wwPDB EM Validation Summary Report (i)

Dec 17, 2022 – 06:07 pm GMT

PDB ID	:	6YMY
EMDB ID	:	EMD-10848
Title	:	Cytochrome c oxidase from Saccharomyces cerevisiae
Authors	:	Berndtsson, J.; Rathore, S.; Ott, M.
Deposited on	:	2020-04-10
Resolution	:	3.41 Å(reported)

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

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

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

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

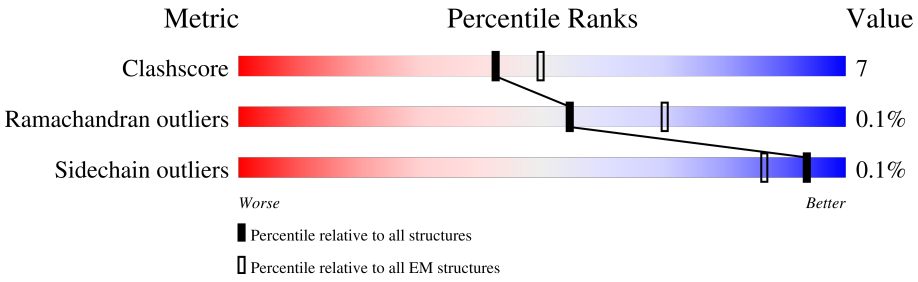
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.41 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	a	530	100%
2	b	236	100%
3	c	268	100%
4	d	117	100%
5	e	128	100%
6	f	99	100%
7	g	55	100%
8	h	51	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	i	52	100%
10	j	78	10% 99%
11	k	114	25% 99%
12	m	38	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	a	602	X	-	-	-
14	HEA	a	603	X	-	-	-

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 14612 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 Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	a	530	4126	2757	641	707	21	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	236	1888	1242	286	350	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	268	2138	1425	343	356	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	117	888	559	147	177	5	0	0

- Molecule 5 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	128	1008	639	175	190	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	99	828	533	134	160	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	g	55	Total	C	N	O	0	0
			456	310	77	69		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	51	Total	C	N	O	S	0	0
			408	278	66	63	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	52	Total	C	N	O	S	0	0
			426	282	71	70	3		

- Molecule 10 is a protein called Cytochrome c oxidase subunit 12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	78	Total	C	N	O	S	0	0
			649	414	111	119	5		

- Molecule 11 is a protein called Cytochrome c oxidase subunit 13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	114	Total	C	N	O	S	0	0
			941	608	163	167	3		

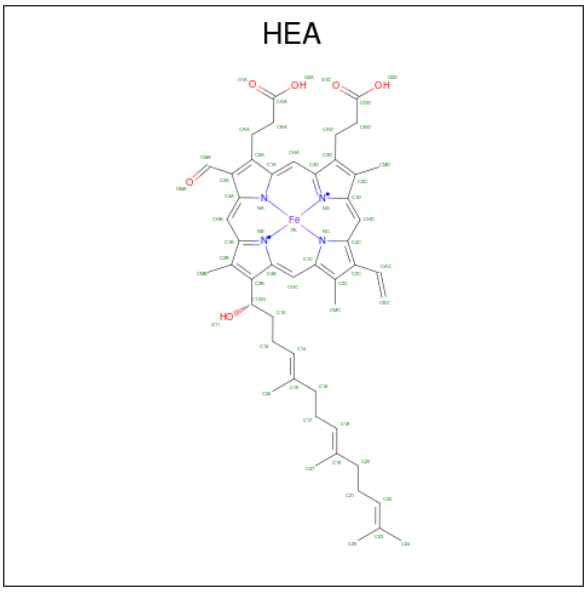
- Molecule 12 is a protein called Cytochrome c oxidase subunit 26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	m	38	Total	C	N	O	S	0	0
			308	207	49	51	1		

- Molecule 13 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

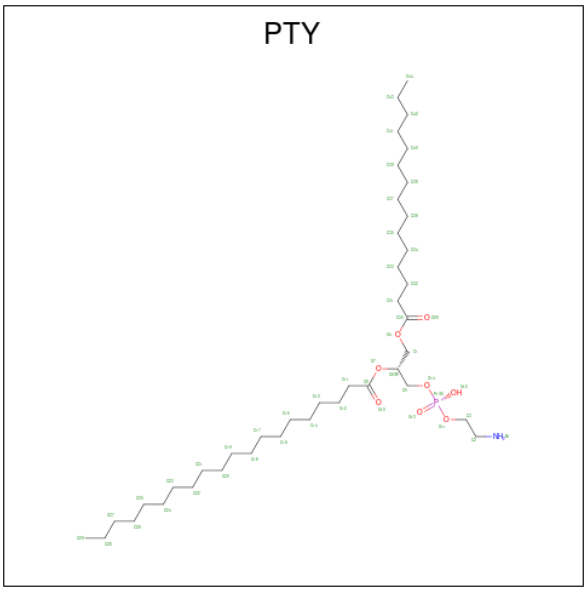
Mol	Chain	Residues	Atoms		AltConf
13	a	1	Total	Cu	0
			1	1	

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total	C	Fe	N	O	0
			120	98	2	8	12	
14	a	1	Total	C	Fe	N	O	0
			120	98	2	8	12	

- Molecule 15 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



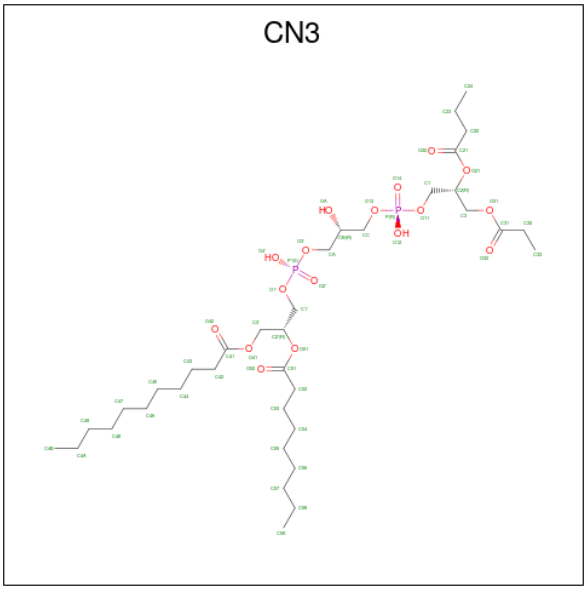
Mol	Chain	Residues	Atoms					AltConf
15	a	1	Total	C	N	O	P	0
			69	49	2	16	2	

Continued on next page...

Continued from previous page...

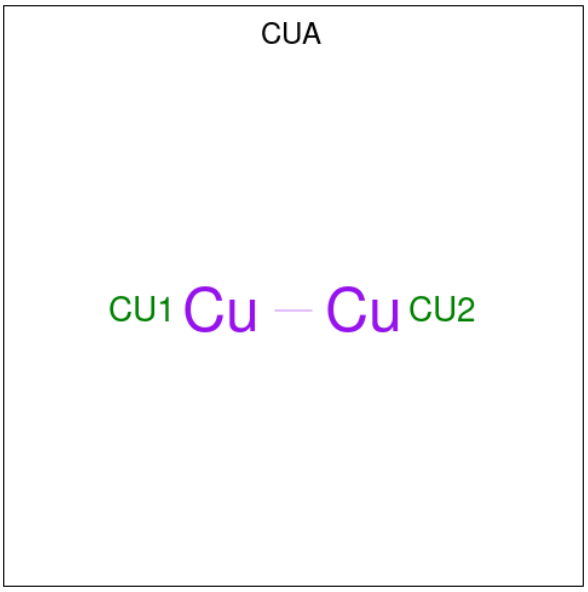
Mol	Chain	Residues	Atoms					AltConf
15	a	1	Total	C	N	O	P	0
			69	49	2	16	2	
15	b	1	Total	C	N	O	P	0
			81	61	2	16	2	
15	b	1	Total	C	N	O	P	0
			81	61	2	16	2	
15	c	1	Total	C	N	O	P	0
			40	30	1	8	1	
15	e	1	Total	C	N	O	P	0
			32	22	1	8	1	
15	i	1	Total	C	N	O	P	0
			30	20	1	8	1	

- Molecule 16 is (2R,5S,11R,14R)-5,8,11-trihydroxy-2-(nonanoyloxy)-5,11-dioxido-16-oxo-14-[(propanoyloxy)methyl]-4,6,10,12,15-pentaoxa-5,11-diphosphanonadec-1-yl undecanoate (three-letter code: CN3) (formula: $C_{36}H_{68}O_{17}P_2$).



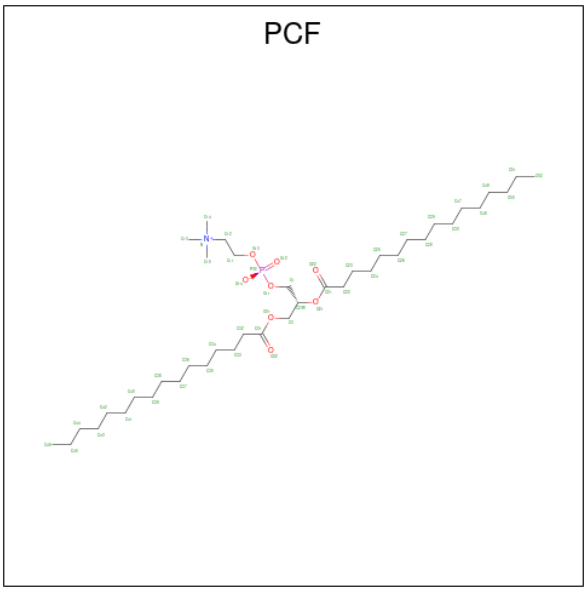
Mol	Chain	Residues	Atoms				AltConf
16	a	1	Total	C	O	P	0
			55	36	17	2	

- Molecule 17 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



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

- Molecule 18 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (three-letter code: PCF) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
18	c	1	Total	C	N	O	P	0
			43	33	1	8	1	
18	e	1	Total	C	N	O	P	0
			36	26	1	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
18	m	1	Total	C	N	O	P	0
			38	28	1	8	1	

- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

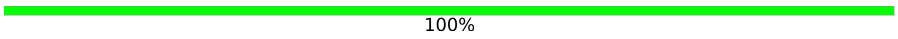
Mol	Chain	Residues	Atoms		AltConf
19	d	1	Total	Zn	0
			1	1	

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: Cytochrome c oxidase subunit 1

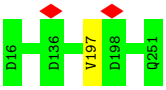
Chain a:



There are no outlier residues recorded for this chain.

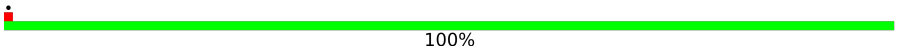
- Molecule 2: Cytochrome c oxidase subunit 2

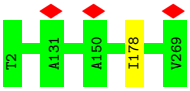
Chain b:



- Molecule 3: Cytochrome c oxidase subunit 3

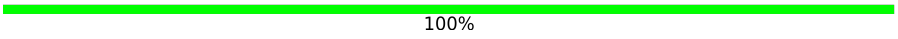
Chain c:





- Molecule 4: Cytochrome c oxidase subunit 4, mitochondrial

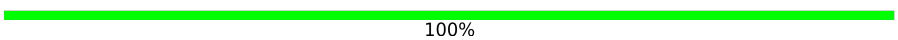
Chain d:



There are no outlier residues recorded for this chain.

- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

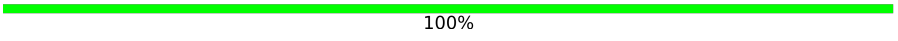
Chain e:



There are no outlier residues recorded for this chain.

- Molecule 6: Cytochrome c oxidase subunit 6, mitochondrial

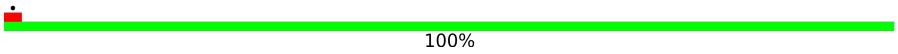
Chain f:

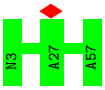


There are no outlier residues recorded for this chain.

• Molecule 7: Cytochrome c oxidase subunit 7, mitochondrial

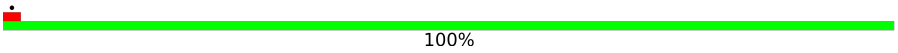
Chain g:





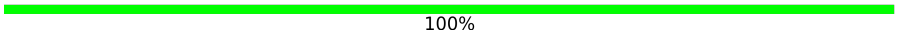
• Molecule 8: Cytochrome c oxidase subunit 8, mitochondrial

Chain h:



• Molecule 9: Cytochrome c oxidase subunit 9, mitochondrial

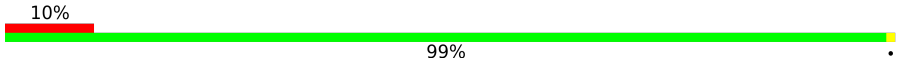
Chain i:

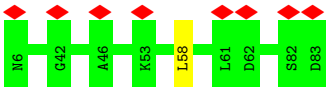


There are no outlier residues recorded for this chain.

• Molecule 10: Cytochrome c oxidase subunit 12, mitochondrial

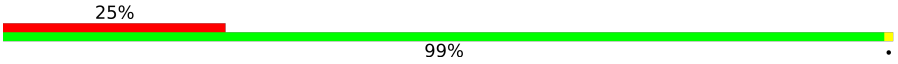
Chain j:

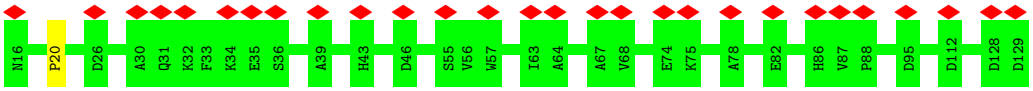




• Molecule 11: Cytochrome c oxidase subunit 13, mitochondrial

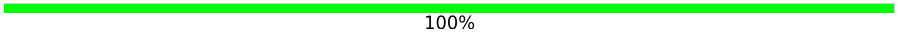
Chain k:





• Molecule 12: Cytochrome c oxidase subunit 26, mitochondrial

Chain m:



There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	201223	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	-1.4	Depositor
Maximum defocus (nm)	-3.0	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.411	Depositor
Minimum map value	-1.211	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.41	Depositor
Map size (Å)	392.2, 392.2, 392.2	wwPDB
Map dimensions	370, 370, 370	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0600001, 1.0600001, 1.0600001	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, HEA, PTY, CU, CN3, PCF, CUA

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	0.38	0/4254	0.55	0/5811
2	b	0.36	0/1940	0.53	0/2653
3	c	0.31	0/2210	0.49	1/3026 (0.0%)
4	d	0.37	0/905	0.60	0/1231
5	e	0.35	0/1032	0.55	0/1396
6	f	0.37	0/845	0.54	0/1143
7	g	0.31	0/472	0.53	0/645
8	h	0.35	0/423	0.51	0/569
9	i	0.34	0/438	0.49	0/590
10	j	0.30	0/671	0.52	1/910 (0.1%)
11	k	0.29	0/974	0.54	0/1324
12	m	0.32	0/319	0.52	0/435
All	All	0.35	0/14483	0.53	2/19733 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	j	58	LEU	CA-CB-CG	6.06	129.24	115.30
3	c	178	ILE	CG1-CB-CG2	-5.19	99.99	111.40

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	a	4126	0	4150	0	0
2	b	1888	0	1868	0	0
3	c	2138	0	2125	0	0
4	d	888	0	885	0	0
5	e	1008	0	988	0	0
6	f	828	0	807	0	0
7	g	456	0	481	0	0
8	h	408	0	408	0	0
9	i	426	0	430	0	0
10	j	649	0	592	0	0
11	k	941	0	902	0	0
12	m	308	0	302	0	0
13	a	1	0	0	0	0
14	a	120	0	108	0	0
15	a	69	0	80	0	0
15	b	81	0	108	0	0
15	c	40	0	53	0	0
15	e	32	0	37	0	0
15	i	30	0	33	0	0
16	a	55	0	66	0	0
17	b	2	0	0	0	0
18	c	43	0	60	0	0
18	e	36	0	46	0	0
18	m	38	0	50	0	0
19	d	1	0	0	0	0
All	All	14612	0	14579	0	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 7.

There are no clashes within the asymmetric unit.

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	528/530 (100%)	489 (93%)	39 (7%)	0	100	100
2	b	234/236 (99%)	215 (92%)	19 (8%)	0	100	100
3	c	266/268 (99%)	252 (95%)	14 (5%)	0	100	100
4	d	115/117 (98%)	90 (78%)	25 (22%)	0	100	100
5	e	126/128 (98%)	115 (91%)	11 (9%)	0	100	100
6	f	97/99 (98%)	88 (91%)	9 (9%)	0	100	100
7	g	53/55 (96%)	47 (89%)	6 (11%)	0	100	100
8	h	49/51 (96%)	45 (92%)	4 (8%)	0	100	100
9	i	50/52 (96%)	45 (90%)	5 (10%)	0	100	100
10	j	76/78 (97%)	66 (87%)	10 (13%)	0	100	100
11	k	112/114 (98%)	101 (90%)	10 (9%)	1 (1%)	17	53
12	m	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
All	All	1742/1766 (99%)	1586 (91%)	155 (9%)	1 (0%)	54	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	k	20	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	443/443 (100%)	443 (100%)	0	100	100
2	b	209/209 (100%)	208 (100%)	1 (0%)	88	95
3	c	227/227 (100%)	227 (100%)	0	100	100
4	d	99/99 (100%)	99 (100%)	0	100	100
5	e	106/106 (100%)	106 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	f	88/88 (100%)	88 (100%)	0	100 100
7	g	48/48 (100%)	48 (100%)	0	100 100
8	h	41/41 (100%)	41 (100%)	0	100 100
9	i	43/43 (100%)	43 (100%)	0	100 100
10	j	70/70 (100%)	70 (100%)	0	100 100
11	k	100/100 (100%)	100 (100%)	0	100 100
12	m	32/32 (100%)	32 (100%)	0	100 100
All	All	1506/1506 (100%)	1505 (100%)	1 (0%)	93 98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	197	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
5	e	63	GLN
7	g	9	GLN
10	j	70	GLN
10	j	6	ASN
6	f	117	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)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
16	CN3	a	606	-	54,54,54	0.51	0	60,66,66	1.20	4 (6%)
15	PTY	e	201	-	31,31,49	1.10	2 (6%)	34,36,54	1.20	4 (11%)
15	PTY	a	605	-	33,33,49	1.05	4 (12%)	36,38,54	1.16	2 (5%)
14	HEA	a	602	1	57,67,67	1.35	7 (12%)	61,103,103	1.61	18 (29%)
14	HEA	a	603	1	57,67,67	1.43	8 (14%)	61,103,103	1.70	14 (22%)
18	PCF	c	302	-	42,42,49	0.63	0	48,50,57	0.57	0
15	PTY	c	301	-	39,39,49	0.99	4 (10%)	42,44,54	1.14	3 (7%)
18	PCF	e	202	-	35,35,49	0.67	0	41,43,57	0.58	0
18	PCF	m	101	-	37,37,49	0.65	0	43,45,57	0.58	0
15	PTY	b	302	-	39,39,49	0.97	4 (10%)	42,44,54	1.09	2 (4%)
15	PTY	a	604	-	32,32,49	1.06	4 (12%)	35,37,54	1.12	2 (5%)
17	CUA	b	301	-	0,1,1	-	-	-		
15	PTY	i	101	-	29,29,49	1.12	4 (13%)	32,34,54	1.21	2 (6%)
15	PTY	b	303	-	40,40,49	0.96	4 (10%)	43,45,54	1.12	2 (4%)

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
16	CN3	a	606	-	-	37/65/65/65	-
15	PTY	e	201	-	-	10/35/35/53	-
15	PTY	a	605	-	-	16/37/37/53	-
14	HEA	a	602	1	3/3/7/16	11/32/76/76	-
14	HEA	a	603	1	3/3/7/16	7/32/76/76	-
18	PCF	c	302	-	-	21/46/46/53	-
15	PTY	c	301	-	-	19/43/43/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	PCF	e	202	-	-	14/39/39/53	-
18	PCF	m	101	-	-	15/41/41/53	-
15	PTY	b	302	-	-	17/43/43/53	-
15	PTY	a	604	-	-	12/36/36/53	-
15	PTY	i	101	-	-	15/33/33/53	-
15	PTY	b	303	-	-	23/44/44/53	-

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	603	HEA	C3C-C2C	-4.66	1.33	1.40
14	a	603	HEA	C3A-CMA	-4.58	1.35	1.46
14	a	602	HEA	C3C-C2C	-4.36	1.34	1.40
14	a	602	HEA	C3A-CMA	-4.29	1.36	1.46
15	e	201	PTY	O4-C30	3.99	1.45	1.33

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	i	101	PTY	O7-C8-C11	4.44	121.07	111.50
15	b	302	PTY	O7-C8-C11	4.22	120.60	111.50
16	a	606	CN3	O51-C51-C52	4.17	120.49	111.50
15	c	301	PTY	O7-C8-C11	4.03	120.19	111.50
15	b	303	PTY	O7-C8-C11	4.00	120.13	111.50

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	a	602	HEA	ND
14	a	602	HEA	NB
14	a	602	HEA	NA
14	a	603	HEA	ND
14	a	603	HEA	NB

5 of 217 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	a	602	HEA	C13-C14-C15-C26
14	a	602	HEA	C17-C18-C19-C27
14	a	602	HEA	C21-C22-C23-C25

Continued on next page...

