



wwPDB EM Validation Summary Report ⓘ

Dec 20, 2022 – 02:14 PM EST

PDB ID : 8DD0
EMDB ID : EMD-27331
Title : The structure of the native cardiac thin filament junction region
Authors : Galkin, V.E.; Risi, C.M.
Deposited on : 2022-06-17
Resolution : 3.50 Å(reported)
Based on initial model : 7KO4

This is a wwPDB EM Validation Summary 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

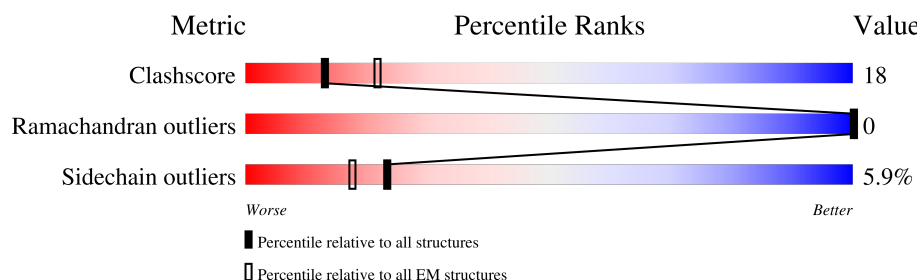
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	377	79% 17% ..
1	B	377	80% 16% ..
1	C	377	79% 17% ..
1	D	377	79% 17% ..
1	E	377	80% 16% ..
1	F	377	81% 15% ..
2	G	284	12% 7% . 81%
2	H	284	11% 7% . 81%

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Mol	Chain	Length	Quality of chain
2	I	284	<div><div><div></div><div></div><div></div></div><div>14%10%.</div><div>75%</div></div>
2	J	284	<div><div><div></div><div></div><div></div></div><div>16%8%</div><div>75%</div></div>
2	L	284	<div><div><div></div><div></div><div></div></div><div>11%8%.</div><div>81%</div></div>
2	M	284	<div><div><div></div><div></div><div></div></div><div>10%9%.</div><div>81%</div></div>
2	N	284	<div><div><div></div><div></div><div></div></div><div>17%7%.</div><div>75%</div></div>
2	O	284	<div><div><div></div><div></div><div></div></div><div>17%7%.</div><div>75%</div></div>
3	K	295	<div><div><div></div><div></div><div></div></div><div>13%11%.</div><div>75%</div></div>
3	P	295	<div><div><div></div><div></div><div></div></div><div>.11%11%.</div><div>75%</div></div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 22892 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 cardiac muscle 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		
1	B	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		
1	C	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		
1	D	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		
1	E	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		
1	F	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		

- Molecule 2 is a protein called Tropomyosin alpha-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	55	Total	C	N	O	S	0	0
			447	277	72	97	1		
2	H	55	Total	C	N	O	S	0	0
			447	277	72	97	1		
2	I	70	Total	C	N	O	S	0	0
			562	343	98	118	3		
2	J	70	Total	C	N	O	S	0	0
			562	343	98	118	3		
2	L	55	Total	C	N	O	S	0	0
			447	277	72	97	1		
2	M	55	Total	C	N	O	S	0	0
			447	277	72	97	1		
2	N	70	Total	C	N	O	S	0	0
			562	343	98	118	3		
2	O	70	Total	C	N	O	S	0	0
			562	343	98	118	3		

- Molecule 3 is a protein called Troponin T2, cardiac type.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	75	Total	C	N	O	S	0	0
			650	394	132	123	1		
3	P	75	Total	C	N	O	S	0	0
			650	394	132	123	1		

- 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	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
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	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	F	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	A	1	Total	Mg	0
			1	1	

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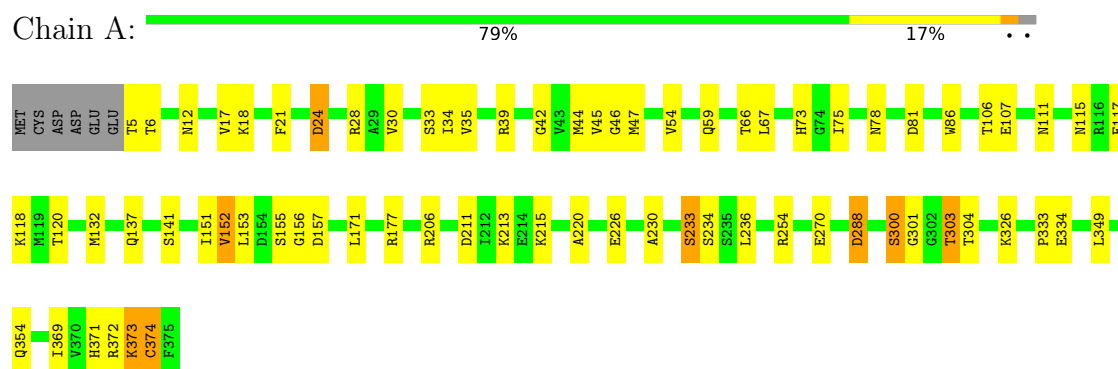
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Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total 1	Mg 1	0
5	C	1	Total 1	Mg 1	0
5	D	1	Total 1	Mg 1	0
5	E	1	Total 1	Mg 1	0
5	F	1	Total 1	Mg 1	0

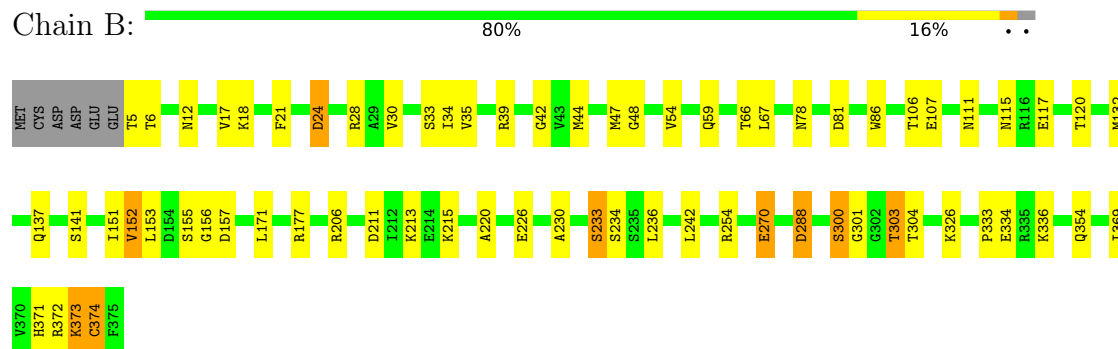
3 Residue-property plots

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.

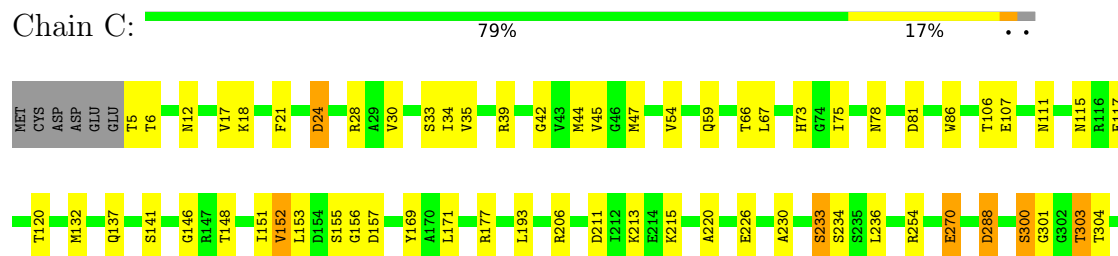
- Molecule 1: Actin, alpha cardiac muscle 1



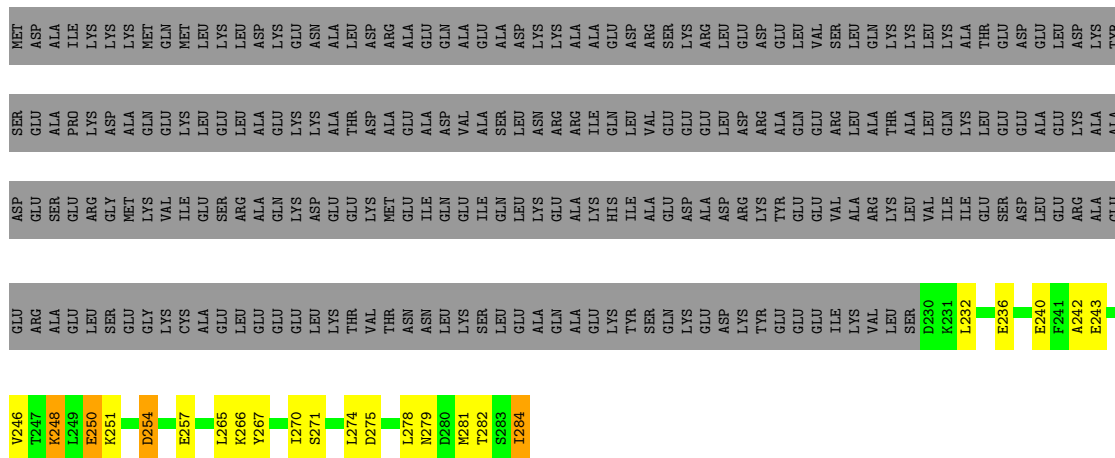
- Molecule 1: Actin, alpha cardiac muscle 1



