Full wwPDB EM Validation Report ⓘ

Mar 17, 2022 – 03:25 pm GMT

PDB ID	:	7P8W
EMDB ID	:	EMD-13256
Title	:	Human erythrocyte catalase cryoEM
Authors	:	Chen, S.; Li, J.; Vinothkumar, K.R.; Henderson, R.
Deposited on	:	2021-07-23
Resolution	:	2.20 Å(reported)
Based on initial models	:	4BLC, 1F4J

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

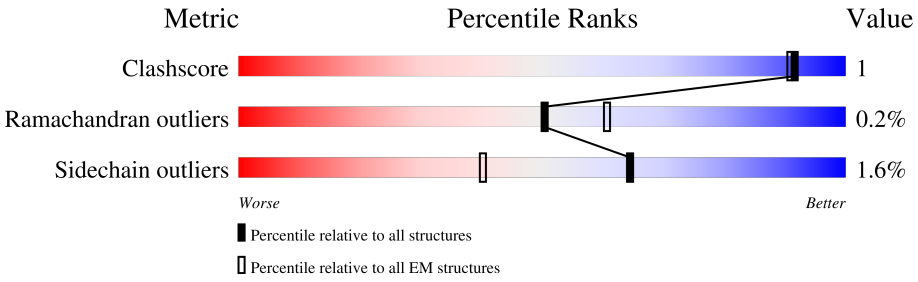
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	527	90% 6% 5%
1	B	527	90% 5% 5%
1	C	527	89% 6% 5%
1	D	527	90% 5% 5%

2 Entry composition

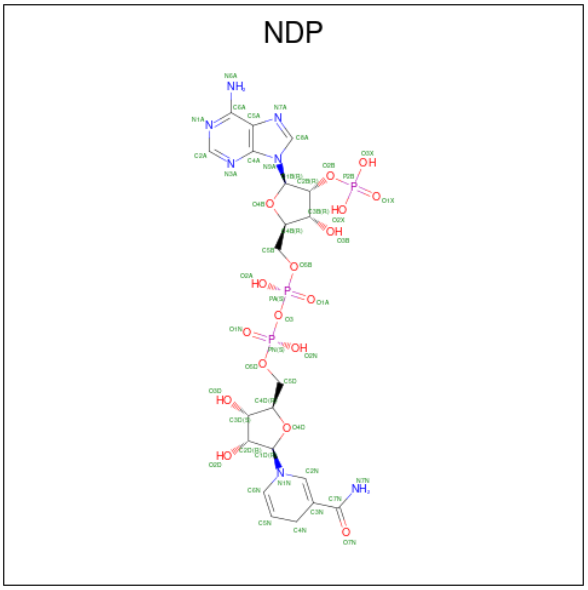
There are 4 unique types of molecules in this entry. The entry contains 17668 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Catalase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	502	Total	C	N	O	S	1	0
			4047	2571	719	744	13		
1	B	502	Total	C	N	O	S	1	0
			4047	2571	719	744	13		
1	C	502	Total	C	N	O	S	1	0
			4047	2571	719	744	13		
1	D	502	Total	C	N	O	S	1	0
			4047	2571	719	744	13		

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	B	1	Total	C	N	O	P	0
			48	21	7	17	3	

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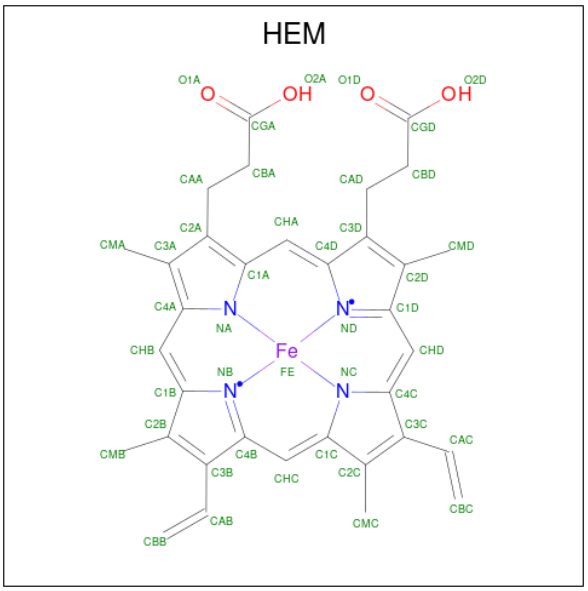
Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	P	0
			48	21	7	17	3	
2	D	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 3 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
3	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
3	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
3	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
3	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	A	279	Total	O	2
			281	281	
4	B	278	Total	O	2
			280	280	
4	C	276	Total	O	1
			277	277	

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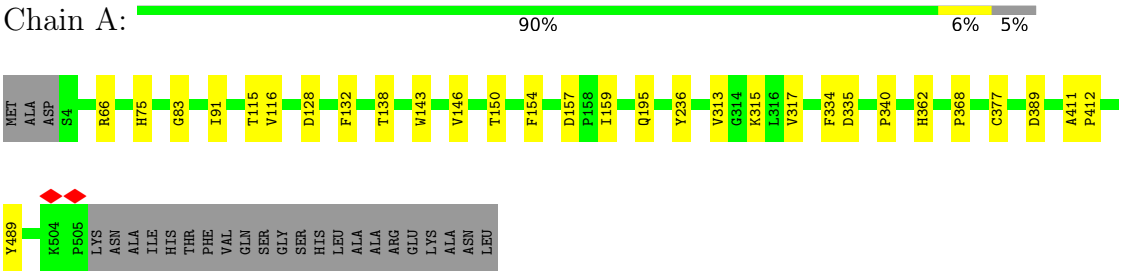
Mol	Chain	Residues	Atoms		AltConf
4	D	277	Total 278	O 278	1

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

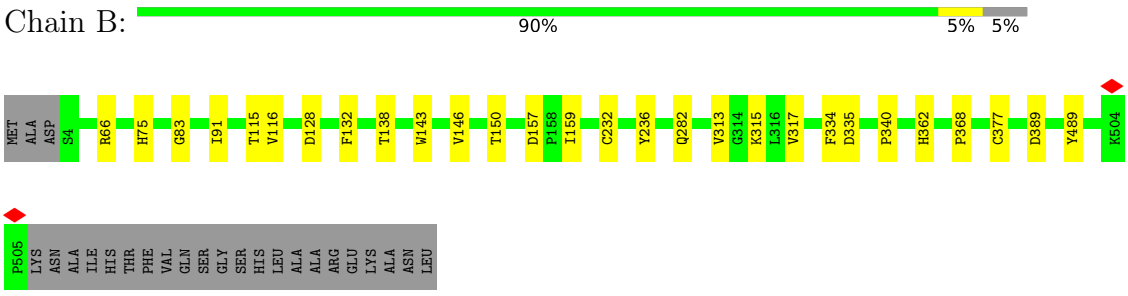
• Molecule 1: Catalase

Chain A:



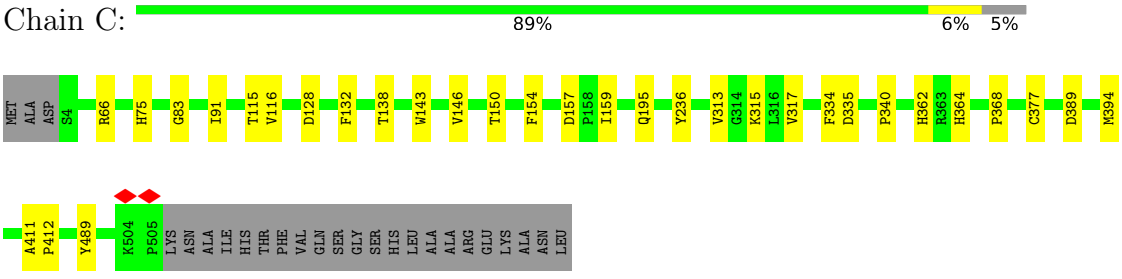
• Molecule 1: Catalase

Chain B:



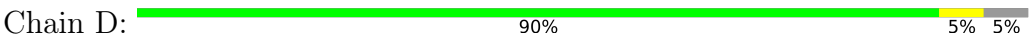
• Molecule 1: Catalase

Chain C:



• Molecule 1: Catalase

Chain D:




MET
ALA
ASP
S4
R66
H75
G83
I91
T115
V116
D128
F132
T138
W143
V146
T150
D157
P158
I159
Y236
V313
G314
K315
L316
V317
F334
D335
P340
H362
P368
C377
D389
M394
Y489
K504
P505
LYS
ASN
ALA
ILE
HIS
THR
PHE
VAL
GLN
SER
GLY
SER
HIS
LEU
ALA
ALA
ARG
GLU
LYS
ALA
ASN
LEU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D2	Depositor
Number of particles used	119169	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	38	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.501	Depositor
Minimum map value	-0.179	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.055	Depositor
Map size (Å)	137.0, 137.0, 137.0	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0703125, 1.0703125, 1.0703125	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, HEM

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	0.60	0/4168	0.79	0/5663
1	B	0.60	0/4168	0.79	0/5663
1	C	0.60	0/4168	0.79	0/5663
1	D	0.60	0/4168	0.79	0/5663
All	All	0.60	0/16672	0.79	0/22652

