



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:58 PM UTC

PDB ID : 9Q06 / pdb_00009q06
EMDB ID : EMD-72088
Title : Symmetric Inactivated Locked State
Authors : Nair, D.; Xu, Y.; Crane, B.
Deposited on : 2025-08-12
Resolution : 3.90 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:

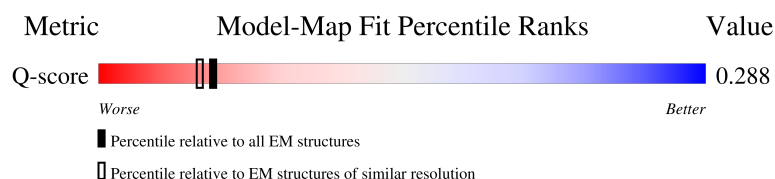
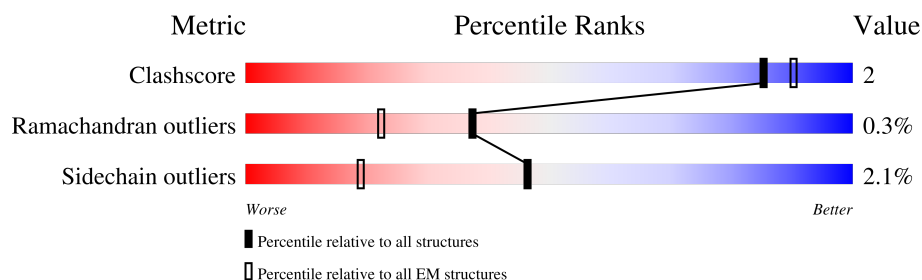
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.90 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	8855 (3.40 - 4.40)

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	
1	B	1468	

2 Entry composition [i](#)

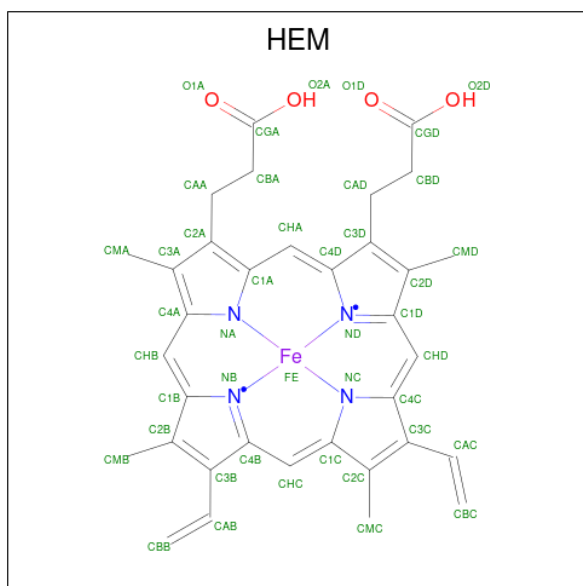
There are 4 unique types of molecules in this entry. The entry contains 44896 atoms, of which 22184 are hydrogens and 0 are deuteriums.

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 Ferredoxin–NADP reductase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1398	Total	C	H	N	O	S	0	0
			22168	7113	10982	1925	2096	52		
1	B	1398	Total	C	H	N	O	S	0	0
			22168	7113	10982	1925	2096	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).

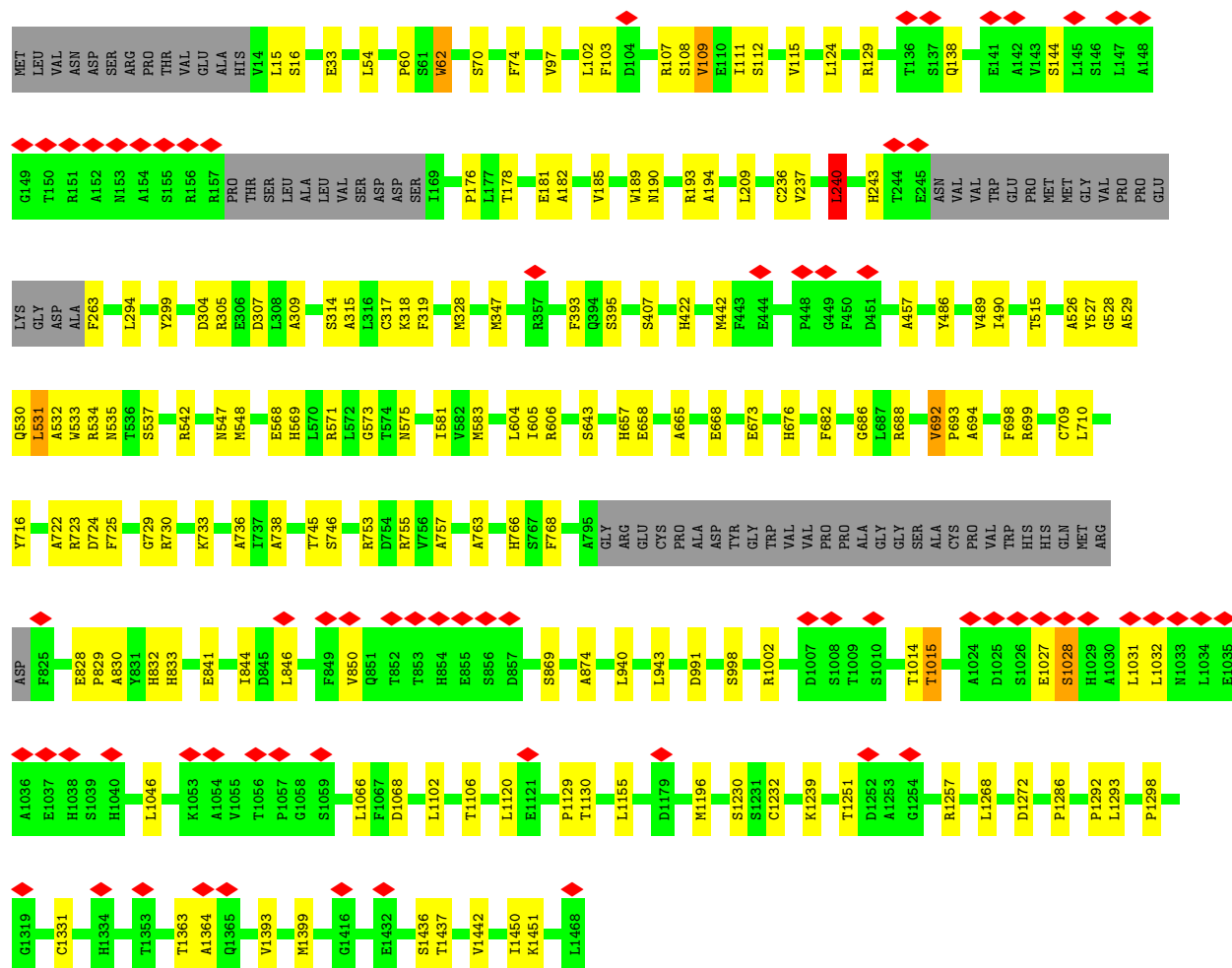


Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
2	A	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
2	B	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
2	B	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- # FAD

The chemical structure of FMN (Flavin Mononucleotide) is shown. It consists of an isoalloxazine ring system (a fused bicyclic system with two nitrogen atoms, N1 and N5) attached to a ribitol chain. The ribitol chain is a five-carbon chain (C1' to C5') with hydroxyl groups at C1', C2', C3', and C4'. The C5' carbon is attached to a phosphate group (O1P, O2P, O3P, O4P). The ribitol chain is shown in a chair conformation. The isoalloxazine ring system is shown in a planar conformation. The atoms are labeled with their respective element symbols and numbers: C1', C2', C3', C4', C5' for the ribitol chain; N1, N5 for the ring nitrogens; C8A, C9A, C10A, C4A, C5A for the ring carbons; O1P, O2P, O3P, O4P for the phosphate group; and O1, O2, O3, O4 for the ring oxygen atoms. The structure is drawn with standard chemical notation, including bond angles and atom labels.

Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	C	H	N	O	P	0
			50	17	19	4	9	1	
4	B	1	Total	C	H	N	O	P	0
			50	17	19	4	9	1	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	133978	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	0.727	Depositor
Minimum map value	-0.179	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.172	Depositor
Map size (Å)	377.27997, 377.27997, 377.27997	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	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, 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	1.06	66/11452 (0.6%)	1.04	106/15545 (0.7%)
1	B	1.06	66/11452 (0.6%)	1.04	106/15545 (0.7%)
All	All	1.06	132/22904 (0.6%)	1.04	212/31090 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	676	HIS	CE1-NE2	-8.73	1.23	1.32
1	B	676	HIS	CE1-NE2	-8.73	1.23	1.32
1	A	243	HIS	CE1-NE2	-8.68	1.23	1.32
1	B	243	HIS	CE1-NE2	-8.68	1.23	1.32
1	B	833	HIS	CE1-NE2	-8.65	1.23	1.32
1	A	569	HIS	CE1-NE2	-8.65	1.24	1.32
1	B	569	HIS	CE1-NE2	-8.65	1.24	1.32
1	A	766	HIS	CE1-NE2	-8.63	1.24	1.32
1	B	766	HIS	CE1-NE2	-8.62	1.24	1.32
1	B	832	HIS	ND1-CE1	-8.60	1.24	1.32
1	A	833	HIS	CE1-NE2	-8.59	1.24	1.32
1	A	832	HIS	ND1-CE1	-8.53	1.24	1.32
1	A	676	HIS	CD2-NE2	-7.99	1.29	1.37
1	B	676	HIS	CD2-NE2	-7.99	1.29	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	766	HIS	CD2-NE2	-7.92	1.29	1.37
1	B	766	HIS	CD2-NE2	-7.92	1.29	1.37
1	A	833	HIS	CD2-NE2	-7.87	1.29	1.37
1	A	569	HIS	CD2-NE2	-7.84	1.29	1.37
1	B	569	HIS	CD2-NE2	-7.84	1.29	1.37
1	A	193	ARG	CZ-NH2	-7.80	1.23	1.33
1	B	193	ARG	CZ-NH2	-7.80	1.23	1.33
1	A	571	ARG	CZ-NH2	-7.79	1.23	1.33
1	B	571	ARG	CZ-NH2	-7.79	1.23	1.33
1	B	730	ARG	CZ-NH2	-7.78	1.23	1.33
1	B	833	HIS	CD2-NE2	-7.78	1.29	1.37
1	A	606	ARG	CZ-NH2	-7.77	1.23	1.33
1	A	755	ARG	CZ-NH2	-7.77	1.23	1.33
1	B	606	ARG	CZ-NH2	-7.77	1.23	1.33
1	B	755	ARG	CZ-NH2	-7.75	1.23	1.33
1	A	107	ARG	CZ-NH2	-7.75	1.23	1.33
1	B	753	ARG	CZ-NH2	-7.74	1.23	1.33
1	B	243	HIS	CD2-NE2	-7.74	1.29	1.37
1	A	129	ARG	CZ-NH2	-7.73	1.23	1.33
1	B	129	ARG	CZ-NH2	-7.73	1.23	1.33
1	A	730	ARG	CZ-NH2	-7.71	1.23	1.33
1	B	107	ARG	CZ-NH2	-7.70	1.23	1.33
1	A	688	ARG	CZ-NH2	-7.70	1.23	1.33
1	B	688	ARG	CZ-NH2	-7.70	1.23	1.33
1	A	243	HIS	CD2-NE2	-7.70	1.29	1.37
1	A	305	ARG	CZ-NH2	-7.68	1.23	1.33
1	B	305	ARG	CZ-NH2	-7.68	1.23	1.33
1	A	753	ARG	CZ-NH2	-7.68	1.23	1.33
1	A	699	ARG	CZ-NH2	-7.67	1.23	1.33
1	B	699	ARG	CZ-NH2	-7.67	1.23	1.33
1	B	723	ARG	CZ-NH2	-7.67	1.23	1.33
1	A	723	ARG	CZ-NH2	-7.67	1.23	1.33
1	B	529	ALA	CA-CB	-6.48	1.43	1.53
1	A	529	ALA	CA-CB	-6.46	1.43	1.53
1	A	532	ALA	CA-CB	-6.46	1.43	1.53
1	B	532	ALA	CA-CB	-6.46	1.43	1.53
1	A	763	ALA	CA-CB	-6.45	1.43	1.53
1	A	757	ALA	CA-CB	-6.45	1.43	1.53
1	B	722	ALA	CA-CB	-6.45	1.43	1.53
1	B	757	ALA	CA-CB	-6.45	1.43	1.53
1	B	763	ALA	CA-CB	-6.44	1.43	1.53
1	A	526	ALA	CA-CB	-6.42	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	526	ALA	CA-CB	-6.42	1.43	1.53
1	A	722	ALA	CA-CB	-6.41	1.43	1.53
1	A	182	ALA	CA-CB	-6.41	1.43	1.53
1	B	182	ALA	CA-CB	-6.41	1.43	1.53
1	A	315	ALA	CA-CB	-6.33	1.43	1.53
1	A	738	ALA	CA-CB	-6.33	1.43	1.53
1	A	194	ALA	CA-CB	-6.32	1.43	1.53
1	B	194	ALA	CA-CB	-6.32	1.43	1.53
1	B	738	ALA	CA-CB	-6.31	1.43	1.53
1	B	730	ARG	CZ-NH1	-6.28	1.24	1.32
1	A	606	ARG	CZ-NH1	-6.28	1.24	1.32
1	B	606	ARG	CZ-NH1	-6.28	1.24	1.32
1	B	315	ALA	CA-CB	-6.27	1.43	1.53
1	A	730	ARG	CZ-NH1	-6.27	1.24	1.32
1	A	107	ARG	CZ-NH1	-6.24	1.24	1.32
1	B	107	ARG	CZ-NH1	-6.24	1.24	1.32
1	A	699	ARG	CZ-NH1	-6.23	1.24	1.32
1	A	129	ARG	CZ-NH1	-6.21	1.24	1.32
1	A	193	ARG	CZ-NH1	-6.19	1.24	1.32
1	A	665	ALA	CA-CB	-6.19	1.43	1.53
1	B	129	ARG	CZ-NH1	-6.19	1.24	1.32
1	B	193	ARG	CZ-NH1	-6.19	1.24	1.32
1	B	699	ARG	CZ-NH1	-6.18	1.24	1.32
1	A	571	ARG	CZ-NH1	-6.17	1.24	1.32
1	B	571	ARG	CZ-NH1	-6.17	1.24	1.32
1	A	305	ARG	CZ-NH1	-6.16	1.24	1.32
1	B	305	ARG	CZ-NH1	-6.16	1.24	1.32
1	A	688	ARG	CZ-NH1	-6.16	1.24	1.32
1	B	688	ARG	CZ-NH1	-6.16	1.24	1.32
1	A	755	ARG	CZ-NH1	-6.15	1.24	1.32
1	B	723	ARG	CZ-NH1	-6.15	1.24	1.32
1	B	755	ARG	CZ-NH1	-6.15	1.24	1.32
1	A	753	ARG	CZ-NH1	-6.14	1.24	1.32
1	B	665	ALA	CA-CB	-6.14	1.43	1.53
1	B	753	ARG	CZ-NH1	-6.14	1.24	1.32
1	A	573	GLY	N-CA	-6.13	1.38	1.45
1	A	723	ARG	CZ-NH1	-6.12	1.24	1.32
1	B	573	GLY	N-CA	-6.12	1.38	1.45
1	B	830	ALA	CA-CB	-6.10	1.43	1.53
1	A	830	ALA	CA-CB	-6.10	1.43	1.53
1	B	528	GLY	N-CA	-6.06	1.38	1.45
1	A	528	GLY	N-CA	-5.98	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	693	PRO	CA-CB	-5.91	1.46	1.53
1	B	693	PRO	CA-CB	-5.91	1.46	1.53
1	B	309	ALA	CA-CB	-5.90	1.43	1.53
1	A	309	ALA	CA-CB	-5.84	1.43	1.53
1	B	730	ARG	CD-NE	-5.46	1.38	1.46
1	B	688	ARG	CD-NE	-5.42	1.38	1.46
1	A	688	ARG	CD-NE	-5.42	1.38	1.46
1	A	730	ARG	CD-NE	-5.40	1.38	1.46
1	A	305	ARG	CD-NE	-5.36	1.38	1.46
1	A	692	VAL	N-CA	-5.36	1.42	1.46
1	B	305	ARG	CD-NE	-5.36	1.38	1.46
1	B	692	VAL	N-CA	-5.36	1.42	1.46
1	B	606	ARG	CD-NE	-5.34	1.38	1.46
1	A	193	ARG	CD-NE	-5.32	1.38	1.46
1	A	606	ARG	CD-NE	-5.32	1.38	1.46
1	B	107	ARG	CD-NE	-5.31	1.38	1.46
1	B	193	ARG	CD-NE	-5.29	1.38	1.46
1	A	753	ARG	CD-NE	-5.28	1.38	1.46
1	B	753	ARG	CD-NE	-5.28	1.38	1.46
1	A	107	ARG	CD-NE	-5.26	1.38	1.46
1	A	699	ARG	CD-NE	-5.25	1.38	1.46
1	B	699	ARG	CD-NE	-5.25	1.38	1.46
1	A	723	ARG	CD-NE	-5.20	1.39	1.46
1	B	723	ARG	CD-NE	-5.16	1.39	1.46
1	A	571	ARG	CD-NE	-5.16	1.39	1.46
1	B	571	ARG	CD-NE	-5.16	1.39	1.46
1	A	294	LEU	CA-CB	-5.14	1.47	1.53
1	A	129	ARG	CD-NE	-5.13	1.39	1.46
1	B	129	ARG	CD-NE	-5.13	1.39	1.46
1	B	755	ARG	CD-NE	-5.10	1.39	1.46
1	A	755	ARG	CD-NE	-5.09	1.39	1.46
1	B	294	LEU	CA-CB	-5.07	1.47	1.53
1	A	686	GLY	N-CA	-5.00	1.38	1.45
1	B	686	GLY	N-CA	-5.00	1.38	1.45