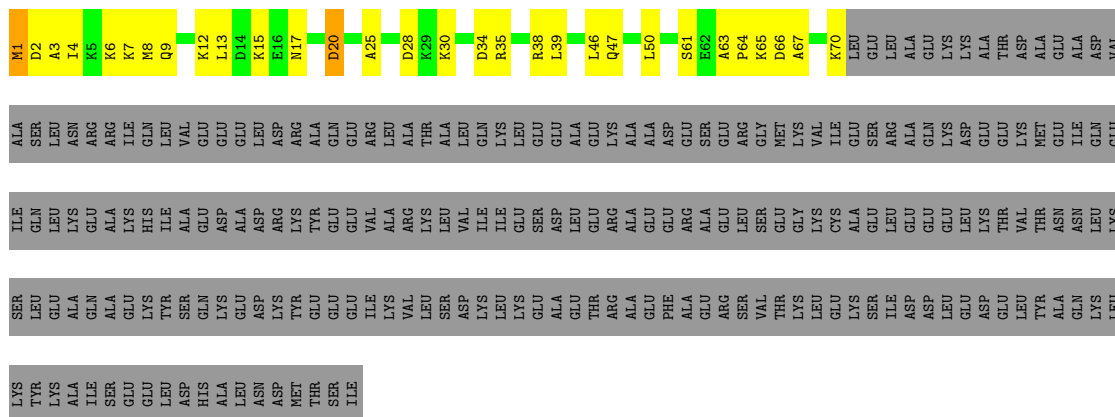
- Molecule 1: Actin, alpha cardiac muscle 1



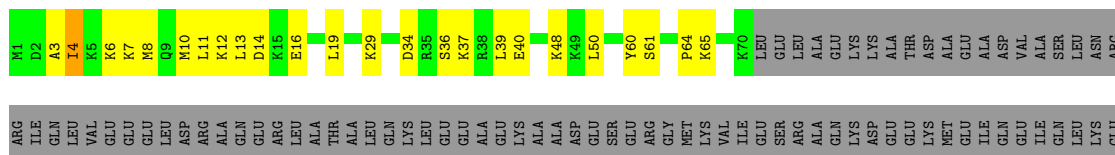
- Molecule 2: Tropomyosin alpha-1 chain



- Molecule 2: Tropomyosin alpha-1 chain



- Molecule 2: Tropomyosin alpha-1 chain



[illegible]

- Molecule 2: Tropomyosin alpha-1 chain

Chain L:  11% 8% 81%

[illegible]

L249		S252		L256		Y261		K264		L265		K266		I270		E273		L274		D275		H276		A277		L278		N279		D280		T281		S282		I284
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- Molecule 2: Tropomyosin alpha-1 chain

Chain M: 10% 9% . 81%

[illegible]

S245	V246	T247	K248	L249	E250	K251	D254	E257	Y261	A262	Q263	K264	L265	K266	Y267	A269	I270	L274	D275	H276	A277	L278	M281	T282	S283	I284
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

- Molecule 2: Tropomyosin alpha-1 chain

Chain N:  17% 7% 75%

M1
D2
A3
I4
K7
M8
Q9
L13
P14
K15
E16
N17
D20
A25
D28
L43
L46
Q47
L50
K51
S61
E62
A63
P64
K65
D66
K70
LEU
GLU
LEU
ALA
ALA
GLY
LYS
THR
ASP
ALA
GLU
ALA
ASP
VAL
ALA
SER
LEU
ASN
ARG
ARG
ILE
CYS

[illegible]

- Molecule 2: Tropomyosin alpha-1 chain



ALA	LEU	LVS	ASP	GLU	M1
ASN	ASP	GLU	ALA	GLU	D2
ASP	ASP	ASP	ASP	LEU	A3
MET	TYR	LVS	ARG	ASP	I4
THR	TYR	GLU	TYR	ALA	K5
SER	GLU	GLU	GLU	GLN	M8
ILE	GLU	GLU	GLU	GLN	Q9
	ILE	VAL	VAL	ARG	M10
	LVS	ALA	ALA	LEU	L11
	VAL	ARG	ARG	ALA	K12
	LEU	LVS	THR	THR	L13
	SER	LEU	LEU	ALA	D14
	ASP	VAL	VAL	LEU	
	ASP	LVS	ILE	GLN	K29
	LEU	LVS	ILE	LVS	K30
	LVS	LVS	GLU	LEU	
	GLU	GLU	SER	GLU	D34
	ALA	ALA	ASP	GLU	
	GLU	THR	LEU	ALA	K37
	THR	ARG	GLU	GLU	R38
	ARG	ARG	ARG	LVS	
	ALA	ALA	ALA	ALA	L46
	GLU	GLU	GLU	ALA	
	PHE	GLU	GLU	ASP	L50
	ALA	ALA	ARG	GLU	
	GLU	GLU	ALA	SER	Y60
	ARG	GLU	GLU	GLU	S61
	SER	SER	LEU	ARG	
	VAL	VAL	SER	GLY	P64
	THR	THR	GLU	MET	K65
	LVS	LVS	GLY	LVS	
	GLU	GLU	CYS	ILE	E69
	LEU	LVS	ALA	GLU	K70
	SER	SER	GLU	SER	LEU
	ILE	ILE	LEU	ARG	GLU
	ASP	ASP	GLU	ALA	ALA
	GLU	GLU	GLU	GLN	GLU
	LEU	LEU	GLU	LVS	LVS
	ASP	GLU	ASP	ASP	LVS
	GLU	THR	THR	GLU	ALA
	LEU	TYR	VAL	LVS	THR
	ALA	ALA	ASN	ILE	ALA
	LVS	LVS	LEU	GLN	ASP
	LEU	LVS	SER	ILE	VAL
	TYR	TYR	LEU	GLN	SER
	LVS	LVS	GLU	LEU	LEU
	ALA	ALA	ALA	LVS	ASN
	ILE	ILE	GLN	GLU	ARG
	SER	SER	ALA	ALA	ARG
	GLU	GLU	GLU	ILE	ARG
	GLU	GLU	LVS	HIS	GLN
	LEU	LEU	TYR	ILE	LEU
	SER	SER	SER	GLU	VAL
	ASN	ASN	GLN	CTR	CTR

- Molecule 3: Troponin T2, cardiac type

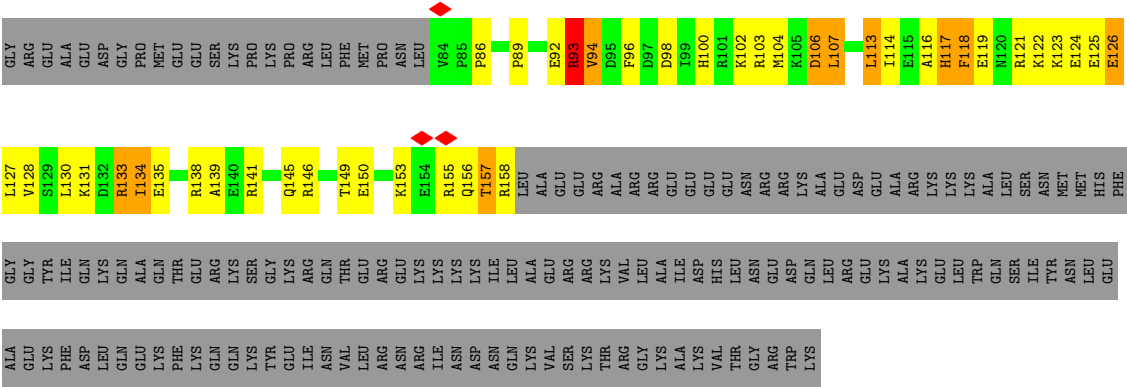


Lys	Gln	K136	Gly	Met
Phe	Thr	R137	Arg	Ser
Lys	Glu	R138	Ala	Asp
Gln	Arg		Glu	Glu
Lys	Ser	R141	Asp	Glu
Lys	Gly	A142	Gly	Thr
Glu	Lys	E143	Pro	Val
Ile	Arg	Q144	Met	Asp
Asn	Gln	R146	Glu	Glu
Val	Thr	I147	Glu	Tyr
Leu	Glu	R148	Ser	Gly
Arg	Arg		Lys	Glu
Asn	Glu	R151	Pro	Glu
Arg	Lys	E152	Lys	Gln
Ile	Lys		Pro	Glu
Asn	Lys	R155	Arg	Glu
Asp	Lys		Leu	Gly
Asn	Ile	R158	Phe	Ala
Gln	Leu	Leu	Met	Ala
Lys	Ala	Ala	Pro	Glu
Lys	Ala	Glu	Asn	Glu
Val	Glu	Glu	Asn	Glu
Ser	Arg	Arg	Leu	Glu
Lys	Arg	Glu	V84	Glu
Thr	Lys	Ala	P85	Ala
Arg	Val	Arg	P86	Trp
Gly	Leu	Arg	K87	Arg
Lys	Ala	Glu	I88	Gln
Ala	Ile	Glu		Asp
Lys	Asp	Glu	G91	Gly
Val	His	Glu	E92	Asp
Thr	Leu	Asn	R93	Glu
Gly	Asn	Arg	V94	Gln
Arg	Glu	Arg		Glu
Trp	Asp	Lys	I99	Glu
Lys	Gln	Ala	H100	Ala
	Leu	Glu	R101	Val
	Arg	Asp	K102	Glu
	Glu	Glu	R103	Glu
	Lys	Ala	M104	Glu
	Ala	Arg	K105	Ala
	Lys	Lys	D106	Gly
	Glu	Lys		Gly
	Leu	Lys	L110	Glu
	Trp	Ala	L113	Ala
	Gln	Leu	I114	Glu
	Ser	Ser		Ala
	Ile	Asn	H117	Glu
	Tyr	Met	F118	Glu
	Asn	Met		Ala
	Leu	His		Asn
	Glu	Phe	R121	Ala
	Ala	Gly	K122	Glu
	Glu	Gly	K123	Glu
	Lys	Ile		Ala
	Phe	Tyr	K131	Gly
	Asp	Asp	D132	Gln
	Leu	Lys	R133	Glu
	Gln	Gln	I134	Glu
	Glu	Ala	F135	Asp

