



## Full wwPDB EM Validation Report ⓘ

Feb 6, 2025 – 12:15 PM EST

PDB ID : 9CFW  
EMDB ID : EMD-45565  
Title : Cryo-EM structure of myosin-1c bound to F-actin in the ADP-B state  
Authors : Chavali, S.S.; Sindelar, C.V.; Ostap, M.E.  
Deposited on : 2024-06-27  
Resolution : 3.00 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.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
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) : 2.40

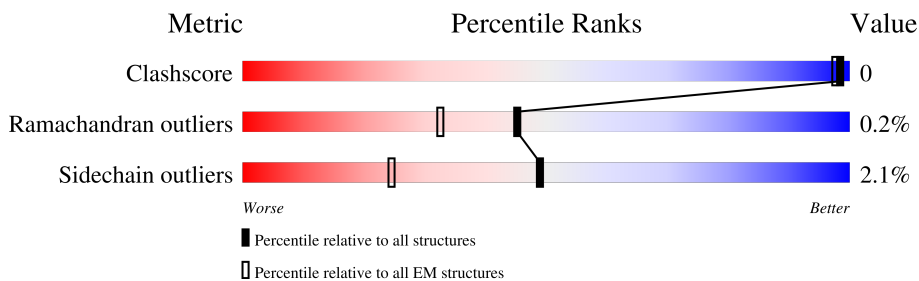
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 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  $\geq 3$ , 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	B	375	
1	C	375	
1	D	375	
2	P	793	
3	R	148	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15838 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	371	2896	1832	489	554	21	0	0
1	C	371	2896	1832	489	554	21	0	0
1	D	371	2896	1832	489	554	21	0	0

- Molecule 2 is a protein called Unconventional myosin-Ic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	P	720	5874	3734	1040	1078	22	0	0

There are 73 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	721	ARG	-	expression tag	UNP Q9WTI7
P	722	VAL	-	expression tag	UNP Q9WTI7
P	723	LYS	-	expression tag	UNP Q9WTI7
P	724	ARG	-	expression tag	UNP Q9WTI7
P	725	SER	-	expression tag	UNP Q9WTI7
P	726	ALA	-	expression tag	UNP Q9WTI7
P	727	ILE	-	expression tag	UNP Q9WTI7
P	728	CYS	-	expression tag	UNP Q9WTI7
P	729	ILE	-	expression tag	UNP Q9WTI7
P	730	GLN	-	expression tag	UNP Q9WTI7
P	731	SER	-	expression tag	UNP Q9WTI7
P	732	TRP	-	expression tag	UNP Q9WTI7
P	733	TRP	-	expression tag	UNP Q9WTI7
P	734	ARG	-	expression tag	UNP Q9WTI7
P	735	GLY	-	expression tag	UNP Q9WTI7
P	736	THR	-	expression tag	UNP Q9WTI7
P	737	LEU	-	expression tag	UNP Q9WTI7

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Chain	Residue	Modelled	Actual	Comment	Reference
P	738	GLY	-	expression tag	UNP Q9WTI7
P	739	ARG	-	expression tag	UNP Q9WTI7
P	740	ARG	-	expression tag	UNP Q9WTI7
P	741	LYS	-	expression tag	UNP Q9WTI7
P	742	ALA	-	expression tag	UNP Q9WTI7
P	743	ALA	-	expression tag	UNP Q9WTI7
P	744	LYS	-	expression tag	UNP Q9WTI7
P	745	ARG	-	expression tag	UNP Q9WTI7
P	746	LYS	-	expression tag	UNP Q9WTI7
P	747	TRP	-	expression tag	UNP Q9WTI7
P	748	ALA	-	expression tag	UNP Q9WTI7
P	749	ALA	-	expression tag	UNP Q9WTI7
P	750	GLN	-	expression tag	UNP Q9WTI7
P	751	THR	-	expression tag	UNP Q9WTI7
P	752	ILE	-	expression tag	UNP Q9WTI7
P	753	ARG	-	expression tag	UNP Q9WTI7
P	754	ARG	-	expression tag	UNP Q9WTI7
P	755	LEU	-	expression tag	UNP Q9WTI7
P	756	ILE	-	expression tag	UNP Q9WTI7
P	757	ARG	-	expression tag	UNP Q9WTI7
P	758	GLY	-	expression tag	UNP Q9WTI7
P	759	PHE	-	expression tag	UNP Q9WTI7
P	760	ILE	-	expression tag	UNP Q9WTI7
P	761	LEU	-	expression tag	UNP Q9WTI7
P	762	ARG	-	expression tag	UNP Q9WTI7
P	763	HIS	-	expression tag	UNP Q9WTI7
P	764	SER	-	expression tag	UNP Q9WTI7
P	765	PRO	-	expression tag	UNP Q9WTI7
P	766	ARG	-	expression tag	UNP Q9WTI7
P	767	CYS	-	expression tag	UNP Q9WTI7
P	768	GLY	-	expression tag	UNP Q9WTI7
P	769	GLY	-	expression tag	UNP Q9WTI7
P	770	LEU	-	expression tag	UNP Q9WTI7
P	771	ASN	-	expression tag	UNP Q9WTI7
P	772	ASP	-	expression tag	UNP Q9WTI7
P	773	ILE	-	expression tag	UNP Q9WTI7
P	774	PHE	-	expression tag	UNP Q9WTI7
P	775	GLU	-	expression tag	UNP Q9WTI7
P	776	ALA	-	expression tag	UNP Q9WTI7
P	777	GLN	-	expression tag	UNP Q9WTI7
P	778	LYS	-	expression tag	UNP Q9WTI7
P	779	ILE	-	expression tag	UNP Q9WTI7

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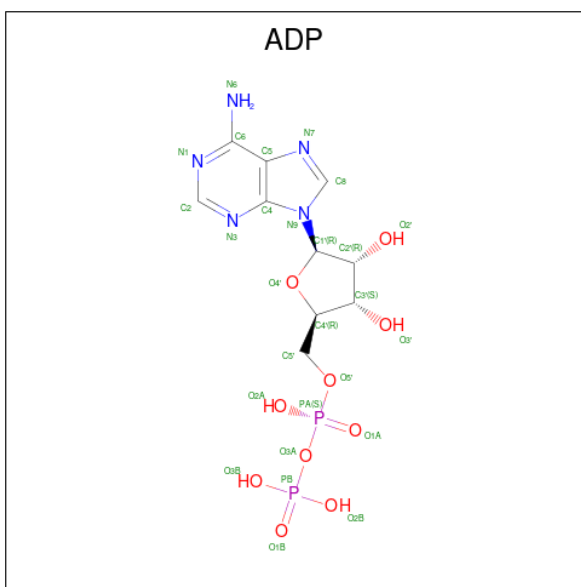
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Chain	Residue	Modelled	Actual	Comment	Reference
P	780	GLU	-	expression tag	UNP Q9WTI7
P	781	TRP	-	expression tag	UNP Q9WTI7
P	782	HIS	-	expression tag	UNP Q9WTI7
P	783	GLU	-	expression tag	UNP Q9WTI7
P	784	ALA	-	expression tag	UNP Q9WTI7
P	785	ALA	-	expression tag	UNP Q9WTI7
P	786	ASP	-	expression tag	UNP Q9WTI7
P	787	TYR	-	expression tag	UNP Q9WTI7
P	788	LYS	-	expression tag	UNP Q9WTI7
P	789	ASP	-	expression tag	UNP Q9WTI7
P	790	ASP	-	expression tag	UNP Q9WTI7
P	791	ASP	-	expression tag	UNP Q9WTI7
P	792	ASP	-	expression tag	UNP Q9WTI7
P	793	LYS	-	expression tag	UNP Q9WTI7

- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			S
3	R	148	1165	713	187	255	10	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	P	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Mg	0
			1	1	
5	C	1	Total	Mg	0
			1	1	
5	D	1	Total	Mg	0
			1	1	

### 3 Residue-property plots [i](#)

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

- Molecule 1: Actin, alpha skeletal muscle

Chain B: 



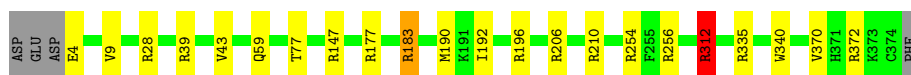
- Molecule 1: Actin, alpha skeletal muscle

Chain C: 




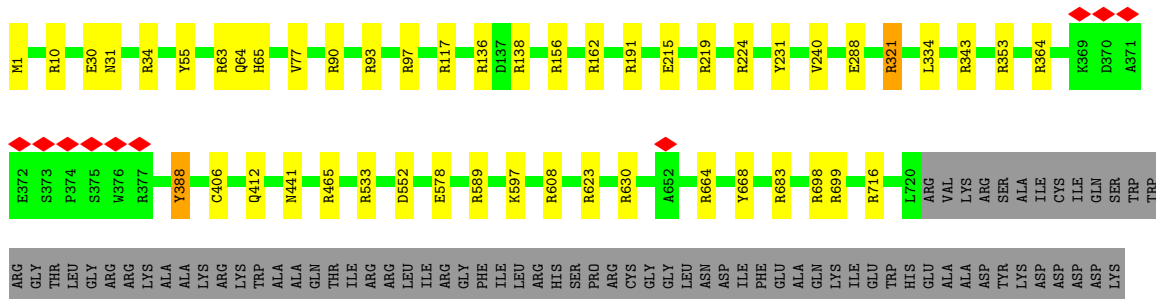
- Molecule 1: Actin, alpha skeletal muscle

Chain D: 