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	682	PHE	CA-CB-CG	7.38	121.19	113.80
1	A	682	PHE	CA-CB-CG	7.36	121.16	113.80
1	B	190	ASN	CA-CB-CG	7.33	119.93	112.60
1	A	190	ASN	CA-CB-CG	7.30	119.90	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	698	PHE	CA-CB-CG	7.17	120.97	113.80
1	B	698	PHE	CA-CB-CG	7.16	120.96	113.80
1	A	725	PHE	CA-CB-CG	7.07	120.87	113.80
1	B	725	PHE	CA-CB-CG	7.07	120.87	113.80
1	B	724	ASP	CA-CB-CG	6.87	119.47	112.60
1	A	724	ASP	CA-CB-CG	6.87	119.47	112.60
1	A	676	HIS	CA-CB-CG	6.86	120.66	113.80
1	B	676	HIS	CA-CB-CG	6.83	120.63	113.80
1	B	535	ASN	CA-CB-CG	6.79	119.39	112.60
1	A	535	ASN	CA-CB-CG	6.76	119.36	112.60
1	A	569	HIS	CA-CB-CG	6.67	120.47	113.80
1	A	575	ASN	CA-CB-CG	6.63	119.23	112.60
1	B	569	HIS	CA-CB-CG	6.62	120.42	113.80
1	B	575	ASN	CA-CB-CG	6.61	119.21	112.60
1	A	547	ASN	CA-CB-CG	6.54	119.14	112.60
1	B	547	ASN	CA-CB-CG	6.51	119.11	112.60
1	A	832	HIS	CA-CB-CG	6.50	120.30	113.80
1	B	833	HIS	CA-CB-CG	6.49	120.29	113.80
1	B	832	HIS	CA-CB-CG	6.47	120.28	113.80
1	A	833	HIS	CA-CB-CG	6.46	120.25	113.80
1	A	548	MET	CA-C-N	6.33	130.80	122.95
1	A	548	MET	C-N-CA	6.33	130.80	122.95
1	B	548	MET	CA-C-N	6.32	130.78	122.95
1	B	548	MET	C-N-CA	6.32	130.78	122.95
1	A	307	ASP	CA-CB-CG	6.23	118.83	112.60
1	B	307	ASP	CA-CB-CG	6.23	118.83	112.60
1	B	725	PHE	CA-C-N	5.99	128.23	120.44
1	B	725	PHE	C-N-CA	5.99	128.23	120.44
1	B	108	SER	CA-C-N	5.99	130.82	123.10
1	B	108	SER	C-N-CA	5.99	130.82	123.10
1	A	108	SER	CA-C-N	5.96	130.79	123.10
1	A	108	SER	C-N-CA	5.96	130.79	123.10
1	A	725	PHE	CA-C-N	5.96	128.19	120.44
1	A	725	PHE	C-N-CA	5.96	128.19	120.44
1	A	755	ARG	CD-NE-CZ	5.90	132.66	124.40
1	B	755	ARG	CD-NE-CZ	5.90	132.66	124.40
1	B	571	ARG	CD-NE-CZ	5.89	132.65	124.40
1	A	571	ARG	CD-NE-CZ	5.88	132.62	124.40
1	B	729	GLY	CA-C-N	5.87	129.86	121.71
1	B	729	GLY	C-N-CA	5.87	129.86	121.71
1	A	129	ARG	CD-NE-CZ	5.86	132.61	124.40
1	A	729	GLY	CA-C-N	5.85	129.84	121.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	729	GLY	C-N-CA	5.85	129.84	121.71
1	B	129	ARG	CD-NE-CZ	5.84	132.58	124.40
1	A	583	MET	CA-C-N	5.80	130.37	122.19
1	A	583	MET	C-N-CA	5.80	130.37	122.19
1	B	583	MET	CA-C-N	5.80	130.37	122.19
1	B	583	MET	C-N-CA	5.80	130.37	122.19
1	A	668	GLU	CA-C-N	5.76	129.80	122.37
1	A	668	GLU	C-N-CA	5.76	129.80	122.37
1	A	766	HIS	CA-CB-CG	5.73	119.53	113.80
1	B	668	GLU	CA-C-N	5.73	129.77	122.37
1	B	668	GLU	C-N-CA	5.73	129.77	122.37
1	B	766	HIS	CA-CB-CG	5.73	119.53	113.80
1	A	568	GLU	CA-C-N	5.67	127.82	120.44
1	A	568	GLU	C-N-CA	5.67	127.82	120.44
1	A	304	ASP	CA-C-N	5.65	127.79	120.44
1	A	304	ASP	C-N-CA	5.65	127.79	120.44
1	A	486	TYR	N-CA-CB	5.65	118.21	110.01
1	B	489	VAL	N-CA-CB	5.63	116.54	110.62
1	B	534	ARG	NE-CZ-NH2	5.63	124.27	119.20
1	B	486	TYR	N-CA-CB	5.63	118.18	110.01
1	B	568	GLU	CA-C-N	5.63	127.76	120.44
1	B	568	GLU	C-N-CA	5.63	127.76	120.44
1	A	489	VAL	N-CA-CB	5.63	116.53	110.62
1	A	604	LEU	CA-C-N	5.61	130.65	123.13
1	A	604	LEU	C-N-CA	5.61	130.65	123.13
1	B	604	LEU	CA-C-N	5.61	130.65	123.13
1	B	604	LEU	C-N-CA	5.61	130.65	123.13
1	A	723	ARG	CD-NE-CZ	5.56	132.19	124.40
1	A	534	ARG	NE-CZ-NH2	5.56	124.20	119.20
1	A	490	ILE	N-CA-CB	5.56	117.05	110.55
1	B	304	ASP	CA-C-N	5.55	127.65	120.44
1	B	304	ASP	C-N-CA	5.55	127.65	120.44
1	B	723	ARG	CD-NE-CZ	5.54	132.16	124.40
1	B	62	TRP	CA-C-N	5.53	130.78	123.05
1	B	62	TRP	C-N-CA	5.53	130.78	123.05
1	A	62	TRP	CA-C-N	5.52	130.78	123.05
1	A	62	TRP	C-N-CA	5.52	130.78	123.05
1	B	490	ILE	N-CA-CB	5.50	116.98	110.55
1	B	299	TYR	CA-C-N	5.46	130.26	122.72
1	B	299	TYR	C-N-CA	5.46	130.26	122.72
1	B	746	SER	CA-C-N	5.43	129.59	121.72
1	B	746	SER	C-N-CA	5.43	129.59	121.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	746	SER	CA-C-N	5.42	129.58	121.72
1	A	746	SER	C-N-CA	5.42	129.58	121.72
1	A	299	TYR	CA-C-N	5.42	130.20	122.72
1	A	299	TYR	C-N-CA	5.42	130.20	122.72
1	B	185	VAL	N-CA-CB	5.41	116.52	110.51
1	A	60	PRO	CA-C-N	5.40	129.61	121.40
1	A	60	PRO	C-N-CA	5.40	129.61	121.40
1	A	185	VAL	N-CA-CB	5.39	116.49	110.51
1	B	60	PRO	CA-C-N	5.36	129.55	121.40
1	B	60	PRO	C-N-CA	5.36	129.55	121.40
1	B	694	ALA	CA-C-N	5.36	127.69	120.50
1	B	694	ALA	C-N-CA	5.36	127.69	120.50
1	A	533	TRP	N-CA-CB	5.34	117.97	110.12
1	A	694	ALA	CA-C-N	5.34	127.65	120.50
1	A	694	ALA	C-N-CA	5.34	127.65	120.50
1	B	533	TRP	N-CA-CB	5.34	117.96	110.12
1	A	736	ALA	CA-C-N	5.33	127.28	120.56
1	A	736	ALA	C-N-CA	5.33	127.28	120.56
1	A	530	GLN	CA-C-N	5.33	127.37	120.44
1	A	530	GLN	C-N-CA	5.33	127.37	120.44
1	B	530	GLN	CA-C-N	5.33	127.37	120.44
1	B	530	GLN	C-N-CA	5.33	127.37	120.44
1	B	736	ALA	CA-C-N	5.33	127.27	120.56
1	B	736	ALA	C-N-CA	5.33	127.27	120.56
1	A	319	PHE	CA-CB-CG	5.33	119.13	113.80
1	A	682	PHE	CA-C-N	5.32	128.40	120.31
1	A	682	PHE	C-N-CA	5.32	128.40	120.31
1	B	319	PHE	CA-CB-CG	5.32	119.12	113.80
1	B	682	PHE	CA-C-N	5.31	128.39	120.31
1	B	682	PHE	C-N-CA	5.31	128.39	120.31
1	A	733	LYS	CA-C-N	5.31	127.34	120.44
1	A	733	LYS	C-N-CA	5.31	127.34	120.44
1	B	733	LYS	CA-C-N	5.28	127.31	120.44
1	B	733	LYS	C-N-CA	5.28	127.31	120.44
1	B	548	MET	N-CA-CB	5.28	117.76	109.69
1	B	176	PRO	CA-C-N	5.26	129.60	122.19
1	B	176	PRO	C-N-CA	5.26	129.60	122.19
1	A	176	PRO	CA-C-N	5.25	129.60	122.19
1	A	176	PRO	C-N-CA	5.25	129.60	122.19
1	B	832	HIS	CE1-NE2-CD2	-5.25	103.75	109.00
1	A	548	MET	N-CA-CB	5.24	117.70	109.69
1	A	753	ARG	CA-CB-CG	5.23	124.56	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	VAL	CA-C-N	5.23	131.02	123.13
1	B	109	VAL	C-N-CA	5.23	131.02	123.13
1	A	317	CYS	N-CA-CB	5.22	117.58	110.01
1	A	109	VAL	CA-C-N	5.22	131.01	123.13
1	A	109	VAL	C-N-CA	5.22	131.01	123.13
1	A	752	TRP	CA-C-N	5.21	127.58	120.54
1	A	752	TRP	C-N-CA	5.21	127.58	120.54
1	B	317	CYS	N-CA-CB	5.21	117.57	110.01
1	A	189	TRP	N-CA-CB	5.21	117.57	110.01
1	B	189	TRP	N-CA-CB	5.21	117.57	110.01
1	B	753	ARG	CA-CB-CG	5.21	124.52	114.10
1	A	832	HIS	CE1-NE2-CD2	-5.21	103.80	109.00
1	A	698	PHE	CA-C-N	5.20	130.87	122.29
1	A	698	PHE	C-N-CA	5.20	130.87	122.29
1	B	698	PHE	CA-C-N	5.20	130.87	122.29
1	B	698	PHE	C-N-CA	5.20	130.87	122.29
1	A	571	ARG	CA-CB-CG	5.19	124.47	114.10
1	B	571	ARG	CA-CB-CG	5.19	124.47	114.10
1	A	581	ILE	CA-C-N	5.18	128.91	121.96
1	A	581	ILE	C-N-CA	5.18	128.91	121.96
1	B	307	ASP	N-CA-CB	5.18	117.52	110.01
1	B	307	ASP	CA-C-N	5.18	127.74	120.28
1	B	307	ASP	C-N-CA	5.18	127.74	120.28
1	A	237	VAL	N-CA-CB	5.18	116.61	110.55
1	B	237	VAL	N-CA-CB	5.18	116.61	110.55
1	B	581	ILE	CA-C-N	5.18	128.90	121.96
1	B	581	ILE	C-N-CA	5.18	128.90	121.96
1	B	755	ARG	CA-C-N	5.17	127.07	120.56
1	B	755	ARG	C-N-CA	5.17	127.07	120.56
1	A	307	ASP	N-CA-CB	5.17	117.50	110.01
1	A	236	CYS	CA-C-N	5.16	127.06	120.56
1	A	236	CYS	C-N-CA	5.16	127.06	120.56
1	B	236	CYS	CA-C-N	5.16	127.06	120.56
1	B	236	CYS	C-N-CA	5.16	127.06	120.56
1	B	317	CYS	CA-C-N	5.16	127.15	120.44
1	B	317	CYS	C-N-CA	5.16	127.15	120.44
1	A	181	GLU	CA-C-N	5.16	127.14	120.44
1	A	181	GLU	C-N-CA	5.16	127.14	120.44
1	A	317	CYS	CA-C-N	5.16	127.14	120.44
1	A	317	CYS	C-N-CA	5.16	127.14	120.44
1	A	307	ASP	CA-C-N	5.15	127.70	120.28
1	A	307	ASP	C-N-CA	5.15	127.70	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	673	GLU	CA-C-N	5.14	128.06	120.91
1	A	673	GLU	C-N-CA	5.14	128.06	120.91
1	B	673	GLU	CA-C-N	5.14	128.06	120.91
1	B	673	GLU	C-N-CA	5.14	128.06	120.91
1	A	755	ARG	CA-C-N	5.14	127.04	120.56
1	A	755	ARG	C-N-CA	5.14	127.04	120.56
1	A	314	SER	N-CA-CB	5.14	117.59	110.04
1	B	181	GLU	CA-C-N	5.13	127.11	120.44
1	B	181	GLU	C-N-CA	5.13	127.11	120.44
1	B	314	SER	N-CA-CB	5.11	117.56	110.04
1	A	531	LEU	CA-C-N	5.11	127.08	120.44
1	A	531	LEU	C-N-CA	5.11	127.08	120.44
1	B	527	TYR	N-CA-CB	5.10	117.62	110.12
1	A	527	TYR	N-CA-CB	5.09	117.60	110.12
1	B	240	LEU	CA-C-N	5.09	127.71	120.49
1	B	240	LEU	C-N-CA	5.09	127.71	120.49
1	B	531	LEU	CA-C-N	5.09	127.05	120.44
1	B	531	LEU	C-N-CA	5.09	127.05	120.44
1	A	832	HIS	ND1-CG-CD2	-5.07	101.03	106.10
1	A	240	LEU	CA-C-N	5.07	127.68	120.49
1	A	240	LEU	C-N-CA	5.07	127.68	120.49
1	B	537	SER	CA-C-N	5.07	127.33	120.44
1	B	537	SER	C-N-CA	5.07	127.33	120.44
1	A	755	ARG	N-CA-CB	5.06	117.48	109.94
1	B	318	LYS	CA-C-N	5.06	127.01	120.44
1	B	318	LYS	C-N-CA	5.06	127.01	120.44
1	A	318	LYS	CA-C-N	5.05	127.01	120.44
1	A	318	LYS	C-N-CA	5.05	127.01	120.44
1	B	305	ARG	CA-C-N	5.05	127.01	120.44
1	B	305	ARG	C-N-CA	5.05	127.01	120.44
1	B	832	HIS	ND1-CG-CD2	-5.05	101.05	106.10
1	A	305	ARG	CA-C-N	5.05	127.00	120.44
1	A	305	ARG	C-N-CA	5.05	127.00	120.44
1	A	832	HIS	CG-CD2-NE2	5.05	112.25	107.20
1	B	832	HIS	CG-CD2-NE2	5.04	112.24	107.20
1	B	185	VAL	CA-C-N	5.03	126.98	120.44
1	B	185	VAL	C-N-CA	5.03	126.98	120.44
1	B	755	ARG	N-CA-CB	5.03	117.43	109.94
1	A	185	VAL	CA-C-N	5.00	126.94	120.44
1	A	185	VAL	C-N-CA	5.00	126.94	120.44

