Full wwPDB EM Validation Report

Dec 16, 2024 – 04:34 PM JST

PDB ID	:	8ZP0
EMDB ID	:	EMD-60323
Title	:	Cryo-EM structure of YF23694-bound porcine bc1 complex
Authors	:	Wang, Y.X.; Sun, J.Y.; Cui, G.R.; Yang, G.F.
Deposited on	:	2024-05-29
Resolution	:	2.44 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:

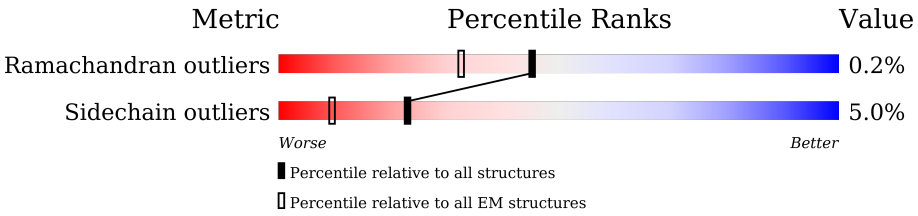
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.44 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	A	378	5% 98%
1	a	378	5% 97%
2	B	241	13% 93% 6%
2	b	241	12% 94% 5%
3	C	196	94% 92% 7%
3	c	196	96% 83% 14%
4	D	446	97%
4	d	446	96%
5	E	418	98%

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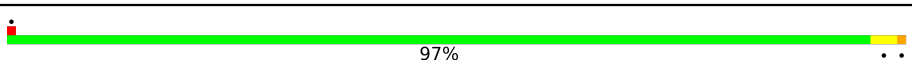
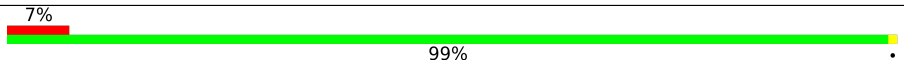
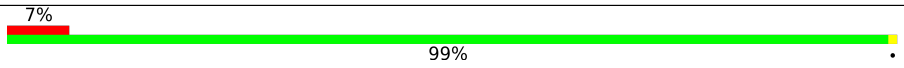
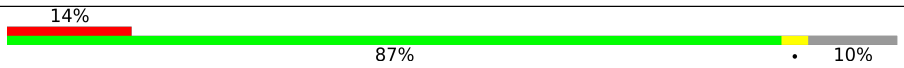
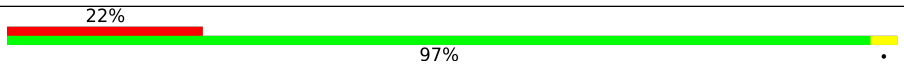
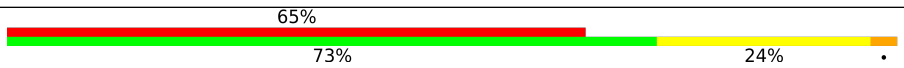
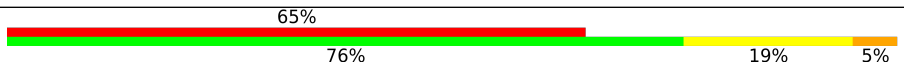
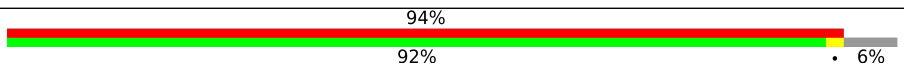
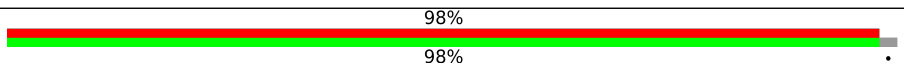
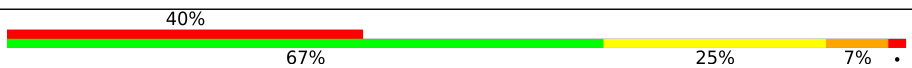
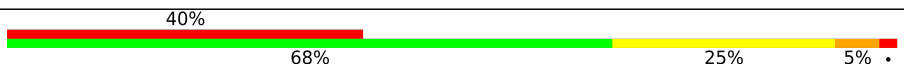
Mol	Chain	Length	Quality of chain
5	e	418	
6	F	64	
6	f	64	
7	G	106	
7	g	106	
8	H	79	
8	h	79	
9	I	62	
9	i	62	
10	J	52	
10	j	52	
11	K	57	
11	k	57	

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 33585 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	378	Total	C	N	O	S	0	0
			3017	2026	470	501	20		
1	a	378	Total	C	N	O	S	0	0
			3017	2026	470	501	20		

- Molecule 2 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	241	Total	C	N	O	S	0	0
			1920	1225	330	349	16		
2	b	239	Total	C	N	O	S	0	0
			1904	1214	327	347	16		

- Molecule 3 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	194	Total	C	N	O	S	0	0
			1502	946	261	288	7		
3	c	196	Total	C	N	O	S	0	0
			1517	954	265	291	7		

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	445	Total	C	N	O	S	0	0
			3452	2157	604	672	19		
4	d	446	Total	C	N	O	S	0	0
			3459	2161	605	674	19		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	418	Total	C	N	O	S	0	0
			3134	1962	556	607	9		
5	e	418	Total	C	N	O	S	0	0
			3134	1962	556	607	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	64	Total	C	N	O	S	0	0
			528	320	97	106	5		
6	f	64	Total	C	N	O	S	0	0
			528	320	97	106	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	106	Total	C	N	O	S	0	0
			921	589	162	168	2		
7	g	106	Total	C	N	O	S	0	0
			921	589	162	168	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	71	Total	C	N	O	S	0	0
			608	399	112	95	2		
8	h	79	Total	C	N	O	S	0	0
			666	434	122	108	2		

- Molecule 9 is a protein called Complex III subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	62	Total	C	N	O	0	0
			507	331	90	86		
9	i	62	Total	C	N	O	0	0
			507	331	90	86		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	49	Total	C	N	O	S	0	0
			405	269	71	63	2		

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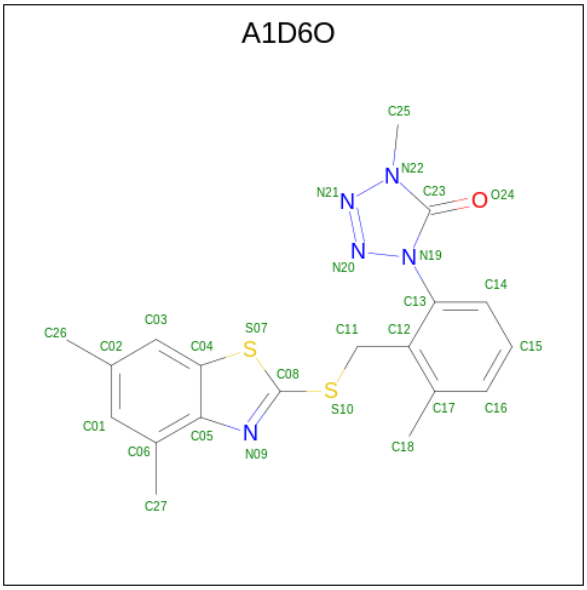
Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	51	Total	C	N	O	S	0	0
			421	281	74	65	1		

- Molecule 11 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

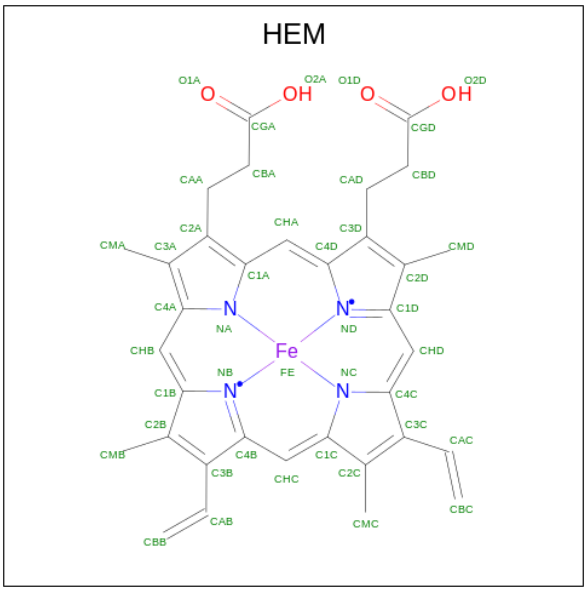
Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	57	Total	C	N	O	S	0	0
			404	252	74	76	2		
11	k	57	Total	C	N	O	S	0	0
			404	252	74	76	2		

- Molecule 12 is 1-[2-[(4,6-dimethyl-1,3-benzothiazol-2-yl)sulfanylmethyl]-3-methyl-phenyl]-4-methyl-1,2,3,4-tetrazol-5-one (three-letter code: A1D6O) (formula: $C_{19}H_{19}N_5OS_2$) (labeled as "Ligand of Interest" by depositor).



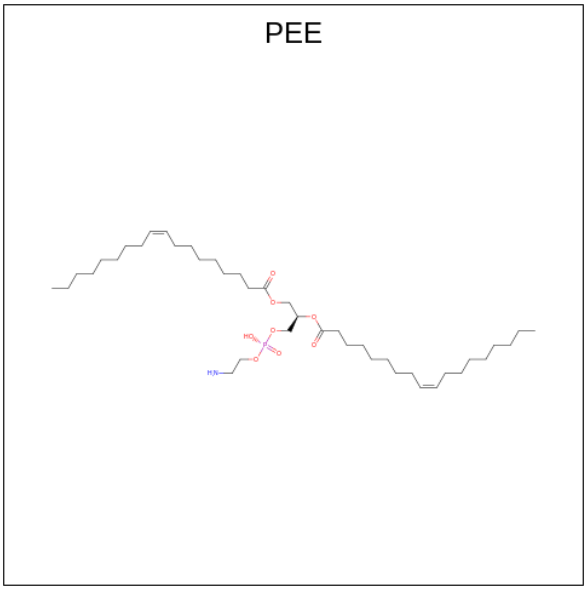
Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	N	O	S	0
			27	19	5	1	2	
12	A	1	Total	C	N	O	S	0
			27	19	5	1	2	
12	a	1	Total	C	N	O	S	0
			27	19	5	1	2	
12	a	1	Total	C	N	O	S	0
			27	19	5	1	2	

- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



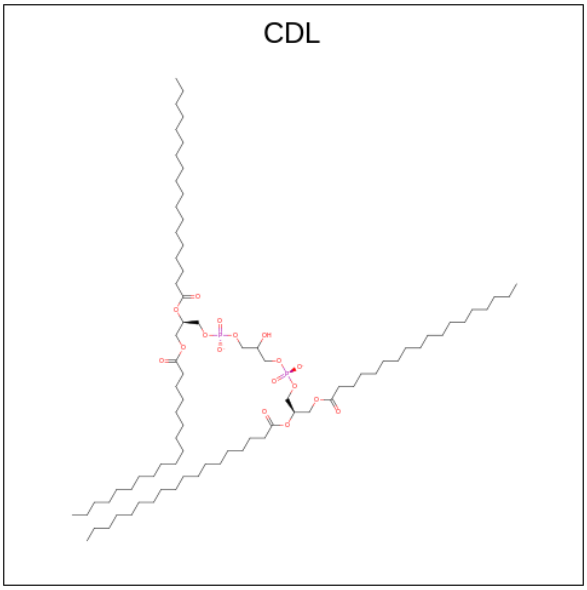
Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	a	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	a	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 14 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$).



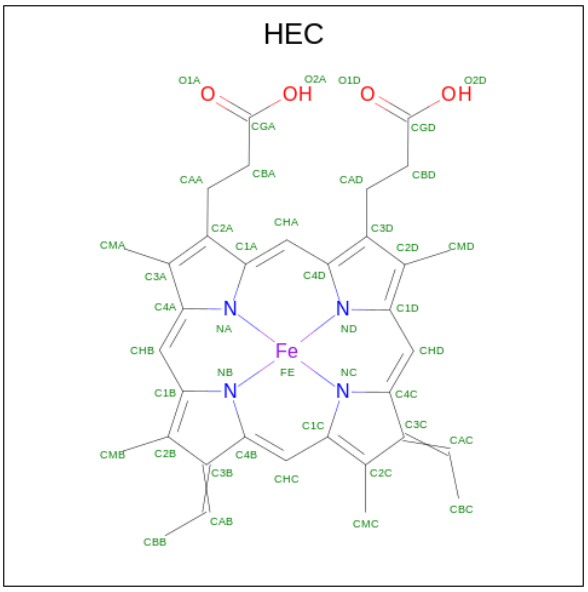
Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
14	D	1	Total	C	N	O	P	0
			49	39	1	8	1	
14	a	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 15 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



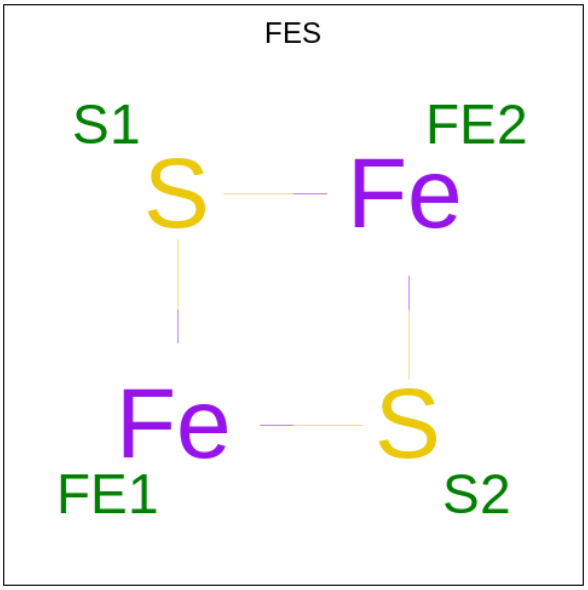
Mol	Chain	Residues	Atoms				AltConf
15	A	1	Total	C	O	P	0
			64	45	17	2	
15	a	1	Total	C	O	P	0
			64	45	17	2	
15	a	1	Total	C	O	P	0
			64	45	17	2	

- Molecule 16 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
16	b	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 17 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

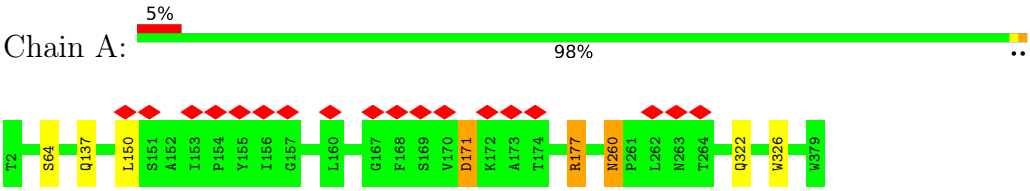


Mol	Chain	Residues	Atoms				AltConf
17	C	1	Total	Fe	S		0
			4	2	2		
17	c	1	Total	Fe	S		0
			4	2	2		

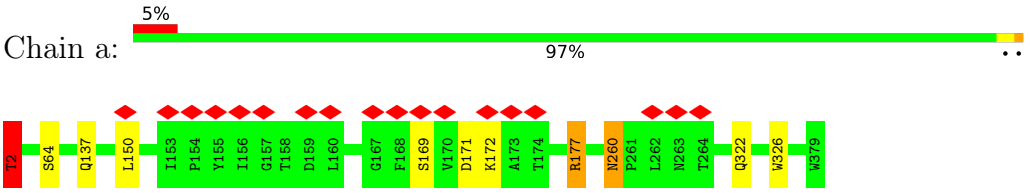
3 Residue-property plots (i)

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.

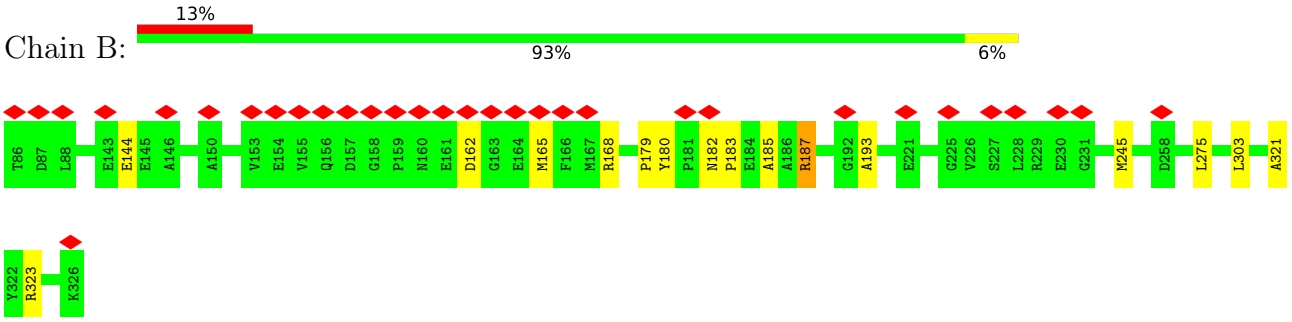
• Molecule 1: Cytochrome b



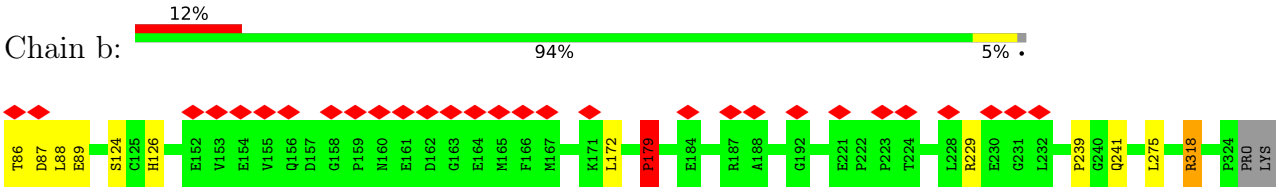
• Molecule 1: Cytochrome b



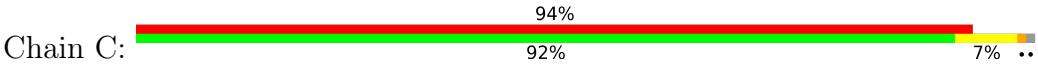
• Molecule 2: Cytochrome c1, heme protein, mitochondrial

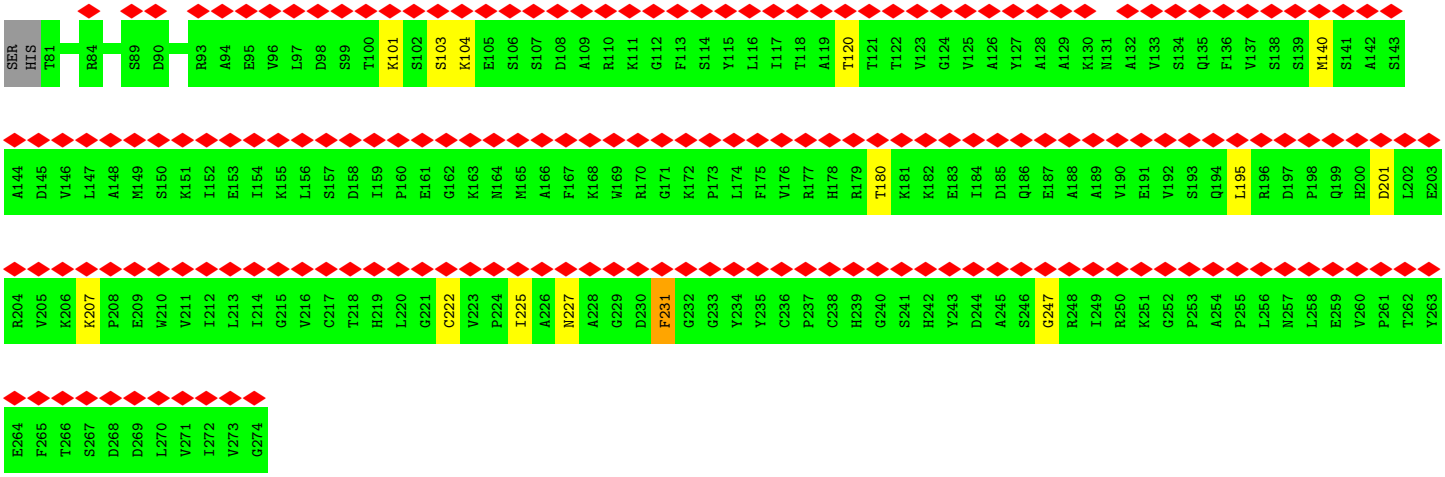


• Molecule 2: Cytochrome c1, heme protein, mitochondrial



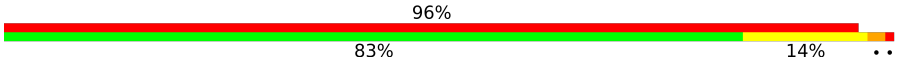
• Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial

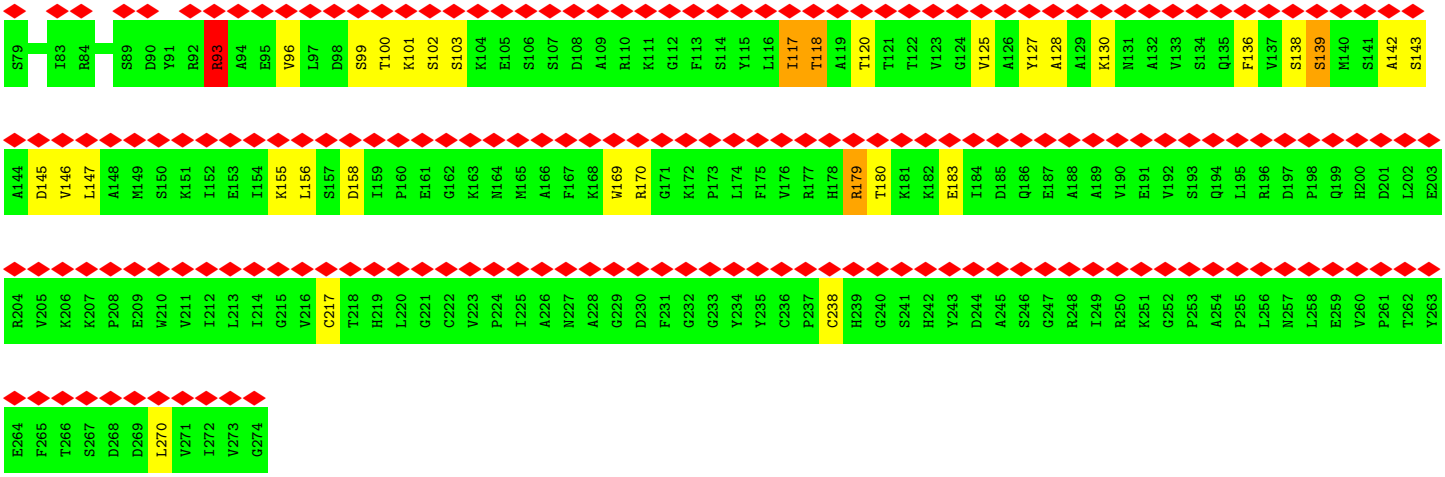




• Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial

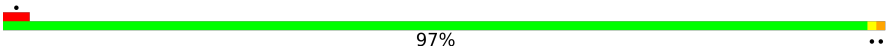
Chain c:





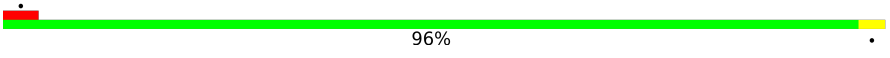
• Molecule 4: Cytochrome b-c1 complex subunit 1, mitochondrial

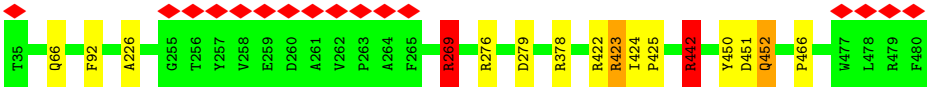
Chain D:



• Molecule 4: Cytochrome b-c1 complex subunit 1, mitochondrial

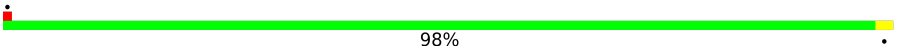
Chain d:

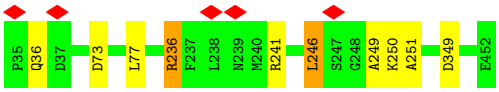




• Molecule 5: Cytochrome b-c1 complex subunit 2, mitochondrial

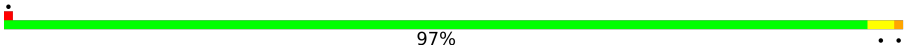
Chain E:

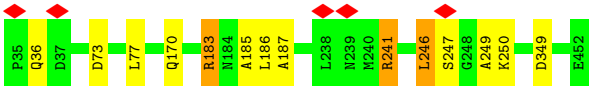




• Molecule 5: Cytochrome b-c1 complex subunit 2, mitochondrial

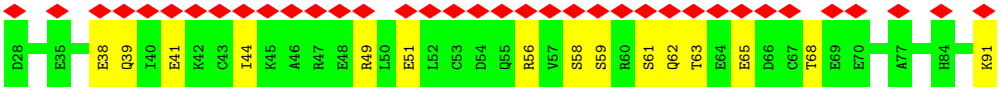
Chain e:





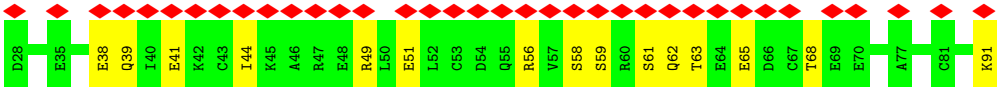
• Molecule 6: Cytochrome b-c1 complex subunit 6

Chain F:



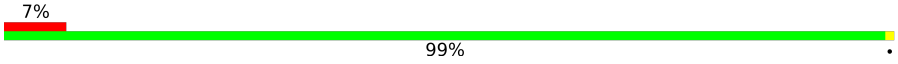
• Molecule 6: Cytochrome b-c1 complex subunit 6

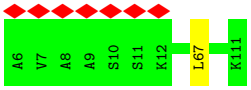
Chain f:



• Molecule 7: Cytochrome b-c1 complex subunit 7

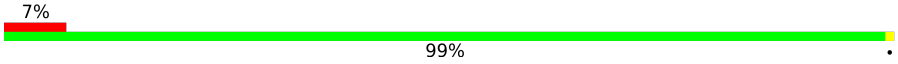
Chain G:

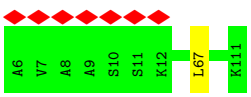




• Molecule 7: Cytochrome b-c1 complex subunit 7

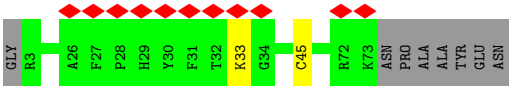
Chain g:





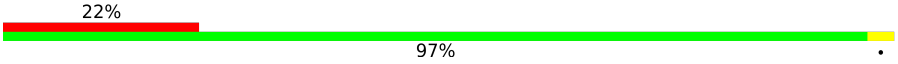
• Molecule 8: Cytochrome b-c1 complex subunit 8

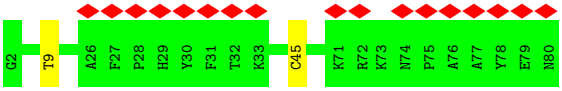
Chain H:



• Molecule 8: Cytochrome b-c1 complex subunit 8

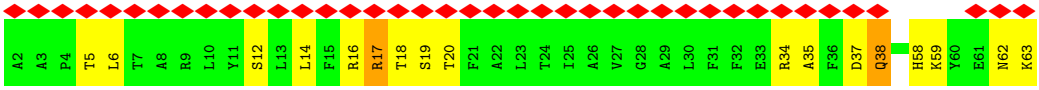
Chain h:





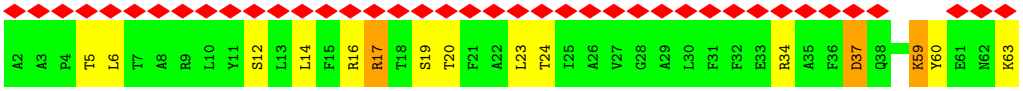
• Molecule 9: Complex III subunit 9

Chain I:



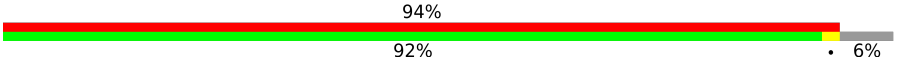
• Molecule 9: Complex III subunit 9

Chain i:



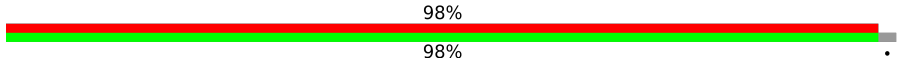
• Molecule 10: Cytochrome b-c1 complex subunit 10

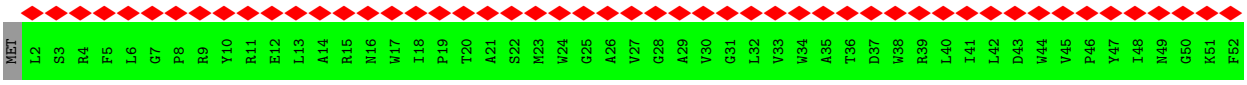
Chain J:



• Molecule 10: Cytochrome b-c1 complex subunit 10

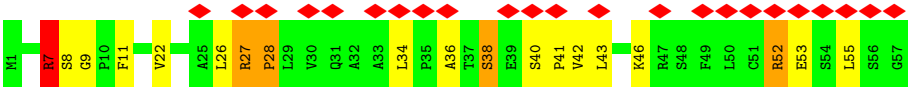
Chain j:





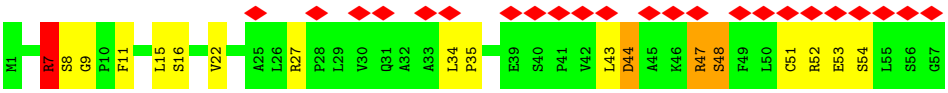
• Molecule 11: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain K:



• Molecule 11: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain k:


M1
R7
S8
G9
P10
F11
L15
S16
V22
A25
L26
R27
P28
L29
V30
Q31
A32
A33
L34
P35
E39
S40
P41
V42
L43
D44
A45
K46
R47
S48
F49
L50
C51
R52
E53
S54
L55
S56
G57

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	493233	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 ($e^-/Å^2$)	49.72	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	10.253	Depositor
Minimum map value	-6.629	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.286	Depositor
Recommended contour level	1.06	Depositor
Map size (Å)	307.19998, 307.19998, 307.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9599999, 0.9599999, 0.9599999	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, FES, A1D6O, CDL, PEE, HEC

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	0.45	0/3115	0.68	3/4259 (0.1%)
1	a	0.48	0/3115	0.72	5/4259 (0.1%)
2	B	0.50	0/1978	0.81	9/2684 (0.3%)
2	b	0.52	0/1961	0.81	5/2661 (0.2%)
3	C	0.43	0/1534	0.75	1/2075 (0.0%)
3	c	0.61	3/1549 (0.2%)	0.94	7/2095 (0.3%)
4	D	0.55	6/3524 (0.2%)	0.73	3/4783 (0.1%)
4	d	0.59	6/3531 (0.2%)	0.77	6/4793 (0.1%)
5	E	0.50	1/3187 (0.0%)	0.67	6/4314 (0.1%)
5	e	0.52	3/3187 (0.1%)	0.70	5/4314 (0.1%)
6	F	0.35	0/534	0.62	0/714
6	f	0.38	0/534	0.73	1/714 (0.1%)
7	G	0.45	0/941	0.59	0/1262
7	g	0.45	0/941	0.59	0/1262
8	H	0.45	0/628	0.71	0/848
8	h	0.41	0/688	0.68	0/931
9	I	0.47	0/520	0.92	2/701 (0.3%)
9	i	0.51	1/520 (0.2%)	0.99	3/701 (0.4%)
10	J	0.33	0/420	0.75	1/576 (0.2%)
10	j	0.35	0/437	0.69	0/598
11	K	1.06	3/410 (0.7%)	1.43	8/556 (1.4%)
11	k	1.11	4/410 (1.0%)	1.36	7/556 (1.3%)
All	All	0.53	27/33664 (0.1%)	0.76	72/45656 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	0	2
2	B	0	2
2	b	0	2
3	C	0	2
3	c	0	6
4	D	0	4
4	d	0	7
5	E	0	3
5	e	0	4
8	h	0	1
9	I	0	3
9	i	0	1
11	K	0	4
11	k	0	5
All	All	0	47

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	46	LYS	C-N	9.61	1.56	1.34
11	k	16	SER	CA-CB	-7.92	1.41	1.52
11	K	9	GLY	C-O	-7.68	1.11	1.23
11	k	9	GLY	C-O	-7.63	1.11	1.23
3	c	102	SER	C-N	6.87	1.49	1.34
4	d	466	PRO	C-O	-6.54	1.10	1.23
11	k	16	SER	C-O	-6.40	1.11	1.23
4	d	378	ARG	C-O	-6.22	1.11	1.23
3	c	142	ALA	C-N	6.08	1.48	1.34
4	D	229	MET	C-O	-5.96	1.12	1.23
4	D	64	SER	C-N	5.96	1.47	1.34
4	d	279	ASP	C-O	-5.92	1.12	1.23
4	D	279	ASP	C-O	-5.91	1.12	1.23
3	c	128	ALA	C-N	5.77	1.47	1.34
4	d	452	GLN	C-O	-5.71	1.12	1.23
4	d	424	ILE	C-O	-5.63	1.12	1.23
4	D	227	PRO	C-O	-5.62	1.12	1.23
4	D	442	ARG	C-O	-5.46	1.12	1.23
9	i	59	LYS	C-N	5.41	1.46	1.34
5	e	187	ALA	C-O	-5.28	1.13	1.23
4	d	442	ARG	C-O	-5.17	1.13	1.23
5	e	249	ALA	CA-CB	-5.17	1.41	1.52
11	k	8	SER	C-O	5.14	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	249	ALA	CA-CB	-5.10	1.41	1.52
5	e	183	ARG	C-O	-5.10	1.13	1.23
11	K	8	SER	C-O	5.09	1.33	1.23
4	D	64	SER	CA-CB	-5.03	1.45	1.52

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	i	60	TYR	N-CA-CB	-11.63	89.66	110.60
4	D	442	ARG	CB-CG-CD	-11.47	81.77	111.60
3	c	118	THR	CB-CA-C	-10.53	83.16	111.60
4	d	425	PRO	N-CA-CB	-10.39	90.83	103.30
1	a	2	THR	CB-CA-C	-10.18	84.11	111.60
11	K	28	PRO	N-CA-CB	-10.14	91.13	103.30
1	a	260	ASN	CB-CA-C	-9.25	91.91	110.40
1	A	260	ASN	CB-CA-C	-8.54	93.31	110.40
6	f	62	GLN	CA-CB-CG	8.32	131.71	113.40
1	A	171	ASP	CB-CG-OD1	8.20	125.68	118.30
1	A	322	GLN	CB-CA-C	7.53	125.45	110.40
1	a	322	GLN	CB-CA-C	7.47	125.34	110.40
2	b	179	PRO	N-CA-CB	-7.43	94.38	103.30
2	B	180	TYR	CB-CA-C	-7.24	95.93	110.40
2	B	183	PRO	N-CA-C	7.21	130.85	112.10
9	I	38	GLN	CB-CA-C	7.13	124.66	110.40
11	k	43	LEU	N-CA-CB	-7.09	96.22	110.40
4	d	450	TYR	O-C-N	-7.07	111.39	122.70
9	i	60	TYR	CA-CB-CG	7.06	126.81	113.40
11	k	7	ARG	CB-CA-C	6.82	124.03	110.40
1	a	2	THR	N-CA-C	6.69	129.06	111.00
11	K	46	LYS	O-C-N	6.66	133.35	122.70
11	k	16	SER	N-CA-CB	-6.51	100.73	110.50
5	E	241	ARG	CB-CA-C	6.48	123.37	110.40
11	K	8	SER	C-N-CA	-6.48	108.69	122.30
11	k	8	SER	C-N-CA	-6.48	108.70	122.30
3	C	195	LEU	CA-CB-CG	6.47	130.19	115.30
2	B	183	PRO	CB-CA-C	-6.44	95.91	112.00
3	c	118	THR	N-CA-CB	6.39	122.43	110.30
2	b	126	HIS	CB-CA-C	6.37	123.14	110.40
11	K	7	ARG	CB-CA-C	6.27	122.93	110.40
10	J	41	ILE	CG1-CB-CG2	-6.27	97.61	111.40
5	e	77	LEU	CA-CB-CG	6.25	129.67	115.30
5	E	77	LEU	CA-CB-CG	6.24	129.66	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	e	246	LEU	CA-CB-CG	6.21	129.58	115.30
5	E	246	LEU	CA-CB-CG	6.20	129.56	115.30
9	I	18	THR	N-CA-CB	6.11	121.91	110.30
4	d	425	PRO	CA-N-CD	6.08	120.21	111.70
4	D	269	ARG	N-CA-CB	-6.05	99.71	110.60
3	c	93	ARG	CB-CA-C	5.94	122.28	110.40
2	B	303	LEU	CB-CG-CD2	-5.91	100.96	111.00
2	B	321	ALA	CB-CA-C	5.89	118.93	110.10
4	d	269	ARG	N-CA-CB	-5.88	100.01	110.60
11	K	28	PRO	CB-CA-C	5.86	126.66	112.00
5	e	249	ALA	N-CA-CB	-5.85	101.91	110.10
11	K	42	VAL	N-CA-C	-5.83	95.25	111.00
4	D	278	ARG	CB-CG-CD	-5.80	96.53	111.60
5	E	249	ALA	N-CA-CB	-5.76	102.03	110.10
3	c	270	LEU	CA-CB-CG	5.72	128.45	115.30
1	a	137	GLN	N-CA-CB	-5.68	100.38	110.60
4	d	442	ARG	CB-CG-CD	-5.68	96.83	111.60
11	K	36	ALA	O-C-N	5.64	131.72	122.70
3	c	139	SER	N-CA-CB	5.58	118.88	110.50
2	B	183	PRO	N-CD-CG	-5.58	94.83	103.20
11	k	44	ASP	N-CA-CB	5.58	120.64	110.60
2	B	275	LEU	CA-CB-CG	5.55	128.07	115.30
3	c	117	ILE	O-C-N	-5.51	113.89	122.70
2	b	275	LEU	CA-CB-CG	5.48	127.91	115.30
11	k	16	SER	N-CA-C	5.37	125.51	111.00
5	e	73	ASP	CB-CG-OD1	5.34	123.10	118.30
5	E	73	ASP	CB-CG-OD1	5.29	123.06	118.30
11	K	38	SER	N-CA-C	-5.18	97.00	111.00
4	d	66	GLN	N-CA-CB	-5.16	101.31	110.60
2	B	180	TYR	CA-CB-CG	-5.11	103.69	113.40
2	b	172	LEU	CA-CB-CG	5.11	127.06	115.30
5	E	251	ALA	CB-CA-C	5.06	117.69	110.10
11	k	48	SER	CB-CA-C	5.05	119.70	110.10
9	i	37	ASP	N-CA-C	-5.04	97.38	111.00
2	B	193	ALA	N-CA-C	-5.02	97.44	111.00
3	c	142	ALA	O-C-N	5.02	130.73	122.70
2	b	179	PRO	N-CA-C	5.00	125.11	112.10
5	e	247	SER	C-N-CA	-5.00	111.79	122.30

There are no chirality outliers.

All (47) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	ARG	Sidechain
2	B	187	ARG	Sidechain
2	B	323	ARG	Sidechain
3	C	231	PHE	Peptide
3	C	247	GLY	Peptide
4	D	269	ARG	Sidechain
4	D	276	ARG	Sidechain
4	D	278	ARG	Sidechain
4	D	442	ARG	Mainchain
5	E	236	ARG	Sidechain
5	E	246	LEU	Peptide
5	E	36	GLN	Peptide
9	I	17	ARG	Sidechain
9	I	35	ALA	Mainchain
9	I	58	HIS	Mainchain
11	K	26	LEU	Mainchain
11	K	27	ARG	Sidechain
11	K	52	ARG	Sidechain
11	K	7	ARG	Sidechain
1	a	177	ARG	Sidechain
1	a	2	THR	Mainchain
2	b	229	ARG	Sidechain
2	b	318	ARG	Sidechain
3	c	117	ILE	Mainchain
3	c	136	PHE	Mainchain
3	c	169	TRP	Peptide
3	c	179	ARG	Sidechain
3	c	93	ARG	Sidechain
3	c	99	SER	Mainchain
4	d	226	ALA	Peptide
4	d	269	ARG	Sidechain
4	d	276	ARG	Sidechain
4	d	422	ARG	Sidechain
4	d	423	ARG	Sidechain
4	d	442	ARG	Mainchain,Sidechain
5	e	183	ARG	Sidechain
5	e	241	ARG	Sidechain
5	e	246	LEU	Peptide
5	e	36	GLN	Peptide
8	h	45	CYS	Peptide
9	i	17	ARG	Sidechain
11	k	27	ARG	Sidechain
11	k	34	LEU	Peptide

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Mol	Chain	Res	Type	Group
11	k	35	PRO	Peptide
11	k	47	ARG	Sidechain
11	k	7	ARG	Sidechain

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	A	376/378 (100%)	370 (98%)	6 (2%)	0	100	100
1	a	376/378 (100%)	368 (98%)	8 (2%)	0	100	100
2	B	239/241 (99%)	209 (87%)	27 (11%)	3 (1%)	10	9
2	b	237/241 (98%)	210 (89%)	24 (10%)	3 (1%)	10	9
3	C	192/196 (98%)	164 (85%)	28 (15%)	0	100	100
3	c	194/196 (99%)	148 (76%)	46 (24%)	0	100	100
4	D	443/446 (99%)	430 (97%)	13 (3%)	0	100	100
4	d	444/446 (100%)	420 (95%)	24 (5%)	0	100	100
5	E	416/418 (100%)	405 (97%)	11 (3%)	0	100	100
5	e	416/418 (100%)	405 (97%)	10 (2%)	1 (0%)	44	53
6	F	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
6	f	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
7	G	104/106 (98%)	103 (99%)	1 (1%)	0	100	100
7	g	104/106 (98%)	103 (99%)	1 (1%)	0	100	100
8	H	69/79 (87%)	66 (96%)	3 (4%)	0	100	100
8	h	77/79 (98%)	70 (91%)	7 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	60/62 (97%)	47 (78%)	13 (22%)	0	100	100
9	i	60/62 (97%)	48 (80%)	12 (20%)	0	100	100
10	J	47/52 (90%)	44 (94%)	3 (6%)	0	100	100
10	j	49/52 (94%)	45 (92%)	4 (8%)	0	100	100
11	K	55/57 (96%)	42 (76%)	13 (24%)	0	100	100
11	k	55/57 (96%)	40 (73%)	15 (27%)	0	100	100
All	All	4137/4198 (98%)	3856 (93%)	274 (7%)	7 (0%)	45	53

