wwPDB EM Validation Summary Report

Nov 23, 2022 – 12:27 pm GMT

PDB ID	:	7ZKQ
EMDB ID	:	EMD-14765
Title	:	Early Pp module assembly intermediate of complex I
Authors	:	Schiller, J.; Laube, E.; Vonck, J.; Zickermann, V.
Deposited on	:	2022-04-13
Resolution	:	3.15 Å(reported)
Based on initial model	:	7O71

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

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

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

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

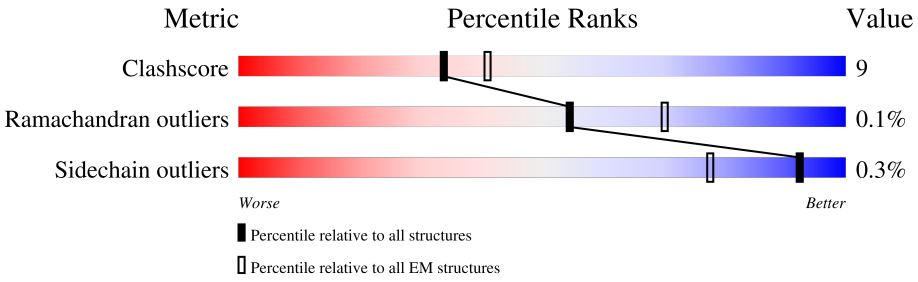
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.15 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	2	469	8% 78% 18% ·
2	b	74	11% 89% 11%
3	A	284	11% 61% 16% 24%
4	C	852	18% 40% 8% 51%
5	T	372	10% 72% 22% · 6%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 12352 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 NADH dehydrogenase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	2	448	3609	2451	525	621	12	0	0

- Molecule 2 is a protein called Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	b	66	502	333	85	84	0	0

- Molecule 3 is a protein called Complex I intermediate-associated protein 30-domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	217	1752	1120	295	331	6	0	0

There are 47 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	238	GLU	-	expression tag	UNP A0A371C5R6
A	239	ASN	-	expression tag	UNP A0A371C5R6
A	240	LEU	-	expression tag	UNP A0A371C5R6
A	241	TYR	-	expression tag	UNP A0A371C5R6
A	242	PHE	-	expression tag	UNP A0A371C5R6
A	243	GLN	-	expression tag	UNP A0A371C5R6
A	244	GLY	-	expression tag	UNP A0A371C5R6
A	245	ALA	-	expression tag	UNP A0A371C5R6
A	246	GLU	-	expression tag	UNP A0A371C5R6
A	247	ALA	-	expression tag	UNP A0A371C5R6
A	248	ALA	-	expression tag	UNP A0A371C5R6
A	249	ALA	-	expression tag	UNP A0A371C5R6
A	250	LYS	-	expression tag	UNP A0A371C5R6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	251	GLU	-	expression tag	UNP A0A371C5R6
A	252	ALA	-	expression tag	UNP A0A371C5R6
A	253	ALA	-	expression tag	UNP A0A371C5R6
A	254	ALA	-	expression tag	UNP A0A371C5R6
A	255	LYS	-	expression tag	UNP A0A371C5R6
A	256	ALA	-	expression tag	UNP A0A371C5R6
A	257	TRP	-	expression tag	UNP A0A371C5R6
A	258	SER	-	expression tag	UNP A0A371C5R6
A	259	HIS	-	expression tag	UNP A0A371C5R6
A	260	PRO	-	expression tag	UNP A0A371C5R6
A	261	GLN	-	expression tag	UNP A0A371C5R6
A	262	PHE	-	expression tag	UNP A0A371C5R6
A	263	GLU	-	expression tag	UNP A0A371C5R6
A	264	LYS	-	expression tag	UNP A0A371C5R6
A	265	GLY	-	expression tag	UNP A0A371C5R6
A	266	GLY	-	expression tag	UNP A0A371C5R6
A	267	GLY	-	expression tag	UNP A0A371C5R6
A	268	SER	-	expression tag	UNP A0A371C5R6
A	269	GLY	-	expression tag	UNP A0A371C5R6
A	270	GLY	-	expression tag	UNP A0A371C5R6
A	271	GLY	-	expression tag	UNP A0A371C5R6
A	272	SER	-	expression tag	UNP A0A371C5R6
A	273	GLY	-	expression tag	UNP A0A371C5R6
A	274	GLY	-	expression tag	UNP A0A371C5R6
A	275	SER	-	expression tag	UNP A0A371C5R6
A	276	ALA	-	expression tag	UNP A0A371C5R6
A	277	TRP	-	expression tag	UNP A0A371C5R6
A	278	SER	-	expression tag	UNP A0A371C5R6
A	279	HIS	-	expression tag	UNP A0A371C5R6
A	280	PRO	-	expression tag	UNP A0A371C5R6
A	281	GLN	-	expression tag	UNP A0A371C5R6
A	282	PHE	-	expression tag	UNP A0A371C5R6
A	283	GLU	-	expression tag	UNP A0A371C5R6
A	284	LYS	-	expression tag	UNP A0A371C5R6

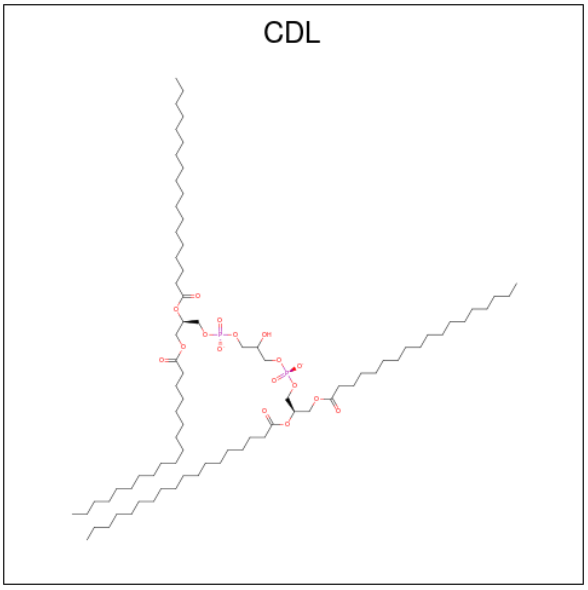
- Molecule 4 is a protein called complex I assembly factor CIA84.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	416	Total	C	N	O	S	0	0
			3396	2153	577	649	17		

- Molecule 5 is a protein called Tafazzin family protein.

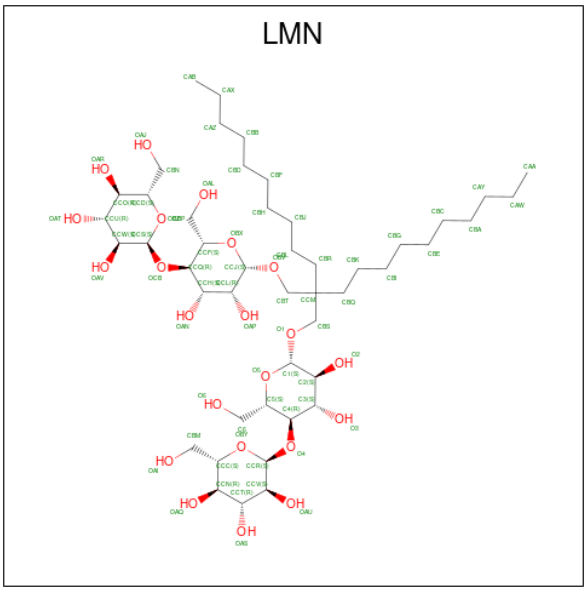
Mol	Chain	Residues	Atoms					AltConf	Trace
5	T	351	Total	C	N	O	S	0	0
			2844	1825	504	498	17		

- Molecule 6 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



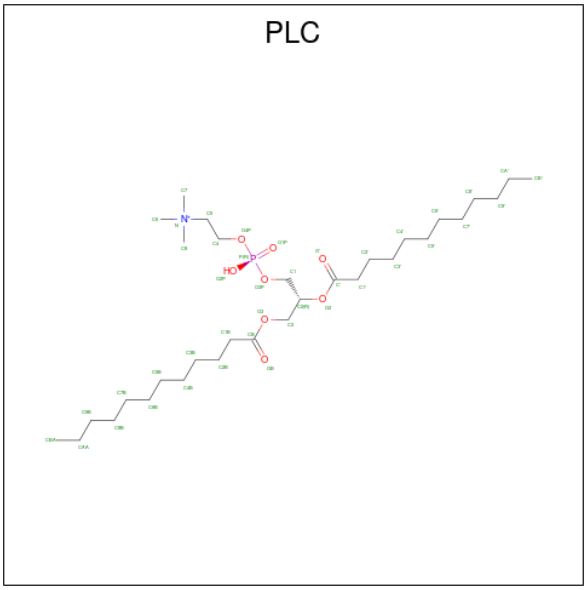
Mol	Chain	Residues	Atoms				AltConf
6	b	1	Total	C	O	P	0
			81	63	16	2	
6	T	1	Total	C	O	P	0
			57	39	16	2	

- Molecule 7 is Lauryl Maltose Neopentyl Glycol (three-letter code: LMN) (formula: $C_{47}H_{88}O_{22}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
7	C	1	69	47	22	0

- Molecule 8 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula: $C_{32}H_{65}NO_8P$).