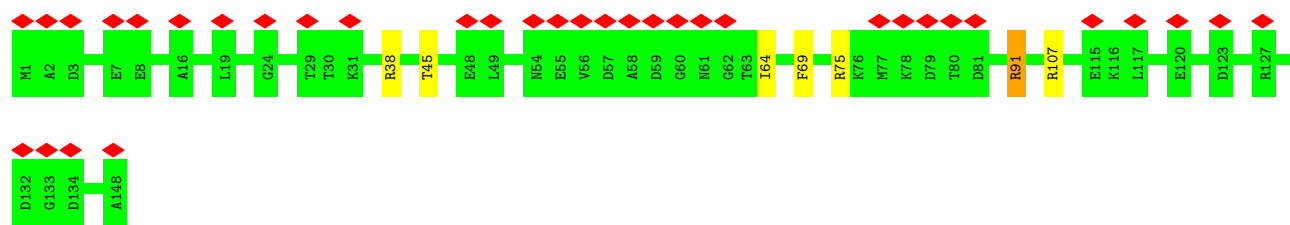


- Molecule 2: Unconventional myosin-Ic

Chain P: 



- Molecule 3: Calmodulin-1





## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=167.88°, rise=27.38 Å, axial sym=C1	Depositor
Number of segments used	126845	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 ( $e^-/\text{Å}^2$ )	52	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.326	Depositor
Minimum map value	-2.151	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	516.864, 516.864, 516.864	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3460001, 1.3460001, 1.3460001	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: ADP, 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	B	0.61	0/2958	1.02	8/4008 (0.2%)
1	C	0.61	0/2958	1.04	17/4008 (0.4%)
1	D	0.62	0/2958	1.03	16/4008 (0.4%)
2	P	0.67	0/5998	1.06	33/8092 (0.4%)
3	R	0.67	0/1177	0.99	4/1579 (0.3%)
All	All	0.64	0/16049	1.04	78/21695 (0.4%)

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	B	0	4
1	C	0	3
1	D	0	2
2	P	0	1
All	All	0	10

There are no bond length outliers.

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	312	ARG	NE-CZ-NH2	12.37	126.48	120.30
1	C	312	ARG	NE-CZ-NH2	11.59	126.09	120.30
1	D	39	ARG	NE-CZ-NH2	9.67	125.13	120.30
2	P	699	ARG	NE-CZ-NH2	9.50	125.05	120.30
1	B	210	ARG	NE-CZ-NH2	9.49	125.05	120.30
1	D	210	ARG	NE-CZ-NH2	9.06	124.83	120.30
1	D	312	ARG	NE-CZ-NH2	8.68	124.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	191	ARG	NE-CZ-NH2	8.58	124.59	120.30
1	D	256	ARG	NE-CZ-NH2	8.14	124.37	120.30
1	C	39	ARG	NE-CZ-NH2	8.09	124.35	120.30
1	B	196	ARG	NE-CZ-NH2	8.03	124.31	120.30
2	P	162	ARG	NE-CZ-NH2	7.91	124.25	120.30
1	C	254	ARG	NE-CZ-NH2	7.75	124.17	120.30
2	P	668	TYR	CB-CG-CD2	-7.68	116.39	121.00
1	C	210	ARG	NE-CZ-NH2	7.67	124.14	120.30
1	C	256	ARG	NE-CZ-NH2	7.65	124.13	120.30
2	P	388	TYR	CB-CG-CD2	-7.64	116.41	121.00
1	B	335	ARG	NE-CZ-NH2	7.60	124.10	120.30
2	P	63	ARG	NE-CZ-NH2	7.50	124.05	120.30
3	R	107	ARG	NE-CZ-NH2	7.25	123.92	120.30
3	R	38	ARG	NE-CZ-NH2	7.15	123.88	120.30
2	P	224	ARG	NE-CZ-NH2	6.85	123.73	120.30
2	P	683	ARG	NE-CZ-NH2	6.78	123.69	120.30
1	B	254	ARG	NE-CZ-NH2	6.74	123.67	120.30
1	C	147	ARG	NE-CZ-NH2	6.74	123.67	120.30
2	P	630	ARG	NE-CZ-NH2	6.71	123.65	120.30
1	C	62	ARG	NE-CZ-NH2	6.67	123.64	120.30
2	P	90	ARG	NE-CZ-NH1	-6.67	116.97	120.30
1	D	335	ARG	NE-CZ-NH2	6.61	123.61	120.30
1	D	183	ARG	NE-CZ-NH1	-6.58	117.01	120.30
2	P	231	TYR	CB-CG-CD2	-6.56	117.06	121.00
2	P	138	ARG	NE-CZ-NH2	6.52	123.56	120.30
3	R	75	ARG	NE-CZ-NH2	6.49	123.54	120.30
2	P	117	ARG	NE-CZ-NH2	6.47	123.54	120.30
2	P	34	ARG	NE-CZ-NH2	6.42	123.51	120.30
1	D	254	ARG	NE-CZ-NH2	6.38	123.49	120.30
2	P	97	ARG	NE-CZ-NH2	6.37	123.49	120.30
1	D	210	ARG	NE-CZ-NH1	-6.25	117.18	120.30
1	C	183	ARG	NE-CZ-NH2	6.22	123.41	120.30
1	D	206	ARG	NE-CZ-NH2	6.21	123.40	120.30
1	B	147	ARG	NE-CZ-NH2	6.17	123.39	120.30
1	C	312	ARG	NE-CZ-NH1	-6.17	117.21	120.30
2	P	63	ARG	NE-CZ-NH1	-6.16	117.22	120.30
2	P	353	ARG	NE-CZ-NH2	6.10	123.35	120.30
2	P	90	ARG	NE-CZ-NH2	6.06	123.33	120.30
2	P	465	ARG	NE-CZ-NH2	5.99	123.30	120.30
2	P	321	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	B	177	ARG	NE-CZ-NH1	-5.93	117.34	120.30
1	D	147	ARG	NE-CZ-NH2	5.90	123.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	335	ARG	NE-CZ-NH2	5.85	123.22	120.30
2	P	219	ARG	NE-CZ-NH2	5.81	123.21	120.30
1	C	166	TYR	CB-CG-CD1	-5.79	117.53	121.00
2	P	343	ARG	NE-CZ-NH2	5.75	123.17	120.30
2	P	93	ARG	NE-CZ-NH2	5.73	123.17	120.30
1	D	196	ARG	NE-CZ-NH2	5.72	123.16	120.30
2	P	664	ARG	NE-CZ-NH2	5.70	123.15	120.30
2	P	156	ARG	NE-CZ-NH2	5.64	123.12	120.30
1	C	372	ARG	NE-CZ-NH2	5.61	123.11	120.30
1	C	206	ARG	NE-CZ-NH2	5.58	123.09	120.30
3	R	91	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	C	183	ARG	NE-CZ-NH1	-5.56	117.52	120.30
2	P	364	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	D	372	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	D	183	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	D	177	ARG	NE-CZ-NH1	-5.37	117.62	120.30
1	C	177	ARG	NE-CZ-NH1	-5.35	117.62	120.30
2	P	388	TYR	CB-CG-CD1	5.33	124.20	121.00
2	P	589	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	C	196	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	D	177	ARG	NE-CZ-NH2	5.26	122.93	120.30
2	P	716	ARG	NE-CZ-NH2	5.23	122.92	120.30
2	P	608	ARG	NE-CZ-NH2	5.18	122.89	120.30
2	P	136	ARG	NE-CZ-NH2	5.17	122.88	120.30
2	P	698	ARG	NE-CZ-NH2	5.17	122.88	120.30
1	B	210	ARG	NE-CZ-NH1	-5.11	117.74	120.30
1	C	28	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	D	28	ARG	NE-CZ-NH2	5.07	122.83	120.30
2	P	668	TYR	CB-CG-CD1	5.00	124.00	121.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	143	TYR	Sidechain
1	B	279	TYR	Sidechain
1	B	306	TYR	Sidechain
1	B	62	ARG	Sidechain
1	C	183	ARG	Sidechain
1	C	279	TYR	Sidechain
1	C	312	ARG	Sidechain
1	D	183	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	312	ARG	Sidechain
2	P	533	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2896	0	2868	1	0
1	C	2896	0	2868	1	0
1	D	2896	0	2868	1	0
2	P	5874	0	5867	2	0
3	R	1165	0	1092	0	0
4	B	27	0	12	0	0
4	C	27	0	12	0	0
4	D	27	0	12	0	0
4	P	27	0	12	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	15838	0	15611	5	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 0.

