wwPDB EM Validation Summary Report

Nov 24, 2021 – 02:14 pm GMT

PDB ID	:	7PLH
EMDB ID	:	EMD-13489
Title	:	Scytonema hofmannii TnsC bound to AMPPNP and DNA
Authors	:	Querques, I.; Jinek, M.
Deposited on	:	2021-08-31
Resolution	:	3.57 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 following versions of software and data (see references ⓘ) were used in the production of this report:

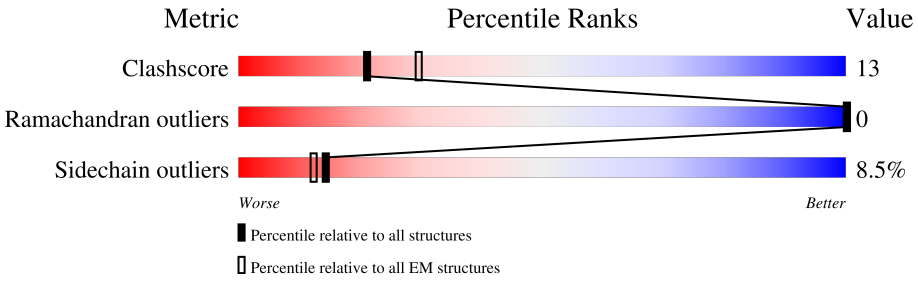
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.4 (270009), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.57 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 <=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	276	70% 22% · 6%
1	B	276	69% 23% · 6%
1	C	276	68% 24% · 6%
1	D	276	5% 68% 23% · 6%
1	E	276	68% 24% · 6%
1	F	276	68% 24% · 6%
1	G	276	67% 25% · 6%
2	H	22	5% 55% 41% 5%

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Mol	Chain	Length	Quality of chain
2	I	22	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15542 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.

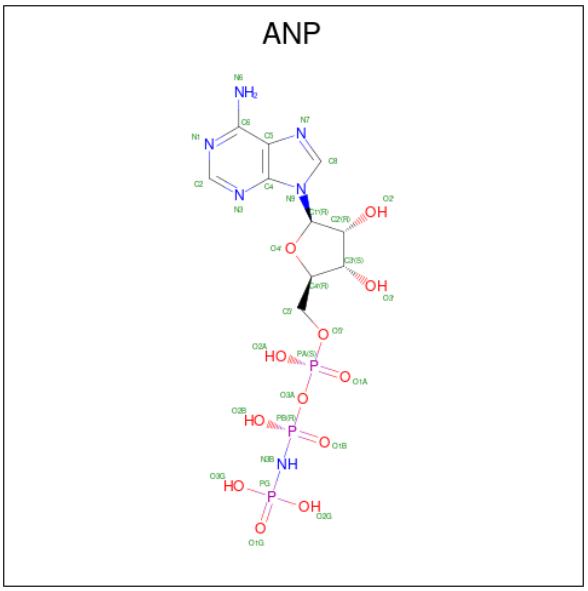
- Molecule 1 is a protein called ShTnsC.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	260	Total	C	N	O	S	0	0
			2060	1298	377	377	8		
1	B	260	Total	C	N	O	S	0	0
			2060	1298	377	377	8		
1	C	260	Total	C	N	O	S	0	0
			2060	1298	377	377	8		
1	D	260	Total	C	N	O	S	0	0
			2060	1298	377	377	8		
1	E	260	Total	C	N	O	S	0	0
			2060	1298	377	377	8		
1	F	260	Total	C	N	O	S	0	0
			2056	1296	377	375	8		
1	G	260	Total	C	N	O	S	0	0
			2060	1298	377	377	8		

- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	22	Total	C	N	O	P	0	0
			451	220	77	132	22		
2	I	22	Total	C	N	O	P	0	0
			451	220	77	132	22		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	B	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	C	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	D	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	E	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	F	1	Total	C	N	O	P	0
			31	10	6	12	3	
3	G	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

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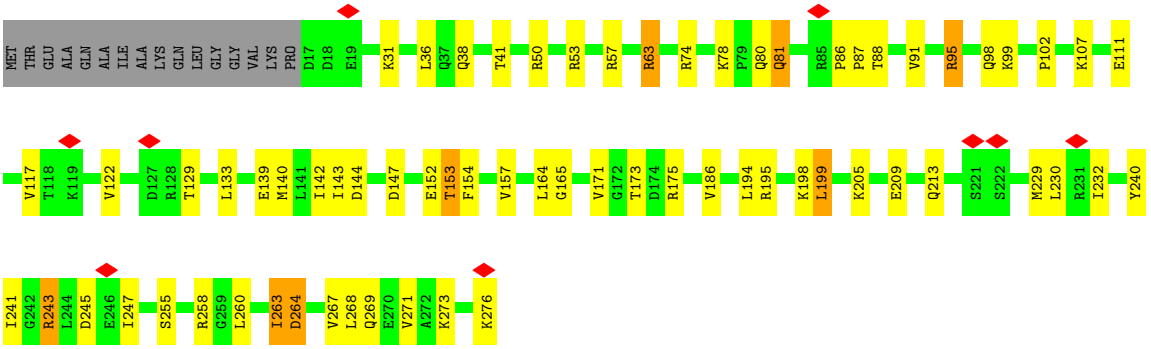
Mol	Chain	Residues	Atoms	AltConf
4	E	1	Total Mg 1 1	0
4	F	1	Total Mg 1 1	0
4	G	1	Total Mg 1 1	0

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.

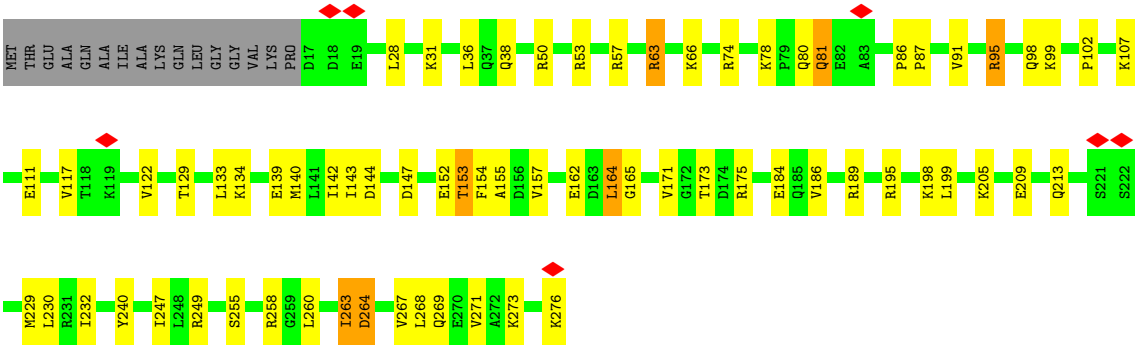
- Molecule 1: ShTnsC

Chain A:



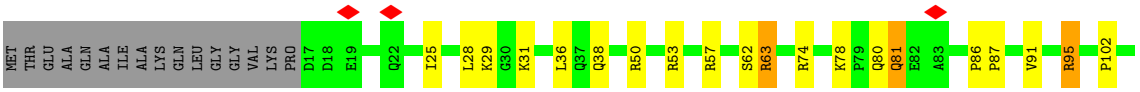
- Molecule 1: ShTnsC

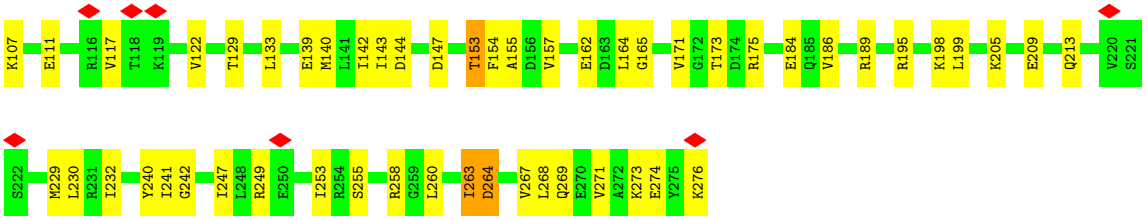
Chain B:



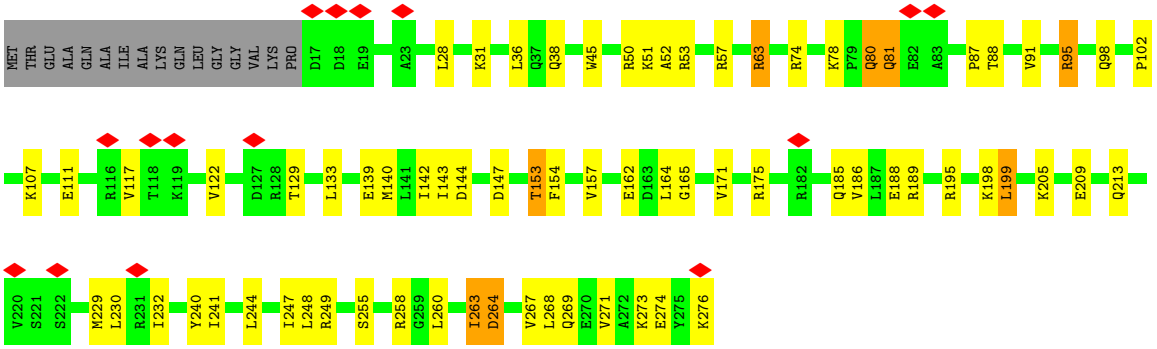
- Molecule 1: ShTnsC

Chain C:

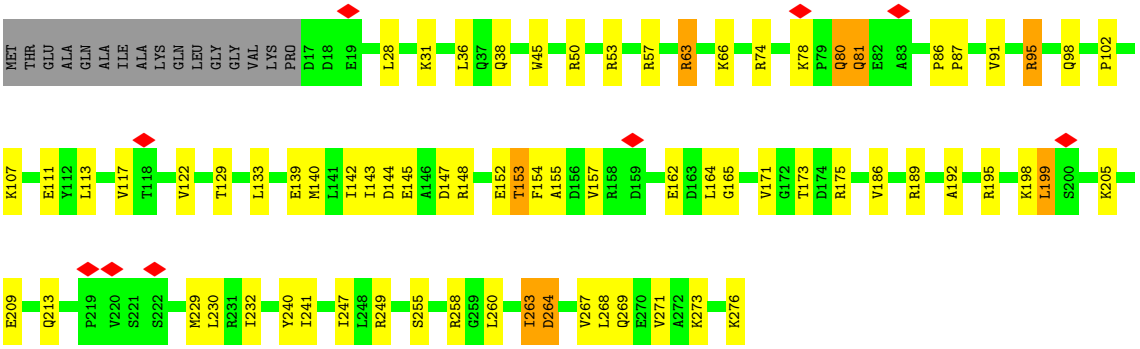




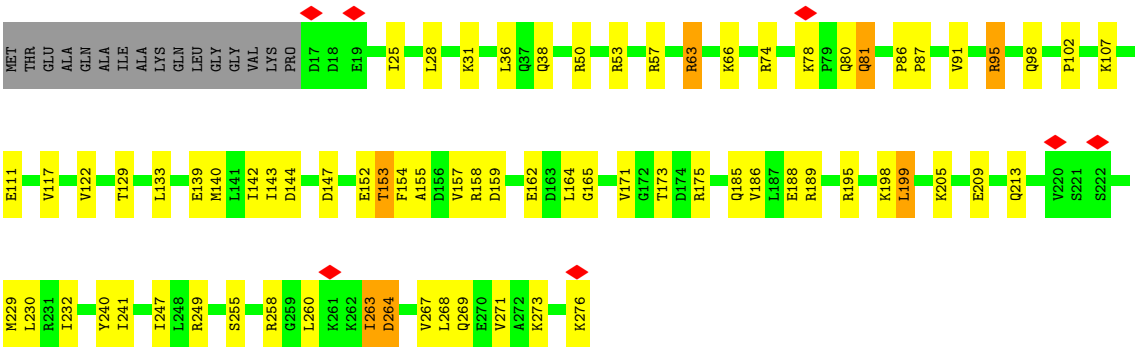
• Molecule 1: ShTnsC



• Molecule 1: ShTnsC

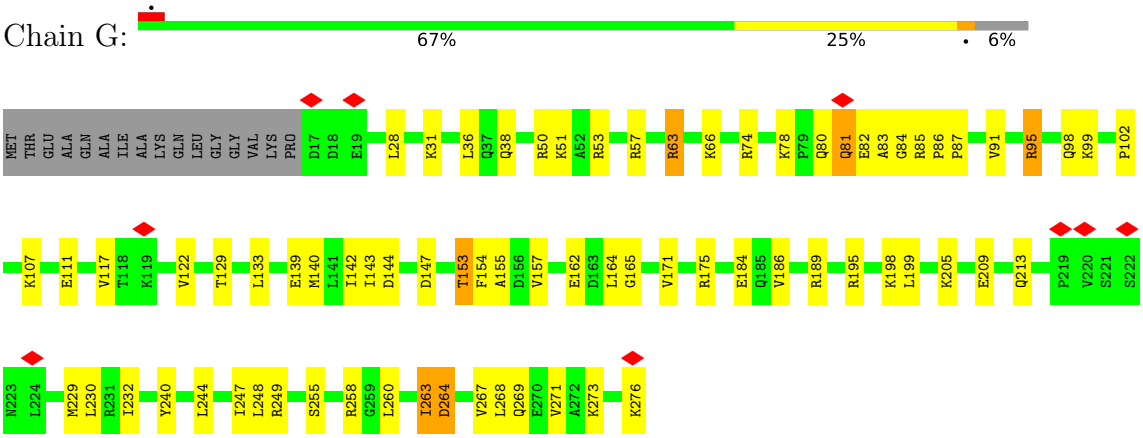


• Molecule 1: ShTnsC



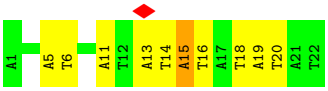
• Molecule 1: ShTnsC

Chain G:



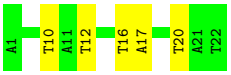
• Molecule 2: DNA (5'-D(P*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*T)-3')

Chain H:



• Molecule 2: DNA (5'-D(P*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*TP*AP*T)-3')

Chain I:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=59.72°, rise=6.78 Å, axial sym=C1	Depositor
Number of segments used	77544	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 ($e^-/Å^2$)	66.39	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	16.846	Depositor
Minimum map value	-9.278	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.1	Depositor
Map size (Å)	228.79999, 228.79999, 228.79999	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.65, 0.65, 0.65	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, ANP

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	0.51	0/2090	0.73	0/2810
1	B	0.51	0/2090	0.74	0/2810
1	C	0.51	0/2090	0.74	0/2810
1	D	0.51	0/2090	0.74	0/2810
1	E	0.50	0/2090	0.74	0/2810
1	F	0.51	0/2086	0.74	0/2805
1	G	0.52	0/2090	0.74	0/2810
2	H	0.68	1/505 (0.2%)	1.05	0/777
2	I	0.58	0/505	0.75	0/777
All	All	0.52	1/15636 (0.0%)	0.75	0/21219

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	15	DA	O3'-P	-5.76	1.54	1.61

There are no bond angle outliers.

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	2060	0	2098	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2060	0	2098	66	0
1	C	2060	0	2098	76	0
1	D	2060	0	2098	73	0
1	E	2060	0	2098	62	0
1	F	2056	0	2094	67	0
1	G	2060	0	2098	60	0
2	H	451	0	254	9	0
2	I	451	0	254	5	0
3	A	31	0	13	7	0
3	B	31	0	13	5	0
3	C	31	0	13	7	0
3	D	31	0	13	7	0
3	E	31	0	13	7	0
3	F	31	0	13	5	0
3	G	31	0	13	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
All	All	15542	0	15281	406	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 13.

