



## wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 04:12 PM EST

PDB ID : 3J7I  
EMDB ID : EMD-2697  
Title : Structure of alpha- and beta- tubulin in GMPCPP-microtubules  
Authors : Yajima, H.; Ogura, T.; Nitta, R.; Okada, Y.; Sato, C.; Hirokawa, N.  
Deposited on : 2014-07-01  
Resolution : 8.90 Å(reported)  
Based on initial model : 1JFF

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

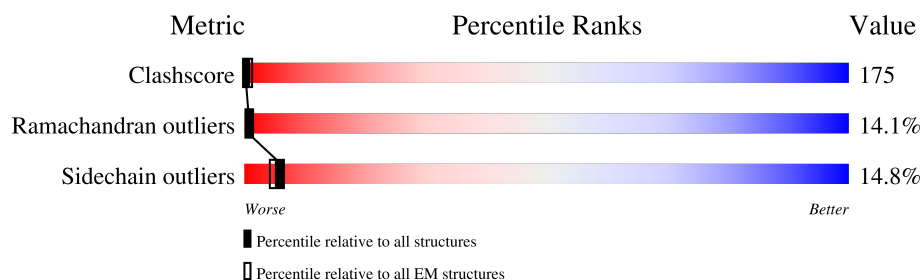
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.90 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	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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	
2	B	445	

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
4	GTP	A	502	-	-	X	-
4	GTP	B	502	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6515 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-1A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	409	Total	C	N	O	S	0	0
			3210	2034	548	608	20		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	GLY	ALA	SEE REMARK 999	UNP P02550

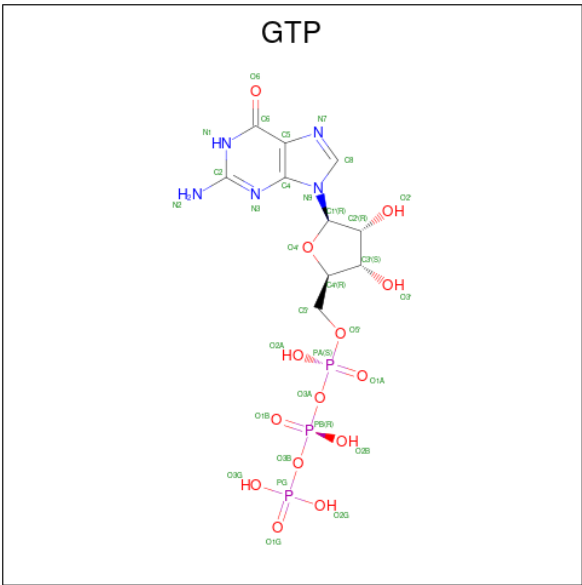
- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	411	Total	C	N	O	S	0	0
			3239	2037	558	620	24		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Mg	0
			1	1	
3	B	1	Total	Mg	0
			1	1	

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).

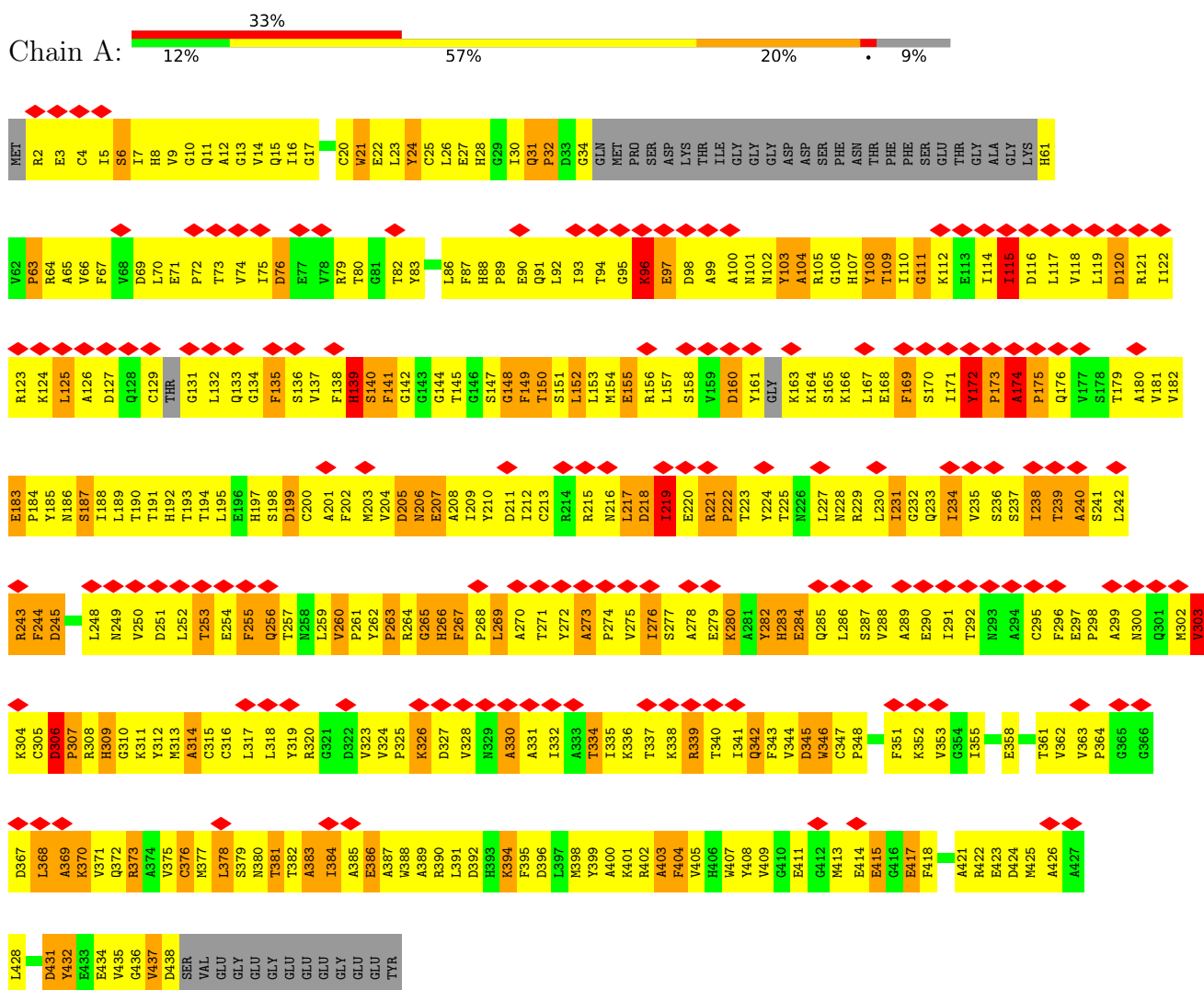


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	B	1	Total	C	N	O	P	0
			32	10	5	14	3	