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	716	TYR	Sidechain
1	B	716	TYR	Sidechain

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	11186	10982	10978	50	0
1	B	11186	10982	10978	45	0
2	A	86	60	60	1	0
2	B	86	60	60	1	0
3	A	53	31	31	0	0
3	B	53	31	31	0	0
4	A	31	19	19	1	0
4	B	31	19	19	1	0
All	All	22712	22184	22176	97	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 2.

All (97) 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:940:LEU:HD13	1:B:943:LEU:HD23	1.66	0.77
1:A:940:LEU:HD13	1:A:943:LEU:HD23	1.66	0.75
1:A:1031:LEU:HD13	1:A:1130:THR:HA	1.73	0.69
1:B:1031:LEU:HD13	1:B:1130:THR:HA	1.73	0.69
1:A:710:LEU:HD12	1:A:710:LEU:O	1.98	0.64
1:B:710:LEU:O	1:B:710:LEU:HD12	1.98	0.64
1:A:940:LEU:CD1	1:A:943:LEU:HD23	2.28	0.63
1:B:115:VAL:HG23	1:B:124:LEU:HD23	1.81	0.63
1:B:347:MET:HE3	1:B:457:ALA:HB1	1.82	0.62
1:B:940:LEU:CD1	1:B:943:LEU:HD23	2.28	0.62
1:B:1196:MET:HE3	1:B:1257:ARG:HB2	1.83	0.61
1:A:115:VAL:HG23	1:A:124:LEU:HD23	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:MET:HE3	1:A:457:ALA:HB1	1.82	0.60
1:A:1196:MET:HE3	1:A:1257:ARG:HB2	1.83	0.59
1:B:209:LEU:CD2	1:B:844:ILE:HD13	2.33	0.59
1:A:209:LEU:CD2	1:A:844:ILE:HD13	2.33	0.58
1:B:347:MET:CE	1:B:457:ALA:HB1	2.33	0.58
1:A:347:MET:CE	1:A:457:ALA:HB1	2.34	0.57
1:A:54:LEU:HD23	1:A:62:TRP:CG	2.42	0.55
1:B:54:LEU:HD23	1:B:62:TRP:CG	2.42	0.54
1:A:1027:GLU:O	1:A:1031:LEU:HG	2.08	0.54
1:B:1027:GLU:O	1:B:1031:LEU:HG	2.08	0.53
1:B:1393:VAL:HG12	1:B:1437:THR:HG22	1.92	0.52
1:A:1393:VAL:HG12	1:A:1437:THR:HG22	1.92	0.52
1:A:1298:PRO:HD2	1:A:1399:MET:HE2	1.91	0.51
1:B:692:VAL:HG13	1:B:692:VAL:O	2.11	0.51
1:B:1066:LEU:HD11	1:B:1239:LYS:HB3	1.92	0.51
1:A:692:VAL:O	1:A:692:VAL:HG13	2.11	0.51
1:A:1298:PRO:CD	1:A:1399:MET:HE2	2.39	0.51
1:A:1031:LEU:HD13	1:A:1130:THR:CA	2.41	0.51
1:B:1298:PRO:CD	1:B:1399:MET:HE2	2.39	0.51
1:A:1066:LEU:HD11	1:A:1239:LYS:HB3	1.92	0.50
1:B:1298:PRO:HD2	1:B:1399:MET:HE2	1.91	0.50
1:B:1031:LEU:HD13	1:B:1130:THR:CA	2.41	0.50
1:A:869:SER:HB3	1:A:874:ALA:HB3	1.94	0.49
1:B:15:LEU:HD23	1:B:138:GLN:NE2	2.28	0.49
1:B:869:SER:HB3	1:B:874:ALA:HB3	1.94	0.49
1:B:846:LEU:O	1:B:850:VAL:HG23	2.13	0.49
1:A:846:LEU:O	1:A:850:VAL:HG23	2.13	0.49
1:A:15:LEU:HD23	1:A:138:GLN:NE2	2.28	0.48
1:A:828:GLU:HB3	1:A:829:PRO:HD3	1.96	0.47
1:A:74:PHE:HB2	1:A:97:VAL:HG23	1.97	0.47
1:B:422:HIS:CE1	2:B:1501:HEM:ND	2.83	0.46
1:B:828:GLU:HB3	1:B:829:PRO:HD3	1.96	0.46
1:A:103:PHE:CD1	1:A:109:VAL:HG23	2.51	0.46
1:A:422:HIS:CE1	2:A:1501:HEM:ND	2.83	0.46
1:A:841:GLU:HB2	1:A:846:LEU:HD11	1.98	0.46
1:B:841:GLU:HB2	1:B:846:LEU:HD11	1.98	0.45
4:B:1504:FMN:H5'1	4:B:1504:FMN:H1'1	1.97	0.45
1:B:74:PHE:HB2	1:B:97:VAL:HG23	1.97	0.45
1:B:1014:THR:O	1:B:1015:THR:C	2.60	0.45
4:A:1504:FMN:H5'1	4:A:1504:FMN:H1'1	1.97	0.45
1:B:102:LEU:HD11	1:B:111:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:PHE:CD1	1:B:109:VAL:HG23	2.51	0.45
1:B:240:LEU:C	1:B:240:LEU:HD23	2.42	0.45
1:B:115:VAL:CG2	1:B:124:LEU:HD23	2.47	0.45
1:B:1046:LEU:HD11	1:B:1068:ASP:HB2	1.99	0.45
1:A:232:MET:HE2	1:A:232:MET:HB3	1.94	0.44
1:A:1014:THR:O	1:A:1015:THR:C	2.60	0.44
1:B:33:GLU:O	1:B:33:GLU:HG2	2.18	0.44
1:A:33:GLU:HG2	1:A:33:GLU:O	2.18	0.44
1:A:102:LEU:HD11	1:A:111:ILE:HD11	1.99	0.44
1:A:1046:LEU:HD11	1:A:1068:ASP:HB2	1.99	0.44
1:A:240:LEU:C	1:A:240:LEU:HD23	2.42	0.43
1:A:1102:LEU:HD11	1:A:1106:THR:CB	2.49	0.43
1:A:1363:THR:HG22	1:A:1364:ALA:N	2.34	0.43
1:B:1196:MET:HE1	1:B:1251:THR:CG2	2.49	0.43
1:B:1196:MET:HE1	1:B:1251:THR:HG21	2.01	0.42
1:A:115:VAL:CG2	1:A:124:LEU:HD23	2.47	0.42
1:B:1286:PRO:HG3	1:B:1293:LEU:HD11	2.01	0.42
1:A:1031:LEU:HD21	1:A:1129:PRO:HB2	2.02	0.42
1:A:1196:MET:HE1	1:A:1251:THR:HG21	2.02	0.42
1:A:1292:PRO:C	1:A:1293:LEU:HD12	2.45	0.42
1:B:991:ASP:OD1	1:B:991:ASP:N	2.53	0.42
1:A:328:MET:N	1:A:328:MET:HE2	2.35	0.42
1:A:1196:MET:HE1	1:A:1251:THR:CG2	2.49	0.42
1:B:1102:LEU:HD11	1:B:1106:THR:CB	2.49	0.42
1:B:1031:LEU:HD21	1:B:1129:PRO:HB2	2.02	0.42
1:A:1102:LEU:HD11	1:A:1106:THR:HG21	2.02	0.42
1:B:1292:PRO:C	1:B:1293:LEU:HD12	2.45	0.42
1:B:1363:THR:HG22	1:B:1364:ALA:N	2.34	0.42
1:B:328:MET:N	1:B:328:MET:HE2	2.35	0.41
1:B:1450:ILE:HG23	1:B:1451:LYS:N	2.36	0.41
1:A:209:LEU:HD23	1:A:844:ILE:HD13	2.03	0.41
1:A:393:PHE:HZ	1:A:442:MET:HE1	1.86	0.41
1:B:1102:LEU:HD11	1:B:1106:THR:HG21	2.02	0.41
1:A:991:ASP:N	1:A:991:ASP:OD1	2.53	0.41
1:A:1268:LEU:HD22	1:A:1272:ASP:HB2	2.03	0.41
1:B:1268:LEU:HD22	1:B:1272:ASP:HB2	2.03	0.41
1:A:328:MET:HE2	1:A:328:MET:HA	2.03	0.41
1:A:1286:PRO:HG3	1:A:1293:LEU:HD11	2.01	0.40
1:B:1028:SER:O	1:B:1032:LEU:HG	2.22	0.40
1:A:1028:SER:O	1:A:1032:LEU:HG	2.22	0.40
1:B:393:PHE:HZ	1:B:442:MET:HE1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:864:LEU:HD23	1:A:864:LEU:HA	1.96	0.40
1:A:1102:LEU:HD12	1:A:1103:SER:N	2.37	0.40
1:A:1450:ILE:HG23	1:A:1451:LYS:N	2.36	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	1390/1468 (95%)	1323 (95%)	63 (4%)	4 (0%)	36	69
1	B	1390/1468 (95%)	1321 (95%)	65 (5%)	4 (0%)	36	69
All	All	2780/2936 (95%)	2644 (95%)	128 (5%)	8 (0%)	37	69

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	SER
1	B	70	SER
1	A	1015	THR
1	B	1015	THR
1	A	542	ARG
1	B	542	ARG
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	1204/1262 (95%)	1180 (98%)	24 (2%)	48	65
1	B	1204/1262 (95%)	1178 (98%)	26 (2%)	45	64
All	All	2408/2524 (95%)	2358 (98%)	50 (2%)	46	65

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	112	SER
1	A	144	SER
1	A	178	THR
1	A	240	LEU
1	A	263	PHE
1	A	515	THR
1	A	531	LEU
1	A	605	ILE
1	A	643	SER
1	A	657	HIS
1	A	709	CYS
1	A	745	THR
1	A	768	PHE
1	A	998	SER
1	A	1002	ARG
1	A	1028	SER
1	A	1120	LEU
1	A	1155	LEU
1	A	1230	SER
1	A	1232	CYS
1	A	1331	CYS
1	A	1436	SER
1	A	1442	VAL
1	B	16	SER
1	B	112	SER
1	B	144	SER
1	B	178	THR
1	B	240	LEU
1	B	263	PHE
1	B	395	SER
1	B	407	SER
1	B	515	THR

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Mol	Chain	Res	Type
1	B	531	LEU
1	B	605	ILE
1	B	643	SER
1	B	657	HIS
1	B	709	CYS
1	B	745	THR
1	B	768	PHE
1	B	998	SER
1	B	1002	ARG
1	B	1028	SER
1	B	1120	LEU
1	B	1155	LEU
1	B	1230	SER
1	B	1232	CYS
1	B	1331	CYS
1	B	1436	SER
1	B	1442	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	467	ASN
1	A	779	GLN
1	A	784	GLN
1	A	832	HIS
1	A	899	ASN
1	A	901	ASN
1	A	930	GLN
1	A	934	GLN
1	A	1085	HIS
1	A	1248	GLN
1	B	467	ASN
1	B	779	GLN
1	B	832	HIS
1	B	1248	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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
3	FAD	B	1503	-	58,58,58	0.53	0	85,89,89	0.64	1 (1%)
2	HEM	B	1501	1	50,50,50	2.69	8 (16%)	67,82,82	1.53	12 (17%)
4	FMN	A	1504	-	33,33,33	0.67	0	48,50,50	0.87	1 (2%)
2	HEM	A	1501	1	50,50,50	2.69	8 (16%)	67,82,82	1.53	12 (17%)
2	HEM	A	1502	1	50,50,50	0.87	1 (2%)	67,82,82	0.68	0
4	FMN	B	1504	-	33,33,33	0.67	0	48,50,50	0.87	1 (2%)
3	FAD	A	1503	-	58,58,58	0.53	0	85,89,89	0.64	1 (1%)
2	HEM	B	1502	1	50,50,50	0.88	1 (2%)	67,82,82	0.69	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	B	1503	-	-	16/34/50/50	0/6/6/6
2	HEM	B	1501	1	-	6/14/54/54	-
4	FMN	A	1504	-	-	7/18/18/18	0/3/3/3
2	HEM	A	1501	1	-	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	1502	1	-	4/14/54/54	-
4	FMN	B	1504	-	-	7/18/18/18	0/3/3/3
3	FAD	A	1503	-	-	16/34/50/50	0/6/6/6
2	HEM	B	1502	1	-	4/14/54/54	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1501	HEM	FE-NB	12.25	2.32	1.94
2	A	1501	HEM	FE-NB	12.24	2.32	1.94
2	B	1501	HEM	FE-NC	8.68	2.23	1.95
2	A	1501	HEM	FE-NC	8.67	2.23	1.95
2	B	1501	HEM	FE-ND	-7.36	1.72	1.94
2	A	1501	HEM	FE-ND	-7.31	1.72	1.94
2	A	1501	HEM	C4D-ND	-3.70	1.33	1.40
2	B	1501	HEM	C4D-ND	-3.70	1.33	1.40
2	A	1501	HEM	C1B-NB	-3.62	1.34	1.40
2	B	1501	HEM	C1B-NB	-3.60	1.34	1.40
2	A	1502	HEM	FE-NB	2.67	2.03	1.94
2	B	1502	HEM	FE-NB	2.65	2.03	1.94
2	A	1501	HEM	C1D-ND	-2.47	1.34	1.38
2	B	1501	HEM	C1D-ND	-2.47	1.34	1.38
2	B	1501	HEM	C4B-NB	-2.38	1.34	1.38
2	A	1501	HEM	C4B-NB	-2.38	1.34	1.38
2	A	1501	HEM	C1C-C2C	-2.23	1.40	1.45
2	B	1501	HEM	C1C-C2C	-2.23	1.40	1.45

