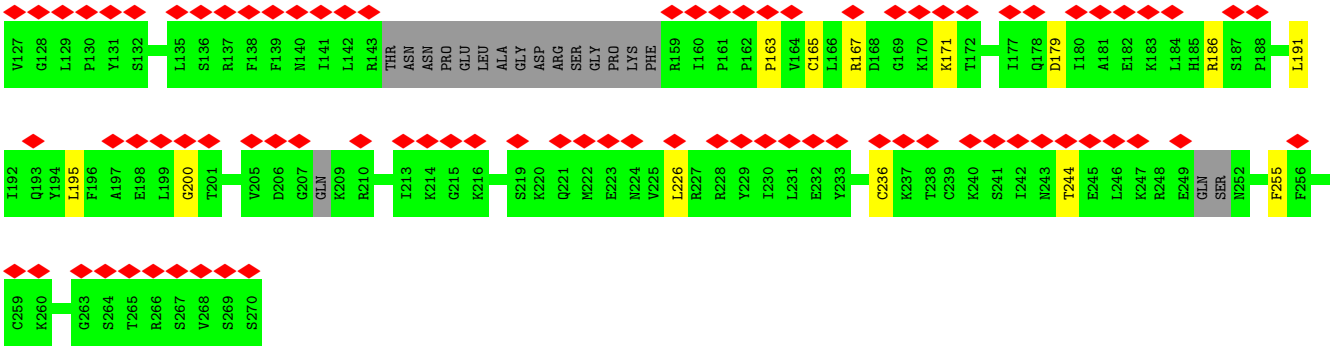
• Molecule 25: Eukaryotic translation initiation factor 2 subunit gamma

Chain k:



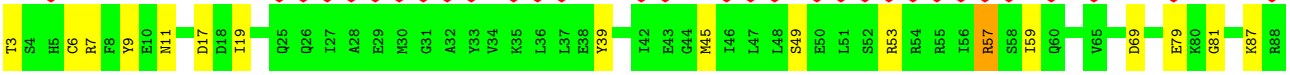
• Molecule 26: Eukaryotic translation initiation factor 2 subunit beta

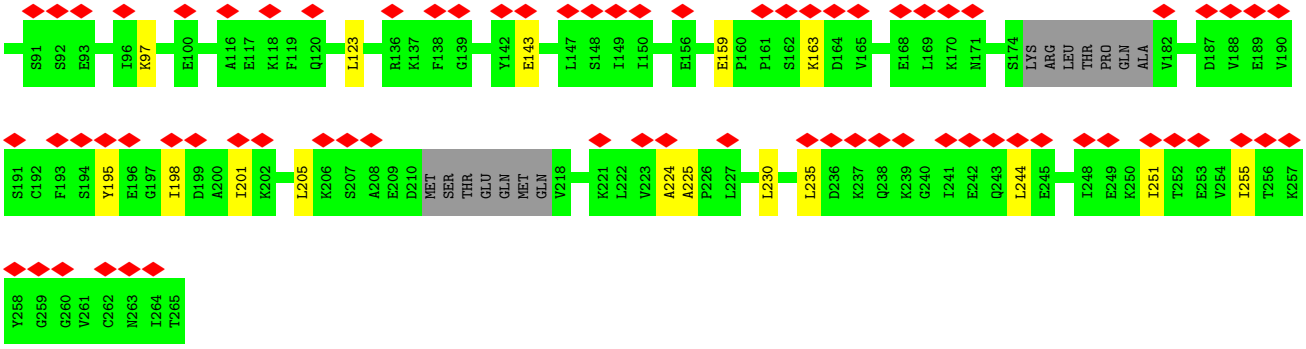
Chain l:



• Molecule 27: Eukaryotic translation initiation factor 2 subunit alpha

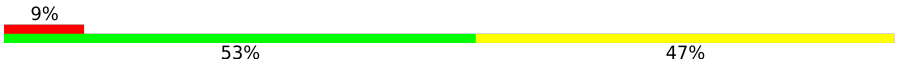
Chain j:

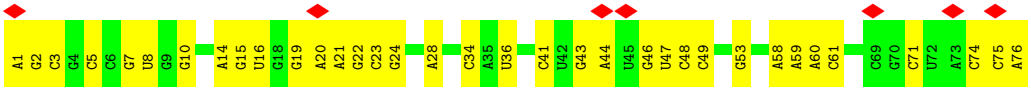




- Molecule 28: tRNAi (75-MER)

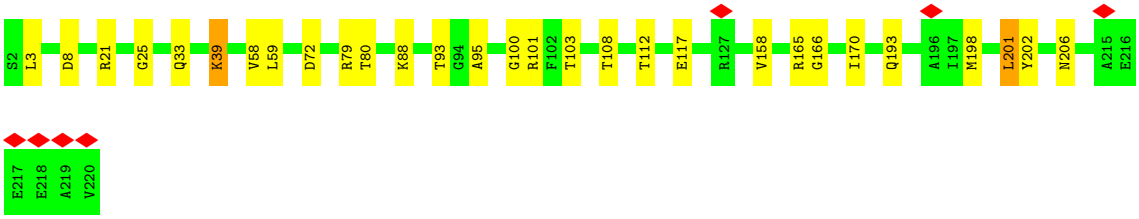
Chain 1:





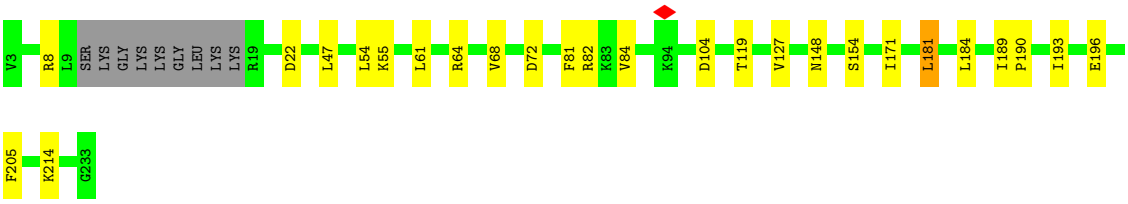
- Molecule 29: 40S ribosomal protein S0

Chain A:



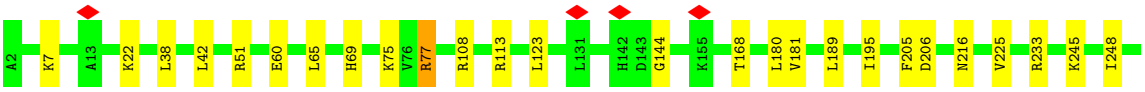
- Molecule 30: 40S ribosomal protein S1

Chain B:



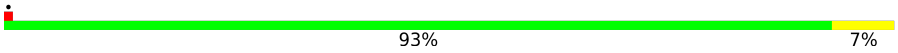
- Molecule 31: 40S ribosomal protein S4

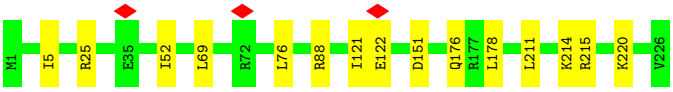
Chain E:



• Molecule 32: 40S ribosomal protein S6

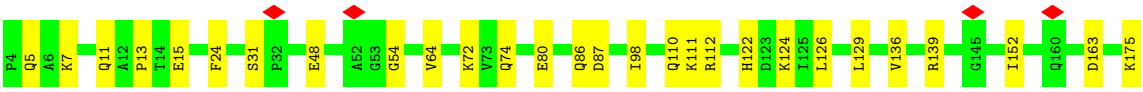
Chain G:





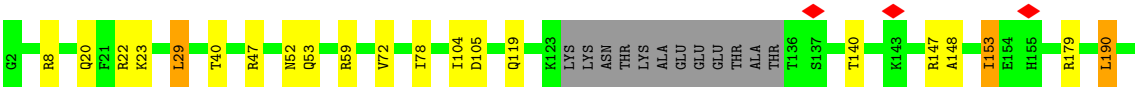
• Molecule 33: 40S ribosomal protein S7

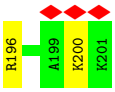
Chain H:



• Molecule 34: 40S ribosomal protein S8

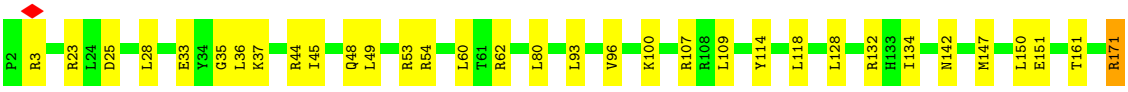
Chain I:

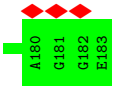




• Molecule 35: KLLA0E23673p

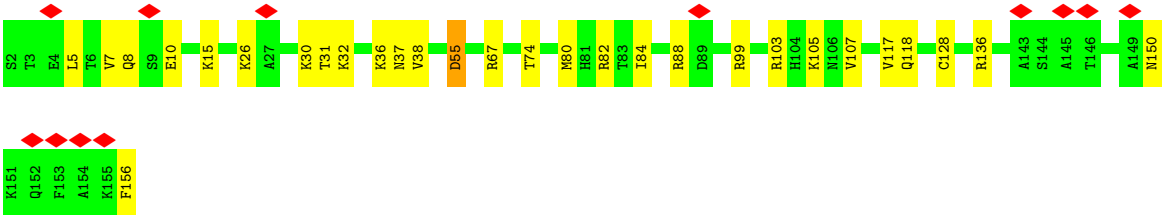
Chain J:





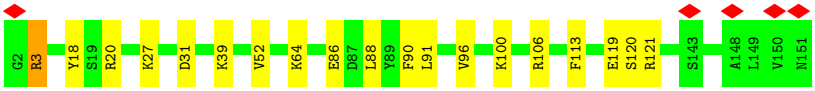
• Molecule 36: KLLA0A10483p

Chain L:



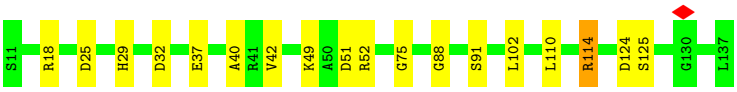
• Molecule 37: KLLA0F18040p

Chain N:



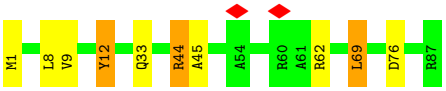
• Molecule 38: 40S ribosomal protein S14

Chain O:



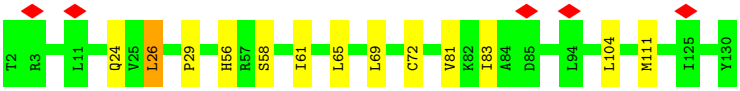
• Molecule 39: 40S ribosomal protein S21

Chain V:



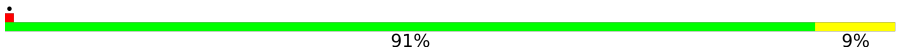
• Molecule 40: 40S ribosomal protein S22

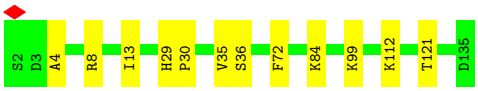
Chain W:



• Molecule 41: 40S ribosomal protein S24

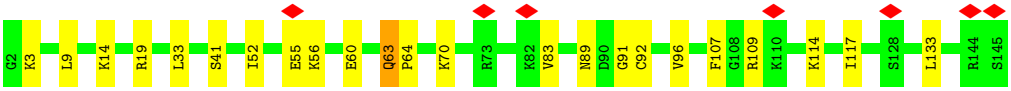
Chain Y:





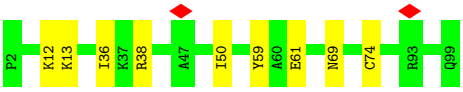
• Molecule 42: RPS23

Chain X:



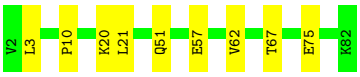
• Molecule 43: 40S ribosomal protein S26

Chain a:



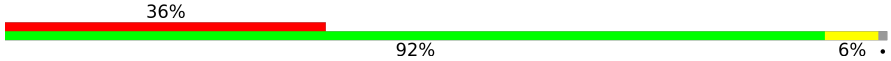
• Molecule 44: 40S ribosomal protein S27

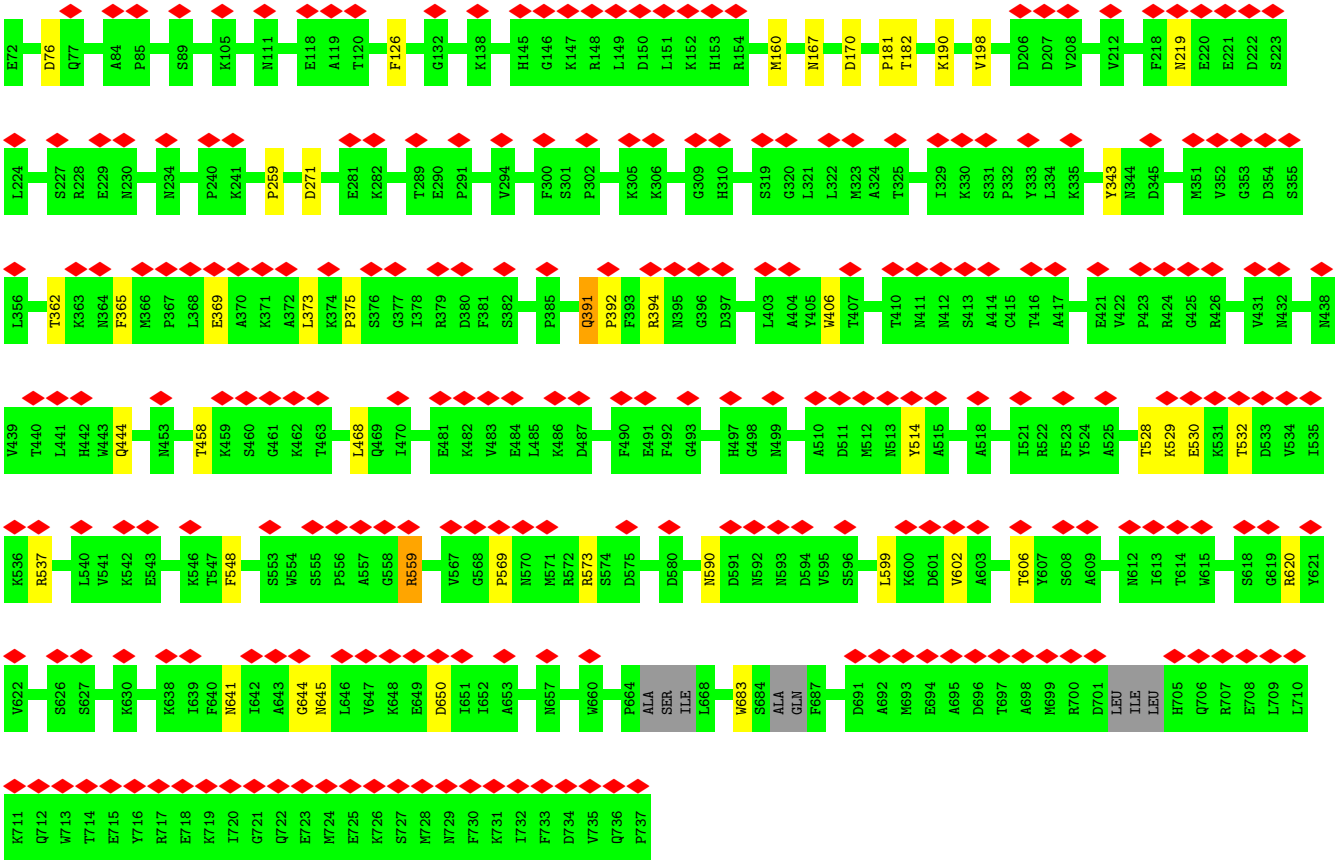
Chain b:



• Molecule 45: Eukaryotic translation initiation factor 3 subunit B

Chain p:





• Molecule 46: Eukaryotic translation initiation factor 3 subunit I

Chain s: 95% 96%

M1 K2 A3 I4 K5 L6 T7 G8 H9 E10 R11 P12 L13 T14 Q15 V16 K17 Y18 N19 K20 E21 G22 D23 L24 L25 F26 S27 C28 S29 K30 D31 S32 S33 A34 S35 V36 W37 Y38 S39 L40 N41 G42 E43 R44 L45 G46 T47 L48 D49 G50 H51 T52 G53 T54 I55 W56 S57 I58 D59 V60

D61 C62 F63 T64 K65 Y66 C67 V68 T69 G70 S71 A72 D73 Y74 S75 I76 K77 L78 W79 D80 V81 S82 N83 G84 Q85 C86 V87 A88 T89 W90 K91 S92 P93 V94 P95 V96 K97 R98 V99 E100 F101 S102 P103 C104 G105 N106 Y107 F108 L109 A110 I111 L112 D113 N114 V115 M116 K117 N118 P119 G120

S121 I122 N123 I124 Y125 E126 I127 E128 R129 D130 S131 A132 T133 H134 E135 L136 T137 K138 V139 S140 E141 E142 P143 I144 H145 K146 I147 I148 T149 H150 E151 G152 L153 D154 A155 A156 T157 V158 A159 G160 W161 S162 T163 K164 G165 K166 Y167 I168 I169 A170 G171 H172 K173 D174 G175 K176 I177 S178 K179 Y180

D181 V182 S183 N184 N185 Y186 E187 Y188 V189 D190 S191 I192 D193 L194 H195 E196 K197 S198 I199 S200 D201 M202 Q203 F204 S205 P206 D207 L208 T209 Y210 F211 I212 T213 S214 S215 R216 D217 T218 N219 S220 F221 L222 V223 D224 V225 S226 T227 L228 Q229 V230 L231 K232 K233 Y234 E235 T236 D237 C238 P239 L240

N241 T242 A243 V244 I245 T246 P247 L248 K249 E250 F251 I252 I253 L254 G255 G256 G257 Q258 GLU ALA LYS ASP VAL THR THR THR SER ALA ASN GLU G271 K272 F273 E274 A275 R276 F277 Y278 H279 K280 I281 F282 E283 E284 E285 I286 G287 R288 V289 Q290 G291 H292 F293 G294 P295 L296 N297 T298 V299 A300

I301 S302 P303 Q304 G305 T306 S307 Y308 A309 S310 G311 G312 E313 D314 G315 F316 I317 R318 L319 H320 H321 F322 E323 K324 S325 Y326 F327 D328 F329 K330 Y331 D332 V333 E334 K335 A336 A337 E338 A339 K340 E341 H342

- Molecule 47: Eukaryotic translation initiation factor 3 subunit G

Chain r: 98% 100%

S48 V49 A50 E51 R52 K53 N54 W55 H56 K57 Y58 G59 S60 E61 K62 G63 S64 P65 A66 G67 P68 S69 A70 V71 T72 A73 R74 L75 G76 E77 E78 V79 E80 L81 R82 L83 S84 R85 N86 W87 K88 Q89 A90 E91 E92 E93 R94 I95 Q96

