



Full wwPDB EM Validation Report ⓘ

Mar 31, 2025 – 05:33 PM JST

PDB ID : 6LZ3 / pdb_00006lz3
EMDB ID : EMD-30022
Title : Structure of cryptochrome in active conformation
Authors : Shao, K.; Zhang, X.; Zhang, P.
Deposited on : 2020-02-18
Resolution : 3.20 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.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

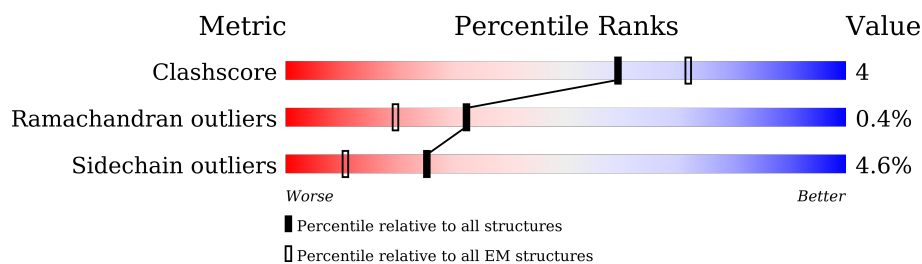
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	688	 60% 10% • 29%
1	B	688	 60% 10% • 29%
1	C	688	 60% 10% • 29%
1	D	688	 60% 10% • 29%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15968 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 Cryptochrome2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	486	Total	C	N	O	S	0	0
			3939	2530	692	705	12		
1	B	486	Total	C	N	O	S	0	0
			3939	2530	692	705	12		
1	C	486	Total	C	N	O	S	0	0
			3939	2530	692	705	12		
1	D	486	Total	C	N	O	S	0	0
			3939	2530	692	705	12		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	368	ALA	TRP	engineered mutation	UNP B8A2L5
B	368	ALA	TRP	engineered mutation	UNP B8A2L5
C	368	ALA	TRP	engineered mutation	UNP B8A2L5
D	368	ALA	TRP	engineered mutation	UNP B8A2L5

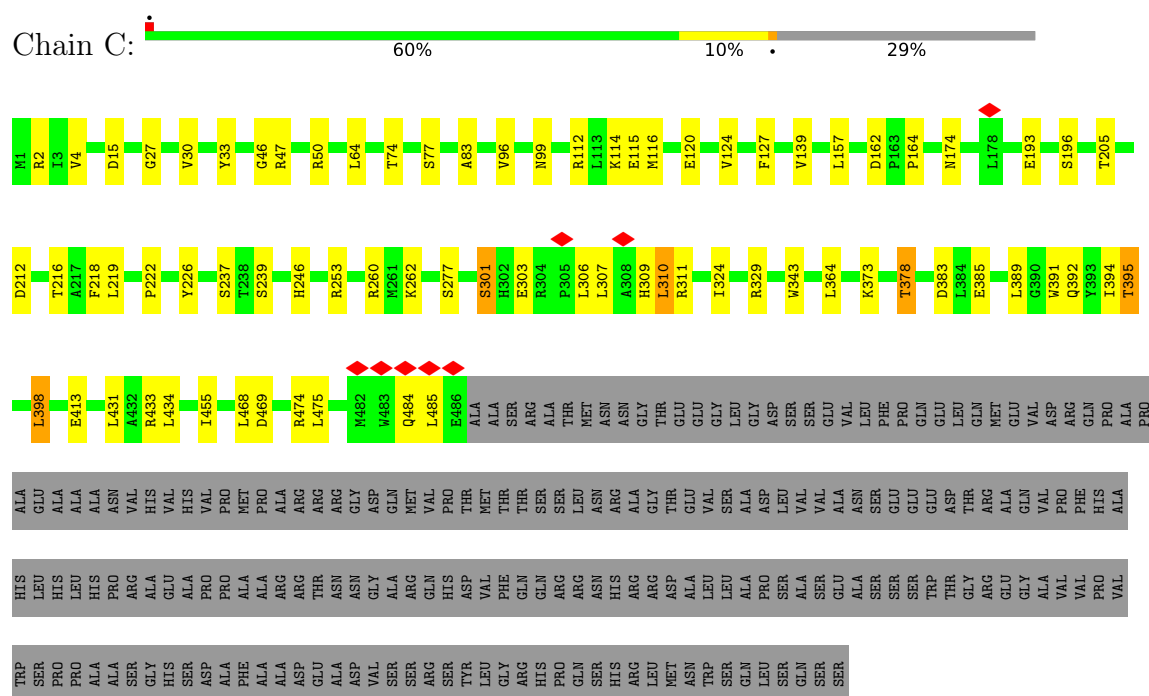
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



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

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

• Molecule 1: Cryptochrome2



ALA
ALA
SER
GLY
HIS
SER
ASP
ALA
PHE
ALA
ALA
ALA
ASP
GLU
ALA
ASP
VAL
SER
SER
ARG
SER
TYR
LEU
GLY
ARG
HIS
PRO
GLN
SER
HIS
ARG
LEU
MET
ASN
TRP
SER
GLN
LEU
SER
GLN
SER

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D2	Depositor
Number of particles used	108059	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.289	Depositor
Minimum map value	-0.147	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.018	Depositor
Map size (\AA)	254.64, 254.64, 254.64	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.061, 1.061, 1.061	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.34	0/4062	0.62	6/5538 (0.1%)
1	B	0.34	0/4062	0.62	6/5538 (0.1%)
1	C	0.34	0/4062	0.62	6/5538 (0.1%)
1	D	0.34	0/4062	0.62	6/5538 (0.1%)
All	All	0.34	0/16248	0.62	24/22152 (0.1%)

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	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	LEU	CA-CB-CG	7.93	133.53	115.30
1	D	306	LEU	CA-CB-CG	7.92	133.52	115.30
1	C	306	LEU	CA-CB-CG	7.91	133.50	115.30
1	B	306	LEU	CA-CB-CG	7.91	133.50	115.30
1	B	310	LEU	CA-CB-CG	7.64	132.87	115.30
1	C	310	LEU	CA-CB-CG	7.62	132.83	115.30
1	A	310	LEU	CA-CB-CG	7.61	132.81	115.30
1	D	310	LEU	CA-CB-CG	7.61	132.81	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	398	LEU	CA-CB-CG	7.31	132.11	115.30
1	A	398	LEU	CA-CB-CG	7.29	132.08	115.30
1	B	398	LEU	CA-CB-CG	7.29	132.07	115.30
1	C	398	LEU	CA-CB-CG	7.29	132.06	115.30
1	B	306	LEU	CB-CG-CD1	-5.83	101.10	111.00
1	A	306	LEU	CB-CG-CD1	-5.82	101.10	111.00
1	C	306	LEU	CB-CG-CD1	-5.82	101.11	111.00
1	D	306	LEU	CB-CG-CD1	-5.80	101.14	111.00
1	A	310	LEU	C-N-CA	5.38	135.16	121.70
1	B	310	LEU	C-N-CA	5.36	135.10	121.70
1	C	310	LEU	C-N-CA	5.36	135.09	121.70
1	D	310	LEU	C-N-CA	5.34	135.06	121.70
1	C	64	LEU	CA-CB-CG	5.10	127.03	115.30
1	D	64	LEU	CA-CB-CG	5.10	127.03	115.30
1	A	64	LEU	CA-CB-CG	5.09	127.01	115.30
1	B	64	LEU	CA-CB-CG	5.08	126.98	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	301	SER	Peptide
1	A	395	THR	Peptide
1	B	301	SER	Peptide
1	B	395	THR	Peptide
1	C	301	SER	Peptide
1	C	395	THR	Peptide
1	D	301	SER	Peptide
1	D	395	THR	Peptide

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	3939	0	3825	38	0
1	B	3939	0	3825	36	0
1	C	3939	0	3825	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3939	0	3825	35	0
2	A	53	0	30	1	0
2	B	53	0	30	1	0
2	C	53	0	30	1	0
2	D	53	0	30	1	0
All	All	15968	0	15420	138	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 4.

