



## wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 01:26 AM EST

PDB ID : 7M2Y  
EMDB ID : EMD-23637  
Title : Closed conformation of the Yeast wild-type gamma-TuRC  
Authors : Brilot, A.F.; Lyon, A.S.; Zelter, A.; Viswanath, S.; Maxwell, A.; MacCoss, M.J.; Muller, E.G.; Sali, A.; Davis, T.N.; Agard, D.A.  
Deposited on : 2021-03-17  
Resolution : 4.03 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](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	:	<b>FAILED</b>
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

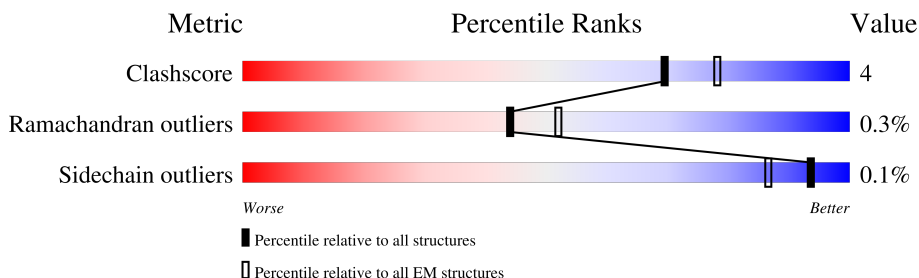
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.03 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	473	85% 8% 7%
1	B	473	87% 7% • 5%
2	C	846	68% 9% • 22%
3	D	823	79% 7% 15%
4	U	220	14% 86%

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
5	GDP	A	501	-	-	X	-
5	GDP	B	501	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18560 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 gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	441	Total	C	N	O	S	0	0
			3447	2156	582	693	16		
1	B	447	Total	C	N	O	S	0	0
			3491	2182	591	701	17		

- Molecule 2 is a protein called Spindle pole body component SPC98.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	656	Total	C	N	O	S	0	0
			5435	3518	899	1002	16		

- Molecule 3 is a protein called Spindle pole body component SPC97.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	703	Total	C	N	O	S	0	0
			5868	3781	984	1074	29		

- Molecule 4 is a protein called Spindle pole body component 110.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	31	Total	C	N	O	S	0	0
			263	162	49	50	2		

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



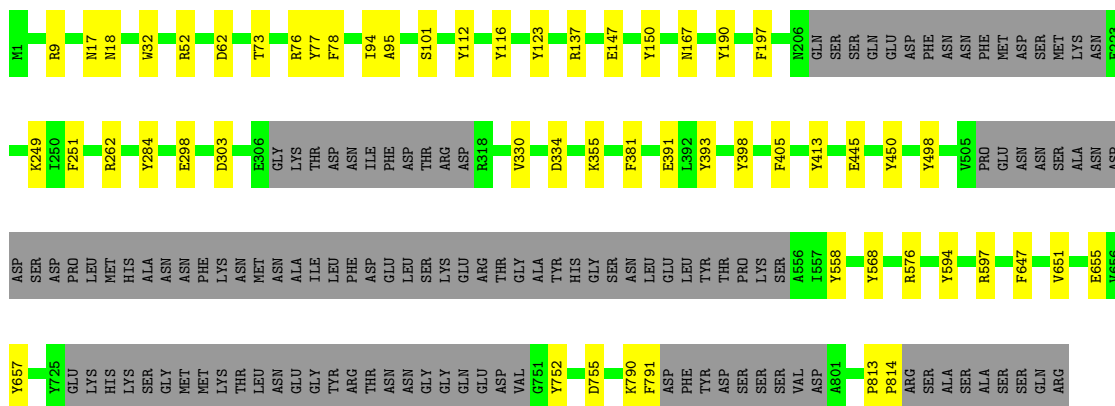
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	B	1	Total	C	N	O	P	0
			28	10	5	11	2	





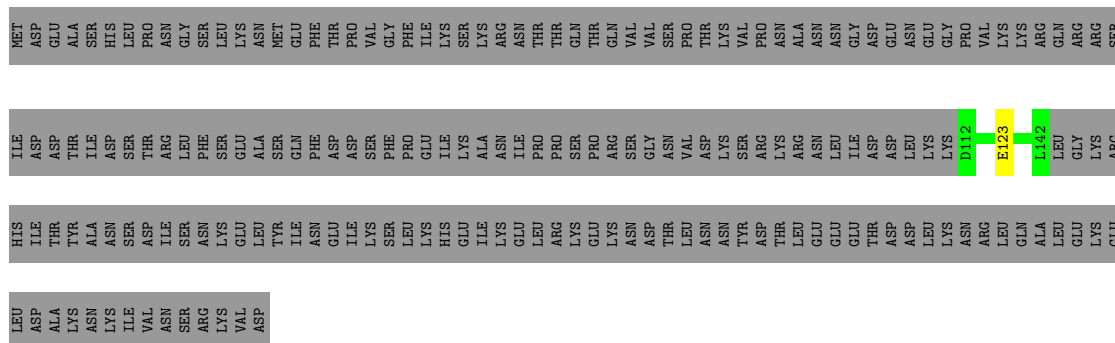
• Molecule 3: Spindle pole body component SPC97

