



## Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 08:53 PM UTC

PDB ID : 9YK0 / pdb\_00009yk0  
EMDB ID : EMD-73041  
Title : cryoEM structure of Aspergillus fumigatus acetolactate synthase (ALS) in complex with a novel inhibitor  
Authors : Hu, Y.  
Deposited on : 2025-10-06  
Resolution : 2.36 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>.

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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

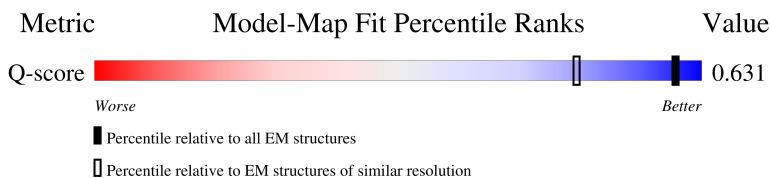
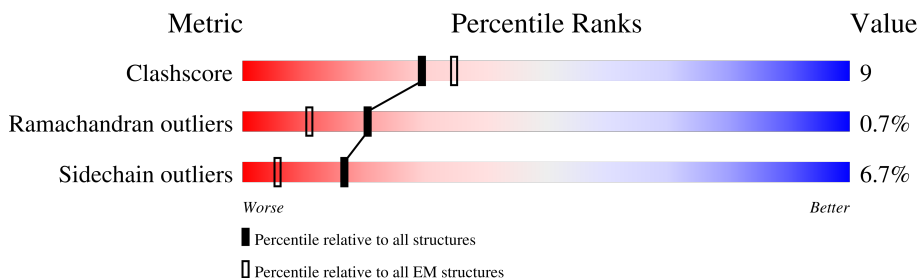
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.36 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	4686 ( 1.86 - 2.86 )

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	641	
1	B	641	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FAD	A	803	X	-	-	-
4	FAD	B	803	X	-	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9092 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.

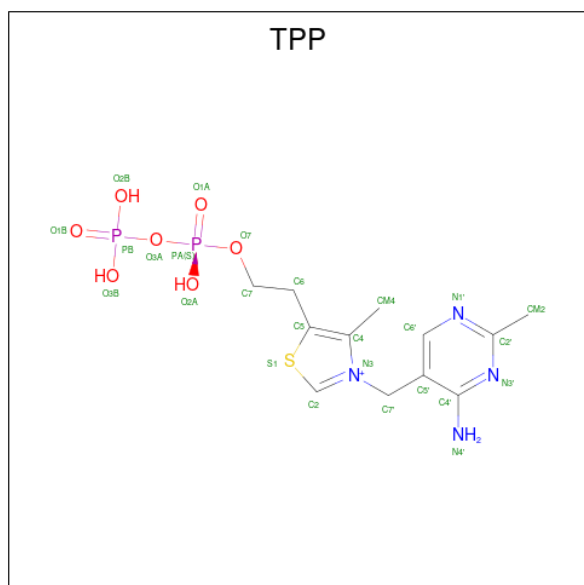
- Molecule 1 is a protein called Acetolactate synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	577	Total	C	N	O	S	0	0
			4438	2821	776	816	25		
1	B	577	Total	C	N	O	S	0	0
			4438	2821	776	816	25		

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

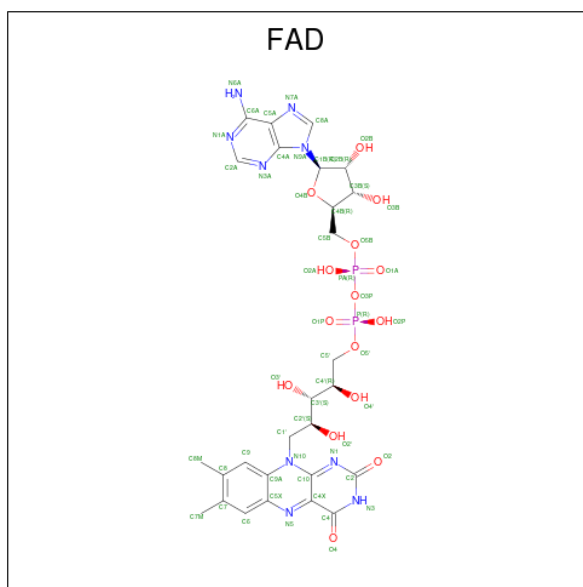
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Mg	0
			1	1	
2	B	1	Total	Mg	0
			1	1	

- Molecule 3 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula:  $C_{12}H_{19}N_4O_7P_2S$ ) (labeled as "Ligand of Interest" by depositor).



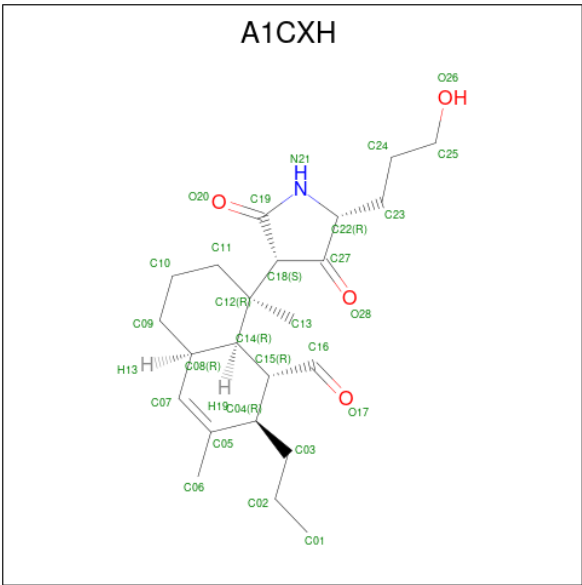
Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total 26	C 12	N 4	O 7	P 2	S 1	0
3	B	1	Total 26	C 12	N 4	O 7	P 2	S 1	0

- Molecule 4 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
4	A	1	Total 53	C 27	N 9	O 15	P 2	0
4	B	1	Total 53	C 27	N 9	O 15	P 2	0

- Molecule 5 is (1R,2R,4aR,8R,8aR)-8-[(3S,5R)-5-(3-hydroxypropyl)-2,4-dioxopyrrolidin-3-yl]-3,8-dimethyl-2-propyl-1,2,4a,5,6,7,8,8a-octahydronaphthalene-1-carbaldehyde (CCD ID: A1CXH) (formula: C<sub>23</sub>H<sub>35</sub>NO<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).

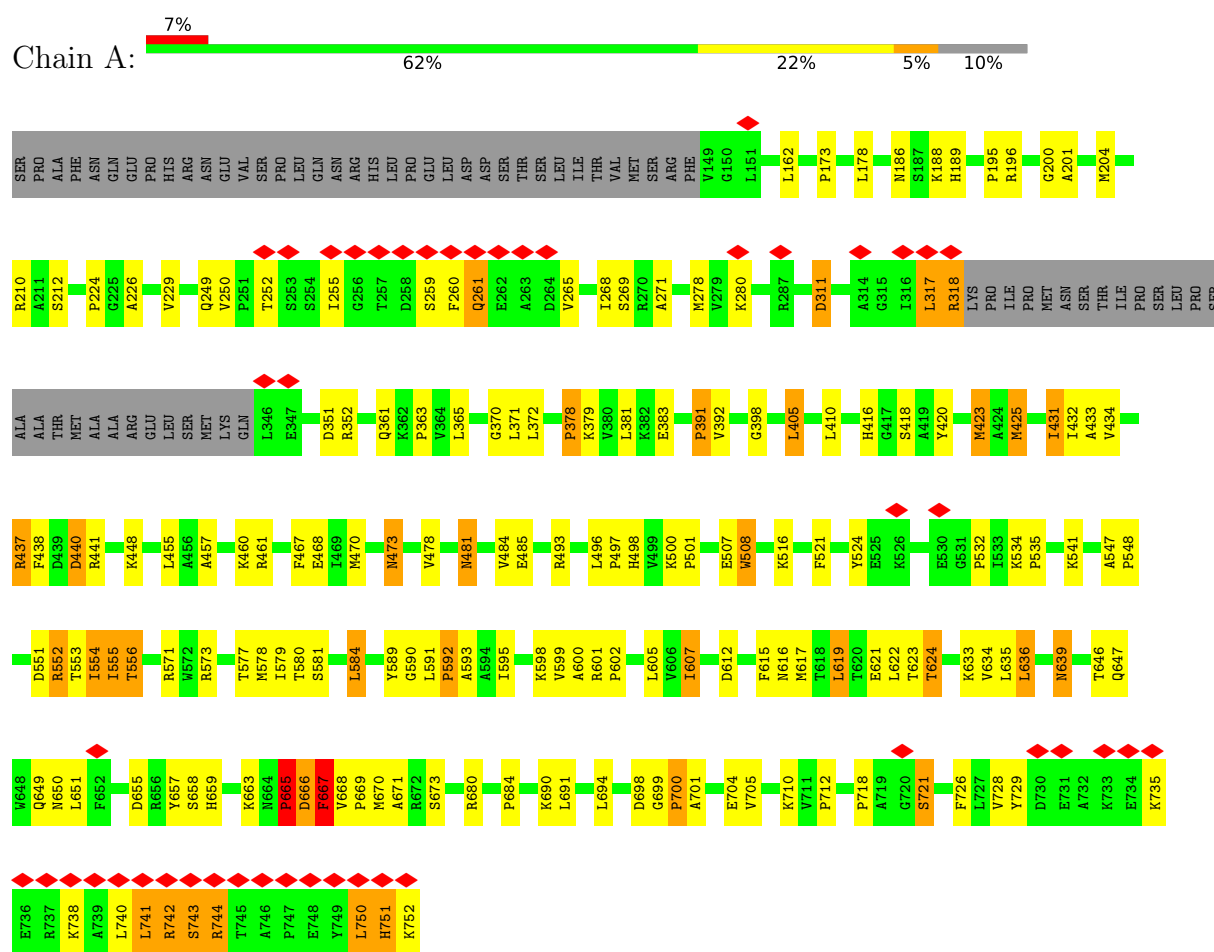


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			28	23	1	4	
5	B	1	Total	C	N	O	0
			28	23	1	4	

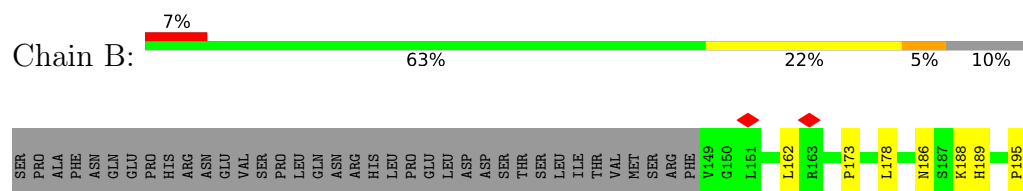
### 3 Residue-property plots

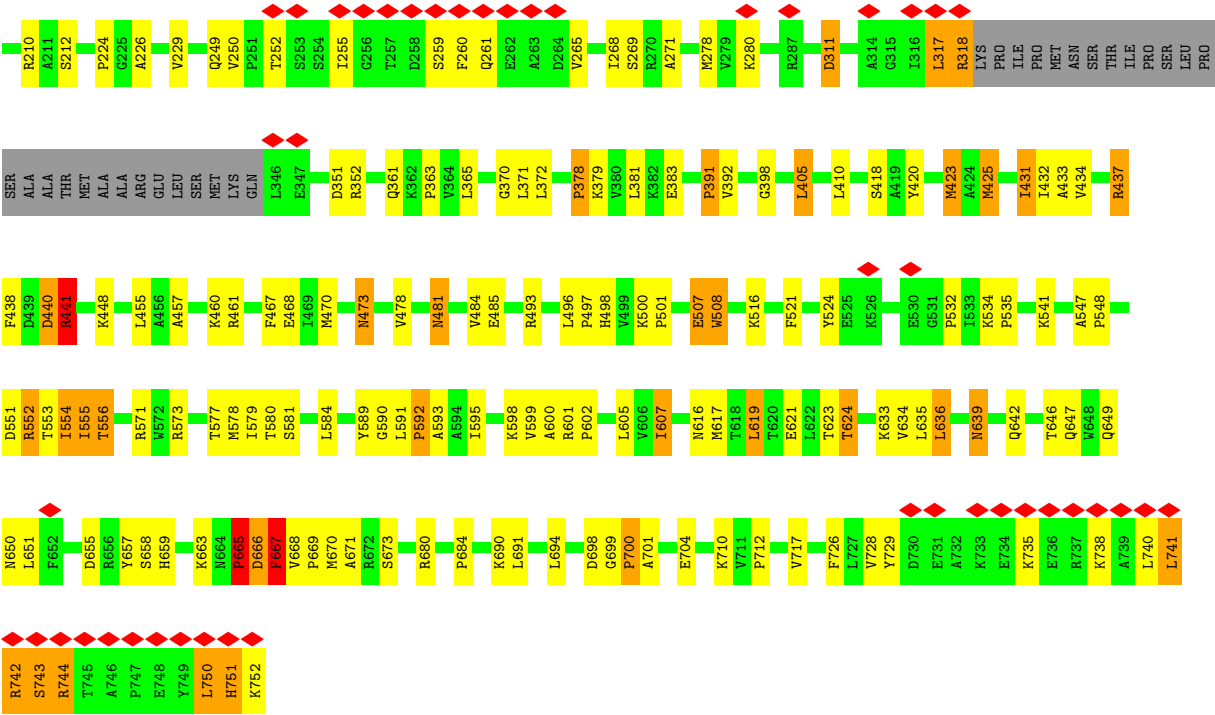
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: Acetolactate synthase



#### • Molecule 1: Acetolactate synthase







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	125472	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	65	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.637	Depositor
Minimum map value	-0.328	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	285.31198, 285.31198, 285.31198	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.743, 0.743, 0.743	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: TPP, FAD, A1CXH, MG

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	1.24	32/4537 (0.7%)	1.36	39/6150 (0.6%)
1	B	1.24	31/4537 (0.7%)	1.34	35/6150 (0.6%)
All	All	1.24	63/9074 (0.7%)	1.35	74/12300 (0.6%)