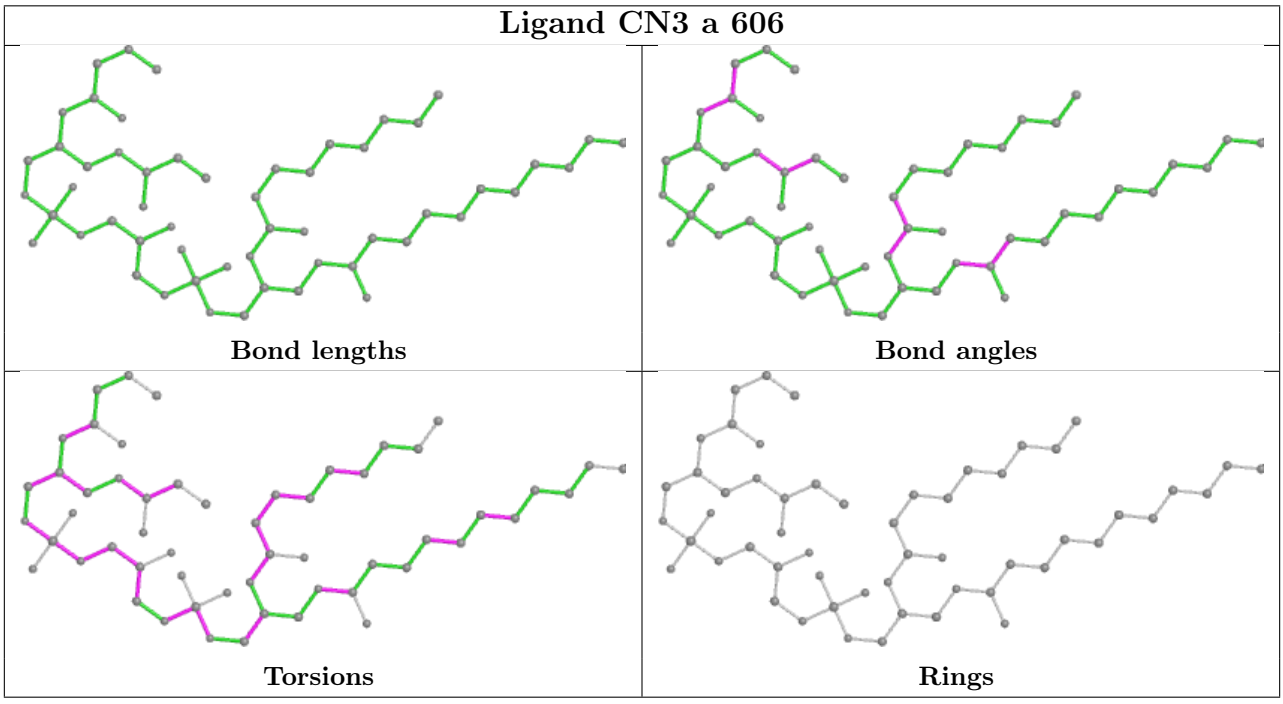
Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a	604	PTY	C3-O11-P1-O13
15	a	604	PTY	C3-O11-P1-O14

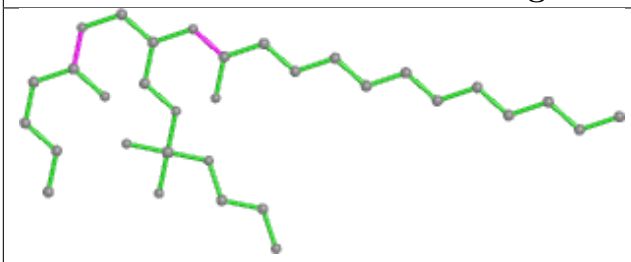
There are no ring outliers.

No monomer is involved in short contacts.

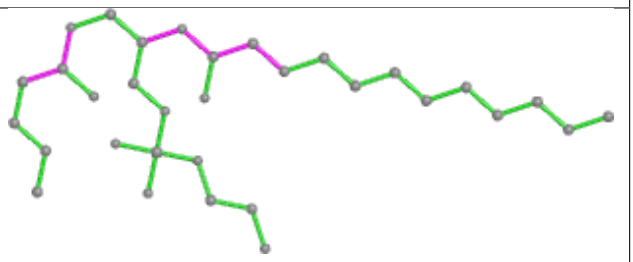
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