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12586	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	32	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.275	Depositor
Minimum map value	-0.119	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	402.0, 402.0, 402.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	2	0.23	0/42691	0.65	3/66521 (0.0%)
2	C	0.40	0/1659	0.68	0/2252
3	D	0.41	0/1769	0.71	0/2378
4	F	0.40	0/1628	0.74	1/2198 (0.0%)
5	K	0.45	0/831	0.70	0/1123
6	M	0.44	0/891	0.75	0/1201
7	P	0.43	0/946	0.72	1/1273 (0.1%)
8	Q	0.43	0/1125	0.72	0/1510
9	R	0.42	0/1038	0.80	1/1395 (0.1%)
10	S	0.41	0/1212	0.76	0/1629
11	T	0.39	0/1129	0.71	0/1520
12	U	0.39	0/857	0.68	0/1158
13	Z	0.41	0/567	0.67	0/762
14	c	0.39	0/489	0.71	0/655
15	f	0.48	0/559	0.69	0/747
16	g	0.41	0/2521	0.59	0/3431
17	d	0.42	0/457	0.62	0/607
18	e	0.40	0/471	0.65	0/628
19	h	0.36	0/234	0.64	0/300
20	3	0.26	0/317	0.68	0/489
21	i	0.36	0/894	0.61	0/1188
22	m	0.41	0/723	0.59	0/965
23	o	0.50	0/3671	0.61	0/4961
24	q	0.50	0/5270	0.62	0/7154
25	k	0.44	0/3167	0.63	1/4278 (0.0%)
26	l	0.47	0/1030	0.61	0/1375
27	j	0.44	0/2034	0.63	1/2737 (0.0%)
28	1	0.34	1/1796 (0.1%)	0.64	0/2795
29	A	0.41	0/1742	0.70	1/2383 (0.0%)
30	B	0.40	0/1793	0.69	2/2414 (0.1%)
31	E	0.39	0/2122	0.65	1/2861 (0.0%)
32	G	0.39	0/1835	0.69	1/2451 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	H	0.41	0/1507	0.69	0/2028
34	I	0.40	0/1515	0.70	2/2029 (0.1%)
35	J	0.40	0/1495	0.77	1/2001 (0.0%)
36	L	0.42	0/1276	0.65	0/1718
37	N	0.40	0/1210	0.74	0/1628
38	O	0.40	0/953	0.66	0/1279
39	V	0.37	0/696	0.66	1/938 (0.1%)
40	W	0.38	0/1039	0.70	2/1399 (0.1%)
41	Y	0.39	0/1075	0.67	0/1433
42	X	0.41	0/1137	0.70	1/1516 (0.1%)
43	a	0.37	0/791	0.65	0/1059
44	b	0.39	0/619	0.63	0/837
45	p	0.45	0/5282	0.57	0/7178
46	s	0.35	0/2669	0.53	0/3611
47	r	0.29	0/399	0.45	0/535
All	All	0.36	1/109131 (0.0%)	0.65	20/156528 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
41	Y	0	1
42	X	0	1
45	p	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	1	1	A	OP3-P	-10.05	1.49	1.61

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	I	190	LEU	CA-CB-CG	7.41	132.35	115.30
7	P	56	LEU	CA-CB-CG	6.99	131.37	115.30
9	R	109	LEU	CA-CB-CG	6.17	129.50	115.30
40	W	26	LEU	CA-CB-CG	6.08	129.29	115.30
1	2	1430	U	C2'-C3'-O3'	6.07	123.41	113.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
42	X	63	GLN	Peptide
41	Y	29	HIS	Peptide
45	p	391	GLN	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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 PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	C	215/217 (99%)	194 (90%)	14 (6%)	7 (3%)	4 26
3	D	221/223 (99%)	196 (89%)	14 (6%)	11 (5%)	2 20
4	F	204/206 (99%)	171 (84%)	22 (11%)	11 (5%)	2 18
5	K	94/96 (98%)	84 (89%)	7 (7%)	3 (3%)	4 26
6	M	113/118 (96%)	86 (76%)	17 (15%)	10 (9%)	1 10
7	P	115/117 (98%)	94 (82%)	15 (13%)	6 (5%)	2 19
8	Q	139/141 (99%)	118 (85%)	11 (8%)	10 (7%)	1 13
9	R	128/130 (98%)	107 (84%)	15 (12%)	6 (5%)	2 21
10	S	143/145 (99%)	118 (82%)	17 (12%)	8 (6%)	2 18
11	T	141/143 (99%)	132 (94%)	7 (5%)	2 (1%)	11 46
12	U	104/106 (98%)	91 (88%)	8 (8%)	5 (5%)	2 20
13	Z	68/70 (97%)	56 (82%)	9 (13%)	3 (4%)	2 22
14	c	60/62 (97%)	53 (88%)	6 (10%)	1 (2%)	9 42
15	f	67/69 (97%)	51 (76%)	7 (10%)	9 (13%)	0 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	g	312/324 (96%)	271 (87%)	33 (11%)	8 (3%)	5	31
17	d	51/53 (96%)	39 (76%)	11 (22%)	1 (2%)	7	37
18	e	56/58 (97%)	45 (80%)	9 (16%)	2 (4%)	3	25
19	h	23/25 (92%)	23 (100%)	0	0	100	100
21	i	109/111 (98%)	90 (83%)	18 (16%)	1 (1%)	17	56
22	m	86/90 (96%)	76 (88%)	7 (8%)	3 (4%)	3	25
23	o	435/567 (77%)	366 (84%)	62 (14%)	7 (2%)	9	43
24	q	667/699 (95%)	577 (86%)	70 (10%)	20 (3%)	4	28
25	k	404/430 (94%)	337 (83%)	60 (15%)	7 (2%)	9	42
26	l	118/144 (82%)	97 (82%)	20 (17%)	1 (1%)	19	60
27	j	243/263 (92%)	210 (86%)	27 (11%)	6 (2%)	5	32
29	A	217/219 (99%)	183 (84%)	24 (11%)	10 (5%)	2	21
30	B	218/231 (94%)	187 (86%)	23 (11%)	8 (4%)	3	24
31	E	258/260 (99%)	240 (93%)	13 (5%)	5 (2%)	8	38
32	G	224/226 (99%)	205 (92%)	18 (8%)	1 (0%)	34	72
33	H	182/184 (99%)	157 (86%)	15 (8%)	10 (6%)	2	18
34	I	184/200 (92%)	166 (90%)	11 (6%)	7 (4%)	3	24
35	J	180/182 (99%)	150 (83%)	25 (14%)	5 (3%)	5	30
36	L	153/155 (99%)	132 (86%)	17 (11%)	4 (3%)	5	31
37	N	148/150 (99%)	135 (91%)	12 (8%)	1 (1%)	22	62
38	O	125/127 (98%)	102 (82%)	12 (10%)	11 (9%)	1	10
39	V	85/87 (98%)	75 (88%)	7 (8%)	3 (4%)	3	25
40	W	127/129 (98%)	113 (89%)	9 (7%)	5 (4%)	3	23
41	Y	132/134 (98%)	116 (88%)	13 (10%)	3 (2%)	6	34
42	X	142/144 (99%)	119 (84%)	14 (10%)	9 (6%)	1	16
43	a	96/98 (98%)	82 (85%)	10 (10%)	4 (4%)	3	22
44	b	79/81 (98%)	70 (89%)	3 (4%)	6 (8%)	1	13
45	p	650/666 (98%)	538 (83%)	93 (14%)	19 (3%)	4	29
46	s	326/342 (95%)	318 (98%)	8 (2%)	0	100	100
47	r	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
All	All	7889/8271 (95%)	6814 (86%)	816 (10%)	259 (3%)	6	26

5 of 259 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	141	VAL
2	C	187	PRO
3	D	220	PRO
4	F	67	SER
6	M	82	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	176/176 (100%)	148 (84%)	28 (16%)	2	13
3	D	185/185 (100%)	148 (80%)	37 (20%)	1	8
4	F	174/174 (100%)	140 (80%)	34 (20%)	1	8
5	K	88/88 (100%)	69 (78%)	19 (22%)	1	6
6	M	93/94 (99%)	79 (85%)	14 (15%)	3	15
7	P	100/100 (100%)	78 (78%)	22 (22%)	1	6
8	Q	117/117 (100%)	100 (86%)	17 (14%)	3	16
9	R	115/118 (98%)	96 (84%)	19 (16%)	2	12
10	S	128/128 (100%)	104 (81%)	24 (19%)	1	9
11	T	117/117 (100%)	93 (80%)	24 (20%)	1	7
12	U	96/96 (100%)	83 (86%)	13 (14%)	4	17
13	Z	60/60 (100%)	49 (82%)	11 (18%)	1	10
14	c	54/54 (100%)	47 (87%)	7 (13%)	4	18
15	f	57/60 (95%)	52 (91%)	5 (9%)	10	31
16	g	265/270 (98%)	236 (89%)	29 (11%)	6	23
17	d	46/46 (100%)	37 (80%)	9 (20%)	1	8
18	e	51/51 (100%)	44 (86%)	7 (14%)	3	17
19	h	23/23 (100%)	18 (78%)	5 (22%)	1	6
21	i	93/93 (100%)	82 (88%)	11 (12%)	5	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	m	77/78 (99%)	71 (92%)	6 (8%)	12	36
23	o	398/438 (91%)	360 (90%)	38 (10%)	8	27
24	q	527/644 (82%)	493 (94%)	34 (6%)	17	42
25	k	332/364 (91%)	307 (92%)	25 (8%)	13	37
26	l	117/132 (89%)	105 (90%)	12 (10%)	7	25
27	j	224/237 (94%)	197 (88%)	27 (12%)	5	20
29	A	180/185 (97%)	160 (89%)	20 (11%)	6	22
30	B	198/210 (94%)	181 (91%)	17 (9%)	10	32
31	E	223/223 (100%)	201 (90%)	22 (10%)	8	26
32	G	192/192 (100%)	179 (93%)	13 (7%)	16	40
33	H	164/164 (100%)	146 (89%)	18 (11%)	6	22
34	I	147/158 (93%)	130 (88%)	17 (12%)	5	21
35	J	153/153 (100%)	125 (82%)	28 (18%)	1	10
36	L	136/136 (100%)	110 (81%)	26 (19%)	1	8
37	N	127/127 (100%)	108 (85%)	19 (15%)	3	15
38	O	96/96 (100%)	88 (92%)	8 (8%)	11	34
39	V	73/73 (100%)	64 (88%)	9 (12%)	4	19
40	W	110/110 (100%)	103 (94%)	7 (6%)	17	42
41	Y	108/108 (100%)	100 (93%)	8 (7%)	13	38
42	X	119/119 (100%)	106 (89%)	13 (11%)	6	23
43	a	83/83 (100%)	78 (94%)	5 (6%)	19	44
44	b	71/71 (100%)	68 (96%)	3 (4%)	30	54
45	p	537/597 (90%)	510 (95%)	27 (5%)	24	49
46	s	287/297 (97%)	286 (100%)	1 (0%)	92	94
47	r	40/40 (100%)	40 (100%)	0	100	100
All	All	6757/7085 (95%)	6019 (89%)	738 (11%)	10	23