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	241	GLN
2	B	179	PRO
2	B	185	ALA
5	e	185	ALA
2	b	239	PRO
2	B	182	ASN
2	b	179	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	331/331 (100%)	324 (98%)	7 (2%)	48	62
1	a	331/331 (100%)	322 (97%)	9 (3%)	40	52
2	B	206/206 (100%)	200 (97%)	6 (3%)	37	49
2	b	204/206 (99%)	197 (97%)	7 (3%)	32	43
3	C	164/166 (99%)	152 (93%)	12 (7%)	11	13
3	c	165/166 (99%)	140 (85%)	25 (15%)	2	1
4	D	371/372 (100%)	362 (98%)	9 (2%)	44	57
4	d	372/372 (100%)	366 (98%)	6 (2%)	58	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	E	327/328 (100%)	324 (99%)	3 (1%)	75 85
5	e	327/328 (100%)	322 (98%)	5 (2%)	60 73
6	F	61/61 (100%)	46 (75%)	15 (25%)	0 0
6	f	61/61 (100%)	47 (77%)	14 (23%)	0 0
7	G	95/95 (100%)	94 (99%)	1 (1%)	70 80
7	g	95/95 (100%)	94 (99%)	1 (1%)	70 80
8	H	65/70 (93%)	63 (97%)	2 (3%)	35 47
8	h	70/70 (100%)	69 (99%)	1 (1%)	62 75
9	I	50/50 (100%)	36 (72%)	14 (28%)	0 0
9	i	50/50 (100%)	36 (72%)	14 (28%)	0 0
10	J	40/42 (95%)	40 (100%)	0	100 100
10	j	41/42 (98%)	41 (100%)	0	100 100
11	K	44/44 (100%)	31 (70%)	13 (30%)	0 0
11	k	44/44 (100%)	33 (75%)	11 (25%)	0 0
All	All	3514/3530 (100%)	3339 (95%)	175 (5%)	23 28

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	SER
1	A	137	GLN
1	A	150	LEU
1	A	171	ASP
1	A	177	ARG
1	A	260	ASN
1	A	326	TRP
2	B	144	GLU
2	B	162	ASP
2	B	165	MET
2	B	168	ARG
2	B	187	ARG
2	B	245	MET
3	C	101	LYS
3	C	103	SER
3	C	104	LYS
3	C	120	THR
3	C	140	MET

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Mol	Chain	Res	Type
3	C	180	THR
3	C	201	ASP
3	C	207	LYS
3	C	222	CYS
3	C	225	ILE
3	C	227	ASN
3	C	231	PHE
4	D	64	SER
4	D	85	LYS
4	D	138	LYS
4	D	195	THR
4	D	225	LYS
4	D	269	ARG
4	D	276	ARG
4	D	278	ARG
4	D	279	ASP
5	E	236	ARG
5	E	250	LYS
5	E	349	ASP
6	F	38	GLU
6	F	39	GLN
6	F	41	GLU
6	F	44	ILE
6	F	49	ARG
6	F	51	GLU
6	F	56	ARG
6	F	58	SER
6	F	59	SER
6	F	61	SER
6	F	62	GLN
6	F	63	THR
6	F	65	GLU
6	F	68	THR
6	F	91	LYS
7	G	67	LEU
8	H	33	LYS
8	H	45	CYS
9	I	5	THR
9	I	6	LEU
9	I	12	SER
9	I	14	LEU
9	I	16	ARG

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Mol	Chain	Res	Type
9	I	17	ARG
9	I	19	SER
9	I	20	THR
9	I	34	ARG
9	I	37	ASP
9	I	38	GLN
9	I	59	LYS
9	I	62	ASN
9	I	63	LYS
11	K	7	ARG
11	K	11	PHE
11	K	22	VAL
11	K	27	ARG
11	K	28	PRO
11	K	34	LEU
11	K	38	SER
11	K	40	SER
11	K	41	PRO
11	K	43	LEU
11	K	52	ARG
11	K	53	GLU
11	K	55	LEU
1	a	2	THR
1	a	64	SER
1	a	150	LEU
1	a	169	SER
1	a	171	ASP
1	a	172	LYS
1	a	177	ARG
1	a	260	ASN
1	a	326	TRP
2	b	86	THR
2	b	87	ASP
2	b	88	LEU
2	b	89	GLU
2	b	124	SER
2	b	179	PRO
2	b	318	ARG
3	c	93	ARG
3	c	96	VAL
3	c	100	THR
3	c	101	LYS

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Mol	Chain	Res	Type
3	c	103	SER
3	c	118	THR
3	c	120	THR
3	c	125	VAL
3	c	127	TYR
3	c	130	LYS
3	c	138	SER
3	c	139	SER
3	c	143	SER
3	c	145	ASP
3	c	146	VAL
3	c	147	LEU
3	c	155	LYS
3	c	156	LEU
3	c	158	ASP
3	c	170	ARG
3	c	179	ARG
3	c	180	THR
3	c	183	GLU
3	c	217	CYS
3	c	238	CYS
4	d	92	PHE
4	d	269	ARG
4	d	423	ARG
4	d	442	ARG
4	d	451	ASP
4	d	452	GLN
5	e	170	GLN
5	e	186	LEU
5	e	241	ARG
5	e	250	LYS
5	e	349	ASP
6	f	38	GLU
6	f	39	GLN
6	f	41	GLU
6	f	44	ILE
6	f	49	ARG
6	f	51	GLU
6	f	56	ARG
6	f	58	SER
6	f	59	SER
6	f	61	SER

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Mol	Chain	Res	Type
6	f	63	THR
6	f	65	GLU
6	f	68	THR
6	f	91	LYS
7	g	67	LEU
8	h	9	THR
9	i	5	THR
9	i	6	LEU
9	i	12	SER
9	i	14	LEU
9	i	16	ARG
9	i	17	ARG
9	i	19	SER
9	i	20	THR
9	i	23	LEU
9	i	24	THR
9	i	34	ARG
9	i	37	ASP
9	i	59	LYS
9	i	63	LYS
11	k	7	ARG
11	k	11	PHE
11	k	15	LEU
11	k	22	VAL
11	k	44	ASP
11	k	47	ARG
11	k	48	SER
11	k	51	CYS
11	k	52	ARG
11	k	53	GLU
11	k	54	SER

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

Mol	Chain	Res	Type
1	A	137	GLN
1	A	255	ASN
2	B	182	ASN
2	B	241	GLN
2	B	266	GLN
3	C	164	ASN
3	C	219	HIS

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Mol	Chain	Res	Type
4	D	66	GLN
4	D	95	HIS
4	D	152	GLN
4	D	153	ASN
4	D	222	GLN
4	D	305	GLN
5	E	75	ASN
5	E	155	GLN
5	E	268	HIS
5	E	290	GLN
5	E	399	GLN
10	J	16	ASN
1	a	114	ASN
1	a	255	ASN
1	a	260	ASN
2	b	283	HIS
3	c	199	GLN
3	c	257	ASN
4	d	49	GLN
4	d	55	ASN
4	d	153	ASN
4	d	222	GLN
4	d	286	HIS
4	d	452	GLN
4	d	469	ASN
5	e	75	ASN
5	e	155	GLN
5	e	168	ASN
5	e	170	GLN
5	e	268	HIS
5	e	290	GLN
5	e	399	GLN
8	h	80	ASN

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 (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

18 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	$\#\|Z\| > 2$
13	HEM	a	404	1	41,50,50	1.48	7 (17%)	45,82,82	1.59	8 (17%)
14	PEE	D	501	-	48,48,50	0.42	0	51,53,55	0.60	1 (1%)
12	A1D6O	A	402	-	27,30,30	1.28	3 (11%)	27,44,44	2.90	9 (33%)
15	CDL	A	406	-	63,63,99	1.09	8 (12%)	69,75,111	1.09	4 (5%)
15	CDL	a	406	-	63,63,99	1.10	6 (9%)	69,75,111	1.07	4 (5%)
13	HEM	a	403	1	41,50,50	1.56	6 (14%)	45,82,82	1.52	10 (22%)
16	HEC	B	401	2	32,50,50	2.12	11 (34%)	24,82,82	3.03	10 (41%)
17	FES	C	301	-	0,4,4	-	-	-		
15	CDL	a	407	-	63,63,99	1.07	6 (9%)	69,75,111	1.12	6 (8%)
17	FES	c	301	-	0,4,4	-	-	-		
14	PEE	A	405	-	44,44,50	0.79	2 (4%)	46,49,55	0.84	2 (4%)
12	A1D6O	a	401	-	27,30,30	1.45	4 (14%)	27,44,44	3.47	12 (44%)
16	HEC	b	401	2	32,50,50	2.10	10 (31%)	24,82,82	3.06	10 (41%)
13	HEM	A	404	1	41,50,50	1.61	5 (12%)	45,82,82	2.04	16 (35%)
14	PEE	a	405	-	48,48,50	0.81	2 (4%)	51,53,55	0.85	2 (3%)
13	HEM	A	403	1	41,50,50	1.47	7 (17%)	45,82,82	1.58	8 (17%)
12	A1D6O	A	401	-	27,30,30	1.45	3 (11%)	27,44,44	3.47	12 (44%)
12	A1D6O	a	402	-	27,30,30	1.28	3 (11%)	27,44,44	2.90	9 (33%)

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
13	HEM	a	404	1	-	2/12/54/54	-
14	PEE	D	501	-	-	34/52/52/54	-
12	A1D6O	A	402	-	-	0/7/9/9	0/4/4/4
15	CDL	A	406	-	-	33/74/74/110	-
15	CDL	a	406	-	-	46/74/74/110	-
13	HEM	a	403	1	-	5/12/54/54	-
16	HEC	B	401	2	-	0/10/54/54	-
17	FES	C	301	-	-	-	0/1/1/1
15	CDL	a	407	-	-	44/74/74/110	-
17	FES	c	301	-	-	-	0/1/1/1
14	PEE	A	405	-	-	23/48/48/54	-
12	A1D6O	a	401	-	-	1/7/9/9	0/4/4/4
16	HEC	b	401	2	-	0/10/54/54	-
13	HEM	A	404	1	-	6/12/54/54	-
14	PEE	a	405	-	-	27/52/52/54	-
13	HEM	A	403	1	-	2/12/54/54	-
12	A1D6O	A	401	-	-	1/7/9/9	0/4/4/4
12	A1D6O	a	402	-	-	0/7/9/9	0/4/4/4

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	b	401	HEC	C2B-C3B	6.22	1.47	1.40
16	B	401	HEC	C2B-C3B	6.20	1.47	1.40
16	B	401	HEC	C3C-C2C	5.38	1.46	1.40
16	b	401	HEC	C3C-C2C	5.19	1.46	1.40
12	A	401	A1D6O	C08-S10	4.53	1.83	1.74
12	a	401	A1D6O	C08-S10	4.51	1.83	1.74
13	A	404	HEM	C3C-C2C	-4.19	1.34	1.40
13	a	403	HEM	C3C-C2C	-4.17	1.34	1.40
13	A	403	HEM	C3C-CAC	3.99	1.56	1.47
13	a	404	HEM	C3C-CAC	3.98	1.56	1.47
12	A	402	A1D6O	C08-S10	3.90	1.81	1.74
12	a	402	A1D6O	C08-S10	3.87	1.81	1.74
13	a	403	HEM	C3C-CAC	3.73	1.55	1.47
13	A	404	HEM	C3C-CAC	3.72	1.55	1.47
13	a	404	HEM	C3C-C2C	-3.54	1.35	1.40
13	A	403	HEM	C3C-C2C	-3.45	1.35	1.40
15	a	406	CDL	OA6-CA4	-3.30	1.38	1.46
16	b	401	HEC	C3D-C2D	3.18	1.47	1.37
16	b	401	HEC	C2A-C3A	3.17	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	401	HEC	C2A-C3A	3.12	1.46	1.37
16	B	401	HEC	C3D-C2D	3.08	1.46	1.37
13	a	404	HEM	CAB-C3B	3.08	1.55	1.47
13	A	403	HEM	CAB-C3B	3.07	1.55	1.47
13	a	403	HEM	CAB-C3B	3.05	1.55	1.47
13	A	404	HEM	CAB-C3B	3.03	1.55	1.47
16	b	401	HEC	C4D-CHA	2.91	1.49	1.41
13	A	404	HEM	FE-ND	2.86	2.11	1.96
16	B	401	HEC	C4D-CHA	2.83	1.48	1.41
15	a	407	CDL	OA6-CA4	-2.70	1.39	1.46
16	B	401	HEC	O2D-CGD	-2.68	1.21	1.30
15	a	407	CDL	OB6-CB5	2.64	1.41	1.34
16	b	401	HEC	O2D-CGD	-2.63	1.21	1.30
13	a	403	HEM	FE-ND	2.62	2.09	1.96
16	B	401	HEC	C1B-CHB	2.58	1.48	1.41
16	b	401	HEC	C1B-CHB	2.58	1.48	1.41
12	a	401	A1D6O	O24-C23	-2.58	1.17	1.22
12	A	401	A1D6O	O24-C23	-2.57	1.17	1.22
12	A	401	A1D6O	C11-C12	2.56	1.55	1.51
14	A	405	PEE	C12-C11	-2.56	1.42	1.52
14	a	405	PEE	C12-C11	-2.56	1.42	1.52
15	a	406	CDL	OA8-CA6	-2.55	1.39	1.45
12	a	401	A1D6O	C11-C12	2.54	1.55	1.51
15	a	406	CDL	OB6-CB4	-2.54	1.40	1.46
15	A	406	CDL	OA8-CA7	2.47	1.40	1.33
12	a	402	A1D6O	O24-C23	-2.43	1.18	1.22
16	b	401	HEC	C2A-C1A	2.41	1.48	1.42
12	a	402	A1D6O	C13-N19	2.40	1.46	1.43
15	A	406	CDL	OA6-CA5	2.39	1.41	1.34
12	A	402	A1D6O	O24-C23	-2.39	1.18	1.22
16	B	401	HEC	C2A-C1A	2.38	1.47	1.42
12	A	402	A1D6O	C13-N19	2.37	1.46	1.43
13	A	404	HEM	FE-NB	2.36	2.08	1.96
15	a	406	CDL	OB8-CB7	2.35	1.40	1.33
15	A	406	CDL	OB8-CB7	2.35	1.40	1.33
15	a	407	CDL	OB8-CB7	2.34	1.40	1.33
14	a	405	PEE	O4-C10	-2.34	1.15	1.22
15	A	406	CDL	OB6-CB4	-2.33	1.40	1.46
15	A	406	CDL	OB8-CB6	-2.32	1.39	1.45
15	A	406	CDL	OA6-CA4	-2.29	1.40	1.46
13	a	404	HEM	FE-ND	2.24	2.07	1.96
15	a	407	CDL	OA8-CA7	2.23	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	401	HEC	C1C-CHC	2.22	1.47	1.41
15	a	406	CDL	OB6-CB5	2.21	1.40	1.34
13	A	403	HEM	FE-ND	2.19	2.07	1.96
13	a	403	HEM	FE-NB	2.19	2.07	1.96
15	A	406	CDL	OA8-CA6	-2.17	1.40	1.45
16	b	401	HEC	C1C-CHC	2.17	1.47	1.41
15	A	406	CDL	OB6-CB5	2.17	1.40	1.34
13	a	404	HEM	CAA-C2A	2.16	1.55	1.52
14	A	405	PEE	O4-C10	-2.16	1.16	1.22
15	a	407	CDL	OA8-CA6	-2.15	1.40	1.45
15	a	407	CDL	OA6-CA5	2.14	1.40	1.34
13	a	404	HEM	CMD-C2D	2.13	1.55	1.50
13	A	403	HEM	CAA-C2A	2.13	1.55	1.52
13	A	403	HEM	CMD-C2D	2.10	1.55	1.50
15	a	406	CDL	OA8-CA7	2.09	1.39	1.33
16	B	401	HEC	O2A-CGA	-2.06	1.23	1.30
16	b	401	HEC	O2A-CGA	-2.06	1.23	1.30
13	A	403	HEM	CMB-C2B	2.04	1.55	1.50
16	B	401	HEC	C4B-C3B	2.04	1.46	1.43
13	a	404	HEM	CMB-C2B	2.03	1.55	1.50
12	a	401	A1D6O	N19-N20	-2.01	1.34	1.36
13	a	403	HEM	CAA-C2A	2.01	1.55	1.52

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	401	A1D6O	C11-S10-C08	12.77	112.14	101.20
12	a	401	A1D6O	C11-S10-C08	12.77	112.14	101.20
16	b	401	HEC	CBD-CAD-C3D	-7.83	99.26	112.62
16	B	401	HEC	CBD-CAD-C3D	-7.74	99.40	112.62
12	a	402	A1D6O	C11-S10-C08	7.23	107.39	101.20
12	A	402	A1D6O	C11-S10-C08	7.22	107.39	101.20
16	b	401	HEC	C1D-C2D-C3D	-6.37	102.56	107.00
16	B	401	HEC	C1D-C2D-C3D	-6.34	102.59	107.00
12	a	402	A1D6O	C06-C01-C02	-6.07	119.42	123.17
12	A	402	A1D6O	C06-C01-C02	-6.03	119.44	123.17
12	a	401	A1D6O	C12-C11-S10	5.72	119.64	107.94
12	A	401	A1D6O	C12-C11-S10	5.69	119.58	107.94
16	B	401	HEC	CMC-C2C-C3C	5.68	132.50	125.82
13	A	404	HEM	CAD-C3D-C4D	5.63	134.49	124.66
16	b	401	HEC	CMC-C2C-C3C	5.60	132.41	125.82
12	A	402	A1D6O	C03-C04-S07	5.16	135.43	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	402	A1D6O	C03-C04-S07	5.15	135.40	125.10
12	A	401	A1D6O	C03-C04-S07	5.11	135.32	125.10
12	a	401	A1D6O	C03-C04-S07	5.11	135.32	125.10
12	a	402	A1D6O	C14-C13-N19	-5.11	112.23	119.08
12	A	402	A1D6O	C14-C13-N19	-5.09	112.25	119.08
12	a	401	A1D6O	C05-C04-S07	-4.99	104.62	112.46
12	A	401	A1D6O	C05-C04-S07	-4.98	104.64	112.46
13	A	404	HEM	CAD-C3D-C2D	-4.97	118.62	127.88
16	b	401	HEC	CMB-C2B-C3B	4.86	131.54	125.82
16	B	401	HEC	CMB-C2B-C3B	4.85	131.52	125.82
12	a	401	A1D6O	C06-C01-C02	-4.73	120.24	123.17
12	A	401	A1D6O	C06-C01-C02	-4.72	120.25	123.17
12	A	402	A1D6O	C05-C04-S07	-4.52	105.35	112.46
12	a	402	A1D6O	C05-C04-S07	-4.52	105.36	112.46
16	B	401	HEC	CAA-CBA-CGA	-4.24	101.88	113.76
15	A	406	CDL	OB6-CB5-C51	4.11	120.37	111.50
16	b	401	HEC	CAA-CBA-CGA	-4.04	102.43	113.76
15	a	406	CDL	OB6-CB5-C51	3.83	119.77	111.50
15	a	407	CDL	OB6-CB5-C51	3.80	119.69	111.50
13	a	404	HEM	C1B-NB-C4B	3.79	108.99	105.07
13	A	403	HEM	C1B-NB-C4B	3.76	108.96	105.07
12	A	402	A1D6O	C12-C11-S10	3.71	115.53	107.94
12	a	402	A1D6O	C12-C11-S10	3.70	115.50	107.94
13	A	404	HEM	C4D-ND-C1D	3.58	108.77	105.07
15	A	406	CDL	OA6-CA5-C11	3.55	119.15	111.50
15	a	407	CDL	OA6-CA5-C11	3.54	119.13	111.50
13	a	404	HEM	C4D-ND-C1D	3.53	108.72	105.07
13	A	403	HEM	C4D-ND-C1D	3.47	108.65	105.07
13	a	404	HEM	C4B-CHC-C1C	3.32	126.94	122.56
13	A	403	HEM	C4B-CHC-C1C	3.32	126.94	122.56
12	A	402	A1D6O	N19-N20-N21	3.29	110.85	107.01
16	b	401	HEC	CMA-C3A-C2A	3.26	131.10	124.94
16	b	401	HEC	CMD-C2D-C3D	3.22	131.01	124.94
12	a	402	A1D6O	N19-N20-N21	3.22	110.77	107.01
13	A	404	HEM	CHA-C4D-C3D	3.20	131.33	125.33
14	a	405	PEE	O2P-P-O4P	-3.16	93.08	107.75
16	B	401	HEC	CMA-C3A-C2A	3.09	130.76	124.94
13	A	403	HEM	C4C-CHD-C1D	3.09	126.63	122.56
13	a	403	HEM	C4D-ND-C1D	3.07	108.25	105.07
13	a	404	HEM	C4C-CHD-C1D	3.07	126.61	122.56
14	a	405	PEE	O4P-P-O1P	3.03	120.92	109.07
13	A	404	HEM	C4C-CHD-C1D	3.00	126.51	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	403	HEM	CMC-C2C-C3C	2.93	130.15	124.68
13	A	404	HEM	CMC-C2C-C3C	2.87	130.04	124.68
12	a	402	A1D6O	C25-N22-N21	2.86	126.21	121.14
12	A	402	A1D6O	C25-N22-N21	2.85	126.20	121.14
15	a	407	CDL	CB4-OB6-CB5	2.84	124.79	117.79
13	a	403	HEM	C1B-NB-C4B	2.84	108.01	105.07
12	a	401	A1D6O	C25-N22-N21	2.84	126.18	121.14
12	A	401	A1D6O	C25-N22-N21	2.83	126.16	121.14
16	B	401	HEC	CMD-C2D-C3D	2.82	130.26	124.94
15	a	406	CDL	OB8-CB7-C71	2.80	120.71	111.91
13	A	404	HEM	C1B-NB-C4B	2.80	107.96	105.07
13	A	404	HEM	CBD-CAD-C3D	2.76	120.29	112.63
12	a	402	A1D6O	C16-C17-C12	2.75	121.58	118.41
12	A	402	A1D6O	C16-C17-C12	2.74	121.57	118.41
13	A	404	HEM	C3D-C4D-ND	-2.71	107.15	110.17
13	a	403	HEM	C4A-C3A-C2A	2.60	108.81	107.00
13	a	403	HEM	C4C-CHD-C1D	2.56	125.93	122.56
15	a	407	CDL	OA8-CA7-C31	2.54	119.89	111.91
13	a	404	HEM	CMC-C2C-C3C	2.54	129.43	124.68
15	A	406	CDL	OA8-CA7-C31	2.54	119.87	111.91
13	A	403	HEM	CMC-C2C-C3C	2.52	129.40	124.68
12	a	401	A1D6O	C14-C13-N19	-2.51	115.71	119.08
15	a	406	CDL	OA6-CA5-C11	2.50	116.90	111.50
14	A	405	PEE	O2P-P-O4P	2.48	119.25	107.75
12	A	401	A1D6O	C14-C13-N19	-2.47	115.77	119.08
13	A	404	HEM	C4A-C3A-C2A	2.47	108.71	107.00
15	a	406	CDL	OA8-CA7-C31	2.44	119.55	111.91
15	A	406	CDL	OB8-CB7-C71	2.43	119.54	111.91
13	a	403	HEM	CMA-C3A-C4A	-2.42	124.74	128.46
13	A	403	HEM	CMB-C2B-C1B	-2.40	121.38	125.04
13	a	404	HEM	CMB-C2B-C1B	-2.38	121.42	125.04
12	a	401	A1D6O	C13-N19-N20	2.37	124.67	120.39
14	A	405	PEE	O3P-P-O1P	-2.36	99.84	109.07
13	A	404	HEM	CMA-C3A-C4A	-2.36	124.84	128.46
12	A	401	A1D6O	C13-N19-N20	2.35	124.64	120.39
13	a	403	HEM	CBA-CAA-C2A	-2.33	108.64	112.62
13	A	404	HEM	CBA-CAA-C2A	-2.33	108.65	112.62
13	a	403	HEM	C4B-CHC-C1C	2.32	125.62	122.56
13	A	404	HEM	CHA-C4D-ND	-2.32	121.52	124.38
16	B	401	HEC	O2A-CGA-CBA	2.30	121.43	114.03
13	A	404	HEM	C1D-C2D-C3D	2.30	109.38	106.96
12	a	401	A1D6O	C18-C17-C16	-2.30	115.82	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	D	501	PEE	O2P-P-O4P	-2.30	97.07	107.75
12	A	401	A1D6O	C18-C17-C16	-2.29	115.84	120.31
13	a	403	HEM	C3D-C4D-ND	-2.28	107.62	110.17
13	A	404	HEM	C4B-CHC-C1C	2.28	125.56	122.56
12	a	401	A1D6O	C11-C12-C17	2.27	121.94	119.58
12	A	401	A1D6O	C11-C12-C17	2.27	121.94	119.58
16	b	401	HEC	O2A-CGA-CBA	2.26	121.30	114.03
16	B	401	HEC	O1A-CGA-CBA	-2.22	115.95	123.08
16	B	401	HEC	C3B-C4B-NB	2.20	115.11	110.94
13	a	404	HEM	C3D-C4D-ND	-2.20	107.72	110.17
16	b	401	HEC	C3B-C4B-NB	2.20	115.09	110.94
15	a	407	CDL	OB8-CB7-C71	2.19	118.79	111.91
16	b	401	HEC	O1A-CGA-CBA	-2.19	116.05	123.08
13	A	403	HEM	C3D-C4D-ND	-2.15	107.78	110.17
12	a	401	A1D6O	N19-N20-N21	2.12	109.49	107.01
12	A	401	A1D6O	N19-N20-N21	2.12	109.49	107.01
15	a	407	CDL	OB6-CB4-CB3	2.12	116.07	108.40
13	a	404	HEM	C2D-C1D-ND	-2.08	107.39	109.88
13	A	403	HEM	C2D-C1D-ND	-2.06	107.42	109.88
13	a	403	HEM	C3B-C2B-C1B	2.05	108.01	106.49
12	a	401	A1D6O	C27-C06-C01	-2.05	117.75	120.74
13	A	404	HEM	C3B-C2B-C1B	2.03	107.99	106.49
12	A	401	A1D6O	C27-C06-C01	-2.01	117.81	120.74

