Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 04:08 pm GMT

PDB ID	:	6SRI
EMDB ID	:	EMD-10290
Title	:	Structure of the Fanconi anaemia core complex
Authors	:	Shakeel, S.; Rajendra, E.; Alcon, P.; He, S.; Scheres, S.H.W.; Passmore, L.A.
Deposited on	:	2019-09-05
Resolution	:	4.20 Å(reported)

This is a Full wwPDB EM Validation 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:

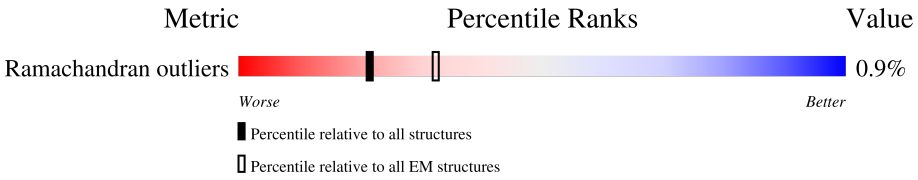
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.20 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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	3	76	78% 100%
1	A	76	25% 100%
1	a	76	26% 100%
2	B	25	8% 100%
2	b	25	8% 100%
3	C	30	23% 100%
3	c	30	17% 100%
4	D	23	30% 100%
4	d	23	30% 100%
5	E	9	11% 100%
5	e	9	100%

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Mol	Chain	Length	Quality of chain
6	F	15	7% 100%
6	Z	15	53% 100%
6	f	15	33% 100%
7	G	26	27% 100%
7	g	26	27% 100%
8	H	17	29% 100%
8	J	17	94% 6%
8	h	17	24% 100%
8	j	17	59% 94% 6%
9	I	37	100%
9	i	37	35% 100%
10	K	21	5% 100%
10	k	21	43% 100%
11	L	18	6% 94% 6%
11	l	18	28% 94% 6%
12	M	120	14% 100%
12	m	120	11% 100%
13	N	43	9% 100%
13	n	43	12% 100%
14	O	279	16% 100%
14	o	279	64% 100%
15	P	276	14% 100%
15	p	276	55% 100%
16	U	227	83% 100%
17	V	27	100% 100%

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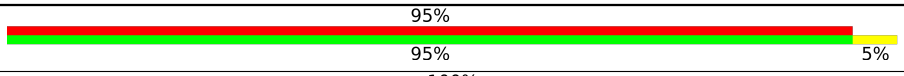
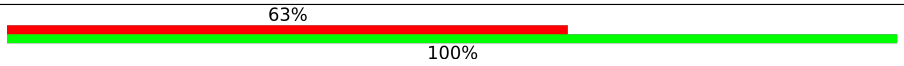
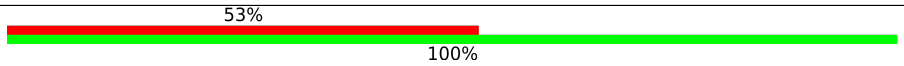
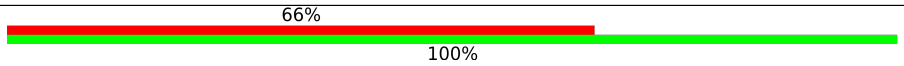
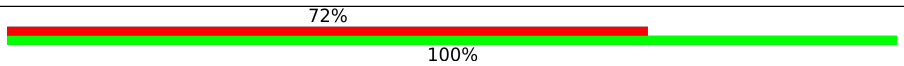
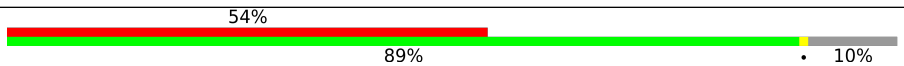
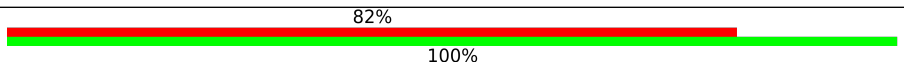
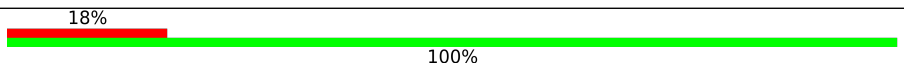
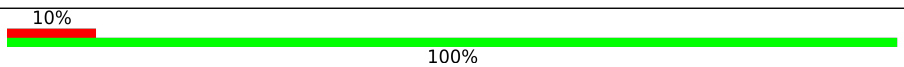
Mol	Chain	Length	Quality of chain
18	W	20	
19	X	13	
20	Y	84	
21	1	109	
22	2	62	
23	4	71	
24	Q	373	
24	q	373	
25	T	201	
26	R	285	
27	S	145	

2 Entry composition (i)

There are 27 unique types of molecules in this entry. The entry contains 15474 atoms, of which 166 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 Unassigned secondary structure elements (central region, proposed FANCB-FAAP100: chain A,a; base region, proposed FANCC-FANC-E-FANCF: chain 3).

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	76	Total 304	C 152	N 76	O 76	0	0
1	a	76	Total 304	C 152	N 76	O 76	0	0
1	3	76	Total 304	C 152	N 76	O 76	0	0

- Molecule 2 is a protein called Unassigned secondary structure elements (central region, proposed FANCB-FAAP100).

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	25	Total 100	C 50	N 25	O 25	0	0
2	b	25	Total 100	C 50	N 25	O 25	0	0

- Molecule 3 is a protein called Unassigned secondary structure elements (central region, proposed FANCB-FAAP100).

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	30	Total 120	C 60	N 30	O 30	0	0
3	c	30	Total 120	C 60	N 30	O 30	0	0

- Molecule 4 is a protein called Unassigned secondary structure elements (central region, proposed FANCB-FAAP100).

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	23	Total 92	C 46	N 23	O 23	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	d	23	Total 92	C 46	N 23	O 23	0	0

- Molecule 5 is a protein called Unassigned secondary structure elements (central region, proposed FANCB-FAAP100).

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	9	Total 36	C 18	N 9	O 9	0	0
5	e	9	Total 36	C 18	N 9	O 9	0	0

- Molecule 6 is a protein called Unassigned secondary structure elements (central region, proposed FANCB-FAAP100: chain F,f; base region, proposed FANCC-FANC-E-FANCF: chain Z).

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	15	Total 60	C 30	N 15	O 15	0	0
6	f	15	Total 60	C 30	N 15	O 15	0	0
6	Z	15	Total 60	C 30	N 15	O 15	0	0

- Molecule 7 is a protein called Unassigned secondary structure elements (central region, proposed FANCB-FAAP100).

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	26	Total 104	C 52	N 26	O 26	0	0
7	g	26	Total 104	C 52	N 26	O 26	0	0

- Molecule 8 is a protein called Unassigned secondary structure elements (central region, proposed FANCB-FAAP100).

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	17	Total 68	C 34	N 17	O 17	0	0
8	J	17	Total 68	C 34	N 17	O 17	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
8	h	17	Total 68	C 34	N 17	O 17	0	0
8	j	17	Total 68	C 34	N 17	O 17	0	0

- Molecule 9 is a protein called Unassigned secondary structure elements (central region, proposed FANCB-FAAP100).

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	37	Total 148	C 74	N 37	O 37	0	0
9	i	37	Total 148	C 74	N 37	O 37	0	0

- Molecule 10 is a protein called Unassigned secondary structure elements (central region, proposed FANCB-FAAP100).

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	21	Total 84	C 42	N 21	O 21	0	0
10	k	21	Total 84	C 42	N 21	O 21	0	0

- Molecule 11 is a protein called Unassigned secondary structure elements (central region, proposed FANCB-FAAP100).

Mol	Chain	Residues	Atoms				AltConf	Trace
11	L	18	Total 72	C 36	N 18	O 18	0	0
11	l	18	Total 72	C 36	N 18	O 18	0	0

- Molecule 12 is a protein called Unassigned secondary structure elements (proposed FANCB).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	120	Total 521	C 240	H 41	N 120	O 120	0	0
12	m	120	Total 521	C 240	H 41	N 120	O 120	0	0

- Molecule 13 is a protein called Unassigned secondary structure elements (proposed FAAP100).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	43	Total	C	H	N	O	0	0
			214	86	42	43	43		
13	n	43	Total	C	H	N	O	0	0
			214	86	42	43	43		

- Molecule 14 is a protein called Unassigned secondary structure elements (proposed FANCB).

Mol	Chain	Residues	Atoms				AltConf	Trace
14	o	279	Total	C	N	O	0	0
			1116	558	279	279		
14	O	279	Total	C	N	O	0	0
			1116	558	279	279		

- Molecule 15 is a protein called Unassigned secondary structure elements (proposed FAAP100).

Mol	Chain	Residues	Atoms				AltConf	Trace
15	p	276	Total	C	N	O	0	0
			1104	552	276	276		
15	P	276	Total	C	N	O	0	0
			1104	552	276	276		

- Molecule 16 is a protein called Unassigned secondary structure elements (base region, proposed FANCC-FANC-E-FANCF).

Mol	Chain	Residues	Atoms				AltConf	Trace
16	U	227	Total	C	N	O	0	0
			908	454	227	227		

- Molecule 17 is a protein called Unassigned secondary structure elements (base region, proposed FANCC-FANC-E-FANCF).

Mol	Chain	Residues	Atoms				AltConf	Trace
17	V	27	Total	C	N	O	0	0
			108	54	27	27		

- Molecule 18 is a protein called Unassigned secondary structure elements (base region, proposed FANCC-FANC-E-FANCF).

Mol	Chain	Residues	Atoms				AltConf	Trace
18	W	20	Total	C	N	O	0	0
			80	40	20	20		

- Molecule 19 is a protein called Unassigned secondary structure elements (base region, proposed FANCC-FANC-E-FANCF).

Mol	Chain	Residues	Atoms				AltConf	Trace
19	X	13	Total	C	N	O	0	0
			52	26	13	13		

- Molecule 20 is a protein called Unassigned secondary structure elements (base region, proposed FANCC-FANC-E-FANCF).

Mol	Chain	Residues	Atoms				AltConf	Trace
20	Y	84	Total	C	N	O	0	0
			336	168	84	84		

- Molecule 21 is a protein called Unassigned secondary structure elements (base region, proposed FANCC-FANC-E-FANCF).

Mol	Chain	Residues	Atoms				AltConf	Trace
21	1	109	Total	C	N	O	0	0
			436	218	109	109		

- Molecule 22 is a protein called Unassigned secondary structure elements (base region, proposed FANCC-FANC-E-FANCF).

Mol	Chain	Residues	Atoms				AltConf	Trace
22	2	62	Total	C	N	O	0	0
			248	124	62	62		

- Molecule 23 is a protein called Unassigned secondary structure elements (base region, proposed FANCC-FANC-E-FANCF).

