wwPDB EM Validation Summary Report (i)

Aug 5, 2026 – 01:24 AM EDT

PDB ID	:	6WWK / pdb_00006wwk
EMDB ID	:	EMD-21938
Title	:	KIF14[391-755] dimer two-heads-bound state - ADP-AlFx in complex with a microtubule
Authors	:	Benoit, M.P.M.H.; Asenjo, A.B.; Paydar, M.; Dhakal, S.; Kwok, B.; Sosa, H.
Deposited on	:	2020-05-09
Resolution	:	3.00 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 (i) 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 (i)) were used in the production of this report:

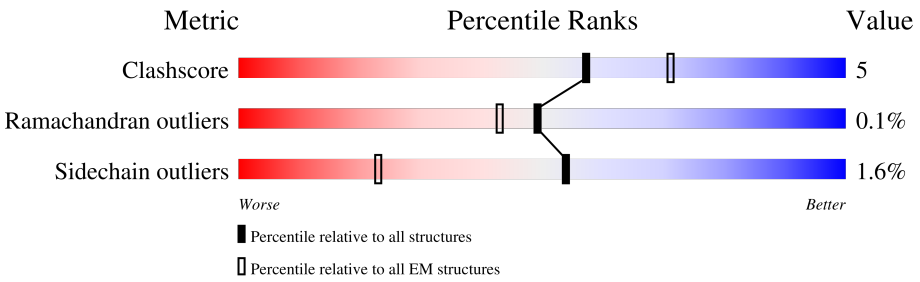
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

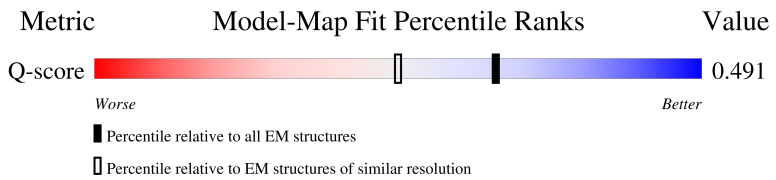
1 Overall quality at a glance (i)

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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 <=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	451	88% 9% •
1	E	451	88% 9% • •
2	B	445	88% 8% •
2	I	445	88% 8% •

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Mol	Chain	Length	Quality of chain
3	K	370	8% 90% 9%
3	N	370	12% 89% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	TA1	B	502	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 19698 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 Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	441	3446	2180	585	659	22	0	0
1	E	441	3458	2189	586	661	22	1	0

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	429	3376	2119	578	652	27	0	0
2	I	429	3376	2119	578	652	27	0	0

- Molecule 3 is a protein called Kinesin-like protein KIF14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	K	368	2878	1800	500	564	14	0	0
3	N	365	2860	1789	497	560	14	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-4	GLY	-	expression tag	UNP L0N7N1
K	-3	PRO	-	expression tag	UNP L0N7N1
K	-2	LEU	-	expression tag	UNP L0N7N1
K	-1	GLY	-	expression tag	UNP L0N7N1
K	0	SER	-	expression tag	UNP L0N7N1
N	386	GLY	-	expression tag	UNP L0N7N1
N	387	PRO	-	expression tag	UNP L0N7N1
N	388	LEU	-	expression tag	UNP L0N7N1
N	389	GLY	-	expression tag	UNP L0N7N1

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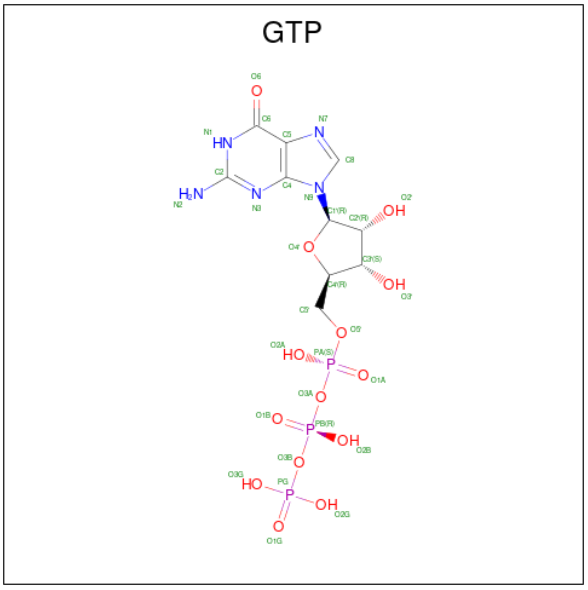
Chain	Residue	Modelled	Actual	Comment	Reference
N	390	SER	-	expression tag	UNP L0N7N1

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

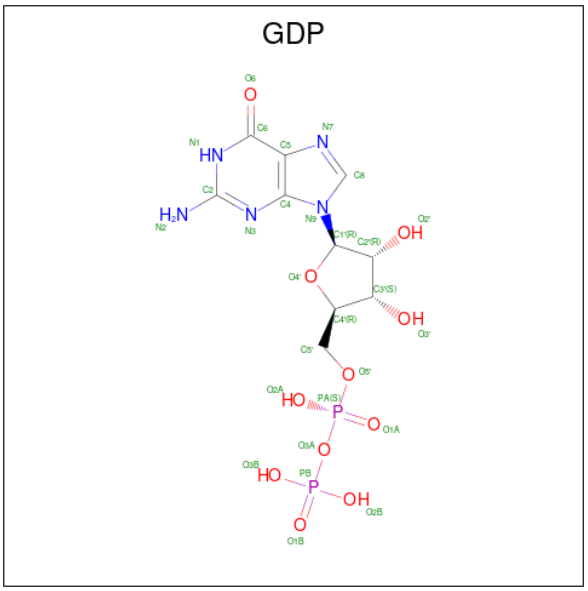


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	E	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

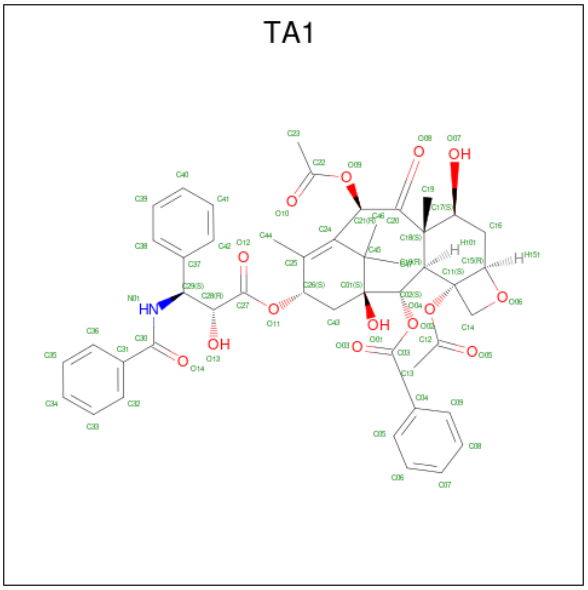
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Mg	0
			1	1	
5	E	1	Total	Mg	0
			1	1	

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



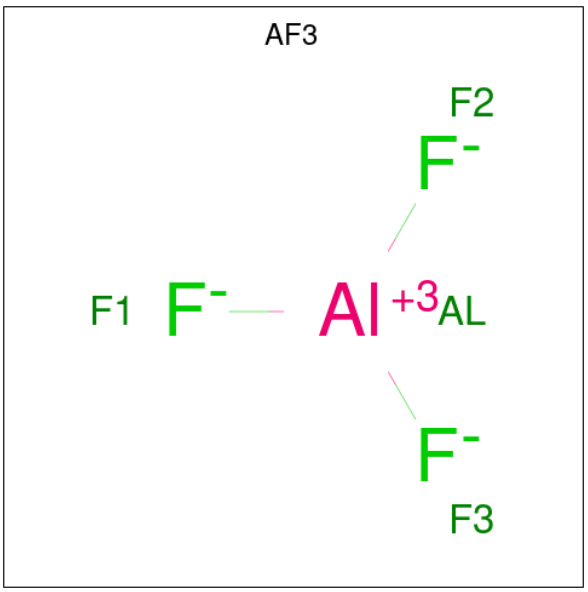
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	B	1	28	10	5	11	2	0
			Total	C	N	O	P	
6	I	1	28	10	5	11	2	0

- Molecule 7 is TAXOL (CCD ID: TA1) (formula: $C_{47}H_{51}NO_{14}$).



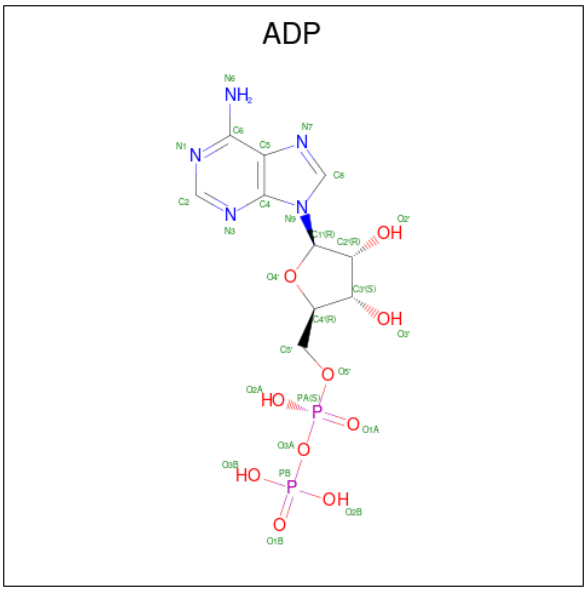
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	B	1	62	47	1	14	0
			Total	C	N	O	
7	I	1	62	47	1	14	0

- Molecule 8 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms			AltConf
			Total	Al	F	
8	K	1	4	1	3	0

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



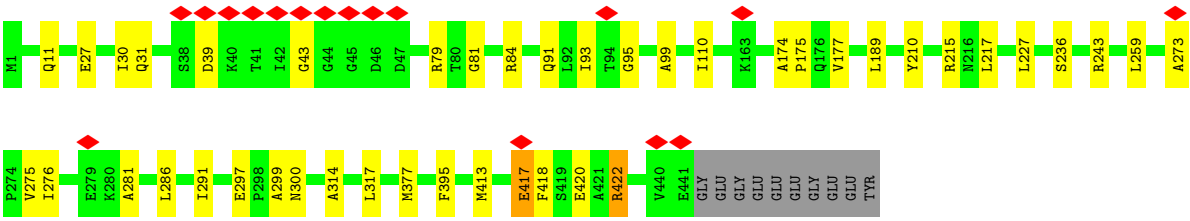
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
9	K	1	27	10	5	10	2	0
			Total	C	N	O	P	
9	N	1	27	10	5	10	2	0

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.