All (5) 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)
2:P:321:ARG:HB2	2:P:334:LEU:HD21	1.98	0.46
1:C:9:VAL:HB	1:C:340:TRP:CH2	2.53	0.43
1:D:9:VAL:HB	1:D:340:TRP:CH2	2.54	0.42
2:P:55:TYR:CZ	2:P:597:LYS:HA	2.55	0.42
1:B:155:SER:HB3	1:B:303:THR:HB	2.02	0.41

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	B	369/375 (98%)	350 (95%)	18 (5%)	1 (0%)	37	70
1	C	369/375 (98%)	354 (96%)	14 (4%)	1 (0%)	37	70
1	D	369/375 (98%)	355 (96%)	14 (4%)	0	100	100
2	P	718/793 (90%)	690 (96%)	27 (4%)	1 (0%)	48	81
3	R	146/148 (99%)	133 (91%)	13 (9%)	0	100	100
All	All	1971/2066 (95%)	1882 (96%)	86 (4%)	3 (0%)	45	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	243	PRO
2	P	240	VAL
1	B	156	GLY

### 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	B	314/318 (99%)	309 (98%)	5 (2%)	58	82
1	C	314/318 (99%)	311 (99%)	3 (1%)	73	88
1	D	314/318 (99%)	306 (98%)	8 (2%)	42	73
2	P	632/692 (91%)	616 (98%)	16 (2%)	42	73
3	R	126/126 (100%)	122 (97%)	4 (3%)	34	67

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1700/1772 (96%)	1664 (98%)	36 (2%)	49 77

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	57	GLU
1	B	80	ASP
1	B	248	ILE
1	B	257	CYS
1	B	340	TRP
1	C	4	GLU
1	C	227	MET
1	C	370	VAL
1	D	4	GLU
1	D	43	VAL
1	D	59	GLN
1	D	77	THR
1	D	190	MET
1	D	192	ILE
1	D	312	ARG
1	D	370	VAL
2	P	1	MET
2	P	10	ARG
2	P	30	GLU
2	P	31	ASN
2	P	64	GLN
2	P	65	HIS
2	P	77	VAL
2	P	215	GLU
2	P	288	GLU
2	P	388	TYR
2	P	406	CYS
2	P	412	GLN
2	P	441	ASN
2	P	552	ASP
2	P	578	GLU
2	P	623	ARG
3	R	45	THR
3	R	64	ILE
3	R	69	PHE
3	R	91	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	P	194	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 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	ADP	B	401	5	24,29,29	1.46	3 (12%)	29,45,45	1.41	5 (17%)
4	ADP	C	401	5	24,29,29	1.41	3 (12%)	29,45,45	1.45	7 (24%)
4	ADP	P	801	-	24,29,29	1.15	1 (4%)	29,45,45	1.24	3 (10%)
4	ADP	D	401	5	24,29,29	1.48	4 (16%)	29,45,45	1.37	4 (13%)

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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	B	401	5	-	4/12/32/32	0/3/3/3
4	ADP	C	401	5	-	1/12/32/32	0/3/3/3
4	ADP	P	801	-	-	1/12/32/32	0/3/3/3
4	ADP	D	401	5	-	0/12/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	401	ADP	PA-O3A	-5.05	1.54	1.59
4	B	401	ADP	PA-O3A	-4.37	1.54	1.59
4	C	401	ADP	PA-O3A	-4.20	1.55	1.59
4	P	801	ADP	O4'-C1'	3.25	1.45	1.40
4	C	401	ADP	PB-O3B	-2.36	1.46	1.54
4	D	401	ADP	C1'-N9	-2.24	1.44	1.49
4	D	401	ADP	PB-O3B	-2.23	1.46	1.54
4	C	401	ADP	PB-O2B	-2.14	1.46	1.54
4	B	401	ADP	O4'-C1'	2.12	1.43	1.40
4	B	401	ADP	PB-O3B	-2.09	1.47	1.54
4	D	401	ADP	C4-N3	-2.05	1.32	1.35

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	401	ADP	C4-C5-N7	4.33	113.91	109.34
4	D	401	ADP	C4-C5-N7	4.32	113.90	109.34
4	P	801	ADP	C4-C5-N7	4.27	113.85	109.34
4	B	401	ADP	C4-C5-N7	4.21	113.79	109.34
4	D	401	ADP	O2A-PA-O3A	3.27	116.12	107.27
4	B	401	ADP	O2A-PA-O3A	3.26	116.08	107.27
4	C	401	ADP	O2B-PB-O1B	-2.83	99.80	110.83
4	C	401	ADP	O2B-PB-O3A	2.72	113.77	104.64
4	C	401	ADP	O2A-PA-O3A	2.28	113.44	107.27
4	D	401	ADP	C5-C6-N6	2.26	123.75	120.31
4	B	401	ADP	N6-C6-N1	-2.21	113.61	118.33
4	C	401	ADP	C5-C6-N6	2.18	123.64	120.31
4	C	401	ADP	N6-C6-N1	-2.15	113.73	118.33
4	P	801	ADP	O3A-PA-O1A	2.09	116.99	110.70
4	P	801	ADP	N6-C6-N1	-2.06	113.93	118.33
4	B	401	ADP	O2B-PB-O3A	2.06	111.53	104.64
4	B	401	ADP	C5-C6-N6	2.04	123.42	120.31
4	C	401	ADP	O3B-PB-O3A	2.03	111.43	104.64
4	D	401	ADP	N6-C6-N1	-2.01	114.05	118.33

There are no chirality outliers.

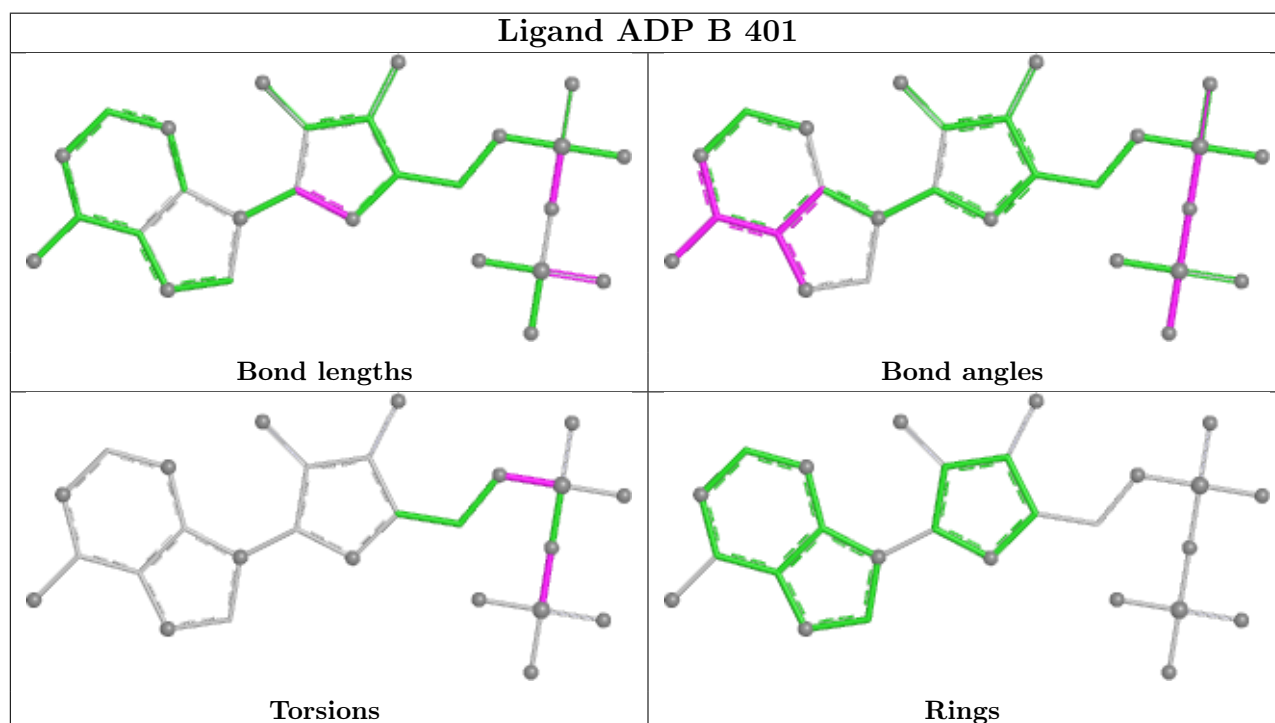
All (6) torsion outliers are listed below:

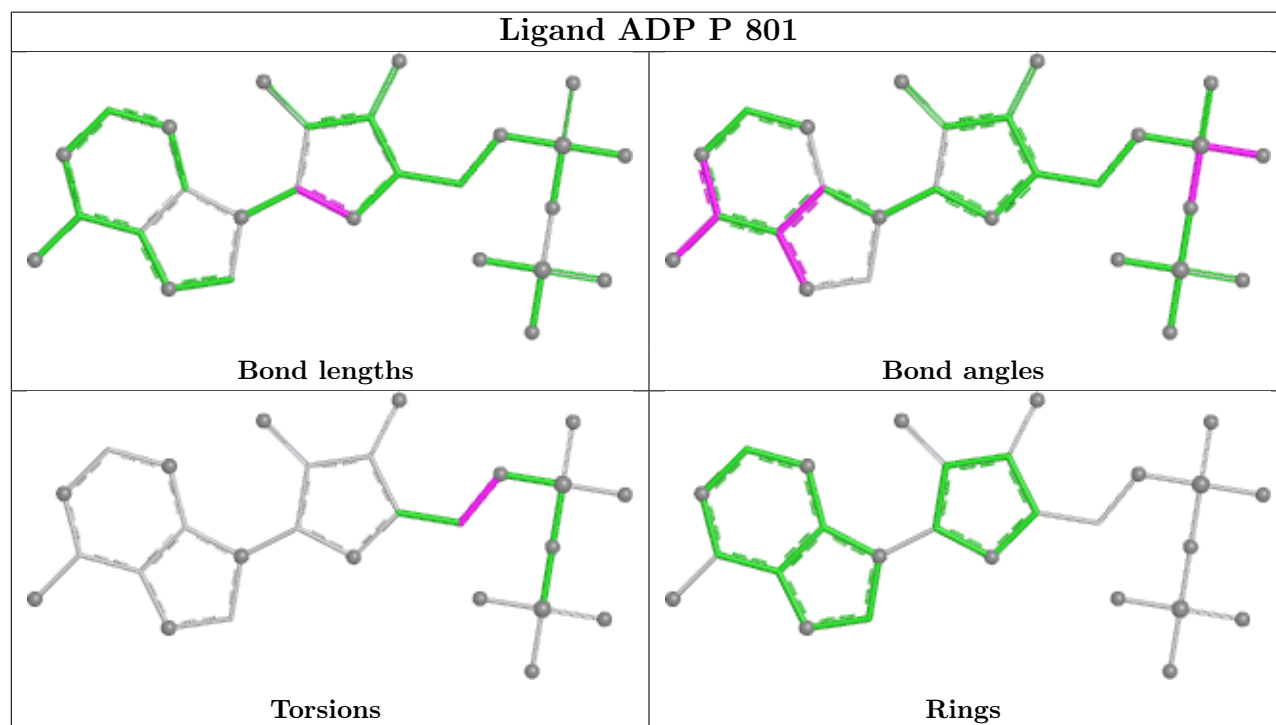
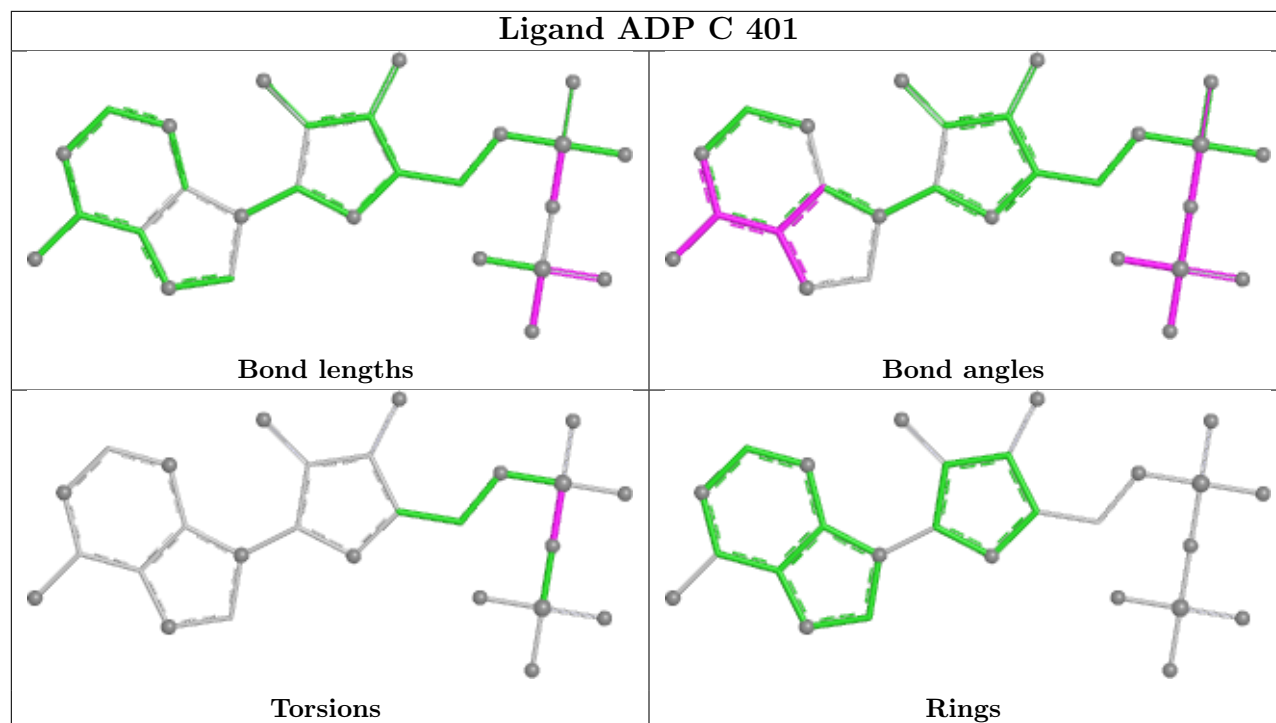
Mol	Chain	Res	Type	Atoms
4	B	401	ADP	PA-O3A-PB-O2B
4	B	401	ADP	PA-O3A-PB-O3B
4	P	801	ADP	C4'-C5'-O5'-PA
4	B	401	ADP	C5'-O5'-PA-O3A
4	B	401	ADP	PA-O3A-PB-O1B
4	C	401	ADP	PB-O3A-PA-O2A

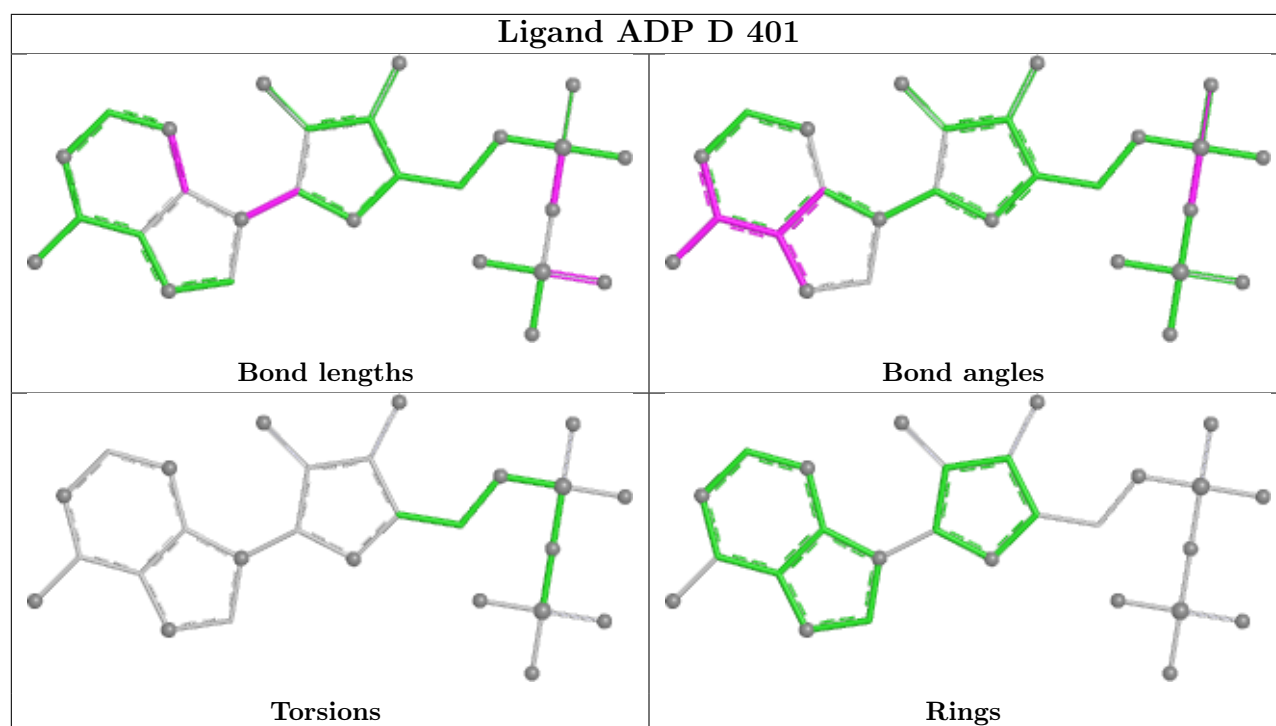
There are no ring outliers.

No monomer is involved in short contacts.

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.

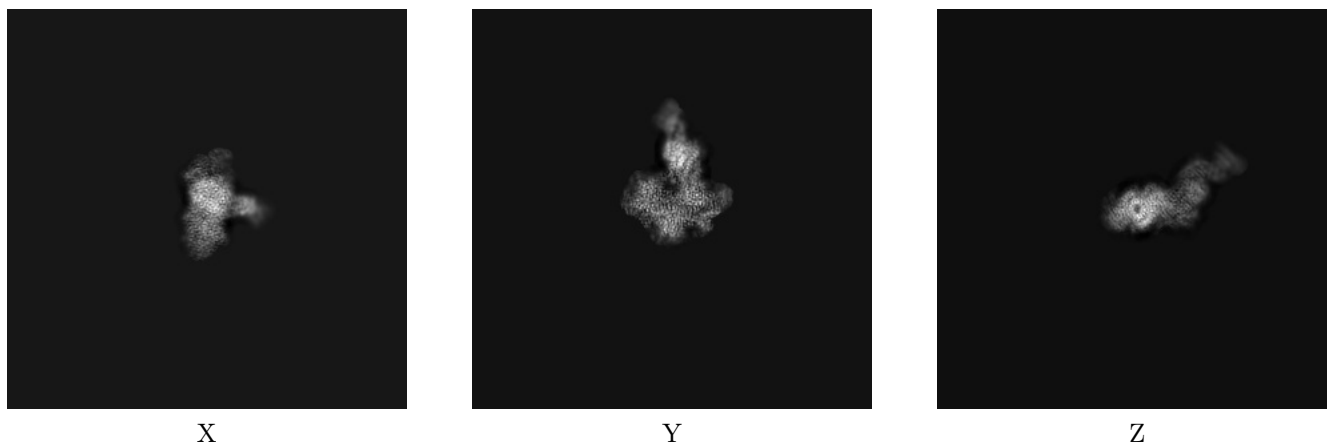
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45565. These allow visual inspection of the internal detail of the map and identification of artifacts.