Mol	Chain	Residues	Atoms				AltConf	Trace
23	4	71	Total	C	N	O	0	0
			284	142	71	71		

- Molecule 24 is a protein called Fanconi anaemia protein FANCL.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	q	337	Total	C	N	O	0	0
			1348	674	337	337		
24	Q	91	Total	C	N	O	0	0
			364	182	91	91		

- Molecule 25 is a protein called base region, proposed FANCF.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	T	201	Total 804	C 402	N 201	O 201	0	0

- Molecule 26 is a protein called Unassigned secondary structure elements (top region, proposed FANCG).

Mol	Chain	Residues	Atoms				AltConf	Trace
26	R	285	Total 1140	C 570	N 285	O 285	0	0

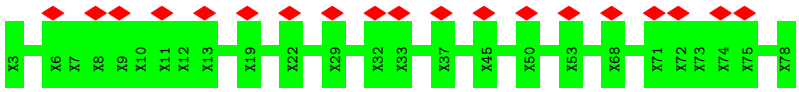
- Molecule 27 is a protein called Unassigned secondary structure elements (top region, proposed FANCG).

Mol	Chain	Residues	Atoms				AltConf	Trace
27	S	145	Total 580	C 290	N 145	O 145	0	0

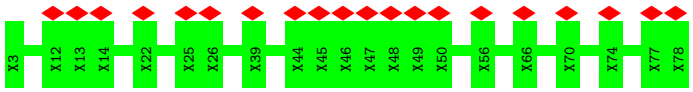
3 Residue-property plots (i)

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.

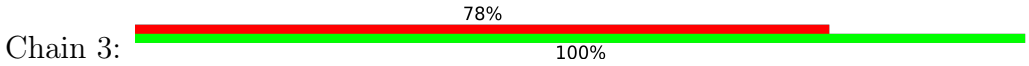
• Molecule 1: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100: chain A,a; base region, proposed FANCC-FANC-E-FANCF: chain 3)

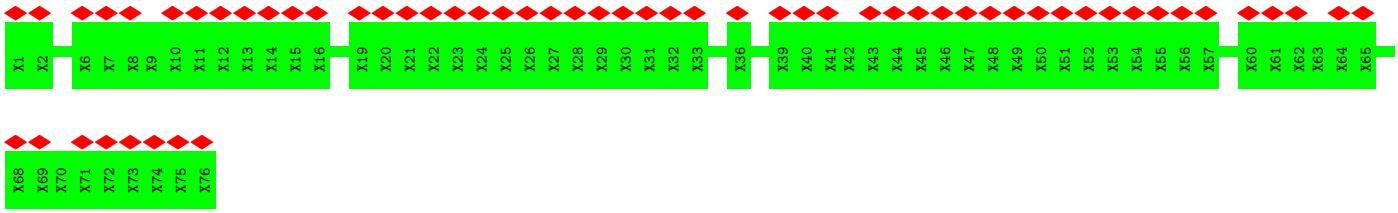


• Molecule 1: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100: chain A,a; base region, proposed FANCC-FANC-E-FANCF: chain 3)

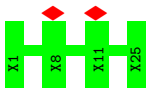


• Molecule 1: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100: chain A,a; base region, proposed FANCC-FANC-E-FANCF: chain 3)



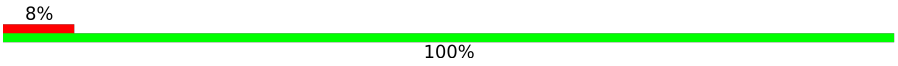


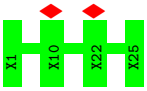
• Molecule 2: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)



• Molecule 2: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

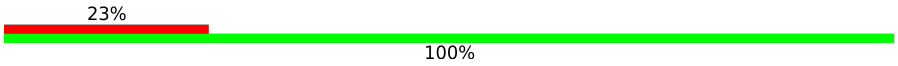
Chain b:

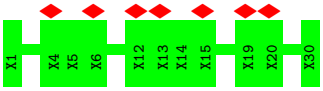




• Molecule 3: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

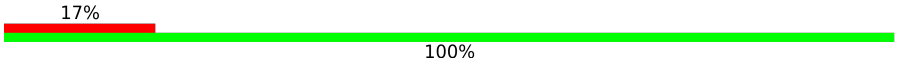
Chain C:

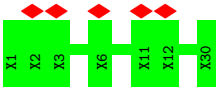




• Molecule 3: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

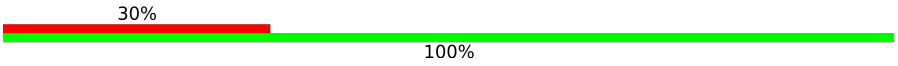
Chain c:

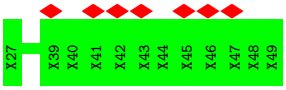




• Molecule 4: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

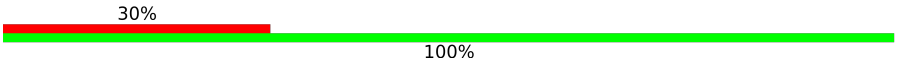
Chain D:

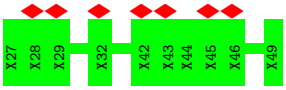




• Molecule 4: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

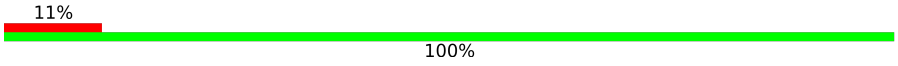
Chain d:





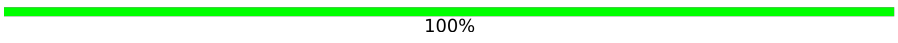
• Molecule 5: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

Chain E:



• Molecule 5: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

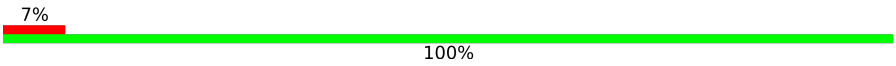
Chain e:

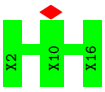


There are no outlier residues recorded for this chain.

• Molecule 6: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100: chain F,f; base region, proposed FANCC-FANC-E-FANCF: chain Z)

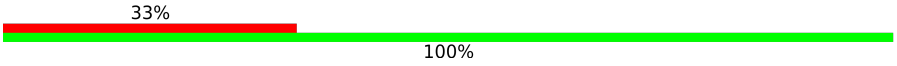
Chain F:

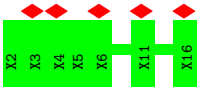




• Molecule 6: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100: chain F,f; base region, proposed FANCC-FANC-E-FANCF: chain Z)

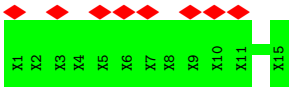
Chain f:





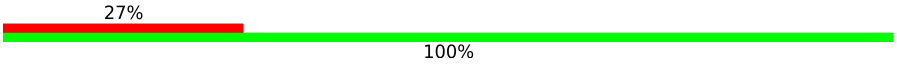
• Molecule 6: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100: chain F,f; base region, proposed FANCC-FANC-E-FANCF: chain Z)

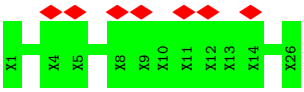
Chain Z:



• Molecule 7: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

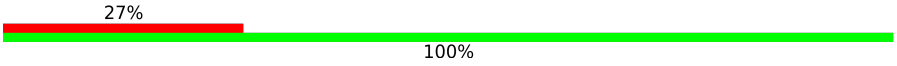
Chain G:

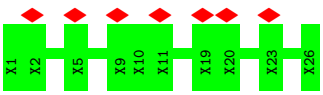




• Molecule 7: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

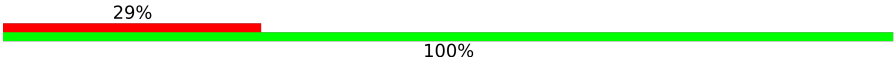
Chain g:

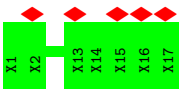




• Molecule 8: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

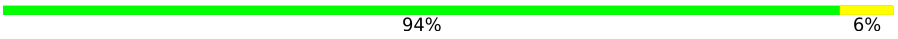
Chain H:





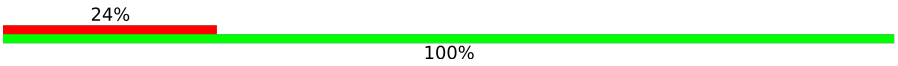
• Molecule 8: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

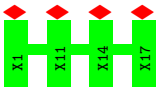
Chain J:



• Molecule 8: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

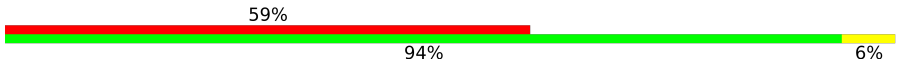
Chain h:

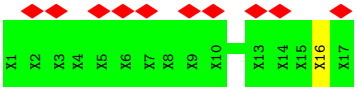




• Molecule 8: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

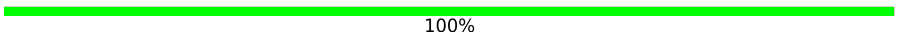
Chain j:





• Molecule 9: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

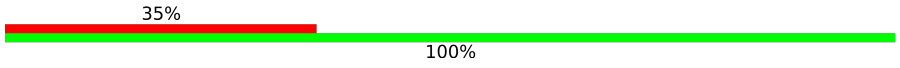
Chain I:

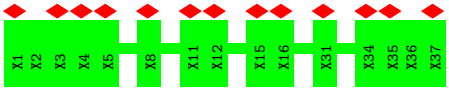


There are no outlier residues recorded for this chain.

