Full wwPDB EM Validation Report (i)

May 5, 2024 – 06:12 PM EDT

PDB ID	:	6D80
EMDB ID	:	EMD-7828
Title	:	Cryo-EM structure of the mitochondrial calcium uniporter from N. fischeri bound to saposin
Authors	:	Nguyen, N.X.; Armache, J.-P.; Cheng, Y.; Bai, X.C.
Deposited on	:	2018-04-25
Resolution	:	5.00 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:

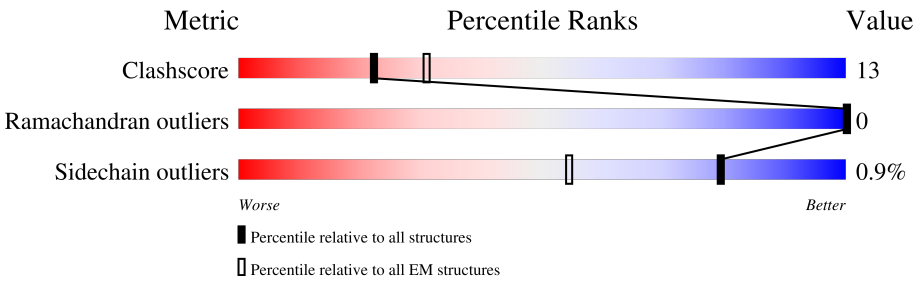
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 5.00 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	F	81	23% 95% 5%
1	G	81	62% 91% 7% •
1	H	81	44% 89% 10% •
1	I	81	27% 98% •
1	J	81	59% 84% 15% •
1	K	81	44% 85% 12% •
2	A	416	21% 55% 11% 34%
2	B	416	18% 49% 16% 35%

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Mol	Chain	Length	Quality of chain
2	C	416	20% 53% 12% • 34%
2	D	416	18% 50% 15% 35%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11351 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 Saposin A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	F	81	405	243	81	81	0	0
1	H	80	400	240	80	80	0	0
1	G	80	400	240	80	80	0	0
1	I	81	405	243	81	81	0	0
1	J	80	400	240	80	80	0	0
1	K	79	395	237	79	79	0	0

- Molecule 2 is a protein called Mitochondrial calcium uniporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	275	2264	1454	395	410	5	0	0
2	B	269	2213	1423	386	399	5	0	0
2	C	274	2255	1449	393	408	5	0	0
2	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
B	73	GLY	-	expression tag	UNP A1CWT6
B	74	SER	-	expression tag	UNP A1CWT6
B	190	PHE	ALA	conflict	UNP A1CWT6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	73	GLY	-	expression tag	UNP A1CWT6
C	74	SER	-	expression tag	UNP A1CWT6
C	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 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

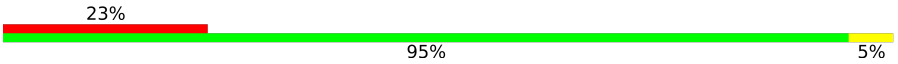
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
3	A	1	1	1	0

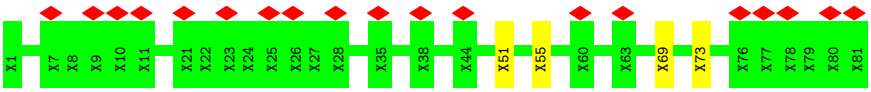
3 Residue-property plots (i)

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: Saposin A

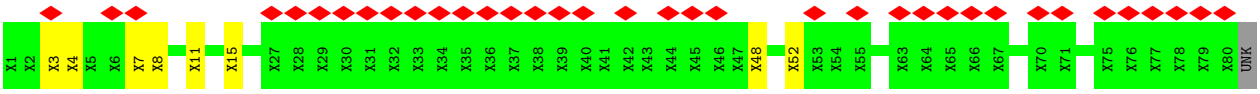
Chain F:





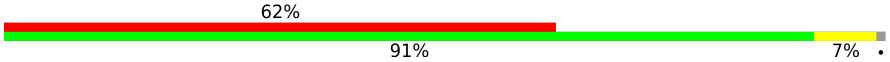
- Molecule 1: Saposin A

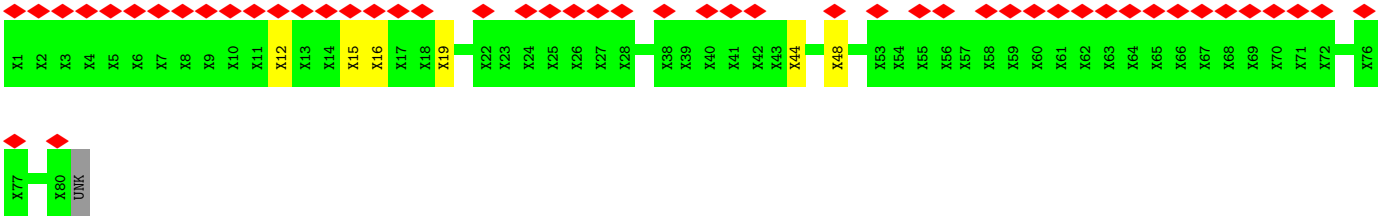
Chain H:



- Molecule 1: Saposin A

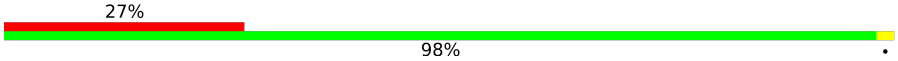
Chain G:

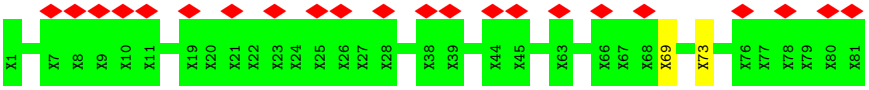




- Molecule 1: Saposin A

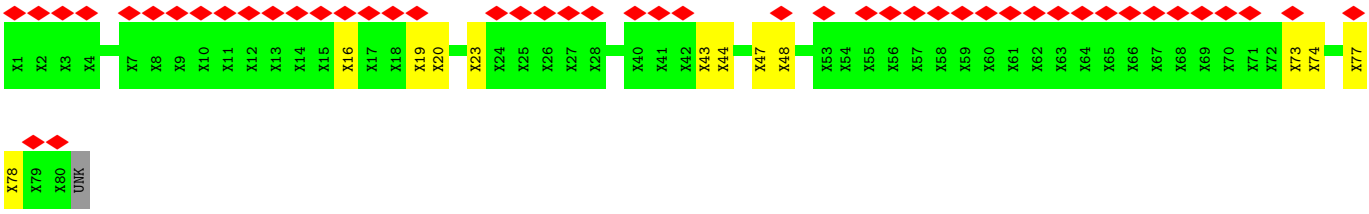
Chain I:





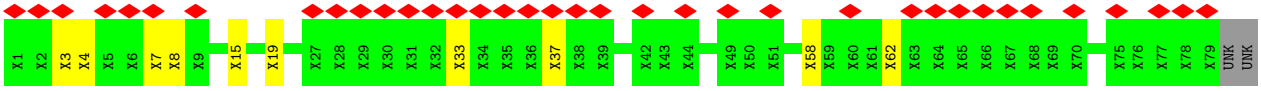
- Molecule 1: Saposin A

Chain J:



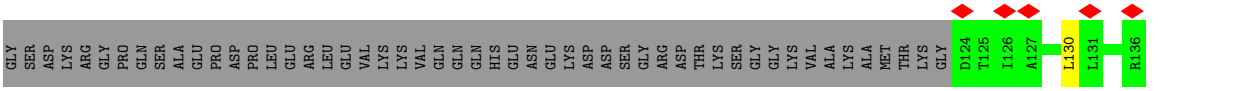
- Molecule 1: Saposin A

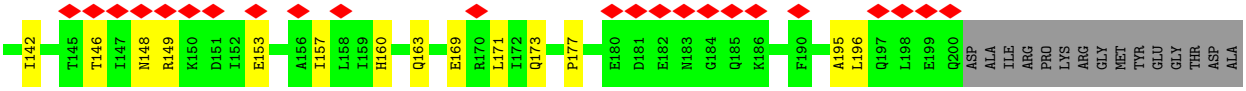
Chain K:

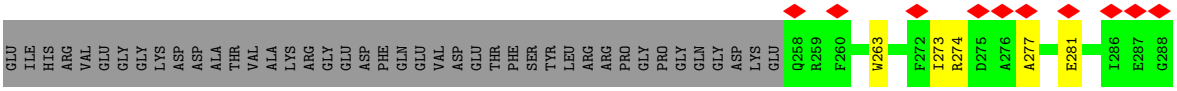


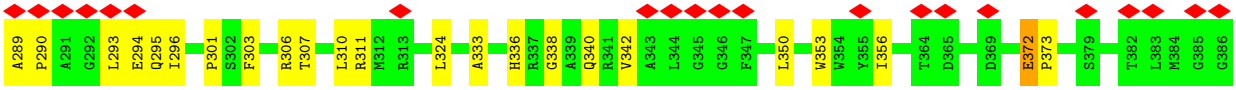
- Molecule 2: Mitochondrial calcium uniporter