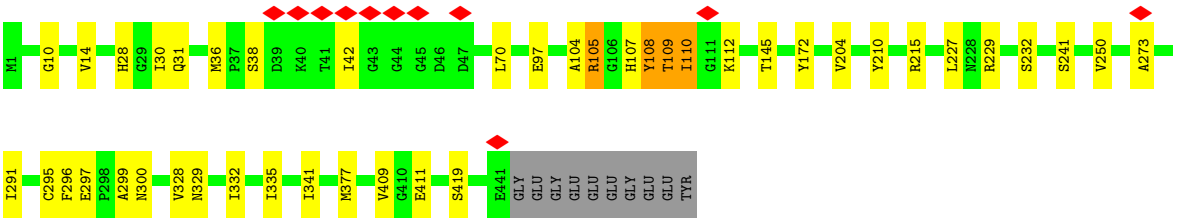
- Molecule 1: Tubulin alpha-1B chain

Chain A:



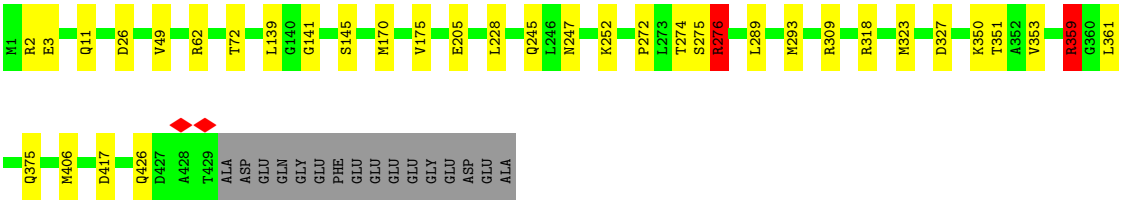
- Molecule 1: Tubulin alpha-1B chain

Chain E:



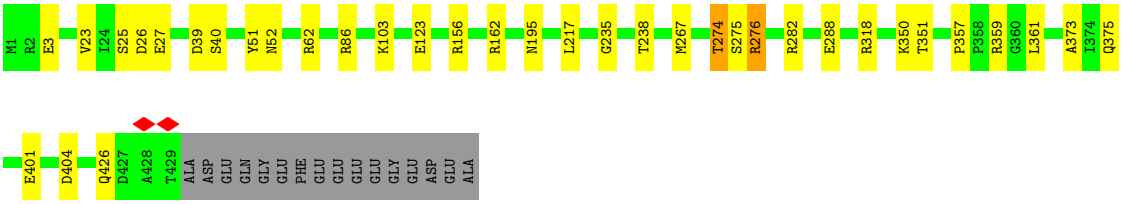
- Molecule 2: Tubulin beta-2B chain

Chain B:



- Molecule 2: Tubulin beta-2B chain

Chain I:

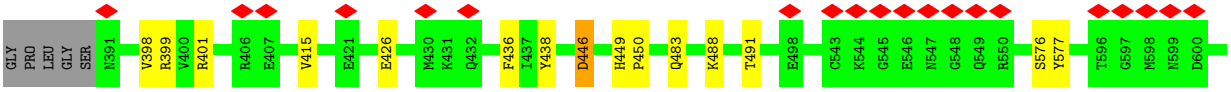


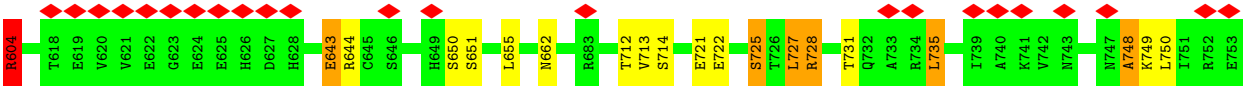
- Molecule 3: Kinesin-like protein KIF14

Chain K:

- Molecule 3: Kinesin-like protein KIF14

Chain N:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=168.07°, rise=5.45 Å, axial sym=C1	Depositor
Number of segments used	146982	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 ($e^-/Å^2$)	73.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	58962	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.109	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0115	Depositor
Map size (Å)	352.768, 352.768, 352.768	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.848, 0.848, 0.848	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: TA1, MG, AF3, ADP, GDP, GTP

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	0.31	0/3524	0.46	1/4784 (0.0%)
1	E	0.35	0/3537	0.51	2/4802 (0.0%)
2	B	0.36	0/3451	0.49	0/4674
2	I	0.35	0/3451	0.50	2/4674 (0.0%)
3	K	0.28	0/2929	0.44	0/3957
3	N	0.34	0/2911	0.53	0/3933
All	All	0.33	0/19803	0.49	5/26824 (0.0%)

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	1
1	E	0	5
2	B	0	3
2	I	0	1
3	K	0	2
3	N	0	3
All	All	0	15

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	108[A]	TYR	CA-C-O	-8.39	114.99	119.77
1	E	108[B]	TYR	CA-C-O	-8.39	114.99	119.77
2	I	357	PRO	CA-C-N	7.03	126.99	120.03
2	I	357	PRO	C-N-CA	7.03	126.99	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	417	GLU	CB-CA-C	-6.65	99.75	110.79

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	422	ARG	Sidechain
2	B	276	ARG	Sidechain
2	B	318	ARG	Sidechain
2	B	359	ARG	Sidechain
3	K	604	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	A	3446	0	3355	29	0
1	E	3458	0	3363	24	0
2	B	3376	0	3257	26	0
2	I	3376	0	3257	19	0
3	K	2878	0	2856	23	0
3	N	2860	0	2834	40	0
4	A	32	0	12	1	0
4	E	32	0	12	0	0
5	A	1	0	0	0	0
5	E	1	0	0	0	0
6	B	28	0	12	0	0
6	I	28	0	12	0	0
7	B	62	0	51	21	0
7	I	62	0	51	18	0
8	K	4	0	0	1	0
9	K	27	0	12	0	0
9	N	27	0	12	0	0
All	All	19698	0	19096	187	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 187 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)
3:N:398:VAL:HG21	3:N:438:TYR:CE1	1.43	1.50
3:N:398:VAL:CG2	3:N:438:TYR:CE1	2.22	1.21
7:B:502:TA1:H142	7:B:502:TA1:H192	1.25	1.17
3:N:398:VAL:CG2	3:N:438:TYR:HE1	1.59	1.12
7:I:502:TA1:H142	7:I:502:TA1:H192	1.22	1.11

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	439/451 (97%)	427 (97%)	12 (3%)	0	100	100
1	E	440/451 (98%)	423 (96%)	16 (4%)	1 (0%)	43	76
2	B	427/445 (96%)	411 (96%)	16 (4%)	0	100	100
2	I	427/445 (96%)	412 (96%)	15 (4%)	0	100	100
3	K	366/370 (99%)	352 (96%)	14 (4%)	0	100	100
3	N	363/370 (98%)	332 (92%)	30 (8%)	1 (0%)	36	70
All	All	2462/2532 (97%)	2357 (96%)	103 (4%)	2 (0%)	49	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	N	749	LYS
1	E	109	THR

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	A	372/379 (98%)	371 (100%)	1 (0%)	86	91
1	E	373/379 (98%)	368 (99%)	5 (1%)	61	81
2	B	371/383 (97%)	365 (98%)	6 (2%)	55	79
2	I	371/383 (97%)	363 (98%)	8 (2%)	45	74
3	K	320/321 (100%)	316 (99%)	4 (1%)	61	81
3	N	318/321 (99%)	307 (96%)	11 (4%)	32	65
All	All	2125/2166 (98%)	2090 (98%)	35 (2%)	54	79

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	N	651	SER
3	N	655	LEU
3	N	728	ARG
1	E	109	THR
1	E	105	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
3	N	483	GLN
3	N	719	ASN
3	K	581	GLN
3	K	626	HIS
3	K	628	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 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
6	GDP	B	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.78	7 (15%)
4	GTP	A	501	5	33,34,34	0.85	0	50,54,54	1.61	8 (16%)
9	ADP	N	801	-	28,29,29	1.40	4 (14%)	43,45,45	1.88	10 (23%)
6	GDP	I	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
9	ADP	K	801	8	28,29,29	1.36	5 (17%)	43,45,45	1.86	11 (25%)
4	GTP	E	501	5	33,34,34	0.87	0	50,54,54	1.62	8 (16%)
7	TA1	B	502	-	68,68,68	1.63	9 (13%)	105,105,105	2.11	27 (25%)
8	AF3	K	800	9,3	0,3,3	-	-	-		
7	TA1	I	502	-	68,68,68	1.66	11 (16%)	105,105,105	2.03	27 (25%)

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
6	GDP	B	501	-	-	5/16/32/32	0/3/3/3
4	GTP	A	501	5	-	8/22/38/38	0/3/3/3
9	ADP	N	801	-	-	5/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GDP	I	501	-	-	5/16/32/32	0/3/3/3
9	ADP	K	801	8	-	3/16/32/32	0/3/3/3
4	GTP	E	501	5	-	3/22/38/38	0/3/3/3
7	TA1	B	502	-	-	18/41/127/127	0/7/7/7
7	TA1	I	502	-	-	14/41/127/127	0/7/7/7

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	502	TA1	O02-C03	5.34	1.45	1.34
7	I	502	TA1	O02-C03	5.13	1.45	1.34
7	B	502	TA1	O09-C22	4.90	1.46	1.35
7	I	502	TA1	O09-C22	4.85	1.45	1.35
7	I	502	TA1	O04-C12	4.84	1.45	1.35

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	502	TA1	C16-C15-C11	-7.23	109.80	119.63
7	B	502	TA1	C01-C02-C10	-7.18	107.45	118.19
7	B	502	TA1	C16-C15-C11	-6.48	110.81	119.63
6	B	501	GDP	C5-C4-N3	-6.20	118.53	128.39
6	I	501	GDP	C5-C4-N3	-6.11	118.66	128.39

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	GTP	C5'-O5'-PA-O3A
4	A	501	GTP	C5'-O5'-PA-O1A
4	A	501	GTP	C5'-O5'-PA-O2A
4	E	501	GTP	C5'-O5'-PA-O3A
4	E	501	GTP	C5'-O5'-PA-O2A

There are no ring outliers.

4 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	GTP	1	0
7	B	502	TA1	21	0

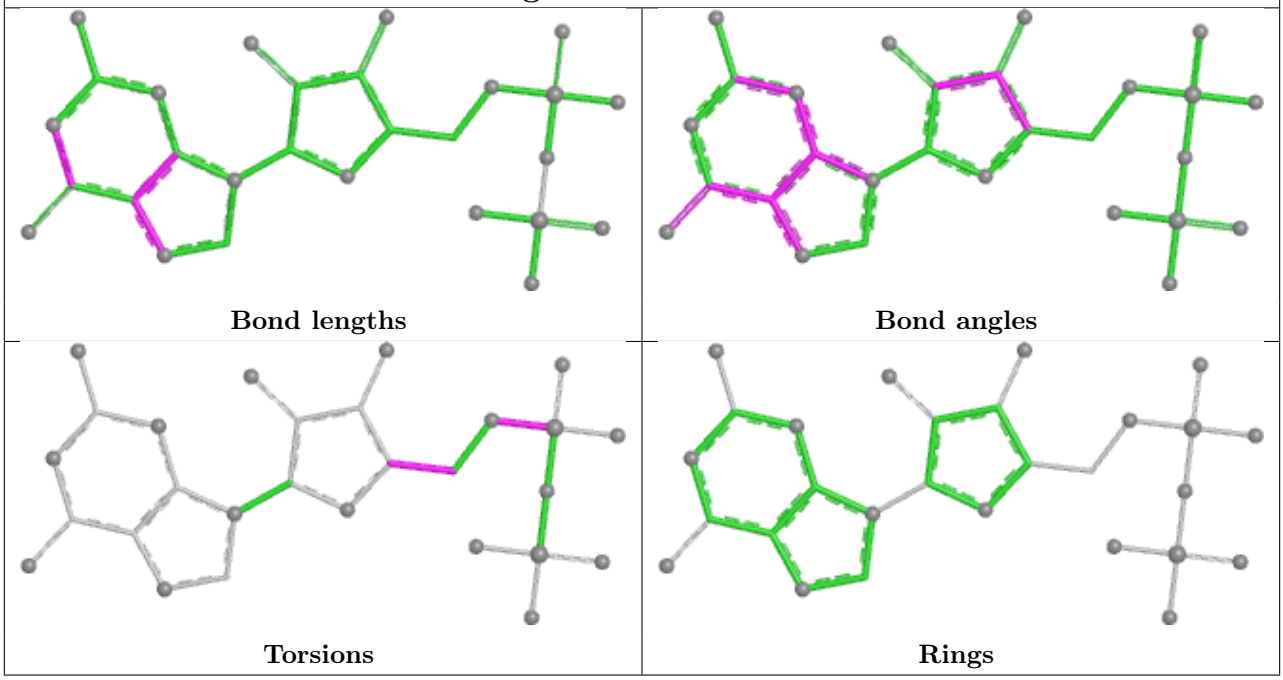
Continued on next page...

Continued from previous page...

