Full wwPDB EM Validation 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 Full wwPDB EM Validation Report for a publicly released PDB entry.

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

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

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

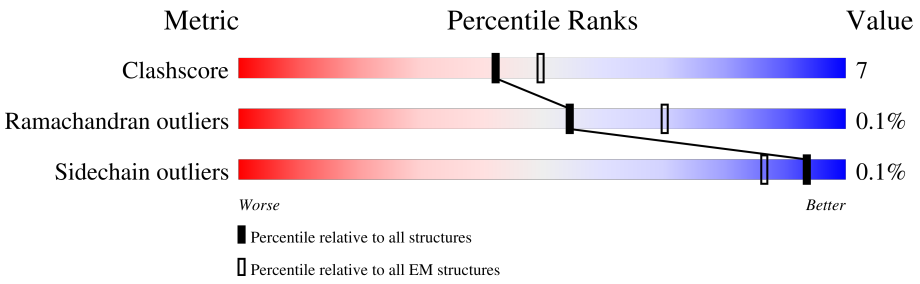
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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%

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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
			Total	C	N	O		
7	g	55	456	310	77	69	0	0

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

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

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

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

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

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

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

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

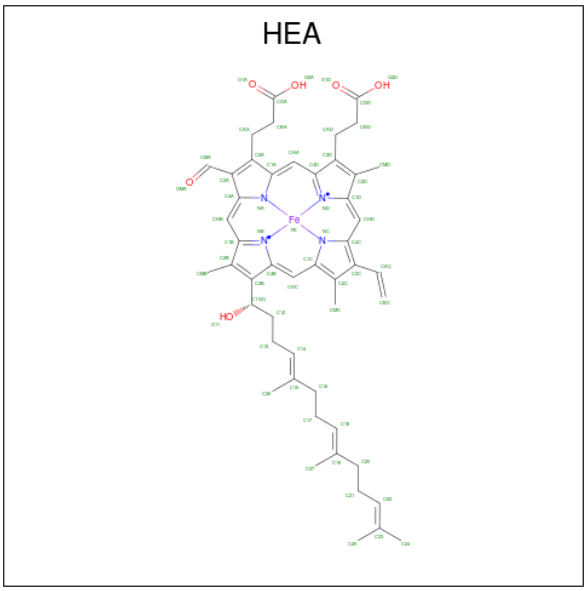
- Molecule 12 is a protein called Cytochrome c oxidase subunit 26, mitochondrial.

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

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

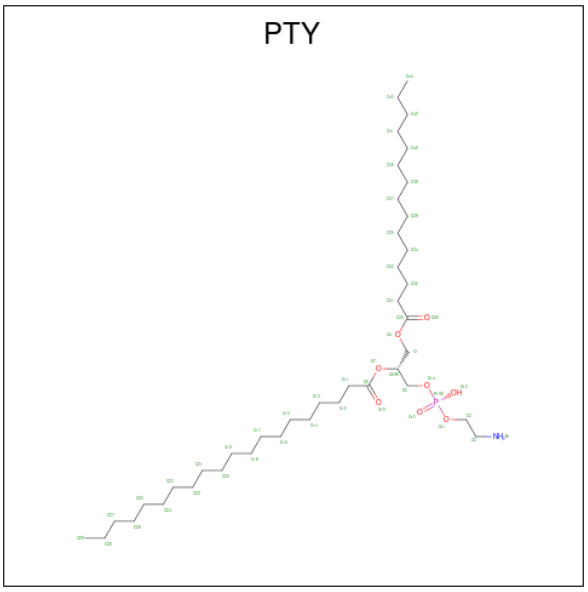
Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
13	a	1	1	1	0

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



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

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



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

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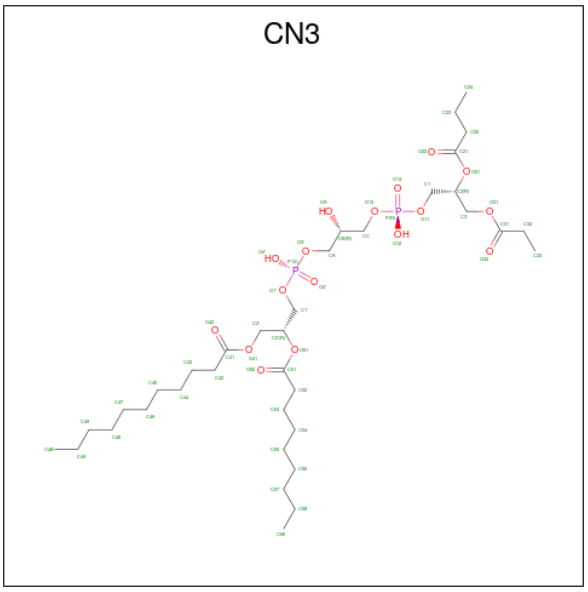
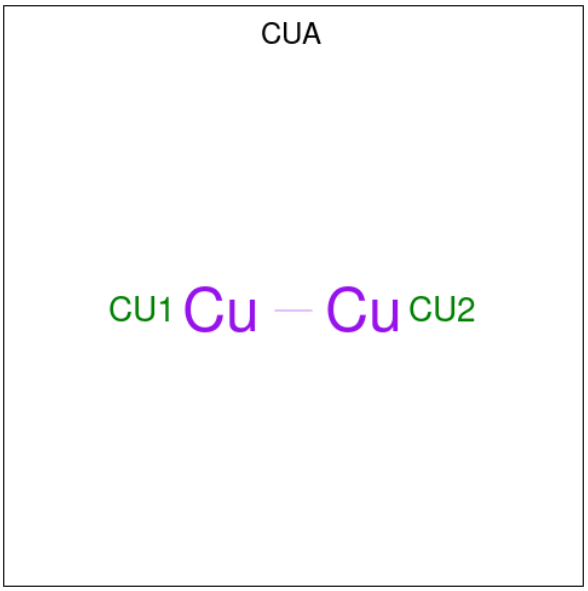
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
15	a	1	69	49	2	16	2	0
15	b	1	81	61	2	16	2	0
15	b	1	81	61	2	16	2	0
15	c	1	40	30	1	8	1	0
15	e	1	32	22	1	8	1	0
15	i	1	30	20	1	8	1	0

- 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: $C_{36}H_{68}O_{17}P_2$).



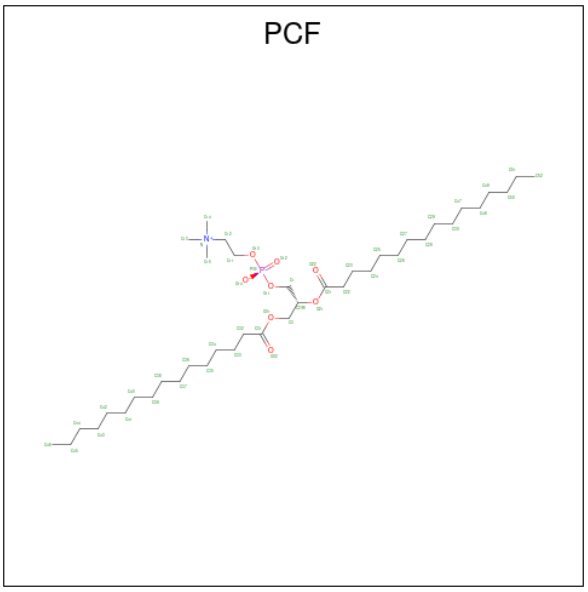
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
16	a	1	55	36	17	2	0

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



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

- 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
			Total	C	N	O	P	
18	c	1	43	33	1	8	1	0
			Total	C	N	O	P	
18	e	1	36	26	1	8	1	0

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

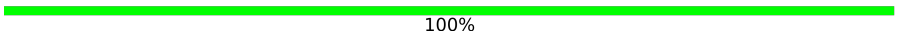
- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

3 Residue-property plots (i)

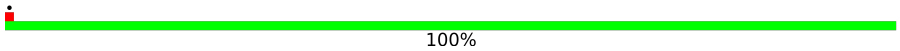
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

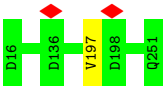
• Molecule 1: Cytochrome c oxidase subunit 1

Chain a: 

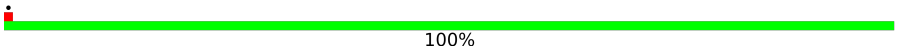
There are no outlier residues recorded for this chain.

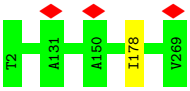
• Molecule 2: Cytochrome c oxidase subunit 2

Chain b: 

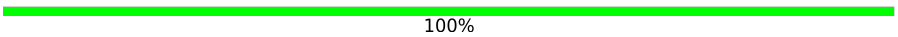


• Molecule 3: Cytochrome c oxidase subunit 3

Chain c: 

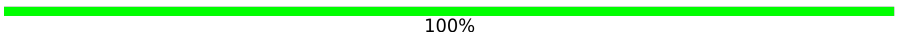


• Molecule 4: Cytochrome c oxidase subunit 4, mitochondrial

Chain d: 

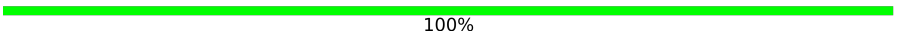
There are no outlier residues recorded for this chain.

• 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: 100%

• Molecule 8: Cytochrome c oxidase subunit 8, mitochondrial

Chain h: 100%

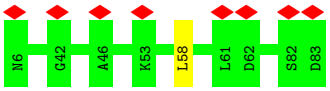
• Molecule 9: Cytochrome c oxidase subunit 9, mitochondrial

Chain i: 100%

There are no outlier residues recorded for this chain.

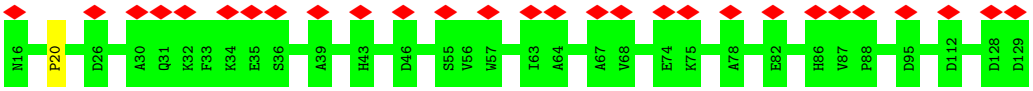
• Molecule 10: Cytochrome c oxidase subunit 12, mitochondrial

Chain j: 10% 99%



• Molecule 11: Cytochrome c oxidase subunit 13, mitochondrial

Chain k: 25% 99%



• Molecule 12: Cytochrome c oxidase subunit 26, mitochondrial

Chain m: 100%

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 (i)

5.1 Standard geometry (i)

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	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

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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. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	215	ASN
1	a	234	HIS
1	a	411	GLN
1	a	451	ASN
1	a	478	ASN
1	a	482	ASN
1	a	528	ASN
2	b	32	ASN
3	c	10	GLN
3	c	47	ASN
3	c	49	ASN
3	c	79	HIS
3	c	226	ASN
5	e	57	GLN
5	e	63	GLN
6	f	75	ASN
6	f	117	ASN
7	g	9	GLN
10	j	6	ASN
10	j	35	HIS
10	j	70	GLN

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	-
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	-

