wwPDB EM Validation Summary Report (i)

Dec 11, 2022 – 10:19 am GMT

PDB ID	:	6S8B
EMDB ID	:	EMD-10117
Title	:	Cryo-EM structure of the Type III-B Cmr-beta bound to cognate target RNA and AMPPnP, state 1
Authors	:	Sofos, N.; Montoya, G.; Stella, S.
Deposited on	:	2019-07-09
Resolution	:	2.41 Å(reported)

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

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

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

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

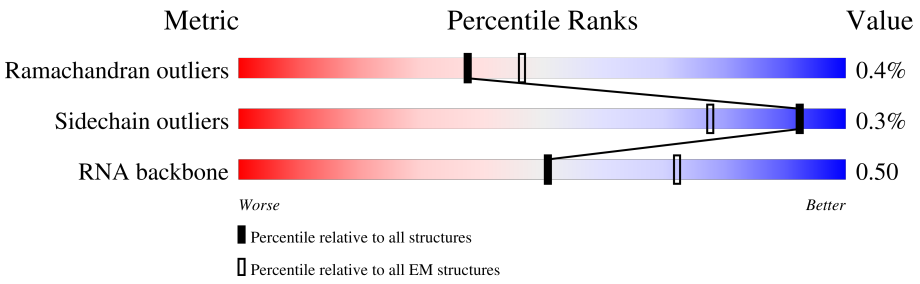
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.41 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	155	99%
1	B	155	99%
1	C	155	99%
2	D	286	100%
2	E	286	99%
2	F	286	99%
2	G	286	100%
3	H	313	97%

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Mol	Chain	Length	Quality of chain
4	I	296	96%
5	J	476	99%
6	U	46	9% 61% 35%
7	V	51	69% 27%
8	L	174	6% 98%
8	M	174	6% 98%
8	N	174	18% 98%
8	O	174	14% 99%
8	P	174	30% 98%
8	Q	174	13% 98%
8	R	174	17% 99%
8	S	174	73% 97%
8	T	174	29% 98%
8	W	174	49% 97%
8	X	174	76% 98%
8	l	174	6% 99%
8	m	174	99%
8	n	174	20% 99%
8	o	174	18% 99%
8	p	174	31% 98%
8	q	174	16% 98%
8	r	174	11% 99%
8	s	174	76% 98%
8	t	174	43% 98%
8	w	174	52% 99%

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Mol	Chain	Length	Quality of chain
8	x	174	82% 99%
9	K	1037	10% 96%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 62151 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 CRISPR-associated protein, Cmr5 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	153	1253	817	205	230	1	0	0
1	B	154	1261	823	206	231	1	0	0
1	C	154	1261	823	206	231	1	0	0

- Molecule 2 is a protein called CRISPR-associated RAMP protein, Cmr4 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	285	2274	1478	369	425	2	0	0
2	E	285	2274	1478	369	425	2	0	0
2	F	285	2274	1478	369	425	2	0	0
2	G	285	2273	1478	369	424	2	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	31	ALA	ASP	conflict	UNP F0NDX6
E	31	ALA	ASP	conflict	UNP F0NDX6
F	31	ALA	ASP	conflict	UNP F0NDX6
G	31	ALA	ASP	conflict	UNP F0NDX6

- Molecule 3 is a protein called CRISPR-associated protein, Cmr3 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	304	2468	1593	408	460	7	0	0

- Molecule 4 is a protein called CRISPR-associated RAMP protein, Cmr6 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	I	284	2282	1470	381	427	4	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	284	ALA	-	expression tag	UNP F0NDX3
I	285	ALA	-	expression tag	UNP F0NDX3
I	286	ALA	-	expression tag	UNP F0NDX3
I	287	HIS	-	expression tag	UNP F0NDX3
I	288	HIS	-	expression tag	UNP F0NDX3
I	289	HIS	-	expression tag	UNP F0NDX3
I	290	HIS	-	expression tag	UNP F0NDX3
I	291	HIS	-	expression tag	UNP F0NDX3
I	292	HIS	-	expression tag	UNP F0NDX3
I	293	HIS	-	expression tag	UNP F0NDX3
I	294	HIS	-	expression tag	UNP F0NDX3
I	295	HIS	-	expression tag	UNP F0NDX3
I	296	HIS	-	expression tag	UNP F0NDX3

- Molecule 5 is a protein called Cmr1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	J	475	3889	2517	632	727	13	0	0

- Molecule 6 is a RNA chain called Cognate target RNA (46-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	U	44	933	418	162	309	44	0	0

- Molecule 7 is a RNA chain called crRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	V	49	1045	470	195	332	48	0	0

- Molecule 8 is a protein called CRISPR-associated protein Cmrx.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	L	173	1378	880	227	269	2	0	0
8	M	173	1378	880	227	269	2	0	0
8	N	173	1378	880	227	269	2	0	0
8	O	173	1378	880	227	269	2	0	0
8	P	173	1378	880	227	269	2	0	0
8	Q	173	1378	880	227	269	2	0	0
8	R	173	1378	880	227	269	2	0	0
8	S	173	1378	880	227	269	2	0	0
8	T	173	1378	880	227	269	2	0	0
8	W	173	1378	880	227	269	2	0	0
8	X	173	1378	880	227	269	2	0	0
8	l	173	1378	880	227	269	2	0	0
8	m	173	1378	880	227	269	2	0	0
8	n	173	1378	880	227	269	2	0	0
8	o	173	1378	880	227	269	2	0	0
8	p	173	1378	880	227	269	2	0	0
8	q	173	1378	880	227	269	2	0	0
8	r	173	1378	880	227	269	2	0	0
8	s	173	1378	880	227	269	2	0	0
8	t	173	1378	880	227	269	2	0	0
8	w	173	1378	880	227	269	2	0	0
8	x	173	1378	880	227	269	2	0	0

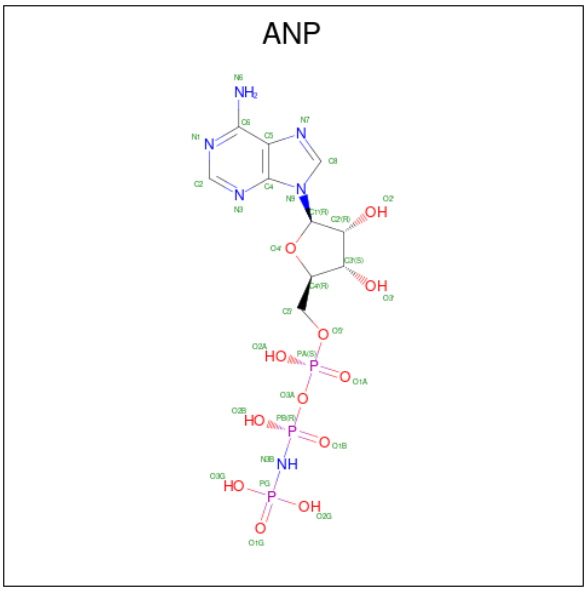
- Molecule 9 is a protein called CRISPR-associated protein, Cmr2 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	K	1009	8282	5360	1366	1532	24	0	0

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
10	K	1	1	1	0

- Molecule 11 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
11	K	1	62	20	12	24	6	0
11	K	1	62	20	12	24	6	0

- Molecule 12 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mn	
12	K	3	3	3	0

3 Residue-property plots (i)

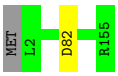
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: CRISPR-associated protein, Cmr5 family

Chain A: 99%

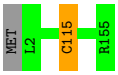
• Molecule 1: CRISPR-associated protein, Cmr5 family

Chain B: 99%



• Molecule 1: CRISPR-associated protein, Cmr5 family

Chain C: 99%

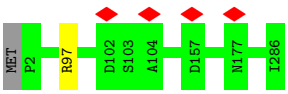


• Molecule 2: CRISPR-associated RAMP protein, Cmr4 family

Chain D: 100%

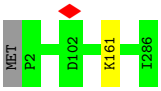
• Molecule 2: CRISPR-associated RAMP protein, Cmr4 family

Chain E: 99%



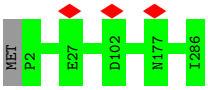
• Molecule 2: CRISPR-associated RAMP protein, Cmr4 family

Chain F: 99%



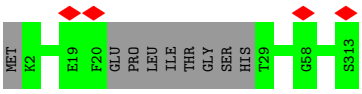
• Molecule 2: CRISPR-associated RAMP protein, Cmr4 family

Chain G: 100%



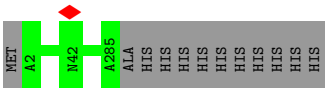
• Molecule 3: CRISPR-associated protein, Cmr3 family

Chain H: 97%



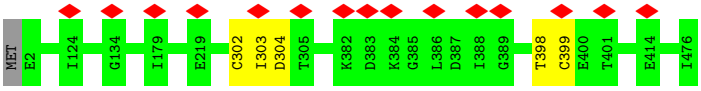
• Molecule 4: CRISPR-associated RAMP protein, Cmr6 family

Chain I: 96%



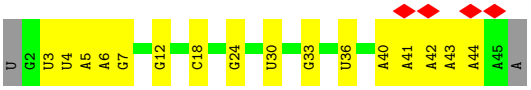
• Molecule 5: Cmr1

Chain J: 99%



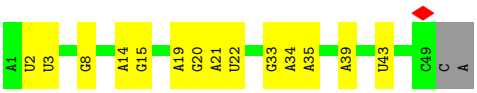
• Molecule 6: Cognate target RNA (46-mer)

Chain U: 9% 61% 35%



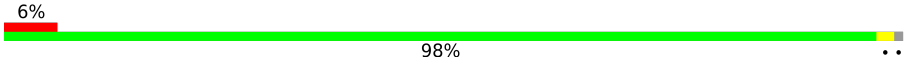
• Molecule 7: crRNA

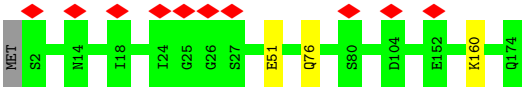
Chain V: 69% 27%



• Molecule 8: CRISPR-associated protein Cmrx

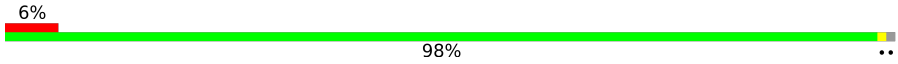
Chain L:

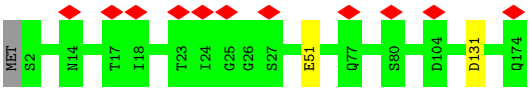




• Molecule 8: CRISPR-associated protein Cmrx

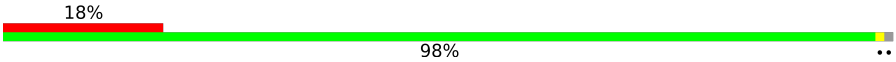
Chain M:

