



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 01:20 PM UTC

PDB ID : 9Q0X / pdb_00009q0x
EMDB ID : EMD-72109
Title : syNOS Turnover State
Authors : Nair, D.; Crane, B.
Deposited on : 2025-08-13
Resolution : 3.77 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
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) : 2.49

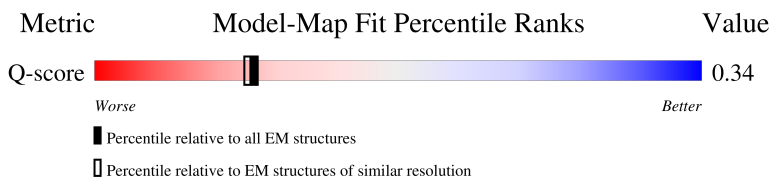
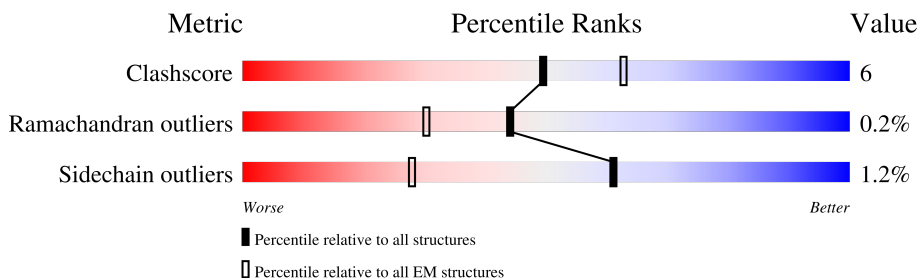
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

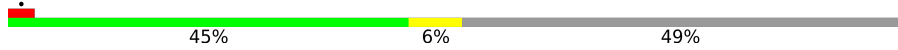
The reported resolution of this entry is 3.77 Å.

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	10146 (3.27 - 4.27)

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	1468	 45% 6% 49%
1	B	1468	 39% 1% 60%

2 Entry composition [i](#)

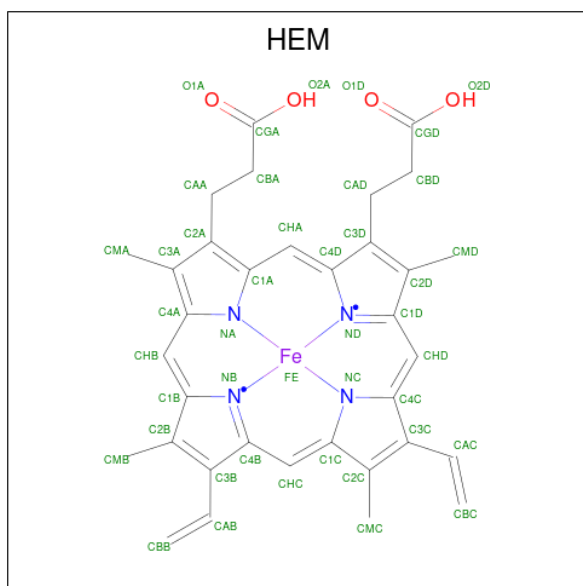
There are 2 unique types of molecules in this entry. The entry contains 22568 atoms, of which 11125 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	752	12087	3922	5975	1047	1107	36	0	0
1	B	628	10189	3320	5030	879	930	30	0	0

- Molecule 2 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
			Total	C	Fe	H	N	O	
2	A	1	73	34	1	30	4	4	0
2	A	1	73	34	1	30	4	4	0
2	B	1	73	34	1	30	4	4	0
2	B	1	73	34	1	30	4	4	0

[illegible]

- Molecule 1: Nitric oxide synthase

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ALA	PRO	GLU	LEU	MET	LEU	ASN	ALA	PHE	THR	CYS	SER	ASP	HIS	THR	SER	GLN	SER	GLY	GLU	VAL	SER	LEU	SER	LEU	ALA	GLY	THR	ARG	ALA	ASN	ALA	SER	ARG	ARG	PRO	THR	SER	LEU	ALA	VAL	SER	ASP	ASP	SER	ILE	E170	T178 Y179	L192	Q199 M200
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L207	L208	L209	L214	L240	E245	ASN	VAL	TRP	GLU	PRO	MET	MET	GLY	VAL	PRO	PRO	GLU	LYS	GLY	ASP	ALA	F263	D264	D268	L272	M291	M292	M293	L294	I297	V324	M328	L343	M347	R357	K358	N359	E360	M361	F365	E371
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G381	R382	A383	D384	M385	D386	G395	L418	L421	H422	V427	S436	M442	P448	G449	A457	W458	I462	L480	E493	V512	I543	I631	M634	P638	V651	E658	V692	L710	E720	D724	M734	M760
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Q779	S780		H787	H788	H789	L790	R791	E792	K793	R794	G795	GLY	ARG	GLU	CYS	PRO	ALA	ASP	THR	LYS	TRP	VAL	VAL	PRO	PRO	ALA	GLY	GLY	SER	SER	ALA	CYS	VAL	HIS	HIS	GLN	MET	ARG	ASP	F825	Y826	D843	ILE	ASP	LEU	GLU	GLN	PHE	VAL	GLN	THR	THR	HIS	GLU	SER
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GLN ARG ASP ARG ARG ILE LEU ILE LEU LEU PHE GLY GLU SER GLY THR THR GLY THR GLU ALA ALA ALA GLY PHE PHE ALA ALA ARG ARG ARG ARG ALA ALA ALA ARG GLN LEU LEU LEU SER SER ALA ALA TYR HIS PRO PRO LYS VAL VAL MET MET ALA ALA LEU LEU ASP ASP ASP ASP TYR TYR ASN ASN VAL VAL ASN ASN THR THR LEU LEU LEU ASP ASP GLU GLU LYS LEU LEU LEU LEU VAL VAL VAL THR THR SER THR THR PHE PHE GLN GLN

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

ALA	GLU	ASN	GLN	THR	GLU	GLY	LYS	ILE	ARG	LEU	GLU	THR	TRP	LEU	GLU	ILE	LEU	ALA	LEU	GLU	ASN	ALA	ALA	ALA	ARG	LYS	MET	LEU	ARG	ASP	ASN	ASP	PHE	MET	SER	VAL	ALA	ALA	ASP	PHE	LEU	GLU	GLY	PHE	PRO	SER	ALA	GLN	ILE	THR	LEU	LEU	GLY	MET	LEU	LEU	GLY	ALA
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[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61553	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.50	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.357	Depositor
Minimum map value	-0.135	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0428	Depositor
Map size (Å)	371.36, 371.36, 371.36	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.844, 0.844, 0.844	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.14	0/6276	0.30	0/8517
1	B	0.12	0/5302	0.27	0/7189
All	All	0.13	0/11578	0.28	0/15706

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	6112	5975	5964	66	0
1	B	5159	5030	5027	45	0
2	A	86	60	60	10	0
2	B	86	60	60	10	0
All	All	11443	11125	11111	129	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 6.

