wwPDB EM Validation Summary Report (i)

Jan 26, 2023 – 05:05 am GMT

PDB ID	:	8BEH
EMDB ID	:	EMD-16003
Title	:	Cryo-EM structure of the Arabidopsis thaliana I+III2 supercomplex (CI membrane tip)
Authors	:	Klusch, N.; Kuehlbrandt, W.
Deposited on	:	2022-10-21
Resolution	:	2.29 Å(reported)

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

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

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

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

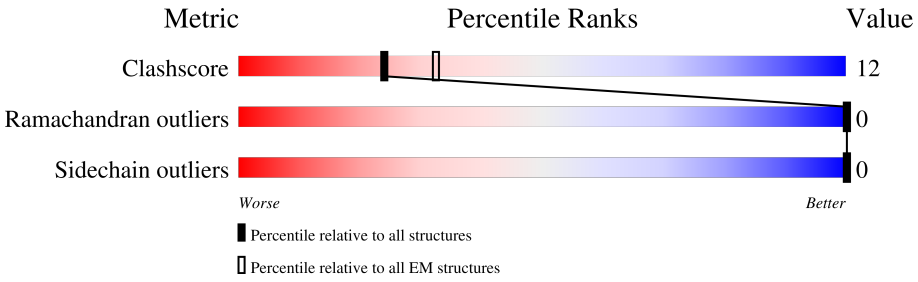
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.29 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	L	669	73% 15% 12%
2	M	495	37% 8% 55%
3	T	122	47% 20% 32%
4	c	88	86% 14%
5	g	114	10% 68% 31%
6	i	98	15% 85%
7	j	69	74% 26%
8	k	72	65% 33%

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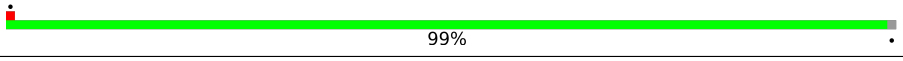
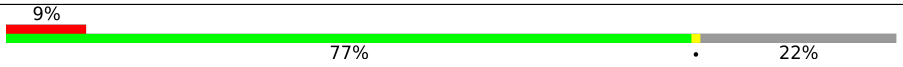
Mol	Chain	Length	Quality of chain
9	l	125	
10	m	71	
11	n	117	
12	o	103	
13	p	106	

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 13555 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-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	L	589	4599	3058	711	794	36	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	91	PHE	SER	variant	UNP P29388
L	288	PHE	SER	variant	UNP P29388
L	537	LEU	PRO	variant	UNP P29388

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	M	225	1761	1170	282	297	12	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	146	PHE	PRO	variant	UNP P93313
M	326	LEU	PRO	variant	UNP P93313
M	383	PHE	SER	variant	UNP P93313

- Molecule 3 is a protein called Acyl carrier protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	T	83	659	417	104	135	3	0	0

- Molecule 4 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	c	76	Total	C	N	O	S	0	0
			617	396	115	100	6		

- Molecule 5 is a protein called ESSS subunit of NADH:ubiquinone oxidoreductase (Complex I) protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	79	Total	C	N	O	S	0	0
			641	412	111	115	3		

- Molecule 6 is a protein called At1g67350.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	i	15	Total	C	N	O	S	0	0
			123	82	19	20	2		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	j	51	Total	C	N	O	S	0	0
			415	275	73	64	3		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	k	48	Total	C	N	O	S	0	0
			382	244	72	63	3		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	l	74	Total	C	N	O	S	0	0
			562	367	91	103	1		

- Molecule 10 is a protein called AT2G31490 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	m	70	Total	C	N	O	S	0	0
			577	370	107	98	2		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	n	109	Total	C	N	O	S	0	0
			911	580	170	160	1		

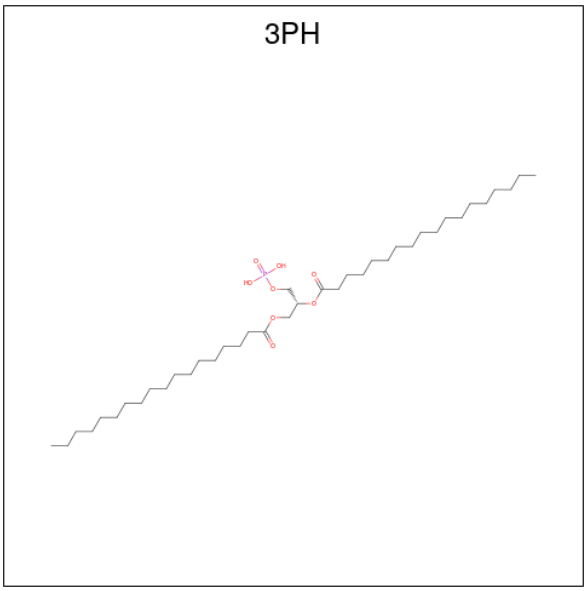
- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	o	80	Total	C	N	O	S	0	0
			657	413	115	119	10		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	p	90	Total	C	N	O	S	0	0
			757	479	141	133	4		

- Molecule 14 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
14	L	1	Total	C	O	P	0
			37	28	8	1	
14	M	1	Total	C	O	P	0
			41	32	8	1	

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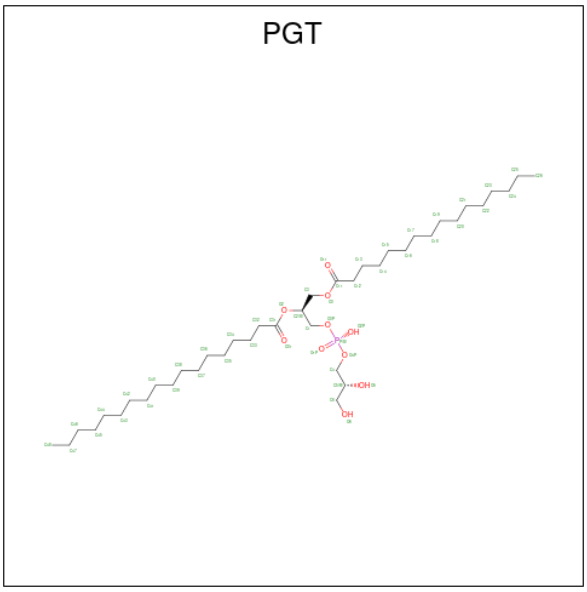
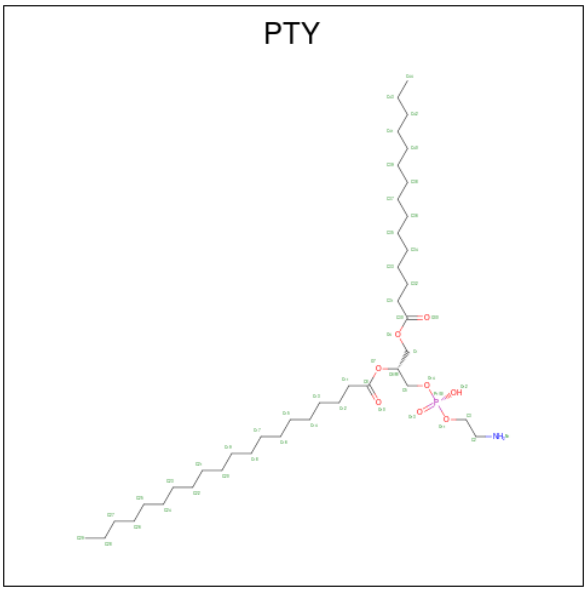
Mol	Chain	Residues	Atoms				AltConf
14	l	1	Total	C	O	P	0
			37	28	8	1	

- Molecule 15 is (1S)-2-{[{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: $C_{40}H_{79}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



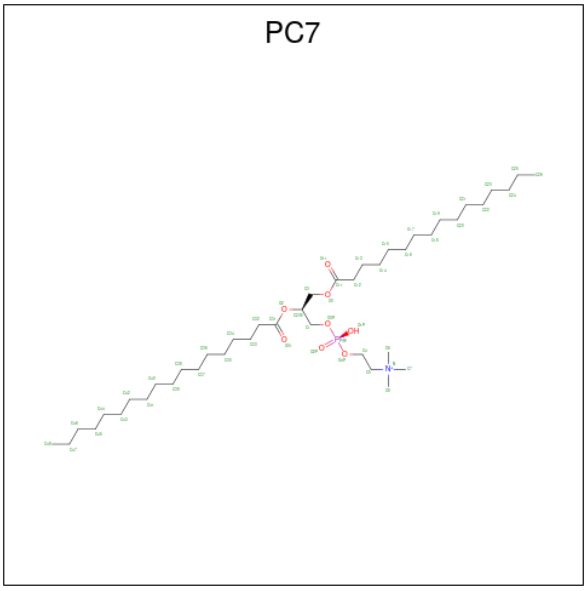
Mol	Chain	Residues	Atoms				AltConf
15	L	1	Total	C	O	P	0
			45	34	10	1	

