



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:21 PM UTC

PDB ID : 9Q15 / pdb\_00009q15  
EMDB ID : EMD-72116  
Title : syNOS Asymmetric Locked State (Composite)  
Authors : Nair, D.; Crane, B.  
Deposited on : 2025-08-13  
Resolution : 3.08 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](mailto: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:

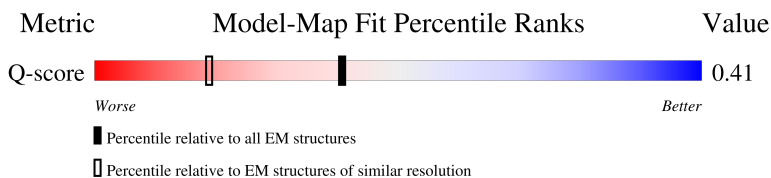
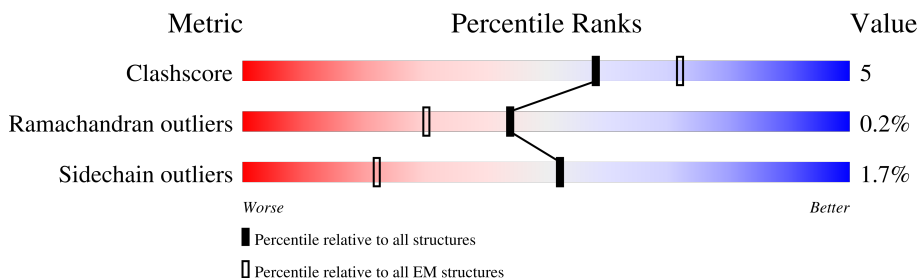
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.08 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	14000 ( 2.58 - 3.58 )

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  $\geq 3$ , 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	<p>88% 7% 6%</p>
1	B	1468	<p>6% 34% 7% 59%</p>

## 2 Entry composition [i](#)

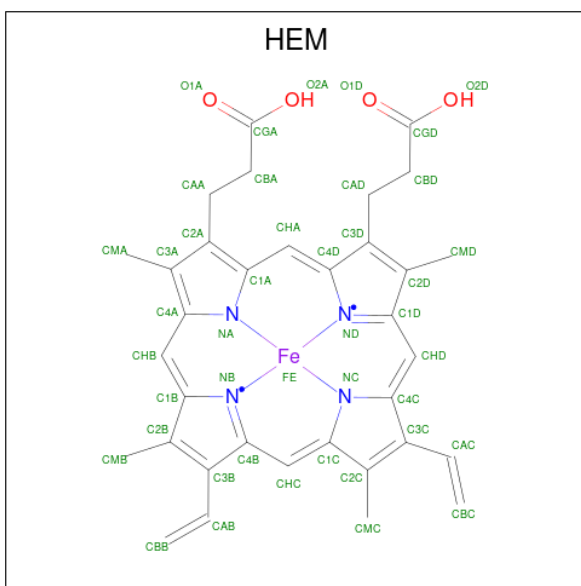
There are 4 unique types of molecules in this entry. The entry contains 32210 atoms, of which 15903 are hydrogens and 0 are deuteriums.

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.

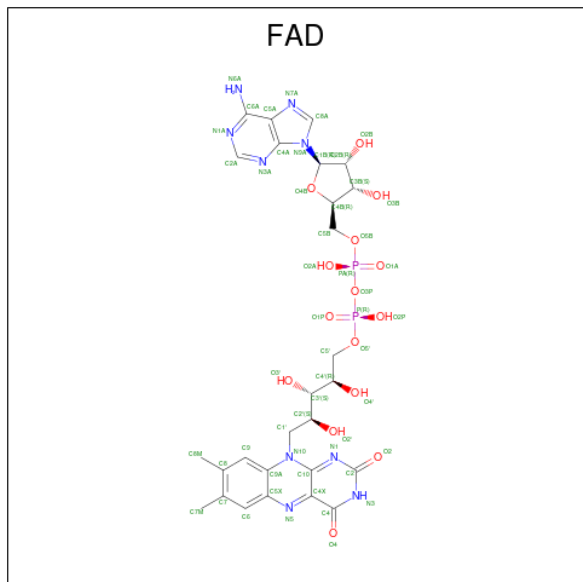
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	B	603	Total	C	H	N	O	S	0	0
			9804	3193	4843	849	889	30		
1	A	1386	Total	C	H	N	O	S	0	0
			21980	7052	10890	1908	2078	52		

- 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).



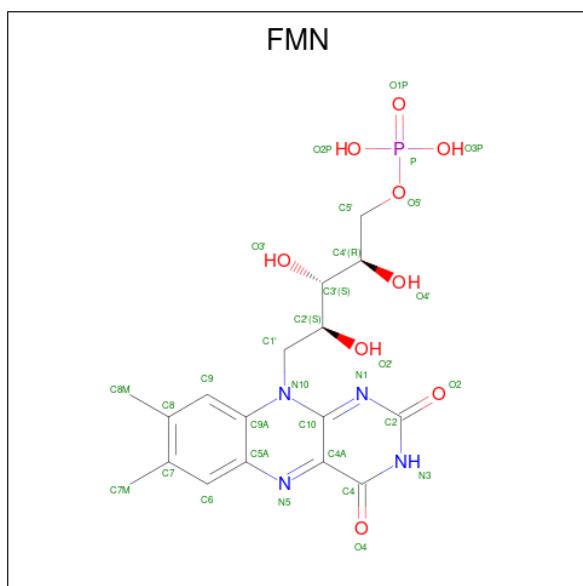
Mol	Chain	Residues	Atoms						AltConf
			Total	C	Fe	H	N	O	
2	B	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
2	B	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
2	A	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
2	A	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
3	A	1	84	27	31	9	15	2	0

- Molecule 4 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ) (labeled as "Ligand of Interest" by depositor).







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70944	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.418	Depositor
Minimum map value	-0.086	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0696	Depositor
Map size ( $\text{\AA}$ )	371.36, 371.36, 371.36	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.844, 0.844, 0.844	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, FAD, 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	0.13	0/11354	0.23	0/15413
1	B	0.13	0/5099	0.28	0/6911
All	All	0.13	0/16453	0.25	0/22324

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11090	10890	10886	63	0
1	B	4961	4843	4841	93	0
2	A	86	60	60	5	0
2	B	86	60	60	9	0
3	A	53	31	31	0	0
4	A	31	19	19	0	0
All	All	16307	15903	15897	150	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 5.

