Full wwPDB EM Validation Report (i)

Aug 5, 2026 – 04:40 AM EDT

PDB ID	:	8UCJ / pdb_00008ucj
EMDB ID	:	EMD-42128
Title	:	CryoEM structure of Komagataella pastoris Cytochrome c oxidase (11 subunits) in complex with human VMAT2
Authors	:	Ye, J.; Liu, B.; Li, W.
Deposited on	:	2023-09-26
Resolution	:	3.20 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 (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 (i)) were used in the production of this report:

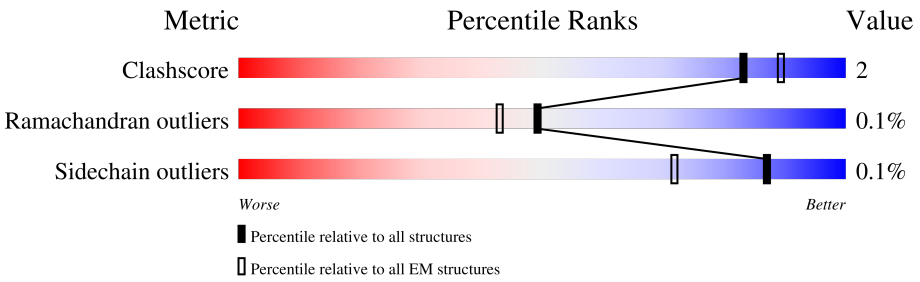
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

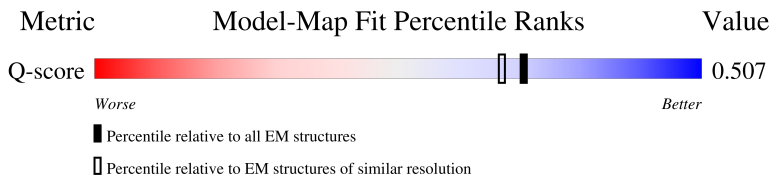
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	514	6% 62% 7% 31%
2	a	535	92% 7%
3	b	236	93% 6% •
4	c	269	93% 7%

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Mol	Chain	Length	Quality of chain
5	d	147	73% 6% 20%
6	e	126	97%
7	f	100	97%
8	g	58	90% 10%
9	h	48	100%
10	i	57	95% 5%
11	j	75	95% 5%
12	k	107	96%

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 16794 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 Synaptic vesicular amine transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	353	2624	1749	409	441	25	0	0

- Molecule 2 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	a	535	4169	2788	646	717	18	0	0

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	4	ILE	MET	conflict	UNP F2R0K8
a	16	ILE	MET	conflict	UNP F2R0K8
a	22	ILE	MET	conflict	UNP F2R0K8
a	33	ILE	MET	conflict	UNP F2R0K8
a	37	ILE	MET	conflict	UNP F2R0K8
a	49	ILE	MET	conflict	UNP F2R0K8
a	78	ILE	MET	conflict	UNP F2R0K8
a	85	LEU	THR	conflict	UNP F2R0K8
a	90	ILE	MET	conflict	UNP F2R0K8
a	121	ILE	MET	conflict	UNP F2R0K8
a	150	ILE	MET	conflict	UNP F2R0K8
a	158	ILE	MET	conflict	UNP F2R0K8
a	165	ILE	MET	conflict	UNP F2R0K8
a	168	ILE	MET	conflict	UNP F2R0K8
a	177	ILE	MET	conflict	UNP F2R0K8
a	232	ILE	MET	conflict	UNP F2R0K8
a	237	LEU	THR	conflict	UNP F2R0K8
a	250	ILE	MET	conflict	UNP F2R0K8
a	256	ILE	MET	conflict	UNP F2R0K8
a	260	ILE	MET	conflict	UNP F2R0K8
a	273	ILE	MET	conflict	UNP F2R0K8

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Chain	Residue	Modelled	Actual	Comment	Reference
a	314	ILE	MET	conflict	UNP F2R0K8
a	320	ILE	MET	conflict	UNP F2R0K8
a	322	ILE	MET	conflict	UNP F2R0K8
a	334	ILE	MET	conflict	UNP F2R0K8
a	367	ILE	MET	conflict	UNP F2R0K8
a	401	LEU	THR	conflict	UNP F2R0K8
a	402	ILE	MET	conflict	UNP F2R0K8
a	421	ILE	MET	conflict	UNP F2R0K8
a	442	ILE	MET	conflict	UNP F2R0K8
a	455	ILE	MET	conflict	UNP F2R0K8
a	462	ILE	MET	conflict	UNP F2R0K8
a	464	ILE	MET	conflict	UNP F2R0K8
a	465	ILE	MET	conflict	UNP F2R0K8
a	510	ILE	MET	conflict	UNP F2R0K8
a	515	ILE	MET	conflict	UNP F2R0K8
a	524	LEU	THR	conflict	UNP F2R0K8

- Molecule 3 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	b	236	1896	1247	287	352	10	0	0

- Molecule 4 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	c	269	2169	1463	338	355	13	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	45	ILE	MET	conflict	UNP F2R0J6
c	55	ILE	MET	conflict	UNP F2R0J6
c	62	ILE	MET	conflict	UNP F2R0J6
c	81	ILE	MET	conflict	UNP F2R0J6
c	89	ILE	MET	conflict	UNP F2R0J6
c	101	ILE	MET	conflict	UNP F2R0J6
c	120	ILE	MET	conflict	UNP F2R0J6
c	129	ILE	MET	conflict	UNP F2R0J6
c	132	ILE	MET	conflict	UNP F2R0J6
c	143	ILE	MET	conflict	UNP F2R0J6

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Chain	Residue	Modelled	Actual	Comment	Reference
c	247	ILE	MET	conflict	UNP F2R0J6
c	248	LEU	THR	conflict	UNP F2R0J6

- Molecule 5 is a protein called Cytochrome c oxidase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	d	117	910	576	147	183	4	0	0

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	e	126	1041	668	178	194	1	0	0

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	f	100	835	531	134	168	2	0	0

- Molecule 8 is a protein called Cytochrome c oxidase subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	g	58	465	309	74	81	1	0	0

- Molecule 9 is a protein called Cytochrome c oxidase subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	h	48	386	260	65	59	2	0	0

- Molecule 10 is a protein called Cytochrome c oxidase subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	i	57	469	307	84	78	0	0

- Molecule 11 is a protein called Cytochrome c oxidase subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	j	75	626	404	104	114	4	0	0

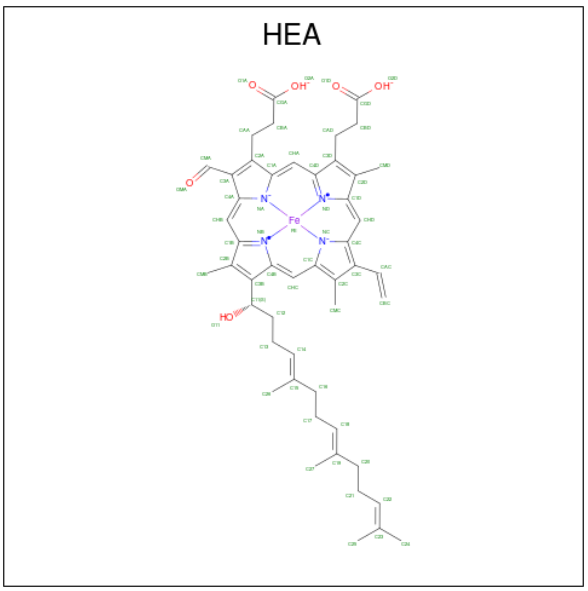
- Molecule 12 is a protein called Cytochrome c oxidase subunit 13.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	k	107	890	576	159	155	0	0

- Molecule 13 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

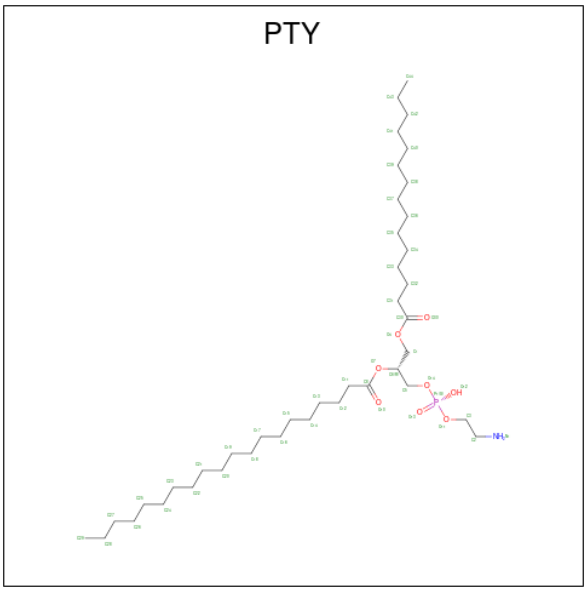
Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
13	a	1	1	1	0

- Molecule 14 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



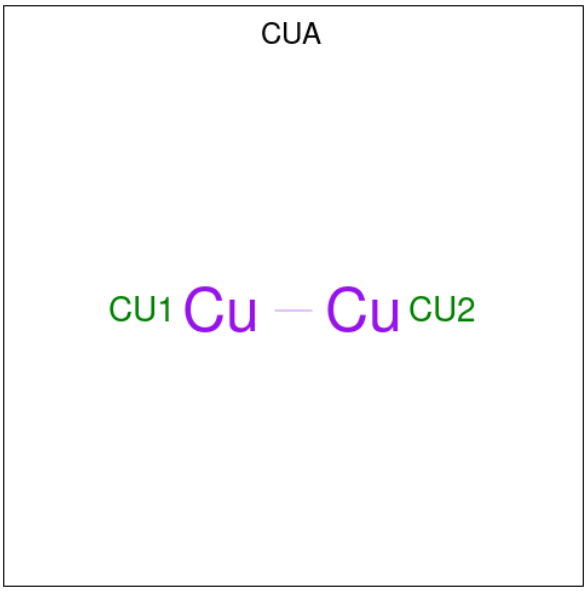
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
14	a	1	60	49	1	4	6	0
14	a	1	60	49	1	4	6	0

- Molecule 15 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
15	a	1	Total	C	N	O	P	0
			34	24	1	8	1	
15	a	1	Total	C	N	O	P	0
			40	30	1	8	1	
15	c	1	Total	C	N	O	P	0
			40	30	1	8	1	
15	e	1	Total	C	N	O	P	0
			33	23	1	8	1	

- Molecule 16 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2) (labeled as "Ligand of Interest" by depositor).

