



wwPDB EM Validation Summary Report ⓘ

Aug 5, 2026 – 05:18 AM EDT

PDB ID : 8T1J / pdb_00008t1j
EMDB ID : EMD-40969
Title : Uncrosslinked nNOS-CaM oxygenase homodimer
Authors : Lee, K.; Pospiech, T.H.; Southworth, D.
Deposited on : 2023-06-02
Resolution : 2.70 Å(reported)

This is a wwPDB EM Validation Summary 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.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

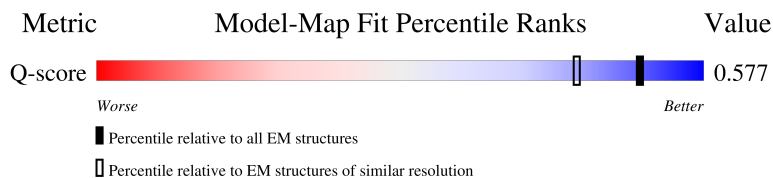
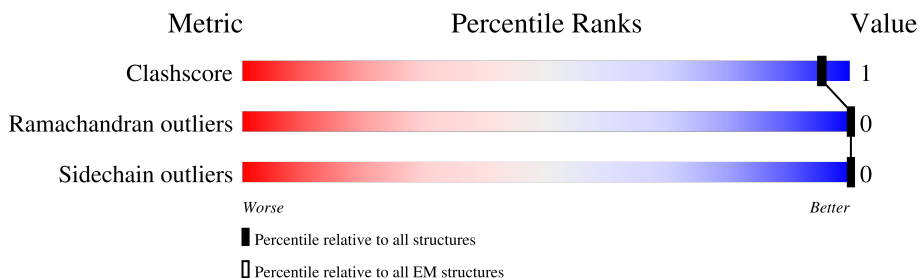
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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 $\leq 5\%$. 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	1429	 28% 71%
1	B	1429	 28% 71%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6973 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.

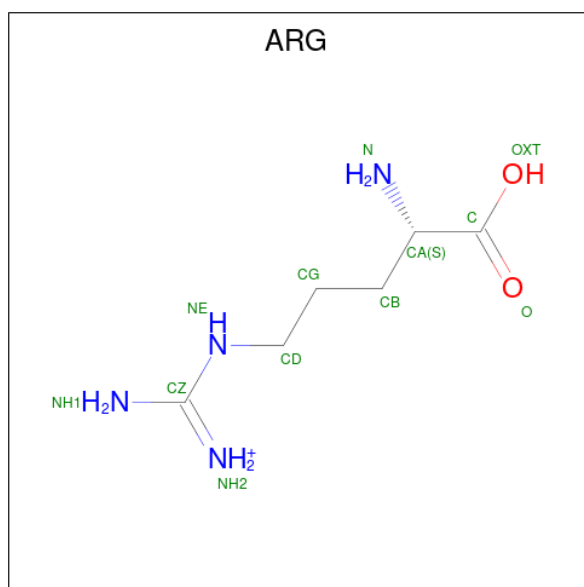
- Molecule 1 is a protein called Nitric oxide synthase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	419	Total	C	N	O	S	0	0
			3414	2181	588	624	21		
1	B	419	Total	C	N	O	S	0	0
			3414	2181	588	624	21		

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	

- Molecule 3 is ARGinine (CCD ID: ARG) (formula: C₆H₁₅N₄O₂) (labeled as "Ligand of Interest" by depositor).



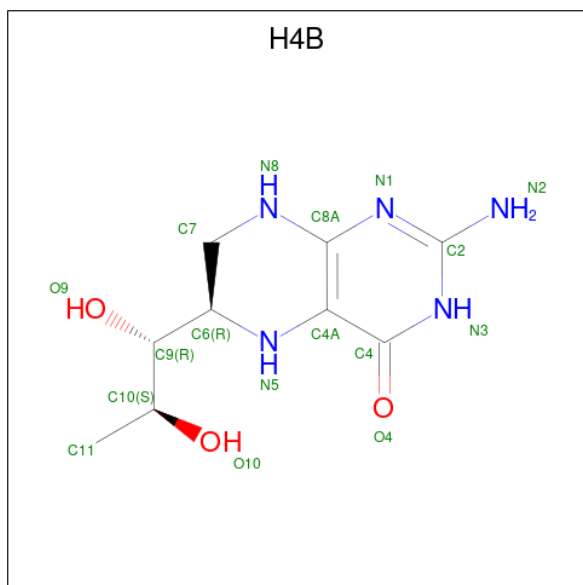
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			12	6	4	2	

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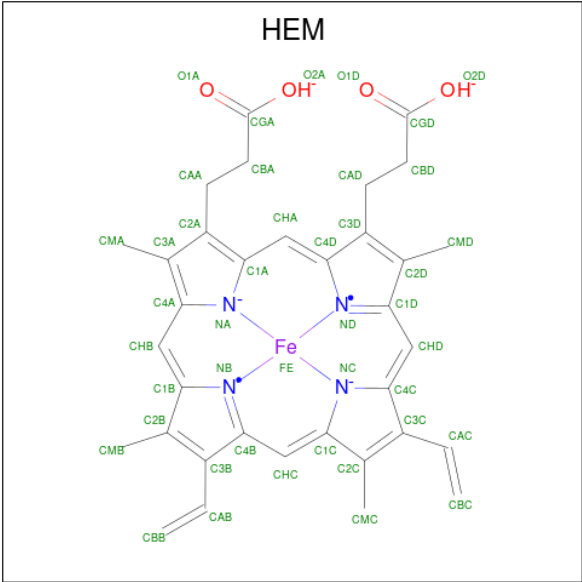
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	B	1	12	6	4	2	0

- Molecule 4 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: $C_9H_{15}N_5O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	17	9	5	3	0
4	B	1	17	9	5	3	0

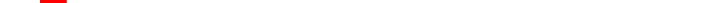
- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

GLU	GLY	CYS	VAL	LEU	PRO	LEU
VAL	GLY	ARG	VAL	LEU	PRO	VAL
THR	HIS	GLN	PRO	THR	THR	ASN
ASN	THR	SER	CYS	GLN	PRO	ALA
ARG	TYR	ILE	VAL	SER	LEU	LEU
LEU	VAL	ILE	ARG	LEU	GLN	ILE
ARG	CYS	ASP	ARG	LEU	GLU	GLU
SER	GLY	HIS	GLY	LEU	GLN	GLN
GLU	ASP	ILE	ALA	LEU	GLN	GLU
SER	VAL	TYR	PRO	PHE	PHE	GLU
ILE	THR	ARG	SER	ARG	ALA	ASP
ALA	MET	GLU	PHE	TYR	SER	ALA
PHE	ALA	GLU	HIS	TYR	LEU	PRO
ILE	ALA	THR	LEU	SER	ALA	ALA
GLU	ASP	GLN	PRO	SER	THR	ASN
GLU	VAL	GLN	ARG	SER	ASN	ASN
SER	LEU	ALA	ASN	SER	GLU	HIS
SER	LYS	LYS	PRO	SER	LYS	VAL
LYS	ALA	ASN	GLN	PRO	GLY	VAL
ASP	ILE	VAL	VAL	ASP	GLY	VAL
ALA	GLN	GLY	PRO	MET	GLN	VAL
ASP	ARG	VAL	CYS	TYR	ARG	GLU
GLU	ILE	PHE	ILE	PRO	LEU	MET
VAL	MET	ARG	LEU	ASP	LEU	LEU
PHE	THR	GLU	VAL	GLU	VAL	GLU
SER	GLN	LEU	GLY	VAL	LEU	GLU
SER	GLY	TYR	ILE	ALA	GLN	LEU
SER	LEU	TYR	GLY	VAL	LEU	ALA
GLU	GLN	GLN	ARG	ILE	GLY	LEU
GLU	GLY	ARG	ILE	ALA	GLN	LEU
GLU	GLU	ARG	ALA	ILE	GLY	GLY
GLU	GLU	GLU	PRO	VAL	TYR	VAL
GLU	ASP	PRO	PHE	PRO	SER	GLU
GLU	ALA	ASP	ARG	TYR	GLU	SER
GLY	GLY	ARG	SER	HIS	TRP	ASN
VAL	VAL	PRO	PHE	THR	LYS	TRP
PHE	PHE	LYS	TRP	ARG	LYS	TRP
ILE	ILE	LYS	GLN	ASP	GLY	ASP
SER	SER	TYR	GLN	GLY	LYS	GLU
ARG	ARG	VAL	ARG	GLU	ASN	SER
LEU	LEU	GLN	GLN	GLY	PRO	ARG
ARG	ARG	ASP	PHE	PRO	THR	LEU
ASP	ASP	VAL	ASP	VAL	MET	PRO
ASN	ASN	LEU	ILE	HIS	VAL	PRO
ARG	ASN	GLN	GLN	HIS	GLU	CYS
ARG	ARG	GLU	HIS	GLY	VAL	THR
TYR	TYR	GLN	LYS	VAL	LEU	ILE
HIS	HIS	LEU	GLY	CYS	GLU	PHE
GLU	GLU	ALA	MET	SER	GLU	GLN
ASP	ASP	GLU	ASN	SER	PHE	ALA
ILE	ILE	SER	PRO	TRP	PRO	LYS
PHE	PHE	VAL	CYS	LEU	SER	LYS
GLY	GLY	TYR	PRO	ASN	ILE	TYR
VAL	VAL	ARG	MET	ARG	GLN	TYR
THR	THR	ALA	VAL	ILE	MET	TYR
LEU	LEU	LEU	VAL	LEU	LEU	ASP
ARG	ARG	LYS	VAL	ALA	ALA	ILE
THR	THR	GLN	PHE	ASP	THR	THR

