



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 12:16 AM UTC

PDB ID : 8KDB / pdb_00008kdb
EMDB ID : EMD-37130
Title : Cryo-EM structure of the human parainfluenza virus hPIV3 L-P polymerase in dimeric form
Authors : Xie, J.; Wang, L.; Zhai, G.; Wu, D.; Lin, Z.; Wang, M.; Yan, X.; Gao, L.; Huang, X.; Fearn, R.; Chen, S.
Deposited on : 2023-08-09
Resolution : 2.70 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
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

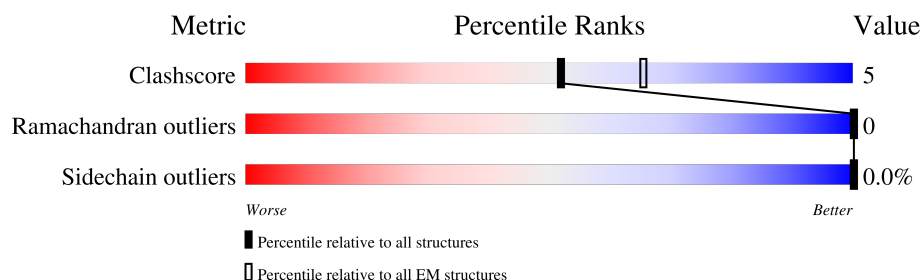
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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	2266	79% 14% 7%
1	G	2266	10% 89%
2	B	609	10% 89%
2	C	609	94%
2	D	609	6% 93%
2	E	609	5% 94%
2	F	609	5% 94%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20861 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 RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2117	Total	C	N	O	S	2	0
			17081	10949	2855	3193	84		
1	G	252	Total	C	N	O	S	0	0
			2039	1321	332	375	11		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2234	ASP	-	expression tag	UNP O89238
A	2235	TYR	-	expression tag	UNP O89238
A	2236	LYS	-	expression tag	UNP O89238
A	2237	ASP	-	expression tag	UNP O89238
A	2238	ASP	-	expression tag	UNP O89238
A	2239	ASP	-	expression tag	UNP O89238
A	2240	ASP	-	expression tag	UNP O89238
A	2241	LYS	-	expression tag	UNP O89238
G	2234	ASP	-	expression tag	UNP O89238
G	2235	TYR	-	expression tag	UNP O89238
G	2236	LYS	-	expression tag	UNP O89238
G	2237	ASP	-	expression tag	UNP O89238
G	2238	ASP	-	expression tag	UNP O89238
G	2239	ASP	-	expression tag	UNP O89238
G	2240	ASP	-	expression tag	UNP O89238
G	2241	LYS	-	expression tag	UNP O89238

- Molecule 2 is a protein called Phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	65	Total	C	N	O	S	0	0
			510	306	90	109	5		
2	C	37	Total	C	N	O	S	0	0
			305	186	58	59	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	41	Total	C	N	O	S	0	0
			335	204	64	65	2		
2	E	38	Total	C	N	O	S	0	0
			309	188	59	60	2		
2	F	34	Total	C	N	O	S	0	0
			279	172	52	53	2		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	604	HIS	-	expression tag	UNP O89234
B	605	HIS	-	expression tag	UNP O89234
B	606	HIS	-	expression tag	UNP O89234
B	607	HIS	-	expression tag	UNP O89234
B	608	HIS	-	expression tag	UNP O89234
B	609	HIS	-	expression tag	UNP O89234
C	604	HIS	-	expression tag	UNP O89234
C	605	HIS	-	expression tag	UNP O89234
C	606	HIS	-	expression tag	UNP O89234
C	607	HIS	-	expression tag	UNP O89234
C	608	HIS	-	expression tag	UNP O89234
C	609	HIS	-	expression tag	UNP O89234
D	604	HIS	-	expression tag	UNP O89234
D	605	HIS	-	expression tag	UNP O89234
D	606	HIS	-	expression tag	UNP O89234
D	607	HIS	-	expression tag	UNP O89234
D	608	HIS	-	expression tag	UNP O89234
D	609	HIS	-	expression tag	UNP O89234
E	604	HIS	-	expression tag	UNP O89234
E	605	HIS	-	expression tag	UNP O89234
E	606	HIS	-	expression tag	UNP O89234
E	607	HIS	-	expression tag	UNP O89234
E	608	HIS	-	expression tag	UNP O89234
E	609	HIS	-	expression tag	UNP O89234
F	604	HIS	-	expression tag	UNP O89234
F	605	HIS	-	expression tag	UNP O89234
F	606	HIS	-	expression tag	UNP O89234
F	607	HIS	-	expression tag	UNP O89234
F	608	HIS	-	expression tag	UNP O89234
F	609	HIS	-	expression tag	UNP O89234

