



wwPDB EM Validation Summary Report ⓘ

Jul 15, 2024 – 04:41 am BST

PDB ID : 8CBJ
EMDB ID : EMD-16541
Title : Cryo-EM structure of Otu2-bound cytoplasmic pre-40S ribosome biogenesis complex
Authors : Ikeuchi, K.; Buschauer, R.; Cheng, J.; Berninghausen, O.; Becker, T.; Beckmann, R.
Deposited on : 2023-01-25
Resolution : 3.80 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:

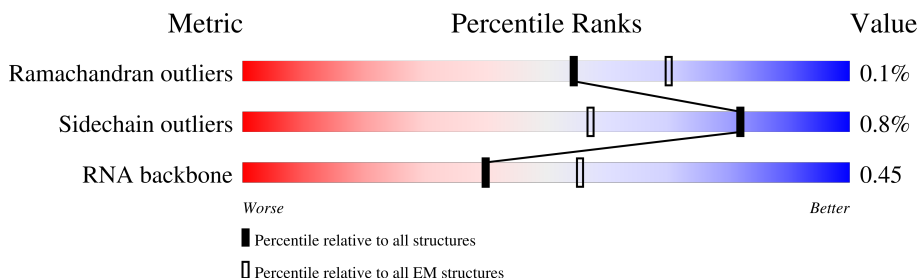
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

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 3.80 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 $\leq 5\%$. 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	b	82	
2	c	67	
3	d	56	
4	e	63	
5	g	319	
6	h	274	
7	i	483	
8	j	463	

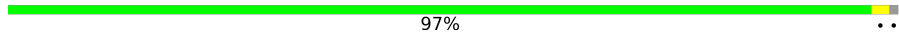





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Mol	Chain	Length	Quality of chain
9	k	788	84% 15%
10	l	425	66% 33%
11	A	252	78% 18%
12	B	255	80% 16%
13	C	254	85% 15%
14	D	240	38% 82% 16%
15	E	261	99%
16	F	225	90% 8%
17	G	236	95%
18	H	190	95%
19	I	200	92% 6%
20	J	197	90% 6%
21	L	156	88% 10%
22	M	143	22% 87% 13%
23	N	151	98%
24	O	137	93% 7%
25	P	142	5% 89% 11%
26	Q	143	87% 11%
27	R	136	5% 90% 8%
28	S	146	90% 8%
29	T	144	8% 97%
30	U	121	8% 85% 15%
31	V	87	98%
32	W	130	96%
33	X	145	5% 99%

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Mol	Chain	Length	Quality of chain
34	Y	135	 97%
35	Z	108	 57% 42%
36	a	459	 59% 41%
37	y	318	 47% 52%
38	2	2012	 51% 31% 5% 12%
39	K	307	 32% 68%

2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 87884 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 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	b	81	610	382	110	113	5	0	0

- Molecule 2 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	c	63	497	306	99	91	1	0	0

- Molecule 3 is a protein called RPS29A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	d	37	302	186	62	50	4	0	0

- Molecule 4 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	e	48	384	242	81	59	2	0	0

- Molecule 5 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	g	317	2431	1538	417	468	8	0	0

- Molecule 6 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	h	181	1436	917	261	254	4	0	0

- Molecule 7 is a protein called ENP1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	i	262	2133	1388	364	378	3	0	0

- Molecule 8 is a protein called LTV1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	j	46	396	242	57	95	2	0	0

- Molecule 9 is a protein called TSR1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	k	670	5402	3449	937	1002	14	0	0

- Molecule 10 is a protein called non-specific serine/threonine protein kinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	l	286	2322	1464	410	430	18	0	0

- Molecule 11 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	A	206	1611	1036	285	288	2	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	206	PHE	ASP	conflict	UNP B3LI22

- Molecule 12 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	B	214	1709	1084	310	311	4	0	0

- Molecule 13 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	C	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 14 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D	202	Total	C	N	O	S	0	0
			1576	998	290	282	6		

- Molecule 15 is a protein called 40S ribosomal protein S4-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 16 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	F	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 17 is a protein called 40S ribosomal protein S6-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	232	Total	C	N	O	S	0	0
			1873	1172	366	332	3		

- Molecule 18 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	H	184	Total	C	N	O	0	0
			1481	951	265	265		

- Molecule 19 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	I	188	Total	C	N	O	S	0	0
			1489	925	298	264	2		

- Molecule 20 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	J	185	1494	943	289	261	1	0	0

- Molecule 21 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	L	140	1129	724	215	187	3	0	0

- Molecule 22 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	M	125	941	591	166	182	2	0	0

- Molecule 23 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	N	150	1192	759	224	207	2	0	0

- Molecule 24 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	O	127	926	569	185	169	3	0	0

- Molecule 25 is a protein called RPS15 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	P	127	1001	637	186	171	7	0	0

- Molecule 26 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
26	Q	127	993	640	177	176	0	0

- Molecule 27 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	R	125	1000	625	188	185	2	0	0

- Molecule 28 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	S	135	1110	696	215	197	2	0	0

- Molecule 29 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	T	143	1112	694	208	208	2	0	0

- Molecule 30 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	U	103	819	519	148	151	1	0	0

- Molecule 31 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	V	87	684	420	125	137	2	0	0

- Molecule 32 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	W	129	1021	650	188	180	3	0	0

- Molecule 33 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	X	144	1121	708	220	191	2	0	0

- Molecule 34 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
34	Y	134	1073	676	208	189	0	0

- Molecule 35 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
35	Z	63	512	328	94	90	0	0

- Molecule 36 is a protein called 20S-pre-rRNA D-site endonuclease NOB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
36	a	272	1343	799	272	272	0	0

- Molecule 37 is a protein called rRNA adenine N(6)-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	y	154	1245	788	223	225	9	0	0

- Molecule 38 is a RNA chain called 20S pre-ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
38	2	1767	37662	16836	6672	12387	1767	0	0

- Molecule 39 is a protein called OTU domain-containing protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
39	K	99	494	296	99	99	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	178	SER	CYS	engineered mutation	UNP P38747

- Molecule 40 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
40	b	1	Total 1	Zn 1	0
40	d	1	Total 1	Zn 1	0

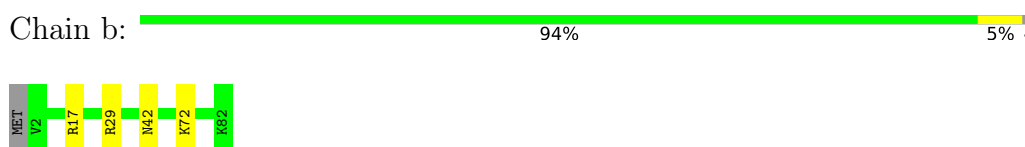
- Molecule 41 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
41	2	46	Total 46	Mg 46	0

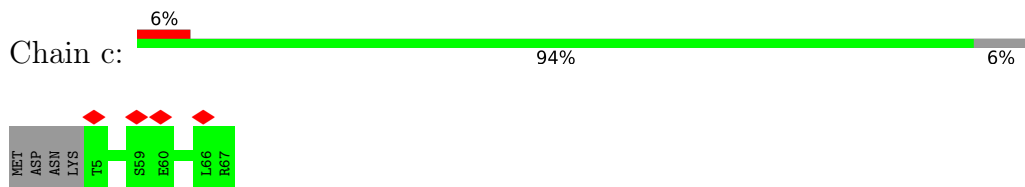
3 Residue-property plots [i](#)

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.

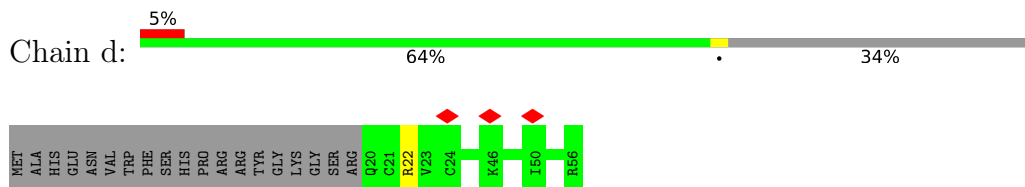
- Molecule 1: 40S ribosomal protein S27-A



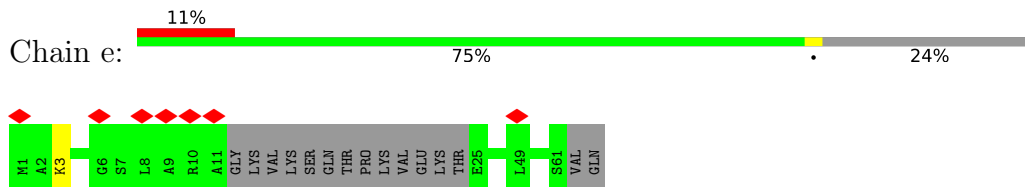
- Molecule 2: 40S ribosomal protein S28-A