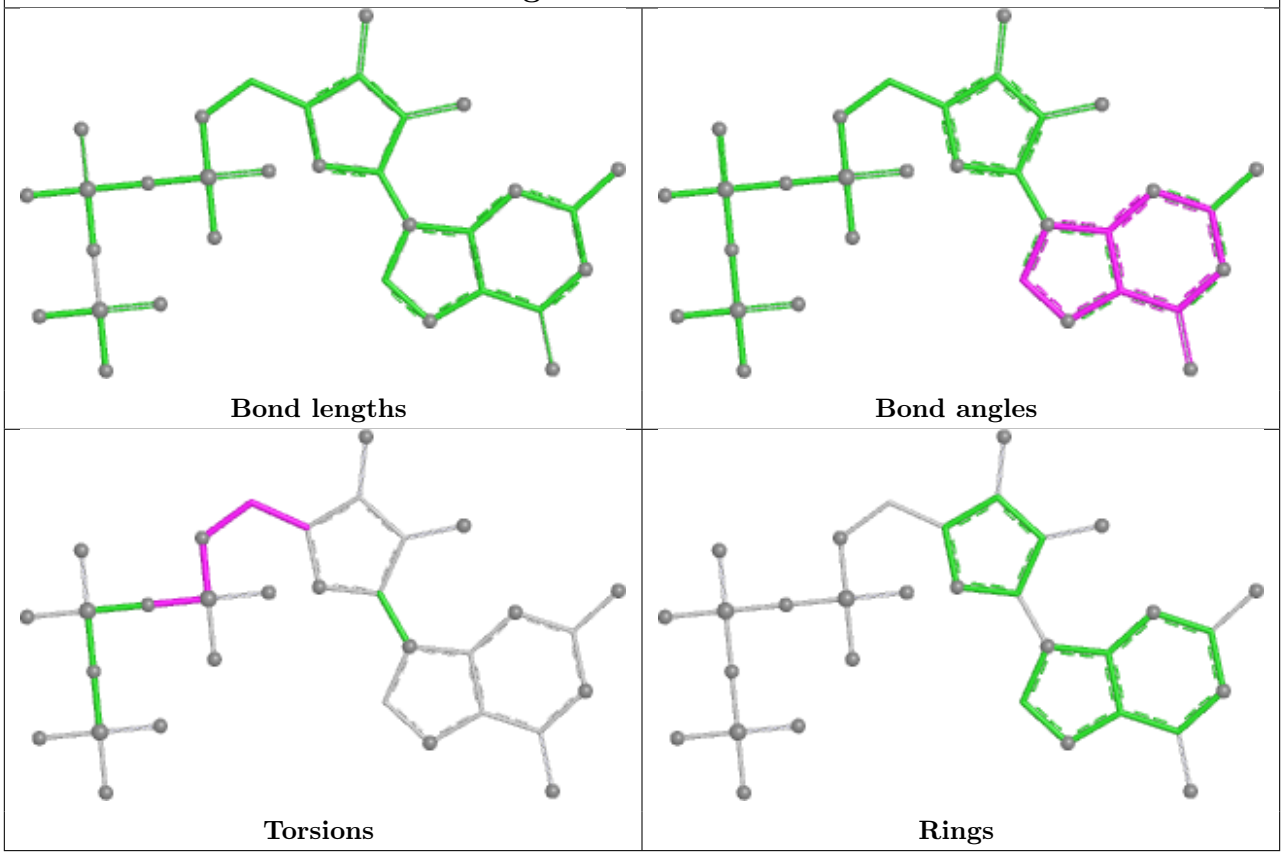
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	K	800	AF3	1	0
7	I	502	TA1	18	0

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 then 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.

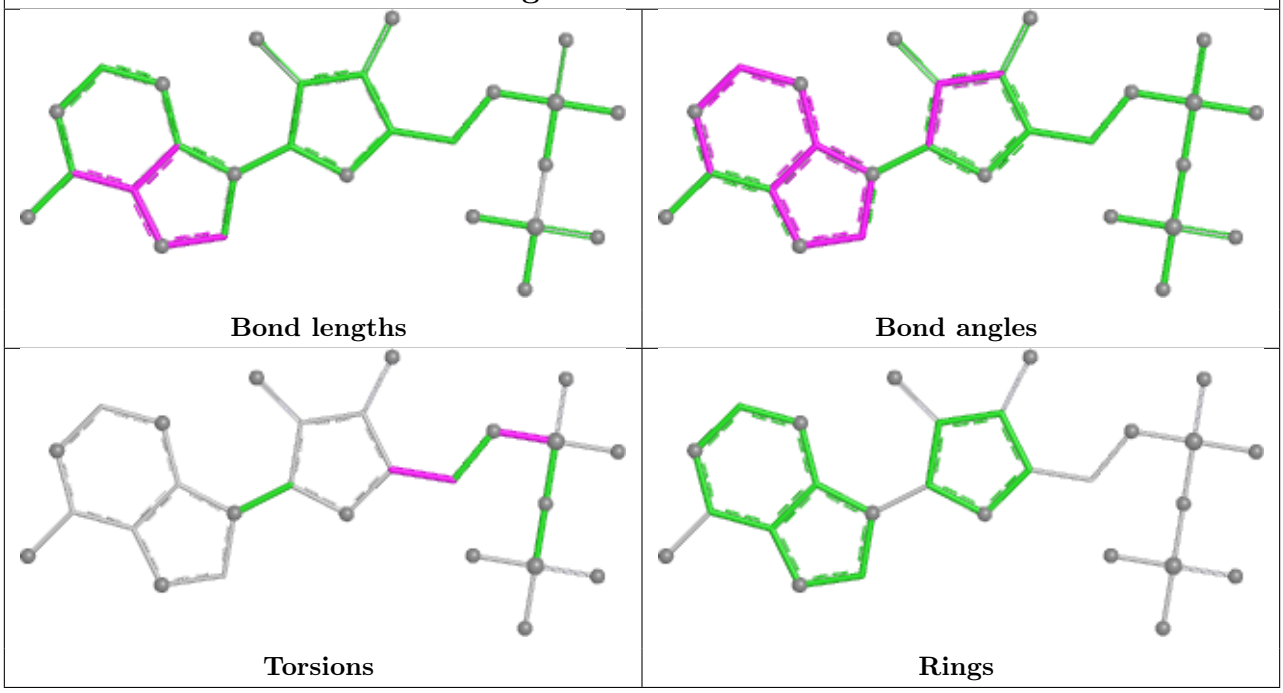
Ligand GDP B 501

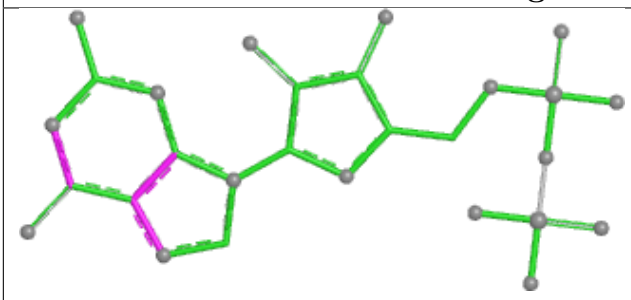
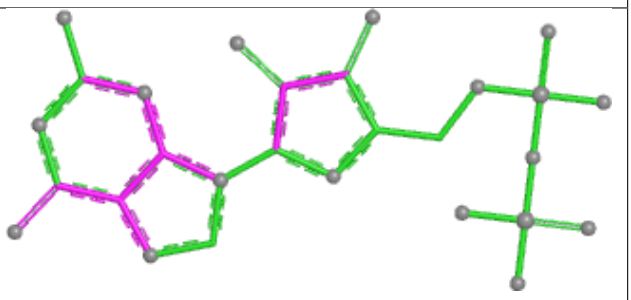
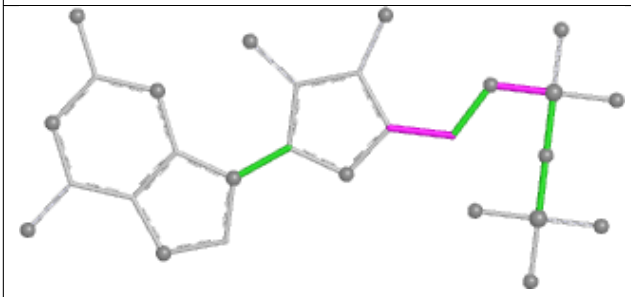
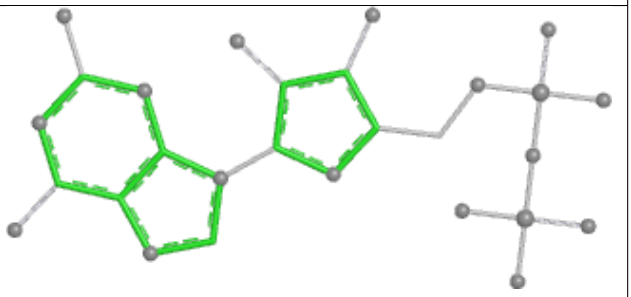


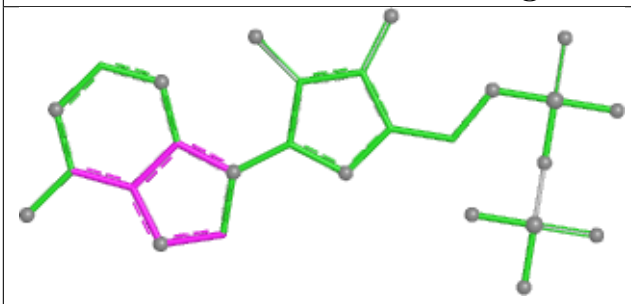
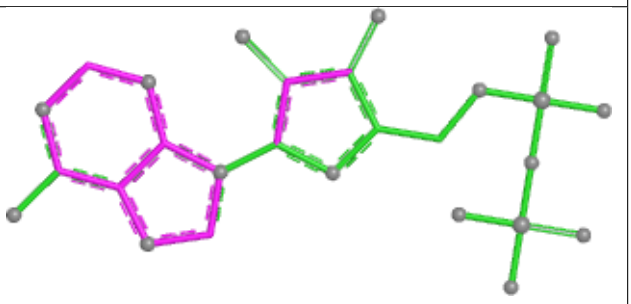
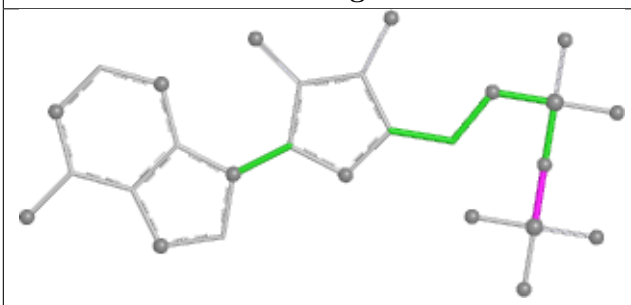
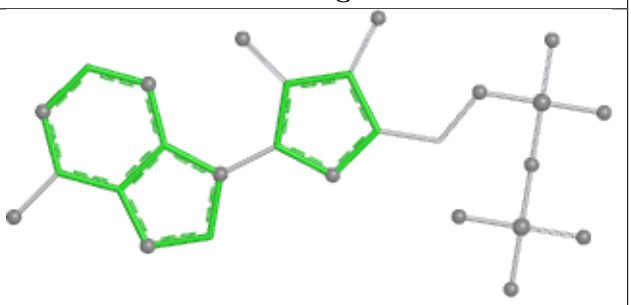
Ligand GTP A 501



