



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 10:13 am BST

PDB ID : 9T3Y / pdb_00009t3y
EMDB ID : EMD-55521
Title : Cryo-EM structure of alphaM/beta2:C3d-anti-CR3-Nb headpiece complex
(HPO2 3D class reconstruction)
Authors : Andersen, G.R.; Fruergaard, M.U.
Deposited on : 2025-10-30
Resolution : 3.44 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:

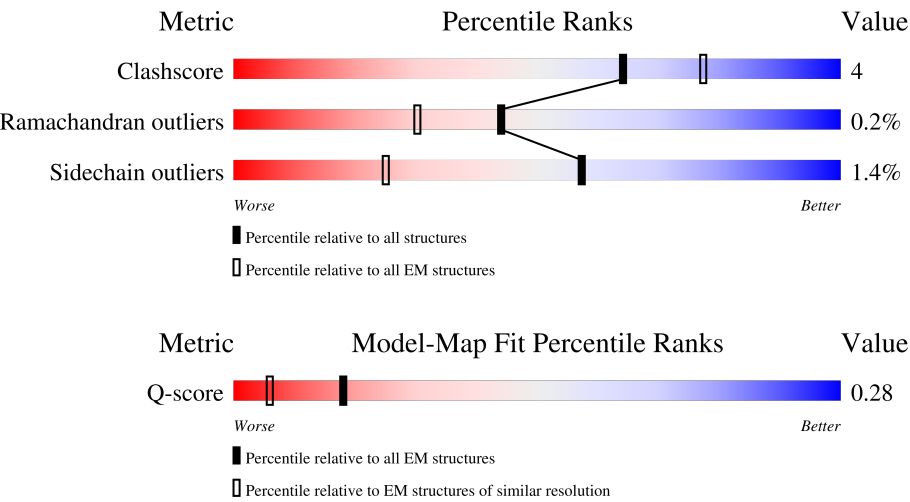
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.44 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	13877 (2.94 - 3.94)

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	763	<div><div></div><div>87%10%..</div></div>
2	B	469	<div><div></div><div>85%13%. .</div></div>
3	C	448	<div><div>67%</div><div>85%9% . 6%</div></div>
4	D	3	<div><div></div><div>100%</div></div>

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Mol	Chain	Length	Quality of chain
5	E	5	<div><div></div>100%</div>
5	F	5	<div><div></div>80%<div></div>20%</div>
6	G	2	<div><div></div>50%<div></div>50%</div>
6	H	2	<div><div></div>100%</div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12937 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 Isoform 2 of Integrin alpha-M.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	751	5803	3636	1036	1106	25	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	755	THR	-	expression tag	UNP P11215
A	756	GLY	-	expression tag	UNP P11215
A	757	GLY	-	expression tag	UNP P11215
A	758	GLU	-	expression tag	UNP P11215
A	759	ASN	-	expression tag	UNP P11215
A	760	LEU	-	expression tag	UNP P11215
A	761	TYR	-	expression tag	UNP P11215
A	762	PHE	-	expression tag	UNP P11215
A	763	GLN	-	expression tag	UNP P11215

- Molecule 2 is a protein called Integrin beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	459	3573	2225	634	685	29	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	461	PRO	-	expression tag	UNP P05107
B	462	ALA	-	expression tag	UNP P05107
B	463	ALA	-	expression tag	UNP P05107
B	464	GLU	-	expression tag	UNP P05107
B	465	ASN	-	expression tag	UNP P05107
B	466	LEU	-	expression tag	UNP P05107
B	467	TYR	-	expression tag	UNP P05107
B	468	PHE	-	expression tag	UNP P05107

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Chain	Residue	Modelled	Actual	Comment	Reference
B	469	GLN	-	expression tag	UNP P05107

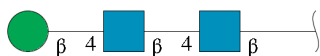
- Molecule 3 is a protein called Nanobody, Complement C3dg fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	422	Total	C	N	O	S	0	0
			3286	2090	554	627	15		

There is a discrepancy between the modelled and reference sequences:

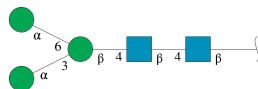
Chain	Residue	Modelled	Actual	Comment	Reference
C	93	SER	CYS	conflict	UNP P01024

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



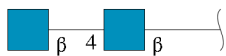
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	5	Total	C	N	O	0	0
			61	34	2	25		
5	F	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 6 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
6	G	2	Total	C	N	O	0	0
			28	16	2	10		
6	H	2	Total	C	N	O	0	0
			28	16	2	10		

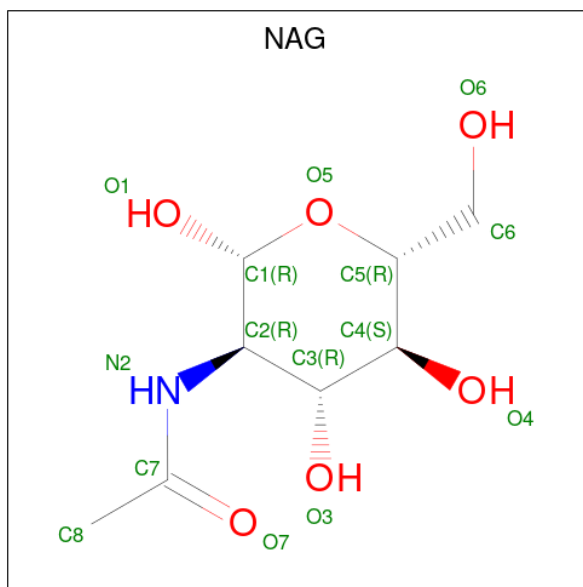
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	A	3	Total	Ca	0
			3	3	
7	B	2	Total	Ca	0
			2	2	

- Molecule 8 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	Mn	0
			1	1	
8	B	1	Total	Mn	0
			1	1	

- Molecule 9 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
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	B	1	Total	C	N	O	0
			14	8	1	5	

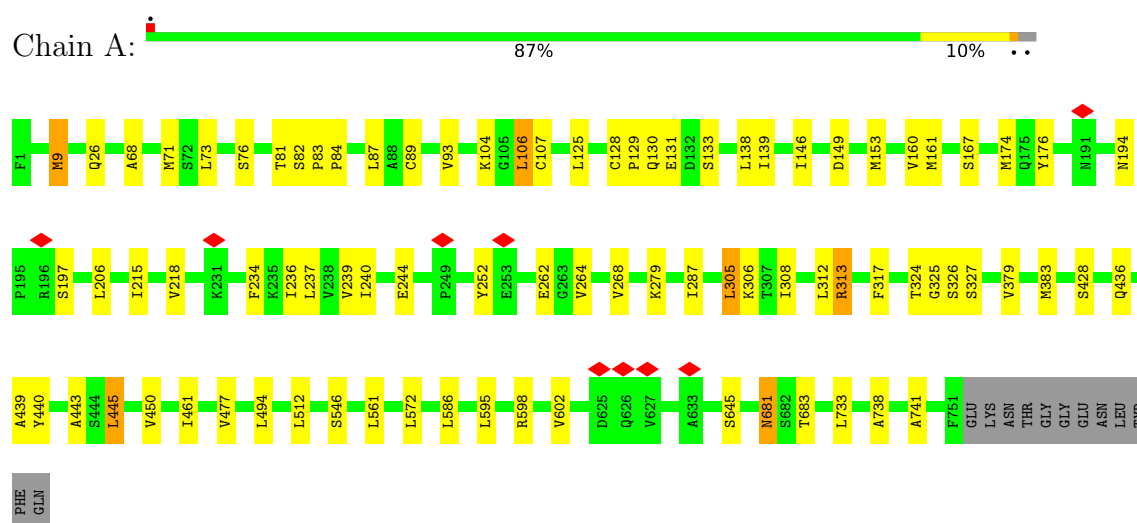
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		AltConf
10	A	4	Total	O	0
			4	4	
10	B	4	Total	O	0
			4	4	
10	C	1	Total	O	0
			1	1	

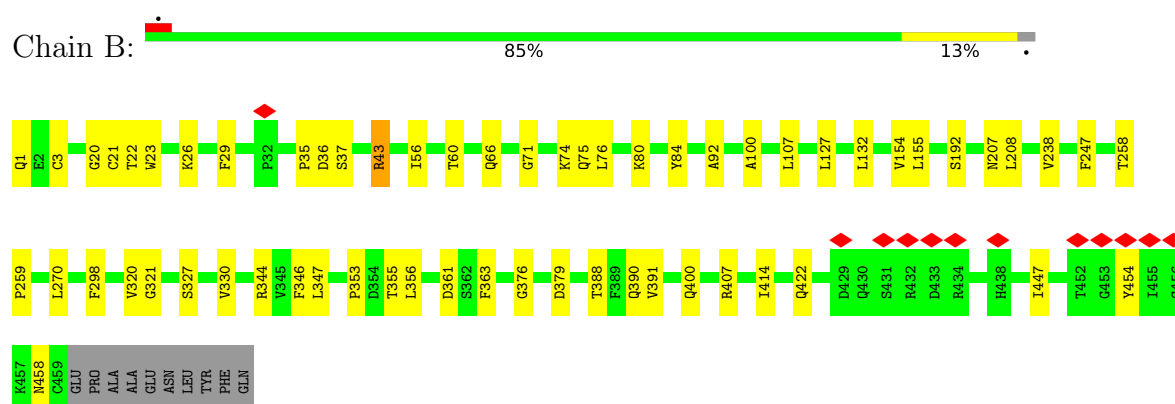
3 Residue-property plots

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.

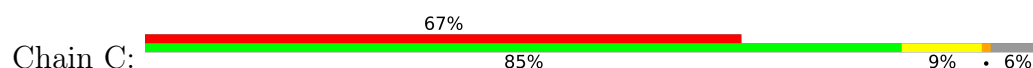
• Molecule 1: Isoform 2 of Integrin alpha-M



• Molecule 2: Integrin beta-2



• Molecule 3: Nanobody, Complement C3dg fragment

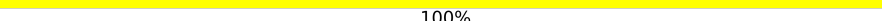


- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  50% 50%

MAG1
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	43930	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 ($e^-/\text{\AA}^2$)	60.1	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.186	Depositor
Minimum map value	-0.496	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.13	Depositor
Map size (\AA)	331.264, 331.264, 331.264	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.294, 1.294, 1.294	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MN, BMA, 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	0.42	0/5914	0.69	7/8007 (0.1%)
2	B	0.39	0/3642	0.70	2/4927 (0.0%)
3	C	0.34	1/3357 (0.0%)	0.71	3/4545 (0.1%)
All	All	0.39	1/12913 (0.0%)	0.70	12/17479 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	412	GLU	C-O	5.46	1.30	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	MET	CA-CB-CG	7.17	128.43	114.10
3	C	33	TYR	N-CA-C	7.04	120.87	109.40
1	A	174	MET	CB-CG-SD	6.34	131.73	112.70
1	A	153	MET	N-CA-CB	6.15	120.42	110.40
2	B	43	ARG	CA-CB-CG	6.12	126.35	114.10
1	A	153	MET	CB-CG-SD	6.02	130.75	112.70
1	A	161	MET	CA-CB-CG	5.46	125.01	114.10
1	A	379	VAL	CA-C-N	5.29	131.65	121.54
1	A	379	VAL	C-N-CA	5.29	131.65	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	224	MET	CB-CG-SD	5.16	128.17	112.70
2	B	155	LEU	CB-CG-CD2	5.12	126.04	110.70
3	C	101	MET	N-CA-CB	5.00	118.31	110.46

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	176	TYR	Peptide
1	A	313	ARG	Sidechain
1	A	82	SER	Peptide

