



wwPDB EM Validation Summary Report ⓘ

Mar 19, 2026 – 07:49 PM UTC

PDB ID : 8AC0 / pdb_00008ac0
EMDB ID : EMD-15329
Title : RNA polymerase at U-rich pause bound to regulatory RNA putL - active, closed clamp state
Authors : Weixlbaumer, A.; Dey, S.
Deposited on : 2022-07-05
Resolution : 4.10 Å(reported)
Based on initial model : 6ALH

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

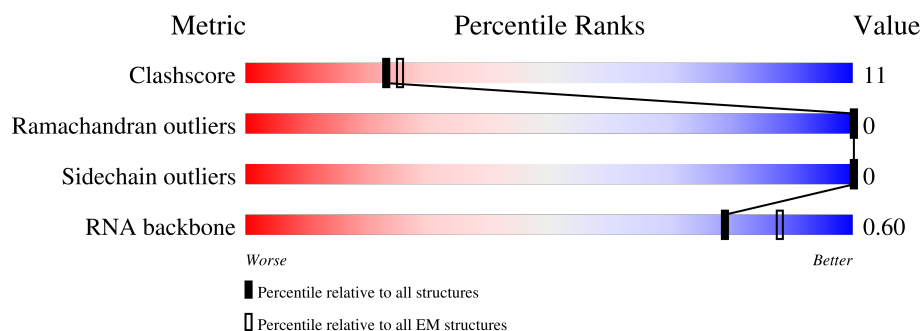
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	329	54% 13% 33%
1	B	329	47% 19% 34%
2	C	1342	76% 24%
3	D	1406	69% 26% 5%
4	E	91	52% 29% 20%
5	N	266	6% 91%
6	R	93	24% 53% 12% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	T	266	6%8%86%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 27948 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	221	Total	C	N	O	S	0	0
			1706	1068	300	332	6		
1	B	218	Total	C	N	O	S	0	0
			1683	1051	297	329	6		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1341	Total	C	N	O	S	0	0
			10577	6636	1842	2056	43		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1335	Total	C	N	O	S	0	0
			10388	6526	1854	1958	50		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	73	Total	C	N	O	S	0	0
			582	355	111	115	1		

- Molecule 5 is a DNA chain called DNA Non-template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	25	Total	C	N	O	P	0	0
			514	245	94	150	25		

- Molecule 6 is a RNA chain called putL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	82	Total	C	N	O	P	0	0
			1756	782	315	577	82		

- Molecule 7 is a DNA chain called DNA Template strand.

