Full wwPDB EM Validation Report (i)

May 5, 2024 – 06:10 PM EDT

PDB ID	:	6D7W
EMDB ID	:	EMD-7826
Title	:	Cryo-EM structure of the mitochondrial calcium uniporter from N. fischeri at 3.8 Angstrom resolution
Authors	:	Nguyen, N.X.; Armache, J.-P.; Cheng, Y.; Bai, X.C.
Deposited on	:	2018-04-25
Resolution	:	3.80 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:

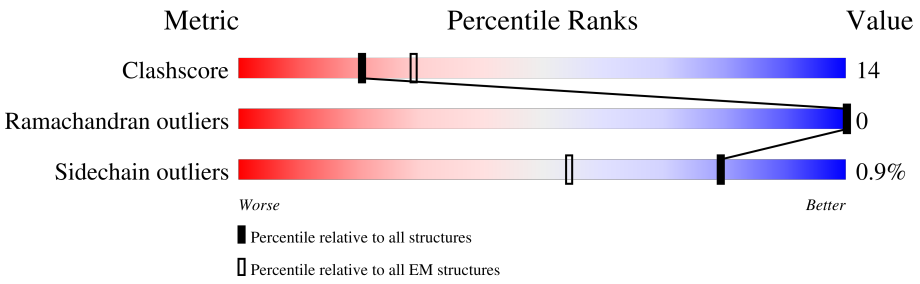
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.80 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	416	22% 55% 11% 34%
1	B	416	22% 53% 12% • 34%
1	C	416	20% 49% 16% 35%
1	D	416	19% 50% 15% 35%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8946 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 Mitochondrial calcium uniporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	275	2264	1454	395	410	5	0	0
1	C	269	2213	1423	386	399	5	0	0
1	B	274	2255	1449	393	408	5	0	0
1	D	269	2213	1423	386	399	5	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	GLY	-	expression tag	UNP A1CWT6
A	74	SER	-	expression tag	UNP A1CWT6
A	190	PHE	ALA	conflict	UNP A1CWT6
C	73	GLY	-	expression tag	UNP A1CWT6
C	74	SER	-	expression tag	UNP A1CWT6
C	190	PHE	ALA	conflict	UNP A1CWT6
B	73	GLY	-	expression tag	UNP A1CWT6
B	74	SER	-	expression tag	UNP A1CWT6
B	190	PHE	ALA	conflict	UNP A1CWT6
D	73	GLY	-	expression tag	UNP A1CWT6
D	74	SER	-	expression tag	UNP A1CWT6
D	190	PHE	ALA	conflict	UNP A1CWT6

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

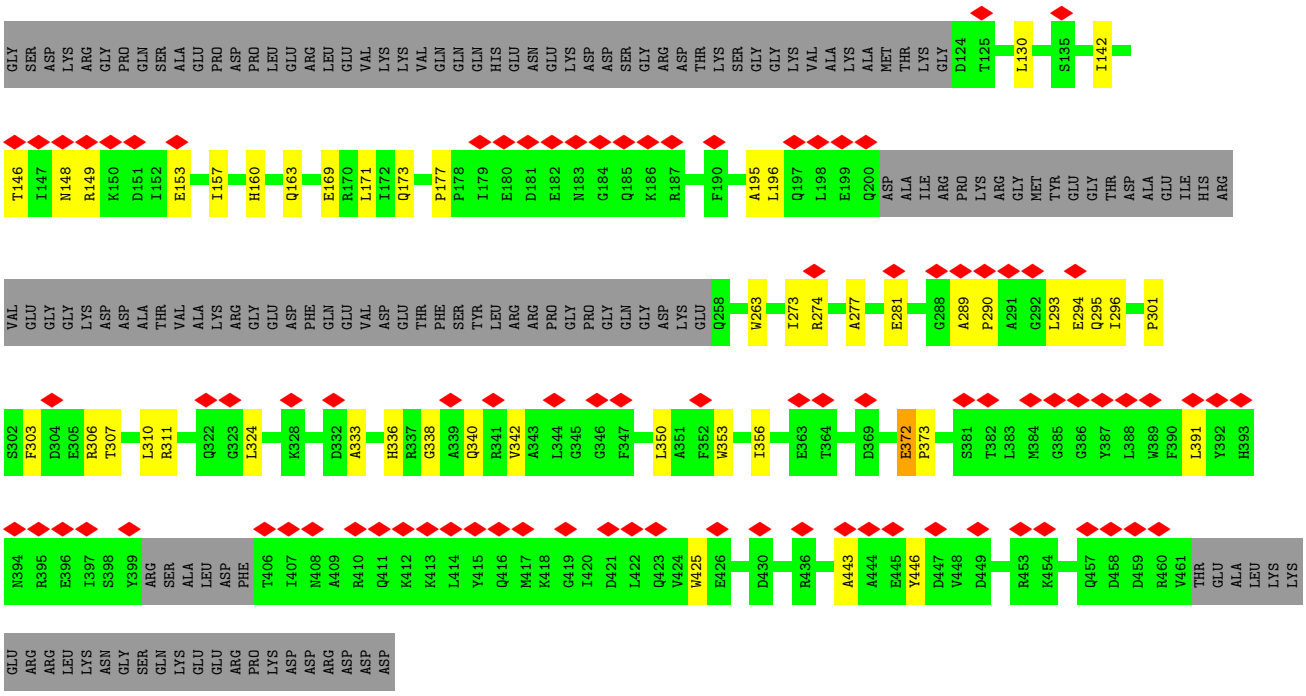
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
2	A	1	1	1	0

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.

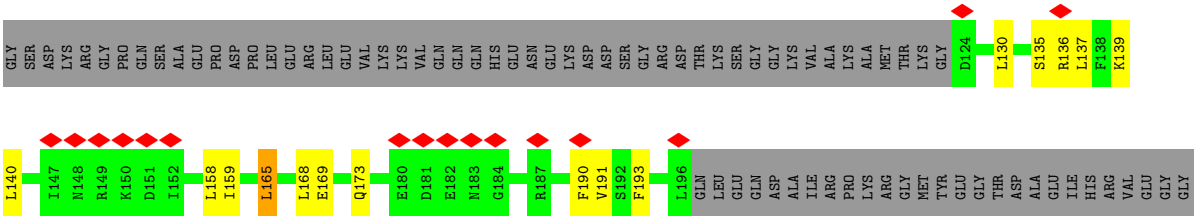
• Molecule 1: Mitochondrial calcium uniporter