5 of 738 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	j	87	LYS
34	I	72	VAL
27	j	255	ILE

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Mol	Chain	Res	Type
27	j	79	GLU
31	E	69	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
32	G	185	GLN
39	V	3	ASN
34	I	84	HIS
37	N	49	GLN
42	X	22	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1797/1798 (99%)	828 (46%)	69 (3%)
20	3	13/14 (92%)	8 (61%)	2 (15%)
28	1	73/75 (97%)	32 (43%)	6 (8%)
All	All	1883/1887 (99%)	868 (46%)	77 (4%)

5 of 868 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	3	U
1	2	4	C
1	2	5	U
1	2	8	U

5 of 77 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1411	U
28	1	7	G
1	2	1455	C
1	2	1613	C
28	1	59	A

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 87 ligands modelled in this entry, 85 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
51	MET	k	603	-	6,7,8	0.46	0	2,7,9	0.14	0
50	GCP	k	602	-	27,34,34	2.16	9 (33%)	34,54,54	1.95	8 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	MET	k	603	-	-	3/5/6/8	-
50	GCP	k	602	-	-	3/15/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	k	602	GCP	PG-O1G	5.41	1.61	1.50
50	k	602	GCP	C5-C6	4.77	1.49	1.41
50	k	602	GCP	PB-O1B	4.16	1.61	1.51
50	k	602	GCP	PB-O2B	-3.39	1.48	1.56
50	k	602	GCP	PB-O3A	3.36	1.62	1.58

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	k	602	GCP	C2-N3-C4	5.53	121.67	115.36
50	k	602	GCP	C2-N1-C6	3.97	122.24	115.93
50	k	602	GCP	C4-C5-C6	-3.90	117.07	120.80
50	k	602	GCP	C5-C6-N1	-3.64	118.46	123.43
50	k	602	GCP	N3-C2-N1	-3.58	122.45	127.22

There are no chirality outliers.

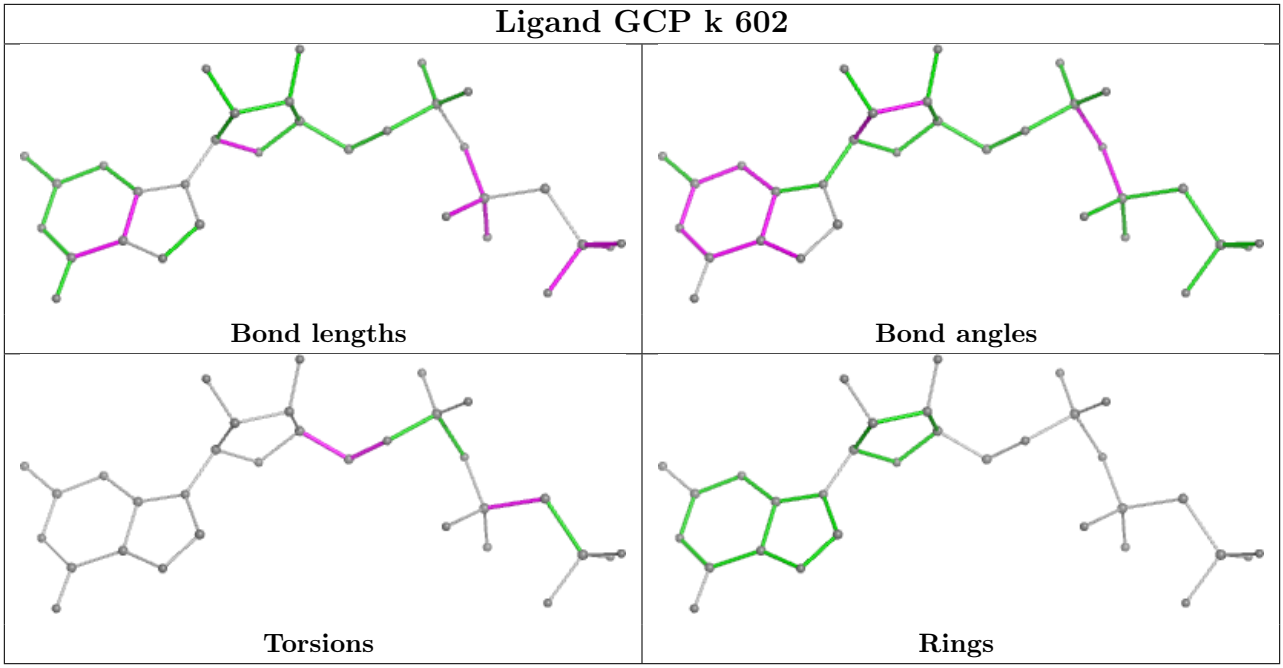
5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
50	k	602	GCP	O4'-C4'-C5'-O5'
51	k	603	MET	O-C-CA-CB
51	k	603	MET	CA-CB-CG-SD
51	k	603	MET	N-CA-CB-CG
50	k	602	GCP	C4'-C5'-O5'-PA

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
23	o	2
28	1	1
22	m	1
25	k	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	o	492:ALA	C	693:UNK	N	230.47
1	1	16:U	O3'	18:G	P	5.21
1	m	75:GLY	C	76:GLU	N	4.38
1	k	372:PRO	C	373:ILE	N	3.76
1	o	5:PRO	C	6:PHE	N	3.57

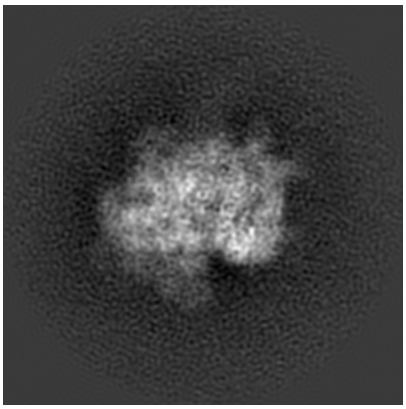
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0058. These allow visual inspection of the internal detail of the map and identification of artifacts.

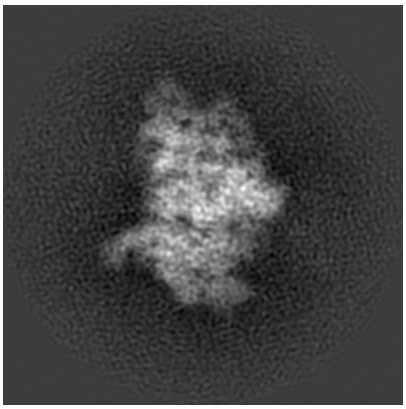
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

