



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 05:33 AM UTC

PDB ID : 9BCQ / pdb_00009bcq
EMDB ID : EMD-44434
Title : Extracellular domain of GC-A bound to ANP
Authors : Liu, S.; Huang, X.
Deposited on : 2024-04-09
Resolution : 3.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

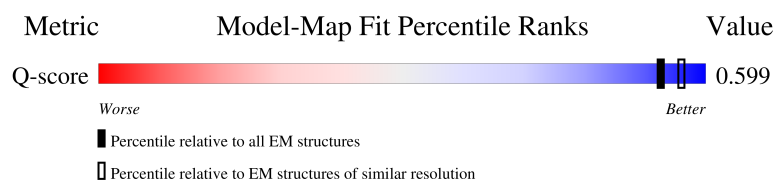
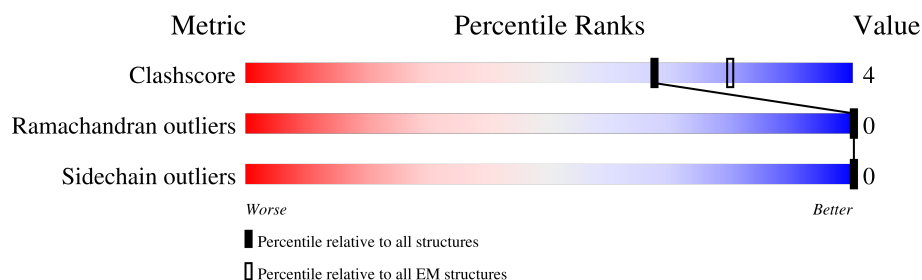
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.10 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	14724 (2.60 - 3.60)

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	1040	
1	B	1040	
2	C	28	
3	D	2	

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Mol	Chain	Length	Quality of chain
3	E	2	 100%
3	F	2	 50% 50%
4	G	3	 67% 33%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13465 atoms, of which 6530 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 Atrial natriuretic peptide receptor 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	425	Total	C	H	N	O	S	0	0
			6460	2122	3150	574	601	13		
1	B	425	Total	C	H	N	O	S	0	0
			6476	2126	3160	571	606	13		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	ASP	-	expression tag	UNP P16066
A	-9	TYR	-	expression tag	UNP P16066
A	-8	LYS	-	expression tag	UNP P16066
A	-7	ASP	-	expression tag	UNP P16066
A	-6	ASP	-	expression tag	UNP P16066
A	-5	ASP	-	expression tag	UNP P16066
A	-4	ASP	-	expression tag	UNP P16066
A	-3	LYS	-	expression tag	UNP P16066
A	-2	ALA	-	expression tag	UNP P16066
A	-1	ALA	-	expression tag	UNP P16066
B	-10	ASP	-	expression tag	UNP P16066
B	-9	TYR	-	expression tag	UNP P16066
B	-8	LYS	-	expression tag	UNP P16066
B	-7	ASP	-	expression tag	UNP P16066
B	-6	ASP	-	expression tag	UNP P16066
B	-5	ASP	-	expression tag	UNP P16066
B	-4	ASP	-	expression tag	UNP P16066
B	-3	LYS	-	expression tag	UNP P16066
B	-2	ALA	-	expression tag	UNP P16066
B	-1	ALA	-	expression tag	UNP P16066

- Molecule 2 is a protein called Atrial natriuretic peptide.

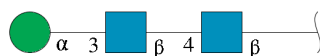
Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	24	Total	C	H	N	O	S	0	0
			326	100	156	35	32	3		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	2	Total	C	H	N	O	0	0
			44	16	16	2	10		
3	E	2	Total	C	H	N	O	0	0
			44	16	16	2	10		
3	F	2	Total	C	H	N	O	0	0
			44	16	16	2	10		

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	3	Total	C	H	N	O	0	0
			47	22	8	2	15		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total Cl 1 1	0
5	B	1	Total Cl 1 1	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
6	B	1	22	8	8	1	5	0

Chain B:  37% 59%

ASP	TYR	LYS	ASP	ASP	ASP	ASP	LYS	ALA	ALA	G1	N13	S19	R22	S53	V70	L82	G83	A91	P92	L104	R143	Y154	A155	V168	T182	F188	L199	L222	M223	F238	D242	G250	Q253	Q253	T281	Y282	F283	D284	ASP											
F293	L297	M309	L313	V314	L327	I366	E373	L392	L401	V402	A403	F425	ASP	ASN	GLU	GLU	ASP	PRO	ALA	CYS	ASN	ASN	GLN	ASP	HIS	LEU	SER	THR	LEU	GLY	SER	LEU	SER	LEU	GLY	THR	THR	GLY	ILE	GLY	LEU	VAL	VAL	GLN	PHE	PHE	ILE	TYR	ALA	
LYS	MET	GLN	LEU	LYS	GLY	LEU	ASN	VAL	GLU	ASN	VAL	THR	ARG	LYS	TRP	GLU	VAL	ARG	HIS	ALA	CYS	ASN	GLN	THR	LEU	GLY	ARG	GLY	ASN	VAL	GLY	THR	LEU	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
PRO	ARG	GLY	SER	LEU	GLN	ASP	ASN	GLU	TRP	MET	PHE	ARG	TYR	LYS	SER	LEU	THR	ASN	ASP	ILE	LEU	VAL	HIS	GLY	GLY	GLY	VAL	ASN	ASN	GLY	LYS	SER	SER	ASN	CYS	ASN	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	
ILE	THR	THR	TYR	GLY	LEU	GLU	ASP	ASP	HIS	THR	VAL	ALA	GLY	GLY	ALA	LYS	LEU	THR	ALA	PRO	GLU	LEU	LEU	PRO	ARG	ILE	GLY	GLN	ASN	GLY	THR	ASP	THR	ASN	GLY	ASN	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	
SER	GLY	PHE	HIS	VAL	VAL	SER	PRO	ILE	GLY	VAL	VAL	ARG	GLY	GLY	GLY	GLY	GLN	ALA	PRO	PRO	SER	GLN	HIS	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY		
GLN	ILE	LEU	THR	THR	THR	ARG	ASN	GLU	THR	ASN	ASN	LEU	LEU	ILE	SER	ARG	GLY	GLY	ARG	PRO	ASN	VAL	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
SER	VAL	ALA	GLN	GLY	LEU	VAL	GLY	ALA	PHE	SER	VAL	ILE	TYR	THR	THR	PHE	THR	ALA	VAL	GLY	LEU	GLY	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY		
ASP	TYR	VAL	LYS	ILE	GLY	ALA	MET	ASP	THR	PRO	VAL	ASN	GLY	GLY	ASN	ARG	LEU	HIS	VAL	VAL	GLY	ALA	ALA	ALA	LEU	ALA	VAL	ARG	PHE	THR	ILE	HIS	ARG	HIS	ASP	THR	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
HIS	THR	GLY	PRO	VAL	CYS	GLY	ALA	VAL	VAL	VAL	VAL	GLY	THR	THR	ASP	THR	THR	ALA	ALA	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY		
GLY	ASP	VAL	GLY	GLY	LYS	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	

- Molecule 2: Atrial natriuretic peptide

Chain C:  86% 14%

SER	LEU	ARG	R4	R27	TYR
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- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  100%

MAG1	MAG2
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- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

MAG1
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  50% 50%

MAG1
MAG2

- Molecule 4: alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  67% 33%

MAG1
MAG2
MAN3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	964634	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 ($e^-/\text{\AA}^2$)	51.13	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.037	Depositor
Minimum map value	-3.722	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.224	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	173.216, 173.216, 173.216	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0826, 1.0826, 1.0826	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NAG, MAN

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	0.27	0/3403	0.37	3/4642 (0.1%)
1	B	0.26	0/3409	0.40	1/4649 (0.0%)
2	C	0.20	0/171	0.32	0/224
All	All	0.26	0/6983	0.38	4/9515 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	373	GLU	CB-CG-CD	5.53	122.01	112.60
1	A	373	GLU	CA-C-O	-5.41	114.31	120.58
1	A	203	MET	CA-CB-CG	5.33	124.77	114.10
1	A	373	GLU	CB-CG-CD	5.16	121.36	112.60

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	3310	3150	3211	24	0
1	B	3316	3160	3216	26	0
2	C	170	156	155	0	0
3	D	28	16	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	28	16	25	1	0
3	F	28	16	25	1	0
4	G	39	8	34	1	0
5	A	1	0	0	0	0
5	B	1	0	0	1	0
6	B	14	8	13	2	0
All	All	6935	6530	6704	52	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 4.