The worst 5 of 406 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:B:173:THR:HG21	1:C:184:GLU:CD	1.93	0.90
1:A:173:THR:HG21	1:B:184:GLU:OE1	1.79	0.83
1:B:134:LYS:HG3	1:B:164:LEU:CD2	2.09	0.82
1:B:173:THR:HG21	1:C:184:GLU:OE1	1.78	0.82
1:E:98:GLN:HE21	1:F:155:ALA:CB	1.92	0.81

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	258/276 (94%)	253 (98%)	5 (2%)	0	100	100
1	B	258/276 (94%)	253 (98%)	5 (2%)	0	100	100
1	C	258/276 (94%)	253 (98%)	5 (2%)	0	100	100
1	D	258/276 (94%)	253 (98%)	5 (2%)	0	100	100
1	E	258/276 (94%)	253 (98%)	5 (2%)	0	100	100
1	F	258/276 (94%)	253 (98%)	5 (2%)	0	100	100
1	G	258/276 (94%)	253 (98%)	5 (2%)	0	100	100
All	All	1806/1932 (94%)	1771 (98%)	35 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	215/238 (90%)	196 (91%)	19 (9%)	10	40
1	B	215/238 (90%)	196 (91%)	19 (9%)	10	40
1	C	215/238 (90%)	197 (92%)	18 (8%)	11	42
1	D	215/238 (90%)	197 (92%)	18 (8%)	11	42
1	E	215/238 (90%)	197 (92%)	18 (8%)	11	42
1	F	214/238 (90%)	196 (92%)	18 (8%)	11	42
1	G	215/238 (90%)	197 (92%)	18 (8%)	11	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1504/1666 (90%)	1376 (92%)	128 (8%)	14 41

5 of 128 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	95	ARG
1	G	153	THR
1	C	195	ARG
1	C	153	THR
1	G	198	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	213	GLN
1	F	185	GLN
1	G	213	GLN
1	F	213	GLN
1	F	98	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

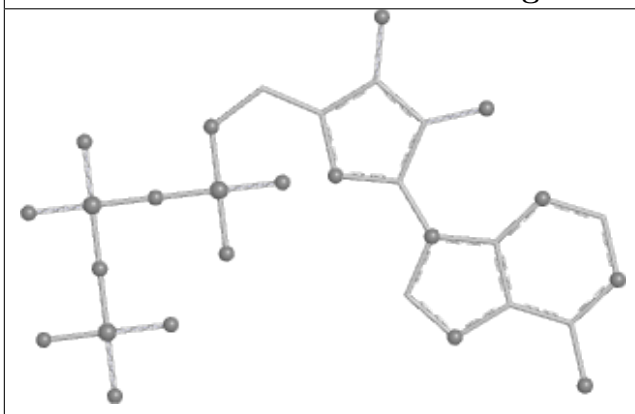
There are no torsion outliers.

There are no ring outliers.

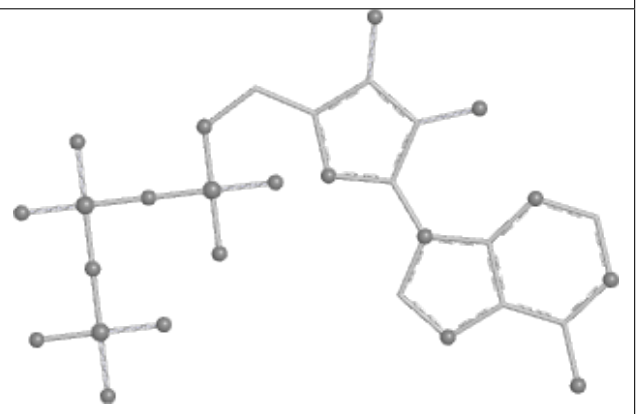
No monomer is involved in short contacts.

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

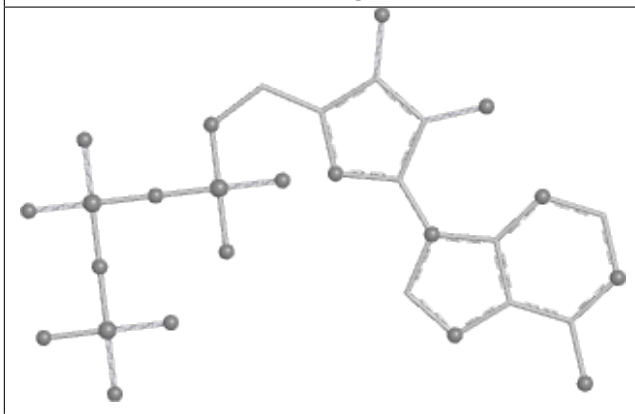
Ligand ANP A 301



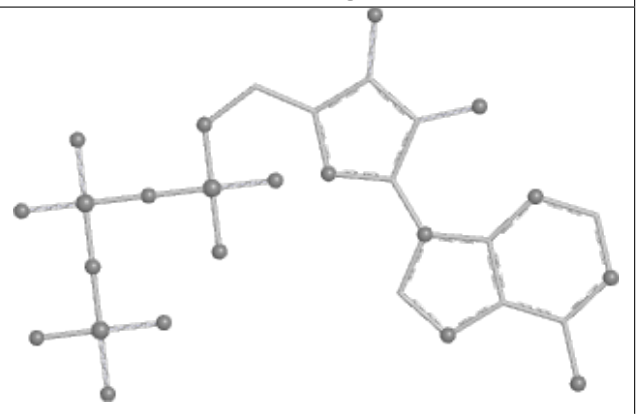
Bond lengths



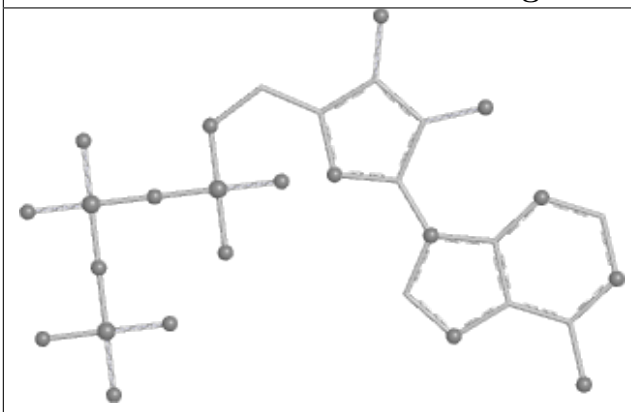
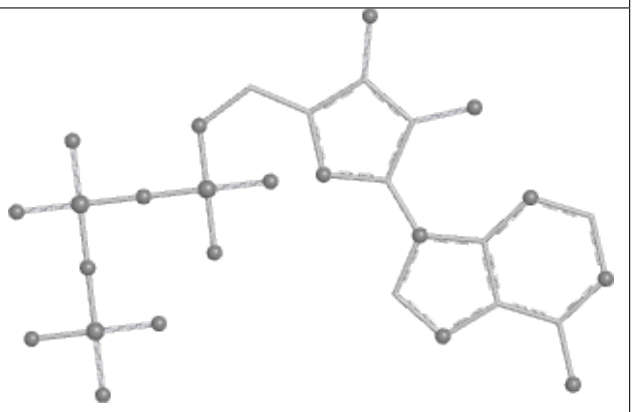
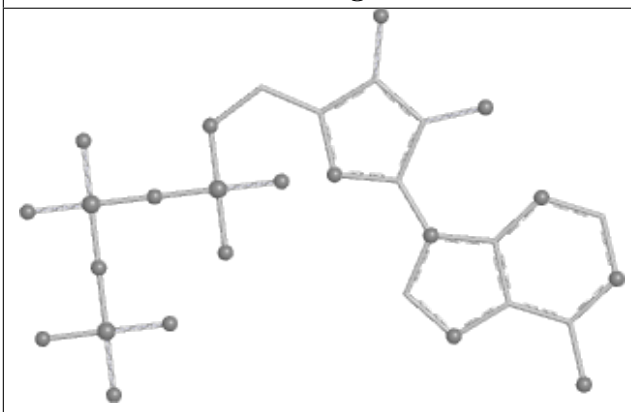
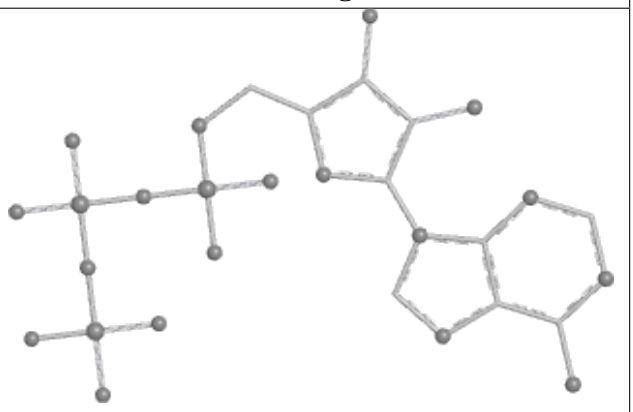
Bond angles