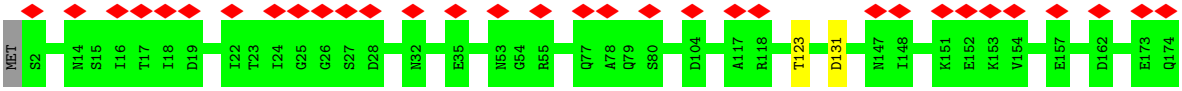




• Molecule 8: CRISPR-associated protein Cmrx

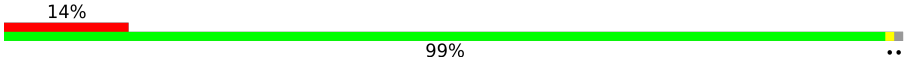
Chain N:

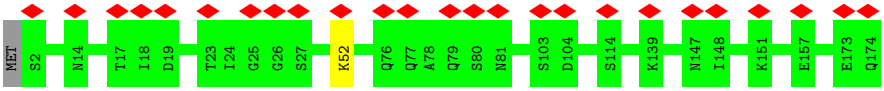




• Molecule 8: CRISPR-associated protein Cmrx

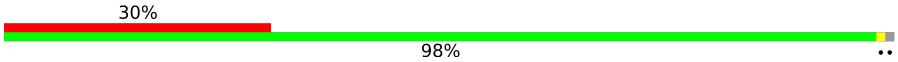
Chain O:

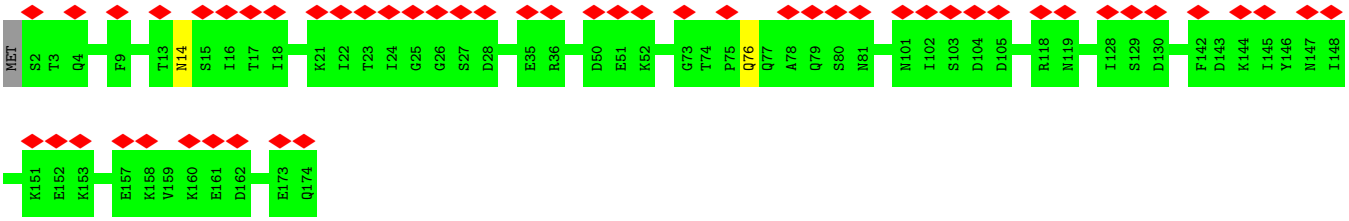




• Molecule 8: CRISPR-associated protein Cmrx

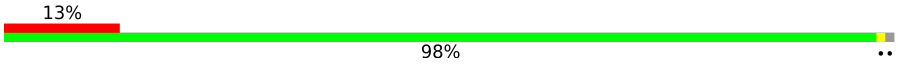
Chain P:

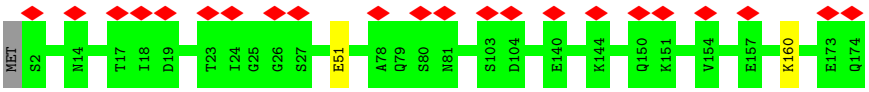




• Molecule 8: CRISPR-associated protein Cmrx

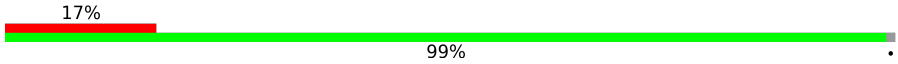
Chain Q:

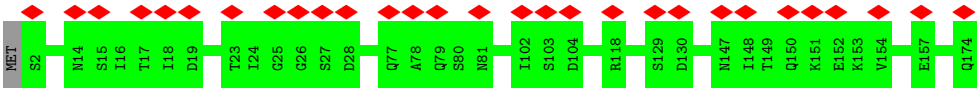




• Molecule 8: CRISPR-associated protein Cmrx

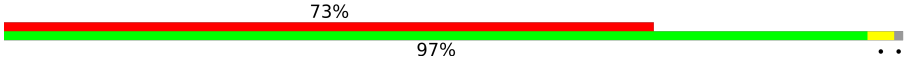
Chain R:

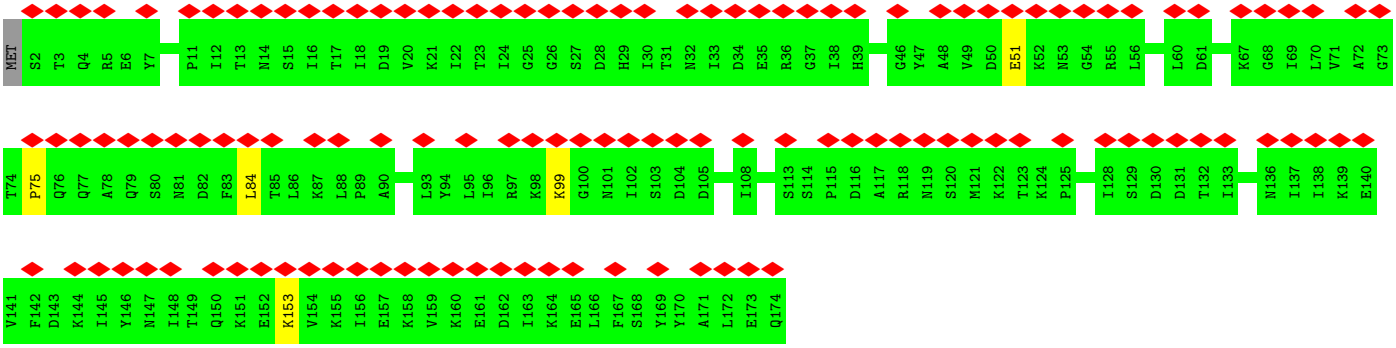




• Molecule 8: CRISPR-associated protein Cmrx

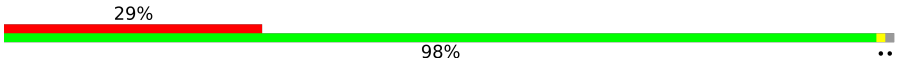
Chain S:

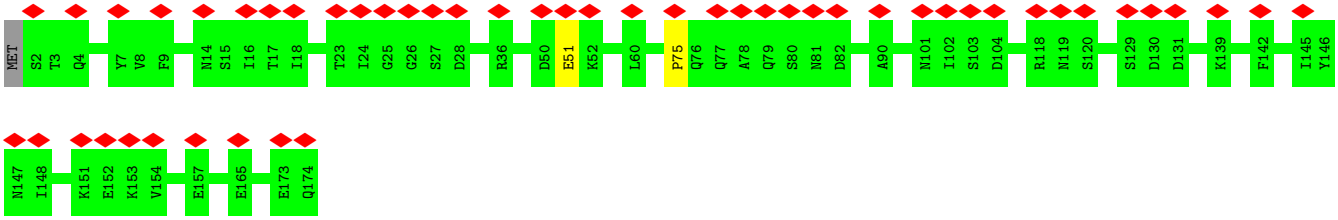




• Molecule 8: CRISPR-associated protein Cmrx

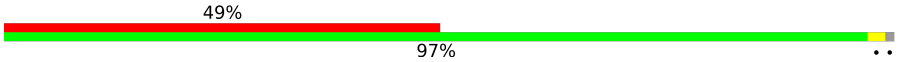
Chain T:

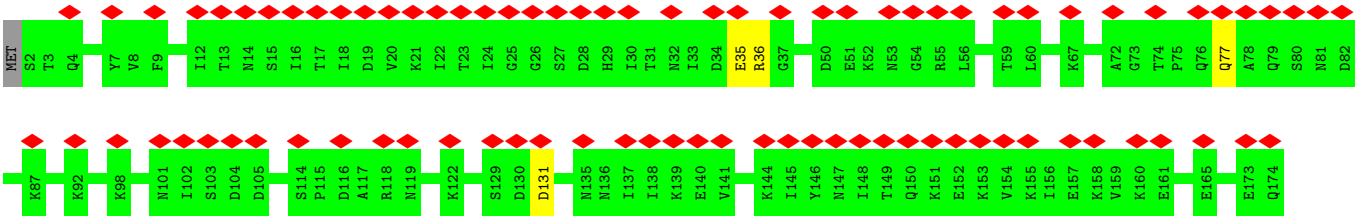




• Molecule 8: CRISPR-associated protein Cmrx

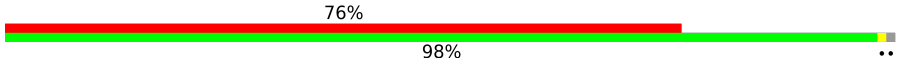
Chain W:

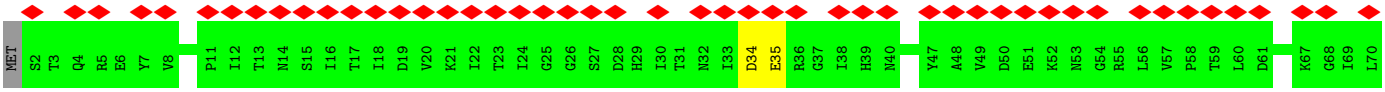


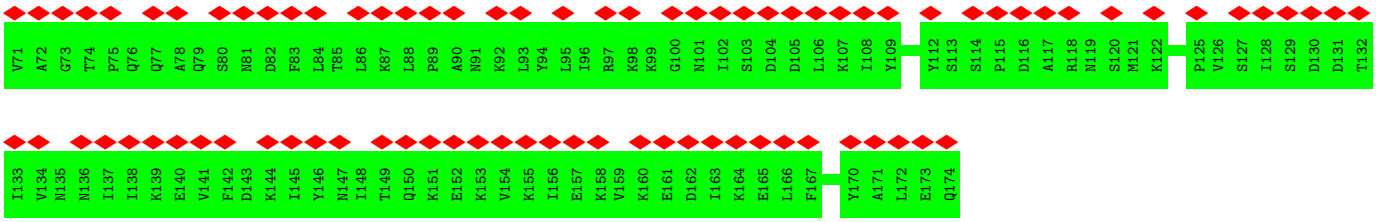


• Molecule 8: CRISPR-associated protein Cmrx

Chain X:

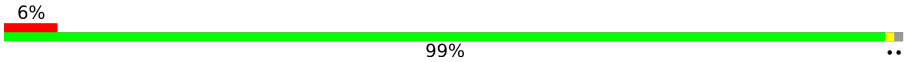


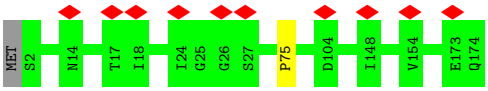




- Molecule 8: CRISPR-associated protein Cmrx

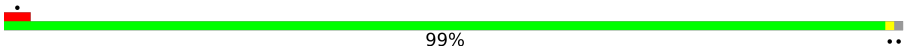
Chain l:

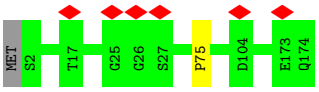




- Molecule 8: CRISPR-associated protein Cmrx

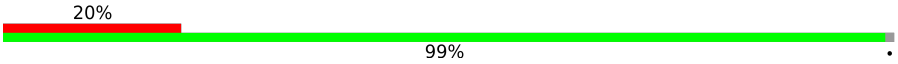
Chain m:

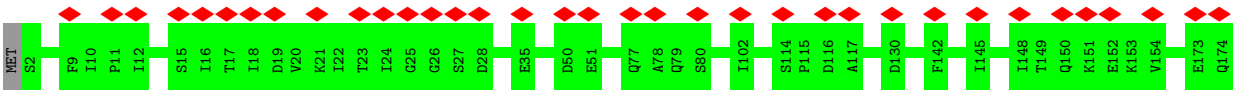




- Molecule 8: CRISPR-associated protein Cmrx

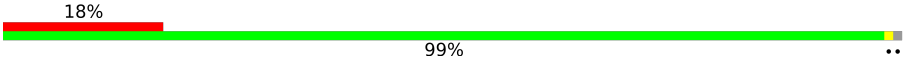
Chain n:

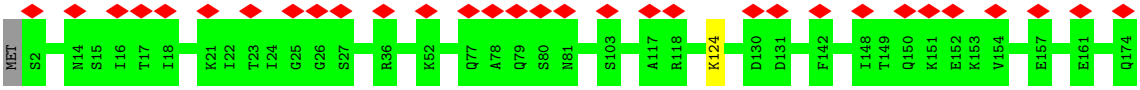




- Molecule 8: CRISPR-associated protein Cmrx

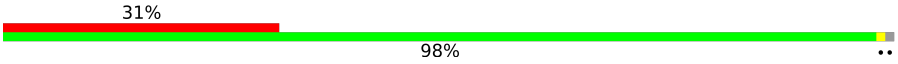
Chain o:

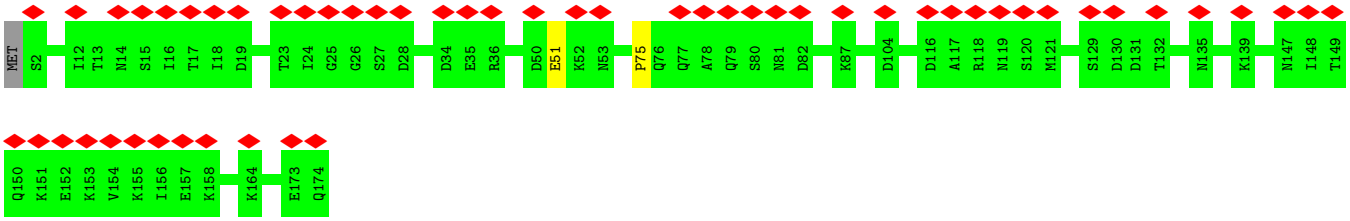




- Molecule 8: CRISPR-associated protein Cmrx

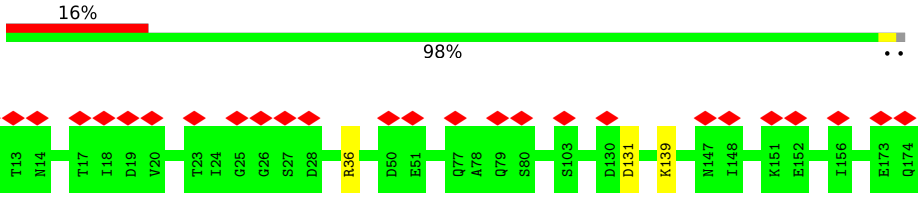
Chain p:





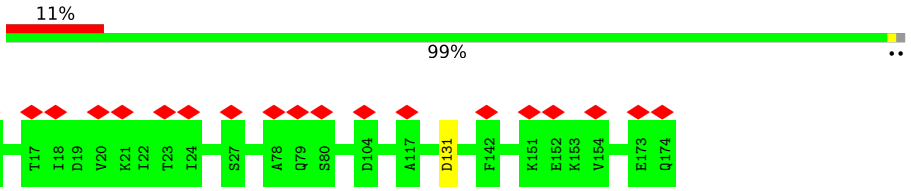
- Molecule 8: CRISPR-associated protein Cmrx

Chain q:



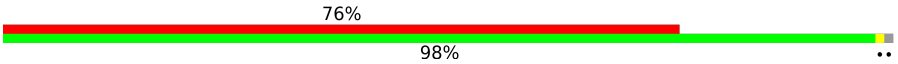
- Molecule 8: CRISPR-associated protein Cmrx

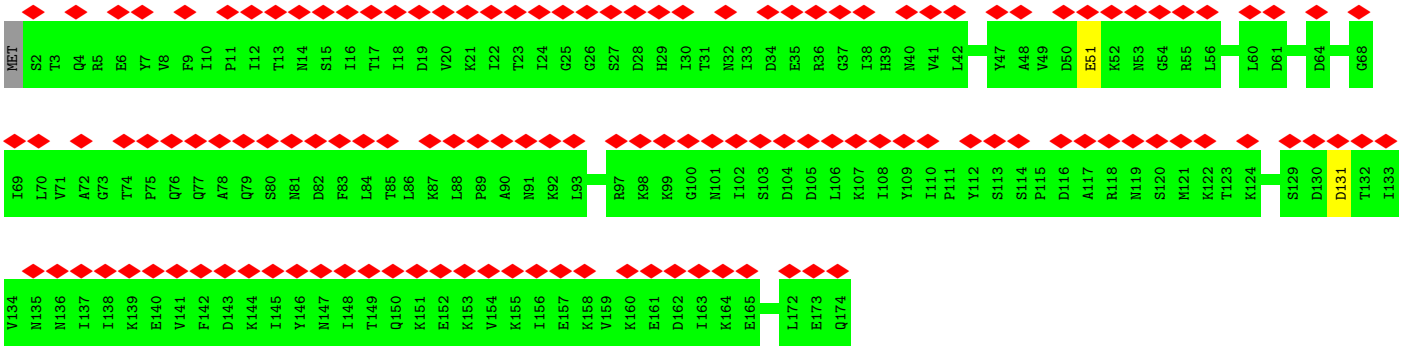
Chain r:



- Molecule 8: CRISPR-associated protein Cmrx

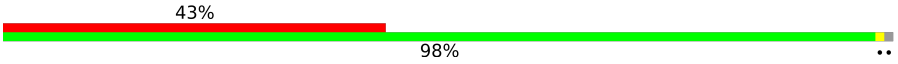
Chain s:

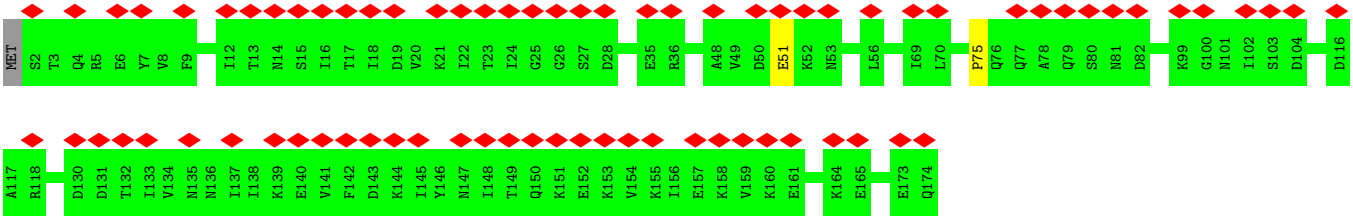




- Molecule 8: CRISPR-associated protein Cmrx

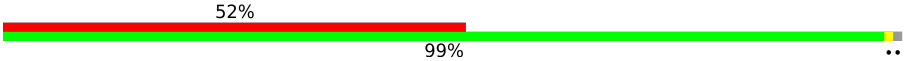
Chain t:

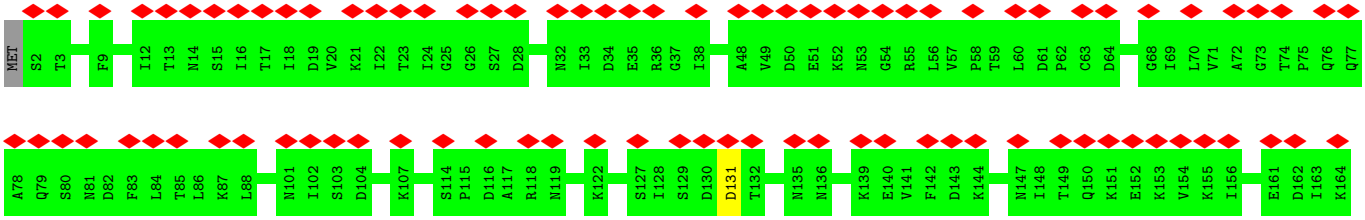




- Molecule 8: CRISPR-associated protein Cmrx

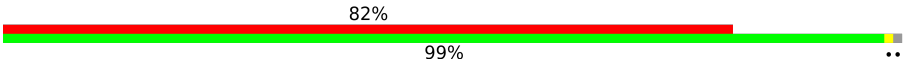
Chain w:

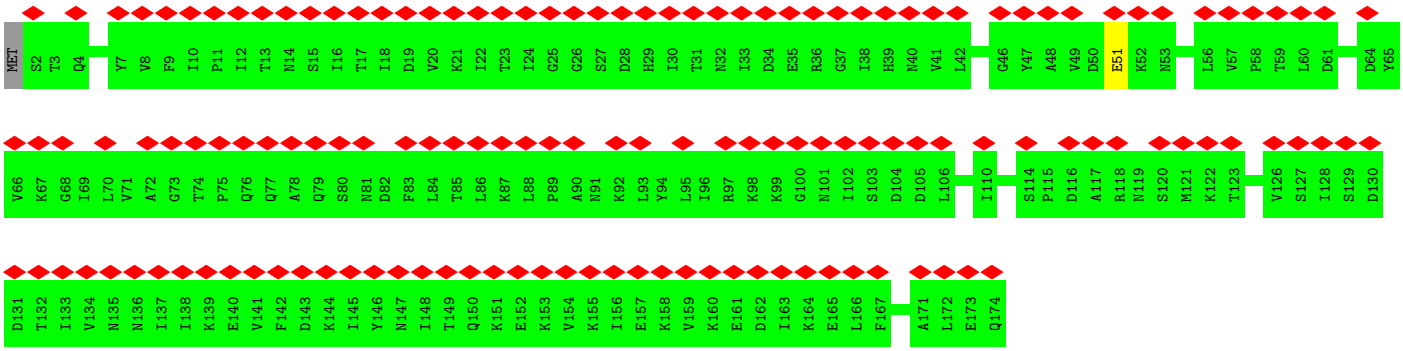




• Molecule 8: CRISPR-associated protein Cmrx

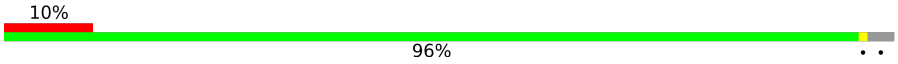
Chain x:

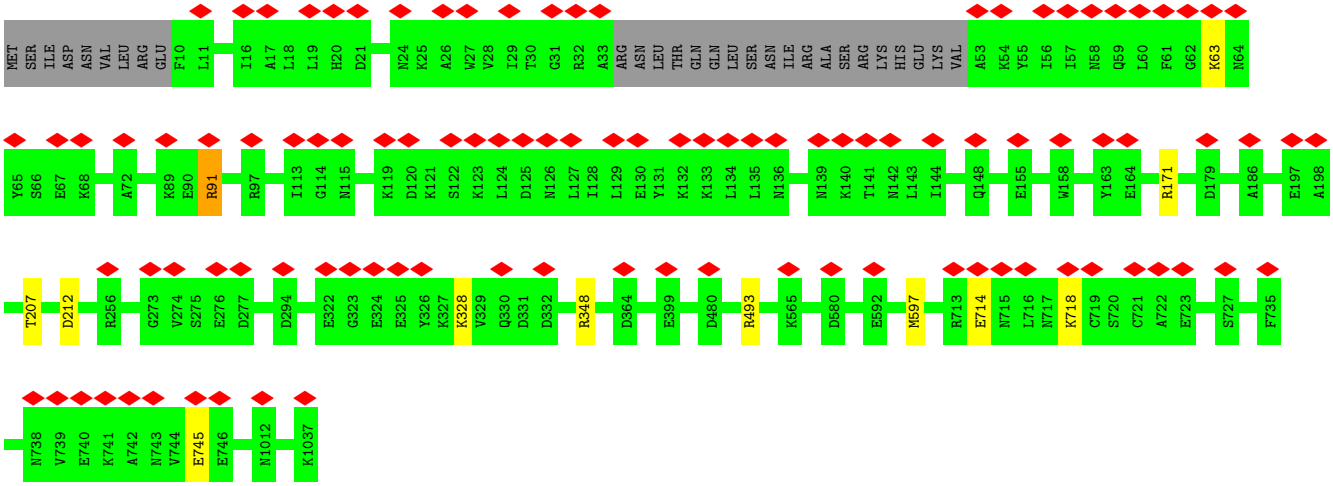




• Molecule 9: CRISPR-associated protein, Cmr2 family

Chain K:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	82571	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	34.130	Depositor
Minimum map value	-15.312	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.723	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	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: MN, ZN, ANP

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	A	0.41	0/1275	0.45	0/1716
1	B	0.42	0/1283	0.51	0/1727
1	C	0.42	0/1283	0.44	0/1727
2	D	0.45	0/2318	0.50	0/3134
2	E	0.45	0/2318	0.49	0/3134
2	F	0.47	0/2318	0.51	0/3134
2	G	0.44	0/2317	0.50	0/3133
3	H	0.36	0/2511	0.49	0/3382
4	I	0.42	0/2325	0.48	0/3138
5	J	0.37	0/3956	0.49	0/5319
6	U	0.78	0/1042	0.81	0/1620
7	V	1.00	0/1171	0.90	5/1823 (0.3%)
8	L	0.33	0/1400	0.50	0/1895
8	M	0.33	0/1400	0.51	0/1895
8	N	0.29	0/1400	0.51	0/1895
8	O	0.30	0/1400	0.52	0/1895
8	P	0.29	0/1400	0.54	0/1895
8	Q	0.28	0/1400	0.51	0/1895
8	R	0.28	0/1400	0.50	0/1895
8	S	0.29	0/1400	0.56	1/1895 (0.1%)
8	T	0.28	0/1400	0.51	0/1895
8	W	0.27	0/1400	0.54	0/1895
8	X	0.28	0/1400	0.53	0/1895
8	l	0.35	0/1400	0.52	0/1895
8	m	0.35	0/1400	0.52	0/1895
8	n	0.28	0/1400	0.52	0/1895
8	o	0.31	0/1400	0.55	0/1895
8	p	0.29	0/1400	0.53	0/1895
8	q	0.31	0/1400	0.51	0/1895
8	r	0.29	0/1400	0.49	0/1895
8	s	0.27	0/1400	0.51	0/1895
8	t	0.27	0/1400	0.55	0/1895

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
8	w	0.27	0/1400	0.52	0/1895
8	x	0.28	0/1400	0.52	0/1895
9	K	0.32	0/8452	0.47	0/11416
All	All	0.38	0/63369	0.52	6/86093 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
5	J	0	2
8	P	0	1
8	S	0	1
8	X	0	1
9	K	0	1
All	All	0	7

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	V	19	A	O4'-C1'-N9	6.92	113.74	108.20
7	V	21	A	O4'-C1'-N9	6.71	113.56	108.20
7	V	15	G	O4'-C1'-N9	6.15	113.12	108.20
7	V	39	A	O4'-C1'-N9	5.73	112.79	108.20
8	S	84	LEU	CA-CB-CG	5.14	127.12	115.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	115	CYS	Peptide
5	J	302	CYS	Peptide
5	J	398	THR	Peptide
8	P	14	ASN	Peptide
8	S	153	LYS	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	A	151/155 (97%)	143 (95%)	8 (5%)	0	100	100
1	B	152/155 (98%)	146 (96%)	5 (3%)	1 (1%)	22	31
1	C	152/155 (98%)	147 (97%)	5 (3%)	0	100	100
2	D	283/286 (99%)	259 (92%)	24 (8%)	0	100	100
2	E	283/286 (99%)	264 (93%)	19 (7%)	0	100	100
2	F	283/286 (99%)	252 (89%)	30 (11%)	1 (0%)	34	47
2	G	283/286 (99%)	242 (86%)	41 (14%)	0	100	100
3	H	300/313 (96%)	270 (90%)	30 (10%)	0	100	100
4	I	282/296 (95%)	263 (93%)	19 (7%)	0	100	100
5	J	473/476 (99%)	424 (90%)	47 (10%)	2 (0%)	34	47
8	L	171/174 (98%)	136 (80%)	33 (19%)	2 (1%)	13	17
8	M	171/174 (98%)	134 (78%)	35 (20%)	2 (1%)	13	17
8	N	171/174 (98%)	138 (81%)	32 (19%)	1 (1%)	25	35
8	O	171/174 (98%)	138 (81%)	33 (19%)	0	100	100
8	P	171/174 (98%)	130 (76%)	40 (23%)	1 (1%)	25	35
8	Q	171/174 (98%)	125 (73%)	45 (26%)	1 (1%)	25	35
8	R	171/174 (98%)	137 (80%)	34 (20%)	0	100	100
8	S	171/174 (98%)	134 (78%)	35 (20%)	2 (1%)	13	17
8	T	171/174 (98%)	130 (76%)	39 (23%)	2 (1%)	13	17
8	W	171/174 (98%)	134 (78%)	34 (20%)	3 (2%)	8	10
8	X	171/174 (98%)	139 (81%)	31 (18%)	1 (1%)	25	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	l	171/174 (98%)	138 (81%)	32 (19%)	1 (1%)	25	35
8	m	171/174 (98%)	131 (77%)	39 (23%)	1 (1%)	25	35
8	n	171/174 (98%)	139 (81%)	32 (19%)	0	100	100
8	o	171/174 (98%)	138 (81%)	33 (19%)	0	100	100
8	p	171/174 (98%)	135 (79%)	34 (20%)	2 (1%)	13	17
8	q	171/174 (98%)	134 (78%)	36 (21%)	1 (1%)	25	35
8	r	171/174 (98%)	138 (81%)	32 (19%)	1 (1%)	25	35
8	s	171/174 (98%)	137 (80%)	32 (19%)	2 (1%)	13	17
8	t	171/174 (98%)	132 (77%)	37 (22%)	2 (1%)	13	17
8	w	171/174 (98%)	137 (80%)	33 (19%)	1 (1%)	25	35
8	x	171/174 (98%)	129 (75%)	41 (24%)	1 (1%)	25	35
9	K	1005/1037 (97%)	892 (89%)	111 (11%)	2 (0%)	47	61
All	All	7409/7559 (98%)	6265 (85%)	1111 (15%)	33 (0%)	38	47

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	161	LYS
8	W	35	GLU
5	J	303	ILE
8	Q	51	GLU
8	S	51	GLU

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	A	134/136 (98%)	134 (100%)	0	100	100
1	B	135/136 (99%)	135 (100%)	0	100	100
1	C	135/136 (99%)	134 (99%)	1 (1%)	84	92
2	D	252/253 (100%)	252 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	252/253 (100%)	251 (100%)	1 (0%)	91	96
2	F	252/253 (100%)	252 (100%)	0	100	100
2	G	251/253 (99%)	251 (100%)	0	100	100
3	H	272/280 (97%)	272 (100%)	0	100	100
4	I	255/266 (96%)	255 (100%)	0	100	100
5	J	442/445 (99%)	441 (100%)	1 (0%)	93	97
8	L	159/160 (99%)	158 (99%)	1 (1%)	86	93
8	M	159/160 (99%)	159 (100%)	0	100	100
8	N	159/160 (99%)	158 (99%)	1 (1%)	86	93
8	O	159/160 (99%)	158 (99%)	1 (1%)	86	93
8	P	159/160 (99%)	159 (100%)	0	100	100
8	Q	159/160 (99%)	158 (99%)	1 (1%)	86	93
8	R	159/160 (99%)	159 (100%)	0	100	100
8	S	159/160 (99%)	158 (99%)	1 (1%)	86	93
8	T	159/160 (99%)	159 (100%)	0	100	100
8	W	159/160 (99%)	158 (99%)	1 (1%)	86	93
8	X	159/160 (99%)	159 (100%)	0	100	100
8	l	159/160 (99%)	159 (100%)	0	100	100
8	m	159/160 (99%)	159 (100%)	0	100	100
8	n	159/160 (99%)	159 (100%)	0	100	100
8	o	159/160 (99%)	158 (99%)	1 (1%)	86	93
8	p	159/160 (99%)	159 (100%)	0	100	100
8	q	159/160 (99%)	157 (99%)	2 (1%)	69	83
8	r	159/160 (99%)	159 (100%)	0	100	100
8	s	159/160 (99%)	159 (100%)	0	100	100
8	t	159/160 (99%)	159 (100%)	0	100	100
8	w	159/160 (99%)	159 (100%)	0	100	100
8	x	159/160 (99%)	159 (100%)	0	100	100
9	K	921/949 (97%)	911 (99%)	10 (1%)	73	86
All	All	6799/6880 (99%)	6777 (100%)	22 (0%)	92	97

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	K	171	ARG
9	K	328	LYS
9	K	212	ASP
9	K	348	ARG
8	Q	160	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
8	m	4	GLN
8	t	29	HIS
8	n	39	HIS
8	q	14	ASN
8	w	76	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	U	43/46 (93%)	16 (37%)	3 (6%)
7	V	48/51 (94%)	9 (18%)	0
All	All	91/97 (93%)	25 (27%)	3 (3%)

5 of 25 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	U	3	U
6	U	4	U
6	U	5	A
6	U	6	A
6	U	7	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	U	5	A
6	U	41	A
6	U	42	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	ANP	K	1103	12	29,33,33	1.04	4 (13%)	31,52,52	1.16	3 (9%)
11	ANP	K	1102	12	29,33,33	1.33	4 (13%)	31,52,52	2.04	7 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ANP	K	1103	12	-	6/14/38/38	0/3/3/3
11	ANP	K	1102	12	-	7/14/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	1102	ANP	PG-O2G	-3.25	1.48	1.56
11	K	1102	ANP	PB-O2B	-3.14	1.48	1.56
11	K	1102	ANP	PG-O3G	-2.77	1.49	1.56
11	K	1103	ANP	PB-O3A	-2.70	1.55	1.59
11	K	1103	ANP	PG-N3B	2.18	1.69	1.63

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	K	1102	ANP	O1B-PB-N3B	6.13	120.80	111.77
11	K	1102	ANP	PB-O3A-PA	-5.36	113.74	132.62
11	K	1102	ANP	O2B-PB-O1B	4.63	119.62	109.92
11	K	1103	ANP	PB-O3A-PA	-3.89	118.93	132.62
11	K	1102	ANP	O3A-PB-N3B	-3.36	97.28	106.59

There are no chirality outliers.