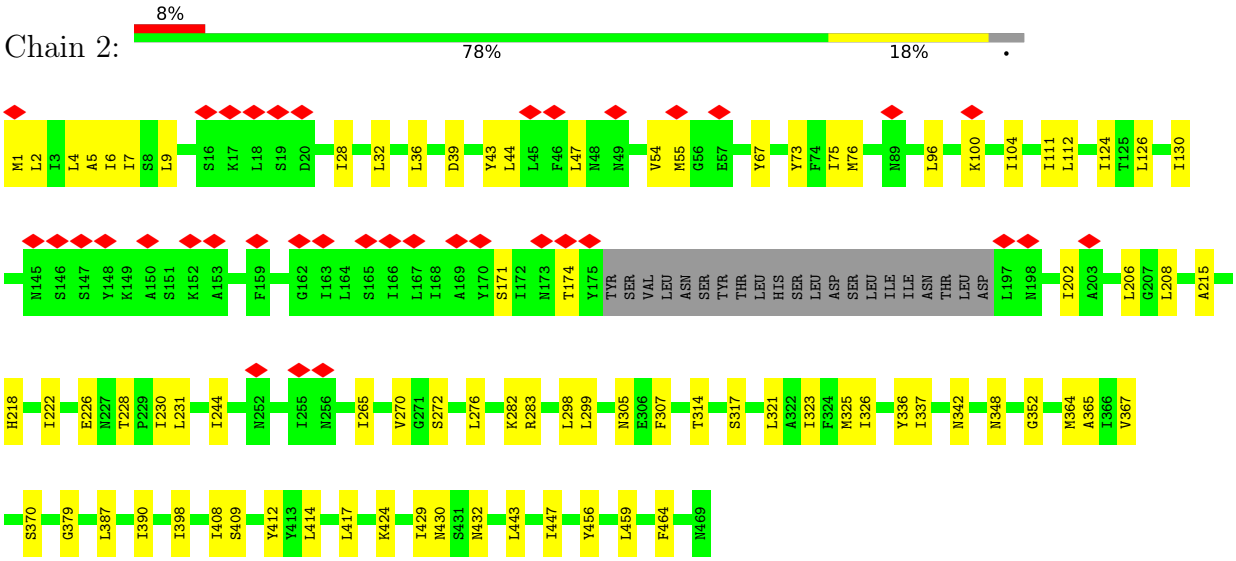
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
8	T	1	42	32	1	8	1	0

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.

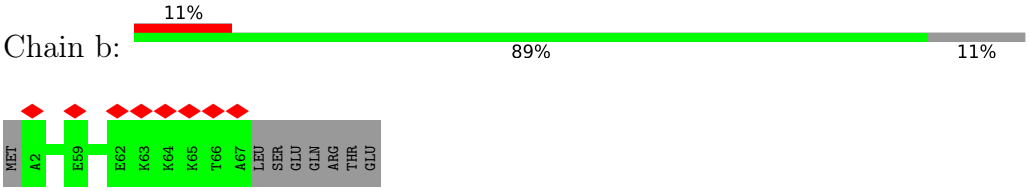
• Molecule 1: NADH dehydrogenase subunit 2

Chain 2:



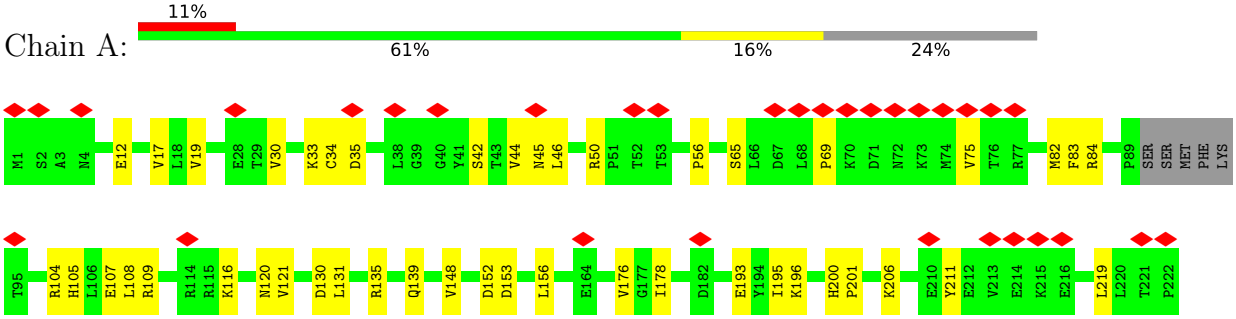
• Molecule 2: Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I)

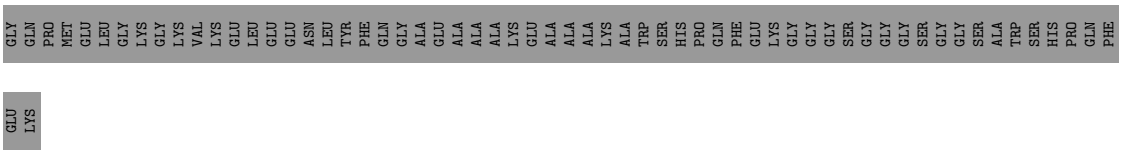
Chain b:



• Molecule 3: Complex I intermediate-associated protein 30-domain-containing protein

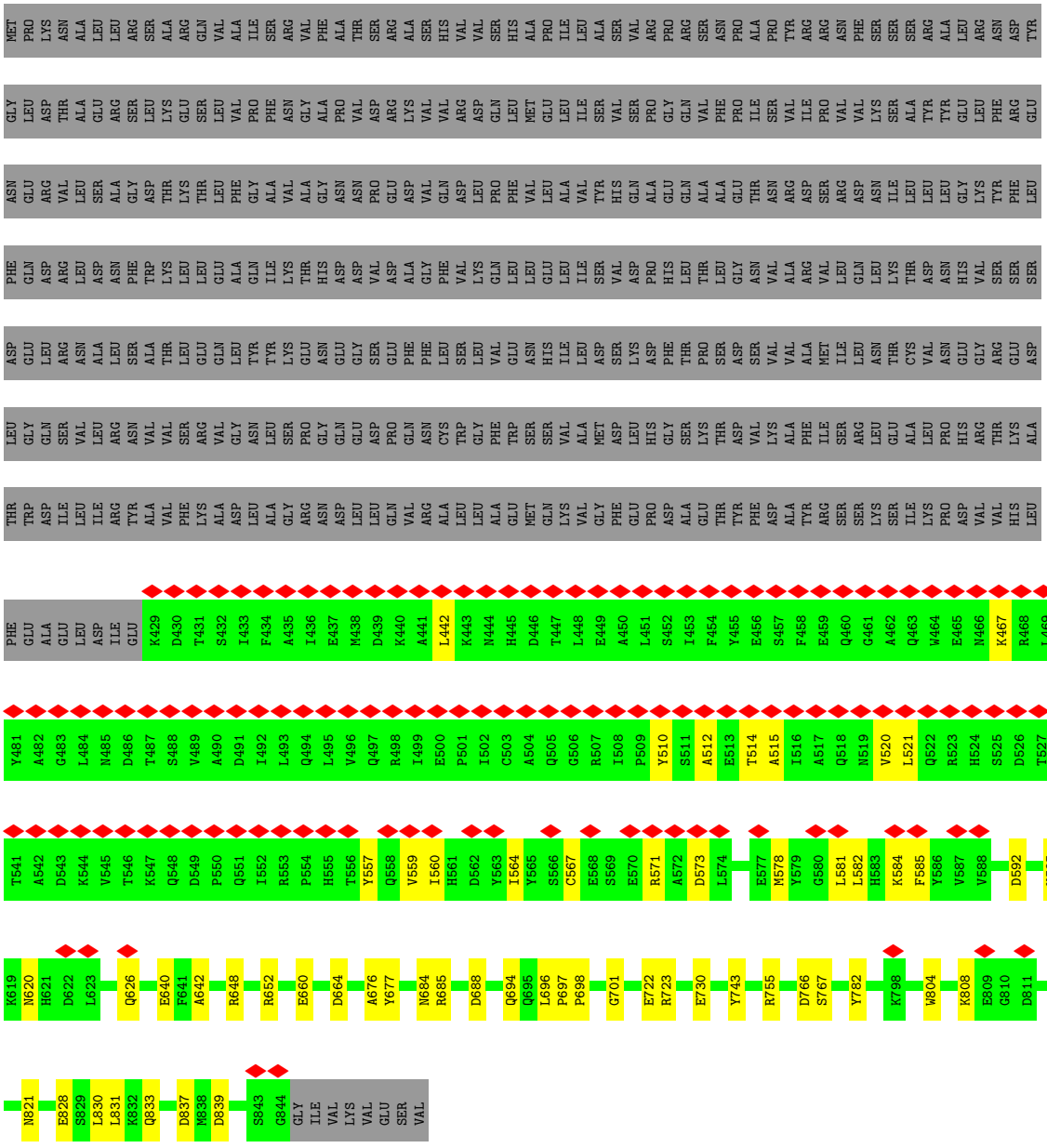
Chain A:





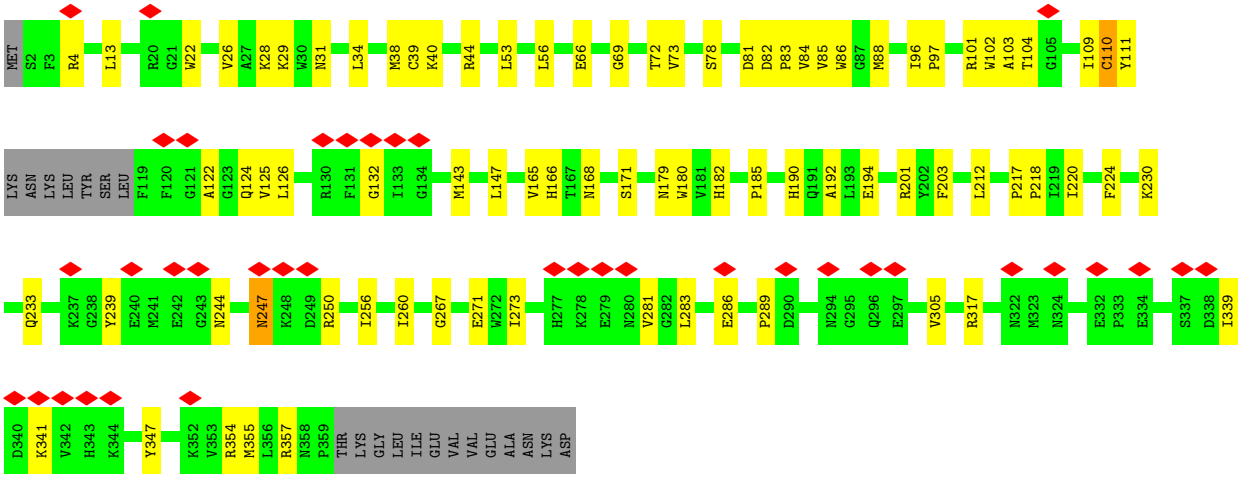
• Molecule 4: complex I assembly factor CIA84

Chain C:



• Molecule 5: Tafazzin family protein

Chain T:


MET S2 F3 R4 L13 R20 G21 W22 V26 A27 K28 K29 W30 N31 L34 M38 C39 K40 R44 L53 L56 E66 G69 T72 V73 S78 D81 D82 P83 V84 V85 W86 G87 M88 I96 P97 R101 W102 A103 T104 G105 I109 C110 Y111
LYS ASN LYS LEU TYR SER LEU F119 F120 G121 A122 G123 Q124 V125 L126 R130 F131 G132 I133 G134 M143 L147 V165 H166 T167 N168 S171 N179 W180 V181 H182 P185 H190 Q191 A192 L193 E194 R201 Y202 F203 L212 P217 P218 I219 I220 F224 K230
Q233 K237 G238 Y239 E240 M241 E242 G243 N244 N247 K248 D249 R250 I256 I260 G267 E271 W272 I273 H277 K278 E279 N280 V281 G282 L283 E286 P289 D290 N294 G295 Q296 E297 V305 R317 N322 M323 N324 E332 P333 E334 S337 D338 I339
D340 K341 V342 H343 K344 Y347 K352 V353 R354 M355 L356 R357 N358 P359 THR LYS GLY LEU ILE GLU VAL VAL GLU ALA ASN LYS ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	376810	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.681	Depositor
Minimum map value	-3.084	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.102	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	251.09967, 251.09967, 251.09967	wwPDB
Map dimensions	208, 208, 208	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.20721, 1.20721, 1.20721	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FME, CDL, PLC, LMN

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	2	0.27	0/3675	0.43	0/5005
2	b	0.26	0/515	0.41	0/696
3	A	0.29	0/1793	0.55	0/2439
4	C	0.25	0/3471	0.45	0/4700
5	T	0.26	0/2925	0.50	0/3965
All	All	0.27	0/12379	0.47	0/16805

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	3609	0	3838	56	0
2	b	502	0	521	0	0
3	A	1752	0	1740	33	0
4	C	3396	0	3296	42	0
5	T	2844	0	2814	79	0
6	T	57	0	64	2	0
6	b	81	0	121	0	0
7	C	69	0	88	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	T	42	0	64	9	0
All	All	12352	0	12546	203	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 9.

The worst 5 of 203 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)
5:T:102:TRP:CD1	5:T:147:LEU:CD2	2.34	1.11
5:T:102:TRP:CD1	5:T:147:LEU:HD22	1.85	1.11
8:T:401:PLC:H11	8:T:401:PLC:H41	1.37	1.06
5:T:102:TRP:CE3	5:T:124:GLN:HG2	1.93	1.02
5:T:102:TRP:HD1	5:T:147:LEU:HD22	1.30	0.96

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	2	444/469 (95%)	435 (98%)	9 (2%)	0	100	100
2	b	64/74 (86%)	63 (98%)	1 (2%)	0	100	100
3	A	213/284 (75%)	202 (95%)	11 (5%)	0	100	100
4	C	414/852 (49%)	404 (98%)	10 (2%)	0	100	100
5	T	347/372 (93%)	333 (96%)	13 (4%)	1 (0%)	41	73
All	All	1482/2051 (72%)	1437 (97%)	44 (3%)	1 (0%)	54	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	T	110	CYS

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	2	411/432 (95%)	411 (100%)	0	100 100
2	b	51/59 (86%)	51 (100%)	0	100 100
3	A	194/240 (81%)	193 (100%)	1 (0%)	88 95
4	C	365/745 (49%)	364 (100%)	1 (0%)	92 97
5	T	306/326 (94%)	304 (99%)	2 (1%)	84 93
All	All	1327/1802 (74%)	1323 (100%)	4 (0%)	92 97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	152	ASP
4	C	648	ARG
5	T	31	ASN
5	T	247	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	200	HIS
5	T	190	HIS
5	T	247	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	FME	2	1	1	8,9,10	0.94	0	7,9,11	0.90	0

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
1	FME	2	1	1	-	5/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	1	FME	O1-CN-N-CA
1	2	1	FME	C-CA-CB-CG
1	2	1	FME	O-C-CA-CB
1	2	1	FME	CA-CB-CG-SD
1	2	1	FME	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	1	FME	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	PLC	T	401	-	41,41,41	0.33	0	47,49,49	0.36	0
6	CDL	T	402	-	56,56,99	0.36	0	61,67,111	0.40	0
7	LMN	C	901	-	72,72,72	1.52	10 (13%)	96,98,98	0.92	2 (2%)
6	CDL	b	101	-	80,80,99	0.30	0	85,91,111	0.35	0

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
8	PLC	T	401	-	-	14/45/45/45	-
6	CDL	T	402	-	-	20/65/65/110	-
7	LMN	C	901	-	-	27/50/130/130	0/4/4/4
6	CDL	b	101	-	-	59/89/89/110	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	901	LMN	CBQ-CCM	4.45	1.62	1.54
7	C	901	LMN	CBR-CCM	4.11	1.61	1.54
7	C	901	LMN	CBS-CCM	3.84	1.62	1.53
7	C	901	LMN	CBT-CCM	3.20	1.60	1.53
7	C	901	LMN	O5-C1	3.14	1.49	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	901	LMN	CCS-OCB-CCQ	-3.32	109.75	117.96
7	C	901	LMN	CCR-O4-C4	-2.44	111.94	117.96

There are no chirality outliers.

5 of 120 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	b	101	CDL	O1-C1-CB2-OB2
6	b	101	CDL	CA2-C1-CB2-OB2
6	b	101	CDL	CA2-OA2-PA1-OA4
6	b	101	CDL	CA3-OA5-PA1-OA3
6	b	101	CDL	C11-CA5-OA6-CA4

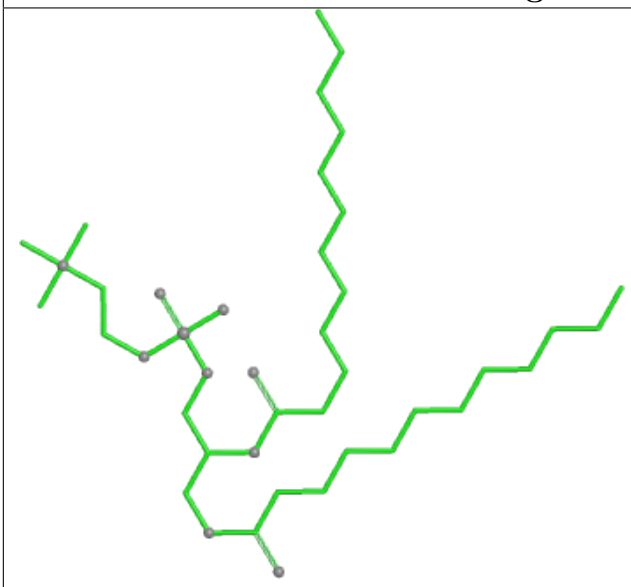
There are no ring outliers.

3 monomers are involved in 13 short contacts:

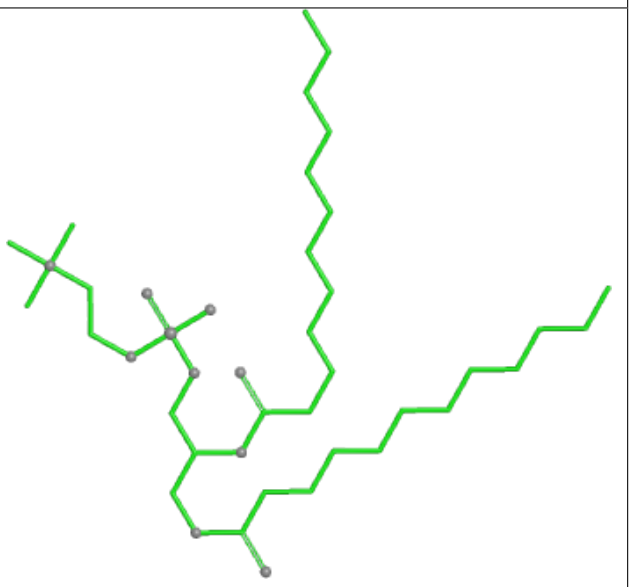
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	T	401	PLC	9	0
6	T	402	CDL	2	0
7	C	901	LMN	3	0

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.