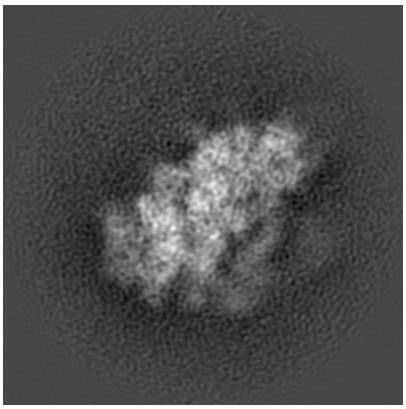
6.1.1 Primary map



X

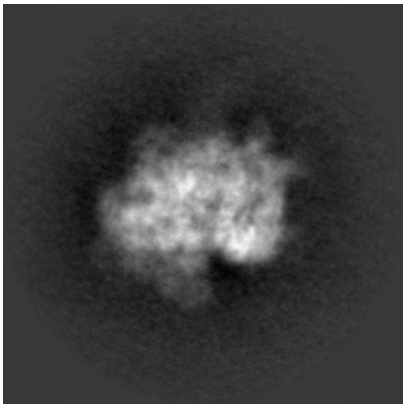


Y

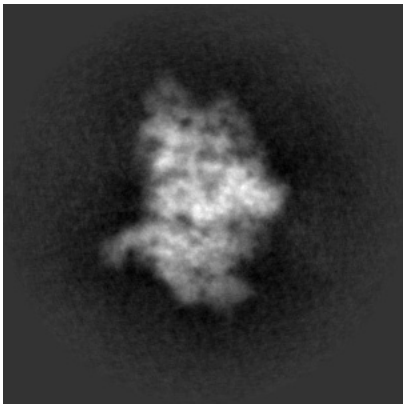


Z

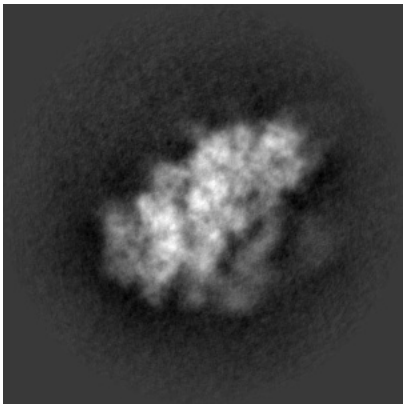
6.1.2 Raw map



X



Y

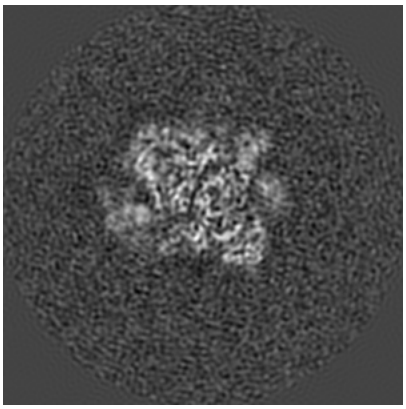


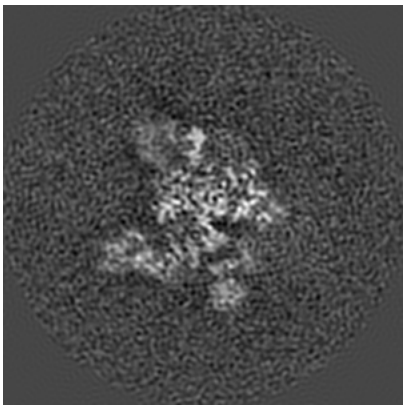
Z

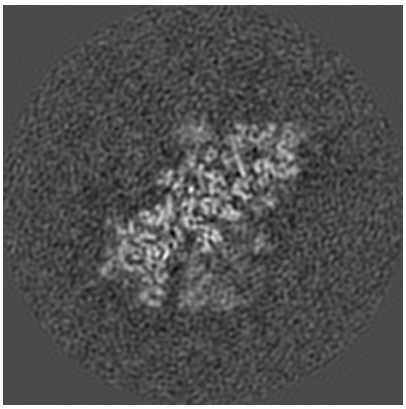
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

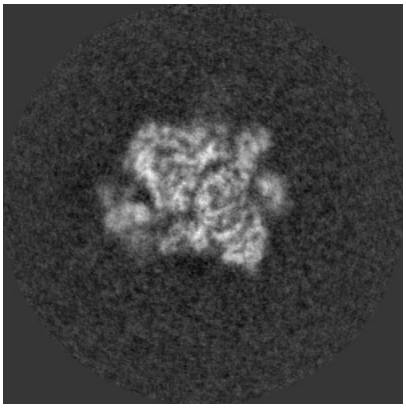
6.2.1 Primary map

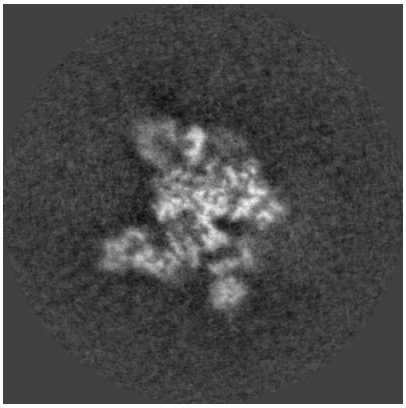

X Index: 150

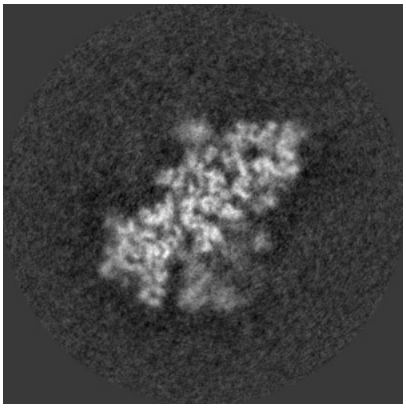

Y Index: 150


Z Index: 150

6.2.2 Raw map


X Index: 150

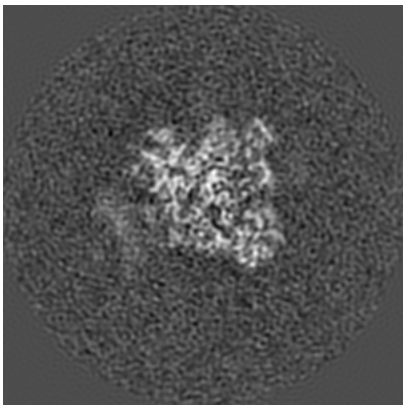

Y Index: 150

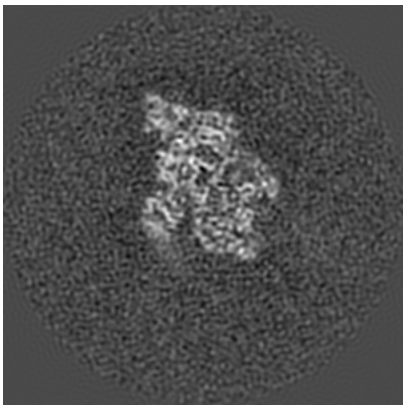

Z Index: 150

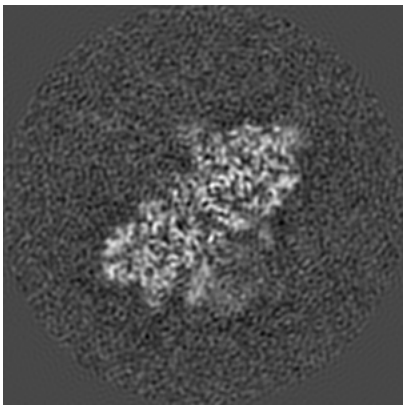
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

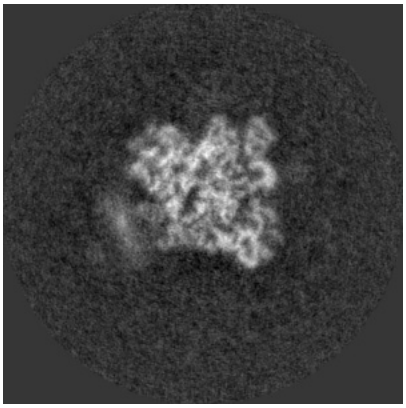
6.3.1 Primary map

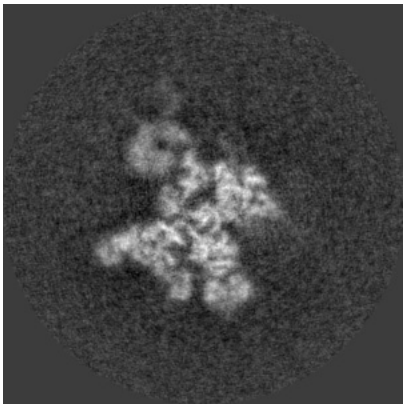

X Index: 160

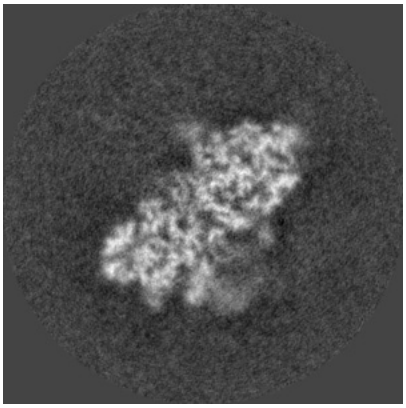

Y Index: 172


Z Index: 143

6.3.2 Raw map


X Index: 158

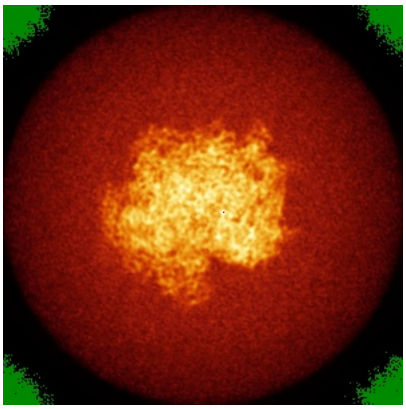

Y Index: 139

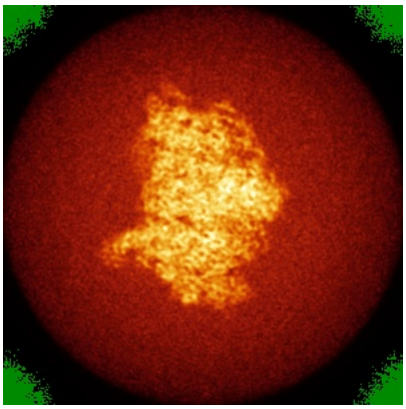

Z Index: 143

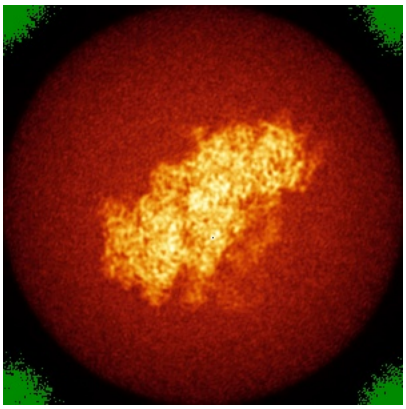
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