All (129) 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:B:200:MET:HE3	1:B:200:MET:HA	1.56	0.86
1:B:268:ASP:O	1:B:272:LEU:HD22	1.90	0.71
1:B:204:PHE:O	1:B:208:LEU:HD12	1.91	0.70
1:A:361:MET:HA	1:A:361:MET:HE2	1.75	0.68
1:A:300:LEU:HD22	1:A:304:ASP:HB2	1.76	0.67
1:A:401:LEU:HD12	1:A:402:CYS:N	2.12	0.64
1:A:612:MET:HE2	1:A:618:MET:CB	2.28	0.64
2:A:1502:HEM:HBB2	2:A:1502:HEM:HHC	1.80	0.63
2:B:1502:HEM:HBB2	2:B:1502:HEM:HHC	1.80	0.63
1:A:392:LEU:O	1:A:396:LEU:HD12	1.99	0.62
1:A:536:THR:HG21	2:A:1502:HEM:HMD3	1.82	0.60
1:B:775:MET:O	1:B:775:MET:HE3	2.02	0.59
2:B:1501:HEM:HMB2	2:B:1501:HEM:HBB2	1.85	0.58
1:B:204:PHE:CE1	1:B:208:LEU:HD11	2.39	0.58
1:A:634:MET:HE3	1:A:634:MET:HA	1.86	0.57
1:A:343:LEU:O	1:A:347:MET:HG2	2.05	0.57
1:A:125:MET:HA	1:A:125:MET:HE2	1.86	0.56
1:A:291:MET:HE3	1:A:291:MET:HA	1.88	0.55
1:B:291:MET:HE2	1:B:291:MET:O	2.07	0.55
2:A:1501:HEM:HBD2	2:A:1501:HEM:HHA	1.88	0.55
1:A:200:MET:HE3	1:A:200:MET:HA	1.89	0.55
1:B:385:MET:O	1:B:385:MET:HE3	2.08	0.54
1:B:293:MET:SD	1:B:294:LEU:HD22	2.49	0.54
2:A:1501:HEM:HMC1	2:A:1501:HEM:HBC2	1.90	0.53
1:A:38:ALA:HB3	1:A:54:LEU:HD22	1.90	0.52
1:A:365:PHE:CE2	1:A:369:LEU:HD12	2.45	0.52
1:A:300:LEU:HD22	1:A:304:ASP:CB	2.40	0.51
1:B:208:LEU:HD12	1:B:208:LEU:H	1.76	0.51
1:B:240:LEU:C	1:B:240:LEU:HD23	2.34	0.51
1:B:365:PHE:HA	1:B:442:MET:HE3	1.93	0.51
1:B:204:PHE:CD1	1:B:208:LEU:HD11	2.45	0.51
1:A:354:PHE:HA	1:A:357:ARG:CZ	2.41	0.50
2:A:1501:HEM:HMB2	2:A:1501:HEM:HBB2	1.92	0.50
1:B:775:MET:HE3	1:B:775:MET:C	2.36	0.50
1:B:631:ILE:HD11	1:B:638:PRO:HD3	1.93	0.50
1:A:344:VAL:HA	1:A:347:MET:HG2	1.94	0.49
2:B:1502:HEM:HMC2	2:B:1502:HEM:HBC2	1.94	0.49
1:A:42:VAL:HG11	1:A:68:HIS:CG	2.48	0.49
1:B:343:LEU:O	1:B:343:LEU:HD12	2.13	0.49
2:B:1501:HEM:HMC2	2:B:1501:HEM:HBC2	1.93	0.49
1:A:612:MET:HE2	1:A:618:MET:HB3	1.95	0.49
1:B:263:PHE:CE2	1:B:272:LEU:HD23	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1501:HEM:HBB2	2:B:1501:HEM:CMB	2.42	0.48
1:B:199:GLN:HB3	1:B:293:MET:HE1	1.96	0.48
1:A:400:PHE:CD1	1:A:400:PHE:C	2.92	0.47
2:A:1501:HEM:HBB2	2:A:1501:HEM:CMB	2.44	0.47
1:A:389:SER:O	1:A:393:PHE:CD1	2.67	0.47
1:A:396:LEU:HD12	1:A:396:LEU:H	1.79	0.47
1:A:15:LEU:HD21	1:A:69:PRO:HB3	1.96	0.47
1:A:446:TYR:O	1:A:447:VAL:HG23	2.14	0.47
1:A:436:SER:HB2	1:A:462:ILE:HG21	1.96	0.47
2:A:1501:HEM:HBC2	2:A:1501:HEM:CMC	2.43	0.47
1:A:21:VAL:O	1:A:63:LEU:HD12	2.15	0.47
2:B:1501:HEM:HBC2	2:B:1501:HEM:CMC	2.45	0.47
1:A:343:LEU:HD21	1:A:457:ALA:HB2	1.97	0.47
1:A:54:LEU:HD23	1:A:62:TRP:CG	2.50	0.46
1:B:209:LEU:O	1:B:209:LEU:HD12	2.16	0.46
1:B:178:THR:HG22	1:B:179:TYR:H	1.80	0.46
1:A:273:PHE:HA	1:A:276:ILE:HG22	1.96	0.46
1:A:377:LEU:HA	1:A:380:PHE:CE1	2.51	0.46
1:A:392:LEU:O	1:A:396:LEU:CD1	2.64	0.46
1:B:543:ILE:HD12	1:B:543:ILE:N	2.30	0.46
1:B:291:MET:HE2	1:B:291:MET:C	2.40	0.46
2:B:1502:HEM:HBC2	2:B:1502:HEM:CMC	2.46	0.46
2:A:1502:HEM:HBC2	2:A:1502:HEM:HMC2	1.97	0.46
1:B:200:MET:HA	1:B:200:MET:CE	2.38	0.46
1:A:341:PRO:O	1:A:344:VAL:HG12	2.16	0.46
1:A:393:PHE:CD1	1:A:393:PHE:N	2.81	0.46
1:A:347:MET:HE3	1:A:458:TRP:CD2	2.51	0.46
1:B:324:VAL:O	1:B:328:MET:HE2	2.16	0.46
1:B:207:LEU:HD11	1:B:214:LEU:CD1	2.46	0.45
1:B:380:PHE:CE1	2:B:1501:HEM:HHB	2.52	0.45
2:B:1502:HEM:HBD1	2:B:1502:HEM:HHA	1.98	0.45
1:B:634:MET:HE3	1:B:634:MET:HA	1.97	0.45
1:A:357:ARG:O	1:A:357:ARG:HG2	2.17	0.45
1:A:361:MET:O	1:A:361:MET:SD	2.75	0.45
1:A:828:GLU:HB2	1:A:829:PRO:HD3	1.99	0.45
1:A:364:GLU:C	1:A:442:MET:HE2	2.42	0.44
2:A:1502:HEM:HBC2	2:A:1502:HEM:CMC	2.47	0.44
1:A:368:THR:O	1:A:372:ARG:HB2	2.18	0.44
1:A:58:LEU:H	1:A:58:LEU:HD23	1.82	0.44
1:A:710:LEU:O	1:A:710:LEU:HG	2.18	0.44
1:B:178:THR:HG22	1:B:179:TYR:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ARG:C	1:A:125:MET:HE1	2.42	0.43
1:B:710:LEU:O	1:B:710:LEU:HG	2.17	0.43
1:A:181:GLU:HA	1:A:184:ILE:HG22	2.00	0.43
1:B:343:LEU:HD21	1:B:457:ALA:HB2	2.01	0.43
2:B:1502:HEM:HBB2	2:B:1502:HEM:CHC	2.46	0.43
1:B:787:ALA:HA	1:B:790:LEU:HD12	1.99	0.43
1:A:298:PRO:O	1:A:299:TYR:CD1	2.72	0.43
1:A:387:TYR:O	1:A:388:LEU:C	2.61	0.43
1:A:362:GLY:HA2	1:A:393:PHE:CZ	2.54	0.43
1:A:399:ILE:HG21	1:A:465:VAL:HG21	1.99	0.43
1:B:543:ILE:HG13	1:B:788:HIS:HB2	2.01	0.42
1:B:204:PHE:O	1:B:208:LEU:CD1	2.63	0.42
1:A:347:MET:HE3	1:A:458:TRP:CE2	2.54	0.42
1:A:443:PHE:HE1	1:A:450:PHE:CZ	2.38	0.42
2:A:1502:HEM:HBB2	2:A:1502:HEM:CHC	2.47	0.42
1:B:357:ARG:CD	1:B:361:MET:HE3	2.50	0.42
1:B:418:LEU:HA	1:B:421:LEU:HD12	2.02	0.42
1:B:480:LEU:HG	1:B:512:VAL:HG11	2.00	0.42
1:A:392:LEU:O	1:A:393:PHE:C	2.61	0.42
1:A:268:ASP:O	1:A:272:LEU:HG	2.19	0.42
1:A:458:TRP:O	1:A:462:ILE:HG12	2.20	0.42
1:B:760:MET:HE2	1:B:760:MET:HA	2.01	0.42
1:A:20:LEU:HD23	1:A:21:VAL:N	2.35	0.41
1:B:343:LEU:O	1:B:347:MET:HG2	2.21	0.41
1:B:427:VAL:O	1:B:427:VAL:HG13	2.20	0.41
1:A:370:PHE:CD1	1:A:377:LEU:HD22	2.55	0.41
1:B:418:LEU:HD11	1:B:422:HIS:CE1	2.56	0.41
1:A:393:PHE:N	1:A:393:PHE:HD1	2.19	0.41
1:A:548:MET:HE3	1:A:548:MET:HB2	1.94	0.41
1:B:192:LEU:HD12	1:B:297:ILE:HD11	2.03	0.41
1:A:74:PHE:N	1:A:74:PHE:CD1	2.88	0.41
1:A:734:MET:HE1	1:A:753:ARG:HG3	2.03	0.41
1:B:347:MET:HE3	1:B:458:TRP:CD2	2.55	0.41
1:B:734:MET:C	1:B:734:MET:SD	3.04	0.41
1:A:465:VAL:O	1:A:469:ILE:HG12	2.21	0.41
1:A:579:ILE:HG21	1:A:714:GLY:O	2.21	0.41
1:B:436:SER:HB2	1:B:462:ILE:HG21	2.02	0.41
1:A:54:LEU:HD23	1:A:62:TRP:CD1	2.57	0.40
1:B:779:GLN:HG2	1:B:780:SER:N	2.37	0.40
1:A:177:LEU:HD11	1:A:322:THR:HG21	2.03	0.40
1:A:180:SER:O	1:A:183:VAL:HG22	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:GLU:O	1:A:367:GLN:HG2	2.21	0.40
1:B:720:GLU:O	1:B:724:ASP:OD1	2.39	0.40
1:A:612:MET:HE2	1:A:618:MET:HB2	2.03	0.40
1:A:347:MET:HB3	1:A:458:TRP:CZ2	2.57	0.40
1:A:717:MET:SD	1:A:776:VAL:HG23	2.61	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	744/1468 (51%)	709 (95%)	33 (4%)	2 (0%)	36	67
1	B	622/1468 (42%)	602 (97%)	19 (3%)	1 (0%)	43	72
All	All	1366/2936 (46%)	1311 (96%)	52 (4%)	3 (0%)	44	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	PRO
1	A	658	GLU
1	B	658	GLU

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	646/1262 (51%)	637 (99%)	9 (1%)	59	70
1	B	541/1262 (43%)	536 (99%)	5 (1%)	70	74
All	All	1187/2524 (47%)	1173 (99%)	14 (1%)	61	71

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	TRP
1	A	90	HIS
1	A	106	GLN
1	A	188	VAL
1	A	398	PHE
1	A	403	LEU
1	A	605	ILE
1	A	700	MET
1	A	765	LEU
1	B	199	GLN
1	B	272	LEU
1	B	493	GLU
1	B	651	VAL
1	B	692	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	51	ASN
1	A	53	GLN
1	A	87	GLN
1	A	345	GLN
1	A	697	ASN
1	B	199	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	HEM	B	1501	-	50,50,50	1.40	8 (16%)	67,82,82	1.05	4 (5%)
2	HEM	A	1501	1	50,50,50	1.31	7 (14%)	67,82,82	0.96	1 (1%)
2	HEM	B	1502	1	50,50,50	1.32	7 (14%)	67,82,82	1.11	5 (7%)
2	HEM	A	1502	1	50,50,50	1.40	7 (14%)	67,82,82	1.10	3 (4%)