- Molecule 3: Troponin T2, cardiac type



MET	SER	ASP	VAL	GLU	THR	VAL	ASP	GLU	TYR	GLU	GLU	GLN	GLU	GLY	ALA	ALA	ARG	ASN	ASP	GLY	ASP	GLU	GLN	GLU	GLU	ALA	VAL	GLU	GLU	ALA	ALA	GLY	GLY	ALA	ASN	GLU	GLU	GLU	GLY	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	236359	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	34	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	10.091	Depositor
Minimum map value	-2.821	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	97.631996, 108.479996, 225.096	wwPDB
Map dimensions	72, 80, 166	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.356, 1.356, 1.356	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.43	0/2961	0.48	0/4011
1	B	0.43	0/2961	0.48	0/4011
1	C	0.43	0/2961	0.48	0/4011
1	D	0.43	0/2961	0.48	0/4011
1	E	0.43	0/2961	0.48	0/4011
1	F	0.43	0/2961	0.48	0/4011
2	G	0.38	0/450	0.65	0/600
2	H	0.40	0/450	0.71	0/600
2	I	0.34	0/563	0.59	0/744
2	J	0.34	0/563	0.61	0/744
2	L	0.39	0/450	0.68	0/600
2	M	0.40	0/450	0.71	0/600
2	N	0.36	0/563	0.65	0/744
2	O	0.35	0/563	0.63	0/744
3	K	0.37	0/656	0.86	1/871 (0.1%)
3	P	0.38	0/656	0.88	1/871 (0.1%)
All	All	0.42	0/23130	0.54	2/31184 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	93	ARG	C-N-CA	6.50	137.96	121.70
3	K	93	ARG	C-N-CA	5.99	136.68	121.70

There are no chirality outliers.

There are no planarity outliers.

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	2898	0	2871	67	0
1	B	2898	0	2871	64	0
1	C	2898	0	2871	95	0
1	D	2898	0	2871	91	0
1	E	2898	0	2871	65	0
1	F	2898	0	2871	60	0
2	G	447	0	441	52	0
2	H	447	0	441	44	0
2	I	562	0	580	67	0
2	J	562	0	580	70	0
2	L	447	0	441	67	0
2	M	447	0	441	73	0
2	N	562	0	580	38	0
2	O	562	0	580	66	0
3	K	650	0	661	117	0
3	P	650	0	661	128	0
4	A	27	0	12	2	0
4	B	27	0	12	2	0
4	C	27	0	12	2	0
4	D	27	0	12	2	0
4	E	27	0	12	3	0
4	F	27	0	12	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
All	All	22892	0	22704	839	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 18.

The worst 5 of 839 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:G:284:ILE:CG2	2:J:12:LYS:CE	1.76	1.57
2:G:281:MET:SD	2:I:7:LYS:HE3	1.44	1.56
2:L:281:MET:SD	2:N:7:LYS:HE3	1.44	1.56
2:G:284:ILE:HG21	2:J:12:LYS:CE	1.35	1.45
2:G:284:ILE:CG2	2:J:12:LYS:HE3	0.98	1.43

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	369/377 (98%)	351 (95%)	18 (5%)	0	100	100
1	B	369/377 (98%)	350 (95%)	19 (5%)	0	100	100
1	C	369/377 (98%)	350 (95%)	19 (5%)	0	100	100
1	D	369/377 (98%)	351 (95%)	18 (5%)	0	100	100
1	E	369/377 (98%)	351 (95%)	18 (5%)	0	100	100
1	F	369/377 (98%)	350 (95%)	19 (5%)	0	100	100
2	G	53/284 (19%)	50 (94%)	3 (6%)	0	100	100
2	H	53/284 (19%)	51 (96%)	2 (4%)	0	100	100
2	I	68/284 (24%)	68 (100%)	0	0	100	100
2	J	68/284 (24%)	68 (100%)	0	0	100	100
2	L	53/284 (19%)	50 (94%)	3 (6%)	0	100	100
2	M	53/284 (19%)	51 (96%)	2 (4%)	0	100	100
2	N	68/284 (24%)	68 (100%)	0	0	100	100
2	O	68/284 (24%)	68 (100%)	0	0	100	100
3	K	73/295 (25%)	69 (94%)	4 (6%)	0	100	100
3	P	73/295 (25%)	70 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2844/5124 (56%)	2716 (96%)	128 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	314/320 (98%)	298 (95%)	16 (5%)	24	57
1	B	314/320 (98%)	298 (95%)	16 (5%)	24	57
1	C	314/320 (98%)	298 (95%)	16 (5%)	24	57
1	D	314/320 (98%)	298 (95%)	16 (5%)	24	57
1	E	314/320 (98%)	298 (95%)	16 (5%)	24	57
1	F	314/320 (98%)	297 (95%)	17 (5%)	22	55
2	G	49/245 (20%)	46 (94%)	3 (6%)	18	51
2	H	49/245 (20%)	42 (86%)	7 (14%)	3	19
2	I	60/245 (24%)	55 (92%)	5 (8%)	11	40
2	J	60/245 (24%)	58 (97%)	2 (3%)	38	68
2	L	49/245 (20%)	46 (94%)	3 (6%)	18	51
2	M	49/245 (20%)	44 (90%)	5 (10%)	7	32
2	N	60/245 (24%)	55 (92%)	5 (8%)	11	40
2	O	60/245 (24%)	58 (97%)	2 (3%)	38	68
3	K	71/257 (28%)	67 (94%)	4 (6%)	21	54
3	P	71/257 (28%)	59 (83%)	12 (17%)	2	12
All	All	2462/4394 (56%)	2317 (94%)	145 (6%)	23	53

5 of 145 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	K	106	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	P	145	GLN
2	L	273	GLU
2	N	46	LEU
1	D	24	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	N	47	GLN
3	P	117	HIS
3	K	100	HIS
3	K	117	HIS
3	K	144	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 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
4	ADP	F	401	5	24,29,29	0.96	1 (4%)	29,45,45	1.46	4 (13%)
4	ADP	A	401	5	24,29,29	0.97	1 (4%)	29,45,45	1.46	4 (13%)
4	ADP	B	401	5	24,29,29	0.97	1 (4%)	29,45,45	1.47	4 (13%)
4	ADP	C	401	5	24,29,29	0.96	1 (4%)	29,45,45	1.46	4 (13%)
4	ADP	D	401	5	24,29,29	0.97	1 (4%)	29,45,45	1.46	4 (13%)
4	ADP	E	401	5	24,29,29	0.96	1 (4%)	29,45,45	1.46	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	F	401	5	-	3/12/32/32	0/3/3/3
4	ADP	A	401	5	-	3/12/32/32	0/3/3/3
4	ADP	B	401	5	-	3/12/32/32	0/3/3/3
4	ADP	C	401	5	-	3/12/32/32	0/3/3/3
4	ADP	D	401	5	-	3/12/32/32	0/3/3/3
4	ADP	E	401	5	-	3/12/32/32	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	401	ADP	C5-C4	2.18	1.46	1.40
4	D	401	ADP	C5-C4	2.18	1.46	1.40
4	E	401	ADP	C5-C4	2.17	1.46	1.40
4	C	401	ADP	C5-C4	2.17	1.46	1.40
4	B	401	ADP	C5-C4	2.16	1.46	1.40

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	401	ADP	PA-O3A-PB	-3.58	120.54	132.83
4	A	401	ADP	PA-O3A-PB	-3.58	120.56	132.83
4	C	401	ADP	PA-O3A-PB	-3.57	120.56	132.83
4	F	401	ADP	PA-O3A-PB	-3.57	120.59	132.83
4	B	401	ADP	PA-O3A-PB	-3.56	120.60	132.83