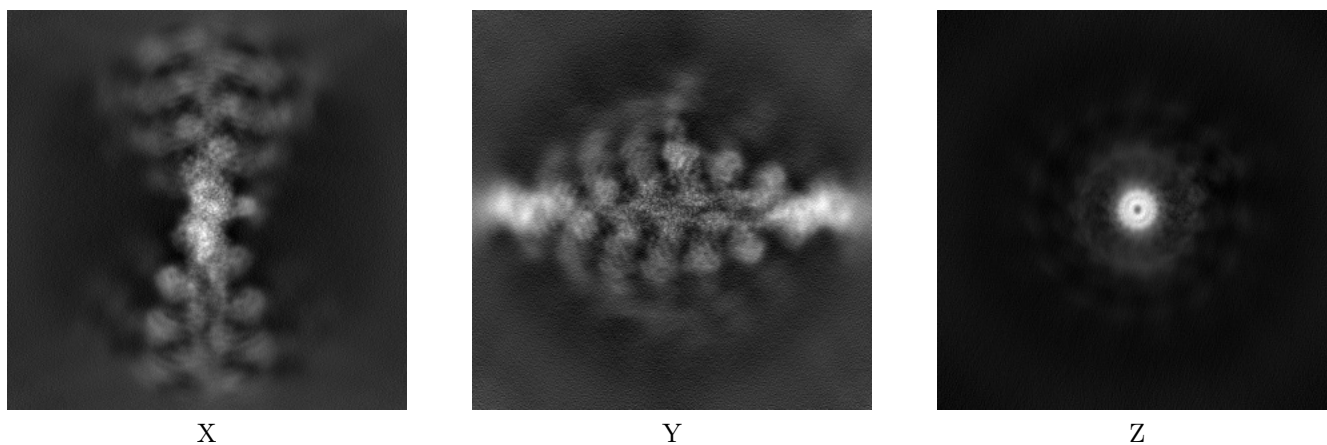
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



#### 6.1.2 Raw map



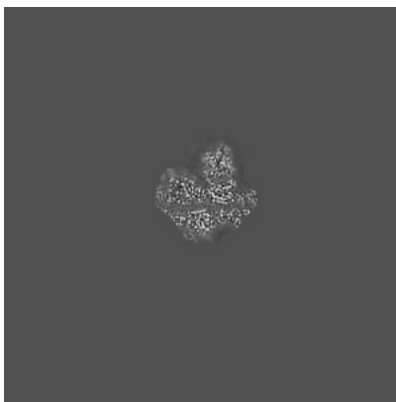
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

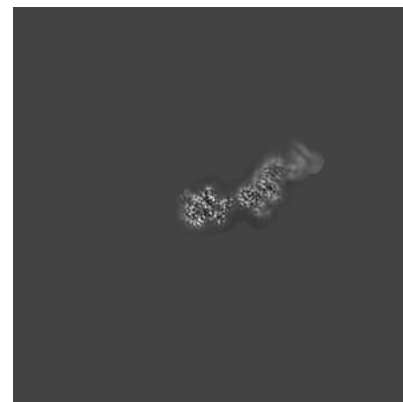
### 6.2.1 Primary map



X Index: 192



Y Index: 192

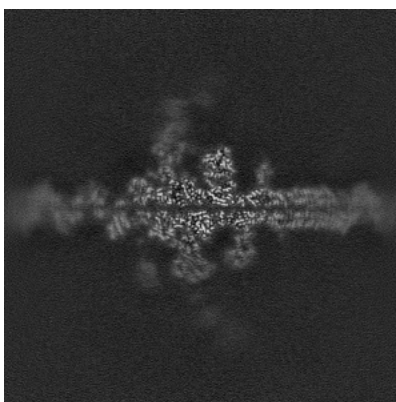


Z Index: 192

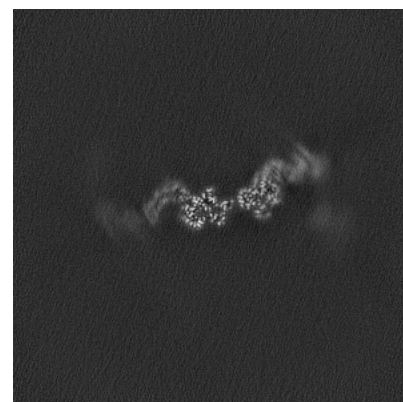
### 6.2.2 Raw map



X Index: 192



Y Index: 192

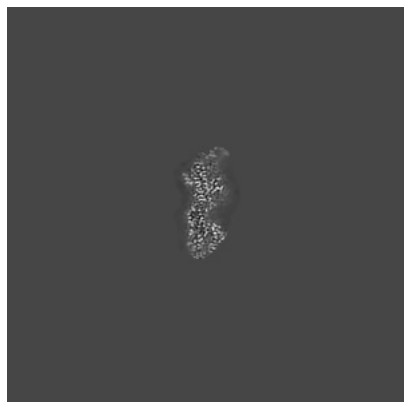


Z Index: 192

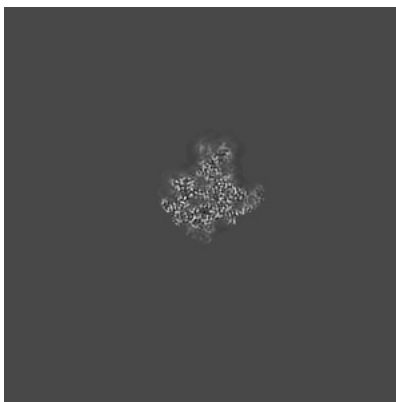
The images above show central slices of the map in three orthogonal directions.

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

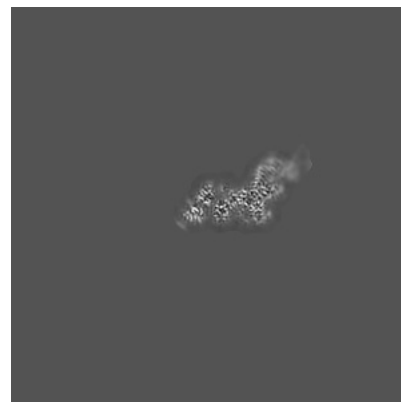
### 6.3.1 Primary map



X Index: 196

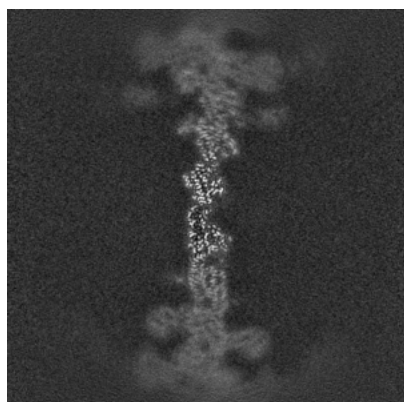


Y Index: 197

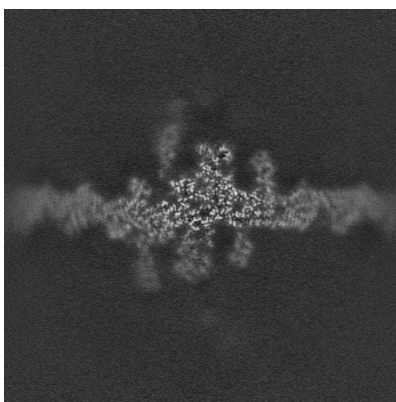


Z Index: 201

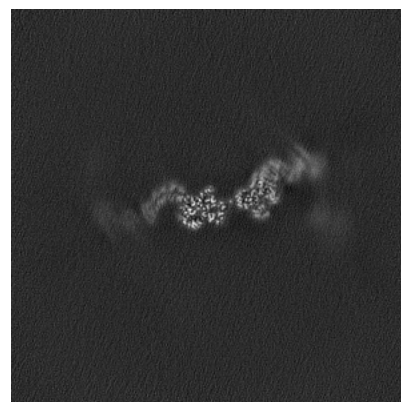
### 6.3.2 Raw map



X Index: 197



Y Index: 197

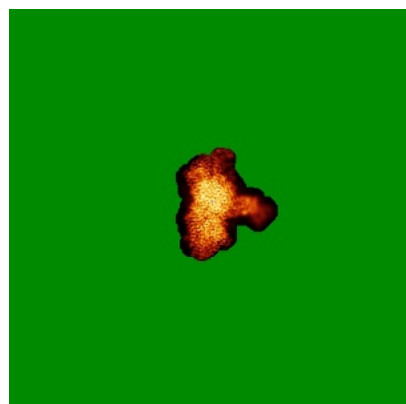


Z Index: 193

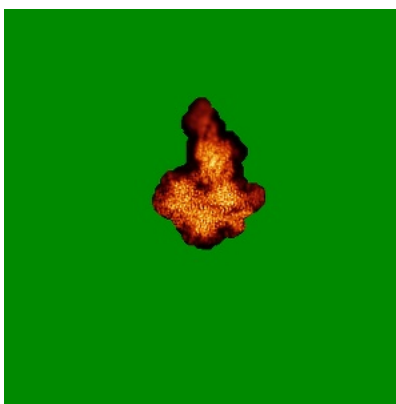
The images above show the largest variance slices of the map in three orthogonal directions.

