



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:10 PM UTC

PDB ID : 8YF1 / pdb_00008yf1
EMDB ID : EMD-39207
Title : Cryo-EM structure of human SV2A in complex with Brivaracetam
Authors : Qu, Q.; Liu, S.; Zhou, Z.
Deposited on : 2024-02-23
Resolution : 3.38 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

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<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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

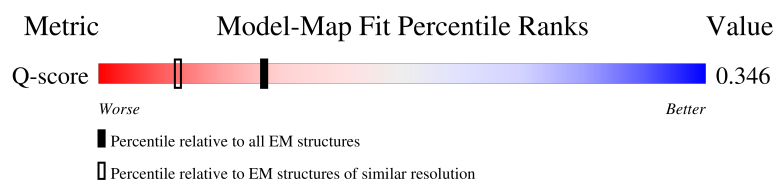
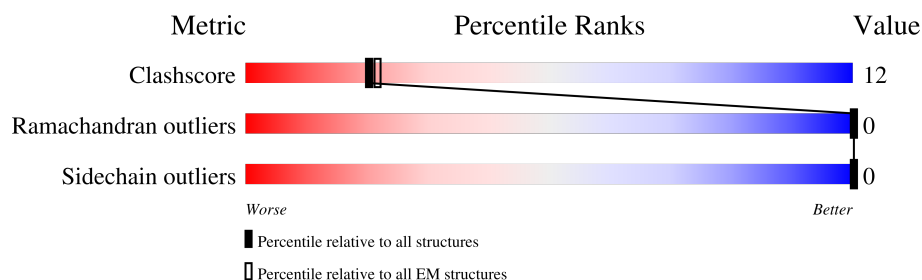
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.38 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14261 (2.88 - 3.88)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	755	
1	B	755	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	VLX	B	801	-	X	-	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9187 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 Synaptic vesicle glycoprotein 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	567	Total	C	N	O	S	0	0
			4505	2937	746	787	35		
1	A	589	Total	C	N	O	S	0	0
			4652	3039	770	808	35		

There are 42 discrepancies between the modelled and reference sequences:

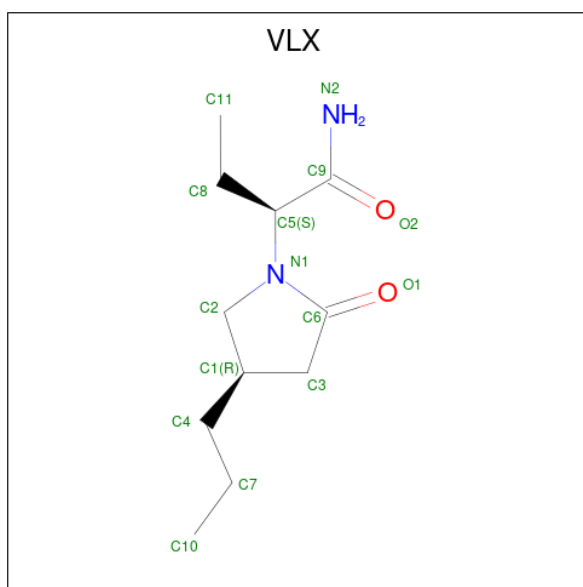
Chain	Residue	Modelled	Actual	Comment	Reference
B	735	SER	-	expression tag	UNP Q7L0J3
B	736	ARG	-	expression tag	UNP Q7L0J3
B	737	LEU	-	expression tag	UNP Q7L0J3
B	738	GLU	-	expression tag	UNP Q7L0J3
B	739	GLU	-	expression tag	UNP Q7L0J3
B	740	GLU	-	expression tag	UNP Q7L0J3
B	741	LEU	-	expression tag	UNP Q7L0J3
B	742	ARG	-	expression tag	UNP Q7L0J3
B	743	ARG	-	expression tag	UNP Q7L0J3
B	744	ARG	-	expression tag	UNP Q7L0J3
B	745	THR	-	expression tag	UNP Q7L0J3
B	746	GLU	-	expression tag	UNP Q7L0J3
B	747	PRO	-	expression tag	UNP Q7L0J3
B	748	GLY	-	expression tag	UNP Q7L0J3
B	749	SER	-	expression tag	UNP Q7L0J3
B	750	LEU	-	expression tag	UNP Q7L0J3
B	751	GLU	-	expression tag	UNP Q7L0J3
B	752	VAL	-	expression tag	UNP Q7L0J3
B	753	LEU	-	expression tag	UNP Q7L0J3
B	754	PHE	-	expression tag	UNP Q7L0J3
B	755	GLN	-	expression tag	UNP Q7L0J3
A	735	SER	-	expression tag	UNP Q7L0J3
A	736	ARG	-	expression tag	UNP Q7L0J3
A	737	LEU	-	expression tag	UNP Q7L0J3
A	738	GLU	-	expression tag	UNP Q7L0J3
A	739	GLU	-	expression tag	UNP Q7L0J3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	740	GLU	-	expression tag	UNP Q7L0J3
A	741	LEU	-	expression tag	UNP Q7L0J3
A	742	ARG	-	expression tag	UNP Q7L0J3
A	743	ARG	-	expression tag	UNP Q7L0J3
A	744	ARG	-	expression tag	UNP Q7L0J3
A	745	THR	-	expression tag	UNP Q7L0J3
A	746	GLU	-	expression tag	UNP Q7L0J3
A	747	PRO	-	expression tag	UNP Q7L0J3
A	748	GLY	-	expression tag	UNP Q7L0J3
A	749	SER	-	expression tag	UNP Q7L0J3
A	750	LEU	-	expression tag	UNP Q7L0J3
A	751	GLU	-	expression tag	UNP Q7L0J3
A	752	VAL	-	expression tag	UNP Q7L0J3
A	753	LEU	-	expression tag	UNP Q7L0J3
A	754	PHE	-	expression tag	UNP Q7L0J3
A	755	GLN	-	expression tag	UNP Q7L0J3

- Molecule 2 is (2S)-2-[(4R)-2-oxidanylidene-4-propyl-pyrrolidin-1-yl]butanamide (CCD ID: VLX) (formula: C₁₁H₂₀N₂O₂) (labeled as "Ligand of Interest" by depositor).

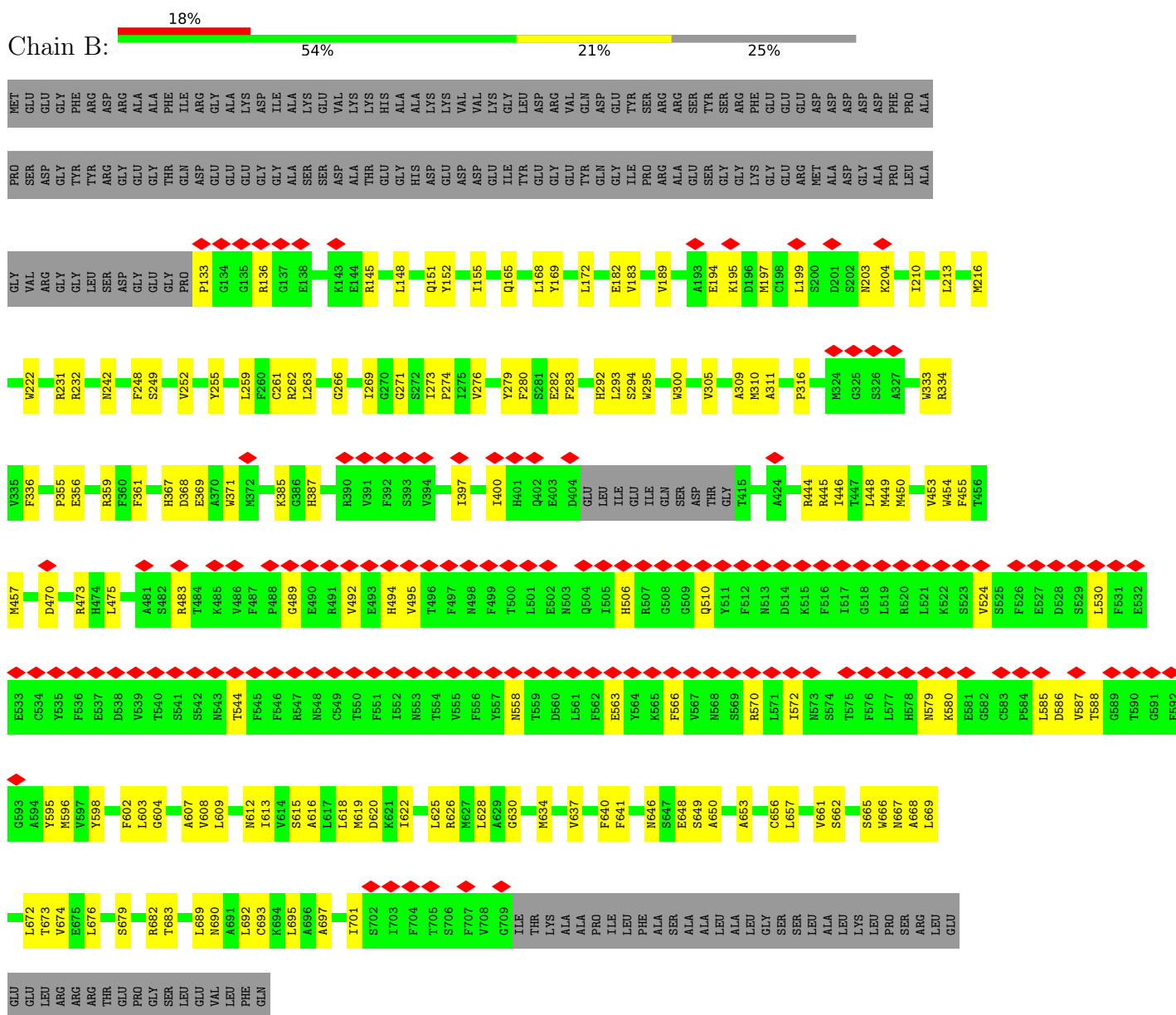


Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	N	O	0
			15	11	2	2	
2	A	1	Total	C	N	O	0
			15	11	2	2	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Synaptic vesicle glycoprotein 2A



• Molecule 1: Synaptic vesicle glycoprotein 2A



MET
GLU
GLY
GLY
PHE
ARG
ASP
ARG
ALA
ALA
PHE
GLN
ILE
ARG
GLY
ALA
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ILE
ALA
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GLU
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HIS
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ALA
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LYS
VAL
VAL
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LYS
GLY
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PRO
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PRO
SER
ASP
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ARG
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THR
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ALA
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GLY
PRO
P133
G134
G136
R136
A139
Q140
R141
R142
K143
E144
R145
Q150
A154
R157
F164
Y169
L172
G173
L174
A175
L176
M177
A178
D179
G180
V181
V189
L190
P191
S192
A193
E194
K195
D196
K197
C198
L199
S200
D201