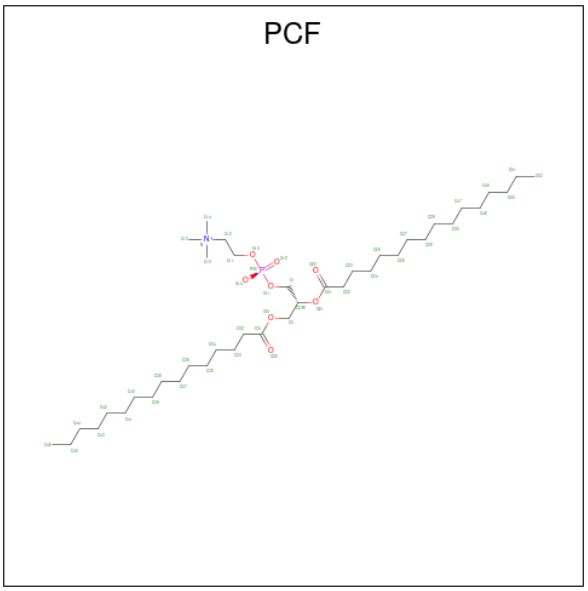


Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
16	b	1	2	2	0

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
17	d	1	1	1	0

- Molecule 18 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (CCD ID: PCF) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



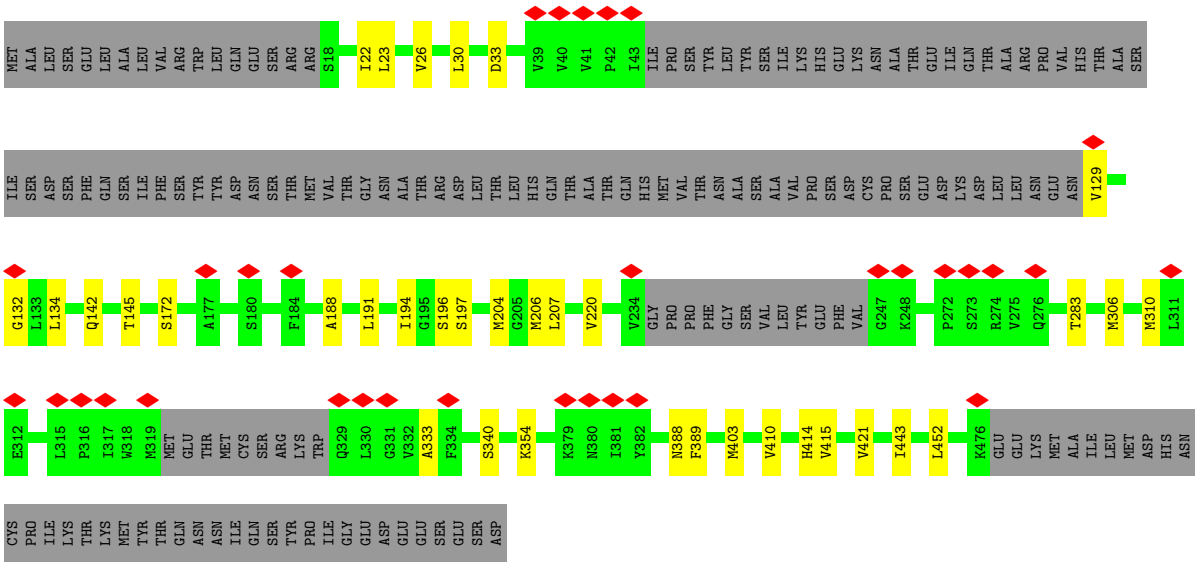
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
18	k	1	43	33	1	8	1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

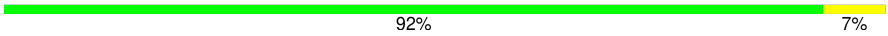
• Molecule 1: Synaptic vesicular amine transporter

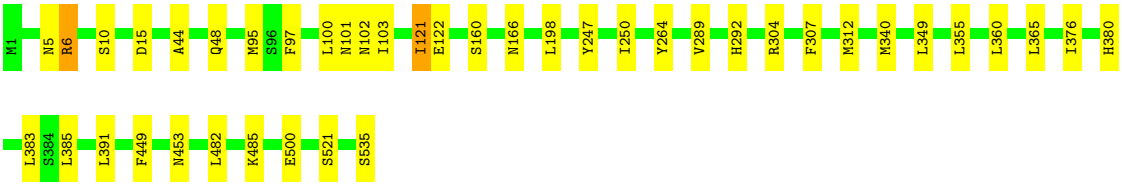
Chain A:



• Molecule 2: Cytochrome c oxidase subunit 1

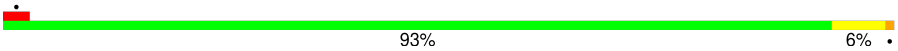
Chain a:





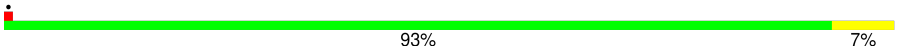
• Molecule 3: Cytochrome c oxidase subunit 2

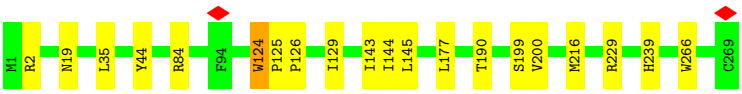
Chain b:



• Molecule 4: Cytochrome c oxidase subunit 3

Chain c:



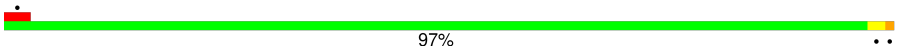


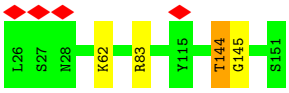
• Molecule 5: Cytochrome c oxidase subunit 4

Chain d:

• Molecule 6: Cytochrome c oxidase subunit 5

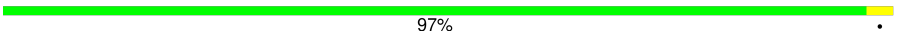
Chain e:

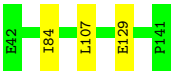




• Molecule 7: Cytochrome c oxidase subunit 6

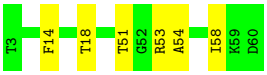
Chain f:





• Molecule 8: Cytochrome c oxidase subunit 7

Chain g:



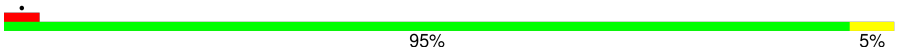
• Molecule 9: Cytochrome c oxidase subunit 8

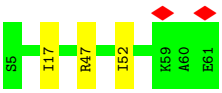
Chain h:

There are no outlier residues recorded for this chain.

• Molecule 10: Cytochrome c oxidase subunit 9

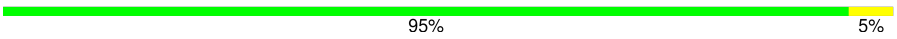
Chain i:





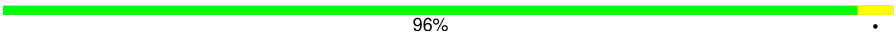
• Molecule 11: Cytochrome c oxidase subunit 12

Chain j:



• Molecule 12: Cytochrome c oxidase subunit 13

Chain k:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	141043	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)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.777	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	281.6, 281.6, 281.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PTY, CUA, HEA, CU, PCF

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	0.27	0/2681	0.61	0/3642
2	a	0.28	0/4300	0.62	1/5878 (0.0%)
3	b	0.26	0/1947	0.58	0/2664
4	c	0.30	0/2240	0.66	1/3065 (0.0%)
5	d	0.26	0/928	0.76	3/1260 (0.2%)
6	e	0.22	0/1069	0.51	0/1449
7	f	0.22	0/851	0.57	0/1148
8	g	0.23	0/478	0.61	0/647
9	h	0.28	0/400	0.65	0/541
10	i	0.20	0/482	0.56	1/650 (0.2%)
11	j	0.26	0/646	0.64	0/874
12	k	0.23	0/922	0.59	1/1254 (0.1%)
All	All	0.27	0/16944	0.61	7/23072 (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
2	a	0	2
4	c	0	1
All	All	0	3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	i	52	ILE	N-CA-C	-6.68	105.97	111.91
12	k	34	VAL	N-CA-C	-6.48	106.48	112.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	d	52	ALA	N-CA-C	-5.53	106.23	114.64
4	c	124	TRP	CA-CB-CG	-5.30	103.53	113.60
5	d	132	SER	CA-C-N	5.17	128.19	120.90
5	d	132	SER	C-N-CA	5.17	128.19	120.90
2	a	6	ARG	CA-CB-CG	5.16	124.42	114.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	a	121	ILE	Peptide
2	a	521	SER	Peptide
4	c	124	TRP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2624	0	2775	20	0
2	a	4169	0	4191	28	0
3	b	1896	0	1865	13	0
4	c	2169	0	2203	14	0
5	d	910	0	887	6	0
6	e	1041	0	1023	3	0
7	f	835	0	794	2	0
8	g	465	0	471	4	0
9	h	386	0	391	0	0
10	i	469	0	479	2	0
11	j	626	0	589	3	0
12	k	890	0	846	3	0
13	a	1	0	0	0	0
14	a	120	0	108	3	0
15	a	74	0	94	3	0
15	c	40	0	53	2	0
15	e	33	0	39	0	0
16	b	2	0	0	0	0
17	d	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	k	43	0	60	1	0
All	All	16794	0	16868	82	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (82) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:145:LEU:HD21	4:c:216:MET:HE1	1.70	0.74
1:A:410:VAL:HG21	1:A:421:VAL:HG21	1.79	0.64
1:A:204:MET:HE3	1:A:403:MET:HE1	1.81	0.61
2:a:6:ARG:NH1	2:a:15:ASP:OD2	2.33	0.61
1:A:306:MET:HG3	1:A:310:MET:HE2	1.82	0.61
4:c:144:ILE:HG23	4:c:177:LEU:HD22	1.83	0.59
3:b:187:CYS:SG	3:b:194:LYS:NZ	2.73	0.59
1:A:33:ASP:OD1	1:A:196:SER:OG	2.21	0.59
4:c:35:LEU:HD13	8:g:51:THR:HG21	1.85	0.58
2:a:349:LEU:HD13	2:a:385:LEU:HD13	1.85	0.58
2:a:5:ASN:O	4:c:19:ASN:ND2	2.36	0.57
4:c:190:THR:O	12:k:112:ASN:ND2	2.38	0.57
2:a:355:LEU:HD22	3:b:45:LEU:HD22	1.87	0.57
5:d:115:ASP:O	5:d:121:ARG:NH1	2.38	0.56
3:b:184:HIS:CD2	3:b:230:MET:HE1	2.42	0.55
4:c:126:PRO:HG2	4:c:129:ILE:HD12	1.90	0.54
1:A:145:THR:HG21	1:A:194:ILE:HG13	1.90	0.54
1:A:172:SER:OG	1:A:188:ALA:O	2.26	0.53
2:a:264:TYR:HB2	2:a:340:MET:HE2	1.91	0.53
1:A:129:VAL:HG13	1:A:132:GLY:H	1.74	0.53
6:e:62:LYS:NZ	7:f:129:GLU:O	2.42	0.52
2:a:312:MET:HB3	3:b:91:LEU:HD22	1.92	0.52
1:A:283:THR:HG23	1:A:415:VAL:HG12	1.91	0.52
1:A:142:GLN:HG3	1:A:197:SER:HB2	1.91	0.52
1:A:354:LYS:NZ	4:c:266:TRP:O	2.44	0.51
4:c:199:SER:OG	4:c:200:VAL:N	2.42	0.51
5:d:133:HIS:CE1	5:d:150:GLU:HB3	2.46	0.51
1:A:191:LEU:HA	1:A:194:ILE:HG22	1.93	0.51
1:A:340:SER:HB3	1:A:389:PHE:HD1	1.75	0.51
5:d:147:ARG:HG3	5:d:154:VAL:HG22	1.92	0.51
3:b:184:HIS:HD2	3:b:230:MET:HE1	1.75	0.51
1:A:30:LEU:HD11	1:A:204:MET:HE1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:44:ALA:HB3	2:a:48:GLN:HE22	1.76	0.51
2:a:500:GLU:O	6:e:83:ARG:NH2	2.44	0.51
4:c:143:ILE:HD12	12:k:60:THR:HG21	1.93	0.51
2:a:247:TYR:HA	2:a:250:ILE:HG22	1.93	0.50
11:j:33:HIS:HA	11:j:36:ILE:HG22	1.94	0.49
2:a:289:VAL:HG23	2:a:307:PHE:HD1	1.77	0.49
1:A:333:ALA:O	1:A:388:ASN:ND2	2.46	0.48
4:c:2:ARG:NH2	5:d:115:ASP:OD2	2.47	0.48
1:A:443:ILE:HG21	1:A:452:LEU:HD13	1.95	0.48
1:A:283:THR:HG21	1:A:414:HIS:HD2	1.78	0.48
3:b:116:LYS:HE2	3:b:129:SER:HB3	1.96	0.48
2:a:449:PHE:O	2:a:453:ASN:ND2	2.44	0.48
2:a:44:ALA:HB3	2:a:48:GLN:NE2	2.29	0.47
2:a:304:ARG:NH2	11:j:19:GLN:OE1	2.47	0.47
3:b:129:SER:HB2	11:j:55:SER:HA	1.97	0.47
12:k:111:TRP:HA	18:k:201:PCF:H132	1.95	0.47
2:a:391:LEU:HB3	14:a:602:HEA:H243	1.97	0.47
2:a:535:SER:HB3	5:d:126:THR:HG22	1.97	0.47
2:a:360:LEU:HB3	14:a:603:HEA:HMA	1.97	0.47
6:e:144:THR:OG1	6:e:145:GLY:N	2.46	0.47
2:a:97:PHE:O	2:a:166:ASN:ND2	2.45	0.46
2:a:121:ILE:HD11	4:c:44:TYR:CZ	2.51	0.46
2:a:100:LEU:HA	2:a:103:ILE:HG22	1.98	0.46
3:b:145:VAL:HG11	3:b:229:ALA:HB1	1.99	0.46
2:a:376:ILE:HG23	2:a:380:HIS:CE1	2.51	0.45
1:A:26:VAL:HG21	1:A:207:LEU:HG	1.99	0.45
2:a:482:LEU:O	2:a:485:LYS:NZ	2.45	0.45
2:a:289:VAL:HG22	2:a:292:HIS:HD1	1.83	0.43
3:b:221:GLU:O	3:b:223:CYS:SG	2.77	0.43
4:c:229:ARG:NH2	15:c:301:PTY:O30	2.51	0.43
7:f:84:ILE:HD13	7:f:107:LEU:HD11	2.01	0.43
5:d:126:THR:C	5:d:133:HIS:HB3	2.45	0.42
2:a:160:SER:HB3	2:a:198:LEU:HD22	2.02	0.42
1:A:23:LEU:HD13	1:A:220:VAL:HG13	2.01	0.42
3:b:219:CYS:SG	3:b:220:SER:N	2.93	0.42
15:a:605:PTY:H202	3:b:51:PHE:HE2	1.85	0.41
2:a:121:ILE:HD12	8:g:54:ALA:HB1	2.01	0.41
15:a:605:PTY:H111	10:i:17:ILE:HD13	2.02	0.41
1:A:134:LEU:HD12	1:A:134:LEU:HA	1.94	0.41
4:c:229:ARG:HH12	15:c:301:PTY:HC11	1.85	0.41
8:g:14:PHE:O	8:g:18:THR:OG1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:365:LEU:HD23	3:b:34:ILE:HG23	2.02	0.41
2:a:95:MET:HG3	2:a:101:ASN:HD21	1.85	0.41
1:A:22:ILE:HG23	1:A:206:MET:HE3	2.03	0.41
4:c:84:ARG:HD3	4:c:239:HIS:CE1	2.56	0.40
2:a:10:SER:H	2:a:102:ASN:HD21	1.69	0.40
15:a:604:PTY:H362	15:a:604:PTY:H181	2.03	0.40
8:g:53:ARG:HG2	8:g:58:ILE:HB	2.03	0.40
3:b:32:GLU:OE2	10:i:47:ARG:NH1	2.54	0.40
2:a:383:LEU:HB3	14:a:602:HEA:HAC	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	345/514 (67%)	333 (96%)	12 (4%)	0	100	100
2	a	533/535 (100%)	503 (94%)	29 (5%)	1 (0%)	43	73
3	b	234/236 (99%)	218 (93%)	16 (7%)	0	100	100
4	c	267/269 (99%)	248 (93%)	18 (7%)	1 (0%)	30	62
5	d	115/147 (78%)	99 (86%)	16 (14%)	0	100	100
6	e	124/126 (98%)	118 (95%)	5 (4%)	1 (1%)	16	50
7	f	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
8	g	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
9	h	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
10	i	55/57 (96%)	52 (94%)	3 (6%)	0	100	100
11	j	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
12	k	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
All	All	2051/2272 (90%)	1925 (94%)	123 (6%)	3 (0%)	49	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	a	122	GLU
6	e	144	THR
4	c	125	PRO

