



wwPDB EM Validation Summary Report ⓘ

Aug 5, 2026 – 09:48 AM EDT

PDB ID : 8T1K / pdb_00008t1k
EMDB ID : EMD-40970
Title : DSBU crosslinked nNOS-CaM oxygenase homodimer
Authors : Lee, K.; Pospiech, T.H.; Southworth, D.
Deposited on : 2023-06-02
Resolution : 3.14 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

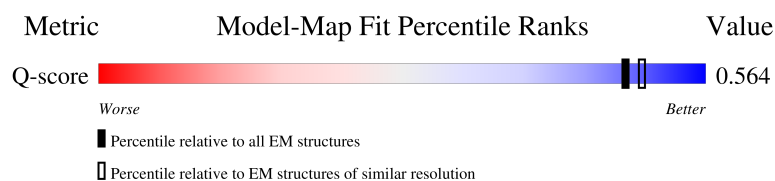
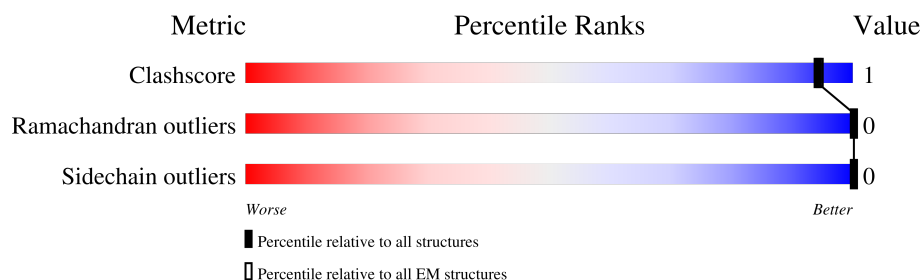
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.14 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	14483 (2.64 - 3.64)

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	 27% 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.

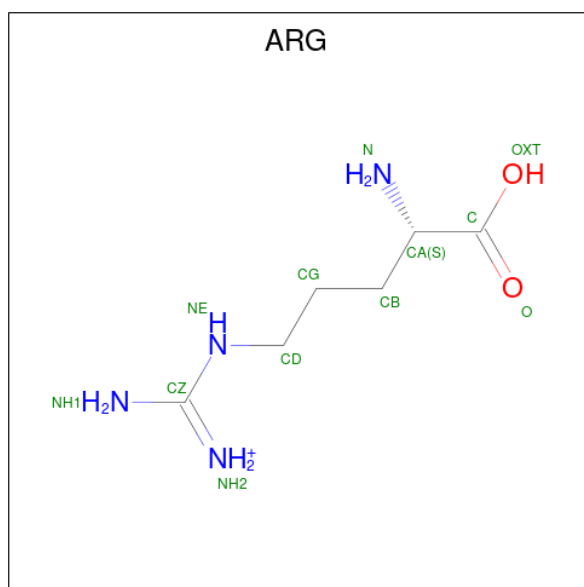
- Molecule 1 is a protein called Nitric oxide synthase 1.

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).



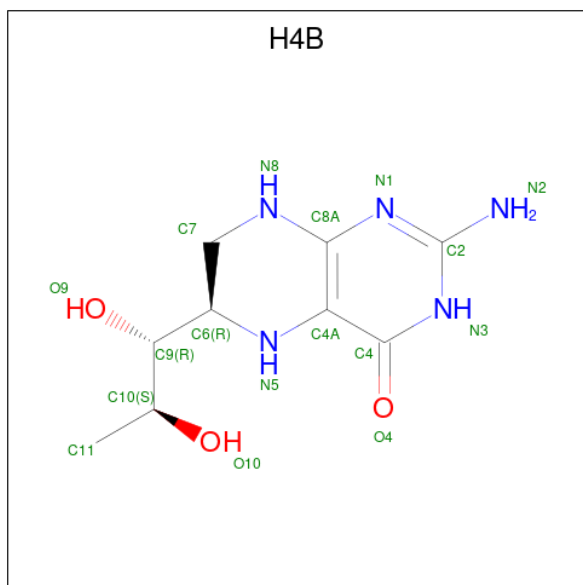
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			12	6	4	2	

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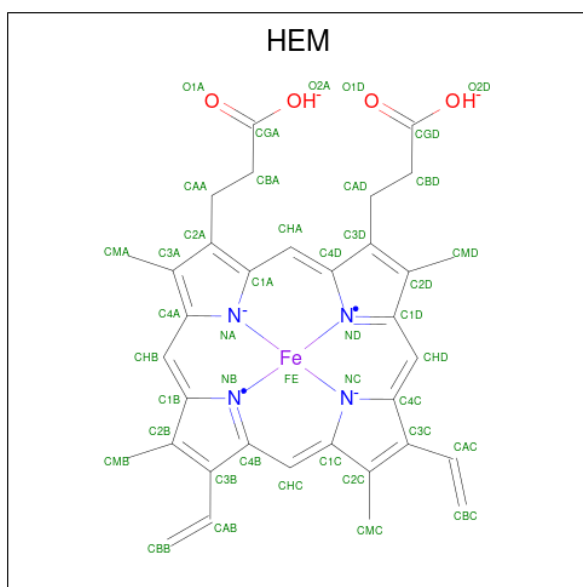
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	B	1	12	6	4	2	0

- 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).

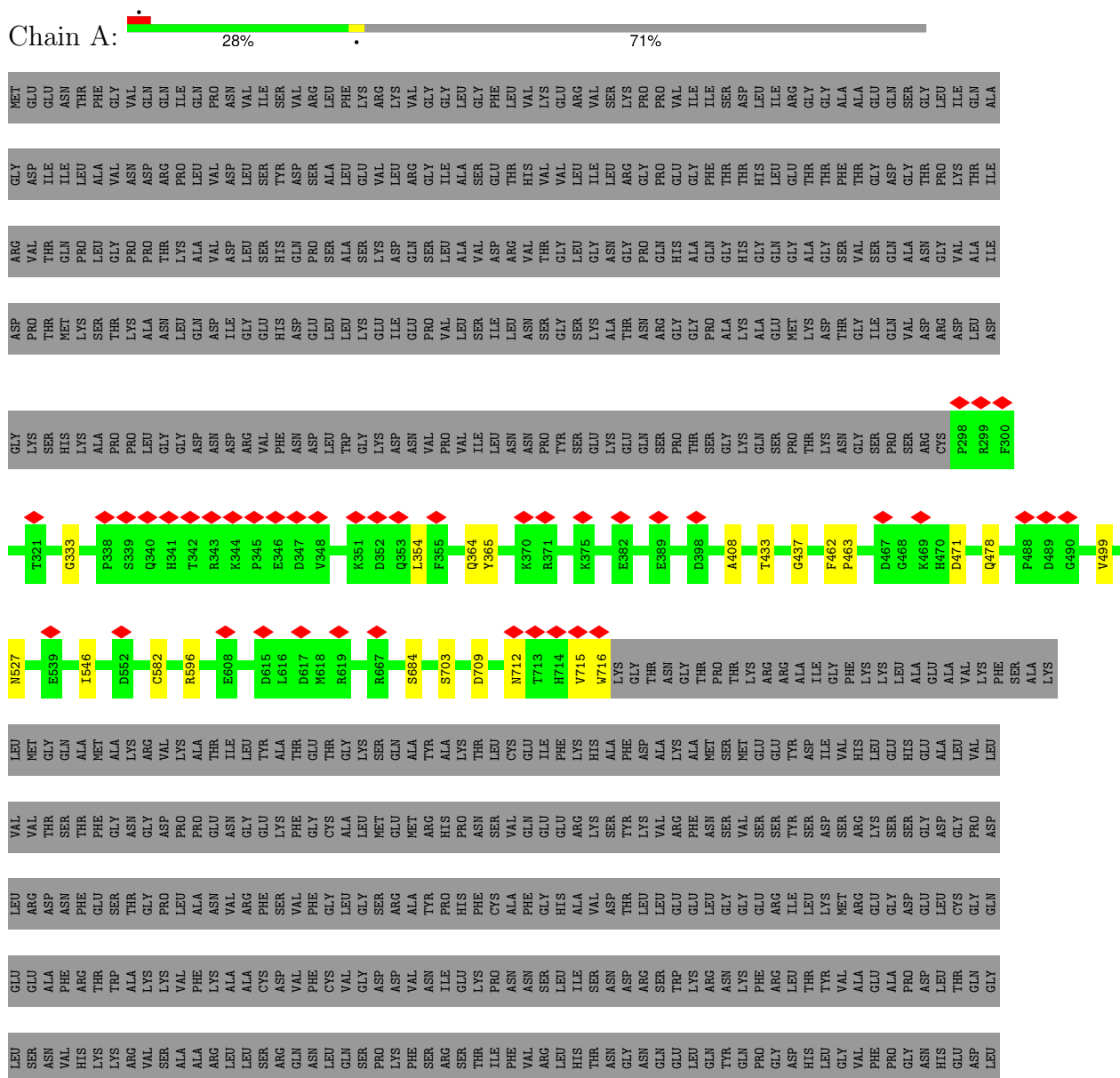


Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0
5	B	1	Total 43	C 34	Fe 1	N 4	O 4	0

3 Residue-property plots

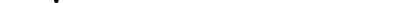
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Nitric oxide synthase 1



[illegible]