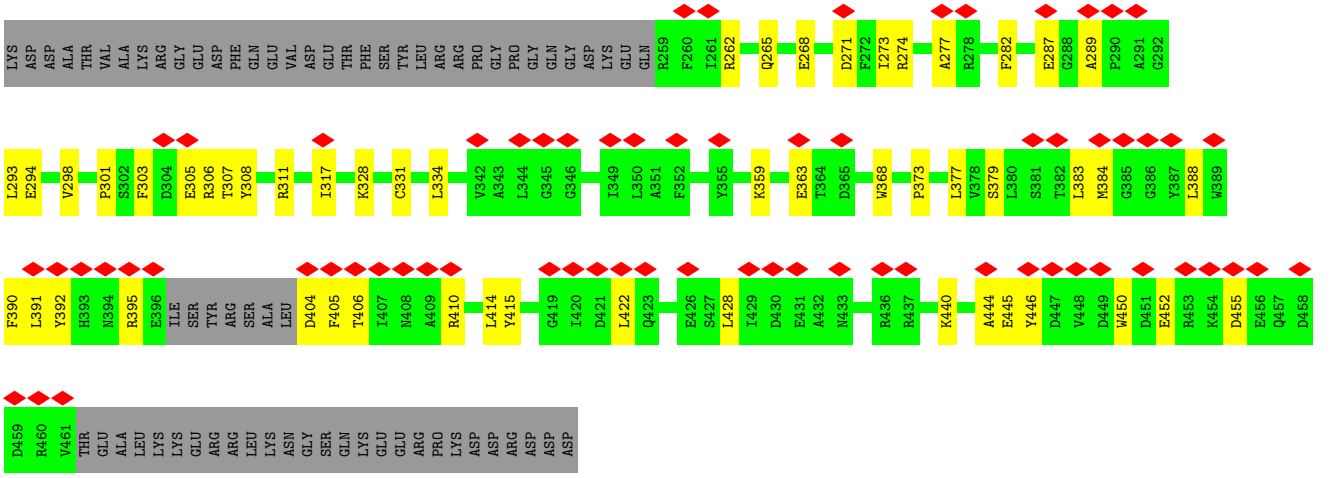
Chain A: 22% 55% 11% 34%



• Molecule 1: Mitochondrial calcium uniporter

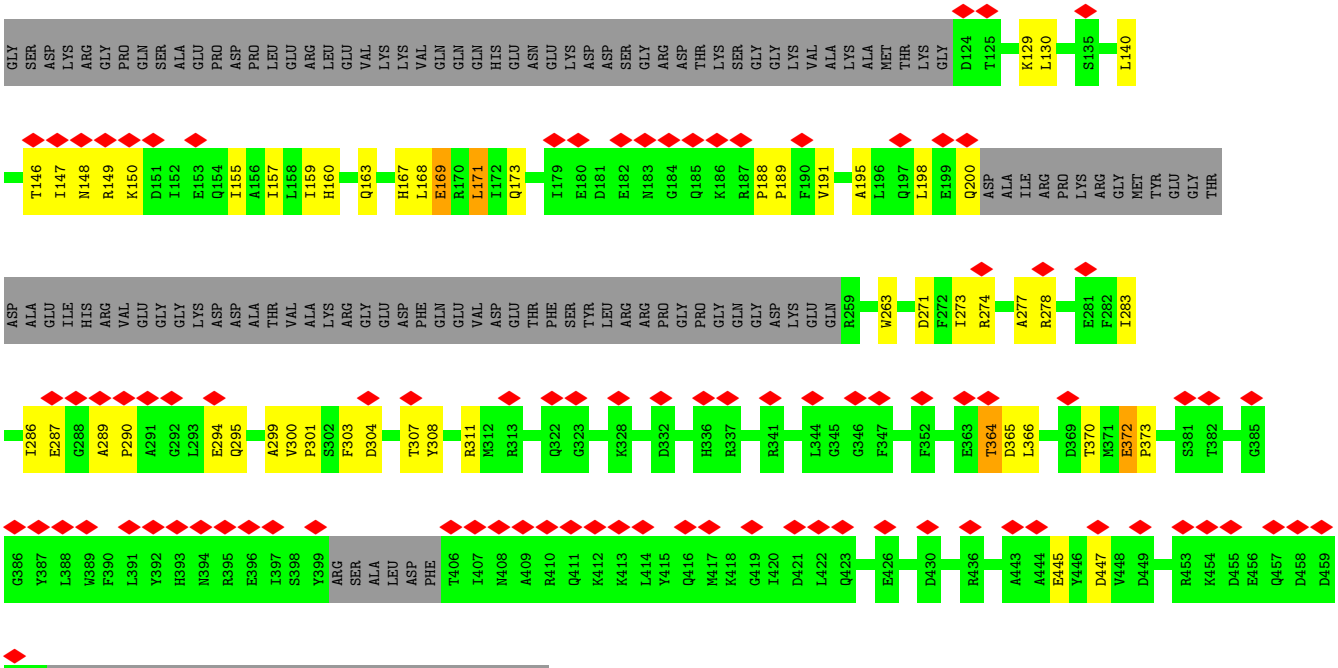
Chain C: 20% 49% 16% 35%





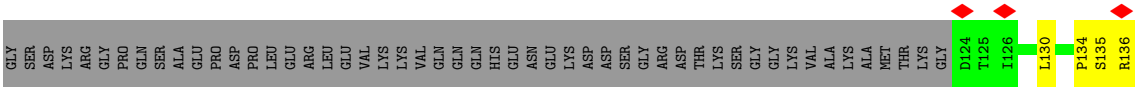
- Molecule 1: Mitochondrial calcium uniporter

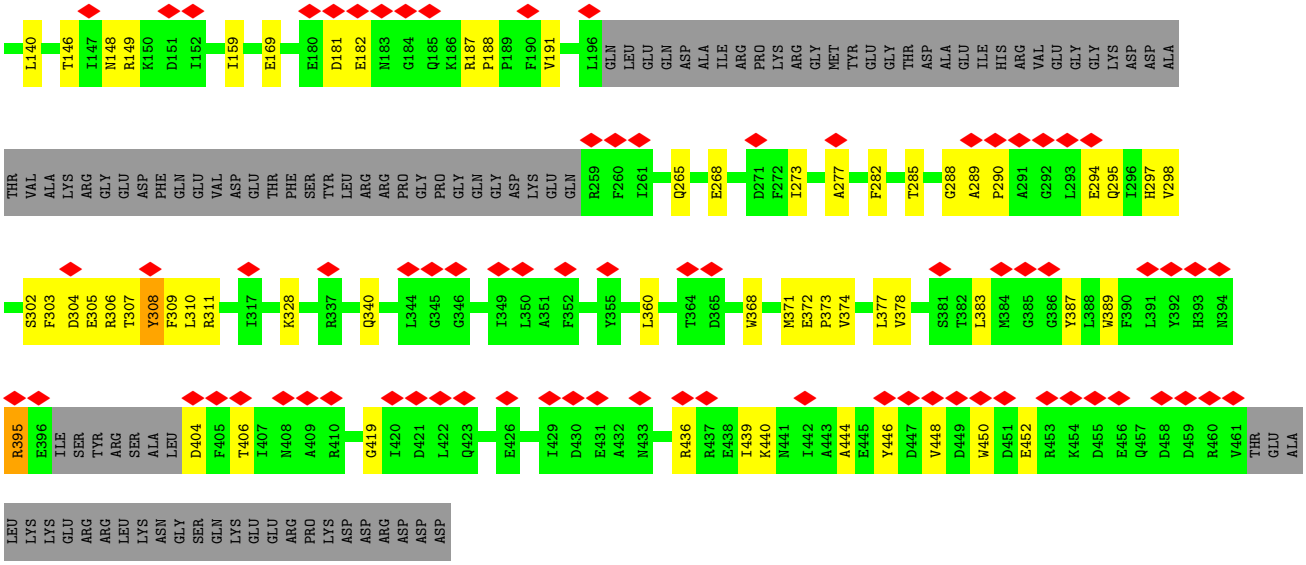
Chain B:



- Molecule 1: Mitochondrial calcium uniporter

Chain D:




L140
T146
I147
N148
R149
K150
D151
I152
I159
E169
E180
D181
E182
N183
G184
Q185
K186
R187
P188
P189
F190
V191
L196
GLN LEU GLU GLN ASP ALA ILE ARG PRO LYS ARG GLY MET TYR GLU GLY THR ASP ALA GLU ILE HIS ARG VAL GLU GLY GLY LYS ASP ASP ALA
THR VAL ALA LYS ARG GLY GLU ASP PHE GLN GLU VAL ASP GLU THR PHE SER TYR LEU ARG ARG PRO GLY PRO GLY GLN GLY ASP LYS GLU GLN
R259
F260
I261
Q265
E268
D271
F272
I273
A277
F282
T285
G288
A289
P290
A291
G292
L293
E294
Q295
I296
H297
V298
S302
F303
D304
E305
R306
T307
Y308
F309
L310
R311
I317
K328
R337
Q340
L344
G345
G346
I349
L350
A351
F352
Y355
L360
T364
D365
W368
M371
E372
P373
V374
L377
V378
S381
T382
L383
M384
G385
G386
Y387
L388
W389
F390
L391
Y392
H393
N394
R395
E396
ILE SER TYR ARG SER ALA LEU
D404
F405
T406
I407
N408
A409
R410
G419
I420
D421
L422
Q423
E426
I429
D430
E431
A432
N433
R436
R437
E438
I439
K440
N441
I442
A443
A444
E445
Y446
D447
V448
D449
W450
D451
E452
R453
K454
D455
E456
Q457
D458
D459
R460
V461
THR GLU ALA
LEU LYS LYS GLU ARG ARG LEU LYS ASN GLY SER GLN LYS GLU GLU ARG PRO LYS ASP ASP ARG ASP ASP ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	83343	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	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	0.060	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	184.79999, 184.79999, 184.79999	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.37	0/2313	0.63	0/3129
1	B	0.37	0/2304	0.64	0/3117
1	C	0.37	0/2262	0.62	0/3060
1	D	0.38	0/2262	0.66	0/3060
All	All	0.37	0/9141	0.64	0/12366

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2264	0	2270	58	0
1	B	2255	0	2262	47	0
1	C	2213	0	2217	72	0
1	D	2213	0	2217	82	0
2	A	1	0	0	0	0
All	All	8946	0	8966	243	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 14.