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	280/427 (66%)	280 (100%)	0	100	100
2	a	452/452 (100%)	452 (100%)	0	100	100
3	b	212/212 (100%)	210 (99%)	2 (1%)	70	81
4	c	235/235 (100%)	235 (100%)	0	100	100
5	d	99/127 (78%)	99 (100%)	0	100	100
6	e	112/112 (100%)	112 (100%)	0	100	100
7	f	90/90 (100%)	90 (100%)	0	100	100
8	g	48/48 (100%)	48 (100%)	0	100	100
9	h	41/41 (100%)	41 (100%)	0	100	100
10	i	48/48 (100%)	48 (100%)	0	100	100
11	j	68/68 (100%)	68 (100%)	0	100	100
12	k	91/91 (100%)	91 (100%)	0	100	100
All	All	1776/1951 (91%)	1774 (100%)	2 (0%)	87	91

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	b	223	CYS
3	b	230	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	a	53	ASN
2	a	64	HIS
2	a	219	ASN
2	a	380	HIS
3	b	62	ASN
3	b	121	GLN
4	c	123	GLN
8	g	26	HIS
12	k	36	HIS
12	k	37	HIS
12	k	94	ASN
12	k	118	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
15	PTY	a	604	-	33,33,49	0.47	0	36,38,54	1.27	4 (11%)
18	PCF	k	201	-	42,42,49	0.65	0	48,50,57	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	PTY	c	301	-	39,39,49	0.43	0	42,44,54	1.30	4 (9%)
15	PTY	e	201	-	32,32,49	0.48	0	35,37,54	1.27	4 (11%)
16	CUA	b	301	3	0,1,1	-	-	-		
14	HEA	a	603	-	67,67,67	1.10	6 (8%)	81,103,103	1.72	16 (19%)
14	HEA	a	602	2	67,67,67	1.04	5 (7%)	81,103,103	1.49	12 (14%)
15	PTY	a	605	-	39,39,49	0.46	0	42,44,54	1.29	4 (9%)

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
15	PTY	a	604	-	-	14/37/37/53	-
18	PCF	k	201	-	-	8/46/46/53	-
15	PTY	c	301	-	-	16/43/43/53	-
15	PTY	e	201	-	-	12/36/36/53	-
14	HEA	a	603	-	-	16/36/76/76	-
14	HEA	a	602	2	-	10/36/76/76	-
15	PTY	a	605	-	-	11/43/43/53	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	603	HEA	C1A-C2A	-4.42	1.37	1.45
14	a	602	HEA	C1A-C2A	-4.34	1.37	1.45
14	a	603	HEA	C3A-C4A	-3.20	1.40	1.46
14	a	602	HEA	C3A-C4A	-3.09	1.40	1.46
14	a	603	HEA	C1C-C2C	-2.64	1.36	1.43
14	a	603	HEA	C1D-ND	-2.22	1.36	1.40
14	a	602	HEA	CHD-C4C	-2.19	1.34	1.39
14	a	603	HEA	CHC-C1C	-2.15	1.34	1.39
14	a	602	HEA	C1D-ND	-2.11	1.36	1.40
14	a	603	HEA	C4B-NB	-2.04	1.36	1.40
14	a	602	HEA	C1C-C2C	-2.03	1.38	1.43

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	603	HEA	C13-C12-C11	-6.72	103.66	114.39
14	a	602	HEA	CHB-C4A-NA	-4.83	119.19	124.45
15	a	605	PTY	O7-C8-C11	4.06	120.26	111.48
14	a	603	HEA	C12-C11-C3B	4.03	118.42	112.12
14	a	603	HEA	CHB-C4A-NA	-3.94	120.16	124.45
15	c	301	PTY	O7-C8-C11	3.83	119.77	111.48
15	a	604	PTY	O7-C8-C11	3.78	119.67	111.48
15	e	201	PTY	O7-C8-C11	3.55	119.17	111.48
14	a	602	HEA	C13-C12-C11	-3.52	108.77	114.39
15	c	301	PTY	P1-O11-C3	-3.36	105.25	121.26
15	e	201	PTY	P1-O11-C3	-3.19	106.08	121.26
14	a	602	HEA	CHB-C4A-C3A	3.17	130.56	125.21
15	a	604	PTY	P1-O11-C3	-3.11	106.44	121.26
15	a	605	PTY	P1-O11-C3	-3.05	106.72	121.26
14	a	603	HEA	C17-C18-C19	-2.96	120.84	127.62
14	a	603	HEA	CHD-C4C-NC	-2.96	118.50	123.86
14	a	603	HEA	C13-C14-C15	-2.95	120.87	127.62
14	a	603	HEA	CMB-C2B-C3B	-2.90	124.67	130.28
14	a	602	HEA	CHB-C1B-NB	-2.89	121.31	124.42
15	a	605	PTY	O4-C30-C31	2.85	120.54	111.83
15	c	301	PTY	O4-C30-C31	2.78	120.31	111.83
14	a	602	HEA	CHD-C4C-NC	-2.76	118.85	123.86
14	a	602	HEA	C4A-CHB-C1B	-2.72	120.24	126.02
15	a	605	PTY	P1-O14-C5	-2.63	106.26	121.35
15	a	604	PTY	O4-C30-C31	2.60	119.76	111.83
14	a	603	HEA	CHB-C1B-NB	-2.60	121.63	124.42
15	e	201	PTY	O4-C30-C31	2.54	119.59	111.83
15	c	301	PTY	P1-O14-C5	-2.49	107.07	121.35
14	a	602	HEA	C17-C18-C19	-2.47	121.96	127.62
14	a	603	HEA	C27-C19-C20	2.46	119.50	115.23
14	a	603	HEA	CHB-C4A-C3A	2.44	129.33	125.21
14	a	603	HEA	C26-C15-C16	2.41	119.41	115.23
14	a	603	HEA	C4A-CHB-C1B	-2.31	121.11	126.02
14	a	603	HEA	O2D-CGD-O1D	-2.30	117.40	123.33
14	a	602	HEA	C13-C14-C15	-2.29	122.37	127.62
15	e	201	PTY	P1-O14-C5	-2.29	108.25	121.35
14	a	602	HEA	OMA-CMA-C3A	-2.27	120.50	125.62
15	a	604	PTY	P1-O14-C5	-2.25	108.46	121.35
14	a	603	HEA	CMB-C2B-C1B	2.24	128.53	125.03
14	a	602	HEA	C4C-CHD-C1D	-2.22	121.03	126.25
14	a	602	HEA	CHD-C1D-ND	-2.18	121.67	124.37
14	a	602	HEA	C27-C19-C20	2.18	119.00	115.23
14	a	603	HEA	CHD-C1D-ND	-2.10	121.77	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	603	HEA	C2D-C1D-ND	2.04	112.19	109.84

