



wwPDB EM Validation Summary Report ⓘ

Jun 19, 2026 – 07:15 am BST

PDB ID : 7R4X / pdb_00007r4x
EMDB ID : EMD-14317
Title : Cryo-EM reconstruction of the human 40S ribosomal subunit - Full map
Authors : Pellegrino, S.; Dent, K.C.; Spikes, T.; Warren, A.J.
Deposited on : 2022-02-09
Resolution : 2.15 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

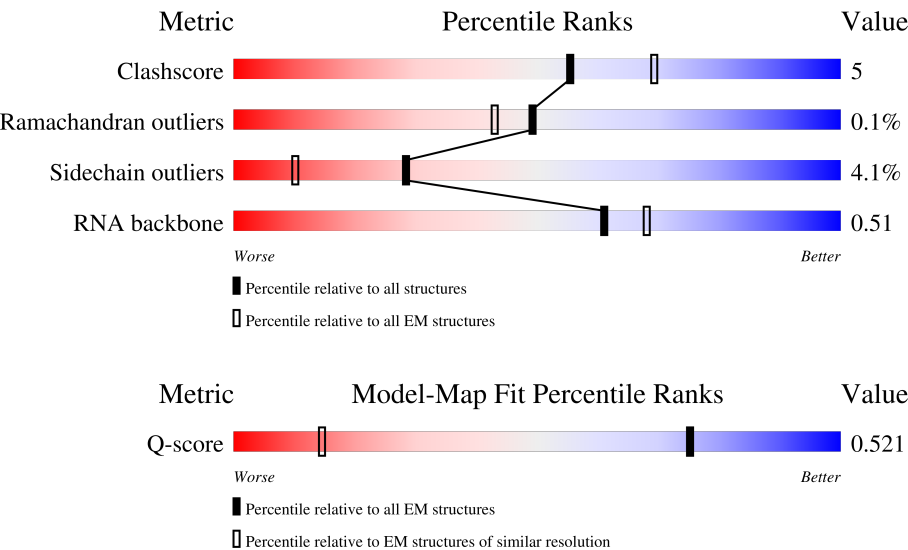
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.15 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	2551 (1.66 - 2.65)

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 $\leq 5\%$. 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	n	25	
2	2	1868	
3	B	264	

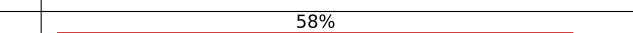
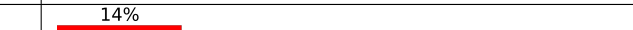
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	243	 79% 75% 17% 8%
5	E	263	 90% 7%
6	F	204	 89% 76% 12% 11%
7	H	194	 36% 77% 13% 5% 5%
8	I	208	 15% 88% 10%
9	K	165	 59% 46% 12% 41%
10	L	158	 5% 79% 10% 11%
11	P	145	 85% 72% 11% 15%
12	Q	146	 93% 80% 14% 5%
13	R	135	 67% 77% 17%
14	S	152	 94% 79% 15% 6%
15	T	145	 99% 94%
16	U	119	 76% 72% 15% 13%
17	V	83	 78% 20%
18	X	143	 86% 12%
19	a	115	 6% 65% 20% 14%
20	c	69	 84% 58% 28% 14%
21	d	56	 84% 91% 5%
22	C	293	 62% 12% 25%
23	G	249	 27% 75% 16% 9%
24	J	194	 5% 79% 15% 5%
25	M	132	 79% 58% 19% 21%
26	N	151	 8% 85% 15%
27	O	151	 70% 13% 16%
28	W	130	 90% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	Y	133	
30	Z	125	
31	b	84	
32	e	59	
33	f	156	
34	g	317	
35	A	295	

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 77936 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 protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	n	20	Total	C	N	O	S	0	0
			193	119	51	20	3		

- Molecule 2 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1646	Total	C	N	O	P	7	0
			35347	15805	6355	11535	1652		

- Molecule 3 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	210	Total	C	N	O	S	0	0
			1711	1086	306	305	14		

- Molecule 4 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	224	Total	C	N	O	S	0	0
			1745	1112	314	312	7		

- Molecule 5 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	257	Total	C	N	O	S	0	0
			2041	1305	379	349	8		

- Molecule 6 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	182	Total	C	N	O	S	0	0
			1445	906	271	261	7		

- Molecule 7 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	184	Total	C	N	O	S	0	0
			1477	942	271	263	1		

- Molecule 8 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 9 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	97	Total	C	N	O	S	0	0
			816	533	144	133	6		

- Molecule 10 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	141	Total	C	N	O	S	0	0
			1157	737	217	197	6		

- Molecule 11 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	123	Total	C	N	O	S	0	0
			1005	638	188	172	7		

- Molecule 12 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	139	Total	C	N	O	S	0	0
			1105	704	207	191	3		

- Molecule 13 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	131	Total	C	N	O	S	0	0
			1064	668	198	194	4		

- Molecule 14 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	143	Total	C	N	O	S	1	0
			1192	751	240	200	1		

- Molecule 15 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 16 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 17 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	83	Total	C	N	O	S	0	0
			639	395	117	122	5		

- Molecule 18 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	140	Total	C	N	O	S	0	0
			1088	687	215	183	3		

- Molecule 19 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	99	Total	C	N	O	S	0	0
			792	492	165	130	5		

- Molecule 20 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	c	59	Total	C	N	O	S	0	0
			464	281	93	88	2		

- Molecule 21 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 22 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	C	219	Total	C	N	O	S	1	0
			1708	1105	295	298	10		

- Molecule 23 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	G	227	Total	C	N	O	S	0	0
			1840	1149	367	317	7		

- Molecule 24 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	J	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 25 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	M	104	Total	C	N	O	S	0	0
			790	494	138	151	7		

- Molecule 26 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	N	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 27 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	O	127	Total	C	N	O	S	0	0
			957	585	189	177	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	138	IAS	ASP	conflict	UNP P62263

- Molecule 28 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	W	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 29 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	122	Total	C	N	O	S	0	0
			1002	635	196	166	5		

- Molecule 30 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	72	Total	C	N	O	S	0	0
			570	366	104	99	1		

- Molecule 31 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

- Molecule 32 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	55	Total	C	N	O	S	0	0
			438	271	95	71	1		

- Molecule 33 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	64	Total	C	N	O	S	0	0
			522	329	99	87	7		

- Molecule 34 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	312	Total	C	N	O	S	0	0
			2429	1531	423	463	12		

- Molecule 35 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	A	206	Total	C	N	O	S	1	0
			1628	1042	287	291	8		

- Molecule 36 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
36	2	76	Total	K	0
			76	76	
36	E	1	Total	K	0
			1	1	
36	L	1	Total	K	0
			1	1	
36	S	1	Total	K	0
			1	1	
36	U	1	Total	K	0
			1	1	
36	d	1	Total	K	0
			1	1	
36	O	1	Total	K	0
			1	1	

- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	2	88	Total	Mg	0
			88	88	

- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
38	a	1	Total	Zn	0
			1	1	
38	d	1	Total	Zn	0
			1	1	
38	f	1	Total	Zn	0
			1	1	

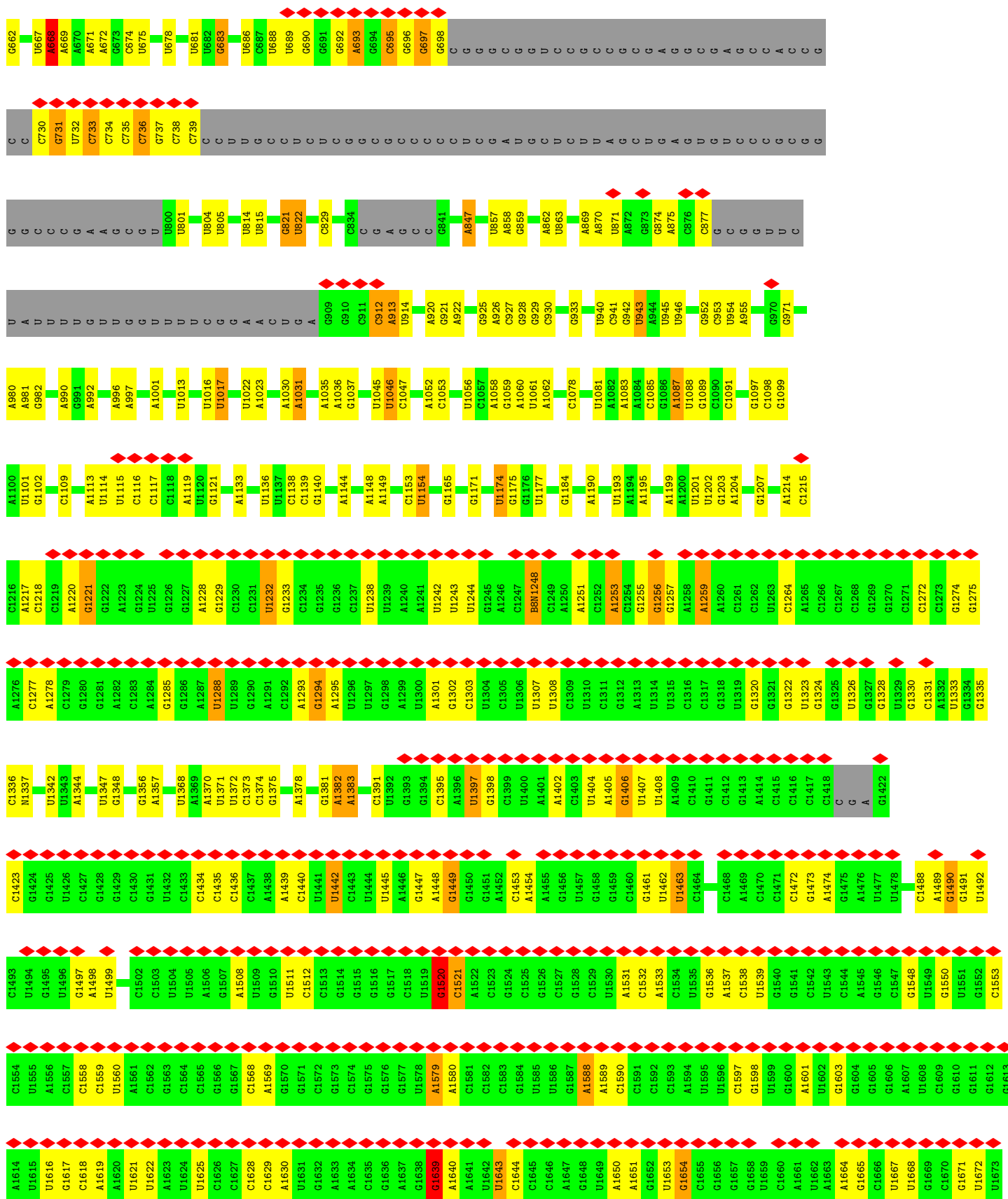
- Molecule 39 is water.

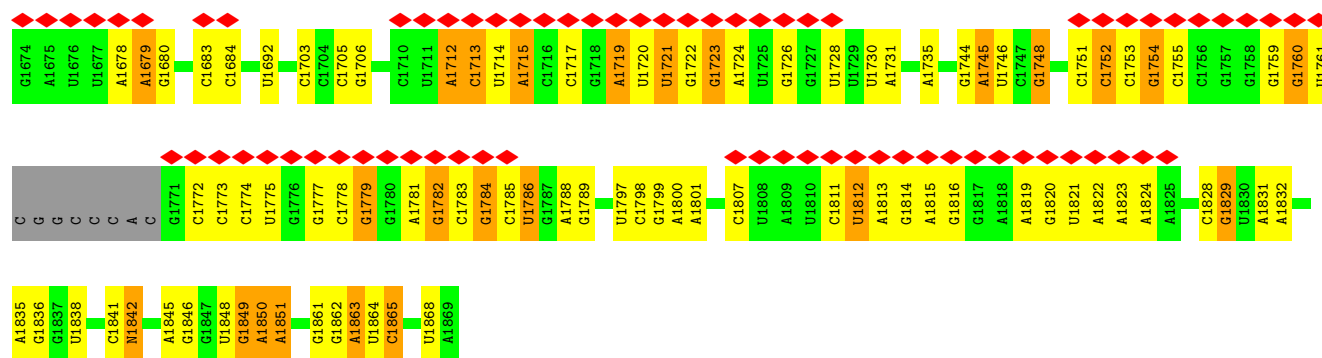
Mol	Chain	Residues	Atoms		AltConf
39	n	10	Total 10	O 10	0
39	2	3102	Total 3102	O 3102	0
39	B	30	Total 30	O 30	0
39	D	24	Total 24	O 24	0
39	E	79	Total 79	O 79	0
39	F	34	Total 34	O 34	0
39	H	8	Total 8	O 8	0
39	I	45	Total 45	O 45	0
39	K	20	Total 20	O 20	0
39	L	62	Total 62	O 62	0
39	P	32	Total 32	O 32	0
39	Q	46	Total 46	O 46	0
39	R	13	Total 13	O 13	0
39	S	30	Total 30	O 30	0
39	T	51	Total 51	O 51	0
39	U	25	Total 25	O 25	0
39	V	19	Total 19	O 19	0
39	X	47	Total 47	O 47	0
39	a	30	Total 30	O 30	0
39	c	6	Total 6	O 6	0
39	d	26	Total 26	O 26	0

Continued on next page...

