



Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 10:51 AM EST

PDB ID : 6UW9
EMDB ID : EMD-20920
Title : Cryo-EM structure of the human TRPV3 K169A mutant in the presence of 2-APB, determined in lipid nanodisc
Authors : Deng, Z.; Yuan, P.
Deposited on : 2019-11-04
Resolution : 4.33 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

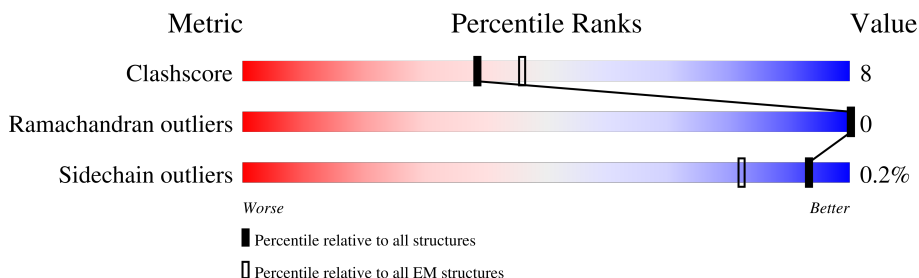
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.33 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	790	
1	B	790	
1	C	790	
1	D	790	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18924 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	582	Total	C	N	O	S	0	0
			4731	3085	784	834	28		
1	B	582	Total	C	N	O	S	0	0
			4731	3085	784	834	28		
1	C	582	Total	C	N	O	S	0	0
			4731	3085	784	834	28		
1	D	582	Total	C	N	O	S	0	0
			4731	3085	784	834	28		

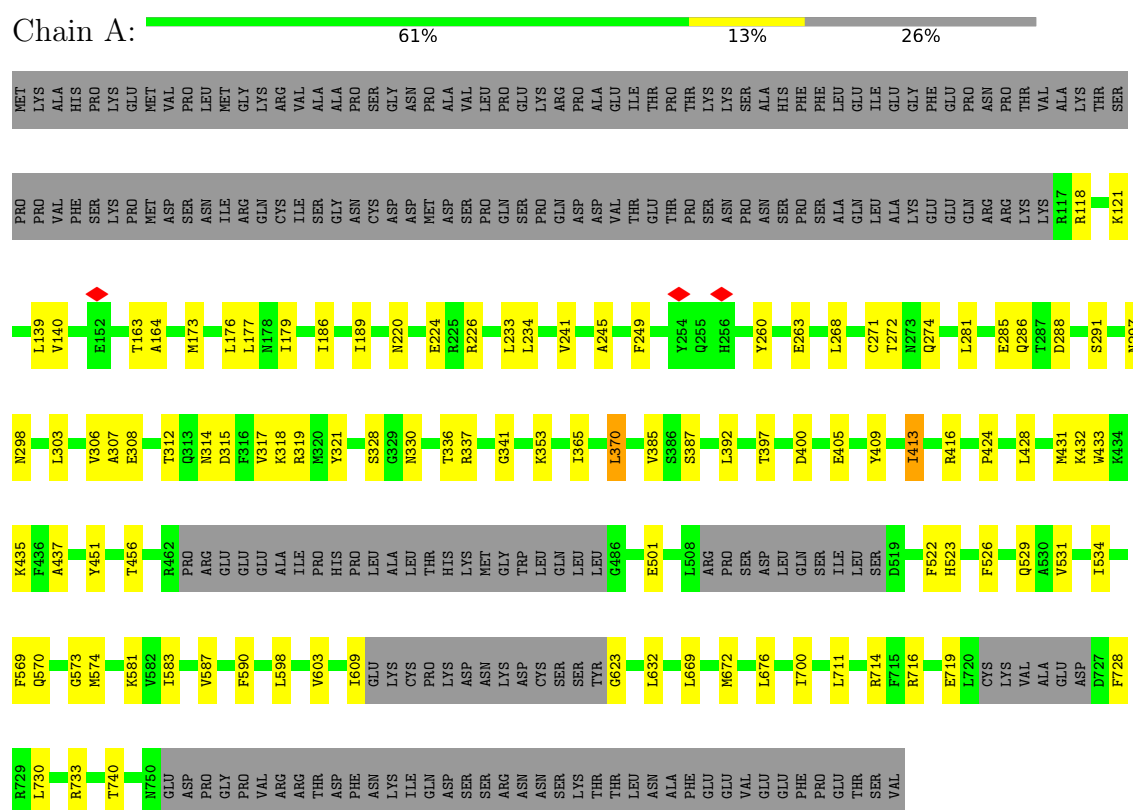
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	VAL	ILE	variant	UNP Q8NET8
A	169	ALA	LYS	engineered mutation	UNP Q8NET8
B	25	VAL	ILE	variant	UNP Q8NET8
B	169	ALA	LYS	engineered mutation	UNP Q8NET8
C	25	VAL	ILE	variant	UNP Q8NET8
C	169	ALA	LYS	engineered mutation	UNP Q8NET8
D	25	VAL	ILE	variant	UNP Q8NET8
D	169	ALA	LYS	engineered mutation	UNP Q8NET8

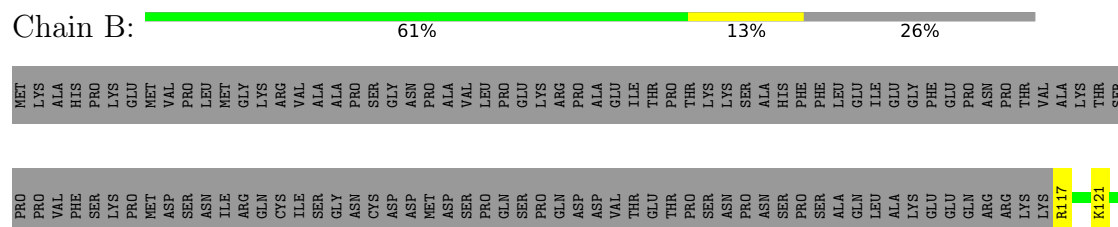
3 Residue-property plots

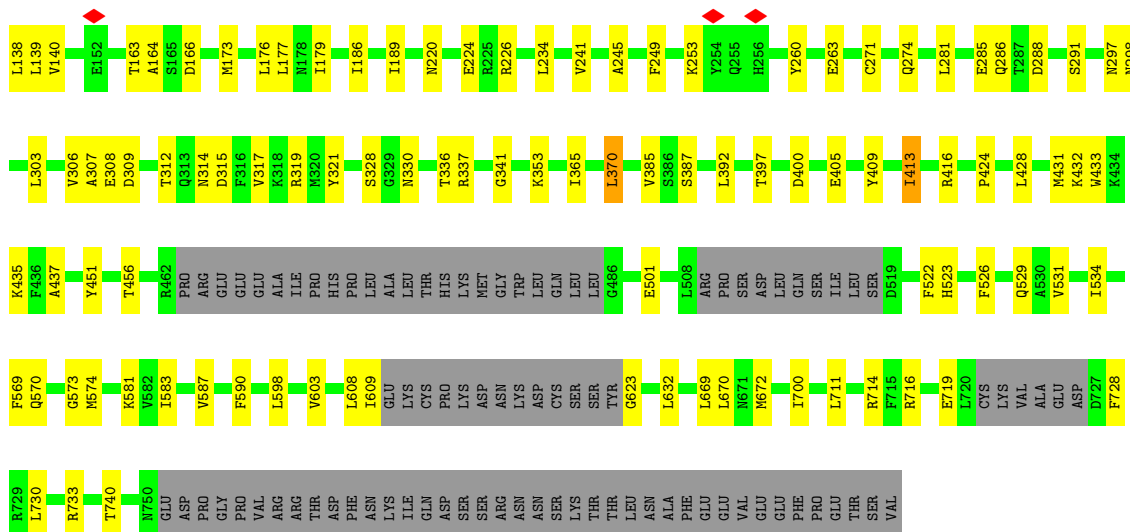
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Transient receptor potential cation channel subfamily V member 3