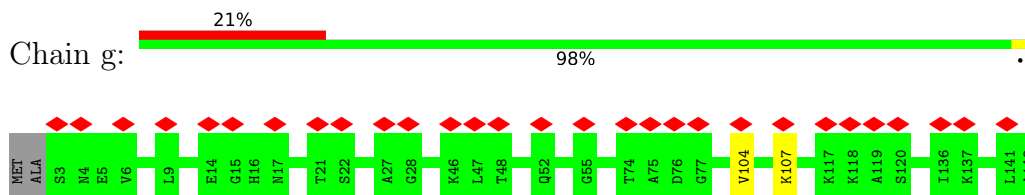
- Molecule 3: RPS29A isoform 1

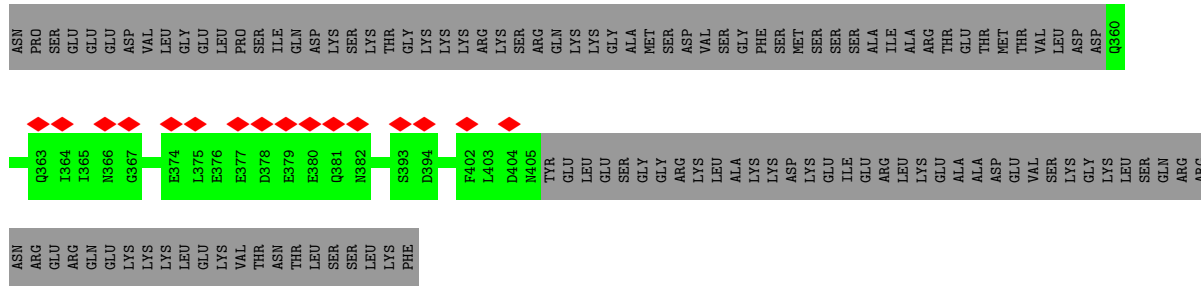


- Molecule 4: 40S ribosomal protein S30-A

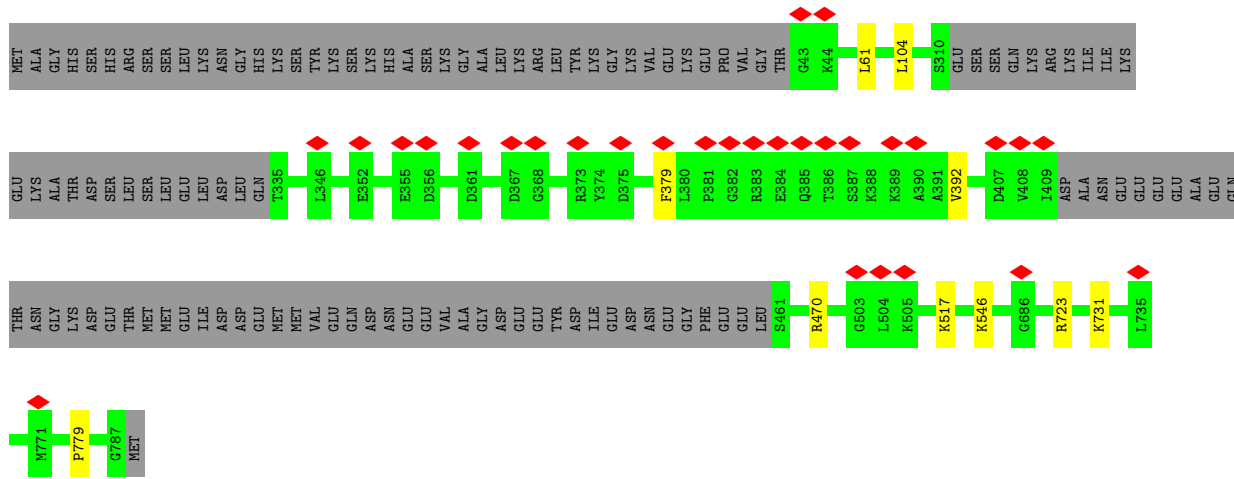
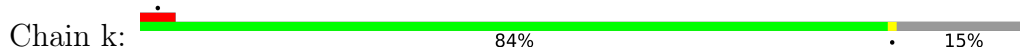


- Molecule 5: Guanine nucleotide-binding protein subunit beta-like protein

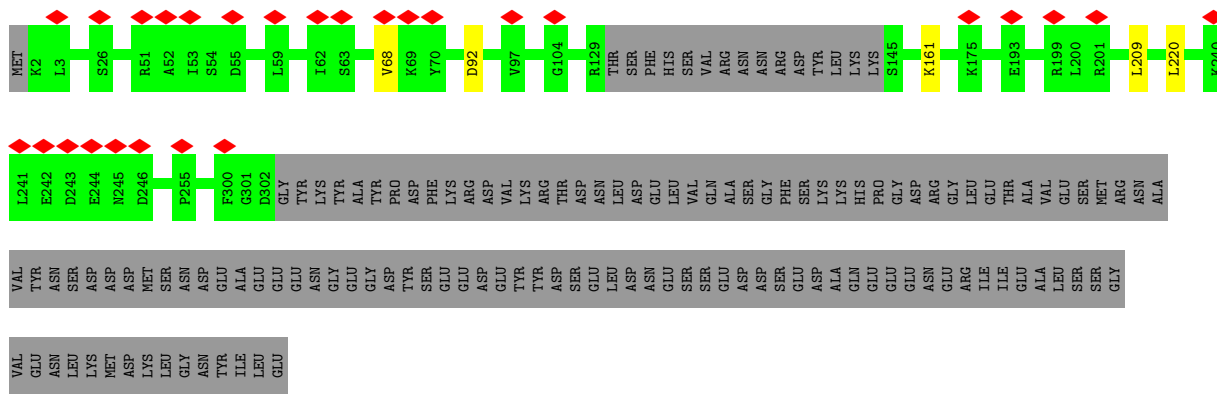




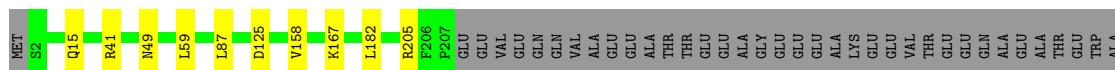
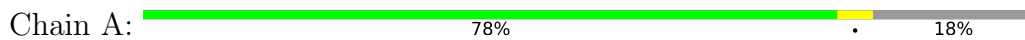
• Molecule 9: TSR1 isoform 1



• Molecule 10: non-specific serine/threonine protein kinase

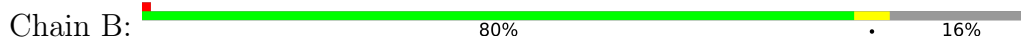


• Molecule 11: 40S ribosomal protein S0-A



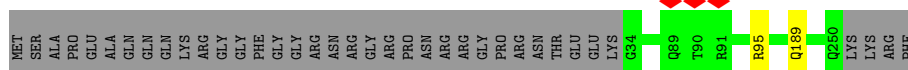
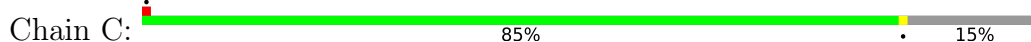
GLU
GLU
ASN
ALA
ASP
ASN
VAL
GLU
TRP

• Molecule 12: 40S ribosomal protein S1-A

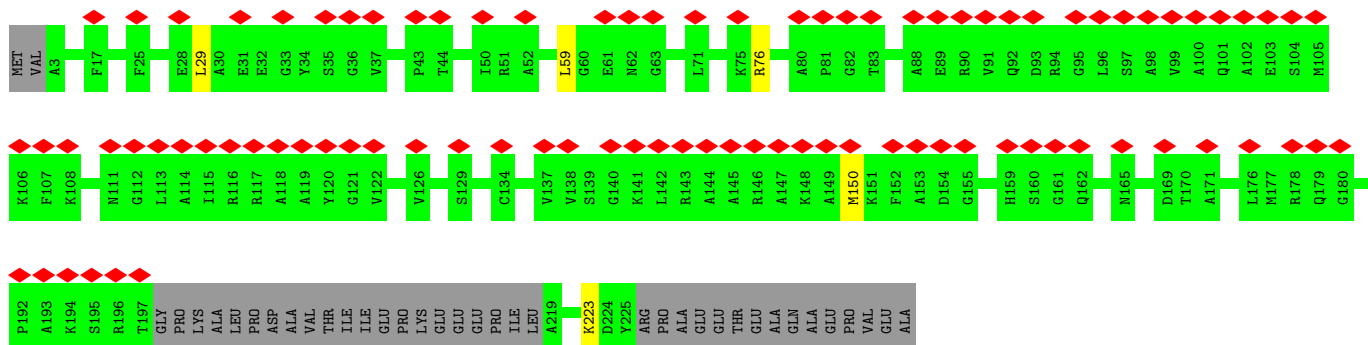
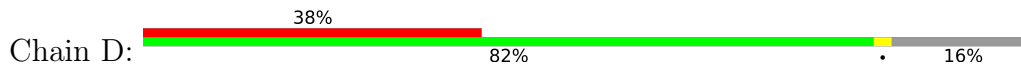


VAL
LEU
GLU
THR
VAL

• Molecule 13: 40S ribosomal protein S2



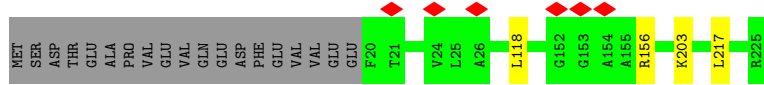
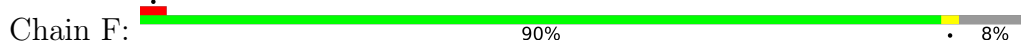
• Molecule 14: 40S ribosomal protein S3



• Molecule 15: 40S ribosomal protein S4-B



• Molecule 16: 40S ribosomal protein S5



- Molecule 17: 40S ribosomal protein S6-B

Chain G:  95%




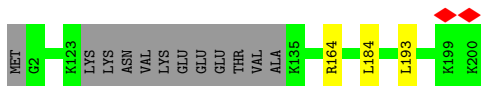
- Molecule 18: 40S ribosomal protein S7-A

Chain H:  95%




- Molecule 19: 40S ribosomal protein S8-A

Chain I:  92% 6%




- Molecule 20: 40S ribosomal protein S9-A

Chain J:  90% 6%




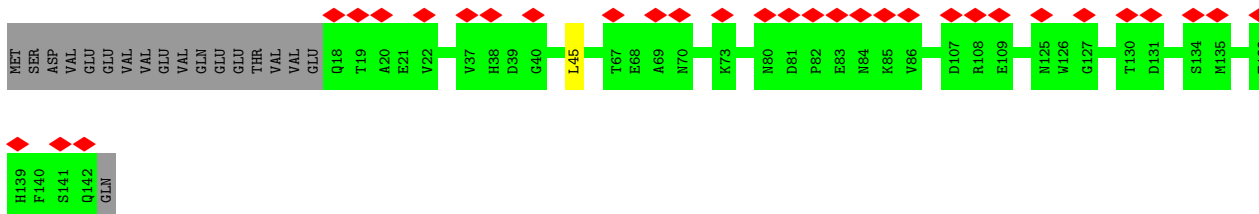
- Molecule 21: 40S ribosomal protein S11-A

Chain L:  88% 10%



- Molecule 22: 40S ribosomal protein S12

Chain M:  22% 87% 13%



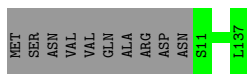
- Molecule 23: 40S ribosomal protein S13

Chain N:  98%




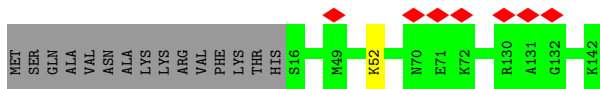
- Molecule 24: 40S ribosomal protein S14-A

