



wwPDB EM Validation Summary Report ⓘ

May 19, 2025 – 03:48 AM EDT

PDB ID : 8UB4 / pdb_00008ub4
EMDB ID : EMD-42076
Title : Cdc48-Shp1 unfolding native substrate, consensus structure
Authors : Cooney, I.; Schubert, H.L.; Cedeno, K.; Carson, R.; Fisher, O.N.; Price, J.C.; Hill, C.P.; Shen, P.S.
Deposited on : 2023-09-22
Resolution : 2.90 Å(reported)

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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

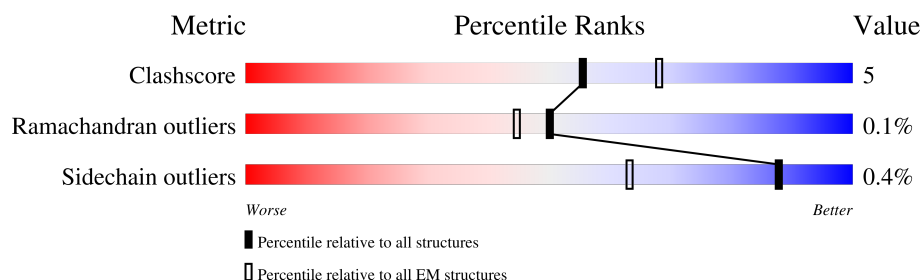
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



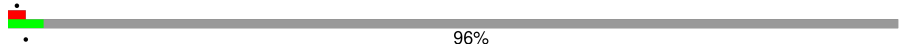
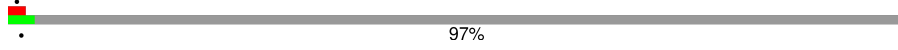
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	835	
1	B	835	
1	C	835	
1	D	835	
1	E	835	
1	F	835	
2	G	22	
3	H	423	

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Mol	Chain	Length	Quality of chain
3	I	423	 96%
3	J	423	 97%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 43895 atoms, of which 20889 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 Cell division control protein 48.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	544	Total	C	H	N	O	S	0	0
			7647	2473	3747	684	726	17		
1	B	561	Total	C	H	N	O	S	0	0
			8242	2637	4076	732	779	18		
1	C	553	Total	C	H	N	O	S	0	0
			8169	2600	4052	722	778	17		
1	D	554	Total	C	H	N	O	S	0	0
			8104	2592	4013	724	757	18		
1	E	513	Total	C	H	N	O	S	0	0
			6986	2291	3375	631	676	13		
1	F	485	Total	C	H	N	O		0	0
			3531	1420	1140	485	486			

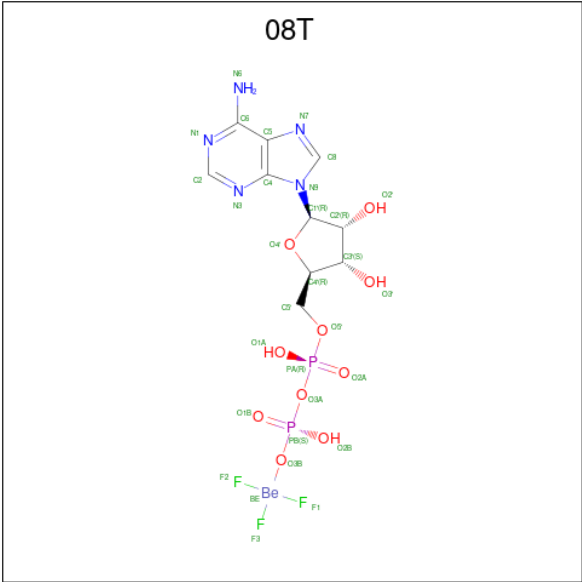
- Molecule 2 is a protein called Substrate.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	22	Total	C	H	N	O	0	0
			246	74	128	22	22		

- Molecule 3 is a protein called UBX domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	H	15	Total	C	H	N	O	S	0	0
			186	65	81	15	23	2		
3	I	15	Total	C	H	N	O	S	0	0
			196	67	87	16	24	2		
3	J	12	Total	C	H	N	O	S	0	0
			162	56	74	13	17	2		

- Molecule 4 is [[[(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxy-tris(fluoranyl)beryllium (CCD ID: 08T) (formula: C₁₀H₁₄BeF₃N₅O₁₀P₂).



Mol	Chain	Residues	Atoms								AltConf
4	A	1	Total	Be	C	F	H	N	O	P	0
			43	1	10	3	12	5	10	2	
4	A	1	Total	Be	C	F	H	N	O	P	0
			42	1	10	3	11	5	10	2	
4	B	1	Total	Be	C	F	H	N	O	P	0
			43	1	10	3	12	5	10	2	
4	B	1	Total	Be	C	F	H	N	O	P	0
			42	1	10	3	11	5	10	2	
4	C	1	Total	Be	C	F	H	N	O	P	0
			43	1	10	3	12	5	10	2	
4	C	1	Total	Be	C	F	H	N	O	P	0
			42	1	10	3	11	5	10	2	
4	D	1	Total	Be	C	F	H	N	O	P	0
			43	1	10	3	12	5	10	2	
4	D	1	Total	Be	C	F	H	N	O	P	0
			42	1	10	3	11	5	10	2	

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

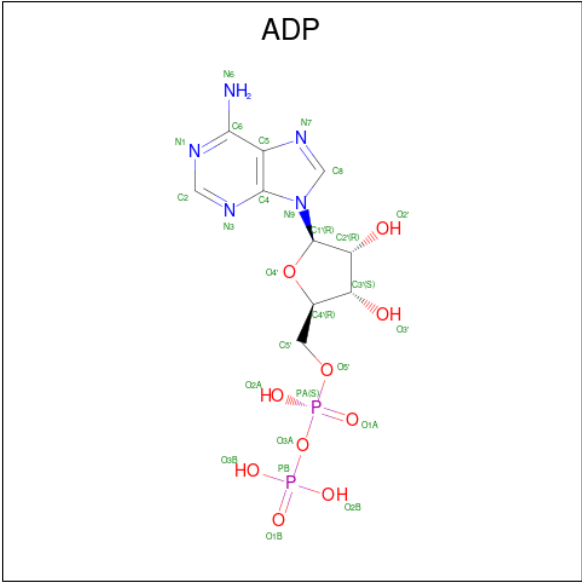
Mol	Chain	Residues	Atoms		AltConf
5	A	2	Total	Mg	0
			2	2	
5	B	2	Total	Mg	0
			2	2	
5	C	2	Total	Mg	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
5	D	2	Total	Mg	0
			2	2	

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

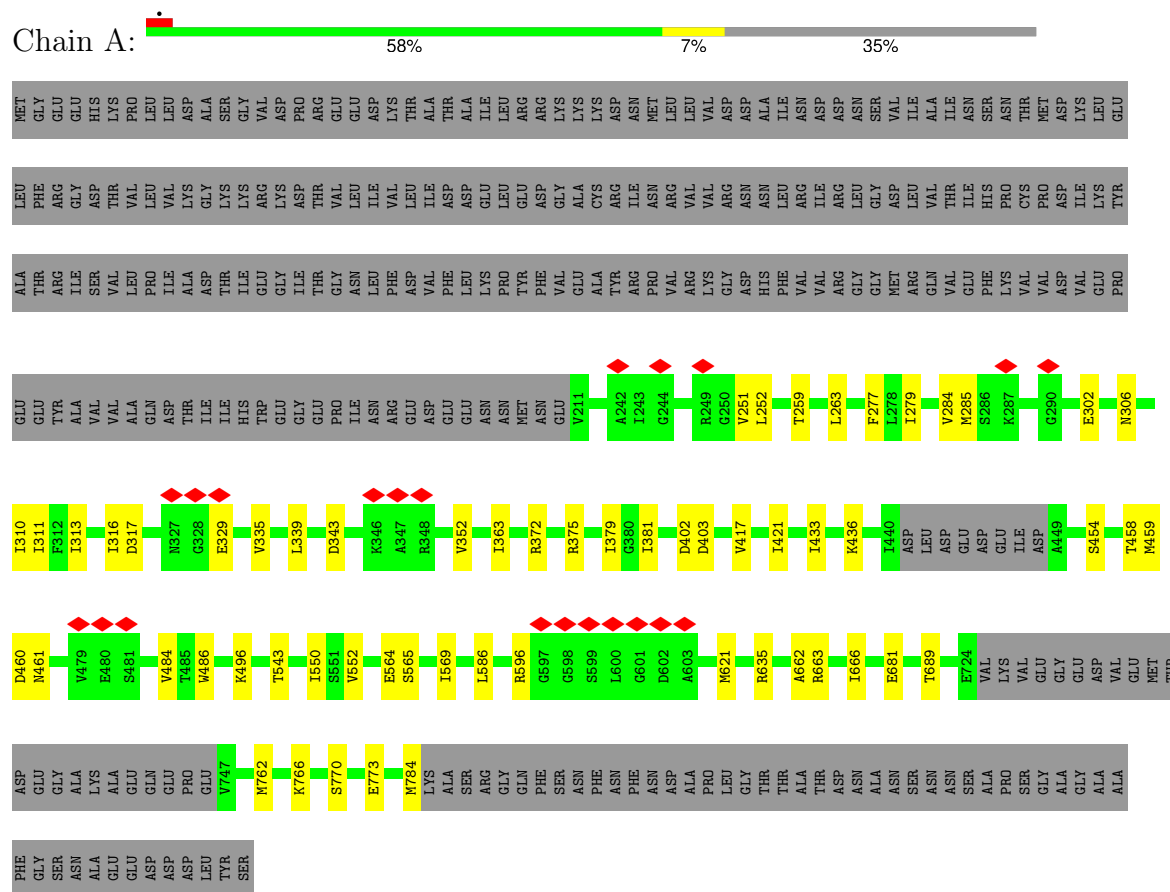


Mol	Chain	Residues	Atoms						AltConf
6	E	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
6	E	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

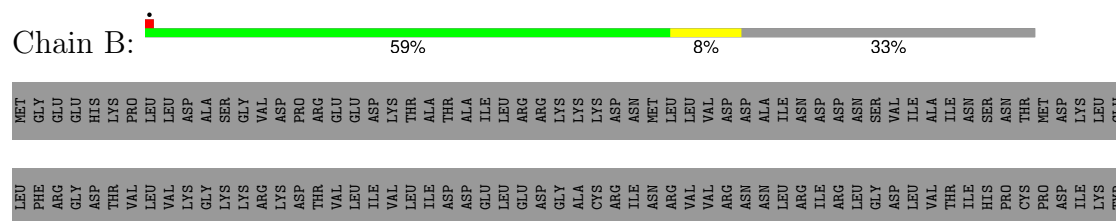
3 Residue-property plots

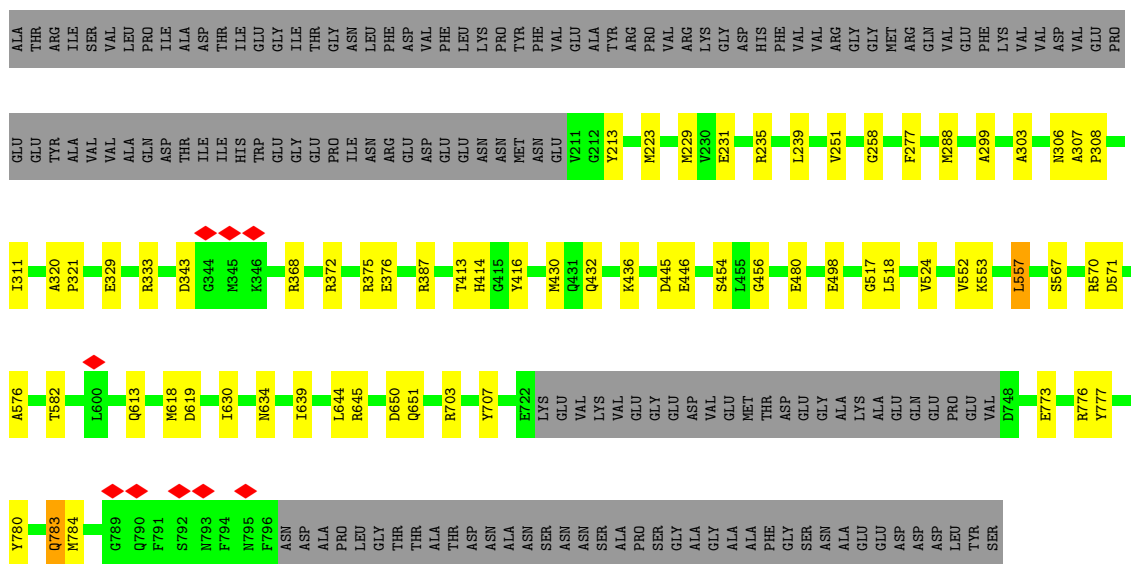
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Cell division control protein 48