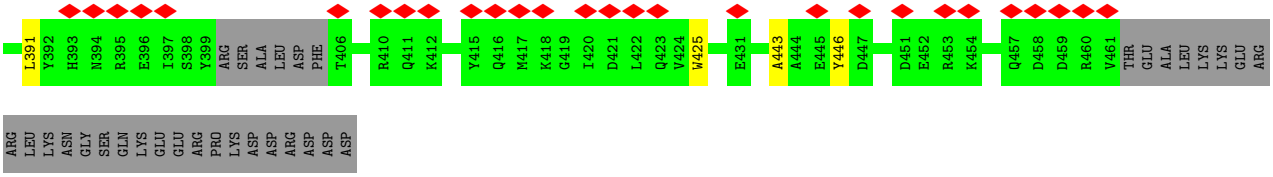
Chain A:





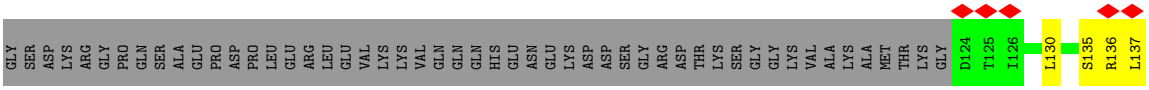


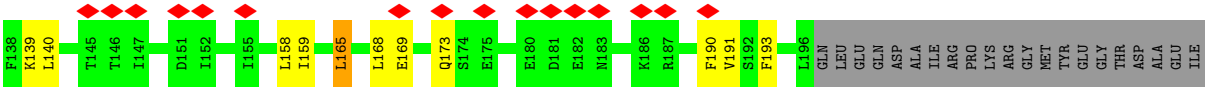


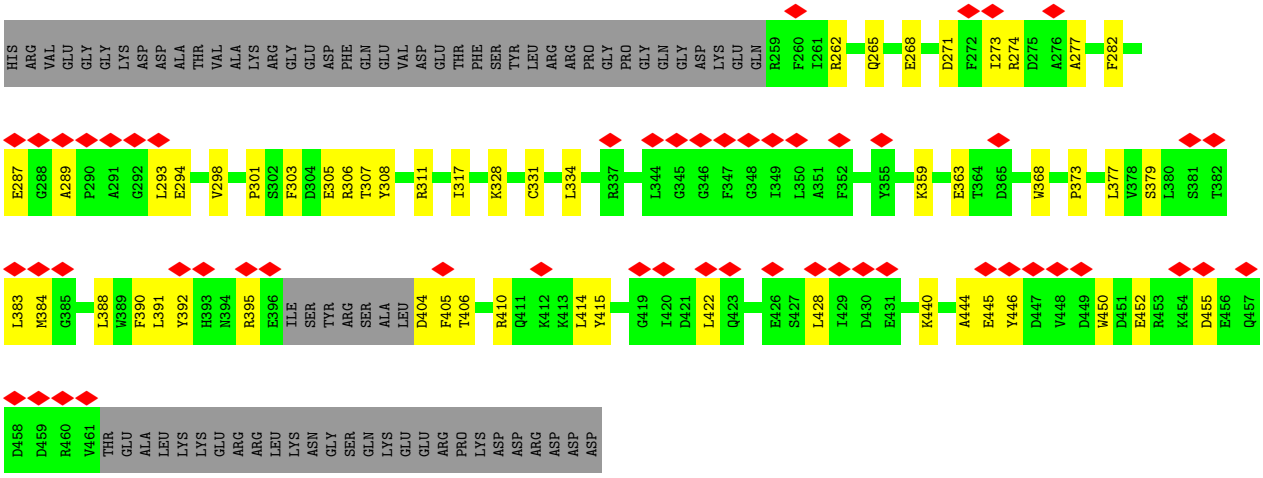


- Molecule 2: Mitochondrial calcium uniporter

Chain B:

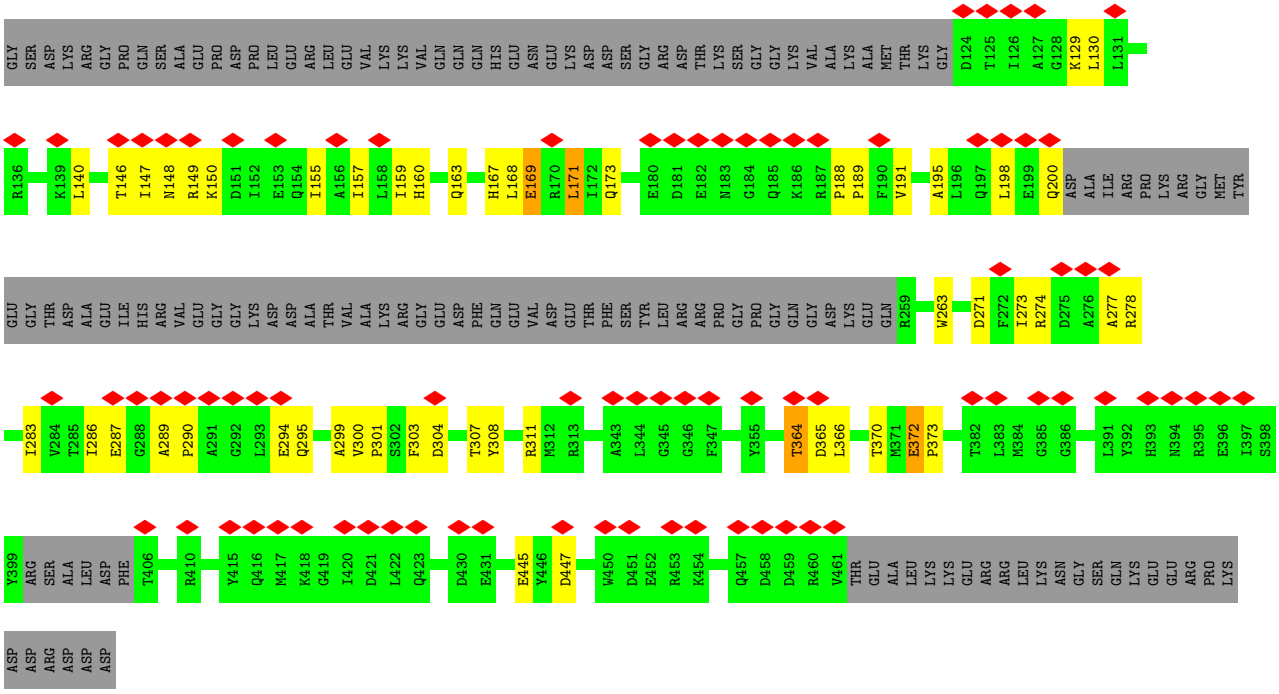






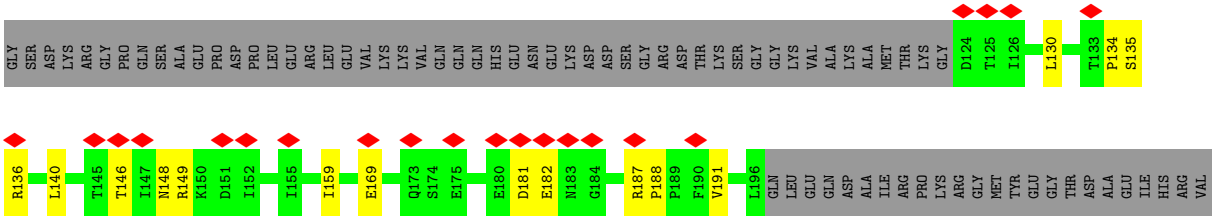
- Molecule 2: Mitochondrial calcium uniporter

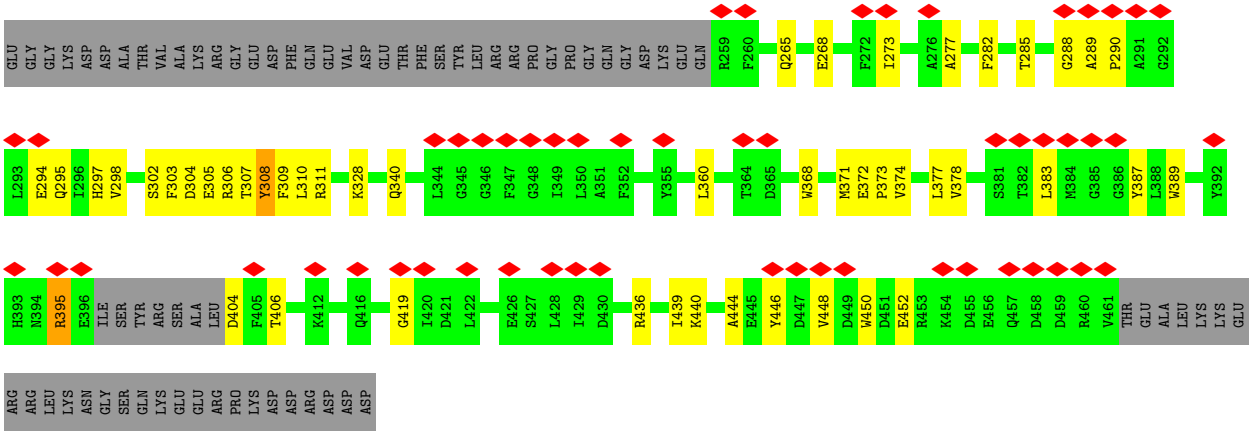
Chain C:



- Molecule 2: Mitochondrial calcium uniporter

Chain D:




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 Q265 E268 F272 I273 A276 A277 F282 T285 G288 A289 P290 A291 G292
L293 E294 Q295 I296 H297 V298 S302 F303 D304 E305 R306 T307 Y308 F309 L310 R311 K328 Q340 L344 G345 G346 F347 G348 I349 L350 A351 F352 Y355 L360 T364 D365 W368 M371 E372 P373 V374 L377 V378 S381 T382 L383 M384 G385 G386 Y387 L388 W389 Y392
H393 N394 R395 E396 ILE SER TYR ARG SER ALA LEU D404 F405 T406 K412 Q416 G419 I420 D421 L422 E426 S427 L428 I429 D430 R436 I439 K440 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, Not provided	
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	0.021	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.009	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	$\#\|Z\|>5$
2	A	0.37	0/2313	0.63	0/3129
2	B	0.37	0/2262	0.62	0/3060
2	C	0.37	0/2304	0.64	0/3117
2	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	F	405	0	83	2	0
1	G	400	0	82	3	0
1	H	400	0	82	4	0
1	I	405	0	83	1	0
1	J	400	0	82	6	0
1	K	395	0	81	5	0
2	A	2264	0	2270	58	0
2	B	2213	0	2217	72	0
2	C	2255	0	2262	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2213	0	2217	82	0
3	A	1	0	0	0	0
All	All	11351	0	9459	264	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 13.