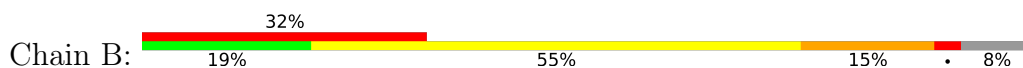
### 3 Residue-property plots

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: Tubulin alpha-1A chain



- Molecule 2: Tubulin beta chain



GLU	A375	P307	Q247	A187	E127	I66	MET
GLN	T376	R308	L248	T188	S128	L67	R2
GLY	F377	H309	N249	L189	CYS	V68	E3
PHE	I378	G310	A250	S190	ASP	I69	I4
GLU	G379	R311	D251	V191	C131	L70	V5
GLU	N380	Y312	L252	H192	L132	E71	H6
GLU	T382	L313	R253	Q193	Q133	G73	I7
GLY	A363	T314	K254	L194	G134	T74	Q8
GLU	I384	V315	L255	V195	F135	M75	A9
ASP	Q385	A316	L256	E196	Q136	D76	G10
GLU	E386	A317	A256	N197	L137	S77	Q11
ALA	L387	V318	V257	T198	T138	V78	C12
	F388	F319	N258	E200	H139	R79	G13
	K389	R320	V260	T201	SER	M14	M14
		G321	P261	Y202	LEU	S90	Q15
		R322	F262	C203	G142	G81	I16
	F395	M323	P263	I204	G143	P82	G17
T396	S324	S324	R264	D205	G144	F83	A18
A397	M325	L265	H266	N206	T145	G84	K19
M398	K326	F267	F268	E207	G146	Q85	F20
F399	E327	F269	M269	A208	S147	I86	W21
R400	V328	P270	P270	L209	G148		E22
R401	D329	G271	G271	M149	M149	P89	V23
K402		F272	F272	D211	G150	D90	I24
A403	E330	A273	A273	T212	T151	N91	S25
F404	M332	P274	P274	C213	L152	D95	D26
	L333	L275	L275	L153	F92	H28	E27
Y408	N334	T276	T276	L154	V93	G29	H28
T409	V335	S277	S277	T155	K156	I30	G29
G410	Q336	R278	R278	L216	GLY	D31	I30
E411	V342	G279	G279	T217	GLN	P32	P32
G412	Q337	S280	S280	K218	S97	I33	I33
N413	N338	Q281	Q281	L219	G98	G34	G34
D414	S340	Q282	Q282	T220	A99	S35	S35
	S341	Y283	Y283	T221	N101	Y36	Y36
	Y342	R284	R284	T222	N102	G38	G38
	F343	A285	A285	T223	W103	D39	D39
	S344	L286	L286	Y224	A104	S40	S40
	E345	T287	T287	G225	K105	D41	D41
	W346	V288	V288	D226	G106	L42	L42
	I347	P289	P289	L227	H107	Q43	Q43
	P348	E290	E290	N228	Y108	L44	L44
	N349	L291	L291	H229	T109	E47	E47
	N350	T292	T292	L230	E110	R48	R48
	V351	Q293	Q293	V231	G111	N50	N50
	K352	Q294	Q294	S232	A112	V51	V51
	T353	M295	M295	A233	E113	Y52	Y52
	A354	F296	F296	T234	L114	N54	N54
	V355	C356	C356	S236	SER	A57	A57
	C356	D297	D297	G237	PRO	G58	G58
	D357	A298	A298	V238	VAL	N59	N59
	I358	K299	K299	T239	SER	P63	P63
	P359	N300	N300	T240	T180	R64	R64
	P360	M301	M301	C241	V181	A65	A65
	R369	M302	M302	L242	V182		
	G370	L303	L303	E183	D120		
	L371	A304	A304	P184	V121		
	K372	M373	M373	N186	Y185		
	S374	D306	D306		R123		
					K124		
					E125		
					S126		

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	320000	Depositor
Resolution determination method	Not provided	
CTF correction method	Each Filament	Depositor
Microscope	JEOL 2010F	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	10	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	40000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	287.504	Depositor
Minimum map value	-8.307	Depositor
Average map value	26.397	Depositor
Map value standard deviation	58.261	Depositor
Recommended contour level	156.0	Depositor
Map size ( $\text{\AA}$ )	152.5, 157.5, 107.5	wwPDB
Map dimensions	61, 63, 43	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	2.5, 2.5, 2.5	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.55	2/3281 (0.1%)	0.78	10/4453 (0.2%)
2	B	0.57	3/3306 (0.1%)	0.87	15/4469 (0.3%)
All	All	0.56	5/6587 (0.1%)	0.83	25/8922 (0.3%)

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
2	B	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	205	ASP	CB-CG	-9.46	1.31	1.51
2	B	205	ASP	CA-CB	-6.95	1.38	1.53
1	A	173	PRO	N-CD	5.43	1.55	1.47
1	A	307	PRO	N-CD	5.16	1.55	1.47
2	B	205	ASP	CA-C	5.08	1.66	1.52

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	ASP	CB-CG-OD1	-9.38	109.85	118.30
2	B	205	ASP	CA-CB-CG	-9.22	93.12	113.40
1	A	383	ALA	CA-C-O	-8.86	101.49	120.10
2	B	203	CYS	C-N-CA	8.78	143.65	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	205	ASP	C-N-CA	-8.20	101.19	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	PHE	Mainchain
2	B	380	ASN	Mainchain

## 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	3210	0	3123	1163	0
2	B	3239	0	3118	1137	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	32	0	12	61	0
4	B	32	0	12	27	0
All	All	6515	0	6265	2233	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 175.