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

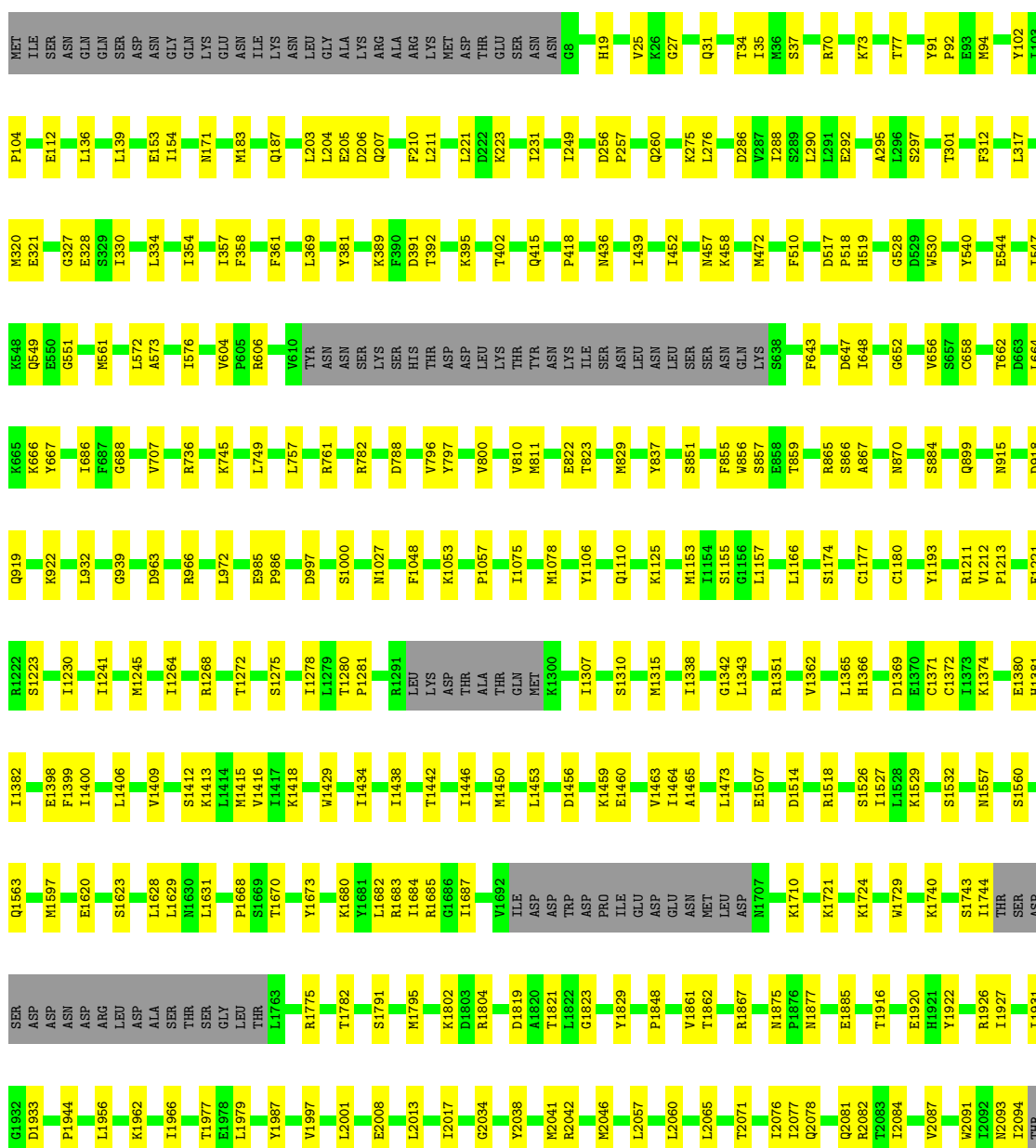
Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Zn	0
			2	2	

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.