There are no chirality outliers.

All (224) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	404	HEM	C2D-C3D-CAD-CBD
13	A	404	HEM	C4D-C3D-CAD-CBD
14	A	405	PEE	C1-O3P-P-O1P
14	A	405	PEE	C4-O4P-P-O2P
14	A	405	PEE	C4-O4P-P-O1P
14	A	405	PEE	O4P-C4-C5-N
14	D	501	PEE	C11-C10-O2-C2
14	D	501	PEE	O4-C10-O2-C2
14	D	501	PEE	O2-C2-C3-O3
14	D	501	PEE	C2-C1-O3P-P
14	a	405	PEE	C4-O4P-P-O2P
14	a	405	PEE	C4-O4P-P-O1P
14	a	405	PEE	O4P-C4-C5-N
15	A	406	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
15	A	406	CDL	CA2-OA2-PA1-OA4
15	A	406	CDL	CA3-OA5-PA1-OA2
15	a	406	CDL	CA2-OA2-PA1-OA3
15	a	406	CDL	CB3-OB5-PB2-OB3
15	a	406	CDL	OB6-CB4-CB6-OB8
15	a	406	CDL	OB7-CB5-OB6-CB4
15	a	406	CDL	C51-CB5-OB6-CB4
15	a	407	CDL	CB3-OB5-PB2-OB2
15	a	407	CDL	CB3-OB5-PB2-OB3
15	a	407	CDL	CB3-OB5-PB2-OB4
15	a	407	CDL	OB7-CB5-OB6-CB4
14	A	405	PEE	O5-C30-O3-C3
15	a	406	CDL	OB9-CB7-OB8-CB6
14	A	405	PEE	C31-C30-O3-C3
15	a	406	CDL	C71-CB7-OB8-CB6
15	a	407	CDL	C51-CB5-OB6-CB4
15	a	406	CDL	OA9-CA7-OA8-CA6
15	A	406	CDL	O1-C1-CA2-OA2
15	a	406	CDL	C31-CA7-OA8-CA6
15	A	406	CDL	C11-CA5-OA6-CA4
14	a	405	PEE	C22-C23-C24-C25
14	D	501	PEE	C21-C22-C23-C24
15	a	406	CDL	C11-C12-C13-C14
14	D	501	PEE	C40-C41-C42-C43
14	a	405	PEE	C14-C15-C16-C17
15	A	406	CDL	CA2-C1-CB2-OB2
15	a	407	CDL	CA2-C1-CB2-OB2
15	A	406	CDL	OA7-CA5-OA6-CA4
14	a	405	PEE	C31-C30-O3-C3
14	A	405	PEE	C15-C16-C17-C18
14	D	501	PEE	C32-C33-C34-C35
14	D	501	PEE	C17-C18-C19-C20
15	a	406	CDL	CB5-C51-C52-C53
15	a	406	CDL	CA5-C11-C12-C13
14	a	405	PEE	O5-C30-O3-C3
15	A	406	CDL	CA7-C31-C32-C33
15	A	406	CDL	O1-C1-CB2-OB2
15	a	406	CDL	O1-C1-CB2-OB2
15	a	407	CDL	O1-C1-CB2-OB2
14	D	501	PEE	C19-C20-C21-C22
14	A	405	PEE	C1-O3P-P-O4P
14	A	405	PEE	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
14	a	405	PEE	C4-O4P-P-O3P
15	A	406	CDL	CA2-OA2-PA1-OA5
15	a	406	CDL	CA2-C1-CB2-OB2
14	D	501	PEE	C39-C40-C41-C42
15	a	407	CDL	C71-C72-C73-C74
14	A	405	PEE	C20-C21-C22-C23
15	a	407	CDL	C54-C55-C56-C57
15	a	407	CDL	CB3-CB4-OB6-CB5
14	D	501	PEE	C31-C32-C33-C34
15	a	406	CDL	C74-C75-C76-C77
15	a	407	CDL	C11-C12-C13-C14
14	A	405	PEE	C31-C32-C33-C34
14	D	501	PEE	C20-C21-C22-C23
15	A	406	CDL	C33-C34-C35-C36
14	A	405	PEE	C14-C15-C16-C17
15	A	406	CDL	C13-C14-C15-C16
15	a	406	CDL	C12-C13-C14-C15
15	a	407	CDL	C72-C73-C74-C75
14	a	405	PEE	C30-C31-C32-C33
14	A	405	PEE	C11-C12-C13-C14
15	A	406	CDL	C51-C52-C53-C54
15	A	406	CDL	C74-C75-C76-C77
15	a	406	CDL	C13-C14-C15-C16
14	a	405	PEE	C34-C35-C36-C37
14	a	405	PEE	C15-C16-C17-C18
14	D	501	PEE	C30-C31-C32-C33
15	A	406	CDL	CB7-C71-C72-C73
15	a	406	CDL	CA7-C31-C32-C33
15	a	406	CDL	C14-C15-C16-C17
15	a	407	CDL	C53-C54-C55-C56
15	A	406	CDL	C73-C74-C75-C76
14	A	405	PEE	C13-C14-C15-C16
14	D	501	PEE	C11-C12-C13-C14
15	a	406	CDL	C54-C55-C56-C57
15	a	407	CDL	CB7-C71-C72-C73
14	D	501	PEE	C41-C42-C43-C44
15	a	407	CDL	C74-C75-C76-C77
14	A	405	PEE	C19-C20-C21-C22
14	A	405	PEE	C23-C24-C25-C26
14	a	405	PEE	C32-C33-C34-C35
15	a	406	CDL	C34-C35-C36-C37
14	D	501	PEE	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
15	a	406	CDL	C52-C53-C54-C55
15	a	406	CDL	C33-C34-C35-C36
14	a	405	PEE	C37-C38-C39-C40
14	D	501	PEE	C24-C25-C26-C27
15	a	407	CDL	CA7-C31-C32-C33
15	A	406	CDL	C53-C54-C55-C56
15	a	407	CDL	C73-C74-C75-C76
14	D	501	PEE	C10-C11-C12-C13
14	a	405	PEE	C20-C21-C22-C23
15	A	406	CDL	OA5-CA3-CA4-OA6
15	a	406	CDL	OA5-CA3-CA4-OA6
14	a	405	PEE	C19-C20-C21-C22
14	a	405	PEE	C35-C36-C37-C38
14	a	405	PEE	C11-C12-C13-C14
14	D	501	PEE	C37-C38-C39-C40
15	a	406	CDL	CA2-OA2-PA1-OA5
15	a	406	CDL	CB3-OB5-PB2-OB2
14	a	405	PEE	C23-C24-C25-C26
15	a	407	CDL	CA5-C11-C12-C13
15	a	406	CDL	C1-CB2-OB2-PB2
15	A	406	CDL	OA5-CA3-CA4-CA6
15	a	407	CDL	OA5-CA3-CA4-CA6
14	A	405	PEE	C34-C35-C36-C37
14	D	501	PEE	C1-C2-C3-O3
15	a	406	CDL	C15-C16-C17-C18
15	a	407	CDL	C15-C16-C17-C18
14	D	501	PEE	C35-C36-C37-C38
14	A	405	PEE	C24-C25-C26-C27
15	A	406	CDL	C12-C11-CA5-OA6
15	a	406	CDL	C31-C32-C33-C34
14	a	405	PEE	C17-C18-C19-C20
15	a	407	CDL	OA6-CA4-CA6-OA8
15	A	406	CDL	C54-C55-C56-C57
15	a	407	CDL	C71-CB7-OB8-CB6
15	a	407	CDL	CB4-CB3-OB5-PB2
14	D	501	PEE	C12-C13-C14-C15
14	a	405	PEE	C31-C32-C33-C34
13	a	403	HEM	C3D-CAD-CBD-CGD
14	a	405	PEE	C1-C2-C3-O3
15	a	406	CDL	CB3-CB4-CB6-OB8
15	A	406	CDL	C75-C76-C77-C78
15	A	406	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
15	a	406	CDL	C75-C76-C77-C78
14	a	405	PEE	O2-C2-C3-O3
15	a	407	CDL	CB2-C1-CA2-OA2
15	A	406	CDL	C1-CA2-OA2-PA1
15	a	407	CDL	C55-C56-C57-C58
15	A	406	CDL	OB5-CB3-CB4-CB6
14	D	501	PEE	C22-C23-C24-C25
15	a	406	CDL	C73-C74-C75-C76
14	D	501	PEE	C1-C2-O2-C10
15	A	406	CDL	CA6-CA4-OA6-CA5
14	a	405	PEE	C40-C41-C42-C43
15	a	406	CDL	CA4-CA3-OA5-PA1
15	a	406	CDL	CA3-CA4-CA6-OA8
15	a	407	CDL	OA5-CA3-CA4-OA6
14	a	405	PEE	C12-C13-C14-C15
15	a	407	CDL	OB9-CB7-OB8-CB6
15	a	406	CDL	OA6-CA4-CA6-OA8
15	a	407	CDL	OB6-CB4-CB6-OB8
14	A	405	PEE	C32-C33-C34-C35
15	A	406	CDL	C71-C72-C73-C74
14	D	501	PEE	C1-O3P-P-O4P
14	D	501	PEE	C4-O4P-P-O3P
15	a	407	CDL	CB2-OB2-PB2-OB5
15	A	406	CDL	C1-CB2-OB2-PB2
15	a	407	CDL	CA4-CA3-OA5-PA1
14	D	501	PEE	C1-O3P-P-O2P
14	D	501	PEE	C4-O4P-P-O2P
15	A	406	CDL	CA2-OA2-PA1-OA3
15	a	406	CDL	CA2-OA2-PA1-OA4
14	A	405	PEE	C33-C34-C35-C36
14	D	501	PEE	C5-C4-O4P-P
15	a	407	CDL	O1-C1-CA2-OA2
15	a	407	CDL	CA3-CA4-CA6-OA8
15	a	407	CDL	CB3-CB4-CB6-OB8
14	A	405	PEE	C12-C13-C14-C15
15	a	406	CDL	O1-C1-CA2-OA2
14	A	405	PEE	C21-C22-C23-C24
15	a	406	CDL	OA5-CA3-CA4-CA6
15	a	407	CDL	C52-C53-C54-C55
15	a	407	CDL	OA9-CA7-OA8-CA6
15	a	406	CDL	CA3-OA5-PA1-OA2
15	a	406	CDL	CB2-OB2-PB2-OB5

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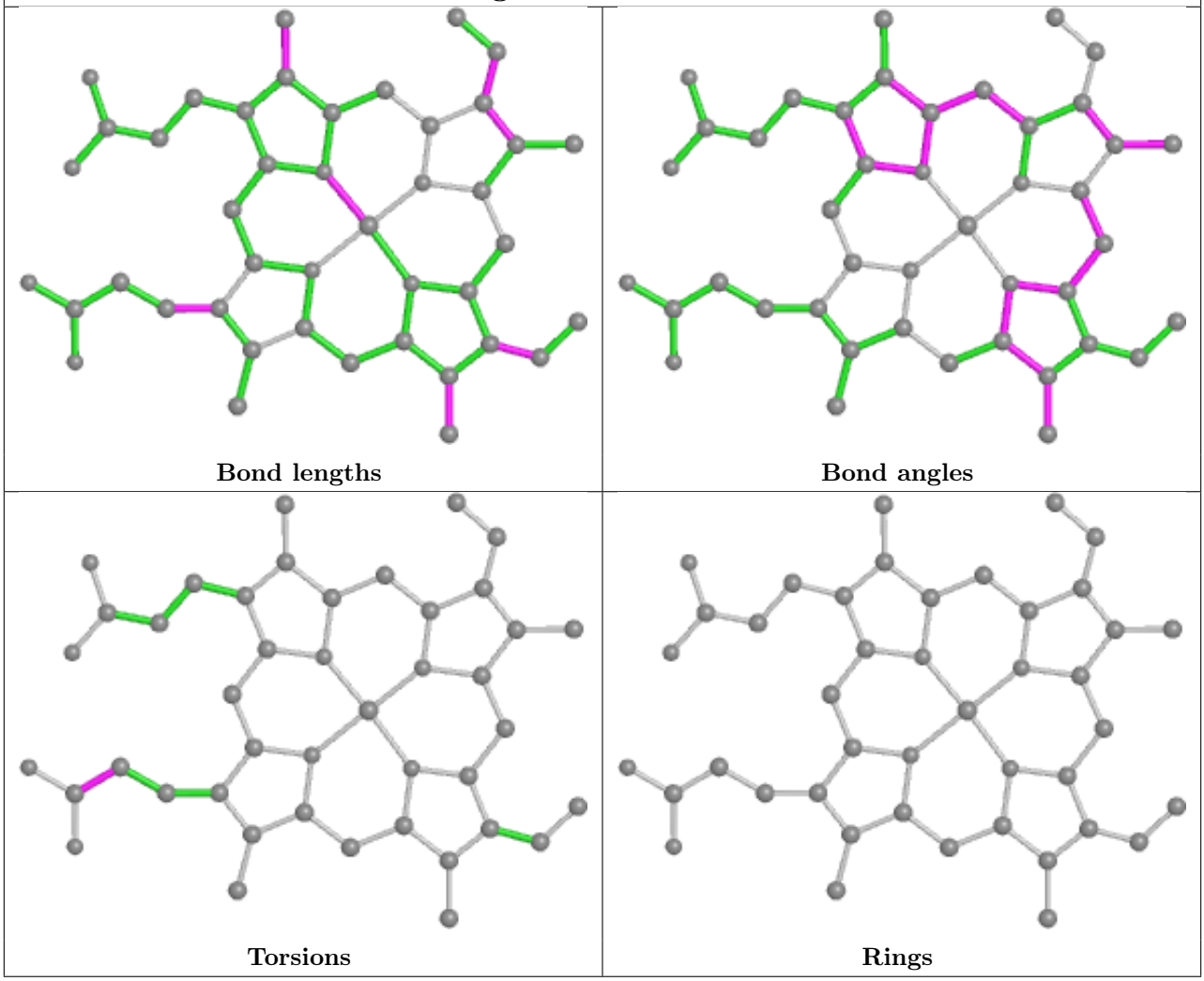
Mol	Chain	Res	Type	Atoms
15	a	407	CDL	CA3-OA5-PA1-OA2
15	a	407	CDL	C32-C33-C34-C35
15	a	407	CDL	C31-CA7-OA8-CA6
15	a	407	CDL	C1-CA2-OA2-PA1
15	A	406	CDL	C12-C11-CA5-OA7
13	a	403	HEM	CAA-CBA-CGA-O1A
14	D	501	PEE	C31-C30-O3-C3
13	A	404	HEM	CAA-CBA-CGA-O1A
14	D	501	PEE	C42-C43-C44-C45
14	D	501	PEE	C16-C17-C18-C19
14	D	501	PEE	O3P-C1-C2-O2
13	A	404	HEM	CAA-CBA-CGA-O2A
13	a	403	HEM	CAA-CBA-CGA-O2A
15	a	407	CDL	C51-C52-C53-C54
15	a	407	CDL	C52-C51-CB5-OB6
13	a	404	HEM	CAA-CBA-CGA-O1A
13	A	403	HEM	CAA-CBA-CGA-O1A
13	A	403	HEM	CAA-CBA-CGA-O2A
13	a	404	HEM	CAA-CBA-CGA-O2A
15	a	407	CDL	C1-CB2-OB2-PB2
15	a	406	CDL	C53-C54-C55-C56
13	a	403	HEM	CAD-CBD-CGD-O1D
15	a	406	CDL	C12-C11-CA5-OA6
15	a	406	CDL	C52-C51-CB5-OB6
14	D	501	PEE	O3P-C1-C2-C3
15	A	406	CDL	OB6-CB4-CB6-OB8
13	a	403	HEM	CAD-CBD-CGD-O2D
14	a	405	PEE	C38-C39-C40-C41
15	a	406	CDL	C32-C31-CA7-OA8
14	A	405	PEE	C16-C17-C18-C19
14	a	405	PEE	C18-C19-C20-C21
12	A	401	A1D6O	S10-C11-C12-C13
12	a	401	A1D6O	S10-C11-C12-C13
15	A	406	CDL	CB3-OB5-PB2-OB4
15	a	407	CDL	CB2-OB2-PB2-OB3
15	a	406	CDL	C52-C51-CB5-OB7
15	a	406	CDL	C12-C11-CA5-OA7
13	A	404	HEM	CAD-CBD-CGD-O2D
14	a	405	PEE	C33-C34-C35-C36
15	a	407	CDL	C72-C71-CB7-OB8
15	A	406	CDL	C72-C73-C74-C75
13	A	404	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

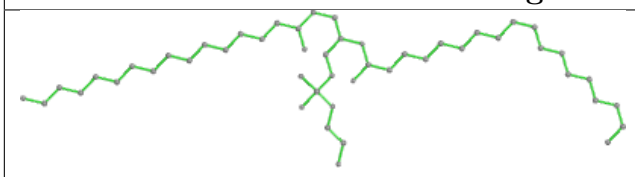
No monomer is involved in short contacts.

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.