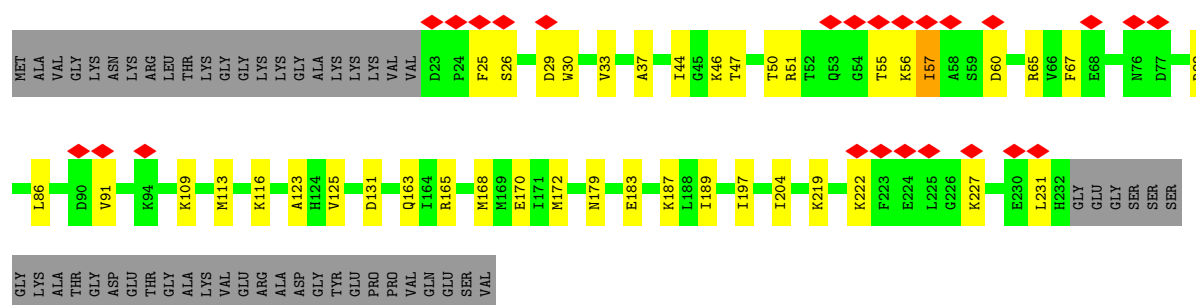
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
39	C	56	Total 56	O 56	0
39	G	18	Total 18	O 18	0
39	J	85	Total 85	O 85	0
39	N	30	Total 30	O 30	0
39	O	28	Total 28	O 28	0
39	W	63	Total 63	O 63	0
39	Y	25	Total 25	O 25	0
39	Z	2	Total 2	O 2	0
39	b	12	Total 12	O 12	0
39	e	13	Total 13	O 13	0
39	g	16	Total 16	O 16	0
39	A	30	Total 30	O 30	0

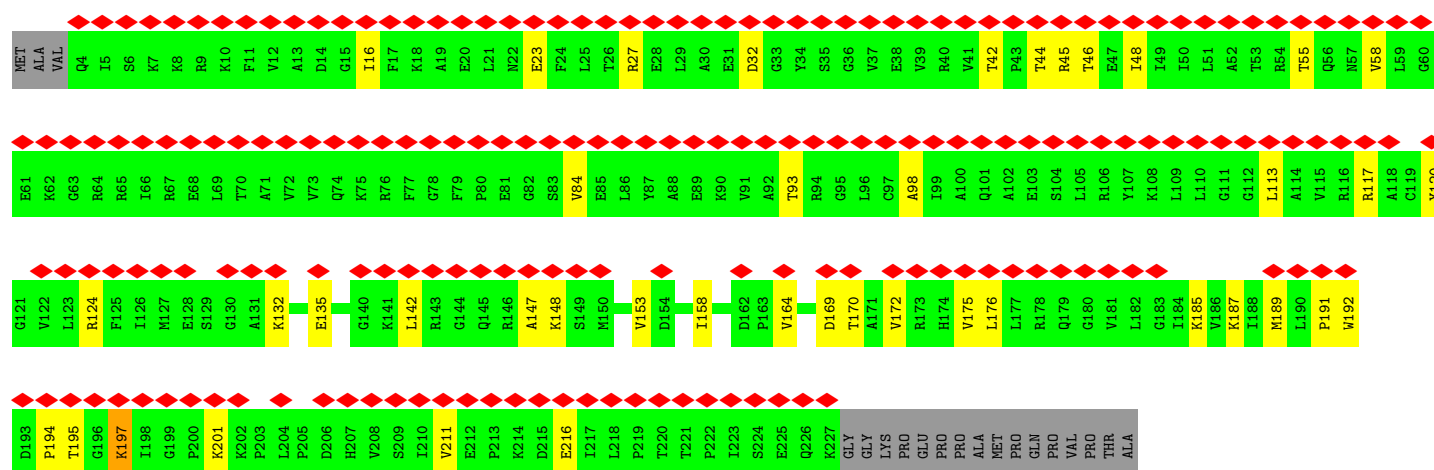
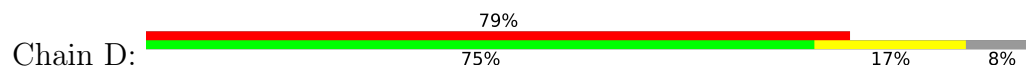




• Molecule 3: 40S ribosomal protein S3a



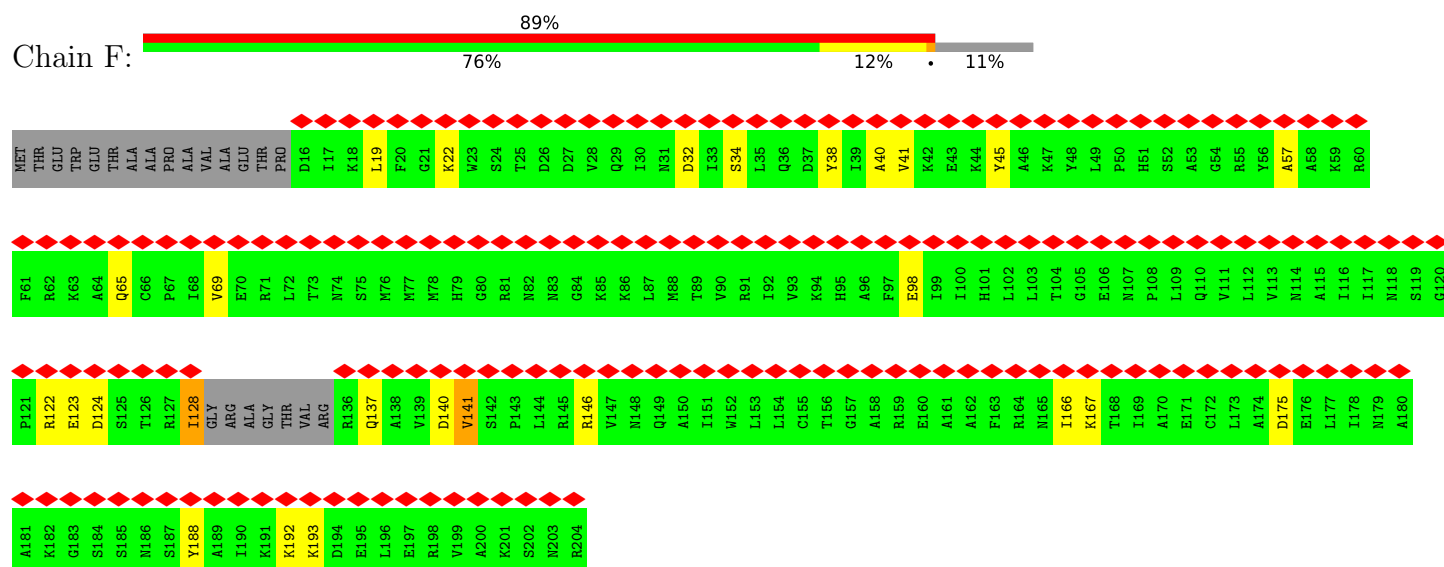
• Molecule 4: 40S ribosomal protein S3



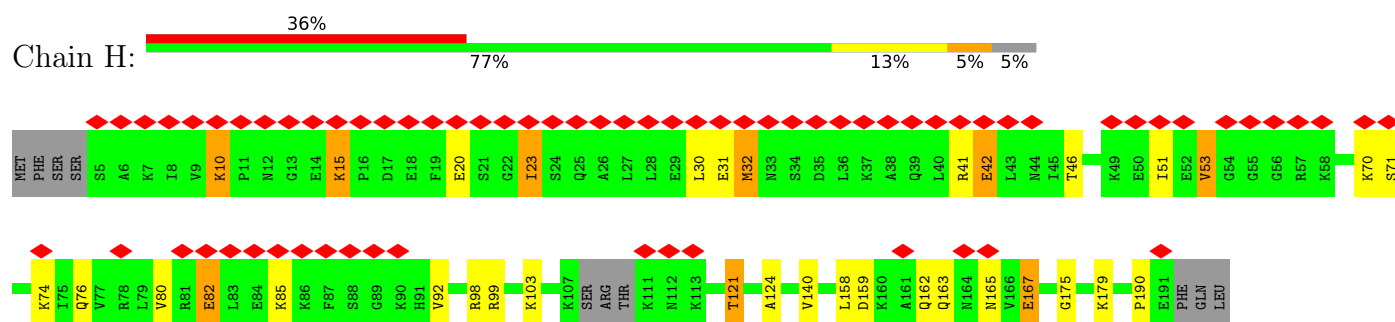
• Molecule 5: 40S ribosomal protein S4, X isoform



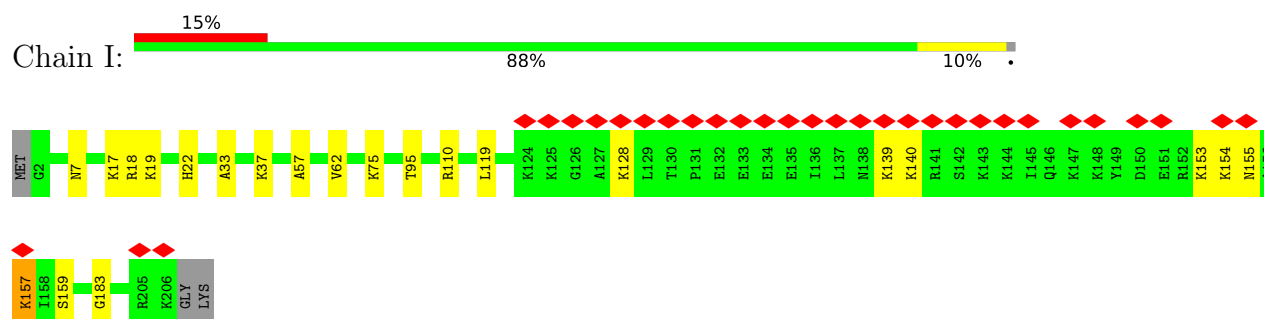
- Molecule 6: 40S ribosomal protein S5



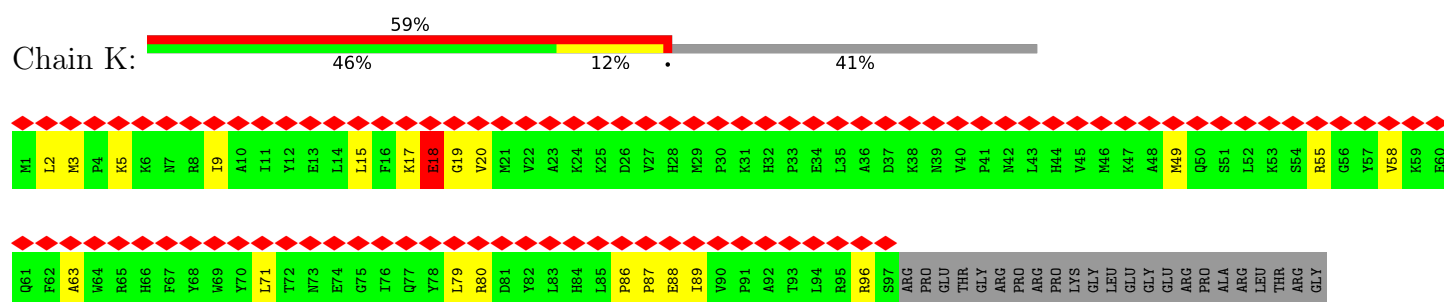
- Molecule 7: 40S ribosomal protein S7



- Molecule 8: 40S ribosomal protein S8



- Molecule 9: 40S ribosomal protein S10



GLU
ALA
ASP
ARG
THR
THR
TYR
ARG
ARG
SER
SER
ALA
VAL
PRO
PRO
GLY
GLY
ALA
ASP
GLY
LYS
LYS
ALA
GLU
GLY
ALA
GLY
SER
SER
THR
THR
GLU
PHE
GLN
PHE
ARG
GLY
GLY
PHE
GLY
ARG
GLY
GLN
GLN
PRO
PRO
GLN

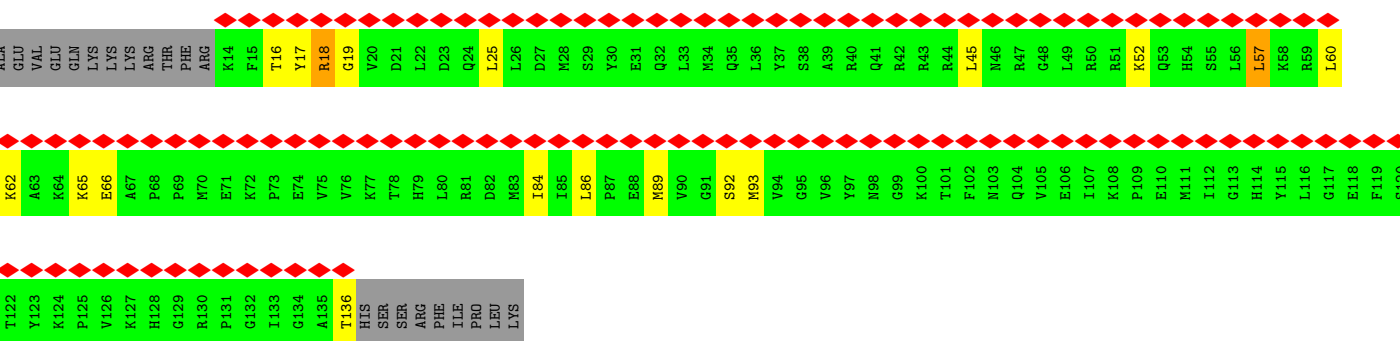
• Molecule 10: 40S ribosomal protein S11

Chain L: 

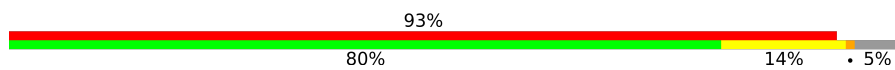

MET ALA D3 I4 K20 K21 ARG VAL ARG LEU LEU GLY THR GLY LYS LYS L33 Y36 E49 I56 S74 M82 T85 I88 D91 K104 M109 D124 R132 K136 K147 A148 A149 G150 T151 K152 K153 Q154 PHE GLN LYS PHE

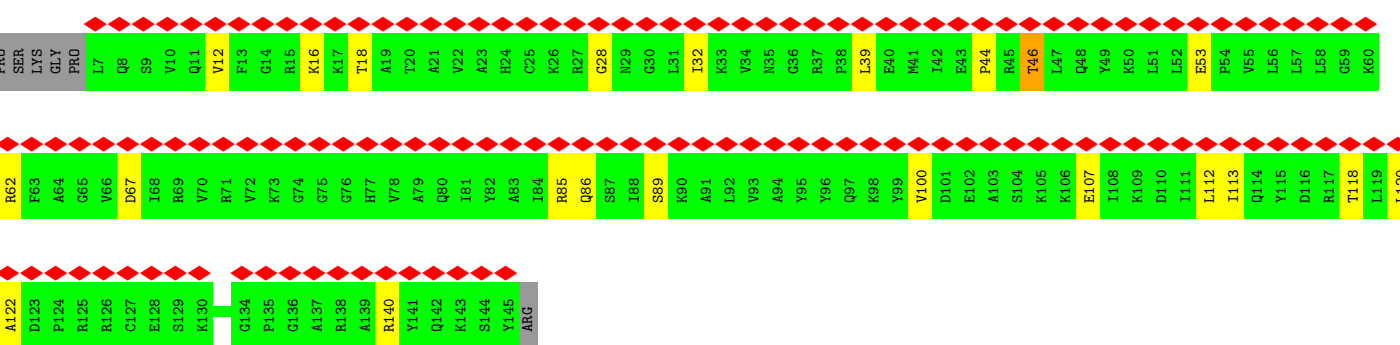
• Molecule 11: 40S ribosomal protein S15

Chain P: 


MET ALA VAL GLU GLN LYS LYS LYS THR PHE ARG K14 F15 T16 Y17 R18 G19 V20 D21 L22 D23 Q24 L25 L26 D27 M28 S29 Y30 E31 Q32 L33 M34 Q35 L36 Y37 S38 A39 R40 Q41 R42 R43 R44 L45 M46 R47 G48 L49 R50 R51 K52 Q53 H54 S55 L56 L57 K58 R59 L60
R61 K62 A63 K64 K65 E66 A67 P68 P69 M70 E71 K72 P73 E74 V75 V76 K77 T78 H79 L80 R81 R82 M83 I84 I85 L86 P87 E88 M89 V90 G91 S92 M93 V94 G95 Y96 Y97 G98 G99 K100 T101 F102 M103 M104 V105 E106 I107 K108 P109 E110 M111 I112 G113 H114 Y115 L116 G117 E118 F119 S120
I121 T122 V123 K124 P125 V126 K127 H128 G129 R130 P131 G132 I133 G134 A135 T136 H137 SER SER ARG PHE ILE PRO LEU LYS

