



## Full wwPDB EM Validation Report ⓘ

Aug 24, 2024 – 12:45 PM EDT

PDB ID : 9B6A  
EMDB ID : EMD-44251  
Title : GluA2 flip Q in complex with TARPgamma2 at pH8, class12, structure of LBD-TMD-TARPgamma2  
Authors : Nakagawa, T.; Greger, I.H.  
Deposited on : 2024-03-23  
Resolution : 3.35 Å (reported)  
Based on initial models : 8FQG, 8FQF

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev112  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.38.2

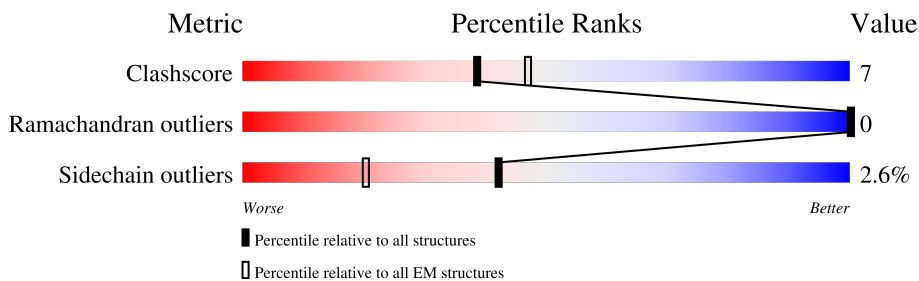
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	E	323	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">16%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 16%, orange 16%, yellow 16%, green 48%, yellow 48%, grey 41%);"></div> <div style="text-align: left;">48%</div> </div>
1	F	323	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">15%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 15%, orange 15%, yellow 7%, green 51%, yellow 51%, grey 42%);"></div> <div style="text-align: left;">51%</div> </div>
1	G	323	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">16%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 16%, orange 16%, yellow 10%, green 48%, yellow 48%, grey 41%);"></div> <div style="text-align: left;">48%</div> </div>
1	H	323	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">14%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 14%, orange 14%, yellow 9%, green 50%, yellow 50%, grey 42%);"></div> <div style="text-align: left;">50%</div> </div>
2	A	889	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">7%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 7%, orange 7%, yellow 9%, green 36%, yellow 36%, grey 55%);"></div> <div style="text-align: left;">36%</div> </div>
2	B	889	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">5%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 5%, orange 5%, yellow 9%, green 37%, yellow 37%, grey 54%);"></div> <div style="text-align: left;">37%</div> </div>
2	C	889	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">•</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 0%, orange 0%, yellow 10%, green 35%, yellow 35%, grey 55%);"></div> <div style="text-align: left;">35%</div> </div>
2	D	889	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">8%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 8%, orange 8%, yellow 10%, green 35%, yellow 35%, grey 54%);"></div> <div style="text-align: left;">35%</div> </div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 18493 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 Voltage-dependent calcium channel gamma-2 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	H	188	1456	949	237	259	11	0	0
1	F	188	1456	949	237	259	11	0	0
1	E	189	1468	960	238	259	11	0	0
1	G	189	1468	960	238	259	11	0	0

- Molecule 2 is a protein called Isoform Flip of Glutamate receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	404	3155	2048	509	577	21	2	0
2	B	408	3177	2063	511	582	21	1	0
2	A	404	3133	2033	503	576	21	0	0
2	D	408	3180	2067	511	581	21	2	0

There are 28 discrepancies between the modelled and reference sequences:

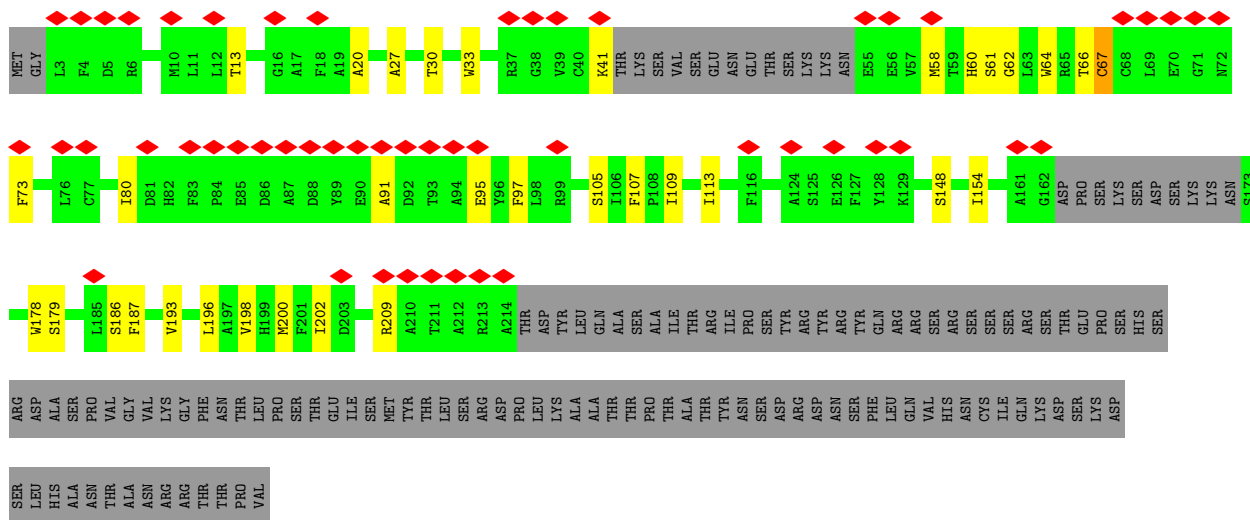
Chain	Residue	Modelled	Actual	Comment	Reference
C	733	ASP	GLY	conflict	UNP P19491
C	848	ASP	-	insertion	UNP P19491
C	850	LYS	-	insertion	UNP P19491
C	851	ASP	-	insertion	UNP P19491
C	852	ASP	-	insertion	UNP P19491
C	853	ASP	-	insertion	UNP P19491
C	854	ASP	-	insertion	UNP P19491
B	733	ASP	GLY	conflict	UNP P19491
B	848	ASP	-	insertion	UNP P19491

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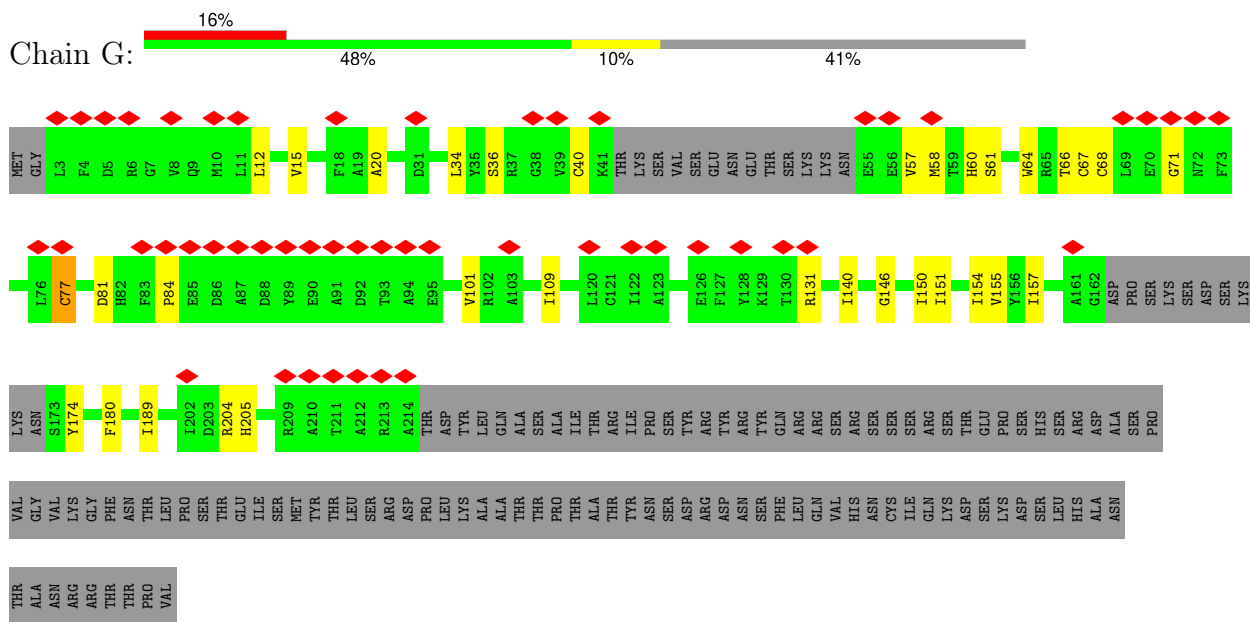
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Chain	Residue	Modelled	Actual	Comment	Reference
B	850	LYS	-	insertion	UNP P19491
B	851	ASP	-	insertion	UNP P19491
B	852	ASP	-	insertion	UNP P19491
B	853	ASP	-	insertion	UNP P19491
B	854	ASP	-	insertion	UNP P19491
A	733	ASP	GLY	conflict	UNP P19491
A	848	ASP	-	insertion	UNP P19491
A	850	LYS	-	insertion	UNP P19491
A	851	ASP	-	insertion	UNP P19491
A	852	ASP	-	insertion	UNP P19491
A	853	ASP	-	insertion	UNP P19491
A	854	ASP	-	insertion	UNP P19491
D	733	ASP	GLY	conflict	UNP P19491
D	848	ASP	-	insertion	UNP P19491
D	850	LYS	-	insertion	UNP P19491
D	851	ASP	-	insertion	UNP P19491
D	852	ASP	-	insertion	UNP P19491
D	853	ASP	-	insertion	UNP P19491
D	854	ASP	-	insertion	UNP P19491