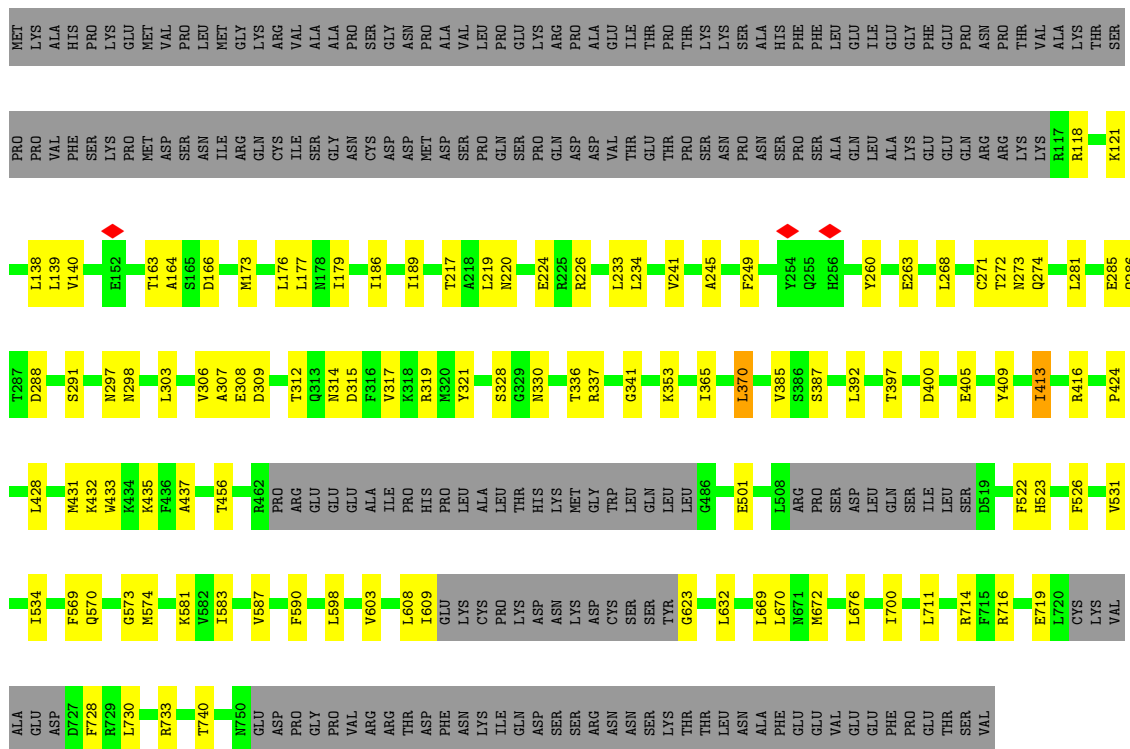


- Molecule 1: Transient receptor potential cation channel subfamily V member 3

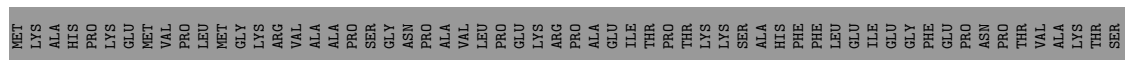




- Molecule 1: Transient receptor potential cation channel subfamily V member 3



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



ALA	GLU	ASP	D727	L730	R733	T740	V746	R750	GLU	ASP	PRO	GLY	PRO	VAL	ARG	THR	ASP	PHE	ASN	LYS	ILE	GLN	ASP	SER	SER	ARG	ASN	ASN	LYS	THR	THR	THR	THR	LEU	ASN	ALA	PHE	GLU	GLU	VAL	GLU	GLU	PHE	GLU	PRO	GLU	THR	SER	VAL
V531	I534	F569	Q570	G573	M574	K581	V582	I583	V587	F590	L598	V603	L608	I609	GLU	LYS	CYS	PRO	LYS	LYS	ASP	ASN	SER	SER	ARG	ASN	ASN	SER	LYS	TYR	G623	L632	L669	L670	M671	M672	L676	I700	L711	R714	F715	R716	L720	CYS	LYS	VAL			
M431	K432	M433	K434	F435	K436	A437	Y451	T456	R462	PRO	ARG	GLU	GLU	GLU	ALA	ILE	PRO	HIS	PRO	LEU	ALA	LEU	THR	LEU	THR	GLN	LEU	LEU	G486	E501	I508	ARG	PRO	SER	ASP	LEU	GLN	SER	ILE	SER	D519	F522	H523	F526	Q529	A530			
S291	N297	N298	L303	V306	A307	E308	D309	T312	Q313	N314	D315	F316	V317	K318	R319	R320	Y321	S328	G329	N330	T336	R337	G341	K353	I365	L370	V385	S386	S387	L392	T397	D400	E405	Y409	I413	R416	P424	L428											
L138	L139	V140	E152	T163	A164	M173	L176	L177	N178	I179	I186	I189	N220	E224	R225	R226	L233	L234	I235	V241	A245	F249	K253	Y254	Q255	H256	Y260	E263	L268	C271	T272	N273	Q274	L281	E285	Q286	T287	D288											
PRO	PRO	VAL	PHE	SER	LYS	PRO	MET	ASP	ASN	ASN	ILE	ARG	GLN	CYS	ILE	SER	GLY	ASN	CYS	ASP	ASP	MET	ASP	SER	PRO	GLN	SER	PRO	SER	ALA	ALA	GLN	LEU	ALA	LYS	GLU	GLU	GLN	ARG	ARG	LYS	R117	R118	K121					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66293	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 ($e^-/\text{\AA}^2$)	62	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	0.094	Depositor
Minimum map value	-0.063	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	281.6, 281.6, 281.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.32	1/4830 (0.0%)	0.62	8/6530 (0.1%)
1	B	0.32	1/4830 (0.0%)	0.62	7/6530 (0.1%)
1	C	0.32	1/4830 (0.0%)	0.62	8/6530 (0.1%)
1	D	0.32	1/4830 (0.0%)	0.62	8/6530 (0.1%)
All	All	0.32	4/19320 (0.0%)	0.62	31/26120 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	424	PRO	C-N	-5.08	1.22	1.34
1	D	424	PRO	C-N	-5.08	1.22	1.34
1	C	424	PRO	C-N	-5.08	1.22	1.34
1	A	424	PRO	C-N	-5.04	1.22	1.34

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	PRO	O-C-N	8.00	135.50	122.70
1	B	424	PRO	O-C-N	8.00	135.49	122.70
1	C	424	PRO	O-C-N	7.99	135.47	122.70
1	D	424	PRO	O-C-N	7.97	135.46	122.70
1	B	370	LEU	CA-CB-CG	6.88	131.12	115.30
1	D	370	LEU	CA-CB-CG	6.87	131.09	115.30
1	C	370	LEU	CA-CB-CG	6.86	131.08	115.30
1	A	370	LEU	CA-CB-CG	6.86	131.07	115.30
1	A	711	LEU	CA-CB-CG	6.83	131.01	115.30
1	C	711	LEU	CA-CB-CG	6.83	131.01	115.30
1	B	711	LEU	CA-CB-CG	6.83	131.01	115.30
1	D	711	LEU	CA-CB-CG	6.82	130.99	115.30
1	A	424	PRO	CA-C-N	-6.41	103.11	117.20
1	C	424	PRO	CA-C-N	-6.38	103.15	117.20
1	B	424	PRO	CA-C-N	-6.38	103.17	117.20
1	D	424	PRO	CA-C-N	-6.38	103.17	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	PRO	C-N-CA	-6.23	106.13	121.70
1	D	424	PRO	C-N-CA	-6.21	106.18	121.70
1	B	424	PRO	C-N-CA	-6.21	106.18	121.70
1	C	424	PRO	C-N-CA	-6.20	106.21	121.70
1	A	315	ASP	CB-CG-OD1	5.83	123.55	118.30
1	B	315	ASP	CB-CG-OD1	5.82	123.54	118.30
1	C	315	ASP	CB-CG-OD1	5.81	123.53	118.30
1	D	315	ASP	CB-CG-OD1	5.81	123.53	118.30
1	D	234	LEU	CA-CB-CG	5.17	127.18	115.30
1	A	234	LEU	CA-CB-CG	5.16	127.17	115.30
1	C	234	LEU	CA-CB-CG	5.16	127.17	115.30
1	B	234	LEU	CA-CB-CG	5.16	127.16	115.30
1	D	233	LEU	CA-CB-CG	5.01	126.83	115.30
1	A	233	LEU	CA-CB-CG	5.01	126.82	115.30
1	C	233	LEU	CA-CB-CG	5.00	126.81	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	4731	0	4783	77	0
1	B	4731	0	4783	79	0
1	C	4731	0	4783	81	0
1	D	4731	0	4783	80	0
All	All	18924	0	19132	301	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 8.