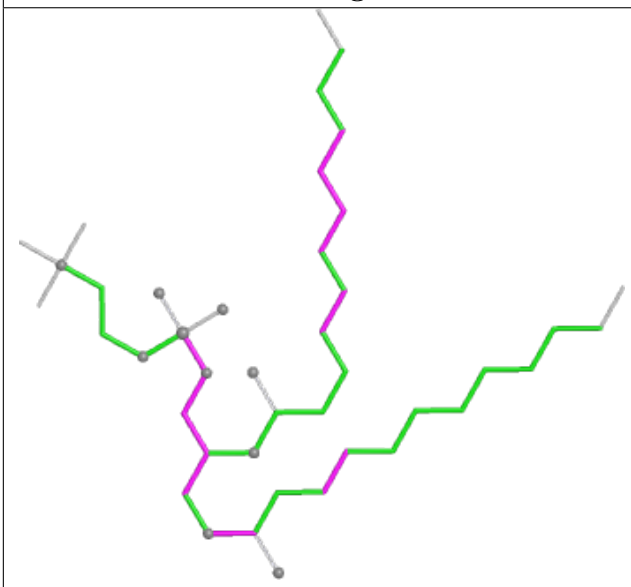
Ligand PLC T 401



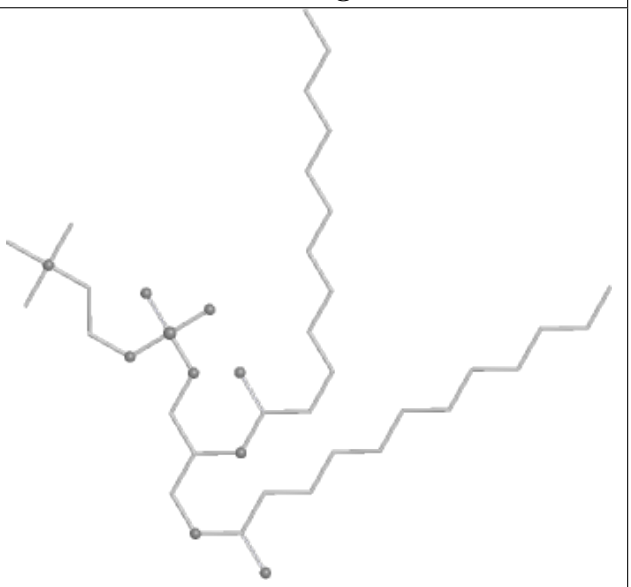
Bond lengths



Bond angles

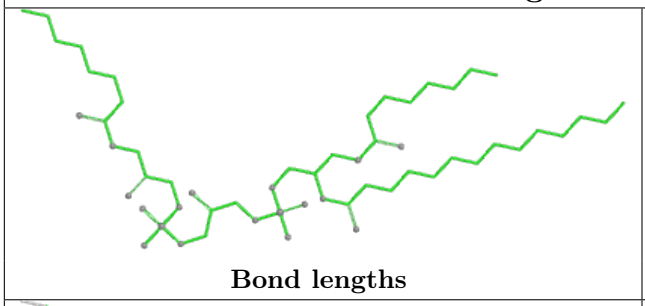


Torsions

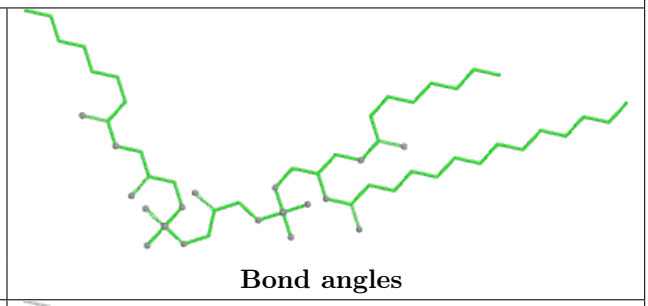


Rings

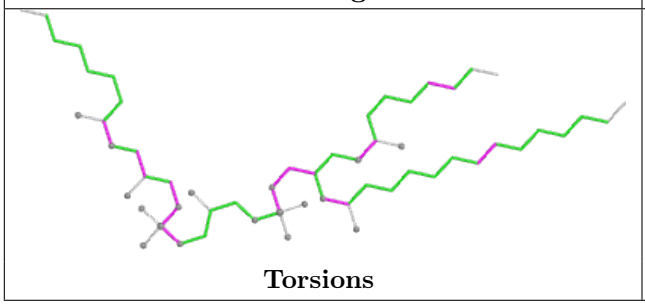
Ligand CDL T 402



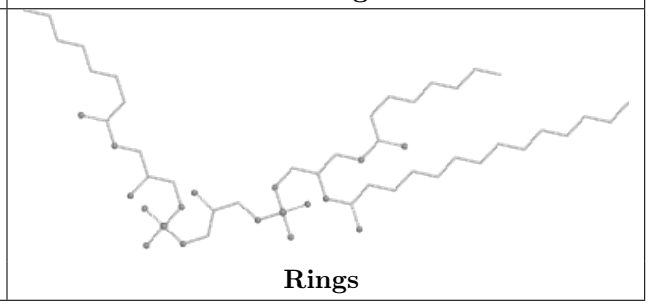
Bond lengths



Bond angles

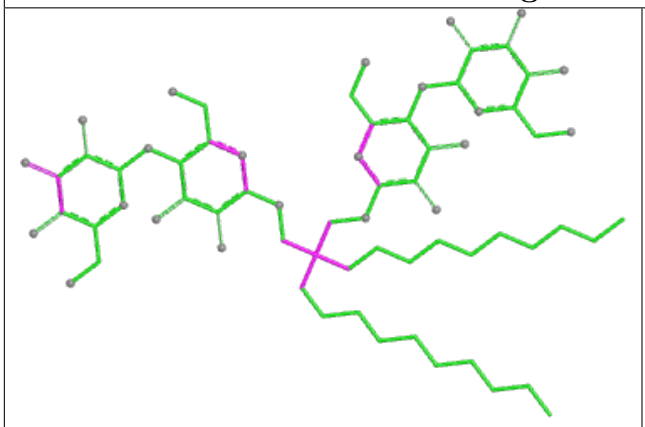


Torsions

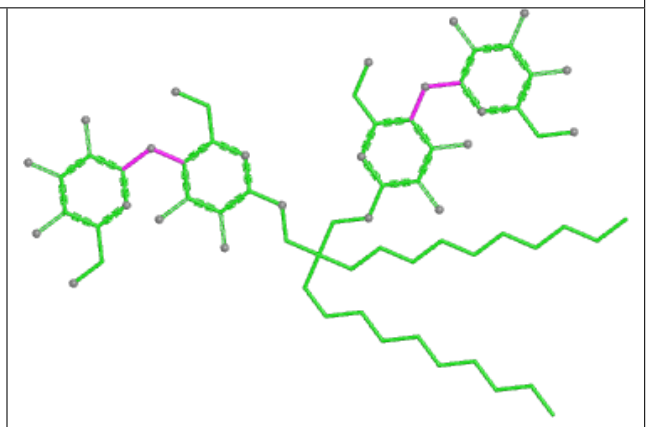


Rings

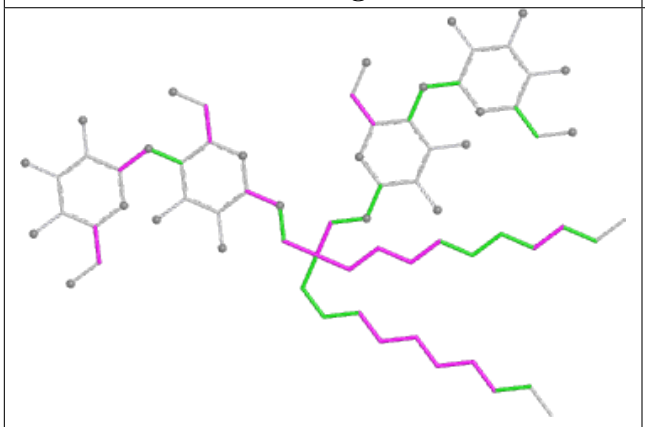
Ligand LMN C 901



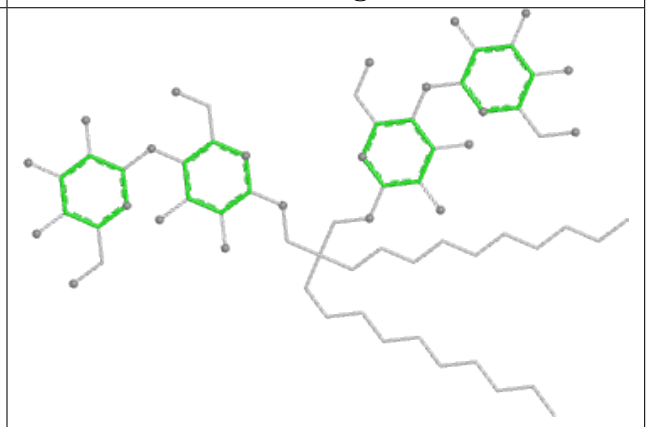
Bond lengths



Bond angles

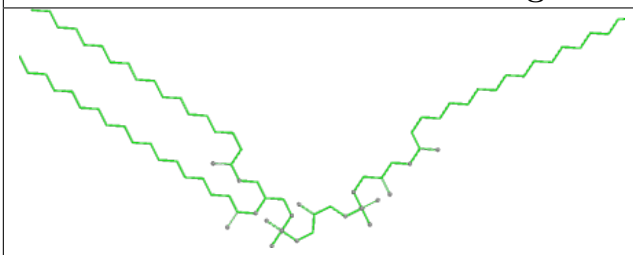


Torsions

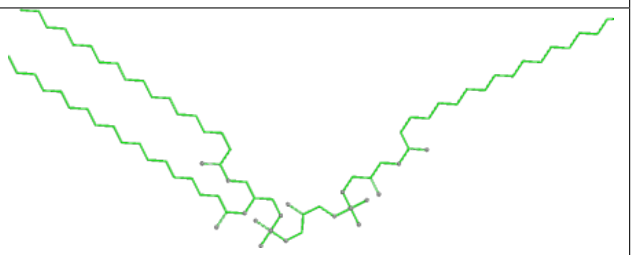


Rings

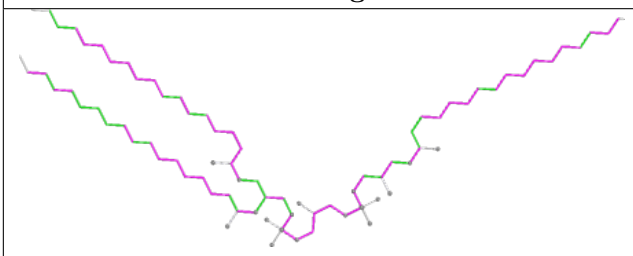
Ligand CDL b 101



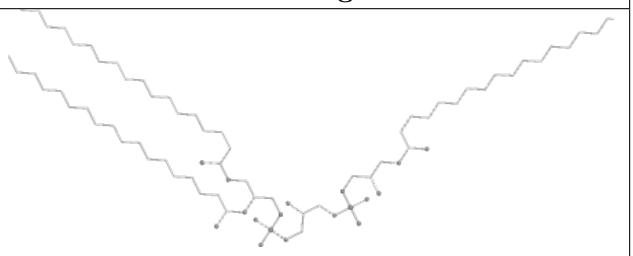
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

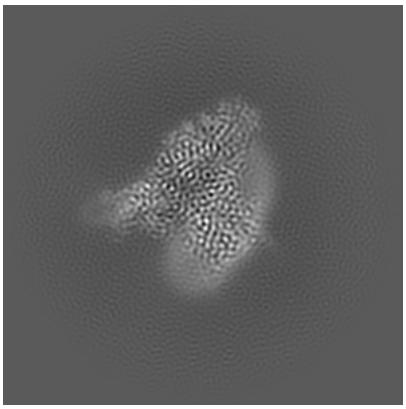
