Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 09:23 PM EST

PDB ID	:	7JRO
EMDB ID	:	EMD-22447
Title	:	Plant Mitochondrial complex IV from Vigna radiata
Authors	:	Maldonado, M.; Letts, J.A.
Deposited on	:	2020-08-12
Resolution	:	3.80 Å(reported)
Based on initial models	:	5B1A, 6Q9E

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 ⓘ symbol.

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

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

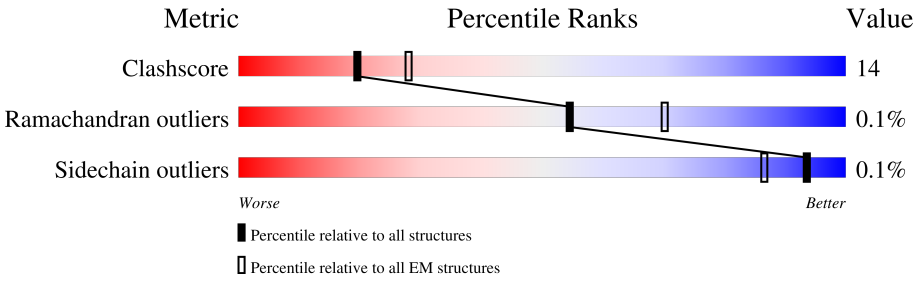
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.80 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	527	99%
2	b	251	8% 95% 5%
3	c	265	100%
4	d	79	8% 95%
5	e	150	9% 63% 37%
6	f	100	17% 58% 41%
7	g	181	7% 41% 59%
8	h	64	9% 77% 23%

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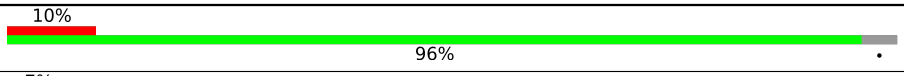
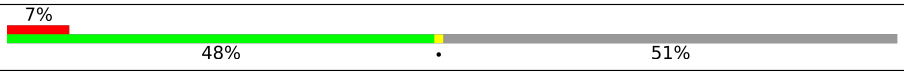
Mol	Chain	Length	Quality of chain
9	i	67	
10	j	96	

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
11	HEA	a	601	X	-	-	-
11	HEA	a	602	X	-	-	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 12747 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 COX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	a	524	4074	2726	640	684	24	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	239	1915	1249	308	348	10	0	0

- Molecule 3 is a protein called COX3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	265	2134	1445	335	347	7	0	0

- Molecule 4 is a protein called COX4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	76	595	387	97	109	2	0	0

- Molecule 5 is a protein called cytochrome c oxidase subunit 5b-2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	94	733	464	124	142	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	59	480	315	76	88	1	0	0

- Molecule 7 is a protein called cytochrome c oxidase subunit 6b-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	74	Total	C	N	O	S	0	0
			612	385	110	113	4		

- Molecule 8 is a protein called Cytochrome c oxidase subunit 5C.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	49	Total	C	N	O	S	0	0
			391	255	67	68	1		

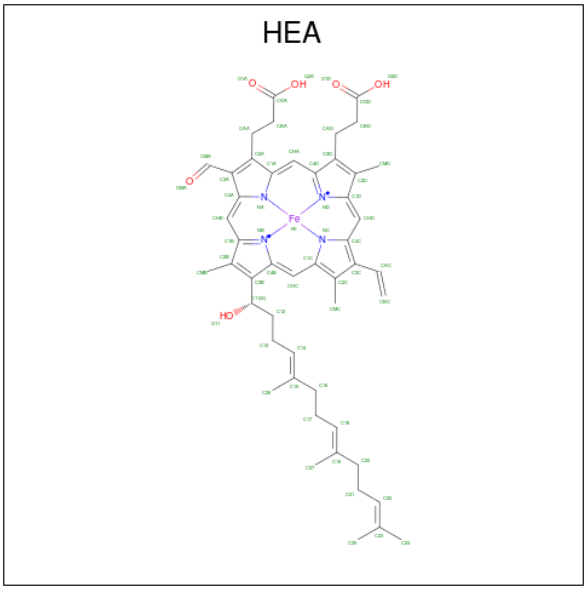
- Molecule 9 is a protein called COX7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	64	Total	C	N	O	S	0	0
			510	331	91	87	1		

- Molecule 10 is a protein called COX7c.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	47	Total	C	N	O	S	0	0
			384	254	67	60	3		

- Molecule 11 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



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

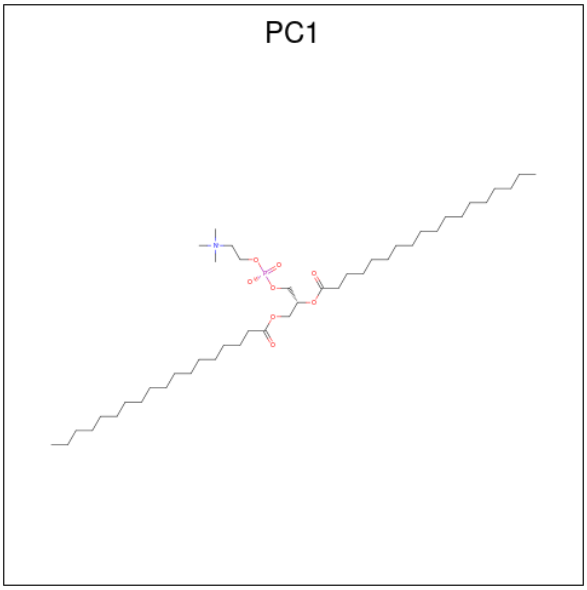
- Molecule 12 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

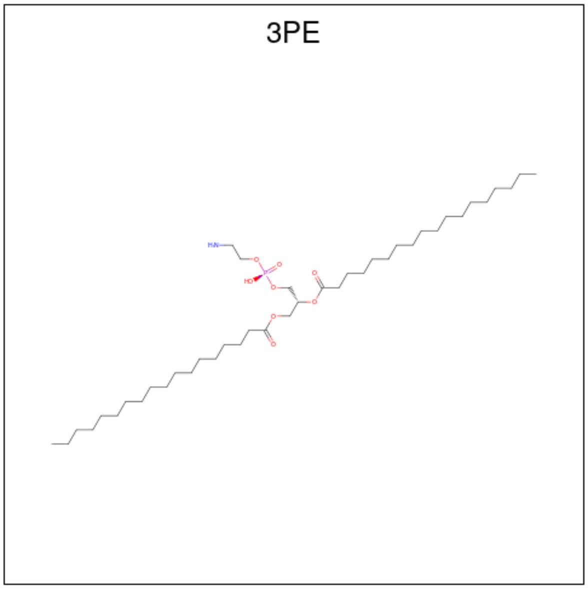
- Molecule 14 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total	C	N	O	P	0
			39	29	1	8	1	
14	i	1	Total	C	N	O	P	0
			36	26	1	8	1	

- Molecule 15 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter

code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
15	a	1	Total 227	C 167	N 6	O 48	P 6	0
15	a	1	Total 227	C 167	N 6	O 48	P 6	0
15	a	1	Total 227	C 167	N 6	O 48	P 6	0
15	a	1	Total 227	C 167	N 6	O 48	P 6	0
15	a	1	Total 227	C 167	N 6	O 48	P 6	0
15	a	1	Total 227	C 167	N 6	O 48	P 6	0
15	b	1	Total 108	C 78	N 3	O 24	P 3	0
15	b	1	Total 108	C 78	N 3	O 24	P 3	0
15	b	1	Total 108	C 78	N 3	O 24	P 3	0
15	c	1	Total 200	C 150	N 5	O 40	P 5	0
15	c	1	Total 200	C 150	N 5	O 40	P 5	0
15	c	1	Total 200	C 150	N 5	O 40	P 5	0
15	c	1	Total 200	C 150	N 5	O 40	P 5	0

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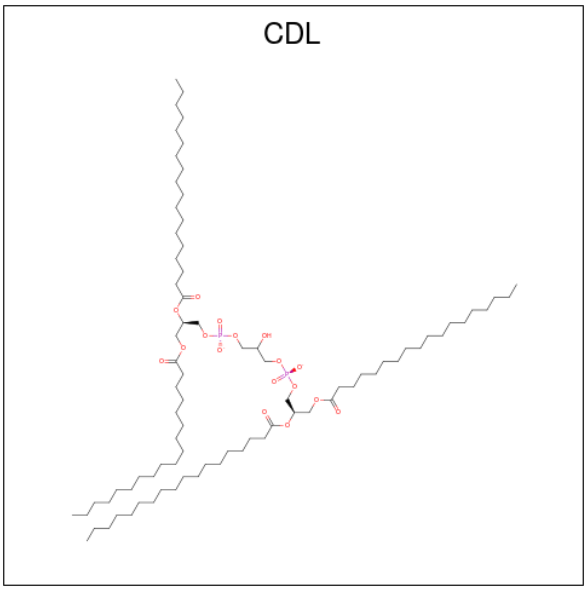
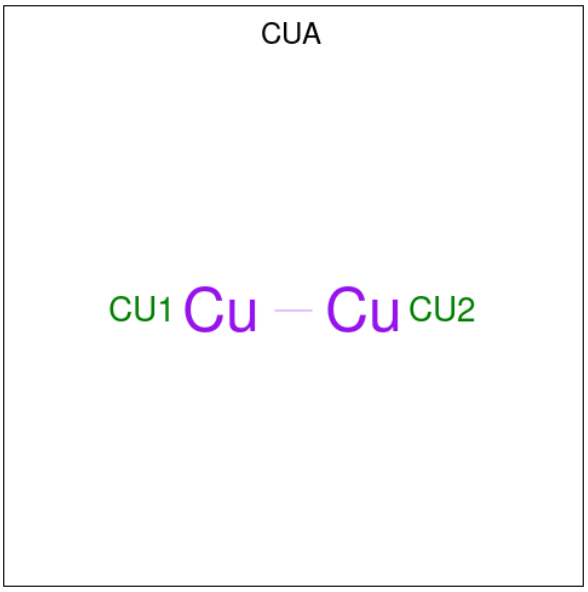
Mol	Chain	Residues	Atoms					AltConf
15	c	1	Total	C	N	O	P	0
			200	150	5	40	5	
15	d	1	Total	C	N	O	P	0
			35	25	1	8	1	
15	h	1	Total	C	N	O	P	0
			38	28	1	8	1	
15	i	1	Total	C	N	O	P	0
			35	25	1	8	1	

- Molecule 16 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
16	a	1	Total	C	O	P	0
			67	48	17	2	

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

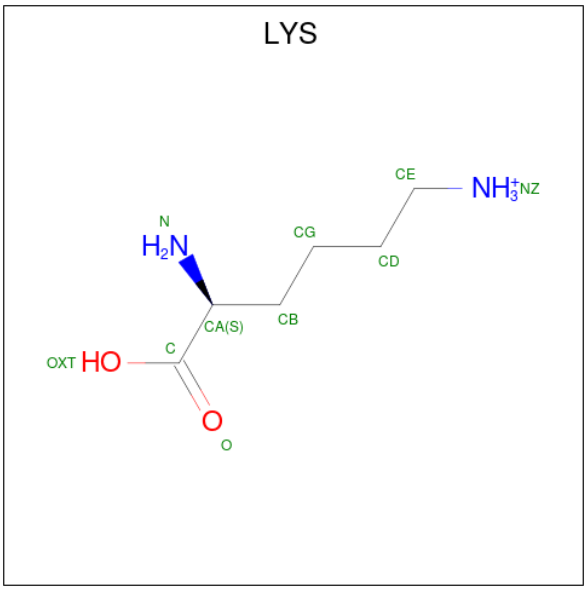


Mol	Chain	Residues	Atoms	AltConf
17	b	1	Total Cu 2 2	0

- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
18	e	1	Total Zn 1 1	0

- Molecule 19 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).



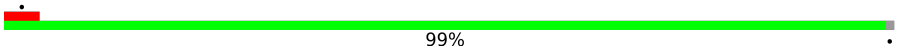
Mol	Chain	Residues	Atoms				AltConf
19	i	1	Total	C	N	O	0
			9	6	2	1	

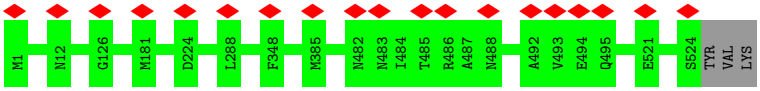
3 Residue-property plots (i)

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: COX1

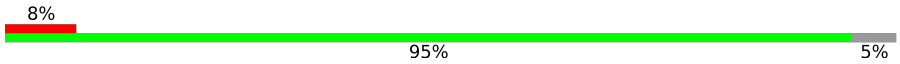
Chain a:

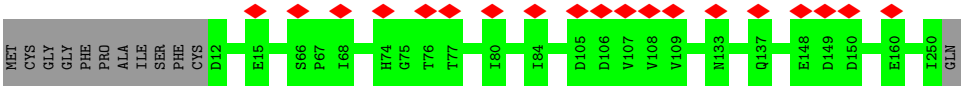




• Molecule 2: Cytochrome c oxidase subunit 2

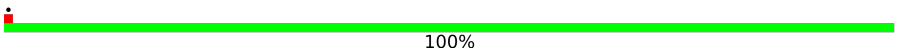
Chain b:

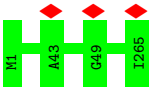




• Molecule 3: COX3

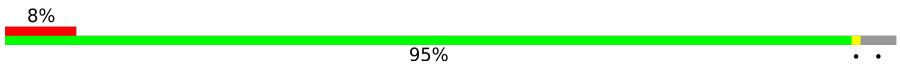
Chain c:

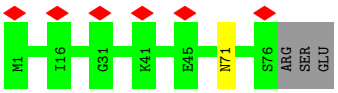




• Molecule 4: COX4

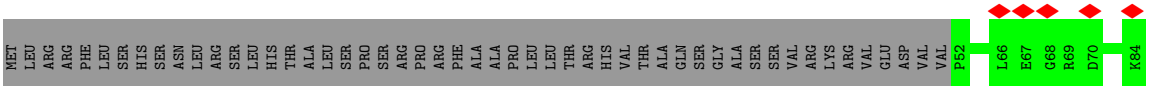
Chain d:

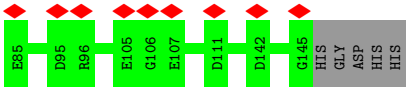




• Molecule 5: cytochrome c oxidase subunit 5b-2, mitochondrial

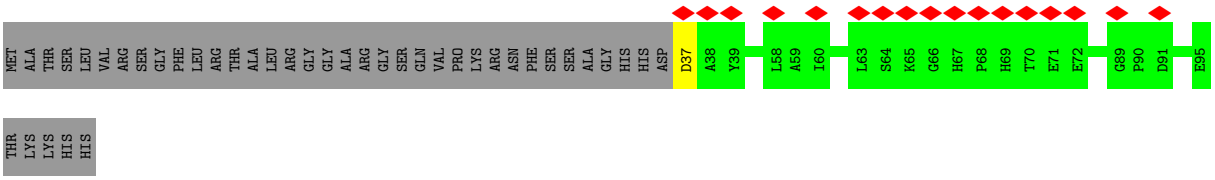
Chain e:





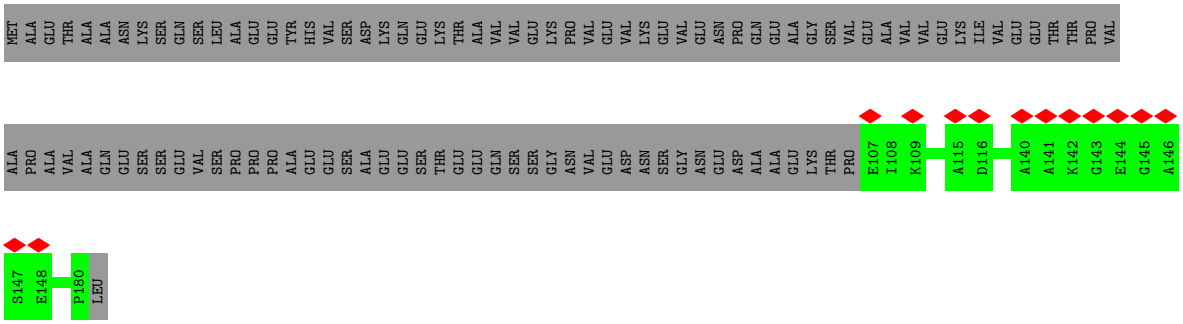
• Molecule 6: cytochrome c oxidase subunit 6a, mitochondrial