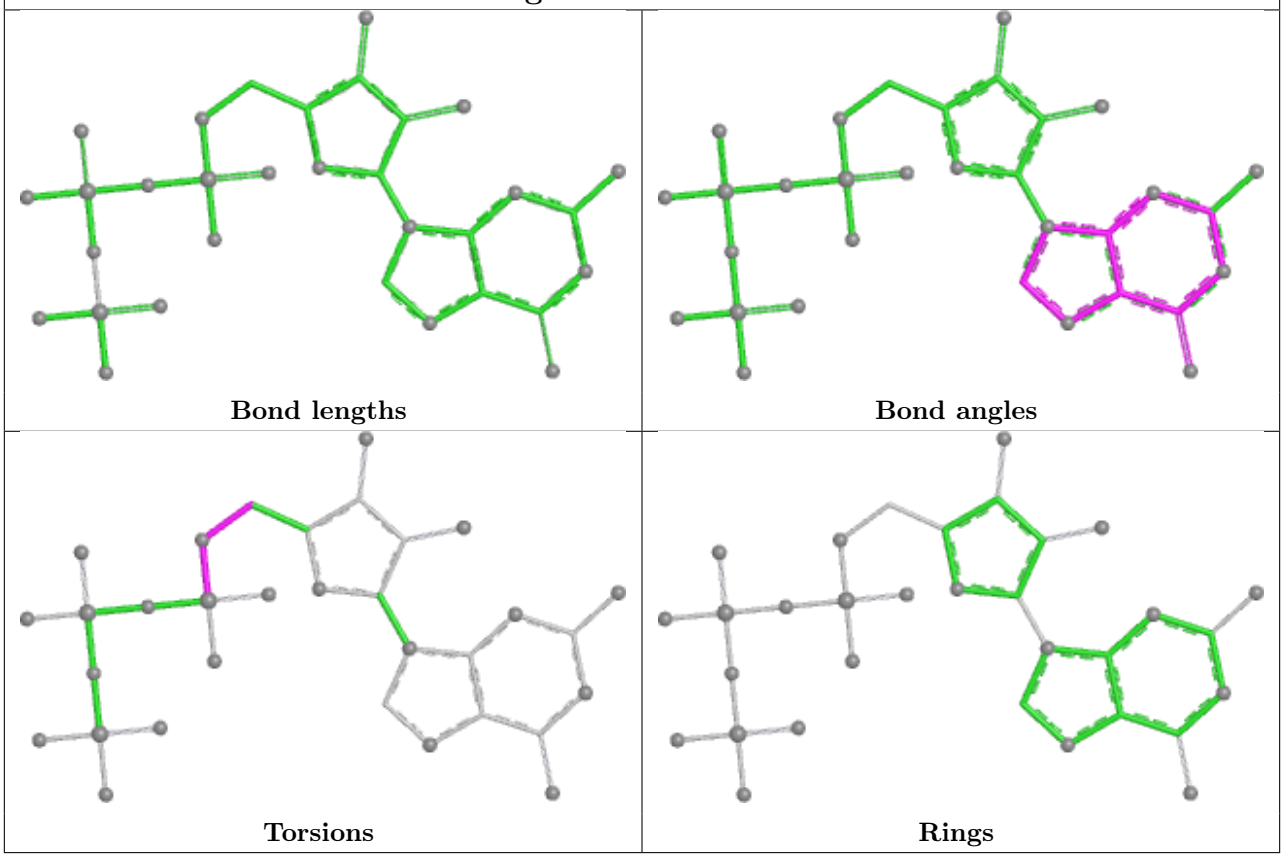
Ligand ADP N 801

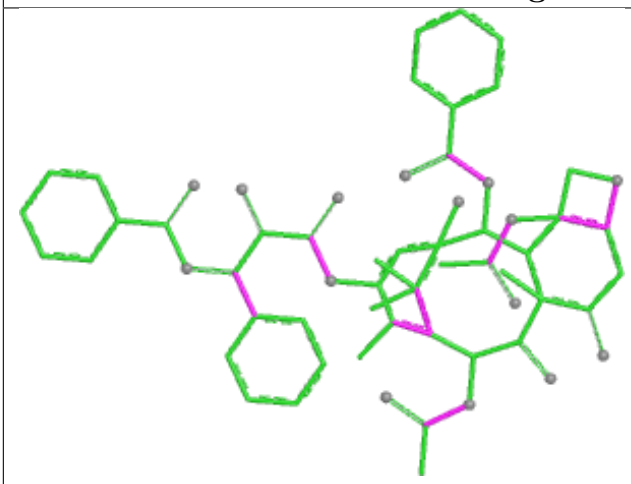
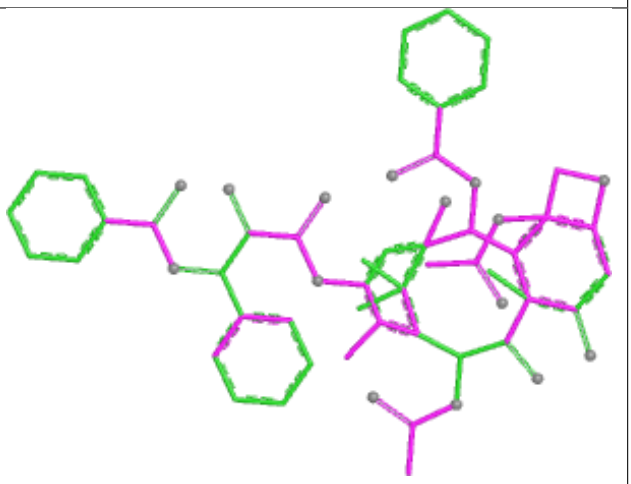
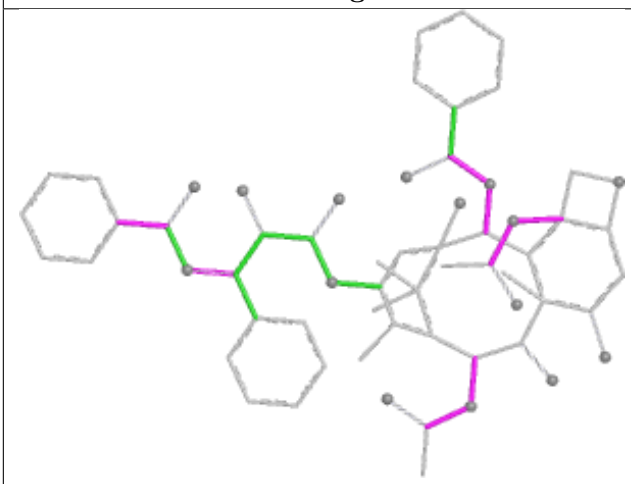
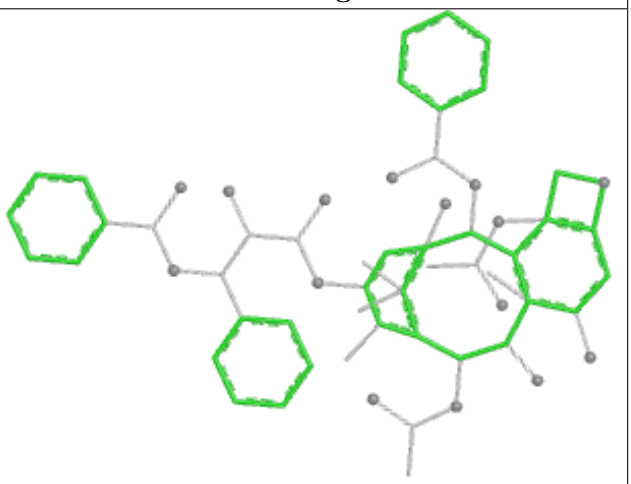


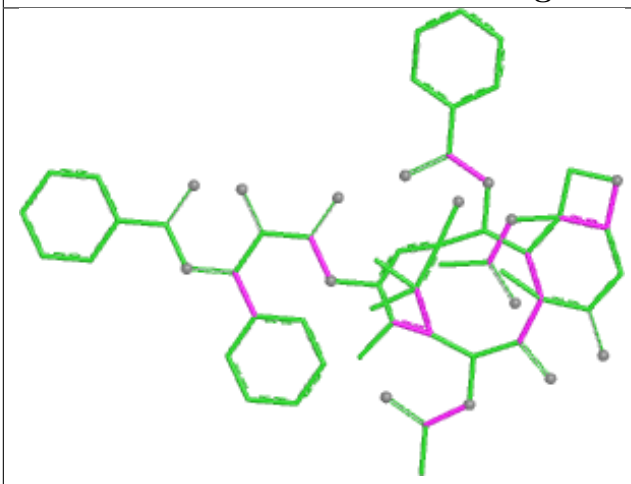
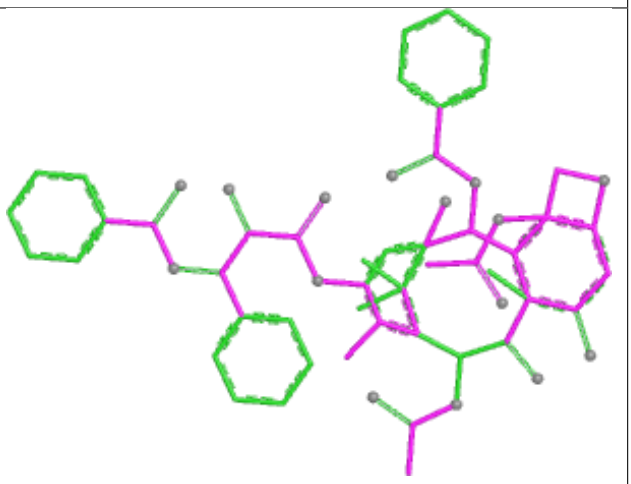
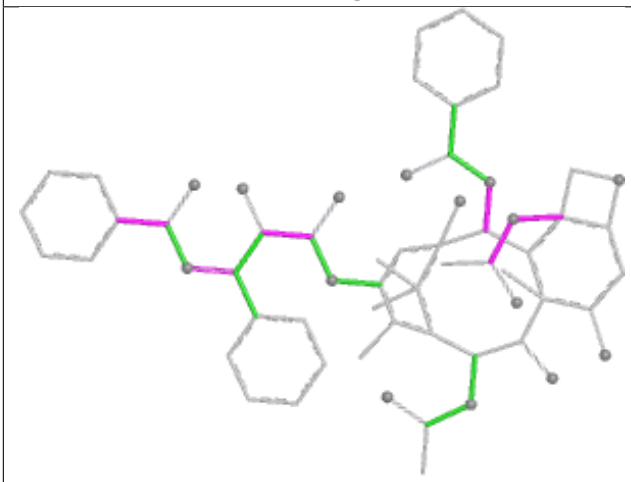
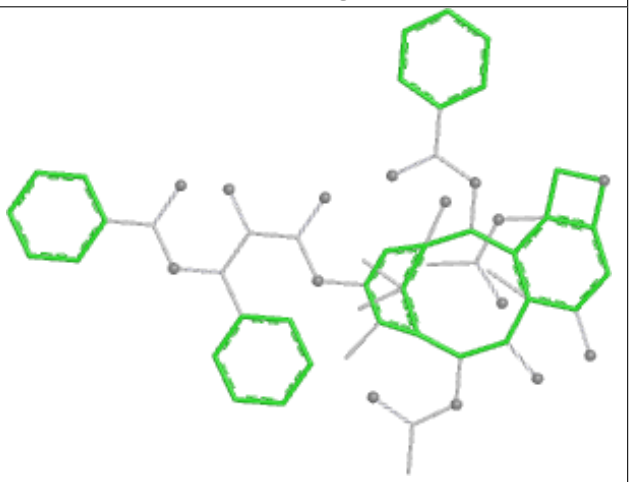
Ligand GDP I 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP K 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GTP E 501



Ligand TA1 B 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand TA1 I 502	
 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.

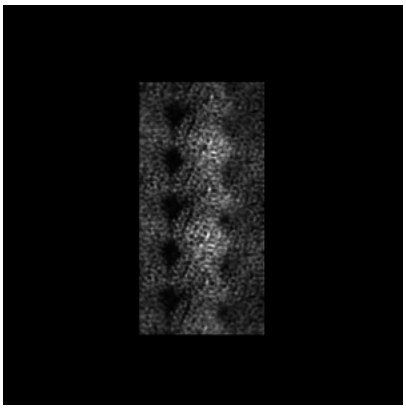
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-21938. These allow visual inspection of the internal detail of the map and identification of artifacts.