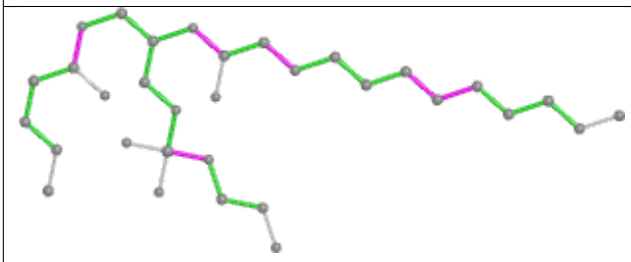
Ligand PTY e 201



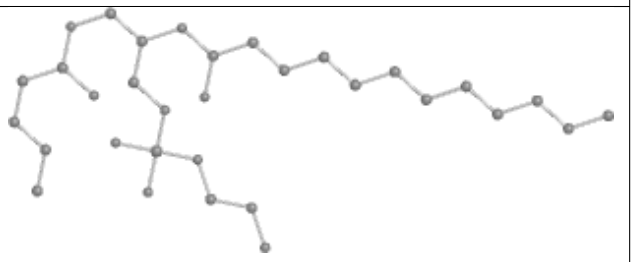
Bond lengths



Bond angles

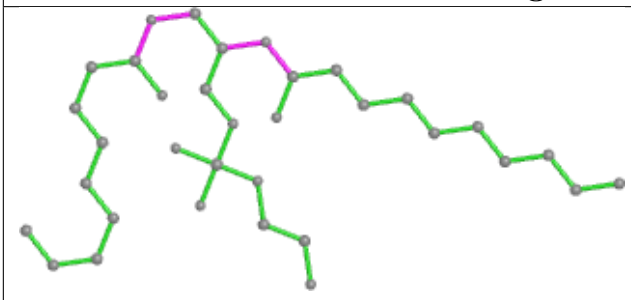


Torsions

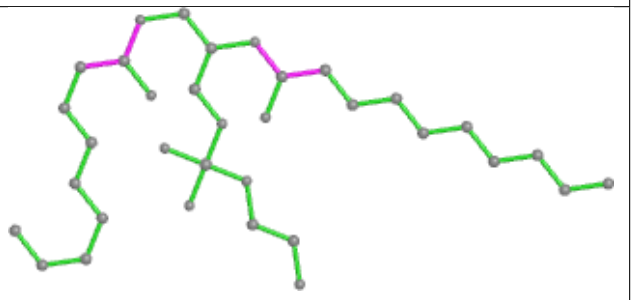


Rings

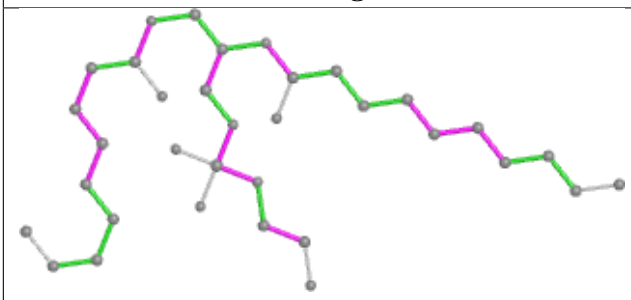
Ligand PTY a 605



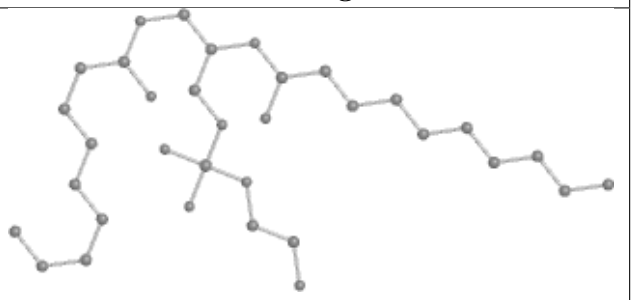
Bond lengths



Bond angles

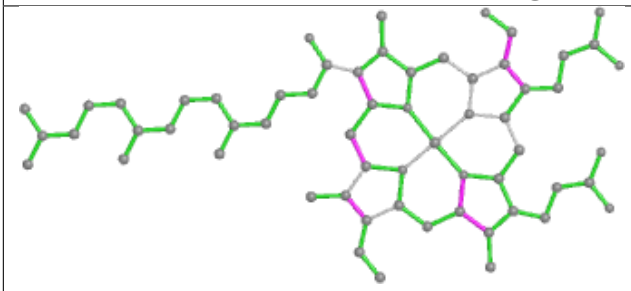


Torsions

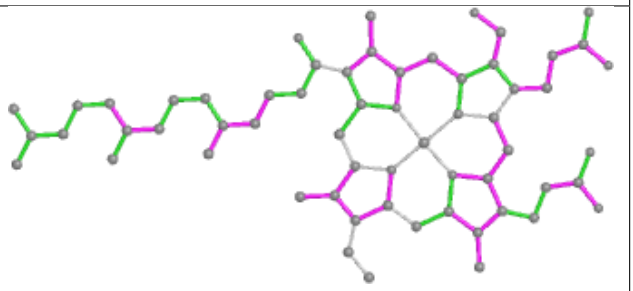


Rings

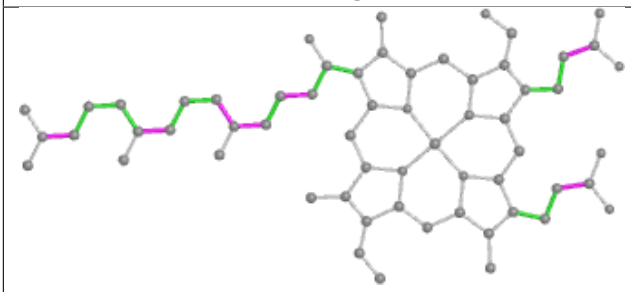
Ligand HEA a 602



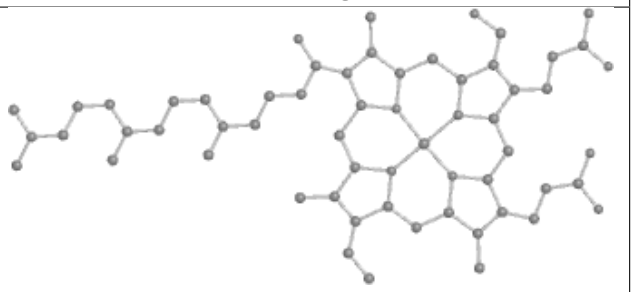
Bond lengths



Bond angles

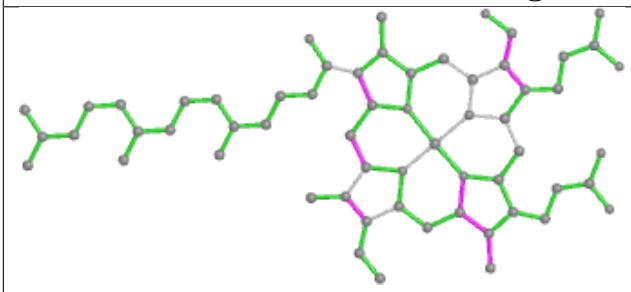


Torsions

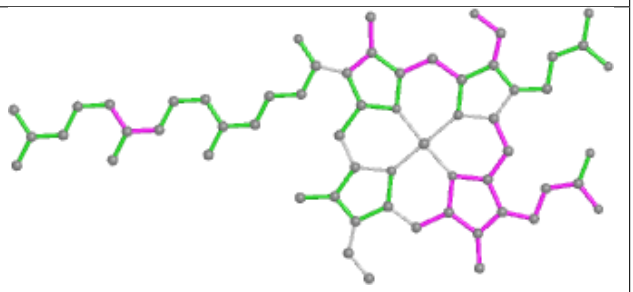


Rings

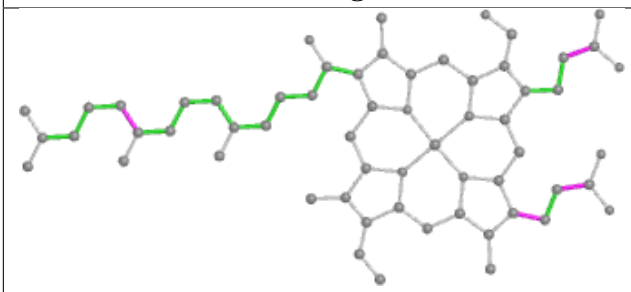
Ligand HEA a 603



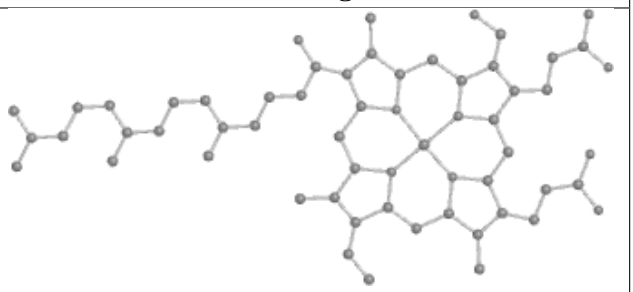
Bond lengths



Bond angles

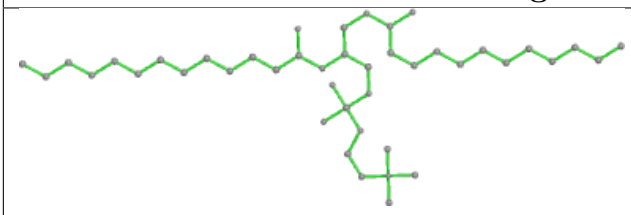


Torsions

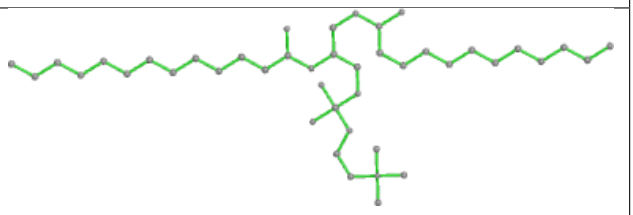


Rings

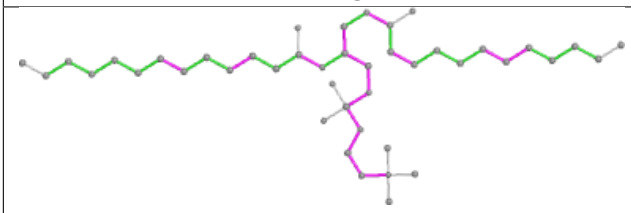
Ligand PCF c 302



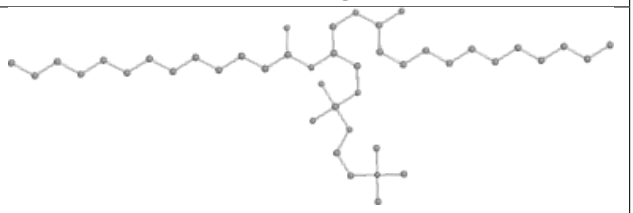
Bond lengths



Bond angles



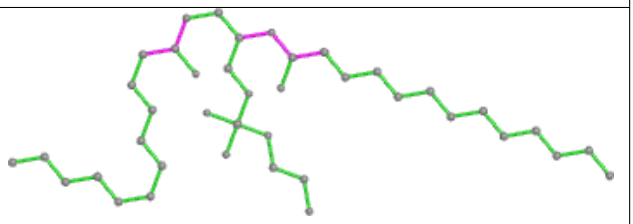
Torsions



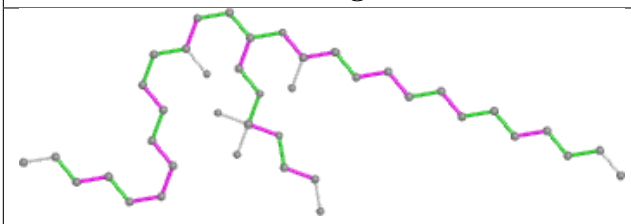
Rings

Ligand PTY c 301

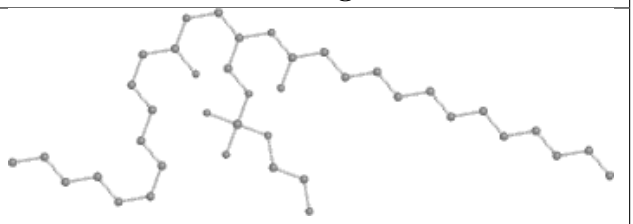
Bond lengths



Bond angles

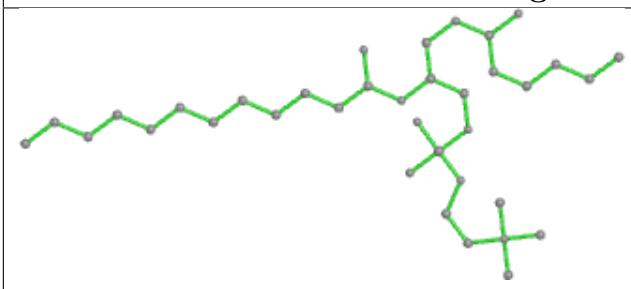


Torsions