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1501	HEM	CHD-C1D-ND	4.38	129.14	124.42
2	B	1501	HEM	CHD-C1D-ND	4.38	129.14	124.42
2	A	1501	HEM	CHC-C4B-NB	4.04	128.77	124.42
2	B	1501	HEM	CHC-C4B-NB	4.00	128.73	124.42
2	A	1501	HEM	C1B-NB-C4B	3.60	109.47	105.21
2	B	1501	HEM	C1B-NB-C4B	3.60	109.47	105.21
2	A	1501	HEM	CHA-C4D-ND	3.54	128.74	124.37
2	B	1501	HEM	CHA-C4D-ND	3.53	128.73	124.37
2	B	1501	HEM	CHD-C1D-C2D	-2.84	120.54	125.03
2	A	1501	HEM	CHD-C1D-C2D	-2.81	120.59	125.03
2	A	1501	HEM	C3B-C4B-NB	-2.47	107.69	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1501	HEM	C3B-C4B-NB	-2.46	107.70	109.47
2	B	1501	HEM	CHB-C1B-NB	2.30	127.22	124.37
2	B	1501	HEM	CHA-C4D-C3D	-2.29	121.00	125.23
2	A	1501	HEM	CHA-C4D-C3D	-2.28	121.02	125.23
2	A	1501	HEM	C4C-CHD-C1D	-2.27	121.19	126.02
2	B	1501	HEM	C4C-CHD-C1D	-2.27	121.19	126.02
2	A	1501	HEM	CHB-C1B-NB	2.27	127.18	124.37
2	A	1501	HEM	C4B-C3B-C2B	-2.25	105.21	107.28
4	A	1504	FMN	C4-N3-C2	-2.25	121.65	125.64
4	B	1504	FMN	C4-N3-C2	-2.23	121.68	125.64
2	B	1501	HEM	C4B-C3B-C2B	-2.21	105.25	107.28
2	A	1501	HEM	CAA-CBA-CGA	-2.12	108.03	113.67
2	B	1501	HEM	CAA-CBA-CGA	-2.12	108.03	113.67
2	B	1501	HEM	C1A-CHA-C4D	-2.09	121.32	126.25
2	A	1501	HEM	C1A-CHA-C4D	-2.08	121.35	126.25
3	A	1503	FAD	C1'-C2'-C3'	2.08	115.30	109.66
3	B	1503	FAD	C1'-C2'-C3'	2.07	115.28	109.66

There are no chirality outliers.

All (66) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
3	A	1503	FAD	C3B-C4B-C5B-O5B
3	B	1503	FAD	C3B-C4B-C5B-O5B
3	A	1503	FAD	P-O3P-PA-O1A
3	A	1503	FAD	PA-O3P-P-O1P
3	B	1503	FAD	P-O3P-PA-O1A
3	B	1503	FAD	PA-O3P-P-O1P
3	A	1503	FAD	C4'-C5'-O5'-P
3	B	1503	FAD	C4'-C5'-O5'-P
3	A	1503	FAD	P-O3P-PA-O5B
3	A	1503	FAD	PA-O3P-P-O5'
3	B	1503	FAD	P-O3P-PA-O5B
3	B	1503	FAD	PA-O3P-P-O5'
4	A	1504	FMN	C5'-O5'-P-O3P
4	B	1504	FMN	C5'-O5'-P-O3P
3	A	1503	FAD	O3'-C3'-C4'-C5'
3	B	1503	FAD	O3'-C3'-C4'-C5'
3	A	1503	FAD	C5B-O5B-PA-O1A
3	A	1503	FAD	C5'-O5'-P-O1P
3	B	1503	FAD	C5B-O5B-PA-O1A
3	B	1503	FAD	C5'-O5'-P-O1P
3	A	1503	FAD	O4B-C4B-C5B-O5B
3	B	1503	FAD	O4B-C4B-C5B-O5B
2	A	1502	HEM	C4B-C3B-CAB-CBB
2	B	1502	HEM	C4B-C3B-CAB-CBB
3	A	1503	FAD	O3'-C3'-C4'-O4'
3	B	1503	FAD	O3'-C3'-C4'-O4'
2	A	1502	HEM	CAA-CBA-CGA-O1A
2	B	1501	HEM	CAD-CBD-CGD-O1D
2	A	1501	HEM	CAD-CBD-CGD-O1D
2	B	1502	HEM	CAA-CBA-CGA-O1A
2	A	1501	HEM	CAD-CBD-CGD-O2D
2	B	1501	HEM	CAD-CBD-CGD-O2D
2	B	1502	HEM	CAA-CBA-CGA-O2A
2	A	1502	HEM	CAA-CBA-CGA-O2A
4	A	1504	FMN	C4'-C5'-O5'-P
4	B	1504	FMN	C4'-C5'-O5'-P
2	A	1501	HEM	CAA-CBA-CGA-O2A
2	B	1501	HEM	CAA-CBA-CGA-O2A
2	A	1501	HEM	CAA-CBA-CGA-O1A
2	B	1501	HEM	CAA-CBA-CGA-O1A
3	A	1503	FAD	C2'-C3'-C4'-O4'
3	B	1503	FAD	C2'-C3'-C4'-O4'

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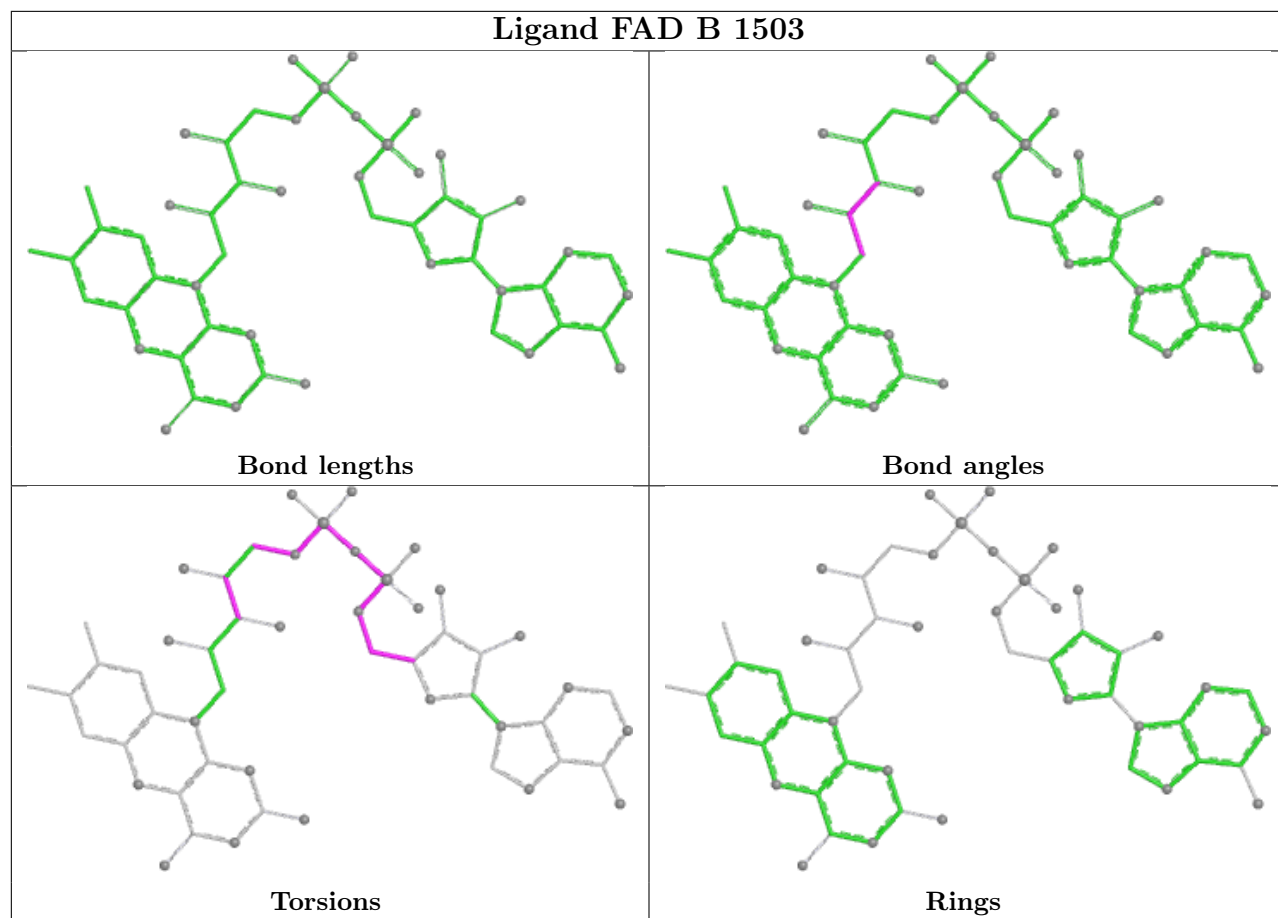
Mol	Chain	Res	Type	Atoms
2	A	1502	HEM	C2C-C3C-CAC-CBC
2	B	1502	HEM	C2C-C3C-CAC-CBC
3	A	1503	FAD	C2'-C3'-C4'-C5'
3	B	1503	FAD	C2'-C3'-C4'-C5'

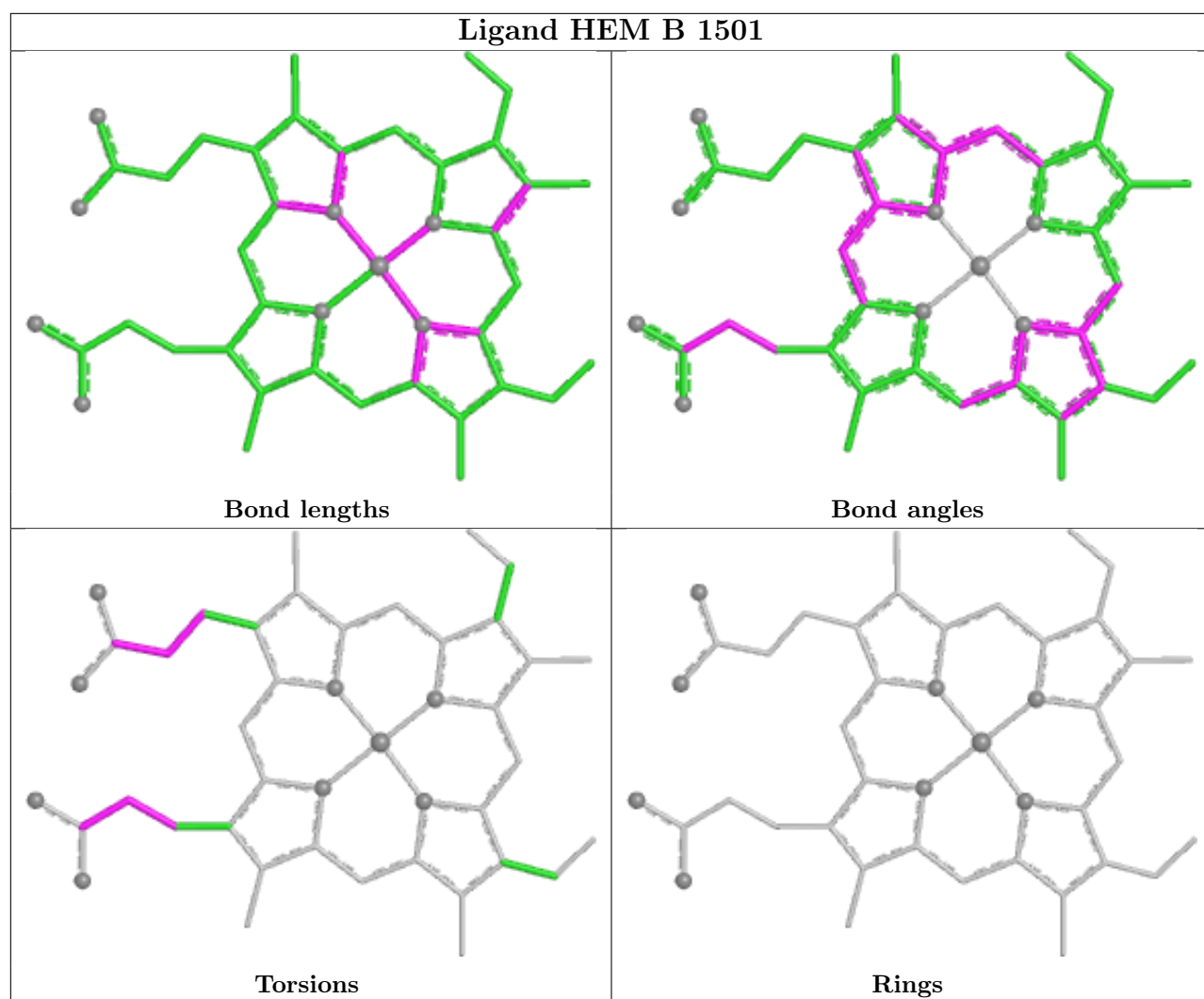
There are no ring outliers.

