Full wwPDB EM Validation Report

May 4, 2025 – 04:18 PM EDT

PDB ID	:	7S1Z / pdb_00007s1z
EMDB ID	:	EMD-24813
Title	:	Cryo-EM structure of Human NKCC1 K289NA492EL671C
Authors	:	Zhao, Y.X.; Cao, E.H.
Deposited on	:	2021-09-02
Resolution	:	3.30 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 (i) 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 (i)) were used in the production of this report:

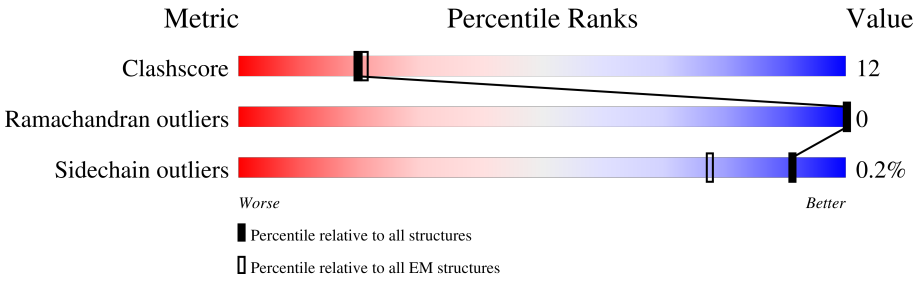
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	1216	29% 9% 61%
1	B	1216	30% 9% 61%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6416 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 Solute carrier family 12 member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	472	Total	C	N	O	S	0	0
			3208	2112	517	562	17		
1	B	472	Total	C	N	O	S	0	0
			3208	2112	517	562	17		

There are 18 discrepancies between the modelled and reference sequences:

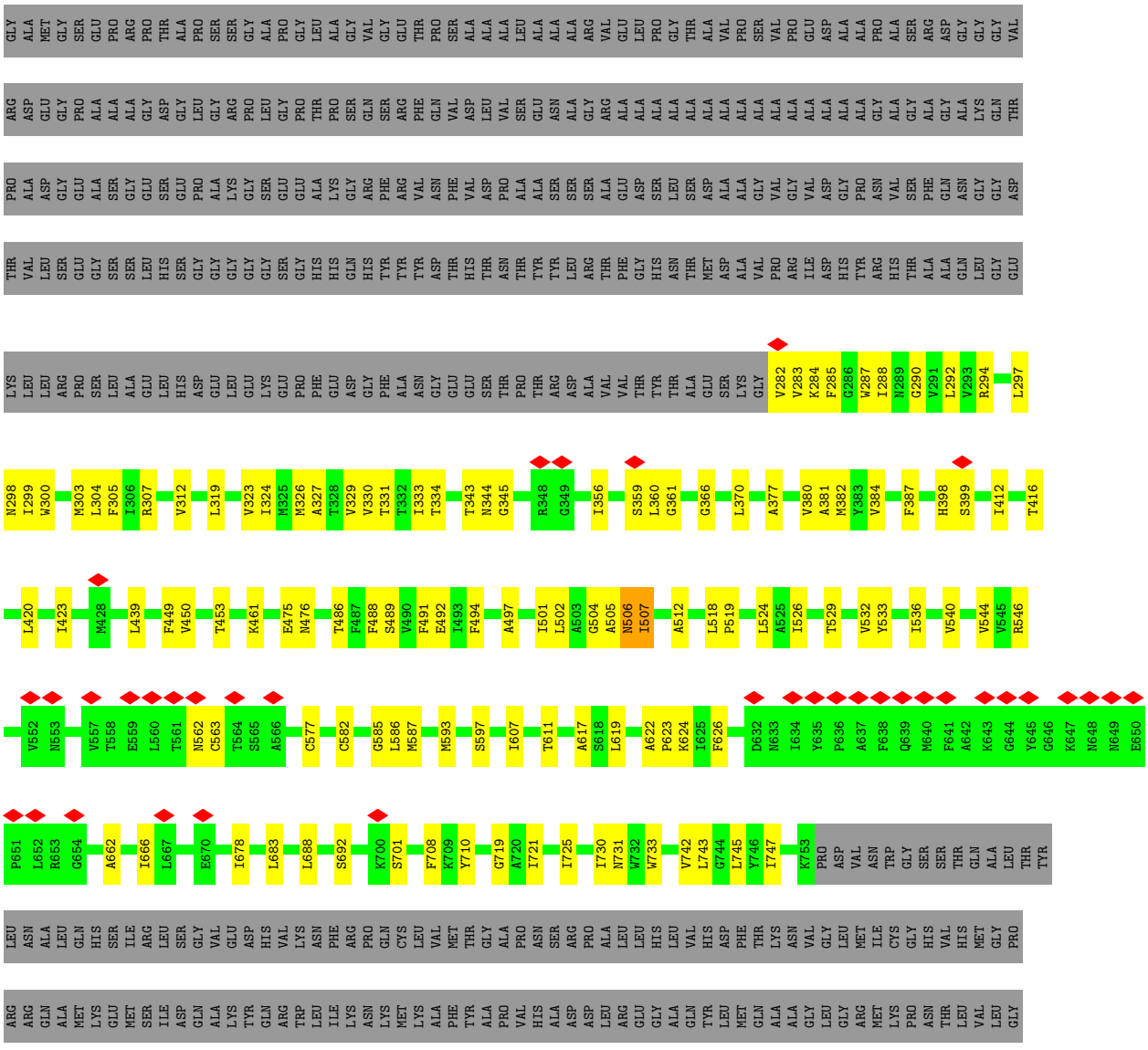
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P55011
A	-2	ALA	-	expression tag	UNP P55011
A	-1	MET	-	expression tag	UNP P55011
A	0	GLY	-	expression tag	UNP P55011
A	1	SER	-	expression tag	UNP P55011
A	289	ASN	LYS	engineered mutation	UNP P55011
A	492	GLU	ALA	engineered mutation	UNP P55011
A	518	LEU	ILE	conflict	UNP P55011
A	671	CYS	LEU	engineered mutation	UNP P55011
B	-3	GLY	-	expression tag	UNP P55011
B	-2	ALA	-	expression tag	UNP P55011
B	-1	MET	-	expression tag	UNP P55011
B	0	GLY	-	expression tag	UNP P55011
B	1	SER	-	expression tag	UNP P55011
B	289	ASN	LYS	engineered mutation	UNP P55011
B	492	GLU	ALA	engineered mutation	UNP P55011
B	518	LEU	ILE	conflict	UNP P55011
B	671	CYS	LEU	engineered mutation	UNP P55011