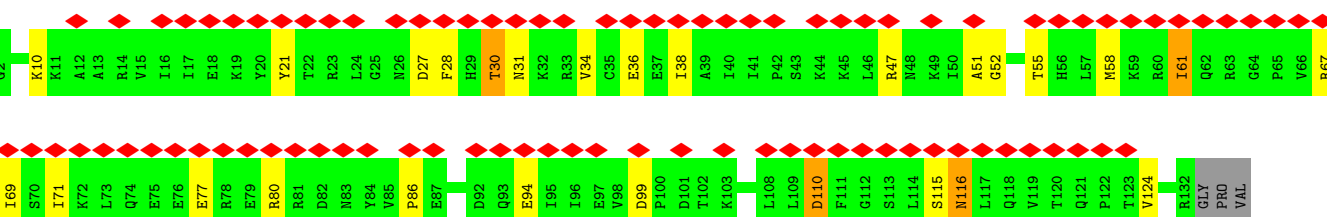
• Molecule 12: 40S ribosomal protein S16

Chain Q: 

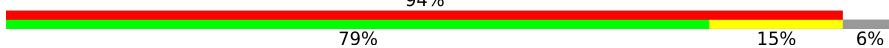

MET PRO SER LYS PRO L7 Q8 S9 V10 Q11 V12 F13 G14 R15 K16 K17 T18 A19 T20 A21 V22 A23 H24 C25 K26 R27 G28 M29 G30 L31 I32 K33 V34 N35 G36 R37 P38 L39 E40 M41 I42 E43 P44 R45 T46 L47 Q48 Y49 K50 L51 L52 E53 P54 V55 L56 L57 G59 K60
E61 R62 F63 A64 G65 V66 D67 I68 R69 V70 R71 V72 K73 G74 G75 G76 H77 V78 A79 Q80 Q81 Y82 I83 A84 R85 Q86 S87 I88 S89 A91 L92 V93 A94 Y95 Y96 Q97 K98 Y99 V100 D101 E102 A103 S104 K105 E107 I108 M109 D110 I111 L112 I113 Q114 Y115 D116 T117 L118 L119 L120
V121 A122 D123 P124 R125 R126 C127 E128 S129 K130 G134 P135 G136 A137 R138 A139 R140 Y141 Q142 K143 S144 Y145 ARG

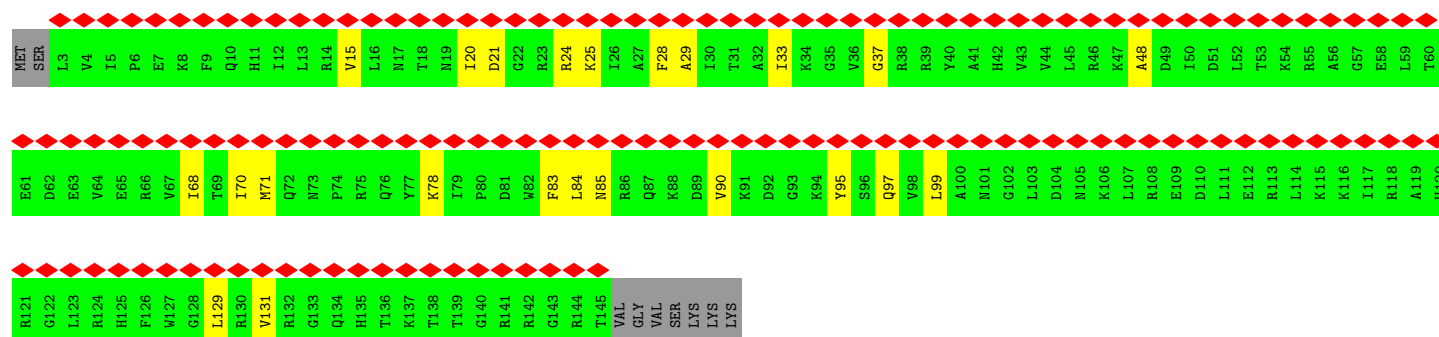
• Molecule 13: 40S ribosomal protein S17

Chain R: 

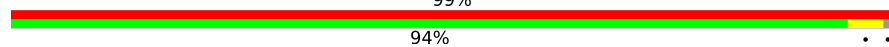

MET G2 K10 K11 A12 A13 R14 V15 I16 I17 E18 K19 Y20 Y21 T22 R23 L24 G25 N26 D27 F28 H29 T30 N31 K32 R33 V34 C35 E36 E37 I38 A39 I40 I41 P42 S43 K44 K45 L46 R47 M48 K49 A51 G52 T55 H56 L57 M58 K59 I61 Q62 R63 G64 P65 V66 R67
G68 I69 S70 I71 K72 L73 Q74 E75 E76 E77 R78 E79 R80 R81 D82 N83 Y84 V85 P86 E87 D82 Q83 E84 I95 I96 E97 V98 D99 P100 D101 T102 K103 L108 L109 D110 F111 G112 S113 L114 S115 N116 L117 Q118 V119 T120 Q121 P122 T123 V124 R132 GLY PRO VAL

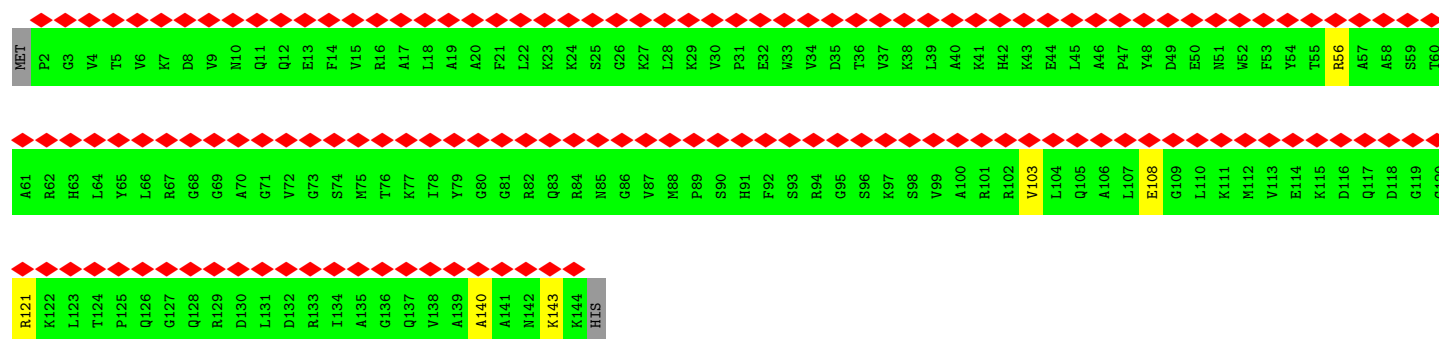
- Molecule 14: 40S ribosomal protein S18

Chain S: 



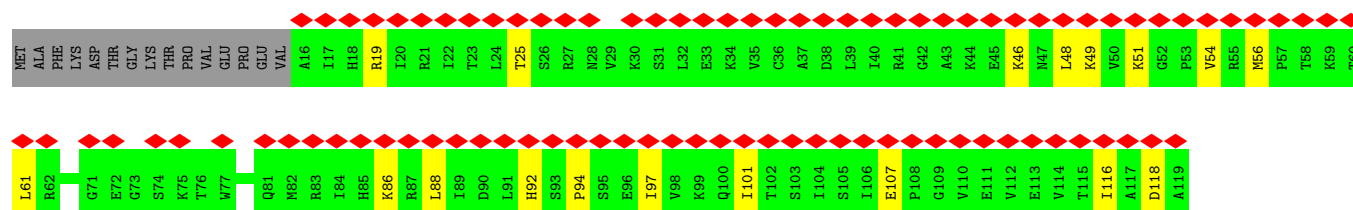
- Molecule 15: 40S ribosomal protein S19

Chain T: 



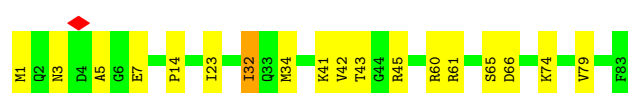
- Molecule 16: 40S ribosomal protein S20

Chain U: 



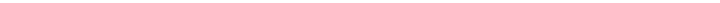
- Molecule 17: 40S ribosomal protein S21

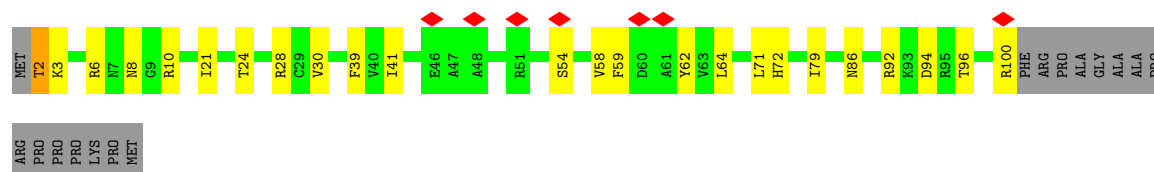
Chain V: 

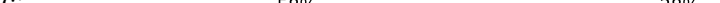


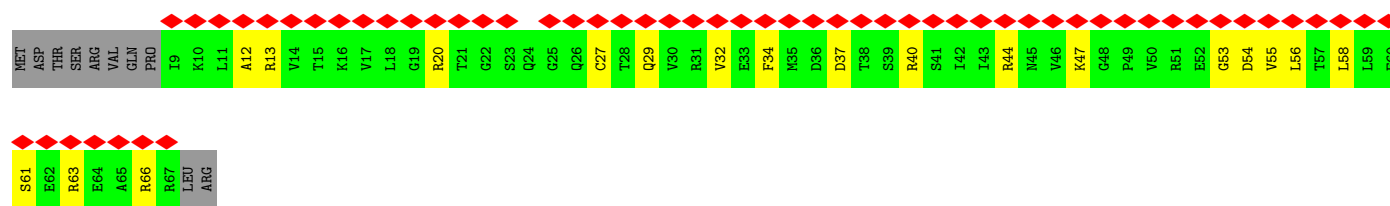
- Molecule 18: 40S ribosomal protein S23

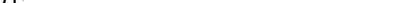
MET	Q2	L7	F41	L52	Q61	P62	N63	SG4	K68	V72	Q73	K76	D88	L91	N92	F93	V102	R119	R140	P141	ARG	SER
-----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	-----	-----

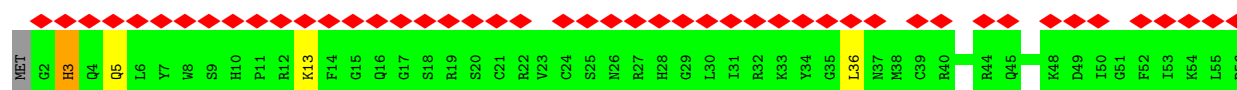
- Chain a:  6% 65% 20% 14%



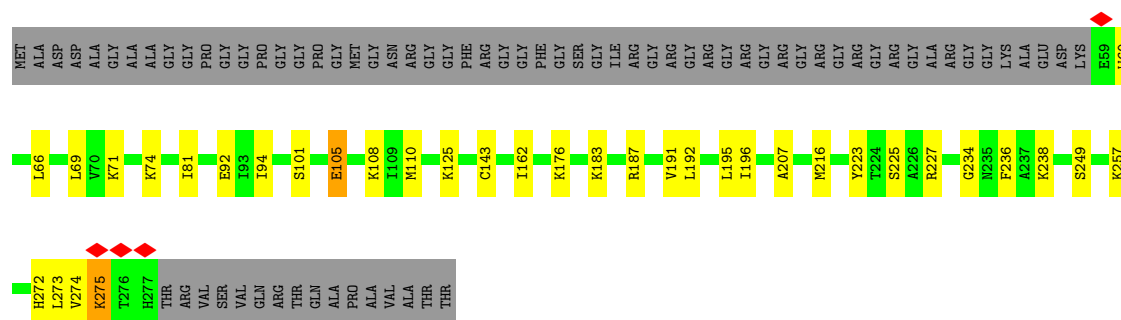
- Chain c:  84% 28% 14%



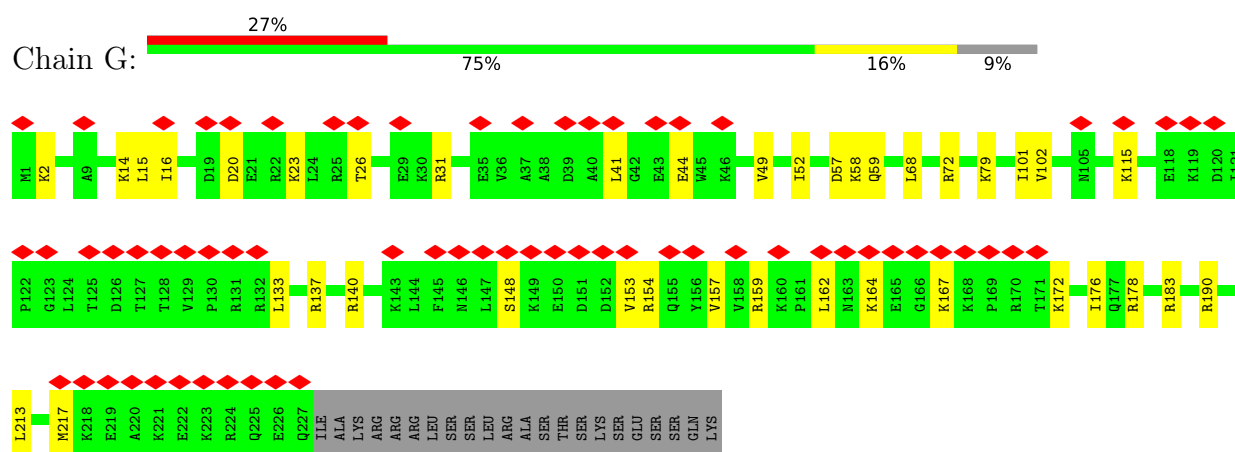
- Chain d:  84% 91% 5% . .