- Molecule 16 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



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

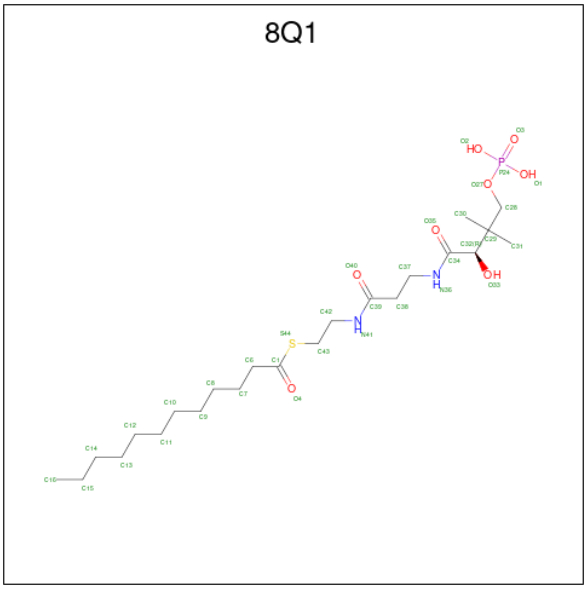
- Molecule 17 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (three-letter code: PC7) (formula: $C_{42}H_{85}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
17	L	1	Total	C	N	O	P	0
			40	30	1	8	1	

- Molecule 18 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta

-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
18	T	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		AltConf
19	L	199	Total	O	0
			199	199	
19	M	116	Total	O	0
			116	116	
19	T	13	Total	O	0
			13	13	
19	c	31	Total	O	0
			31	31	
19	g	30	Total	O	0
			30	30	
19	i	6	Total	O	0
			6	6	
19	j	3	Total	O	0
			3	3	
19	k	10	Total	O	0
			10	10	
19	l	25	Total	O	0
			25	25	

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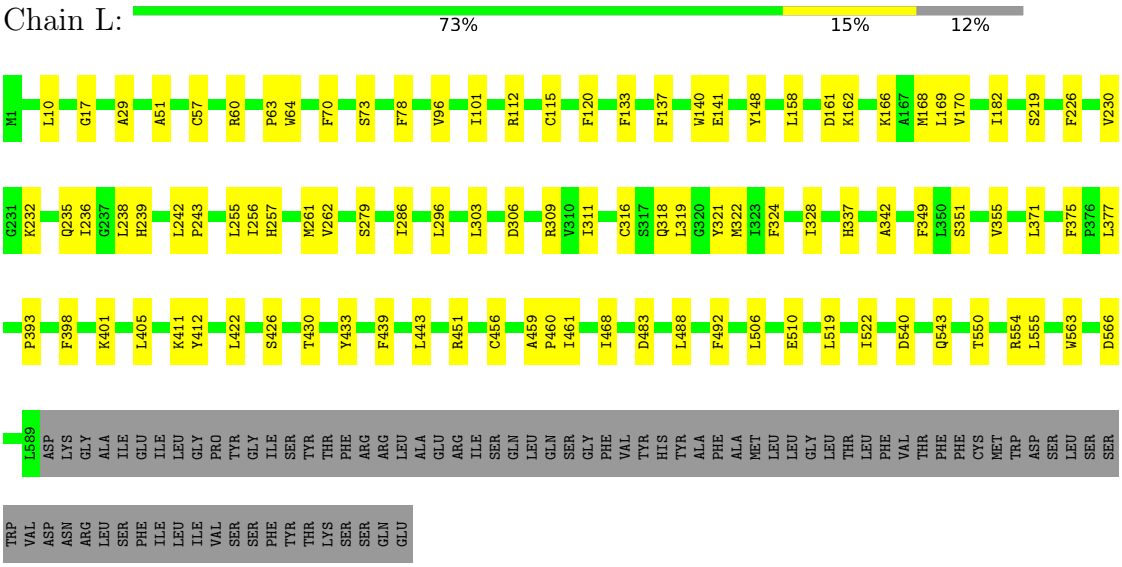
Mol	Chain	Residues	Atoms	AltConf
19	m	29	Total O 29 29	0
19	n	48	Total O 48 48	0
19	o	50	Total O 50 50	0
19	p	57	Total O 57 57	0

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.

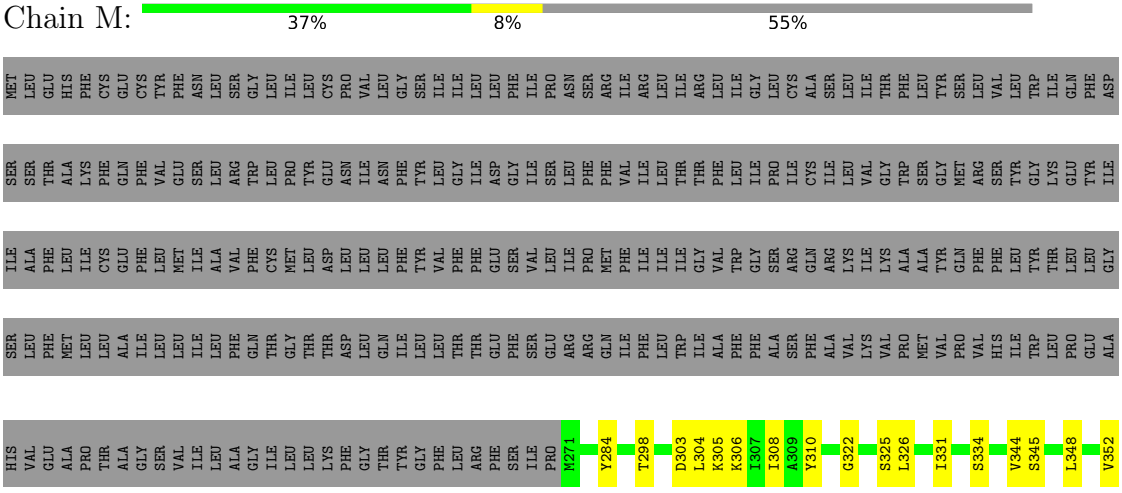
• Molecule 1: NADH-ubiquinone oxidoreductase chain 5

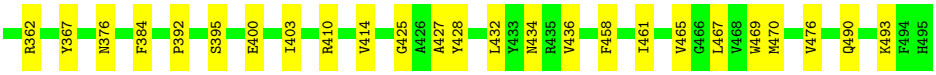
Chain L:



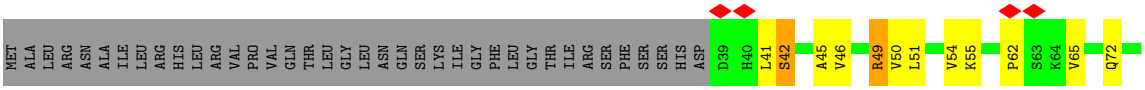
• Molecule 2: NADH-ubiquinone oxidoreductase chain 4

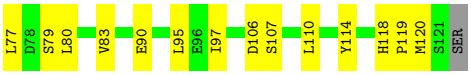
Chain M:



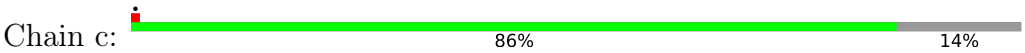


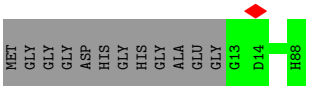
• Molecule 3: Acyl carrier protein 1, mitochondrial



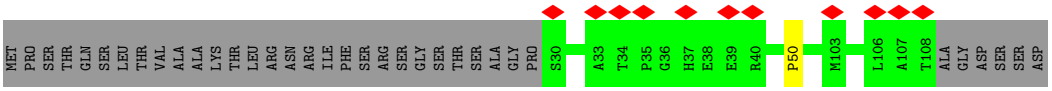


• Molecule 4: Transmembrane protein

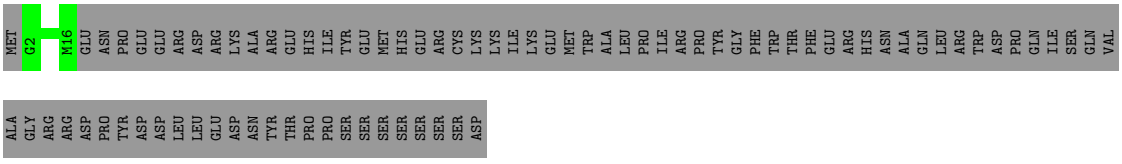




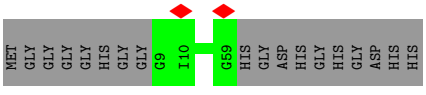
• Molecule 5: ESSS subunit of NADH:ubiquinone oxidoreductase (Complex I) protein



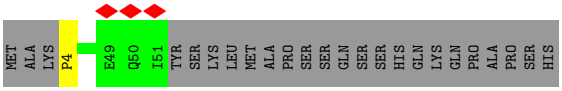
• Molecule 6: At1g67350



• Molecule 7: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2

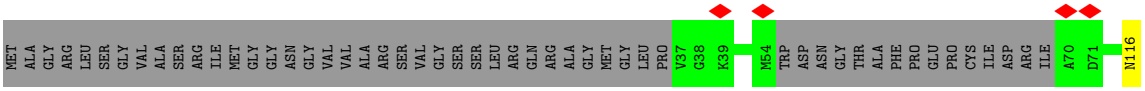


• Molecule 8: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3-A



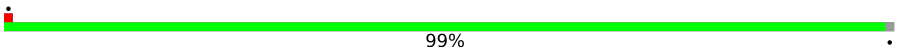
• Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain l:



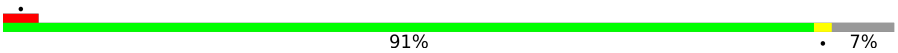
• Molecule 10: AT2G31490 protein

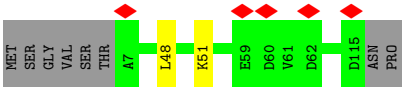
Chain m:



• Molecule 11: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

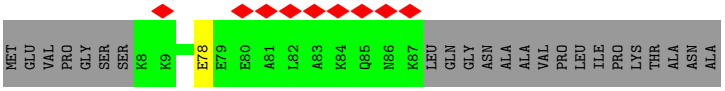
Chain n:





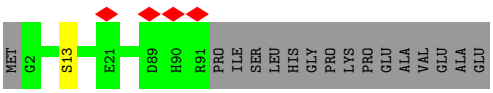
• Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o:



• Molecule 13: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10-B

Chain p:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	213993	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)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	215000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	5.588	Depositor
Minimum map value	-3.808	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.329	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	126.633, 139.812, 140.38501	wwPDB
Map dimensions	245, 244, 221	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.573, 0.573, 0.573	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PH, PC7, PGT, PTY, 8Q1

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	L	0.53	0/4726	0.72	2/6421 (0.0%)
2	M	0.49	0/1807	0.65	0/2452
3	T	0.57	1/671 (0.1%)	0.74	1/911 (0.1%)
4	c	0.40	0/637	0.58	0/860
5	g	0.35	0/661	0.66	2/899 (0.2%)
6	i	0.45	0/124	0.82	0/164
7	j	0.42	0/433	0.63	0/592
8	k	0.46	0/392	0.81	2/526 (0.4%)
9	l	0.41	0/575	0.63	1/781 (0.1%)
10	m	0.45	0/592	0.67	0/793
11	n	0.67	2/938 (0.2%)	0.83	0/1273
12	o	0.56	0/666	0.82	1/886 (0.1%)
13	p	0.64	1/777 (0.1%)	0.84	0/1043
All	All	0.52	4/12999 (0.0%)	0.72	9/17601 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	n	51	LYS	C-O	10.09	1.42	1.23
3	T	42	SER	CA-CB	-5.56	1.44	1.52
13	p	13	SER	CA-CB	-5.36	1.45	1.52
11	n	48	LEU	C-O	5.20	1.33	1.23

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	70	PHE	CB-CA-C	7.74	125.89	110.40
5	g	50	PRO	N-CD-CG	-7.55	91.88	103.20
5	g	50	PRO	CA-CB-CG	-6.48	91.69	104.00
1	L	540	ASP	CB-CA-C	5.74	121.88	110.40
9	l	116	ASN	CB-CA-C	5.64	121.69	110.40

There are no chirality outliers.

There are no planarity outliers.

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	L	4599	0	4633	75	0
2	M	1761	0	1809	38	0
3	T	659	0	644	34	0
4	c	617	0	619	0	0
5	g	641	0	632	0	0
6	i	123	0	127	0	0
7	j	415	0	406	0	0
8	k	382	0	380	0	0
9	l	562	0	567	0	0
10	m	577	0	564	0	0
11	n	911	0	879	0	0
12	o	657	0	669	0	0
13	p	757	0	745	0	0
14	L	37	0	47	3	0
14	M	41	0	58	7	0
14	l	37	0	47	0	0
15	L	45	0	63	4	0
16	L	42	0	60	2	0
17	L	40	0	54	6	0
18	T	35	0	0	0	0
19	L	199	0	0	16	0
19	M	116	0	0	14	0
19	T	13	0	0	1	0
19	c	31	0	0	0	0
19	g	30	0	0	0	0
19	i	6	0	0	0	0
19	j	3	0	0	0	0
19	k	10	0	0	0	0
19	l	25	0	0	0	0
19	m	29	0	0	0	0
19	n	48	0	0	0	0
19	o	50	0	0	0	0
19	p	57	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13555	0	13003	151	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 12.

The worst 5 of 151 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)
1:L:243:PRO:O	1:L:309:ARG:NH1	1.56	1.34
1:L:262:VAL:HB	19:L:947:HOH:O	1.30	1.29
1:L:451:ARG:NH2	19:L:801:HOH:O	1.69	1.26
3:T:41:LEU:CD1	3:T:49:ARG:HH21	1.65	1.10
2:M:400:GLU:HG3	19:M:677:HOH:O	1.54	1.07

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	L	587/669 (88%)	567 (97%)	20 (3%)	0	100	100
2	M	223/495 (45%)	222 (100%)	1 (0%)	0	100	100
3	T	81/122 (66%)	78 (96%)	3 (4%)	0	100	100
4	c	74/88 (84%)	74 (100%)	0	0	100	100
5	g	77/114 (68%)	77 (100%)	0	0	100	100
6	i	13/98 (13%)	13 (100%)	0	0	100	100
7	j	49/69 (71%)	47 (96%)	2 (4%)	0	100	100
8	k	46/72 (64%)	45 (98%)	1 (2%)	0	100	100
9	l	70/125 (56%)	69 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	m	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
11	n	107/117 (92%)	106 (99%)	1 (1%)	0	100	100
12	o	78/103 (76%)	75 (96%)	3 (4%)	0	100	100
13	p	88/106 (83%)	86 (98%)	2 (2%)	0	100	100
All	All	1561/2249 (69%)	1526 (98%)	35 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	L	497/568 (88%)	497 (100%)	0	100	100
2	M	194/434 (45%)	194 (100%)	0	100	100
3	T	78/112 (70%)	78 (100%)	0	100	100
4	c	66/71 (93%)	66 (100%)	0	100	100
5	g	68/96 (71%)	68 (100%)	0	100	100
6	i	13/90 (14%)	13 (100%)	0	100	100
7	j	42/51 (82%)	42 (100%)	0	100	100
8	k	39/60 (65%)	39 (100%)	0	100	100
9	l	60/97 (62%)	60 (100%)	0	100	100
10	m	58/59 (98%)	58 (100%)	0	100	100
11	n	92/99 (93%)	92 (100%)	0	100	100
12	o	70/87 (80%)	70 (100%)	0	100	100
13	p	80/93 (86%)	80 (100%)	0	100	100
All	All	1357/1917 (71%)	1357 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	318	GLN
2	M	341	HIS
3	T	118	HIS
11	n	39	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

7 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	$\#\|Z\| > 2$
14	3PH	L	701	-	36,36,47	0.55	0	40,41,52	0.73	2 (5%)
18	8Q1	T	200	-	31,34,34	0.38	0	40,43,43	1.14	3 (7%)
16	PTY	L	703	-	41,41,49	0.96	4 (9%)	44,46,54	1.07	2 (4%)
15	PGT	L	702	-	44,44,50	1.13	4 (9%)	47,50,56	1.06	2 (4%)
14	3PH	l	201	-	36,36,47	0.71	1 (2%)	40,41,52	0.71	1 (2%)
17	PC7	L	704	-	39,39,51	1.08	3 (7%)	45,47,59	1.10	3 (6%)
14	3PH	M	501	-	40,40,47	0.70	1 (2%)	44,45,52	0.66	1 (2%)

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
14	3PH	L	701	-	-	14/38/38/49	-
18	8Q1	T	200	-	-	24/41/41/41	-
16	PTY	L	703	-	-	20/45/45/53	-
15	PGT	L	702	-	-	29/49/49/55	-
14	3PH	l	201	-	-	11/38/38/49	-
17	PC7	L	704	-	-	17/43/43/55	-
14	3PH	M	501	-	-	19/42/42/49	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	501	3PH	P-O11	3.29	1.70	1.60
14	l	201	3PH	P-O11	3.23	1.70	1.60
15	L	702	PGT	O3-C11	3.09	1.42	1.33
15	L	702	PGT	O2-C31	2.70	1.41	1.34
17	L	704	PC7	O2-C2	-2.63	1.40	1.46

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	T	200	8Q1	C37-C38-C39	-4.18	105.40	112.36
15	L	702	PGT	O2-C31-C32	3.93	119.98	111.50
16	L	703	PTY	O7-C8-C11	3.85	119.79	111.50
17	L	704	PC7	O2-C31-C32	3.55	119.16	111.50
17	L	704	PC7	O3-C11-C12	2.92	121.08	111.91

There are no chirality outliers.

5 of 134 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	L	701	3PH	O22-C21-O21-C2
14	L	701	3PH	C22-C21-O21-C2
14	l	201	3PH	O22-C21-O21-C2
14	l	201	3PH	C22-C21-O21-C2
15	L	702	PGT	C32-C31-O2-C2

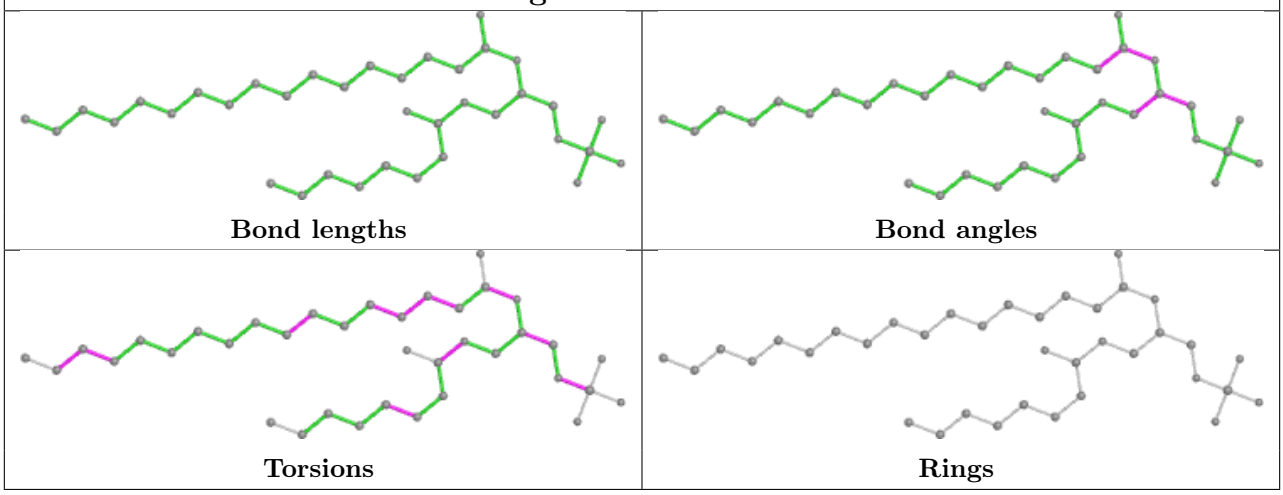
There are no ring outliers.