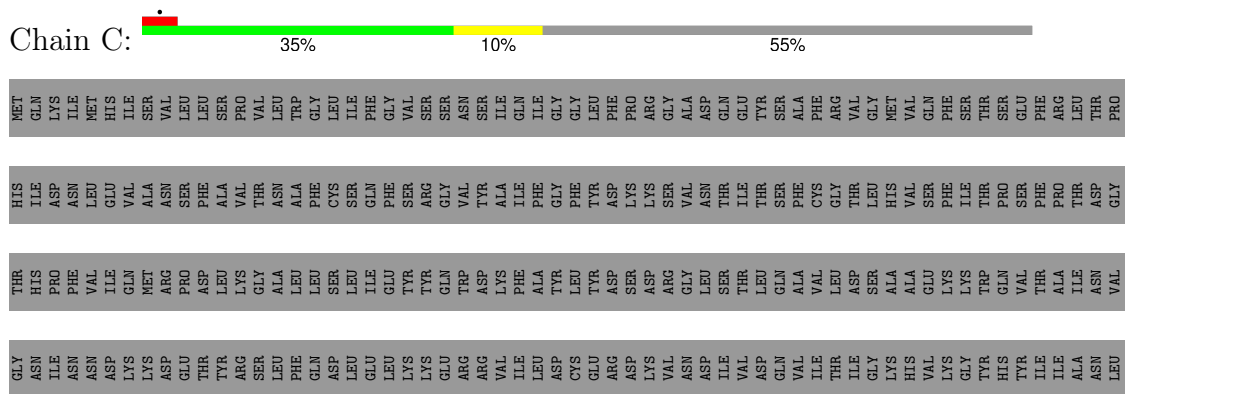


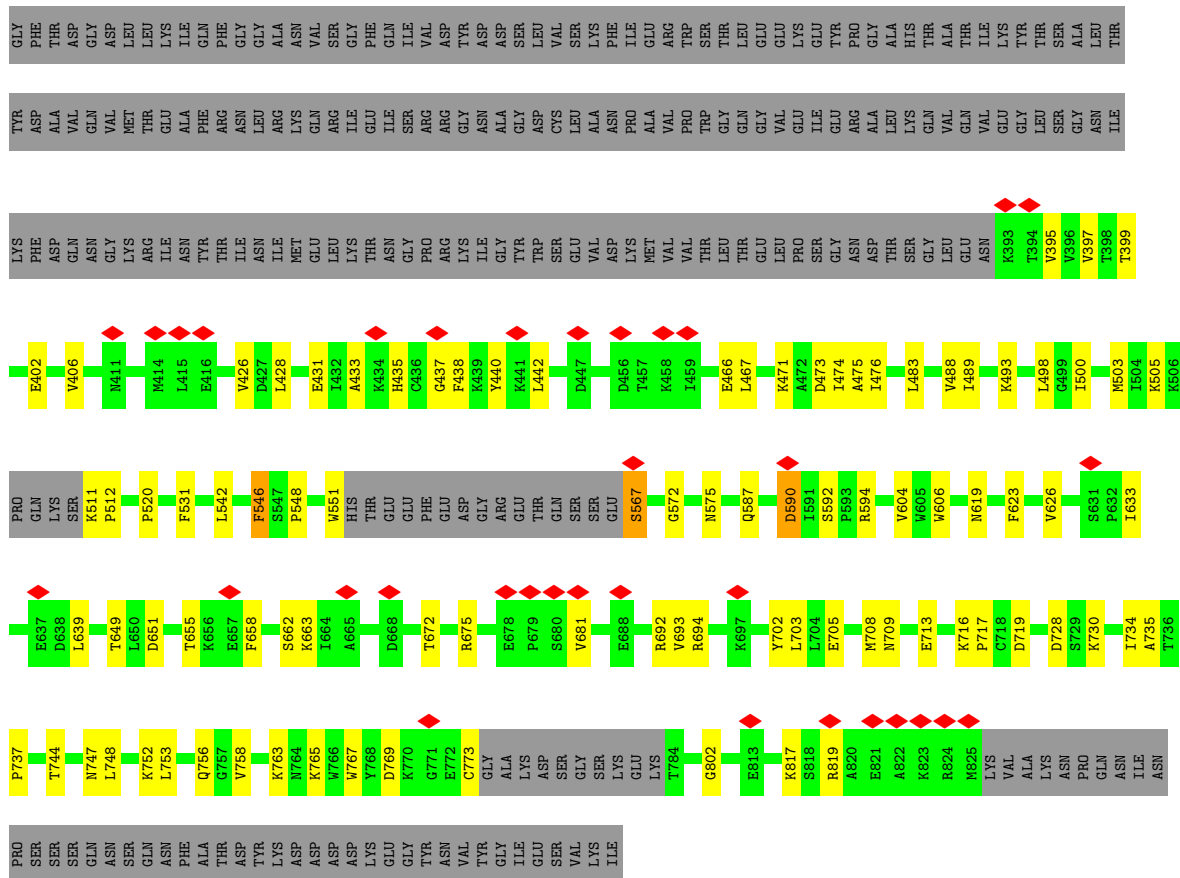


• Molecule 1: Voltage-dependent calcium channel gamma-2 subunit

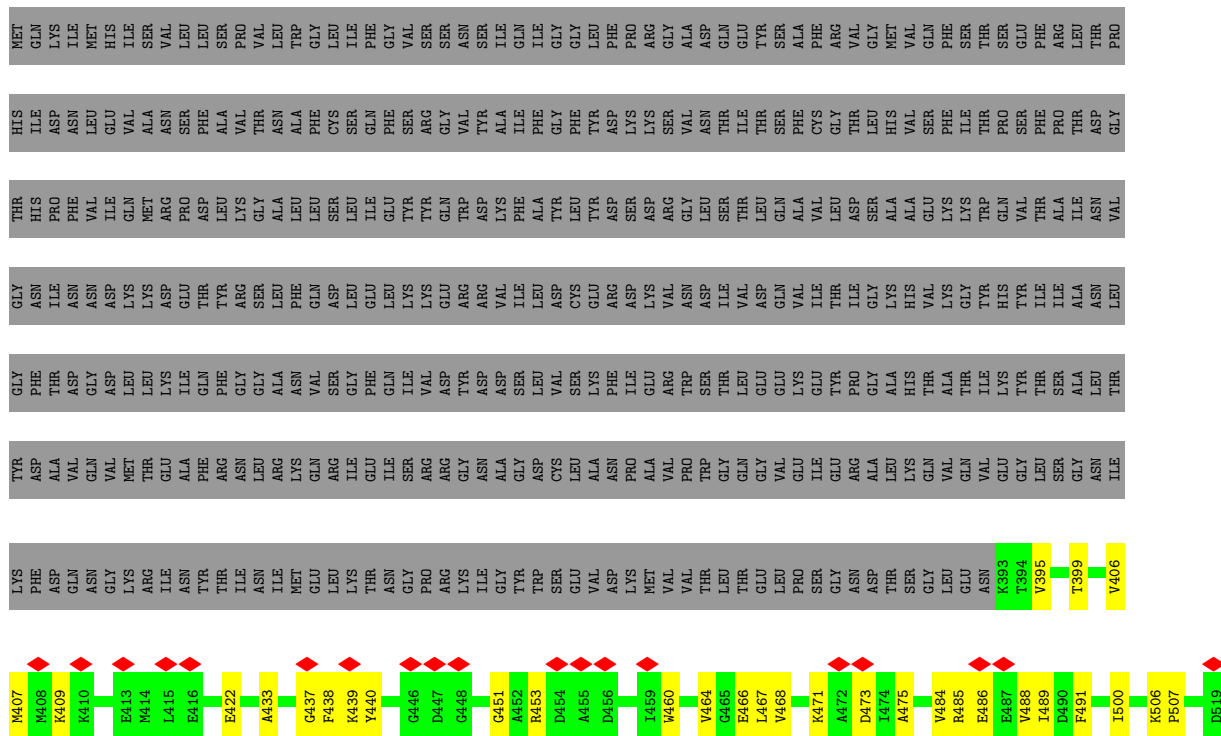
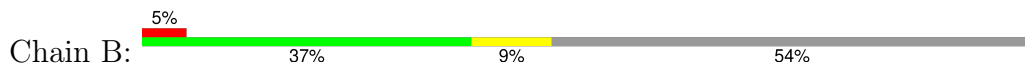


• Molecule 2: Isoform Flip of Glutamate receptor 2





● Molecule 2: Isoform Flip of Glutamate receptor 2









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	48399	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	52.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.107	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0155	Depositor
Map size (Å)	295.2, 295.2, 295.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82000005, 0.82000005, 0.82000005	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	E	0.25	0/1502	0.45	0/2030
1	F	0.25	0/1489	0.44	0/2013
1	G	0.29	0/1502	0.50	1/2030 (0.0%)
1	H	0.25	0/1489	0.43	0/2013
2	A	0.25	0/3200	0.44	0/4324
2	B	0.25	0/3247	0.46	1/4388 (0.0%)
2	C	0.25	0/3227	0.45	0/4361
2	D	0.31	1/3254 (0.0%)	0.51	3/4399 (0.1%)
All	All	0.26	1/18910 (0.0%)	0.46	5/25558 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	548	PRO	CG-CD	-8.24	1.23	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	548	PRO	N-CD-CG	-9.83	88.45	103.20
1	G	77	CYS	CA-CB-SG	8.16	128.68	114.00
2	D	548	PRO	CA-CB-CG	-7.73	89.31	104.00
2	D	548	PRO	N-CA-CB	-6.12	95.87	102.60
2	B	745	PRO	CA-N-CD	-5.51	103.78	111.50

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	E	1468	0	1446	17	0
1	F	1456	0	1433	11	0
1	G	1468	0	1446	23	0
1	H	1456	0	1433	16	0
2	A	3133	0	3132	55	0
2	B	3177	0	3186	49	0
2	C	3155	0	3148	56	0
2	D	3180	0	3184	68	0
All	All	18493	0	18408	263	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 7.