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	HEM	B	1501	-	-	1/14/54/54	-
2	HEM	A	1501	1	-	3/14/54/54	-
2	HEM	B	1502	1	-	3/14/54/54	-
2	HEM	A	1502	1	-	1/14/54/54	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1502	HEM	FE-NB	3.73	2.06	1.94
2	B	1501	HEM	FE-NB	3.34	2.05	1.94
2	B	1501	HEM	FE-ND	3.29	2.05	1.94
2	A	1502	HEM	FE-ND	3.18	2.04	1.94
2	B	1501	HEM	FE-NA	3.01	2.05	1.95
2	B	1502	HEM	FE-ND	2.98	2.04	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1501	HEM	CAC-C3C	2.96	1.55	1.47
2	B	1502	HEM	CAB-C3B	2.95	1.55	1.47
2	B	1501	HEM	CAB-C3B	2.94	1.55	1.47
2	A	1501	HEM	CAC-C3C	2.85	1.55	1.47
2	B	1502	HEM	CAC-C3C	2.84	1.55	1.47
2	A	1501	HEM	CAB-C3B	2.84	1.55	1.47
2	A	1501	HEM	FE-NB	2.82	2.03	1.94
2	A	1502	HEM	CAC-C3C	2.82	1.54	1.47
2	A	1502	HEM	CAB-C3B	2.79	1.54	1.47
2	B	1502	HEM	FE-NB	2.76	2.03	1.94
2	B	1501	HEM	FE-NC	2.76	2.04	1.95
2	A	1502	HEM	FE-NC	2.41	2.03	1.95
2	A	1502	HEM	FE-NA	2.38	2.03	1.95
2	A	1501	HEM	FE-NA	2.31	2.02	1.95
2	A	1501	HEM	FE-ND	2.25	2.01	1.94
2	A	1501	HEM	FE-NC	2.13	2.02	1.95
2	B	1502	HEM	C2A-C3A	-2.07	1.33	1.38
2	B	1501	HEM	CMB-C2B	2.06	1.55	1.50
2	A	1502	HEM	C2A-C3A	-2.04	1.33	1.38
2	B	1501	HEM	CMC-C2C	2.04	1.55	1.50
2	B	1502	HEM	FE-NC	2.04	2.01	1.95
2	A	1501	HEM	C2A-C3A	-2.04	1.33	1.38
2	B	1502	HEM	CMD-C2D	2.02	1.54	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1502	HEM	C3B-C2B-C1B	2.81	108.52	106.41
2	A	1502	HEM	C3B-C2B-C1B	2.71	108.44	106.41
2	B	1502	HEM	C1B-NB-C4B	2.44	108.09	105.21
2	B	1501	HEM	C4D-ND-C1D	2.33	107.96	105.21
2	B	1501	HEM	C1B-NB-C4B	2.20	107.81	105.21
2	B	1501	HEM	C2A-C1A-NA	-2.13	107.79	110.15
2	B	1502	HEM	C4D-ND-C1D	2.11	107.71	105.21
2	B	1502	HEM	C3B-C4B-NB	-2.11	107.95	109.47
2	A	1501	HEM	C4D-ND-C1D	2.10	107.69	105.21
2	A	1502	HEM	C1B-NB-C4B	2.09	107.69	105.21
2	B	1502	HEM	C2A-C1A-NA	-2.05	107.88	110.15
2	B	1501	HEM	C3D-C4D-ND	-2.03	107.94	110.17
2	A	1502	HEM	C2A-C1A-NA	-2.02	107.91	110.15

There are no chirality outliers.

All (8) torsion outliers are listed below:

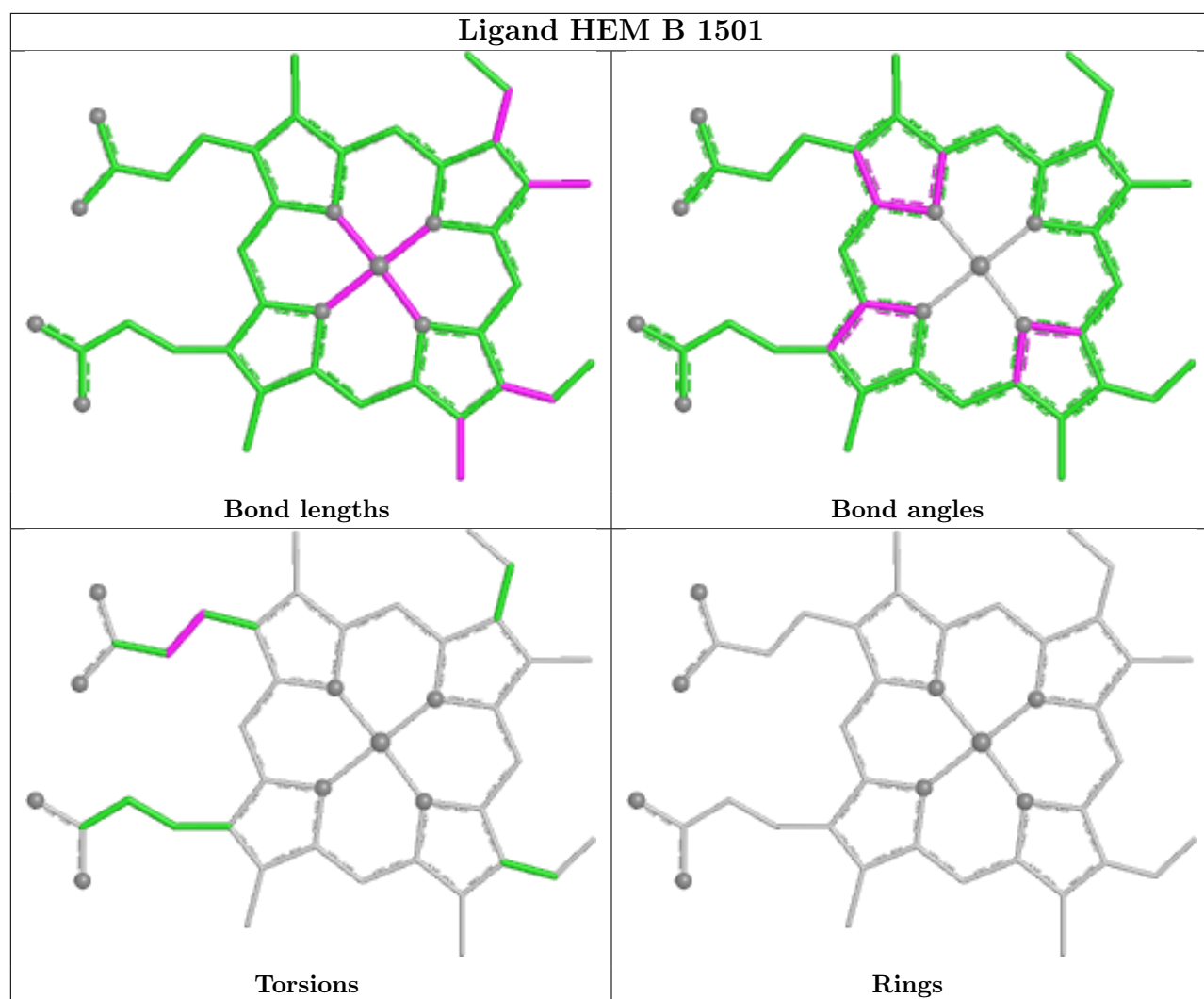
Mol	Chain	Res	Type	Atoms
2	A	1501	HEM	C4D-C3D-CAD-CBD
2	A	1501	HEM	C2D-C3D-CAD-CBD
2	B	1502	HEM	C4B-C3B-CAB-CBB
2	A	1502	HEM	C4B-C3B-CAB-CBB
2	B	1502	HEM	C4D-C3D-CAD-CBD
2	B	1501	HEM	C3D-CAD-CBD-CGD
2	B	1502	HEM	C2D-C3D-CAD-CBD
2	A	1501	HEM	C3D-CAD-CBD-CGD

There are no ring outliers.

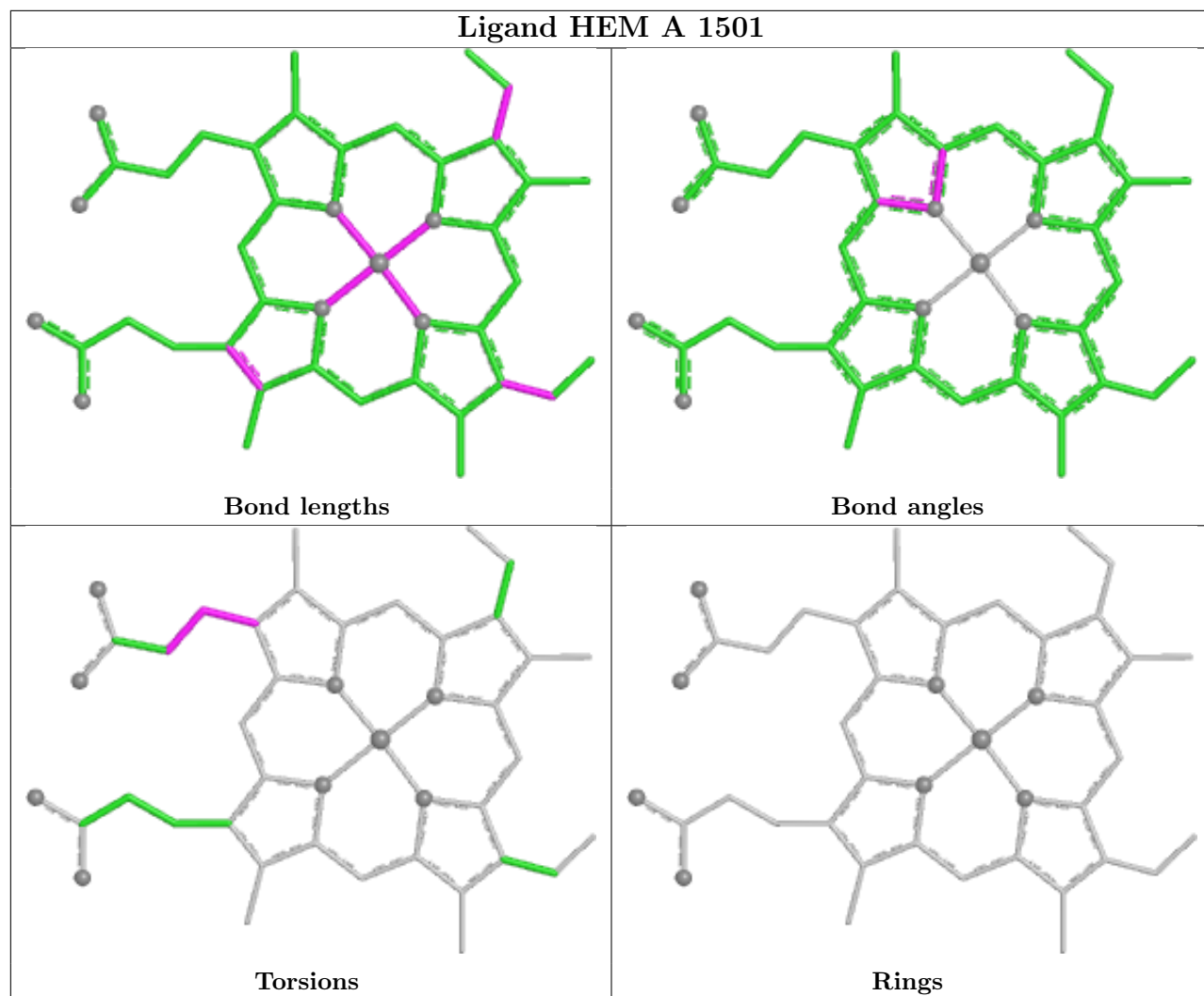
4 monomers are involved in 20 short contacts:

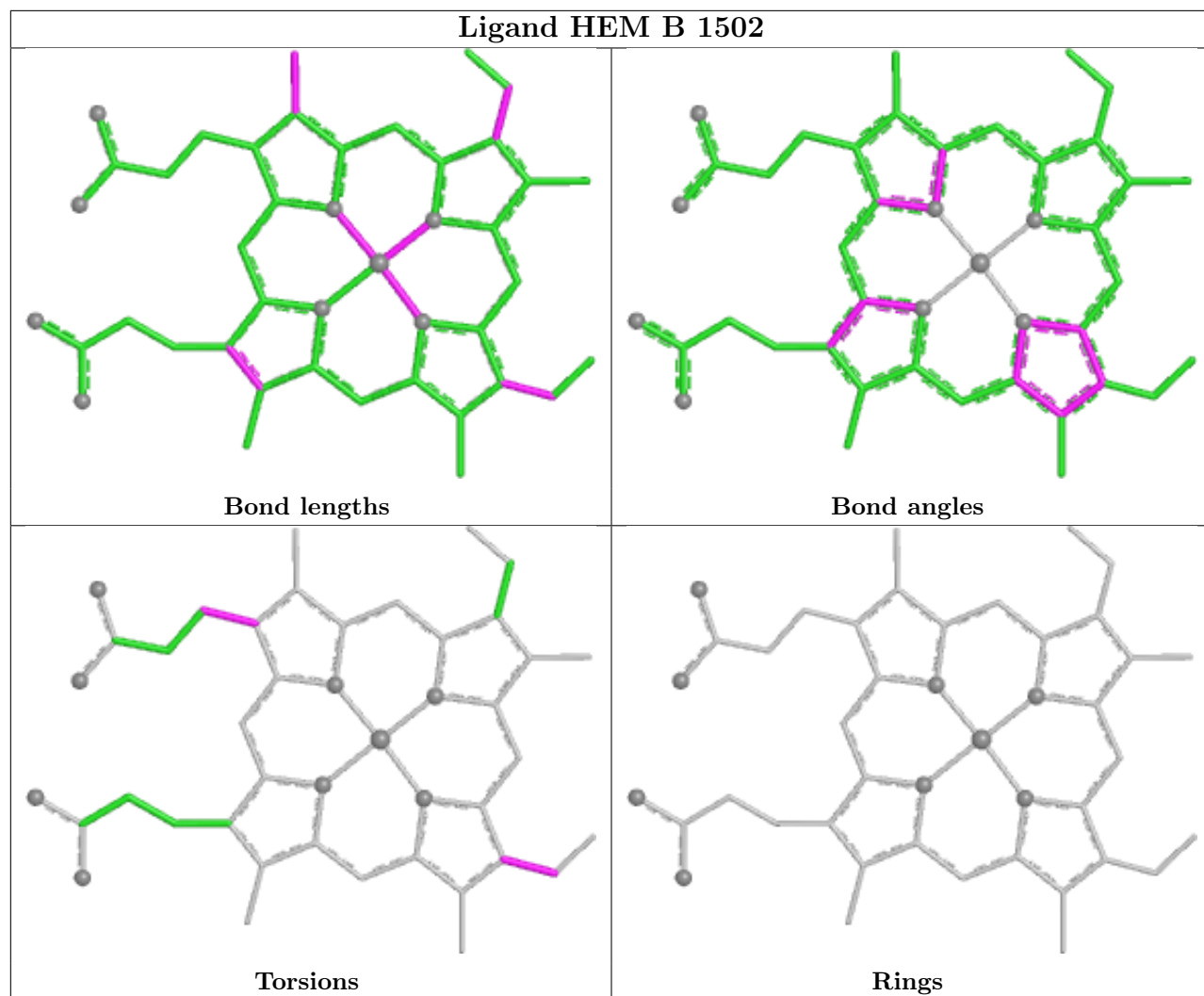
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1501	HEM	5	0
2	A	1501	HEM	5	0
2	B	1502	HEM	5	0
2	A	1502	HEM	5	0

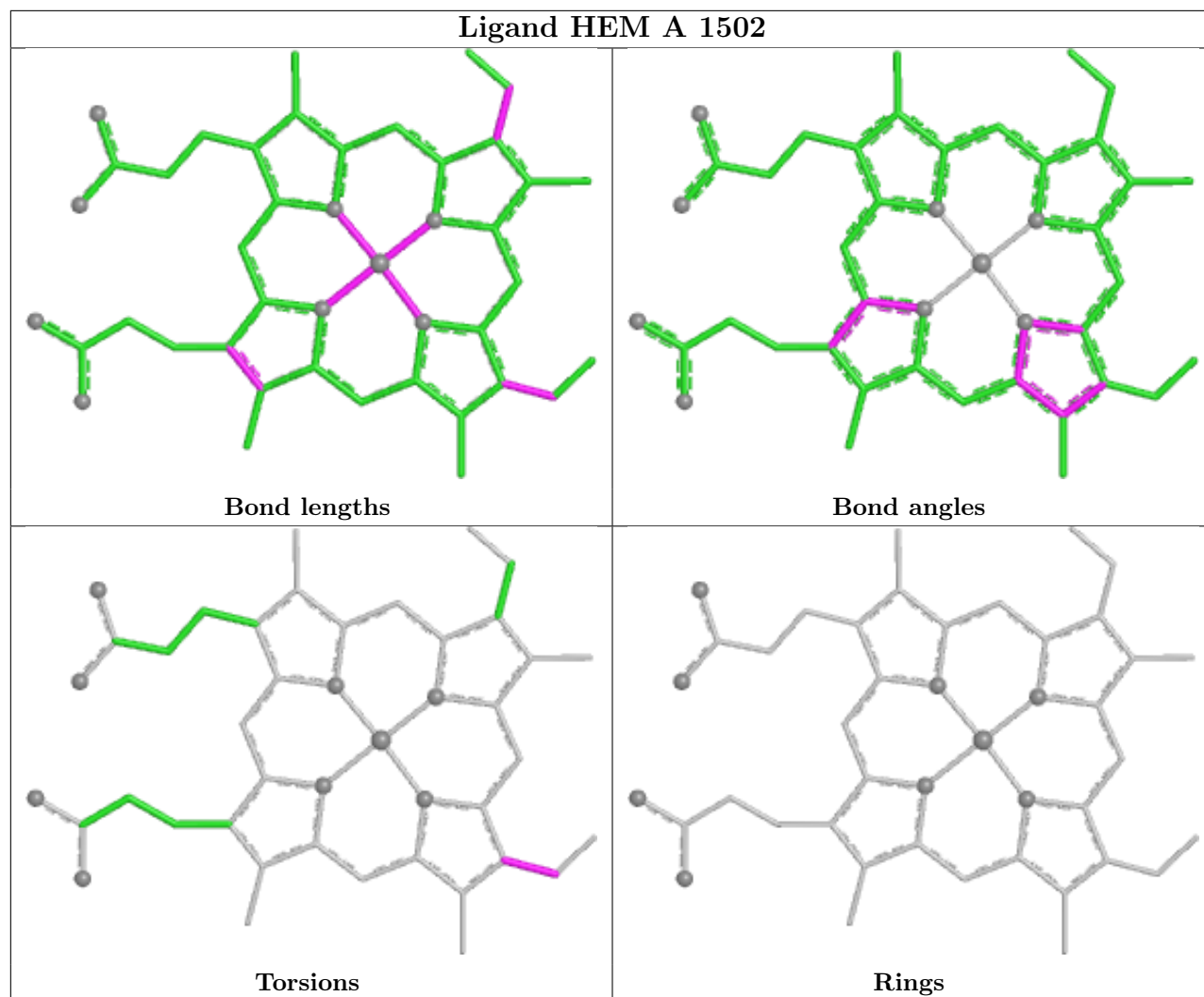
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 A 1501







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.

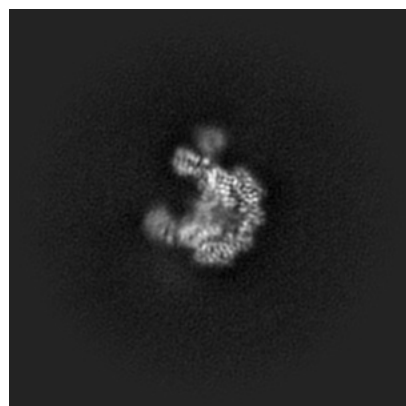
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72109. These allow visual inspection of the internal detail of the map and identification of artifacts.