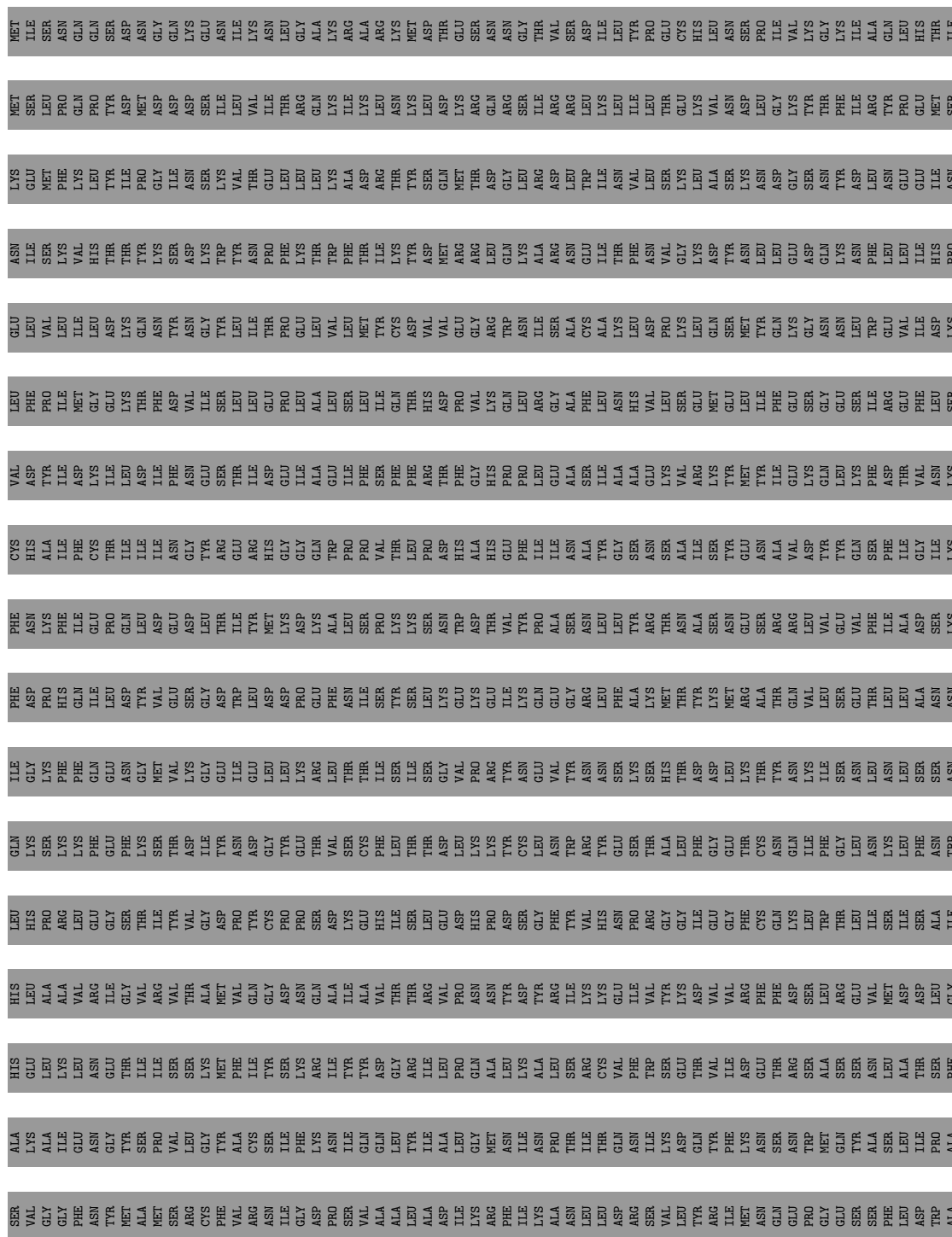
• Molecule 1: RNA-directed RNA polymerase L

Chain A: 



- Molecule 1: RNA-directed RNA polymerase L

Chain G: 10% . 89%



Chain B: 10% 89%

T544
R545
L546
I547
Q603
HIS
HIS
HIS
HIS
HIS
HIS

Chain C: 94%



LEU	VAL	ALA	VAL	ILE	SER	ASN	SER	ASN	GLN	SER	THR	LYS	GLN	SER	SER	TYR	ILE	ASN	GLY	LEU	LYS	HIS	CYS	LYS	ASN	ASP	GLU	GLU	VAL	SER	SER	GLU	LEU	MET	ASP	PHE	MET	ASN	GLU	ASP	VAL	ASN	CYS	GLN	HIS	HIS	HIS	HIS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

Chain D: 6% 93%

[illegible]