All (243) 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:D:307:THR:HG21	1:D:439:ILE:CD1	1.66	1.23
1:C:130:LEU:HD11	1:C:301:PRO:CD	1.74	1.15
1:D:307:THR:HG22	1:D:311:ARG:HD3	1.20	1.09
1:D:395:ARG:HH21	1:D:395:ARG:HG3	1.10	1.09
1:D:289:ALA:N	1:D:290:PRO:HD2	1.67	1.08
1:D:395:ARG:HH21	1:D:395:ARG:CG	1.67	1.07
1:D:307:THR:HG21	1:D:439:ILE:HD12	1.37	1.07
1:A:303:PHE:CE2	1:A:443:ALA:HA	1.93	1.03
1:D:307:THR:CG2	1:D:439:ILE:HD12	1.94	0.98
1:D:307:THR:HG21	1:D:439:ILE:HD11	1.41	0.98
1:C:307:THR:O	1:C:311:ARG:HG3	1.63	0.97
1:C:130:LEU:HD11	1:C:301:PRO:HD2	1.48	0.95
1:D:134:PRO:HA	1:D:309:PHE:CZ	2.04	0.92
1:A:303:PHE:HE2	1:A:443:ALA:HA	1.35	0.92
1:D:134:PRO:HB3	1:D:309:PHE:HZ	1.36	0.91
1:D:285:THR:HG23	1:D:294:GLU:O	1.73	0.89
1:C:130:LEU:CD1	1:C:301:PRO:CD	2.52	0.88
1:A:303:PHE:HE2	1:A:443:ALA:CA	1.86	0.87
1:C:130:LEU:CD1	1:C:301:PRO:HD3	2.04	0.86
1:D:289:ALA:N	1:D:290:PRO:CD	2.40	0.85
1:C:130:LEU:HD11	1:C:301:PRO:HD3	1.59	0.84
1:D:307:THR:HG22	1:D:311:ARG:CD	2.06	0.84
1:D:308:TYR:HA	1:D:311:ARG:NE	1.93	0.83
1:B:304:ASP:O	1:B:308:TYR:HB2	1.82	0.80
1:D:288:GLY:C	1:D:290:PRO:HD2	2.02	0.79
1:D:395:ARG:HG3	1:D:395:ARG:NH2	1.85	0.79
1:C:334:LEU:HD12	1:C:414:LEU:HD21	1.65	0.78
1:D:303:PHE:HB3	1:D:446:TYR:HD2	1.46	0.78
1:C:130:LEU:HD12	1:C:130:LEU:O	1.85	0.77
1:C:331:CYS:SG	1:C:415:TYR:HB3	2.24	0.77
1:A:336:HIS:O	1:A:340:GLN:HG2	1.85	0.77
1:B:163:GLN:OE1	1:B:167:HIS:CD2	2.38	0.76
1:A:130:LEU:HD12	1:A:301:PRO:HD3	1.67	0.76
1:A:307:THR:HG22	1:A:311:ARG:HG3	1.67	0.76
1:B:171:LEU:HD13	1:B:171:LEU:O	1.85	0.76
1:D:395:ARG:CG	1:D:395:ARG:NH2	2.38	0.76
1:D:307:THR:CG2	1:D:439:ILE:CD1	2.53	0.75
1:D:308:TYR:HB2	1:D:311:ARG:HH21	1.52	0.74
1:D:307:THR:CG2	1:D:311:ARG:HD3	2.09	0.73
1:A:130:LEU:HD12	1:A:130:LEU:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:303:PHE:CZ	1:D:448:VAL:HG21	2.23	0.73
1:B:273:ILE:O	1:B:277:ALA:HB2	1.90	0.72
1:D:134:PRO:CB	1:D:309:PHE:HZ	2.03	0.72
1:A:169:GLU:O	1:A:173:GLN:HB2	1.88	0.71
1:A:273:ILE:O	1:A:277:ALA:HB2	1.89	0.71
1:D:134:PRO:CA	1:D:309:PHE:CZ	2.73	0.70
1:A:303:PHE:CE2	1:A:443:ALA:CA	2.65	0.70
1:C:165:LEU:HD11	1:C:193:PHE:CD1	2.27	0.70
1:D:134:PRO:HA	1:D:309:PHE:CE1	2.26	0.69
1:C:311:ARG:HD2	1:C:455:ASP:OD2	1.92	0.69
1:C:373:PRO:O	1:C:377:LEU:HB2	1.93	0.69
1:C:293:LEU:HD12	1:C:293:LEU:C	2.14	0.68
1:C:334:LEU:HD13	1:C:334:LEU:C	2.14	0.68
1:A:130:LEU:CD1	1:A:301:PRO:HD3	2.24	0.68
1:C:368:TRP:NE1	1:B:372:GLU:HG2	2.09	0.67
1:C:293:LEU:HD12	1:C:293:LEU:O	1.95	0.67
1:D:308:TYR:HA	1:D:311:ARG:HE	1.57	0.67
1:C:395:ARG:HG2	1:C:405:PHE:HB2	1.76	0.66
1:D:273:ILE:O	1:D:277:ALA:HB2	1.94	0.66
1:A:149:ARG:HG2	1:A:153:GLU:HB2	1.78	0.65
1:C:287:GLU:OE2	1:C:287:GLU:HA	1.97	0.65
1:B:370:THR:HG22	1:B:370:THR:O	1.97	0.65
1:C:379:SER:O	1:C:383:LEU:HD23	1.98	0.64
1:A:290:PRO:CG	1:A:294:GLU:HB3	2.27	0.64
1:C:273:ILE:O	1:C:277:ALA:HB2	1.98	0.64
1:D:307:THR:O	1:D:308:TYR:C	2.34	0.63
1:C:317:ILE:HD11	1:C:428:LEU:HD22	1.81	0.63
1:C:308:TYR:HB3	1:C:311:ARG:NH2	2.14	0.63
1:B:159:ILE:HD11	1:B:168:LEU:HD13	1.81	0.62
1:A:372:GLU:HG2	1:D:368:TRP:NE1	2.14	0.62
1:C:169:GLU:HG2	1:C:191:VAL:HG22	1.82	0.62
1:C:328:LYS:HE3	1:C:415:TYR:CZ	2.35	0.62
1:D:307:THR:O	1:D:310:LEU:N	2.33	0.62
1:A:293:LEU:O	1:A:294:GLU:HG2	1.99	0.61
1:A:293:LEU:O	1:A:295:GLN:HG2	2.01	0.61
1:A:163:GLN:NE2	1:D:265:GLN:O	2.34	0.60
1:C:395:ARG:C	1:C:395:ARG:HD2	2.21	0.60
1:A:290:PRO:HG3	1:A:294:GLU:HB2	1.83	0.60
1:A:350:LEU:HD23	1:C:384:MET:SD	2.41	0.60
1:B:278:ARG:NH1	1:B:445:GLU:O	2.35	0.60
1:B:364:THR:O	1:B:364:THR:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:GLN:O	1:B:163:GLN:NE2	2.36	0.58
1:D:295:GLN:HG2	1:D:297:HIS:CD2	2.38	0.58
1:B:191:VAL:HG12	1:B:286:ILE:HA	1.84	0.58
1:B:146:THR:HG22	1:B:147:ILE:HD12	1.86	0.58
1:C:271:ASP:OD1	1:C:274:ARG:NH1	2.37	0.57
1:C:130:LEU:HD12	1:C:130:LEU:C	2.24	0.57
1:D:187:ARG:HG3	1:D:188:PRO:HD2	1.87	0.57
1:C:306:ARG:NH1	1:C:446:TYR:OH	2.37	0.57
1:A:290:PRO:CG	1:A:294:GLU:CB	2.83	0.56
1:C:328:LYS:HE3	1:C:415:TYR:CE1	2.40	0.56
1:C:190:PHE:HE2	1:C:262:ARG:HH22	1.53	0.56
1:A:350:LEU:HG	1:C:384:MET:HE2	1.86	0.56
1:D:308:TYR:CB	1:D:311:ARG:NH2	2.69	0.56
1:D:360:LEU:HB3	1:D:371:MET:CE	2.36	0.56
1:B:147:ILE:HG22	1:B:148:ASN:H	1.69	0.56
1:D:302:SER:O	1:D:306:ARG:N	2.32	0.56
1:C:388:LEU:HD11	1:C:392:TYR:CD2	2.41	0.56
1:C:130:LEU:HA	1:C:140:LEU:HA	1.88	0.55
1:D:373:PRO:O	1:D:377:LEU:HB2	2.06	0.55
1:C:130:LEU:HD11	1:C:301:PRO:CG	2.34	0.55
1:D:305:GLU:HA	1:D:308:TYR:HD2	1.72	0.55
1:B:365:ASP:N	1:B:365:ASP:OD1	2.40	0.54
1:A:196:LEU:HB2	1:A:281:GLU:HG2	1.90	0.54
1:C:169:GLU:OE2	1:C:173:GLN:NE2	2.41	0.54
1:D:383:LEU:O	1:D:387:TYR:HB2	2.08	0.54
1:C:404:ASP:HB3	1:C:406:THR:HG23	1.89	0.54
1:C:440:LYS:O	1:C:444:ALA:HB2	2.08	0.54
1:B:171:LEU:HD13	1:B:171:LEU:C	2.28	0.54
1:A:303:PHE:HB2	1:A:446:TYR:CG	2.42	0.53
1:B:273:ILE:O	1:B:277:ALA:CB	2.56	0.53
1:C:359:LYS:NZ	1:C:363:GLU:OE1	2.40	0.53
1:A:290:PRO:HG3	1:A:294:GLU:CB	2.38	0.53
1:C:130:LEU:CG	1:C:301:PRO:HD3	2.39	0.53
1:D:308:TYR:HB2	1:D:311:ARG:NH2	2.21	0.52
1:C:135:SER:OG	1:C:136:ARG:N	2.41	0.52
1:B:271:ASP:OD1	1:B:274:ARG:NH2	2.38	0.52
1:A:146:THR:HG23	1:A:177:PRO:HD3	1.91	0.52
1:C:334:LEU:HD13	1:C:334:LEU:O	2.10	0.52
1:B:149:ARG:HH21	1:B:150:LYS:HD3	1.75	0.51
1:C:410:ARG:O	1:C:414:LEU:HB2	2.09	0.51
1:B:304:ASP:O	1:B:308:TYR:CB	2.55	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:LYS:HZ3	1:D:419:GLY:HA3	1.76	0.51
1:B:372:GLU:HB3	1:B:373:PRO:HD3	1.92	0.51
1:B:372:GLU:N	1:B:373:PRO:CD	2.73	0.51
1:A:350:LEU:HG	1:C:384:MET:CE	2.40	0.51
1:D:134:PRO:HB3	1:D:309:PHE:CZ	2.28	0.51