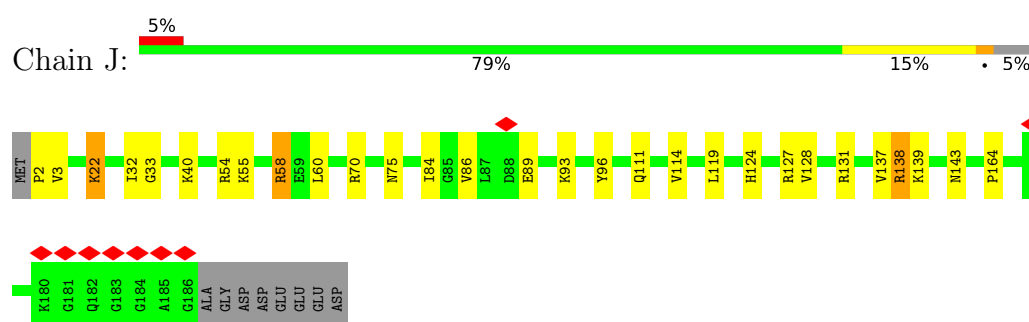
- Chain C: 62% 12% 25%



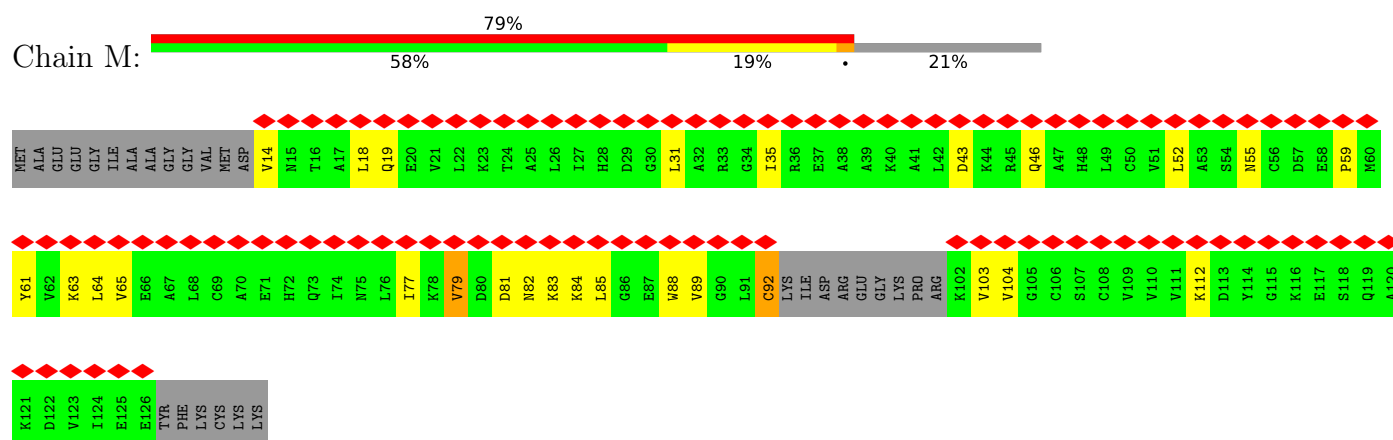
- WORLDWIDE
PDB
PROTEIN DATA BANK



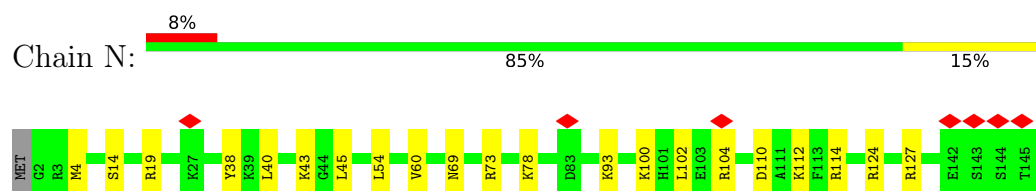
• Molecule 24: 40S ribosomal protein S9



• Molecule 25: 40S ribosomal protein S12

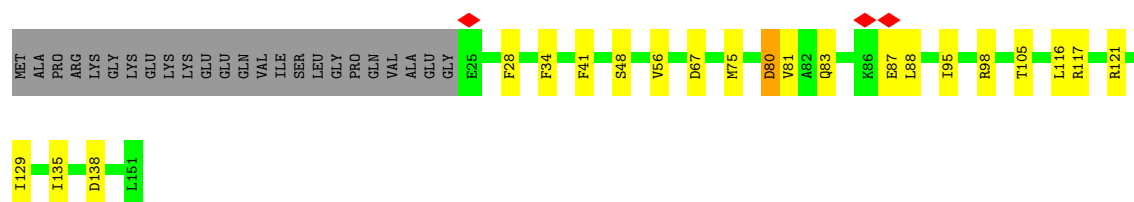


• Molecule 26: 40S ribosomal protein S13



• Molecule 27: 40S ribosomal protein S14





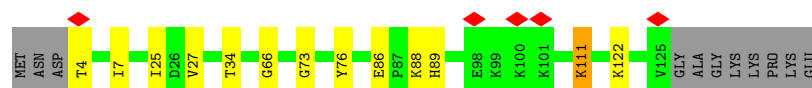
- Molecule 28: 40S ribosomal protein S15a

Chain W: 90% 9%



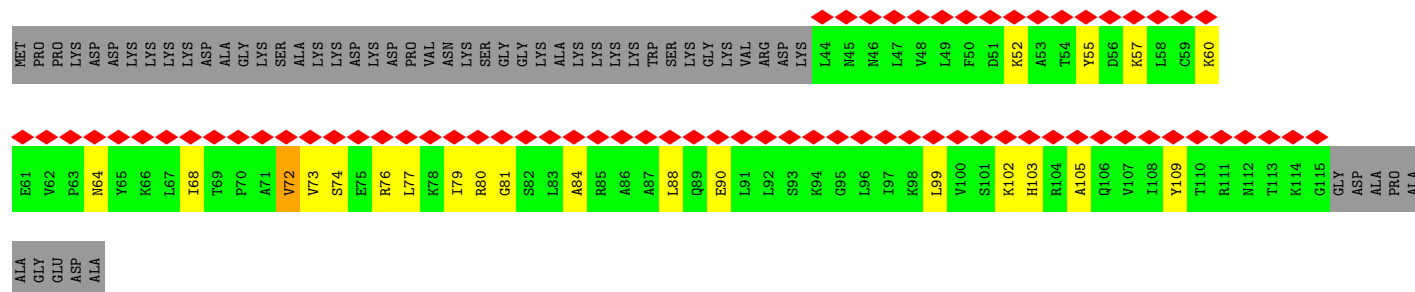
- Molecule 29: 40S ribosomal protein S24

Chain Y: 82% 9% 8%



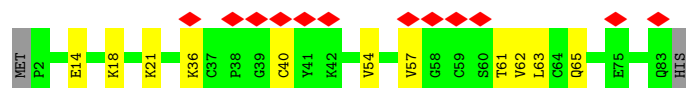
- Molecule 30: 40S ribosomal protein S25

Chain Z: 58% 40% 17% 42%



- Molecule 31: 40S ribosomal protein S27

Chain b: 14% 85% 13%

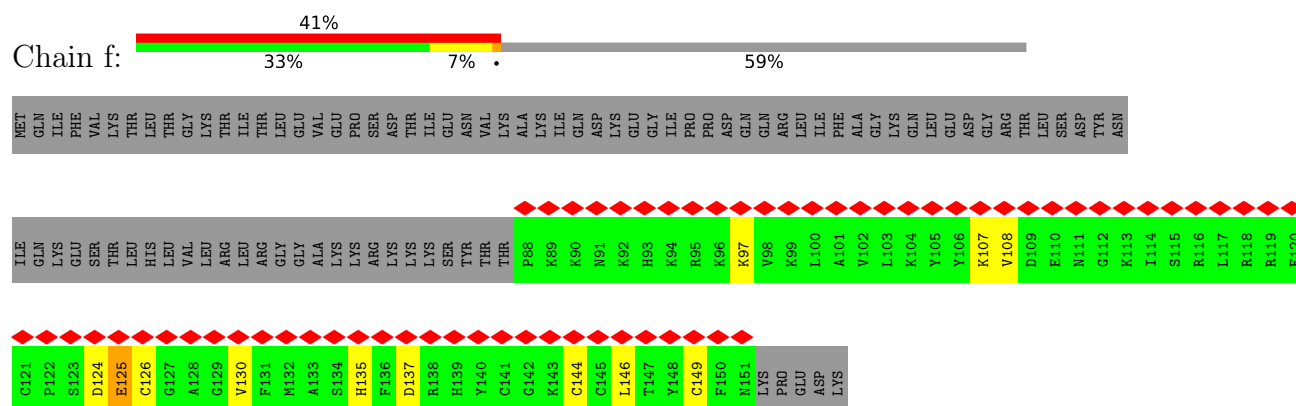


- Molecule 32: 40S ribosomal protein S30

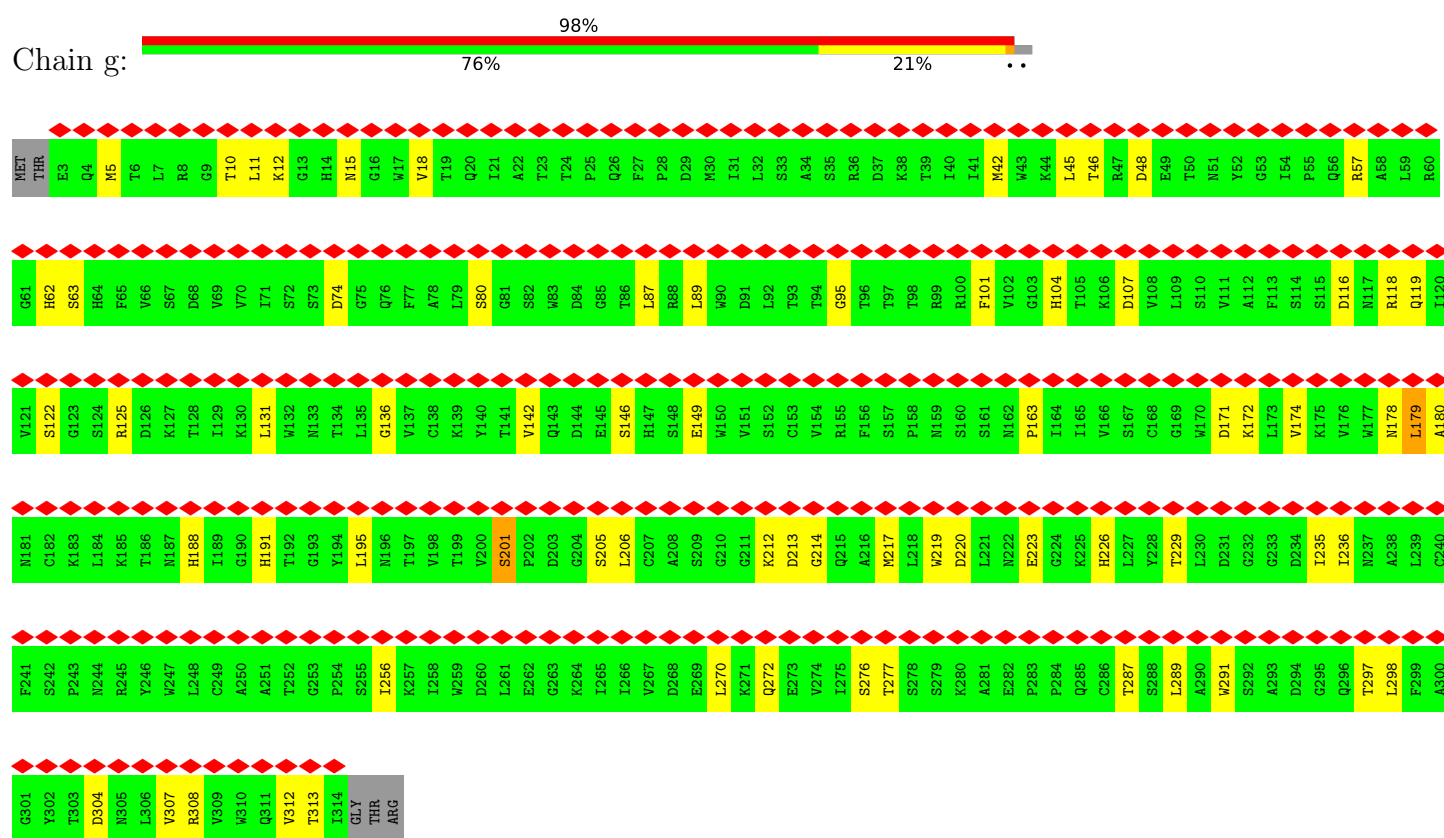
Chain e: 17% 68% 24% 7%



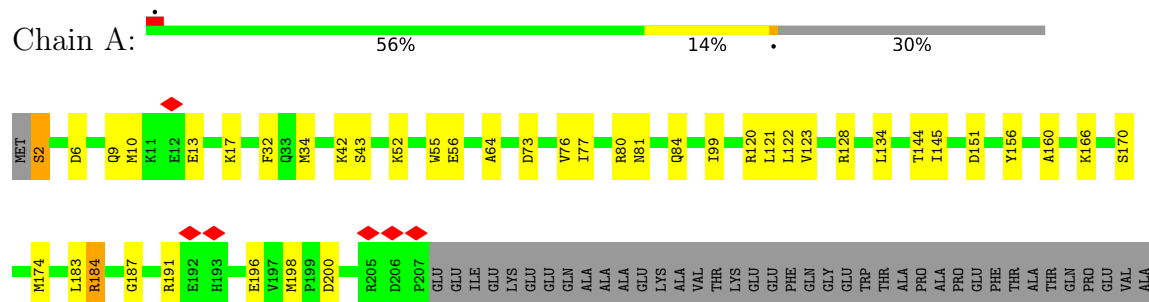
• Molecule 33: Ubiquitin-40S ribosomal protein S27a



• Molecule 34: Receptor of activated protein C kinase 1



• Molecule 35: 40S ribosomal protein SA



ASP	TRP	SER	GLU	GLY	VAL	GLN	VAL	PRO	SER	VAL	PRO	ILE	GLN	GLN	PHE	PRO	THR	GLU	ASP	TRP	SER	ALA	GLN	PRO	ALA	THR	GLU	ASP	TRP	SER	ALA	ALA	PRO	THR	ALA	GLN	ALA	THR	GLU	TRP	VAL	GLY	ALA	THR	THR	ASP	TRP	SER
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	474276	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 ($e^-/\text{\AA}^2$)	40.56	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.283	Depositor
Minimum map value	-0.102	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	423.2704, 423.2704, 423.2704	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8267, 0.8267, 0.8267	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: SAC, PSU, 7MG, HY3, MG, B8N, MA6, A2M, K, 4AC, AME, OMG, OMC, 6MZ, IAS, OMU, ZN

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	n	0.50	0/194	0.78	0/246
2	2	0.55	2/37770 (0.0%)	0.54	2/58857 (0.0%)
3	B	0.40	0/1738	0.49	0/2325
4	D	0.49	0/1773	0.64	0/2387
5	E	0.41	0/2083	0.53	0/2805
6	F	0.46	0/1465	0.65	0/1969
7	H	0.30	0/1498	0.55	0/2005
8	I	0.51	0/1711	0.67	0/2282
9	K	0.48	0/840	0.67	3/1133 (0.3%)
10	L	0.44	0/1177	0.53	0/1574
11	P	0.34	0/1024	0.52	0/1369
12	Q	0.40	0/1122	0.59	2/1503 (0.1%)
13	R	0.42	0/1078	0.59	2/1447 (0.1%)
14	S	0.39	0/1214	0.59	0/1626
15	T	0.41	0/1131	0.52	0/1515
16	U	0.37	0/831	0.57	0/1115
17	V	0.44	0/635	0.54	0/850
18	X	0.48	0/1096	0.61	0/1461
19	a	0.58	0/805	0.67	0/1079
20	c	0.52	0/465	0.70	0/621
21	d	0.39	0/470	0.51	0/623
22	C	0.54	0/1748	0.62	0/2361
23	G	0.34	0/1863	0.52	0/2481
24	J	0.52	0/1550	0.71	0/2069
25	M	0.26	0/796	0.48	0/1072
26	N	0.37	0/1232	0.55	0/1656
27	O	0.54	0/960	0.66	0/1284
28	W	0.52	0/1051	0.64	0/1406
29	Y	0.41	0/1019	0.49	0/1354
30	Z	0.29	0/576	0.59	0/774
31	b	0.36	0/653	0.49	0/876
32	e	0.39	0/443	0.56	0/582