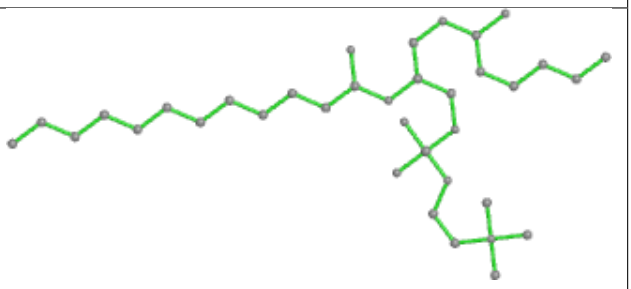


Rings

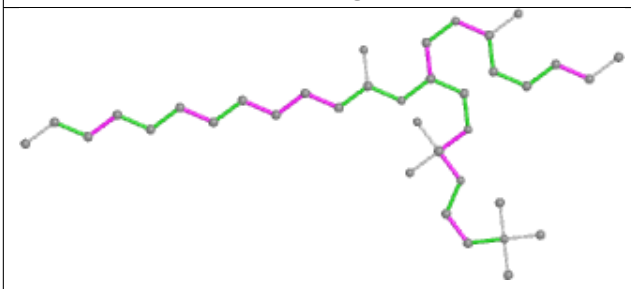
Ligand PCF e 202



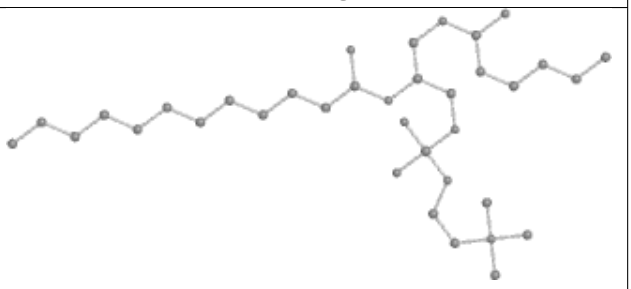
Bond lengths



Bond angles

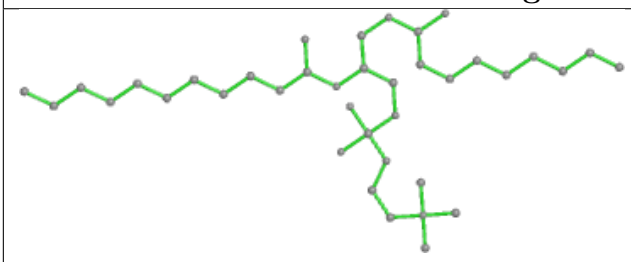


Torsions

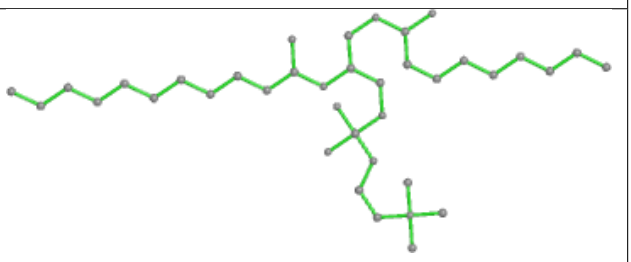


Rings

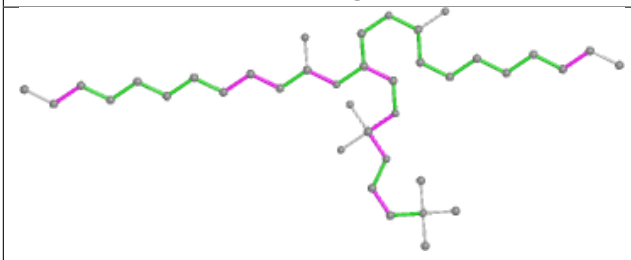
Ligand PCF m 101



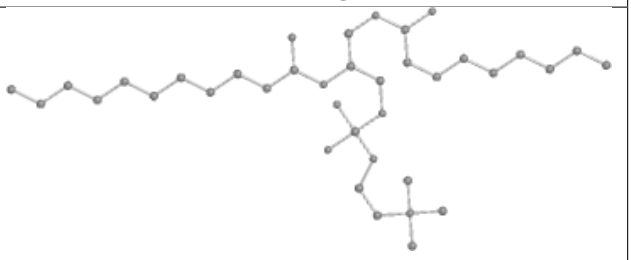
Bond lengths



Bond angles

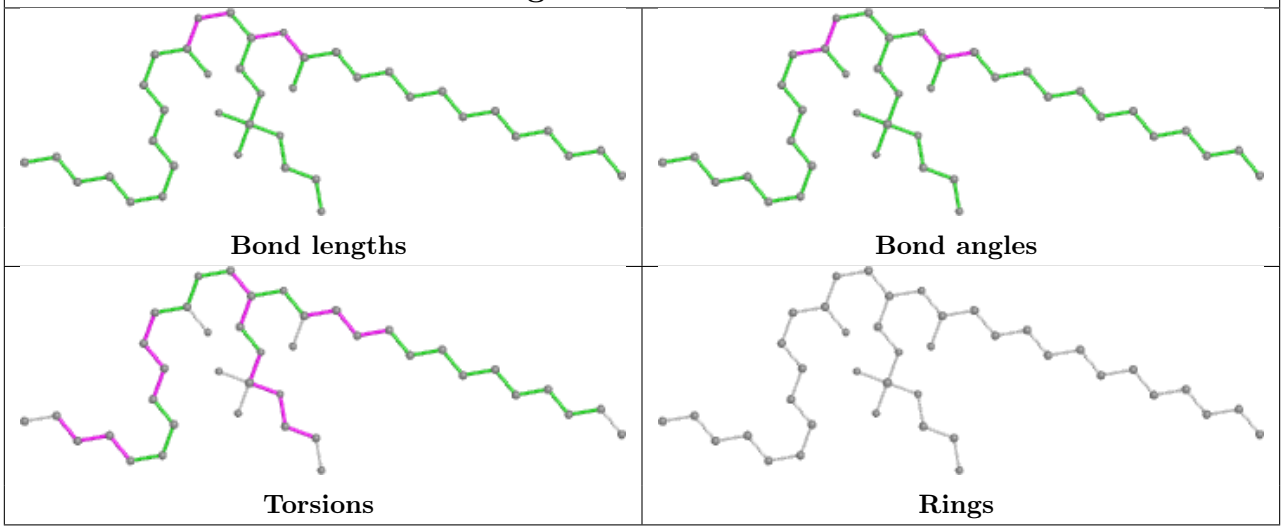


Torsions

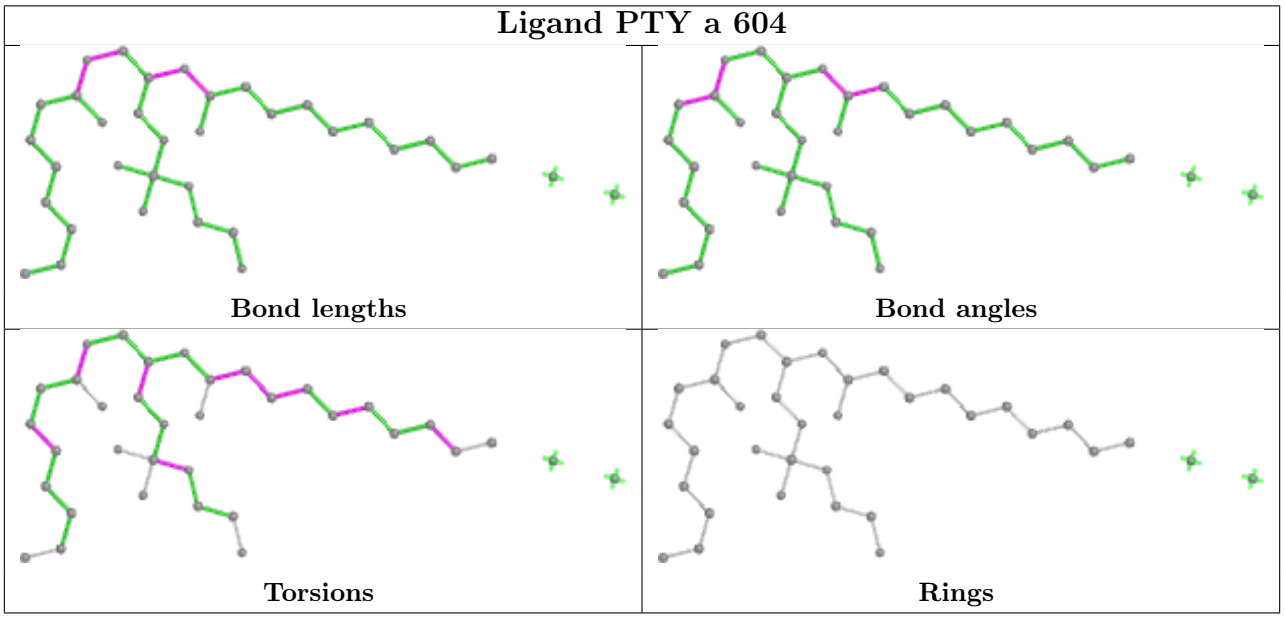


Rings

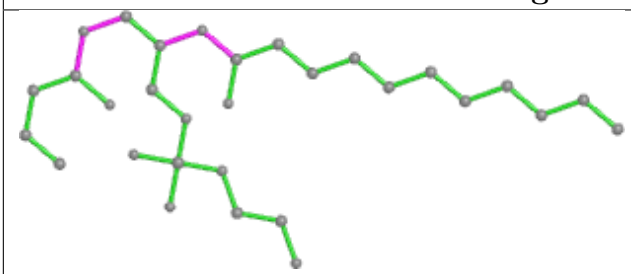
Ligand PTY b 302



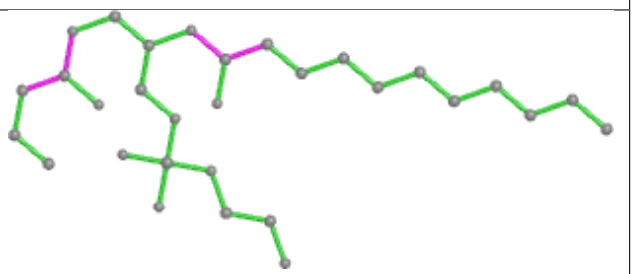
Ligand PTY a 604



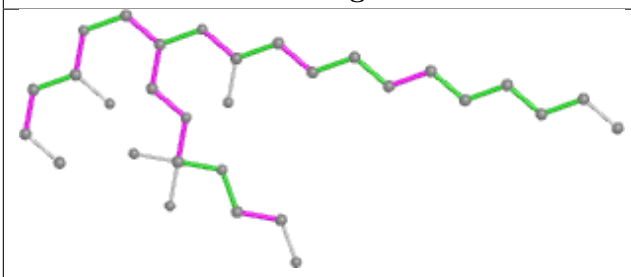
Ligand PTY i 101



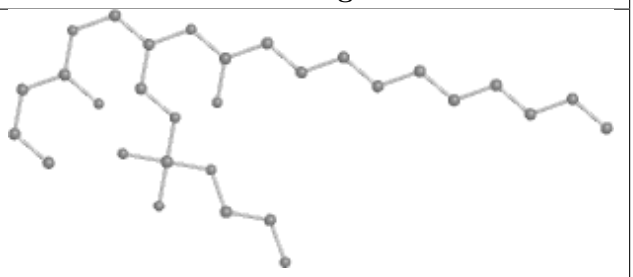
Bond lengths



Bond angles

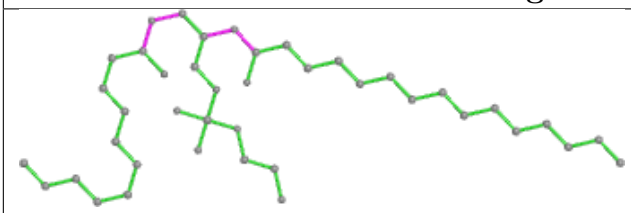


Torsions

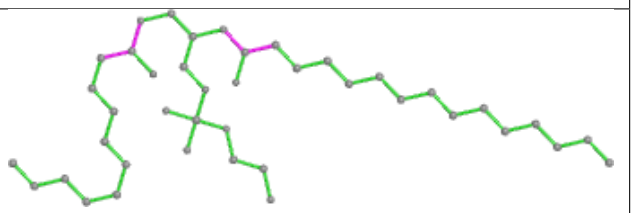


Rings

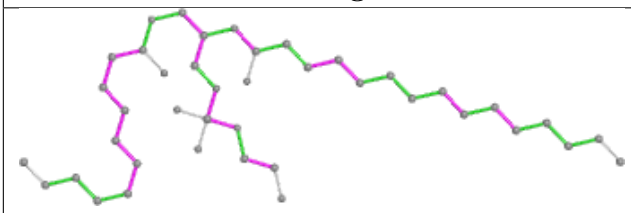
Ligand PTY b 303



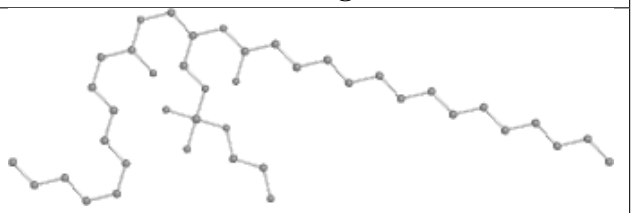
Bond lengths



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.

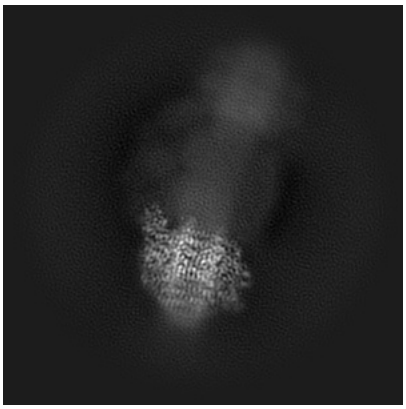
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10848. These allow visual inspection of the internal detail of the map and identification of artifacts.

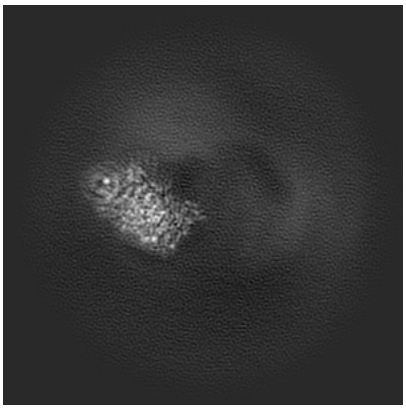
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