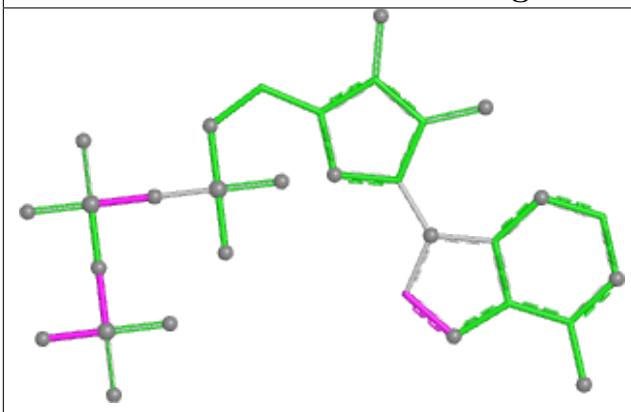
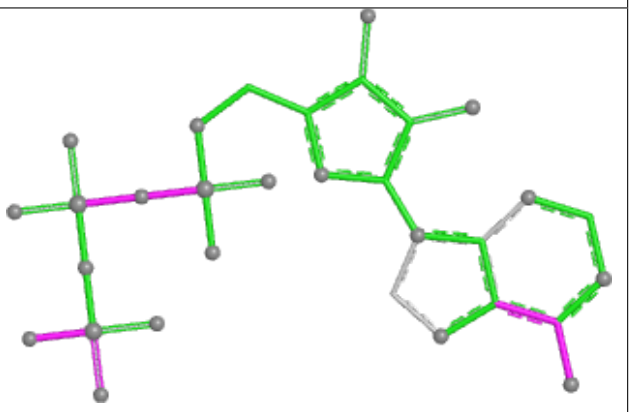
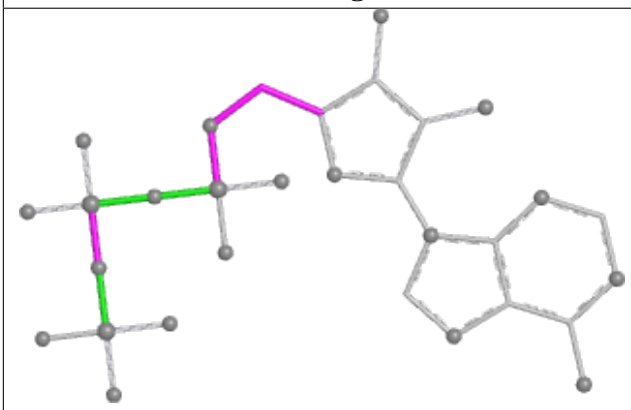
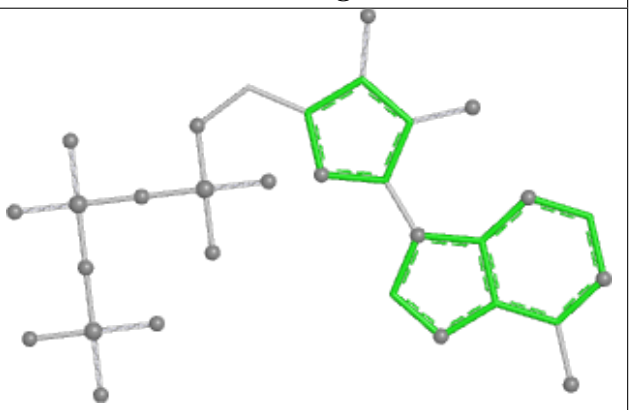
5 of 13 torsion outliers are listed below:

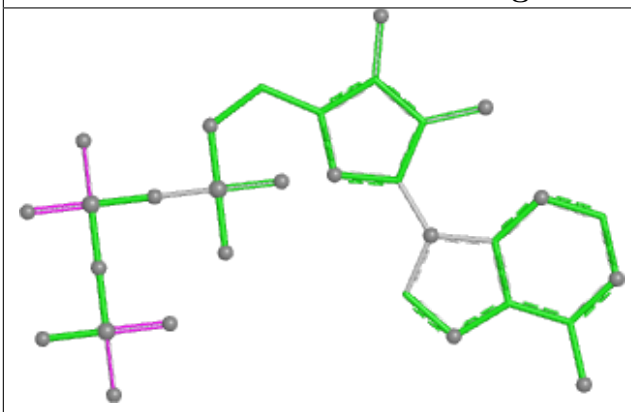
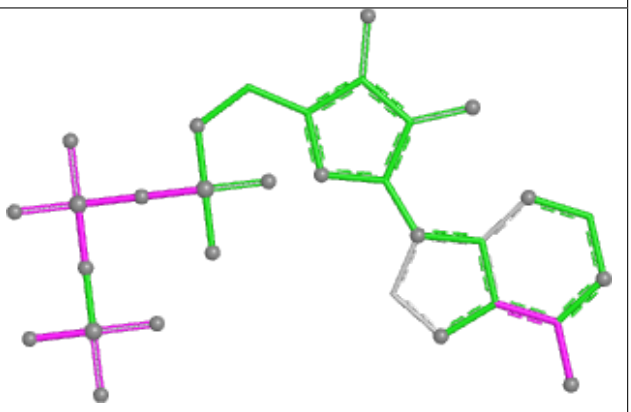
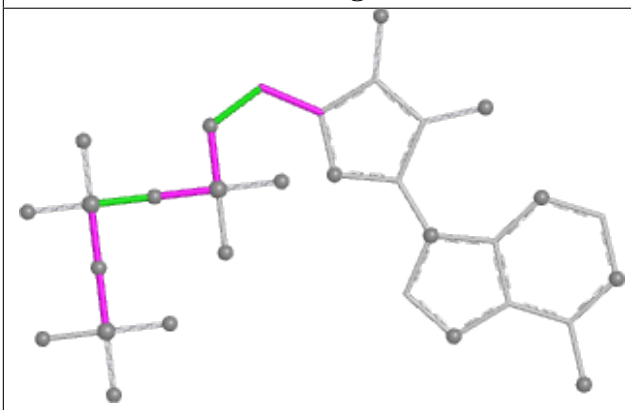
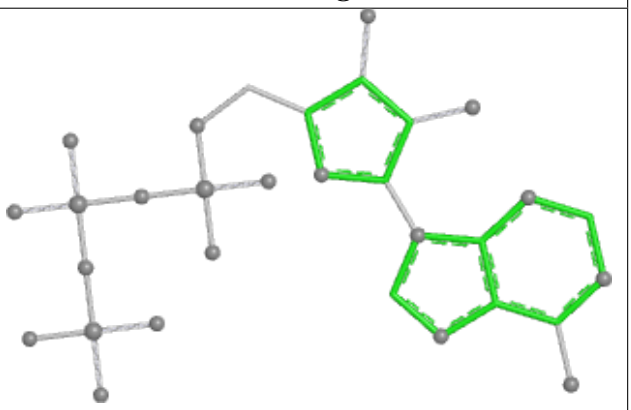
Mol	Chain	Res	Type	Atoms
11	K	1102	ANP	PB-N3B-PG-O1G
11	K	1102	ANP	PG-N3B-PB-O1B
11	K	1102	ANP	C5'-O5'-PA-O1A
11	K	1102	ANP	C5'-O5'-PA-O2A
11	K	1102	ANP	C5'-O5'-PA-O3A

There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand ANP K 1103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ANP K 1102	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

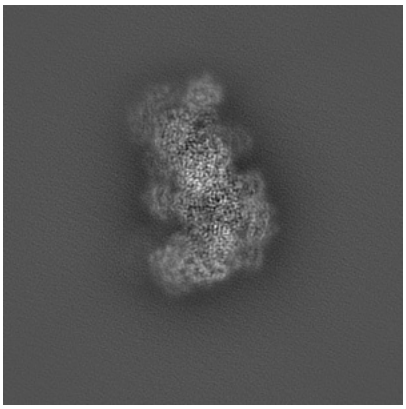
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10117. These allow visual inspection of the internal detail of the map and identification of artifacts.

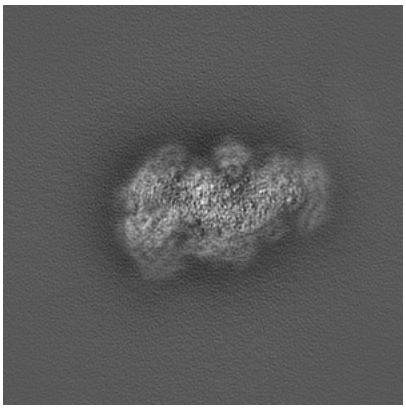
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