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	f	0.56	0/533	0.80	0/706
34	g	0.40	0/2486	0.59	1/3384 (0.0%)
35	A	0.46	0/1659	0.53	0/2254
All	All	0.49	2/76689 (0.0%)	0.56	10/111051 (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
7	H	0	2
14	S	0	1
16	U	0	1
24	J	0	1
35	A	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1622	U	O3'-P	-13.48	1.41	1.61
2	2	99	A2M	O3'-P	5.80	1.62	1.56

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	R	86	PRO	N-CD-CG	-7.13	92.51	103.20
2	2	1622	U	P-O3'-C3'	6.93	130.59	120.20
9	K	18	GLU	N-CA-C	-6.08	97.38	108.02
9	K	63	ALA	CA-C-N	5.88	132.78	121.54
9	K	63	ALA	C-N-CA	5.88	132.78	121.54

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	H	15	LYS	Peptide
7	H	42	GLU	Peptide
24	J	137	VAL	Peptide
14	S	99	LEU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
16	U	107	GLU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	n	193	0	237	3	0
2	2	35347	0	17896	284	0
3	B	1711	0	1782	23	0
4	D	1745	0	1839	19	0
5	E	2041	0	2143	12	0
6	F	1445	0	1495	13	0
7	H	1477	0	1573	24	0
8	I	1682	0	1769	11	0
9	K	816	0	841	10	0
10	L	1157	0	1222	9	0
11	P	1005	0	1053	13	0
12	Q	1105	0	1172	10	0
13	R	1064	0	1118	17	0
14	S	1192	0	1253	15	0
15	T	1112	0	1146	3	0
16	U	821	0	883	11	0
17	V	639	0	638	14	0
18	X	1088	0	1149	10	0
19	a	792	0	841	16	0
20	c	464	0	488	10	0
21	d	459	0	448	4	0
22	C	1708	0	1797	25	0
23	G	1840	0	1989	26	0
24	J	1525	0	1640	18	0
25	M	790	0	808	12	0
26	N	1208	0	1293	13	0
27	O	957	0	981	9	0
28	W	1034	0	1080	7	0
29	Y	1002	0	1075	8	0
30	Z	570	0	626	11	0
31	b	640	0	665	5	0
32	e	438	0	484	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	f	522	0	529	8	0
34	g	2429	0	2386	34	0
35	A	1628	0	1649	28	0
36	2	76	0	0	0	0
36	E	1	0	0	0	0
36	L	1	0	0	0	0
36	O	1	0	0	0	0
36	S	1	0	0	0	0
36	U	1	0	0	0	0
36	d	1	0	0	0	0
37	2	88	0	0	0	0
38	a	1	0	0	0	0
38	d	1	0	0	0	0
38	f	1	0	0	0	0
39	2	3102	0	0	16	0
39	A	30	0	0	1	0
39	B	30	0	0	1	0
39	C	56	0	0	3	0
39	D	24	0	0	0	0
39	E	79	0	0	0	0
39	F	34	0	0	0	0
39	G	18	0	0	0	0
39	H	8	0	0	0	0
39	I	45	0	0	0	0
39	J	85	0	0	0	0
39	K	20	0	0	0	0
39	L	62	0	0	0	0
39	N	30	0	0	1	0
39	O	28	0	0	0	0
39	P	32	0	0	0	0
39	Q	46	0	0	0	0
39	R	13	0	0	0	0
39	S	30	0	0	0	0
39	T	51	0	0	0	0
39	U	25	0	0	0	0
39	V	19	0	0	0	0
39	W	63	0	0	1	0
39	X	47	0	0	0	0
39	Y	25	0	0	0	0
39	Z	2	0	0	0	0
39	a	30	0	0	2	0
39	b	12	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	c	6	0	0	1	0
39	d	26	0	0	0	0
39	e	13	0	0	1	0
39	g	16	0	0	0	0
39	n	10	0	0	0	0
All	All	77936	0	57988	651	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 651 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:J:54:ARG:O	24:J:58:ARG:HG3	1.65	0.95
26:N:73:ARG:HD2	39:N:201:HOH:O	1.67	0.95
2:2:925:G:H1	2:2:1017:U:H3	1.18	0.88
2:2:928:G:H1	2:2:1013:U:H3	1.21	0.86
39:2:4896:HOH:O	14:S:28[B]:PHE:HE1	1.60	0.85

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
1	n	18/25 (72%)	17 (94%)	1 (6%)	0	100	100
3	B	208/264 (79%)	202 (97%)	6 (3%)	0	100	100
4	D	222/243 (91%)	218 (98%)	4 (2%)	0	100	100
5	E	255/263 (97%)	251 (98%)	4 (2%)	0	100	100
6	F	178/204 (87%)	171 (96%)	7 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	H	180/194 (93%)	156 (87%)	24 (13%)	0	100	100
8	I	203/208 (98%)	199 (98%)	4 (2%)	0	100	100
9	K	95/165 (58%)	86 (90%)	8 (8%)	1 (1%)	11	7
10	L	137/158 (87%)	131 (96%)	6 (4%)	0	100	100
11	P	121/145 (83%)	118 (98%)	2 (2%)	1 (1%)	16	10
12	Q	137/146 (94%)	131 (96%)	6 (4%)	0	100	100
13	R	129/135 (96%)	121 (94%)	8 (6%)	0	100	100
14	S	142/152 (93%)	138 (97%)	4 (3%)	0	100	100
15	T	141/145 (97%)	139 (99%)	2 (1%)	0	100	100
16	U	102/119 (86%)	98 (96%)	4 (4%)	0	100	100
17	V	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
18	X	137/143 (96%)	135 (98%)	2 (2%)	0	100	100
19	a	97/115 (84%)	95 (98%)	2 (2%)	0	100	100
20	c	57/69 (83%)	53 (93%)	4 (7%)	0	100	100
21	d	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
22	C	218/293 (74%)	212 (97%)	6 (3%)	0	100	100
23	G	225/249 (90%)	221 (98%)	4 (2%)	0	100	100
24	J	183/194 (94%)	177 (97%)	5 (3%)	1 (0%)	24	20
25	M	100/132 (76%)	92 (92%)	8 (8%)	0	100	100
26	N	148/151 (98%)	144 (97%)	4 (3%)	0	100	100
27	O	123/151 (82%)	120 (98%)	3 (2%)	0	100	100
28	W	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
29	Y	120/133 (90%)	118 (98%)	2 (2%)	0	100	100
30	Z	70/125 (56%)	68 (97%)	2 (3%)	0	100	100
31	b	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
32	e	53/59 (90%)	48 (91%)	5 (9%)	0	100	100
33	f	62/156 (40%)	56 (90%)	6 (10%)	0	100	100
34	g	310/317 (98%)	286 (92%)	24 (8%)	0	100	100
35	A	205/295 (70%)	200 (98%)	5 (2%)	0	100	100
All	All	4717/5501 (86%)	4535 (96%)	179 (4%)	3 (0%)	49	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	K	19	GLY
24	J	138	ARG
11	P	18	ARG

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
1	n	19/24 (79%)	19 (100%)	0	100	100
3	B	192/231 (83%)	184 (96%)	8 (4%)	26	25
4	D	188/202 (93%)	174 (93%)	14 (7%)	13	8
5	E	220/225 (98%)	218 (99%)	2 (1%)	70	77
6	F	155/170 (91%)	146 (94%)	9 (6%)	18	14
7	H	164/174 (94%)	155 (94%)	9 (6%)	19	15
8	I	178/180 (99%)	168 (94%)	10 (6%)	19	15
9	K	88/136 (65%)	83 (94%)	5 (6%)	18	14
10	L	128/142 (90%)	126 (98%)	2 (2%)	55	61
11	P	109/130 (84%)	106 (97%)	3 (3%)	38	40
12	Q	115/121 (95%)	111 (96%)	4 (4%)	32	32
13	R	119/122 (98%)	112 (94%)	7 (6%)	18	13
14	S	125/132 (95%)	123 (98%)	2 (2%)	55	61
15	T	113/115 (98%)	113 (100%)	0	100	100
16	U	94/107 (88%)	91 (97%)	3 (3%)	34	36
17	V	66/66 (100%)	65 (98%)	1 (2%)	57	64
18	X	111/114 (97%)	107 (96%)	4 (4%)	31	31
19	a	86/98 (88%)	82 (95%)	4 (5%)	23	21
20	c	52/62 (84%)	47 (90%)	5 (10%)	8	4
21	d	48/49 (98%)	47 (98%)	1 (2%)	47	52
22	C	186/225 (83%)	181 (97%)	5 (3%)	39	41
23	G	198/218 (91%)	191 (96%)	7 (4%)	32	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	J	161/168 (96%)	153 (95%)	8 (5%)	22	18
25	M	86/108 (80%)	77 (90%)	9 (10%)	6	3
26	N	130/131 (99%)	126 (97%)	4 (3%)	35	37
27	O	99/118 (84%)	92 (93%)	7 (7%)	13	8
28	W	112/113 (99%)	111 (99%)	1 (1%)	70	77
29	Y	107/115 (93%)	104 (97%)	3 (3%)	38	40
30	Z	63/103 (61%)	61 (97%)	2 (3%)	34	36
31	b	74/76 (97%)	72 (97%)	2 (3%)	39	41
32	e	45/48 (94%)	39 (87%)	6 (13%)	4	1
33	f	57/140 (41%)	54 (95%)	3 (5%)	20	17
34	g	271/275 (98%)	255 (94%)	16 (6%)	18	13
35	A	172/242 (71%)	170 (99%)	2 (1%)	63	70
All	All	4131/4680 (88%)	3963 (96%)	168 (4%)	28	26

5 of 168 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	M	43	ASP
32	e	43	VAL
25	M	79	VAL
27	O	105	THR
34	g	12	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
14	S	73	ASN
35	A	9	GLN
18	X	26	GLN
35	A	141	ASN
34	g	76	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2	1628/1868 (87%)	263 (16%)	7 (0%)

5 of 263 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	2	4	C
2	2	17	C
2	2	33	G
2	2	46	A
2	2	56	G

5 of 7 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	1165	G
2	2	1434	C
2	2	1679	A
2	2	1520	G
2	2	912	C

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

77 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	A2M	2	590	2	22,25,26	3.18	9 (40%)	31,36,39	3.21	14 (45%)
2	A2M	2	99	37,2	22,25,26	3.19	9 (40%)	31,36,39	3.05	11 (35%)
2	PSU	2	1692	36,2	18,21,22	3.74	7 (38%)	22,30,33	1.79	4 (18%)
2	OMC	2	1391	2	19,22,23	2.70	8 (42%)	26,31,34	0.91	0
2	OMU	2	354	2	19,22,23	2.88	8 (42%)	26,31,34	1.91	6 (23%)
2	OMG	2	1490	37,2	23,26,27	1.22	3 (13%)	33,38,41	1.95	7 (21%)
2	PSU	2	119	2	18,21,22	3.99	7 (38%)	22,30,33	1.80	5 (22%)
2	A2M	2	166	2	22,25,26	3.28	10 (45%)	31,36,39	3.04	12 (38%)
2	OMU	2	121	2	19,22,23	2.73	8 (42%)	26,31,34	1.75	5 (19%)
2	A2M	2	468	2	22,25,26	3.23	11 (50%)	31,36,39	3.17	11 (35%)
2	PSU	2	572	36,2	18,21,22	4.06	7 (38%)	22,30,33	1.88	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	4AC	2	1842	2	21,24,25	3.02	10 (47%)	29,34,37	1.51	4 (13%)
2	OMC	2	462	2	19,22,23	2.73	8 (42%)	26,31,34	0.77	0
2	PSU	2	681	2	18,21,22	3.93	8 (44%)	22,30,33	1.83	4 (18%)
2	PSU	2	814	2	18,21,22	3.86	7 (38%)	22,30,33	1.66	3 (13%)
2	PSU	2	296	2	18,21,22	3.97	7 (38%)	22,30,33	1.81	5 (22%)
2	A2M	2	484	2	22,25,26	1.45	4 (18%)	31,36,39	2.03	9 (29%)
2	OMG	2	509	37,2	23,26,27	2.30	8 (34%)	33,38,41	2.12	14 (42%)
2	A2M	2	576	36,2	22,25,26	3.33	11 (50%)	31,36,39	2.98	13 (41%)
2	PSU	2	406	2	18,21,22	3.94	7 (38%)	22,30,33	1.78	4 (18%)
2	A2M	2	1383	2	22,25,26	3.41	11 (50%)	31,36,39	3.02	14 (45%)
2	A2M	2	668	37,2	22,25,26	1.46	5 (22%)	31,36,39	2.11	11 (35%)
2	PSU	2	1244	2	18,21,22	3.98	7 (38%)	22,30,33	2.12	5 (22%)
2	PSU	2	1046	36,2	18,21,22	4.00	7 (38%)	22,30,33	1.78	3 (13%)
2	A2M	2	512	2	22,25,26	3.28	10 (45%)	31,36,39	3.12	14 (45%)
2	B8N	2	1248	2	24,29,30	2.86	7 (29%)	29,42,45	1.91	7 (24%)
2	OMU	2	1326	37,2	19,22,23	2.86	8 (42%)	26,31,34	2.02	5 (19%)
2	OMC	2	174	37,2	19,22,23	2.75	8 (42%)	26,31,34	0.93	0
2	PSU	2	1445	2	18,21,22	3.99	7 (38%)	22,30,33	1.78	4 (18%)
2	OMU	2	172	2	19,22,23	2.86	7 (36%)	26,31,34	1.85	6 (23%)
2	PSU	2	1625	2	18,21,22	3.95	7 (38%)	22,30,33	1.92	5 (22%)
35	SAC	A	2	35	7,8,9	1.57	2 (28%)	8,9,11	1.45	2 (25%)
2	PSU	2	105	36,2	18,21,22	3.91	7 (38%)	22,30,33	2.12	5 (22%)
2	A2M	2	1678	2	22,25,26	1.39	4 (18%)	31,36,39	2.15	9 (29%)
2	PSU	2	36	2	18,21,22	1.45	4 (22%)	22,30,33	1.80	4 (18%)
2	PSU	2	649	2	18,21,22	4.06	7 (38%)	22,30,33	1.93	5 (22%)
2	OMU	2	428	37,2	19,22,23	2.86	8 (42%)	26,31,34	1.59	5 (19%)
2	OMU	2	1288	2	19,22,23	2.86	7 (36%)	26,31,34	1.75	4 (15%)
2	PSU	2	93	2	18,21,22	4.01	7 (38%)	22,30,33	1.66	4 (18%)
2	MA6	2	1851	2	23,26,27	1.46	5 (21%)	34,38,41	2.40	14 (41%)
2	OMG	2	601	2	23,26,27	2.26	8 (34%)	33,38,41	2.24	14 (42%)
2	PSU	2	1056	2	18,21,22	3.82	7 (38%)	22,30,33	2.08	5 (22%)
27	IAS	O	138	27	6,7,8	0.99	0	6,8,10	1.97	3 (50%)
2	6MZ	2	1832	36,37,2	22,25,26	3.56	6 (27%)	30,36,39	2.33	10 (33%)
2	OMC	2	1272	2	19,22,23	2.71	8 (42%)	26,31,34	0.68	0
2	7MG	2	1639	2	22,26,27	1.38	3 (13%)	29,39,42	2.53	7 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	4AC	2	1337	2	21,24,25	3.37	10 (47%)	29,34,37	1.63	6 (20%)
2	OMG	2	683	2	23,26,27	2.34	8 (34%)	33,38,41	2.16	14 (42%)
2	PSU	2	1081	2	18,21,22	3.99	8 (44%)	22,30,33	1.87	6 (27%)
2	PSU	2	1643	37,2	18,21,22	1.48	4 (22%)	22,30,33	1.89	4 (18%)
2	OMG	2	644	2	23,26,27	2.26	9 (39%)	33,38,41	2.17	12 (36%)
2	PSU	2	109	36,2	18,21,22	4.06	7 (38%)	22,30,33	1.82	4 (18%)
2	PSU	2	1174	36,2	18,21,22	1.41	3 (16%)	22,30,33	1.83	3 (13%)
2	PSU	2	1232	2	18,21,22	3.98	7 (38%)	22,30,33	1.74	4 (18%)
2	OMG	2	1328	36,2	23,26,27	2.33	9 (39%)	33,38,41	2.44	11 (33%)
2	OMC	2	517	2	19,22,23	2.68	8 (42%)	26,31,34	0.79	0
2	MA6	2	1850	2	23,26,27	1.46	3 (13%)	34,38,41	2.52	13 (38%)
2	OMC	2	1703	2	19,22,23	2.67	8 (42%)	26,31,34	0.86	0
2	A2M	2	27	37,2	22,25,26	1.44	4 (18%)	31,36,39	2.31	12 (38%)
17	AME	V	1	17	9,10,11	1.36	1 (11%)	9,11,13	2.01	2 (22%)
2	OMU	2	1442	37,2	19,22,23	2.87	8 (42%)	26,31,34	1.81	5 (19%)
2	PSU	2	822	2	18,21,22	3.94	8 (44%)	22,30,33	1.77	4 (18%)
2	PSU	2	1177	2	18,21,22	1.36	4 (22%)	22,30,33	1.89	4 (18%)
2	PSU	2	651	2	18,21,22	3.93	8 (44%)	22,30,33	2.29	5 (22%)
2	OMU	2	116	2	19,22,23	2.78	7 (36%)	26,31,34	1.56	5 (19%)
2	A2M	2	1031	2	22,25,26	3.24	11 (50%)	31,36,39	3.16	12 (38%)
2	PSU	2	1238	2	18,21,22	3.92	7 (38%)	22,30,33	1.79	4 (18%)
2	PSU	2	1136	2	18,21,22	3.86	8 (44%)	22,30,33	1.96	4 (18%)
2	OMG	2	1447	2	23,26,27	2.26	9 (39%)	33,38,41	2.28	12 (36%)
18	HY3	X	62	36,18	6,8,9	8.45	4 (66%)	5,10,12	1.18	0
2	PSU	2	1347	2	18,21,22	1.44	3 (16%)	22,30,33	1.90	4 (18%)
2	PSU	2	815	2	18,21,22	4.01	7 (38%)	22,30,33	1.85	4 (18%)
2	PSU	2	686	2	18,21,22	4.08	7 (38%)	22,30,33	1.98	5 (22%)
2	PSU	2	863	2	18,21,22	3.72	7 (38%)	22,30,33	2.05	5 (22%)
2	PSU	2	1045	2	18,21,22	4.14	7 (38%)	22,30,33	1.94	5 (22%)
2	OMG	2	436	2	23,26,27	2.33	8 (34%)	33,38,41	2.15	14 (42%)
2	A2M	2	159	2	22,25,26	3.22	9 (40%)	31,36,39	3.13	14 (45%)