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	a	602	HEA	C2A-C3A-CMA-OMA
14	a	602	HEA	C4A-C3A-CMA-OMA
14	a	602	HEA	C2C-C3C-CAC-CBC
14	a	602	HEA	C4C-C3C-CAC-CBC
14	a	602	HEA	C17-C18-C19-C20
14	a	602	HEA	C17-C18-C19-C27
14	a	603	HEA	C2A-C3A-CMA-OMA
14	a	603	HEA	C4A-C3A-CMA-OMA
14	a	603	HEA	C2C-C3C-CAC-CBC
14	a	603	HEA	C4C-C3C-CAC-CBC
15	a	604	PTY	O30-C30-O4-C1
15	a	604	PTY	O10-C8-O7-C6
15	a	604	PTY	C11-C8-O7-C6
15	a	604	PTY	C5-O14-P1-O11
15	a	604	PTY	C5-O14-P1-O12
15	a	604	PTY	C5-O14-P1-O13
15	a	605	PTY	N1-C2-C3-O11
15	a	605	PTY	C11-C8-O7-C6
15	c	301	PTY	N1-C2-C3-O11
15	e	201	PTY	C5-O14-P1-O11
15	e	201	PTY	C5-O14-P1-O12
15	e	201	PTY	C5-O14-P1-O13
18	k	201	PCF	C11-O13-P-O11
18	k	201	PCF	C11-O13-P-O14
18	k	201	PCF	C22-C21-O21-C2
15	e	201	PTY	O30-C30-O4-C1
15	a	605	PTY	O10-C8-O7-C6
18	k	201	PCF	O22-C21-O21-C2
15	a	604	PTY	C31-C30-O4-C1
15	e	201	PTY	C31-C30-O4-C1
14	a	603	HEA	C13-C14-C15-C26
14	a	603	HEA	C17-C18-C19-C20
15	c	301	PTY	O30-C30-O4-C1
15	c	301	PTY	C31-C30-O4-C1
14	a	603	HEA	C17-C18-C19-C27
15	c	301	PTY	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
14	a	603	HEA	C21-C22-C23-C25
14	a	603	HEA	C15-C16-C17-C18
14	a	603	HEA	C3D-CAD-CBD-CGD
14	a	603	HEA	C21-C22-C23-C24
15	c	301	PTY	C36-C37-C38-C39
15	c	301	PTY	C11-C8-O7-C6
15	a	604	PTY	C14-C15-C16-C17
14	a	602	HEA	C21-C22-C23-C25
15	e	201	PTY	C11-C12-C13-C14
15	c	301	PTY	C35-C36-C37-C38
15	c	301	PTY	C37-C38-C39-C40
15	a	604	PTY	C15-C16-C17-C18
15	c	301	PTY	O10-C8-O7-C6
15	e	201	PTY	C34-C35-C36-C37
15	a	605	PTY	O4-C1-C6-O7
15	c	301	PTY	C13-C14-C15-C16
15	c	301	PTY	C14-C15-C16-C17
15	a	605	PTY	C11-C12-C13-C14
15	a	605	PTY	O14-C5-C6-O7
15	a	604	PTY	O4-C1-C6-O7
15	a	605	PTY	C31-C32-C33-C34
15	a	604	PTY	C34-C35-C36-C37
18	k	201	PCF	O13-C11-C12-N
15	a	604	PTY	C30-C31-C32-C33
15	e	201	PTY	C8-C11-C12-C13
14	a	602	HEA	C26-C15-C16-C17
18	k	201	PCF	C27-C28-C29-C30
15	c	301	PTY	C16-C17-C18-C19
15	c	301	PTY	O14-C5-C6-O7
15	a	605	PTY	O4-C1-C6-C5
14	a	602	HEA	C11-C12-C13-C14
15	a	604	PTY	C3-O11-P1-O13
15	a	605	PTY	C3-O11-P1-O13
15	e	201	PTY	C3-O11-P1-O13
15	a	605	PTY	O14-C5-C6-C1
14	a	603	HEA	CAA-CBA-CGA-O2A
14	a	602	HEA	C19-C20-C21-C22
15	c	301	PTY	C17-C18-C19-C20
15	a	605	PTY	C36-C37-C38-C39
18	k	201	PCF	C29-C30-C47-C48
14	a	603	HEA	CAA-CBA-CGA-O1A
14	a	603	HEA	CAD-CBD-CGD-O2D

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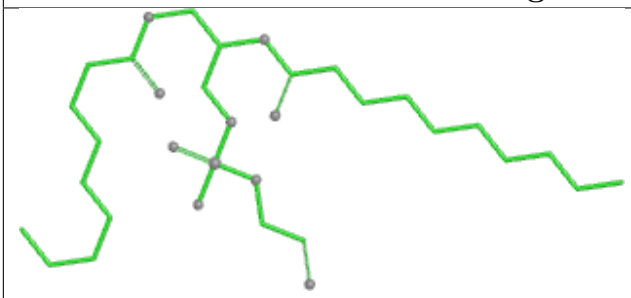
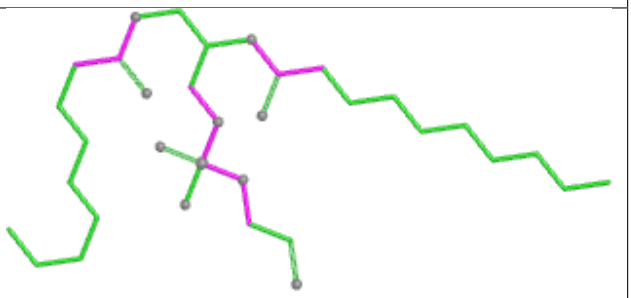
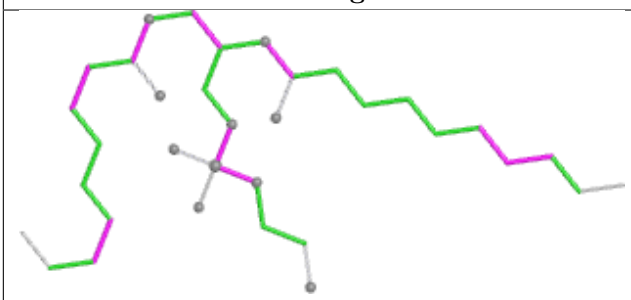
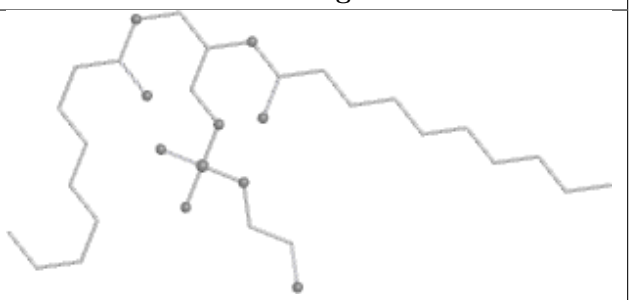
Mol	Chain	Res	Type	Atoms
14	a	603	HEA	CAD-CBD-CGD-O1D
15	e	201	PTY	C31-C32-C33-C34
15	a	604	PTY	O4-C1-C6-C5
15	e	201	PTY	O14-C5-C6-C1
18	k	201	PCF	C28-C29-C30-C47
15	e	201	PTY	O14-C5-C6-O7
15	c	301	PTY	C18-C19-C20-C21
15	c	301	PTY	O14-C5-C6-C1
14	a	603	HEA	C13-C14-C15-C16

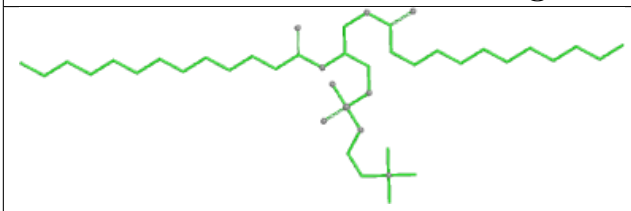
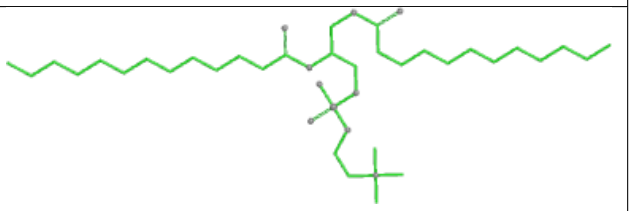
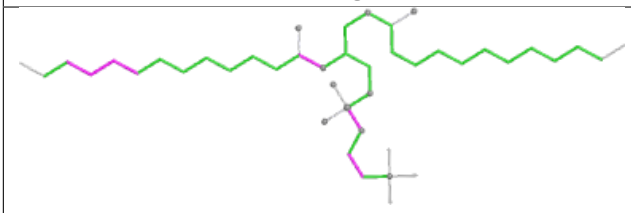
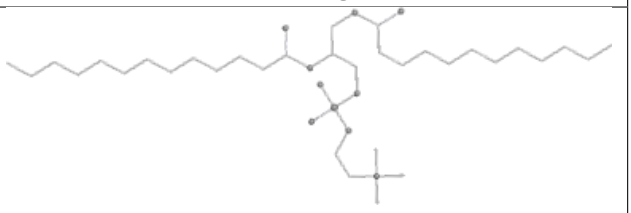
There are no ring outliers.

6 monomers are involved in 9 short contacts:

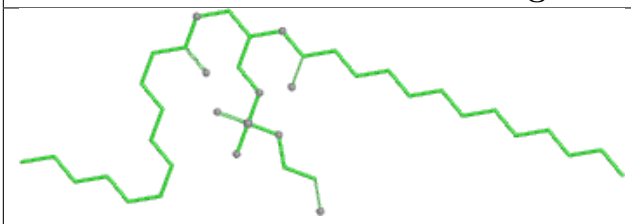
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	a	604	PTY	1	0
18	k	201	PCF	1	0
15	c	301	PTY	2	0
14	a	603	HEA	1	0
14	a	602	HEA	2	0
15	a	605	PTY	2	0

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.