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4047	0	3875	13	0
1	B	4047	0	3875	12	0
1	C	4047	0	3875	15	0
1	D	4047	0	3875	12	0
2	A	48	0	26	0	0
2	B	48	0	26	0	0
2	C	48	0	26	0	0
2	D	48	0	26	0	0
3	A	43	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	43	0	30	0	0
3	C	43	0	30	0	0
3	D	43	0	30	0	0
4	A	281	0	0	1	0
4	B	280	0	0	1	0
4	C	277	0	0	2	0
4	D	278	0	0	1	0
All	All	17668	0	15724	47	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (47) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:CYS:SG	4:A:858[A]:HOH:O	2.49	0.70
1:C:377:CYS:SG	4:C:853[A]:HOH:O	2.50	0.70
1:B:377:CYS:SG	4:B:857[A]:HOH:O	2.50	0.69
1:D:377:CYS:SG	4:D:847[A]:HOH:O	2.52	0.66
1:B:75:HIS:HA	1:B:115:THR:O	2.08	0.54
1:D:75:HIS:HA	1:D:115:THR:O	2.08	0.54
1:C:75:HIS:HA	1:C:115:THR:O	2.08	0.53
1:A:75:HIS:HA	1:A:115:THR:O	2.08	0.53
1:A:157:ASP:OD1	1:A:159:ILE:HG22	2.09	0.52
1:C:157:ASP:OD1	1:C:159:ILE:HG22	2.09	0.52
1:B:157:ASP:OD1	1:B:159:ILE:HG22	2.09	0.51
1:C:364:HIS:ND1	4:C:701:HOH:O	2.34	0.51
1:D:157:ASP:OD1	1:D:159:ILE:HG22	2.09	0.51
1:C:394:MET:HE1	1:D:394:MET:HG3	1.94	0.50
1:C:91:ILE:HG21	1:C:313:VAL:HG22	1.94	0.49
1:A:91:ILE:HG21	1:A:313:VAL:HG22	1.94	0.49
1:B:143:TRP:HB2	1:B:340:PRO:HD3	1.95	0.49
1:D:143:TRP:HB2	1:D:340:PRO:HD3	1.95	0.49
1:B:91:ILE:HG21	1:B:313:VAL:HG22	1.94	0.48
1:D:91:ILE:HG21	1:D:313:VAL:HG22	1.94	0.48
1:C:143:TRP:HB2	1:C:340:PRO:HD3	1.95	0.48
1:A:146:VAL:HG22	1:A:334:PHE:HB3	1.95	0.48
1:A:143:TRP:HB2	1:A:340:PRO:HD3	1.95	0.48
1:C:146:VAL:HG22	1:C:334:PHE:HB3	1.95	0.48
1:B:146:VAL:HG22	1:B:334:PHE:HB3	1.95	0.47
1:D:146:VAL:HG22	1:D:334:PHE:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:HIS:CE1	1:B:116:VAL:HG22	2.51	0.46
1:D:75:HIS:CE1	1:D:116:VAL:HG22	2.51	0.45
1:A:75:HIS:CE1	1:A:116:VAL:HG22	2.51	0.44
1:B:335:ASP:OD1	1:B:362:HIS:ND1	2.51	0.44
1:C:75:HIS:CE1	1:C:116:VAL:HG22	2.51	0.44
1:D:335:ASP:OD1	1:D:362:HIS:ND1	2.51	0.44
1:A:335:ASP:OD1	1:A:362:HIS:ND1	2.51	0.44
1:A:368:PRO:HG3	1:B:66:ARG:HD3	1.98	0.44
1:C:335:ASP:OD1	1:C:362:HIS:ND1	2.51	0.44
1:C:368:PRO:HG3	1:D:66:ARG:HD3	1.99	0.44
1:C:66:ARG:HD3	1:D:368:PRO:HG3	1.99	0.44
1:A:66:ARG:HD3	1:B:368:PRO:HG3	1.99	0.44
1:B:83:GLY:HA3	1:B:317:VAL:O	2.19	0.43
1:D:83:GLY:HA3	1:D:317:VAL:O	2.19	0.42
1:A:83:GLY:HA3	1:A:317:VAL:O	2.19	0.41
1:C:83:GLY:HA3	1:C:317:VAL:O	2.19	0.41
1:A:154:PHE:CE1	1:A:195:GLN:HG3	2.57	0.40
1:A:411:ALA:HB1	1:A:412:PRO:CD	2.52	0.40
1:C:411:ALA:HB1	1:C:412:PRO:CD	2.52	0.40
1:B:232:CYS:HA	1:B:282:GLN:O	2.22	0.40
1:C:154:PHE:CE1	1:C:195:GLN:HG3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	501/527 (95%)	481 (96%)	19 (4%)	1 (0%)	47 55
1	B	501/527 (95%)	481 (96%)	19 (4%)	1 (0%)	47 55
1	C	501/527 (95%)	481 (96%)	19 (4%)	1 (0%)	47 55
1	D	501/527 (95%)	481 (96%)	19 (4%)	1 (0%)	47 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2004/2108 (95%)	1924 (96%)	76 (4%)	4 (0%)	50 55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	389	ASP
1	B	389	ASP
1	C	389	ASP
1	D	389	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	433/451 (96%)	426 (98%)	7 (2%)	62 76
1	B	433/451 (96%)	426 (98%)	7 (2%)	62 76
1	C	433/451 (96%)	426 (98%)	7 (2%)	62 76
1	D	433/451 (96%)	426 (98%)	7 (2%)	62 76
All	All	1732/1804 (96%)	1704 (98%)	28 (2%)	64 76

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	ASP
1	A	132	PHE
1	A	138	THR
1	A	150	THR
1	A	236	TYR
1	A	315	LYS
1	A	489	TYR
1	B	128	ASP
1	B	132	PHE
1	B	138	THR
1	B	150	THR

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Mol	Chain	Res	Type
1	B	236	TYR
1	B	315	LYS
1	B	489	TYR
1	C	128	ASP
1	C	132	PHE
1	C	138	THR
1	C	150	THR
1	C	236	TYR
1	C	315	LYS
1	C	489	TYR
1	D	128	ASP
1	D	132	PHE
1	D	138	THR
1	D	150	THR
1	D	236	TYR
1	D	315	LYS
1	D	489	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	GLN
1	A	492	HIS
1	B	168	GLN
1	B	492	HIS
1	C	168	GLN
1	C	492	HIS
1	D	168	GLN
1	D	492	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
2	NDP	D	601	-	45,52,52	0.64	0	53,80,80	0.84	2 (3%)
2	NDP	A	601	-	45,52,52	0.65	0	53,80,80	0.84	2 (3%)
2	NDP	C	601	-	45,52,52	0.65	0	53,80,80	0.84	2 (3%)
3	HEM	A	602	1	27,50,50	0.91	1 (3%)	17,82,82	1.78	5 (29%)
3	HEM	B	602	1	27,50,50	0.91	1 (3%)	17,82,82	1.78	5 (29%)
2	NDP	B	601	-	45,52,52	0.64	0	53,80,80	0.84	2 (3%)
3	HEM	C	602	1	27,50,50	0.92	1 (3%)	17,82,82	1.79	5 (29%)
3	HEM	D	602	1	27,50,50	0.91	1 (3%)	17,82,82	1.78	5 (29%)

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
2	NDP	D	601	-	-	3/30/77/77	0/5/5/5
2	NDP	A	601	-	-	2/30/77/77	0/5/5/5
2	NDP	C	601	-	-	3/30/77/77	0/5/5/5
3	HEM	A	602	1	-	0/6/54/54	-
3	HEM	B	602	1	-	0/6/54/54	-
2	NDP	B	601	-	-	2/30/77/77	0/5/5/5
3	HEM	C	602	1	-	0/6/54/54	-
3	HEM	D	602	1	-	0/6/54/54	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	HEM	C3B-C2B	-2.81	1.36	1.40
3	C	602	HEM	C3B-C2B	-2.81	1.36	1.40
3	B	602	HEM	C3B-C2B	-2.76	1.36	1.40
3	D	602	HEM	C3B-C2B	-2.74	1.36	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	602	HEM	CAD-CBD-CGD	-3.56	106.69	112.67
3	C	602	HEM	CAD-CBD-CGD	-3.56	106.69	112.67
3	A	602	HEM	CAD-CBD-CGD	-3.55	106.71	112.67
3	D	602	HEM	CAD-CBD-CGD	-3.54	106.73	112.67
3	B	602	HEM	CMA-C3A-C4A	-3.27	123.44	128.46
3	C	602	HEM	CMA-C3A-C4A	-3.26	123.46	128.46
3	D	602	HEM	CMA-C3A-C4A	-3.26	123.46	128.46
3	A	602	HEM	CMA-C3A-C4A	-3.24	123.48	128.46
2	C	601	NDP	C5A-C6A-N6A	2.59	124.29	120.35
3	A	602	HEM	CBA-CAA-C2A	-2.57	107.74	112.49
2	A	601	NDP	C5A-C6A-N6A	2.57	124.26	120.35
3	C	602	HEM	CBA-CAA-C2A	-2.57	107.74	112.49
3	B	602	HEM	CBA-CAA-C2A	-2.56	107.77	112.49
2	B	601	NDP	C5A-C6A-N6A	2.55	124.23	120.35
2	D	601	NDP	C5A-C6A-N6A	2.55	124.23	120.35
3	D	602	HEM	CBA-CAA-C2A	-2.54	107.80	112.49
2	C	601	NDP	C3D-C2D-C1D	2.36	105.92	101.43
2	A	601	NDP	C3D-C2D-C1D	2.36	105.92	101.43
2	D	601	NDP	C3D-C2D-C1D	2.36	105.91	101.43
2	B	601	NDP	C3D-C2D-C1D	2.35	105.89	101.43
3	A	602	HEM	CMA-C3A-C2A	2.18	129.05	124.94
3	B	602	HEM	CMA-C3A-C2A	2.18	129.05	124.94
3	C	602	HEM	CMA-C3A-C2A	2.16	129.02	124.94
3	D	602	HEM	CMA-C3A-C2A	2.15	128.99	124.94
3	C	602	HEM	CMC-C2C-C3C	2.06	128.53	124.68
3	B	602	HEM	CMC-C2C-C3C	2.05	128.52	124.68
3	D	602	HEM	CMC-C2C-C3C	2.04	128.50	124.68
3	A	602	HEM	CMC-C2C-C3C	2.02	128.45	124.68

There are no chirality outliers.