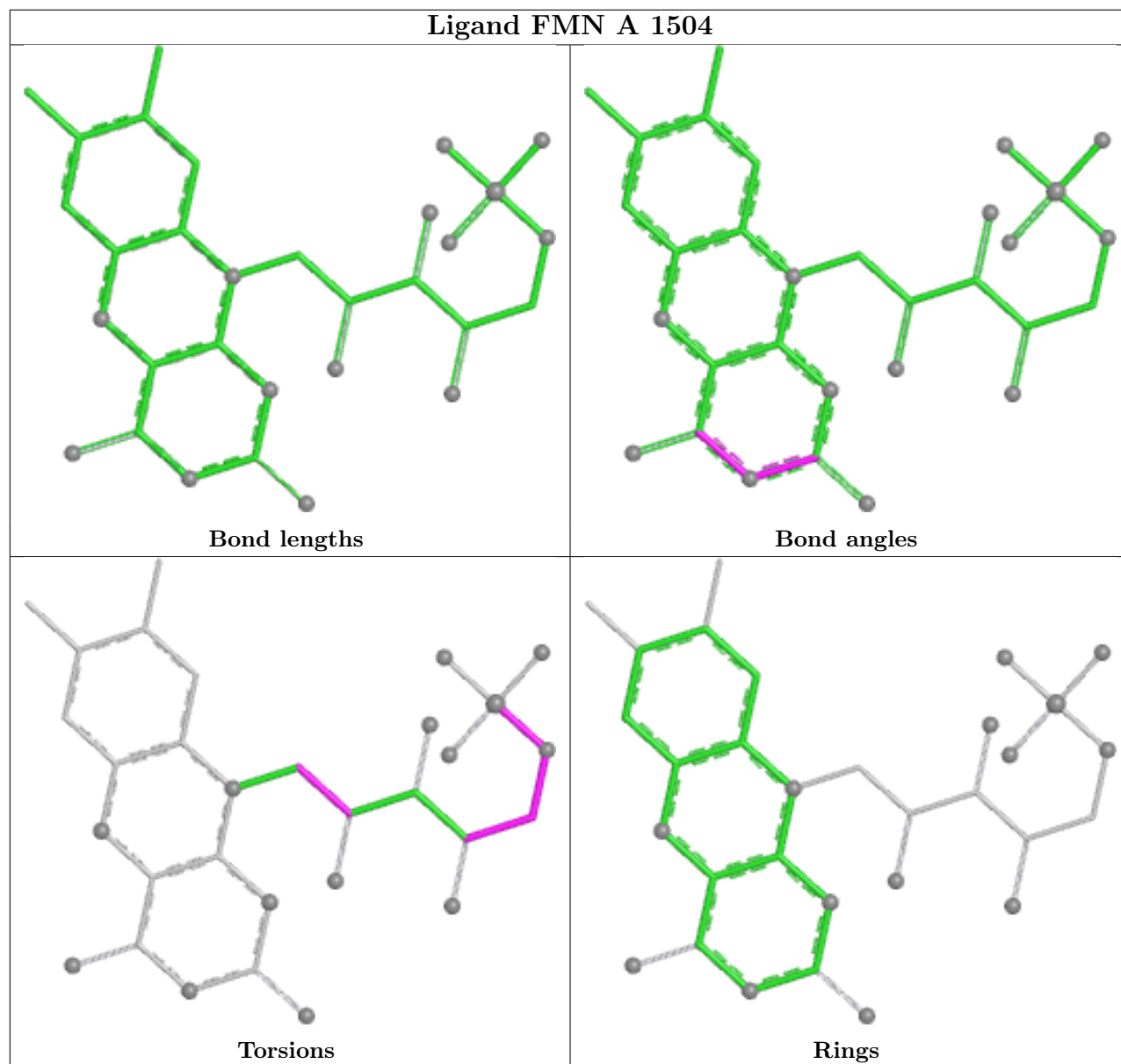
4 monomers are involved in 4 short contacts:

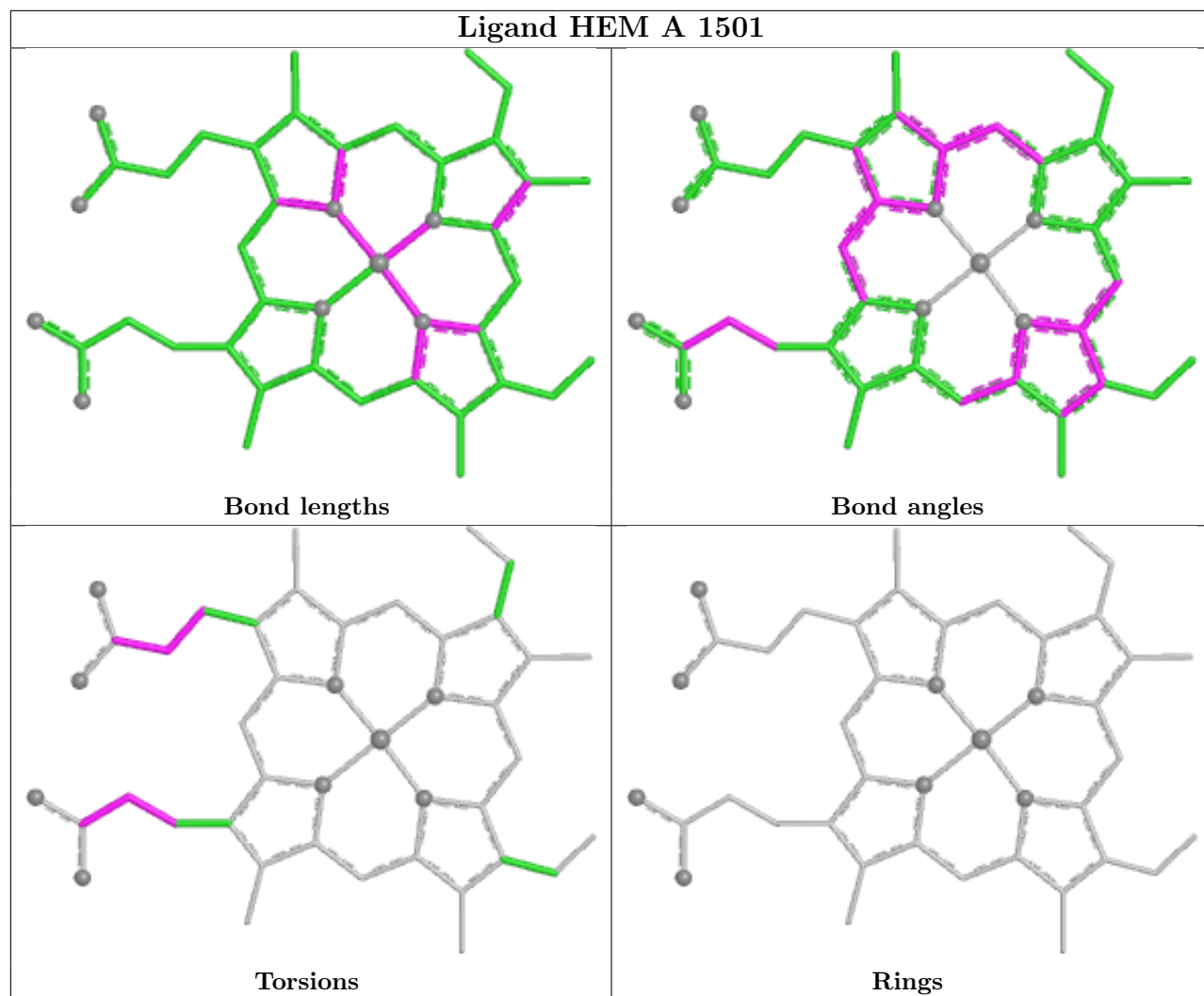
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1501	HEM	1	0
4	A	1504	FMN	1	0
2	A	1501	HEM	1	0
4	B	1504	FMN	1	0

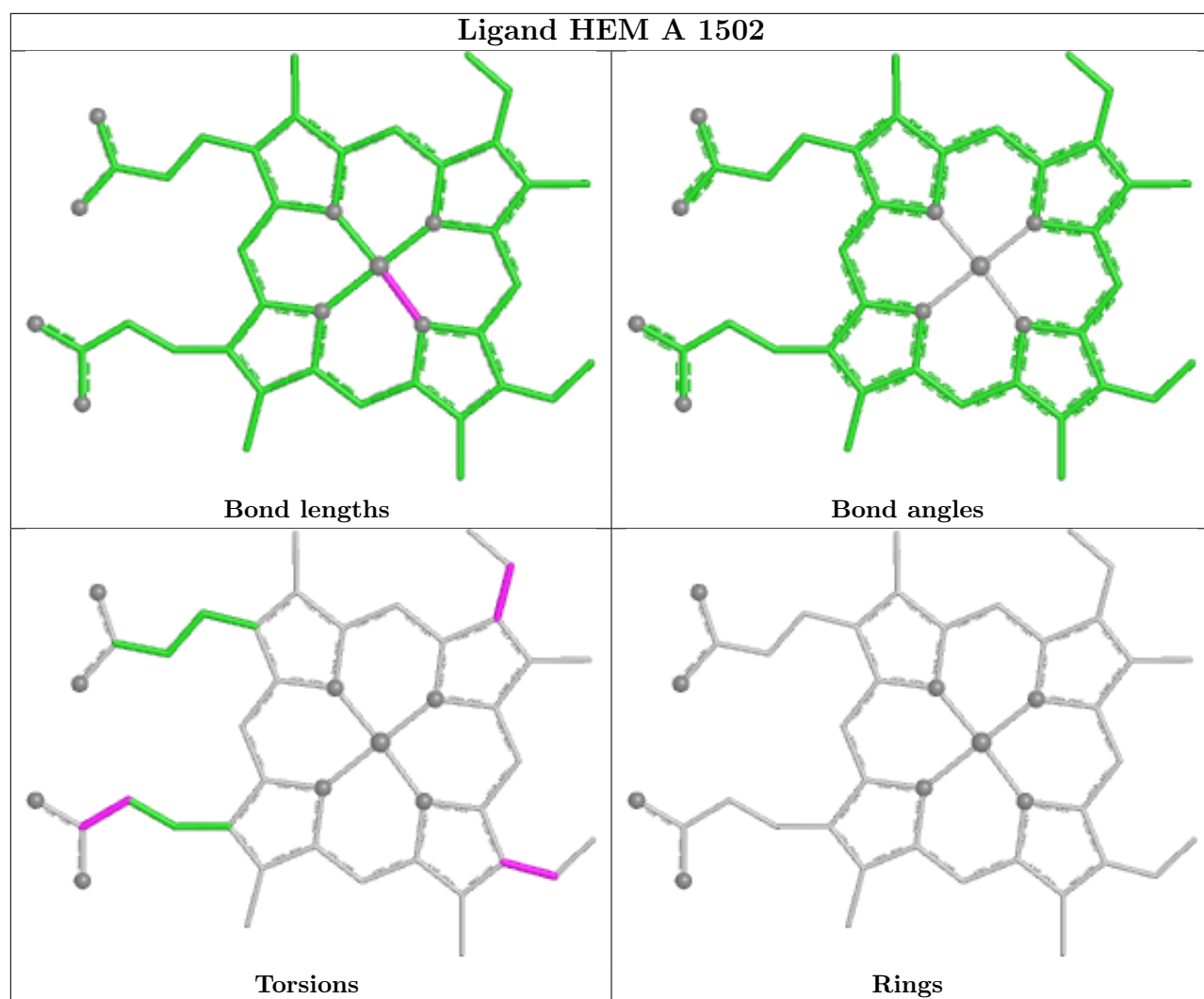
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