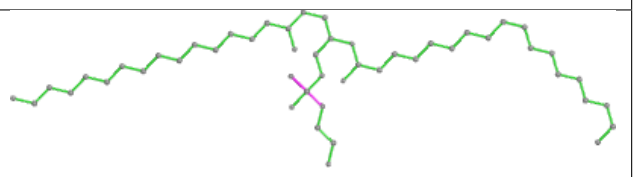
Ligand HEM a 404



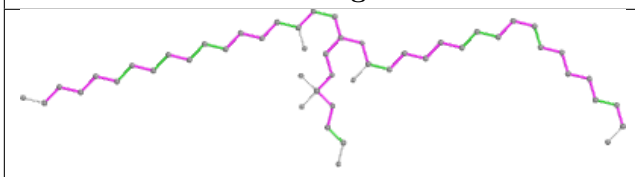
Ligand PEE D 501



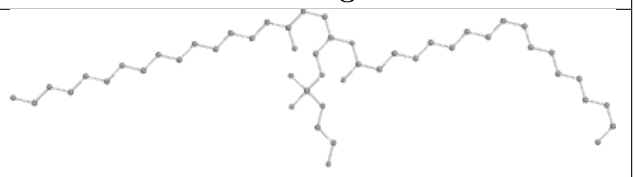
Bond lengths



Bond angles

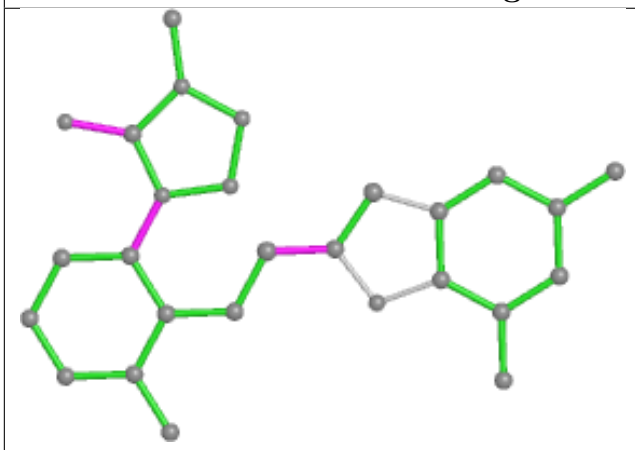


Torsions



Rings

Ligand A1D6O A 402



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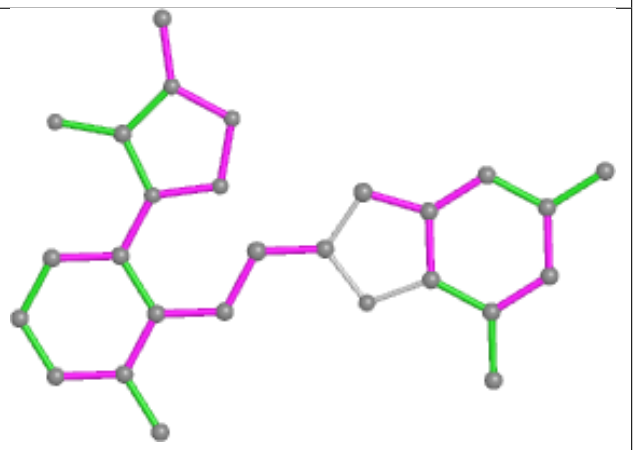
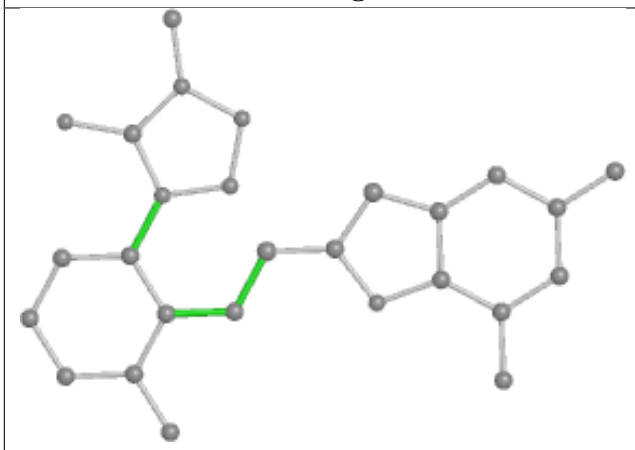
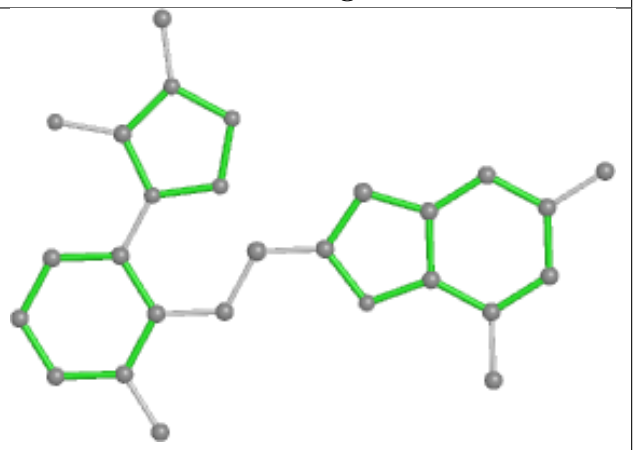


Bond angles

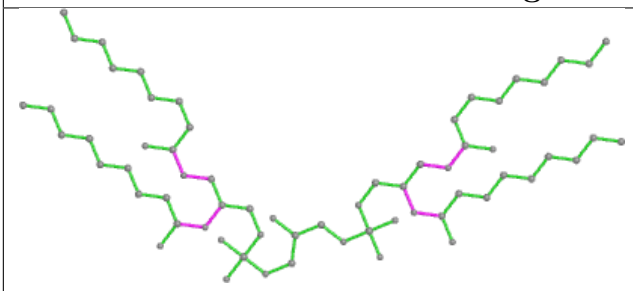


Torsions

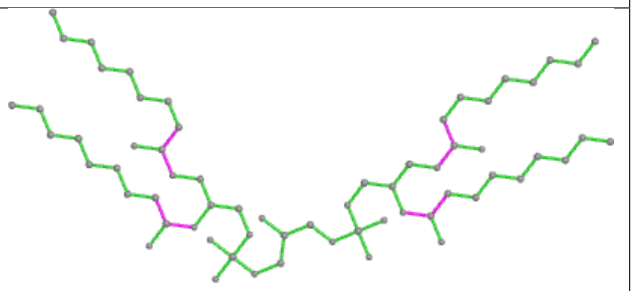


Rings

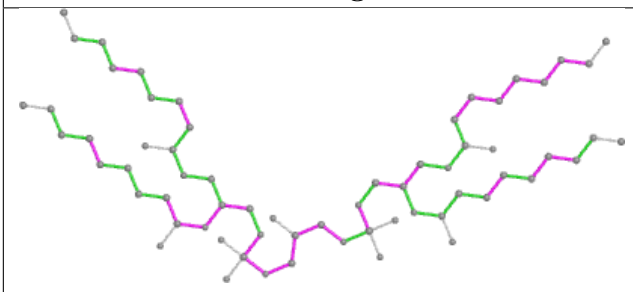
Ligand CDL A 406



Bond lengths



Bond angles



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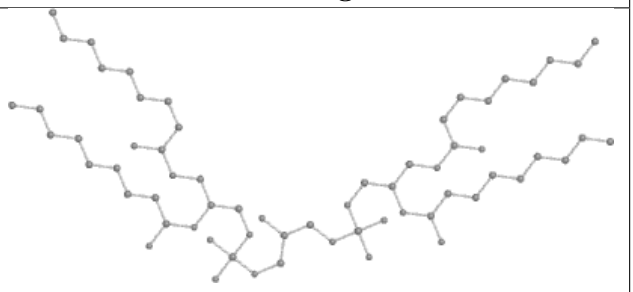
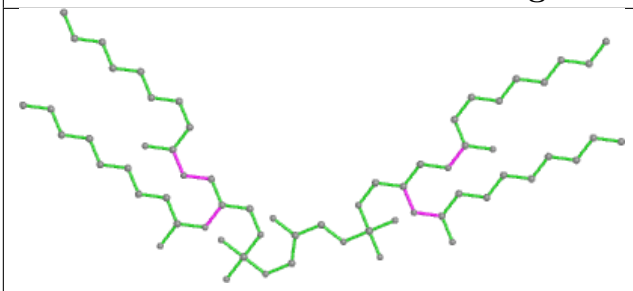


Rings

Ligand CDL a 406



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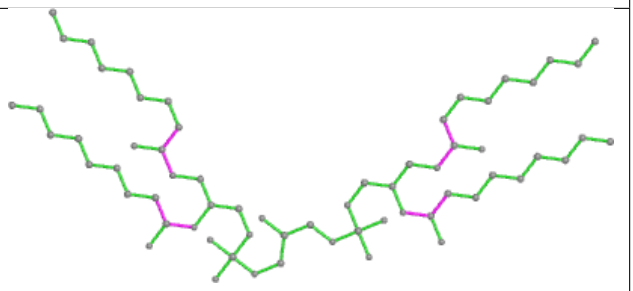
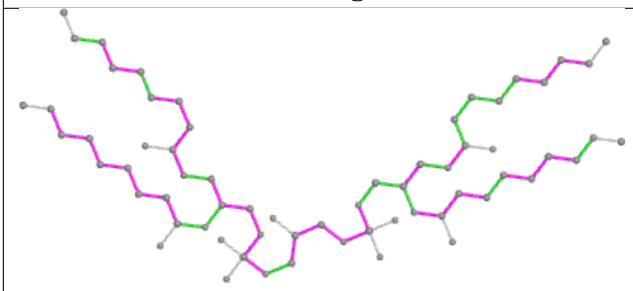


Bond angles



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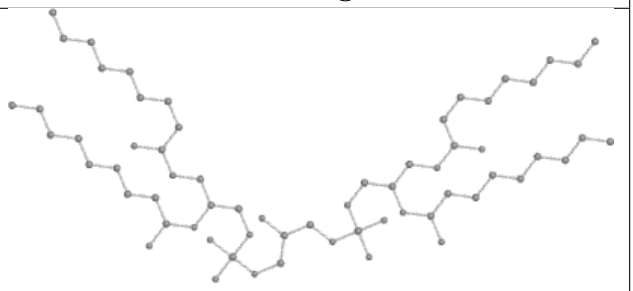
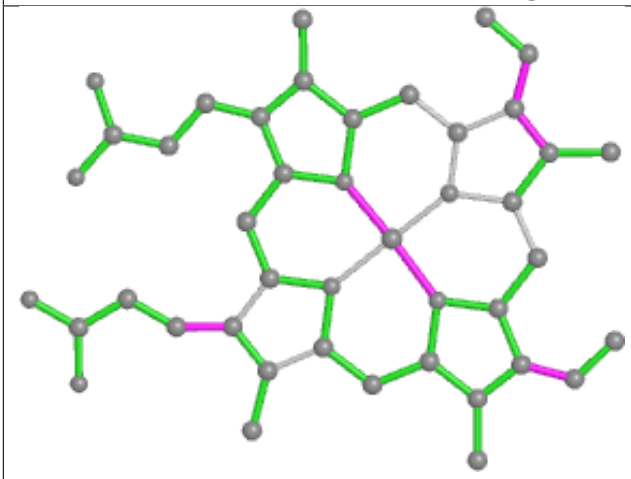


Rings

Ligand HEM a 403



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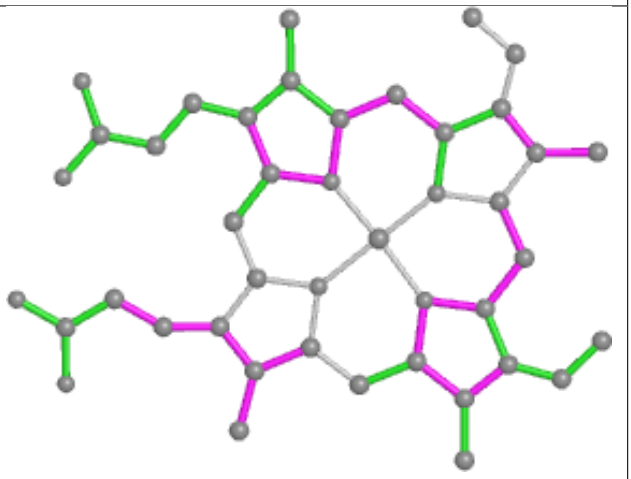

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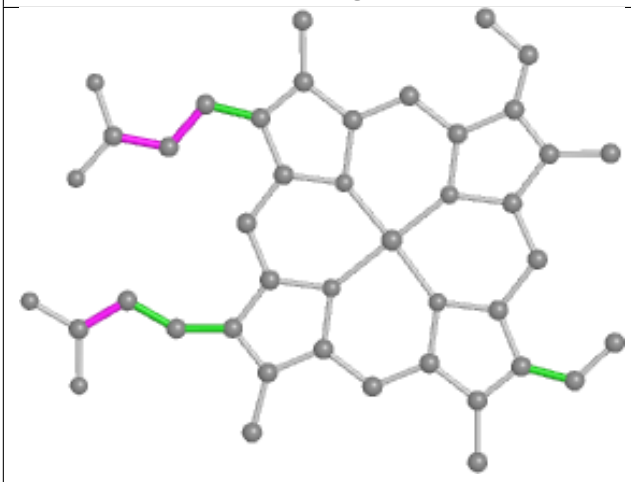

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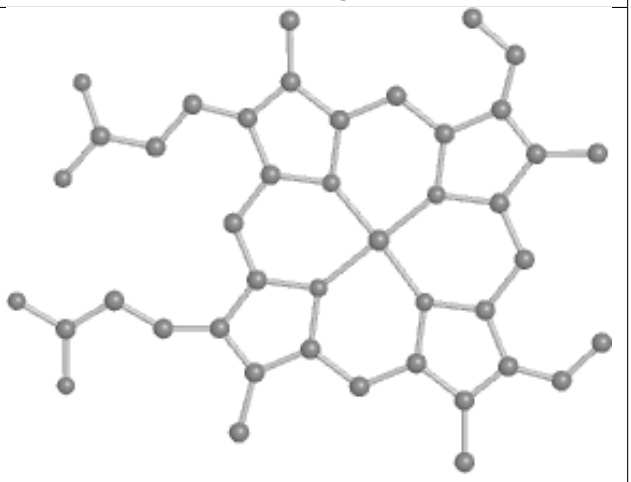
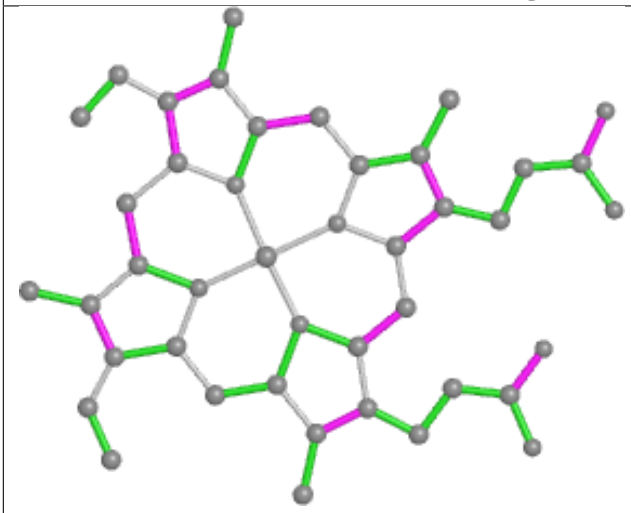


Rings

Ligand HEC B 401



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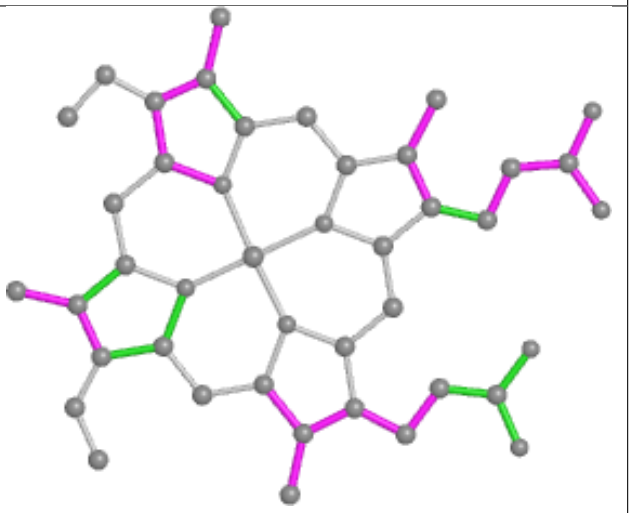

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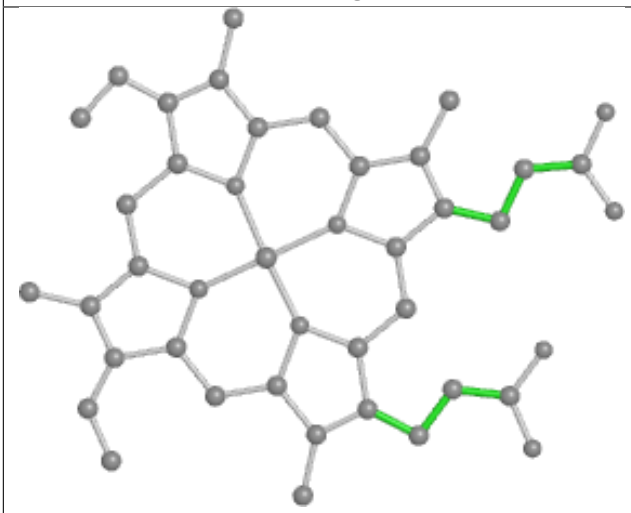

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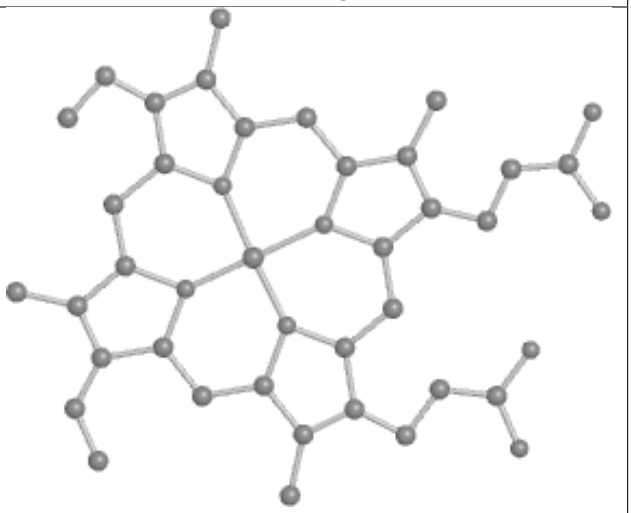
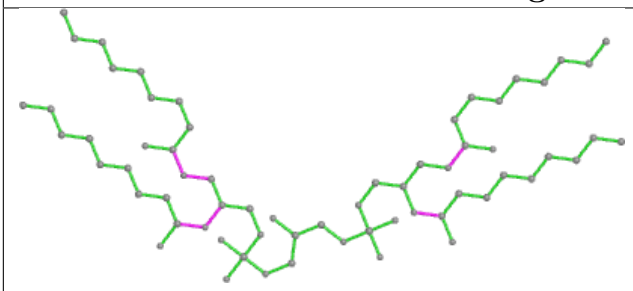


Rings

Ligand CDL a 407



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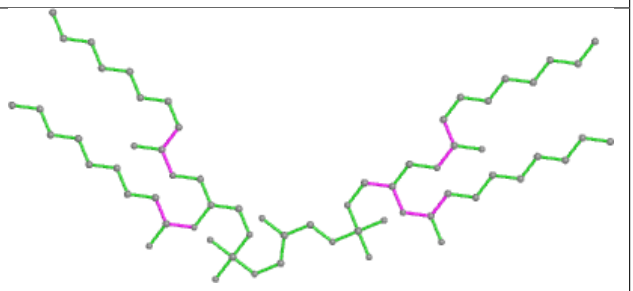

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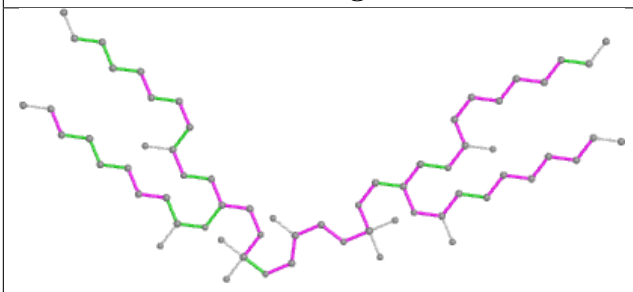

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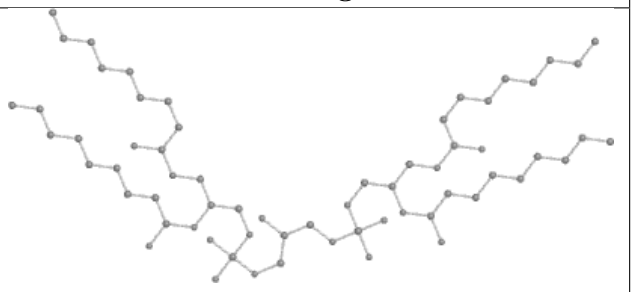
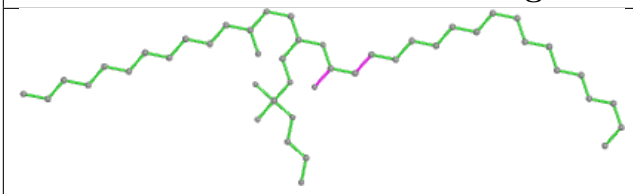


Rings

Ligand PEE A 405



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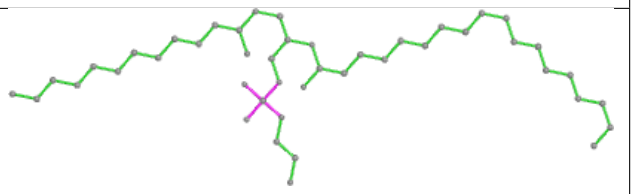
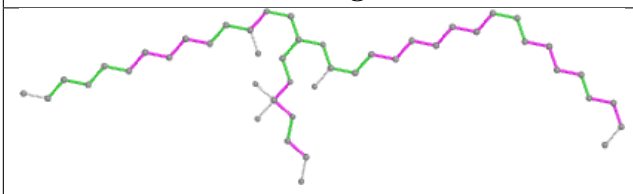


Bond angles



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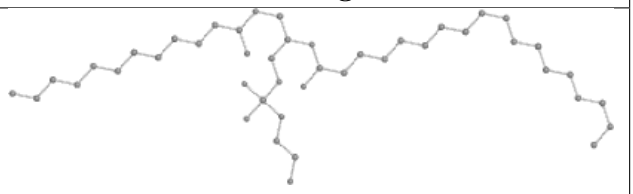
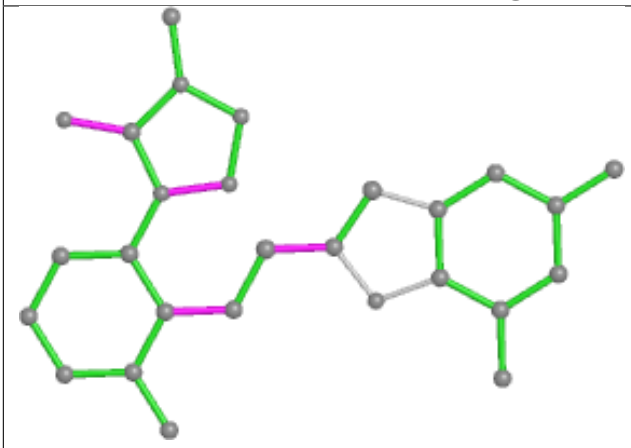


