Full wwPDB EM Validation Report ⓘ

Nov 24, 2024 – 01:46 AM JST

PDB ID	:	8IBC
EMDB ID	:	EMD-35339
Title	:	Respiratory complex CIII2, focus-refined of type IB, Wild type mouse under cold temperature
Authors	:	Shin, Y.-C.; Liao, M.
Deposited on	:	2023-02-10
Resolution	:	3.60 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 ⓘ 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:

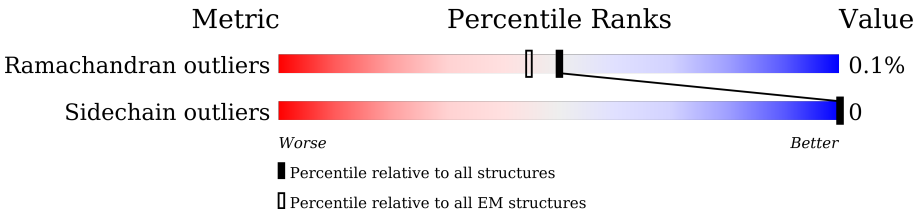
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	AA	480	5% 83% 17%
1	Aa	480	83% 16%
2	AB	453	5% 91% 9%
2	Ab	453	91% 9%
3	AC	381	13% 98%
3	Ac	381	7% 97%
4	AD	325	11% 73% 27%
4	Ad	325	5% 73% 27%
5	AE	274	55% 68% 32%

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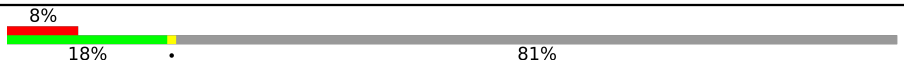
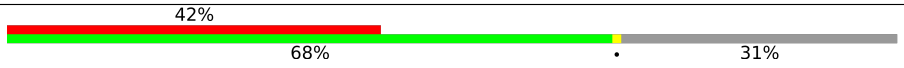
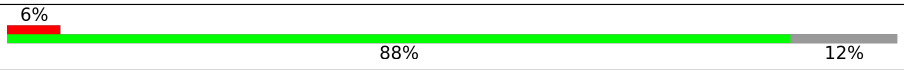
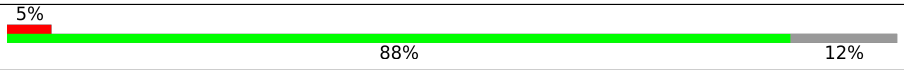
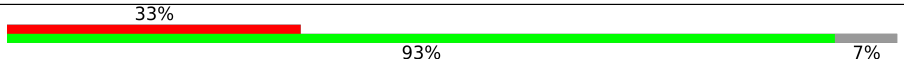
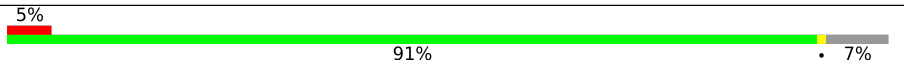
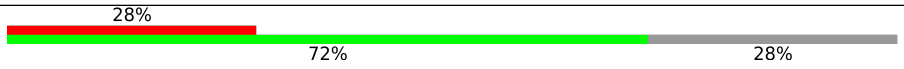
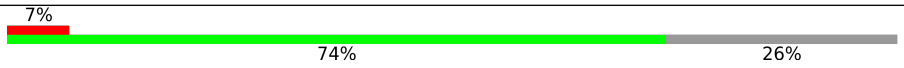
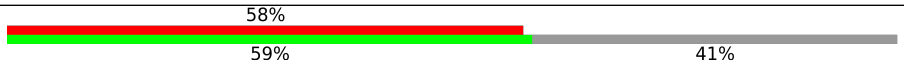
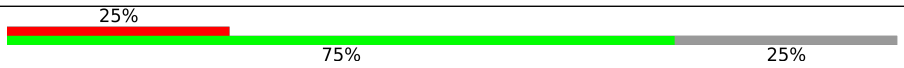
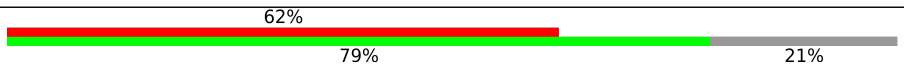
Mol	Chain	Length	Quality of chain
5	AI	274	
5	Ae	274	
6	AF	111	
6	Af	111	
7	AG	82	
7	Ag	82	
8	AH	89	
8	Ah	89	
9	AJ	64	
9	Aj	64	
10	AK	56	
10	Ak	56	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 31431 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 b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	399	Total	C	N	O	S	0	0
			3117	1943	554	604	16		
1	Aa	401	Total	C	N	O	S	0	0
			3131	1955	555	605	16		

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	414	Total	C	N	O	S	0	0
			3107	1954	546	598	9		
2	Ab	413	Total	C	N	O	S	0	0
			3101	1948	543	601	9		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	373	Total	C	N	O	S	0	0
			2988	2018	461	489	20		
3	Ac	373	Total	C	N	O	S	0	0
			2988	2018	461	489	20		

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	238	Total	C	N	O	S	0	0
			1896	1211	326	345	14		
4	Ad	238	Total	C	N	O	S	0	0
			1895	1211	325	345	14		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	185	Total	C	N	O	S	0	0
			1427	902	250	268	7		
5	AI	51	Total	C	N	O		0	0
			347	221	65	61			
5	Ae	188	Total	C	N	O	S	0	0
			1451	916	254	274	7		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	98	Total	C	N	O	S	0	0
			864	552	154	155	3		
6	Af	98	Total	C	N	O	S	0	0
			864	552	154	155	3		

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	76	Total	C	N	O	S	0	0
			643	418	116	108	1		
7	Ag	76	Total	C	N	O	S	0	0
			643	418	116	108	1		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	64	Total	C	N	O	S	0	0
			527	321	98	103	5		
8	Ah	66	Total	C	N	O	S	0	0
			544	333	101	105	5		

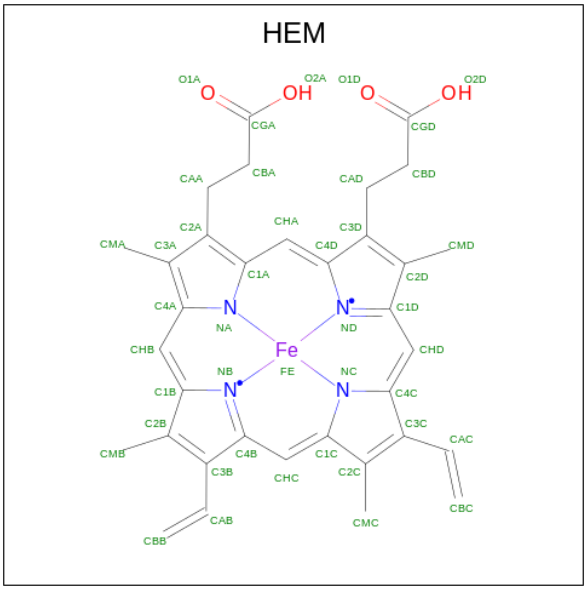
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	AJ	38	Total	C	N	O	0	0
			307	201	51	55		
9	Aj	48	Total	C	N	O	0	0
			392	257	67	68		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 10.

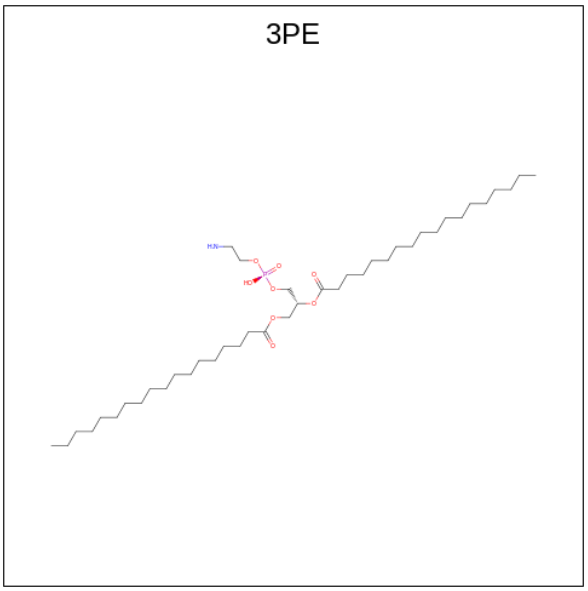
Mol	Chain	Residues	Atoms					AltConf	Trace
10	AK	34	Total	C	N	O	S	0	0
			278	183	51	43	1		
10	Ak	44	Total	C	N	O	S	0	0
			357	236	63	57	1		

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



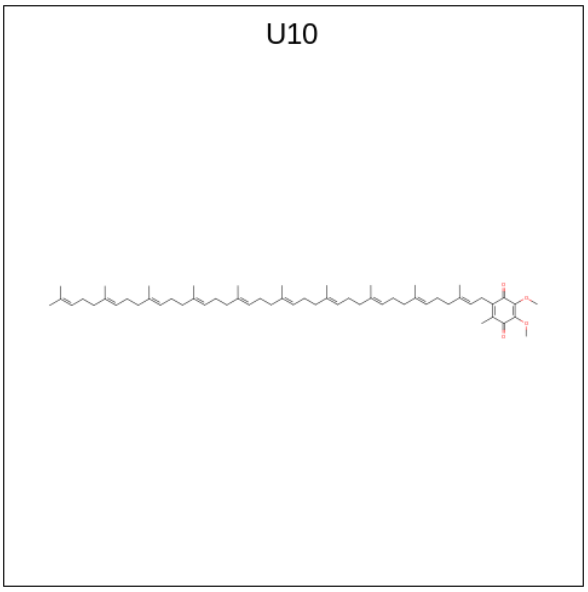
Mol	Chain	Residues	Atoms					AltConf
11	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 12 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
12	AC	1	Total	C	N	O	P	0
			25	15	1	8	1	
12	Ac	1	Total	C	N	O	P	0
			35	25	1	8	1	

- Molecule 13 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
13	AC	1	Total	C	O	0
			23	19	4	

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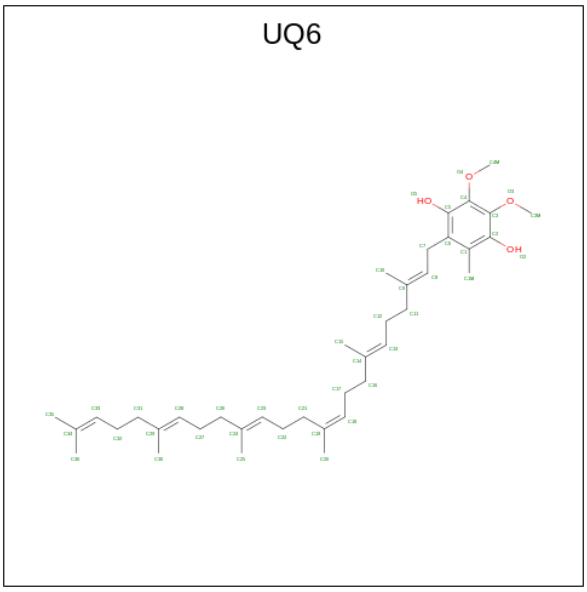
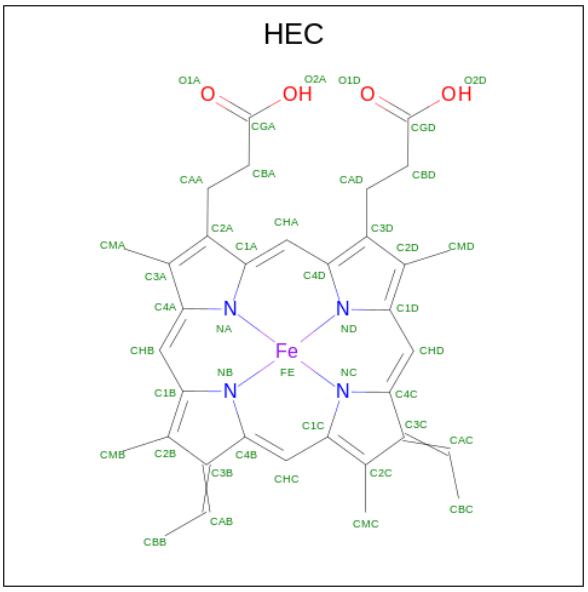
Mol	Chain	Residues	Atoms			AltConf
13	Ac	1	Total	C	O	0
			23	19	4	

- Molecule 14 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXAENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (three-letter code: UQ6) (formula: $C_{39}H_{60}O_4$) (labeled as "Ligand of Interest" by depositor).



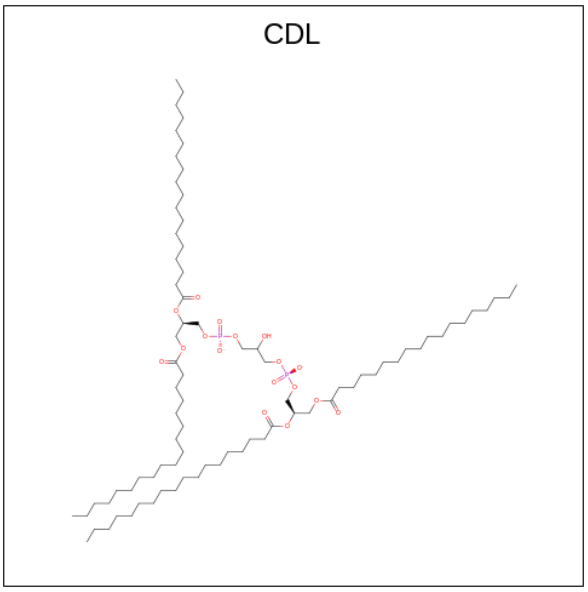
Mol	Chain	Residues	Atoms			AltConf
14	AC	1	Total	C	O	0
			28	24	4	
14	Ac	1	Total	C	O	0
			28	24	4	

- Molecule 15 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
15	AD	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
15	Ad	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 16 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
16	Aa	1	Total	C	O	P	0
			46	27	17	2	

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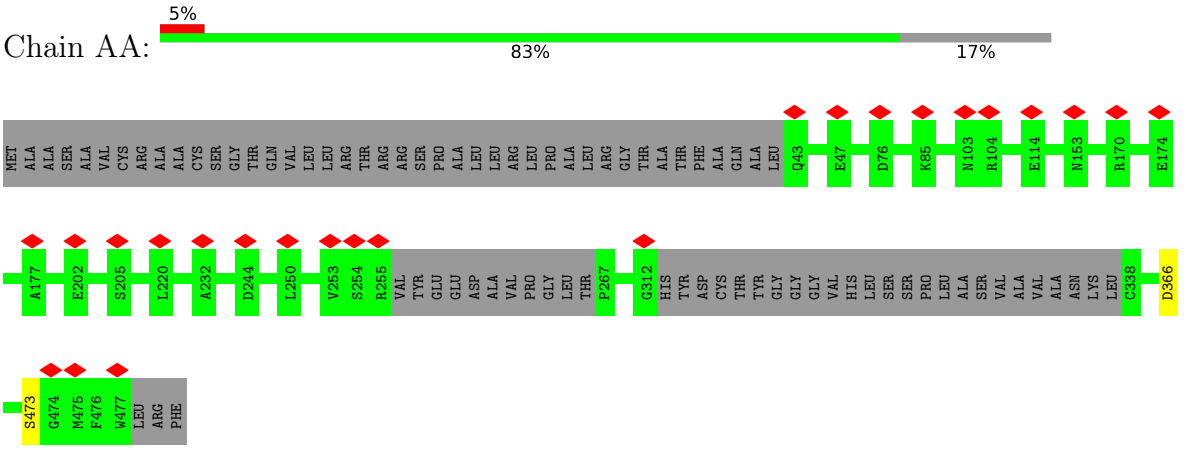
Mol	Chain	Residues	Atoms				AltConf
16	Ac	1	Total	C	O	P	0
			42	23	17	2	
16	Ag	1	Total	C	O	P	0
			56	37	17	2	

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.

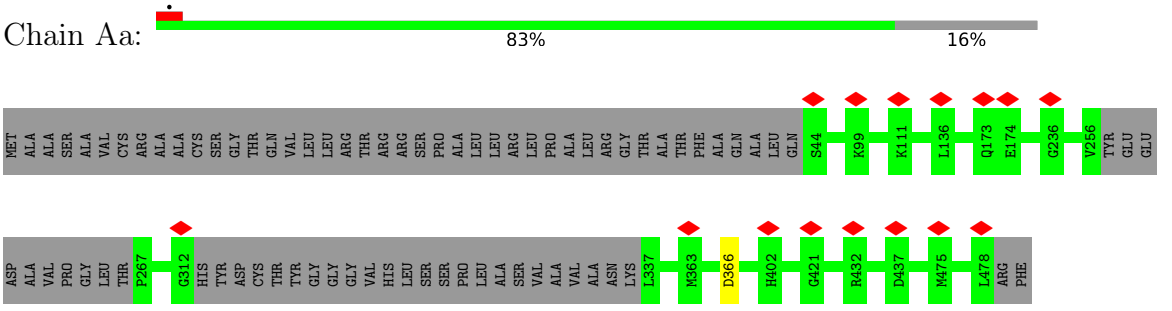
• Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain AA:



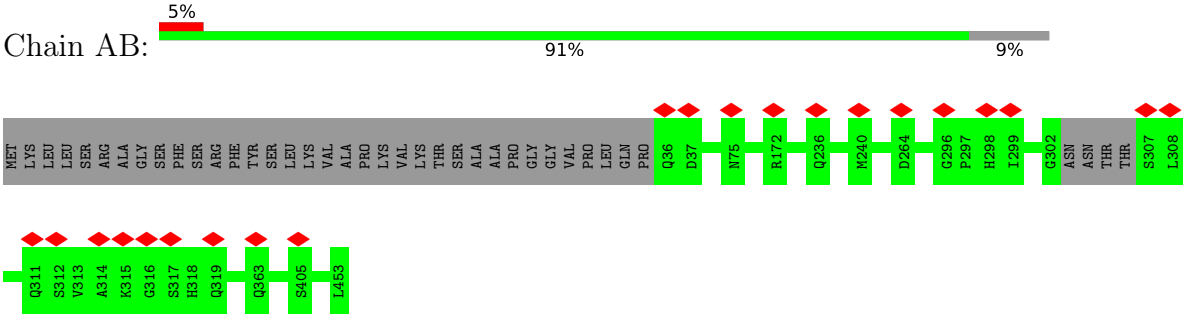
• Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain Aa:



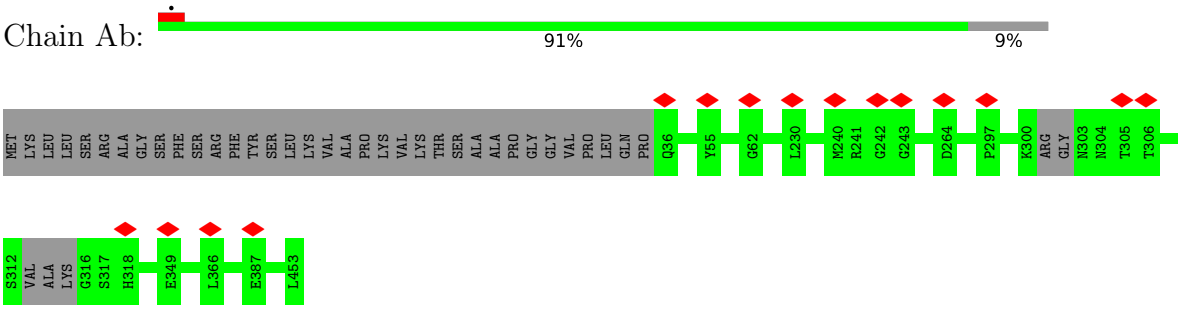
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain AB:



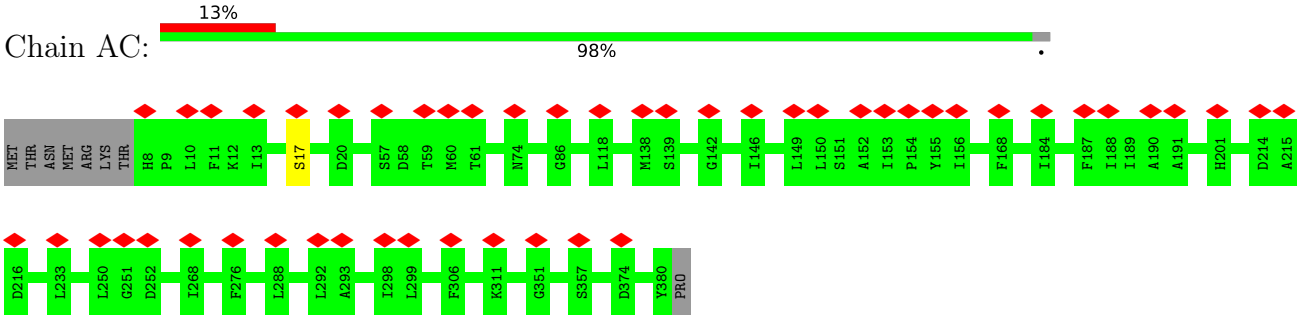
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain Ab:



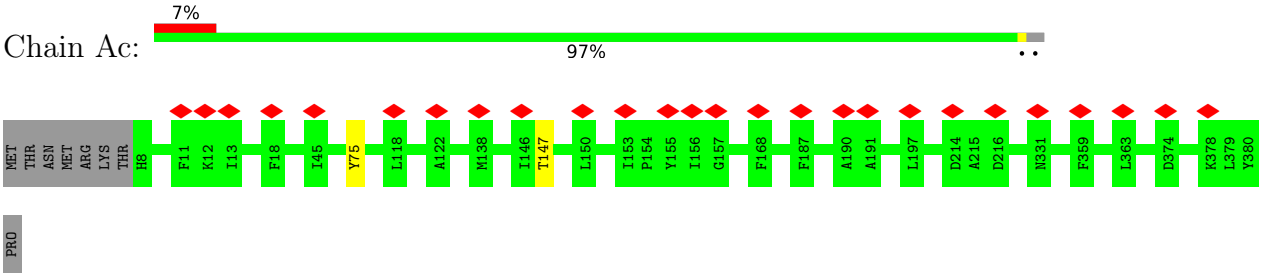
• Molecule 3: Cytochrome b

Chain AC:



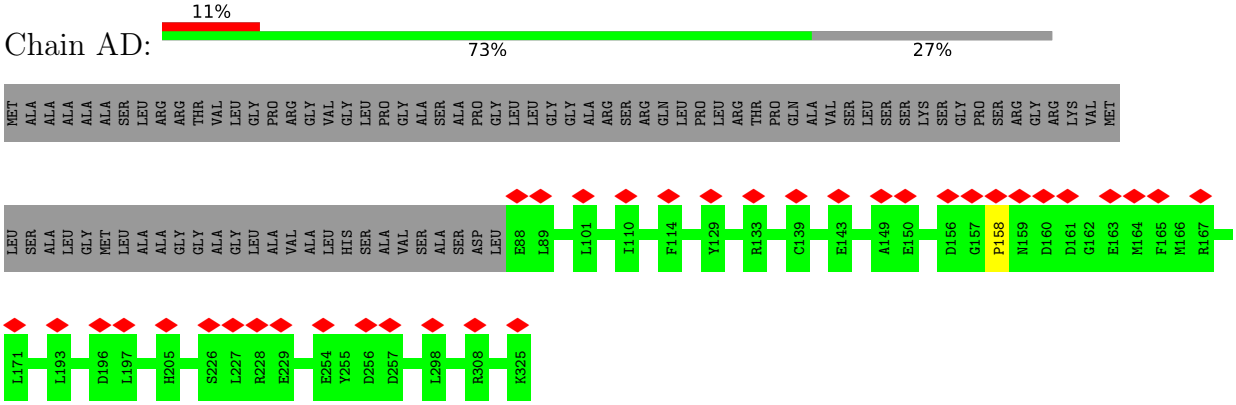
• Molecule 3: Cytochrome b

Chain Ac:



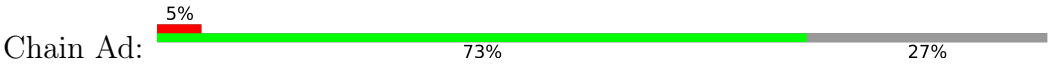
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

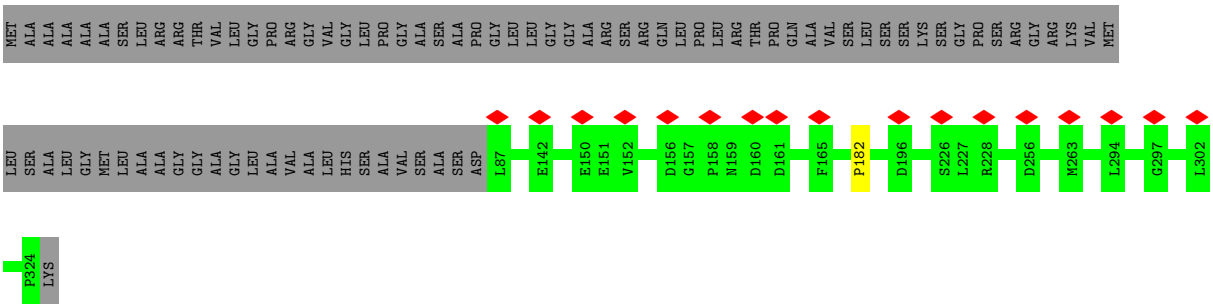
Chain AD:



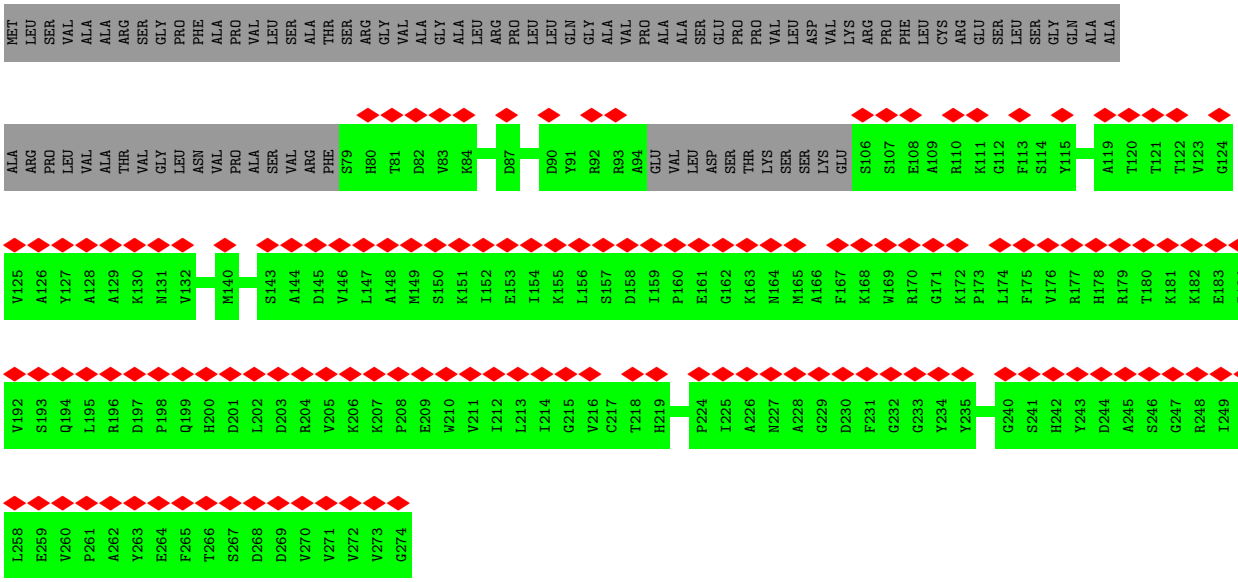
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain Ad:

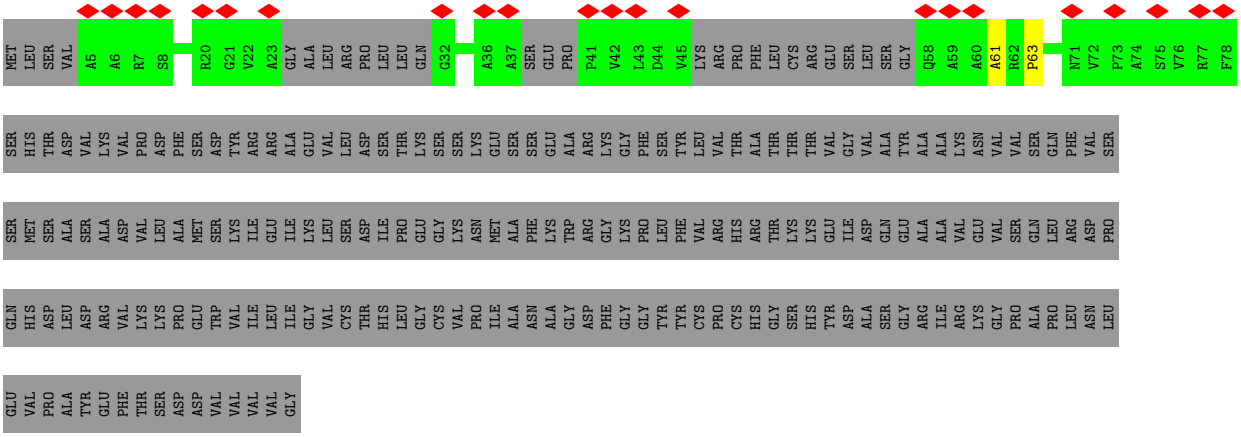




• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

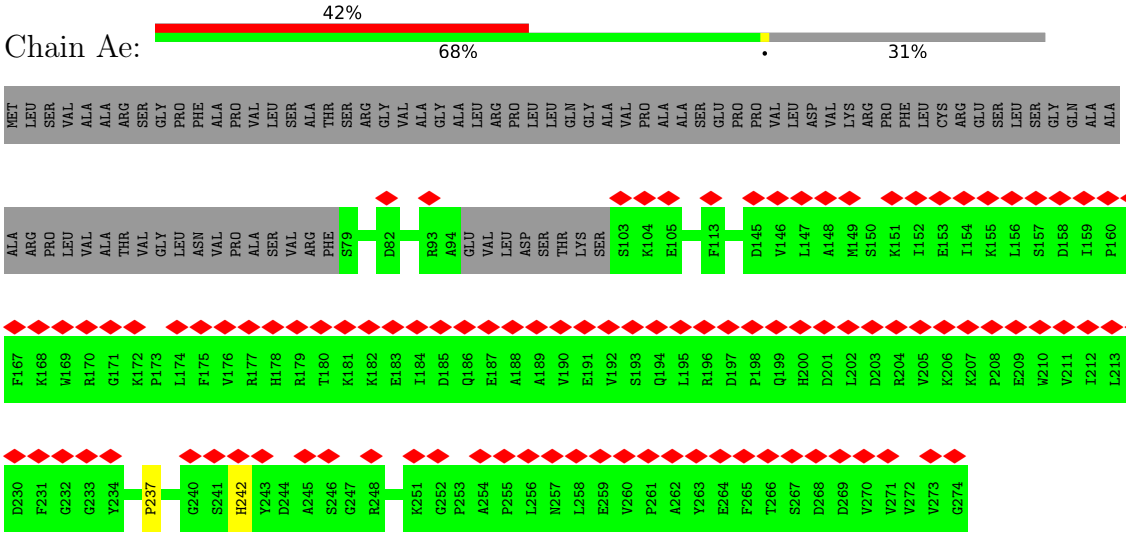


• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



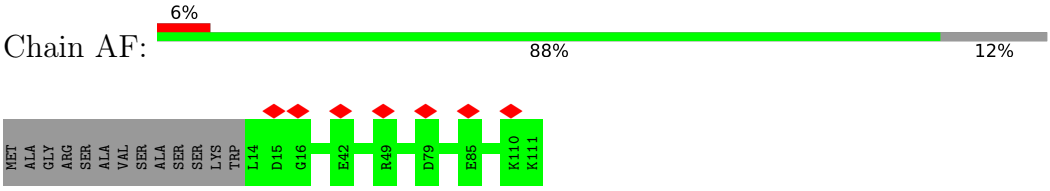
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain Ae:



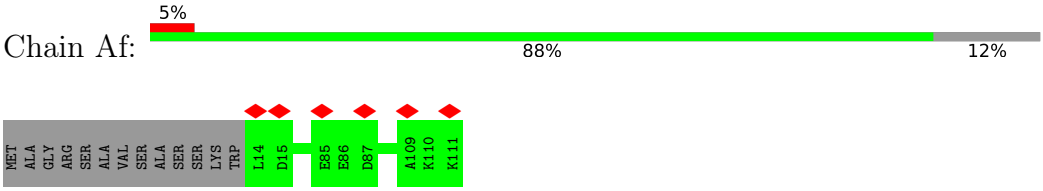
• Molecule 6: Cytochrome b-c1 complex subunit 7

Chain AF:



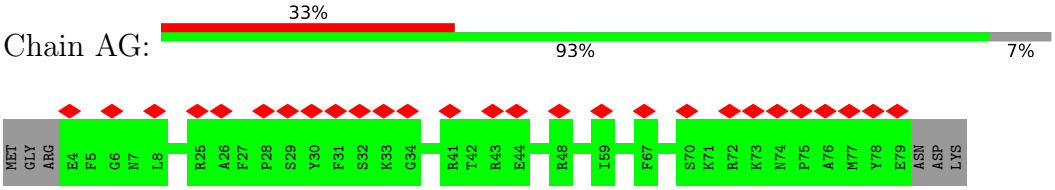
• Molecule 6: Cytochrome b-c1 complex subunit 7

Chain Af:



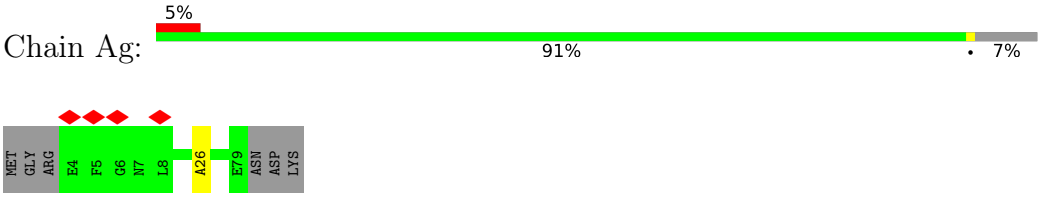
• Molecule 7: Cytochrome b-c1 complex subunit 8

Chain AG:



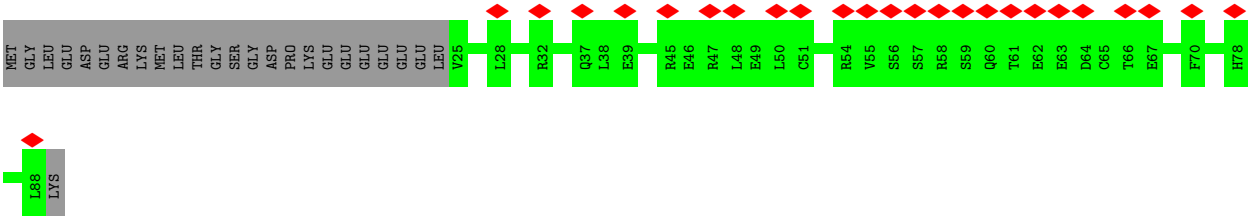
• Molecule 7: Cytochrome b-c1 complex subunit 8

Chain Ag:

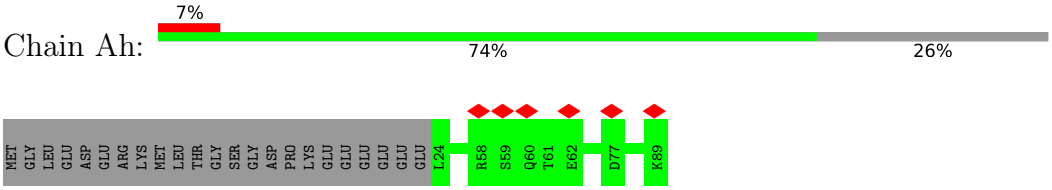


• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

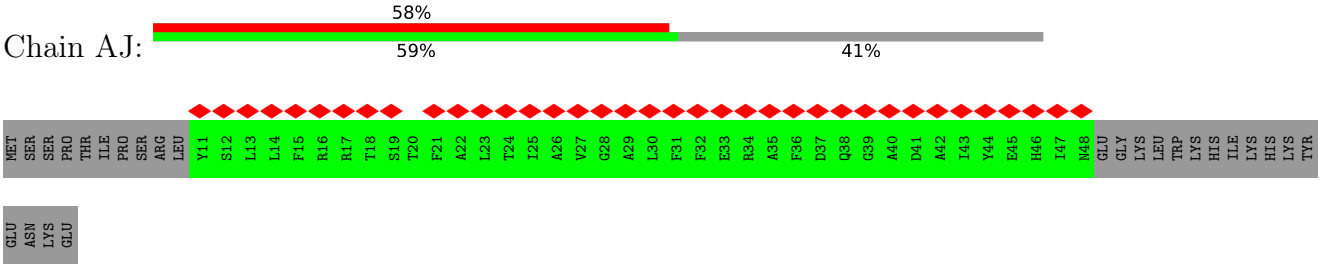
Chain AH:



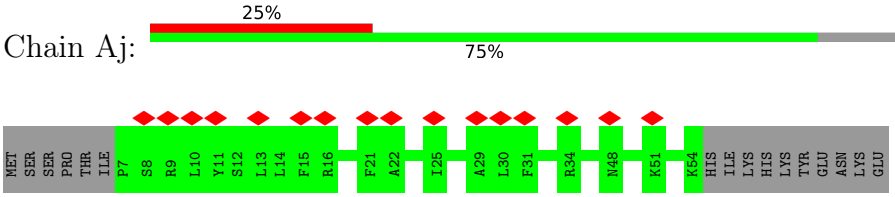
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



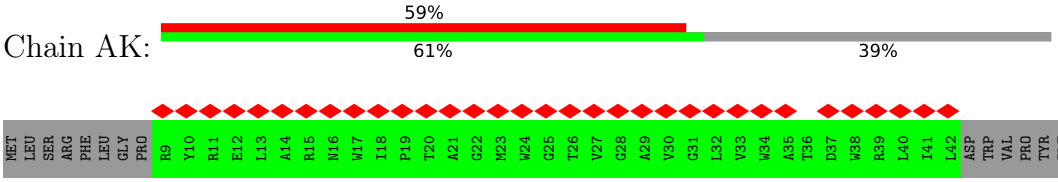
• Molecule 9: Cytochrome b-c1 complex subunit 9



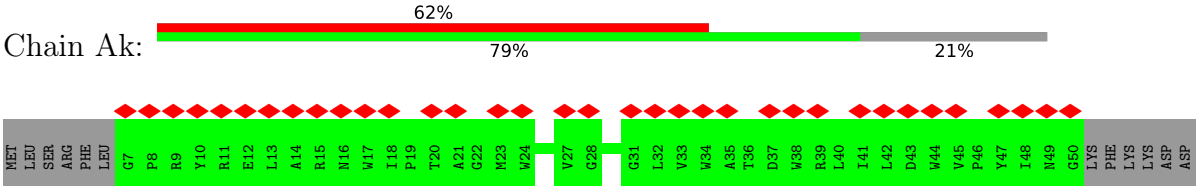
• Molecule 9: Cytochrome b-c1 complex subunit 9



• Molecule 10: Cytochrome b-c1 complex subunit 10



• Molecule 10: Cytochrome b-c1 complex subunit 10



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	147426	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	46.1, 45.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.469	Depositor
Minimum map value	-1.236	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, HEM, CDL, HEC, UQ6, U10