All (138) 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:394:ILE:HG23	1:A:395:THR:HG23	1.82	0.61
1:C:394:ILE:HG23	1:C:395:THR:HG23	1.82	0.61
1:B:394:ILE:HG23	1:B:395:THR:HG23	1.82	0.61
1:D:394:ILE:HG23	1:D:395:THR:HG23	1.82	0.61
1:B:114:LYS:HG2	1:B:124:VAL:HG21	1.84	0.60
1:D:114:LYS:HG2	1:D:124:VAL:HG21	1.84	0.60
1:B:391:TRP:O	1:B:395:THR:OG1	2.20	0.59
1:D:391:TRP:O	1:D:395:THR:OG1	2.20	0.59
1:C:114:LYS:HG2	1:C:124:VAL:HG21	1.84	0.58
1:A:114:LYS:HG2	1:A:124:VAL:HG21	1.84	0.58
1:B:343:TRP:O	1:C:433:ARG:NH1	2.36	0.58
1:C:391:TRP:O	1:C:395:THR:OG1	2.20	0.55
1:A:391:TRP:O	1:A:395:THR:OG1	2.20	0.55
1:C:47:ARG:NE	1:C:193:GLU:OE1	2.40	0.55
1:A:47:ARG:NE	1:A:193:GLU:OE1	2.40	0.55
1:B:222:PRO:HB3	1:B:237:SER:HB2	1.89	0.55
1:D:222:PRO:HB3	1:D:237:SER:HB2	1.89	0.55
1:A:46:GLY:O	1:A:50:ARG:NH1	2.40	0.55
1:B:47:ARG:NE	1:B:193:GLU:OE1	2.40	0.55
1:C:46:GLY:O	1:C:50:ARG:NH1	2.40	0.55
1:B:46:GLY:O	1:B:50:ARG:NH1	2.40	0.55
1:D:46:GLY:O	1:D:50:ARG:NH1	2.40	0.55
1:D:47:ARG:NE	1:D:193:GLU:OE1	2.40	0.55
1:B:378:THR:O	1:B:378:THR:OG1	2.25	0.54
1:D:378:THR:O	1:D:378:THR:OG1	2.25	0.54
1:A:378:THR:O	1:A:378:THR:OG1	2.25	0.54
1:C:378:THR:O	1:C:378:THR:OG1	2.25	0.54
1:A:431:LEU:HD12	1:A:455:ILE:HG12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:SER:OG	2:C:701:FAD:O2A	2.26	0.54
1:A:239:SER:OG	2:A:701:FAD:O2A	2.26	0.54
1:C:431:LEU:HD12	1:C:455:ILE:HG12	1.90	0.54
1:A:168:LEU:HD21	1:B:260:ARG:HG2	1.90	0.54
1:B:431:LEU:HD12	1:B:455:ILE:HG12	1.90	0.54
1:C:222:PRO:HB3	1:C:237:SER:HB2	1.89	0.54
1:D:431:LEU:HD12	1:D:455:ILE:HG12	1.90	0.54
1:B:239:SER:OG	2:B:701:FAD:O2A	2.26	0.53
1:A:222:PRO:HB3	1:A:237:SER:HB2	1.89	0.53
1:D:239:SER:OG	2:D:701:FAD:O2A	2.26	0.53
1:D:96:VAL:HB	1:D:124:VAL:HG12	1.91	0.52
1:B:96:VAL:HB	1:B:124:VAL:HG12	1.91	0.52
1:A:96:VAL:HB	1:A:124:VAL:HG12	1.91	0.51
1:C:96:VAL:HB	1:C:124:VAL:HG12	1.91	0.51
1:B:99:ASN:N	1:B:99:ASN:OD1	2.43	0.51
1:C:260:ARG:HG2	1:D:168:LEU:HD21	1.92	0.51
1:D:99:ASN:N	1:D:99:ASN:OD1	2.43	0.51
1:B:77:SER:HB2	1:B:83:ALA:HB2	1.93	0.50
1:B:433:ARG:NH1	1:C:343:TRP:O	2.44	0.50
1:C:162:ASP:OD2	1:D:24:ARG:NH1	2.40	0.50
1:D:77:SER:HB2	1:D:83:ALA:HB2	1.94	0.50
1:A:99:ASN:N	1:A:99:ASN:OD1	2.43	0.50
1:C:99:ASN:N	1:C:99:ASN:OD1	2.43	0.49
1:C:77:SER:HB2	1:C:83:ALA:HB2	1.94	0.49
1:A:77:SER:HB2	1:A:83:ALA:HB2	1.94	0.48
1:A:343:TRP:O	1:D:433:ARG:NH1	2.46	0.48
1:A:469:ASP:OD2	1:A:469:ASP:N	2.46	0.48
1:C:469:ASP:OD2	1:C:469:ASP:N	2.46	0.48
1:A:99:ASN:HA	1:A:127:PHE:H	1.79	0.48
1:C:99:ASN:HA	1:C:127:PHE:H	1.79	0.48
1:B:99:ASN:HA	1:B:127:PHE:H	1.79	0.48
1:D:99:ASN:HA	1:D:127:PHE:H	1.79	0.48
1:A:2:ARG:HD3	1:A:27:GLY:HA3	1.96	0.47
1:B:193:GLU:HG3	1:B:196:SER:HB3	1.96	0.47
1:C:2:ARG:HD3	1:C:27:GLY:HA3	1.96	0.47
1:D:193:GLU:HG3	1:D:196:SER:HB3	1.96	0.47
1:A:246:HIS:CD2	1:A:383:ASP:HB3	2.50	0.47
1:D:246:HIS:CD2	1:D:383:ASP:HB3	2.50	0.47
1:B:246:HIS:CD2	1:B:383:ASP:HB3	2.50	0.47
1:C:246:HIS:CD2	1:C:383:ASP:HB3	2.50	0.47
1:B:301:SER:O	1:B:301:SER:OG	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:GLU:HG3	1:A:196:SER:HB3	1.96	0.46
1:A:433:ARG:NH1	1:D:343:TRP:O	2.49	0.46
1:B:164:PRO:HG2	1:B:253:ARG:HH12	1.80	0.46
1:A:301:SER:O	1:A:301:SER:OG	2.33	0.46
1:B:2:ARG:HD3	1:B:27:GLY:HA3	1.96	0.46
1:D:164:PRO:HG2	1:D:253:ARG:HH12	1.80	0.46
1:C:193:GLU:HG3	1:C:196:SER:HB3	1.96	0.46
1:C:301:SER:OG	1:C:301:SER:O	2.33	0.46
1:A:164:PRO:HG2	1:A:253:ARG:HH12	1.80	0.46
1:D:2:ARG:HD3	1:D:27:GLY:HA3	1.96	0.46
1:C:164:PRO:HG2	1:C:253:ARG:HH12	1.80	0.46
1:C:218:PHE:HA	1:C:222:PRO:HD2	1.98	0.46
1:D:174:ASN:N	1:D:174:ASN:OD1	2.49	0.46
1:A:218:PHE:HA	1:A:222:PRO:HD2	1.98	0.45
1:B:174:ASN:N	1:B:174:ASN:OD1	2.49	0.45
1:C:262:LYS:HB2	1:C:262:LYS:HE3	1.78	0.45
1:A:262:LYS:HE3	1:A:262:LYS:HB2	1.78	0.45
1:B:324:ILE:HD12	1:B:329:ARG:HB2	1.99	0.45
1:D:324:ILE:HD12	1:D:329:ARG:HB2	1.99	0.45
1:B:218:PHE:HA	1:B:222:PRO:HD2	1.98	0.45
1:D:218:PHE:HA	1:D:222:PRO:HD2	1.98	0.45
1:B:216:THR:HA	1:B:219:LEU:HD12	1.98	0.45
1:C:4:VAL:HG12	1:C:30:VAL:HG23	1.99	0.45
1:D:216:THR:HA	1:D:219:LEU:HD12	1.98	0.45
1:C:216:THR:HA	1:C:219:LEU:HD12	1.98	0.45
1:A:4:VAL:HG12	1:A:30:VAL:HG23	1.99	0.44
1:C:174:ASN:OD1	1:C:174:ASN:N	2.49	0.44
1:D:4:VAL:HG12	1:D:30:VAL:HG23	1.99	0.44
1:A:216:THR:HA	1:A:219:LEU:HD12	1.98	0.44
1:B:4:VAL:HG12	1:B:30:VAL:HG23	1.99	0.44
1:A:174:ASN:N	1:A:174:ASN:OD1	2.49	0.44
1:C:385:GLU:O	1:C:389:LEU:N	2.45	0.44
1:A:385:GLU:O	1:A:389:LEU:N	2.45	0.44
1:C:324:ILE:HD12	1:C:329:ARG:HB2	1.99	0.44
1:A:324:ILE:HD12	1:A:329:ARG:HB2	1.99	0.44
1:D:221:GLY:HA3	1:D:222:PRO:HD3	1.81	0.43
1:D:301:SER:O	1:D:301:SER:OG	2.33	0.43
1:C:373:LYS:HA	1:C:373:LYS:HD3	1.86	0.43
1:C:364:LEU:HD23	1:C:364:LEU:HA	1.90	0.43
1:A:24:ARG:NH1	1:B:162:ASP:OD2	2.44	0.43
1:B:221:GLY:HA3	1:B:222:PRO:HD3	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:TYR:HB3	1:C:277:SER:HB2	2.01	0.43
1:A:226:TYR:HB3	1:A:277:SER:HB2	2.01	0.42
1:A:364:LEU:HD23	1:A:364:LEU:HA	1.91	0.42
1:B:234:ASP:OD1	1:B:234:ASP:N	2.52	0.42
1:A:373:LYS:HA	1:A:373:LYS:HD3	1.86	0.42
1:D:226:TYR:HB3	1:D:277:SER:HB2	2.01	0.42
1:B:226:TYR:HB3	1:B:277:SER:HB2	2.01	0.42
1:A:239:SER:OG	1:A:239:SER:O	2.37	0.42
1:C:239:SER:OG	1:C:239:SER:O	2.37	0.42
1:A:431:LEU:HG	1:A:434:LEU:HD12	2.02	0.41
1:D:237:SER:O	1:D:237:SER:OG	2.34	0.41
1:C:431:LEU:HG	1:C:434:LEU:HD12	2.02	0.41
1:B:364:LEU:HD23	1:B:364:LEU:HA	1.90	0.41
1:B:237:SER:O	1:B:237:SER:OG	2.35	0.41
1:B:431:LEU:HG	1:B:434:LEU:HD12	2.02	0.41
1:D:364:LEU:HD23	1:D:364:LEU:HA	1.90	0.41
1:D:431:LEU:HG	1:D:434:LEU:HD12	2.02	0.41
1:A:33:TYR:HB3	1:A:74:THR:HG22	2.03	0.41
1:C:33:TYR:HB3	1:C:74:THR:HG22	2.03	0.41
1:A:392:GLN:HG2	1:A:398:LEU:HD22	2.03	0.41
1:B:385:GLU:O	1:B:389:LEU:N	2.45	0.41
1:C:392:GLN:HG2	1:C:398:LEU:HD22	2.03	0.41
1:B:33:TYR:HB3	1:B:74:THR:HG22	2.03	0.40
1:D:385:GLU:O	1:D:389:LEU:N	2.45	0.40
1:D:33:TYR:HB3	1:D:74:THR:HG22	2.03	0.40
1:A:381:ASP:OD1	1:A:381:ASP:N	2.48	0.40
1:D:484:GLN:H	1:D:484:GLN:HG3	1.71	0.40
1:B:484:GLN:H	1:B:484:GLN:HG3	1.72	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	484/688 (70%)	440 (91%)	42 (9%)	2 (0%)	30	64
1	B	484/688 (70%)	440 (91%)	42 (9%)	2 (0%)	30	64
1	C	484/688 (70%)	440 (91%)	42 (9%)	2 (0%)	30	64
1	D	484/688 (70%)	440 (91%)	42 (9%)	2 (0%)	30	64
All	All	1936/2752 (70%)	1760 (91%)	168 (9%)	8 (0%)	32	64

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	311	ARG
1	B	311	ARG
1	C	311	ARG
1	D	311	ARG
1	A	15	ASP
1	B	15	ASP
1	C	15	ASP
1	D	15	ASP

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	414/576 (72%)	395 (95%)	19 (5%)	23	56
1	B	414/576 (72%)	395 (95%)	19 (5%)	23	56
1	C	414/576 (72%)	395 (95%)	19 (5%)	23	56
1	D	414/576 (72%)	395 (95%)	19 (5%)	23	56
All	All	1656/2304 (72%)	1580 (95%)	76 (5%)	25	56

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	ARG
1	A	115	GLU
1	A	116	MET

