



wwPDB EM Validation Summary Report ⓘ

Jul 28, 2026 – 02:22 pm BST

PDB ID : 9TD2 / pdb_00009td2
EMDB ID : EMD-55800
Title : Integrin AlphaIIbBeta3 bound to Fab of the anti-HPA-1a antibody 26.4
Authors : de Pereda, J.M.; Stam, W.; Gragera, M.; van der Meer, F.; Chichon, F.J.;
Zarkadas, E.; van der Schoot, E.; Vidarsson, G.; Takagi, J.; Margadant, C.
Deposited on : 2025-11-22
Resolution : 2.64 Å (reported)
Based on initial models : 3FCS, .

This is a wwPDB EM Validation Summary 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:

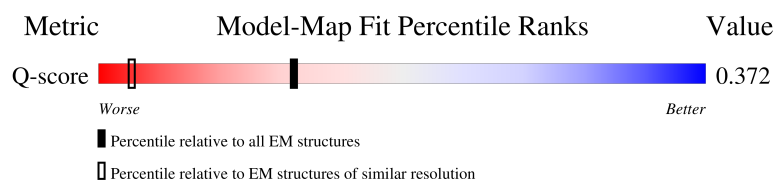
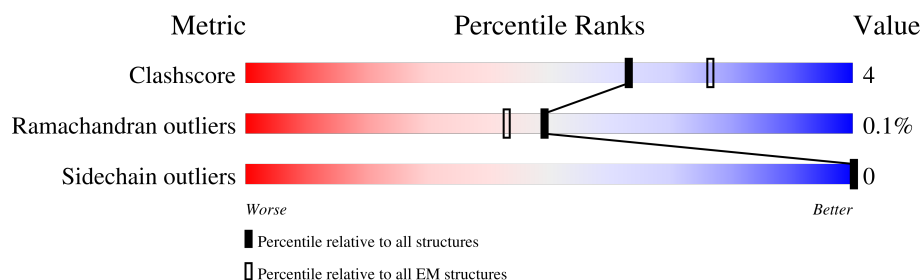
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance

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

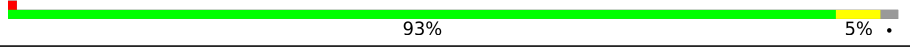
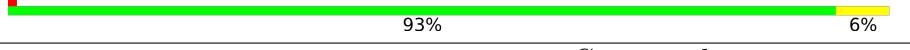
The reported resolution of this entry is 2.64 Å.

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.



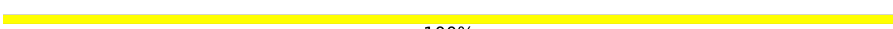
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8968 (2.14 - 3.14)

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	993	
2	B	735	
3	H	242	
4	L	215	

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Mol	Chain	Length	Quality of chain
5	E	2	 50% 50%
5	I	2	 50% 50%
6	F	4	 50% 50%
7	G	3	 33% 67%
7	J	3	 100%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 25007 atoms, of which 12241 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 Integrin alpha-IIb.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	599	Total	C	H	N	O	S	0	0
			9008	2895	4431	800	867	15		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	964	ALA	-	expression tag	UNP P08514
A	965	GLN	-	expression tag	UNP P08514
A	966	CYS	-	expression tag	UNP P08514
A	967	GLU	-	expression tag	UNP P08514
A	968	LYS	-	expression tag	UNP P08514
A	969	GLU	-	expression tag	UNP P08514
A	970	LEU	-	expression tag	UNP P08514
A	971	GLN	-	expression tag	UNP P08514
A	972	ALA	-	expression tag	UNP P08514
A	973	LEU	-	expression tag	UNP P08514
A	974	GLU	-	expression tag	UNP P08514
A	975	LYS	-	expression tag	UNP P08514
A	976	GLU	-	expression tag	UNP P08514
A	977	ASN	-	expression tag	UNP P08514
A	978	ALA	-	expression tag	UNP P08514
A	979	GLN	-	expression tag	UNP P08514
A	980	LEU	-	expression tag	UNP P08514
A	981	GLU	-	expression tag	UNP P08514
A	982	TRP	-	expression tag	UNP P08514
A	983	GLU	-	expression tag	UNP P08514
A	984	LEU	-	expression tag	UNP P08514
A	985	GLN	-	expression tag	UNP P08514
A	986	ALA	-	expression tag	UNP P08514
A	987	LEU	-	expression tag	UNP P08514
A	988	GLU	-	expression tag	UNP P08514
A	989	LYS	-	expression tag	UNP P08514
A	990	GLU	-	expression tag	UNP P08514
A	991	LEU	-	expression tag	UNP P08514