1:A:289:ALA:N	1:A:290:PRO:HD2	2.26	0.51
1:C:165:LEU:HD13	1:C:165:LEU:O	2.10	0.51
1:B:198:LEU:HG	1:B:200:GLN:H	1.74	0.51
1:D:389:TRP:HD1	1:D:395:ARG:NH2	2.09	0.51
1:A:273:ILE:O	1:A:277:ALA:CB	2.58	0.51
1:D:148:ASN:O	1:D:149:ARG:NE	2.41	0.50
1:D:307:THR:HG23	1:D:439:ILE:HD12	1.88	0.50
1:D:360:LEU:HB3	1:D:371:MET:HE3	1.92	0.50
1:D:395:ARG:HH21	1:D:395:ARG:HG2	1.66	0.50
1:C:190:PHE:CE2	1:C:262:ARG:NH2	2.79	0.50
1:C:273:ILE:O	1:C:277:ALA:CB	2.59	0.50
1:B:168:LEU:HD12	1:B:168:LEU:O	2.12	0.50
1:B:289:ALA:N	1:B:290:PRO:HD3	2.27	0.50
1:A:372:GLU:OE2	1:D:372:GLU:OE2	2.29	0.50
1:C:388:LEU:HD11	1:C:392:TYR:CE2	2.45	0.50
1:B:130:LEU:CD1	1:B:301:PRO:HD3	2.42	0.50
1:B:195:ALA:HB3	1:B:263:TRP:HE1	1.77	0.50
1:D:135:SER:OG	1:D:136:ARG:N	2.45	0.49
1:A:340:GLN:HE21	1:A:340:GLN:HA	1.78	0.49
1:B:189:PRO:HB3	1:B:287:GLU:HB3	1.93	0.49
1:D:273:ILE:O	1:D:277:ALA:CB	2.58	0.49
1:B:173:GLN:HE21	1:B:188:PRO:HB2	1.77	0.49
1:A:290:PRO:HB2	1:A:294:GLU:HB3	1.95	0.49
1:A:290:PRO:CB	1:A:294:GLU:HB3	2.43	0.49
1:A:391:LEU:HD11	1:D:340:GLN:HG2	1.94	0.49
1:C:390:PHE:HD1	1:C:395:ARG:NH2	2.11	0.48
1:C:190:PHE:HE2	1:C:262:ARG:NH2	2.10	0.48
1:A:303:PHE:CE2	1:A:443:ALA:CB	2.96	0.48
1:D:372:GLU:N	1:D:373:PRO:CD	2.76	0.48
1:A:160:HIS:NE2	1:D:268:GLU:OE2	2.36	0.48
1:D:303:PHE:HB3	1:D:446:TYR:CD2	2.37	0.48
1:D:308:TYR:C	1:D:308:TYR:CD1	2.86	0.48
1:A:340:GLN:HA	1:A:340:GLN:NE2	2.29	0.48
1:C:328:LYS:NZ	1:C:422:LEU:HD21	2.29	0.48
1:D:187:ARG:CG	1:D:188:PRO:HD2	2.44	0.48
1:C:268:GLU:OE2	1:B:160:HIS:NE2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:374:VAL:O	1:D:378:VAL:HB	2.14	0.48
1:C:303:PHE:HB3	1:C:446:TYR:HD2	1.79	0.47
1:C:289:ALA:HB2	1:C:294:GLU:HB3	1.96	0.47
1:C:305:GLU:HA	1:C:308:TYR:CD2	2.49	0.47
1:A:307:THR:O	1:A:310:LEU:N	2.47	0.47
1:D:134:PRO:CA	1:D:309:PHE:HZ	2.23	0.47
1:C:450:TRP:HE1	1:C:452:GLU:HG3	1.80	0.47
1:D:440:LYS:O	1:D:444:ALA:HB2	2.15	0.47
1:D:304:ASP:O	1:D:308:TYR:HB3	2.14	0.47
1:B:140:LEU:HD23	1:B:157:ILE:HB	1.98	0.46
1:C:440:LYS:O	1:C:444:ALA:CB	2.64	0.46
1:D:306:ARG:NH1	1:D:446:TYR:OH	2.47	0.46
1:D:450:TRP:HE1	1:D:452:GLU:HG3	1.80	0.46
1:A:307:THR:CG2	1:A:311:ARG:HG3	2.43	0.45
1:A:333:ALA:HA	1:A:336:HIS:CD2	2.51	0.45
1:C:130:LEU:HG	1:C:301:PRO:HD3	1.97	0.45
1:B:370:THR:O	1:B:370:THR:CG2	2.61	0.45
1:A:373:PRO:HG3	1:D:368:TRP:CD2	2.50	0.45
1:B:169:GLU:HB2	1:B:191:VAL:CG2	2.46	0.45
1:B:289:ALA:HB2	1:B:294:GLU:HG3	1.98	0.45
1:C:308:TYR:HA	1:C:311:ARG:HB2	1.99	0.45
1:D:181:ASP:HA	1:D:182:GLU:HB2	1.99	0.45
1:D:404:ASP:HB3	1:D:406:THR:HG23	1.97	0.45
1:A:340:GLN:NE2	1:C:391:LEU:HD22	2.32	0.45
1:B:163:GLN:OE1	1:B:167:HIS:HD2	1.93	0.44
1:A:340:GLN:HE22	1:C:391:LEU:HD22	1.82	0.44
1:B:129:LYS:HG2	1:B:299:ALA:HB3	1.98	0.44
1:D:140:LEU:HD22	1:D:159:ILE:HD11	1.99	0.44
1:D:282:PHE:HB3	1:D:298:VAL:HG22	1.98	0.44
1:B:171:LEU:C	1:B:171:LEU:CD1	2.86	0.44
1:D:290:PRO:HB2	1:D:294:GLU:H	1.83	0.44
1:D:368:TRP:HA	1:D:371:MET:HB3	1.99	0.44
1:A:146:THR:HG22	1:A:148:ASN:H	1.82	0.44
1:B:307:THR:O	1:B:311:ARG:HB2	2.18	0.44
1:A:274:ARG:HH22	1:C:137:LEU:HD21	1.81	0.43
1:A:306:ARG:HD3	1:A:446:TYR:OH	2.18	0.43
1:A:142:ILE:HG23	1:A:296:ILE:HG21	2.00	0.43
1:D:436:ARG:HA	1:D:439:ILE:HG22	2.01	0.43
1:C:395:ARG:C	1:C:395:ARG:CD	2.86	0.43
1:B:155:ILE:H	1:B:155:ILE:HG13	1.62	0.43
1:A:293:LEU:O	1:A:294:GLU:CG	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:PHE:HE2	1:A:443:ALA:CB	2.32	0.43
1:D:302:SER:O	1:D:306:ARG:HB2	2.19	0.43
1:D:383:LEU:O	1:D:387:TYR:CB	2.67	0.43
1:C:159:ILE:HD11	1:C:168:LEU:HD13	2.01	0.43
1:D:440:LYS:O	1:D:444:ALA:CB	2.66	0.43
1:A:195:ALA:HB3	1:A:263:TRP:HE1	1.83	0.43
1:A:303:PHE:CD1	1:A:303:PHE:C	2.91	0.43
1:A:372:GLU:HG2	1:D:368:TRP:HE1	1.79	0.43
1:B:277:ALA:HA	1:B:300:VAL:HG11	2.01	0.43
1:B:283:ILE:HG21	1:B:295:GLN:NE2	2.33	0.43
1:C:334:LEU:C	1:C:334:LEU:CD1	2.85	0.43
1:C:307:THR:O	1:C:311:ARG:CG	2.52	0.42
1:D:169:GLU:HG3	1:D:191:VAL:HG22	2.01	0.42
1:D:304:ASP:O	1:D:308:TYR:N	2.32	0.42
1:C:282:PHE:HB3	1:C:298:VAL:HG22	2.01	0.42
1:D:360:LEU:HB3	1:D:371:MET:HE1	2.01	0.42
1:D:130:LEU:HA	1:D:140:LEU:HA	2.01	0.42
1:A:293:LEU:C	1:A:294:GLU:HG2	2.39	0.42
1:A:324:LEU:HD23	1:A:425:TRP:HE3	1.84	0.42
1:A:303:PHE:CE2	1:A:443:ALA:HB2	2.55	0.42
1:B:289:ALA:CB	1:B:294:GLU:HG3	2.50	0.42
1:C:130:LEU:CD1	1:C:301:PRO:CG	2.97	0.42
1:B:294:GLU:O	1:B:294:GLU:HG2	2.20	0.41
1:B:365:ASP:OD1	1:B:366:LEU:N	2.53	0.41
1:A:306:ARG:CD	1:A:446:TYR:OH	2.68	0.41
1:B:278:ARG:NH2	1:B:447:ASP:OD2	2.52	0.41
1:B:289:ALA:HA	1:B:294:GLU:HG3	2.02	0.41
1:A:353:TRP:HA	1:A:356:ILE:HG22	2.03	0.41
1:D:308:TYR:HA	1:D:311:ARG:CZ	2.49	0.41
1:D:303:PHE:CE1	1:D:448:VAL:HG21	2.55	0.41
1:D:307:THR:O	1:D:309:PHE:N	2.54	0.41
1:D:308:TYR:CB	1:D:311:ARG:HH21	2.21	0.41
1:C:274:ARG:HD2	1:C:445:GLU:HB3	2.03	0.40
1:A:157:ILE:HG23	1:A:171:LEU:HD12	2.02	0.40
1:B:130:LEU:HD12	1:B:301:PRO:HD3	2.03	0.40
1:B:303:PHE:O	1:B:307:THR:OG1	2.27	0.40
1:A:338:GLY:O	1:A:342:VAL:HG23	2.22	0.40
1:C:139:LYS:HB3	1:C:158:LEU:HD23	2.03	0.40
1:C:388:LEU:CD1	1:C:392:TYR:CD2	3.05	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	269/416 (65%)	256 (95%)	13 (5%)	0	100	100
1	B	268/416 (64%)	254 (95%)	14 (5%)	0	100	100
1	C	263/416 (63%)	242 (92%)	21 (8%)	0	100	100
1	D	263/416 (63%)	240 (91%)	23 (9%)	0	100	100
All	All	1063/1664 (64%)	992 (93%)	71 (7%)	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	241/358 (67%)	240 (100%)	1 (0%)	91	95
1	B	240/358 (67%)	236 (98%)	4 (2%)	60	78
1	C	235/358 (66%)	234 (100%)	1 (0%)	91	95
1	D	235/358 (66%)	232 (99%)	3 (1%)	69	82
All	All	951/1432 (66%)	942 (99%)	9 (1%)	79	88