5 monomers are involved in 22 short contacts:

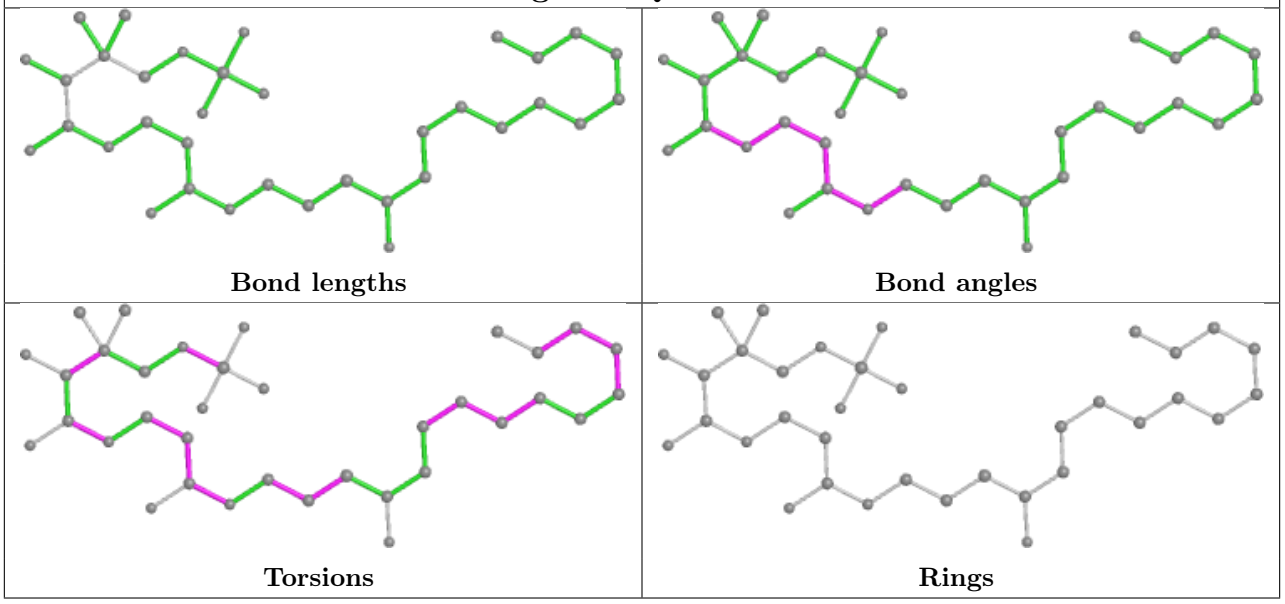
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	L	701	3PH	3	0
16	L	703	PTY	2	0
15	L	702	PGT	4	0
17	L	704	PC7	6	0
14	M	501	3PH	7	0

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.

