Full wwPDB EM Validation Report

Nov 19, 2026 – 05:01 PM JST

PDB ID	:	25OU / pdb_000025ou
EMDB ID	:	EMD-80278
Title	:	Structure of mouse iNOS(S594E) mutant in the non-productive intermediate state
Authors	:	Chen, L.; Shi, Y.
Deposited on	:	2026-04-12
Resolution	:	4.23 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:

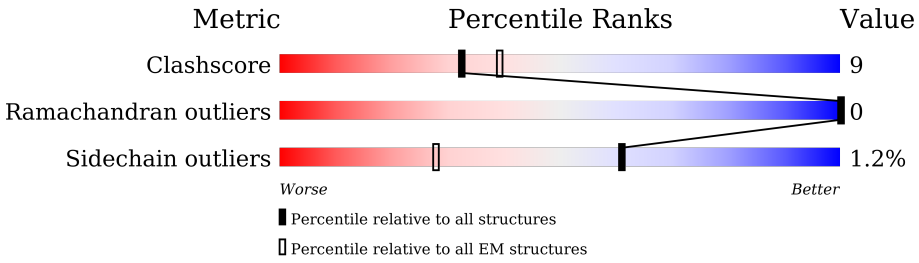
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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)	:	2.51

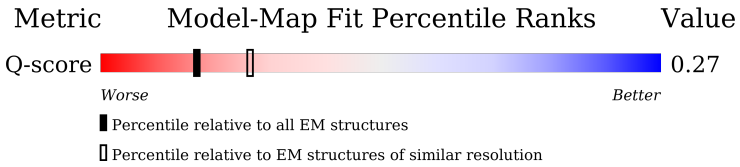
1 Overall quality at a glance

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

The reported resolution of this entry is 4.23 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	4685 (3.74 - 4.73)

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

Mol	Chain	Length	Quality of chain
1	A	1152	28% 8% 64%
1	B	1152	12% 71% 19% 9%
2	D	155	23% 68% 25% 6%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 13051 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, inducible.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	420	Total	C	N	O	S	1	0
			3421	2191	589	620	21		
1	B	1043	Total	C	N	O	S	0	0
			8279	5284	1437	1513	45		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	594	GLU	SER	engineered mutation	UNP P29477
A	1145	LEU	-	expression tag	UNP P29477
A	1146	GLU	-	expression tag	UNP P29477
A	1147	LEU	-	expression tag	UNP P29477
A	1148	GLU	-	expression tag	UNP P29477
A	1149	VAL	-	expression tag	UNP P29477
A	1150	LEU	-	expression tag	UNP P29477
A	1151	PHE	-	expression tag	UNP P29477
A	1152	GLN	-	expression tag	UNP P29477
B	594	GLU	SER	engineered mutation	UNP P29477
B	1145	LEU	-	expression tag	UNP P29477
B	1146	GLU	-	expression tag	UNP P29477
B	1147	LEU	-	expression tag	UNP P29477
B	1148	GLU	-	expression tag	UNP P29477
B	1149	VAL	-	expression tag	UNP P29477
B	1150	LEU	-	expression tag	UNP P29477
B	1151	PHE	-	expression tag	UNP P29477
B	1152	GLN	-	expression tag	UNP P29477

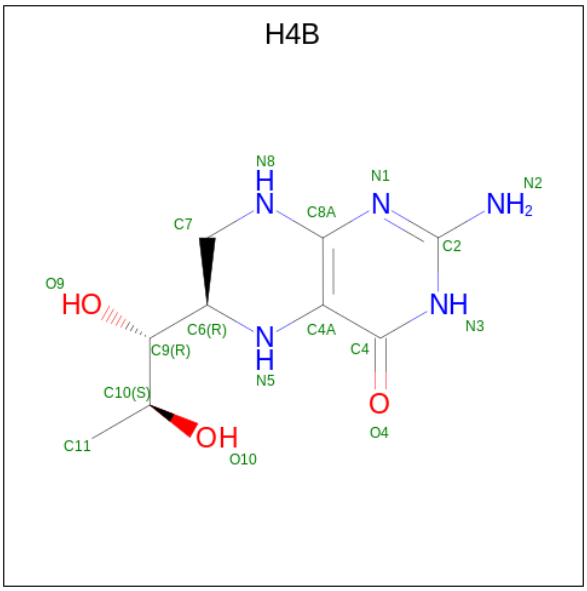
- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	145	Total	C	N	O	S	0	0
			1087	673	177	229	8		

There are 6 discrepancies between the modelled and reference sequences:

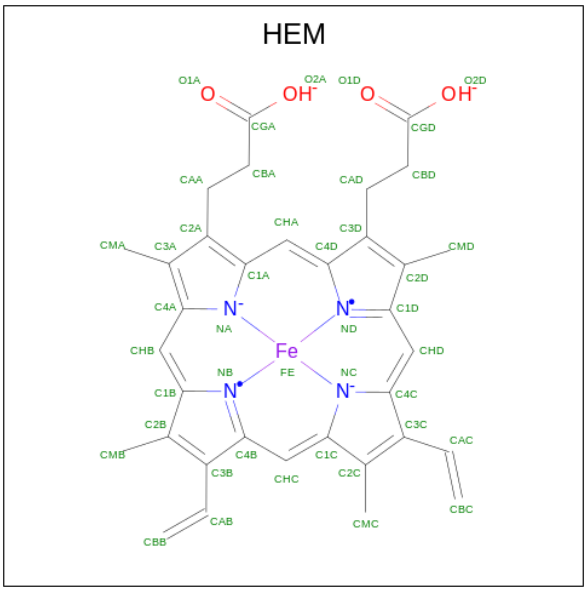
Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLY	-	expression tag	UNP P0DP26
D	-5	PRO	-	expression tag	UNP P0DP26
D	-4	GLY	-	expression tag	UNP P0DP26
D	-3	GLY	-	expression tag	UNP P0DP26
D	-2	GLU	-	expression tag	UNP P0DP26
D	-1	PHE	-	expression tag	UNP P0DP26

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: $C_9H_{15}N_5O_3$).



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

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

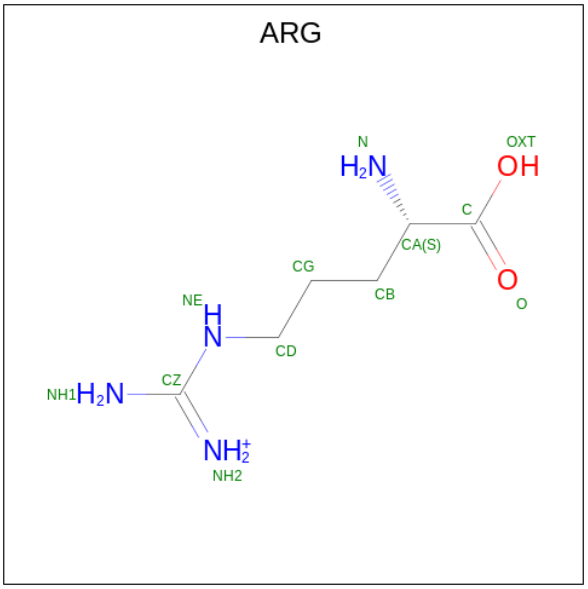


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
4	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

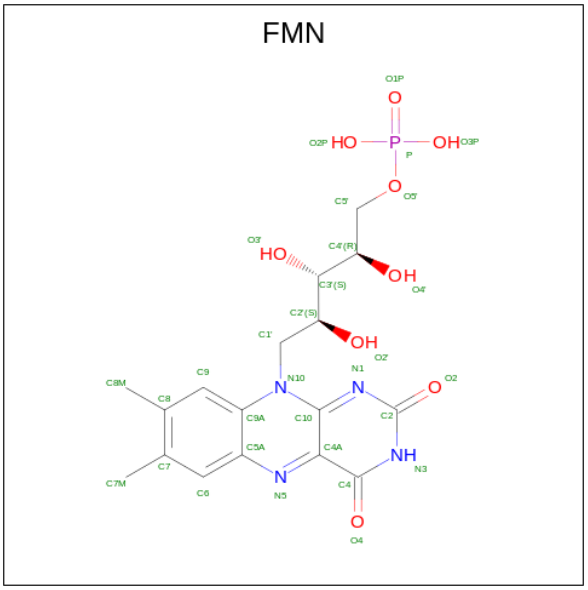
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	

- Molecule 6 is ARGININE (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



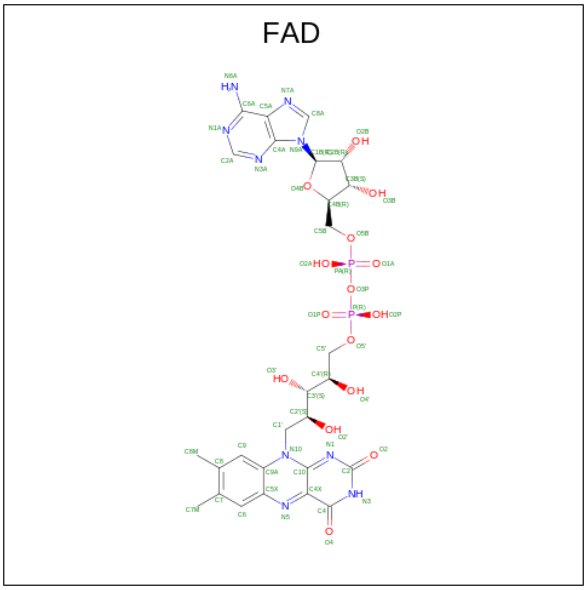
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			12	6	4	2	
6	B	1	Total	C	N	O	0
			12	6	4	2	

- Molecule 7 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



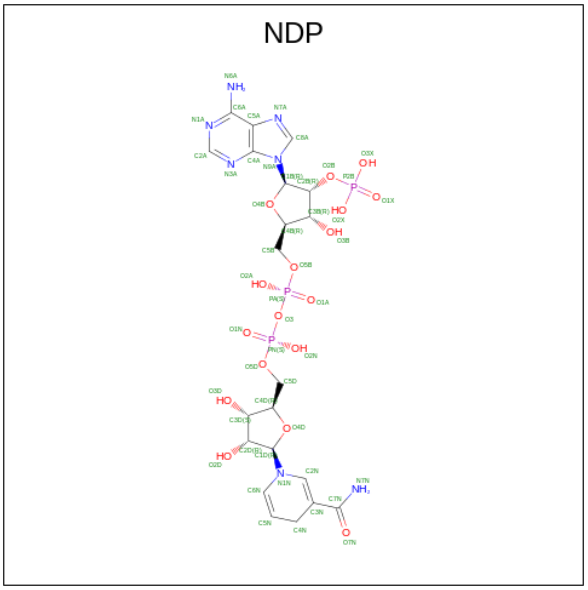
Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					AltConf
8	B	1	Total	C	N	O	P	0
			53	27	9	15	2	

- Molecule 9 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					AltConf
9	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
10	D	4	Total	Ca	0
			4	4	

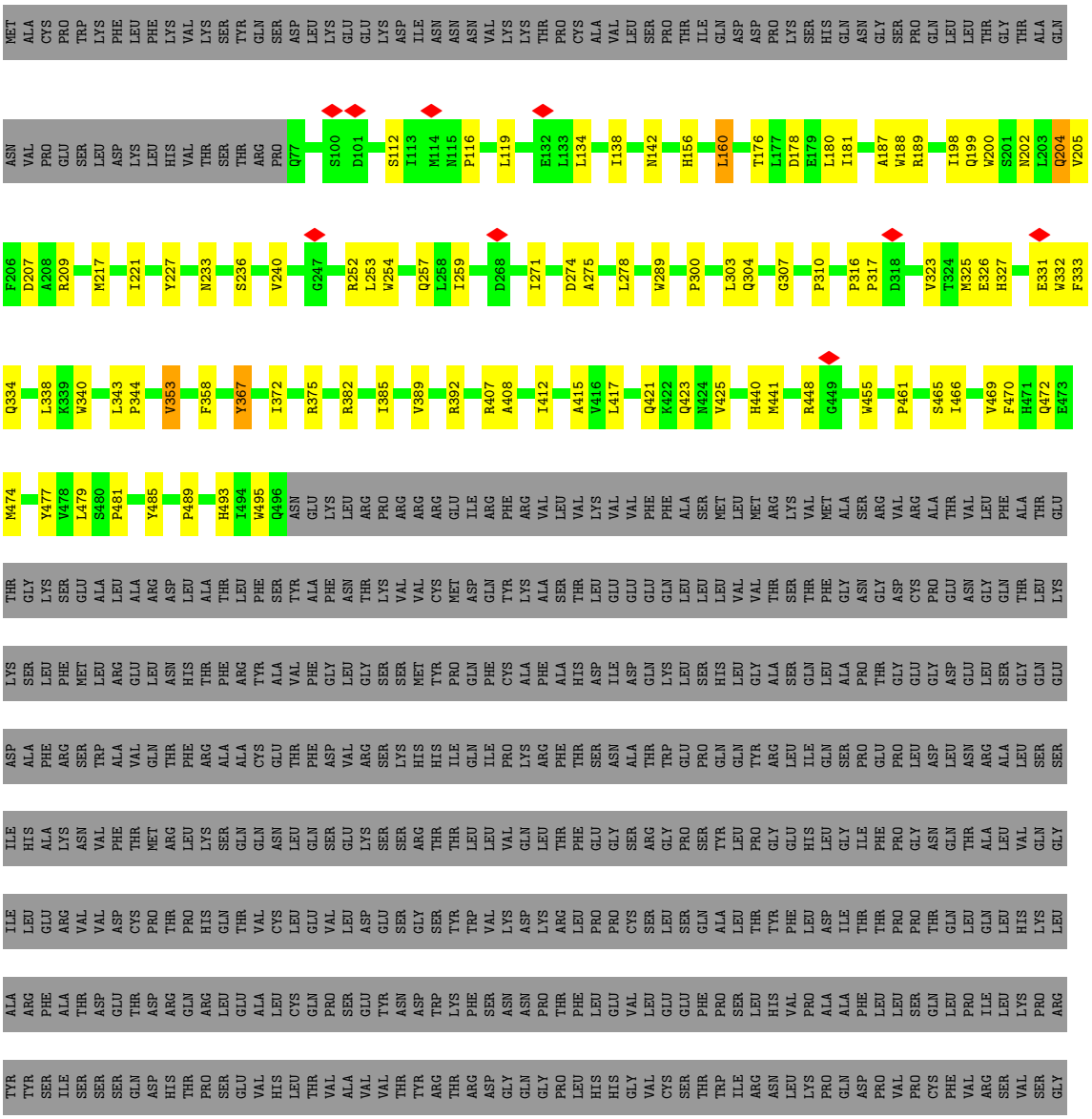
3 Residue-property plots (i)