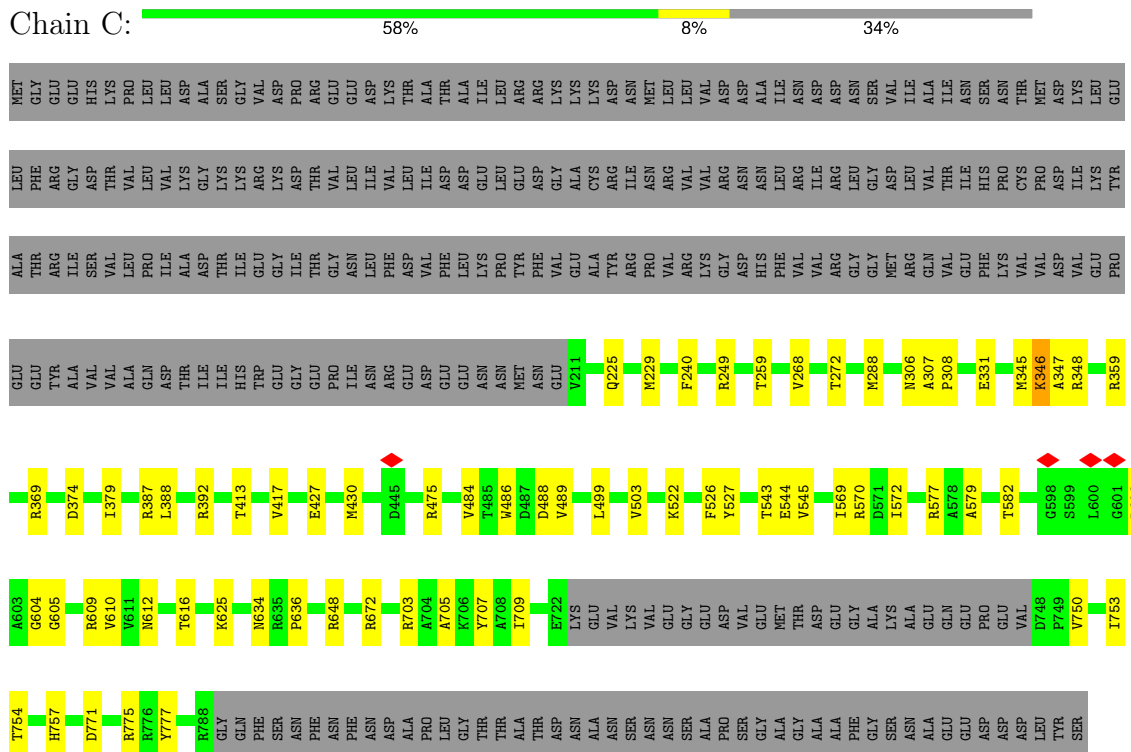


• Molecule 1: Cell division control protein 48

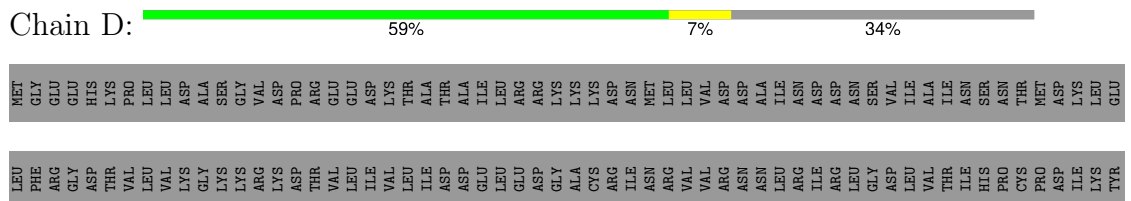




- Molecule 1: Cell division control protein 48



- Molecule 1: Cell division control protein 48





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

- Molecule 3: UBX domain-containing protein 1

Chain I:  96%

[illegible]

- Molecule 3: UBX domain-containing protein 1

Chain J: 97%

[illegible]

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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	325377	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 ($e^-/\text{\AA}^2$)	33	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.216	Depositor
Minimum map value	-0.353	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	311.04, 311.04, 311.04	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 08T, 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	0.14	0/3965	0.31	0/5398
1	B	0.19	0/4238	0.32	0/5751
1	C	0.20	0/4186	0.32	0/5679
1	D	0.18	0/4162	0.31	0/5644
1	E	0.14	0/3668	0.29	0/5004
1	F	0.06	0/2383	0.23	0/3302
2	G	0.10	0/117	0.23	0/163
3	H	0.22	0/106	0.45	0/141
3	I	0.19	0/110	0.18	0/146
3	J	0.21	0/89	0.27	0/117
All	All	0.16	0/23024	0.30	0/31345

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	C	0	3
1	E	0	1
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	596	ARG	Sidechain
1	A	635	ARG	Sidechain
1	C	348	ARG	Sidechain
1	C	570	ARG	Sidechain
1	C	577	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3900	3747	3745	39	0
1	B	4166	4076	4076	44	0
1	C	4117	4052	4052	44	0
1	D	4091	4013	4012	43	0
1	E	3611	3375	3373	47	0
1	F	2391	1140	1142	2	0
2	G	118	128	128	1	0
3	H	105	81	83	1	0
3	I	109	87	89	0	0
3	J	88	74	76	0	0
4	A	62	23	24	0	0
4	B	62	23	24	1	0
4	C	62	23	24	0	0
4	D	62	23	24	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	E	54	24	24	3	0
All	All	23006	20889	20896	207	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 5.

The worst 5 of 207 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:D:399:LYS:NZ	1:E:242:ALA:O	2.14	0.80
1:D:436:LYS:NZ	1:D:454:SER:O	2.16	0.78
1:E:579:ALA:O	1:E:582:THR:OG1	2.02	0.76
1:A:564:GLU:OE1	1:A:564:GLU:N	2.20	0.75
1:B:634:ASN:O	1:B:777:TYR:OH	2.02	0.74

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	538/835 (64%)	511 (95%)	27 (5%)	0	100	100
1	B	557/835 (67%)	534 (96%)	23 (4%)	0	100	100
1	C	549/835 (66%)	512 (93%)	36 (7%)	1 (0%)	44	73
1	D	548/835 (66%)	514 (94%)	34 (6%)	0	100	100
1	E	503/835 (60%)	480 (95%)	23 (5%)	0	100	100
1	F	469/835 (56%)	437 (93%)	31 (7%)	1 (0%)	44	73
2	G	20/22 (91%)	18 (90%)	2 (10%)	0	100	100
3	H	13/423 (3%)	13 (100%)	0	0	100	100
3	I	13/423 (3%)	13 (100%)	0	0	100	100
3	J	10/423 (2%)	10 (100%)	0	0	100	100
All	All	3220/6301 (51%)	3042 (94%)	176 (6%)	2 (0%)	50	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	287	LYS
1	C	346	LYS

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	366/695 (53%)	364 (100%)	2 (0%)	86	96
1	B	411/695 (59%)	407 (99%)	4 (1%)	73	91
1	C	412/695 (59%)	411 (100%)	1 (0%)	92	98
1	D	401/695 (58%)	401 (100%)	0	100	100
1	E	324/695 (47%)	324 (100%)	0	100	100
1	F	1/695 (0%)	1 (100%)	0	100	100
2	G	4/4 (100%)	4 (100%)	0	100	100
3	H	10/362 (3%)	10 (100%)	0	100	100
3	I	11/362 (3%)	11 (100%)	0	100	100
3	J	9/362 (2%)	9 (100%)	0	100	100
All	All	1949/5260 (37%)	1942 (100%)	7 (0%)	88	97

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	557	LEU
1	B	618	MET
1	C	572	ILE
1	B	783	GLN
1	B	553	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	512	GLN
1	D	280	ASN
1	E	394	HIS
1	D	651	GLN
1	B	651	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](#)

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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	08T	A	903	-	27,33,33	0.89	0	27,52,52	0.88	2 (7%)
6	ADP	E	901	-	24,29,29	0.77	0	29,45,45	1.27	2 (6%)
4	08T	C	903	5	27,33,33	0.87	0	27,52,52	0.89	2 (7%)
6	ADP	E	902	-	24,29,29	0.80	0	29,45,45	1.03	1 (3%)
4	08T	B	901	5	27,33,33	0.95	1 (3%)	27,52,52	0.87	2 (7%)
4	08T	D	903	5	27,33,33	0.90	0	27,52,52	0.87	2 (7%)
4	08T	D	901	5	27,33,33	0.91	1 (3%)	27,52,52	1.02	2 (7%)
4	08T	B	903	5	27,33,33	0.91	1 (3%)	27,52,52	0.90	2 (7%)
4	08T	C	901	5	27,33,33	0.91	1 (3%)	27,52,52	0.88	2 (7%)
4	08T	A	901	5	27,33,33	0.84	0	27,52,52	0.89	2 (7%)

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	08T	A	903	-	-	5/12/38/38	0/3/3/3
6	ADP	E	901	-	-	5/12/32/32	0/3/3/3
4	08T	C	903	5	-	0/12/38/38	0/3/3/3
6	ADP	E	902	-	-	7/12/32/32	0/3/3/3
4	08T	B	901	5	-	5/12/38/38	0/3/3/3
4	08T	D	903	5	-	5/12/38/38	0/3/3/3
4	08T	D	901	5	-	5/12/38/38	0/3/3/3
4	08T	B	903	5	-	0/12/38/38	0/3/3/3
4	08T	C	901	5	-	5/12/38/38	0/3/3/3
4	08T	A	901	5	-	5/12/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	901	08T	PA-O3A	-2.40	1.56	1.59
4	C	901	08T	PA-O3A	-2.16	1.57	1.59
4	D	901	08T	PA-O3A	-2.08	1.57	1.59
4	B	903	08T	PA-O3A	-2.07	1.57	1.59

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	901	ADP	C4'-O4'-C1'	-4.04	106.23	109.92
4	D	901	08T	C5-C6-N6	2.30	123.81	120.31
6	E	902	ADP	C5-C6-N6	2.30	123.81	120.31
4	C	901	08T	C5-C6-N6	2.29	123.80	120.31
4	A	903	08T	C5-C6-N6	2.29	123.80	120.31

