W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB EM Validation Summary Report ⓘ

Apr 1, 2025 – 06:44 pm BST

PDB ID	:	6ZRQ / pdb_00006zrq
EMDB ID	:	EMD-11382
Title	:	two-protofilament amyloid structure of S20G variant of human amylin (IAPP - islet amyloid polypeptide)
Authors	:	Gallardo, R.U.; Iadanza, M.G.; Ranson, N.A.; Radford, S.E.
Deposited on	:	2020-07-14
Resolution	:	3.90 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 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:

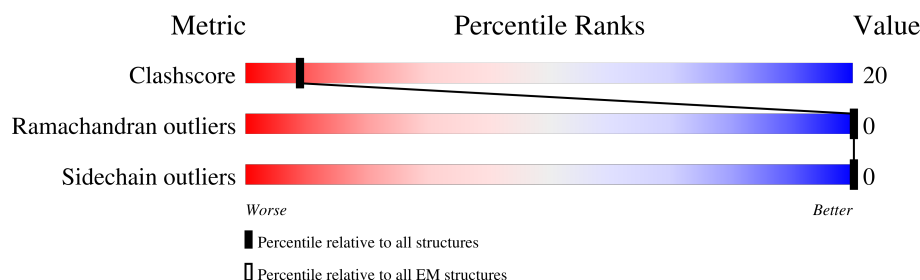|		
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 3.90 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.
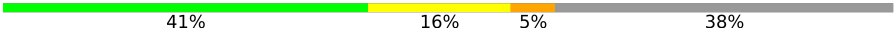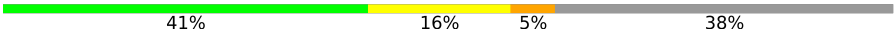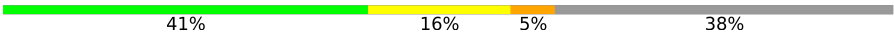
Metric	Percentile Ranks	Value
Clashscore		20
Ramachandran outliers		0
Sidechain outliers		0

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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%

Mol	Chain	Length	Quality of chain
1	A	37	41% 16% 5% 38%
1	B	37	43% 14% 5% 38%
1	C	37	43% 14% 5% 38%
1	D	37	43% 14% 5% 38%
1	E	37	49% 11% • 38%
1	F	37	43% 16% • 38%
1	G	37	43% 16% • 38%
1	H	37	41% 16% 5% 38%
1	I	37	43% 14% 5% 38%

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Mol	Chain	Length	Quality of chain
1	J	37	41% 16% 5% 38%
1	K	37	41% 16% 5% 38%
1	L	37	41% 16% 5% 38%

2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 3948 atoms, of which 1908 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 Islet amyloid polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	23	Total 329	C 106	H 159	N 30	O 34	0	0
1	B	23	Total 329	C 106	H 159	N 30	O 34	0	0
1	C	23	Total 329	C 106	H 159	N 30	O 34	0	0
1	D	23	Total 329	C 106	H 159	N 30	O 34	0	0
1	E	23	Total 329	C 106	H 159	N 30	O 34	0	0
1	F	23	Total 329	C 106	H 159	N 30	O 34	0	0
1	G	23	Total 329	C 106	H 159	N 30	O 34	0	0
1	H	23	Total 329	C 106	H 159	N 30	O 34	0	0
1	I	23	Total 329	C 106	H 159	N 30	O 34	0	0
1	J	23	Total 329	C 106	H 159	N 30	O 34	0	0
1	K	23	Total 329	C 106	H 159	N 30	O 34	0	0
1	L	23	Total 329	C 106	H 159	N 30	O 34	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLY	SER	engineered mutation	UNP P10997
A	37	TYC	TYR	modified residue	UNP P10997
B	20	GLY	SER	engineered mutation	UNP P10997
B	37	TYC	TYR	modified residue	UNP P10997
C	20	GLY	SER	engineered mutation	UNP P10997
C	37	TYC	TYR	modified residue	UNP P10997