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	7
1	B	0	7
All	All	0	14

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	392	VAL	C-O	-7.40	1.16	1.24
1	A	392	VAL	C-O	-7.35	1.16	1.24
1	B	579	ILE	C-O	-6.95	1.16	1.24
1	A	579	ILE	C-O	-6.89	1.16	1.24
1	B	363	PRO	C-O	-6.83	1.16	1.23
1	A	363	PRO	C-O	-6.82	1.16	1.23
1	A	700	PRO	C-O	-6.48	1.15	1.23
1	B	700	PRO	C-O	-6.47	1.15	1.23
1	B	634	VAL	C-O	-6.41	1.17	1.24
1	A	634	VAL	C-O	-6.37	1.17	1.24
1	B	391	PRO	C-O	-6.27	1.16	1.23
1	A	391	PRO	C-O	-6.24	1.16	1.23
1	A	665	PRO	C-O	-6.23	1.15	1.24
1	B	665	PRO	C-O	-6.23	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	607	ILE	C-O	-6.22	1.17	1.24
1	B	607	ILE	C-O	-6.16	1.17	1.24
1	B	712	PRO	C-O	-6.11	1.17	1.23
1	A	712	PRO	C-O	-6.09	1.17	1.23
1	A	532	PRO	C-O	-6.02	1.16	1.23
1	B	532	PRO	C-O	-6.02	1.16	1.23
1	B	555	ILE	C-O	-5.94	1.17	1.24
1	A	555	ILE	C-O	-5.94	1.17	1.24
1	A	671	ALA	C-O	-5.88	1.17	1.24
1	B	671	ALA	C-O	-5.85	1.17	1.24
1	A	592	PRO	C-O	-5.73	1.16	1.24
1	B	592	PRO	C-O	-5.73	1.16	1.24
1	B	694	LEU	C-O	-5.57	1.17	1.24
1	B	633	LYS	C-O	-5.49	1.17	1.24
1	A	556	THR	C-O	-5.48	1.17	1.24
1	A	633	LYS	C-O	-5.48	1.17	1.24
1	A	694	LEU	C-O	-5.47	1.17	1.24
1	B	556	THR	C-O	-5.45	1.17	1.24
1	B	602	PRO	C-O	-5.44	1.16	1.24
1	A	602	PRO	C-O	-5.38	1.17	1.24
1	B	370	GLY	C-O	-5.35	1.17	1.24
1	B	635	LEU	C-O	-5.33	1.17	1.24
1	A	370	GLY	C-O	-5.32	1.17	1.24
1	A	431	ILE	C-O	-5.31	1.18	1.24
1	A	635	LEU	C-O	-5.29	1.17	1.24
1	A	581	SER	CA-CB	-5.26	1.46	1.53
1	B	581	SER	CA-CB	-5.26	1.46	1.53
1	B	431	ILE	C-O	-5.23	1.18	1.24
1	A	434	VAL	C-O	-5.23	1.18	1.24
1	A	577	THR	C-O	-5.23	1.17	1.24
1	B	554	ILE	C-O	-5.21	1.17	1.24
1	A	554	ILE	C-O	-5.21	1.17	1.24
1	B	684	PRO	C-O	-5.21	1.17	1.24
1	B	433	ALA	CA-CB	-5.18	1.46	1.53
1	B	577	THR	C-O	-5.18	1.17	1.24
1	A	636	LEU	C-O	-5.17	1.17	1.24
1	B	636	LEU	C-O	-5.17	1.17	1.24
1	A	684	PRO	C-O	-5.16	1.17	1.24
1	A	433	ALA	CA-CB	-5.14	1.46	1.53
1	B	434	VAL	C-O	-5.13	1.18	1.24
1	A	701	ALA	C-O	-5.13	1.17	1.23
1	B	701	ALA	C-O	-5.13	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	484	VAL	C-O	-5.10	1.18	1.24
1	B	484	VAL	C-O	-5.10	1.18	1.24
1	B	673	SER	CA-CB	-5.07	1.45	1.53
1	A	700	PRO	N-CA	-5.06	1.41	1.47
1	A	705	VAL	C-O	-5.06	1.18	1.24
1	B	700	PRO	N-CA	-5.02	1.41	1.47
1	A	673	SER	CA-CB	-5.02	1.45	1.53

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	416	HIS	CB-CG-CD2	-12.82	114.53	131.20
1	A	416	HIS	CB-CG-ND1	9.94	137.61	122.70
1	A	650	ASN	N-CA-C	-8.51	102.06	114.39
1	B	650	ASN	N-CA-C	-8.48	102.10	114.39
1	A	378	PRO	N-CA-CB	-7.89	94.97	103.25
1	B	378	PRO	N-CA-CB	-7.89	94.97	103.25
1	B	363	PRO	N-CA-CB	-7.50	96.07	103.19
1	A	363	PRO	N-CA-CB	-7.42	96.14	103.19
1	B	698	ASP	CB-CA-C	-7.24	100.02	111.17
1	A	698	ASP	CB-CA-C	-7.23	100.03	111.17
1	B	363	PRO	N-CA-C	7.23	123.69	111.32
1	A	363	PRO	N-CA-C	7.17	123.58	111.32
1	A	639	ASN	CA-CB-CG	6.58	119.18	112.60
1	B	639	ASN	CA-CB-CG	6.47	119.07	112.60
1	A	391	PRO	N-CA-CB	-6.44	97.58	103.31
1	B	391	PRO	N-CA-CB	-6.43	97.59	103.31
1	A	437	ARG	CB-CG-CD	-6.37	96.66	111.30
1	B	437	ARG	CB-CG-CD	-6.35	96.70	111.30
1	A	416	HIS	CA-CB-CG	6.14	119.94	113.80
1	B	589	TYR	N-CA-CB	-6.07	100.88	110.28
1	A	589	TYR	N-CA-CB	-6.06	100.89	110.28
1	B	752	LYS	CB-CA-C	-6.04	98.62	110.10
1	B	501	PRO	N-CA-C	6.04	119.92	110.80
1	B	438	PHE	CA-CB-CG	6.03	119.83	113.80
1	A	501	PRO	N-CA-C	6.02	119.89	110.80
1	A	752	LYS	CB-CA-C	-6.00	98.71	110.10
1	A	438	PHE	CA-CB-CG	5.98	119.78	113.80
1	A	691	LEU	N-CA-C	-5.92	106.19	113.41
1	B	691	LEU	N-CA-C	-5.90	106.22	113.41
1	A	261	GLN	CB-CA-C	5.81	119.25	111.82
1	A	535	PRO	N-CA-CB	-5.68	97.08	103.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	467	PHE	CA-CB-CG	5.68	119.48	113.80
1	B	441	ARG	N-CA-C	-5.64	106.17	113.16
1	A	467	PHE	CA-CB-CG	5.64	119.44	113.80
1	B	535	PRO	N-CA-CB	-5.63	97.13	103.33
1	A	667	PHE	CA-CB-CG	5.61	119.41	113.80
1	B	667	PHE	CA-CB-CG	5.60	119.40	113.80
1	B	508	TRP	N-CA-C	-5.58	105.28	111.36
1	A	508	TRP	N-CA-C	-5.54	105.32	111.36
1	A	729	TYR	CB-CA-C	-5.47	101.31	110.29
1	B	729	TYR	CB-CA-C	-5.47	101.31	110.29
1	B	448	LYS	N-CA-CB	-5.42	102.62	110.70
1	B	553	THR	CB-CA-C	-5.42	102.44	110.62
1	B	577	THR	N-CA-C	-5.41	106.54	114.39
1	A	455	LEU	N-CA-C	-5.40	105.83	112.90
1	B	481	ASN	CB-CA-C	5.39	120.02	110.85
1	A	448	LYS	N-CA-CB	-5.38	102.68	110.70
1	A	577	THR	N-CA-C	-5.38	106.59	114.39
1	B	455	LEU	N-CA-C	-5.38	105.85	112.90
1	A	481	ASN	CB-CA-C	5.38	119.99	110.85
1	A	553	THR	CB-CA-C	-5.38	102.50	110.62
1	A	639	ASN	N-CA-C	-5.31	106.80	113.28
1	A	602	PRO	CB-CA-C	-5.31	102.81	111.56
1	B	602	PRO	CB-CA-C	-5.31	102.81	111.56
1	B	481	ASN	N-CA-C	-5.30	105.58	111.36
1	B	639	ASN	N-CA-C	-5.29	106.83	113.28
1	A	524	TYR	CA-CB-CG	5.29	123.42	113.90
1	A	481	ASN	N-CA-C	-5.28	105.61	111.36
1	B	524	TYR	CA-CB-CG	5.27	123.38	113.90
1	A	521	PHE	CA-CB-CG	5.24	119.04	113.80
1	A	712	PRO	N-CA-CB	-5.21	98.23	103.19
1	B	670	MET	CA-C-O	-5.20	115.34	120.70
1	B	521	PHE	CA-CB-CG	5.19	118.99	113.80
1	A	670	MET	CA-C-O	-5.19	115.36	120.70
1	B	712	PRO	N-CA-CB	-5.15	98.30	103.19
1	A	598	LYS	N-CA-C	-5.14	107.01	113.28
1	B	598	LYS	N-CA-C	-5.14	107.02	113.28
1	A	473	ASN	N-CA-C	-5.11	106.83	113.16
1	A	584	LEU	N-CA-C	-5.09	106.76	113.12
1	B	381	LEU	N-CA-C	-5.07	105.93	111.82
1	B	473	ASN	N-CA-C	-5.07	106.87	113.16
1	A	381	LEU	N-CA-C	-5.06	105.95	111.82
1	B	717	VAL	N-CA-C	-5.04	102.97	107.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	612	ASP	CB-CA-C	5.00	118.74	110.88