All (263) 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:G:67:CYS:HA	1:G:77:CYS:HB3	1.38	1.05
1:G:67:CYS:CA	1:G:77:CYS:HB3	2.08	0.81
2:B:547:SER:HB2	2:B:550:GLU:HG2	1.63	0.80
2:D:488:VAL:HG23	2:D:489:ILE:HG23	1.68	0.75
1:F:34:LEU:HD11	1:F:174:TYR:HB2	1.68	0.74
2:D:475:ALA:HB3	2:D:735:ALA:HB3	1.70	0.74
2:A:763:LYS:O	2:A:767:TRP:HB2	1.88	0.73
2:C:466:GLU:HG2	2:C:471:LYS:HB3	1.73	0.71
2:B:763:LYS:O	2:B:767:TRP:HB2	1.92	0.70
2:B:475:ALA:HB3	2:B:735:ALA:HB3	1.73	0.70
2:D:765:LYS:HA	2:D:769:ASP:HB2	1.74	0.70
2:C:475:ALA:HB3	2:C:735:ALA:HB3	1.73	0.70
2:D:520:PRO:HB3	2:D:619:ASN:HB3	1.76	0.68
1:H:6:ARG:NH1	1:H:10:MET:SD	2.67	0.68
2:A:420:ARG:NH2	2:A:421:TYR:OH	2.28	0.67
2:A:802:GLY:HA3	2:D:604:VAL:HG11	1.77	0.67
2:A:756:GLN:HA	2:D:661:ARG:HH12	1.60	0.66
2:C:672:THR:HG22	2:C:675:ARG:HH21	1.60	0.66
2:C:756:GLN:HA	2:B:661:ARG:HH12	1.61	0.65
2:C:520:PRO:O	2:C:619:ASN:ND2	2.27	0.65
2:C:488:VAL:HG13	2:C:489:ILE:HG23	1.80	0.64
2:D:681:VAL:HA	2:D:692:ARG:HH22	1.63	0.64
2:C:604:VAL:HG11	2:D:802:GLY:HA3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:765:LYS:HA	2:B:769:ASP:HB2	1.81	0.63
2:C:431:GLU:O	2:C:435[B]:HIS:ND1	2.32	0.63
2:C:756:GLN:HG3	2:C:758:VAL:HG23	1.81	0.63
1:G:34:LEU:HD21	1:G:174:TYR:HB2	1.81	0.62
1:H:59:THR:HG22	1:H:68:CYS:HA	1.79	0.62
2:A:663:LYS:HB3	2:D:761:LYS:HE2	1.80	0.62
2:C:681:VAL:HA	2:C:692:ARG:HH22	1.64	0.62
1:H:95:GLU:O	1:H:99:ARG:HG3	1.99	0.62
2:A:719:ASP:OD1	2:A:719:ASP:N	2.33	0.62
2:D:763:LYS:O	2:D:767:TRP:HB2	1.99	0.62
1:E:91:ALA:HB1	1:E:95:GLU:HB3	1.82	0.61
2:B:466:GLU:HG3	2:B:471:LYS:HB2	1.82	0.61
2:D:505:LYS:NZ	2:D:694:ARG:O	2.31	0.60
1:F:33:TRP:HB2	1:F:62:GLY:HA2	1.83	0.60
2:C:765:LYS:HA	2:C:769:ASP:HB2	1.83	0.59
2:C:719:ASP:OD1	2:C:719:ASP:N	2.36	0.58
2:A:666:VAL:O	2:A:670:MET:HG3	2.03	0.58
2:A:520:PRO:O	2:A:619:ASN:ND2	2.33	0.58
2:C:500:ILE:HD12	2:C:655:THR:HG22	1.85	0.58
2:A:475:ALA:HB3	2:A:735:ALA:HB3	1.86	0.58
2:A:500:ILE:HD13	2:A:655:THR:HG23	1.86	0.57
2:D:409:LYS:HB3	2:D:412:HIS:HB3	1.86	0.57
1:G:20:ALA:HB2	1:G:189:ILE:HG22	1.86	0.56
1:E:20:ALA:O	1:E:186:SER:OG	2.22	0.56
1:E:33:TRP:HB2	1:E:62:GLY:HA2	1.88	0.56
1:H:157:ILE:HD13	2:D:524:GLU:HB3	1.88	0.56
2:C:802:GLY:HA3	2:B:604:VAL:HG11	1.88	0.56
2:C:744:THR:O	2:C:748:LEU:HG	2.06	0.55
2:B:464:VAL:O	2:B:468:VAL:HG13	2.06	0.55
2:D:496:MET:HG2	2:D:732:TYR:HB2	1.88	0.55
2:A:480:THR:HG22	2:A:732:TYR:HE1	1.71	0.55
2:D:467:LEU:HD21	2:D:475:ALA:HB2	1.89	0.55
2:C:693:VAL:HG21	2:C:702:TYR:HB2	1.87	0.55
1:G:60:HIS:CE1	1:G:67:CYS:HB2	2.42	0.55
1:H:92:ASP:OD1	1:H:92:ASP:N	2.37	0.55
2:C:663:LYS:HG3	2:B:761:LYS:HE2	1.88	0.54
2:D:548:PRO:HG2	2:D:549:TYR:N	2.21	0.54
2:C:716:LYS:HG3	2:C:717:PRO:HA	1.89	0.54
2:A:489:ILE:HD12	2:A:735:ALA:HB1	1.90	0.54
2:A:520:PRO:HB3	2:A:619:ASN:HB3	1.88	0.54
1:H:33:TRP:HB2	1:H:62:GLY:HA2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:151:ILE:HD11	2:A:800:VAL:HG11	1.90	0.54
2:D:401:LEU:HD23	2:D:406:VAL:HG12	1.90	0.53
1:G:81:ASP:HB3	1:G:84:PRO:HG3	1.90	0.53
2:B:674:MET:HG2	2:B:681:VAL:HG21	1.90	0.53
2:B:395:VAL:HG13	2:B:473:ASP:HB2	1.91	0.53
2:D:631:SER:O	2:D:631:SER:OG	2.20	0.53
2:C:542:LEU:HD21	1:G:140:ILE:HD13	1.91	0.53
2:B:796:PHE:HB3	1:E:154:ILE:HD13	1.90	0.53
1:E:107:PHE:O	1:E:148:SER:OG	2.27	0.53
2:A:756:GLN:HG2	2:D:661:ARG:HH22	1.74	0.52
1:F:41:LYS:HA	1:F:78:LYS:HB2	1.92	0.52
2:A:683:VAL:HG11	2:A:689:GLY:N	2.24	0.52
1:F:132:HIS:O	1:F:135:ILE:HG22	2.09	0.52
2:D:422:GLU:HA	2:D:426:VAL:HG21	1.90	0.52
1:E:13:THR:HG23	1:E:193:VAL:HG13	1.90	0.52
1:F:71:GLY:H	1:F:74:LYS:HB2	1.75	0.52
2:A:500:ILE:HB	2:A:727:LEU:HB2	1.92	0.52
2:A:405:TYR:HA	2:A:424:TYR:HB3	1.91	0.52
1:F:202:ILE:HD11	2:B:546:PHE:HA	1.91	0.52
2:C:428:LEU:HD21	2:C:734:ILE:HD11	1.91	0.52
2:D:454:ASP:OD2	2:D:457:THR:OG1	2.27	0.51
2:C:500:ILE:HG12	2:C:728:ASP:OD1	2.11	0.51
2:D:433:ALA:O	2:D:437:GLY:N	2.43	0.51
2:D:749:ALA:O	2:D:753:LEU:HD13	2.09	0.51
2:C:763:LYS:O	2:C:767:TRP:HB2	2.11	0.51
2:D:462:GLY:O	2:D:466:GLU:HG2	2.10	0.51
2:B:784:THR:HG23	2:A:626:VAL:HG21	1.92	0.51
2:B:715:ARG:HH12	2:B:771:GLY:HA2	1.75	0.51
2:C:747:ASN:ND2	2:B:486:GLU:OE2	2.44	0.51
2:C:752:LYS:O	2:C:756:GLN:HG2	2.10	0.51
2:D:545:ARG:NH1	2:D:569:ASN:O	2.44	0.51
2:B:551:TRP:HA	2:B:567:SER:HA	1.93	0.51
2:B:752:LYS:O	2:B:756:GLN:HG2	2.10	0.51
2:A:401:LEU:HG	2:A:444:ILE:HG12	1.93	0.51
1:F:92:ASP:OD1	1:F:92:ASP:N	2.40	0.50
2:A:665:ALA:O	2:A:669:LYS:HG3	2.12	0.50
1:E:198:VAL:O	1:E:202:ILE:HG13	2.10	0.50
2:D:406:VAL:HG23	2:D:425:CYS:HB2	1.94	0.50
2:D:683:VAL:HG21	2:D:702:TYR:HE2	1.77	0.50
2:C:606:TRP:CG	2:D:587:GLN:HG3	2.46	0.50
2:C:633:ILE:HG21	2:C:639:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:467:LEU:HB3	2:D:737:PRO:HG3	1.94	0.50
2:D:463:MET:O	2:D:467:LEU:HG	2.12	0.50
2:A:408:MET:SD	2:A:408:MET:N	2.79	0.50
2:B:433:ALA:O	2:B:437:GLY:N	2.45	0.49
2:B:464:VAL:HA	2:B:467:LEU:HD12	1.93	0.49
2:A:450:TYR:HE1	2:A:478:PRO:HG2	1.77	0.49
2:D:690:VAL:HG12	2:D:694:ARG:HD2	1.93	0.49
2:C:551:TRP:HA	2:C:567:SER:HB2	1.93	0.49
2:B:438:PHE:HE1	2:B:440:TYR:HB3	1.78	0.49
2:D:485:ARG:HB3	2:D:491:PHE:HE2	1.77	0.49
2:C:626:VAL:HG21	2:D:784:THR:HG23	1.95	0.49
2:C:649:THR:HG22	2:C:703:LEU:HB2	1.94	0.49
2:B:520:PRO:O	2:B:619:ASN:ND2	2.46	0.49
1:H:24:MET:HB2	1:H:186:SER:OG	2.13	0.48
2:D:511:LYS:HG2	2:D:512:PRO:HD2	1.95	0.48
2:C:397:VAL:HG12	2:C:474:ILE:HG23	1.95	0.48
1:G:146:GLY:O	1:G:150:ILE:HG12	2.14	0.48
2:B:656:LYS:O	2:B:660:ARG:HG3	2.13	0.48
2:A:476:ILE:HG22	2:A:734:ILE:HG12	1.94	0.48
1:F:191:GLU:O	1:F:195:VAL:HG23	2.14	0.48
2:B:485:ARG:HB3	2:B:491:PHE:HE2	1.79	0.48
2:B:753:LEU:HD22	2:B:758:VAL:HG11	1.95	0.48
2:A:651:ASP:HA	2:A:682:PHE:HB3	1.96	0.48
2:C:435[B]:HIS:HE1	2:C:753:LEU:HD21	1.78	0.48
2:A:476:ILE:HG13	2:A:476:ILE:O	2.12	0.48
2:D:551:TRP:HA	2:D:567:SER:HA	1.95	0.48
1:G:12:LEU:HA	1:G:15:VAL:HG22	1.96	0.48
2:C:651:ASP:N	2:C:651:ASP:OD1	2.47	0.48
2:B:660:ARG:HG2	2:B:671:TRP:CZ2	2.49	0.48
2:A:693:VAL:HG21	2:A:702:TYR:HB2	1.94	0.48
2:D:702:TYR:CE1	2:D:704:LEU:HB3	2.49	0.48
2:A:715:ARG:HH12	2:A:771:GLY:HA2	1.79	0.47
2:C:483:LEU:HD22	2:B:752:LYS:HB2	1.96	0.47
2:B:802:GLY:HA3	2:A:604:VAL:HG11	1.97	0.47
2:A:427:ASP:HB3	2:A:762:LEU:HD11	1.95	0.47
1:G:64:TRP:HH2	1:G:109:ILE:HD11	1.77	0.47
1:F:60:HIS:CE1	1:F:67:CYS:HB2	2.49	0.47
1:G:57:VAL:HG21	1:G:71:GLY:HA2	1.96	0.47
2:B:666:VAL:O	2:B:670:MET:HG3	2.15	0.47
2:D:456:ASP:OD1	2:D:456:ASP:N	2.48	0.47
1:E:66:THR:HG23	1:E:80:ILE:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:40:CYS:HB2	1:G:68:CYS:HB2	1.75	0.47
2:C:705:GLU:OE2	2:C:730:LYS:NZ	2.48	0.47
2:A:670:MET:O	2:A:674:MET:HG2	2.15	0.47
2:D:548:PRO:HG2	2:D:549:TYR:H	1.78	0.47
1:H:9:GLN:O	1:H:13:THR:OG1	2.22	0.47
1:F:198:VAL:O	1:F:202:ILE:HG12	2.15	0.47
2:D:505:LYS:HZ2	2:D:697:LYS:HA	1.79	0.47
2:D:428:LEU:HD23	2:D:476:ILE:HG23	1.97	0.46
2:B:489:ILE:HD12	2:B:735:ALA:HB1	1.97	0.46
2:B:587:GLN:HG3	2:A:606:TRP:CG	2.51	0.46
2:D:415:LEU:HD13	2:D:419:GLU:HG3	1.96	0.46
2:C:402:GLU:HA	2:C:402:GLU:OE2	2.15	0.46
2:A:454:ASP:OD2	2:A:457:THR:OG1	2.33	0.46
2:B:685:THR:HG22	2:B:687:ALA:H	1.81	0.46
2:B:693:VAL:HG21	2:B:702:TYR:HB2	1.98	0.46
2:D:694:ARG:HH21	2:D:717:PRO:HD2	1.81	0.46
2:C:426:VAL:HG13	2:C:442:LEU:HD11	1.97	0.46
2:C:694:ARG:HG2	2:C:719:ASP:OD2	2.15	0.46
2:A:466:GLU:HG2	2:A:471:LYS:HD2	1.98	0.46
2:A:803:LEU:HD21	2:D:536:VAL:HG22	1.97	0.46
2:A:447:ASP:OD1	2:A:447:ASP:N	2.44	0.45
2:D:405:TYR:HB3	2:D:425:CYS:SG	2.56	0.45
2:D:633:ILE:HG22	2:D:723:VAL:HG21	1.98	0.45
2:C:395:VAL:HG23	2:C:473:ASP:HB2	1.98	0.45
2:C:493:LYS:N	2:C:747:ASN:OD1	2.45	0.45
1:H:61:SER:HB3	1:H:66:THR:HG23	1.99	0.45
1:E:61:SER:HA	1:E:66:THR:HA	1.99	0.45
2:C:590:ASP:OD1	2:C:590:ASP:N	2.35	0.45
2:A:762:LEU:HD23	2:A:762:LEU:HA	1.86	0.45
2:A:808:LEU:O	2:A:812:ILE:HG12	2.16	0.45
2:D:692:ARG:HA	2:D:695:LYS:HG2	1.99	0.45
1:E:41:LYS:HB2	1:E:73:PHE:CE2	2.52	0.45
2:C:572:GLY:H	2:C:575:ASN:HB2	1.81	0.45
2:C:531:PHE:HB3	1:G:150:ILE:HD12	1.98	0.44
2:D:683:VAL:HG11	2:D:689:GLY:HA2	1.98	0.44
1:H:131:ARG:HG3	1:H:134:ILE:HG13	1.99	0.44
2:C:587:GLN:HG3	2:B:606:TRP:CG	2.52	0.44
1:H:101:VAL:HG12	1:H:155:VAL:HG11	1.97	0.44
2:B:451:GLY:HA3	2:B:464:VAL:HG12	2.00	0.44
2:B:635:SER:OG	2:B:637:GLU:HG2	2.18	0.44
2:A:823:LYS:HE2	2:A:823:LYS:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:669:LYS:HA	2:D:672:THR:HG22	2.00	0.44
1:E:64:TRP:HH2	1:E:109:ILE:HD11	1.82	0.44
1:E:27:ALA:HA	1:E:179:SER:HB3	2.00	0.44
2:C:467:LEU:HD22	2:C:737:PRO:HD3	2.00	0.44
2:B:751:LEU:HD23	2:B:751:LEU:HA	1.83	0.44
1:G:61:SER:HA	1:G:66:THR:HA	2.00	0.44
2:A:485:ARG:O	2:A:489:ILE:HG12	2.18	0.43
1:H:191:GLU:HB3	2:D:538:VAL:HG21	2.00	0.43
2:C:542:LEU:O	2:C:546:PHE:HB3	2.18	0.43
2:C:663:LYS:H	2:C:663:LYS:HG2	1.66	0.43
2:A:647:TYR:HB3	2:A:701:ALA:HB3	2.00	0.43
2:C:399:THR:HB	2:C:406:VAL:HG21	1.99	0.43
2:D:702:TYR:CD1	2:D:704:LEU:HB3	2.54	0.43
1:F:129:LYS:HA	1:F:129:LYS:HD3	1.76	0.43
2:B:500:ILE:HD12	2:B:728:ASP:OD2	2.18	0.43
2:B:409:LYS:HG2	2:B:422:GLU:HG2	2.00	0.43
2:D:666:VAL:HA	2:D:669:LYS:HE3	2.00	0.43
2:D:495:PHE:N	2:D:732:TYR:O	2.52	0.43
2:D:656:LYS:HB3	2:D:656:LYS:HE3	1.80	0.43
2:A:651:ASP:N	2:A:683:VAL:O	2.44	0.43
2:C:817:LYS:HB3	2:B:549:TYR:CZ	2.54	0.42
2:B:399:THR:HB	2:B:406:VAL:HG21	2.01	0.42
2:B:439:LYS:HA	2:B:439:LYS:HD3	1.76	0.42
2:A:451:GLY:HA2	2:A:461:ASN:O	2.20	0.42
1:H:98:LEU:HD23	1:H:98:LEU:HA	1.86	0.42
2:A:587:GLN:HG3	2:D:606:TRP:CG	2.55	0.42
2:A:663:LYS:HD2	2:A:663:LYS:O	2.19	0.42
2:A:714:GLN:HA	2:A:714:GLN:OE1	2.20	0.42
2:D:689:GLY:HA3	2:D:702:TYR:HE2	1.84	0.42
1:H:31:ASP:OD2	1:H:65:ARG:NE	2.52	0.42
2:D:405:TYR:CD2	2:D:478:PRO:HG3	2.55	0.42
1:G:131:ARG:HD2	1:G:131:ARG:HA	1.88	0.42
2:C:476:ILE:HG12	2:C:734:ILE:HG23	2.02	0.42
2:D:693:VAL:HG21	2:D:702:TYR:HB2	2.02	0.42
2:C:658:PHE:O	2:C:662:SER:HB2	2.20	0.42
2:A:431:GLU:HB3	2:A:753:LEU:HD21	2.02	0.42
1:E:196:LEU:O	1:E:200:MET:HG3	2.19	0.42
2:B:506:LYS:HG3	2:B:507:PRO:HD2	2.01	0.42
1:G:34:LEU:HD22	1:G:36:SER:HB3	2.02	0.42
1:E:30:THR:HG21	1:E:178:TRP:CH2	2.55	0.41
2:B:484:VAL:O	2:B:488:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:823:LYS:HB3	2:B:823:LYS:HE3	1.76	0.41
2:D:689:GLY:HA3	2:D:702:TYR:CE2	2.54	0.41
2:C:511:LYS:HA	2:C:512:PRO:HD3	1.94	0.41
2:A:463:MET:HE2	2:A:475:ALA:HB1	2.02	0.41
2:A:691:ALA:O	2:A:695:LYS:HG2	2.21	0.41
2:D:404:PRO:HB3	2:D:711:TYR:CE1	2.55	0.41
2:C:438:PHE:HE2	2:C:440:TYR:HB3	1.85	0.41
2:A:699:LYS:HA	2:A:699:LYS:HD3	1.75	0.41
2:D:457:THR:HB	2:D:459:ILE:HG13	2.03	0.41
2:D:792:VAL:O	2:D:795:VAL:HG12	2.21	0.41
1:G:157:ILE:HD11	1:G:180:PHE:HZ	1.85	0.41
1:G:101:VAL:HG12	1:G:155:VAL:HG11	2.02	0.41
2:C:503:MET:HB2	2:C:709:ASN:OD1	2.20	0.41
2:A:422:GLU:HA	2:A:426:VAL:HG21	2.02	0.41
2:A:734:ILE:HG21	2:A:746:VAL:HG11	2.03	0.41
2:D:503:MET:HB2	2:D:709:ASN:OD1	2.20	0.41
2:D:796:PHE:HB3	1:G:154:ILE:HD13	2.02	0.41
1:G:34:LEU:CD2	1:G:174:TYR:HB2	2.50	0.41
2:C:548:PRO:HG3	1:G:205:HIS:CE1	2.56	0.40
2:A:429:ALA:HB2	2:A:476:ILE:HD11	2.03	0.40
1:E:60:HIS:CE1	1:E:67:CYS:HB3	2.56	0.40
1:E:64:TRP:O	1:E:80:ILE:HG13	2.21	0.40
1:E:109:ILE:O	1:E:113:ILE:HG23	2.20	0.40
2:C:681:VAL:HA	2:C:692:ARG:NH2	2.33	0.40
2:D:542:LEU:O	2:D:546:PHE:HB3	2.21	0.40
2:D:800:VAL:HG11	1:G:151:ILE:HG12	2.04	0.40
1:G:57:VAL:HG22	1:G:58:MET:H	1.87	0.40
1:H:143:VAL:HG21	2:D:542:LEU:HD13	2.02	0.40
2:B:488:VAL:HG23	2:B:489:ILE:HG23	2.02	0.40
2:B:792:VAL:O	2:B:795:VAL:HG12	2.21	0.40
2:C:433:ALA:O	2:C:437:GLY:N	2.55	0.40
2:D:425:CYS:SG	2:D:477:ALA:HA	2.61	0.40
2:B:453:ARG:HB2	2:B:460:TRP:CE2	2.57	0.40
2:B:810:ALA:HB1	2:A:546:PHE:HE1	1.87	0.40
2:A:787:LEU:HD13	2:D:619:ASN:OD1	2.21	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	E	183/323 (57%)	174 (95%)	9 (5%)	0	100	100
1	F	182/323 (56%)	178 (98%)	4 (2%)	0	100	100
1	G	183/323 (57%)	175 (96%)	8 (4%)	0	100	100
1	H	182/323 (56%)	178 (98%)	4 (2%)	0	100	100
2	A	396/889 (44%)	388 (98%)	8 (2%)	0	100	100
2	B	403/889 (45%)	398 (99%)	5 (1%)	0	100	100
2	C	398/889 (45%)	391 (98%)	7 (2%)	0	100	100
2	D	404/889 (45%)	400 (99%)	4 (1%)	0	100	100
All	All	2331/4848 (48%)	2282 (98%)	49 (2%)	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	E	151/275 (55%)	145 (96%)	6 (4%)	27	52
1	F	150/275 (54%)	145 (97%)	5 (3%)	33	59
1	G	151/275 (55%)	150 (99%)	1 (1%)	81	89
1	H	150/275 (54%)	148 (99%)	2 (1%)	65	79
2	A	333/764 (44%)	322 (97%)	11 (3%)	33	59
2	B	339/764 (44%)	334 (98%)	5 (2%)	60	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	335/764 (44%)	323 (96%)	12 (4%)	30	56
2	D	339/764 (44%)	331 (98%)	8 (2%)	44	67
All	All	1948/4156 (47%)	1898 (97%)	50 (3%)	42	65