All (10) torsion outliers are listed below:

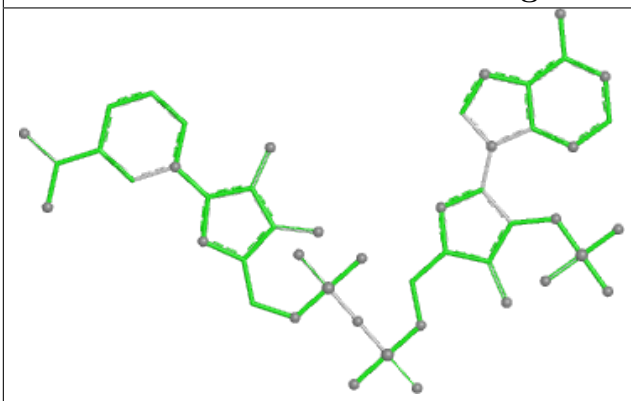
Mol	Chain	Res	Type	Atoms
2	A	601	NDP	O4D-C1D-N1N-C6N
2	B	601	NDP	O4D-C1D-N1N-C6N
2	C	601	NDP	O4D-C1D-N1N-C6N
2	D	601	NDP	O4D-C1D-N1N-C6N
2	A	601	NDP	O4B-C4B-C5B-O5B
2	B	601	NDP	O4B-C4B-C5B-O5B
2	C	601	NDP	O4B-C4B-C5B-O5B
2	D	601	NDP	O4B-C4B-C5B-O5B
2	C	601	NDP	PA-O3-PN-O2N
2	D	601	NDP	PA-O3-PN-O2N

There are no ring outliers.

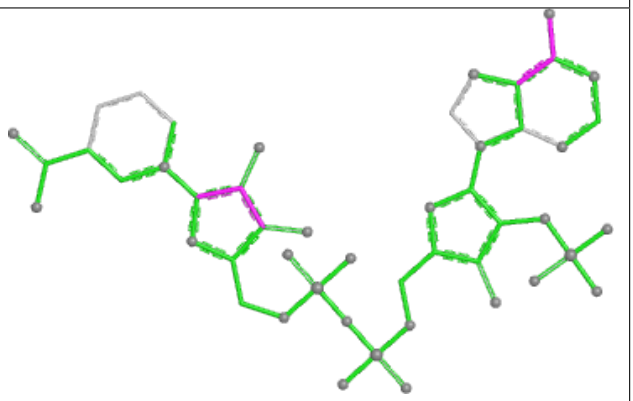
No monomer is involved in short contacts.

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.