Chain O:  93% 7%




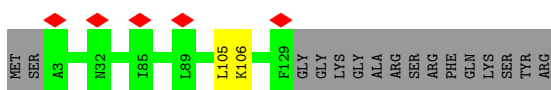
- Molecule 25: RPS15 isoform 1

Chain P:  5% 89% 11%

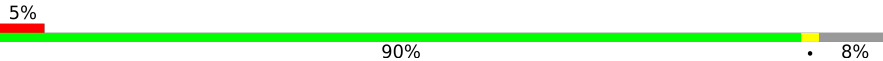


- Molecule 26: 40S ribosomal protein S16-A

Chain Q:  87% 11%




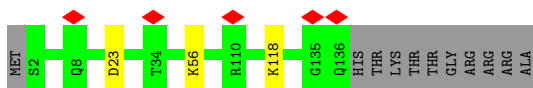
- Molecule 27: 40S ribosomal protein S17-A

Chain R:  5% 90% 8%



- Molecule 28: 40S ribosomal protein S18-A

Chain S:  90% 8%

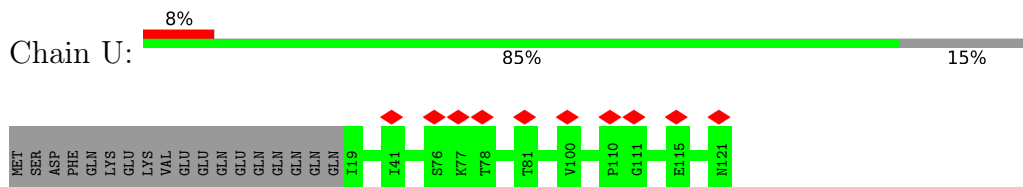


- Molecule 29: 40S ribosomal protein S19-A

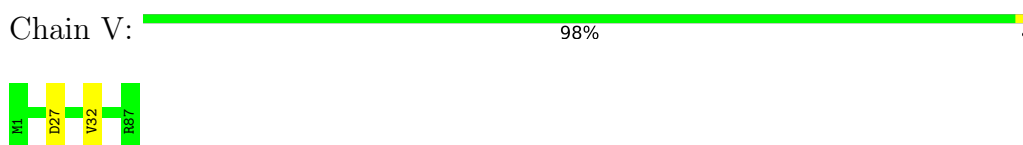
Chain T:  8% 97%



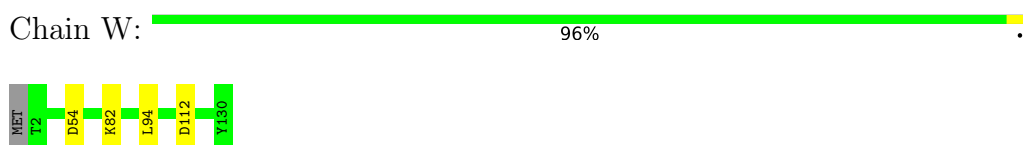
- Molecule 30: 40S ribosomal protein S20



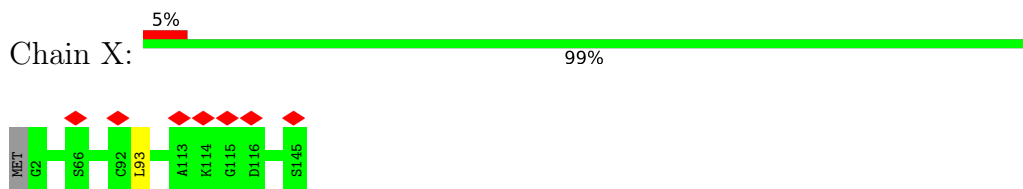
- Molecule 31: 40S ribosomal protein S21-A



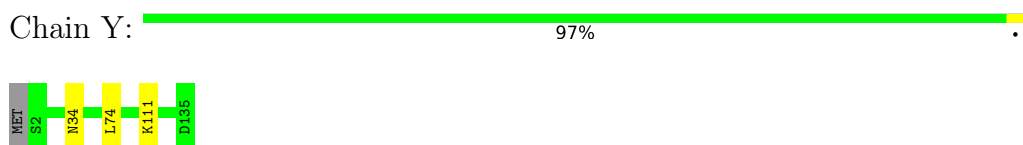
- Molecule 32: 40S ribosomal protein S22-A



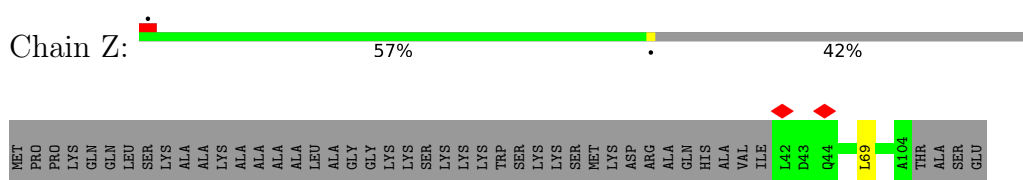
- Molecule 33: 40S ribosomal protein S23-A



- Molecule 34: 40S ribosomal protein S24-A



- Molecule 35: 40S ribosomal protein S25-A



- Molecule 36: 20S-pre-rRNA D-site endonuclease NOB1



G C U D U G C C C U U V U A A C U D U G C G C C G G U U C U D U G C C U U A A G G G C U U U G U U A A G U U C U U C U U A G C U U A U C C A A A C

G G U U G A C A G A U U D C C U D U G C C G C U D U U G U D U A U A A G G C A C U U A U U C C U U C U U A A G C U U C C A A A C

• Molecule 39: OTU domain-containing protein 2

Chain K: 32% 68%

MET	THR	GLY	MET	GLU	SER	GLY	GLU	ASN	LEU	GLU	ASN	H13	H72	ASN	GLU	VAL	PHE	ASP	ALA	GLN	GLU	ASP	GLU	H84	H94	ILE	SER	ARG	ASP	GLU	LYS	GLY	GLN	GLN	ASN	VAL	VAL	VAL	GLN	GLN	GLN	GLY	GLN	THR	LYS	ARG	H120	H139	H140	H141	H142									
E143	A144	S145	K146	Q147	PRO	ASP	LEU	LYS	VAL	MET	GLU	GLN	GLU	SER	ILE	ASP	GLN	LEU	CYS	GLU	LEU	LYS	LYS	LEU	LYS	GLN	PHE	ASP	ILE	GLN	PRO	ASP	GLY	HIS	SER	LEU	PHE	ALA	ILE	LEU	ASP	GLN	TRP	GLY	GLY	ARG	HIS	ASP	PRO	LYS	ALA	LYS	LEU	ASP	GLN	ASP	VAL			
MET	LYS	LEU	ARG	TRP	LEU	SER	CYS	ASN	TYR	VAL	GLN	HIS	ARG	ASP	ASP	PHE	ILE	PRO	TYR	LEU	PHE	ASP	GLU	GLU	THR	MET	LYS	MET	LYS	ASP	ILE	GLN	PRO	ASP	GLY	TYR	THR	LYS	GLU	MET	GLU	HIS	THR	ALA	GLN	TRP	GLY	GLY	ILE	GLU	ILE	LEU	ALA	LYS	LEU	SER	HIS	VAL	PHE	ASP
CYS	PRO	ILE	SER	ILE	LEU	MET	SER	GLY	ARG	PRO	ILE	GLN	VAL	TYR	ASN	GLY	LYS	ASN	PRO	GLU	LEU	LYS	LEU	VAL	TYR	TYR	LYS	HIS	SER	TYR	ALA	LEU	GLY	GLY	HIS	TYR	ASN	SER	LEU	HIS	ASP	SER	PRO	GLY	GLY	ILE	LEU	ALA	LYS	LEU	SER	HIS	VAL	PHE	ASP					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	4908	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 ($e^-/\text{\AA}^2$)	46.4	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.970	Depositor
Minimum map value	-1.474	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.067	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	438.9, 438.9, 438.9	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	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: MG, 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	b	0.39	0/620	0.75	1/838 (0.1%)
2	c	0.29	0/499	0.79	0/670
3	d	0.32	0/306	0.68	0/404
4	e	0.40	0/390	0.79	0/517
5	g	0.28	0/2484	0.61	2/3382 (0.1%)
6	h	0.39	0/1462	0.89	2/1969 (0.1%)
7	i	0.32	0/2188	0.65	2/2970 (0.1%)
8	j	0.28	0/403	0.48	0/543
9	k	0.33	0/5528	0.68	5/7477 (0.1%)
10	l	0.32	0/2368	0.75	3/3181 (0.1%)
11	A	0.39	0/1653	0.80	4/2261 (0.2%)
12	B	0.33	0/1735	0.79	4/2335 (0.2%)
13	C	0.39	0/1665	0.75	1/2263 (0.0%)
14	D	0.30	0/1596	0.70	3/2142 (0.1%)
15	E	0.45	0/2109	0.81	2/2839 (0.1%)
16	F	0.34	0/1629	0.74	2/2202 (0.1%)
17	G	0.34	0/1897	0.74	4/2532 (0.2%)
18	H	0.37	0/1506	0.79	2/2028 (0.1%)
19	I	0.45	0/1514	0.78	2/2021 (0.1%)
20	J	0.46	0/1519	0.88	5/2035 (0.2%)
21	L	0.47	0/1155	0.71	0/1557
22	M	0.28	0/949	0.59	1/1284 (0.1%)
23	N	0.38	0/1215	0.82	2/1638 (0.1%)
24	O	0.34	0/937	0.74	0/1261
25	P	0.31	0/1022	0.74	0/1373
26	Q	0.30	0/1011	0.68	2/1362 (0.1%)
27	R	0.35	0/1010	0.83	1/1355 (0.1%)
28	S	0.29	0/1128	0.70	1/1518 (0.1%)
29	T	0.33	0/1130	0.70	2/1517 (0.1%)
30	U	0.25	0/829	0.58	0/1121
31	V	0.46	0/693	0.89	2/935 (0.2%)
32	W	0.51	0/1038	0.93	4/1395 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	X	0.41	0/1139	0.74	1/1518 (0.1%)
34	Y	0.42	0/1087	0.77	2/1449 (0.1%)
35	Z	0.31	0/519	0.79	1/696 (0.1%)
36	a	0.24	0/1340	0.38	0/1861
37	y	0.31	0/1265	0.80	2/1702 (0.1%)
38	2	0.61	0/42123	1.33	587/65631 (0.9%)
39	K	0.24	0/491	0.25	0/682
All	All	0.49	0/93152	1.07	652/134464 (0.5%)

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
9	k	0	1
12	B	0	1
20	J	0	1
21	L	0	1
27	R	0	1
37	y	0	1
All	All	0	6

There are no bond length outliers.