All (301) 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:522:PHE:O	1:A:526:PHE:CD2	2.18	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:522:PHE:O	1:C:526:PHE:CD2	2.18	0.96
1:D:522:PHE:O	1:D:526:PHE:HD2	1.49	0.96
1:A:522:PHE:O	1:A:526:PHE:HD2	1.48	0.96
1:B:522:PHE:O	1:B:526:PHE:CD2	2.18	0.95
1:D:522:PHE:O	1:D:526:PHE:CD2	2.18	0.95
1:B:522:PHE:O	1:B:526:PHE:HD2	1.48	0.95
1:C:522:PHE:O	1:C:526:PHE:HD2	1.49	0.92
1:A:433:TRP:HB2	1:A:700:ILE:HD11	1.57	0.86
1:B:433:TRP:HB2	1:B:700:ILE:HD11	1.57	0.86
1:D:433:TRP:HB2	1:D:700:ILE:HD11	1.57	0.86
1:C:433:TRP:HB2	1:C:700:ILE:HD11	1.57	0.86
1:C:428:LEU:HD23	1:C:428:LEU:O	1.79	0.82
1:B:428:LEU:O	1:B:428:LEU:HD23	1.79	0.82
1:A:433:TRP:CE3	1:A:437:ALA:HB3	2.16	0.81
1:D:428:LEU:O	1:D:428:LEU:HD23	1.79	0.81
1:B:433:TRP:CE3	1:B:437:ALA:HB3	2.16	0.80
1:A:428:LEU:HD23	1:A:428:LEU:O	1.79	0.80
1:C:433:TRP:HB2	1:C:700:ILE:CD1	2.12	0.80
1:C:433:TRP:CE3	1:C:437:ALA:HB3	2.16	0.80
1:A:433:TRP:HB2	1:A:700:ILE:CD1	2.12	0.80
1:D:433:TRP:HB2	1:D:700:ILE:CD1	2.12	0.80
1:D:433:TRP:CE3	1:D:437:ALA:HB3	2.16	0.80
1:B:433:TRP:HB2	1:B:700:ILE:CD1	2.12	0.79
1:A:431:MET:O	1:A:435:LYS:HB2	1.94	0.67
1:D:431:MET:O	1:D:435:LYS:HB2	1.94	0.67
1:B:431:MET:O	1:B:435:LYS:HB2	1.94	0.67
1:C:433:TRP:CE3	1:C:437:ALA:CB	2.78	0.67
1:B:433:TRP:CE3	1:B:437:ALA:CB	2.78	0.67
1:C:431:MET:O	1:C:435:LYS:HB2	1.94	0.66
1:D:433:TRP:CE3	1:D:437:ALA:CB	2.78	0.66
1:A:433:TRP:CE3	1:A:437:ALA:CB	2.78	0.66
1:A:583:ILE:HA	1:A:587:VAL:HG12	1.79	0.64
1:C:583:ILE:HA	1:C:587:VAL:HG12	1.79	0.64
1:B:583:ILE:HA	1:B:587:VAL:HG12	1.79	0.63
1:D:583:ILE:HA	1:D:587:VAL:HG12	1.79	0.62
1:B:431:MET:O	1:B:435:LYS:CB	2.49	0.61
1:C:431:MET:O	1:C:435:LYS:CB	2.49	0.61
1:C:431:MET:CE	1:C:716:ARG:HD2	2.24	0.61
1:A:428:LEU:HD21	1:A:432:LYS:HE3	1.82	0.61
1:A:431:MET:O	1:A:435:LYS:CB	2.49	0.61
1:D:431:MET:O	1:D:435:LYS:CB	2.49	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:MET:CE	1:B:716:ARG:HD2	2.24	0.60
1:A:433:TRP:HE3	1:A:437:ALA:HB3	1.66	0.60
1:B:428:LEU:HD21	1:B:432:LYS:HE3	1.82	0.60
1:D:428:LEU:HD21	1:D:432:LYS:HE3	1.82	0.60
1:D:428:LEU:HD23	1:D:428:LEU:C	2.22	0.60
1:C:428:LEU:HD21	1:C:432:LYS:HE3	1.82	0.60
1:A:428:LEU:HD23	1:A:428:LEU:C	2.22	0.59
1:B:428:LEU:HD23	1:B:428:LEU:C	2.22	0.59
1:C:428:LEU:HD23	1:C:428:LEU:C	2.22	0.58
1:A:397:THR:HG22	1:A:432:LYS:HZ1	1.67	0.58
1:D:433:TRP:CE3	1:D:700:ILE:HD11	2.38	0.58
1:D:433:TRP:HE3	1:D:437:ALA:HB3	1.66	0.58
1:C:433:TRP:CE3	1:C:700:ILE:HD11	2.39	0.58
1:A:433:TRP:CE3	1:A:700:ILE:HD11	2.38	0.57
1:B:433:TRP:HE3	1:B:437:ALA:HB3	1.66	0.57
1:B:433:TRP:CE3	1:B:700:ILE:HD11	2.38	0.57
1:B:397:THR:HG22	1:B:432:LYS:HZ1	1.69	0.57
1:C:433:TRP:HE3	1:C:437:ALA:HB3	1.66	0.56
1:A:220:ASN:O	1:A:224:GLU:HB2	2.05	0.56
1:C:220:ASN:O	1:C:224:GLU:HB2	2.05	0.56
1:B:220:ASN:O	1:B:224:GLU:HB2	2.05	0.56
1:D:220:ASN:O	1:D:224:GLU:HB2	2.05	0.56
1:B:433:TRP:HE3	1:B:700:ILE:CD1	2.20	0.55
1:D:176:LEU:HD23	1:D:179:ILE:HD11	1.88	0.55
1:A:176:LEU:HD23	1:A:179:ILE:HD11	1.89	0.55
1:A:433:TRP:HE3	1:A:700:ILE:CD1	2.20	0.55
1:D:431:MET:CE	1:D:716:ARG:HD2	2.24	0.55
1:C:433:TRP:HE3	1:C:700:ILE:CD1	2.20	0.55
1:B:714:ARG:O	1:B:716:ARG:NH2	2.41	0.55
1:D:433:TRP:HE3	1:D:700:ILE:CD1	2.20	0.55
1:A:433:TRP:CE3	1:A:700:ILE:CD1	2.90	0.54
1:C:433:TRP:CE3	1:C:700:ILE:CD1	2.90	0.54
1:B:176:LEU:HD23	1:B:179:ILE:HD11	1.89	0.54
1:B:392:LEU:HB2	1:B:730:LEU:HB2	1.89	0.54
1:B:433:TRP:CE3	1:B:700:ILE:CD1	2.90	0.54
1:A:392:LEU:HB2	1:A:730:LEU:HB2	1.89	0.54
1:C:714:ARG:O	1:C:716:ARG:NH2	2.41	0.54
1:D:433:TRP:CE3	1:D:700:ILE:CD1	2.90	0.54
1:A:431:MET:CE	1:A:716:ARG:HD2	2.24	0.54
1:D:392:LEU:HB2	1:D:730:LEU:HB2	1.89	0.54
1:B:314:ASN:O	1:B:319:ARG:NH2	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:LEU:HD23	1:C:179:ILE:HD11	1.88	0.53
1:D:714:ARG:O	1:D:716:ARG:NH2	2.40	0.53
1:A:298:ASN:ND2	1:A:336:THR:OG1	2.41	0.53
1:C:433:TRP:HE3	1:C:700:ILE:HD13	1.74	0.53
1:B:298:ASN:ND2	1:B:336:THR:OG1	2.41	0.53
1:C:298:ASN:ND2	1:C:336:THR:OG1	2.41	0.53
1:D:298:ASN:ND2	1:D:336:THR:OG1	2.41	0.53
1:A:714:ARG:O	1:A:716:ARG:NH2	2.41	0.53
1:C:397:THR:HG22	1:C:432:LYS:HZ1	1.73	0.53
1:D:433:TRP:HE3	1:D:700:ILE:HD13	1.74	0.53
1:B:433:TRP:HE3	1:B:700:ILE:HD13	1.74	0.52
1:C:392:LEU:HB2	1:C:730:LEU:HB2	1.89	0.52
1:B:397:THR:HG22	1:B:432:LYS:NZ	2.24	0.52
1:A:314:ASN:O	1:A:319:ARG:NH2	2.39	0.52
1:A:397:THR:HG22	1:A:432:LYS:NZ	2.24	0.52
1:A:433:TRP:HE3	1:A:700:ILE:HD13	1.74	0.52
1:A:249:PHE:HZ	1:B:385:VAL:HG11	1.75	0.52
1:C:309:ASP:OD1	1:C:309:ASP:N	2.43	0.52
1:D:285:GLU:HG3	1:D:286:GLN:HG2	1.92	0.52
1:A:308:GLU:HA	1:A:353:LYS:HG2	1.92	0.52