Chain D: 79% 7% 15%



• Molecule 4: Spindle pole body component 110

Chain U: 14% 86%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=0°, rise=0.01 Å, axial sym=C1	Depositor
Number of segments used	20420	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Final reconstruction in cis-TEM	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	80	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	47214	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	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: GDP

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	1.10	7/3518 (0.2%)	0.98	6/4778 (0.1%)
1	B	1.07	7/3563 (0.2%)	1.02	11/4837 (0.2%)
2	C	1.28	31/5551 (0.6%)	0.99	20/7500 (0.3%)
3	D	1.22	28/5984 (0.5%)	0.96	12/8078 (0.1%)
4	U	1.21	1/266 (0.4%)	0.86	0/352
All	All	1.19	74/18882 (0.4%)	0.98	49/25545 (0.2%)

The worst 5 of 74 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	190	TYR	CB-CG	-11.62	1.34	1.51
2	C	288	TYR	CB-CG	-10.94	1.35	1.51
3	D	78	PHE	CB-CG	-10.01	1.34	1.51
2	C	349	TRP	CB-CG	-9.95	1.32	1.50
2	C	267	PHE	CB-CG	-9.22	1.35	1.51

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	413	TYR	CB-CG-CD2	-11.02	114.39	121.00
2	C	612	ARG	NE-CZ-NH2	-9.92	115.34	120.30
2	C	612	ARG	NE-CZ-NH1	8.36	124.48	120.30
2	C	533	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	A	217	PHE	CB-CG-CD1	8.11	126.48	120.80

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	3447	0	3305	29	0
1	B	3491	0	3349	40	0
2	C	5435	0	5462	54	0
3	D	5868	0	5932	13	0
4	U	263	0	266	0	0
5	A	28	0	12	13	0
5	B	28	0	11	31	0
All	All	18560	0	18337	135	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 4.

The worst 5 of 135 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:621:ASN:HB3	2:C:622:PRO:CD	1.17	1.46
1:B:174:PRO:CD	5:B:501:GDP:O3'	1.63	1.42
2:C:621:ASN:CB	2:C:622:PRO:CD	2.09	1.25
1:B:174:PRO:HD3	5:B:501:GDP:O3'	1.02	1.18
1:B:143:ALA:HB3	5:B:501:GDP:H4'	1.13	1.11

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	437/473 (92%)	420 (96%)	15 (3%)	2 (0%)	29	67
1	B	443/473 (94%)	432 (98%)	11 (2%)	0	100	100
2	C	650/846 (77%)	634 (98%)	12 (2%)	4 (1%)	25	63
3	D	691/823 (84%)	681 (99%)	10 (1%)	0	100	100
4	U	29/220 (13%)	28 (97%)	1 (3%)	0	100	100
All	All	2250/2835 (79%)	2195 (98%)	49 (2%)	6 (0%)	44	75

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	555	TRP
2	C	628	ILE
1	A	135	GLY
1	A	341	ARG
2	C	621	ASN

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	393/420 (94%)	393 (100%)	0	100	100
1	B	397/420 (94%)	395 (100%)	2 (0%)	88	93
2	C	613/787 (78%)	613 (100%)	0	100	100
3	D	659/766 (86%)	659 (100%)	0	100	100
4	U	30/206 (15%)	30 (100%)	0	100	100
All	All	2092/2599 (80%)	2090 (100%)	2 (0%)	93	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	192	ARG
1	B	248	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	12	GLN
3	D	485	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	$\# Z  > 2$
5	GDP	A	501	-	24,30,30	0.97	0	30,47,47	1.17	4 (13%)
5	GDP	B	501	-	24,30,30	0.96	0	30,47,47	1.17	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GDP	A	501	-	-	3/12/32/32	0/3/3/3
5	GDP	B	501	-	-	3/12/32/32	0/3/3/3

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	GDP	C5-C6-N1	2.71	118.73	113.95
5	A	501	GDP	C5-C6-N1	2.69	118.70	113.95
5	B	501	GDP	PA-O3A-PB	-2.65	123.73	132.83
5	A	501	GDP	PA-O3A-PB	-2.64	123.77	132.83
5	B	501	GDP	C8-N7-C5	2.39	107.55	102.99