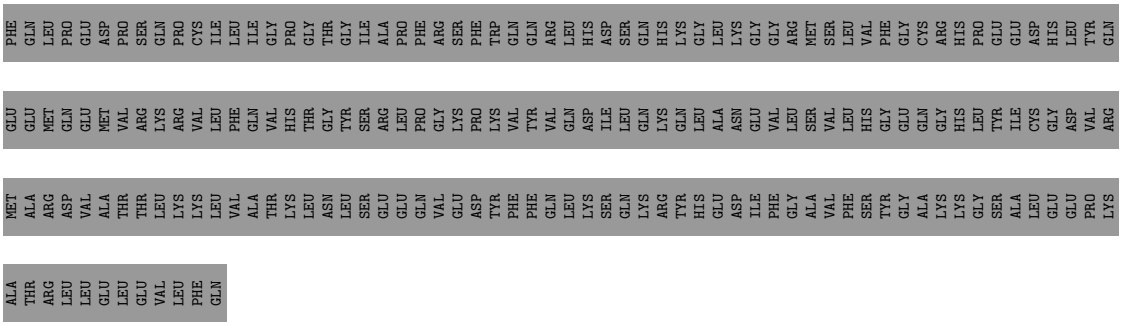
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Nitric oxide synthase, inducible

Chain A:



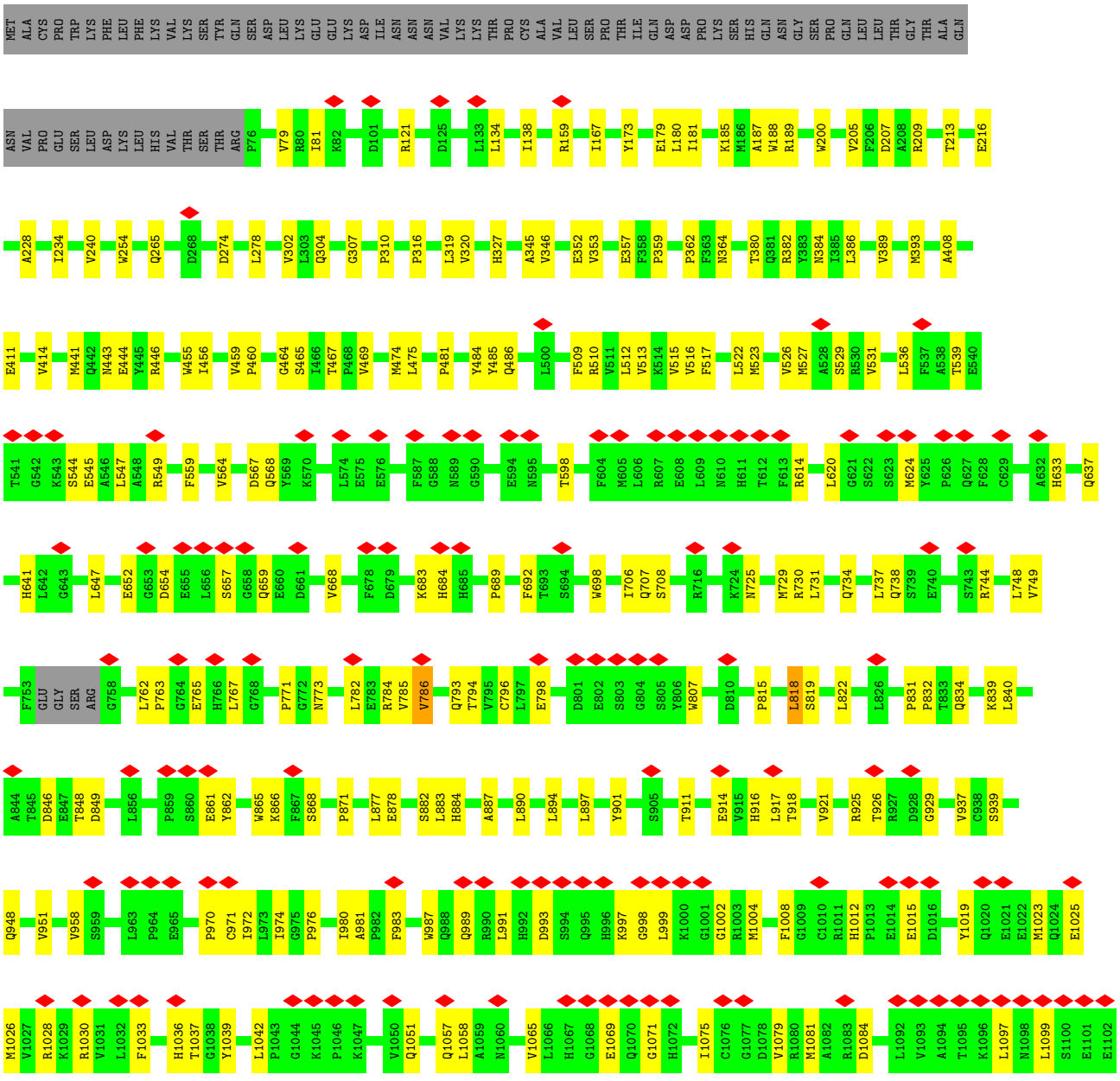


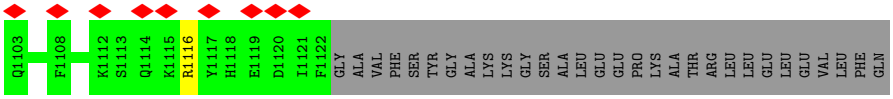


• Molecule 1: Nitric oxide synthase, inducible

Chain B:



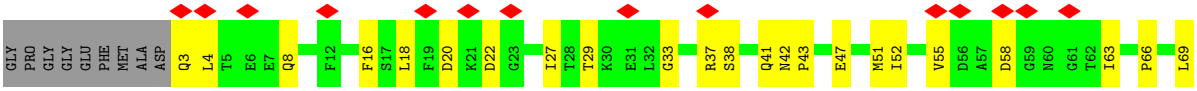


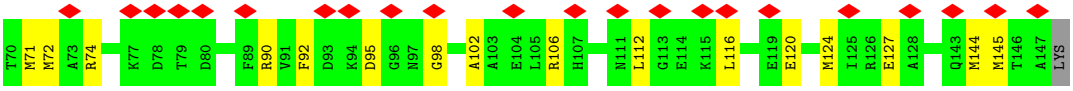


• Molecule 2: Calmodulin-1

Chain D:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55156	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.644	Depositor
Minimum map value	-1.436	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	320.1, 320.1, 320.1	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.067, 1.067, 1.067	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.12	0/3521	0.28	0/4789
1	B	0.14	0/8499	0.33	0/11553
2	D	0.09	0/1099	0.24	0/1483
All	All	0.13	0/13119	0.31	0/17825

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	3421	0	3300	61	0
1	B	8279	0	8027	141	0
2	D	1087	0	997	29	0
3	A	17	0	15	1	0
3	B	17	0	15	0	0
4	A	43	0	30	2	0
4	B	43	0	30	3	0
5	A	1	0	0	0	0
6	A	12	0	12	2	0
6	B	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	31	0	19	1	0
8	B	53	0	31	1	0
9	B	31	0	11	1	0
10	D	4	0	0	0	0
All	All	13051	0	12499	218	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 9.