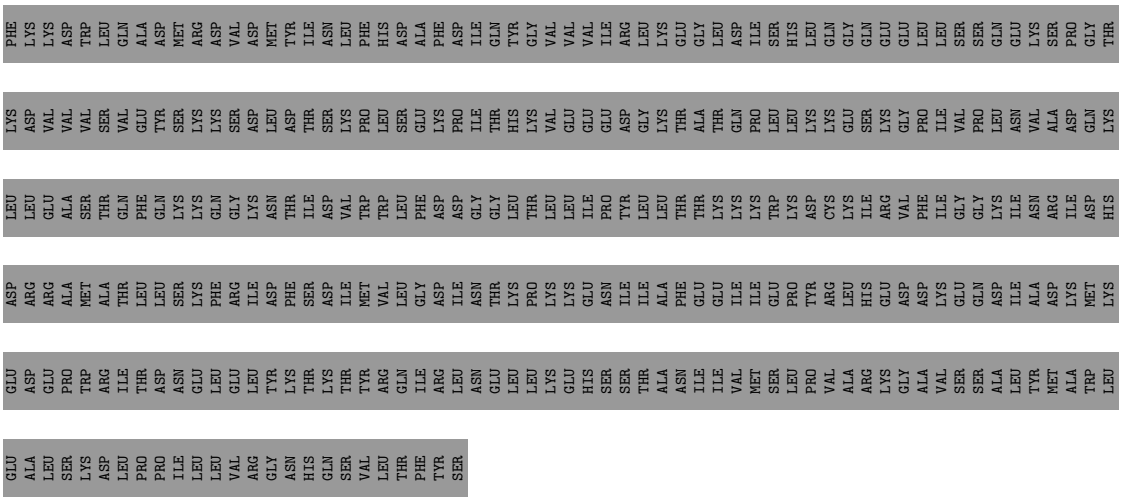
3 Residue-property plots (i)

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: Solute carrier family 12 member 2

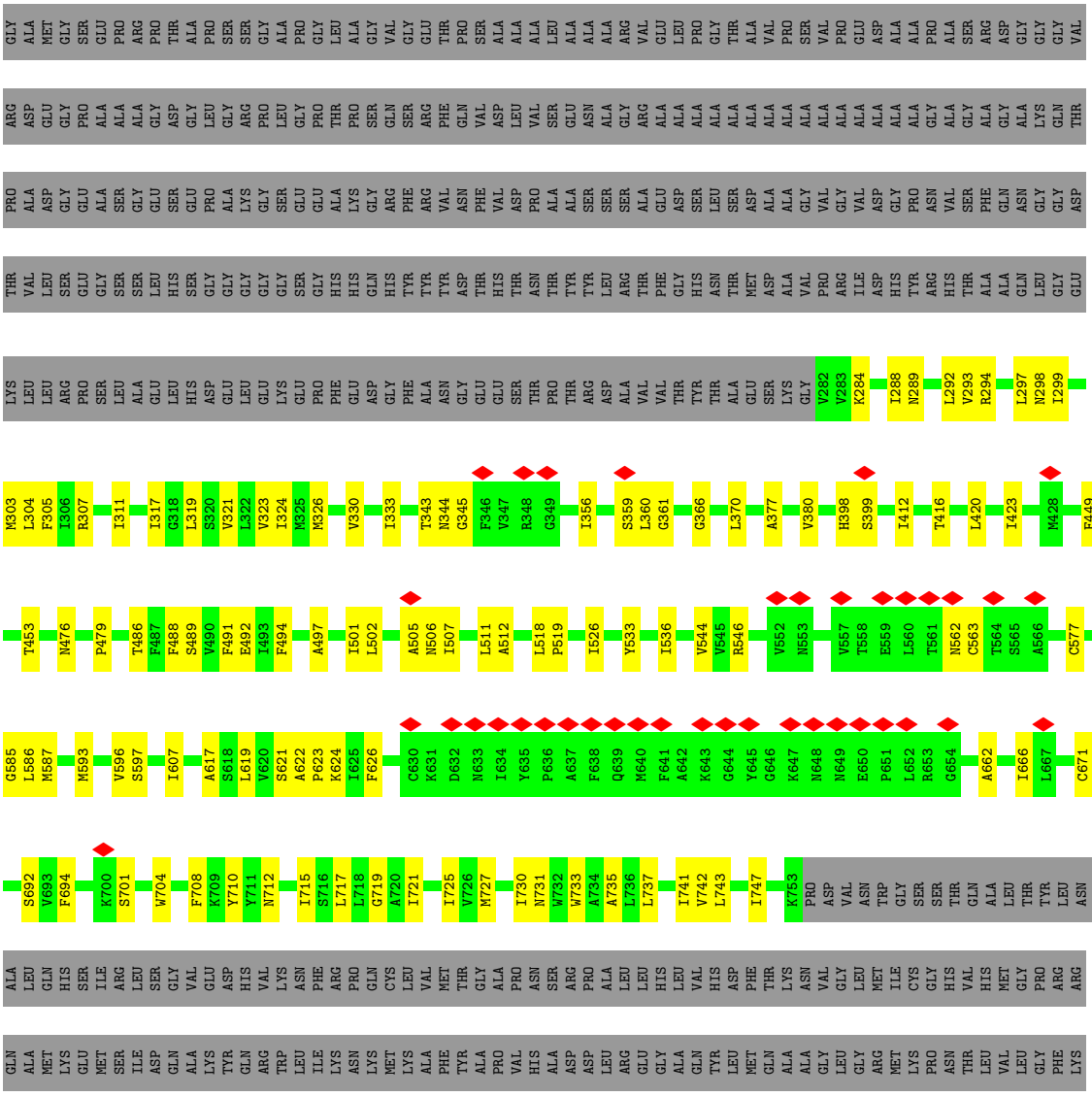
Chain A:





• Molecule 1: Solute carrier family 12 member 2

Chain B:



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

VAL VAL VAL SER VAL GLU TYR SER LYS LYS SER ASP LEU ASP THR SER LYS PRO LEU SER GLU LYS PRO ILE THR HIS LYS VAL GLU GLU GLU ASP GLY LYS THR ALA THR GLN PRO LEU LEU LYS LYS GLU SER LYS GLY PRO ILE VAL PRO LEU ASN VAL ALA ASP GLN LYS LEU LEU

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

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

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

LEU SER LYS ASP LEU PRO PRO ILE LEU LEU LEU VAL ARG GLY ASN HIS GLN SER VAL LEU THR PHE TYR SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	536763	Depositor
Resolution determination method	DIFFRACTION PATTERN/LAYERLINES	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.175	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	7.275	Depositor
Minimum map value	-5.775	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.150	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	271.36, 271.36, 271.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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	0.15	0/3280	0.42	1/4490 (0.0%)
1	B	0.15	0/3280	0.41	0/4490
All	All	0.15	0/6560	0.42	1/8980 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	507	ILE	N-CA-C	-5.77	106.16	112.80

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	3208	0	2984	80	0
1	B	3208	0	2984	72	0
All	All	6416	0	5968	152	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 12.