Rings

Ligand A1D6O a 401



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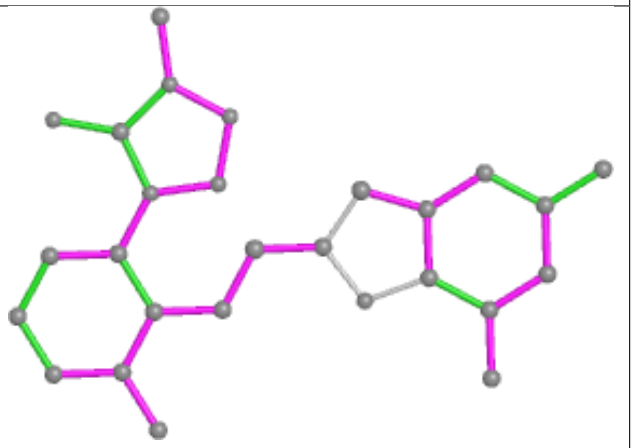
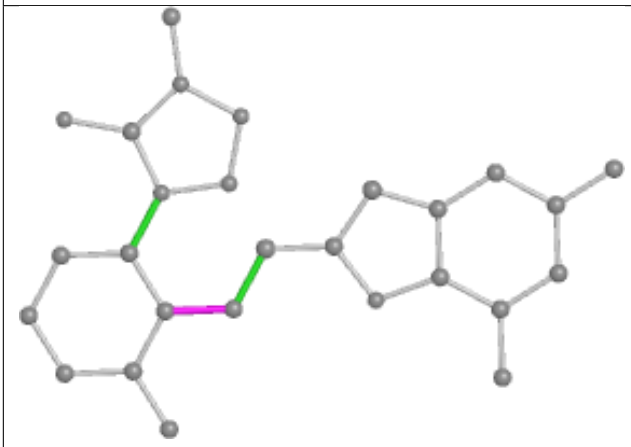


Bond angles



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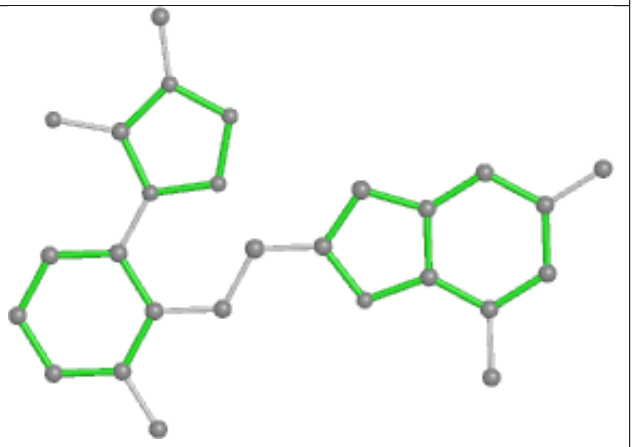
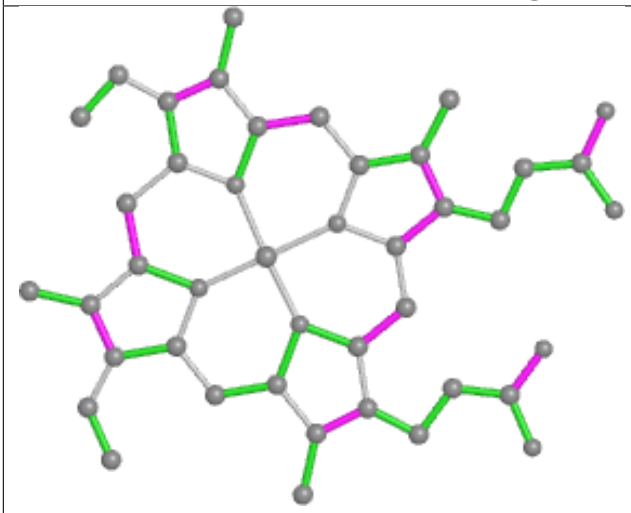


Rings

Ligand HEC b 401



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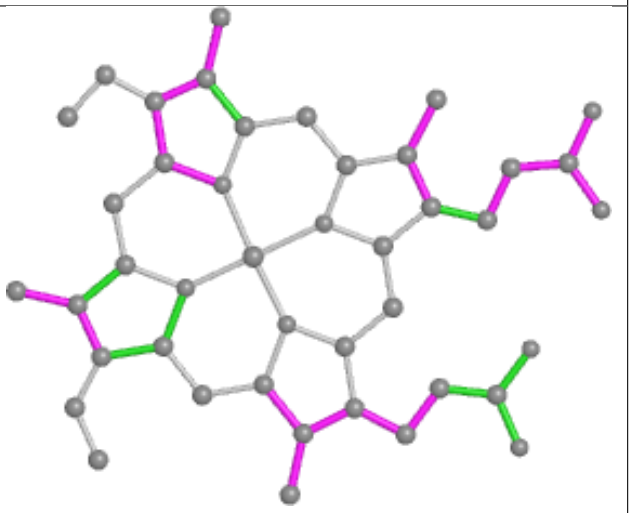

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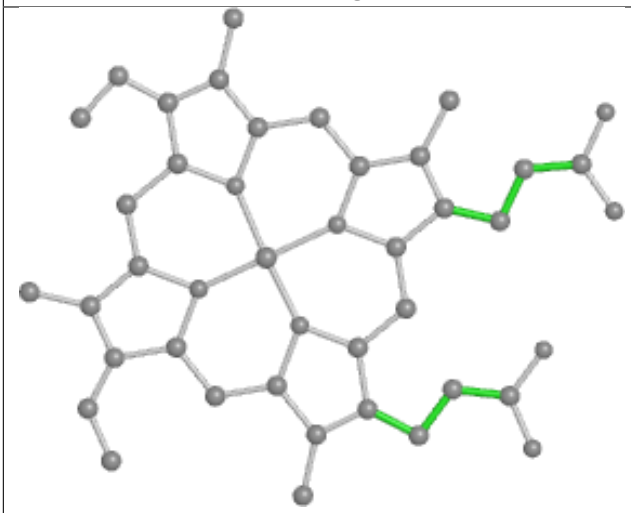

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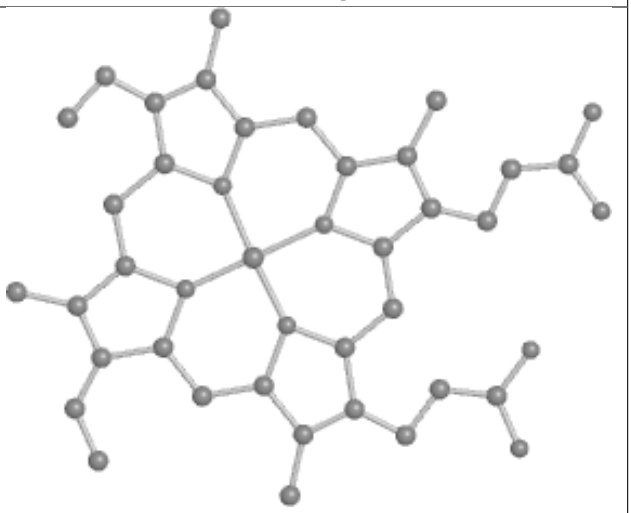
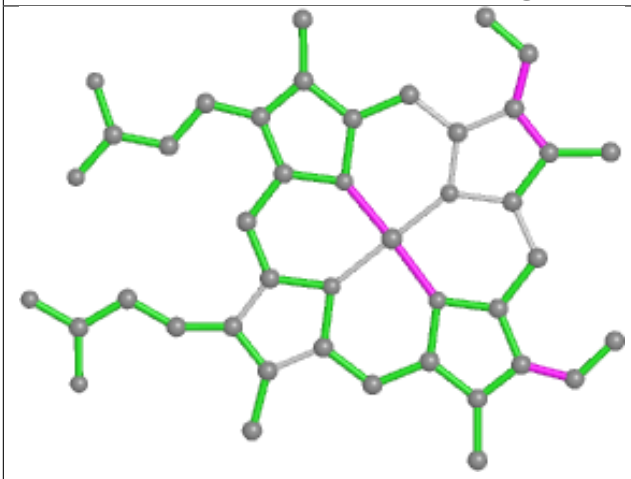


Rings

Ligand HEM A 404



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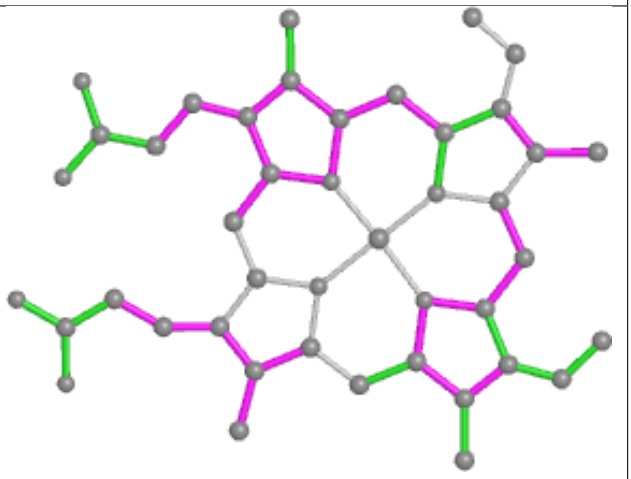
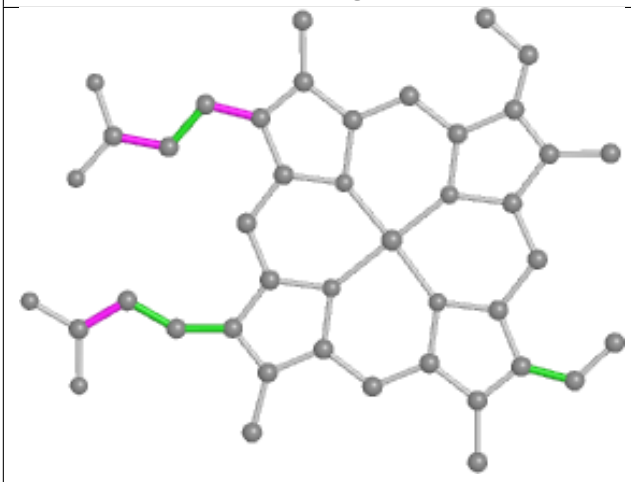


Bond angles



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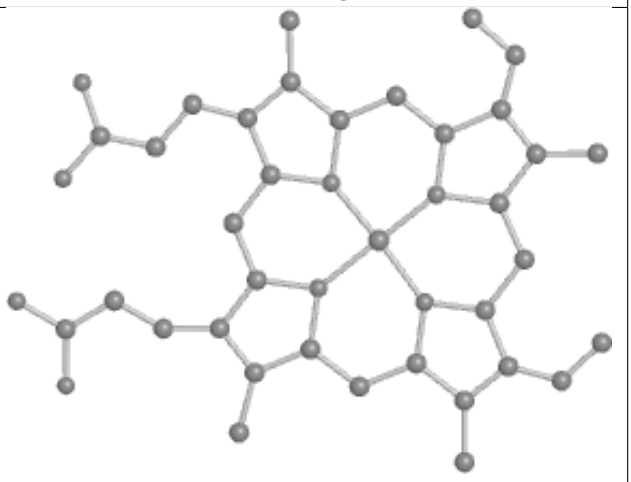
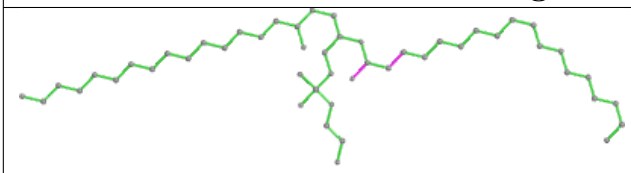
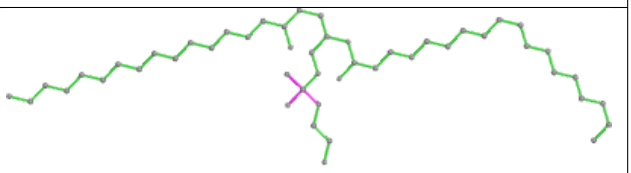


Rings

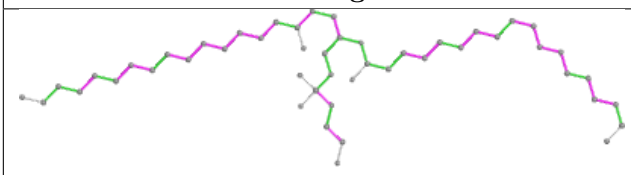
Ligand PEE a 405



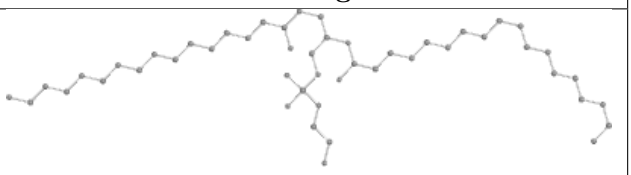
Bond lengths



Bond angles

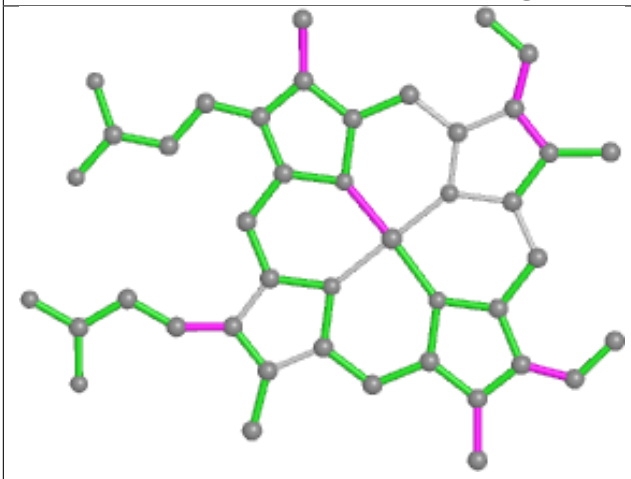


Torsions



Rings

Ligand HEM A 403



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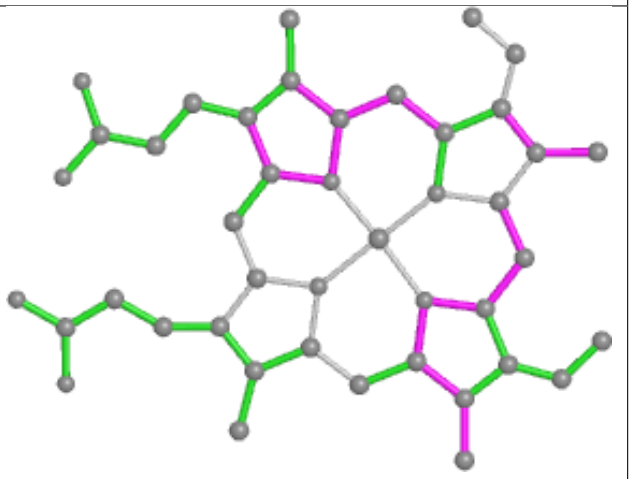
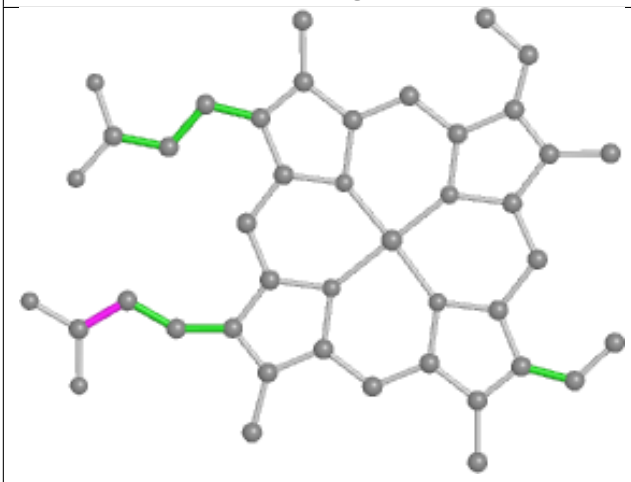
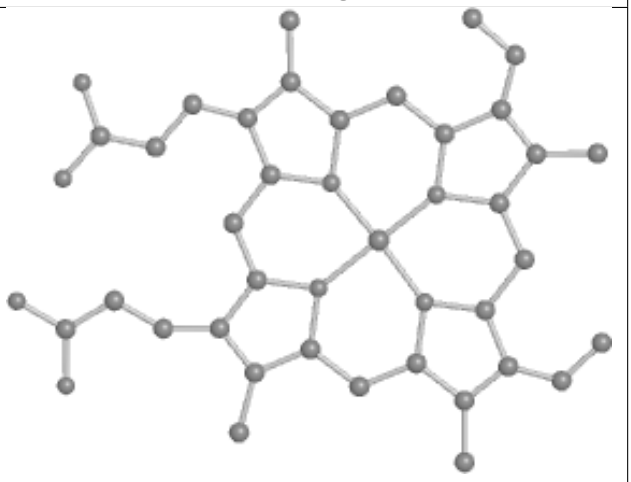


Bond angles

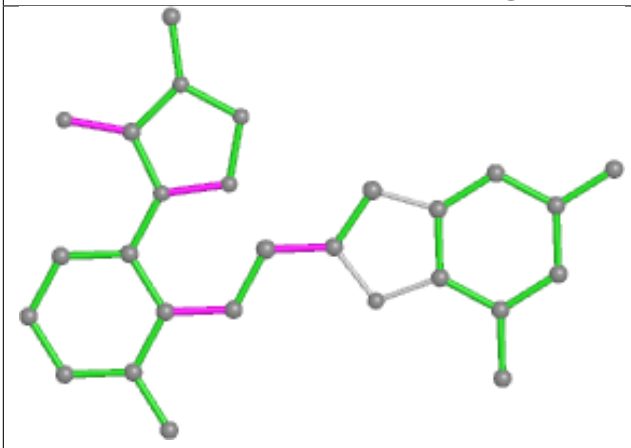


Torsions

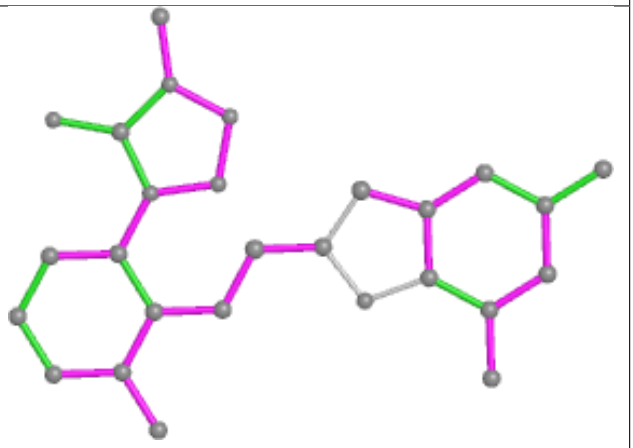


Rings

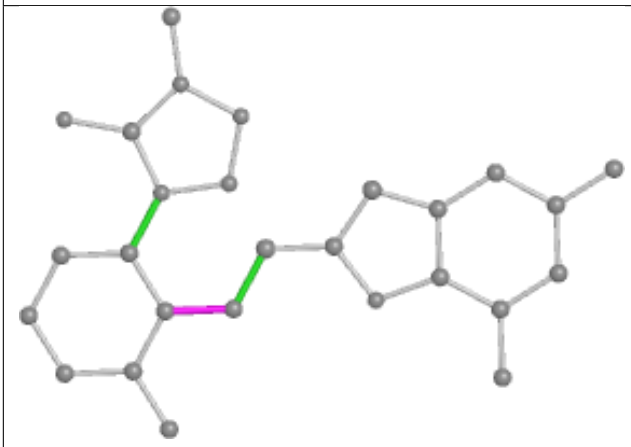
Ligand A1D6O A 401



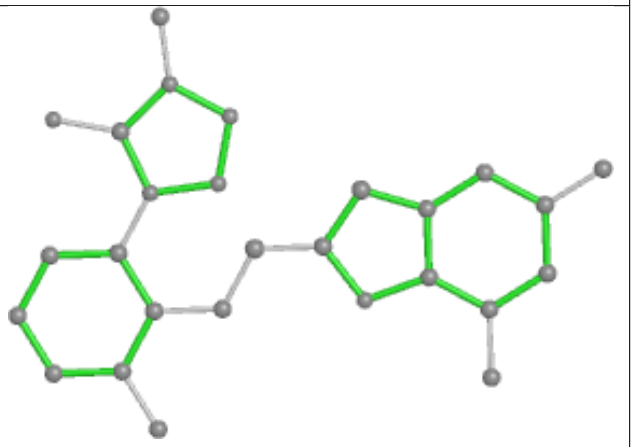
Bond lengths



Bond angles

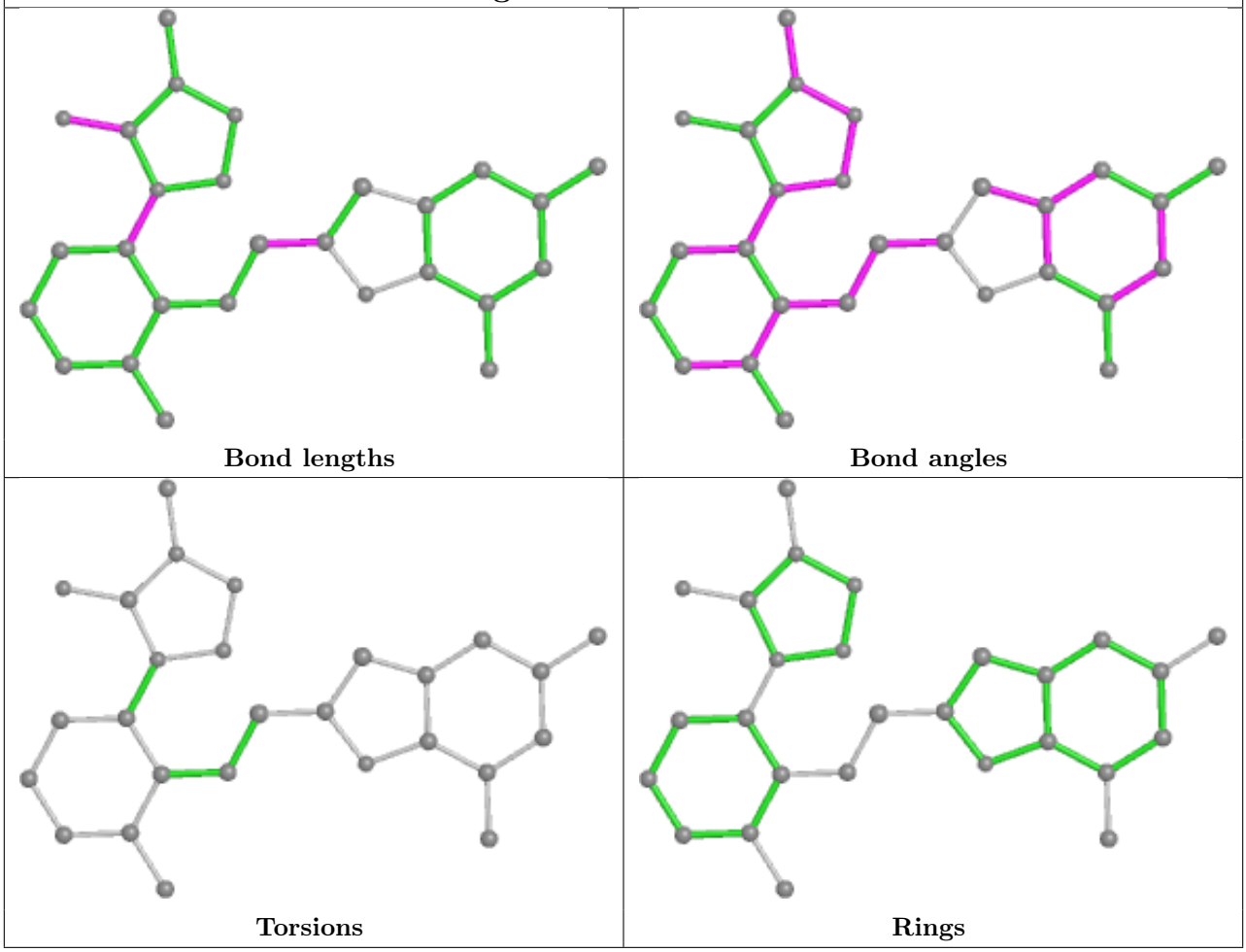


Torsions



Rings

Ligand A1D6O a 402



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.