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

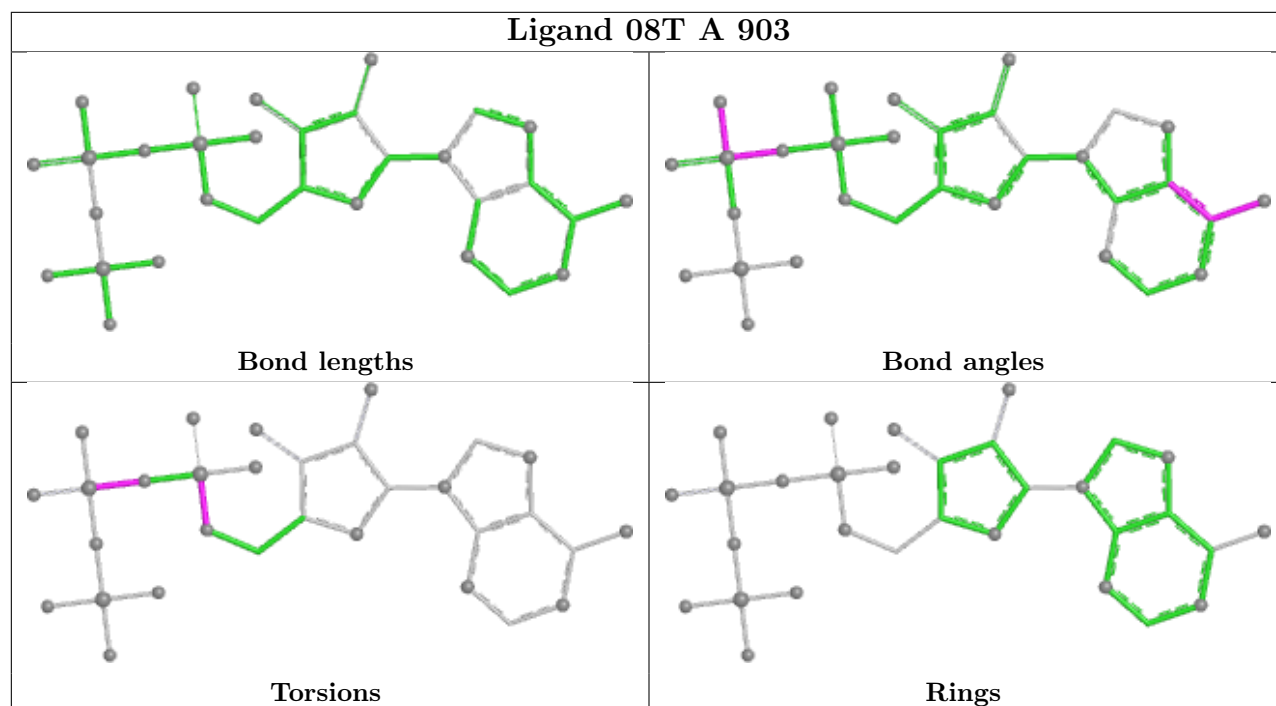
Mol	Chain	Res	Type	Atoms
4	A	901	08T	C5'-O5'-PA-O1A
4	A	901	08T	C5'-O5'-PA-O2A
4	A	901	08T	C5'-O5'-PA-O3A
4	A	901	08T	O4'-C4'-C5'-O5'
4	A	903	08T	C5'-O5'-PA-O1A

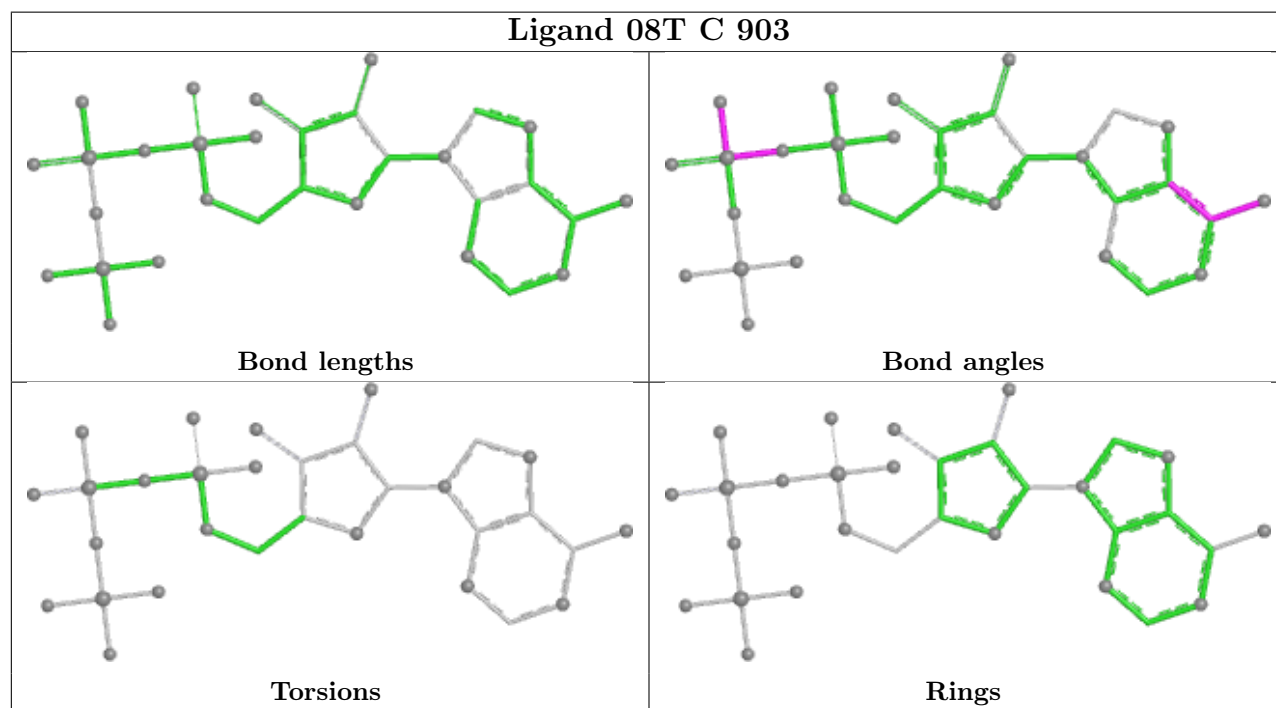
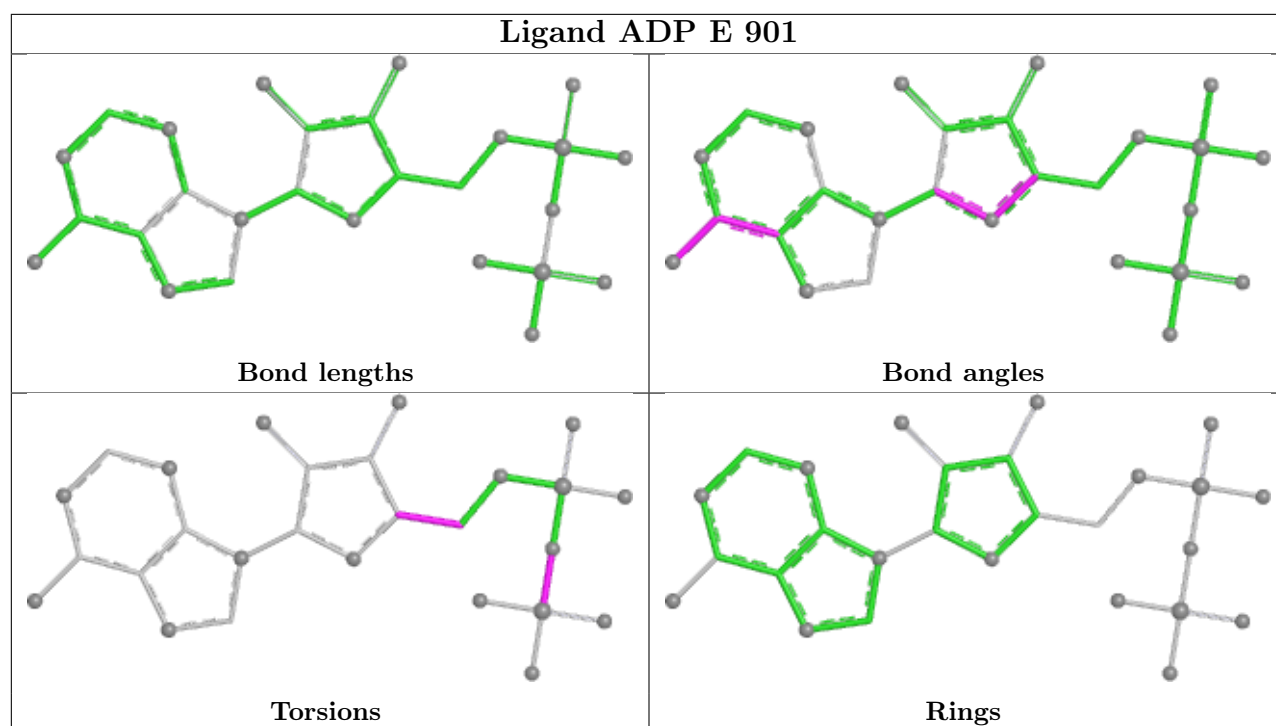
There are no ring outliers.

