



Full wwPDB EM Validation Report ⓘ

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PDB ID : 7L2N / pdb_00007l2n
EMDB ID : EMD-23134
Title : Cryo-EM structure of RTX-bound full-length TRPV1 in C1 state
Authors : Zhang, K.; Julius, D.; Cheng, Y.
Deposited on : 2020-12-17
Resolution : 3.09 Å(reported)

This is a Full wwPDB EM Validation 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

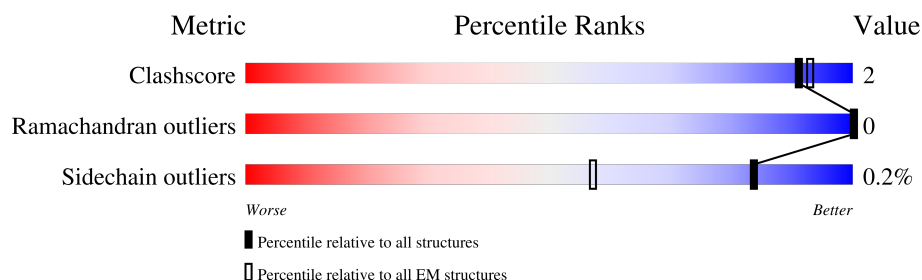
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.09 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

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	842	
1	B	842	
1	C	842	
1	D	842	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14724 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 Transient receptor potential cation channel subfamily V member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	445	Total	C	N	O	S	0	0
			3635	2387	582	643	23		
1	C	445	Total	C	N	O	S	0	0
			3635	2387	582	643	23		
1	D	445	Total	C	N	O	S	0	0
			3635	2387	582	643	23		
1	B	445	Total	C	N	O	S	0	0
			3635	2387	582	643	23		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP O35433
A	-2	ALA	-	expression tag	UNP O35433
A	-1	MET	-	expression tag	UNP O35433
A	0	GLY	-	expression tag	UNP O35433
A	1	SER	-	expression tag	UNP O35433
C	-3	GLY	-	expression tag	UNP O35433
C	-2	ALA	-	expression tag	UNP O35433
C	-1	MET	-	expression tag	UNP O35433
C	0	GLY	-	expression tag	UNP O35433
C	1	SER	-	expression tag	UNP O35433
D	-3	GLY	-	expression tag	UNP O35433
D	-2	ALA	-	expression tag	UNP O35433
D	-1	MET	-	expression tag	UNP O35433
D	0	GLY	-	expression tag	UNP O35433
D	1	SER	-	expression tag	UNP O35433
B	-3	GLY	-	expression tag	UNP O35433
B	-2	ALA	-	expression tag	UNP O35433
B	-1	MET	-	expression tag	UNP O35433
B	0	GLY	-	expression tag	UNP O35433
B	1	SER	-	expression tag	UNP O35433

- # 6EU

Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total 46	C 37	O 9	0
2	C	1	Total 46	C 37	O 9	0
2	D	1	Total 46	C 37	O 9	0
2	B	1	Total 46	C 37	O 9	0

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24855	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
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: 6EU

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	0.26	0/3721	0.39	0/5032
1	B	0.26	0/3721	0.38	0/5032
1	C	0.26	0/3721	0.39	0/5032
1	D	0.26	0/3721	0.38	0/5032
All	All	0.26	0/14884	0.39	0/20128

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	3635	0	3673	14	0
1	B	3635	0	3673	12	0
1	C	3635	0	3673	11	0
1	D	3635	0	3673	12	0
2	A	46	0	0	1	0
2	B	46	0	0	2	0
2	C	46	0	0	1	0
2	D	46	0	0	1	0
All	All	14724	0	14692	46	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 2.