• Molecule 9: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

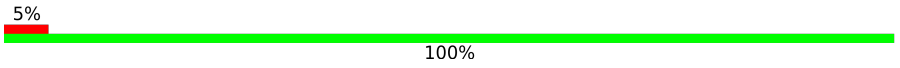
Chain i:

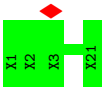




• Molecule 10: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

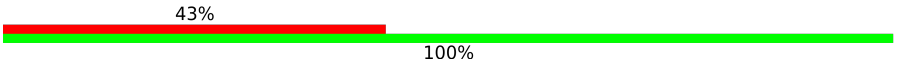
Chain K:

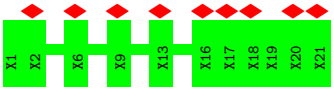




• Molecule 10: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

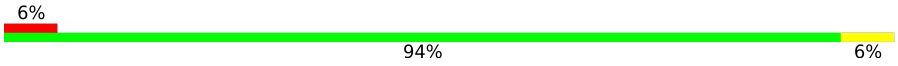
Chain k:

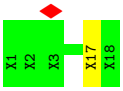




• Molecule 11: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

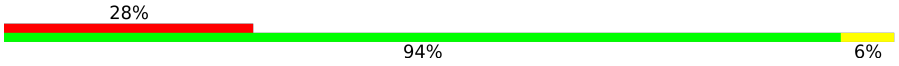
Chain L:

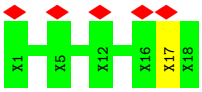




• Molecule 11: Unassigned secondary structure elements (central region, proposed FANCB-FAAP100)

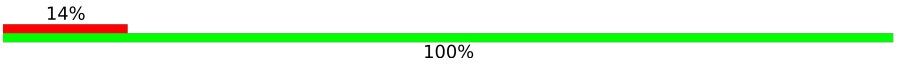
Chain l:

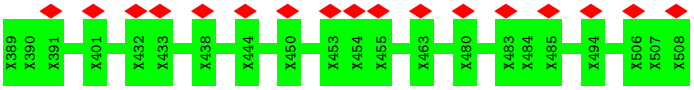




• Molecule 12: Unassigned secondary structure elements (proposed FANCB)

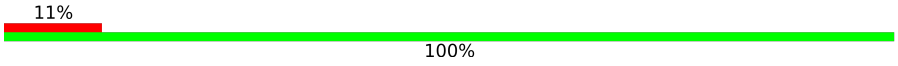
Chain M:

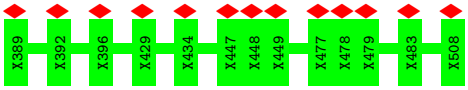




• Molecule 12: Unassigned secondary structure elements (proposed FANCB)

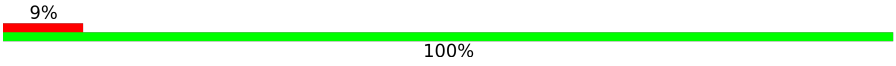
Chain m:

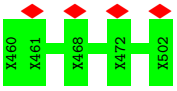




• Molecule 13: Unassigned secondary structure elements (proposed FAAP100)

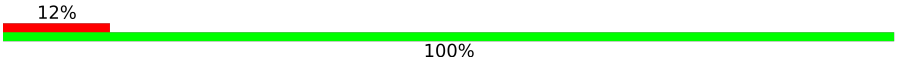
Chain N:

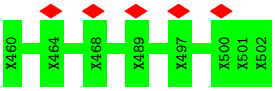




• Molecule 13: Unassigned secondary structure elements (proposed FAAP100)

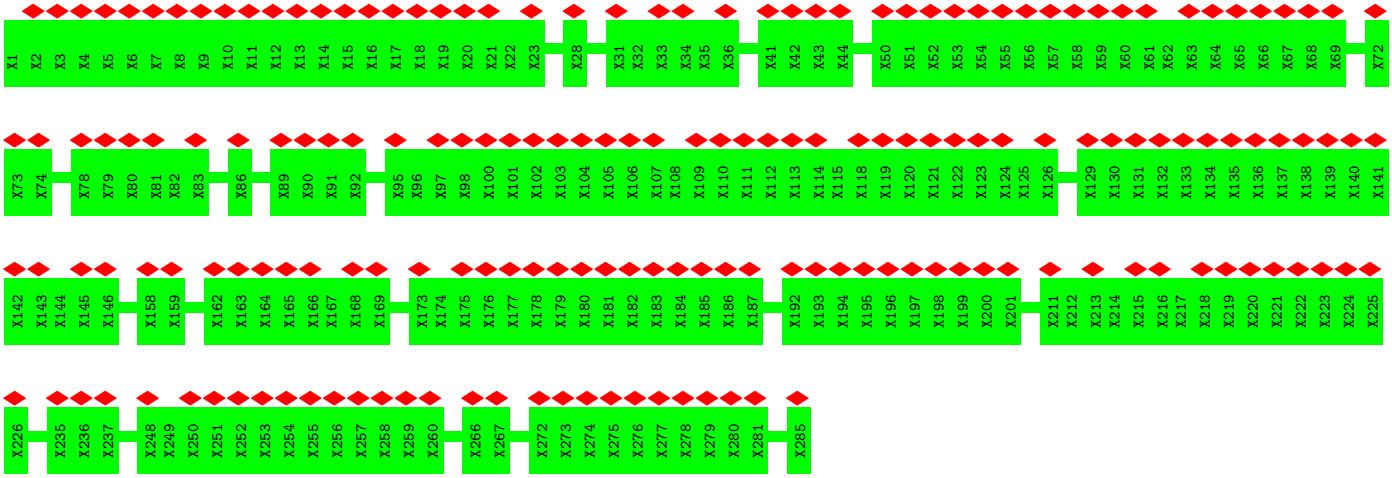
Chain n:





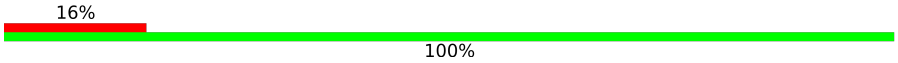
• Molecule 14: Unassigned secondary structure elements (proposed FANCB)

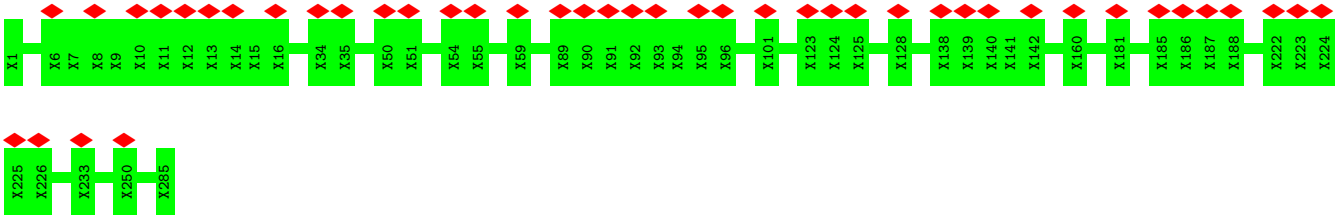
Chain o:



• Molecule 14: Unassigned secondary structure elements (proposed FANCB)

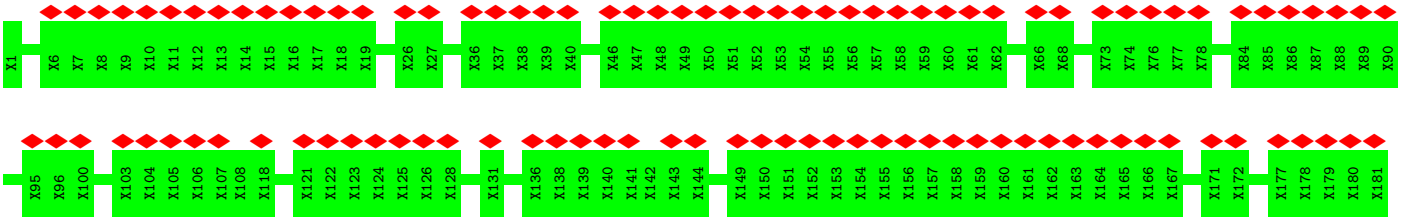
Chain O:





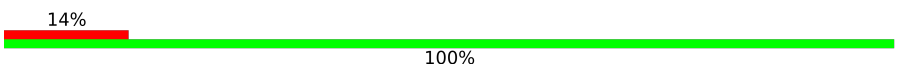
• Molecule 15: Unassigned secondary structure elements (proposed FAAP100)

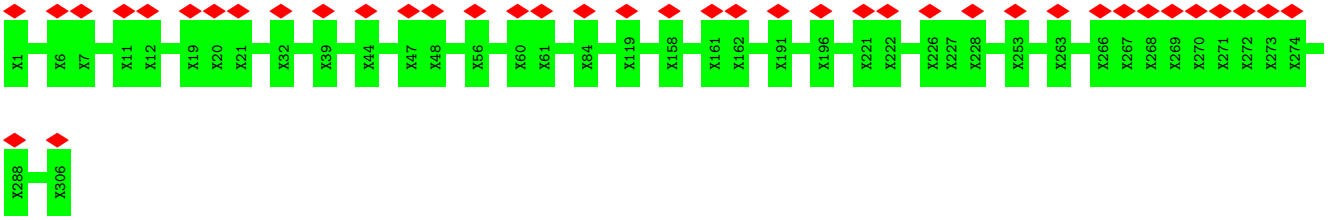
Chain p:



• Molecule 15: Unassigned secondary structure elements (proposed FAAP100)

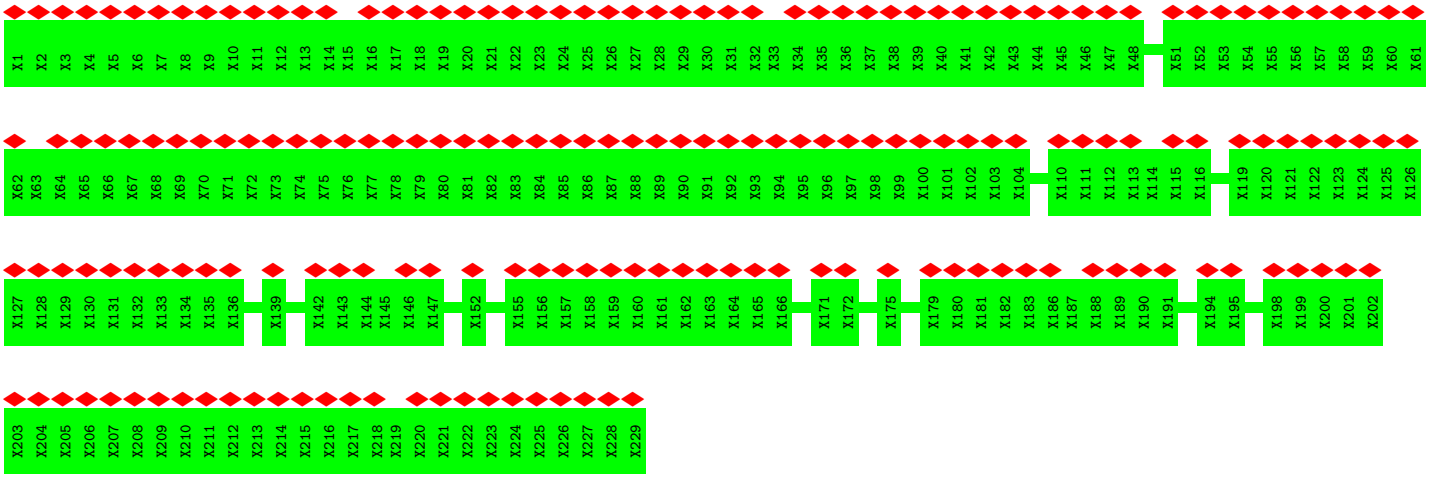
Chain P:





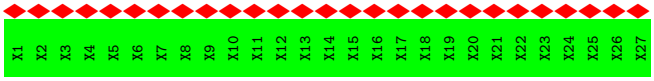
• Molecule 16: Unassigned secondary structure elements (base region, proposed FANCC-FANC-E-FANCF)

Chain U:



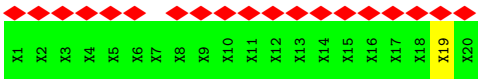
• Molecule 17: Unassigned secondary structure elements (base region, proposed FANCC-FANC-E-FANCF)

Chain V:



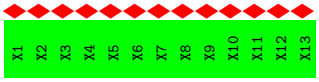
• Molecule 18: Unassigned secondary structure elements (base region, proposed FANCC-FANC-E-FANCF)

Chain W:



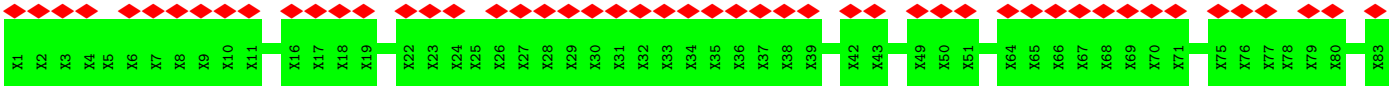
• Molecule 19: Unassigned secondary structure elements (base region, proposed FANCC-FANC-E-FANCF)

Chain X:



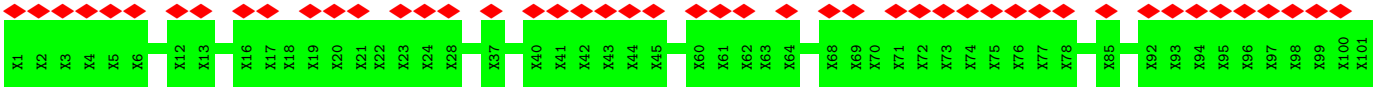
• Molecule 20: Unassigned secondary structure elements (base region, proposed FANCC-FANC-E-FANCF)

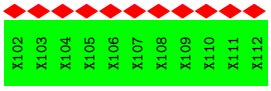
Chain Y:



• Molecule 21: Unassigned secondary structure elements (base region, proposed FANCC-FANC-E-FANCF)

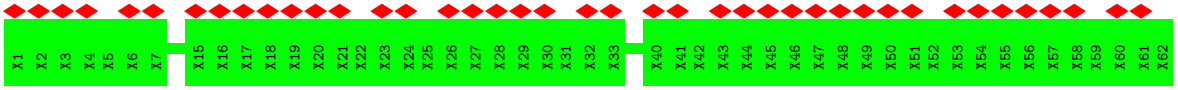
Chain 1:





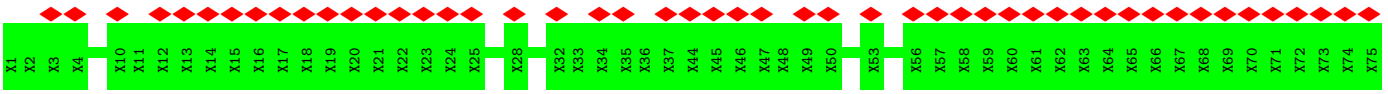
• Molecule 22: Unassigned secondary structure elements (base region, proposed FANCC-FANC-E-FANCF)

Chain 2:



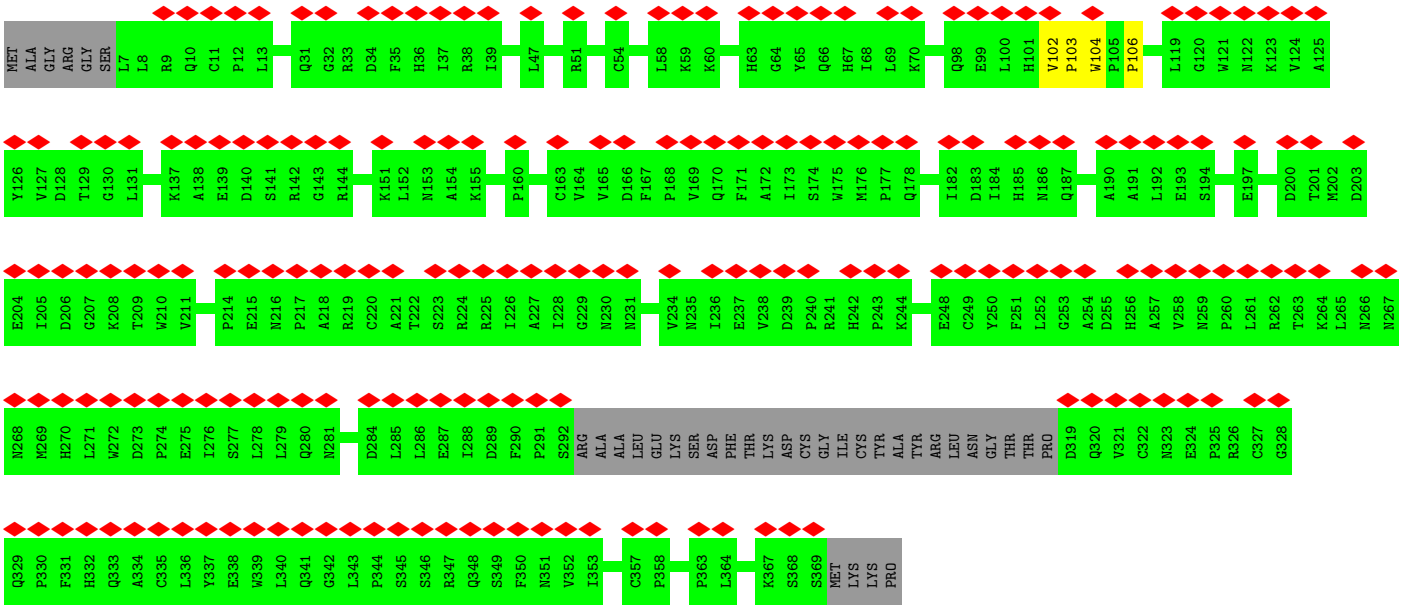
• Molecule 23: Unassigned secondary structure elements (base region, proposed FANCC-FANC-E-FANCF)

Chain 4:



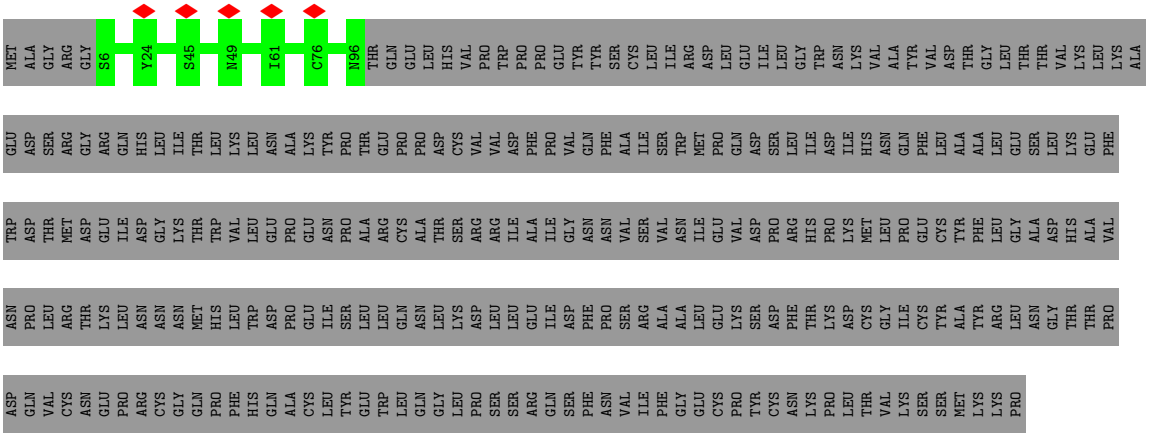
• Molecule 24: Fanconi anaemia protein FANCL

Chain q:



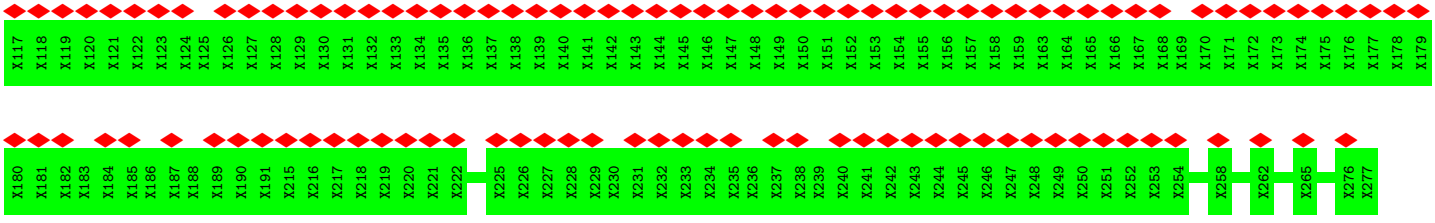
• Molecule 24: Fanconi anaemia protein FANCL

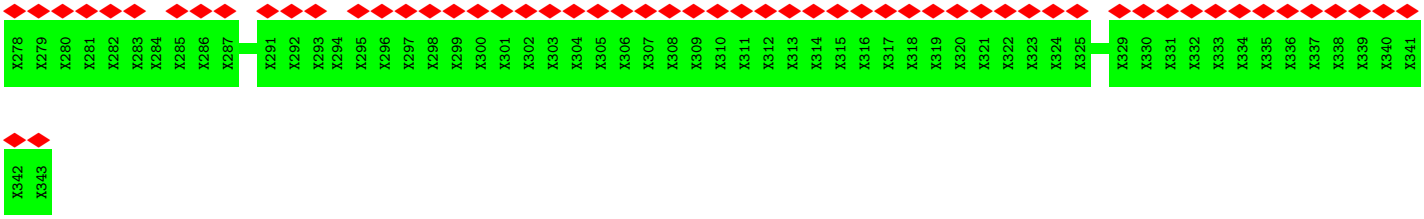
Chain Q:



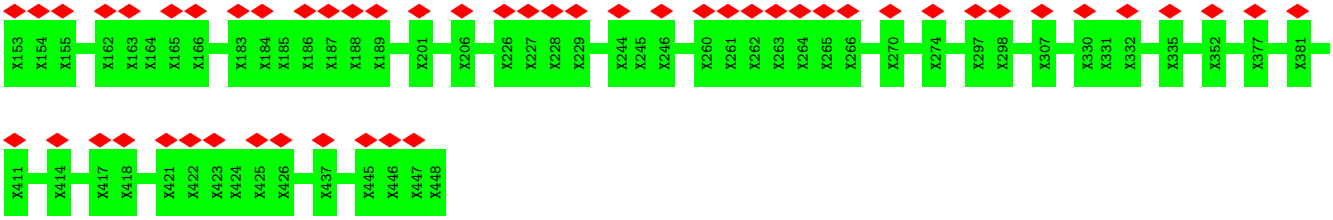
• Molecule 25: base region, proposed FANCF