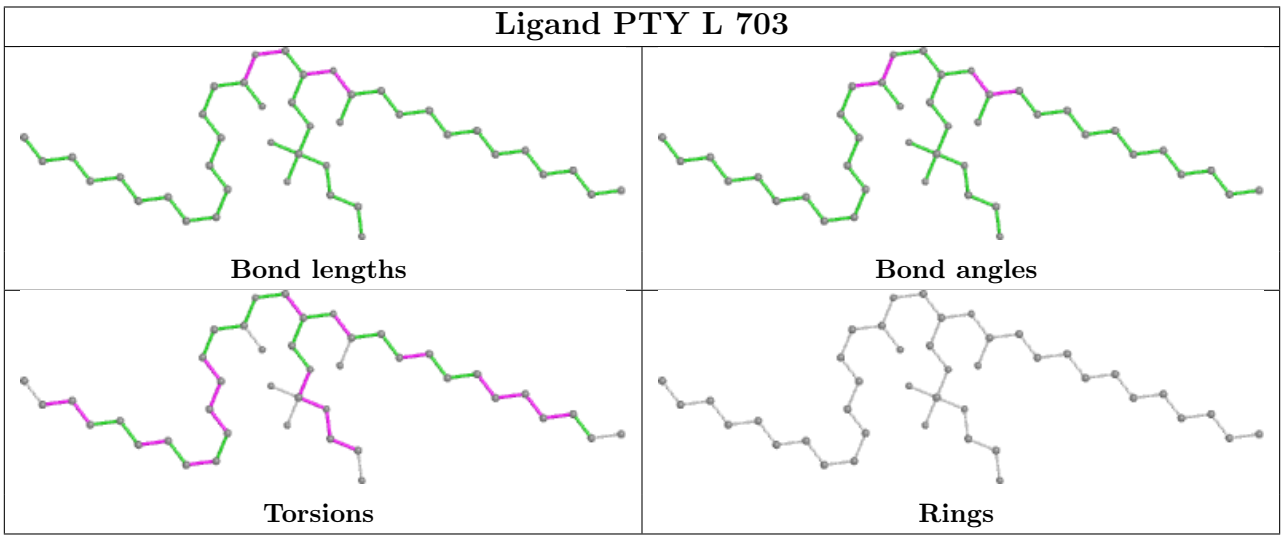
Ligand 3PH L 701



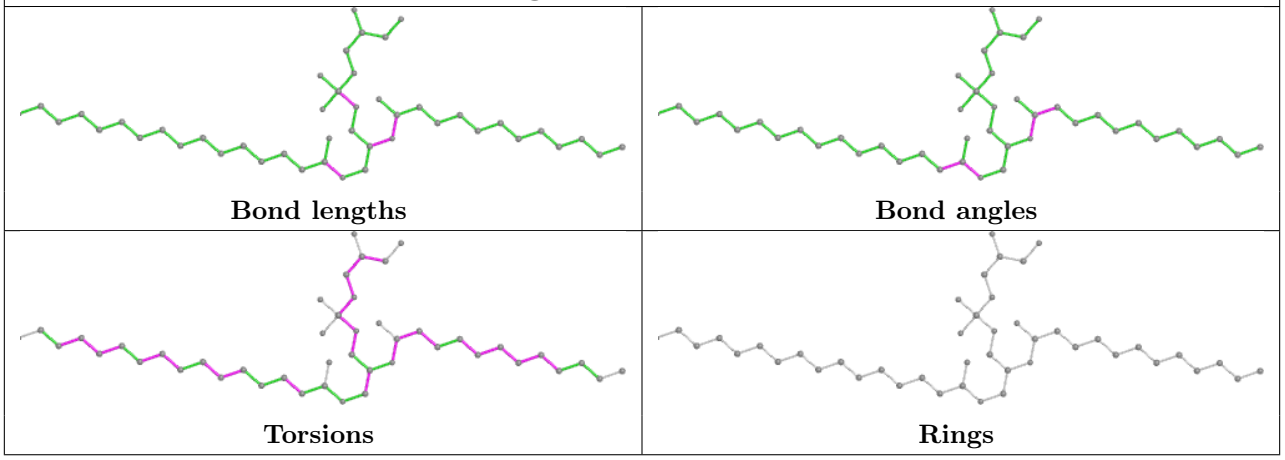
Ligand 8Q1 T 200



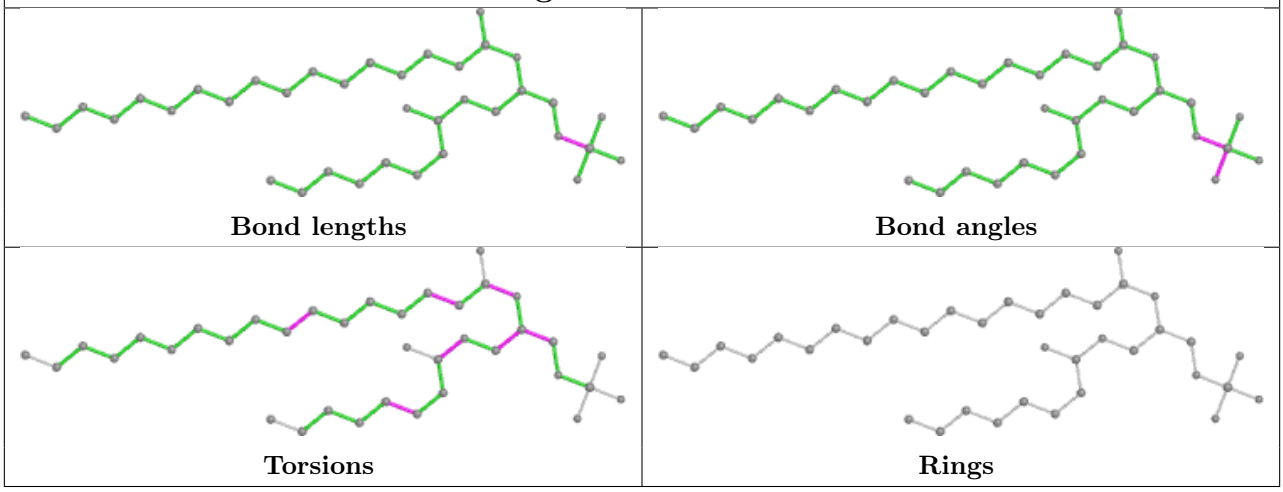
Ligand PTY L 703



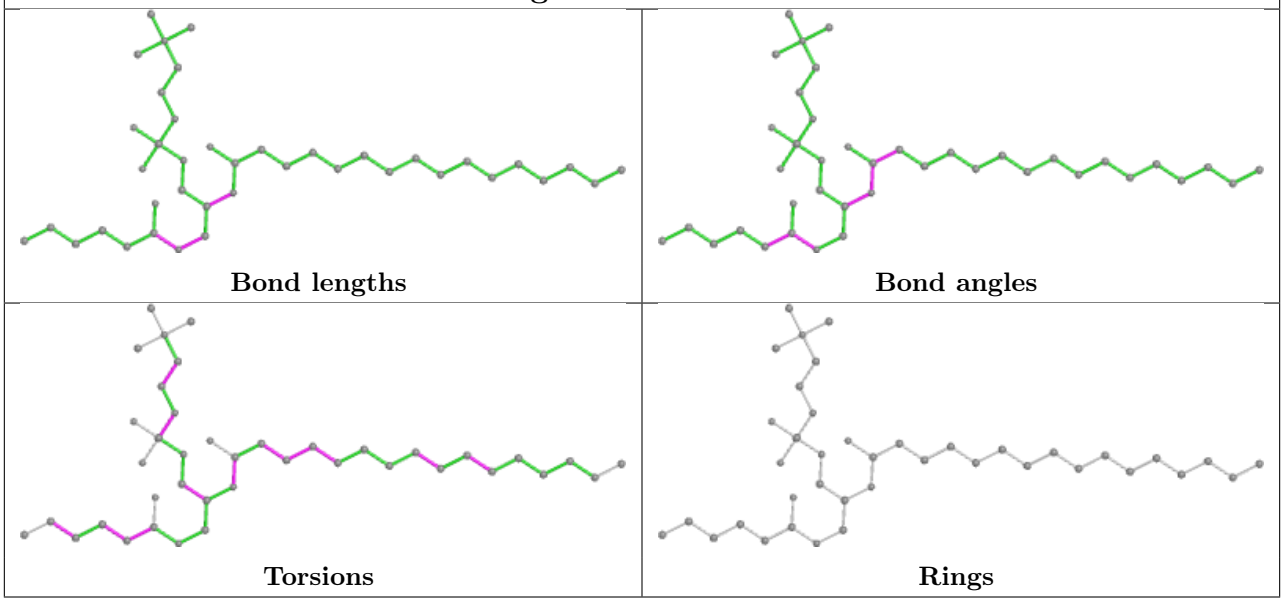
Ligand PGT L 702



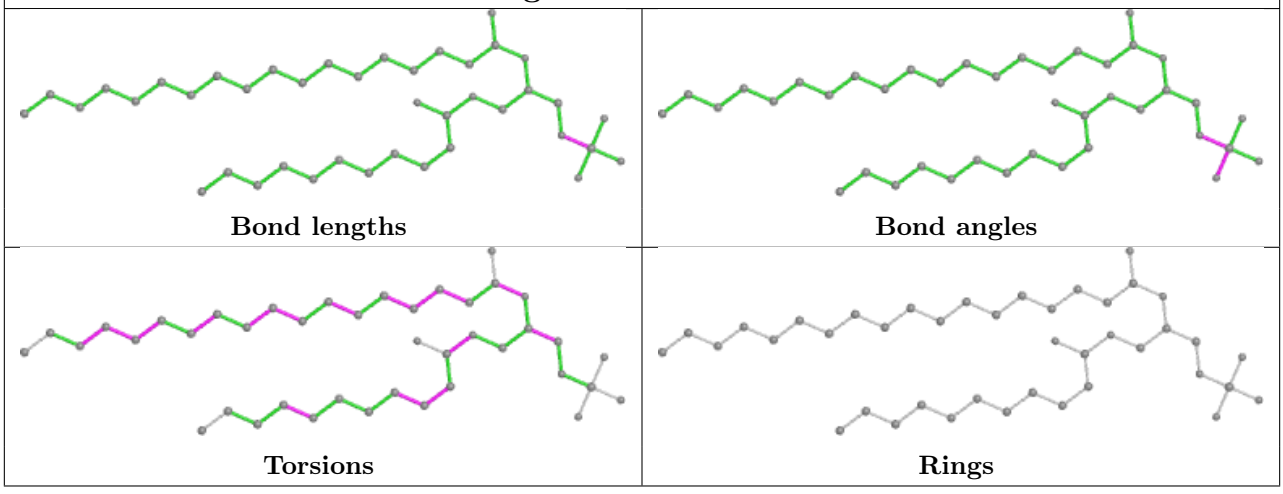
Ligand 3PH l 201



Ligand PC7 L 704



Ligand 3PH M 501



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.

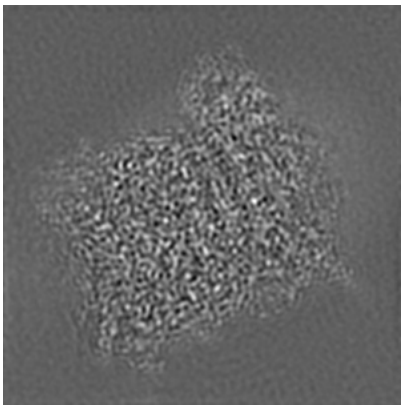
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16003. These allow visual inspection of the internal detail of the map and identification of artifacts.

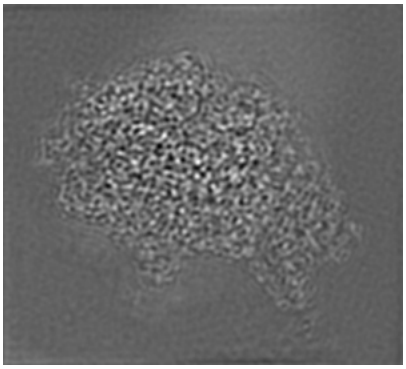
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

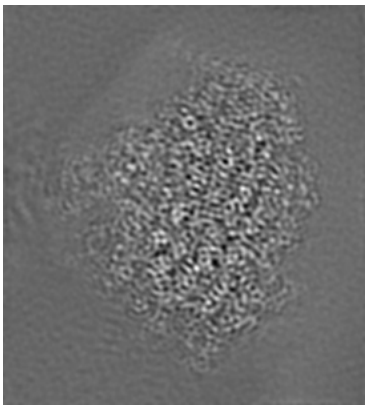
6.1.1 Primary map



X

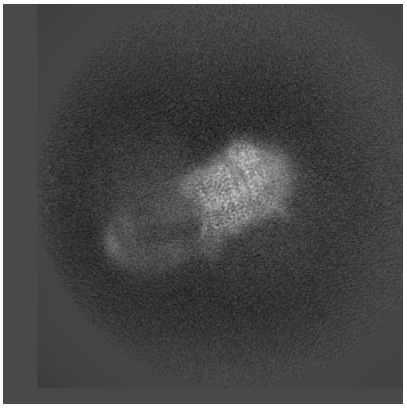


Y

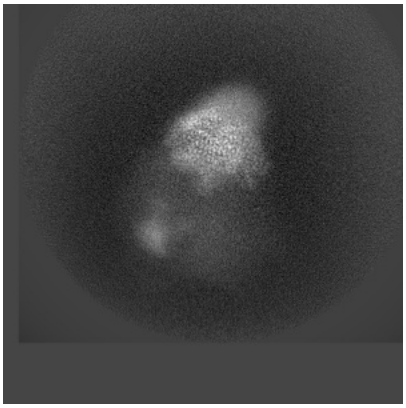


Z

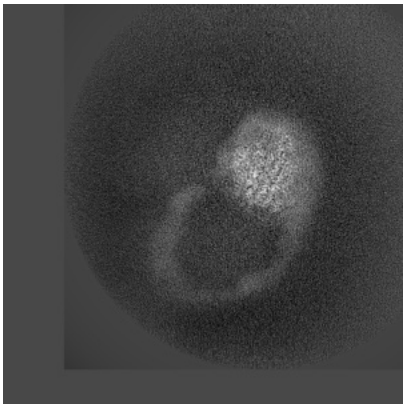
6.1.2 Raw map



X



Y

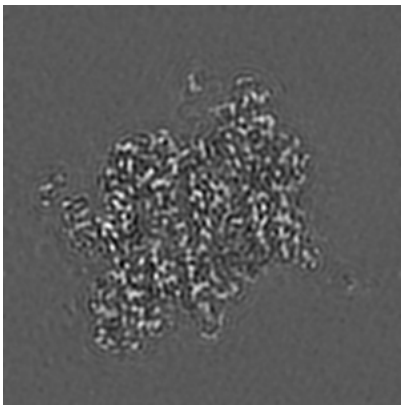


Z

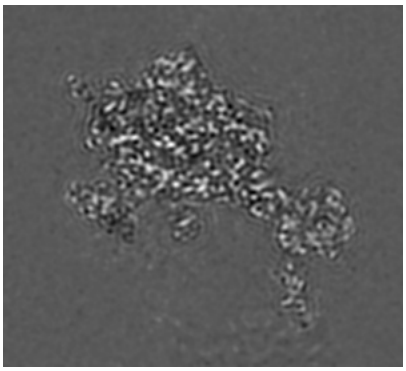
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