All (264) 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)
2:D:307:THR:HG21	2:D:439:ILE:CD1	1.66	1.23
2:B:130:LEU:HD11	2:B:301:PRO:CD	1.74	1.15
2:D:307:THR:HG22	2:D:311:ARG:HD3	1.20	1.09
2:D:395:ARG:HH21	2:D:395:ARG:HG3	1.10	1.09
2:D:289:ALA:N	2:D:290:PRO:HD2	1.67	1.08
2:D:395:ARG:HH21	2:D:395:ARG:CG	1.67	1.07
2:D:307:THR:HG21	2:D:439:ILE:HD12	1.37	1.07
2:A:303:PHE:CE2	2:A:443:ALA:HA	1.93	1.03
2:D:307:THR:CG2	2:D:439:ILE:HD12	1.94	0.98
2:D:307:THR:HG21	2:D:439:ILE:HD11	1.41	0.98
2:B:307:THR:O	2:B:311:ARG:HG3	1.63	0.97
2:B:130:LEU:HD11	2:B:301:PRO:HD2	1.48	0.95
2:D:134:PRO:HA	2:D:309:PHE:CZ	2.04	0.92
2:A:303:PHE:HE2	2:A:443:ALA:HA	1.35	0.92
2:D:134:PRO:HB3	2:D:309:PHE:HZ	1.36	0.91
2:D:285:THR:HG23	2:D:294:GLU:O	1.73	0.89
2:B:130:LEU:CD1	2:B:301:PRO:CD	2.52	0.88
2:A:303:PHE:HE2	2:A:443:ALA:CA	1.86	0.87
2:B:130:LEU:CD1	2:B:301:PRO:HD3	2.04	0.86
2:D:289:ALA:N	2:D:290:PRO:CD	2.40	0.85
2:B:130:LEU:HD11	2:B:301:PRO:HD3	1.59	0.84
2:D:307:THR:HG22	2:D:311:ARG:CD	2.06	0.84
2:D:308:TYR:HA	2:D:311:ARG:NE	1.93	0.83
2:C:304:ASP:O	2:C:308:TYR:HB2	1.82	0.80
2:D:288:GLY:C	2:D:290:PRO:HD2	2.02	0.79
2:D:395:ARG:HG3	2:D:395:ARG:NH2	1.85	0.79
2:B:334:LEU:HD12	2:B:414:LEU:HD21	1.65	0.78
2:D:303:PHE:HB3	2:D:446:TYR:HD2	1.46	0.78
2:B:130:LEU:HD12	2:B:130:LEU:O	1.85	0.77
2:B:331:CYS:SG	2:B:415:TYR:HB3	2.24	0.77
2:A:336:HIS:O	2:A:340:GLN:HG2	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:163:GLN:OE1	2:C:167:HIS:CD2	2.38	0.76
2:A:130:LEU:HD12	2:A:301:PRO:HD3	1.67	0.76
2:A:307:THR:HG22	2:A:311:ARG:HG3	1.67	0.76
2:C:171:LEU:HD13	2:C:171:LEU:O	1.85	0.76
2:D:395:ARG:CG	2:D:395:ARG:NH2	2.38	0.76
2:D:307:THR:CG2	2:D:439:ILE:CD1	2.53	0.75
2:D:308:TYR:HB2	2:D:311:ARG:HH21	1.52	0.74
2:D:307:THR:CG2	2:D:311:ARG:HD3	2.09	0.73
2:A:130:LEU:HD12	2:A:130:LEU:O	1.89	0.73
2:D:303:PHE:CZ	2:D:448:VAL:HG21	2.23	0.73
2:C:273:ILE:O	2:C:277:ALA:HB2	1.90	0.72
2:D:134:PRO:CB	2:D:309:PHE:HZ	2.03	0.72
2:A:169:GLU:O	2:A:173:GLN:HB2	1.88	0.71
2:A:273:ILE:O	2:A:277:ALA:HB2	1.89	0.71
2:D:134:PRO:CA	2:D:309:PHE:CZ	2.73	0.70
2:A:303:PHE:CE2	2:A:443:ALA:CA	2.65	0.70
2:B:165:LEU:HD11	2:B:193:PHE:CD1	2.27	0.70
2:D:134:PRO:HA	2:D:309:PHE:CE1	2.26	0.69
2:B:311:ARG:HD2	2:B:455:ASP:OD2	1.92	0.69
2:B:373:PRO:O	2:B:377:LEU:HB2	1.93	0.69
2:B:293:LEU:C	2:B:293:LEU:HD12	2.14	0.68
2:B:334:LEU:C	2:B:334:LEU:HD13	2.14	0.68
2:A:130:LEU:CD1	2:A:301:PRO:HD3	2.24	0.68
2:B:368:TRP:NE1	2:C:372:GLU:HG2	2.09	0.67
2:B:293:LEU:HD12	2:B:293:LEU:O	1.95	0.67
2:D:308:TYR:HA	2:D:311:ARG:HE	1.57	0.67
2:B:395:ARG:HG2	2:B:405:PHE:HB2	1.76	0.66
2:D:273:ILE:O	2:D:277:ALA:HB2	1.94	0.66
2:A:149:ARG:HG2	2:A:153:GLU:HB2	1.78	0.65
2:B:287:GLU:OE2	2:B:287:GLU:HA	1.97	0.65
2:C:370:THR:O	2:C:370:THR:HG22	1.97	0.65
2:B:379:SER:O	2:B:383:LEU:HD23	1.98	0.64
2:A:290:PRO:CG	2:A:294:GLU:HB3	2.27	0.64
2:B:273:ILE:O	2:B:277:ALA:HB2	1.98	0.64
2:D:307:THR:O	2:D:308:TYR:C	2.34	0.63
2:B:317:ILE:HD11	2:B:428:LEU:HD22	1.81	0.63
2:B:308:TYR:HB3	2:B:311:ARG:NH2	2.14	0.63
2:C:159:ILE:HD11	2:C:168:LEU:HD13	1.81	0.62
2:A:372:GLU:HG2	2:D:368:TRP:NE1	2.14	0.62
2:B:169:GLU:HG2	2:B:191:VAL:HG22	1.82	0.62
2:B:328:LYS:HE3	2:B:415:TYR:CZ	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:307:THR:O	2:D:310:LEU:N	2.33	0.62
2:A:293:LEU:O	2:A:294:GLU:HG2	1.99	0.61
2:A:293:LEU:O	2:A:295:GLN:HG2	2.01	0.61
2:A:163:GLN:NE2	2:D:265:GLN:O	2.34	0.60
2:B:395:ARG:HD2	2:B:395:ARG:C	2.21	0.60
2:A:290:PRO:HG3	2:A:294:GLU:HB2	1.83	0.60
2:A:350:LEU:HD23	2:B:384:MET:SD	2.41	0.60
2:C:278:ARG:NH1	2:C:445:GLU:O	2.35	0.60
2:C:364:THR:HG23	2:C:364:THR:O	2.01	0.60
2:B:265:GLN:O	2:C:163:GLN:NE2	2.36	0.58
2:D:295:GLN:HG2	2:D:297:HIS:CD2	2.38	0.58
2:C:191:VAL:HG12	2:C:286:ILE:HA	1.84	0.58
2:C:146:THR:HG22	2:C:147:ILE:HD12	1.86	0.58
2:B:271:ASP:OD1	2:B:274:ARG:NH1	2.37	0.57
2:B:130:LEU:HD12	2:B:130:LEU:C	2.24	0.57
2:D:187:ARG:HG3	2:D:188:PRO:HD2	1.87	0.57
2:B:306:ARG:NH1	2:B:446:TYR:OH	2.37	0.57
2:A:290:PRO:CG	2:A:294:GLU:CB	2.83	0.56
2:B:328:LYS:HE3	2:B:415:TYR:CE1	2.40	0.56
2:B:190:PHE:HE2	2:B:262:ARG:HH22	1.53	0.56
2:A:350:LEU:HG	2:B:384:MET:HE2	1.86	0.56
2:D:308:TYR:CB	2:D:311:ARG:NH2	2.69	0.56
2:D:360:LEU:HB3	2:D:371:MET:CE	2.36	0.56
2:C:147:ILE:HG22	2:C:148:ASN:H	1.69	0.56
2:D:302:SER:O	2:D:306:ARG:N	2.32	0.56
2:B:388:LEU:HD11	2:B:392:TYR:CD2	2.41	0.56
2:B:130:LEU:HA	2:B:140:LEU:HA	1.88	0.55
2:D:373:PRO:O	2:D:377:LEU:HB2	2.06	0.55
2:B:130:LEU:HD11	2:B:301:PRO:CG	2.34	0.55
2:D:305:GLU:HA	2:D:308:TYR:HD2	1.72	0.55
2:C:365:ASP:OD1	2:C:365:ASP:N	2.40	0.54
2:A:196:LEU:HB2	2:A:281:GLU:HG2	1.90	0.54
2:B:169:GLU:OE2	2:B:173:GLN:NE2	2.41	0.54
2:D:383:LEU:O	2:D:387:TYR:HB2	2.08	0.54
2:B:404:ASP:HB3	2:B:406:THR:HG23	1.89	0.54
2:B:440:LYS:O	2:B:444:ALA:HB2	2.08	0.54
2:C:171:LEU:HD13	2:C:171:LEU:C	2.28	0.54
2:A:303:PHE:HB2	2:A:446:TYR:CG	2.42	0.53
2:C:273:ILE:O	2:C:277:ALA:CB	2.56	0.53
2:B:359:LYS:NZ	2:B:363:GLU:OE1	2.40	0.53
2:A:290:PRO:HG3	2:A:294:GLU:CB	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:LEU:CG	2:B:301:PRO:HD3	2.39	0.53
2:D:308:TYR:HB2	2:D:311:ARG:NH2	2.21	0.52
2:B:135:SER:OG	2:B:136:ARG:N	2.41	0.52
2:C:271:ASP:OD1	2:C:274:ARG:NH2	2.38	0.52
2:A:146:THR:HG23	2:A:177:PRO:HD3	1.91	0.52
2:B:334:LEU:HD13	2:B:334:LEU:O	2.10	0.52
2:C:149:ARG:HH21	2:C:150:LYS:HD3	1.75	0.51
2:B:410:ARG:O	2:B:414:LEU:HB2	2.09	0.51
2:C:304:ASP:O	2:C:308:TYR:CB	2.55	0.51
2:D:328:LYS:HZ3	2:D:419:GLY:HA3	1.76	0.51
2:C:372:GLU:N	2:C:373:PRO:CD	2.73	0.51
2:C:372:GLU:HB3	2:C:373:PRO:HD3	1.92	0.51
2:A:350:LEU:HG	2:B:384:MET:CE	2.40	0.51
2:D:134:PRO:HB3	2:D:309:PHE:CZ	2.28	0.51
2:A:289:ALA:N	2:A:290:PRO:HD2	2.26	0.51
2:B:165:LEU:HD13	2:B:165:LEU:O	2.10	0.51
2:C:198:LEU:HG	2:C:200:GLN:H	1.74	0.51
2:D:389:TRP:HD1	2:D:395:ARG:NH2	2.09	0.51
2:A:273:ILE:O	2:A:277:ALA:CB	2.58	0.51
1:H:4:UNK:O	1:H:8:UNK:CB	2.59	0.50
2:D:148:ASN:O	2:D:149:ARG:NE	2.41	0.50
2:D:307:THR:HG23	2:D:439:ILE:HD12	1.88	0.50
2:D:360:LEU:HB3	2:D:371:MET:HE3	1.92	0.50
2:D:395:ARG:HH21	2:D:395:ARG:HG2	1.66	0.50
2:B:190:PHE:CE2	2:B:262:ARG:NH2	2.79	0.50
2:B:273:ILE:O	2:B:277:ALA:CB	2.59	0.50
2:C:168:LEU:HD12	2:C:168:LEU:O	2.12	0.50
2:C:289:ALA:N	2:C:290:PRO:HD3	2.27	0.50
2:A:372:GLU:OE2	2:D:372:GLU:OE2	2.29	0.50
2:B:388:LEU:HD11	2:B:392:TYR:CE2	2.45	0.50
2:C:130:LEU:CD1	2:C:301:PRO:HD3	2.42	0.50
2:C:195:ALA:HB3	2:C:263:TRP:HE1	1.77	0.50
2:D:135:SER:OG	2:D:136:ARG:N	2.45	0.49
2:A:340:GLN:HE21	2:A:340:GLN:HA	1.78	0.49
2:C:189:PRO:HB3	2:C:287:GLU:HB3	1.93	0.49
2:D:273:ILE:O	2:D:277:ALA:CB	2.58	0.49
2:C:173:GLN:HE21	2:C:188:PRO:HB2	1.77	0.49
2:A:290:PRO:HB2	2:A:294:GLU:HB3	1.95	0.49
2:A:290:PRO:CB	2:A:294:GLU:HB3	2.43	0.49
2:A:391:LEU:HD11	2:D:340:GLN:HG2	1.94	0.49
2:B:390:PHE:HD1	2:B:395:ARG:NH2	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:PHE:HE2	2:B:262:ARG:NH2	2.10	0.48
2:A:303:PHE:CE2	2:A:443:ALA:CB	2.96	0.48
2:D:372:GLU:N	2:D:373:PRO:CD	2.76	0.48
2:A:160:HIS:NE2	2:D:268:GLU:OE2	2.36	0.48
2:D:303:PHE:HB3	2:D:446:TYR:CD2	2.37	0.48
2:D:308:TYR:C	2:D:308:TYR:CD1	2.86	0.48
2:A:340:GLN:HA	2:A:340:GLN:NE2	2.29	0.48
2:B:328:LYS:NZ	2:B:422:LEU:HD21	2.29	0.48
2:D:187:ARG:CG	2:D:188:PRO:HD2	2.44	0.48
2:B:268:GLU:OE2	2:C:160:HIS:NE2	2.45	0.48
2:D:374:VAL:O	2:D:378:VAL:HB	2.14	0.48
1:H:11:UNK:O	1:H:15:UNK:CB	2.62	0.48
1:F:69:UNK:O	1:F:73:UNK:CB	2.62	0.47
2:B:303:PHE:HB3	2:B:446:TYR:HD2	1.79	0.47
2:B:289:ALA:HB2	2:B:294:GLU:HB3	1.96	0.47
2:B:305:GLU:HA	2:B:308:TYR:CD2	2.49	0.47
2:A:307:THR:O	2:A:310:LEU:N	2.47	0.47
2:D:134:PRO:CA	2:D:309:PHE:HZ	2.23	0.47
1:G:44:UNK:O	1:G:48:UNK:CB	2.63	0.47
2:B:450:TRP:HE1	2:B:452:GLU:HG3	1.80	0.47
2:D:440:LYS:O	2:D:444:ALA:HB2	2.15	0.47
2:D:304:ASP:O	2:D:308:TYR:HB3	2.14	0.47
1:I:69:UNK:O	1:I:73:UNK:CB	2.63	0.47
1:J:74:UNK:O	1:J:78:UNK:CB	2.63	0.46
2:C:140:LEU:HD23	2:C:157:ILE:HB	1.98	0.46
1:K:4:UNK:O	1:K:8:UNK:CB	2.64	0.46
1:J:73:UNK:O	1:J:77:UNK:CB	2.63	0.46
2:B:440:LYS:O	2:B:444:ALA:CB	2.64	0.46
1:J:19:UNK:O	1:J:23:UNK:CB	2.64	0.46
2:D:306:ARG:NH1	2:D:446:TYR:OH	2.47	0.46
2:D:450:TRP:HE1	2:D:452:GLU:HG3	1.80	0.46
1:J:44:UNK:O	1:J:48:UNK:CB	2.63	0.45
2:A:307:THR:CG2	2:A:311:ARG:HG3	2.43	0.45
2:A:333:ALA:HA	2:A:336:HIS:CD2	2.51	0.45
2:B:130:LEU:HG	2:B:301:PRO:HD3	1.97	0.45
2:C:370:THR:O	2:C:370:THR:CG2	2.61	0.45
2:A:373:PRO:HG3	2:D:368:TRP:CD2	2.50	0.45
2:C:169:GLU:HB2	2:C:191:VAL:CG2	2.46	0.45
2:C:289:ALA:HB2	2:C:294:GLU:HG3	1.98	0.45
2:B:308:TYR:HA	2:B:311:ARG:HB2	1.99	0.45
2:D:181:ASP:HA	2:D:182:GLU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:404:ASP:HB3	2:D:406:THR:HG23	1.97	0.45
1:F:51:UNK:O	1:F:55:UNK:CB	2.65	0.45
2:A:340:GLN:NE2	2:B:391:LEU:HD22	2.32	0.45
2:C:163:GLN:OE1	2:C:167:HIS:HD2	1.93	0.44
1:H:48:UNK:O	1:H:52:UNK:CB	2.66	0.44
2:A:340:GLN:HE22	2:B:391:LEU:HD22	1.82	0.44
2:C:129:LYS:HG2	2:C:299:ALA:HB3	1.98	0.44
2:D:140:LEU:HD22	2:D:159:ILE:HD11	1.99	0.44
2:D:282:PHE:HB3	2:D:298:VAL:HG22	1.98	0.44
1:K:15:UNK:O	1:K:19:UNK:CB	2.66	0.44
2:C:171:LEU:C	2:C:171:LEU:CD1	2.86	0.44
2:D:290:PRO:HB2	2:D:294:GLU:H	1.83	0.44
2:D:368:TRP:HA	2:D:371:MET:HB3	1.99	0.44
2:A:146:THR:HG22	2:A:148:ASN:H	1.82	0.44
2:C:307:THR:O	2:C:311:ARG:HB2	2.18	0.44
2:A:274:ARG:HH22	2:B:137:LEU:HD21	1.81	0.43
2:A:306:ARG:HD3	2:A:446:TYR:OH	2.18	0.43
1:H:3:UNK:O	1:H:7:UNK:CB	2.65	0.43
2:A:142:ILE:HG23	2:A:296:ILE:HG21	2.00	0.43
2:D:436:ARG:HA	2:D:439:ILE:HG22	2.01	0.43
2:B:395:ARG:C	2:B:395:ARG:CD	2.86	0.43
2:C:155:ILE:H	2:C:155:ILE:HG13	1.62	0.43
2:A:293:LEU:O	2:A:294:GLU:CG	2.65	0.43
1:J:43:UNK:O	1:J:47:UNK:CB	2.66	0.43
2:A:303:PHE:HE2	2:A:443:ALA:CB	2.32	0.43
2:D:302:SER:O	2:D:306:ARG:HB2	2.19	0.43
2:D:383:LEU:O	2:D:387:TYR:CB	2.67	0.43
2:B:159:ILE:HD11	2:B:168:LEU:HD13	2.01	0.43
2:D:440:LYS:O	2:D:444:ALA:CB	2.66	0.43
2:A:195:ALA:HB3	2:A:263:TRP:HE1	1.83	0.43
2:A:303:PHE:CD1	2:A:303:PHE:C	2.91	0.43
2:A:372:GLU:HG2	2:D:368:TRP:HE1	1.79	0.43
2:C:277:ALA:HA	2:C:300:VAL:HG11	2.01	0.43
2:C:283:ILE:HG21	2:C:295:GLN:NE2	2.33	0.43
2:B:334:LEU:C	2:B:334:LEU:CD1	2.85	0.43
1:G:12:UNK:O	1:G:16:UNK:CB	2.67	0.42
2:B:307:THR:O	2:B:311:ARG:CG	2.52	0.42
2:D:169:GLU:HG3	2:D:191:VAL:HG22	2.01	0.42
2:D:304:ASP:O	2:D:308:TYR:N	2.32	0.42
2:B:282:PHE:HB3	2:B:298:VAL:HG22	2.01	0.42
1:J:16:UNK:O	1:J:20:UNK:CB	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:360:LEU:HB3	2:D:371:MET:HE1	2.01	0.42
2:D:130:LEU:HA	2:D:140:LEU:HA	2.01	0.42
2:A:293:LEU:C	2:A:294:GLU:HG2	2.39	0.42
2:A:324:LEU:HD23	2:A:425:TRP:HE3	1.84	0.42
2:A:303:PHE:CE2	2:A:443:ALA:HB2	2.55	0.42
2:C:289:ALA:CB	2:C:294:GLU:HG3	2.50	0.42
2:B:130:LEU:CD1	2:B:301:PRO:CG	2.97	0.42
1:K:3:UNK:O	1:K:7:UNK:CB	2.68	0.41
1:K:58:UNK:O	1:K:62:UNK:N	2.53	0.41
2:C:294:GLU:O	2:C:294:GLU:HG2	2.20	0.41
2:C:365:ASP:OD1	2:C:366:LEU:N	2.53	0.41
2:A:306:ARG:CD	2:A:446:TYR:OH	2.68	0.41
2:C:278:ARG:NH2	2:C:447:ASP:OD2	2.52	0.41
2:C:289:ALA:HA	2:C:294:GLU:HG3	2.02	0.41
1:G:15:UNK:O	1:G:19:UNK:CB	2.69	0.41
1:K:33:UNK:O	1:K:37:UNK:CB	2.69	0.41
2:A:353:TRP:HA	2:A:356:ILE:HG22	2.03	0.41
2:D:308:TYR:HA	2:D:311:ARG:CZ	2.49	0.41
2:D:303:PHE:CE1	2:D:448:VAL:HG21	2.55	0.41
2:D:307:THR:O	2:D:309:PHE:N	2.54	0.41
2:D:308:TYR:CB	2:D:311:ARG:HH21	2.21	0.41
2:B:274:ARG:HD2	2:B:445:GLU:HB3	2.03	0.40
2:A:157:ILE:HG23	2:A:171:LEU:HD12	2.02	0.40
2:C:130:LEU:HD12	2:C:301:PRO:HD3	2.03	0.40
2:C:303:PHE:O	2:C:307:THR:OG1	2.27	0.40
2:A:338:GLY:O	2:A:342:VAL:HG23	2.22	0.40
2:B:139:LYS:HB3	2:B:158:LEU:HD23	2.03	0.40
2:B:388:LEU:CD1	2:B: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	
2	A	269/416 (65%)	256 (95%)	13 (5%)	0	100	100
2	B	263/416 (63%)	242 (92%)	21 (8%)	0	100	100
2	C	268/416 (64%)	254 (95%)	14 (5%)	0	100	100
2	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	
2	A	241/358 (67%)	240 (100%)	1 (0%)	91	94
2	B	235/358 (66%)	234 (100%)	1 (0%)	91	94
2	C	240/358 (67%)	236 (98%)	4 (2%)	60	78
2	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
2	A	372	GLU
2	B	165	LEU
2	C	169	GLU
2	C	171	LEU
2	C	364	THR
2	C	372	GLU
2	D	146	THR
2	D	308	TYR
2	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
2	A	162	GLN
2	A	295	GLN
2	A	340	GLN
2	A	408	ASN
2	B	173	GLN
2	B	441	ASN
2	C	167	HIS
2	C	295	GLN
2	C	340	GLN
2	D	154	GLN
2	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.