1:C:308:GLU:HA	1:C:353:LYS:HG2	1.92	0.52
1:D:397:THR:HG22	1:D:432:LYS:NZ	2.24	0.52
1:B:285:GLU:HG3	1:B:286:GLN:HG2	1.92	0.51
1:C:397:THR:HG22	1:C:432:LYS:NZ	2.24	0.51
1:B:166:ASP:OD1	1:B:166:ASP:N	2.44	0.51
1:C:433:TRP:CB	1:C:700:ILE:HD11	2.37	0.51
1:D:308:GLU:HA	1:D:353:LYS:HG2	1.92	0.51
1:C:166:ASP:OD1	1:C:166:ASP:N	2.44	0.51
1:A:285:GLU:HG3	1:A:286:GLN:HG2	1.92	0.51
1:B:308:GLU:HA	1:B:353:LYS:HG2	1.92	0.51
1:C:314:ASN:O	1:C:319:ARG:NH2	2.39	0.51
1:C:307:ALA:HB2	1:C:317:VAL:HG11	1.93	0.51
1:A:307:ALA:HB2	1:A:317:VAL:HG11	1.93	0.50
1:A:609:ILE:O	1:A:623:GLY:N	2.44	0.50
1:A:400:ASP:OD1	1:A:400:ASP:N	2.45	0.50
1:B:609:ILE:O	1:B:623:GLY:N	2.44	0.50
1:A:433:TRP:CB	1:A:700:ILE:HD11	2.37	0.50
1:C:387:SER:OG	1:C:733:ARG:NH2	2.45	0.50
1:C:609:ILE:O	1:C:623:GLY:N	2.44	0.50
1:C:285:GLU:HG3	1:C:286:GLN:HG2	1.92	0.50
1:C:400:ASP:OD1	1:C:400:ASP:N	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:ALA:HB2	1:D:317:VAL:HG11	1.93	0.50
1:D:314:ASN:O	1:D:319:ARG:NH2	2.39	0.50
1:B:241:VAL:HG11	1:B:281:LEU:HD11	1.94	0.49
1:D:365:ILE:HG21	1:D:370:LEU:HG	1.95	0.49
1:A:385:VAL:HG11	1:D:249:PHE:HZ	1.76	0.49
1:B:400:ASP:OD1	1:B:400:ASP:N	2.45	0.49
1:C:433:TRP:HB2	1:C:700:ILE:HD12	1.93	0.49
1:A:365:ILE:HG21	1:A:370:LEU:HG	1.95	0.49
1:B:433:TRP:HB2	1:B:700:ILE:HD12	1.93	0.49
1:D:186:ILE:HA	1:D:189:ILE:HG12	1.94	0.49
1:D:400:ASP:OD1	1:D:400:ASP:N	2.45	0.49
1:D:609:ILE:O	1:D:623:GLY:N	2.44	0.49
1:A:387:SER:OG	1:A:733:ARG:NH2	2.45	0.49
1:B:307:ALA:HB2	1:B:317:VAL:HG11	1.93	0.49
1:B:387:SER:OG	1:B:733:ARG:NH2	2.45	0.49
1:C:245:ALA:H	1:C:263:GLU:HB2	1.78	0.49
1:D:387:SER:OG	1:D:733:ARG:NH2	2.45	0.49
1:B:186:ILE:HA	1:B:189:ILE:HG12	1.94	0.49
1:D:241:VAL:HG11	1:D:281:LEU:HD11	1.94	0.49
1:B:245:ALA:H	1:B:263:GLU:HB2	1.78	0.49
1:B:433:TRP:CB	1:B:700:ILE:HD11	2.37	0.49
1:C:241:VAL:HG11	1:C:281:LEU:HD11	1.94	0.49
1:C:365:ILE:HG21	1:C:370:LEU:HG	1.95	0.49
1:D:433:TRP:HB2	1:D:700:ILE:HD12	1.93	0.49
1:A:186:ILE:HA	1:A:189:ILE:HG12	1.94	0.49
1:A:241:VAL:HG11	1:A:281:LEU:HD11	1.94	0.48
1:C:186:ILE:HA	1:C:189:ILE:HG12	1.94	0.48
1:A:245:ALA:H	1:A:263:GLU:HB2	1.78	0.48
1:B:365:ILE:HG21	1:B:370:LEU:HG	1.95	0.48
1:D:245:ALA:H	1:D:263:GLU:HB2	1.78	0.48
1:D:501:GLU:OE1	1:D:523:HIS:ND1	2.47	0.48
1:C:501:GLU:OE1	1:C:523:HIS:ND1	2.47	0.48
1:B:220:ASN:OD1	1:B:220:ASN:N	2.47	0.48
1:B:501:GLU:OE1	1:B:523:HIS:ND1	2.47	0.48
1:A:220:ASN:OD1	1:A:220:ASN:N	2.47	0.47
1:A:501:GLU:OE1	1:A:523:HIS:ND1	2.47	0.47
1:D:260:TYR:OH	1:D:297:ASN:ND2	2.47	0.47
1:B:260:TYR:OH	1:B:297:ASN:ND2	2.47	0.47
1:B:590:PHE:HB2	1:B:672:MET:HG3	1.96	0.47
1:A:590:PHE:HB2	1:A:672:MET:HG3	1.96	0.47
1:C:260:TYR:OH	1:C:297:ASN:ND2	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:TYR:OH	1:A:297:ASN:ND2	2.47	0.47
1:C:590:PHE:HB2	1:C:672:MET:HG3	1.97	0.47
1:A:226:ARG:HD3	1:A:274:GLN:HE21	1.80	0.47
1:C:220:ASN:OD1	1:C:220:ASN:N	2.47	0.47
1:D:226:ARG:HD3	1:D:274:GLN:HE21	1.80	0.47
1:D:303:LEU:HD23	1:D:321:TYR:HD1	1.80	0.47
1:C:570:GLN:HG2	1:C:574:MET:HE2	1.98	0.46
1:B:603:VAL:HG11	1:C:456:THR:HG23	1.97	0.46
1:D:590:PHE:HB2	1:D:672:MET:HG3	1.97	0.46
1:A:433:TRP:HB2	1:A:700:ILE:HD12	1.93	0.46
1:B:413:ILE:O	1:B:416:ARG:NH1	2.49	0.46
1:D:397:THR:HG22	1:D:432:LYS:HZ1	1.79	0.46
1:D:413:ILE:O	1:D:416:ARG:NH1	2.49	0.46
1:D:220:ASN:OD1	1:D:220:ASN:N	2.47	0.46
1:C:413:ILE:O	1:C:416:ARG:NH1	2.49	0.45
1:D:271:CYS:HB3	1:D:306:VAL:HG21	1.98	0.45
1:D:570:GLN:HG2	1:D:574:MET:HE2	1.98	0.45
1:A:303:LEU:HD23	1:A:321:TYR:HD1	1.80	0.45
1:B:226:ARG:HD3	1:B:274:GLN:HE21	1.80	0.45
1:B:303:LEU:HD23	1:B:321:TYR:HD1	1.80	0.45
1:C:226:ARG:HD3	1:C:274:GLN:HE21	1.80	0.45
1:C:433:TRP:HE3	1:C:437:ALA:CB	2.25	0.45
1:B:173:MET:O	1:B:177:LEU:HB2	2.17	0.45
1:B:451:TYR:OH	1:B:529:GLN:NE2	2.47	0.45
1:A:268:LEU:O	1:A:272:THR:OG1	2.33	0.45
1:C:303:LEU:HD23	1:C:321:TYR:HD1	1.81	0.45
1:D:173:MET:O	1:D:177:LEU:HB2	2.17	0.45
1:A:740:THR:HG23	1:D:312:THR:HG23	1.99	0.45
1:B:570:GLN:HG2	1:B:574:MET:HE2	1.98	0.45
1:C:271:CYS:HB3	1:C:306:VAL:HG21	1.98	0.45
1:C:173:MET:O	1:C:177:LEU:HB2	2.17	0.45
1:D:268:LEU:O	1:D:272:THR:OG1	2.32	0.45
1:A:413:ILE:O	1:A:416:ARG:NH1	2.49	0.45
1:A:603:VAL:HG11	1:B:456:THR:HG23	1.99	0.45
1:D:328:SER:OG	1:D:330:ASN:OD1	2.30	0.45
1:D:451:TYR:OH	1:D:529:GLN:NE2	2.48	0.45
1:A:271:CYS:HB3	1:A:306:VAL:HG21	1.98	0.45
1:B:307:ALA:O	1:B:353:LYS:NZ	2.42	0.45
1:C:288:ASP:HB3	1:C:291:SER:HB3	1.99	0.45
1:D:581:LYS:HD3	1:D:581:LYS:HA	1.80	0.45
1:A:581:LYS:HA	1:A:581:LYS:HD3	1.80	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:583:ILE:HA	1:C:587:VAL:CG1	2.47	0.44
1:C:603:VAL:HG11	1:D:456:THR:HG23	1.99	0.44