All (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
15	e	201	PTY	O7-C8	3.57	1.44	1.34
14	a	603	HEA	C1D-C2D	2.72	1.49	1.44
15	c	301	PTY	O7-C6	-2.70	1.39	1.46
15	b	303	PTY	O7-C6	-2.63	1.40	1.46
15	a	605	PTY	O7-C6	-2.59	1.40	1.46
14	a	603	HEA	C1C-CHC	-2.50	1.34	1.41
15	a	604	PTY	O7-C6	-2.48	1.40	1.46
15	i	101	PTY	O4-C30	2.47	1.40	1.33
15	b	302	PTY	O7-C6	-2.47	1.40	1.46
14	a	602	HEA	C4B-C3B	2.46	1.48	1.44
15	i	101	PTY	O7-C6	-2.44	1.40	1.46
15	c	301	PTY	O4-C30	2.44	1.40	1.33
15	b	303	PTY	O4-C30	2.43	1.40	1.33
15	b	302	PTY	O4-C30	2.41	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	a	605	PTY	O4-C30	2.36	1.40	1.33
15	a	605	PTY	O4-C1	-2.33	1.39	1.45
14	a	603	HEA	C3A-C2A	-2.32	1.37	1.40
14	a	602	HEA	C1C-CHC	-2.31	1.34	1.41
15	a	604	PTY	O4-C30	2.28	1.40	1.33
15	a	604	PTY	O4-C1	-2.27	1.40	1.45
14	a	603	HEA	C1D-ND	-2.26	1.36	1.40
14	a	603	HEA	CMD-C2D	2.24	1.55	1.50
15	b	302	PTY	O4-C1	-2.21	1.40	1.45
15	i	101	PTY	O7-C8	2.21	1.40	1.34
14	a	602	HEA	C3A-C2A	-2.20	1.37	1.40
15	a	605	PTY	O7-C8	2.19	1.40	1.34
14	a	602	HEA	C1D-C2D	2.17	1.48	1.44
15	b	302	PTY	O7-C8	2.16	1.40	1.34
15	c	301	PTY	O4-C1	-2.15	1.40	1.45
15	a	604	PTY	O7-C8	2.14	1.40	1.34
15	b	303	PTY	O4-C1	-2.13	1.40	1.45
15	i	101	PTY	O4-C1	-2.10	1.40	1.45
14	a	603	HEA	C4B-C3B	2.08	1.48	1.44
15	c	301	PTY	O7-C8	2.05	1.40	1.34
15	b	303	PTY	O7-C8	2.05	1.40	1.34
14	a	602	HEA	C1D-ND	-2.02	1.36	1.40

All (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
16	a	606	CN3	O21-C21-C22	3.99	120.11	111.50
15	a	604	PTY	O7-C8-C11	3.92	119.95	111.50
15	a	605	PTY	O7-C8-C11	3.92	119.95	111.50
15	e	201	PTY	C6-O7-C8	-3.75	108.55	117.79
14	a	602	HEA	CMD-C2D-C1D	3.58	130.49	125.04
14	a	602	HEA	C4A-CHB-C1B	3.34	126.96	122.56
14	a	603	HEA	C3D-C4D-ND	3.33	113.58	110.36
14	a	603	HEA	CBD-CAD-C3D	3.30	121.79	112.63
16	a	606	CN3	O31-C31-C32	3.25	119.92	111.38
14	a	602	HEA	CBA-CAA-C2A	3.23	118.05	112.60
14	a	603	HEA	CAD-C3D-C2D	3.14	133.72	127.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	e	201	PTY	O7-C8-C11	3.05	118.06	111.50
14	a	603	HEA	CAD-C3D-C4D	-3.03	119.36	124.66
14	a	603	HEA	OMA-CMA-C3A	-3.03	118.31	124.91
14	a	603	HEA	CHA-C4D-C3D	-2.85	120.64	124.84
14	a	603	HEA	C20-C19-C18	-2.84	115.36	121.12
14	a	603	HEA	C1D-C2D-C3D	-2.80	104.01	106.96
16	a	606	CN3	O41-C41-C42	2.77	120.59	111.91
15	a	605	PTY	O4-C30-C31	2.76	120.58	111.91
14	a	602	HEA	C26-C15-C14	-2.73	116.68	123.68
15	i	101	PTY	O4-C30-C31	2.68	120.32	111.91
14	a	603	HEA	C4A-CHB-C1B	2.67	126.08	122.56
14	a	603	HEA	CMD-C2D-C1D	2.64	129.05	125.04
14	a	602	HEA	CMC-C2C-C1C	-2.63	124.42	128.46
14	a	603	HEA	C4D-CHA-C1A	2.59	125.97	122.56
15	a	604	PTY	O4-C30-C31	2.58	120.01	111.91
15	b	303	PTY	O4-C30-C31	2.57	119.97	111.91
14	a	602	HEA	OMA-CMA-C3A	-2.53	119.40	124.91
15	c	301	PTY	O4-C30-C31	2.50	119.75	111.91
14	a	602	HEA	C3D-C4D-ND	2.43	112.71	110.36
14	a	602	HEA	CMC-C2C-C3C	2.43	129.22	124.68
14	a	602	HEA	C4D-CHA-C1A	2.38	125.70	122.56
15	b	302	PTY	O4-C30-C31	2.36	119.32	111.91
14	a	603	HEA	CMB-C2B-C3B	-2.36	125.84	130.34
14	a	602	HEA	C1D-C2D-C3D	-2.34	104.49	106.96
14	a	602	HEA	O1D-CGD-CBD	-2.32	115.63	123.08
14	a	602	HEA	C2B-C1B-NB	2.32	112.66	109.88
14	a	602	HEA	C13-C14-C15	-2.24	122.27	127.66
14	a	602	HEA	O1A-CGA-CBA	-2.24	115.89	123.08
14	a	603	HEA	CHD-C1D-ND	-2.23	121.62	124.38
14	a	602	HEA	C3C-C4C-NC	2.21	112.07	109.21
15	e	201	PTY	O4-C30-C31	2.19	118.78	111.91
14	a	602	HEA	CHA-C4D-C3D	-2.18	121.64	124.84
15	c	301	PTY	C6-O7-C8	-2.14	112.52	117.79
14	a	602	HEA	C20-C19-C18	-2.13	116.81	121.12
14	a	603	HEA	O1D-CGD-CBD	-2.13	116.24	123.08
14	a	602	HEA	CMB-C2B-C3B	-2.13	126.28	130.34
15	e	201	PTY	C12-C11-C8	-2.03	106.25	113.62

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	a	602	HEA	ND

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

All (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
15	a	604	PTY	C3-O11-P1-O13
15	a	604	PTY	C3-O11-P1-O14
15	a	605	PTY	C3-O11-P1-O12
15	a	605	PTY	C5-O14-P1-O13
15	b	303	PTY	O10-C8-O7-C6
15	b	303	PTY	C11-C8-O7-C6
15	b	303	PTY	C5-O14-P1-O12
15	b	303	PTY	C5-O14-P1-O13
15	c	301	PTY	N1-C2-C3-O11
15	c	301	PTY	O14-C5-C6-O7
15	e	201	PTY	C11-C8-O7-C6
15	e	201	PTY	C3-O11-P1-O12
15	e	201	PTY	C3-O11-P1-O13
15	e	201	PTY	C3-O11-P1-O14
15	i	101	PTY	O4-C1-C6-O7
15	i	101	PTY	O10-C8-O7-C6
15	i	101	PTY	C11-C8-O7-C6
15	i	101	PTY	C5-O14-P1-O13
16	a	606	CN3	C1-O11-P-O12
16	a	606	CN3	C1-O11-P-O14
16	a	606	CN3	C1'-O1'-P'-O2'
16	a	606	CN3	CA-O3'-P'-O1'
16	a	606	CN3	CA-O3'-P'-O4'
16	a	606	CN3	O1'-C1'-C2'-O51
16	a	606	CN3	C52-C51-O51-C2'
18	c	302	PCF	C1-O11-P-O12
18	c	302	PCF	C1-O11-P-O13
18	c	302	PCF	O13-C11-C12-N
18	c	302	PCF	C22-C21-O21-C2
18	m	101	PCF	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
18	m	101	PCF	C11-O13-P-O12
18	m	101	PCF	C11-O13-P-O14
18	m	101	PCF	O13-C11-C12-N
15	a	605	PTY	O30-C30-O4-C1
15	a	604	PTY	O30-C30-O4-C1
15	e	201	PTY	O10-C8-O7-C6
16	a	606	CN3	O52-C51-O51-C2'
18	c	302	PCF	O22-C21-O21-C2
15	a	604	PTY	C31-C30-O4-C1
15	a	605	PTY	C31-C30-O4-C1
16	a	606	CN3	OA-CB-CC-O13
14	a	602	HEA	C21-C22-C23-C24
16	a	606	CN3	O3'-CA-CB-CC
14	a	602	HEA	C17-C18-C19-C20
18	c	302	PCF	C11-C12-N-C13
18	c	302	PCF	C11-C12-N-C15
16	a	606	CN3	O3'-CA-CB-OA
16	a	606	CN3	O21-C2-C3-O31
15	a	604	PTY	C8-C11-C12-C13
15	b	302	PTY	C8-C11-C12-C13
15	b	303	PTY	C30-C31-C32-C33
15	a	605	PTY	C30-C31-C32-C33
14	a	603	HEA	C4D-C3D-CAD-CBD
15	a	605	PTY	C3-O11-P1-O14
15	b	303	PTY	C5-O14-P1-O11
16	a	606	CN3	C1-O11-P-O13
16	a	606	CN3	C1'-O1'-P'-O3'
18	e	202	PCF	C21-C22-C23-C24
15	a	605	PTY	C11-C8-O7-C6
15	b	303	PTY	C33-C34-C35-C36
15	e	201	PTY	C14-C15-C16-C17
15	a	605	PTY	O10-C8-O7-C6
15	i	101	PTY	C8-C11-C12-C13
16	a	606	CN3	C51-C52-C53-C54
15	c	301	PTY	C33-C34-C35-C36
15	a	605	PTY	C31-C32-C33-C34
18	c	302	PCF	C36-C37-C38-C39
15	a	605	PTY	C12-C13-C14-C15
15	b	303	PTY	C32-C33-C34-C35
16	a	606	CN3	C52-C53-C54-C55
15	b	302	PTY	C30-C31-C32-C33
15	c	301	PTY	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
15	b	303	PTY	C34-C35-C36-C37
15	e	201	PTY	C15-C16-C17-C18
15	a	604	PTY	C13-C14-C15-C16
15	c	301	PTY	C34-C35-C36-C37
15	b	303	PTY	C18-C19-C20-C21
18	c	302	PCF	C11-C12-N-C14
15	a	605	PTY	C32-C33-C34-C35
15	i	101	PTY	C13-C14-C15-C16
15	a	605	PTY	C13-C14-C15-C16
14	a	603	HEA	C27-C19-C20-C21
15	c	301	PTY	O10-C8-O7-C6
15	e	201	PTY	C8-C11-C12-C13
16	a	606	CN3	C42-C41-O41-C3'
18	c	302	PCF	C32-C31-O31-C3
18	c	302	PCF	C31-C32-C33-C34
15	c	301	PTY	C11-C8-O7-C6
18	m	101	PCF	C22-C21-O21-C2
18	m	101	PCF	O22-C21-O21-C2
16	a	606	CN3	CC-O13-P-O11
18	m	101	PCF	C1-O11-P-O13
15	b	302	PTY	O14-C5-C6-C1
16	a	606	CN3	O11-C1-C2-C3
16	a	606	CN3	O1'-C1'-C2'-C3'
15	b	303	PTY	C12-C13-C14-C15
18	e	202	PCF	C23-C24-C25-C26
15	b	302	PTY	O4-C1-C6-C5
16	a	606	CN3	C1-C2-C3-O31
18	e	202	PCF	C1-C2-C3-O31
16	a	606	CN3	O42-C41-O41-C3'
15	b	303	PTY	O4-C30-C31-C32
18	c	302	PCF	O32-C31-O31-C3
14	a	602	HEA	C11-C12-C13-C14
15	b	302	PTY	O4-C1-C6-O7
14	a	603	HEA	C2D-C3D-CAD-CBD
15	c	301	PTY	C12-C13-C14-C15
15	e	201	PTY	C31-C30-O4-C1
15	a	604	PTY	O14-C5-C6-C1
15	a	605	PTY	N1-C2-C3-O11
15	b	302	PTY	N1-C2-C3-O11
18	e	202	PCF	C25-C26-C27-C28
18	e	202	PCF	C32-C31-O31-C3
15	b	303	PTY	O4-C1-C6-C5