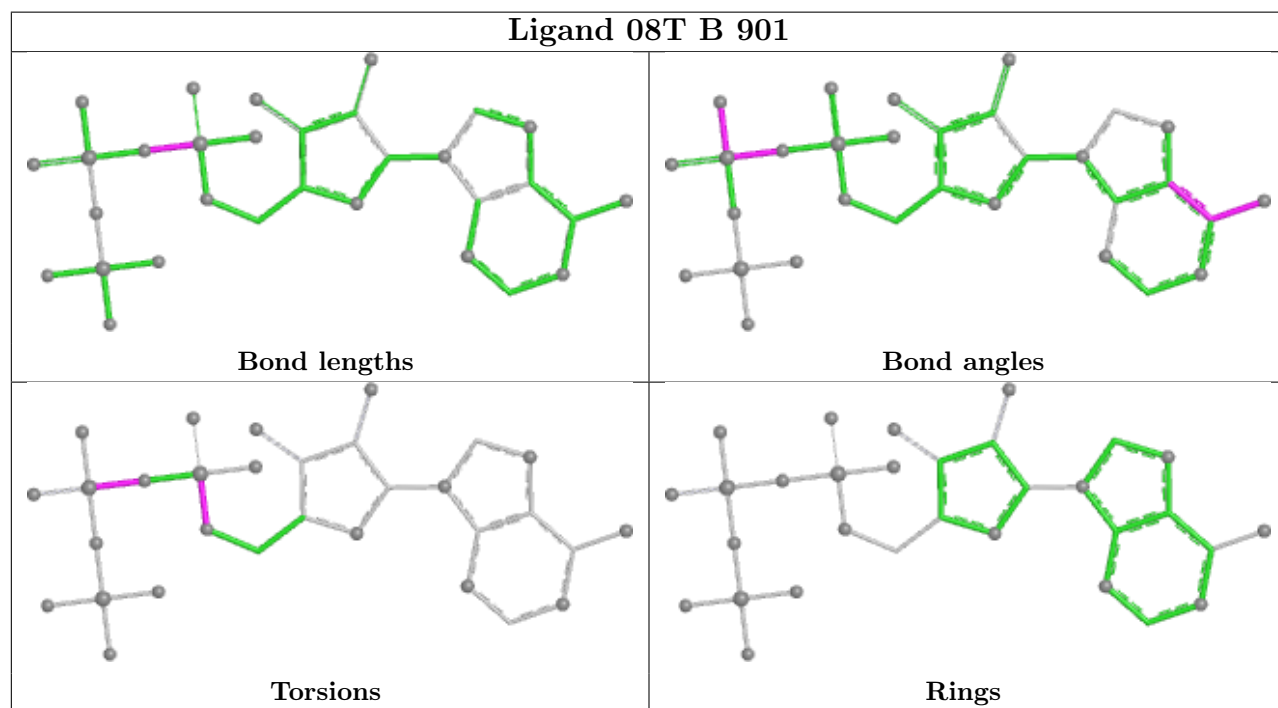
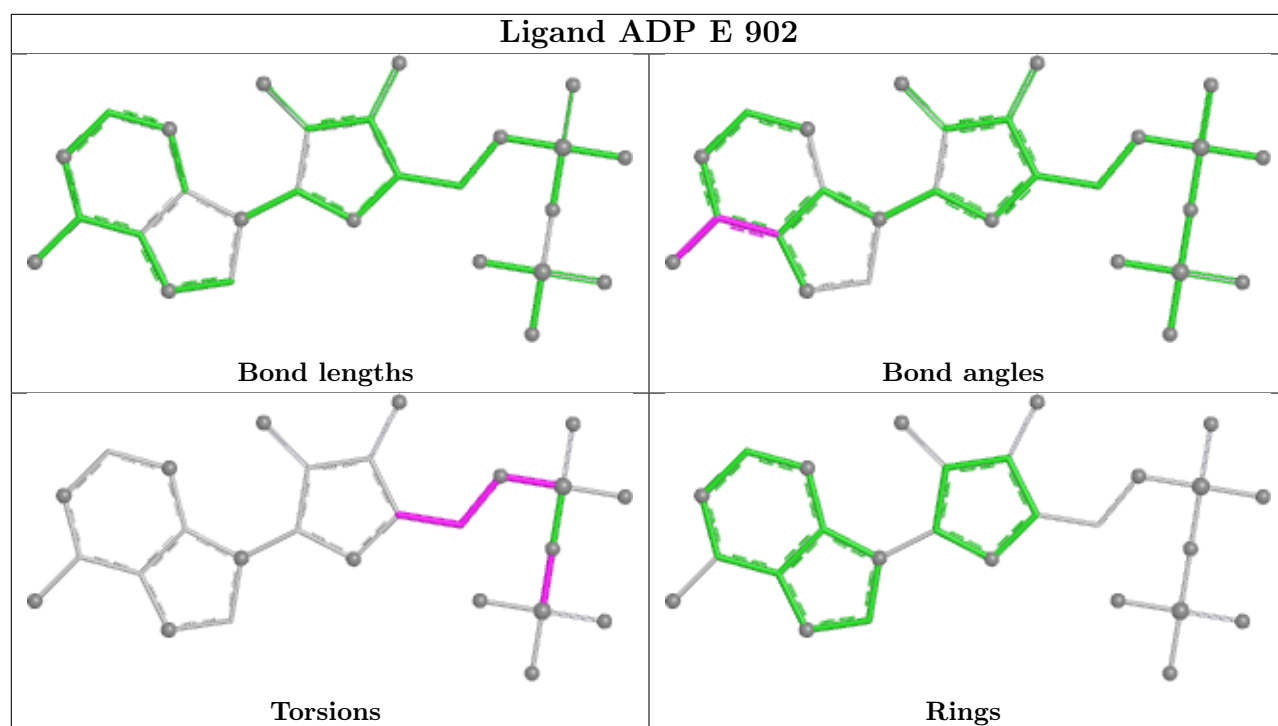
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	901	ADP	1	0
6	E	902	ADP	2	0
4	B	903	08T	1	0

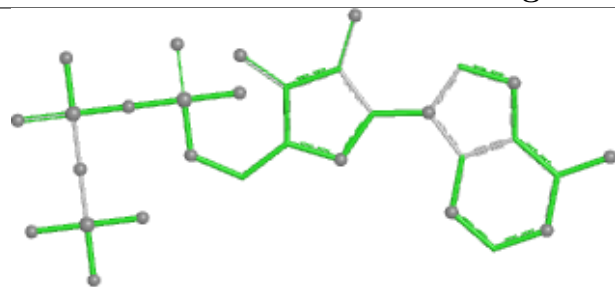
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