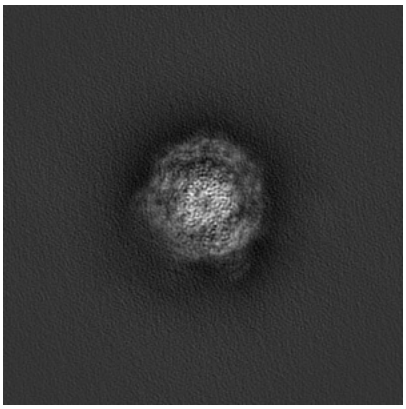
6.1.1 Primary map



X

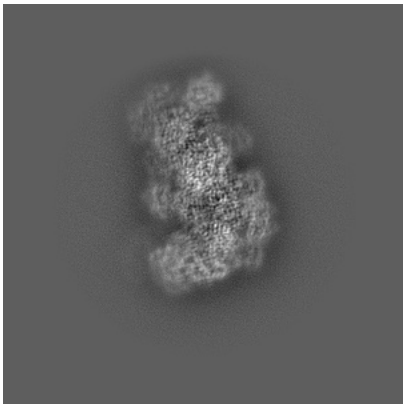


Y

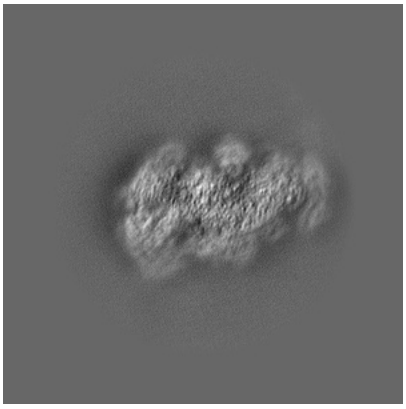


Z

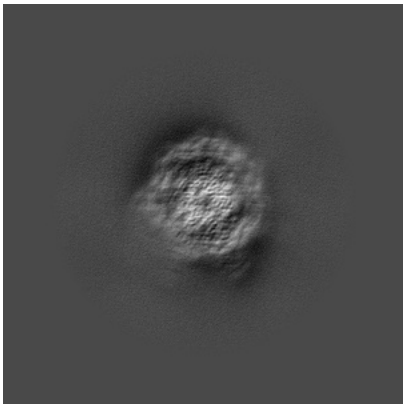
6.1.2 Raw map



X



Y

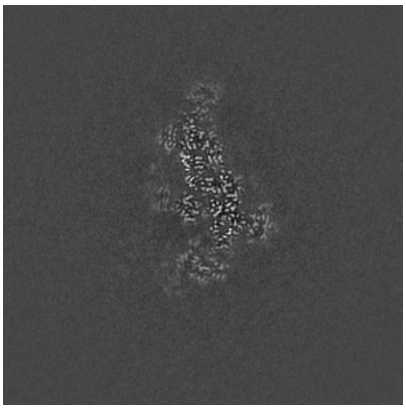


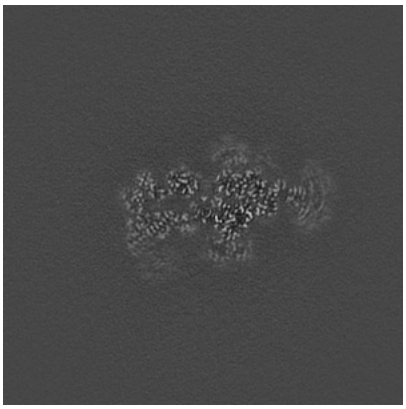
Z

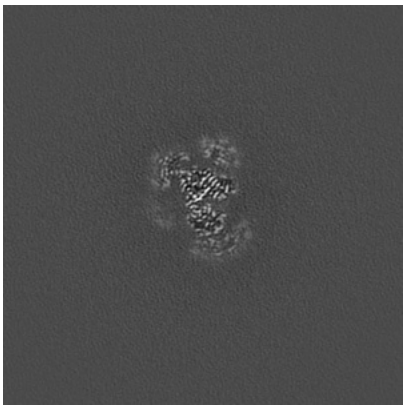
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

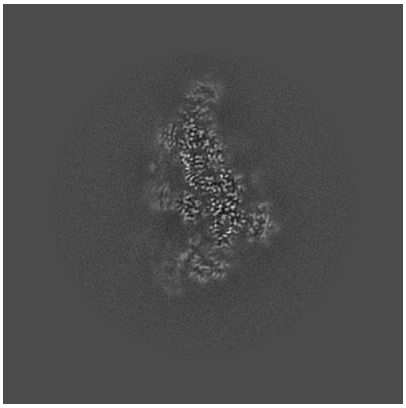
6.2.1 Primary map

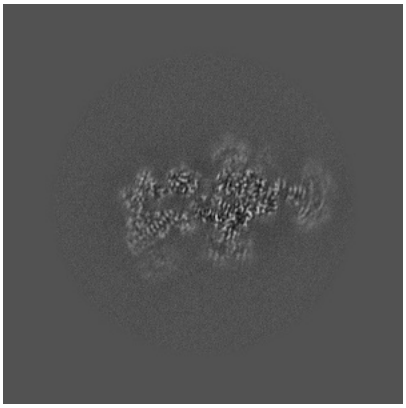

X Index: 250

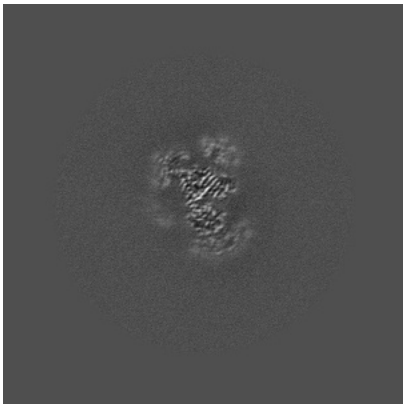

Y Index: 250


Z Index: 250

6.2.2 Raw map


X Index: 250

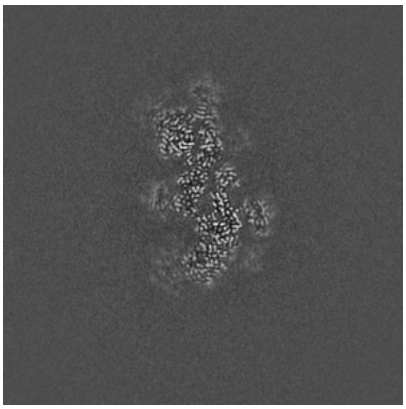

Y Index: 250

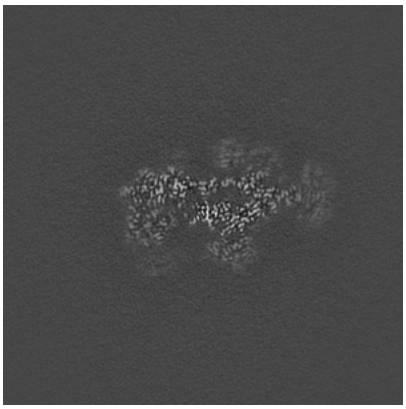

Z Index: 250

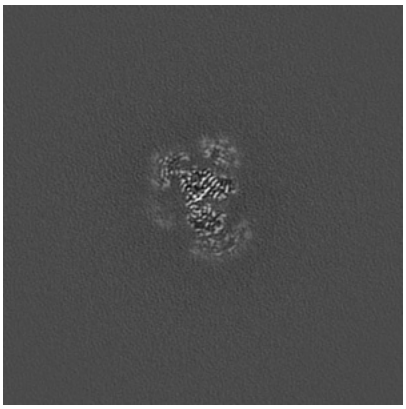
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

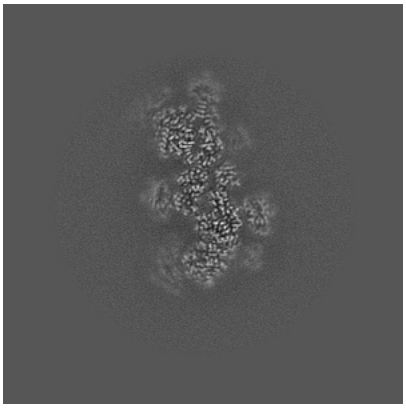
6.3.1 Primary map

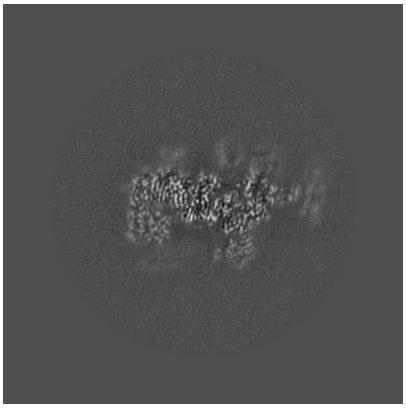

X Index: 267

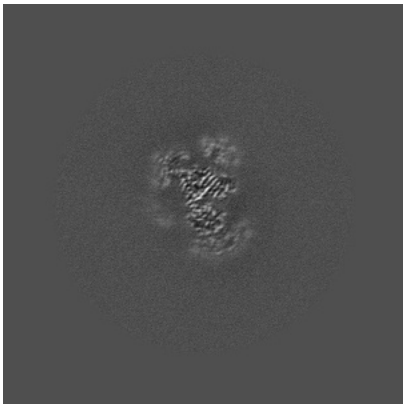

Y Index: 259


Z Index: 250

6.3.2 Raw map


X Index: 267


Y Index: 264


Z Index: 250

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 2.5. 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.

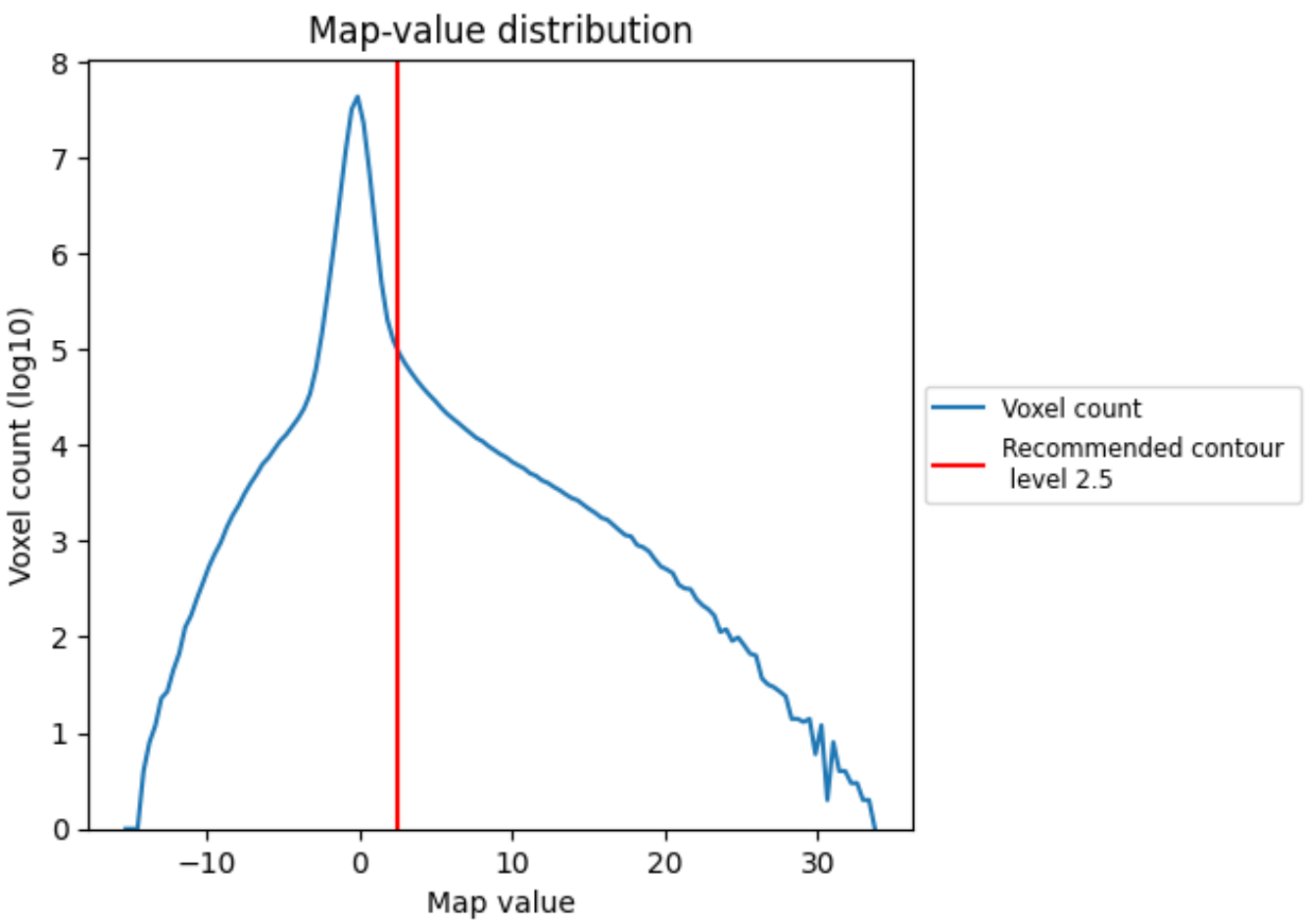
6.5 Mask visualisation (i)