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Mol	Chain	Res	Type	Atoms
18	c	302	PCF	C1-C2-C3-O31
15	i	101	PTY	C5-O14-P1-O11
16	a	606	CN3	O11-C1-C2-O21
18	m	101	PCF	O11-C1-C2-O21
16	a	606	CN3	C43-C44-C45-C46
15	b	303	PTY	O4-C1-C6-O7
18	e	202	PCF	O21-C2-C3-O31
16	a	606	CN3	CA-CB-CC-O13
15	c	301	PTY	C31-C32-C33-C34
18	c	302	PCF	C22-C23-C24-C25
15	a	605	PTY	C14-C15-C16-C17
15	i	101	PTY	O14-C5-C6-C1
18	m	101	PCF	O11-C1-C2-C3
15	c	301	PTY	C11-C12-C13-C14
18	e	202	PCF	C28-C29-C30-C47
15	b	302	PTY	C32-C33-C34-C35
15	e	201	PTY	O30-C30-O4-C1
18	e	202	PCF	O32-C31-O31-C3
15	b	302	PTY	C31-C32-C33-C34
15	b	302	PTY	C5-O14-P1-O11
15	b	303	PTY	C3-O11-P1-O14
16	a	606	CN3	CB-CC-O13-P
15	b	303	PTY	C16-C17-C18-C19
16	a	606	CN3	CC-O13-P-O12
16	a	606	CN3	CA-O3'-P'-O2'
18	m	101	PCF	C1-O11-P-O12
18	m	101	PCF	C1-O11-P-O14
15	b	303	PTY	O14-C5-C6-C1
15	c	301	PTY	O14-C5-C6-C1
16	a	606	CN3	C45-C46-C47-C48
15	b	302	PTY	C11-C12-C13-C14
15	a	604	PTY	O14-C5-C6-O7
15	a	605	PTY	O14-C5-C6-O7
15	b	302	PTY	O14-C5-C6-O7
15	b	303	PTY	O14-C5-C6-O7
15	i	101	PTY	O14-C5-C6-O7
18	c	302	PCF	C35-C36-C37-C38
15	i	101	PTY	O4-C1-C6-C5
18	e	202	PCF	O13-C11-C12-N
18	m	101	PCF	C28-C29-C30-C47
15	i	101	PTY	C30-C31-C32-C33
18	m	101	PCF	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
15	a	605	PTY	O14-C5-C6-C1
15	b	303	PTY	C11-C12-C13-C14
16	a	606	CN3	C32-C31-O31-C3
15	b	302	PTY	C3-O11-P1-O14
15	c	301	PTY	C3-O11-P1-O14
18	c	302	PCF	C11-O13-P-O11
18	e	202	PCF	C1-O11-P-O13
18	e	202	PCF	C11-O13-P-O11
15	i	101	PTY	C6-C5-O14-P1
15	c	301	PTY	C31-C30-O4-C1
15	b	303	PTY	O30-C30-C31-C32
16	a	606	CN3	O32-C31-O31-C3
15	c	301	PTY	O30-C30-O4-C1
15	c	301	PTY	C14-C15-C16-C17
15	a	604	PTY	C16-C17-C18-C19
18	c	302	PCF	C2-C1-O11-P
14	a	602	HEA	CAD-CBD-CGD-O1D
15	a	604	PTY	C31-C32-C33-C34
18	m	101	PCF	C22-C23-C24-C25
14	a	603	HEA	CAA-CBA-CGA-O2A
14	a	602	HEA	CAA-CBA-CGA-O2A
14	a	603	HEA	CAA-CBA-CGA-O1A
18	m	101	PCF	C21-C22-C23-C24
14	a	603	HEA	C18-C19-C20-C21
18	c	302	PCF	O21-C2-C3-O31
15	a	604	PTY	C11-C12-C13-C14
15	b	303	PTY	C31-C32-C33-C34
15	a	604	PTY	C12-C11-C8-O7
15	b	302	PTY	C38-C39-C40-C41
18	e	202	PCF	C22-C23-C24-C25
14	a	602	HEA	C26-C15-C16-C17
16	a	606	CN3	O32-C31-C32-C33
15	b	302	PTY	C12-C11-C8-O7
14	a	603	HEA	CAD-CBD-CGD-O2D
15	c	301	PTY	C35-C36-C37-C38
15	c	301	PTY	C37-C38-C39-C40
18	c	302	PCF	O11-C1-C2-O21
14	a	602	HEA	CAA-CBA-CGA-O1A
18	e	202	PCF	C33-C34-C35-C36
16	a	606	CN3	O31-C31-C32-C33
16	a	606	CN3	O51-C51-C52-C53
18	c	302	PCF	C25-C26-C27-C28

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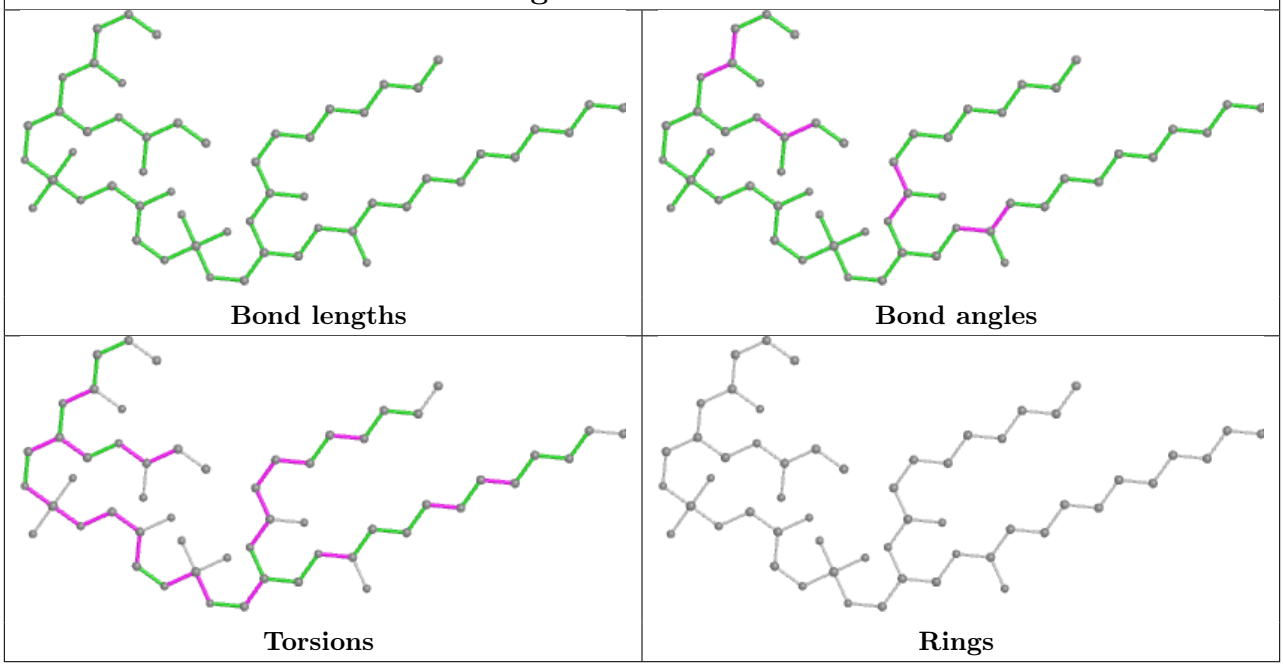
Mol	Chain	Res	Type	Atoms
16	a	606	CN3	O22-C21-O21-C2
15	b	303	PTY	C3-O11-P1-O13
18	e	202	PCF	C11-O13-P-O12
15	b	302	PTY	C36-C37-C38-C39
15	i	101	PTY	O30-C30-O4-C1
15	b	303	PTY	N1-C2-C3-O11
15	i	101	PTY	N1-C2-C3-O11
15	i	101	PTY	C31-C30-O4-C1
14	a	602	HEA	CAD-CBD-CGD-O2D
15	b	302	PTY	C2-C3-O11-P1
18	c	302	PCF	C12-C11-O13-P
16	a	606	CN3	C54-C55-C56-C57
16	a	606	CN3	O52-C51-C52-C53
15	c	301	PTY	C12-C11-C8-O7
15	b	302	PTY	C37-C38-C39-C40
15	c	301	PTY	C12-C11-C8-O10

There are no ring outliers.

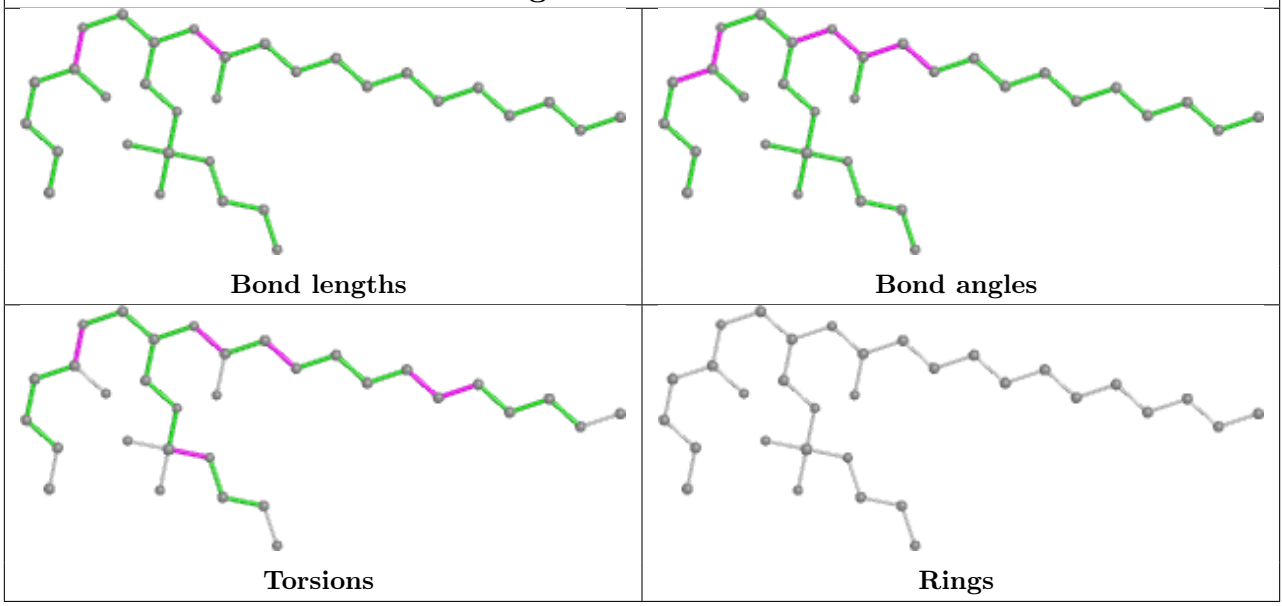
No monomer is involved in short contacts.

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.

