



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 08:10 AM UTC

PDB ID : 6DVZ / pdb_00006dvz
EMDB ID : EMD-8921
Title : Cryo-EM structure of mouse TRPV3-Y564A in complex with 2-Aminoethoxy diphenyl borate (2-APB)
Authors : Singh, A.K.; McGoldrick, L.L.; Sobolevsky, A.I.
Deposited on : 2018-06-25
Resolution : 4.24 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:

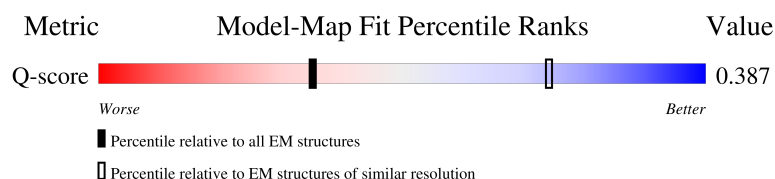
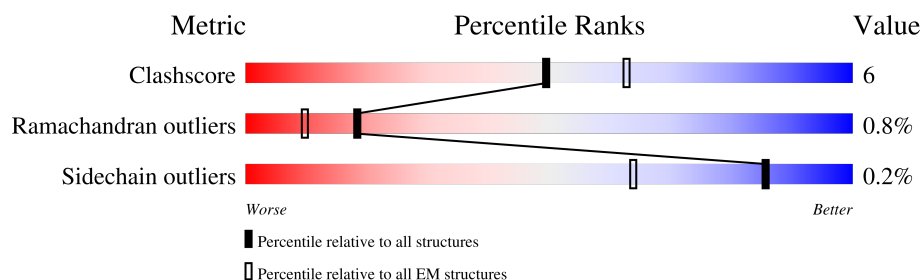
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 4.24 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4688 (3.74 - 4.74)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	791	44% 67% 13% • 19%
1	B	791	44% 67% 14% • 19%
1	C	791	44% 67% 14% • 19%
1	D	791	44% 67% 14% • 19%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20976 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.

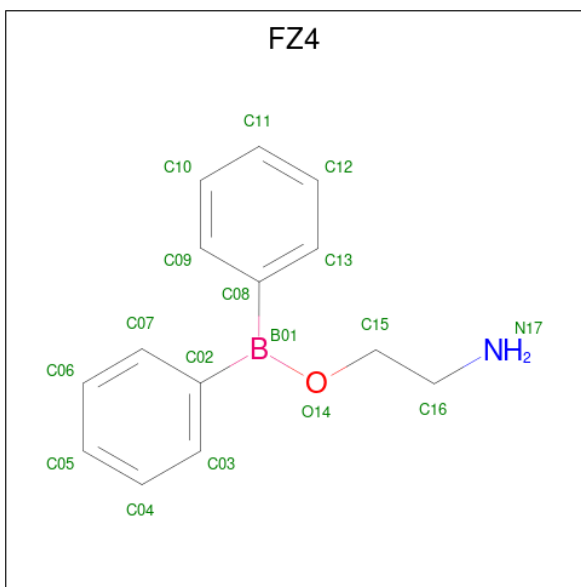
- Molecule 1 is a protein called Transient receptor potential cation channel subfamily V member 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	643	Total	C	N	O	S	0	0
			5193	3372	860	930	31		
1	B	643	Total	C	N	O	S	0	0
			5193	3372	860	930	31		
1	C	643	Total	C	N	O	S	0	0
			5193	3372	860	930	31		
1	D	643	Total	C	N	O	S	0	0
			5193	3372	860	930	31		

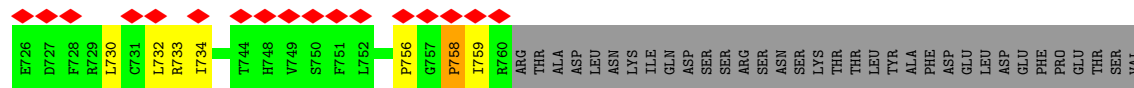
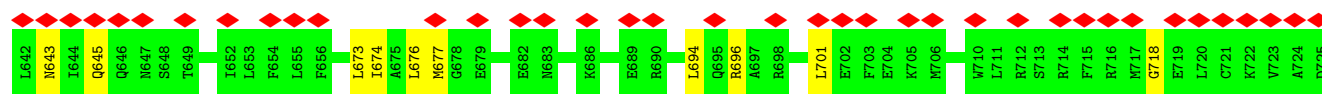
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q8K424
A	2	GLY	-	expression tag	UNP Q8K424
A	564	ALA	TYR	engineered mutation	UNP Q8K424
B	1	MET	-	initiating methionine	UNP Q8K424
B	2	GLY	-	expression tag	UNP Q8K424
B	564	ALA	TYR	engineered mutation	UNP Q8K424
C	1	MET	-	initiating methionine	UNP Q8K424
C	2	GLY	-	expression tag	UNP Q8K424
C	564	ALA	TYR	engineered mutation	UNP Q8K424
D	1	MET	-	initiating methionine	UNP Q8K424
D	2	GLY	-	expression tag	UNP Q8K424
D	564	ALA	TYR	engineered mutation	UNP Q8K424

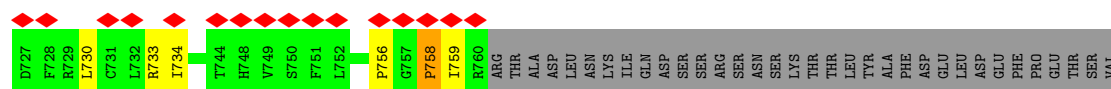
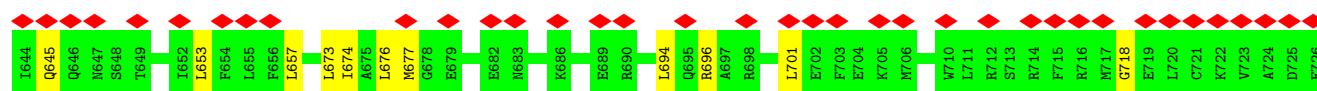
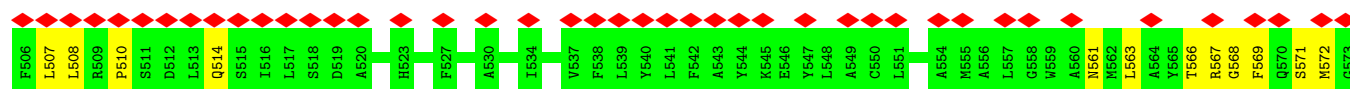
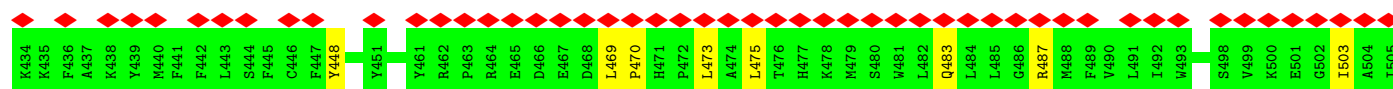
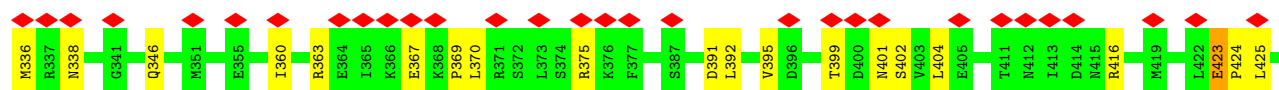
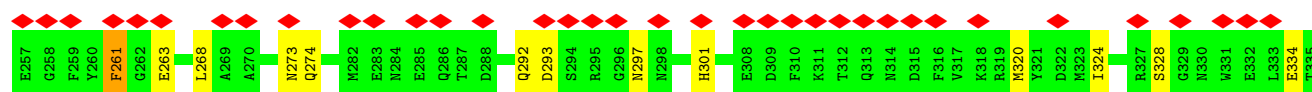
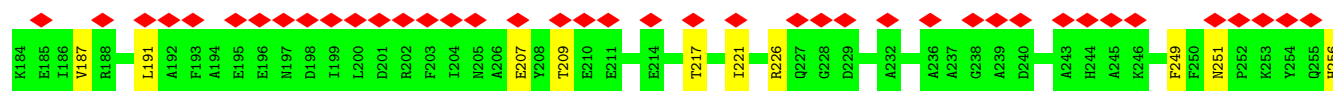
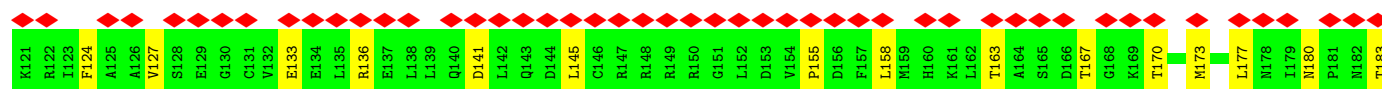
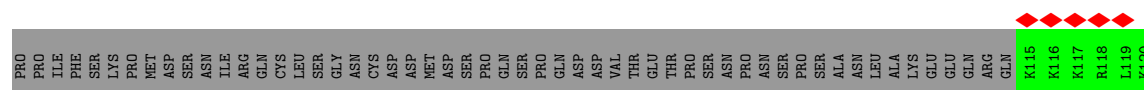
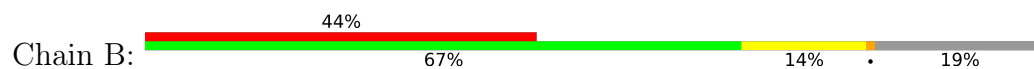
- Molecule 2 is 2-aminoethyl diphenylborinate (CCD ID: FZ4) (formula: C₁₄H₁₆BNO).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	B	C	N	O	0
			17	1	14	1	1	
2	A	1	Total	B	C	N	O	0
			17	1	14	1	1	
2	A	1	Total	B	C	N	O	0
			17	1	14	1	1	
2	B	1	Total	B	C	N	O	0
			17	1	14	1	1	
2	B	1	Total	B	C	N	O	0
			17	1	14	1	1	
2	B	1	Total	B	C	N	O	0
			17	1	14	1	1	
2	C	1	Total	B	C	N	O	0
			17	1	14	1	1	
2	C	1	Total	B	C	N	O	0
			17	1	14	1	1	
2	C	1	Total	B	C	N	O	0
			17	1	14	1	1	
2	D	1	Total	B	C	N	O	0
			17	1	14	1	1	
2	D	1	Total	B	C	N	O	0
			17	1	14	1	1	
2	D	1	Total	B	C	N	O	0
			17	1	14	1	1	