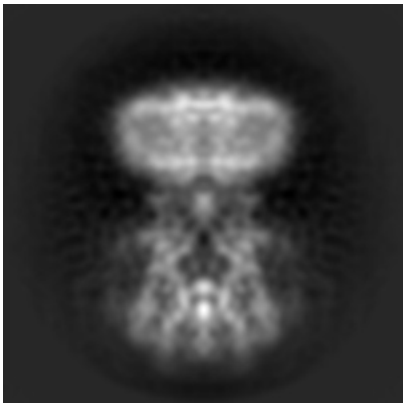
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-7828. These allow visual inspection of the internal detail of the map and identification of artifacts.

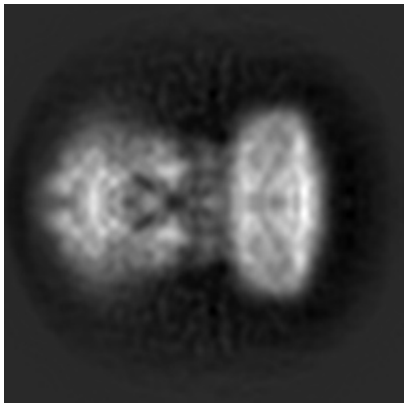
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

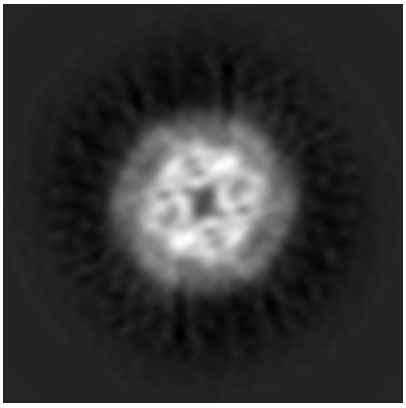
6.1.1 Primary map



X



Y

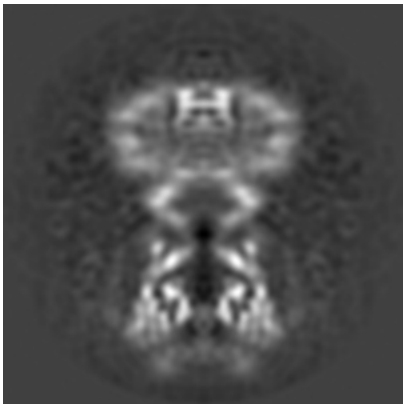


Z

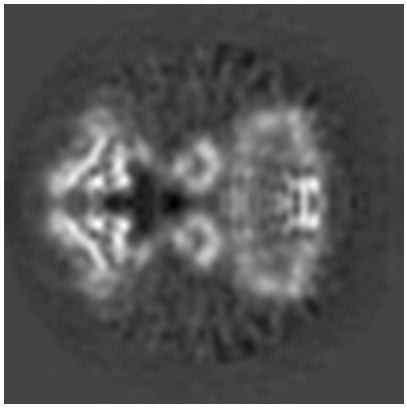
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