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	78	LYS
1	H	97	PHE
1	F	40	CYS
1	F	78	LYS
1	F	104	SER
1	F	186	SER
1	F	203	ASP
2	C	498	LEU
2	C	505	LYS
2	C	546	PHE
2	C	567	SER
2	C	590	ASP
2	C	592	SER
2	C	594	ARG
2	C	623	PHE
2	C	708	MET
2	C	713	GLU
2	C	773	CYS
2	C	819	ARG
2	B	407	MET
2	B	523	TYR
2	B	708	MET
2	B	754	SER
2	B	767	TRP
2	A	491	PHE
2	A	498	LEU
2	A	506	LYS
2	A	519	ASP
2	A	541	PHE
2	A	567	SER
2	A	760	ASP
2	A	761	LYS
2	A	767	TRP
2	A	773	CYS

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Mol	Chain	Res	Type
2	A	818	SER
2	D	523	TYR
2	D	546	PHE
2	D	619	ASN
2	D	631	SER
2	D	663	LYS
2	D	684	ARG
2	D	719	ASP
2	D	773	CYS
1	E	58	MET
1	E	67	CYS
1	E	97	PHE
1	E	105	SER
1	E	187	PHE
1	E	209	ARG
1	G	204	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

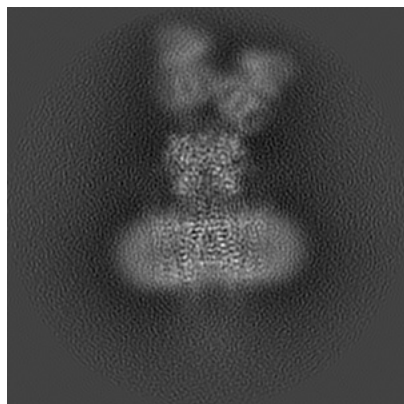
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44251. These allow visual inspection of the internal detail of the map and identification of artifacts.