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	5803	0	5725	47	0
2	B	3573	0	3487	31	0
3	C	3286	0	3214	30	0
4	D	39	0	34	0	0
5	E	61	0	52	0	0
5	F	61	0	52	1	0
6	G	28	0	25	0	0
6	H	28	0	25	0	0
7	A	3	0	0	0	0
7	B	2	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	28	0	26	0	0
9	B	14	0	13	0	0
10	A	4	0	0	1	0
10	B	4	0	0	0	0
10	C	1	0	0	0	0
All	All	12937	0	12653	104	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 (104) 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)
3:C:300:LYS:HG3	3:C:331:PHE:CE2	1.70	1.25
3:C:300:LYS:CG	3:C:331:PHE:CE2	2.55	0.89
1:A:206:LEU:HB2	3:C:300:LYS:HD3	1.59	0.84
3:C:300:LYS:HG3	3:C:331:PHE:CD2	2.18	0.77
2:B:71:GLY:HA3	2:B:74:LYS:HD3	1.65	0.77
2:B:75:GLN:HE22	2:B:100:ALA:H	1.41	0.69
2:B:35:PRO:HB2	2:B:447:ILE:HG23	1.81	0.63
1:A:206:LEU:CB	3:C:300:LYS:HD3	2.29	0.61
2:B:407:ARG:HG2	2:B:414:ILE:HG22	1.83	0.61
3:C:29:THR:HG22	3:C:32:ASP:H	1.65	0.61
3:C:300:LYS:HE2	3:C:331:PHE:CD2	2.38	0.59
1:A:324:THR:HA	5:F:5:MAN:H62	1.84	0.58
2:B:346:PHE:HA	2:B:376:GLY:O	2.04	0.58
1:A:572:LEU:HD22	1:A:586:LEU:HD11	1.87	0.57
2:B:35:PRO:HB2	2:B:447:ILE:HA	1.87	0.57
3:C:300:LYS:HG3	3:C:331:PHE:HE2	1.57	0.56
3:C:300:LYS:HE2	3:C:331:PHE:CG	2.39	0.56
1:A:206:LEU:HB3	3:C:300:LYS:NZ	2.20	0.56
1:A:129:PRO:HG2	1:A:317:PHE:HZ	1.71	0.56
3:C:320:LEU:HD11	3:C:336:VAL:HG12	1.89	0.55
2:B:355:THR:HG23	2:B:356:LEU:HD22	1.89	0.55
3:C:35:ILE:HA	3:C:410:ALA:O	2.08	0.53
2:B:35:PRO:HD3	2:B:458:ASN:ND2	2.24	0.53
1:A:436:GLN:HB3	1:A:439:ALA:HB2	1.91	0.53
2:B:298:PHE:HB2	2:B:320:VAL:HG22	1.91	0.53
2:B:344:ARG:HD2	2:B:379:ASP:HB2	1.91	0.52
2:B:66:GLN:NE2	2:B:80:LYS:NZ	2.58	0.52
2:B:353:PRO:HG2	2:B:356:LEU:HD23	1.90	0.52
3:C:320:LEU:HD22	3:C:361:ALA:HB1	1.91	0.51
3:C:404:THR:HG23	3:C:433:THR:HA	1.91	0.51
1:A:106:LEU:HG	1:A:125:LEU:HD21	1.92	0.51
3:C:166:VAL:HG23	3:C:183:LEU:HG	1.93	0.51
1:A:139:ILE:HG22	1:A:240:ILE:HG13	1.91	0.51
3:C:320:LEU:HD12	3:C:335:VAL:HG12	1.92	0.51
1:A:87:LEU:HD11	1:A:107:CYS:HB3	1.93	0.51
2:B:66:GLN:NE2	2:B:80:LYS:HZ3	2.10	0.50
1:A:244:GLU:HA	1:A:279:LYS:HZ1	1.77	0.50
1:A:236:ILE:HD11	1:A:308:ILE:HD11	1.95	0.49
2:B:84:TYR:HB3	2:B:422:GLN:HB2	1.93	0.49
1:A:68:ALA:HA	1:A:93:VAL:HG13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ILE:O	1:A:149:ASP:N	2.44	0.49
1:A:681:ASN:HB3	1:A:683:THR:H	1.80	0.47
3:C:412:GLU:HG3	3:C:423:PRO:HA	1.96	0.47
1:A:598:ARG:HG3	10:A:1302:HOH:O	2.14	0.47
1:A:128:CYS:HB2	1:A:130:GLN:HG3	1.96	0.47
1:A:325:GLY:O	1:A:327:SER:N	2.47	0.46
1:A:146:ILE:HD12	1:A:146:ILE:H	1.81	0.46
1:A:239:VAL:HG13	1:A:268:VAL:HG23	1.98	0.46
1:A:313:ARG:HD3	1:A:313:ARG:HA	1.74	0.46
1:A:598:ARG:HE	1:A:733:LEU:HD13	1.81	0.46
1:A:133:SER:HA	1:A:234:PHE:H	1.81	0.46
2:B:363:PHE:HD2	2:B:388:THR:HG23	1.80	0.46
1:A:383:MET:HB3	1:A:383:MET:HE3	1.80	0.46
1:A:93:VAL:HB	1:A:104:LYS:O	2.16	0.45
3:C:321:LEU:HD23	3:C:357:MET:HE1	1.97	0.45
2:B:321:GLY:HA3	2:B:330:VAL:HG12	1.97	0.45
1:A:738:ALA:HB3	1:A:741:ALA:HB2	1.98	0.45
2:B:23:TRP:HH2	2:B:36:ASP:HB2	1.81	0.45
1:A:561:LEU:HD23	1:A:595:LEU:HD22	1.99	0.45
3:C:103:PRO:HA	3:C:106:ILE:HG22	1.99	0.45
1:A:26:GLN:HB3	1:A:81:THR:HG22	1.99	0.45
1:A:194:ASN:HD21	1:A:197:SER:HB2	1.82	0.44
3:C:87:ILE:HA	3:C:104:THR:HG22	1.99	0.44
1:A:215:ILE:HA	1:A:218:VAL:HG12	2.00	0.44
2:B:22:THR:HG22	2:B:43:ARG:HH21	1.82	0.44
3:C:407:TYR:O	3:C:429:GLY:CA	2.66	0.44
1:A:262:GLU:HB2	1:A:264:VAL:HG23	1.99	0.44
2:B:26:LYS:HB3	2:B:29:PHE:HB2	2.00	0.44
3:C:216:LEU:HD22	3:C:226:LEU:HD23	2.00	0.44
2:B:107:LEU:HD11	2:B:238:VAL:HG23	2.00	0.43
1:A:76:SER:HB2	1:A:89:CYS:HB2	1.99	0.43
3:C:101:MET:HE1	3:C:139:GLN:HG3	2.00	0.43
1:A:450:VAL:HG21	1:A:546:SER:HA	1.99	0.43
1:A:440:TYR:HD2	1:A:443:ALA:HB2	1.84	0.42
3:C:300:LYS:CD	3:C:331:PHE:CZ	3.02	0.42
1:A:252:TYR:HE2	1:A:287:ILE:HB	1.85	0.42
3:C:285:LEU:HD12	3:C:326:LEU:HD11	2.01	0.42
1:A:83:PRO:HA	1:A:84:PRO:HD3	1.82	0.42
2:B:127:LEU:HD13	2:B:327:SER:HB2	2.02	0.42
2:B:3:CYS:HB2	2:B:21:CYS:HB2	1.86	0.42
1:A:71:MET:HE3	1:A:73:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:GLU:OE2	1:A:167:SER:OG	2.37	0.42
2:B:1:GLN:HB2	2:B:20:GLY:HA3	2.01	0.42
2:B:74:LYS:O	2:B:75:GLN:C	2.63	0.42
3:C:249:PRO:HA	3:C:252:ILE:HG12	2.02	0.42
3:C:272:VAL:HG11	3:C:296:THR:HG21	2.02	0.42
2:B:132:LEU:HD21	2:B:192:SER:HB2	2.02	0.42
3:C:139:GLN:HB3	3:C:149:PHE:HZ	1.84	0.41
1:A:445:LEU:HD12	1:A:461:ILE:HG12	2.01	0.41
1:A:306:LYS:HE2	1:A:306:LYS:HB3	1.83	0.41
1:A:512:LEU:HD21	1:A:586:LEU:HD13	2.02	0.41
2:B:74:LYS:C	2:B:76:LEU:N	2.78	0.41
1:A:160:VAL:HG22	1:A:305:LEU:HB3	2.01	0.41
1:A:206:LEU:HB3	3:C:300:LYS:HZ2	1.84	0.41
2:B:23:TRP:CZ2	2:B:36:ASP:HA	2.56	0.41
2:B:92:ALA:HA	2:B:391:VAL:O	2.21	0.41
2:B:361:ASP:HB2	2:B:390:GLN:HB3	2.03	0.41
2:B:258:THR:HA	2:B:259:PRO:HD3	1.95	0.41
3:C:184:CYS:HA	3:C:187:VAL:HG12	2.02	0.41
1:A:9:MET:HE3	1:A:9:MET:HB2	1.97	0.41
1:A:71:MET:HG3	1:A:93:VAL:HG22	2.03	0.40
1:A:602:VAL:HG23	1:A:645:SER:HB2	2.03	0.40
2:B:22:THR:HG21	2:B:56:ILE:HG23	2.02	0.40
1:A:138:LEU:HD23	1:A:237:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	749/763 (98%)	704 (94%)	44 (6%)	1 (0%)	48 78
2	B	457/469 (97%)	429 (94%)	25 (6%)	3 (1%)	18 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	418/448 (93%)	397 (95%)	21 (5%)	0	100	100
All	All	1624/1680 (97%)	1530 (94%)	90 (6%)	4 (0%)	44	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	326	SER
2	B	454	TYR
2	B	37	SER
2	B	60	THR

5.3.2 Protein sidechains ⓘ

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	634/644 (98%)	625 (99%)	9 (1%)	59	71
2	B	400/408 (98%)	393 (98%)	7 (2%)	51	68
3	C	346/360 (96%)	342 (99%)	4 (1%)	63	73
All	All	1380/1412 (98%)	1360 (99%)	20 (1%)	57	71

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	MET
1	A	106	LEU
1	A	305	LEU
1	A	312	LEU
1	A	428	SER
1	A	445	LEU
1	A	477	VAL
1	A	494	LEU
1	A	681	ASN
2	B	154	VAL
2	B	207	ASN

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Mol	Chain	Res	Type
2	B	208	LEU
2	B	247	PHE
2	B	270	LEU
2	B	347	LEU
2	B	400	GLN
3	C	33	TYR
3	C	242	GLU
3	C	259	LEU
3	C	362	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	175	GLN
1	A	298	GLN
1	A	401	GLN
1	A	624	ASN
1	A	656	GLN
2	B	66	GLN
2	B	75	GLN
2	B	167	ASN
2	B	191	ASN
2	B	390	GLN
2	B	400	GLN
3	C	195	GLN
3	C	262	ASN
3	C	281	GLN
3	C	390	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

17 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
4	NAG	D	1	1,4	14,14,15	0.78	1 (7%)	17,19,21	1.31	1 (5%)
4	NAG	D	2	4	14,14,15	0.74	0	17,19,21	1.24	1 (5%)
4	BMA	D	3	4	11,11,12	0.97	1 (9%)	15,15,17	2.63	5 (33%)
5	NAG	E	1	1,5	14,14,15	0.86	0	17,19,21	1.26	1 (5%)
5	NAG	E	2	5	14,14,15	0.76	0	17,19,21	1.22	1 (5%)
5	BMA	E	3	5	11,11,12	0.89	1 (9%)	15,15,17	2.97	5 (33%)
5	MAN	E	4	5	11,11,12	0.62	0	15,15,17	2.00	1 (6%)
5	MAN	E	5	5	11,11,12	0.77	0	15,15,17	1.28	1 (6%)
5	NAG	F	1	1,5	14,14,15	0.88	1 (7%)	17,19,21	1.61	3 (17%)
5	NAG	F	2	5	14,14,15	0.80	0	17,19,21	2.17	4 (23%)
5	BMA	F	3	5	11,11,12	0.93	1 (9%)	15,15,17	2.76	8 (53%)
5	MAN	F	4	5	11,11,12	0.79	0	15,15,17	1.57	2 (13%)
5	MAN	F	5	5	11,11,12	0.80	0	15,15,17	1.58	1 (6%)
6	NAG	G	1	2,6	14,14,15	0.73	0	17,19,21	0.99	0
6	NAG	G	2	6	14,14,15	0.80	0	17,19,21	1.00	1 (5%)
6	NAG	H	1	2,6	14,14,15	0.84	0	17,19,21	1.87	2 (11%)
6	NAG	H	2	6	14,14,15	0.79	0	17,19,21	1.35	3 (17%)