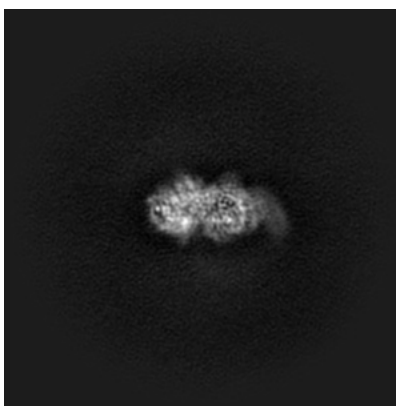
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

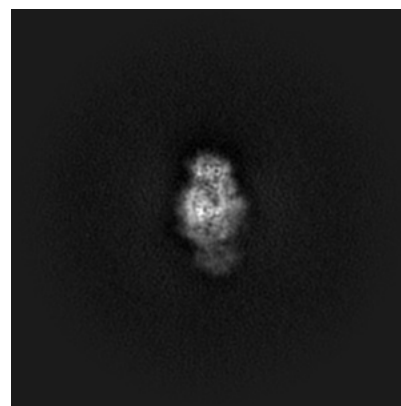
6.1.1 Primary map



X

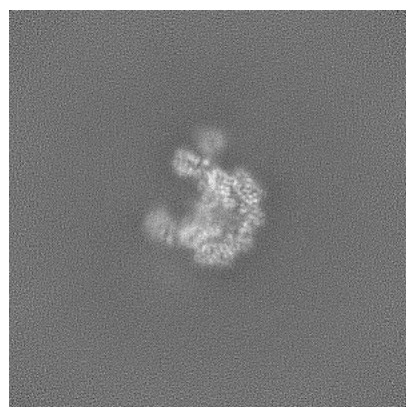


Y

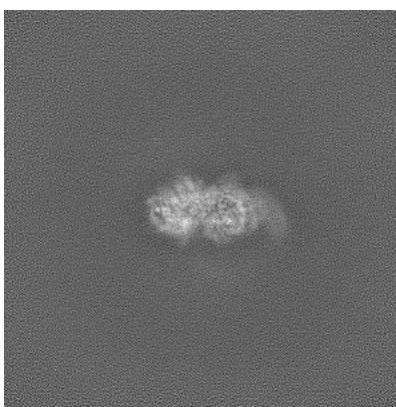


Z

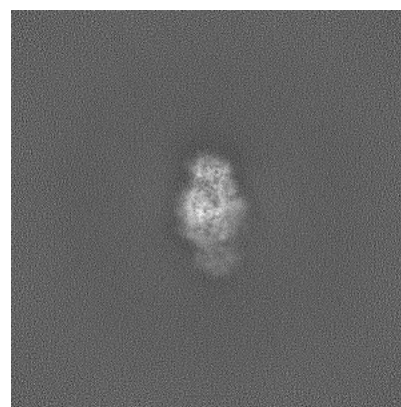
6.1.2 Raw map



X



Y

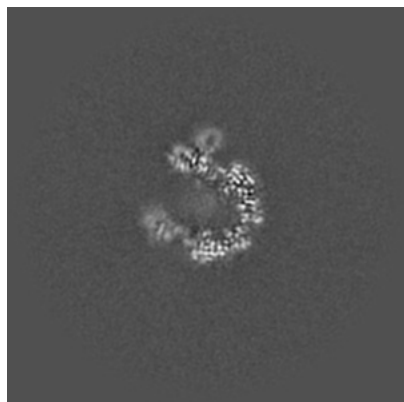


Z

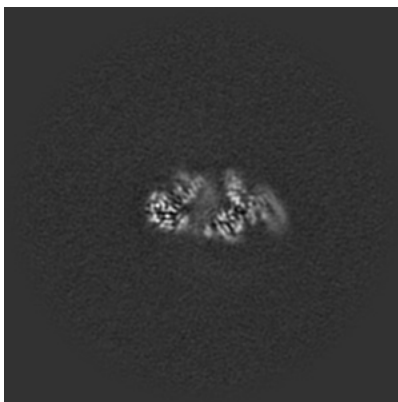
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

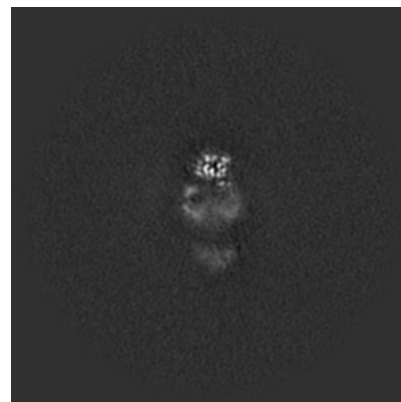
6.2.1 Primary map



X Index: 220

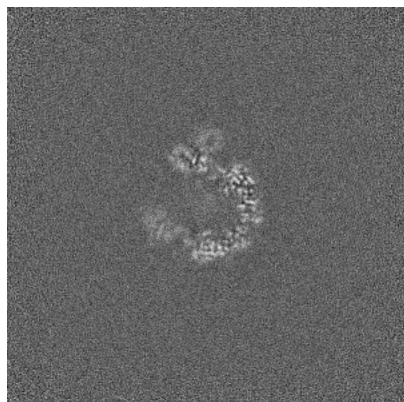


Y Index: 220

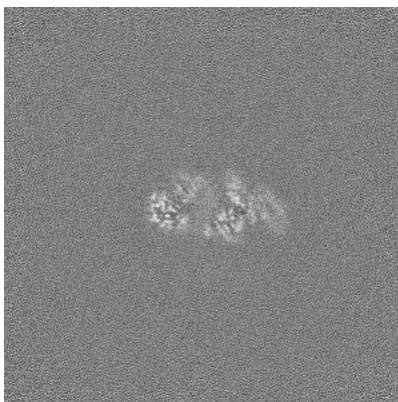


Z Index: 220

6.2.2 Raw map



X Index: 220



Y Index: 220

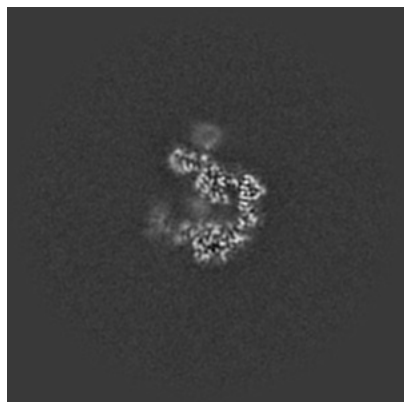


Z Index: 220

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

6.3 Largest variance slices [i](#)

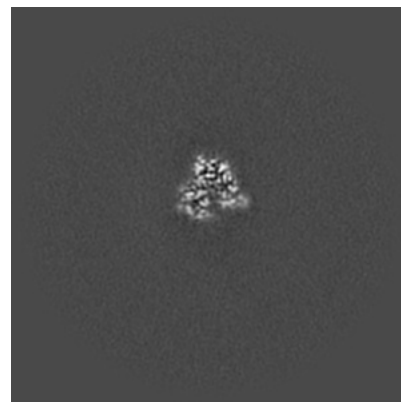
6.3.1 Primary map



X Index: 208

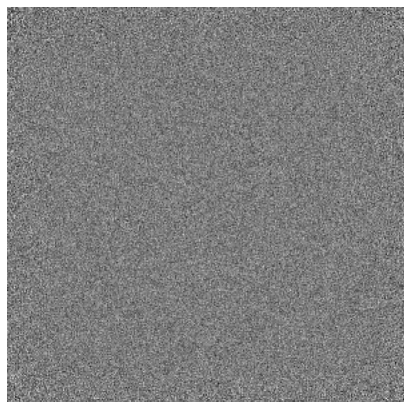


Y Index: 226

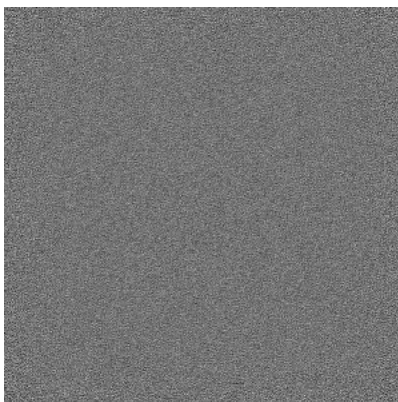


Z Index: 246

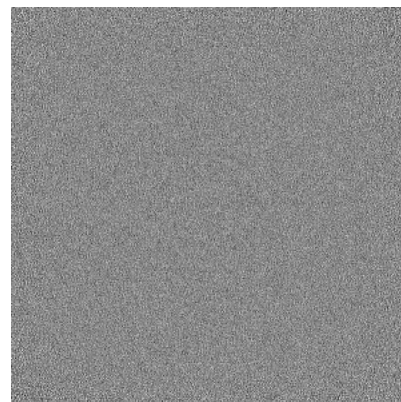
6.3.2 Raw map



X Index: 0



Y Index: 0



Z Index: 0

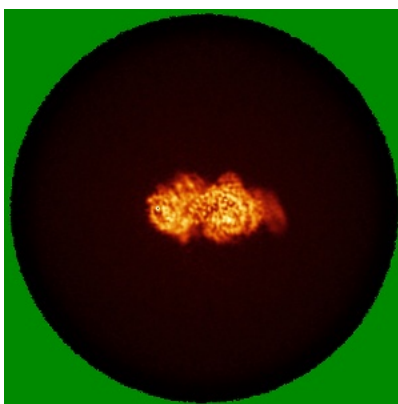
The images above show the largest variance slices of the map in three orthogonal directions.