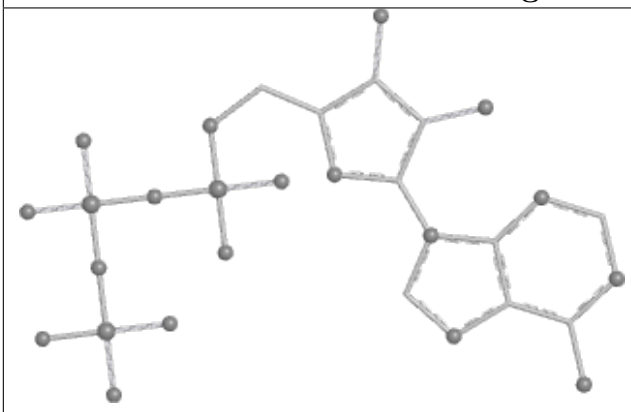
Torsions



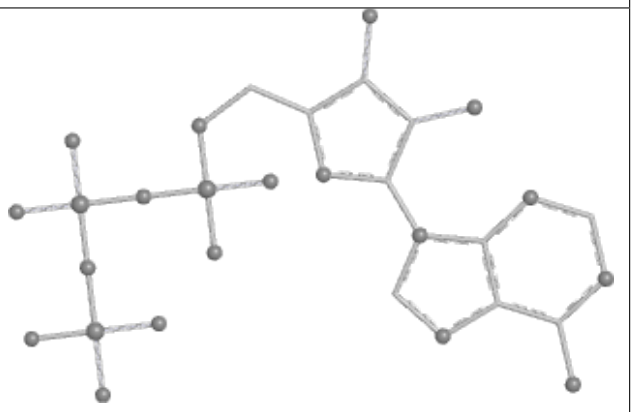
Rings

Ligand ANP B 301	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

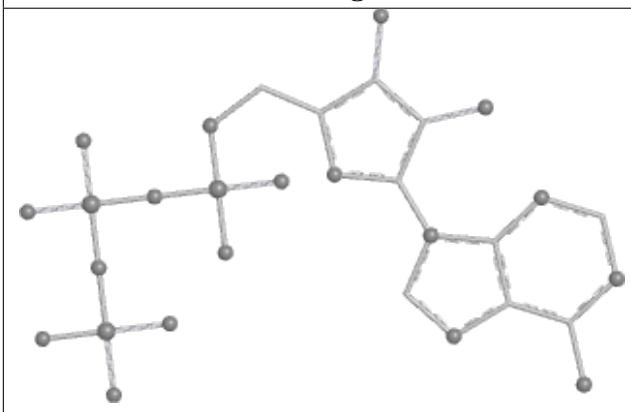
Ligand ANP C 301



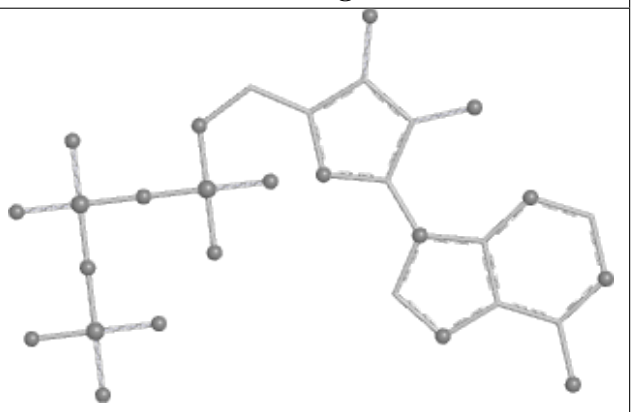
Bond lengths



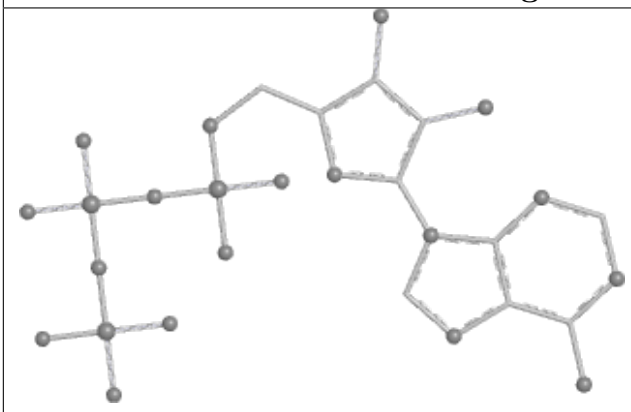
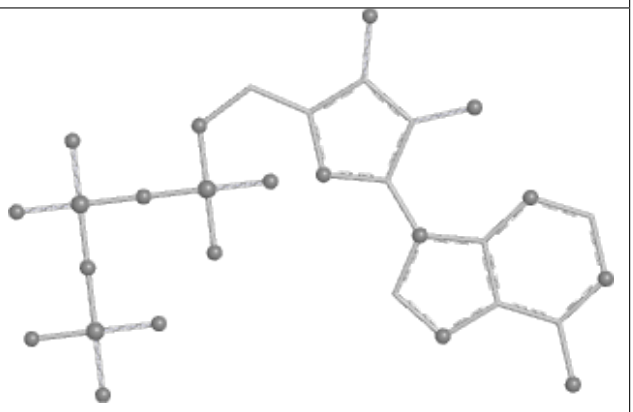
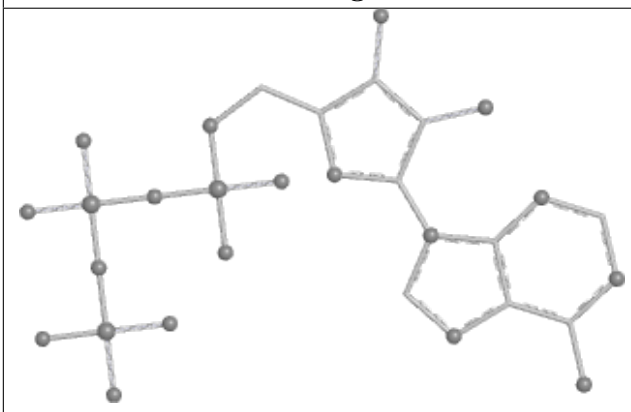
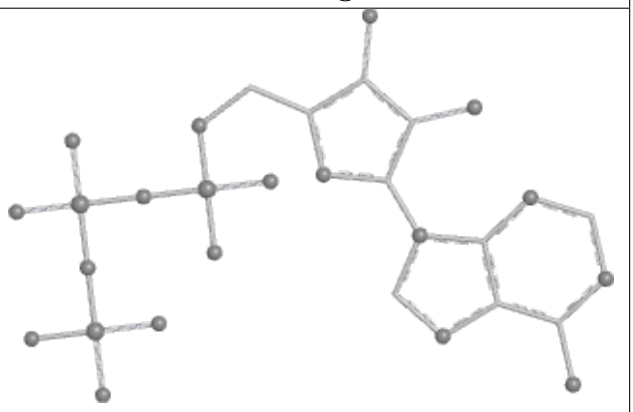
Bond angles