L210
L213
G218
V222
G223
A226
R231
S238
F248
V252
Q253
G254
L259
R262
V267
G268
L269
L273
F274
L275
V276
F280
S281
E282
F283
K288
H292
L296
C297
M298
F299
I302
G303
M310
I314
I315
P316
S326
A327
Y328

V335
F336
P343
S344
V345
T348
S357
P358
W371
R372
L374
K375
G376
V377
H378
D379
T380
N381
M382
R383
E389
R390
V391
F392
S393
V394
T395
H396
I397
K398
T399
I400
H401
Q402
GLU
ASP
GLU
LEU
ILE
ILE
ILE
GLN
SER
ASP
THR
GLY
THR
W416
Y417
Q418
R419
W420

R423
Q440
E442
I446
V453
T456
G463
L464
T465
V466
W467
F468
P469
I472
R473
Q476
Y480
A481
S482
R483
T484
K485
V486
F487
P488
G489
E490
R491
V492
E493
H494
V495
T496
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F499
T500
L501
E502
N503
Q504
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H506
R507
G508
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Y511
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D514

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K522
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S529
L530
F531
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Y564
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F566
N568
S569
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N573
S574

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C583
P584
L585
D586
V587
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T590
G591
V597
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A607
V608
L609
P610
I613
W619
M627
S638
F641
E648
S649
A650
W651
I652
A653
L654
L655
C656
L657
F658
W666
N667
A668
L672
L676
Y677
P678

K681
R682
T683
L695
A696
A697
V698
I701
G709
K712
A719
L723
G726
A730
L733
F734
SER
ARG
LEU
GLU
GLU
GLU
LEU
ARG
ARG
ARG
THR
GLU
PRO
GLY
SER
LEU
GLU
VAL
PHE
GLN

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	112317	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	4.147	Depositor
Minimum map value	-3.394	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.090	Depositor
Recommended contour level	0.23	Depositor
Map size ($\text{\AA}$)	251.64, 251.64, 251.64	wwPDB
Map dimensions	270, 270, 270	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.932, 0.932, 0.932	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.17	0/4781	0.35	0/6468
1	B	0.17	1/4631 (0.0%)	0.32	0/6263
All	All	0.17	1/9412 (0.0%)	0.34	0/12731

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	282	GLU	CA-C	-5.17	1.45	1.52

There are no bond angle outliers.