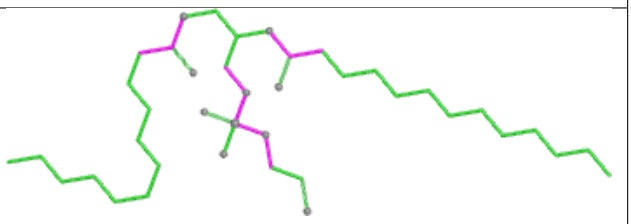
Ligand PTY a 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PCF k 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

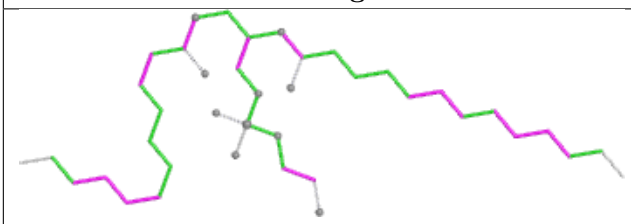
Ligand PTY c 301



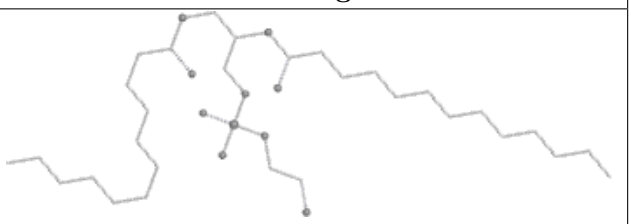
Bond lengths



Bond angles

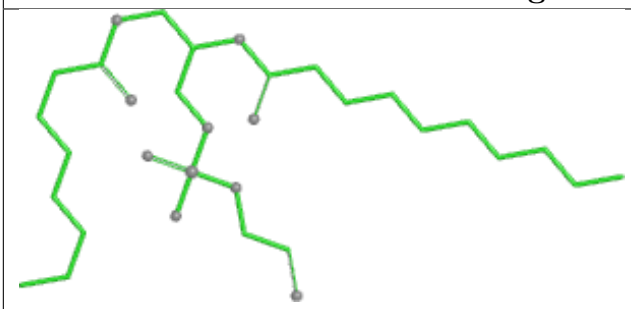


Torsions

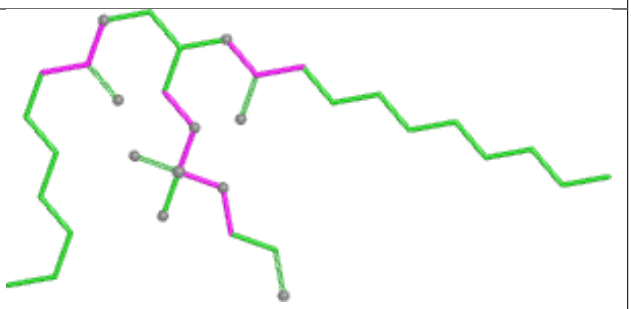


Rings

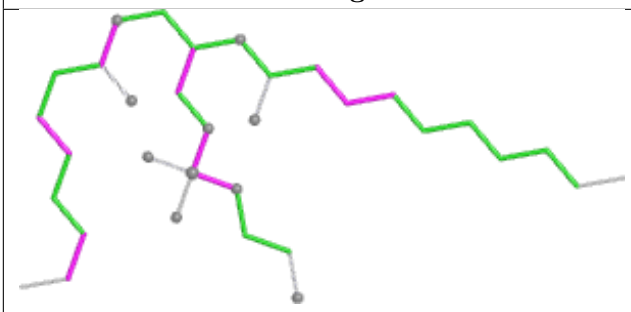
Ligand PTY e 201



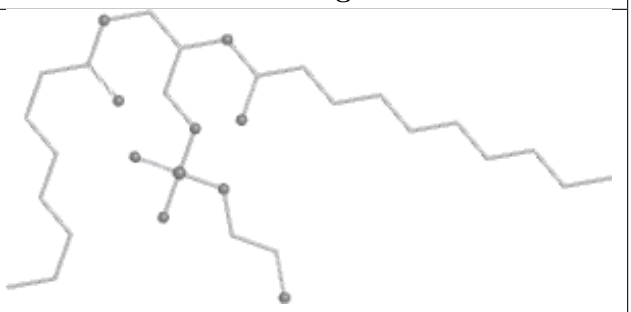
Bond lengths



Bond angles

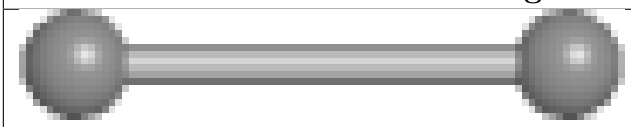


Torsions

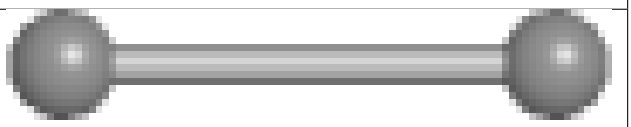


Rings

Ligand CUA b 301

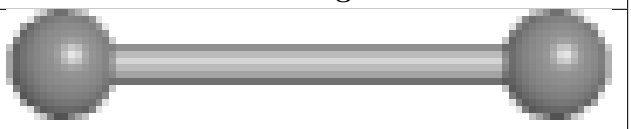


Bond lengths

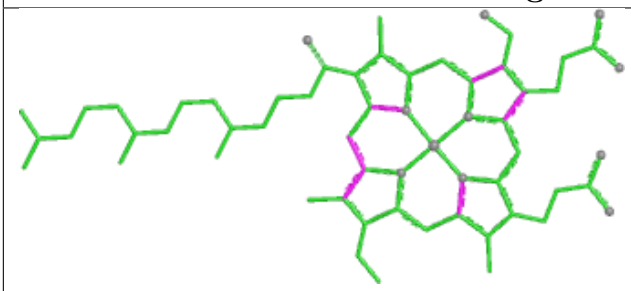
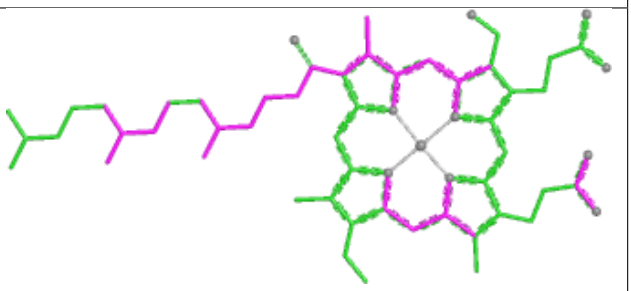
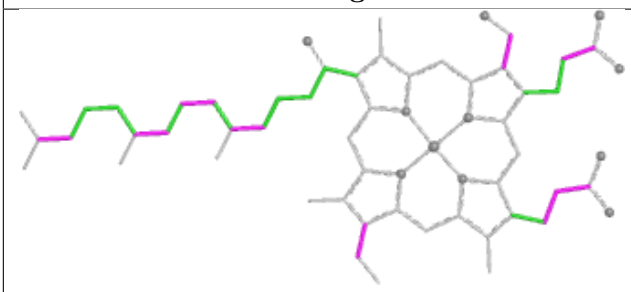
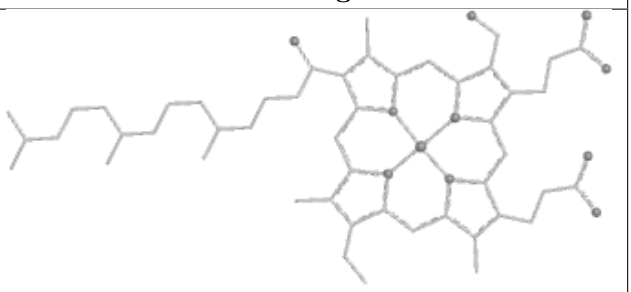


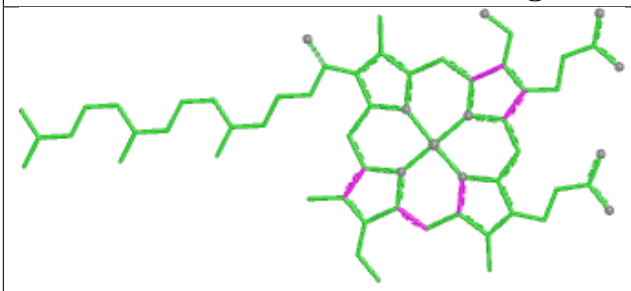
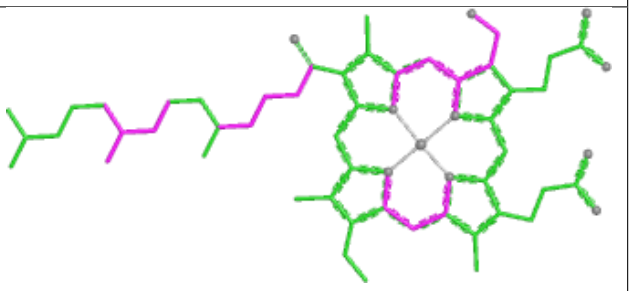
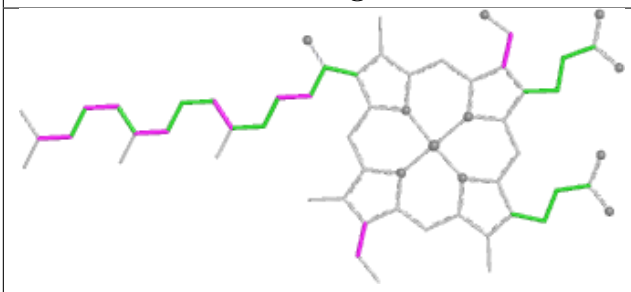
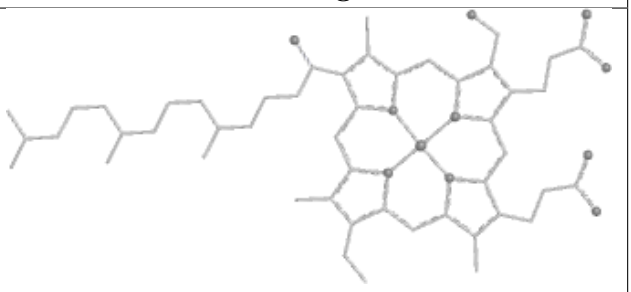
Bond angles

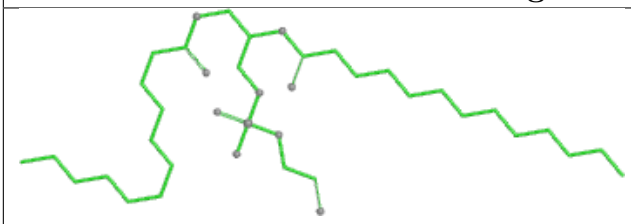
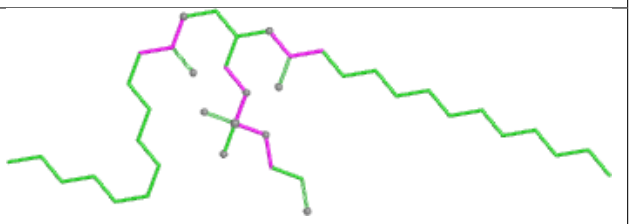
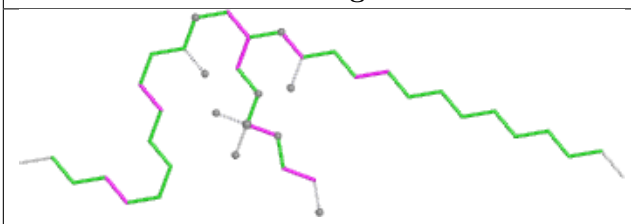
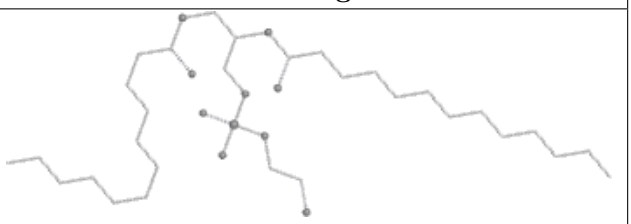
Torsions



Rings

Ligand HEA a 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEA a 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PTY a 605	
 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.

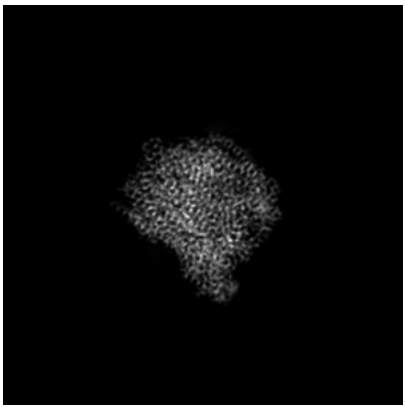
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-42128. These allow visual inspection of the internal detail of the map and identification of artifacts.