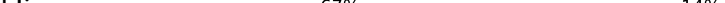


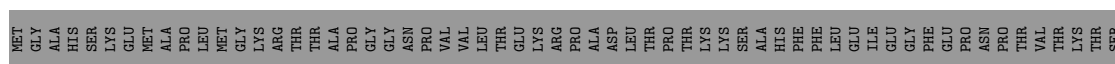
- Molecule 1: Transient receptor potential cation channel subfamily V member 3



- Chain C:



- Chain D:  44% 67% 14% 19%



WORLDWIDE
PDB
PROTEIN DATA BANK

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28075	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 ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.139	Depositor
Minimum map value	-0.084	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.057	Depositor
Map size ($\text{\AA}$)	233.19998, 233.19998, 233.19998	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FZ4

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	0.39	0/5301	0.73	6/7171 (0.1%)
1	B	0.39	0/5301	0.73	4/7171 (0.1%)
1	C	0.39	0/5301	0.73	6/7171 (0.1%)
1	D	0.39	0/5301	0.73	6/7171 (0.1%)
All	All	0.39	0/21204	0.73	22/28684 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	5
1	C	0	5
1	D	0	5
All	All	0	20

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	756	PRO	N-CA-CB	7.87	110.78	103.15
1	B	756	PRO	N-CA-CB	7.83	110.74	103.15
1	A	756	PRO	N-CA-CB	7.83	110.74	103.15
1	C	756	PRO	N-CA-CB	7.83	110.74	103.15
1	C	758	PRO	N-CA-CB	7.58	111.21	103.25
1	D	758	PRO	N-CA-CB	7.57	111.20	103.25
1	A	758	PRO	N-CA-CB	7.57	111.20	103.25
1	B	758	PRO	N-CA-CB	7.54	111.17	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	614	LYS	CA-C-N	5.40	131.85	121.54
1	A	614	LYS	C-N-CA	5.40	131.85	121.54
1	C	614	LYS	CA-C-N	5.40	131.85	121.54
1	C	614	LYS	C-N-CA	5.40	131.85	121.54
1	B	614	LYS	CA-C-N	5.38	131.81	121.54
1	B	614	LYS	C-N-CA	5.38	131.81	121.54
1	D	614	LYS	CA-C-N	5.36	131.78	121.54
1	D	614	LYS	C-N-CA	5.36	131.78	121.54
1	A	262	GLY	CA-C-N	5.17	131.41	121.54
1	A	262	GLY	C-N-CA	5.17	131.41	121.54
1	C	262	GLY	CA-C-N	5.16	131.40	121.54
1	C	262	GLY	C-N-CA	5.16	131.40	121.54
1	D	262	GLY	CA-C-N	5.16	131.40	121.54
1	D	262	GLY	C-N-CA	5.16	131.40	121.54

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	249	PHE	Peptide
1	A	261	PHE	Peptide
1	A	423	GLU	Peptide
1	A	469	LEU	Peptide
1	A	733	ARG	Peptide
1	B	249	PHE	Peptide
1	B	261	PHE	Peptide
1	B	423	GLU	Peptide
1	B	469	LEU	Peptide
1	B	733	ARG	Peptide
1	C	249	PHE	Peptide
1	C	261	PHE	Peptide
1	C	423	GLU	Peptide
1	C	469	LEU	Peptide
1	C	733	ARG	Peptide
1	D	249	PHE	Peptide
1	D	261	PHE	Peptide
1	D	423	GLU	Peptide
1	D	469	LEU	Peptide
1	D	733	ARG	Peptide

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	5193	0	5243	61	0
1	B	5193	0	5243	60	0
1	C	5193	0	5243	61	0
1	D	5193	0	5243	61	0
2	A	51	0	0	1	0
2	B	51	0	0	1	0
2	C	51	0	0	1	0
2	D	51	0	0	1	0
All	All	20976	0	20972	239	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 6.