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	AA	0.41	0/3176	0.62	2/4305 (0.0%)
1	Aa	0.37	0/3190	0.62	1/4325 (0.0%)
2	AB	0.36	0/3156	0.56	0/4263
2	Ab	0.35	0/3149	0.56	0/4255
3	AC	0.34	0/3089	0.56	1/4221 (0.0%)
3	Ac	0.37	0/3089	0.57	1/4221 (0.0%)
4	AD	0.38	0/1955	0.50	0/2655
4	Ad	0.49	1/1954 (0.1%)	0.57	2/2655 (0.1%)
5	AE	0.33	0/1459	0.53	0/1976
5	AI	0.84	1/351 (0.3%)	0.92	3/478 (0.6%)
5	Ae	0.36	0/1483	0.61	2/2007 (0.1%)
6	AF	0.33	0/884	0.50	0/1184
6	Af	0.45	0/884	0.48	0/1184
7	AG	0.37	0/662	0.56	0/895
7	Ag	0.39	0/662	0.60	1/895 (0.1%)
8	AH	0.34	0/534	0.56	0/717
8	Ah	0.41	0/551	0.52	0/739
9	AJ	0.33	0/314	0.41	0/424
9	Aj	0.38	0/402	0.50	0/541
10	AK	0.31	0/287	0.54	0/393
10	Ak	0.33	0/371	0.47	0/511
All	All	0.38	2/31602 (0.0%)	0.57	13/42844 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AI	63	PRO	N-CD	-13.60	1.28	1.47
4	Ad	182	PRO	N-CD	-11.74	1.31	1.47

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	366	ASP	CB-CG-OD1	9.56	126.90	118.30
1	Aa	366	ASP	CB-CG-OD1	9.47	126.83	118.30
5	AI	63	PRO	CA-N-CD	9.36	124.81	111.70
4	Ad	182	PRO	CA-N-CD	8.60	123.75	111.70
5	AI	63	PRO	N-CA-CB	-7.88	93.84	103.30
5	AI	61	ALA	CB-CA-C	-6.68	100.07	110.10
3	Ac	147	THR	N-CA-CB	6.04	121.77	110.30
4	Ad	182	PRO	N-CA-CB	-5.88	96.14	102.60
3	AC	17	SER	N-CA-CB	-5.59	102.12	110.50
5	Ae	221	GLY	N-CA-C	5.48	126.81	113.10
5	Ae	242	HIS	N-CA-C	5.32	125.36	111.00
1	AA	473	SER	N-CA-CB	-5.28	102.58	110.50
7	Ag	26	ALA	N-CA-CB	-5.15	102.89	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	AA	393/480 (82%)	378 (96%)	15 (4%)	0	100	100
1	Aa	395/480 (82%)	384 (97%)	11 (3%)	0	100	100
2	AB	410/453 (90%)	400 (98%)	10 (2%)	0	100	100
2	Ab	407/453 (90%)	397 (98%)	10 (2%)	0	100	100
3	AC	371/381 (97%)	367 (99%)	4 (1%)	0	100	100
3	Ac	371/381 (97%)	362 (98%)	8 (2%)	1 (0%)	37	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	AD	236/325 (73%)	229 (97%)	6 (2%)	1 (0%)	30 63
4	Ad	236/325 (73%)	224 (95%)	12 (5%)	0	100 100
5	AE	181/274 (66%)	168 (93%)	13 (7%)	0	100 100
5	AI	43/274 (16%)	41 (95%)	2 (5%)	0	100 100
5	Ae	184/274 (67%)	171 (93%)	12 (6%)	1 (0%)	25 59
6	AF	96/111 (86%)	96 (100%)	0	0	100 100
6	Af	96/111 (86%)	96 (100%)	0	0	100 100
7	AG	74/82 (90%)	74 (100%)	0	0	100 100
7	Ag	74/82 (90%)	73 (99%)	1 (1%)	0	100 100
8	AH	62/89 (70%)	62 (100%)	0	0	100 100
8	Ah	64/89 (72%)	63 (98%)	1 (2%)	0	100 100
9	AJ	36/64 (56%)	36 (100%)	0	0	100 100
9	Aj	46/64 (72%)	45 (98%)	1 (2%)	0	100 100
10	AK	32/56 (57%)	31 (97%)	1 (3%)	0	100 100
10	Ak	42/56 (75%)	41 (98%)	1 (2%)	0	100 100
All	All	3849/4904 (78%)	3738 (97%)	108 (3%)	3 (0%)	50 79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	Ac	75	TYR
4	AD	158	PRO
5	Ae	237	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	AA	337/398 (85%)	337 (100%)	0	100 100
1	Aa	339/398 (85%)	339 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	324/356 (91%)	324 (100%)	0	100	100
2	Ab	325/356 (91%)	325 (100%)	0	100	100
3	AC	325/333 (98%)	325 (100%)	0	100	100
3	Ac	325/333 (98%)	325 (100%)	0	100	100
4	AD	203/260 (78%)	203 (100%)	0	100	100
4	Ad	203/260 (78%)	203 (100%)	0	100	100
5	AE	155/224 (69%)	155 (100%)	0	100	100
5	AI	34/224 (15%)	34 (100%)	0	100	100
5	Ae	158/224 (70%)	158 (100%)	0	100	100
6	AF	90/99 (91%)	90 (100%)	0	100	100
6	Af	90/99 (91%)	90 (100%)	0	100	100
7	AG	69/74 (93%)	69 (100%)	0	100	100
7	Ag	69/74 (93%)	69 (100%)	0	100	100
8	AH	61/83 (74%)	61 (100%)	0	100	100
8	Ah	63/83 (76%)	63 (100%)	0	100	100
9	AJ	30/55 (54%)	30 (100%)	0	100	100
9	Aj	39/55 (71%)	39 (100%)	0	100	100
10	AK	26/46 (56%)	26 (100%)	0	100	100
10	Ak	34/46 (74%)	34 (100%)	0	100	100
All	All	3299/4080 (81%)	3299 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	43	GLN
1	AA	55	ASN
1	AA	87	ASN
1	AA	103	ASN
1	AA	173	GLN
1	AA	207	ASN
1	AA	286	HIS
1	AA	342	GLN
1	AA	402	HIS

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Mol	Chain	Res	Type
2	AB	167	GLN
2	AB	415	GLN
3	AC	341	GLN
4	AD	98	HIS
4	AD	189	ASN
4	AD	190	ASN
7	AG	69	GLN
8	AH	34	HIS
8	AH	37	GLN
8	AH	82	HIS
1	Aa	87	ASN
1	Aa	119	HIS
1	Aa	173	GLN
1	Aa	181	ASN
1	Aa	193	GLN
1	Aa	207	ASN
2	Ab	227	HIS
2	Ab	284	ASN
2	Ab	298	HIS
2	Ab	304	ASN
2	Ab	311	GLN
2	Ab	343	GLN
2	Ab	415	GLN
3	Ac	148	ASN
3	Ac	341	GLN
4	Ad	155	GLN
4	Ad	190	ASN
5	Ae	242	HIS
6	Af	80	GLN
7	Ag	24	GLN
8	Ah	82	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	HEM	AC	402	3	41,50,50	1.36	6 (14%)	45,82,82	1.95	9 (20%)
12	3PE	AC	403	-	24,24,50	1.30	2 (8%)	27,29,55	1.17	2 (7%)
11	HEM	AC	401	3	41,50,50	1.38	6 (14%)	45,82,82	2.08	13 (28%)
15	HEC	Ad	401	4	32,50,50	2.18	11 (34%)	24,82,82	2.94	8 (33%)
11	HEM	Ac	401	3	41,50,50	1.37	5 (12%)	45,82,82	1.91	11 (24%)
15	HEC	AD	401	4	32,50,50	2.24	12 (37%)	24,82,82	2.28	6 (25%)
12	3PE	Ac	403	-	34,34,50	1.09	2 (5%)	37,39,55	1.20	3 (8%)
16	CDL	Ag	101	16	55,55,99	1.21	4 (7%)	61,67,111	1.20	6 (9%)
13	U10	AC	404	-	23,23,63	1.75	2 (8%)	28,31,79	1.70	7 (25%)
11	HEM	Ac	402	3	41,50,50	1.32	4 (9%)	45,82,82	1.94	10 (22%)
16	CDL	Ac	406	16	41,41,99	1.39	4 (9%)	47,53,111	1.45	7 (14%)
13	U10	Ac	404	-	23,23,63	1.24	3 (13%)	28,31,79	2.09	7 (25%)
14	UQ6	Ac	405	-	28,28,43	0.81	1 (3%)	33,37,55	0.75	0
14	UQ6	AC	405	-	28,28,43	2.44	6 (21%)	33,37,55	1.65	8 (24%)
16	CDL	Aa	501	-	45,45,99	1.34	4 (8%)	51,57,111	1.32	6 (11%)

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
11	HEM	AC	402	3	-	7/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	3PE	AC	403	-	-	7/28/28/54	-
11	HEM	AC	401	3	-	6/12/54/54	-
15	HEC	Ad	401	4	-	2/10/54/54	-
11	HEM	Ac	401	3	-	7/12/54/54	-
15	HEC	AD	401	4	-	3/10/54/54	-
12	3PE	Ac	403	-	-	3/38/38/54	-
16	CDL	Ag	101	16	-	22/66/66/110	-
13	U10	AC	404	-	-	5/15/39/87	0/1/1/1
11	HEM	Ac	402	3	-	6/12/54/54	-
16	CDL	Ac	406	16	-	18/52/52/110	-
13	U10	Ac	404	-	-	6/15/39/87	0/1/1/1
14	UQ6	Ac	405	-	-	13/21/21/39	0/1/1/1
14	UQ6	AC	405	-	-	3/21/21/39	0/1/1/1
16	CDL	Aa	501	-	-	12/56/56/110	-

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	AC	404	U10	C6-C1	7.36	1.48	1.35
15	AD	401	HEC	C3C-C2C	6.33	1.47	1.40
15	AD	401	HEC	C2B-C3B	6.19	1.47	1.40
14	AC	405	UQ6	C2-C3	5.91	1.49	1.39
15	Ad	401	HEC	C2B-C3B	5.86	1.46	1.40
14	AC	405	UQ6	C5-C4	5.85	1.48	1.39
15	Ad	401	HEC	C3C-C2C	5.84	1.46	1.40
14	AC	405	UQ6	C5-C6	5.74	1.48	1.40
14	AC	405	UQ6	C6-C1	4.98	1.48	1.40
14	AC	405	UQ6	C4-C3	4.58	1.48	1.39
16	Aa	501	CDL	OA8-CA7	4.23	1.45	1.33
16	Ac	406	CDL	OB8-CB7	4.22	1.45	1.33
12	Ac	403	3PE	O31-C31	4.20	1.45	1.33
16	Ag	101	CDL	OB8-CB7	4.19	1.45	1.33
16	Aa	501	CDL	OB8-CB7	4.19	1.45	1.33
12	AC	403	3PE	O31-C31	4.17	1.45	1.33
16	Ag	101	CDL	OA8-CA7	4.14	1.45	1.33
16	Aa	501	CDL	OB6-CB5	4.10	1.45	1.34
16	Ac	406	CDL	OA8-CA7	4.10	1.45	1.33
16	Aa	501	CDL	OA6-CA5	4.09	1.45	1.34
14	AC	405	UQ6	C2-C1	4.08	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Ac	406	CDL	OA6-CA5	4.05	1.45	1.34
16	Ag	101	CDL	OA6-CA5	4.02	1.45	1.34
12	Ac	403	3PE	O21-C21	4.02	1.45	1.34
12	AC	403	3PE	O21-C21	4.01	1.45	1.34
16	Ag	101	CDL	OB6-CB5	3.98	1.45	1.34
16	Ac	406	CDL	OB6-CB5	3.97	1.45	1.34
11	AC	402	HEM	C4D-ND	-3.85	1.33	1.40
11	AC	401	HEM	C1B-NB	-3.79	1.33	1.40
11	Ac	401	HEM	C4D-ND	-3.55	1.34	1.40
11	Ac	402	HEM	C1B-NB	-3.51	1.34	1.40
11	AC	402	HEM	C1B-NB	-3.47	1.34	1.40
11	AC	401	HEM	C4D-ND	-3.46	1.34	1.40
11	Ac	401	HEM	C1B-NB	-3.28	1.34	1.40
15	Ad	401	HEC	C2A-C3A	3.27	1.47	1.37
15	Ad	401	HEC	C3D-C2D	3.25	1.47	1.37
15	AD	401	HEC	C2A-C3A	3.23	1.47	1.37
11	Ac	402	HEM	C4D-ND	-3.18	1.34	1.40
13	AC	404	U10	C4-C3	3.14	1.49	1.36
15	AD	401	HEC	C3D-C2D	3.12	1.46	1.37
15	Ad	401	HEC	C4B-C3B	2.95	1.48	1.43
14	Ac	405	UQ6	O2-C2	-2.92	1.30	1.37
13	Ac	404	U10	C6-C5	-2.92	1.38	1.46
15	Ad	401	HEC	C2A-C1A	2.87	1.49	1.42
11	Ac	401	HEM	FE-NB	2.87	2.11	1.96
13	Ac	404	U10	C4-C3	2.86	1.48	1.36
15	AD	401	HEC	C4B-C3B	2.81	1.48	1.43
15	AD	401	HEC	C3A-C4A	2.77	1.48	1.42
15	AD	401	HEC	C3C-C4C	2.77	1.48	1.43
11	Ac	402	HEM	FE-NB	2.77	2.10	1.96
15	AD	401	HEC	C2A-C1A	2.75	1.48	1.42
15	Ad	401	HEC	C3C-C4C	2.73	1.48	1.43
11	AC	402	HEM	FE-NB	2.68	2.10	1.96
11	AC	401	HEM	FE-NB	2.64	2.09	1.96
13	Ac	404	U10	C3-C2	-2.50	1.41	1.48
15	Ad	401	HEC	C3A-C4A	2.48	1.48	1.42
15	Ad	401	HEC	C1C-CHC	2.46	1.47	1.41
15	Ad	401	HEC	C1D-CHD	2.45	1.47	1.41
15	Ad	401	HEC	C4D-CHA	2.39	1.47	1.41
15	AD	401	HEC	C1B-CHB	2.38	1.47	1.41
11	Ac	401	HEM	C1D-ND	-2.34	1.34	1.38
15	AD	401	HEC	C1D-CHD	2.31	1.47	1.41
15	AD	401	HEC	C4D-CHA	2.30	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	AD	401	HEC	C1C-CHC	2.27	1.47	1.41
11	Ac	401	HEM	C4B-NB	-2.15	1.34	1.38
11	AC	402	HEM	C1D-ND	-2.12	1.34	1.38
11	AC	401	HEM	C1D-ND	-2.11	1.34	1.38
11	AC	401	HEM	C4B-NB	-2.10	1.34	1.38
11	AC	402	HEM	FE-ND	-2.08	1.86	1.96
11	Ac	402	HEM	C4B-NB	-2.03	1.34	1.38
11	AC	401	HEM	FE-ND	-2.02	1.86	1.96
11	AC	402	HEM	C4B-NB	-2.01	1.34	1.38

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	Ad	401	HEC	CMB-C2B-C3B	9.37	136.84	125.82
13	Ac	404	U10	C6-C1-C2	7.85	125.39	119.18
15	AD	401	HEC	C1D-C2D-C3D	-6.39	102.55	107.00
11	AC	401	HEM	CHC-C4B-NB	6.03	130.98	124.43
15	Ad	401	HEC	C1D-C2D-C3D	-5.89	102.90	107.00
11	AC	402	HEM	CHC-C4B-NB	5.74	130.67	124.43
11	Ac	402	HEM	CHC-C4B-NB	5.37	130.26	124.43
11	Ac	401	HEM	CHC-C4B-NB	5.19	130.07	124.43
11	Ac	402	HEM	CHD-C1D-ND	5.10	129.97	124.43
11	AC	401	HEM	CHD-C1D-ND	4.85	129.70	124.43
11	AC	402	HEM	CHD-C1D-ND	4.72	129.56	124.43
13	AC	404	U10	C7-C8-C9	-4.63	119.08	126.79
15	AD	401	HEC	CMC-C2C-C3C	4.59	131.22	125.82
16	Ac	406	CDL	OB6-CB5-C51	4.56	121.32	111.50
15	Ad	401	HEC	CBD-CAD-C3D	-4.52	104.91	112.62
11	AC	401	HEM	CHB-C1B-NB	4.36	129.77	124.38
11	Ac	402	HEM	CHA-C4D-ND	4.26	129.65	124.38
11	Ac	401	HEM	CHD-C1D-ND	4.26	129.06	124.43
15	AD	401	HEC	CMB-C2B-C3B	4.14	130.69	125.82
14	AC	405	UQ6	C7-C8-C9	-4.10	120.89	127.24
15	Ad	401	HEC	CMB-C2B-C1B	-4.08	122.20	128.46
13	Ac	404	U10	C1-C6-C5	-4.07	115.75	119.58
16	Aa	501	CDL	OA6-CA5-C11	4.06	120.26	111.50
12	Ac	403	3PE	O21-C21-C22	3.99	120.11	111.50
13	AC	404	U10	C1M-C1-C6	-3.95	117.95	124.40
11	AC	401	HEM	C1B-NB-C4B	3.94	109.14	105.07
11	AC	402	HEM	CHA-C4D-ND	3.90	129.20	124.38
11	AC	402	HEM	C1B-NB-C4B	3.86	109.06	105.07
11	AC	402	HEM	CBD-CAD-C3D	-3.85	101.92	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Ac	402	HEM	C1B-NB-C4B	3.85	109.05	105.07
11	AC	401	HEM	CHA-C4D-ND	3.78	129.05	124.38
16	Ag	101	CDL	OB6-CB5-C51	3.75	119.59	111.50
11	Ac	401	HEM	CHB-C1B-NB	3.75	129.01	124.38
16	Ag	101	CDL	OA6-CA5-C11	3.73	119.53	111.50
11	Ac	401	HEM	CHA-C4D-ND	3.72	128.98	124.38
11	Ac	401	HEM	C1B-NB-C4B	3.71	108.91	105.07
15	Ad	401	HEC	CMC-C2C-C3C	3.58	130.03	125.82
15	AD	401	HEC	CBD-CAD-C3D	-3.56	106.54	112.62
11	Ac	402	HEM	CHB-C1B-NB	3.56	128.78	124.38
11	AC	402	HEM	CHB-C1B-NB	3.55	128.77	124.38
14	AC	405	UQ6	C12-C13-C14	-3.55	119.12	127.66
12	AC	403	3PE	O21-C21-C22	3.49	119.02	111.50
16	Ac	406	CDL	OB8-CB7-C71	3.46	120.46	111.38
16	Aa	501	CDL	OB6-CB5-C51	3.32	120.07	110.80
16	Aa	501	CDL	OB8-CB7-C71	3.32	120.09	111.38
16	Ac	406	CDL	CB4-OB6-CB5	-3.24	109.81	117.79
16	Ac	406	CDL	OA6-CA5-C11	3.24	119.83	110.80
14	AC	405	UQ6	C15-C14-C16	3.23	120.70	115.27
13	Ac	404	U10	C4-C3-C2	-3.22	114.35	120.68
11	Ac	401	HEM	CBA-CAA-C2A	-3.21	107.15	112.62
11	Ac	402	HEM	C4D-ND-C1D	2.99	108.16	105.07
11	AC	401	HEM	C4D-ND-C1D	2.91	108.08	105.07
11	AC	401	HEM	CHD-C1D-C2D	-2.84	120.54	124.98
11	Ac	401	HEM	CAD-CBD-CGD	-2.80	107.57	113.60
12	Ac	403	3PE	O31-C31-C32	2.78	120.64	111.91
11	AC	402	HEM	CHD-C1D-C2D	-2.77	120.65	124.98
13	AC	404	U10	C12-C13-C14	-2.72	118.47	127.75
16	Ag	101	CDL	CB4-OB6-CB5	-2.66	111.23	117.79
13	AC	404	U10	C10-C9-C11	2.66	119.74	115.27
14	AC	405	UQ6	C10-C9-C11	2.64	119.71	115.27
14	AC	405	UQ6	C6-C7-C8	-2.63	108.01	112.17
16	Aa	501	CDL	OA8-CA7-C31	2.62	120.12	111.91
11	AC	402	HEM	CHA-C4D-C3D	-2.60	120.44	125.33
12	Ac	403	3PE	C2-O21-C21	-2.59	111.42	117.79
13	Ac	404	U10	O4-C4-C5	-2.57	107.88	116.56
11	AC	401	HEM	C4B-C3B-C2B	-2.56	105.08	107.11
11	Ac	401	HEM	CHD-C1D-C2D	-2.56	120.99	124.98
14	AC	405	UQ6	C21-C19-C20	2.55	120.24	114.60
12	AC	403	3PE	O31-C31-C32	2.54	119.89	111.91
16	Ag	101	CDL	OA8-CA7-C31	2.54	119.89	111.91
11	Ac	402	HEM	CHD-C1D-C2D	-2.53	121.03	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	Ac	404	U10	C7-C6-C5	2.50	121.48	118.48
11	AC	401	HEM	CMC-C2C-C3C	2.48	129.32	124.68
16	Ac	406	CDL	OA8-CA7-C31	2.46	119.63	111.91
11	AC	401	HEM	C3B-C2B-C1B	2.43	108.29	106.49
14	AC	405	UQ6	C4M-O4-C4	2.43	121.44	114.78
11	AC	401	HEM	CBD-CAD-C3D	-2.42	105.89	112.63
15	Ad	401	HEC	CBA-CAA-C2A	-2.42	108.53	112.60
11	AC	401	HEM	CHC-C4B-C3B	-2.41	120.88	124.57
11	Ac	402	HEM	CHA-C4D-C3D	-2.41	120.80	125.33
16	Aa	501	CDL	CA4-OA6-CA5	-2.36	111.98	117.79
11	Ac	401	HEM	CHA-C4D-C3D	-2.36	120.90	125.33
13	AC	404	U10	C16-C14-C15	2.35	119.79	114.60
15	Ad	401	HEC	CMA-C3A-C2A	2.33	129.34	124.94
16	Ag	101	CDL	OB8-CB7-C71	2.33	119.22	111.91
16	Aa	501	CDL	CB4-OB6-CB5	-2.25	112.26	117.79
11	Ac	401	HEM	C4D-ND-C1D	2.24	107.39	105.07
11	Ac	402	HEM	CBD-CAD-C3D	-2.22	106.45	112.63
15	Ad	401	HEC	CMD-C2D-C3D	2.17	129.04	124.94
11	AC	402	HEM	C4D-ND-C1D	2.17	107.31	105.07
16	Ag	101	CDL	CA4-OA6-CA5	-2.17	112.46	117.79
14	AC	405	UQ6	C17-C18-C19	-2.16	120.35	127.75
16	Ac	406	CDL	OB6-CB5-OB7	-2.16	118.49	123.70
11	Ac	401	HEM	CHB-C1B-C2B	-2.13	120.83	126.72
11	AC	401	HEM	CHB-C1B-C2B	-2.11	120.89	126.72
15	AD	401	HEC	CAA-CBA-CGA	-2.10	107.88	113.76
13	AC	404	U10	C7-C6-C5	2.08	120.99	118.48
11	Ac	402	HEM	CHB-C1B-C2B	-2.04	121.07	126.72
15	AD	401	HEC	CMA-C3A-C2A	2.04	128.79	124.94
13	Ac	404	U10	O4-C4-C3	2.04	131.32	123.64
13	AC	404	U10	C6-C1-C2	2.03	120.79	119.18
13	Ac	404	U10	C3M-O3-C3	2.02	123.64	116.47
16	Ac	406	CDL	CA4-OA6-CA5	-2.01	112.85	117.79