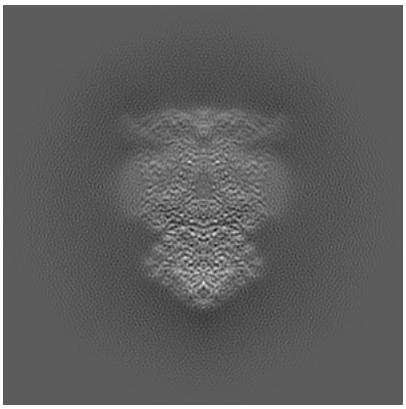
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-60323. These allow visual inspection of the internal detail of the map and identification of artifacts.

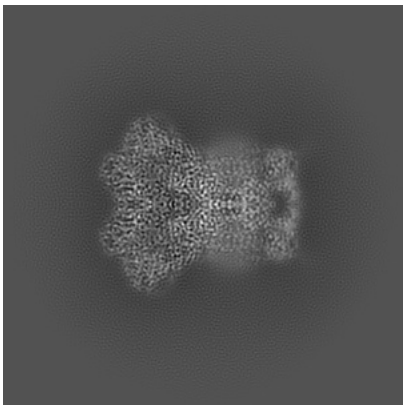
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

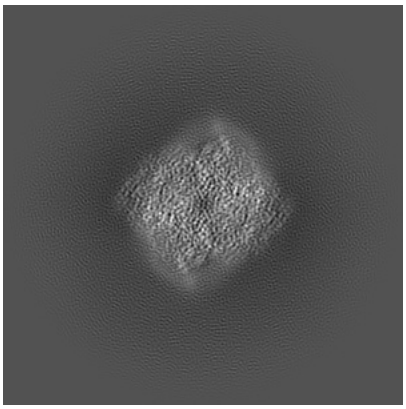
6.1.1 Primary map



X

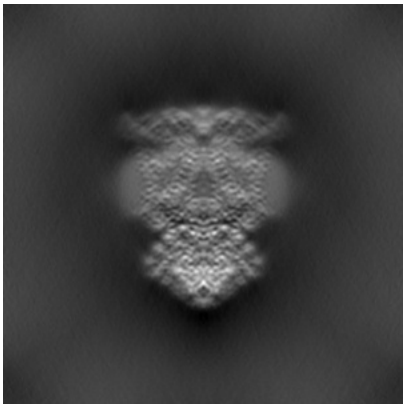


Y

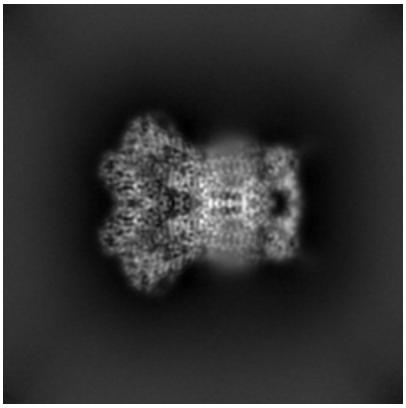


Z

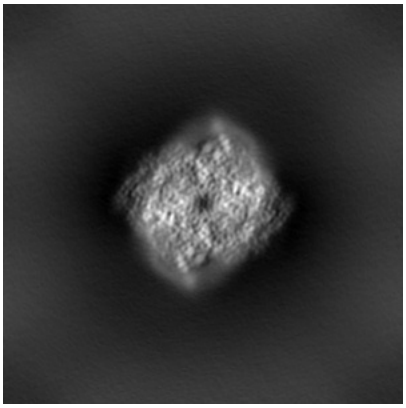
6.1.2 Raw map



X



Y

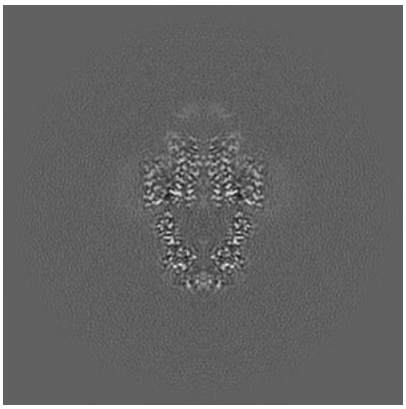


Z

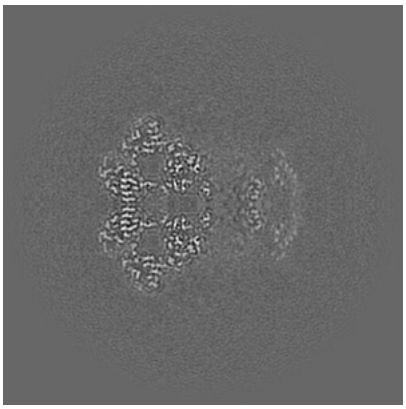
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

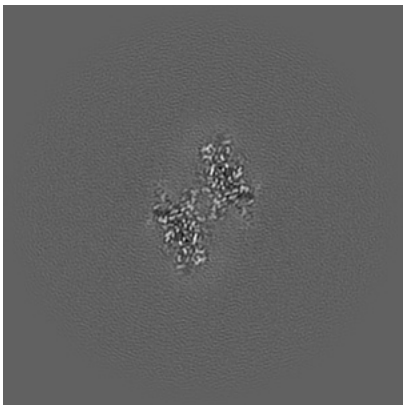
6.2.1 Primary map



X Index: 160

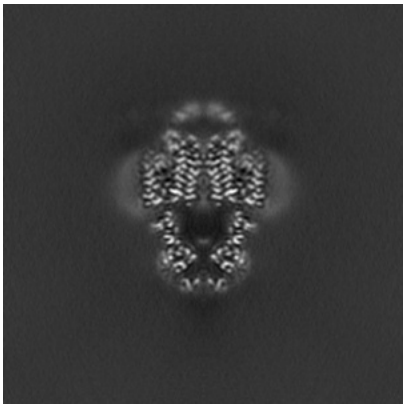


Y Index: 160

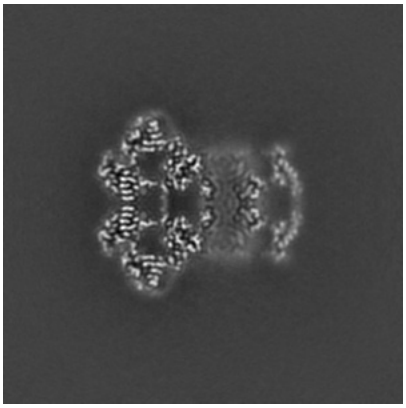


Z Index: 160

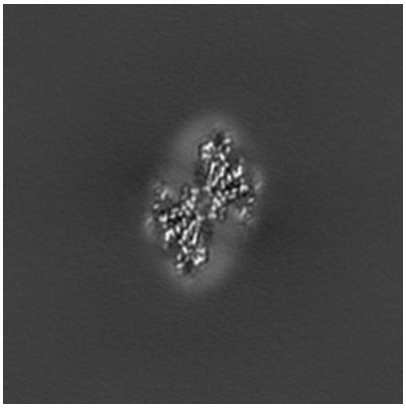
6.2.2 Raw map



X Index: 160



Y Index: 160

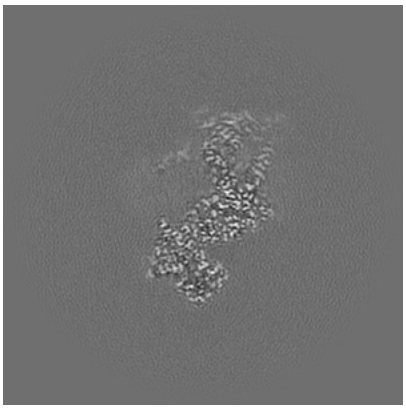


Z Index: 160

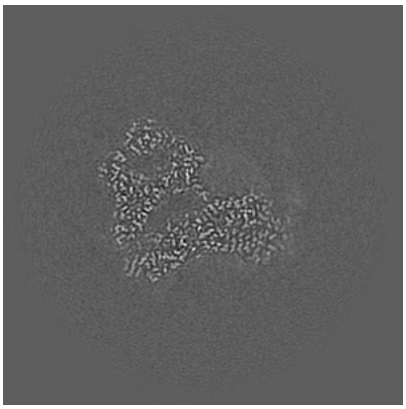
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

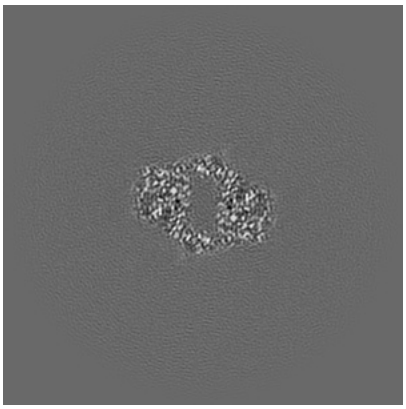
6.3.1 Primary map



X Index: 176

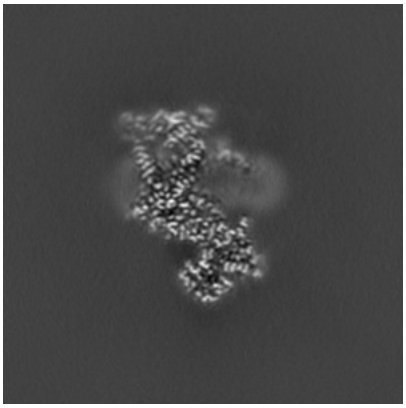


Y Index: 150

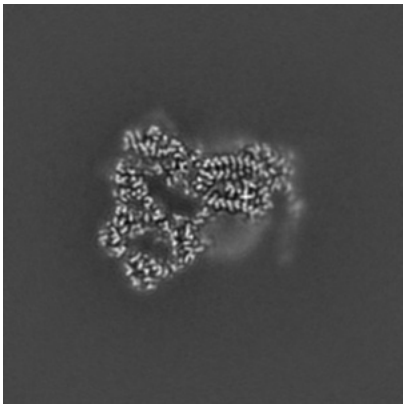


Z Index: 138

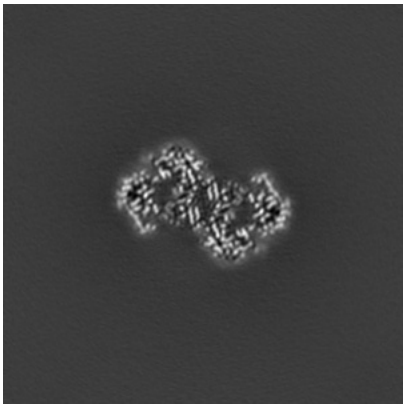
6.3.2 Raw map



X Index: 144



Y Index: 170

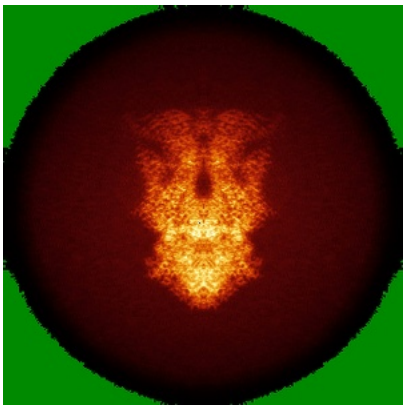


Z Index: 108

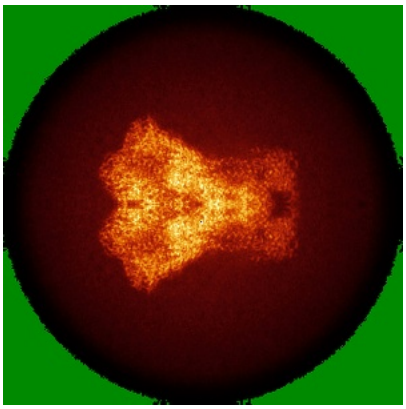
The images above show the largest variance slices of the map in three orthogonal directions.

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

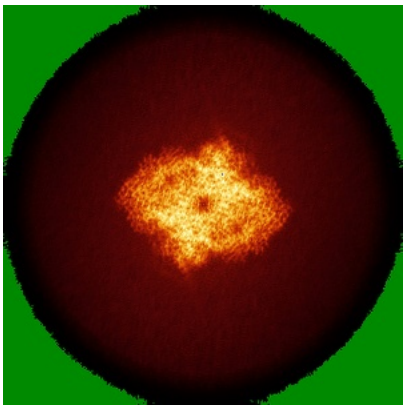
6.4.1 Primary map



X

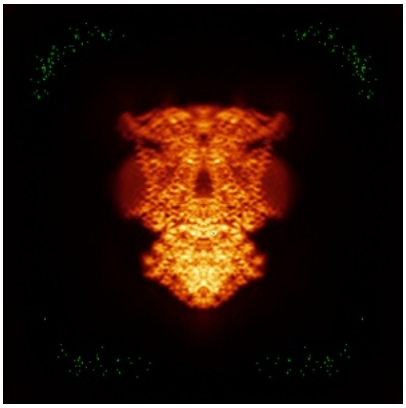


Y

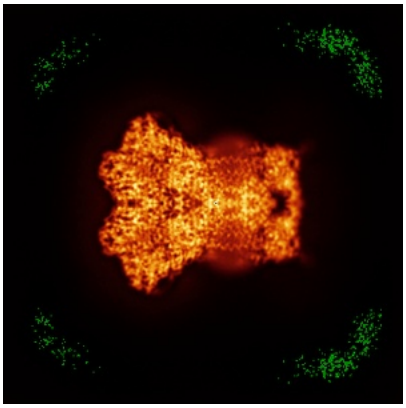


Z

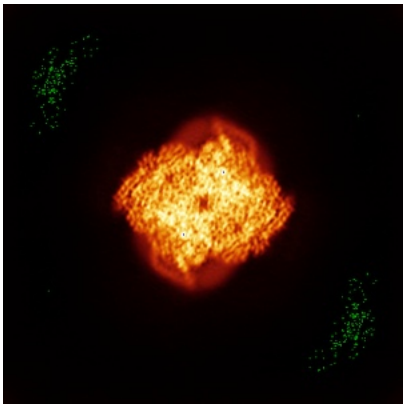
6.4.2 Raw map



X



Y

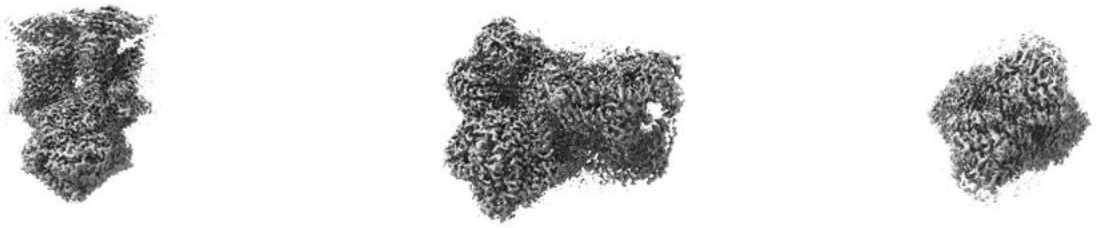


Z

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)

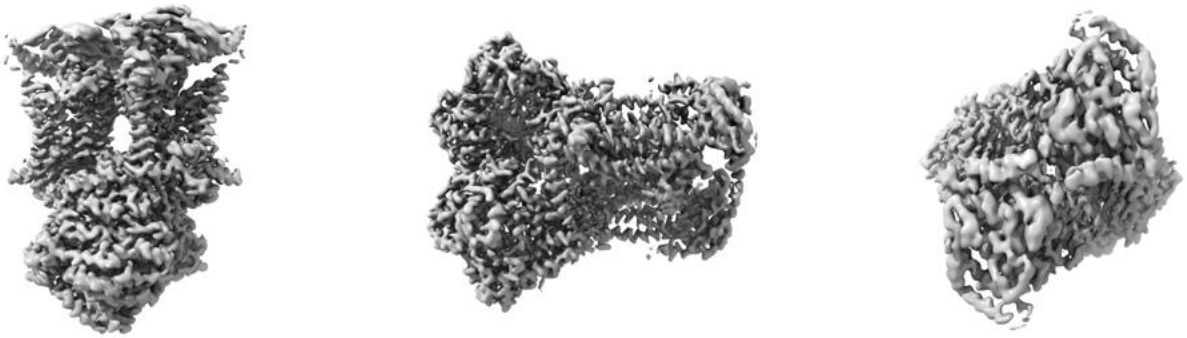
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.06. 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.