Chain f:



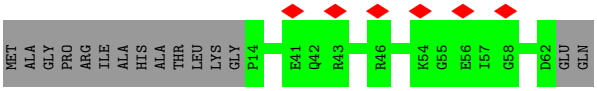
• Molecule 7: cytochrome c oxidase subunit 6b-1

Chain g:



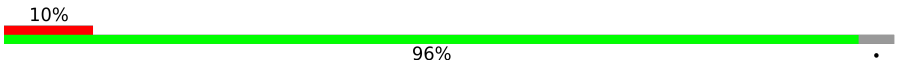
• Molecule 8: Cytochrome c oxidase subunit 5C

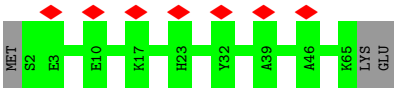
Chain h:



• Molecule 9: COX7a

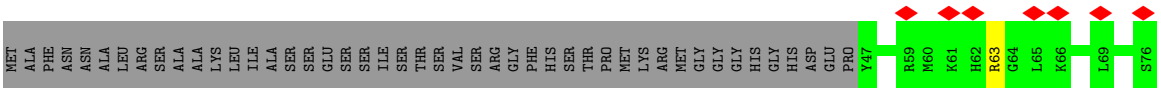
Chain i:





• Molecule 10: COX7c

Chain j:




T93
ALA
SER
ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	29348	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 ($e^-/Å^2$)	86.4	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	60010	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.071	Depositor
Minimum map value	-0.056	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	426.5984, 426.5984, 426.5984	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8332, 0.8332, 0.8332	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEA, CU, CDL, ZN, PC1, 3PE, MG, 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	0/4214	0.52	0/5758
2	b	0.35	0/1971	0.53	0/2697
3	c	0.38	0/2217	0.46	0/3030
4	d	0.34	0/612	0.48	0/832
5	e	0.33	0/756	0.47	0/1026
6	f	0.29	0/499	0.50	1/682 (0.1%)
7	g	0.39	0/631	0.58	0/853
8	h	0.34	0/399	0.44	0/538
9	i	0.33	0/524	0.50	0/705
10	j	0.33	0/394	0.47	0/528
All	All	0.36	0/12217	0.50	1/16649 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	f	37	ASP	CB-CG-OD2	5.21	122.99	118.30

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	4074	0	4063	0	0
2	b	1915	0	1876	0	0
3	c	2134	0	2098	0	0
4	d	595	0	596	0	0
5	e	733	0	677	0	0
6	f	480	0	452	0	0
7	g	612	0	563	0	0
8	h	391	0	405	0	0
9	i	510	0	528	0	0
10	j	384	0	398	0	0
11	a	120	0	108	0	0
12	a	1	0	0	0	0
13	a	1	0	0	0	0
14	a	39	0	52	0	0
14	i	36	0	46	0	0
15	a	227	0	301	0	0
15	b	108	0	141	0	0
15	c	200	0	270	0	0
15	d	35	0	44	0	0
15	h	38	0	50	0	0
15	i	35	0	44	0	0
16	a	67	0	78	0	0
17	b	2	0	0	0	0
18	e	1	0	0	0	0
19	i	9	0	12	0	0
All	All	12747	0	12802	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 14.

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	522/527 (99%)	472 (90%)	50 (10%)	0	100	100
2	b	237/251 (94%)	206 (87%)	31 (13%)	0	100	100
3	c	263/265 (99%)	249 (95%)	14 (5%)	0	100	100
4	d	74/79 (94%)	67 (90%)	7 (10%)	0	100	100
5	e	92/150 (61%)	82 (89%)	10 (11%)	0	100	100
6	f	57/100 (57%)	54 (95%)	3 (5%)	0	100	100
7	g	72/181 (40%)	63 (88%)	9 (12%)	0	100	100
8	h	47/64 (73%)	46 (98%)	1 (2%)	0	100	100
9	i	62/67 (92%)	57 (92%)	5 (8%)	0	100	100
10	j	45/96 (47%)	39 (87%)	5 (11%)	1 (2%)	6	39
All	All	1471/1780 (83%)	1335 (91%)	135 (9%)	1 (0%)	54	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	j	63	ARG

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	433/436 (99%)	433 (100%)	0	100	100
2	b	213/222 (96%)	213 (100%)	0	100	100
3	c	219/219 (100%)	219 (100%)	0	100	100
4	d	65/68 (96%)	64 (98%)	1 (2%)	65	81
5	e	77/126 (61%)	77 (100%)	0	100	100
6	f	50/82 (61%)	50 (100%)	0	100	100
7	g	63/153 (41%)	63 (100%)	0	100	100
8	h	42/52 (81%)	42 (100%)	0	100	100
9	i	55/58 (95%)	55 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	j	40/77 (52%)	40 (100%)	0	100 100
All	All	1257/1493 (84%)	1256 (100%)	1 (0%)	93 97

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

Mol	Chain	Res	Type
4	d	71	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	12	ASN
1	a	219	ASN
1	a	259	HIS
1	a	431	HIS
1	a	505	GLN
2	b	121	GLN
7	g	124	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 27 ligands modelled in this entry, 3 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	3PE	a	609	-	37,37,50	0.35	0	40,42,55	0.40	0
11	HEA	a	602	1	57,67,67	1.24	5 (8%)	61,103,103	1.53	14 (22%)
15	3PE	a	611	-	37,37,50	0.35	0	40,42,55	0.31	0
15	3PE	c	305	-	39,39,50	0.35	0	42,44,55	0.32	0
15	3PE	c	303	-	36,36,50	0.35	0	39,41,55	0.34	0
15	3PE	h	101	-	37,37,50	0.35	0	40,42,55	0.33	0
15	3PE	a	612	-	38,38,50	0.34	0	41,43,55	0.32	0
15	3PE	a	606	-	31,31,50	0.37	0	34,36,55	0.39	0
15	3PE	d	101	-	34,34,50	0.36	0	37,39,55	0.32	0
15	3PE	a	610	-	39,39,50	0.34	0	42,44,55	0.31	0
14	PC1	a	605	-	38,38,53	0.35	0	44,46,61	0.36	0
15	3PE	c	301	-	39,39,50	0.35	0	42,44,55	0.38	0
16	CDL	a	608	-	66,66,99	0.36	0	72,78,111	0.37	0
15	3PE	c	304	-	42,42,50	0.35	0	45,47,55	0.45	0
15	3PE	c	302	-	39,39,50	0.36	0	42,44,55	0.49	0
15	3PE	b	303	-	28,28,50	0.40	0	31,33,55	0.43	0
15	3PE	b	304	-	42,42,50	0.32	0	45,47,55	0.33	0
19	LYS	i	102	-	7,8,9	0.47	0	3,8,10	0.42	0
15	3PE	b	302	-	35,35,50	0.36	0	38,40,55	0.34	0
15	3PE	i	103	-	34,34,50	0.37	0	37,39,55	0.29	0
17	CUA	b	301	2	0,1,1	-	-	-		
11	HEA	a	601	1	57,67,67	1.22	5 (8%)	61,103,103	1.84	16 (26%)
14	PC1	i	101	-	35,35,53	0.35	0	41,43,61	0.40	0
15	3PE	a	607	-	39,39,50	0.35	0	42,44,55	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	3PE	a	609	-	-	14/41/41/54	-
11	HEA	a	602	1	3/3/7/16	9/32/76/76	-
15	3PE	a	611	-	-	5/41/41/54	-
15	3PE	c	305	-	-	7/43/43/54	-
15	3PE	c	303	-	-	9/40/40/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	3PE	h	101	-	-	3/41/41/54	-
15	3PE	a	612	-	-	5/42/42/54	-
15	3PE	a	606	-	-	11/35/35/54	-
15	3PE	d	101	-	-	15/38/38/54	-
15	3PE	a	610	-	-	10/43/43/54	-
14	PC1	a	605	-	-	15/42/42/57	-
15	3PE	c	301	-	-	12/43/43/54	-
16	CDL	a	608	-	-	15/77/77/110	-
15	3PE	c	304	-	-	12/46/46/54	-
15	3PE	c	302	-	-	10/43/43/54	-
15	3PE	b	303	-	-	10/32/32/54	-
15	3PE	b	304	-	-	6/46/46/54	-
19	LYS	i	102	-	-	1/6/7/9	-
15	3PE	b	302	-	-	11/39/39/54	-
15	3PE	i	103	-	-	10/38/38/54	-
11	HEA	a	601	1	3/3/7/16	8/32/76/76	-
14	PC1	i	101	-	-	6/39/39/57	-
15	3PE	a	607	-	-	5/43/43/54	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	602	HEA	C3A-C2A	-4.32	1.34	1.40
11	a	601	HEA	C3A-C2A	-3.83	1.35	1.40
11	a	601	HEA	C1D-ND	-3.39	1.34	1.40
11	a	602	HEA	C1D-ND	-3.30	1.34	1.40
11	a	601	HEA	C4D-C3D	3.01	1.50	1.45
11	a	601	HEA	C4B-NB	-2.83	1.35	1.40
11	a	602	HEA	C3C-C2C	-2.78	1.36	1.40
11	a	602	HEA	C4D-C3D	2.72	1.49	1.45
11	a	602	HEA	C4B-NB	-2.71	1.35	1.40
11	a	601	HEA	C3C-C2C	-2.43	1.37	1.40

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	601	HEA	C13-C12-C11	-4.70	107.28	114.35
11	a	601	HEA	C1D-ND-C4D	4.64	109.87	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	601	HEA	C4B-NB-C1B	3.83	109.03	105.07
11	a	601	HEA	C3D-C4D-ND	-3.34	107.12	110.36
11	a	601	HEA	CAA-CBA-CGA	-3.32	104.44	113.76
11	a	601	HEA	C13-C14-C15	-3.10	120.19	127.66
11	a	602	HEA	C13-C12-C11	-3.09	109.70	114.35
11	a	602	HEA	C17-C18-C19	-2.96	120.52	127.66
11	a	602	HEA	CAA-CBA-CGA	-2.89	105.67	113.76
11	a	601	HEA	OMA-CMA-C3A	-2.84	118.72	124.91
11	a	602	HEA	CMC-C2C-C1C	-2.78	124.19	128.46
11	a	602	HEA	C13-C14-C15	-2.77	120.98	127.66
11	a	602	HEA	CAD-CBD-CGD	-2.68	107.83	113.60
11	a	602	HEA	C1D-ND-C4D	2.67	107.83	105.07
11	a	601	HEA	C21-C22-C23	-2.60	118.85	127.75
11	a	602	HEA	C4B-NB-C1B	2.58	107.74	105.07
11	a	601	HEA	C3C-C4C-NC	-2.57	105.89	109.21
11	a	601	HEA	C17-C18-C19	-2.56	121.48	127.66
11	a	601	HEA	CMB-C2B-C3B	-2.52	125.53	130.34
11	a	601	HEA	CHA-C4D-C3D	2.40	128.37	124.84
11	a	601	HEA	CMC-C2C-C1C	-2.37	124.82	128.46
11	a	601	HEA	C26-C15-C14	-2.29	117.80	123.68
11	a	601	HEA	C27-C19-C20	2.28	119.10	115.27
11	a	602	HEA	C26-C15-C16	2.19	118.95	115.27
11	a	602	HEA	C25-C23-C24	2.17	119.40	114.60
11	a	602	HEA	CMB-C2B-C3B	-2.13	126.28	130.34
11	a	601	HEA	C25-C23-C24	2.13	119.31	114.60
11	a	602	HEA	C21-C22-C23	-2.05	120.74	127.75
11	a	602	HEA	C27-C19-C20	2.03	118.68	115.27
11	a	602	HEA	O2D-CGD-O1D	-2.01	118.28	123.30

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	a	601	HEA	NB
11	a	601	HEA	ND
11	a	601	HEA	NA
11	a	602	HEA	NB
11	a	602	HEA	ND
11	a	602	HEA	NA

All (209) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	a	602	HEA	C3B-C11-C12-C13
11	a	602	HEA	C15-C16-C17-C18
14	a	605	PC1	C1-O11-P-O12
14	i	101	PC1	C11-O13-P-O12
14	i	101	PC1	C11-O13-P-O14
14	i	101	PC1	C11-O13-P-O11
15	a	606	3PE	C11-O13-P-O12
15	a	606	3PE	O13-C11-C12-N
15	a	607	3PE	C11-O13-P-O14
15	a	607	3PE	O13-C11-C12-N
15	a	609	3PE	C11-O13-P-O14
15	a	609	3PE	O13-C11-C12-N
15	a	610	3PE	C11-O13-P-O14
15	a	610	3PE	O13-C11-C12-N
15	a	611	3PE	C11-O13-P-O12
15	a	611	3PE	O13-C11-C12-N
15	a	612	3PE	C1-O11-P-O12
15	b	302	3PE	O13-C11-C12-N
15	b	303	3PE	C1-O11-P-O12
15	b	303	3PE	O13-C11-C12-N
15	b	304	3PE	C1-O11-P-O12
15	b	304	3PE	C11-O13-P-O12
15	b	304	3PE	O13-C11-C12-N
15	c	301	3PE	C11-O13-P-O11
15	c	301	3PE	C11-O13-P-O12
15	c	301	3PE	C11-O13-P-O14
15	c	301	3PE	O13-C11-C12-N
15	c	302	3PE	O13-C11-C12-N
15	c	303	3PE	C1-O11-P-O12
15	c	303	3PE	C11-O13-P-O11
15	c	304	3PE	C11-O13-P-O11
15	c	305	3PE	C11-O13-P-O12
15	c	305	3PE	O13-C11-C12-N
15	d	101	3PE	C1-O11-P-O12
15	d	101	3PE	C1-O11-P-O13
15	d	101	3PE	C11-O13-P-O12
15	d	101	3PE	C11-O13-P-O14
15	d	101	3PE	O13-C11-C12-N
15	i	103	3PE	C1-O11-P-O12
15	i	103	3PE	C11-O13-P-O12
15	i	103	3PE	C11-O13-P-O14
15	i	103	3PE	O13-C11-C12-N
16	a	608	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
16	a	608	CDL	CA2-OA2-PA1-OA4
16	a	608	CDL	CB3-OB5-PB2-OB3
19	i	102	LYS	O-C-CA-CB
11	a	601	HEA	C21-C22-C23-C25
11	a	601	HEA	C21-C22-C23-C24
11	a	601	HEA	C13-C14-C15-C26
11	a	602	HEA	C21-C22-C23-C25
11	a	602	HEA	C13-C14-C15-C26
14	a	605	PC1	C11-C12-N-C15
14	a	605	PC1	C21-C22-C23-C24
15	a	610	3PE	C21-C22-C23-C24
14	a	605	PC1	C11-C12-N-C13
15	a	606	3PE	C11-O13-P-O11
15	a	609	3PE	C1-O11-P-O13
15	a	609	3PE	C11-O13-P-O11
15	a	611	3PE	C1-O11-P-O13
15	a	611	3PE	C11-O13-P-O11
15	b	303	3PE	C1-O11-P-O13
15	b	304	3PE	C1-O11-P-O13
15	b	304	3PE	C11-O13-P-O11
15	c	302	3PE	C11-O13-P-O11
15	c	303	3PE	C1-O11-P-O13
15	d	101	3PE	C11-O13-P-O11
15	i	103	3PE	C11-O13-P-O11
16	a	608	CDL	CA2-OA2-PA1-OA5
16	a	608	CDL	CA3-OA5-PA1-OA2
15	c	301	3PE	C31-C32-C33-C34
15	c	304	3PE	C32-C33-C34-C35
14	a	605	PC1	C33-C34-C35-C36
15	b	302	3PE	C29-C2A-C2B-C2C
15	c	305	3PE	C23-C24-C25-C26
15	i	103	3PE	C22-C23-C24-C25
14	a	605	PC1	C11-C12-N-C14
11	a	602	HEA	C21-C22-C23-C24
15	a	606	3PE	O21-C2-C3-O31
14	a	605	PC1	C1-O11-P-O13
15	a	610	3PE	C11-O13-P-O11
15	c	304	3PE	C1-O11-P-O13
15	i	103	3PE	C1-O11-P-O13
15	a	610	3PE	O11-C1-C2-C3
11	a	602	HEA	O11-C11-C12-C13
15	c	304	3PE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
15	a	609	3PE	C36-C37-C38-C39
15	c	305	3PE	C37-C38-C39-C3A
15	c	304	3PE	O21-C2-C3-O31
14	a	605	PC1	C32-C33-C34-C35
15	c	304	3PE	C23-C24-C25-C26
15	c	302	3PE	O11-C1-C2-C3
15	d	101	3PE	O11-C1-C2-C3
15	b	302	3PE	C32-C33-C34-C35
15	a	609	3PE	C21-C22-C23-C24
15	a	606	3PE	C1-C2-C3-O31
15	b	302	3PE	C1-C2-C3-O31
15	b	303	3PE	C1-C2-C3-O31
15	c	301	3PE	C1-C2-C3-O31
16	a	608	CDL	CB3-CB4-CB6-OB8
15	a	609	3PE	C24-C25-C26-C27
15	b	302	3PE	C11-O13-P-O11
15	c	305	3PE	C11-O13-P-O11
15	h	101	3PE	C11-O13-P-O11
15	c	302	3PE	O11-C1-C2-O21
15	b	303	3PE	O21-C2-C3-O31
15	d	101	3PE	O21-C2-C3-O31
15	d	101	3PE	C2-C1-O11-P
15	c	303	3PE	O11-C1-C2-C3
11	a	602	HEA	C13-C14-C15-C16
15	a	610	3PE	C2-C1-O11-P
15	c	302	3PE	C2-C1-O11-P
15	c	301	3PE	O21-C2-C3-O31
15	a	607	3PE	C11-O13-P-O11
15	a	612	3PE	C1-O11-P-O13
15	b	303	3PE	C11-O13-P-O11
15	a	606	3PE	C2-C1-O11-P
14	a	605	PC1	C1-O11-P-O14
15	a	609	3PE	C1-O11-P-O12
15	a	609	3PE	C1-O11-P-O14
15	a	609	3PE	C11-O13-P-O12
15	a	610	3PE	C11-O13-P-O12
15	a	611	3PE	C1-O11-P-O14
15	a	612	3PE	C1-O11-P-O14
15	b	302	3PE	C11-O13-P-O12
15	b	303	3PE	C11-O13-P-O12
15	c	302	3PE	C11-O13-P-O14
15	c	303	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
15	c	304	3PE	C1-O11-P-O12
15	c	304	3PE	C1-O11-P-O14
15	c	304	3PE	C11-O13-P-O12
15	c	305	3PE	C11-O13-P-O14
15	d	101	3PE	C1-O11-P-O14
15	i	103	3PE	C1-O11-P-O14
16	a	608	CDL	CA3-OA5-PA1-OA3
16	a	608	CDL	CB3-OB5-PB2-OB4
14	a	605	PC1	C31-C32-C33-C34
15	c	303	3PE	O11-C1-C2-O21
15	d	101	3PE	O11-C1-C2-O21
16	a	608	CDL	OB5-CB3-CB4-OB6
14	i	101	PC1	O13-C11-C12-N
15	b	302	3PE	O21-C2-C3-O31
16	a	608	CDL	OB6-CB4-CB6-OB8
15	b	304	3PE	O31-C31-C32-C33
15	c	301	3PE	O31-C31-C32-C33
15	c	303	3PE	C2-C1-O11-P
15	a	606	3PE	C34-C35-C36-C37
15	a	610	3PE	O11-C1-C2-O21
15	c	305	3PE	O31-C31-C32-C33
15	c	301	3PE	C37-C38-C39-C3A
15	a	606	3PE	C1-O11-P-O13
15	b	302	3PE	C1-O11-P-O13
15	c	301	3PE	C1-O11-P-O13
15	c	302	3PE	C1-O11-P-O13
15	c	304	3PE	C1-C2-C3-O31
15	b	303	3PE	C2-C1-O11-P
15	a	607	3PE	C26-C27-C28-C29
11	a	601	HEA	CAD-CBD-CGD-O1D
15	a	609	3PE	C31-C32-C33-C34
15	c	302	3PE	C1-C2-O21-C21
15	c	304	3PE	C3-C2-O21-C21
15	a	609	3PE	C39-C3A-C3B-C3C
15	b	302	3PE	C33-C34-C35-C36
16	a	608	CDL	C54-C55-C56-C57
11	a	601	HEA	CAA-CBA-CGA-O2A
11	a	601	HEA	CAD-CBD-CGD-O2D
11	a	601	HEA	CAA-CBA-CGA-O1A
14	i	101	PC1	C32-C33-C34-C35
15	a	606	3PE	O31-C31-C32-C33
14	a	605	PC1	C3-C2-O21-C21