All (52) 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)
6:B:1102:NAG:H3	6:B:1102:NAG:H83	1.61	0.81
1:A:11:LEU:HD21	1:A:50:LEU:HD12	1.72	0.71
1:B:282:TYR:HB2	1:B:313:LEU:HD21	1.73	0.71
1:B:313:LEU:O	1:B:313:LEU:HD23	1.95	0.65
1:B:223:MET:HE1	1:B:238:PHE:CD2	2.31	0.65
1:B:242:ASP:O	1:B:281:THR:HG22	1.98	0.63
1:B:223:MET:HE1	1:B:238:PHE:CG	2.34	0.62
1:A:155:ALA:HB1	1:A:190:GLU:HG3	1.84	0.60
4:G:2:NAG:O3	4:G:2:NAG:O7	2.20	0.60
1:A:357:PHE:O	1:A:364:LEU:N	2.34	0.59
6:B:1102:NAG:H3	6:B:1102:NAG:C8	2.34	0.57
1:B:91:ALA:HB3	1:B:92:PRO:HD3	1.86	0.57
1:A:252:GLN:HG3	1:A:284:ASP:OD2	2.05	0.55
1:A:175:VAL:HG22	1:A:175:VAL:O	2.07	0.55
1:A:196:TYR:O	1:A:200:LEU:HD23	2.08	0.54
1:A:223:MET:HE1	1:A:238:PHE:CG	2.43	0.53
1:B:143:ARG:HD2	1:B:401:LEU:HD23	1.90	0.52
1:B:297:LEU:CD2	1:B:309:MET:HE2	2.40	0.52
1:B:83:GLY:CA	1:B:104:LEU:HD11	2.41	0.51
1:B:154:TYR:HB3	1:B:168:VAL:HG21	1.93	0.50
1:B:252:GLN:HG2	1:B:284:ASP:OD2	2.12	0.50
1:B:199:LEU:HD23	1:B:222:LEU:HD11	1.93	0.49
1:A:328:TYR:O	1:A:332:VAL:HG23	2.13	0.48
1:A:8:VAL:HG12	1:A:53:SER:HB3	1.95	0.48
1:B:327:LEU:HD21	1:B:366:ILE:HD12	1.95	0.48
1:A:70:VAL:HG11	1:B:70:VAL:HG11	1.95	0.48
1:A:11:LEU:CD2	1:A:50:LEU:HD12	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ASN:OD1	1:A:397:THR:HG22	2.14	0.47
1:B:83:GLY:HA2	1:B:104:LEU:HD11	1.97	0.47
1:B:13:ASN:ND2	3:F:1:NAG:O7	2.50	0.45
1:A:155:ALA:HB2	1:A:188:PHE:CZ	2.52	0.45
1:A:397:THR:HG21	3:E:1:NAG:H5	2.00	0.44
1:A:66:PRO:O	1:A:70:VAL:HG23	2.18	0.44
1:A:161:GLU:O	1:A:161:GLU:HG2	2.18	0.43
1:A:91:ALA:HB3	1:A:92:PRO:CD	2.49	0.43
1:B:155:ALA:HB2	1:B:188:PHE:CZ	2.54	0.42
1:B:182:THR:O	1:B:182:THR:HG23	2.19	0.42
1:B:53:SER:OG	5:B:1101:CL:CL	2.65	0.42
1:A:155:ALA:HB1	1:A:190:GLU:CG	2.47	0.42
1:A:204:PRO:O	1:A:208:ARG:NH1	2.43	0.42
1:A:237:VAL:O	1:A:237:VAL:HG13	2.19	0.41
1:A:65:ALA:HB3	1:A:66:PRO:HD3	2.02	0.41
1:B:250:GLY:O	1:B:313:LEU:HB2	2.21	0.41
1:A:317:ILE:HB	1:A:318:PRO:CD	2.50	0.41
1:B:82:LEU:HD23	1:B:82:LEU:HA	1.96	0.41
1:B:392:LEU:HD23	1:B:403:ALA:HA	2.03	0.40
1:B:293:PHE:CZ	1:B:297:LEU:HD12	2.55	0.40
1:A:200:LEU:O	1:A:204:PRO:HD3	2.22	0.40
1:B:314:VAL:HG22	1:B:314:VAL:O	2.22	0.40
1:A:390:VAL:O	1:A:407:ARG:NH1	2.55	0.40
1:B:19:SER:O	1:B:22:ARG:N	2.51	0.40
1:B:402:VAL:O	1:B:402:VAL:HG13	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	423/1040 (41%)	408 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	423/1040 (41%)	406 (96%)	17 (4%)	0	100	100
2	C	22/28 (79%)	22 (100%)	0	0	100	100
All	All	868/2108 (41%)	836 (96%)	32 (4%)	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	340/879 (39%)	340 (100%)	0	100	100
1	B	342/879 (39%)	342 (100%)	0	100	100
2	C	17/22 (77%)	17 (100%)	0	100	100
All	All	699/1780 (39%)	699 (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 (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	240	HIS
1	B	299	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

9 monosaccharides 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$
3	NAG	D	1	3,1	14,14,15	0.46	0	17,19,21	0.54	0
3	NAG	D	2	3	14,14,15	0.33	0	17,19,21	0.43	0
3	NAG	E	1	3,1	14,14,15	0.26	0	17,19,21	0.49	0
3	NAG	E	2	3	14,14,15	0.26	0	17,19,21	0.72	1 (5%)
3	NAG	F	1	3,1	14,14,15	0.41	0	17,19,21	0.45	0
3	NAG	F	2	3	14,14,15	0.27	0	17,19,21	0.39	0
4	NAG	G	1	4,1	14,14,15	0.66	1 (7%)	17,19,21	1.48	3 (17%)
4	NAG	G	2	4	14,14,15	0.94	1 (7%)	17,19,21	0.74	1 (5%)
4	MAN	G	3	4	11,11,12	0.81	0	15,15,17	1.25	2 (13%)

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
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/23/26	0/1/1/1
4	MAN	G	3	4	-	1/2/19/22	1/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	2	NAG	O5-C1	-3.47	1.37	1.43
4	G	1	NAG	O5-C1	2.22	1.47	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	NAG	C1-O5-C5	4.27	117.92	112.19
4	G	3	MAN	C1-O5-C5	3.67	117.11	112.19
4	G	1	NAG	O4-C4-C5	3.11	116.98	109.32
3	E	2	NAG	C1-O5-C5	2.43	115.44	112.19
4	G	3	MAN	O2-C2-C3	-2.35	105.29	110.15
4	G	2	NAG	C1-O5-C5	2.34	115.32	112.19
4	G	1	NAG	C4-C3-C2	-2.06	108.00	111.02

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	F	1	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
4	G	3	MAN	O5-C5-C6-O6
4	G	2	NAG	C3-C2-N2-C7

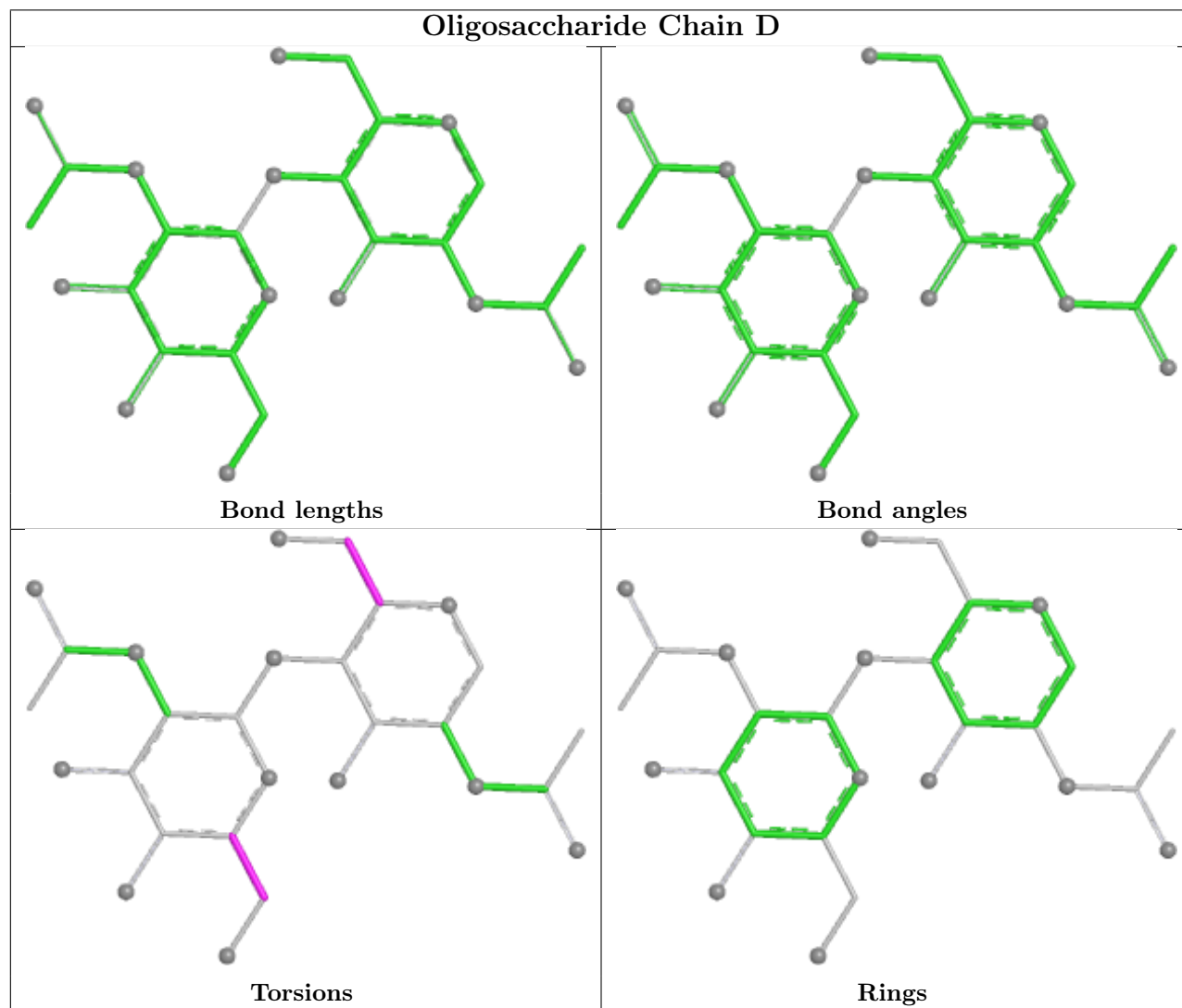
All (1) ring outliers are listed below:

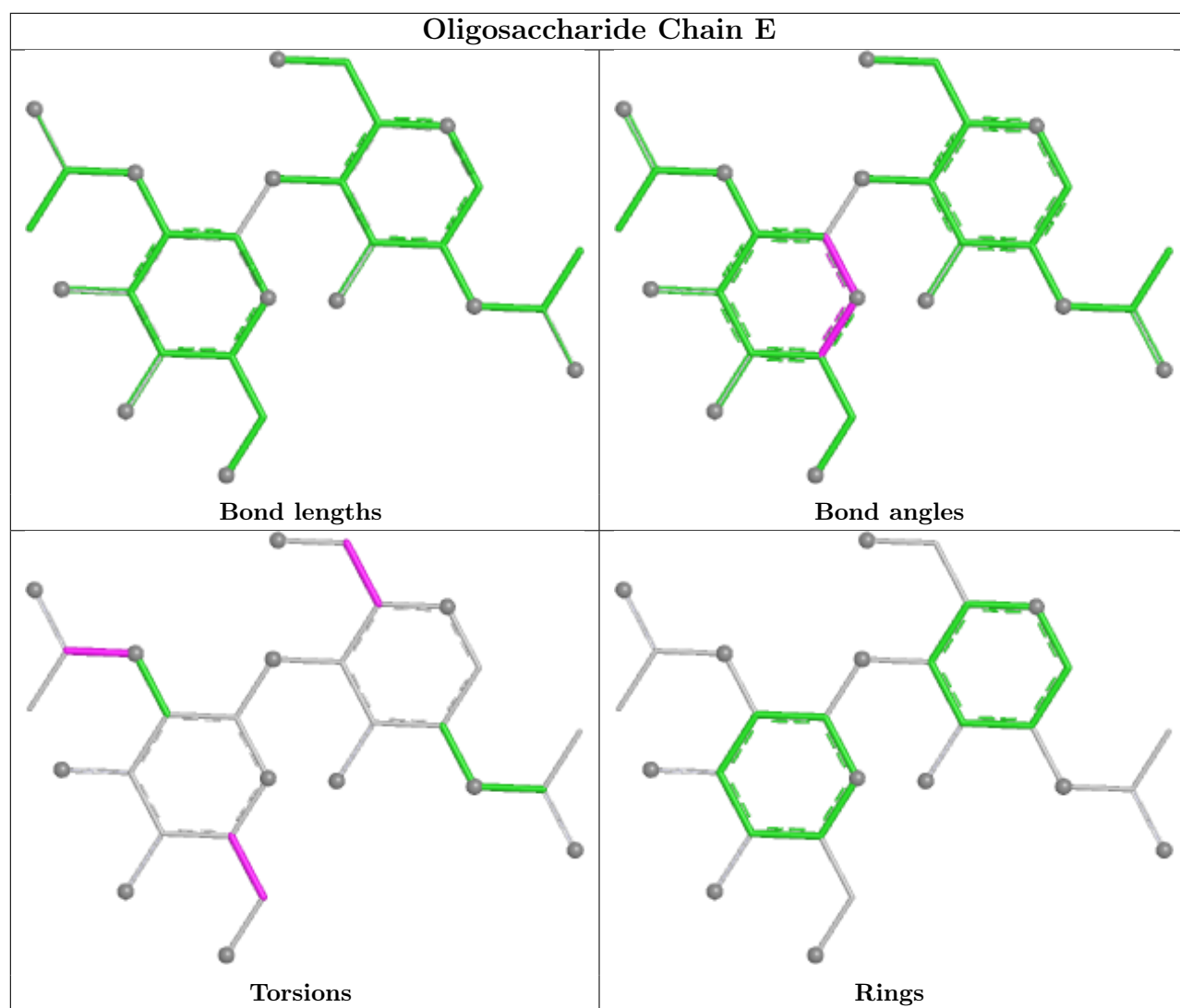
Mol	Chain	Res	Type	Atoms
4	G	3	MAN	C1-C2-C3-C4-C5-O5

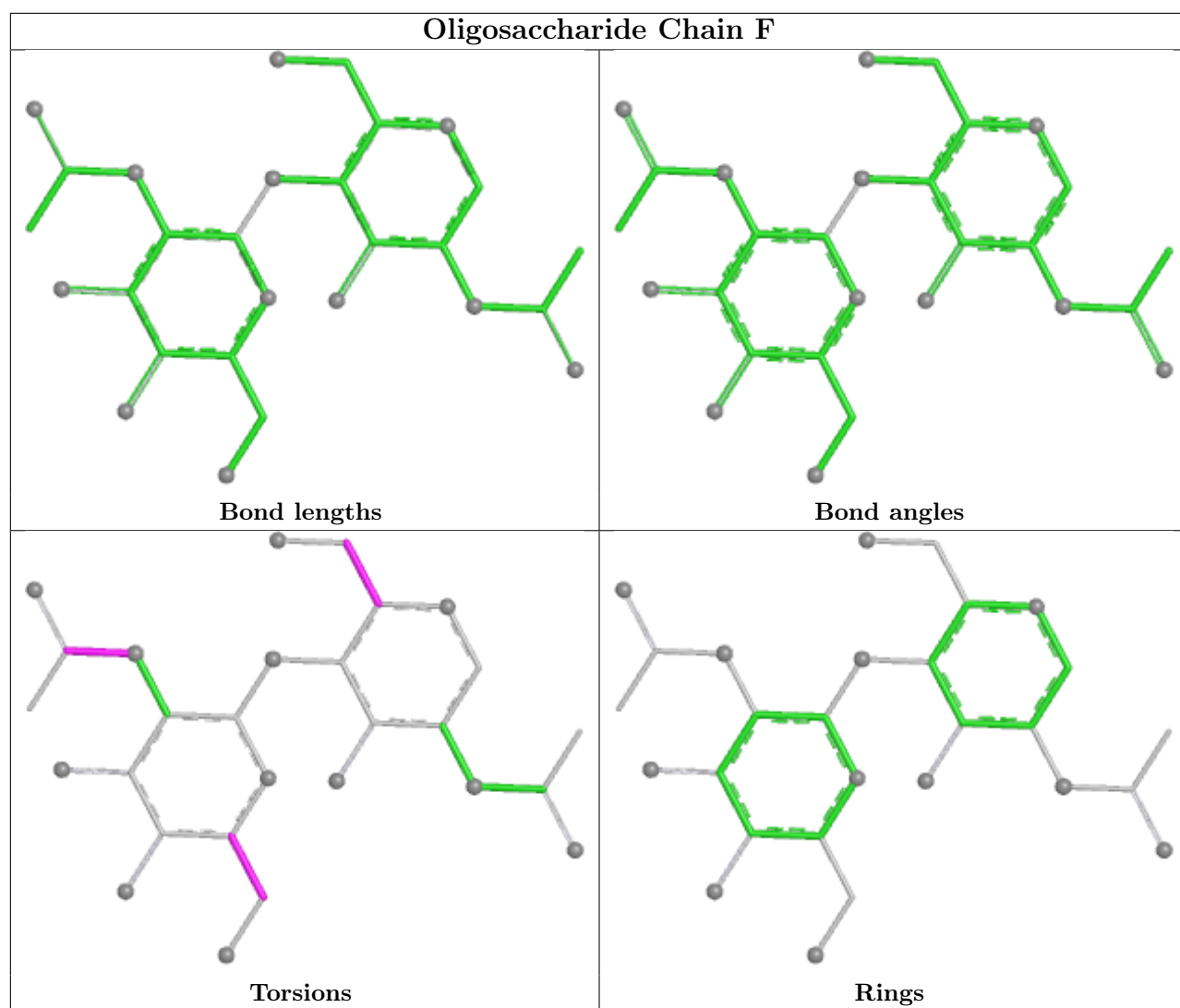
3 monomers are involved in 3 short contacts:

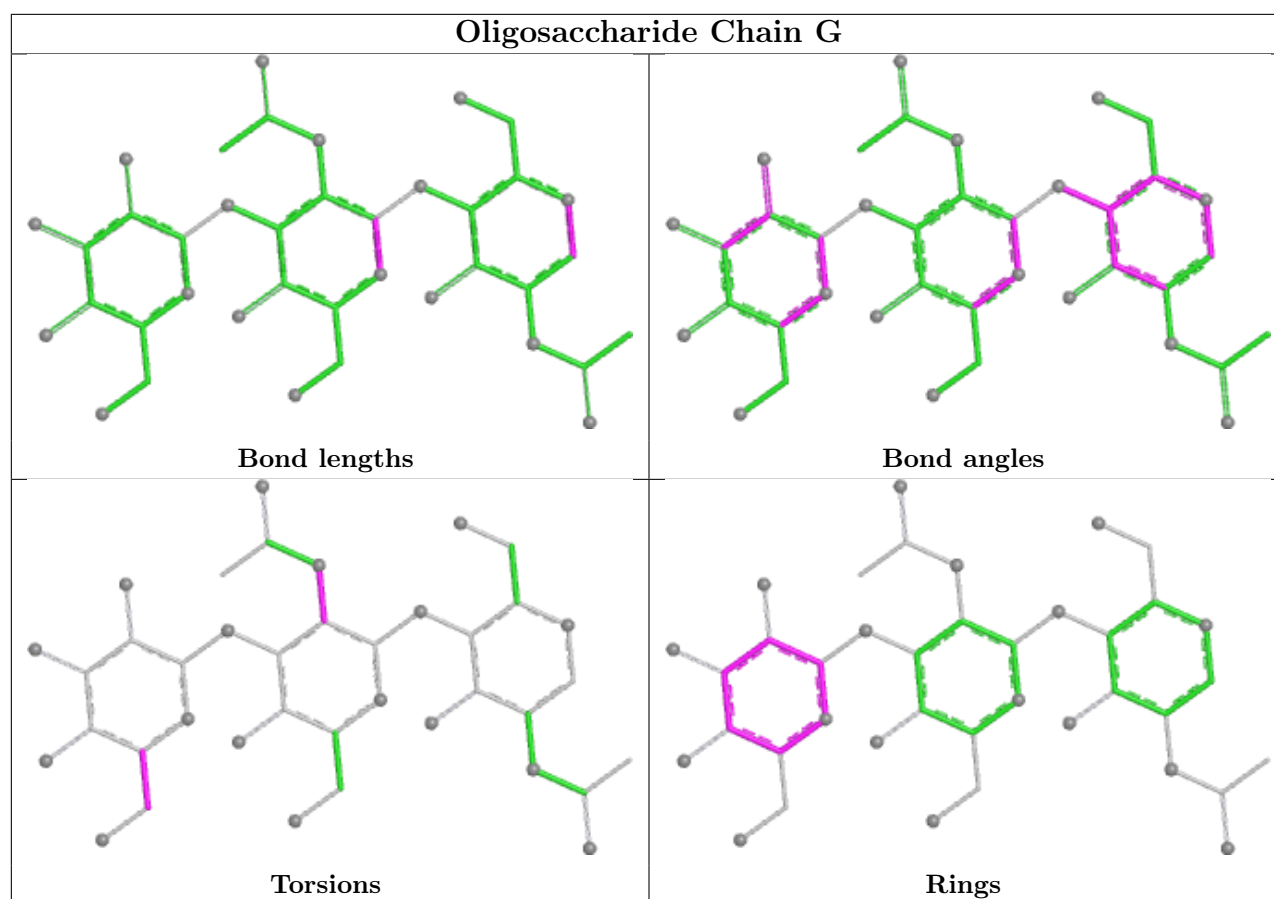
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	1	0
4	G	2	NAG	1	0
3	E	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
6	NAG	B	1102	1	14,14,15	0.42	0	17,19,21	0.81	1 (5%)

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
6	NAG	B	1102	1	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1102	NAG	C2-N2-C7	2.41	126.12	122.90

There are no chirality outliers.

All (5) torsion outliers are listed below:

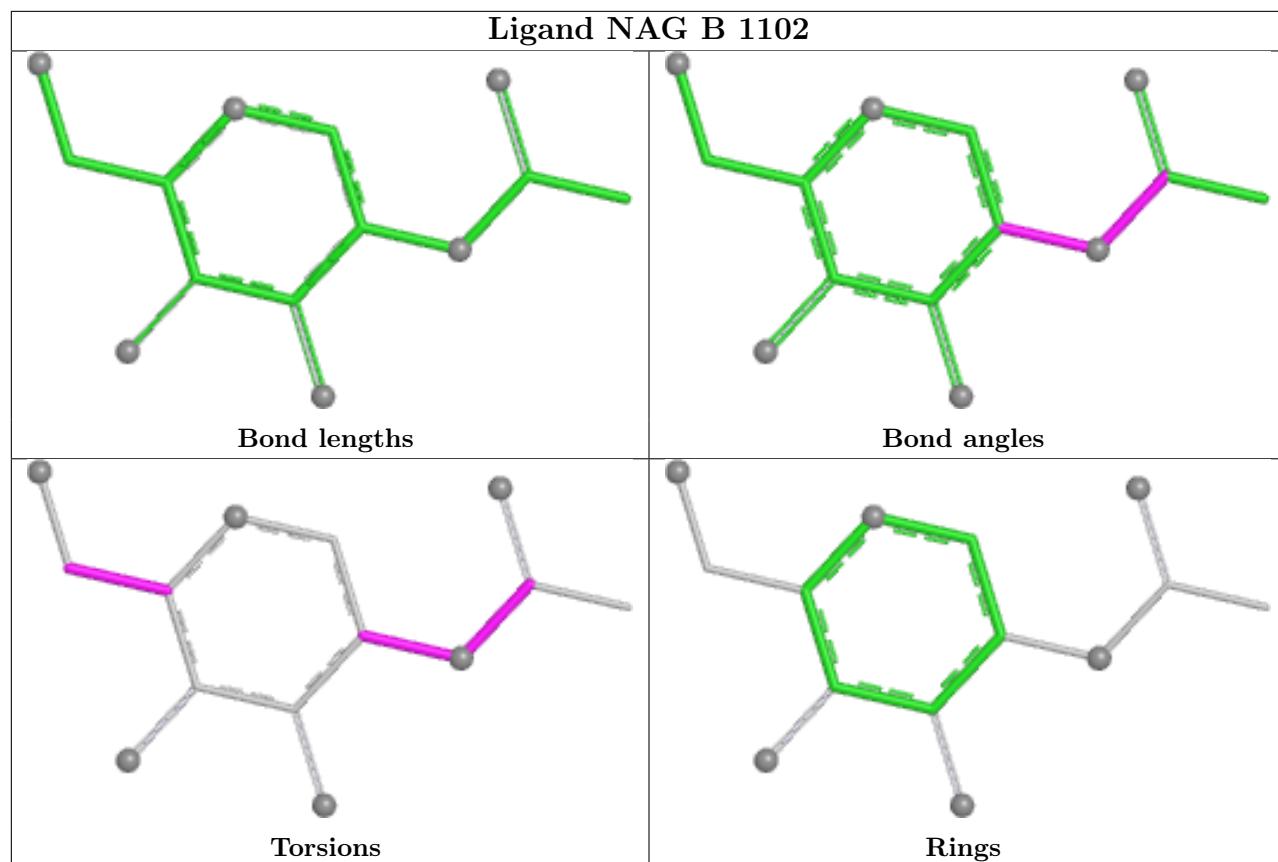
Mol	Chain	Res	Type	Atoms
6	B	1102	NAG	C8-C7-N2-C2
6	B	1102	NAG	O7-C7-N2-C2
6	B	1102	NAG	O5-C5-C6-O6
6	B	1102	NAG	C3-C2-N2-C7
6	B	1102	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1102	NAG	2	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.

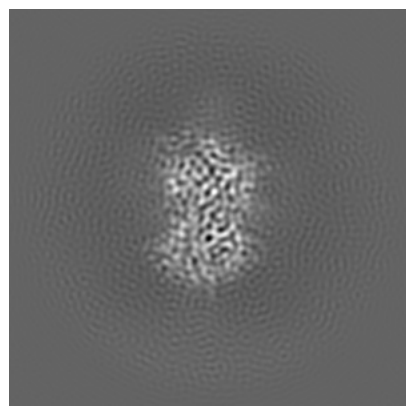
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44434. These allow visual inspection of the internal detail of the map and identification of artifacts.

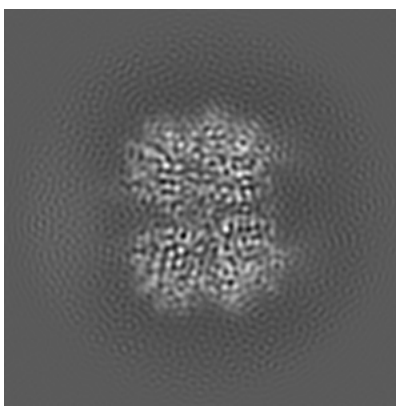
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