All (152) 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:B:333:ILE:HG21	1:B:719:GLY:HA3	1.71	0.71
1:A:476:ASN:OD1	1:A:546:ARG:NH1	2.24	0.69
1:A:285:PHE:CE2	1:A:290:GLY:HA3	2.30	0.67
1:A:333:ILE:HG21	1:A:719:GLY:HA3	1.76	0.66
1:A:506:ASN:HD22	1:A:624:LYS:HD2	1.59	0.66
1:B:324:ILE:HD12	1:B:533:TYR:HB3	1.79	0.64
1:B:674:ILE:HA	1:B:677:ILE:HD12	1.80	0.64
1:B:712:ASN:HB3	1:B:715:ILE:HG12	1.81	0.63
1:B:476:ASN:HA	1:B:546:ARG:HH22	1.64	0.62
1:A:303:MET:HB2	1:A:497:ALA:HB2	1.81	0.62
1:A:324:ILE:HD12	1:A:533:TYR:HB3	1.82	0.61
1:B:294:ARG:HD2	1:B:507:ILE:HG13	1.81	0.61
1:B:488:PHE:HB3	1:B:730:ILE:HD11	1.81	0.60
1:B:288:ILE:O	1:B:292:LEU:HB3	2.01	0.60
1:A:504:GLY:O	1:A:507:ILE:HG22	2.01	0.60
1:A:488:PHE:HB3	1:A:730:ILE:HD11	1.84	0.59
1:B:731:ASN:OD1	1:B:733:TRP:NE1	2.36	0.59
1:B:303:MET:HB2	1:B:497:ALA:HB2	1.83	0.58
1:A:288:ILE:O	1:A:292:LEU:HB3	2.04	0.58
1:A:662:ALA:O	1:A:666:ILE:HG12	2.04	0.57
1:A:449:PHE:HA	1:A:597:SER:HB2	1.87	0.57
1:B:299:ILE:HD13	1:B:501:ILE:HG23	1.85	0.57
1:A:398:HIS:CG	1:A:399:SER:H	2.23	0.57
1:B:492:GLU:HG3	1:B:730:ILE:HG21	1.87	0.57
1:B:323:VAL:HG13	1:B:491:PHE:HD2	1.70	0.57
1:B:662:ALA:O	1:B:666:ILE:HG12	2.04	0.56
1:B:398:HIS:CG	1:B:399:SER:H	2.23	0.56
1:B:743:LEU:O	1:B:747:ILE:HD12	2.05	0.56
1:B:449:PHE:HA	1:B:597:SER:HB2	1.87	0.56
1:A:731:ASN:OD1	1:A:733:TRP:NE1	2.37	0.56
1:B:305:PHE:HB3	1:B:607:ILE:HG12	1.89	0.55
1:A:420:LEU:HA	1:A:423:ILE:HG22	1.88	0.55
1:A:359:SER:HB3	1:A:701:SER:HB3	1.89	0.55
1:B:476:ASN:ND2	1:B:544:VAL:O	2.39	0.55
1:B:511:LEU:HD12	1:B:512:ALA:H	1.72	0.55
1:B:562:ASN:OD1	1:B:563:CYS:N	2.34	0.54
1:A:743:LEU:O	1:A:747:ILE:HD12	2.07	0.54
1:A:305:PHE:HB3	1:A:607:ILE:HG12	1.90	0.54
1:A:501:ILE:HD13	1:A:526:ILE:HD11	1.89	0.54
1:A:502:LEU:O	1:A:505:ALA:HB3	2.07	0.54
1:A:562:ASN:OD1	1:A:563:CYS:N	2.35	0.53
1:B:356:ILE:O	1:B:692:SER:OG	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:LEU:HD11	1:A:439:LEU:HB2	1.91	0.53
1:B:294:ARG:HB2	1:B:294:ARG:NH1	2.24	0.53
1:B:359:SER:HB3	1:B:701:SER:HB3	1.92	0.52
1:B:502:LEU:O	1:B:505:ALA:HB3	2.09	0.52
1:B:343:THR:HG21	1:B:708:PHE:HB2	1.92	0.52
1:A:356:ILE:O	1:A:692:SER:OG	2.27	0.51
1:A:299:ILE:HD13	1:A:501:ILE:HG23	1.91	0.51
1:A:323:VAL:HG13	1:A:491:PHE:HD2	1.75	0.51
1:B:708:PHE:HE1	1:B:710:TYR:HB2	1.74	0.51
1:B:380:VAL:HG21	1:B:619:LEU:HB2	1.91	0.51
1:B:298:ASN:HD22	1:B:617:ALA:HB3	1.76	0.50
1:A:343:THR:HG21	1:A:708:PHE:HB2	1.94	0.50
1:B:737:LEU:O	1:B:741:ILE:HG12	2.11	0.50
1:B:420:LEU:HA	1:B:423:ILE:HG22	1.93	0.50
1:B:476:ASN:HA	1:B:546:ARG:HH12	1.77	0.49
1:B:326:MET:O	1:B:330:VAL:HG23	2.12	0.49
1:A:285:PHE:HE2	1:A:290:GLY:HA3	1.73	0.49
1:A:721:ILE:O	1:A:725:ILE:HG12	2.13	0.49
1:A:506:ASN:ND2	1:A:624:LYS:HD2	2.25	0.49
1:B:721:ILE:O	1:B:725:ILE:HG12	2.13	0.49
1:A:708:PHE:HE1	1:A:710:TYR:HB2	1.78	0.49
1:A:298:ASN:HD22	1:A:617:ALA:HB3	1.78	0.48
1:B:324:ILE:HD13	1:B:494:PHE:CZ	2.49	0.48
1:A:505:ALA:HA	1:A:518:LEU:HD12	1.95	0.48
1:A:324:ILE:HD13	1:A:494:PHE:CZ	2.49	0.47
1:A:688:LEU:HD11	1:A:742:VAL:HG21	1.95	0.47
1:B:671:CYS:HA	1:B:674:ILE:HD12	1.95	0.47
1:B:289:ASN:O	1:B:293:VAL:HB	2.14	0.47
1:A:577:CYS:HB2	1:A:582:CYS:HB3	1.43	0.47
1:B:577:CYS:HB2	1:B:582:CYS:HB3	1.45	0.47
1:A:412:ILE:O	1:A:416:THR:HG22	2.15	0.47
1:B:727:MET:HG2	1:B:735:ALA:HB1	1.96	0.46
1:A:382:MET:HE2	1:A:678:ILE:HG13	1.98	0.46
1:B:506:ASN:ND2	1:B:621:SER:OG	2.49	0.46
1:A:300:TRP:NE1	1:A:529:THR:OG1	2.49	0.45
1:A:329:VAL:O	1:A:333:ILE:HG12	2.16	0.45
1:B:486:THR:H	1:B:489:SER:HB3	1.81	0.45
1:B:317:ILE:O	1:B:321:VAL:HG23	2.17	0.45