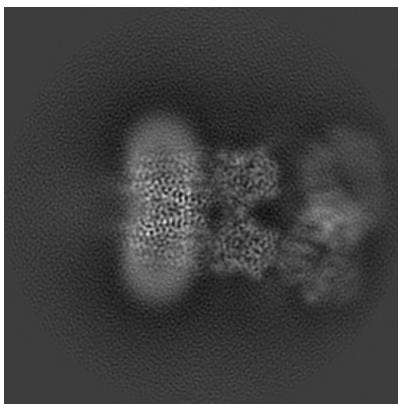
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

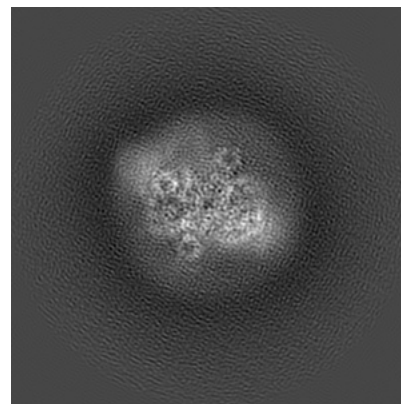
#### 6.1.1 Primary map



X

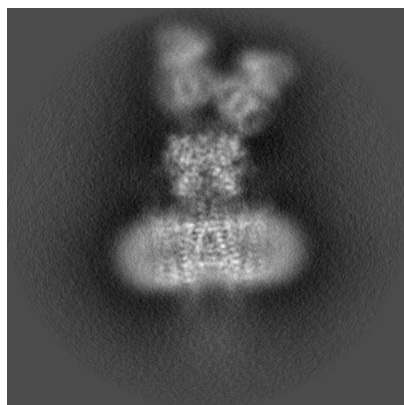


Y

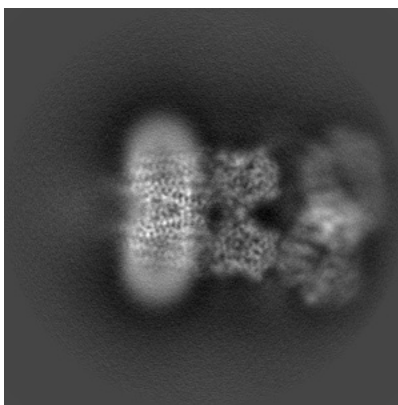


Z

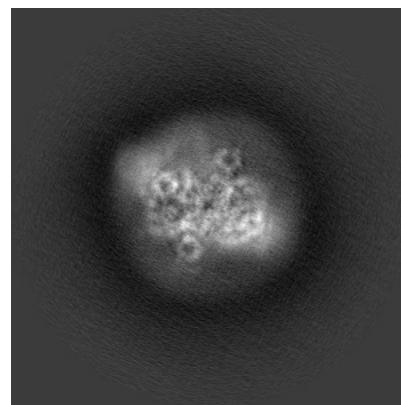
#### 6.1.2 Raw map



X



Y

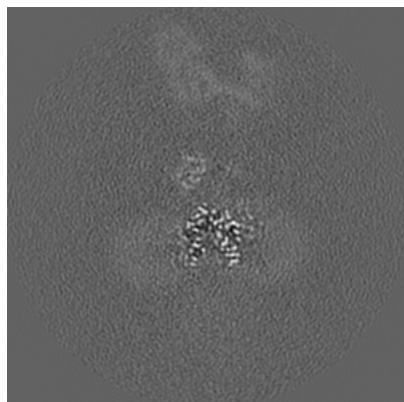


Z

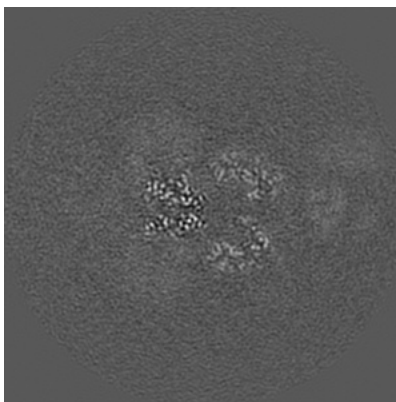
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