The worst 5 of 652 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	2	1004	U	C2-N1-C1'	12.75	133.00	117.70
38	2	1389	C	N1-C2-O2	12.39	126.33	118.90
38	2	1185	U	OP2-P-O3'	-12.33	78.07	105.20
38	2	1389	C	C2-N1-C1'	12.29	132.32	118.80
38	2	1389	C	N3-C2-O2	-11.72	113.69	121.90

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	B	144	ARG	Peptide
20	J	112	GLN	Peptide
21	L	10	GLU	Peptide
27	R	21	TYR	Peptide

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Mol	Chain	Res	Type	Group
9	k	392	VAL	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	
1	b	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
2	c	61/67 (91%)	57 (93%)	4 (7%)	0	100	100
3	d	35/56 (62%)	33 (94%)	2 (6%)	0	100	100
4	e	44/63 (70%)	42 (96%)	2 (4%)	0	100	100
5	g	315/319 (99%)	296 (94%)	18 (6%)	1 (0%)	41	74
6	h	179/274 (65%)	176 (98%)	3 (2%)	0	100	100
7	i	260/483 (54%)	251 (96%)	9 (4%)	0	100	100
8	j	44/463 (10%)	41 (93%)	3 (7%)	0	100	100
9	k	664/788 (84%)	632 (95%)	32 (5%)	0	100	100
10	l	282/425 (66%)	263 (93%)	18 (6%)	1 (0%)	34	70
11	A	204/252 (81%)	191 (94%)	12 (6%)	1 (0%)	29	66
12	B	212/255 (83%)	203 (96%)	9 (4%)	0	100	100
13	C	215/254 (85%)	205 (95%)	10 (5%)	0	100	100
14	D	198/240 (82%)	190 (96%)	8 (4%)	0	100	100
15	E	258/261 (99%)	242 (94%)	16 (6%)	0	100	100
16	F	204/225 (91%)	192 (94%)	12 (6%)	0	100	100
17	G	230/236 (98%)	222 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	H	182/190 (96%)	173 (95%)	9 (5%)	0	100	100
19	I	184/200 (92%)	175 (95%)	9 (5%)	0	100	100
20	J	183/197 (93%)	176 (96%)	7 (4%)	0	100	100
21	L	138/156 (88%)	133 (96%)	5 (4%)	0	100	100
22	M	123/143 (86%)	118 (96%)	5 (4%)	0	100	100
23	N	148/151 (98%)	142 (96%)	6 (4%)	0	100	100
24	O	125/137 (91%)	118 (94%)	7 (6%)	0	100	100
25	P	125/142 (88%)	118 (94%)	7 (6%)	0	100	100
26	Q	125/143 (87%)	121 (97%)	4 (3%)	0	100	100
27	R	123/136 (90%)	117 (95%)	6 (5%)	0	100	100
28	S	133/146 (91%)	129 (97%)	4 (3%)	0	100	100
29	T	141/144 (98%)	137 (97%)	4 (3%)	0	100	100
30	U	101/121 (84%)	100 (99%)	1 (1%)	0	100	100
31	V	85/87 (98%)	78 (92%)	7 (8%)	0	100	100
32	W	127/130 (98%)	113 (89%)	14 (11%)	0	100	100
33	X	142/145 (98%)	136 (96%)	6 (4%)	0	100	100
34	Y	132/135 (98%)	130 (98%)	1 (1%)	1 (1%)	19	57
35	Z	61/108 (56%)	59 (97%)	2 (3%)	0	100	100
36	a	266/459 (58%)	266 (100%)	0	0	100	100
37	y	150/318 (47%)	134 (89%)	16 (11%)	0	100	100
39	K	93/307 (30%)	93 (100%)	0	0	100	100
All	All	6371/8438 (76%)	6077 (95%)	290 (5%)	4 (0%)	54	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	g	237	GLN
34	Y	34	ASN
10	l	68	VAL
11	A	158	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	
1	b	70/71 (99%)	67 (96%)	3 (4%)	29	58
2	c	56/60 (93%)	56 (100%)	0	100	100
3	d	33/49 (67%)	32 (97%)	1 (3%)	41	66
4	e	40/54 (74%)	39 (98%)	1 (2%)	47	70
5	g	259/262 (99%)	257 (99%)	2 (1%)	81	89
6	h	158/238 (66%)	155 (98%)	3 (2%)	57	76
7	i	234/424 (55%)	234 (100%)	0	100	100
8	j	44/419 (10%)	44 (100%)	0	100	100
9	k	580/703 (82%)	576 (99%)	4 (1%)	84	91
10	l	260/384 (68%)	259 (100%)	1 (0%)	91	95
11	A	171/210 (81%)	166 (97%)	5 (3%)	42	67
12	B	191/224 (85%)	187 (98%)	4 (2%)	53	74
13	C	176/205 (86%)	175 (99%)	1 (1%)	86	92
14	D	164/195 (84%)	162 (99%)	2 (1%)	71	84
15	E	221/222 (100%)	221 (100%)	0	100	100
16	F	173/191 (91%)	171 (99%)	2 (1%)	71	84
17	G	198/201 (98%)	195 (98%)	3 (2%)	65	81
18	H	165/170 (97%)	164 (99%)	1 (1%)	86	92
19	I	150/161 (93%)	149 (99%)	1 (1%)	84	91
20	J	158/166 (95%)	157 (99%)	1 (1%)	86	92
21	L	125/137 (91%)	123 (98%)	2 (2%)	62	79
22	M	101/119 (85%)	101 (100%)	0	100	100
23	N	127/128 (99%)	127 (100%)	0	100	100
24	O	91/105 (87%)	91 (100%)	0	100	100
25	P	105/118 (89%)	104 (99%)	1 (1%)	76	86
26	Q	107/119 (90%)	106 (99%)	1 (1%)	78	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	R	113/124 (91%)	112 (99%)	1 (1%)	78	88
28	S	120/129 (93%)	118 (98%)	2 (2%)	60	78
29	T	115/116 (99%)	114 (99%)	1 (1%)	78	88
30	U	96/114 (84%)	96 (100%)	0	100	100
31	V	74/74 (100%)	74 (100%)	0	100	100
32	W	110/111 (99%)	110 (100%)	0	100	100
33	X	119/120 (99%)	119 (100%)	0	100	100
34	Y	112/113 (99%)	111 (99%)	1 (1%)	78	88
35	Z	56/89 (63%)	56 (100%)	0	100	100
37	y	141/283 (50%)	141 (100%)	0	100	100
All	All	5213/6608 (79%)	5169 (99%)	44 (1%)	82	89

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	F	203	LYS
21	L	11	ARG
17	G	31	ARG
18	H	141	ARG
25	P	52	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	b	42	ASN
3	d	48	ASN
11	A	49	ASN
18	H	74	GLN
32	W	80	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
38	2	1761/2012 (87%)	604 (34%)	18 (1%)

5 of 604 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
38	2	4	C
38	2	6	G
38	2	17	C
38	2	25	C
38	2	26	A

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
38	2	1570	A
38	2	1700	C
38	2	1652	C
38	2	1229	G
38	2	1481	C

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 48 ligands modelled in this entry, 48 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
38	2	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1377:U	O3'	1378:U	P	3.49
1	2	902:G	O3'	903:U	P	3.34

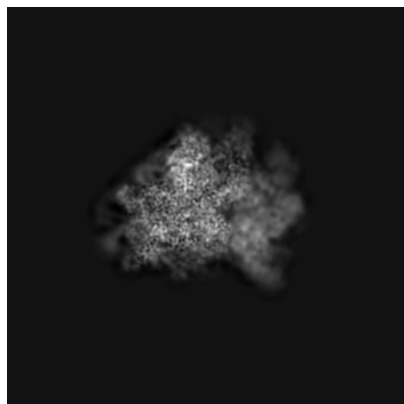
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16541. These allow visual inspection of the internal detail of the map and identification of artifacts.

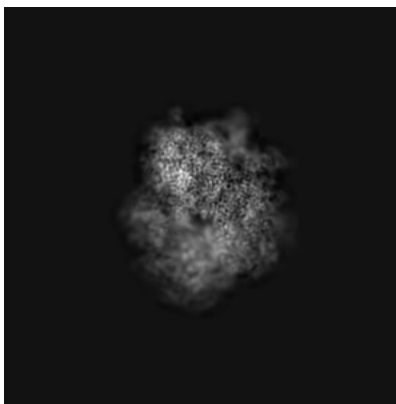
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