All (46) 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:557:ARG:NH1	1:A:570:GLU:OE1	2.17	0.78
1:B:557:ARG:NH1	1:B:570:GLU:OE1	2.17	0.77
1:D:557:ARG:NH1	1:D:570:GLU:OE1	2.18	0.76
1:A:458:GLU:OE1	1:A:458:GLU:N	2.29	0.66
1:C:458:GLU:N	1:C:458:GLU:OE1	2.31	0.63
1:C:547:MET:SD	2:C:901:6EU:OAD	2.57	0.63
1:A:411:ASP:OD1	1:A:695:ASN:ND2	2.32	0.62
1:D:425:LYS:NZ	1:D:709:GLU:OE1	2.33	0.61
1:D:458:GLU:N	1:D:458:GLU:OE1	2.36	0.58
1:A:326:GLU:N	1:A:326:GLU:OE1	2.36	0.58
1:B:672:ILE:O	1:B:676:ASN:ND2	2.40	0.55
1:B:737:ASP:OD1	1:B:738:TYR:N	2.40	0.54
1:C:737:ASP:OD1	1:C:738:TYR:N	2.41	0.54
1:D:737:ASP:OD1	1:D:738:TYR:N	2.41	0.54
1:A:737:ASP:OD1	1:A:738:TYR:N	2.41	0.53
1:B:458:GLU:OE1	1:B:458:GLU:N	2.43	0.52
1:B:536:GLU:N	1:B:536:GLU:OE1	2.41	0.52
1:C:411:ASP:OD1	1:C:695:ASN:ND2	2.42	0.52
1:D:553:LEU:HD12	2:D:901:6EU:CBM	2.39	0.52
1:A:569:ILE:HG12	1:D:677:MET:HE1	1.92	0.51
1:A:553:LEU:HD12	2:A:901:6EU:CBM	2.41	0.50
1:A:536:GLU:OE1	1:A:536:GLU:N	2.43	0.50
1:C:536:GLU:N	1:C:536:GLU:OE1	2.43	0.49
1:D:536:GLU:N	1:D:536:GLU:OE1	2.43	0.49
1:D:693:SER:HA	1:D:696:ILE:HG22	1.95	0.48
1:C:577:LEU:HD13	1:B:673:LEU:HD11	1.96	0.47
1:B:553:LEU:HD12	2:B:901:6EU:CBM	2.44	0.47
1:A:693:SER:HA	1:A:696:ILE:HG22	1.96	0.47
1:A:404:SER:O	1:A:409:ARG:NH1	2.50	0.45
1:A:569:ILE:CG1	1:D:677:MET:HE1	2.47	0.45
1:D:672:ILE:O	1:D:676:ASN:ND2	2.50	0.44
1:D:736:ASP:OD1	1:D:737:ASP:N	2.47	0.44
1:C:736:ASP:OD1	1:C:737:ASP:N	2.49	0.43
1:B:736:ASP:OD1	1:B:737:ASP:N	2.48	0.43
1:A:672:ILE:O	1:A:676:ASN:ND2	2.52	0.43
1:B:512:SER:OG	2:B:901:6EU:OAI	2.36	0.43
1:A:736:ASP:OD1	1:A:737:ASP:N	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:THR:HA	1:A:596:VAL:HG12	2.01	0.42
1:C:289:HIS:NE2	1:C:334:LEU:O	2.52	0.42
1:C:672:ILE:O	1:C:676:ASN:ND2	2.52	0.42
1:B:415:VAL:HG12	1:B:417:PRO:HD2	2.00	0.42
1:C:384:LEU:HD22	1:C:421:LEU:HD11	2.01	0.42
1:B:388:ASP:OD1	1:B:388:ASP:N	2.53	0.42
1:D:355:ARG:NH1	1:D:365:LEU:O	2.52	0.41
1:B:666:TYR:CE1	1:B:670:THR:HG21	2.55	0.41
1:C:666:TYR:CE1	1:C:670:THR:HG21	2.57	0.40

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	441/842 (52%)	421 (96%)	20 (4%)	0	100	100
1	B	441/842 (52%)	420 (95%)	21 (5%)	0	100	100
1	C	441/842 (52%)	417 (95%)	24 (5%)	0	100	100
1	D	441/842 (52%)	416 (94%)	25 (6%)	0	100	100
All	All	1764/3368 (52%)	1674 (95%)	90 (5%)	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	400/743 (54%)	399 (100%)	1 (0%)	86	87
1	B	400/743 (54%)	399 (100%)	1 (0%)	86	87
1	C	400/743 (54%)	399 (100%)	1 (0%)	86	87
1	D	400/743 (54%)	399 (100%)	1 (0%)	86	87
All	All	1600/2972 (54%)	1596 (100%)	4 (0%)	84	87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	687	ASN
1	C	687	ASN
1	D	687	ASN
1	B	687	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	676	ASN
1	C	676	ASN
1	C	687	ASN
1	D	700	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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$
2	6EU	A	901	-	45,52,52	4.88	24 (53%)	44,83,83	2.16	11 (25%)
2	6EU	C	901	-	45,52,52	4.88	24 (53%)	44,83,83	2.11	11 (25%)
2	6EU	B	901	-	45,52,52	4.89	24 (53%)	44,83,83	2.11	11 (25%)
2	6EU	D	901	-	45,52,52	4.90	25 (55%)	44,83,83	2.12	11 (25%)

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
2	6EU	A	901	-	-	5/20/101/101	0/8/7/7
2	6EU	C	901	-	-	5/20/101/101	0/8/7/7
2	6EU	B	901	-	-	5/20/101/101	0/8/7/7
2	6EU	D	901	-	-	5/20/101/101	0/8/7/7