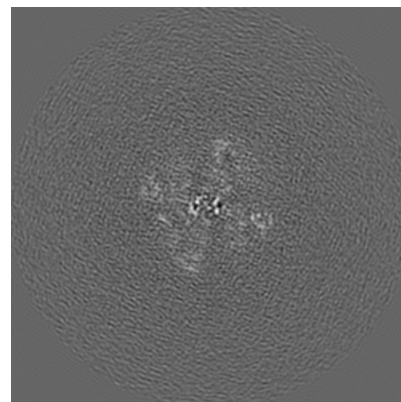
### 6.2.1 Primary map



X Index: 180

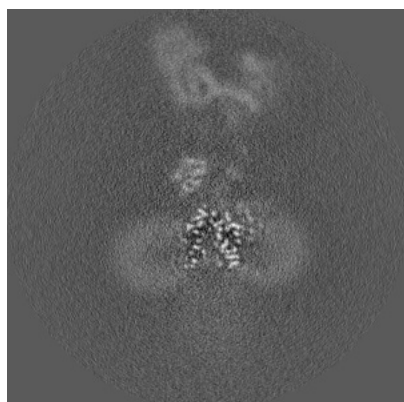


Y Index: 180

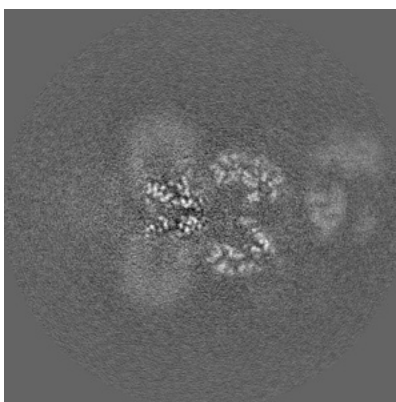


Z Index: 180

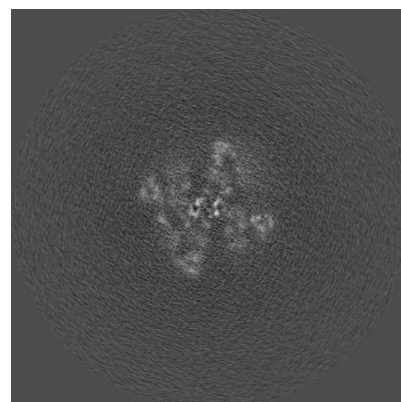
### 6.2.2 Raw map



X Index: 180



Y Index: 180



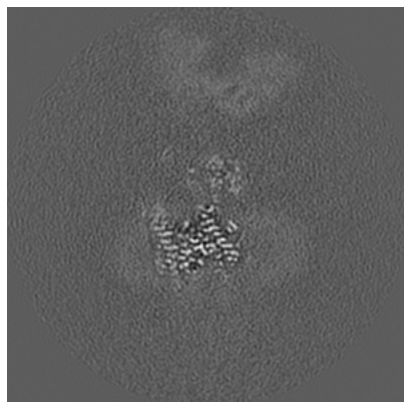
Z Index: 180

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

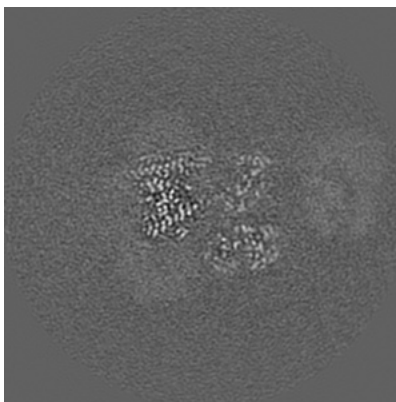


## 6.3 Largest variance slices [i](#)

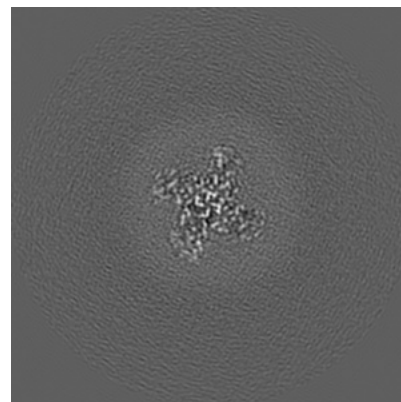
### 6.3.1 Primary map



X Index: 166

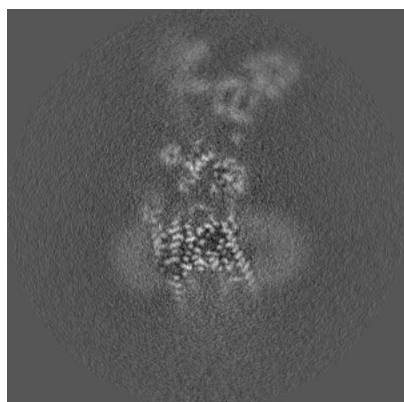


Y Index: 171

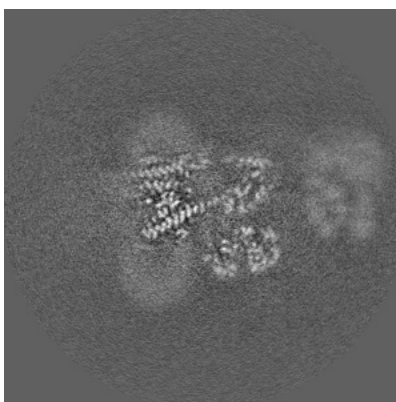


Z Index: 161

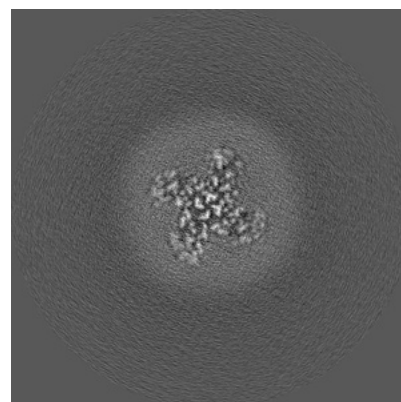
### 6.3.2 Raw map



X Index: 160



Y Index: 172

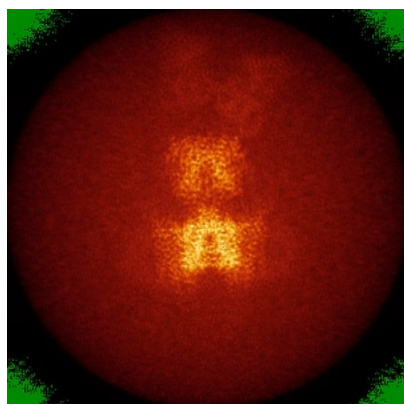


Z Index: 161

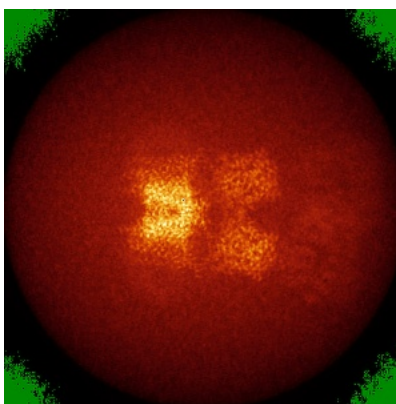
The images above show the largest variance slices of the map in three orthogonal directions.

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

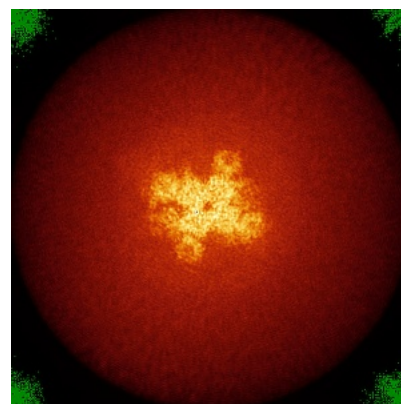
### 6.4.1 Primary map



X

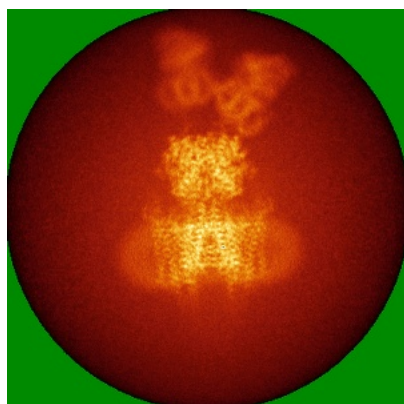


Y

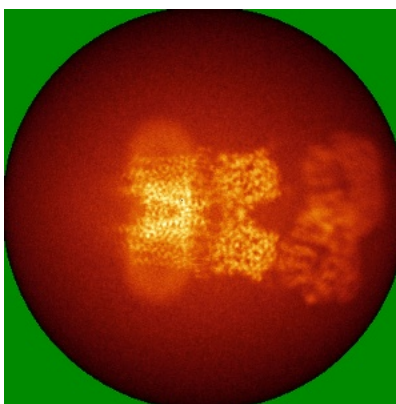


Z

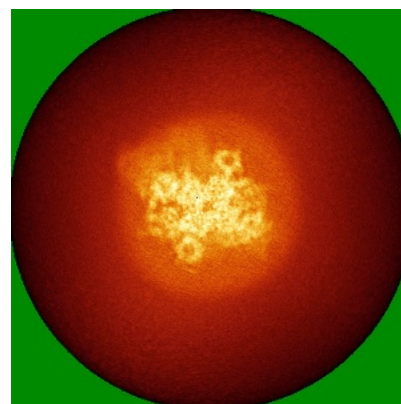
### 6.4.2 Raw map



X



Y

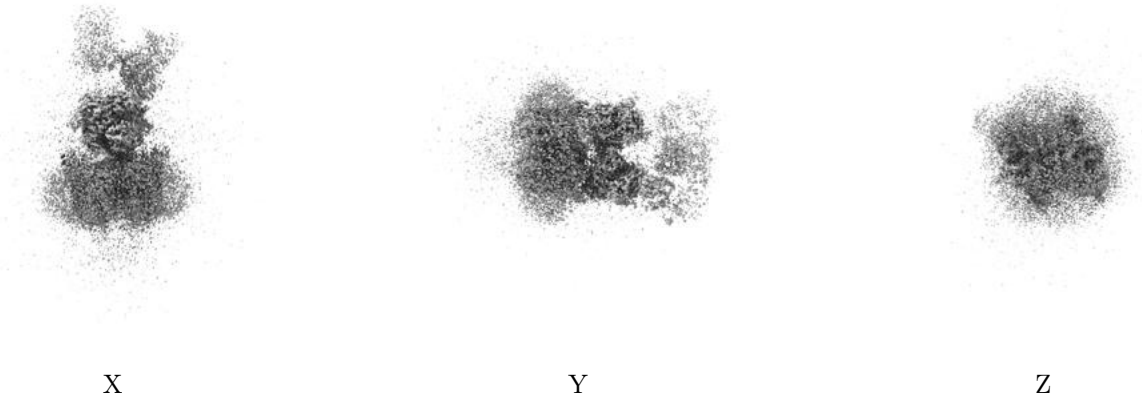


Z

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.

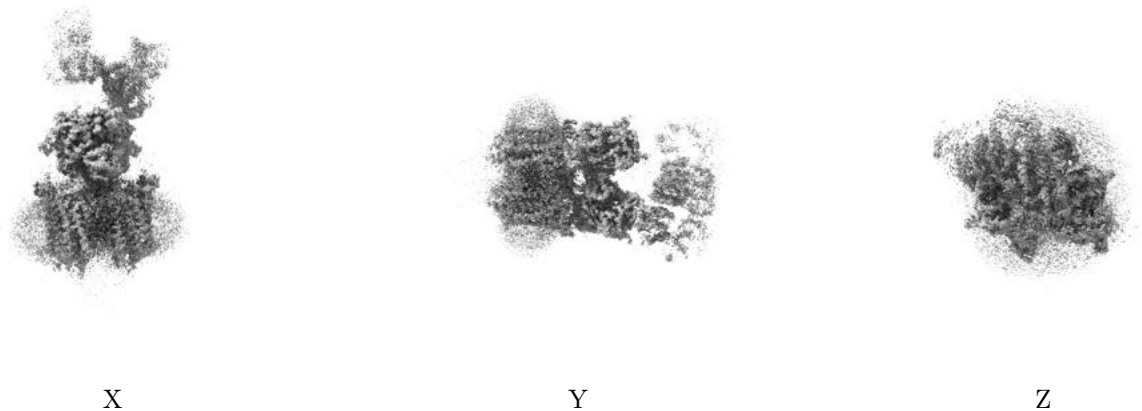
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0155. 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.

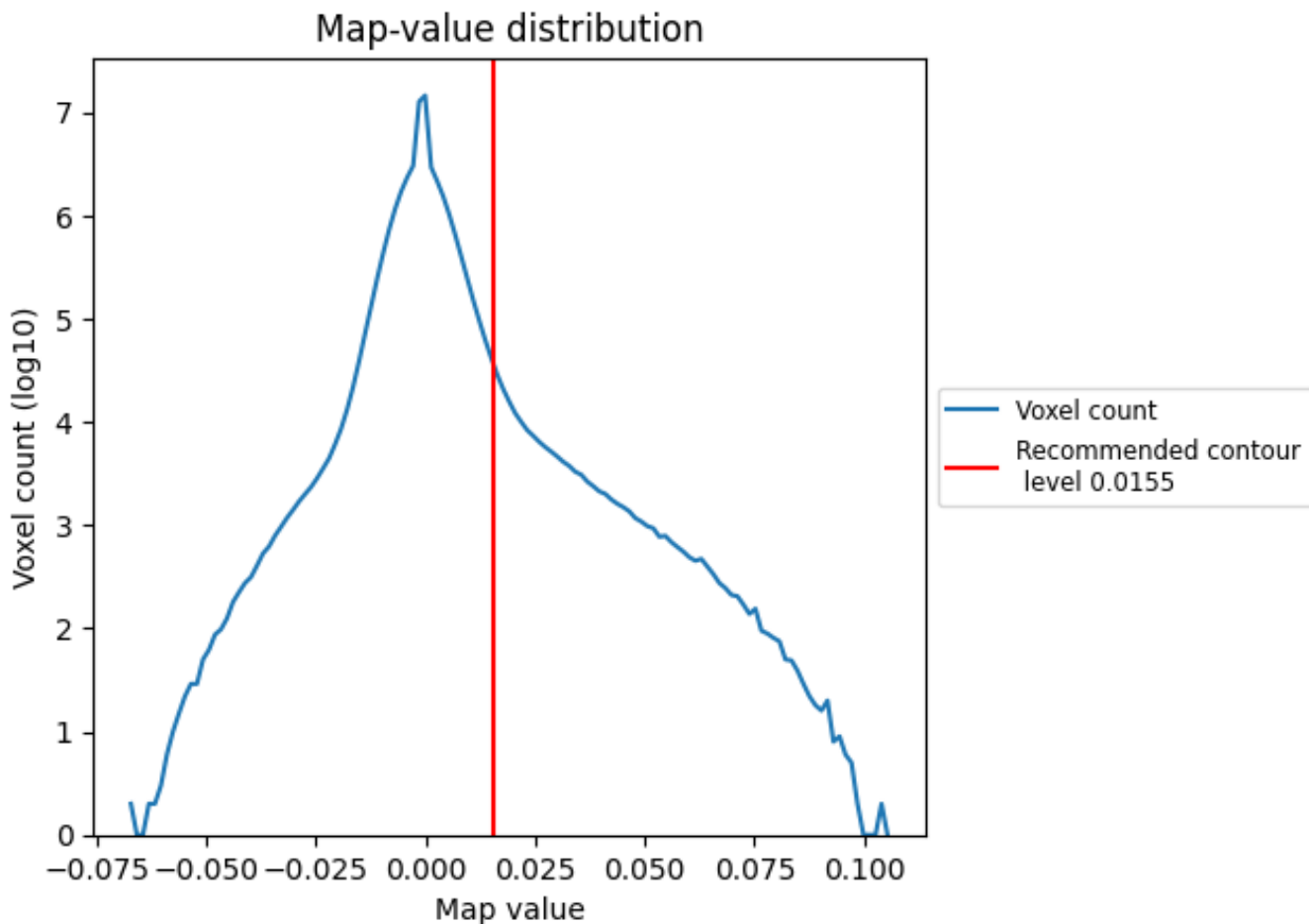
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