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

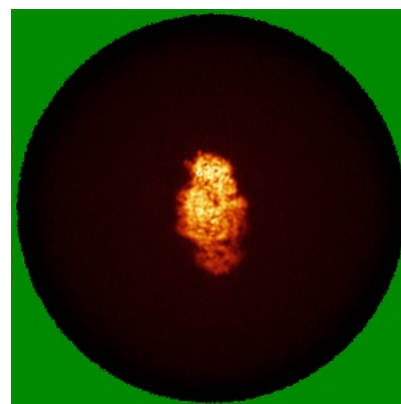
6.4.1 Primary map



X

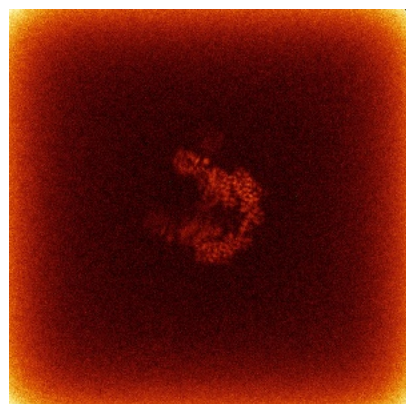


Y

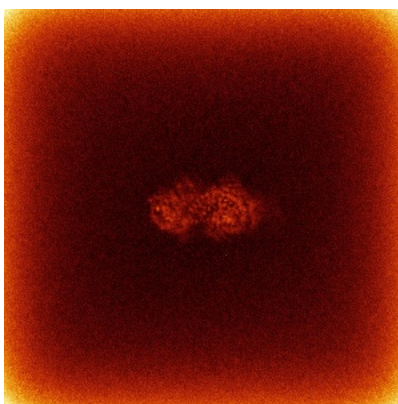


Z

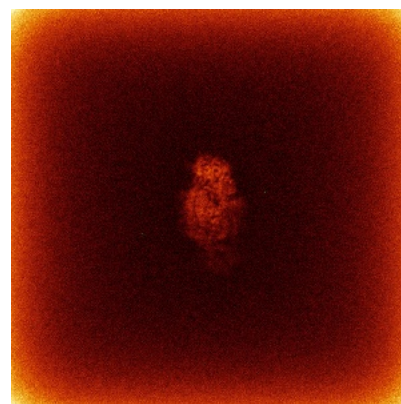
6.4.2 Raw map



X



Y



Z

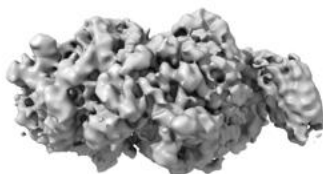
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



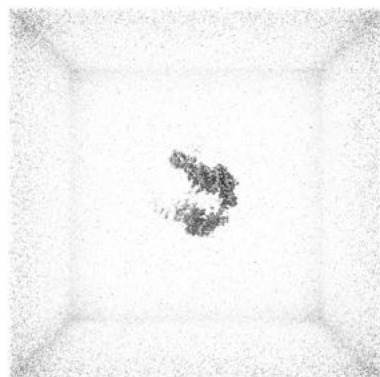
Y



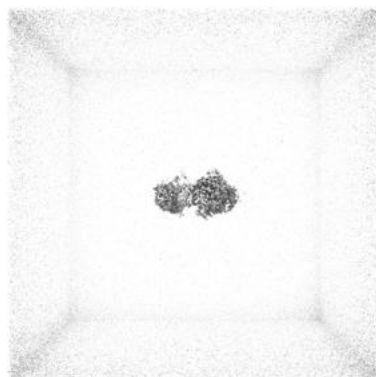
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0428. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

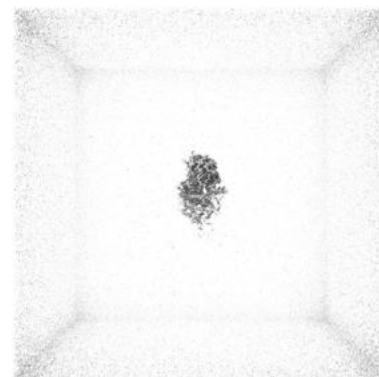
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

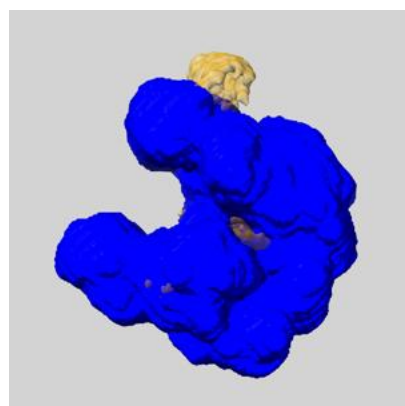
6.6 Mask visualisation [i](#)

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

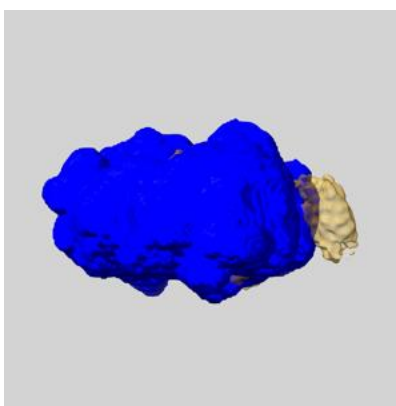
A mask typically either:

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

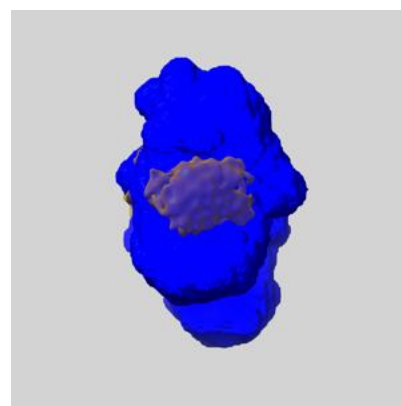
6.6.1 emd_72109_msk_1.map [i](#)