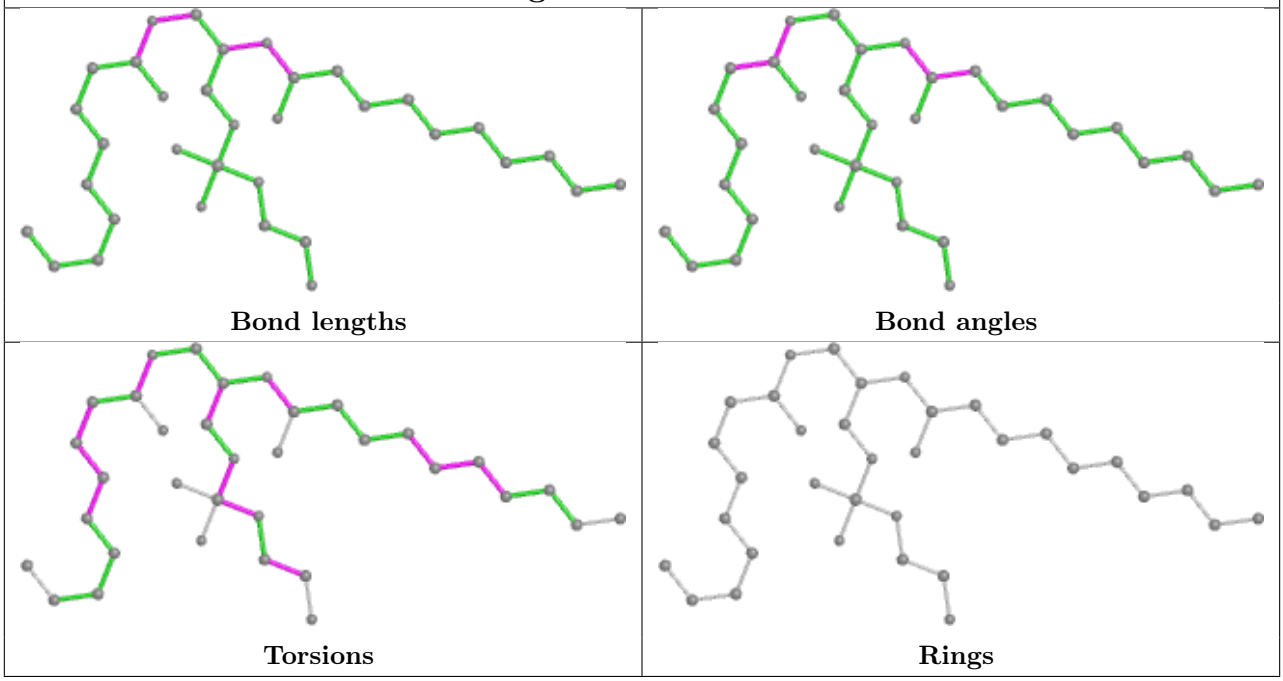
Ligand CN3 a 606



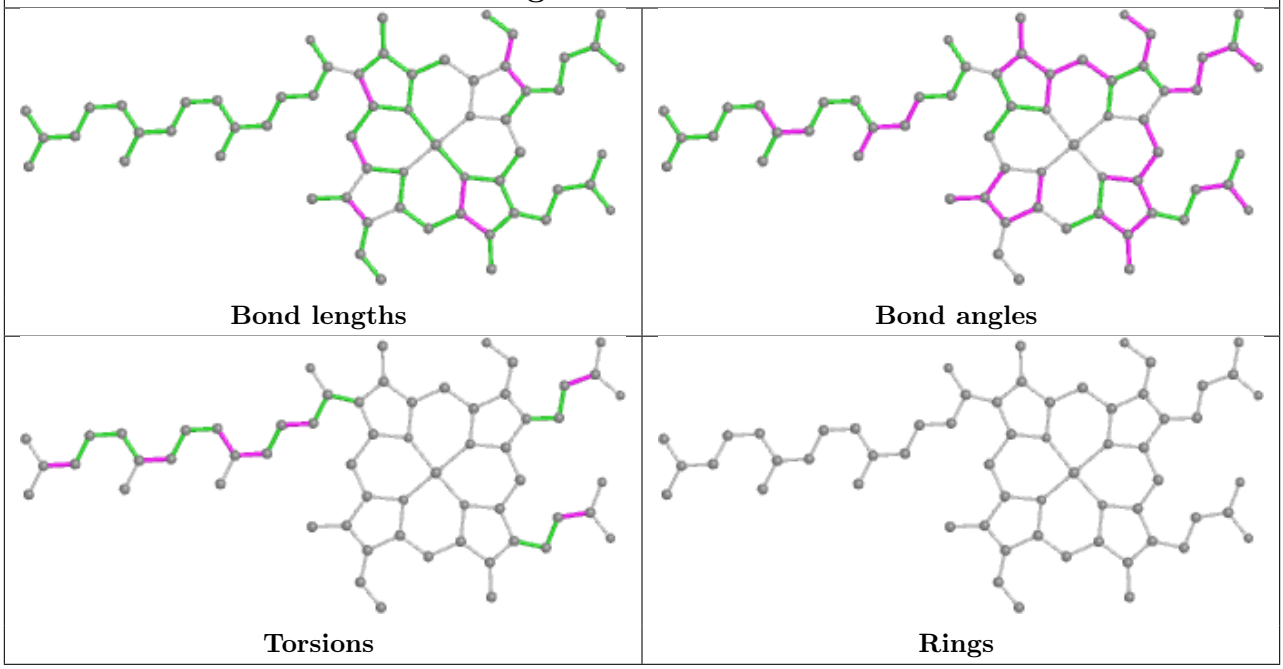
Ligand PTY e 201



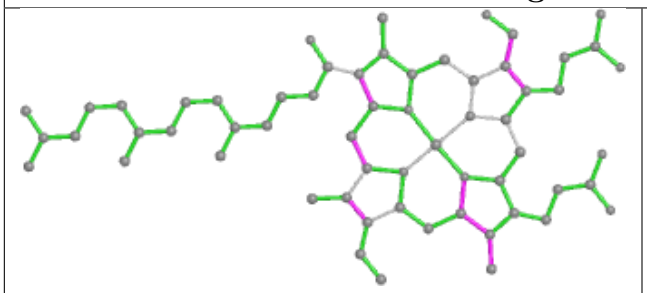
Ligand PTY a 605



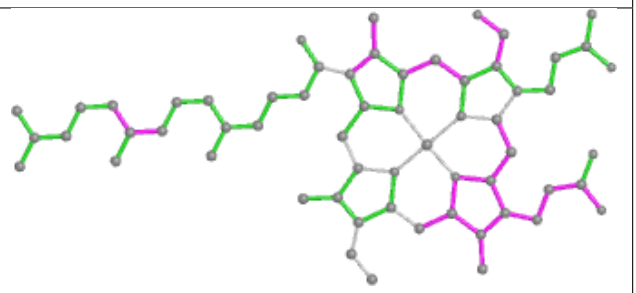
Ligand HEA a 602



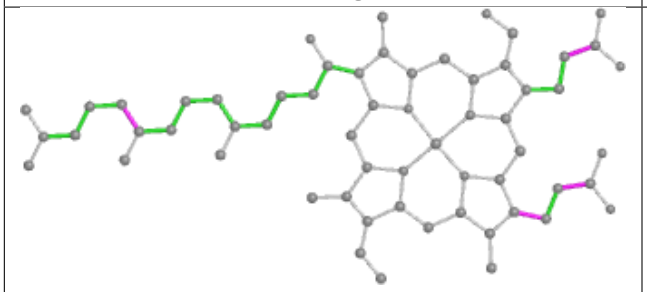
Ligand HEA a 603



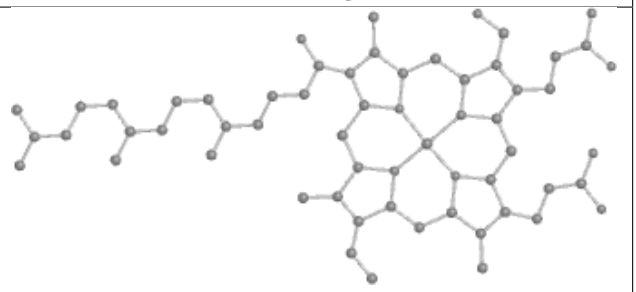
Bond lengths



Bond angles

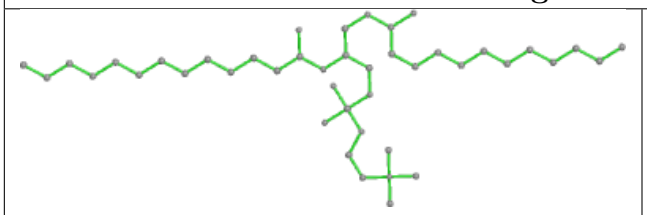


Torsions

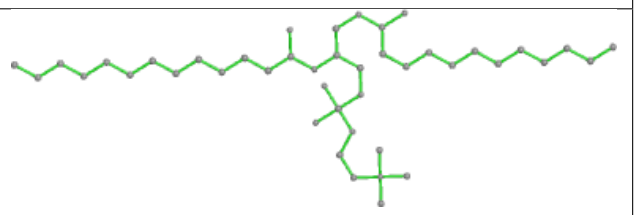


Rings

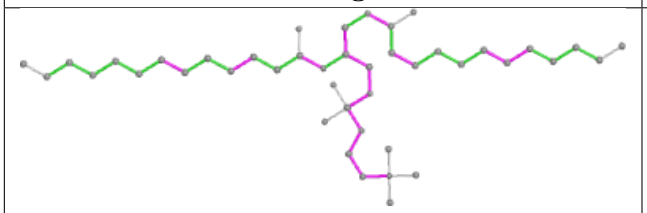
Ligand PCF c 302



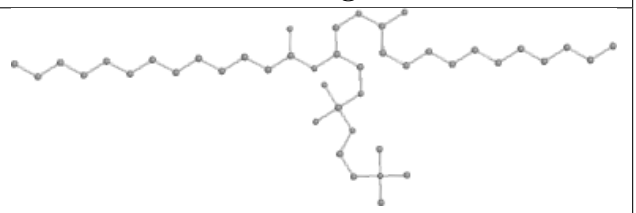
Bond lengths



Bond angles

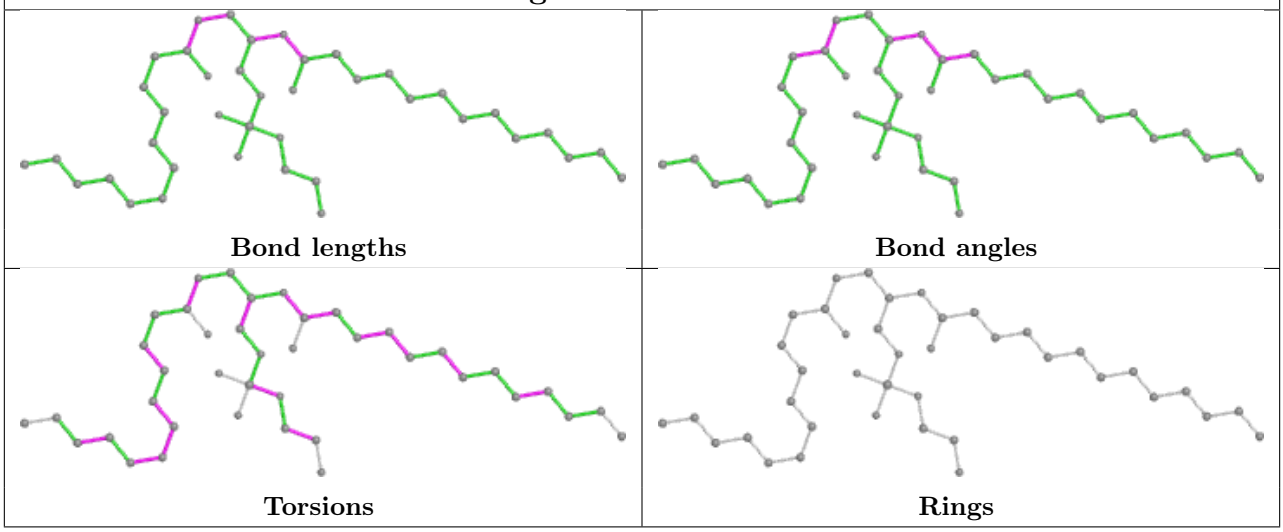


Torsions

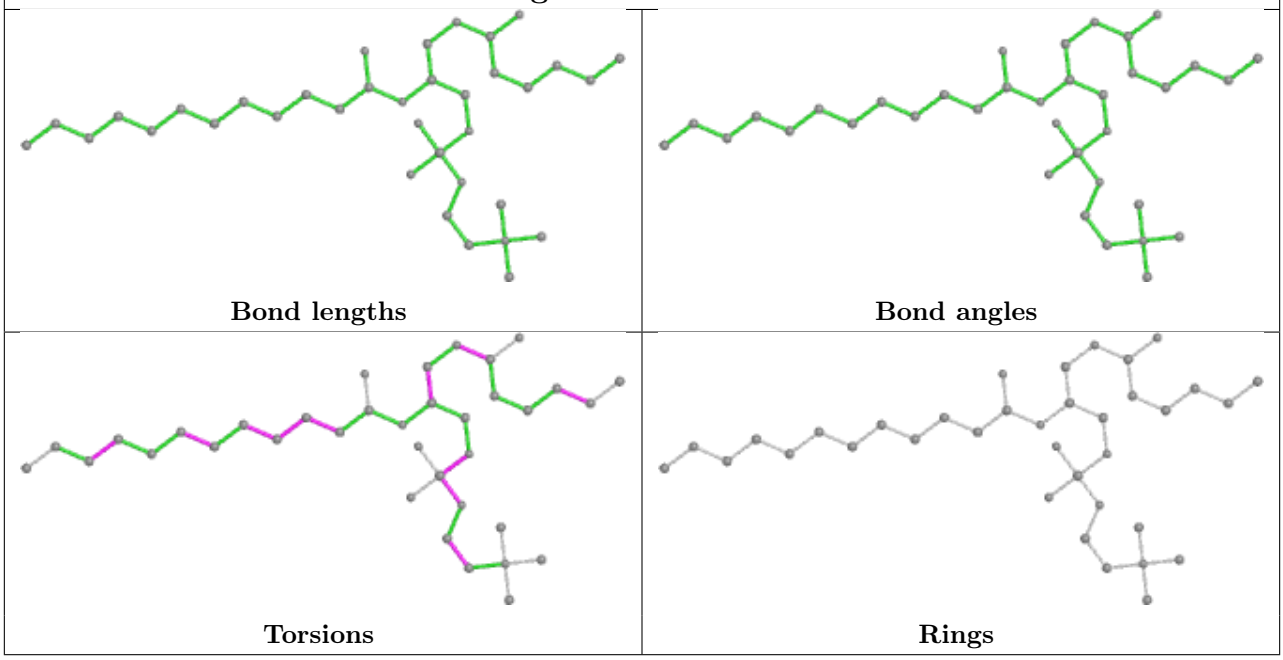


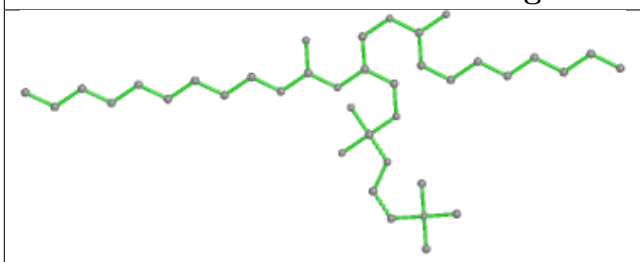
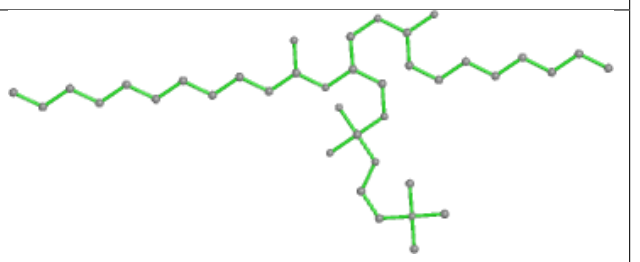
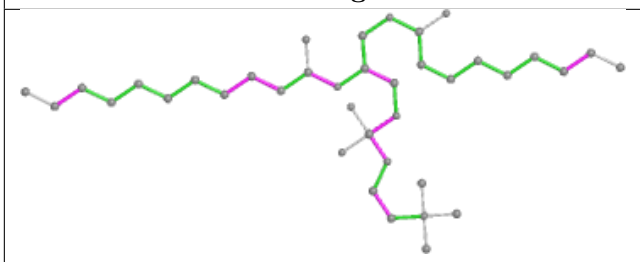
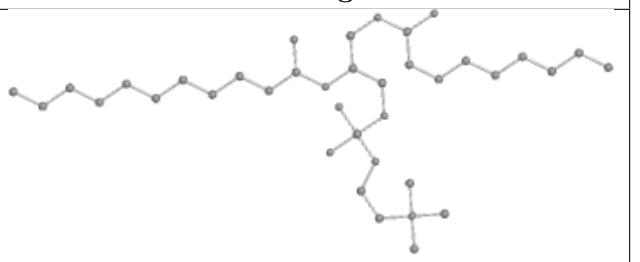
Rings

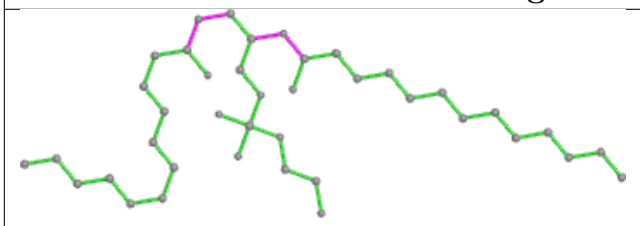