- Molecule 1: Nitric oxide synthase 1

Chain B:  27% 71%

SER	ALA	ASN	K469	GLY	T321	ASP	ARG	GLY	ALA	MET
		GLY	T321	PRO	VAL	LYS	THR	GLY	ASP	
TYR	PHE	THR	Q478	SER	E328	THR	THR	SER	THR	GLU
VAL	ALA	PRO	R481	THR	E328	THR	GLN	HIS	ASN	ASN
ARG	LYS	THR		LYS		LYS	LYS	LYS	PRO	THR
PHE	ALA	LYS		ALA	G333	SER	LEU	LEU	ALA	PHE
ASN	MET	ARG					GLY	VAL	GLY	GLY
ASN	SER	ARG	P488	ARG	P338	THR	THR	PRO	THR	VAL
VAL	MET	ALA	D489	ALA	D489	LYS	LYS	PRO	ASN	VAL
GLN	GLU	ILE	G490	ILE	G490	ALA	ALA	LEU	THR	GLN
SER	GLU	GLY		GLY	S339	ASN	ASN	GLY	ARG	GLN
SER	GLU	PHE	V499	PHE	Q340	LEU	LYS	PRO	LYS	ILE
TYR	TYR	LYS		LYS	H341	GLN	ALA	LEU	GLN	PRO
SER	ASP	LYS		LYS	T342	ASP	ASP	VAL	VAL	ASN
ASP	ILE	LYS	K511	ILE	T342	ILE	ASP	ASP	ASN	ASN
SER	VAL	VAL	A512	VAL	R343	GLY	LEU	LEU	VAL	VAL
ARG	HIS	ALA	P513	ALA	K344	GLU	SER	TYR	ILE	SER
LYS	LEU	GLU		GLU	P345	HIS	HIS	TYR	SER	VAL
SER	GLU	ALA	N527	ALA	ASP	ASP	GLN	ASP	VAL	VAL
SER	HIS	VAL		VAL	E346	GLU	PRO	SER	ARG	ARG
GLY	GLU	LYS	D530	LYS	D347	LEU	LEU	LEU	ALA	PHE
ASP	ALA	PHE		PHE	V348	TRP	LEU	GLY	SER	LYS
GLY	LEU	SER		SER	E539	GLY	LYS	LYS	LEU	VAL
PRO	VAL	ALA		ALA	R349	ILE	ASP	ILE	ASP	ARG
ASP	LEU	LYS		LYS		ASP	ILE	LEU	LEU	LYS
LEU	VAL	LEU	I546	LEU	D352	GLU	GLN	ARG	VAL	VAL
ASP	THR	MET		MET	Q353	PRO	PRO	GLY	GLY	GLY
ASP	THR	GLY	D552	GLY	L354	VAL	VAL	ILE	LEU	ILE
ASN	SER	GLN		GLN	F355	LEU	ALA	ALA	LEU	ALA
PHE	THR	ALA		ALA		SER	VAL	VAL	SER	GLY
GLU	PHE	MET	D556	MET		ILE	ASP	GLU	GLU	PHE
SER	GLY	ALA		ALA	K359	ILE	ASP	LEU	THR	VAL
THR	ASN	LYS	C582	LYS	D363	ASN	ASN	ASN	HIS	VAL
GLY	ASP	ARG		ARG	Q364	SER	THR	VAL	LYS	VAL
PRO	GLY	VAL	Y588	VAL	Y365	GLY	GLY	VAL	VAL	GLY
LEU	PRO	LYS		LYS		SER	SER	LEU	LEU	ARG
ALA	PRO	ALA	R596	ALA		GLU	LYS	ILE	VAL	VAL
ASN	GLU	THR		THR	K370	ALA	ALA	SER	LEU	SER
VAL	ASN	ILE	E608	ILE	R371	THR	GLY	ARG	LYS	LYS
ARG	GLY	LEU		LEU		ASN	ASN	PRO	GLY	PRO
PHE	GLU	TYR		TYR	K375	ARG	GLN	GLN	PRO	VAL
SER	LYS	ALA	D615	ALA		GLY	ALA	HIS	GLY	ILE
VAL	PHE	THR	L616	THR		GLY	ALA	PHE	THR	ILE
PHE	GLY	GLU	D617	GLU	M378	PRO	GLN	THR	SER	THR
GLY	CYS	THR	M618	THR	D379	ALA	GLY	ALA	GLY	ASP
LEU	ALA	GLY	R619	GLY		LYS	LYS	ALA	LEU	LEU
GLY	LEU	LYS		LYS	E382	ALA	ALA	GLY	HIS	ILE
SER	MET	SER	D650	SER		GLU	GLN	SER	LEU	GLY
ARG	GLU	GLN		GLN		GLY	GLY	GLY	GLY	ARG
ALA	MET	ALA	R667	ALA	E387	MET	GLY	GLY	THR	GLY
TYR	ARG	TYR		TYR	I388	ASP	ASP	THR	THR	THR
PRO	HIS	ALA	S684	ALA	E389	LYS	SER	GLY	PHE	ALA
HIS	PRO	LYS		LYS		GLY	VAL	THR	ALA	ALA
PHE	ASN	THR	S703	THR	S392	ILE	SER	GLY	GLY	GLU
CYS	SER	LEU		LEU		GLN	GLN	ASP	ASP	GLN
ALA	VAL	CYS	D709	CYS	D398	VAL	VAL	GLY	GLY	SER
PHE	GLN	GLU		GLU		ASN	ASN	THR	THR	GLY
GLY	GLU	ILE	N712	ILE	A408	ARG	ARG	GLY	VAL	LEU
HIS	GLU	PHE	T713	PHE		CYS	ARG	ASP	GLY	LYS
ALA	ARG	LYS	H714	LYS	T433	ASN	ASN	THR	THR	ALA
ALA	LYS	THR		THR		LEU	LEU	LEU	THR	GLN

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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	294924	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	62.00	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	8.752	Depositor
Minimum map value	-6.717	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.141	Depositor
Recommended contour level	1.8	Depositor
Map size (Å)	310.08, 310.08, 310.08	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.91199994, 0.91199994, 0.91199994	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.97	12/4764 (0.3%)
1	B	0.66	2/3511 (0.1%)	0.99	12/4764 (0.3%)
All	All	0.64	2/7022 (0.0%)	0.98	24/9528 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	588	TYR	C-O	-7.97	1.14	1.23
1	B	588	TYR	CA-C	-7.94	1.42	1.52

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	588	TYR	CA-C-O	-8.14	111.77	120.80
1	B	354	LEU	N-CA-C	7.12	119.12	111.36
1	A	354	LEU	N-CA-C	7.06	119.06	111.36
1	A	712	ASN	N-CA-C	-6.04	105.56	113.17
1	B	712	ASN	N-CA-C	-5.99	105.62	113.17

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	3414	0	3322	7	0
1	B	3414	0	3322	11	0
2	A	1	0	0	0	0
3	A	12	0	12	1	0
3	B	12	0	12	0	0
4	A	17	0	15	1	0
4	B	17	0	15	1	0
5	A	43	0	30	0	0
5	B	43	0	30	0	0
All	All	6973	0	6758	17	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 17 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:478:GLN:HE22	3:A:1502:ARG:C	2.19	0.51
1:B:478:GLN:OE1	1:B:481:ARG:NH2	2.47	0.48
1:B:359:LYS:NZ	1:B:363:ASP:OD2	2.43	0.47
1:A:715:VAL:O	1:A:716:TRP:HB2	2.16	0.46
1:B:462:PHE:HB3	1:B:463:PRO:HD2	1.98	0.45

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%)	405 (97%)	12 (3%)	0	100	100
All	All	834/2858 (29%)	812 (97%)	22 (3%)	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	478	GLN
1	A	525	GLN
1	A	527	ASN
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	$\# Z > 2$
3	ARG	B	1501	-	10,11,11	0.65	0	9,13,13	0.36	0
3	ARG	A	1502	-	10,11,11	0.61	0	9,13,13	0.26	0
4	H4B	B	1502	-	17,18,18	1.49	4 (23%)	14,26,26	1.91	2 (14%)
5	HEM	B	1503	-	50,50,50	1.56	8 (16%)	67,82,82	1.30	7 (10%)
4	H4B	A	1503	-	17,18,18	1.68	5 (29%)	14,26,26	1.90	3 (21%)
5	HEM	A	1504	1	50,50,50	1.51	4 (8%)	67,82,82	1.16	8 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ARG	B	1501	-	-	0/11/11/11	-
3	ARG	A	1502	-	-	4/11/11/11	-
4	H4B	B	1502	-	-	0/8/17/17	0/2/2/2
5	HEM	B	1503	-	-	3/14/54/54	-
4	H4B	A	1503	-	-	0/8/17/17	0/2/2/2
5	HEM	A	1504	1	-	4/14/54/54	-

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1504	HEM	FE-NC	6.74	2.17	1.95
5	B	1503	HEM	FE-NC	5.85	2.14	1.95
4	A	1503	H4B	C4A-N5	3.90	1.47	1.37
5	A	1504	HEM	FE-NA	3.16	2.05	1.95
5	B	1503	HEM	FE-NA	3.16	2.05	1.95

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1503	H4B	C2-N1-C8A	5.18	122.50	113.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1502	H4B	C2-N1-C8A	5.16	122.47	113.36
5	A	1504	HEM	CHD-C4C-NC	-3.61	120.52	124.45
5	B	1503	HEM	C3B-C2B-C1B	3.38	108.95	106.41
4	B	1502	H4B	N3-C2-N1	-3.34	117.21	123.32