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
2	A2M	2	590	2	-	0/9/27/28	0/3/3/3
2	A2M	2	99	37,2	-	2/9/27/28	0/3/3/3
2	PSU	2	1692	36,2	-	0/7/25/26	0/2/2/2
2	OMC	2	1391	2	-	0/9/27/28	0/2/2/2
2	OMU	2	354	2	-	0/9/27/28	0/2/2/2
2	OMG	2	1490	37,2	-	1/9/27/28	0/3/3/3
2	PSU	2	119	2	-	0/7/25/26	0/2/2/2
2	A2M	2	166	2	-	0/9/27/28	0/3/3/3
2	OMU	2	121	2	-	0/9/27/28	0/2/2/2
2	A2M	2	468	2	-	1/9/27/28	0/3/3/3
2	PSU	2	572	36,2	-	0/7/25/26	0/2/2/2
2	4AC	2	1842	2	-	2/11/29/30	0/2/2/2
2	OMC	2	462	2	-	0/9/27/28	0/2/2/2
2	PSU	2	681	2	-	0/7/25/26	0/2/2/2
2	PSU	2	814	2	-	0/7/25/26	0/2/2/2
2	PSU	2	296	2	-	0/7/25/26	0/2/2/2
2	A2M	2	484	2	-	1/9/27/28	0/3/3/3
2	OMG	2	509	37,2	-	0/9/27/28	0/3/3/3
2	A2M	2	576	36,2	-	2/9/27/28	0/3/3/3
2	PSU	2	406	2	-	0/7/25/26	0/2/2/2
2	A2M	2	1383	2	-	0/9/27/28	0/3/3/3
2	A2M	2	668	37,2	-	3/9/27/28	0/3/3/3
2	PSU	2	1244	2	-	0/7/25/26	0/2/2/2
2	PSU	2	1046	36,2	-	0/7/25/26	0/2/2/2
2	A2M	2	512	2	-	0/9/27/28	0/3/3/3
2	B8N	2	1248	2	-	2/16/34/35	0/2/2/2
2	OMU	2	1326	37,2	-	0/9/27/28	0/2/2/2
2	OMC	2	174	37,2	-	1/9/27/28	0/2/2/2
2	PSU	2	1445	2	-	0/7/25/26	0/2/2/2
2	OMU	2	172	2	-	1/9/27/28	0/2/2/2
2	PSU	2	1625	2	-	0/7/25/26	0/2/2/2
35	SAC	A	2	35	-	0/7/8/10	-
2	PSU	2	105	36,2	-	0/7/25/26	0/2/2/2
2	A2M	2	1678	2	-	1/9/27/28	0/3/3/3
2	PSU	2	36	2	-	0/7/25/26	0/2/2/2
2	PSU	2	649	2	-	0/7/25/26	0/2/2/2
2	OMU	2	428	37,2	-	4/9/27/28	0/2/2/2
2	OMU	2	1288	2	-	0/9/27/28	0/2/2/2
2	PSU	2	93	2	-	0/7/25/26	0/2/2/2
2	MA6	2	1851	2	-	6/11/29/30	0/3/3/3
2	OMG	2	601	2	-	0/9/27/28	0/3/3/3
2	PSU	2	1056	2	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	IAS	O	138	27	-	2/7/7/8	-
2	6MZ	2	1832	36,37,2	-	0/9/27/28	0/3/3/3
2	OMC	2	1272	2	-	0/9/27/28	0/2/2/2
2	7MG	2	1639	2	-	0/7/37/38	0/3/3/3
2	4AC	2	1337	2	-	2/11/29/30	0/2/2/2
2	OMG	2	683	2	-	0/9/27/28	0/3/3/3
2	PSU	2	1081	2	-	1/7/25/26	0/2/2/2
2	PSU	2	1643	37,2	-	0/7/25/26	0/2/2/2
2	OMG	2	644	2	-	1/9/27/28	0/3/3/3
2	PSU	2	109	36,2	-	0/7/25/26	0/2/2/2
2	PSU	2	1174	36,2	-	0/7/25/26	0/2/2/2
2	PSU	2	1232	2	-	0/7/25/26	0/2/2/2
2	OMG	2	1328	36,2	-	0/9/27/28	0/3/3/3
2	OMC	2	517	2	-	0/9/27/28	0/2/2/2
2	MA6	2	1850	2	-	2/11/29/30	0/3/3/3
2	OMC	2	1703	2	-	0/9/27/28	0/2/2/2
2	A2M	2	27	37,2	-	1/9/27/28	0/3/3/3
17	AME	V	1	17	-	3/9/10/12	-
2	OMU	2	1442	37,2	-	0/9/27/28	0/2/2/2
2	PSU	2	822	2	-	0/7/25/26	0/2/2/2
2	PSU	2	1177	2	-	0/7/25/26	0/2/2/2
2	PSU	2	651	2	-	0/7/25/26	0/2/2/2
2	OMU	2	116	2	-	1/9/27/28	0/2/2/2
2	A2M	2	1031	2	-	0/9/27/28	0/3/3/3
2	PSU	2	1238	2	-	0/7/25/26	0/2/2/2
2	PSU	2	1136	2	-	0/7/25/26	0/2/2/2
2	OMG	2	1447	2	-	2/9/27/28	0/3/3/3
18	HY3	X	62	36,18	-	1/1/12/14	0/1/1/1
2	PSU	2	1347	2	-	1/7/25/26	0/2/2/2
2	PSU	2	815	2	-	0/7/25/26	0/2/2/2
2	PSU	2	686	2	-	0/7/25/26	0/2/2/2
2	PSU	2	863	2	-	0/7/25/26	0/2/2/2
2	PSU	2	1045	2	-	0/7/25/26	0/2/2/2
2	OMG	2	436	2	-	0/9/27/28	0/3/3/3
2	A2M	2	159	2	-	0/9/27/28	0/3/3/3

The worst 5 of 535 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	X	62	HY3	C3-CA	-19.76	1.35	1.55
2	2	1832	6MZ	C6-N6	14.91	1.50	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	686	PSU	C6-C5	10.90	1.48	1.35
2	2	93	PSU	C6-C5	10.88	1.48	1.35
2	2	815	PSU	C6-C5	10.84	1.47	1.35

The worst 5 of 497 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1639	7MG	N9-C4-N3	8.72	138.51	125.47
2	2	468	A2M	N6-C6-N1	-6.94	103.14	118.35
2	2	590	A2M	N6-C6-N1	-6.78	103.51	118.35
2	2	1328	OMG	C1'-N9-C8	-6.77	107.43	126.70
2	2	590	A2M	C5-C4-N3	-6.64	118.09	126.75

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	X	62	HY3	O-C-CA-C3
2	2	27	A2M	C1'-C2'-O2'-CM'
2	2	116	OMU	C1'-C2'-O2'-CM2
2	2	174	OMC	C1'-C2'-O2'-CM2
2	2	468	A2M	C1'-C2'-O2'-CM'

There are no ring outliers.

24 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	468	A2M	1	0
2	2	1842	4AC	4	0
2	2	462	OMC	2	0
2	2	296	PSU	1	0
2	2	484	A2M	1	0
2	2	509	OMG	1	0
2	2	576	A2M	2	0
2	2	1383	A2M	1	0
2	2	668	A2M	1	0
2	2	1046	PSU	1	0
2	2	174	OMC	1	0
2	2	1288	OMU	1	0
2	2	1639	7MG	1	0
2	2	683	OMG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	1643	PSU	1	0
2	2	1174	PSU	2	0
2	2	1232	PSU	2	0
2	2	1850	MA6	2	0
2	2	27	A2M	1	0
2	2	1442	OMU	1	0
2	2	116	OMU	3	0
2	2	1031	A2M	1	0
2	2	436	OMG	1	0
2	2	159	A2M	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 173 ligands modelled in this entry, 173 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

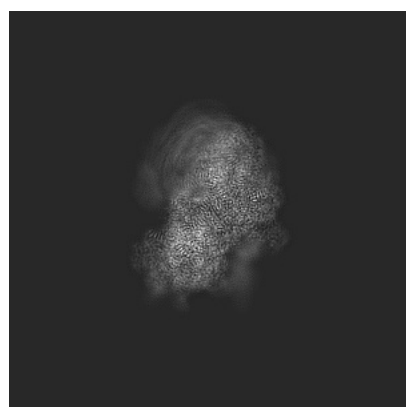
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14317. These allow visual inspection of the internal detail of the map and identification of artifacts.

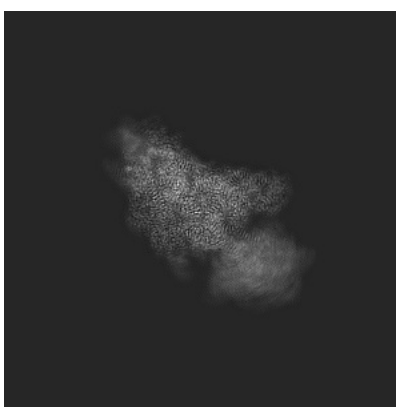
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

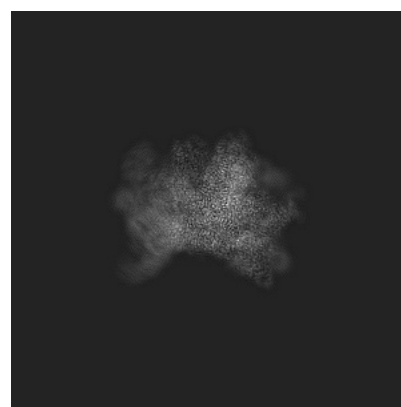
6.1.1 Primary map



X



Y

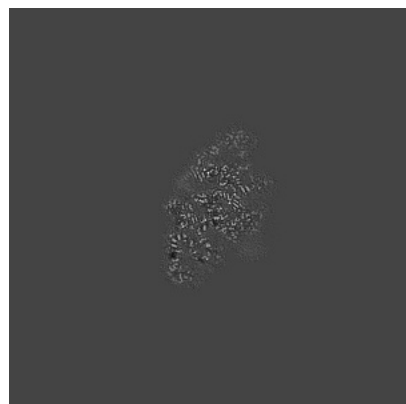


Z

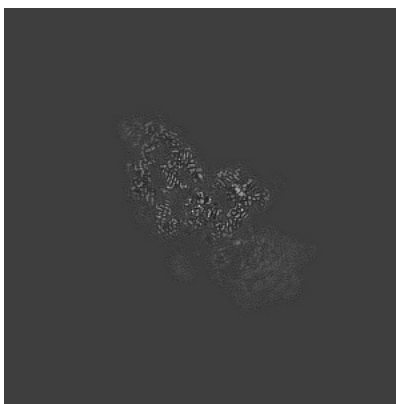
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

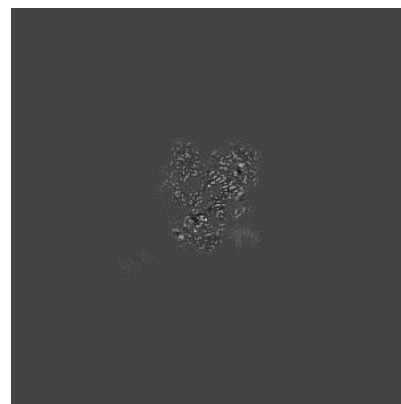
6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