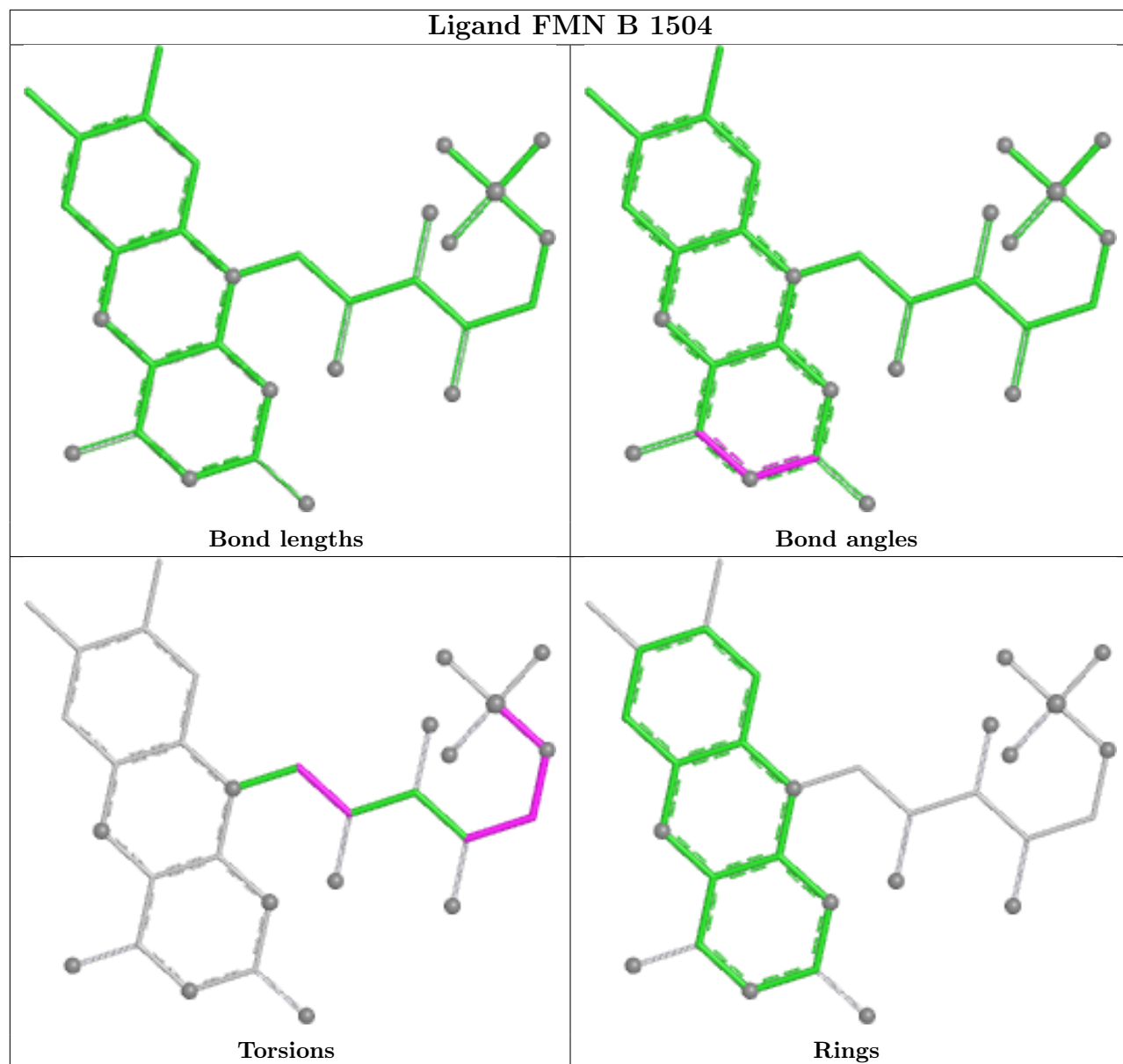


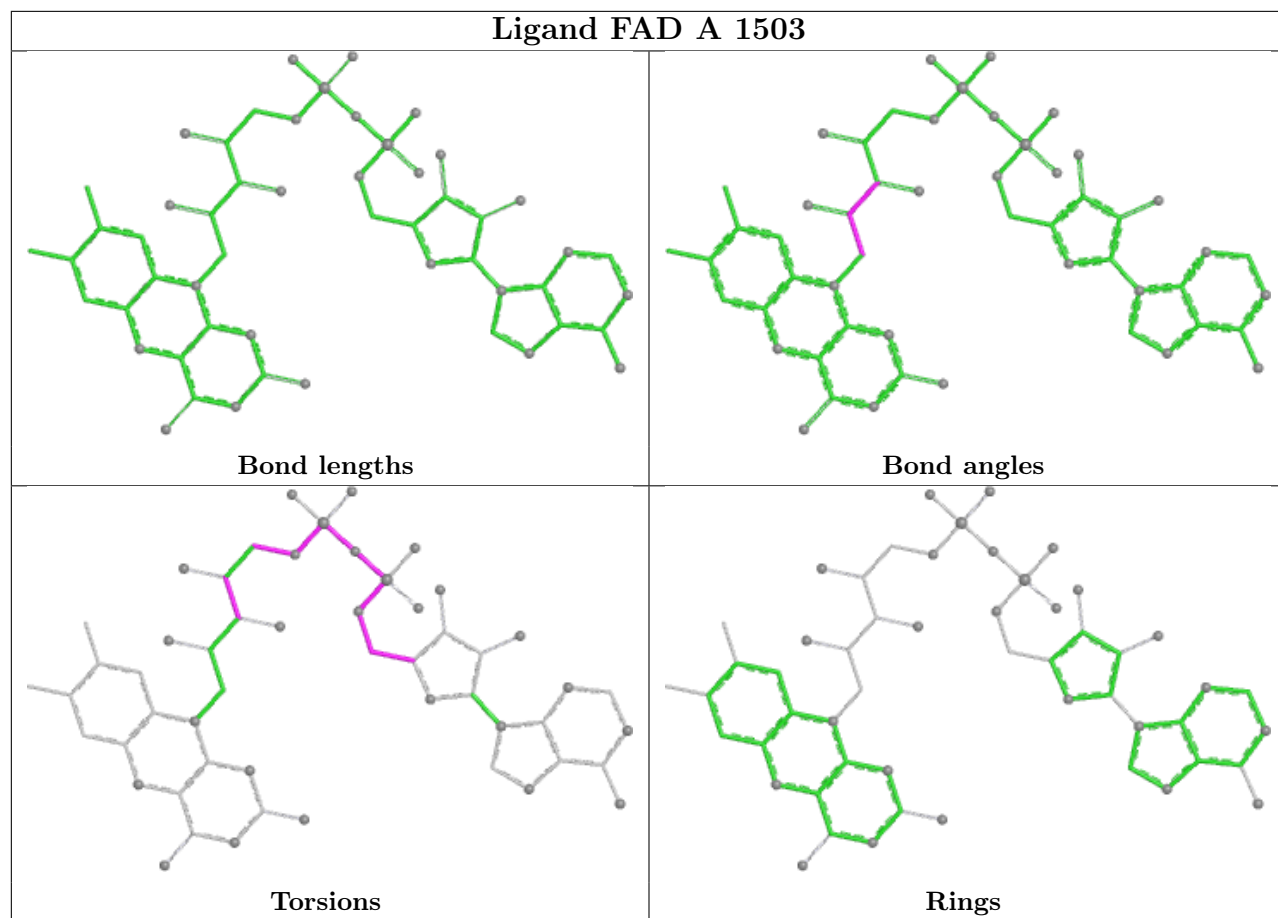


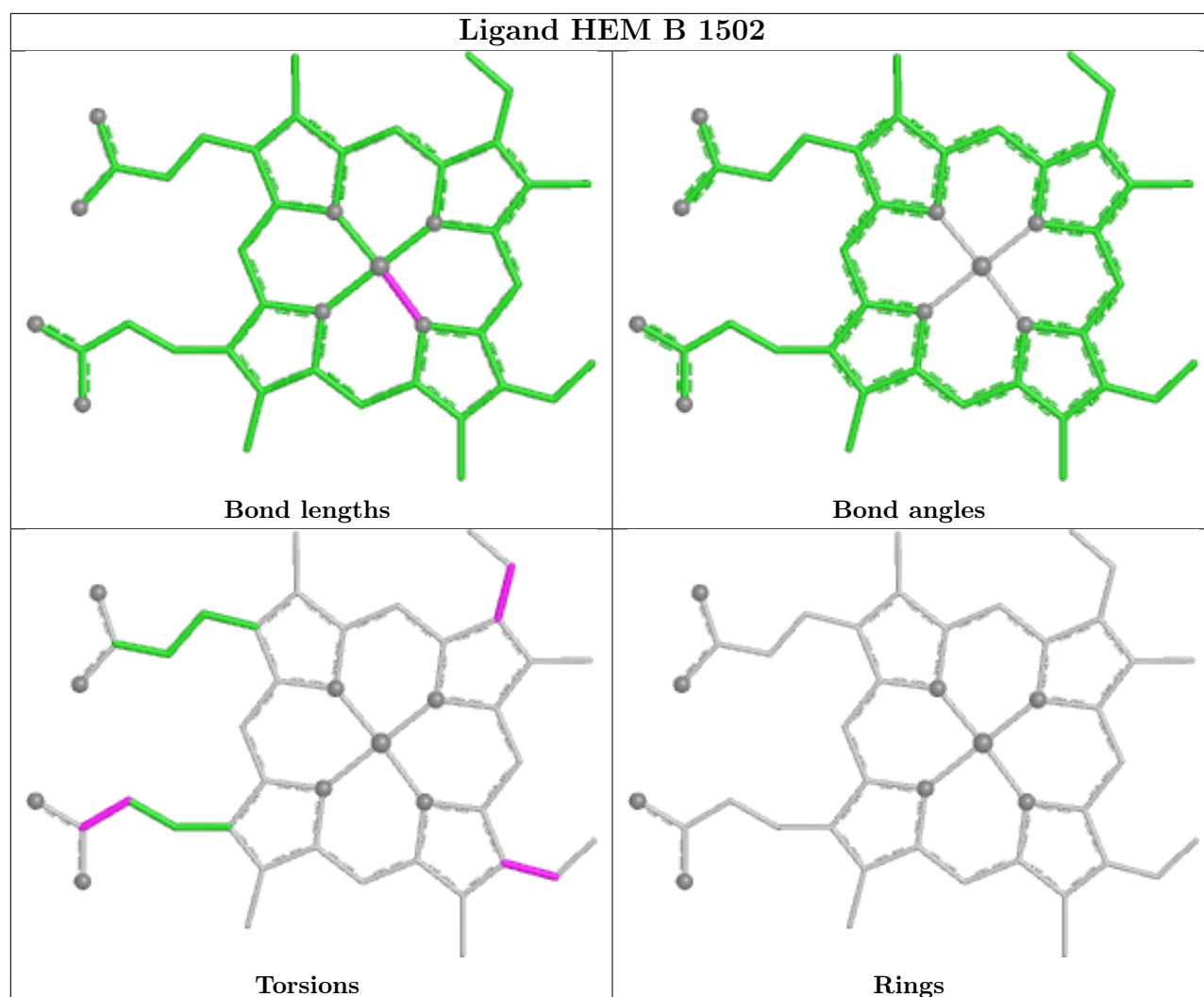












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

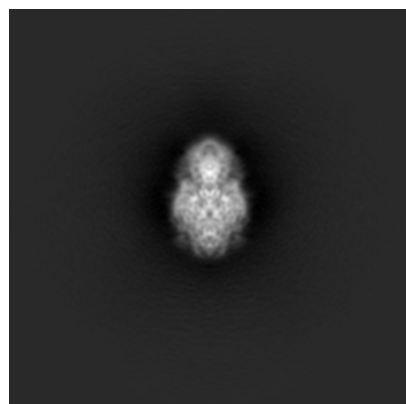
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72088. These allow visual inspection of the internal detail of the map and identification of artifacts.

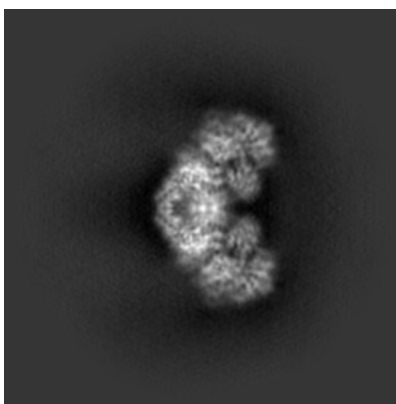
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

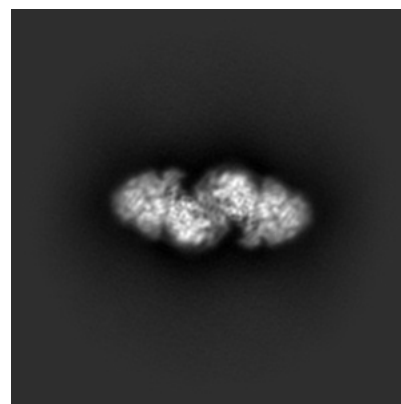
6.1.1 Primary map



X

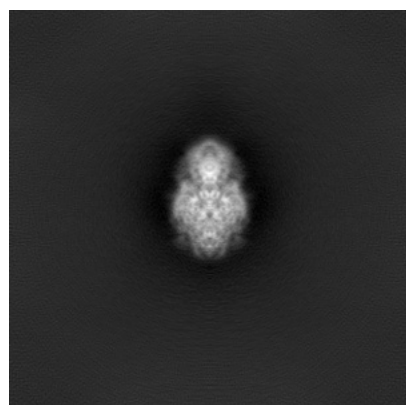


Y

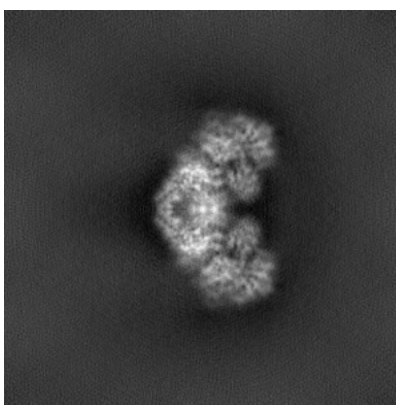


Z

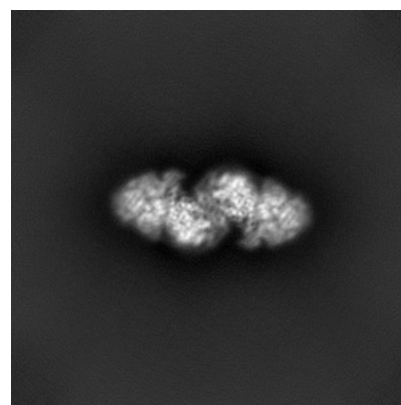
6.1.2 Raw map



X



Y

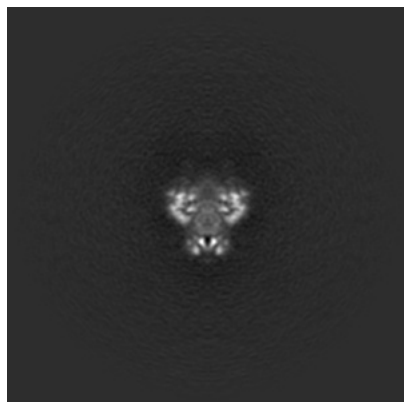


Z

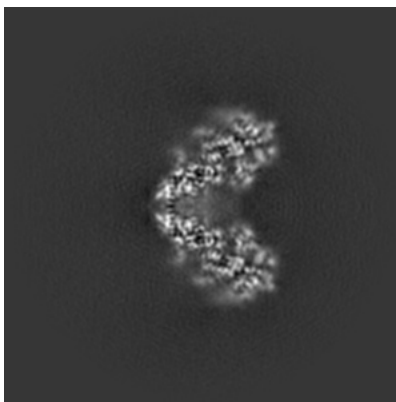
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

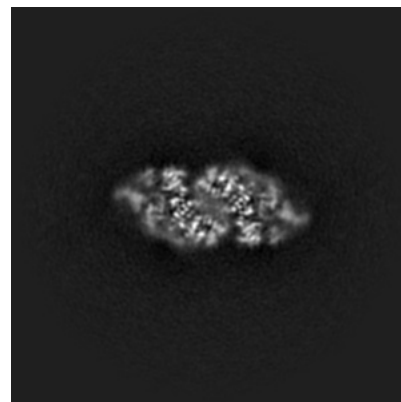
6.2.1 Primary map



X Index: 144

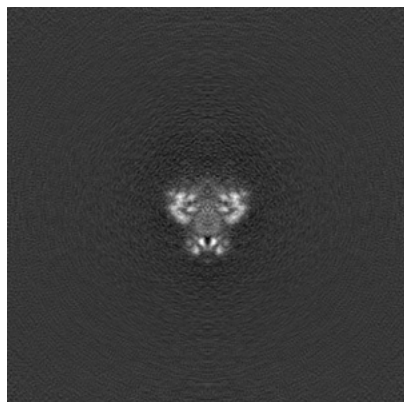


Y Index: 144

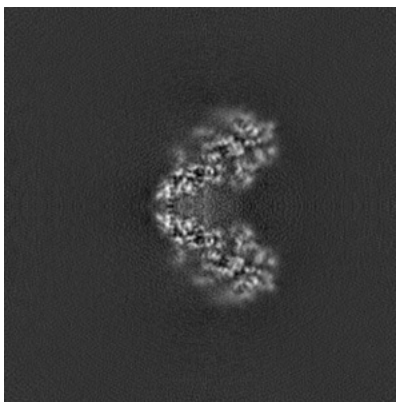


Z Index: 144

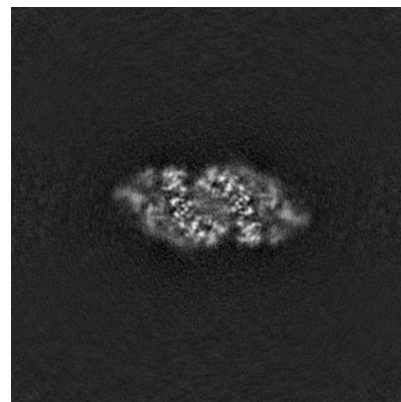
6.2.2 Raw map



X Index: 144



Y Index: 144

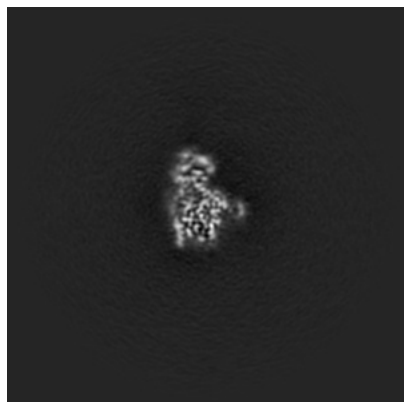


Z Index: 144

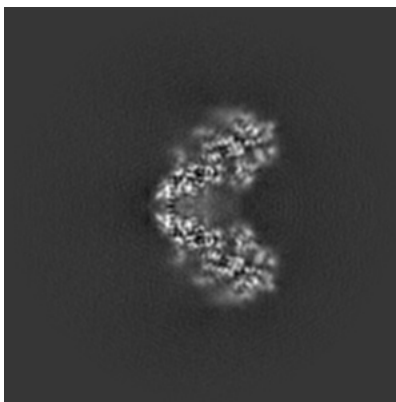
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