All (150) 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:531:LEU:HD11	1:B:827:LEU:HD22	1.59	0.84
1:B:399:ILE:HG23	1:B:411:LEU:HD13	1.66	0.78
1:A:940:LEU:HD13	1:A:943:LEU:HD23	1.67	0.76
1:B:366:TYR:OH	1:B:388:LEU:HD12	1.87	0.71
1:A:710:LEU:HD12	1:A:710:LEU:O	1.91	0.70
1:A:1031:LEU:HD13	1:A:1130:THR:HA	1.73	0.69
1:B:758:LEU:HD23	1:A:758:LEU:HD23	1.74	0.69
1:B:609:ALA:HB2	1:B:620:ASP:O	1.94	0.67
1:B:263:PHE:CD2	1:B:272:LEU:HD22	2.30	0.66
1:B:531:LEU:CD1	1:B:827:LEU:HD22	2.27	0.64
1:A:940:LEU:CD1	1:A:943:LEU:HD23	2.29	0.62
1:B:373:TYR:O	1:B:376:VAL:HG22	1.99	0.62
1:B:749:GLN:O	1:A:765:LEU:HD13	2.00	0.62
1:B:347:MET:HE3	1:B:458:TRP:CE2	2.34	0.61
1:A:115:VAL:HG23	1:A:124:LEU:HD23	1.82	0.61
1:A:347:MET:HE3	1:A:457:ALA:HB1	1.83	0.61
1:B:351:TRP:HH2	1:B:396:LEU:HD23	1.66	0.61
1:A:431:ALA:C	2:A:1501:HEM:HBB1	2.26	0.60
1:B:358:LYS:HB3	1:B:390:THR:HG22	1.84	0.59
1:B:758:LEU:HD13	1:A:754:ASP:OD1	2.02	0.59
1:B:435:ILE:HG21	2:B:1501:HEM:HAB	1.85	0.58
1:A:347:MET:CE	1:A:457:ALA:HB1	2.34	0.58
1:A:1196:MET:HE3	1:A:1257:ARG:HB2	1.84	0.58
1:A:209:LEU:CD2	1:A:844:ILE:HD13	2.33	0.58
1:A:435:ILE:HD13	2:A:1501:HEM:HAB	1.86	0.58
1:A:717:MET:HG3	1:A:776:VAL:HG13	1.85	0.57
1:A:1298:PRO:CD	1:A:1399:MET:HE2	2.34	0.57
1:A:1298:PRO:HD2	1:A:1399:MET:HE2	1.87	0.57
1:B:758:LEU:HD21	1:A:755:ARG:HA	1.87	0.57
1:B:717:MET:HA	1:B:717:MET:HE2	1.87	0.56
1:B:464:ARG:O	1:B:468:VAL:HG23	2.05	0.56
1:B:670:LEU:HD23	1:B:671:GLU:N	2.22	0.55
1:B:755:ARG:HA	1:A:758:LEU:HD21	1.89	0.54
1:B:388:LEU:C	1:B:388:LEU:HD13	2.33	0.54
1:A:54:LEU:HD23	1:A:62:TRP:CG	2.44	0.53
1:A:1027:GLU:O	1:A:1031:LEU:HG	2.08	0.53
1:B:351:TRP:CH2	1:B:396:LEU:HD23	2.43	0.53
1:B:486:TYR:O	1:B:490:ILE:HG22	2.09	0.53
1:B:293:MET:HE3	1:B:294:LEU:HD23	1.91	0.53
1:B:380:PHE:CZ	1:B:435:ILE:HD12	2.44	0.52
1:B:569:HIS:CD2	1:B:582:VAL:HG13	2.44	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1066:LEU:HD11	1:A:1239:LYS:HB3	1.92	0.52
1:B:485:GLU:O	1:B:489:VAL:HG23	2.10	0.51
1:B:751:LEU:HD21	1:A:765:LEU:CD1	2.41	0.51
1:B:758:LEU:HD12	1:B:758:LEU:O	2.11	0.51
2:B:1502:HEM:HBB2	2:B:1502:HEM:HHC	1.92	0.51
1:B:600:TRP:CH2	1:B:634:MET:HE1	2.45	0.51
1:B:533:TRP:CD1	1:B:533:TRP:O	2.63	0.51
1:B:599:ILE:HD11	1:B:709:CYS:SG	2.50	0.51
1:B:343:LEU:HD21	1:B:457:ALA:HB2	1.93	0.50
1:B:465:VAL:HG12	1:B:469:ILE:HD12	1.93	0.50
1:B:347:MET:HE3	1:B:458:TRP:CZ2	2.46	0.50
1:A:1393:VAL:HG12	1:A:1437:THR:HG22	1.93	0.50
1:B:411:LEU:C	1:B:411:LEU:HD12	2.36	0.50
1:B:379:ILE:HG21	1:B:428:PRO:CD	2.42	0.49
1:B:734:MET:SD	1:B:734:MET:C	2.95	0.49
1:B:291:MET:C	1:B:291:MET:SD	2.95	0.49
1:B:443:PHE:CE2	1:B:458:TRP:CE2	3.01	0.49
1:B:664:PHE:HB2	1:B:669:ILE:HD11	1.94	0.49
1:B:325:ILE:O	1:B:329:VAL:HG23	2.13	0.49
1:A:1031:LEU:HD13	1:A:1130:THR:CA	2.41	0.49
1:B:388:LEU:HD13	1:B:388:LEU:O	2.13	0.49
1:A:869:SER:HB3	1:A:874:ALA:HB3	1.94	0.48
1:A:15:LEU:HD23	1:A:138:GLN:NE2	2.29	0.48
1:B:750:THR:O	1:A:762:ILE:HD12	2.13	0.48
1:B:536:THR:HG21	2:B:1502:HEM:C3D	2.48	0.48
1:B:347:MET:CE	1:B:458:TRP:CE2	2.97	0.48
1:A:74:PHE:HB2	1:A:97:VAL:HG23	1.96	0.47
1:A:846:LEU:O	1:A:850:VAL:HG23	2.13	0.47
1:B:351:TRP:CZ3	1:B:458:TRP:CH2	3.02	0.47
1:B:431:ALA:C	2:B:1501:HEM:HBB1	2.40	0.47
1:A:692:VAL:O	1:A:692:VAL:HG13	2.14	0.47
1:B:365:PHE:HZ	1:B:435:ILE:HD11	1.78	0.47
1:B:530:GLN:HA	1:B:548:MET:CE	2.45	0.47
1:B:750:THR:O	1:B:750:THR:HG22	2.15	0.47
1:B:217:ILE:CG2	1:B:276:ILE:HG22	2.44	0.46
1:B:634:MET:HE3	1:B:659:PRO:HB2	1.96	0.46
1:B:762:ILE:HA	1:A:751:LEU:HD13	1.97	0.46
2:A:1502:HEM:HBC2	2:A:1502:HEM:HMC2	1.96	0.46
1:B:436:SER:HB2	1:B:462:ILE:HG23	1.98	0.46
1:B:480:LEU:HG	1:B:512:VAL:HG11	1.97	0.46
1:B:634:MET:SD	1:B:634:MET:N	2.88	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:718:GLY:N	1:B:775:MET:HE2	2.31	0.46
1:A:291:MET:HE3	1:A:317:CYS:HB2	1.97	0.46
1:A:1014:THR:O	1:A:1015:THR:C	2.59	0.46
1:B:508:ILE:O	1:B:512:VAL:HG23	2.16	0.45
1:B:207:LEU:HA	1:B:289:VAL:HG21	1.99	0.45
1:B:277:GLY:O	1:B:278:MET:C	2.59	0.45
1:B:391:HIS:HB3	2:B:1501:HEM:O1D	2.17	0.45
1:A:841:GLU:HB2	1:A:846:LEU:HD11	1.98	0.45
1:B:710:LEU:O	1:B:710:LEU:HD12	2.17	0.44
1:B:391:HIS:CB	2:B:1501:HEM:O1D	2.66	0.44
1:B:481:LYS:O	1:B:485:GLU:HG2	2.18	0.44
1:B:435:ILE:O	1:B:438:VAL:HG12	2.17	0.44
1:B:347:MET:SD	1:B:454:LEU:HD23	2.58	0.43
1:A:102:LEU:HD11	1:A:111:ILE:HD11	2.00	0.43
1:B:293:MET:CE	1:B:294:LEU:HD23	2.48	0.43
1:A:828:GLU:HB3	1:A:829:PRO:HD3	1.99	0.43
1:B:196:LYS:O	1:B:200:MET:HG2	2.18	0.43
1:B:386:ASP:O	1:B:390:THR:HG23	2.18	0.43
1:B:531:LEU:HD12	1:B:531:LEU:O	2.18	0.43
1:A:750:THR:C	1:A:751:LEU:HD12	2.43	0.43
1:B:232:MET:SD	1:B:328:MET:HE3	2.58	0.43
1:A:178:THR:HG22	1:A:179:TYR:H	1.84	0.43
1:A:232:MET:HE3	1:A:233:PHE:CD1	2.54	0.43
1:A:1292:PRO:C	1:A:1293:LEU:HD12	2.44	0.43
1:B:379:ILE:HG21	1:B:428:PRO:HD3	2.01	0.42
1:B:439:MET:HA	1:B:439:MET:HE2	2.01	0.42
1:B:347:MET:CE	1:B:458:TRP:CD2	3.03	0.42
1:B:443:PHE:CE2	1:B:458:TRP:CZ2	3.08	0.42
1:B:579:ILE:HB	1:B:715:TRP:HB3	2.02	0.42
1:A:103:PHE:CD1	1:A:109:VAL:HG23	2.55	0.42
1:A:184:ILE:HG21	1:A:307:ASP:OD2	2.20	0.42
1:B:765:LEU:HD23	1:B:765:LEU:O	2.20	0.42
1:A:33:GLU:HG2	1:A:33:GLU:O	2.19	0.42
1:B:380:PHE:CE2	1:B:435:ILE:HD12	2.54	0.42
1:B:456:GLU:O	1:B:460:VAL:HG23	2.20	0.42
1:B:458:TRP:O	1:B:459:GLN:C	2.63	0.42
1:A:1102:LEU:HD11	1:A:1106:THR:CB	2.49	0.42
1:A:1363:THR:HG22	1:A:1364:ALA:N	2.35	0.42
1:A:115:VAL:CG2	1:A:124:LEU:HD23	2.47	0.41
1:A:232:MET:HE2	1:A:232:MET:HB3	1.91	0.41
1:A:1196:MET:HE1	1:A:1251:THR:CG2	2.51	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:758:LEU:HD22	1:A:754:ASP:OD1	2.20	0.41
1:A:393:PHE:HZ	1:A:442:MET:HE1	1.85	0.41
1:A:1046:LEU:HD11	1:A:1068:ASP:HB2	2.01	0.41
1:B:374:PRO:HA	1:B:377:LEU:HD12	2.02	0.41
1:B:539:CYS:HA	2:B:1502:HEM:C1A	2.55	0.41
1:A:435:ILE:CD1	2:A:1501:HEM:HAB	2.50	0.41
1:A:991:ASP:N	1:A:991:ASP:OD1	2.53	0.41
1:A:1031:LEU:HD21	1:A:1129:PRO:HB2	2.02	0.41
1:B:285:ARG:O	1:B:289:VAL:HG23	2.21	0.41
1:B:358:LYS:CB	1:B:390:THR:HG22	2.49	0.41
1:B:369:LEU:HB2	1:B:438:VAL:HG11	2.03	0.41
1:B:481:LYS:N	1:B:481:LYS:HD2	2.36	0.41
1:B:562:MET:SD	1:B:586:PHE:CD1	3.14	0.41
1:A:240:LEU:HD23	1:A:240:LEU:C	2.46	0.41
1:A:1196:MET:HE1	1:A:1251:THR:HG21	2.03	0.41
1:B:533:TRP:C	1:B:535:ASN:H	2.29	0.41
1:A:182:ALA:HB1	1:A:240:LEU:HD21	2.03	0.40
1:A:1286:PRO:HG3	1:A:1293:LEU:HD11	2.01	0.40
1:B:366:TYR:CD2	1:B:385:MET:HA	2.56	0.40
1:A:726:LEU:HD11	1:A:757:ALA:HA	2.03	0.40
1:A:1102:LEU:HD11	1:A:1106:THR:HG21	2.03	0.40
1:A:1373:MET:HE1	1:A:1407:PHE:CE1	2.57	0.40
1:B:533:TRP:CZ2	2:B:1502:HEM:C1C	3.09	0.40
1:B:347:MET:HE3	1:B:458:TRP:CD2	2.56	0.40
1:B:392:LEU:CD1	2:B:1501:HEM:C3C	3.04	0.40
1:A:1450:ILE:HG23	1:A:1451:LYS:N	2.36	0.40
2:A:1502:HEM:HHC	2:A:1502:HEM:HBB2	2.04	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	1378/1468 (94%)	1309 (95%)	66 (5%)	3 (0%)	43	71
1	B	597/1468 (41%)	579 (97%)	18 (3%)	0	100	100
All	All	1975/2936 (67%)	1888 (96%)	84 (4%)	3 (0%)	44	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	SER
1	A	1015	THR
1	A	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	1195/1263 (95%)	1176 (98%)	19 (2%)	55	72
1	B	521/1263 (41%)	511 (98%)	10 (2%)	50	70
All	All	1716/2526 (68%)	1687 (98%)	29 (2%)	52	71

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	225	ILE
1	B	347	MET
1	B	365	PHE
1	B	366	TYR
1	B	411	LEU
1	B	493	GLU
1	B	673	GLU
1	B	675	GLU
1	B	716	TYR
1	B	828	GLU
1	A	240	LEU
1	A	263	PHE
1	A	388	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	460	VAL
1	A	643	SER
1	A	657	HIS
1	A	709	CYS
1	A	750	THR
1	A	783	ARG
1	A	865	ILE
1	A	998	SER
1	A	1002	ARG
1	A	1028	SER
1	A	1120	LEU
1	A	1155	LEU
1	A	1232	CYS
1	A	1331	CYS
1	A	1436	SER
1	A	1442	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	B	391	HIS
1	B	494	GLN
1	A	106	GLN
1	A	467	ASN
1	A	575	ASN
1	A	766	HIS
1	A	1248	GLN