There are no chirality outliers.

All (120) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	AC	402	HEM	C2B-C3B-CAB-CBB
11	AC	402	HEM	C4B-C3B-CAB-CBB
11	Ac	401	HEM	C2A-CAA-CBA-CGA
11	Ac	402	HEM	C1A-C2A-CAA-CBA
11	Ac	402	HEM	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	AC	403	3PE	C1-O11-P-O12
12	Ac	403	3PE	C1-O11-P-O12
13	Ac	404	U10	C7-C8-C9-C10
13	Ac	404	U10	C7-C8-C9-C11
14	Ac	405	UQ6	C1-C6-C7-C8
14	Ac	405	UQ6	C7-C8-C9-C10
14	Ac	405	UQ6	C7-C8-C9-C11
14	Ac	405	UQ6	C12-C13-C14-C15
14	Ac	405	UQ6	C12-C13-C14-C16
14	Ac	405	UQ6	C13-C14-C16-C17
14	Ac	405	UQ6	C15-C14-C16-C17
14	Ac	405	UQ6	C17-C18-C19-C20
16	Aa	501	CDL	CA3-OA5-PA1-OA3
16	Aa	501	CDL	CB2-OB2-PB2-OB4
16	Ac	406	CDL	CA2-OA2-PA1-OA3
16	Ac	406	CDL	CA2-OA2-PA1-OA4
16	Ac	406	CDL	CB2-OB2-PB2-OB3
16	Ac	406	CDL	CB2-OB2-PB2-OB4
16	Ag	101	CDL	C1-CB2-OB2-PB2
16	Ag	101	CDL	CB2-OB2-PB2-OB3
16	Ag	101	CDL	CB2-OB2-PB2-OB4
16	Ag	101	CDL	CB3-OB5-PB2-OB2
16	Ag	101	CDL	CB3-OB5-PB2-OB3
16	Ag	101	CDL	CB3-OB5-PB2-OB4
13	Ac	404	U10	C12-C13-C14-C15
13	Ac	404	U10	C12-C13-C14-C16
16	Ac	406	CDL	OB9-CB7-OB8-CB6
16	Ac	406	CDL	C71-CB7-OB8-CB6
14	Ac	405	UQ6	C17-C18-C19-C21
13	AC	404	U10	C12-C11-C9-C10
13	AC	404	U10	C12-C11-C9-C8
16	Aa	501	CDL	OB9-CB7-OB8-CB6
12	AC	403	3PE	C32-C31-O31-C3
16	Aa	501	CDL	C71-CB7-OB8-CB6
12	AC	403	3PE	O32-C31-O31-C3
14	Ac	405	UQ6	C9-C11-C12-C13
14	Ac	405	UQ6	C14-C16-C17-C18
16	Ac	406	CDL	CB4-CB6-OB8-CB7
16	Aa	501	CDL	C31-CA7-OA8-CA6
11	AC	402	HEM	C2A-CAA-CBA-CGA
16	Ag	101	CDL	CA4-CA3-OA5-PA1
16	Aa	501	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
12	AC	403	3PE	C22-C21-O21-C2
12	AC	403	3PE	C1-O11-P-O13
16	Aa	501	CDL	CA3-OA5-PA1-OA2
16	Ac	406	CDL	CA2-OA2-PA1-OA5
16	Ac	406	CDL	CB2-OB2-PB2-OB5
16	Ag	101	CDL	CA2-OA2-PA1-OA5
16	Ag	101	CDL	CA3-OA5-PA1-OA2
16	Ag	101	CDL	CB2-OB2-PB2-OB5
12	AC	403	3PE	O22-C21-O21-C2
16	Ag	101	CDL	C74-C75-C76-C77
16	Ac	406	CDL	OA7-CA5-OA6-CA4
11	Ac	401	HEM	C2B-C3B-CAB-CBB
16	Ac	406	CDL	C11-CA5-OA6-CA4
16	Aa	501	CDL	CB2-OB2-PB2-OB5
12	AC	403	3PE	C23-C24-C25-C26
16	Ag	101	CDL	C31-CA7-OA8-CA6
16	Ag	101	CDL	CB4-CB3-OB5-PB2
16	Ag	101	CDL	OA9-CA7-OA8-CA6
13	AC	404	U10	C9-C11-C12-C13
14	AC	405	UQ6	C15-C14-C16-C17
16	Ag	101	CDL	C51-CB5-OB6-CB4
11	AC	401	HEM	C2B-C3B-CAB-CBB
11	Ac	402	HEM	C2B-C3B-CAB-CBB
11	Ac	401	HEM	C4B-C3B-CAB-CBB
16	Ac	406	CDL	OB7-CB5-OB6-CB4
16	Ag	101	CDL	OB7-CB5-OB6-CB4
16	Ac	406	CDL	C51-CB5-OB6-CB4
16	Ag	101	CDL	C1-CA2-OA2-PA1
16	Aa	501	CDL	CA3-OA5-PA1-OA4
16	Aa	501	CDL	CB2-OB2-PB2-OB3
16	Ag	101	CDL	CA2-OA2-PA1-OA3
16	Ag	101	CDL	CA3-OA5-PA1-OA3
16	Ag	101	CDL	CA3-OA5-PA1-OA4
16	Ag	101	CDL	C71-CB7-OB8-CB6
16	Ag	101	CDL	OB9-CB7-OB8-CB6
16	Ac	406	CDL	CA6-CA4-OA6-CA5
15	AD	401	HEC	C3D-CAD-CBD-CGD
16	Aa	501	CDL	CA2-OA2-PA1-OA5
16	Aa	501	CDL	CA4-CA3-OA5-PA1
11	Ac	401	HEM	CAA-CBA-CGA-O1A
11	AC	402	HEM	CAD-CBD-CGD-O1D
11	AC	401	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
11	AC	402	HEM	CAA-CBA-CGA-O2A
11	Ac	402	HEM	CAD-CBD-CGD-O1D
11	AC	401	HEM	CAD-CBD-CGD-O1D
11	AC	402	HEM	CAA-CBA-CGA-O1A
13	Ac	404	U10	C12-C11-C9-C10
11	AC	401	HEM	CAA-CBA-CGA-O2A
11	Ac	401	HEM	CAD-CBD-CGD-O2D
11	Ac	402	HEM	CAD-CBD-CGD-O2D
11	Ac	401	HEM	CAD-CBD-CGD-O1D
11	AC	402	HEM	CAD-CBD-CGD-O2D
11	Ac	401	HEM	CAA-CBA-CGA-O2A
13	Ac	404	U10	C12-C11-C9-C8
11	AC	401	HEM	CAD-CBD-CGD-O2D
14	Ac	405	UQ6	C5-C6-C7-C8
16	Ac	406	CDL	CA4-CA3-OA5-PA1
13	AC	404	U10	C1-C6-C7-C8
14	AC	405	UQ6	C13-C14-C16-C17
13	AC	404	U10	C5-C6-C7-C8
15	AD	401	HEC	CAA-CBA-CGA-O2A
15	Ad	401	HEC	CAA-CBA-CGA-O2A
11	AC	401	HEM	C4B-C3B-CAB-CBB
11	Ac	402	HEM	C4B-C3B-CAB-CBB
15	AD	401	HEC	CAA-CBA-CGA-O1A
15	Ad	401	HEC	CAA-CBA-CGA-O1A
14	AC	405	UQ6	C1-C6-C7-C8
14	Ac	405	UQ6	C6-C7-C8-C9
16	Ac	406	CDL	C1-CA2-OA2-PA1
12	Ac	403	3PE	C1-O11-P-O14
16	Ac	406	CDL	C52-C51-CB5-OB6
12	Ac	403	3PE	C23-C24-C25-C26
16	Ac	406	CDL	C52-C51-CB5-OB7

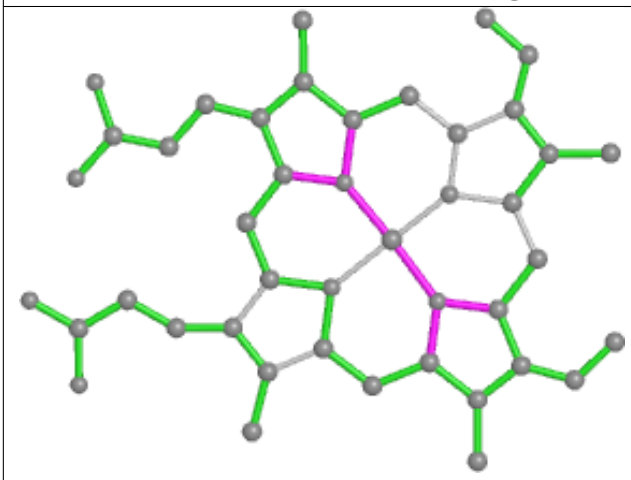
There are no ring outliers.

No monomer is involved in short contacts.

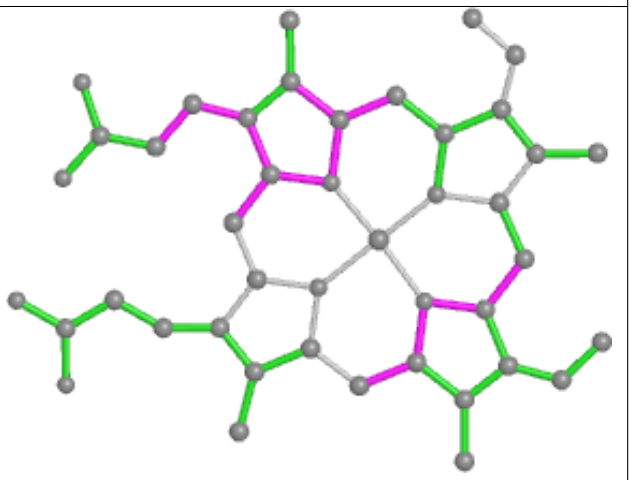
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