The worst 5 of 2233 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:A:154:MET:HE2	1:A:197:HIS:CE1	1.22	1.68
2:B:185:TYR:CE1	2:B:399:PHE:HD1	1.02	1.63
1:A:189:LEU:HD21	1:A:418:PHE:CD2	1.12	1.63
2:B:413:MET:HE3	2:B:418:PHE:CE1	1.25	1.62
2:B:169:PHE:CZ	2:B:235:MET:CB	1.83	1.62

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	401/451 (89%)	257 (64%)	83 (21%)	61 (15%)	0	4
2	B	399/445 (90%)	262 (66%)	85 (21%)	52 (13%)	0	5
All	All	800/896 (89%)	519 (65%)	168 (21%)	113 (14%)	1	4

5 of 113 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	LYS
1	A	108	TYR
1	A	109	THR
1	A	175	PRO
1	A	183	GLU

### 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	345/377 (92%)	293 (85%)	52 (15%)	3	14
2	B	353/381 (93%)	302 (86%)	51 (14%)	3	16
All	All	698/758 (92%)	595 (85%)	103 (15%)	6	15

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	68	VAL

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Mol	Chain	Res	Type
2	B	205	ASP
2	B	382	THR
2	B	90	ASP
2	B	153	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	334	ASN
2	B	337	ASN
2	B	424	ASN
2	B	14	ASN
1	A	380	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	GTP	A	502	3	26,34,34	1.30	4 (15%)	32,54,54	1.10	2 (6%)
4	GTP	B	502	3	26,34,34	1.29	4 (15%)	32,54,54	1.10	2 (6%)

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	GTP	A	502	3	-	3/18/38/38	0/3/3/3
4	GTP	B	502	3	-	3/18/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	GTP	C5-C6	-3.66	1.40	1.47
4	B	502	GTP	C5-C6	-3.66	1.40	1.47
4	A	502	GTP	C6-N1	2.59	1.41	1.37
4	B	502	GTP	C6-N1	2.58	1.41	1.37
4	A	502	GTP	C8-N7	-2.45	1.30	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	502	GTP	O2G-PG-O3B	2.66	113.54	104.64
4	A	502	GTP	O2G-PG-O3B	2.64	113.49	104.64
4	A	502	GTP	O5'-C5'-C4'	2.07	116.12	108.99
4	B	502	GTP	O5'-C5'-C4'	2.07	116.12	108.99

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

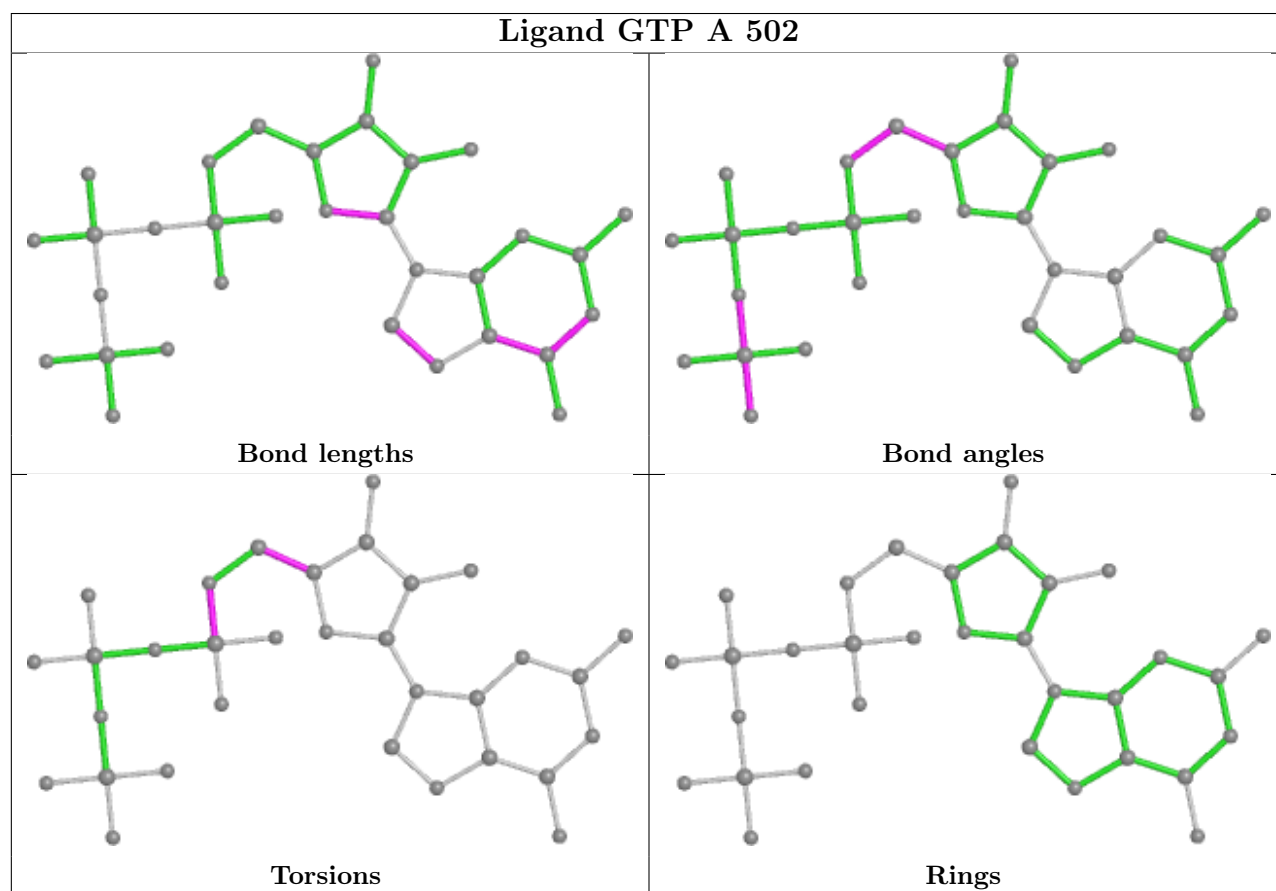
Mol	Chain	Res	Type	Atoms
4	A	502	GTP	C3'-C4'-C5'-O5'
4	B	502	GTP	C3'-C4'-C5'-O5'
4	A	502	GTP	O4'-C4'-C5'-O5'
4	B	502	GTP	O4'-C4'-C5'-O5'
4	A	502	GTP	C5'-O5'-PA-O1A