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Mol	Chain	Res	Type
1	A	120	GLU
1	A	139	VAL
1	A	157	LEU
1	A	205	THR
1	A	212	ASP
1	A	303	GLU
1	A	307	LEU
1	A	309	HIS
1	A	310	LEU
1	A	378	THR
1	A	413	GLU
1	A	468	LEU
1	A	474	ARG
1	A	475	LEU
1	A	484	GLN
1	A	485	LEU
1	B	112	ARG
1	B	115	GLU
1	B	116	MET
1	B	120	GLU
1	B	139	VAL
1	B	157	LEU
1	B	205	THR
1	B	212	ASP
1	B	303	GLU
1	B	307	LEU
1	B	309	HIS
1	B	310	LEU
1	B	378	THR
1	B	413	GLU
1	B	468	LEU
1	B	474	ARG
1	B	475	LEU
1	B	484	GLN
1	B	485	LEU
1	C	112	ARG
1	C	115	GLU
1	C	116	MET
1	C	120	GLU
1	C	139	VAL
1	C	157	LEU
1	C	205	THR

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Mol	Chain	Res	Type
1	C	212	ASP
1	C	303	GLU
1	C	307	LEU
1	C	309	HIS
1	C	310	LEU
1	C	378	THR
1	C	413	GLU
1	C	468	LEU
1	C	474	ARG
1	C	475	LEU
1	C	484	GLN
1	C	485	LEU
1	D	112	ARG
1	D	115	GLU
1	D	116	MET
1	D	120	GLU
1	D	139	VAL
1	D	157	LEU
1	D	205	THR
1	D	212	ASP
1	D	303	GLU
1	D	307	LEU
1	D	309	HIS
1	D	310	LEU
1	D	378	THR
1	D	413	GLU
1	D	468	LEU
1	D	474	ARG
1	D	475	LEU
1	D	484	GLN
1	D	485	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	59	HIS
1	A	154	ASN
1	A	210	ASN
1	A	244	HIS
1	A	263	GLN
1	B	58	ASN

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Mol	Chain	Res	Type
1	B	59	HIS
1	B	154	ASN
1	B	210	ASN
1	B	244	HIS
1	B	263	GLN
1	C	58	ASN
1	C	59	HIS
1	C	154	ASN
1	C	210	ASN
1	C	244	HIS
1	C	263	GLN
1	D	58	ASN
1	D	59	HIS
1	D	154	ASN
1	D	210	ASN
1	D	244	HIS
1	D	263	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	D	701	1	53,58,58	0.59	0	68,89,89	0.70	2 (2%)
2	FAD	C	701	1	53,58,58	0.59	0	68,89,89	0.70	2 (2%)
2	FAD	B	701	1	53,58,58	0.59	0	68,89,89	0.70	2 (2%)
2	FAD	A	701	1	53,58,58	0.59	0	68,89,89	0.70	2 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	D	701	1	-	16/30/50/50	0/6/6/6
2	FAD	C	701	1	-	16/30/50/50	0/6/6/6
2	FAD	B	701	1	-	16/30/50/50	0/6/6/6
2	FAD	A	701	1	-	16/30/50/50	0/6/6/6

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	FAD	C3B-C2B-C1B	2.21	104.30	100.98
2	A	701	FAD	C5A-C6A-N6A	2.20	123.69	120.35
2	C	701	FAD	C5A-C6A-N6A	2.19	123.68	120.35
2	D	701	FAD	C3B-C2B-C1B	2.19	104.27	100.98
2	A	701	FAD	C3B-C2B-C1B	2.18	104.26	100.98
2	B	701	FAD	C5A-C6A-N6A	2.18	123.66	120.35
2	C	701	FAD	C3B-C2B-C1B	2.18	104.26	100.98
2	D	701	FAD	C5A-C6A-N6A	2.17	123.66	120.35

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	FAD	C5B-O5B-PA-O2A
2	A	701	FAD	N10-C1'-C2'-O2'
2	A	701	FAD	N10-C1'-C2'-C3'
2	A	701	FAD	C1'-C2'-C3'-O3'
2	A	701	FAD	C1'-C2'-C3'-C4'
2	A	701	FAD	O2'-C2'-C3'-O3'

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Mol	Chain	Res	Type	Atoms
2	A	701	FAD	O2'-C2'-C3'-C4'
2	A	701	FAD	C2'-C3'-C4'-C5'
2	A	701	FAD	O3'-C3'-C4'-O4'
2	A	701	FAD	O3'-C3'-C4'-C5'
2	A	701	FAD	C3'-C4'-C5'-O5'
2	A	701	FAD	O4'-C4'-C5'-O5'
2	B	701	FAD	C5B-O5B-PA-O2A
2	B	701	FAD	N10-C1'-C2'-O2'
2	B	701	FAD	N10-C1'-C2'-C3'
2	B	701	FAD	C1'-C2'-C3'-O3'
2	B	701	FAD	C1'-C2'-C3'-C4'
2	B	701	FAD	O2'-C2'-C3'-O3'
2	B	701	FAD	O2'-C2'-C3'-C4'
2	B	701	FAD	C2'-C3'-C4'-C5'
2	B	701	FAD	O3'-C3'-C4'-O4'
2	B	701	FAD	O3'-C3'-C4'-C5'
2	B	701	FAD	C3'-C4'-C5'-O5'
2	B	701	FAD	O4'-C4'-C5'-O5'
2	C	701	FAD	C5B-O5B-PA-O2A
2	C	701	FAD	N10-C1'-C2'-O2'
2	C	701	FAD	N10-C1'-C2'-C3'
2	C	701	FAD	C1'-C2'-C3'-O3'
2	C	701	FAD	C1'-C2'-C3'-C4'
2	C	701	FAD	O2'-C2'-C3'-O3'
2	C	701	FAD	O2'-C2'-C3'-C4'
2	C	701	FAD	C2'-C3'-C4'-C5'
2	C	701	FAD	O3'-C3'-C4'-O4'
2	C	701	FAD	O3'-C3'-C4'-C5'
2	C	701	FAD	C3'-C4'-C5'-O5'
2	C	701	FAD	O4'-C4'-C5'-O5'
2	D	701	FAD	C5B-O5B-PA-O2A
2	D	701	FAD	N10-C1'-C2'-O2'
2	D	701	FAD	N10-C1'-C2'-C3'
2	D	701	FAD	C1'-C2'-C3'-O3'
2	D	701	FAD	C1'-C2'-C3'-C4'
2	D	701	FAD	O2'-C2'-C3'-O3'
2	D	701	FAD	O2'-C2'-C3'-C4'
2	D	701	FAD	C2'-C3'-C4'-C5'
2	D	701	FAD	O3'-C3'-C4'-O4'
2	D	701	FAD	O3'-C3'-C4'-C5'
2	D	701	FAD	C3'-C4'-C5'-O5'
2	D	701	FAD	O4'-C4'-C5'-O5'

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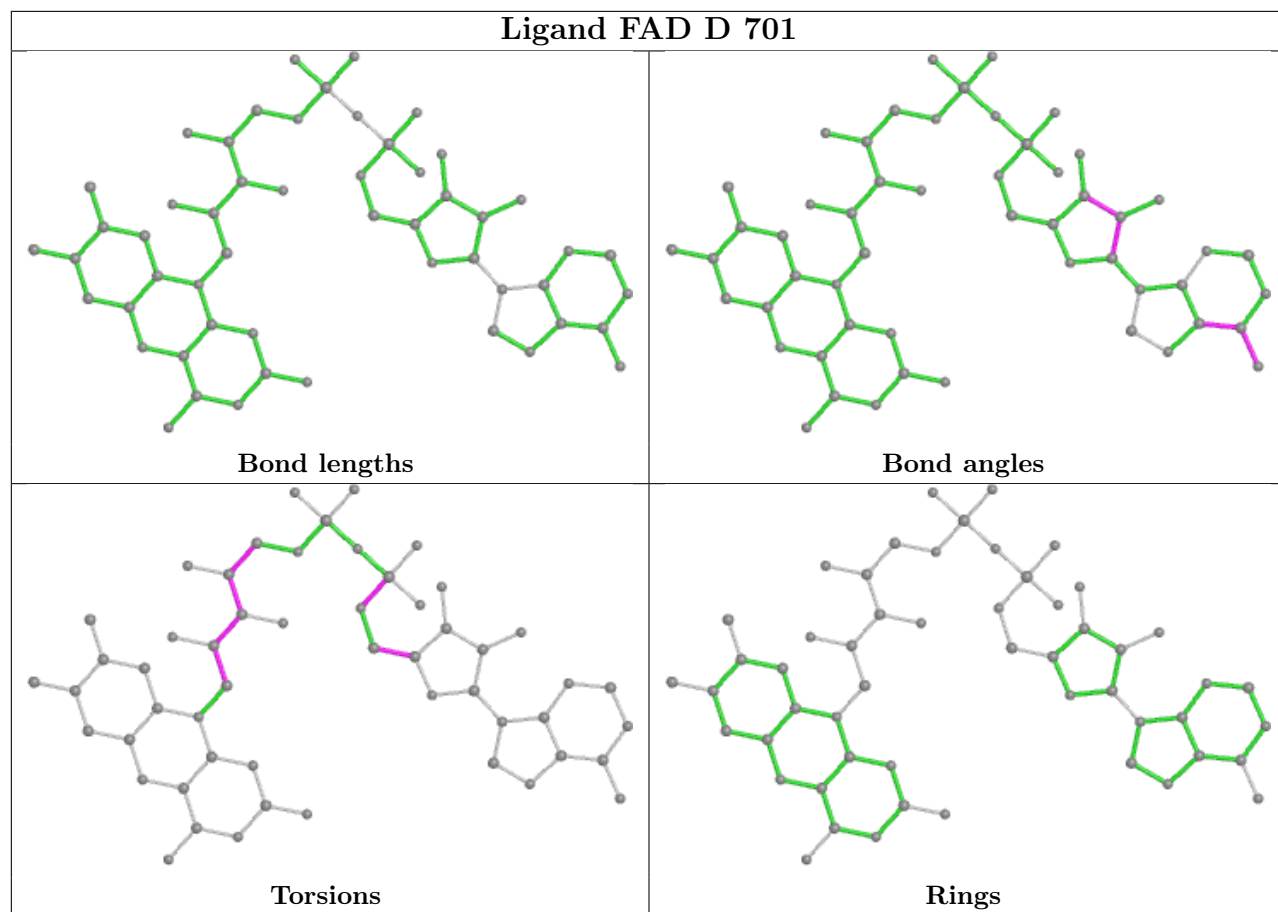
Mol	Chain	Res	Type	Atoms
2	A	701	FAD	C2'-C3'-C4'-O4'
2	B	701	FAD	C2'-C3'-C4'-O4'
2	C	701	FAD	C2'-C3'-C4'-O4'
2	D	701	FAD	C2'-C3'-C4'-O4'
2	A	701	FAD	C5B-O5B-PA-O3P
2	B	701	FAD	C5B-O5B-PA-O3P
2	C	701	FAD	C5B-O5B-PA-O3P
2	D	701	FAD	C5B-O5B-PA-O3P
2	A	701	FAD	C5B-O5B-PA-O1A
2	B	701	FAD	C5B-O5B-PA-O1A
2	C	701	FAD	C5B-O5B-PA-O1A
2	D	701	FAD	C5B-O5B-PA-O1A
2	C	701	FAD	O4B-C4B-C5B-O5B
2	A	701	FAD	O4B-C4B-C5B-O5B
2	B	701	FAD	O4B-C4B-C5B-O5B
2	D	701	FAD	O4B-C4B-C5B-O5B