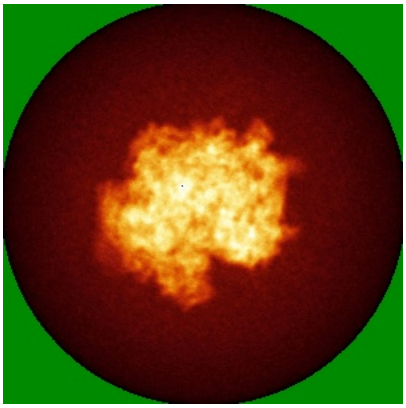
6.4.1 Primary map

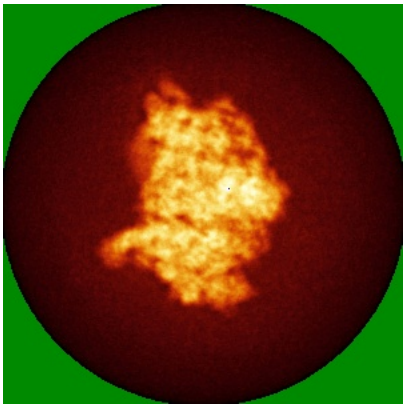

X

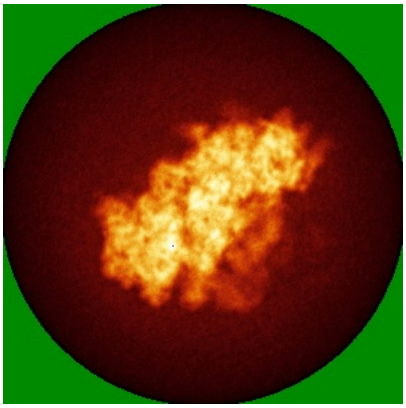

Y


Z

6.4.2 Raw map


X

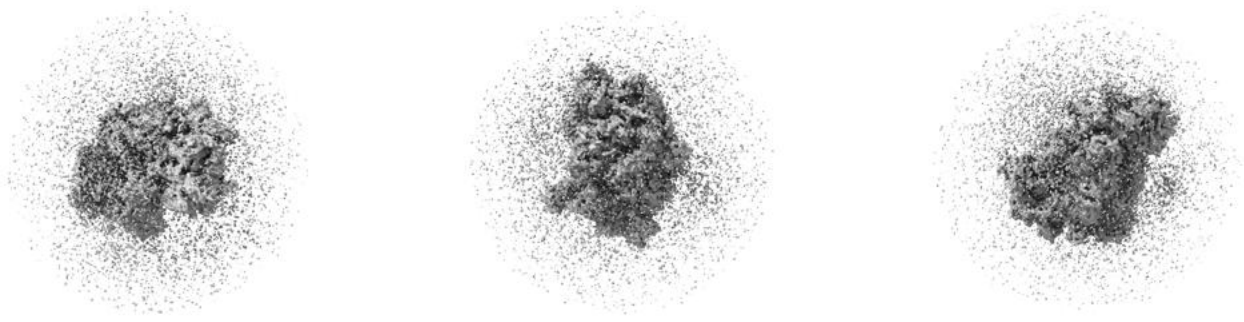

Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

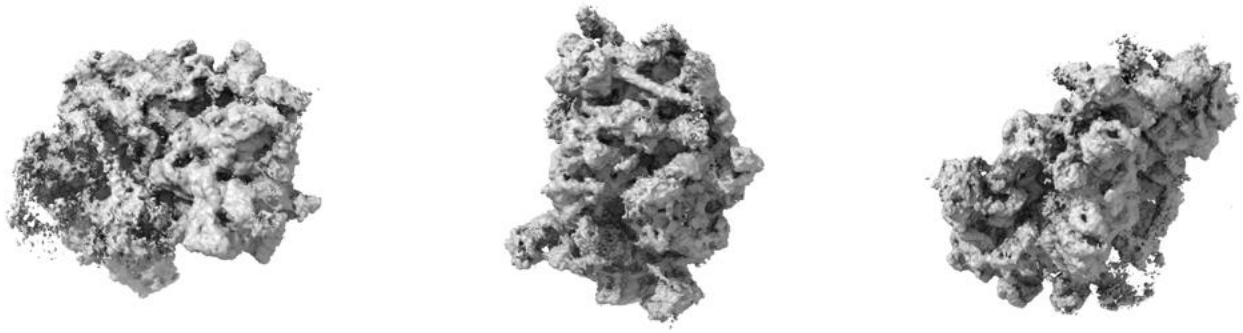
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

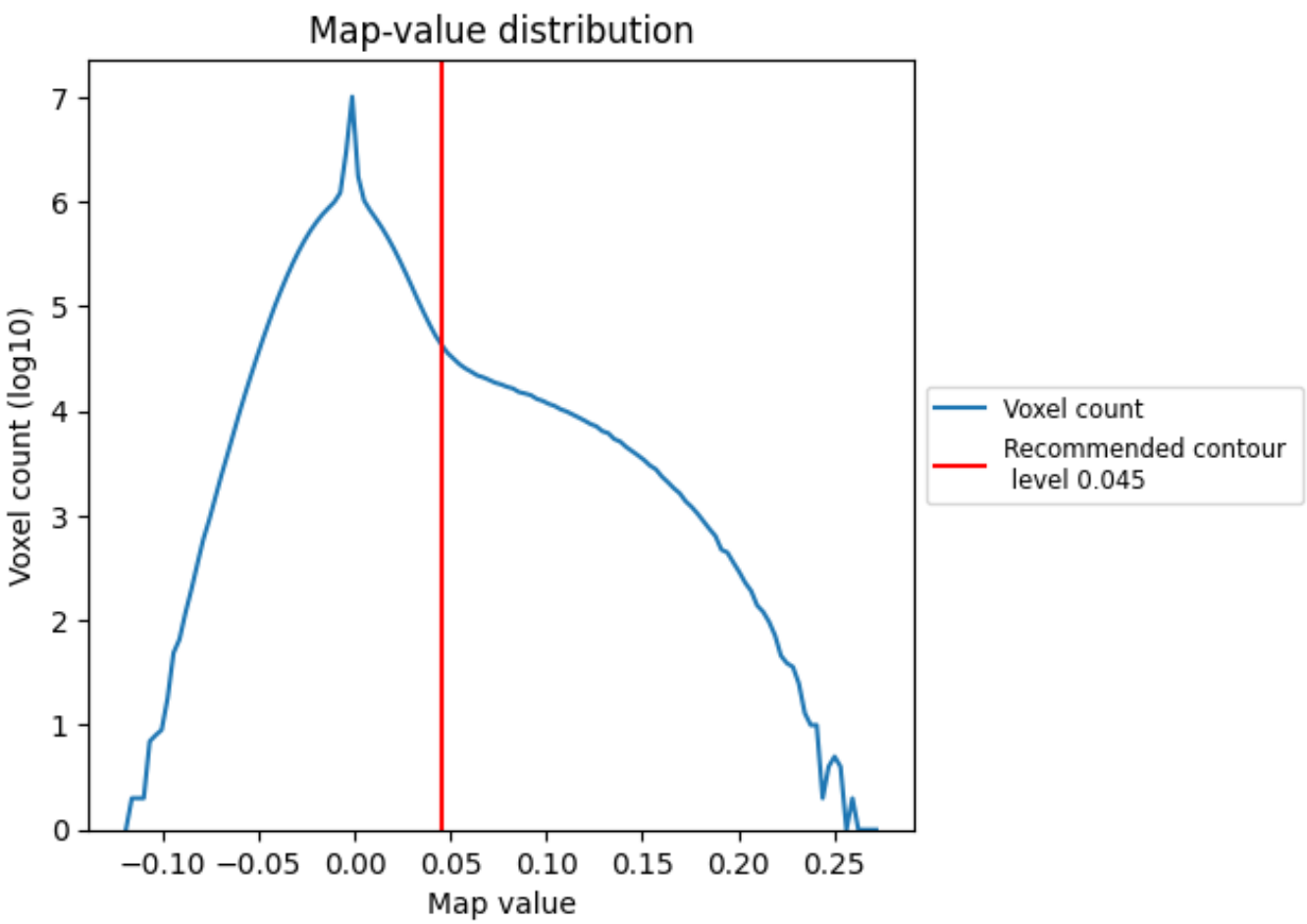
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

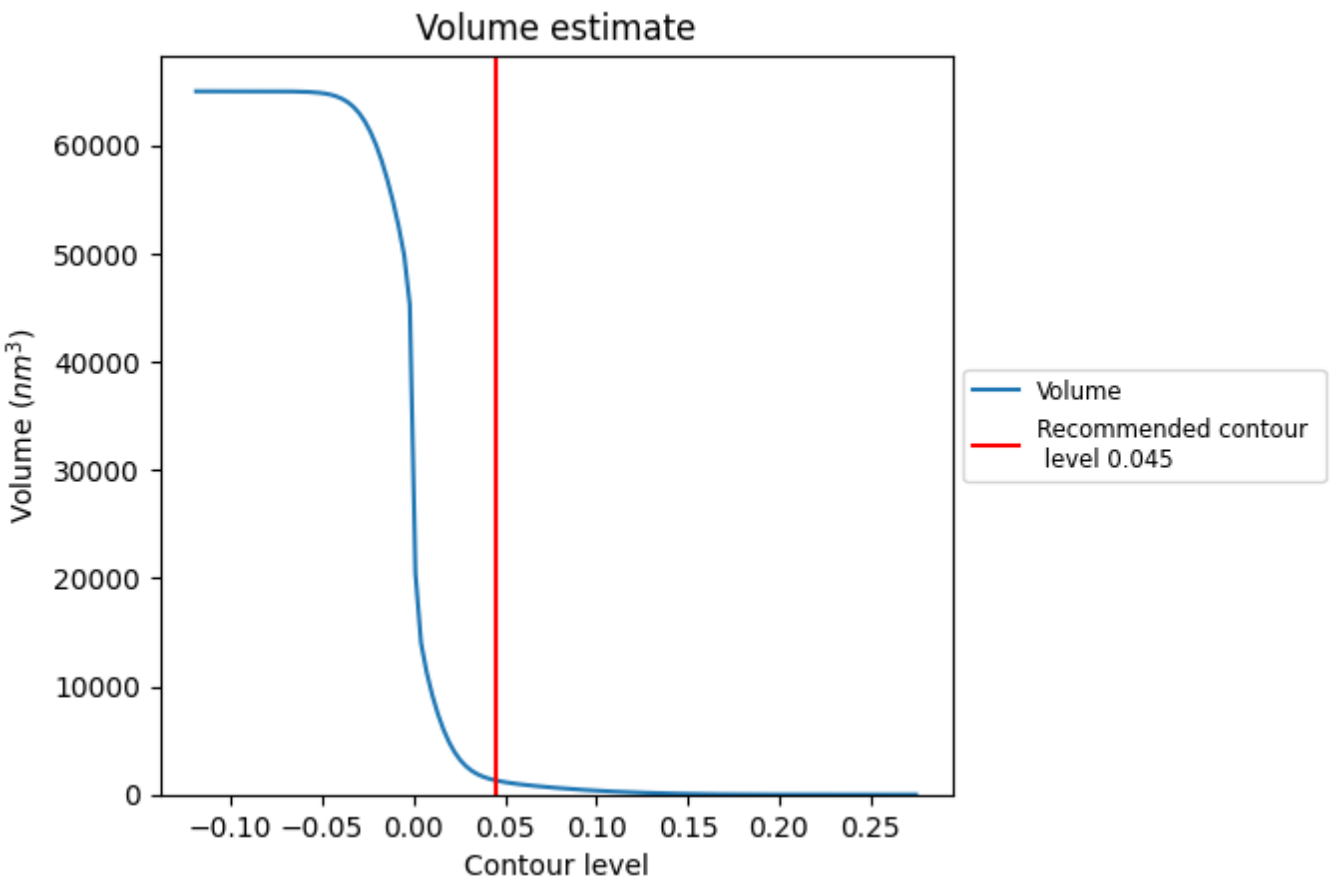
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