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Chain	Residue	Modelled	Actual	Comment	Reference
D	20	GLY	SER	engineered mutation	UNP P10997
D	37	TYC	TYR	modified residue	UNP P10997
E	20	GLY	SER	engineered mutation	UNP P10997
E	37	TYC	TYR	modified residue	UNP P10997
F	20	GLY	SER	engineered mutation	UNP P10997
F	37	TYC	TYR	modified residue	UNP P10997
G	20	GLY	SER	engineered mutation	UNP P10997
G	37	TYC	TYR	modified residue	UNP P10997
H	20	GLY	SER	engineered mutation	UNP P10997
H	37	TYC	TYR	modified residue	UNP P10997
I	20	GLY	SER	engineered mutation	UNP P10997
I	37	TYC	TYR	modified residue	UNP P10997
J	20	GLY	SER	engineered mutation	UNP P10997
J	37	TYC	TYR	modified residue	UNP P10997
K	20	GLY	SER	engineered mutation	UNP P10997
K	37	TYC	TYR	modified residue	UNP P10997
L	20	GLY	SER	engineered mutation	UNP P10997
L	37	TYC	TYR	modified residue	UNP P10997

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. 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. 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.
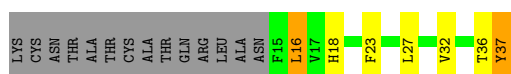
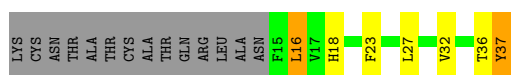• Molecule 1: Islet amyloid polypeptide

Chain A:
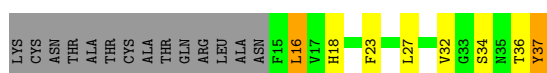
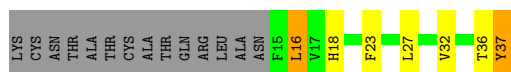• Molecule 1: Islet amyloid polypeptide

Chain B:

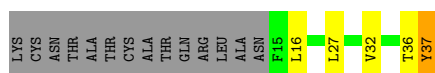• Molecule 1: Islet amyloid polypeptide

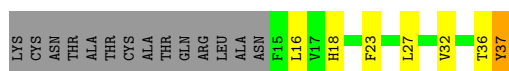Chain C:

• Molecule 1: Islet amyloid polypeptide

Chain D:

• Molecule 1: Islet amyloid polypeptide

Chain E:

• Molecule 1: Islet amyloid polypeptide

Chain F:

LYS CYS ASN THR ALA THR CYS ALA THR GLN ARG LEU ALA ASN F15 L16 V17 H18 F23 L27 V32 T36 Y37

• Molecule 1: Islet amyloid polypeptide

Chain G: 43%   16%   •   38%

LYS CYS ASN THR ALA THR CYS ALA THR GLN ARG LEU ALA ASN F15 L16 V17 H18 F23 L27 V32 T36 Y37

• Molecule 1: Islet amyloid polypeptide

Chain H: 41%   16%   5%   38%

LYS CYS ASN THR ALA THR CYS ALA THR GLN ARG LEU ALA ASN F15 L16 V17 H18 F23 L27 V32 G33 S34 N35 T36 Y37

• Molecule 1: Islet amyloid polypeptide

Chain I: 43%   14%   5%   38%

LYS CYS ASN THR ALA THR CYS ALA THR GLN ARG LEU ALA ASN F15 L16 V17 H18 F23 L27 V32 T36 Y37

• Molecule 1: Islet amyloid polypeptide

Chain J: 41%   16%   5%   38%

LYS CYS ASN THR ALA THR CYS ALA THR GLN ARG LEU ALA ASN F15 L16 V17 H18 F23 L27 V32 G33 S34 N35 T36 Y37

• Molecule 1: Islet amyloid polypeptide

Chain K: 41%   16%   5%   38%

LYS CYS ASN THR ALA THR CYS ALA THR GLN ARG LEU ALA ASN F15 L16 V17 H18 F23 L27 V32 G33 S34 N35 T36 Y37

• Molecule 1: Islet amyloid polypeptide

Chain L: 41%   16%   5%   38%

LYS CYS ASN THR ALA THR CYS ALA THR GLN ARG LEU ALA ASN F15 L16 V17 H18 F23 L27 V32 G33 S34 N35 T36 Y37

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=179.05°, rise=2.41 Å, axial sym=C1	Depositor
Number of segments used	11901	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 $(e^-/\text{Å}^2)$	54.73	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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