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	318	ARG	Sidechain
1	A	352	ARG	Sidechain
1	A	441	ARG	Sidechain
1	A	461	ARG	Sidechain
1	A	552	ARG	Sidechain
1	A	571	ARG	Sidechain
1	A	744	ARG	Sidechain
1	B	318	ARG	Sidechain
1	B	352	ARG	Sidechain
1	B	441	ARG	Sidechain
1	B	461	ARG	Sidechain
1	B	552	ARG	Sidechain
1	B	571	ARG	Sidechain
1	B	744	ARG	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	4438	0	4468	82	0
1	B	4438	0	4468	88	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	26	0	16	2	0
3	B	26	0	16	3	0
4	A	53	0	25	2	0
4	B	53	0	25	2	0
5	A	28	0	0	1	0
5	B	28	0	0	1	0
All	All	9092	0	9018	166	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 (166) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:PRO:O	1:A:721:SER:OG	1.79	1.00
1:A:224:PRO:HD3	1:B:584:LEU:HG	1.54	0.88
1:A:584:LEU:HG	1:B:224:PRO:HD3	1.54	0.87
1:A:646:THR:HA	1:A:649:GLN:HG2	1.69	0.73
1:B:741:LEU:HD22	1:B:750:LEU:HD21	1.71	0.73
1:B:646:THR:HA	1:B:649:GLN:HG2	1.69	0.73
1:A:741:LEU:HD22	1:A:750:LEU:HD21	1.71	0.72
1:A:278:MET:HG2	1:A:280:LYS:NZ	2.05	0.72
1:B:278:MET:HG2	1:B:280:LYS:NZ	2.05	0.71
1:B:441:ARG:HH21	1:B:441:ARG:HG3	1.59	0.68
1:A:252:THR:HA	1:A:255:ILE:HD12	1.76	0.68
1:B:710:LYS:HG3	1:B:750:LEU:HD13	1.76	0.68
1:B:252:THR:HA	1:B:255:ILE:HD12	1.76	0.68
1:B:655:ASP:HB2	1:B:744:ARG:HD2	1.76	0.67
1:A:710:LYS:HG3	1:A:750:LEU:HD13	1.76	0.67
1:A:655:ASP:HB2	1:A:744:ARG:HD2	1.76	0.67
1:B:740:LEU:O	1:B:744:ARG:HG2	1.95	0.66
1:A:740:LEU:O	1:A:744:ARG:HG2	1.95	0.66
1:A:554:ILE:HD11	1:A:601:ARG:HD3	1.78	0.65
1:B:554:ILE:HD11	1:B:601:ARG:HD3	1.78	0.65
1:A:311:ASP:OD1	1:A:311:ASP:N	2.30	0.64
1:A:584:LEU:O	1:B:261:GLN:HG2	1.98	0.64
1:A:200:GLY:O	1:A:204:MET:HG3	1.99	0.63
1:B:200:GLY:O	1:B:204:MET:HG3	1.99	0.62
1:A:741:LEU:C	1:A:743:SER:H	2.08	0.61
1:B:741:LEU:C	1:B:743:SER:H	2.08	0.61
1:A:666:ASP:HB3	1:A:669:PRO:HD2	1.82	0.61
1:B:666:ASP:HB3	1:B:669:PRO:HD2	1.83	0.60
1:B:437:ARG:HB3	4:B:803:FAD:H52A	1.84	0.59
1:A:437:ARG:HB3	4:A:803:FAD:H52A	1.85	0.59
1:A:278:MET:HG2	1:A:280:LYS:HZ2	1.68	0.58
1:B:642:GLN:HB3	3:B:802:TPP:H61	1.87	0.57
1:A:457:ALA:HB1	1:A:481:ASN:ND2	2.21	0.56
1:B:260:PHE:CE2	1:B:261:GLN:HG3	2.41	0.55
1:A:379:LYS:O	1:A:383:GLU:HG2	2.06	0.55
1:B:457:ALA:HB1	1:B:481:ASN:ND2	2.21	0.55
1:B:556:THR:HG21	1:B:593:ALA:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:SER:OG	1:A:600:ALA:HB1	2.07	0.55
1:B:186:ASN:O	1:B:188:LYS:NZ	2.40	0.55
1:A:556:THR:HG21	1:A:593:ALA:HB3	1.87	0.55
1:B:379:LYS:O	1:B:383:GLU:HG2	2.06	0.55
1:B:212:SER:OG	1:B:600:ALA:HB1	2.07	0.55
1:A:210:ARG:NH1	1:A:580:THR:O	2.40	0.54
1:A:265:VAL:O	1:A:269:SER:OG	2.24	0.54
1:B:372:LEU:HD21	1:B:398:GLY:HA2	1.89	0.54
1:B:210:ARG:NH1	1:B:580:THR:O	2.40	0.54
1:A:186:ASN:O	1:A:188:LYS:NZ	2.40	0.54
1:B:278:MET:HG2	1:B:280:LYS:HZ2	1.73	0.54
1:A:493:ARG:HG2	1:A:493:ARG:HH11	1.74	0.53
1:A:665:PRO:HG2	1:A:667:PHE:CE1	2.45	0.52
1:B:265:VAL:O	1:B:269:SER:OG	2.24	0.52
1:B:493:ARG:HG2	1:B:493:ARG:HH11	1.74	0.52
1:B:278:MET:HG2	1:B:280:LYS:HZ3	1.73	0.52
5:B:804:A1CXH:C16	5:B:804:A1CXH:C18	2.88	0.52
1:A:372:LEU:HD21	1:A:398:GLY:HA2	1.91	0.51
1:B:591:LEU:HB3	1:B:592:PRO:HD3	1.93	0.51
1:A:496:LEU:O	1:A:498:HIS:N	2.44	0.51
5:A:804:A1CXH:C16	5:A:804:A1CXH:C18	2.88	0.51
1:B:665:PRO:HG2	1:B:667:PHE:CE1	2.45	0.51
1:A:659:HIS:O	1:B:173:PRO:HG2	2.11	0.51
1:A:440:ASP:OD2	1:A:440:ASP:N	2.40	0.50
1:A:668:VAL:HB	1:A:669:PRO:HD3	1.93	0.50
1:B:668:VAL:HB	1:B:669:PRO:HD3	1.93	0.50
1:A:591:LEU:HB3	1:A:592:PRO:HD3	1.93	0.50
1:A:605:LEU:HD21	1:A:607:ILE:HD11	1.94	0.50
1:A:173:PRO:HG2	1:B:659:HIS:O	2.11	0.50
1:A:391:PRO:HB2	1:A:410:LEU:HD11	1.94	0.50
1:A:425:MET:HE1	1:A:431:ILE:HG23	1.94	0.50
1:B:496:LEU:O	1:B:498:HIS:N	2.44	0.50
1:B:425:MET:HE1	1:B:431:ILE:HG23	1.94	0.49
1:B:311:ASP:OD1	1:B:311:ASP:N	2.30	0.49
1:A:457:ALA:HB1	1:A:481:ASN:HD21	1.77	0.49
1:A:699:GLY:O	1:A:700:PRO:C	2.55	0.49
1:B:195:PRO:HG3	1:B:201:ALA:HB2	1.95	0.49
1:B:605:LEU:HD21	1:B:607:ILE:HD11	1.93	0.49
1:A:556:THR:HG22	1:A:590:GLY:HA2	1.94	0.49
1:A:500:LYS:HB3	1:A:500:LYS:HE2	1.30	0.48
1:B:226:ALA:O	1:B:229:VAL:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:PRO:HB2	1:B:410:LEU:HD11	1.94	0.48
1:A:226:ALA:O	1:A:229:VAL:HG22	2.14	0.48
1:B:710:LYS:HG3	1:B:750:LEU:CD1	2.42	0.48
1:A:195:PRO:HG3	1:A:201:ALA:HB2	1.95	0.48
1:A:735:LYS:NZ	1:A:735:LYS:HB3	2.28	0.48
1:B:405:LEU:HD22	1:B:573:ARG:HD2	1.95	0.48
1:B:440:ASP:OD2	1:B:440:ASP:N	2.42	0.48
1:B:556:THR:HG22	1:B:590:GLY:HA2	1.94	0.48
1:B:547:ALA:HB3	1:B:548:PRO:HD3	1.95	0.48
1:B:457:ALA:HB1	1:B:481:ASN:HD21	1.78	0.47
1:B:735:LYS:NZ	1:B:735:LYS:HB3	2.28	0.47
1:A:547:ALA:HB3	1:A:548:PRO:HD3	1.95	0.47
1:B:699:GLY:O	1:B:700:PRO:C	2.55	0.47
1:A:405:LEU:HD22	1:A:573:ARG:HD2	1.95	0.47
1:B:741:LEU:O	1:B:743:SER:N	2.48	0.47
1:A:361:GLN:HE21	1:A:361:GLN:HA	1.80	0.47
1:B:647:GLN:O	1:B:651:LEU:HG	2.14	0.47
1:A:261:GLN:HG2	1:B:584:LEU:O	2.15	0.47
1:A:271:ALA:HB3	1:B:268:ILE:HG13	1.97	0.47
1:A:710:LYS:HG3	1:A:750:LEU:CD1	2.42	0.47
1:A:259:SER:OG	1:A:260:PHE:N	2.47	0.46
1:A:647:GLN:O	1:A:651:LEU:HG	2.15	0.46
1:B:361:GLN:HA	1:B:361:GLN:HE21	1.80	0.46
1:B:616:ASN:HA	1:B:619:LEU:HD23	1.98	0.46
1:B:649:GLN:HG3	1:B:657:TYR:CD1	2.51	0.46
1:B:423:MET:HE2	1:B:423:MET:HB3	1.66	0.46
1:A:741:LEU:C	1:A:743:SER:N	2.73	0.46
3:A:802:TPP:HN42	3:A:802:TPP:C2	2.29	0.46
1:B:259:SER:OG	1:B:260:PHE:N	2.49	0.46
1:A:655:ASP:HB2	1:A:744:ARG:CD	2.46	0.46
1:A:649:GLN:HG3	1:A:657:TYR:CD1	2.51	0.45
1:B:666:ASP:O	1:B:667:PHE:HB2	2.17	0.45
1:A:268:ILE:HG13	1:B:271:ALA:HB3	1.97	0.45
1:A:621:GLU:HA	1:A:624:THR:HG23	1.99	0.45
1:B:441:ARG:HG3	1:B:441:ARG:NH2	2.25	0.45
1:B:741:LEU:C	1:B:743:SER:N	2.73	0.45
1:A:616:ASN:HA	1:A:619:LEU:HD23	1.98	0.45
1:B:500:LYS:HE2	1:B:500:LYS:HB3	1.31	0.45
1:A:666:ASP:O	1:A:667:PHE:HB2	2.16	0.45
1:B:162:LEU:HD22	1:B:189:HIS:CE1	2.52	0.45
1:B:655:ASP:HB2	1:B:744:ARG:CD	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:GLN:HG3	1:A:250:VAL:N	2.32	0.45
1:B:249:GLN:HG3	1:B:250:VAL:N	2.32	0.45
1:B:423:MET:HG2	1:B:726:PHE:HE2	1.82	0.45
1:B:468:GLU:OE2	4:B:803:FAD:O2B	2.34	0.45
1:B:507:GLU:H	1:B:507:GLU:HG2	1.46	0.45
1:A:162:LEU:HD22	1:A:189:HIS:CE1	2.52	0.44
1:B:621:GLU:HA	1:B:624:THR:HG23	1.98	0.44
1:A:468:GLU:OE2	4:A:803:FAD:O2B	2.35	0.44
1:A:741:LEU:O	1:A:743:SER:N	2.48	0.44
1:B:372:LEU:CD2	1:B:398:GLY:HA2	2.47	0.44
1:A:420:TYR:CG	1:A:516:LYS:HG2	2.53	0.44
1:A:496:LEU:N	1:A:497:PRO:HD2	2.33	0.44
1:B:551:ASP:OD1	1:B:552:ARG:HG2	2.18	0.43
1:A:278:MET:HG2	1:A:280:LYS:HZ3	1.79	0.43
1:A:423:MET:HG2	1:A:726:PHE:HE2	1.82	0.43
1:A:551:ASP:OD1	1:A:552:ARG:HG2	2.18	0.43
3:A:802:TPP:HN42	3:A:802:TPP:H2	1.83	0.43
1:A:460:LYS:N	1:A:460:LYS:HD2	2.34	0.43
1:A:372:LEU:CD2	1:A:398:GLY:HA2	2.47	0.43
1:B:496:LEU:N	1:B:497:PRO:HD2	2.33	0.43
1:B:260:PHE:CZ	1:B:261:GLN:HG3	2.54	0.43
1:B:420:TYR:CG	1:B:516:LYS:HG2	2.54	0.43
1:B:595:ILE:O	1:B:599:VAL:HG23	2.19	0.42
1:A:365:LEU:HD23	1:A:432:ILE:HB	2.02	0.42
1:B:738:LYS:HD3	1:B:742:ARG:HH12	1.84	0.42
1:B:317:LEU:O	1:B:318:ARG:HB2	2.19	0.42
1:A:595:ILE:O	1:A:599:VAL:HG23	2.19	0.42
1:B:460:LYS:N	1:B:460:LYS:HD2	2.34	0.42
1:A:317:LEU:O	1:A:318:ARG:HB2	2.20	0.42
1:B:178:LEU:HD12	1:B:178:LEU:HA	1.88	0.41
1:B:365:LEU:HD23	1:B:432:ILE:HB	2.02	0.41
1:A:178:LEU:HD12	1:A:178:LEU:HA	1.88	0.41
1:B:750:LEU:O	1:B:751:HIS:CB	2.68	0.41
1:A:636:LEU:HD23	1:A:704:GLU:HG3	2.02	0.41
1:A:680:ARG:O	1:A:690:LYS:NZ	2.53	0.41
1:A:617:MET:HG2	1:B:196:ARG:O	2.20	0.41
1:A:738:LYS:HD3	1:A:742:ARG:HH12	1.86	0.41
1:B:636:LEU:HD23	1:B:704:GLU:HG3	2.02	0.41
1:A:196:ARG:O	1:B:617:MET:HG2	2.21	0.41
1:A:252:THR:HG23	1:A:311:ASP:OD2	2.21	0.41
1:A:615:PHE:HZ	1:A:622:LEU:HD11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:750:LEU:O	1:A:751:HIS:CB	2.68	0.41
3:B:802:TPP:C2	3:B:802:TPP:HN42	2.34	0.40
3:B:802:TPP:HN42	3:B:802:TPP:H2	1.86	0.40
1:B:252:THR:HG23	1:B:311:ASP:OD2	2.21	0.40
1:B:680:ARG:O	1:B:690:LYS:NZ	2.53	0.40
1:B:742:ARG:HH11	1:B:742:ARG:HD3	1.77	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	573/641 (89%)	544 (95%)	25 (4%)	4 (1%)	18	20
1	B	573/641 (89%)	544 (95%)	25 (4%)	4 (1%)	18	20
All	All	1146/1282 (89%)	1088 (95%)	50 (4%)	8 (1%)	20	20

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	751	HIS
1	B	751	HIS
1	A	667	PHE
1	B	667	PHE
1	A	742	ARG
1	B	742	ARG
1	A	665	PRO
1	B	665	PRO

### 5.3.2 Protein sidechains ⓘ

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	473/532 (89%)	441 (93%)	32 (7%)	14	16
1	B	473/532 (89%)	442 (93%)	31 (7%)	15	17
All	All	946/1064 (89%)	883 (93%)	63 (7%)	17	17

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	311	ASP
1	A	317	LEU
1	A	351	ASP
1	A	371	LEU
1	A	378	PRO
1	A	405	LEU
1	A	418	SER
1	A	423	MET
1	A	425	MET
1	A	440	ASP
1	A	470	MET
1	A	473	ASN
1	A	478	VAL
1	A	485	GLU
1	A	507	GLU
1	A	508	TRP
1	A	534	LYS
1	A	541	LYS
1	A	555	ILE
1	A	578	MET
1	A	619	LEU
1	A	623	THR
1	A	624	THR
1	A	639	ASN
1	A	658	SER
1	A	663	LYS
1	A	666	ASP

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Mol	Chain	Res	Type
1	A	721	SER
1	A	728	VAL
1	A	741	LEU
1	A	743	SER
1	A	750	LEU
1	B	311	ASP
1	B	317	LEU
1	B	351	ASP
1	B	371	LEU
1	B	378	PRO
1	B	405	LEU
1	B	418	SER
1	B	423	MET
1	B	425	MET
1	B	440	ASP
1	B	470	MET
1	B	473	ASN
1	B	478	VAL
1	B	485	GLU
1	B	507	GLU
1	B	508	TRP
1	B	534	LYS
1	B	541	LYS
1	B	555	ILE
1	B	578	MET
1	B	619	LEU
1	B	623	THR
1	B	624	THR
1	B	639	ASN
1	B	658	SER
1	B	663	LYS
1	B	666	ASP
1	B	728	VAL
1	B	741	LEU
1	B	743	SER
1	B	750	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	361	GLN
1	A	416	HIS

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Mol	Chain	Res	Type
1	A	426	GLN
1	A	452	GLN
1	A	479	GLN
1	A	481	ASN
1	A	561	GLN
1	A	563	GLN
1	A	574	HIS
1	A	638	ASN
1	B	361	GLN
1	B	426	GLN
1	B	452	GLN
1	B	473	ASN
1	B	481	ASN
1	B	561	GLN
1	B	563	GLN
1	B	574	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	A1CXH	A	804	1	28,30,30	1.72	1 (3%)	27,44,44	2.62	5 (18%)
4	FAD	A	803	-	58,58,58	2.76	19 (32%)	85,89,89	2.18	27 (31%)
5	A1CXH	B	804	1	28,30,30	1.72	1 (3%)	27,44,44	2.62	5 (18%)
3	TPP	A	802	2	26,27,27	1.12	2 (7%)	38,40,40	1.66	3 (7%)
3	TPP	B	802	2	26,27,27	2.91	11 (42%)	38,40,40	4.19	11 (28%)
4	FAD	B	803	-	58,58,58	2.75	19 (32%)	85,89,89	2.19	28 (32%)

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
5	A1CXH	A	804	1	-	2/11/64/64	0/3/3/3
4	FAD	A	803	-	1/1/9/9	7/34/50/50	0/6/6/6
5	A1CXH	B	804	1	-	2/11/64/64	0/3/3/3
3	TPP	A	802	2	-	4/17/17/17	0/2/2/2
3	TPP	B	802	2	-	5/17/17/17	0/2/2/2
4	FAD	B	803	-	1/1/9/9	6/34/50/50	0/6/6/6