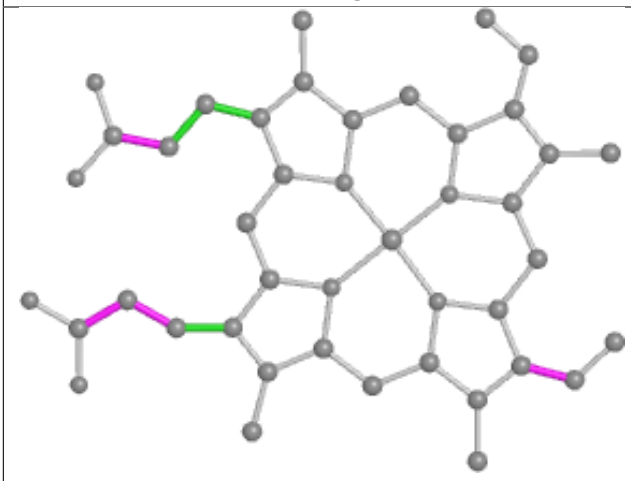
Ligand HEM AC 402



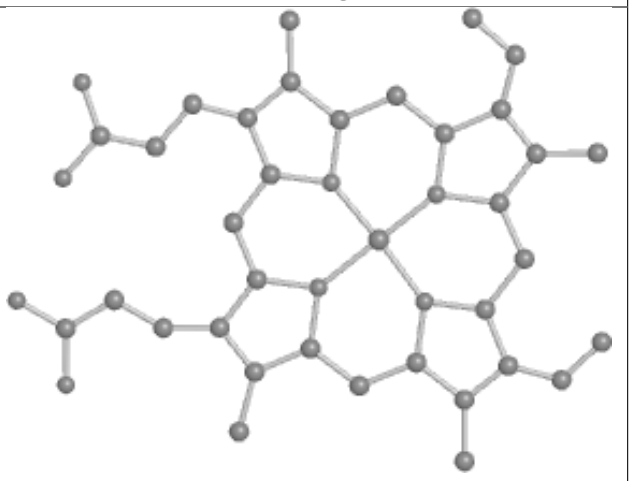
Bond lengths



Bond angles

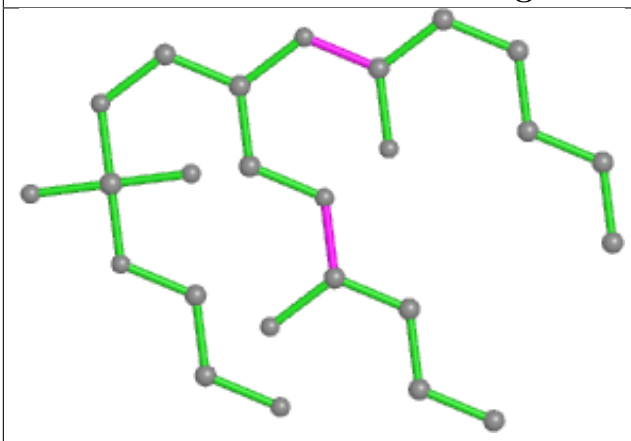


Torsions

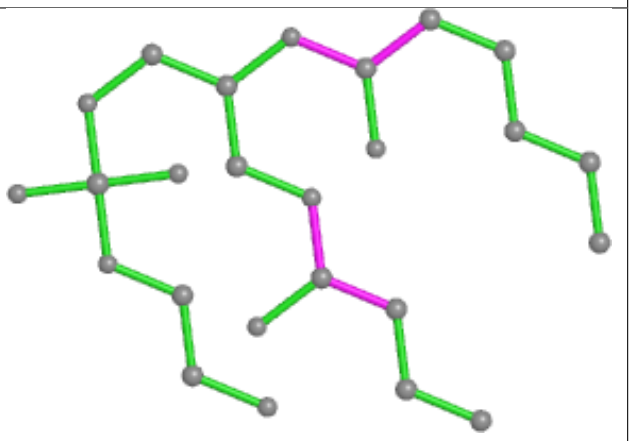


Rings

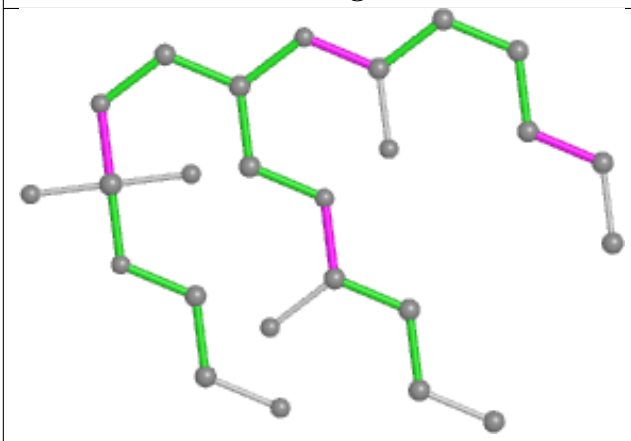
Ligand 3PE AC 403



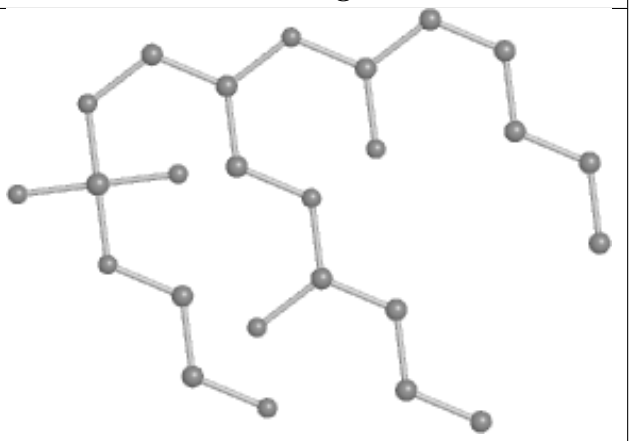
Bond lengths



Bond angles

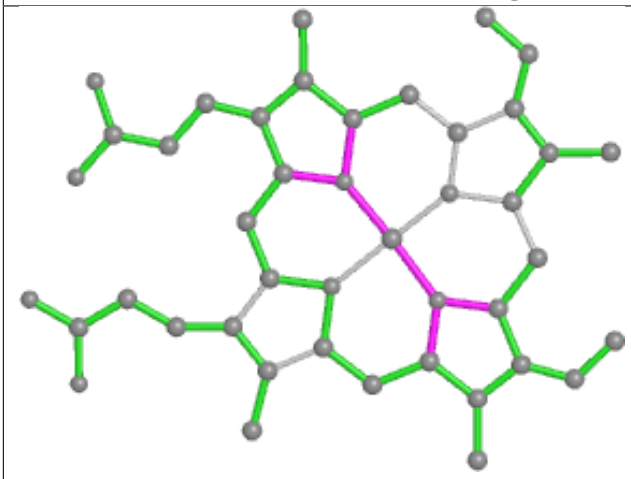


Torsions

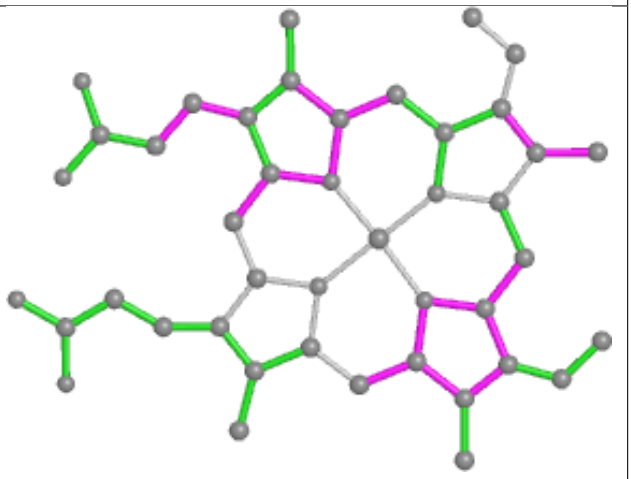


Rings

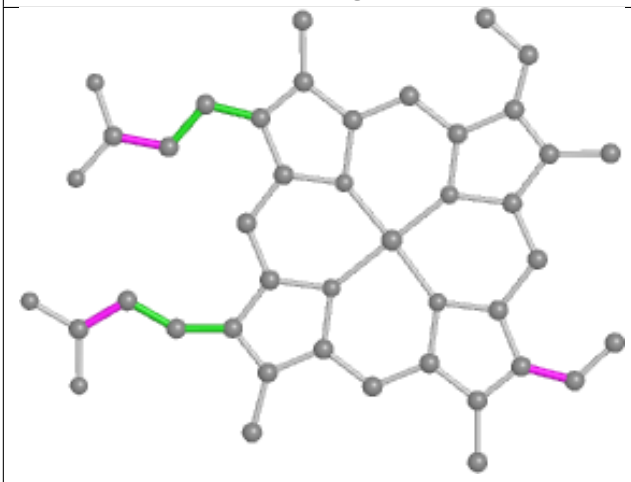
Ligand HEM AC 401



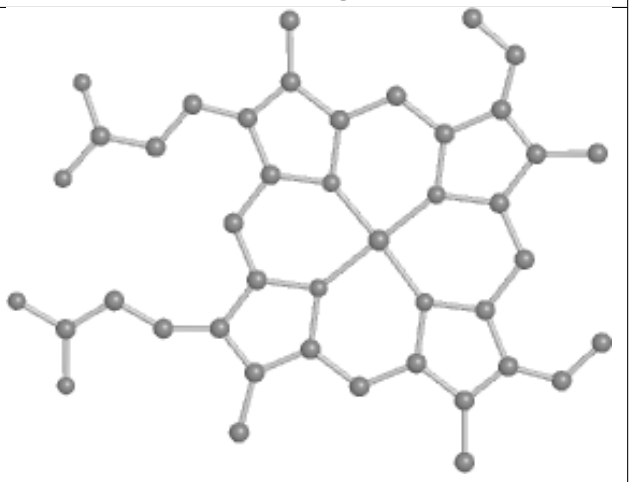
Bond lengths



Bond angles

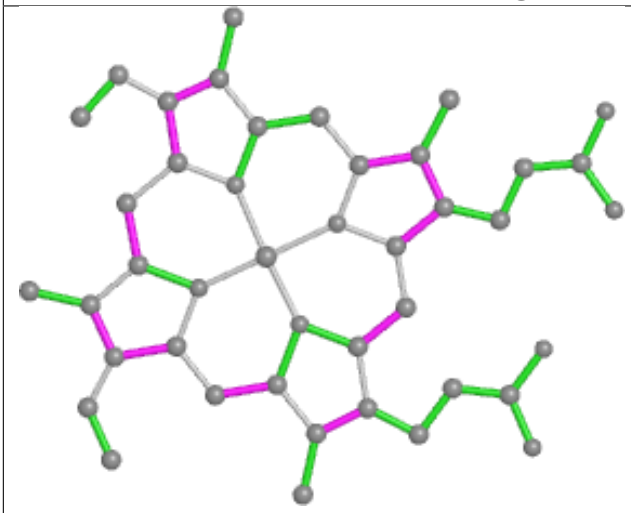


Torsions

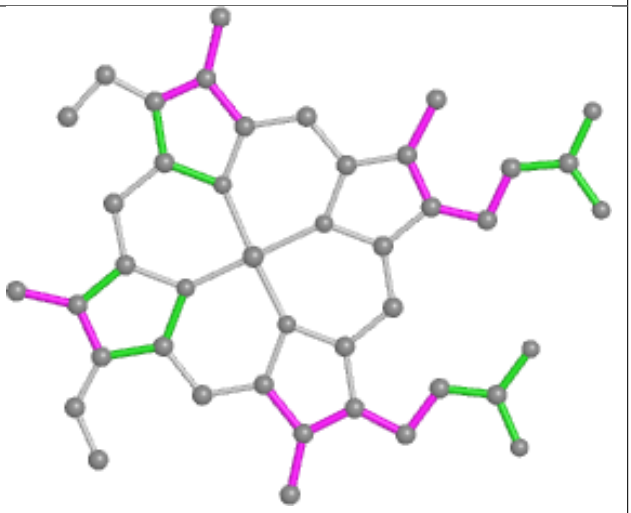


Rings

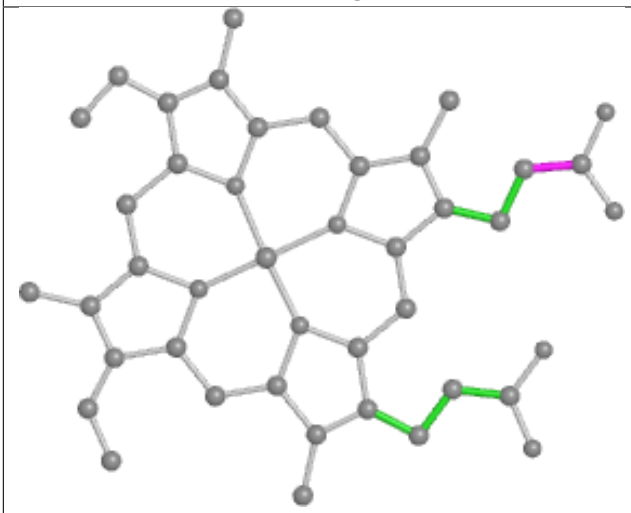
Ligand HEC Ad 401



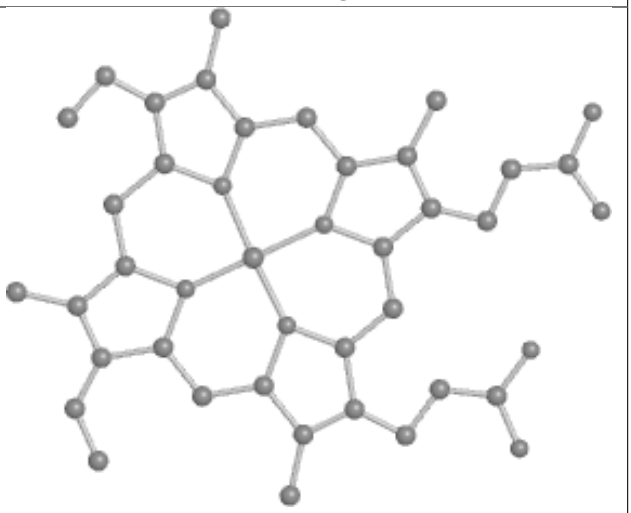
Bond lengths



Bond angles

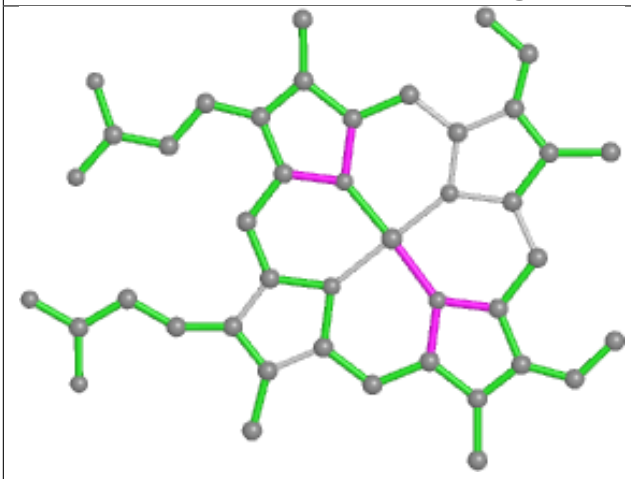


Torsions

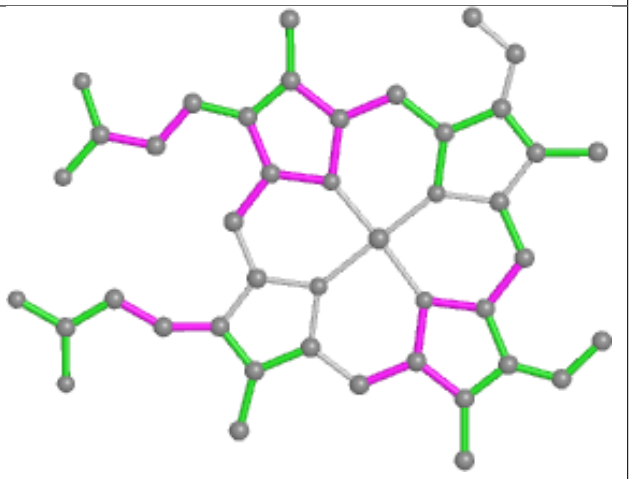


Rings

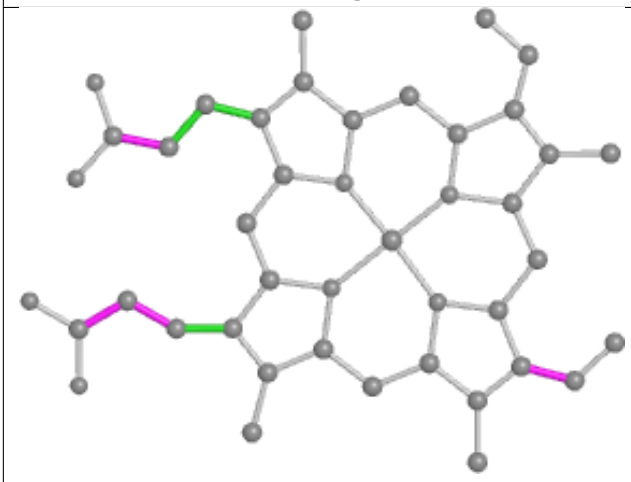
Ligand HEM Ac 401



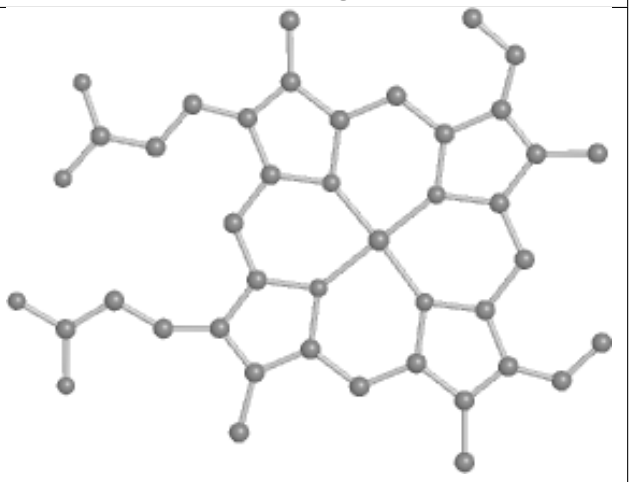
Bond lengths



Bond angles

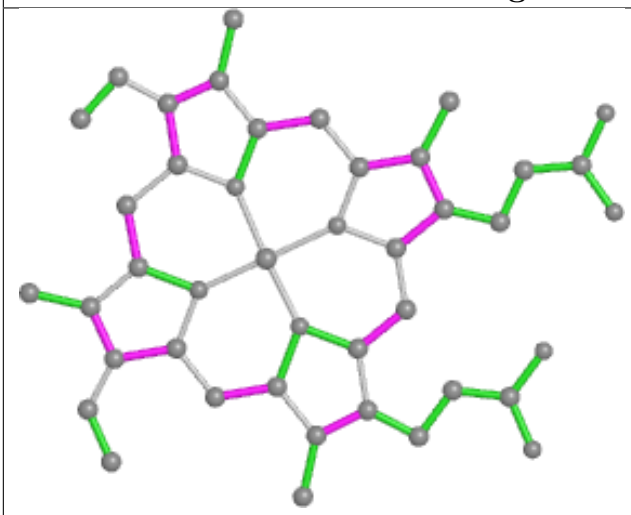


Torsions

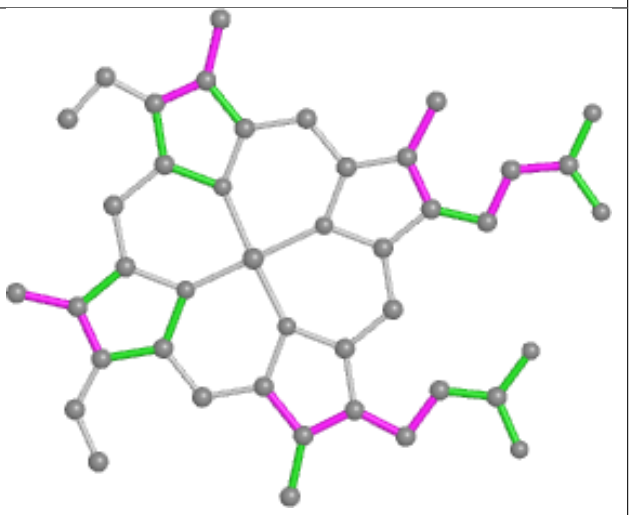


Rings

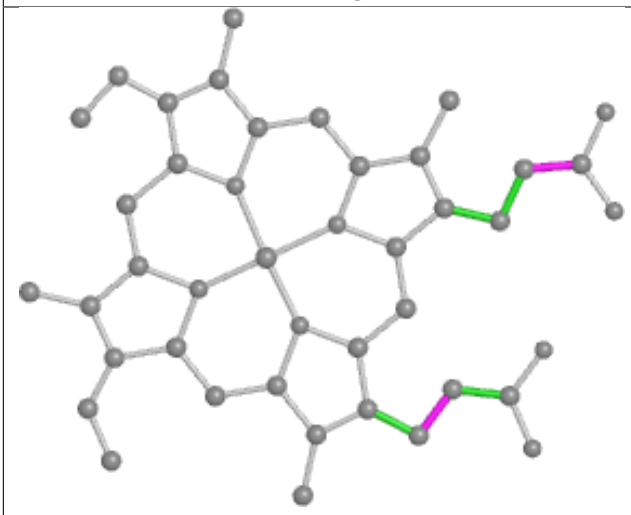
Ligand HEC AD 401



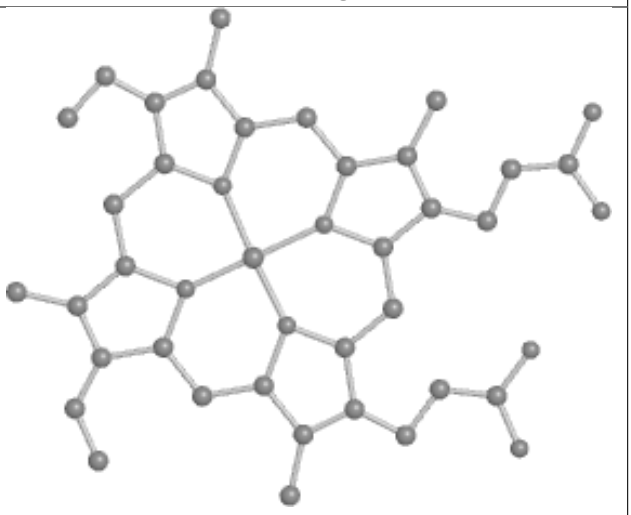
Bond lengths



Bond angles

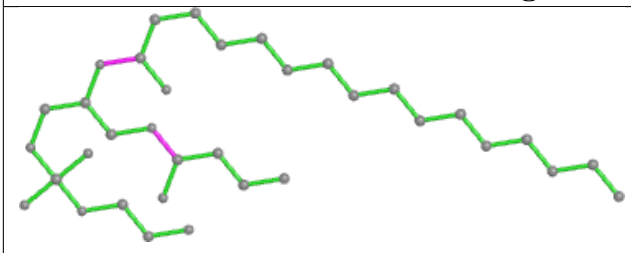


Torsions

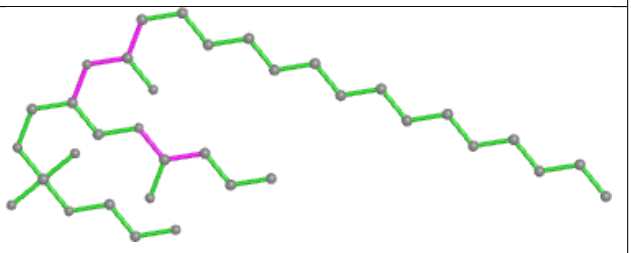


Rings

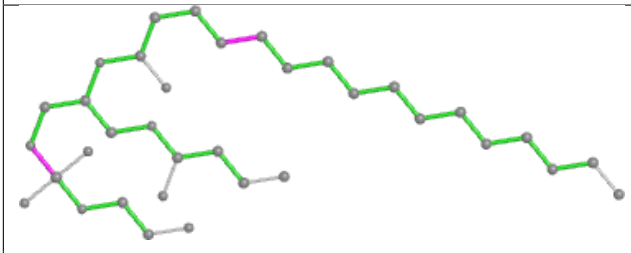
Ligand 3PE Ac 403



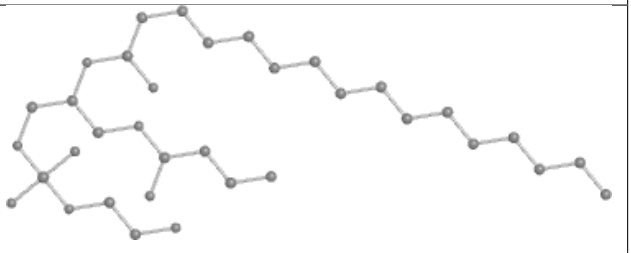
Bond lengths



Bond angles

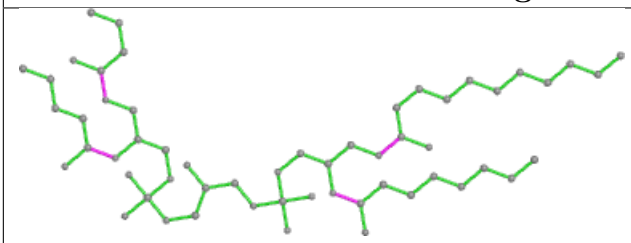


Torsions

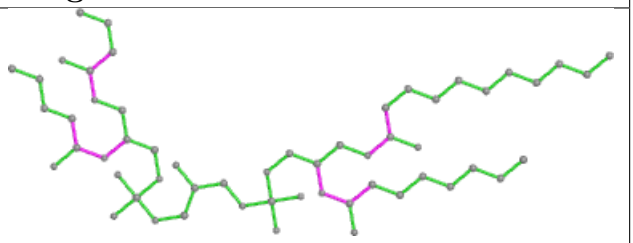


Rings

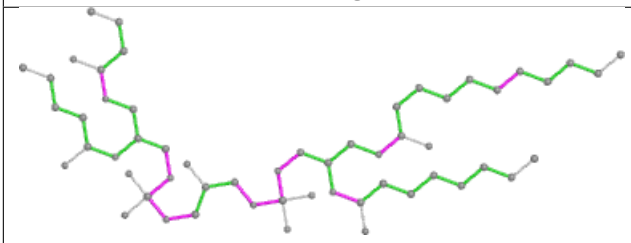
Ligand CDL Ag 101