X



Y

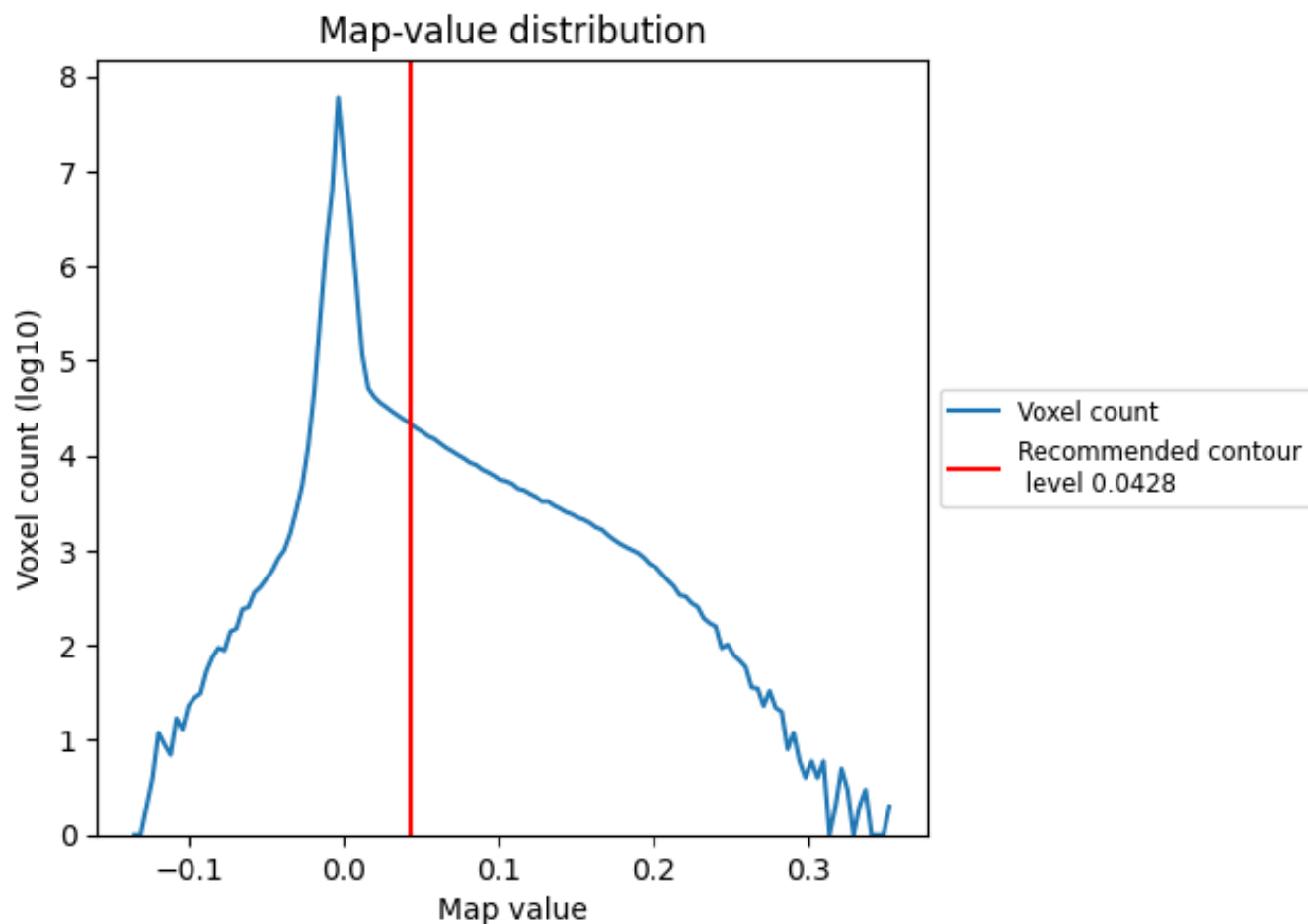


Z

7 Map analysis [i](#)

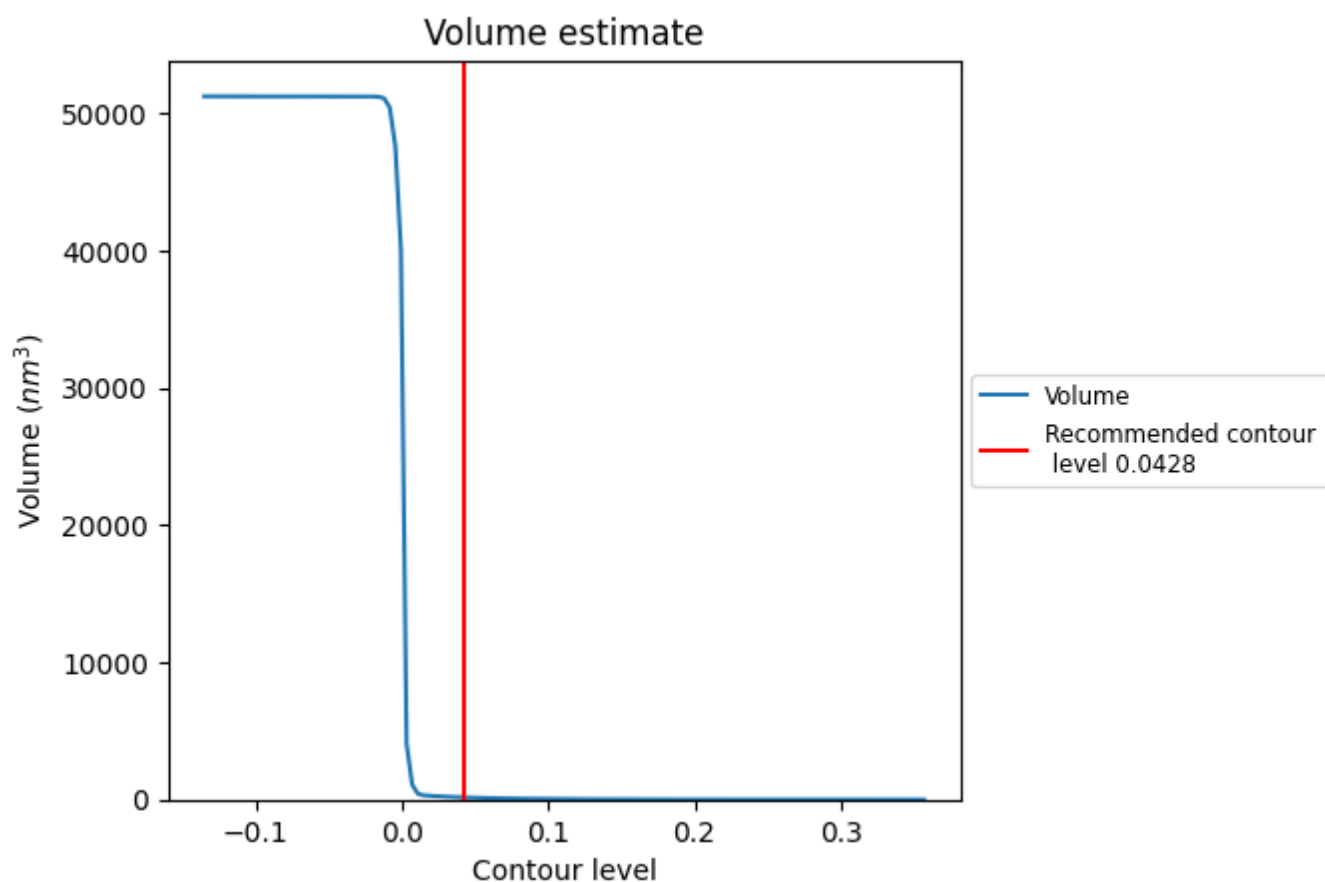
This section contains the results of statistical analysis of the map.

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.

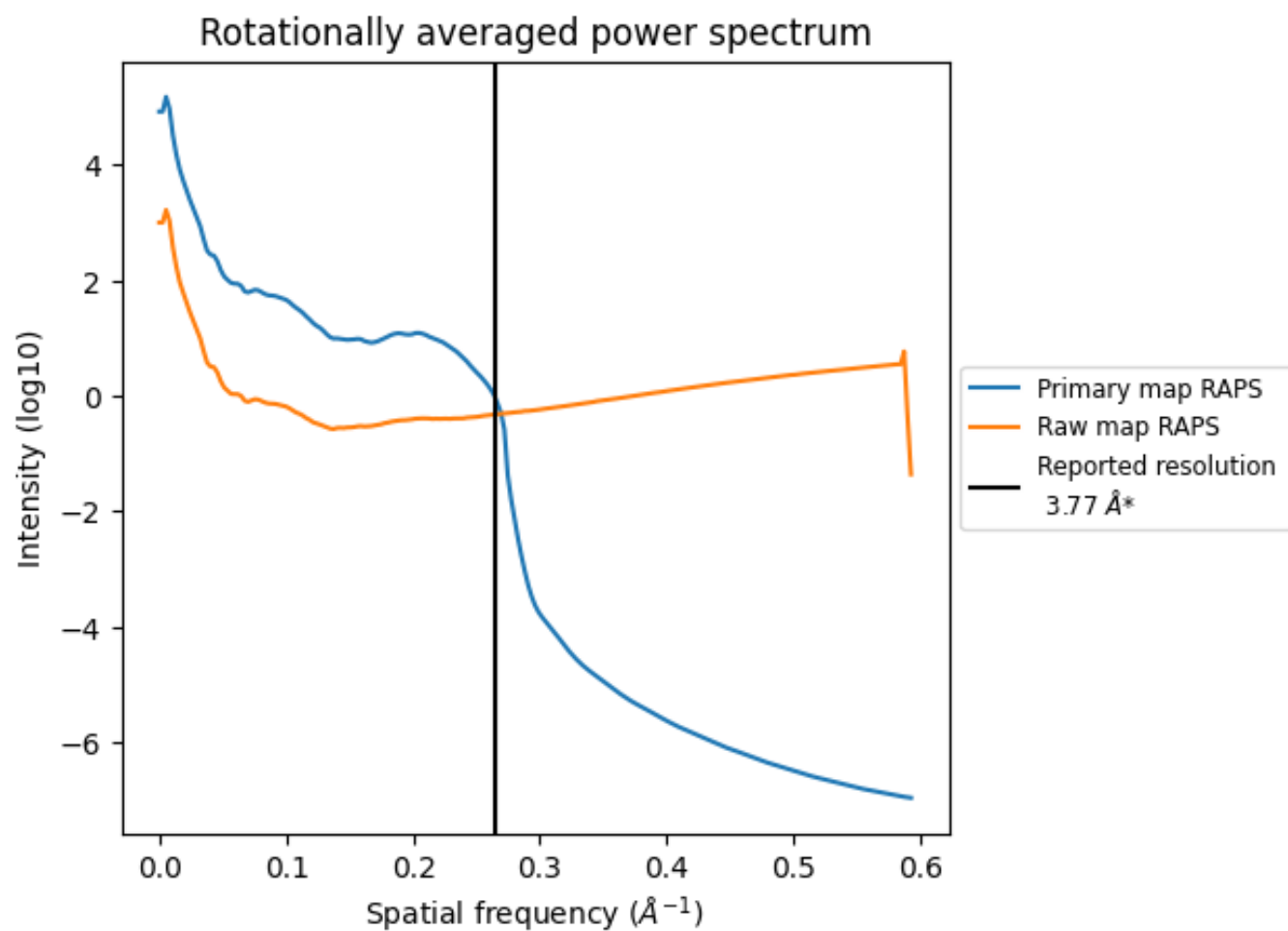
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 154 nm³; this corresponds to an approximate mass of 139 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 ⓘ

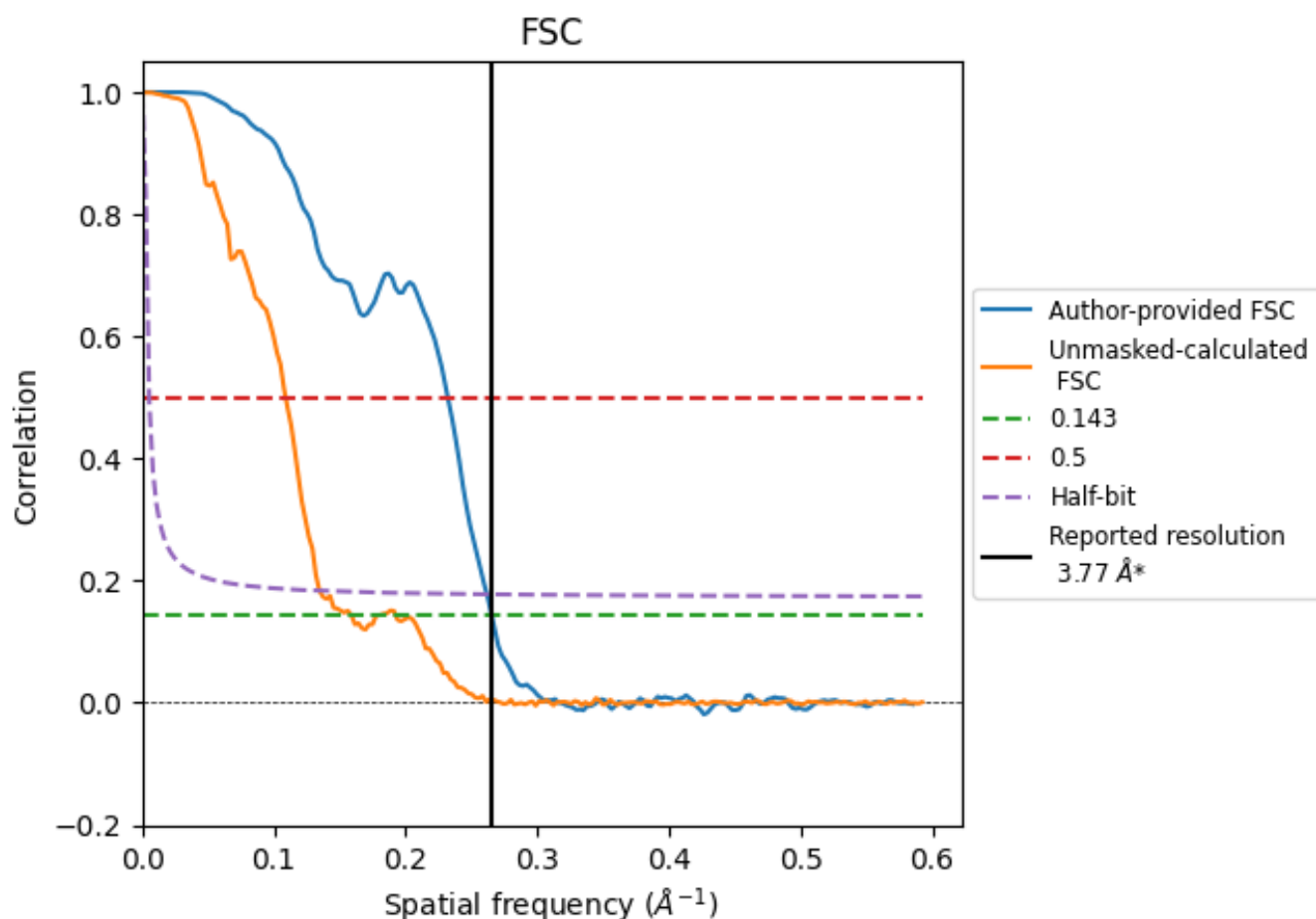


*Reported resolution corresponds to spatial frequency of $0.265 \text{ \AA}^{-1}$