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	FAD	O2'-C2'	-10.87	1.20	1.43
4	B	803	FAD	O2'-C2'	-10.81	1.20	1.43
5	A	804	A1CXH	C11-C10	-8.63	1.32	1.52
5	B	804	A1CXH	C11-C10	-8.61	1.32	1.52
3	B	802	TPP	C2-S1	-7.05	1.47	1.69
4	A	803	FAD	O4B-C4B	-6.71	1.30	1.45
4	B	803	FAD	O4B-C4B	-6.69	1.30	1.45
4	B	803	FAD	O4'-C4'	-6.05	1.30	1.43
4	A	803	FAD	O4'-C4'	-6.05	1.30	1.43
3	B	802	TPP	C5-C4	6.03	1.47	1.35
3	B	802	TPP	C4-N3	5.46	1.51	1.39
4	A	803	FAD	O4B-C1B	-5.40	1.29	1.42
4	B	803	FAD	O4B-C1B	-5.33	1.29	1.42
4	B	803	FAD	O3'-C3'	-4.48	1.31	1.43
4	A	803	FAD	O3'-C3'	-4.47	1.31	1.43
4	A	803	FAD	O5B-C5B	-4.39	1.28	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	803	FAD	O5B-C5B	-4.37	1.28	1.44
4	B	803	FAD	O2B-C2B	-4.32	1.32	1.43
4	A	803	FAD	O2B-C2B	-4.29	1.32	1.43
4	A	803	FAD	O3B-C3B	-4.27	1.32	1.43
4	B	803	FAD	O3B-C3B	-4.24	1.32	1.43
4	A	803	FAD	O5'-C5'	-4.19	1.28	1.44
4	B	803	FAD	O5'-C5'	-4.18	1.28	1.44
3	B	802	TPP	C5'-C4'	-3.95	1.36	1.42
3	B	802	TPP	C4'-N4'	3.90	1.44	1.34
3	B	802	TPP	C2-N3	3.54	1.41	1.32
3	B	802	TPP	PB-O3B	-3.14	1.43	1.54
3	A	802	TPP	C5-S1	-3.03	1.64	1.72
3	B	802	TPP	PB-O2B	-3.02	1.43	1.54
4	A	803	FAD	C4-N3	-3.00	1.33	1.38
4	B	803	FAD	C4-N3	-3.00	1.33	1.38
4	B	803	FAD	C4X-N5	2.94	1.37	1.30
4	B	803	FAD	PA-O2A	-2.83	1.42	1.55
4	A	803	FAD	PA-O2A	-2.83	1.42	1.55
3	B	802	TPP	PA-O2A	-2.76	1.42	1.55
4	A	803	FAD	C4X-N5	2.75	1.36	1.30
4	B	803	FAD	C2-N3	-2.63	1.33	1.39
4	B	803	FAD	PA-O5B	2.61	1.69	1.59
4	A	803	FAD	PA-O5B	2.59	1.69	1.59
4	A	803	FAD	C2-N3	-2.58	1.33	1.39
4	A	803	FAD	C3B-C4B	-2.52	1.46	1.53
3	A	802	TPP	C5-C4	2.47	1.40	1.35
4	A	803	FAD	C4X-C4	-2.43	1.35	1.44
4	B	803	FAD	C3B-C4B	-2.42	1.46	1.53
3	B	802	TPP	C4'-N3'	-2.39	1.31	1.35
4	B	803	FAD	C4X-C4	-2.38	1.35	1.44
3	B	802	TPP	PB-O1B	-2.34	1.43	1.50
4	A	803	FAD	P-O1P	-2.23	1.43	1.50
4	B	803	FAD	P-O1P	-2.23	1.43	1.50
4	B	803	FAD	C4'-C3'	-2.18	1.49	1.53
4	A	803	FAD	C4X-C10	-2.17	1.37	1.44
4	B	803	FAD	C4X-C10	-2.15	1.37	1.44
4	A	803	FAD	C4'-C3'	-2.11	1.49	1.53

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	TPP	C2-S1-C5	22.84	106.34	91.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	804	A1CXH	C10-C11-C12	8.81	123.55	113.19
5	A	804	A1CXH	C10-C11-C12	8.77	123.50	113.19
3	A	802	TPP	C2-S1-C5	8.62	96.92	91.22
5	A	804	A1CXH	C11-C10-C09	7.38	123.25	111.33
5	B	804	A1CXH	C11-C10-C09	7.36	123.23	111.33
4	A	803	FAD	C4-N3-C2	-7.05	113.11	125.64
4	B	803	FAD	C4-N3-C2	-7.03	113.16	125.64
4	A	803	FAD	C1'-C2'-C3'	6.96	128.53	109.66
4	B	803	FAD	C1'-C2'-C3'	6.93	128.46	109.66
5	B	804	A1CXH	C13-C12-C11	-5.59	99.42	108.31
5	A	804	A1CXH	C13-C12-C11	-5.57	99.45	108.31
4	A	803	FAD	O2-C2-N1	-5.30	113.00	121.80
4	B	803	FAD	O2-C2-N1	-5.27	113.05	121.80
4	A	803	FAD	C4X-C4-N3	4.78	125.41	113.25
4	B	803	FAD	C4X-C4-N3	4.77	125.38	113.25
4	B	803	FAD	C4-C4X-N5	4.35	124.21	118.21
3	B	802	TPP	CM2-C2'-N1'	4.23	121.70	117.20
4	A	803	FAD	C4-C4X-N5	4.20	124.00	118.21
3	B	802	TPP	S1-C2-N3	-4.18	107.00	112.30
4	A	803	FAD	C9A-C5X-N5	-4.17	118.02	122.45
4	B	803	FAD	C9A-C5X-N5	-4.15	118.06	122.45
3	B	802	TPP	N1'-C2'-N3'	-3.95	118.97	125.53
3	B	802	TPP	O2B-PB-O3A	3.61	116.75	104.64
3	B	802	TPP	C5-C4-N3	-3.59	105.14	111.67
3	B	802	TPP	C4-C5-S1	-3.45	105.19	110.56
4	B	803	FAD	N3-C2-N1	3.35	126.61	119.50
4	A	803	FAD	N3-C2-N1	3.34	126.59	119.50
4	B	803	FAD	C9A-C9-C8	3.29	125.83	119.22
4	A	803	FAD	C9A-C9-C8	3.26	125.79	119.22
4	B	803	FAD	O2'-C2'-C3'	3.24	116.83	109.25
4	A	803	FAD	O2'-C2'-C3'	3.23	116.80	109.25
3	B	802	TPP	C6'-N1'-C2'	3.10	121.17	116.07
4	B	803	FAD	C4X-C10-N10	3.04	120.84	116.48
4	B	803	FAD	O3B-C3B-C4B	-2.95	102.60	111.08
4	A	803	FAD	O3B-C3B-C4B	-2.95	102.61	111.08
4	A	803	FAD	C4X-C10-N10	2.95	120.70	116.48
4	B	803	FAD	O4B-C1B-N9A	2.80	113.47	108.09
4	A	803	FAD	O4-C4-C4X	-2.80	119.14	126.53
4	B	803	FAD	C10-C4X-N5	-2.79	119.11	124.81
4	A	803	FAD	O4B-C1B-N9A	2.76	113.40	108.09
4	B	803	FAD	C6-C5X-N5	2.74	122.99	118.44
4	A	803	FAD	C10-C4X-N5	-2.70	119.29	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	803	FAD	O4-C4-C4X	-2.69	119.44	126.53
4	A	803	FAD	C6-C5X-N5	2.68	122.89	118.44
4	A	803	FAD	C5B-C4B-C3B	-2.66	105.62	115.21
4	B	803	FAD	O4B-C1B-C2B	-2.65	100.95	106.62
4	B	803	FAD	O4-C4-N3	-2.63	115.18	120.11
4	A	803	FAD	O4B-C1B-C2B	-2.62	101.01	106.62
3	B	802	TPP	CM4-C4-N3	2.59	126.55	120.57
4	B	803	FAD	C5B-C4B-C3B	-2.58	105.91	115.21
4	A	803	FAD	O4B-C4B-C5B	2.56	117.55	109.33
4	B	803	FAD	O4B-C4B-C5B	2.56	117.54	109.33
4	A	803	FAD	C5A-C4A-N9A	2.52	108.56	105.81
4	B	803	FAD	C5A-C4A-N9A	2.52	108.56	105.81
3	B	802	TPP	O3B-PB-O3A	2.51	113.05	104.64
5	B	804	A1CXH	C03-C04-C15	-2.48	109.97	114.16
4	A	803	FAD	O4-C4-N3	-2.48	115.45	120.11
5	A	804	A1CXH	C03-C04-C15	-2.45	110.03	114.16
3	A	802	TPP	C6-C5-C4	2.32	133.99	128.17
4	A	803	FAD	O4'-C4'-C5'	-2.31	104.88	109.99
4	B	803	FAD	O4'-C4'-C5'	-2.30	104.92	109.99
3	B	802	TPP	O2A-PA-O1A	-2.28	101.86	112.44
4	A	803	FAD	O2P-P-O1P	2.26	122.95	112.44
4	B	803	FAD	O2P-P-O1P	2.25	122.92	112.44
4	A	803	FAD	O5'-P-O1P	-2.21	100.17	108.94
4	B	803	FAD	O5'-P-O1P	-2.21	100.19	108.94
4	A	803	FAD	C5A-C4A-N3A	-2.20	123.69	126.72
4	B	803	FAD	C5A-C4A-N3A	-2.19	123.69	126.72
5	A	804	A1CXH	C13-C12-C14	-2.19	108.28	111.83
4	A	803	FAD	O5B-PA-O1A	-2.19	100.24	108.94
4	B	803	FAD	O5B-PA-O1A	-2.18	100.31	108.94
4	A	803	FAD	O2A-PA-O3P	2.17	113.14	107.27
4	B	803	FAD	O2A-PA-O3P	2.16	113.11	107.27
5	B	804	A1CXH	C13-C12-C14	-2.15	108.35	111.83
4	A	803	FAD	C9-C8-C7	-2.02	116.72	119.69
4	B	803	FAD	C9-C8-C7	-2.02	116.72	119.69
4	B	803	FAD	C4A-N9A-C1B	2.02	131.36	126.63
3	A	802	TPP	C4-C5-S1	-2.01	107.43	110.56

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	803	FAD	C2'
4	B	803	FAD	C2'

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	TPP	PA-O3A-PB-O2B
3	B	802	TPP	C5-C6-C7-O7
3	B	802	TPP	C7-O7-PA-O2A
3	B	802	TPP	PA-O3A-PB-O2B
3	B	802	TPP	PA-O3A-PB-O3B
4	A	803	FAD	N10-C1'-C2'-O2'
4	A	803	FAD	C1'-C2'-C3'-C4'
4	B	803	FAD	N10-C1'-C2'-O2'
4	B	803	FAD	C1'-C2'-C3'-C4'
5	A	804	A1CXH	C11-C12-C18-C19
5	A	804	A1CXH	C11-C12-C18-C27
5	B	804	A1CXH	C11-C12-C18-C19
5	B	804	A1CXH	C11-C12-C18-C27
4	A	803	FAD	O2'-C2'-C3'-C4'
4	B	803	FAD	O2'-C2'-C3'-C4'
4	A	803	FAD	O2'-C2'-C3'-O3'
4	B	803	FAD	O2'-C2'-C3'-O3'
4	A	803	FAD	C1'-C2'-C3'-O3'
3	A	802	TPP	PA-O3A-PB-O3B
3	B	802	TPP	C7-O7-PA-O3A
4	A	803	FAD	PA-O3P-P-O1P
4	B	803	FAD	PA-O3P-P-O1P
4	B	803	FAD	PA-O3P-P-O2P
3	A	802	TPP	PA-O3A-PB-O1B
3	A	802	TPP	C5-C6-C7-O7
4	A	803	FAD	PA-O3P-P-O2P

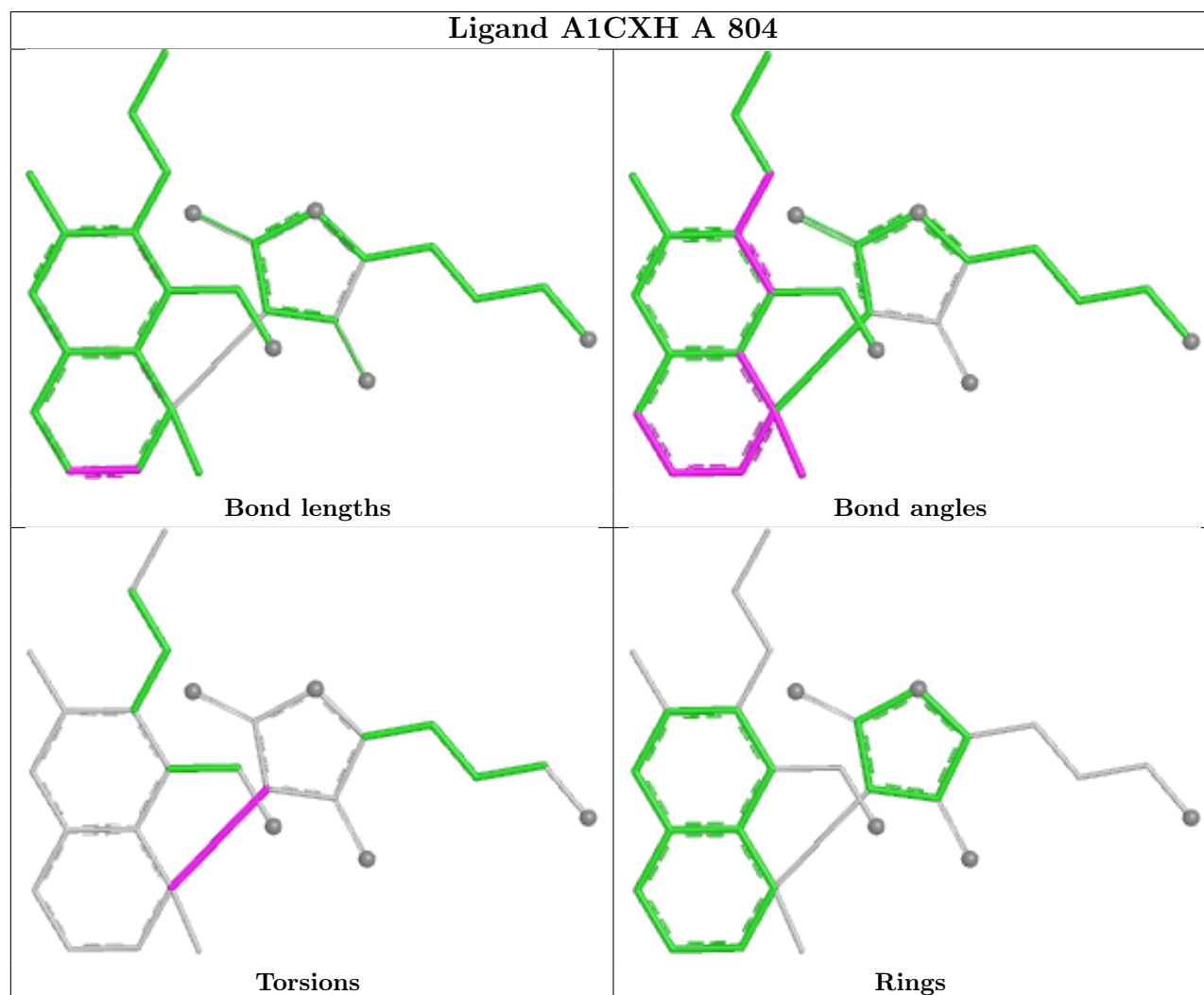
There are no ring outliers.