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

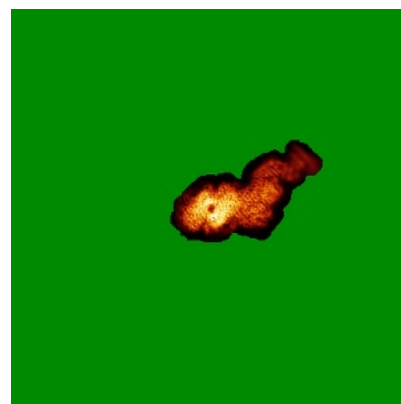
### 6.4.1 Primary map



X

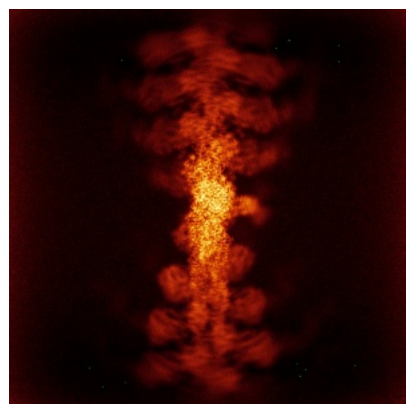


Y

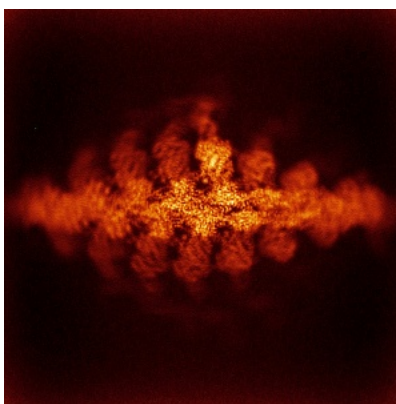


Z

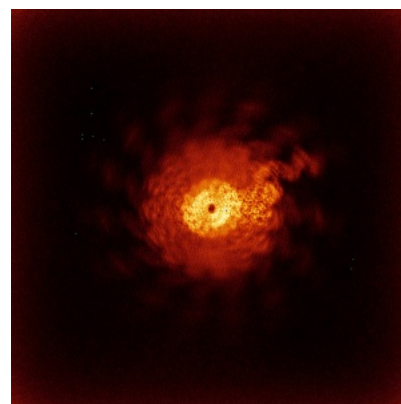
### 6.4.2 Raw map



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.



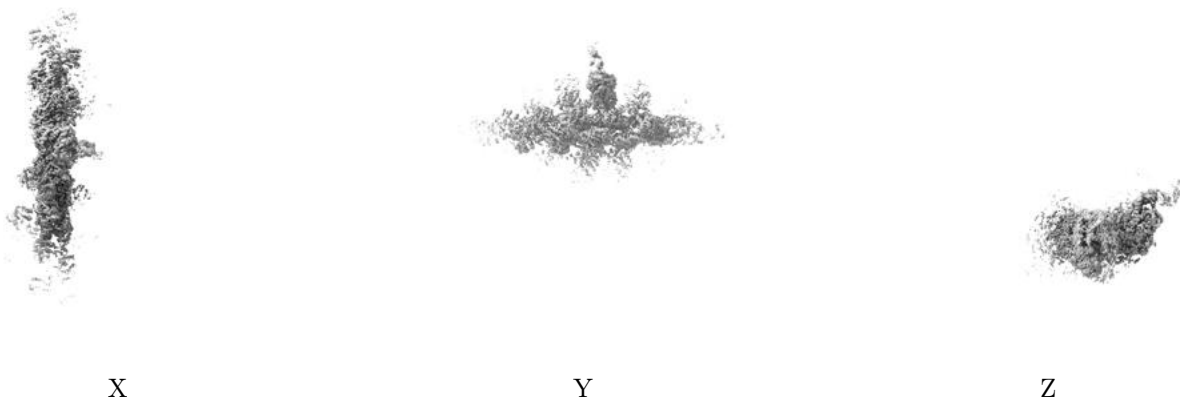
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

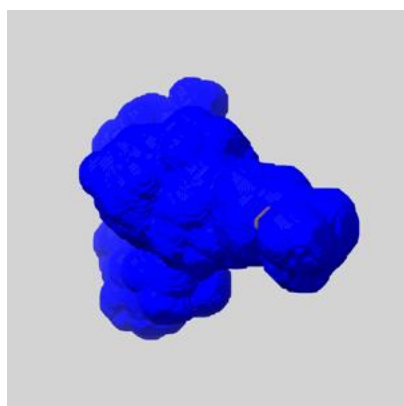
## 6.6 Mask visualisation [i](#)

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

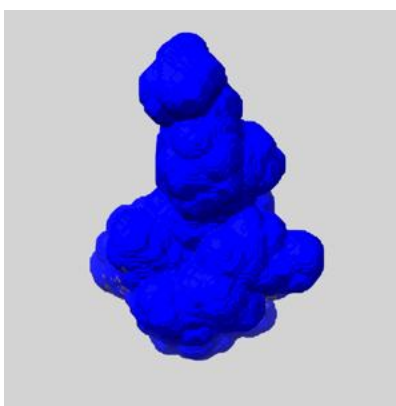
A mask typically either:

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

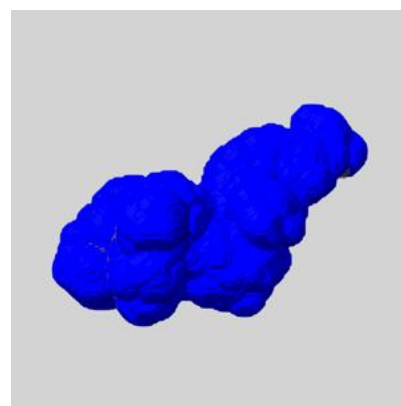
### 6.6.1 emd\_45565\_msk\_1.map [i](#)