Chain E: 5% . 94%

GLY	GLN	THR	ILE	MET
GLY	GLN	VAL	TYR	GLU
GLY	SER	VAL	GLN	SER
GLY	ARG	SER	PRO	ASP
GLY	ASN	GLY	LYS	ALA
ASP	SER	GLY	ILE	LYS
THR	ASP	ILE	LYS	ASN
PHE	HIS	SER	PRO	TYR
LYS	GLY	ARG	THR	GLN
GLN	ARG	SER	GLU	ILE
SER	SER	ILE	THR	MET
LYS	LEU	THR	SER	ASP
ASP	GLU	ASN	GLU	SER
THR	ILE	SER	LYS	THR
ASP	ILE	LYS	ASP	GLY
ASN	SER	ASN	SER	GLU
GLN	THR	GLY	GLY	GLU
ILE	PRO	THR	SER	SER
PRO	ASP	GLN	THR	ARG
THR	THR	ASN	ASP	ASP
SER	ARG	THR	LYS	SER
ASP	SER	GLU	ASN	SER
TYR	ILE	ASP	ARG	THR
ARG	SER	ILE	GLN	ASN
SER	VAL	ASP	SER	ILE
THR	VAL	LEU	GLY	SER
SER	THR	ASN	SER	SER
GLY	ALA	GLU	SER	ALA
ALA	ALA	ILE	HIS	LEU
THR	THR	ARG	GLU	ASN
PRO	PRO	LYS	CYS	ILE
LYS	ASP	MET	THR	ILE
ILE	ILE	ASP	THR	GLU
GLU	ASP	LYS	GLU	PHE
LYS	GLU	ASP	ALA	ILE
THR	GLU	SER	LYS	LEU
ILE	ILE	ILE	ASP	SER
THR	LEU	GLU	ARG	THR
THR	MET	GLY	THR	ASP
ILE	LYS	LYS	ILE	PRO
ASN	ASN	VAL	ASP	GLN
ASP	SER	ARG	GLN	GLU
THR	ARG	GLN	GLU	ASP
LYS	THR	SER	THR	LEU
GLY	LYS	ALA	VAL	SER
GLN	GLN	ASP	GLN	GLU
THR	SER	VAL	ARG	ASN
GLU	SER	PRO	GLY	ASP
ILE	SER	SER	PHO	THR
GLN	ILE	GLU	GLY	ILE
THR	HIS	ILE	ARG	ASN
GLU	GLN	SER	ARG	THR
SER	GLU	GLY	SER	ARG
SER	ASP	SER	SER	THR
GLY	LYS	ASP	ASP	GLN
THR	THR	VAL	SER	GLN
GLN	ARG	ILE	SER	LEU
SER	ILE	PHE	ARG	SER
SER	LYS	THR	ALA	THR
THR	LYS	THR	GLU	THR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT, POINT, POINT	Depositor
Number of particles used	102956, 102956, 102956, 102956	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.00	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (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: MG, ZN

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	0.13	0/17429	0.30	0/23589
1	G	0.11	0/2078	0.31	0/2818
2	B	0.09	0/513	0.25	0/689
2	C	0.17	0/305	0.42	0/404
2	D	0.21	0/335	0.40	0/442
2	E	0.13	0/309	0.28	0/409
2	F	0.12	0/279	0.24	0/370
All	All	0.13	0/21248	0.30	0/28721

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	17081	0	17225	186	0
1	G	2039	0	2076	20	0
2	B	510	0	499	2	0
2	C	305	0	322	7	0
2	D	335	0	355	7	0
2	E	309	0	325	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	279	0	298	5	0
3	A	1	0	0	0	0
4	A	2	0	0	0	0
All	All	20861	0	21100	225	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 5.