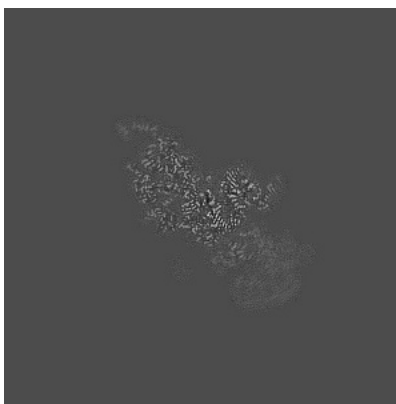
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

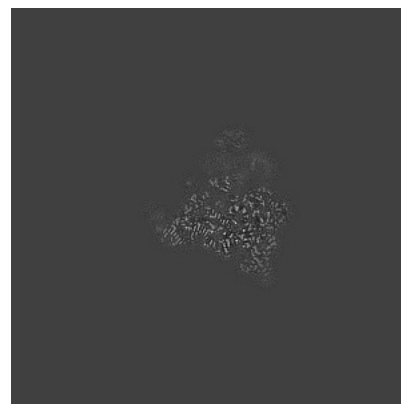
6.3.1 Primary map



X Index: 279



Y Index: 264

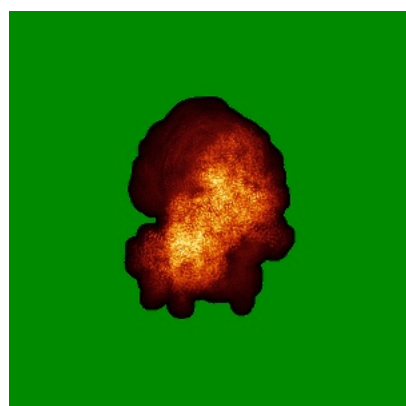


Z Index: 213

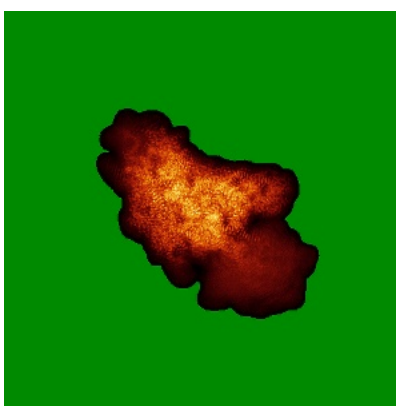
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

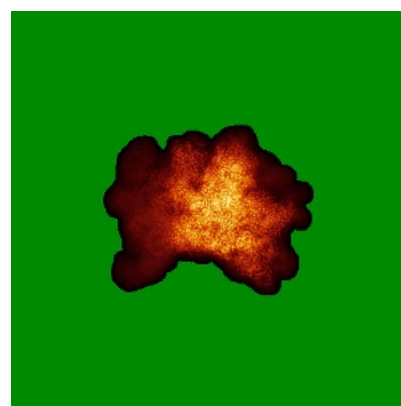
6.4.1 Primary map



X



Y

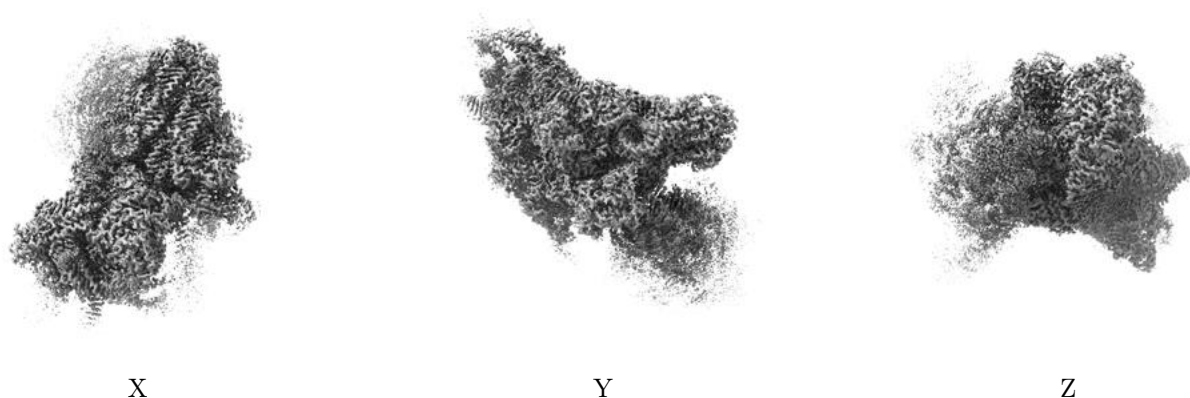


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

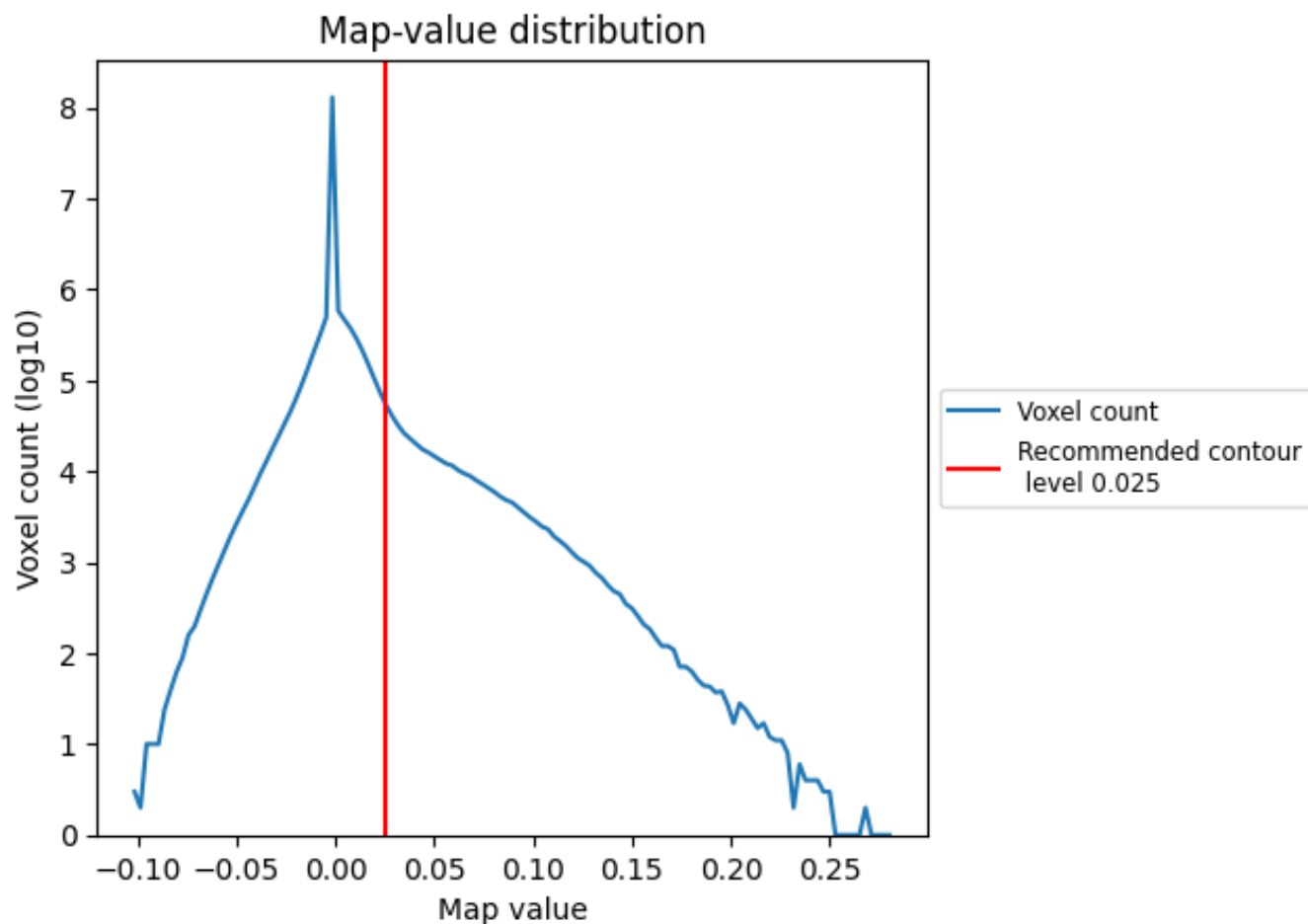
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

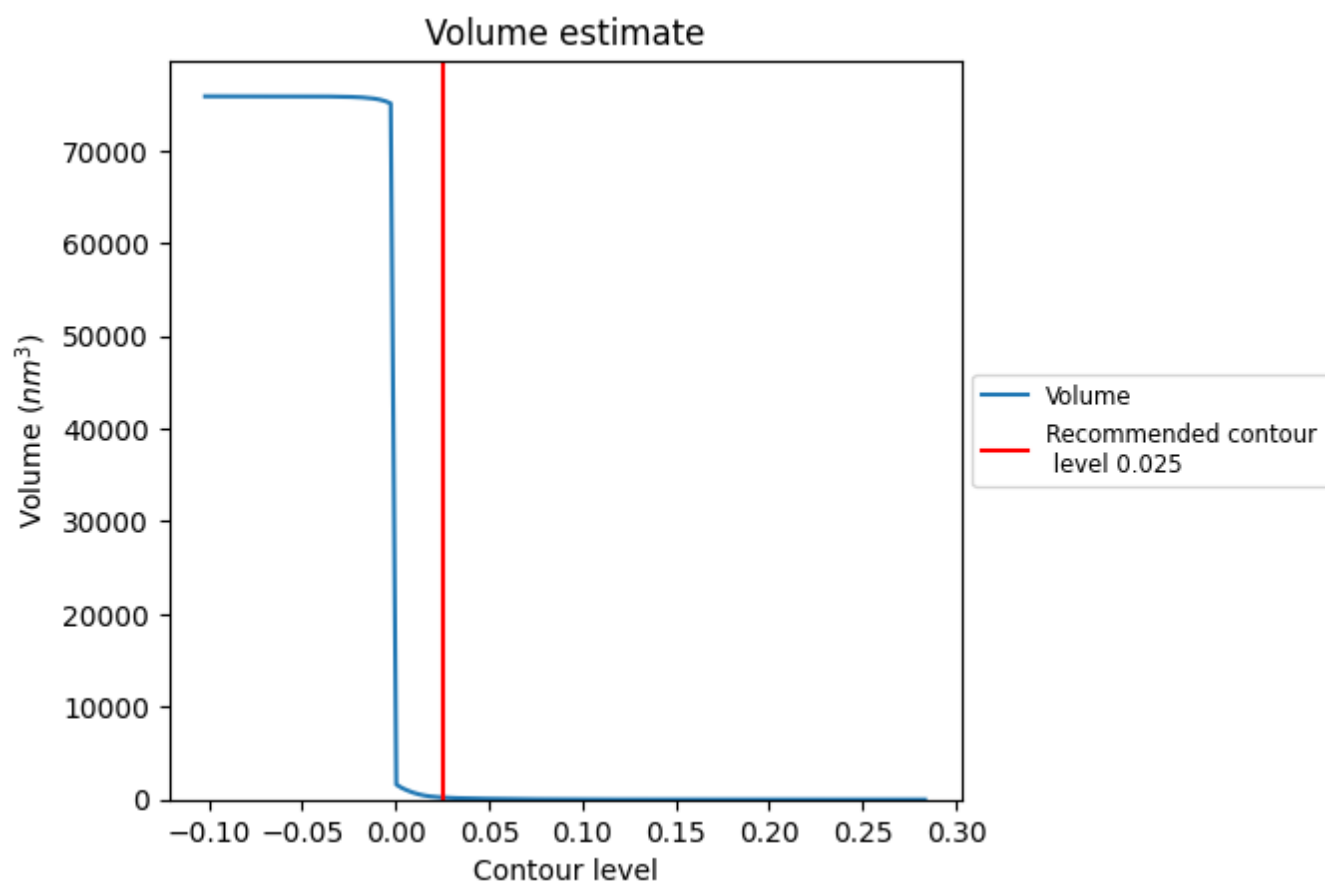
This section contains the results of statistical analysis of the map.

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.

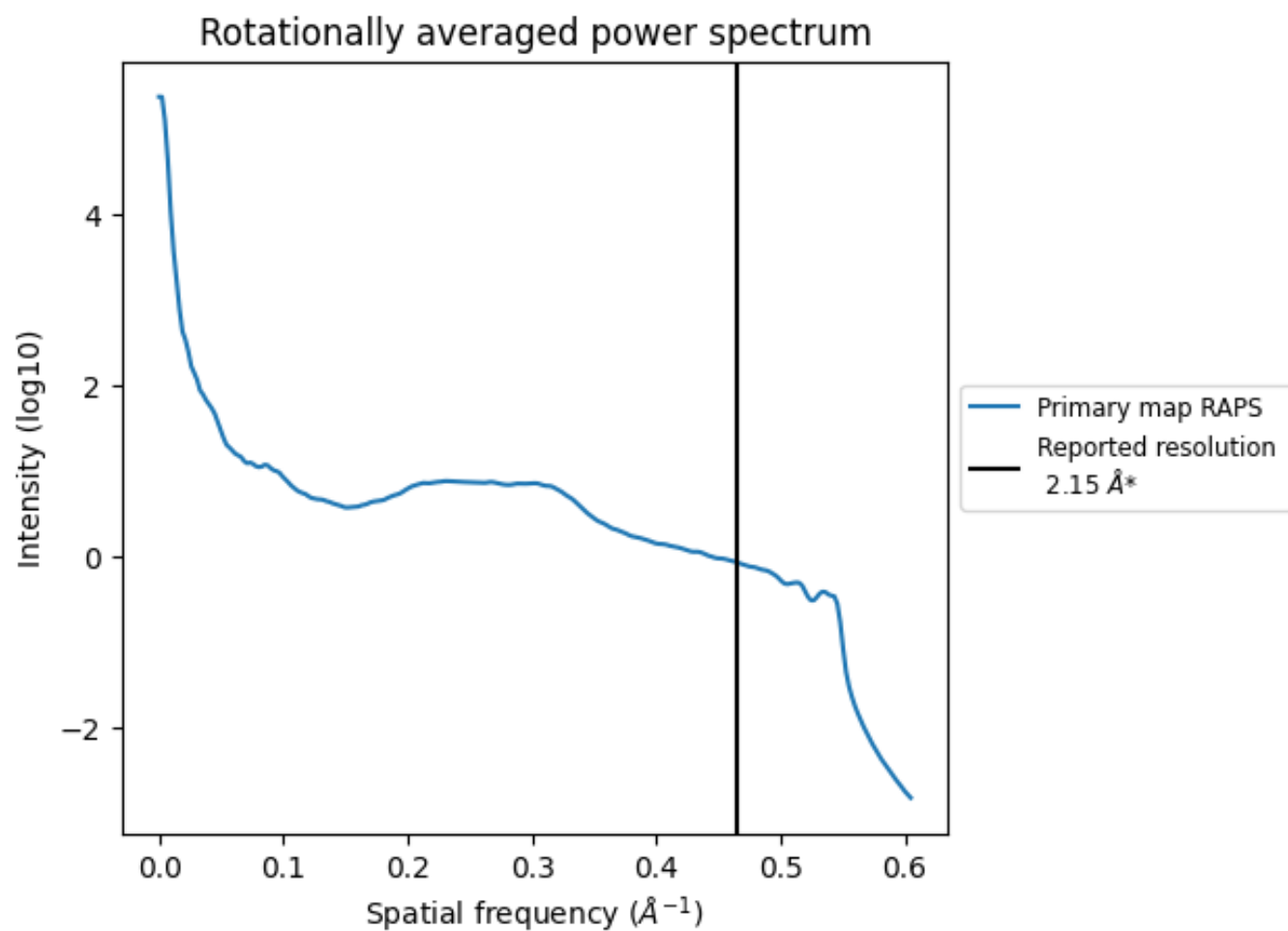
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 225 nm^3 ; this corresponds to an approximate mass of 203 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 ⓘ