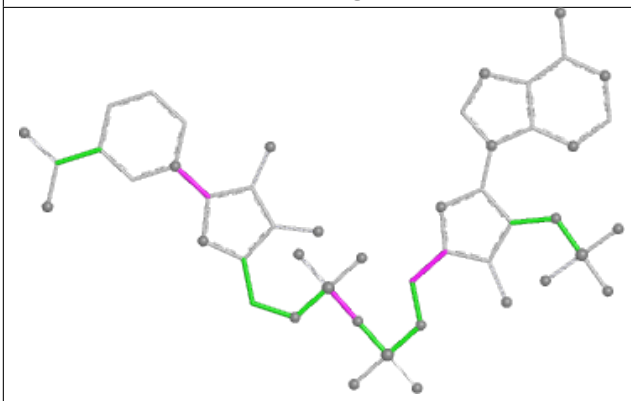
Ligand NDP D 601



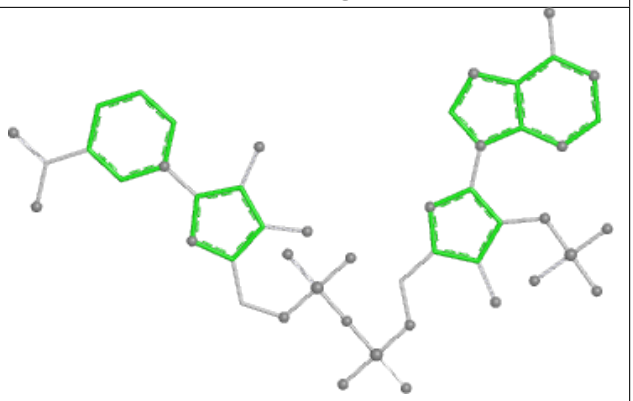
Bond lengths



Bond angles

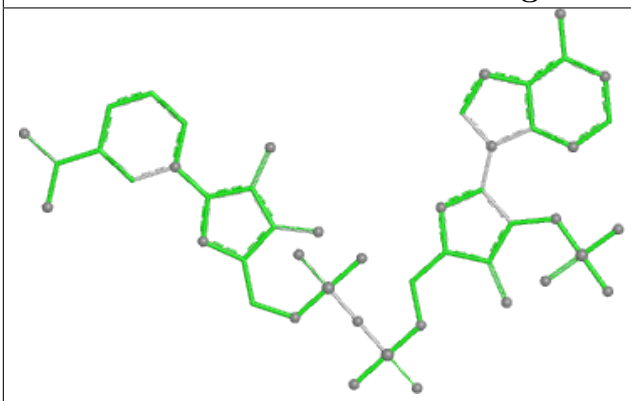


Torsions

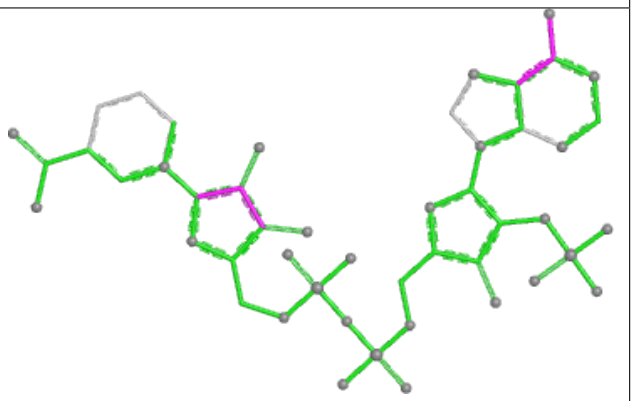


Rings

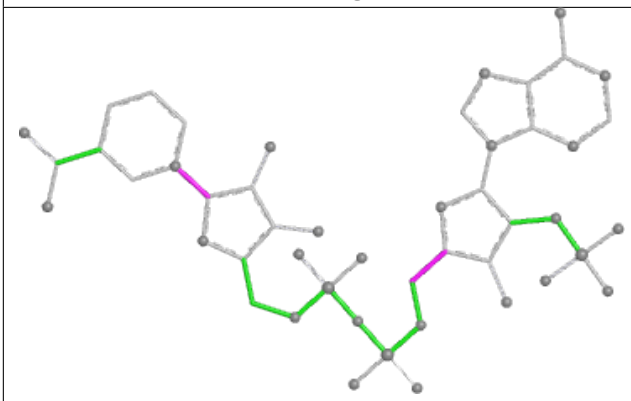
Ligand NDP A 601



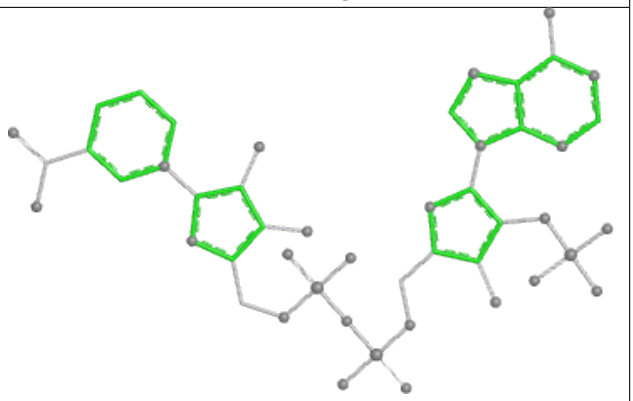
Bond lengths



Bond angles

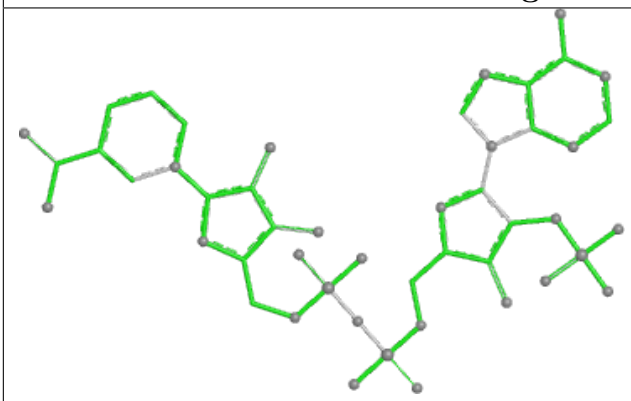


Torsions

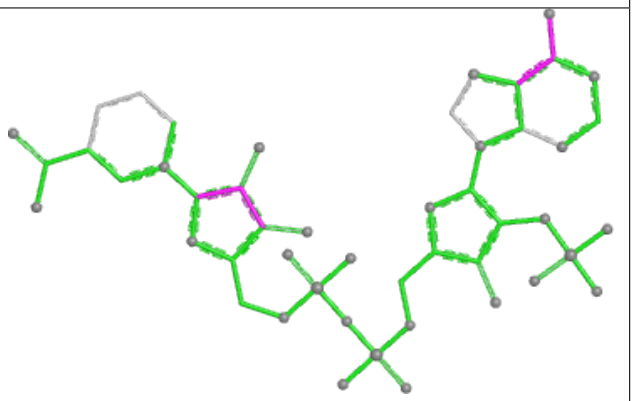


Rings

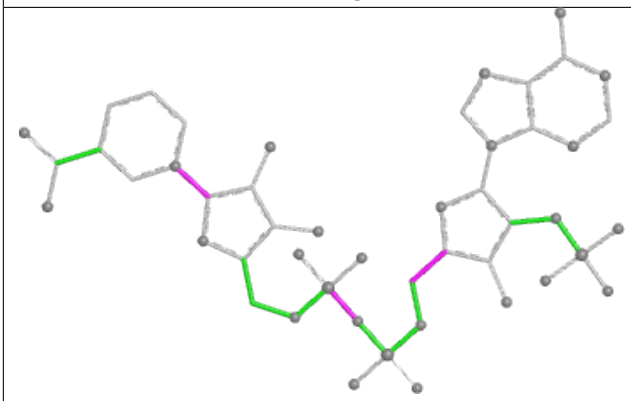
Ligand NDP C 601



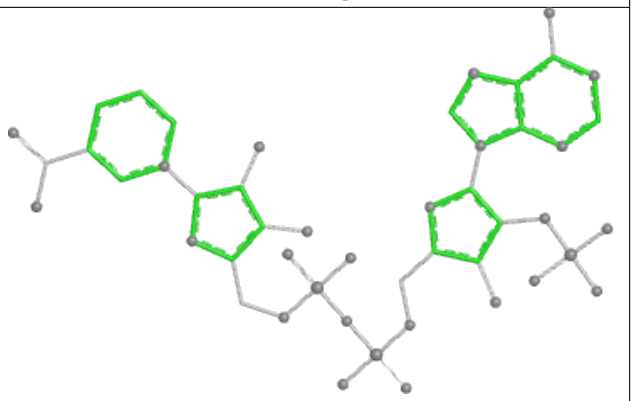
Bond lengths



Bond angles

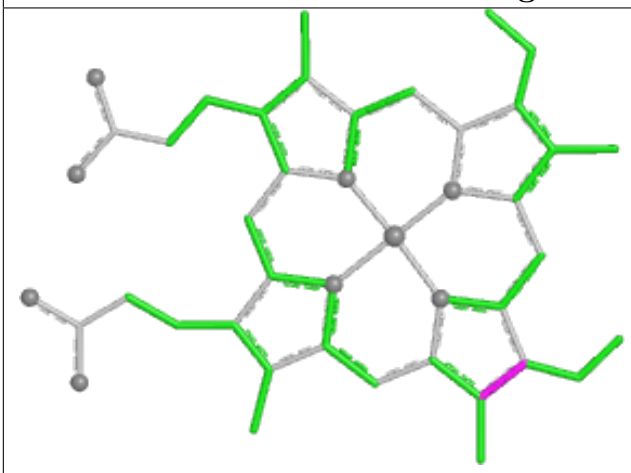


Torsions

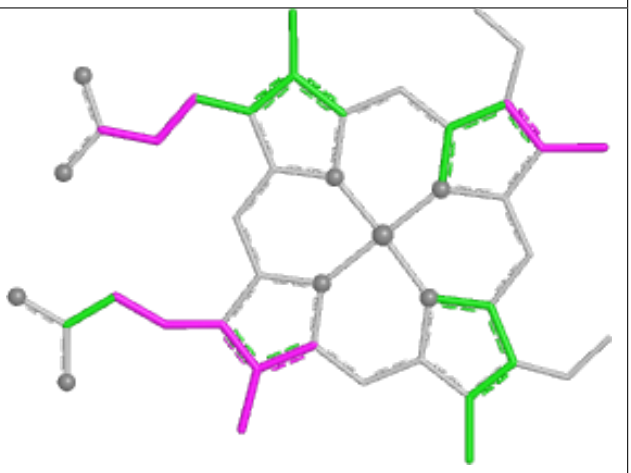


Rings

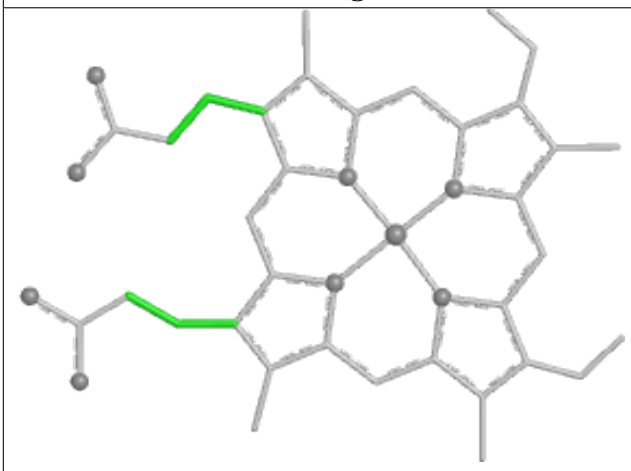
Ligand HEM A 602



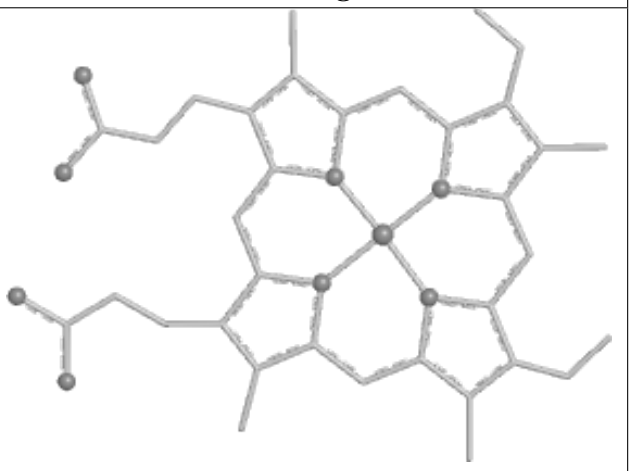
Bond lengths



Bond angles

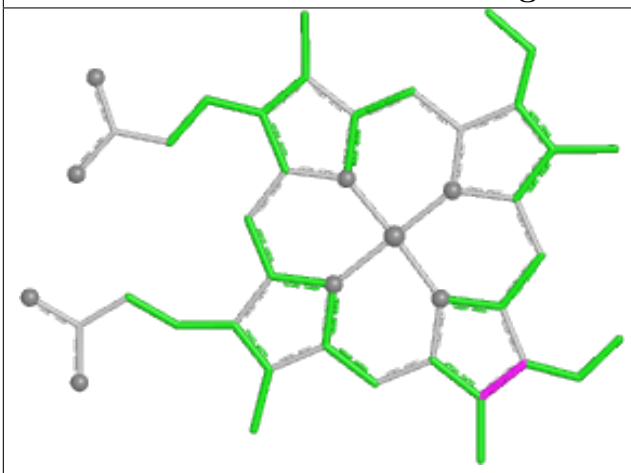


Torsions