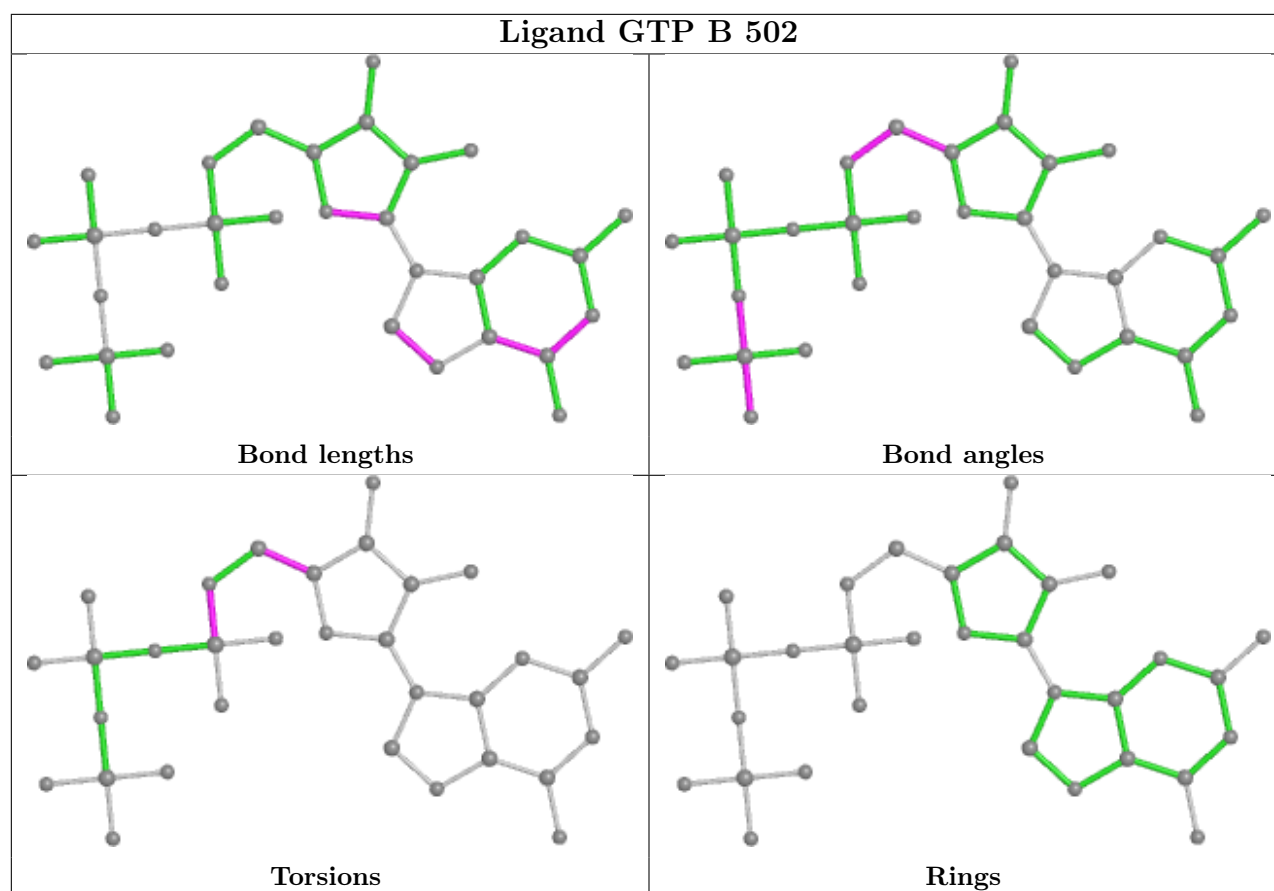
There are no ring outliers.

2 monomers are involved in 88 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	GTP	61	0
4	B	502	GTP	27	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

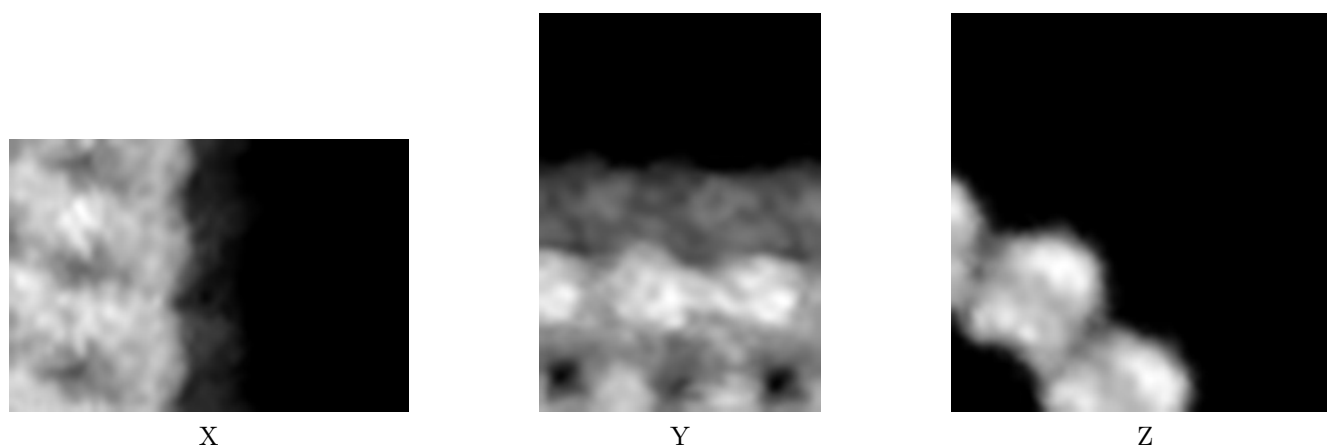
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2697. 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 [i](#)