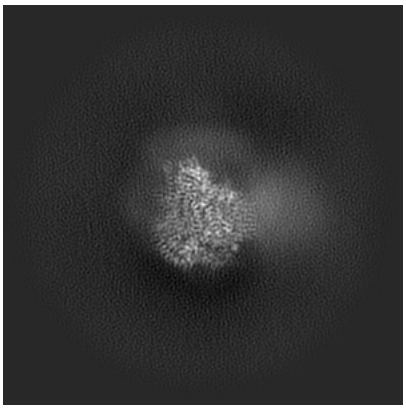
6.1.1 Primary map



X

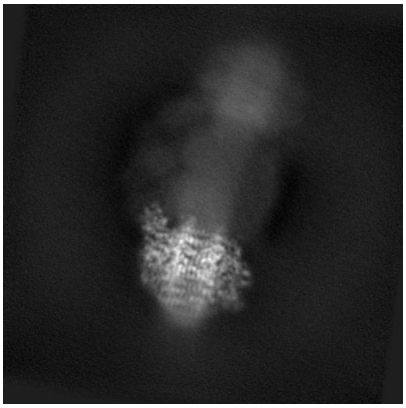


Y

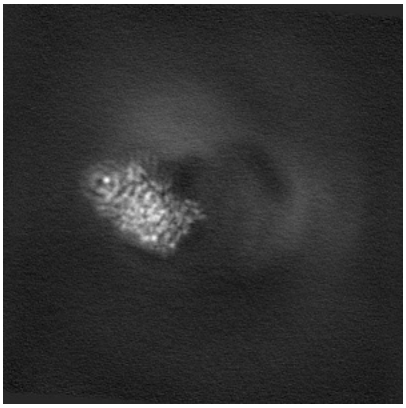


Z

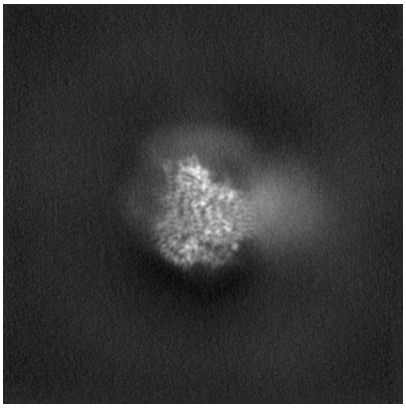
6.1.2 Raw map



X



Y

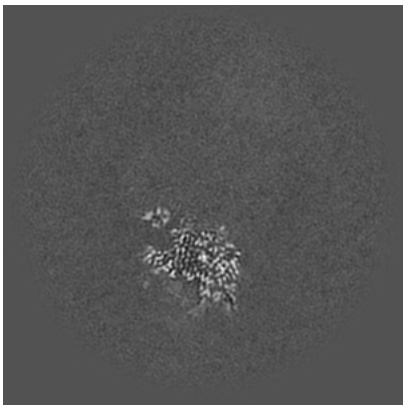


Z

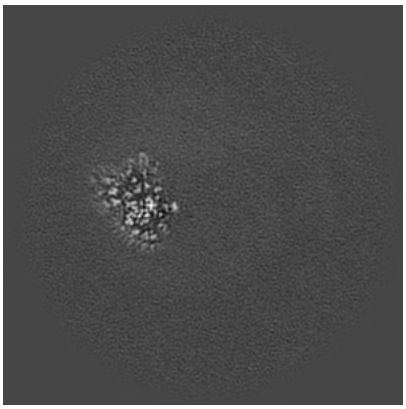
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

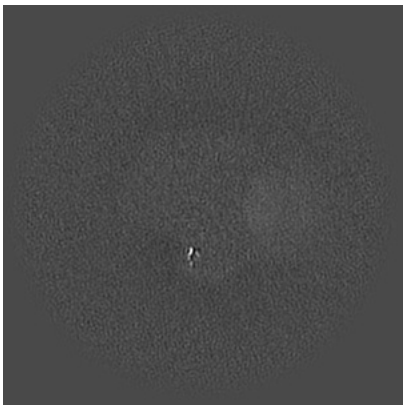
6.2.1 Primary map



X Index: 185

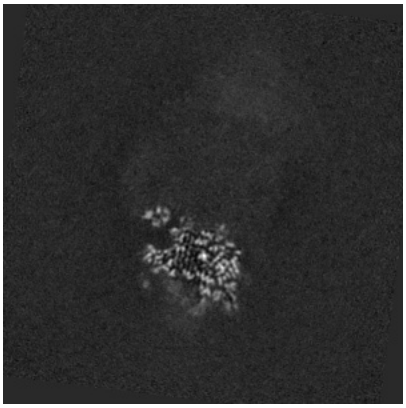


Y Index: 185

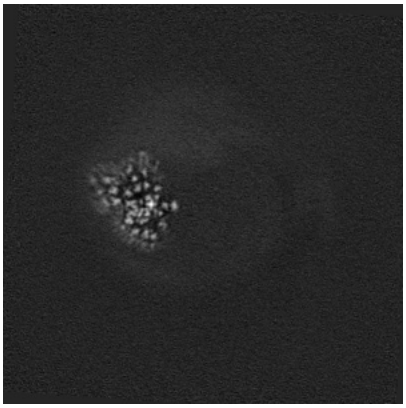


Z Index: 185

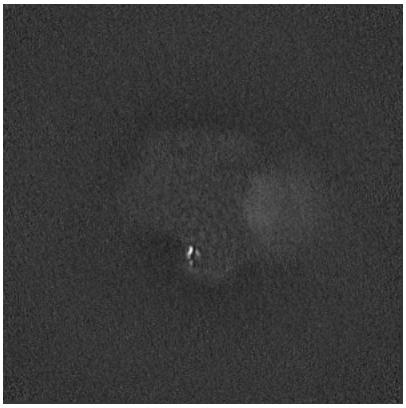
6.2.2 Raw map



X Index: 185



Y Index: 185

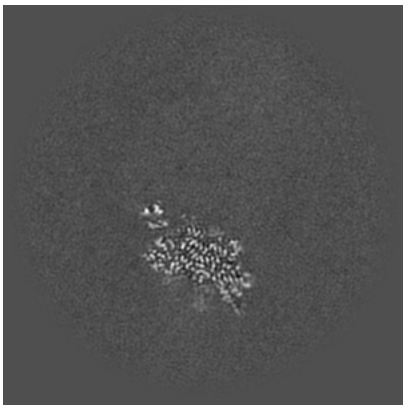


Z Index: 185

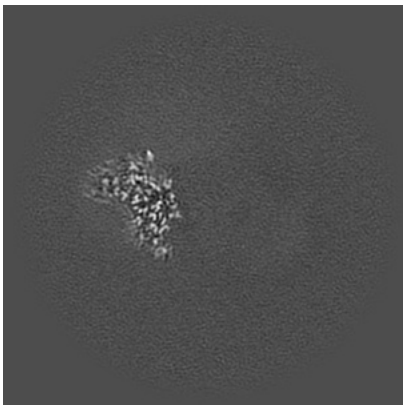
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

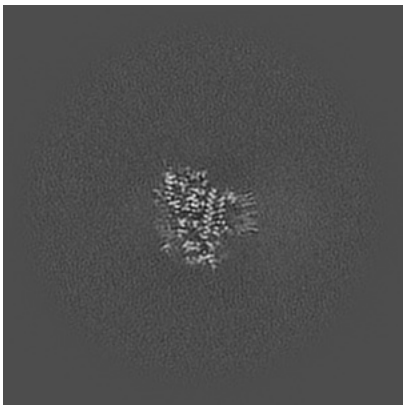
6.3.1 Primary map



X Index: 178

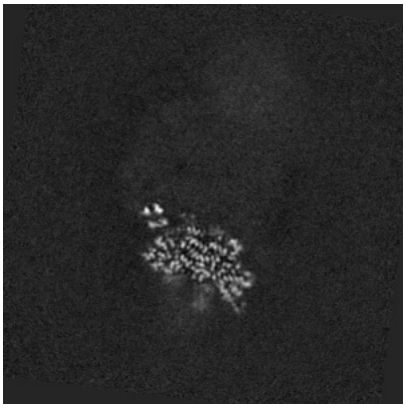


Y Index: 162

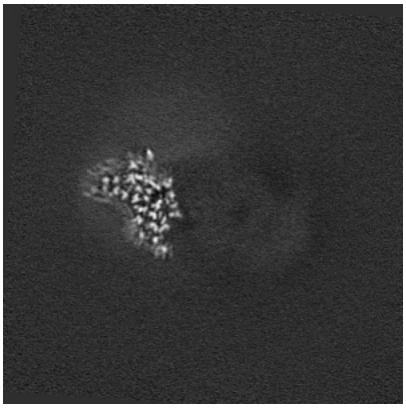


Z Index: 133

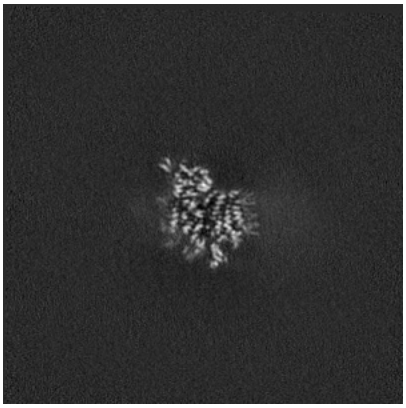
6.3.2 Raw map



X Index: 178



Y Index: 162

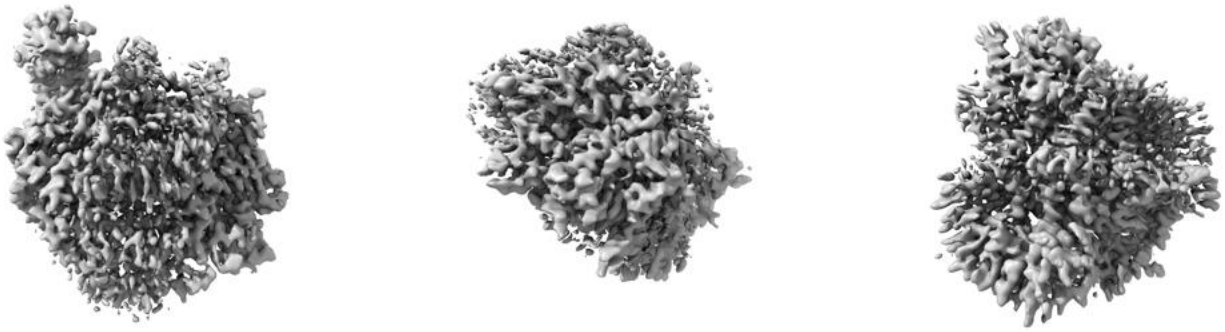


Z Index: 126

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

6.4 Orthogonal surface views (i)

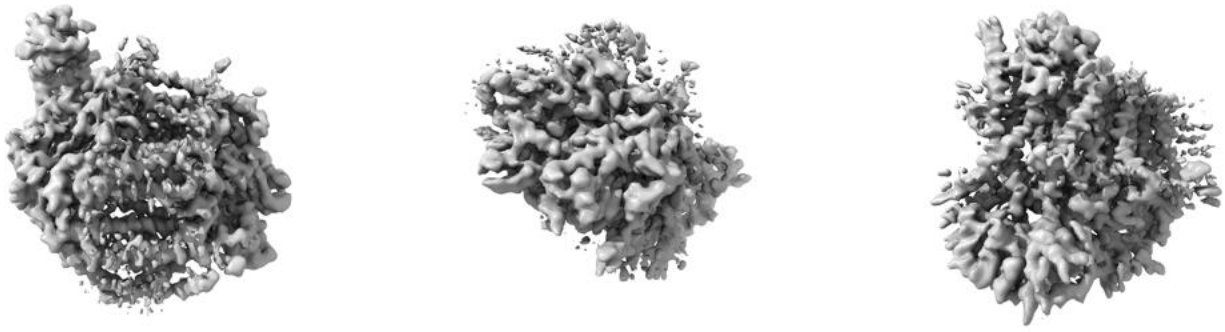
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.41. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

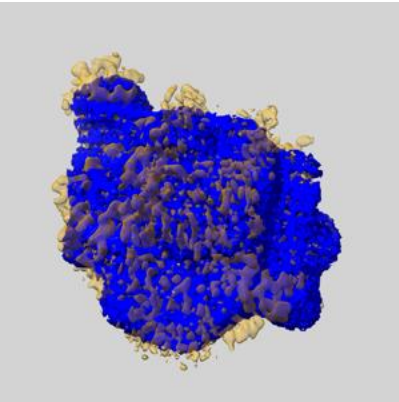
6.5 Mask visualisation (i)