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	901	6EU	OAC-CAM	-15.95	1.20	1.44
2	B	901	6EU	OAC-CAM	-15.92	1.20	1.44
2	C	901	6EU	OAC-CAM	-15.92	1.20	1.44
2	A	901	6EU	OAC-CAM	-15.91	1.20	1.44
2	B	901	6EU	OAB-CAL	-12.93	1.24	1.43
2	A	901	6EU	OAB-CAL	-12.91	1.24	1.43
2	C	901	6EU	OAB-CAL	-12.90	1.24	1.43
2	D	901	6EU	OAB-CAL	-12.89	1.24	1.43
2	A	901	6EU	CBP-CBR	9.08	1.53	1.38
2	C	901	6EU	CBP-CBR	9.05	1.53	1.38
2	B	901	6EU	CBP-CBR	9.03	1.53	1.38
2	D	901	6EU	CBP-CBR	9.02	1.53	1.38
2	C	901	6EU	CBO-CBN	8.08	1.53	1.39
2	D	901	6EU	CBO-CBN	8.06	1.52	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	6EU	CBO-CBN	8.02	1.52	1.39
2	B	901	6EU	CBO-CBN	8.01	1.52	1.39
2	B	901	6EU	CBI-CBG	7.95	1.52	1.38
2	D	901	6EU	CBI-CBG	7.92	1.52	1.38
2	C	901	6EU	CBI-CBG	7.89	1.52	1.38
2	A	901	6EU	CBI-CBG	7.87	1.52	1.38
2	A	901	6EU	CBH-CBE	7.42	1.53	1.38
2	D	901	6EU	CBH-CBE	7.42	1.53	1.38
2	B	901	6EU	CBH-CBE	7.39	1.53	1.38
2	C	901	6EU	CBH-CBE	7.39	1.53	1.38
2	B	901	6EU	OAA-CAJ	7.18	1.59	1.44
2	C	901	6EU	OAA-CAJ	7.16	1.59	1.44
2	D	901	6EU	OAA-CAJ	7.08	1.59	1.44
2	A	901	6EU	OAA-CAJ	6.99	1.59	1.44
2	A	901	6EU	CBS-CBQ	6.59	1.51	1.40
2	D	901	6EU	CBJ-CBL	6.58	1.52	1.38
2	C	901	6EU	CBJ-CBL	6.57	1.52	1.38
2	B	901	6EU	CBJ-CBL	6.56	1.52	1.38
2	D	901	6EU	CBS-CBQ	6.55	1.51	1.40
2	A	901	6EU	CBJ-CBL	6.54	1.52	1.38
2	B	901	6EU	CBS-CBQ	6.44	1.51	1.40
2	C	901	6EU	CBS-CBQ	6.36	1.51	1.40
2	D	901	6EU	CAW-CBA	5.59	1.44	1.33
2	A	901	6EU	CAW-CBA	5.57	1.44	1.33
2	C	901	6EU	CAW-CBA	5.54	1.44	1.33
2	B	901	6EU	CAW-CBA	5.54	1.44	1.33
2	A	901	6EU	OAB-CAQ	-5.23	1.32	1.41
2	C	901	6EU	OAB-CAQ	-5.23	1.32	1.41
2	B	901	6EU	OAB-CAQ	-5.21	1.32	1.41
2	D	901	6EU	OAB-CAQ	-5.21	1.32	1.41
2	B	901	6EU	CBR-CBS	-4.82	1.31	1.39
2	C	901	6EU	CBR-CBS	-4.80	1.31	1.39
2	D	901	6EU	CBR-CBS	-4.77	1.31	1.39
2	D	901	6EU	CBJ-CBH	-4.69	1.30	1.38
2	C	901	6EU	CBJ-CBH	-4.68	1.30	1.38
2	A	901	6EU	CBR-CBS	-4.68	1.31	1.39
2	A	901	6EU	CBJ-CBH	-4.66	1.30	1.38
2	B	901	6EU	CBJ-CBH	-4.66	1.30	1.38
2	D	901	6EU	CBO-CBQ	-4.42	1.31	1.38
2	B	901	6EU	CBO-CBQ	-4.36	1.31	1.38
2	A	901	6EU	CBO-CBQ	-4.35	1.31	1.38
2	D	901	6EU	CBP-CBN	-4.34	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	901	6EU	CBO-CBQ	-4.30	1.31	1.38
2	C	901	6EU	CBP-CBN	-4.29	1.30	1.38
2	A	901	6EU	CBP-CBN	-4.26	1.30	1.38
2	B	901	6EU	CBP-CBN	-4.24	1.30	1.38
2	D	901	6EU	CBG-CBE	-4.22	1.30	1.38
2	B	901	6EU	CBG-CBE	-4.19	1.30	1.38
2	C	901	6EU	CBG-CBE	-4.18	1.30	1.38
2	A	901	6EU	CBG-CBE	-4.14	1.30	1.38
2	D	901	6EU	CBB-CAV	3.79	1.52	1.34
2	C	901	6EU	CBB-CAV	3.79	1.52	1.34
2	A	901	6EU	CBB-CAV	3.78	1.52	1.34
2	B	901	6EU	CBB-CAV	3.77	1.52	1.34
2	C	901	6EU	CAZ-CBA	3.57	1.58	1.47
2	B	901	6EU	CAZ-CBA	3.57	1.58	1.47
2	A	901	6EU	CAZ-CBA	3.56	1.58	1.47
2	D	901	6EU	CAZ-CBA	3.54	1.58	1.47
2	D	901	6EU	OAF-CBK	3.34	1.43	1.33
2	A	901	6EU	OAF-CBK	3.31	1.43	1.33
2	B	901	6EU	OAF-CBK	3.31	1.43	1.33
2	C	901	6EU	OAF-CBK	3.25	1.42	1.33
2	D	901	6EU	CBL-CBI	-3.04	1.31	1.38
2	B	901	6EU	CBL-CBI	-3.02	1.31	1.38
2	A	901	6EU	CBL-CBI	-3.00	1.31	1.38
2	C	901	6EU	CBL-CBI	-2.98	1.31	1.38
2	A	901	6EU	CAR-CAO	-2.36	1.49	1.55
2	C	901	6EU	CAR-CAO	-2.35	1.49	1.55
2	D	901	6EU	CAR-CAO	-2.34	1.49	1.55
2	B	901	6EU	CAR-CAO	-2.30	1.49	1.55
2	D	901	6EU	OAH-CBQ	2.27	1.40	1.37
2	A	901	6EU	OAH-CBQ	2.19	1.40	1.37
2	B	901	6EU	OAI-CBS	2.17	1.40	1.36
2	C	901	6EU	OAI-CBS	2.16	1.40	1.36
2	C	901	6EU	OAH-CBQ	2.14	1.40	1.37
2	B	901	6EU	OAH-CBQ	2.14	1.40	1.37
2	A	901	6EU	OAE-CAZ	-2.10	1.18	1.22
2	B	901	6EU	OAE-CAZ	-2.09	1.18	1.22
2	D	901	6EU	OAE-CAZ	-2.08	1.18	1.22
2	C	901	6EU	OAE-CAZ	-2.06	1.18	1.22
2	D	901	6EU	OAI-CBS	2.03	1.40	1.36
2	D	901	6EU	CBM-CBN	2.02	1.54	1.51
2	A	901	6EU	OAI-CBS	2.02	1.40	1.36