All (218) 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:624:MET:SD	1:B:901:TYR:OH	2.42	0.78
1:B:763:PRO:HG3	1:B:989:GLN:HG3	1.67	0.77
1:B:707:GLN:N	1:B:707:GLN:OE1	2.21	0.73
1:A:469:VAL:HG13	1:A:474:MET:HE1	1.72	0.72
1:B:921:VAL:HA	1:B:939:SER:HB2	1.72	0.72
4:A:1202:HEM:HHC	4:A:1202:HEM:HBB2	1.71	0.71
1:B:539:THR:HB	1:B:544:SER:HB3	1.73	0.71
1:A:389:VAL:HG21	1:A:412:ILE:HD11	1.73	0.70
1:A:441:MET:HE1	1:A:472:GLN:HG2	1.75	0.68
1:B:1071:GLY:O	1:B:1116:ARG:NH1	2.27	0.67
1:A:417:LEU:O	1:A:421:GLN:HG2	1.96	0.65
1:B:353:VAL:HG22	1:B:481:PRO:HB3	1.79	0.65
1:B:189:ARG:NH2	1:B:444:GLU:OE1	2.29	0.64
1:A:323:VAL:HG13	1:A:423:GLN:HG3	1.78	0.63
1:B:515:VAL:HG21	2:D:18:LEU:HD23	1.80	0.63
1:A:304:GLN:HE21	1:A:307:GLY:HA2	1.64	0.62
1:B:991:LEU:HB2	1:B:1026:MET:HE1	1.80	0.62
4:B:1203:HEM:HHC	4:B:1203:HEM:HBB2	1.80	0.61
2:D:43:PRO:HB2	2:D:47:GLU:HB3	1.82	0.61
1:A:332:TRP:HB2	1:A:392:ARG:HH21	1.64	0.61
1:B:460:PRO:HG2	1:B:467:THR:HG21	1.83	0.61
1:B:1039:TYR:HB2	1:B:1042:LEU:HG	1.83	0.61
4:A:1202:HEM:HBC2	4:A:1202:HEM:HMC2	1.84	0.60
1:B:997:LYS:HB3	1:B:999:LEU:HD13	1.84	0.60
1:B:393:MET:HE1	1:B:408:ALA:HA	1.84	0.60
1:B:976:PRO:HG3	1:B:1081:MET:HE1	1.84	0.59
1:B:773:ASN:ND2	1:B:822:LEU:O	2.34	0.59
1:B:767:LEU:HD22	1:B:917:LEU:HD11	1.85	0.59
1:B:993:ASP:O	1:B:998:GLY:N	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1065:VAL:HA	1:B:1069:GLU:HB2	1.83	0.58
4:B:1203:HEM:HBC2	4:B:1203:HEM:HMC2	1.86	0.58
1:A:323:VAL:HG21	1:A:425:VAL:HG21	1.86	0.58
1:B:1051:GLN:HE22	9:B:1206:NDP:H2A	1.69	0.58
1:B:181:ILE:O	1:B:185:LYS:HG2	2.04	0.57
1:B:614:ARG:HD3	1:B:647:LEU:HD21	1.86	0.57
1:B:784:ARG:HH12	1:B:878:GLU:HA	1.70	0.57
1:B:1008:PHE:HD2	1:B:1037:THR:HG23	1.70	0.57
1:A:461:PRO:HB3	1:B:465:SER:HB3	1.87	0.57
1:B:786:VAL:HB	1:B:884:HIS:HB3	1.87	0.56
1:A:180:LEU:HD22	1:A:209:ARG:HE	1.70	0.56
1:A:199:GLN:HE21	1:A:202:ASN:HD21	1.51	0.56
1:B:510:ARG:NH1	2:D:127:GLU:OE2	2.39	0.56
2:D:29:THR:HG22	2:D:52:ILE:HG21	1.88	0.56
1:B:469:VAL:HG13	1:B:474:MET:HE1	1.88	0.56
1:B:738:GLN:NE2	1:B:744:ARG:O	2.39	0.56
1:A:253:LEU:HD13	1:A:303:LEU:HD23	1.88	0.56
1:B:846:ASP:OD2	1:B:848:THR:OG1	2.21	0.55
1:A:331:GLU:O	1:A:334:GLN:NE2	2.39	0.55
1:B:911:THR:HB	1:B:914:GLU:HB2	1.89	0.55
1:B:187:ALA:HB2	1:B:481:PRO:HB2	1.89	0.54
1:B:937:VAL:N	8:B:1205:FAD:O1P	2.40	0.54
1:B:121:ARG:NH1	1:B:357:GLU:OE2	2.41	0.53
1:A:204:GLN:HG3	1:A:227:TYR:HE1	1.72	0.53
1:A:289:TRP:CD1	1:A:300:PRO:HG3	2.43	0.53
1:B:265:GLN:HB2	1:B:278:LEU:HD11	1.90	0.53
2:D:33:GLY:O	2:D:37:ARG:HD3	2.09	0.53
1:B:316:PRO:HD2	1:B:319:LEU:HD12	1.91	0.53
1:B:352:GLU:HG2	1:B:484:TYR:CE2	2.44	0.53
2:D:3:GLN:HG2	2:D:4:LEU:HG	1.90	0.53
1:A:338:LEU:HD21	1:A:385:ILE:HD13	1.90	0.52
1:B:389:VAL:HG22	1:B:393:MET:HE2	1.91	0.52
1:B:765:GLU:HA	1:B:958:VAL:HG12	1.91	0.52
1:B:730:ARG:HB3	1:B:948:GLN:HA	1.91	0.52
1:B:1051:GLN:NE2	1:B:1084:ASP:OD2	2.43	0.52
1:B:861:GLU:OE1	1:B:861:GLU:HA	2.10	0.52
1:A:204:GLN:HG3	1:A:227:TYR:CE1	2.44	0.52
1:B:274:ASP:OD2	1:B:382:ARG:NH2	2.43	0.52
2:D:55:VAL:HB	2:D:63:ILE:HD12	1.92	0.52
1:A:407:ARG:HH21	1:B:414:VAL:HG21	1.75	0.51
1:B:167:ILE:HD11	1:B:173:TYR:HD1	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:LEU:HD12	1:B:620:LEU:HD11	1.93	0.51
1:B:633:HIS:NE2	1:B:652:GLU:OE2	2.34	0.51
1:B:1097:LEU:HB3	1:B:1099:LEU:HG	1.92	0.51
1:A:327:HIS:HD2	1:A:415:ALA:HB2	1.75	0.51
1:A:181:ILE:HG22	1:A:205:VAL:HB	1.93	0.51
1:B:523:MET:HE1	2:D:43:PRO:HD3	1.93	0.51
2:D:90:ARG:HH22	2:D:98:GLY:HA2	1.76	0.50
1:A:112:SER:OG	1:B:474:MET:O	2.28	0.50
1:B:1097:LEU:HD23	1:B:1099:LEU:HD11	1.93	0.50
1:B:346:VAL:O	1:B:362:PRO:HA	2.10	0.50
1:B:831:PRO:HD2	1:B:866:LYS:HZ2	1.77	0.50
1:A:187:ALA:HB2	1:A:481:PRO:HB2	1.93	0.50
1:A:344:PRO:HB3	1:A:367:TYR:CE1	2.46	0.50
1:B:654:ASP:HB3	1:B:657:SER:HB3	1.94	0.49
1:A:326:GLU:HG2	1:A:334:GLN:HB3	1.94	0.49
2:D:116:LEU:HB3	2:D:120:GLU:HG3	1.94	0.49
1:B:359:PRO:O	1:B:486:GLN:NE2	2.39	0.49
1:B:516:VAL:HG11	2:D:92:PHE:HE2	1.77	0.49
1:A:325:MET:HB3	1:A:333:PHE:HE2	1.78	0.48
1:B:345:ALA:HB2	1:B:364:ASN:HB3	1.95	0.48
1:A:204:GLN:NE2	1:A:236:SER:O	2.46	0.48
1:A:252:ARG:HH21	1:A:489:PRO:HD3	1.79	0.48
1:B:708:SER:O	1:B:794:THR:CB	2.62	0.48
1:A:180:LEU:HD11	1:A:240:VAL:HG11	1.95	0.48
1:B:459:VAL:HG22	1:B:469:VAL:HG12	1.95	0.48
1:B:531:VAL:HB	1:B:559:PHE:HD1	1.78	0.48
1:B:1012:HIS:HB3	1:B:1015:GLU:HB2	1.96	0.48
1:A:189:ARG:CZ	1:A:448:ARG:HD2	2.44	0.48
1:A:466:ILE:HD12	1:B:386:LEU:HD11	1.96	0.48
1:B:327:HIS:NE2	1:B:411:GLU:OE1	2.47	0.48
1:B:918:THR:HB	1:B:981:ALA:HB2	1.95	0.48
1:B:1036:HIS:CD2	1:B:1058:LEU:HD21	2.48	0.47
1:B:1019:TYR:O	1:B:1023:MET:HG2	2.14	0.47
1:A:340:TRP:CD1	1:A:372:ILE:HD12	2.50	0.47
1:B:798:GLU:HB3	1:B:807:TRP:HB3	1.97	0.47
1:A:408:ALA:O	1:A:412:ILE:HG12	2.14	0.47
1:B:637:GLN:OE1	1:B:641:HIS:NE2	2.44	0.47
1:B:659:GLN:NE2	7:B:1201:FMN:O4'	2.39	0.47
1:B:784:ARG:NH2	1:B:877:LEU:O	2.48	0.47
1:B:707:GLN:HB2	1:B:793:GLN:HE21	1.79	0.47
1:A:233:ASN:HD21	1:B:725:ASN:HD22	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:TRP:HA	1:A:489:PRO:HG3	1.97	0.46
1:B:545:GLU:O	1:B:549:ARG:HG2	2.16	0.46
1:B:980:ILE:HD12	1:B:983:PHE:HD2	1.81	0.46
1:B:840:LEU:HD13	1:B:883:LEU:HD21	1.97	0.46
1:A:116:PRO:HG2	1:A:119:LEU:HB2	1.98	0.46
1:A:119:LEU:O	1:A:485:TYR:N	2.44	0.46
1:A:257:GLN:HE22	6:A:1204:ARG:HB3	1.80	0.46
1:B:134:LEU:O	1:B:138:ILE:HG12	2.16	0.46
1:A:207:ASP:OD2	1:A:209:ARG:NH2	2.49	0.46
1:B:81:ILE:HD11	1:B:475:LEU:HD13	1.98	0.46
1:B:974:ILE:HB	1:B:1075:ILE:HD13	1.98	0.46
1:B:868:SER:O	1:B:926:THR:OG1	2.33	0.46
1:A:375:ARG:HH12	3:A:1201:H4B:C4	2.29	0.46
1:B:167:ILE:HD11	1:B:173:TYR:CD1	2.51	0.46
1:B:972:ILE:HD11	1:B:1065:VAL:HG21	1.98	0.46
1:B:748:LEU:HD11	1:B:916:HIS:HB3	1.98	0.46
1:B:980:ILE:HB	1:B:1008:PHE:HE1	1.81	0.45
1:B:180:LEU:HD11	1:B:240:VAL:HG11	1.97	0.45
1:A:493:HIS:CE1	1:A:495:TRP:HD1	2.35	0.45
1:B:509:PHE:HD2	2:D:144:MET:HE3	1.81	0.45
1:B:567:ASP:OD1	1:B:568:GLN:N	2.49	0.45
1:B:834:GLN:HG3	1:B:862:TYR:HE2	1.82	0.45
1:B:181:ILE:HA	1:B:205:VAL:HG21	1.98	0.45
1:B:304:GLN:HE21	1:B:307:GLY:HA2	1.81	0.45
1:A:198:ILE:HB	1:A:440:HIS:HB2	1.99	0.45
1:B:987:TRP:CD1	1:B:1026:MET:HE2	2.52	0.45
2:D:38:SER:HB3	2:D:112:LEU:HD22	1.98	0.45
1:A:353:VAL:HB	1:A:481:PRO:HB3	1.99	0.45
1:B:734:GLN:HB3	1:B:749:VAL:HG12	1.98	0.44
1:A:259:ILE:HD12	1:A:343:LEU:HB3	1.98	0.44
1:B:731:LEU:H	1:B:731:LEU:HD23	1.82	0.44
1:B:925:ARG:HB3	1:B:929:GLY:HA2	1.99	0.44
1:B:1036:HIS:ND1	1:B:1057:GLN:OE1	2.49	0.44
2:D:27:ILE:HB	2:D:63:ILE:HB	1.99	0.44
2:D:58:ASP:OD1	2:D:58:ASP:N	2.48	0.44
2:D:95:ASP:OD1	2:D:95:ASP:N	2.51	0.44
1:A:233:ASN:ND2	1:B:725:ASN:ND2	2.65	0.44
2:D:144:MET:HE2	2:D:144:MET:HB2	1.90	0.44
1:A:477:TYR:HD1	1:A:479:LEU:HD13	1.82	0.44
1:B:862:TYR:CD1	1:B:862:TYR:C	2.93	0.44
2:D:66:PRO:O	2:D:69:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ILE:HG23	1:A:278:LEU:HD21	1.99	0.44
1:A:274:ASP:OD1	1:A:382:ARG:NE	2.49	0.44
1:B:464:GLY:O	1:B:467:THR:OG1	2.29	0.44
1:B:737:LEU:HD11	1:B:748:LEU:HB2	2.00	0.43
1:A:209:ARG:HD3	1:A:358:PHE:HE2	1.83	0.43
1:B:207:ASP:OD1	1:B:209:ARG:NE	2.46	0.43
1:A:257:GLN:NE2	6:A:1204:ARG:HB3	2.34	0.43
1:B:771:PRO:HG2	1:B:897:LEU:HD21	2.00	0.43
1:A:254:TRP:CH2	1:A:310:PRO:HG3	2.54	0.43
1:B:523:MET:HG3	2:D:41:GLN:CD	2.43	0.43
1:B:254:TRP:HB2	1:B:302:VAL:HB	2.01	0.43
1:B:441:MET:HE1	1:B:474:MET:HG2	2.00	0.43
1:A:275:ALA:HA	1:A:278:LEU:HG	1.99	0.43
1:B:689:PRO:HG2	1:B:692:PHE:CB	2.49	0.43
1:B:834:GLN:HG3	1:B:862:TYR:CE2	2.54	0.43
1:B:849:ASP:OD2	1:B:882:SER:OG	2.25	0.42
1:B:862:TYR:CD1	1:B:862:TYR:O	2.72	0.42
1:A:303:LEU:O	1:A:310:PRO:HA	2.18	0.42
1:B:683:LYS:HG3	1:B:684:HIS:ND1	2.33	0.42
1:B:698:TRP:HB2	1:B:839:LYS:HD3	2.01	0.42
1:B:818:LEU:HD12	1:B:819:SER:N	2.34	0.42
1:B:513:VAL:HA	1:B:516:VAL:HG12	2.00	0.42
1:A:138:ILE:HD13	1:A:160:LEU:HD12	2.01	0.42
1:B:485:TYR:OH	4:B:1203:HEM:O1D	2.32	0.42
1:B:517:PHE:HD2	2:D:72:MET:HE1	1.85	0.42
2:D:4:LEU:HA	2:D:8:GLN:HE21	1.84	0.42
1:B:254:TRP:CH2	1:B:310:PRO:HG3	2.54	0.42
1:B:1025:GLU:HA	1:B:1028:ARG:HD2	2.02	0.42
1:B:785:VAL:HG11	1:B:887:ALA:HB2	2.01	0.42
1:A:188:TRP:CE3	1:A:200:TRP:HA	2.55	0.42
1:B:188:TRP:CE3	1:B:200:TRP:HA	2.54	0.42
1:A:134:LEU:O	1:A:138:ILE:HG12	2.20	0.42
1:A:142:ASN:HA	1:A:156:HIS:HE1	1.84	0.42
1:A:455:TRP:CZ3	1:B:456:ILE:HG23	2.55	0.42
1:B:890:LEU:HD22	1:B:894:LEU:HD11	2.00	0.42
2:D:16:PHE:O	2:D:20:ASP:N	2.42	0.42
1:A:316:PRO:HA	1:A:317:PRO:HD3	1.96	0.42
1:B:443:ASN:OD1	1:B:446:ARG:NH2	2.53	0.42
1:B:274:ASP:OD1	1:B:382:ARG:NE	2.53	0.41
1:B:380:THR:HA	1:B:384:ASN:HD22	1.85	0.41
1:B:522:LEU:HB3	2:D:51:MET:SD	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1030:ARG:HH22	1:B:1033:PHE:HD1	1.68	0.41
1:B:782:LEU:HD22	1:B:818:LEU:HD13	2.03	0.41
1:B:971:CYS:HB2	1:B:1004:MET:SD	2.59	0.41
2:D:71:MET:O	2:D:74:ARG:HG3	2.20	0.41
2:D:102:ALA:O	2:D:106:ARG:HG2	2.19	0.41
1:B:865:TRP:CZ2	1:B:871:PRO:HG3	2.55	0.41
2:D:22:ASP:OD1	2:D:22:ASP:N	2.53	0.41
1:A:217:MET:O	1:A:221:ILE:HG12	2.20	0.41
1:B:228:ALA:O	1:B:234:ILE:HA	2.21	0.41
1:B:796:CYS:HB3	1:B:815:PRO:HB3	2.02	0.41
1:B:970:PRO:HA	1:B:1002:GLY:O	2.20	0.41
1:B:509:PHE:HD1	2:D:124:MET:HE3	1.86	0.41
1:B:527:MET:C	1:B:529:SER:N	2.77	0.41
1:B:729:MET:HE3	1:B:729:MET:HB3	1.89	0.41
1:B:79:VAL:HG11	1:B:475:LEU:HD11	2.03	0.41
1:B:159:ARG:NH2	1:B:179:GLU:OE1	2.53	0.41
1:B:213:THR:HG23	1:B:216:GLU:H	1.85	0.41
1:B:1008:PHE:N	1:B:1036:HIS:O	2.51	0.41
1:B:536:LEU:HA	1:B:564:VAL:O	2.21	0.41
1:B:831:PRO:HA	1:B:832:PRO:HD3	1.94	0.41
1:A:176:THR:OG1	1:A:178:ASP:OD1	2.32	0.40
1:B:523:MET:HE3	2:D:41:GLN:HG3	2.03	0.40
1:A:465:SER:HA	1:A:470:PHE:CG	2.57	0.40
1:B:455:TRP:CZ2	1:B:459:VAL:HG21	2.56	0.40
2:D:37:ARG:HE	2:D:42:ASN:CG	2.29	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	419/1152 (36%)	410 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1039/1152 (90%)	1017 (98%)	22 (2%)	0	100	100
2	D	143/155 (92%)	142 (99%)	1 (1%)	0	100	100
All	All	1601/2459 (65%)	1569 (98%)	32 (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	366/1021 (36%)	362 (99%)	4 (1%)	65	73
1	B	890/1021 (87%)	879 (99%)	11 (1%)	63	73
2	D	110/130 (85%)	109 (99%)	1 (1%)	70	76
All	All	1366/2172 (63%)	1350 (99%)	16 (1%)	61	73

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	LEU
1	A	204	GLN
1	A	353	VAL
1	A	367	TYR
1	B	320	VAL
1	B	512	LEU
1	B	526	VAL
1	B	598	THR
1	B	668	VAL
1	B	706	ILE
1	B	762	LEU
1	B	786	VAL
1	B	818	LEU
1	B	951	VAL
1	B	1079	VAL
2	D	145	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	GLN
1	A	215	GLN
1	A	224	HIS
1	A	364	ASN
1	A	442	GLN
1	B	95	HIS
1	B	96	HIS
1	B	364	ASN
1	B	725	ASN
1	B	738	GLN
1	B	793	GLN
1	B	908	GLN
1	B	935	HIS
1	B	969	GLN
1	B	1067	HIS
1	B	1118	HIS