All (239) 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:718:GLY:HA2	1:A:730:LEU:HB2	1.78	0.66
1:D:718:GLY:HA2	1:D:730:LEU:HB2	1.78	0.66
1:B:718:GLY:HA2	1:B:730:LEU:HB2	1.78	0.65
1:C:718:GLY:HA2	1:C:730:LEU:HB2	1.78	0.64
1:A:483:GLN:HG3	1:A:487:ARG:HH11	1.63	0.63
1:D:483:GLN:HG3	1:D:487:ARG:HH11	1.63	0.62
1:C:483:GLN:HG3	1:C:487:ARG:HH11	1.63	0.62
1:B:483:GLN:HG3	1:B:487:ARG:HH11	1.63	0.62
1:A:367:GLU:HB3	1:A:370:LEU:HB2	1.82	0.61
1:B:367:GLU:HG3	1:B:369:PRO:HD2	1.83	0.61
1:B:367:GLU:HB3	1:B:370:LEU:HB2	1.82	0.61
1:A:367:GLU:HG3	1:A:369:PRO:HD2	1.83	0.60
1:C:367:GLU:HG3	1:C:369:PRO:HD2	1.83	0.60
1:D:367:GLU:HB3	1:D:370:LEU:HB2	1.82	0.60
1:C:367:GLU:HB3	1:C:370:LEU:HB2	1.82	0.59
1:C:510:PRO:O	1:C:514:GLN:NE2	2.36	0.59
1:D:367:GLU:HG3	1:D:369:PRO:HD2	1.83	0.59
1:A:510:PRO:O	1:A:514:GLN:NE2	2.35	0.59
1:D:163:THR:HG22	1:D:170:THR:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:PRO:O	1:B:514:GLN:NE2	2.36	0.59
1:D:510:PRO:O	1:D:514:GLN:NE2	2.35	0.58
1:A:163:THR:HG22	1:A:170:THR:HA	1.84	0.58
1:C:163:THR:HG22	1:C:170:THR:HA	1.85	0.58
1:A:346:GLN:NE2	1:A:401:ASN:O	2.37	0.58
1:D:346:GLN:NE2	1:D:401:ASN:O	2.37	0.58
1:C:251:ASN:ND2	1:C:256:HIS:O	2.37	0.58
1:C:346:GLN:NE2	1:C:401:ASN:O	2.37	0.58
1:B:251:ASN:ND2	1:B:256:HIS:O	2.37	0.57
1:B:163:THR:HG22	1:B:170:THR:HA	1.84	0.57
1:B:346:GLN:NE2	1:B:401:ASN:O	2.37	0.57
1:A:251:ASN:ND2	1:A:256:HIS:O	2.37	0.57
2:D:801:FZ4:C03	2:D:801:FZ4:C08	2.83	0.57
1:D:251:ASN:ND2	1:D:256:HIS:O	2.37	0.56
1:A:448:TYR:OH	1:A:561:ASN:ND2	2.39	0.56
2:A:801:FZ4:C03	2:A:801:FZ4:C08	2.83	0.56
2:B:801:FZ4:C03	2:B:801:FZ4:C08	2.83	0.56
1:C:334:GLU:OE2	1:C:363:ARG:NH1	2.39	0.55
1:D:448:TYR:OH	1:D:561:ASN:ND2	2.39	0.55
1:C:448:TYR:OH	1:C:561:ASN:ND2	2.39	0.55
1:A:334:GLU:OE2	1:A:363:ARG:NH1	2.39	0.55
1:B:334:GLU:OE2	1:B:363:ARG:NH1	2.39	0.55
1:B:416:ARG:HD2	1:B:694:LEU:HD21	1.89	0.54
1:B:448:TYR:OH	1:B:561:ASN:ND2	2.39	0.54
1:D:334:GLU:OE2	1:D:363:ARG:NH1	2.39	0.54
1:A:416:ARG:HD2	1:A:694:LEU:HD21	1.89	0.54
1:A:674:ILE:HA	1:A:677:MET:HB3	1.90	0.54
2:C:801:FZ4:C03	2:C:801:FZ4:C08	2.83	0.54
1:C:416:ARG:HD2	1:C:694:LEU:HD21	1.89	0.54
1:D:674:ILE:HA	1:D:677:MET:HB3	1.90	0.54
1:C:674:ILE:HA	1:C:677:MET:HB3	1.90	0.54
1:B:674:ILE:HA	1:B:677:MET:HB3	1.90	0.53
1:C:261:PHE:HB2	1:C:263:GLU:H	1.73	0.53
1:D:416:ARG:HD2	1:D:694:LEU:HD21	1.89	0.53
1:D:261:PHE:HB2	1:D:263:GLU:H	1.73	0.53
1:B:392:LEU:HD12	1:B:395:VAL:HB	1.91	0.53
1:B:261:PHE:HB2	1:B:263:GLU:H	1.73	0.53
1:C:392:LEU:HD12	1:C:395:VAL:HB	1.91	0.53
1:D:292:GLN:NE2	1:D:336:MET:SD	2.76	0.53
1:D:226:ARG:HG2	1:D:274:GLN:HE21	1.74	0.52
1:A:261:PHE:HB2	1:A:263:GLU:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:GLN:NE2	1:B:336:MET:SD	2.76	0.52
1:B:375:ARG:NH1	1:B:391:ASP:OD2	2.43	0.52
1:C:375:ARG:NH1	1:C:391:ASP:OD2	2.43	0.52
1:D:392:LEU:HD12	1:D:395:VAL:HB	1.91	0.52
1:A:167:THR:O	1:A:209:THR:OG1	2.27	0.52
1:A:226:ARG:HG2	1:A:274:GLN:HE21	1.74	0.52
1:B:226:ARG:HG2	1:B:274:GLN:HE21	1.74	0.52
1:D:643:ASN:HA	1:D:645:GLN:HE22	1.75	0.52
1:A:392:LEU:HD12	1:A:395:VAL:HB	1.91	0.52
1:B:643:ASN:HA	1:B:645:GLN:HE22	1.75	0.51
1:C:643:ASN:HA	1:C:645:GLN:HE22	1.75	0.51
1:D:167:THR:O	1:D:209:THR:OG1	2.27	0.51
1:D:360:ILE:O	1:D:363:ARG:NH2	2.44	0.51
1:A:360:ILE:O	1:A:363:ARG:NH2	2.44	0.51
1:A:643:ASN:HA	1:A:645:GLN:HE22	1.75	0.51
1:C:226:ARG:HG2	1:C:274:GLN:HE21	1.74	0.51
1:C:292:GLN:NE2	1:C:336:MET:SD	2.76	0.51
1:D:375:ARG:NH1	1:D:391:ASP:OD2	2.43	0.51
1:A:292:GLN:NE2	1:A:336:MET:SD	2.76	0.51
1:B:598:LEU:HD11	1:B:629:VAL:HG13	1.93	0.51
1:C:360:ILE:O	1:C:363:ARG:NH2	2.44	0.51
1:C:598:LEU:HD11	1:C:629:VAL:HG13	1.93	0.51
1:A:375:ARG:NH1	1:A:391:ASP:OD2	2.43	0.50
1:B:360:ILE:O	1:B:363:ARG:NH2	2.44	0.50
1:B:167:THR:O	1:B:209:THR:OG1	2.27	0.50
1:D:598:LEU:HD11	1:D:629:VAL:HG13	1.93	0.50
1:A:598:LEU:HD11	1:A:629:VAL:HG13	1.93	0.50
1:C:167:THR:O	1:C:209:THR:OG1	2.27	0.49
1:B:676:LEU:HD11	1:C:578:MET:HE1	1.93	0.49
1:D:133:GLU:OE2	1:D:136:ARG:NH2	2.46	0.49
1:A:273:ASN:HA	1:A:320:MET:HE1	1.94	0.49
1:C:676:LEU:HD11	1:D:578:MET:HE1	1.93	0.49
1:C:273:ASN:HA	1:C:320:MET:HE1	1.94	0.49
1:A:578:MET:HE1	1:D:676:LEU:HD11	1.93	0.48
1:D:423:GLU:O	1:D:425:LEU:N	2.46	0.48
1:B:273:ASN:HA	1:B:320:MET:HE1	1.94	0.48
1:B:423:GLU:O	1:B:425:LEU:N	2.46	0.48
1:D:273:ASN:HA	1:D:320:MET:HE1	1.94	0.48
1:A:676:LEU:HD11	1:B:578:MET:HE1	1.93	0.48
1:D:293:ASP:HB3	1:D:297:ASN:H	1.79	0.48
1:A:133:GLU:OE2	1:A:136:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:ILE:HD13	1:B:623:GLY:HA2	1.96	0.48
1:C:133:GLU:OE2	1:C:136:ARG:NH2	2.46	0.48
1:C:423:GLU:O	1:C:425:LEU:N	2.46	0.48
1:B:293:ASP:HB3	1:B:297:ASN:H	1.79	0.48
1:A:423:GLU:O	1:A:425:LEU:N	2.46	0.48
1:B:399:THR:O	1:B:402:SER:OG	2.30	0.48
1:C:293:ASP:HB3	1:C:297:ASN:H	1.78	0.48
1:B:133:GLU:OE2	1:B:136:ARG:NH2	2.46	0.48
1:C:609:ILE:HD13	1:C:623:GLY:HA2	1.96	0.48
1:C:399:THR:O	1:C:402:SER:OG	2.30	0.48
1:A:293:ASP:HB3	1:A:297:ASN:H	1.78	0.47
1:C:367:GLU:HG2	1:C:370:LEU:HD12	1.96	0.47
1:D:367:GLU:HG2	1:D:370:LEU:HD12	1.96	0.47
1:D:609:ILE:HD13	1:D:623:GLY:HA2	1.96	0.47
1:C:613:SER:HB3	1:C:617:LYS:HA	1.97	0.47
1:B:187:VAL:O	1:B:191:LEU:N	2.42	0.47
1:B:367:GLU:HG2	1:B:370:LEU:HD12	1.96	0.47
1:D:187:VAL:O	1:D:191:LEU:N	2.42	0.47
1:D:613:SER:HB3	1:D:617:LYS:HA	1.97	0.47
1:A:613:SER:HB3	1:A:617:LYS:HA	1.97	0.47
1:B:613:SER:HB3	1:B:617:LYS:HA	1.97	0.47
1:A:367:GLU:HG2	1:A:370:LEU:HD12	1.96	0.46
1:A:568:GLY:O	1:A:696:ARG:NH2	2.49	0.46
1:A:609:ILE:HD13	1:A:623:GLY:HA2	1.96	0.46
1:C:568:GLY:O	1:C:696:ARG:NH2	2.49	0.46
1:B:566:THR:HB	1:B:572:MET:HB3	1.97	0.46
1:A:566:THR:HB	1:A:572:MET:HB3	1.97	0.46
1:B:568:GLY:O	1:B:696:ARG:NH2	2.49	0.46
1:C:207:GLU:HB3	1:C:217:THR:HG22	1.98	0.46
1:D:207:GLU:HB3	1:D:217:THR:HG22	1.98	0.46
1:D:566:THR:HB	1:D:572:MET:HB3	1.97	0.46
1:D:568:GLY:O	1:D:696:ARG:NH2	2.49	0.46
1:A:187:VAL:O	1:A:191:LEU:N	2.42	0.45
1:C:566:THR:HB	1:C:572:MET:HB3	1.97	0.45
1:A:634:LYS:HB3	1:A:639:LEU:HB2	1.97	0.45
1:B:207:GLU:HB3	1:B:217:THR:HG22	1.98	0.45
1:B:567:ARG:O	1:B:569:PHE:N	2.50	0.45
1:C:634:LYS:HB3	1:C:639:LEU:HB2	1.97	0.45
1:D:634:LYS:HB3	1:D:639:LEU:HB2	1.97	0.45
1:B:324:ILE:O	1:B:328:SER:N	2.50	0.45
1:C:653:LEU:O	1:C:657:LEU:N	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:567:ARG:O	1:D:569:PHE:N	2.50	0.45
1:B:124:PHE:HA	1:B:127:VAL:HB	1.98	0.45
1:B:634:LYS:HB3	1:B:639:LEU:HB2	1.97	0.45
1:D:324:ILE:O	1:D:328:SER:N	2.50	0.45
1:A:567:ARG:O	1:A:569:PHE:N	2.50	0.45
1:A:399:THR:O	1:A:402:SER:OG	2.30	0.45
1:A:124:PHE:HA	1:A:127:VAL:HB	1.99	0.44
1:A:207:GLU:HB3	1:A:217:THR:HG22	1.98	0.44
1:A:261:PHE:HD1	1:A:268:LEU:HD13	1.83	0.44
1:C:124:PHE:HA	1:C:127:VAL:HB	1.99	0.44
1:B:563:LEU:O	1:B:566:THR:OG1	2.32	0.44
1:C:567:ARG:O	1:C:569:PHE:N	2.50	0.44
1:D:261:PHE:HD1	1:D:268:LEU:HD13	1.83	0.44
1:C:324:ILE:O	1:C:328:SER:N	2.50	0.44
1:D:399:THR:O	1:D:402:SER:OG	2.30	0.44
1:B:141:ASP:O	1:B:145:LEU:N	2.47	0.44
1:C:673:LEU:O	1:C:677:MET:N	2.40	0.43
1:D:124:PHE:HA	1:D:127:VAL:HB	1.99	0.43
1:C:261:PHE:HD1	1:C:268:LEU:HD13	1.83	0.43
1:A:324:ILE:O	1:A:328:SER:N	2.50	0.43
1:B:624:SER:O	1:B:628:ALA:N	2.48	0.43
1:B:261:PHE:HD1	1:B:268:LEU:HD13	1.83	0.43
1:A:673:LEU:O	1:A:677:MET:N	2.41	0.43
1:D:624:SER:O	1:D:628:ALA:N	2.48	0.43
1:A:227:GLN:O	1:A:231:THR:OG1	2.29	0.43
1:B:226:ARG:HG2	1:B:274:GLN:NE2	2.34	0.43
1:C:404:LEU:HG	1:C:701:LEU:HD11	2.01	0.43
1:D:375:ARG:HB3	1:D:391:ASP:HB2	2.01	0.43
1:A:375:ARG:HB3	1:A:391:ASP:HB2	2.01	0.43
1:C:155:PRO:HA	1:C:158:LEU:HD12	2.01	0.43
1:A:155:PRO:HA	1:A:158:LEU:HD12	2.01	0.42
1:C:177:LEU:HG	1:C:221:ILE:HD11	2.01	0.42
1:C:226:ARG:HG2	1:C:274:GLN:NE2	2.34	0.42
1:B:673:LEU:O	1:B:677:MET:N	2.41	0.42
1:D:155:PRO:HA	1:D:158:LEU:HD12	2.01	0.42
1:B:177:LEU:HG	1:B:221:ILE:HD11	2.01	0.42
1:A:589:LYS:HE2	1:B:571:SER:HB2	2.02	0.42
1:A:624:SER:O	1:A:628:ALA:N	2.48	0.42
1:D:362:SER:OG	1:D:363:ARG:N	2.53	0.42
1:D:732:LEU:HD23	1:D:732:LEU:HA	1.89	0.42
1:B:375:ARG:HB3	1:B:391:ASP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:ASN:OD1	1:C:183:THR:OG1	2.27	0.42
1:D:177:LEU:HG	1:D:221:ILE:HD11	2.01	0.42
1:A:362:SER:OG	1:A:363:ARG:N	2.53	0.42
1:B:404:LEU:HG	1:B:701:LEU:HD11	2.01	0.42
1:B:589:LYS:HE2	1:C:571:SER:HB2	2.02	0.42
1:C:170:THR:HG23	1:C:173:MET:HE2	2.02	0.42
1:D:673:LEU:O	1:D:677:MET:N	2.40	0.42
1:B:155:PRO:HA	1:B:158:LEU:HD12	2.01	0.42
1:C:187:VAL:O	1:C:191:LEU:N	2.42	0.42
1:C:362:SER:OG	1:C:363:ARG:N	2.53	0.42
1:A:177:LEU:HG	1:A:221:ILE:HD11	2.01	0.42
1:D:180:ASN:OD1	1:D:183:THR:OG1	2.26	0.42
1:B:653:LEU:O	1:B:657:LEU:N	2.36	0.41
1:C:375:ARG:HB3	1:C:391:ASP:HB2	2.01	0.41
1:D:170:THR:HG23	1:D:173:MET:HE2	2.02	0.41
1:D:226:ARG:HG2	1:D:274:GLN:NE2	2.34	0.41
1:A:404:LEU:HG	1:A:701:LEU:HD11	2.01	0.41
1:D:404:LEU:HG	1:D:701:LEU:HD11	2.01	0.41
1:C:589:LYS:HE2	1:D:571:SER:HB2	2.02	0.41
1:C:669:LEU:HD23	1:C:669:LEU:HA	1.86	0.41
1:A:170:THR:HG23	1:A:173:MET:HE2	2.02	0.41
1:A:226:ARG:HG2	1:A:274:GLN:NE2	2.34	0.41
1:D:563:LEU:O	1:D:566:THR:OG1	2.32	0.41
1:B:734:ILE:HD11	1:B:759:ILE:HA	2.03	0.41
1:C:448:TYR:HH	1:C:561:ASN:HD21	1.68	0.41
1:A:508:LEU:HD13	1:A:508:LEU:HA	1.93	0.41
1:A:732:LEU:HD23	1:A:732:LEU:HA	1.89	0.41
1:B:503:ILE:HG22	1:B:507:LEU:HG	2.03	0.41
1:D:503:ILE:HG22	1:D:507:LEU:HG	2.03	0.41
1:D:653:LEU:O	1:D:657:LEU:N	2.36	0.41
1:A:301:HIS:HE1	1:A:338:ASN:HB3	1.86	0.41
1:A:503:ILE:HG22	1:A:507:LEU:HG	2.03	0.41
1:A:571:SER:HB2	1:D:589:LYS:HE2	2.02	0.41
1:B:180:ASN:OD1	1:B:183:THR:OG1	2.27	0.41
1:B:301:HIS:HE1	1:B:338:ASN:HB3	1.86	0.41
1:B:473:LEU:HD11	1:B:475:LEU:HD23	2.03	0.41
1:C:141:ASP:O	1:C:145:LEU:N	2.47	0.41
1:C:734:ILE:HD11	1:C:759:ILE:HA	2.03	0.41
1:D:669:LEU:HA	1:D:672:MET:HB3	2.03	0.41
1:B:170:THR:HG23	1:B:173:MET:HE2	2.02	0.41
1:D:411:THR:OG1	1:D:412:ASN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:LEU:HD11	1:A:475:LEU:HD23	2.03	0.40
1:D:219:LEU:HD23	1:D:219:LEU:HA	1.92	0.40
1:D:473:LEU:HD11	1:D:475:LEU:HD23	2.03	0.40
1:A:734:ILE:HD11	1:A:759:ILE:HA	2.03	0.40
1:C:301:HIS:HE1	1:C:338:ASN:HB3	1.86	0.40
1:C:473:LEU:HD11	1:C:475:LEU:HD23	2.03	0.40
1:C:503:ILE:HG22	1:C:507:LEU:HG	2.03	0.40
1:D:325:LEU:HD23	1:D:325:LEU:HA	1.90	0.40
1:A:325:LEU:HA	1:A:325:LEU:HD23	1.90	0.40
1:A:701:LEU:HD23	1:A:701:LEU:HA	1.90	0.40
1:A:320:MET:HE3	1:A:320:MET:HB2	1.97	0.40
1:B:508:LEU:HD13	1:B:508:LEU:HA	1.93	0.40
1:C:669:LEU:HA	1:C:672:MET:HB3	2.03	0.40
1:B:320:MET:HE3	1:B:320:MET:HB2	1.97	0.40
1:C:411:THR:OG1	1:C:412:ASN:N	2.54	0.40