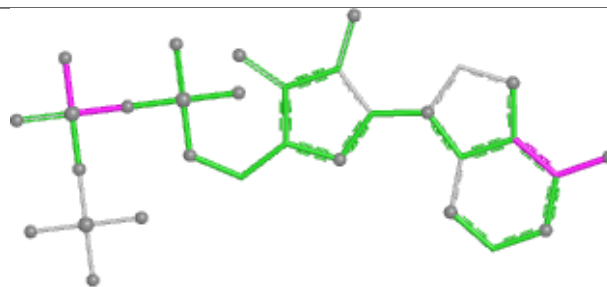




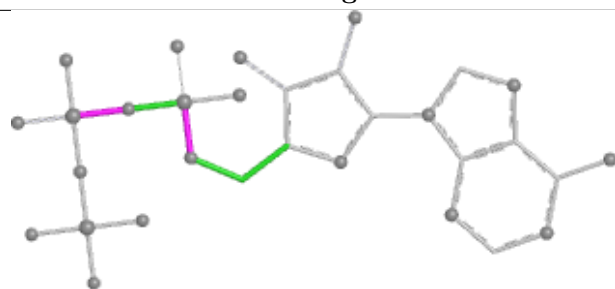
Ligand 08T D 903



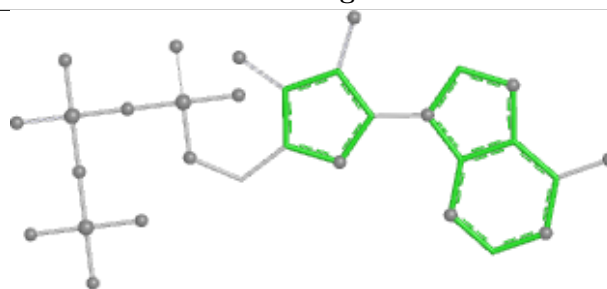
Bond lengths



Bond angles

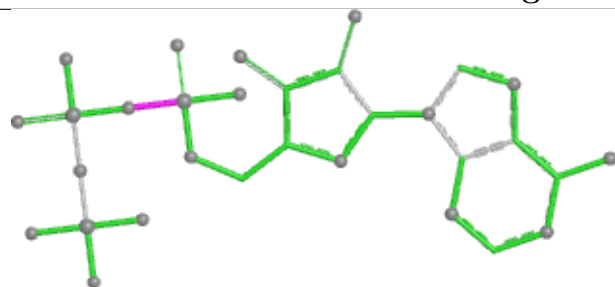


Torsions

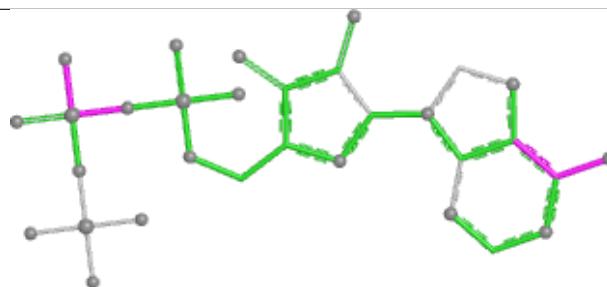


Rings

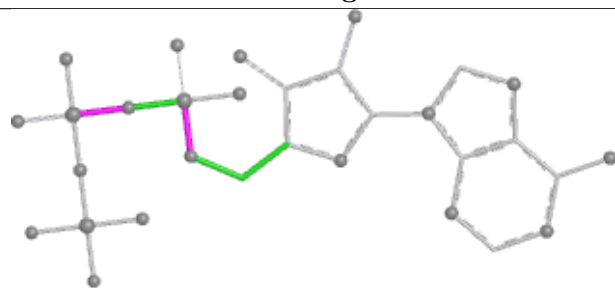
Ligand 08T D 901



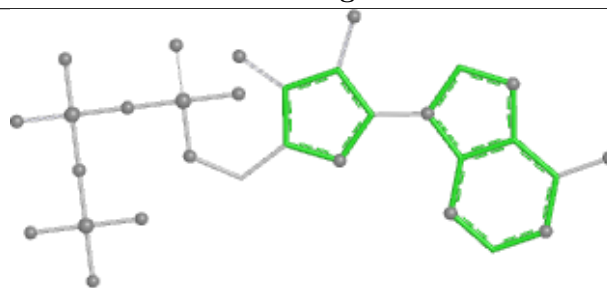
Bond lengths



Bond angles

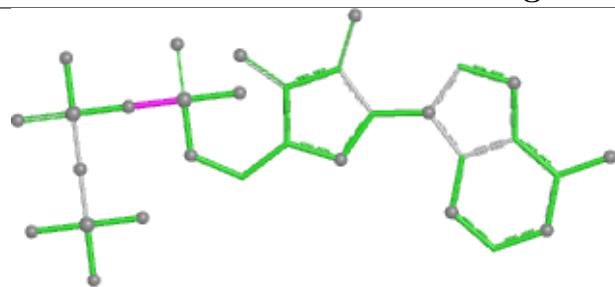


Torsions

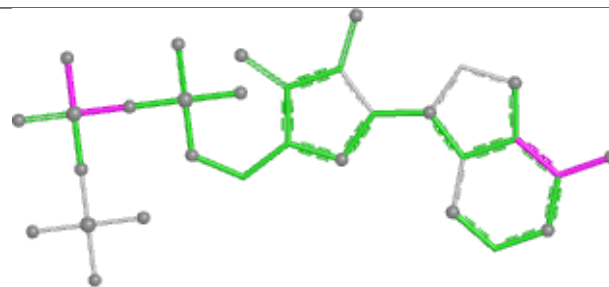


Rings

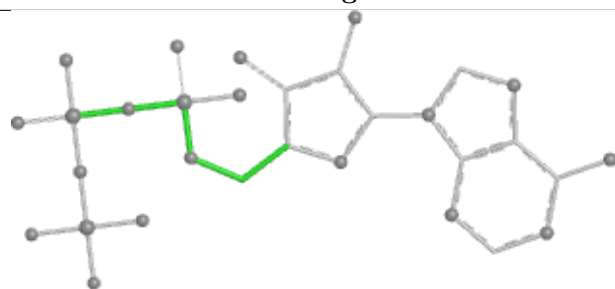
Ligand 08T B 903



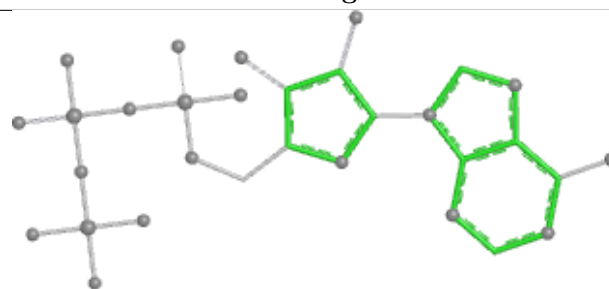
Bond lengths



Bond angles

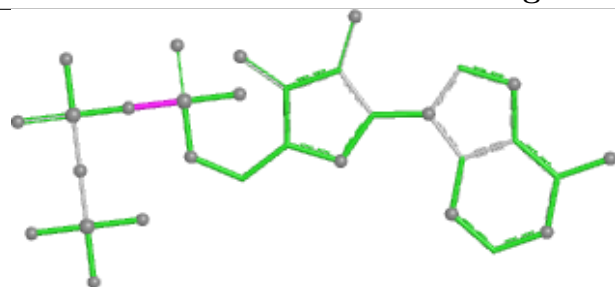


Torsions

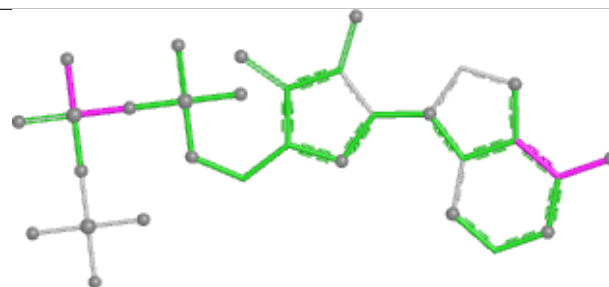


Rings

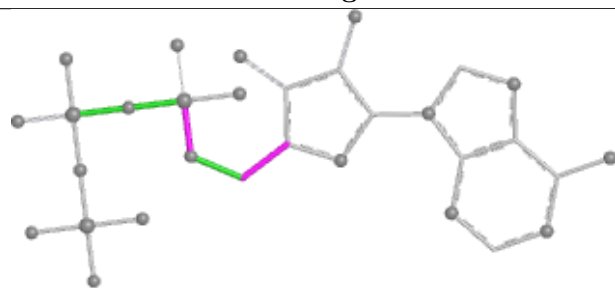
Ligand 08T C 901



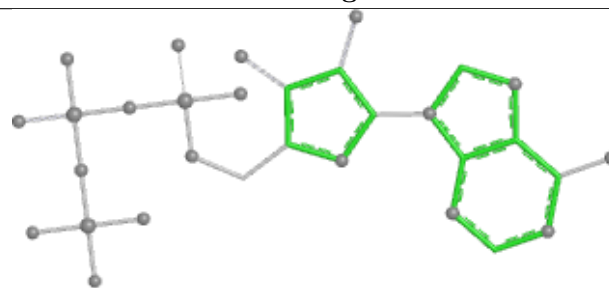
Bond lengths



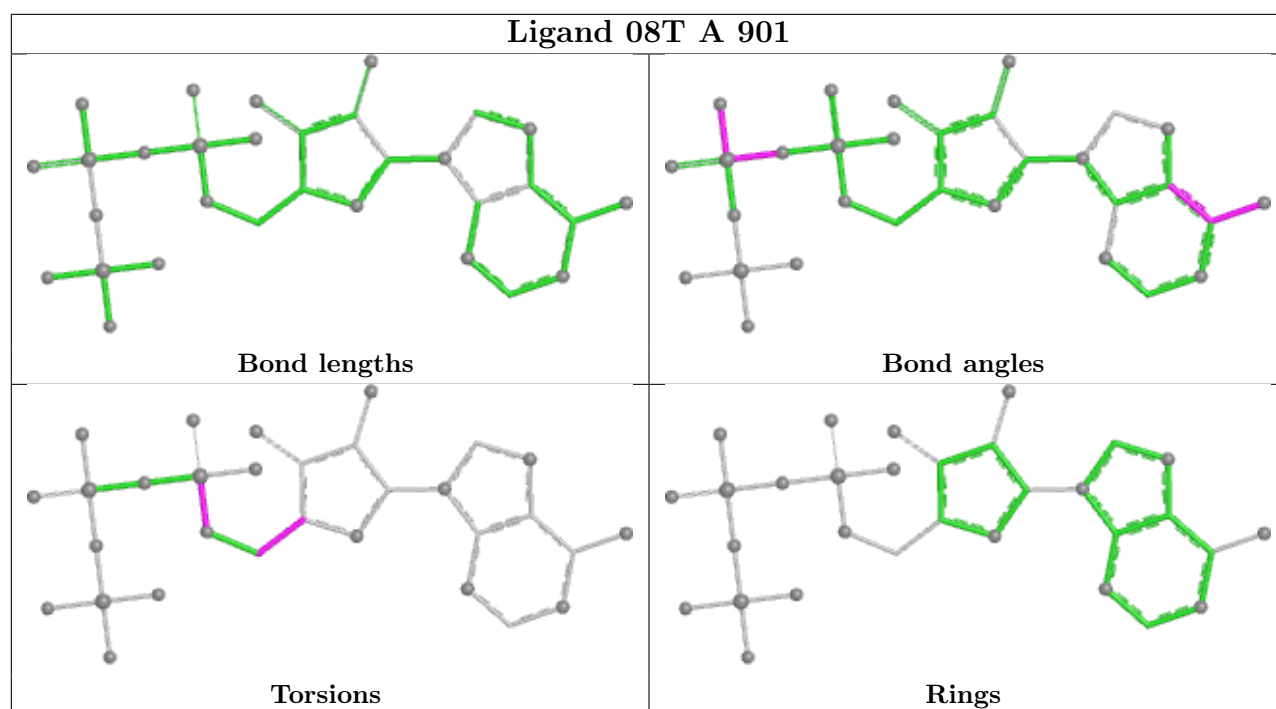
Bond angles



Torsions



Rings



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.

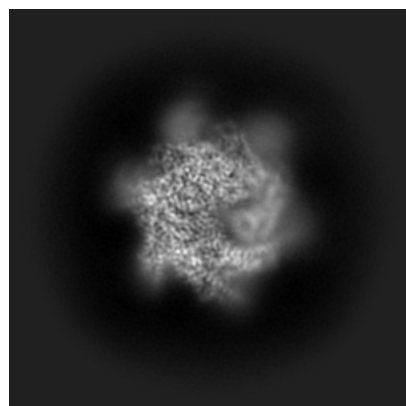
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42076. These allow visual inspection of the internal detail of the map and identification of artifacts.

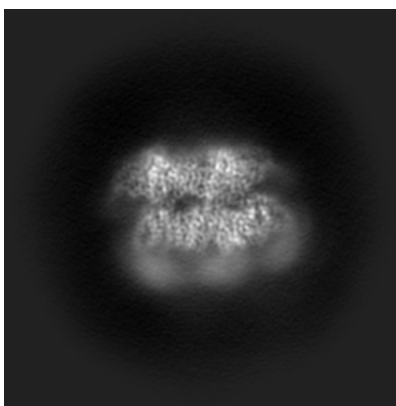
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

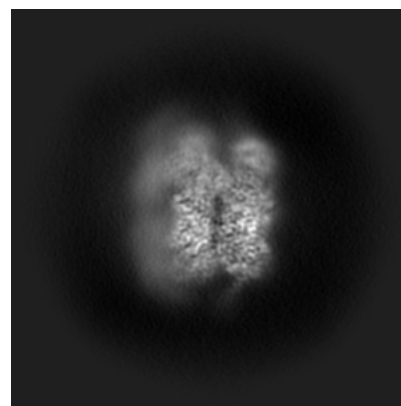
6.1.1 Primary map



X

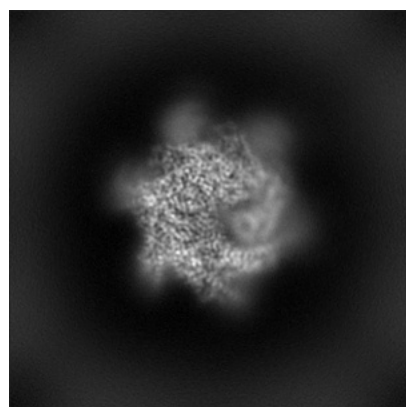


Y

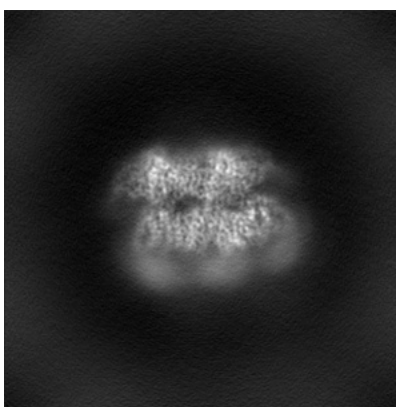


Z

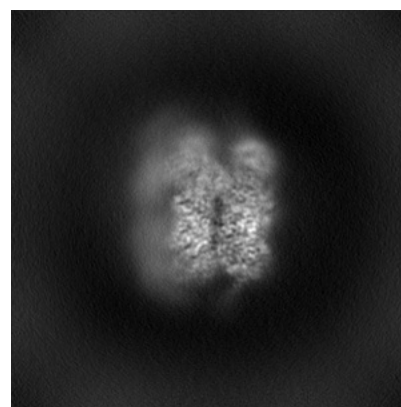
6.1.2 Raw map



X



Y

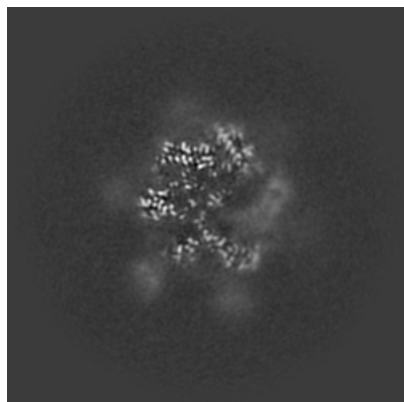


Z

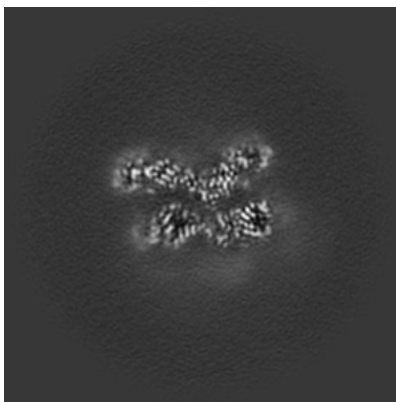
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

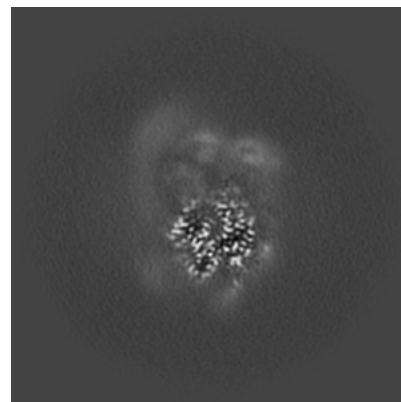
6.2.1 Primary map



X Index: 144

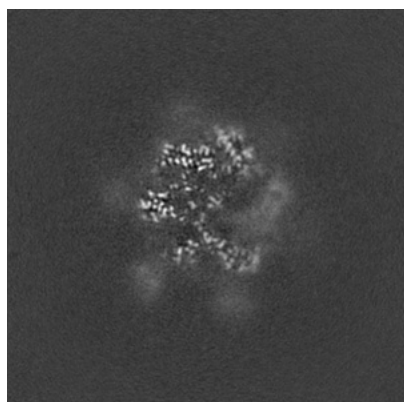


Y Index: 144

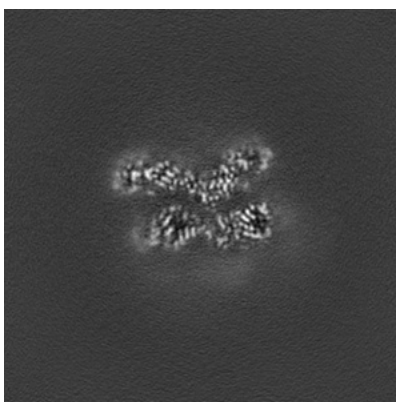


Z Index: 144

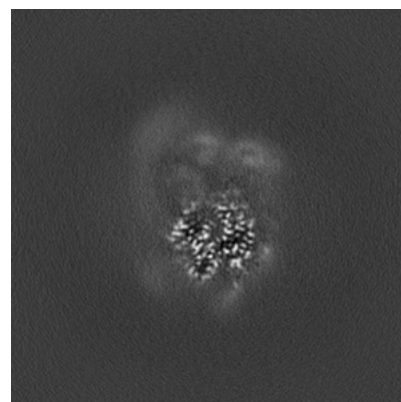
6.2.2 Raw map



X Index: 144



Y Index: 144

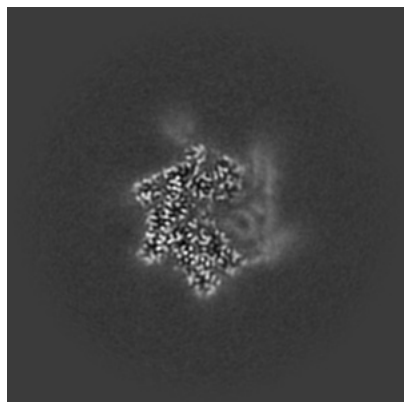


Z Index: 144

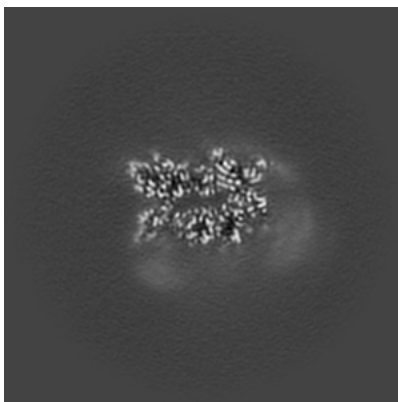
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