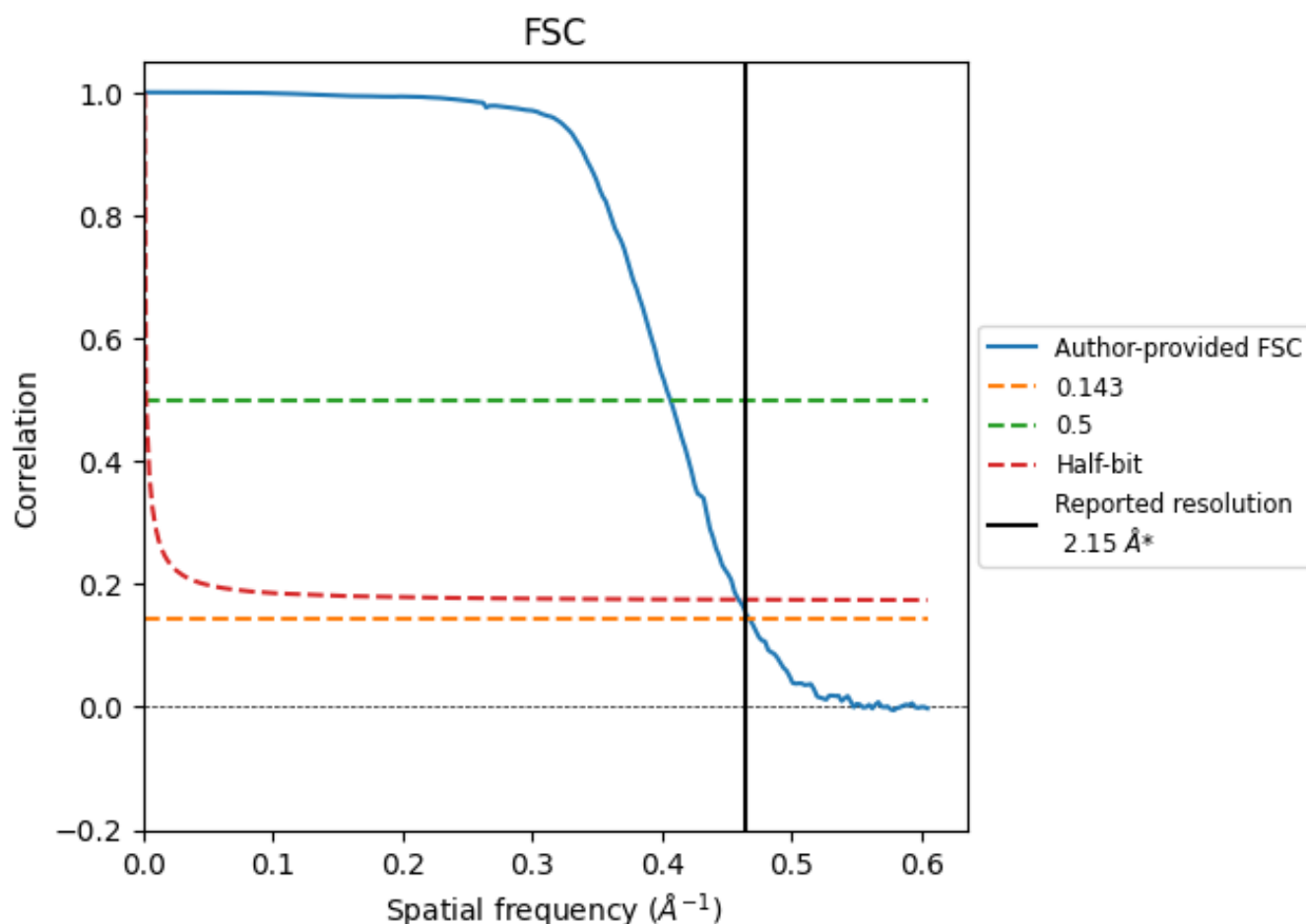


*Reported resolution corresponds to spatial frequency of 0.465 Å⁻¹

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 0.465 Å⁻¹

8.2 Resolution estimates [i](#)

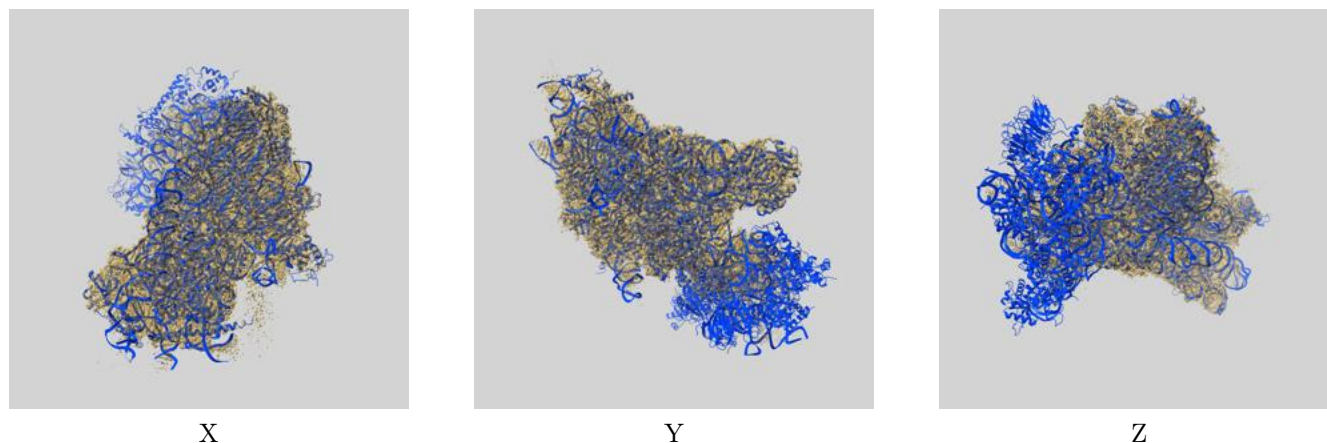
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.15	-	-
Author-provided FSC curve	2.14	2.46	2.18
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

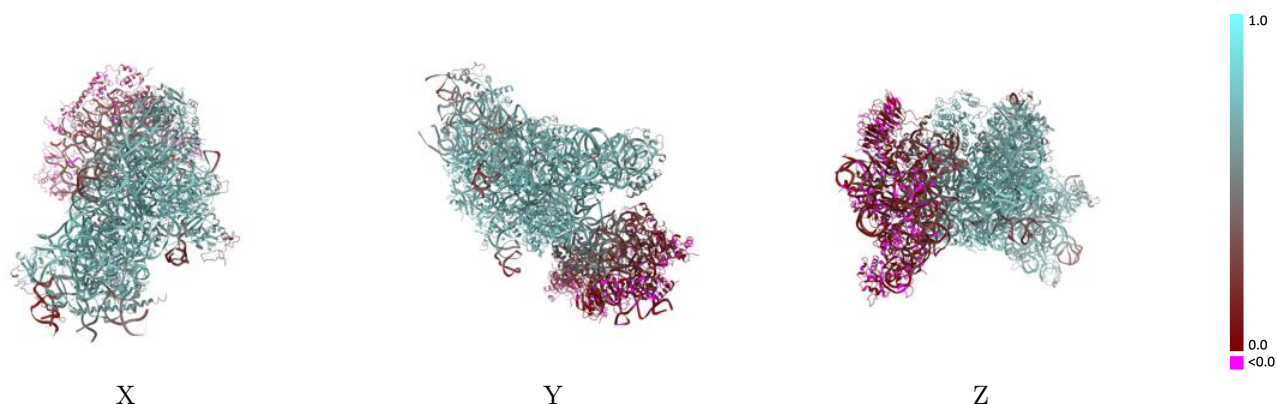
This section contains information regarding the fit between EMDB map EMD-14317 and PDB model 7R4X. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



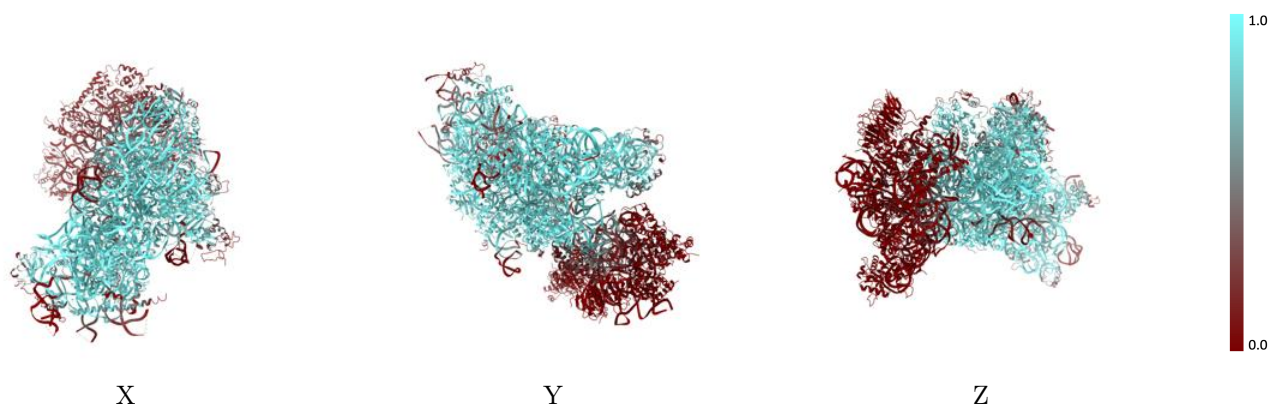
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



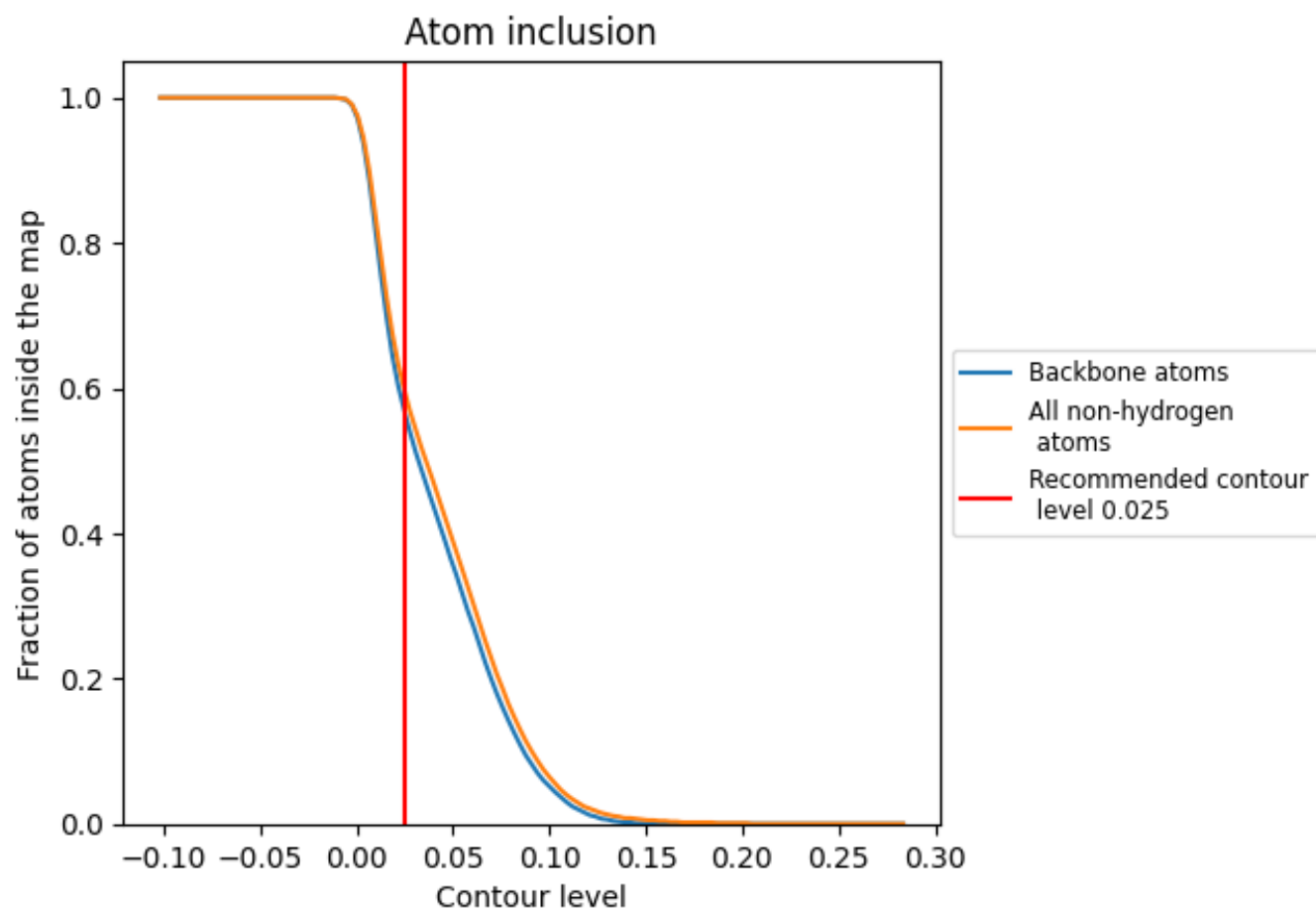
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5950	 0.5210
2	 0.6770	 0.5580
A	 0.9030	 0.7170
B	 0.7650	 0.6480
C	 0.9130	 0.7440
D	 0.1730	 0.3590
E	 0.9420	 0.7390
F	 0.0210	 0.1930
G	 0.6250	 0.6060
H	 0.5390	 0.5700
I	 0.7720	 0.6420
J	 0.8950	 0.7330
K	 0.0290	 0.1770
L	 0.8970	 0.7170
M	 0.0010	 0.0580
N	 0.8610	 0.6950
O	 0.8390	 0.6690
P	 0.0060	 0.1180
Q	 0.0500	 0.1560
R	 0.2950	 0.4730
S	 0.0050	 0.0860
T	 0.0050	 0.1020
U	 0.1150	 0.2440
V	 0.8940	 0.7250
W	 0.9680	 0.7720
X	 0.9490	 0.7620
Y	 0.8870	 0.7050
Z	 0.0000	 0.0570
a	 0.8450	 0.6970
b	 0.7610	 0.6650
c	 0.0490	 0.2810
d	 0.2170	 0.3440
e	 0.7350	 0.6540
f	 0.0000	 0.0280
g	 0.0070	 0.1120
n	 0.8010	 0.6940