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	639/791 (81%)	528 (83%)	106 (17%)	5 (1%)	16	52
1	B	639/791 (81%)	528 (83%)	106 (17%)	5 (1%)	16	52
1	C	639/791 (81%)	528 (83%)	106 (17%)	5 (1%)	16	52
1	D	639/791 (81%)	527 (82%)	107 (17%)	5 (1%)	16	52
All	All	2556/3164 (81%)	2111 (83%)	425 (17%)	20 (1%)	18	52

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	758	PRO
1	B	758	PRO
1	C	758	PRO
1	D	758	PRO
1	A	586	ASP
1	A	615	ASP
1	B	586	ASP
1	B	615	ASP
1	C	586	ASP
1	C	615	ASP
1	D	586	ASP
1	D	615	ASP
1	A	424	PRO
1	B	424	PRO
1	C	424	PRO
1	D	424	PRO
1	A	470	PRO
1	B	470	PRO
1	C	470	PRO
1	D	470	PRO

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	561/706 (80%)	560 (100%)	1 (0%)	87	85
1	B	561/706 (80%)	560 (100%)	1 (0%)	87	85
1	C	561/706 (80%)	560 (100%)	1 (0%)	87	85
1	D	561/706 (80%)	560 (100%)	1 (0%)	87	85
All	All	2244/2824 (80%)	2240 (100%)	4 (0%)	85	85

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

Mol	Chain	Res	Type
1	A	609	ILE
1	B	609	ILE

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Mol	Chain	Res	Type
1	C	609	ILE
1	D	609	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	A	143	GLN
1	A	178	ASN
1	A	205	ASN
1	A	255	GLN
1	A	274	GLN
1	A	645	GLN
1	A	647	ASN
1	A	683	ASN
1	B	140	GLN
1	B	143	GLN
1	B	178	ASN
1	B	274	GLN
1	B	645	GLN
1	B	647	ASN
1	B	683	ASN
1	C	140	GLN
1	C	143	GLN
1	C	178	ASN
1	C	205	ASN
1	C	274	GLN
1	C	645	GLN
1	C	647	ASN
1	C	683	ASN
1	D	140	GLN
1	D	143	GLN
1	D	178	ASN
1	D	274	GLN
1	D	645	GLN
1	D	647	ASN
1	D	683	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 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	FZ4	A	802	-	17,18,18	0.70	0	18,22,22	1.62	6 (33%)
2	FZ4	A	803	-	17,18,18	0.73	0	18,22,22	1.63	3 (16%)
2	FZ4	C	802	-	17,18,18	0.68	0	18,22,22	1.62	6 (33%)
2	FZ4	B	802	-	17,18,18	0.69	0	18,22,22	1.62	6 (33%)
2	FZ4	C	803	-	17,18,18	0.72	0	18,22,22	1.62	3 (16%)
2	FZ4	A	801	-	17,18,18	0.93	1 (5%)	18,22,22	1.84	6 (33%)
2	FZ4	D	802	-	17,18,18	0.69	0	18,22,22	1.63	6 (33%)
2	FZ4	D	803	-	17,18,18	0.72	0	18,22,22	1.61	3 (16%)
2	FZ4	B	801	-	17,18,18	0.93	1 (5%)	18,22,22	1.84	6 (33%)
2	FZ4	C	801	-	17,18,18	0.93	1 (5%)	18,22,22	1.83	6 (33%)
2	FZ4	B	803	-	17,18,18	0.72	0	18,22,22	1.63	4 (22%)
2	FZ4	D	801	-	17,18,18	0.92	1 (5%)	18,22,22	1.84	6 (33%)

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	FZ4	A	802	-	-	4/12/12/12	0/2/2/2
2	FZ4	A	803	-	-	8/12/12/12	0/2/2/2
2	FZ4	C	802	-	-	4/12/12/12	0/2/2/2
2	FZ4	B	802	-	-	4/12/12/12	0/2/2/2
2	FZ4	C	803	-	-	8/12/12/12	0/2/2/2
2	FZ4	A	801	-	-	6/12/12/12	0/2/2/2
2	FZ4	D	802	-	-	4/12/12/12	0/2/2/2
2	FZ4	D	803	-	-	8/12/12/12	0/2/2/2
2	FZ4	B	801	-	-	6/12/12/12	0/2/2/2
2	FZ4	C	801	-	-	6/12/12/12	0/2/2/2
2	FZ4	B	803	-	-	8/12/12/12	0/2/2/2
2	FZ4	D	801	-	-	6/12/12/12	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	FZ4	C03-C02	-2.35	1.37	1.40
2	A	801	FZ4	C03-C02	-2.28	1.37	1.40
2	C	801	FZ4	C03-C02	-2.26	1.37	1.40
2	D	801	FZ4	C03-C02	-2.24	1.37	1.40