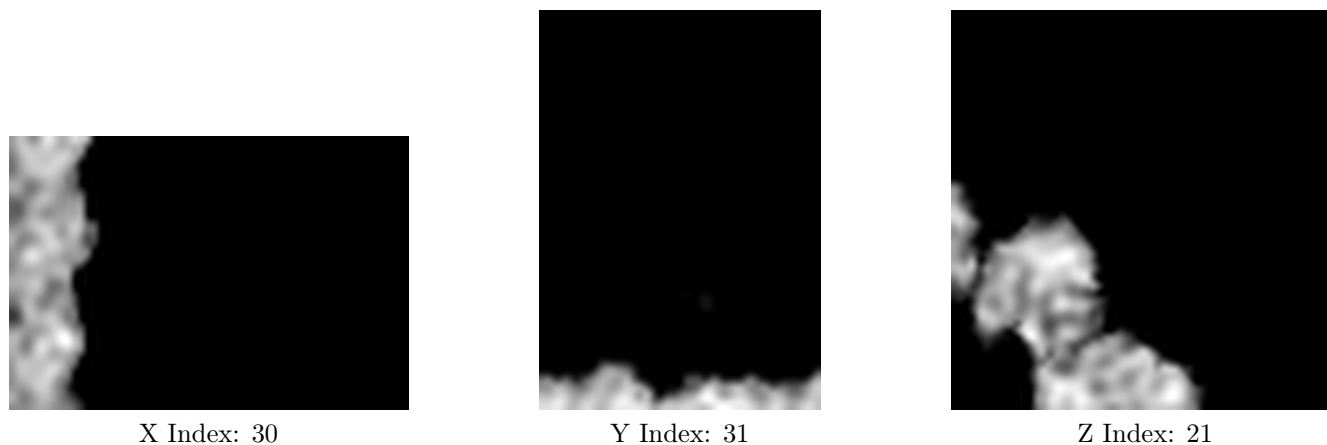
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

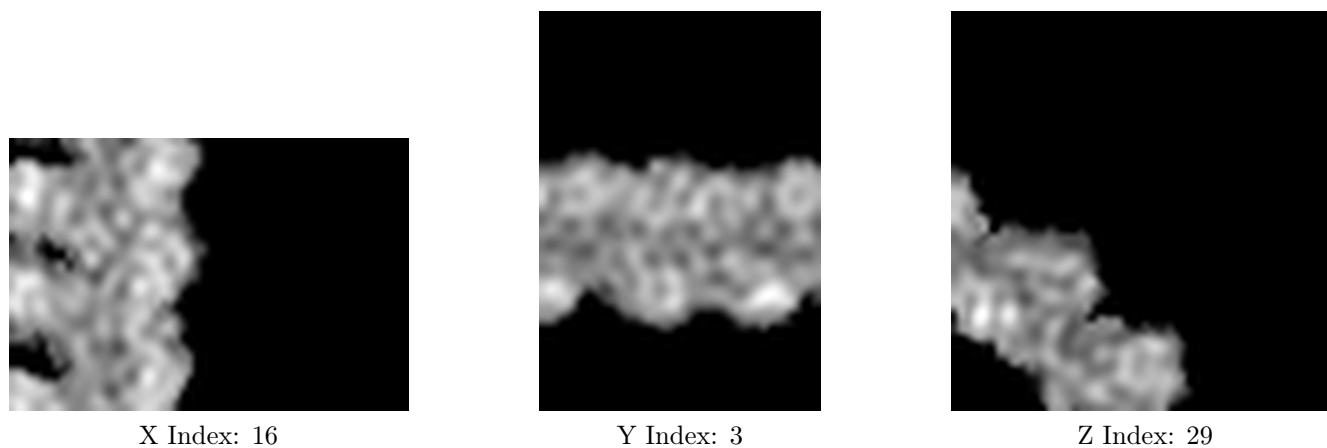
#### 6.2.1 Primary map



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

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

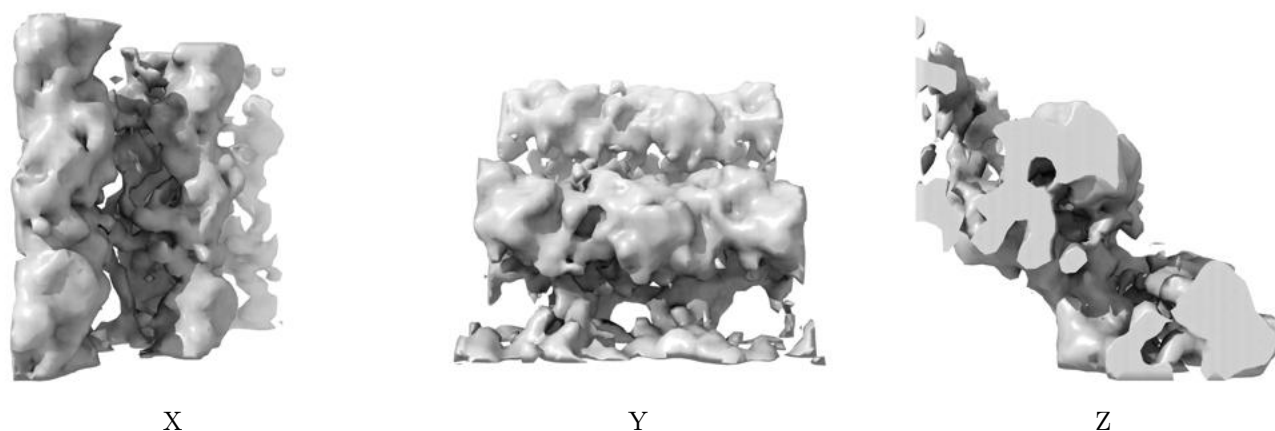
### 6.3.1 Primary map



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

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

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 156.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