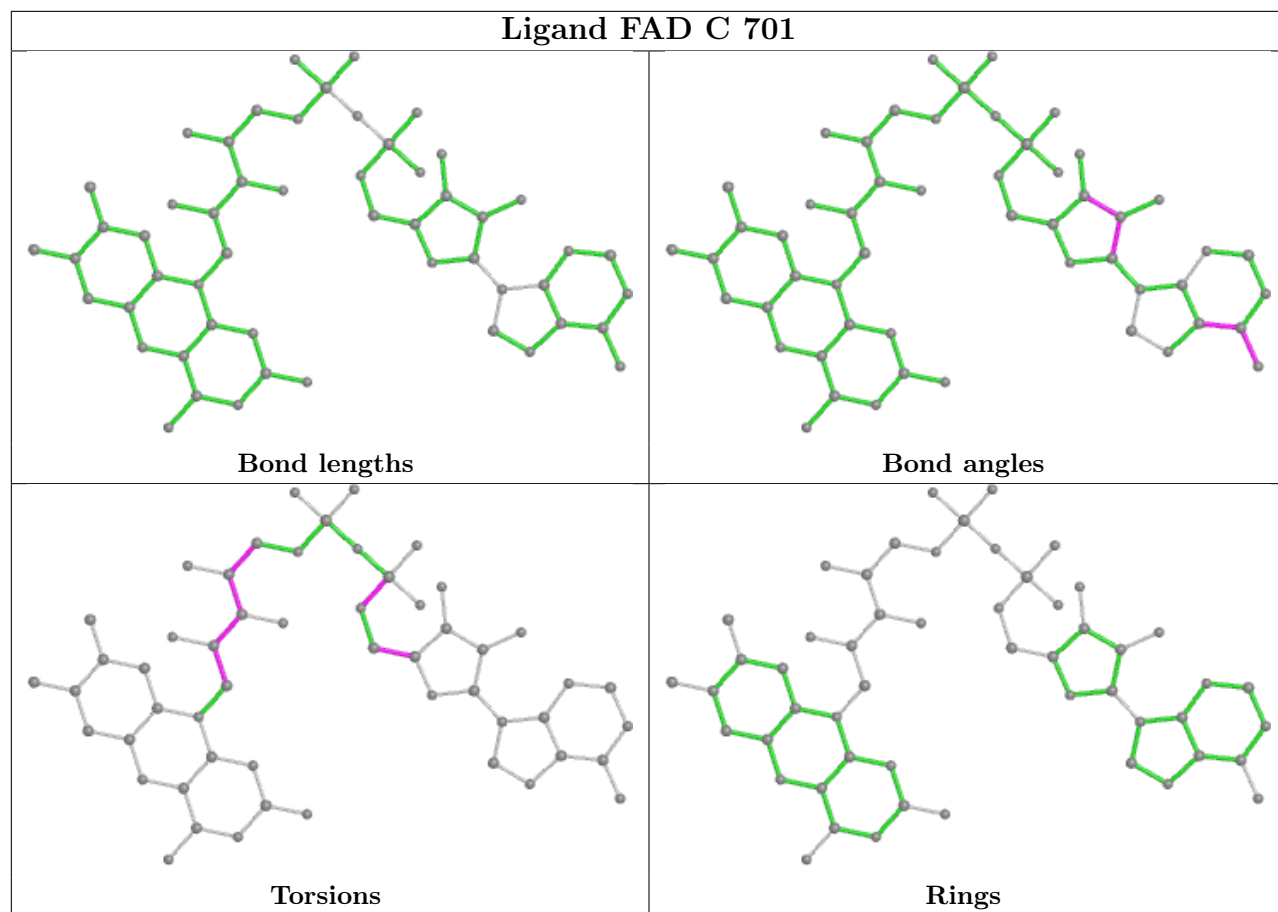
There are no ring outliers.

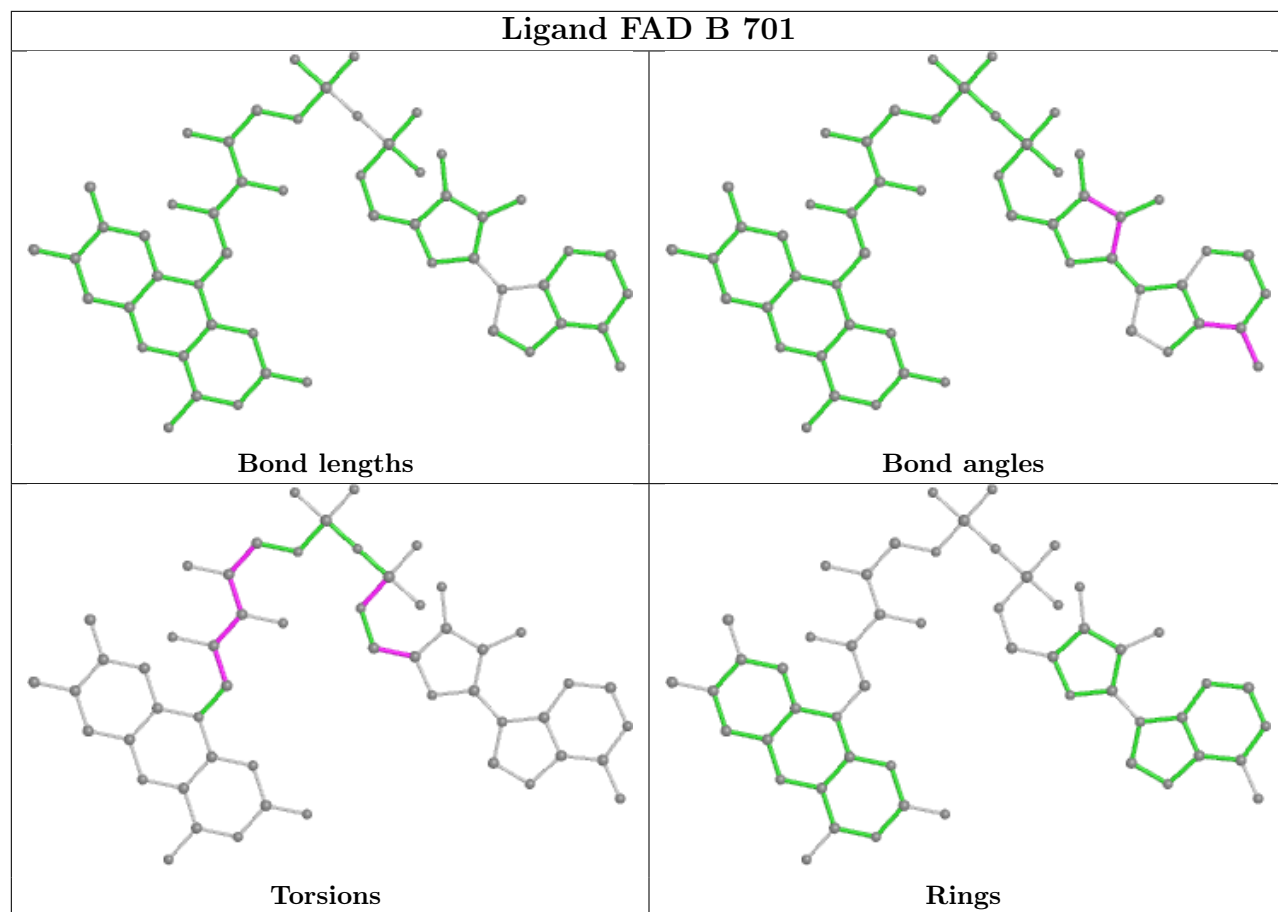
4 monomers are involved in 4 short contacts:

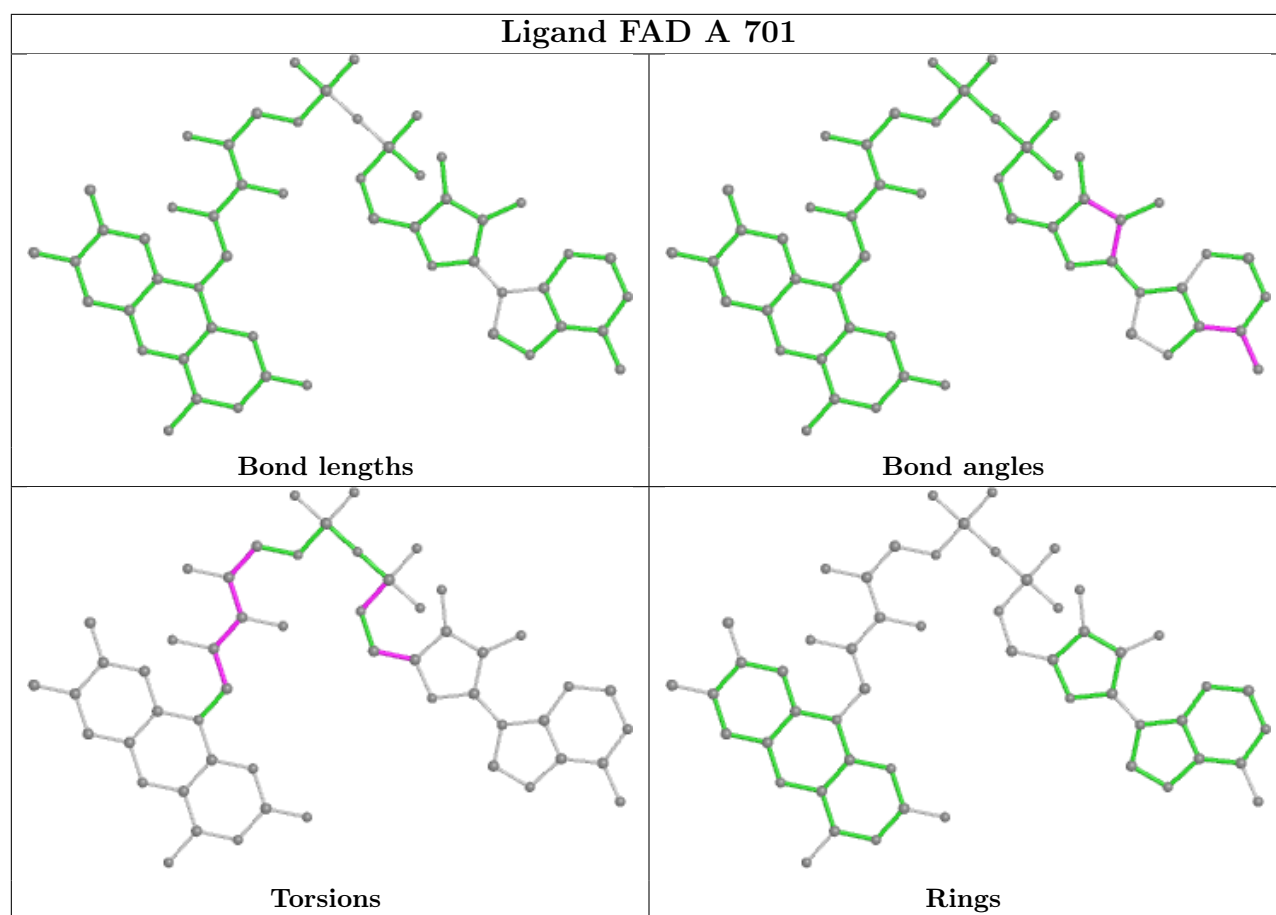
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	701	FAD	1	0
2	C	701	FAD	1	0
2	B	701	FAD	1	0
2	A	701	FAD	1	0

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.