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FZ4	B01-C02-C03	-4.43	115.10	121.51
2	A	801	FZ4	B01-C02-C03	-4.41	115.12	121.51
2	B	801	FZ4	B01-C02-C03	-4.39	115.15	121.51
2	C	801	FZ4	B01-C02-C03	-4.39	115.15	121.51
2	C	802	FZ4	C07-C02-C03	3.80	121.22	116.86
2	D	802	FZ4	C07-C02-C03	3.79	121.21	116.86
2	B	802	FZ4	C07-C02-C03	3.76	121.18	116.86
2	A	802	FZ4	C07-C02-C03	3.75	121.17	116.86
2	A	803	FZ4	C13-C08-C09	3.37	120.73	116.86
2	C	803	FZ4	C13-C08-C09	3.34	120.70	116.86
2	D	803	FZ4	C13-C08-C09	3.32	120.67	116.86
2	B	803	FZ4	C13-C08-C09	3.31	120.66	116.86
2	B	801	FZ4	C07-C02-C03	3.07	120.38	116.86
2	B	803	FZ4	C07-C02-C03	3.04	120.35	116.86
2	A	801	FZ4	C07-C02-C03	3.04	120.34	116.86
2	D	801	FZ4	C07-C02-C03	3.03	120.34	116.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	FZ4	C07-C02-C03	3.00	120.30	116.86
2	A	803	FZ4	C07-C02-C03	2.99	120.30	116.86
2	C	803	FZ4	C07-C02-C03	2.97	120.27	116.86
2	D	803	FZ4	C07-C02-C03	2.93	120.22	116.86
2	A	802	FZ4	C13-C08-C09	2.70	119.96	116.86
2	B	802	FZ4	C13-C08-C09	2.66	119.92	116.86
2	D	802	FZ4	C04-C03-C02	-2.64	119.05	121.58
2	D	802	FZ4	C13-C08-C09	2.64	119.89	116.86
2	A	802	FZ4	C04-C03-C02	-2.64	119.06	121.58
2	C	802	FZ4	C04-C03-C02	-2.64	119.06	121.58
2	C	802	FZ4	C13-C08-C09	2.63	119.88	116.86
2	B	802	FZ4	C04-C03-C02	-2.62	119.07	121.58
2	A	803	FZ4	C10-C09-C08	-2.53	119.16	121.58
2	D	803	FZ4	C10-C09-C08	-2.51	119.18	121.58
2	B	803	FZ4	C10-C09-C08	-2.50	119.19	121.58
2	C	803	FZ4	C10-C09-C08	-2.50	119.19	121.58
2	D	801	FZ4	C04-C03-C02	-2.46	119.22	121.58
2	B	801	FZ4	C04-C03-C02	-2.44	119.25	121.58
2	A	801	FZ4	C04-C03-C02	-2.43	119.25	121.58
2	C	801	FZ4	C04-C03-C02	-2.40	119.28	121.58
2	B	802	FZ4	C10-C09-C08	-2.31	119.37	121.58
2	A	802	FZ4	C10-C09-C08	-2.31	119.37	121.58
2	A	801	FZ4	C05-C04-C03	2.29	123.07	120.24
2	B	801	FZ4	C05-C04-C03	2.29	123.07	120.24
2	C	801	FZ4	C05-C04-C03	2.29	123.07	120.24
2	D	801	FZ4	C05-C04-C03	2.29	123.07	120.24
2	D	802	FZ4	C10-C09-C08	-2.28	119.40	121.58
2	C	802	FZ4	C10-C09-C08	-2.26	119.42	121.58
2	C	802	FZ4	C06-C07-C02	-2.12	119.55	121.58
2	D	801	FZ4	B01-C02-C07	2.10	124.55	121.51
2	D	802	FZ4	C06-C07-C02	-2.10	119.57	121.58
2	C	801	FZ4	B01-C02-C07	2.09	124.54	121.51
2	D	802	FZ4	B01-C02-C07	-2.09	118.48	121.51
2	A	801	FZ4	B01-C02-C07	2.08	124.52	121.51
2	C	802	FZ4	B01-C02-C07	-2.08	118.50	121.51
2	B	802	FZ4	C06-C07-C02	-2.07	119.60	121.58
2	B	802	FZ4	B01-C02-C07	-2.07	118.51	121.51
2	A	802	FZ4	C06-C07-C02	-2.05	119.62	121.58
2	A	802	FZ4	B01-C02-C07	-2.04	118.56	121.51
2	A	801	FZ4	C13-C08-C09	2.04	119.20	116.86
2	B	801	FZ4	C13-C08-C09	2.04	119.20	116.86
2	C	801	FZ4	C13-C08-C09	2.04	119.20	116.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FZ4	C13-C08-C09	2.04	119.20	116.86
2	B	801	FZ4	B01-C02-C07	2.04	124.46	121.51
2	B	803	FZ4	C06-C07-C02	-2.02	119.65	121.58

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	FZ4	O14-B01-C08-C09
2	A	801	FZ4	O14-B01-C08-C13
2	A	801	FZ4	C02-B01-O14-C15
2	A	801	FZ4	C08-B01-O14-C15
2	A	802	FZ4	C08-B01-O14-C15
2	A	802	FZ4	O14-C15-C16-N17
2	A	803	FZ4	O14-B01-C02-C03
2	A	803	FZ4	O14-B01-C02-C07
2	A	803	FZ4	C02-B01-O14-C15
2	A	803	FZ4	C08-B01-O14-C15
2	A	803	FZ4	O14-C15-C16-N17
2	B	801	FZ4	O14-B01-C08-C09
2	B	801	FZ4	O14-B01-C08-C13
2	B	801	FZ4	C02-B01-O14-C15
2	B	801	FZ4	C08-B01-O14-C15
2	B	802	FZ4	C08-B01-O14-C15
2	B	802	FZ4	O14-C15-C16-N17
2	B	803	FZ4	O14-B01-C02-C03
2	B	803	FZ4	O14-B01-C02-C07
2	B	803	FZ4	C02-B01-O14-C15
2	B	803	FZ4	C08-B01-O14-C15
2	B	803	FZ4	O14-C15-C16-N17
2	C	801	FZ4	O14-B01-C08-C09
2	C	801	FZ4	O14-B01-C08-C13
2	C	801	FZ4	C02-B01-O14-C15
2	C	801	FZ4	C08-B01-O14-C15
2	C	802	FZ4	C08-B01-O14-C15
2	C	802	FZ4	O14-C15-C16-N17
2	C	803	FZ4	O14-B01-C02-C03
2	C	803	FZ4	O14-B01-C02-C07
2	C	803	FZ4	C02-B01-O14-C15
2	C	803	FZ4	C08-B01-O14-C15
2	C	803	FZ4	O14-C15-C16-N17
2	D	801	FZ4	O14-B01-C08-C09

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Mol	Chain	Res	Type	Atoms
2	D	801	FZ4	O14-B01-C08-C13
2	D	801	FZ4	C02-B01-O14-C15
2	D	801	FZ4	C08-B01-O14-C15
2	D	802	FZ4	C08-B01-O14-C15
2	D	802	FZ4	O14-C15-C16-N17
2	D	803	FZ4	O14-B01-C02-C03
2	D	803	FZ4	O14-B01-C02-C07
2	D	803	FZ4	C02-B01-O14-C15
2	D	803	FZ4	C08-B01-O14-C15
2	D	803	FZ4	O14-C15-C16-N17
2	A	801	FZ4	C02-B01-C08-C13
2	B	801	FZ4	C02-B01-C08-C13
2	C	801	FZ4	C02-B01-C08-C13
2	D	801	FZ4	C02-B01-C08-C13
2	A	801	FZ4	C02-B01-C08-C09
2	A	803	FZ4	C08-B01-C02-C03
2	A	803	FZ4	C08-B01-C02-C07
2	B	801	FZ4	C02-B01-C08-C09
2	B	803	FZ4	C08-B01-C02-C03
2	B	803	FZ4	C08-B01-C02-C07
2	C	801	FZ4	C02-B01-C08-C09
2	C	803	FZ4	C08-B01-C02-C03
2	C	803	FZ4	C08-B01-C02-C07
2	D	801	FZ4	C02-B01-C08-C09
2	D	803	FZ4	C08-B01-C02-C03
2	D	803	FZ4	C08-B01-C02-C07
2	A	802	FZ4	O14-B01-C08-C09
2	A	802	FZ4	O14-B01-C08-C13
2	A	803	FZ4	O14-B01-C08-C09
2	B	802	FZ4	O14-B01-C08-C09
2	B	802	FZ4	O14-B01-C08-C13
2	B	803	FZ4	O14-B01-C08-C09
2	C	802	FZ4	O14-B01-C08-C09
2	C	802	FZ4	O14-B01-C08-C13
2	C	803	FZ4	O14-B01-C08-C09
2	D	802	FZ4	O14-B01-C08-C09
2	D	802	FZ4	O14-B01-C08-C13
2	D	803	FZ4	O14-B01-C08-C09

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	FZ4	1	0
2	B	801	FZ4	1	0
2	C	801	FZ4	1	0
2	D	801	FZ4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1
1	C	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	744:THR	C	748:HIS	N	35.64
1	B	744:THR	C	748:HIS	N	35.64
1	C	744:THR	C	748:HIS	N	35.64
1	D	744:THR	C	748:HIS	N	35.64

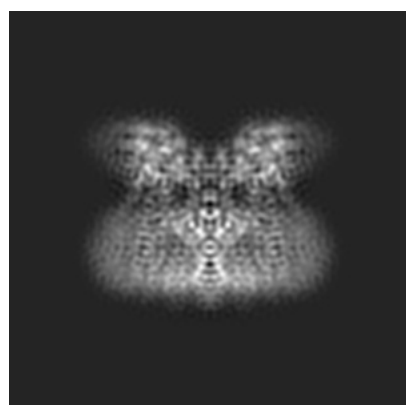
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8921. These allow visual inspection of the internal detail of the map and identification of artifacts.