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	4652	0	4584	112	0
1	B	4505	0	4404	115	0
2	A	15	0	0	1	0
2	B	15	0	0	1	0
All	All	9187	0	8988	222	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (222) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:619:MET:HE1	1:B:668:ALA:HB2	1.58	0.84
1:B:607:ALA:HB2	1:A:654:LEU:HD13	1.63	0.81
1:B:603:LEU:HD22	1:A:650:ALA:HB1	1.70	0.74
1:A:164:PHE:HB2	1:A:380:THR:HB	1.68	0.74
1:B:194:GLU:HG3	1:B:204:LYS:HB2	1.73	0.71
1:A:375:LYS:HA	1:A:378:HIS:CE1	2.26	0.69
1:B:222:TRP:HB2	1:B:271:GLY:HA3	1.74	0.69
1:B:273:ILE:HD11	2:B:801:VLX:C8	2.24	0.67
1:B:475:LEU:HD13	1:B:648:GLU:HB2	1.77	0.67
1:B:649:SER:HB3	1:A:653:ALA:HB2	1.76	0.67
1:B:646:ASN:HB3	1:A:603:LEU:HD12	1.76	0.66
1:B:367:HIS:HB3	1:B:400:ILE:HD13	1.78	0.66
1:B:199:LEU:HD12	1:B:203:ASN:HB3	1.79	0.65
1:B:197:MET:SD	1:B:334:ARG:NH2	2.71	0.63
1:A:314:ILE:HD12	1:A:335:VAL:HG12	1.79	0.63
1:A:179:ASP:HA	1:A:269:ILE:HD12	1.78	0.63
1:B:172:LEU:HB3	1:B:276:VAL:HG23	1.79	0.63
1:B:619:MET:O	1:B:626:ARG:NH1	2.28	0.63
1:B:165:GLN:NE2	1:B:283:PHE:O	2.33	0.62
1:B:640:PHE:HE1	1:B:653:ALA:HB1	1.64	0.61
1:B:674:VAL:HG23	1:B:682:ARG:HD3	1.80	0.61
1:B:273:ILE:HA	1:B:276:VAL:HG12	1.82	0.61
1:B:622:ILE:HD11	1:B:626:ARG:HA	1.84	0.60
1:B:455:PHE:HE1	1:B:692:LEU:HG	1.68	0.59
1:A:194:GLU:HA	1:A:199:LEU:HB3	1.85	0.59
1:B:669:LEU:O	1:B:673:THR:HG23	2.03	0.59
1:A:142:ARG:HB2	1:A:145:ARG:HH21	1.66	0.58
1:B:274:PRO:HG3	1:B:690:ASN:HD22	1.66	0.58
1:A:299:PHE:HA	1:A:302:ILE:HG22	1.85	0.58
1:A:172:LEU:HD13	1:A:280:PHE:HB2	1.86	0.58
1:A:558:ASN:HB3	1:A:580:LYS:HE3	1.85	0.58
1:A:382:MET:HG2	1:A:389:GLU:HB2	1.86	0.58
1:A:373:VAL:O	1:A:377:VAL:HG23	2.04	0.58
1:A:486:VAL:HG11	1:A:507:ARG:HE	1.69	0.58
1:B:558:ASN:HA	1:B:580:LYS:H	1.69	0.57
1:B:280:PHE:CE2	1:B:292:HIS:HB3	2.40	0.57
1:B:195:LYS:HB3	1:B:587:VAL:H	1.70	0.57
1:B:359:ARG:HE	1:B:679:SER:CB	2.17	0.57
1:A:314:ILE:HD11	1:A:336:PHE:HA	1.86	0.57
1:B:595:TYR:CD2	1:B:596:MET:HG2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:LEU:O	1:B:613:ILE:HD12	2.05	0.57
1:B:607:ALA:HB3	1:B:656:CYS:SG	2.44	0.57
1:B:199:LEU:HD13	1:B:255:TYR:HB2	1.86	0.56
1:A:169:TYR:HB2	1:A:292:HIS:HE1	1.70	0.56
1:A:238:SER:OG	1:A:268:GLY:O	2.23	0.56
1:B:359:ARG:HE	1:B:679:SER:HB3	1.71	0.56
1:B:607:ALA:HB1	1:A:657:LEU:HD11	1.86	0.56
1:A:523:SER:HA	1:A:543:ASN:HB2	1.88	0.56
1:A:226:ALA:HB3	1:A:683:THR:HG21	1.87	0.55
1:A:375:LYS:HA	1:A:378:HIS:ND1	2.21	0.55
1:A:191:PRO:HG3	1:A:473:ARG:NE	2.22	0.55
1:A:571:LEU:HD12	1:A:574:SER:HB3	1.89	0.55
1:A:213:LEU:HD12	1:A:698:VAL:HG21	1.88	0.55
1:B:625:LEU:HD11	1:B:628:LEU:HD23	1.89	0.55
1:B:242:ASN:ND2	1:B:269:ILE:HD13	2.22	0.55
1:B:371:TRP:CE2	1:B:397:ILE:HG12	2.42	0.55
1:B:613:ILE:HD12	1:B:613:ILE:H	1.73	0.54
1:A:418:GLN:HG2	1:A:419:ARG:HG2	1.90	0.54
1:B:210:ILE:HG21	1:B:259:LEU:HD11	1.90	0.54
1:B:279:TYR:OH	1:B:355:PRO:O	2.21	0.53
1:B:634:MET:SD	1:B:661:VAL:HG11	2.48	0.53
1:A:154:ALA:HA	1:A:157:ARG:HE	1.73	0.53
1:A:672:LEU:HD21	1:A:733:LEU:HD13	1.90	0.53
1:B:630:GLY:O	1:B:634:MET:HG2	2.08	0.53
1:B:231:ARG:NH2	1:B:683:THR:OG1	2.42	0.52
1:A:638:SER:HB2	1:A:658:PHE:CE2	2.44	0.52
1:A:218:GLY:HA3	1:A:267:VAL:HA	1.92	0.52
1:B:145:ARG:HD3	1:B:148:LEU:HD21	1.92	0.52
1:B:450:MET:SD	1:B:673:THR:HG22	2.50	0.52
1:A:139:ALA:O	1:A:142:ARG:HD3	2.09	0.52
1:A:399:THR:O	1:A:402:GLN:HG3	2.10	0.52
1:A:609:LEU:HB3	1:A:610:PRO:HD3	1.92	0.52
1:A:210:ILE:HG21	1:A:259:LEU:HD11	1.91	0.52
1:B:524:VAL:H	1:B:544:THR:HG22	1.75	0.51
1:B:172:LEU:HB3	1:B:276:VAL:CG2	2.40	0.51
1:B:595:TYR:O	1:B:596:MET:HE2	2.10	0.51
1:A:393:SER:HA	1:A:396:HIS:CD2	2.46	0.51
1:A:587:VAL:HG12	1:A:588:THR:HG23	1.92	0.51
1:B:293:LEU:O	1:B:667:ASN:ND2	2.33	0.51
1:B:310:MET:HE2	1:B:310:MET:HA	1.93	0.51
1:A:231:ARG:NH2	1:A:282:GLU:OE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:604:GLY:HA2	1:B:656:CYS:SG	2.50	0.51
1:B:637:VAL:HG22	1:B:657:LEU:HD23	1.92	0.51
1:A:310:MET:O	1:A:314:ILE:HG12	2.10	0.51
1:B:618:LEU:O	1:B:622:ILE:HG12	2.11	0.50
1:B:470:ASP:HA	1:B:473:ARG:NH1	2.27	0.50
1:A:375:LYS:HG2	1:A:378:HIS:HE1	1.76	0.50
1:A:177:MET:HG3	1:A:303:GLY:HA2	1.92	0.50
1:A:542:SER:OG	1:A:588:THR:OG1	2.25	0.49
1:B:697:ALA:O	1:B:701:ILE:HG23	2.12	0.49
1:B:266:GLY:HA2	1:B:269:ILE:HG22	1.94	0.49
1:B:510:GLN:HG3	1:B:530:LEU:H	1.78	0.49
1:B:169:TYR:HB2	1:B:280:PHE:CZ	2.48	0.49
1:A:195:LYS:HD2	1:A:589:GLY:H	1.77	0.49
1:A:383:ARG:O	1:A:383:ARG:NE	2.45	0.49
1:A:480:TYR:HD1	1:A:483:ARG:HE	1.60	0.49
1:A:190:LEU:HG	1:A:191:PRO:HD3	1.95	0.48
1:B:168:LEU:HG	1:B:172:LEU:HD13	1.96	0.48
1:B:457:MET:HE1	1:B:665:SER:HB2	1.95	0.48
1:B:152:TYR:CZ	1:B:359:ARG:HB2	2.48	0.48
1:B:210:ILE:HG22	1:B:263:LEU:HD13	1.95	0.48
1:A:173:GLY:HA3	1:A:299:PHE:CD1	2.48	0.48
1:A:223:GLY:HA2	1:A:683:THR:HG22	1.95	0.48
1:A:556:PHE:H	1:A:576:PHE:HD1	1.61	0.48
1:B:494:HIS:O	1:B:494:HIS:ND1	2.47	0.48
1:A:641:PHE:CE1	1:A:654:LEU:HD23	2.48	0.48
1:B:619:MET:HE3	1:B:619:MET:HB2	1.61	0.48
1:A:273:ILE:HG21	2:A:801:VLX:O1	2.13	0.48
1:B:563:GLU:HA	1:B:566:PHE:HB2	1.96	0.48
1:A:181:VAL:HG21	1:A:343:PRO:HG3	1.95	0.48
1:A:193:ALA:HB3	1:A:199:LEU:HD22	1.95	0.48
1:A:172:LEU:HB3	1:A:276:VAL:HG13	1.96	0.48
1:A:491:ARG:NH2	1:A:510:GLN:O	2.46	0.47
1:B:273:ILE:HG22	1:B:274:PRO:HD3	1.96	0.47
1:A:377:VAL:O	1:A:381:ASN:ND2	2.38	0.47
1:A:420:TRP:HA	1:A:423:ARG:HG2	1.96	0.47
1:B:450:MET:HA	1:B:453:VAL:HG12	1.97	0.47
1:A:446:ILE:HG21	1:A:676:LEU:HD21	1.96	0.47
1:A:697:ALA:O	1:A:701:ILE:HG12	2.15	0.47
1:B:294:SER:HA	1:B:667:ASN:ND2	2.29	0.47
1:B:455:PHE:CE1	1:B:692:LEU:HG	2.47	0.46
1:A:719:ALA:O	1:A:723:LEU:HG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:GLN:HE22	1:B:283:PHE:HB3	1.80	0.46
1:B:616:ALA:O	1:B:620:ASP:HB2	2.16	0.46
1:A:177:MET:HG3	1:A:303:GLY:CA	2.44	0.46
1:A:607:ALA:O	1:A:610:PRO:HD2	2.15	0.46
1:B:182:GLU:OE1	1:B:262:ARG:NH2	2.48	0.46
1:A:579:ASN:ND2	1:A:581:GLU:OE2	2.48	0.46
1:A:176:LEU:HD12	1:A:296:LEU:HD22	1.98	0.46
1:B:454:TRP:HZ3	1:B:666:TRP:HZ3	1.64	0.46
1:B:641:PHE:CD1	1:B:650:ALA:HB1	2.51	0.46
1:B:333:TRP:HE1	1:B:587:VAL:HG21	1.81	0.45
1:A:150:GLN:OE1	1:A:157:ARG:NH2	2.47	0.45
1:A:490:GLU:OE1	1:A:511:TYR:OH	2.34	0.45
1:B:232:ARG:HB3	1:B:356:GLU:HG2	1.98	0.45
1:B:295:TRP:CH2	1:B:613:ILE:HG23	2.51	0.45
1:A:142:ARG:HA	1:A:145:ARG:HE	1.81	0.45
1:A:189:VAL:HG12	1:A:189:VAL:O	2.17	0.45
1:A:371:TRP:CZ3	1:A:400:ILE:HD12	2.52	0.45
1:A:678:PRO:HG2	1:A:681:LYS:HB2	1.99	0.45
1:B:558:ASN:H	1:B:579:ASN:HA	1.81	0.44
1:A:288:LYS:HD3	1:A:288:LYS:N	2.32	0.44
1:B:450:MET:HG3	1:B:454:TRP:CD1	2.52	0.44
1:A:222:TRP:HB3	1:A:275:ILE:HD11	1.99	0.44
1:A:466:VAL:C	1:A:469:PRO:HD2	2.43	0.44
1:B:586:ASP:O	1:B:588:THR:N	2.49	0.44
1:A:543:ASN:ND2	1:A:588:THR:O	2.47	0.44
1:B:249:SER:O	1:B:252:VAL:HG12	2.17	0.44
1:B:305:VAL:HG13	1:B:602:PHE:HE1	1.83	0.44
1:A:681:LYS:HB3	1:A:681:LYS:HZ2	1.82	0.44
1:A:283:PHE:CE2	1:A:357:SER:HA	2.53	0.44
1:B:168:LEU:HD23	1:B:280:PHE:HD1	1.83	0.44
1:A:154:ALA:HA	1:A:157:ARG:NE	2.33	0.44
1:A:453:VAL:O	1:A:456:THR:HB	2.18	0.44
1:B:248:PHE:HB3	1:B:261:CYS:SG	2.57	0.43
1:B:368:ASP:OD1	1:B:368:ASP:N	2.49	0.43
1:A:468:PHE:HB2	1:A:655:LEU:HD13	1.98	0.43
1:B:662:SER:O	1:B:666:TRP:HD1	2.01	0.43
1:A:375:LYS:HA	1:A:378:HIS:HD1	1.82	0.43
1:A:491:ARG:HH22	1:A:511:TYR:HA	1.82	0.43
1:B:189:VAL:HG22	1:B:598:TYR:HE1	1.84	0.43
1:A:549:CYS:O	1:A:569:SER:OG	2.28	0.43
1:B:454:TRP:CD1	1:B:689:LEU:HD22	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:615:SER:O	1:B:619:MET:HG2	2.17	0.43
1:A:345:VAL:HA	1:A:348:ILE:HG22	1.99	0.43
1:A:393:SER:HA	1:A:396:HIS:NE2	2.33	0.43
1:B:483:ARG:HD2	1:B:483:ARG:HA	1.71	0.43
1:A:283:PHE:CZ	1:A:358:PRO:HD3	2.53	0.43
1:B:570:ARG:HB3	1:B:572:ILE:HG12	2.00	0.43
1:A:648:GLU:O	1:A:652:ILE:HG13	2.18	0.43
1:B:445:ARG:HG3	1:B:449:MET:HE3	2.01	0.42
1:A:392:PHE:CD2	1:A:396:HIS:HB3	2.54	0.42
1:A:383:ARG:HA	1:A:389:GLU:HG3	2.00	0.42
1:A:463:GLY:HA2	1:A:467:TRP:HB3	2.01	0.42
1:A:608:VAL:HG22	1:A:656:CYS:O	2.18	0.42
1:B:295:TRP:HH2	1:B:613:ILE:HG23	1.83	0.42
1:B:489:GLY:HA2	1:B:506:HIS:HD2	1.85	0.42
1:A:494:HIS:O	1:A:494:HIS:ND1	2.53	0.42
1:A:371:TRP:HE1	1:A:396:HIS:HB2	1.84	0.42
1:A:678:PRO:O	1:A:682:ARG:N	2.53	0.42
1:B:672:LEU:O	1:B:676:LEU:HG	2.19	0.42
1:A:627:MET:HB3	1:A:668:ALA:HB1	2.02	0.42
1:B:151:GLN:O	1:B:155:ILE:HG13	2.19	0.42
1:B:197:MET:HG2	1:B:333:TRP:CH2	2.54	0.42
1:B:172:LEU:HD21	1:B:279:TYR:CD2	2.54	0.42
1:B:311:ALA:HB2	1:B:336:PHE:CE1	2.55	0.42
1:B:585:LEU:HD23	1:B:585:LEU:H	1.85	0.42
1:A:172:LEU:HD22	1:A:276:VAL:HG13	2.01	0.42
1:B:213:LEU:O	1:B:216:MET:HB3	2.20	0.42
1:A:195:LYS:HD3	1:A:591:GLY:H	1.85	0.42
1:A:619:MET:SD	1:A:668:ALA:HB2	2.60	0.42
1:B:294:SER:HA	1:B:667:ASN:CG	2.45	0.41
1:A:174:LEU:HD23	1:A:174:LEU:HA	1.89	0.41
1:B:385:LYS:HB2	1:B:387:HIS:NE2	2.35	0.41
1:A:464:LEU:HD23	1:A:666:TRP:CH2	2.55	0.41
1:A:466:VAL:HG11	1:A:701:ILE:HD12	2.01	0.41
1:A:472:ILE:HD12	1:A:600:VAL:HG11	2.02	0.41
1:B:309:ALA:HB2	1:B:602:PHE:CE1	2.55	0.41
1:B:608:VAL:O	1:B:612:ASN:HB2	2.21	0.41
1:A:476:GLN:HG3	1:A:597:VAL:HG22	2.03	0.41
1:B:133:PRO:HB2	1:B:136:ARG:HB2	2.03	0.41
1:B:595:TYR:HD2	1:B:596:MET:HG2	1.82	0.41
1:B:666:TRP:HH2	1:B:693:CYS:SG	2.43	0.41
1:A:695:LEU:HA	1:A:698:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LEU:HD23	1:B:276:VAL:HG23	2.01	0.41
1:A:610:PRO:HA	1:A:613:ILE:HD12	2.00	0.41
1:B:145:ARG:HD3	1:B:145:ARG:HA	1.87	0.41
1:B:183:VAL:HG11	1:B:300:TRP:CZ2	2.56	0.41
1:A:726:GLY:O	1:A:730:ALA:HB3	2.21	0.41
1:B:444:ARG:O	1:B:448:LEU:HD23	2.21	0.41
1:B:446:ILE:HD12	1:B:446:ILE:HA	1.94	0.41
1:B:216:MET:HE2	1:B:695:LEU:N	2.35	0.41
1:A:315:ILE:HB	1:A:316:PRO:HD3	2.02	0.41
1:A:709:GLY:HA2	1:A:712:LYS:HE2	2.03	0.41
1:A:262:ARG:HA	1:A:262:ARG:HD2	1.76	0.41
1:B:316:PRO:HG3	1:B:596:MET:HE1	2.02	0.40
1:A:196:ASP:C	1:A:197:MET:HG2	2.46	0.40
1:A:248:PHE:O	1:A:252:VAL:HG13	2.20	0.40
1:A:197:MET:HE2	1:A:197:MET:HB3	1.97	0.40
1:A:298:MET:HE3	1:A:298:MET:HB3	1.93	0.40
1:B:361:PHE:CE2	1:B:369:GLU:HB3	2.56	0.40
1:B:492:VAL:O	1:B:495:VAL:HG12	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	585/755 (78%)	568 (97%)	17 (3%)	0	100	100
1	B	563/755 (75%)	546 (97%)	17 (3%)	0	100	100
All	All	1148/1510 (76%)	1114 (97%)	34 (3%)	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	491/622 (79%)	491 (100%)	0	100	100
1	B	477/622 (77%)	477 (100%)	0	100	100
All	All	968/1244 (78%)	968 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	161	HIS
1	B	242	ASN
1	B	354	GLN
1	B	690	ASN
1	A	331	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	VLX	B	801	-	15,15,15	3.69	7 (46%)	16,20,20	2.47	8 (50%)
2	VLX	A	801	-	15,15,15	3.89	6 (40%)	16,20,20	1.75	7 (43%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	VLX	B	801	-	-	10/13/25/25	0/1/1/1
2	VLX	A	801	-	-	9/13/25/25	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	VLX	C6-N1	12.47	1.52	1.35
2	B	801	VLX	C6-N1	11.68	1.51	1.35
2	A	801	VLX	C9-N2	5.78	1.46	1.32
2	B	801	VLX	C9-N2	5.64	1.46	1.32
2	A	801	VLX	C5-N1	3.58	1.50	1.46
2	B	801	VLX	O2-C9	-3.01	1.18	1.23
2	A	801	VLX	C3-C6	-2.86	1.46	1.50
2	B	801	VLX	C3-C6	-2.83	1.46	1.50
2	A	801	VLX	O2-C9	-2.68	1.19	1.23
2	B	801	VLX	C5-N1	2.56	1.49	1.46
2	B	801	VLX	C2-N1	-2.39	1.43	1.47
2	B	801	VLX	O1-C6	-2.14	1.18	1.23
2	A	801	VLX	O1-C6	-2.06	1.18	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	VLX	C8-C5-C9	-5.04	106.94	111.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	VLX	C9-C5-N1	3.79	118.04	111.46
2	B	801	VLX	C5-C9-N2	3.31	123.98	116.57
2	A	801	VLX	C2-N1-C5	3.14	127.81	123.21
2	B	801	VLX	C5-N1-C6	3.01	126.58	123.08
2	B	801	VLX	O1-C6-C3	-2.72	123.30	127.28
2	B	801	VLX	C8-C5-N1	2.41	115.45	112.18
2	A	801	VLX	O1-C6-N1	2.38	127.52	124.87
2	B	801	VLX	O2-C9-C5	-2.31	116.37	120.22
2	A	801	VLX	C4-C1-C3	-2.29	108.37	115.42
2	B	801	VLX	O1-C6-N1	2.27	127.40	124.87
2	A	801	VLX	O1-C6-C3	-2.26	123.98	127.28
2	A	801	VLX	C7-C4-C1	-2.22	109.42	115.67
2	A	801	VLX	C5-N1-C6	2.16	125.58	123.08
2	A	801	VLX	C1-C3-C6	-2.14	101.86	105.05