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	372	GLU
1	C	165	LEU

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Mol	Chain	Res	Type
1	B	169	GLU
1	B	171	LEU
1	B	364	THR
1	B	372	GLU
1	D	146	THR
1	D	308	TYR
1	D	395	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	GLN
1	A	295	GLN
1	A	340	GLN
1	A	408	ASN
1	C	173	GLN
1	C	441	ASN
1	B	167	HIS
1	B	295	GLN
1	B	340	GLN
1	D	154	GLN
1	D	441	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

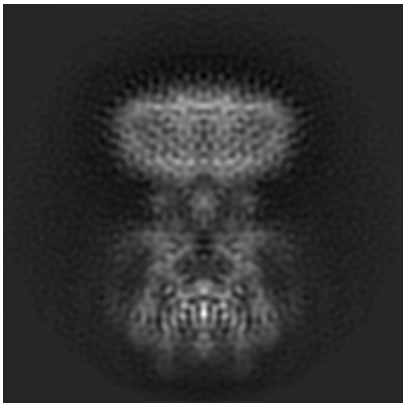
6 Map visualisation (i)

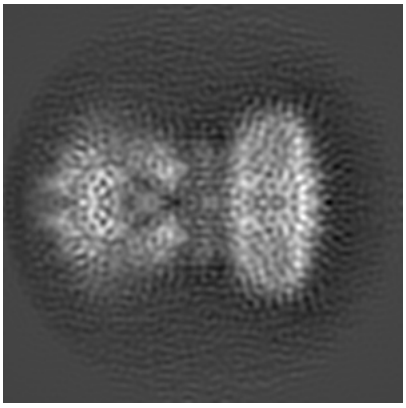
This section contains visualisations of the EMDB entry EMD-7826. These allow visual inspection of the internal detail of the map and identification of artifacts.

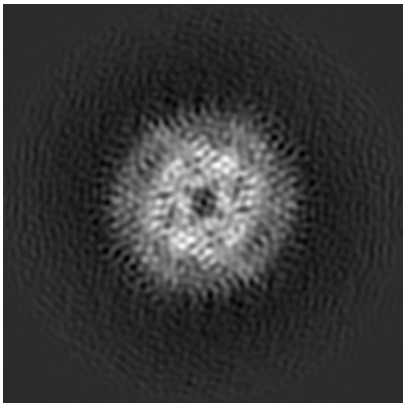
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

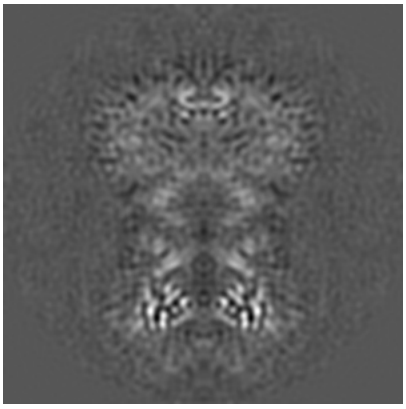

Y

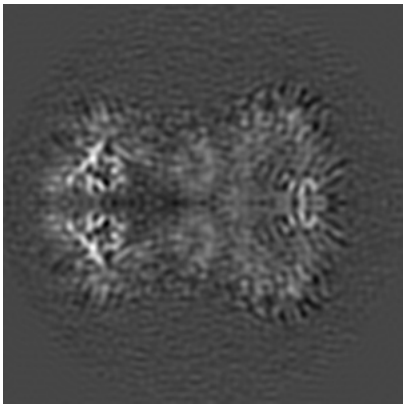

Z

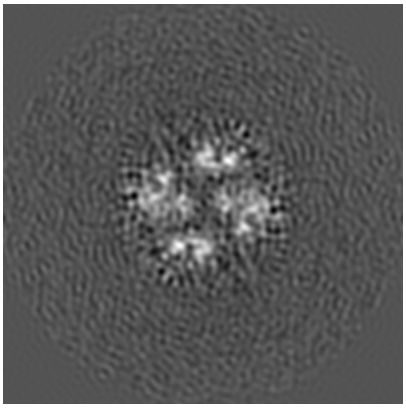
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 110