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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
4	HEM	A	1202	6	50,50,50	1.32	7 (14%)	66,82,82	1.27	7 (10%)
6	ARG	B	1204	-	10,11,11	0.73	1 (10%)	11,13,13	1.02	2 (18%)
7	FMN	B	1201	-	33,33,33	1.09	2 (6%)	48,50,50	1.18	7 (14%)
8	FAD	B	1205	-	56,58,58	0.28	0	81,89,89	0.42	1 (1%)
6	ARG	A	1204	4	10,11,11	0.73	1 (10%)	11,13,13	1.02	2 (18%)
3	H4B	B	1202	-	15,18,18	1.77	3 (20%)	11,26,26	1.93	4 (36%)
3	H4B	A	1201	-	15,18,18	1.78	3 (20%)	11,26,26	1.90	3 (27%)
4	HEM	B	1203	-	50,50,50	1.35	7 (14%)	66,82,82	1.27	7 (10%)
9	NDP	B	1206	-	31,33,52	2.83	5 (16%)	48,52,80	1.86	11 (22%)

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
4	HEM	A	1202	6	-	3/14/54/54	-
6	ARG	B	1204	-	-	2/11/11/11	-
7	FMN	B	1201	-	-	8/18/18/18	0/3/3/3
8	FAD	B	1205	-	-	20/34/50/50	0/6/6/6
6	ARG	A	1204	4	-	4/11/11/11	-
3	H4B	B	1202	-	-	0/8/17/17	0/2/2/2
3	H4B	A	1201	-	-	0/8/17/17	0/2/2/2
4	HEM	B	1203	-	-	2/14/54/54	-
9	NDP	B	1206	-	-	5/21/37/77	0/3/3/5

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1206	NDP	P2B-O2B	12.90	1.83	1.59
9	B	1206	NDP	PN-O5D	5.50	1.76	1.54
3	A	1201	H4B	C4A-C8A	5.36	1.47	1.38
3	B	1202	H4B	C4A-C8A	5.31	1.47	1.38
7	B	1201	FMN	C4A-N5	3.93	1.38	1.30
4	B	1203	HEM	FE-NB	3.11	2.04	1.94
4	B	1203	HEM	FE-ND	3.03	2.04	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1202	HEM	CAC-C3C	2.99	1.55	1.47
4	B	1203	HEM	CAC-C3C	2.97	1.55	1.47
9	B	1206	NDP	O2B-C2B	-2.92	1.33	1.44
4	A	1202	HEM	FE-NB	2.85	2.03	1.94
4	A	1202	HEM	CAB-C3B	2.85	1.55	1.47
4	A	1202	HEM	FE-ND	2.80	2.03	1.94
4	B	1203	HEM	CAB-C3B	2.79	1.55	1.47
4	B	1203	HEM	FE-NC	2.64	2.04	1.95
4	B	1203	HEM	FE-NA	2.62	2.04	1.95
9	B	1206	NDP	C5A-C4A	2.53	1.43	1.39
4	A	1202	HEM	FE-NC	2.52	2.03	1.95
3	A	1201	H4B	C4-N3	-2.52	1.34	1.38
7	B	1201	FMN	C10-N1	2.52	1.38	1.33
3	B	1202	H4B	C4-N3	-2.49	1.34	1.38
4	A	1202	HEM	FE-NA	2.47	2.03	1.95
9	B	1206	NDP	C2A-N1A	2.29	1.38	1.33
3	B	1202	H4B	C4A-C4	2.28	1.48	1.42
3	A	1201	H4B	C4A-C4	2.28	1.48	1.42
6	A	1204	ARG	OXT-C	-2.13	1.23	1.30
6	B	1204	ARG	OXT-C	-2.13	1.23	1.30
4	B	1203	HEM	CMC-C2C	2.03	1.55	1.50
4	A	1202	HEM	CMC-C2C	2.01	1.55	1.50

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	1206	NDP	PA-O3-PN	-7.17	108.21	132.83
3	B	1202	H4B	C2-N1-C8A	4.38	121.34	113.43
3	A	1201	H4B	C2-N1-C8A	4.32	121.22	113.43
9	B	1206	NDP	O2B-P2B-O1X	-3.35	96.46	109.39
9	B	1206	NDP	O2N-PN-O1N	3.29	123.56	110.68
4	A	1202	HEM	C1B-NB-C4B	3.18	108.36	105.07
4	B	1203	HEM	C3B-C2B-C1B	3.10	108.79	106.49
7	B	1201	FMN	C4-N3-C2	-3.08	119.94	125.64
8	B	1205	FAD	P-O3P-PA	-3.07	122.29	132.83
9	B	1206	NDP	PA-O5B-C5B	-3.05	103.77	121.68
4	A	1202	HEM	C3B-C2B-C1B	3.02	108.73	106.49
4	A	1202	HEM	C4D-ND-C1D	3.01	108.18	105.07
4	B	1203	HEM	C4D-ND-C1D	2.94	108.11	105.07
4	B	1203	HEM	C1B-NB-C4B	2.92	108.09	105.07
9	B	1206	NDP	O2N-PN-O3	2.92	114.44	104.64
4	A	1202	HEM	C4A-NA-C1A	2.86	108.15	105.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1201	H4B	O4-C4-C4A	-2.82	120.77	127.24
3	B	1202	H4B	O4-C4-C4A	-2.79	120.85	127.24
4	B	1203	HEM	C4A-NA-C1A	2.77	108.06	105.35
7	B	1201	FMN	C4A-C4-N3	2.66	119.95	113.19
9	B	1206	NDP	O5D-PN-O1N	-2.62	100.42	110.68
9	B	1206	NDP	O3X-P2B-O2X	2.55	117.38	107.64
4	A	1202	HEM	C4C-NC-C1C	2.51	107.81	105.35
7	B	1201	FMN	C4A-C10-N10	2.51	120.15	116.48
6	B	1204	ARG	OXT-C-O	-2.50	118.41	124.09
9	B	1206	NDP	N3A-C4A-N9A	2.49	131.19	127.08
6	A	1204	ARG	OXT-C-O	-2.44	118.54	124.09
9	B	1206	NDP	C2A-N1A-C6A	-2.39	114.67	118.77
3	B	1202	H4B	C4-C4A-N5	2.37	123.12	116.76
4	B	1203	HEM	C4C-NC-C1C	2.35	107.65	105.35
7	B	1201	FMN	O4-C4-C4A	-2.33	120.41	126.60
9	B	1206	NDP	C5A-C4A-N3A	-2.32	123.73	126.75
7	B	1201	FMN	C10-C4A-N5	-2.28	120.02	124.86
7	B	1201	FMN	C4A-C10-N1	-2.27	119.47	124.73
3	A	1201	H4B	C4-C4A-N5	2.25	122.79	116.76
4	B	1203	HEM	C3D-C4D-ND	-2.22	107.70	110.17
4	B	1203	HEM	C2A-C1A-NA	-2.21	107.68	110.15
9	B	1206	NDP	O4B-C4B-C3B	2.17	109.41	105.11
6	B	1204	ARG	OXT-C-CA	2.17	120.77	113.38
6	A	1204	ARG	OXT-C-CA	2.17	120.76	113.38
4	A	1202	HEM	C2A-C1A-NA	-2.16	107.73	110.15
7	B	1201	FMN	C9A-C5A-N5	-2.10	120.15	122.43
4	A	1202	HEM	C3D-C4D-ND	-2.07	107.86	110.17
3	B	1202	H4B	C4A-C4-N3	2.04	118.39	112.31

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1204	ARG	O-C-CA-N
7	B	1201	FMN	C3'-C4'-C5'-O5'
7	B	1201	FMN	O4'-C4'-C5'-O5'
7	B	1201	FMN	C5'-O5'-P-O2P
7	B	1201	FMN	C5'-O5'-P-O3P
8	B	1205	FAD	C5B-O5B-PA-O1A
8	B	1205	FAD	C5B-O5B-PA-O2A
8	B	1205	FAD	N10-C1'-C2'-O2'
8	B	1205	FAD	N10-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
8	B	1205	FAD	C1'-C2'-C3'-O3'
8	B	1205	FAD	C1'-C2'-C3'-C4'
8	B	1205	FAD	C2'-C3'-C4'-C5'
8	B	1205	FAD	O3'-C3'-C4'-C5'
8	B	1205	FAD	C3'-C4'-C5'-O5'
8	B	1205	FAD	O4'-C4'-C5'-O5'
8	B	1205	FAD	C5'-O5'-P-O1P
8	B	1205	FAD	C5'-O5'-P-O2P
9	B	1206	NDP	C5B-O5B-PA-O3
9	B	1206	NDP	C2B-O2B-P2B-O2X
8	B	1205	FAD	O3'-C3'-C4'-O4'
8	B	1205	FAD	C2'-C3'-C4'-O4'
8	B	1205	FAD	C4B-C5B-O5B-PA
6	A	1204	ARG	OXT-C-CA-N
8	B	1205	FAD	O2'-C2'-C3'-O3'
4	A	1202	HEM	C3D-CAD-CBD-CGD
7	B	1201	FMN	C5'-O5'-P-O1P
7	B	1201	FMN	C2'-C3'-C4'-O4'
7	B	1201	FMN	C2'-C3'-C4'-C5'
9	B	1206	NDP	PN-O3-PA-O5B
9	B	1206	NDP	C2B-O2B-P2B-O1X
8	B	1205	FAD	O2'-C2'-C3'-C4'
4	A	1202	HEM	C4B-C3B-CAB-CBB
4	B	1203	HEM	C4B-C3B-CAB-CBB
8	B	1205	FAD	C5'-O5'-P-O3P
9	B	1206	NDP	C5B-O5B-PA-O2A
6	B	1204	ARG	OXT-C-CA-CB
6	A	1204	ARG	O-C-CA-CB
7	B	1201	FMN	O3'-C3'-C4'-O4'
4	A	1202	HEM	C2A-CAA-CBA-CGA
6	B	1204	ARG	O-C-CA-CB
4	B	1203	HEM	C1A-C2A-CAA-CBA
8	B	1205	FAD	C5B-O5B-PA-O3P
6	A	1204	ARG	OXT-C-CA-CB
8	B	1205	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1202	HEM	2	0
7	B	1201	FMN	1	0

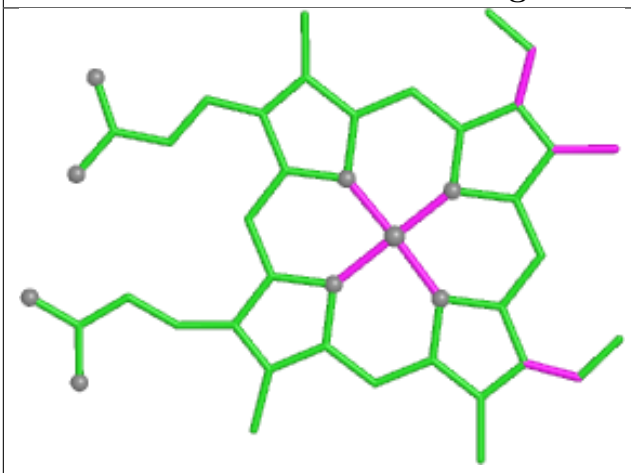
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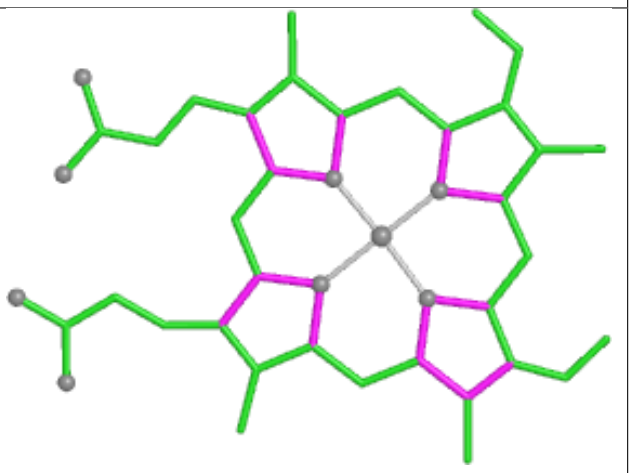
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1205	FAD	1	0
6	A	1204	ARG	2	0
3	A	1201	H4B	1	0
4	B	1203	HEM	3	0
9	B	1206	NDP	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