1:B:505:ALA:HA	1:B:518:LEU:HD12	1.99	0.45
1:A:492:GLU:HG3	1:A:730:ILE:HG21	1.99	0.45
1:A:287:TRP:CD1	1:A:287:TRP:O	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LEU:HD23	1:A:319:LEU:HA	1.84	0.44
1:A:384:VAL:HG13	1:A:666:ILE:HD11	2.00	0.44
1:A:518:LEU:HB2	1:A:519:PRO:HD3	2.00	0.44
1:B:307:ARG:O	1:B:311:ILE:HG12	2.18	0.44
1:B:449:PHE:CE2	1:B:536:ILE:HG13	2.52	0.44
1:A:476:ASN:ND2	1:A:544:VAL:O	2.47	0.43
1:B:593:MET:HA	1:B:596:VAL:HG12	2.00	0.43
1:B:727:MET:HG2	1:B:735:ALA:CB	2.49	0.43
1:A:380:VAL:HG21	1:A:619:LEU:HB2	2.00	0.43
1:A:623:PRO:HA	1:A:626:PHE:HB2	2.00	0.43
1:B:344:ASN:OD1	1:B:345:GLY:N	2.51	0.43
1:B:412:ILE:O	1:B:416:THR:HG22	2.19	0.43
1:A:622:ALA:HB3	1:A:623:PRO:HD3	2.00	0.43
1:A:524:LEU:HD12	1:A:524:LEU:HA	1.86	0.43
1:B:366:GLY:O	1:B:370:LEU:HD23	2.19	0.43
1:A:307:ARG:HA	1:A:307:ARG:HD2	1.88	0.43
1:A:344:ASN:OD1	1:A:345:GLY:N	2.51	0.43
1:A:449:PHE:CE2	1:A:536:ILE:HG13	2.54	0.43
1:A:300:TRP:CZ2	1:A:532:VAL:HG11	2.54	0.43
1:B:450:VAL:O	1:B:453:THR:OG1	2.30	0.43
1:B:694:PHE:CZ	1:B:717:LEU:HD12	2.54	0.42
1:A:312:VAL:HG11	1:A:540:VAL:HG13	2.01	0.42
1:A:326:MET:O	1:A:330:VAL:HG23	2.19	0.42
1:A:449:PHE:O	1:A:453:THR:HG23	2.20	0.42
1:A:334:THR:HG22	1:A:502:LEU:HD21	2.01	0.42
1:B:398:HIS:CG	1:B:399:SER:N	2.87	0.42
1:B:518:LEU:HB2	1:B:519:PRO:HD3	2.00	0.42
1:B:501:ILE:HG21	1:B:526:ILE:HD11	2.02	0.42
1:A:366:GLY:O	1:A:370:LEU:HD23	2.19	0.42
1:A:683:LEU:HD23	1:A:683:LEU:HA	1.92	0.42
1:B:622:ALA:HB3	1:B:623:PRO:HD3	2.01	0.42
1:A:450:VAL:O	1:A:453:THR:OG1	2.30	0.42
1:A:360:LEU:HD12	1:A:361:GLY:O	2.19	0.42
1:B:297:LEU:HD23	1:B:297:LEU:HA	1.78	0.42
1:B:688:LEU:HD11	1:B:742:VAL:HG21	2.02	0.42
1:A:304:LEU:HD13	1:A:533:TYR:CE1	2.55	0.41
1:A:593:MET:HE2	1:A:593:MET:HB3	1.89	0.41
1:B:304:LEU:HD13	1:B:533:TYR:CE1	2.55	0.41
1:A:284:LYS:HB3	1:A:512:ALA:HB2	2.02	0.41
1:B:585:GLY:C	1:B:587:MET:H	2.29	0.41
1:A:745:LEU:HD23	1:A:745:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:LEU:HD12	1:B:361:GLY:O	2.21	0.41
1:A:585:GLY:C	1:A:587:MET:H	2.29	0.41
1:B:294:ARG:HB2	1:B:294:ARG:CZ	2.50	0.41
1:B:319:LEU:HD12	1:B:479:PRO:HB3	2.02	0.41
1:A:294:ARG:HB2	1:A:294:ARG:NH1	2.35	0.41
1:A:377:ALA:O	1:A:380:VAL:HG12	2.21	0.41
1:A:529:THR:HA	1:A:532:VAL:HG12	2.01	0.41
1:A:387:PHE:HB2	1:A:611:THR:HB	2.03	0.41
1:A:475:GLU:HG3	1:A:546:ARG:HH22	1.86	0.41
1:B:546:ARG:HA	1:B:586:LEU:HD22	2.00	0.41
1:A:398:HIS:CG	1:A:399:SER:N	2.87	0.41
1:B:623:PRO:HA	1:B:626:PHE:HB2	2.03	0.41
1:A:461:LYS:HD2	1:A:461:LYS:HA	1.93	0.41
1:B:284:LYS:HB3	1:B:512:ALA:HB2	2.02	0.41
1:A:501:ILE:HG13	1:A:502:LEU:HD22	2.02	0.40
1:B:377:ALA:O	1:B:380:VAL:HG12	2.21	0.40
1:A:327:ALA:O	1:A:331:THR:HG22	2.21	0.40
1:A:486:THR:H	1:A:489:SER:HB3	1.86	0.40
1:B:701:SER:HB2	1:B:704:TRP:HB2	2.03	0.40
1:A:282:VAL:HG13	1:A:283:VAL:HG13	2.02	0.40
1:B:416:THR:O	1:B:420:LEU:HD23	2.21	0.40
1:B:501:ILE:HD13	1:B:526:ILE:HD11	2.03	0.40
1:B:586:LEU:HD23	1:B:586:LEU:O	2.21	0.40
1:A:299:ILE:HG23	1:A:300:TRP:CD1	2.57	0.40
1:A:381:ALA:HB2	1:A:662:ALA:HA	2.04	0.40
1:A:416:THR:O	1:A:420:LEU:HD23	2.22	0.40
1:A:586:LEU:HD23	1:A:586:LEU:O	2.22	0.40
1:B:507:ILE:HD13	1:B:624:LYS:HE3	2.03	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	470/1216 (39%)	426 (91%)	44 (9%)	0	100	100
1	B	470/1216 (39%)	426 (91%)	44 (9%)	0	100	100
All	All	940/2432 (39%)	852 (91%)	88 (9%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	281/985 (28%)	280 (100%)	1 (0%)	89	93
1	B	281/985 (28%)	281 (100%)	0	100	100
All	All	562/1970 (28%)	561 (100%)	1 (0%)	91	95