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Chain	Residue	Modelled	Actual	Comment	Reference
A	992	ALA	-	expression tag	UNP P08514
A	993	GLN	-	expression tag	UNP P08514

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	592	Total	C	H	N	O	S	0	0
			8821	2781	4300	773	907	60		

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	693	GLY	-	expression tag	UNP P05106
B	694	GLY	-	expression tag	UNP P05106
B	695	LEU	-	expression tag	UNP P05106
B	696	GLU	-	expression tag	UNP P05106
B	697	ASN	-	expression tag	UNP P05106
B	698	LEU	-	expression tag	UNP P05106
B	699	TYR	-	expression tag	UNP P05106
B	700	PHE	-	expression tag	UNP P05106
B	701	GLN	-	expression tag	UNP P05106
B	702	GLY	-	expression tag	UNP P05106
B	703	GLY	-	expression tag	UNP P05106
B	704	LYS	-	expression tag	UNP P05106
B	705	ASN	-	expression tag	UNP P05106
B	706	ALA	-	expression tag	UNP P05106
B	707	GLN	-	expression tag	UNP P05106
B	708	CYS	-	expression tag	UNP P05106
B	709	LYS	-	expression tag	UNP P05106
B	710	LYS	-	expression tag	UNP P05106
B	711	LYS	-	expression tag	UNP P05106
B	712	LEU	-	expression tag	UNP P05106
B	713	GLN	-	expression tag	UNP P05106
B	714	ALA	-	expression tag	UNP P05106
B	715	LEU	-	expression tag	UNP P05106
B	716	LYS	-	expression tag	UNP P05106
B	717	LYS	-	expression tag	UNP P05106
B	718	LYS	-	expression tag	UNP P05106
B	719	ASN	-	expression tag	UNP P05106
B	720	ALA	-	expression tag	UNP P05106
B	721	GLN	-	expression tag	UNP P05106
B	722	LEU	-	expression tag	UNP P05106

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Chain	Residue	Modelled	Actual	Comment	Reference
B	723	LYS	-	expression tag	UNP P05106
B	724	TRP	-	expression tag	UNP P05106
B	725	LYS	-	expression tag	UNP P05106
B	726	LEU	-	expression tag	UNP P05106
B	727	GLN	-	expression tag	UNP P05106
B	728	ALA	-	expression tag	UNP P05106
B	729	LEU	-	expression tag	UNP P05106
B	730	LYS	-	expression tag	UNP P05106
B	731	LYS	-	expression tag	UNP P05106
B	732	LYS	-	expression tag	UNP P05106
B	733	LEU	-	expression tag	UNP P05106
B	734	ALA	-	expression tag	UNP P05106
B	735	GLN	-	expression tag	UNP P05106

- Molecule 3 is a protein called Antibody 26.4 Fab heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	H	238	Total	C	H	N	O	S	0	0
			3525	1127	1727	309	355	7		

- Molecule 4 is a protein called Antibody 26.4 Fab light chain.

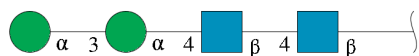
Mol	Chain	Residues	Atoms						AltConf	Trace
4	L	214	Total	C	H	N	O	S	0	0
			3238	1027	1596	279	331	5		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



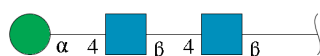
Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	2	Total	C	H	N	O		0	0
			53	16	25	2	10			
5	I	2	Total	C	H	N	O		0	0
			53	16	25	2	10			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-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
6	F	4	Total	C	H	N	O	0	0
			93	28	43	2	20		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

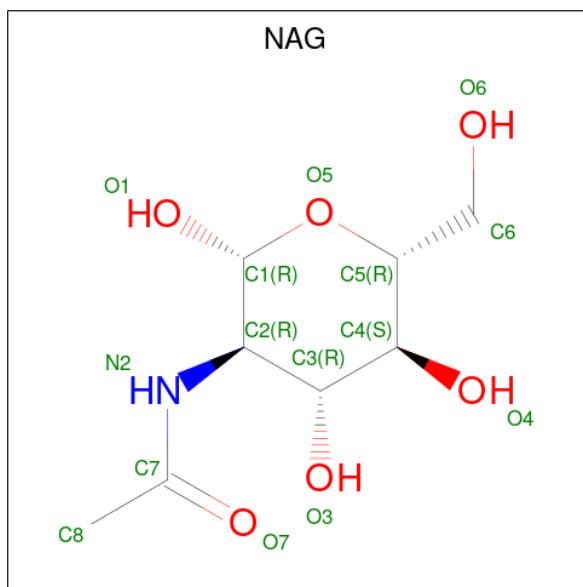


Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	3	Total	C	H	N	O	0	0
			73	22	34	2	15		
7	J	3	Total	C	H	N	O	0	0
			73	22	34	2	15		