Chain T:

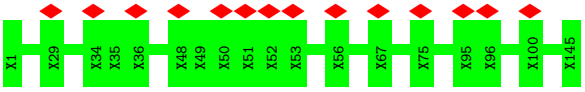




• Molecule 26: Unassigned secondary structure elements (top region, proposed FANCG)



• Molecule 27: Unassigned secondary structure elements (top region, proposed FANCG)



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	169000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.0	Depositor
Minimum defocus (nm)	-1800	Depositor
Maximum defocus (nm)	-4000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.073	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0138	Depositor
Map size (Å)	609.44, 609.44, 609.44	wwPDB
Map dimensions	586, 586, 586	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

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
24	Q	0.22	0/363	0.50	0/452
24	q	0.23	0/1346	0.49	0/1679
All	All	0.22	0/1709	0.49	0/2131

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
8	J	0	1
8	j	0	1
11	L	0	1
11	l	0	1
18	W	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	J	16	UNK	Mainchain
11	L	17	UNK	Mainchain
18	W	19	UNK	Mainchain
8	j	16	UNK	Mainchain
11	l	17	UNK	Mainchain

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
24	Q	89/373 (24%)	88 (99%)	1 (1%)	0	100	100
24	q	333/373 (89%)	312 (94%)	17 (5%)	4 (1%)	13	50
All	All	422/746 (57%)	400 (95%)	18 (4%)	4 (1%)	21	56

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
24	q	103	PRO
24	q	106	PRO
24	q	104	TRP
24	q	102	VAL

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
14	o	12
15	p	10
15	P	10
14	O	10
1	A	3
1	a	3
25	T	2
7	G	2
7	g	2
27	S	1
23	4	1
26	R	1
16	U	1
21	1	1
12	m	1
4	D	1
4	d	1
20	Y	1
12	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	p	240:UNK	C	244:UNK	N	21.69
1	p	96:UNK	C	100:UNK	N	15.16

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	p	281:UNK	C	288:UNK	N	12.83
1	P	228:UNK	C	232:UNK	N	12.83
1	T	191:UNK	C	215:UNK	N	11.77
1	S	123:UNK	C	124:UNK	N	11.75
1	o	98:UNK	C	100:UNK	N	11.66
1	O	128:UNK	C	129:UNK	N	11.32
1	p	228:UNK	C	232:UNK	N	11.25
1	o	146:UNK	C	150:UNK	N	11.15
1	P	240:UNK	C	244:UNK	N	10.60
1	O	146:UNK	C	150:UNK	N	10.44
1	p	108:UNK	C	118:UNK	N	10.20
1	p	136:UNK	C	138:UNK	N	9.73
1	P	108:UNK	C	118:UNK	N	8.98
1	A	65:UNK	C	66:UNK	N	8.86
1	a	65:UNK	C	66:UNK	N	8.85
1	T	159:UNK	C	163:UNK	N	8.85
1	O	115:UNK	C	118:UNK	N	8.75
1	O	98:UNK	C	100:UNK	N	8.42
1	P	126:UNK	C	128:UNK	N	8.35
1	G	18:UNK	C	19:UNK	N	7.93
1	g	18:UNK	C	19:UNK	N	7.93
1	4	37:UNK	C	44:UNK	N	7.80
1	P	136:UNK	C	138:UNK	N	7.73
1	p	27:UNK	C	30:UNK	N	7.32
1	R	381:UNK	C	393:UNK	N	7.27
1	o	166:UNK	C	167:UNK	N	7.09
1	U	183:UNK	C	186:UNK	N	6.98
1	P	66:UNK	C	68:UNK	N	6.98
1	1	24:UNK	C	28:UNK	N	6.89
1	O	60:UNK	C	61:UNK	N	6.67
1	O	95:UNK	C	96:UNK	N	6.59
1	G	16:UNK	C	17:UNK	N	6.48
1	g	16:UNK	C	17:UNK	N	6.48
1	m	430:UNK	C	431:UNK	N	6.48
1	P	27:UNK	C	30:UNK	N	6.48
1	P	96:UNK	C	100:UNK	N	6.41
1	o	80:UNK	C	81:UNK	N	6.30
1	p	66:UNK	C	68:UNK	N	6.12
1	p	74:UNK	C	76:UNK	N	5.97
1	p	126:UNK	C	128:UNK	N	5.94
1	P	281:UNK	C	288:UNK	N	5.92
1	A	61:UNK	C	62:UNK	N	5.82

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	a	61:UNK	C	62:UNK	N	5.82
1	o	128:UNK	C	129:UNK	N	5.35
1	A	43:UNK	C	44:UNK	N	5.29
1	a	43:UNK	C	44:UNK	N	5.29
1	P	74:UNK	C	76:UNK	N	5.16
1	D	43:UNK	C	44:UNK	N	5.02
1	d	43:UNK	C	44:UNK	N	5.02
1	o	39:UNK	C	40:UNK	N	4.73
1	O	39:UNK	C	40:UNK	N	4.73
1	o	95:UNK	C	96:UNK	N	4.61
1	O	188:UNK	C	189:UNK	N	4.58
1	o	60:UNK	C	61:UNK	N	4.51
1	o	115:UNK	C	118:UNK	N	4.46
1	o	188:UNK	C	189:UNK	N	4.24
1	O	80:UNK	C	81:UNK	N	3.77
1	o	19:UNK	C	20:UNK	N	3.73
1	Y	51:UNK	C	54:UNK	N	3.73
1	M	430:UNK	C	431:UNK	N	3.57
1	O	51:UNK	C	52:UNK	N	3.57
1	o	31:UNK	C	32:UNK	N	3.35

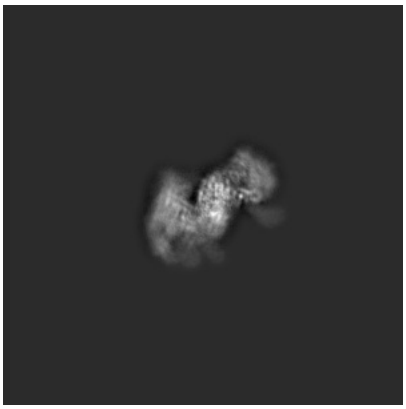
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10290. 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.

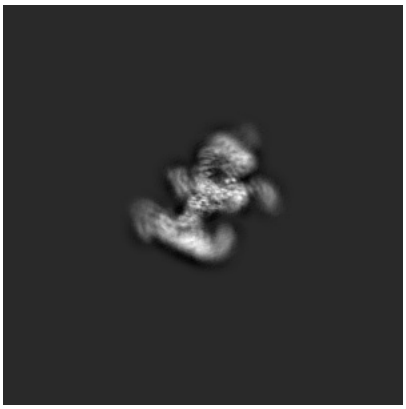
6.1 Orthogonal projections

6.1.1 Primary map



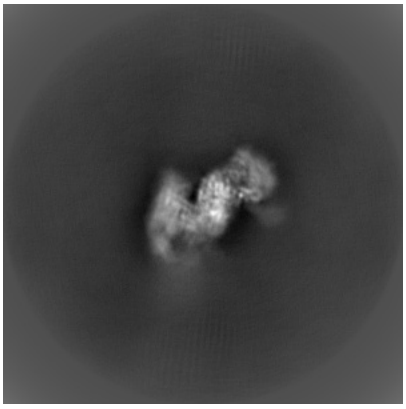
X

Y

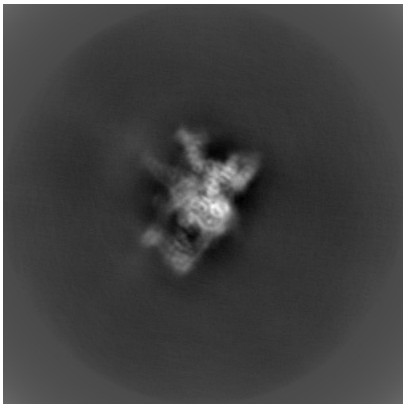


Z

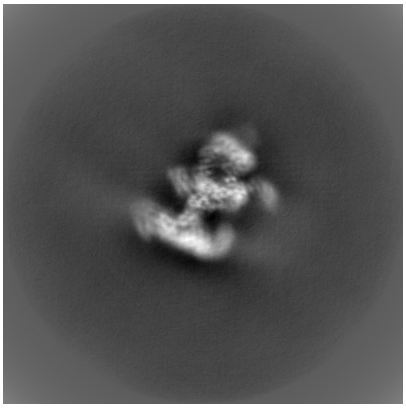
6.1.2 Raw map



X



Y

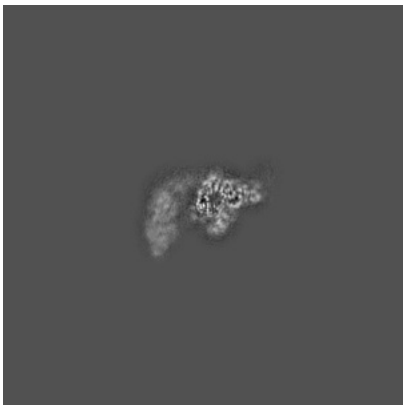


Z

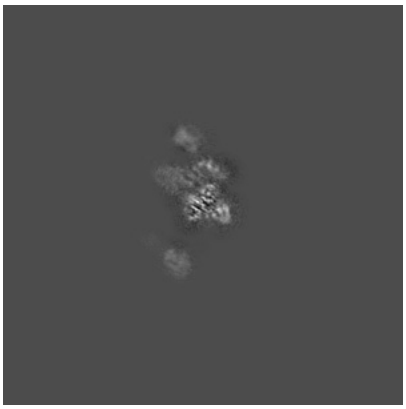
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