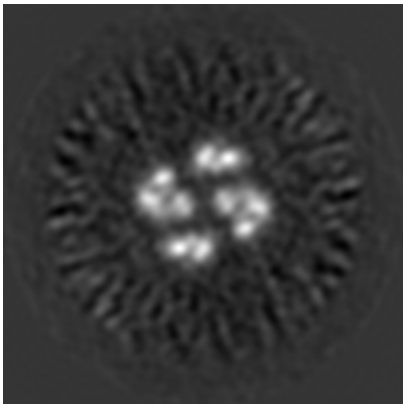
6.2.1 Primary map



X Index: 110



Y Index: 110

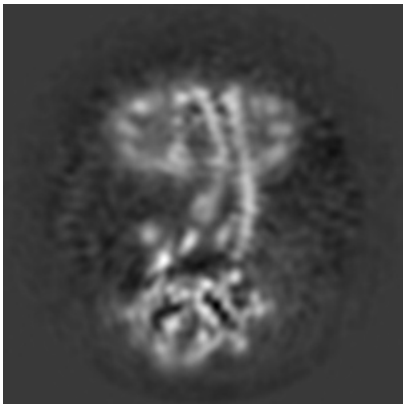


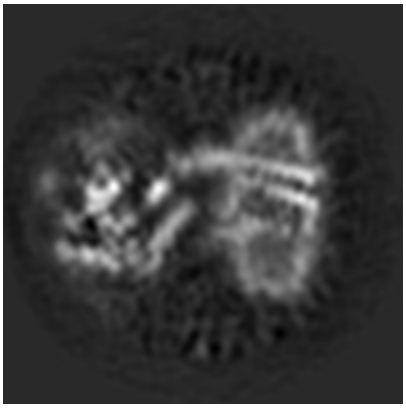
Z Index: 110

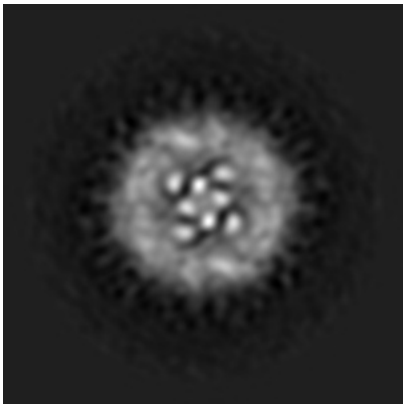
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 122

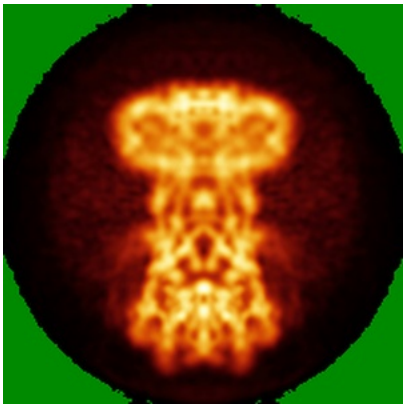

Y Index: 99

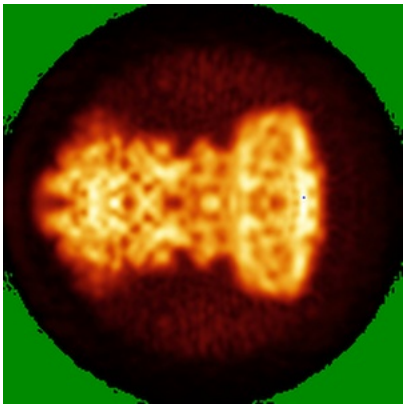

Z Index: 163

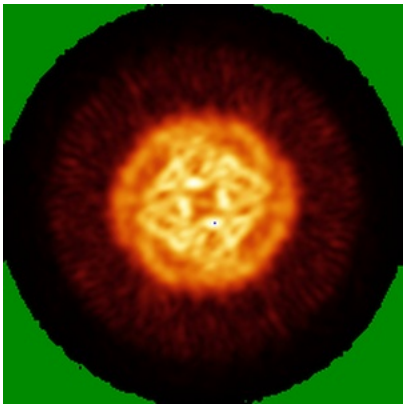
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

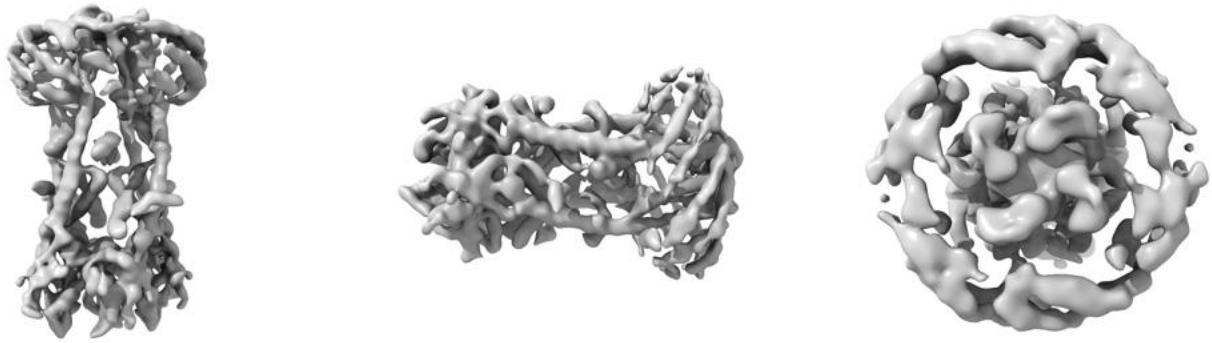

Y


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

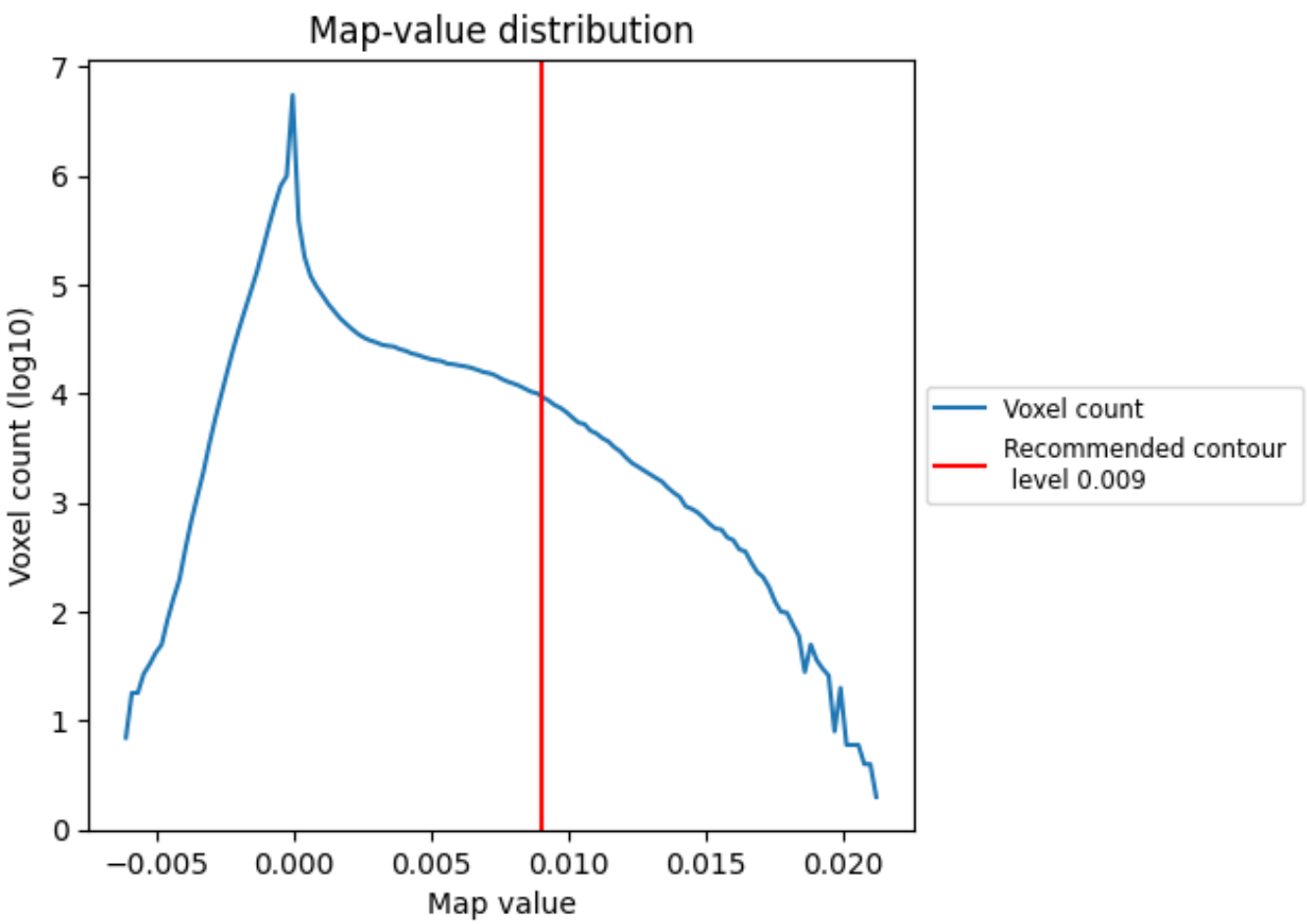
6.6 Mask visualisation (i)