There are no chirality outliers.

All (19) torsion outliers are listed below:

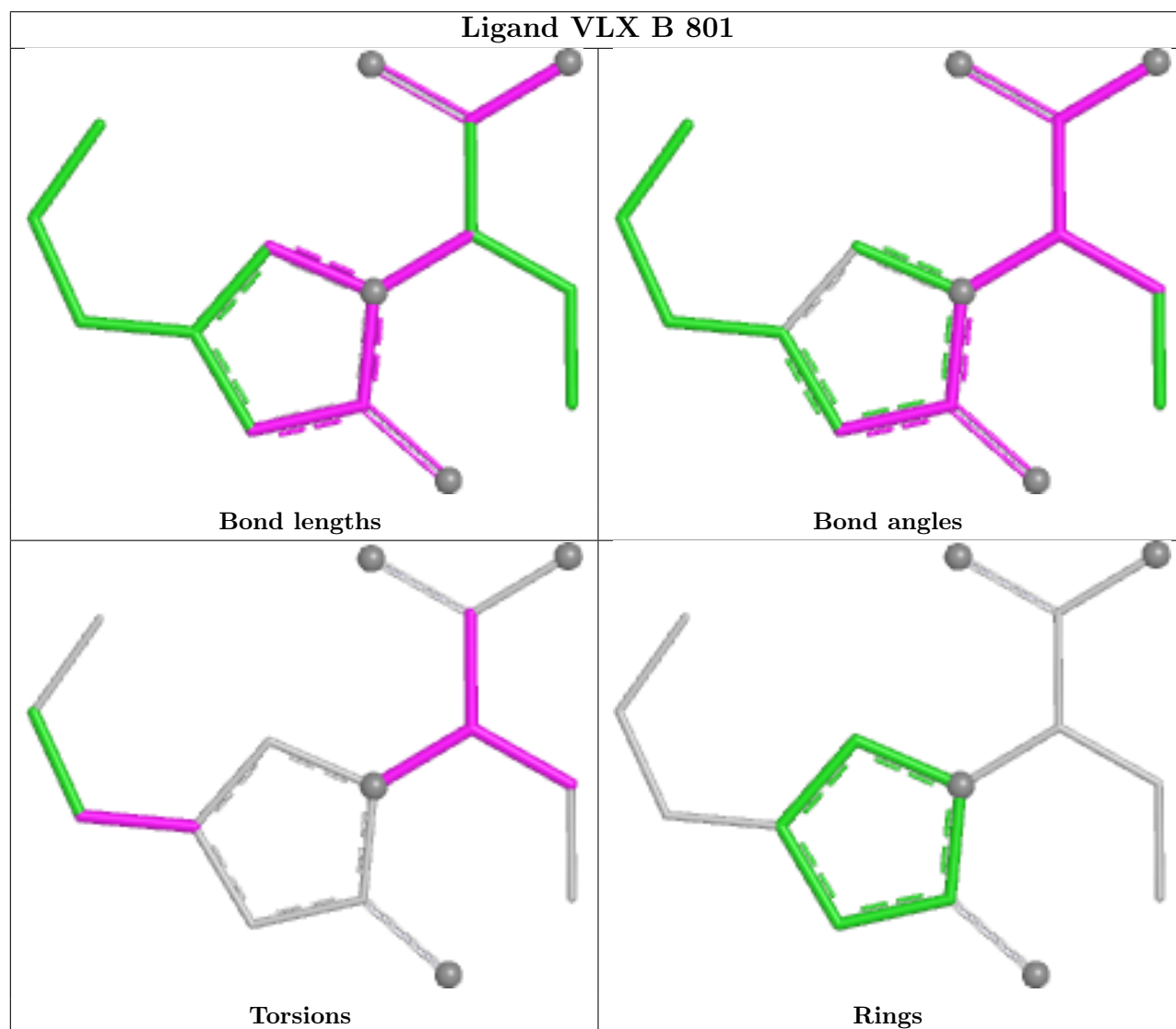
Mol	Chain	Res	Type	Atoms
2	B	801	VLX	C9-C5-C8-C11
2	B	801	VLX	N1-C5-C8-C11
2	B	801	VLX	C9-C5-N1-C2
2	B	801	VLX	C9-C5-N1-C6
2	B	801	VLX	C3-C1-C4-C7
2	A	801	VLX	C9-C5-C8-C11
2	A	801	VLX	N1-C5-C8-C11
2	A	801	VLX	C1-C4-C7-C10
2	B	801	VLX	C2-C1-C4-C7
2	A	801	VLX	C8-C5-C9-N2
2	B	801	VLX	C8-C5-N1-C6
2	A	801	VLX	C3-C1-C4-C7
2	B	801	VLX	C8-C5-C9-N2
2	B	801	VLX	C8-C5-C9-O2
2	A	801	VLX	C8-C5-C9-O2
2	A	801	VLX	C9-C5-N1-C2
2	A	801	VLX	C8-C5-N1-C2
2	B	801	VLX	C8-C5-N1-C2
2	A	801	VLX	C2-C1-C4-C7

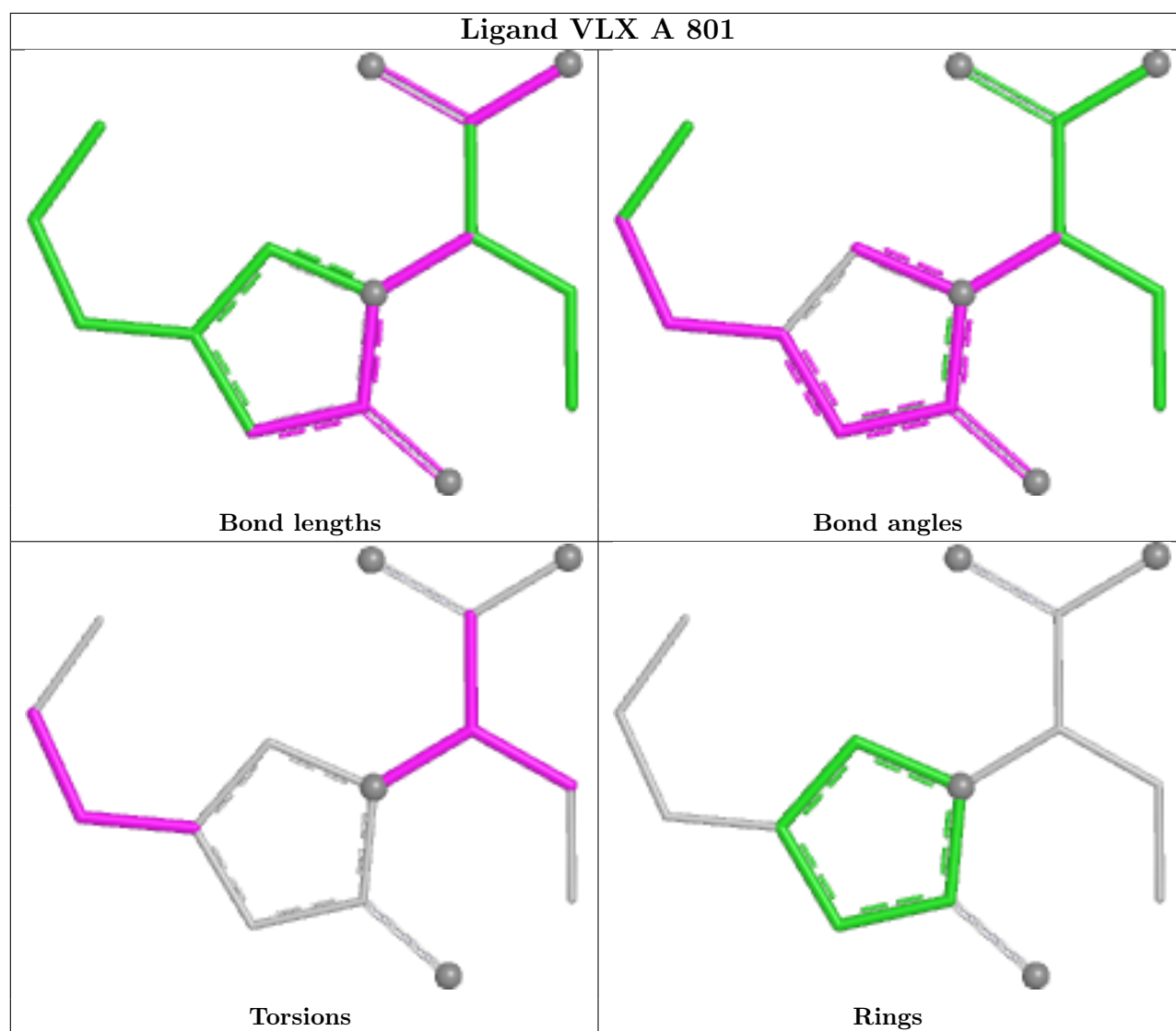
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	VLX	1	0
2	A	801	VLX	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

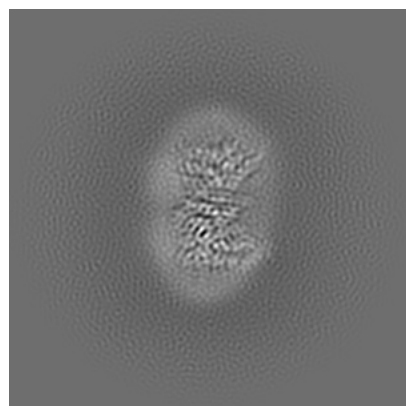
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39207. These allow visual inspection of the internal detail of the map and identification of artifacts.