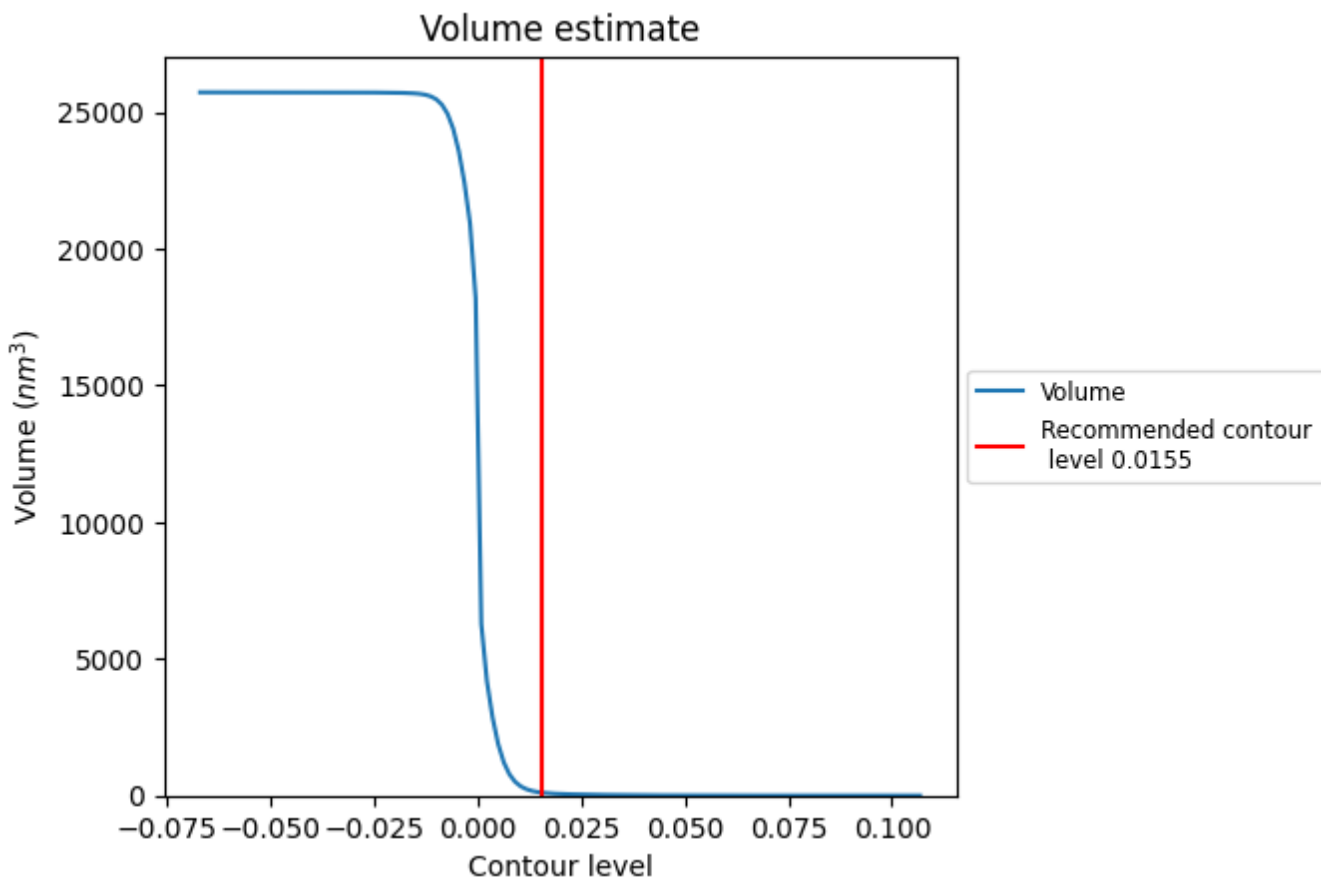
This section contains the results of statistical analysis of the map.

### 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.

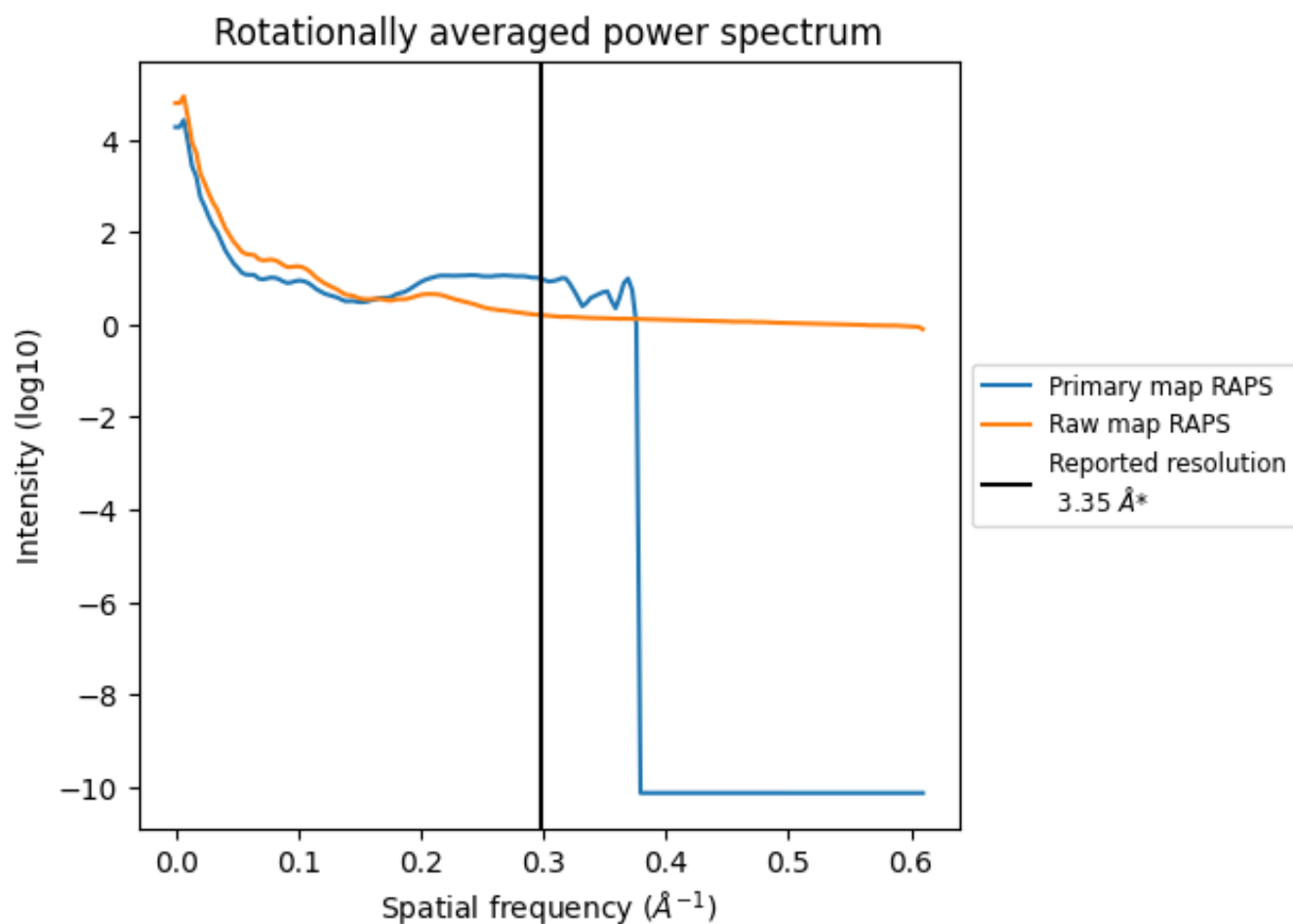
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 107 nm<sup>3</sup>; this corresponds to an approximate mass of 96 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 [\(i\)](#)

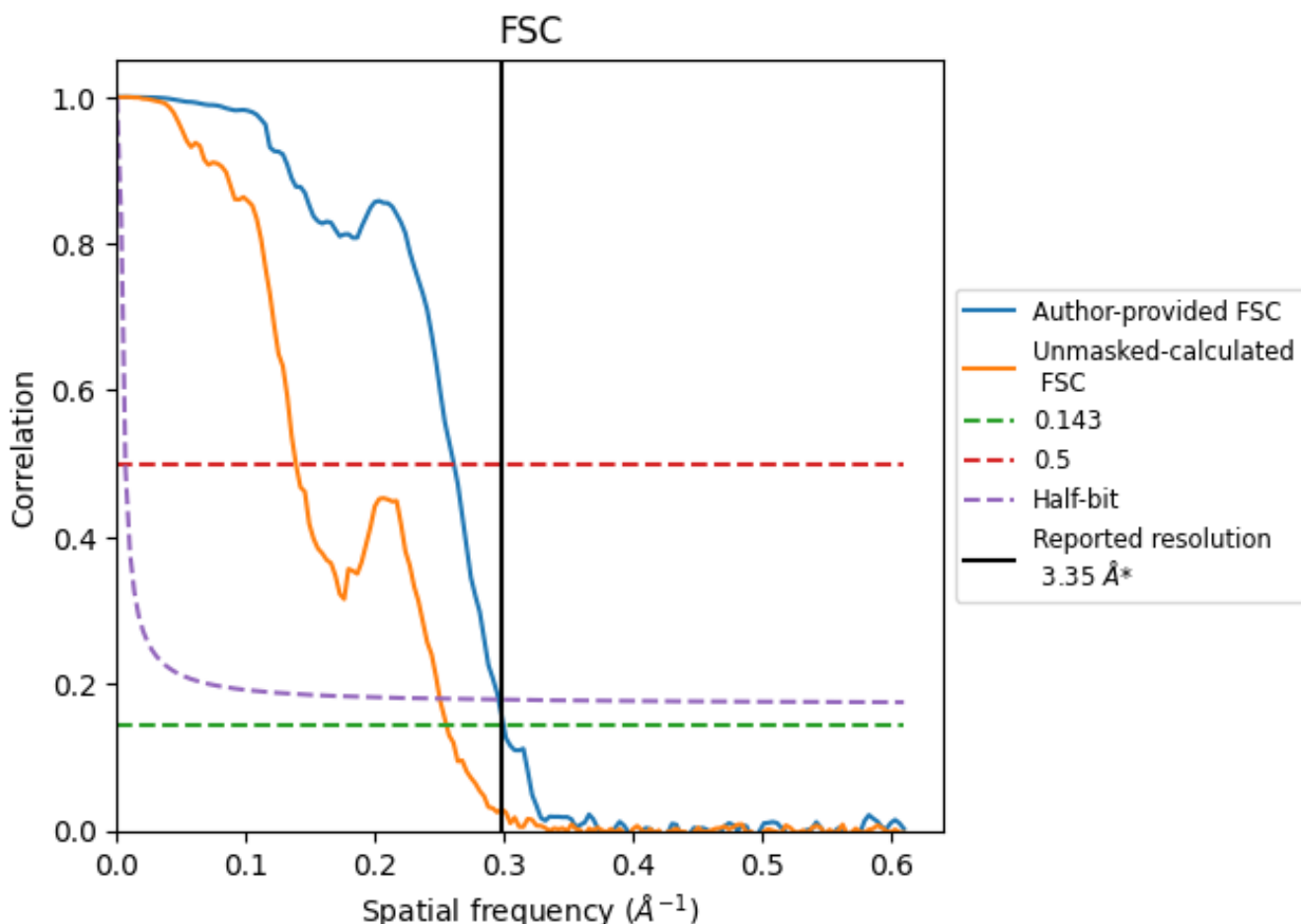


\*Reported resolution corresponds to spatial frequency of 0.299 Å<sup>-1</sup>

## 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 0.299 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.35	-	-
Author-provided FSC curve	3.34	3.83	3.38
Unmasked-calculated*	3.91	7.20	4.00