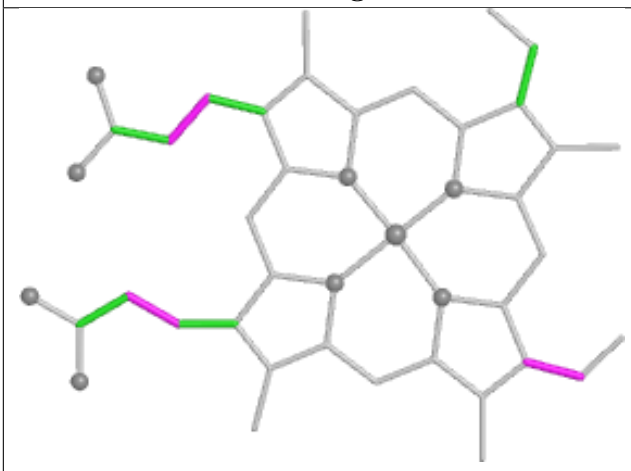
Ligand HEM A 1202



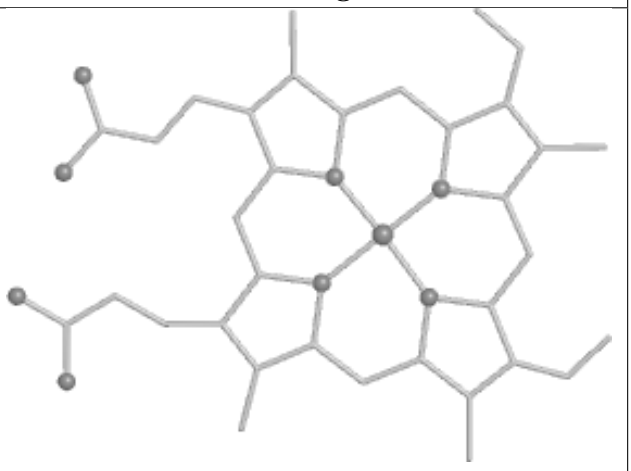
Bond lengths



Bond angles

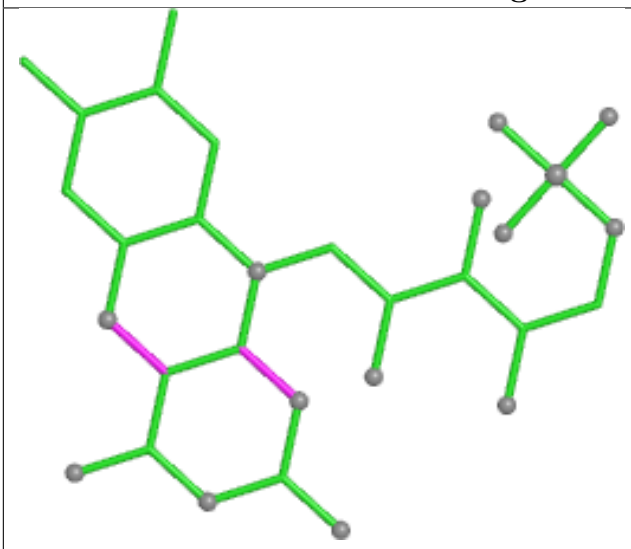


Torsions

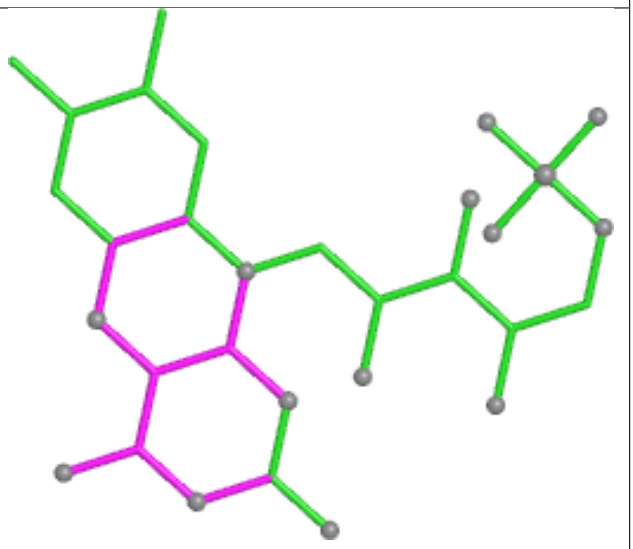


Rings

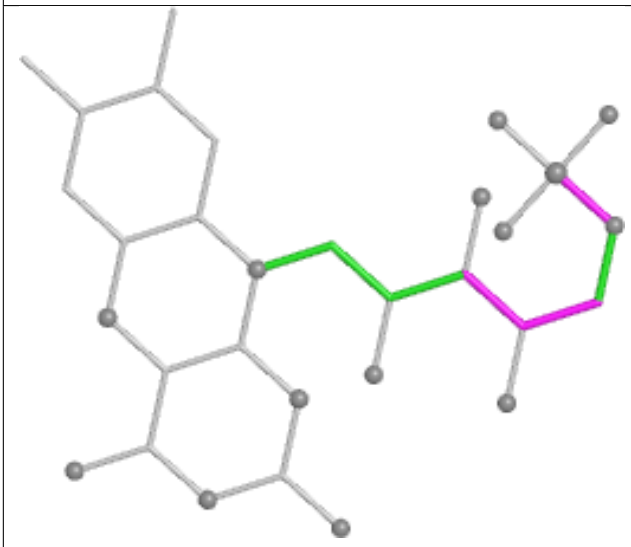
Ligand FMN B 1201



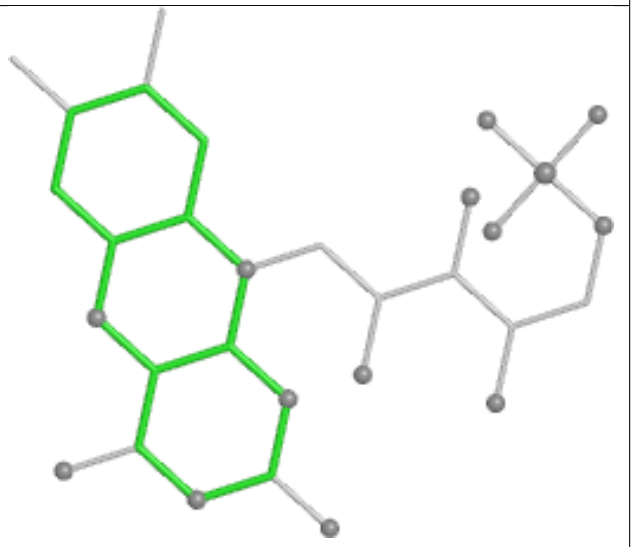
Bond lengths



Bond angles

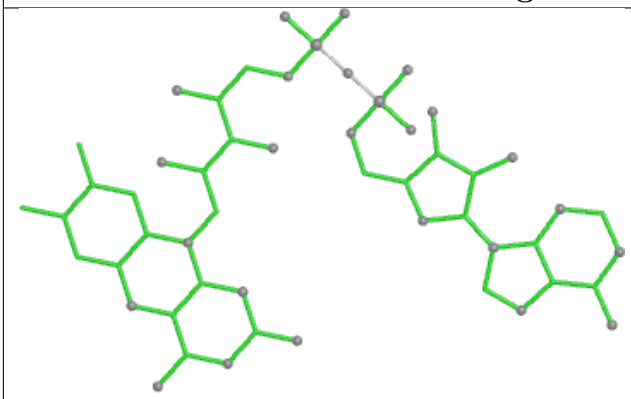


Torsions

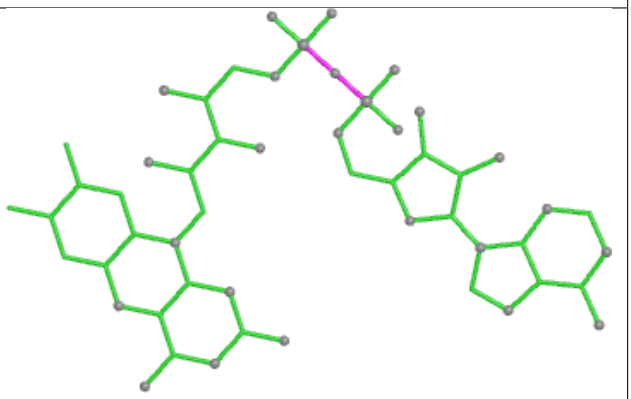


Rings

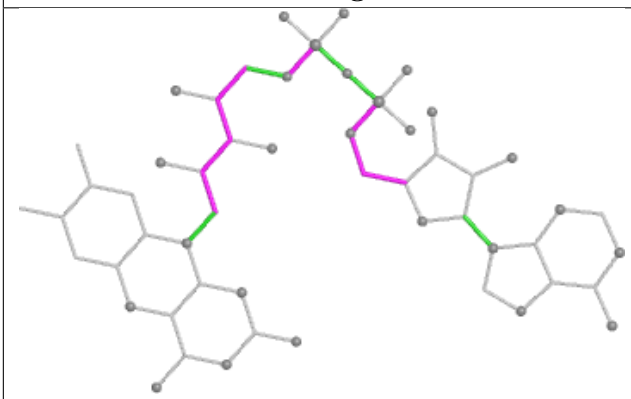
Ligand FAD B 1205



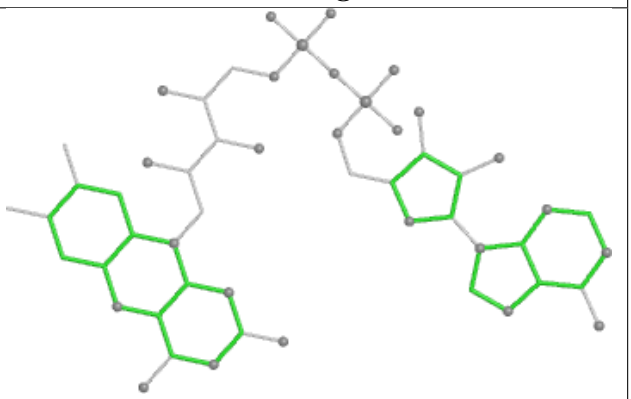
Bond lengths



Bond angles

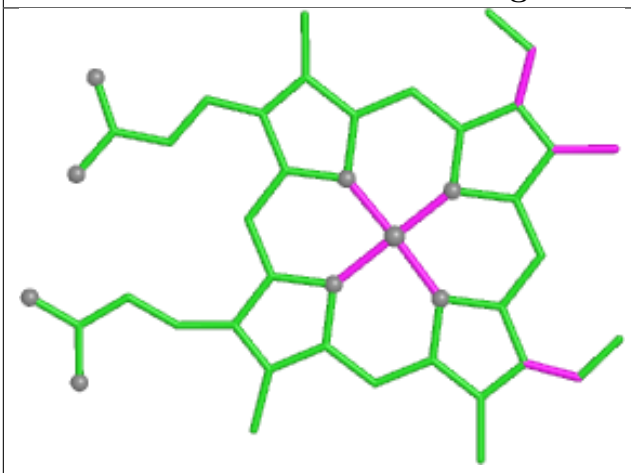


Torsions

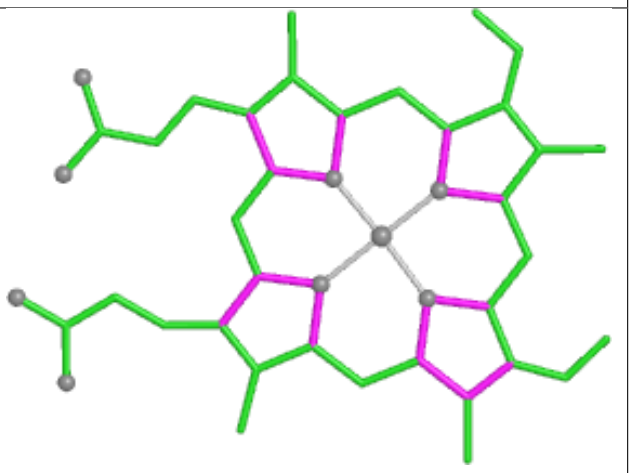


Rings

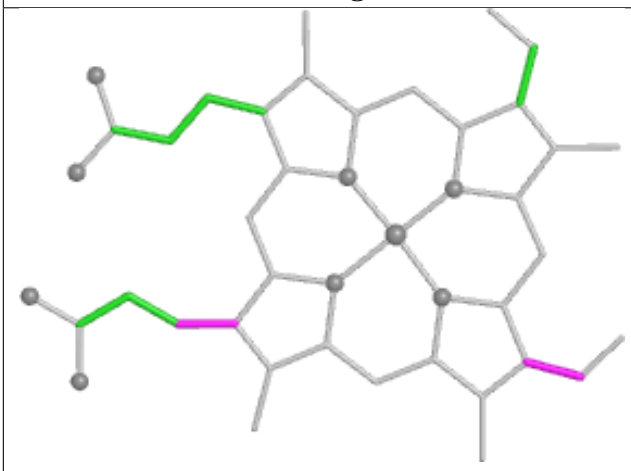
Ligand HEM B 1203



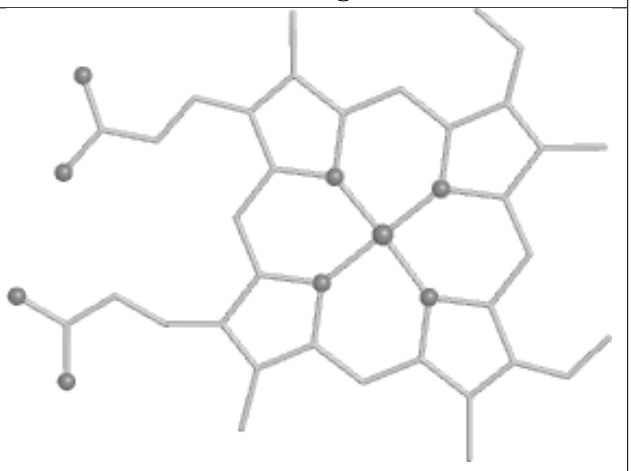
Bond lengths



Bond angles

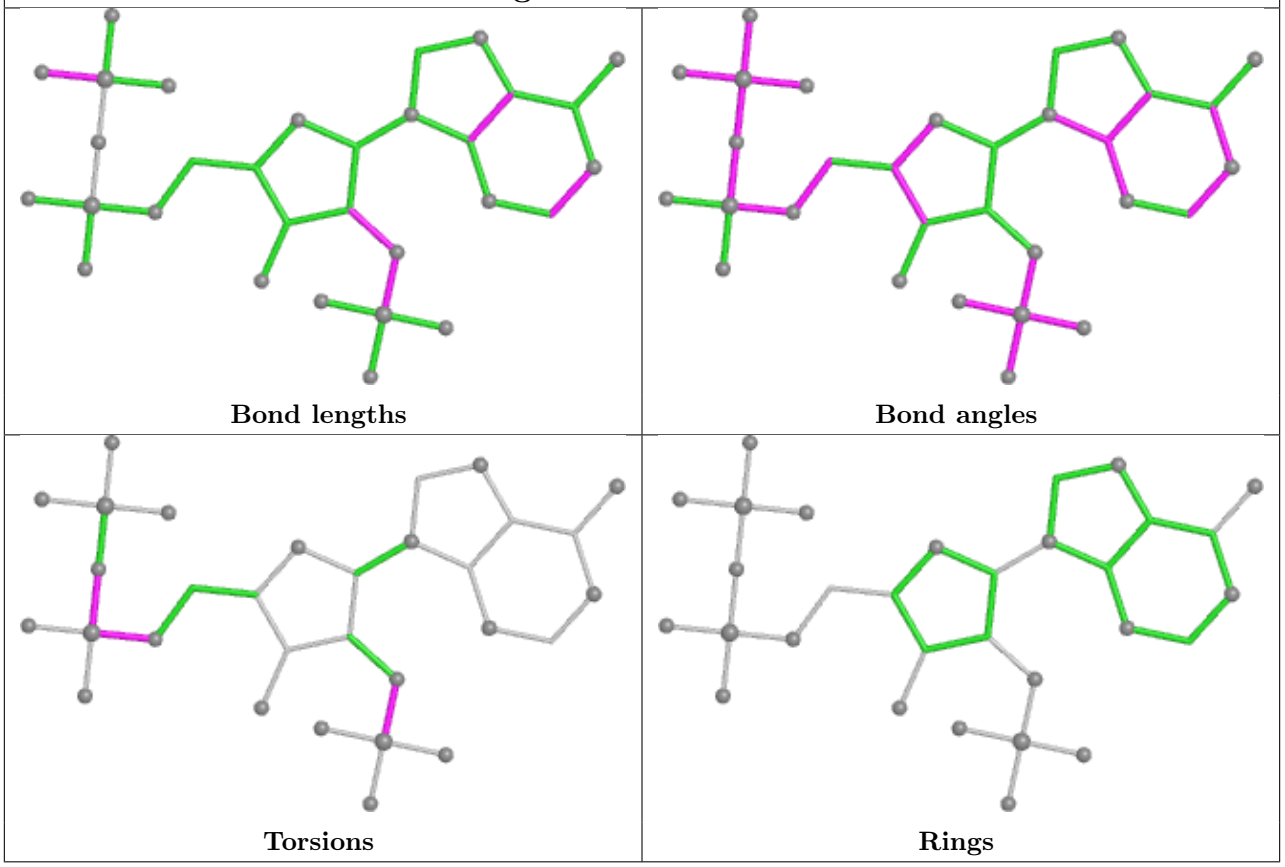


Torsions



Rings

Ligand NDP B 1206



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

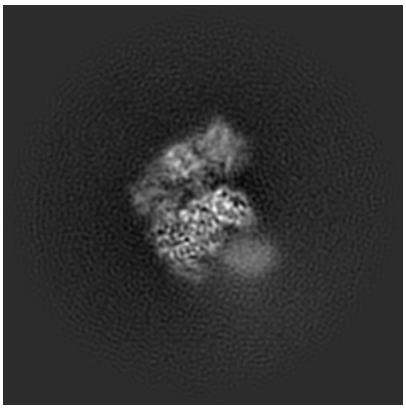
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-80278. These allow visual inspection of the internal detail of the map and identification of artifacts.

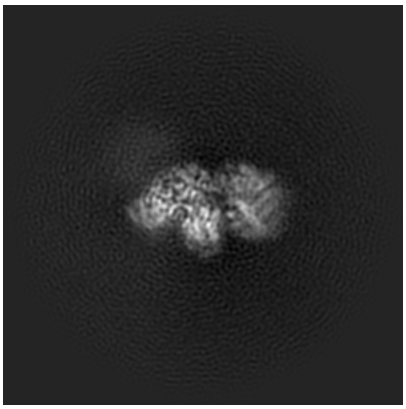
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