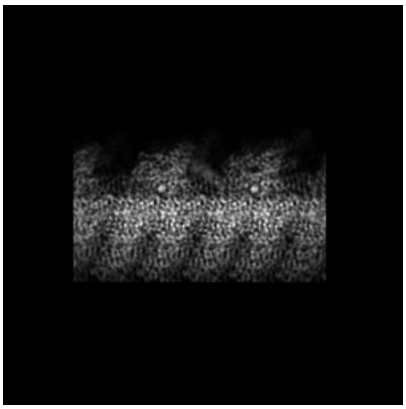
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

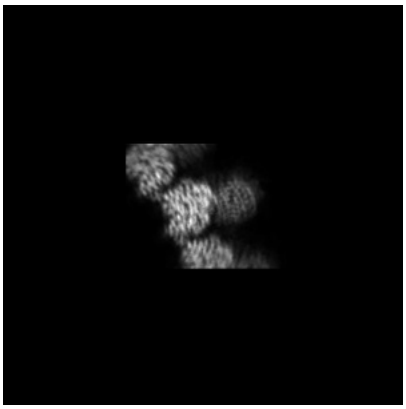
6.1.1 Primary map



X

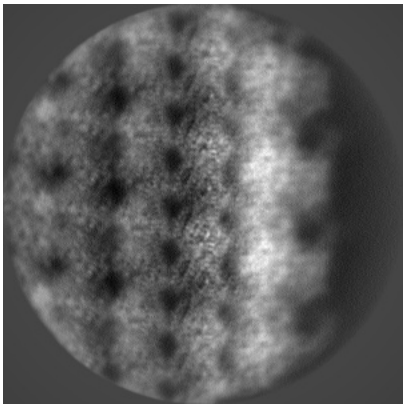


Y

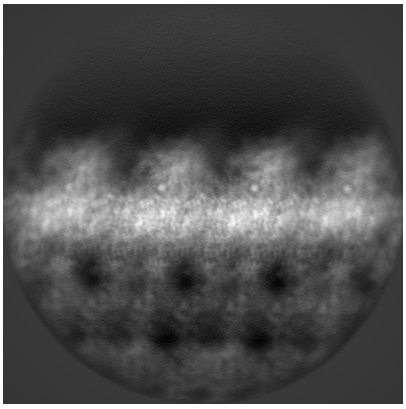


Z

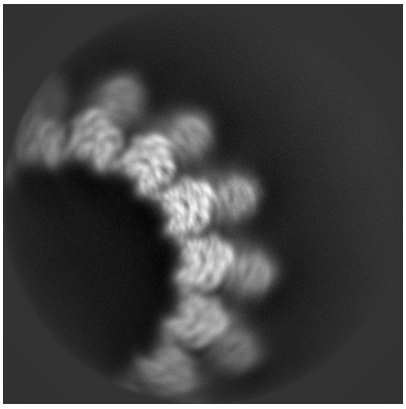
6.1.2 Raw map



X



Y

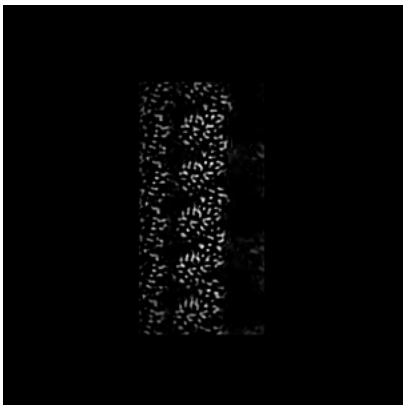


Z

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

6.2 Central slices (i)

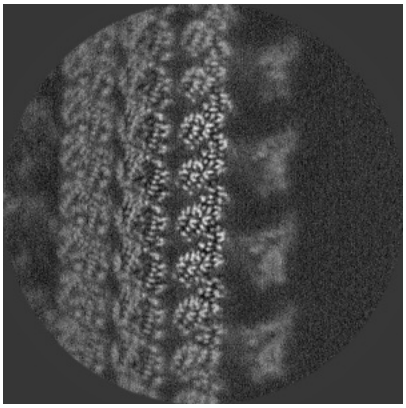
6.2.1 Primary map

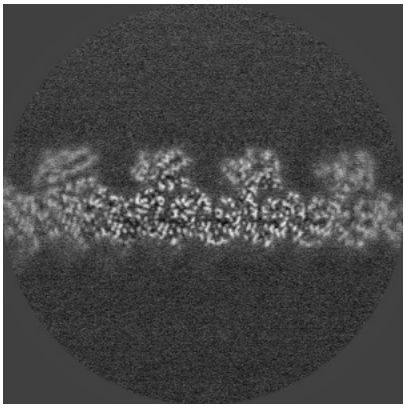

X Index: 208

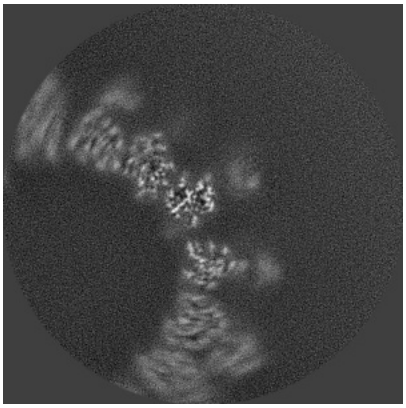
Y Index: 208

Z Index: 208

6.2.2 Raw map


X Index: 208


Y Index: 208

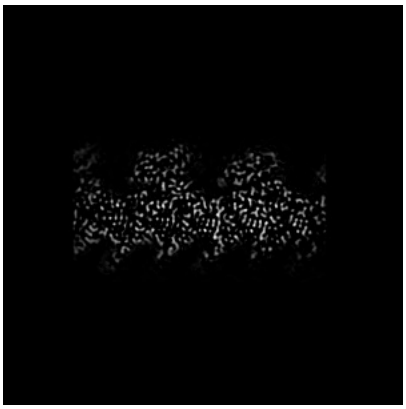

Z Index: 208

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

6.3 Largest variance slices (i)

6.3.1 Primary map

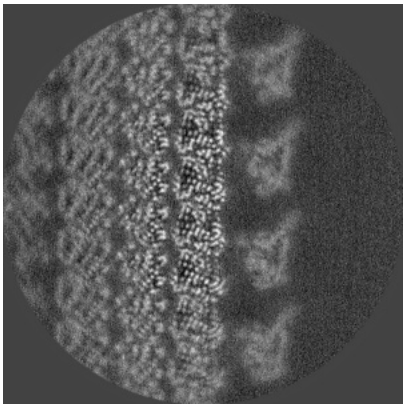
X Index: 199



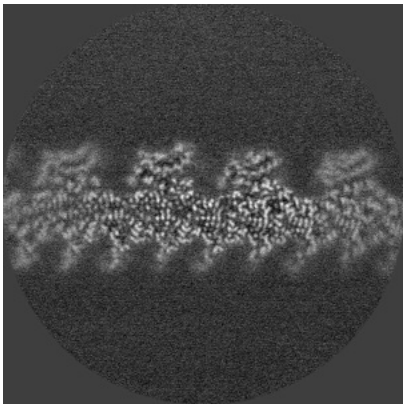
Y Index: 214

Z Index: 176

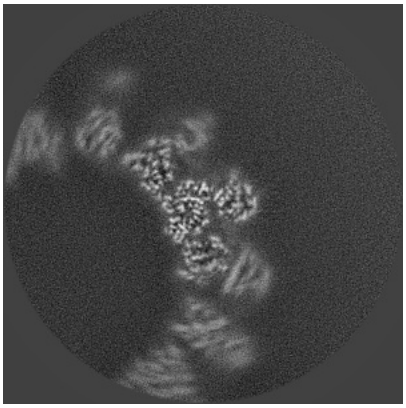
6.3.2 Raw map



X Index: 199



Y Index: 216

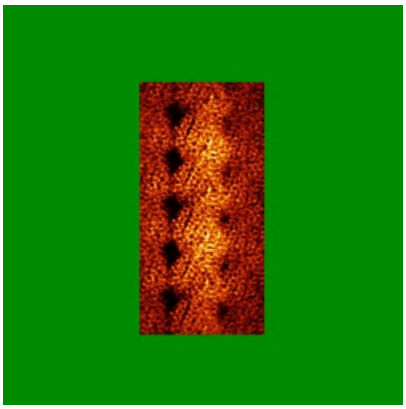


Z Index: 176

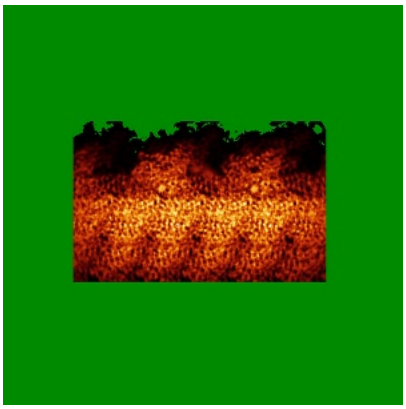
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

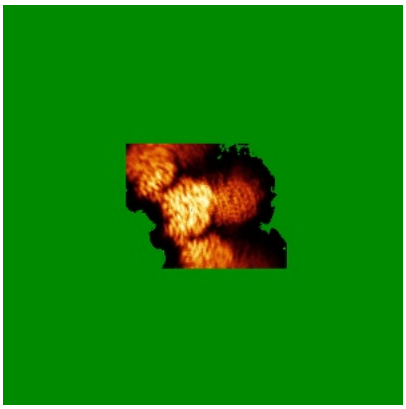
6.4.1 Primary map



X

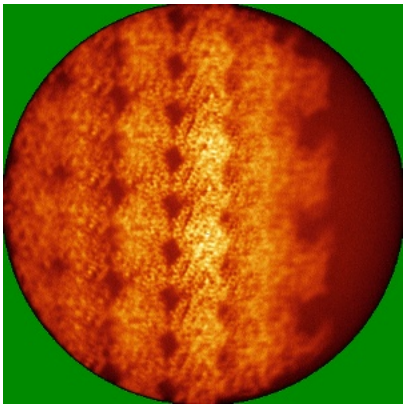


Y

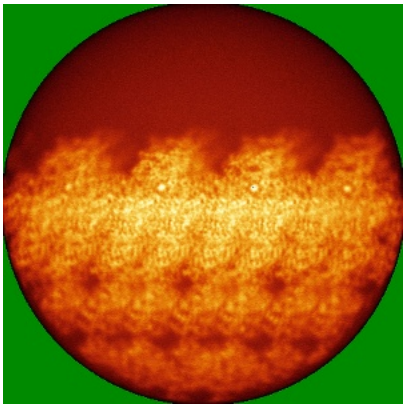


Z

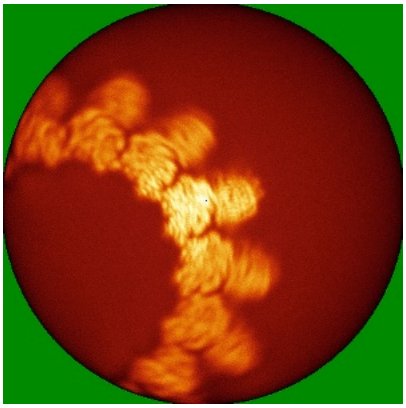
6.4.2 Raw map



X



Y

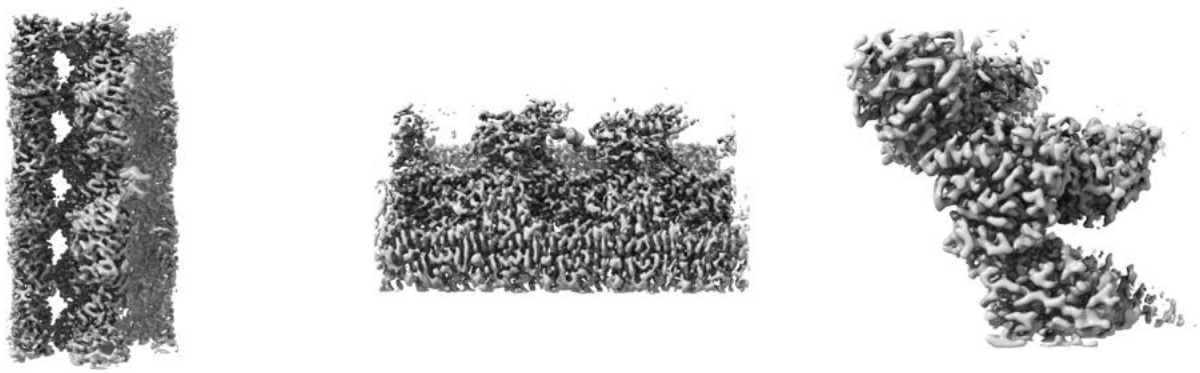


Z

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)

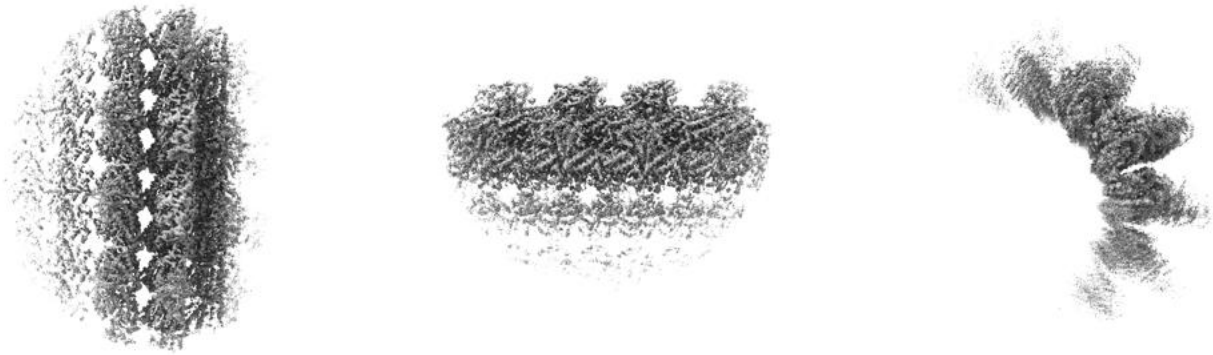
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0115. 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



X Y Z

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.