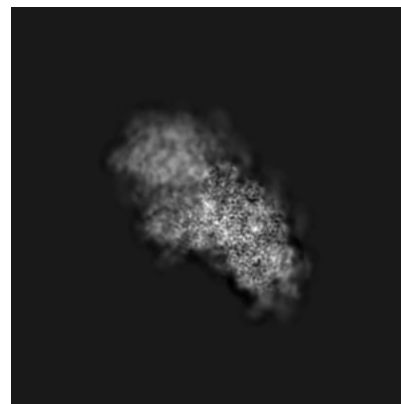
6.1.1 Primary map



X

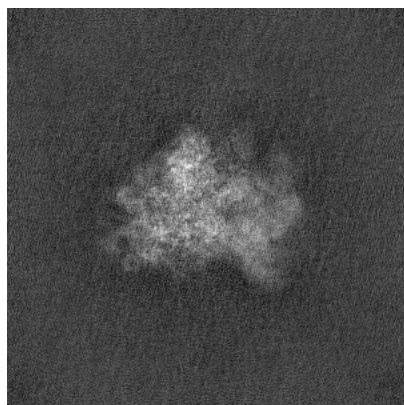


Y

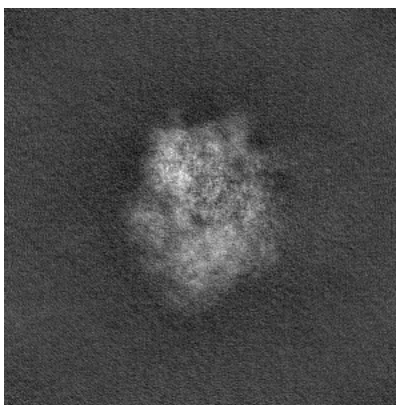


Z

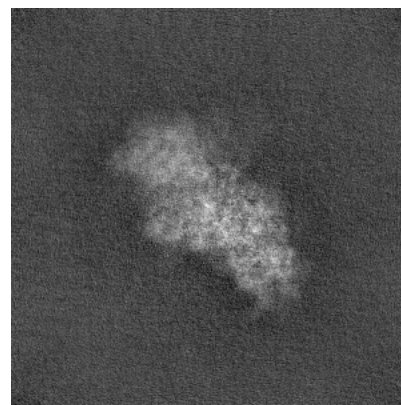
6.1.2 Raw map



X



Y

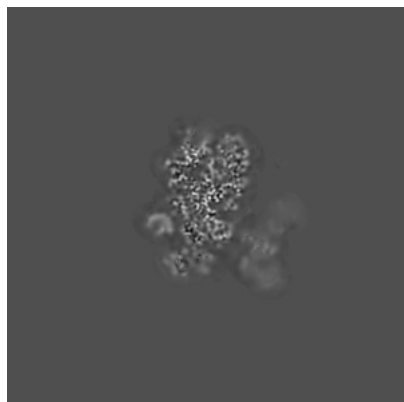


Z

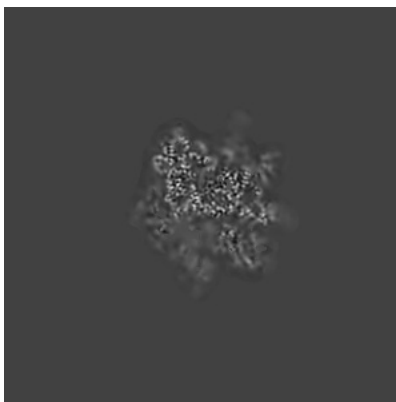
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

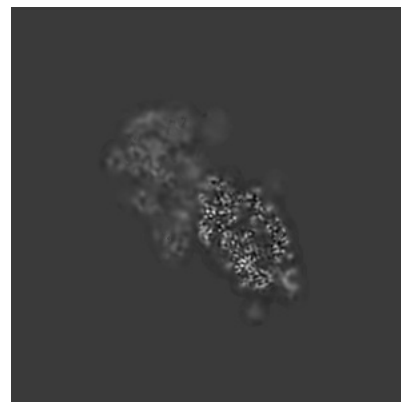
6.2.1 Primary map



X Index: 210

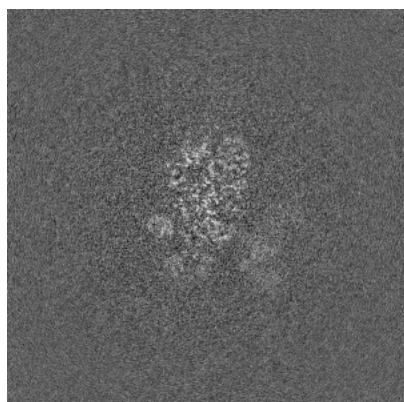


Y Index: 210

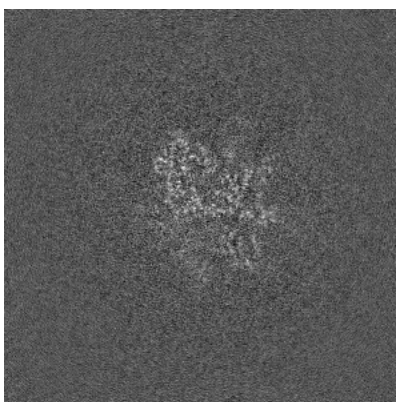


Z Index: 210

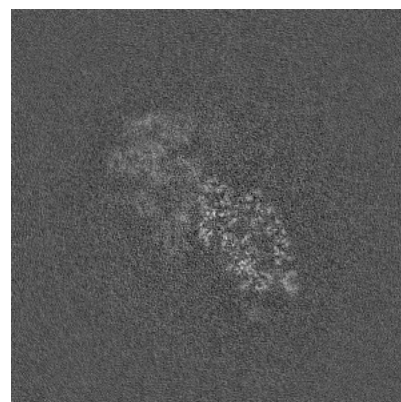
6.2.2 Raw map



X Index: 210



Y Index: 210

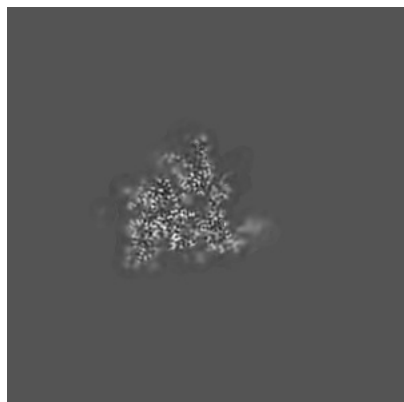


Z Index: 210

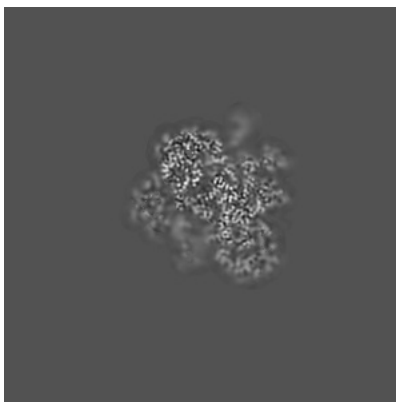
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

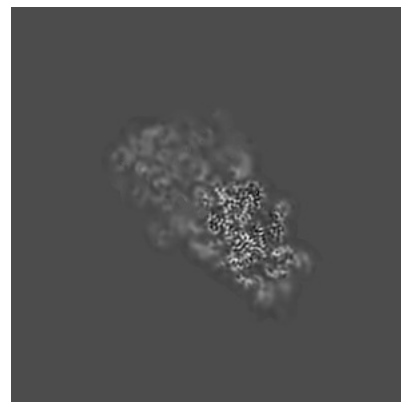
6.3.1 Primary map



X Index: 245

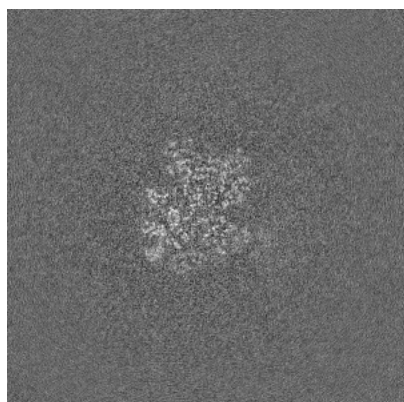


Y Index: 187

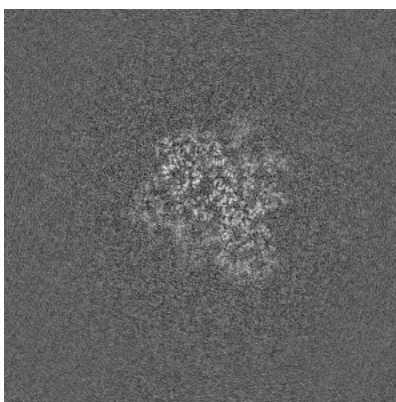


Z Index: 185

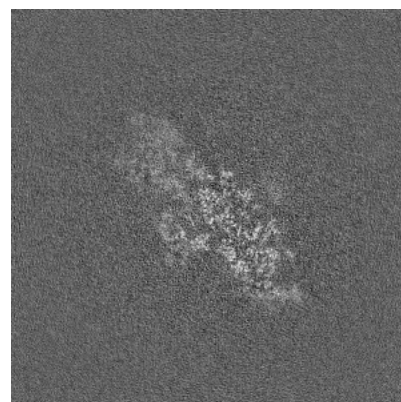
6.3.2 Raw map



X Index: 232



Y Index: 187

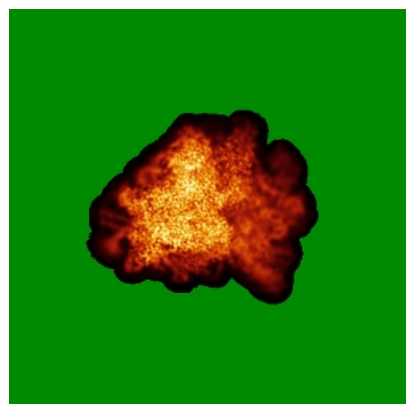


Z Index: 223

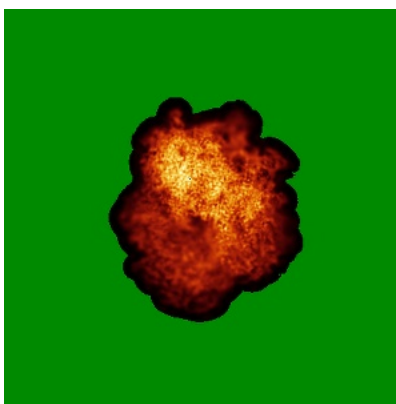
The images above show the largest variance slices of the map in three orthogonal directions.