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
8	A	4	Total	Ca	0
			4	4	
8	B	2	Total	Ca	0
			2	2	

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



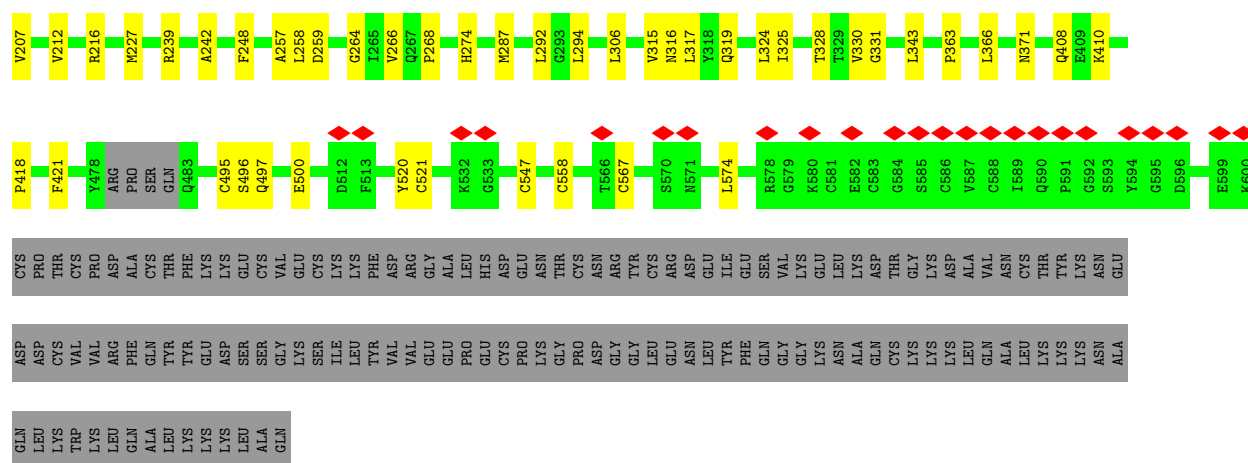
Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
9	A	1	Total	C	H	N	O	0
			27	8	13	1	5	

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	B	1	Total	Mg	0
			1	1	

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		AltConf
11	A	3	Total	O	0
			3	3	
11	B	6	Total	O	0
			6	6	



- Molecule 3: Antibody 26.4 Fab heavy chain

Chain H: 93% 5%



- Molecule 4: Antibody 26.4 Fab light chain

Chain L: 93% 6%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 50% 50%



- Molecule 6: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 50% 50%



- Molecule 7: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  33% 67%



- Molecule 7: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	84349	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 ($e^-/\text{\AA}^2$)	41.57	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	165000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.723	Depositor
Minimum map value	-0.798	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	309.52, 309.52, 309.52	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0317333, 1.0317333, 1.0317333	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.25	0/4691	0.44	0/6390
2	B	0.17	0/4601	0.41	0/6223
3	H	0.11	0/1848	0.28	0/2528
4	L	0.14	0/1677	0.27	0/2276
All	All	0.19	0/12817	0.39	0/17417

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4577	4431	4445	46	0
2	B	4521	4300	4309	51	0
3	H	1798	1727	1731	6	0
4	L	1642	1596	1598	9	0
5	E	28	25	25	3	0
5	I	28	25	25	0	0
6	F	50	43	43	1	0
7	G	39	34	34	5	0
7	J	39	34	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	4	0	0	0	0
8	B	2	0	0	0	0
9	A	28	26	26	0	0
10	B	1	0	0	0	0
11	A	3	0	0	1	0
11	B	6	0	0	1	0
All	All	12766	12241	12270	105	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.