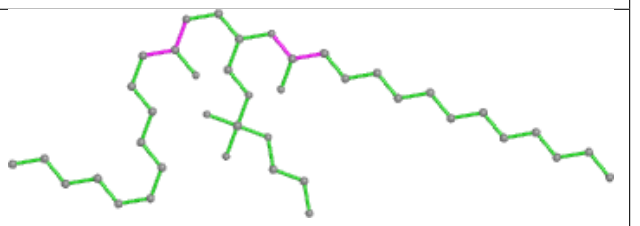
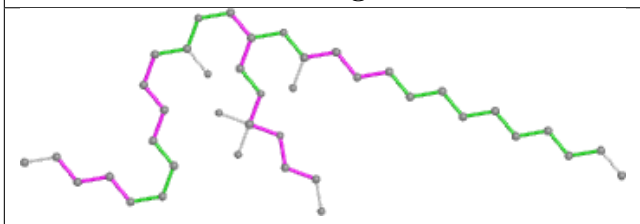
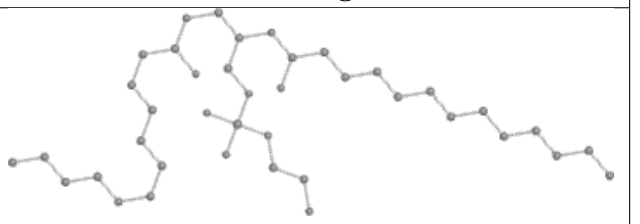
Ligand PTY c 301



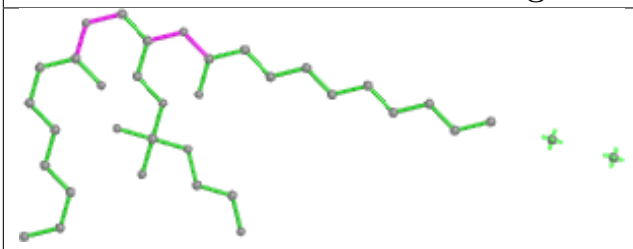
Ligand PCF e 202



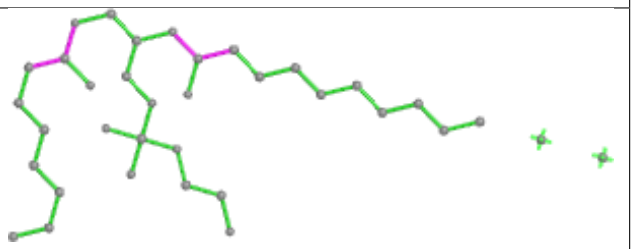
Ligand PCF m 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PTY b 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

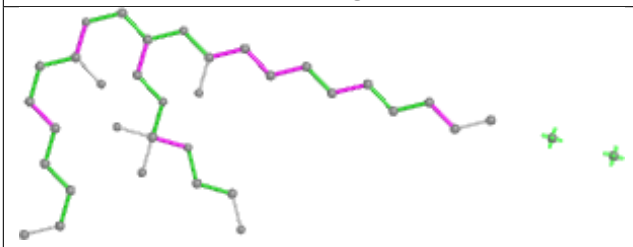
Ligand PTY a 604



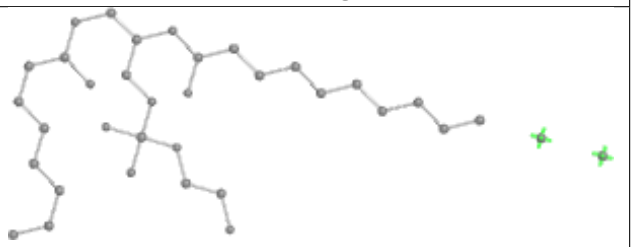
Bond lengths



Bond angles

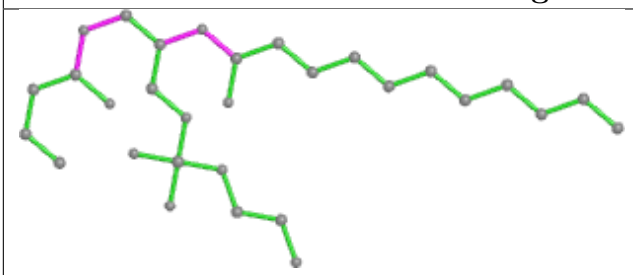


Torsions

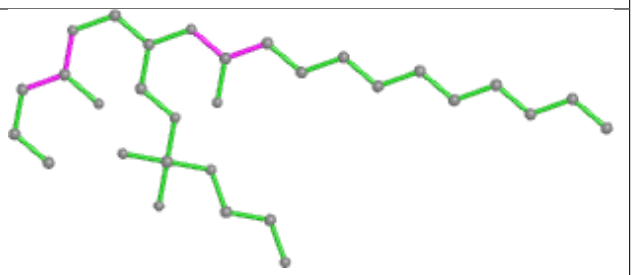


Rings

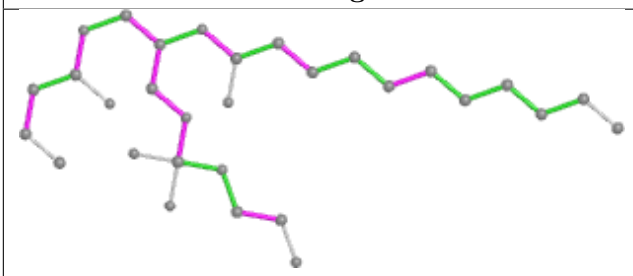
Ligand PTY i 101



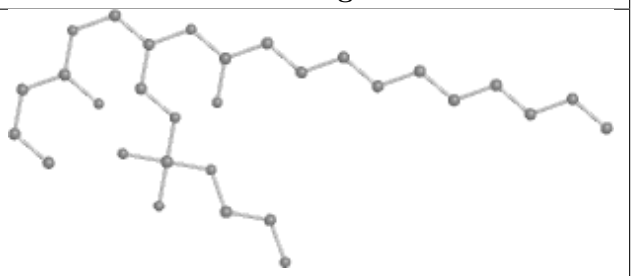
Bond lengths



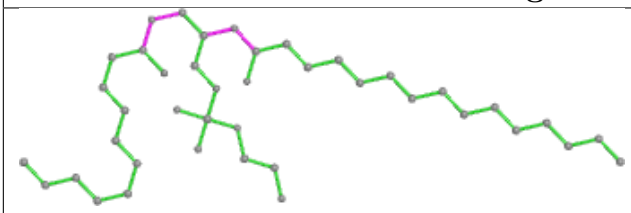
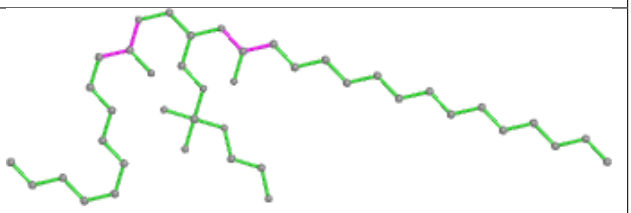
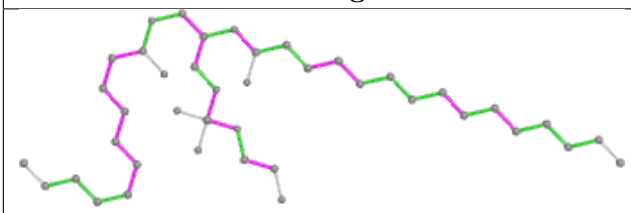
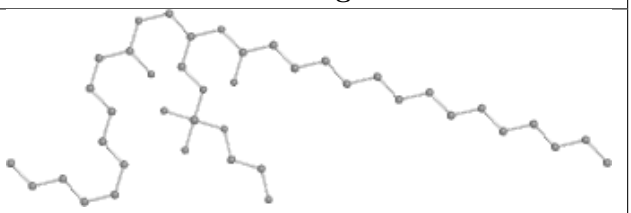
Bond angles