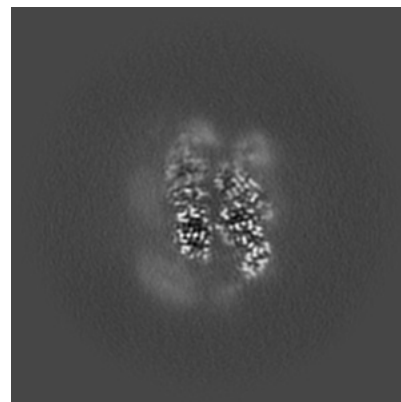
6.3.1 Primary map



X Index: 168

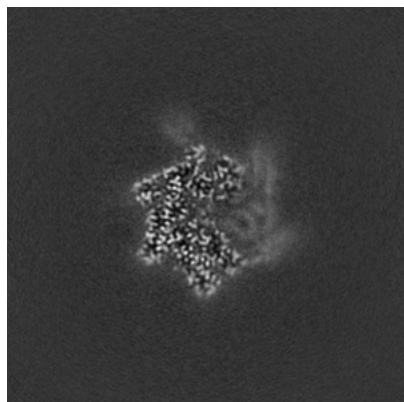


Y Index: 130

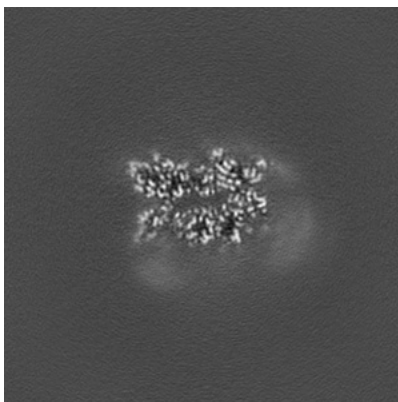


Z Index: 162

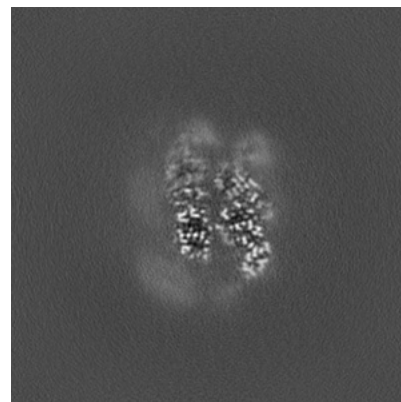
6.3.2 Raw map



X Index: 168



Y Index: 130

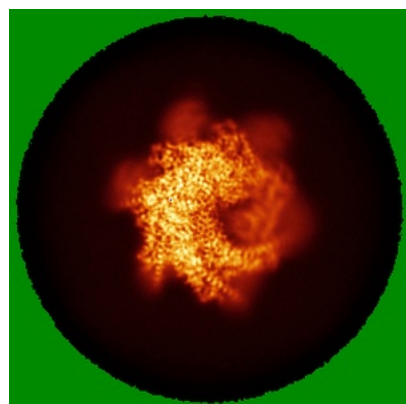


Z Index: 162

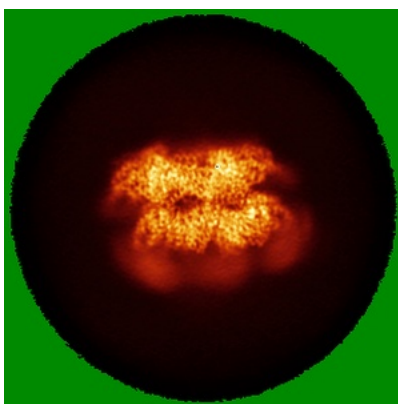
The images above show the largest variance slices of the map in three orthogonal directions.

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

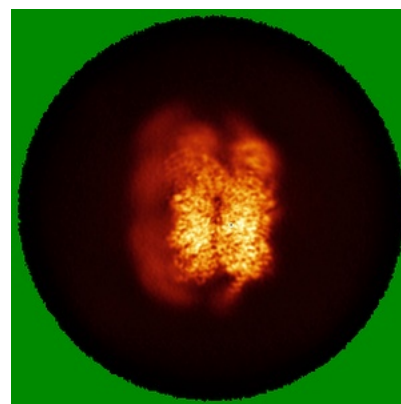
6.4.1 Primary map



X

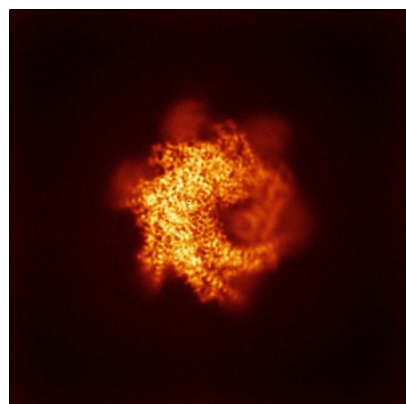


Y

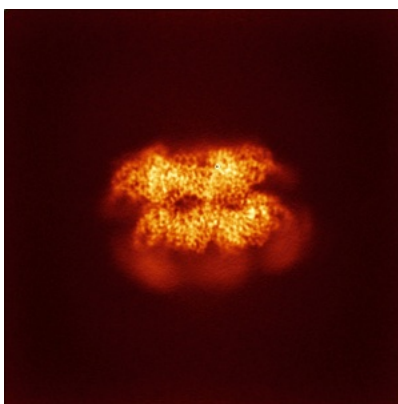


Z

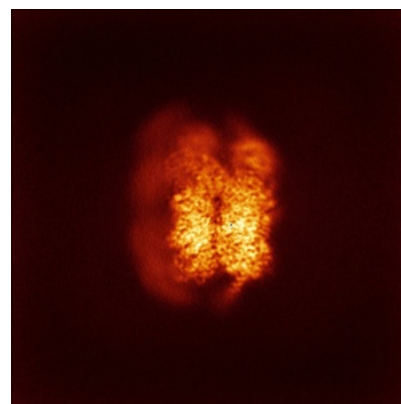
6.4.2 Raw map



X



Y

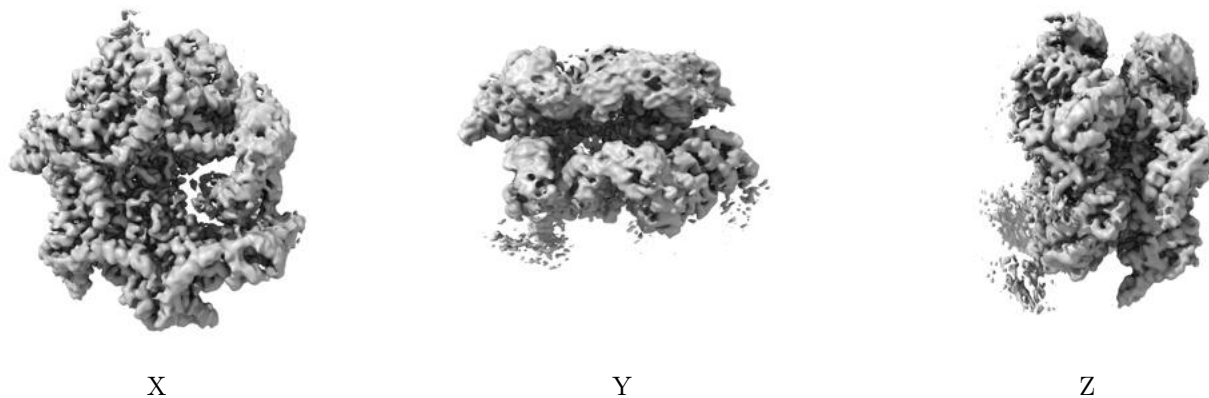


Z

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 0.16. 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.

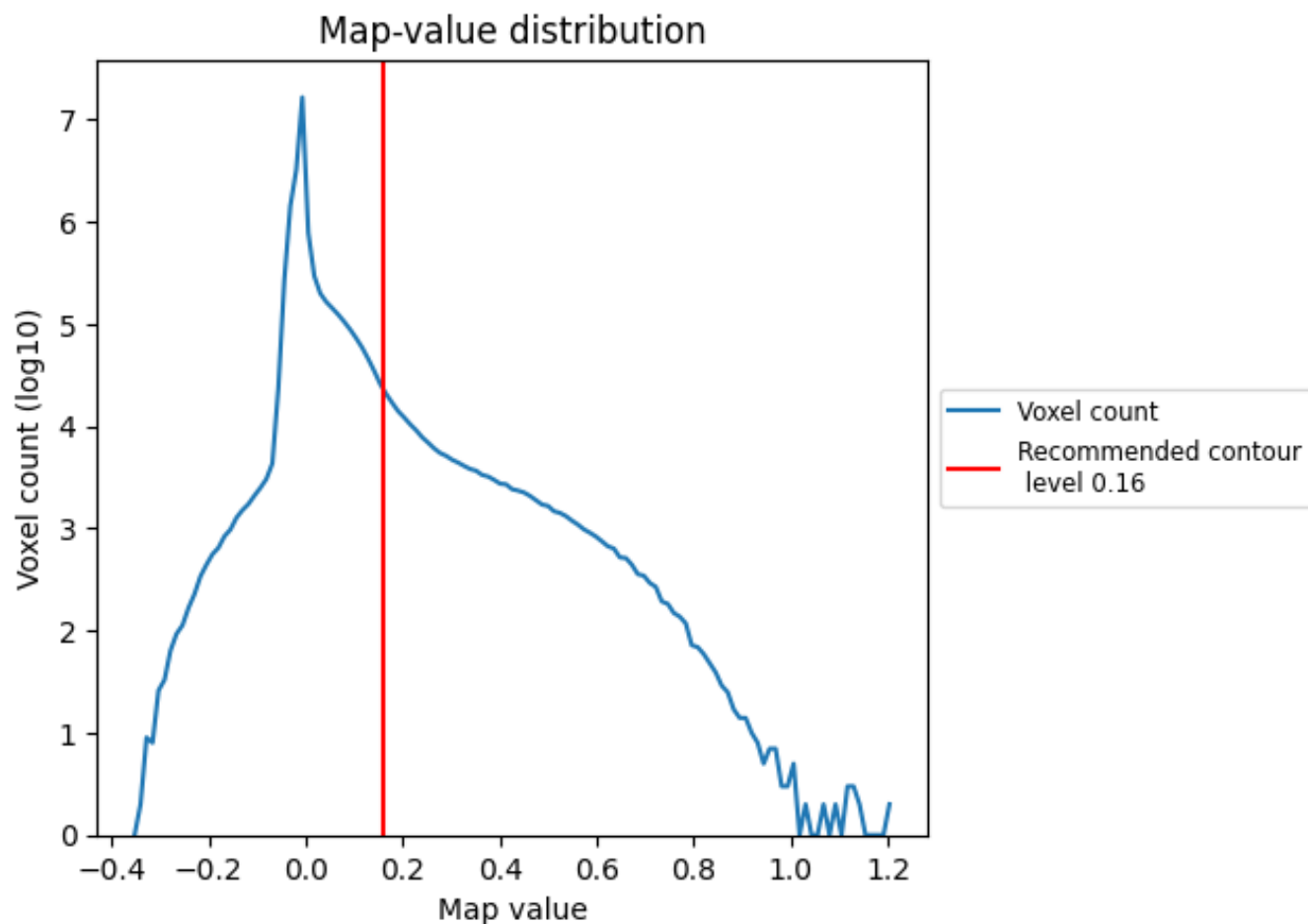
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