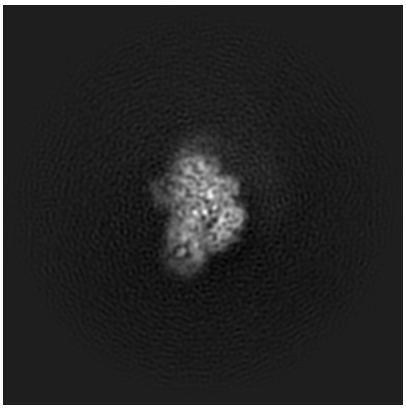
6.1.1 Primary map



X

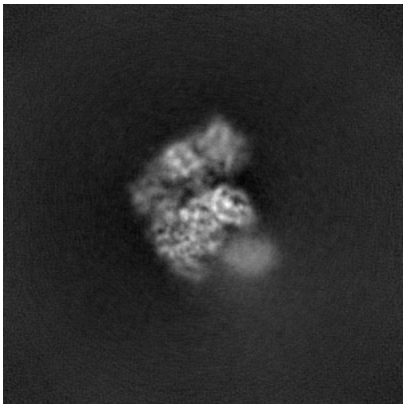


Y

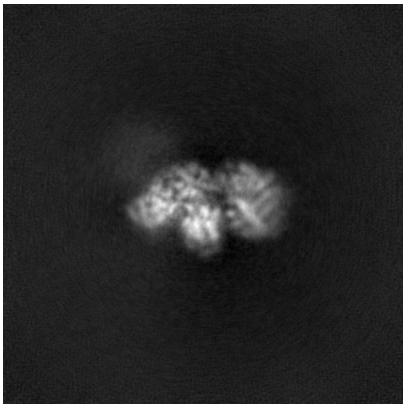


Z

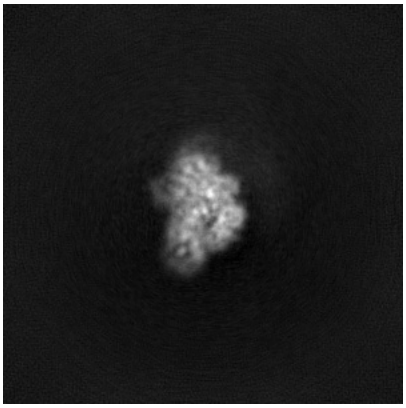
6.1.2 Raw map



X



Y

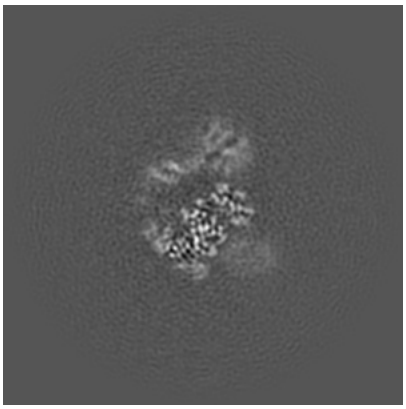


Z

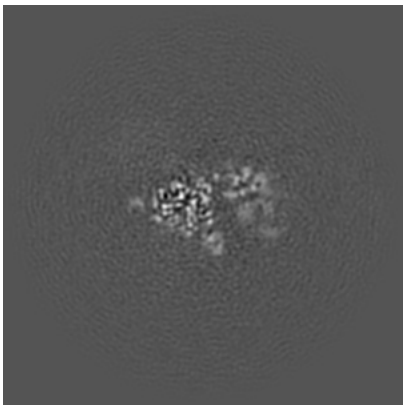
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

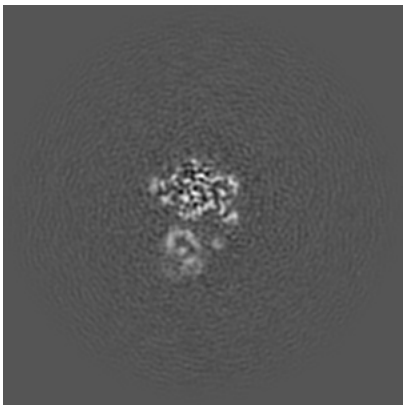
6.2.1 Primary map



X Index: 150

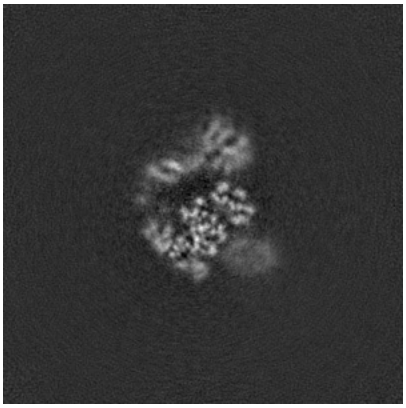


Y Index: 150

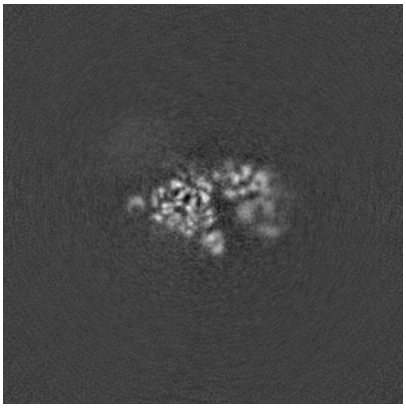


Z Index: 150

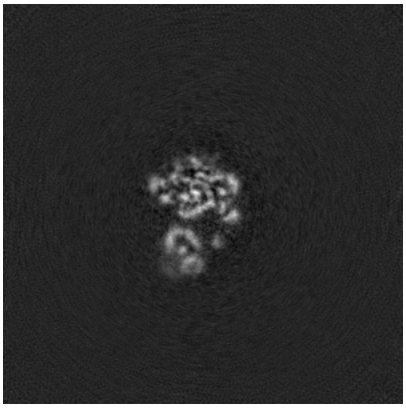
6.2.2 Raw map



X Index: 150



Y Index: 150

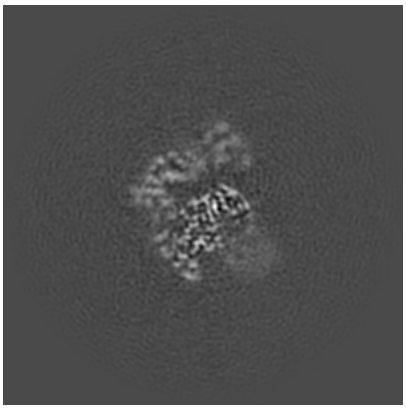


Z Index: 150

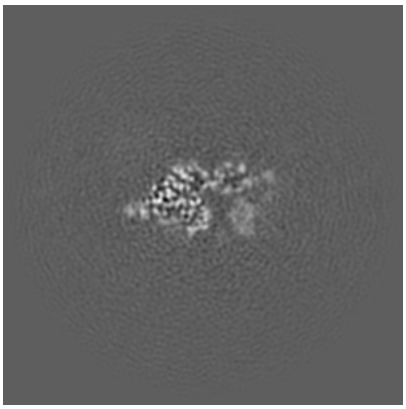
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

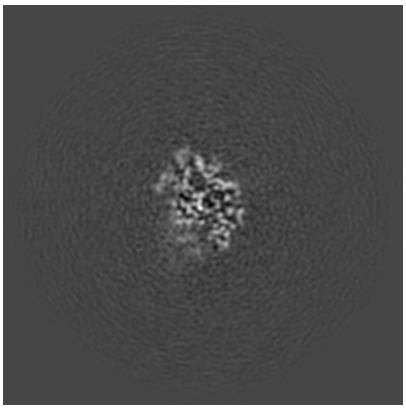
6.3.1 Primary map



X Index: 143

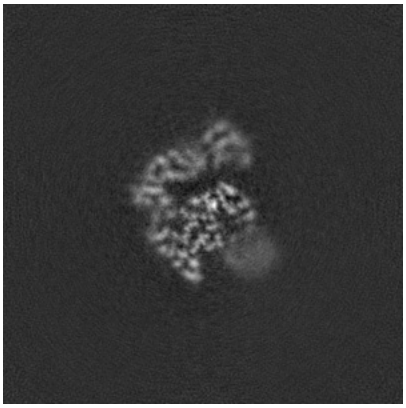


Y Index: 143

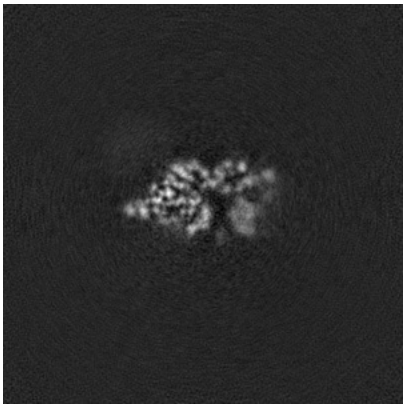


Z Index: 139

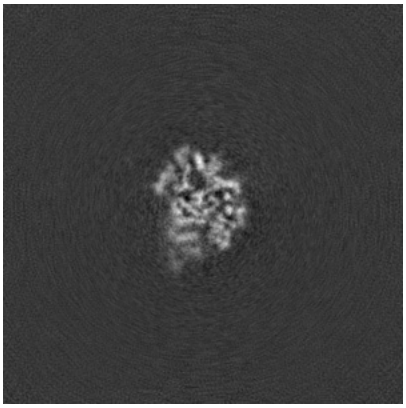
6.3.2 Raw map



X Index: 144



Y Index: 143

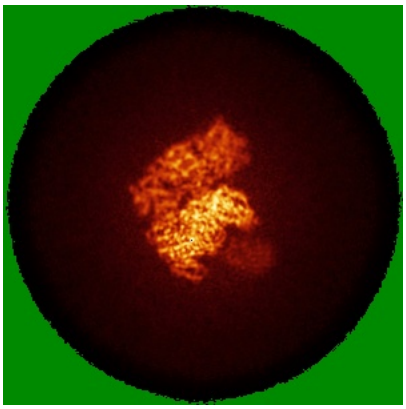


Z Index: 140

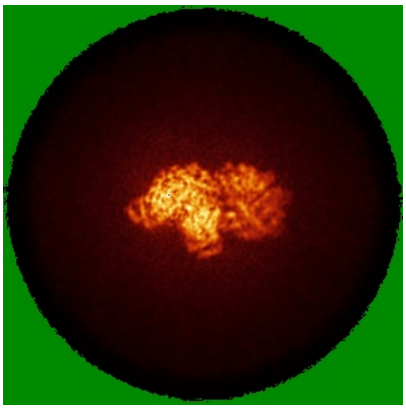
The images above show the largest variance slices of the map in three orthogonal directions.