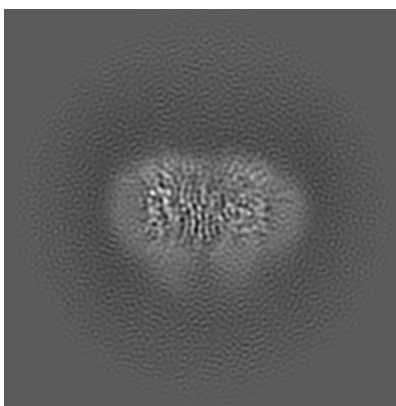
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

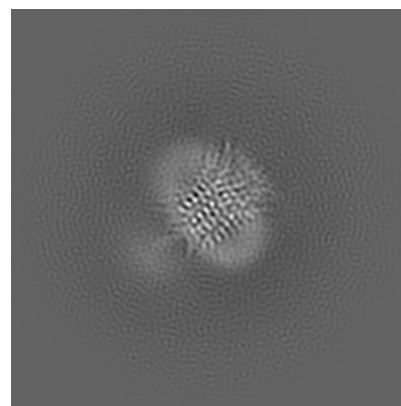
6.1.1 Primary map



X

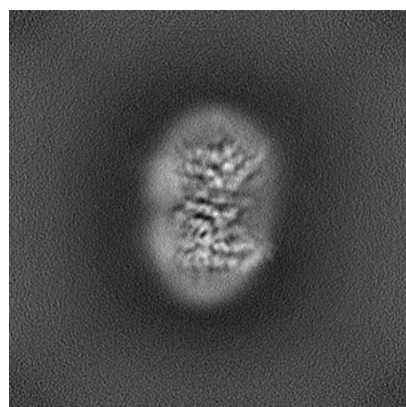


Y

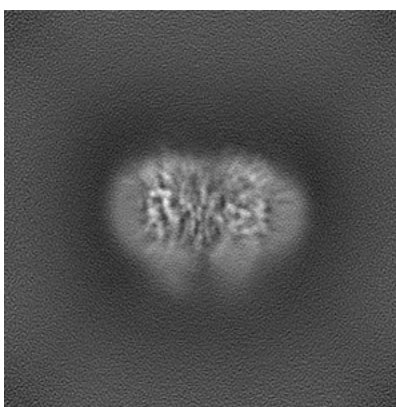


Z

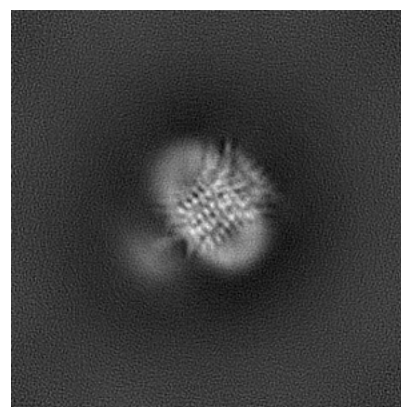
6.1.2 Raw map



X



Y

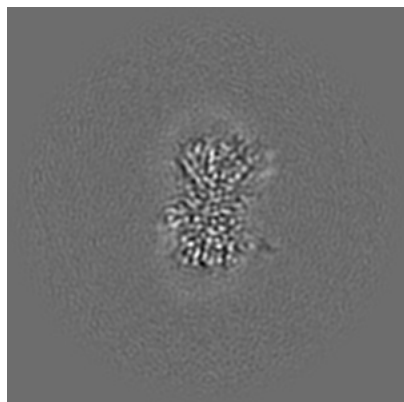


Z

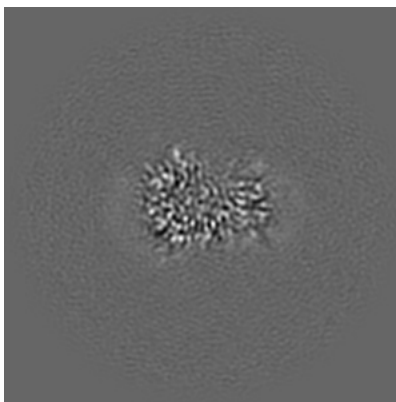
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

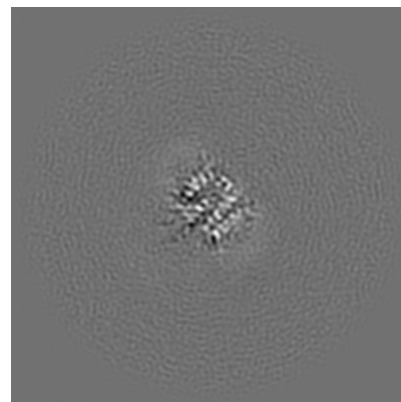
6.2.1 Primary map



X Index: 135

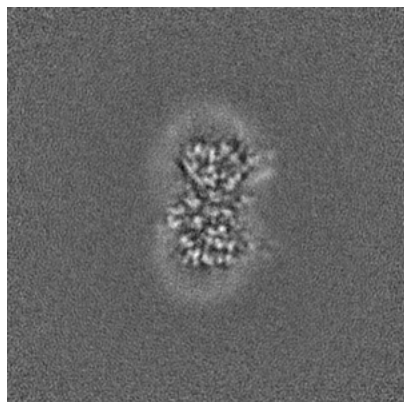


Y Index: 135

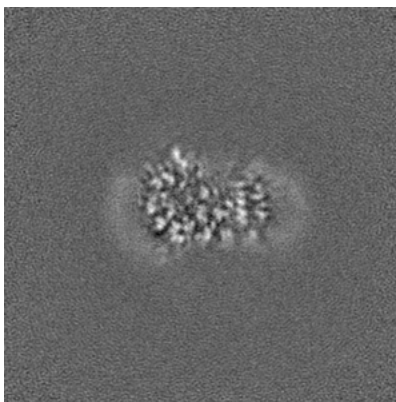


Z Index: 135

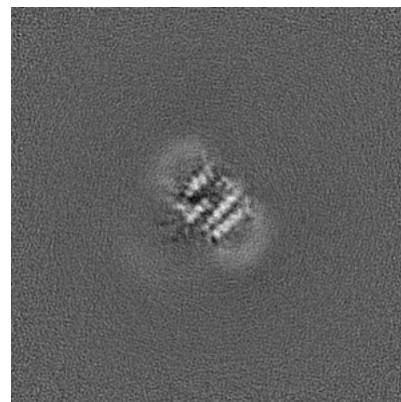
6.2.2 Raw map



X Index: 135



Y Index: 135

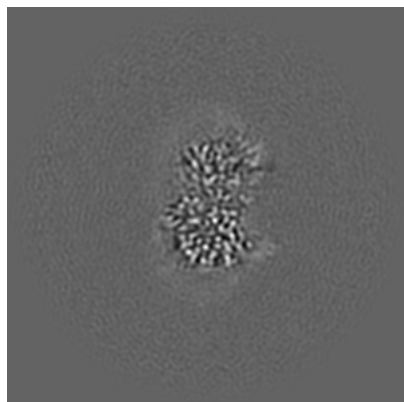


Z Index: 135

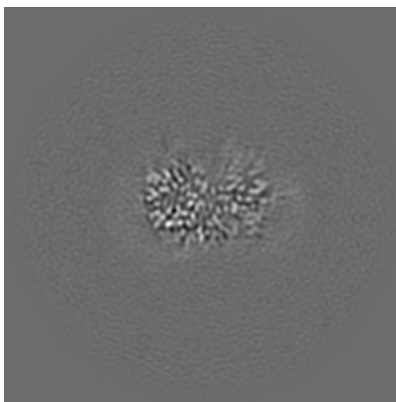
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

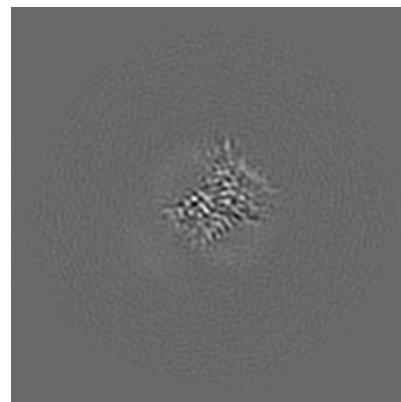
6.3.1 Primary map



X Index: 137

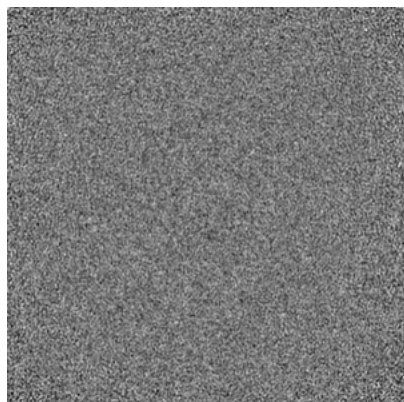


Y Index: 140

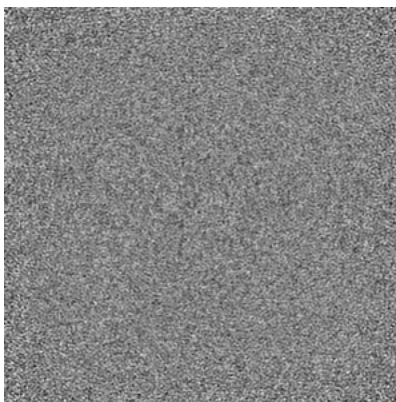


Z Index: 111

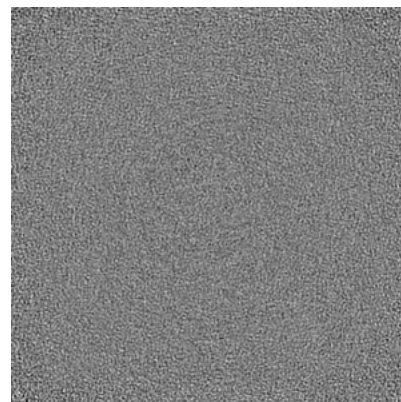
6.3.2 Raw map



X Index: 0



Y Index: 0

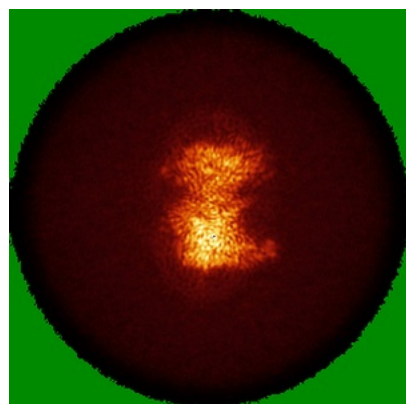


Z Index: 0

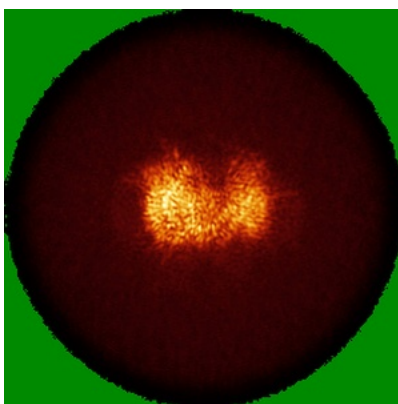
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