All (225) 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:G:1532:SER:HB3	1:G:1563:GLN:HB3	1.51	0.90
2:D:450:GLN:HG3	2:E:454:LEU:HD11	1.53	0.88
1:A:1166:LEU:HD21	1:A:1338:ILE:HG12	1.61	0.83
1:A:2087:VAL:HG23	1:A:2121:LEU:HB3	1.70	0.74
1:A:472[B]:MET:HG3	1:A:1078:MET:HG3	1.72	0.72
1:A:1862:THR:O	1:A:1867:ARG:NH1	2.23	0.72
1:A:206:ASP:OD1	1:A:207:GLN:N	2.26	0.68
1:A:1307:ILE:HG23	1:A:1310:SER:HB2	1.75	0.68
2:C:440:ASP:OD1	2:F:443:HIS:NE2	2.26	0.68
1:A:204:LEU:HD12	1:A:211:LEU:HD23	1.76	0.68
1:A:295:ALA:HB2	1:A:357:ILE:HD11	1.76	0.67
1:A:1962:LYS:HG2	1:A:1987:TYR:HB2	1.75	0.67
1:G:1478:LEU:HD11	1:G:1539:LYS:HB3	1.78	0.65
2:D:439:MET:HE1	2:E:439:MET:HE1	1.79	0.65
1:A:1213:PRO:HG3	1:A:1307:ILE:HG21	1.78	0.64
1:A:1721:LYS:HZ2	1:A:1795:MET:HE2	1.62	0.64
1:A:1245:MET:HE2	1:A:1281:PRO:HD2	1.80	0.64
1:A:286:ASP:OD2	1:A:549:GLN:NE2	2.33	0.62
2:E:450:GLN:HE21	2:F:451:ARG:HB2	1.65	0.61
1:A:205:GLU:OE2	1:A:223:LYS:NZ	2.32	0.61
1:A:35:ILE:O	1:A:70:ARG:NH1	2.34	0.61
1:A:2077:ILE:O	1:A:2081:GLN:HG3	2.00	0.60
1:A:855:PHE:O	1:A:899:GLN:NE2	2.34	0.60
1:A:829:MET:HA	1:A:837:TYR:O	2.03	0.59
1:A:402:THR:HG23	1:A:439:ILE:HG23	1.85	0.59
1:A:415:GLN:OE1	1:A:436:ASN:ND2	2.36	0.59
1:A:2041:MET:HB2	1:A:2046:MET:HE2	1.84	0.59
1:A:1371:CYS:O	1:A:1374:LYS:NZ	2.36	0.59
1:A:1875:ASN:ND2	1:A:1877:ASN:OD1	2.35	0.58
1:A:1241:ILE:HG23	1:A:1280:THR:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1463:VAL:HG11	1:A:1526:SER:HB2	1.85	0.58
1:A:94:MET:HE1	1:A:231:ILE:HG22	1.87	0.57
1:A:1791:SER:HB3	1:A:1821:THR:HG21	1.87	0.57
1:A:31:GLN:HA	1:A:34:THR:HG22	1.87	0.57
1:G:1676:LYS:O	1:G:1680:LYS:HG3	2.04	0.57
1:A:2038:TYR:HA	1:A:2210:PRO:HG3	1.86	0.57
1:A:963:ASP:OD1	1:A:966:ARG:NH1	2.38	0.56
1:A:857:SER:O	1:A:870:ASN:ND2	2.35	0.56
1:G:1517:MET:HE2	1:G:1572:GLU:HG2	1.87	0.55
1:A:2076:ILE:HG22	1:A:2132:LEU:HD23	1.87	0.55
1:A:37:SER:O	1:A:73:LYS:NZ	2.40	0.55
1:A:1802:LYS:NZ	1:A:1933:ASP:OD2	2.37	0.55
1:A:2078:GLN:O	1:A:2082:ARG:NE	2.39	0.55
1:A:1721:LYS:NZ	1:A:1795:MET:HE2	2.22	0.55
1:A:1966:ILE:HD11	1:A:1979:LEU:HD13	1.88	0.55
1:G:1628:LEU:HB3	1:G:1636:ARG:HE	1.71	0.55
1:A:530:TRP:HB2	1:A:561:MET:HE1	1.89	0.54
1:A:656:VAL:HG23	1:A:796:VAL:HG21	1.90	0.54
1:G:1454:ASP:CG	1:G:1603:ARG:HH21	2.16	0.54
1:A:327:GLY:HA3	1:A:330:ILE:HD12	1.89	0.54
1:A:361:PHE:CE1	1:A:547:ILE:HD11	2.43	0.54
1:G:1654:LEU:HD21	1:G:1659:ILE:HD11	1.90	0.53
1:A:1268:ARG:NH1	1:A:1400:ILE:O	2.39	0.53
1:A:2065:LEU:HA	1:A:2127:LEU:HD12	1.91	0.53
2:C:443:HIS:O	2:C:447:ILE:HG12	2.10	0.52
1:A:1956:LEU:HD13	1:A:2001:LEU:HD21	1.91	0.52
1:A:256:ASP:OD1	1:A:1351:ARG:NH2	2.43	0.52
1:A:1429:TRP:O	1:A:1685:ARG:NH1	2.40	0.52
1:A:102:TYR:CD1	1:A:171:ASN:HB3	2.44	0.52
1:A:1944:PRO:HG2	1:A:1977:THR:HB	1.91	0.52
1:A:540:TYR:HB2	1:A:707:VAL:HA	1.91	0.51
1:A:312:PHE:HE1	1:A:822:GLU:HA	1.76	0.51
1:G:1631:LEU:HD21	1:G:1635:GLU:HB2	1.92	0.51