1:A:456:THR:HG23	1:D:603:VAL:HG11	2.00	0.44
1:D:433:TRP:CB	1:D:700:ILE:HD11	2.37	0.44
1:A:428:LEU:C	1:A:428:LEU:CD2	2.85	0.44
1:C:312:THR:HG23	1:D:740:THR:HG23	1.98	0.44
1:B:271:CYS:HB3	1:B:306:VAL:HG21	1.98	0.44
1:D:288:ASP:HB3	1:D:291:SER:HB3	1.99	0.44
1:A:173:MET:O	1:A:177:LEU:HB2	2.17	0.44
1:B:433:TRP:HE3	1:B:437:ALA:CB	2.25	0.44
1:A:570:GLN:HG2	1:A:574:MET:HE2	1.99	0.44
1:B:117:ARG:O	1:B:121:LYS:NZ	2.44	0.44
1:B:583:ILE:HA	1:B:587:VAL:CG1	2.47	0.44
1:C:669:LEU:HD12	1:C:672:MET:HE3	2.00	0.44
1:D:138:LEU:HD23	1:D:138:LEU:HA	1.89	0.44
1:C:428:LEU:C	1:C:428:LEU:CD2	2.86	0.43
1:B:288:ASP:HB3	1:B:291:SER:HB3	1.99	0.43
1:B:428:LEU:C	1:B:428:LEU:CD2	2.85	0.43
1:C:328:SER:OG	1:C:330:ASN:OD1	2.30	0.43
1:D:431:MET:HB3	1:D:716:ARG:HH12	1.04	0.43
1:A:288:ASP:HB3	1:A:291:SER:HB3	1.99	0.43
1:C:138:LEU:HD23	1:C:138:LEU:HA	1.89	0.43
1:A:337:ARG:HB3	1:A:341:GLY:HA2	2.01	0.43
1:B:337:ARG:HB3	1:B:341:GLY:HA2	2.01	0.43
1:C:268:LEU:O	1:C:272:THR:OG1	2.33	0.43
1:D:428:LEU:C	1:D:428:LEU:CD2	2.86	0.43
1:A:433:TRP:HE3	1:A:437:ALA:CB	2.25	0.43
1:B:309:ASP:N	1:B:309:ASP:OD1	2.42	0.43
1:C:249:PHE:HZ	1:D:385:VAL:HG11	1.83	0.43
1:C:273:ASN:ND2	1:D:746:VAL:O	2.47	0.43
1:D:337:ARG:HB3	1:D:341:GLY:HA2	2.01	0.43
1:D:669:LEU:HD12	1:D:672:MET:HE3	2.00	0.43
1:A:676:LEU:HD21	1:D:670:LEU:HD21	2.01	0.43
1:C:531:VAL:HA	1:C:534:ILE:HG22	2.01	0.43
1:A:328:SER:OG	1:A:330:ASN:OD1	2.30	0.42
1:B:138:LEU:HD23	1:B:138:LEU:HA	1.89	0.42
1:B:534:ILE:HD12	1:B:534:ILE:HA	1.92	0.42
1:B:669:LEU:HD12	1:B:672:MET:HE3	2.00	0.42
1:C:405:GLU:O	1:C:409:TYR:HB2	2.19	0.42
1:C:608:LEU:HD12	1:C:608:LEU:HA	1.91	0.42
1:D:309:ASP:OD1	1:D:309:ASP:N	2.43	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:569:PHE:O	1:D:573:GLY:N	2.48	0.42
1:A:405:GLU:O	1:A:409:TYR:HB2	2.19	0.42
1:D:583:ILE:HA	1:D:587:VAL:CG1	2.47	0.42
1:D:598:LEU:HD12	1:D:632:LEU:HD23	2.02	0.42
1:B:531:VAL:HA	1:B:534:ILE:HG22	2.01	0.42
1:D:405:GLU:O	1:D:409:TYR:HB2	2.19	0.42
1:A:598:LEU:HD12	1:A:632:LEU:HD23	2.02	0.42
1:C:337:ARG:HB3	1:C:341:GLY:HA2	2.01	0.42
1:B:405:GLU:O	1:B:409:TYR:HB2	2.19	0.42
1:D:118:ARG:O	1:D:121:LYS:NZ	2.53	0.42
1:A:531:VAL:HA	1:A:534:ILE:HG22	2.01	0.41
1:A:118:ARG:O	1:A:121:LYS:NZ	2.53	0.41
1:B:569:PHE:O	1:B:573:GLY:N	2.48	0.41
1:D:531:VAL:HA	1:D:534:ILE:HG22	2.01	0.41
1:A:719:GLU:HB3	1:A:728:PHE:HA	2.03	0.41
1:B:598:LEU:HD12	1:B:632:LEU:HD23	2.02	0.41
1:A:312:THR:HG23	1:B:740:THR:HG23	2.02	0.41
1:D:253:LYS:HB2	1:D:253:LYS:HE2	1.91	0.41
1:A:669:LEU:HD12	1:A:672:MET:HE3	2.01	0.41
1:A:431:MET:O	1:A:435:LYS:HB3	2.21	0.41
1:A:318:LYS:HE2	1:A:318:LYS:HB3	1.91	0.41
1:A:285:GLU:H	1:A:285:GLU:HG2	1.72	0.41
1:A:451:TYR:OH	1:A:529:GLN:NE2	2.47	0.41
1:A:569:PHE:O	1:A:573:GLY:N	2.48	0.41
1:A:733:ARG:HE	1:A:733:ARG:HB3	1.73	0.41
1:B:328:SER:OG	1:B:330:ASN:OD1	2.30	0.41
1:B:719:GLU:HB3	1:B:728:PHE:HA	2.03	0.41
1:C:139:LEU:HD12	1:C:140:VAL:HG13	2.03	0.41
1:C:163:THR:OG1	1:C:164:ALA:N	2.54	0.41
1:C:431:MET:HB3	1:C:716:ARG:HH12	1.04	0.41
1:C:581:LYS:HD3	1:C:581:LYS:HA	1.80	0.41
1:D:608:LEU:HD12	1:D:608:LEU:HA	1.91	0.41
1:B:249:PHE:HZ	1:C:385:VAL:HG11	1.86	0.41
1:B:608:LEU:HD12	1:B:608:LEU:HA	1.91	0.41
1:C:598:LEU:HD12	1:C:632:LEU:HD23	2.02	0.41
1:A:431:MET:HB3	1:A:716:ARG:HH12	1.04	0.40
1:B:139:LEU:HD12	1:B:140:VAL:HG13	2.03	0.40
1:B:163:THR:OG1	1:B:164:ALA:N	2.54	0.40
1:C:569:PHE:O	1:C:573:GLY:N	2.48	0.40
1:A:163:THR:OG1	1:A:164:ALA:N	2.54	0.40
1:B:312:THR:HG23	1:C:740:THR:HG23	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:431:MET:O	1:C:435:LYS:HB3	2.21	0.40
1:D:235:ILE:HD12	1:D:235:ILE:HA	1.96	0.40
1:B:581:LYS:HA	1:B:581:LYS:HD3	1.80	0.40
1:C:670:LEU:HD21	1:D:676:LEU:HD21	2.04	0.40
1:D:139:LEU:HD12	1:D:140:VAL:HG13	2.03	0.40
1:A:139:LEU:HD12	1:A:140:VAL:HG13	2.03	0.40
1:C:217:THR:HG23	1:C:219:LEU:H	1.87	0.40
1:C:719:GLU:HB3	1:C:728:PHE:HA	2.03	0.40
1:D:163:THR:OG1	1:D:164:ALA:N	2.54	0.40
1:D:318:LYS:HE2	1:D:318:LYS:HB3	1.91	0.40
1:B:253:LYS:HE2	1:B:253:LYS:HB2	1.91	0.40
1:B:670:LEU:HD21	1:C:676:LEU:HD21	2.04	0.40
1:C:118:ARG:O	1:C:121:LYS:NZ	2.53	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	572/790 (72%)	530 (93%)	42 (7%)	0	100	100
1	B	572/790 (72%)	530 (93%)	42 (7%)	0	100	100
1	C	572/790 (72%)	530 (93%)	42 (7%)	0	100	100
1	D	572/790 (72%)	530 (93%)	42 (7%)	0	100	100
All	All	2288/3160 (72%)	2120 (93%)	168 (7%)	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	508/702 (72%)	507 (100%)	1 (0%)	93	96
1	B	508/702 (72%)	507 (100%)	1 (0%)	93	96
1	C	508/702 (72%)	507 (100%)	1 (0%)	93	96
1	D	508/702 (72%)	507 (100%)	1 (0%)	93	96
All	All	2032/2808 (72%)	2028 (100%)	4 (0%)	93	96