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

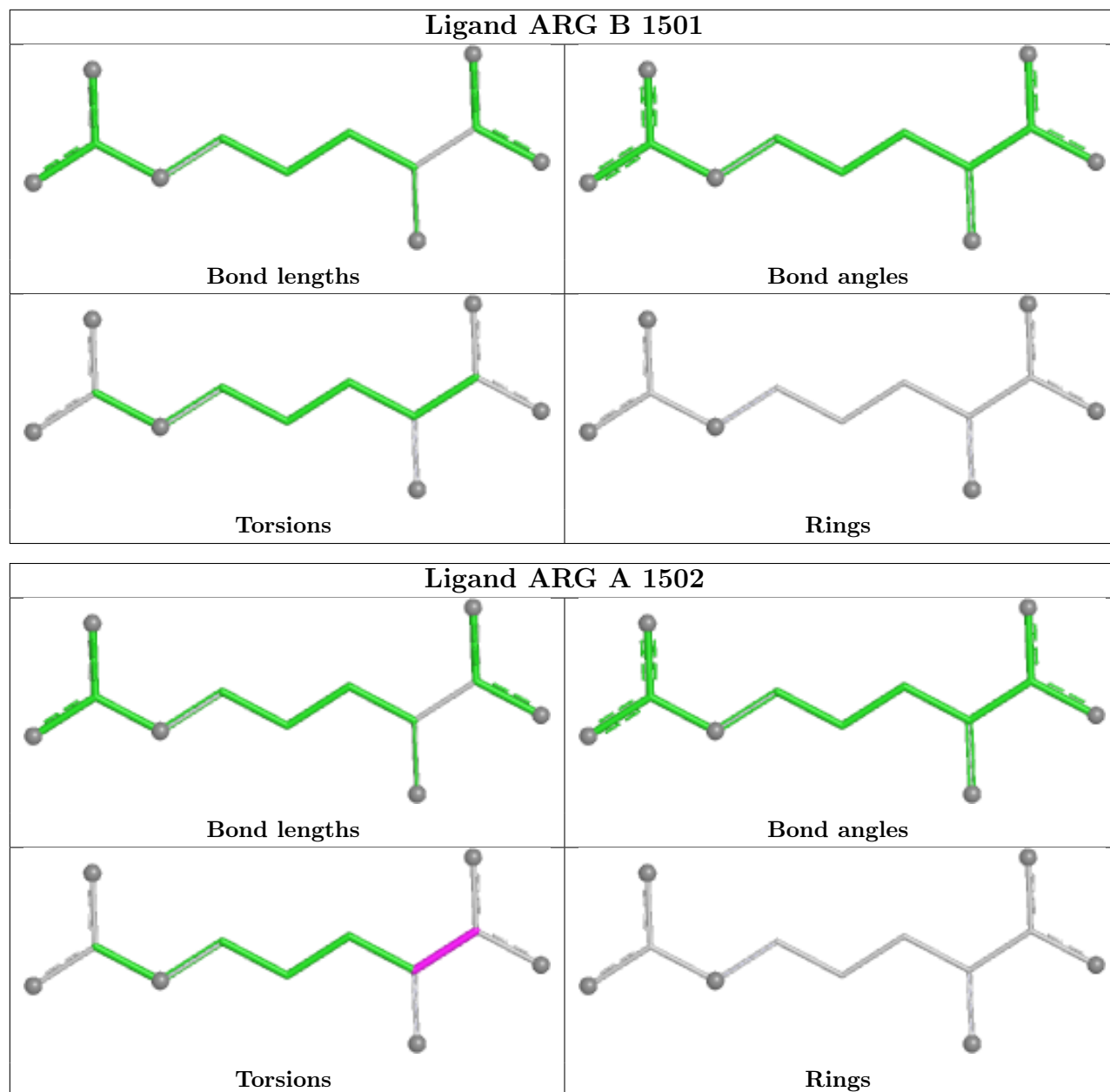
Mol	Chain	Res	Type	Atoms
3	A	1502	ARG	O-C-CA-N
5	A	1504	HEM	C2B-C3B-CAB-CBB
5	A	1504	HEM	C4B-C3B-CAB-CBB
5	B	1503	HEM	C2B-C3B-CAB-CBB
3	A	1502	ARG	OXT-C-CA-N

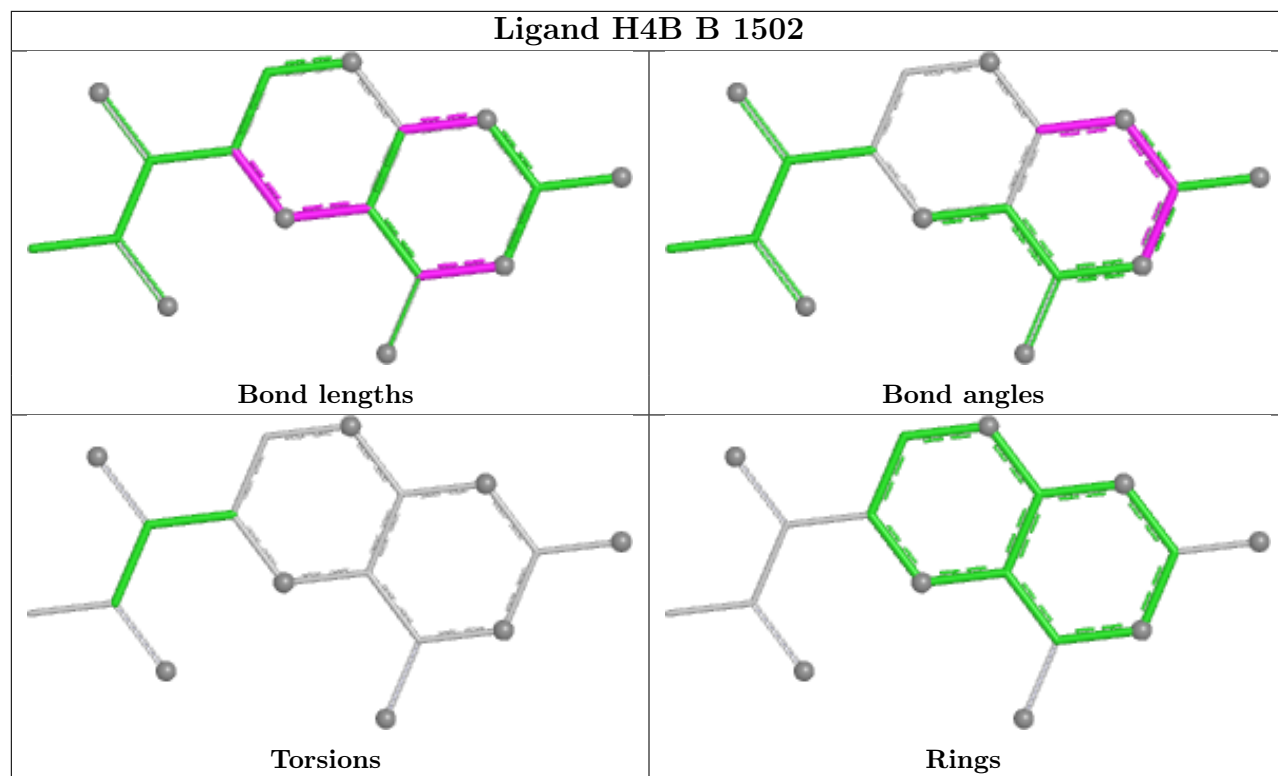
There are no ring outliers.

3 monomers are involved in 3 short contacts:

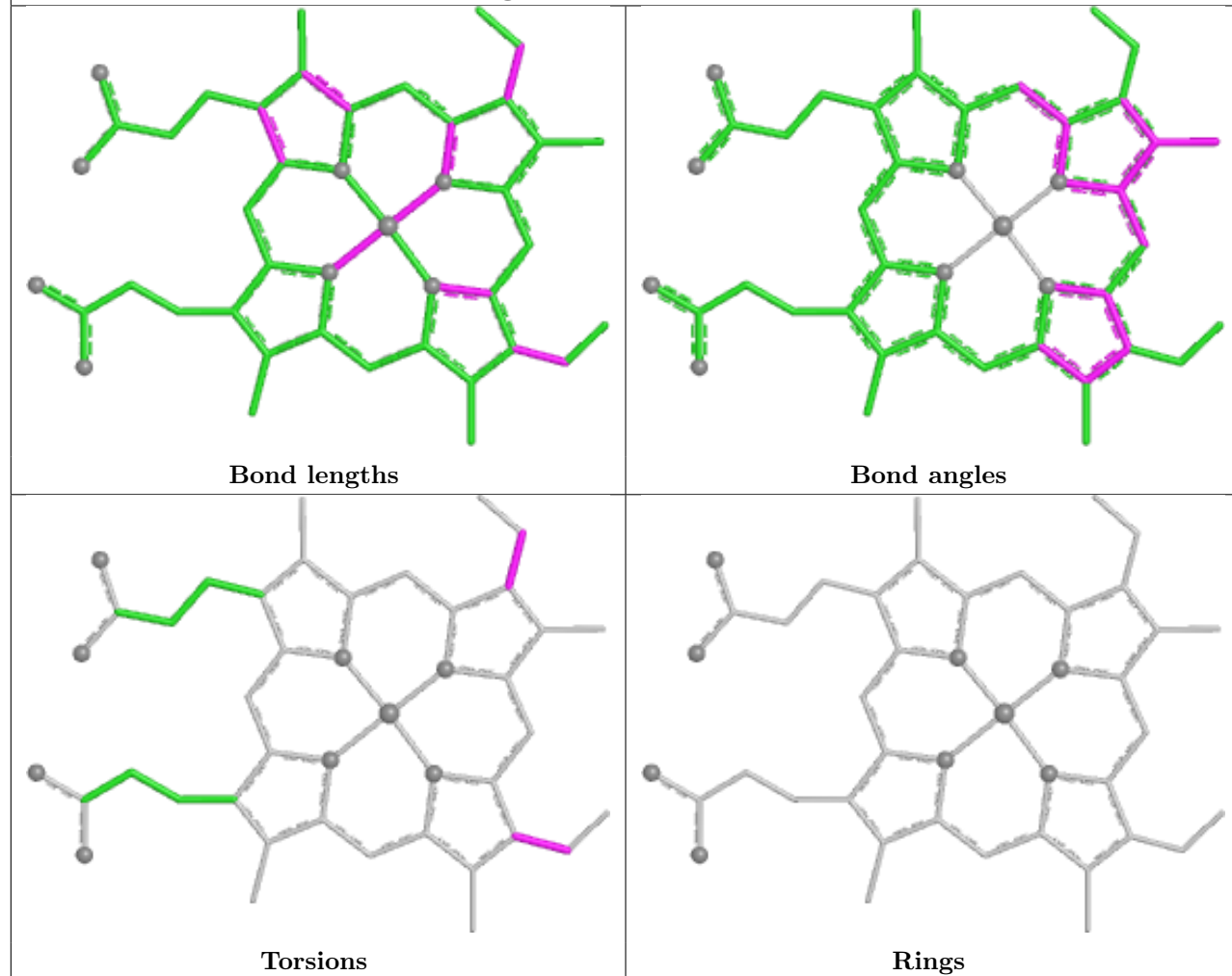
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1502	ARG	1	0
4	B	1502	H4B	1	0
4	A	1503	H4B	1	0