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

Mol	Chain	Res	Type
1	A	506	ASN

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

Mol	Chain	Res	Type
1	A	298	ASN
1	B	298	ASN
1	B	506	ASN
1	B	690	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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.

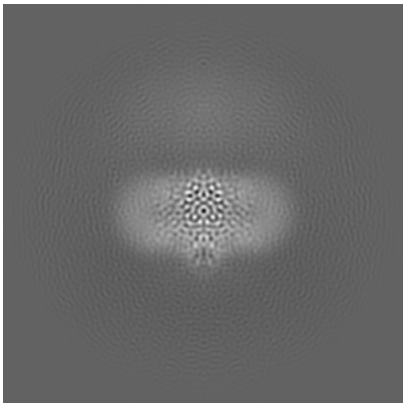
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24813. These allow visual inspection of the internal detail of the map and identification of artifacts.

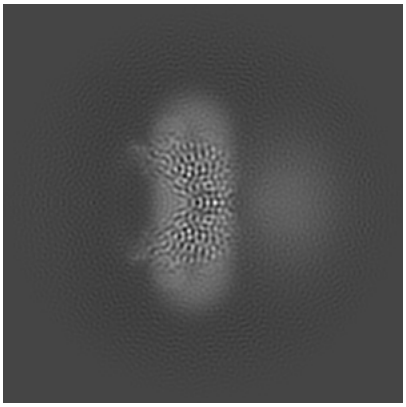
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

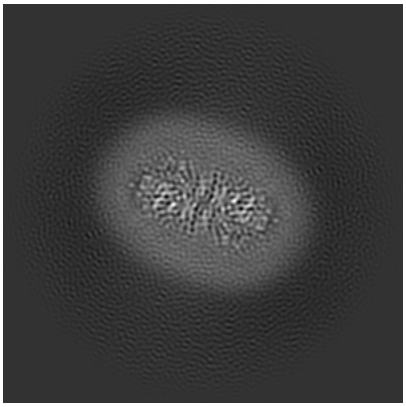
6.1.1 Primary map



X



Y

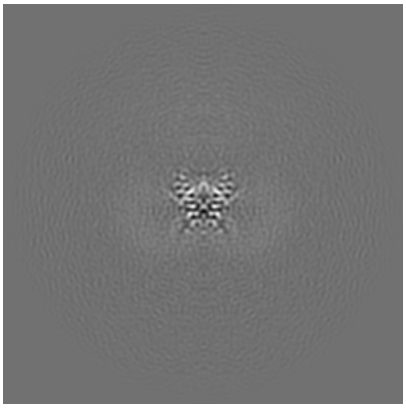


Z

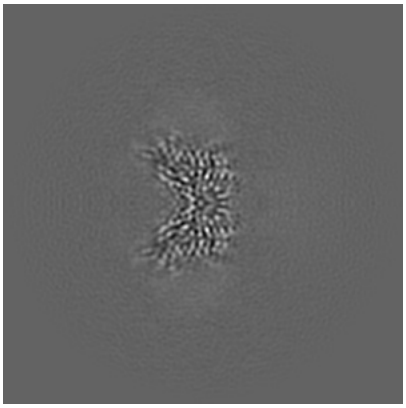
The images above show the map projected in three orthogonal directions.

6.2 Central slices

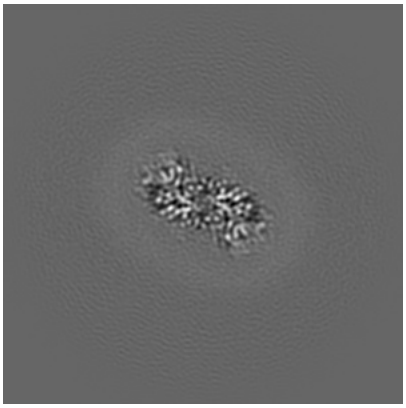
6.2.1 Primary map



X Index: 128



Y Index: 128

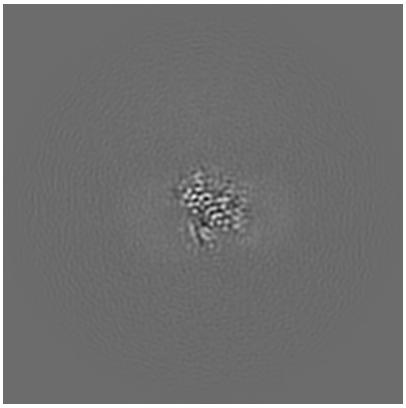


Z Index: 128

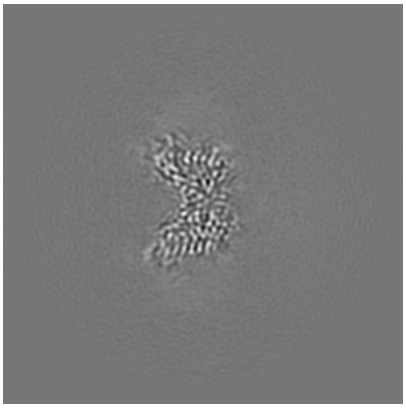
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

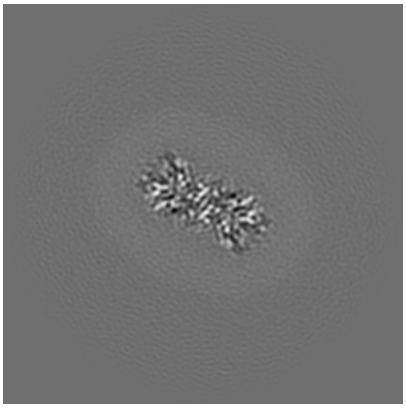
6.3.1 Primary map



X Index: 115



Y Index: 126

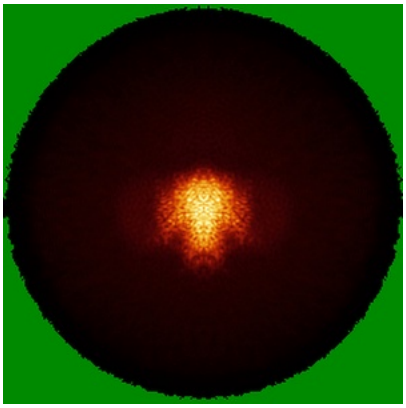


Z Index: 126

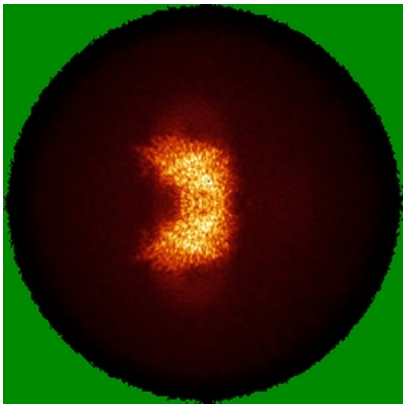
The images above show the largest variance slices of the map in three orthogonal directions.