- Molecule 1: Nitric oxide synthase 1

Chain B:  28% 71%

ARG	VAL	MET	R481	D309	GLY	GLY	ASP	ARG	GLY	ASP	ARG	GLY	MET	GLU
ASN	THR	GLY	K486	D309	LYS	LYS	PRO	VAL	THR	PRO	VAL	THR	THR	GLU
PHE	THR	ALA	Q487	T321	SER	HIS	THR	THR	MET	ASN	GLN	THR	GLN	ILE
GLU	PHE	THR	P488	T321	LYS	LYS	LYS	PRO	LYS	LYS	PRO	PRO	ILE	ILE
SER	GLY	ALA	D489	G333	ALA	ALA	SER	GLY	SER	GLY	GLY	ALA	ALA	THR
THR	ASN	LYS	D489	G333	PRO	PRO	THR	THR	THR	THR	THR	VAL	VAL	GLY
ASN	GLY	LYS	G490	F338	ASP	ASP	LYS	LYS	LYS	PRO	ASN	ASN	ASN	GLY
GLY	GLY	VAL	S491	F338	PRO	PRO	ALA	ALA	ALA	ALA	THR	THR	THR	GLN
VAL	PRO	VAL	S491	F338	LEU	LEU	LEU	LEU	LEU	LEU	VAL	VAL	VAL	PRO
ALA	PRO	ALA	V499	Q340	GLY	GLY	GLN	GLN	GLN	GLN	ALA	ALA	ALA	LEU
ASN	GLU	THR	V499	Q340	ASP	ASP	ASP	ASP	ASP	ASP	VAL	VAL	VAL	LEU
GLU	ASN	ILE	N527	H341	ASN	ASN	ASN	ASN	ASN	ASN	GLN	GLN	GLN	PRO
THR	GLY	LEU	N527	H341	ASP	ASP	ASP	ASP	ILE	ILE	ASP	ASP	ASP	ASN
GLY	GLY	TYR	I546	R343	ARG	ARG	VAL	VAL	GLY	GLY	LEU	LEU	LEU	ASN
LYS	LYS	ALA	I546	R343	VAL	PHE	PHE	PHE	HIS	HIS	SER	SER	SER	THR
PHE	PHE	THR	C582	P345	ASN	ASN	ASN	ASP	ASP	GLU	GLN	GLN	GLN	VAL
GLY	GLY	GLU	C582	P345	ASP	ASP	ASP	ASP	GLU	LEU	LEU	LEU	LEU	ARG
CYS	CYS	THR	D615	E346	ASP	ASP	ILE	ILE	THR	THR	LYS	LYS	LYS	ARG
GLY	ALA	GLY	L616	D347	LEU	LEU	TRP	LEU	LEU	LEU	GLY	GLY	GLY	VAL
LEU	LEU	LYS	D617	V348	GLY	GLY	GLY	GLY	LYS	LYS	SER	SER	SER	PHE
GLU	GLU	GLN	M618	V348	LYS	LYS	LYS	GLU	GLU	GLU	ASP	ASP	ASP	ARG
ALA	MET	ALA	R619	K351	ASN	ASN	ASP	ASP	VAL	VAL	LYS	LYS	LYS	GLY
TYR	ARG	THR	R619	K351	ASN	ASN	GLU	GLU	GLU	GLU	GLN	GLN	GLN	LEU
PRO	HIS	ALA	D650	D352	VAL	VAL	VAL	VAL	PRO	PRO	SER	SER	SER	ARG
HIS	PRO	LYS	D650	D352	VAL	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	VAL
PHE	ASN	THR	S703	L354	VAL	VAL	VAL	SER	ASN	ASN	VAL	VAL	VAL	GLY
CYS	SER	LEU	S703	L354	ILE	ILE	SER	SER	SER	SER	VAL	VAL	VAL	GLY
ALA	VAL	CYS	N712	Q364	LEU	LEU	LEU	ILE	ILE	ILE	ASP	ASP	ASP	PHE
PHE	GLN	GLU	T713	Y365	ASN	ASN	ASN	ASN	LEU	LEU	ARG	ARG	ARG	GLU
GLY	GLY	ILE	T713	Y365	ASN	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR
HIS	ALA	PHE	H714	K370	PRO	PRO	PRO	VAL	ASN	ASN	VAL	VAL	VAL	VAL
ARG	ARG	GLU	V715	R371	TYR	TYR	GLY	GLY	GLY	GLY	THR	THR	THR	GLY
LYS	LYS	HIS	W716	R371	SER	SER	SER	SER	SER	SER	LEU	LEU	LEU	ARG
SER	SER	ALA	W716	R375	GLU	GLU	GLU	LYS	LYS	LYS	LEU	LEU	LEU	VAL
TYR	TYR	PHE	GLY	K375	LYS	LYS	LYS	ASN	ALA	ALA	ASN	ASN	ASN	SER
LYS	LYS	ASP	THR	K375	GLY	GLY	GLY	GLY	ALA	ALA	GLY	GLY	GLY	LEU
VAL	VAL	ALA	ASN	K378	THR	THR	THR	THR	ASN	ASN	PRO	PRO	PRO	LYS
ARG	ARG	LYS	GLY	D379	SER	SER	SER	ARG	GLN	GLN	PRO	PRO	PRO	PRO
PHE	PHE	ALA	THR	D379	SER	SER	PRO	GLY	GLY	GLY	HIS	HIS	HIS	VAL
ASN	ASN	MET	PRO	K386	THR	THR	THR	GLY	GLY	PRO	ALA	ALA	ALA	GLY
SER	SER	THR	THR	K386	SER	SER	SER	THR	THR	THR	GLY	GLY	GLY	THR
GLY	GLY	MET	LYS	F399	GLY	GLY	GLY	ALA	ALA	ALA	GLY	GLY	GLY	THR
GLU	GLU	ARG	ARG	F399	GLN	GLN	GLN	SER	ALA	ALA	HIS	HIS	HIS	LEU
ILE	ILE	THR	THR	D398	SER	SER	SER	PRO	PRO	PRO	GLU	GLU	GLU	ARG
LEU	LEU	ALA	ALA	D398	PRO	PRO	PRO	MET	MET	MET	GLY	GLY	GLY	GLY
LEU	LEU	ILE	ILE	A408	THR	THR	THR	ALA	ALA	ALA	GLY	GLY	GLY	THR
LYS	LYS	GLY	GLY	A408	LYS	LYS	LYS	ASN	ASN	ASN	GLY	GLY	GLY	THR
VAL	VAL	PHE	PHE	C415	ASN	ASN	GLY	THR	THR	THR	VAL	VAL	VAL	THR
GLU	GLU	LYS	LYS	C415	SER	SER	GLY	ILE	ILE	ILE	GLN	GLN	GLN	ASP
GLY	GLY	LEU	LEU	R418	GLY	GLY	SER	THR	THR	THR	GLY	GLY	GLY	GLY
THR	THR	LYS	LYS	R418	PRO	PRO	PRO	THR	THR	THR	THR	THR	THR	THR
SER	SER	HIS	HIS	T433	ASN	ASN	ASN	VAL	VAL	VAL	GLN	GLN	GLN	ASP
GLY	GLY	ALA	ALA	T433	SER	SER	SER	ARG	ARG	ARG	VAL	VAL	VAL	THR
ASP	ASP	GLU	GLU	G437	ARG	ARG	ARG	GLY	GLY	GLY	ASP	ASP	ASP	GLY
GLY	GLY	VAL	VAL	G437	CYS	CYS	CYS	THR	THR	THR	GLY	GLY	GLY	LYS
VAL	VAL	LEU	LEU	F462	THR	THR	THR	ASP	ASP	ASP	VAL	VAL	VAL	LYS
THR	THR	PHE	PHE	F462	LYS	LYS	LYS	GLY	GLY	GLY	ALA	ALA	ALA	THR
GLN	GLN	ILE	ILE	R299	R298	R298	R298	ASP	ASP	ASP	THR	THR	THR	THR



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138304	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 ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	8.483	Depositor
Minimum map value	-5.012	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.121	Depositor
Recommended contour level	1.6	Depositor
Map size (Å)	338.88, 338.88, 338.88	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, HEM, H4B

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	0.62	0/3511	0.96	10/4764 (0.2%)
1	B	0.61	0/3511	0.98	10/4764 (0.2%)
All	All	0.61	0/7022	0.97	20/9528 (0.2%)

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	LEU	N-CA-C	7.13	119.13	111.36
1	B	354	LEU	N-CA-C	7.12	119.12	111.36
1	B	499	VAL	N-CA-C	6.00	116.17	110.42
1	A	712	ASN	N-CA-C	-5.96	105.66	113.17
1	B	712	ASN	N-CA-C	-5.92	105.70	113.17

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3414	0	3322	6	0
1	B	3414	0	3322	7	0
2	A	1	0	0	0	0
3	A	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	12	0	0
4	A	17	0	15	0	0
4	B	17	0	15	0	0
5	A	43	0	30	0	0
5	B	43	0	30	0	0
All	All	6973	0	6758	13	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.