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
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	1/2/19/22	0/1/1/1
5	NAG	E	1	1,5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	BMA	E	3	5	-	1/2/19/22	0/1/1/1
5	MAN	E	4	5	-	2/2/19/22	0/1/1/1
5	MAN	E	5	5	-	0/2/19/22	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1
5	MAN	F	4	5	-	0/2/19/22	0/1/1/1
5	MAN	F	5	5	-	0/2/19/22	0/1/1/1
6	NAG	G	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	G	2	6	-	0/6/23/26	0/1/1/1
6	NAG	H	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	H	2	6	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3	BMA	C2-C3	2.29	1.55	1.52
5	F	3	BMA	C2-C3	2.10	1.55	1.52
5	F	1	NAG	C2-N2	-2.07	1.42	1.46
5	E	3	BMA	C2-C3	2.03	1.55	1.52
4	D	1	NAG	C2-N2	-2.03	1.42	1.46

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	3	BMA	C1-O5-C5	8.78	124.08	112.19
4	D	3	BMA	C1-O5-C5	8.09	123.16	112.19
5	F	3	BMA	C1-O5-C5	7.57	122.45	112.19
5	E	4	MAN	C1-O5-C5	6.99	121.66	112.19
6	H	1	NAG	C1-O5-C5	5.79	120.04	112.19
5	F	2	NAG	C1-O5-C5	5.73	119.96	112.19
5	F	5	MAN	C1-O5-C5	4.38	118.12	112.19
5	E	3	BMA	C2-C3-C4	4.18	118.14	110.89
5	F	2	NAG	O3-C3-C2	-4.06	101.06	109.47
5	F	4	MAN	C1-O5-C5	4.05	117.68	112.19
5	F	2	NAG	O4-C4-C3	3.99	119.58	110.35
6	H	1	NAG	O4-C4-C5	3.92	119.04	109.30
5	E	3	BMA	O3-C3-C2	-3.84	102.64	109.99
5	E	5	MAN	C1-O5-C5	3.81	117.35	112.19
5	F	1	NAG	C1-O5-C5	3.66	117.16	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3	BMA	C2-C3-C4	3.60	117.12	110.89
5	E	2	NAG	C1-O5-C5	3.44	116.85	112.19
4	D	1	NAG	C1-O5-C5	3.39	116.78	112.19
4	D	2	NAG	C1-O5-C5	3.32	116.70	112.19
5	F	3	BMA	C3-C4-C5	3.22	115.98	110.24
6	H	2	NAG	O5-C1-C2	-2.97	106.59	111.29
5	F	3	BMA	O2-C2-C3	2.86	115.87	110.14
5	F	1	NAG	O3-C3-C2	-2.77	103.73	109.47
5	F	3	BMA	C2-C3-C4	2.73	115.62	110.89
5	F	3	BMA	O4-C4-C3	-2.67	104.18	110.35
6	G	2	NAG	C1-O5-C5	2.59	115.70	112.19
5	F	3	BMA	C1-C2-C3	-2.55	106.53	109.67
5	F	4	MAN	O5-C1-C2	-2.37	107.12	110.77
5	F	2	NAG	C3-C4-C5	-2.34	106.06	110.24
5	F	3	BMA	O3-C3-C4	2.34	115.76	110.35
5	E	3	BMA	C1-C2-C3	2.32	112.52	109.67
5	F	1	NAG	O5-C1-C2	-2.28	107.69	111.29
5	E	1	NAG	C1-O5-C5	2.27	115.26	112.19
4	D	3	BMA	O3-C3-C2	-2.25	105.68	109.99
6	H	2	NAG	C1-O5-C5	2.25	115.24	112.19
4	D	3	BMA	C3-C4-C5	2.19	114.15	110.24
5	F	3	BMA	O5-C5-C4	2.19	116.15	110.83
4	D	3	BMA	O4-C4-C3	-2.17	105.32	110.35
6	H	2	NAG	C4-C3-C2	2.16	114.18	111.02
5	E	3	BMA	O4-C4-C3	-2.01	105.70	110.35

There are no chirality outliers.

All (10) torsion outliers are listed below:

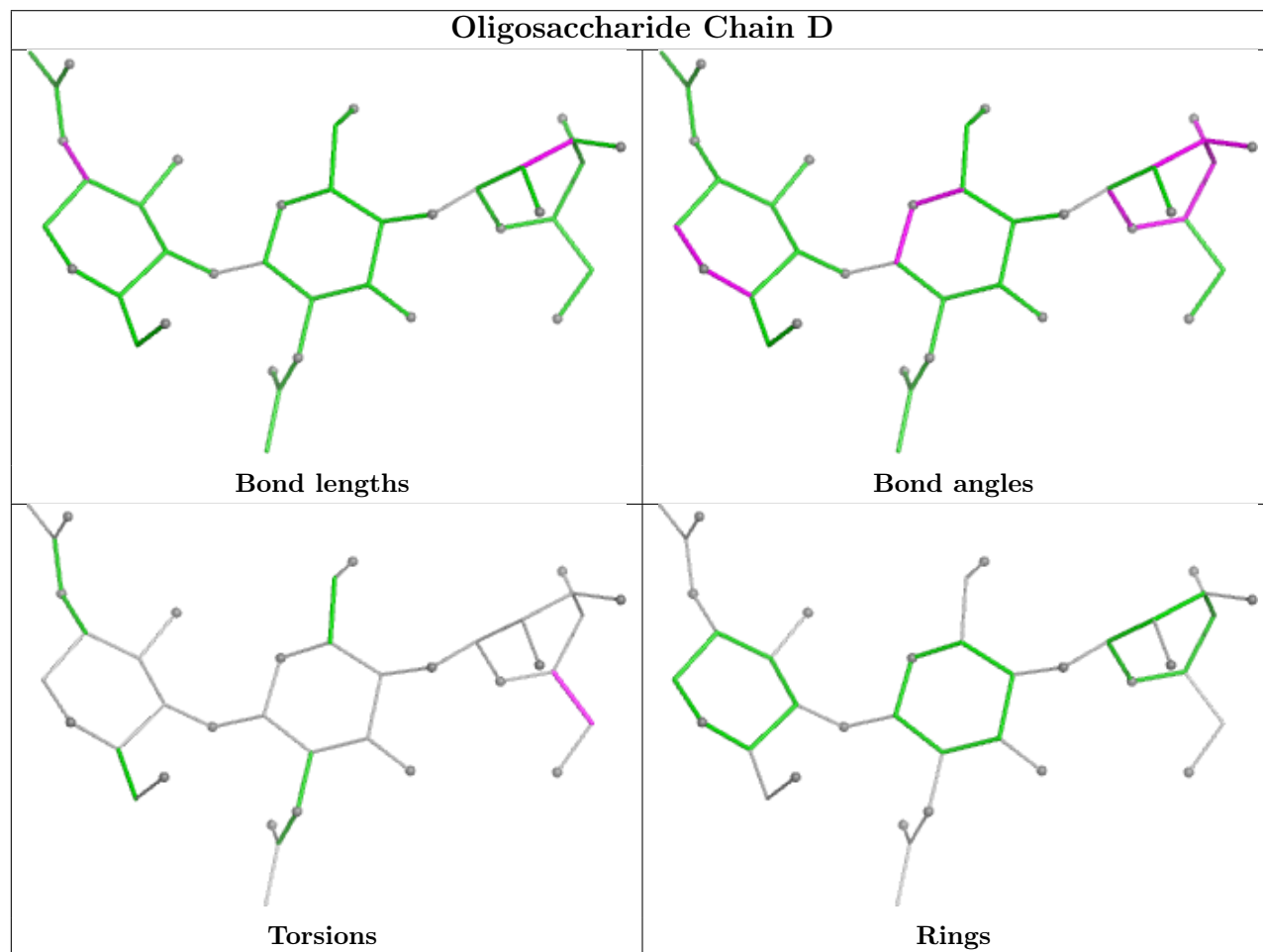
Mol	Chain	Res	Type	Atoms
5	F	2	NAG	O5-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
6	H	1	NAG	C4-C5-C6-O6
5	E	3	BMA	O5-C5-C6-O6
5	E	4	MAN	O5-C5-C6-O6
6	H	1	NAG	O5-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
6	H	2	NAG	O5-C5-C6-O6
6	H	2	NAG	C4-C5-C6-O6
5	E	4	MAN	C4-C5-C6-O6

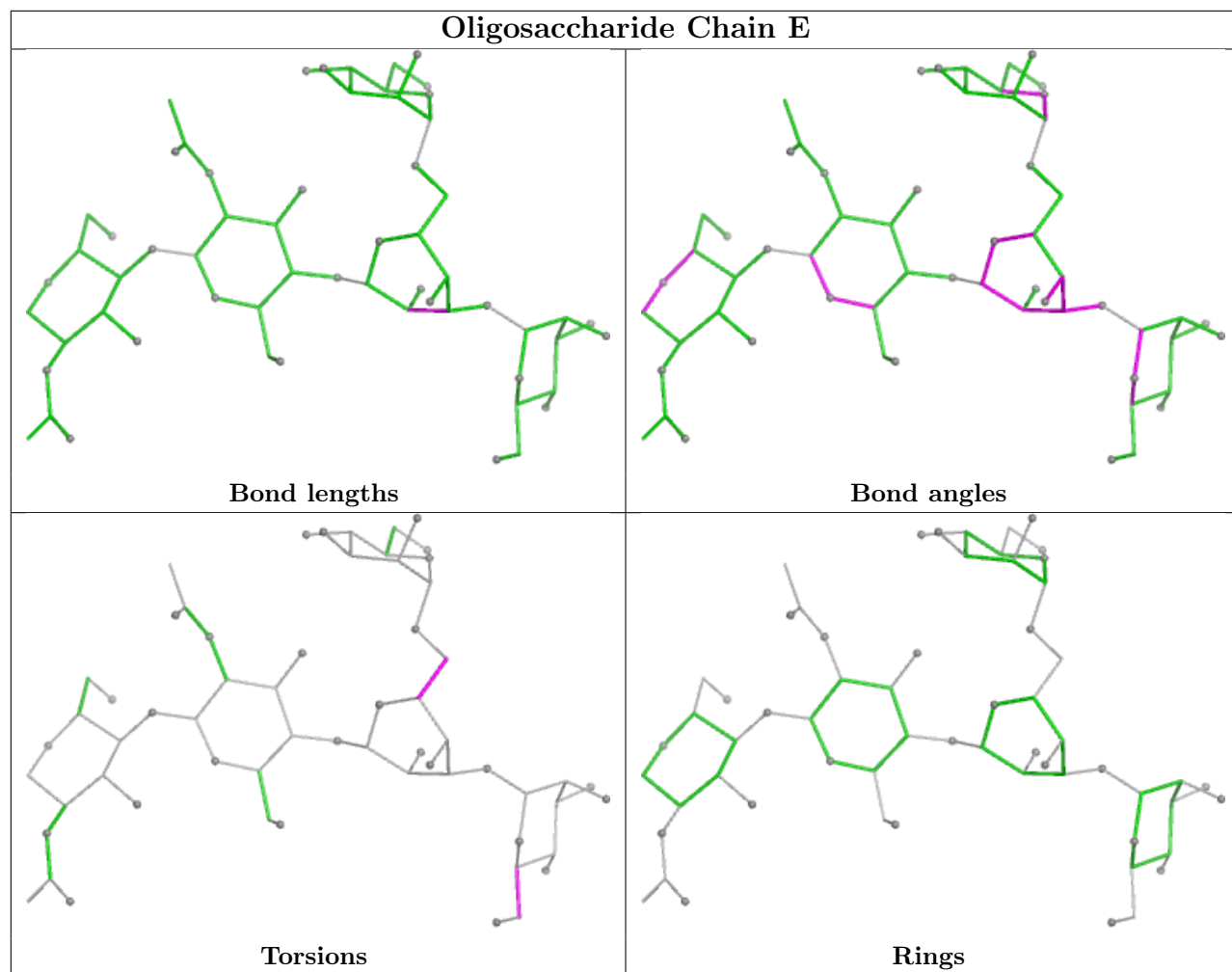
There are no ring outliers.