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	901	6EU	OAA-CAJ-CAN	-7.34	96.80	106.34
2	A	901	6EU	OAA-CAJ-CAN	-7.32	96.83	106.34
2	B	901	6EU	OAA-CAJ-CAN	-7.26	96.91	106.34
2	C	901	6EU	OAA-CAJ-CAN	-7.14	97.06	106.34
2	A	901	6EU	OAF-CBK-CBM	6.21	120.90	111.21
2	C	901	6EU	OAF-CBK-CBM	6.17	120.85	111.21
2	D	901	6EU	OAF-CBK-CBM	5.89	120.41	111.21
2	B	901	6EU	OAF-CBK-CBM	5.79	120.25	111.21
2	D	901	6EU	CAQ-CAY-CBE	-4.60	108.20	113.60
2	B	901	6EU	CAQ-CAY-CBE	-4.49	108.33	113.60
2	A	901	6EU	CAQ-CAY-CBE	-4.44	108.39	113.60
2	C	901	6EU	CAQ-CAY-CBE	-4.43	108.40	113.60
2	C	901	6EU	CAM-CAV-CBB	-3.60	112.18	121.88
2	D	901	6EU	CAM-CAV-CBB	-3.59	112.23	121.88
2	B	901	6EU	CAM-CAV-CBB	-3.57	112.27	121.88
2	A	901	6EU	CAM-CAV-CBB	-3.52	112.42	121.88
2	A	901	6EU	OAH-CBQ-CBS	3.38	119.62	114.55
2	D	901	6EU	OAH-CBQ-CBS	3.13	119.24	114.55
2	B	901	6EU	OAH-CBQ-CBS	3.12	119.23	114.55
2	C	901	6EU	OAH-CBQ-CBS	3.07	119.15	114.55
2	A	901	6EU	CBT-OAH-CBQ	-2.91	113.25	117.51
2	B	901	6EU	CBT-OAH-CBQ	-2.82	113.37	117.51
2	D	901	6EU	CBT-OAH-CBQ	-2.80	113.41	117.51
2	C	901	6EU	CBT-OAH-CBQ	-2.62	113.67	117.51
2	A	901	6EU	OAH-CBQ-CBO	-2.52	119.74	124.08
2	C	901	6EU	OAC-CAM-CAP	2.45	111.51	109.40
2	C	901	6EU	CBD-CAV-CAM	-2.42	110.88	116.79
2	A	901	6EU	OAC-CAM-CAP	2.35	111.43	109.40
2	B	901	6EU	OAC-CAM-CAP	2.30	111.39	109.40
2	A	901	6EU	CBD-CAV-CBB	-2.30	112.84	121.12
2	A	901	6EU	CBD-CAV-CAM	-2.29	111.19	116.79
2	B	901	6EU	CBD-CAV-CBB	-2.29	112.86	121.12
2	D	901	6EU	CBD-CAV-CBB	-2.28	112.89	121.12
2	C	901	6EU	CBD-CAV-CBB	-2.28	112.90	121.12
2	D	901	6EU	OAH-CBQ-CBO	-2.27	120.17	124.08
2	D	901	6EU	CBD-CAV-CAM	-2.26	111.25	116.79
2	B	901	6EU	CBD-CAV-CAM	-2.26	111.27	116.79
2	B	901	6EU	OAH-CBQ-CBO	-2.23	120.23	124.08
2	A	901	6EU	OAB-CAL-CAK	-2.23	104.51	107.51
2	C	901	6EU	OAH-CBQ-CBO	-2.23	120.24	124.08
2	D	901	6EU	OAC-CAM-CAP	2.19	111.29	109.40
2	B	901	6EU	OAB-CAL-CAK	-2.16	104.60	107.51
2	D	901	6EU	OAB-CAL-CAK	-2.16	104.60	107.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	901	6EU	OAB-CAL-CAK	-2.11	104.67	107.51