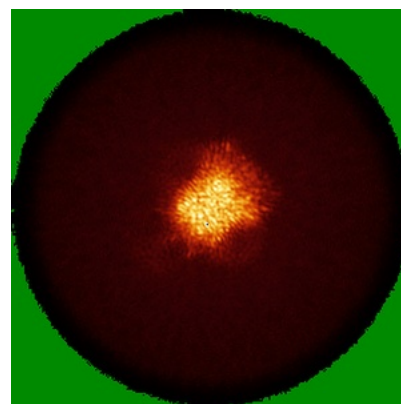
6.4.1 Primary map



X

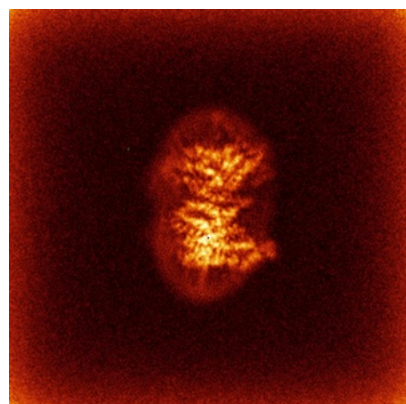


Y

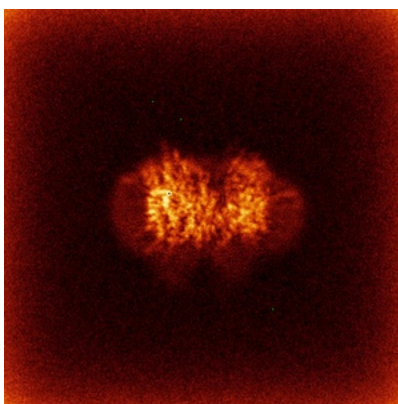


Z

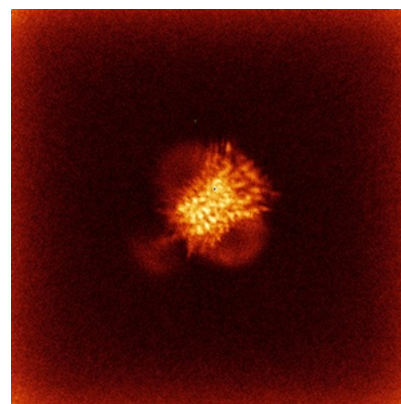
6.4.2 Raw map



X



Y

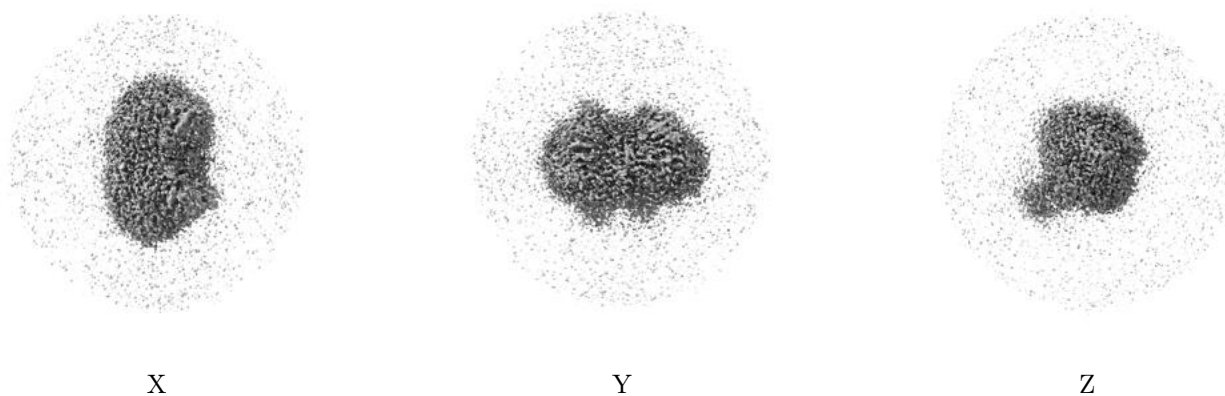


Z

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.

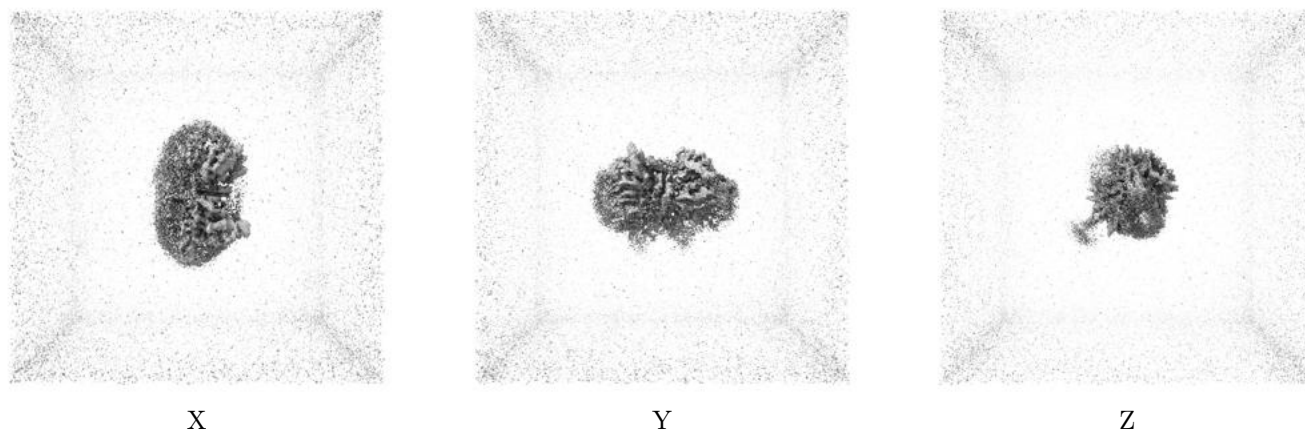
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.23. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

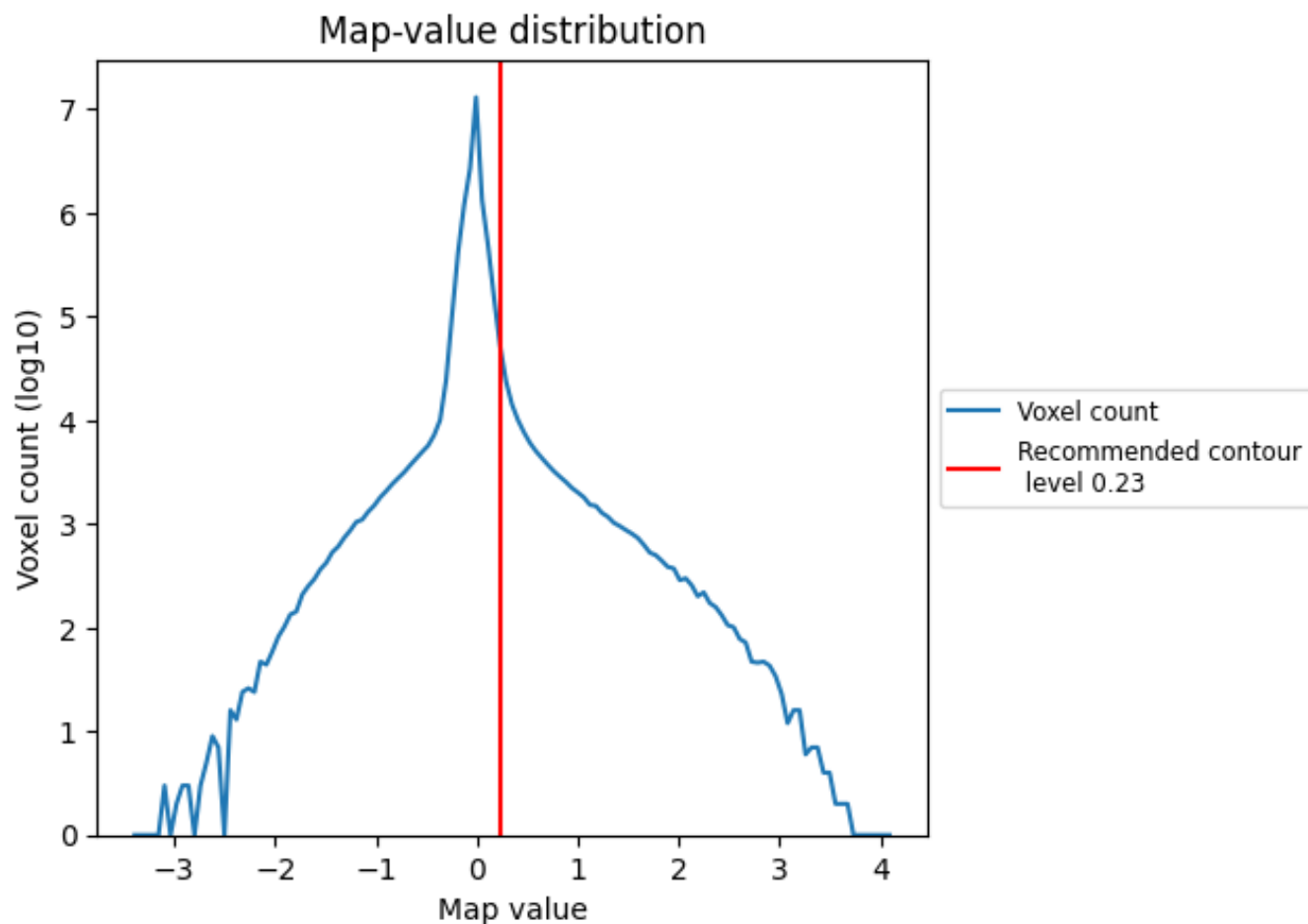
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