### 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

6 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	A	1501	1	50,50,50	1.65	9 (18%)	67,82,82	1.56	11 (16%)
3	FAD	A	1503	-	58,58,58	1.31	4 (6%)	85,89,89	0.78	2 (2%)
4	FMN	A	1504	-	33,33,33	1.07	2 (6%)	48,50,50	1.25	8 (16%)
2	HEM	B	1501	1	50,50,50	1.65	9 (18%)	67,82,82	1.55	11 (16%)
2	HEM	B	1502	-	50,50,50	1.68	10 (20%)	67,82,82	1.58	11 (16%)
2	HEM	A	1502	1	50,50,50	1.66	10 (20%)	67,82,82	1.53	10 (14%)

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	A	1501	1	-	8/14/54/54	-
3	FAD	A	1503	-	-	10/34/50/50	0/6/6/6
4	FMN	A	1504	-	-	11/18/18/18	0/3/3/3
2	HEM	B	1501	1	-	6/14/54/54	-
2	HEM	B	1502	-	-	6/14/54/54	-
2	HEM	A	1502	1	-	2/14/54/54	-

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1503	FAD	P-O3P	6.47	1.66	1.59
2	B	1502	HEM	FE-NB	5.30	2.11	1.94
2	A	1502	HEM	FE-NB	5.28	2.11	1.94
2	B	1501	HEM	FE-NB	5.04	2.10	1.94
2	A	1501	HEM	FE-NB	4.92	2.10	1.94

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1502	HEM	FE-NC	4.03	2.08	1.95
2	A	1501	HEM	FE-NC	4.00	2.08	1.95
2	A	1502	HEM	FE-NC	3.88	2.08	1.95
2	B	1501	HEM	C4D-ND	-3.84	1.33	1.40
2	A	1501	HEM	C4D-ND	-3.79	1.33	1.40
2	B	1501	HEM	C1B-NB	-3.78	1.33	1.40
2	B	1501	HEM	FE-NC	3.76	2.07	1.95
3	A	1503	FAD	PA-O3P	3.68	1.63	1.59
2	A	1502	HEM	C4D-ND	-3.65	1.33	1.40
2	B	1502	HEM	C4D-ND	-3.59	1.34	1.40
2	A	1502	HEM	C1B-NB	-3.51	1.34	1.40
2	A	1501	HEM	C1B-NB	-3.46	1.34	1.40
2	B	1502	HEM	C1B-NB	-3.34	1.34	1.40
4	A	1504	FMN	C4A-N5	3.30	1.37	1.30
2	A	1501	HEM	FE-ND	-2.87	1.86	1.94
2	B	1502	HEM	C3B-C4B	2.86	1.50	1.44
2	A	1501	HEM	C1D-ND	-2.81	1.33	1.38
2	B	1501	HEM	FE-ND	-2.76	1.86	1.94
2	B	1502	HEM	C1D-ND	-2.68	1.33	1.38
2	B	1502	HEM	FE-ND	-2.65	1.86	1.94
2	A	1502	HEM	FE-ND	-2.63	1.86	1.94
2	A	1502	HEM	C1D-ND	-2.55	1.33	1.38
3	A	1503	FAD	C5X-N5	-2.49	1.34	1.39
4	A	1504	FMN	C10-N1	2.46	1.38	1.33
2	A	1501	HEM	C4B-NB	-2.40	1.34	1.38
2	B	1501	HEM	C4B-NB	-2.39	1.34	1.38
2	B	1501	HEM	C1C-C2C	-2.34	1.40	1.45
2	A	1502	HEM	C3B-C4B	2.31	1.49	1.44
2	B	1501	HEM	C1D-ND	-2.27	1.34	1.38
2	A	1502	HEM	C4B-NB	-2.22	1.34	1.38
2	B	1502	HEM	C3C-C4C	-2.12	1.42	1.46
2	A	1501	HEM	C1C-C2C	-2.10	1.41	1.45
2	A	1501	HEM	C1A-C2A	-2.10	1.40	1.44
2	A	1502	HEM	C1C-C2C	-2.09	1.41	1.45
3	A	1503	FAD	C6-C7	-2.07	1.36	1.39
2	B	1502	HEM	C1C-C2C	-2.06	1.41	1.45
2	B	1502	HEM	C4B-NB	-2.06	1.34	1.38
2	A	1502	HEM	C1A-C2A	-2.03	1.40	1.44
2	B	1501	HEM	C1C-NC	-2.01	1.35	1.39

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1501	HEM	CHC-C4B-NB	5.20	130.01	124.42
2	B	1501	HEM	CHC-C4B-NB	4.97	129.77	124.42
2	B	1502	HEM	CHD-C1D-ND	4.69	129.47	124.42
2	A	1502	HEM	CHD-C1D-ND	4.43	129.19	124.42
2	A	1501	HEM	CHD-C1D-ND	4.33	129.08	124.42
2	A	1502	HEM	CHC-C4B-NB	4.21	128.96	124.42
2	B	1501	HEM	CHA-C4D-ND	4.10	129.44	124.37
2	A	1502	HEM	CHA-C4D-ND	3.69	128.93	124.37
2	B	1501	HEM	CHD-C1D-ND	3.68	128.38	124.42
2	A	1501	HEM	C1B-NB-C4B	3.63	109.51	105.21
2	B	1502	HEM	C1B-NB-C4B	3.57	109.43	105.21
2	B	1502	HEM	CHD-C1D-C2D	-3.34	119.75	125.03
2	A	1501	HEM	CHA-C4D-ND	3.31	128.46	124.37
2	B	1502	HEM	CHA-C4D-ND	3.29	128.44	124.37
4	A	1504	FMN	C4-N3-C2	-3.27	119.83	125.64
2	B	1501	HEM	C1B-NB-C4B	3.27	109.08	105.21
2	A	1502	HEM	C1B-NB-C4B	3.15	108.94	105.21
2	B	1502	HEM	CHC-C4B-NB	3.10	127.76	124.42
2	B	1502	HEM	C3B-C4B-NB	-3.05	107.28	109.47
2	A	1502	HEM	CHD-C1D-C2D	-2.78	120.64	125.03
2	B	1501	HEM	CHB-C1B-NB	2.76	127.78	124.37
2	B	1501	HEM	CHA-C4D-C3D	-2.74	120.18	125.23
2	B	1502	HEM	CHB-C1B-NB	2.69	127.69	124.37
4	A	1504	FMN	C4A-C4-N3	2.68	120.08	113.25
2	A	1501	HEM	C3B-C4B-NB	-2.66	107.56	109.47
2	A	1502	HEM	CHA-C4D-C3D	-2.65	120.35	125.23
2	A	1502	HEM	CHB-C1B-NB	2.63	127.62	124.37
4	A	1504	FMN	C4A-C10-N10	2.58	120.18	116.48
4	A	1504	FMN	O4-C4-C4A	-2.58	119.73	126.53
2	A	1501	HEM	C1A-CHA-C4D	-2.55	120.26	126.25
2	B	1501	HEM	C1A-CHA-C4D	-2.54	120.28	126.25
2	B	1502	HEM	C1A-CHA-C4D	-2.51	120.34	126.25
2	A	1501	HEM	CHD-C1D-C2D	-2.47	121.14	125.03
2	A	1502	HEM	C1A-CHA-C4D	-2.45	120.50	126.25
2	B	1502	HEM	C4C-NC-C1C	2.36	109.67	105.82
2	A	1501	HEM	C4D-ND-C1D	2.35	107.98	105.21
3	A	1503	FAD	C9-C9A-N10	2.33	124.99	121.85
4	A	1504	FMN	C5A-C9A-N10	2.33	120.07	117.97
2	A	1501	HEM	C4C-NC-C1C	2.28	109.53	105.82
2	A	1502	HEM	C4B-C3B-C2B	-2.26	105.20	107.28
2	A	1502	HEM	CHA-C1A-NA	2.26	127.95	123.86
2	A	1501	HEM	CHB-C1B-NB	2.25	127.16	124.37
2	B	1501	HEM	C4C-CHD-C1D	-2.25	121.24	126.02

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1504	FMN	C9A-C5A-N5	-2.19	120.13	122.45
2	B	1502	HEM	CHA-C1A-NA	2.16	127.78	123.86
2	B	1501	HEM	C4B-C3B-C2B	-2.15	105.31	107.28
4	A	1504	FMN	C4A-C10-N1	-2.14	119.34	124.59
4	A	1504	FMN	C10-C4A-N5	-2.14	120.45	124.81
2	B	1501	HEM	C4D-ND-C1D	2.12	107.72	105.21
2	B	1502	HEM	CHA-C4D-C3D	-2.08	121.40	125.23
2	B	1501	HEM	C4C-NC-C1C	2.06	109.18	105.82
3	A	1503	FAD	O2P-P-O1P	2.04	121.92	112.44
2	A	1501	HEM	C4C-CHD-C1D	-2.02	121.72	126.02

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1503	FAD	C5B-O5B-PA-O3P
3	A	1503	FAD	P-O3P-PA-O5B
3	A	1503	FAD	C5'-O5'-P-O3P
4	A	1504	FMN	N10-C1'-C2'-O2'
4	A	1504	FMN	N10-C1'-C2'-C3'
4	A	1504	FMN	C3'-C4'-C5'-O5'
4	A	1504	FMN	O4'-C4'-C5'-O5'
4	A	1504	FMN	C5'-O5'-P-O2P
4	A	1504	FMN	C5'-O5'-P-O3P
2	B	1501	HEM	C3D-CAD-CBD-CGD
2	B	1502	HEM	C2A-CAA-CBA-CGA
2	A	1501	HEM	C2A-CAA-CBA-CGA
2	A	1501	HEM	C3D-CAD-CBD-CGD
2	B	1501	HEM	C2A-CAA-CBA-CGA
3	A	1503	FAD	C3B-C4B-C5B-O5B
4	A	1504	FMN	C2'-C3'-C4'-O4'
4	A	1504	FMN	C2'-C3'-C4'-C5'
3	A	1503	FAD	C4B-C5B-O5B-PA
4	A	1504	FMN	C5'-O5'-P-O1P
4	A	1504	FMN	O3'-C3'-C4'-O4'
3	A	1503	FAD	PA-O3P-P-O5'
2	B	1502	HEM	C4B-C3B-CAB-CBB
3	A	1503	FAD	C5B-O5B-PA-O1A
3	A	1503	FAD	C5'-O5'-P-O1P
3	A	1503	FAD	C4'-C5'-O5'-P
2	A	1501	HEM	CAD-CBD-CGD-O1D
2	B	1502	HEM	CAD-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