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

7 Map analysis (i)

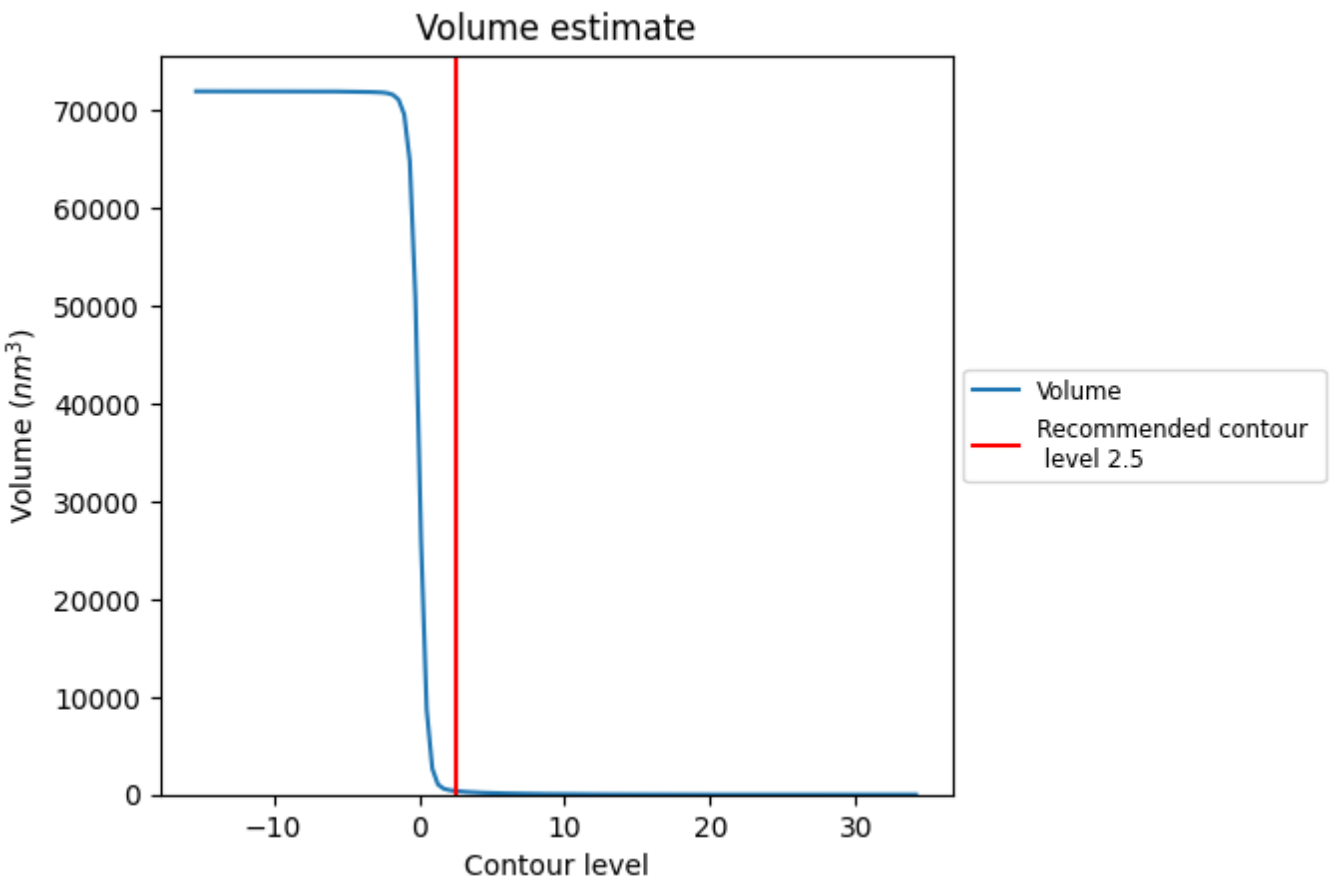
This section contains the results of statistical analysis of the map.

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.

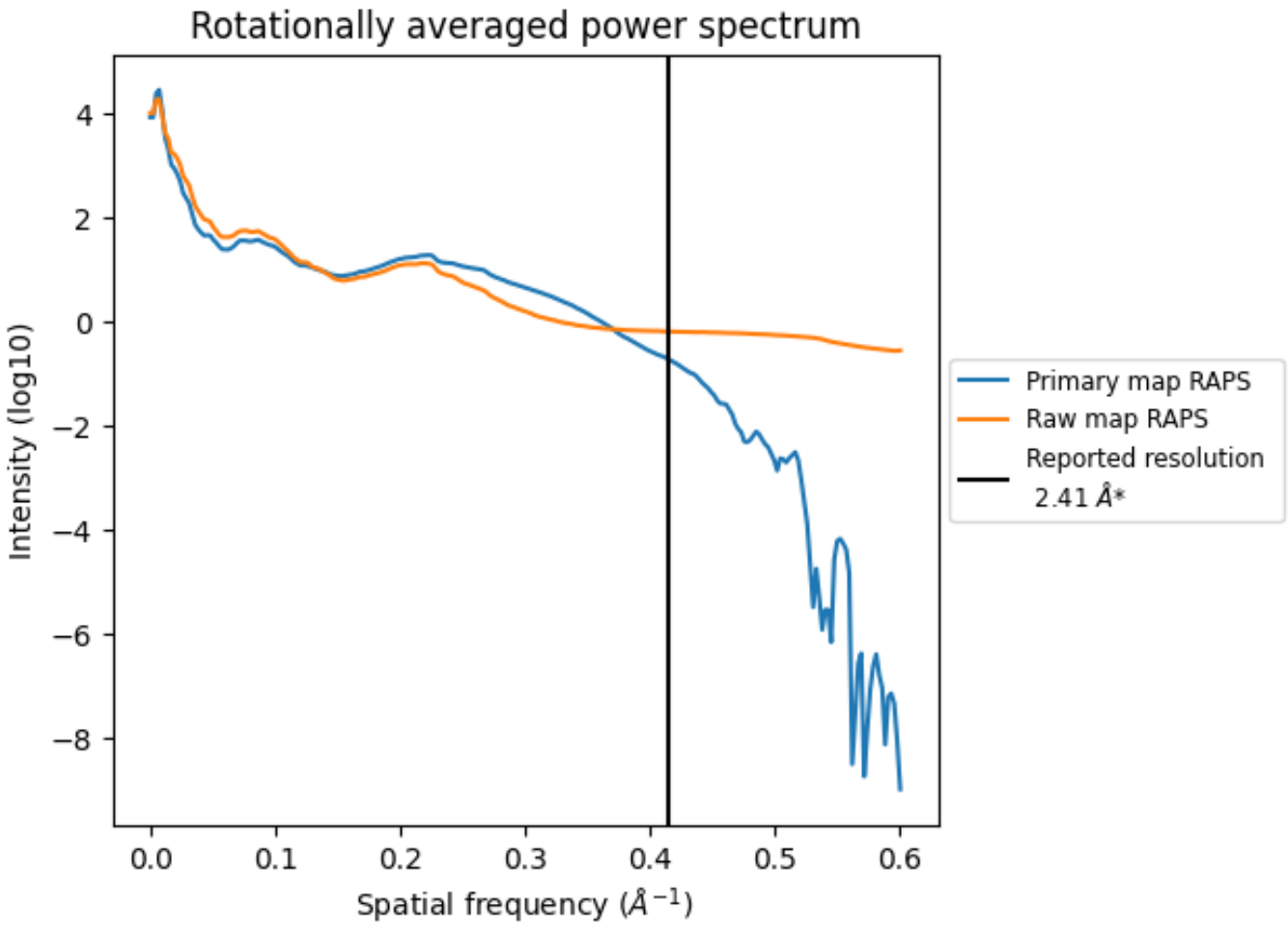
7.2 Volume estimate (i)



The volume at the recommended contour level is 367 nm^3; this corresponds to an approximate mass of 332 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)