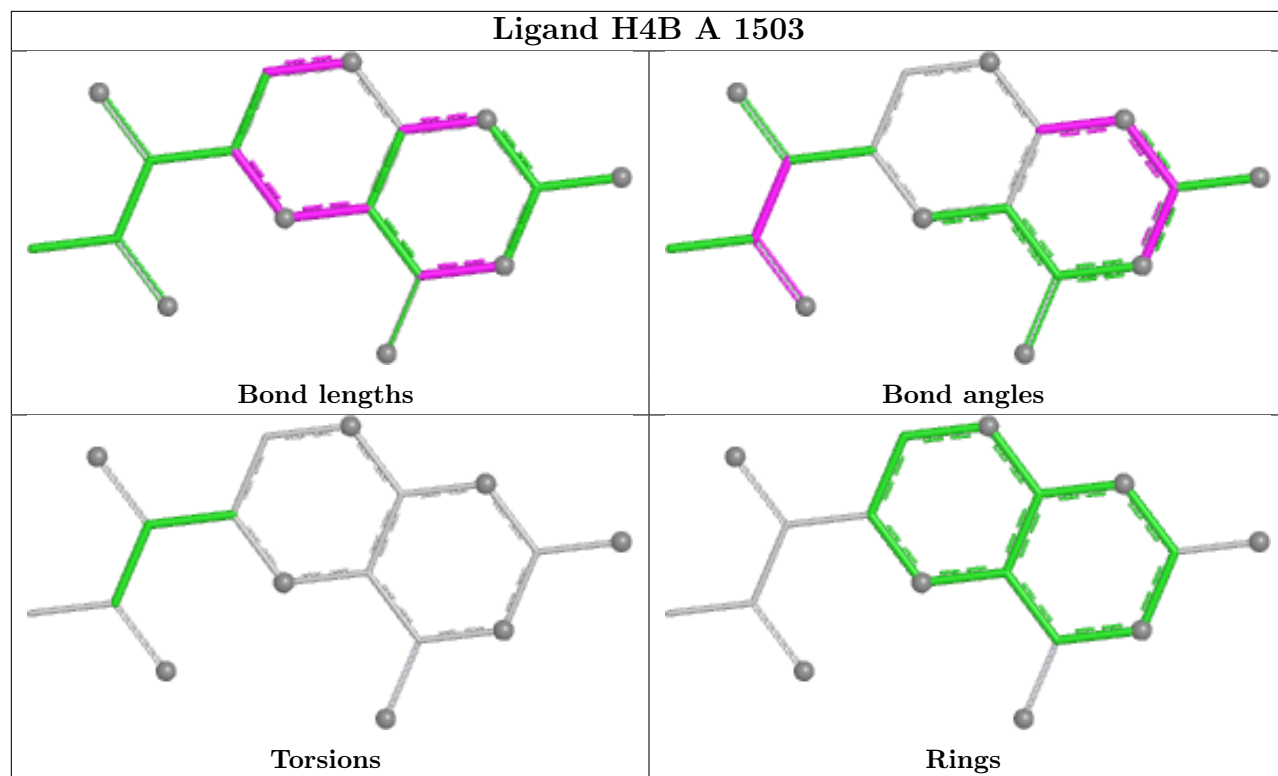
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

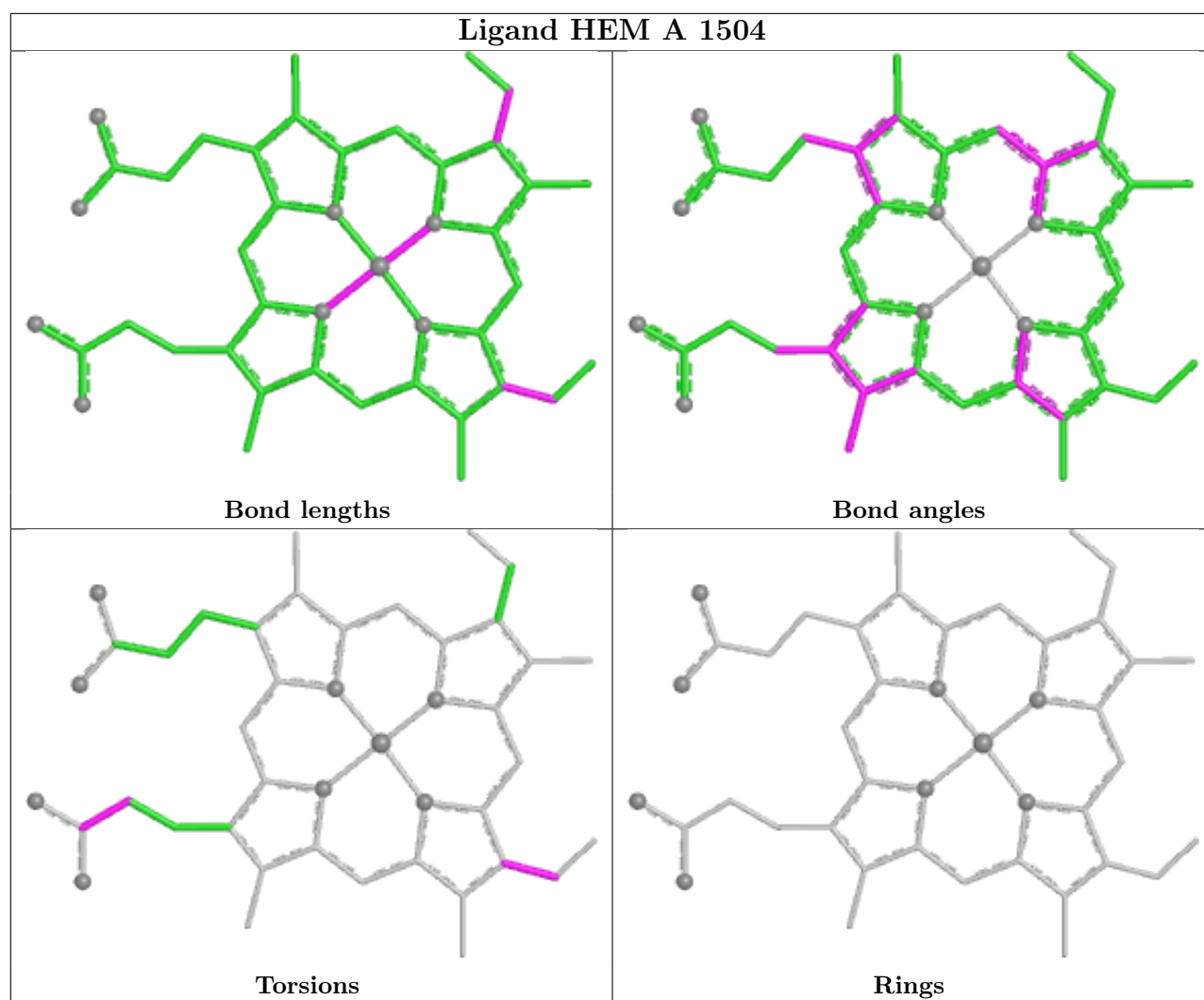




Ligand HEM B 1503







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.

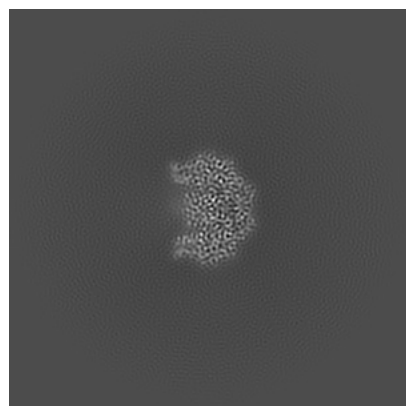
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40970. These allow visual inspection of the internal detail of the map and identification of artifacts.

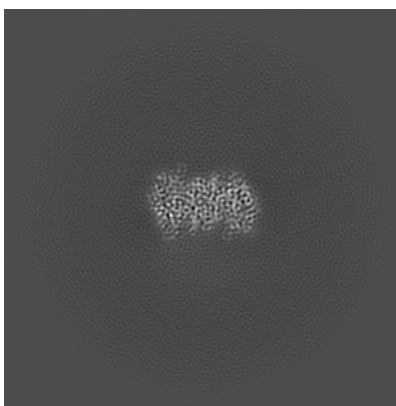
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