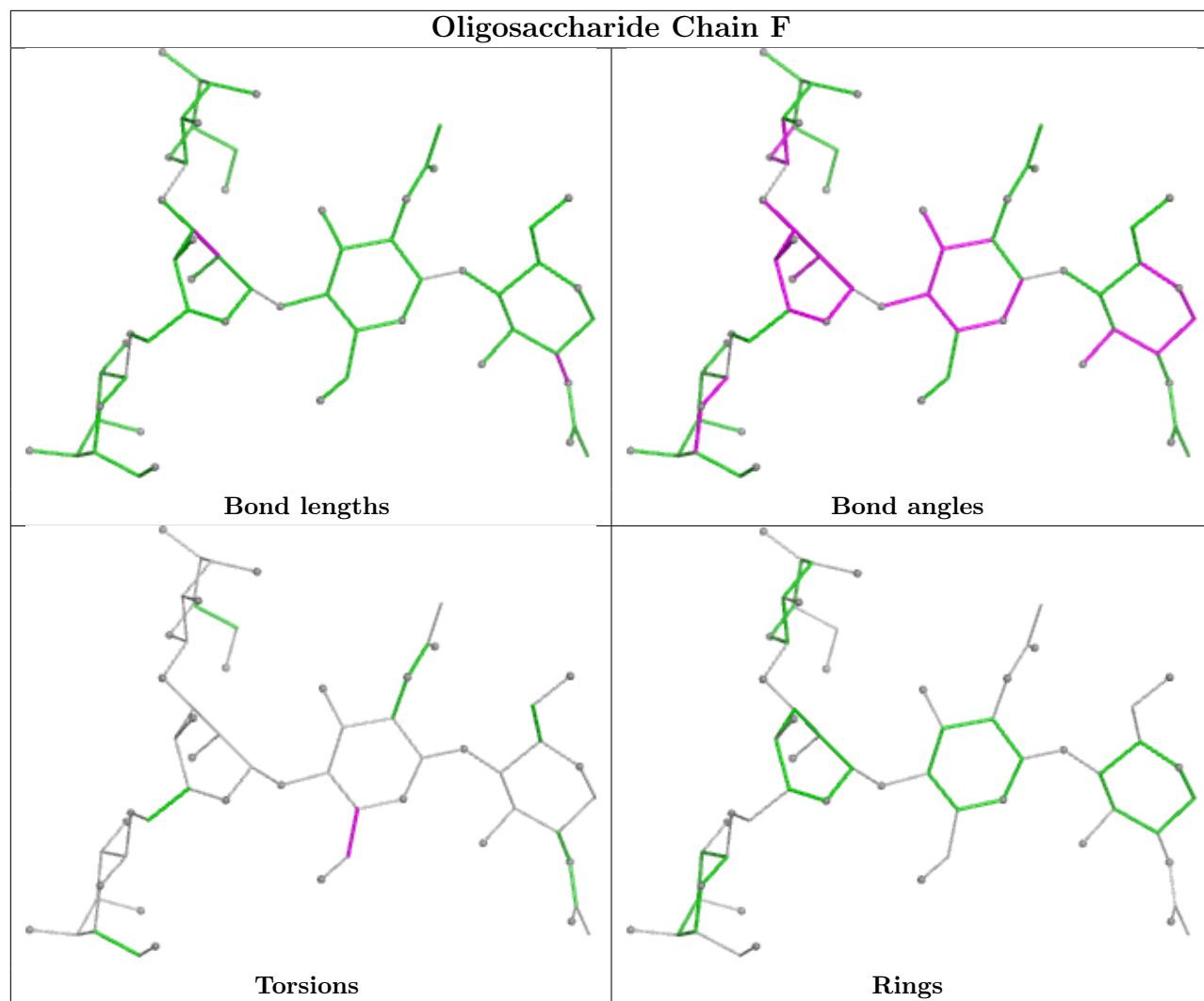
1 monomer is involved in 1 short contact:

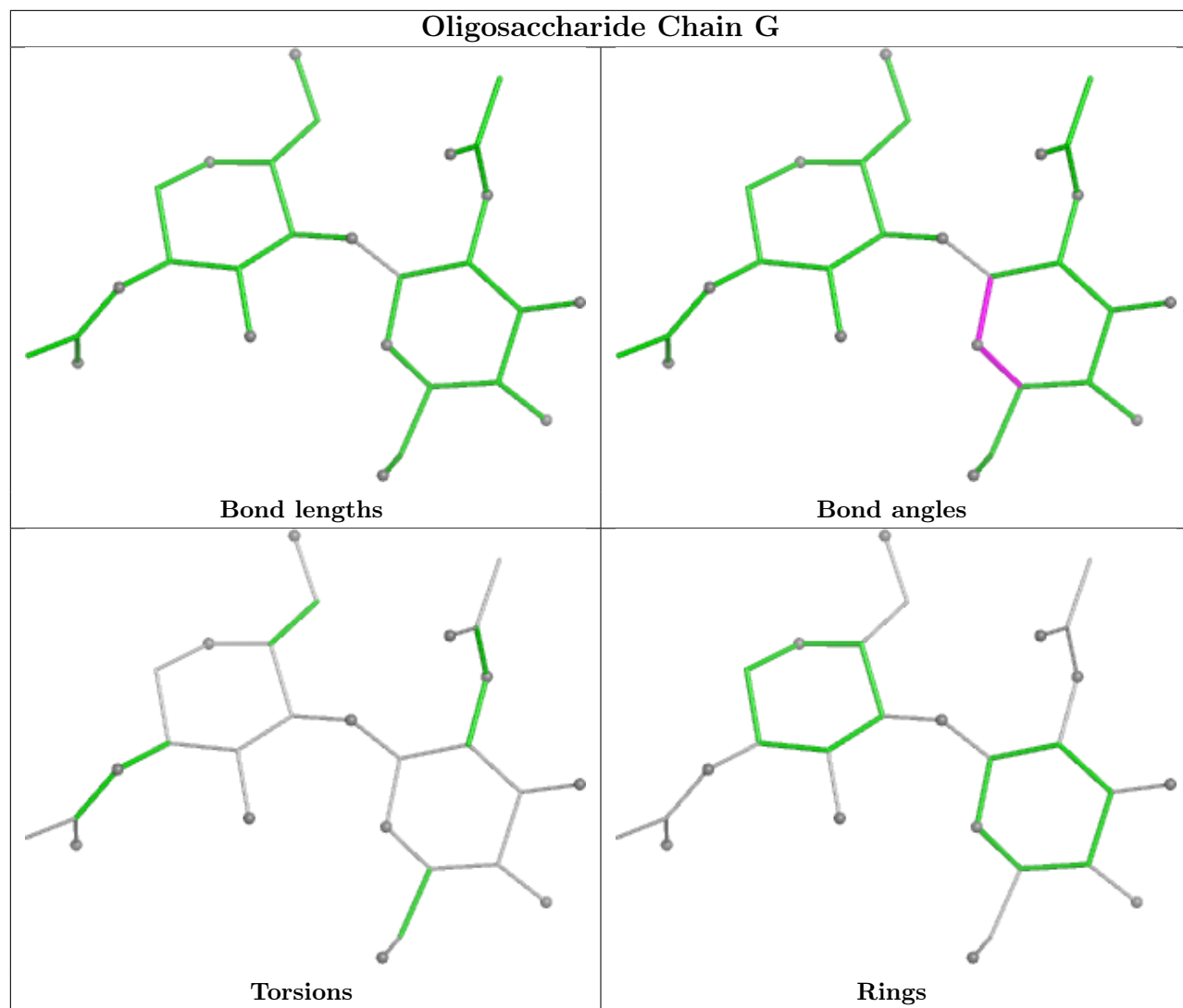
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	5	MAN	1	0

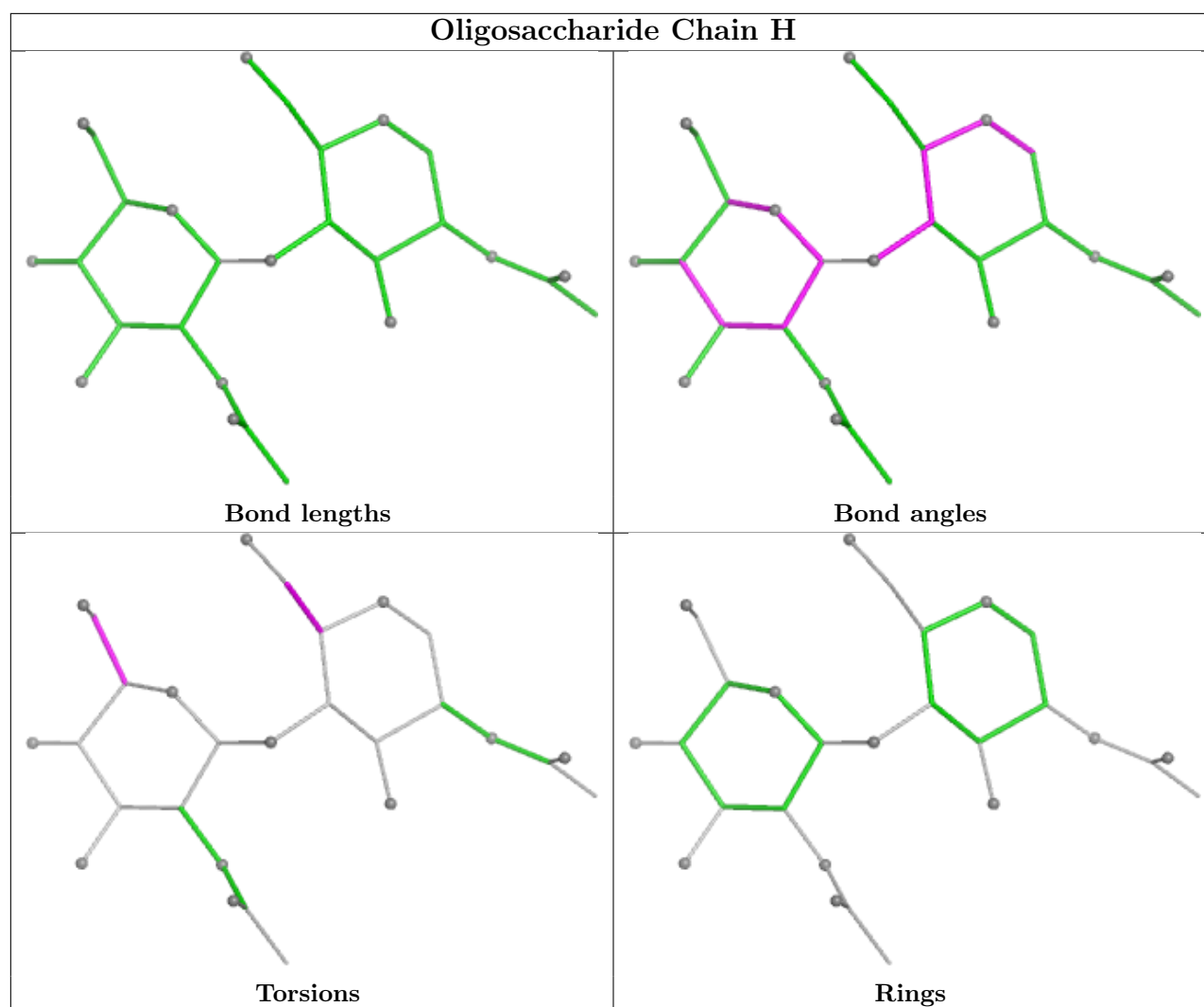
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 7 are monoatomic - leaving 3 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$
9	NAG	A	1205	1	14,14,15	0.96	1 (7%)	17,19,21	2.52	4 (23%)
9	NAG	B	2004	2	14,14,15	0.60	0	17,19,21	1.01	1 (5%)
9	NAG	A	1206	1	14,14,15	0.83	0	17,19,21	1.39	3 (17%)

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
9	NAG	A	1205	1	-	0/6/23/26	0/1/1/1
9	NAG	B	2004	2	-	2/6/23/26	0/1/1/1
9	NAG	A	1206	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1205	NAG	C1-C2	3.24	1.57	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1205	NAG	C1-O5-C5	8.50	123.71	112.19
9	A	1205	NAG	C2-N2-C7	4.01	128.61	122.90
9	A	1206	NAG	C1-O5-C5	2.84	116.05	112.19
9	A	1206	NAG	C4-C3-C2	2.66	114.91	111.02
9	B	2004	NAG	C1-O5-C5	2.64	115.77	112.19
9	A	1205	NAG	O5-C1-C2	2.59	115.38	111.29
9	A	1206	NAG	C2-N2-C7	2.48	126.44	122.90
9	A	1205	NAG	O7-C7-N2	2.00	125.63	121.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