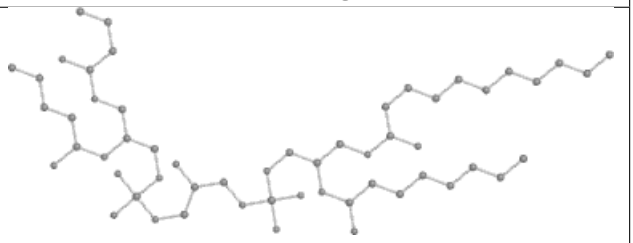
Bond lengths



Bond angles

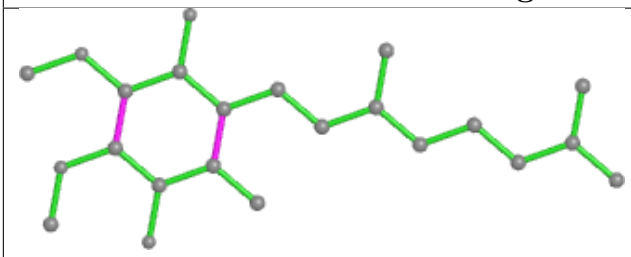


Torsions

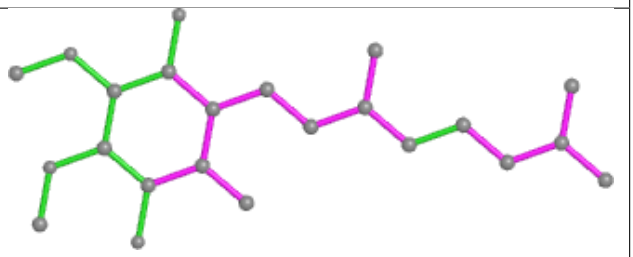


Rings

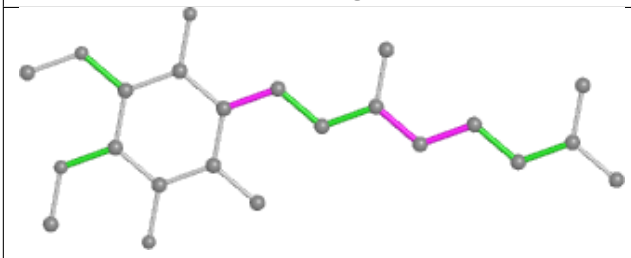
Ligand U10 AC 404



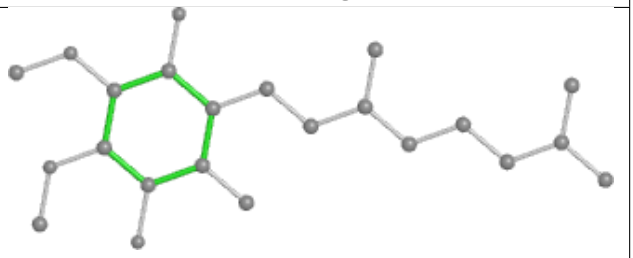
Bond lengths



Bond angles

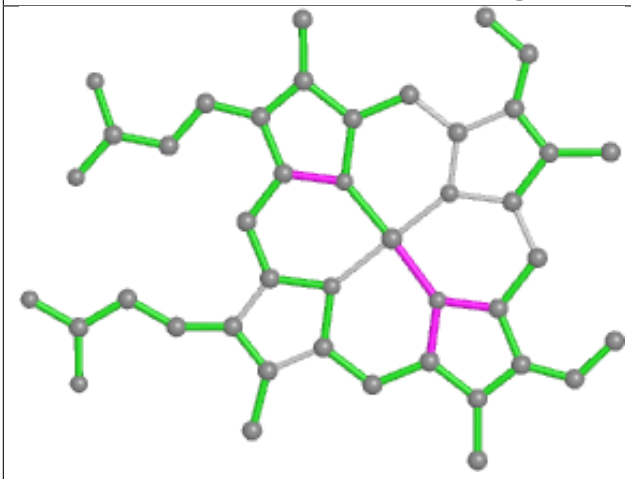


Torsions

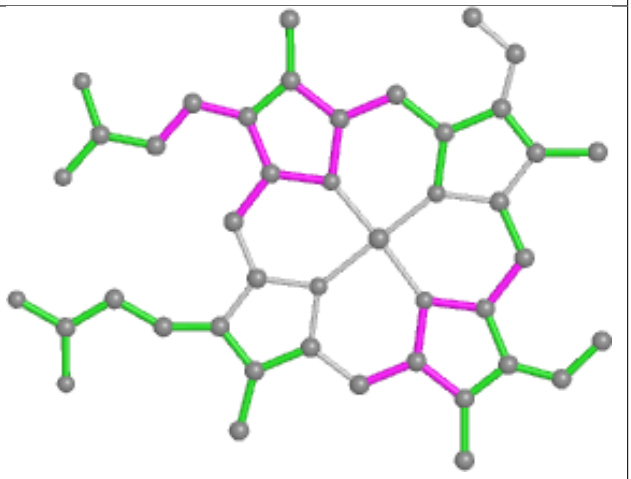


Rings

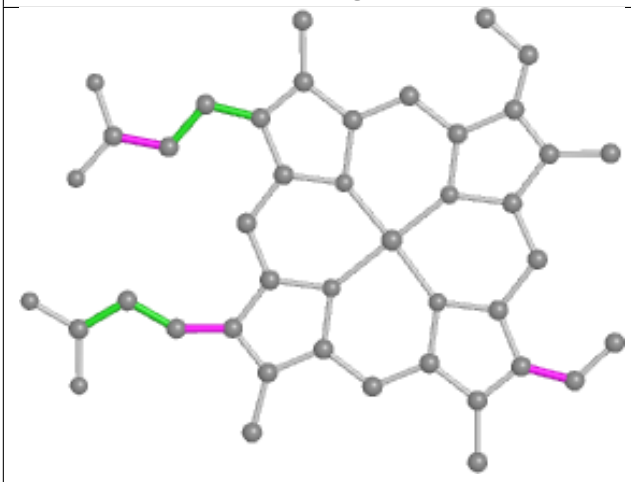
Ligand HEM Ac 402



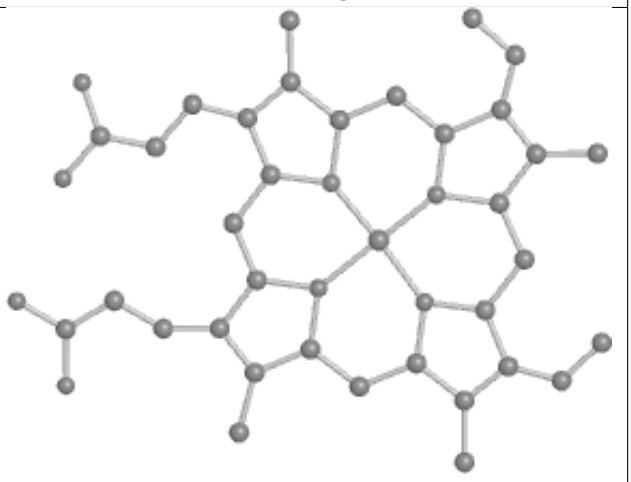
Bond lengths



Bond angles

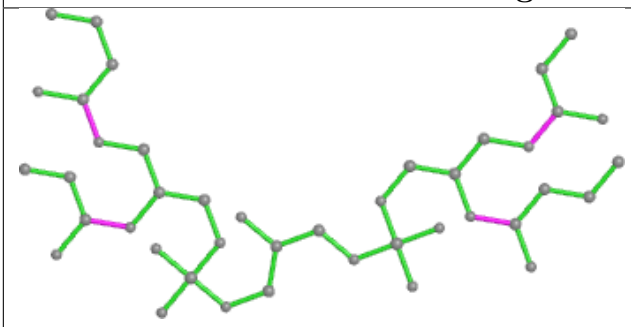


Torsions

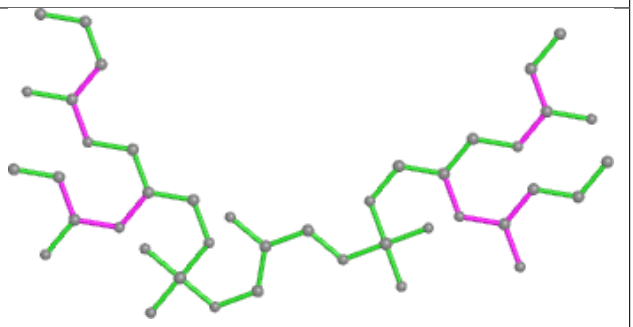


Rings

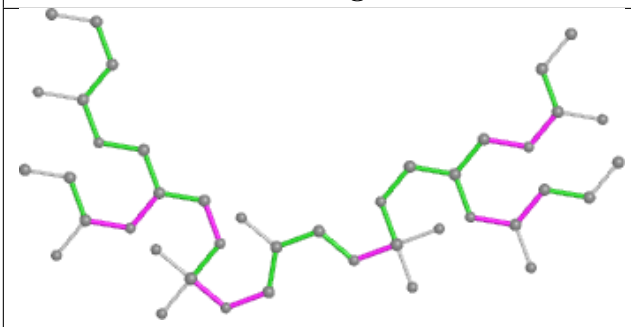
Ligand CDL Ac 406



Bond lengths



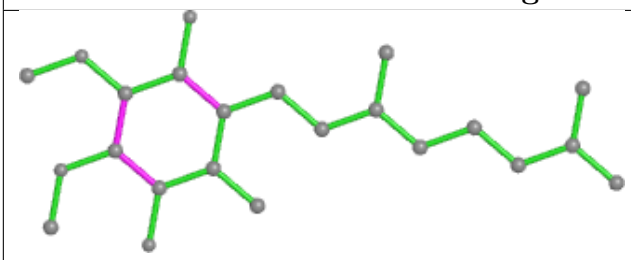
Bond angles



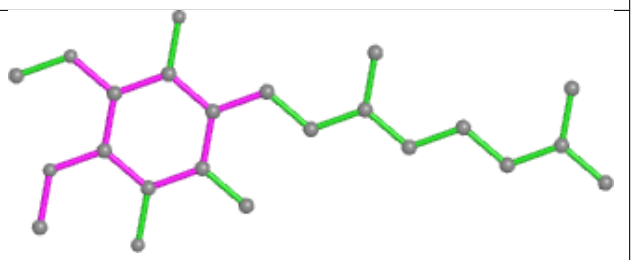
Torsions

Rings

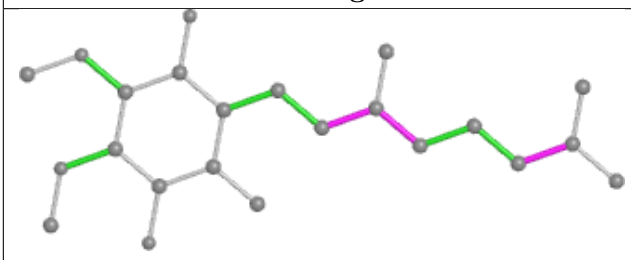
Ligand U10 Ac 404



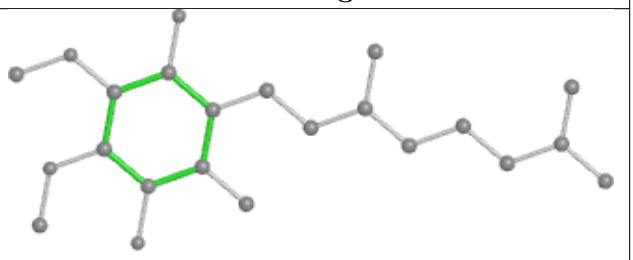
Bond lengths



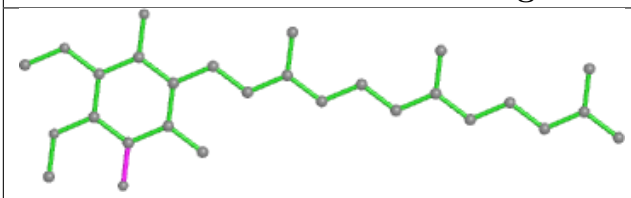
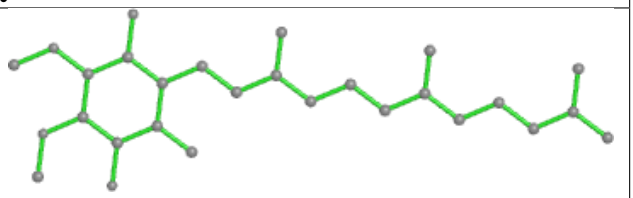
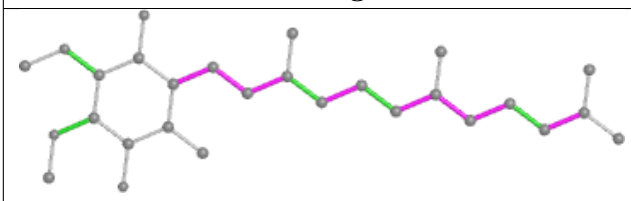
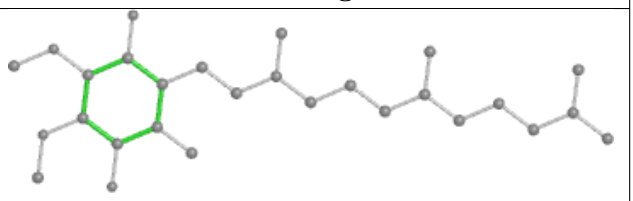
Bond angles

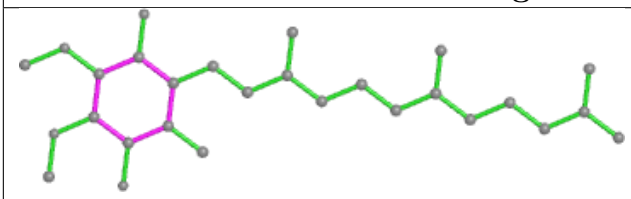
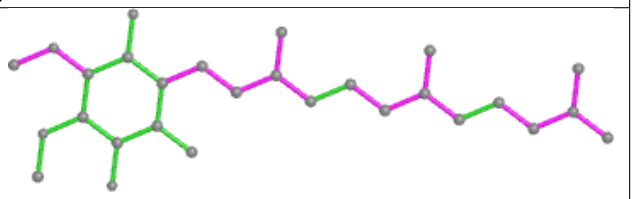
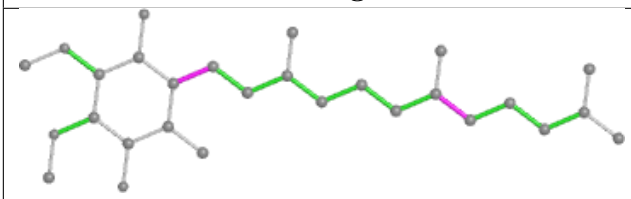
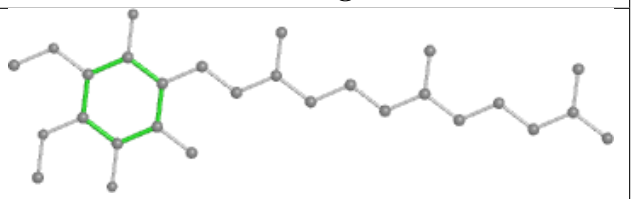


Torsions

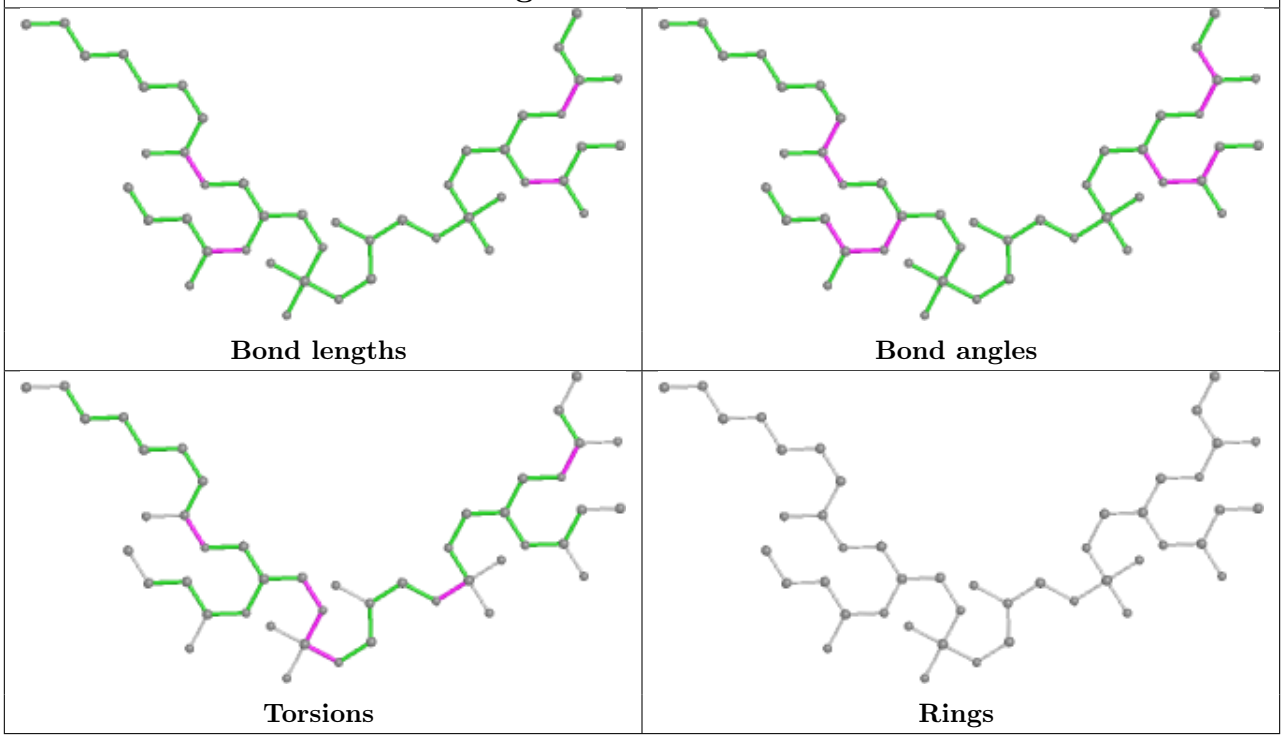


Rings

Ligand UQ6 Ac 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand UQ6 AC 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL Aa 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

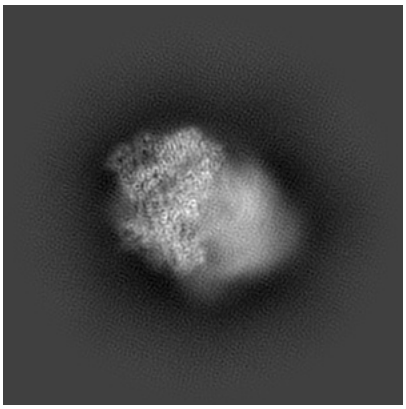
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35339. These allow visual inspection of the internal detail of the map and identification of artifacts.

