Full wwPDB EM Validation Report ⓘ

Jun 20, 2024 – 03:51 AM JST

PDB ID	:	7X5V
EMDB ID	:	EMD-33016
Title	:	NaVEh Sodium channel, and NaVEh from the coccolithophore Emiliania huxleyi
Authors	:	Jiang, D.; Zhang, J.
Deposited on	:	2022-03-05
Resolution	:	2.83 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:

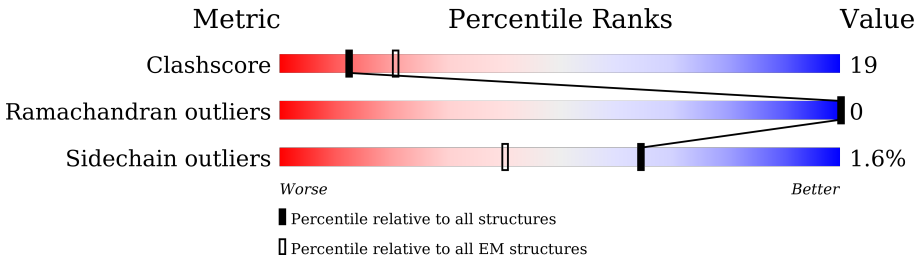
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.83 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 <=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	815	22% 13% 64%
1	B	815	22% 13% 64%
1	C	815	23% 12% 64%
1	D	815	23% 13% 64%
2	E	17	82% 65% 29% 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9504 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 ion channel,GFP-TwinStrep.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	290	Total	C	N	O	S	0	0
			2345	1547	370	414	14		
1	B	290	Total	C	N	O	S	0	0
			2345	1547	370	414	14		
1	C	290	Total	C	N	O	S	0	0
			2345	1547	370	414	14		
1	D	290	Total	C	N	O	S	0	0
			2345	1547	370	414	14		

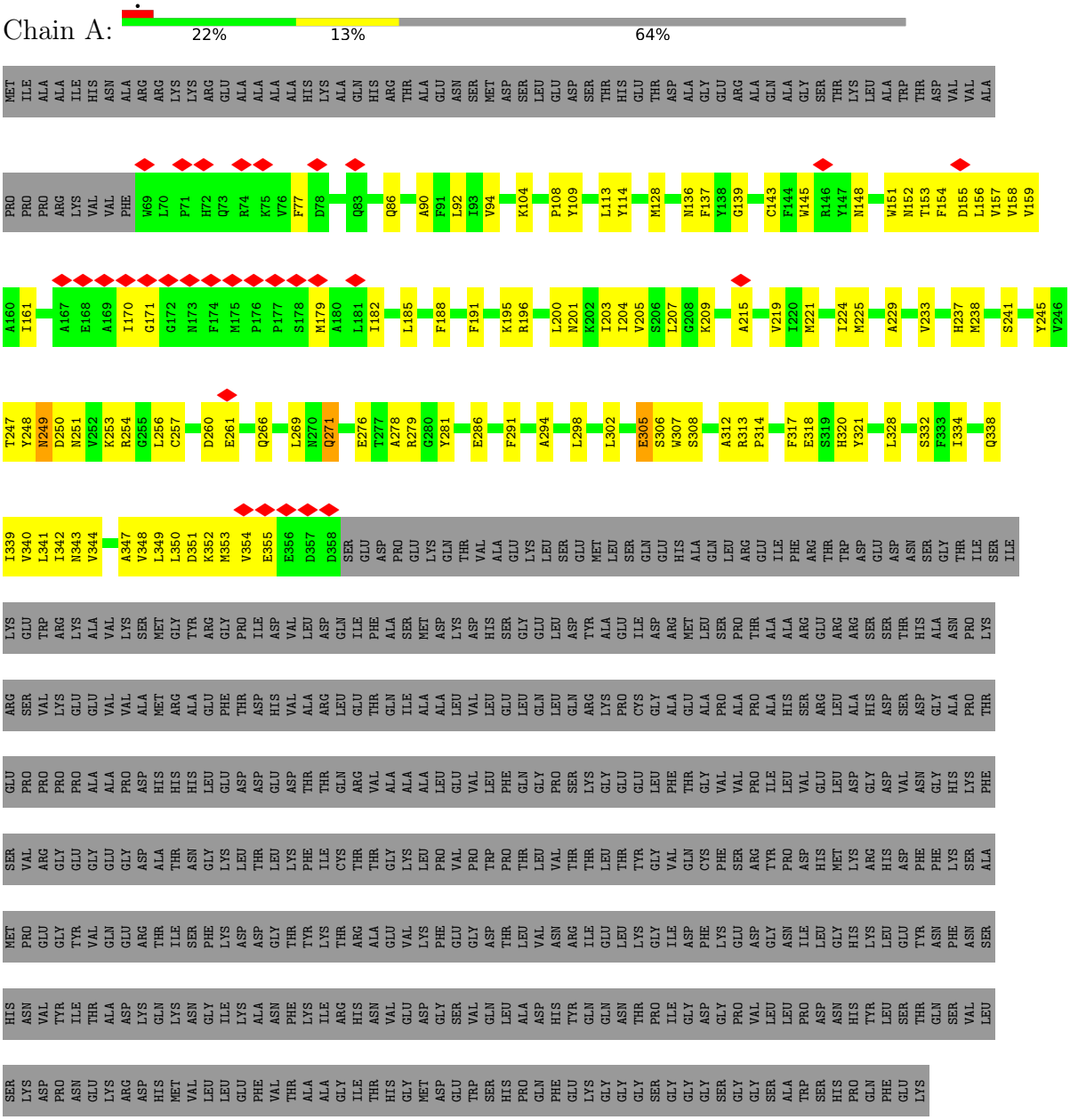
- Molecule 2 is a protein called ion channel.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	16	Total	C	N	O	0	0
			124	75	30	19		

3 Residue-property plots (i)

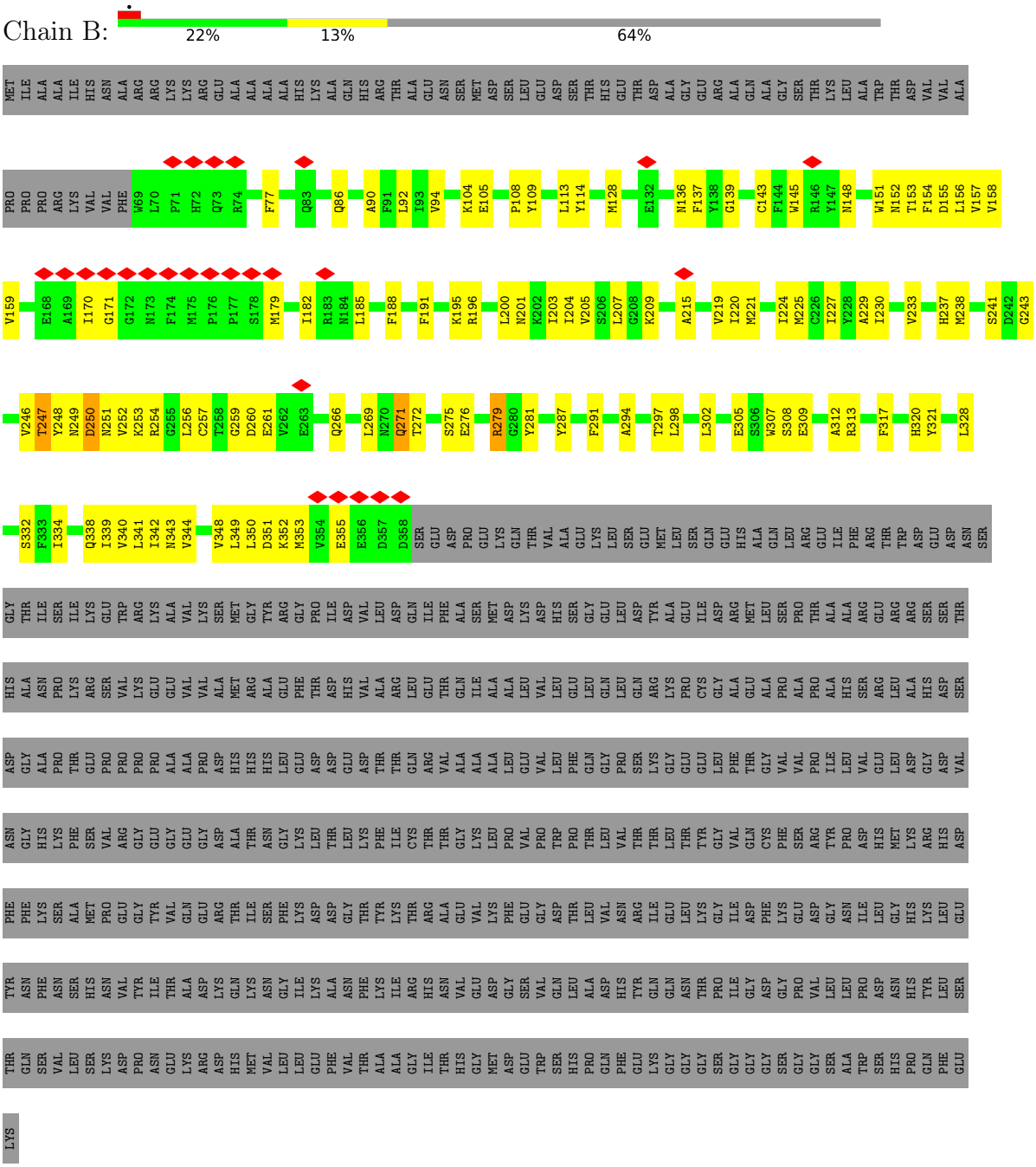
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: ion channel,GFP-TwinStrep