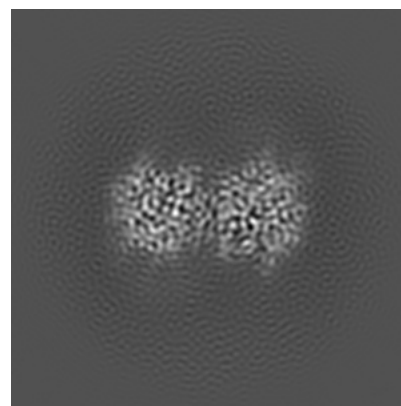
6.1.1 Primary map



X

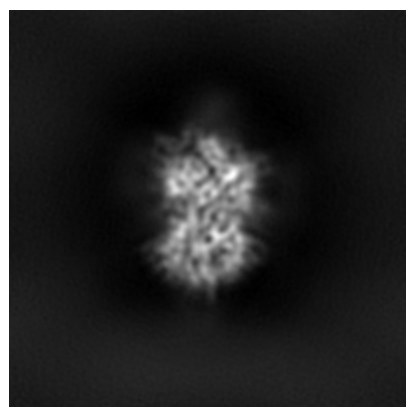


Y

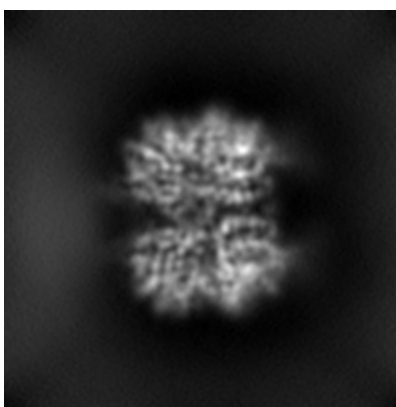


Z

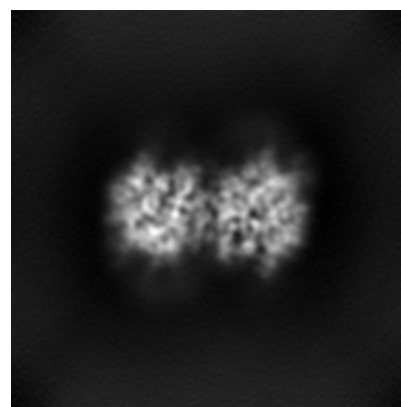
6.1.2 Raw map



X



Y

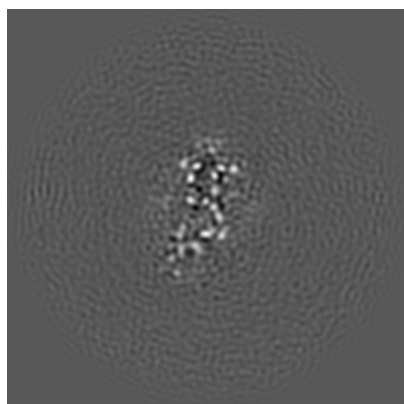


Z

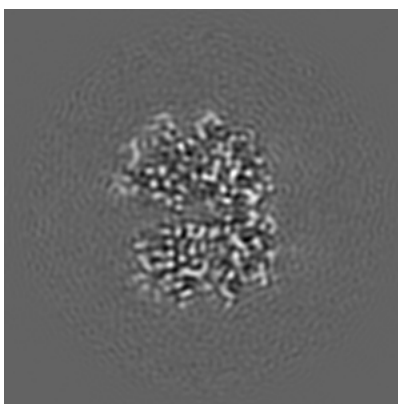
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

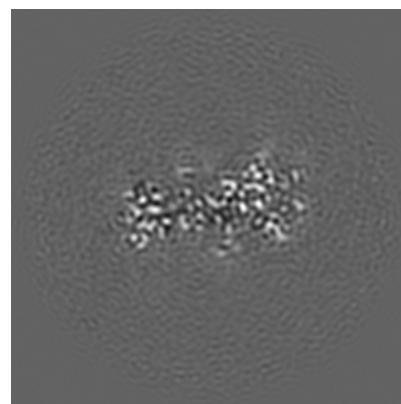
6.2.1 Primary map



X Index: 80

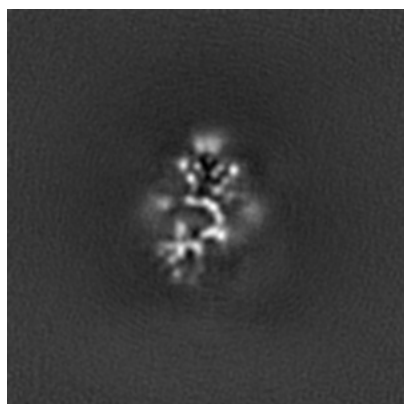


Y Index: 80

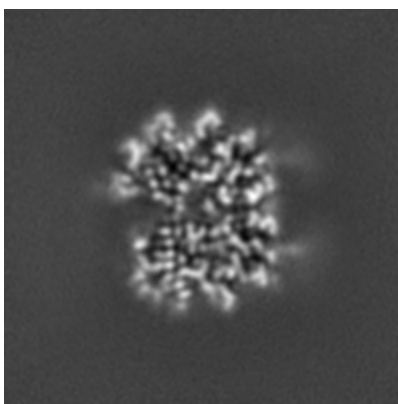


Z Index: 80

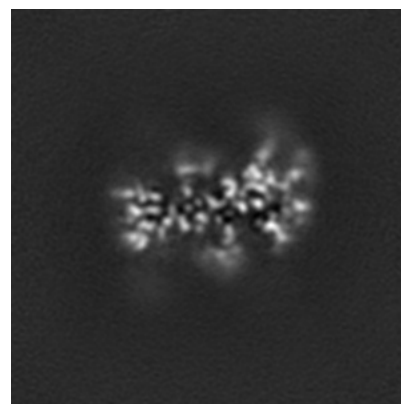
6.2.2 Raw map



X Index: 80



Y Index: 80

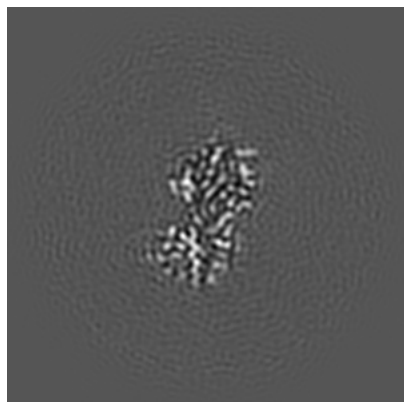


Z Index: 80

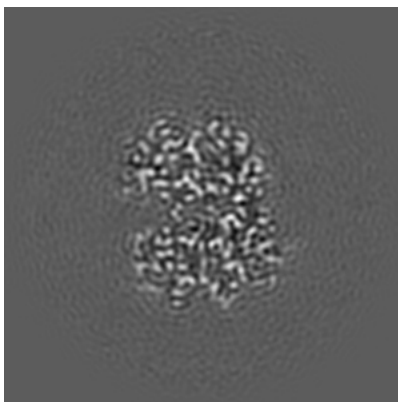
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

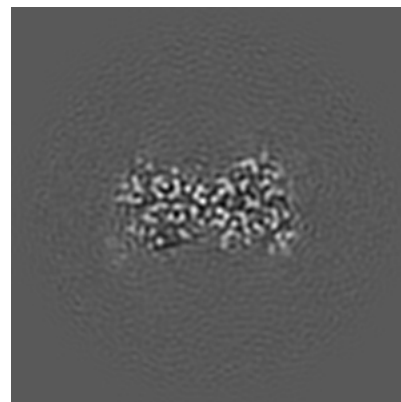
6.3.1 Primary map



X Index: 97

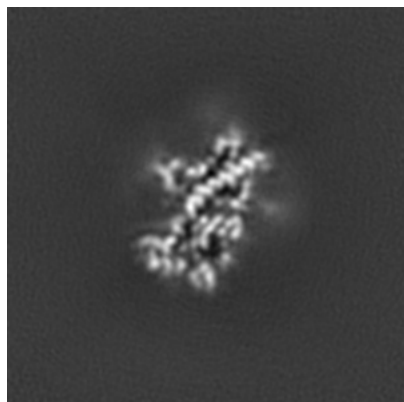


Y Index: 78

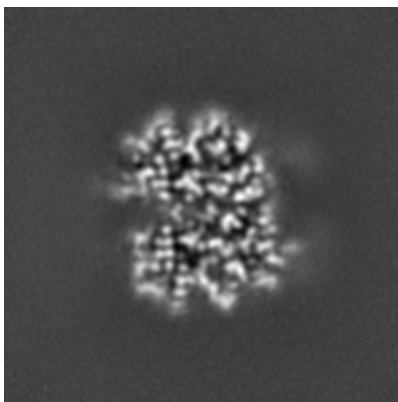


Z Index: 93

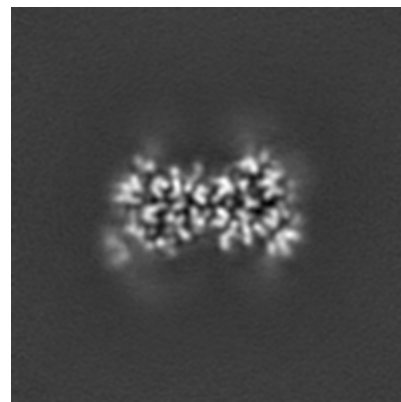
6.3.2 Raw map



X Index: 104



Y Index: 78

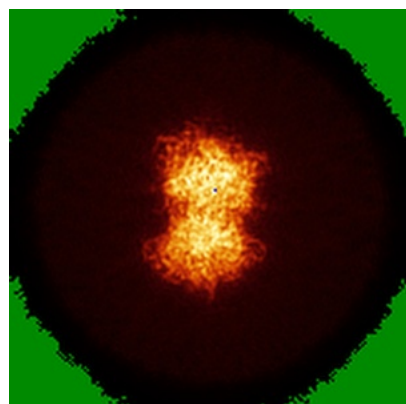


Z Index: 93

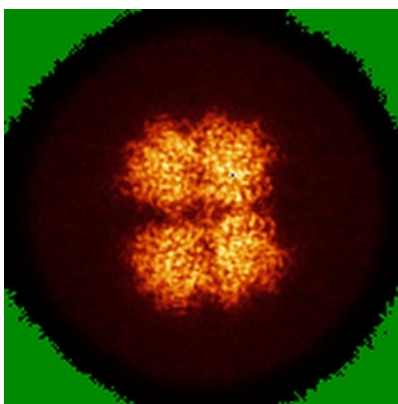
The images above show the largest variance slices of the map in three orthogonal directions.