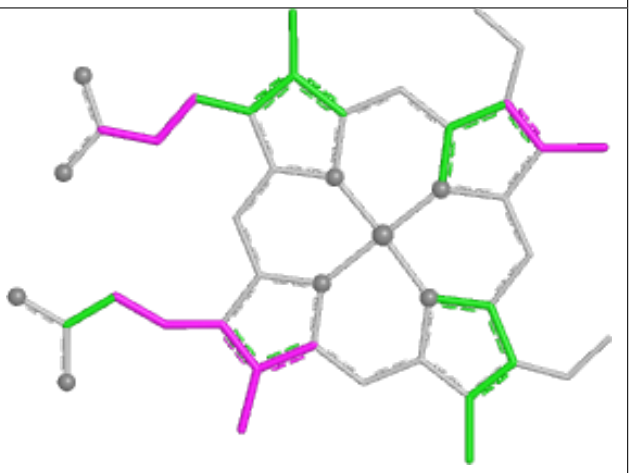


Rings

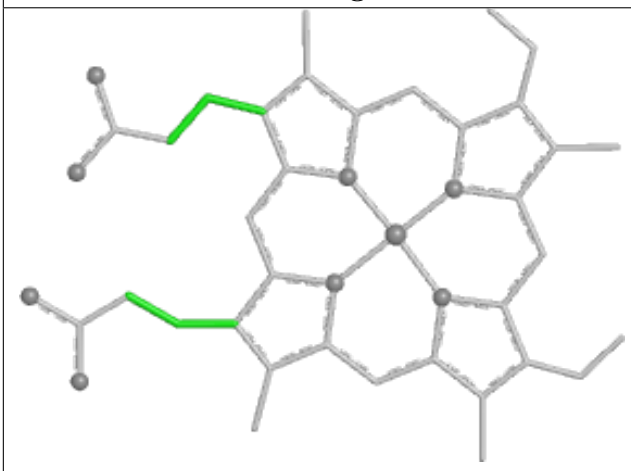
Ligand HEM B 602



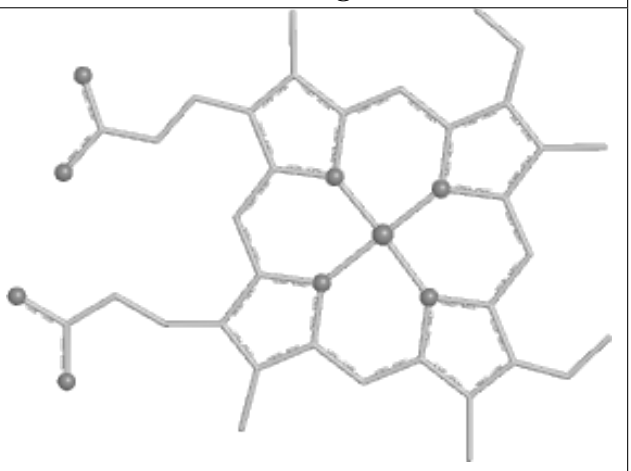
Bond lengths



Bond angles

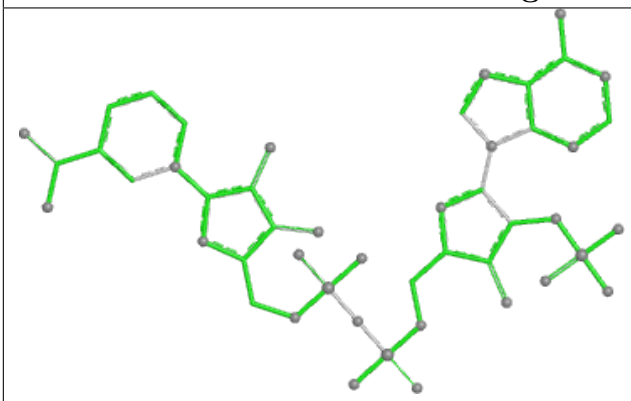


Torsions

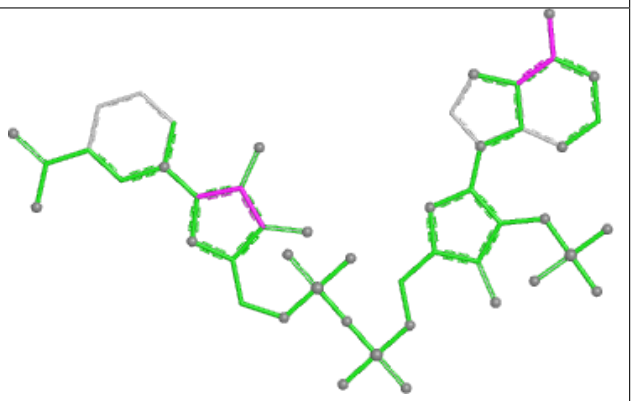


Rings

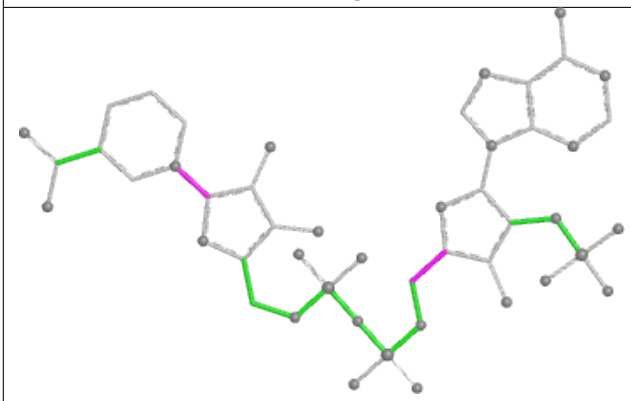
Ligand NDP B 601



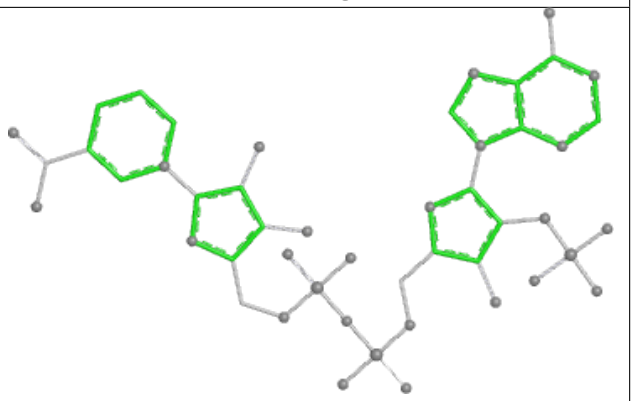
Bond lengths



Bond angles

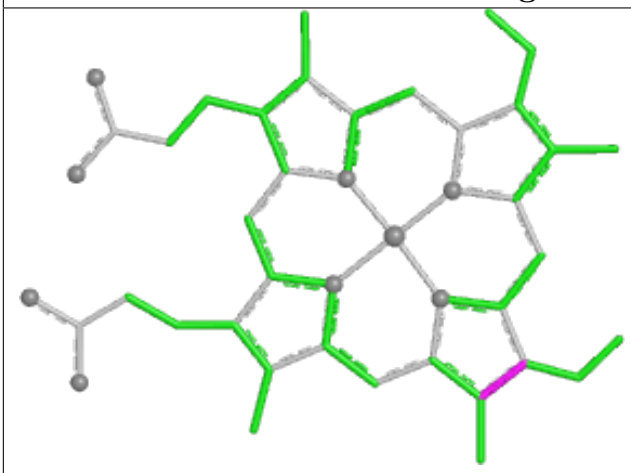


Torsions

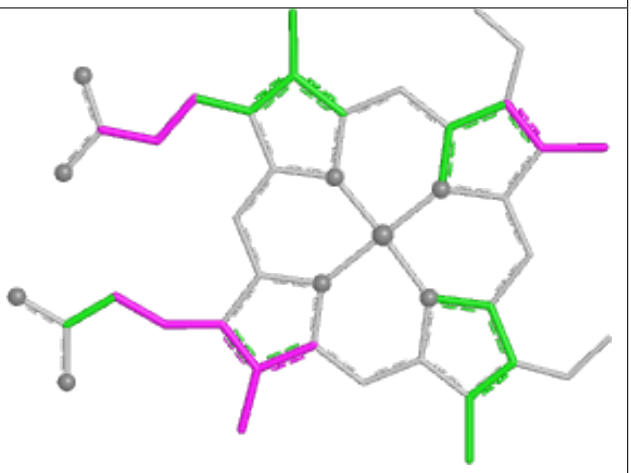


Rings

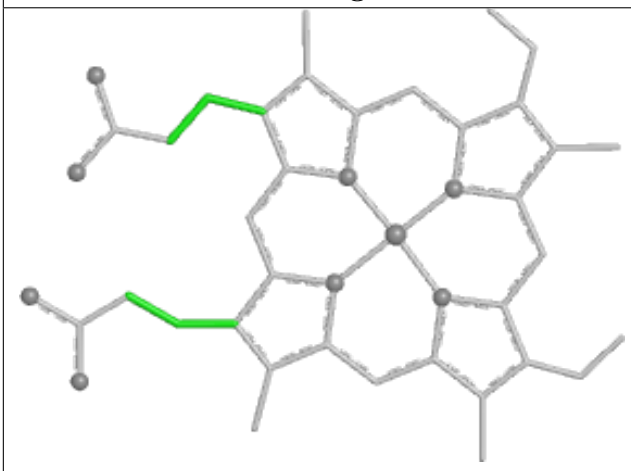
Ligand HEM C 602



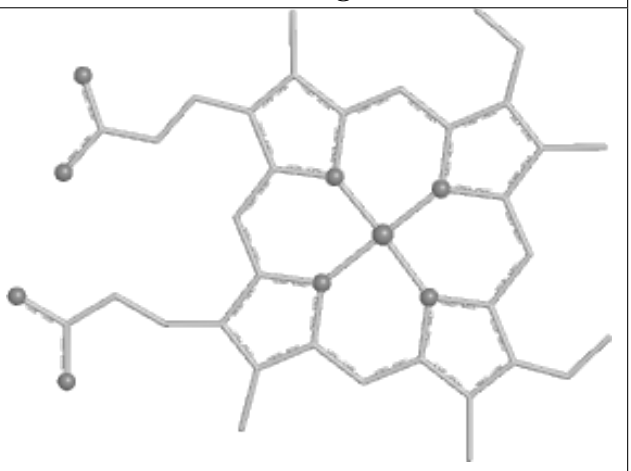
Bond lengths



Bond angles

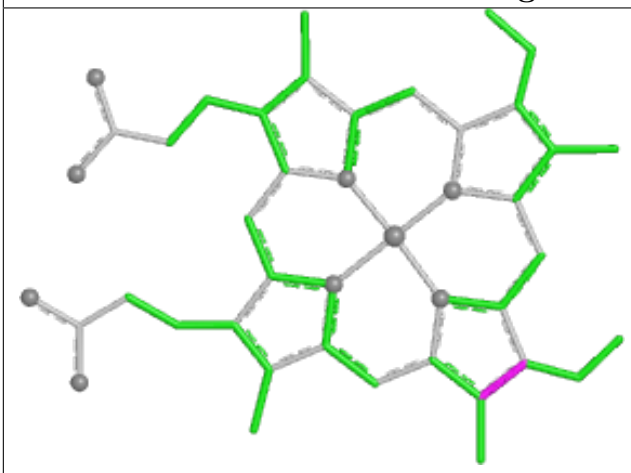


Torsions

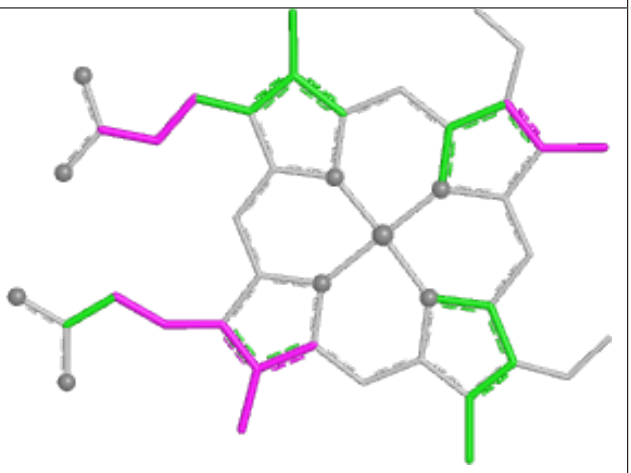


Rings

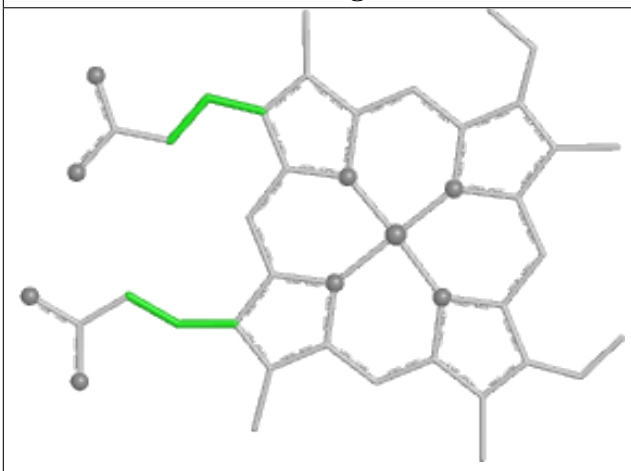
Ligand HEM D 602



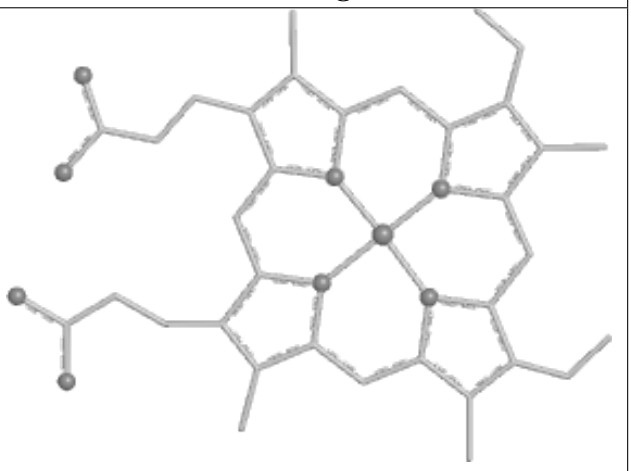
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