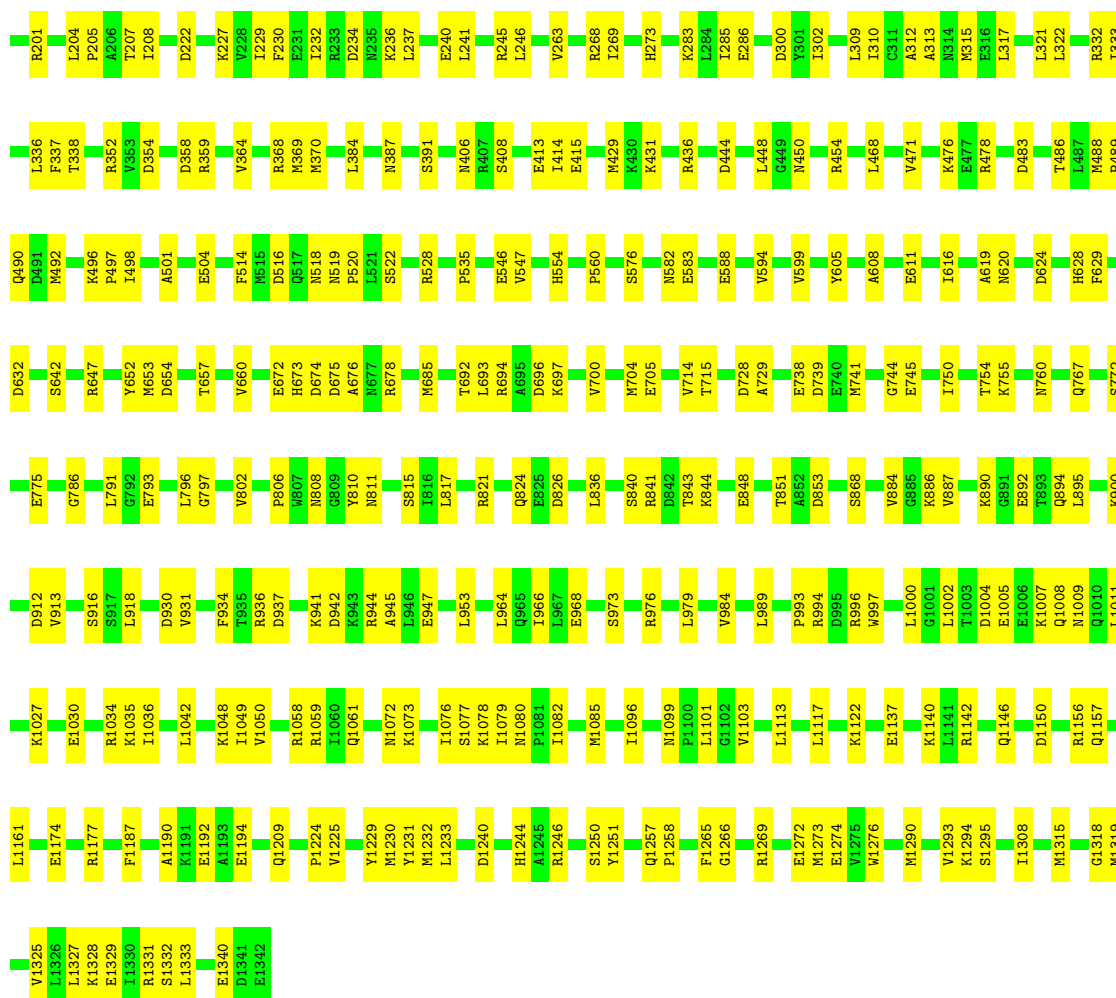
Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	36	Total	C	N	O	P	0	0
			739	351	141	211	36		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
8	D	1	Total	Mg	0
			1	1	

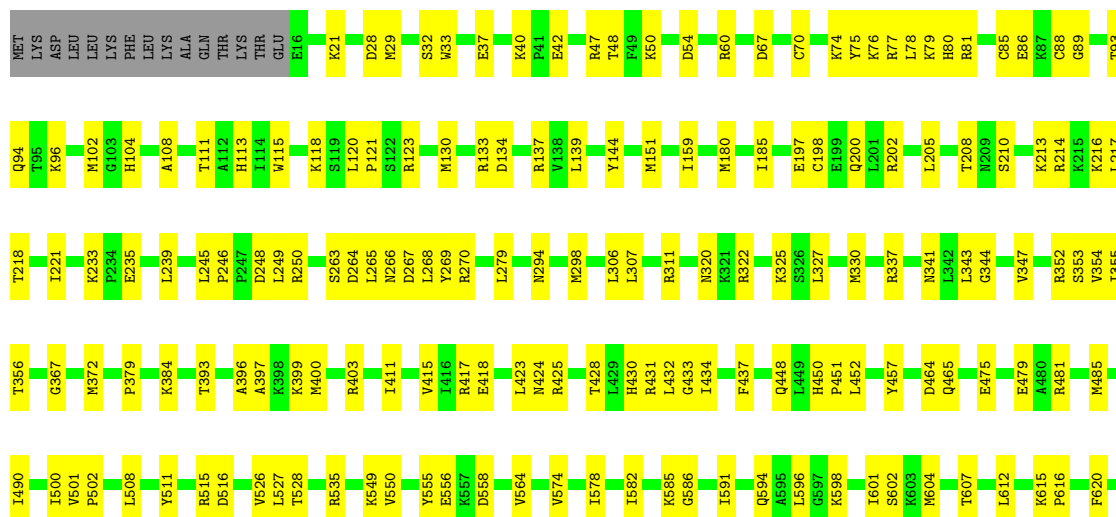
- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
9	D	2	Total	Zn	0
			2	2	