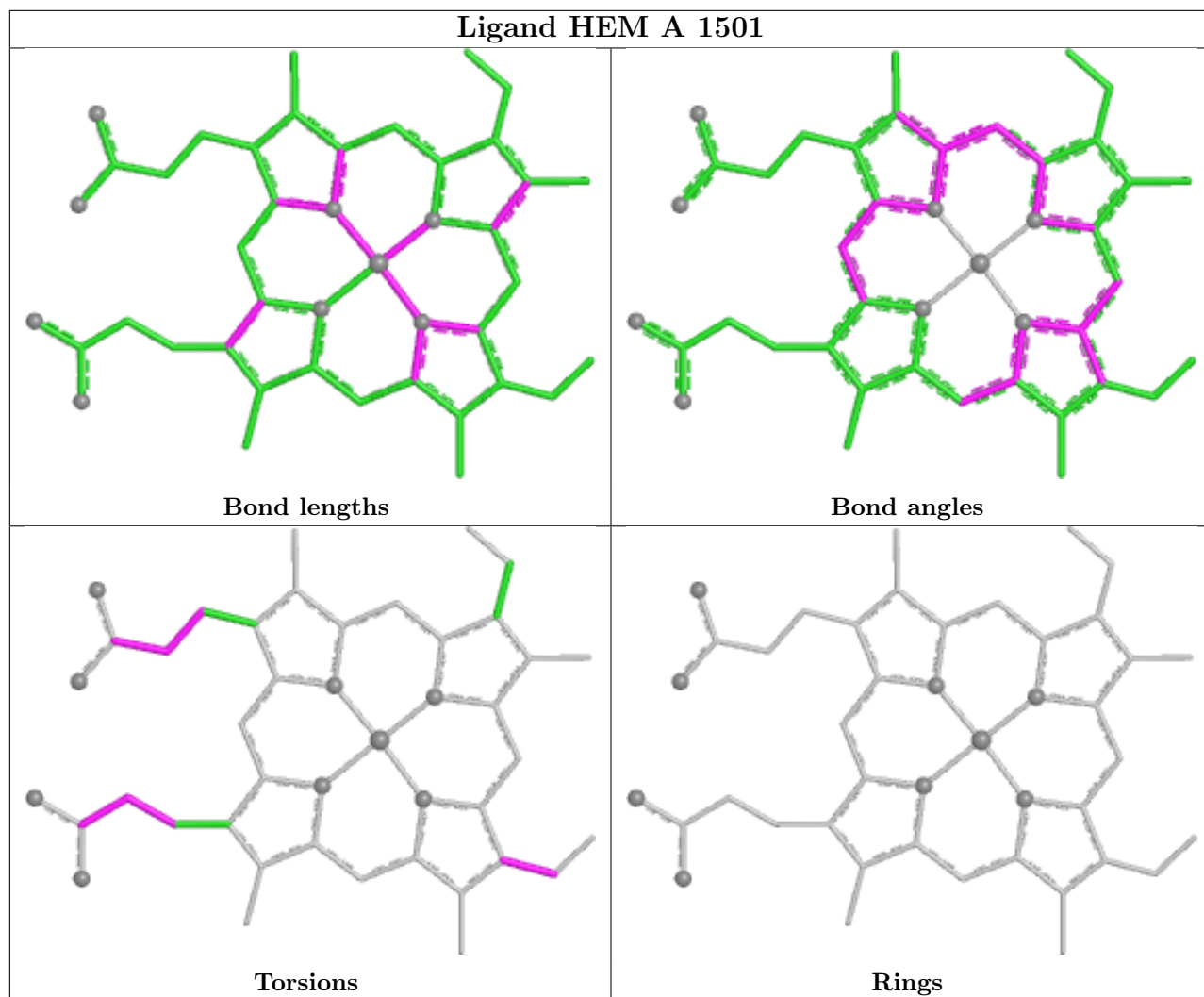
Mol	Chain	Res	Type	Atoms
4	A	1504	FMN	O3'-C3'-C4'-C5'
2	B	1502	HEM	CAA-CBA-CGA-O2A
2	A	1502	HEM	CAA-CBA-CGA-O2A
2	A	1501	HEM	CAD-CBD-CGD-O2D
2	B	1502	HEM	CAA-CBA-CGA-O1A
2	A	1501	HEM	CAA-CBA-CGA-O2A
2	B	1501	HEM	CAA-CBA-CGA-O2A
2	B	1501	HEM	CAD-CBD-CGD-O2D
2	B	1502	HEM	CAD-CBD-CGD-O1D
2	A	1501	HEM	CAA-CBA-CGA-O1A
2	A	1501	HEM	C4B-C3B-CAB-CBB
2	A	1502	HEM	CAA-CBA-CGA-O1A
2	B	1501	HEM	CAD-CBD-CGD-O1D
3	A	1503	FAD	PA-O3P-P-O1P
2	B	1501	HEM	CAA-CBA-CGA-O1A
2	A	1501	HEM	C2B-C3B-CAB-CBB

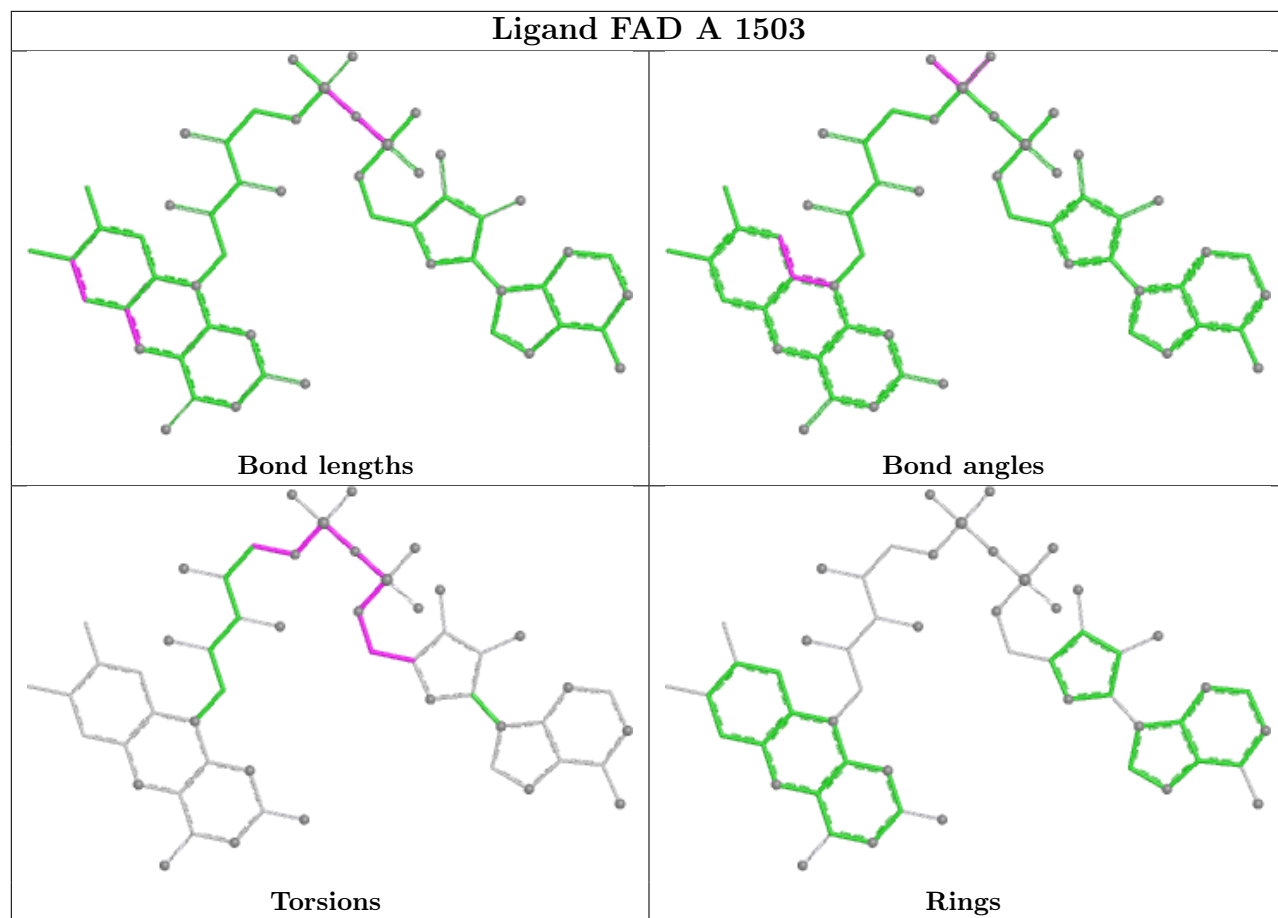
There are no ring outliers.

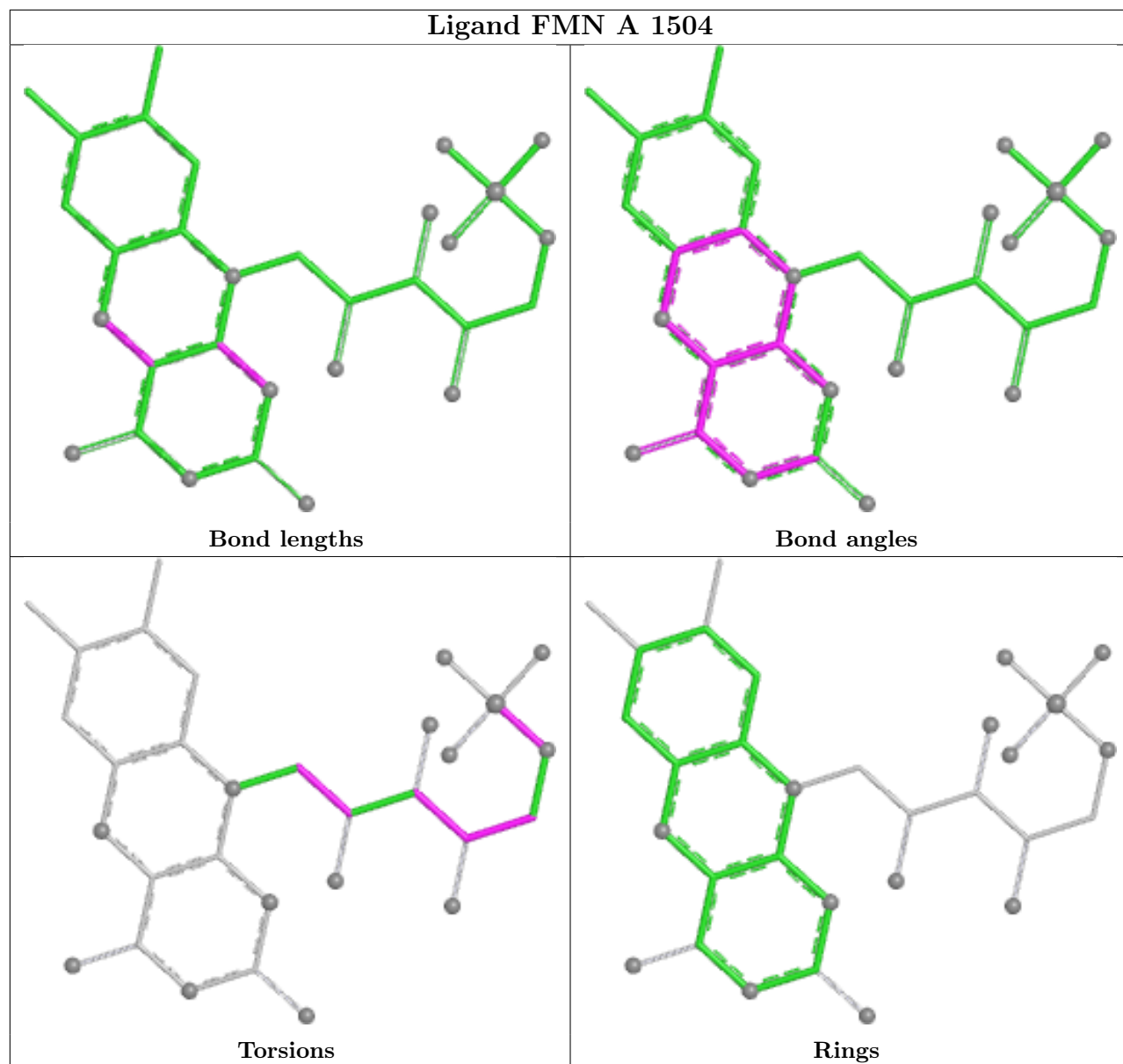
4 monomers are involved in 14 short contacts:

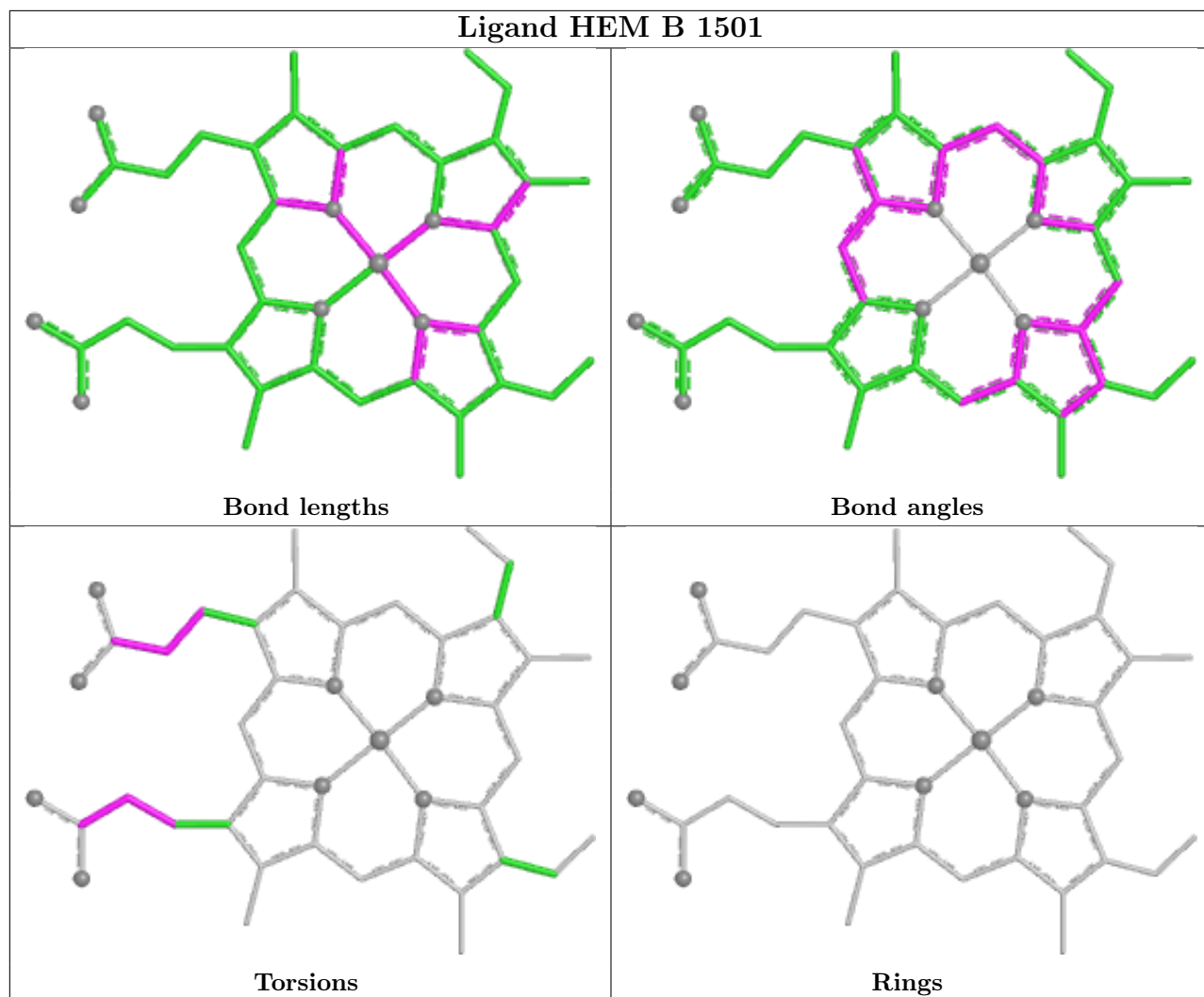
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1501	HEM	3	0
2	B	1501	HEM	5	0
2	B	1502	HEM	4	0
2	A	1502	HEM	2	0

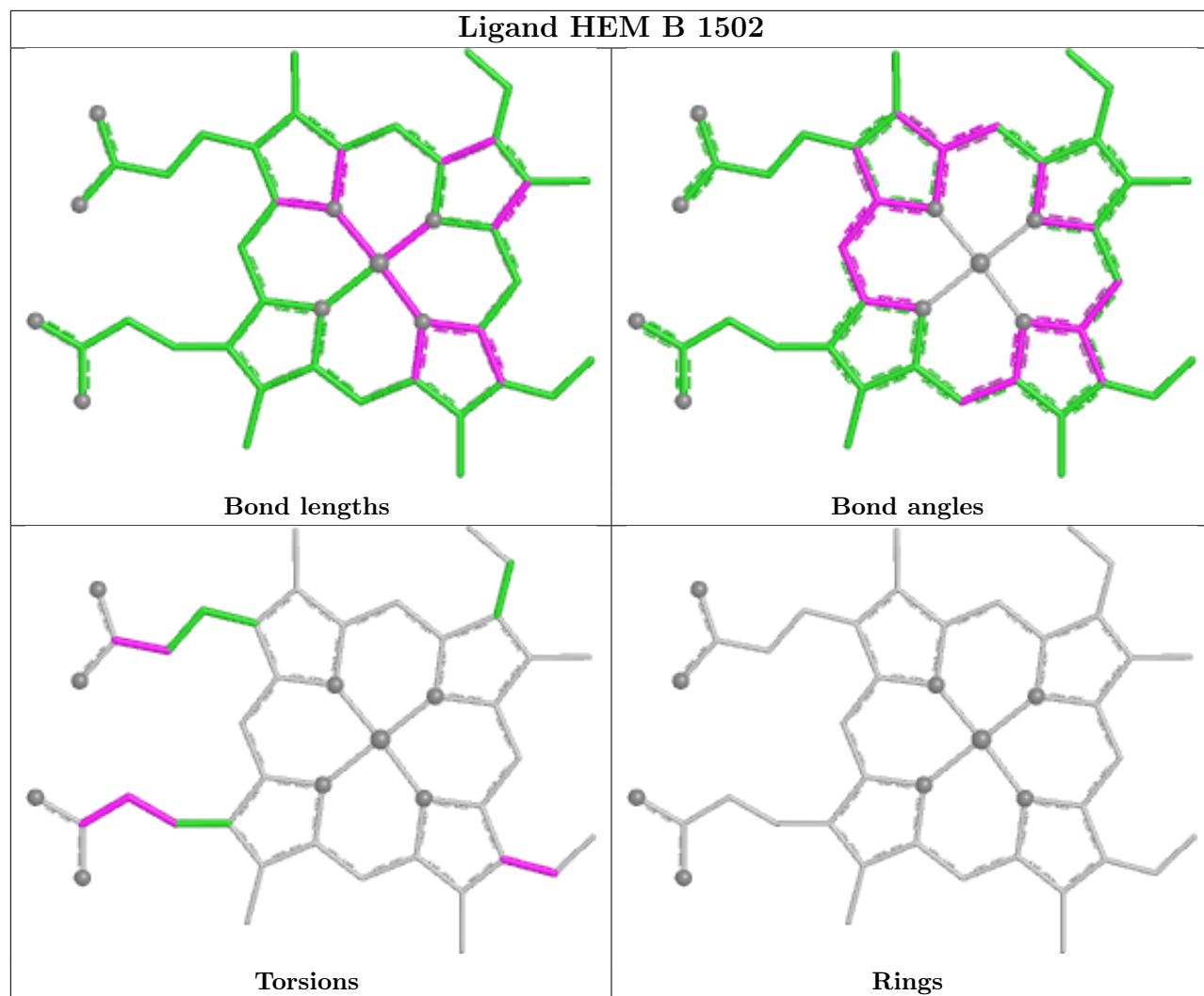
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