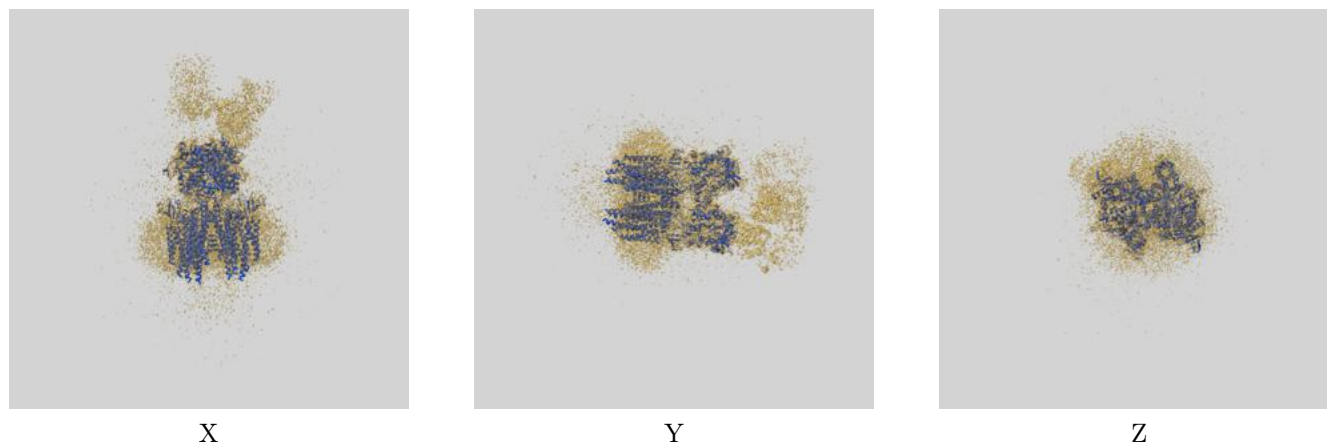
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.91 differs from the reported value 3.35 by more than 10 %



## 9 Map-model fit [i](#)

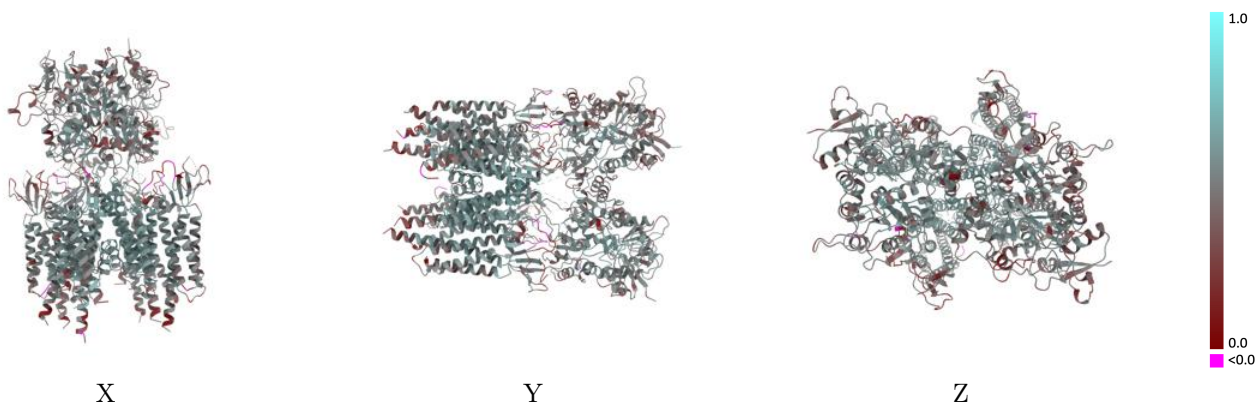
This section contains information regarding the fit between EMDB map EMD-44251 and PDB model 9B6A. Per-residue inclusion information can be found in section 3 on page 5.

### 9.1 Map-model overlay [i](#)



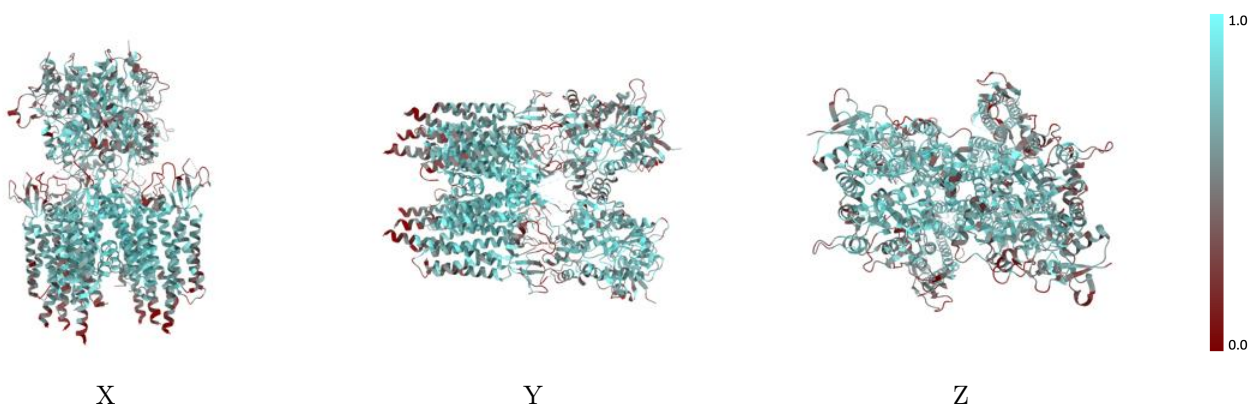
The images above show the 3D surface view of the map at the recommended contour level 0.0155 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



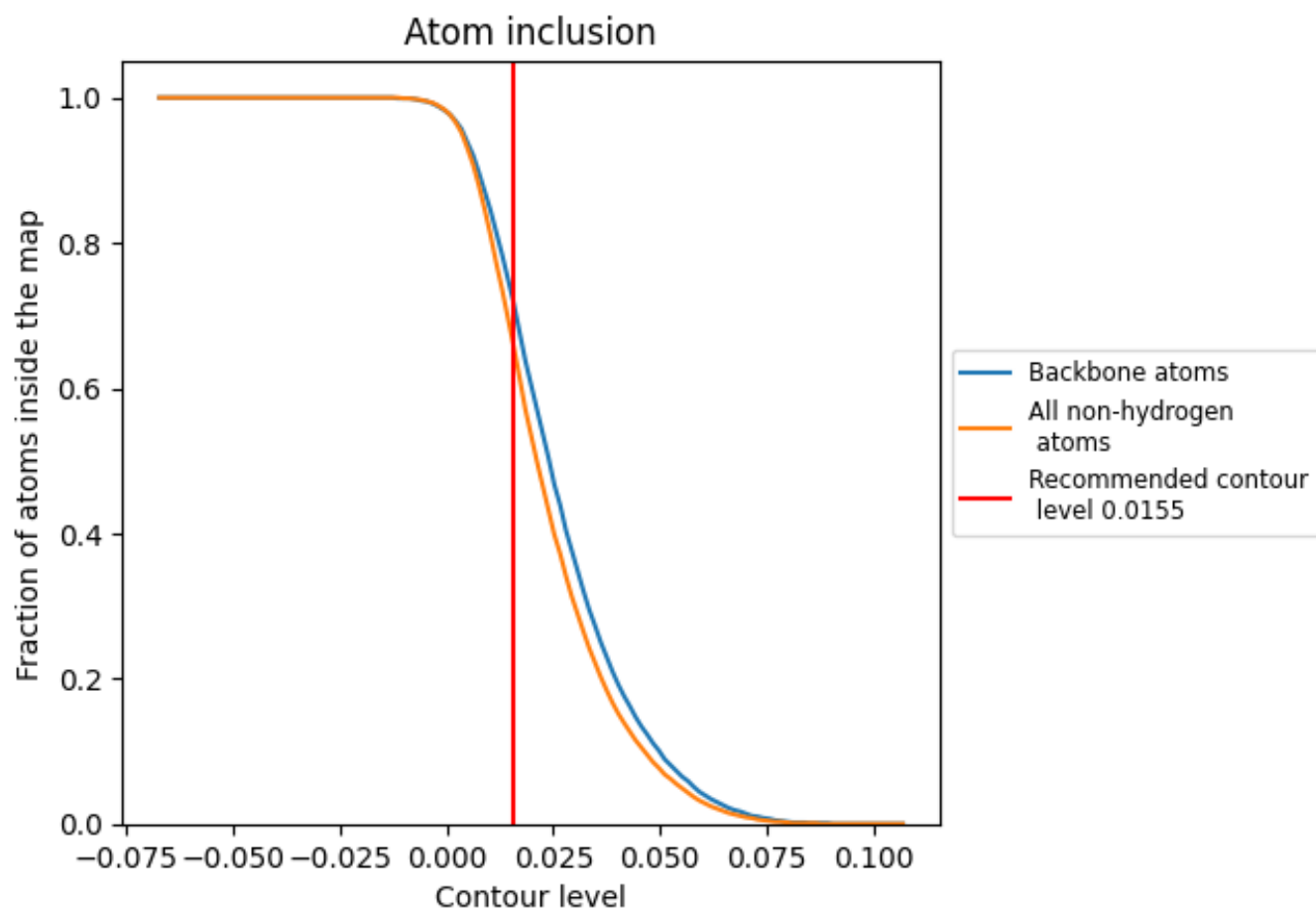
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0155).



















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 72% 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 (0.0155) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6650	 0.4880
A	 0.6800	 0.4990
B	 0.7170	 0.5120
C	 0.7370	 0.5180
D	 0.6840	 0.4980
E	 0.5740	 0.4310
F	 0.5810	 0.4550
G	 0.5690	 0.4430
H	 0.5920	 0.4590