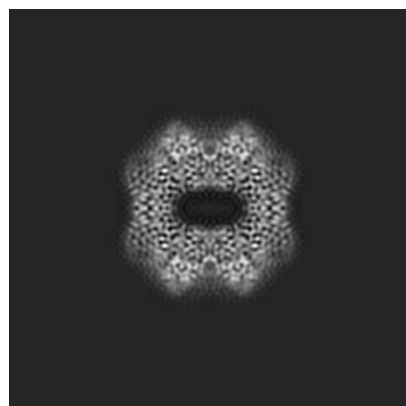
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30022. These allow visual inspection of the internal detail of the map and identification of artifacts.

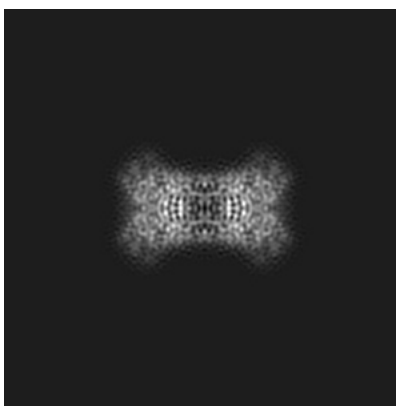
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

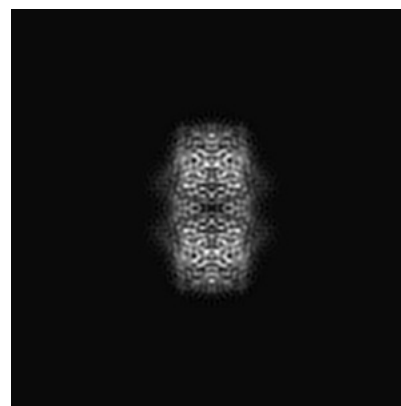
6.1.1 Primary map



X

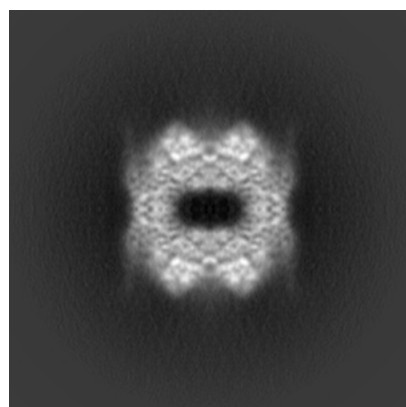


Y

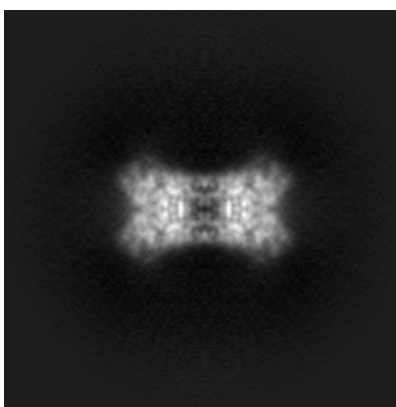


Z

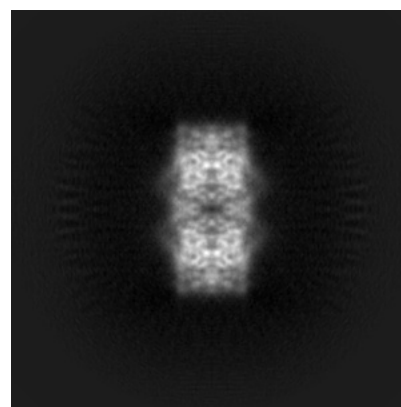
6.1.2 Raw map



X



Y

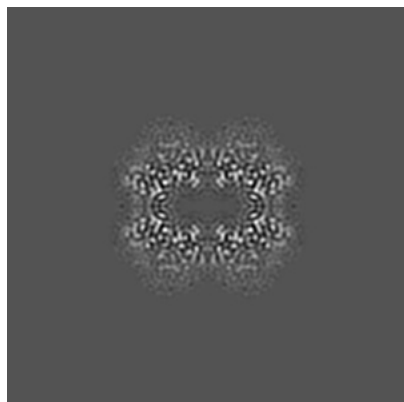


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 120

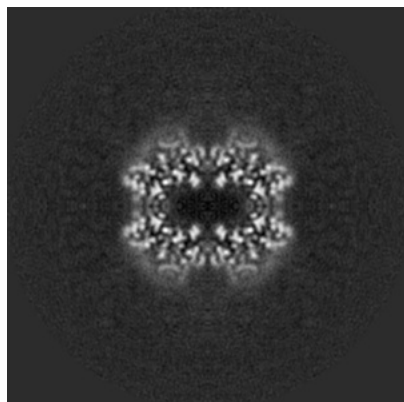


Y Index: 120

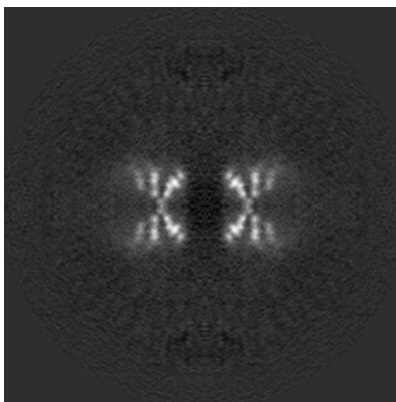


Z Index: 120

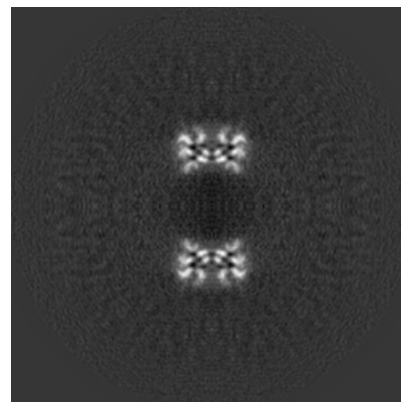
6.2.2 Raw map



X Index: 120



Y Index: 120

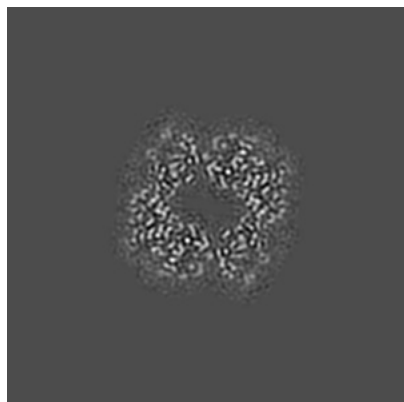


Z Index: 120

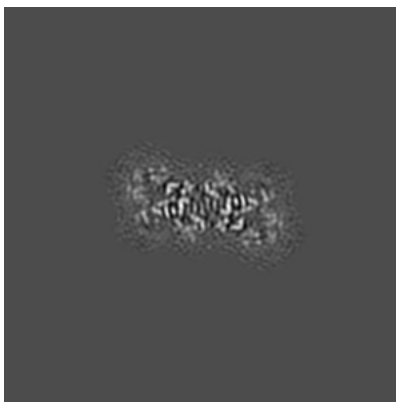
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 128

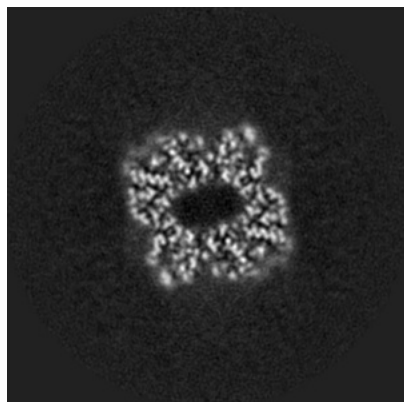


Y Index: 146

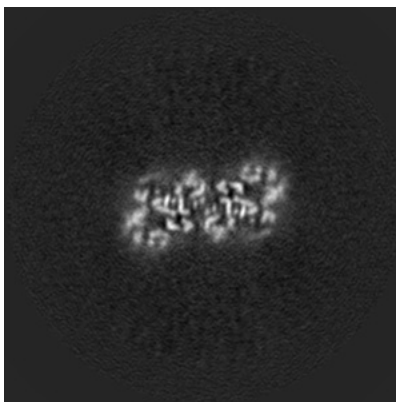


Z Index: 97

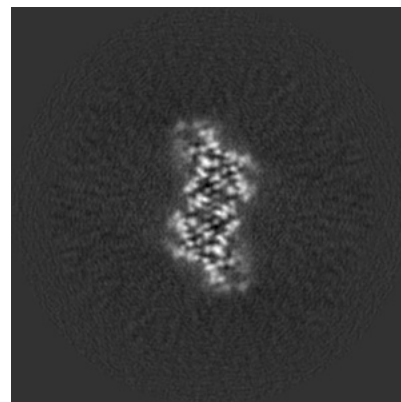
6.3.2 Raw map



X Index: 111



Y Index: 94

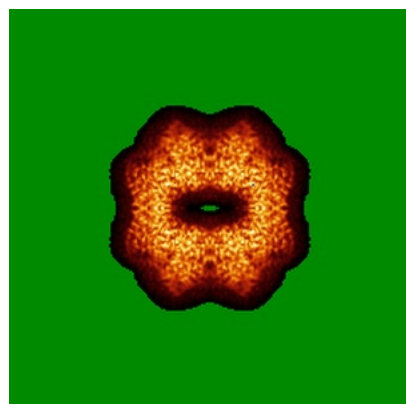


Z Index: 97

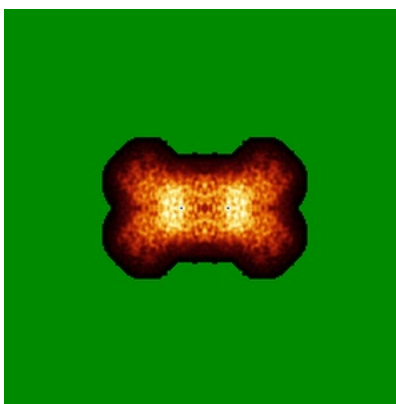
The images above show the largest variance slices of the map in three orthogonal directions.