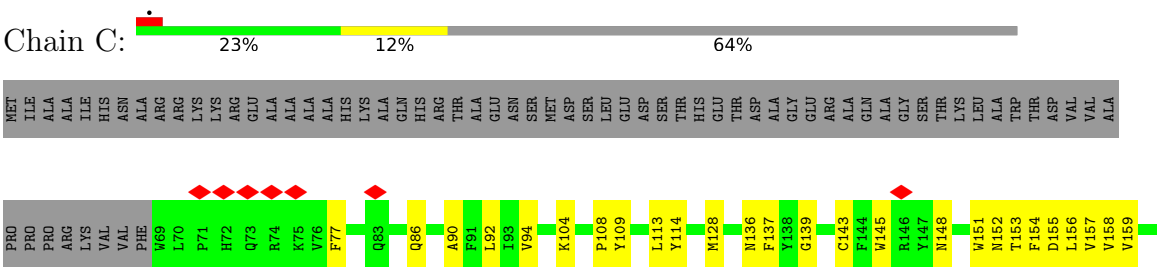
• Molecule 1: ion channel,GFP-TwinStrep

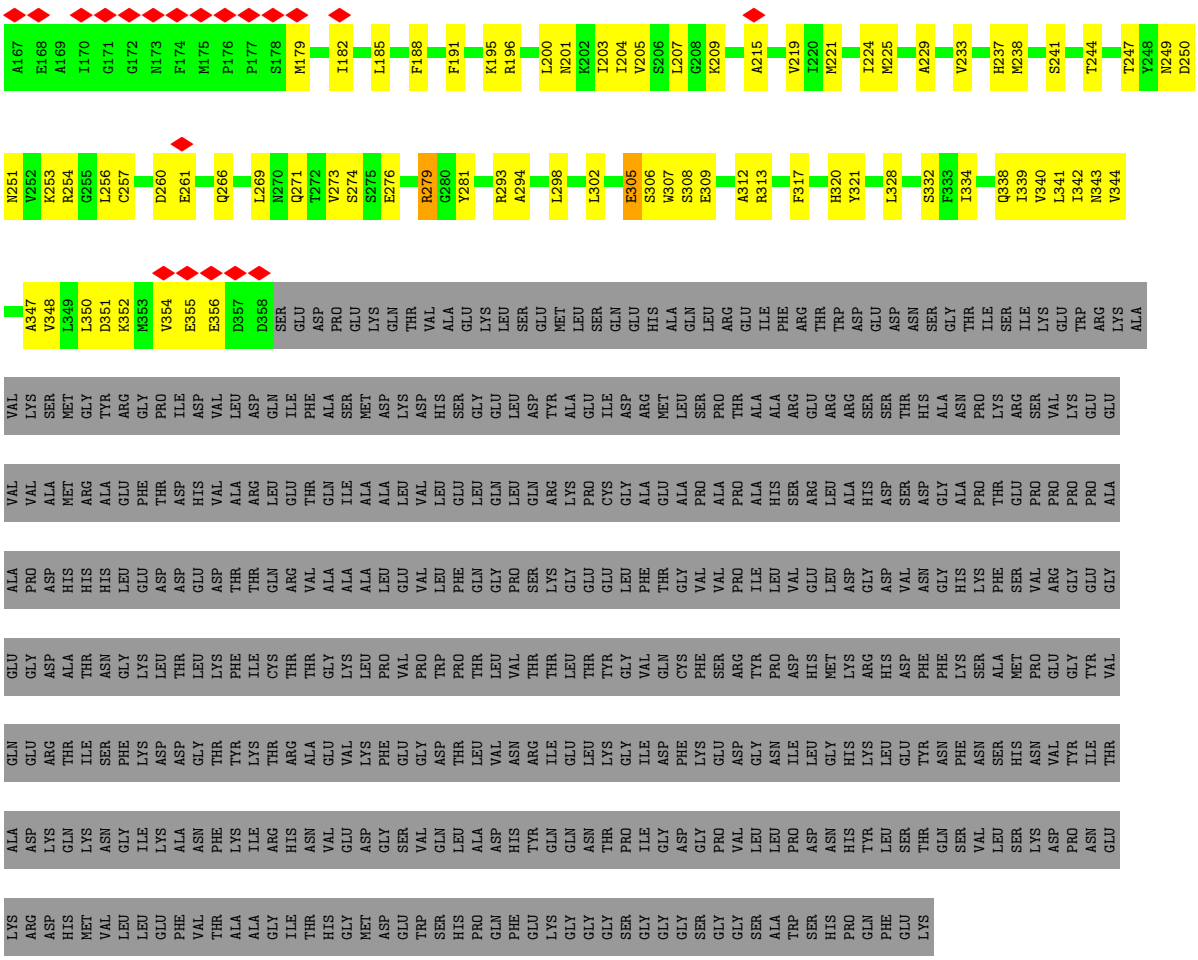
Chain B:



• Molecule 1: ion channel,GFP-TwinStrep

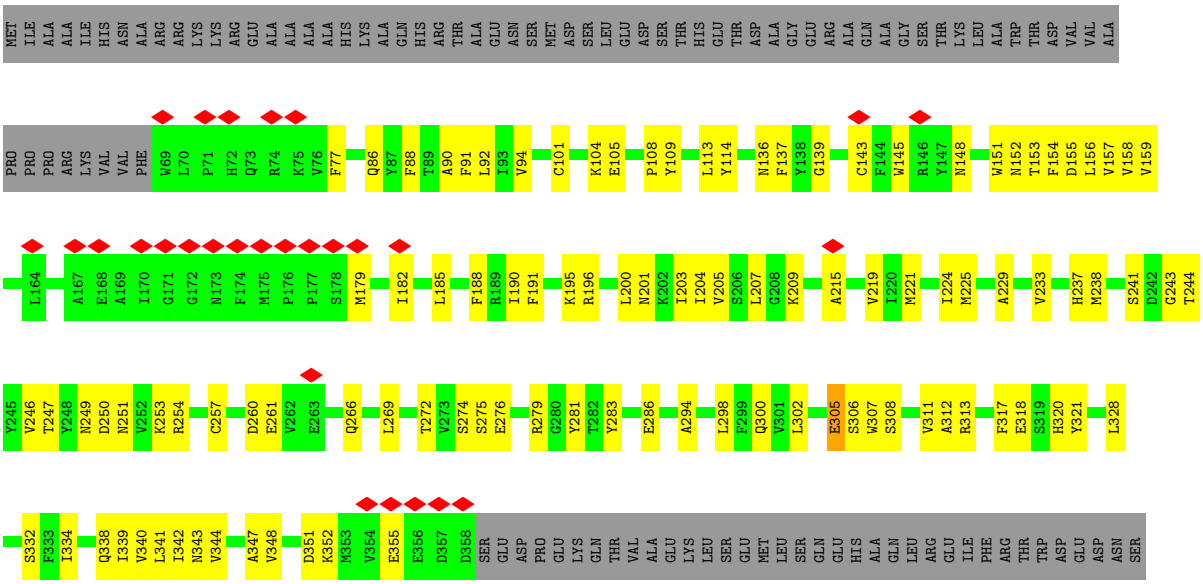
Chain C:





• Molecule 1: ion channel,GFP-TwinStrep

Chain D:



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

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

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

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

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

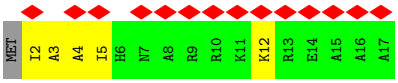
TYR ASN PHE ASN SER HIS ASN VAL TYR ILE THR ALA ASP LYS GLN LYS ASN GLY ILE LYS ALA ASN PHE LYS ILE ARG HIS ASN VAL GLU ASP GLY SER VAL GLN LEU ALA ASP HIS TYR GLN GLN ASN THR PRO ILE GLY ASP GLY PRO VAL LEU LEU PRO ASP ASN HIS TYR LEU SER

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

LYS

- Molecule 2: ion channel

Chain E:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61065	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 ($e^-/Å^2$)	60.0	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.044	Depositor
Minimum map value	-3.520	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.109	Depositor
Recommended contour level	0.56	Depositor
Map size (Å)	266.24, 266.24, 266.24	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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	0.39	0/2411	0.50	1/3278 (0.0%)
1	B	0.39	0/2411	0.49	1/3278 (0.0%)
1	C	0.39	0/2411	0.50	1/3278 (0.0%)
1	D	0.42	0/2411	0.49	1/3278 (0.0%)
2	E	0.32	0/124	0.45	0/163
All	All	0.39	0/9768	0.50	4/13275 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	260	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	260	ASP	CB-CG-OD2	5.19	122.97	118.30
1	D	260	ASP	CB-CG-OD2	5.16	122.94	118.30
1	C	260	ASP	CB-CG-OD2	5.12	122.91	118.30

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	2345	0	2286	111	0
1	B	2345	0	2286	102	0
1	C	2345	0	2286	105	0
1	D	2345	0	2286	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	124	0	135	11	0
All	All	9504	0	9279	357	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 19.