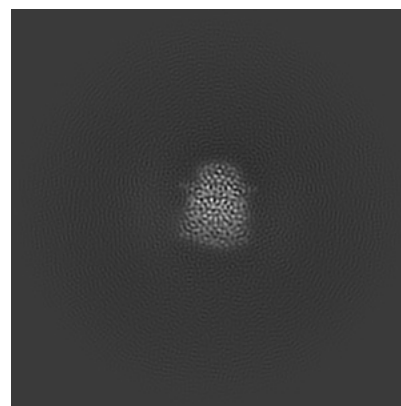
6.1.1 Primary map



X

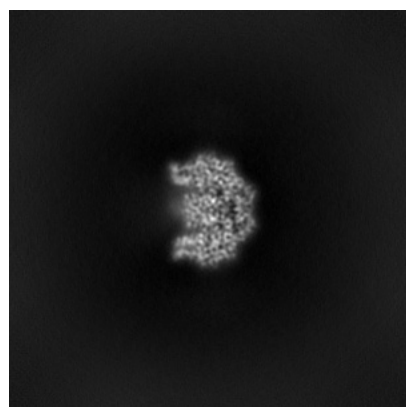


Y

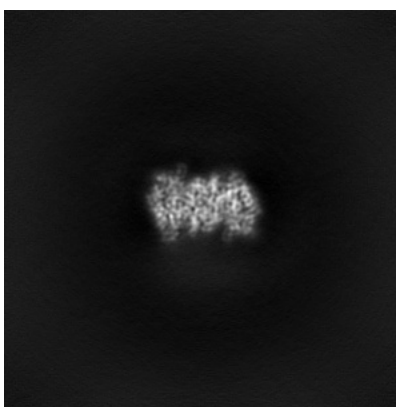


Z

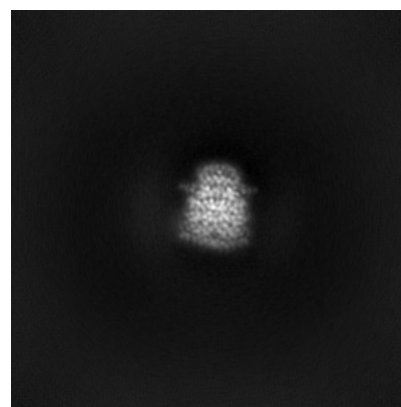
6.1.2 Raw map



X



Y

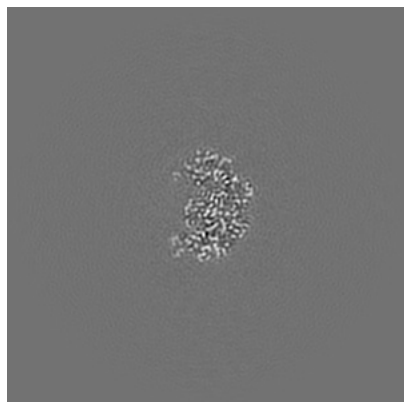


Z

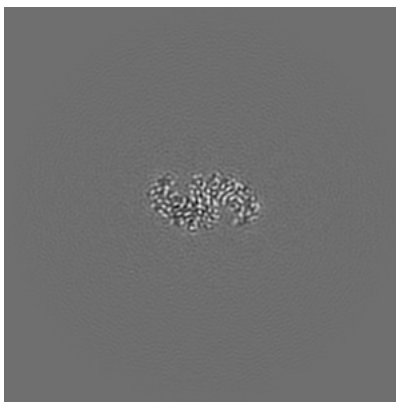
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

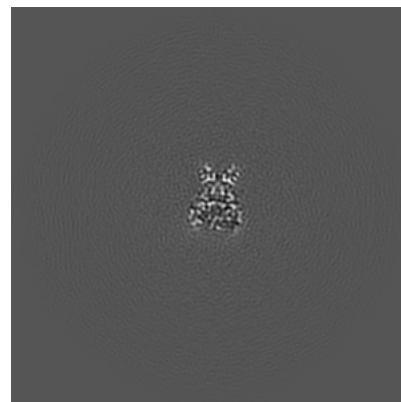
6.2.1 Primary map



X Index: 170

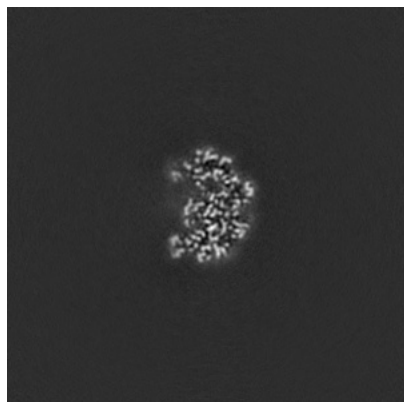


Y Index: 170

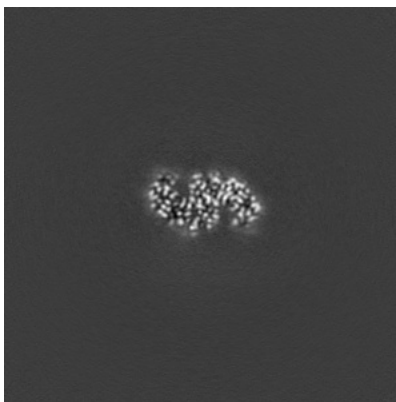


Z Index: 170

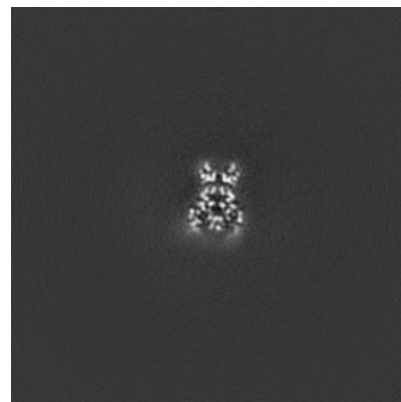
6.2.2 Raw map



X Index: 170



Y Index: 170

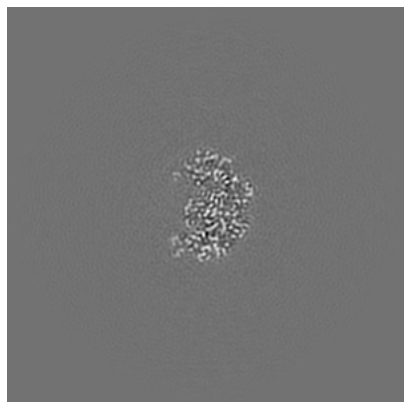


Z Index: 170

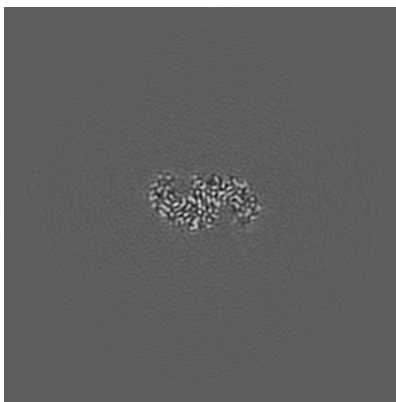
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

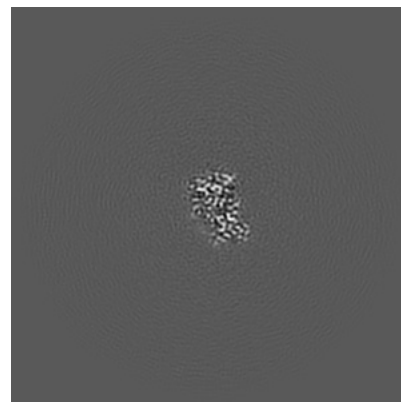
6.3.1 Primary map



X Index: 170

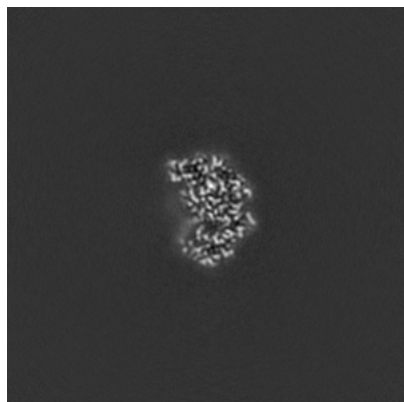


Y Index: 171

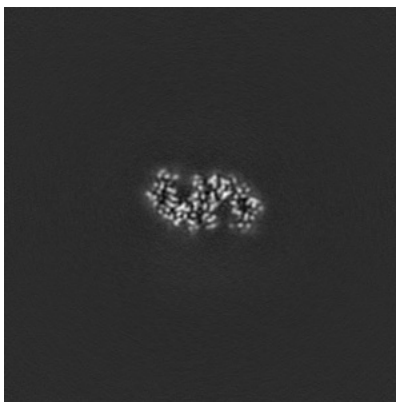


Z Index: 196

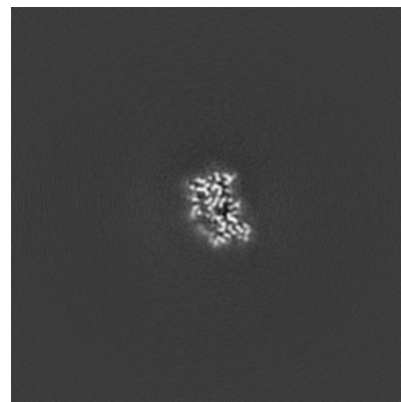
6.3.2 Raw map



X Index: 180



Y Index: 173

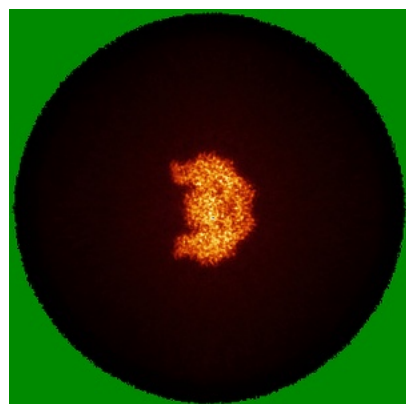


Z Index: 196

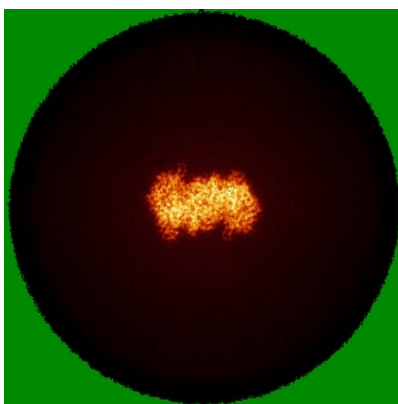
The images above show the largest variance slices of the map in three orthogonal directions.