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

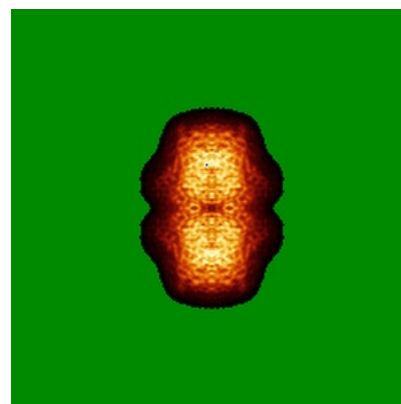
6.4.1 Primary map



X

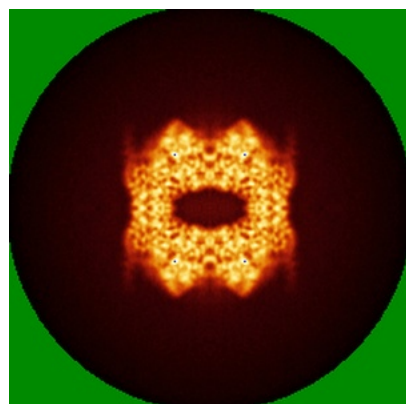


Y

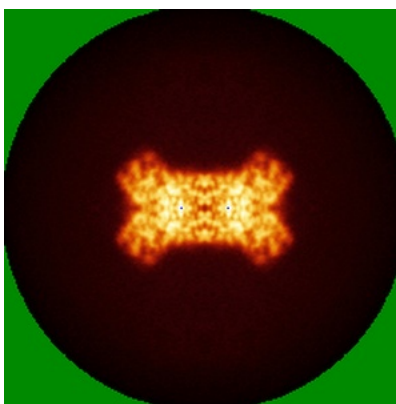


Z

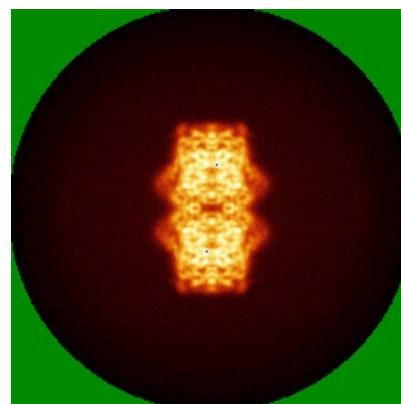
6.4.2 Raw map



X



Y

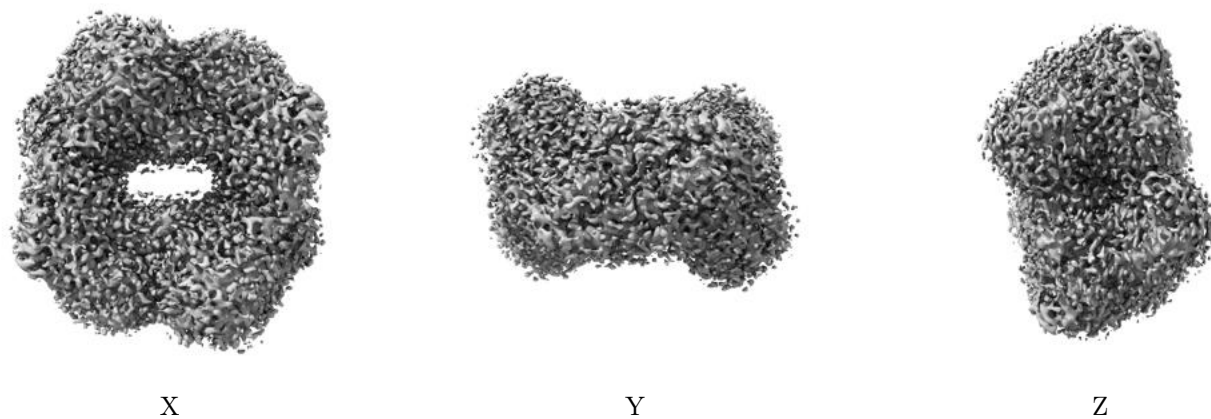


Z

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.

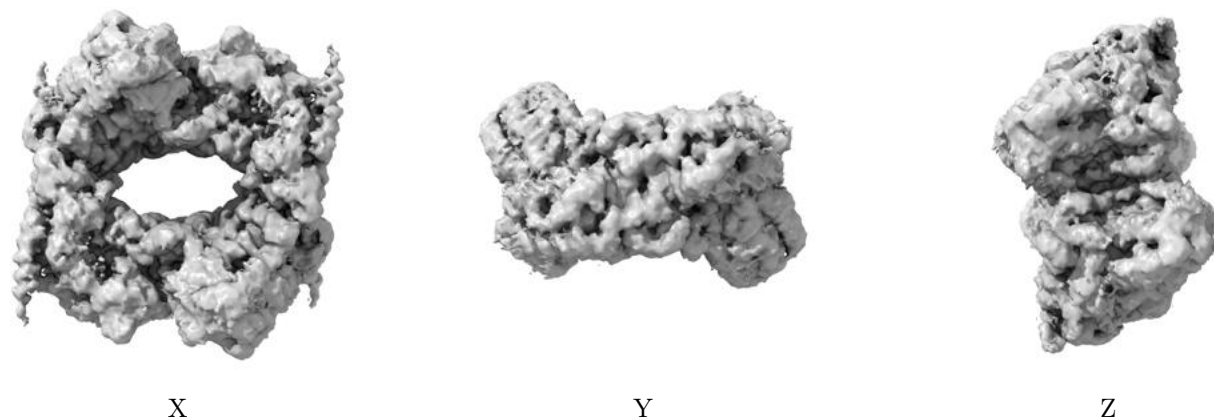
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. 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.

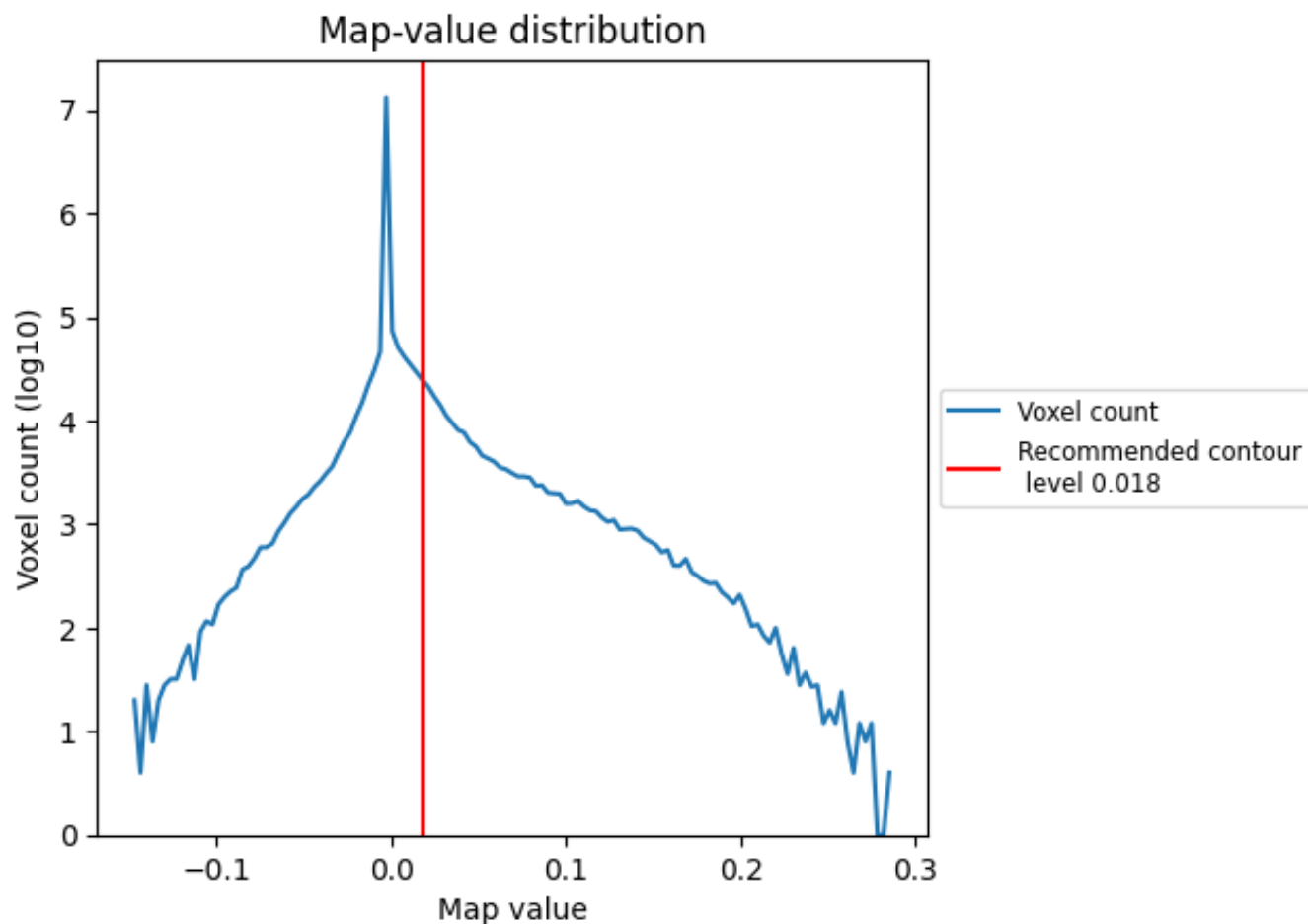
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