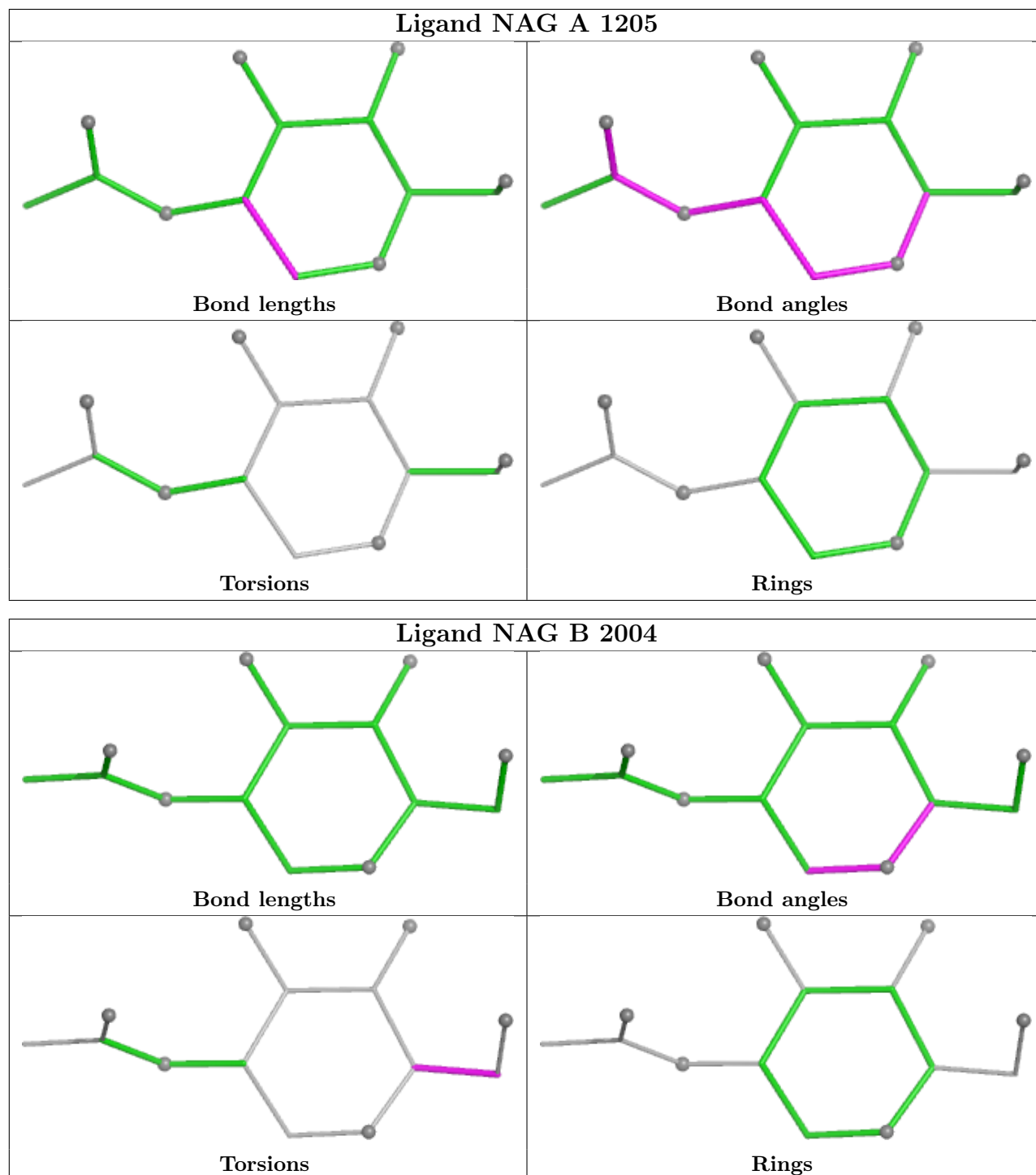
Mol	Chain	Res	Type	Atoms
9	B	2004	NAG	C4-C5-C6-O6
9	B	2004	NAG	O5-C5-C6-O6

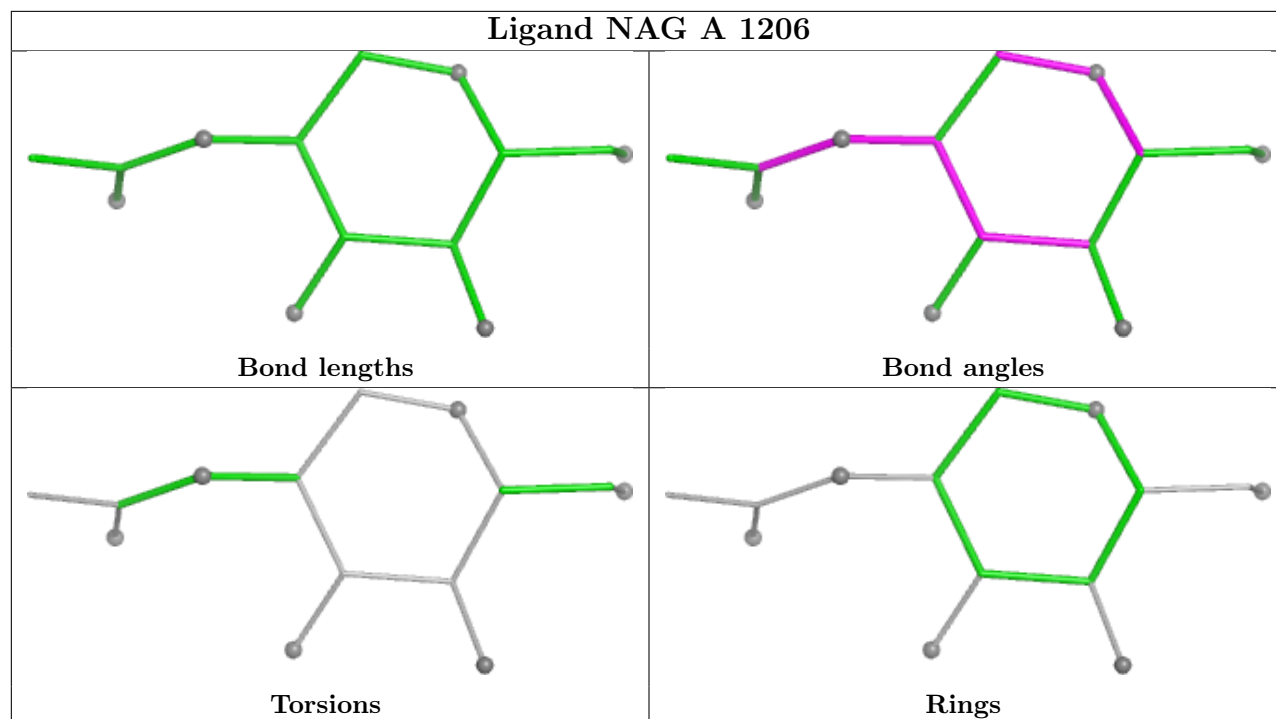
There are no ring outliers.

No monomer is involved in short contacts.

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.

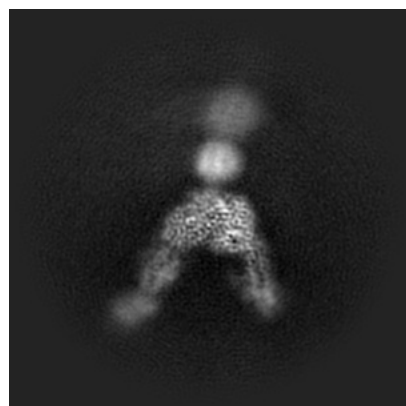
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55521. These allow visual inspection of the internal detail of the map and identification of artifacts.

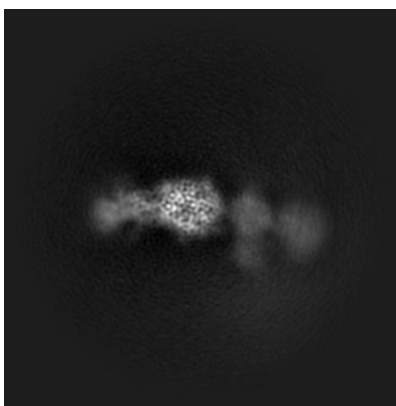
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

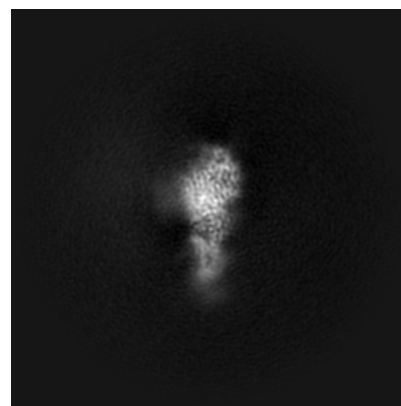
6.1.1 Primary map



X

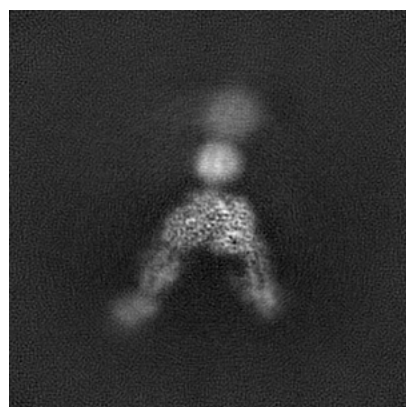


Y

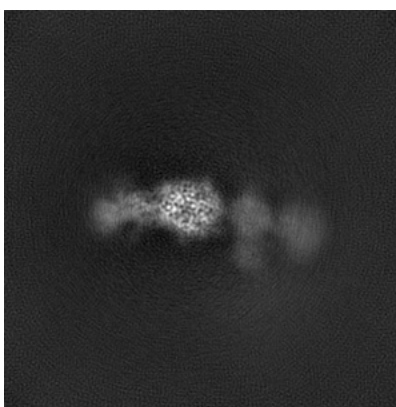


Z

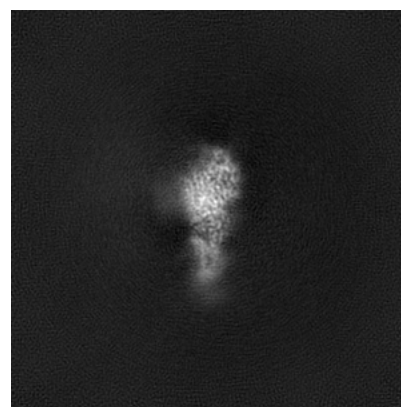
6.1.2 Raw map



X



Y

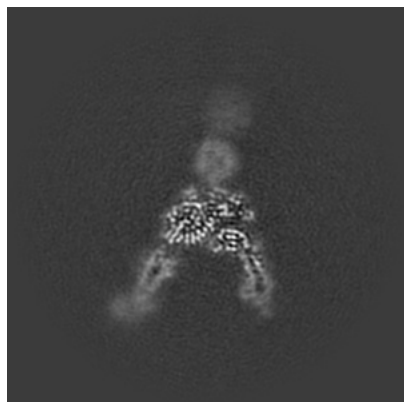


Z

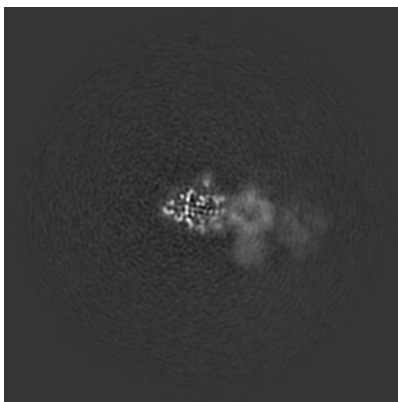
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