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

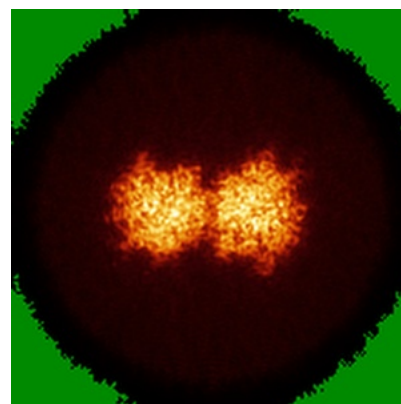
6.4.1 Primary map



X

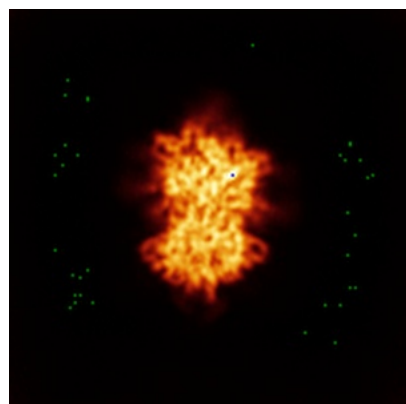


Y

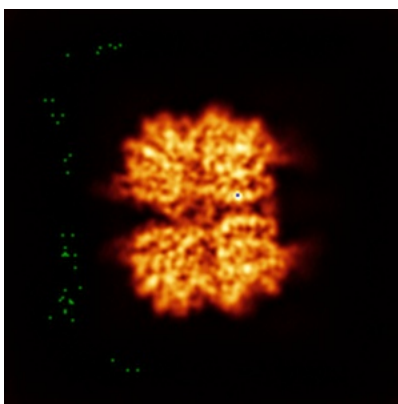


Z

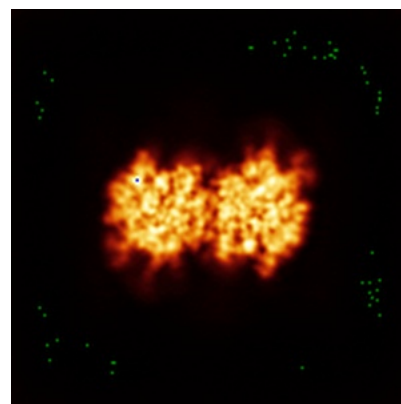
6.4.2 Raw map



X



Y

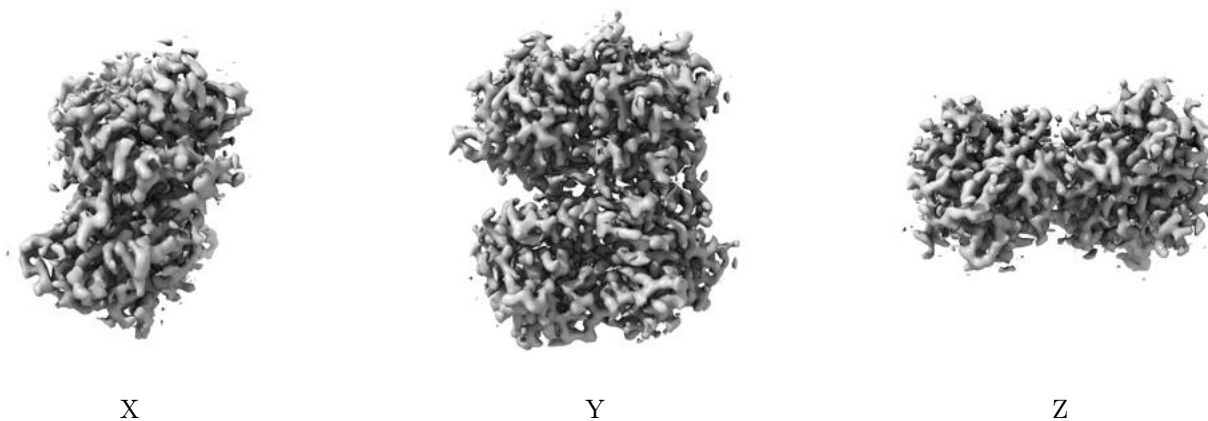


Z

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.

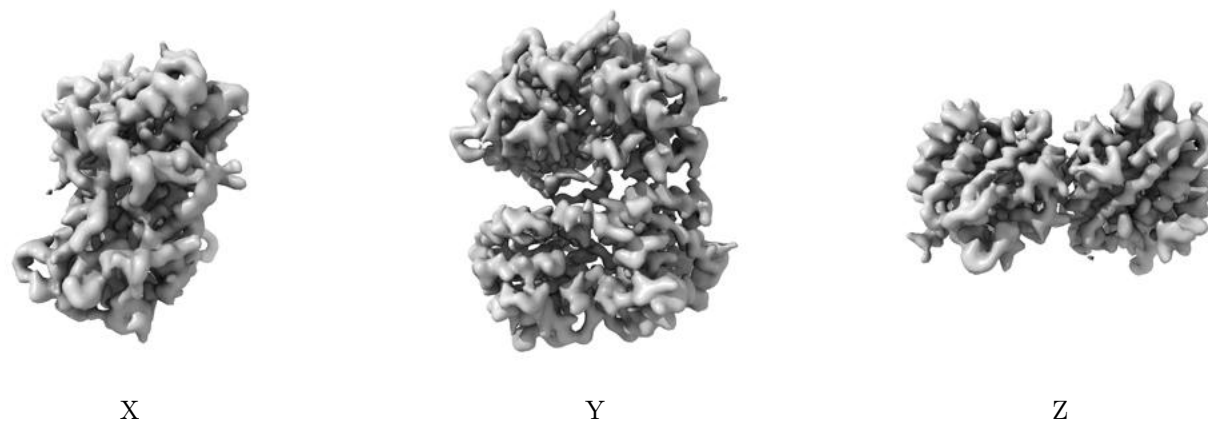
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.8. 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.

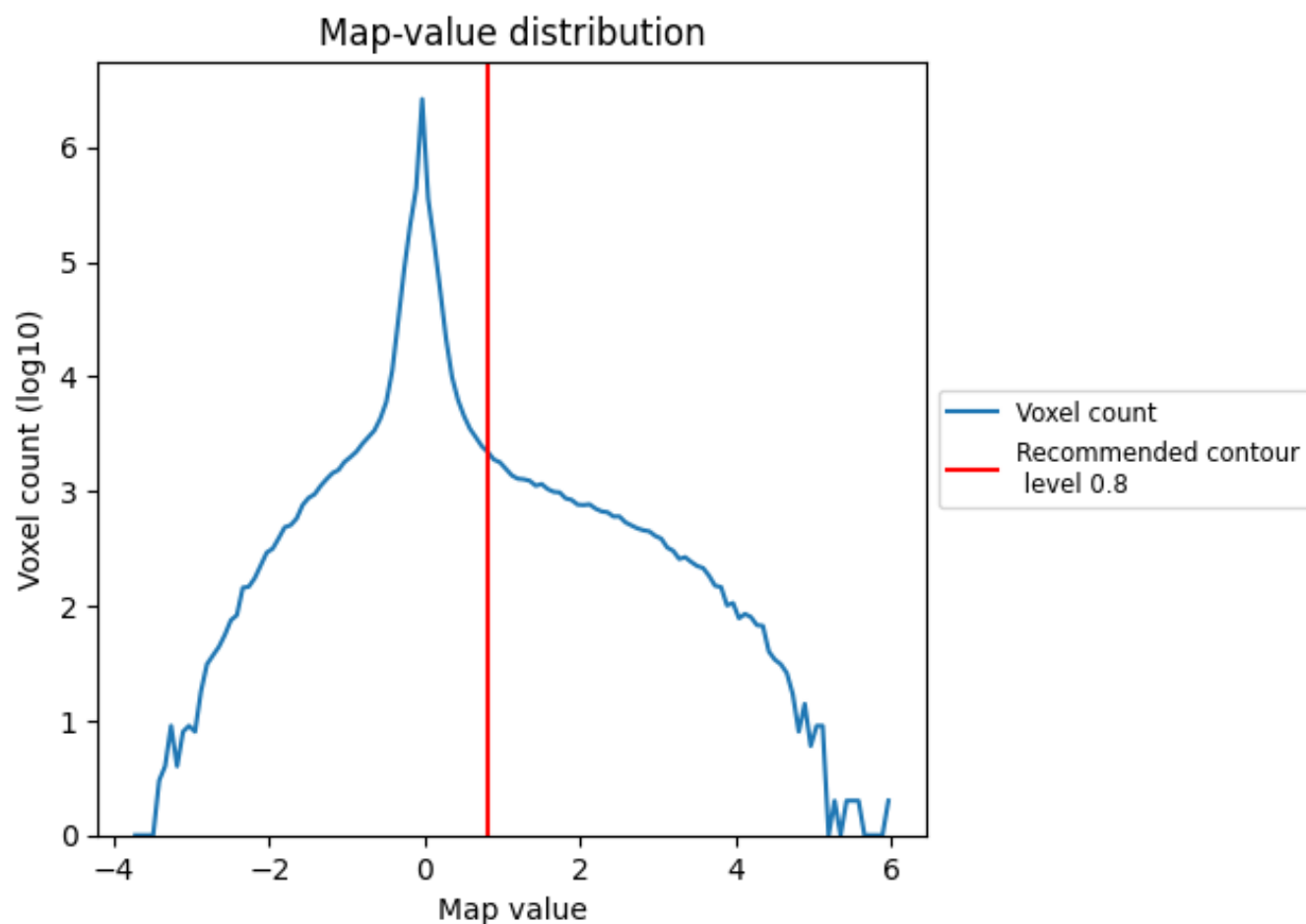
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