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14765. These allow visual inspection of the internal detail of the map and identification of artifacts.

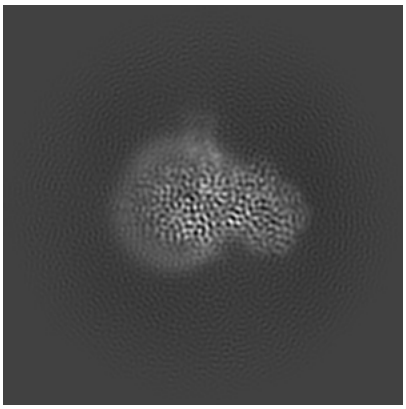
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

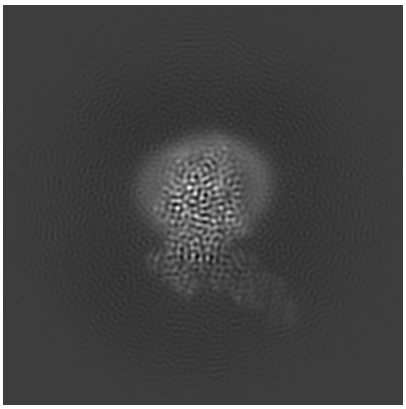
6.1.1 Primary map



X

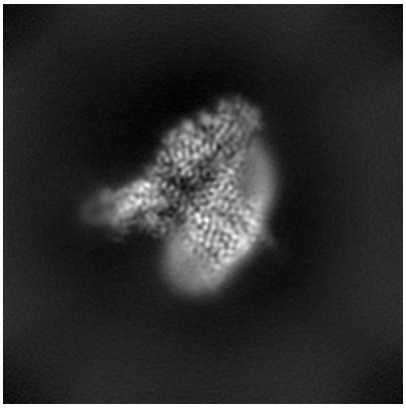


Y

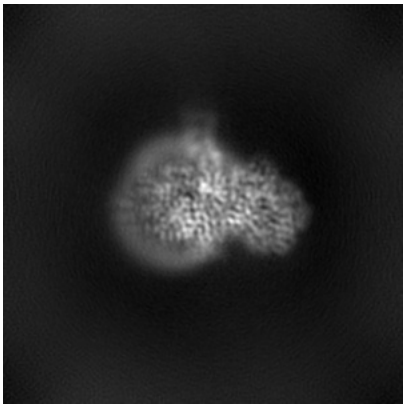


Z

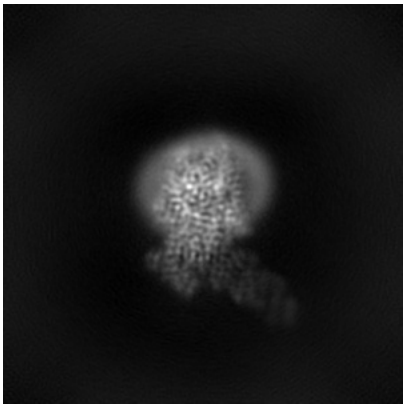
6.1.2 Raw map



X



Y

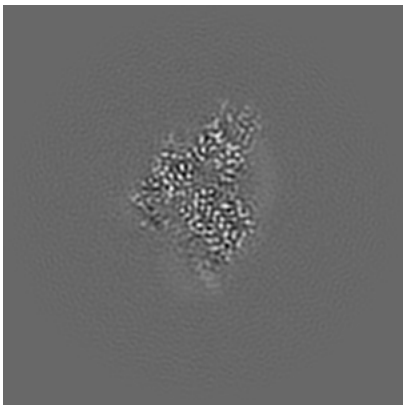


Z

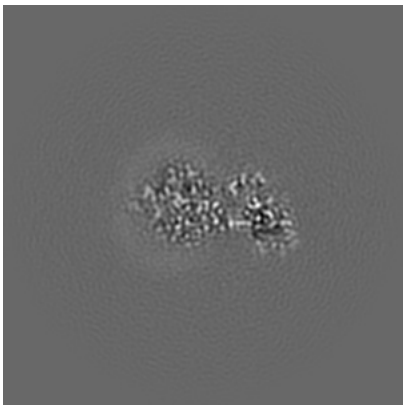
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

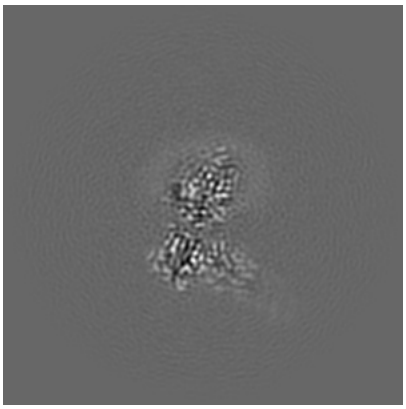
6.2.1 Primary map



X Index: 104

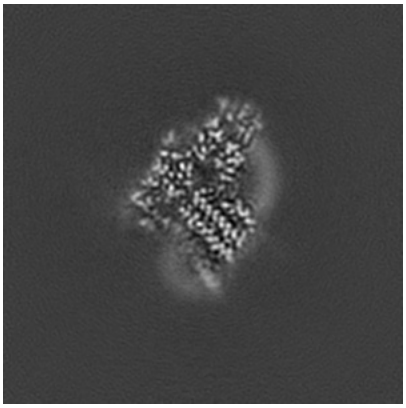


Y Index: 104

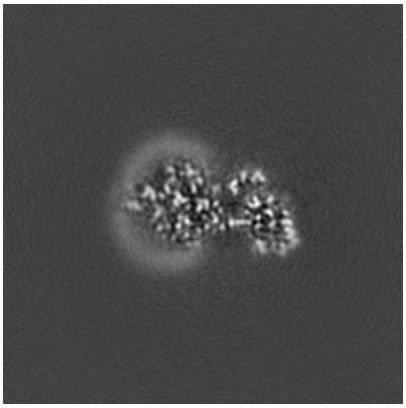


Z Index: 104

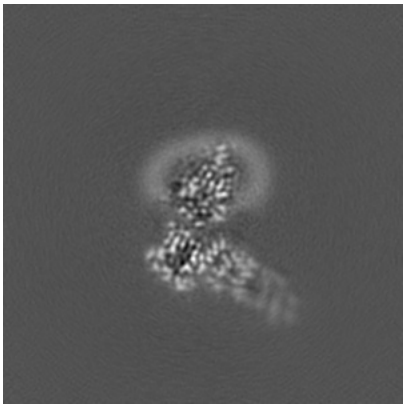
6.2.2 Raw map



X Index: 104



Y Index: 104

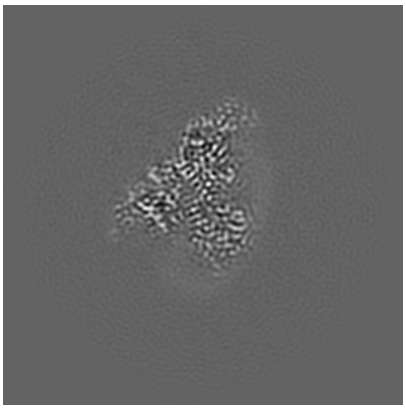


Z Index: 104

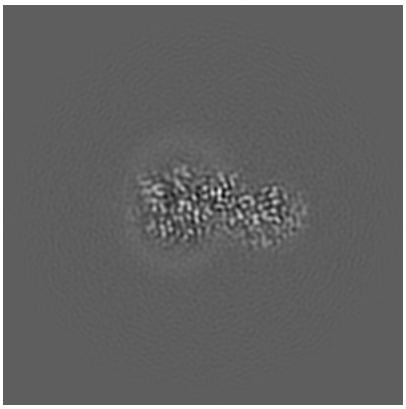
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