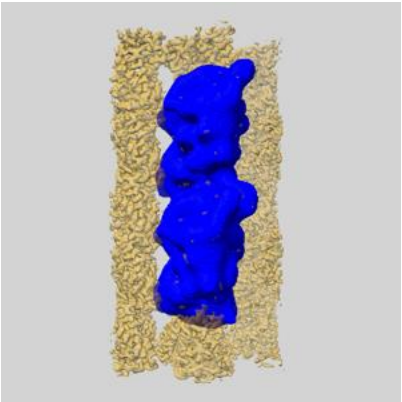
6.6 Mask visualisation (i)

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

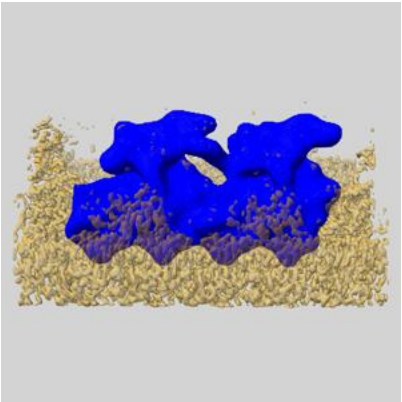
A mask typically either:

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

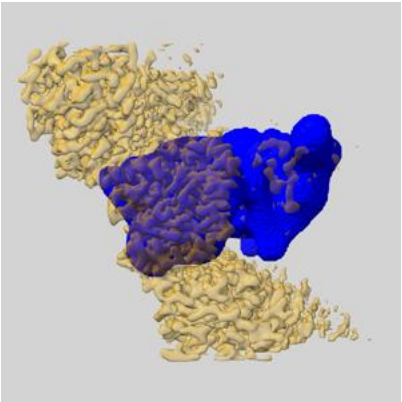
6.6.1 emd_21938_msk_4.map (i)



X

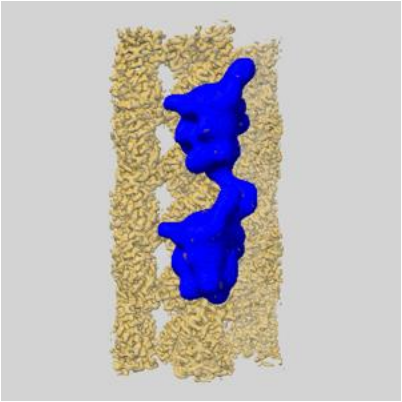


Y

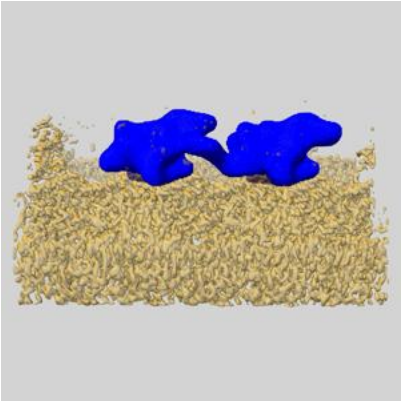


Z

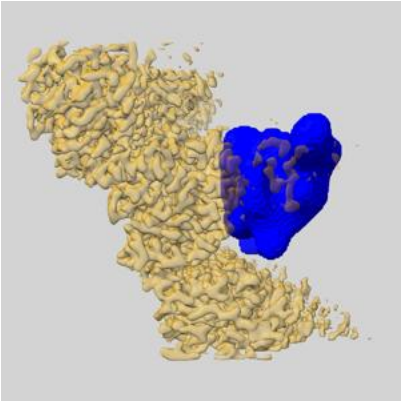
6.6.2 emd_21938_msk_3.map (i)



X

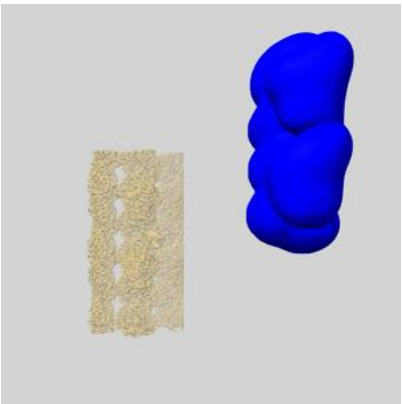


Y



Z

6.6.3 emd_21938_msk_7.map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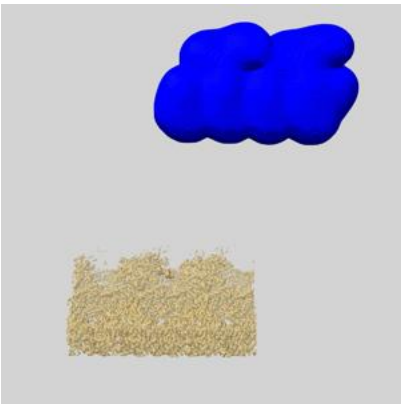
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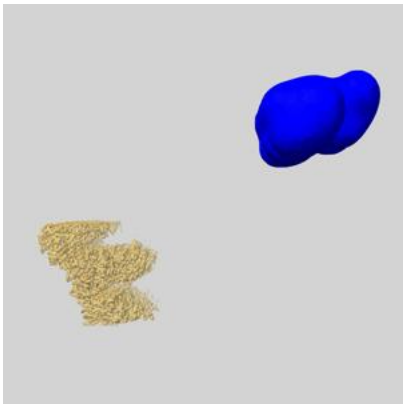
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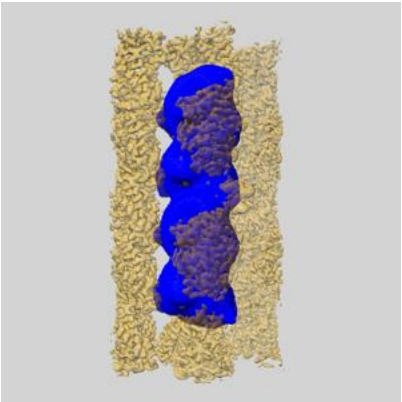
6.6.4 emd_21938_msk_6.map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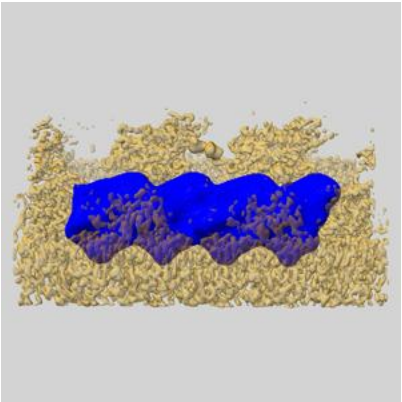
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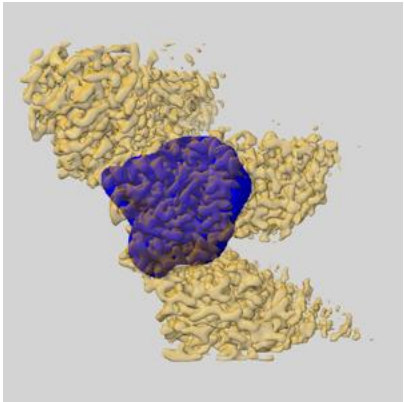
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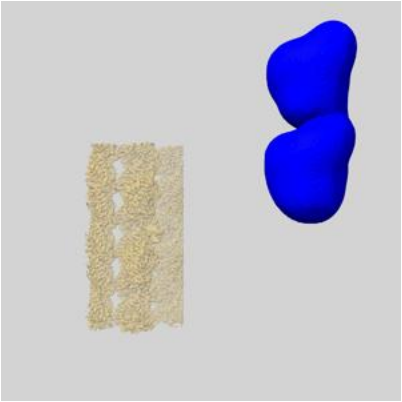
6.6.5 emd_21938_msk_5.map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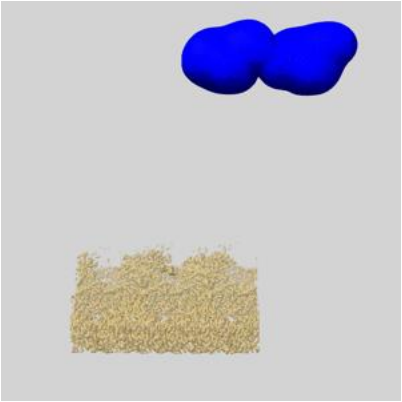
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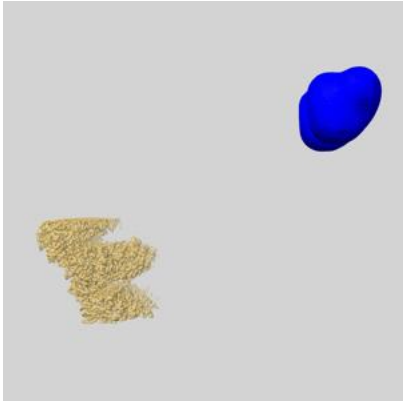
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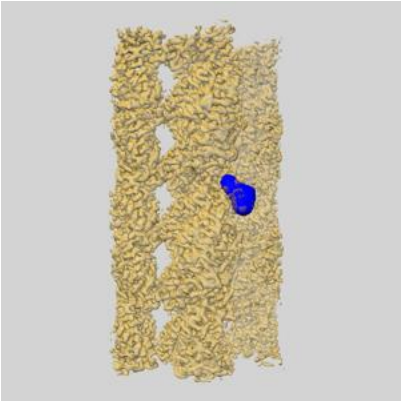
6.6.6 emd_21938_msk_2.map (i)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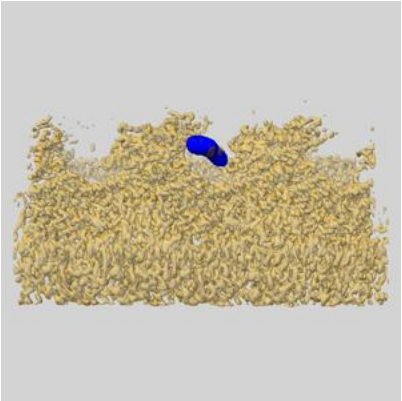
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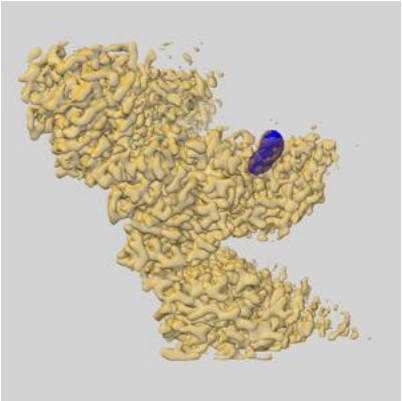
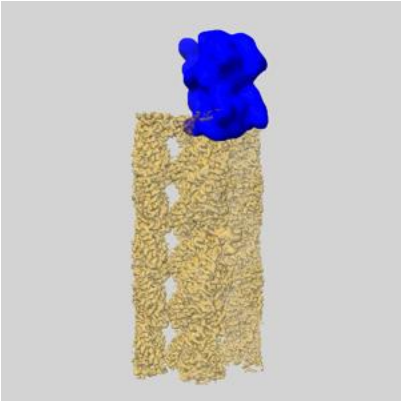