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

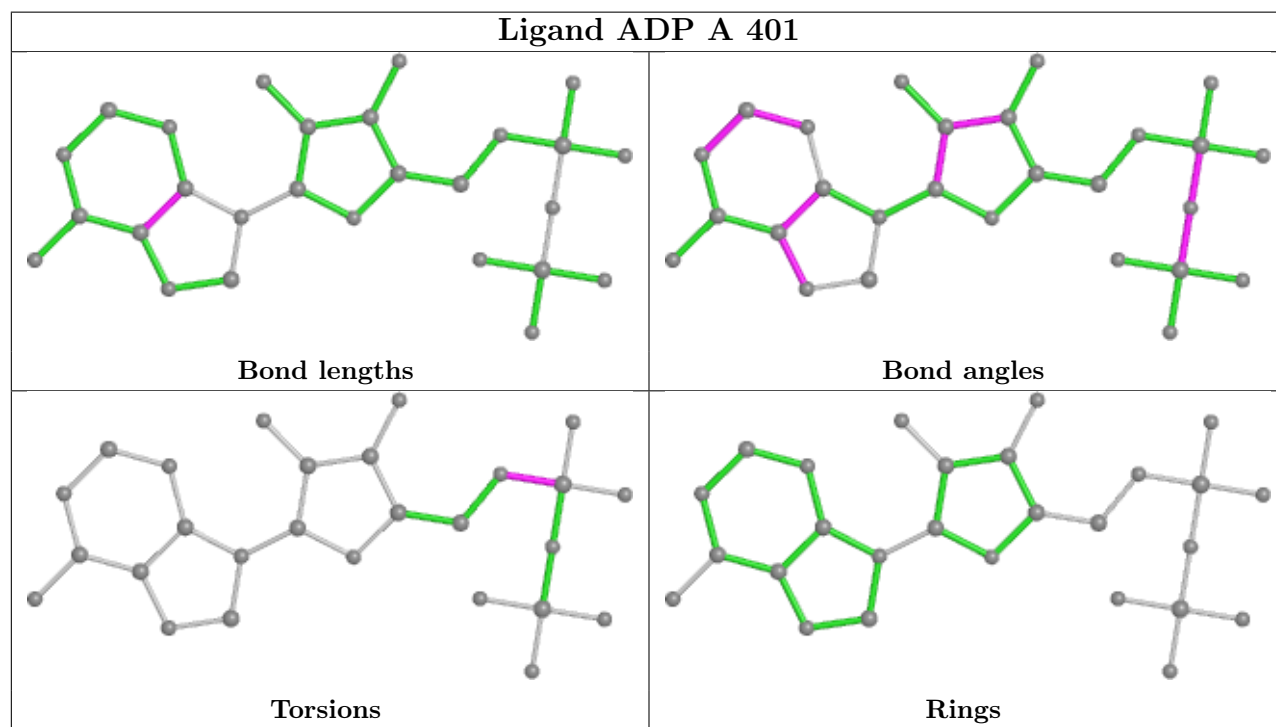
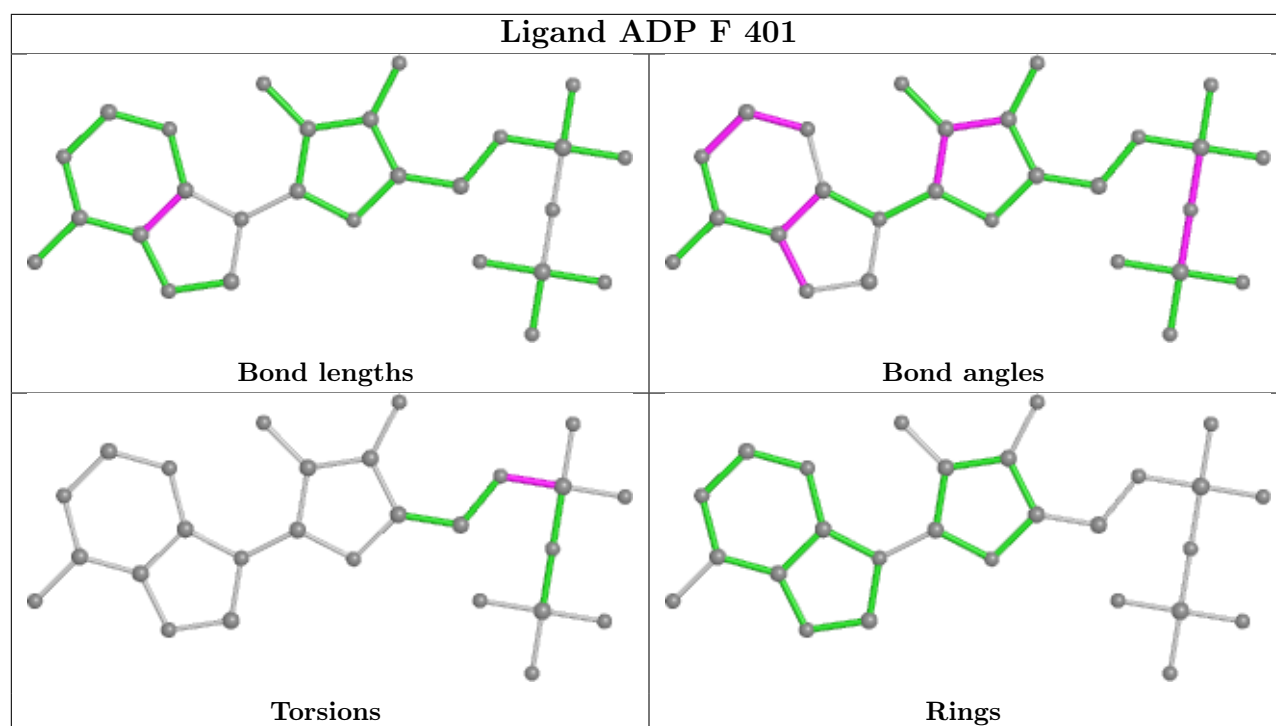
Mol	Chain	Res	Type	Atoms
4	A	401	ADP	C5'-O5'-PA-O1A
4	A	401	ADP	C5'-O5'-PA-O2A
4	B	401	ADP	C5'-O5'-PA-O1A
4	B	401	ADP	C5'-O5'-PA-O2A
4	C	401	ADP	C5'-O5'-PA-O1A

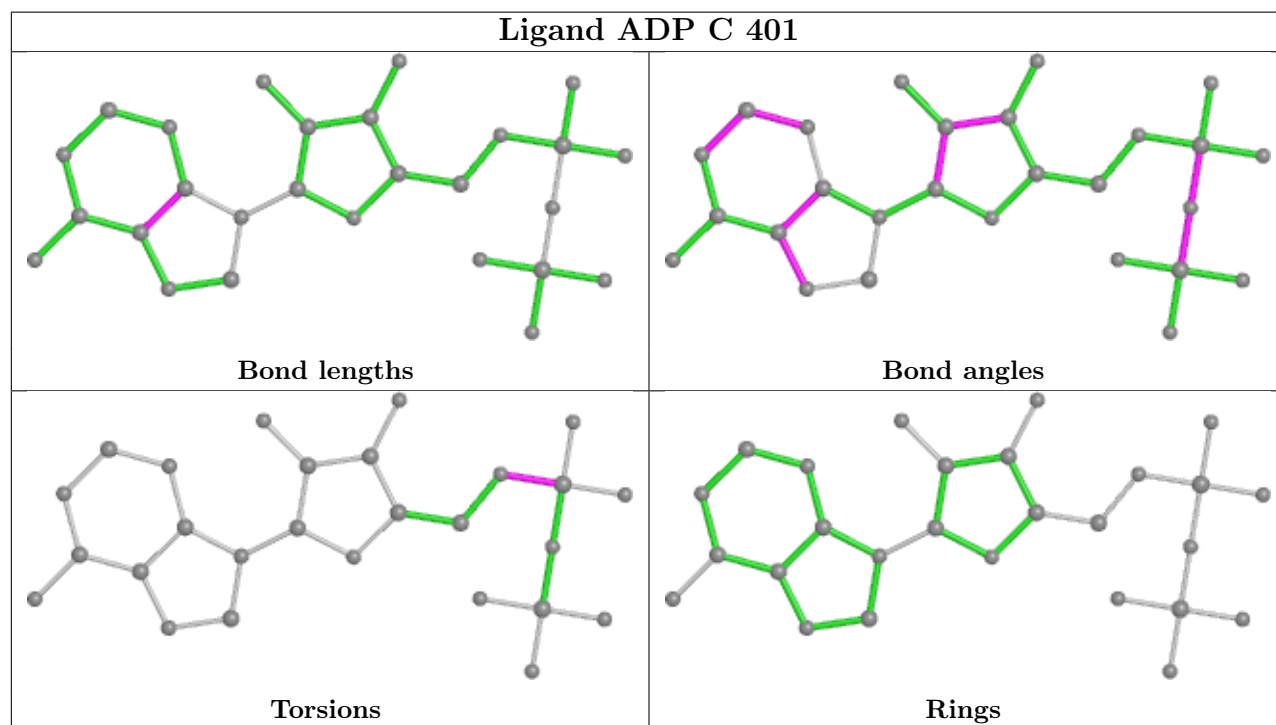
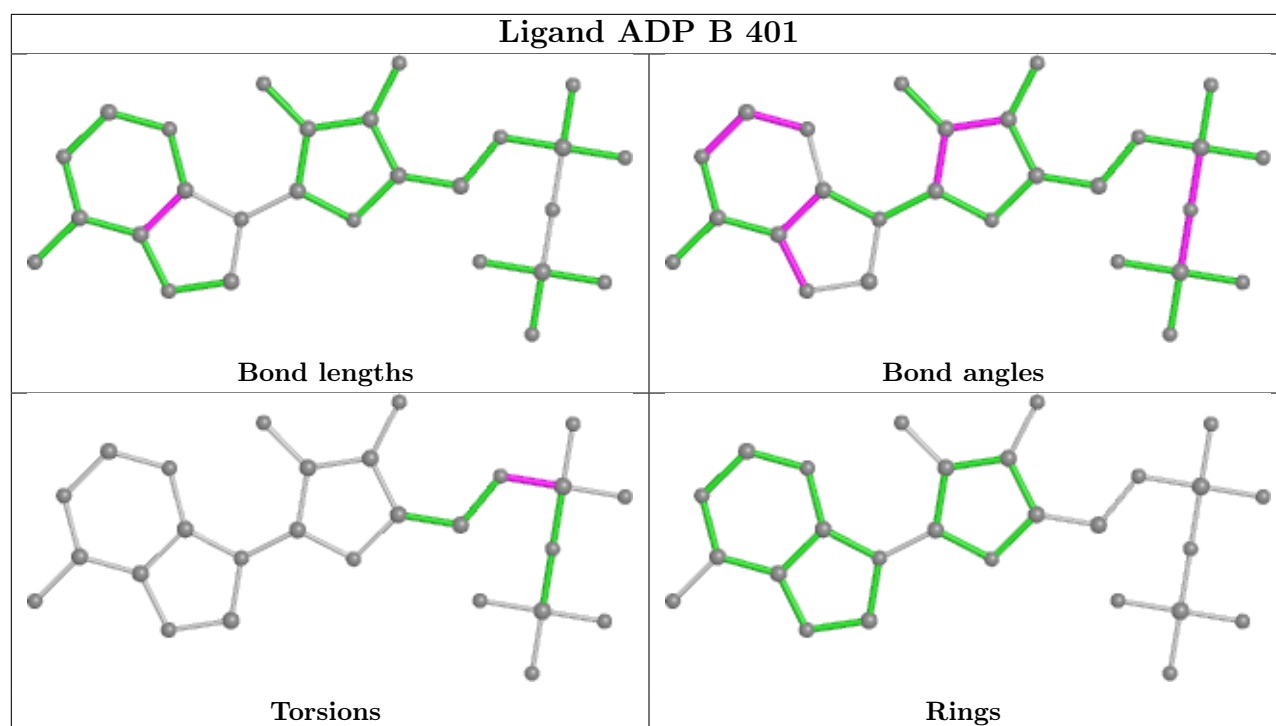
There are no ring outliers.