All (357) 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:279:ARG:HH21	1:C:313:ARG:HD3	0.99	1.08
1:A:279:ARG:NH2	1:C:313:ARG:HD3	1.72	1.04
1:B:313:ARG:HD3	1:D:279:ARG:NH2	1.76	1.01
1:A:237:HIS:O	1:C:254:ARG:NH2	1.93	1.00
1:A:279:ARG:HG3	1:A:286:GLU:OE2	1.62	1.00
1:A:347:ALA:HA	2:E:4:ALA:HB1	1.46	0.98
1:C:279:ARG:HH12	1:D:313:ARG:HD3	1.26	0.98
1:A:249:ASN:OD1	1:A:271:GLN:NE2	1.98	0.96
1:B:313:ARG:HD3	1:D:279:ARG:HH21	1.28	0.96
1:B:109:TYR:OH	1:C:253:LYS:HE2	1.67	0.92
1:A:253:LYS:HD3	1:D:109:TYR:OH	1.69	0.91
1:A:247:THR:OG1	1:A:271:GLN:OE1	1.89	0.89
1:B:251:ASN:HB3	1:B:257:CYS:SG	2.12	0.89
1:A:320:HIS:CE1	1:A:321:TYR:CZ	2.61	0.89
1:C:247:THR:HG22	1:C:317:PHE:O	1.73	0.89
1:B:113:LEU:HD11	1:C:253:LYS:HE3	1.56	0.87
1:C:251:ASN:HB3	1:C:257:CYS:SG	2.17	0.84
1:A:203:ILE:O	1:A:207:LEU:HD13	1.78	0.84
1:B:203:ILE:O	1:B:207:LEU:HD13	1.78	0.83
1:C:279:ARG:NH1	1:D:313:ARG:HB3	1.93	0.83
1:A:109:TYR:OH	1:D:253:LYS:HE3	1.78	0.83
1:C:203:ILE:O	1:C:207:LEU:HD13	1.78	0.83
1:D:203:ILE:O	1:D:207:LEU:HD13	1.78	0.82
1:B:109:TYR:CZ	1:C:253:LYS:HE2	2.14	0.82
1:C:279:ARG:NH1	1:D:313:ARG:CB	2.42	0.82
1:C:347:ALA:HA	2:E:5:ILE:HD13	1.62	0.81
1:B:253:LYS:HE2	1:C:113:LEU:HD11	1.63	0.81
1:C:320:HIS:CE1	1:C:321:TYR:CZ	2.70	0.80
1:D:320:HIS:CE1	1:D:321:TYR:CZ	2.70	0.80
1:B:320:HIS:CE1	1:B:321:TYR:CZ	2.70	0.79
1:D:279:ARG:HG3	1:D:286:GLU:OE2	1.83	0.79
1:C:179:MET:O	1:C:182:ILE:HG22	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:MET:O	1:D:182:ILE:HG22	1.84	0.78
1:C:250:ASP:O	1:C:254:ARG:HG3	1.84	0.78
1:A:179:MET:O	1:A:182:ILE:HG22	1.84	0.77
1:A:158:VAL:O	1:A:161:ILE:HG22	1.84	0.77
1:A:251:ASN:HB3	1:A:257:CYS:SG	2.24	0.76
1:B:179:MET:O	1:B:182:ILE:HG22	1.84	0.76
1:C:261:GLU:HG2	1:C:266:GLN:OE1	1.86	0.76
1:D:251:ASN:HB3	1:D:257:CYS:SG	2.26	0.76
1:A:261:GLU:HG2	1:A:266:GLN:OE1	1.86	0.76
1:C:320:HIS:NE2	1:C:321:TYR:CE1	2.54	0.76
1:B:320:HIS:NE2	1:B:321:TYR:CE1	2.54	0.76
1:D:261:GLU:HG2	1:D:266:GLN:OE1	1.85	0.76
1:B:261:GLU:HG2	1:B:266:GLN:OE1	1.86	0.75
1:D:320:HIS:NE2	1:D:321:TYR:CE1	2.54	0.75
1:C:281:TYR:OH	1:D:247:THR:HG22	1.87	0.75
1:A:109:TYR:OH	1:D:253:LYS:CE	2.35	0.74
1:A:279:ARG:NH2	1:C:309:GLU:OE1	2.20	0.73
1:B:291:PHE:HB3	1:D:105:GLU:HB2	1.71	0.73
1:A:109:TYR:CZ	1:D:253:LYS:HE3	2.25	0.72
1:C:279:ARG:HH11	1:D:313:ARG:HB3	1.53	0.72
1:B:109:TYR:CE2	1:C:253:LYS:HE2	2.25	0.70
1:D:250:ASP:O	1:D:254:ARG:HG3	1.91	0.70
1:B:109:TYR:CZ	1:C:253:LYS:HG2	2.28	0.69
1:B:253:LYS:HG2	1:C:109:TYR:CZ	2.26	0.69
1:C:249:ASN:HB2	1:C:269:LEU:HA	1.72	0.69
1:B:334:ILE:HG23	1:B:338:GLN:OE1	1.93	0.69
1:C:279:ARG:HH12	1:D:313:ARG:CD	2.05	0.69
1:D:334:ILE:HG23	1:D:338:GLN:OE1	1.93	0.68
1:A:334:ILE:HG23	1:A:338:GLN:OE1	1.93	0.68
1:A:313:ARG:HD3	1:B:279:ARG:HH21	1.58	0.68
1:C:281:TYR:OH	1:D:247:THR:CG2	2.41	0.67
1:C:334:ILE:HG23	1:C:338:GLN:OE1	1.93	0.67
1:A:245:TYR:HB2	1:A:318:GLU:HG2	1.75	0.67
1:A:249:ASN:ND2	1:A:269:LEU:HA	2.10	0.66
1:D:88:PHE:O	1:D:92:LEU:HD23	1.95	0.66
1:C:249:ASN:HB2	1:C:269:LEU:CA	2.25	0.66
1:A:250:ASP:O	1:A:254:ARG:HG3	1.95	0.66
1:A:170:ILE:HG23	1:A:171:GLY:N	2.10	0.66
1:B:170:ILE:HG23	1:B:171:GLY:N	2.10	0.65
1:B:247:THR:HG22	1:B:317:PHE:O	1.96	0.65
1:B:224:ILE:HD12	1:B:341:LEU:HD11	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:HIS:CE1	1:A:321:TYR:CE2	2.86	0.64
1:C:279:ARG:HH12	1:D:313:ARG:CB	2.10	0.64
1:A:253:LYS:HD3	1:D:109:TYR:CZ	2.33	0.64
1:C:224:ILE:HD12	1:C:341:LEU:HD11	1.78	0.64
1:A:224:ILE:HD12	1:A:341:LEU:HD11	1.78	0.63
1:D:224:ILE:HD12	1:D:341:LEU:HD11	1.78	0.63
1:A:161:ILE:CD1	1:A:182:ILE:HG13	2.27	0.63
1:A:248:TYR:HA	1:A:269:LEU:O	1.99	0.62
1:A:86:GLN:OE1	1:A:196:ARG:NH1	2.33	0.62
1:C:205:VAL:HG12	1:C:209:LYS:HD2	1.81	0.62
1:A:205:VAL:HG12	1:A:209:LYS:HD2	1.81	0.62
1:C:86:GLN:OE1	1:C:196:ARG:NH1	2.33	0.62
1:D:205:VAL:HG12	1:D:209:LYS:HD2	1.81	0.61
1:B:86:GLN:OE1	1:B:196:ARG:NH1	2.33	0.61
1:B:109:TYR:CE2	1:C:253:LYS:HG2	2.35	0.61
1:A:317:PHE:CD1	1:B:281:TYR:HE2	2.19	0.61
1:B:348:VAL:O	1:B:352:LYS:HG2	2.00	0.61
1:D:86:GLN:OE1	1:D:196:ARG:NH1	2.33	0.61
1:A:313:ARG:HD3	1:B:279:ARG:NH2	2.15	0.61
1:B:205:VAL:HG12	1:B:209:LYS:HD2	1.80	0.60
1:B:250:ASP:HB2	1:B:254:ARG:HG3	1.81	0.60
1:A:279:ARG:HE	1:C:313:ARG:HB3	1.66	0.60
1:B:251:ASN:CB	1:B:257:CYS:SG	2.89	0.60
1:A:328:LEU:O	1:A:332:SER:OG	2.16	0.60
1:A:279:ARG:CG	1:A:286:GLU:OE2	2.44	0.60
1:D:279:ARG:CG	1:D:286:GLU:OE2	2.50	0.59
1:C:201:ASN:O	1:C:205:VAL:HG23	2.03	0.59
1:C:279:ARG:NH1	1:D:313:ARG:HB2	2.15	0.59
1:C:279:ARG:NH1	1:D:313:ARG:HD3	2.08	0.59
1:A:201:ASN:O	1:A:205:VAL:HG23	2.03	0.58
1:D:201:ASN:O	1:D:205:VAL:HG23	2.03	0.58
1:B:252:VAL:HA	1:B:257:CYS:O	2.04	0.58
1:B:328:LEU:O	1:B:332:SER:OG	2.16	0.57
1:A:109:TYR:CE2	1:D:253:LYS:HE3	2.39	0.57
1:B:201:ASN:O	1:B:205:VAL:HG23	2.03	0.57
1:C:328:LEU:O	1:C:332:SER:OG	2.16	0.57
1:D:91:PHE:HD1	1:D:92:LEU:HD22	1.68	0.57
1:B:249:ASN:OD1	1:B:269:LEU:HA	2.05	0.57
1:C:244:THR:HG22	1:C:274:SER:HA	1.86	0.57
1:C:249:ASN:OD1	1:C:271:GLN:NE2	2.38	0.57
1:D:91:PHE:CD1	1:D:92:LEU:HD22	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ILE:O	1:A:207:LEU:CD1	2.53	0.56
1:B:203:ILE:O	1:B:207:LEU:CD1	2.53	0.56
1:C:148:ASN:OD1	1:C:151:TRP:HB2	2.06	0.56
1:A:348:VAL:O	1:A:352:LYS:HG2	2.06	0.56
1:B:248:TYR:HA	1:B:269:LEU:O	2.05	0.56
1:D:148:ASN:OD1	1:D:151:TRP:HB2	2.06	0.56
1:C:92:LEU:HD21	1:C:128:MET:SD	2.46	0.56
1:A:253:LYS:HE2	1:D:113:LEU:HD11	1.87	0.55