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

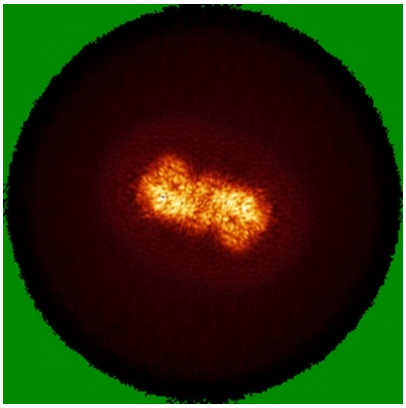
6.4.1 Primary map



X



Y

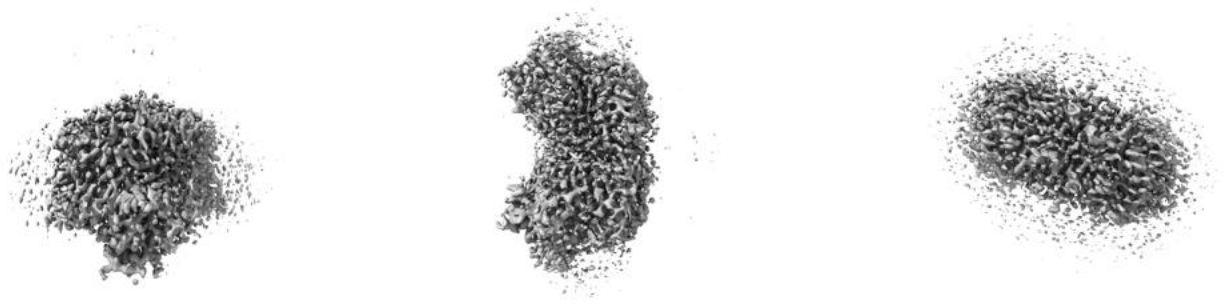


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

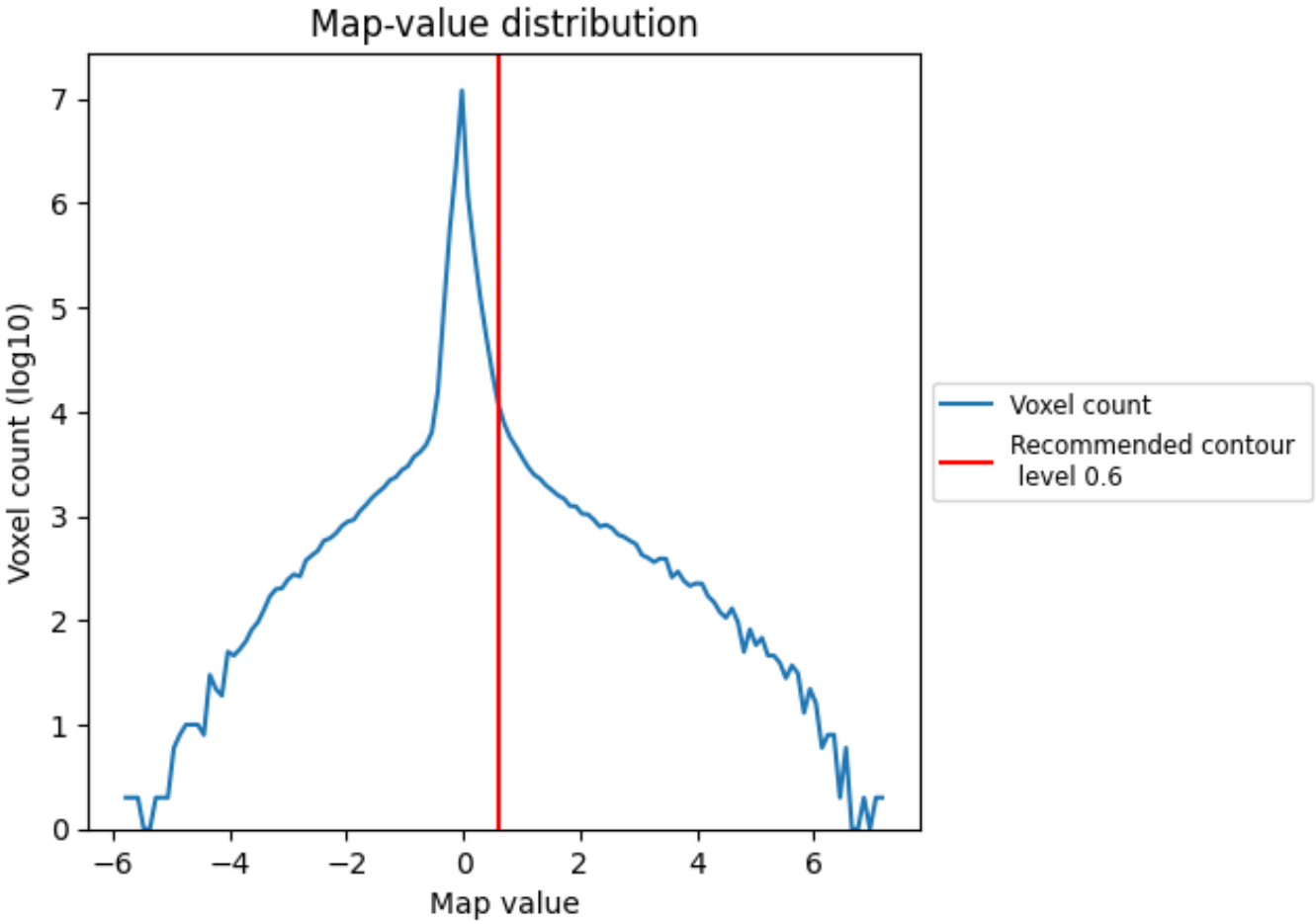
6.6 Mask visualisation (i)

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

7 Map analysis

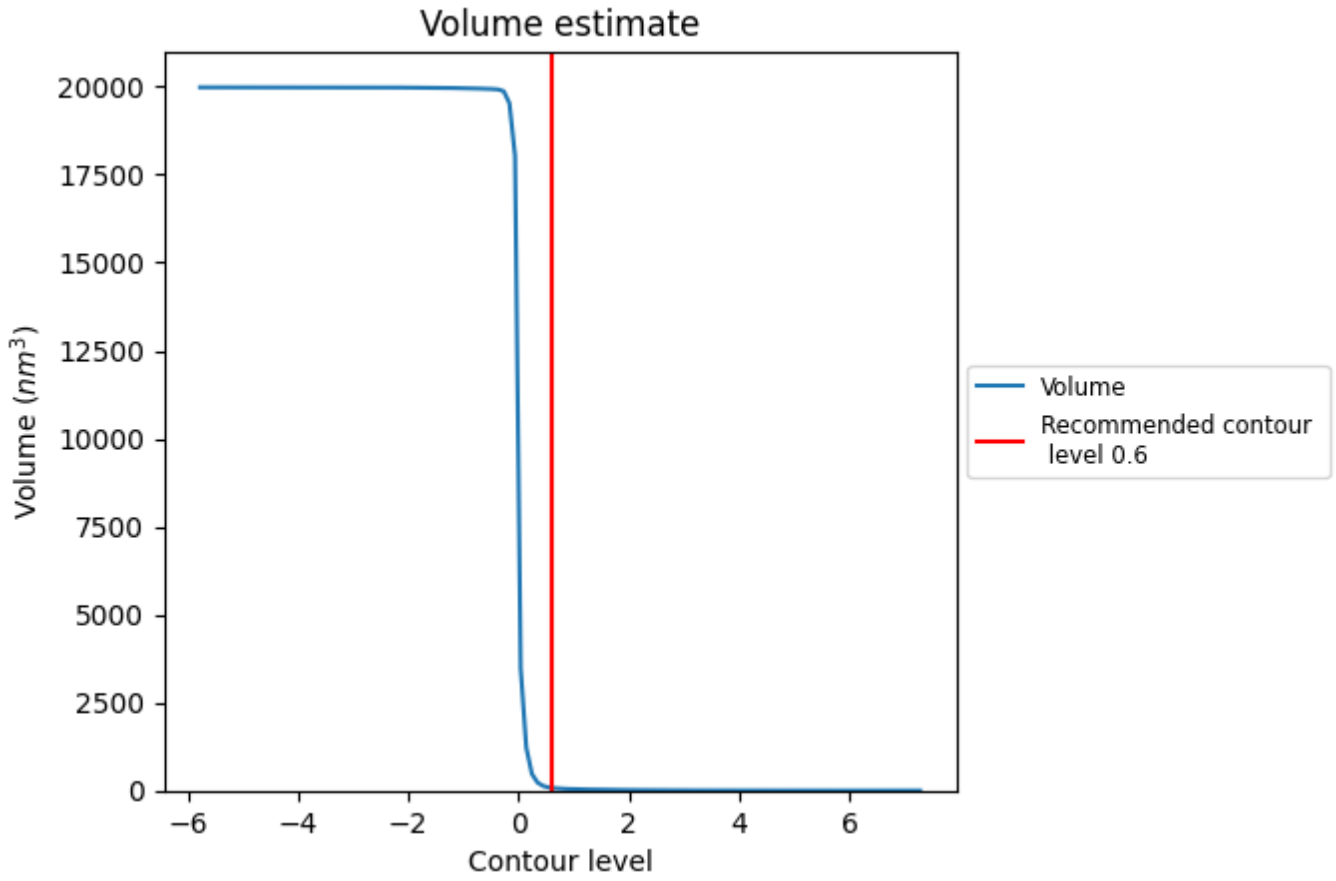
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