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

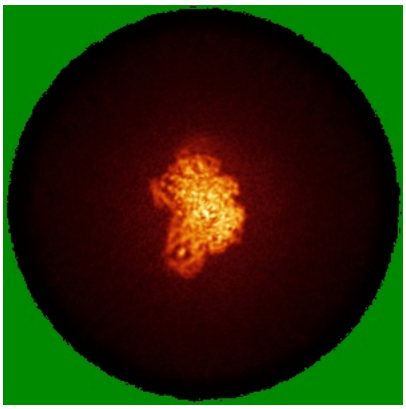
6.4.1 Primary map



X

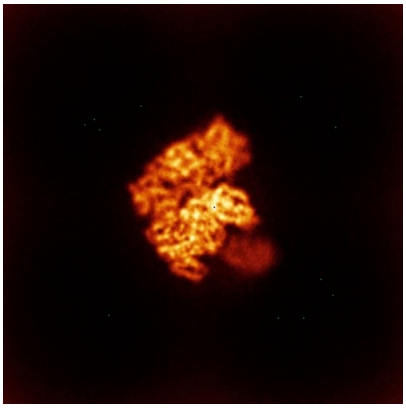


Y

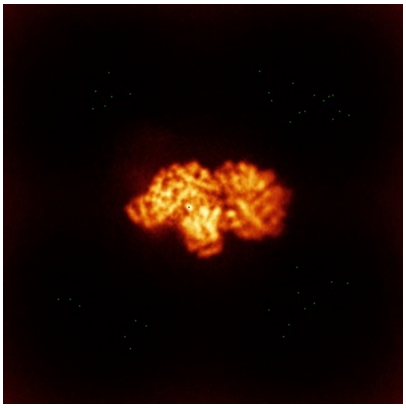


Z

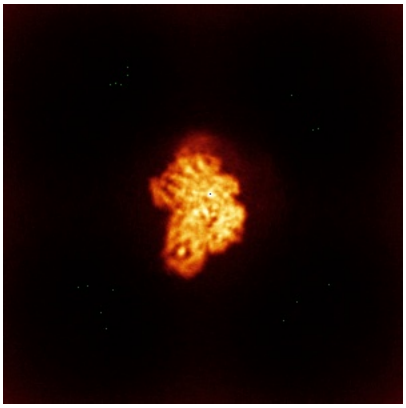
6.4.2 Raw map



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 0.4. 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.

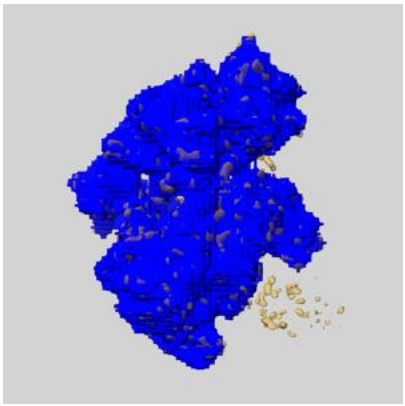
6.6 Mask visualisation (i)

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

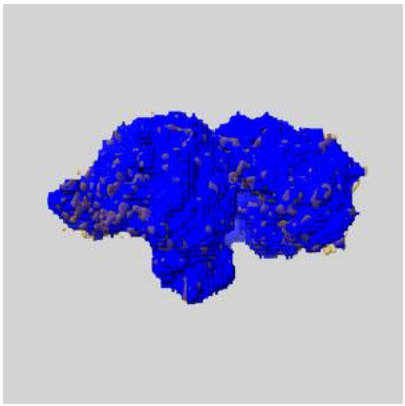
A mask typically either:

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

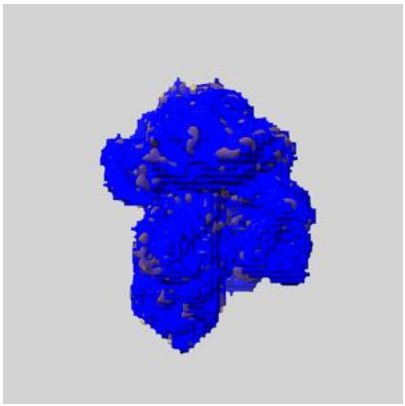
6.6.1 emd_80278_msk_1.map (i)



X



Y

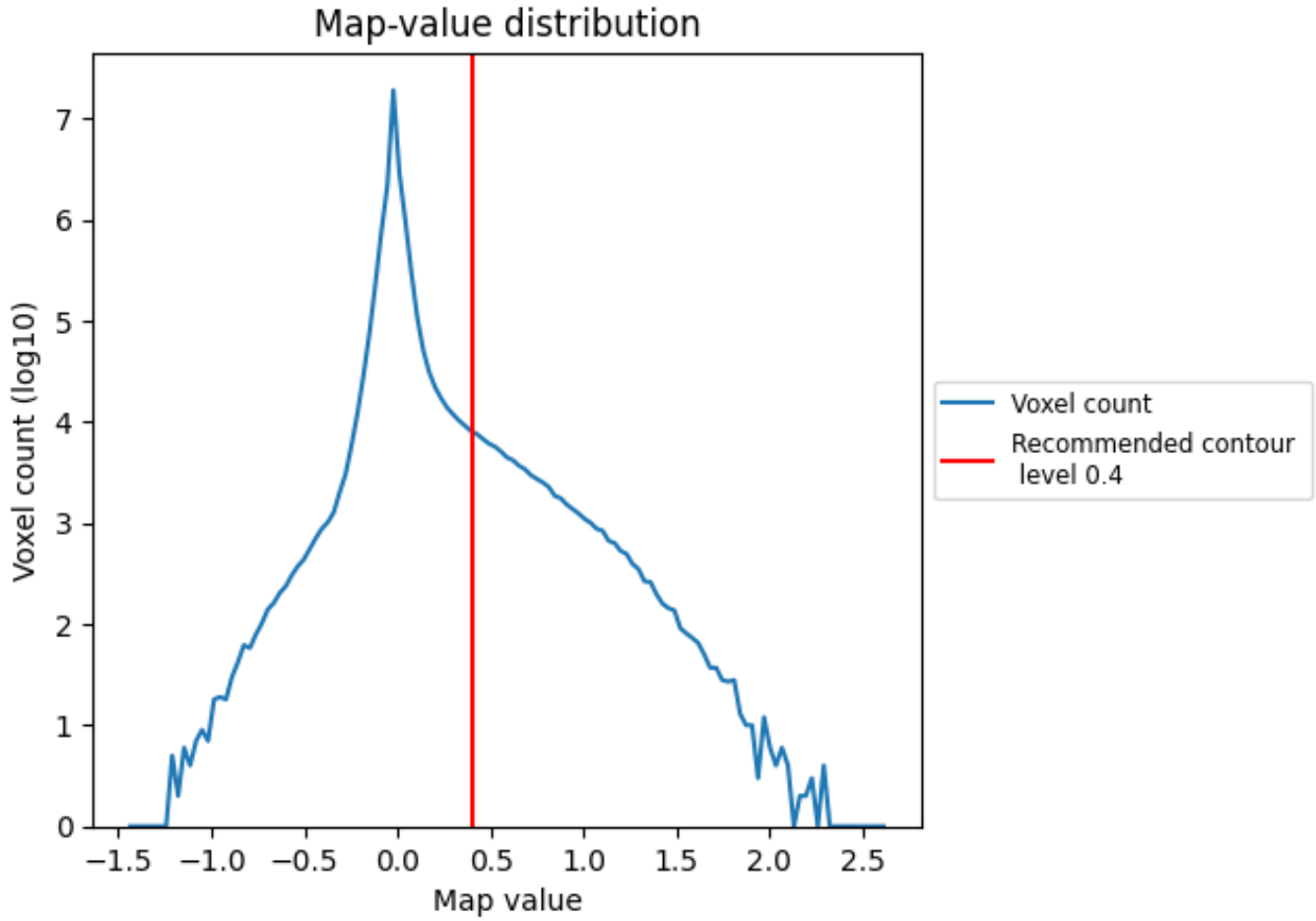


Z

7 Map analysis

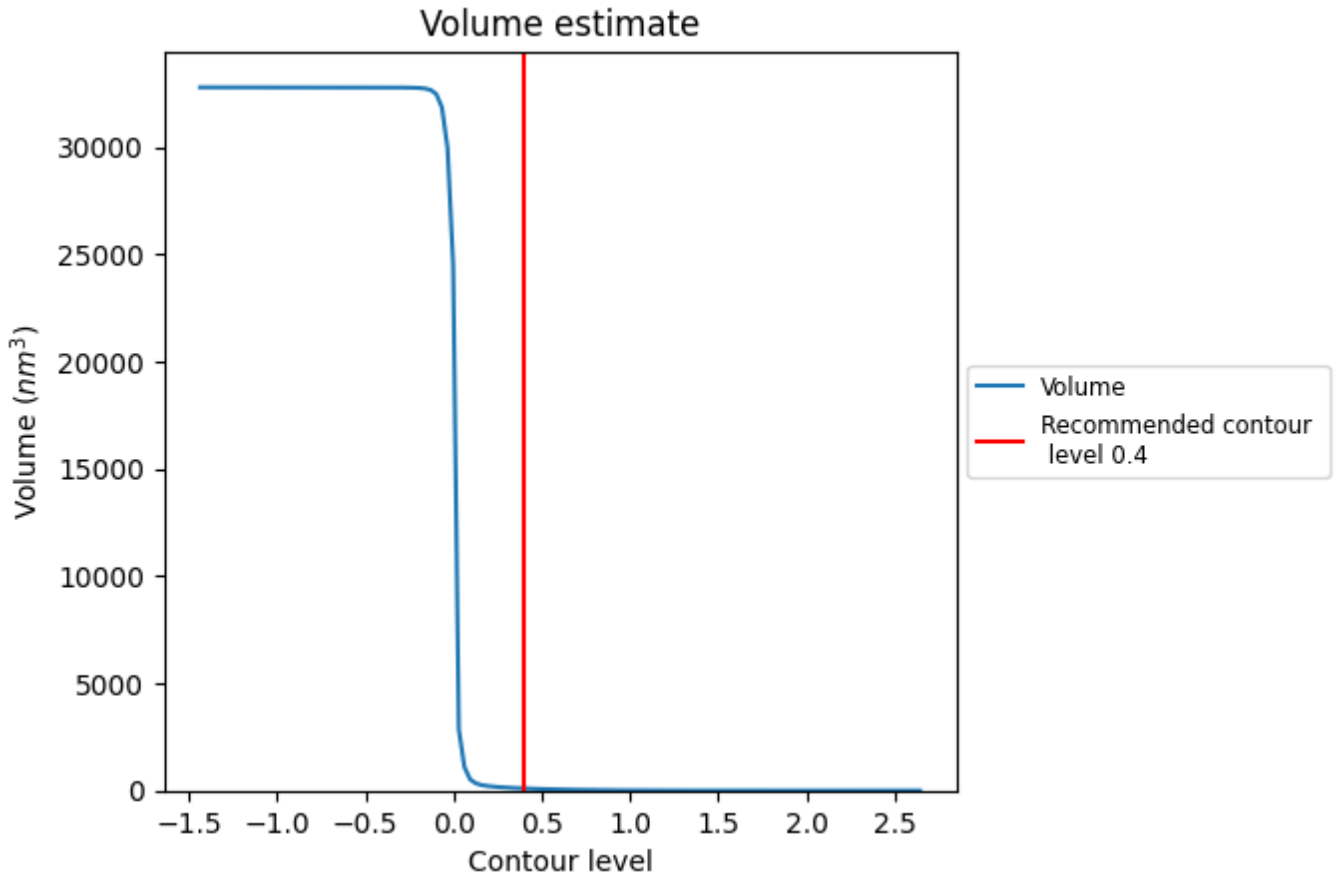
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

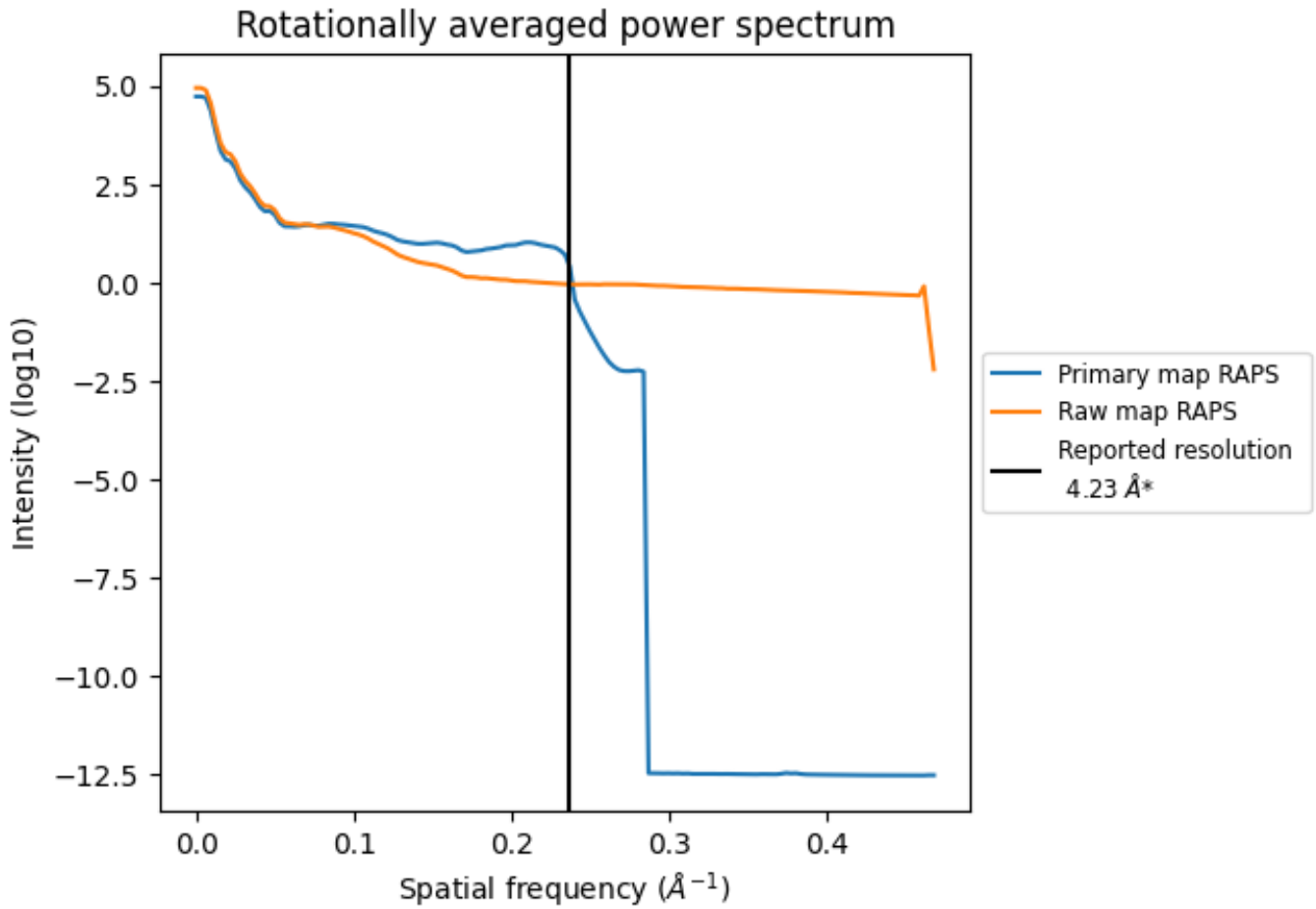
7.2 Volume estimate



The volume at the recommended contour level is 98 nm^3; this corresponds to an approximate mass of 89 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