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

Mol	Chain	Res	Type
1	A	413	ILE
1	B	413	ILE
1	C	413	ILE
1	D	413	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	ASN
1	A	570	GLN
1	A	580	GLN
1	B	297	ASN
1	B	570	GLN
1	B	580	GLN
1	C	297	ASN
1	C	570	GLN
1	C	580	GLN
1	D	297	ASN
1	D	570	GLN
1	D	580	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

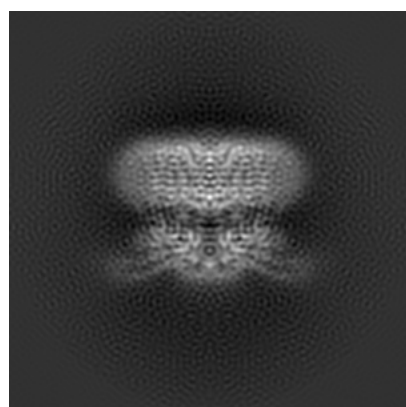
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20920. These allow visual inspection of the internal detail of the map and identification of artifacts.

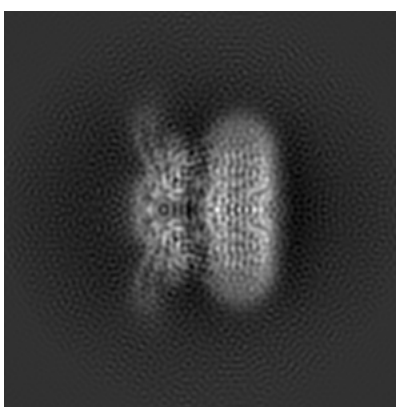
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

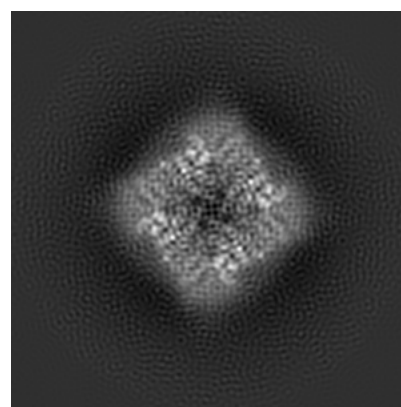
6.1.1 Primary map



X



Y

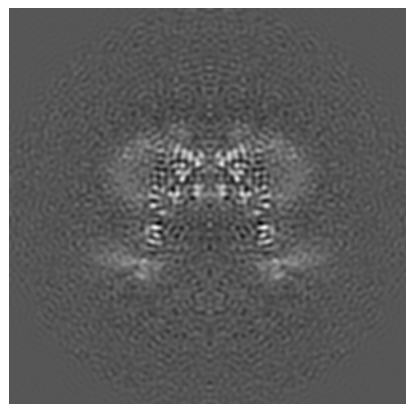


Z

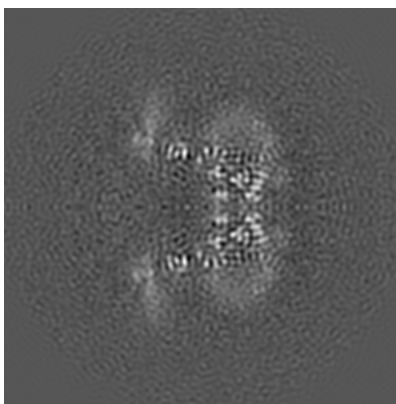
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

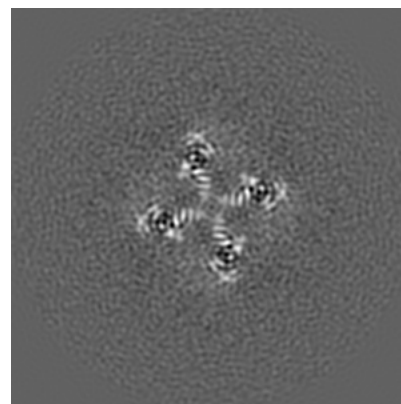
6.2.1 Primary map



X Index: 128



Y Index: 128

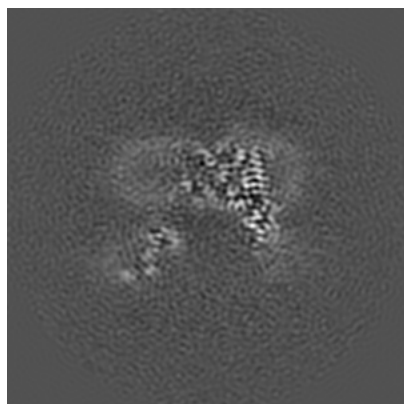


Z Index: 128

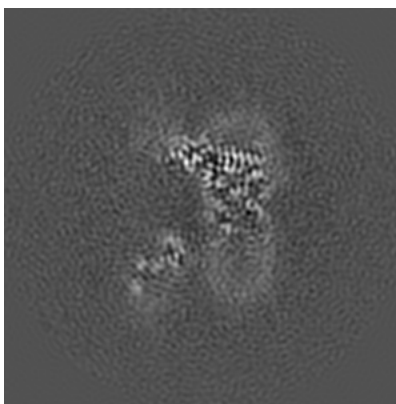
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