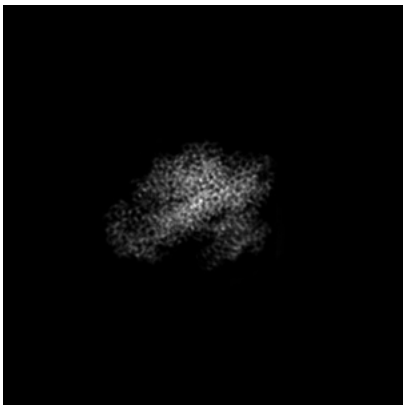
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

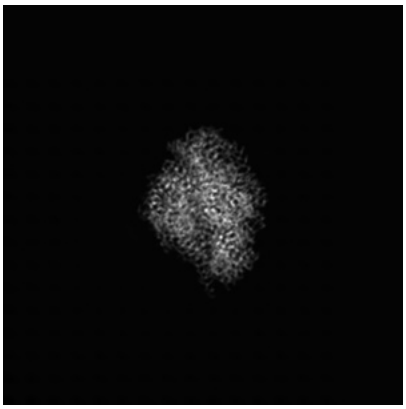
6.1.1 Primary map



X

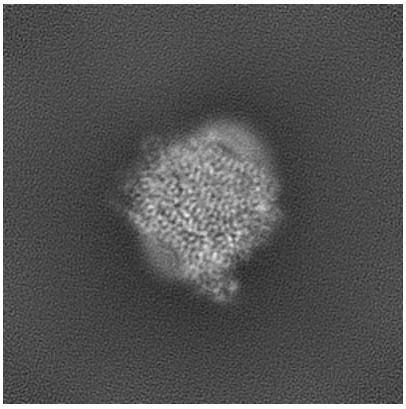


Y

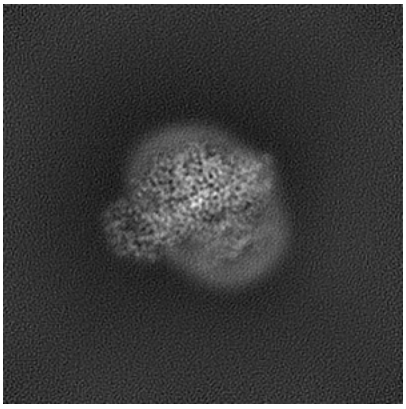


Z

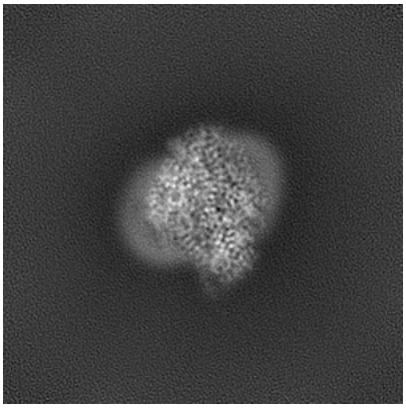
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

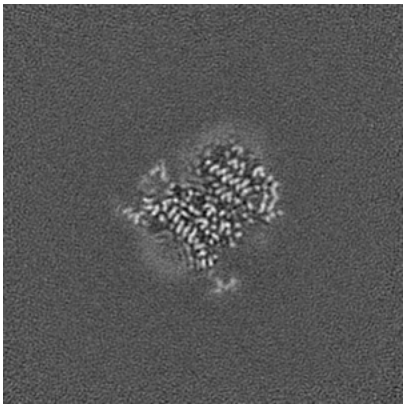
6.2.1 Primary map

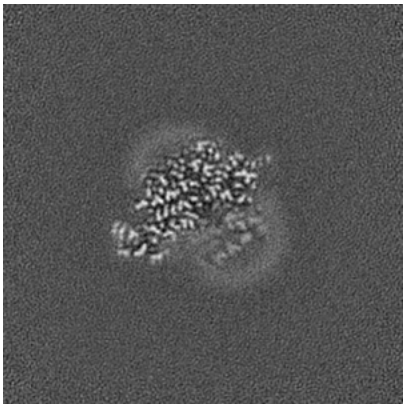
X Index: 128

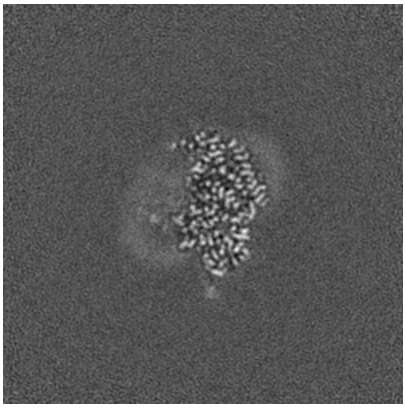
Y Index: 128

Z Index: 128

6.2.2 Raw map


X Index: 128


Y Index: 128


Z Index: 128

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

6.3 Largest variance slices (i)

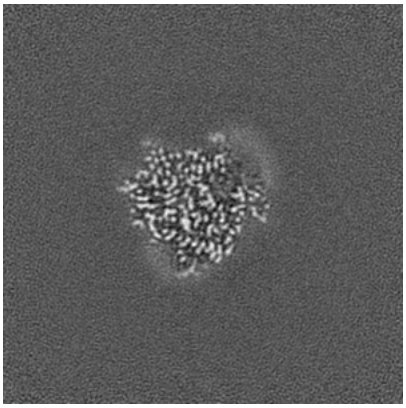
6.3.1 Primary map

X Index: 136

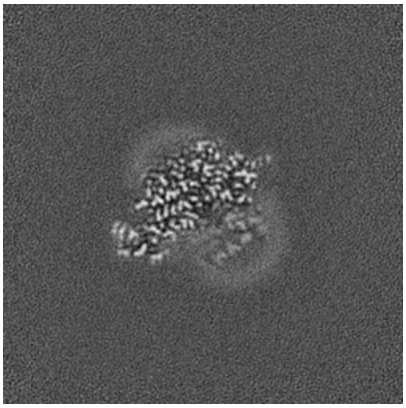
Y Index: 128

Z Index: 120

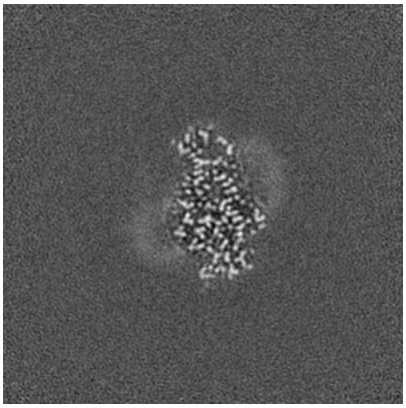
6.3.2 Raw map



X Index: 143



Y Index: 128

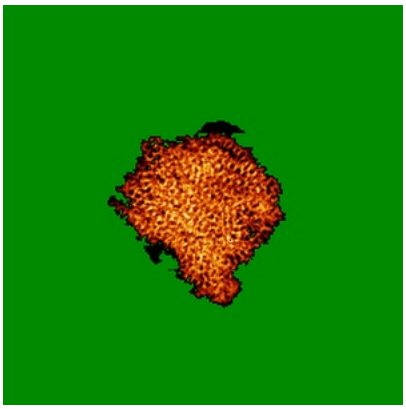


Z Index: 120

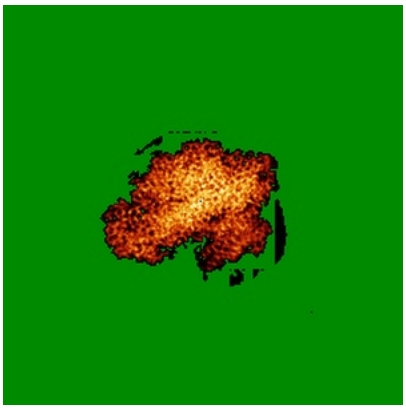
The images above show the largest variance slices of the map in three orthogonal directions.

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

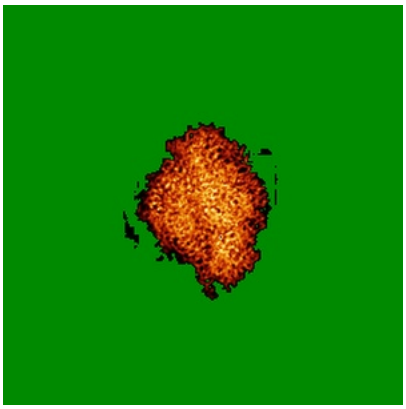
6.4.1 Primary map



X

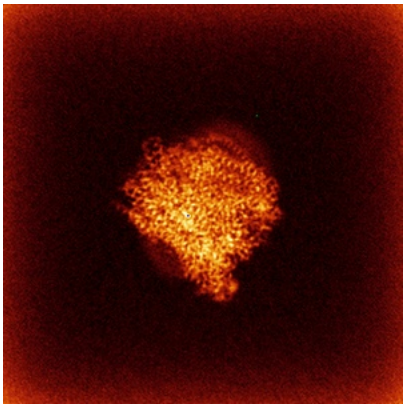


Y

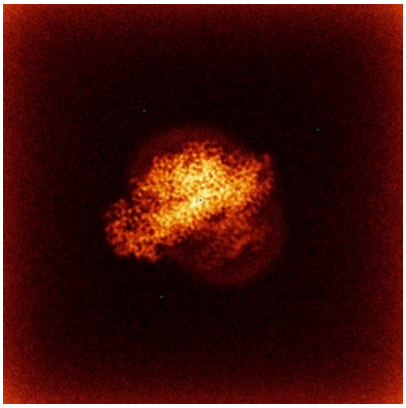


Z

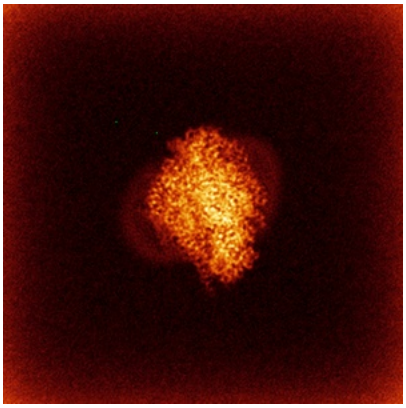
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