1:A:109:TYR:CZ	1:D:253:LYS:HG2	2.41	0.55
1:C:351:ASP:O	1:C:355:GLU:HG3	2.07	0.55
1:C:148:ASN:O	1:C:152:ASN:ND2	2.38	0.55
1:A:351:ASP:O	1:A:355:GLU:HG3	2.07	0.55
1:D:320:HIS:CE1	1:D:321:TYR:CE1	2.95	0.54
1:A:148:ASN:OD1	1:A:151:TRP:HB2	2.06	0.54
1:A:155:ASP:O	1:A:159:VAL:HG23	2.07	0.54
1:A:354:VAL:CG1	2:E:12:LYS:HD3	2.37	0.54
1:B:148:ASN:O	1:B:152:ASN:ND2	2.38	0.54
1:B:148:ASN:OD1	1:B:151:TRP:HB2	2.06	0.54
1:B:302:LEU:HG	1:B:342:ILE:HD11	1.90	0.54
1:B:113:LEU:CD1	1:C:253:LYS:HE3	2.34	0.54
1:D:351:ASP:O	1:D:355:GLU:HG3	2.07	0.54
1:C:155:ASP:O	1:C:159:VAL:HG23	2.07	0.54
1:B:351:ASP:O	1:B:355:GLU:HG3	2.07	0.54
1:A:281:TYR:HE2	1:C:317:PHE:CD1	2.25	0.54
1:D:302:LEU:HG	1:D:342:ILE:HD11	1.90	0.54
1:B:155:ASP:O	1:B:159:VAL:HG23	2.07	0.54
1:B:320:HIS:CE1	1:B:321:TYR:CE1	2.95	0.54
1:A:254:ARG:NH2	1:B:237:HIS:O	2.40	0.53
1:D:328:LEU:O	1:D:332:SER:OG	2.16	0.53
1:A:302:LEU:HG	1:A:342:ILE:HD11	1.90	0.53
1:B:227:ILE:HD11	1:D:190:ILE:CG2	2.38	0.53
1:A:347:ALA:HA	2:E:4:ALA:CB	2.29	0.53
1:C:77:PHE:HB2	1:C:139:GLY:O	2.08	0.53
1:B:253:LYS:CE	1:C:113:LEU:HD11	2.36	0.53
1:C:302:LEU:HG	1:C:342:ILE:HD11	1.90	0.53
1:D:155:ASP:O	1:D:159:VAL:HG23	2.07	0.53
1:D:249:ASN:OD1	1:D:269:LEU:HA	2.09	0.53
1:A:77:PHE:HB2	1:A:139:GLY:O	2.09	0.53
1:A:314:PRO:O	1:A:318:GLU:HB2	2.08	0.53
1:D:237:HIS:CD2	1:D:238:MET:HG2	2.45	0.53
1:D:203:ILE:O	1:D:207:LEU:CD1	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:PHE:HB2	1:D:139:GLY:O	2.08	0.52
1:B:237:HIS:CD2	1:B:238:MET:HG2	2.44	0.52
1:A:245:TYR:HB2	1:A:318:GLU:CG	2.40	0.52
1:A:317:PHE:CD1	1:B:281:TYR:CE2	2.97	0.52
1:A:161:ILE:HD13	1:A:182:ILE:HG13	1.90	0.52
1:A:237:HIS:CD2	1:A:238:MET:HG2	2.44	0.52
1:C:229:ALA:O	1:C:233:VAL:HG23	2.10	0.52
1:C:215:ALA:O	1:C:219:VAL:HG23	2.10	0.52
1:C:237:HIS:CD2	1:C:238:MET:HG2	2.44	0.52
1:A:92:LEU:HD21	1:A:128:MET:SD	2.50	0.52
1:A:229:ALA:O	1:A:233:VAL:HG23	2.10	0.52
1:D:229:ALA:O	1:D:233:VAL:HG23	2.10	0.52
1:B:215:ALA:O	1:B:219:VAL:HG23	2.10	0.52
1:B:229:ALA:O	1:B:233:VAL:HG23	2.10	0.51
1:D:238:MET:O	1:D:241:SER:OG	2.28	0.51
1:A:215:ALA:O	1:A:219:VAL:HG23	2.11	0.51
1:D:247:THR:HG23	1:D:317:PHE:O	2.10	0.51
1:A:354:VAL:HG12	2:E:12:LYS:HD3	1.92	0.51
1:C:320:HIS:CE1	1:C:321:TYR:CE1	2.95	0.51
1:C:203:ILE:O	1:C:207:LEU:CD1	2.53	0.51
1:C:293:ARG:HE	1:D:317:PHE:HE1	1.58	0.51
1:C:238:MET:O	1:C:241:SER:OG	2.28	0.51
1:D:276:GLU:HA	1:D:281:TYR:O	2.11	0.51
1:A:238:MET:O	1:A:241:SER:OG	2.28	0.51
1:D:215:ALA:O	1:D:219:VAL:HG23	2.10	0.51
1:D:244:THR:HG22	1:D:274:SER:HA	1.93	0.51
1:A:158:VAL:O	1:A:161:ILE:CG2	2.57	0.50
1:B:238:MET:O	1:B:241:SER:OG	2.28	0.50
1:B:276:GLU:HA	1:B:281:TYR:O	2.11	0.50
1:C:347:ALA:HA	2:E:5:ILE:CD1	2.38	0.50
1:A:340:VAL:O	1:A:344:VAL:HG23	2.11	0.50
1:D:340:VAL:O	1:D:344:VAL:HG23	2.11	0.50
1:D:348:VAL:O	1:D:352:LYS:HG2	2.12	0.50
1:A:109:TYR:OH	1:D:253:LYS:HE2	2.11	0.50
1:D:148:ASN:O	1:D:152:ASN:ND2	2.38	0.50
1:D:185:LEU:HG	1:D:185:LEU:O	2.11	0.50
1:B:340:VAL:O	1:B:344:VAL:HG23	2.11	0.50
1:C:276:GLU:HA	1:C:281:TYR:O	2.11	0.50
1:C:340:VAL:O	1:C:344:VAL:HG23	2.11	0.50
1:A:148:ASN:O	1:A:152:ASN:ND2	2.38	0.50
1:B:320:HIS:CD2	1:B:321:TYR:CE1	3.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:GLU:HA	1:A:281:TYR:O	2.11	0.49
1:A:320:HIS:CE1	1:A:321:TYR:OH	2.65	0.49
1:B:153:THR:O	1:B:157:VAL:HG23	2.12	0.49
1:C:185:LEU:O	1:C:185:LEU:HG	2.11	0.49
1:C:320:HIS:CD2	1:C:321:TYR:CE1	3.00	0.49
1:C:348:VAL:O	1:C:352:LYS:HG2	2.12	0.49
1:D:153:THR:O	1:D:157:VAL:HG23	2.12	0.49
1:D:305:GLU:OE1	1:D:306:SER:OG	2.21	0.49
1:A:153:THR:O	1:A:157:VAL:HG23	2.12	0.49
1:C:153:THR:O	1:C:157:VAL:HG23	2.12	0.49
1:B:185:LEU:O	1:B:185:LEU:HG	2.11	0.49
1:B:339:ILE:O	1:B:343:ASN:ND2	2.46	0.49
1:D:339:ILE:O	1:D:343:ASN:ND2	2.46	0.49
1:A:281:TYR:CE2	1:C:317:PHE:CD1	3.00	0.49
1:A:185:LEU:HG	1:A:185:LEU:O	2.11	0.49
1:B:109:TYR:CE2	1:C:253:LYS:CE	2.95	0.49
1:A:339:ILE:O	1:A:343:ASN:ND2	2.46	0.49
1:B:250:ASP:HB3	1:B:253:LYS:HB3	1.94	0.49
1:D:320:HIS:CD2	1:D:321:TYR:CE1	3.00	0.49
1:B:230:ILE:HD11	1:D:101:CYS:SG	2.53	0.48
1:C:339:ILE:O	1:C:343:ASN:ND2	2.46	0.48
1:D:246:VAL:HG22	1:D:272:THR:HG22	1.95	0.48
1:A:109:TYR:HH	1:D:253:LYS:HE3	1.75	0.48
1:A:221:MET:O	1:A:225:MET:HG3	2.13	0.48
1:D:221:MET:O	1:D:225:MET:HG3	2.13	0.48
1:A:305:GLU:HG3	1:C:307:TRP:CD1	2.49	0.48
1:B:221:MET:O	1:B:225:MET:HG3	2.13	0.48
1:C:221:MET:O	1:C:225:MET:HG3	2.13	0.48
1:B:308:SER:HA	1:B:312:ALA:HB3	1.96	0.48
1:A:241:SER:HB3	1:C:256:LEU:HD21	1.95	0.47
1:B:249:ASN:ND2	1:B:271:GLN:HE21	2.12	0.47
1:B:334:ILE:O	1:B:338:GLN:HB3	2.14	0.47
1:D:104:LYS:HA	1:D:104:LYS:HD3	1.59	0.47
1:D:308:SER:HA	1:D:312:ALA:HB3	1.96	0.47
1:B:151:TRP:CE2	1:B:195:LYS:HB2	2.50	0.47
1:D:151:TRP:CE2	1:D:195:LYS:HB2	2.50	0.47
1:C:308:SER:HA	1:C:312:ALA:HB3	1.96	0.47
1:C:334:ILE:O	1:C:338:GLN:HB3	2.14	0.47
1:A:151:TRP:CE2	1:A:195:LYS:HB2	2.50	0.47
1:B:350:LEU:HD12	2:E:3:ALA:HB3	1.96	0.47
1:D:136:ASN:ND2	1:D:152:ASN:OD1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:ILE:O	1:D:338:GLN:HB3	2.14	0.47
1:A:308:SER:HA	1:A:312:ALA:HB3	1.96	0.46
1:A:334:ILE:O	1:A:338:GLN:HB3	2.14	0.46
1:A:109:TYR:CE2	1:D:253:LYS:HG2	2.51	0.46
1:B:77:PHE:HB2	1:B:139:GLY:O	2.16	0.46
1:B:246:VAL:HG12	1:B:272:THR:HG22	1.98	0.46
1:C:151:TRP:CE2	1:C:195:LYS:HB2	2.50	0.46
1:C:279:ARG:HH11	1:D:313:ARG:CB	2.15	0.46
1:D:88:PHE:CZ	1:D:92:LEU:HD21	2.51	0.46
1:C:261:GLU:HB3	1:C:266:GLN:HB2	1.98	0.46