1:A:1724:LYS:HD2	1:A:1729:TRP:H	1.75	0.51
1:G:1568:LEU:O	1:G:1572:GLU:HG3	2.10	0.51
1:A:297:SER:O	1:A:301:THR:HG23	2.11	0.50
1:A:1804:ARG:NH2	1:A:1823:GLY:O	2.40	0.50
1:A:2091:TRP:O	1:A:2094:ILE:HG12	2.12	0.50
1:A:573:ALA:HB2	1:A:745:LYS:HE2	1.94	0.50
1:A:648:ILE:HD11	1:A:652:GLY:HA3	1.93	0.50
1:A:153:GLU:OE2	1:A:884:SER:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2034:GLY:HA2	1:A:2042:ARG:NH1	2.26	0.50
1:A:867:ALA:HB1	1:A:899:GLN:HE21	1.77	0.50
1:A:1053:LYS:HE2	1:A:1382:ILE:HA	1.92	0.50
1:A:1682:LEU:HD12	1:A:1687:ILE:HD12	1.93	0.50
1:A:288:ILE:HG22	1:A:547:ILE:HD12	1.94	0.50
1:A:519:HIS:NE2	1:A:1398:GLU:OE2	2.42	0.50
2:C:462:SER:O	2:C:466:ILE:HG12	2.12	0.49
1:A:1371:CYS:SG	1:A:1372:CYS:N	2.86	0.49
2:F:435:ASP:N	2:F:435:ASP:OD1	2.45	0.49
1:A:249:ILE:HD11	1:A:851:SER:HB3	1.93	0.49
1:A:1507:GLU:OE2	1:A:1623:SER:OG	2.31	0.49
1:A:1272:THR:HG23	1:A:1275:SER:H	1.77	0.49
1:A:136:LEU:HD12	1:A:154:ILE:HD11	1.93	0.49
1:A:662:THR:HB	1:A:823:THR:HG23	1.94	0.49
1:A:1453:LEU:HD22	1:A:1527:ILE:HA	1.93	0.49
1:G:1452:GLN:N	1:G:1455:ARG:HH21	2.10	0.49
1:A:2084:ILE:HA	1:A:2087:VAL:HG12	1.93	0.49
1:G:1473:LEU:HD12	1:G:1476:GLU:OE2	2.13	0.49
1:A:1507:GLU:HB3	1:A:1620:GLU:HA	1.95	0.49
1:G:1456:ASP:CG	1:G:1610:ARG:HH21	2.20	0.49
1:A:452:ILE:HG22	2:C:459:SER:HB3	1.95	0.48
1:A:915:ASN:O	1:A:919:GLN:HB2	2.13	0.48
1:A:1597:MET:HE2	1:A:1668:PRO:HB3	1.95	0.48
1:A:91:TYR:HB3	1:A:92:PRO:HD3	1.95	0.48
1:A:354:ILE:O	1:A:357:ILE:HG12	2.13	0.48
1:A:664:LEU:HD22	1:A:667:TYR:HD1	1.79	0.48
1:A:210:PHE:HB3	1:A:221:LEU:HB2	1.95	0.48
1:A:276:LEU:HD22	1:A:334:LEU:HD11	1.96	0.48
1:A:576:ILE:HD11	1:A:686:ILE:HG21	1.96	0.47
1:A:1057:PRO:HG2	1:A:1157:LEU:HD21	1.96	0.47
1:A:1791:SER:O	1:A:1795:MET:HG3	2.14	0.47
1:A:1177:CYS:HB3	1:A:1180:CYS:HB2	1.97	0.47
1:A:369:LEU:HD22	1:A:551:GLY:H	1.80	0.47
1:G:1648:ILE:HD11	1:G:1654:LEU:HD22	1.97	0.47
1:A:604:VAL:O	1:A:606:ARG:NH1	2.47	0.47
2:E:450:GLN:O	2:E:454:LEU:HG	2.15	0.47
1:G:1454:ASP:OD2	1:G:1603:ARG:NH2	2.46	0.47
1:A:418:PRO:HB2	1:A:457:ASN:HB2	1.96	0.47
1:A:1683:ARG:HH11	1:A:1683:ARG:HG2	1.80	0.46
1:A:1412:SER:HA	1:A:1415:MET:HE2	1.97	0.46
1:A:369:LEU:HD22	1:A:551:GLY:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ASP:OD1	1:A:392:THR:N	2.47	0.46
1:A:1442:THR:HG23	1:A:1473:LEU:HD23	1.98	0.46
1:A:658:CYS:HB3	1:A:800:VAL:HG21	1.97	0.46
1:A:1446:ILE:O	1:A:1450:MET:HG2	2.15	0.46
1:A:317:LEU:O	1:A:321:GLU:HG3	2.16	0.46
1:A:1922:TYR:O	1:A:1926:ARG:HG3	2.16	0.46
1:A:528:GLY:HA2	1:A:530:TRP:CZ3	2.51	0.46
1:A:112:GLU:OE1	1:A:112:GLU:N	2.49	0.46
1:A:2190:LEU:O	1:A:2194:VAL:HG23	2.16	0.46
1:G:1593:CYS:HB3	1:G:1669:SER:O	2.16	0.46
1:A:292:GLU:HG2	1:A:358:PHE:CD1	2.51	0.45
1:A:1211:ARG:HB2	1:A:1464:ILE:O	2.16	0.45
1:A:1048:PHE:HE2	1:A:1264:ILE:HD11	1.81	0.45
1:A:1459:LYS:HD3	1:A:1526:SER:OG	2.17	0.45
1:A:1278:ILE:HD11	1:A:1418:LYS:HG3	1.99	0.45