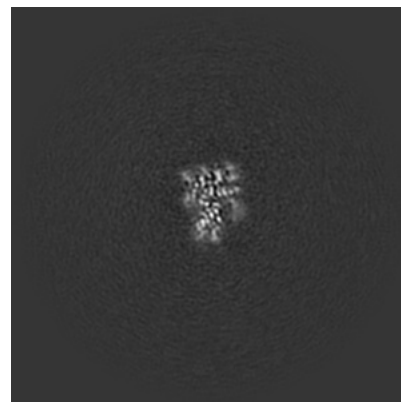
6.2.1 Primary map



X Index: 128

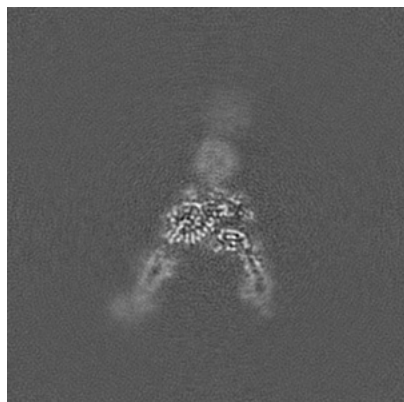


Y Index: 128

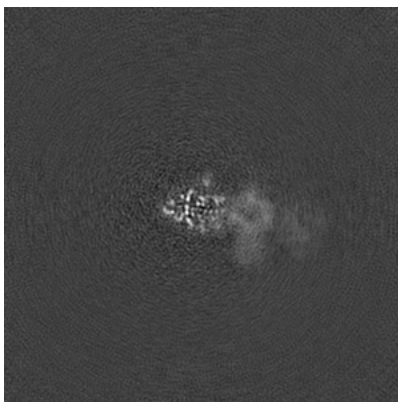


Z Index: 128

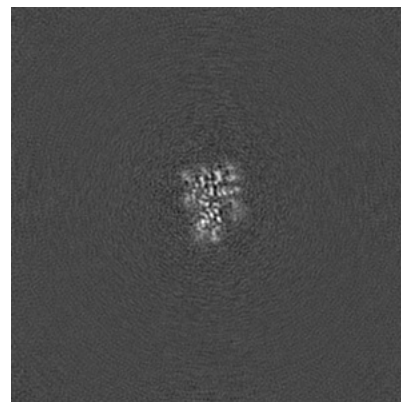
6.2.2 Raw map



X Index: 128



Y Index: 128

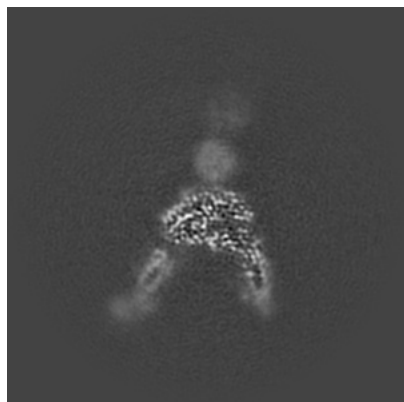


Z Index: 128

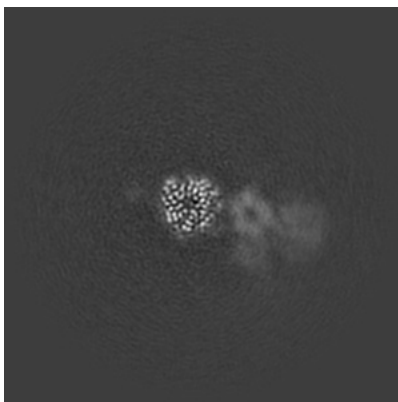
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

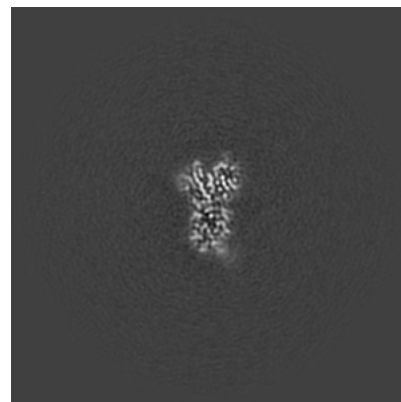
6.3.1 Primary map



X Index: 130

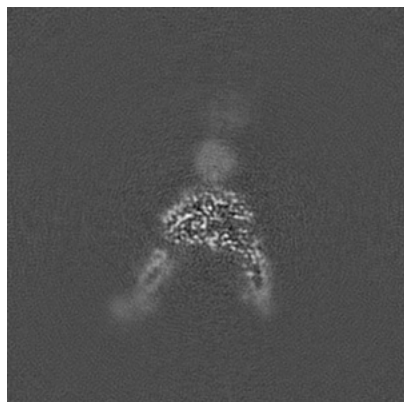


Y Index: 138

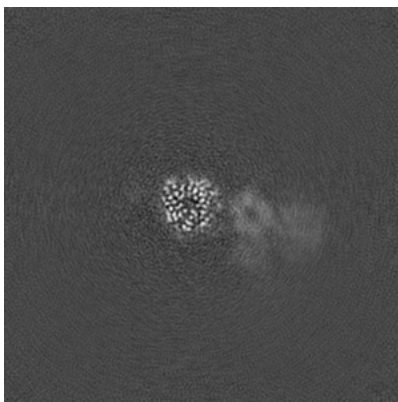


Z Index: 112

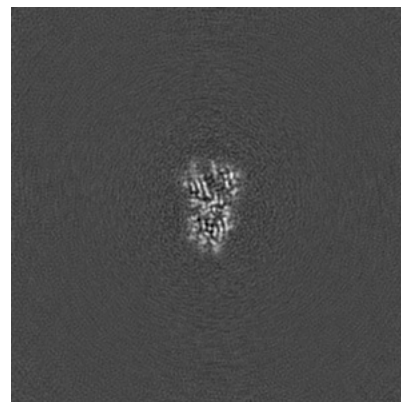
6.3.2 Raw map



X Index: 130



Y Index: 138

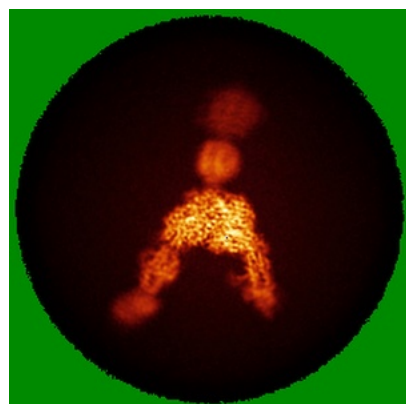


Z Index: 120

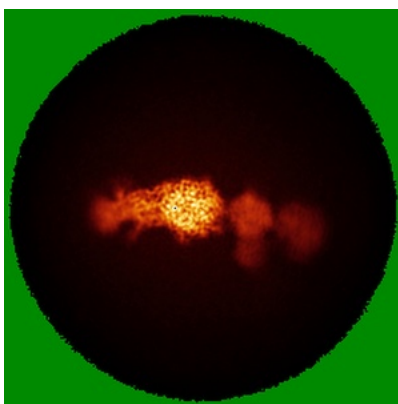
The images above show the largest variance slices of the map in three orthogonal directions.

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

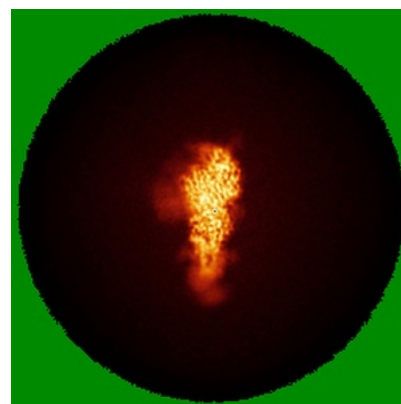
6.4.1 Primary map



X

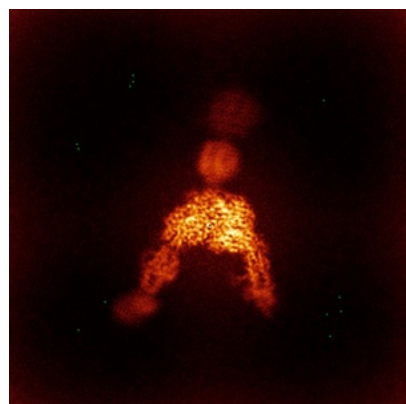


Y

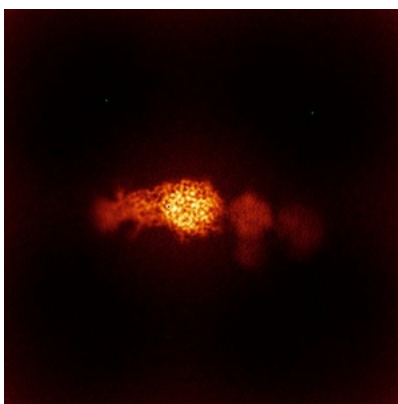


Z

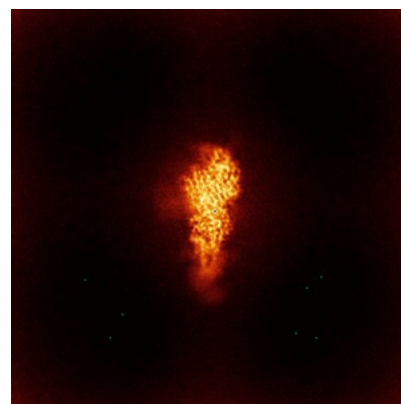
6.4.2 Raw map



X



Y

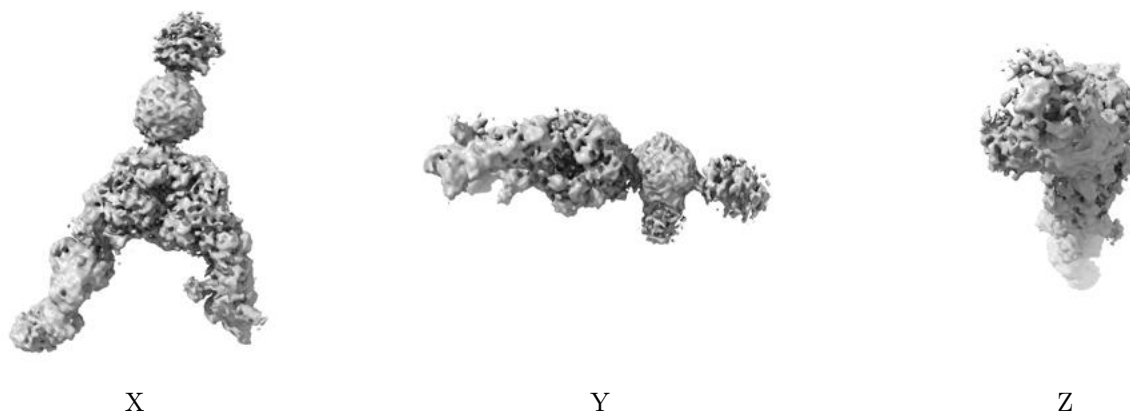


Z

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.

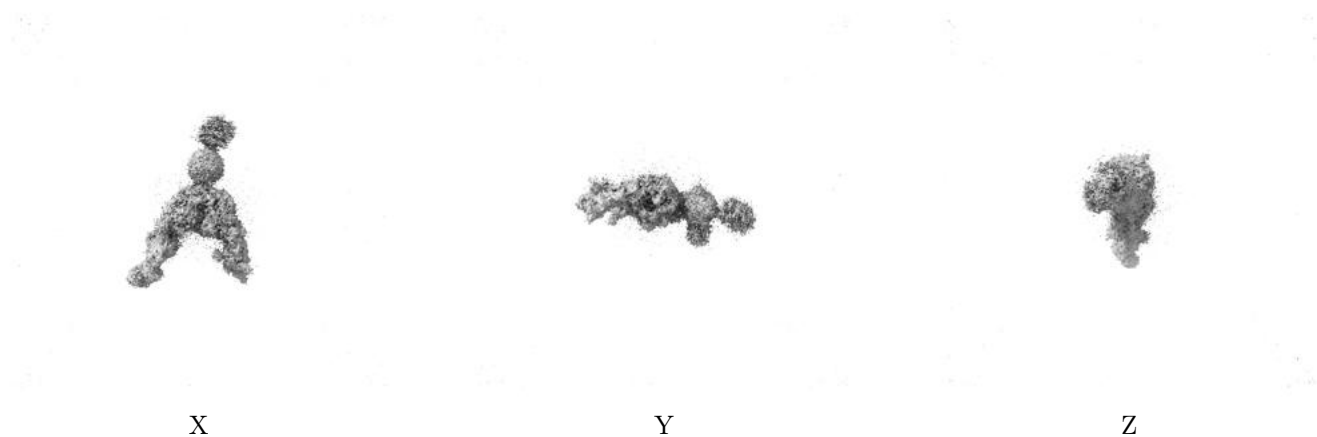
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.13. 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.