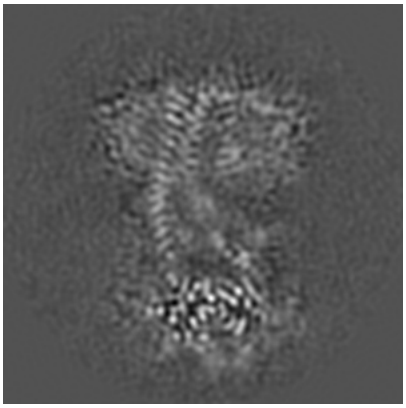

Y Index: 110

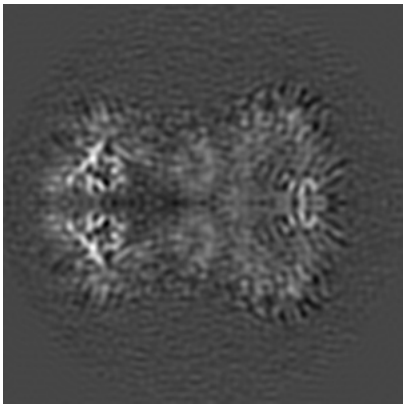

Z Index: 110

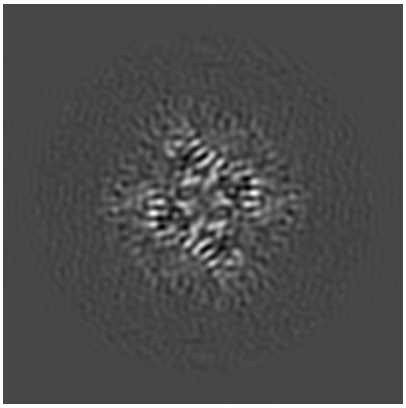
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 98

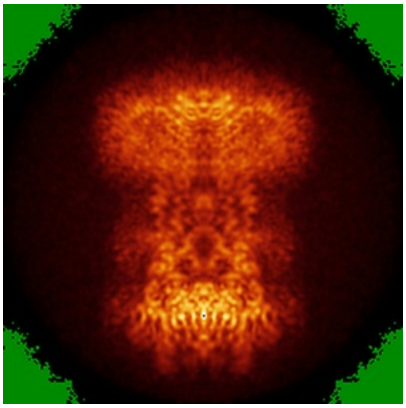

Y Index: 110

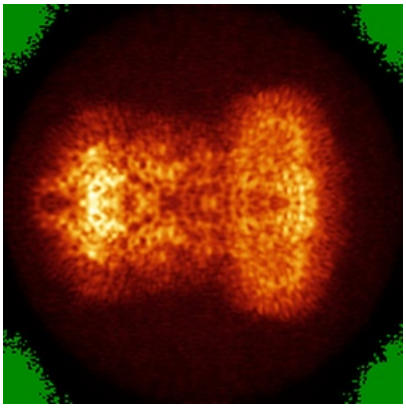

Z Index: 48

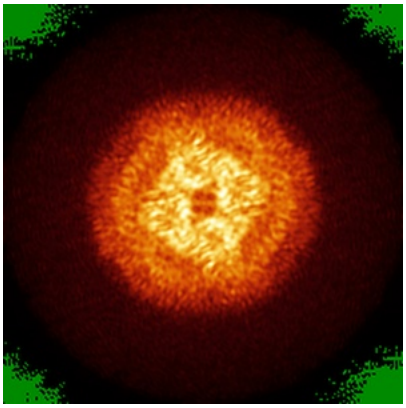
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

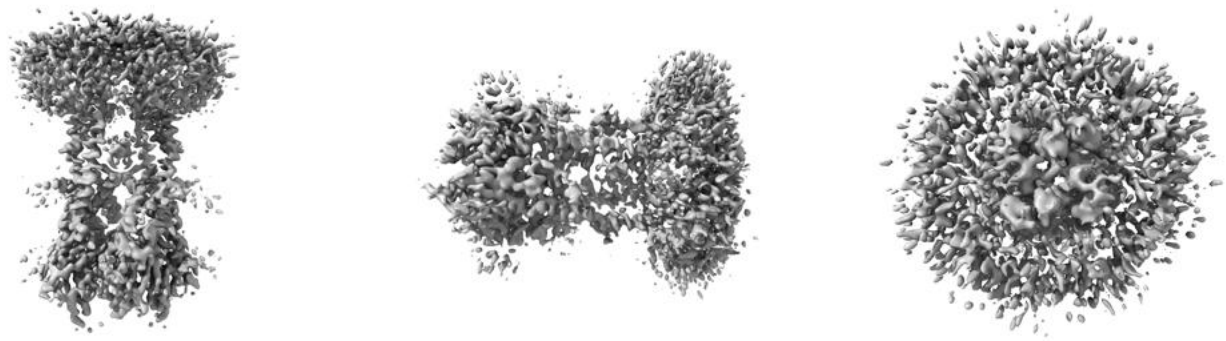

Y


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

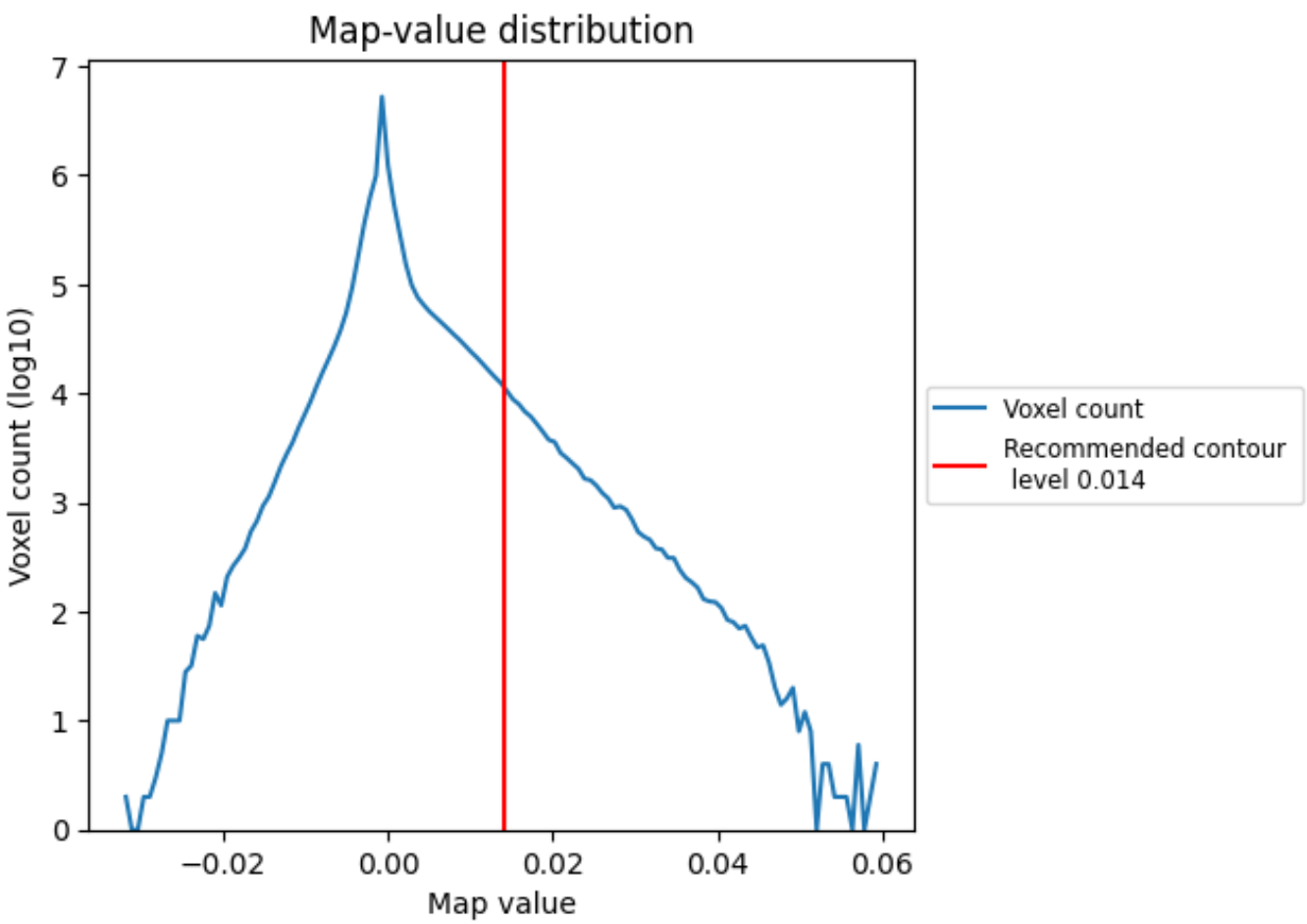
6.6 Mask visualisation (i)