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

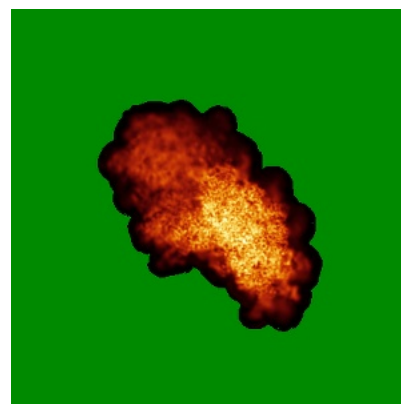
6.4.1 Primary map



X

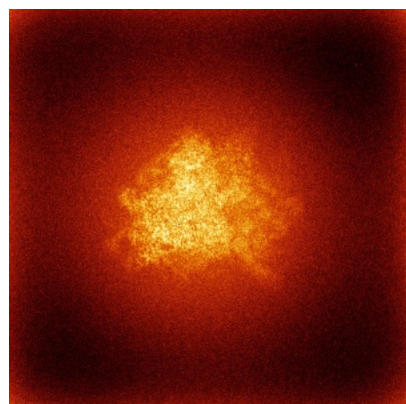


Y

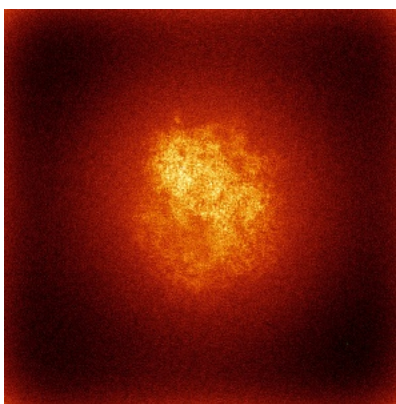


Z

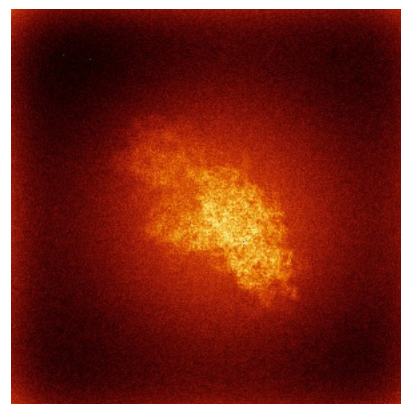
6.4.2 Raw map



X



Y

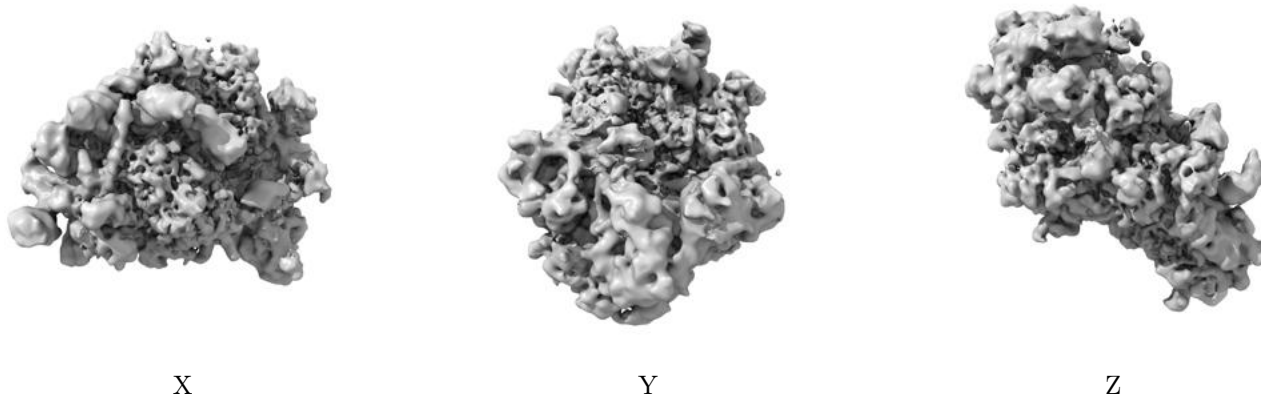


Z

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.

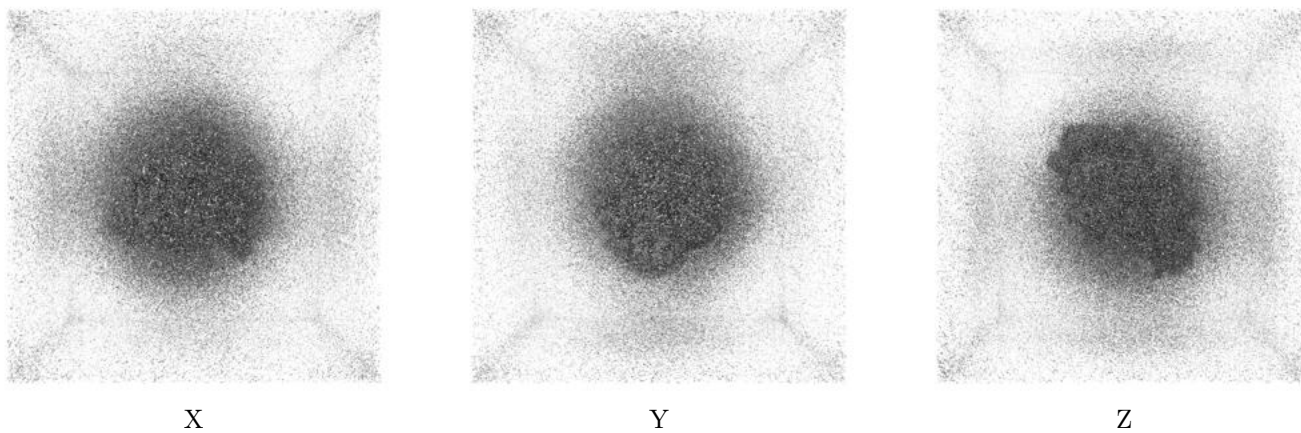
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.14. 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



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.

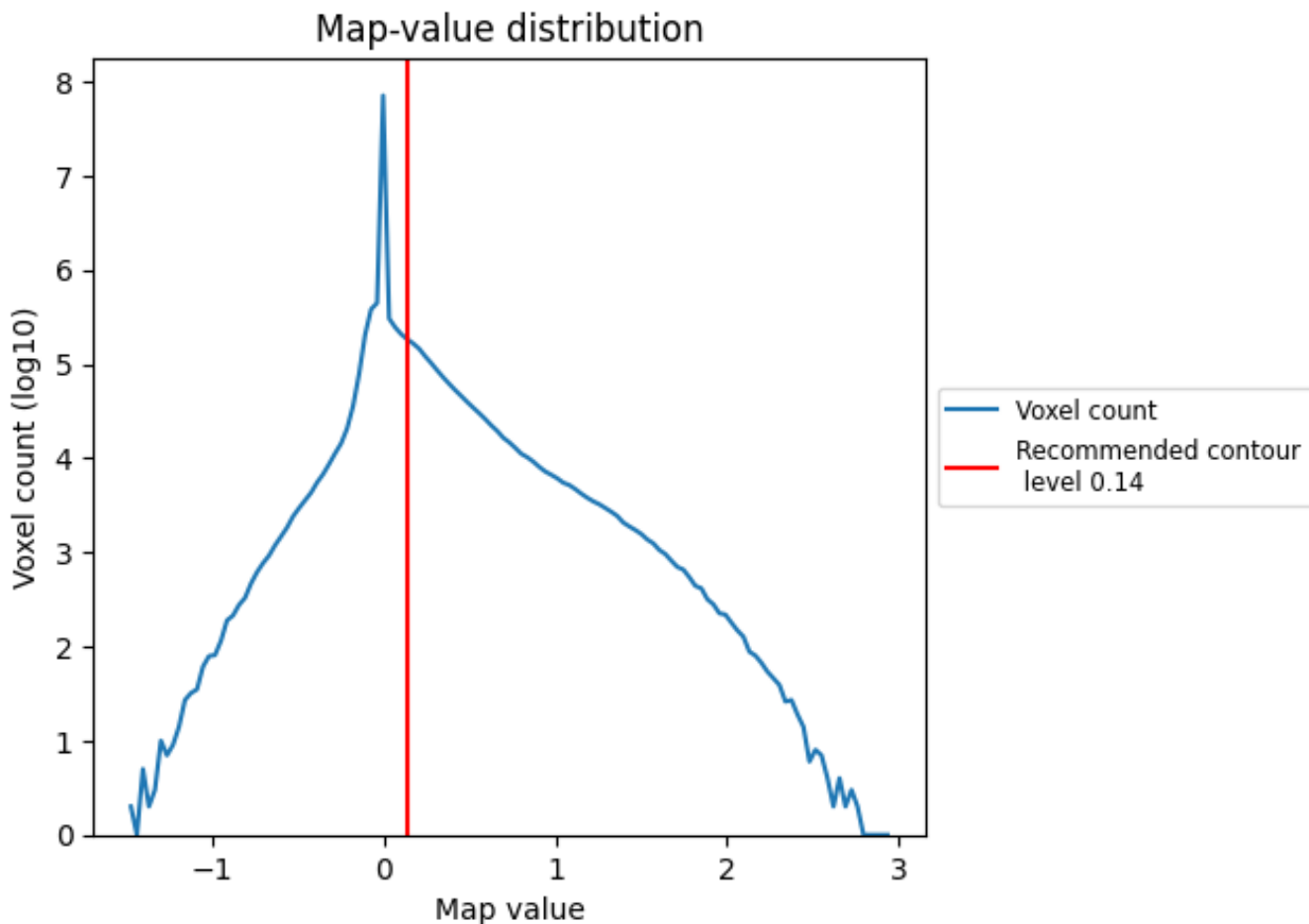
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