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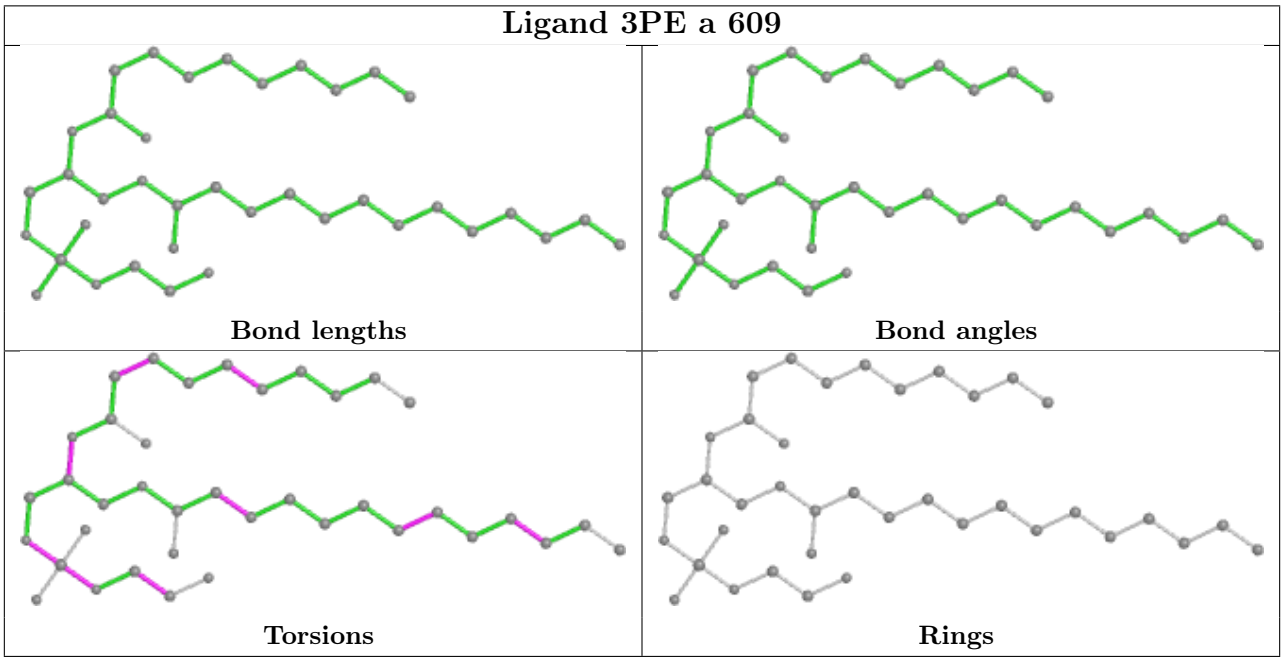
Mol	Chain	Res	Type	Atoms
15	a	609	3PE	C1-C2-O21-C21
15	b	303	3PE	C3-C2-O21-C21
11	a	602	HEA	C11-C12-C13-C14
14	a	605	PC1	O21-C21-C22-C23
15	d	101	3PE	C1-C2-C3-O31
15	c	303	3PE	O21-C21-C22-C23
15	d	101	3PE	O31-C31-C32-C33
15	d	101	3PE	O21-C21-C22-C23
15	h	101	3PE	C26-C27-C28-C29
15	c	301	3PE	C27-C28-C29-C2A
16	a	608	CDL	C14-C15-C16-C17
15	a	612	3PE	O21-C2-C3-O31
15	a	610	3PE	O31-C31-C32-C33
16	a	608	CDL	C52-C51-CB5-OB6
15	a	607	3PE	C25-C26-C27-C28
15	a	612	3PE	C23-C24-C25-C26
15	d	101	3PE	O32-C31-C32-C33
11	a	601	HEA	C26-C15-C16-C17
15	a	606	3PE	O21-C21-C22-C23
15	a	606	3PE	O32-C31-C32-C33
15	c	303	3PE	O22-C21-C22-C23
14	a	605	PC1	C11-O13-P-O14
15	b	302	3PE	C1-O11-P-O14
15	c	301	3PE	C1-O11-P-O14
15	c	302	3PE	C11-O13-P-O12
15	h	101	3PE	C11-O13-P-O14
14	a	605	PC1	O22-C21-C22-C23
15	a	610	3PE	O32-C31-C32-C33
11	a	602	HEA	CAD-CBD-CGD-O2D
15	c	302	3PE	C33-C34-C35-C36
14	a	605	PC1	C1-C2-O21-C21
15	a	609	3PE	C3-C2-O21-C21
15	b	303	3PE	C1-C2-O21-C21
15	c	304	3PE	C1-C2-O21-C21
16	a	608	CDL	C52-C51-CB5-OB7
15	i	103	3PE	O31-C31-C32-C33
15	b	302	3PE	O31-C31-C32-C33
14	i	101	PC1	C38-C39-C3A-C3B
16	a	608	CDL	C12-C11-CA5-OA6
15	i	103	3PE	O32-C31-C32-C33

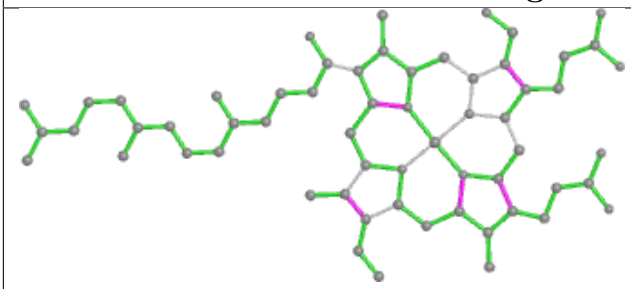
There are no ring outliers.

No monomer is involved in short contacts.

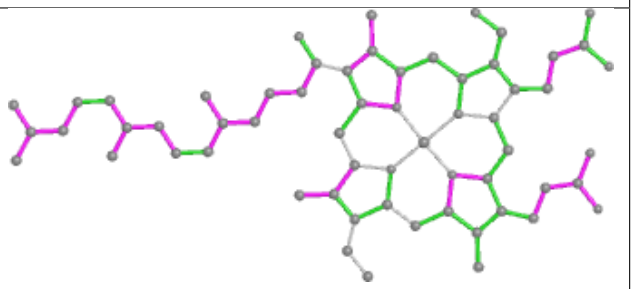
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