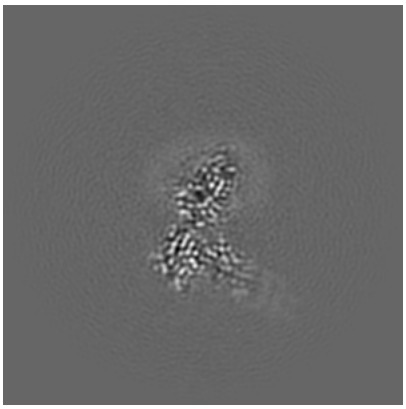
6.3.1 Primary map



X Index: 95

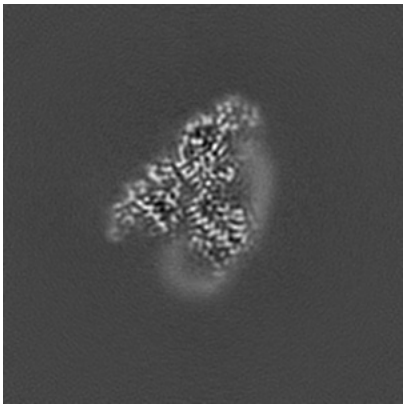


Y Index: 113

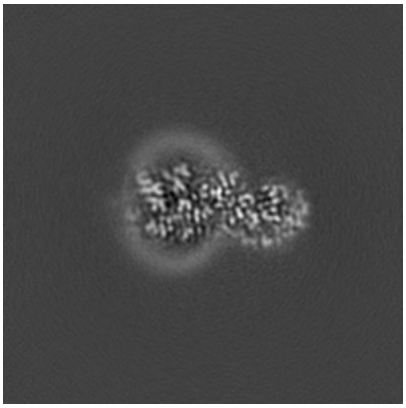


Z Index: 105

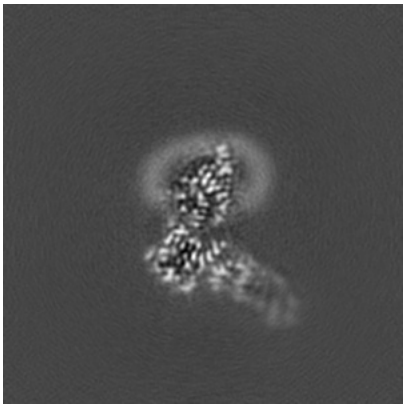
6.3.2 Raw map



X Index: 95



Y Index: 113



Z Index: 103

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

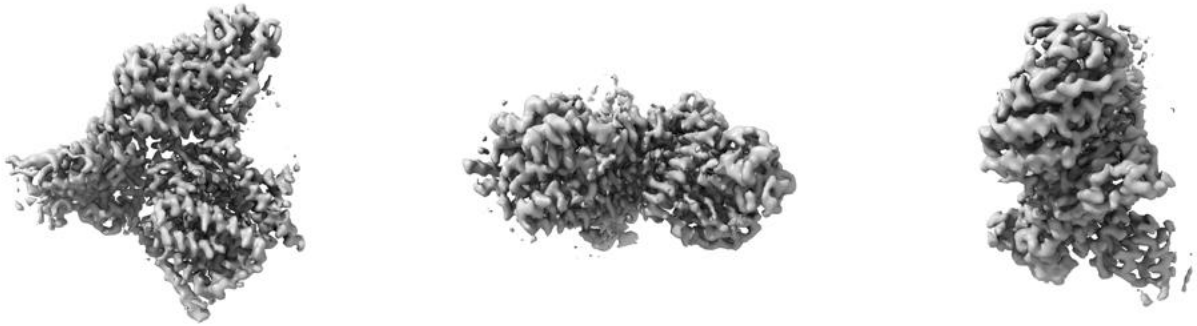
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

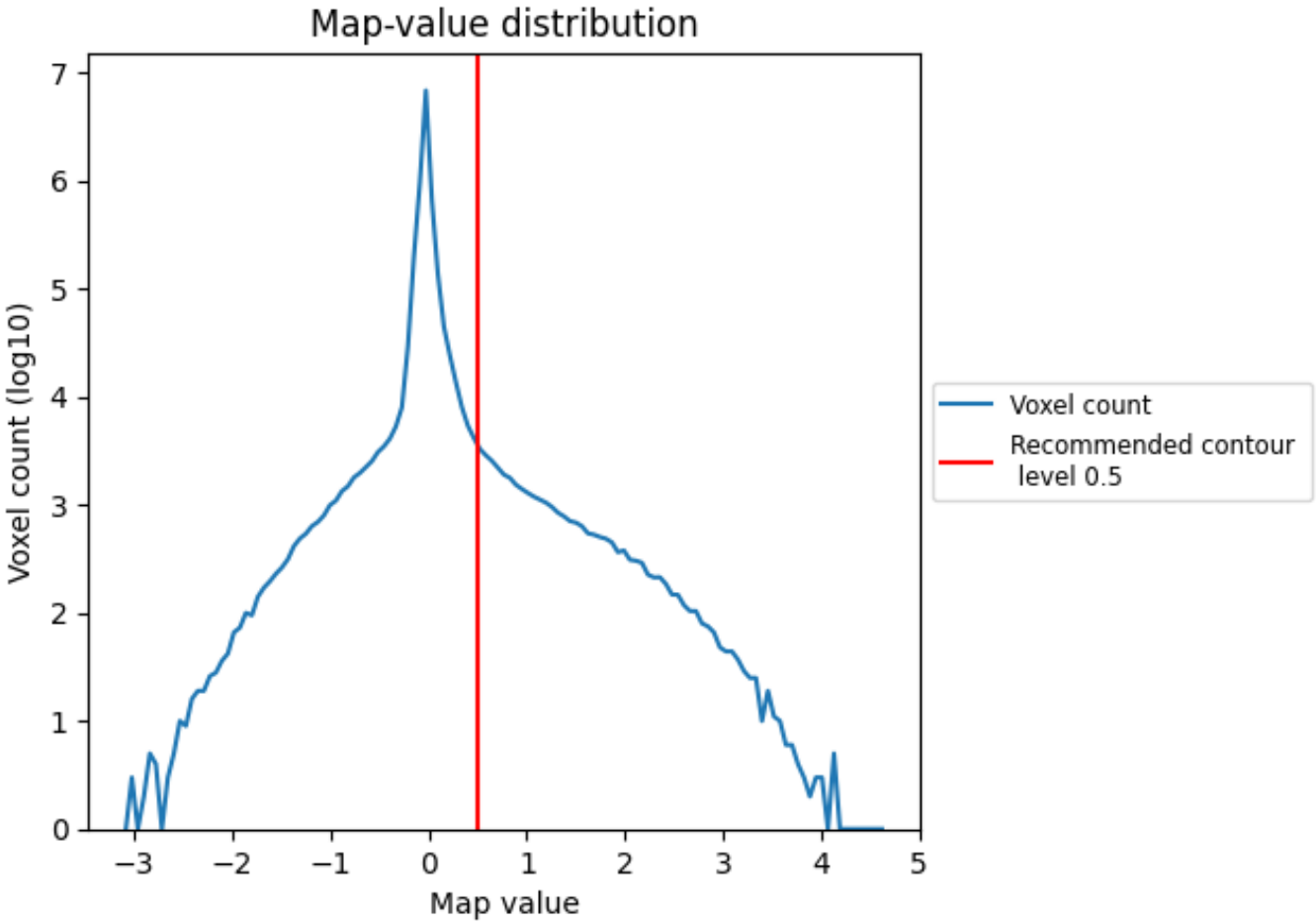
6.5 Mask visualisation (i)