1:A:170:ILE:CG2	1:A:171:GLY:N	2.78	0.46
1:B:261:GLU:HB3	1:B:266:GLN:HB2	1.98	0.46
1:C:137:PHE:HE1	1:C:156:LEU:HD12	1.81	0.46
1:C:350:LEU:HD11	2:E:2:ILE:HG21	1.97	0.46
1:D:261:GLU:HB3	1:D:266:GLN:HB2	1.98	0.46
1:A:307:TRP:CD2	1:A:334:ILE:HD11	2.51	0.45
1:C:104:LYS:HA	1:C:104:LYS:HD3	1.63	0.45
1:D:307:TRP:CD2	1:D:334:ILE:HD11	2.51	0.45
1:A:233:VAL:O	1:A:237:HIS:HB3	2.17	0.45
1:A:261:GLU:HB3	1:A:266:GLN:HB2	1.98	0.45
1:B:137:PHE:HE1	1:B:156:LEU:HD12	1.81	0.45
1:B:136:ASN:ND2	1:B:152:ASN:OD1	2.48	0.45
1:B:170:ILE:CG2	1:B:171:GLY:N	2.78	0.45
1:D:233:VAL:O	1:D:237:HIS:HB3	2.17	0.45
1:A:136:ASN:ND2	1:A:152:ASN:OD1	2.48	0.45
1:C:294:ALA:O	1:C:298:LEU:HG	2.17	0.45
1:B:313:ARG:CB	1:D:279:ARG:HH21	2.30	0.45
1:A:104:LYS:HA	1:A:104:LYS:HD3	1.63	0.45
1:B:307:TRP:CD2	1:B:334:ILE:HD11	2.51	0.45
1:D:137:PHE:HE1	1:D:156:LEU:HD12	1.81	0.45
1:C:305:GLU:CD	1:D:306:SER:HA	2.37	0.45
1:C:307:TRP:CD2	1:C:334:ILE:HD11	2.51	0.45
1:A:137:PHE:HE1	1:A:156:LEU:HD12	1.81	0.45
1:A:294:ALA:O	1:A:298:LEU:HG	2.17	0.45
1:B:294:ALA:O	1:B:298:LEU:HG	2.17	0.45
1:A:256:LEU:HD21	1:B:241:SER:HB3	1.99	0.44
1:B:233:VAL:O	1:B:237:HIS:HB3	2.17	0.44
1:B:338:GLN:O	1:B:342:ILE:HB	2.17	0.44
1:C:233:VAL:O	1:C:237:HIS:HB3	2.16	0.44
1:B:249:ASN:HD22	1:B:271:GLN:HE21	1.64	0.44
1:B:254:ARG:NH2	1:D:237:HIS:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:GLN:O	1:C:342:ILE:HB	2.17	0.44
1:D:338:GLN:O	1:D:342:ILE:HB	2.17	0.44
1:D:347:ALA:HA	2:E:2:ILE:HD11	1.99	0.44
1:A:185:LEU:HD12	1:A:188:PHE:CD2	2.53	0.44
1:B:309:GLU:HG2	1:D:305:GLU:OE2	2.17	0.44
1:D:185:LEU:HD12	1:D:188:PHE:CD2	2.53	0.44
1:D:294:ALA:O	1:D:298:LEU:HG	2.17	0.44
1:B:104:LYS:HA	1:B:104:LYS:HD3	1.63	0.44
1:C:185:LEU:HD12	1:C:188:PHE:CD2	2.53	0.44
1:C:249:ASN:HB2	1:C:269:LEU:O	2.18	0.44
1:D:320:HIS:NE2	1:D:321:TYR:CZ	2.85	0.44
1:B:256:LEU:HD21	1:D:241:SER:HB3	1.98	0.44
1:A:249:ASN:N	1:A:269:LEU:O	2.48	0.43
1:A:338:GLN:O	1:A:342:ILE:HB	2.17	0.43
1:B:185:LEU:HD12	1:B:188:PHE:CD2	2.53	0.43
1:B:252:VAL:HG21	1:B:259:GLY:CA	2.48	0.43
1:C:320:HIS:NE2	1:C:321:TYR:CZ	2.84	0.43
1:B:143:CYS:O	1:B:145:TRP:CE3	2.71	0.43
1:A:286:GLU:HG2	1:C:313:ARG:HH21	1.84	0.43
1:C:154:PHE:O	1:C:158:VAL:HG22	2.19	0.43
1:B:154:PHE:O	1:B:158:VAL:HG22	2.19	0.43
1:C:136:ASN:ND2	1:C:152:ASN:OD1	2.48	0.43
1:D:154:PHE:O	1:D:158:VAL:HG22	2.19	0.43
1:A:143:CYS:O	1:A:145:TRP:CE3	2.72	0.43
1:B:220:ILE:HD11	1:D:200:LEU:HA	2.00	0.43
1:B:221:MET:HA	1:B:341:LEU:HD13	2.00	0.43
1:D:143:CYS:O	1:D:145:TRP:CE3	2.72	0.43
1:A:170:ILE:HG23	1:A:171:GLY:H	1.83	0.43
1:A:305:GLU:OE1	1:A:306:SER:OG	2.21	0.43
1:A:350:LEU:HD13	2:E:5:ILE:HG12	2.01	0.43
1:C:143:CYS:O	1:C:145:TRP:CE3	2.71	0.43
1:C:305:GLU:OE1	1:C:306:SER:OG	2.21	0.43
1:B:287:TYR:O	1:B:297:THR:OG1	2.27	0.43
1:A:161:ILE:HD11	1:A:182:ILE:HG13	2.01	0.42
1:A:154:PHE:O	1:A:158:VAL:HG22	2.19	0.42
1:A:188:PHE:HD1	1:A:191:PHE:HE2	1.67	0.42
1:D:283:TYR:OH	1:D:311:VAL:O	2.33	0.42
1:C:188:PHE:HD1	1:C:191:PHE:HE2	1.67	0.42
1:C:281:TYR:CZ	1:D:247:THR:CG2	3.02	0.42
1:D:188:PHE:HD1	1:D:191:PHE:HE2	1.67	0.42
1:D:221:MET:HA	1:D:341:LEU:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:PHE:HD1	1:B:191:PHE:HE2	1.68	0.42
1:D:243:GLY:O	1:D:275:SER:N	2.42	0.42
1:C:221:MET:HA	1:C:341:LEU:HD13	2.00	0.42
1:B:243:GLY:O	1:B:275:SER:N	2.42	0.42
1:B:108:PRO:HD2	1:B:109:TYR:CE2	2.55	0.42
1:A:221:MET:HA	1:A:341:LEU:HD13	2.00	0.42
1:A:349:LEU:HG	1:A:353:MET:HE3	2.02	0.42
1:B:250:ASP:O	1:B:254:ARG:HG3	2.19	0.42
1:B:279:ARG:HD3	1:B:279:ARG:N	2.35	0.42
1:A:109:TYR:CZ	1:D:253:LYS:CE	3.00	0.41
1:B:92:LEU:HD21	1:B:128:MET:SD	2.60	0.41
1:B:349:LEU:HG	1:B:353:MET:HE3	2.02	0.41
1:A:161:ILE:HD13	1:A:182:ILE:CG1	2.50	0.41
1:D:108:PRO:HD2	1:D:109:TYR:CE2	2.55	0.41
1:C:281:TYR:CZ	1:D:247:THR:HG21	2.56	0.41
1:A:278:ALA:O	1:C:273:VAL:HG21	2.20	0.41
1:C:108:PRO:HD2	1:C:109:TYR:CE2	2.55	0.41
1:A:90:ALA:O	1:A:94:VAL:HG23	2.21	0.41
1:A:108:PRO:HD2	1:A:109:TYR:CE2	2.55	0.41
1:A:350:LEU:HD13	2:E:5:ILE:CG1	2.51	0.41
1:B:90:ALA:O	1:B:94:VAL:HG23	2.21	0.41
1:B:170:ILE:HG23	1:B:171:GLY:H	1.83	0.41
1:C:237:HIS:O	1:D:254:ARG:NH2	2.51	0.41
1:A:291:PHE:HB3	1:B:105:GLU:HB2	2.03	0.41
1:C:90:ALA:O	1:C:94:VAL:HG23	2.21	0.41
1:D:90:ALA:O	1:D:94:VAL:HG23	2.21	0.41
1:B:200:LEU:O	1:B:204:ILE:HG12	2.21	0.40
1:C:200:LEU:O	1:C:204:ILE:HG12	2.21	0.40
1:B:227:ILE:HD11	1:D:190:ILE:HG21	2.02	0.40
1:B:313:ARG:NH1	1:D:300:GLN:OE1	2.54	0.40
1:C:249:ASN:HB2	1:C:269:LEU:C	2.42	0.40
1:C:350:LEU:O	1:C:354:VAL:HG22	2.21	0.40
1:D:281:TYR:CD2	1:D:286:GLU:HB2	2.57	0.40
1:A:200:LEU:O	1:A:204:ILE:HG12	2.21	0.40
1:D:200:LEU:O	1:D:204:ILE:HG12	2.21	0.40
1:A:113:LEU:HD11	1:D:253:LYS:HD2	2.04	0.40
1:A:233:VAL:O	1:A:237:HIS:ND1	2.55	0.40
1:C:356:GLU:OE2	1:C:356:GLU:HA	2.22	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	288/815 (35%)	273 (95%)	15 (5%)	0	100	100
1	B	288/815 (35%)	270 (94%)	18 (6%)	0	100	100
1	C	288/815 (35%)	272 (94%)	16 (6%)	0	100	100
1	D	288/815 (35%)	271 (94%)	17 (6%)	0	100	100
2	E	14/17 (82%)	14 (100%)	0	0	100	100
All	All	1166/3277 (36%)	1100 (94%)	66 (6%)	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	247/688 (36%)	243 (98%)	4 (2%)	62	81
1	B	247/688 (36%)	241 (98%)	6 (2%)	49	72
1	C	247/688 (36%)	244 (99%)	3 (1%)	71	85
1	D	247/688 (36%)	244 (99%)	3 (1%)	71	85
2	E	10/11 (91%)	10 (100%)	0	100	100
All	All	998/2763 (36%)	982 (98%)	16 (2%)	64	81