The worst 5 of 105 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:A:219:GLN:HE21	1:A:221:LEU:HD11	1.43	0.83
1:A:327:ARG:NH1	1:A:346:LEU:HD13	2.02	0.74
4:L:37:GLN:HB2	4:L:47:LEU:HD11	1.70	0.72
2:B:26:CYS:HB2	2:B:44:LEU:HD23	1.75	0.69
2:B:274:HIS:CE1	2:B:287:MET:HE1	2.29	0.67

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	597/993 (60%)	578 (97%)	18 (3%)	1 (0%)	43	58
2	B	586/735 (80%)	555 (95%)	31 (5%)	0	100	100
3	H	236/242 (98%)	224 (95%)	12 (5%)	0	100	100
4	L	212/215 (99%)	201 (95%)	11 (5%)	0	100	100
All	All	1631/2185 (75%)	1558 (96%)	72 (4%)	1 (0%)	49	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU

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	488/827 (59%)	488 (100%)	0	100	100
2	B	522/648 (81%)	522 (100%)	0	100	100
3	H	204/208 (98%)	204 (100%)	0	100	100
4	L	184/185 (100%)	184 (100%)	0	100	100
All	All	1398/1868 (75%)	1398 (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. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
3	H	116	HIS
4	L	210	ASN
4	L	199	GLN
2	B	14	GLN
3	H	81	GLN

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 ⓘ

14 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
5	NAG	E	1	5,2	14,14,15	0.85	0	17,19,21	1.36	2 (11%)
5	NAG	E	2	5	14,14,15	0.77	0	17,19,21	0.95	0
6	NAG	F	1	2,6	14,14,15	0.80	0	17,19,21	1.72	4 (23%)
6	NAG	F	2	6	14,14,15	1.14	1 (7%)	17,19,21	1.32	3 (17%)
6	MAN	F	3	6	11,11,12	0.74	0	15,15,17	1.72	3 (20%)
6	MAN	F	4	6	11,11,12	0.66	0	15,15,17	2.89	4 (26%)
7	NAG	G	1	2,7	14,14,15	0.76	0	17,19,21	0.87	0
7	NAG	G	2	7	14,14,15	0.84	1 (7%)	17,19,21	1.66	3 (17%)
7	MAN	G	3	7	11,11,12	0.69	0	15,15,17	1.63	1 (6%)
5	NAG	I	1	5,2	14,14,15	0.88	1 (7%)	17,19,21	1.34	2 (11%)
5	NAG	I	2	5	14,14,15	0.82	0	17,19,21	0.93	0
7	NAG	J	1	2,7	14,14,15	0.78	0	17,19,21	0.91	1 (5%)
7	NAG	J	2	7	14,14,15	0.87	1 (7%)	17,19,21	1.61	3 (17%)
7	MAN	J	3	7	11,11,12	0.66	0	15,15,17	1.61	1 (6%)

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
5	NAG	E	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
6	NAG	F	1	2,6	-	1/6/23/26	0/1/1/1
6	NAG	F	2	6	-	0/6/23/26	0/1/1/1
6	MAN	F	3	6	-	0/2/19/22	1/1/1/1
6	MAN	F	4	6	-	1/2/19/22	0/1/1/1
7	NAG	G	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	G	2	7	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	G	3	7	-	2/2/19/22	1/1/1/1
5	NAG	I	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
7	NAG	J	1	2,7	-	1/6/23/26	0/1/1/1
7	NAG	J	2	7	-	2/6/23/26	0/1/1/1
7	MAN	J	3	7	-	2/2/19/22	1/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	2	NAG	O5-C1	-3.54	1.38	1.43
7	J	2	NAG	O5-C1	-2.59	1.39	1.43
7	G	2	NAG	O5-C1	-2.44	1.39	1.43
5	I	1	NAG	O5-C1	-2.28	1.40	1.43

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	4	MAN	C1-O5-C5	9.11	124.53	112.19
7	J	3	MAN	C1-O5-C5	5.18	119.22	112.19
7	G	3	MAN	C1-O5-C5	5.18	119.21	112.19
6	F	1	NAG	C2-N2-C7	5.06	130.10	122.90
7	G	2	NAG	O5-C1-C2	-4.65	103.94	111.29

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	1	NAG	C3-C2-N2-C7
7	G	3	MAN	O5-C5-C6-O6
7	J	3	MAN	O5-C5-C6-O6
7	J	2	NAG	C8-C7-N2-C2
7	J	2	NAG	O7-C7-N2-C2