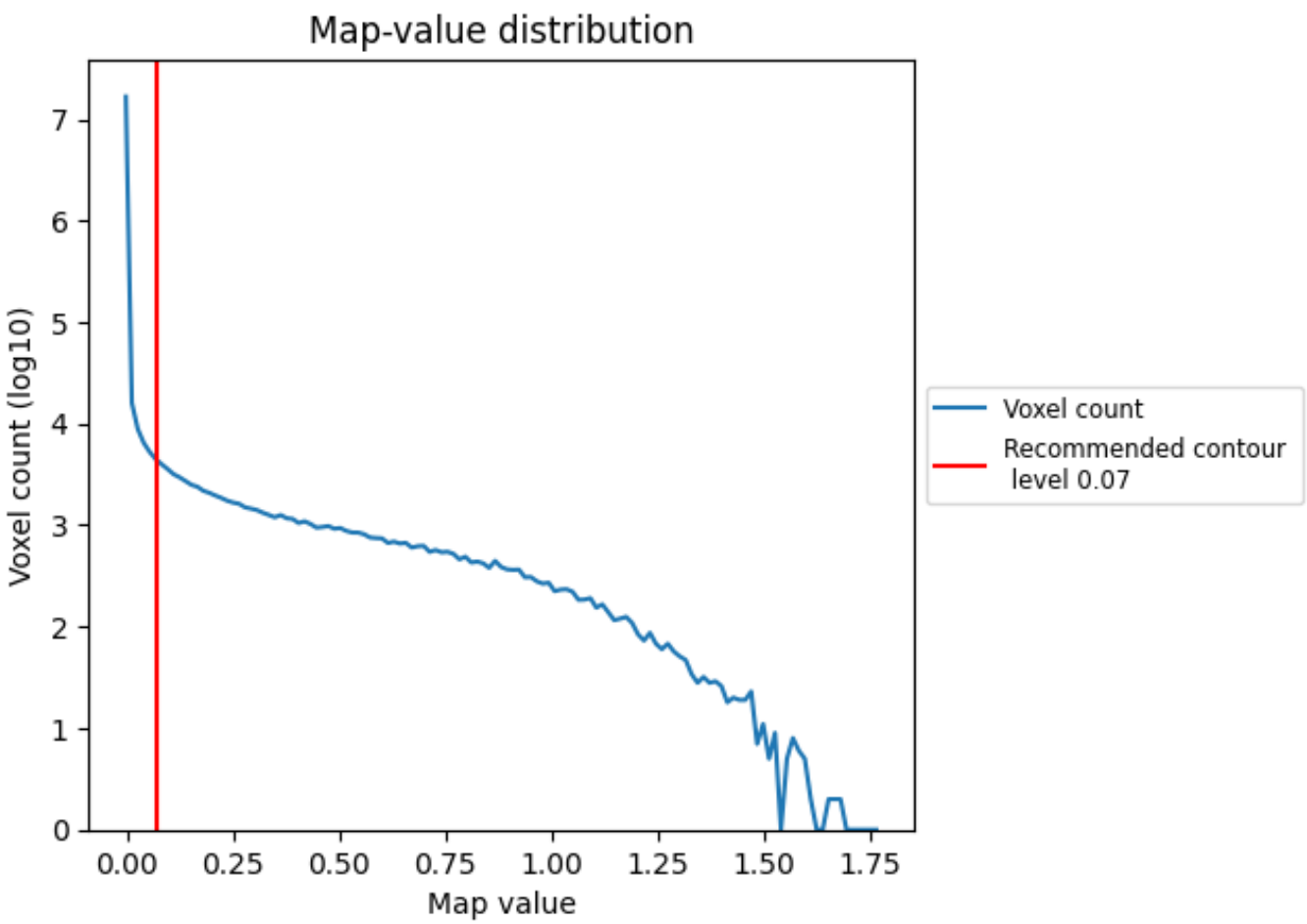
6.6 Mask visualisation (i)

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

7 Map analysis (i)

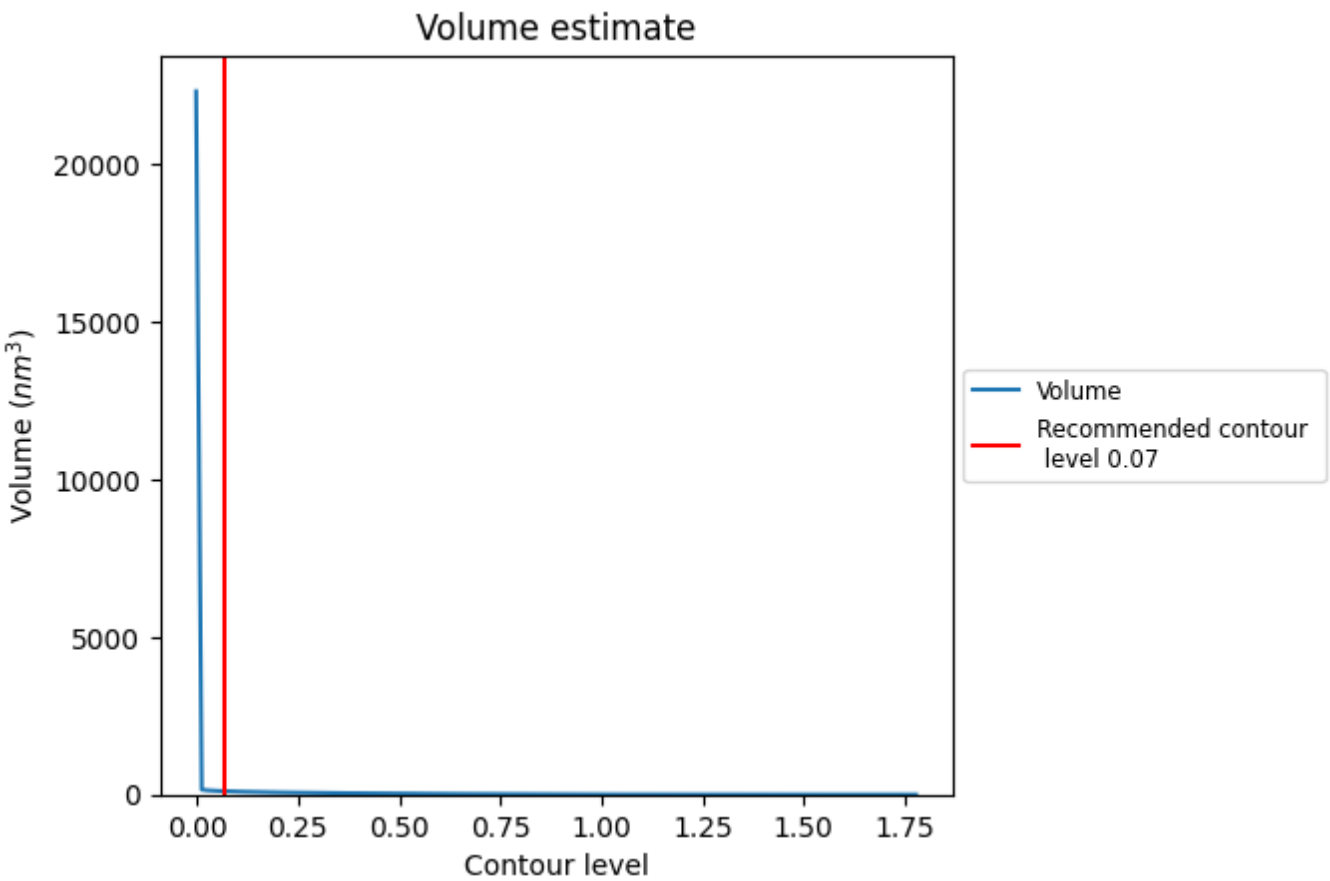
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

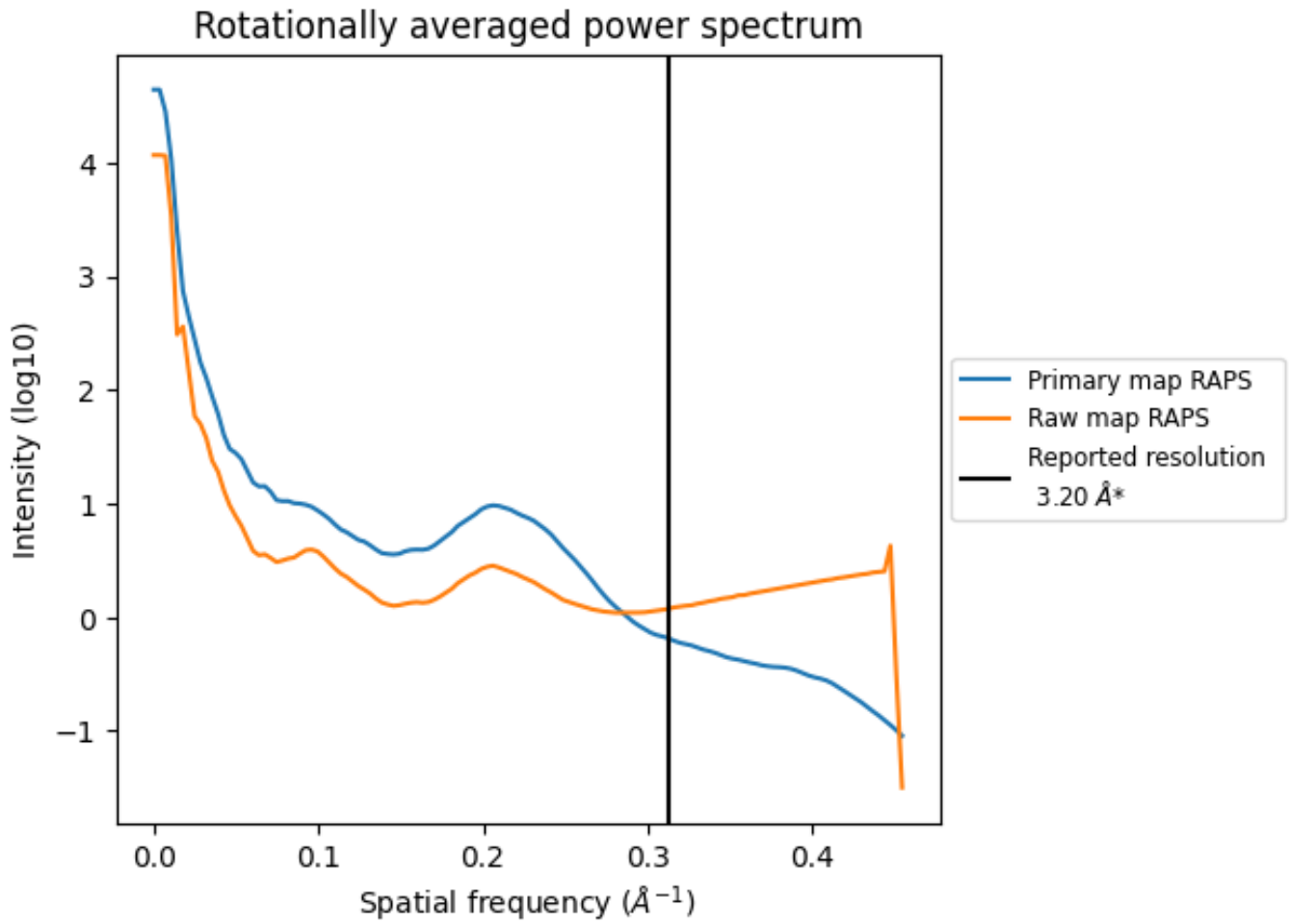
7.2 Volume estimate (i)



The volume at the recommended contour level is 107 nm^3; this corresponds to an approximate mass of 96 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)