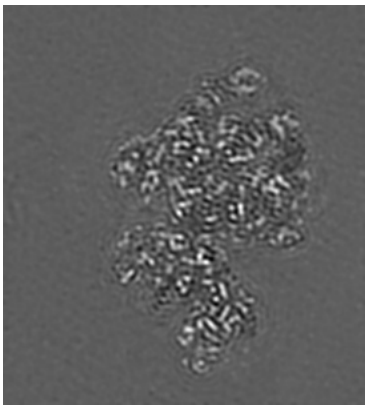
6.2.1 Primary map



X Index: 110

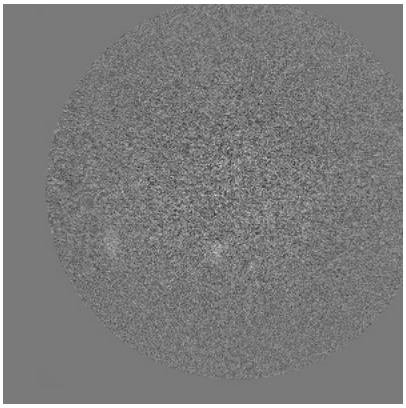


Y Index: 122

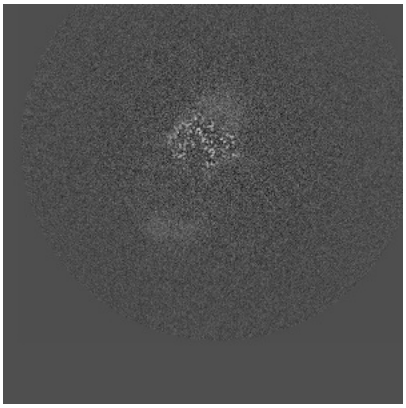


Z Index: 122

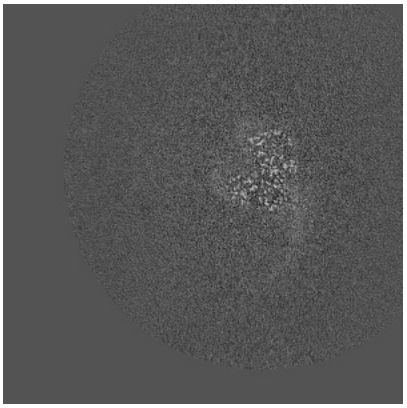
6.2.2 Raw map



X Index: 375



Y Index: 375

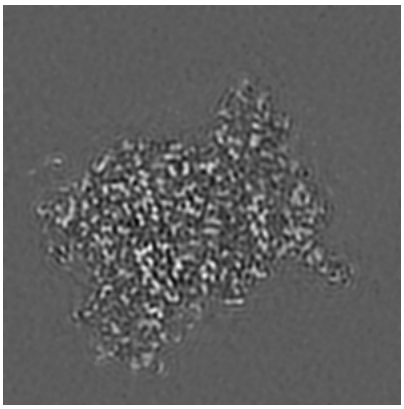


Z Index: 375

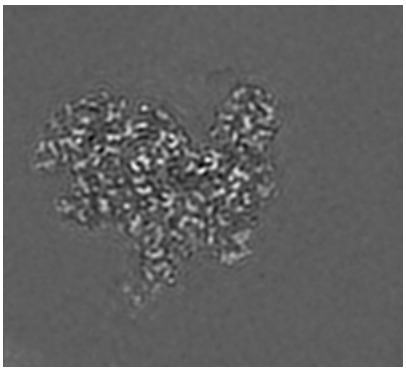
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

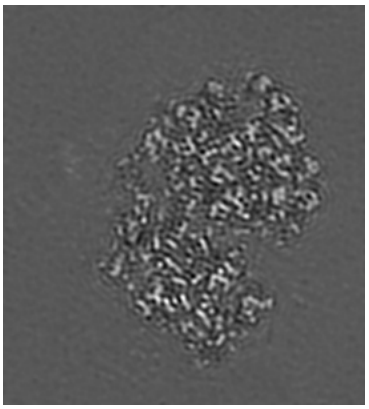
6.3.1 Primary map



X Index: 125

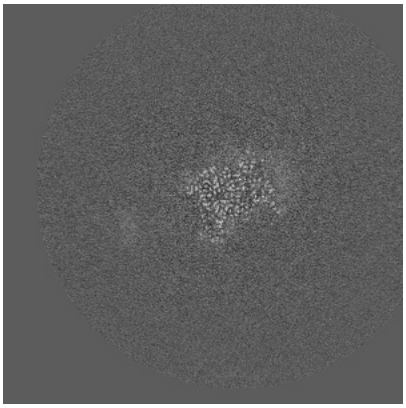


Y Index: 90

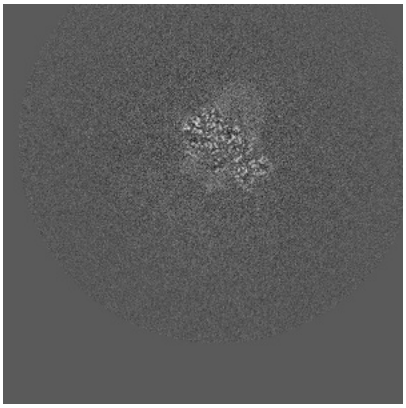


Z Index: 109

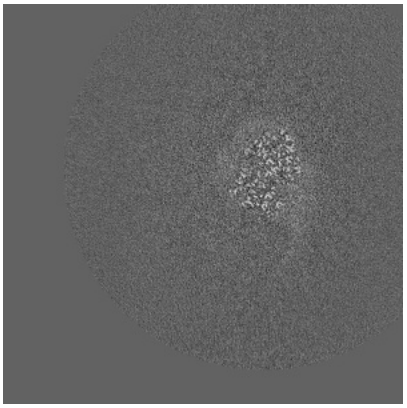
6.3.2 Raw map



X Index: 492



Y Index: 452



Z Index: 391

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

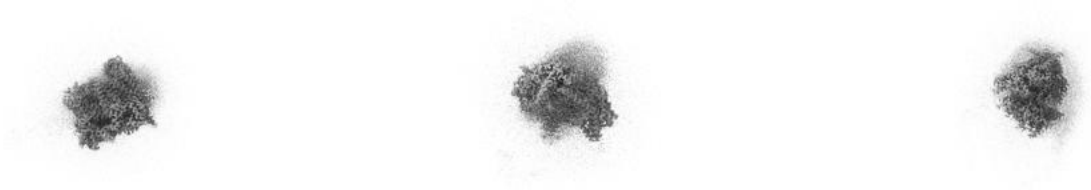
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. 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.

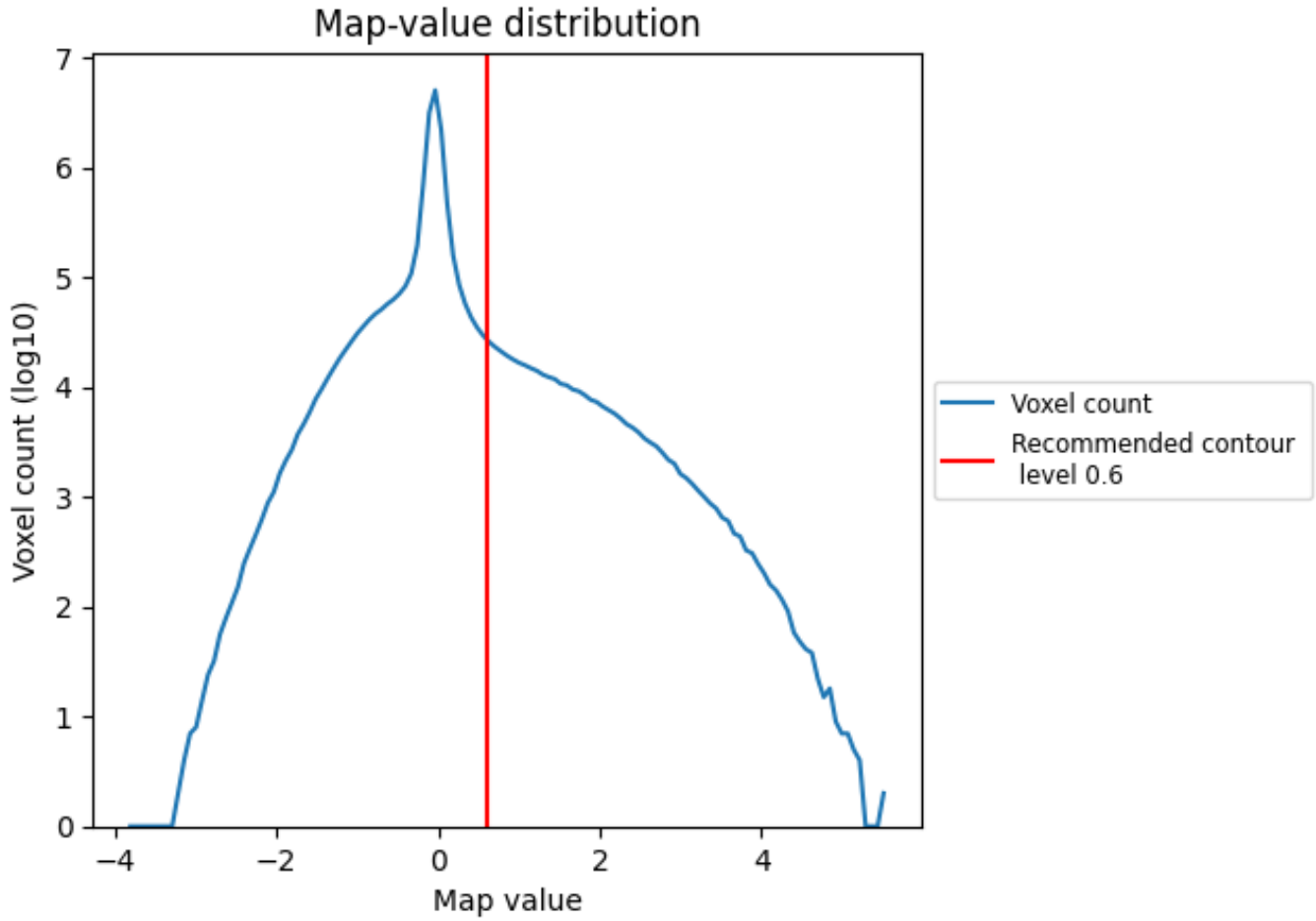
6.5 Mask visualisation (i)