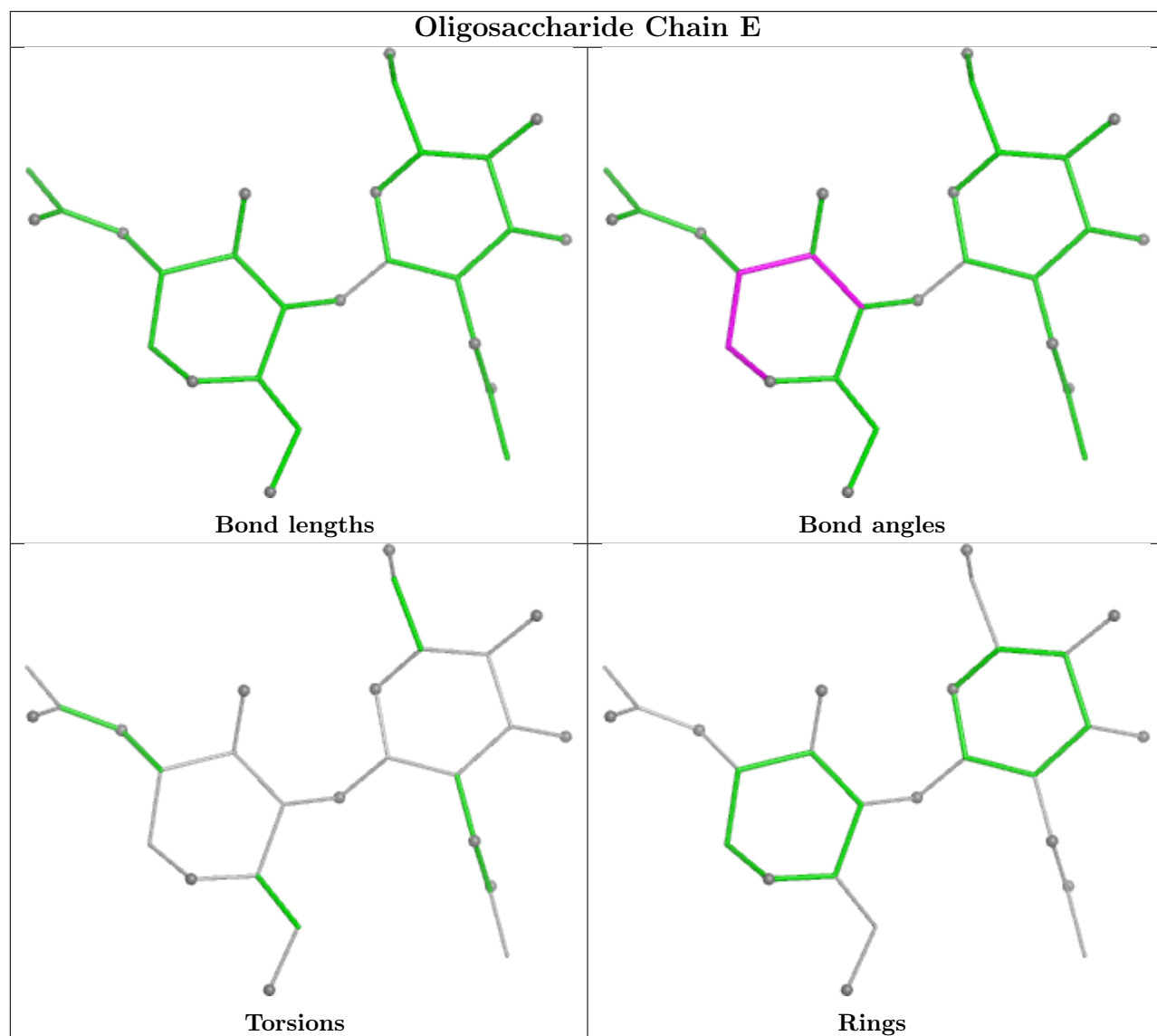
All (3) ring outliers are listed below:

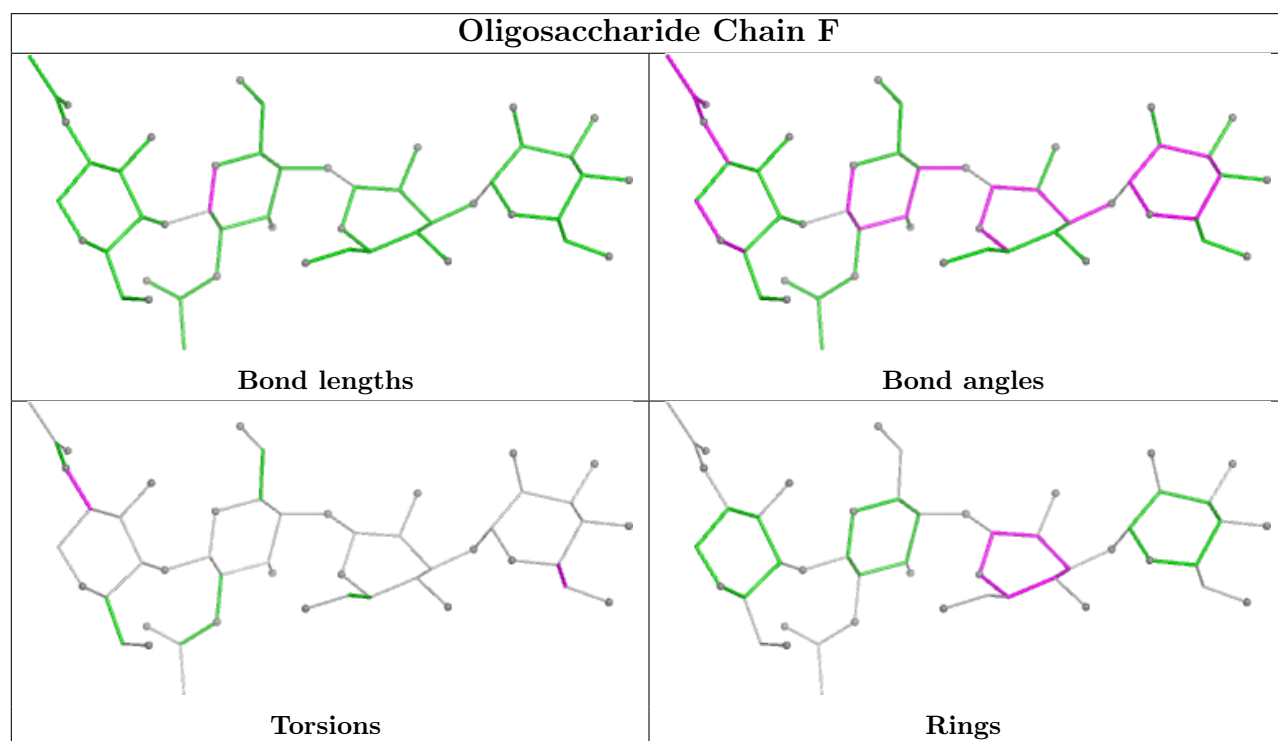
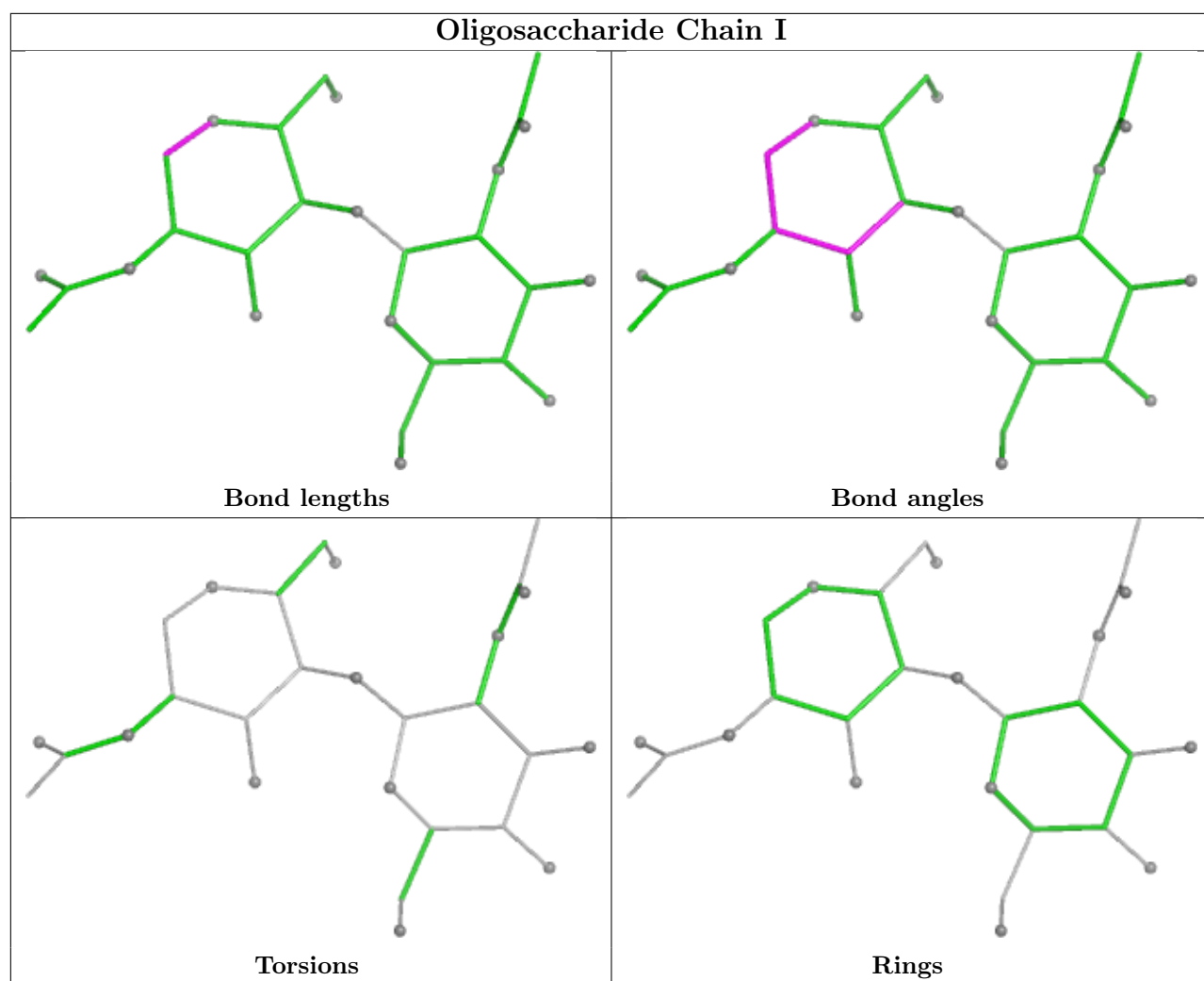
Mol	Chain	Res	Type	Atoms
6	F	3	MAN	C1-C2-C3-C4-C5-O5
7	J	3	MAN	C1-C2-C3-C4-C5-O5
7	G	3	MAN	C1-C2-C3-C4-C5-O5