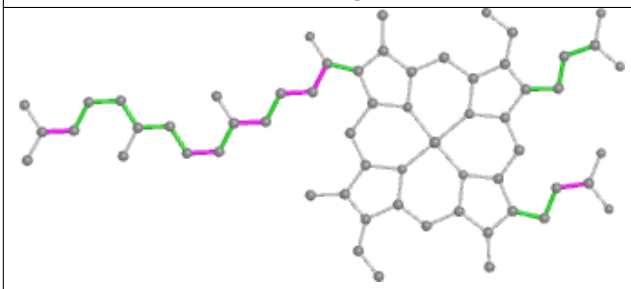
Ligand HEA a 602



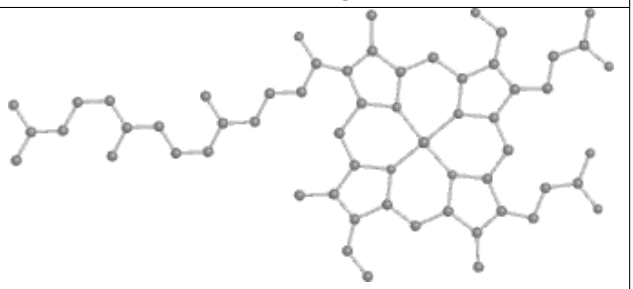
Bond lengths



Bond angles

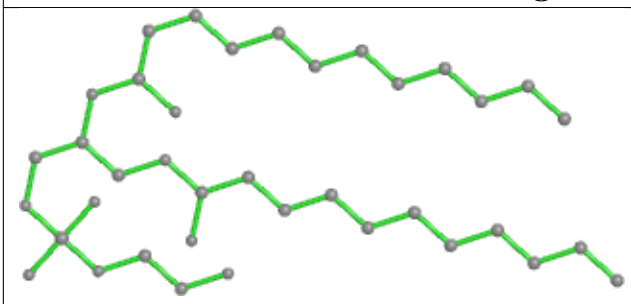


Torsions

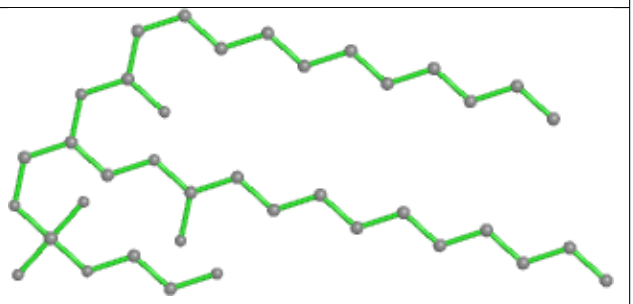


Rings

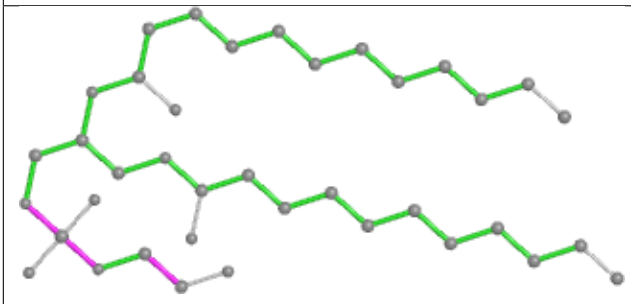
Ligand 3PE a 611



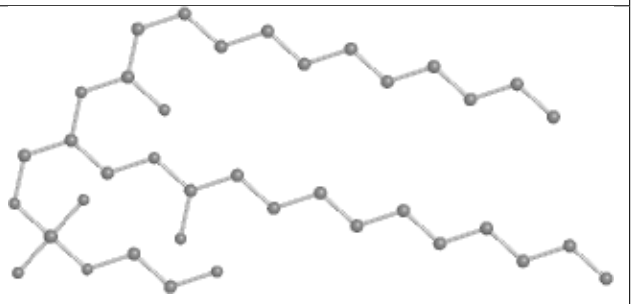
Bond lengths



Bond angles

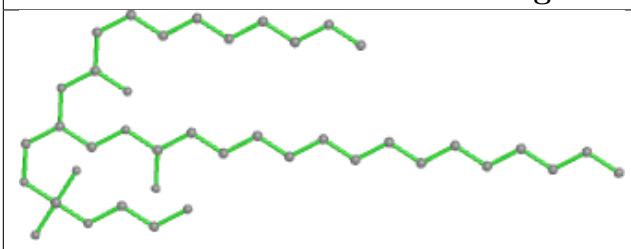


Torsions

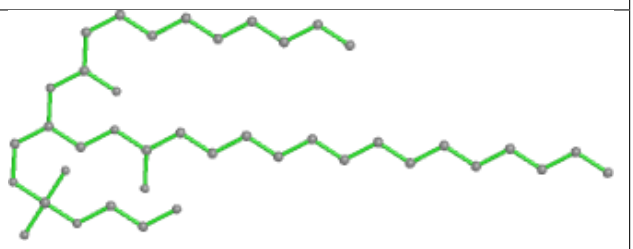


Rings

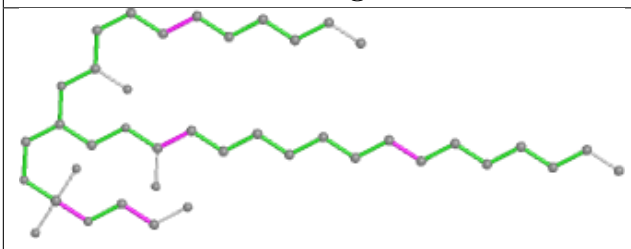
Ligand 3PE c 305



Bond lengths



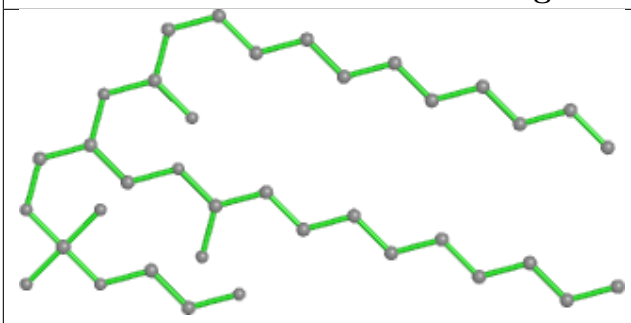
Bond angles



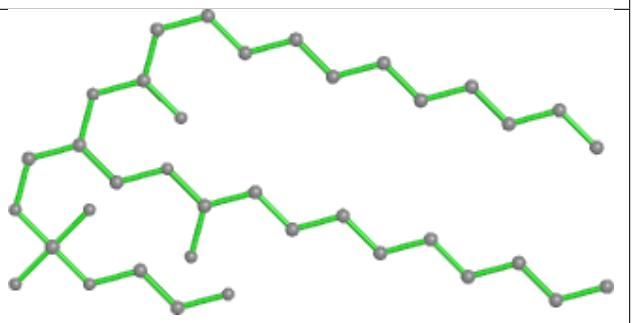
Torsions

Rings

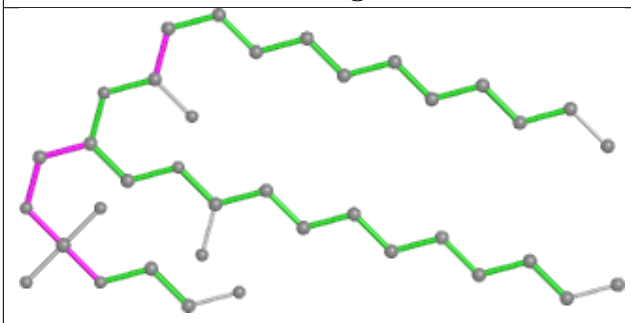
Ligand 3PE c 303



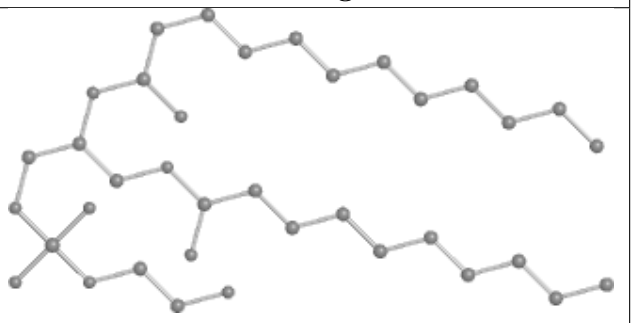
Bond lengths



Bond angles

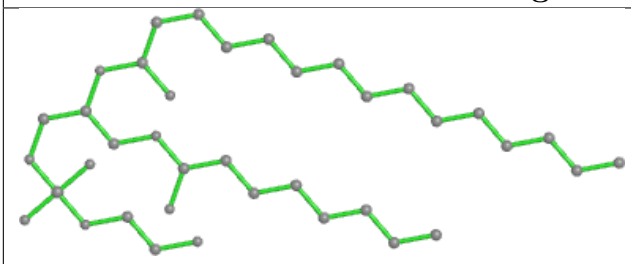


Torsions

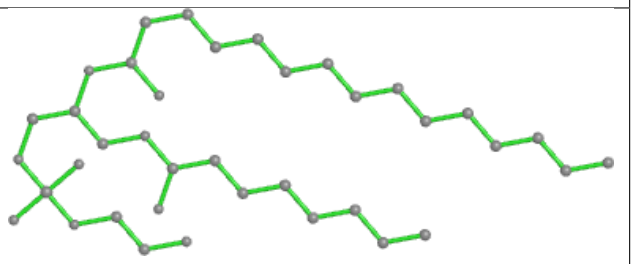


Rings

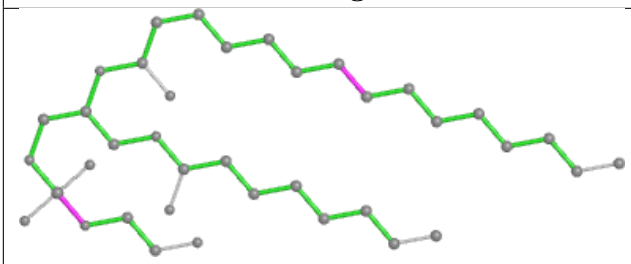
Ligand 3PE h 101



Bond lengths



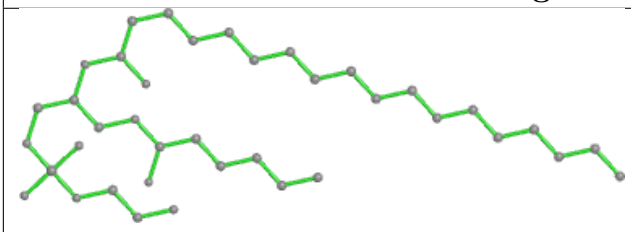
Bond angles



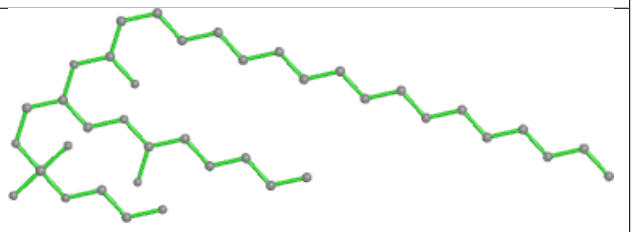
Torsions

Rings

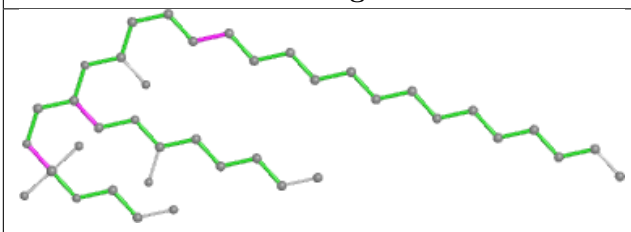
Ligand 3PE a 612



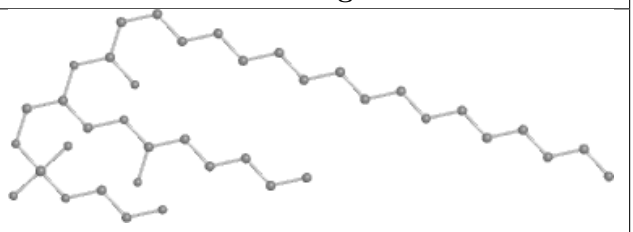
Bond lengths



Bond angles

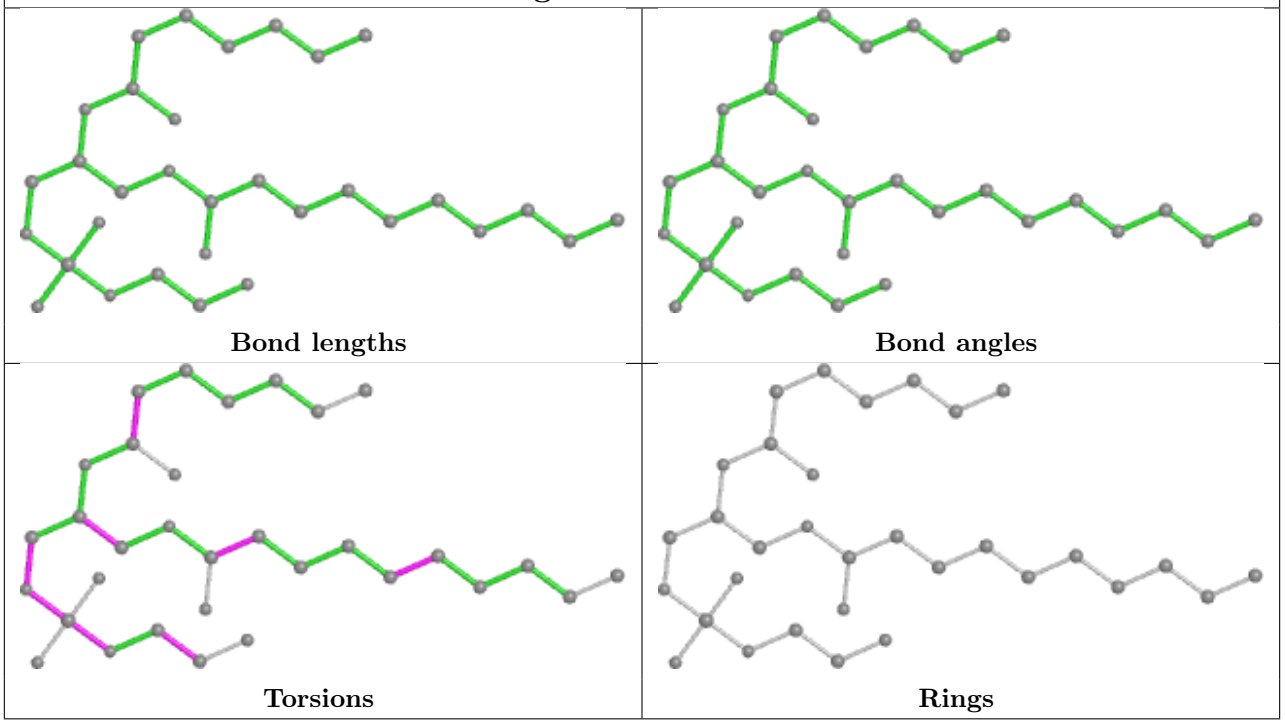


Torsions

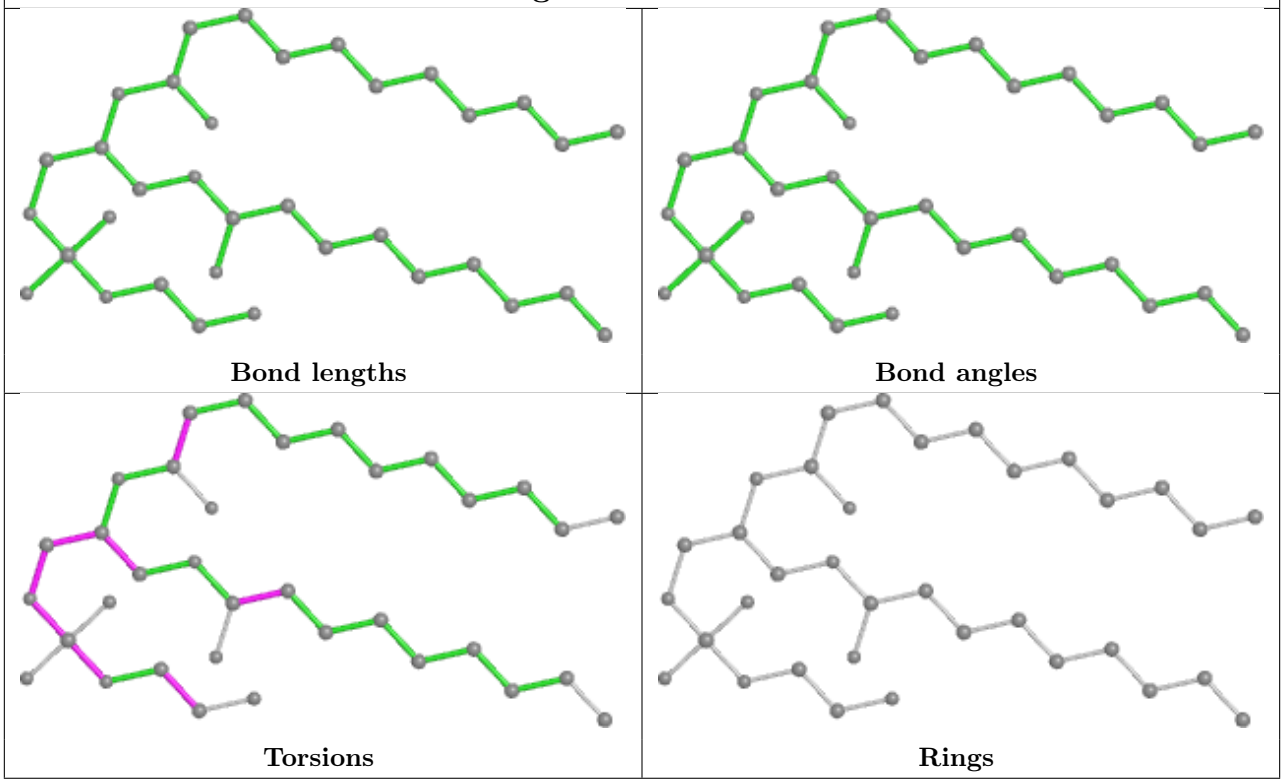


Rings

Ligand 3PE a 606



Ligand 3PE d 101



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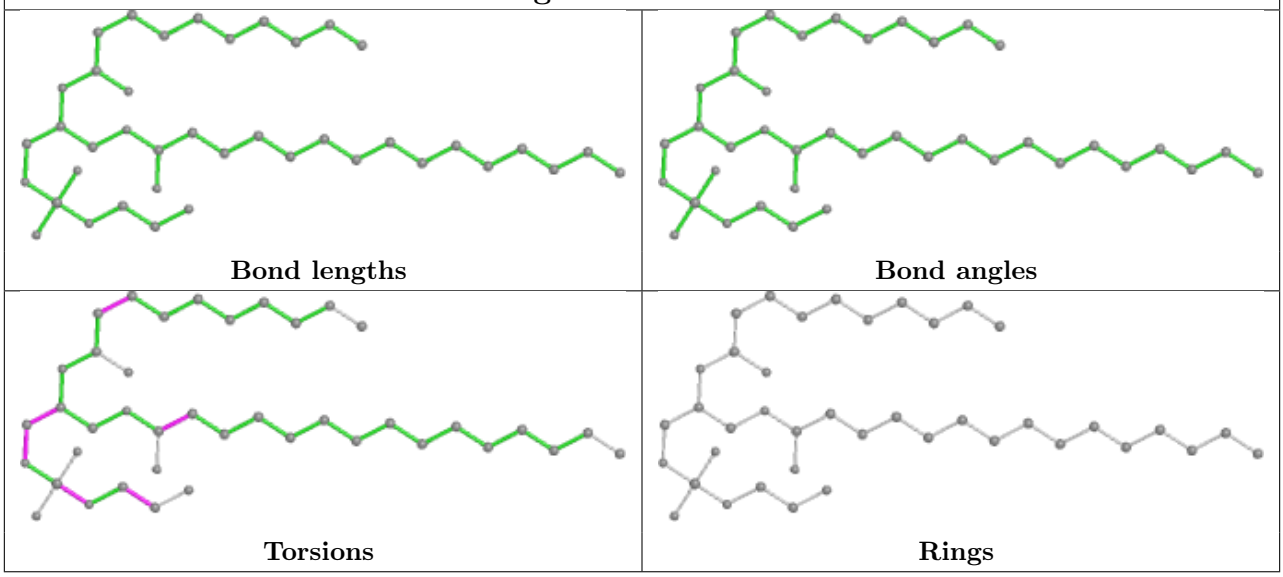
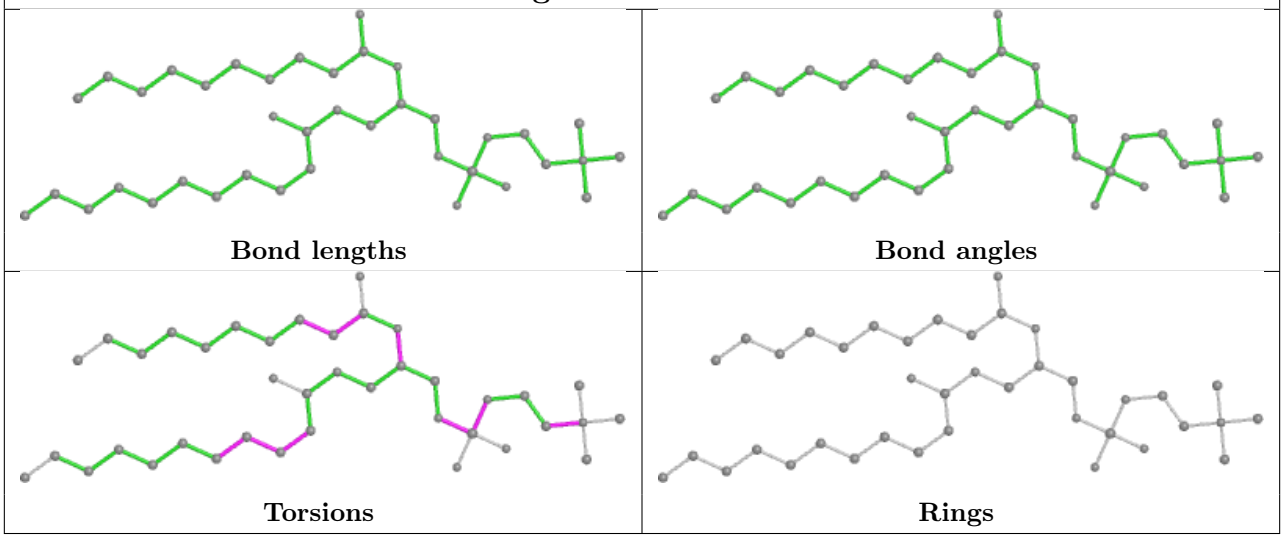
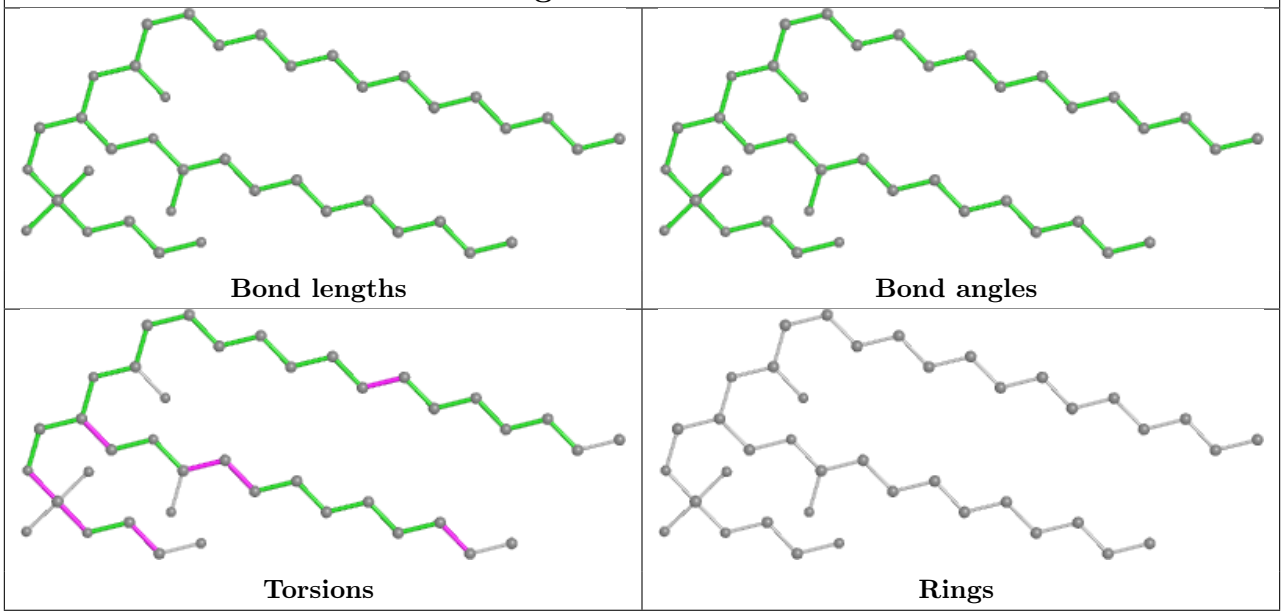