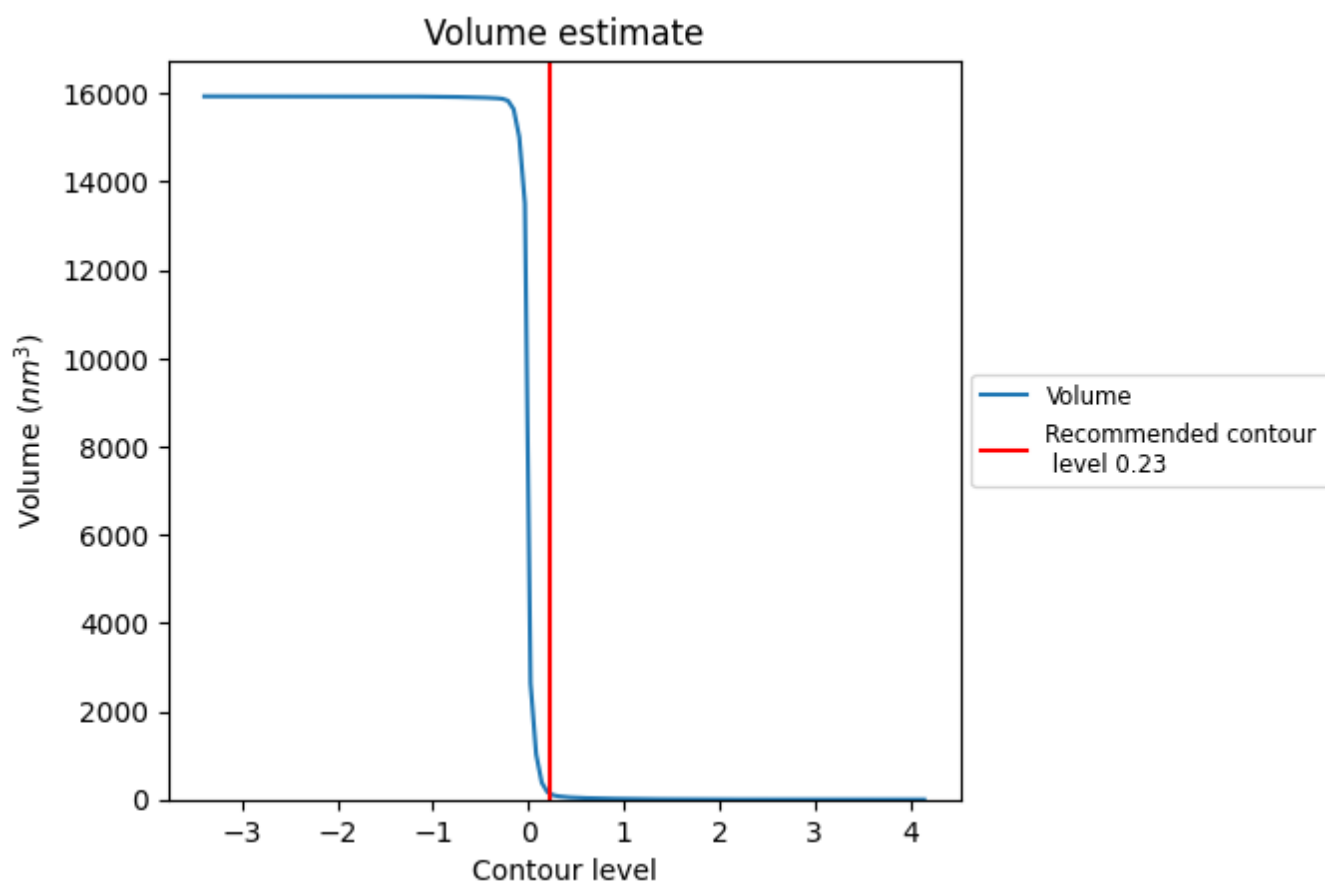
This section contains the results of statistical analysis of the map.

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.

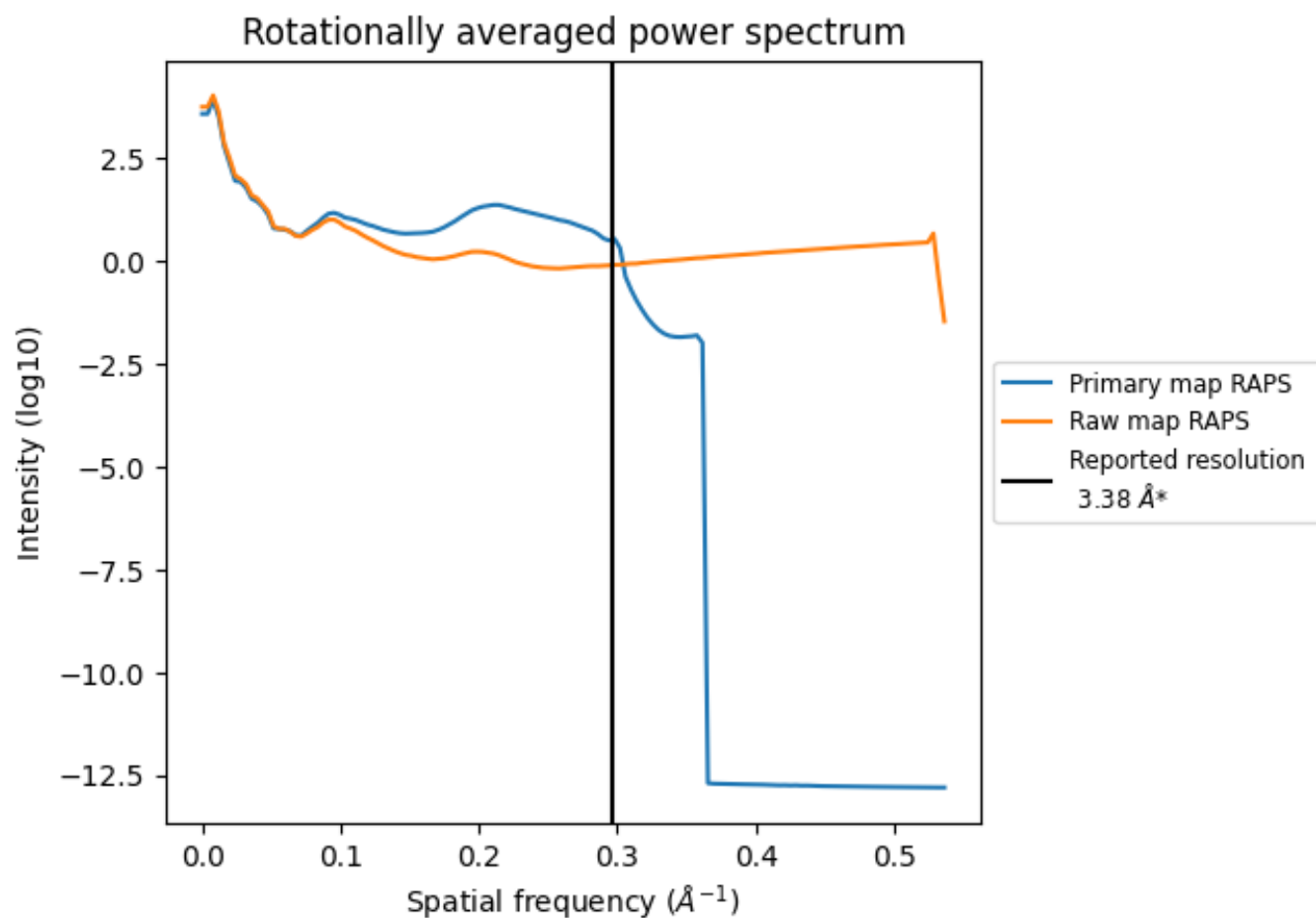
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 134 nm³; this corresponds to an approximate mass of 121 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](#)

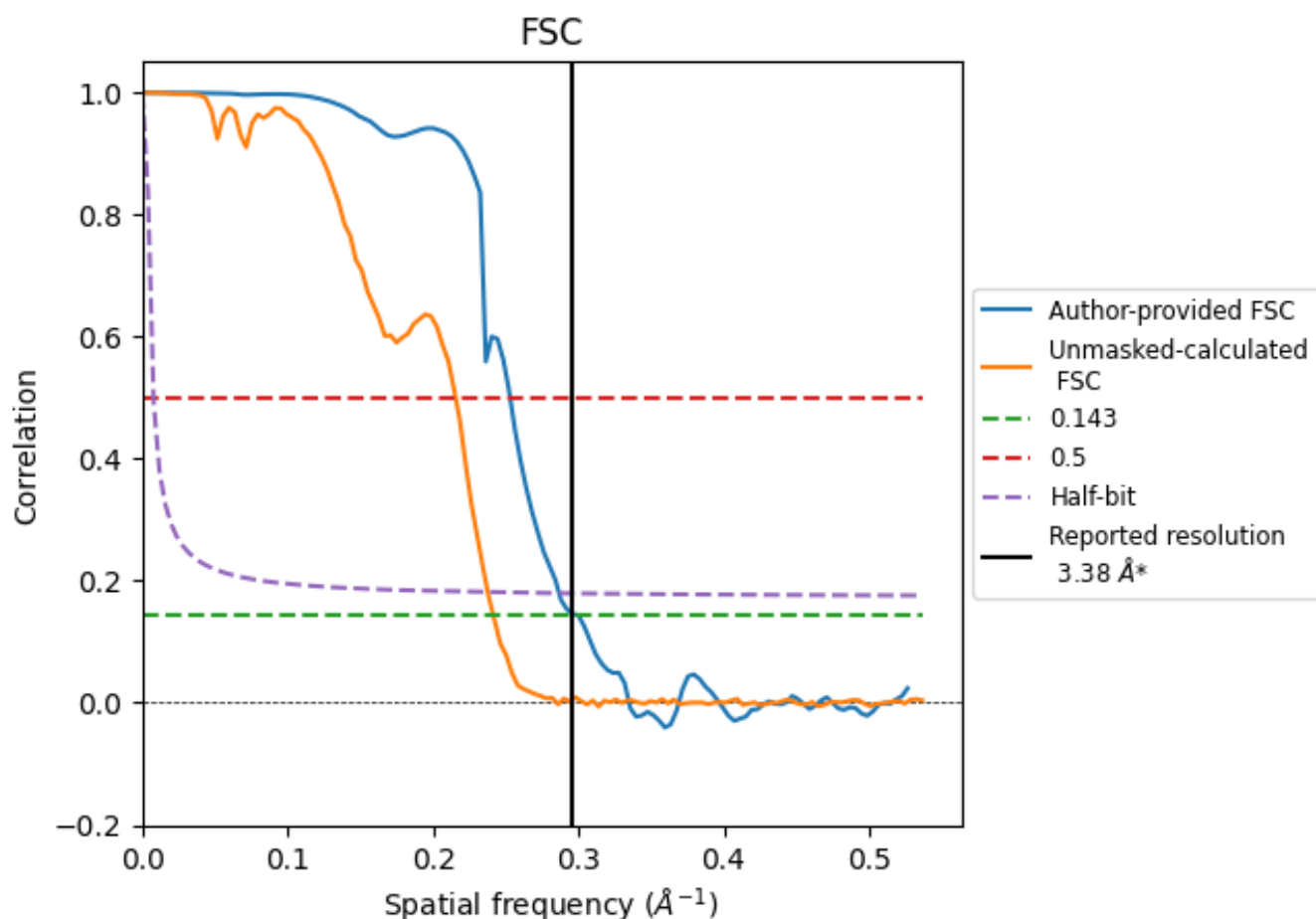


*Reported resolution corresponds to spatial frequency of 0.296 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.296 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