The worst 5 of 13 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:462:PHE:HB3	1:A:463:PRO:HD2	1.97	0.47
1:B:462:PHE:HB3	1:B:463:PRO:HD2	1.97	0.46
1:A:715:VAL:O	1:A:716:TRP:HB2	2.17	0.45
1:B:715:VAL:O	1:B:716:TRP:HB2	2.18	0.44
1:A:650:ASP:OD1	1:A:650:ASP:C	2.61	0.44

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	417/1429 (29%)	407 (98%)	10 (2%)	0	100	100
1	B	417/1429 (29%)	407 (98%)	10 (2%)	0	100	100
All	All	834/2858 (29%)	814 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	375/1241 (30%)	375 (100%)	0	100	100
1	B	375/1241 (30%)	375 (100%)	0	100	100
All	All	750/2482 (30%)	750 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	525	GLN
1	A	527	ASN
1	A	714	HIS
1	B	527	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	HEM	A	1504	-	50,50,50	1.50	4 (8%)	67,82,82	1.16	7 (10%)
4	H4B	B	1502	-	17,18,18	1.48	4 (23%)	14,26,26	1.93	2 (14%)
5	HEM	B	1503	-	50,50,50	1.56	7 (14%)	67,82,82	1.29	7 (10%)
3	ARG	B	1501	-	10,11,11	0.66	0	9,13,13	0.38	0
4	H4B	A	1503	-	17,18,18	1.66	5 (29%)	14,26,26	1.90	3 (21%)
3	ARG	A	1502	-	10,11,11	0.70	0	9,13,13	0.26	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	A	1504	-	-	4/14/54/54	-
4	H4B	B	1502	-	-	0/8/17/17	0/2/2/2
5	HEM	B	1503	-	-	5/14/54/54	-
3	ARG	B	1501	-	-	0/11/11/11	-
4	H4B	A	1503	-	-	0/8/17/17	0/2/2/2
3	ARG	A	1502	-	-	2/11/11/11	-

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1504	HEM	FE-NC	6.72	2.17	1.95
5	B	1503	HEM	FE-NC	5.82	2.14	1.95
4	A	1503	H4B	C4A-N5	3.88	1.47	1.37
5	B	1503	HEM	FE-NA	3.19	2.05	1.95
5	A	1504	HEM	FE-NA	3.17	2.05	1.95

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1503	H4B	C2-N1-C8A	5.22	122.57	113.36
4	B	1502	H4B	C2-N1-C8A	5.19	122.52	113.36
5	A	1504	HEM	CHD-C4C-NC	-3.69	120.44	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1502	H4B	N3-C2-N1	-3.37	117.15	123.32
5	B	1503	HEM	C3B-C2B-C1B	3.37	108.94	106.41

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

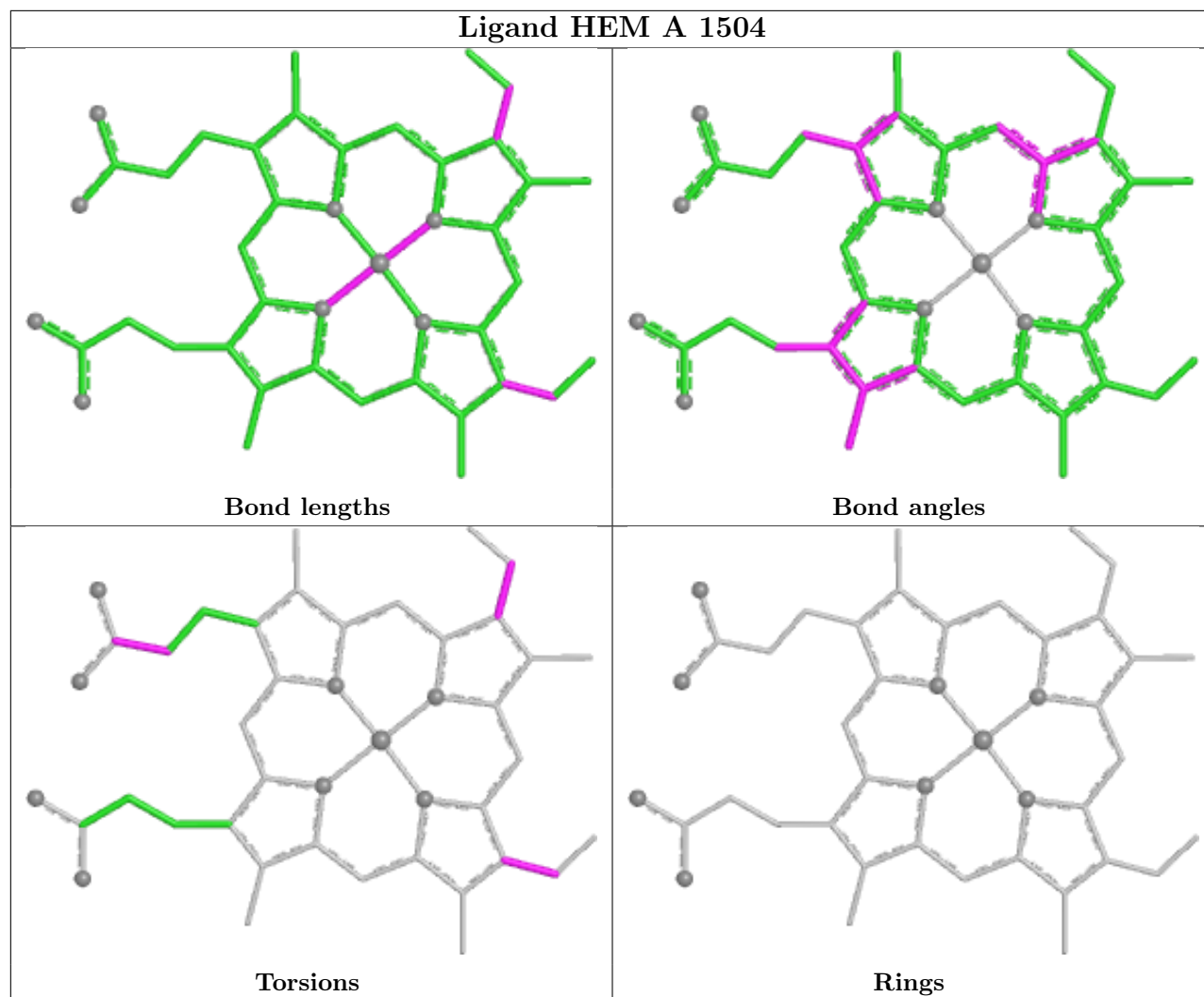
Mol	Chain	Res	Type	Atoms
5	A	1504	HEM	C2B-C3B-CAB-CBB
5	A	1504	HEM	C4B-C3B-CAB-CBB
5	B	1503	HEM	C2B-C3B-CAB-CBB
5	B	1503	HEM	C4B-C3B-CAB-CBB
3	A	1502	ARG	OXT-C-CA-CB

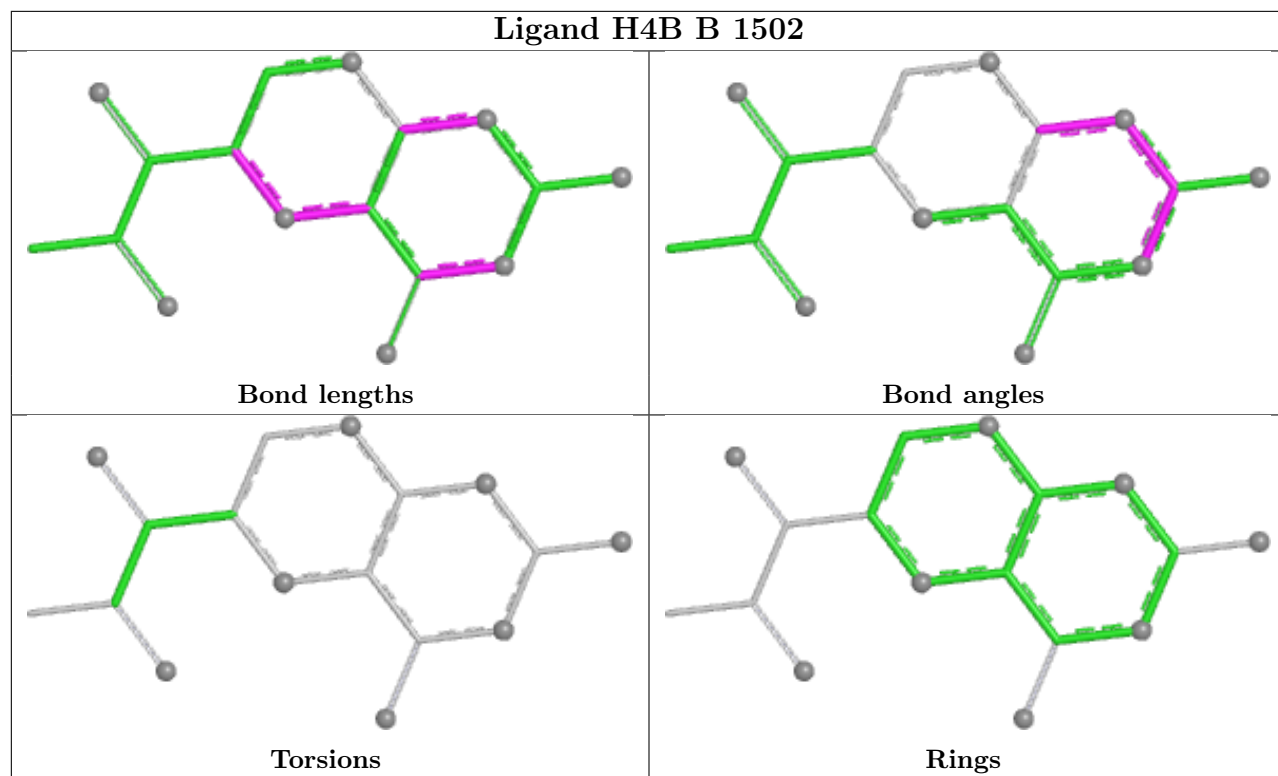
There are no ring outliers.

No monomer is involved in short contacts.