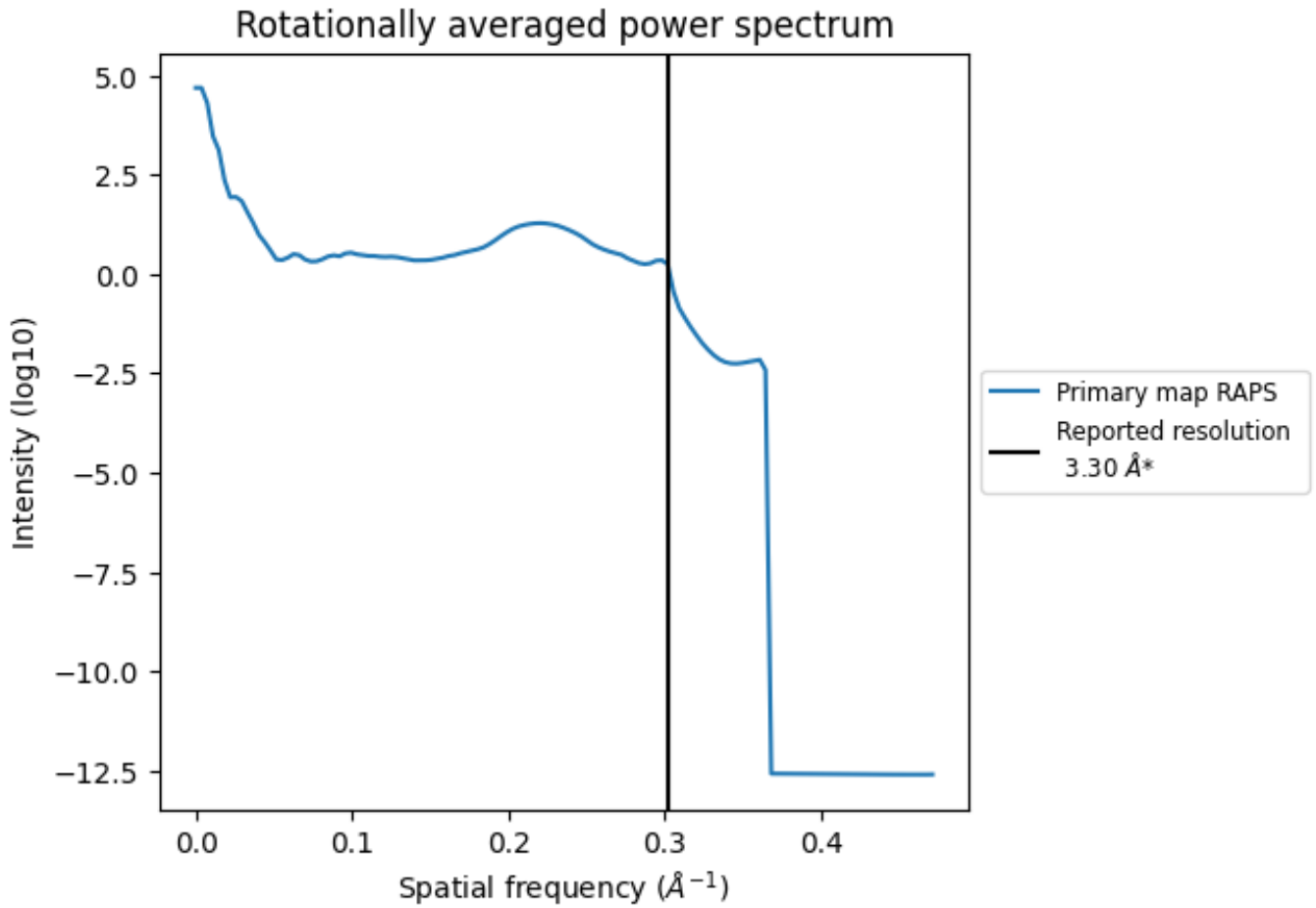
7.2 Volume estimate



The volume at the recommended contour level is 77 nm^3; this corresponds to an approximate mass of 69 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 (i)



*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

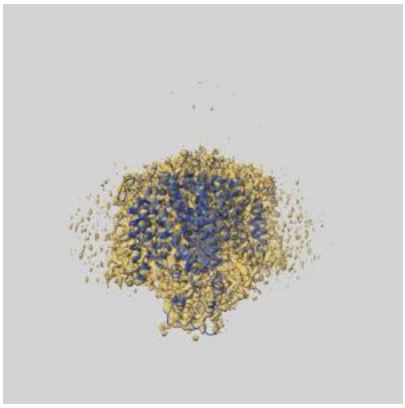
8 Fourier-Shell correlation (i)

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

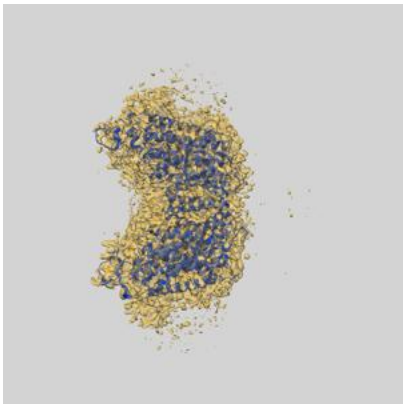
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24813 and PDB model 7S1Z. Per-residue inclusion information can be found in section 3 on page 4.