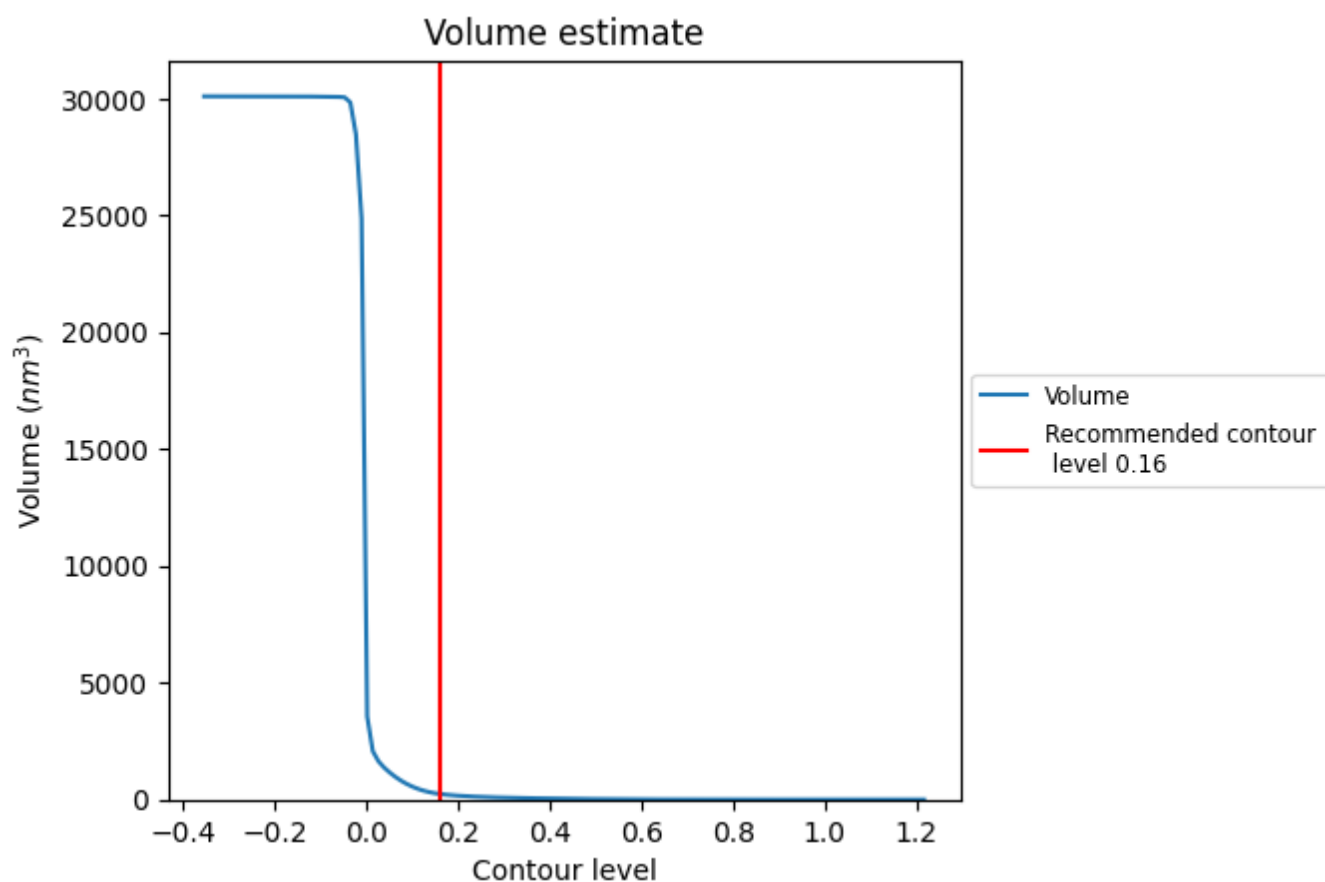
This section contains the results of statistical analysis of the map.

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.

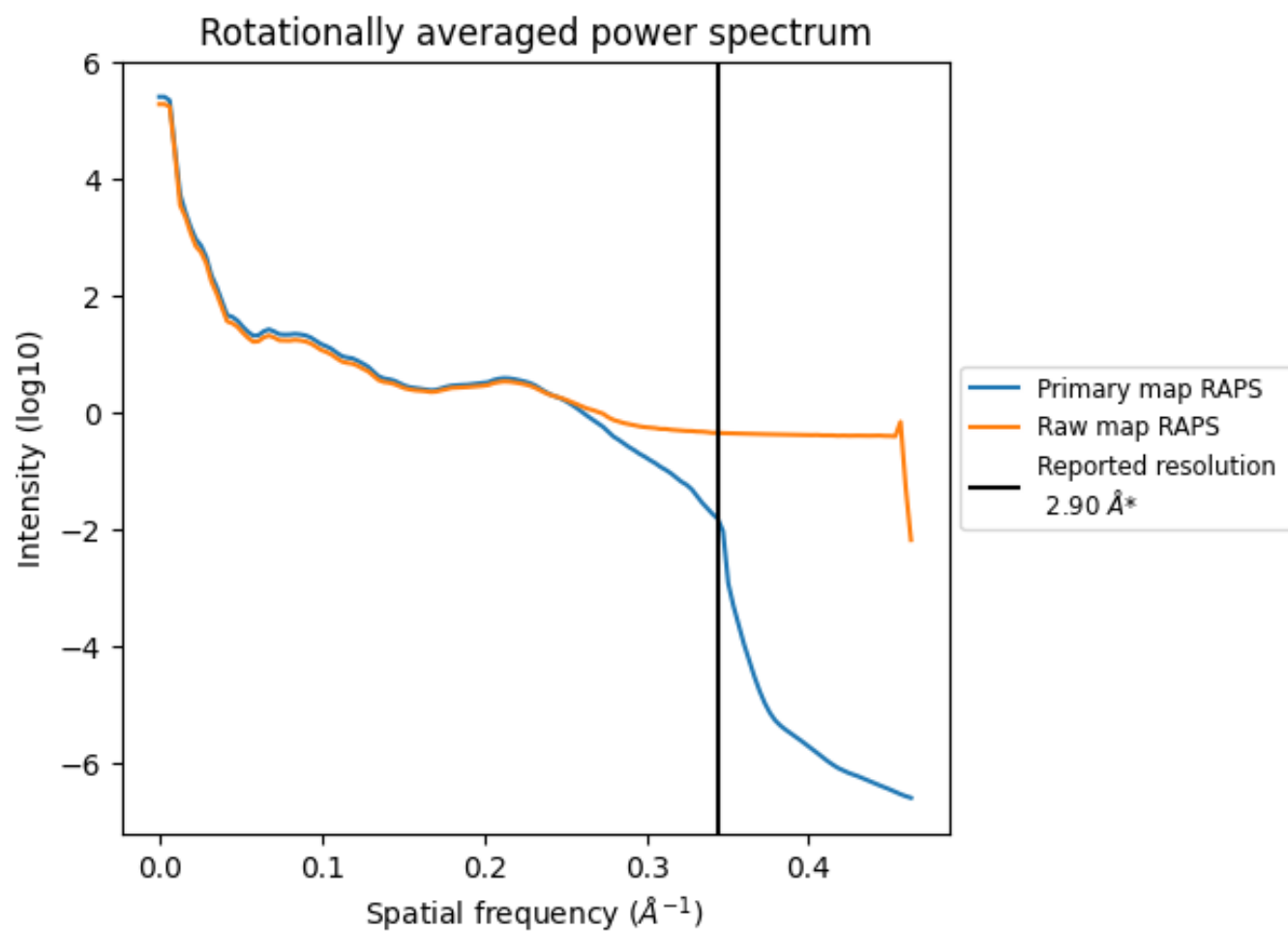
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 242 nm³; this corresponds to an approximate mass of 219 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 ⓘ