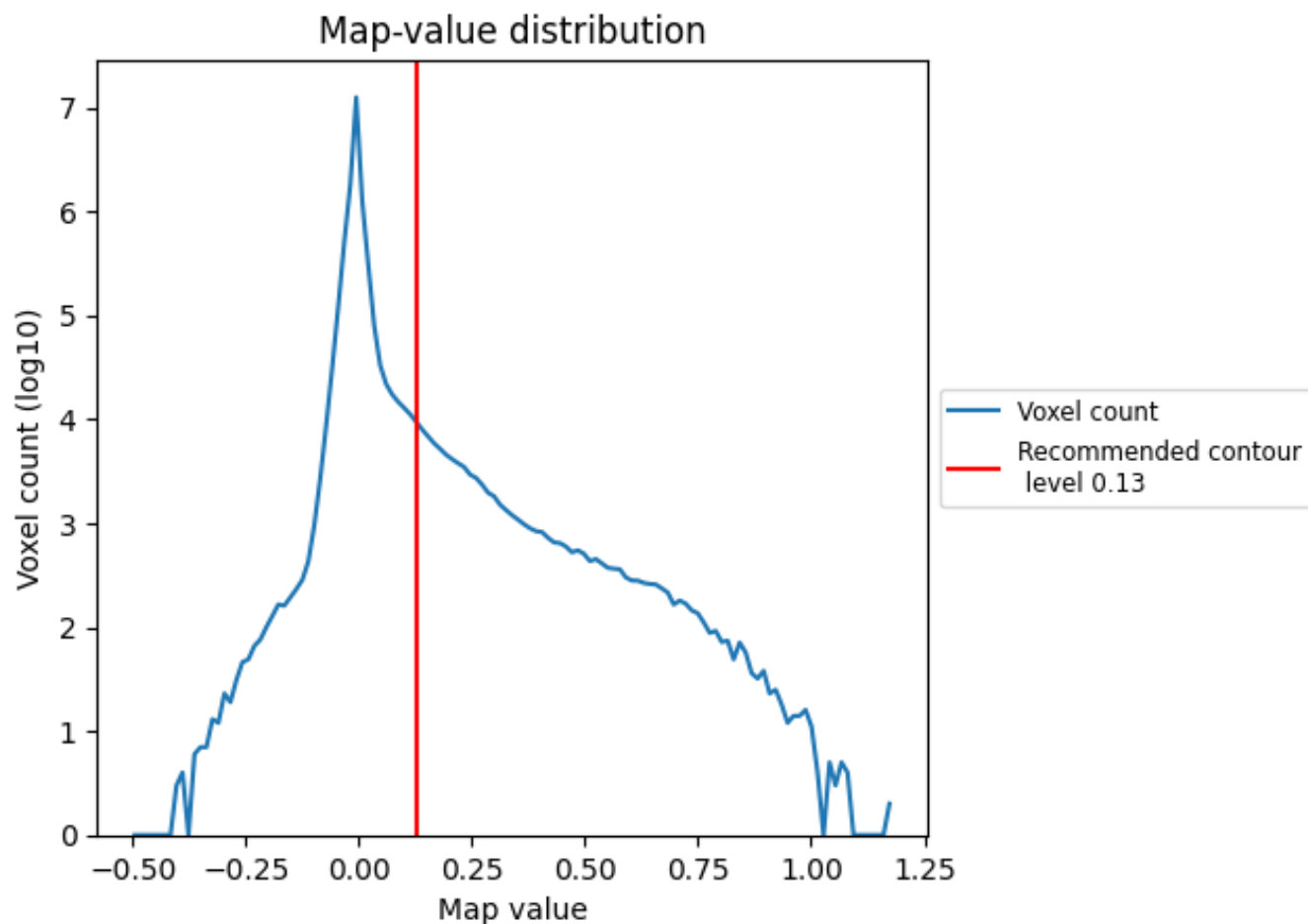
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

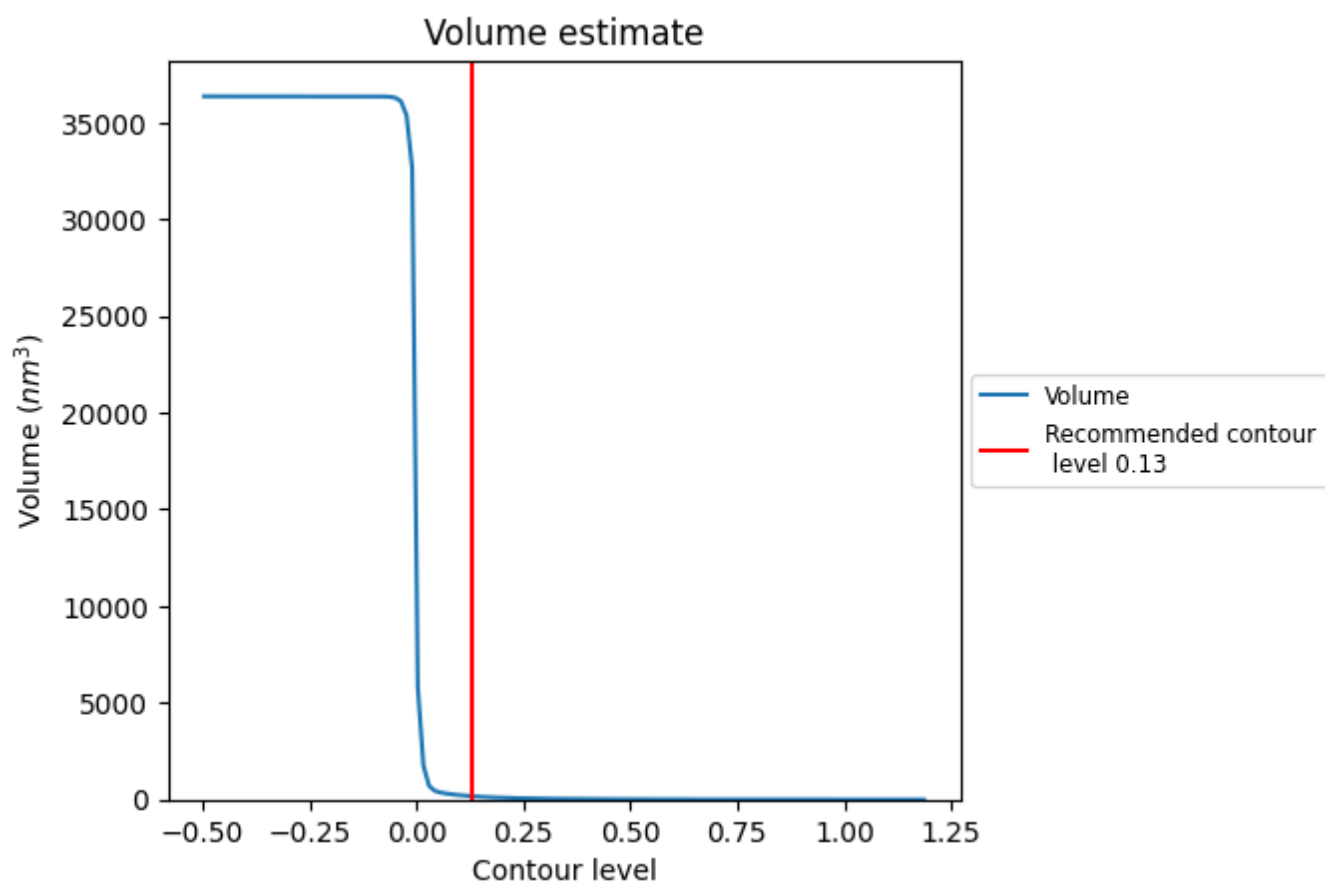
This section contains the results of statistical analysis of the map.

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.

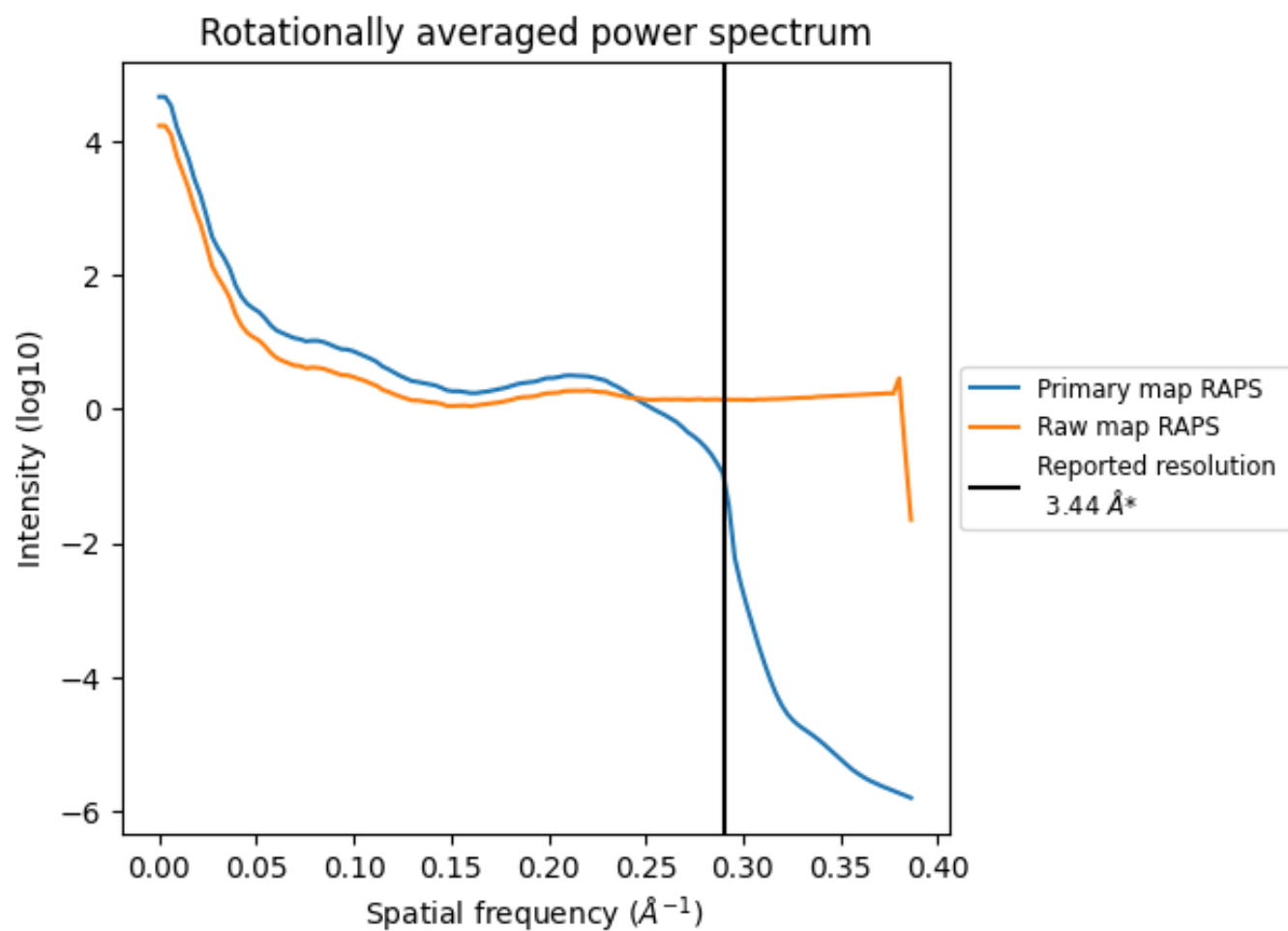
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 173 nm³; this corresponds to an approximate mass of 156 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](#)