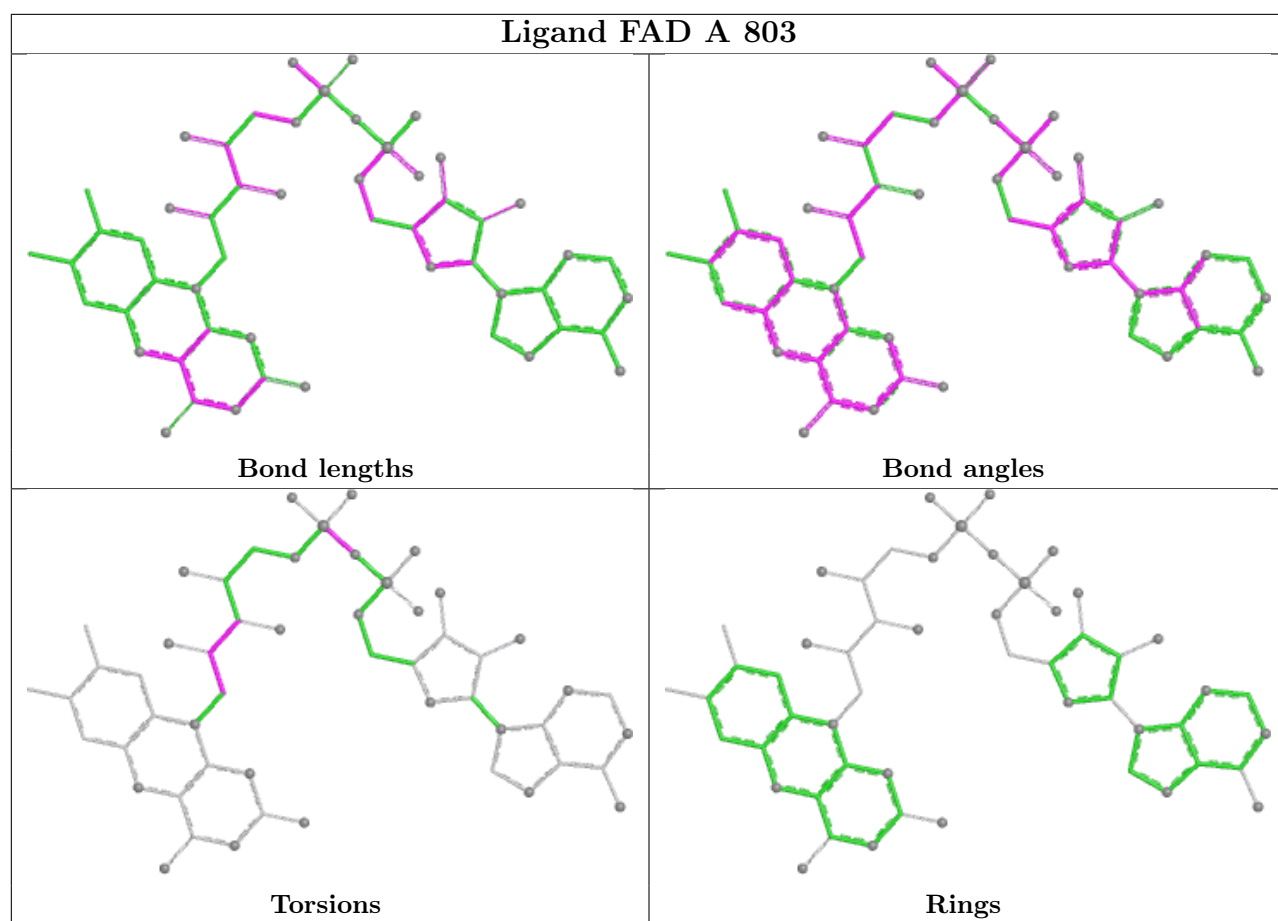
6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	804	A1CXH	1	0
4	A	803	FAD	2	0
5	B	804	A1CXH	1	0
3	A	802	TPP	2	0
3	B	802	TPP	3	0
4	B	803	FAD	2	0

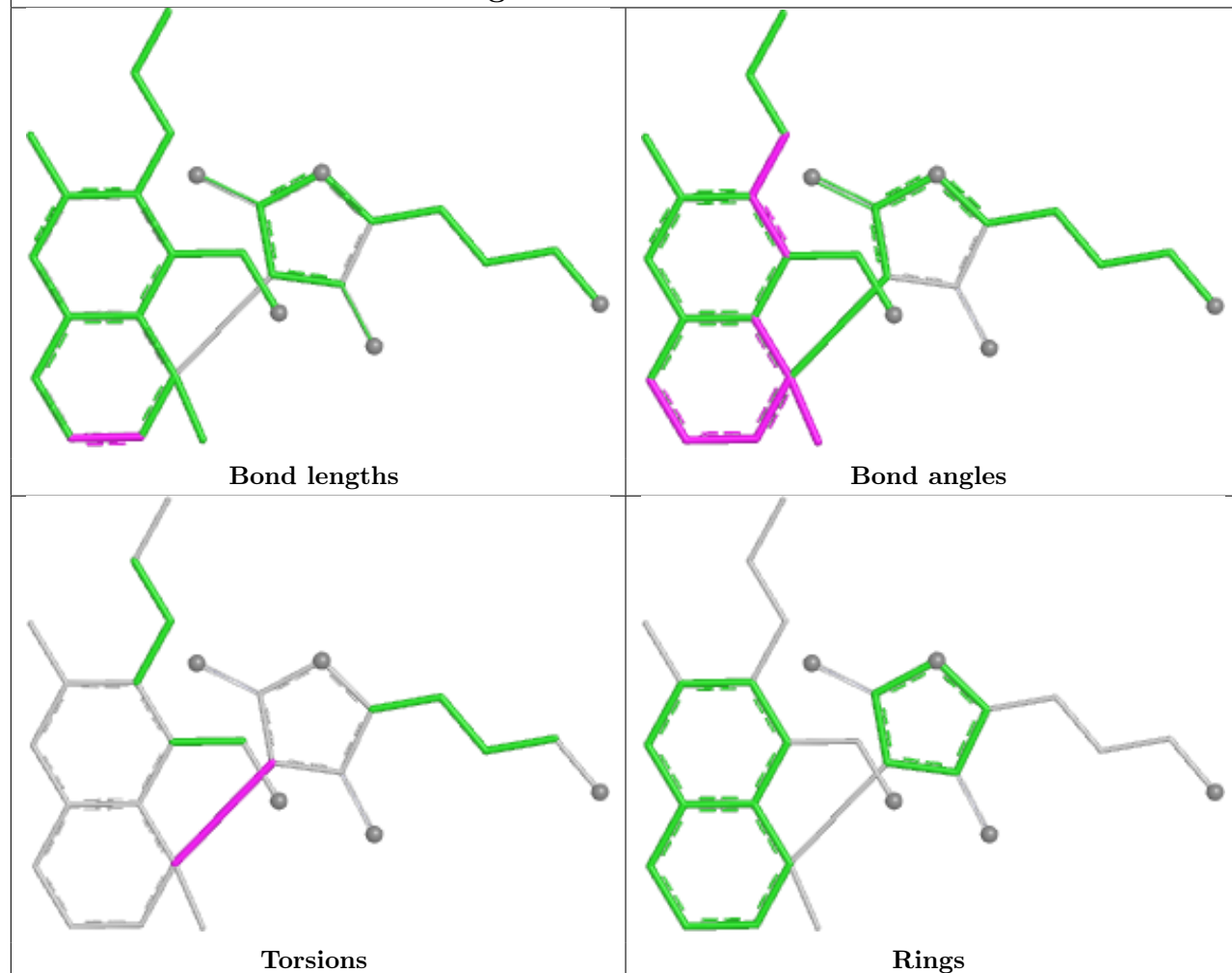
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

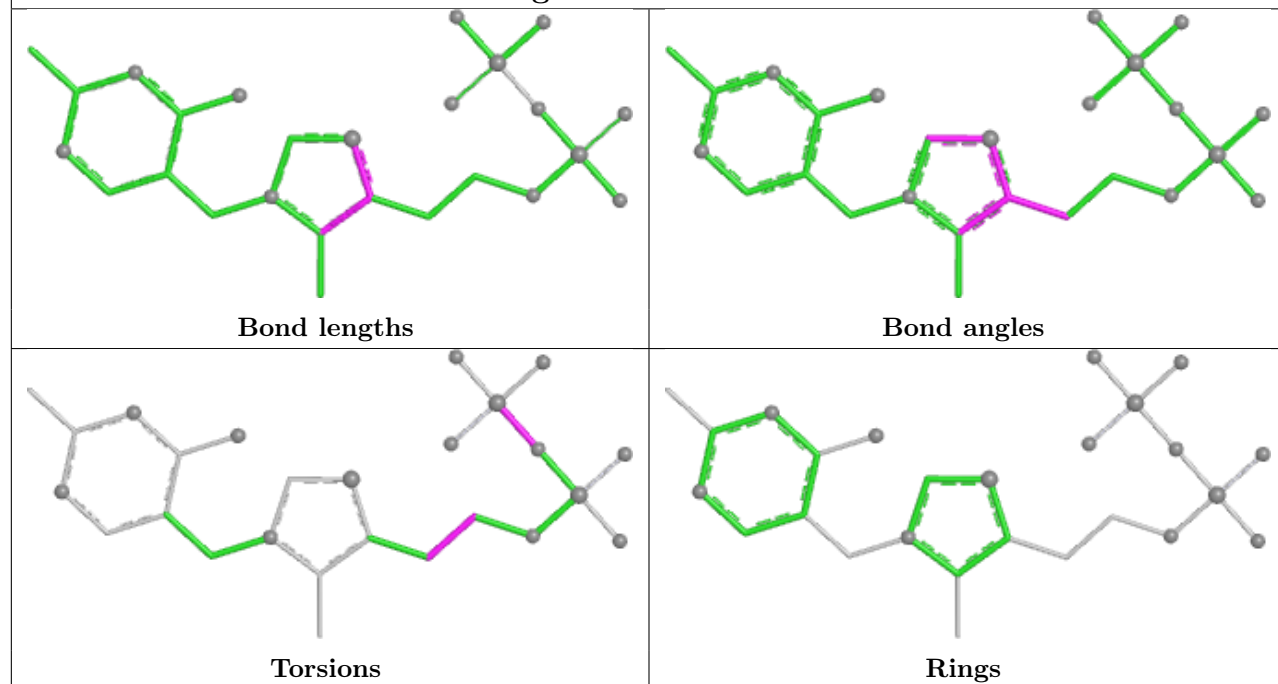


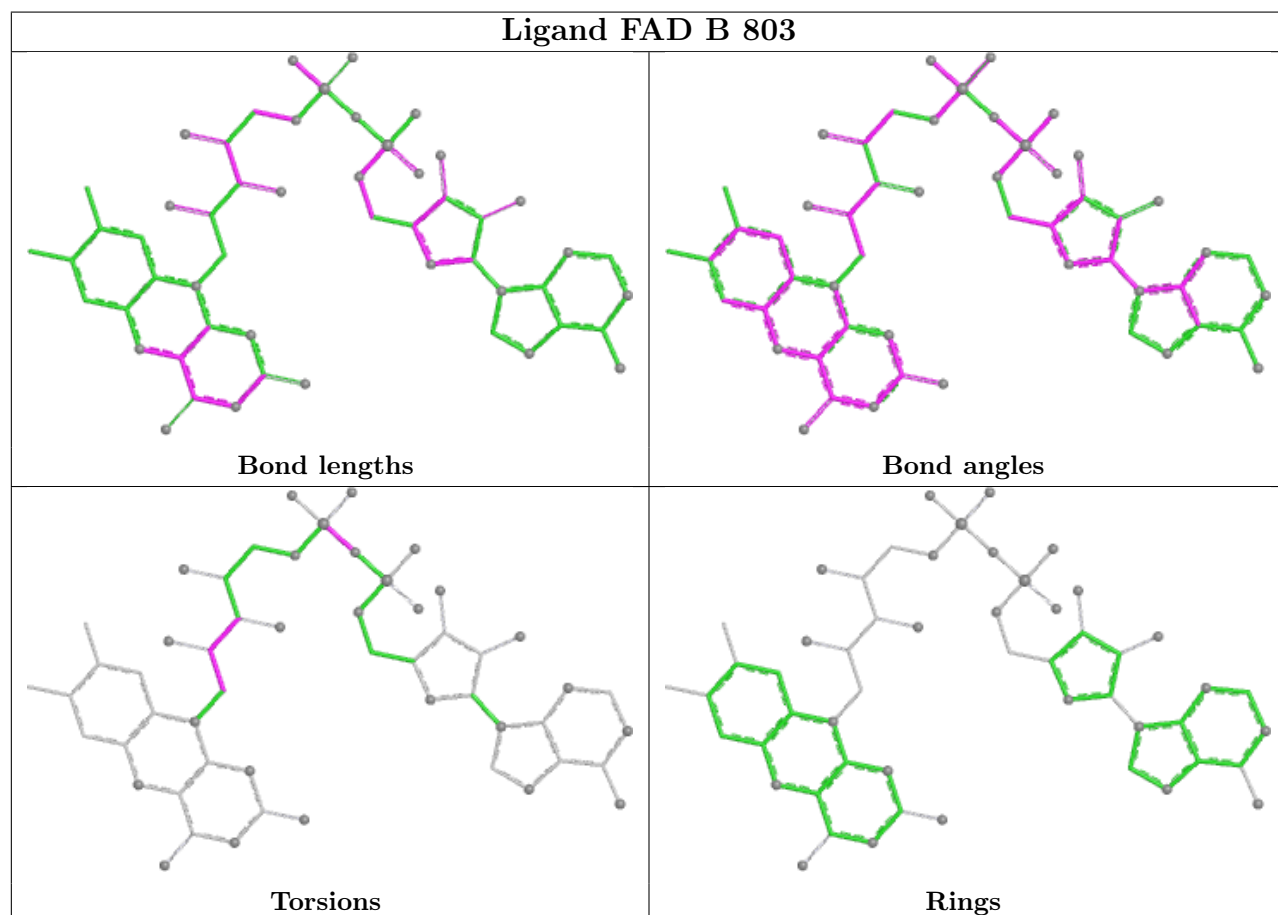
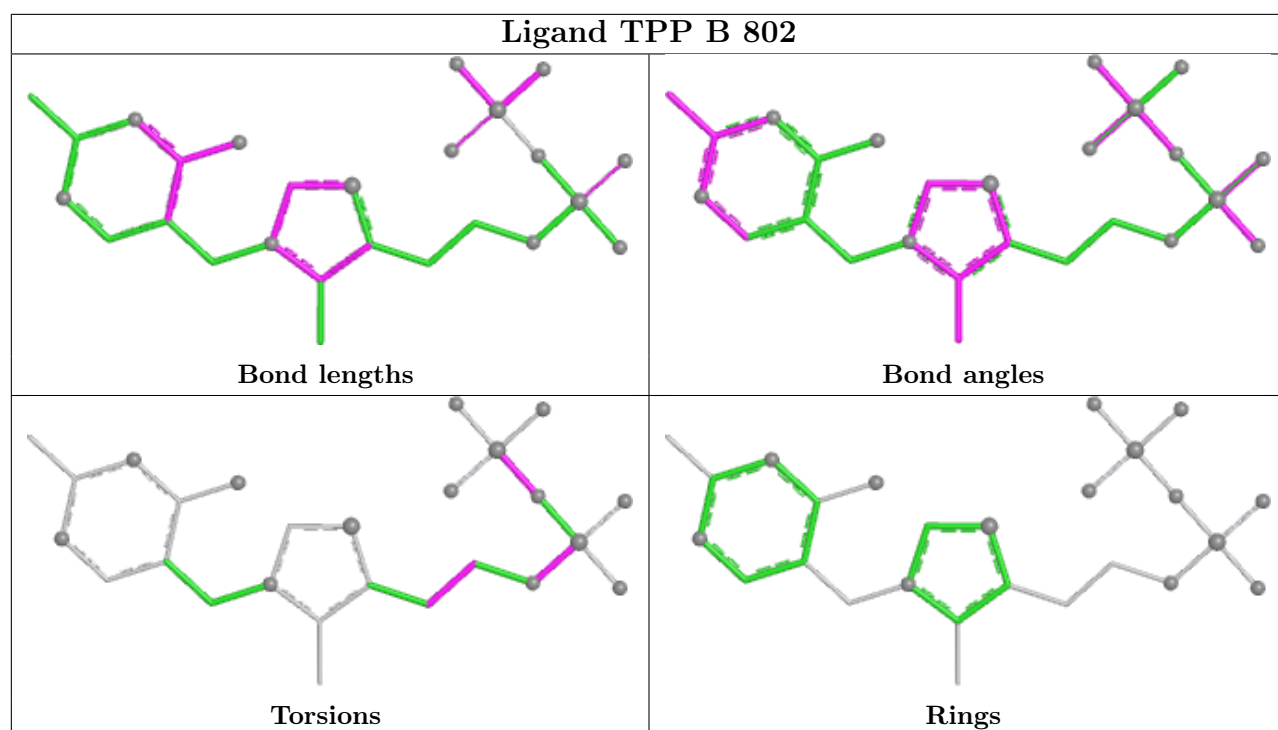