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

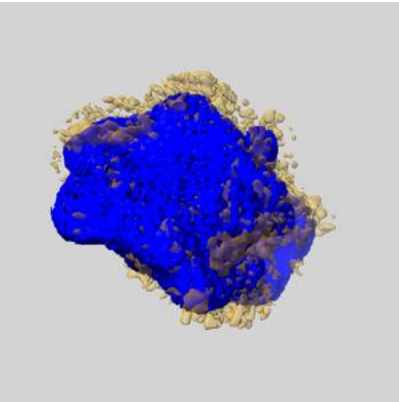
A mask typically either:

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

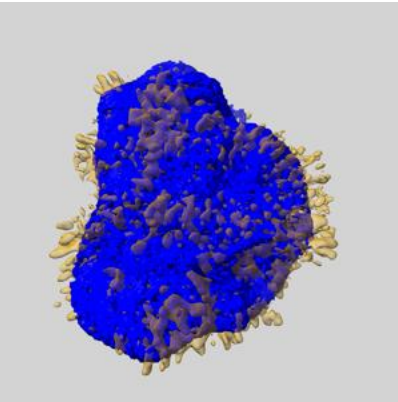
6.5.1 emd_10848_msk_1.map (i)



X



Y

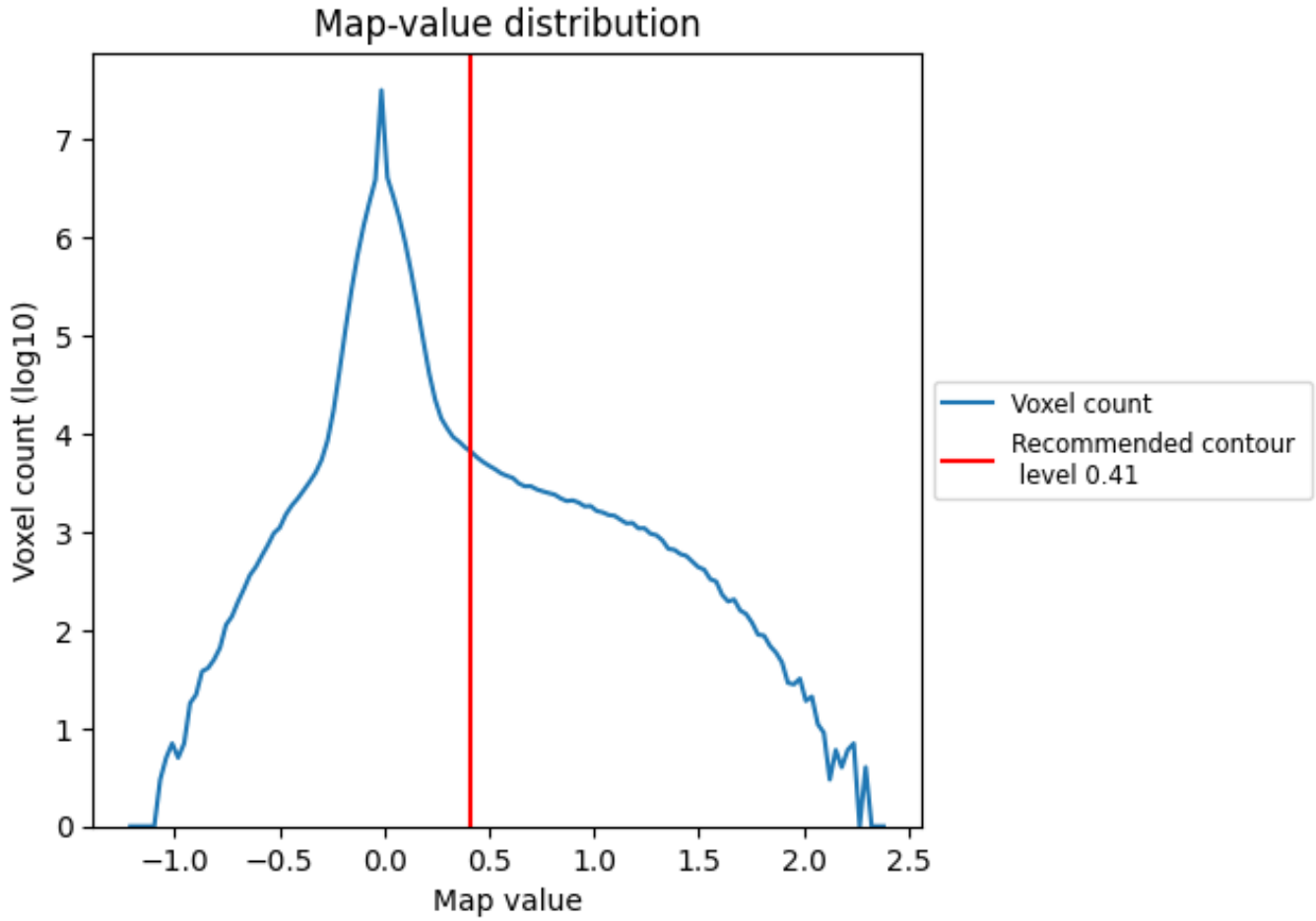


Z

7 Map analysis

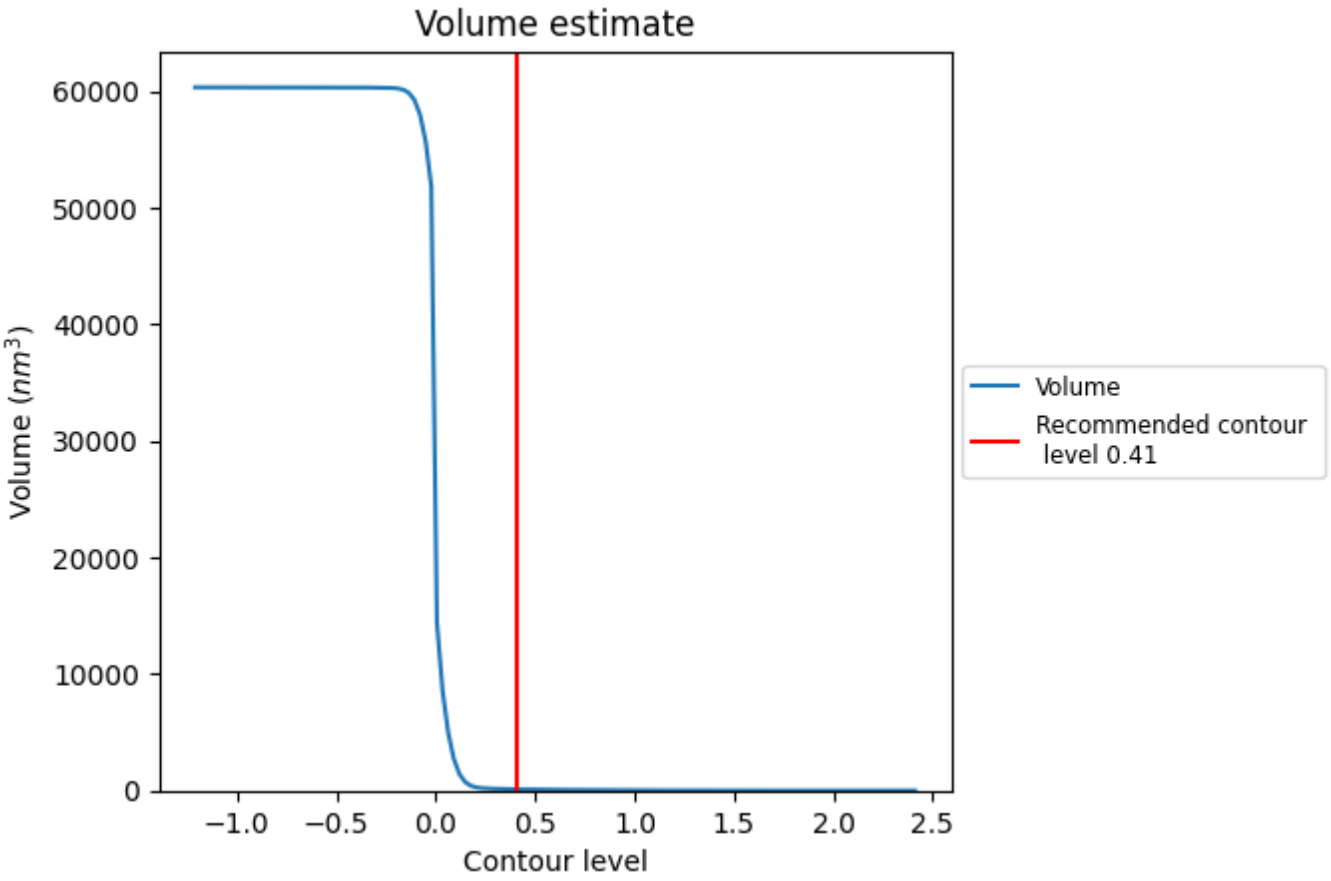
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

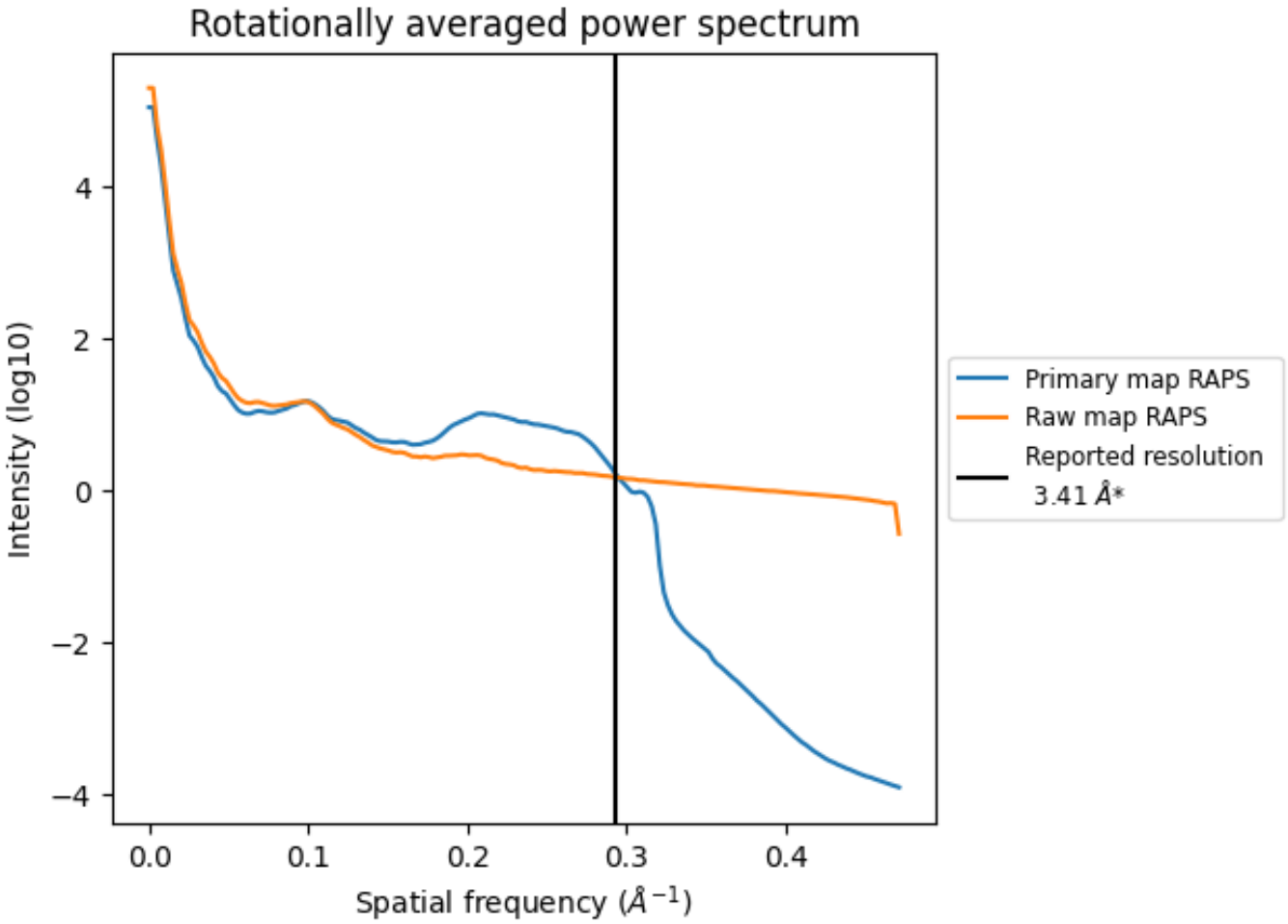
7.2 Volume estimate (i)