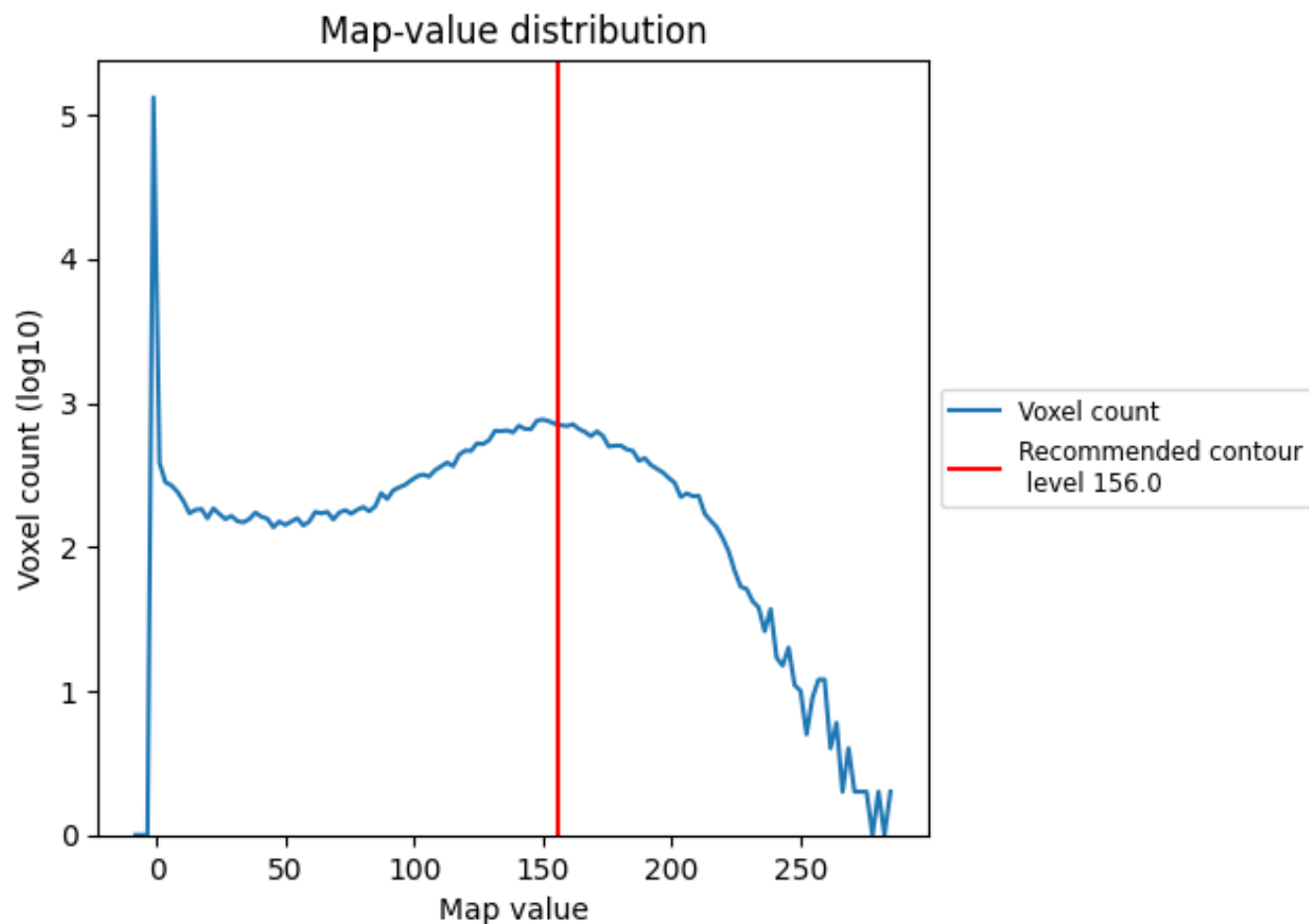
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