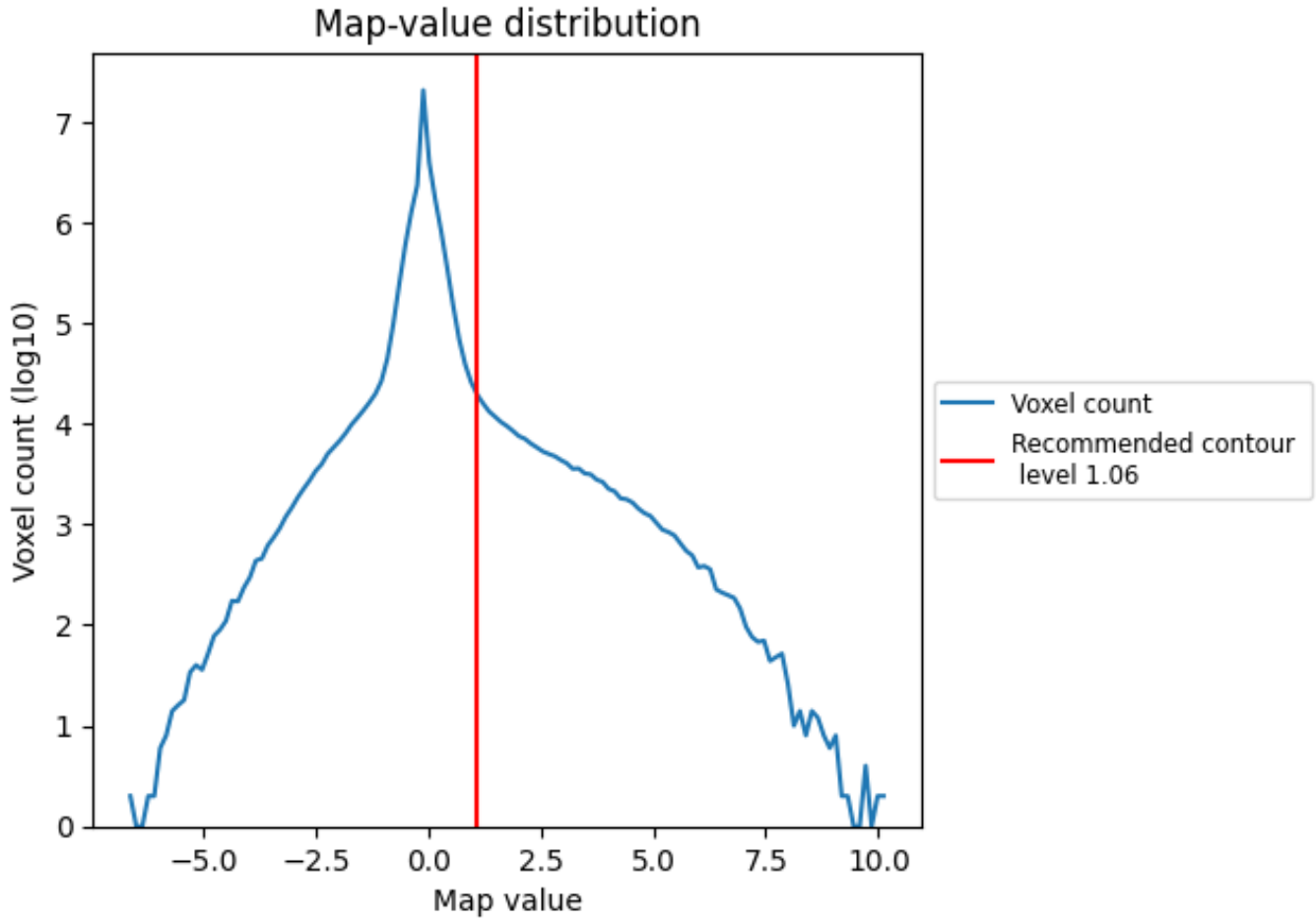
6.6 Mask visualisation (i)

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

7 Map analysis

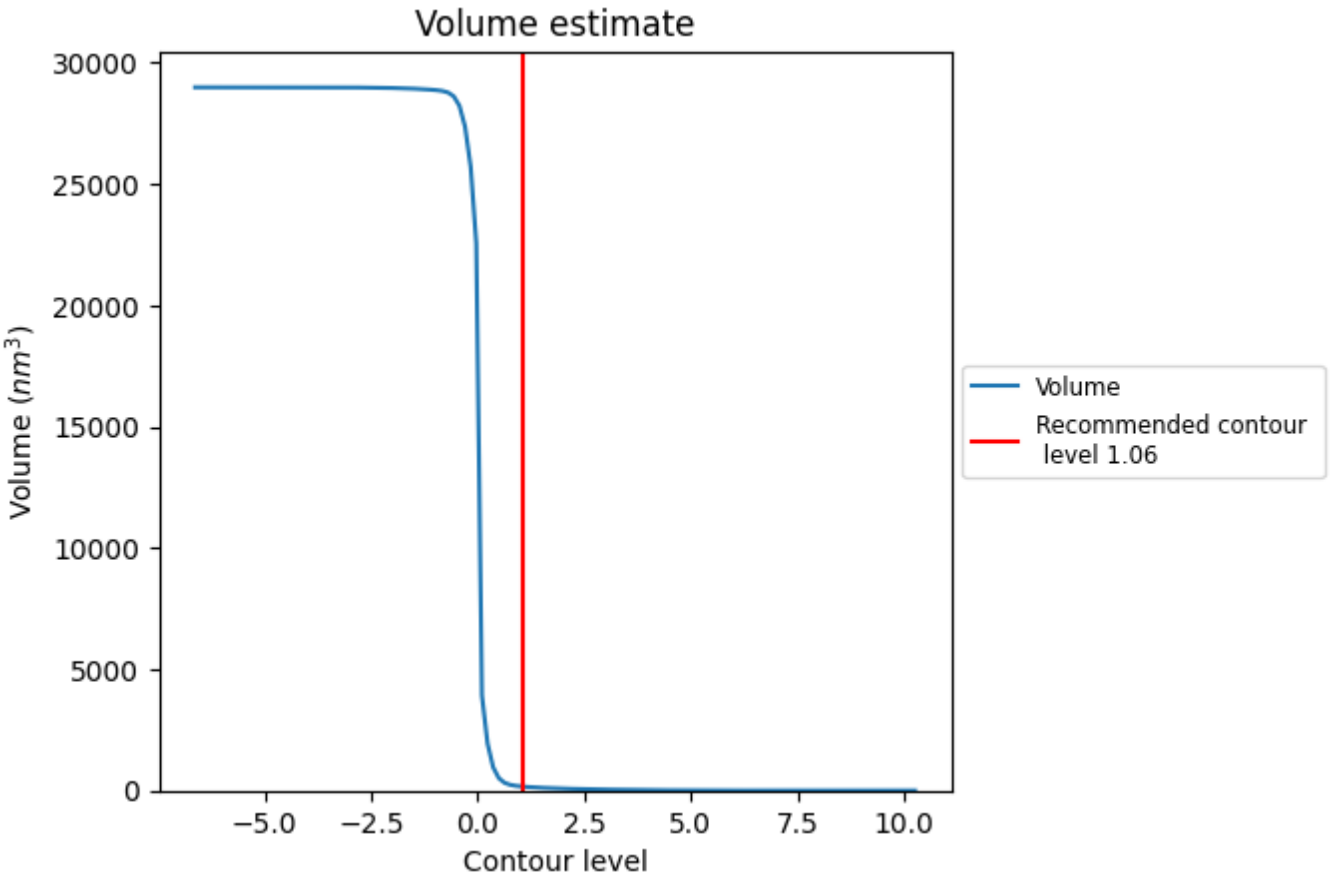
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

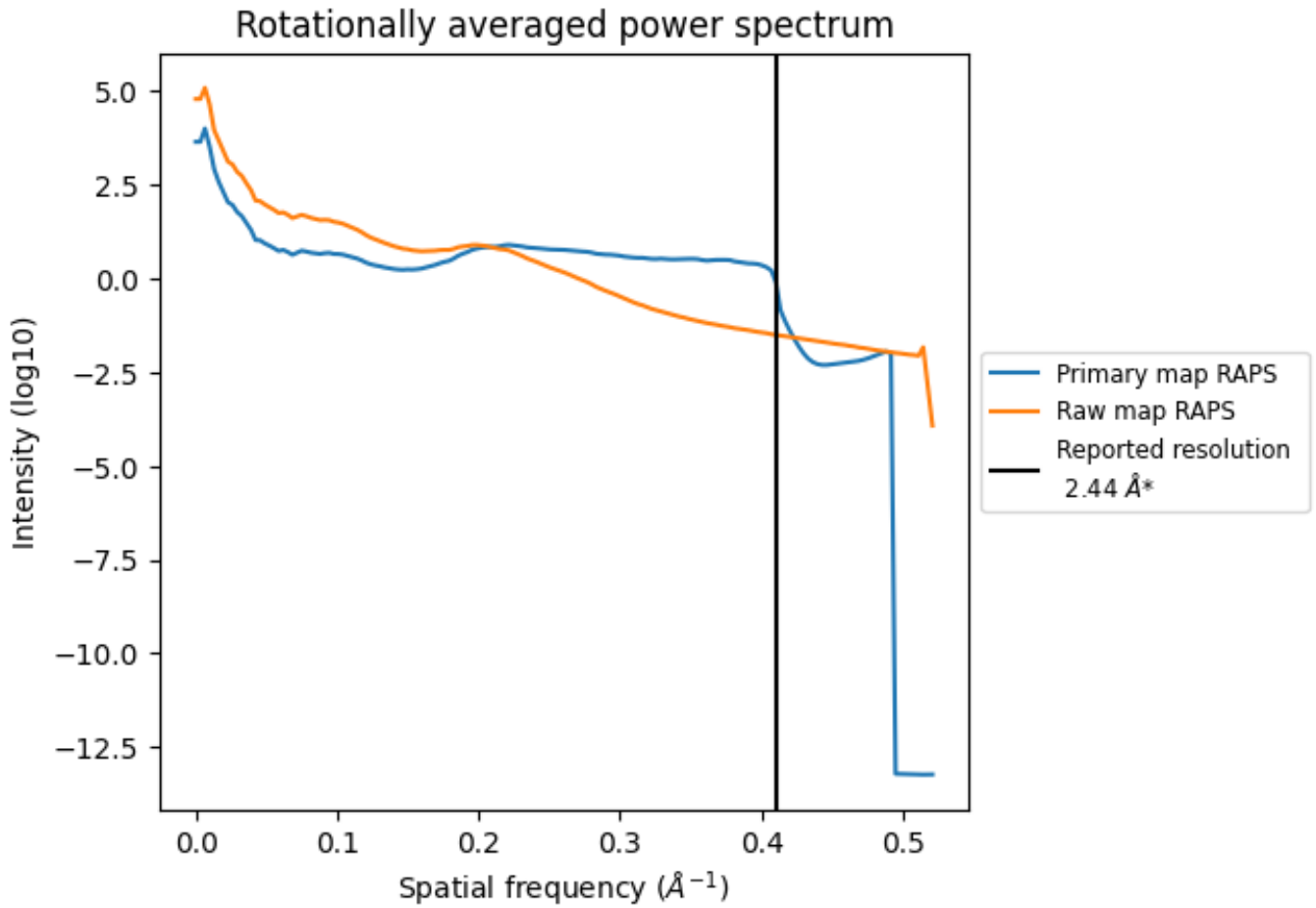
7.2 Volume estimate



The volume at the recommended contour level is 163 nm^3; this corresponds to an approximate mass of 147 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)

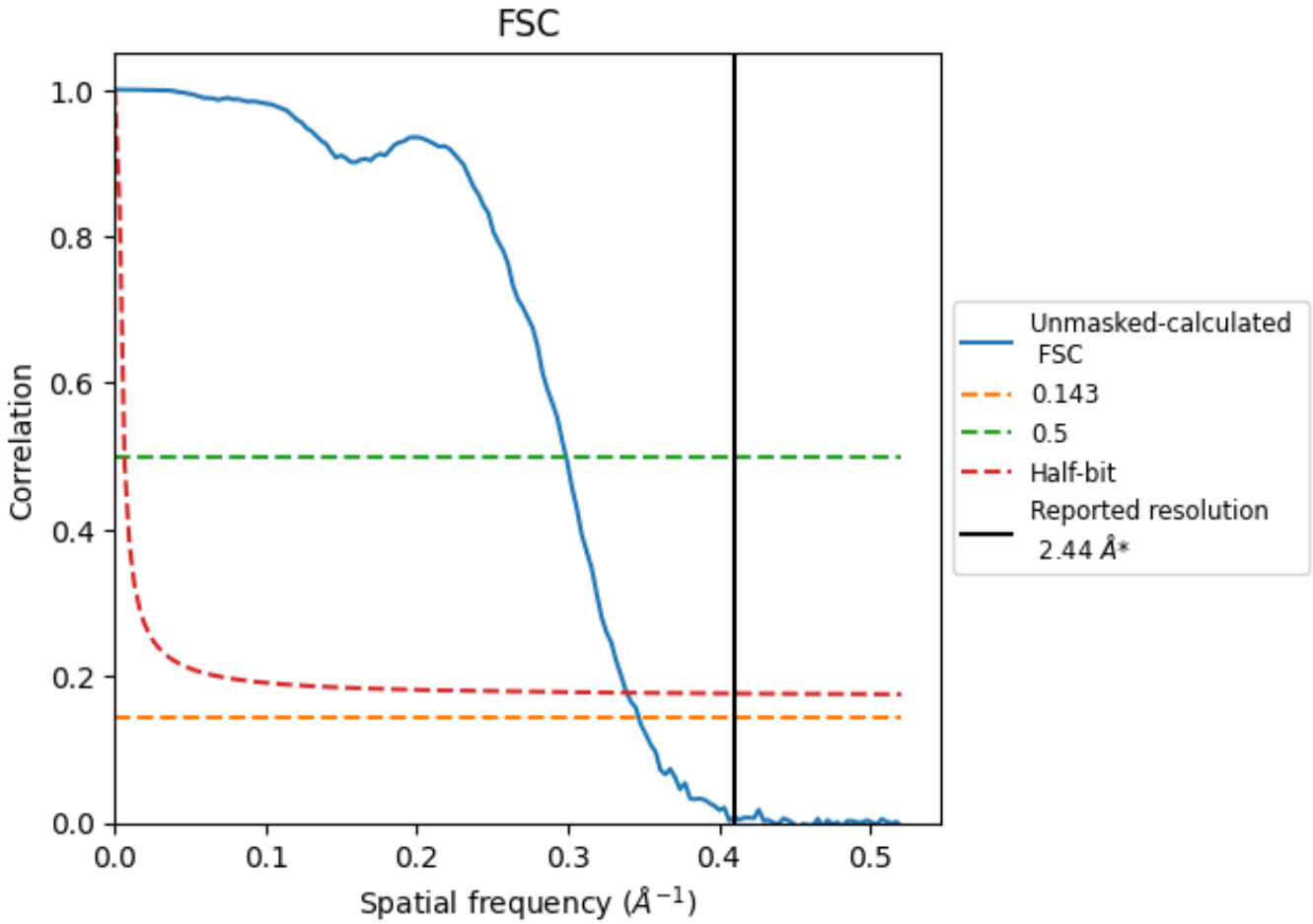


*Reported resolution corresponds to spatial frequency of 0.410 $Å^{-1}$

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 0.410 Å^{-1}

8.2 Resolution estimates (i)

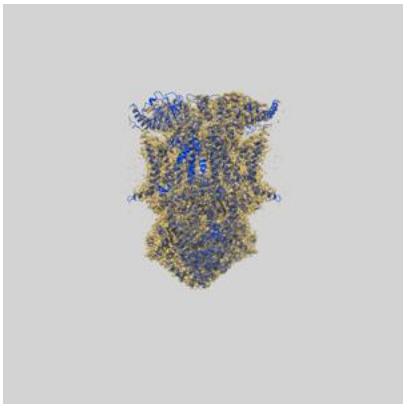
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.44	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.88	3.35	2.95

*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 2.88 differs from the reported value 2.44 by more than 10 %

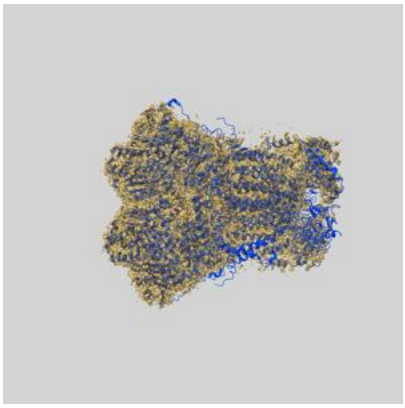
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-60323 and PDB model 8ZP0. Per-residue inclusion information can be found in section 3 on page 10.

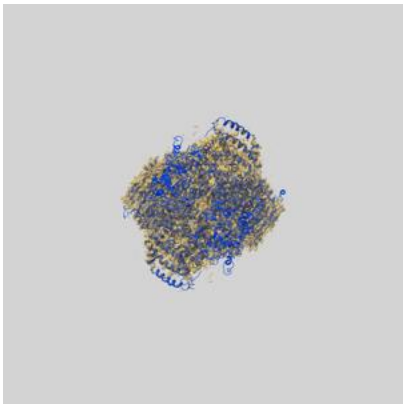
9.1 Map-model overlay



X



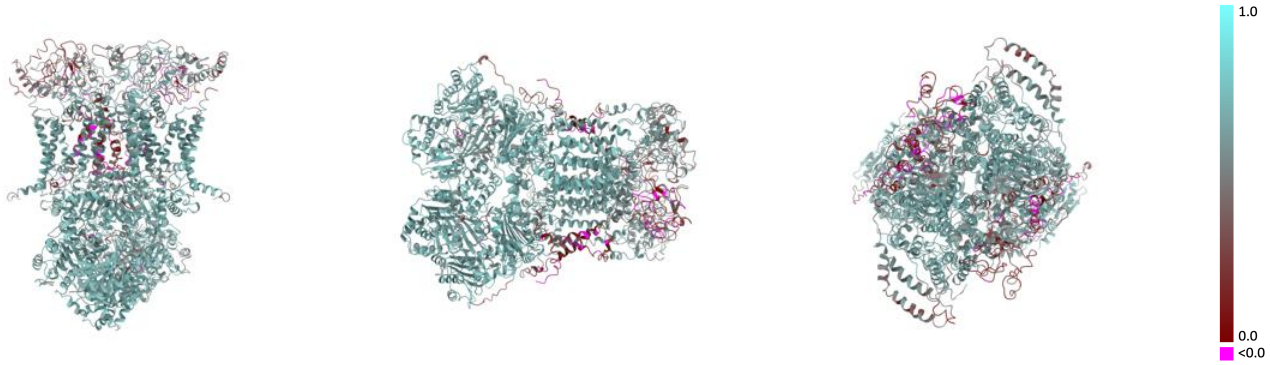
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.06 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.

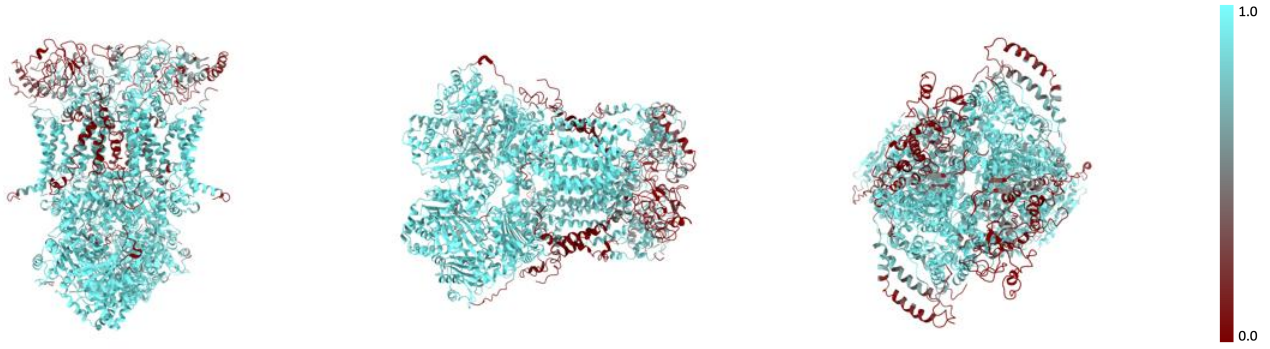
9.2 Q-score mapped to coordinate model (i)



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.

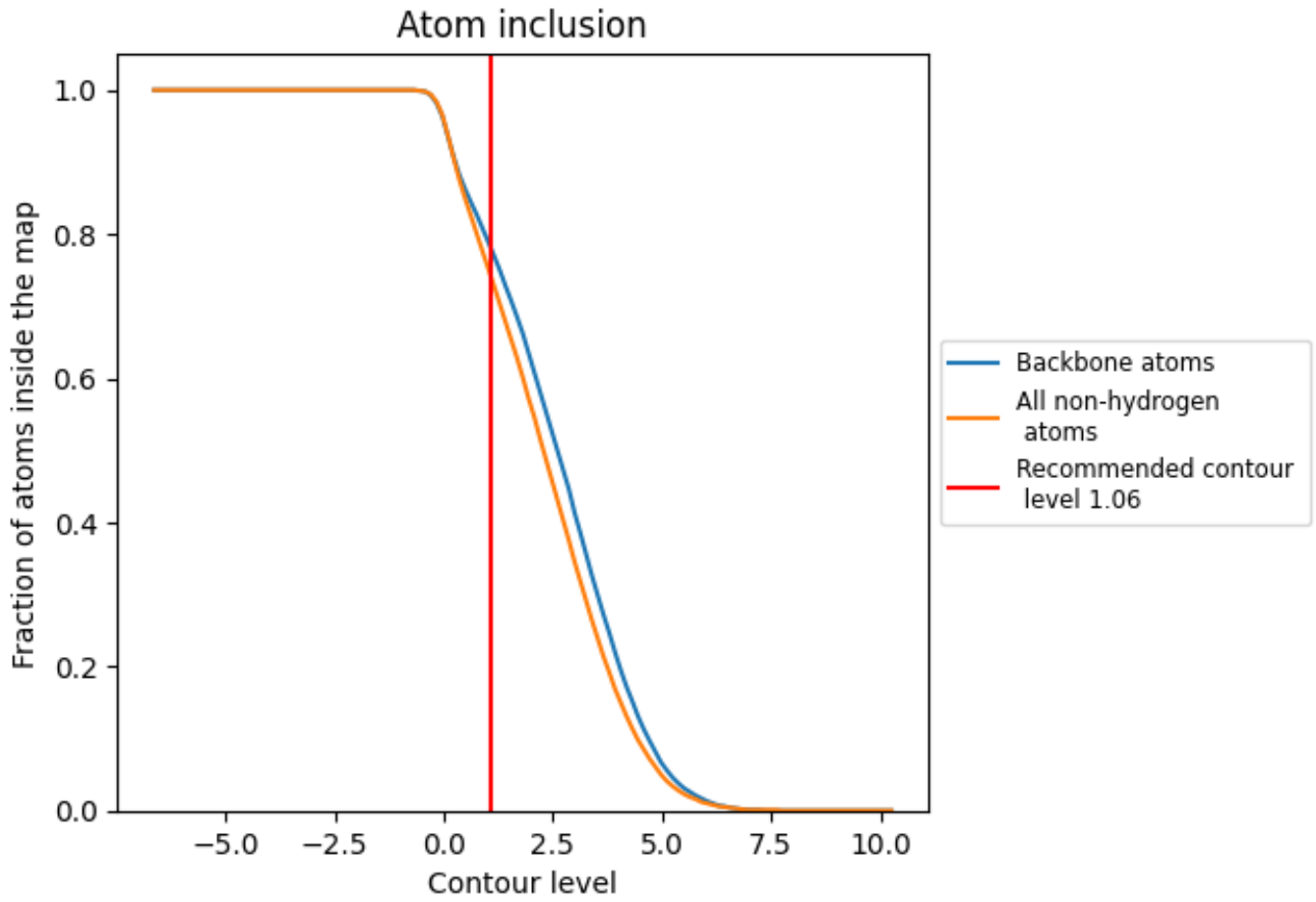
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.06).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 74% 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 (1.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7450	0.5780
A	0.8930	0.6450
B	0.7460	0.5820
C	0.0530	0.2900
D	0.9110	0.6610
E	0.9440	0.6680
F	0.3820	0.4860
G	0.8940	0.6630
H	0.7760	0.6080
I	0.3170	0.3120
J	0.0050	0.1980
K	0.4870	0.4200
a	0.8860	0.6430
b	0.7610	0.5910
c	0.0600	0.2220
d	0.9160	0.6620
e	0.9450	0.6690
f	0.3900	0.4780
g	0.8930	0.6630
h	0.7240	0.5740
i	0.3190	0.2970
j	0.0030	0.1840
k	0.5000	0.4250