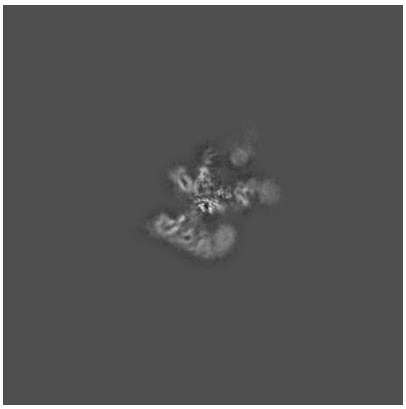
6.2.1 Primary map



X Index: 293

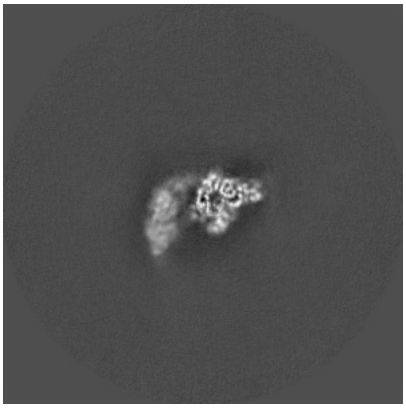


Y Index: 293

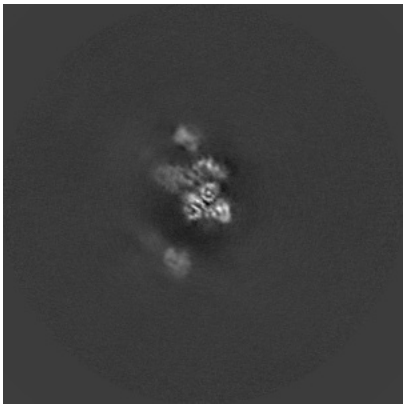


Z Index: 293

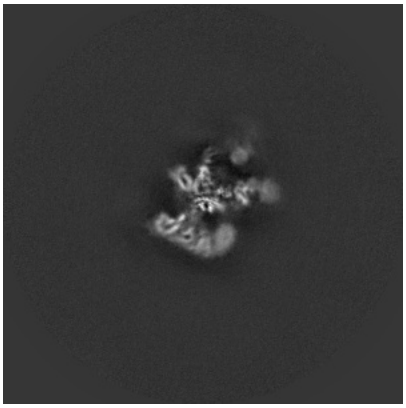
6.2.2 Raw map



X Index: 293



Y Index: 293

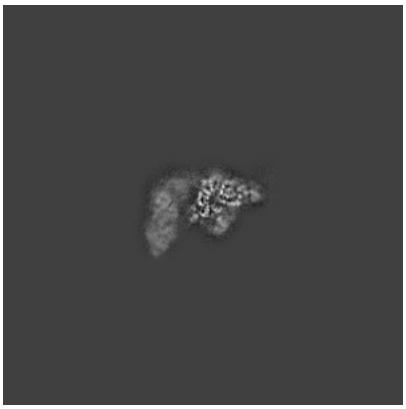


Z Index: 293

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

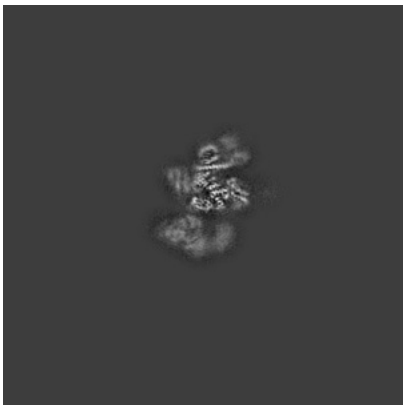
6.3 Largest variance slices (i)

6.3.1 Primary map



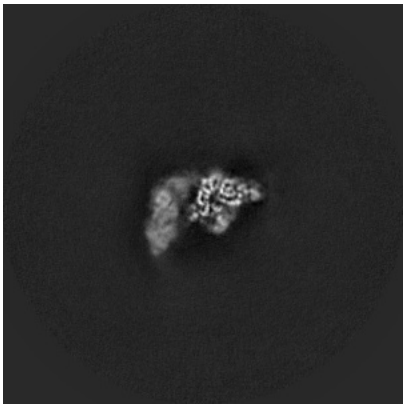
X Index: 290

Y Index: 311

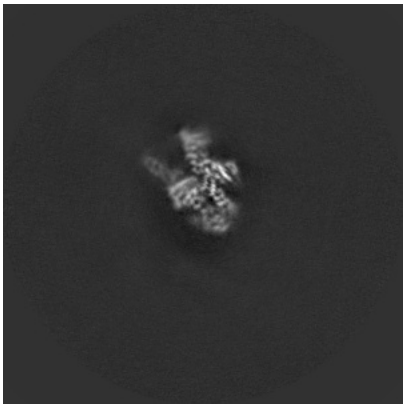


Z Index: 306

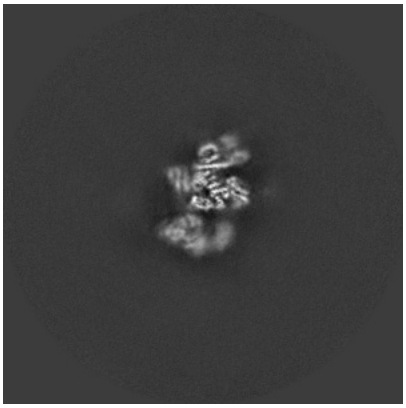
6.3.2 Raw map



X Index: 290



Y Index: 312



Z Index: 306

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0138. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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

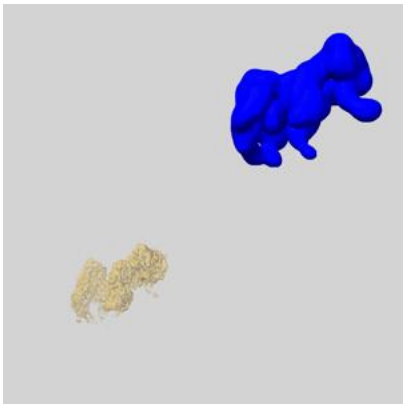
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

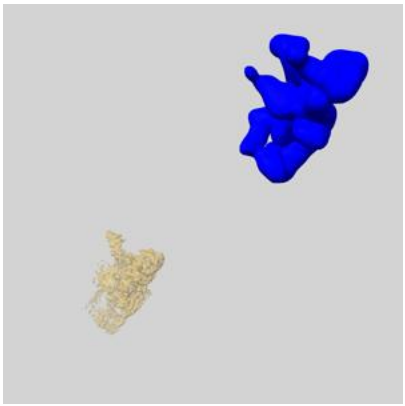
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

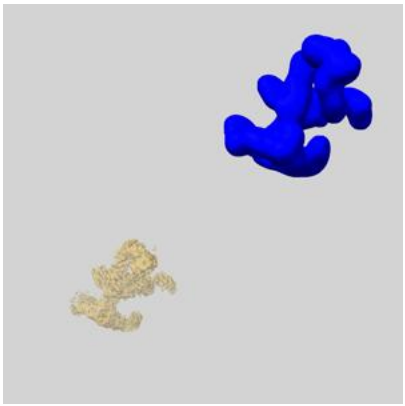
6.5.1 emd_10290_msk_1.map (i)