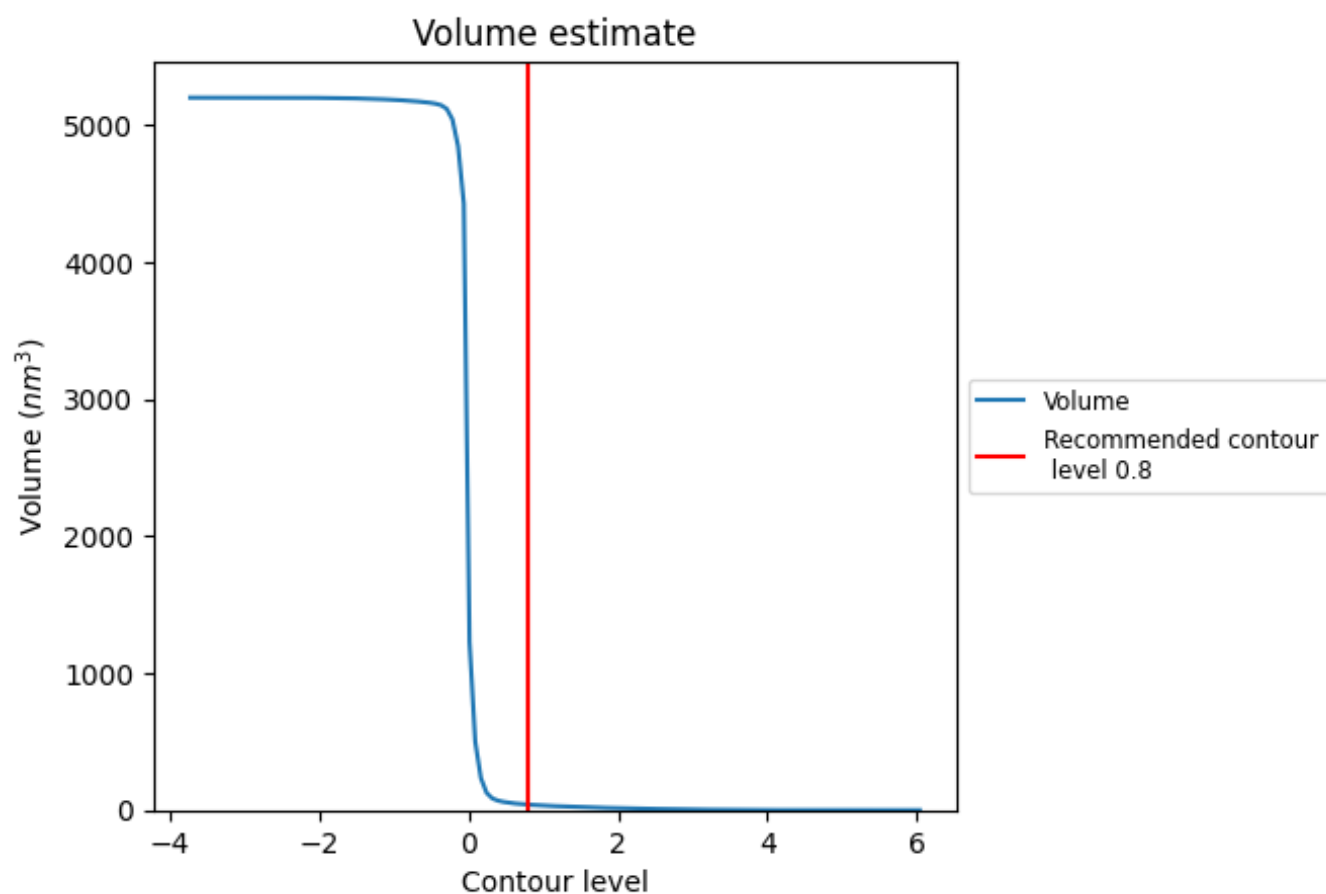
This section contains the results of statistical analysis of the map.

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.

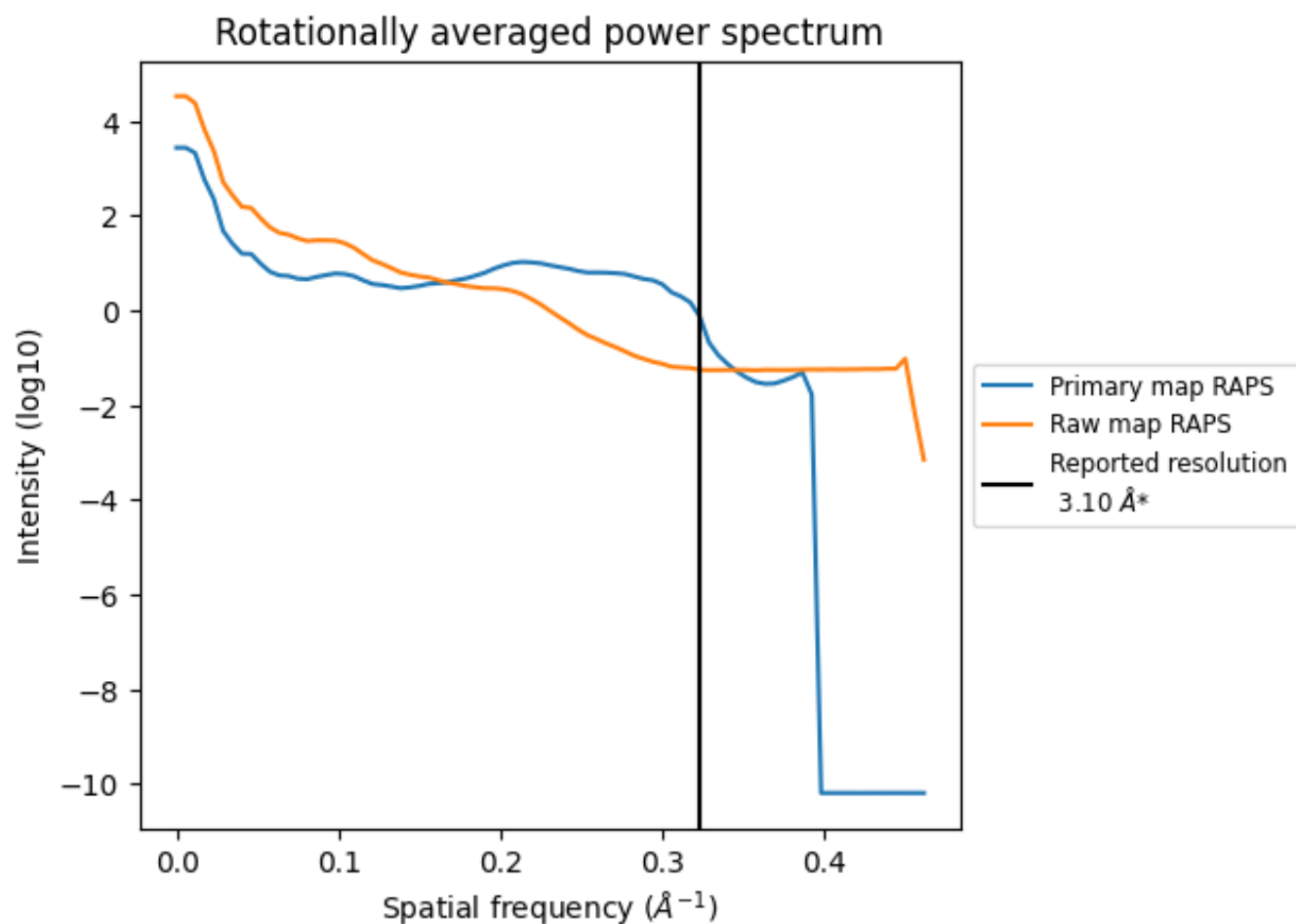
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 40 nm³; this corresponds to an approximate mass of 36 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 ⓘ