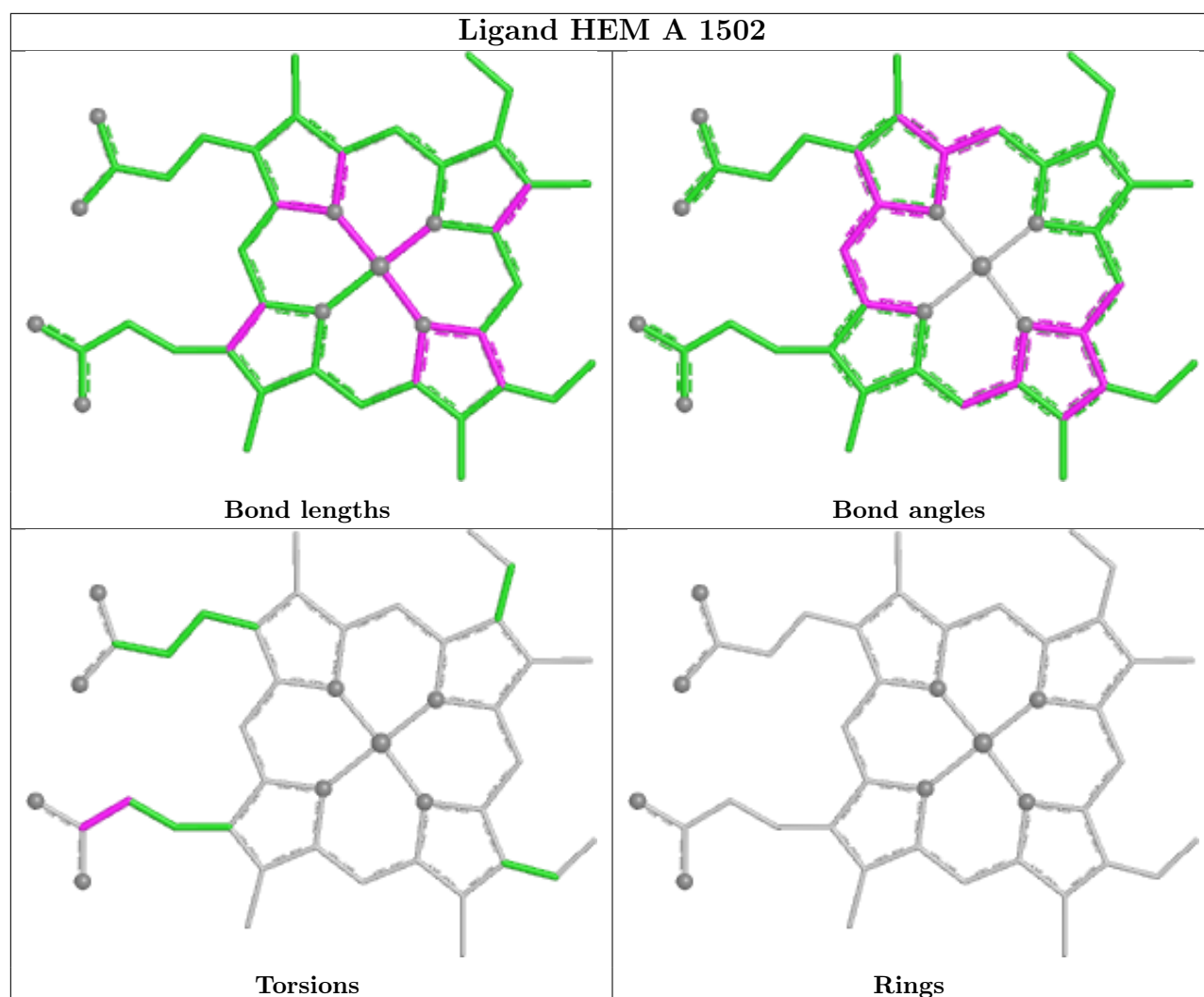












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

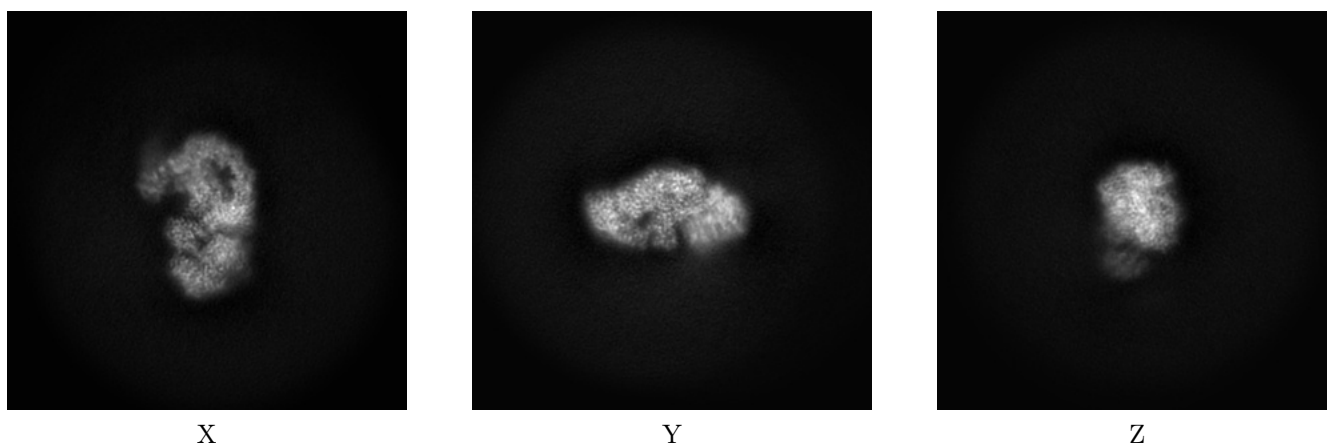
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72116. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 6.1 Orthogonal projections [i](#)

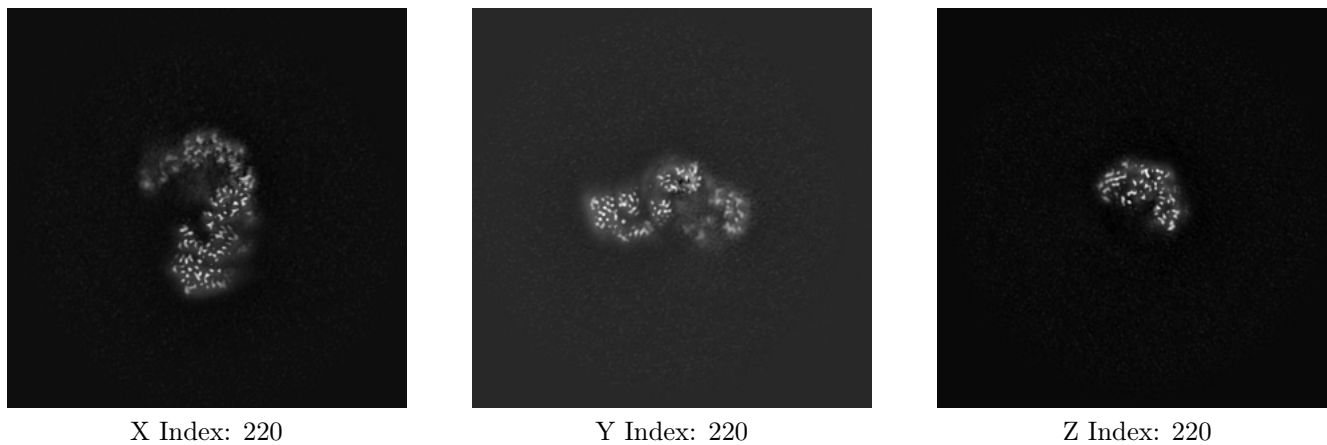
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

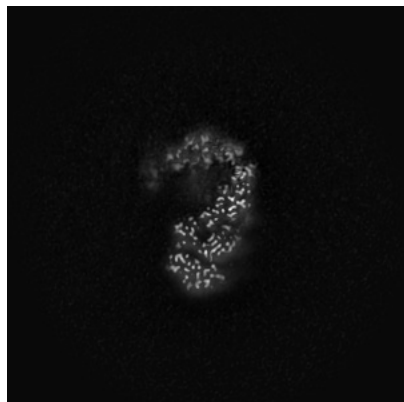
#### 6.2.1 Primary map



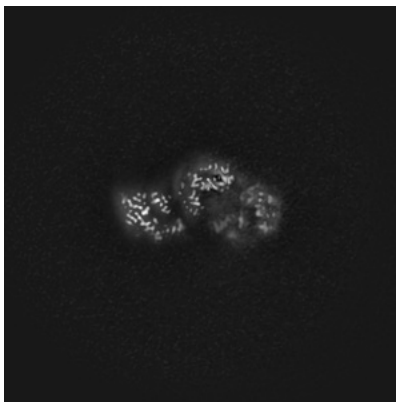
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

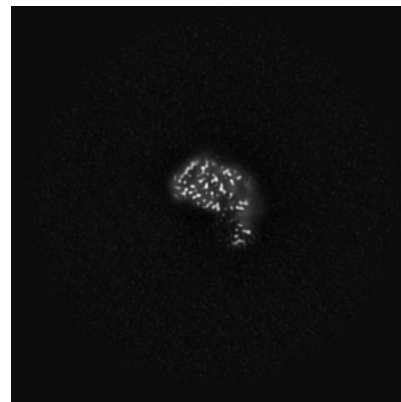
### 6.3.1 Primary map



X Index: 226



Y Index: 218

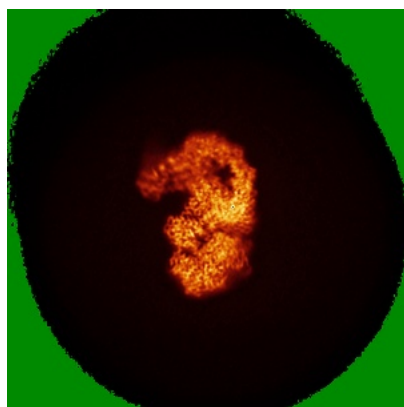


Z Index: 211

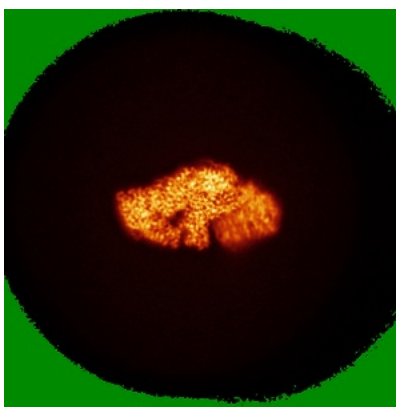
The images above show the largest variance slices of the map in three orthogonal directions.