2:E:454:LEU:O	2:E:458:THR:HG23	2.16	0.45
1:A:664:LEU:HD21	1:A:811:MET:HE2	1.99	0.45
1:A:1710:LYS:HG2	1:A:1861:VAL:HG22	1.97	0.45
1:A:2013:LEU:O	1:A:2017:ILE:HG12	2.16	0.45
1:A:19:HIS:NE2	1:A:856:TRP:O	2.50	0.44
1:G:1625:GLY:HA2	1:G:1643:TYR:CE2	2.52	0.44
2:D:437:LYS:O	2:D:441:GLU:OE1	2.35	0.44
1:A:2071:THR:HA	1:A:2139:LEU:HD21	1.99	0.44
1:A:865:ARG:NH1	1:A:939:GLY:O	2.51	0.44
1:A:643:PHE:CE2	1:A:2185:ILE:HD11	2.52	0.44
1:A:1680:LYS:O	1:A:1684:ILE:HG12	2.18	0.44
1:A:643:PHE:HE2	1:A:2185:ILE:HD11	1.82	0.44
1:A:757:LEU:O	1:A:761:ARG:HG3	2.18	0.44
1:A:2060:LEU:HD22	1:A:2196:ILE:HG23	2.00	0.44
1:A:997:ASP:CG	1:A:1000:SER:HB3	2.43	0.44
2:C:450:GLN:NE2	2:D:447:ILE:HG23	2.33	0.44
1:A:25:VAL:HG12	1:A:27:GLY:H	1.82	0.43
1:A:761:ARG:HH11	1:A:810:VAL:HG23	1.83	0.43
1:A:1406:LEU:HD12	1:A:1406:LEU:O	2.18	0.43
1:A:2122:SER:O	1:A:2126:VAL:HG23	2.17	0.43
2:B:545:ARG:HE	2:B:547:ILE:HD11	1.84	0.43
1:A:389:LYS:HD3	2:D:465:LYS:HE2	2.00	0.43
1:A:2057:LEU:HD12	1:A:2200:LEU:HD23	2.00	0.43
1:G:1446:ILE:HD11	1:G:1473:LEU:HD21	1.99	0.43
1:A:391:ASP:O	1:A:395:LYS:HG3	2.19	0.43
1:A:458:LYS:HD2	1:A:688:GLY:HA3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:439:MET:HE3	2:F:439:MET:HE1	2.01	0.43
1:A:1211:ARG:HA	1:A:1464:ILE:HD12	2.01	0.43
1:A:932:LEU:HD21	1:A:972:LEU:HB3	2.00	0.43
1:A:918:ASP:HB2	1:A:922:LYS:HD2	2.01	0.43
1:A:736:ARG:HA	1:A:736:ARG:HD2	1.86	0.43
1:A:1180:CYS:SG	1:A:1366:HIS:CE1	3.12	0.43
1:A:1775:ARG:HB3	1:A:1782:THR:HB	2.01	0.43
1:A:2123:ARG:O	1:A:2127:LEU:HD23	2.18	0.43
1:A:183:MET:O	1:A:187:GLN:HG3	2.20	0.42
1:A:1213:PRO:HG3	1:A:1307:ILE:CG2	2.49	0.42
1:A:1629:LEU:HD23	1:A:1629:LEU:HA	1.89	0.42
2:C:446:LEU:HD23	2:D:447:ILE:HG21	2.00	0.42
1:G:1447:ALA:O	1:G:1449:THR:N	2.51	0.42
1:A:275:LYS:HE2	1:A:275:LYS:HB2	1.71	0.42
1:A:518:PRO:HD2	1:A:1399:PHE:CE2	2.54	0.42
1:A:328:GLU:OE1	1:A:328:GLU:N	2.47	0.42
1:A:1106:TYR:O	1:A:1110:GLN:HG2	2.20	0.42
1:A:1153:MET:SD	1:A:1155:SER:HB3	2.59	0.42
1:A:1962:LYS:HD3	1:A:1987:TYR:CD1	2.54	0.42
1:G:1426:MET:HA	1:G:1429:TRP:CD1	2.54	0.42
1:G:1632:THR:O	1:G:1636:ARG:HG3	2.20	0.42
1:A:517:ASP:N	1:A:517:ASP:OD1	2.52	0.42
2:E:462:SER:O	2:E:466:ILE:HG12	2.20	0.42
1:A:102:TYR:CE2	1:A:104:PRO:HG3	2.54	0.42
1:A:203:LEU:HD11	1:A:210:PHE:CZ	2.54	0.42
1:A:782:ARG:NH1	1:A:1460:GLU:OE2	2.53	0.42
1:A:1230:ILE:HD12	1:A:1409:VAL:HG21	2.02	0.42
1:A:1740:LYS:HB2	1:A:1743:SER:OG	2.19	0.42
1:A:257:PRO:HA	1:A:260:GLN:HG3	2.01	0.42
1:A:544:GLU:OE1	1:A:544:GLU:N	2.50	0.42
1:A:1193:TYR:HD1	1:A:1362:VAL:HG22	1.83	0.42
1:A:1342:GLY:HA3	1:A:1365:LEU:HD11	2.02	0.42
1:A:1413:LYS:HA	1:A:1416:VAL:HG12	2.02	0.42
1:A:1927:ILE:O	1:A:1931:ILE:HG12	2.20	0.42
1:A:139:LEU:HD23	1:A:139:LEU:HA	1.94	0.41
1:A:1532:SER:HB2	1:A:1563:GLN:HB3	2.02	0.41
1:A:1557:ASN:OD1	1:A:1560:SER:HB3	2.19	0.41
1:A:1174:SER:HB3	1:A:1885:GLU:HB3	2.02	0.41
1:A:1819:ASP:OD2	1:A:1867:ARG:NH2	2.53	0.41