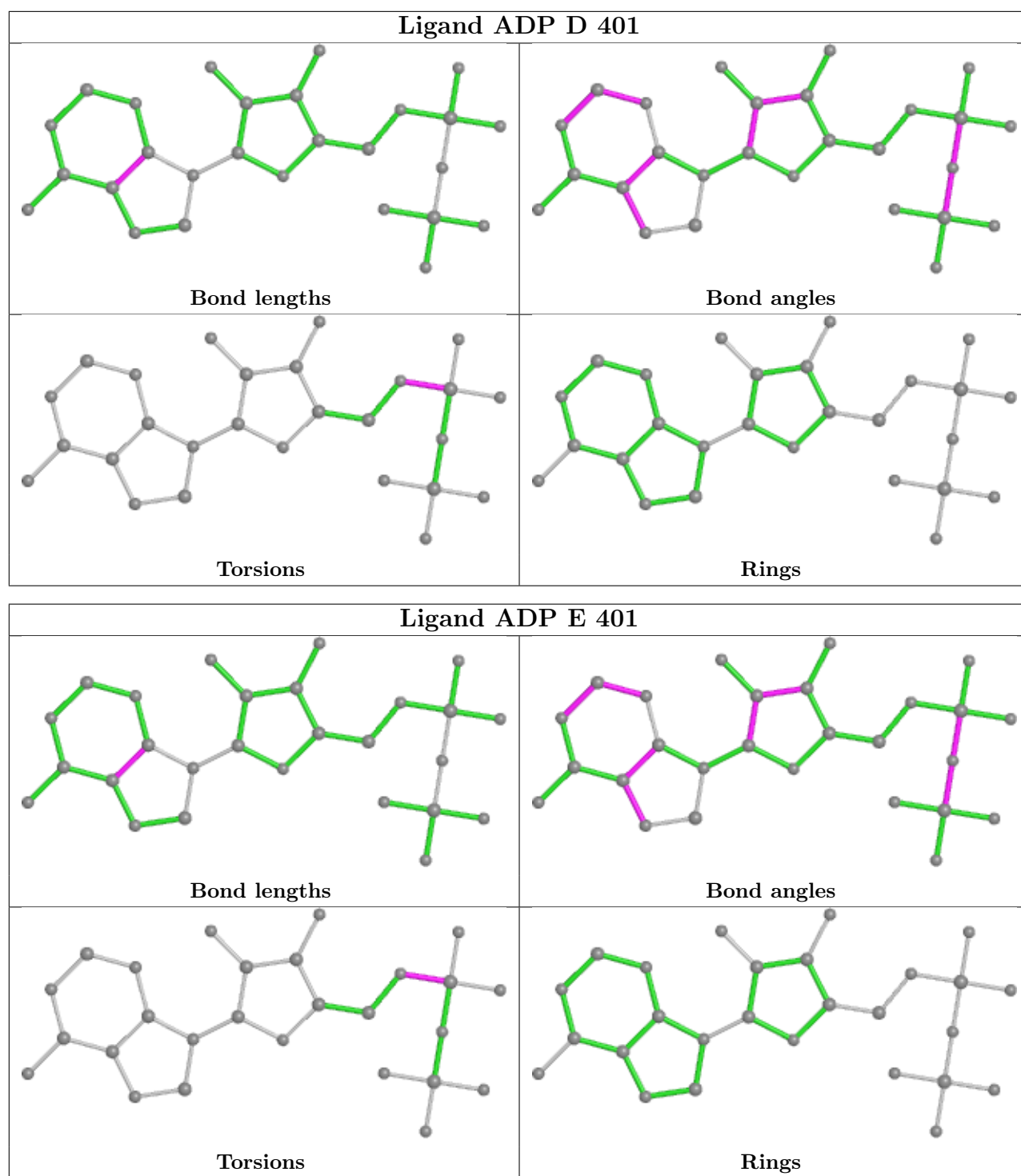
6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	401	ADP	2	0
4	A	401	ADP	2	0
4	B	401	ADP	2	0
4	C	401	ADP	2	0
4	D	401	ADP	2	0
4	E	401	ADP	3	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

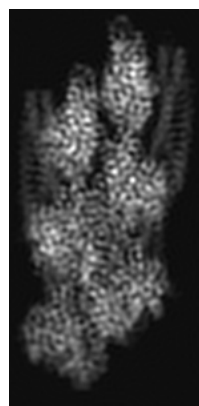
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27331. These allow visual inspection of the internal detail of the map and identification of artifacts.

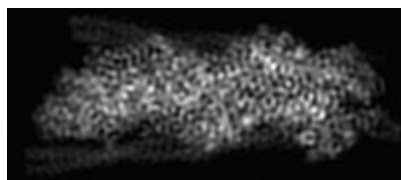
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