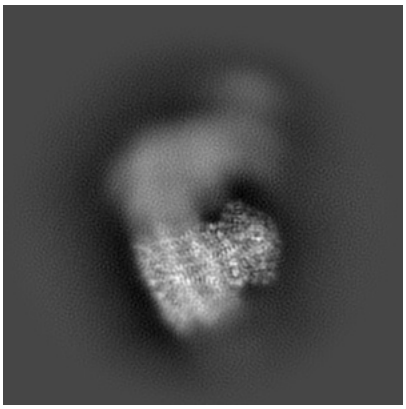
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

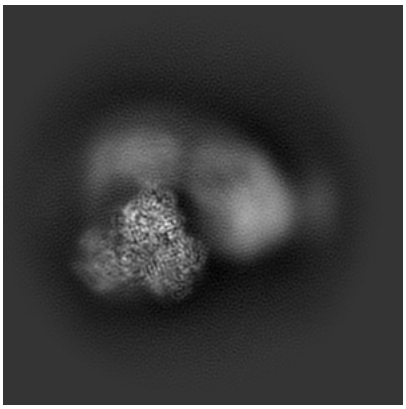
6.1.1 Primary map



X

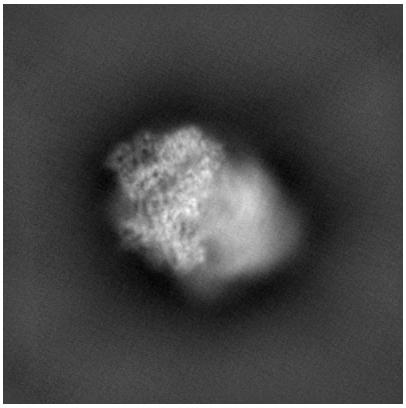


Y

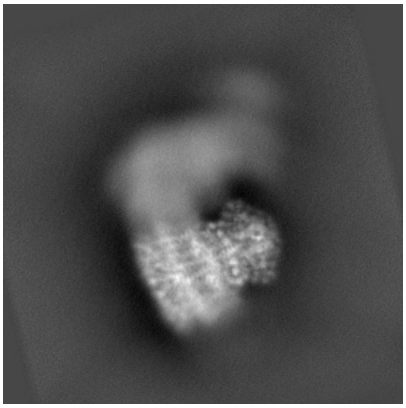


Z

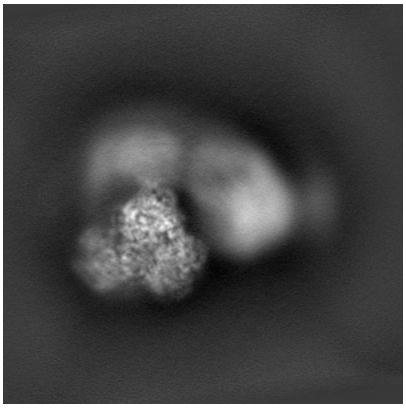
6.1.2 Raw map



X



Y

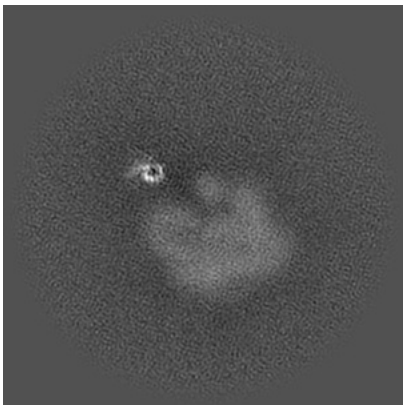


Z

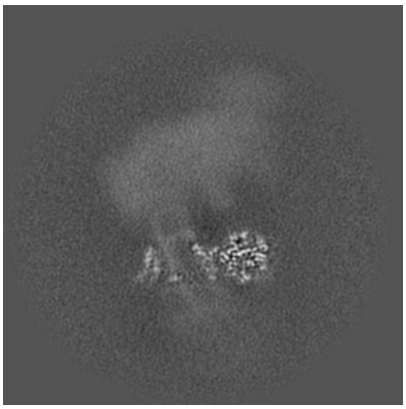
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

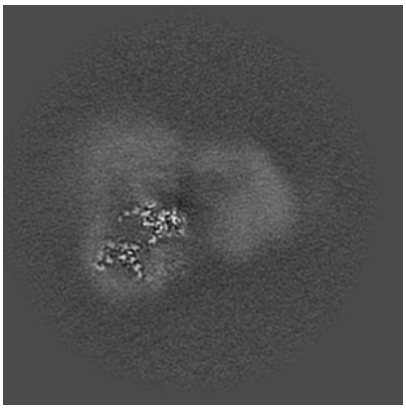
6.2.1 Primary map



X Index: 192

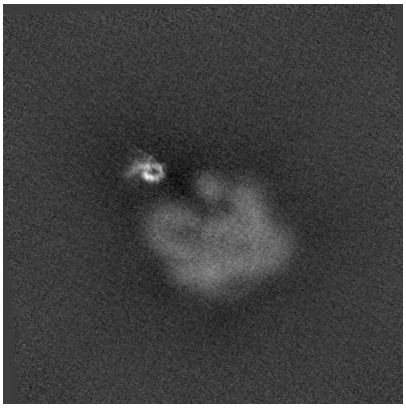


Y Index: 192

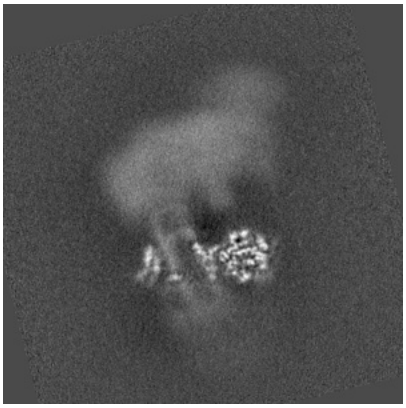


Z Index: 192

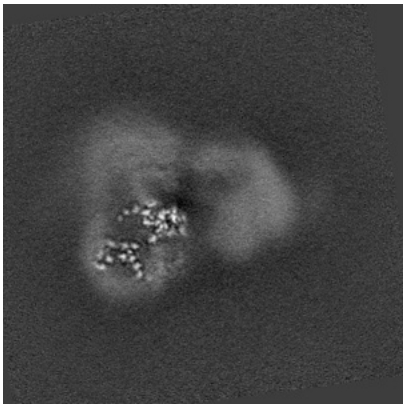
6.2.2 Raw map



X Index: 192



Y Index: 192

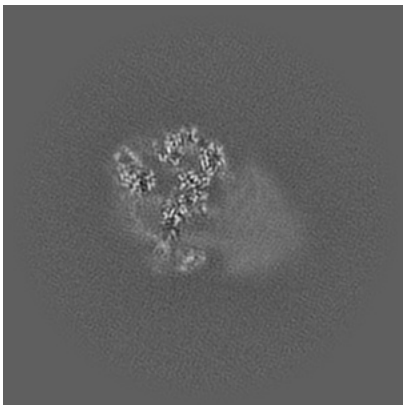


Z Index: 192

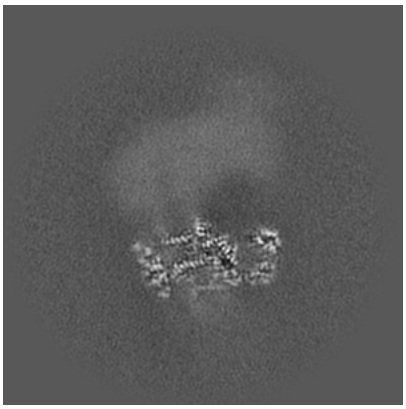
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

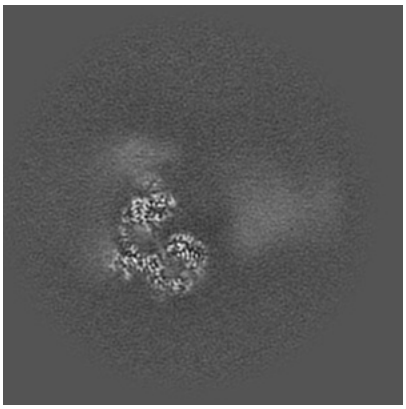
6.3.1 Primary map



X Index: 146

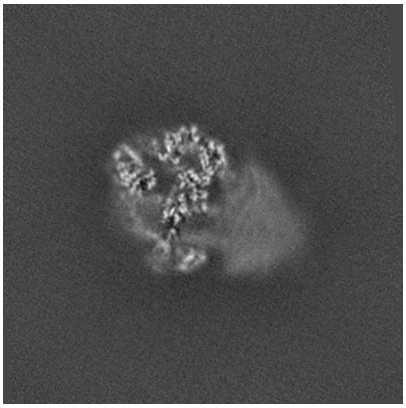


Y Index: 177

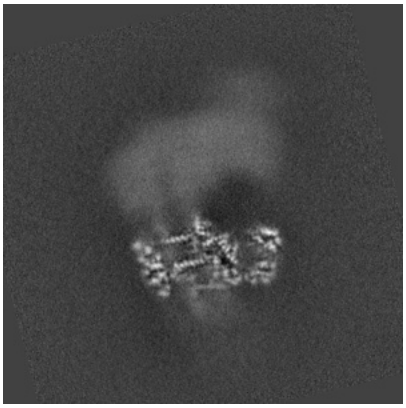


Z Index: 222

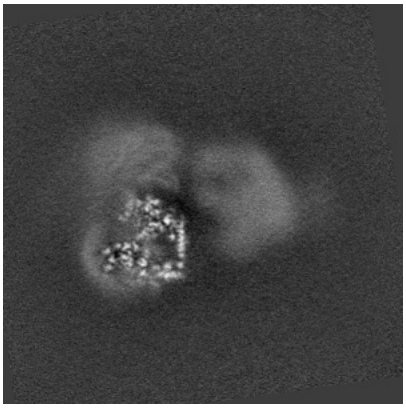
6.3.2 Raw map



X Index: 146



Y Index: 177

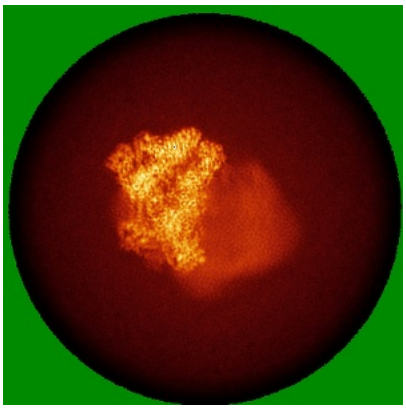


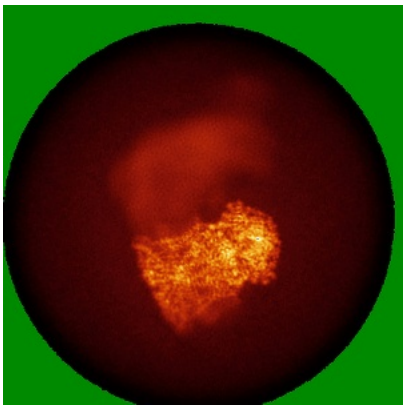
Z Index: 200

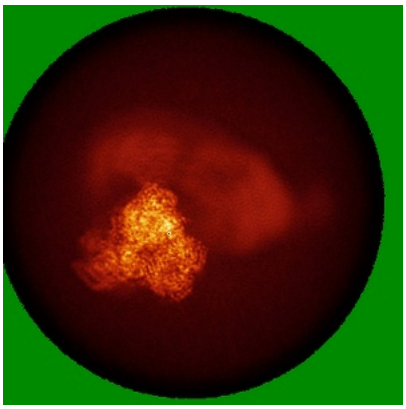
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

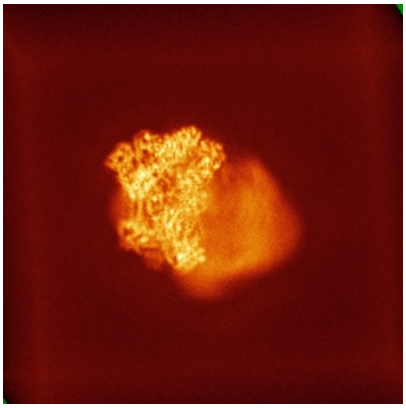
6.4.1 Primary map

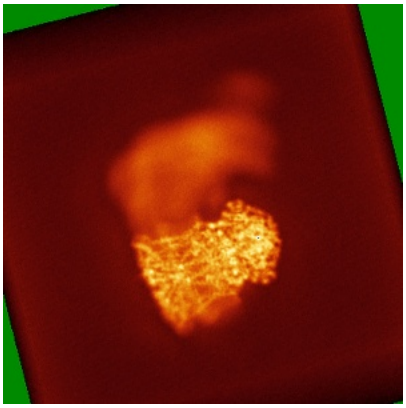

X

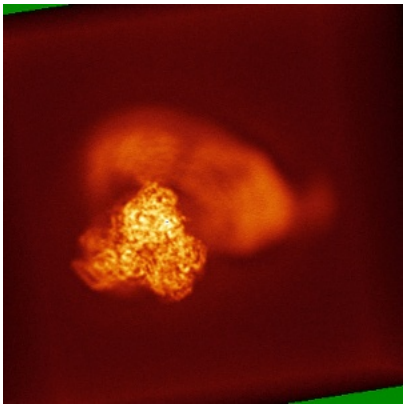

Y


Z

6.4.2 Raw map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

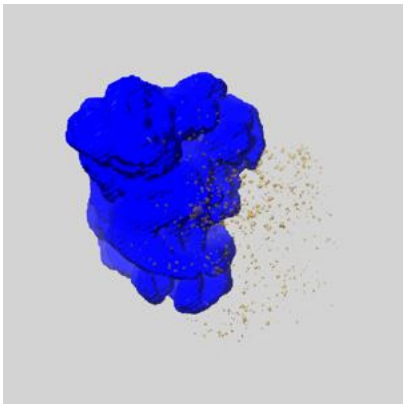
6.6 Mask visualisation (i)

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

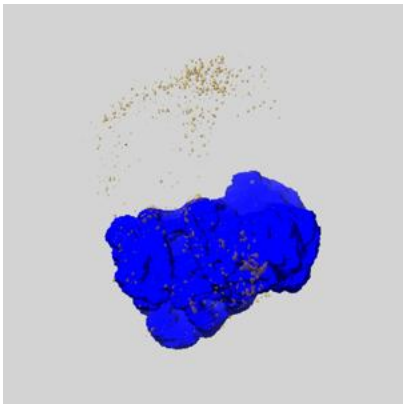
A mask typically either:

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

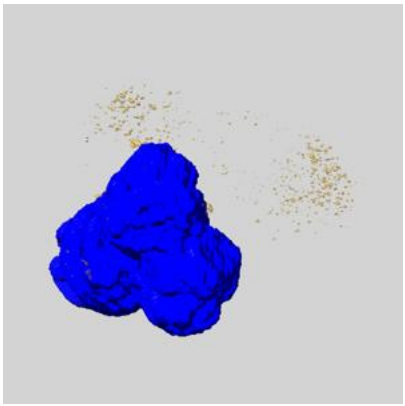
6.6.1 emd_35339_msk_1.map (i)



X



Y

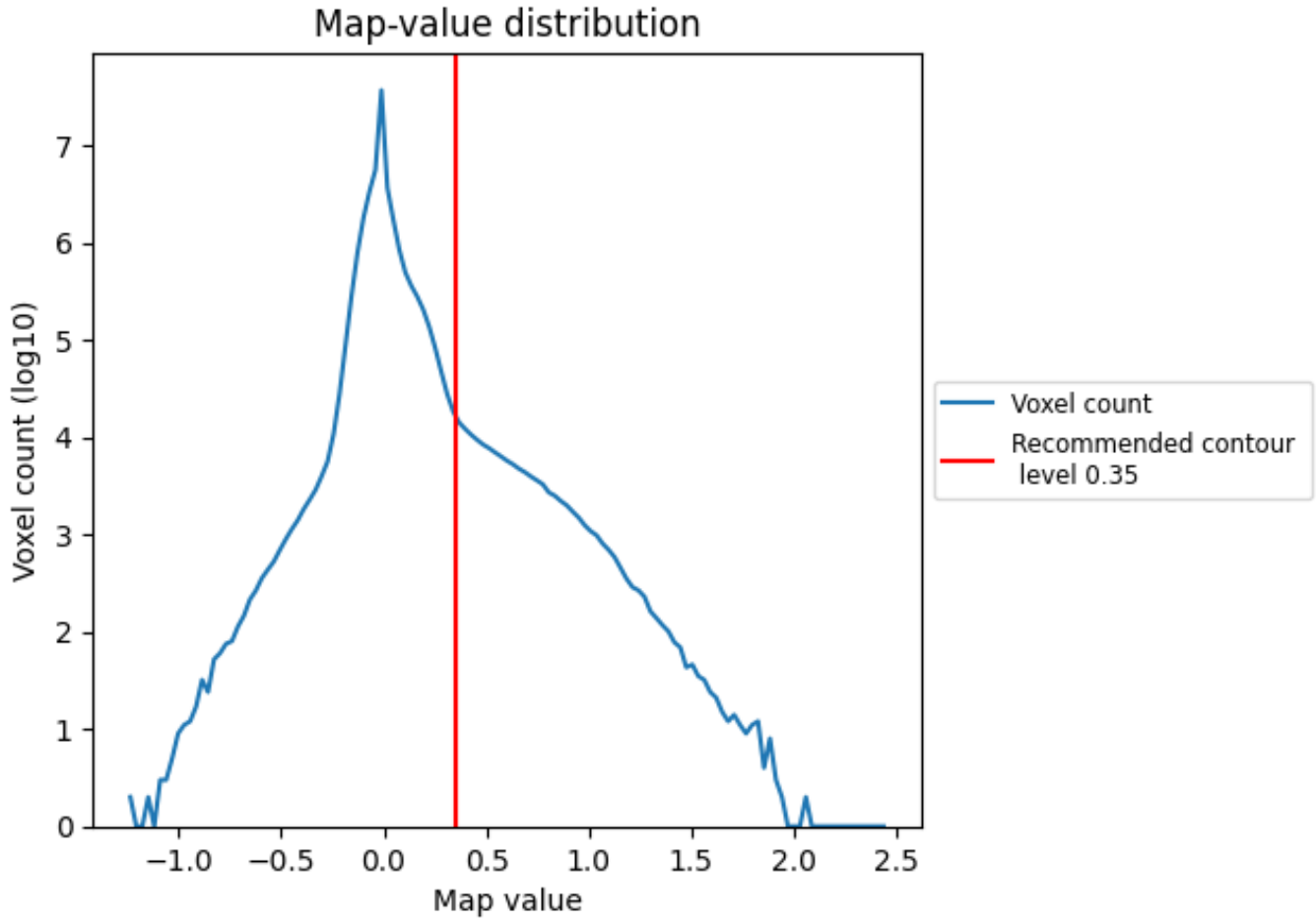


Z

7 Map analysis

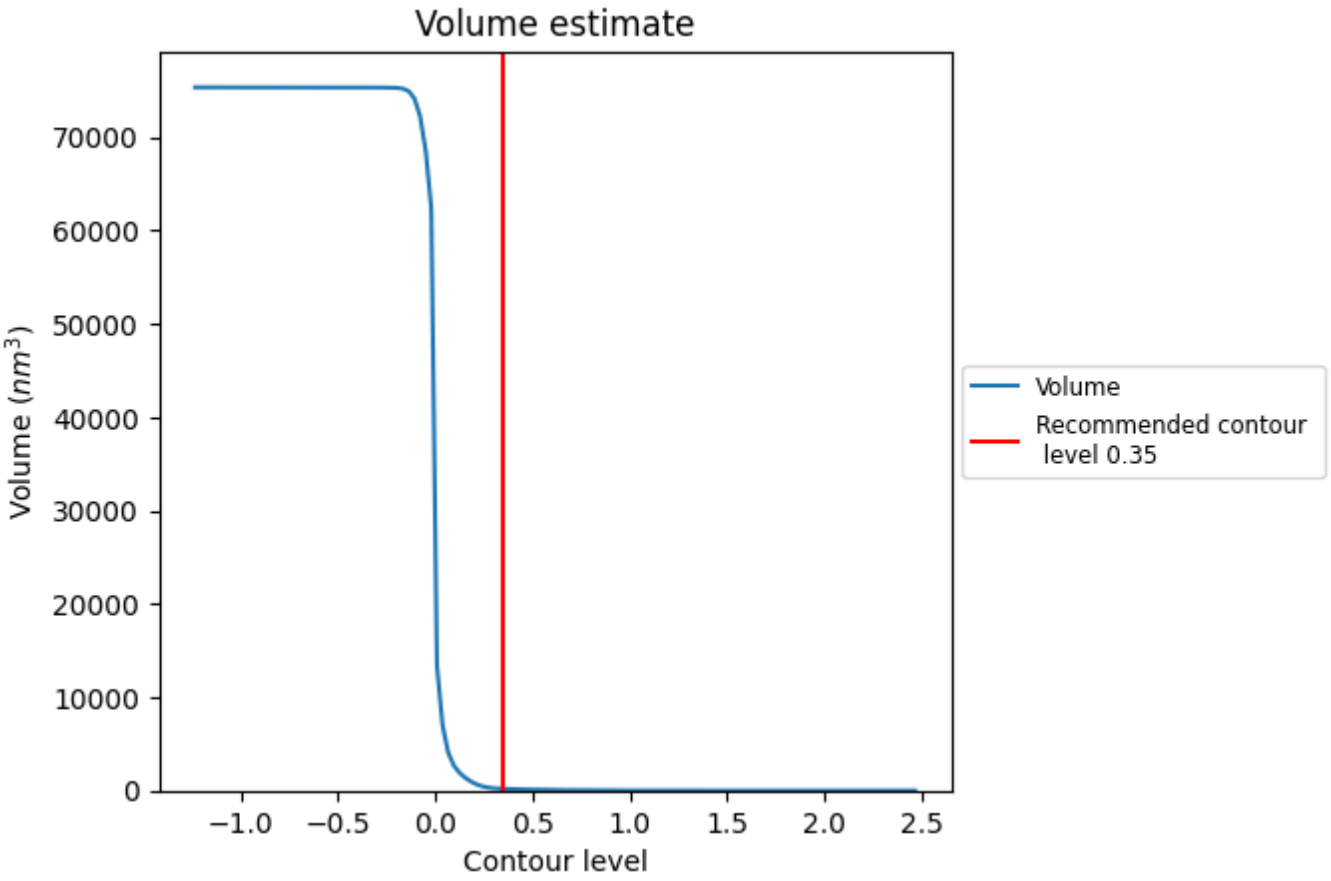
This section contains the results of statistical analysis of the map.