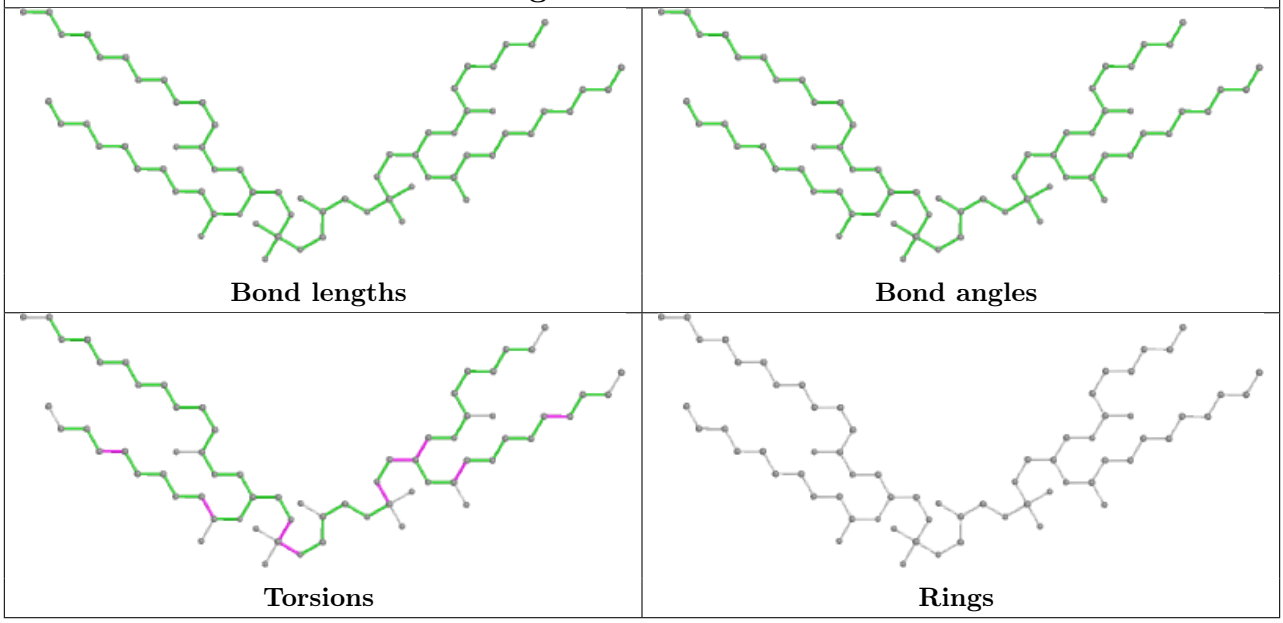
Ligand PC1 a 605



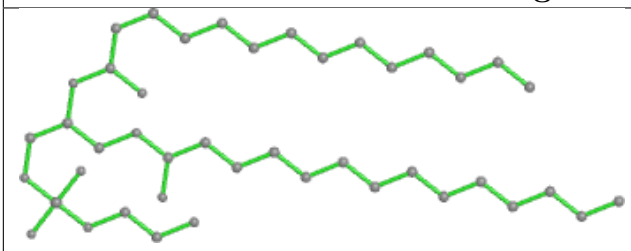
Ligand 3PE c 301



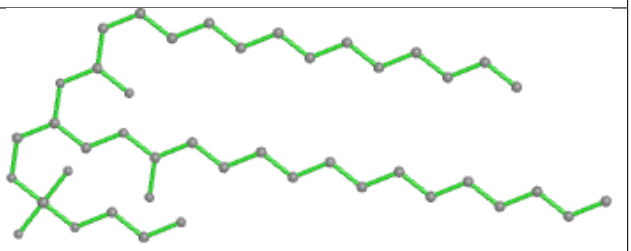
Ligand CDL a 608



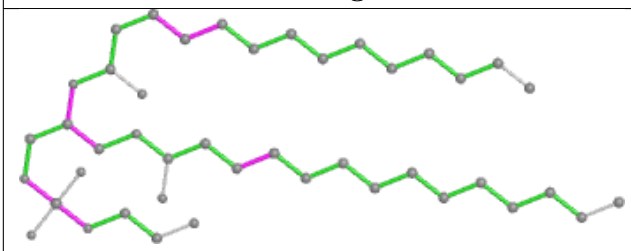
Ligand 3PE c 304



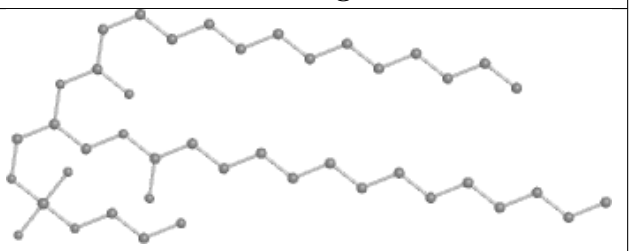
Bond lengths



Bond angles

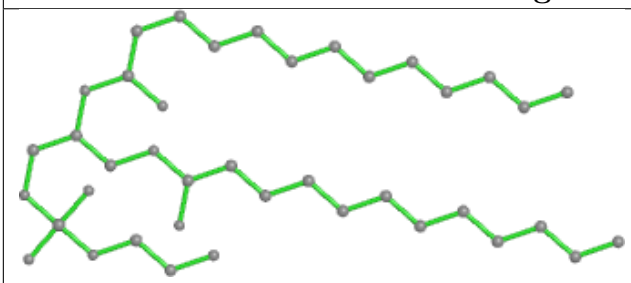


Torsions

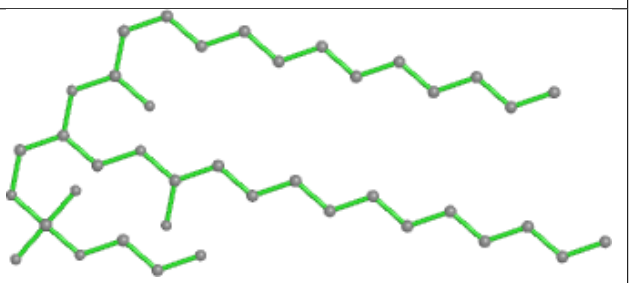


Rings

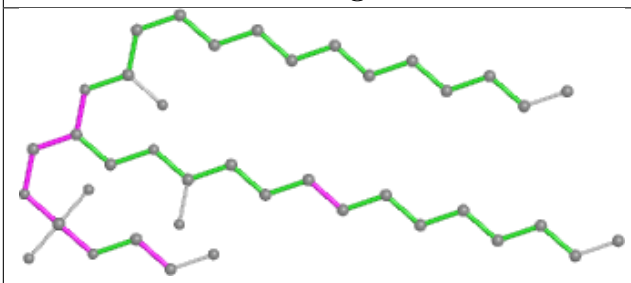
Ligand 3PE c 302



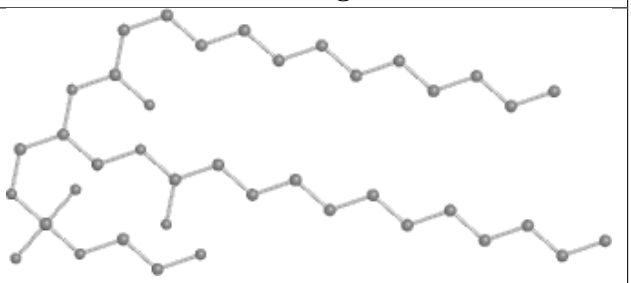
Bond lengths



Bond angles

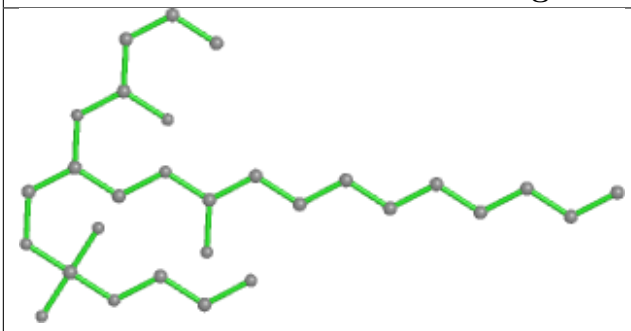


Torsions

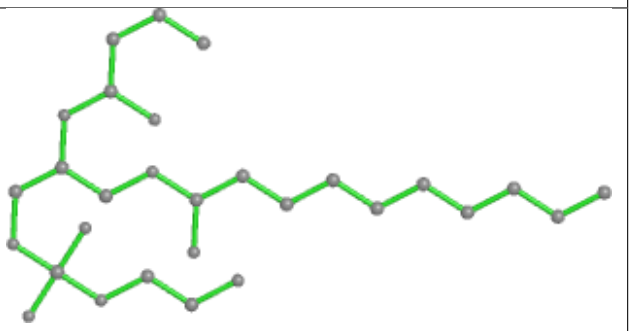


Rings

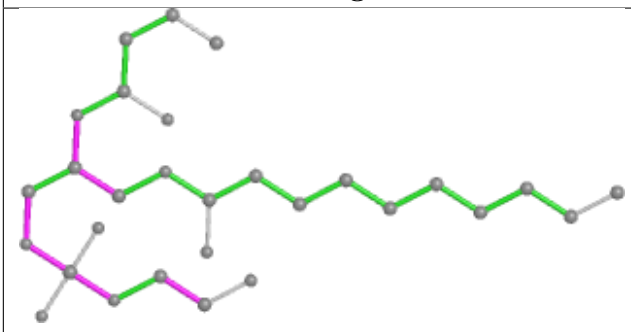
Ligand 3PE b 303



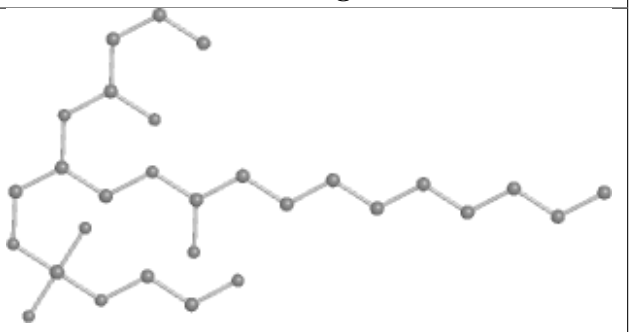
Bond lengths



Bond angles

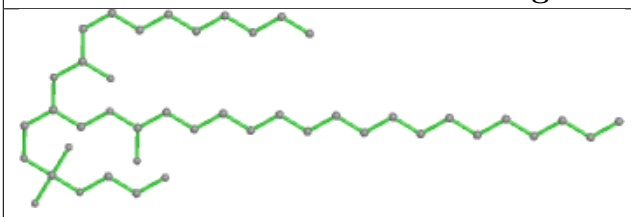


Torsions

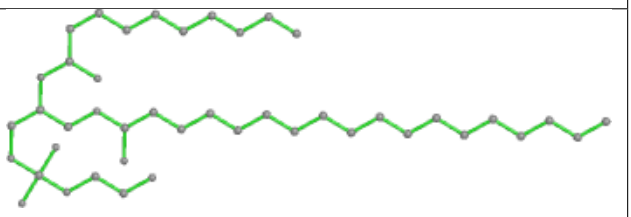


Rings

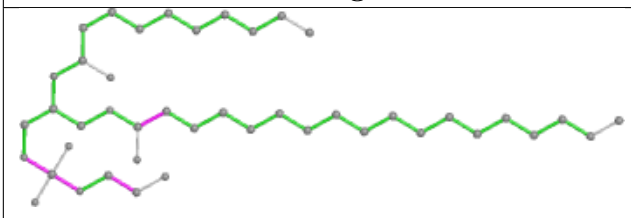
Ligand 3PE b 304



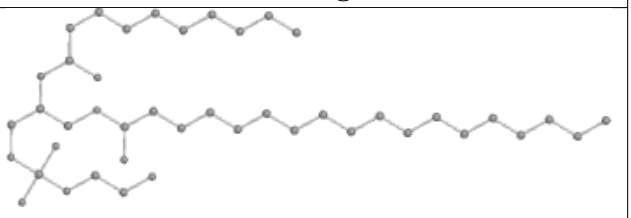
Bond lengths



Bond angles

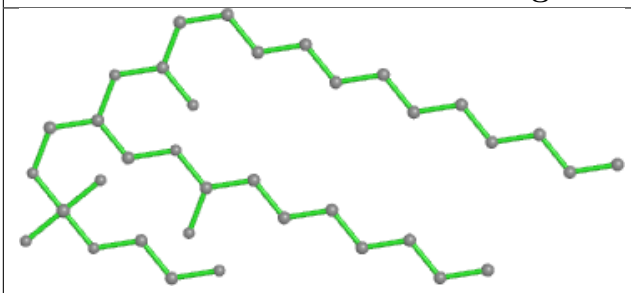


Torsions

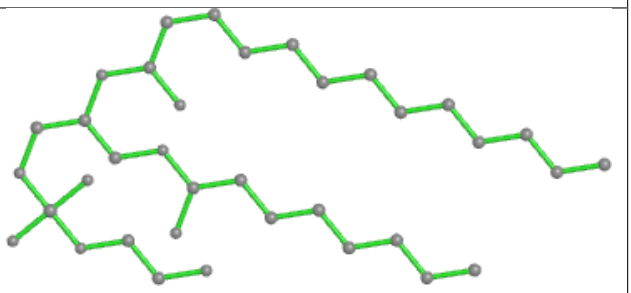


Rings

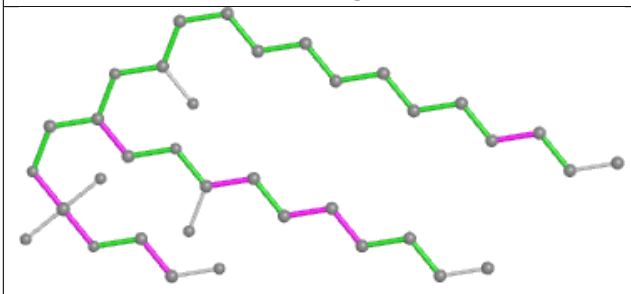
Ligand 3PE b 302



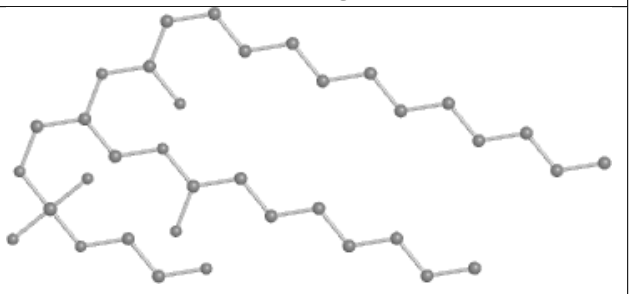
Bond lengths



Bond angles

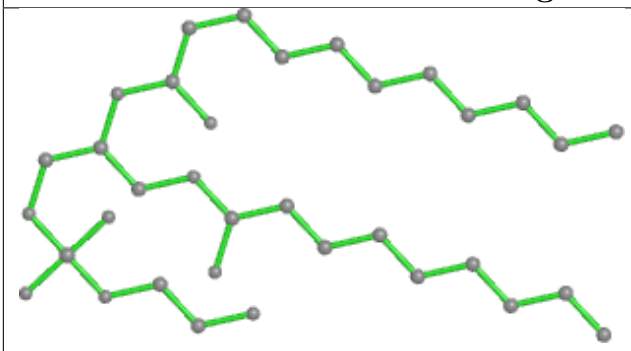


Torsions

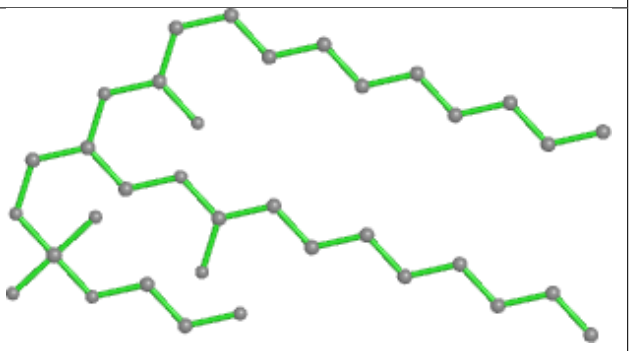


Rings