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	TYR
1	A	249	ASN
1	A	271	GLN
1	A	305	GLU
1	B	114	TYR
1	B	247	THR
1	B	250	ASP
1	B	271	GLN
1	B	279	ARG
1	B	305	GLU
1	C	114	TYR
1	C	279	ARG
1	C	305	GLU
1	D	114	TYR
1	D	305	GLU
1	D	318	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	184	ASN
1	A	320	HIS
1	A	343	ASN
1	B	115	GLN
1	B	184	ASN
1	B	249	ASN
1	B	320	HIS
1	B	343	ASN
1	C	115	GLN
1	C	184	ASN
1	C	320	HIS
1	C	343	ASN
1	D	73	GLN
1	D	115	GLN
1	D	184	ASN
1	D	320	HIS
1	D	343	ASN

5.3.3 RNA

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.

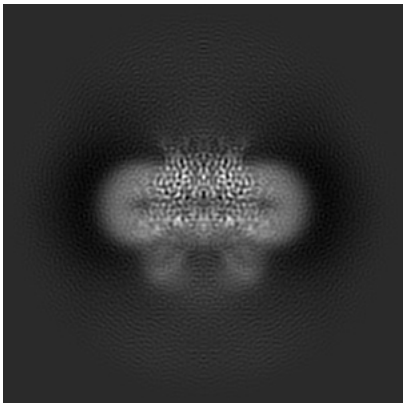
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33016. These allow visual inspection of the internal detail of the map and identification of artifacts.

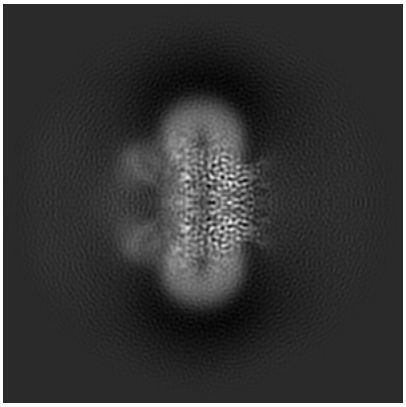
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

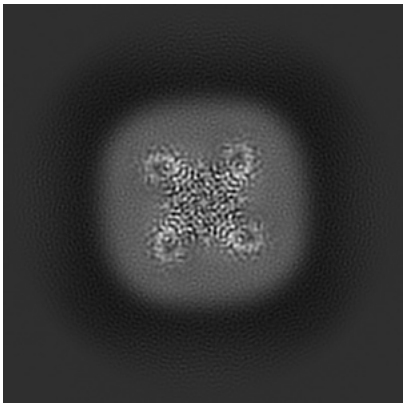
6.1.1 Primary map



X



Y

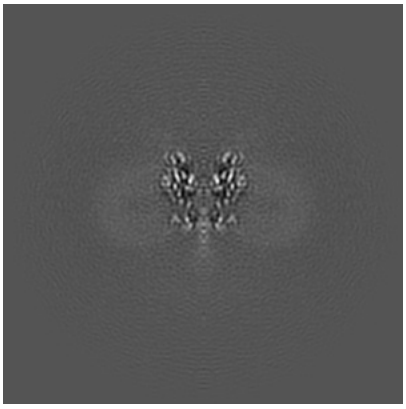


Z

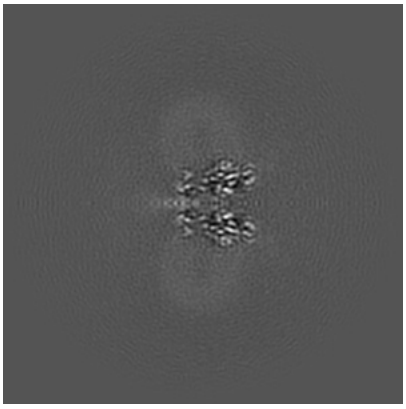
The images above show the map projected in three orthogonal directions.

6.2 Central slices

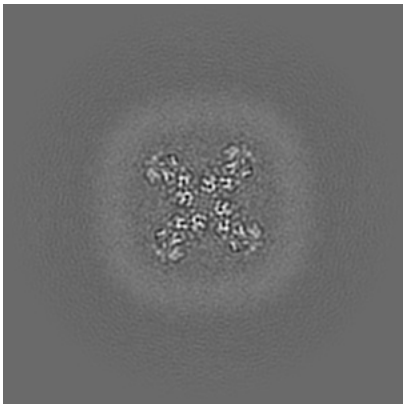
6.2.1 Primary map



X Index: 128



Y Index: 128

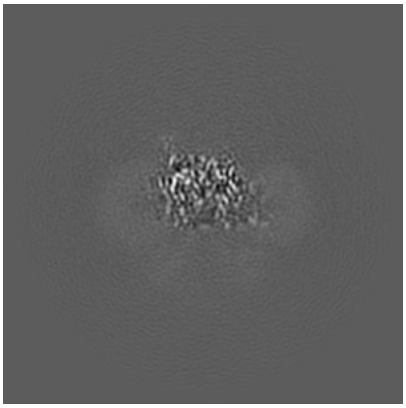


Z Index: 128

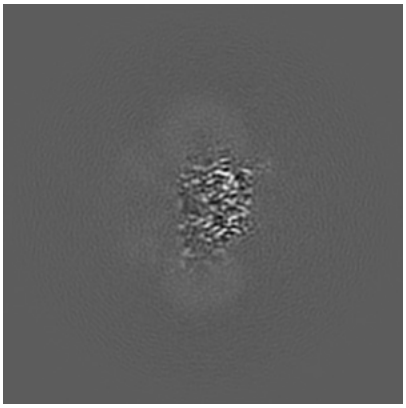
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

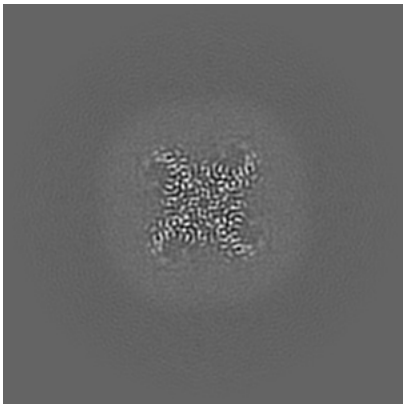
6.3.1 Primary map



X Index: 141



Y Index: 141

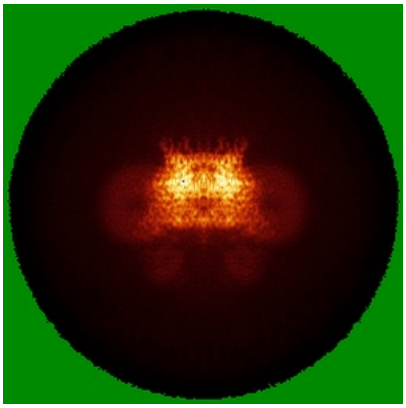


Z Index: 141

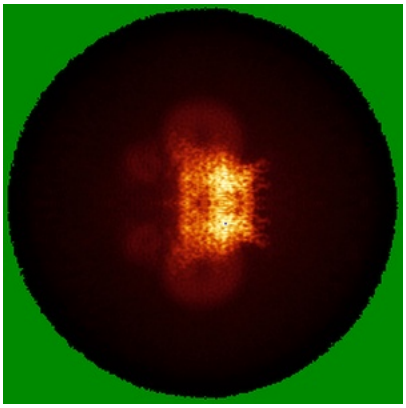
The images above show the largest variance slices of the map in three orthogonal directions.

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

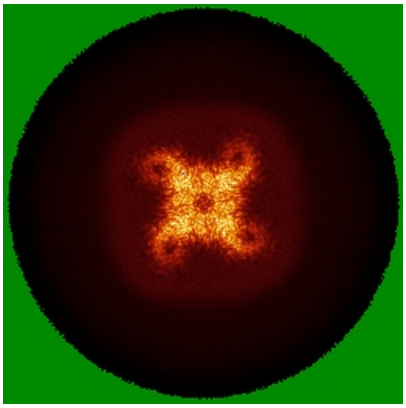
6.4.1 Primary map



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 0.56. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