1:A:1997:VAL:O	1:A:2001:LEU:HG	2.19	0.41
1:A:1369:ASP:OD1	1:A:1369:ASP:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1434:ILE:O	1:A:1438:ILE:HG13	2.20	0.41
1:A:1514:ASP:OD2	1:A:1518:ARG:NH1	2.54	0.41
1:A:788:ASP:OD1	1:A:788:ASP:N	2.50	0.41
1:A:572:LEU:HD23	1:A:745:LYS:HB2	2.02	0.41
1:A:1221:GLU:CD	1:A:1223:SER:HB3	2.46	0.41
1:A:1670:THR:HG23	1:A:1673:TYR:H	1.86	0.41
1:A:1829:TYR:CE1	1:A:1848:PRO:HG3	2.54	0.41
1:A:2060:LEU:HD23	1:A:2060:LEU:HA	1.90	0.41
1:A:510:PHE:O	1:A:1027:ASN:ND2	2.50	0.41
2:C:444:ARG:O	2:C:448:GLU:OE1	2.37	0.41
2:D:439:MET:HE3	2:D:443:HIS:CE1	2.56	0.41
1:A:647:ASP:OD1	1:A:647:ASP:N	2.46	0.41
1:A:797:TYR:OH	2:B:544:THR:O	2.25	0.41
1:A:1380:GLU:HG2	1:A:1381:HIS:CD2	2.55	0.41
1:A:1463:VAL:HA	1:A:1529:LYS:HD3	2.02	0.41
1:A:1916:THR:O	1:A:1920:GLU:HG3	2.20	0.41
1:A:472[B]:MET:SD	1:A:1075:ILE:HG12	2.60	0.41
1:A:381:TYR:CE2	1:A:666:LYS:HE2	2.56	0.40
1:A:745:LYS:O	1:A:749:LEU:HG	2.21	0.40
2:E:443:HIS:O	2:E:447:ILE:HG12	2.21	0.40
1:A:73:LYS:O	1:A:77:THR:HG23	2.21	0.40
1:A:1212:VAL:HB	1:A:1465:ALA:HA	2.02	0.40
1:A:1628:LEU:HA	1:A:1631:LEU:HD12	2.03	0.40
2:F:443:HIS:O	2:F:447:ILE:HG12	2.21	0.40
1:A:1315:MET:HE1	1:A:1343:LEU:HD11	2.03	0.40
1:A:1744:ILE:HD13	1:A:2008:GLU:HB3	2.02	0.40
1:A:290:LEU:HD13	1:A:320:MET:HG2	2.03	0.40
1:A:859:THR:HG22	1:A:866:SER:OG	2.21	0.40
1:A:985:GLU:HA	1:A:986:PRO:HD3	1.90	0.40
1:A:1125:LYS:HA	1:A:1125:LYS:HD3	1.89	0.40
1:A:1456:ASP:O	1:A:1459:LYS:NZ	2.39	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	2107/2266 (93%)	2063 (98%)	44 (2%)	0	100	100
1	G	248/2266 (11%)	243 (98%)	5 (2%)	0	100	100
2	B	63/609 (10%)	62 (98%)	1 (2%)	0	100	100
2	C	35/609 (6%)	35 (100%)	0	0	100	100
2	D	39/609 (6%)	39 (100%)	0	0	100	100
2	E	36/609 (6%)	36 (100%)	0	0	100	100
2	F	32/609 (5%)	32 (100%)	0	0	100	100
All	All	2560/7577 (34%)	2510 (98%)	50 (2%)	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	1921/2059 (93%)	1920 (100%)	1 (0%)	88	96
1	G	230/2059 (11%)	230 (100%)	0	100	100
2	B	63/567 (11%)	63 (100%)	0	100	100
2	C	36/567 (6%)	36 (100%)	0	100	100
2	D	39/567 (7%)	39 (100%)	0	100	100
2	E	36/567 (6%)	36 (100%)	0	100	100
2	F	33/567 (6%)	33 (100%)	0	100	100
All	All	2358/6953 (34%)	2357 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2093	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	187	GLN
1	A	214	HIS
1	A	267	ASN
1	A	302	HIS
1	A	501	ASN
1	A	549	GLN
1	A	896	ASN
1	A	899	GLN
1	A	1020	ASN
1	A	1027	ASN
1	A	1142	GLN
1	A	1187	ASN
1	A	1336	GLN
1	A	1358	HIS
1	A	1359	ASN
1	A	1533	ASN
1	A	1537	HIS
1	A	1551	ASN
1	A	1601	ASN
1	A	1605	GLN
1	A	1715	ASN
1	A	1772	HIS
1	A	1780	ASN
1	A	1827	ASN
1	A	1875	ASN
1	A	2049	GLN
1	A	2054	GLN
2	B	573	GLN
2	F	450	GLN
1	G	1561	GLN
1	G	1647	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

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-37130. 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.