Z

6.6.7 emd_21938_msk_1.map (i)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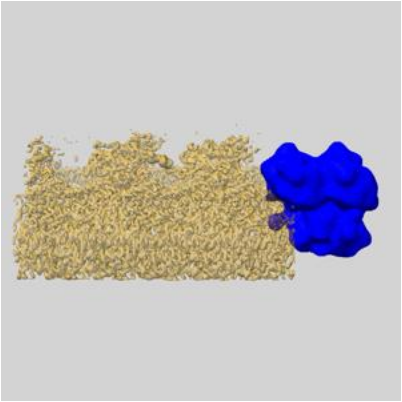
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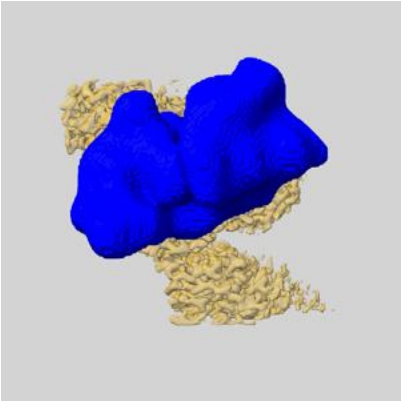
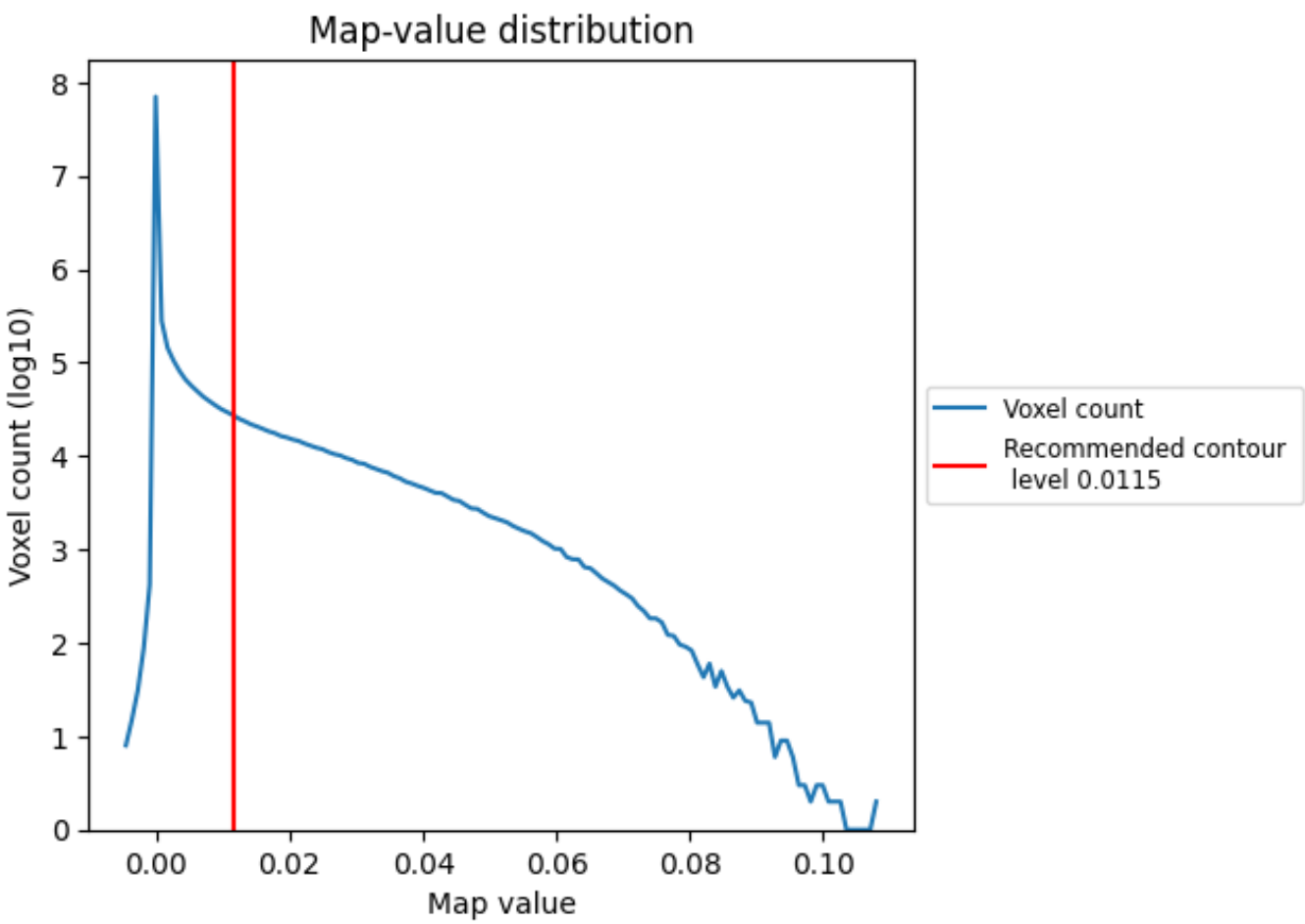

Z

7 Map analysis (i)

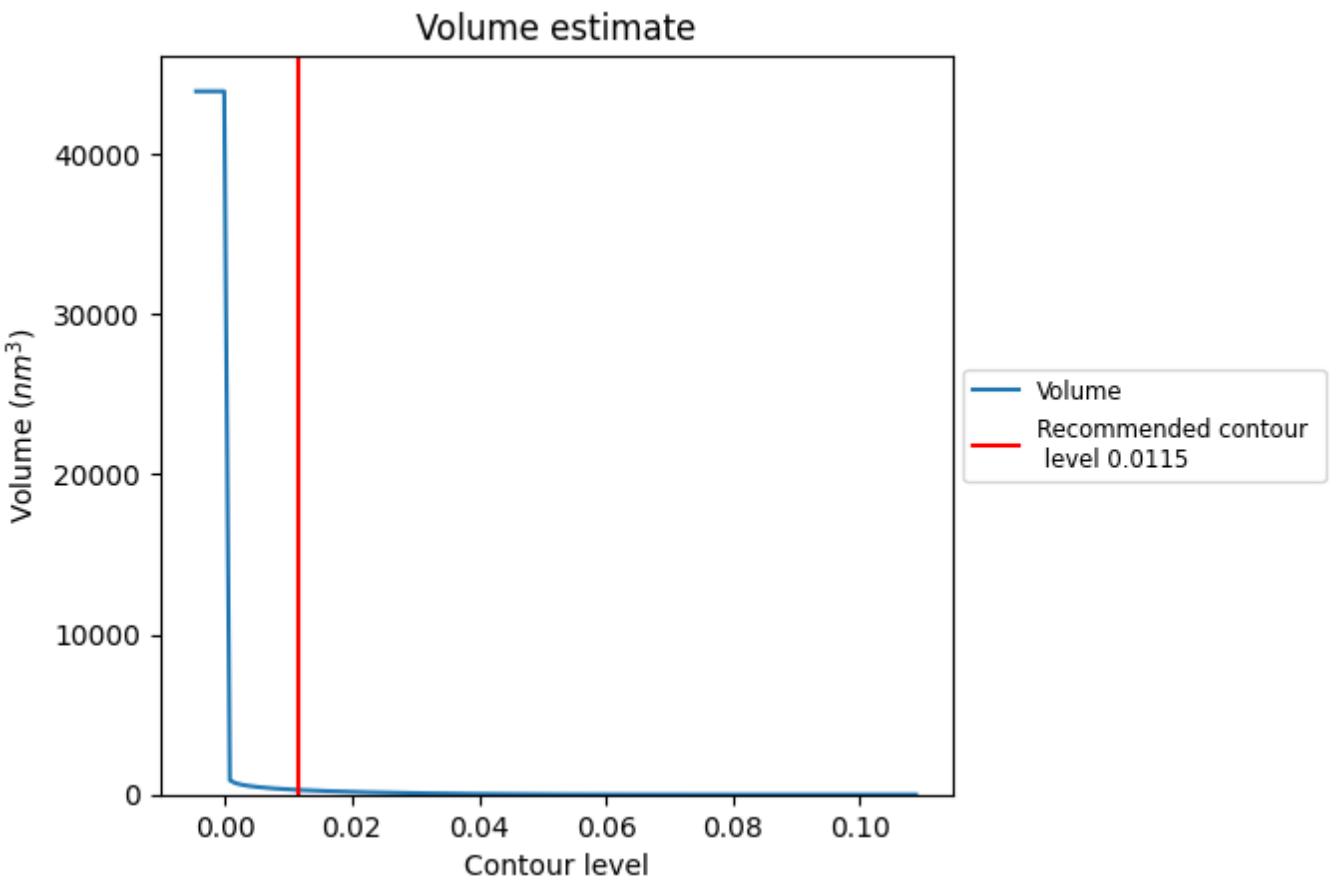
This section contains the results of statistical analysis of the map.

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.

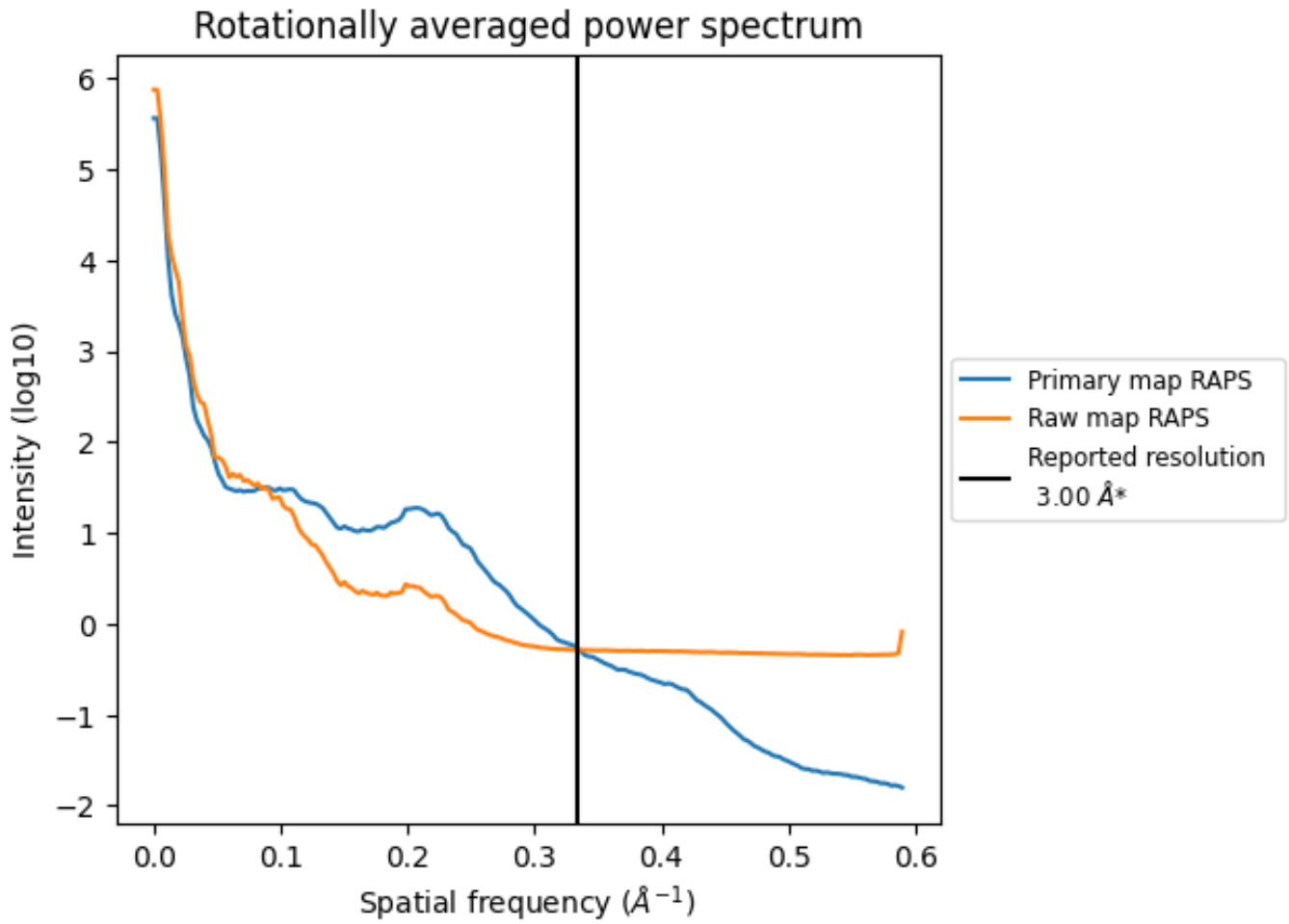
7.2 Volume estimate (i)



The volume at the recommended contour level is 291 nm^3; this corresponds to an approximate mass of 263 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)