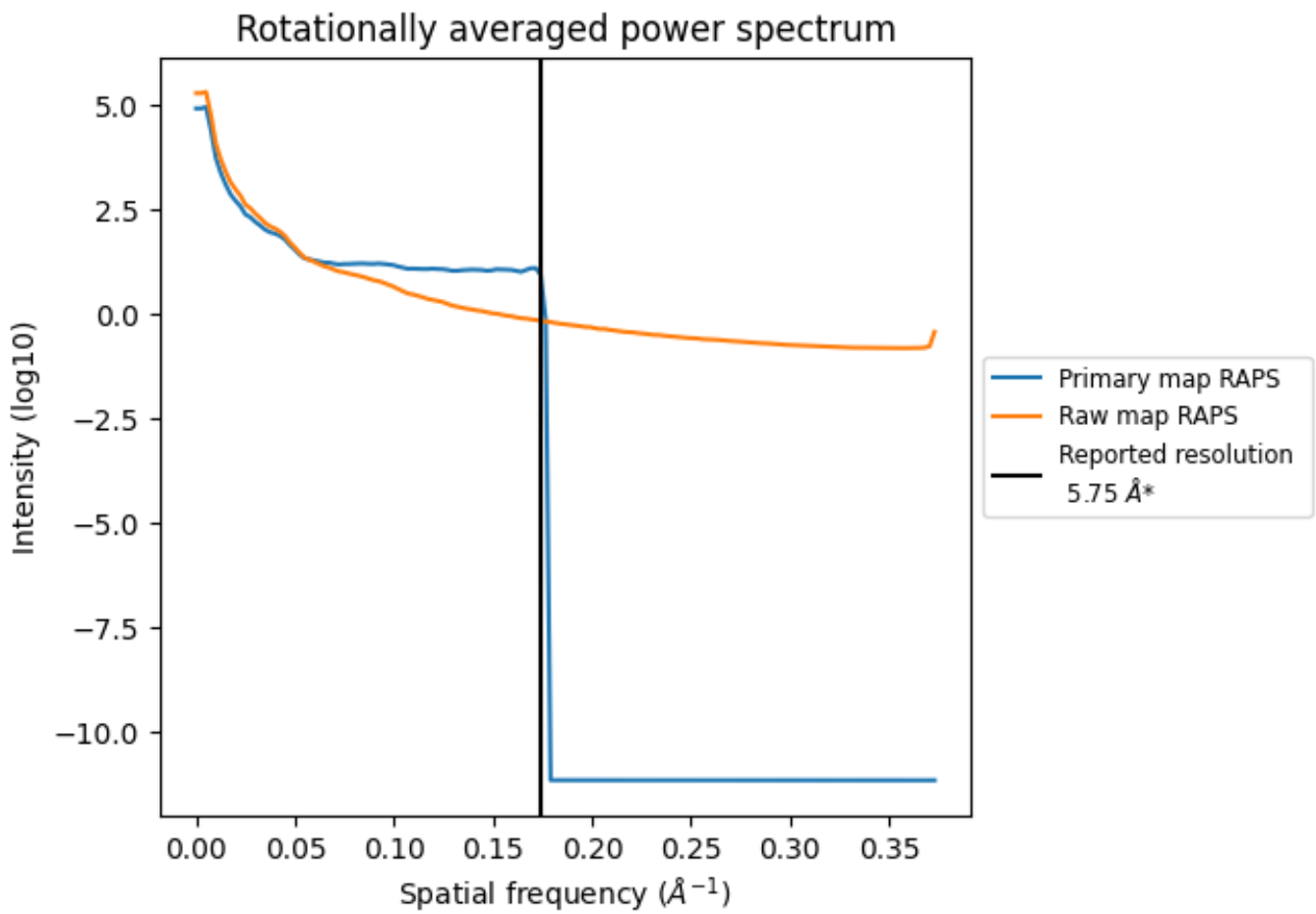
7.2 Volume estimate (i)



The volume at the recommended contour level is 1308 nm^3; this corresponds to an approximate mass of 1181 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

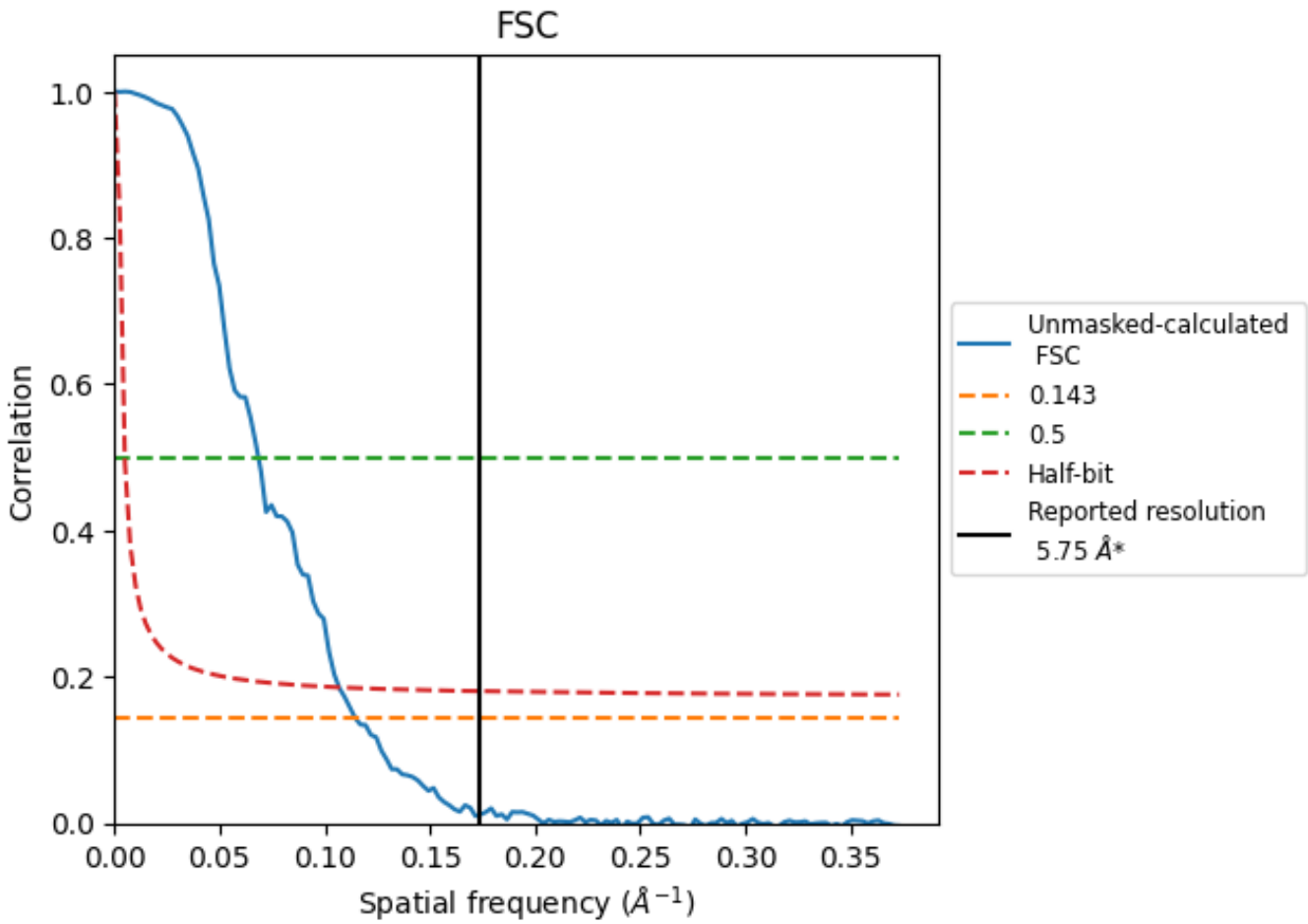


*Reported resolution corresponds to spatial frequency of 0.174 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.174 Å^{-1}

8.2 Resolution estimates (i)

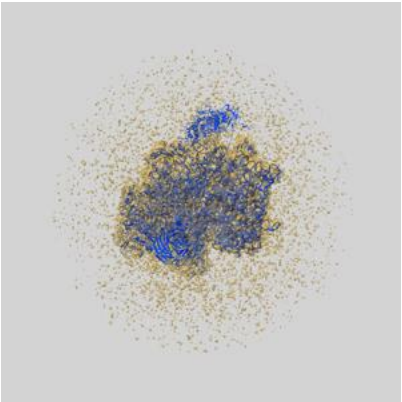
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.75	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.73	14.62	9.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.73 differs from the reported value 5.75 by more than 10 %

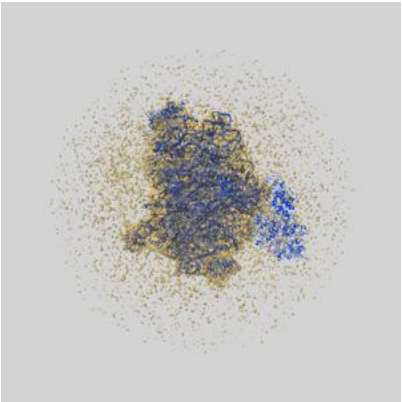
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0058 and PDB model 6GSN. Per-residue inclusion information can be found in section 3 on page 14.