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

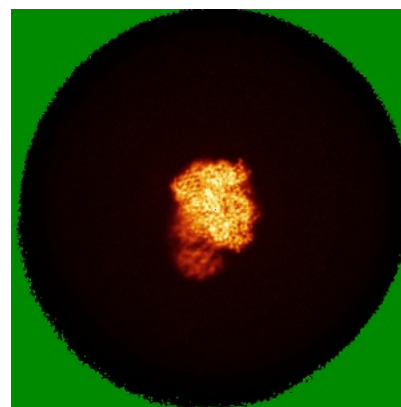
### 6.4.1 Primary map



X



Y

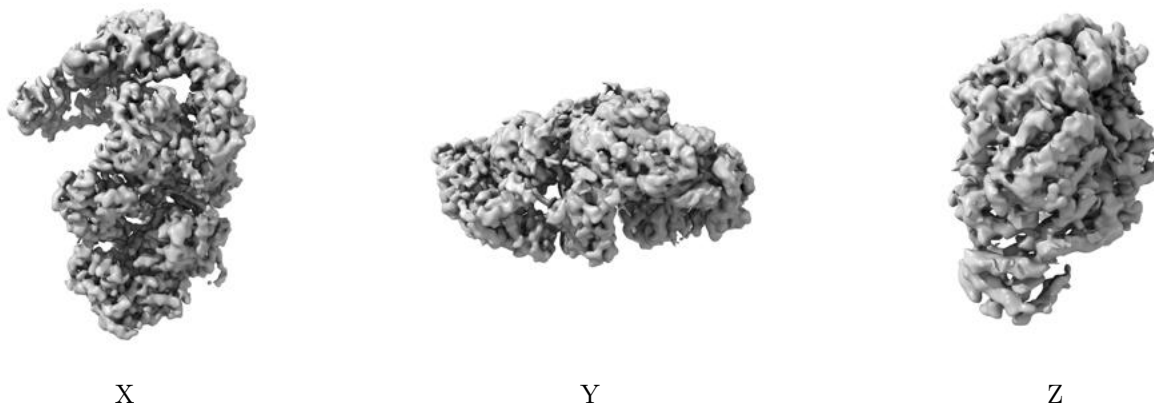


Z

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 0.0696. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

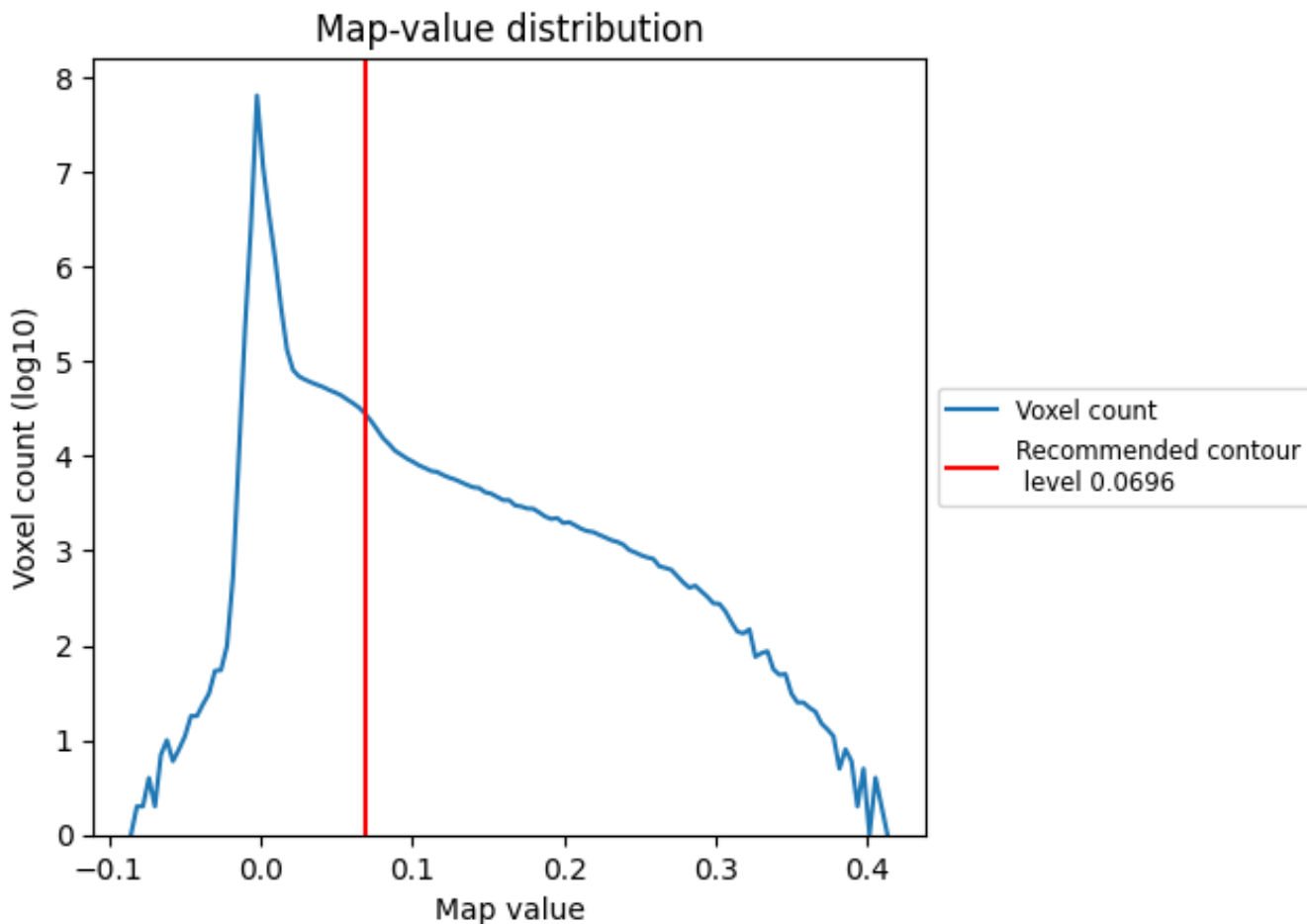
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

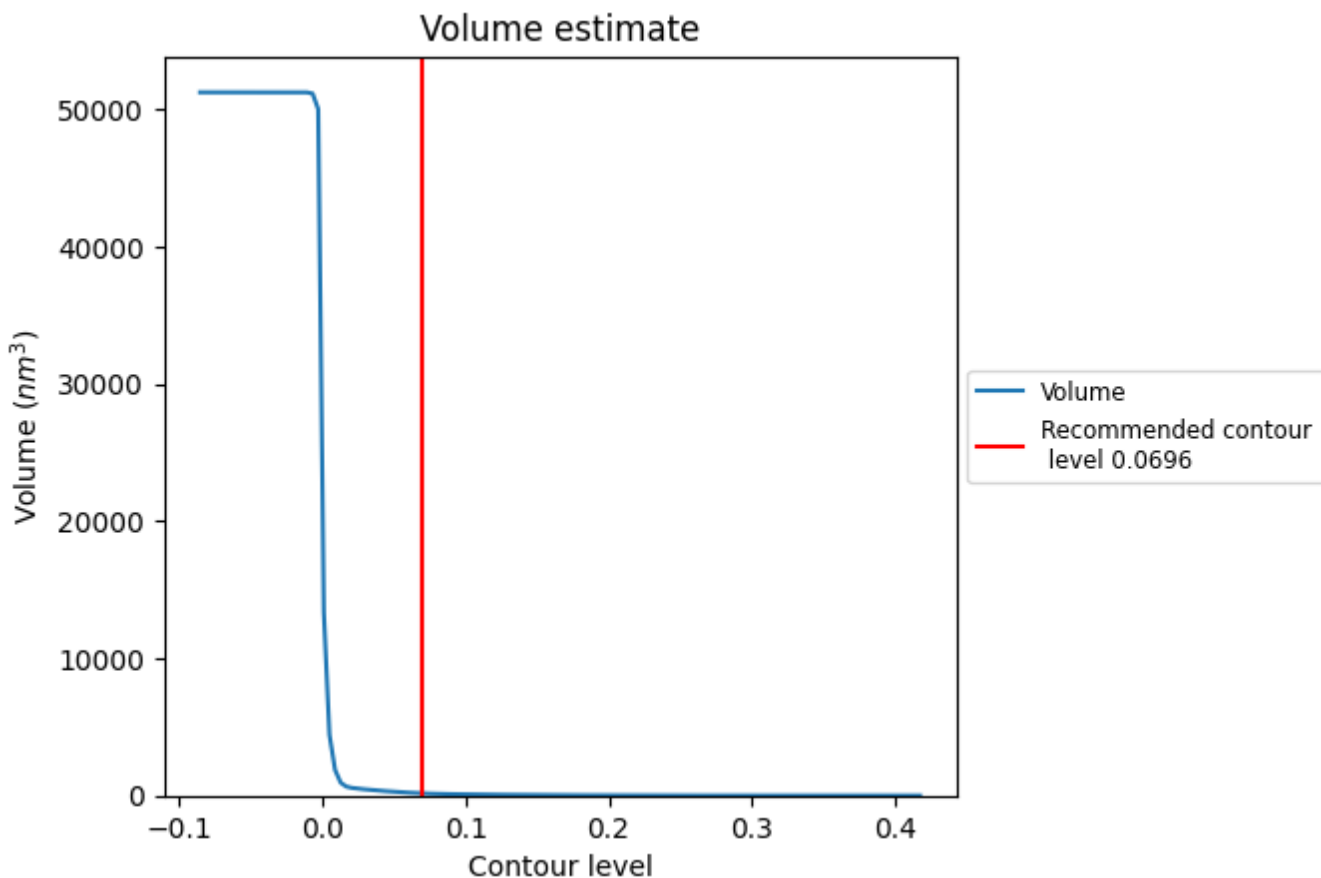
This section contains the results of statistical analysis of the map.