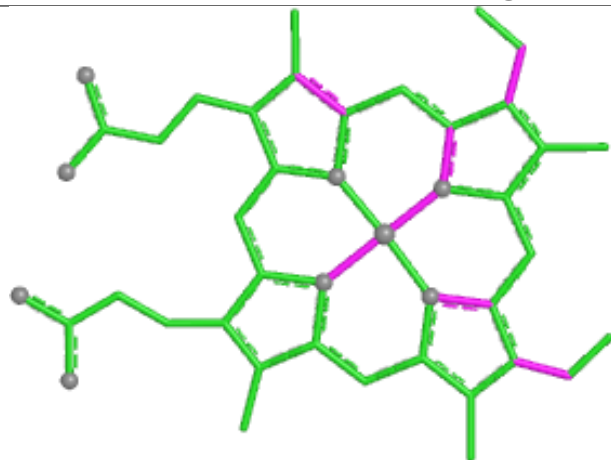
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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 1504

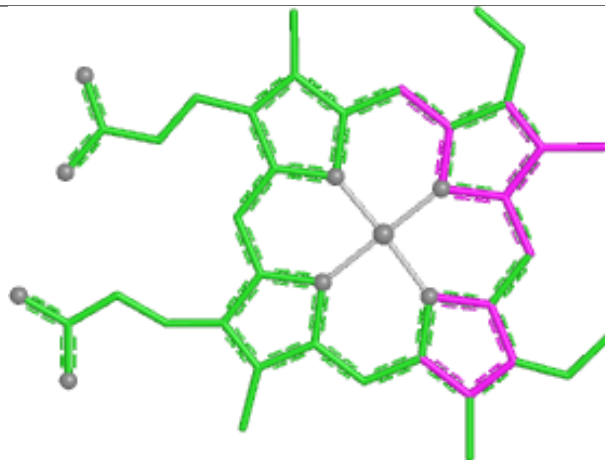




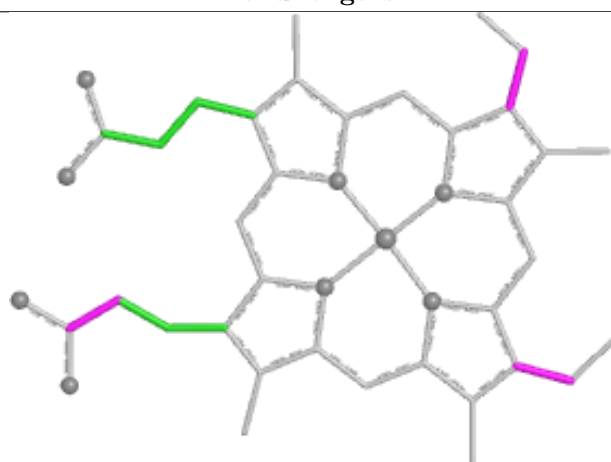
Ligand HEM B 1503



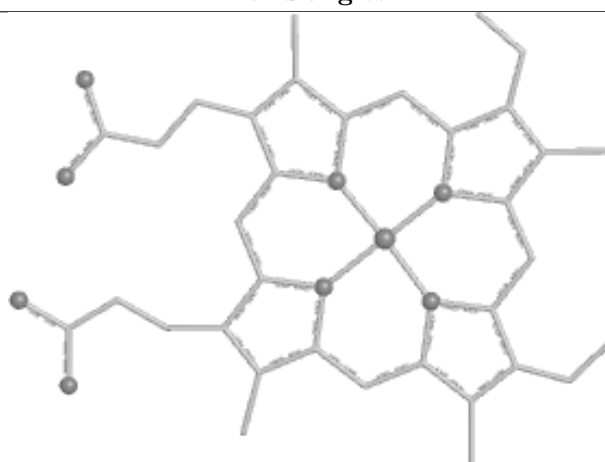
Bond lengths



Bond angles

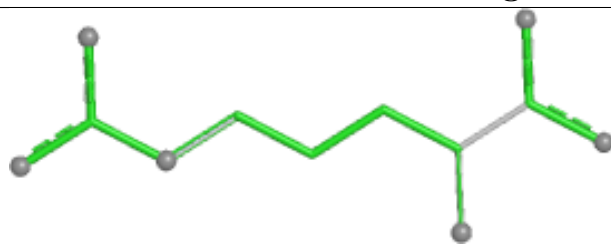


Torsions

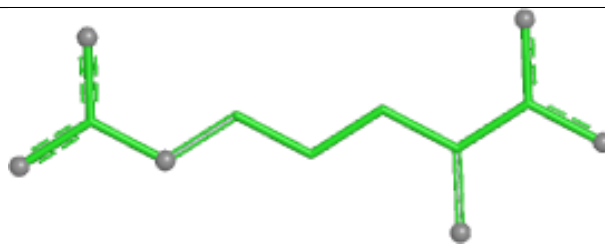


Rings

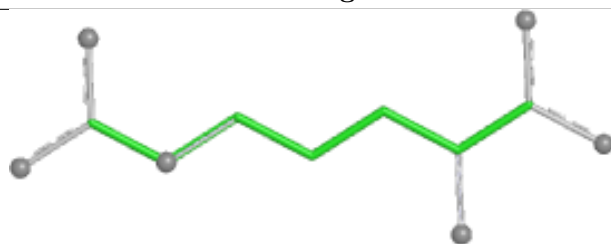
Ligand ARG B 1501



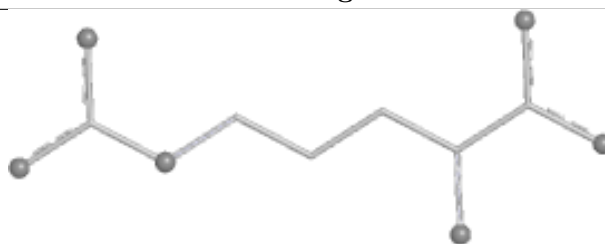
Bond lengths



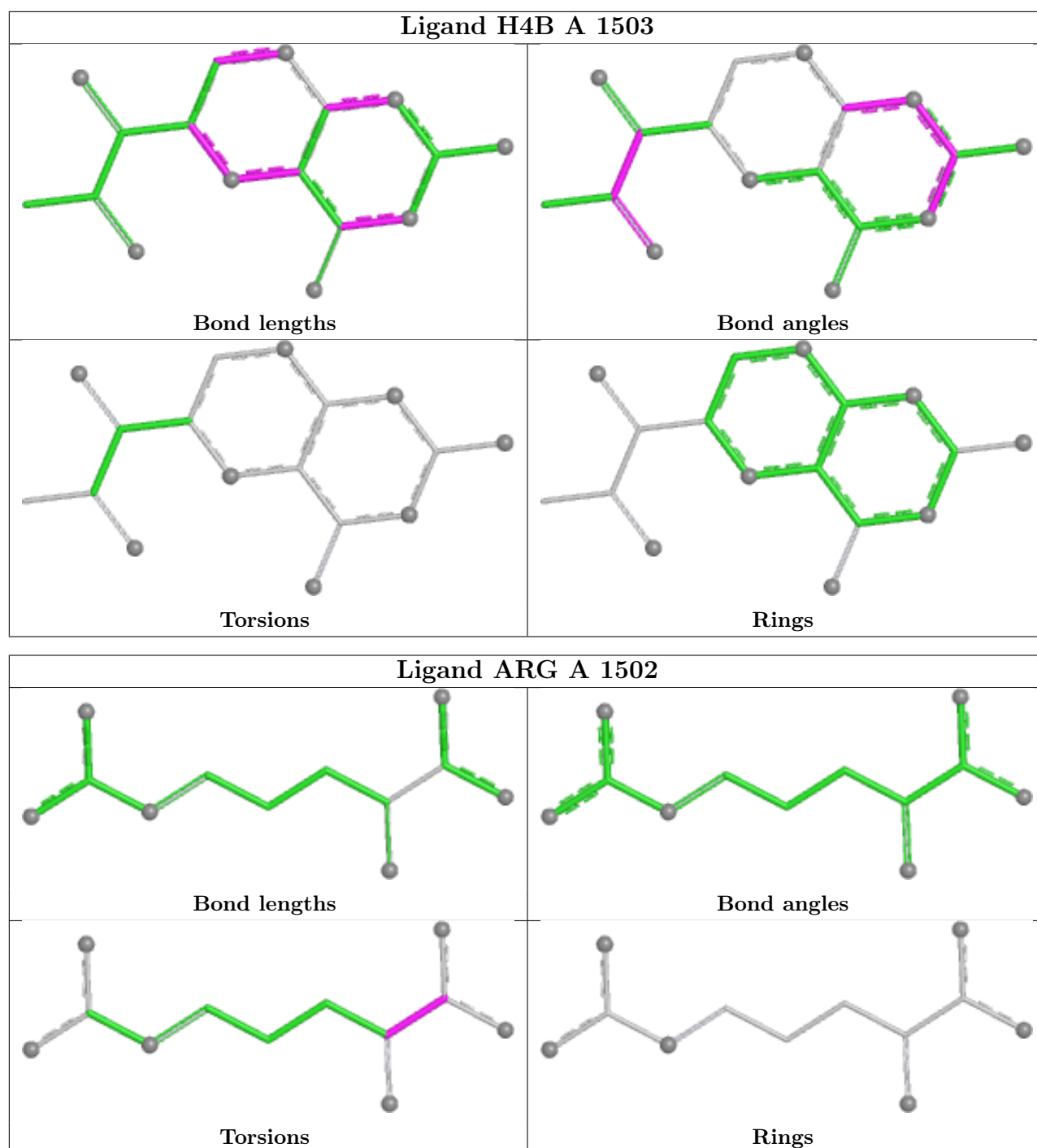
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

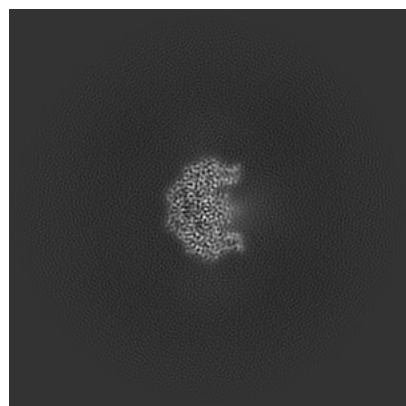
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40969. These allow visual inspection of the internal detail of the map and identification of artifacts.