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	6EU	CAL-CAM-CAV-CBB
2	C	901	6EU	CAL-CAM-CAV-CBB
2	D	901	6EU	OAC-CAM-CAV-CBB
2	D	901	6EU	CAL-CAM-CAV-CBB
2	B	901	6EU	OAC-CAM-CAV-CBB
2	B	901	6EU	CAL-CAM-CAV-CBB
2	A	901	6EU	CBM-CBK-OAF-CBC
2	C	901	6EU	CBM-CBK-OAF-CBC
2	D	901	6EU	CBM-CBK-OAF-CBC
2	B	901	6EU	CBM-CBK-OAF-CBC
2	A	901	6EU	OAG-CBK-OAF-CBC
2	C	901	6EU	OAG-CBK-OAF-CBC
2	D	901	6EU	OAG-CBK-OAF-CBC
2	B	901	6EU	OAG-CBK-OAF-CBC
2	A	901	6EU	CAP-CAM-CAV-CBB
2	C	901	6EU	CAP-CAM-CAV-CBB
2	D	901	6EU	CAP-CAM-CAV-CBB
2	B	901	6EU	CAP-CAM-CAV-CBB
2	A	901	6EU	OAC-CAM-CAV-CBB
2	C	901	6EU	OAC-CAM-CAV-CBB