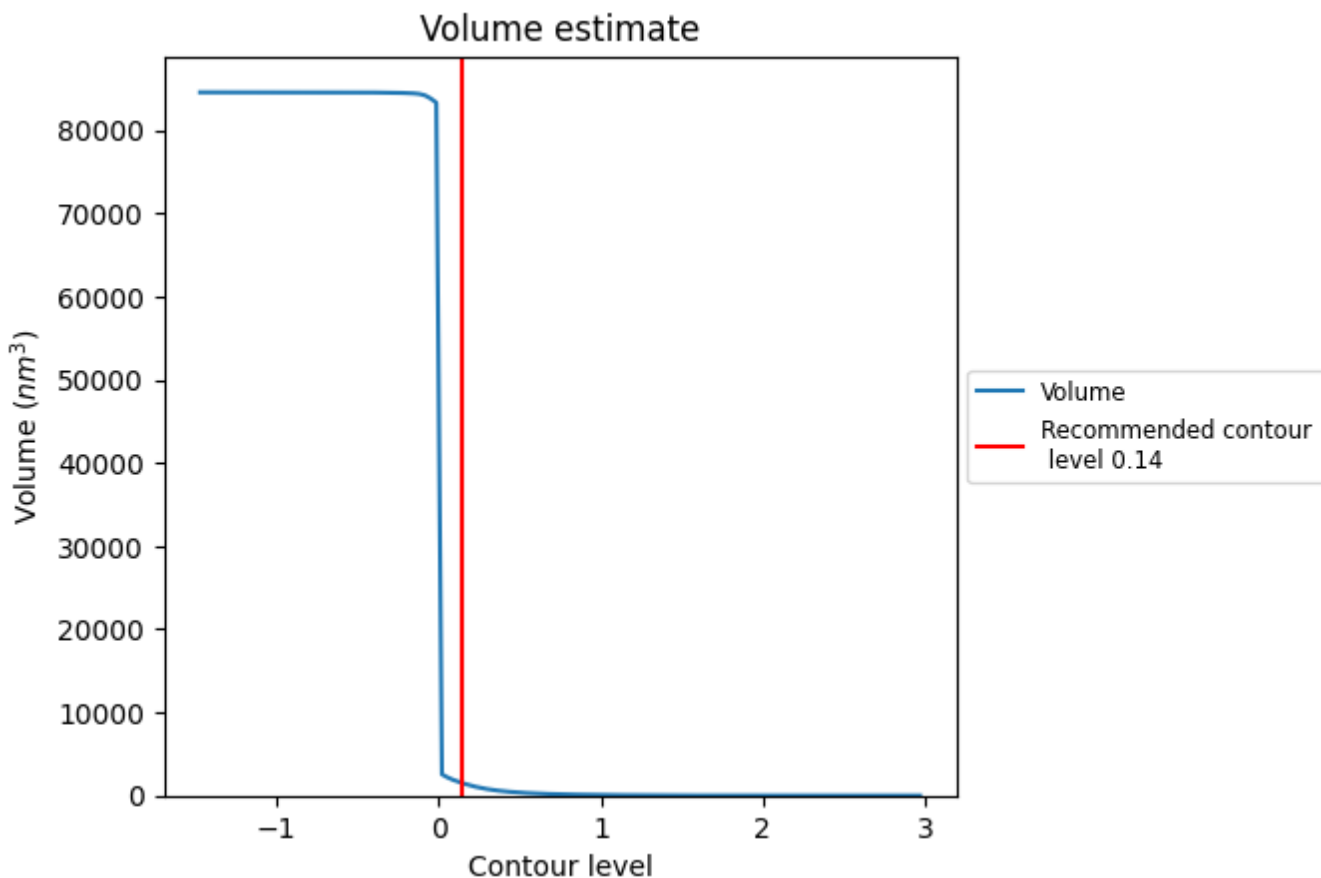
This section contains the results of statistical analysis of the map.

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.

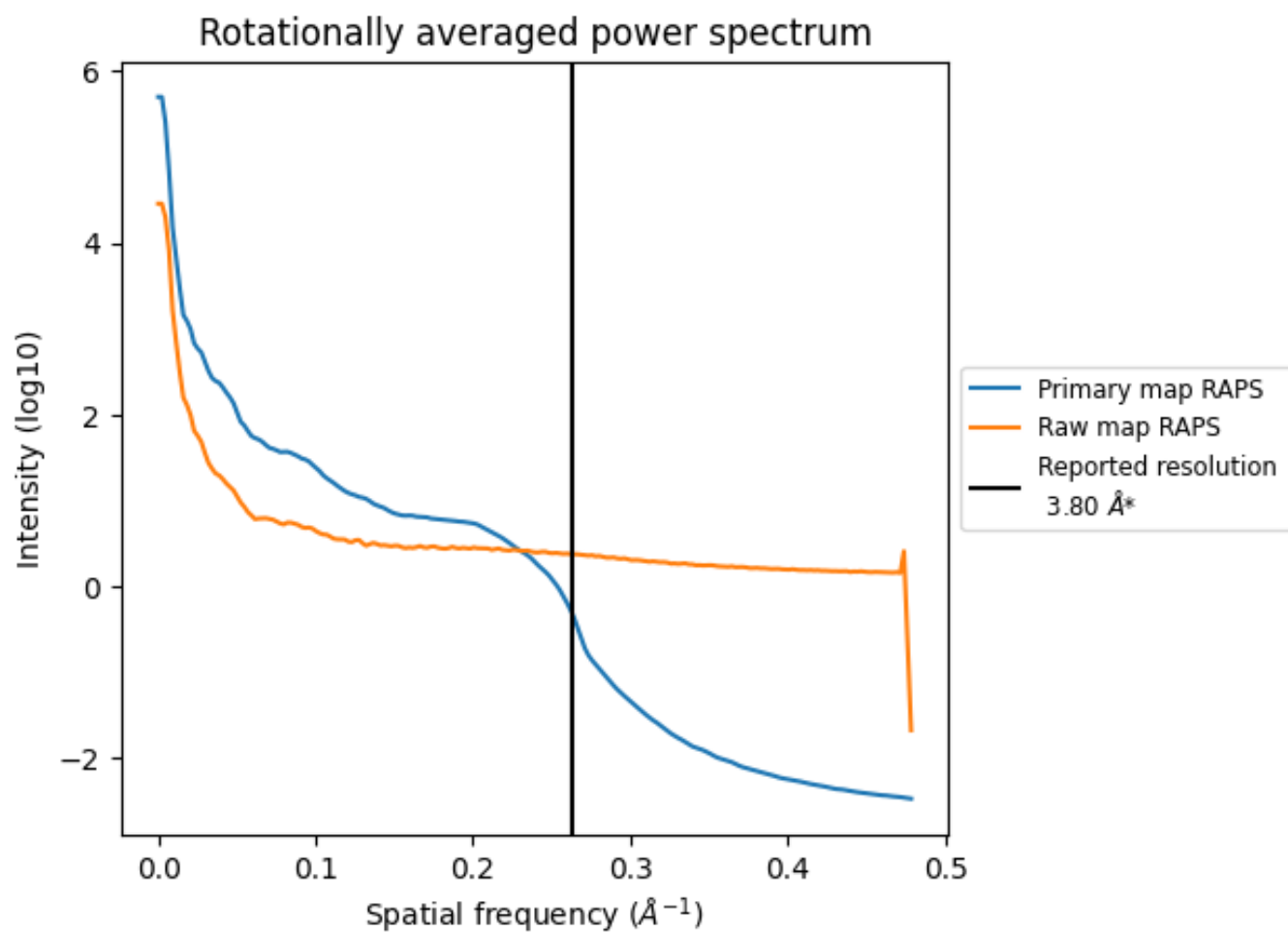
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1532 nm³; this corresponds to an approximate mass of 1384 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 [\(i\)](#)

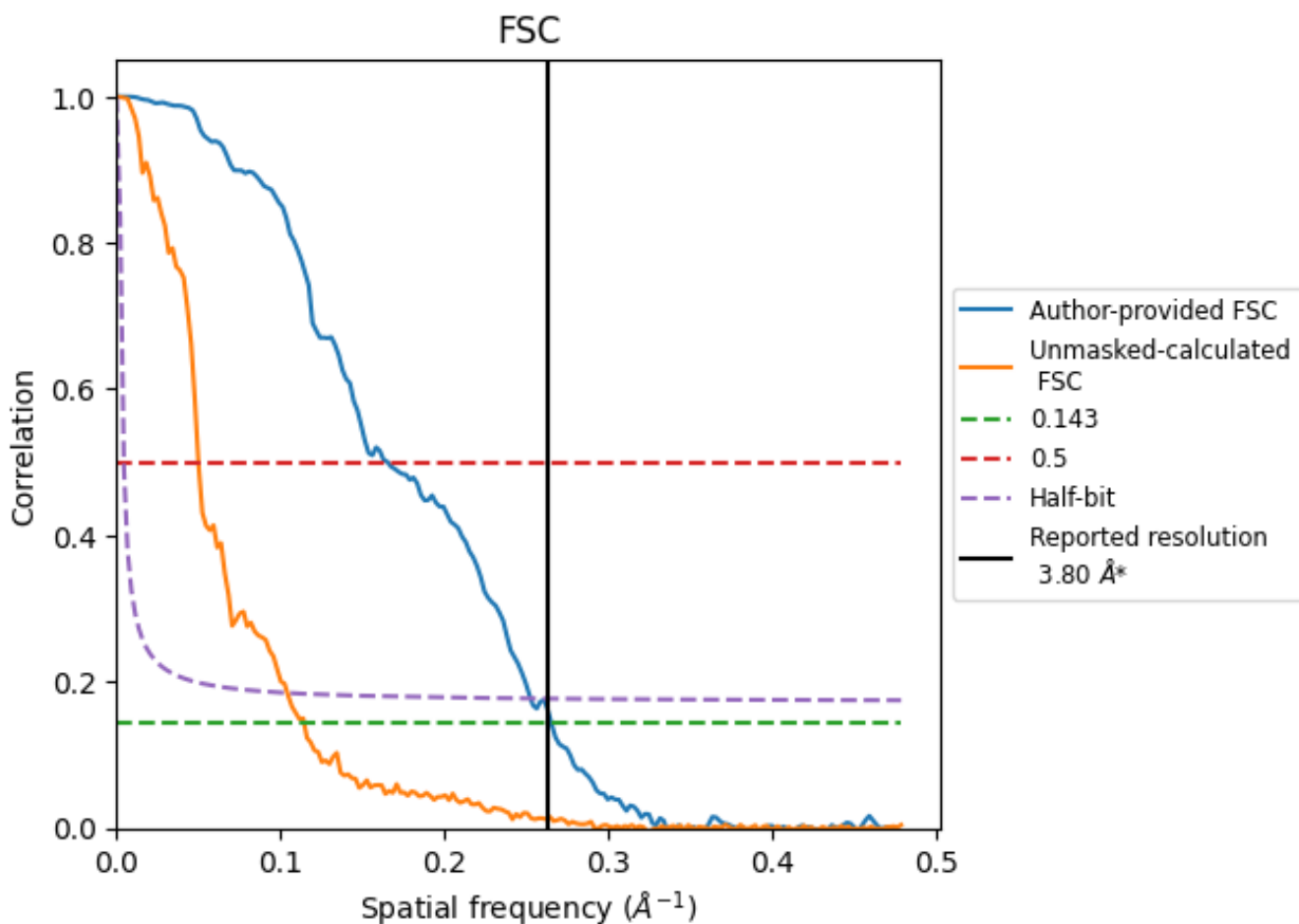


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

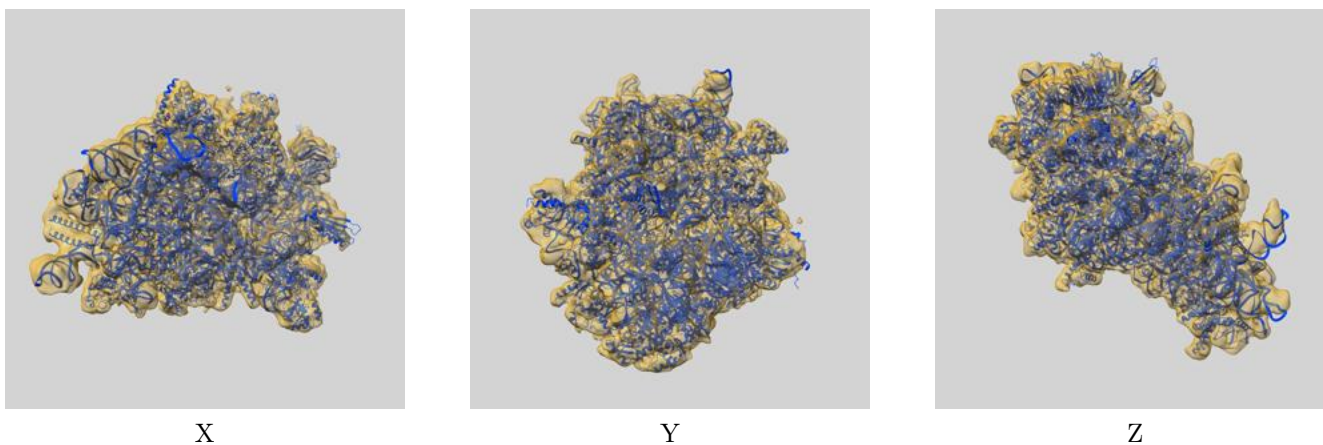
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.77	6.05	3.96
Unmasked-calculated*	8.73	20.00	9.59