X



Y

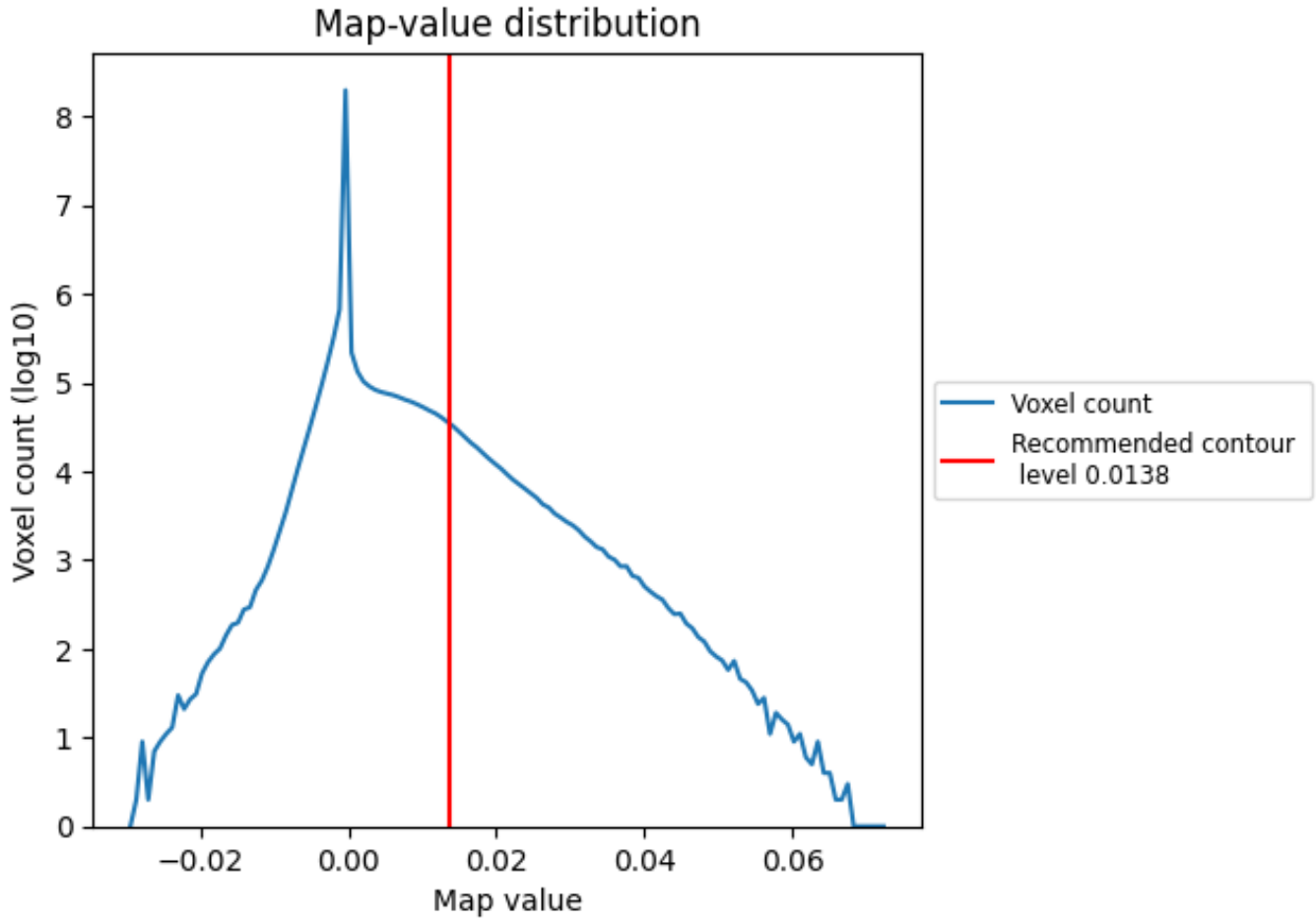


Z

7 Map analysis

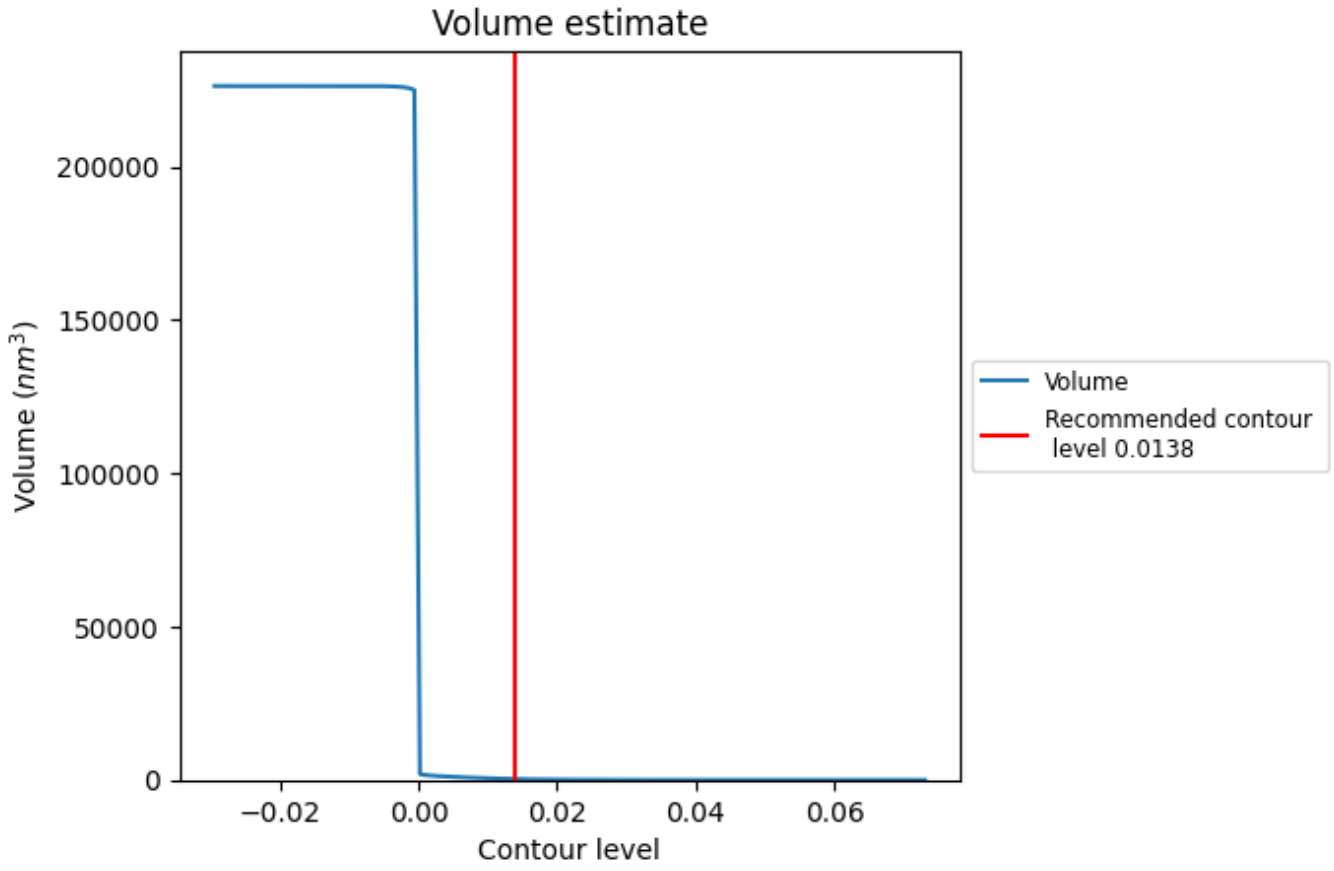
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

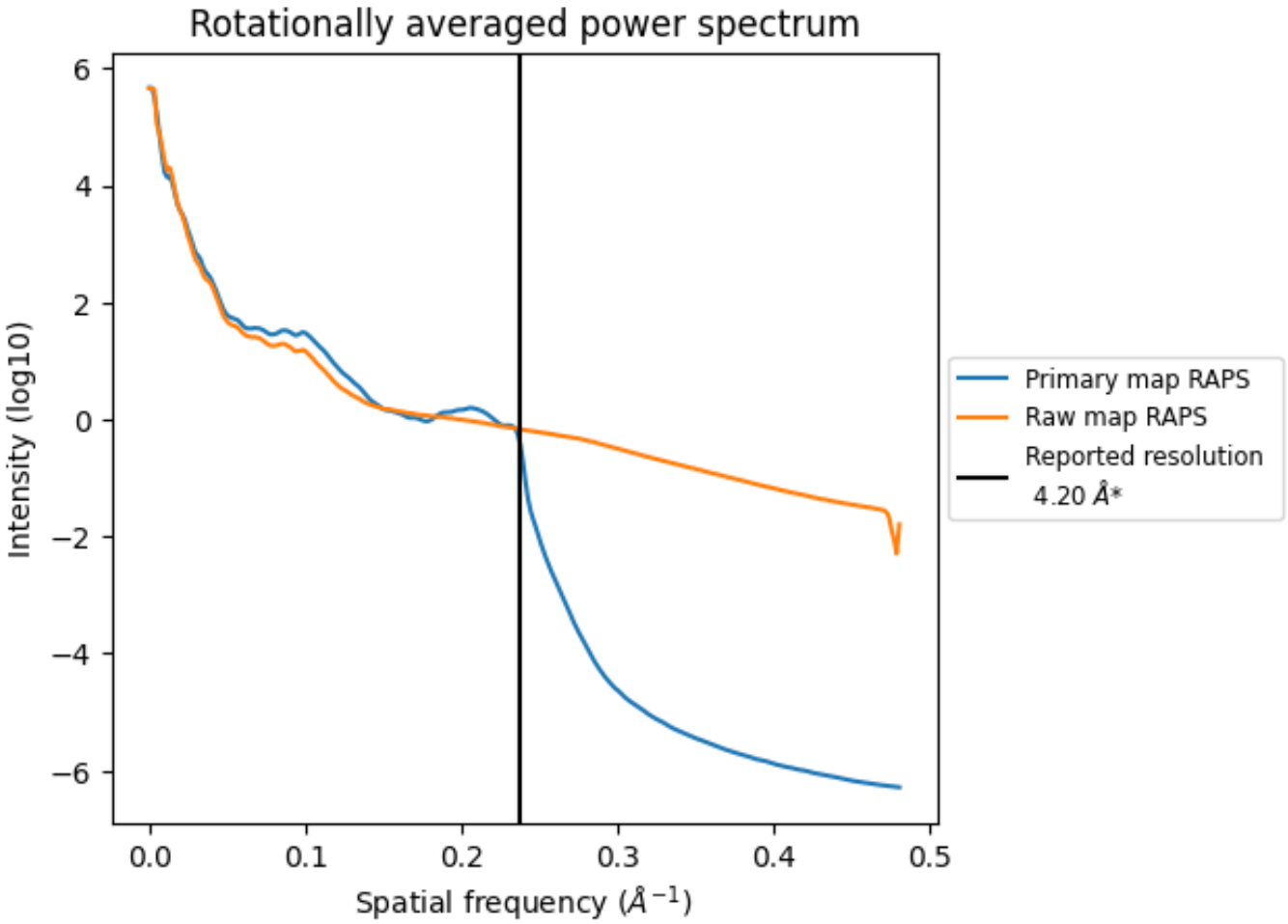
7.2 Volume estimate



The volume at the recommended contour level is 306 nm^3; this corresponds to an approximate mass of 276 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)

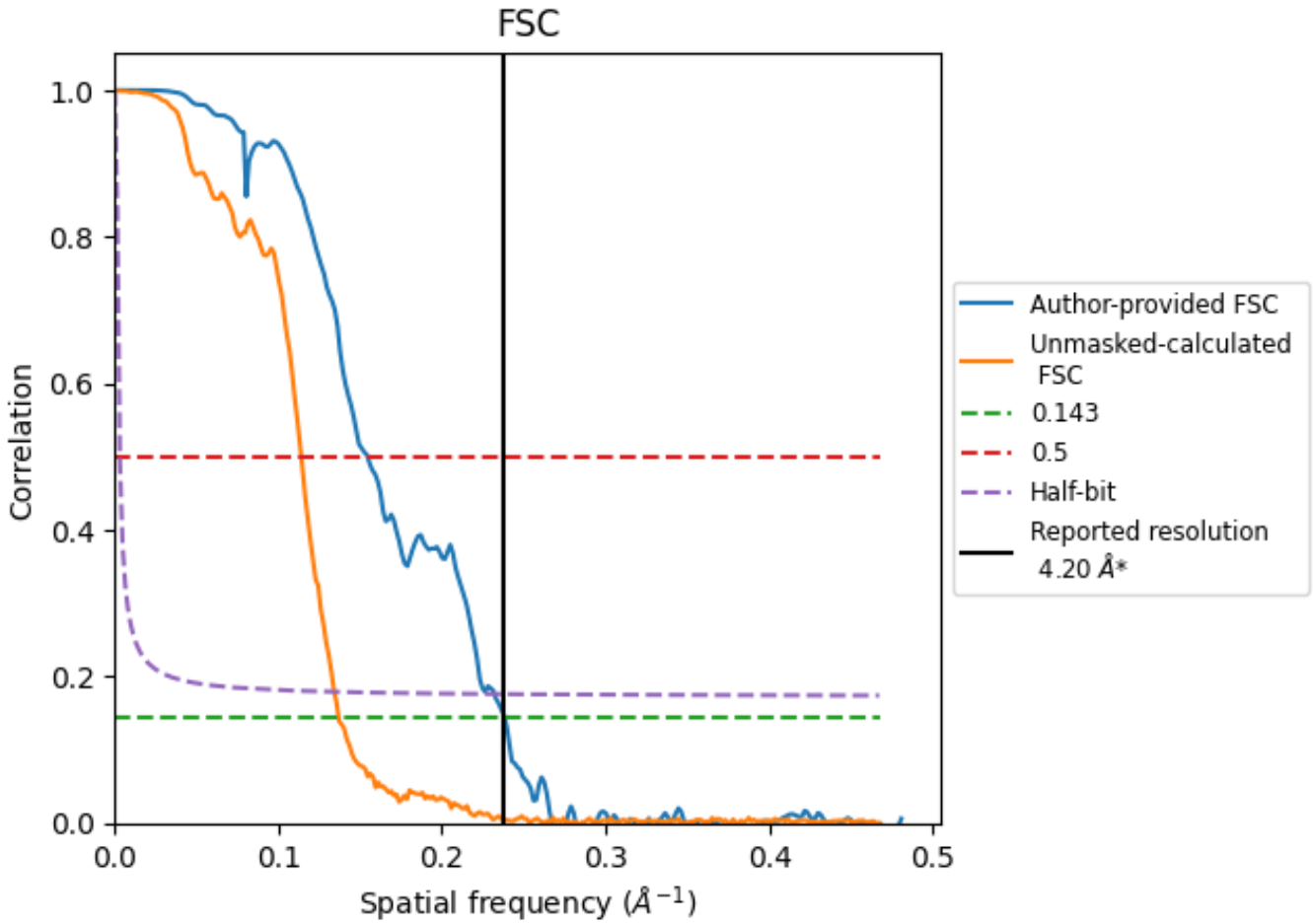


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8.2 Resolution estimates (i)

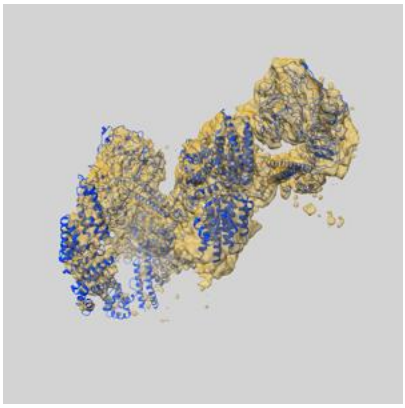
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.20	6.47	4.31
Unmasked-calculated*	7.30	8.76	7.45

*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 7.30 differs from the reported value 4.2 by more than 10 %

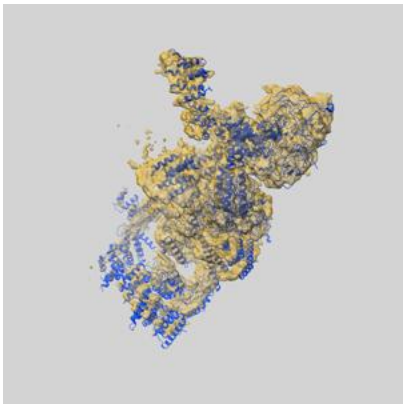
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10290 and PDB model 6SRI. Per-residue inclusion information can be found in section 3 on page 11.