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

7 Map analysis (i)

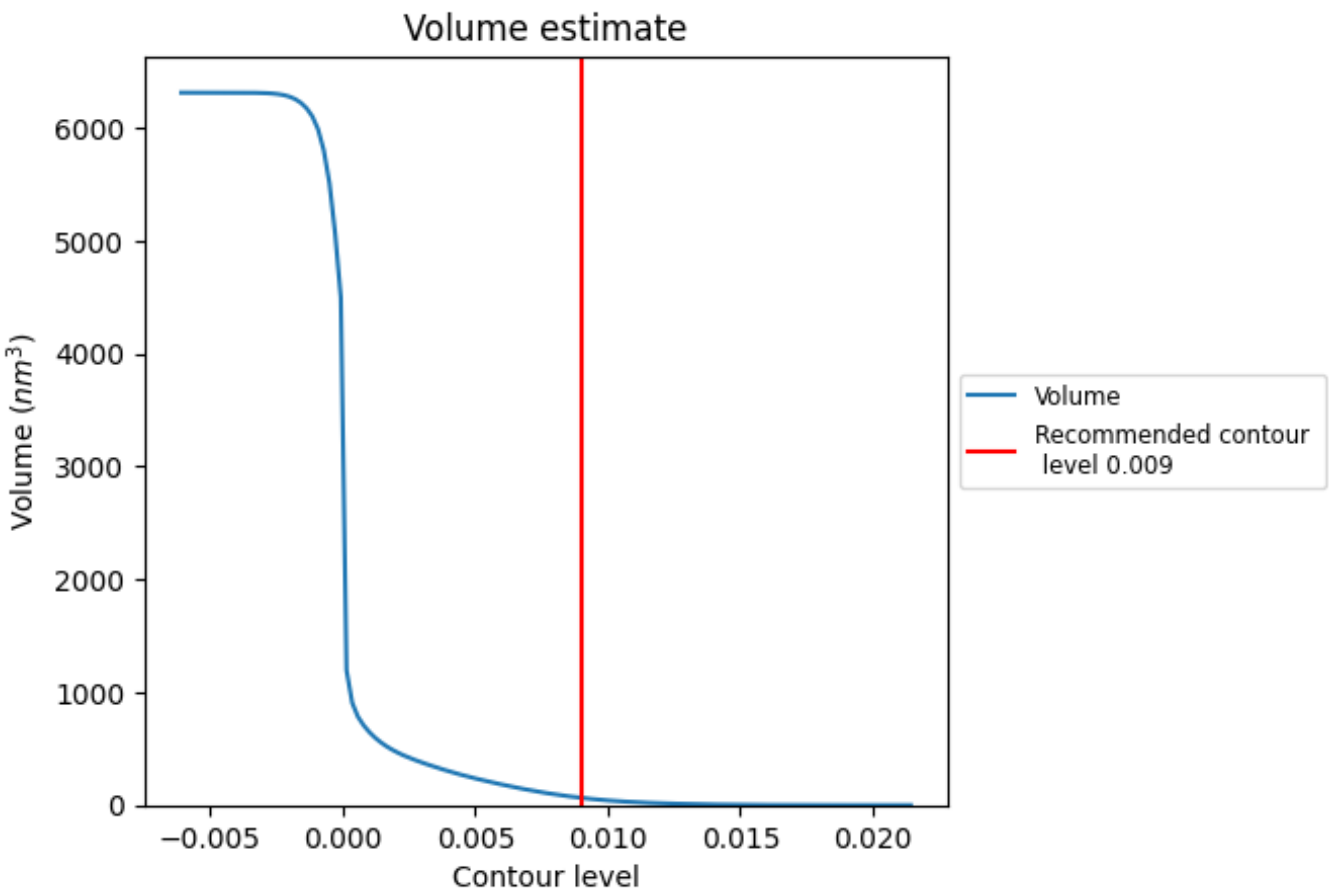
This section contains the results of statistical analysis of the map.

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.

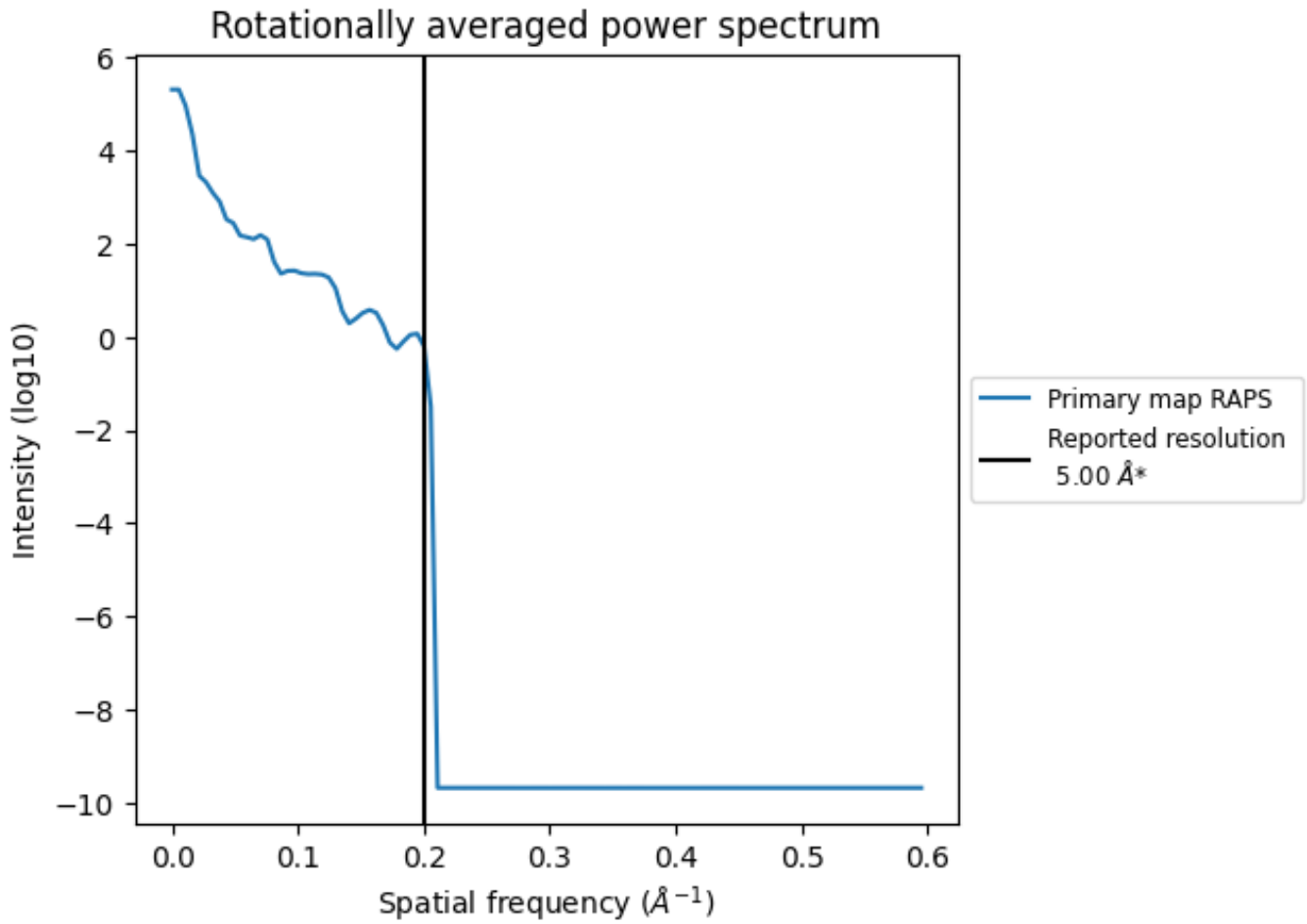
7.2 Volume estimate (i)



The volume at the recommended contour level is 65 nm^3; this corresponds to an approximate mass of 59 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 0.200 Å^{-1}

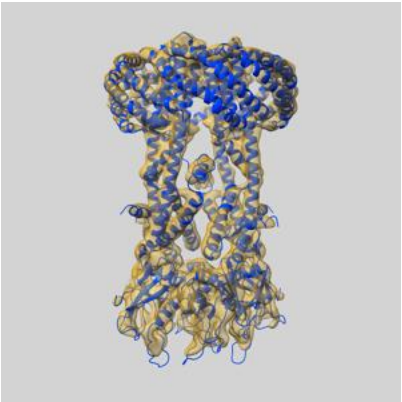
8 Fourier-Shell correlation (i)

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

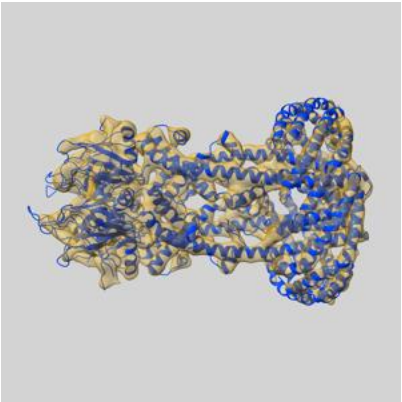
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-7828 and PDB model 6D80. Per-residue inclusion information can be found in section 3 on page 6.