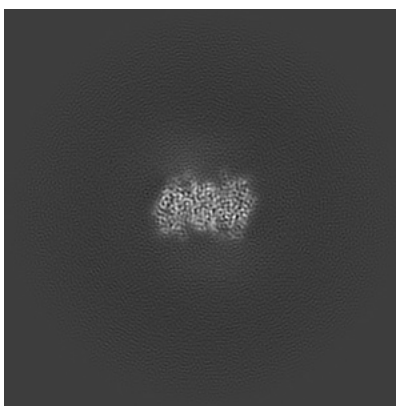
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

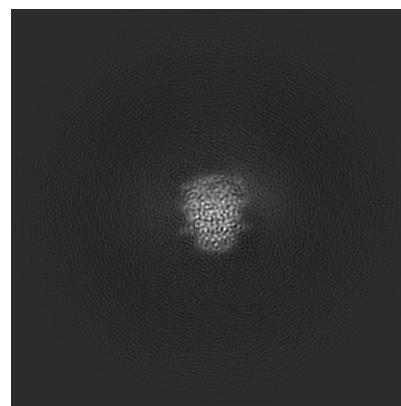
6.1.1 Primary map



X

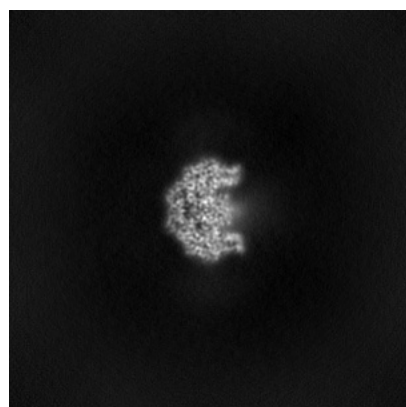


Y

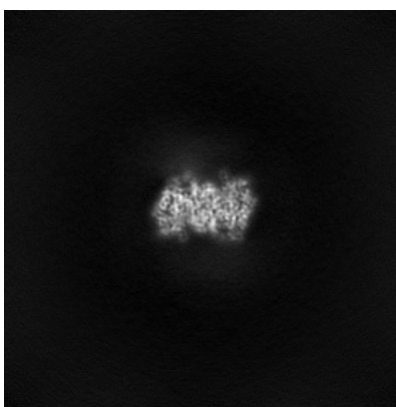


Z

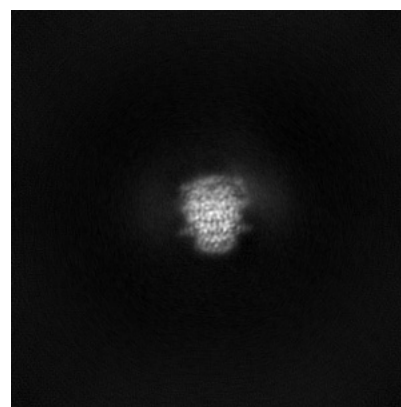
6.1.2 Raw map



X



Y

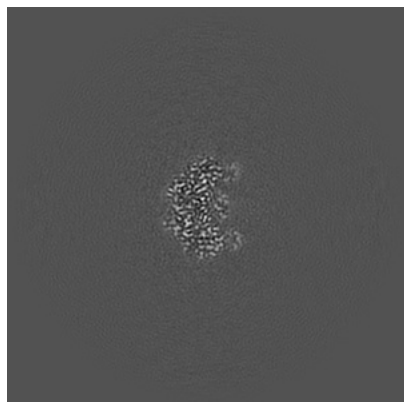


Z

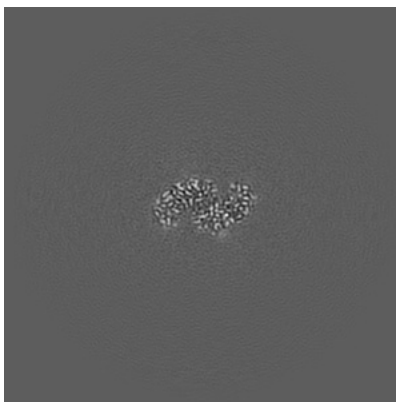
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

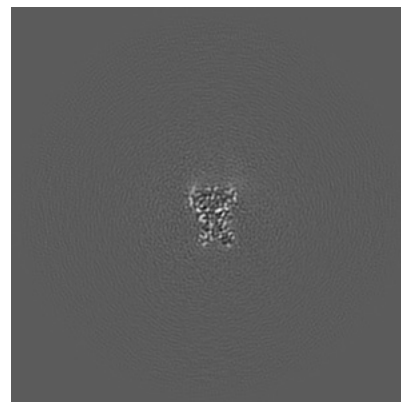
6.2.1 Primary map



X Index: 160

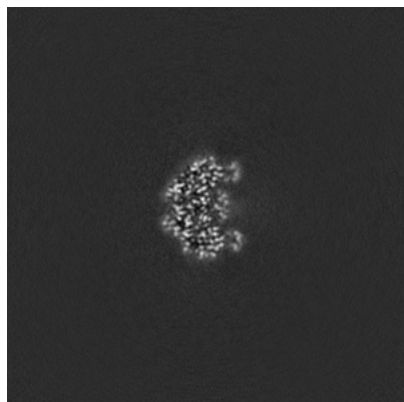


Y Index: 160

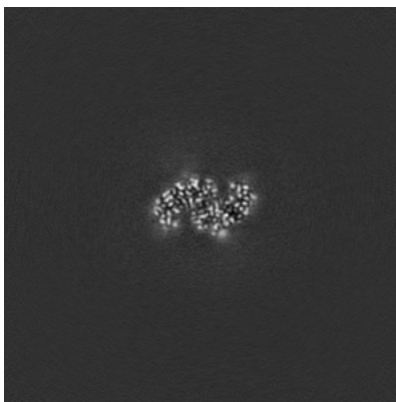


Z Index: 160

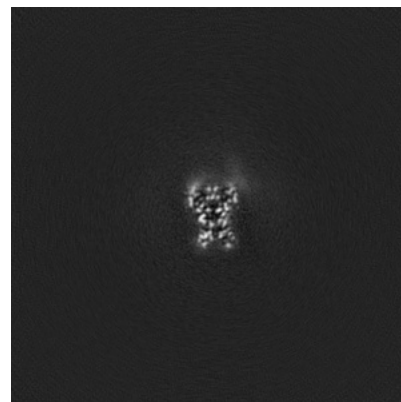
6.2.2 Raw map



X Index: 160



Y Index: 160

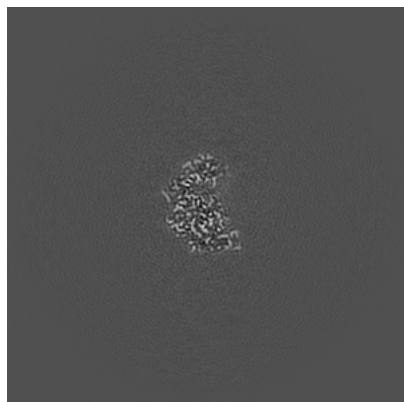


Z Index: 160

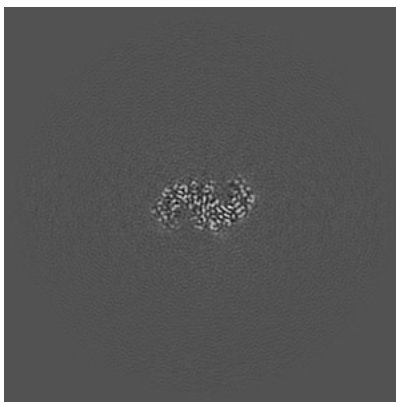
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

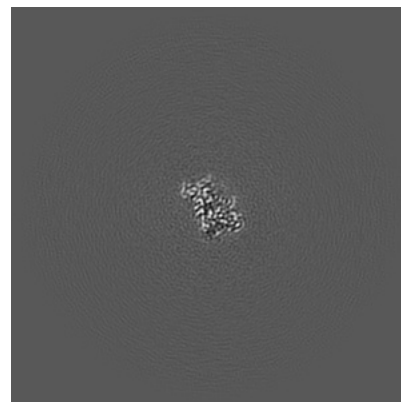
6.3.1 Primary map



X Index: 167

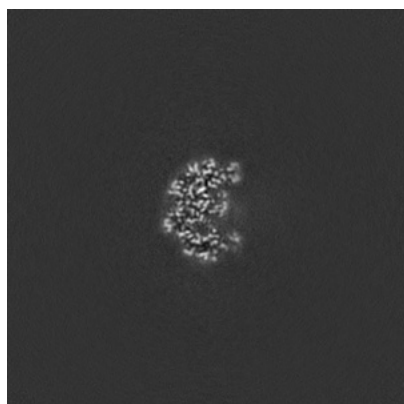


Y Index: 157

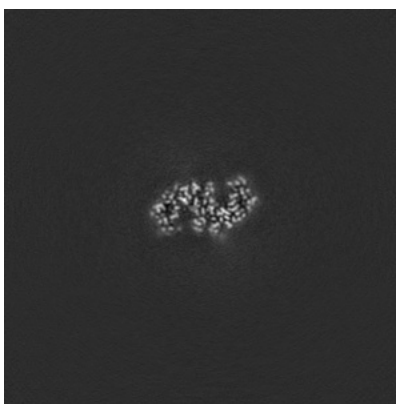


Z Index: 183

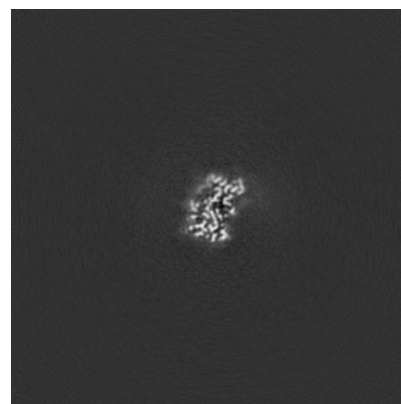
6.3.2 Raw map



X Index: 158



Y Index: 156

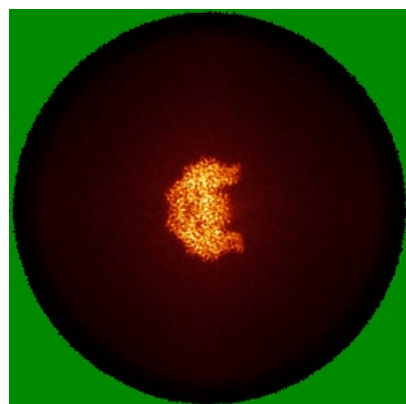


Z Index: 137

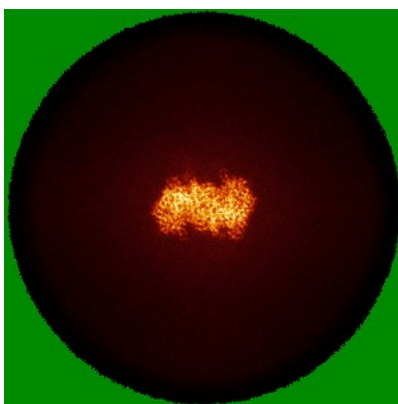
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