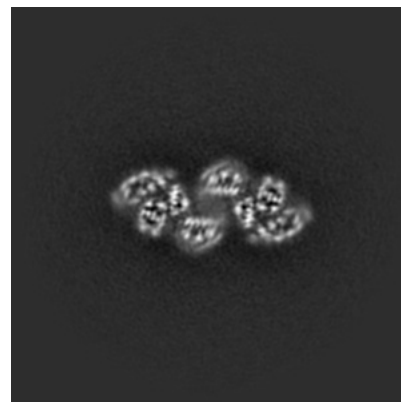
6.3.1 Primary map



X Index: 123

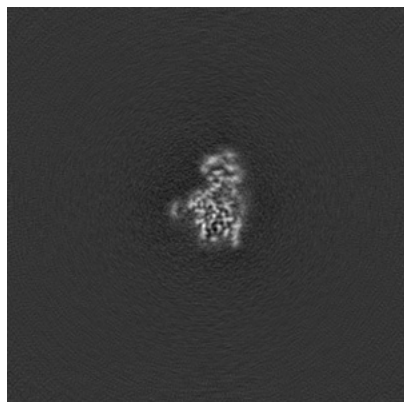


Y Index: 144

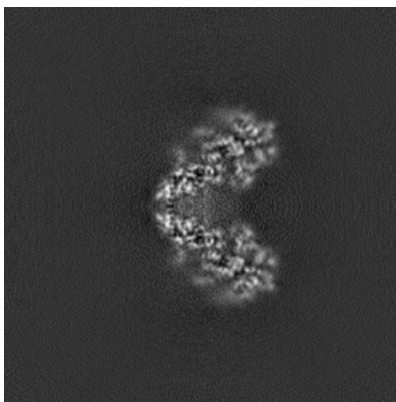


Z Index: 152

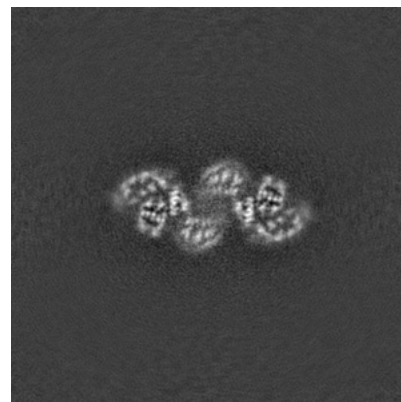
6.3.2 Raw map



X Index: 165



Y Index: 144

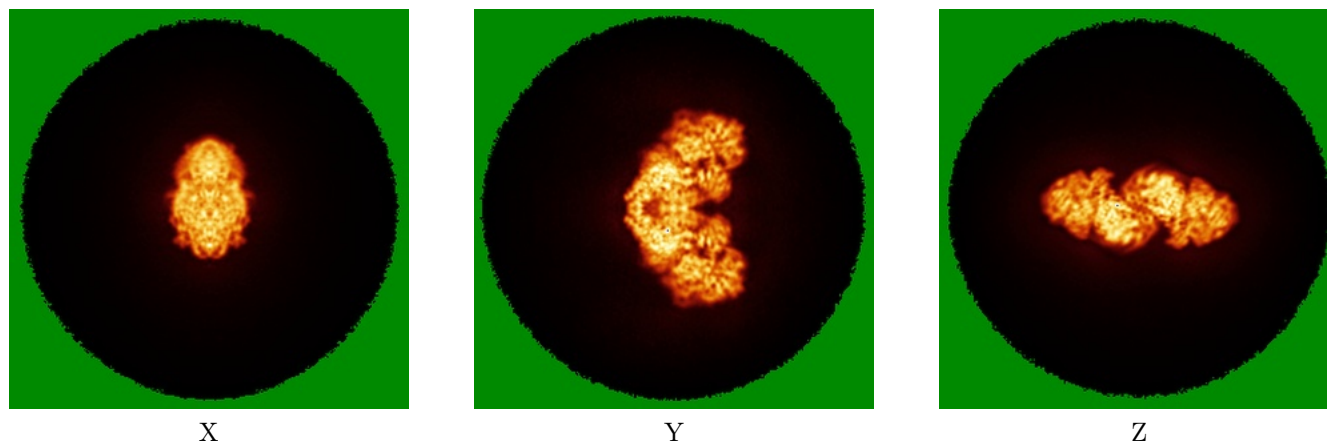


Z Index: 153

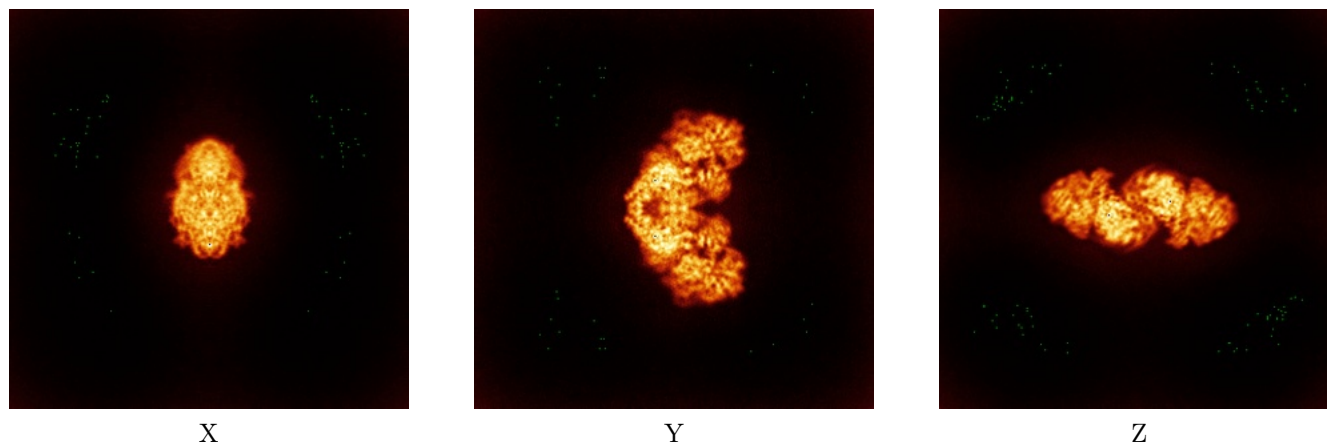
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



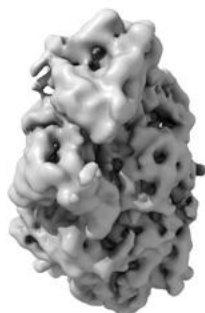
6.4.2 Raw map



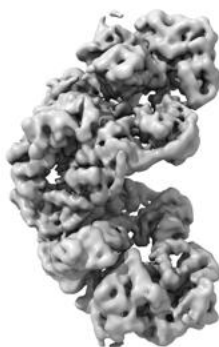
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

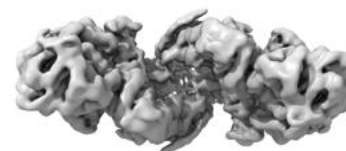
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.172. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

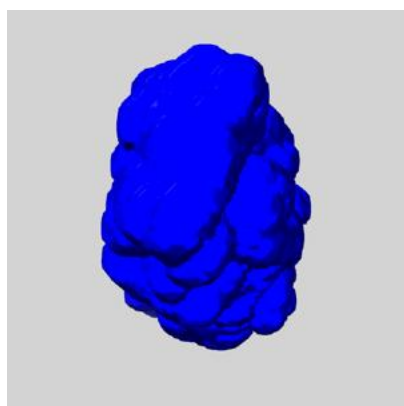
6.6 Mask visualisation [i](#)

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

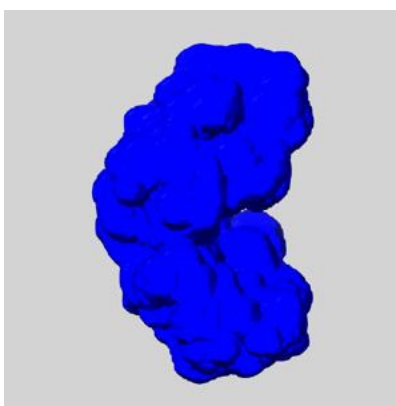
A mask typically either:

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

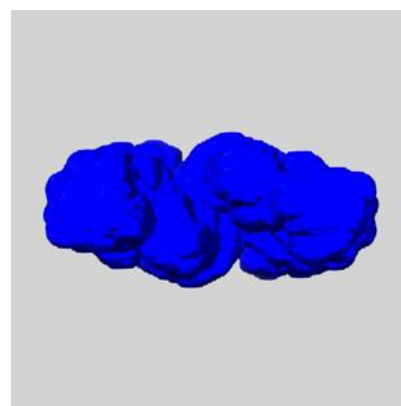
6.6.1 emd_72088_msk_1.map [i](#)



X



Y

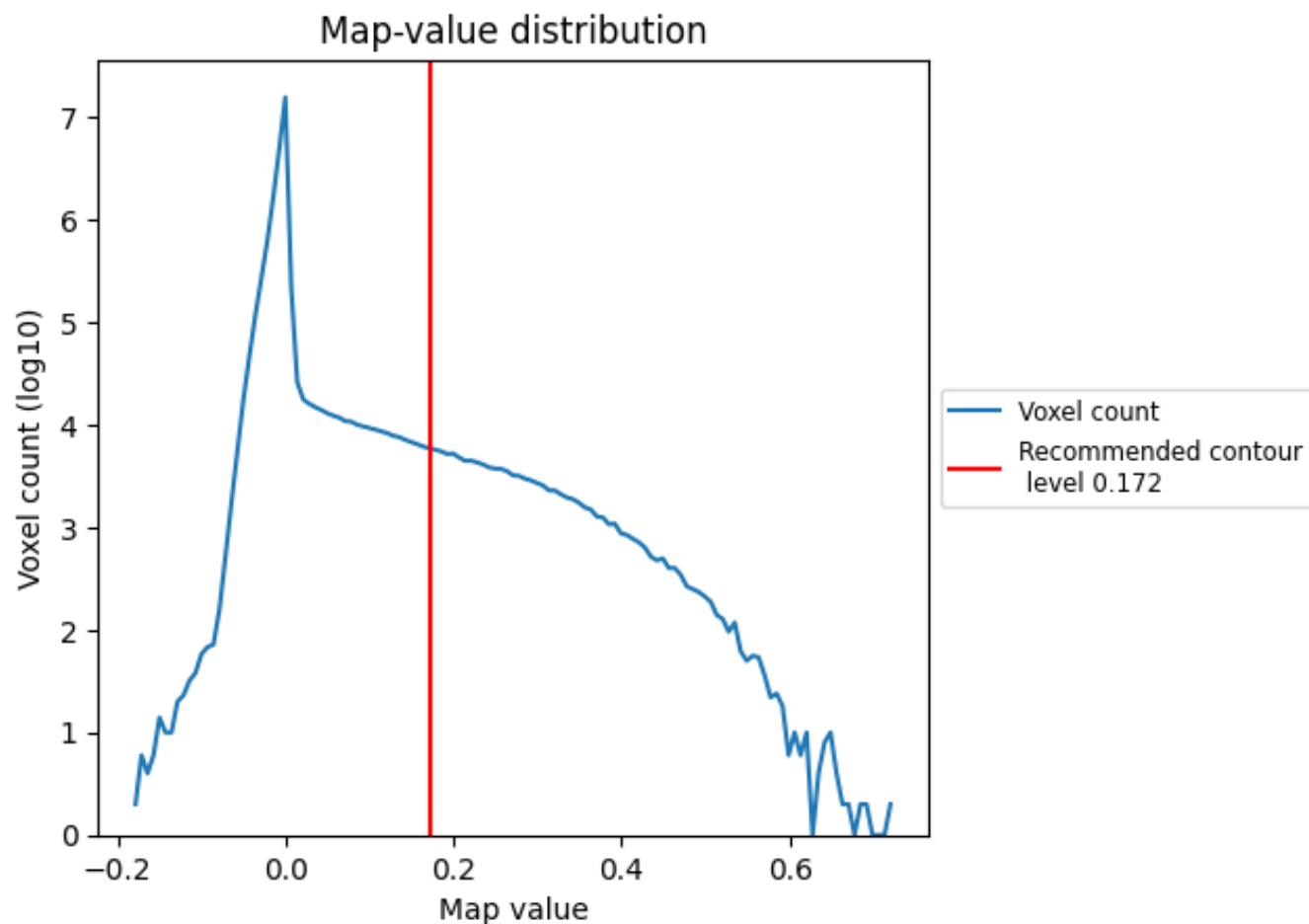


Z

7 Map analysis [i](#)

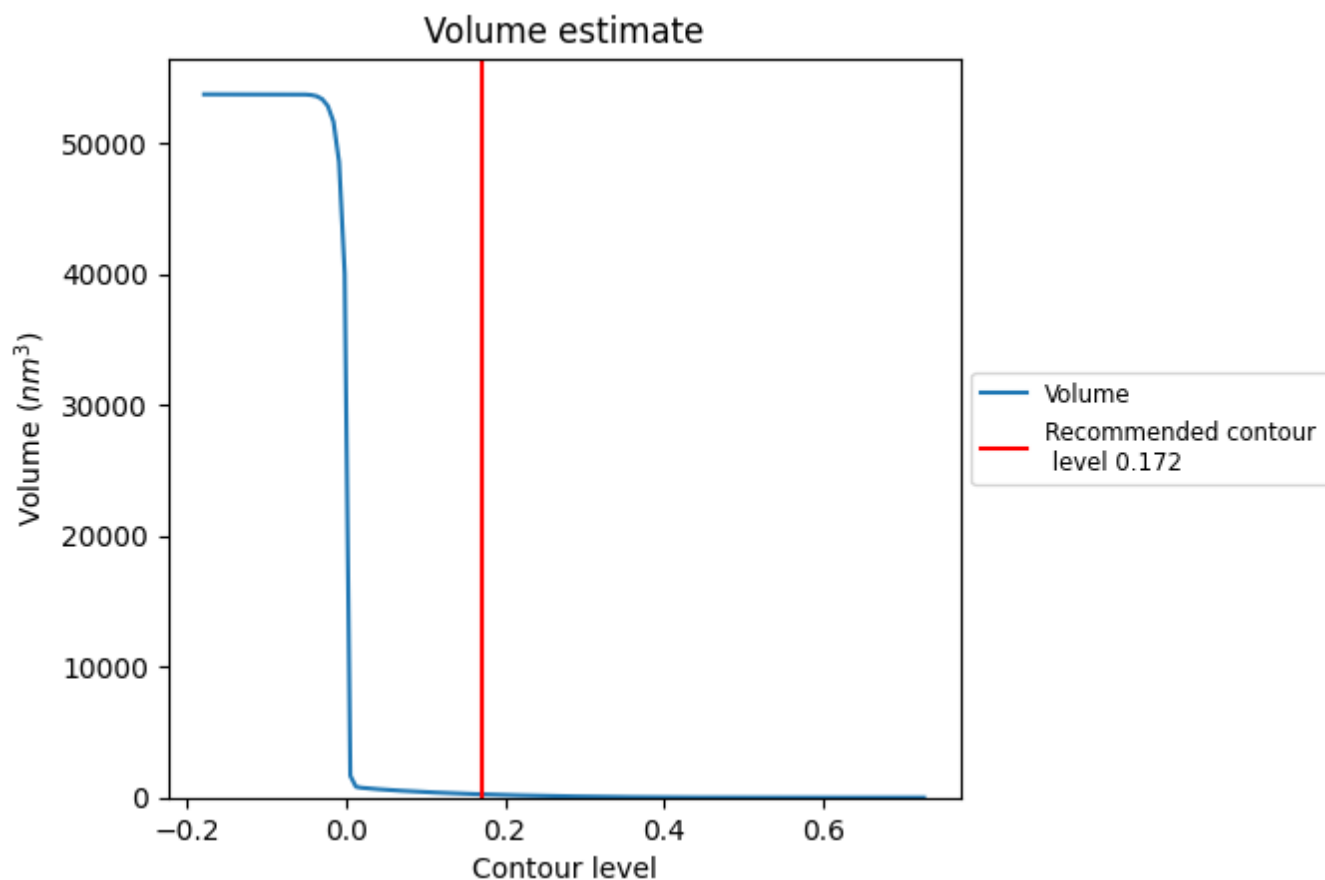
This section contains the results of statistical analysis of the map.

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.