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

7 Map analysis (i)

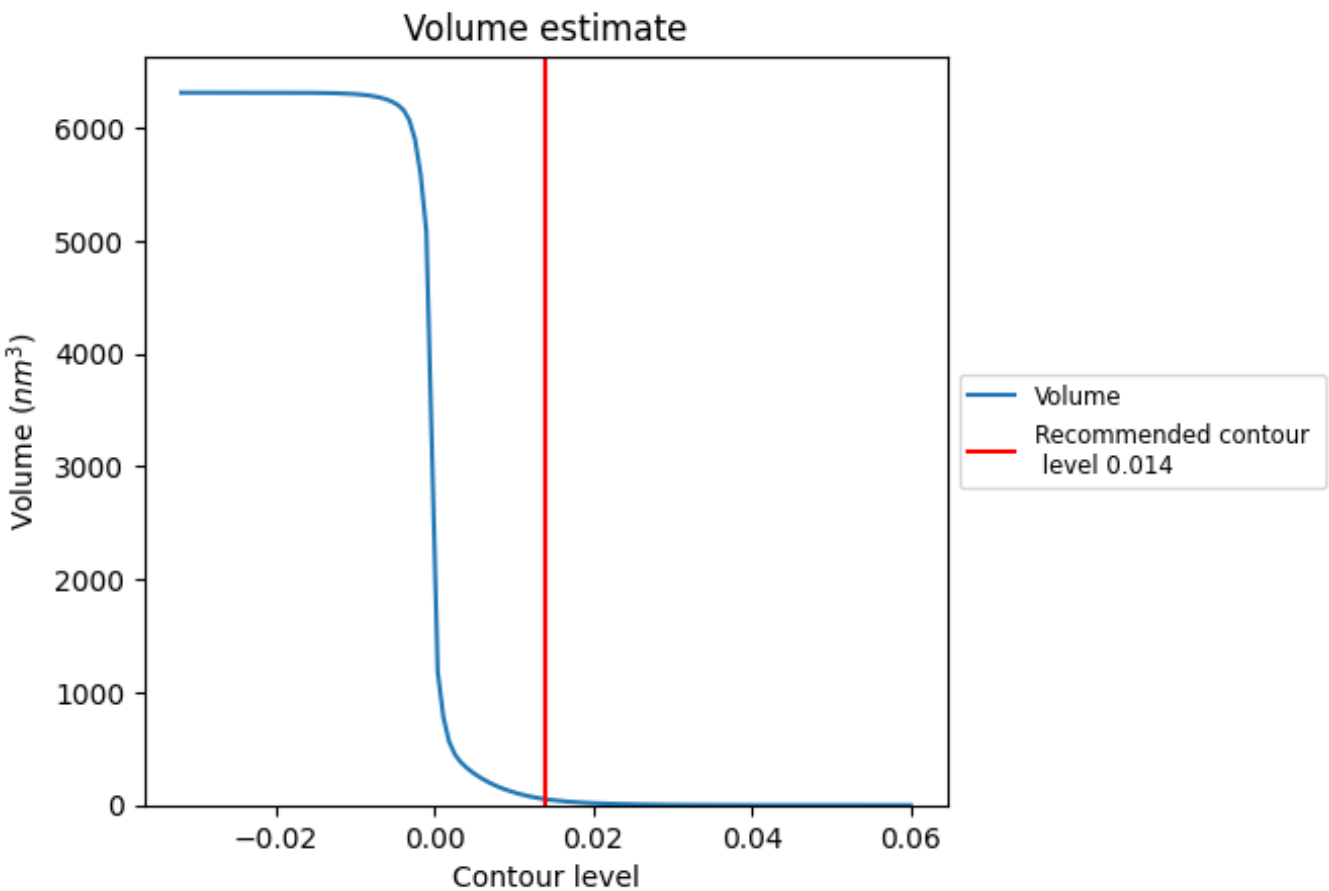
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

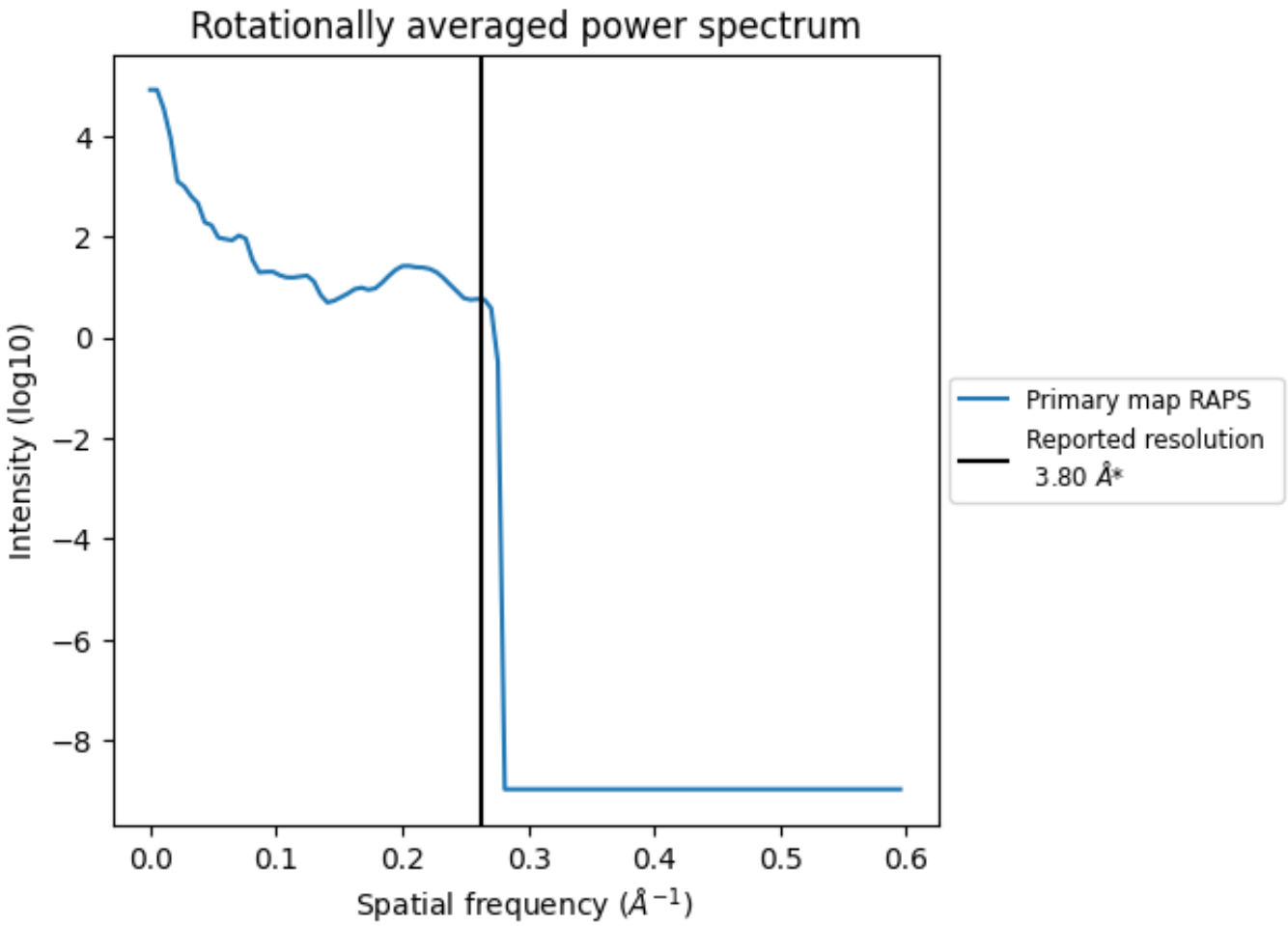
7.2 Volume estimate (i)



The volume at the recommended contour level is 53 nm^3; this corresponds to an approximate mass of 48 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 0.263 Å^{-1}

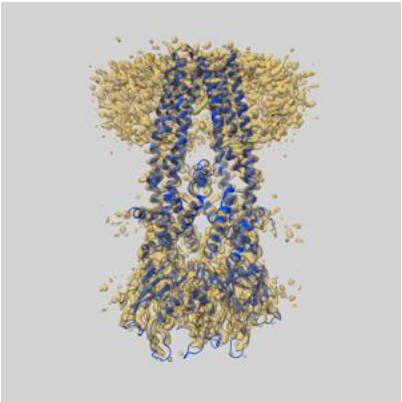
8 Fourier-Shell correlation (i)

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

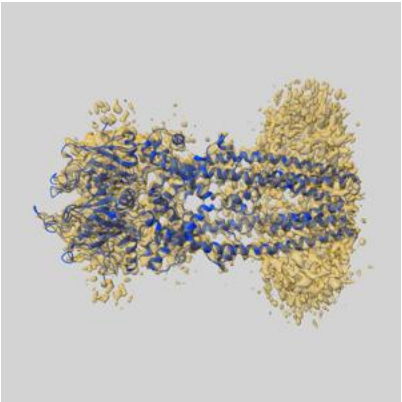
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-7826 and PDB model 6D7W. Per-residue inclusion information can be found in section 3 on page 4.