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

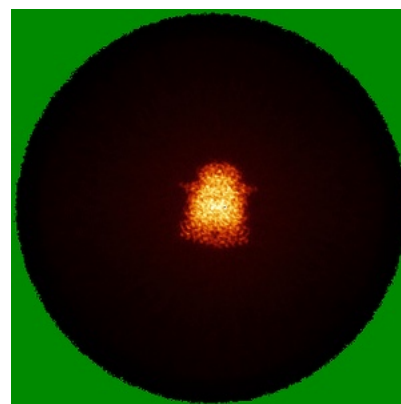
6.4.1 Primary map



X

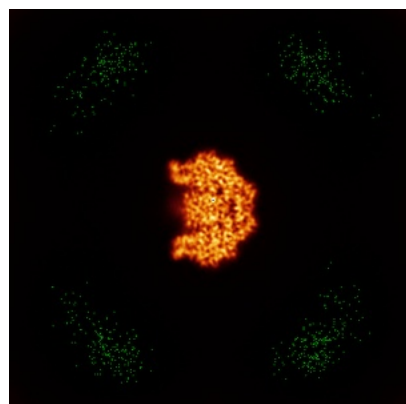


Y

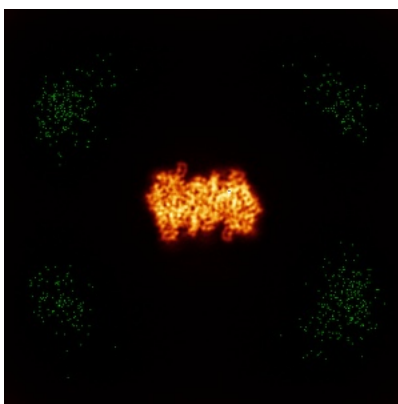


Z

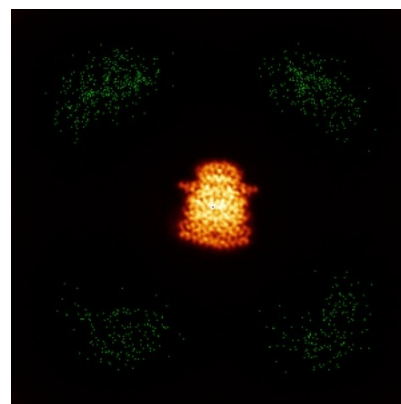
6.4.2 Raw map



X



Y

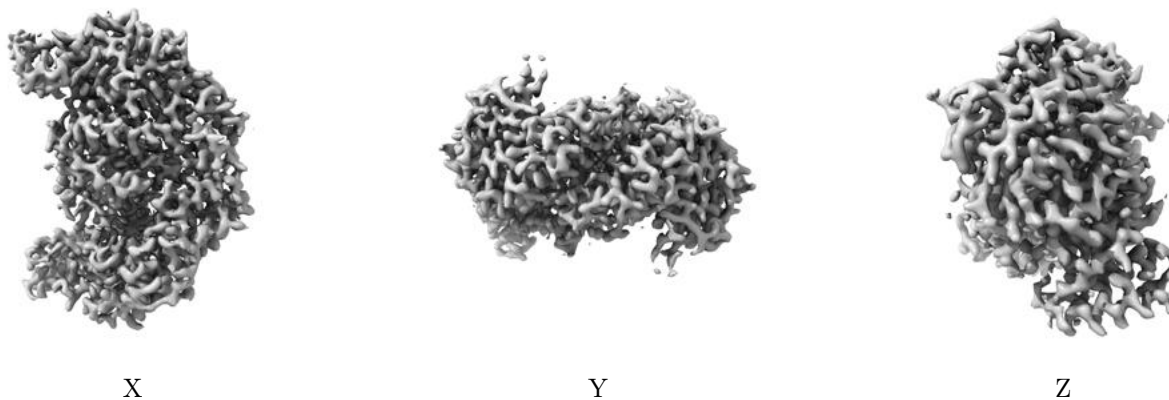


Z

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.

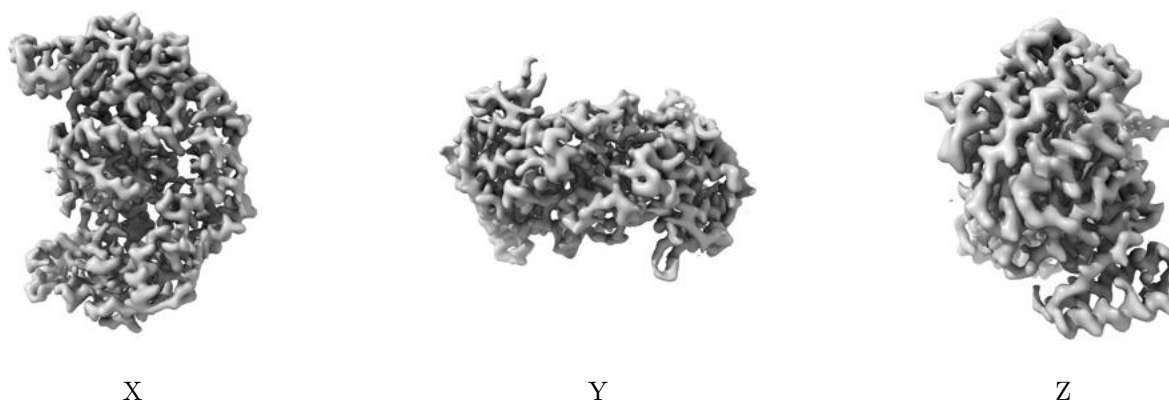
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.8. 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.

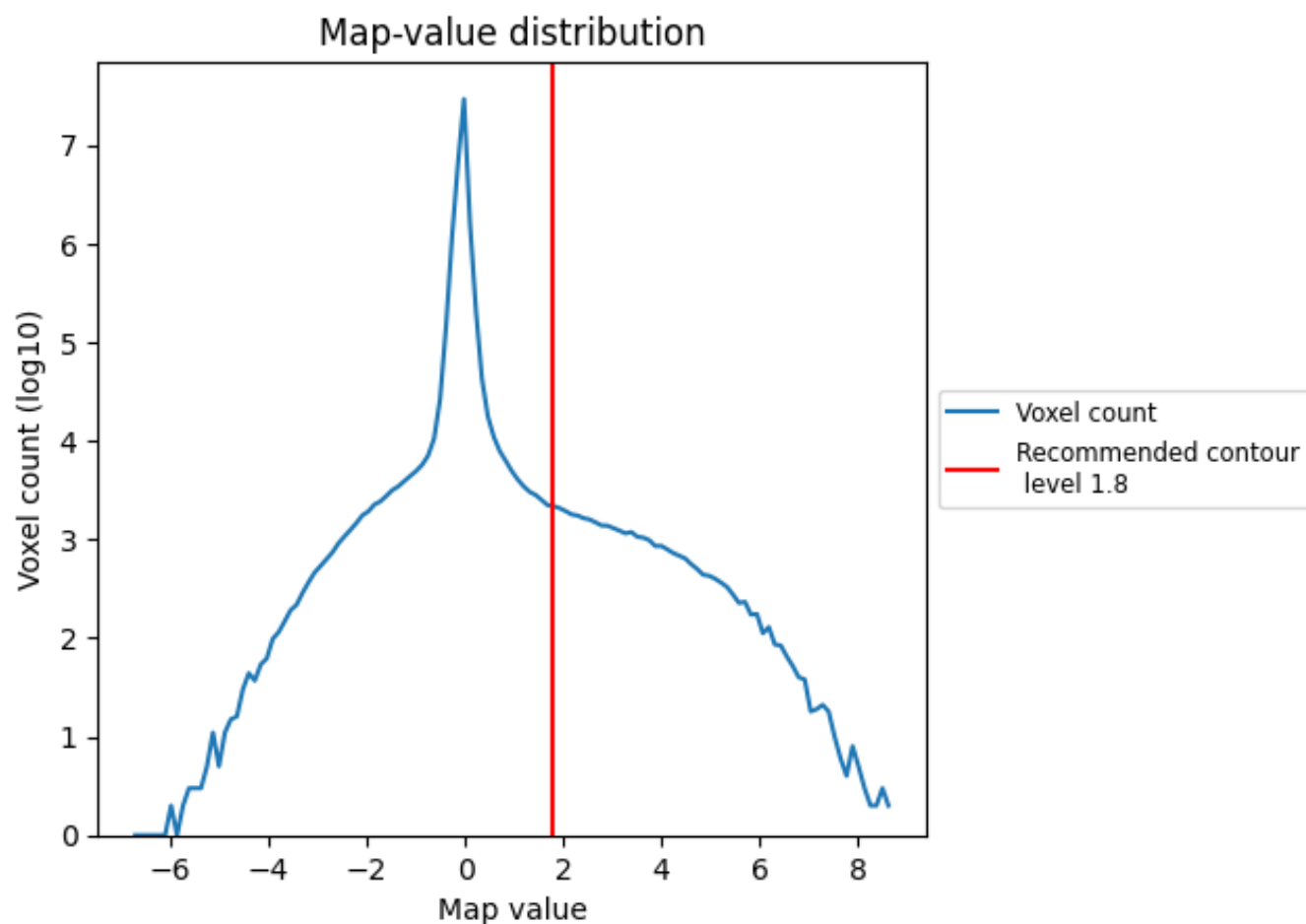
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