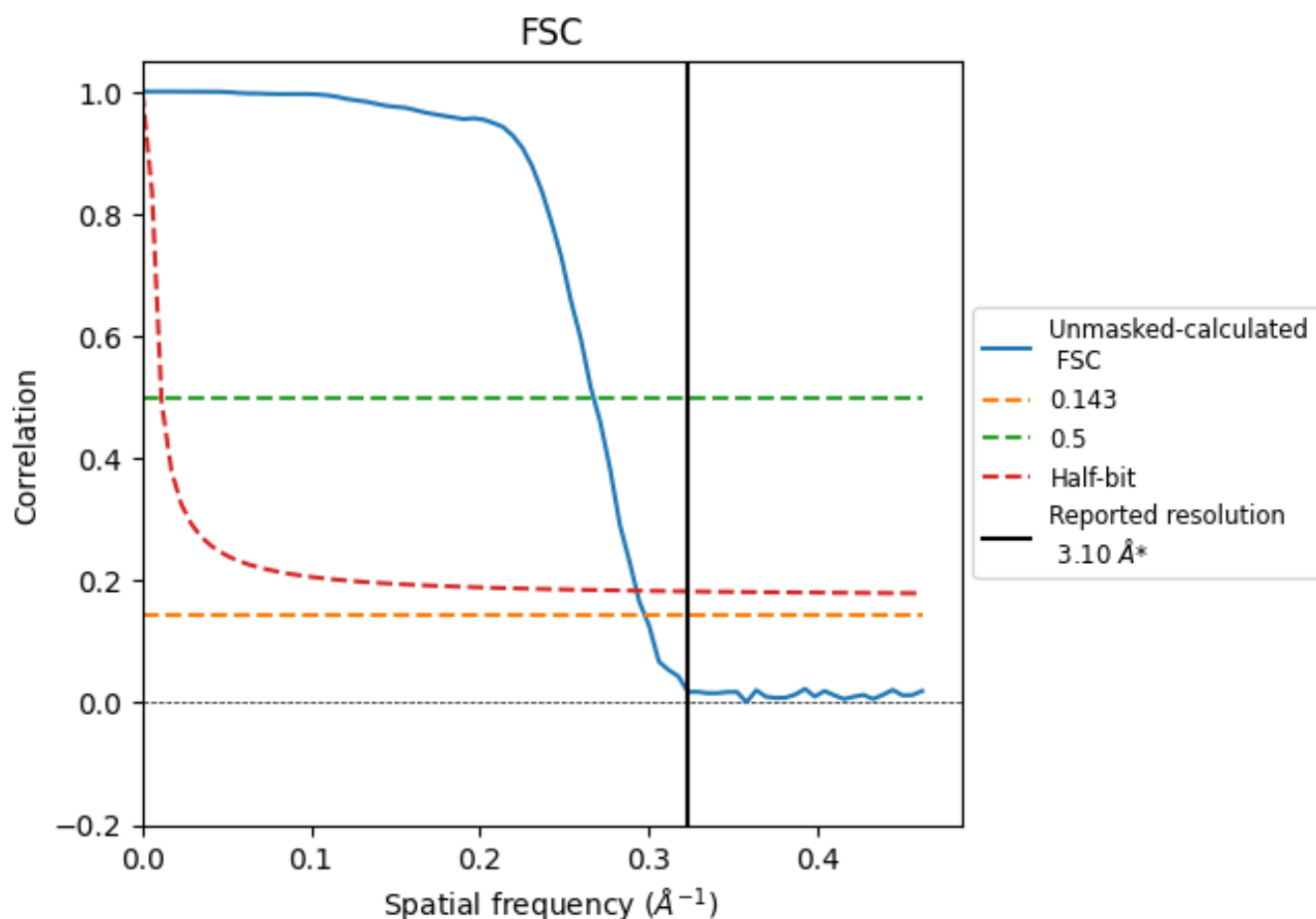


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 $0.323 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

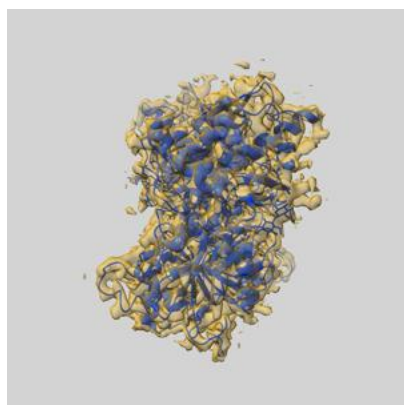
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.36	3.74	3.42

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

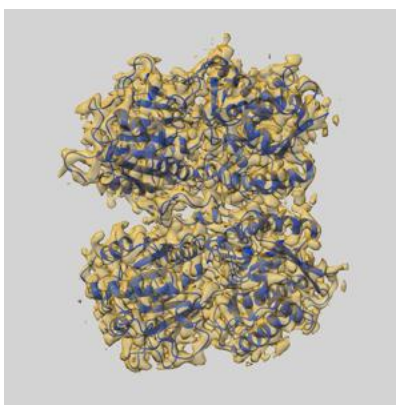
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44434 and PDB model 9BCQ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

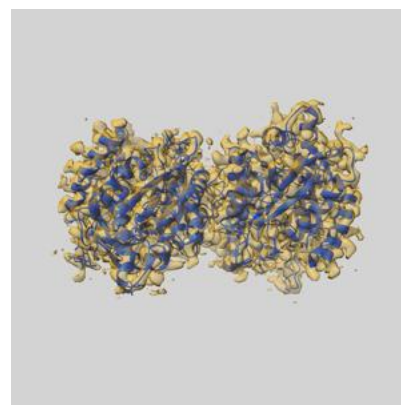
9.1 Map-model overlay [i](#)



X



Y



Z

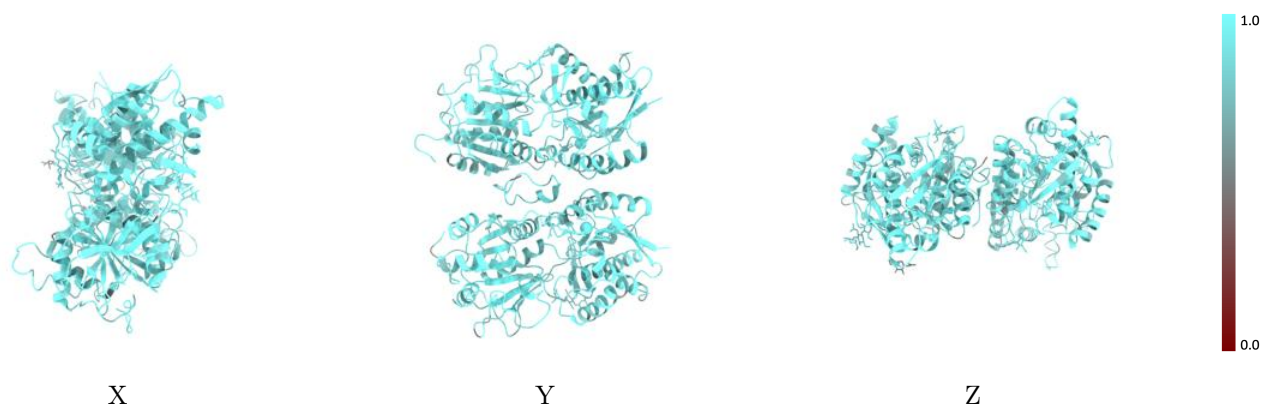
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



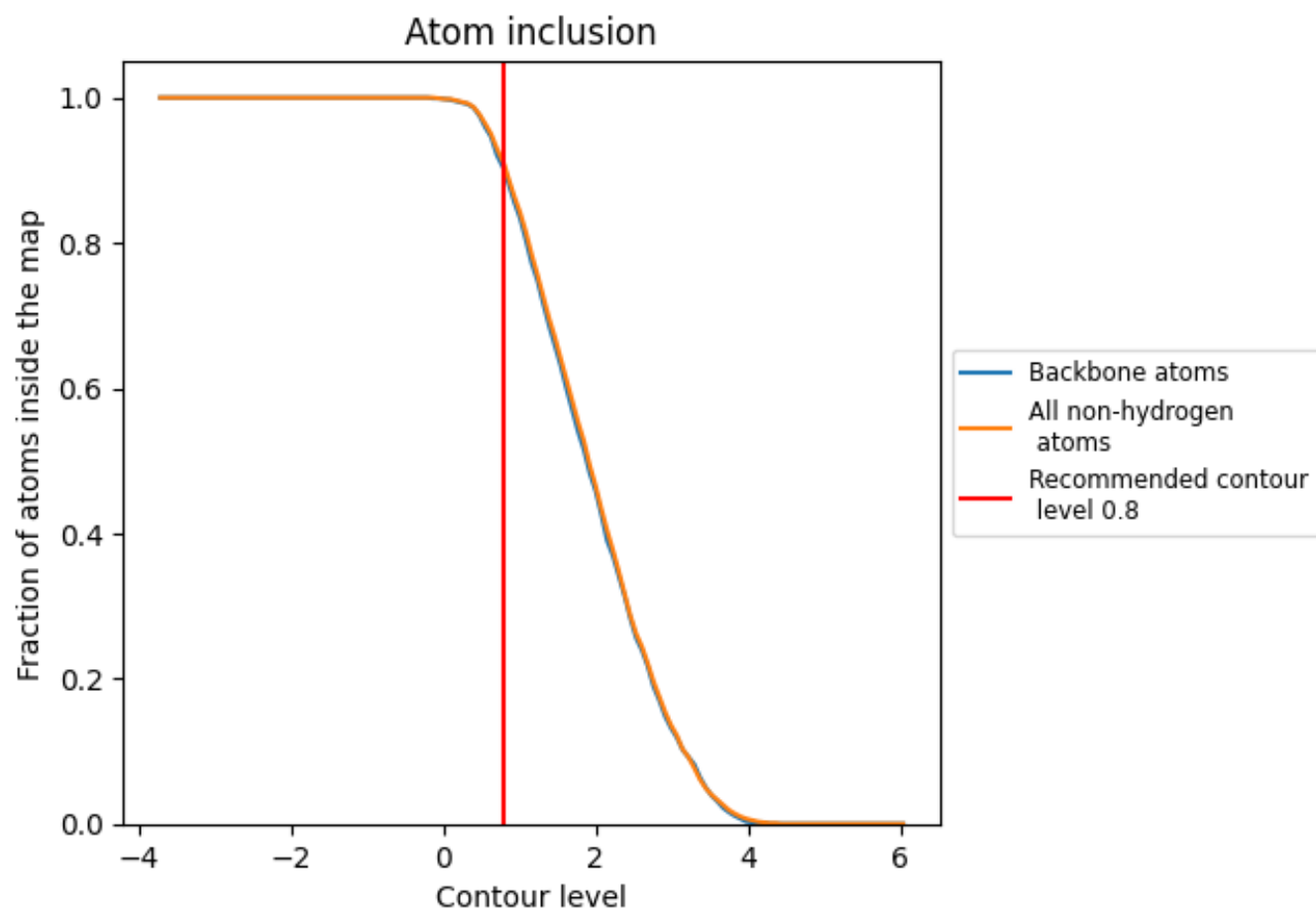
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 91% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9070	0.5990
A	0.9130	0.6000
B	0.9060	0.5980
C	0.9210	0.6000
D	0.8210	0.5760
E	0.8930	0.5900
F	0.8570	0.5970
G	0.8210	0.5690

1.0

0.0

<0.0