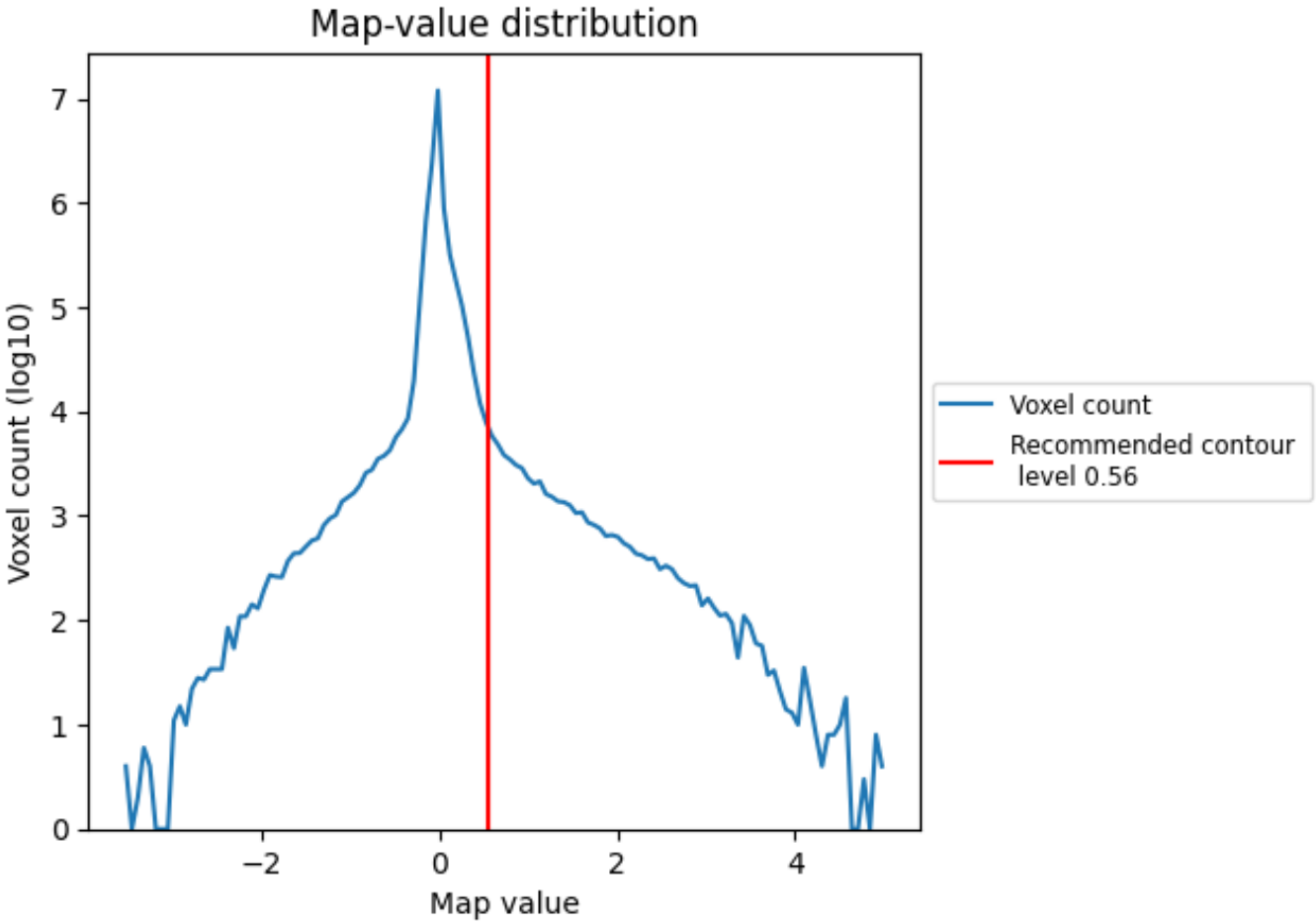
6.6 Mask visualisation (i)

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

7 Map analysis

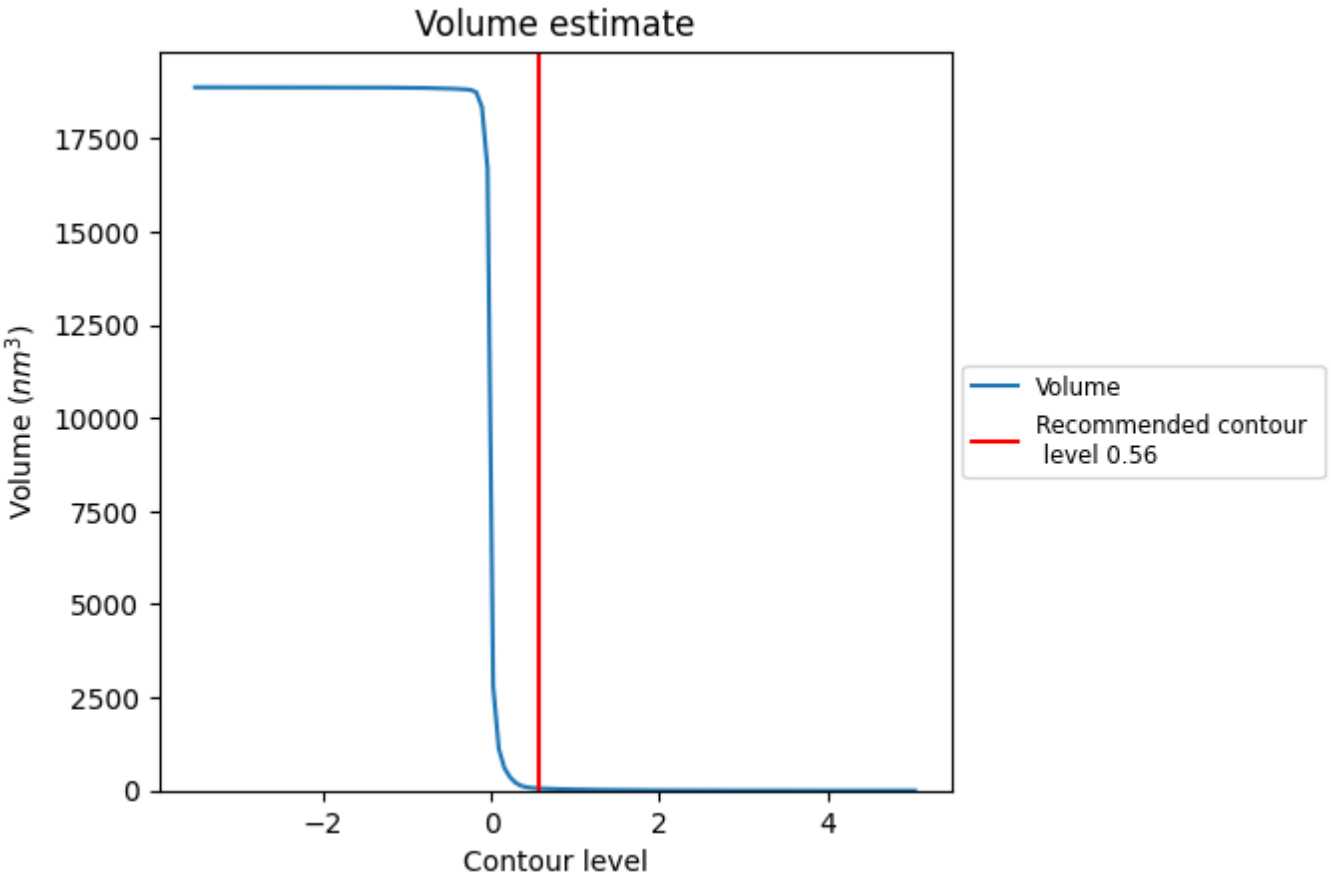
This section contains the results of statistical analysis of the map.

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.

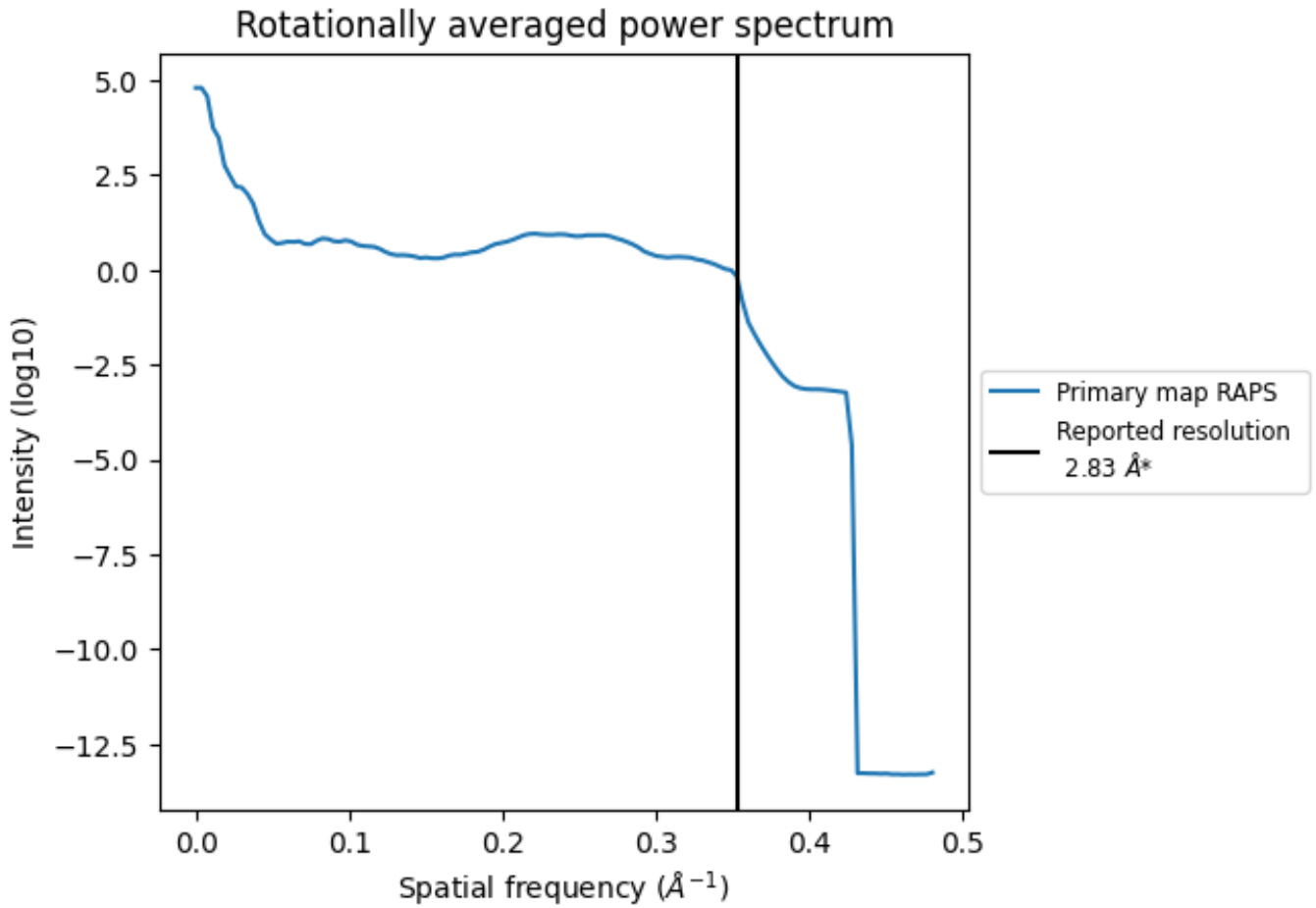
7.2 Volume estimate



The volume at the recommended contour level is 60 nm^3; 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 (i)