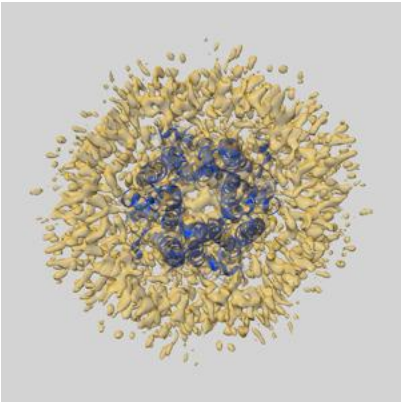
9.1 Map-model overlay (i)



X



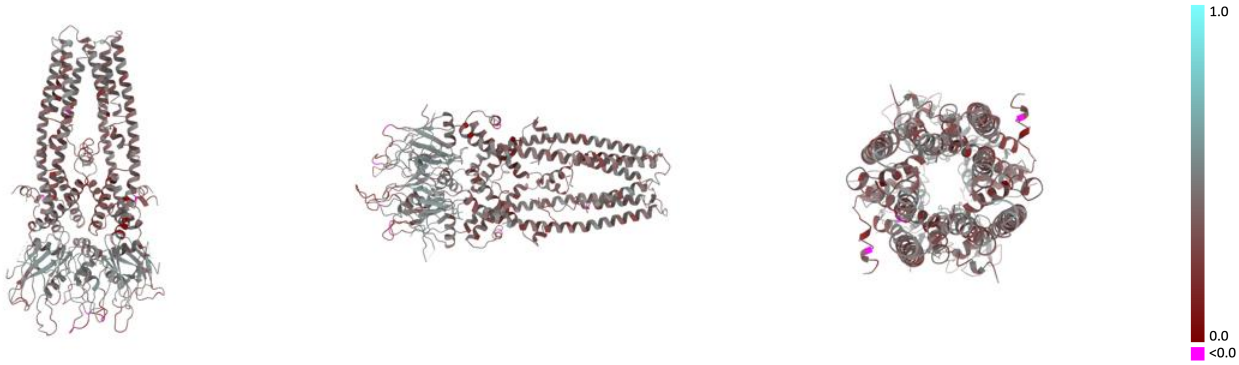
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014 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.

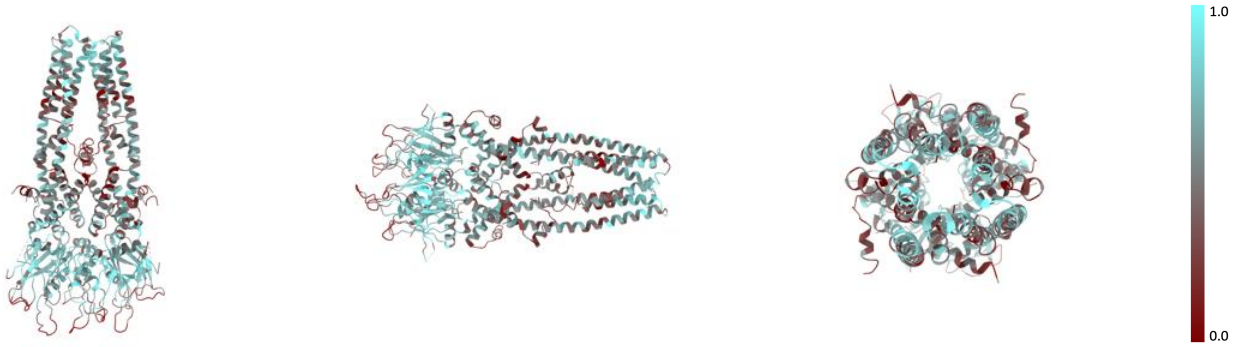
9.2 Q-score mapped to coordinate model (i)



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.

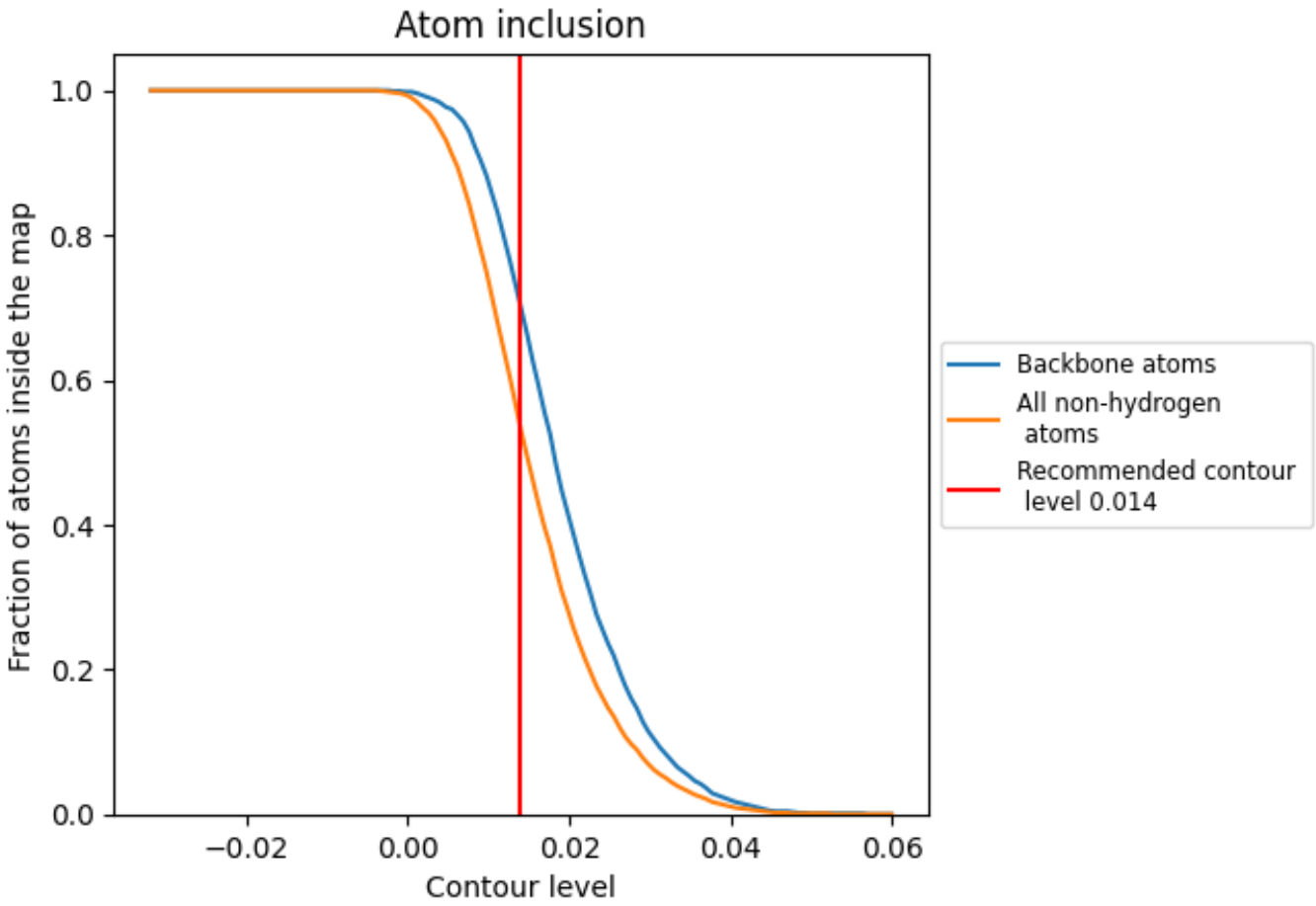
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.014).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 53% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5320	0.3980
A	0.5240	0.4040
B	0.5280	0.3980
C	0.5360	0.3940
D	0.5410	0.3950