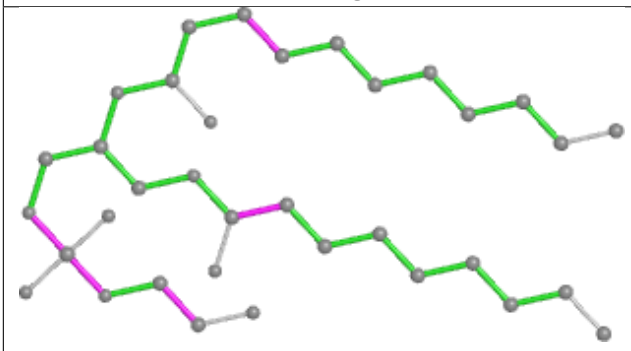
Ligand 3PE i 103



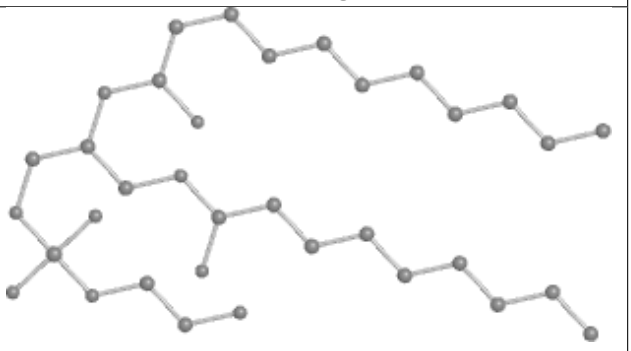
Bond lengths



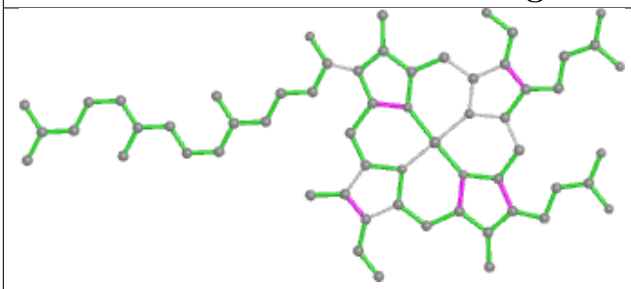
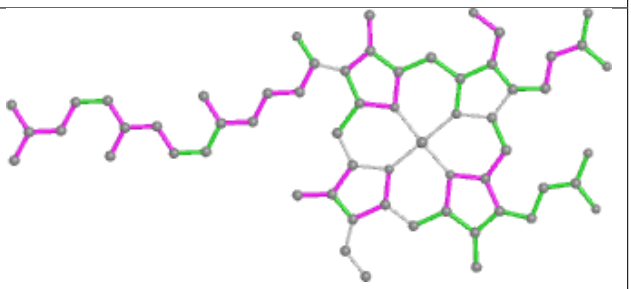
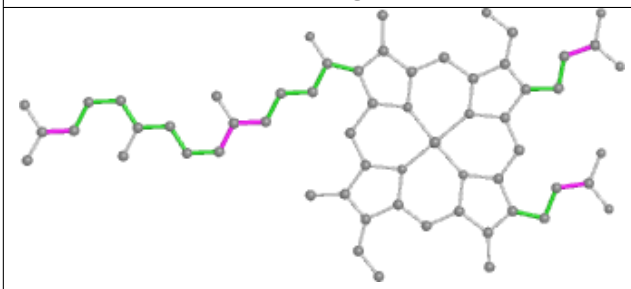
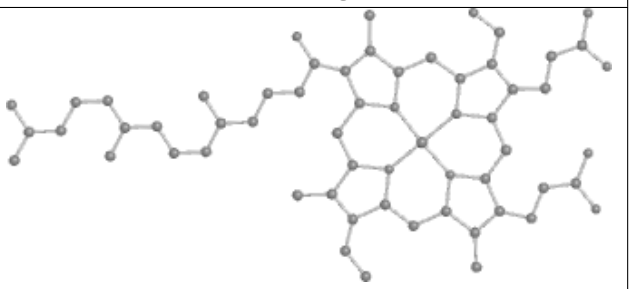
Bond angles

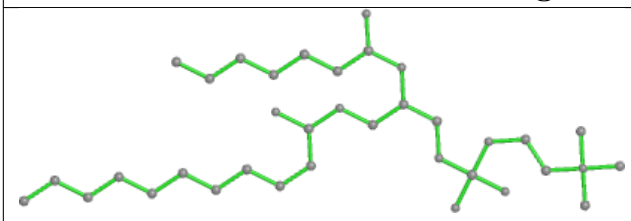
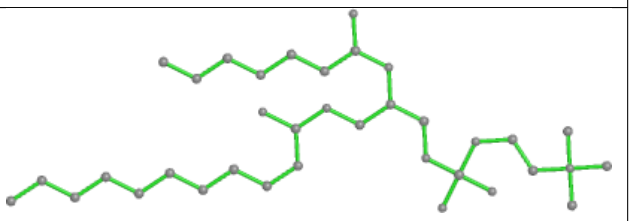
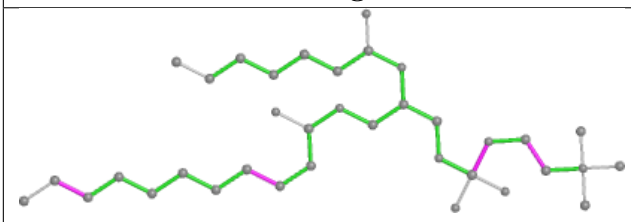
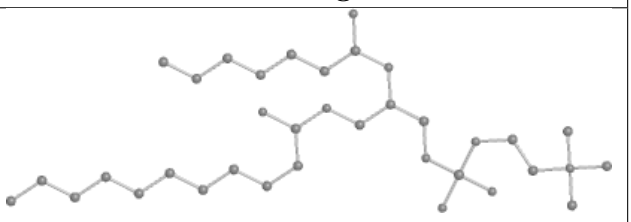


Torsions

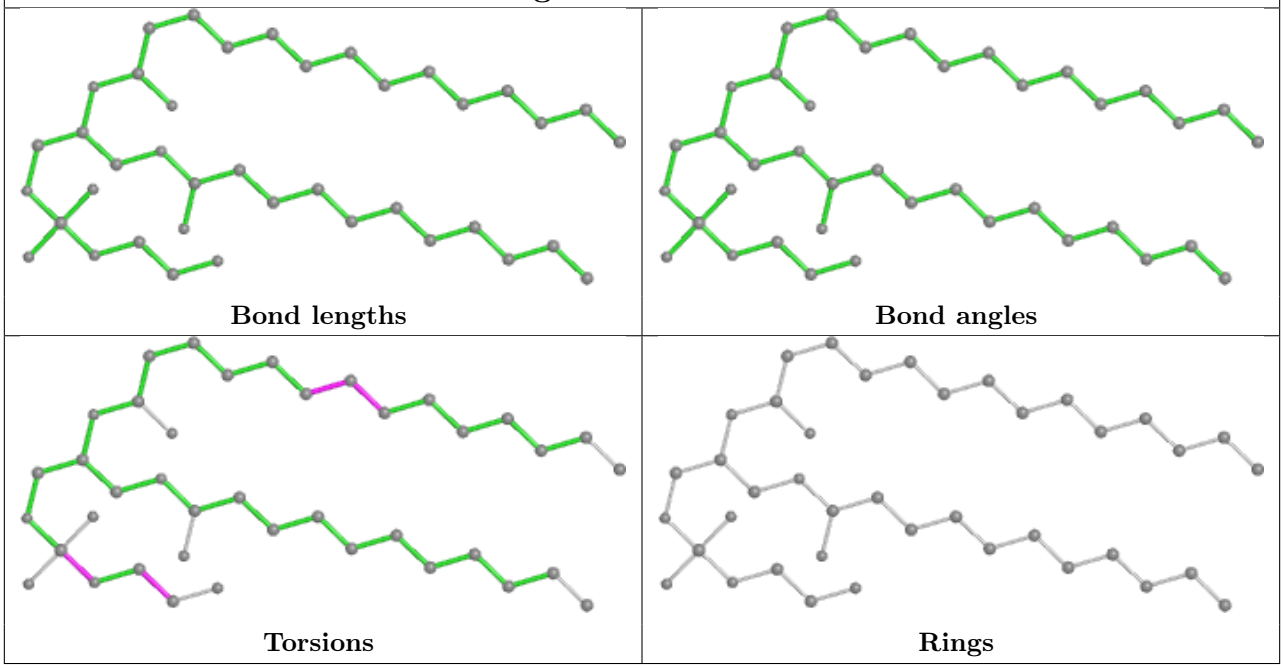


Rings

Ligand HEA a 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 i 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE a 607



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

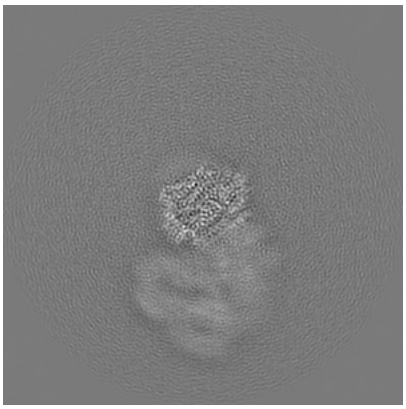
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22447. These allow visual inspection of the internal detail of the map and identification of artifacts.

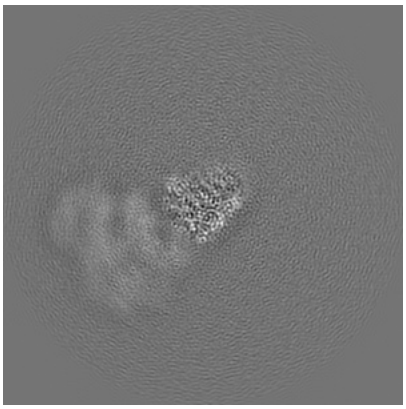
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

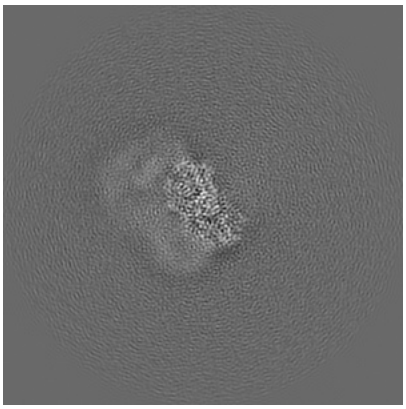
6.1.1 Primary map



X

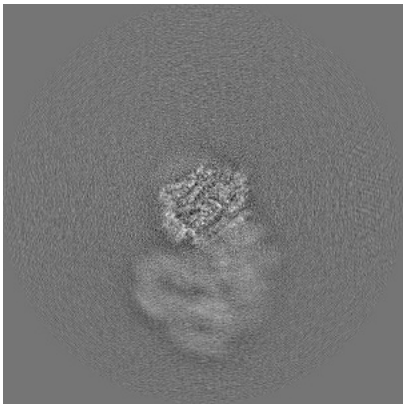


Y

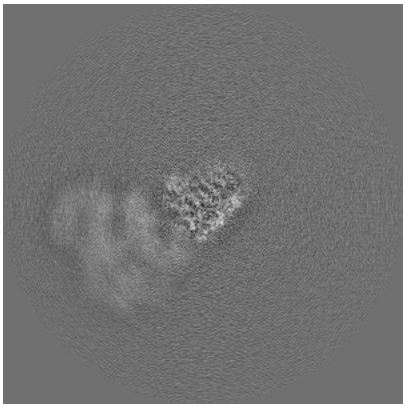


Z

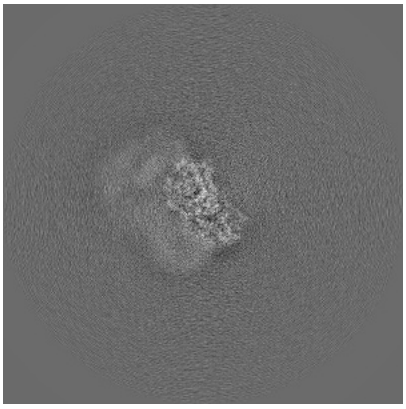
6.1.2 Raw map



X



Y

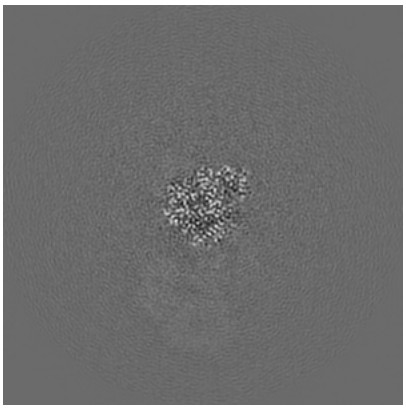


Z

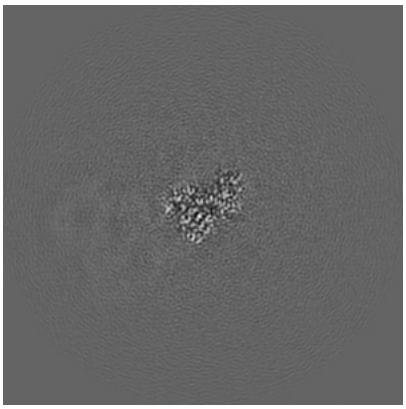
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