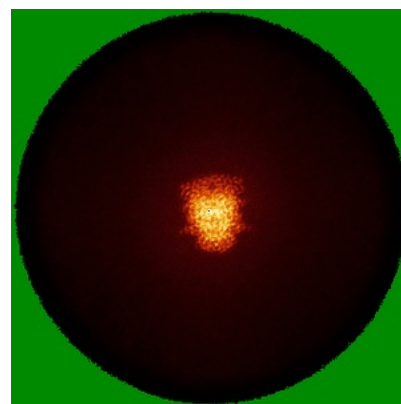
6.4.1 Primary map



X

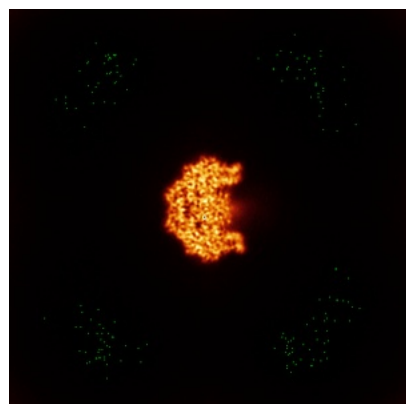


Y

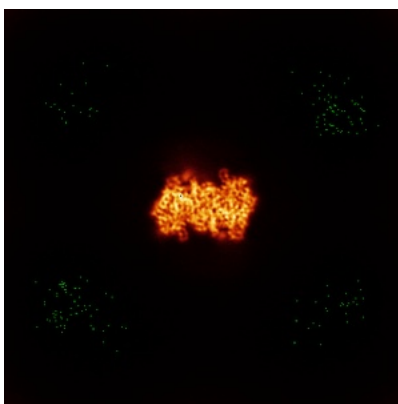


Z

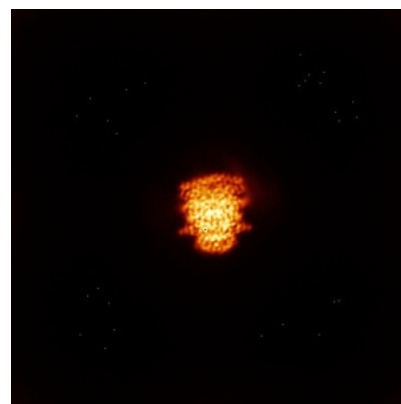
6.4.2 Raw map



X



Y

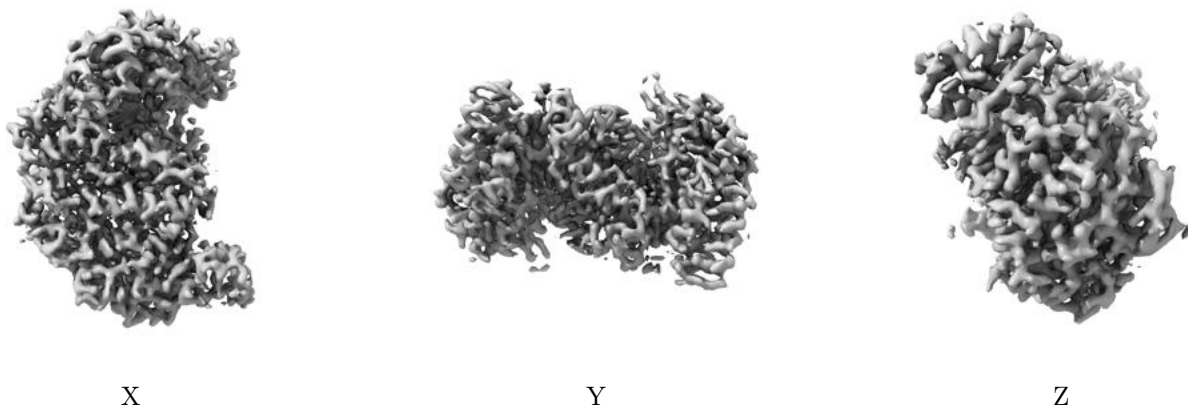


Z

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.

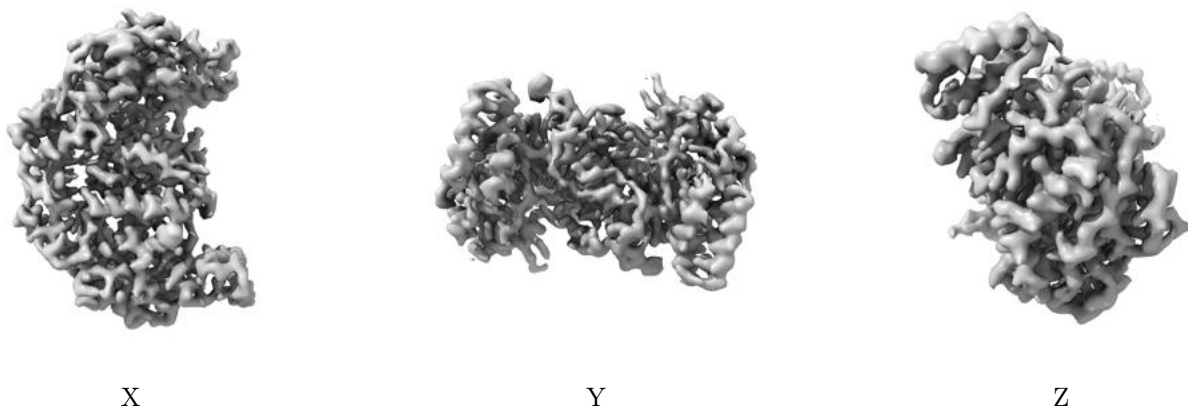
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.6. 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



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.

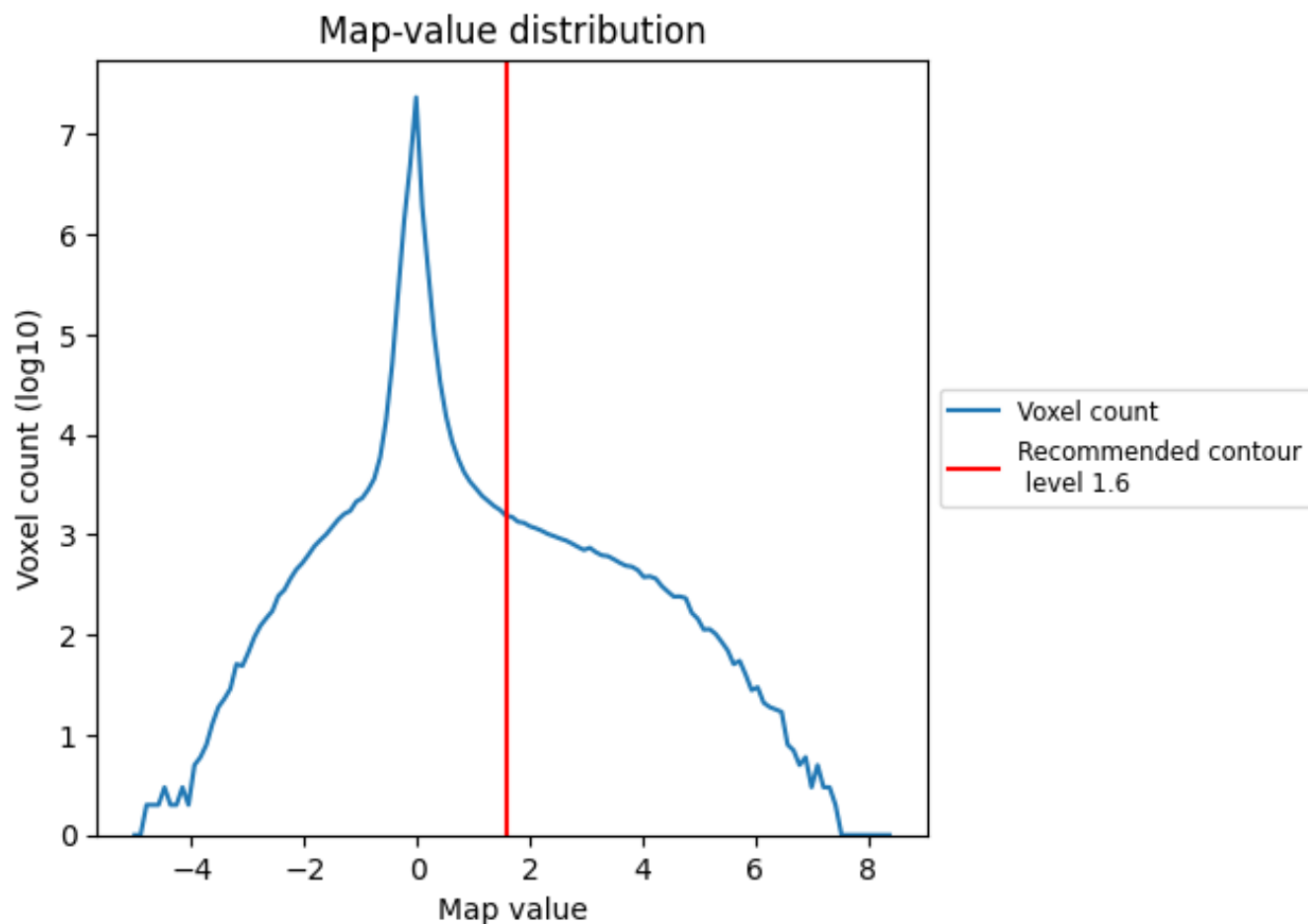
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