Torsions



Rings

Ligand PTY b 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

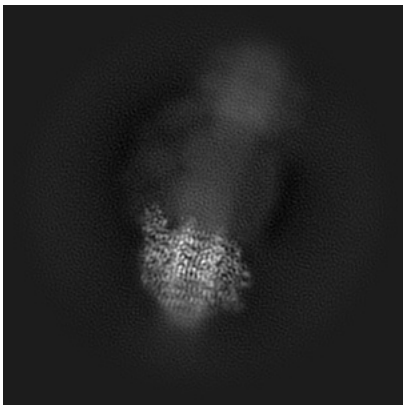
6 Map visualisation (i)

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

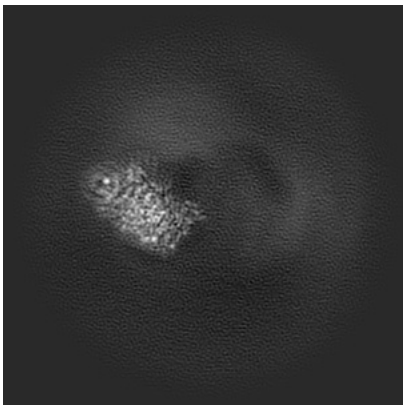
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

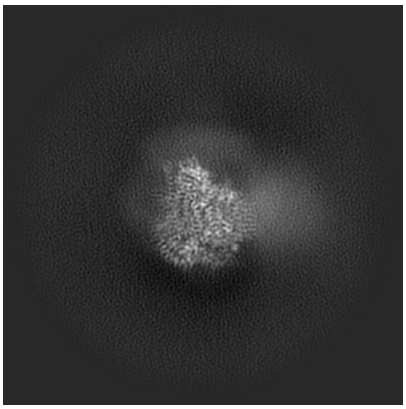
6.1.1 Primary map



X

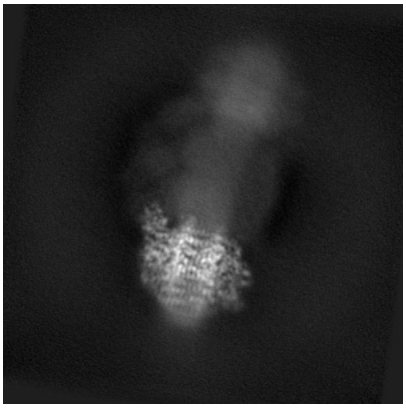


Y

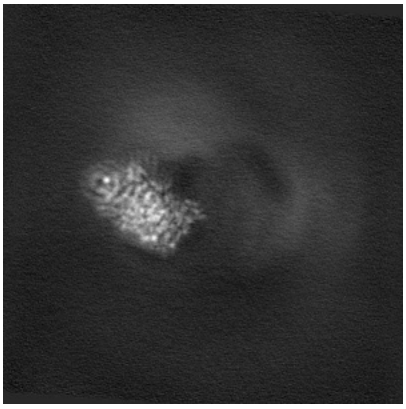


Z

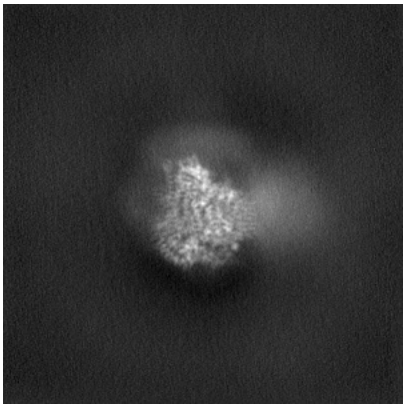
6.1.2 Raw map



X



Y

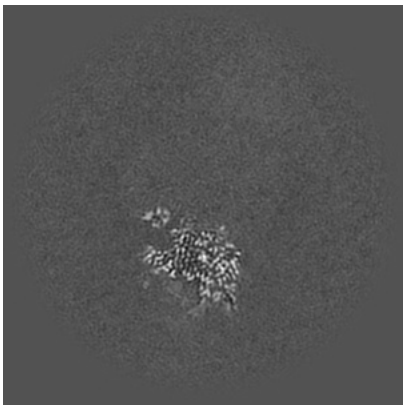


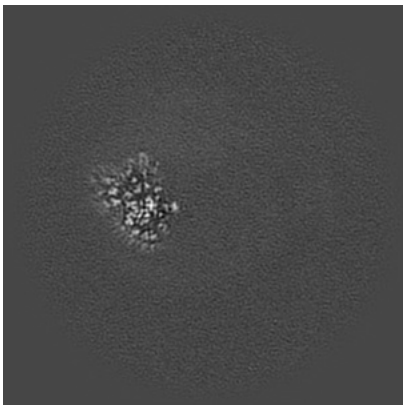
Z

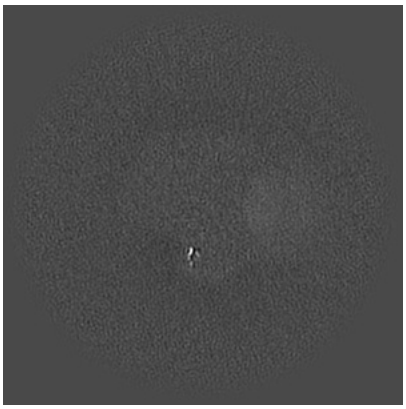
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

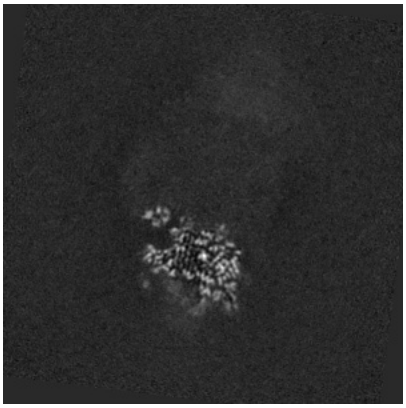
6.2.1 Primary map

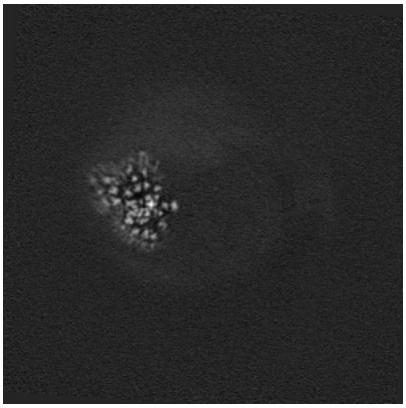

X Index: 185

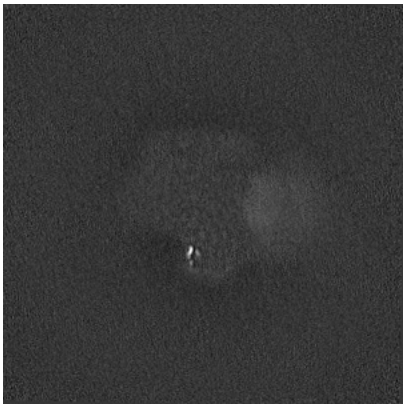

Y Index: 185


Z Index: 185

6.2.2 Raw map


X Index: 185

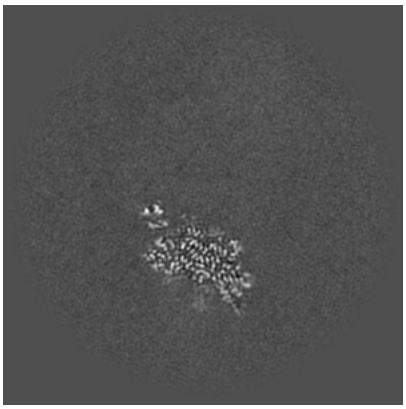

Y Index: 185

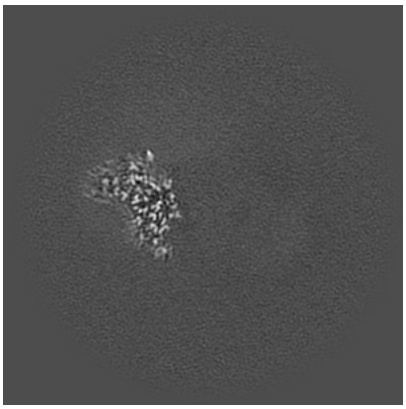

Z Index: 185

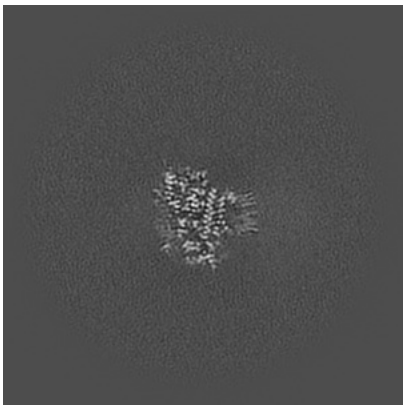
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

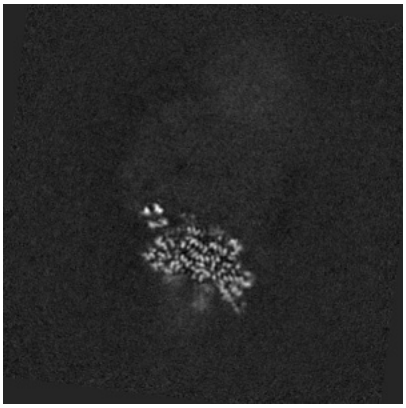
6.3.1 Primary map

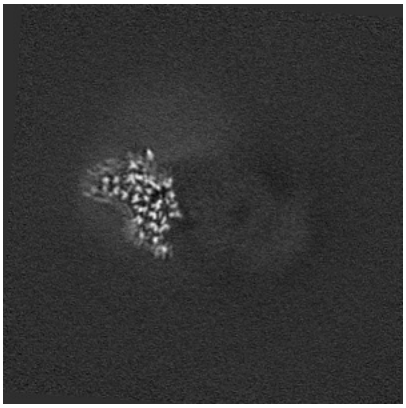

X Index: 178

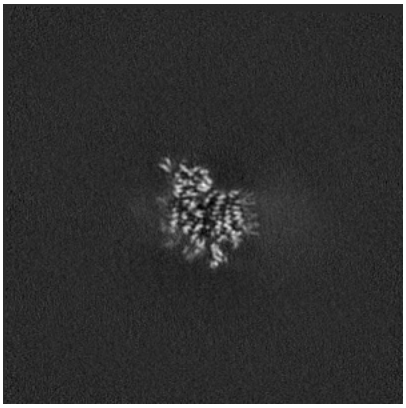

Y Index: 162


Z Index: 133

6.3.2 Raw map


X Index: 178

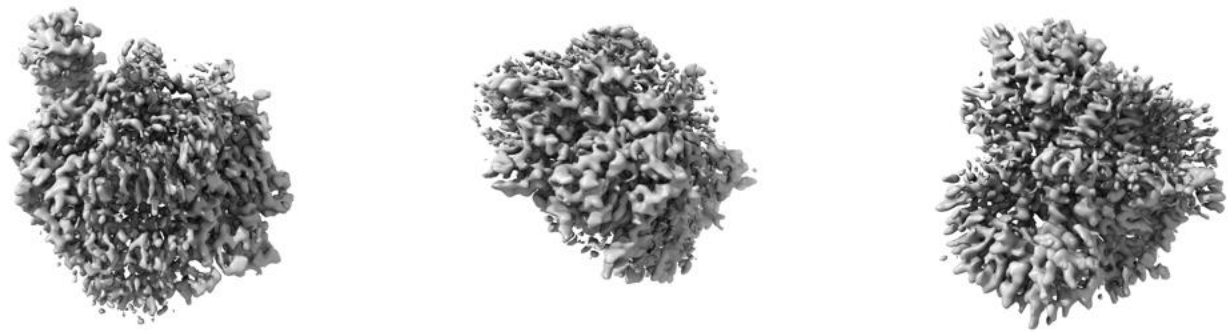

Y Index: 162


Z Index: 126

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

6.4 Orthogonal surface views (i)

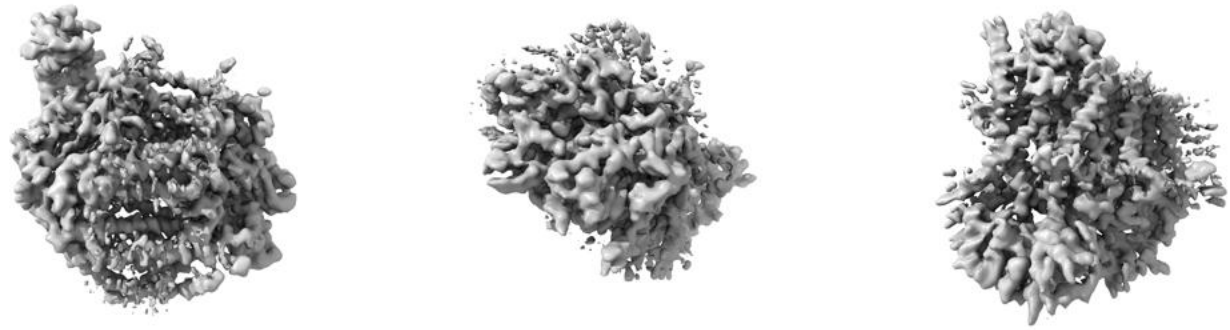
6.4.1 Primary map



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.