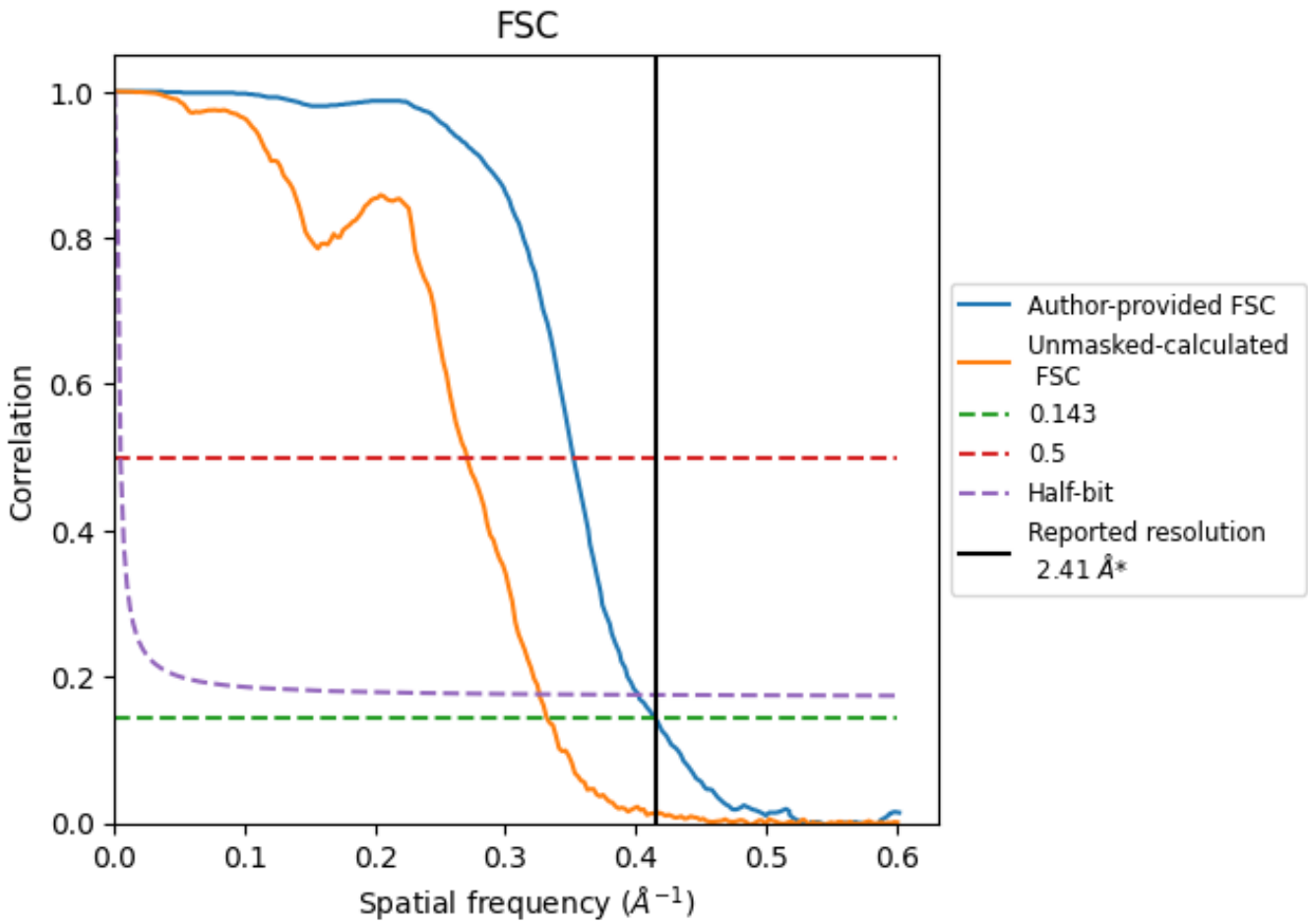


*Reported resolution corresponds to spatial frequency of 0.415 Å^{-1}

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 0.415 Å^{-1}

8.2 Resolution estimates (i)

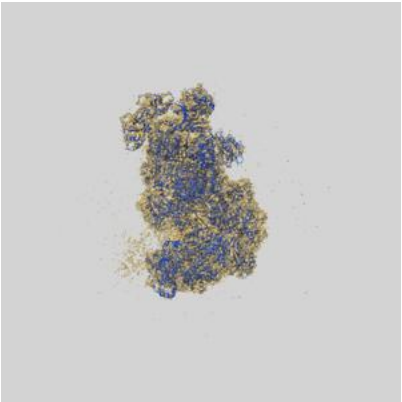
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.41	-	-
Author-provided FSC curve	2.41	2.84	2.49
Unmasked-calculated*	3.01	3.70	3.07

*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 3.01 differs from the reported value 2.41 by more than 10 %

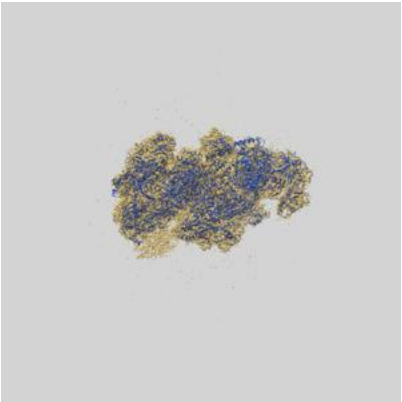
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-10117 and PDB model 6S8B. Per-residue inclusion information can be found in section 3 on page 9.

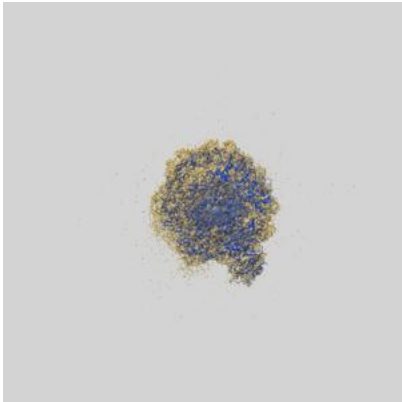
9.1 Map-model overlay (i)



X



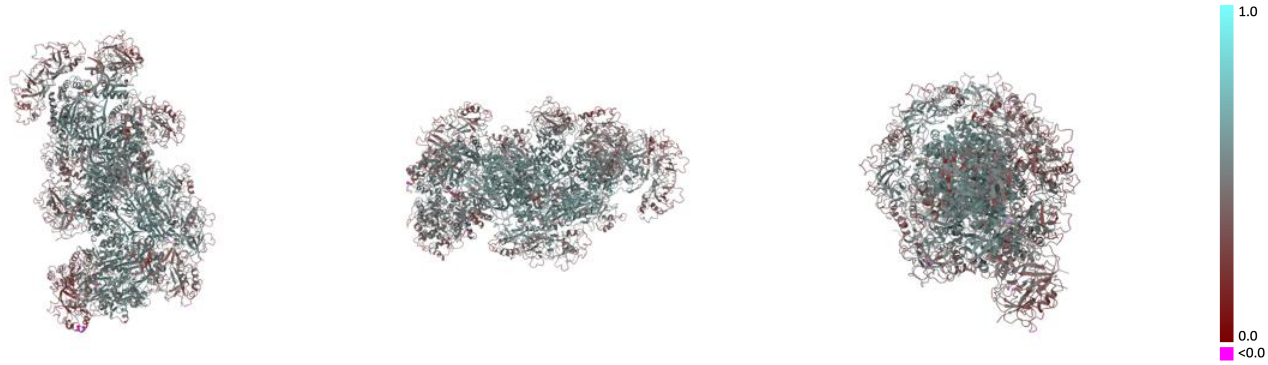
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

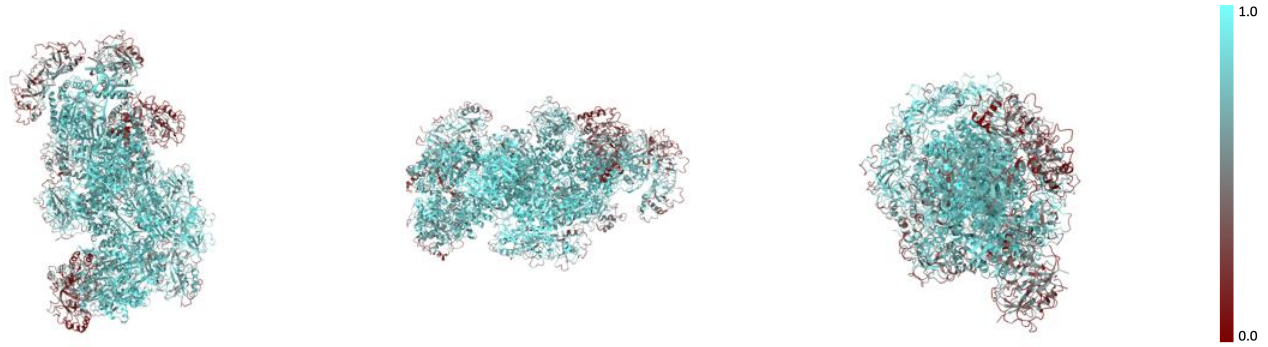
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

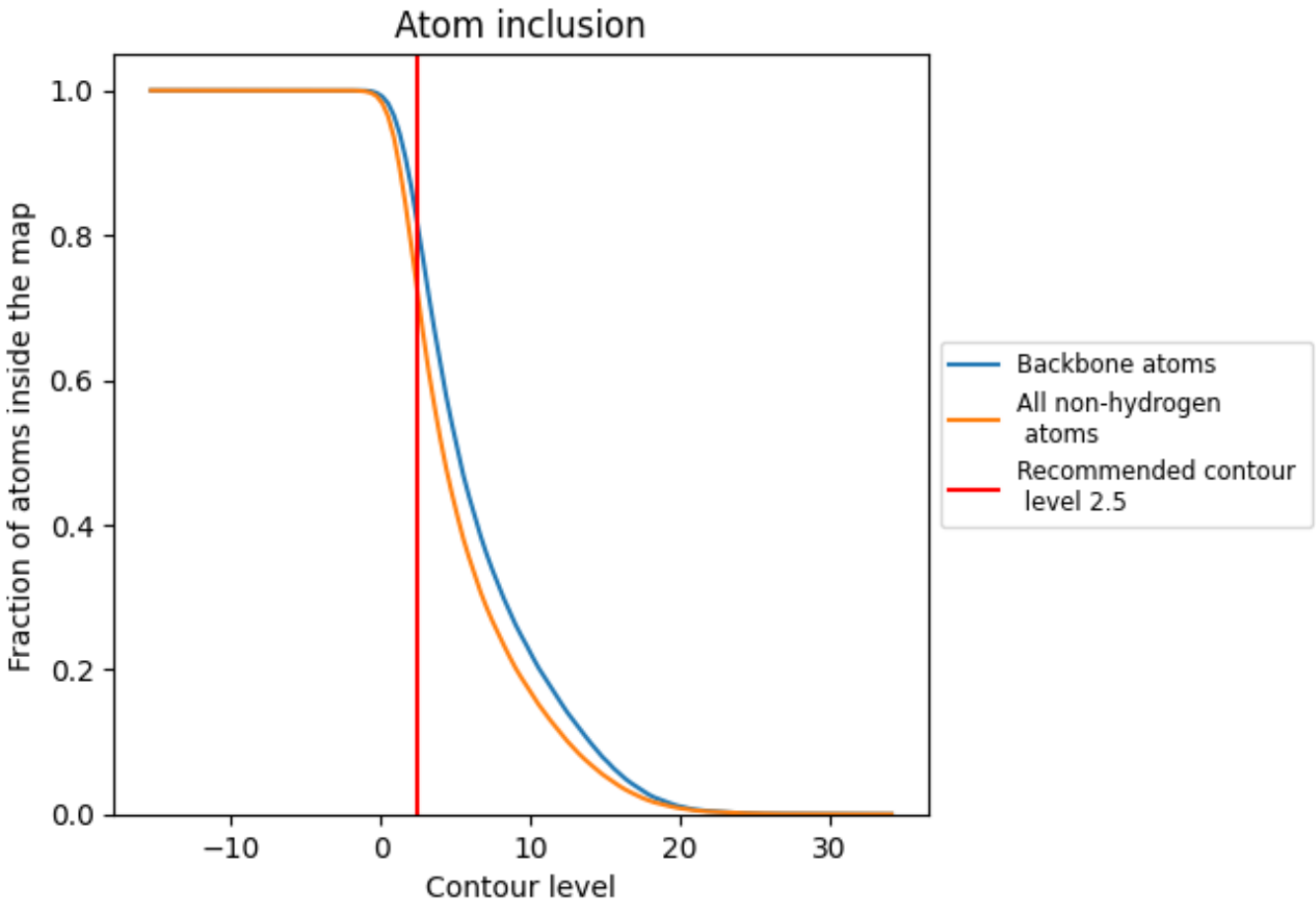
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.5).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7179	0.4800
A	0.9124	0.5820
B	0.9195	0.5870
C	0.9154	0.5820
D	0.9337	0.5970
E	0.9243	0.5950
F	0.9301	0.5920
G	0.9059	0.5720
H	0.8893	0.5450
I	0.9156	0.5850
J	0.8341	0.5320
K	0.7502	0.4600
L	0.8028	0.4670
M	0.8175	0.4750
N	0.6181	0.4050
O	0.6895	0.4550
P	0.5408	0.4470
Q	0.6630	0.4240
R	0.6799	0.4240
S	0.2465	0.3730
T	0.5563	0.3890
U	0.8875	0.5720
V	0.9617	0.6020
W	0.3900	0.3870
X	0.2531	0.3200
l	0.8035	0.4730
m	0.8396	0.4810
n	0.6012	0.3830
o	0.6865	0.4550
p	0.5820	0.4470
q	0.6755	0.4250
r	0.7123	0.4340
s	0.2539	0.3800
t	0.4467	0.3670
w	0.3870	0.3600
x	0.2031	0.3260