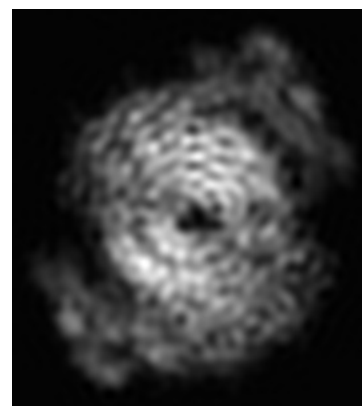
6.1.1 Primary map



X

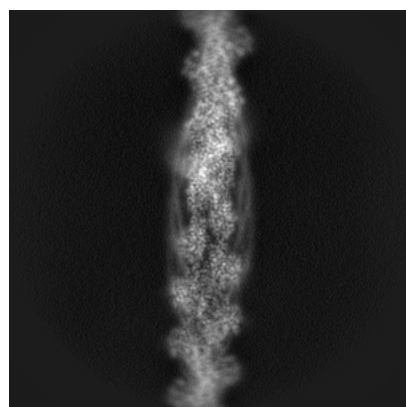


Y

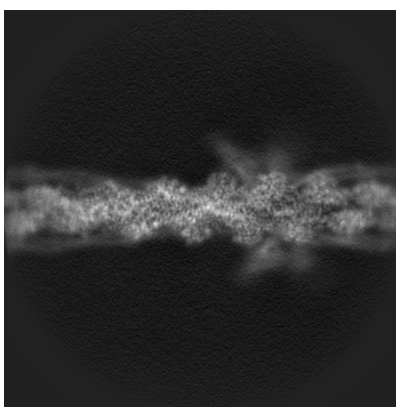


Z

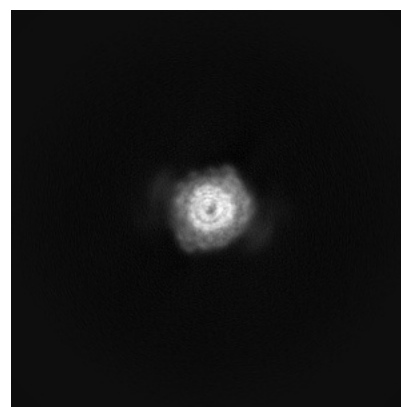
6.1.2 Raw map



X



Y

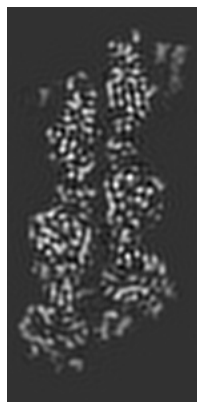


Z

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

6.2 Central slices [i](#)

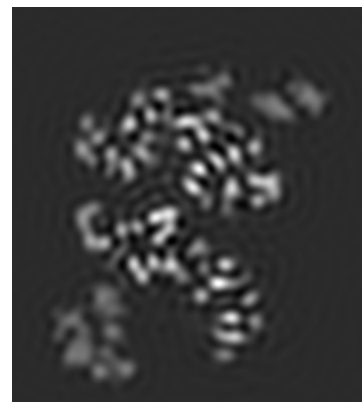
6.2.1 Primary map



X Index: 36

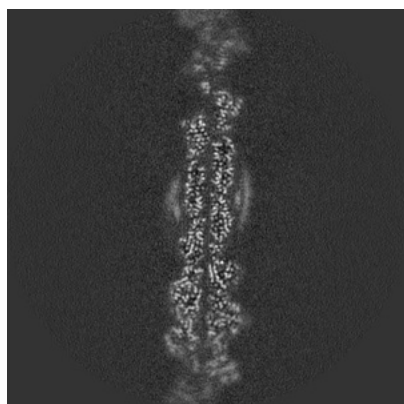


Y Index: 40

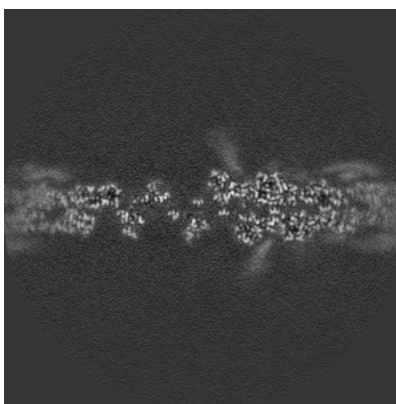


Z Index: 83

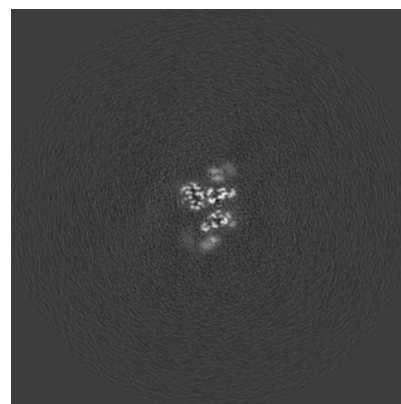
6.2.2 Raw map



X Index: 162



Y Index: 162

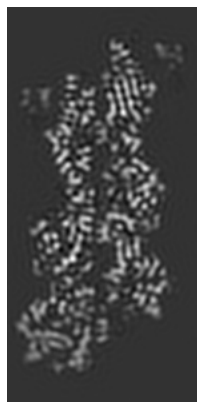


Z Index: 162

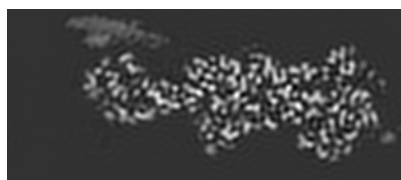
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

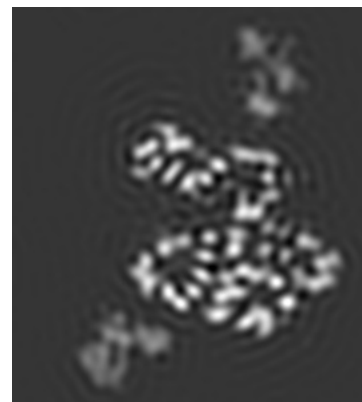
6.3.1 Primary map



X Index: 34

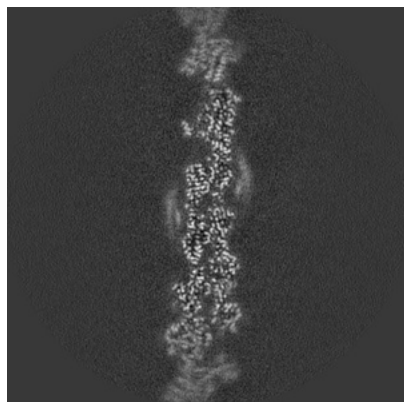


Y Index: 50

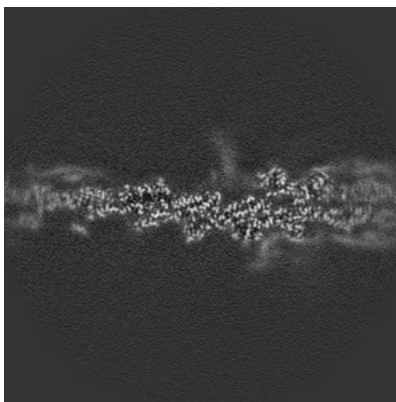


Z Index: 107

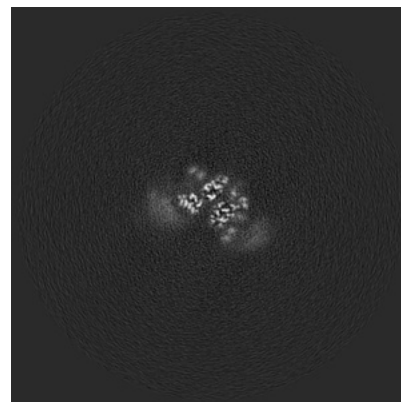
6.3.2 Raw map



X Index: 158



Y Index: 169

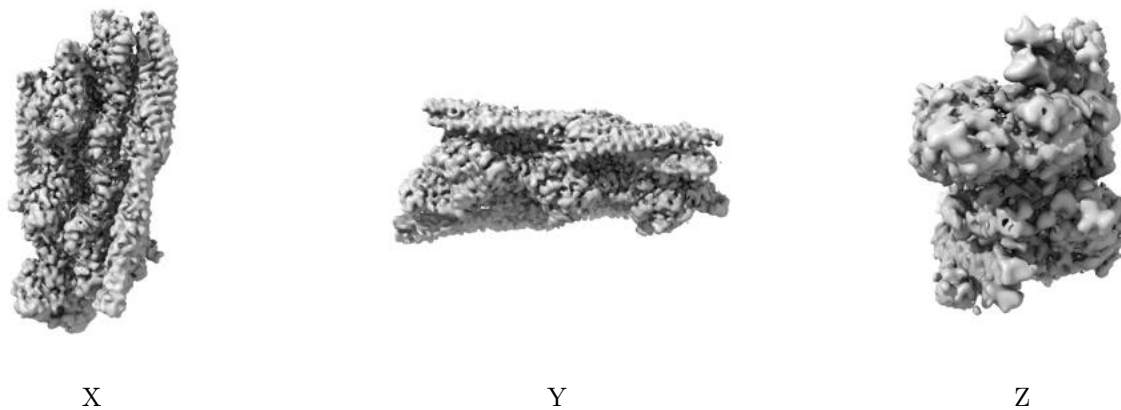


Z Index: 206

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

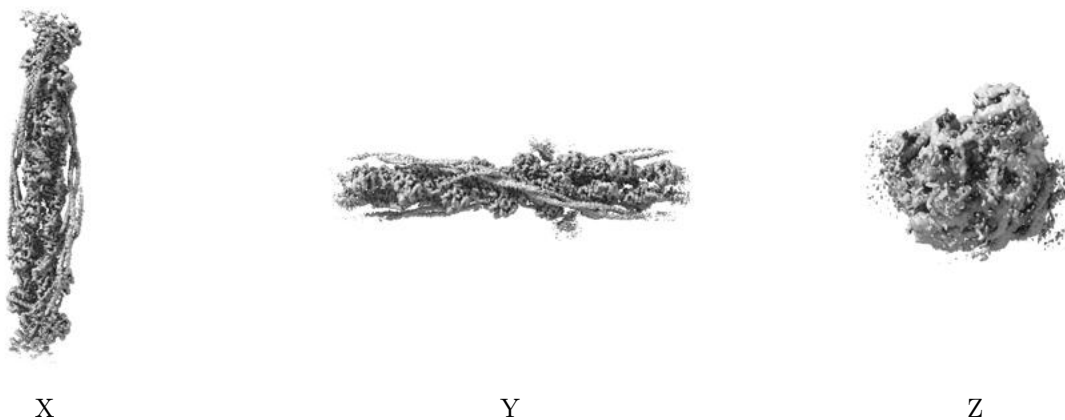
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

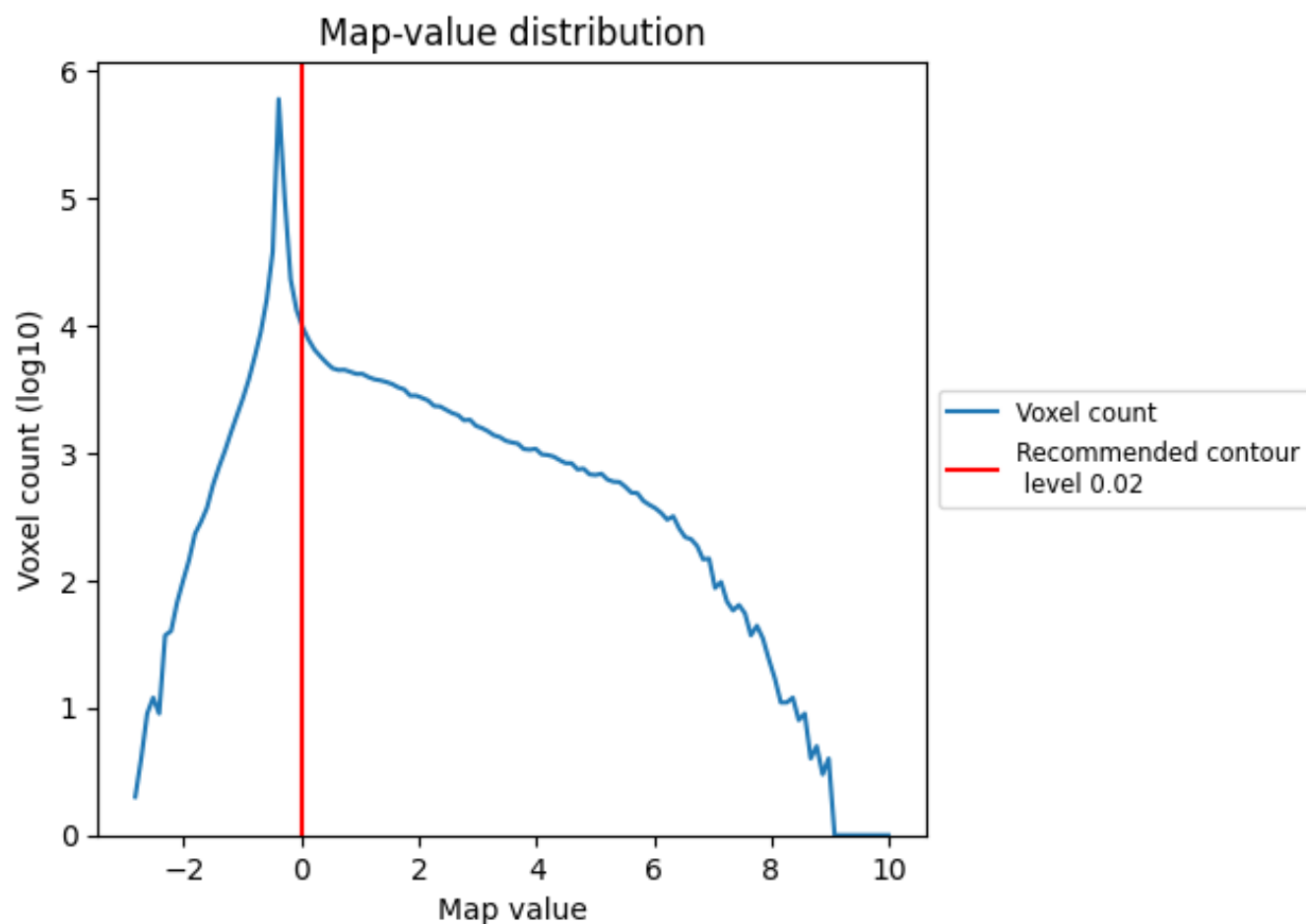
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