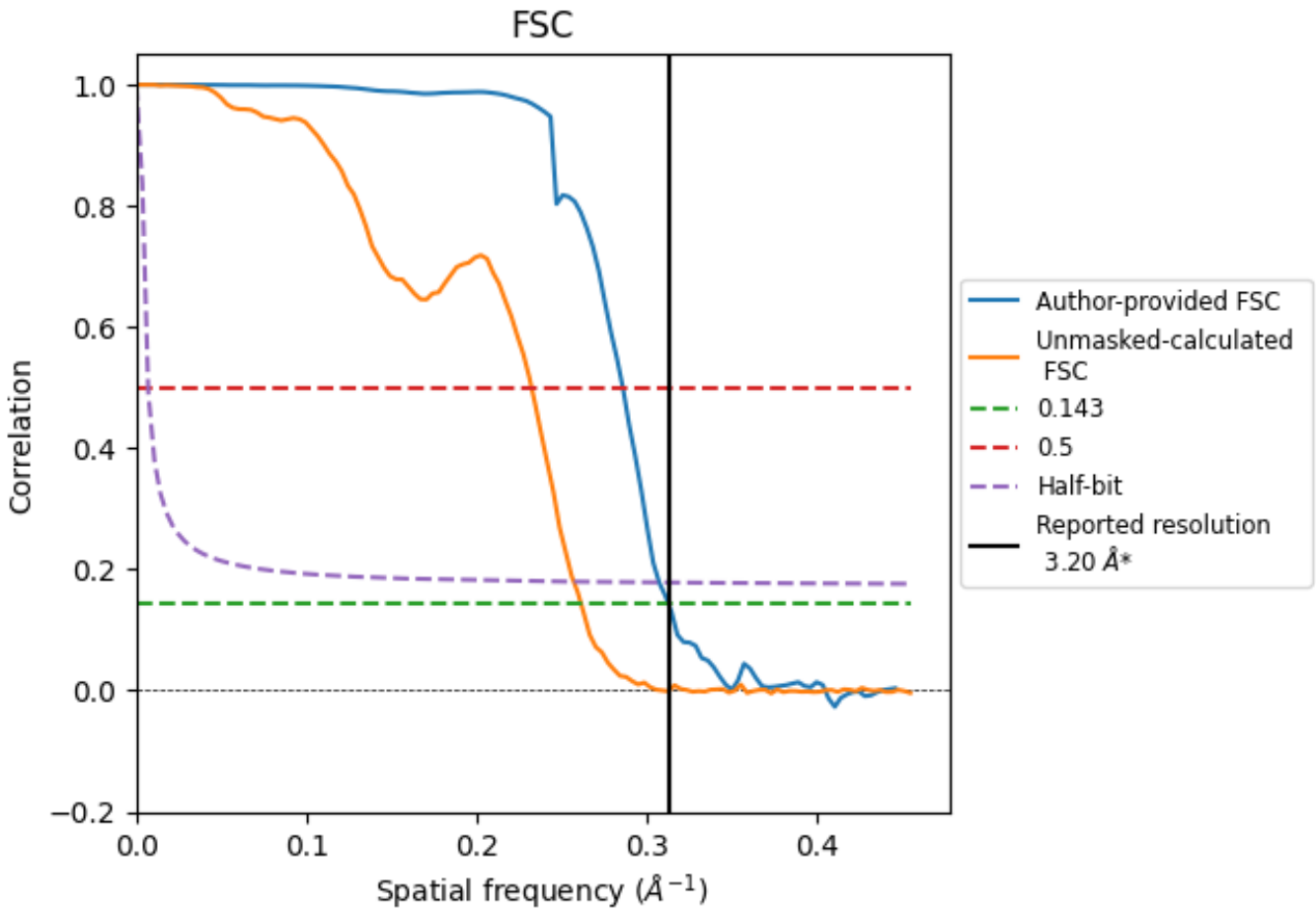


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

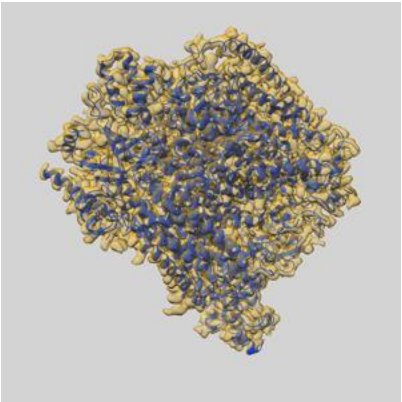
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.20	3.50	3.26
Unmasked-calculated*	3.83	4.31	3.89

*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 3.83 differs from the reported value 3.2 by more than 10 %

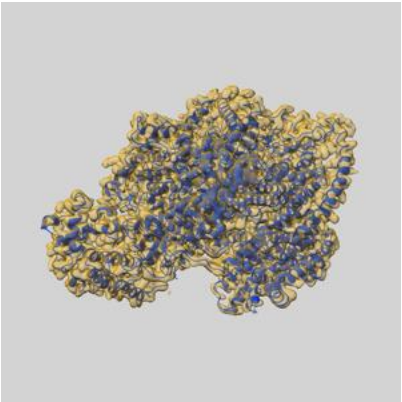
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-42128 and PDB model 8UCJ. Per-residue inclusion information can be found in section 3 on page 10.

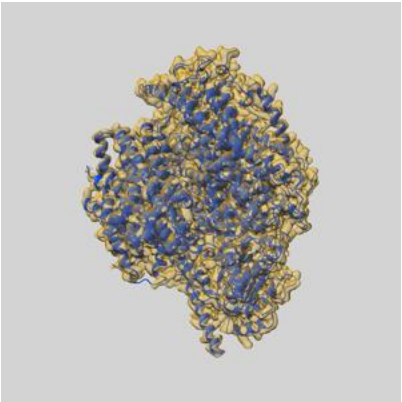
9.1 Map-model overlay (i)



X



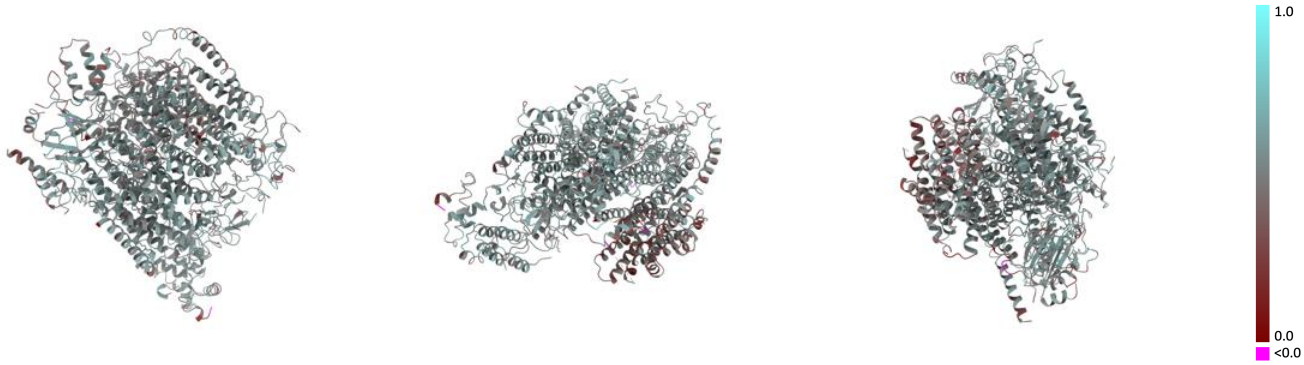
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

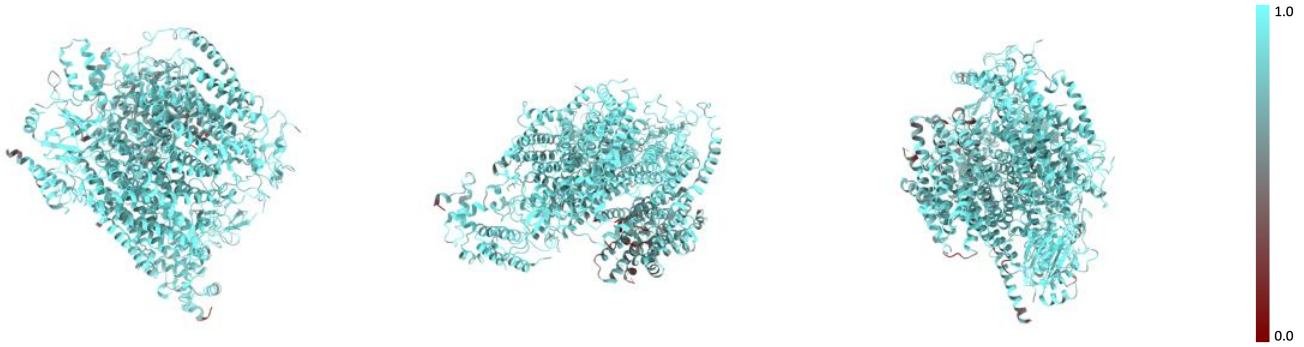
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

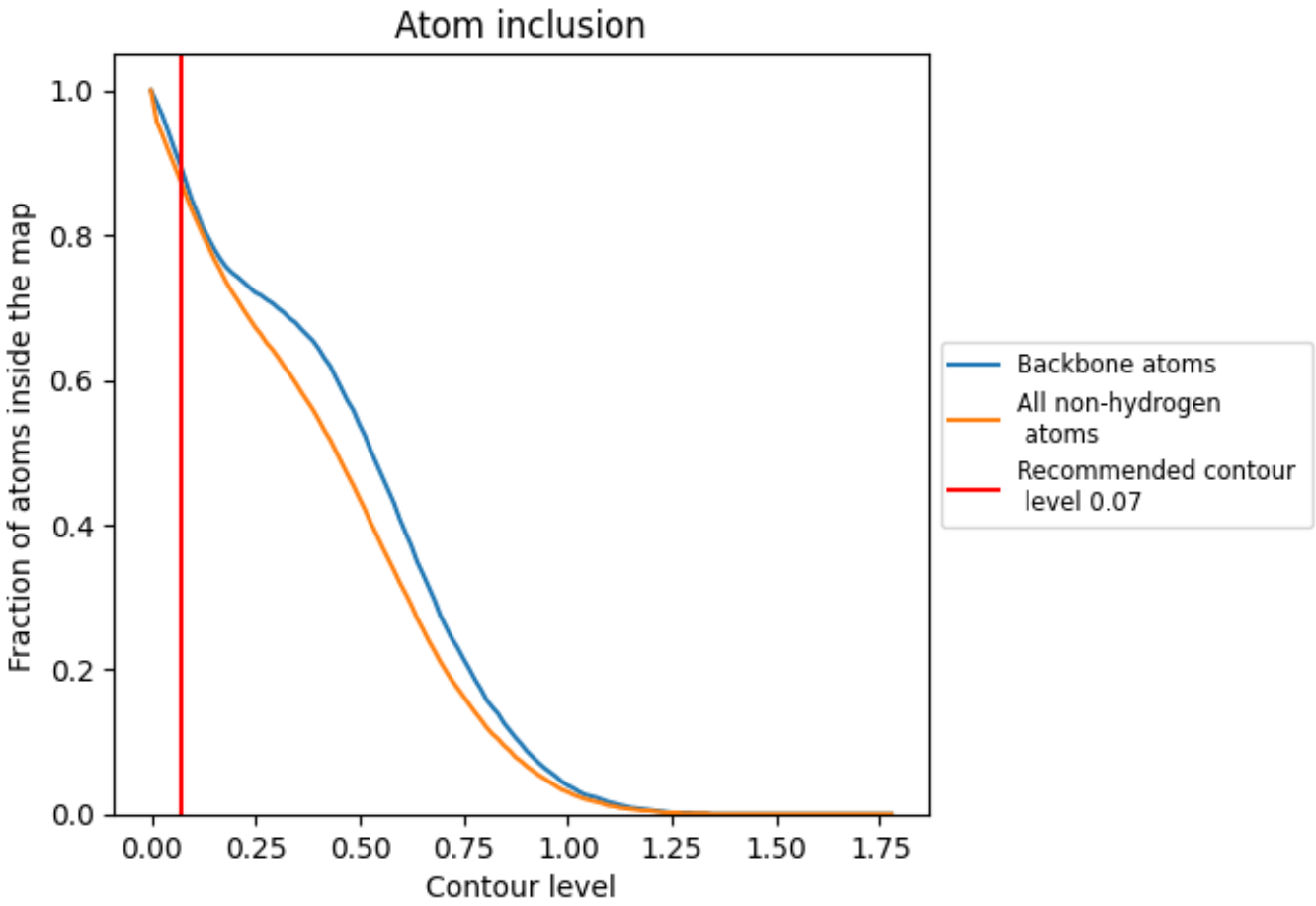
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8740	0.5070
A	0.7560	0.4190
a	0.9240	0.5380
b	0.9010	0.5220
c	0.9180	0.5320
d	0.8920	0.5160
e	0.8430	0.5040
f	0.8800	0.5300
g	0.9100	0.5330
h	0.8910	0.5240
i	0.8440	0.5040
j	0.8630	0.4880
k	0.8260	0.4840