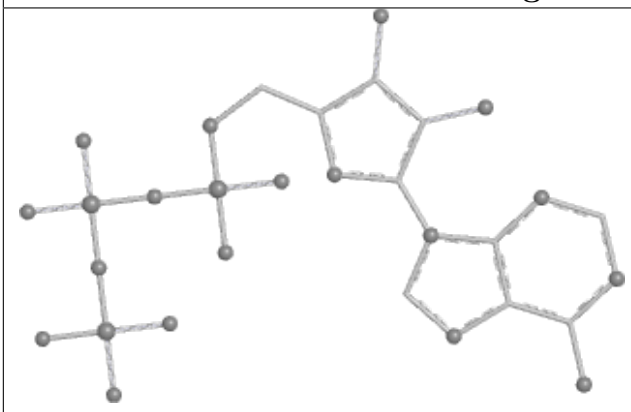
Torsions



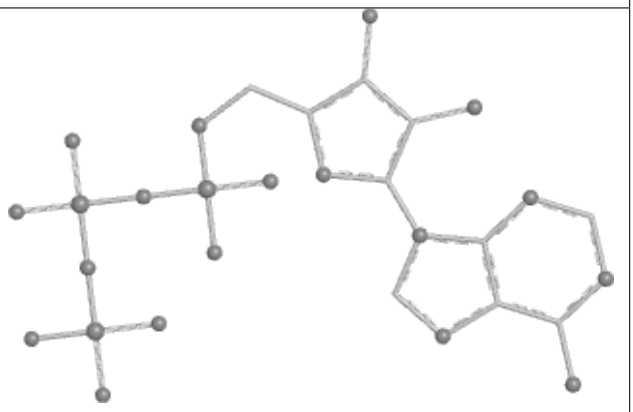
Rings

Ligand ANP D 301	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

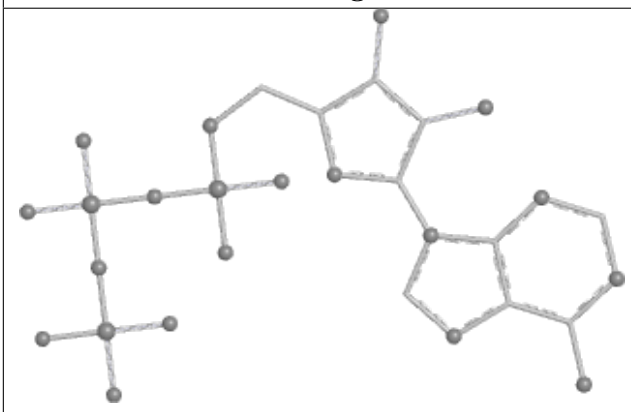
Ligand ANP E 301



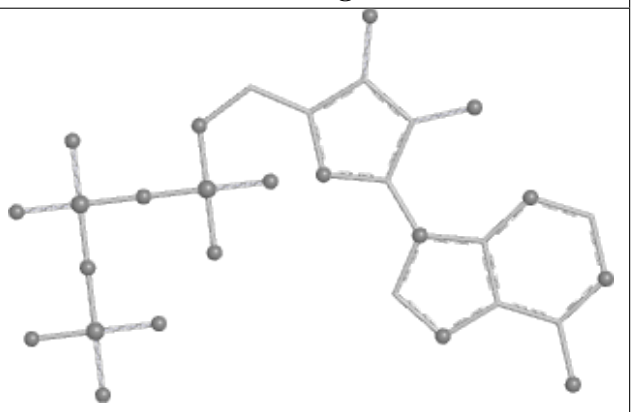
Bond lengths



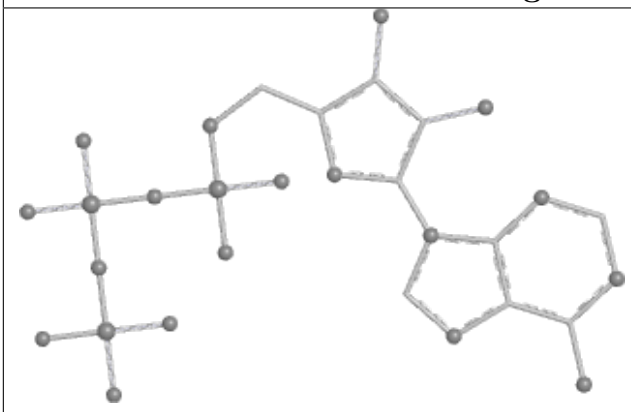
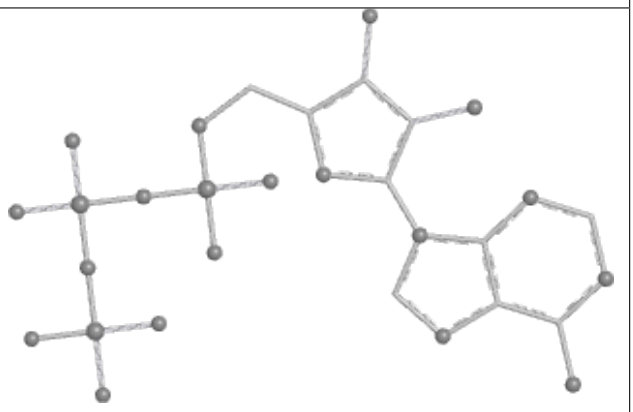
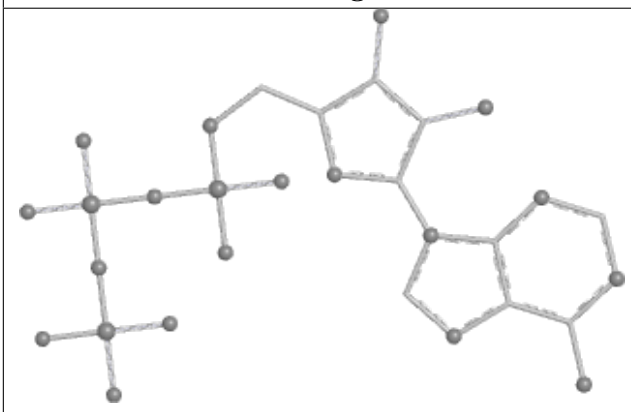
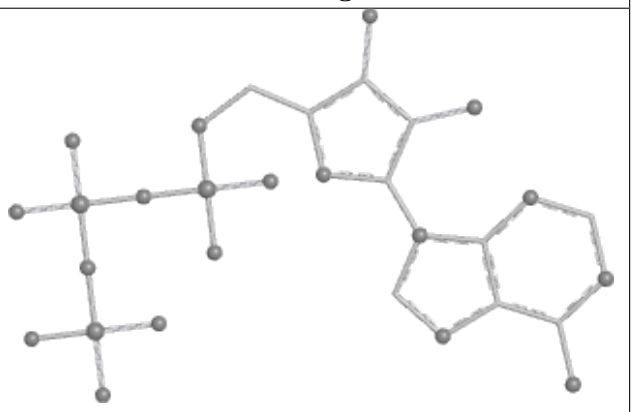
Bond angles

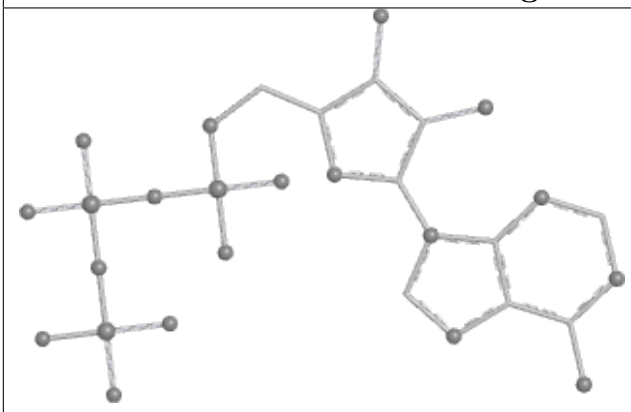
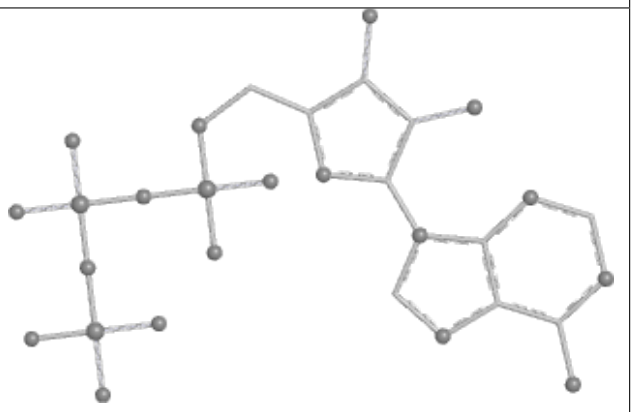
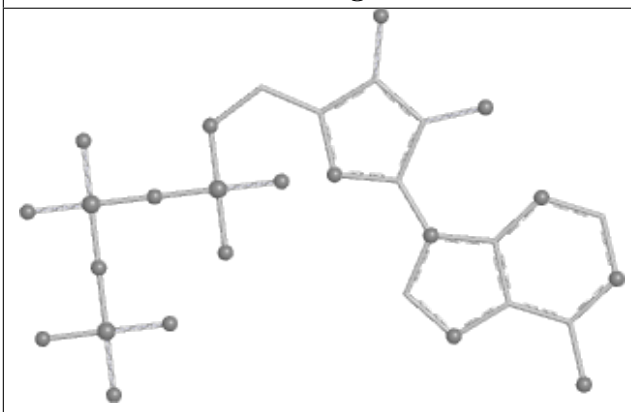
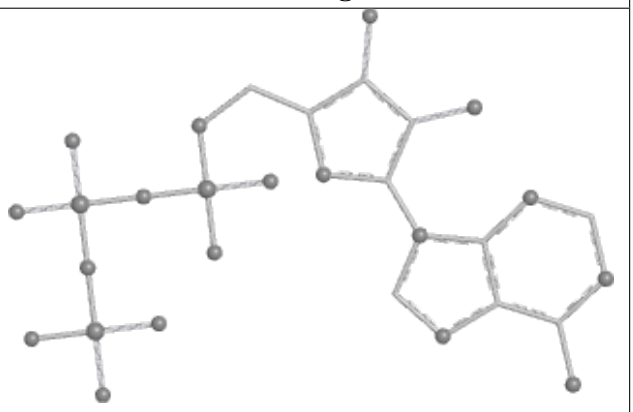


Torsions



Rings

Ligand ANP F 301	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand ANP G 301	
 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.