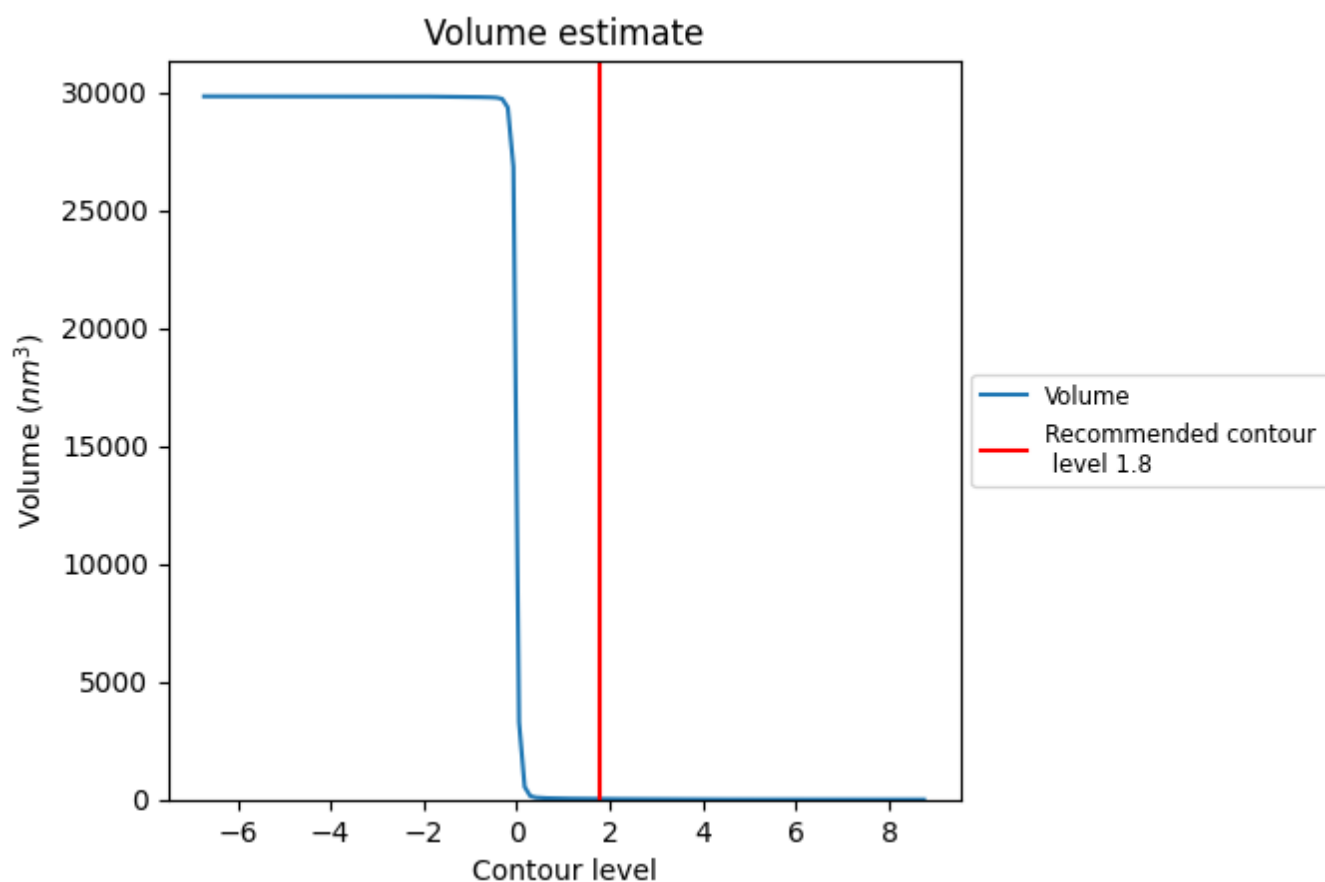
This section contains the results of statistical analysis of the map.

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.

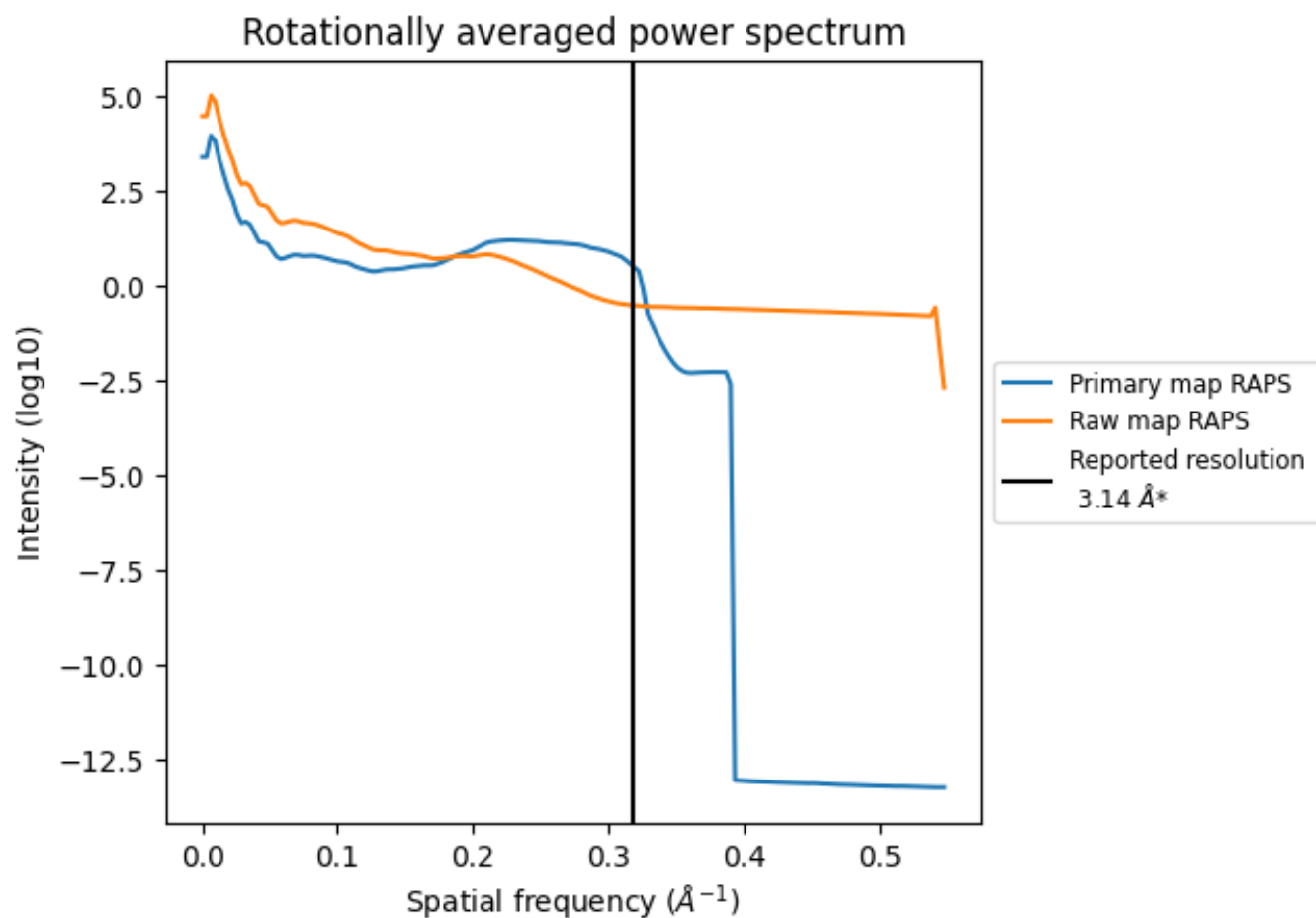
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 26 nm³; this corresponds to an approximate mass of 24 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 ⓘ

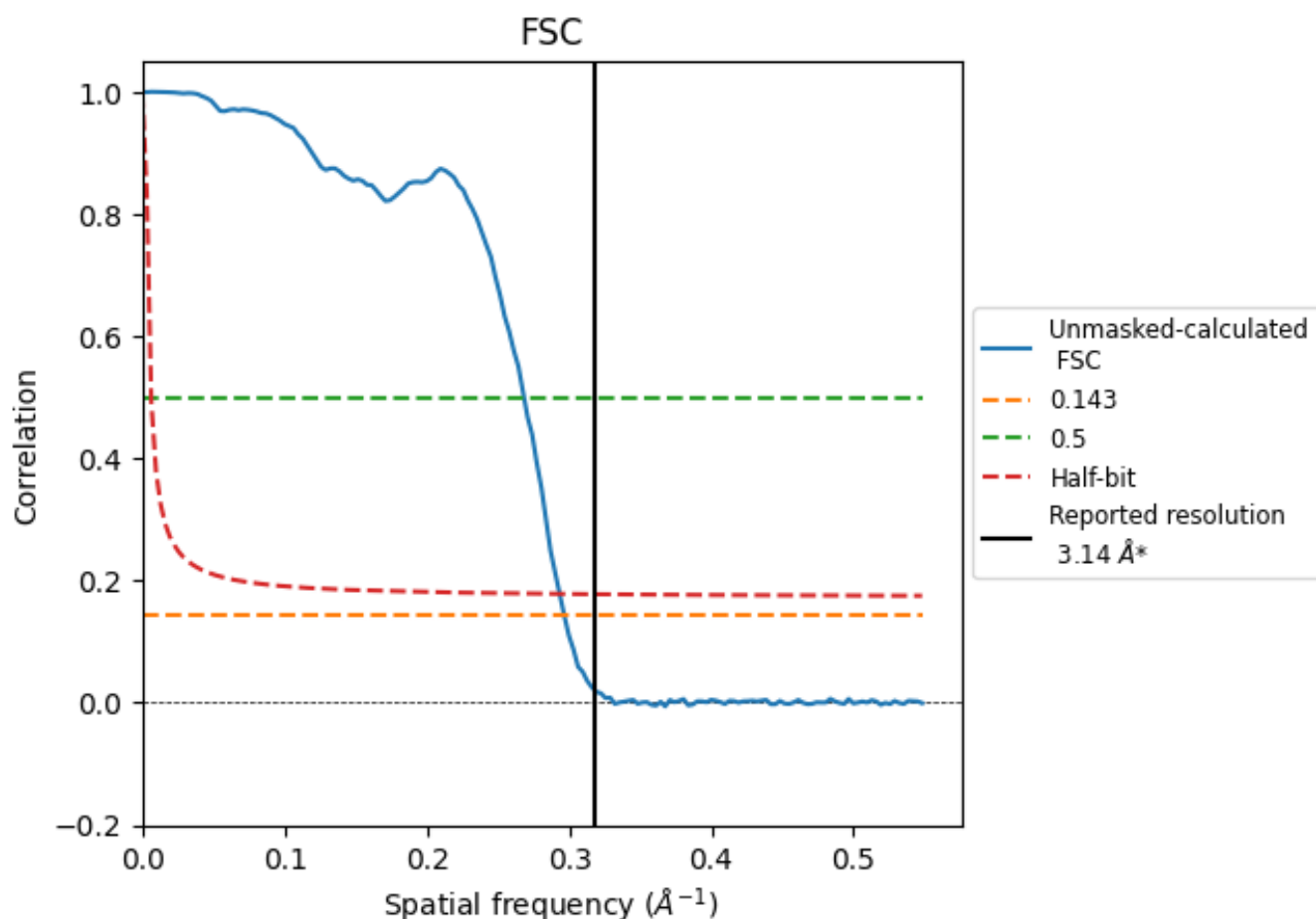


*Reported resolution corresponds to spatial frequency of 0.318 $\text{\AA}^{-1}$

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 0.318 Å⁻¹

8.2 Resolution estimates [i](#)

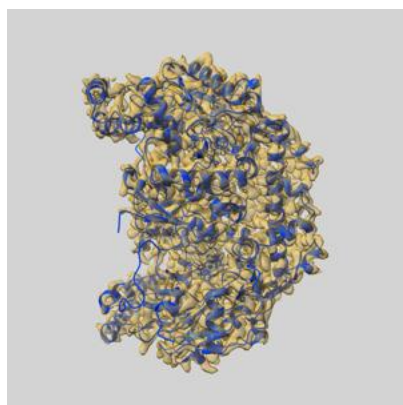
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.14	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.37	3.73	3.41