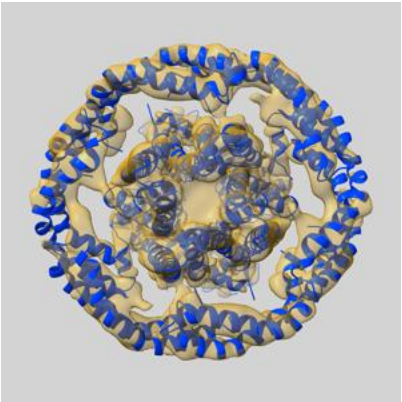
9.1 Map-model overlay (i)



X



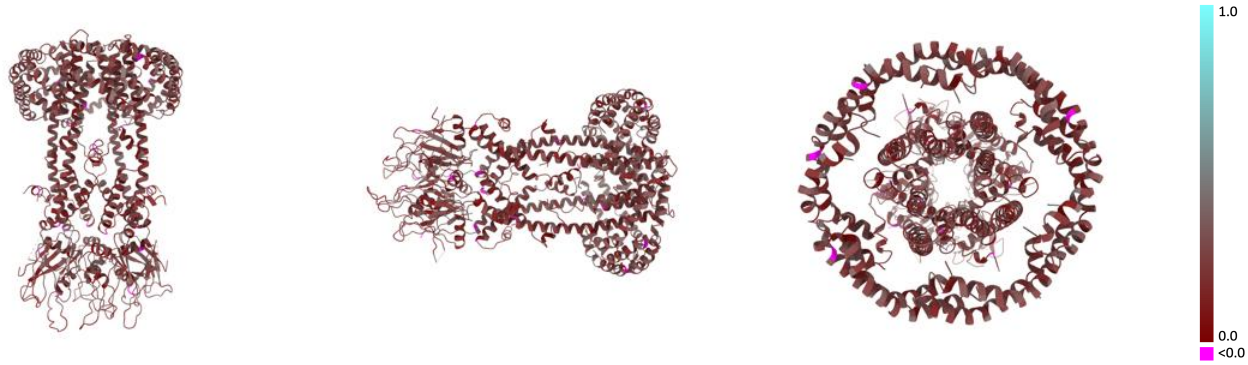
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.009 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.

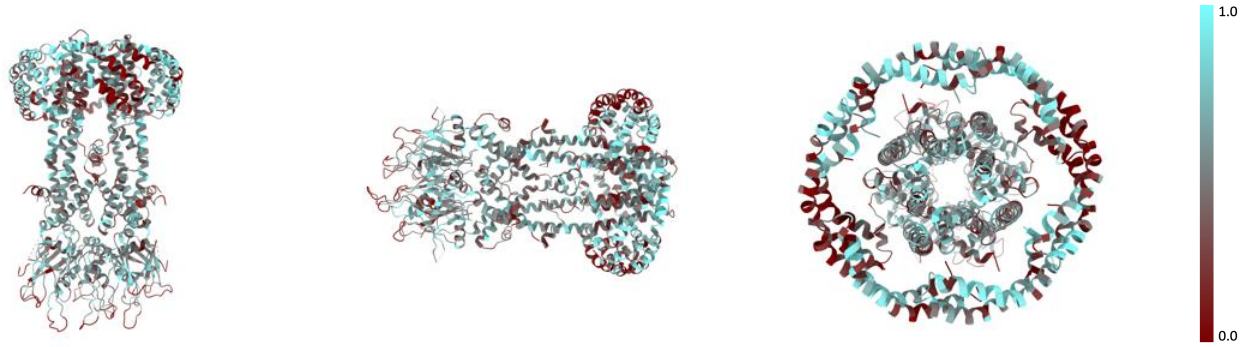
9.2 Q-score mapped to coordinate model (i)



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.

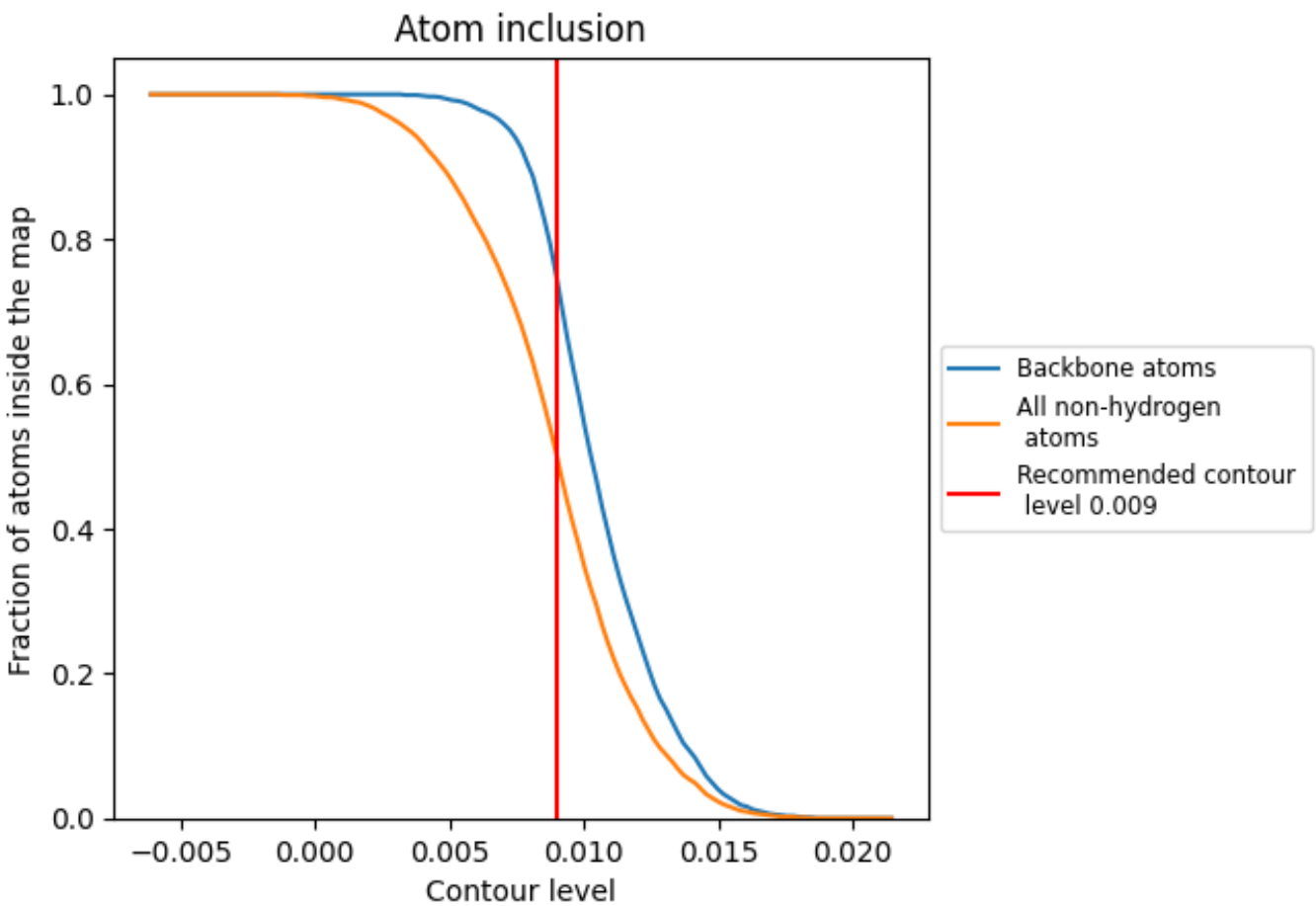
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.009).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 50% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4990	0.2350
A	0.4840	0.2270
B	0.5140	0.2230
C	0.4810	0.2290
D	0.5120	0.2280
F	0.6320	0.2730
G	0.3700	0.2530
H	0.5120	0.2650
I	0.6200	0.2710
J	0.3780	0.2620
K	0.5090	0.2700