## Ligand A1CXH B 804



## Ligand TPP A 802





## 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.



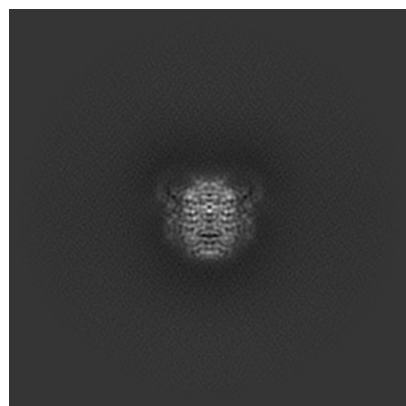
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73041. These allow visual inspection of the internal detail of the map and identification of artifacts.

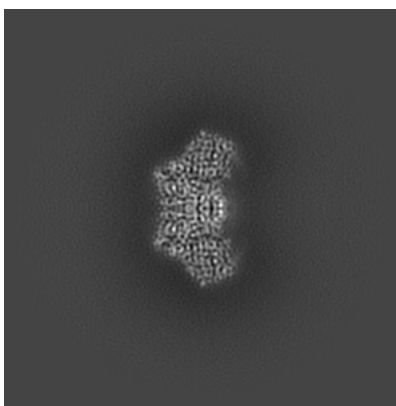
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

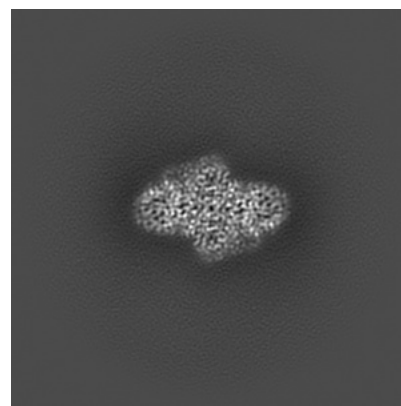
#### 6.1.1 Primary map



X

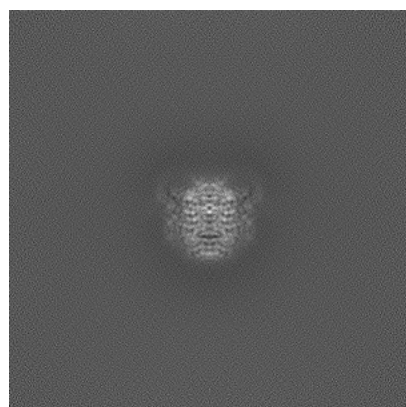


Y

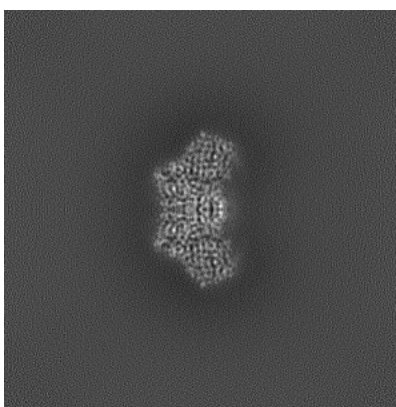


Z

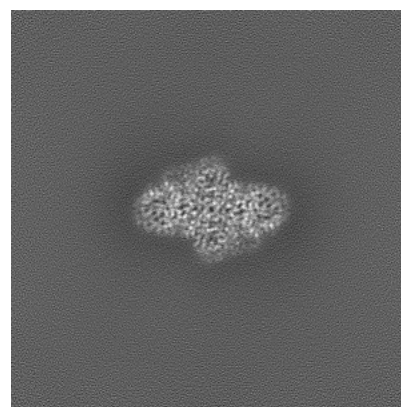
#### 6.1.2 Raw map



X



Y

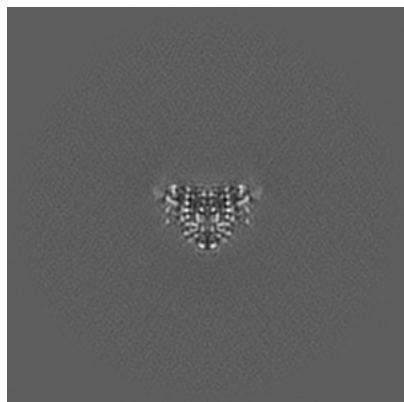


Z

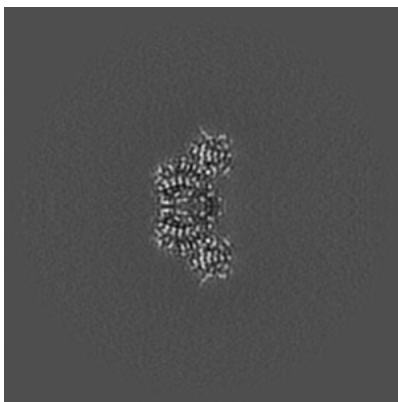
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

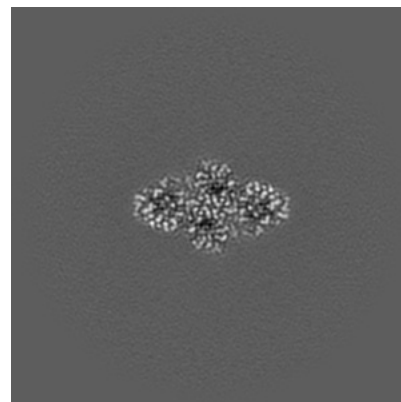
### 6.2.1 Primary map



X Index: 192

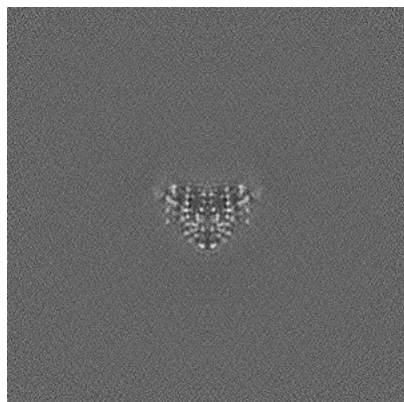


Y Index: 192

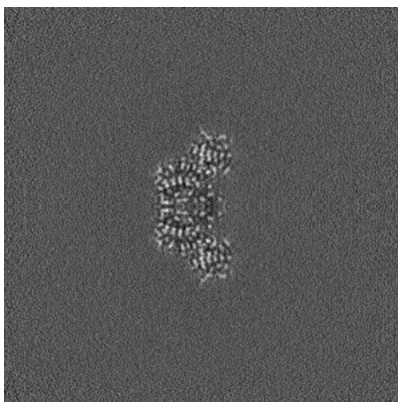


Z Index: 192

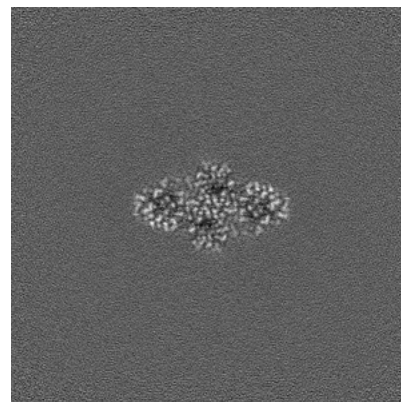
### 6.2.2 Raw map



X Index: 192



Y Index: 192

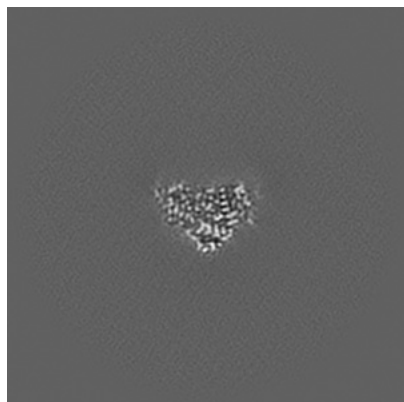


Z Index: 192

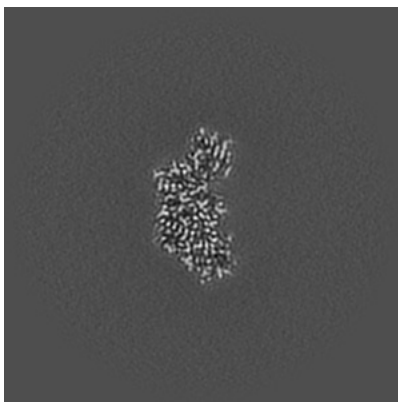
The images above show central slices of the map in three orthogonal directions.