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.

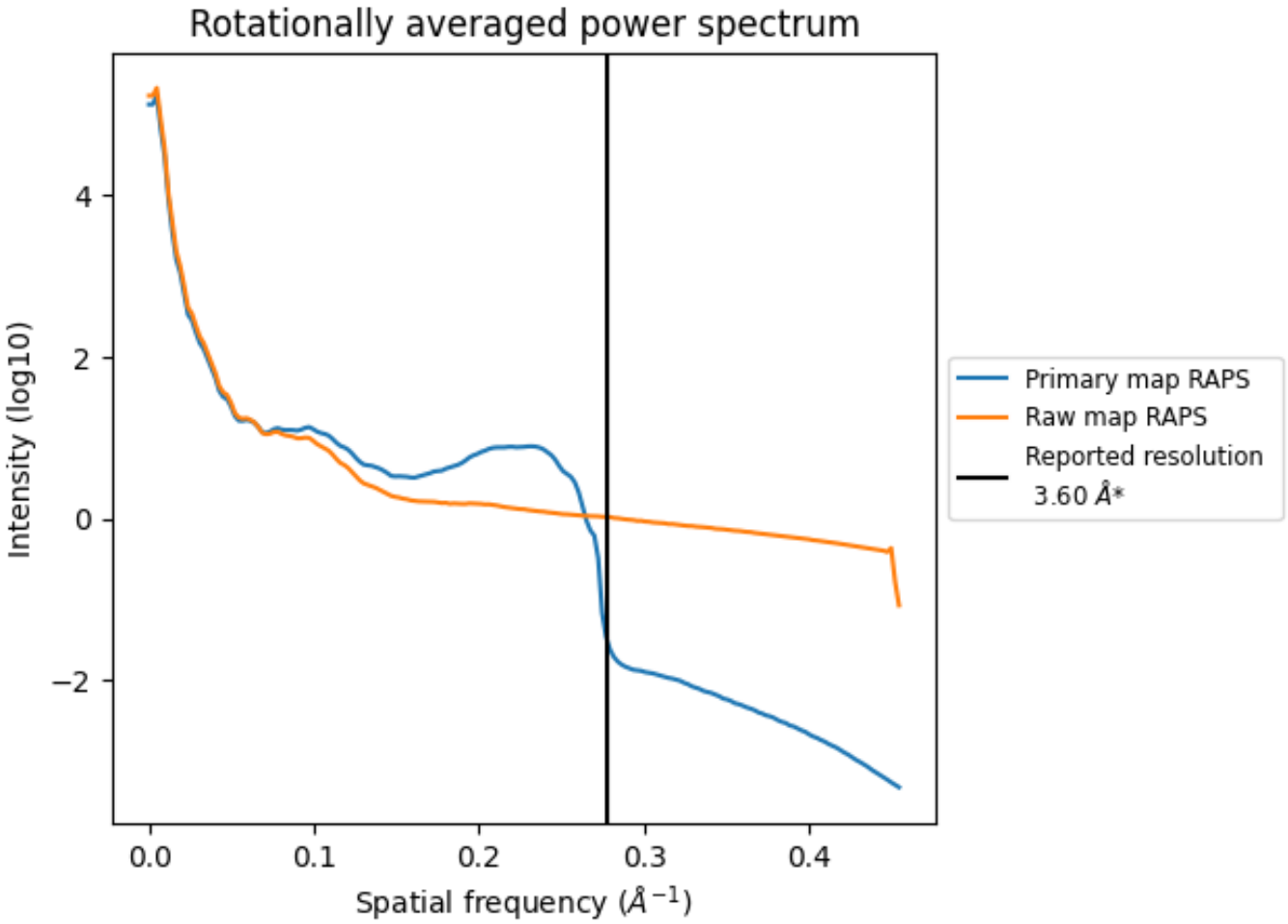
7.2 Volume estimate



The volume at the recommended contour level is 184 nm^3; this corresponds to an approximate mass of 166 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)

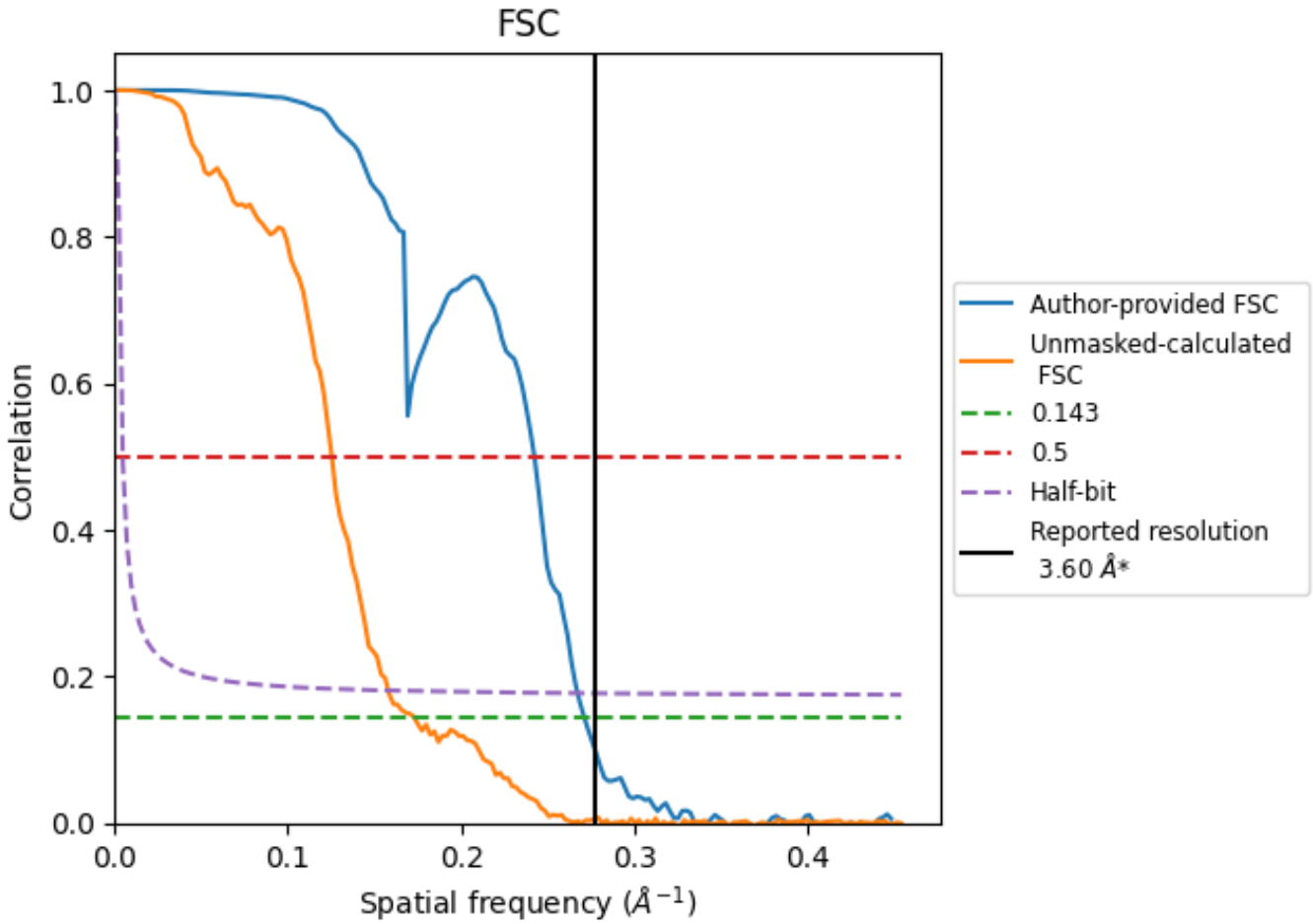


*Reported resolution corresponds to spatial frequency of 0.278 $Å^{-1}$

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 0.278 Å^{-1}

8.2 Resolution estimates (i)

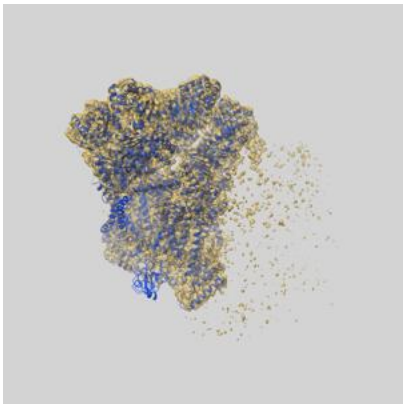
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.68	4.13	3.74
Unmasked-calculated*	5.77	7.97	6.33

*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 5.77 differs from the reported value 3.6 by more than 10 %

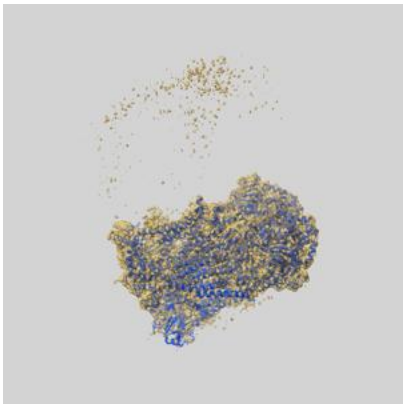
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35339 and PDB model 8IBC. Per-residue inclusion information can be found in section 3 on page 11.

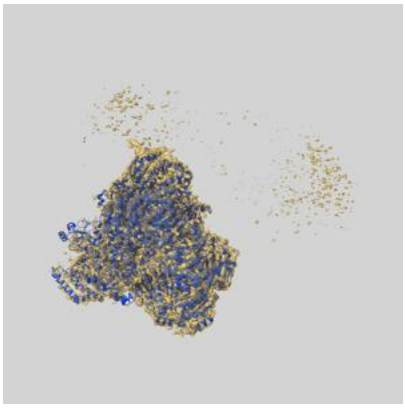
9.1 Map-model overlay



X



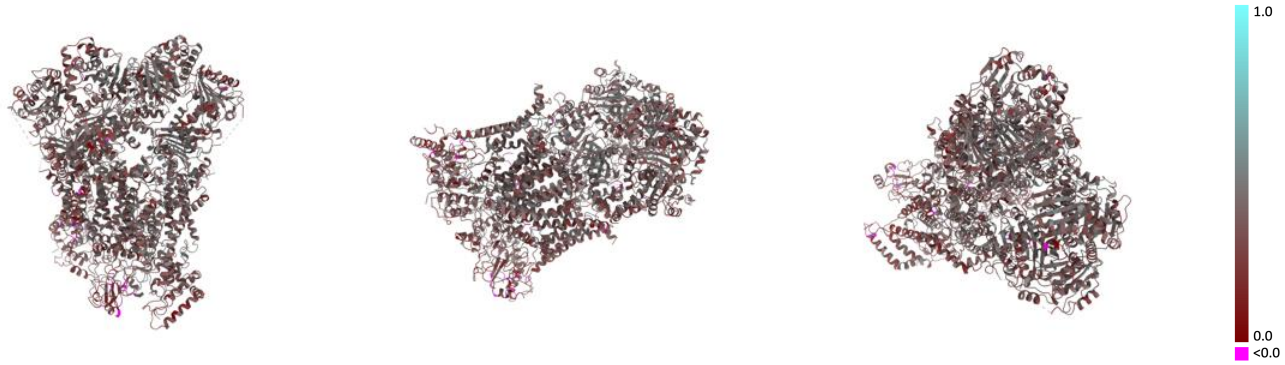
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 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.

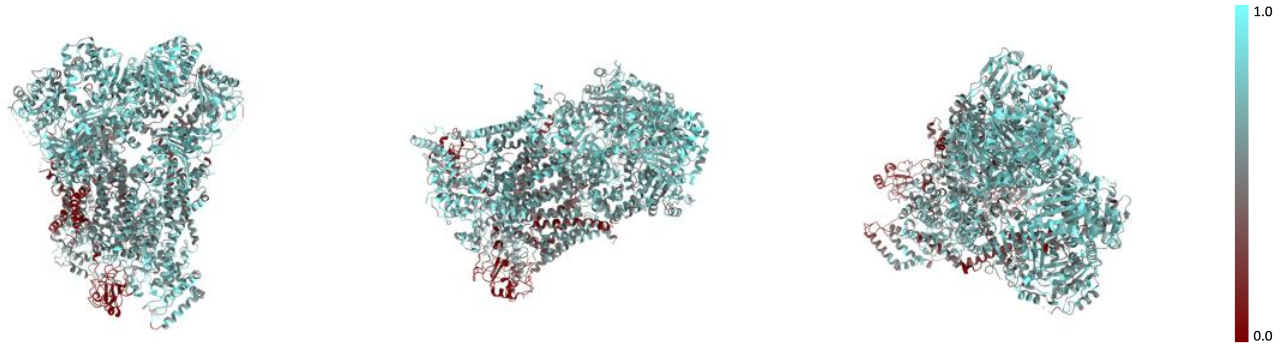
9.2 Q-score mapped to coordinate model (i)



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.

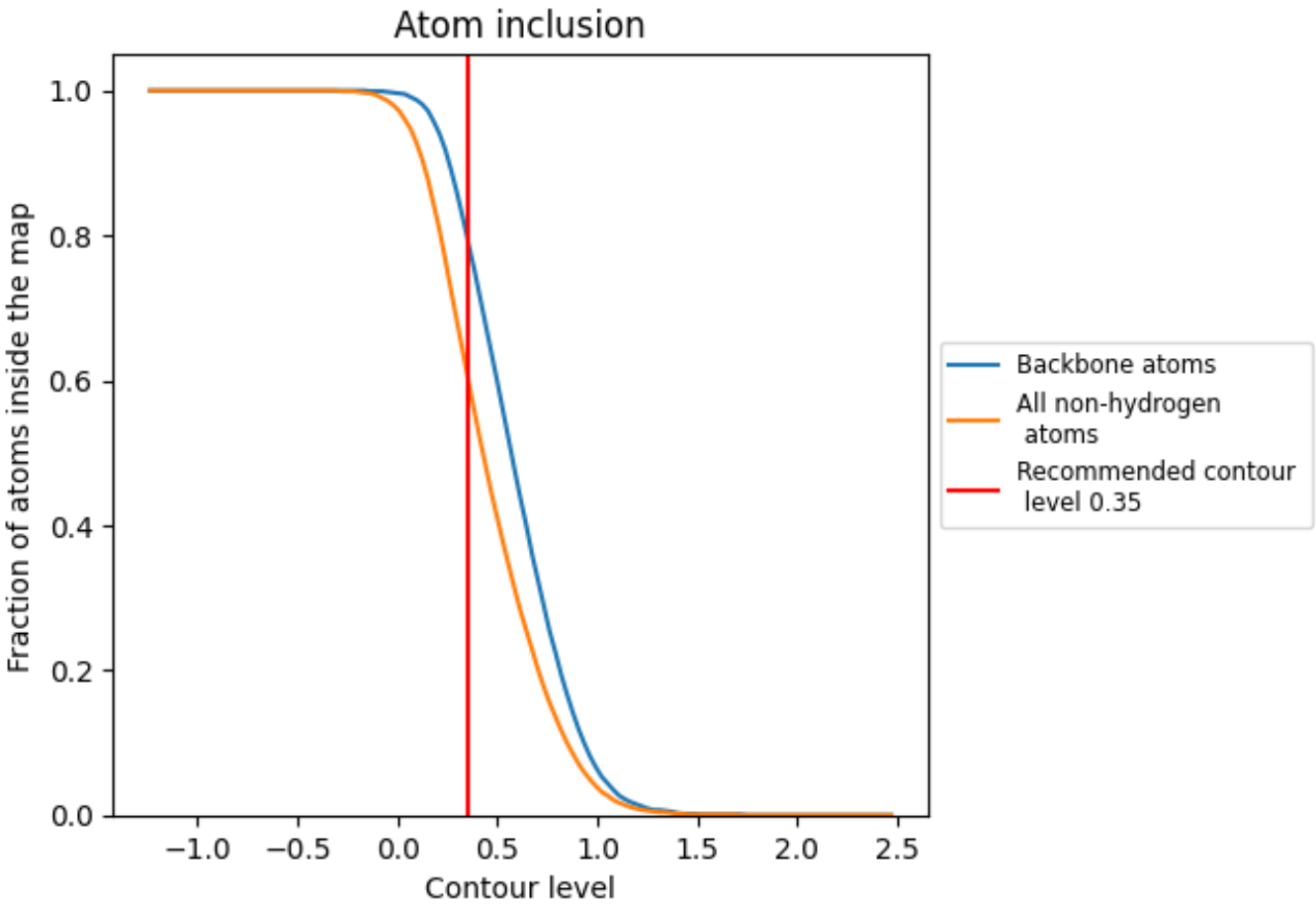
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 61% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6070	0.3520
AA	0.6840	0.3640
AB	0.6980	0.3750
AC	0.6010	0.3510
AD	0.6050	0.3210
AE	0.1820	0.2700
AF	0.6630	0.3670
AG	0.4890	0.2910
AH	0.4760	0.2710
AI	0.4430	0.3720
AJ	0.1100	0.2680
AK	0.0790	0.2310
Aa	0.7000	0.3710
Ab	0.7250	0.3760
Ac	0.6580	0.3840
Ad	0.7040	0.3580
Ae	0.3000	0.2900
Af	0.7040	0.4130
Ag	0.6610	0.3730
Ah	0.6540	0.2950
Aj	0.4930	0.3430
Ak	0.2600	0.3220