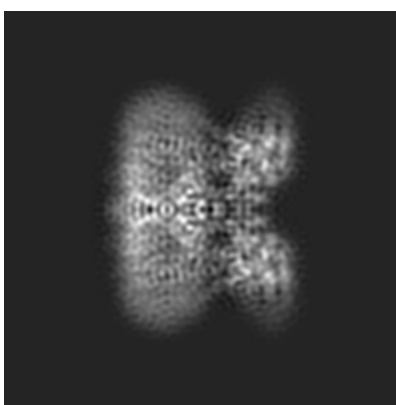
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

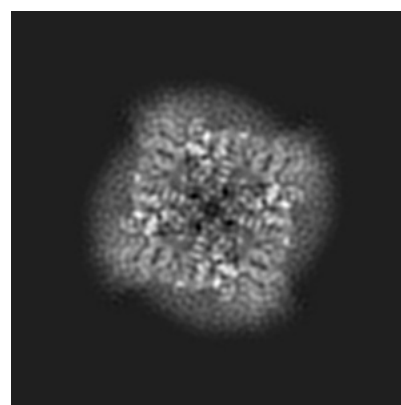
6.1.1 Primary map



X



Y

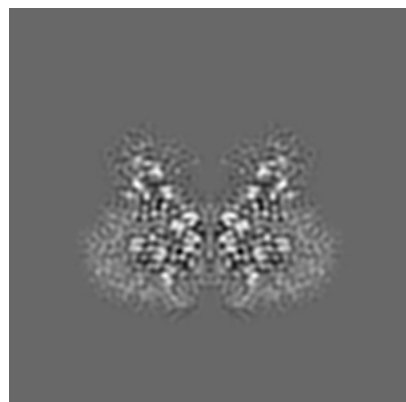


Z

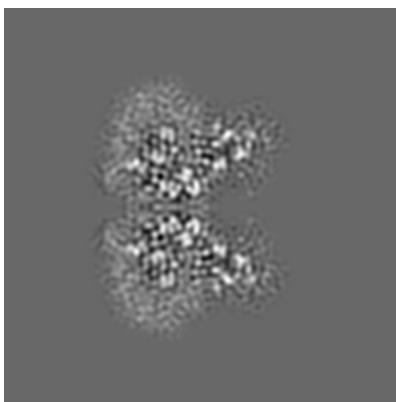
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

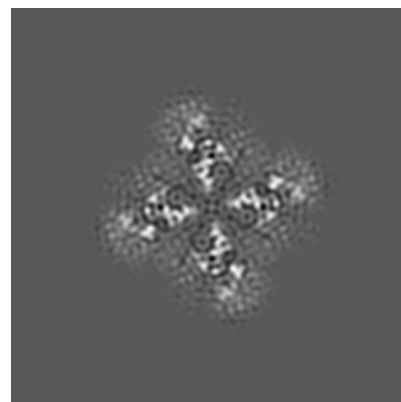
6.2.1 Primary map



X Index: 110



Y Index: 110



Z Index: 110

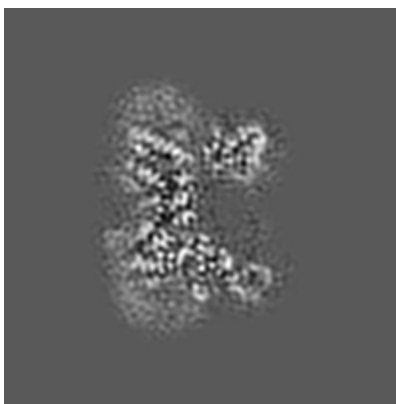
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

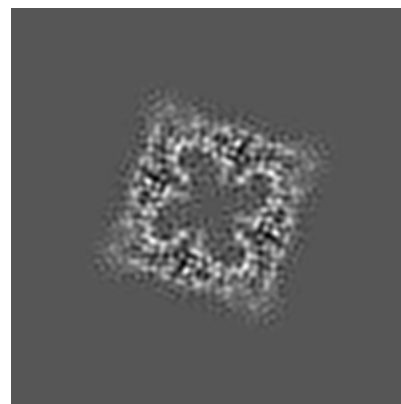
6.3.1 Primary map



X Index: 104



Y Index: 104

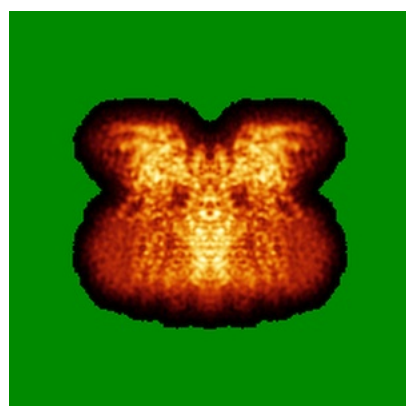


Z Index: 134

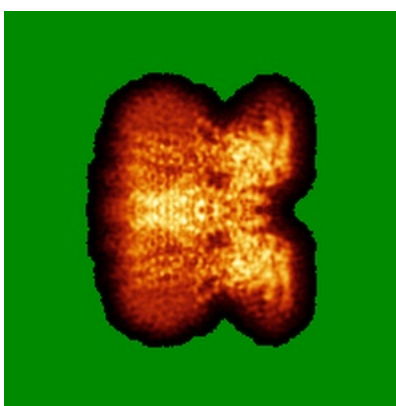
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

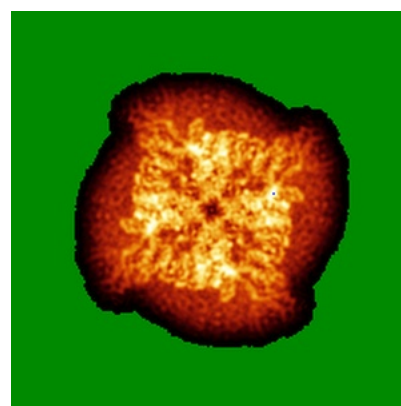
6.4.1 Primary map



X



Y

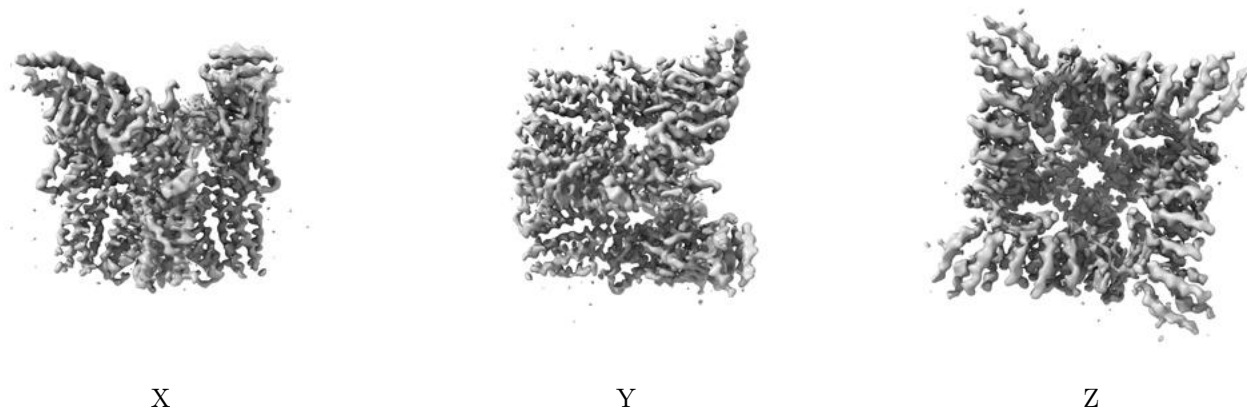


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.057. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