### 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.

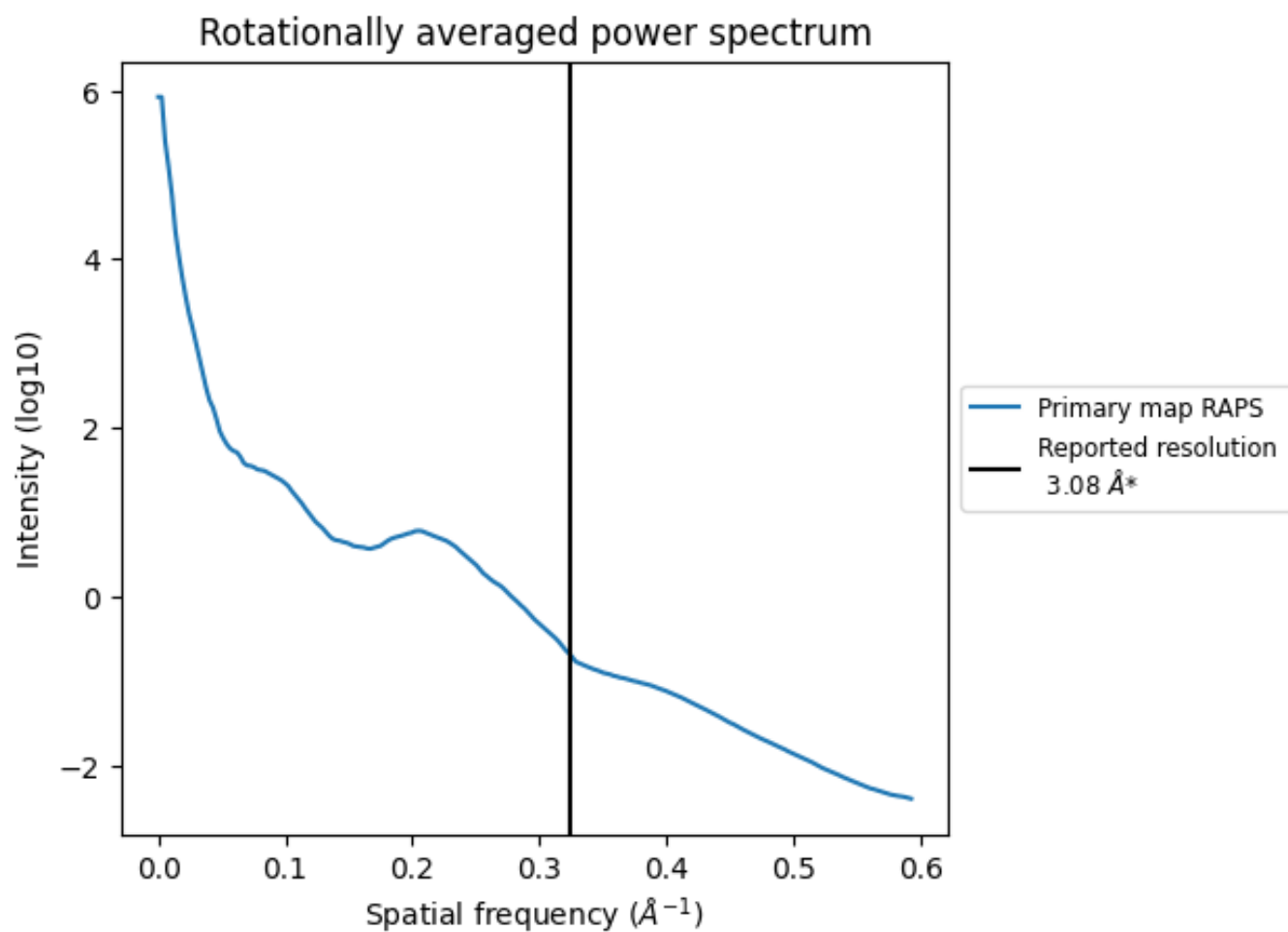
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 162 nm<sup>3</sup>; this corresponds to an approximate mass of 146 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  $0.325 \text{ \AA}^{-1}$

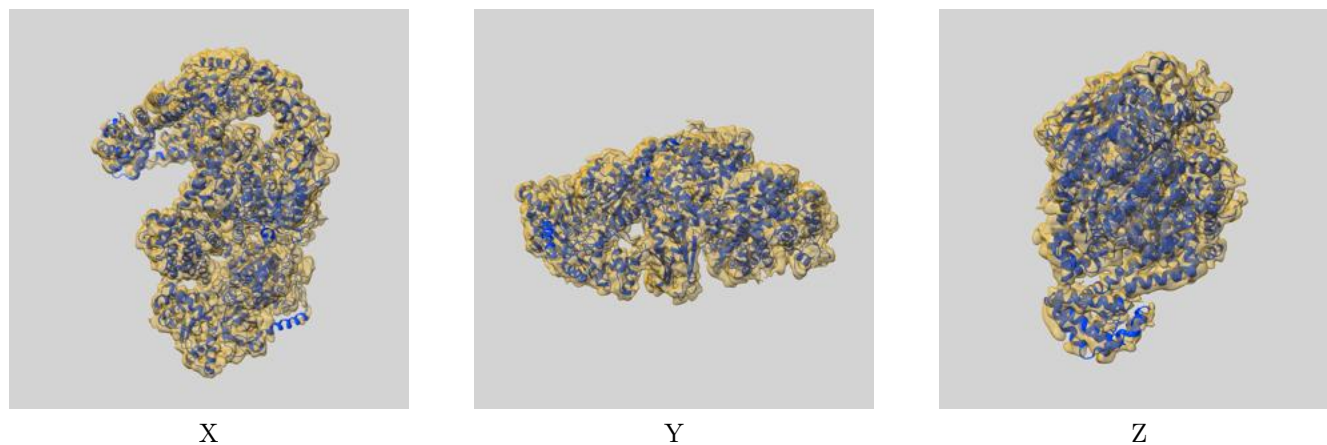
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72116 and PDB model 9Q15. Per-residue inclusion information can be found in section 3 on page 5.

### 9.1 Map-model overlay [i](#)



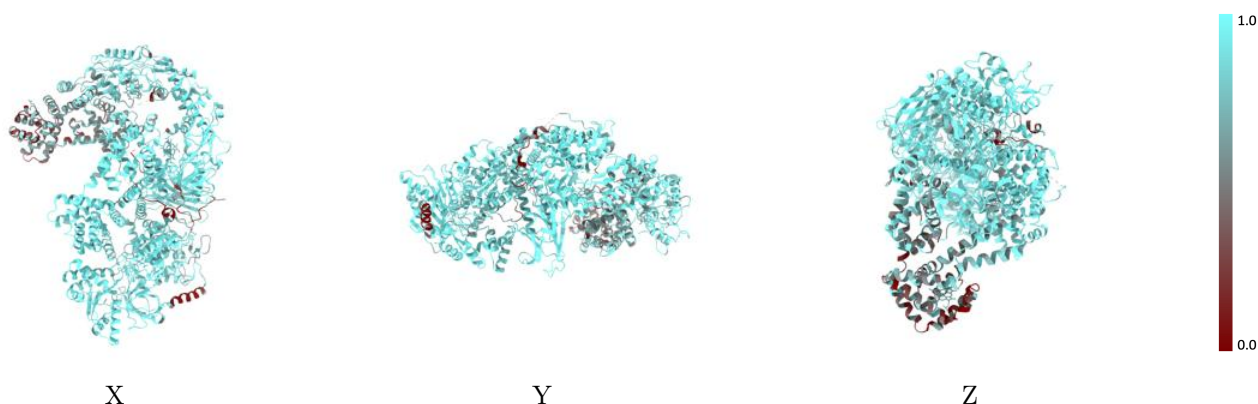
The images above show the 3D surface view of the map at the recommended contour level 0.0696 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



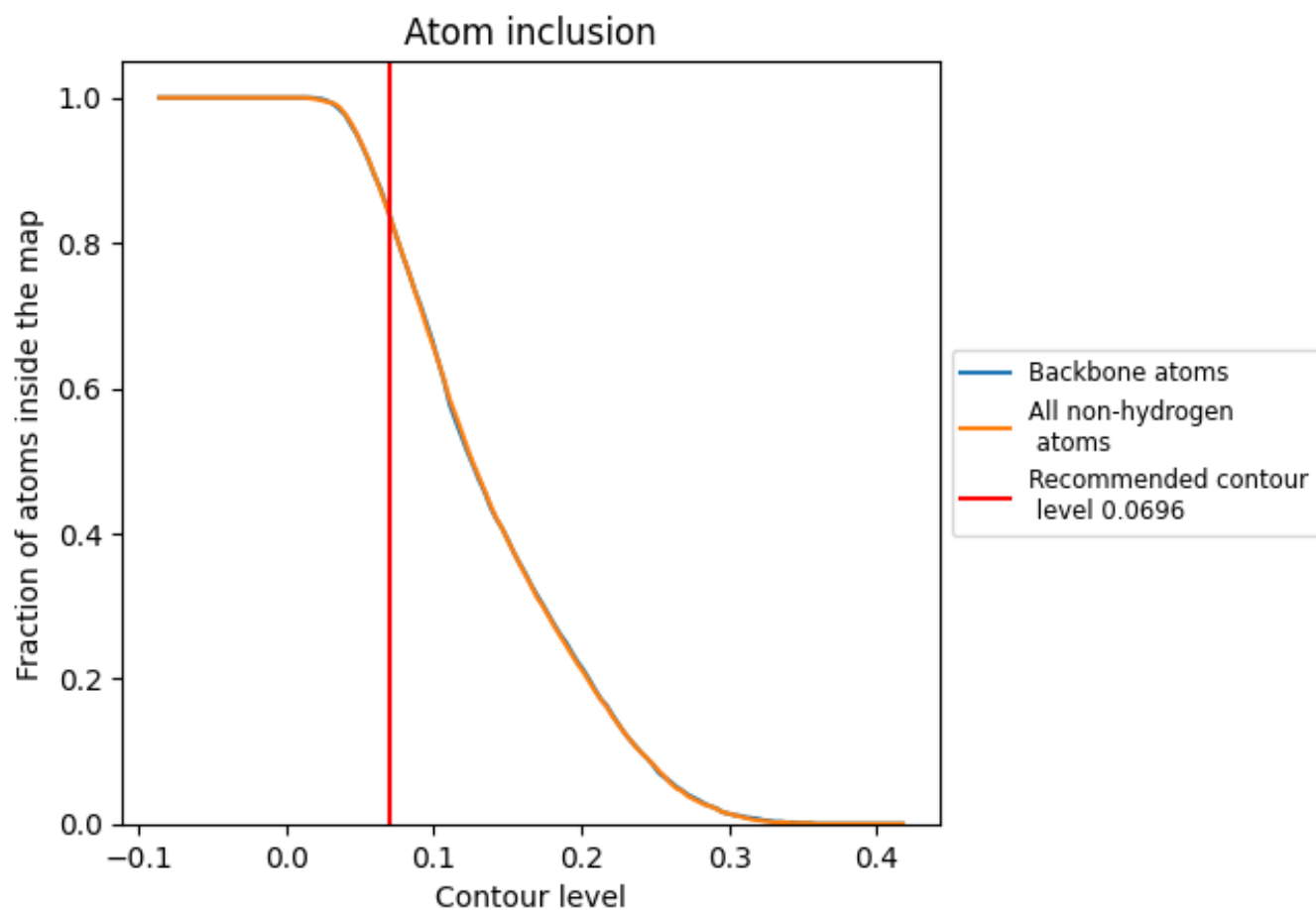
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0696).







## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.0696) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8410	 0.4100
A	 0.9060	 0.4770
B	 0.7030	 0.2620