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

7 Map analysis

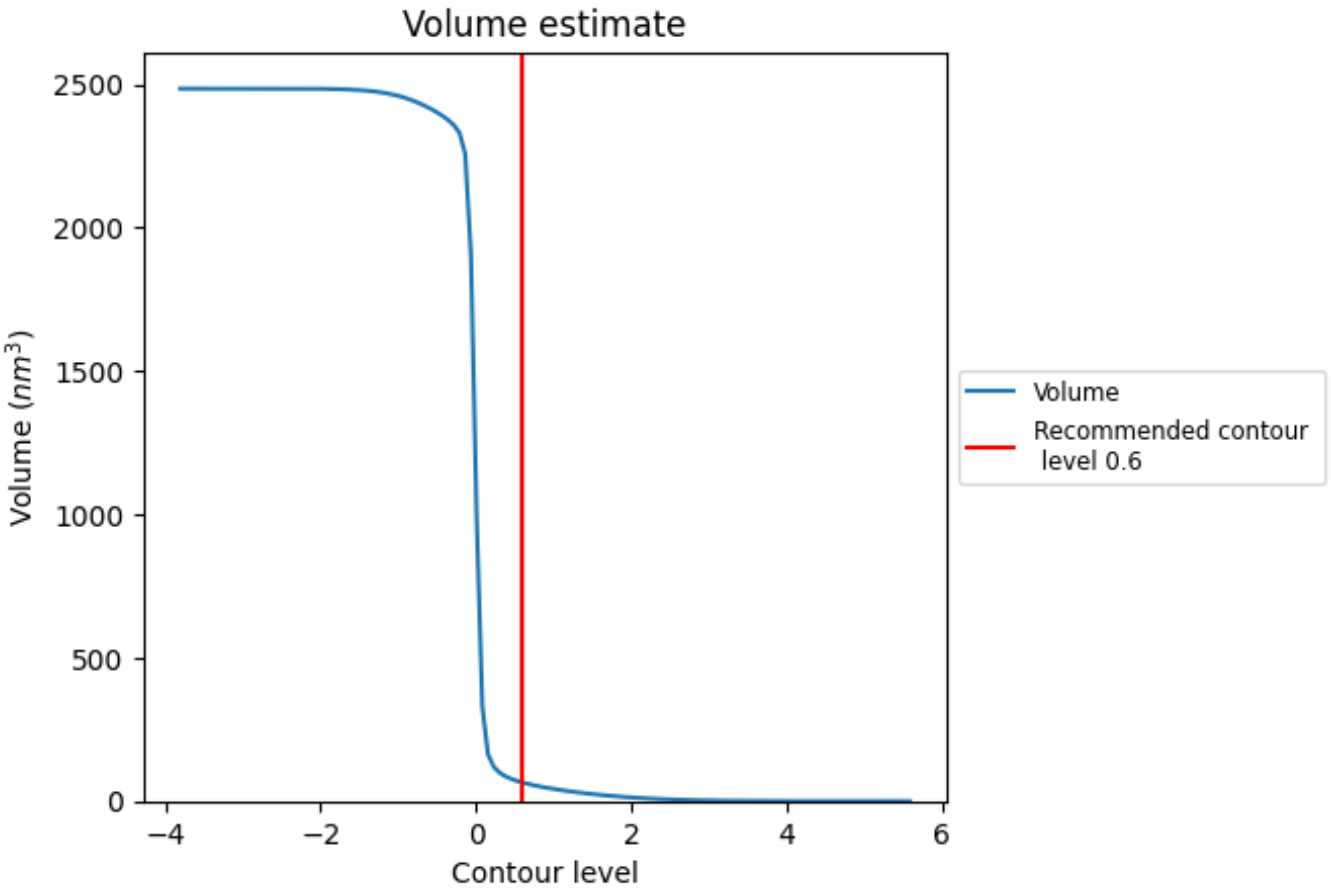
This section contains the results of statistical analysis of the map.

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 65 nm^3; this corresponds to an approximate mass of 59 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.

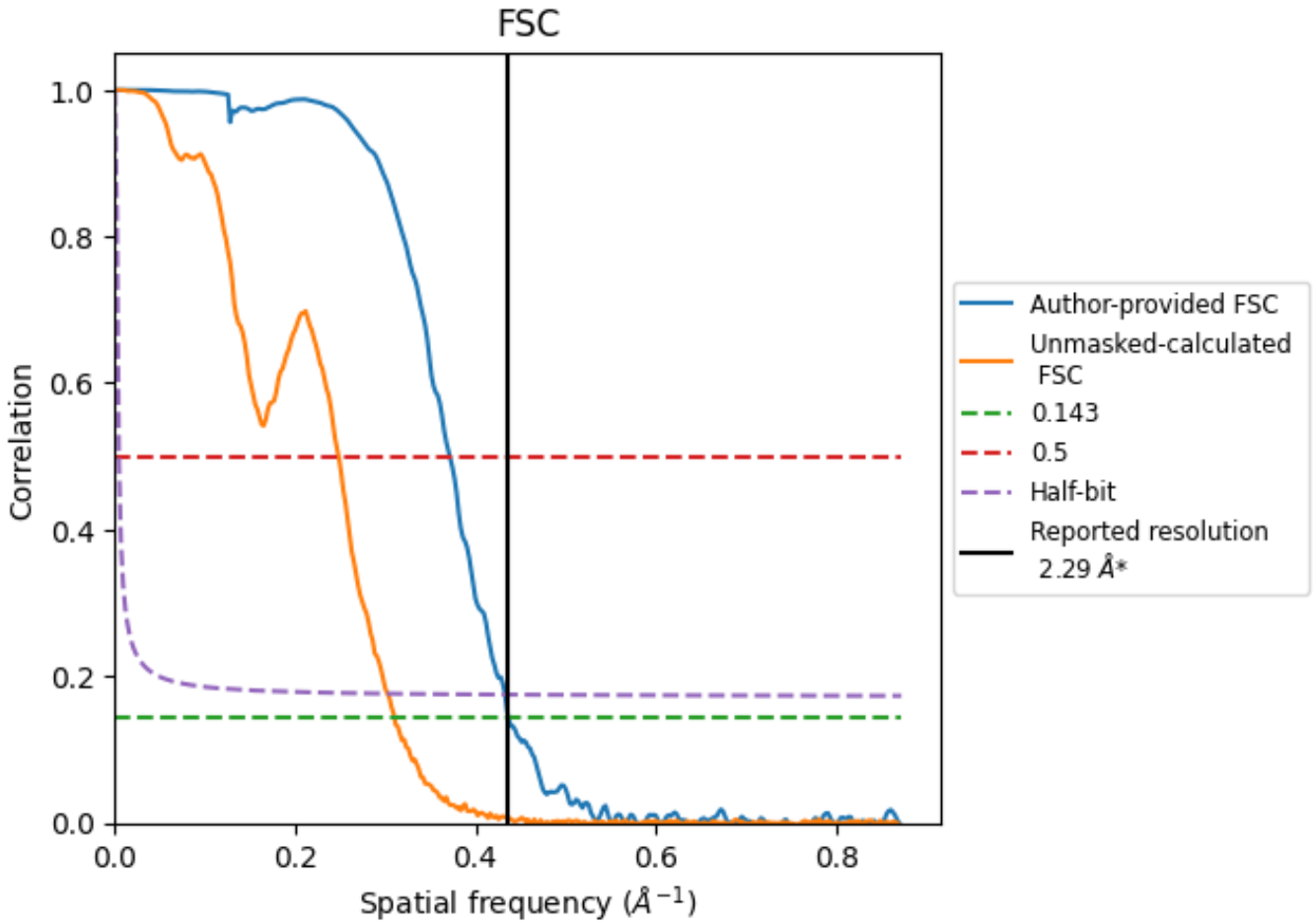
7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.437 Å^{-1}