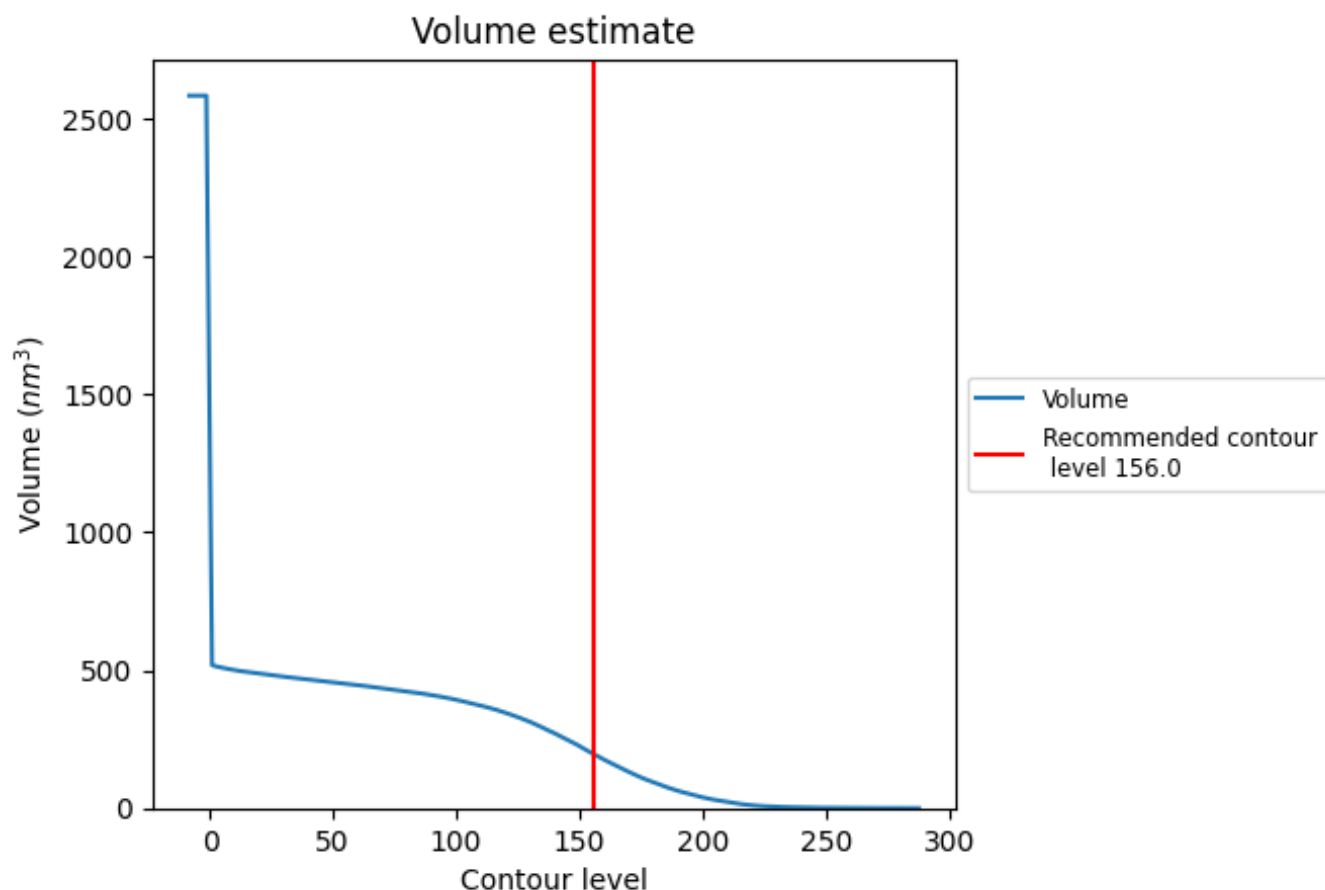
This section contains the results of statistical analysis of the map.

### 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 194 nm<sup>3</sup>; this corresponds to an approximate mass of 175 kDa.

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

## 7.3 Rotationally averaged power spectrum [i](#)

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

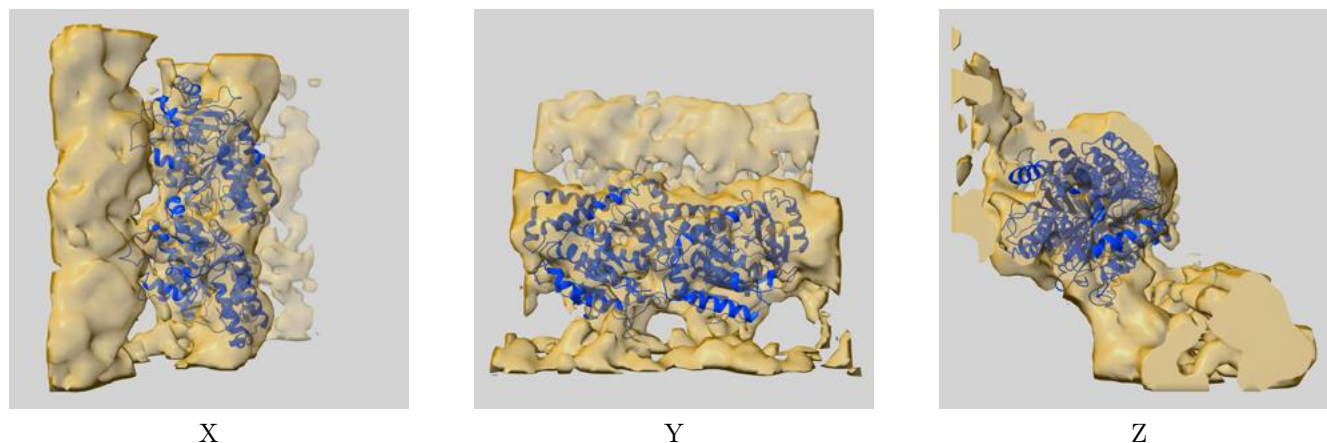
## 8 Fourier-Shell correlation

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

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

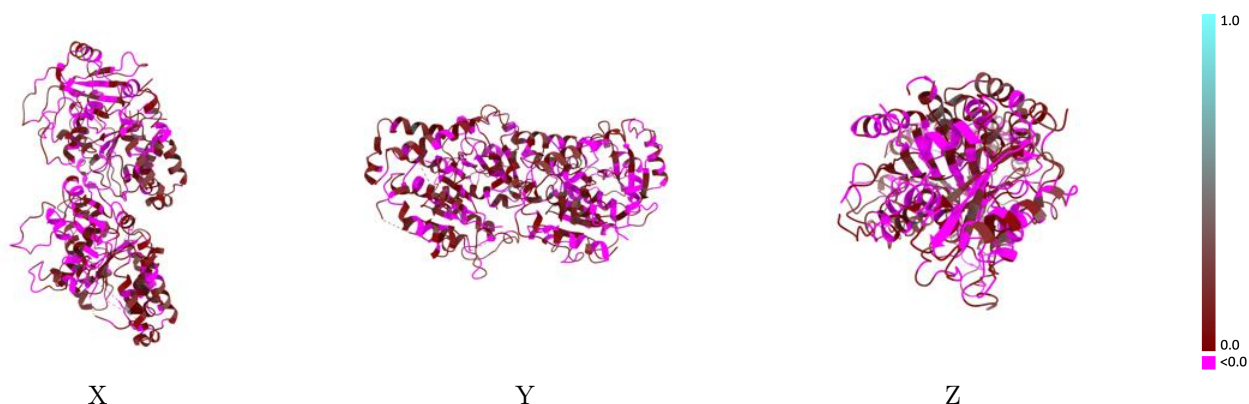
This section contains information regarding the fit between EMDB map EMD-2697 and PDB model 3J7I. Per-residue inclusion information can be found in section [3](#) on page [5](#).