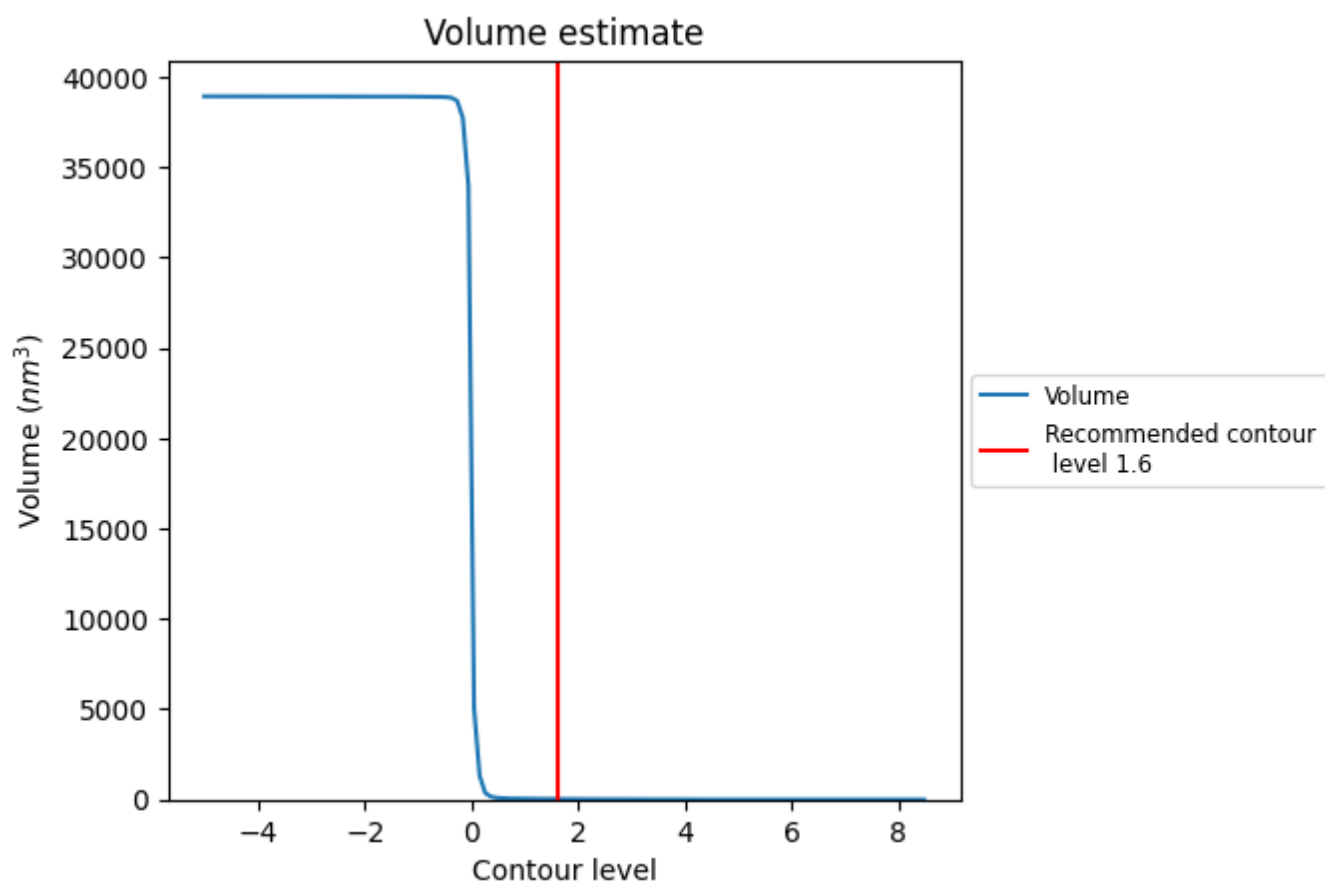
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

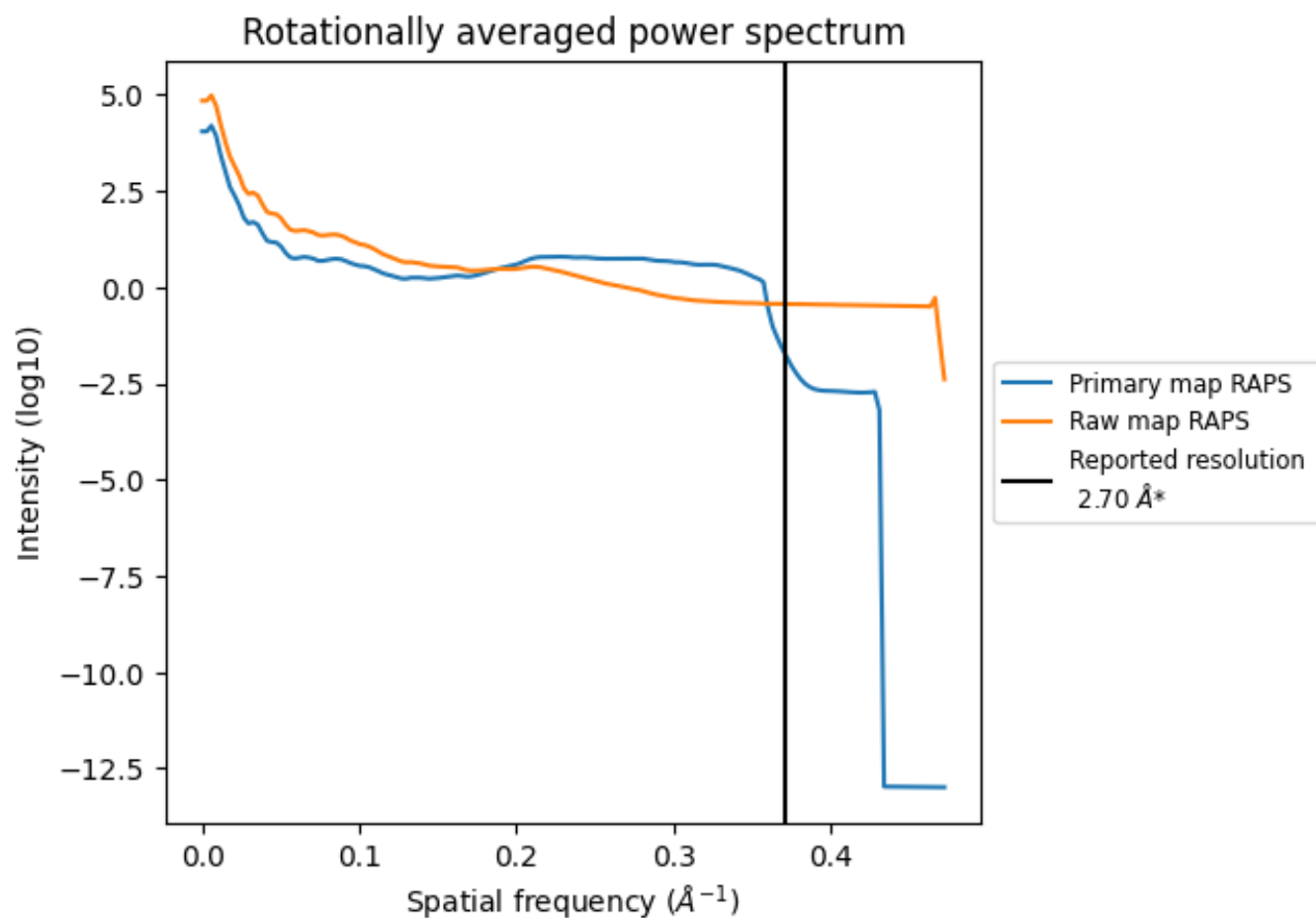
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 28 nm³; this corresponds to an approximate mass of 25 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 ⓘ

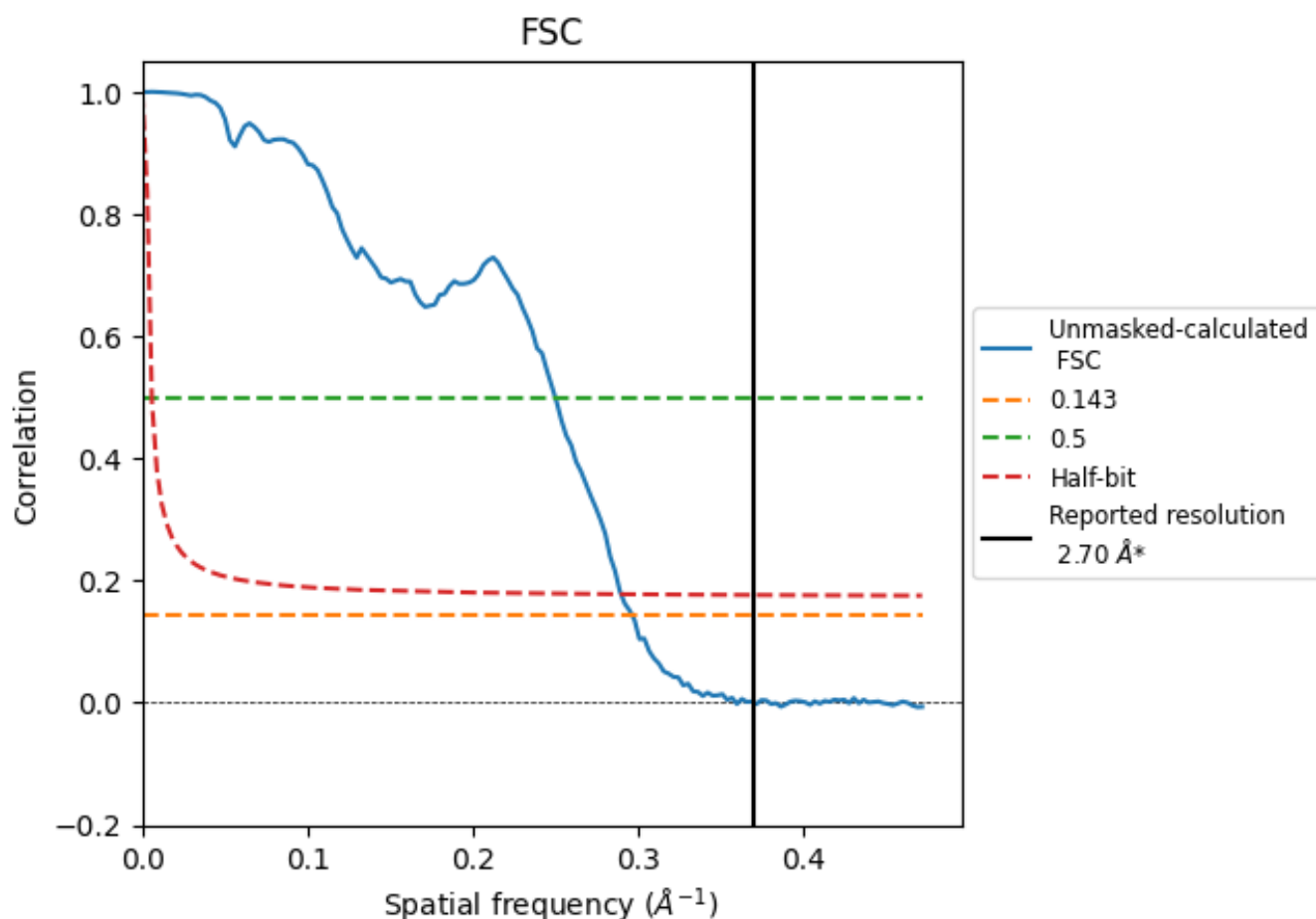


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8.2 Resolution estimates [i](#)