8.2 Resolution estimates (i)

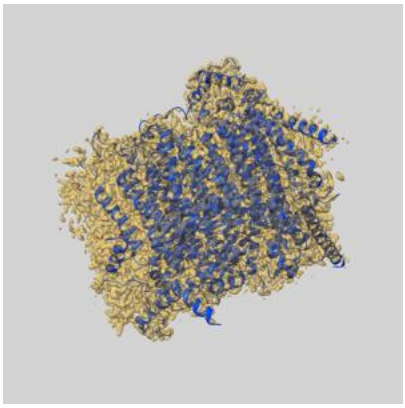
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.29	-	-
Author-provided FSC curve	2.29	2.69	2.31
Unmasked-calculated*	3.22	4.03	3.30

*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 3.22 differs from the reported value 2.29 by more than 10 %

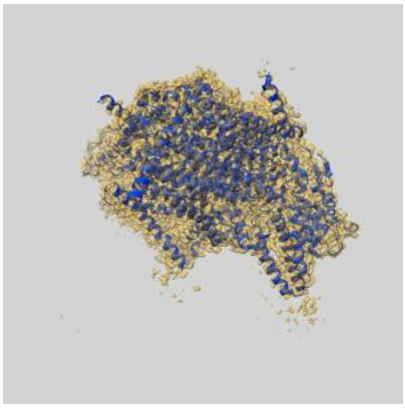
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16003 and PDB model 8BEH. Per-residue inclusion information can be found in section 3 on page 11.

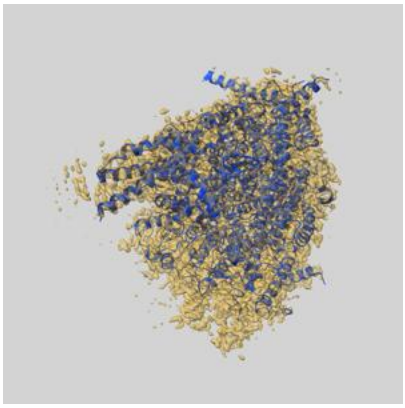
9.1 Map-model overlay



X



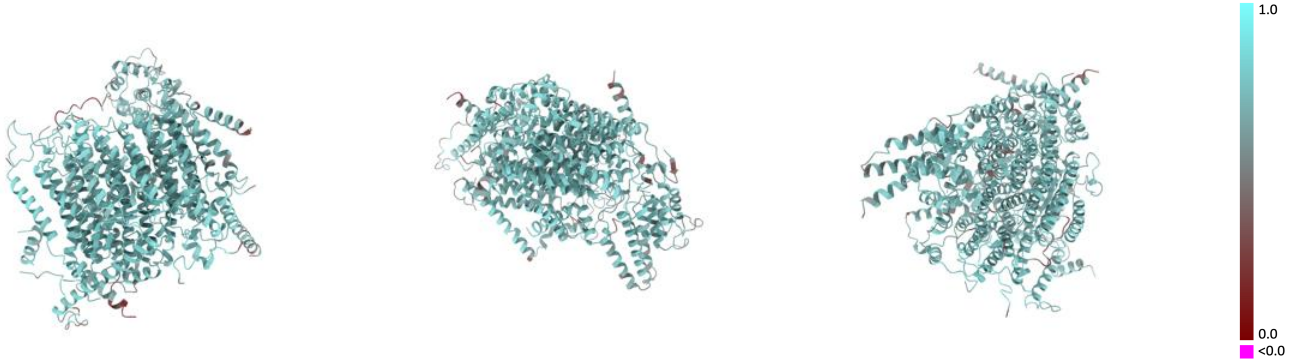
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

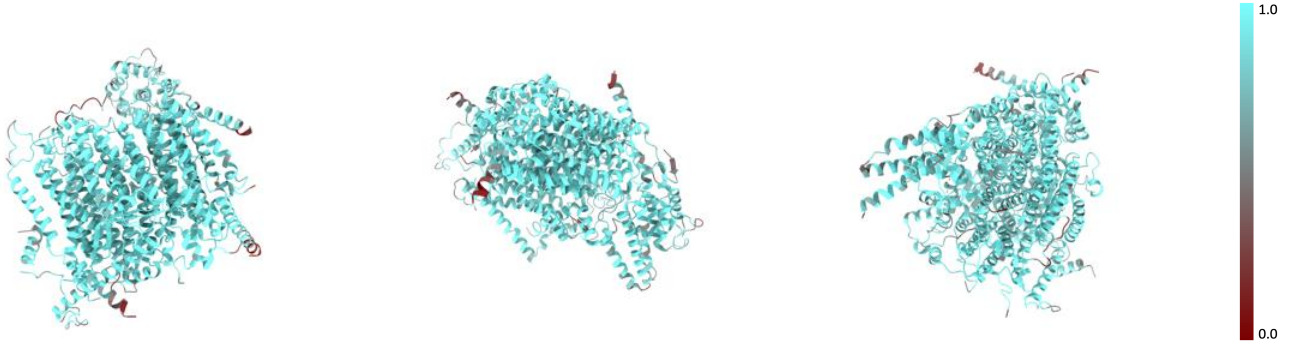
9.2 Q-score mapped to coordinate model



X Y Z

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

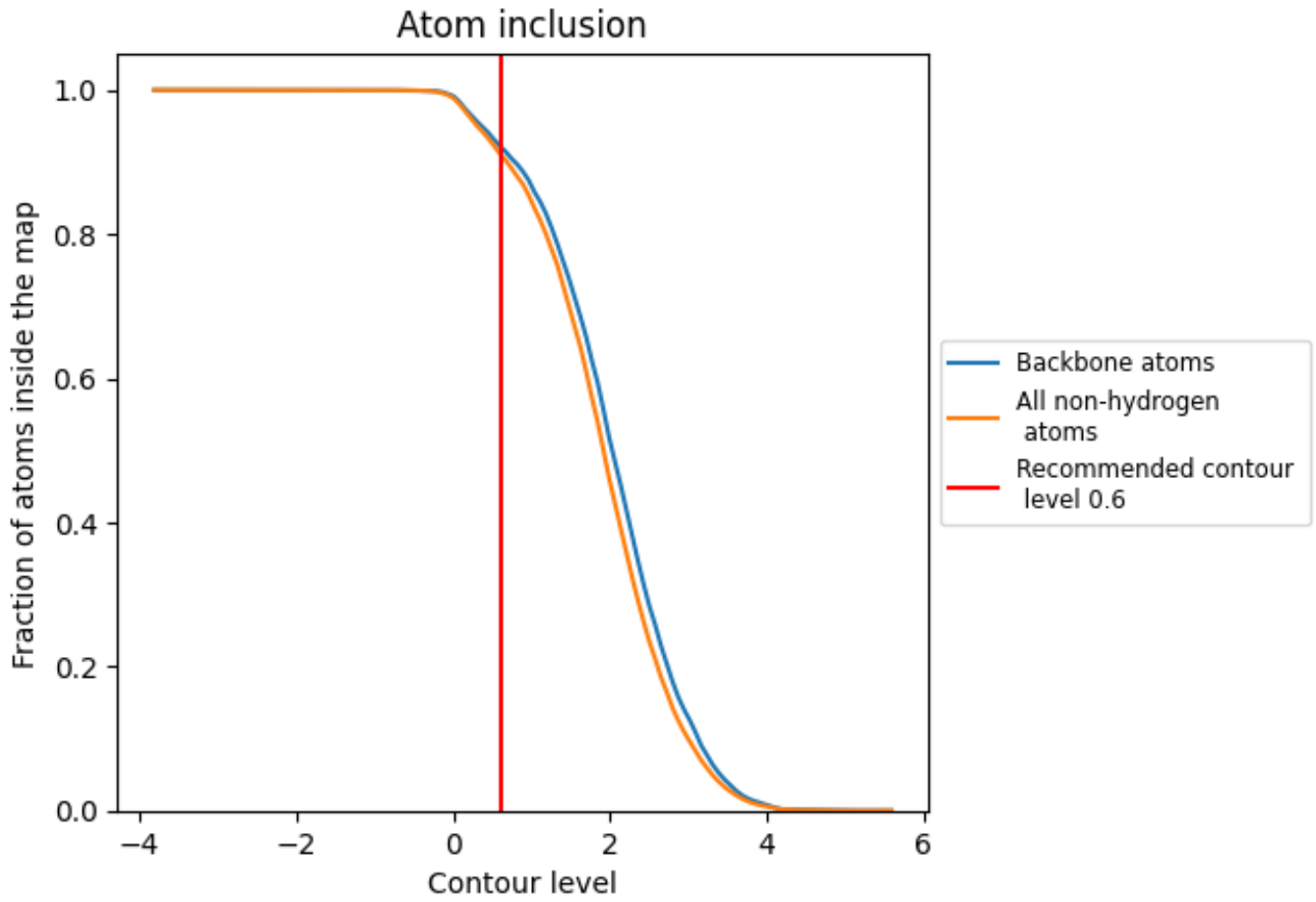
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.6).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9112	0.7110
L	0.9627	0.7370
M	0.9876	0.7690
T	0.8241	0.6610
c	0.9318	0.7110
g	0.8016	0.6400
i	0.7851	0.6630
j	0.8589	0.6590
k	0.8216	0.6410
l	0.8102	0.6570
m	0.8879	0.6940
n	0.8894	0.6950
o	0.8367	0.6850
p	0.8569	0.6830