• Molecule 3: DNA-directed RNA polymerase subunit beta'

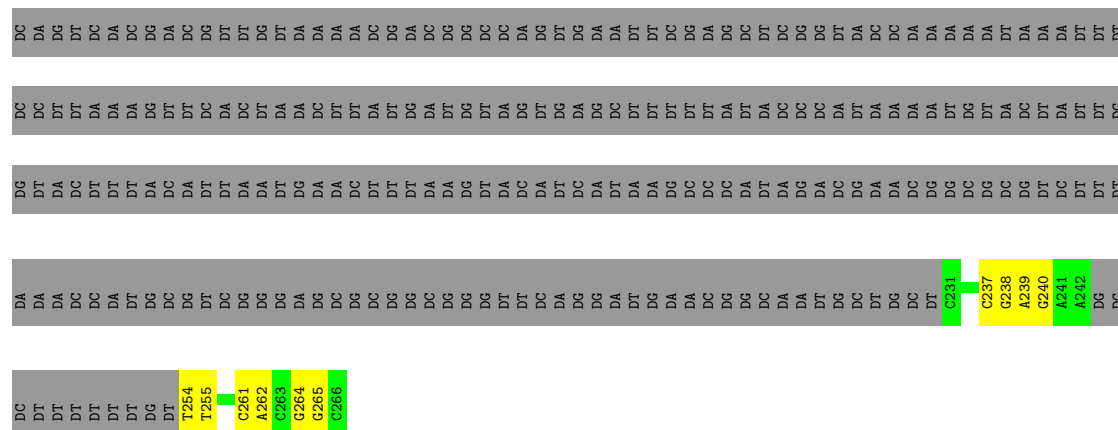
Chain D: 69% 26% 5%



- Molecule 4: DNA-directed RNA polymerase subunit omega



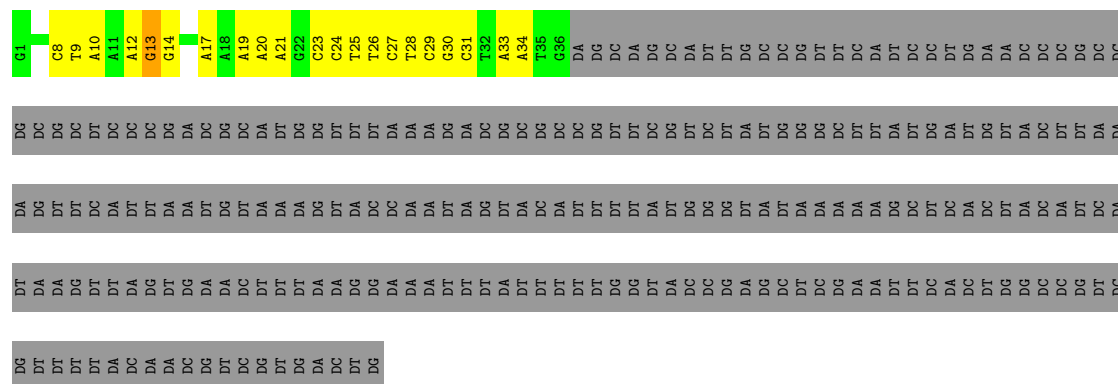
- Molecule 5: DNA Non-template strand



- Molecule 6: putL RNA



- Molecule 7: DNA Template strand



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	81468	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k 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: ZN, IGU, 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	0.10	0/1726	0.29	0/2338
1	B	0.09	0/1702	0.25	0/2306
2	C	0.10	0/10746	0.28	0/14499
3	D	0.11	0/10545	0.30	0/14236
4	E	0.16	0/584	0.43	0/786
5	N	0.17	0/575	0.38	0/883
6	R	0.10	0/1962	0.27	0/3056
7	T	0.19	0/779	0.38	0/1196
All	All	0.11	0/28619	0.30	0/39300