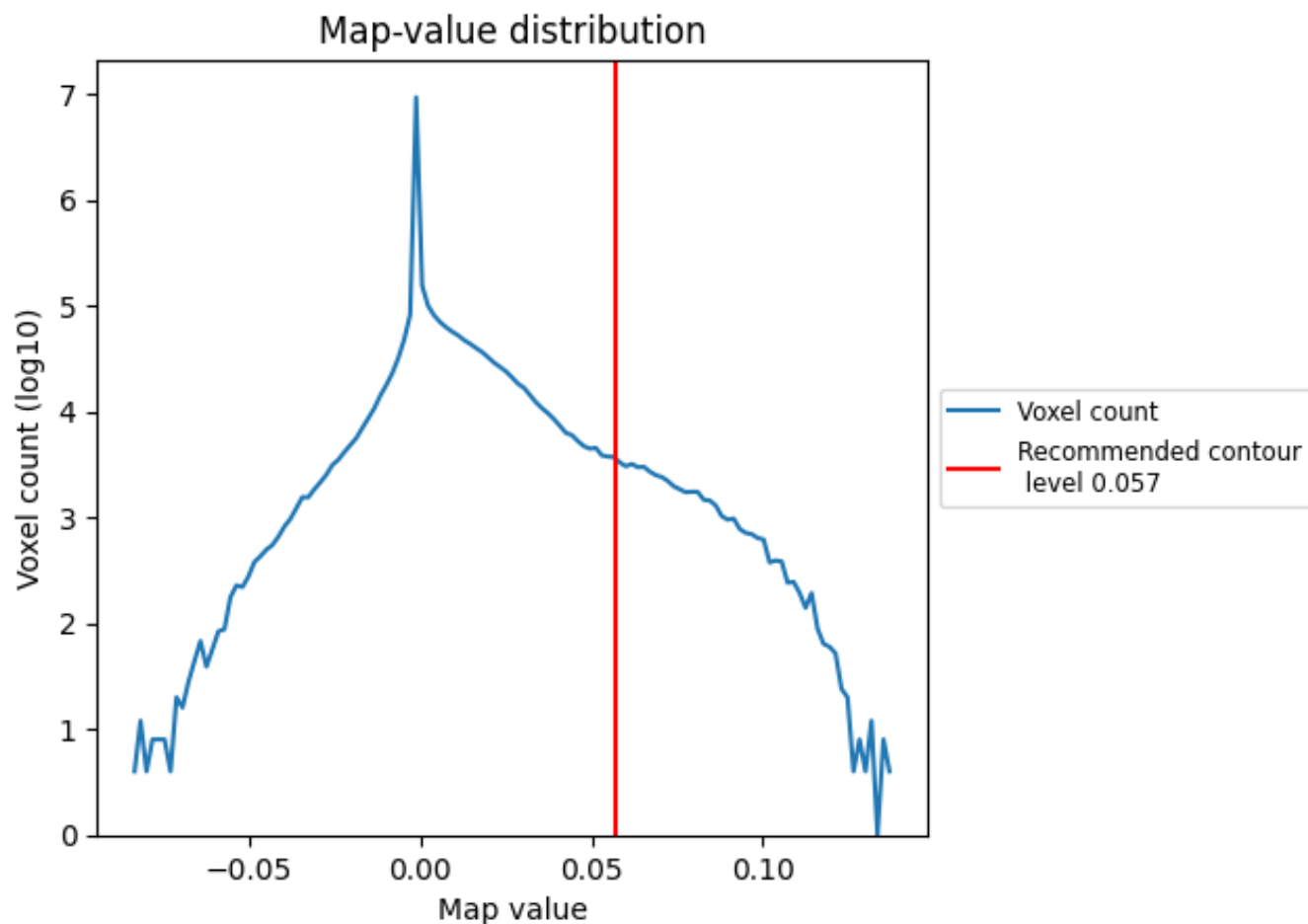
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

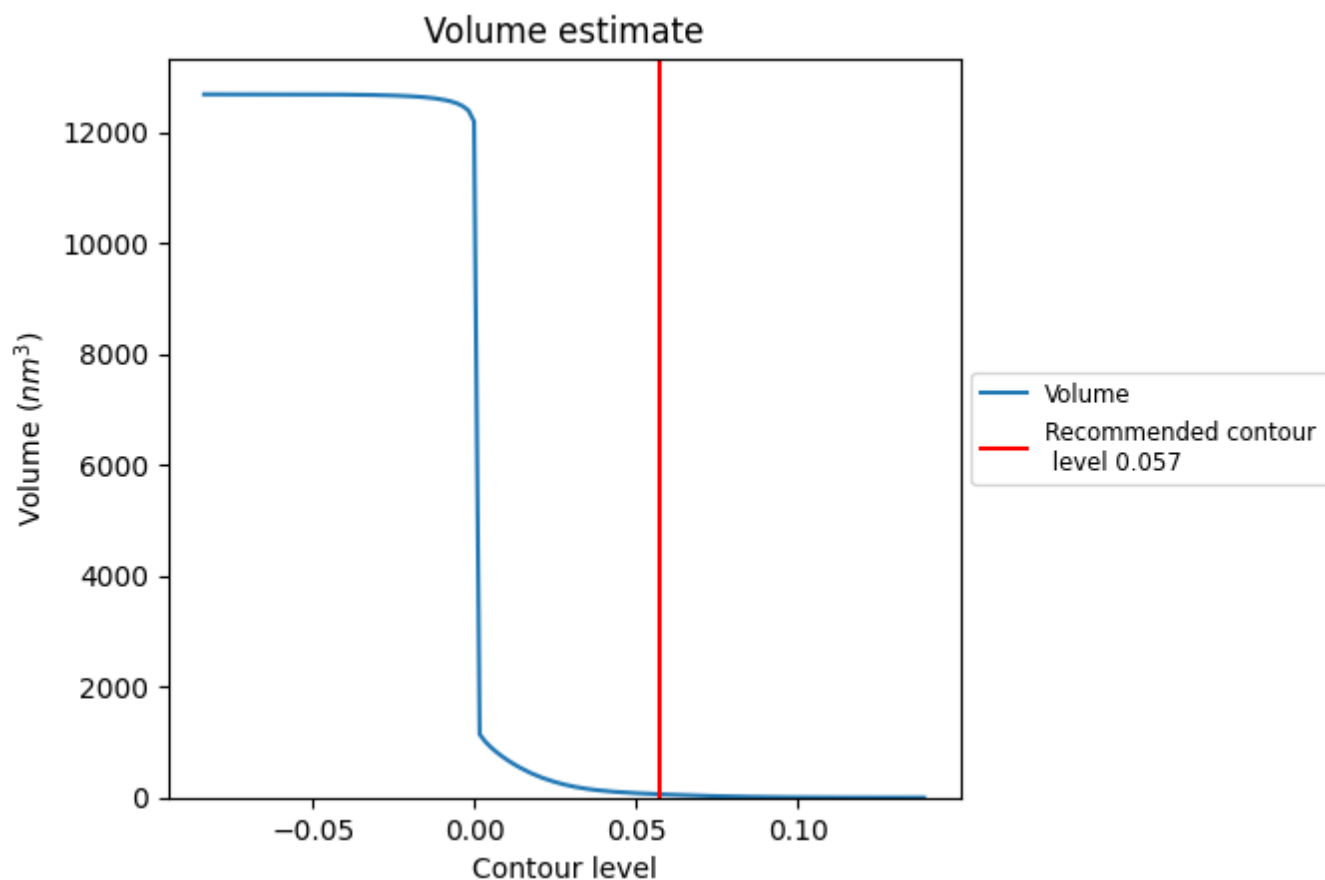
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

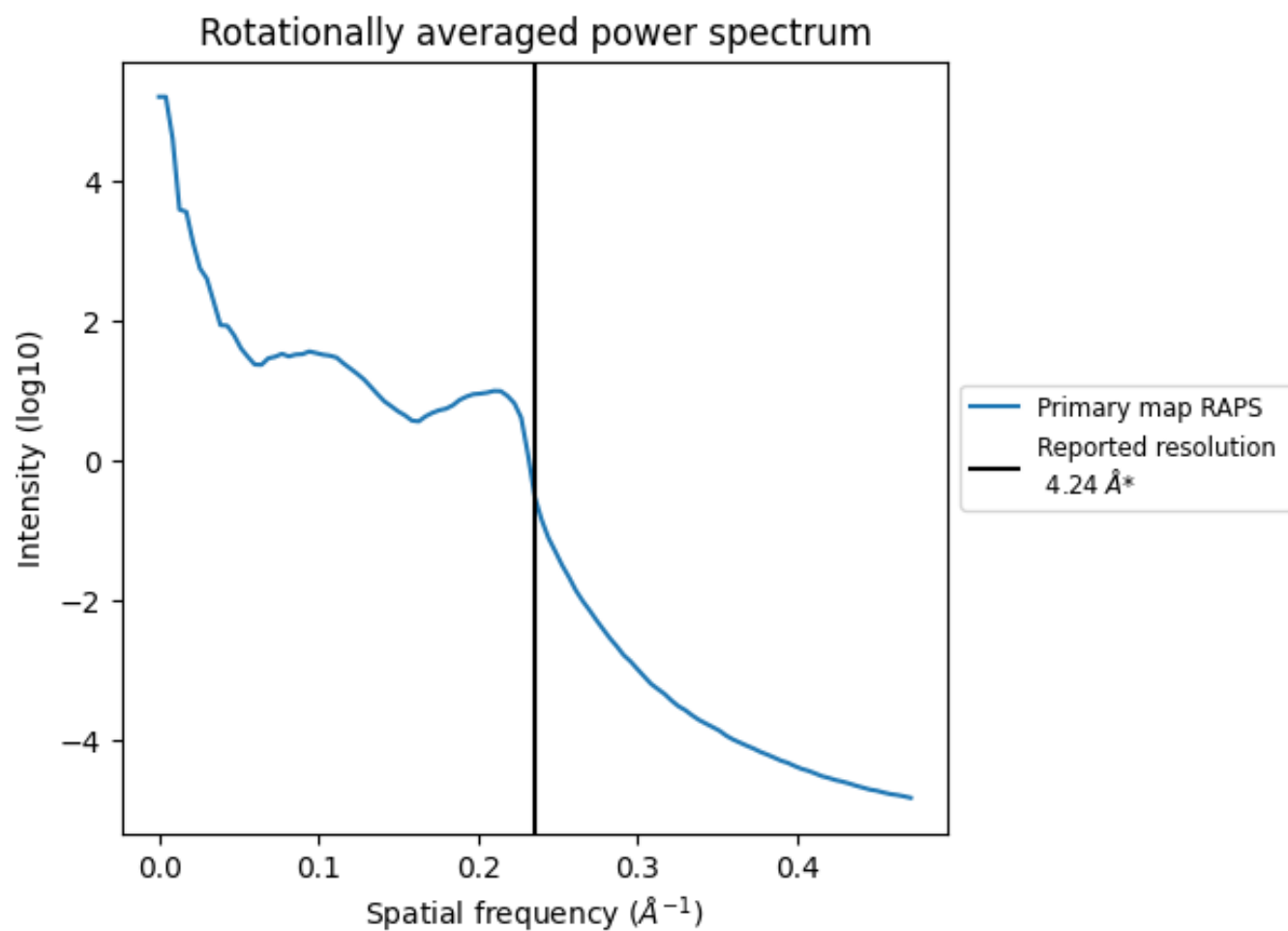
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 60 nm³; this corresponds to an approximate mass of 54 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.236 Å⁻¹