X



Y

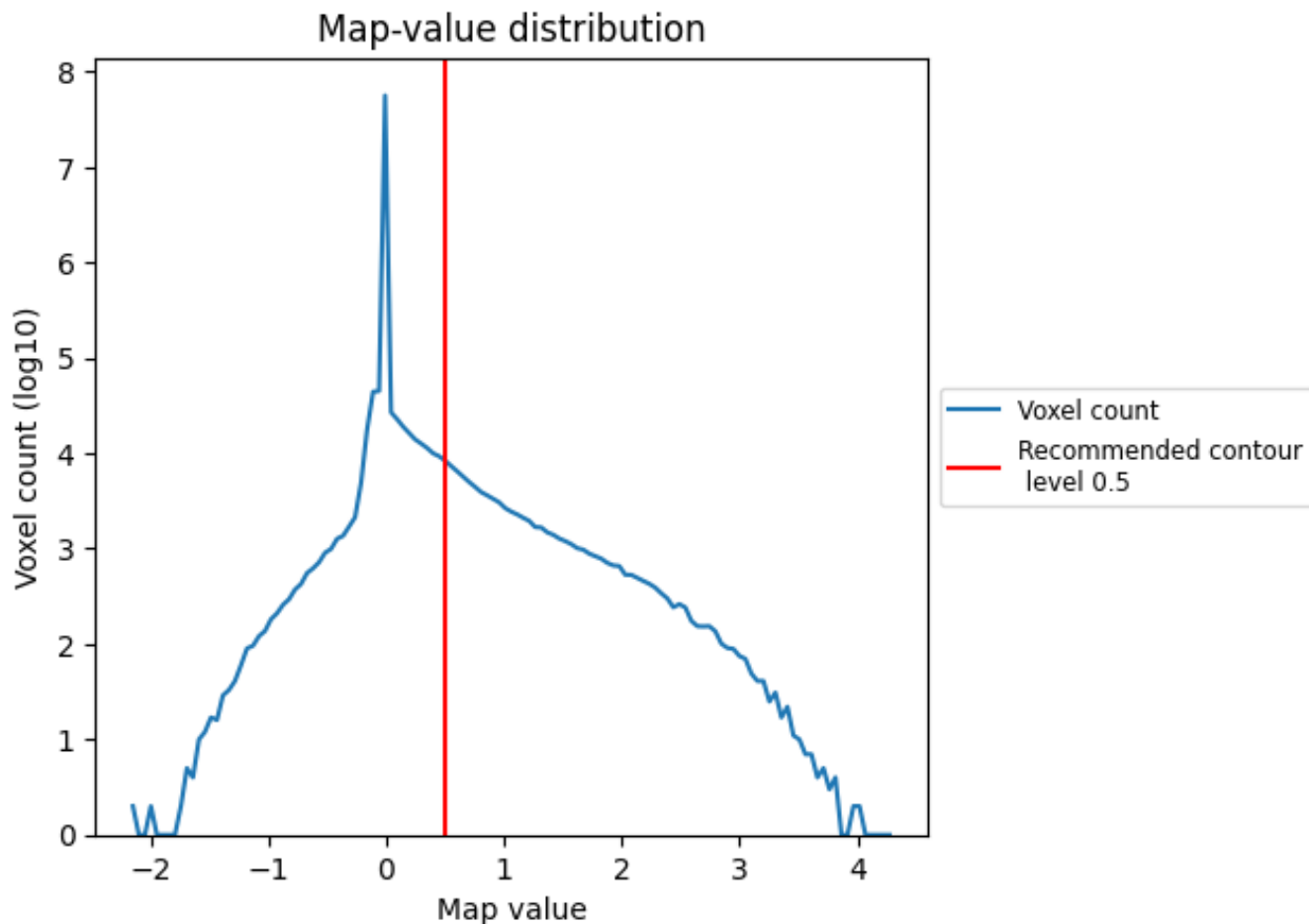


Z

## 7 Map analysis [i](#)

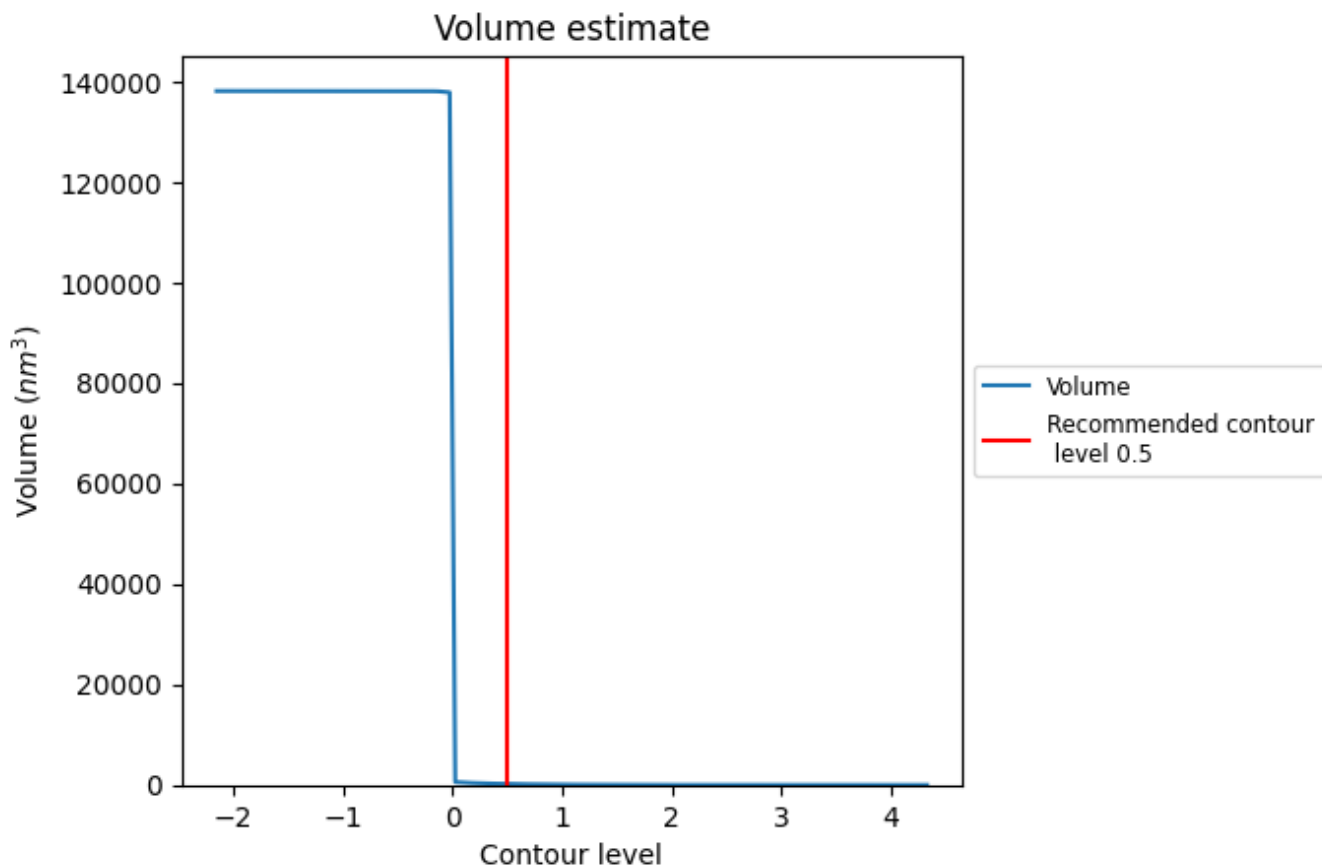
This section contains the results of statistical analysis of the map.

### 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.

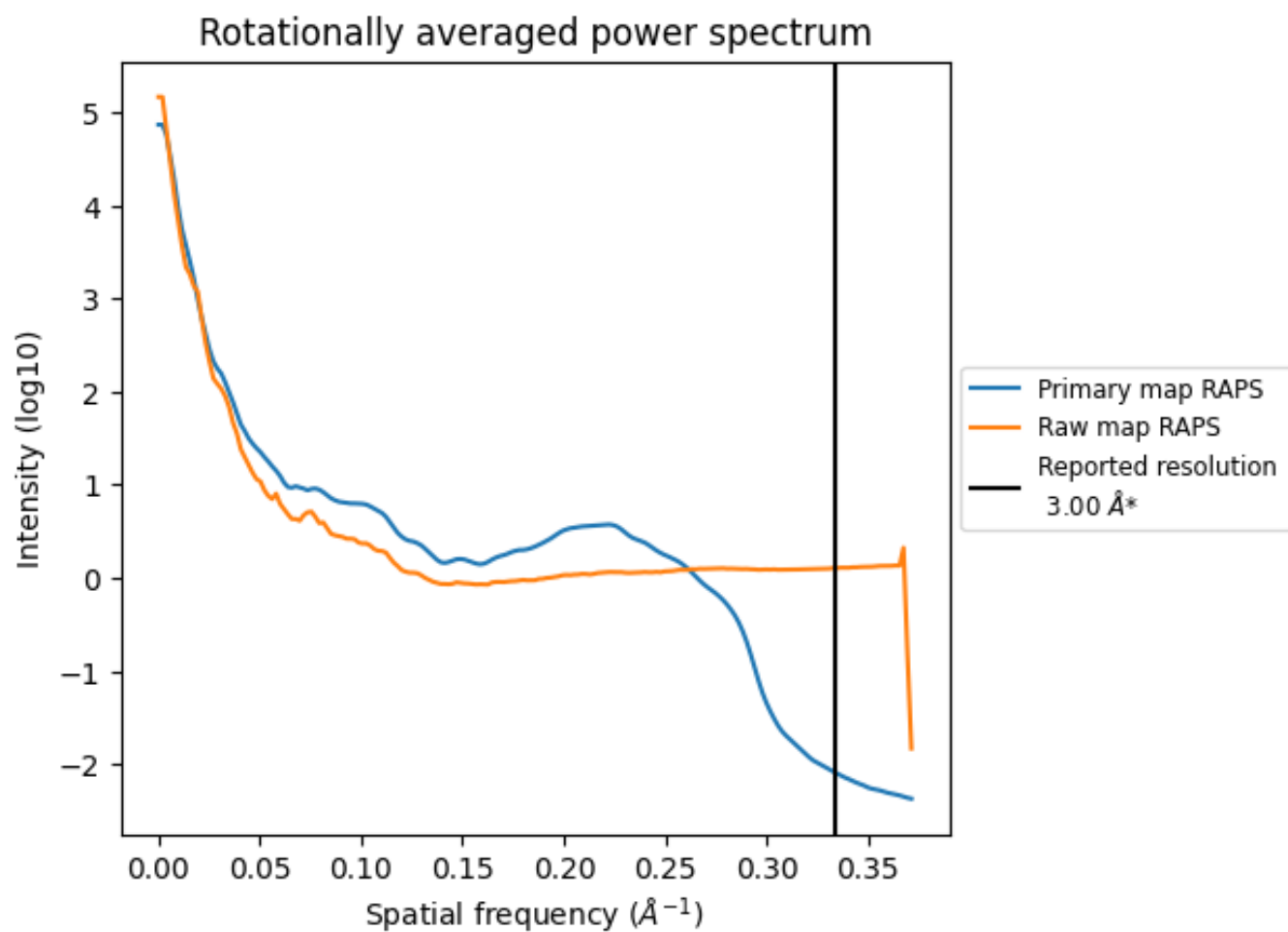
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 207 nm<sup>3</sup>; this corresponds to an approximate mass of 187 kDa.