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

7 Map analysis

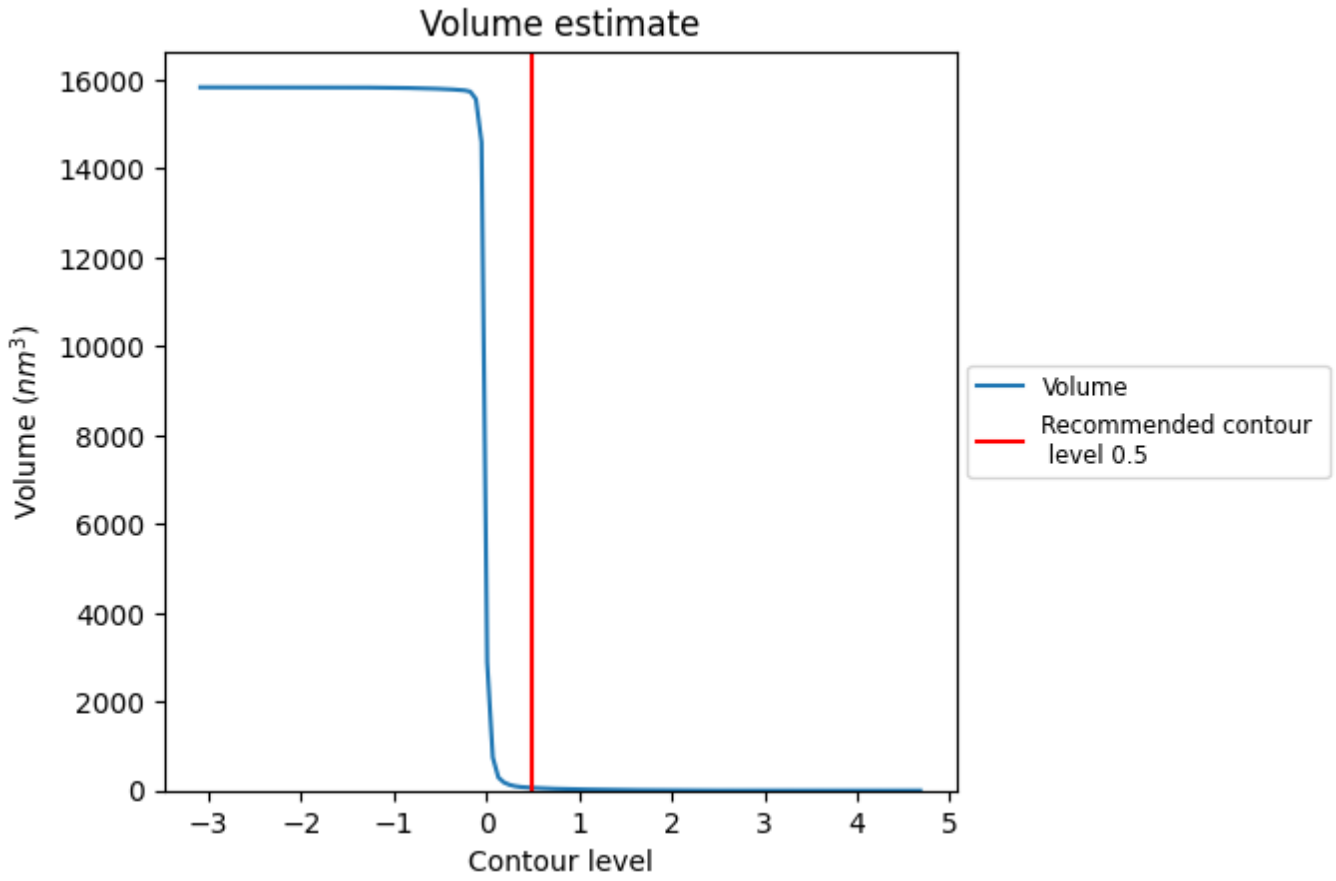
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

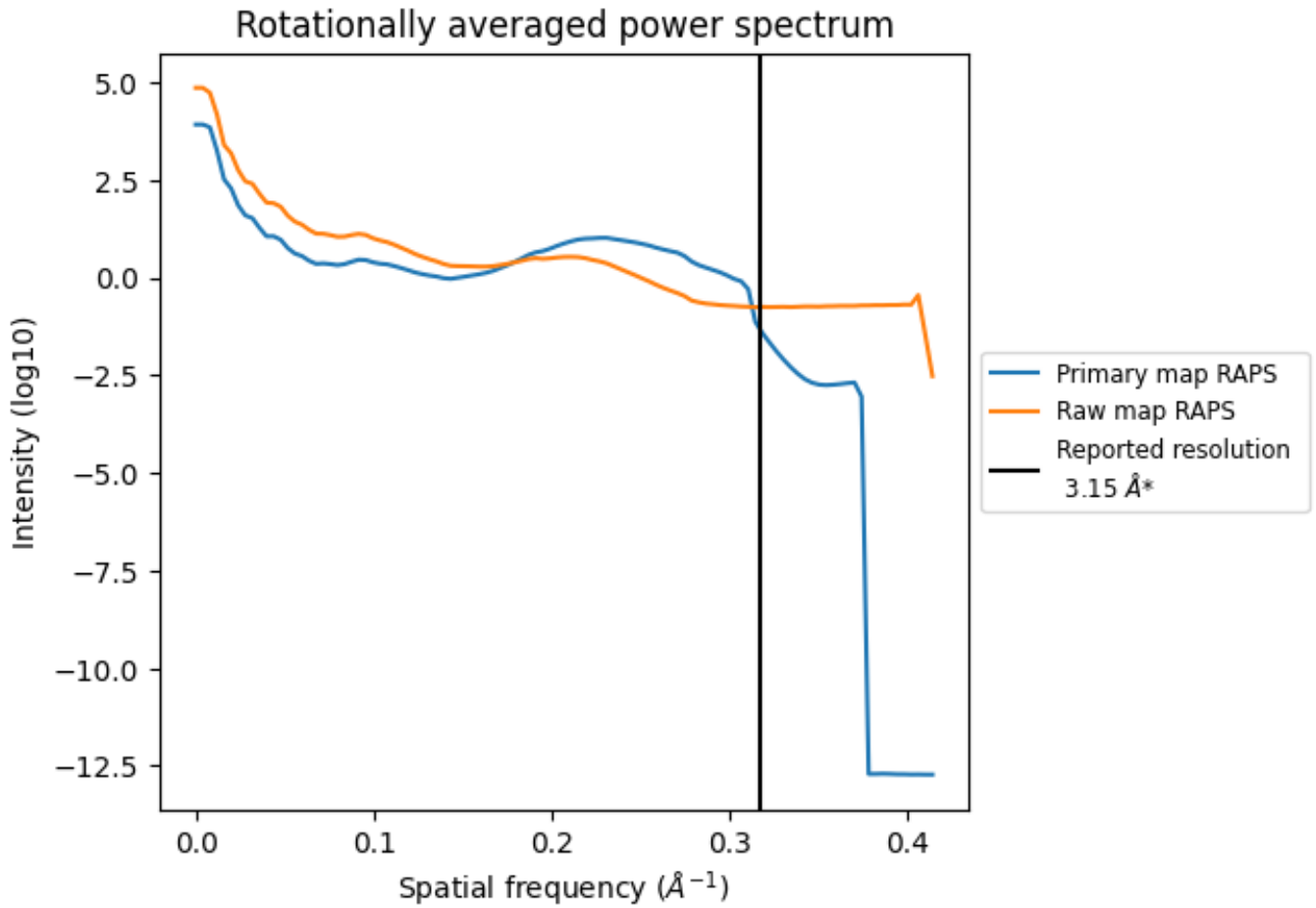
7.2 Volume estimate (i)



The volume at the recommended contour level is 61 nm^3; this corresponds to an approximate mass of 55 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)

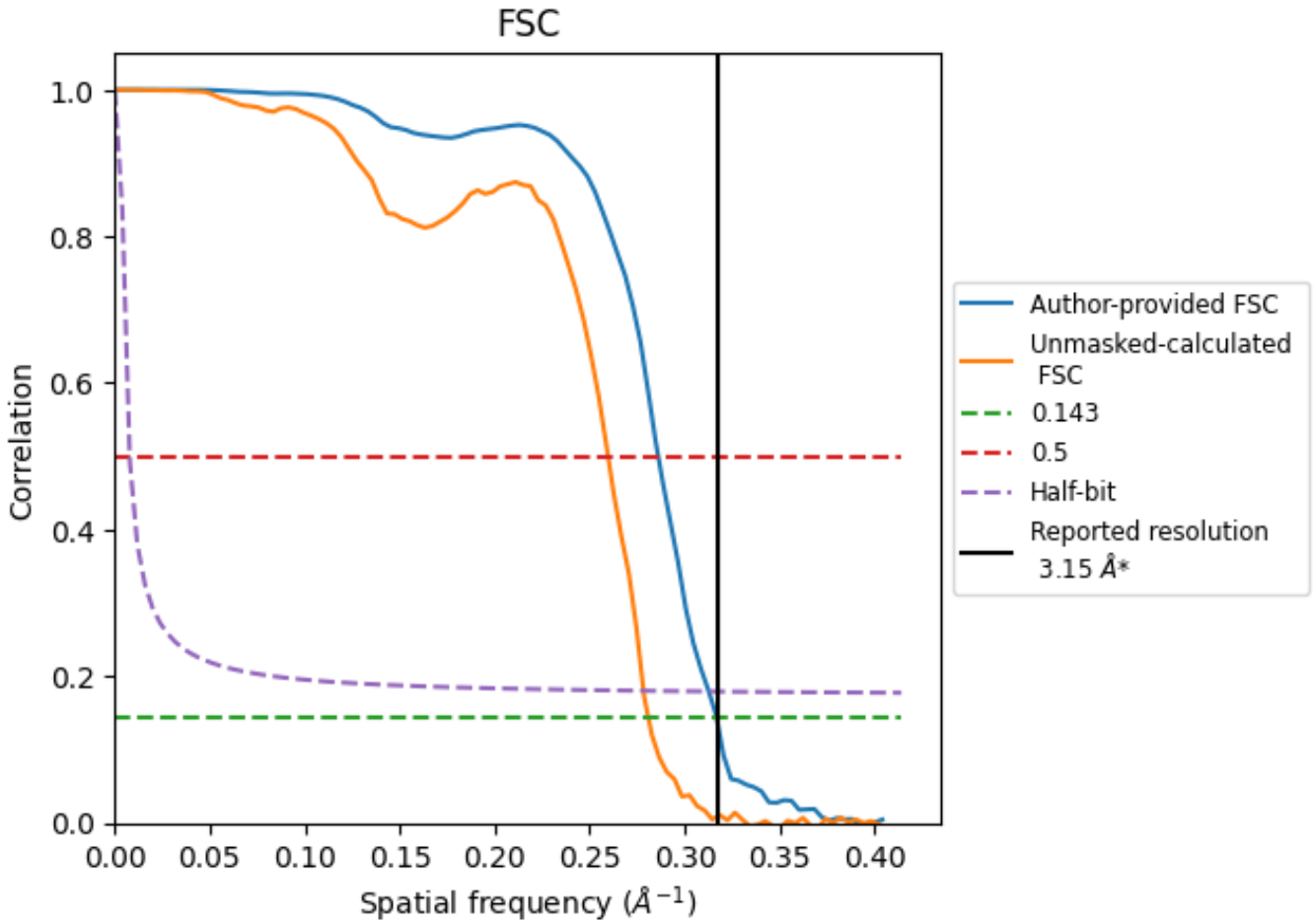


*Reported resolution corresponds to spatial frequency of 0.317 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.317 Å^{-1}