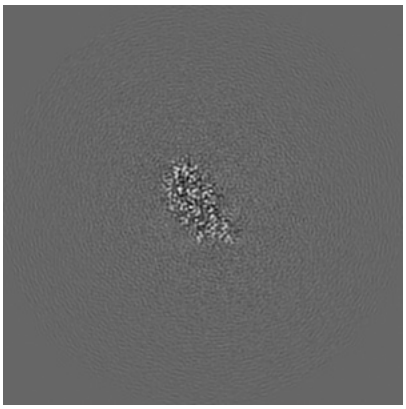
6.2.1 Primary map



X Index: 256

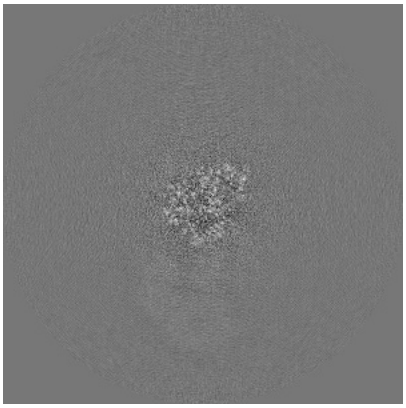


Y Index: 256

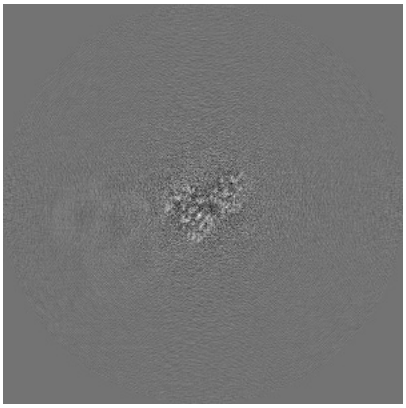


Z Index: 256

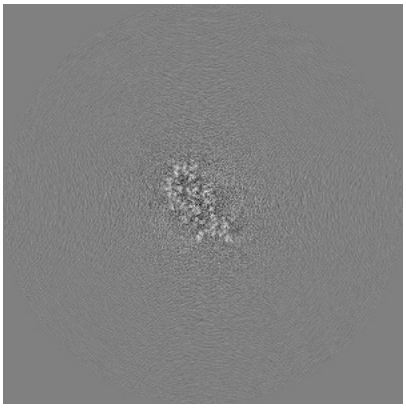
6.2.2 Raw map



X Index: 256



Y Index: 256

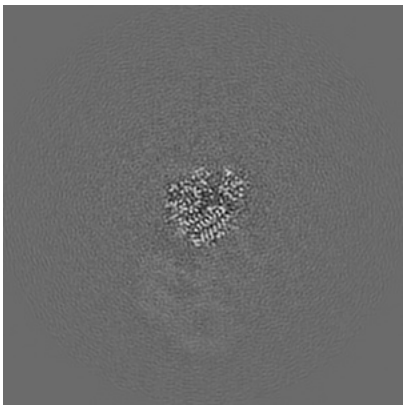


Z Index: 256

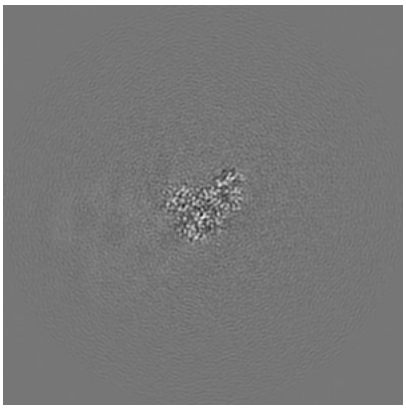
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

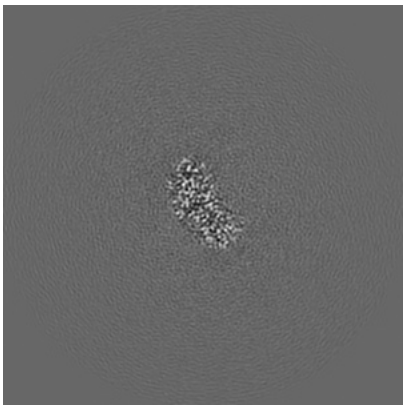
6.3.1 Primary map



X Index: 252

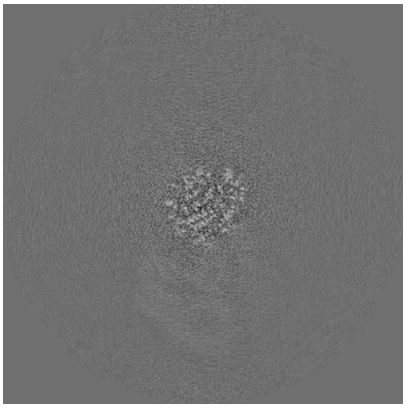


Y Index: 253

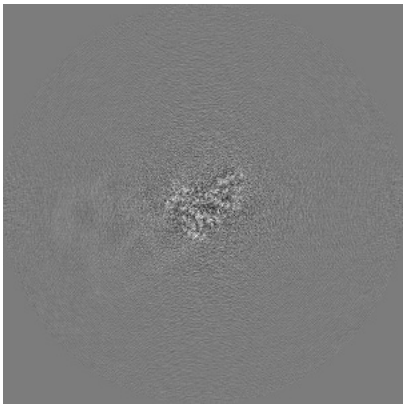


Z Index: 266

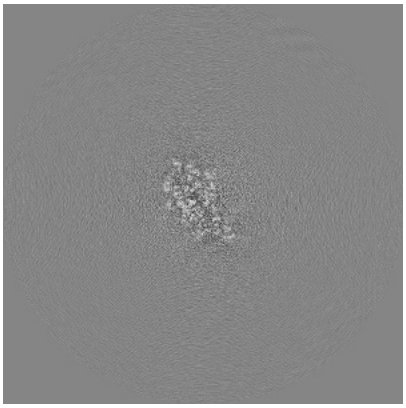
6.3.2 Raw map



X Index: 250



Y Index: 254



Z Index: 253

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

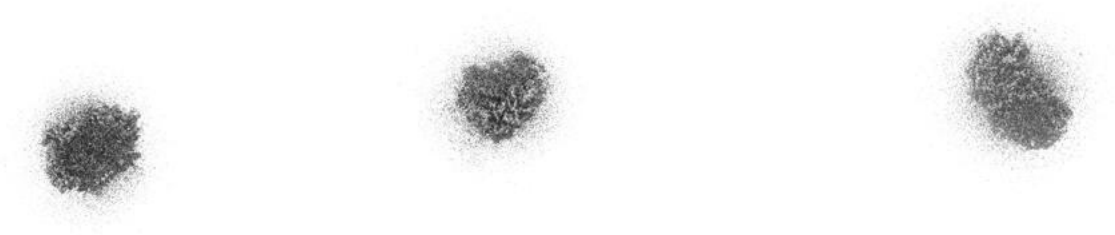
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. 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.

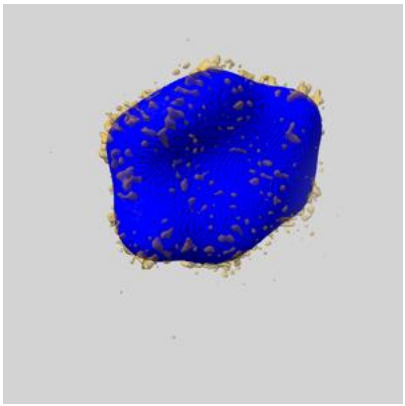
6.5 Mask visualisation (i)

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

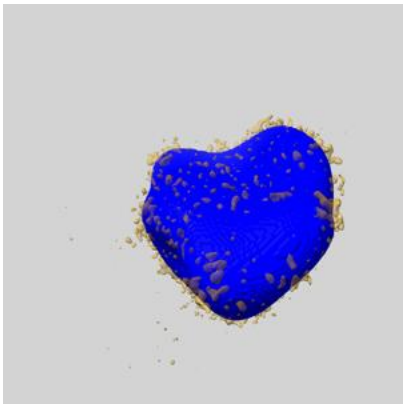
A mask typically either:

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

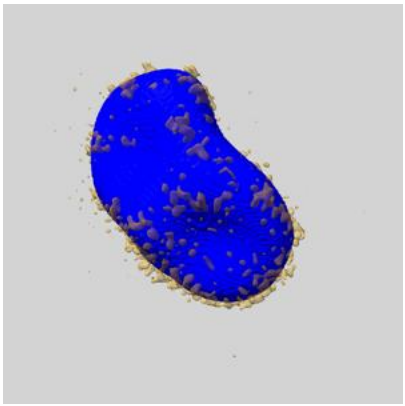
6.5.1 emd_22447_msk_1.map (i)



X



Y

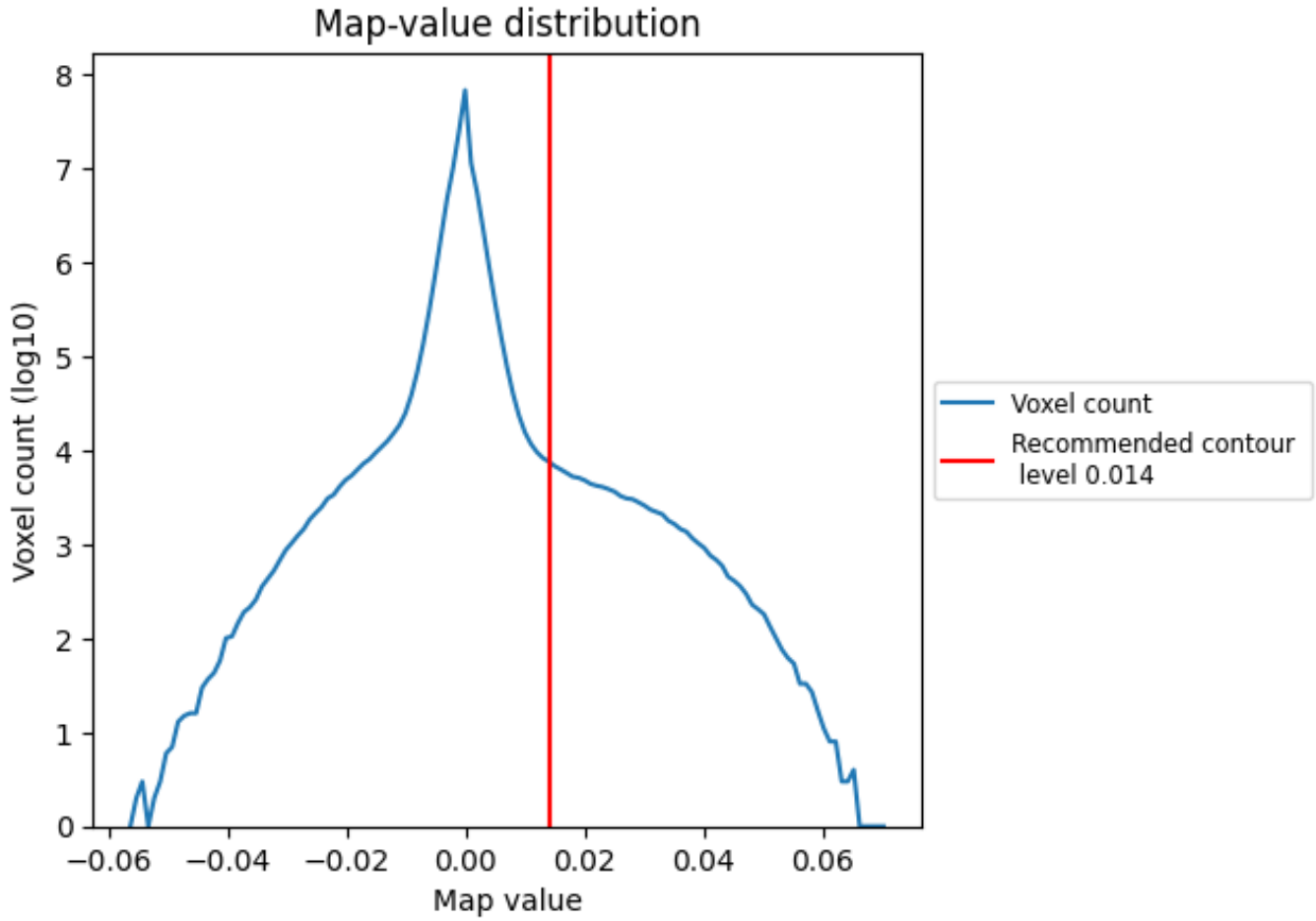


Z

7 Map analysis

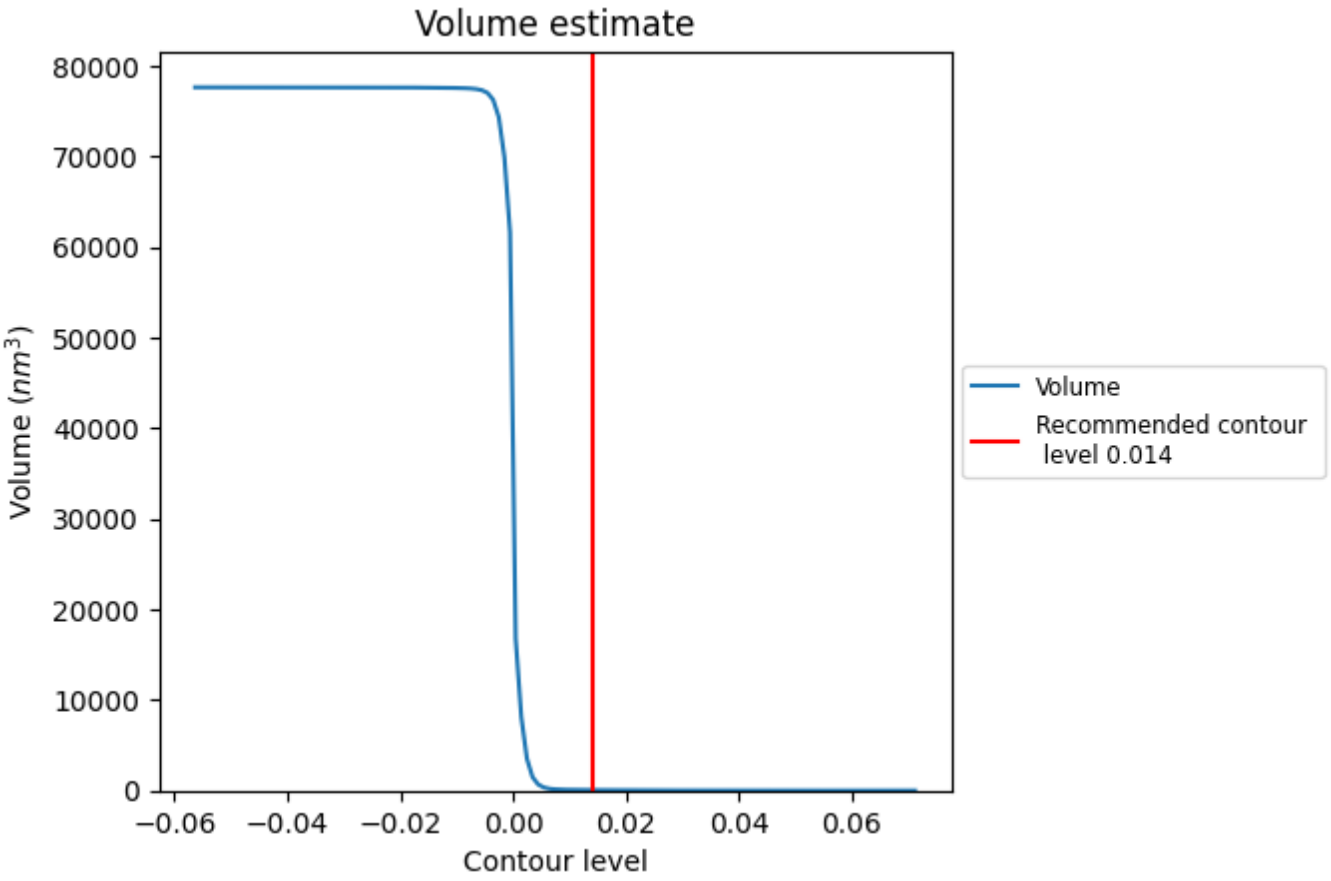
This section contains the results of statistical analysis of the map.

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.