The volume at the recommended contour level is 109 nm^3; this corresponds to an approximate mass of 98 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 0.293 Å^{-1}

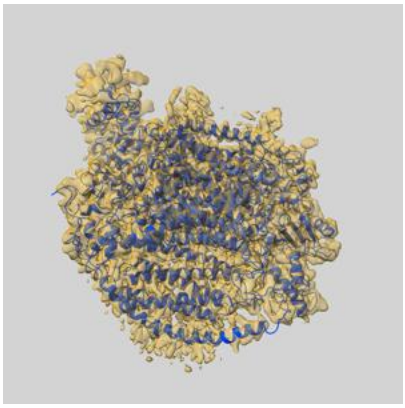
8 Fourier-Shell correlation

This section was not generated.

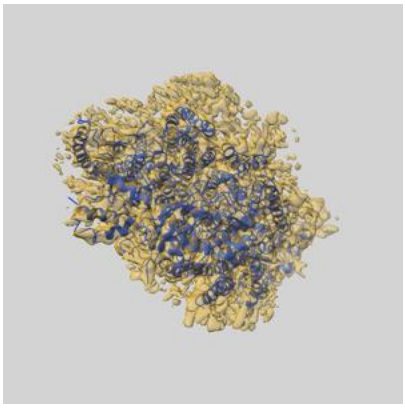
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10848 and PDB model 6YMY. Per-residue inclusion information can be found in section 3 on page 10.

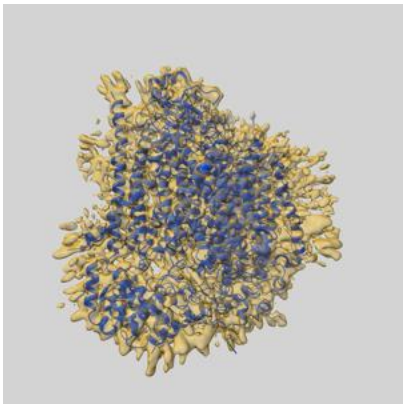
9.1 Map-model overlay



X



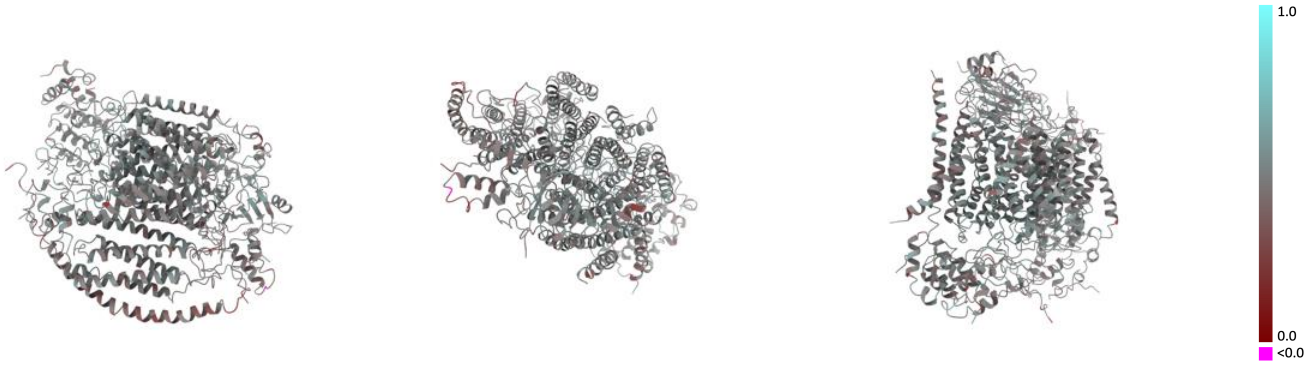
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.41 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.

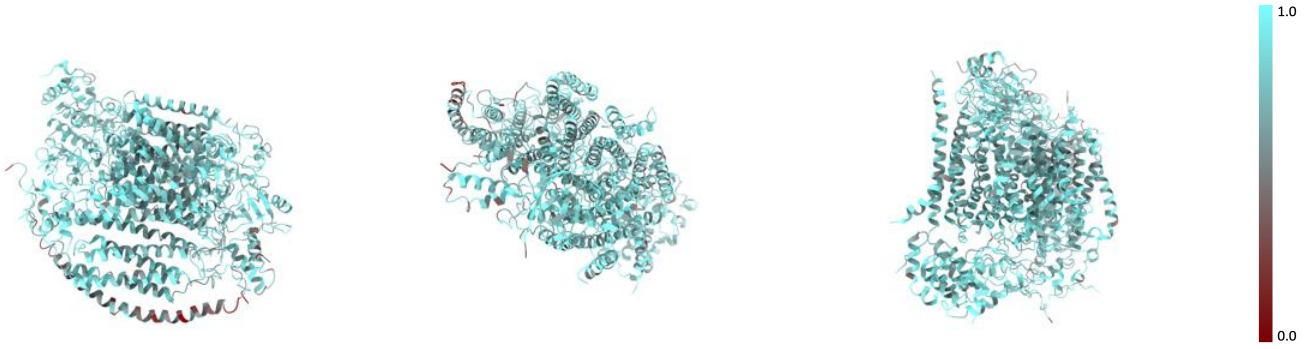
9.2 Q-score mapped to coordinate model



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.

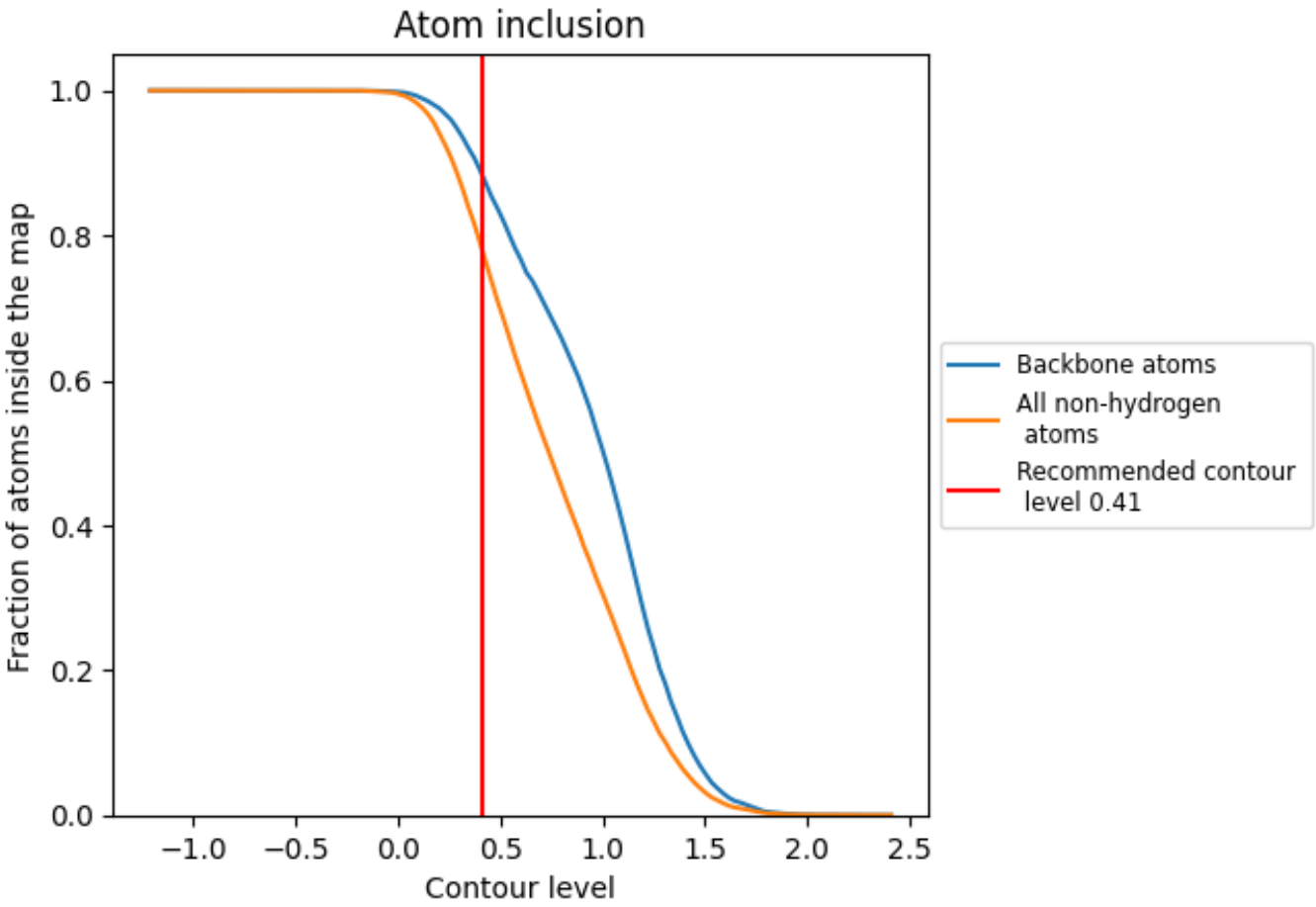
9.3 Atom inclusion mapped to coordinate model



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 (0.41).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 78% 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 (0.41) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7817	0.4830
a	0.7974	0.5060
b	0.8020	0.4950
c	0.7870	0.4830
d	0.8206	0.4760
e	0.7812	0.4710
f	0.8267	0.4750
g	0.8423	0.4810
h	0.8065	0.4900
i	0.7708	0.4730
j	0.7429	0.4430
k	0.5832	0.4130
m	0.7456	0.4720