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 0.265 Å⁻¹

8.2 Resolution estimates [i](#)

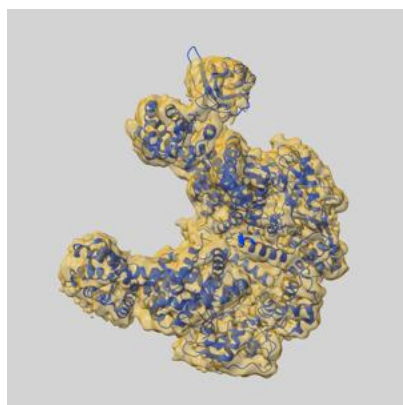
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.77	-	-
Author-provided FSC curve	3.77	4.31	3.82
Unmasked-calculated*	6.29	9.18	7.42

*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 6.29 differs from the reported value 3.77 by more than 10 %

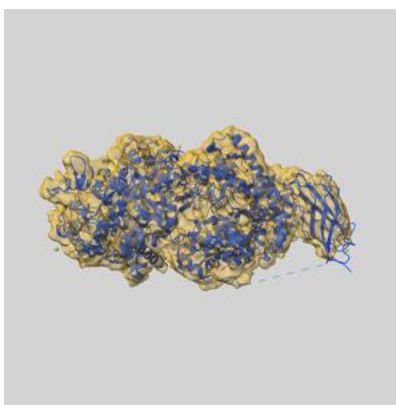
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72109 and PDB model 9Q0X. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

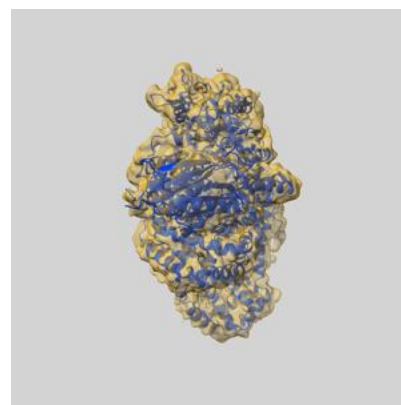
9.1 Map-model overlay [i](#)



X



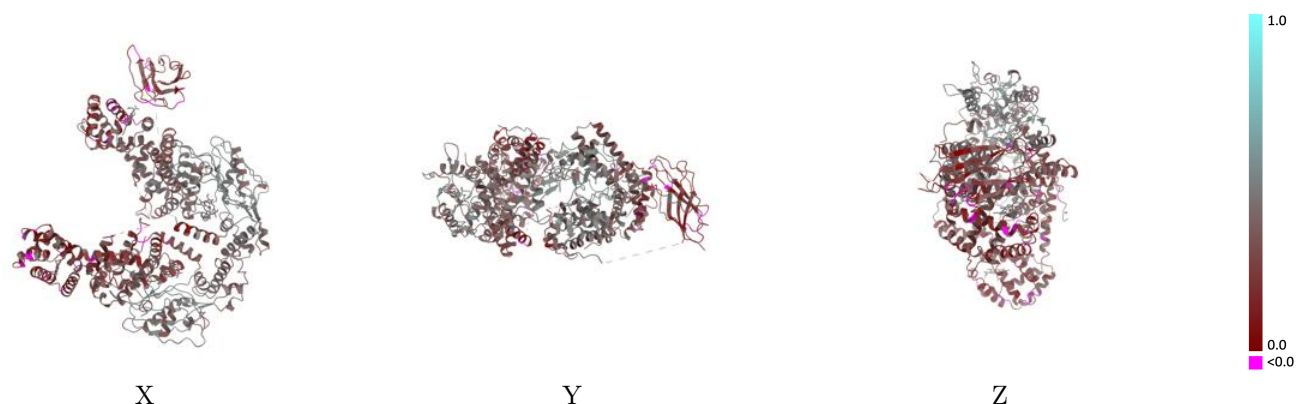
Y



Z

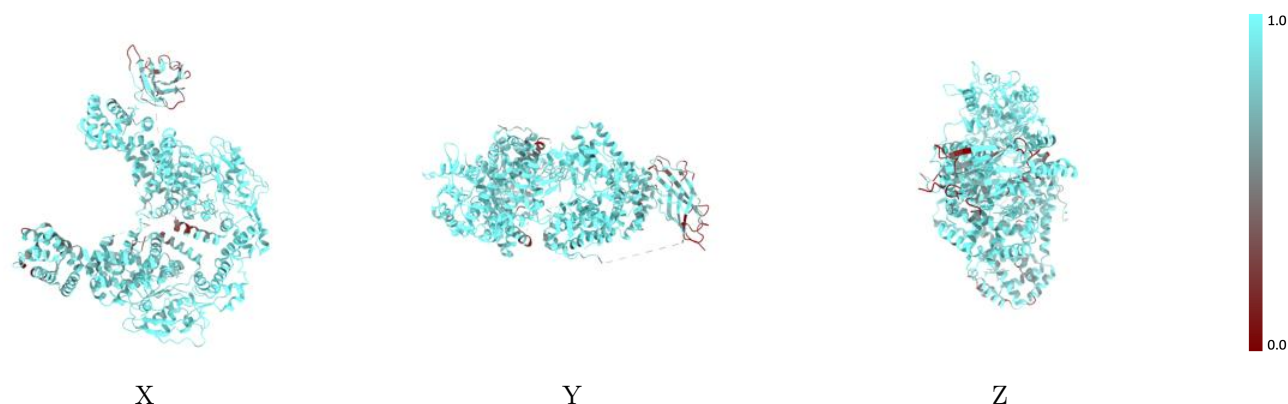
The images above show the 3D surface view of the map at the recommended contour level 0.0428 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



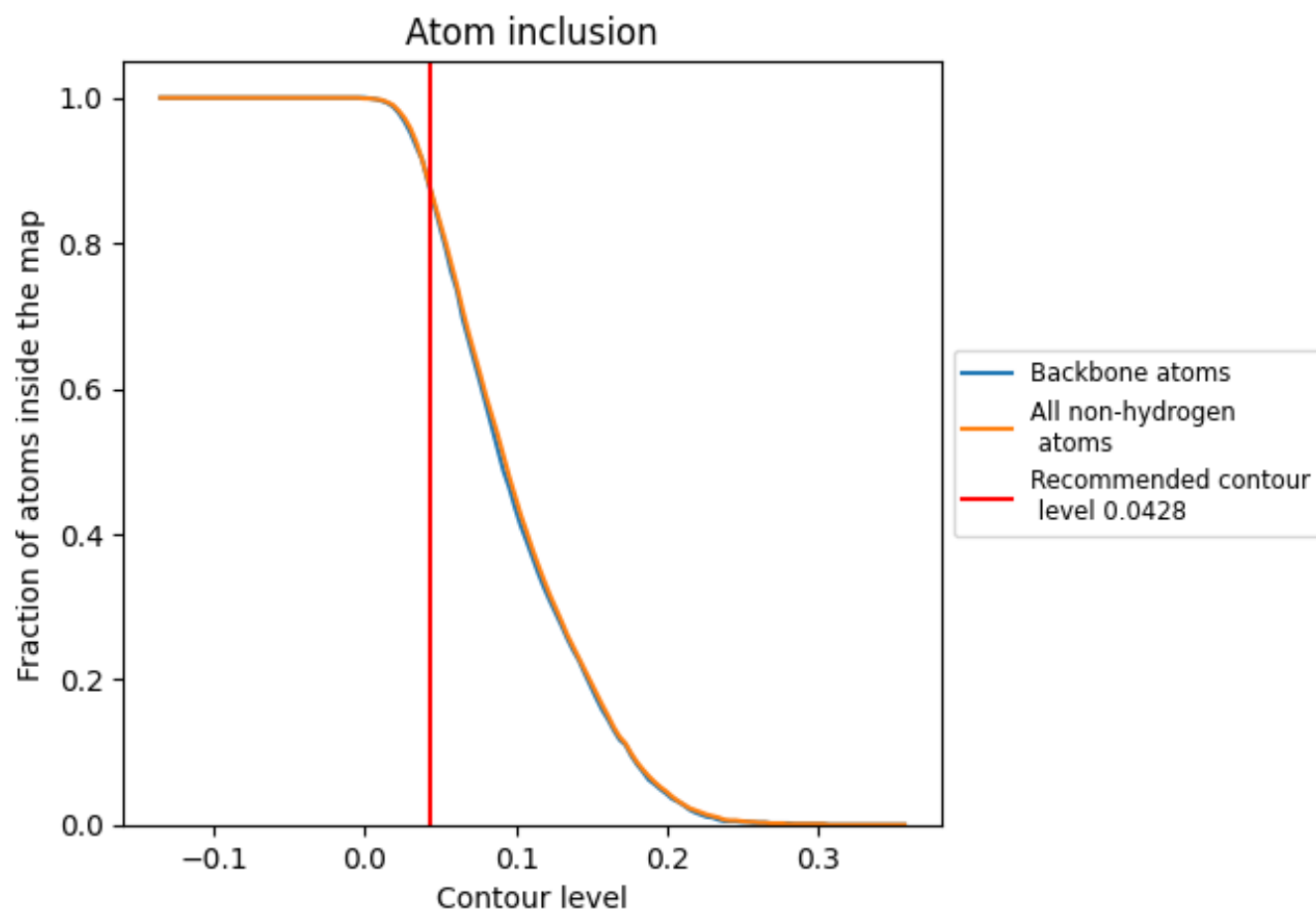
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0428).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 88% 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 (0.0428) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8780	0.3400
A	0.8830	0.3570
B	0.8840	0.3200