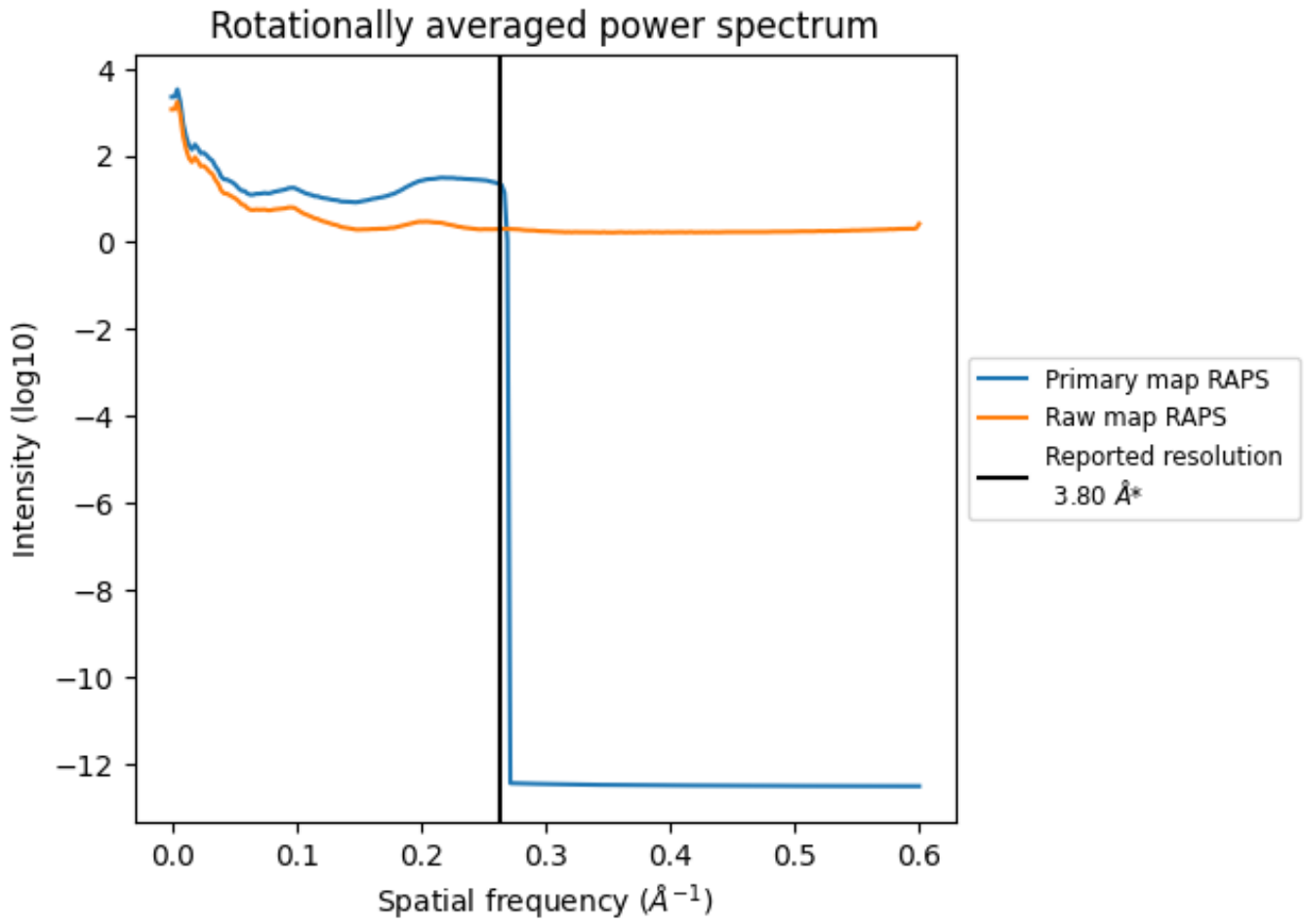
7.2 Volume estimate



The volume at the recommended contour level is 56 nm^3; this corresponds to an approximate mass of 51 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)

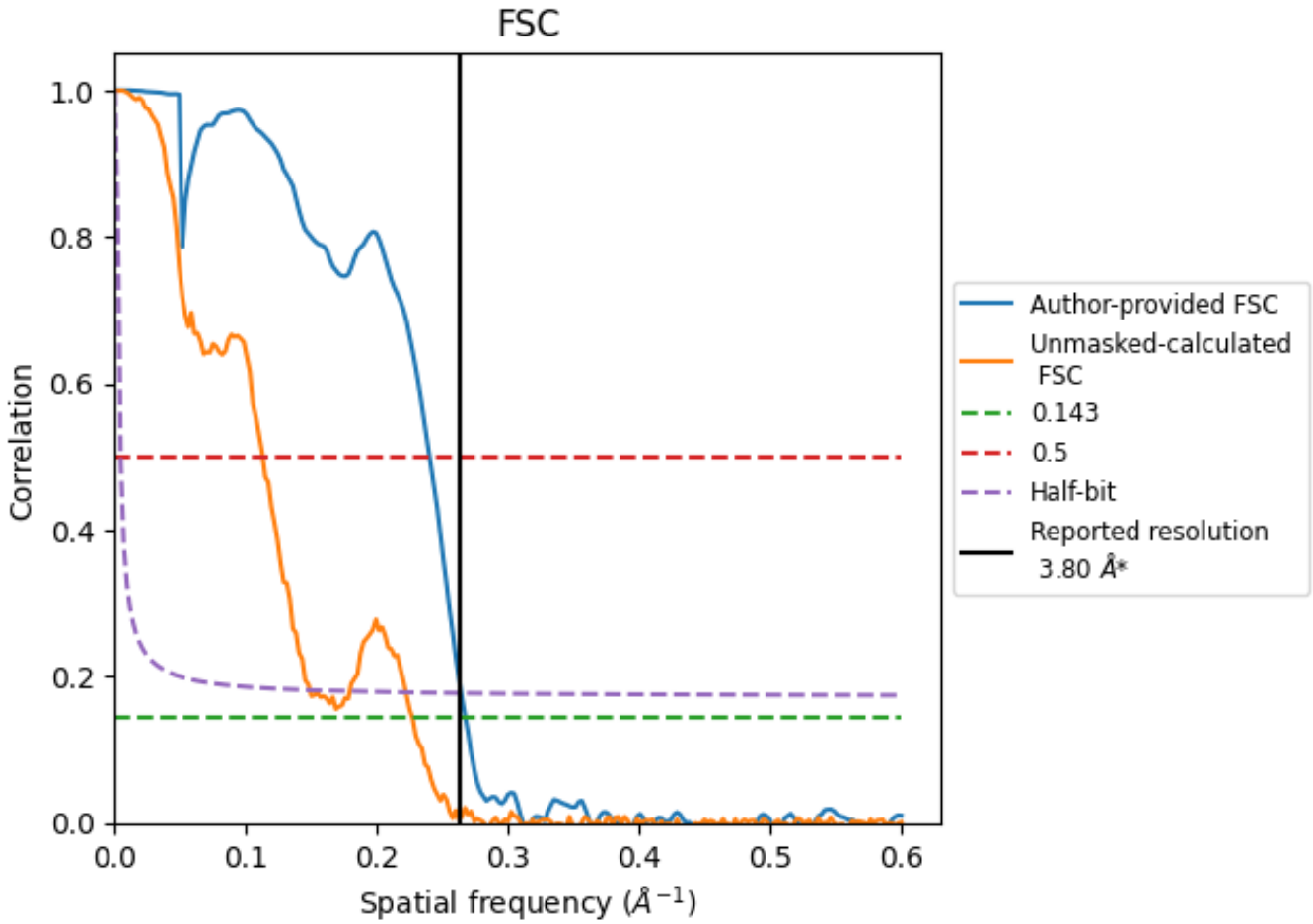


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8.2 Resolution estimates (i)

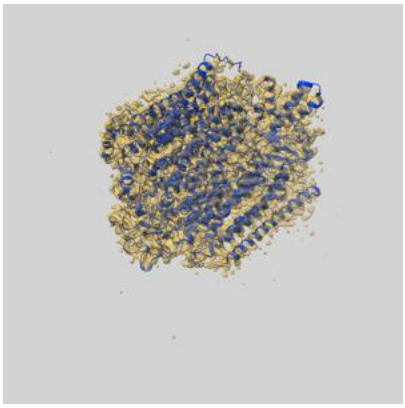
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.74	4.17	3.78
Unmasked-calculated*	4.40	8.86	6.72

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.40 differs from the reported value 3.8 by more than 10 %

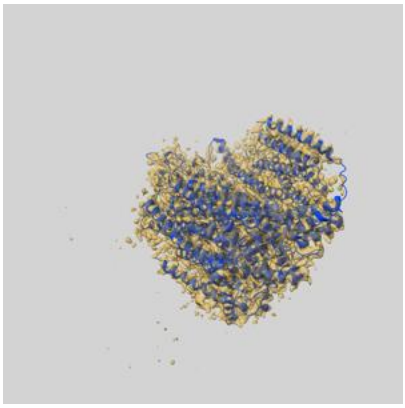
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22447 and PDB model 7JRO. Per-residue inclusion information can be found in section 3 on page 11.

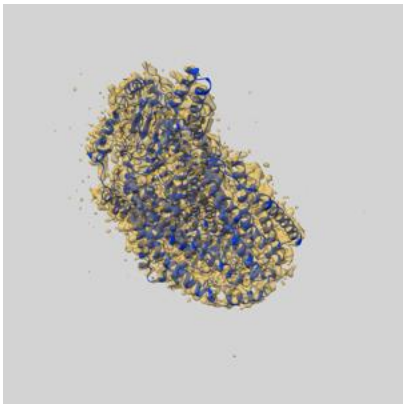
9.1 Map-model overlay



X



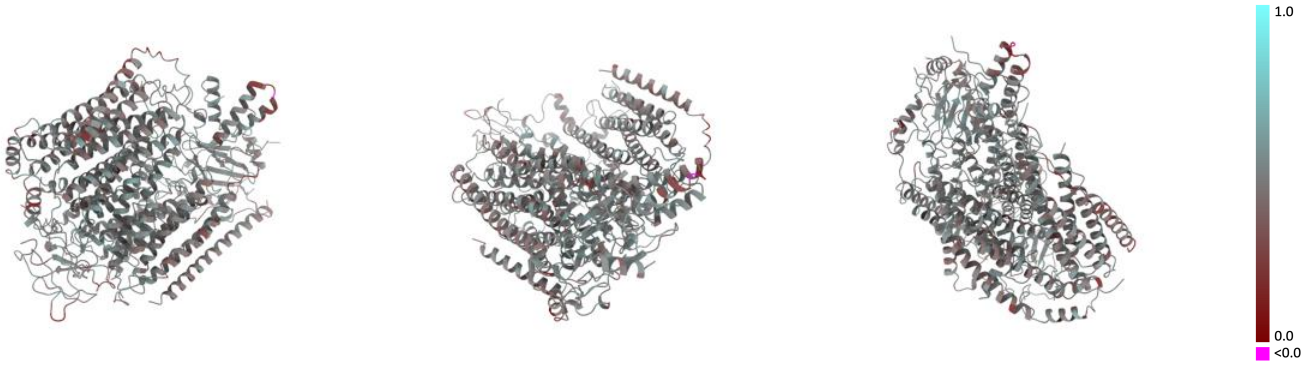
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014 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.

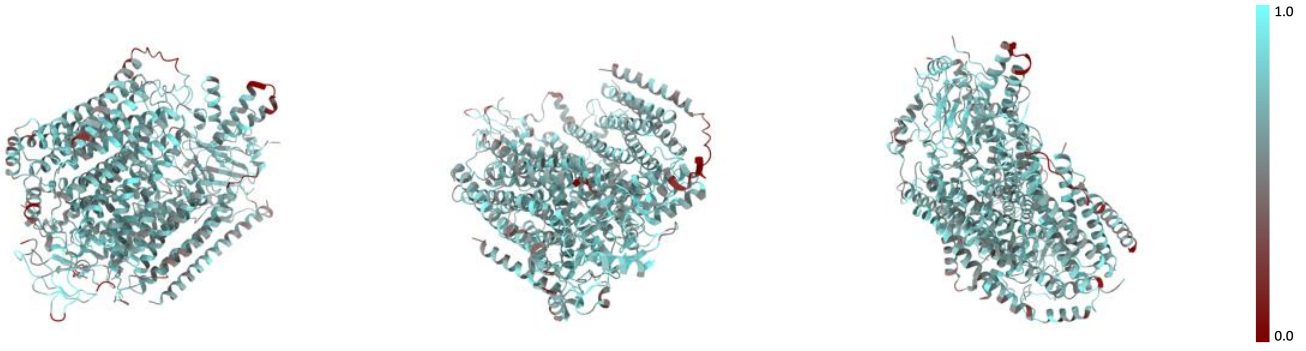
9.2 Q-score mapped to coordinate model (i)



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.

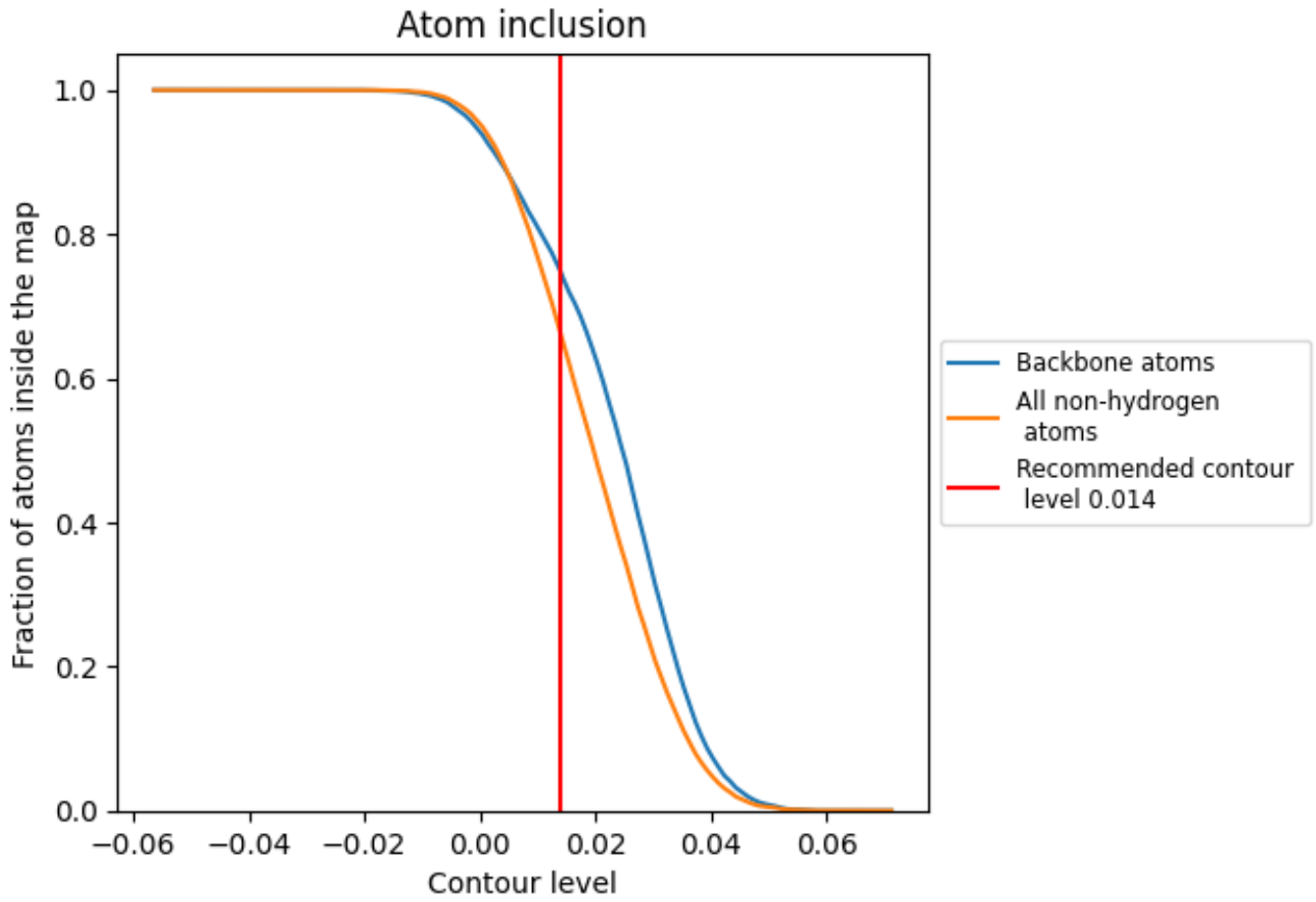
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.014).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6607	0.4820
a	0.6897	0.4980
b	0.6675	0.4910
c	0.6854	0.4900
d	0.6290	0.4580
e	0.6338	0.4450
f	0.5329	0.4400
g	0.6368	0.4530
h	0.5735	0.4370
i	0.5966	0.4750
j	0.6277	0.4700