*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 3.8 by more than 10 %

9 Map-model fit [i](#)

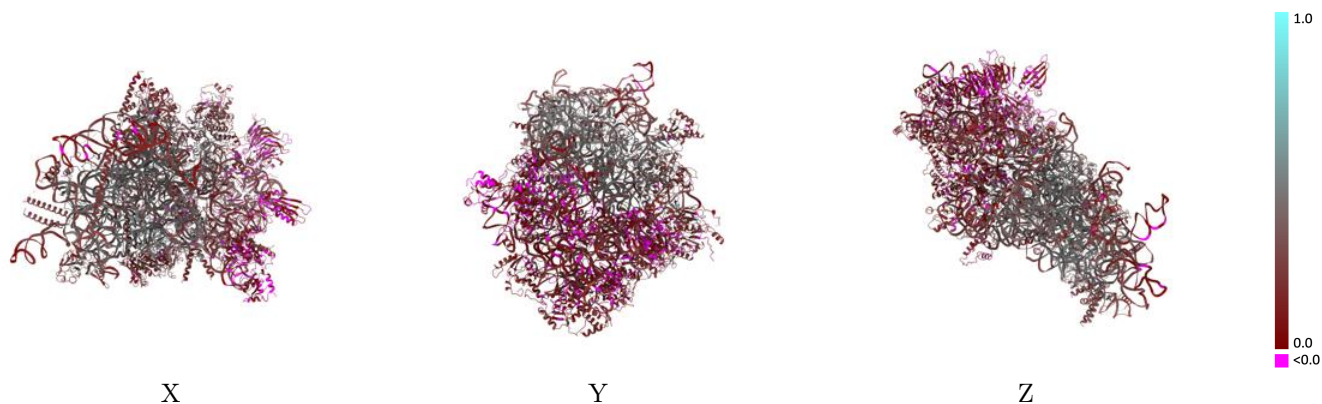
This section contains information regarding the fit between EMDB map EMD-16541 and PDB model 8CBJ. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



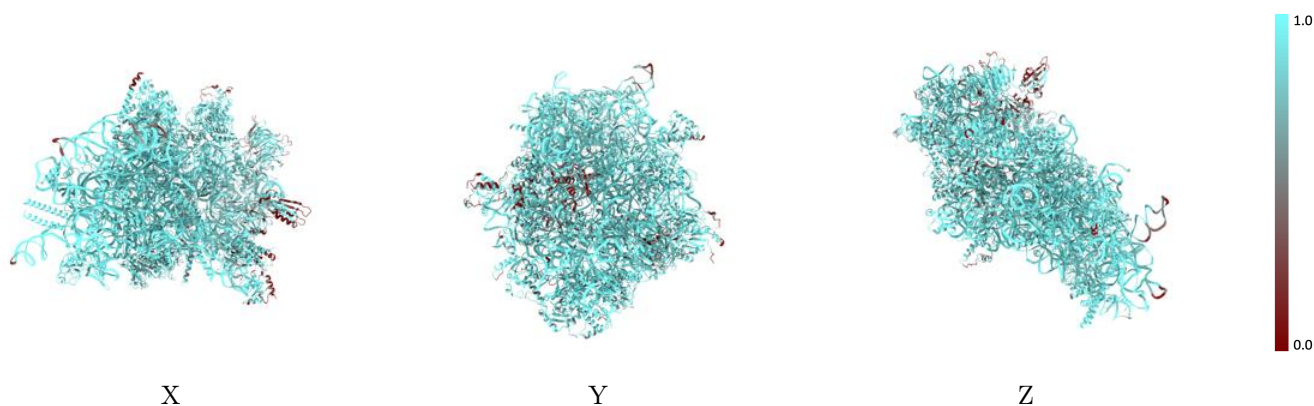
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



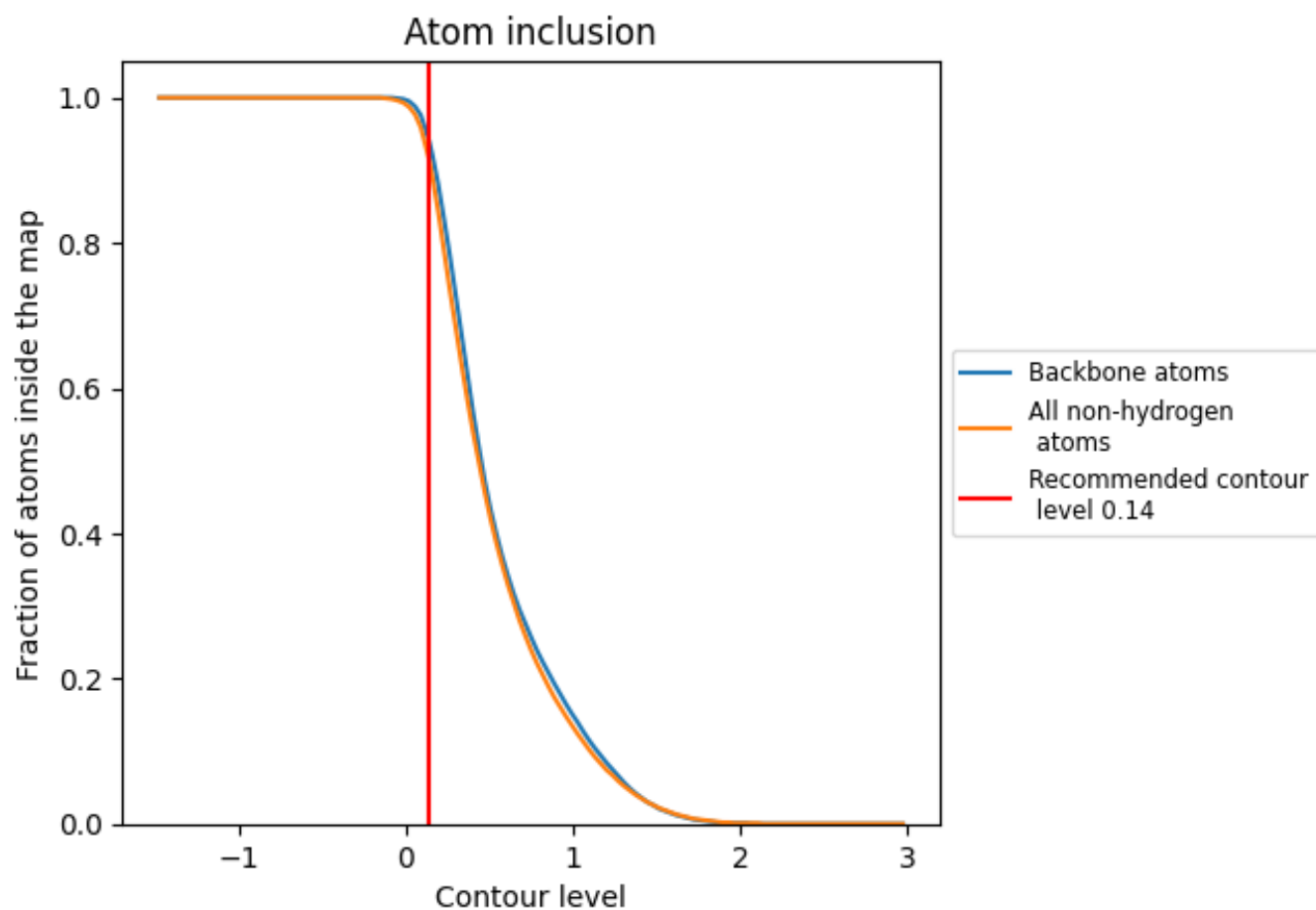
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.14).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 91% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9130	 0.2630
2	 0.9730	 0.3030
A	 0.9240	 0.3220
B	 0.8670	 0.2470
C	 0.9470	 0.3950
D	 0.4960	 0.0690
E	 0.9600	 0.4290
F	 0.8850	 0.1280
G	 0.9700	 0.3040
H	 0.9350	 0.2810
I	 0.9680	 0.4050
J	 0.9480	 0.4090
K	 0.9130	 0.2550
L	 0.9600	 0.4520
M	 0.6920	 0.0350
N	 0.9520	 0.3580
O	 0.8890	 0.2580
P	 0.8960	 0.1490
Q	 0.9280	 0.1010
R	 0.8970	 0.1390
S	 0.8720	 0.1350
T	 0.8620	 0.1110
U	 0.8570	 0.0760
V	 0.9650	 0.3930
W	 0.9710	 0.4450
X	 0.9020	 0.3890
Y	 0.9570	 0.3960
Z	 0.8950	 0.1390
a	 0.8880	 0.2310
b	 0.9500	 0.3760
c	 0.9200	 0.1280
d	 0.8940	 0.0880
e	 0.8370	 0.3070
g	 0.7250	 0.0640
h	 0.8500	 0.2060



Continued on next page...

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Chain	Atom inclusion	Q-score
i	 0.8260	 0.0880
j	 0.5820	 0.0820
k	 0.8260	 0.2090
l	 0.8040	 0.1030
y	 0.7850	 0.1410