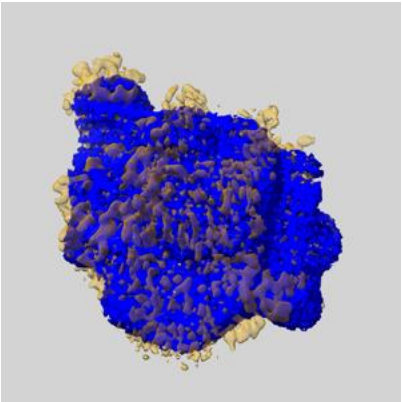
6.5 Mask visualisation (i)

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

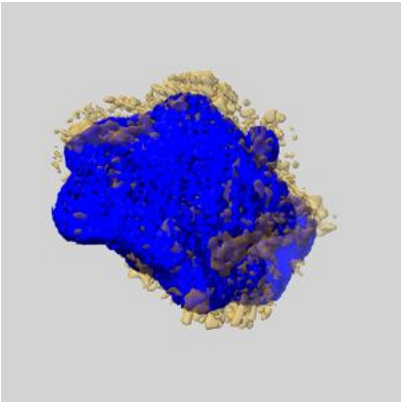
A mask typically either:

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

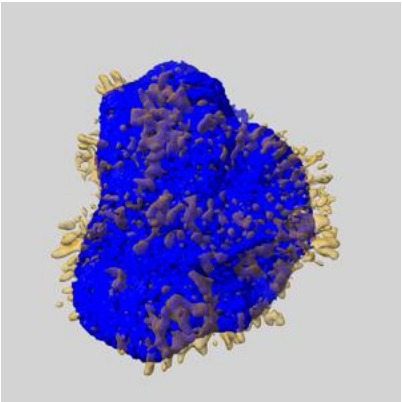
6.5.1 emd_10848_msk_1.map (i)



X



Y

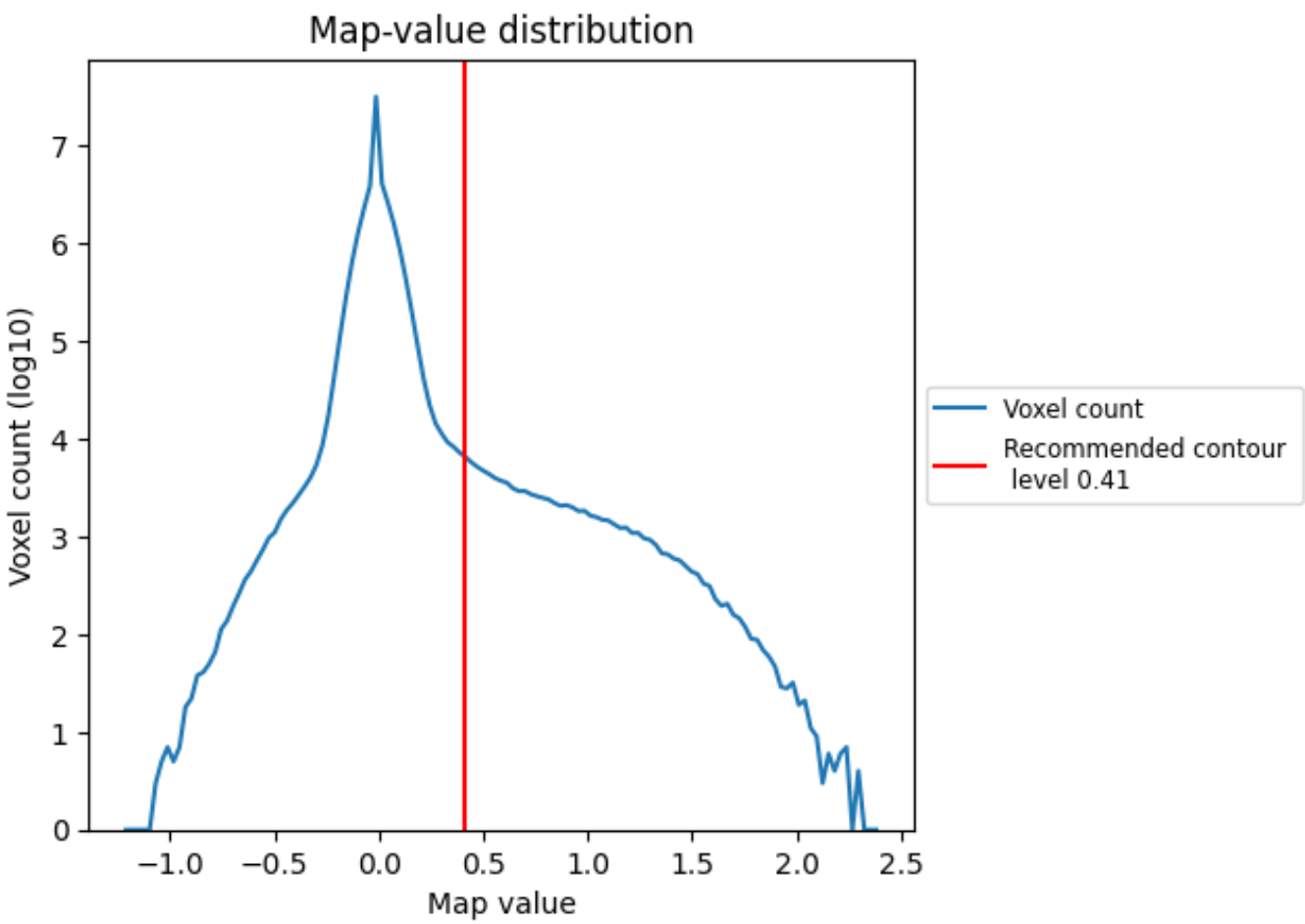


Z

7 Map analysis (i)

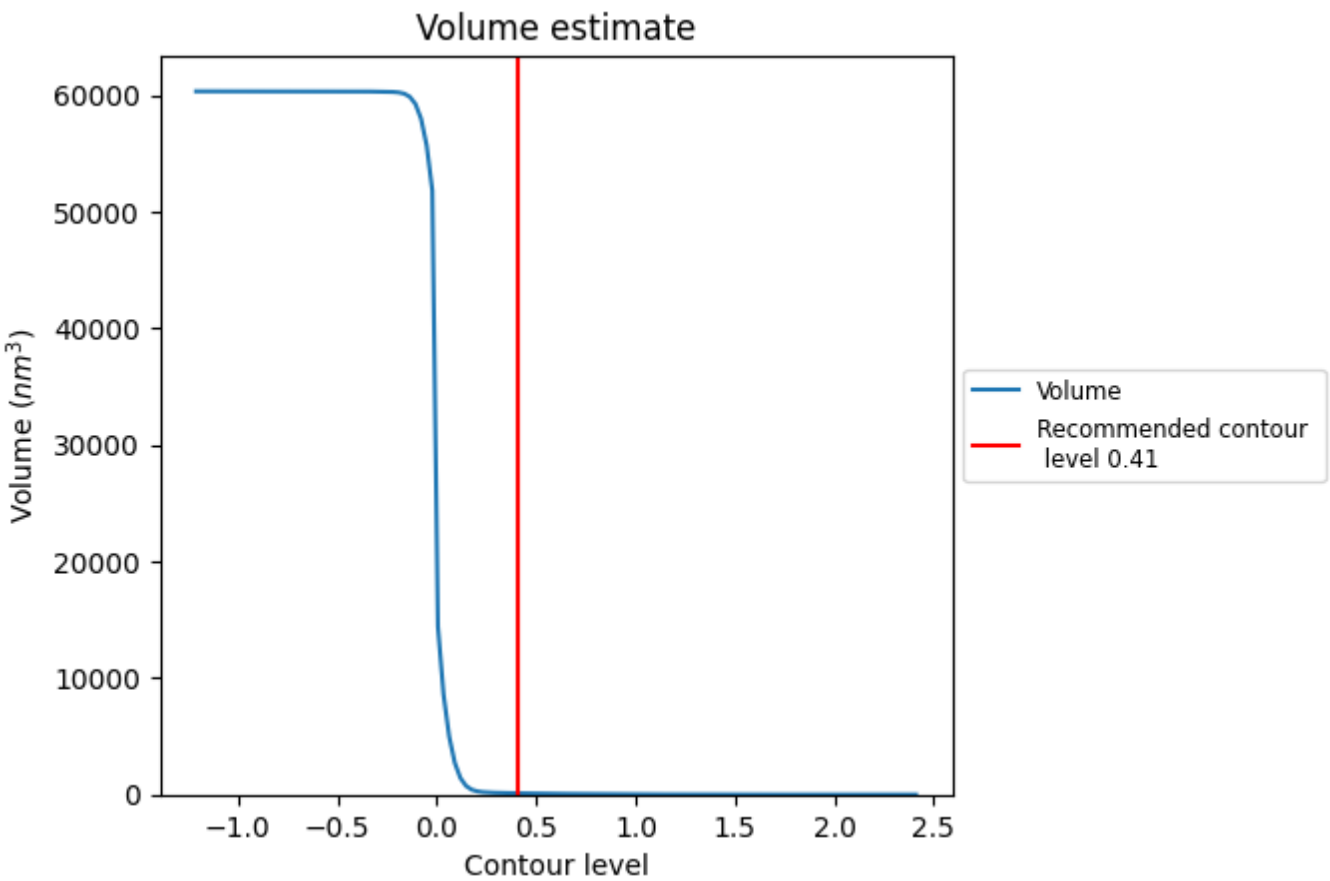
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