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	0.44	0/159	0.69	1/215 (0.5%)
1	B	0.44	0/159	0.69	1/215 (0.5%)
1	C	0.44	0/159	0.69	1/215 (0.5%)
1	D	0.44	0/159	0.69	1/215 (0.5%)
1	E	0.44	0/159	0.69	1/215 (0.5%)
1	F	0.43	0/159	0.69	1/215 (0.5%)
1	G	0.44	0/159	0.69	1/215 (0.5%)
1	H	0.44	0/159	0.69	1/215 (0.5%)
1	I	0.44	0/159	0.69	1/215 (0.5%)
1	J	0.44	0/159	0.69	1/215 (0.5%)
1	K	0.44	0/159	0.69	1/215 (0.5%)
1	L	0.44	0/159	0.69	1/215 (0.5%)
All	All	0.44	0/1908	0.69	12/2580 (0.5%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	16	LEU	CA-CB-CG	5.55	128.07	115.30
1	K	16	LEU	CA-CB-CG	5.54	128.05	115.30
1	C	16	LEU	CA-CB-CG	5.54	128.04	115.30
1	D	16	LEU	CA-CB-CG	5.54	128.03	115.30
1	F	16	LEU	CA-CB-CG	5.53	128.03	115.30

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	170	159	157	9	0
1	B	170	159	157	11	0
1	C	170	159	157	10	0
1	D	170	159	157	14	0
1	E	170	159	157	6	0
1	F	170	159	157	10	0
1	G	170	159	157	8	0
1	H	170	159	157	11	0
1	I	170	159	157	14	0
1	J	170	159	157	15	0
1	K	170	159	157	11	0
1	L	170	159	157	12	0
All	All	2040	1908	1884	80	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 20.

The worst 5 of 80 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:J:36:THR:HA	1:L:36:THR:HG22	1.83	0.59
1:H:32:VAL:HG12	1:H:32:VAL:O	2.03	0.59
1:B:32:VAL:HG12	1:B:32:VAL:O	2.03	0.59
1:J:32:VAL:HG12	1:J:32:VAL:O	2.03	0.59
1:D:32:VAL:HG12	1:D:32:VAL:O	2.03	0.58

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	21/37 (57%)	20 (95%)	1 (5%)	0	100	100
1	B	21/37 (57%)	20 (95%)	1 (5%)	0	100	100
1	C	21/37 (57%)	20 (95%)	1 (5%)	0	100	100
1	D	21/37 (57%)	20 (95%)	1 (5%)	0	100	100
1	E	21/37 (57%)	20 (95%)	1 (5%)	0	100	100
1	F	21/37 (57%)	20 (95%)	1 (5%)	0	100	100
1	G	21/37 (57%)	20 (95%)	1 (5%)	0	100	100
1	H	21/37 (57%)	20 (95%)	1 (5%)	0	100	100
1	I	21/37 (57%)	20 (95%)	1 (5%)	0	100	100
1	J	21/37 (57%)	20 (95%)	1 (5%)	0	100	100
1	K	21/37 (57%)	20 (95%)	1 (5%)	0	100	100
1	L	21/37 (57%)	20 (95%)	1 (5%)	0	100	100
All	All	252/444 (57%)	240 (95%)	12 (5%)	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	18/29 (62%)	18 (100%)	0	100	100
1	B	18/29 (62%)	18 (100%)	0	100	100
1	C	18/29 (62%)	18 (100%)	0	100	100
1	D	18/29 (62%)	18 (100%)	0	100	100
1	E	18/29 (62%)	18 (100%)	0	100	100
1	F	18/29 (62%)	18 (100%)	0	100	100
1	G	18/29 (62%)	18 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	18/29 (62%)	18 (100%)	0	100	100
1	I	18/29 (62%)	18 (100%)	0	100	100
1	J	18/29 (62%)	18 (100%)	0	100	100
1	K	18/29 (62%)	18 (100%)	0	100	100
1	L	18/29 (62%)	18 (100%)	0	100	100
All	All	216/348 (62%)	216 (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 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	35	ASN
1	L	35	ASN
1	F	35	ASN
1	G	35	ASN
1	H	18	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)