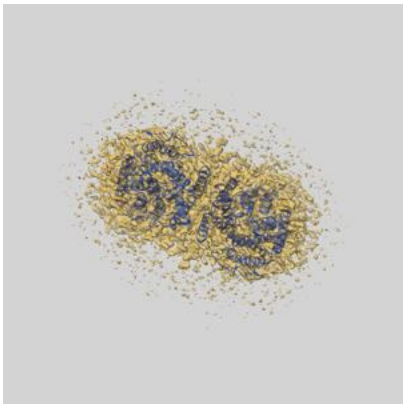
9.1 Map-model overlay



X



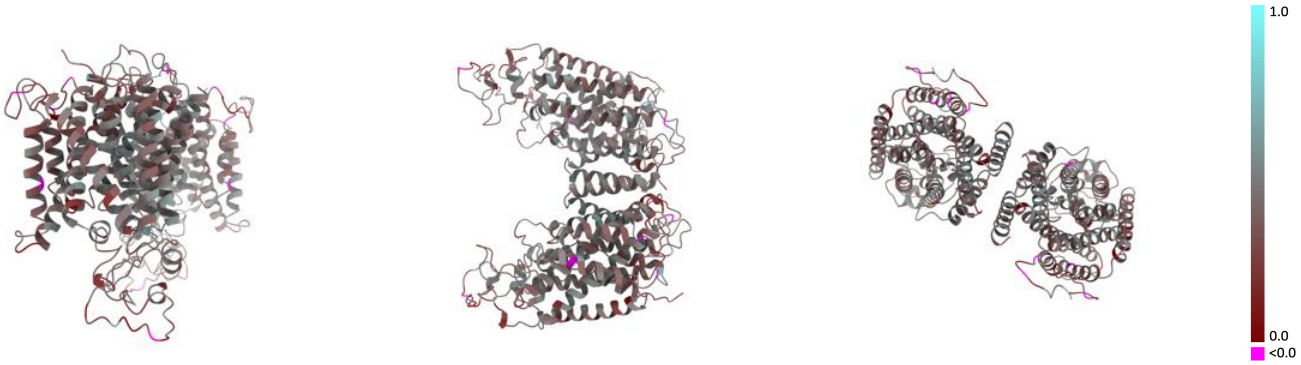
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6 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.

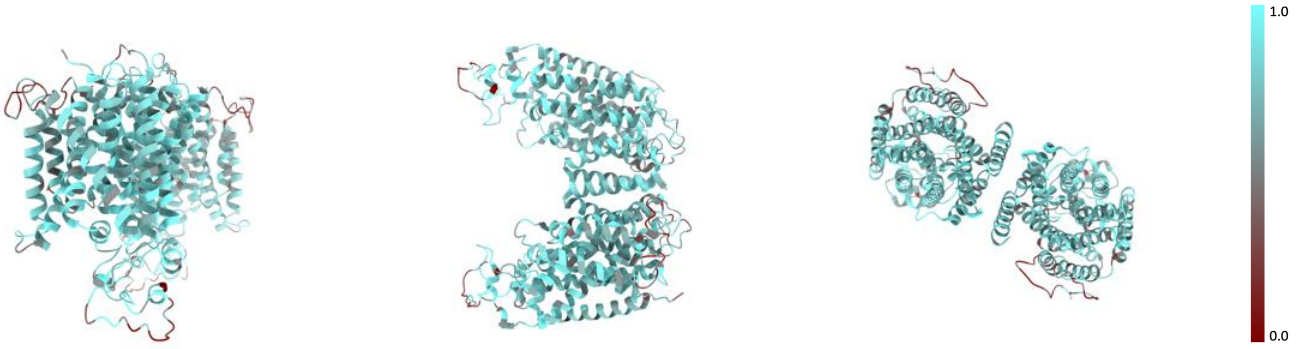
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

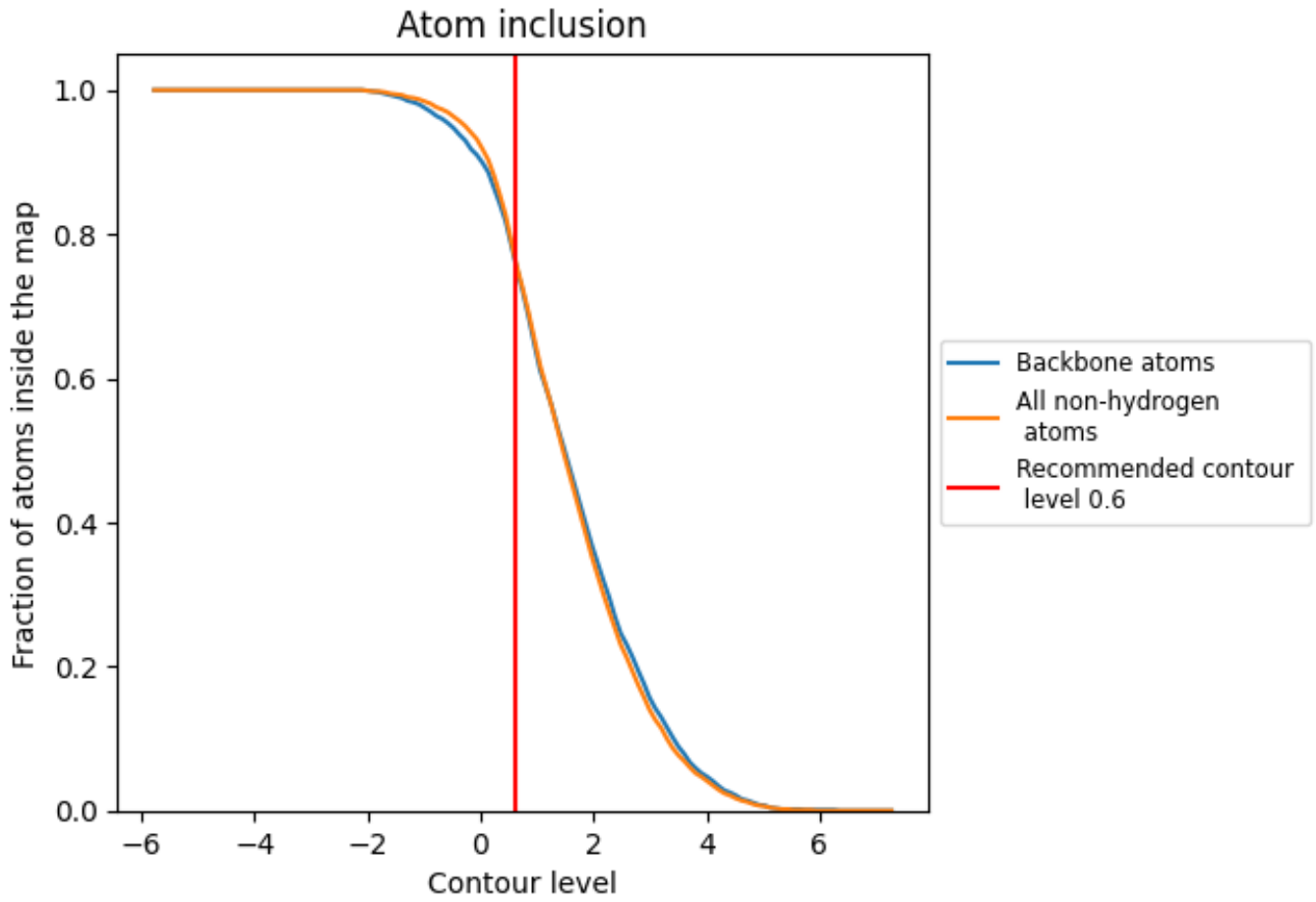
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.6).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7700	0.4040
A	0.7700	0.4050
B	0.7700	0.4030