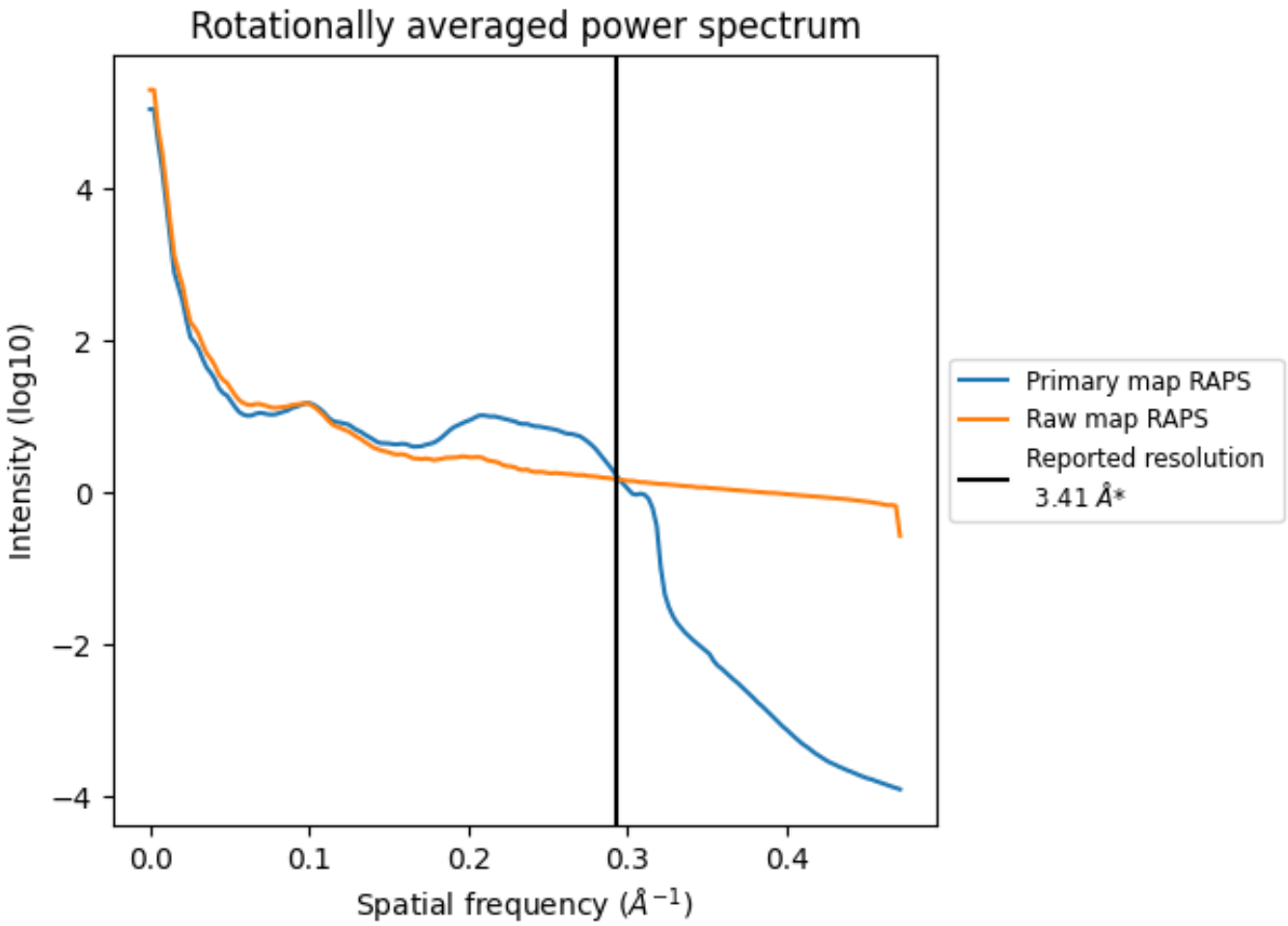
7.2 Volume estimate (i)



The volume at the recommended contour level is 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}

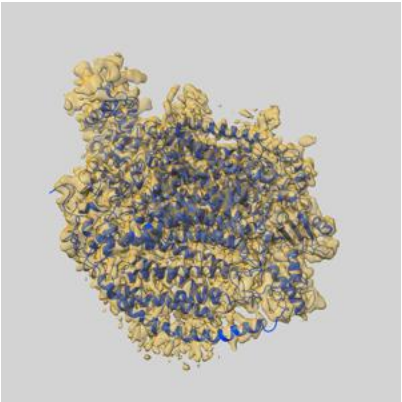
8 Fourier-Shell correlation (i)

This section was not generated.

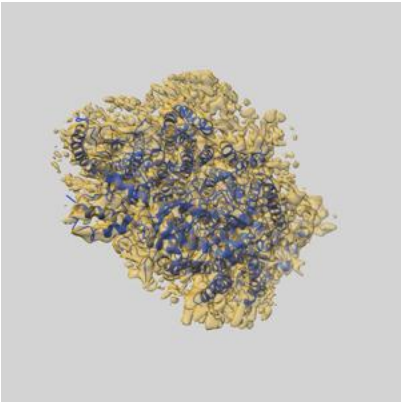
9 Map-model fit (i)

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.

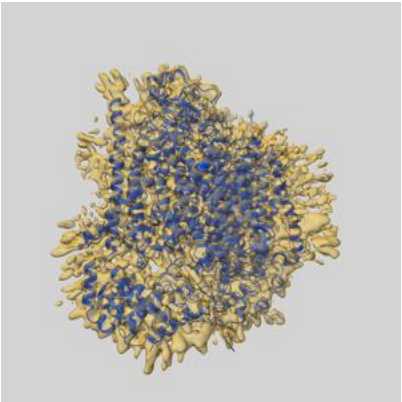
9.1 Map-model overlay (i)



X



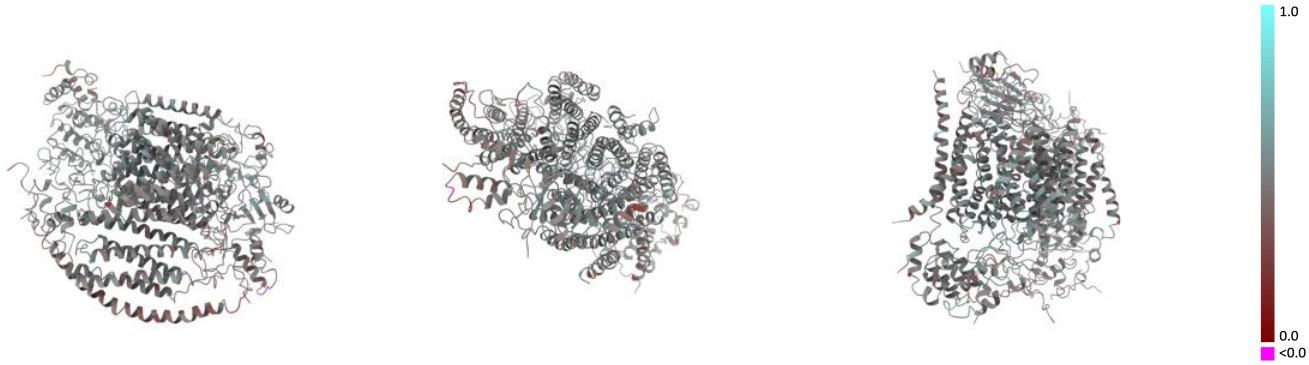
Y



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.

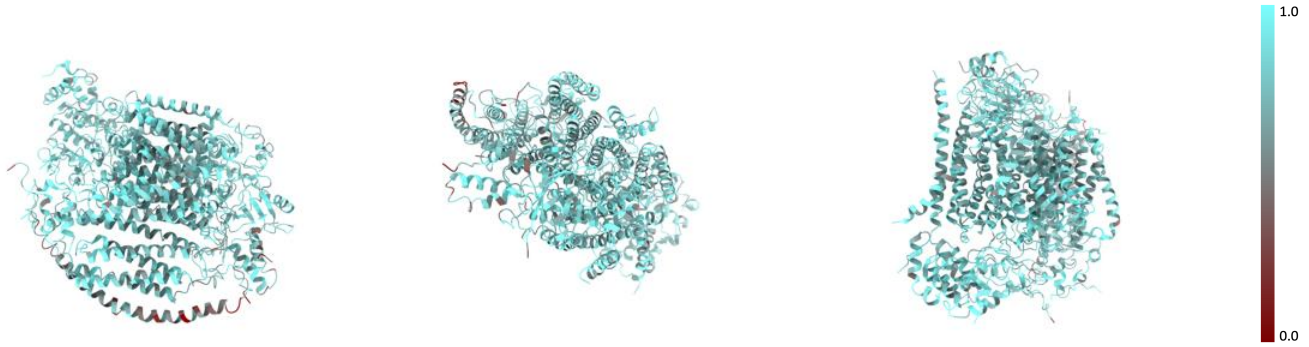
9.2 Q-score mapped to coordinate model (i)



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.

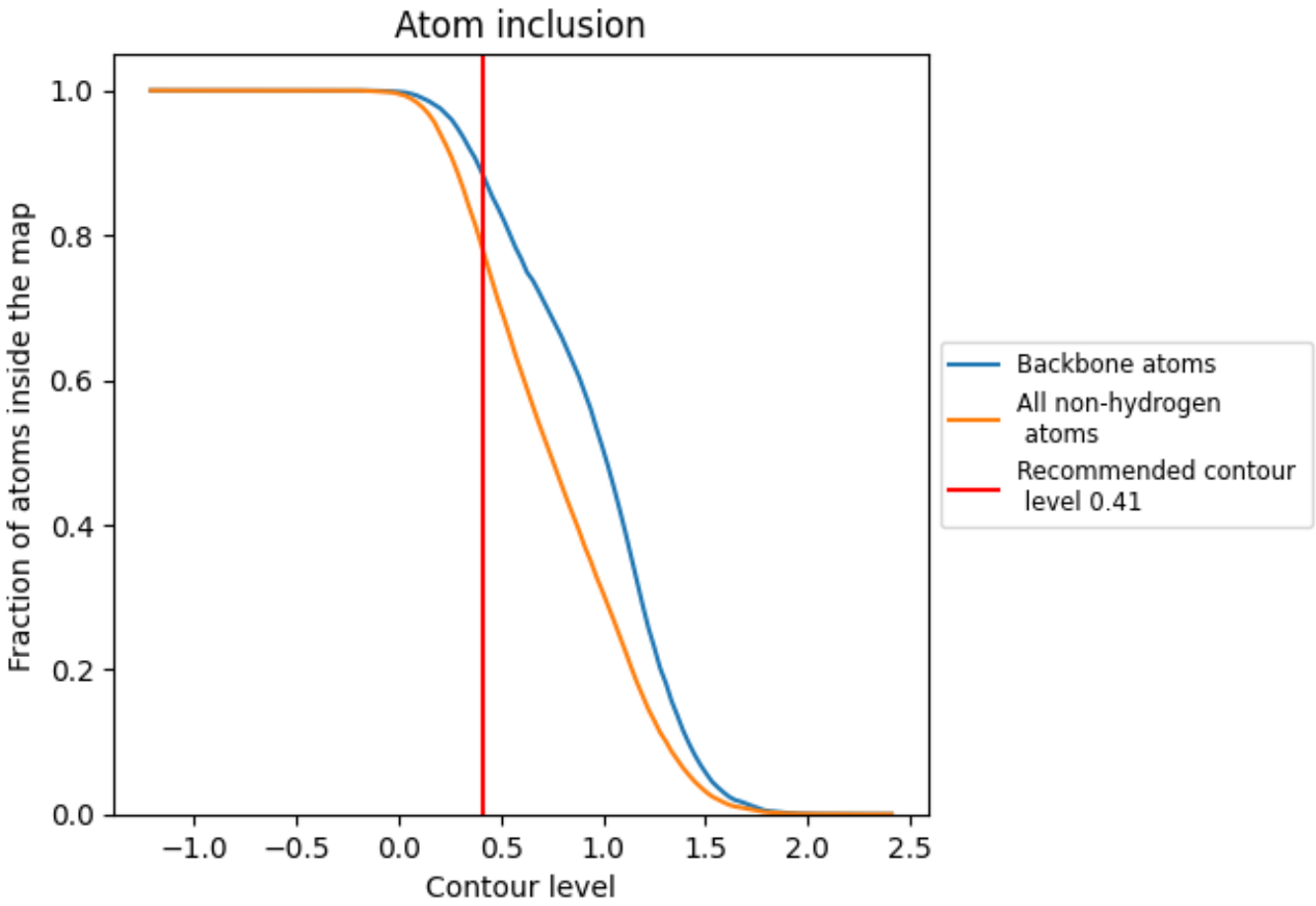
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.41).

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 (i)

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