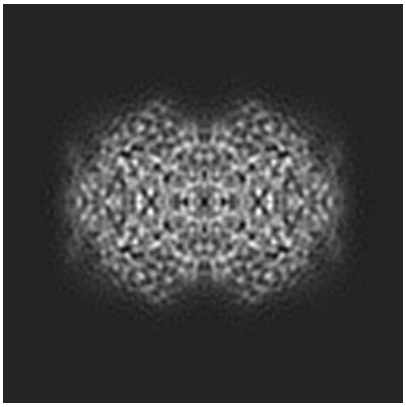
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13256. These allow visual inspection of the internal detail of the map and identification of artifacts.

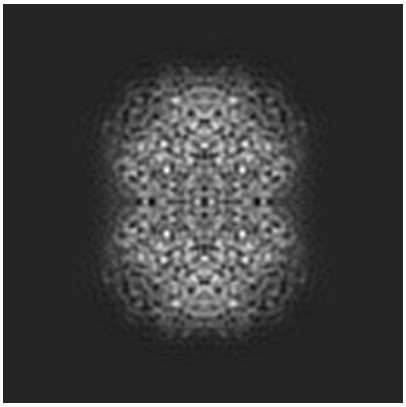
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

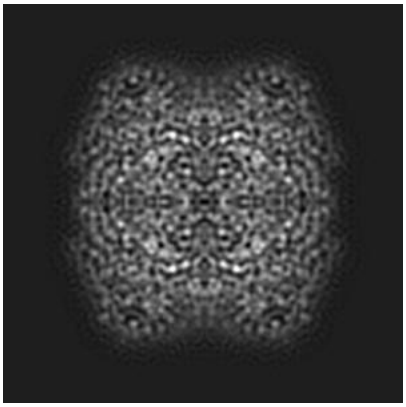
6.1.1 Primary map



X



Y

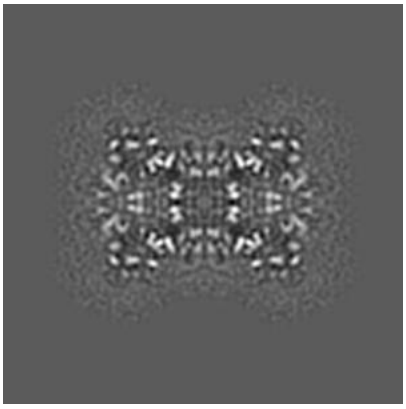


Z

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

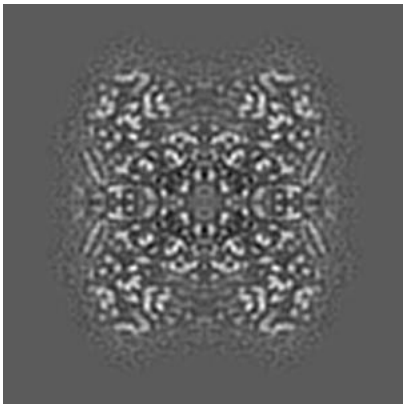
6.2 Central slices

6.2.1 Primary map



X Index: 64

Y Index: 64

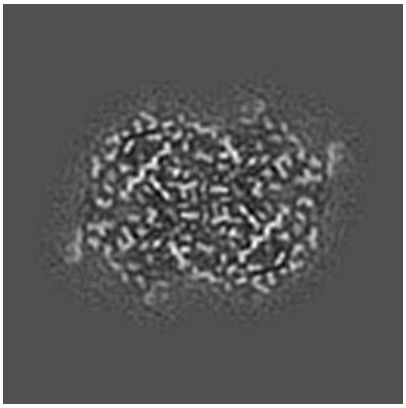


Z Index: 64

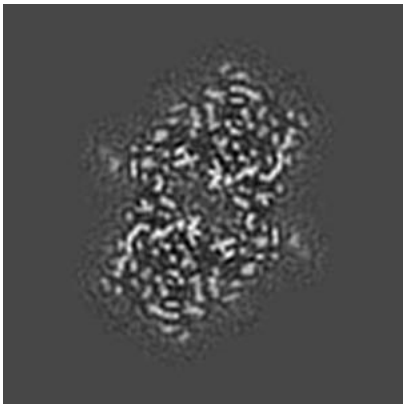
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

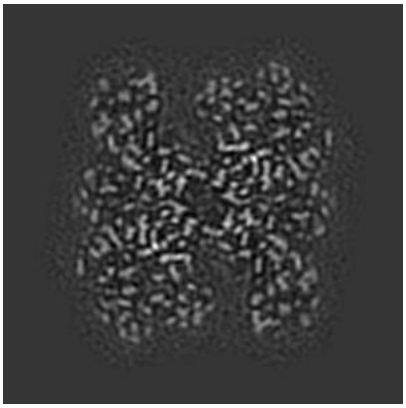
6.3.1 Primary map



X Index: 78



Y Index: 47

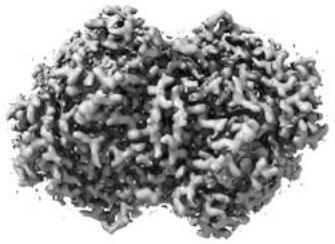


Z Index: 60

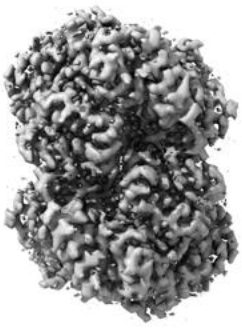
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

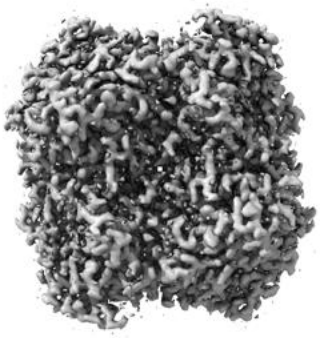
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

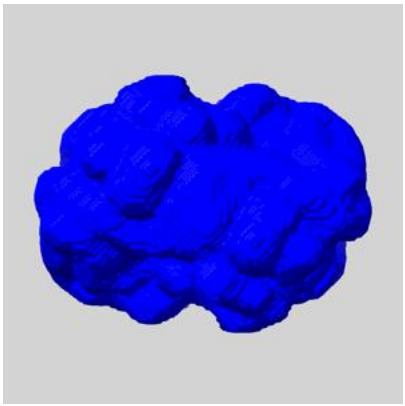
6.5 Mask visualisation (i)

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

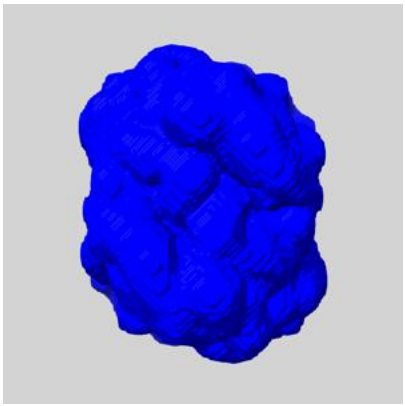
A mask typically either:

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

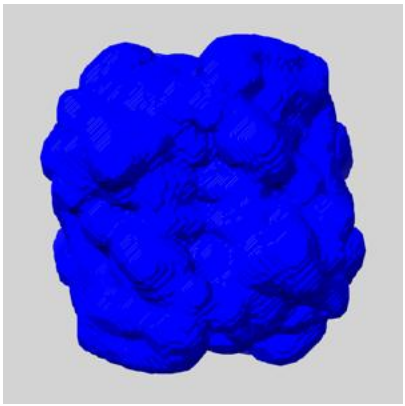
6.5.1 emd_13256_msk_1.map (i)