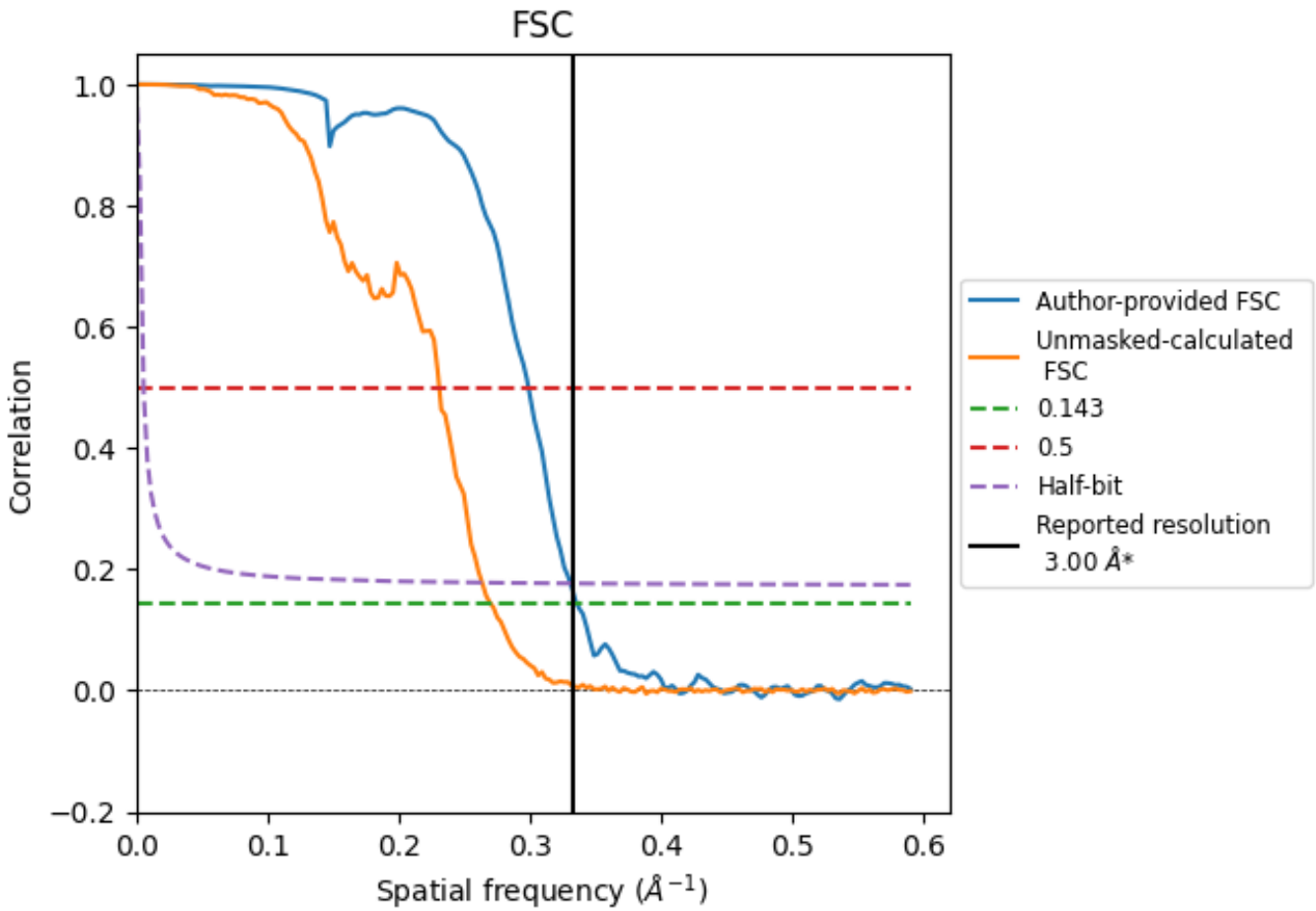


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

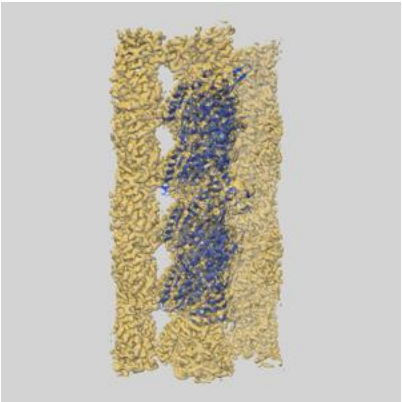
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.98	3.35	3.02
Unmasked-calculated*	3.70	4.33	3.80

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

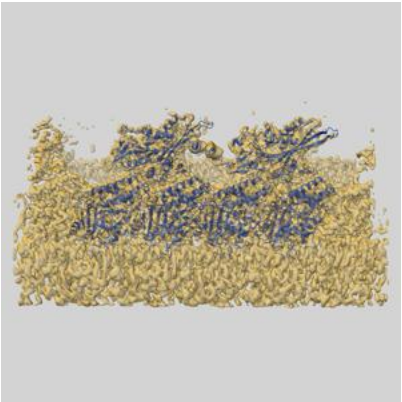
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-21938 and PDB model 6WWK. Per-residue inclusion information can be found in section 3 on page 8.

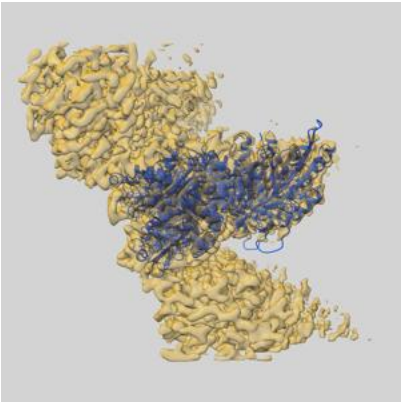
9.1 Map-model overlay (i)



X



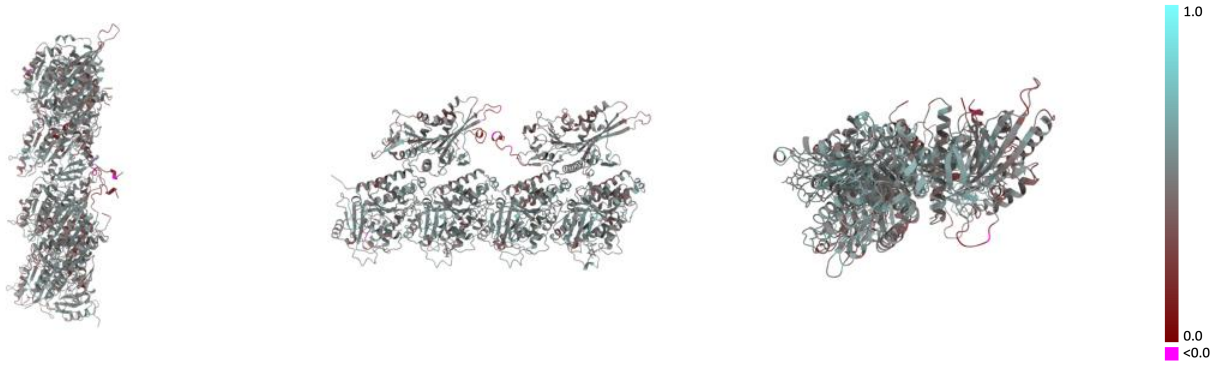
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0115 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.

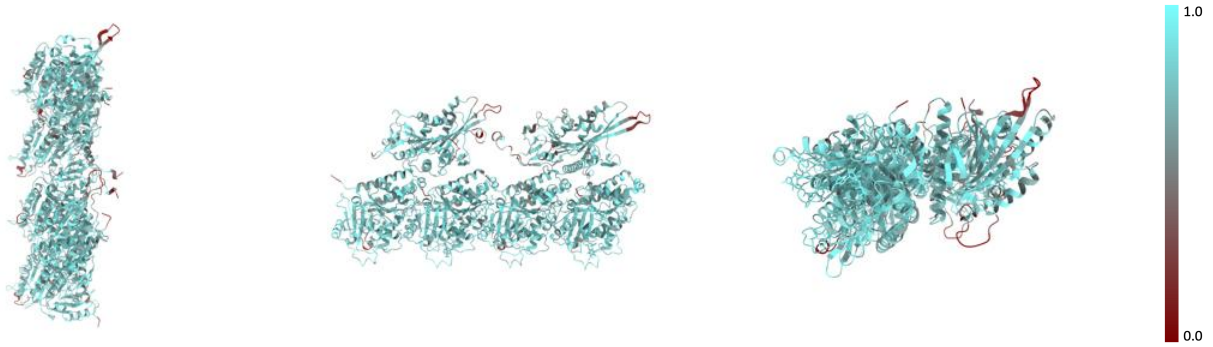
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

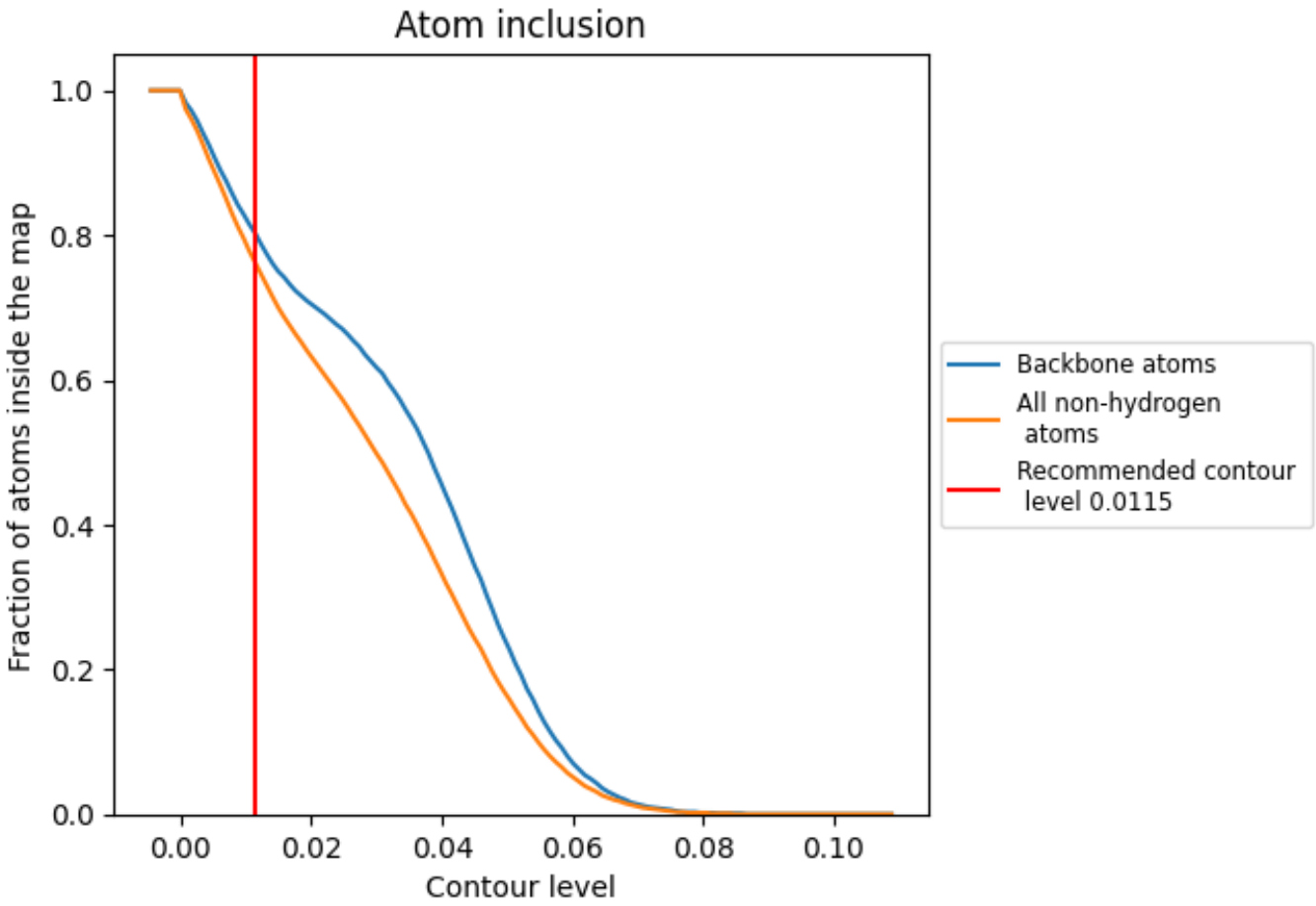
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0115).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 76% 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 (0.0115) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7600	0.4910
A	0.7760	0.4990
B	0.8020	0.5190
E	0.7850	0.5030
I	0.7920	0.5110
K	0.7070	0.4550
N	0.6770	0.4460