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



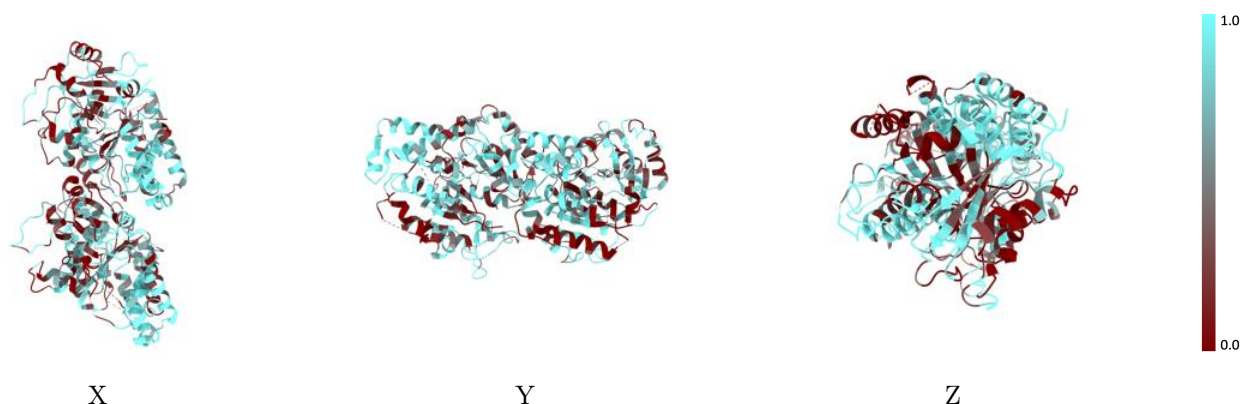
The images above show the 3D surface view of the map at the recommended contour level 156.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



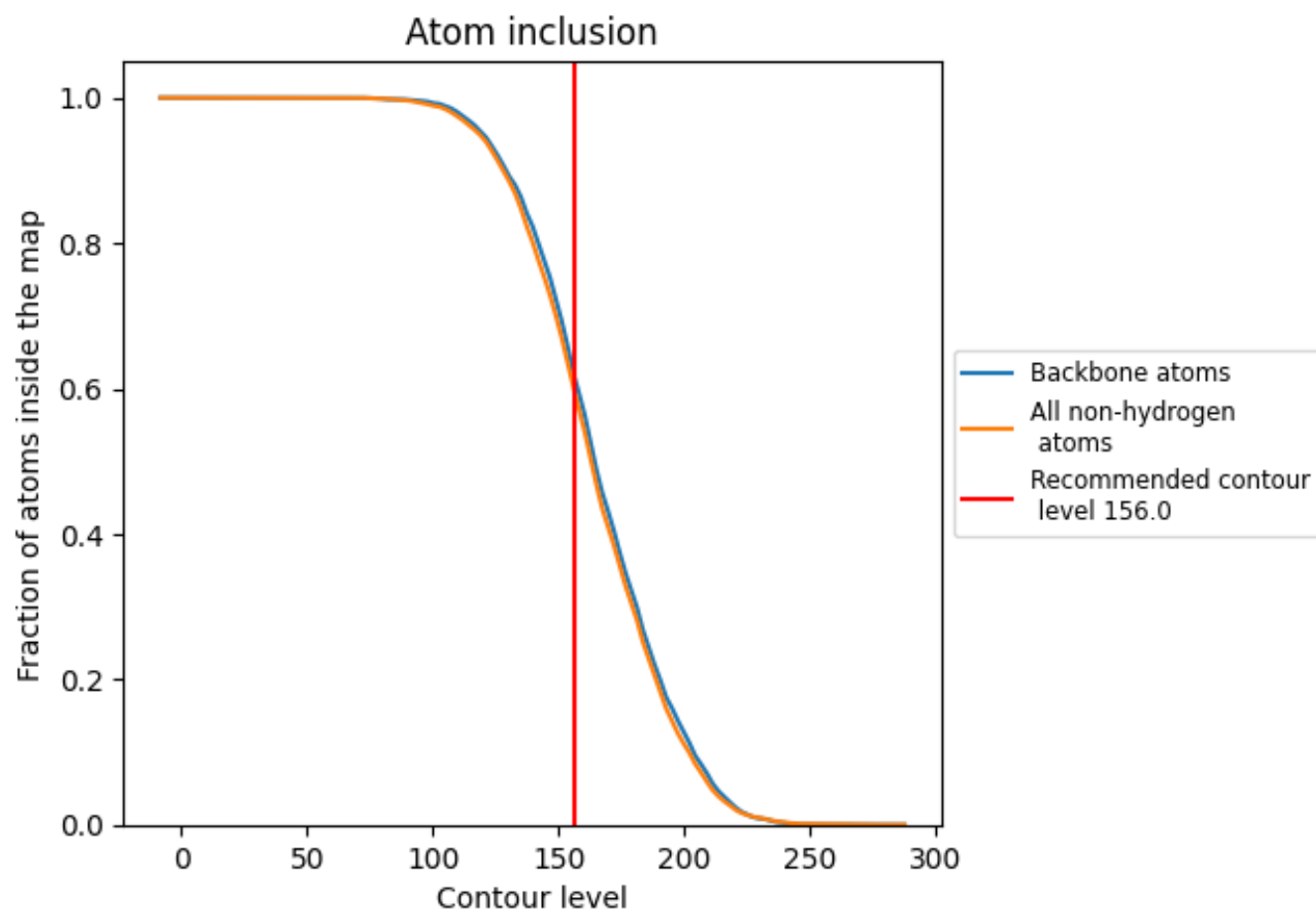
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (156.0).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 60% 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 (156.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5999	<div></div> 0.0380
A	<div></div> 0.5917	<div></div> 0.0340
B	<div></div> 0.6080	<div></div> 0.0420