*Reported resolution corresponds to spatial frequency of 0.353 $Å^{-1}$

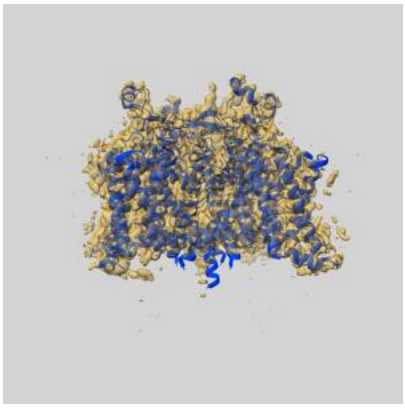
8 Fourier-Shell correlation

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

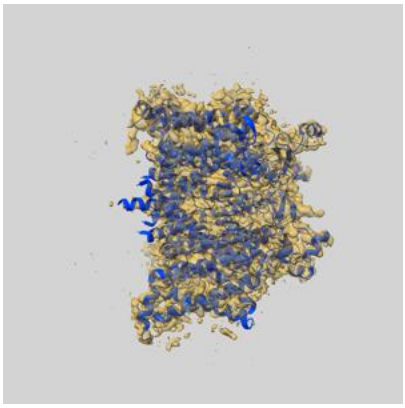
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33016 and PDB model 7X5V. Per-residue inclusion information can be found in section 3 on page 4.

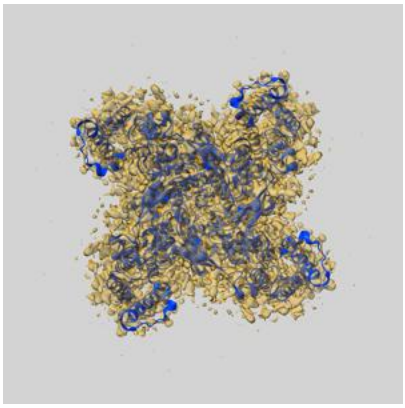
9.1 Map-model overlay



X



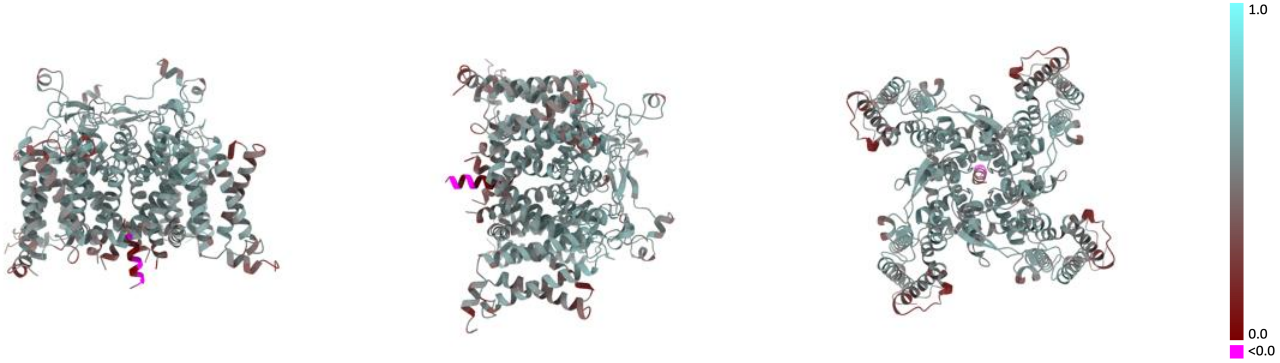
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.56 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.

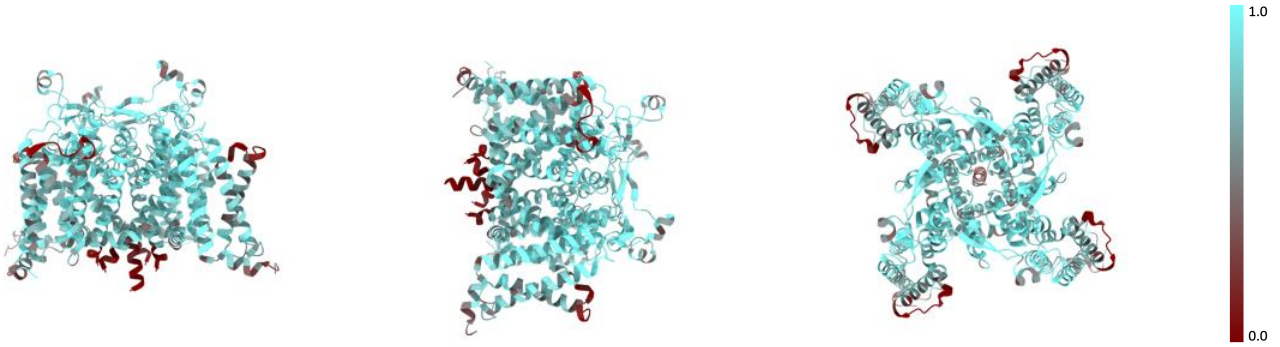
9.2 Q-score mapped to coordinate model (i)



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.

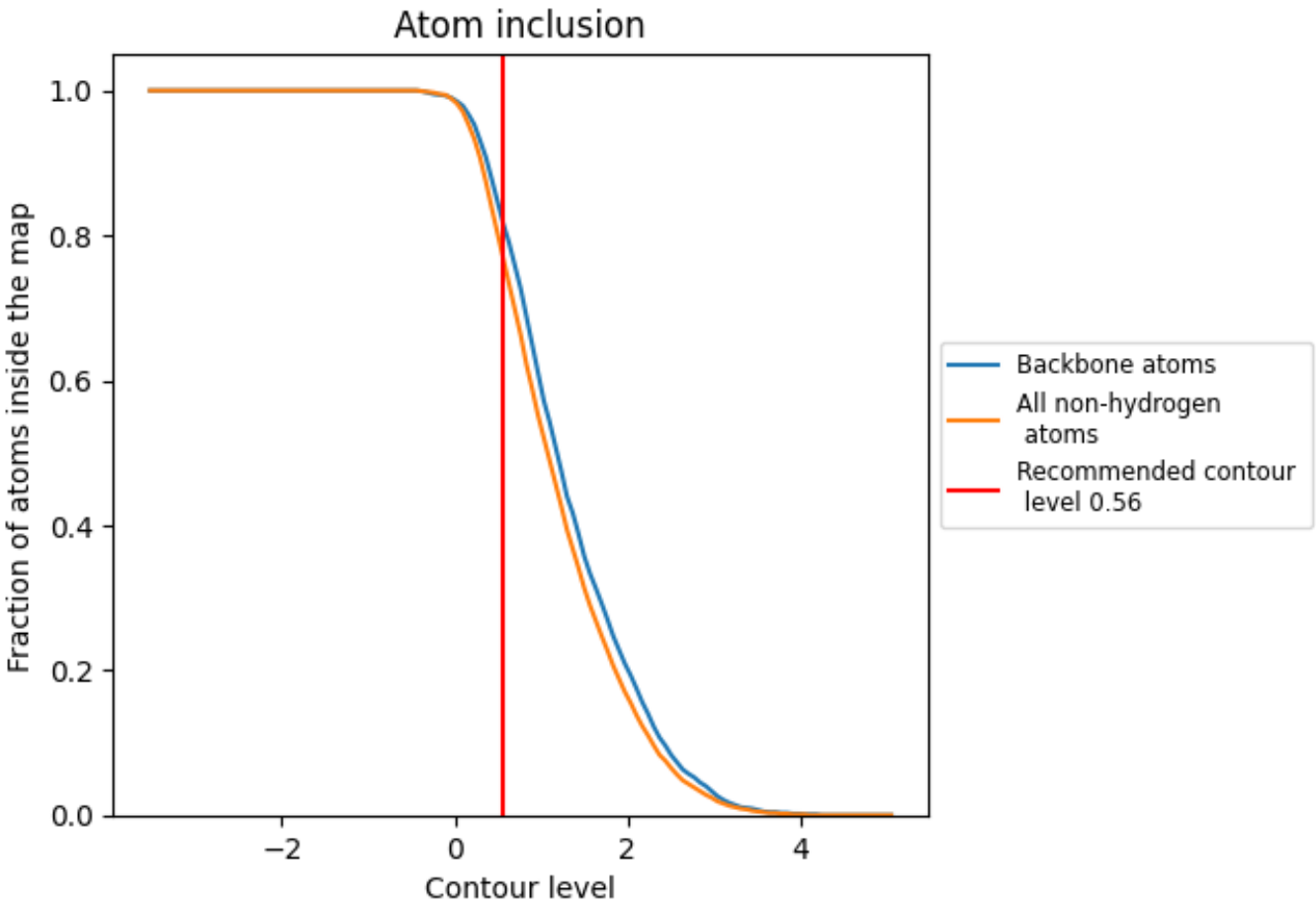
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.56).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 77% 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 (0.56) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7690	0.5180
A	0.7720	0.5250
B	0.7790	0.5220
C	0.7770	0.5260
D	0.7790	0.5220
E	0.1440	0.0530