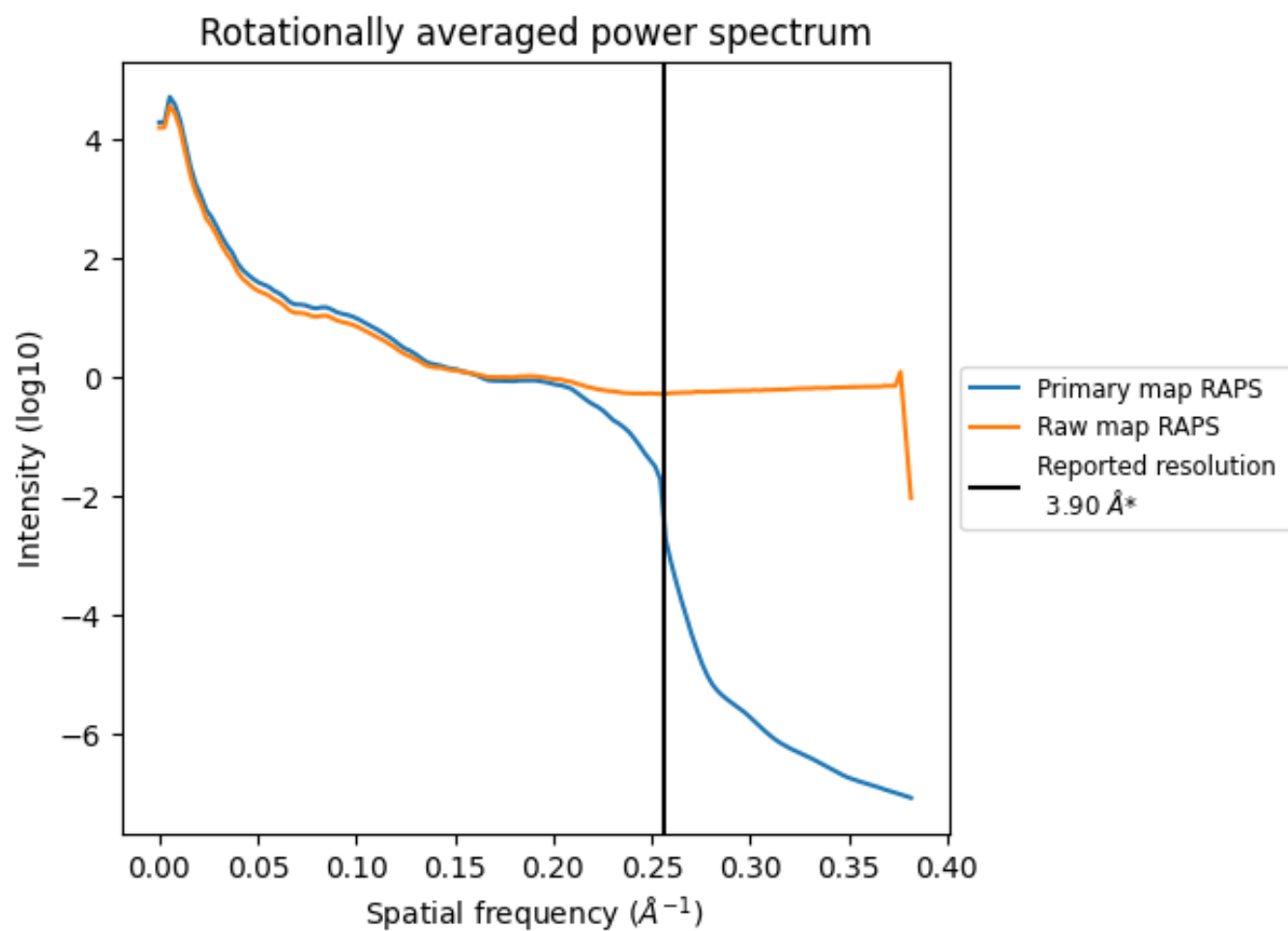
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 246 nm^3 ; this corresponds to an approximate mass of 223 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 ⓘ

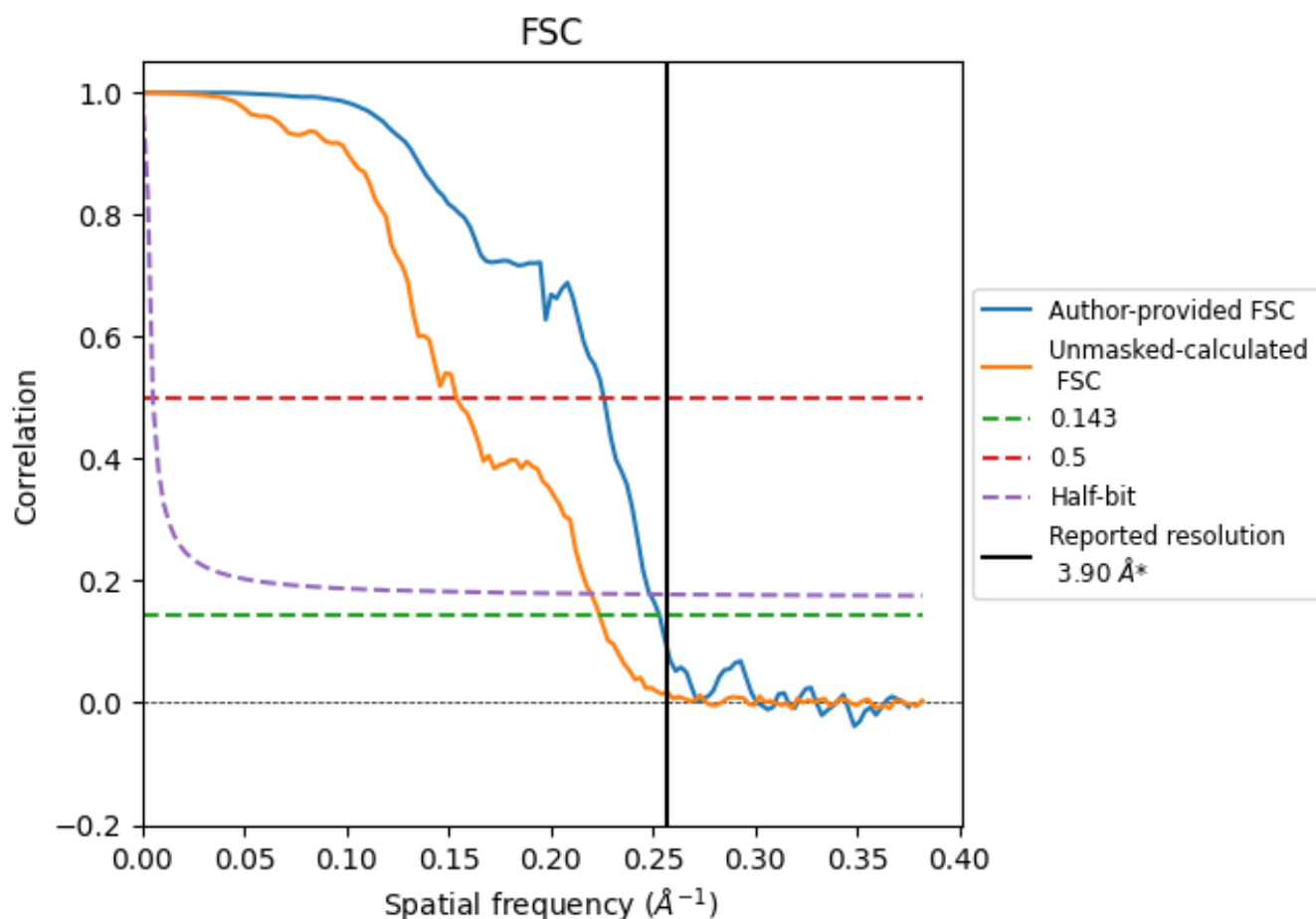


*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

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 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

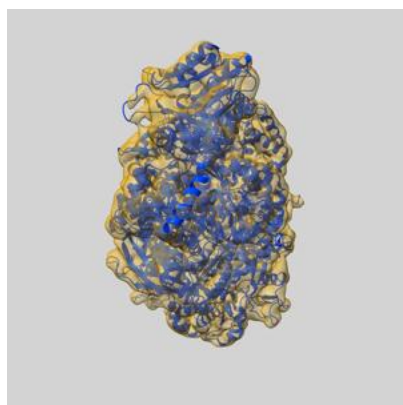
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.95	4.43	4.02
Unmasked-calculated*	4.47	6.51	4.55

*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 4.47 differs from the reported value 3.9 by more than 10 %

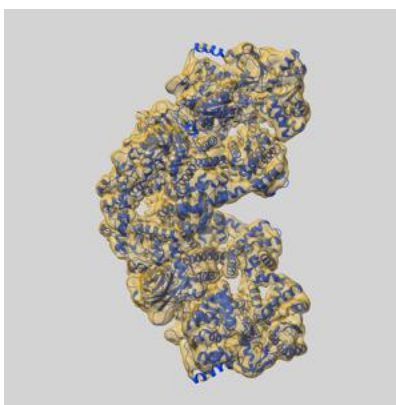
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-72088 and PDB model 9Q06. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

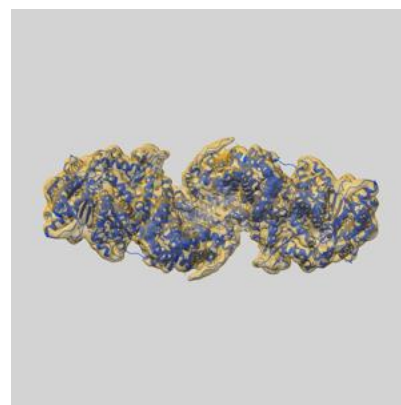
9.1 Map-model overlay [i](#)



X



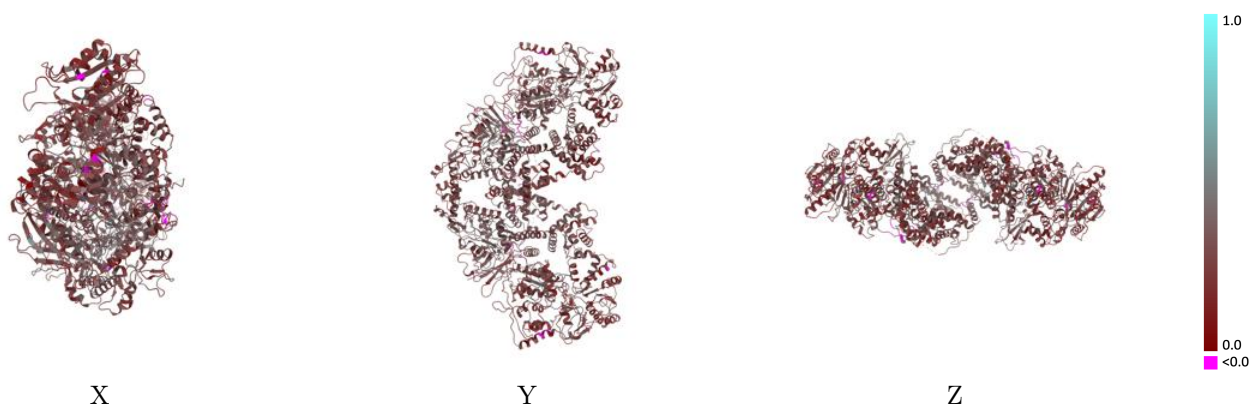
Y



Z

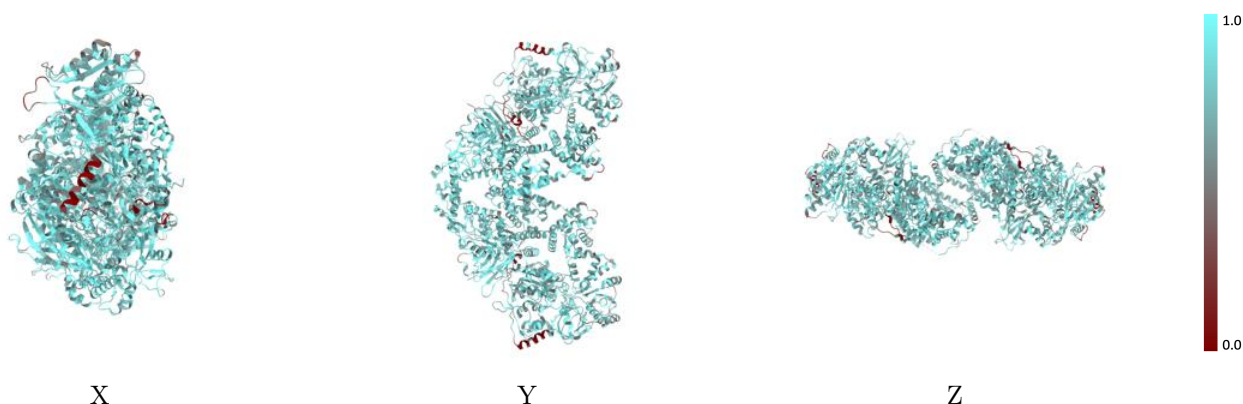
The images above show the 3D surface view of the map at the recommended contour level 0.172 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



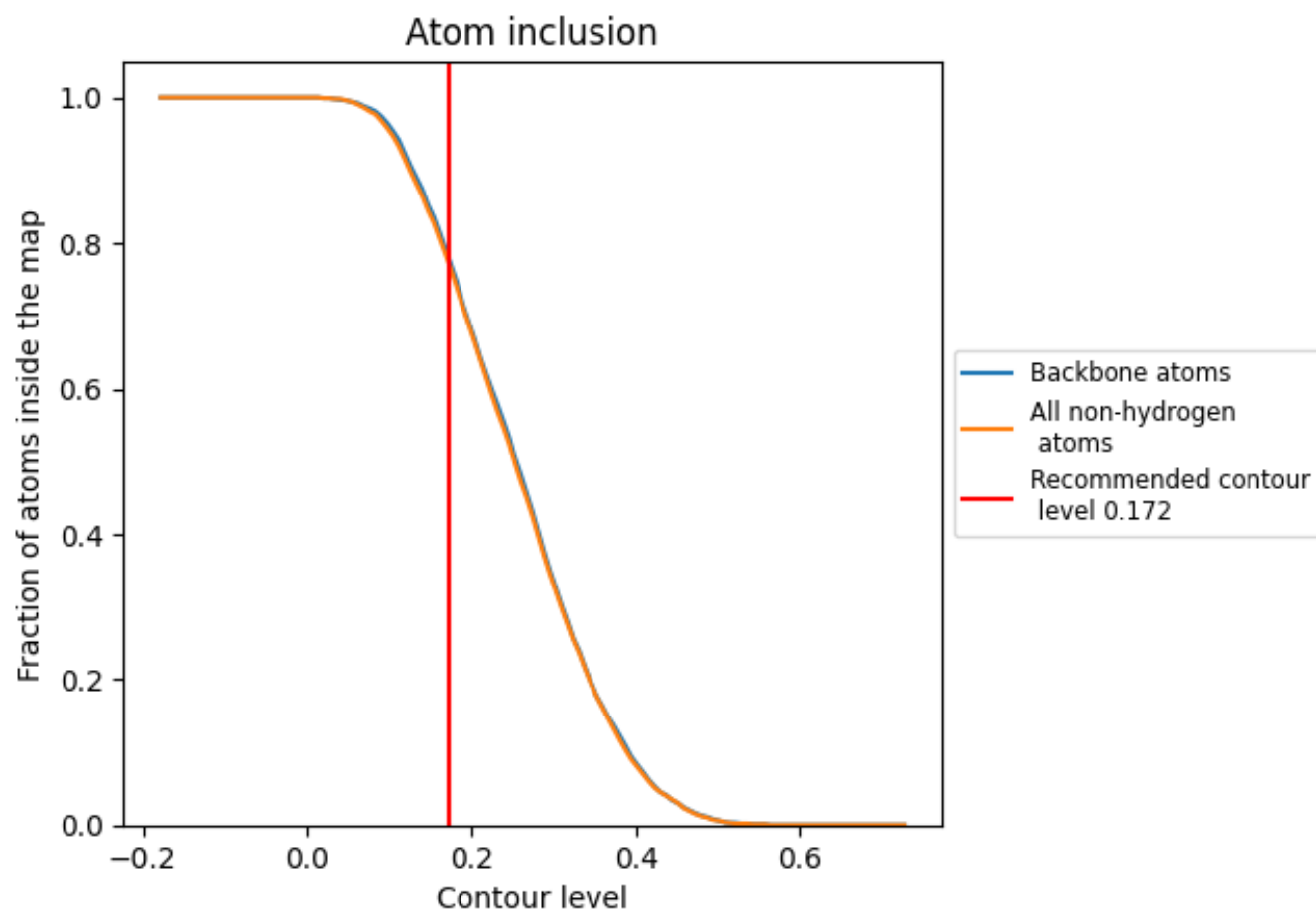
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.172).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 77% 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 (0.172) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7720	0.2880
A	0.7860	0.2880
B	0.7860	0.2890