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1706	0	1746	30	0
1	B	1683	0	1719	44	0
2	C	10577	0	10591	220	0
3	D	10388	0	10610	259	0
4	E	582	0	593	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	N	514	0	284	8	0
6	R	1756	0	884	61	0
7	T	739	0	404	16	0
8	D	1	0	0	0	0
9	D	2	0	0	0	0
All	All	27948	0	26831	606	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 11.

The worst 5 of 606 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:D:245:LEU:HD12	3:D:246:PRO:HD2	1.59	0.84
6:R:12:G:H1	6:R:32:U:H3	1.29	0.81
4:E:72:GLN:HE22	4:E:73:GLN:HE21	1.33	0.77
3:D:481:ARG:HA	3:D:485:MET:HE3	1.70	0.74
1:A:12:ARG:H	1:A:29:GLU:HB2	1.53	0.73

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	217/329 (66%)	209 (96%)	8 (4%)	0	100	100
1	B	214/329 (65%)	210 (98%)	4 (2%)	0	100	100
2	C	1339/1342 (100%)	1285 (96%)	54 (4%)	0	100	100
3	D	1329/1406 (94%)	1277 (96%)	52 (4%)	0	100	100
4	E	71/91 (78%)	65 (92%)	6 (8%)	0	100	100
All	All	3170/3497 (91%)	3046 (96%)	124 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	189/286 (66%)	189 (100%)	0	100	100
1	B	187/286 (65%)	187 (100%)	0	100	100
2	C	1156/1157 (100%)	1156 (100%)	0	100	100
3	D	1120/1167 (96%)	1120 (100%)	0	100	100
4	E	63/75 (84%)	63 (100%)	0	100	100
All	All	2715/2971 (91%)	2715 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
4	E	29	GLN
3	D	954	ASN
2	C	1237	HIS
3	D	865	HIS
2	C	1220	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	R	80/93 (86%)	17 (21%)	1 (1%)

5 of 17 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	R	3	A
6	R	8	A
6	R	9	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	R	22	A
6	R	23	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	R	54	A

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

2 non-standard protein/DNA/RNA residues 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
7	IGU	T	13	5,7	21,24,25	1.24	3 (14%)	29,35,38	1.72	5 (17%)
7	IGU	T	14	7	21,24,25	1.24	2 (9%)	29,35,38	1.81	6 (20%)

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
7	IGU	T	13	5,7	-	2/7/21/22	0/3/3/3
7	IGU	T	14	7	-	1/7/21/22	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	14	IGU	C5-C6	3.66	1.48	1.40
7	T	13	IGU	C5-C6	3.03	1.46	1.40
7	T	13	IGU	C5-N7	-2.44	1.34	1.39
7	T	13	IGU	C4-N9	-2.33	1.32	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	14	IGU	C5-N7	-2.26	1.34	1.39

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	13	IGU	C6-C5-N7	4.53	135.79	130.21
7	T	14	IGU	C6-C5-N7	4.42	135.65	130.21
7	T	14	IGU	C5-C4-N3	-4.33	118.72	127.60
7	T	13	IGU	C5-C4-N3	-3.48	120.46	127.60
7	T	14	IGU	N9-C4-N3	3.43	134.89	127.05

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	T	13	IGU	C3'-C4'-C5'-O5'
7	T	13	IGU	O4'-C4'-C5'-O5'
7	T	14	IGU	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	13	IGU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 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.

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-15329. 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 standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 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.