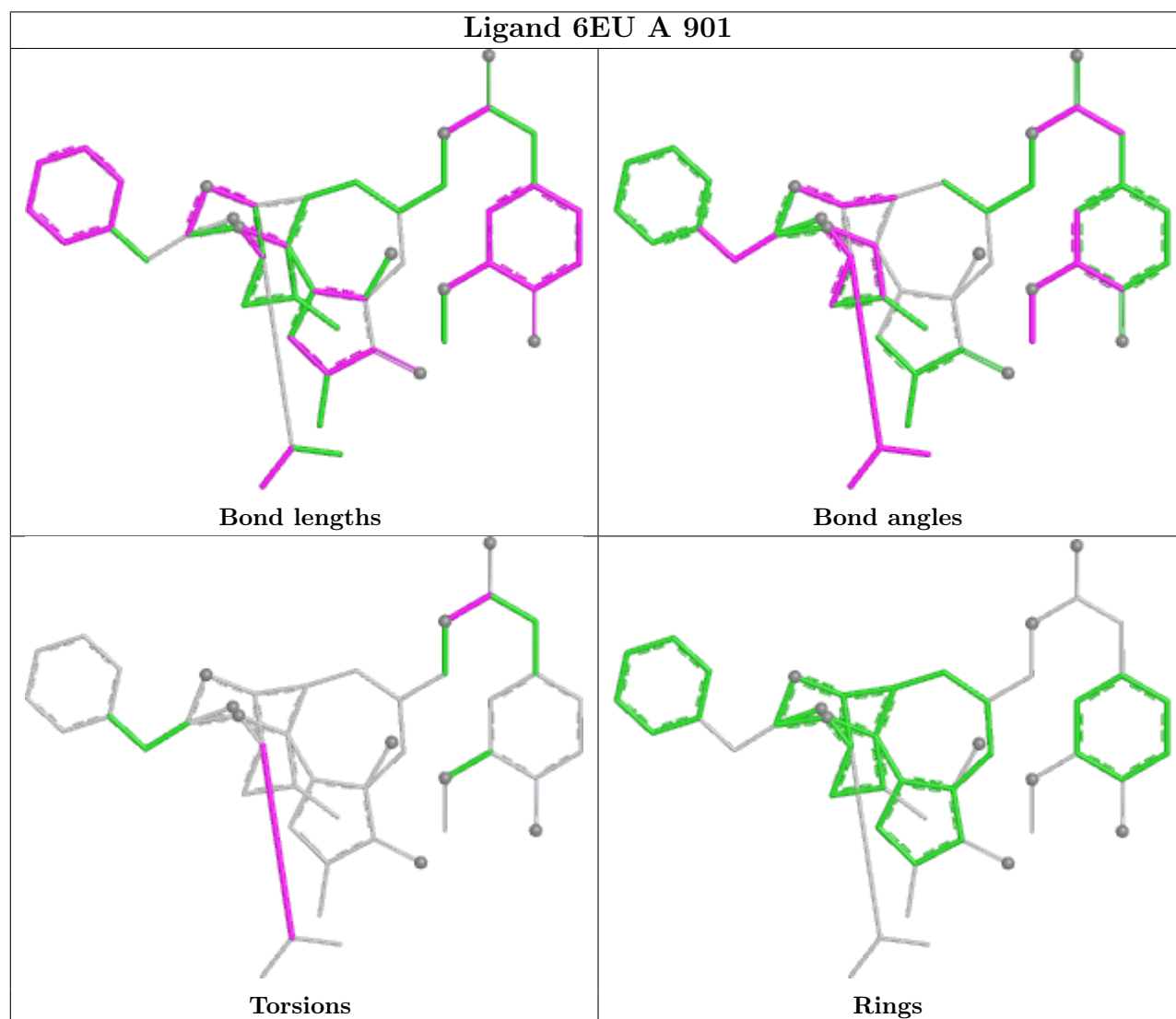
There are no ring outliers.

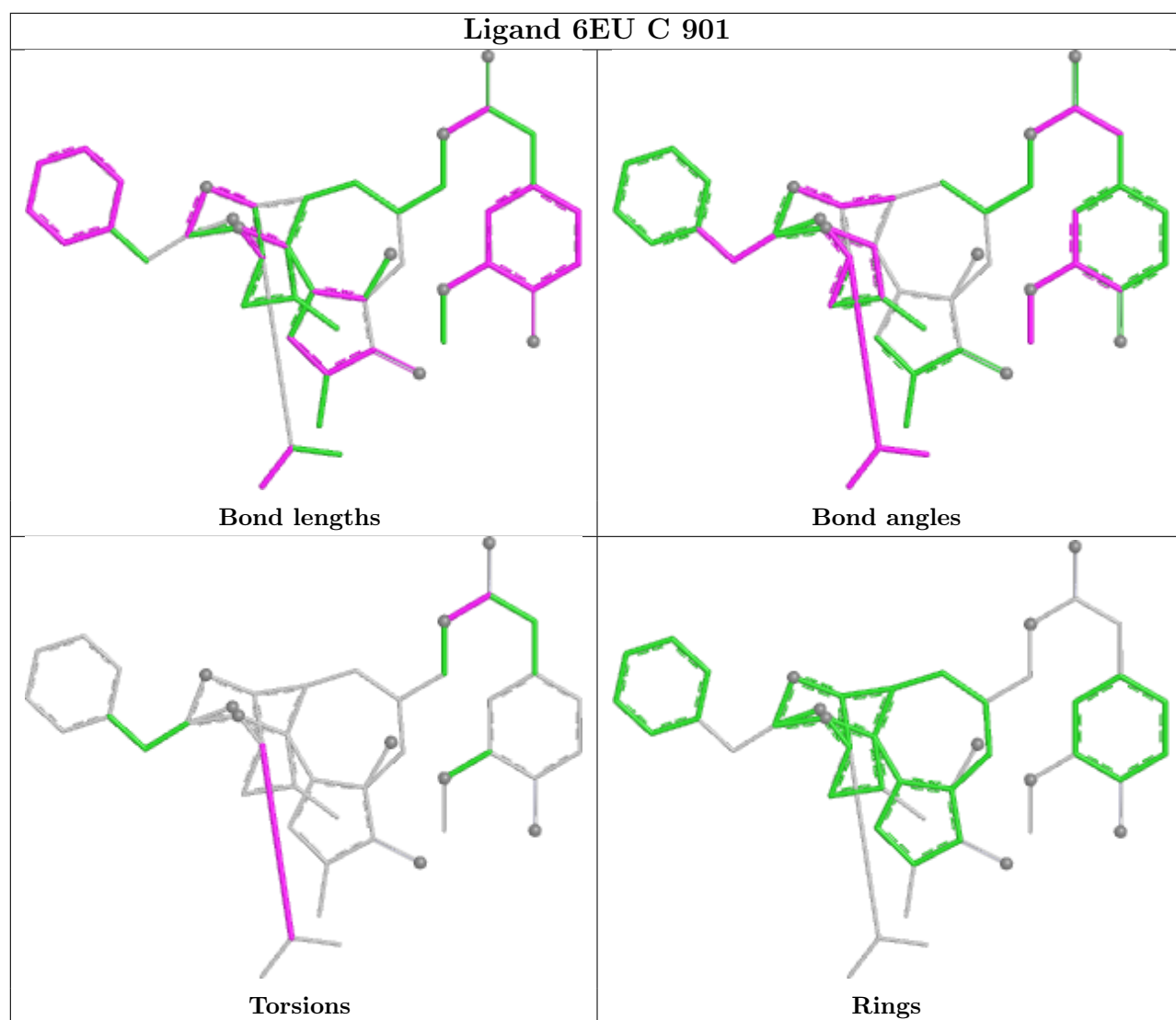
4 monomers are involved in 5 short contacts:

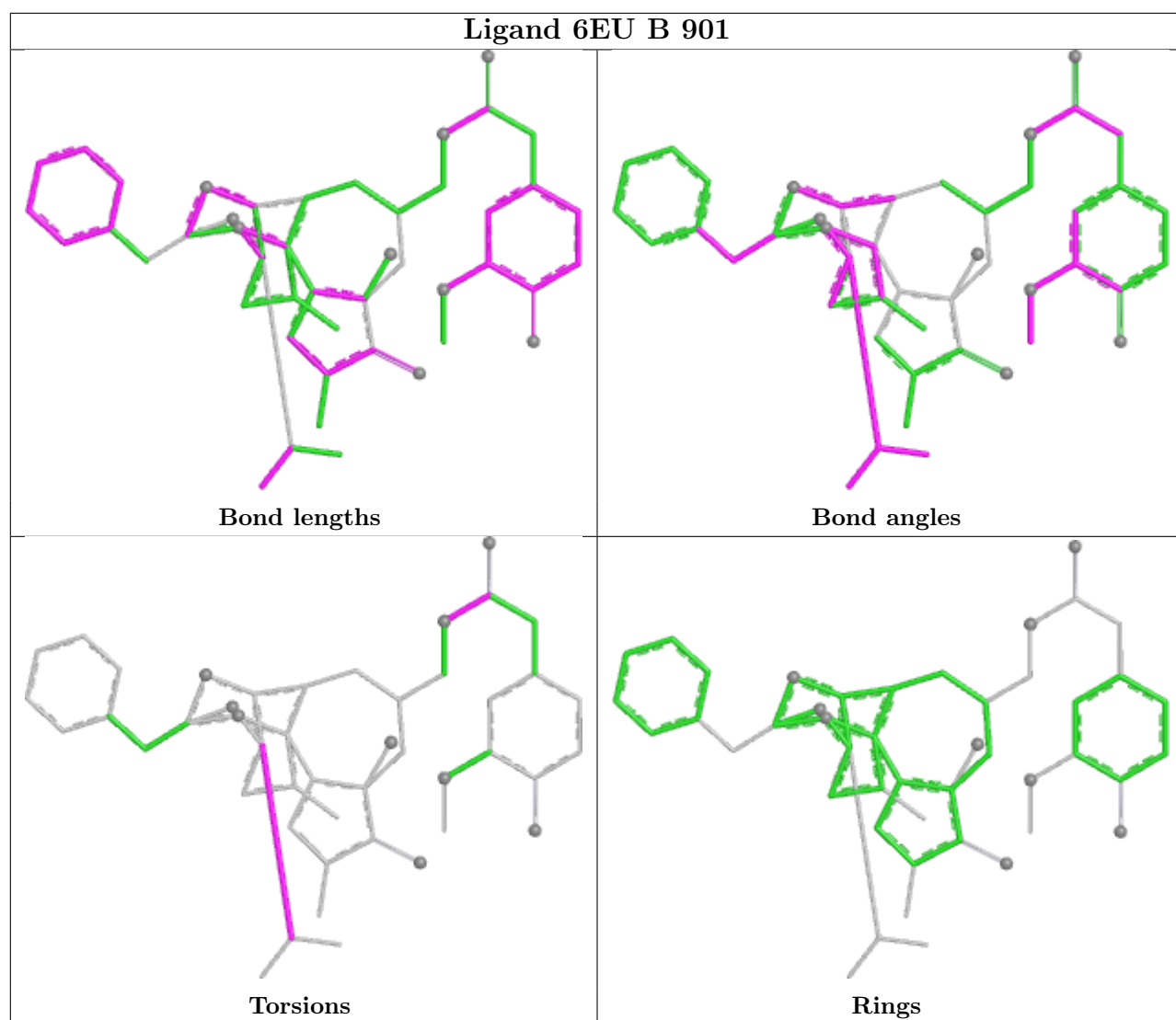
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	6EU	1	0
2	C	901	6EU	1	0
2	B	901	6EU	2	0
2	D	901	6EU	1	0