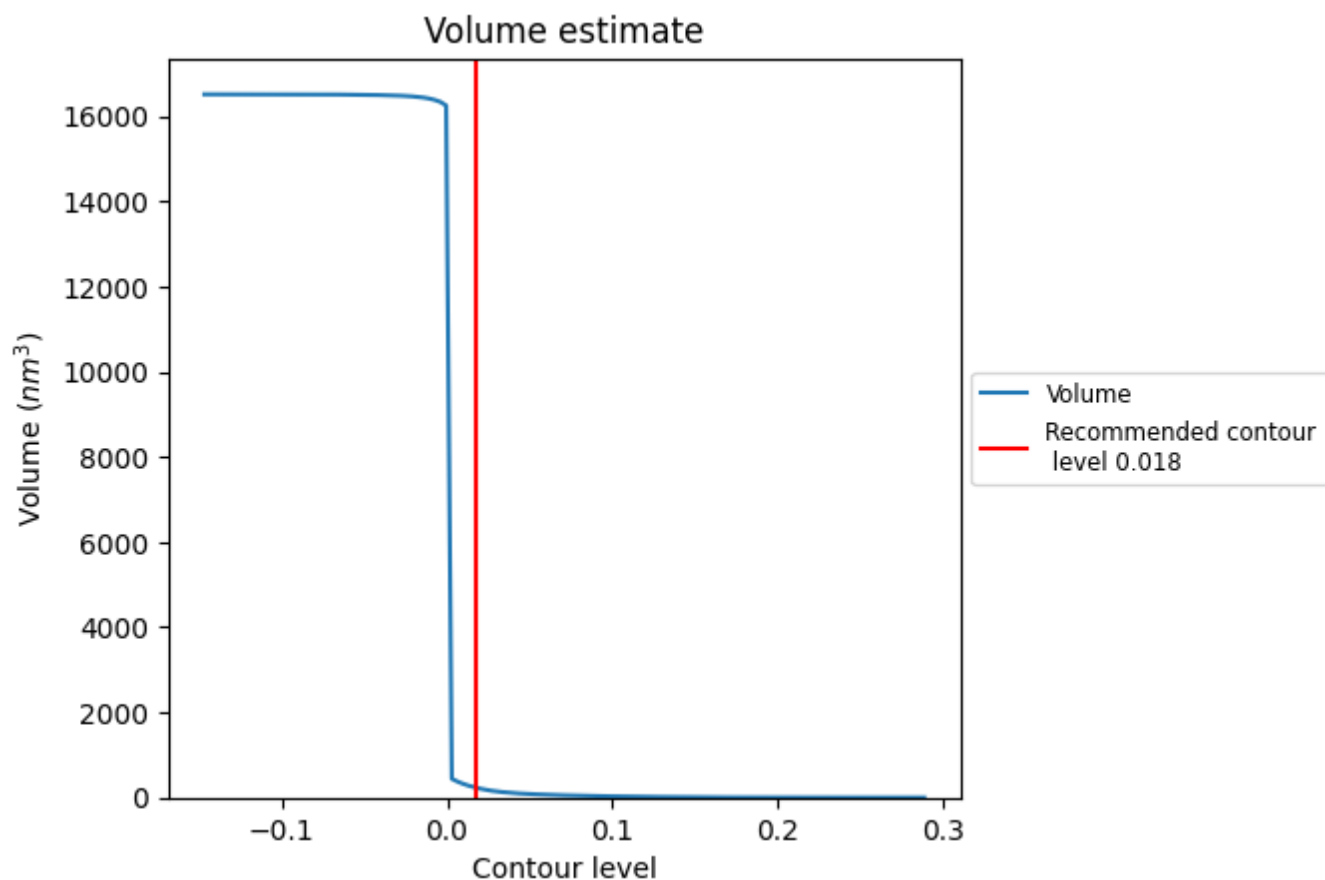
This section contains the results of statistical analysis of the map.

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.

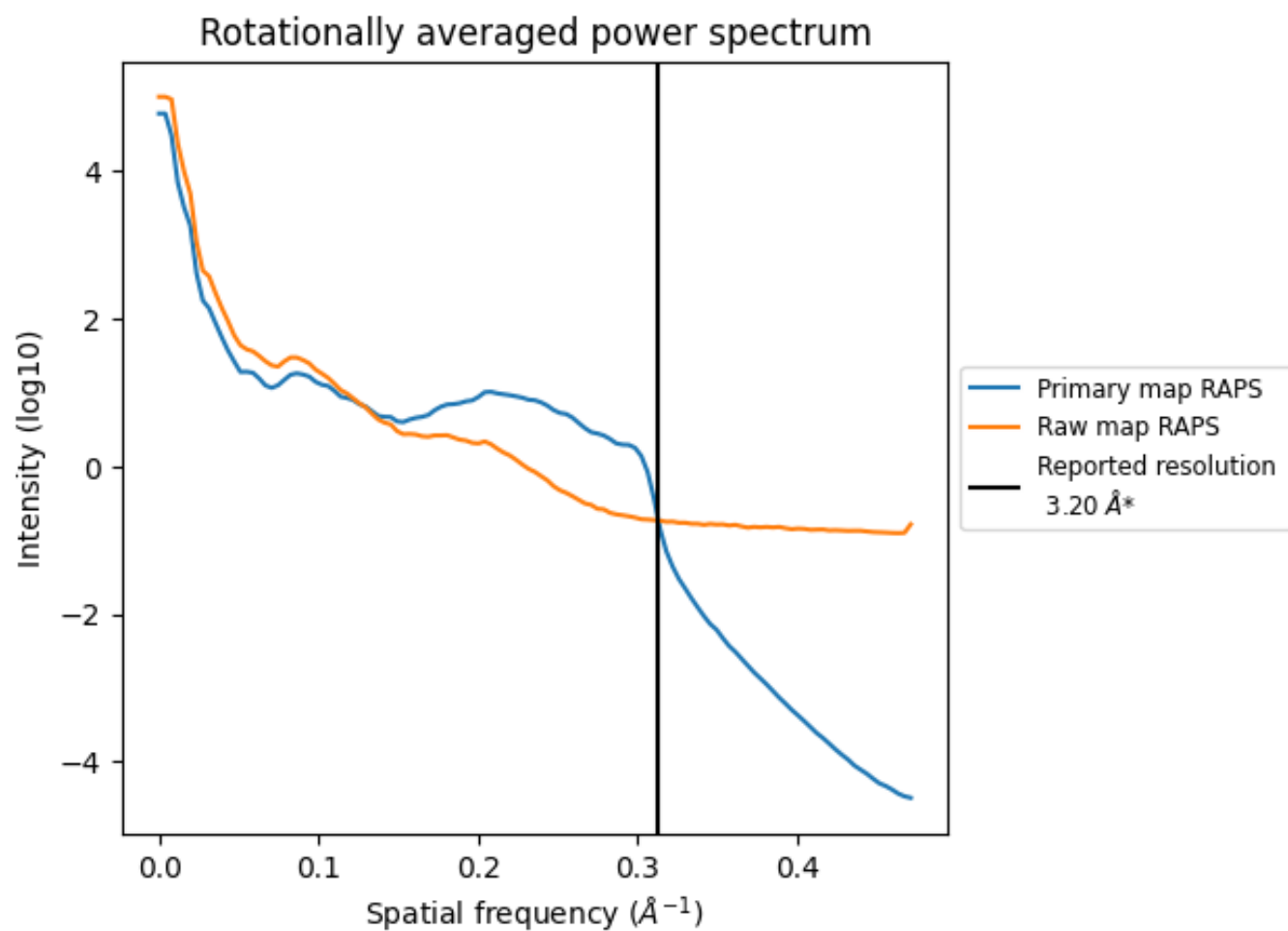
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 228 nm³; this corresponds to an approximate mass of 206 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 ⓘ