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

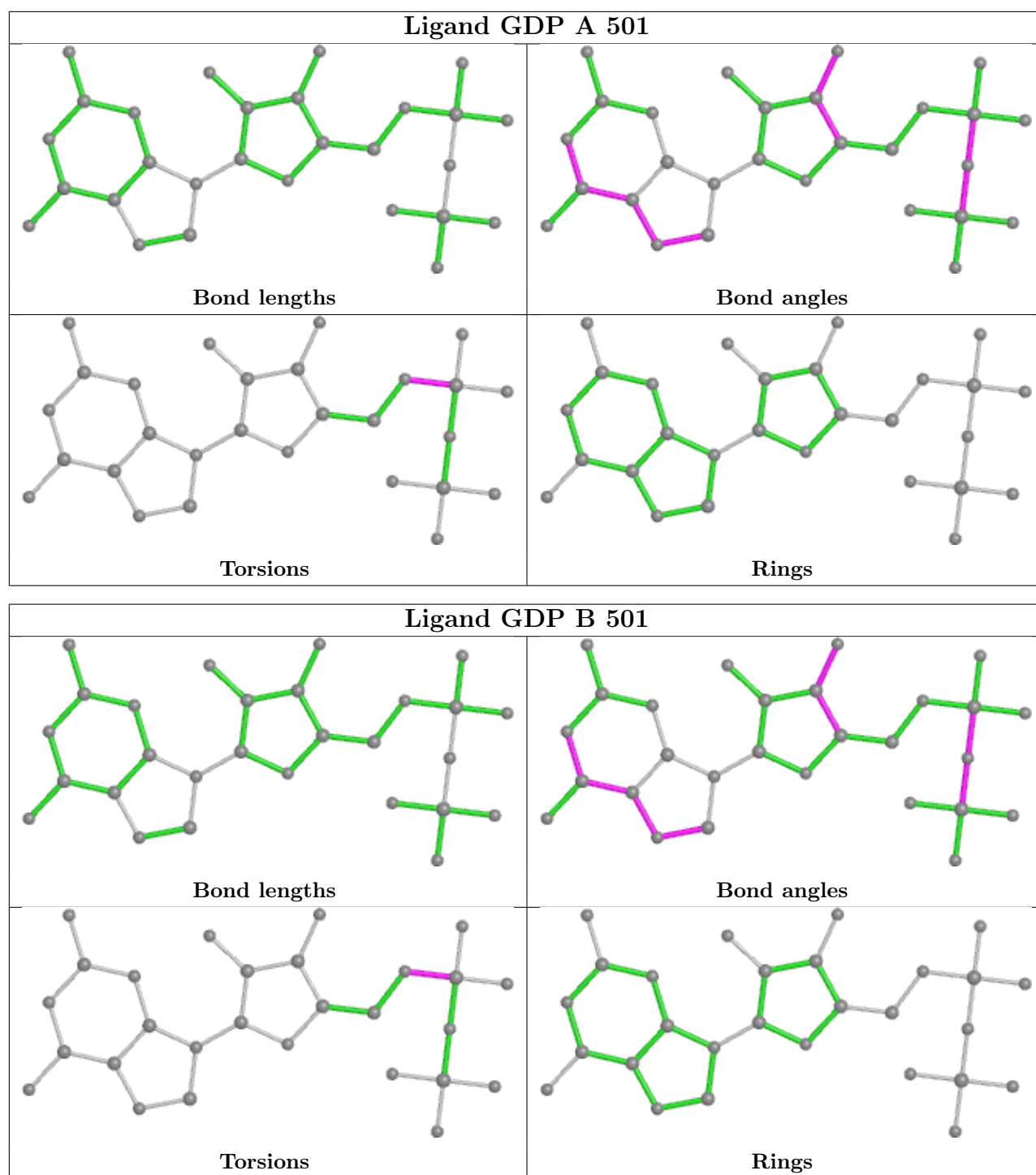
Mol	Chain	Res	Type	Atoms
5	A	501	GDP	C5'-O5'-PA-O2A
5	B	501	GDP	C5'-O5'-PA-O2A
5	A	501	GDP	C5'-O5'-PA-O3A
5	B	501	GDP	C5'-O5'-PA-O3A
5	A	501	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

2 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GDP	13	0
5	B	501	GDP	31	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

This section contains visualisations of the EMDB entry EMD-23637. 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

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal surface views

This section was not generated.

### 6.5 Mask visualisation

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 ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.



## 8 Fourier-Shell correlation

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

## 9 Map-model fit

This section was not generated.