12 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	$\#\|Z\| > 2$
1	TYC	F	37	1	13,13,13	0.26	0	17,17,17	0.81	1 (5%)
1	TYC	C	37	1	13,13,13	0.26	0	17,17,17	0.82	1 (5%)
1	TYC	J	37	1	13,13,13	0.26	0	17,17,17	0.80	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	TYC	G	37	1	13,13,13	0.26	0	17,17,17	0.82	1 (5%)
1	TYC	H	37	1	13,13,13	0.27	0	17,17,17	0.81	1 (5%)
1	TYC	I	37	1	13,13,13	0.26	0	17,17,17	0.81	1 (5%)
1	TYC	K	37	1	13,13,13	0.27	0	17,17,17	0.81	1 (5%)
1	TYC	A	37	1	13,13,13	0.26	0	17,17,17	0.81	1 (5%)
1	TYC	B	37	1	13,13,13	0.26	0	17,17,17	0.82	1 (5%)
1	TYC	L	37	1	13,13,13	0.27	0	17,17,17	0.81	1 (5%)
1	TYC	E	37	1	13,13,13	0.27	0	17,17,17	0.82	1 (5%)
1	TYC	D	37	1	13,13,13	0.27	0	17,17,17	0.81	1 (5%)

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
1	TYC	F	37	1	-	4/8/8/8	0/1/1/1
1	TYC	C	37	1	-	4/8/8/8	0/1/1/1
1	TYC	J	37	1	-	4/8/8/8	0/1/1/1
1	TYC	G	37	1	-	4/8/8/8	0/1/1/1
1	TYC	H	37	1	-	4/8/8/8	0/1/1/1
1	TYC	I	37	1	-	4/8/8/8	0/1/1/1
1	TYC	K	37	1	-	4/8/8/8	0/1/1/1
1	TYC	A	37	1	-	4/8/8/8	0/1/1/1
1	TYC	B	37	1	-	4/8/8/8	0/1/1/1
1	TYC	L	37	1	-	4/8/8/8	0/1/1/1
1	TYC	E	37	1	-	4/8/8/8	0/1/1/1
1	TYC	D	37	1	-	4/8/8/8	0/1/1/1

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	37	TYC	CG-CB-CA	-2.07	109.81	114.13
1	I	37	TYC	CG-CB-CA	-2.07	109.82	114.13
1	E	37	TYC	CG-CB-CA	-2.07	109.82	114.13
1	K	37	TYC	CG-CB-CA	-2.07	109.82	114.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	37	TYC	CG-CB-CA	-2.07	109.83	114.13

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	37	TYC	O-C-CA-N
1	A	37	TYC	NXT-C-CA-N
1	A	37	TYC	O-C-CA-CB
1	A	37	TYC	NXT-C-CA-CB
1	B	37	TYC	O-C-CA-N

There are no ring outliers.

12 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	37	TYC	2	0
1	C	37	TYC	3	0
1	J	37	TYC	3	0
1	G	37	TYC	1	0
1	H	37	TYC	2	0
1	I	37	TYC	2	0
1	K	37	TYC	2	0
1	A	37	TYC	2	0
1	B	37	TYC	3	0
1	L	37	TYC	3	0
1	E	37	TYC	2	0
1	D	37	TYC	3	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11382. 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)

This section was not generated.

6.2   Central slices (i)

This section was not generated.

6.3   Largest variance slices (i)

This section was not generated.

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

This section was not generated.

6.5   Orthogonal surface views (i)

This section was not generated.

6.6   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 ⓘ

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 (i)

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

9 Map-model fit (i)

This section was not generated.