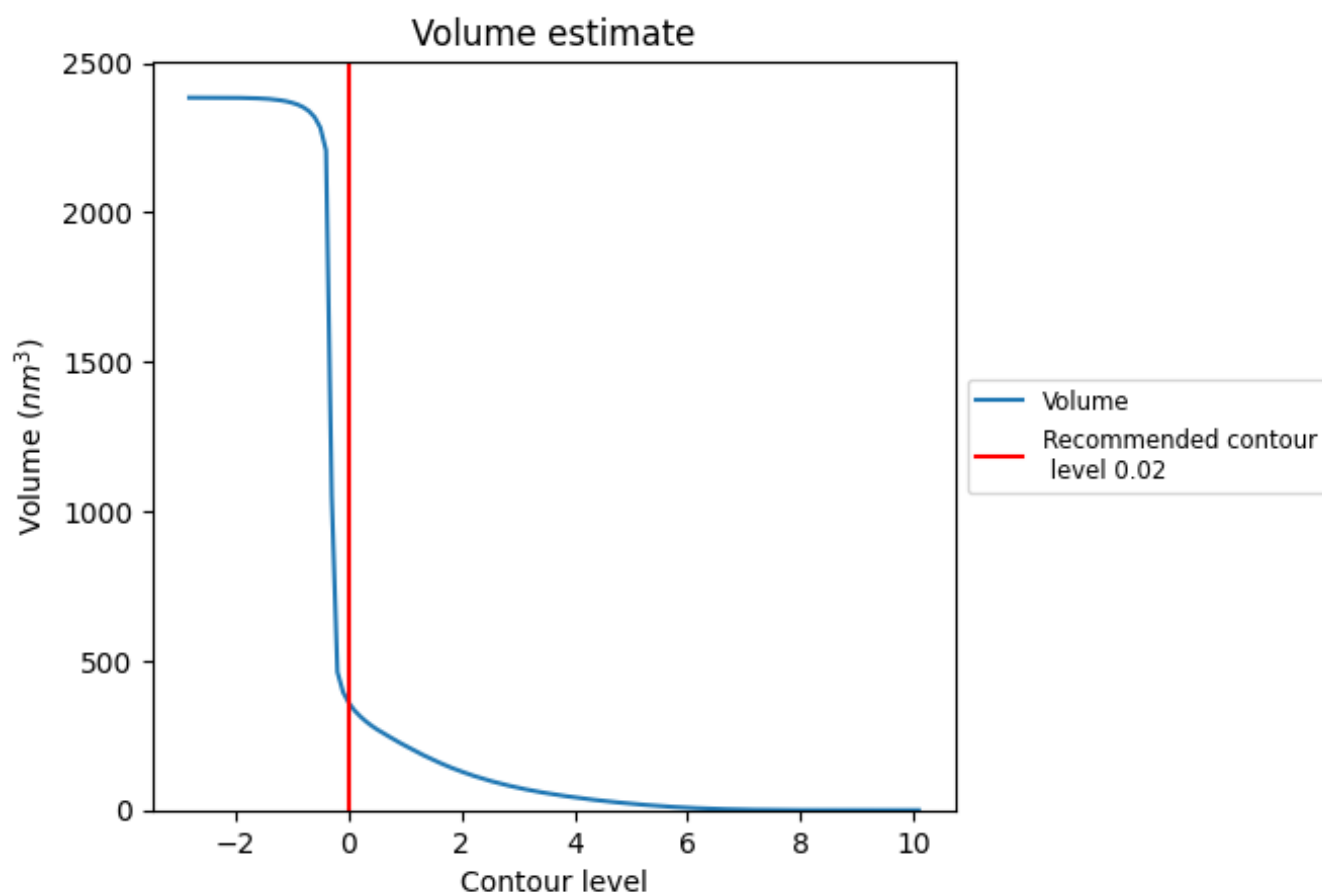
This section contains the results of statistical analysis of the map.

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 355 nm³; this corresponds to an approximate mass of 320 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.

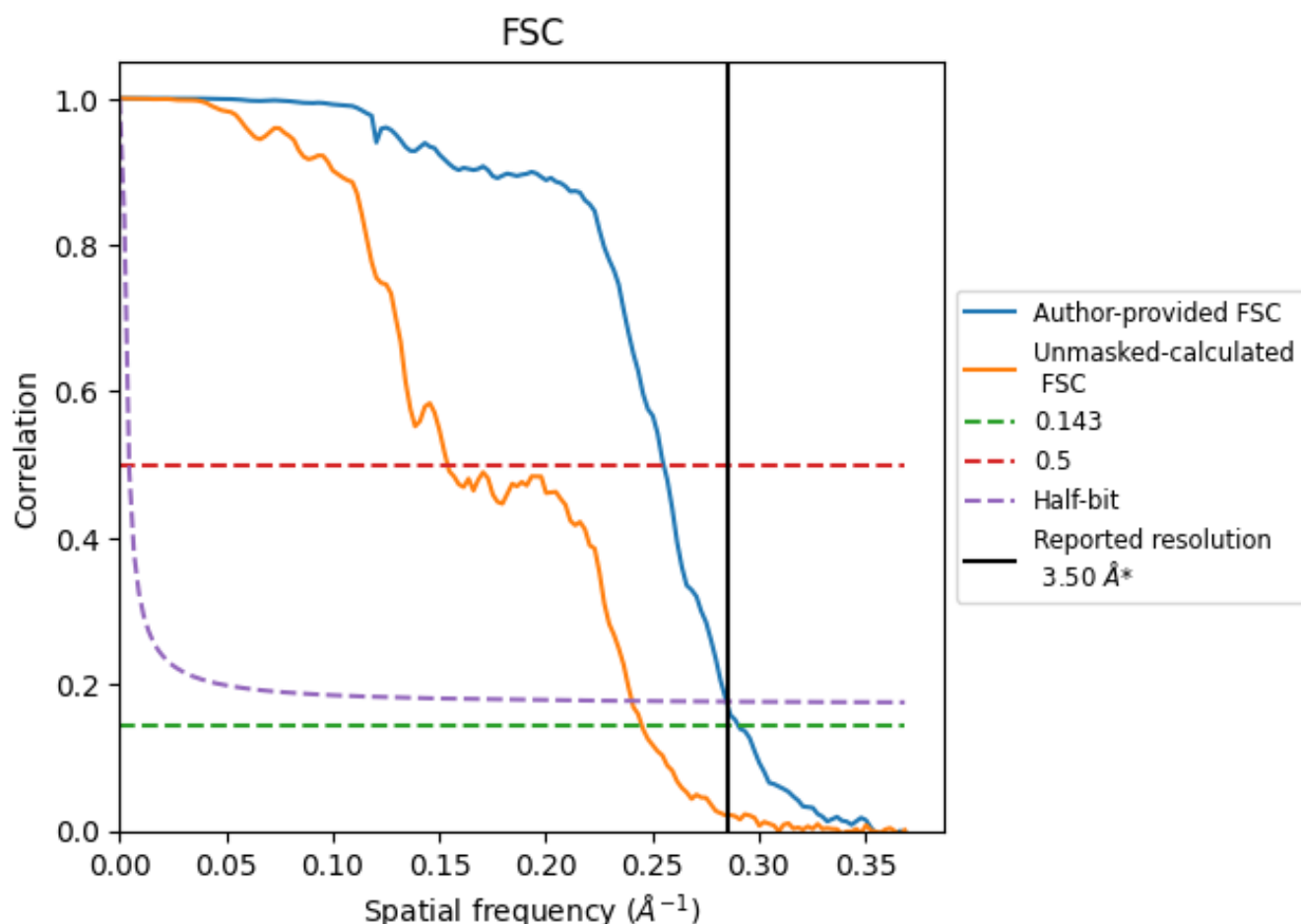
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