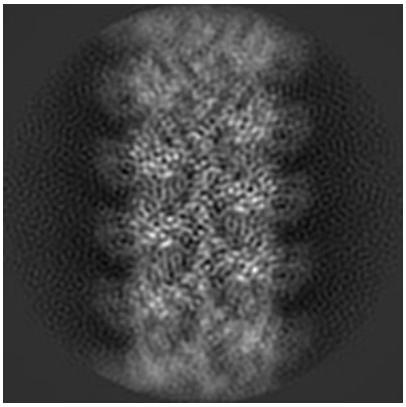
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13489. These allow visual inspection of the internal detail of the map and identification of artifacts.

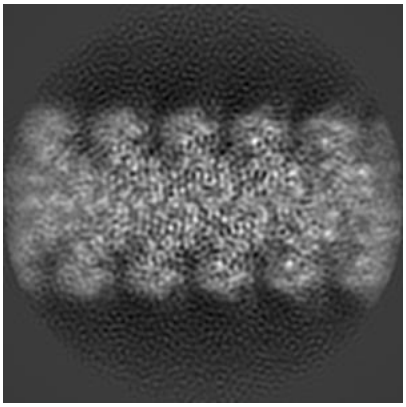
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

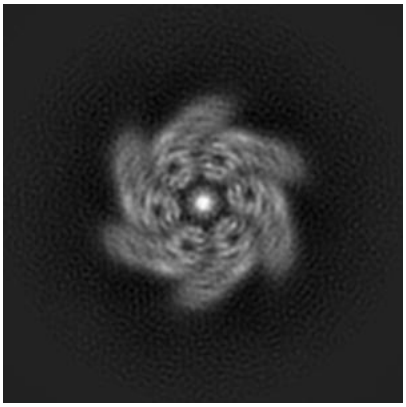
6.1.1 Primary map



X



Y

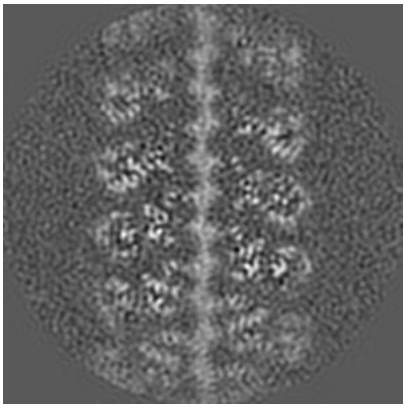


Z

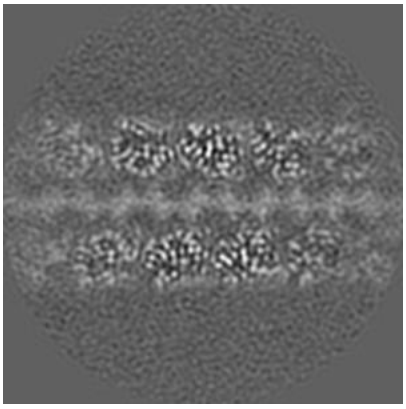
The images above show the map projected in three orthogonal directions.

6.2 Central slices

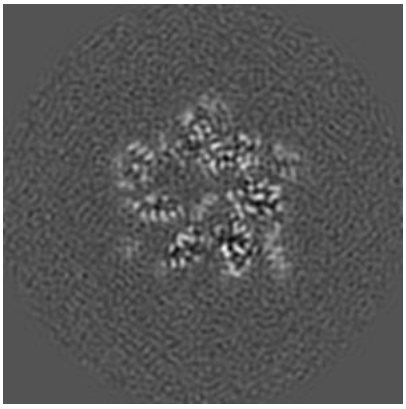
6.2.1 Primary map



X Index: 176



Y Index: 176

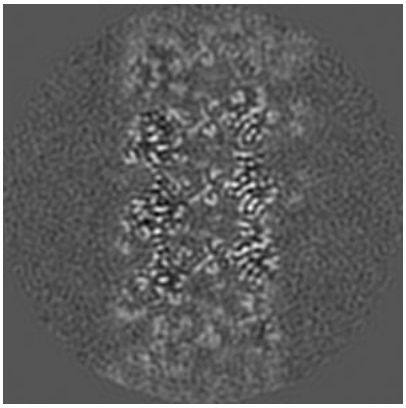


Z Index: 176

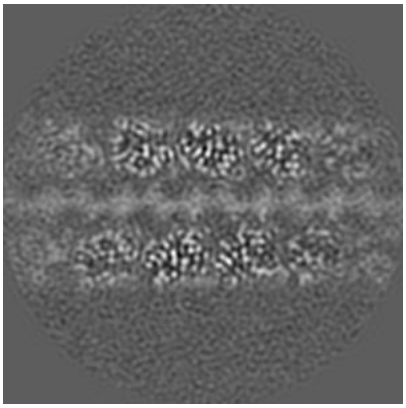
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

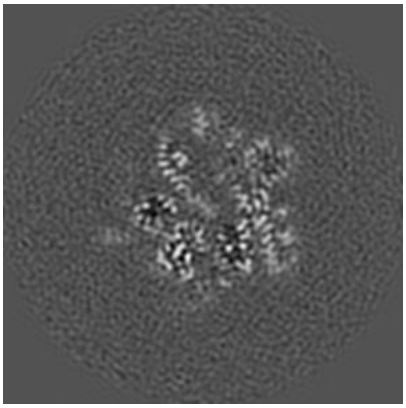
6.3.1 Primary map



X Index: 200



Y Index: 175

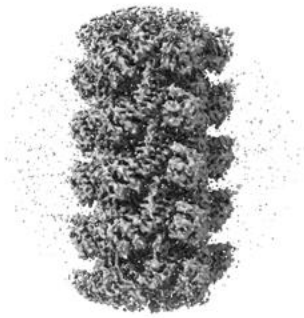


Z Index: 161

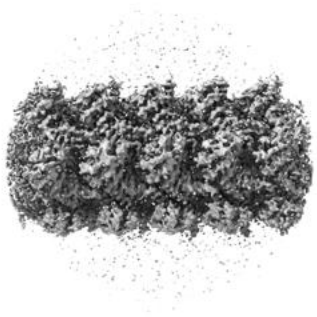
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

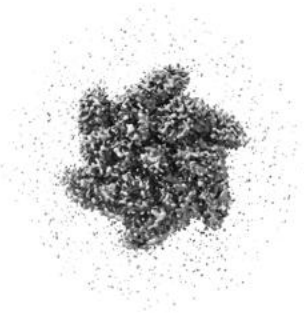
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