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

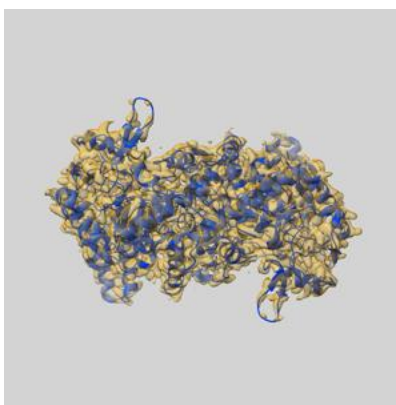
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40970 and PDB model 8T1K. Per-residue inclusion information can be found in section [3](#) on page [6](#).

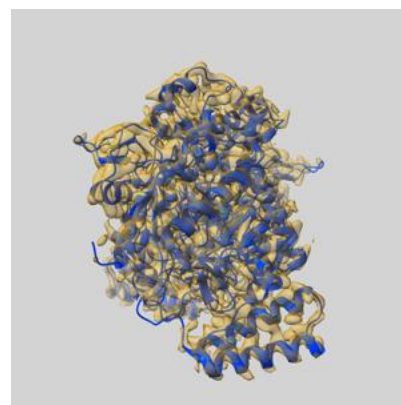
9.1 Map-model overlay [i](#)



X



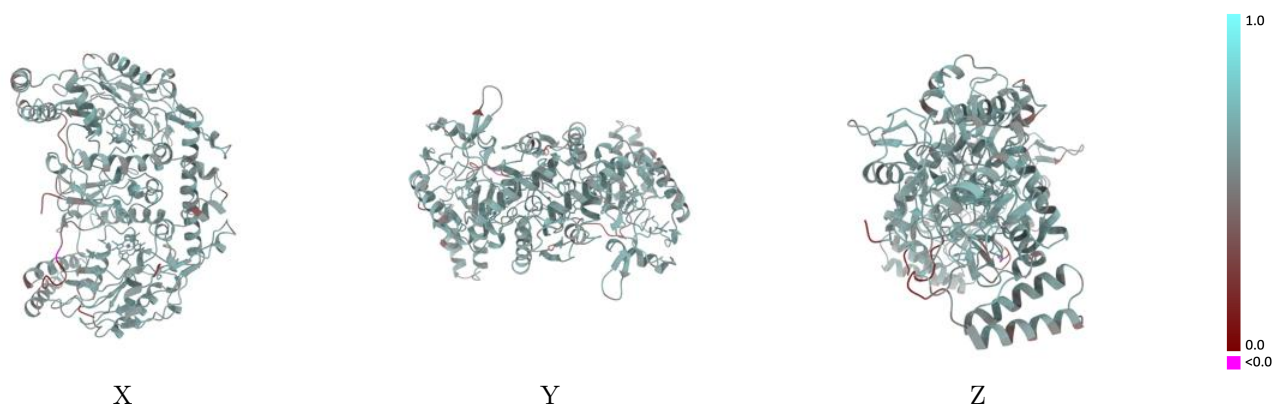
Y



Z

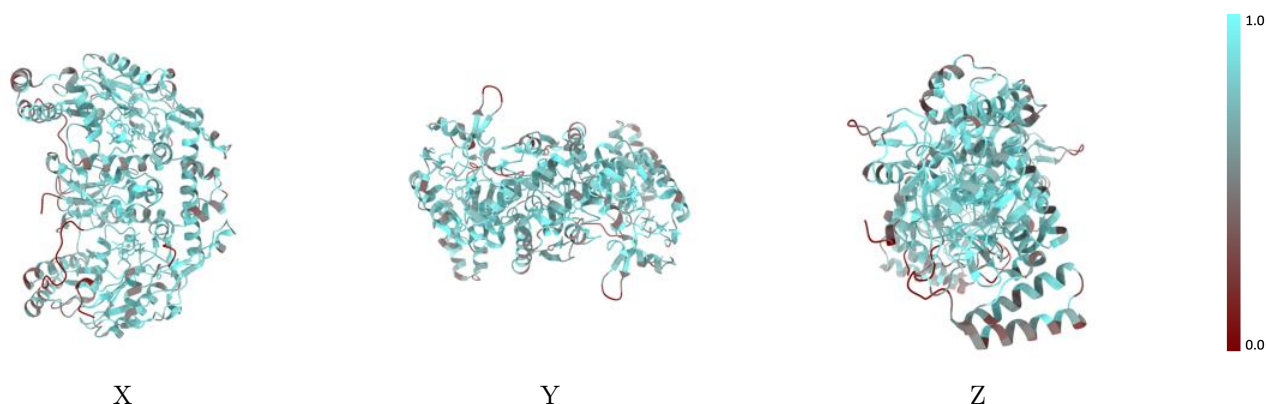
The images above show the 3D surface view of the map at the recommended contour level 1.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



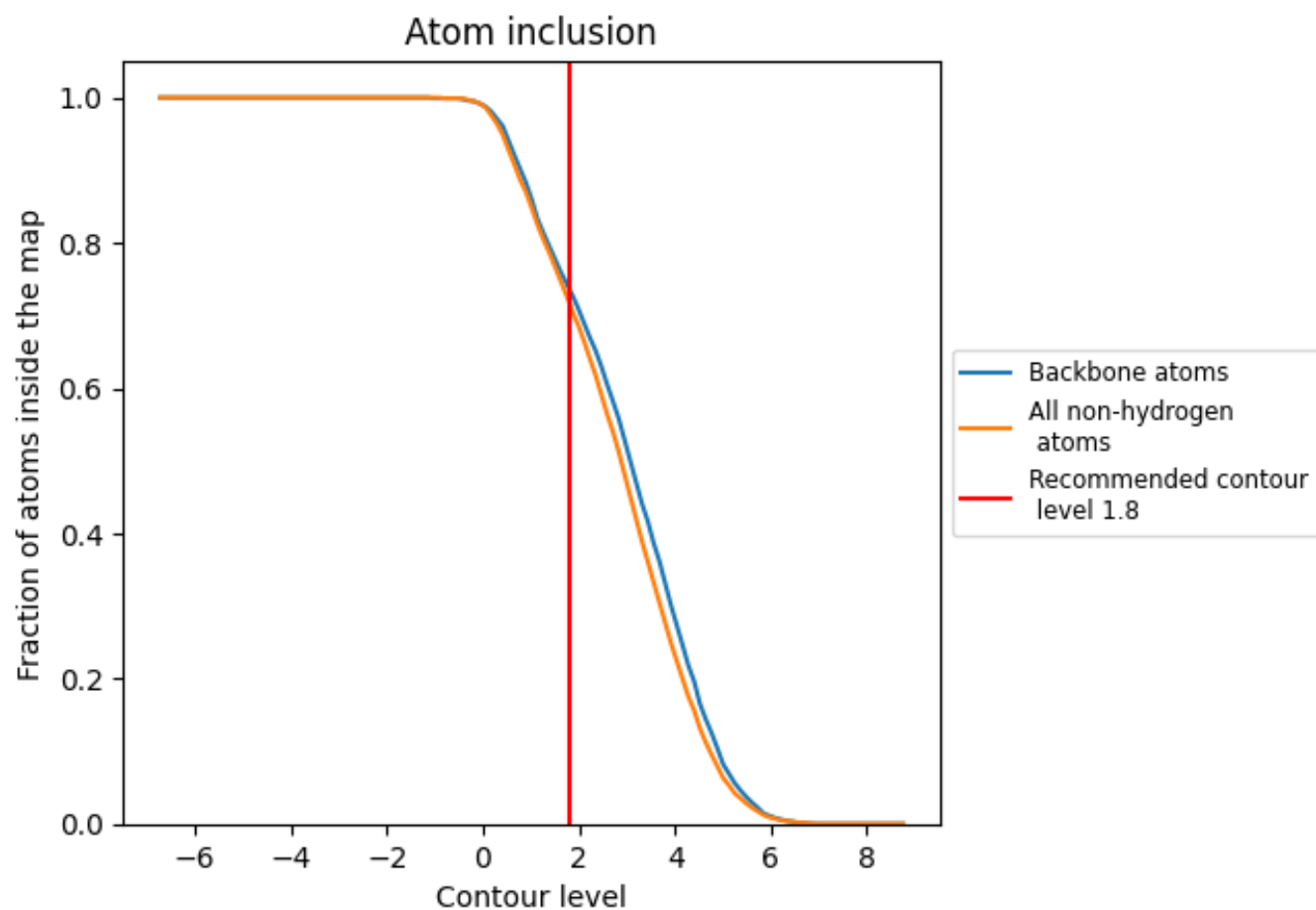
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 72% 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 (1.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7180	0.5640
A	0.7190	0.5640
B	0.7170	0.5640