X



Y

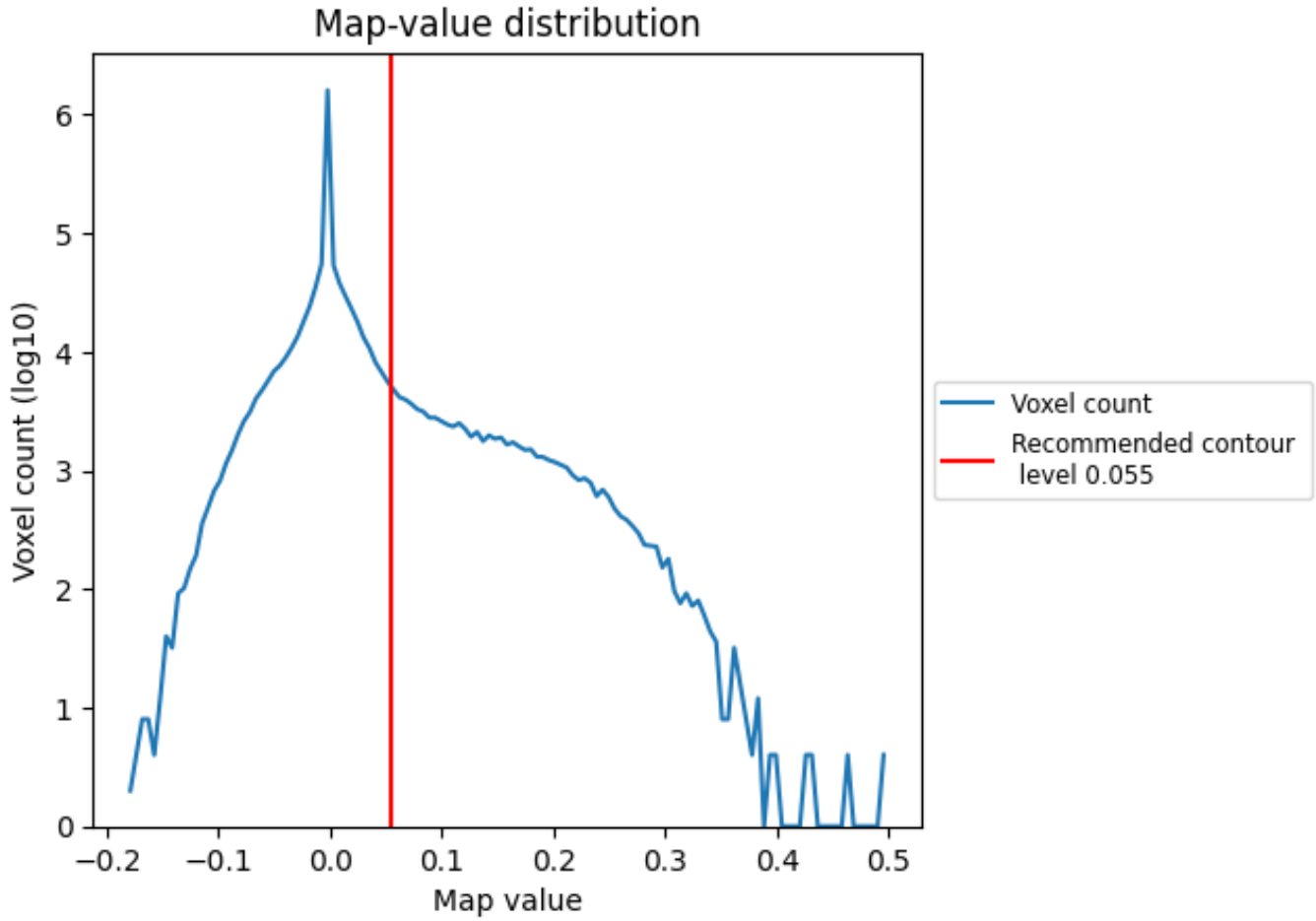


Z

7 Map analysis

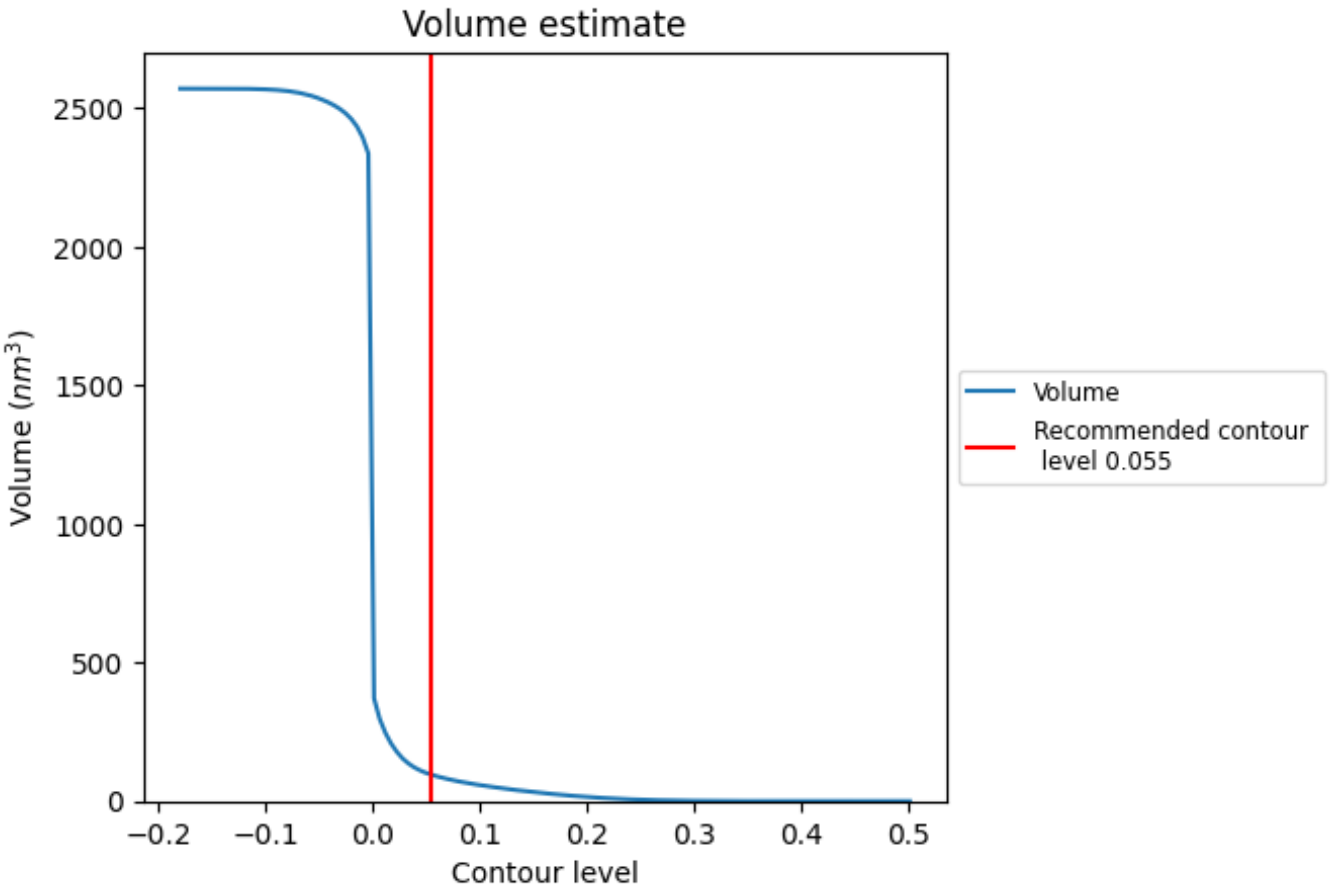
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

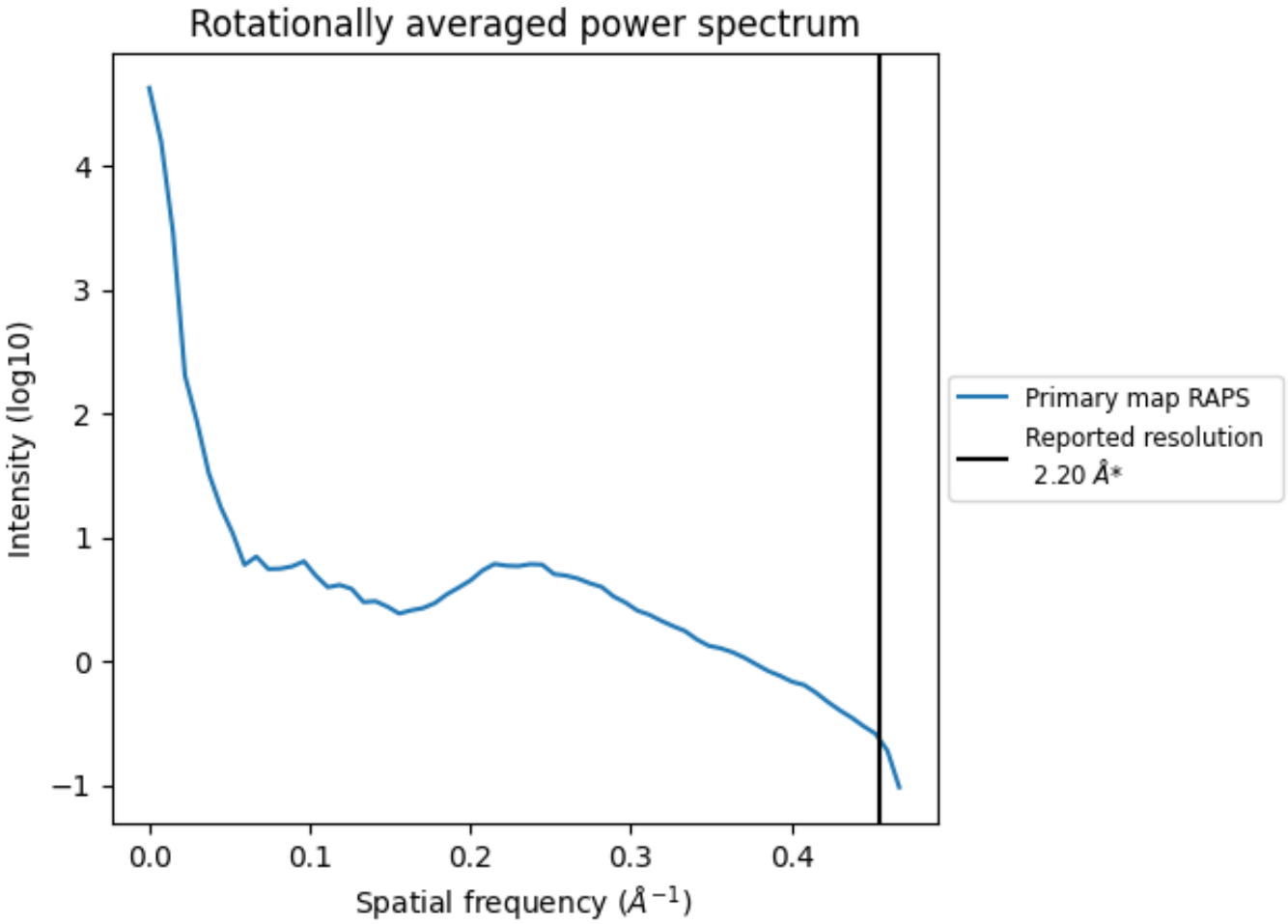
7.2 Volume estimate (i)