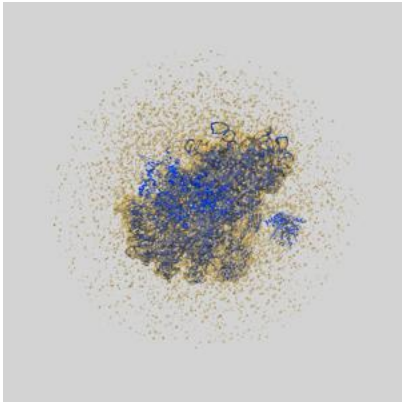
9.1 Map-model overlay (i)



X



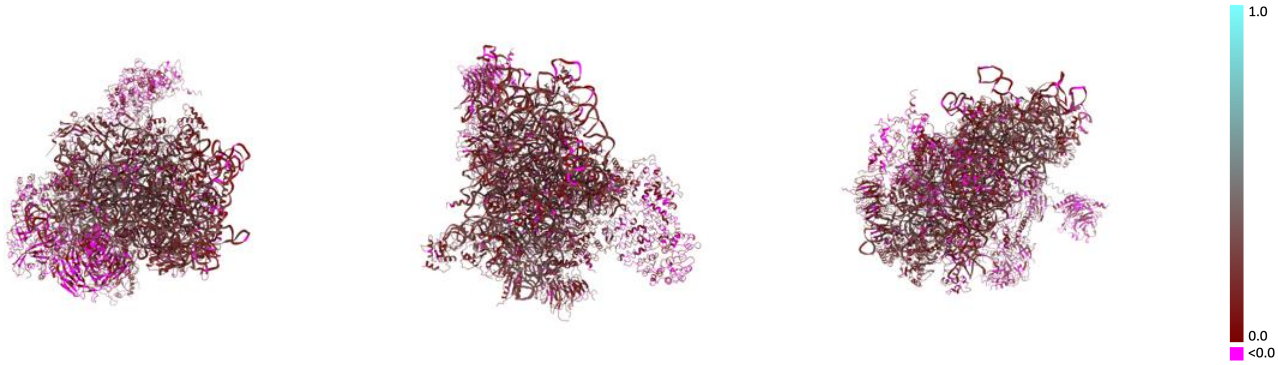
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

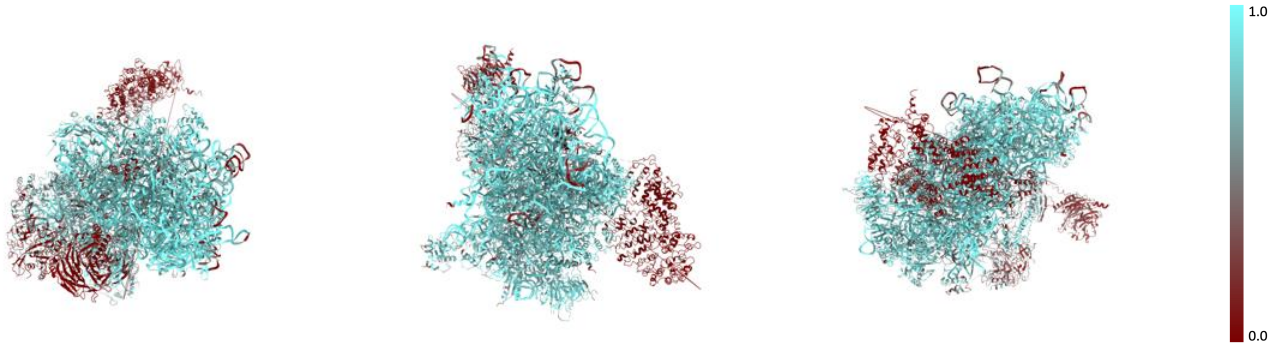
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

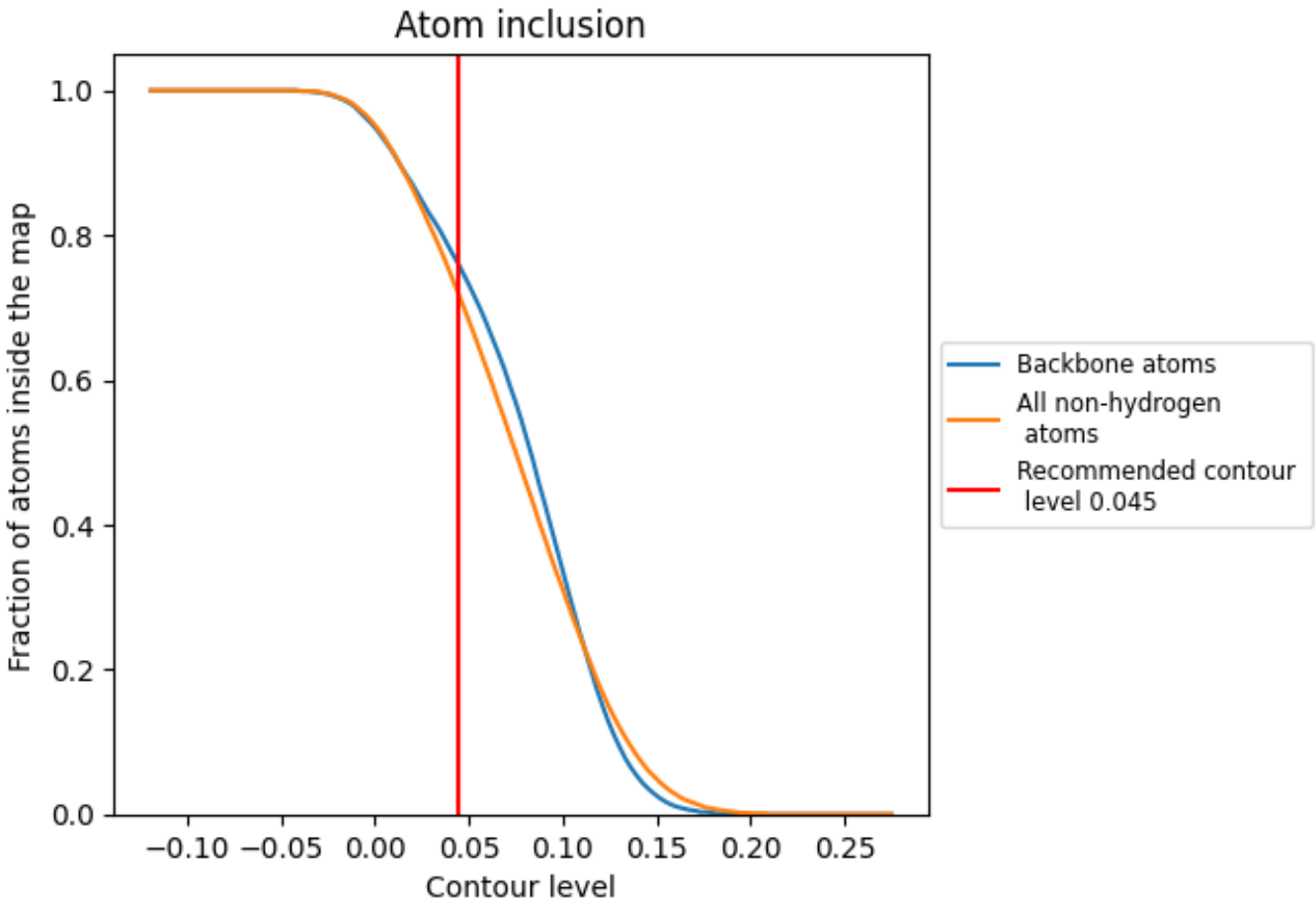
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.045).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7170	0.1850
1	0.8130	0.1580
2	0.9260	0.2360
3	0.7350	0.1800
A	0.8200	0.2010
B	0.8440	0.1950
C	0.7730	0.2070
D	0.7760	0.2120
E	0.7920	0.1980
F	0.7870	0.1950
G	0.8350	0.1770
H	0.8230	0.1830
I	0.8020	0.1920
J	0.7920	0.2000
K	0.8250	0.1880
L	0.7670	0.2080
M	0.6960	0.1600
N	0.8170	0.1930
O	0.8550	0.2030
P	0.8400	0.1940
Q	0.8150	0.1760
R	0.7820	0.1940
S	0.7940	0.1800
T	0.8270	0.1810
U	0.7510	0.1810
V	0.8430	0.2120
W	0.7920	0.1980
X	0.7260	0.2060
Y	0.8330	0.2070
Z	0.7350	0.1580
a	0.8330	0.2220
b	0.8410	0.2140
c	0.7940	0.2100
d	0.7840	0.1930
e	0.6930	0.2070

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
f	0.7900	0.1870
g	0.8280	0.1720
h	0.5400	0.1350
i	0.7160	0.2200
j	0.4780	0.1290
k	0.2490	0.0930
l	0.3020	0.1060
m	0.4460	0.1650
o	0.0950	0.0710
p	0.5480	0.1290
q	0.0460	0.0870
r	0.0210	0.0550
s	0.0230	0.0020