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

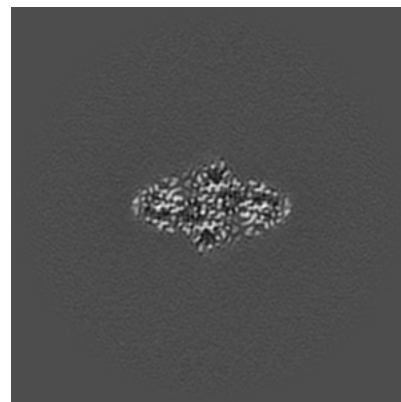
### 6.3.1 Primary map



X Index: 198

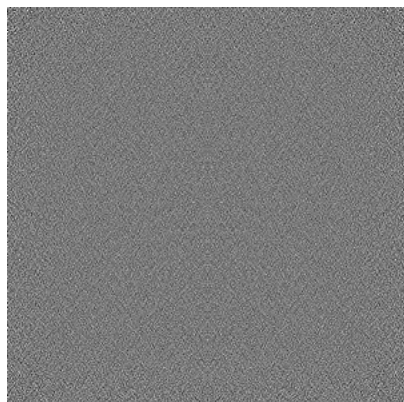


Y Index: 187

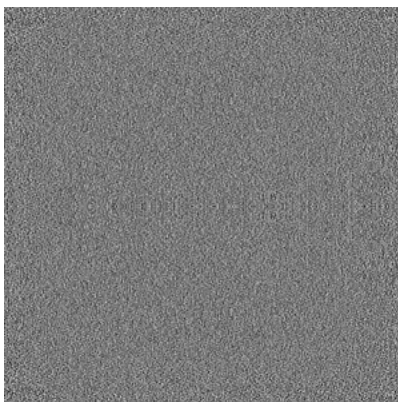


Z Index: 189

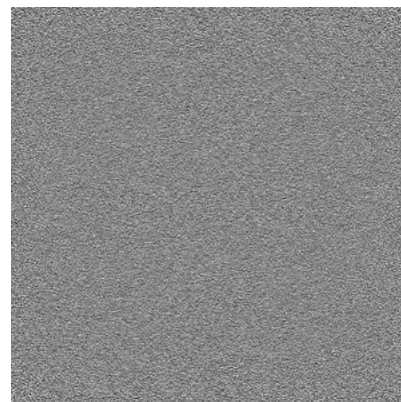
### 6.3.2 Raw map



X Index: 0



Y Index: 0



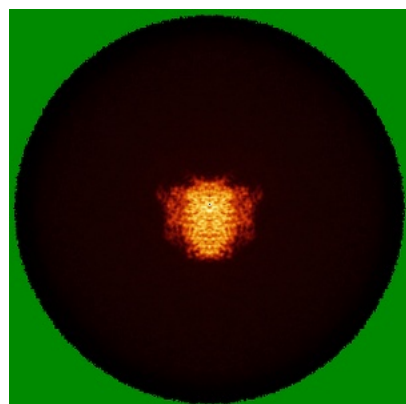
Z Index: 383

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

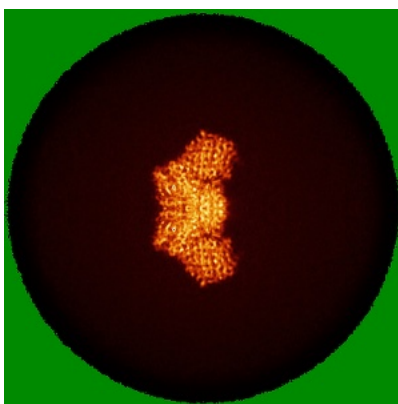


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

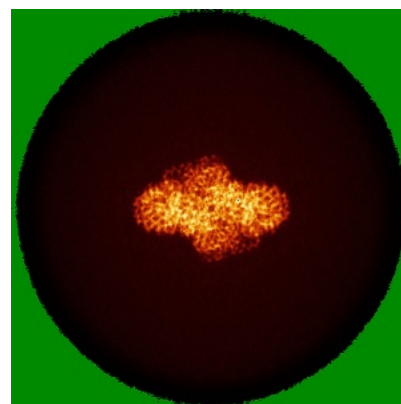
### 6.4.1 Primary map



X

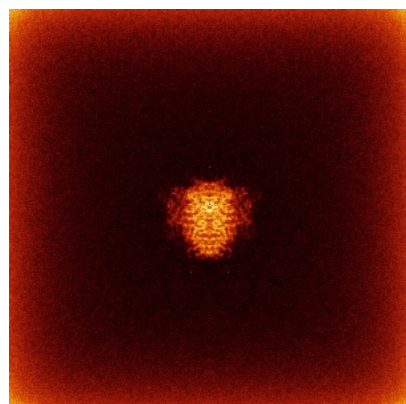


Y

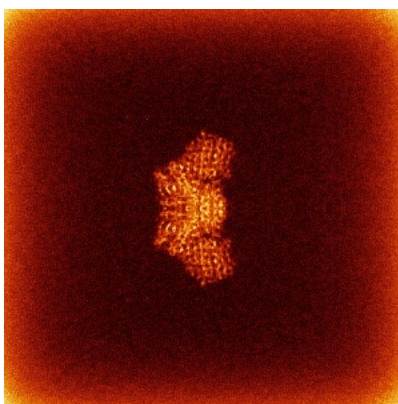


Z

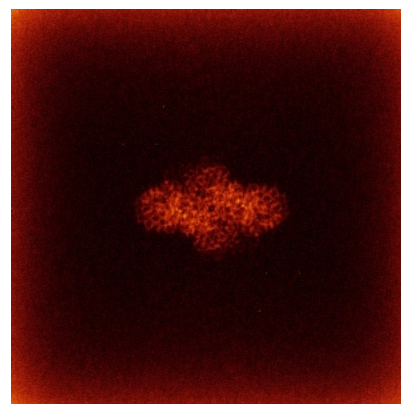
### 6.4.2 Raw map



X



Y

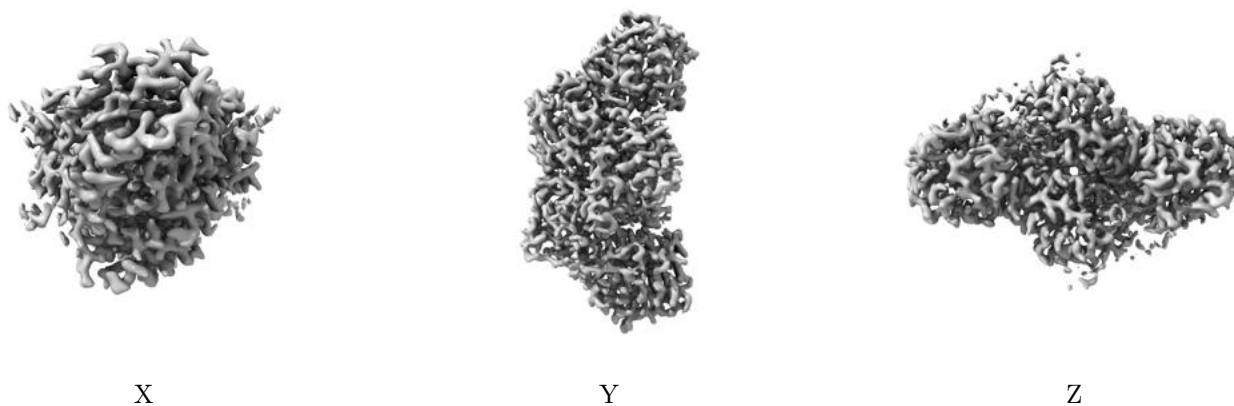


Z

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

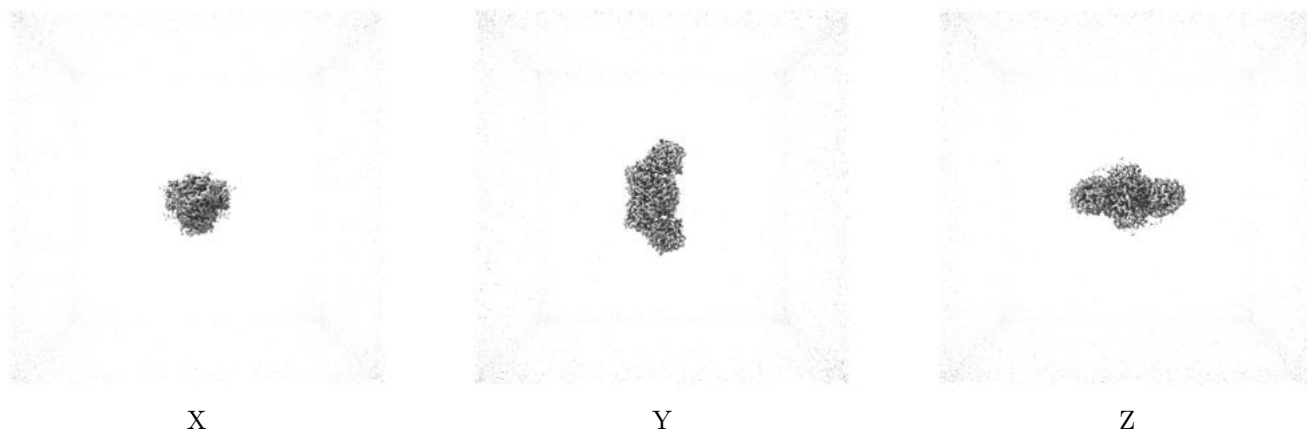
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

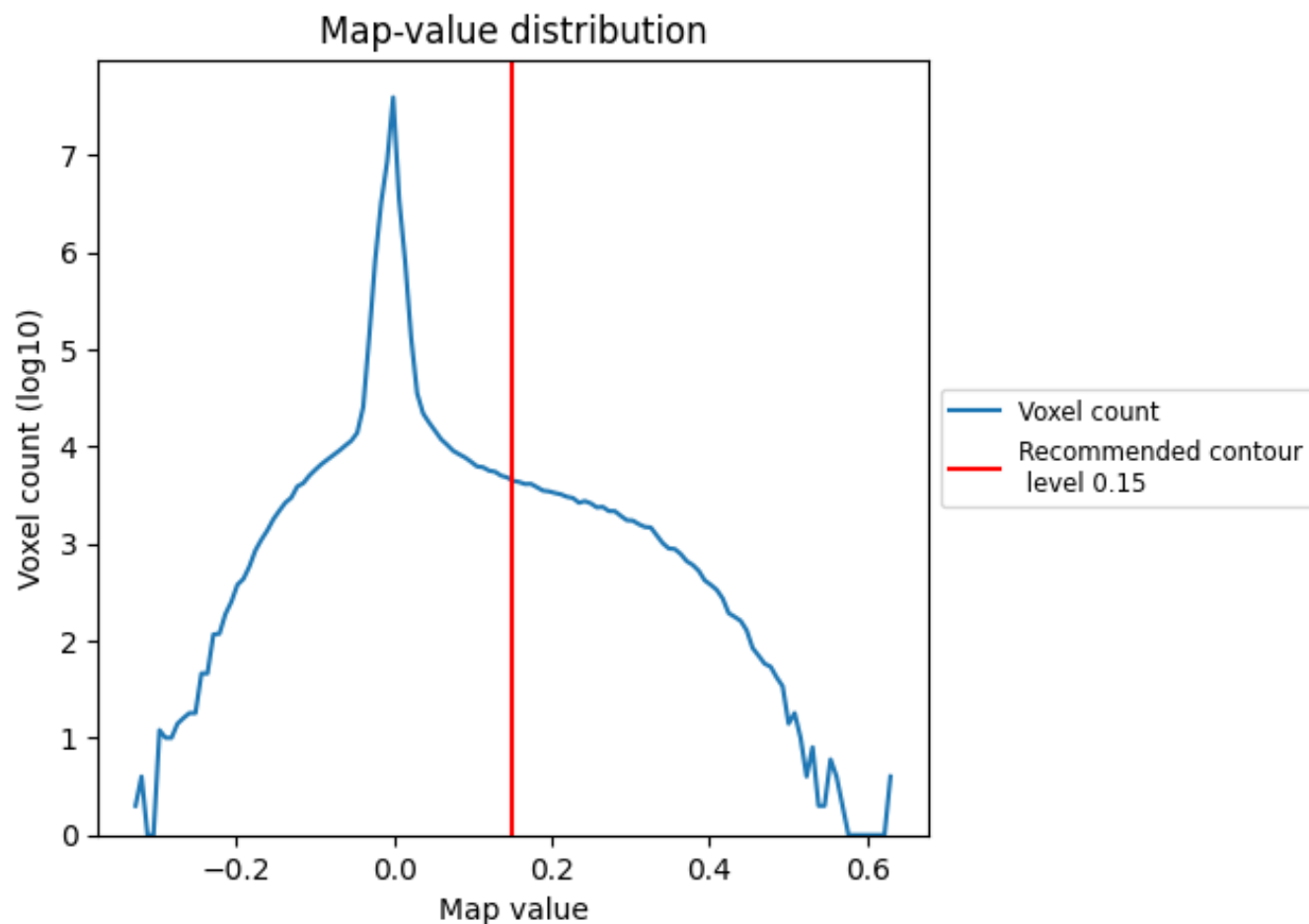
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

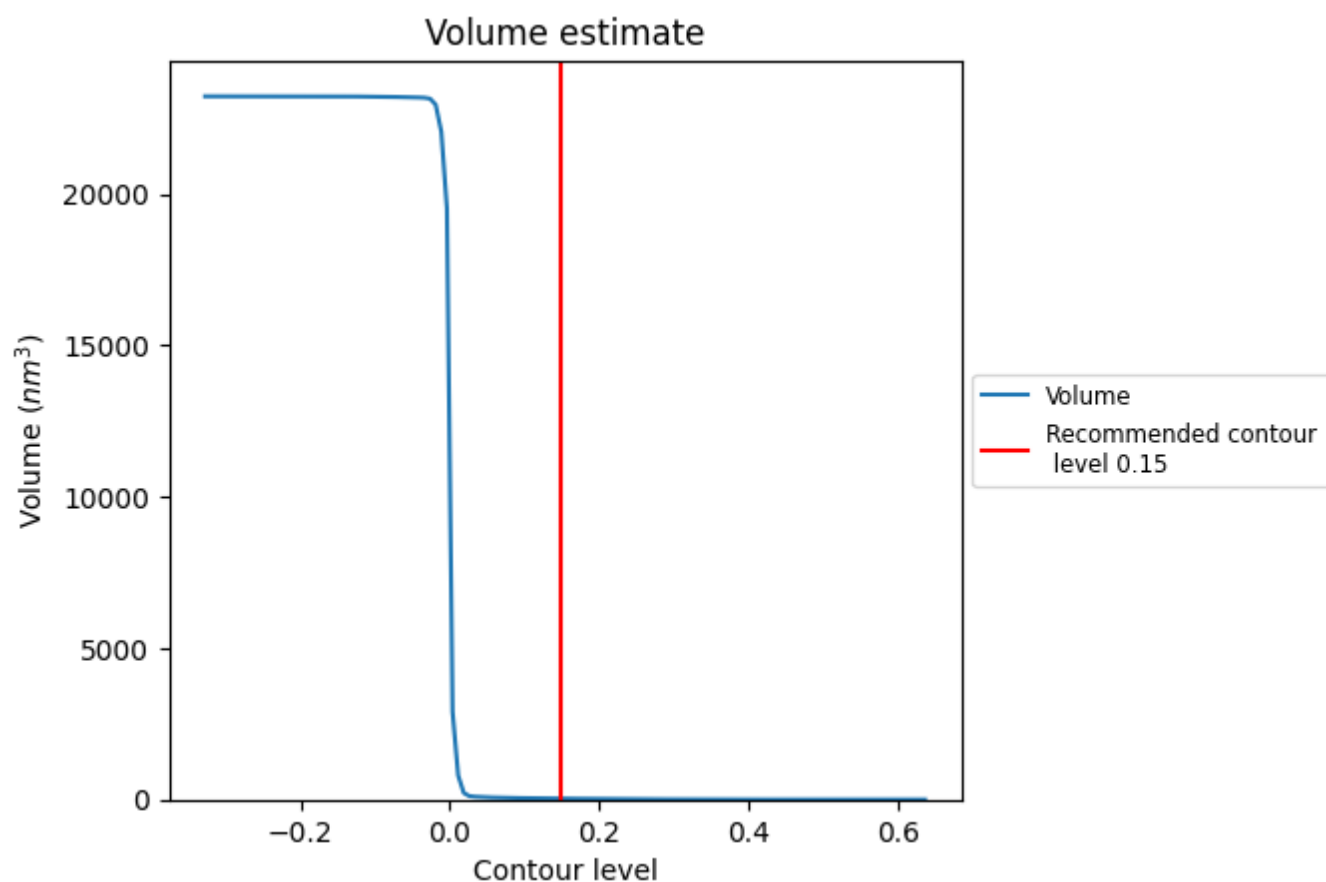
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

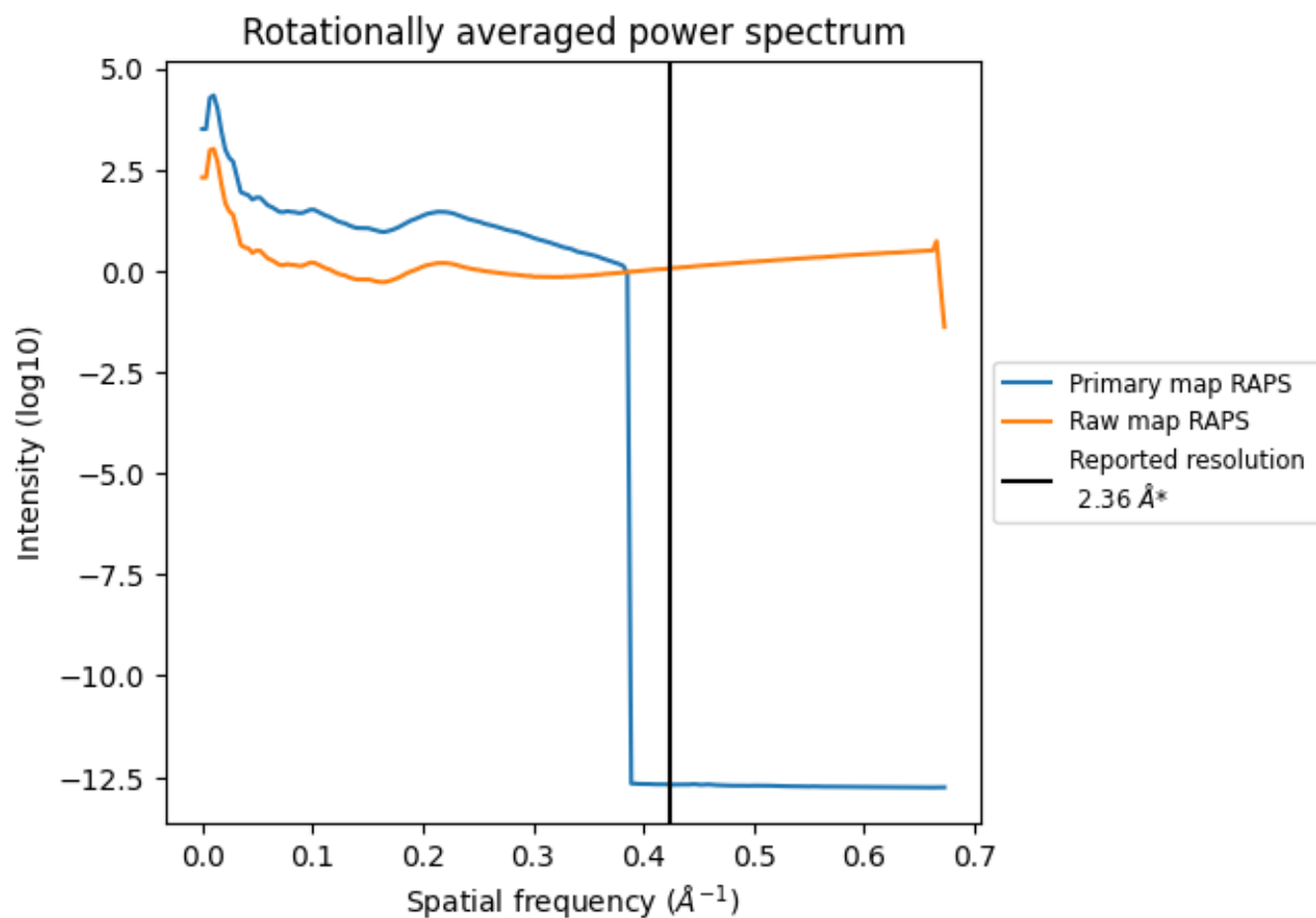
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 31 nm<sup>3</sup>; this corresponds to an approximate mass of 28 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 ⓘ