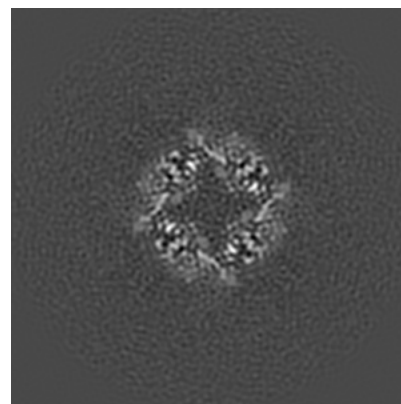
6.3.1 Primary map



X Index: 122



Y Index: 134

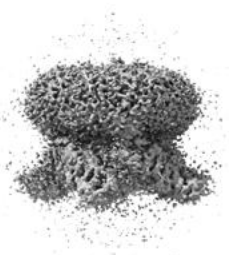


Z Index: 110

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

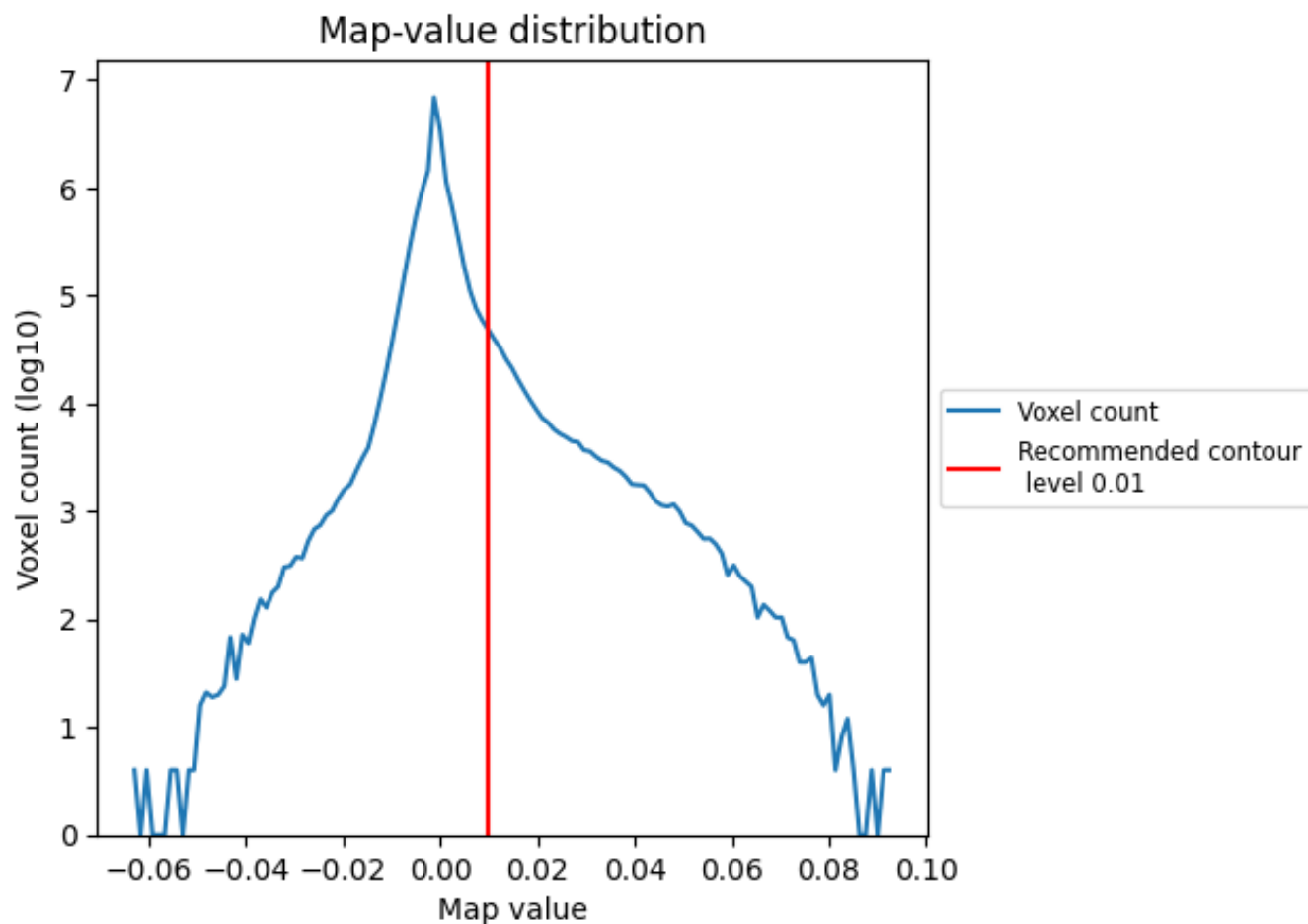
6.5 Mask visualisation

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

7 Map analysis [i](#)

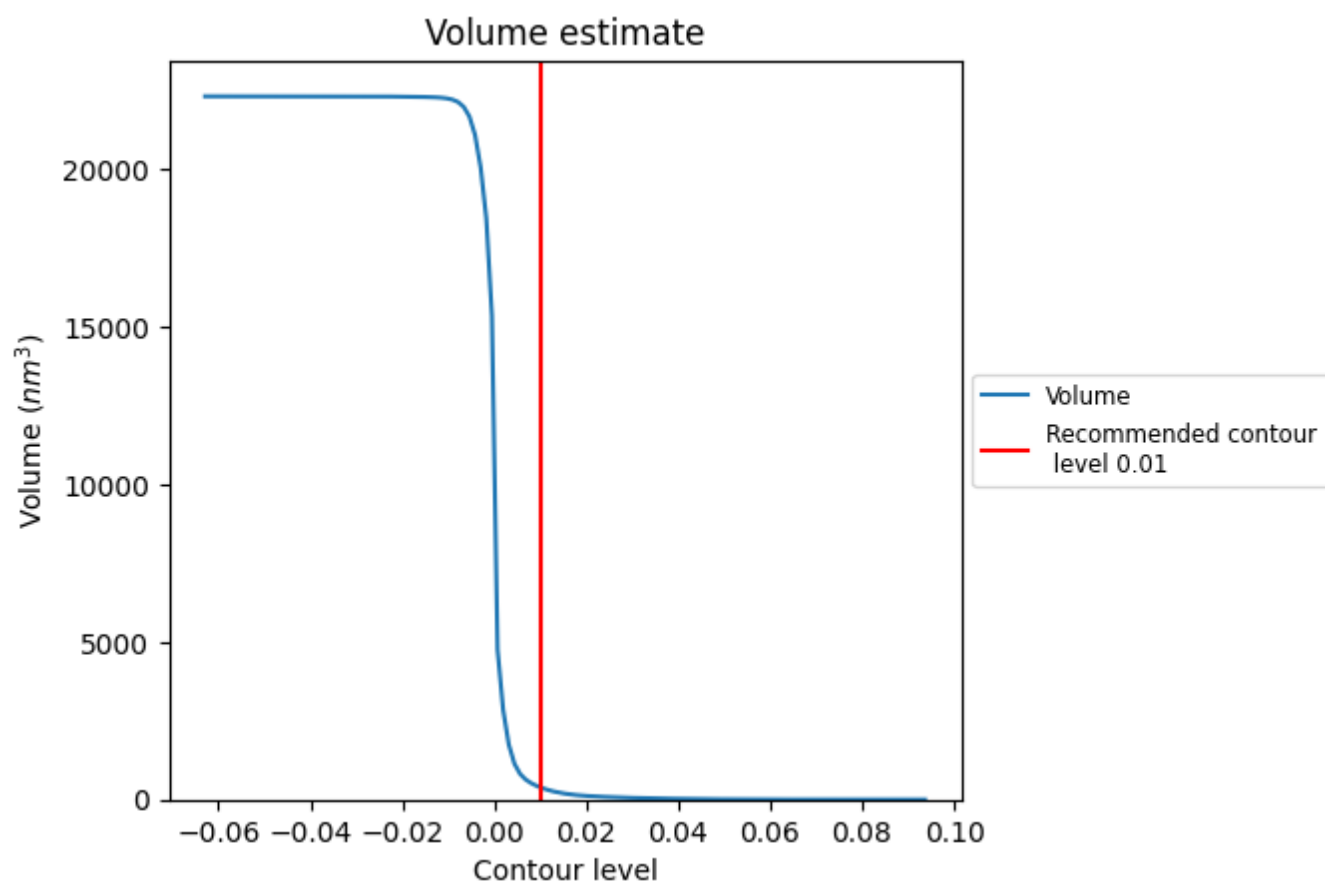
This section contains the results of statistical analysis of the map.

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.

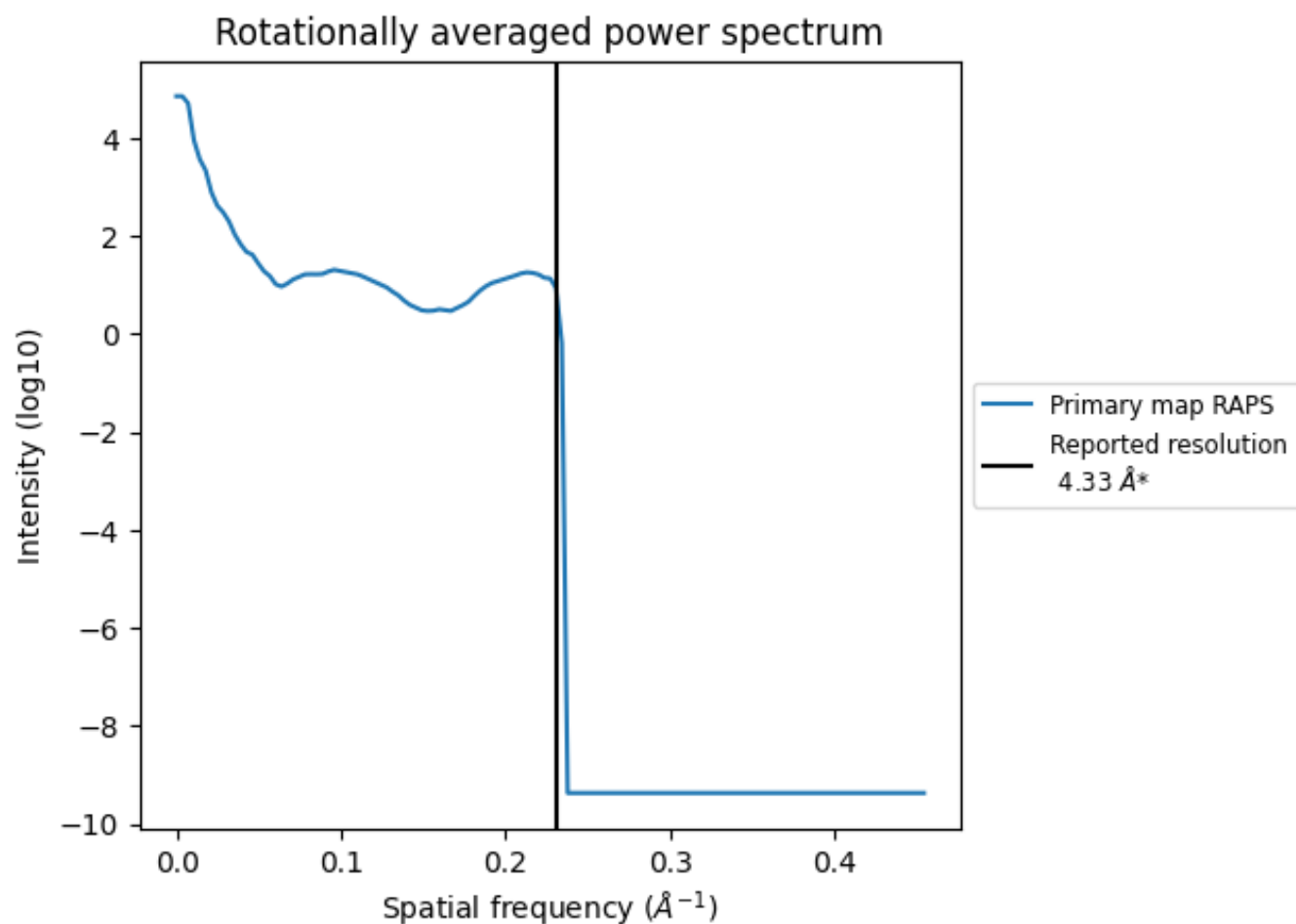
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 391 nm³; this corresponds to an approximate mass of 353 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 0.231 Å⁻¹