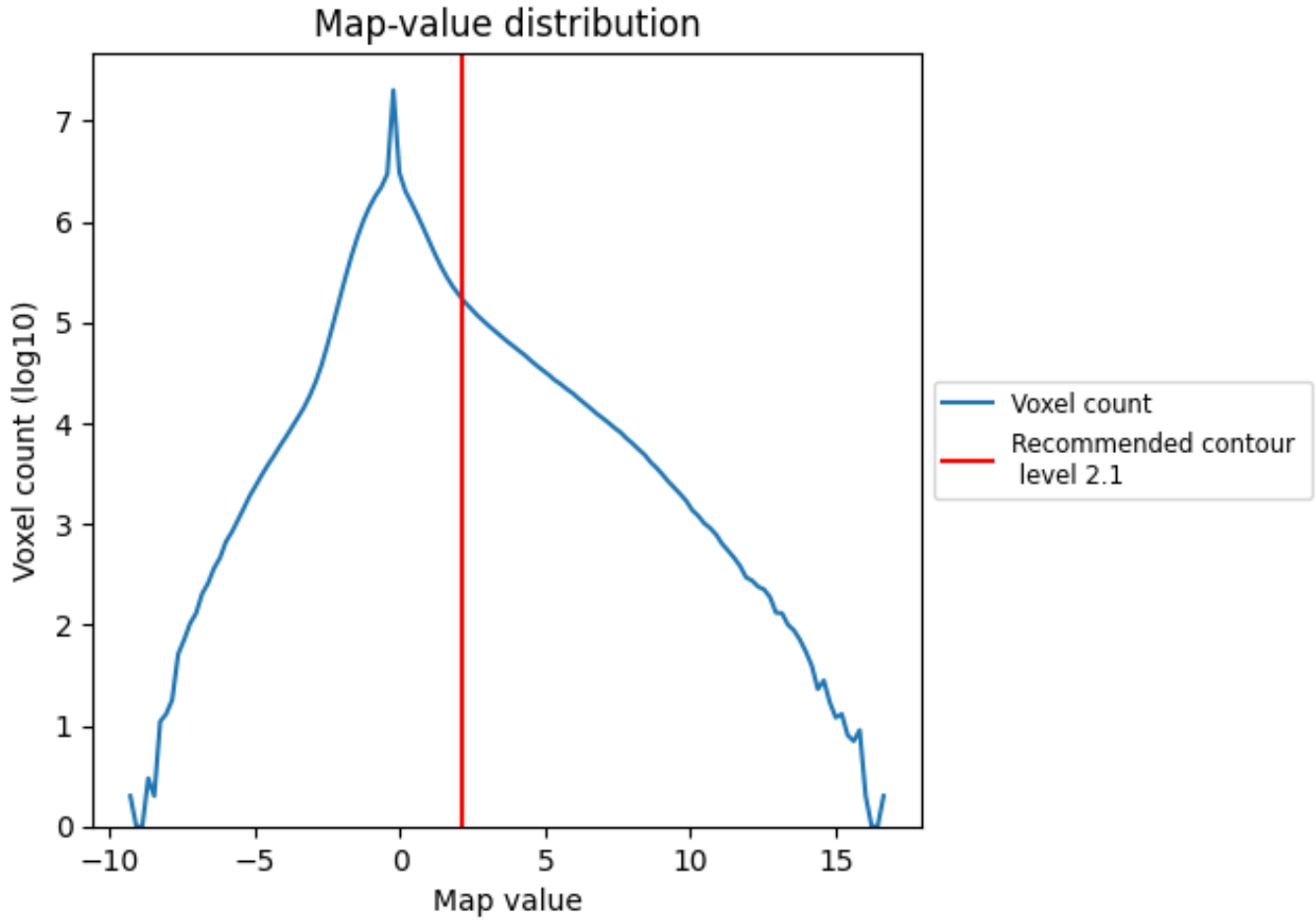
6.5 Mask visualisation (i)

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

7 Map analysis

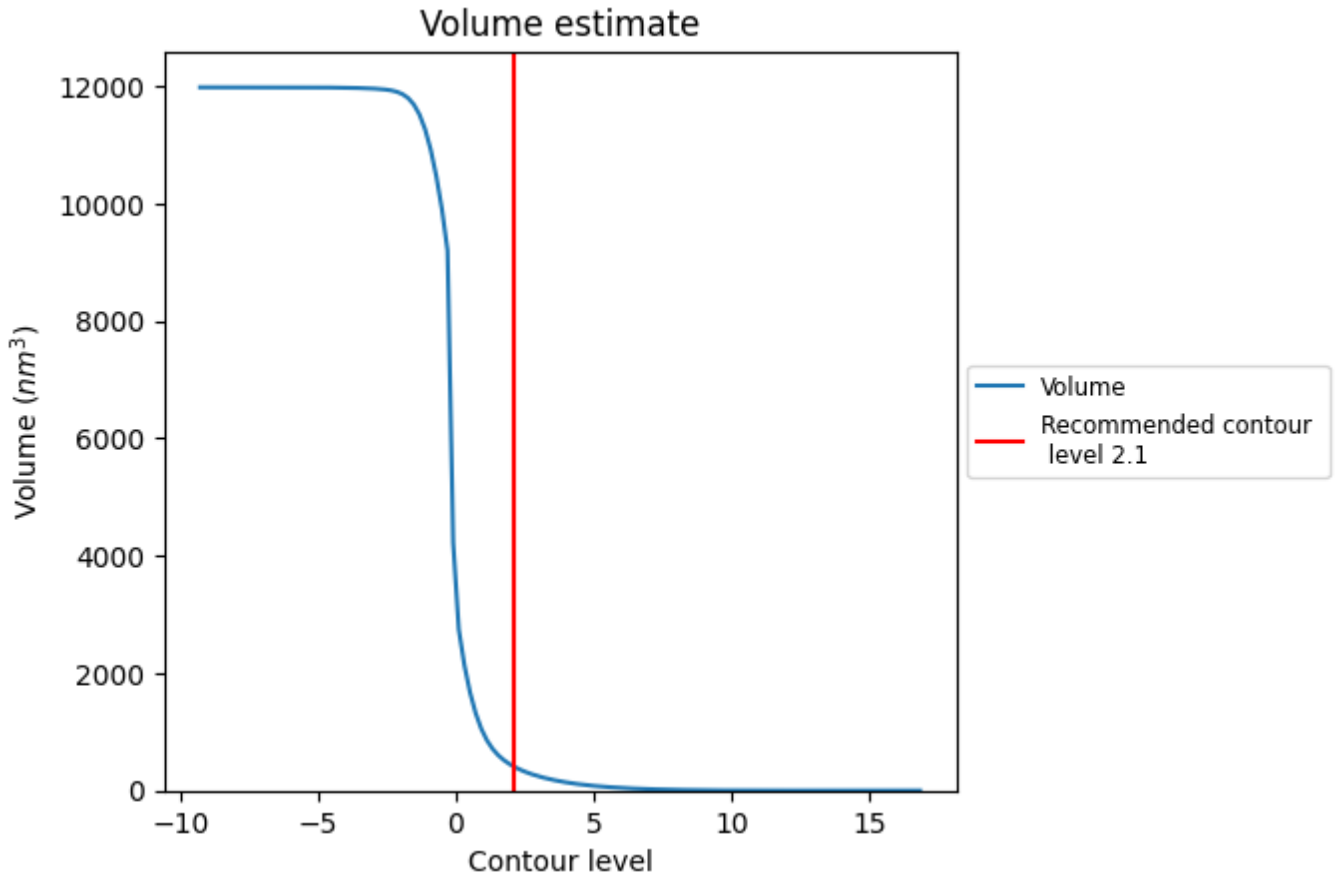
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