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

### 7.3 Rotationally averaged power spectrum i

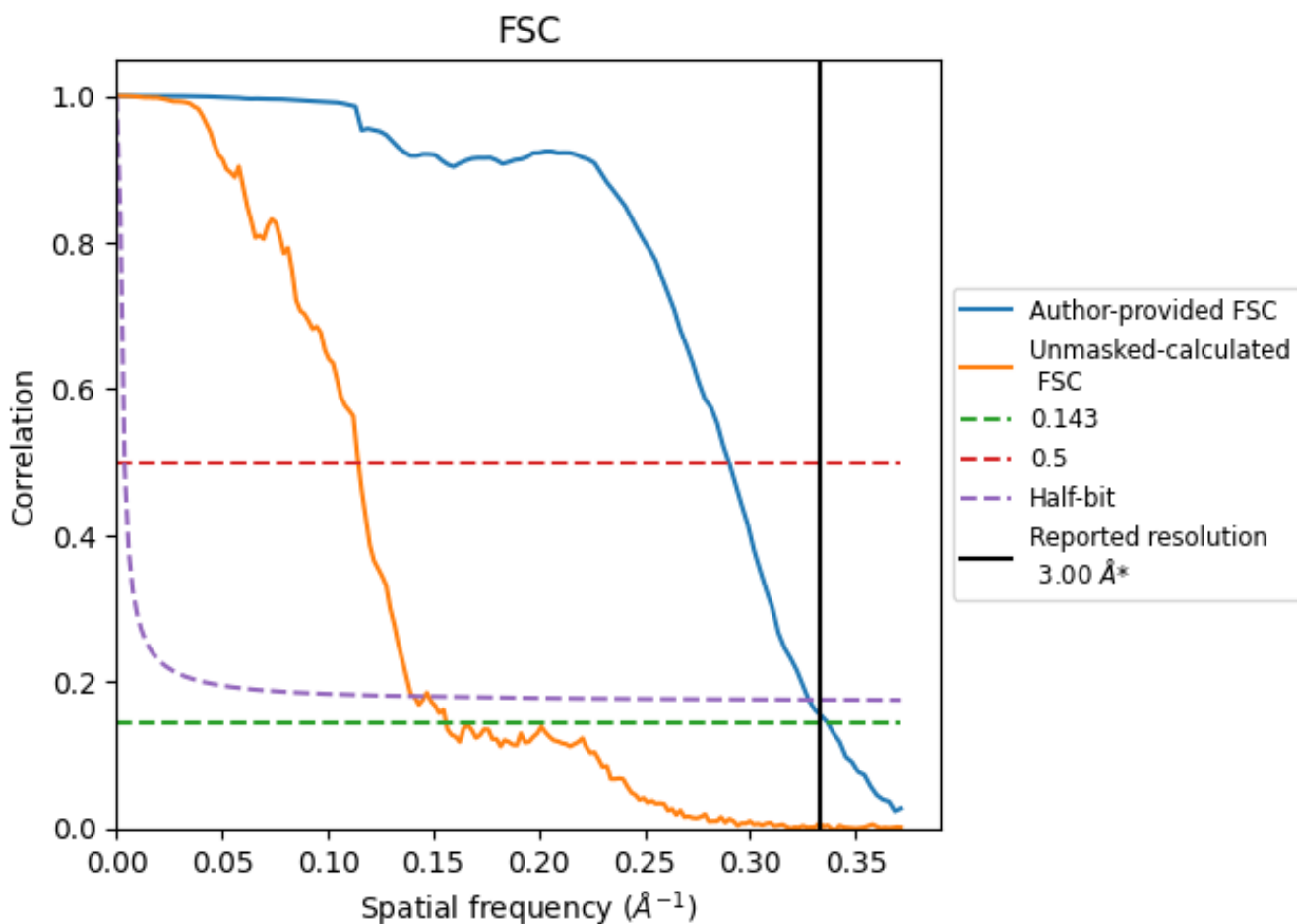


\*Reported resolution corresponds to spatial frequency of  $0.333 \text{ \AA}^{-1}$

## 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 0.333 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

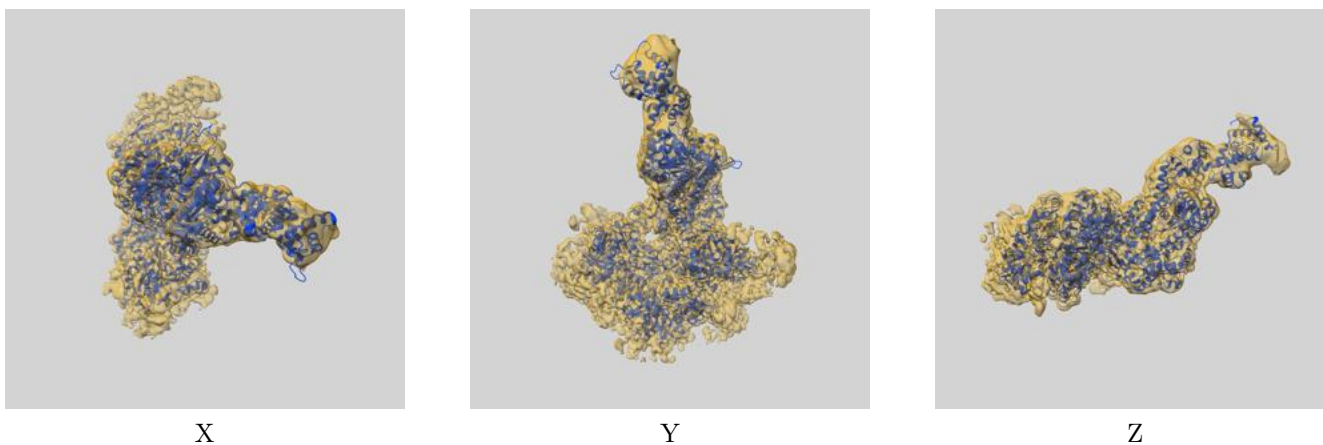
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.97	3.45	3.05
Unmasked-calculated*	6.41	8.73	7.10

\*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 6.41 differs from the reported value 3.0 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-45565 and PDB model 9CFW. Per-residue inclusion information can be found in section [3](#) on page [7](#).

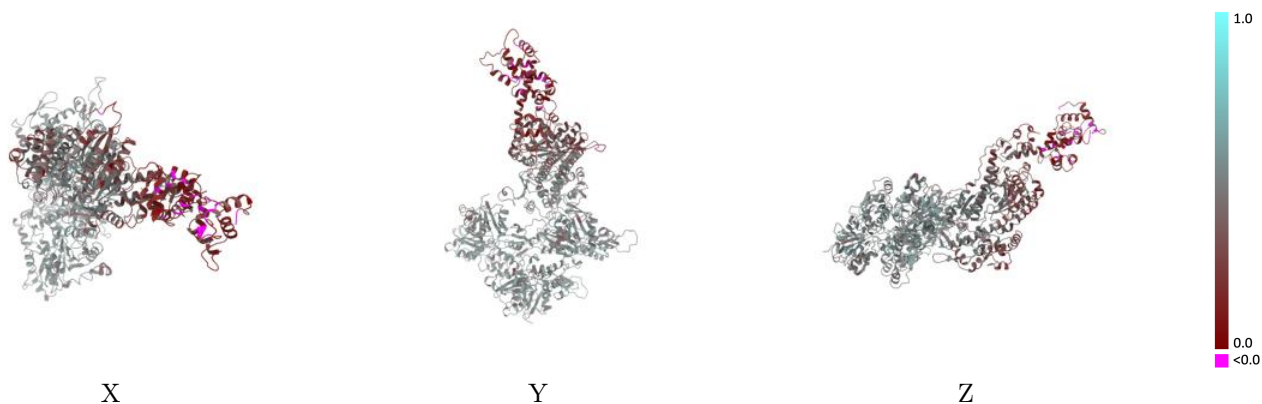
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.5 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](#)



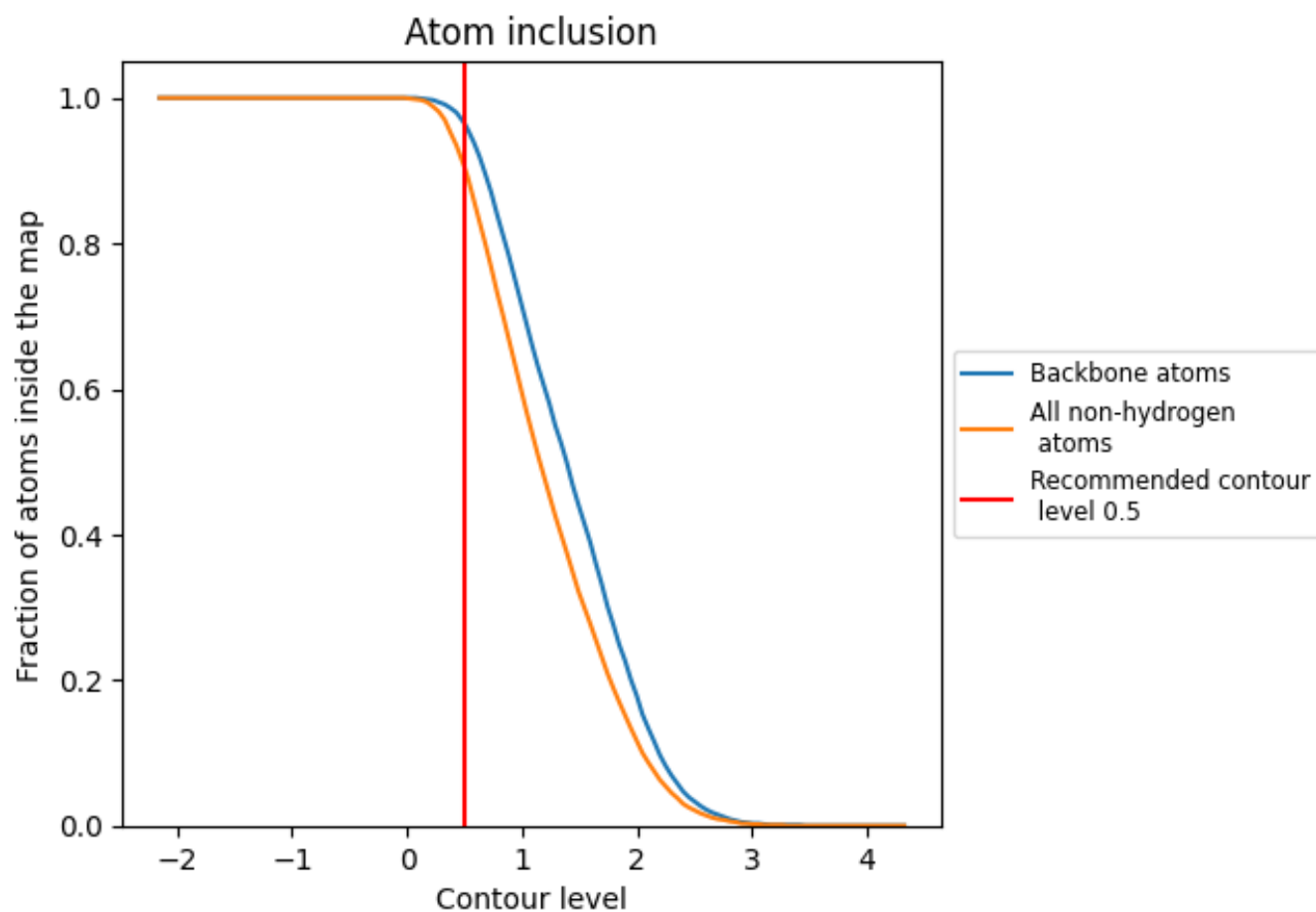
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).













## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

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

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9050	 0.4380
B	 0.9280	 0.5130
C	 0.9560	 0.5080
D	 0.9550	 0.5120
P	 0.8960	 0.3840
R	 0.6410	 0.1560