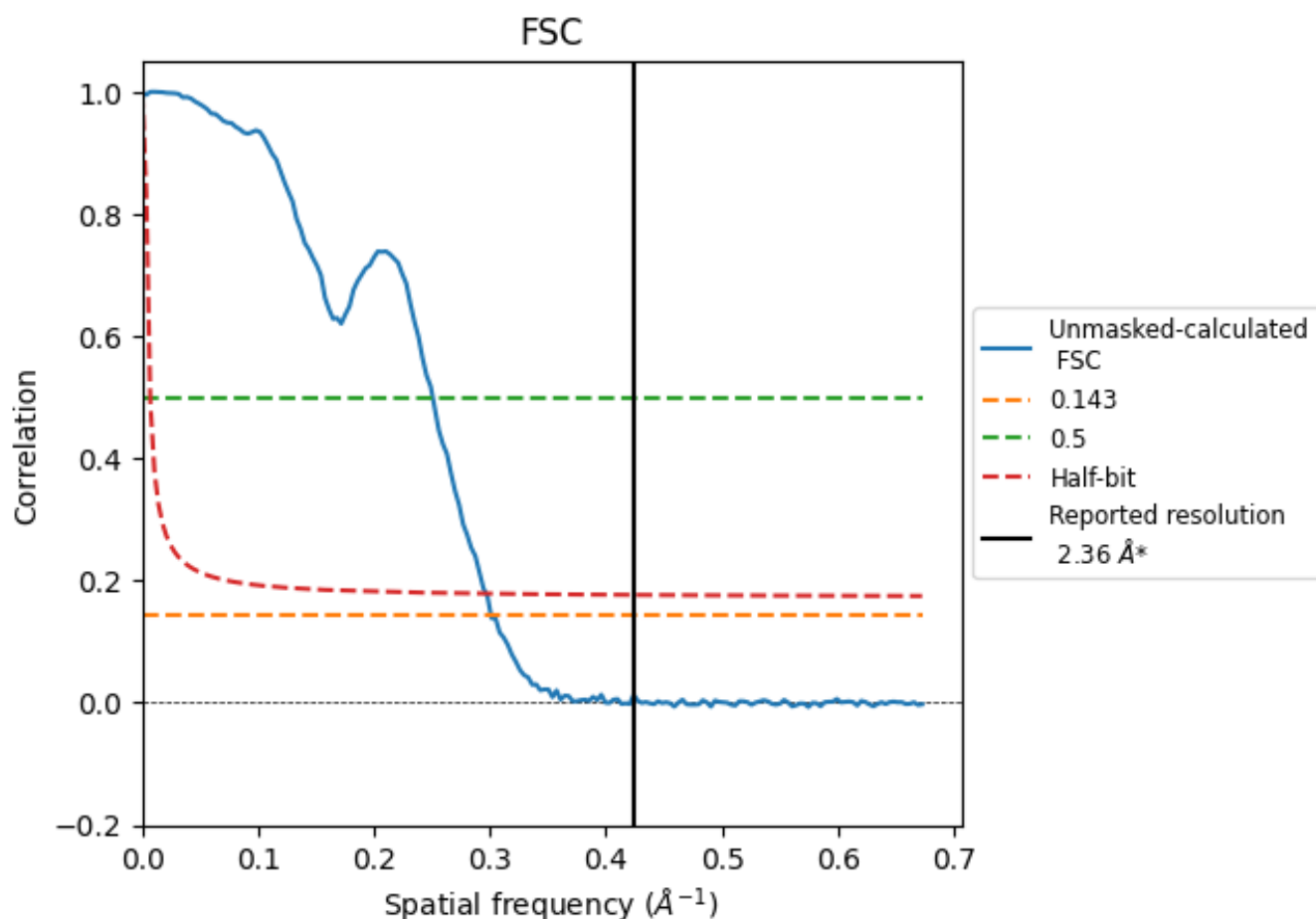
\*Reported resolution corresponds to spatial frequency of 0.424 Å<sup>-1</sup>



## 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 0.424  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

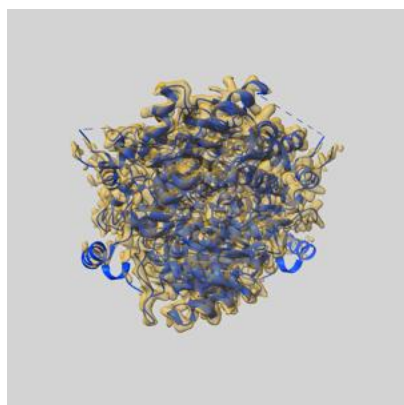
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.36	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.32	3.99	3.37

\*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 3.32 differs from the reported value 2.36 by more than 10 %

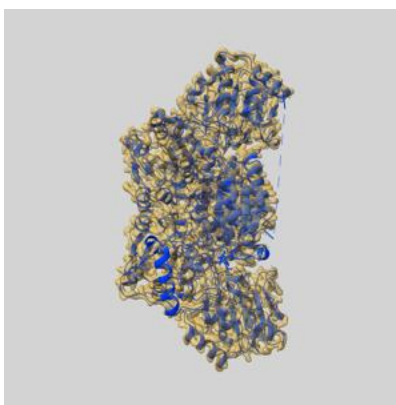
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-73041 and PDB model 9YK0. Per-residue inclusion information can be found in section 3 on page 7.

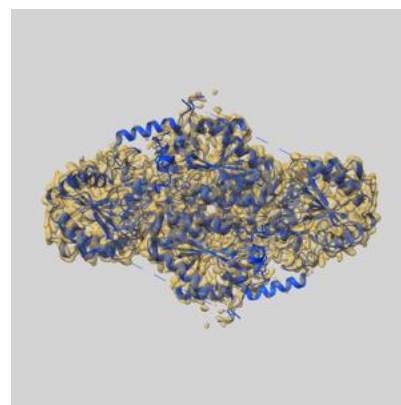
### 9.1 Map-model overlay [i](#)



X



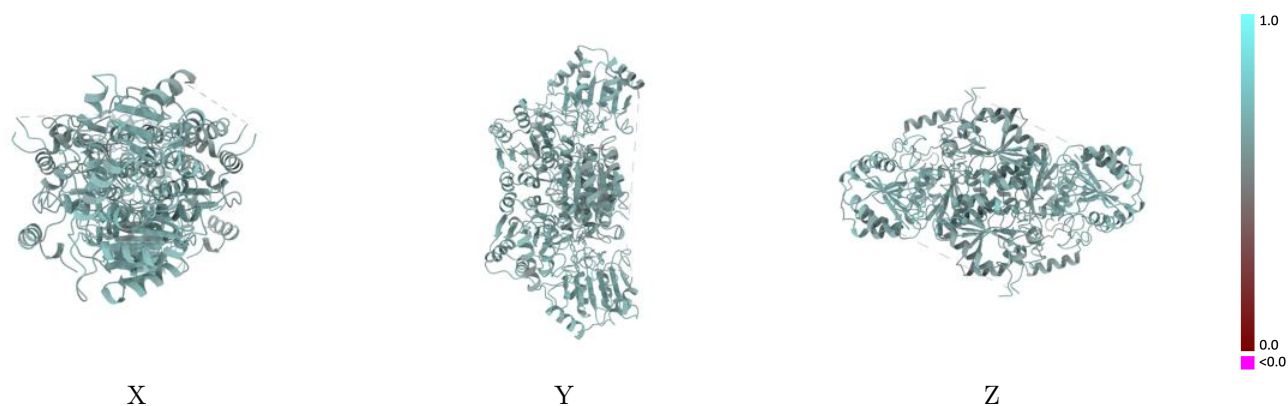
Y



Z

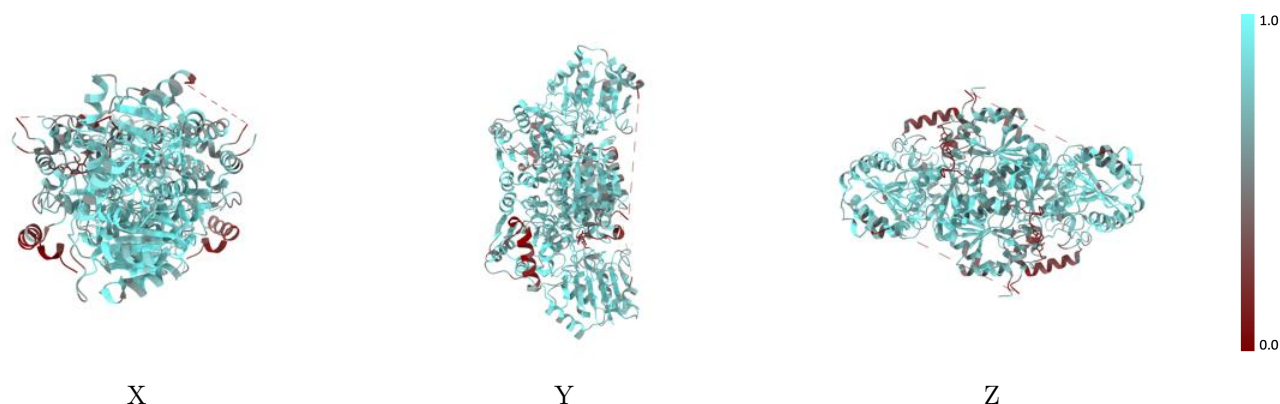
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



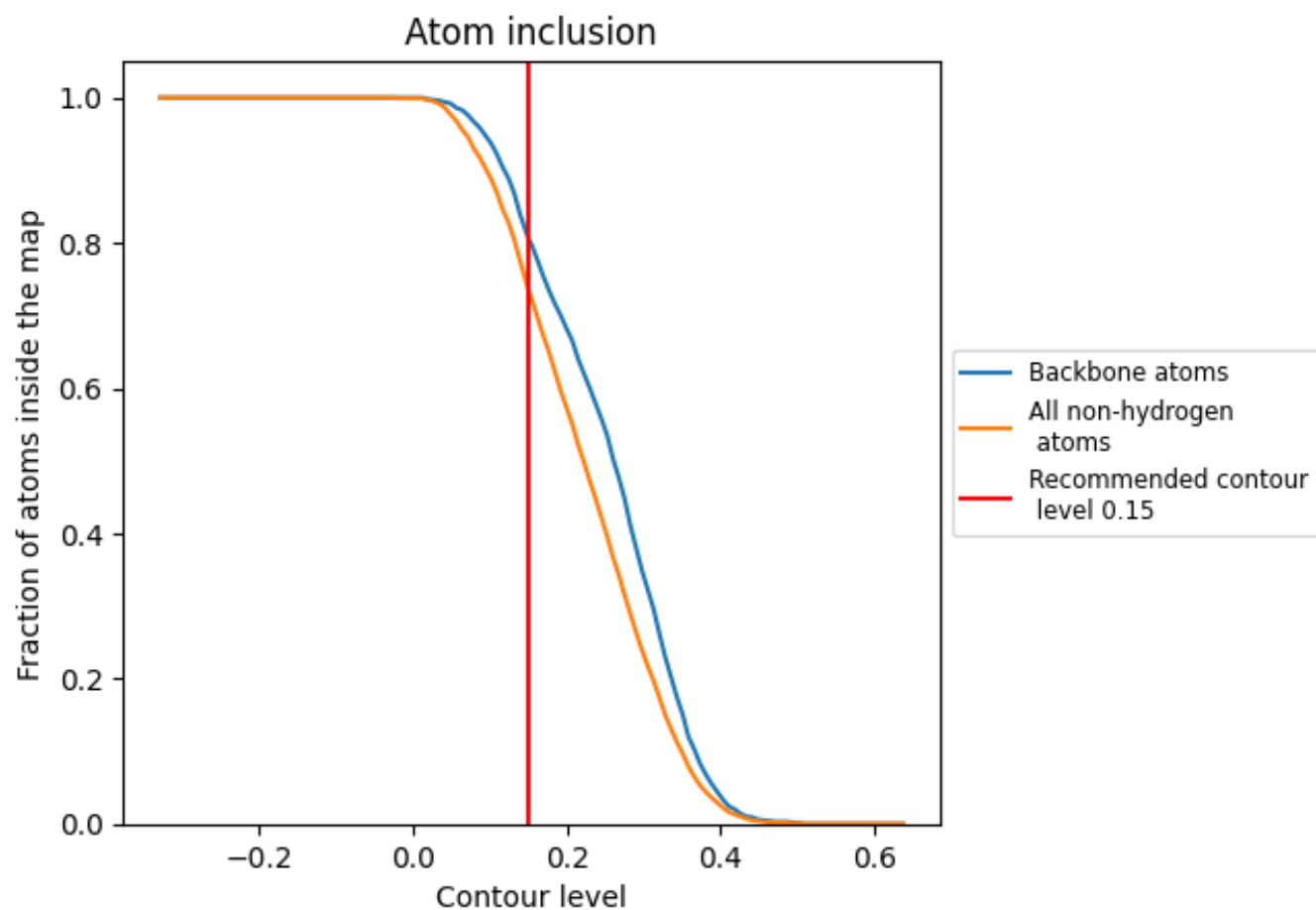
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 74% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7360	<div></div> 0.6310
A	<div></div> 0.7360	<div></div> 0.6310
B	<div></div> 0.7360	<div></div> 0.6310