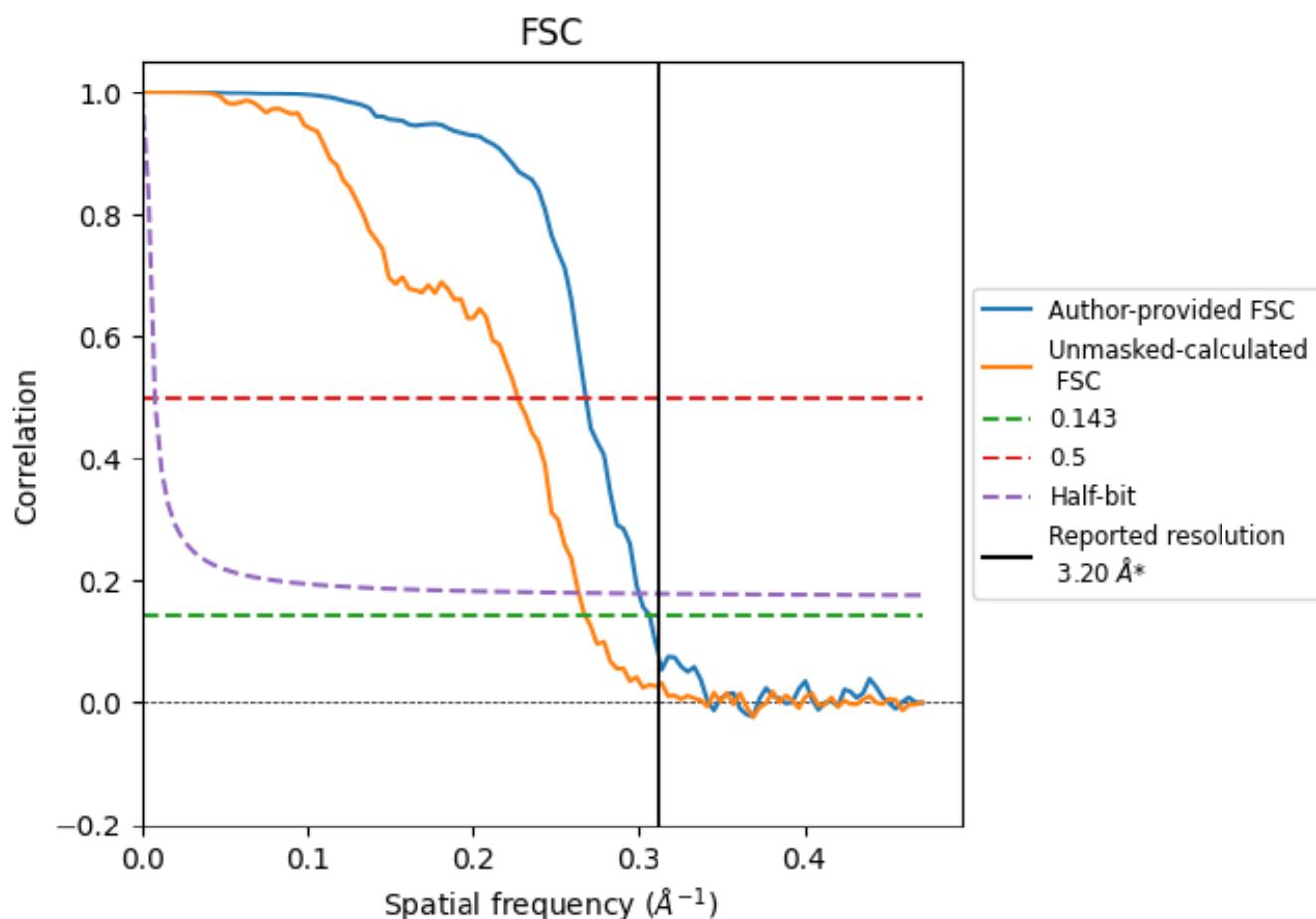


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

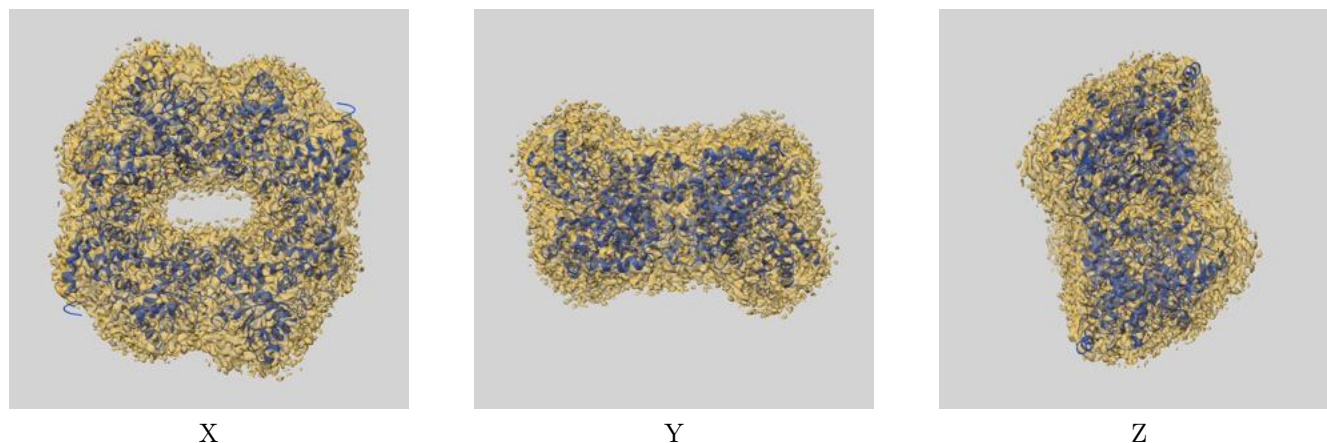
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.26	3.73	3.33
Unmasked-calculated*	3.74	4.40	3.79

*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 3.74 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

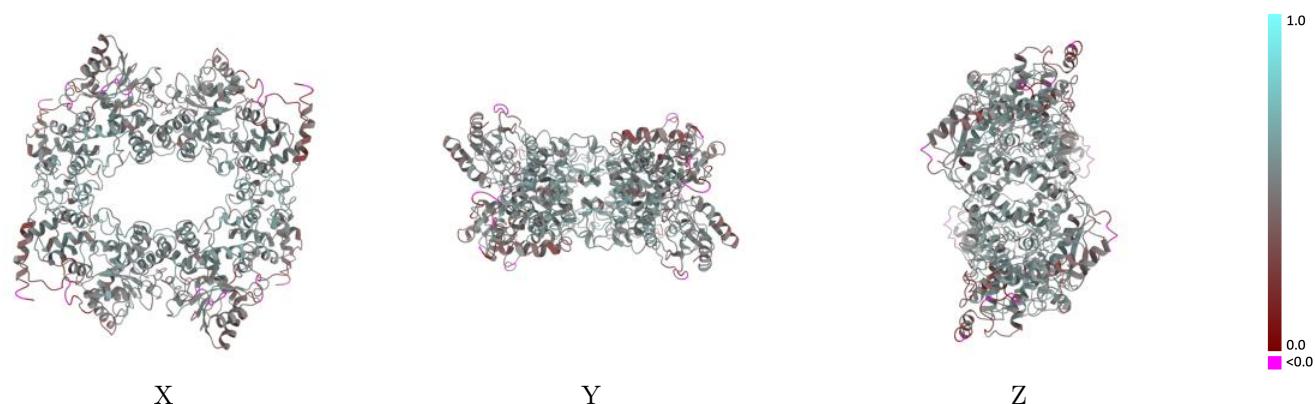
This section contains information regarding the fit between EMDB map EMD-30022 and PDB model 6LZ3. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



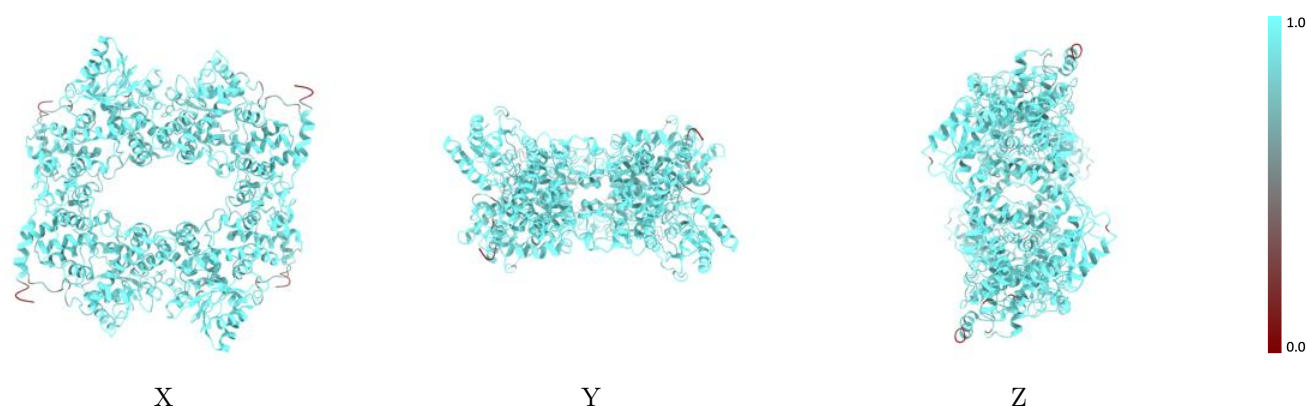
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



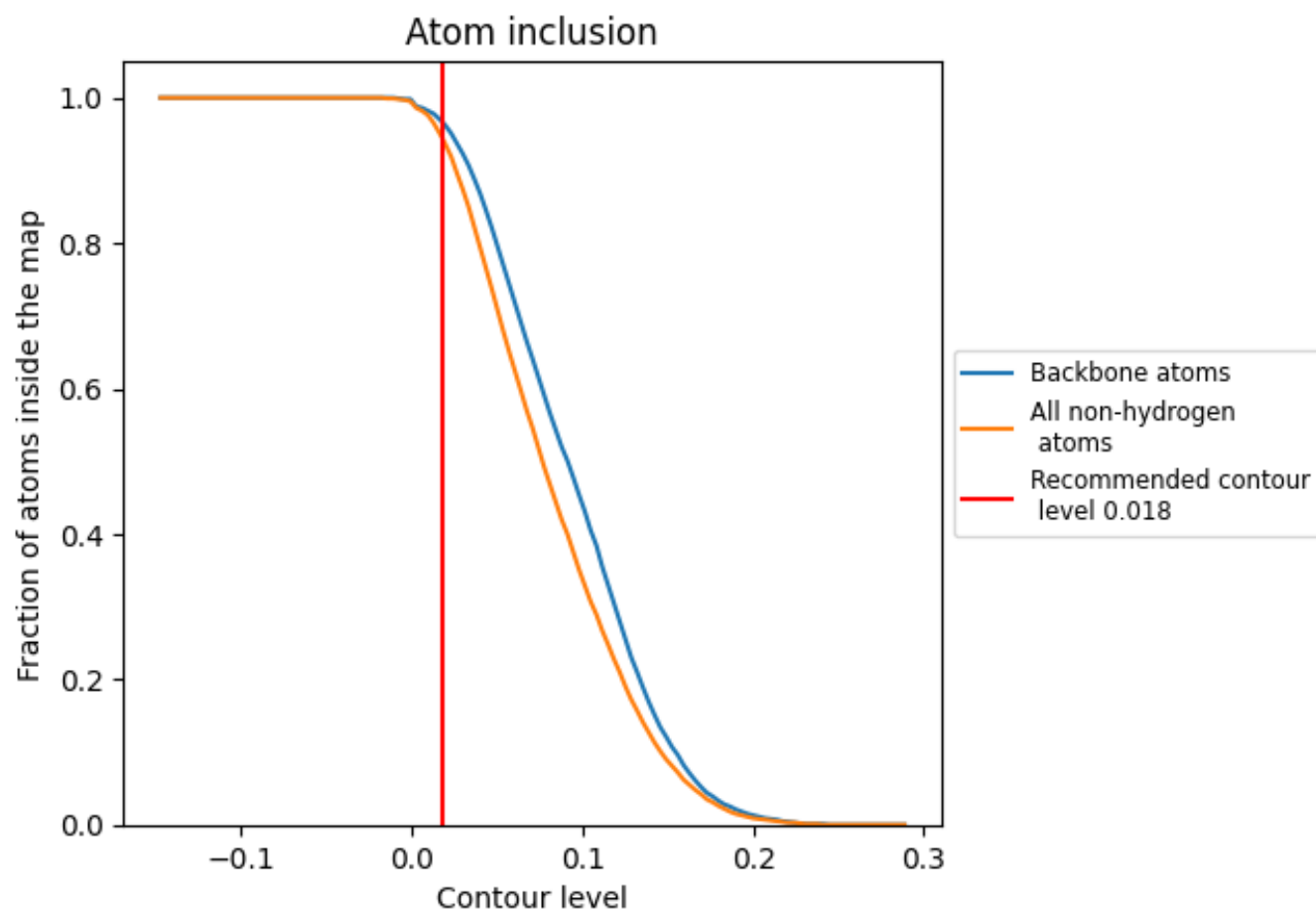
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 94% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9450	<div></div> 0.4760
A	<div></div> 0.9440	<div></div> 0.4760
B	<div></div> 0.9430	<div></div> 0.4740
C	<div></div> 0.9470	<div></div> 0.4770
D	<div></div> 0.9470	<div></div> 0.4790