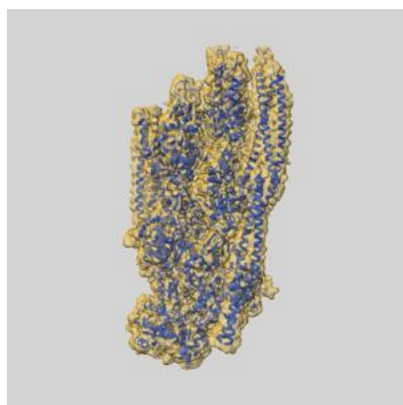
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.44	3.92	3.51
Unmasked-calculated*	4.08	6.49	4.16

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.08 differs from the reported value 3.5 by more than 10 %

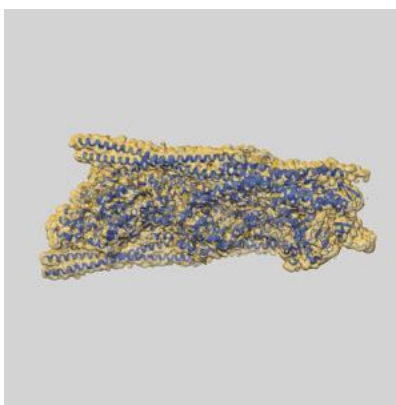
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27331 and PDB model 8DD0. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

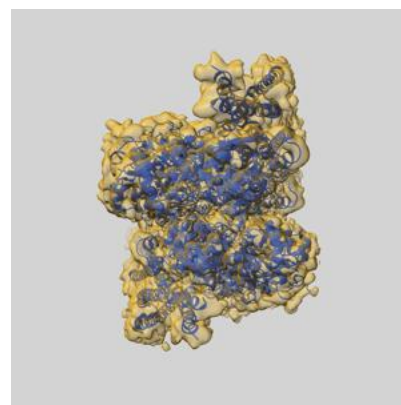
9.1 Map-model overlay [i](#)



X



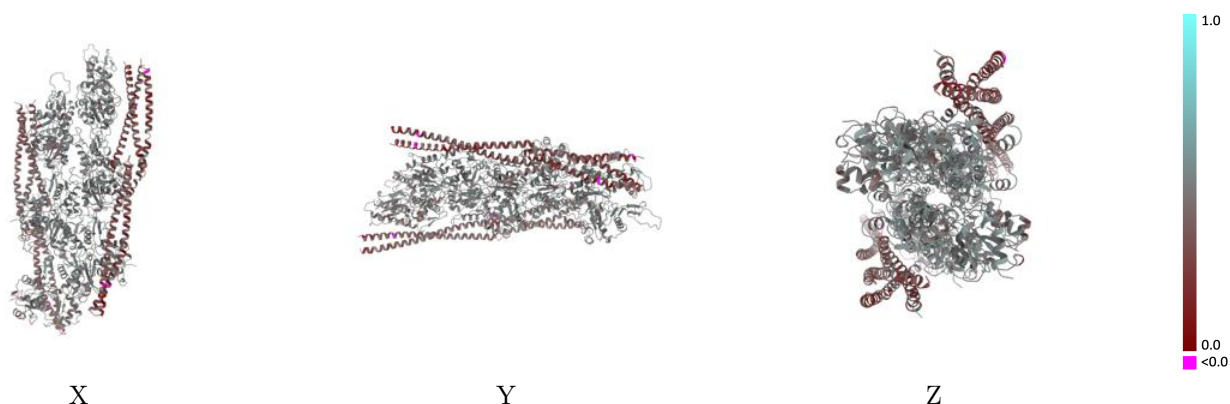
Y



Z

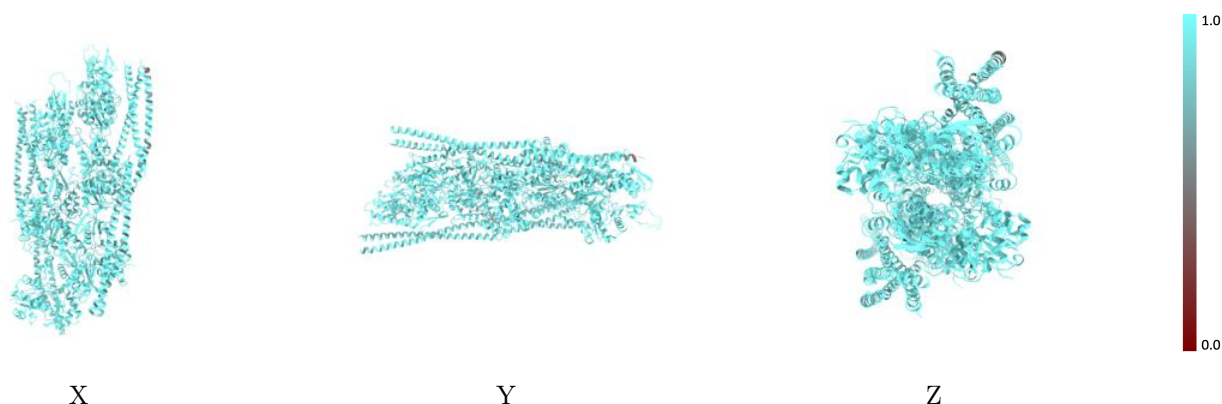
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



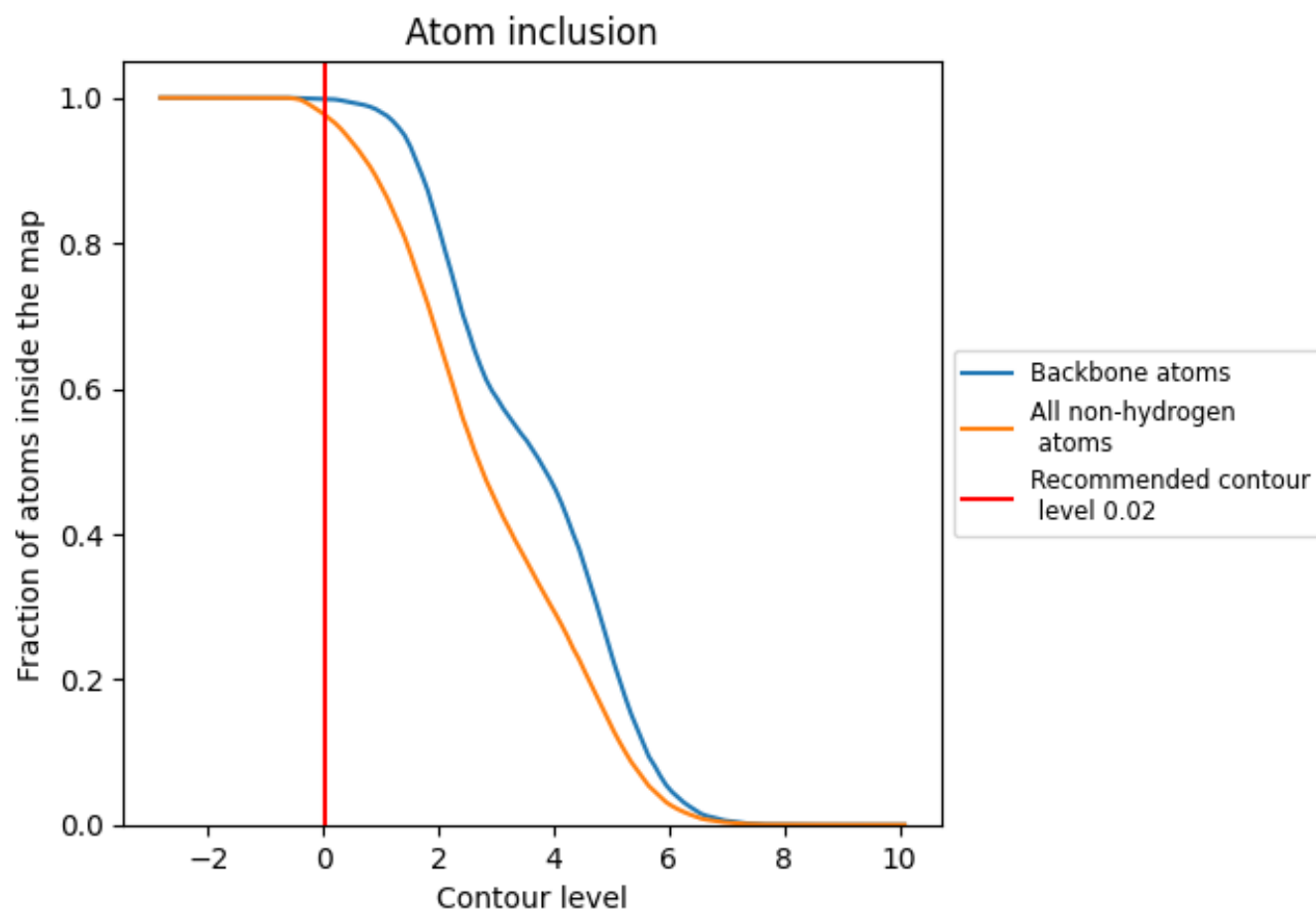
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 98% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9772	 0.4430
A	 0.9875	 0.4650
B	 0.9895	 0.4820
C	 0.9941	 0.4900
D	 0.9920	 0.4910
E	 0.9934	 0.4900
F	 0.9902	 0.4840
G	 0.9592	 0.3200
H	 0.9841	 0.3420
I	 0.9207	 0.2980
J	 0.9441	 0.3300
K	 0.9215	 0.3360
L	 0.9342	 0.2880
M	 0.9660	 0.2870
N	 0.8919	 0.2860
O	 0.9441	 0.3120
P	 0.8798	 0.3050