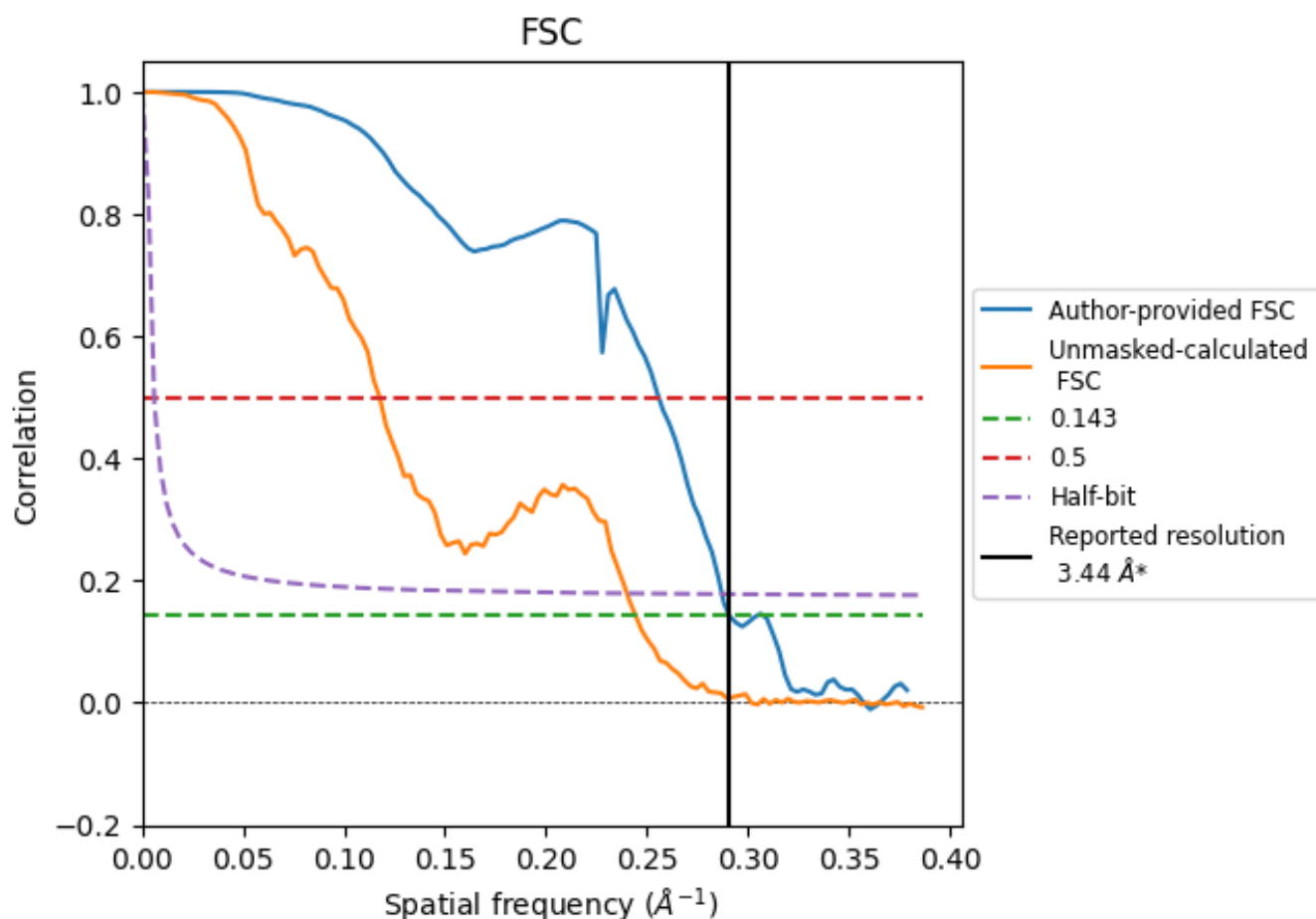


*Reported resolution corresponds to spatial frequency of 0.291 Å⁻¹

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 0.291 \AA^{-1}

8.2 Resolution estimates [i](#)

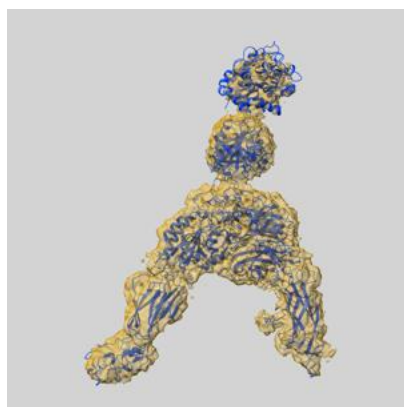
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.44	-	-
Author-provided FSC curve	3.44	3.91	3.48
Unmasked-calculated*	4.09	8.50	4.16

*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 4.09 differs from the reported value 3.44 by more than 10 %

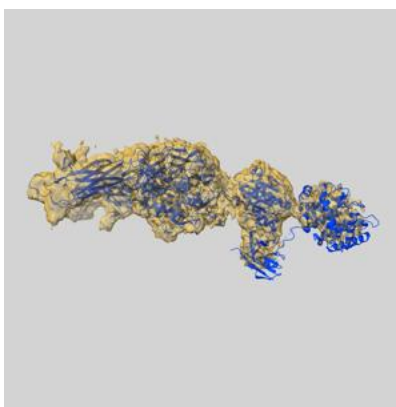
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55521 and PDB model 9T3Y. Per-residue inclusion information can be found in section [3](#) on page [8](#).

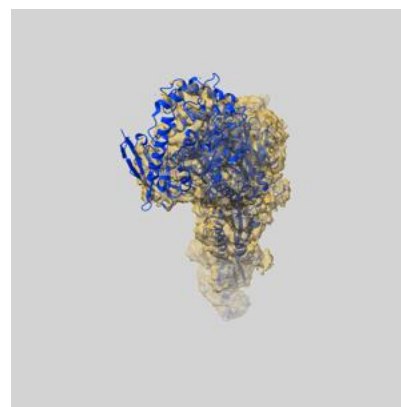
9.1 Map-model overlay [i](#)



X



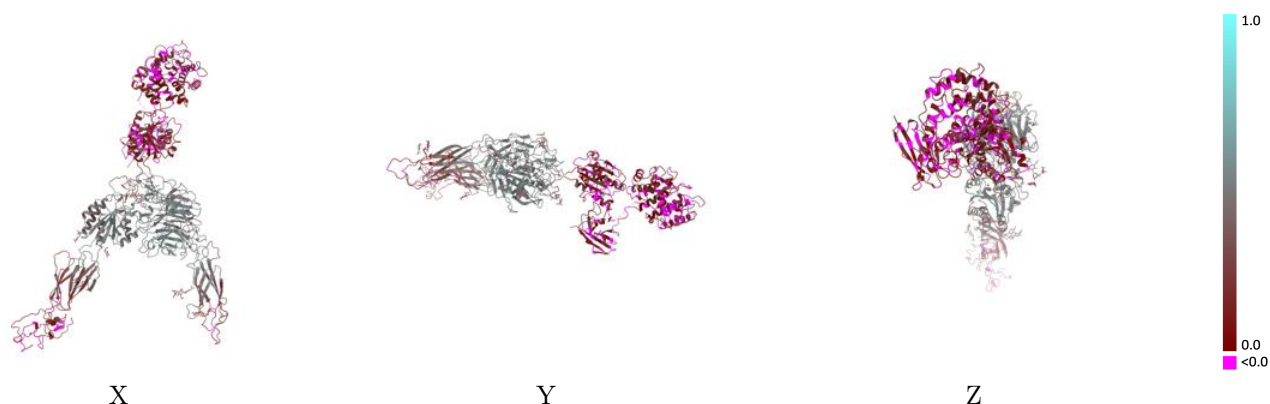
Y



Z

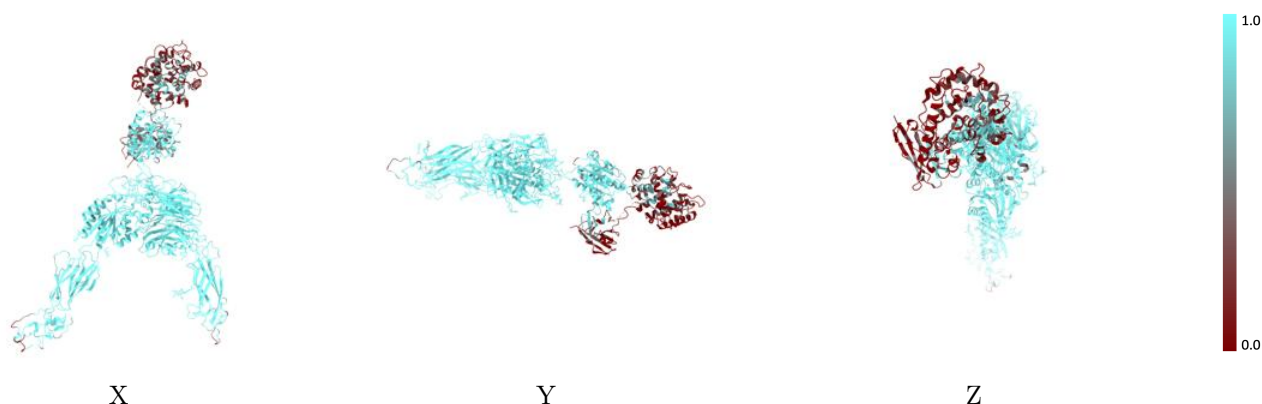
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



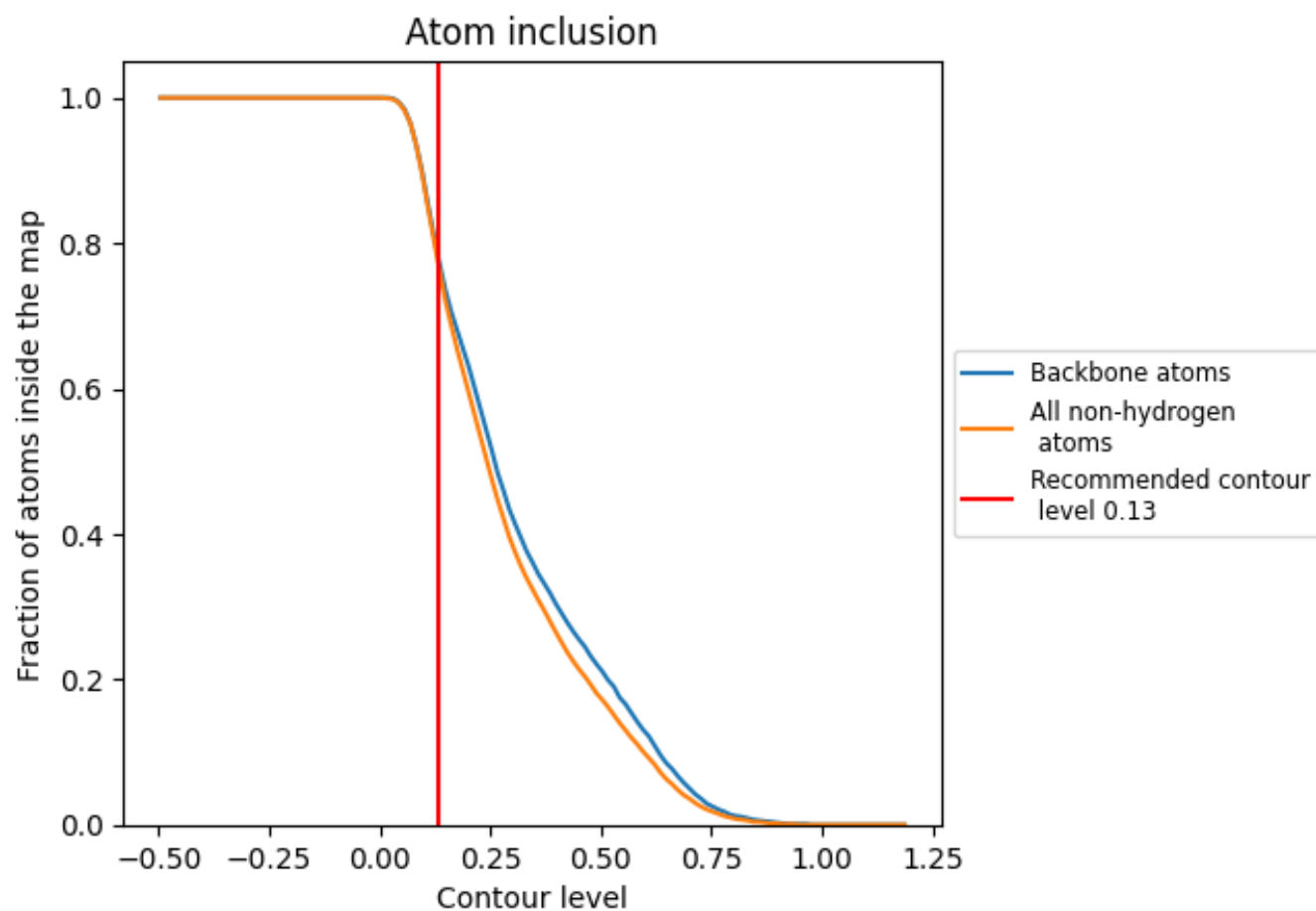
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.13).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 78% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7780	<div></div> 0.2800
A	<div></div> 0.9570	<div></div> 0.3500
B	<div></div> 0.9430	<div></div> 0.3530
C	<div></div> 0.2720	<div></div> 0.0690
D	<div></div> 0.9490	<div></div> 0.3440
E	<div></div> 0.9340	<div></div> 0.3410
F	<div></div> 0.9670	<div></div> 0.4290
G	<div></div> 1.0000	<div></div> 0.4040
H	<div></div> 0.9640	<div></div> 0.2610

1.0

0.0

<0.0