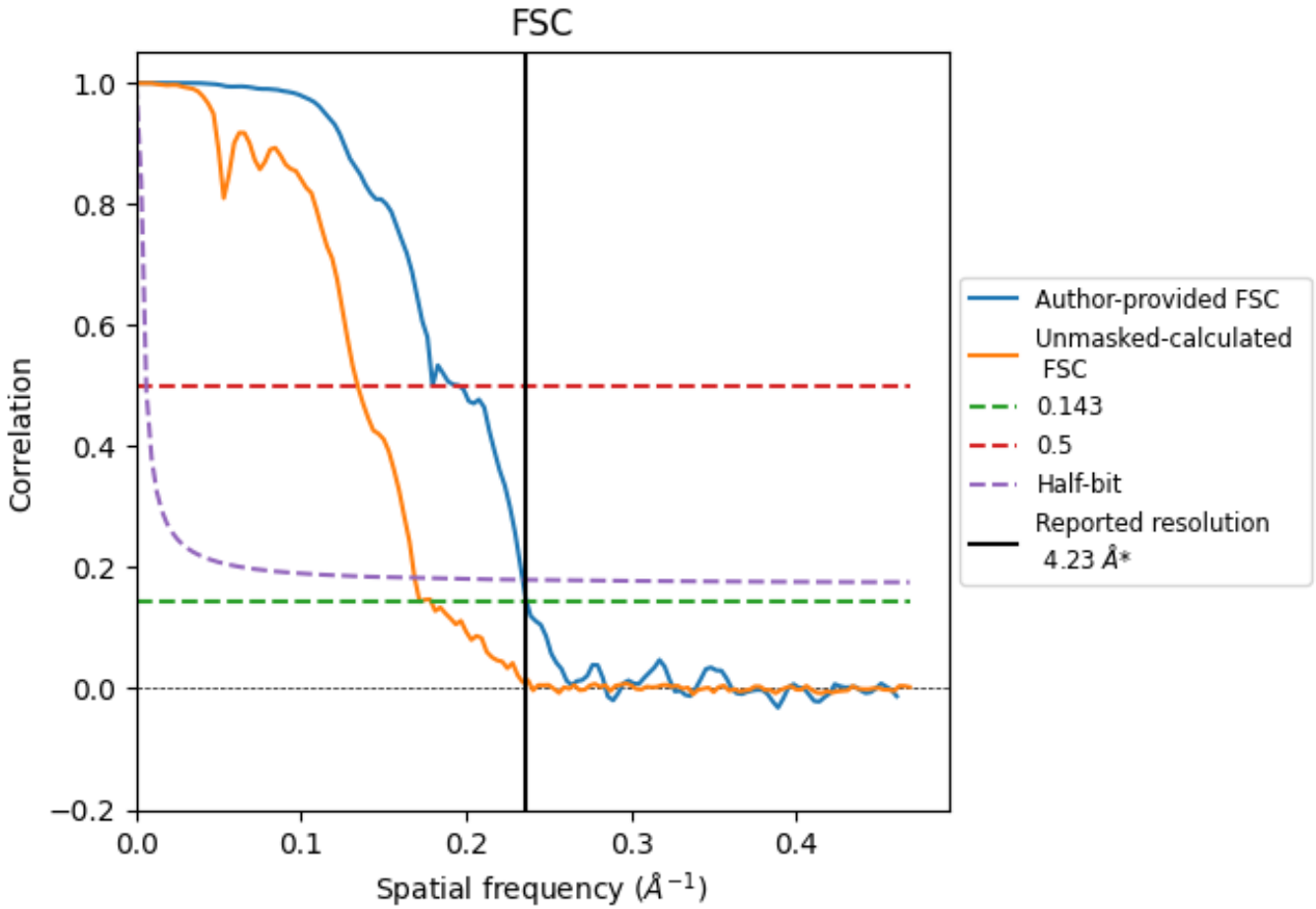


*Reported resolution corresponds to spatial frequency of 0.236 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.236 Å^{-1}

8.2 Resolution estimates (i)

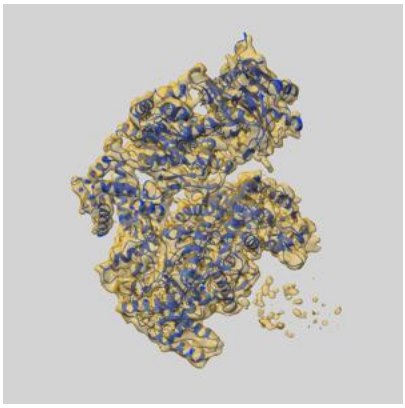
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.23	-	-
Author-provided FSC curve	4.23	5.12	4.27
Unmasked-calculated*	5.59	7.45	5.92

*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 5.59 differs from the reported value 4.23 by more than 10 %

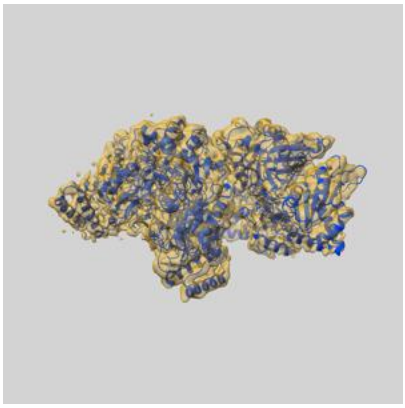
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-80278 and PDB model 25OU. Per-residue inclusion information can be found in section 3 on page 8.

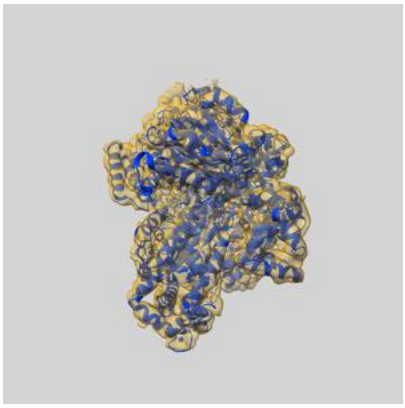
9.1 Map-model overlay



X



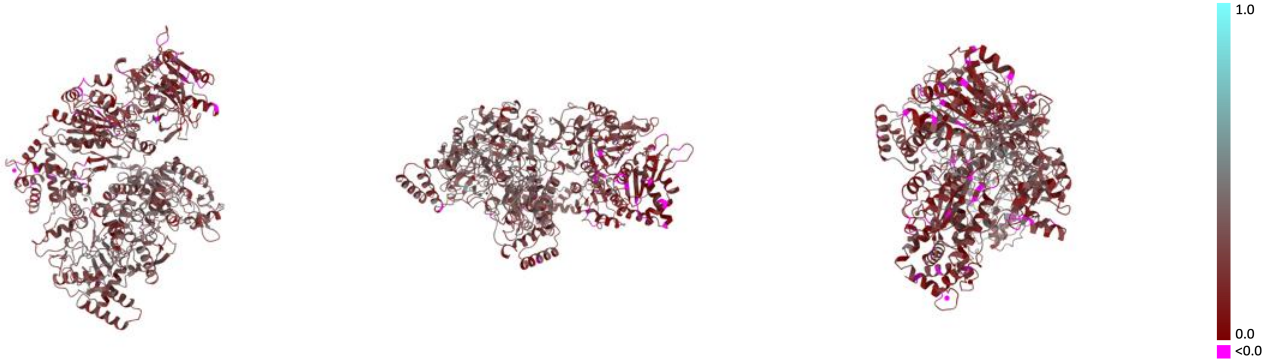
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

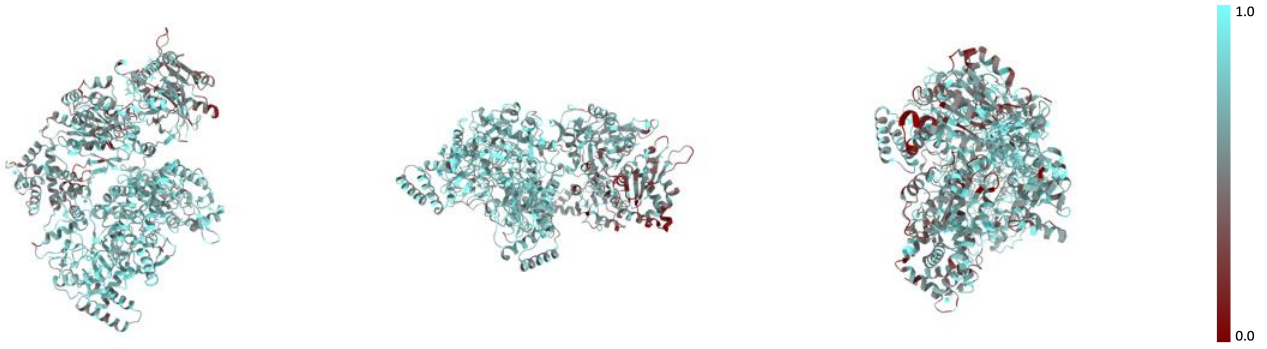
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

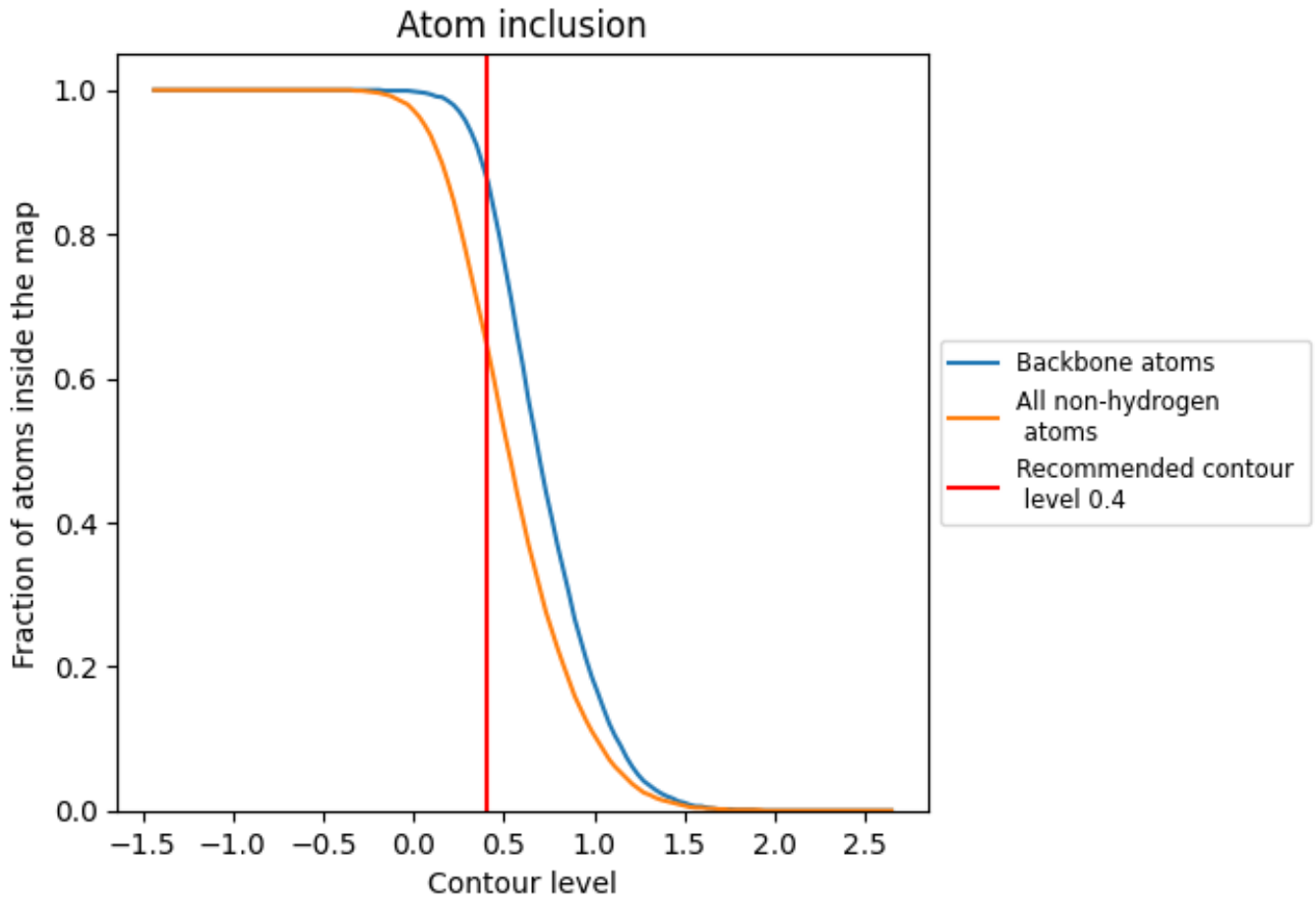
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 65% 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 (0.4) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.6510	0.2700
A	0.7240	0.3250
B	0.6310	0.2570
D	0.5700	0.1890