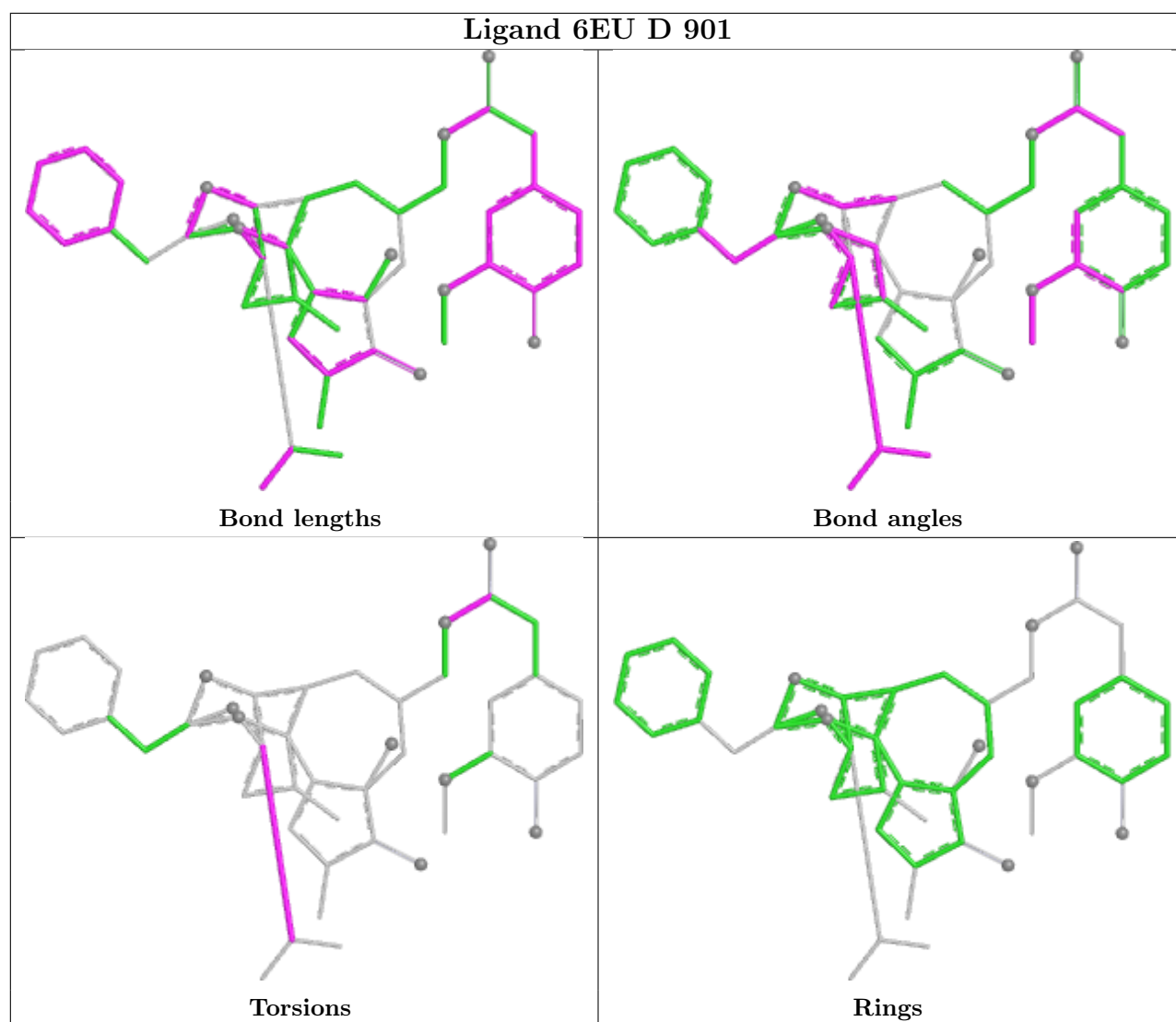
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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-23134. 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.