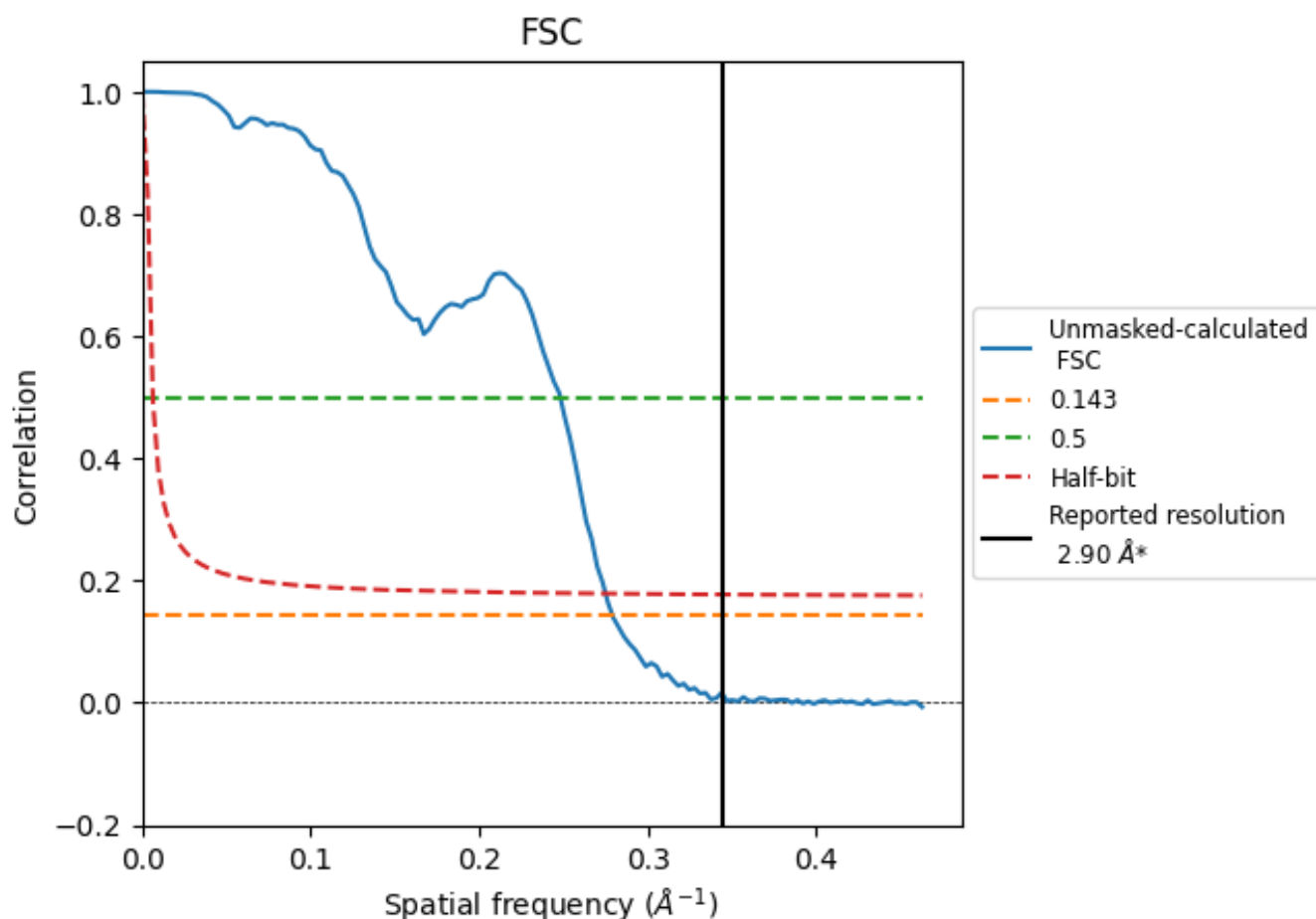


*Reported resolution corresponds to spatial frequency of 0.345 \AA^{-1}

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

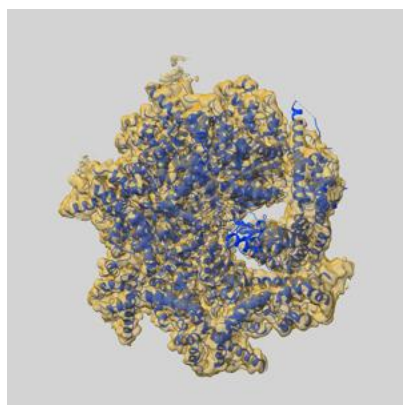
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.58	4.03	3.64

*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 3.58 differs from the reported value 2.9 by more than 10 %

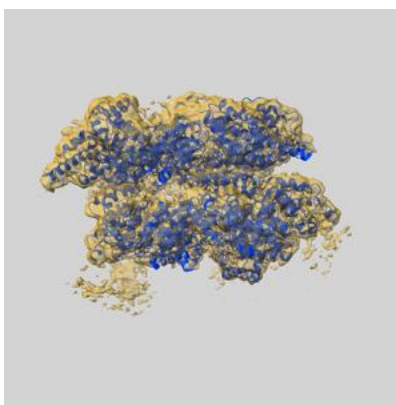
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42076 and PDB model 8UB4. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

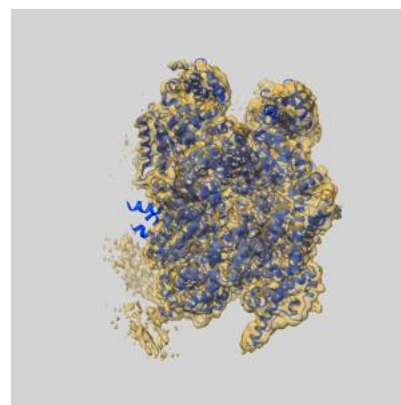
9.1 Map-model overlay [i](#)



X



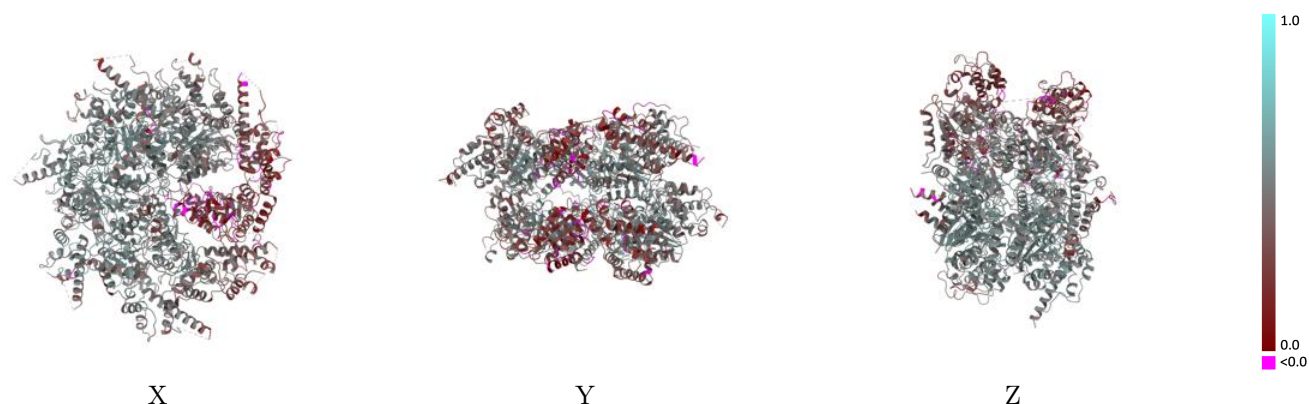
Y



Z

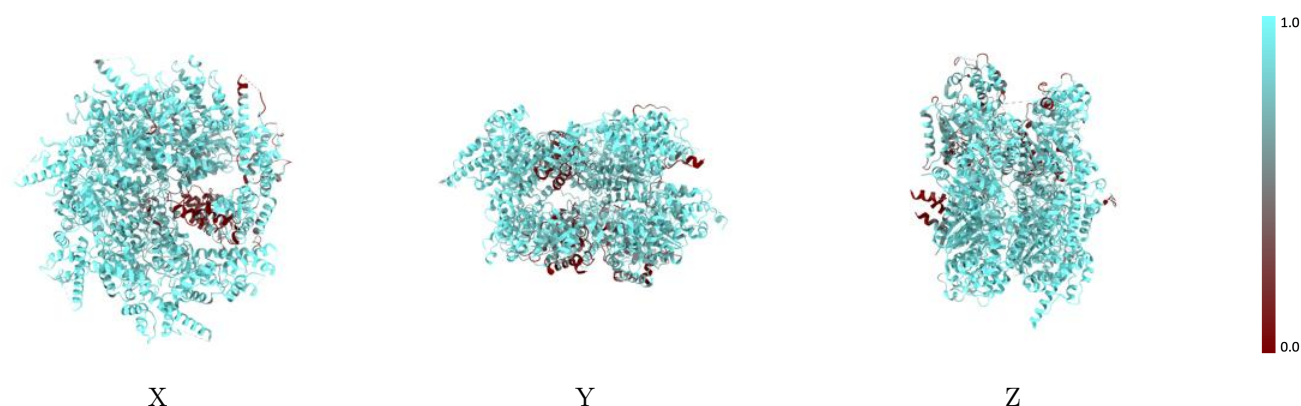
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



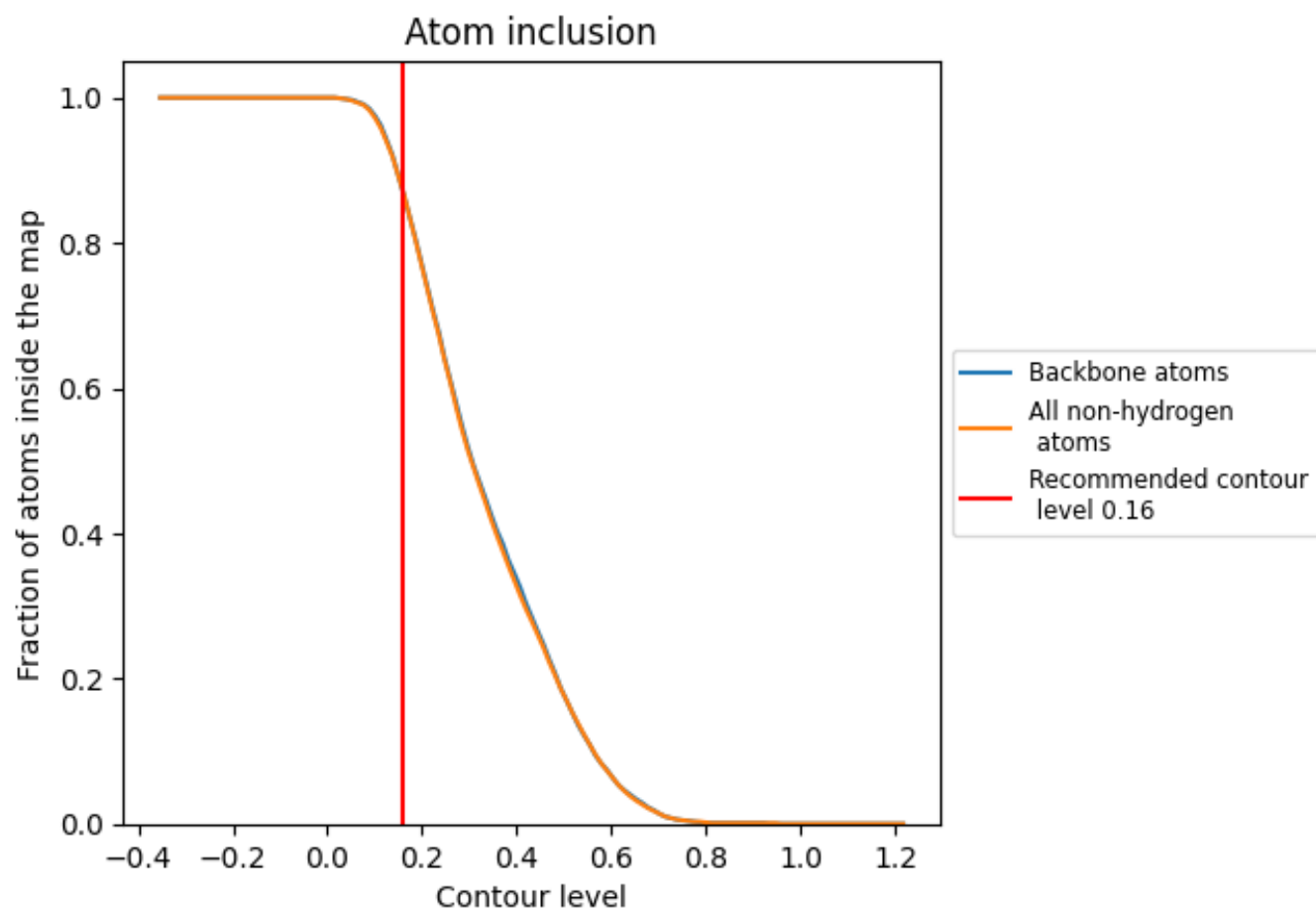
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 87% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8700	<div></div> 0.4550
A	<div></div> 0.8600	<div></div> 0.4400
B	<div></div> 0.9260	<div></div> 0.5070
C	<div></div> 0.9430	<div></div> 0.5240
D	<div></div> 0.9370	<div></div> 0.5080
E	<div></div> 0.8960	<div></div> 0.4470
F	<div></div> 0.5870	<div></div> 0.1900
G	<div></div> 0.8310	<div></div> 0.5200
H	<div></div> 0.1140	<div></div> 0.2990
I	<div></div> 0.4040	<div></div> 0.4350
J	<div></div> 0.2840	<div></div> 0.4520

1.0
0.0
<0.0