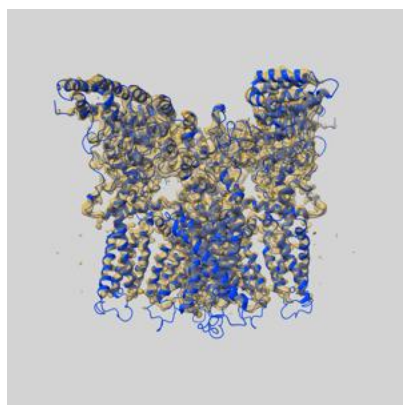
8 Fourier-Shell correlation ⓘ

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

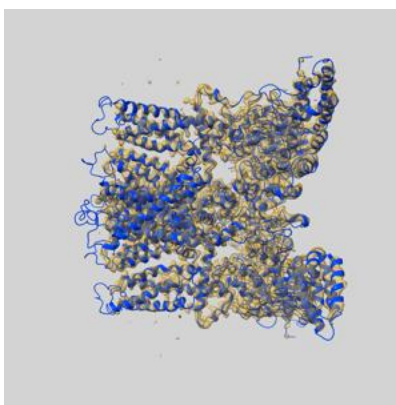
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8921 and PDB model 6DVZ. Per-residue inclusion information can be found in section 3 on page 5.

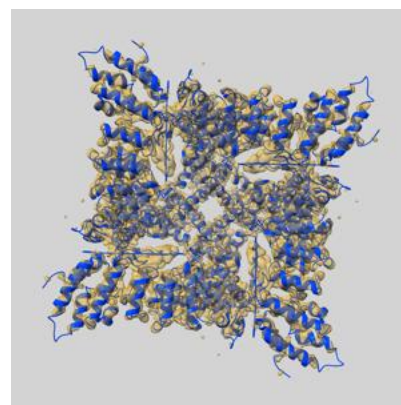
9.1 Map-model overlay [i](#)



X



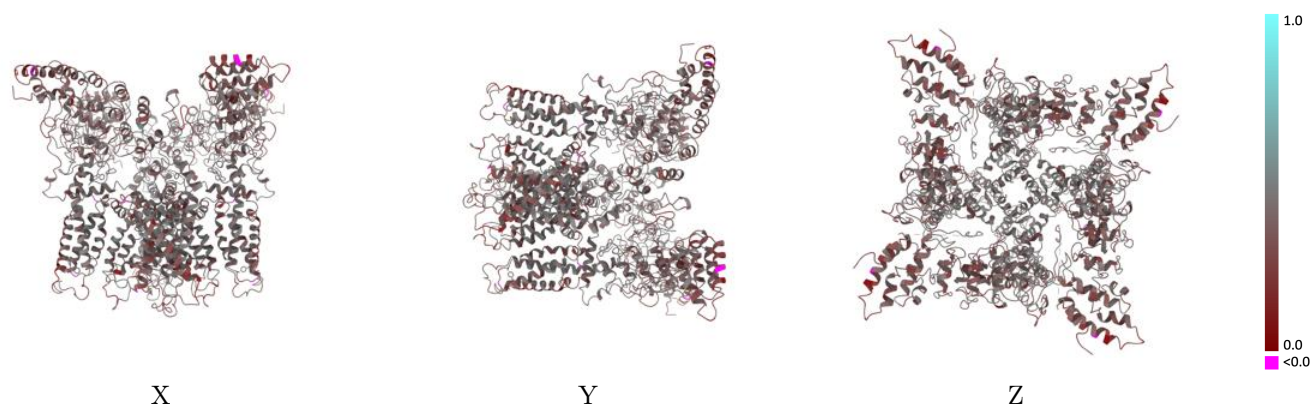
Y



Z

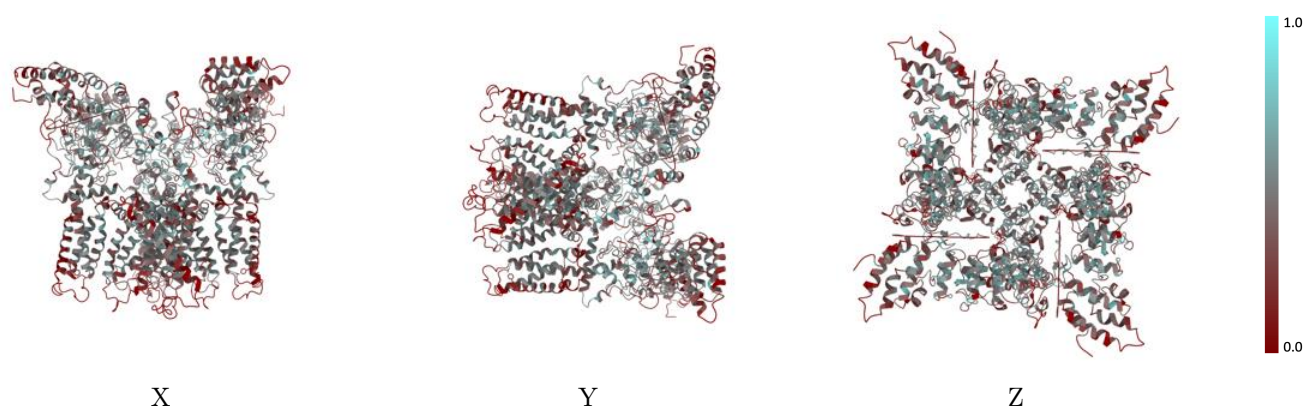
The images above show the 3D surface view of the map at the recommended contour level 0.057 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



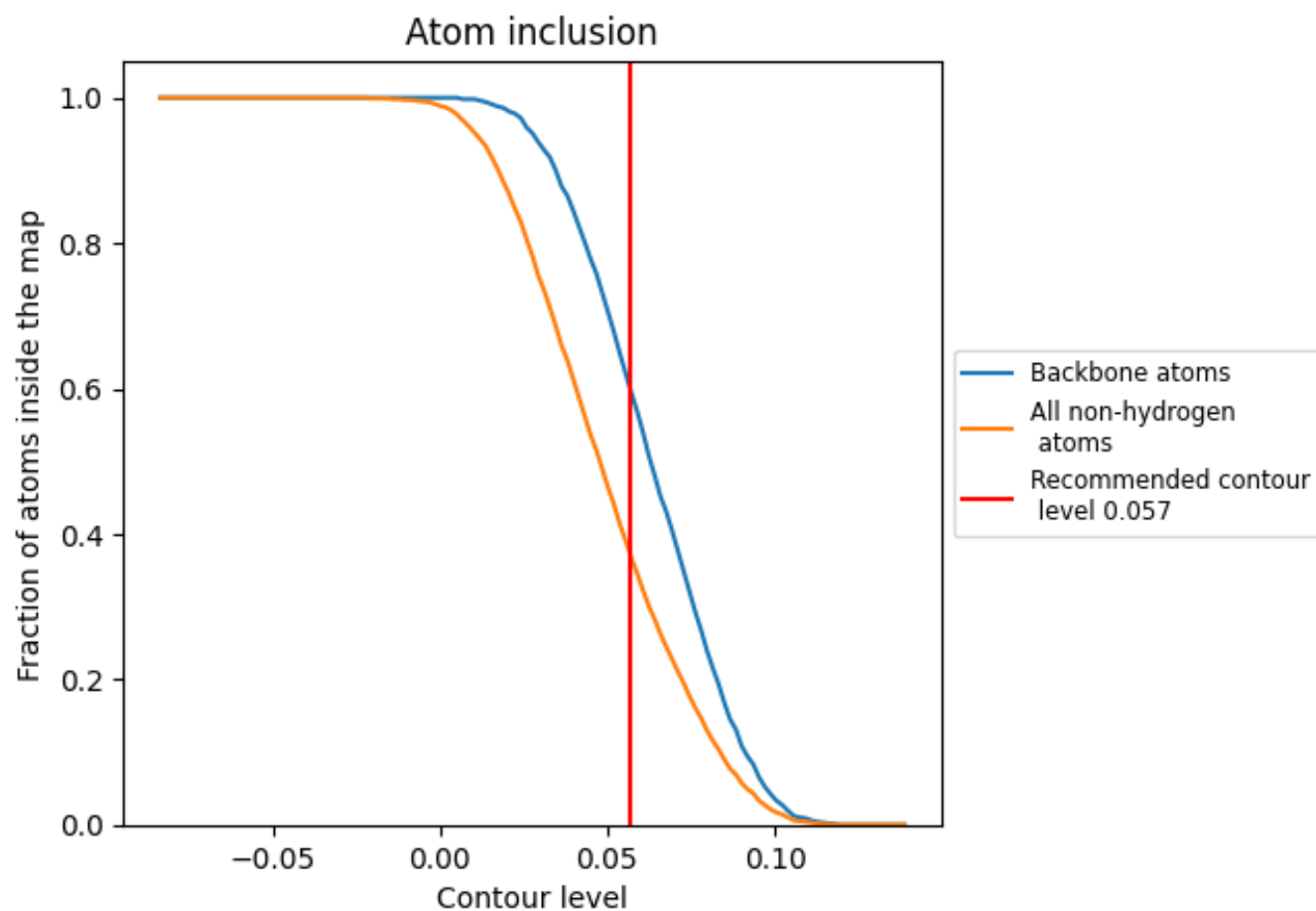
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.057).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 37% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.057) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3710	0.3870
A	0.3700	0.3850
B	0.3700	0.3870
C	0.3700	0.3880
D	0.3710	0.3860