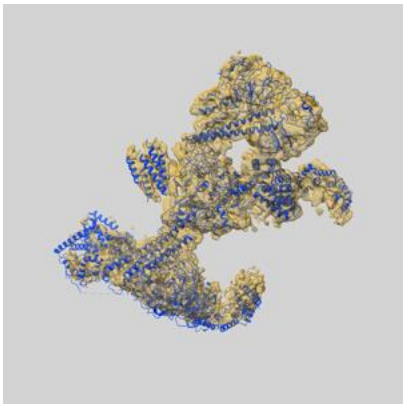
9.1 Map-model overlay



X



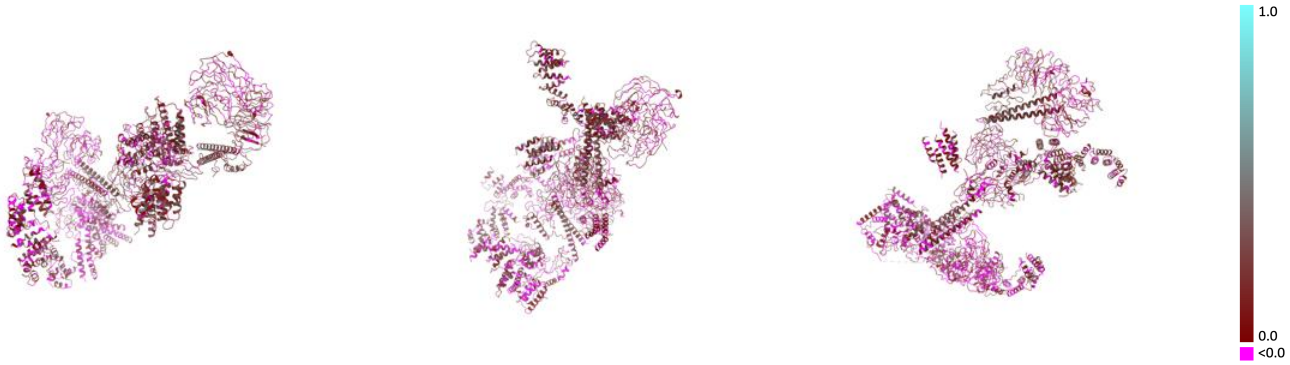
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0138 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.

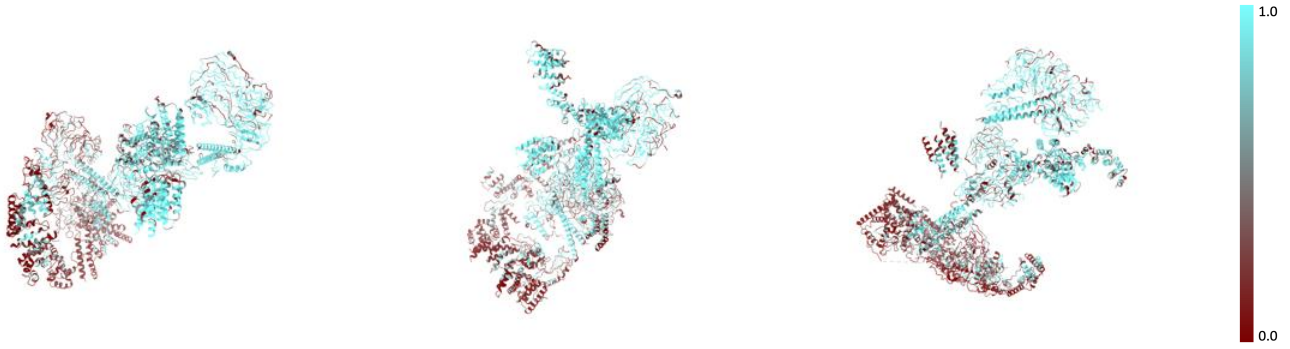
9.2 Q-score mapped to coordinate model



X Y Z

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

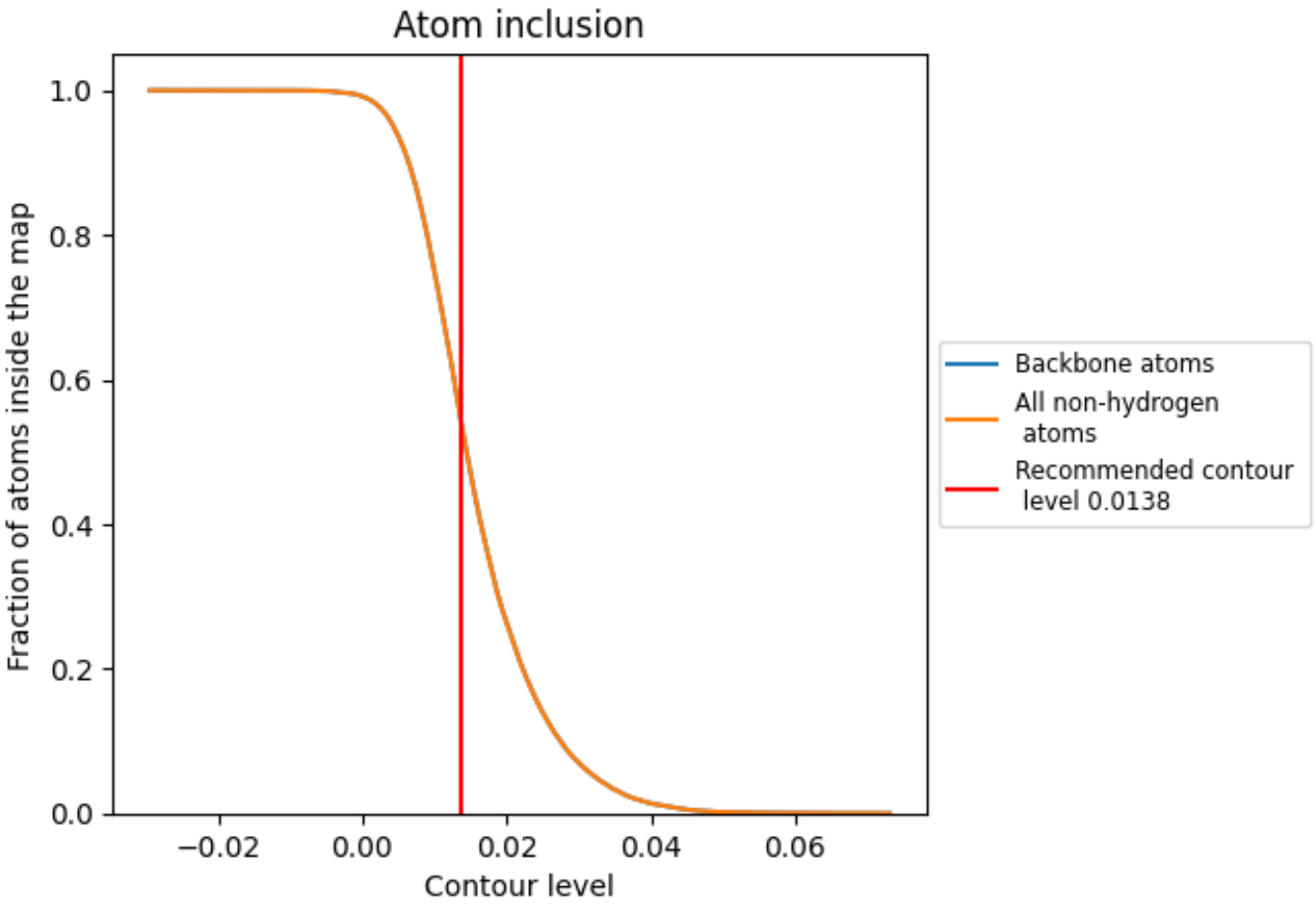
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0138).

9.4 Atom inclusion (i)



At the recommended contour level, 54% of all backbone atoms, 54% 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 (0.0138) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5356	0.1120
1	0.4014	0.0790
2	0.3065	0.0630
3	0.1875	0.1120
4	0.2430	0.0610
A	0.6546	0.1280
B	0.9100	0.2070
C	0.6167	0.1490
D	0.6630	0.2030
E	0.7500	0.0570
F	0.8500	0.1690
G	0.6250	0.1510
H	0.5588	0.1280
I	0.9527	0.2390
J	0.9559	0.2570
K	0.9405	0.2970
L	0.9167	0.2790
M	0.7708	0.1690
N	0.8488	0.2690
O	0.7616	0.0940
P	0.7799	0.1480
Q	0.9066	0.2590
R	0.7474	0.1880
S	0.8466	0.2100
T	0.1530	0.1190
U	0.1487	0.0420
V	0.0093	-0.0140
W	0.0250	0.0990
X	0.0000	-0.0720
Y	0.3095	0.0680
Z	0.2833	0.0020
a	0.6678	0.0570
b	0.8400	0.2290
c	0.7667	0.1970
d	0.5326	0.0410

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Chain	Atom inclusion	Q-score
e	0.7500	0.0130
f	0.5167	0.0700
g	0.7019	0.1310
h	0.6029	0.0830
i	0.6014	0.1020
j	0.3676	0.0930
k	0.4881	0.0860
l	0.6944	0.1320
m	0.8063	0.1970
n	0.7733	0.1620
o	0.3244	0.0370
p	0.3976	0.0150
q	0.3605	0.0610