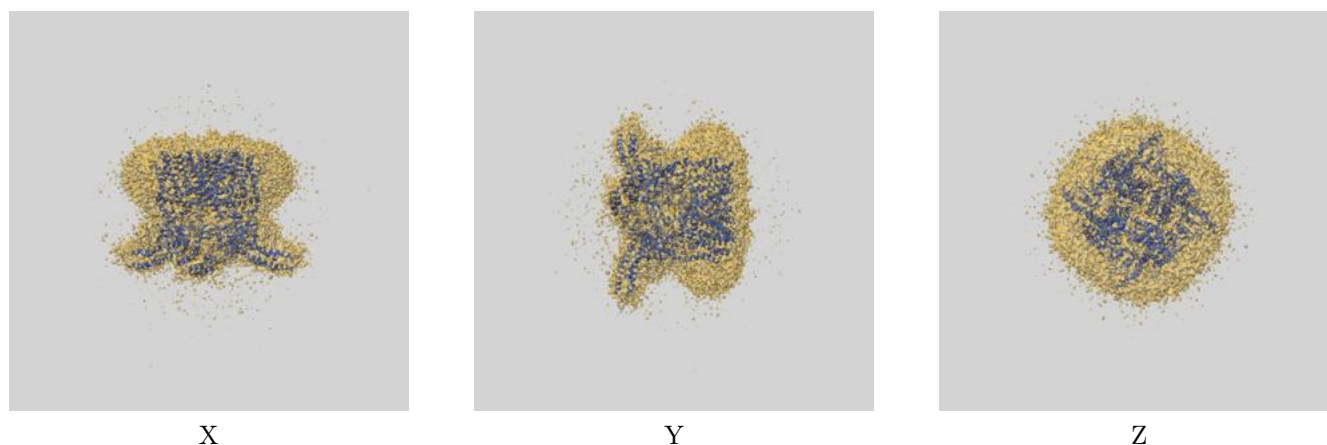
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

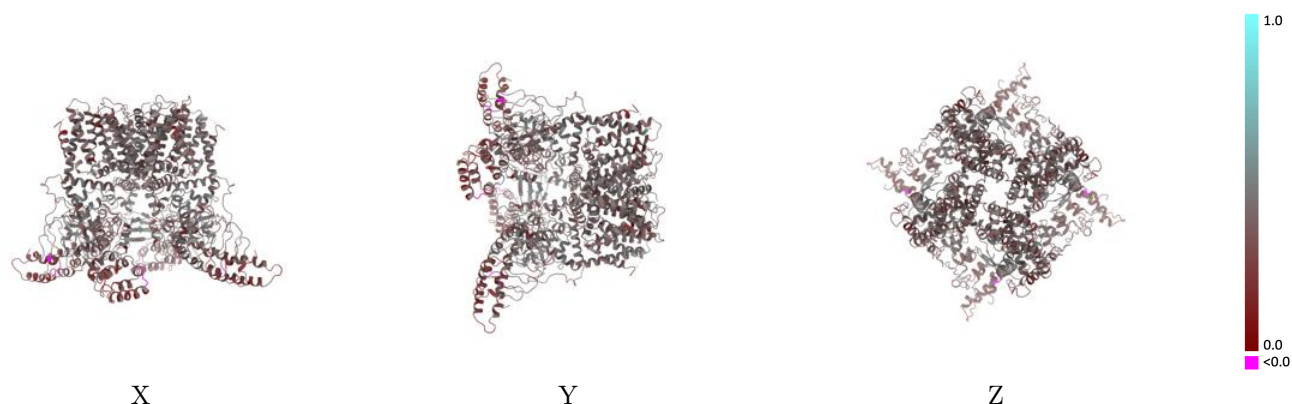
This section contains information regarding the fit between EMDB map EMD-20920 and PDB model 6UW9. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



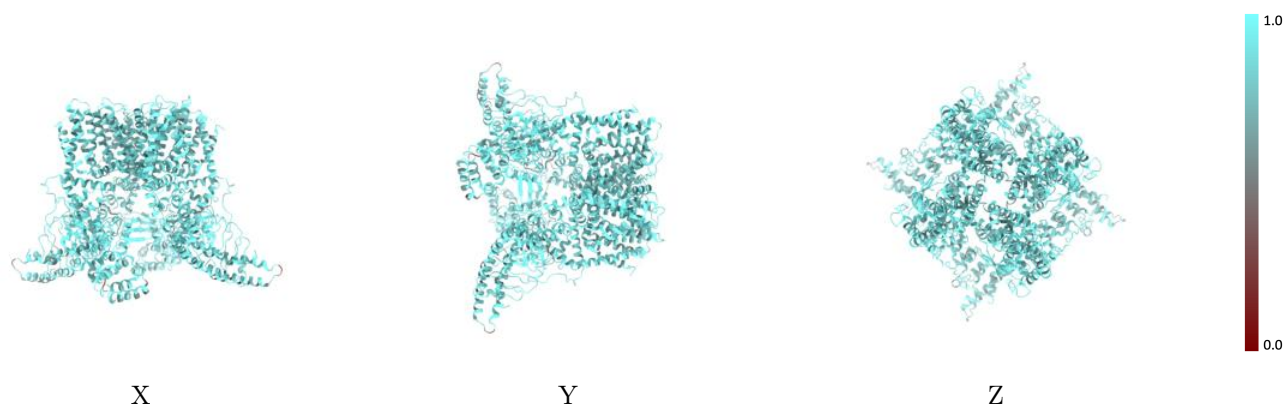
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



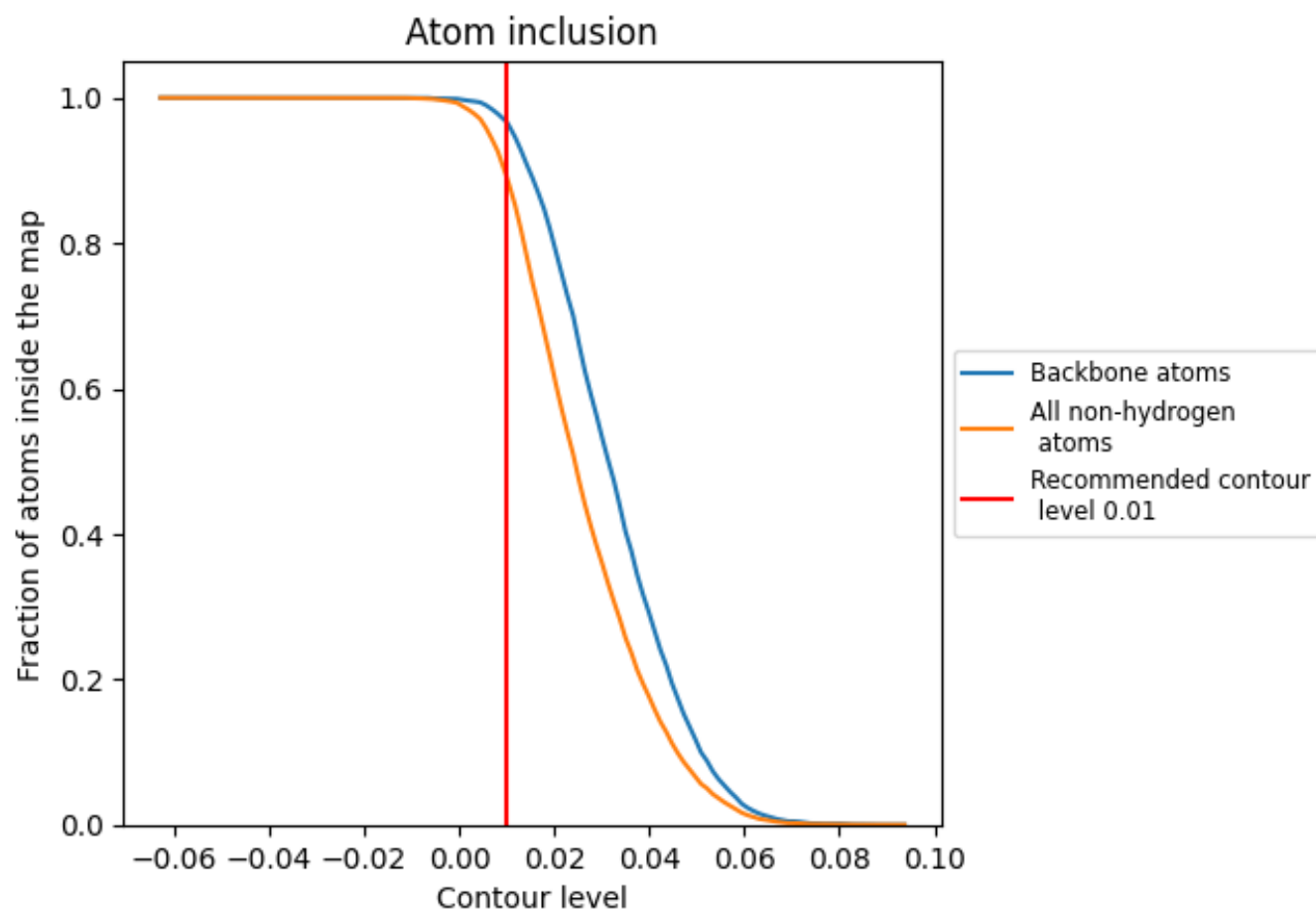
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 89% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8904	<div></div> 0.3830
A	<div></div> 0.8904	<div></div> 0.3840
B	<div></div> 0.8904	<div></div> 0.3830
C	<div></div> 0.8902	<div></div> 0.3820
D	<div></div> 0.8906	<div></div> 0.3830