The volume at the recommended contour level is 96 nm^3; this corresponds to an approximate mass of 86 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)

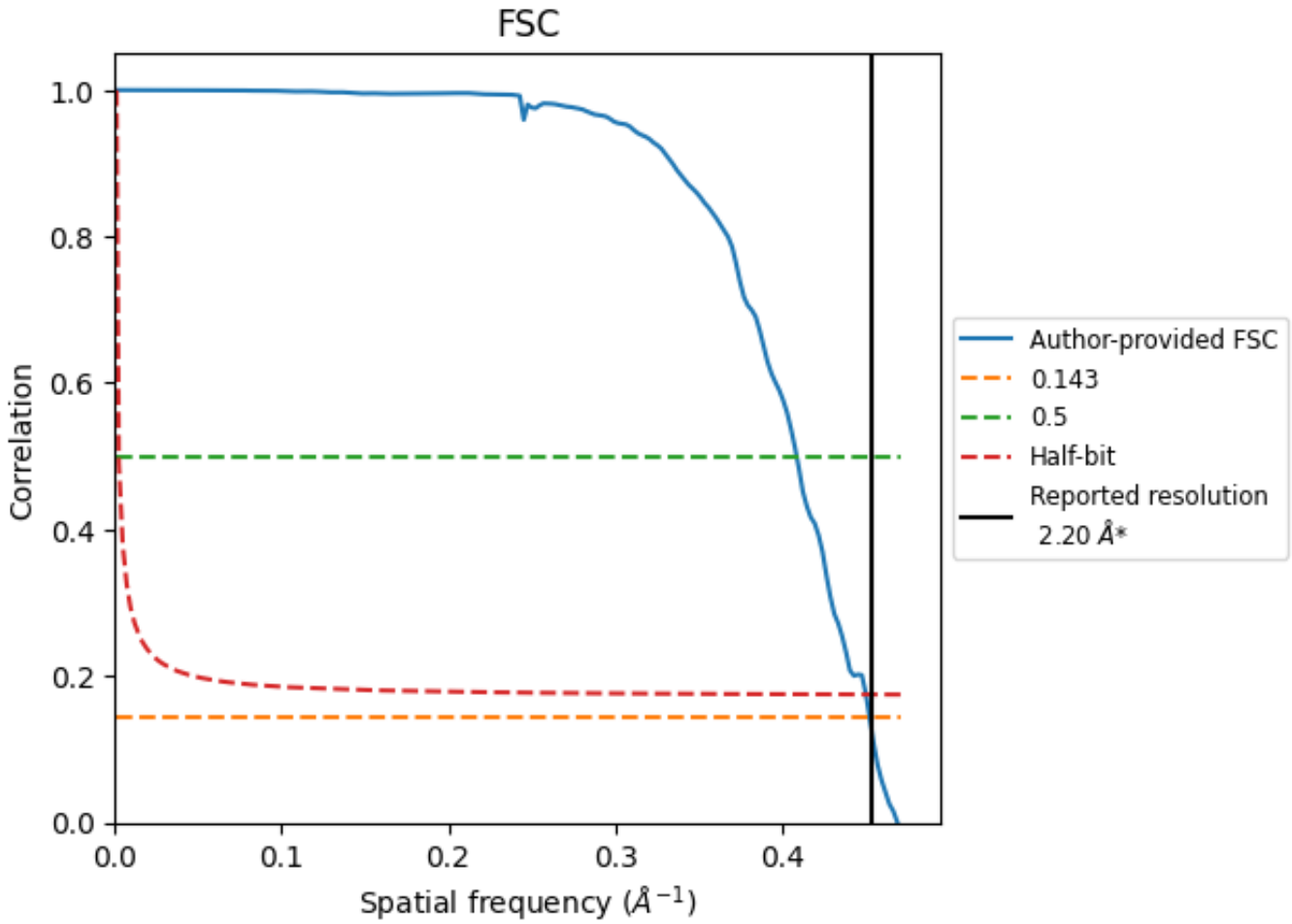


*Reported resolution corresponds to spatial frequency of 0.455 $Å^{-1}$

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 0.455 Å^{-1}

8.2 Resolution estimates (i)

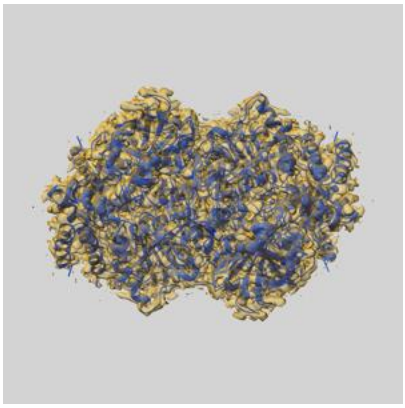
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.21	2.44	2.22
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

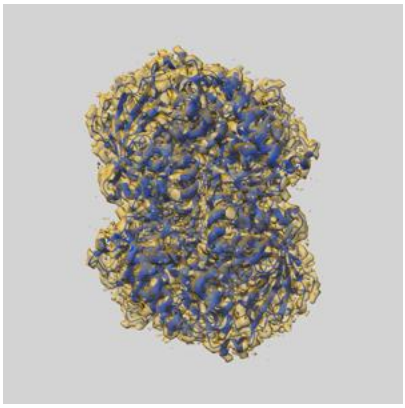
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13256 and PDB model 7P8W. Per-residue inclusion information can be found in section 3 on page 6.

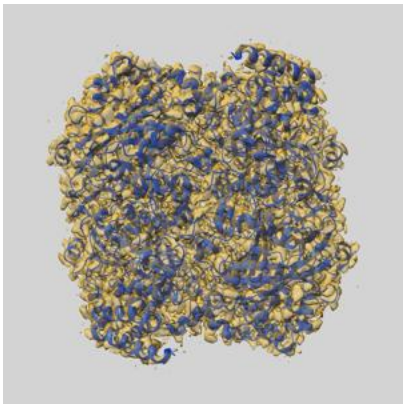
9.1 Map-model overlay



X



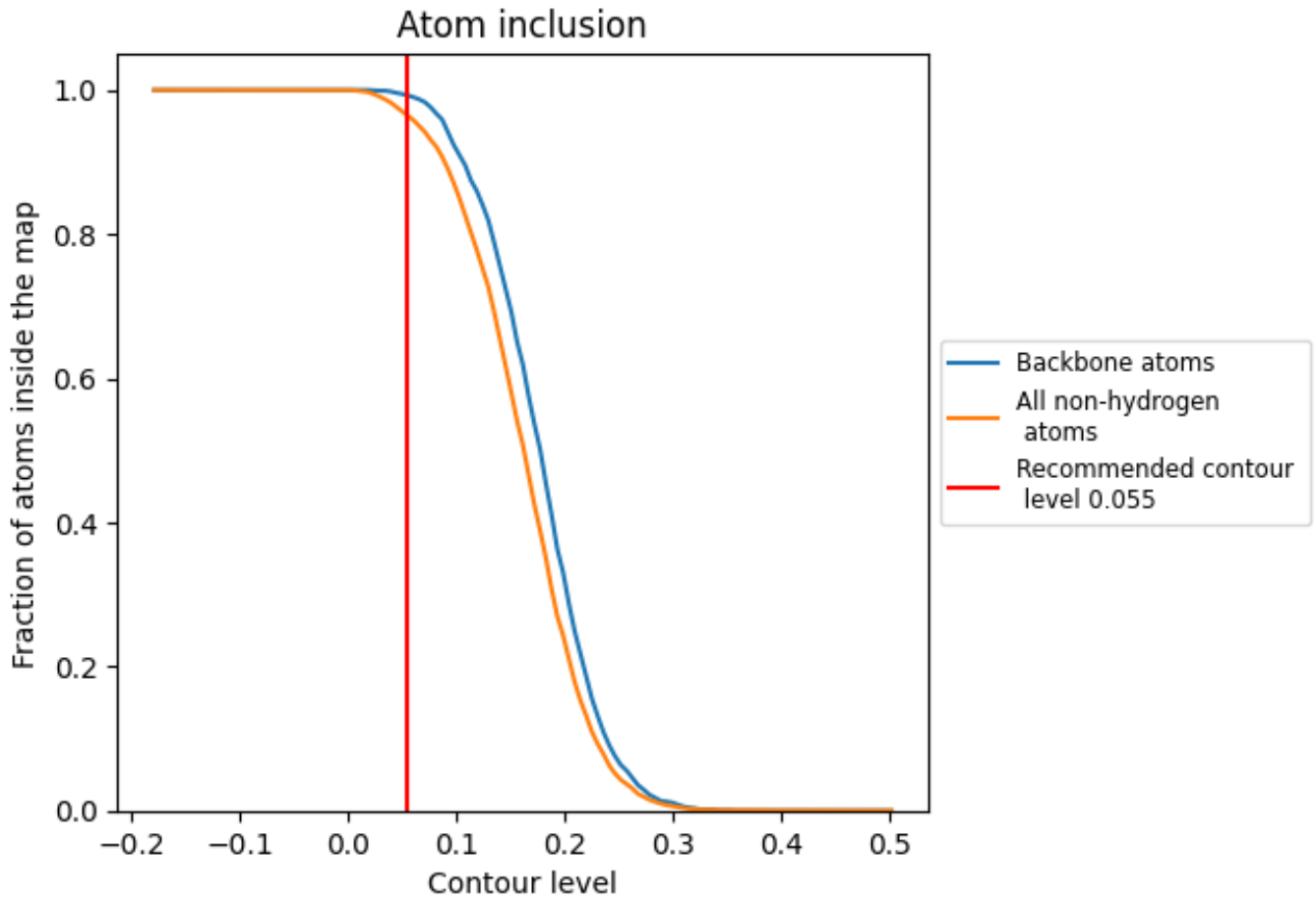
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.055 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 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.