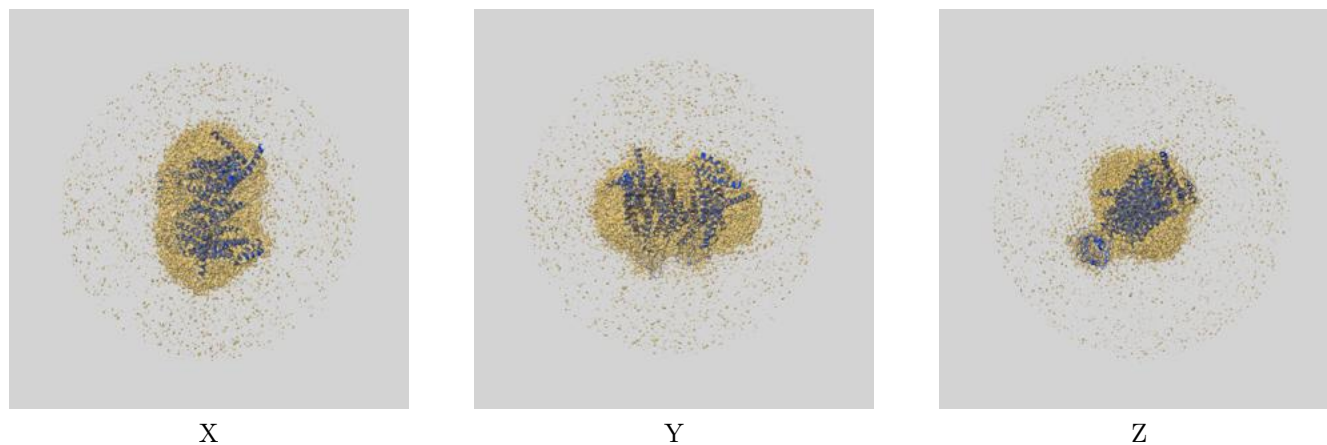
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.38	-	-
Author-provided FSC curve	3.33	3.95	3.49
Unmasked-calculated*	4.14	4.64	4.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.14 differs from the reported value 3.38 by more than 10 %

9 Map-model fit [i](#)

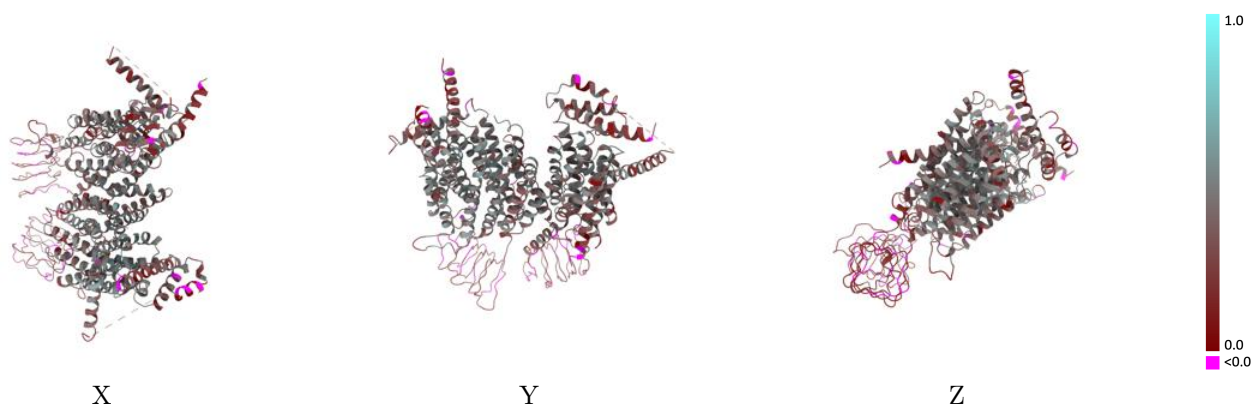
This section contains information regarding the fit between EMDB map EMD-39207 and PDB model 8YF1. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



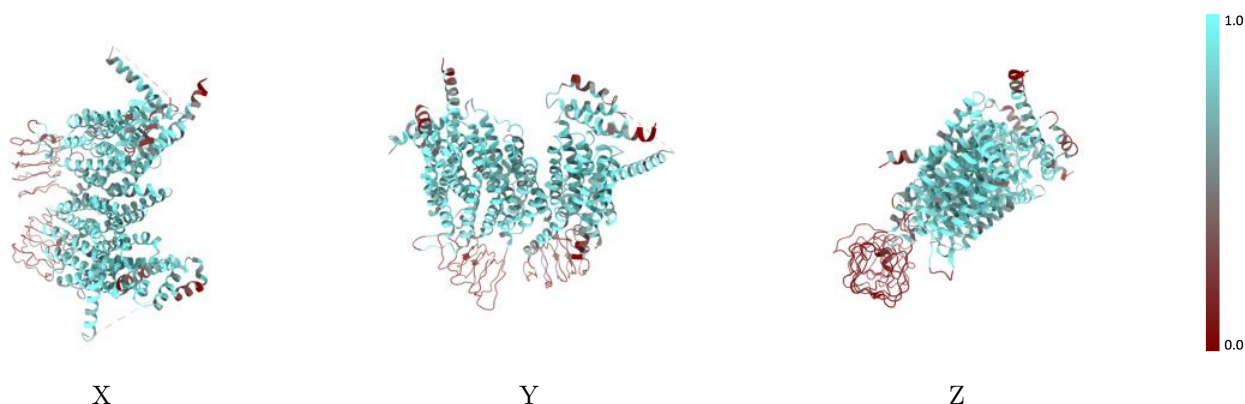
The images above show the 3D surface view of the map at the recommended contour level 0.23 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



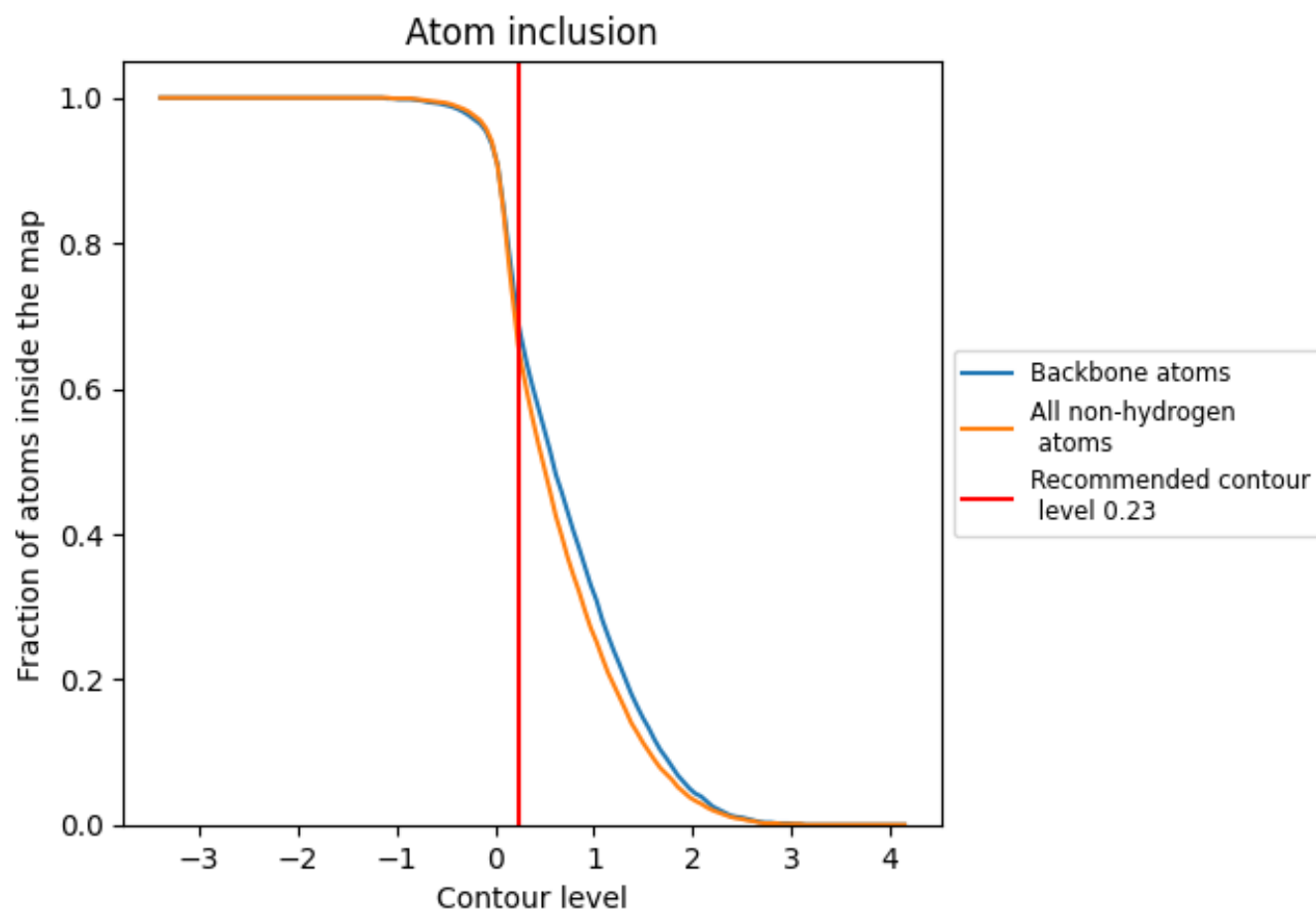
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.23).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 66% 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 (0.23) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6610	0.3460
A	0.6750	0.3620
B	0.6460	0.3290