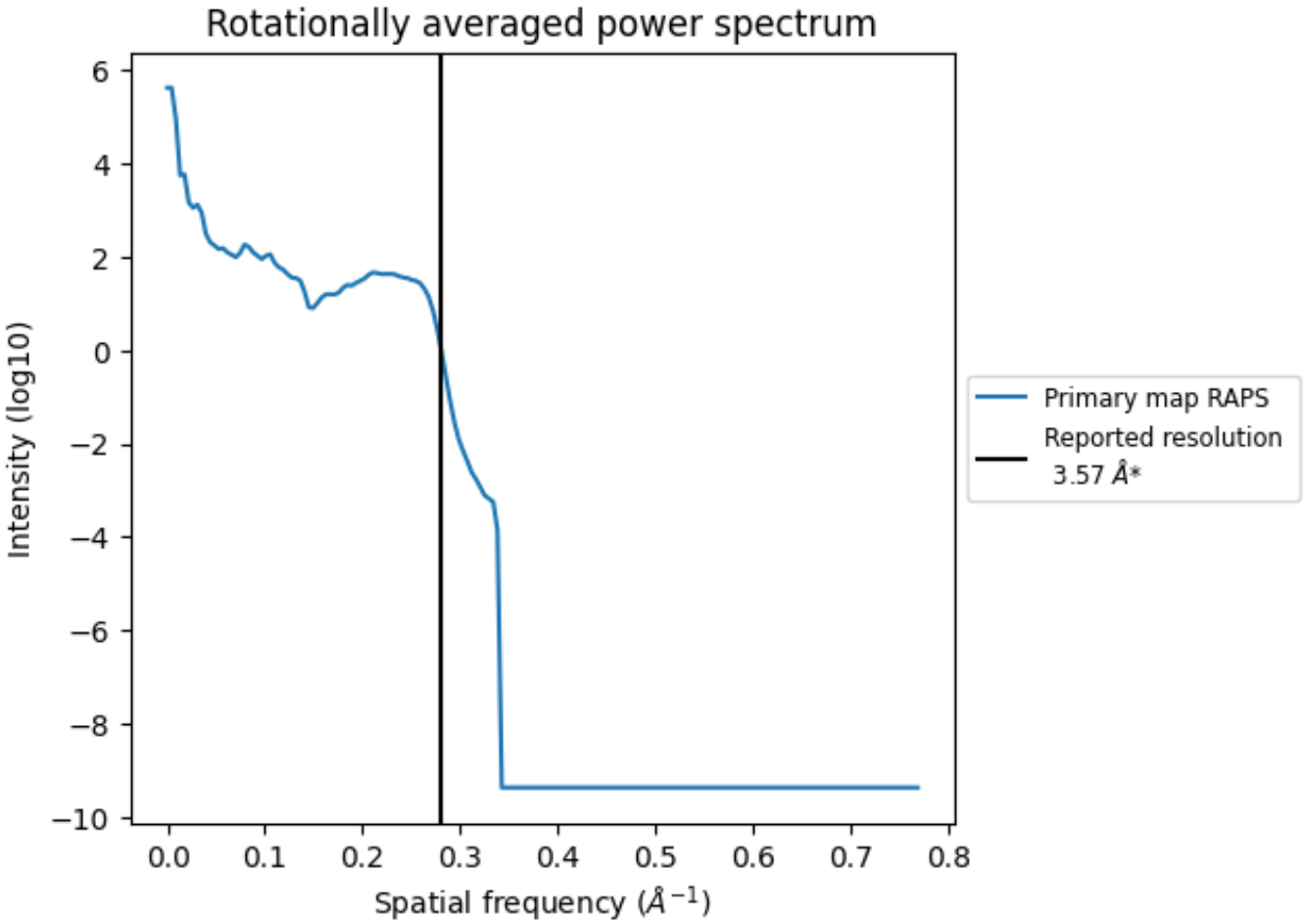
7.2 Volume estimate (i)



The volume at the recommended contour level is 412 nm^3; this corresponds to an approximate mass of 372 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 0.280 $Å^{-1}$

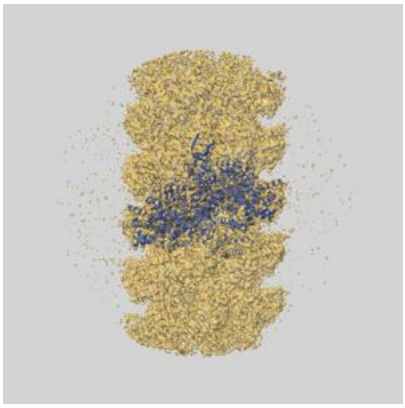
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

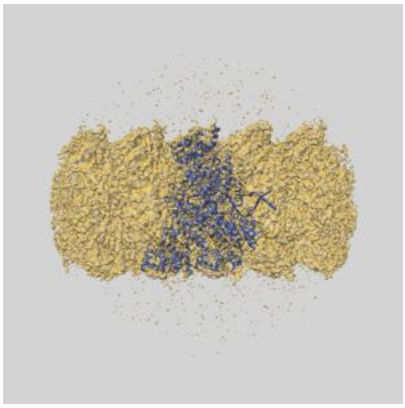
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13489 and PDB model 7PLH. Per-residue inclusion information can be found in section 3 on page 7.

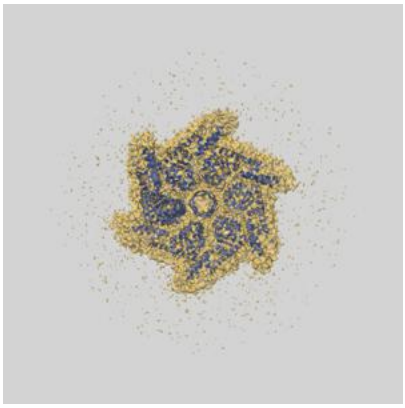
9.1 Map-model overlay



X



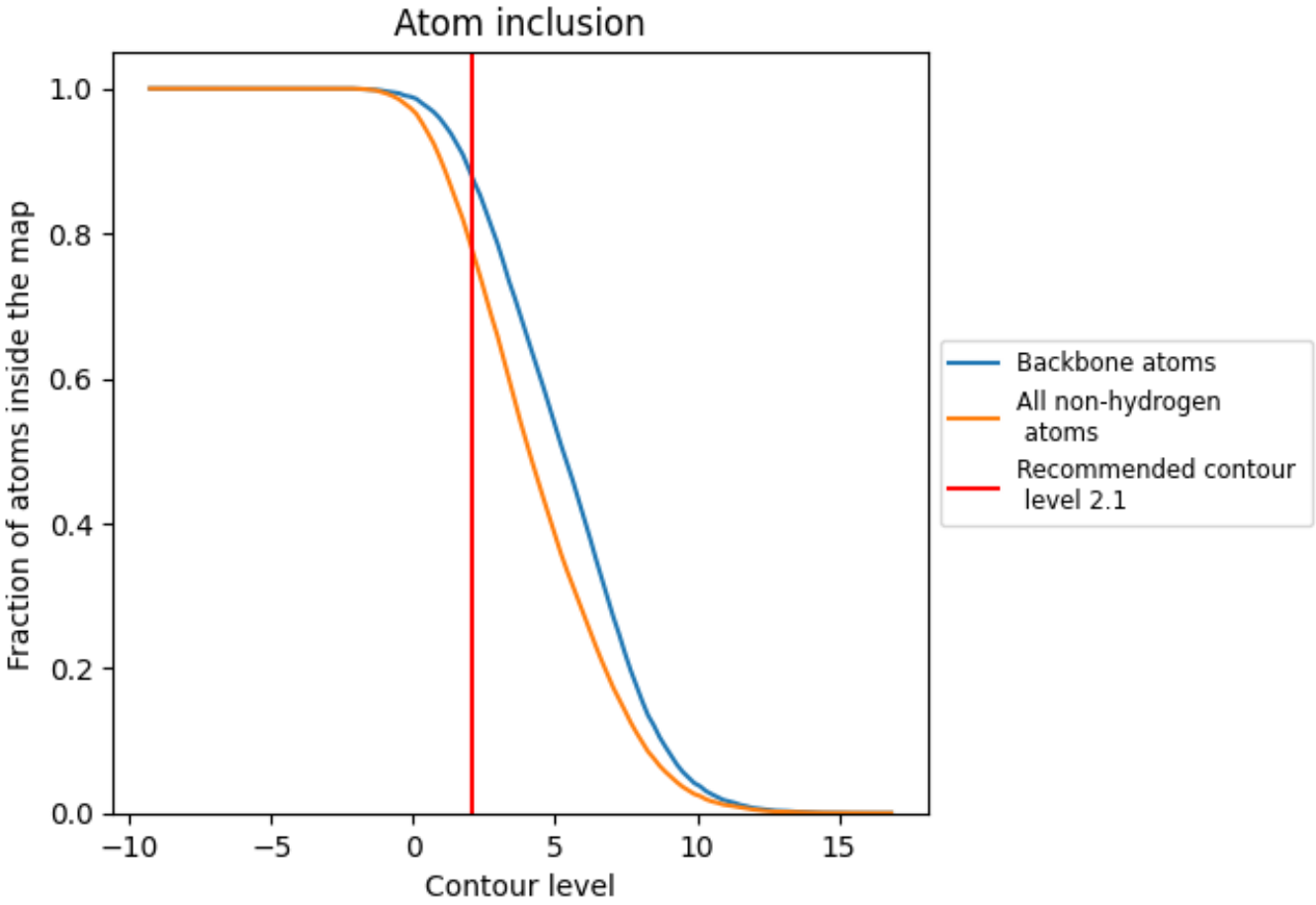
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.1 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 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.