8.2 Resolution estimates (i)

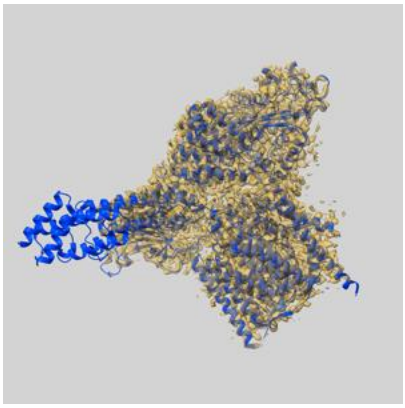
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.15	-	-
Author-provided FSC curve	3.16	3.49	3.20
Unmasked-calculated*	3.56	3.85	3.59

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.56 differs from the reported value 3.15 by more than 10 %

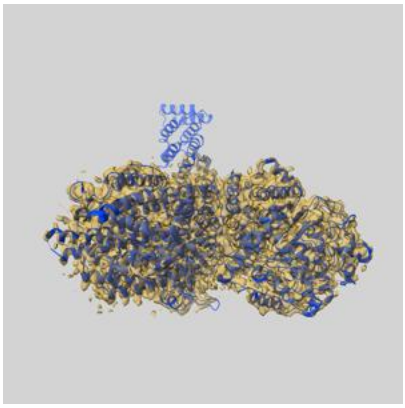
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14765 and PDB model 7ZKQ. Per-residue inclusion information can be found in section 3 on page 7.

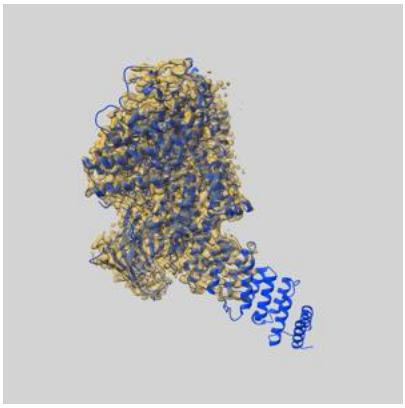
9.1 Map-model overlay



X



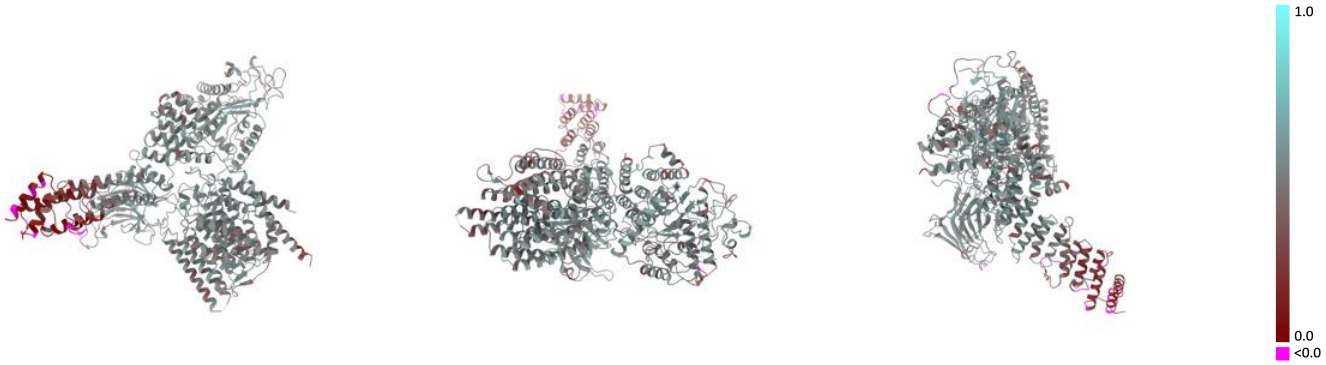
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

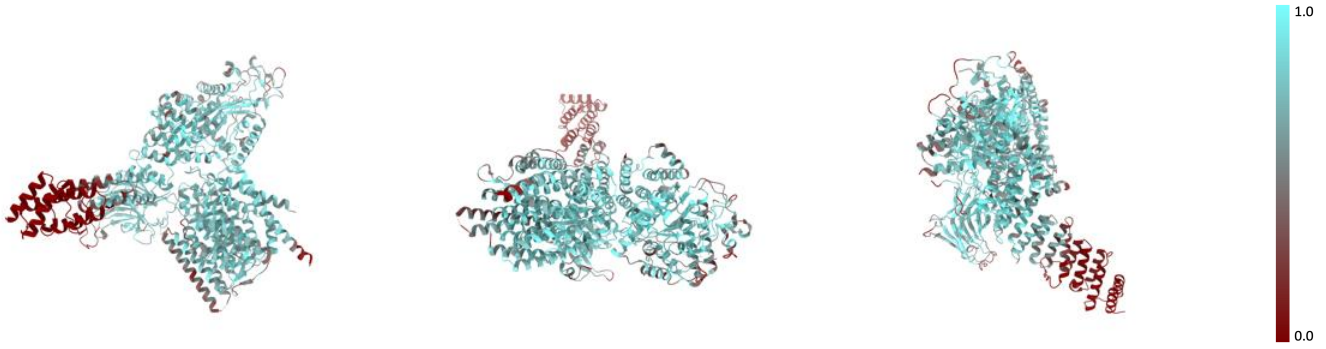
9.2 Q-score mapped to coordinate model (i)



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.

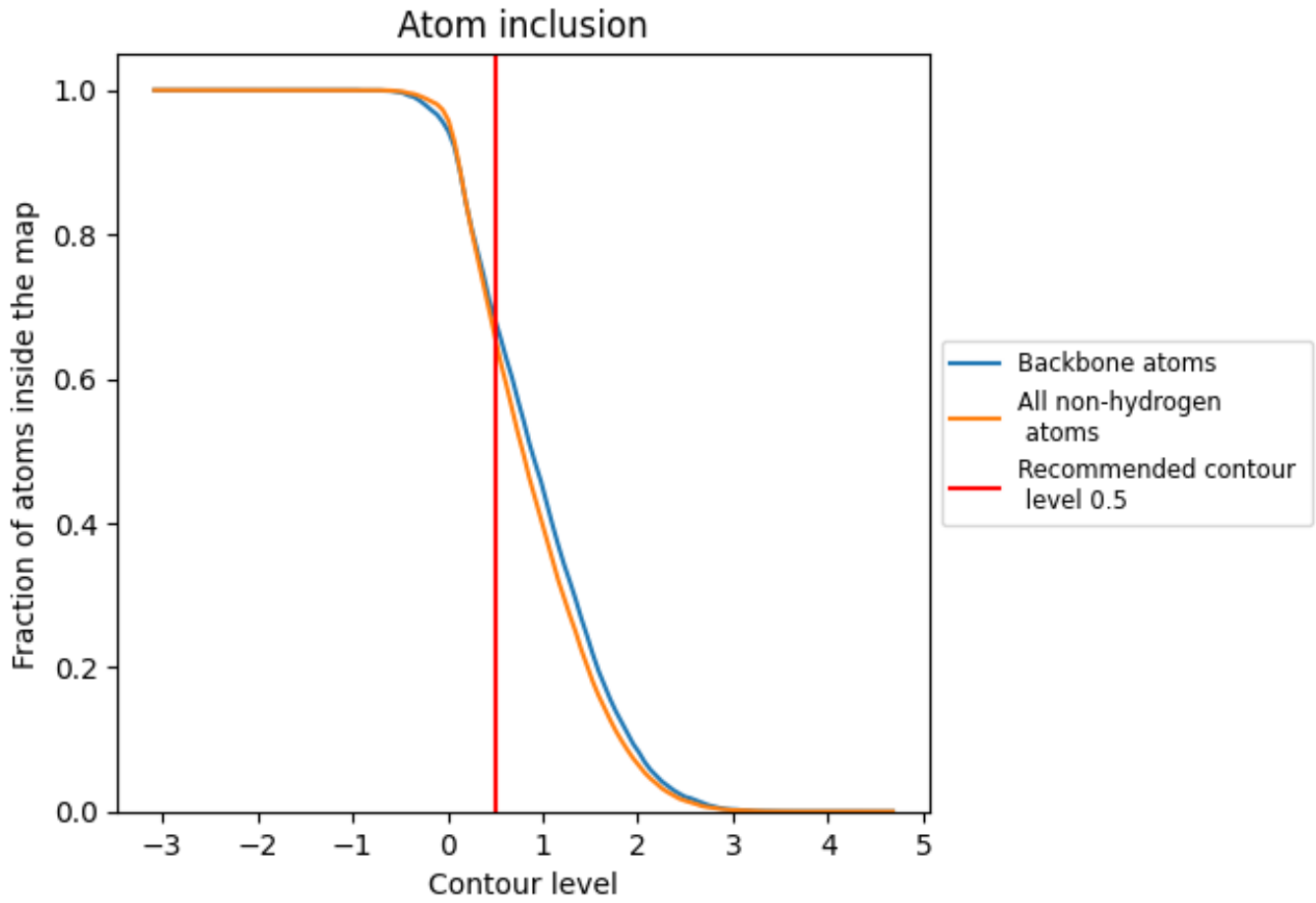
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6558	0.4740
2	0.7405	0.5020
A	0.6741	0.4940
C	0.5025	0.4020
T	0.7128	0.5050
b	0.6967	0.5030