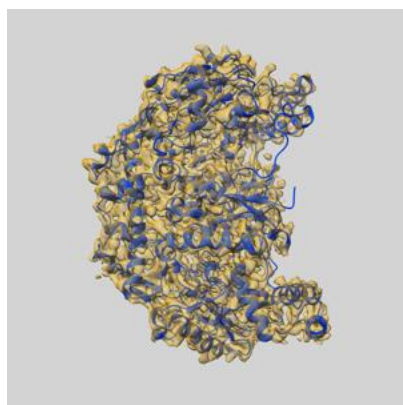
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.37	4.00	3.45

*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 3.37 differs from the reported value 2.7 by more than 10 %

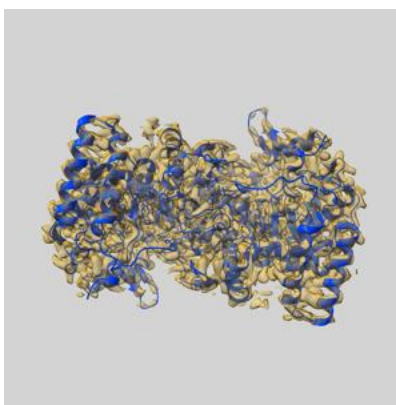
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40969 and PDB model 8T1J. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

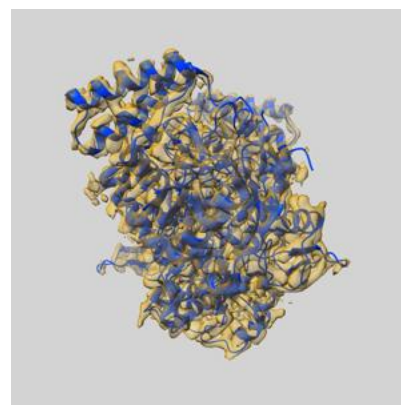
9.1 Map-model overlay [i](#)



X



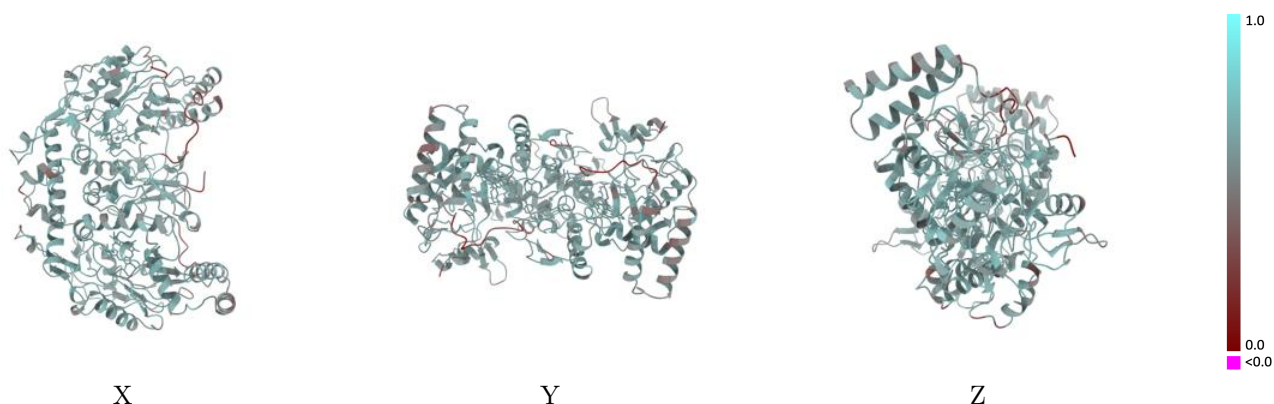
Y



Z

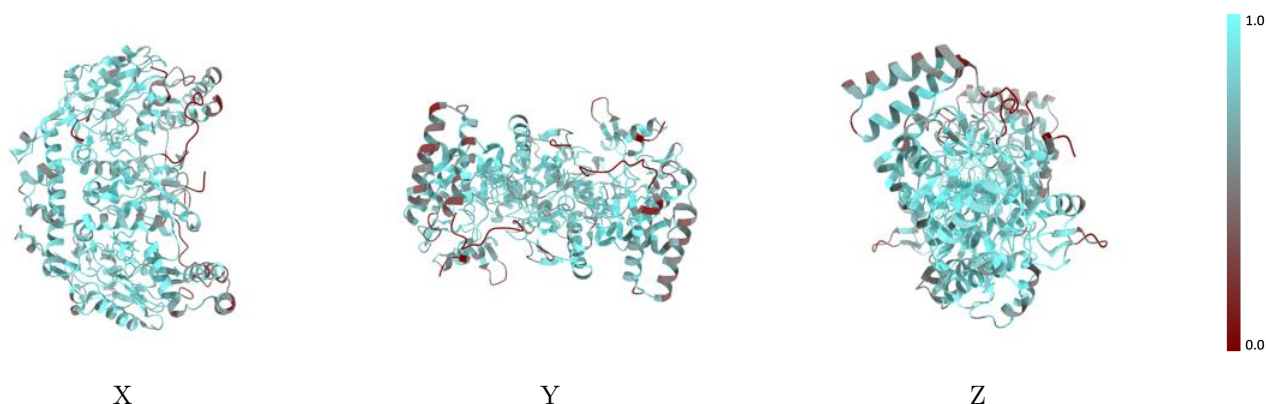
The images above show the 3D surface view of the map at the recommended contour level 1.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



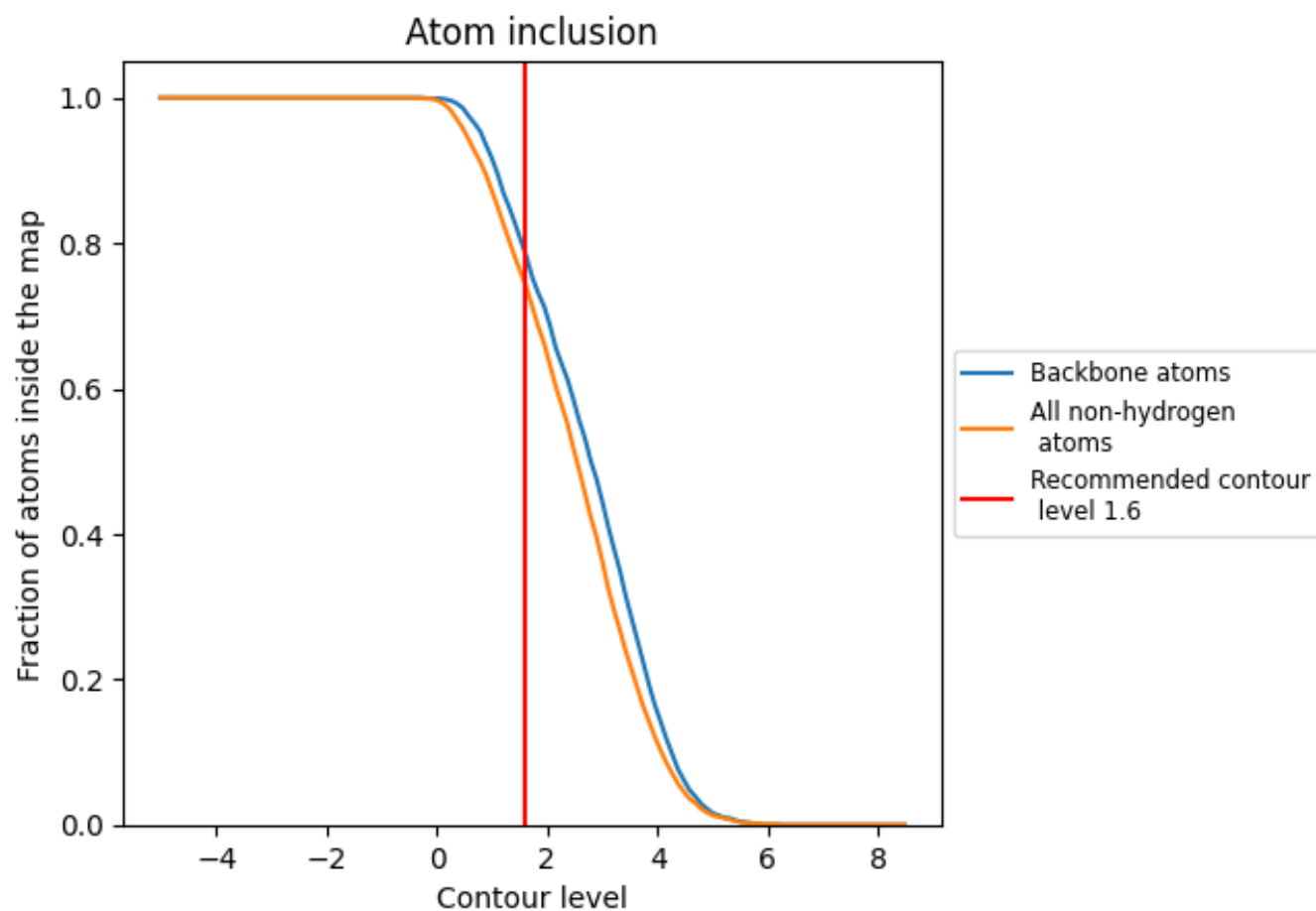
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (1.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% 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 (1.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7440	0.5770
A	0.7350	0.5760
B	0.7530	0.5790