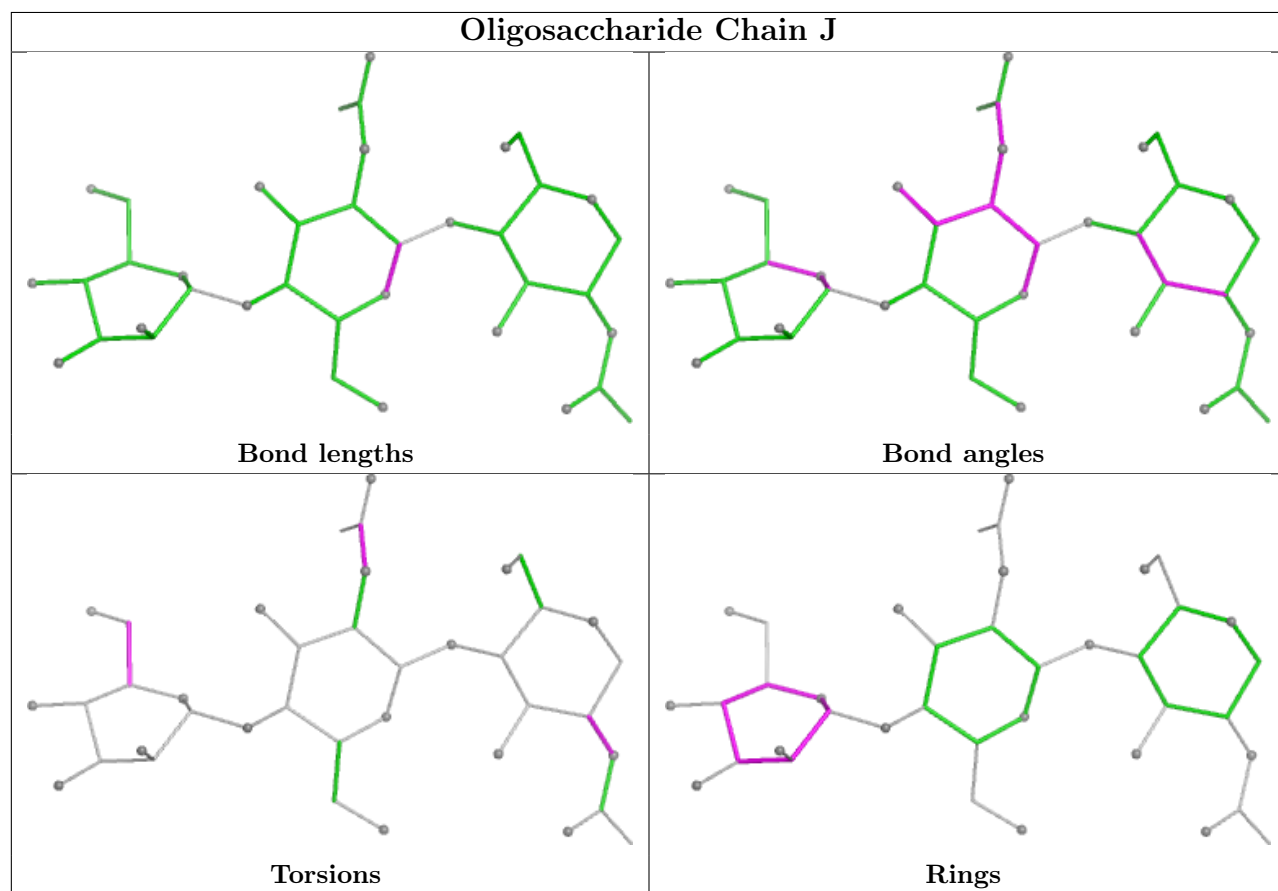
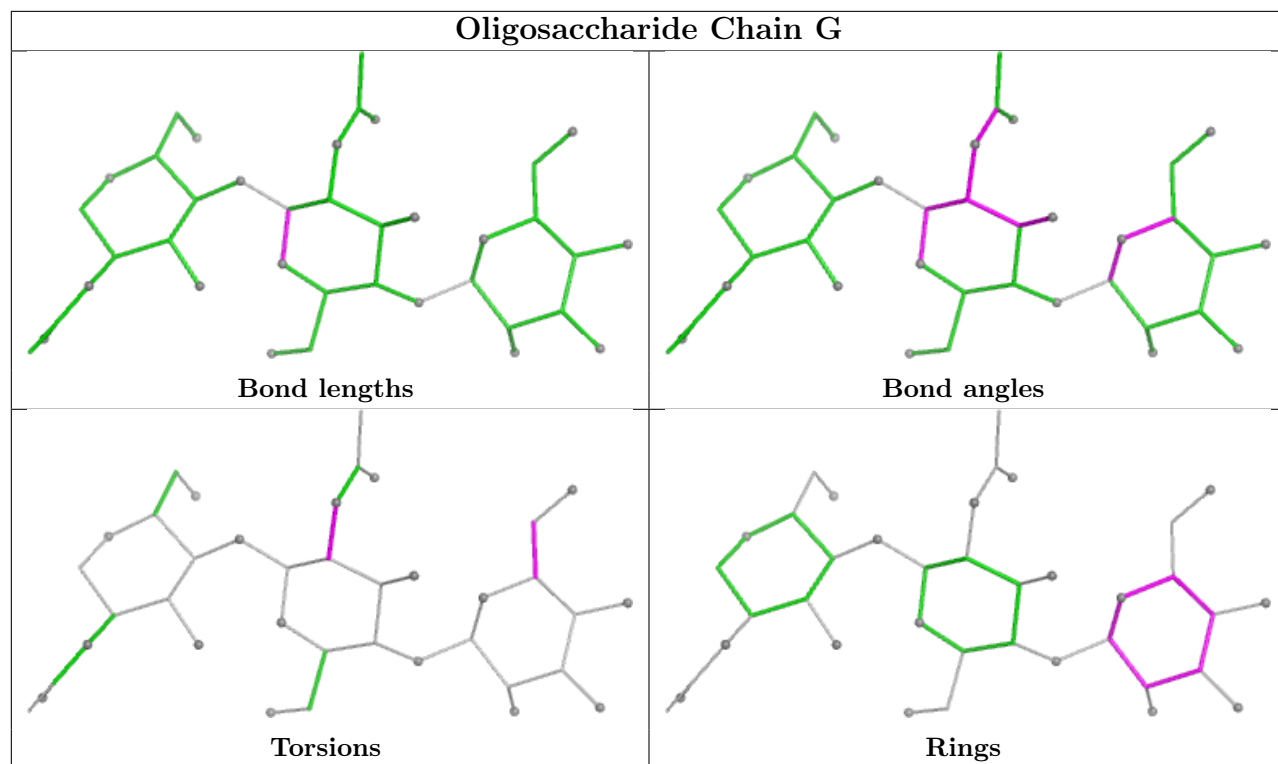
6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	2	NAG	5	0
5	E	1	NAG	3	0
7	G	1	NAG	1	0
6	F	2	NAG	1	0
6	F	3	MAN	1	0
7	G	3	MAN	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 oligosaccharide.







5.6 Ligand geometry

Of 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 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	1006	1	14,14,15	0.81	0	17,19,21	1.88	4 (23%)
9	NAG	A	1005	1	14,14,15	0.73	0	17,19,21	0.85	0

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	1006	1	-	2/6/23/26	0/1/1/1
9	NAG	A	1005	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1006	NAG	C1-O5-C5	5.54	119.70	112.19
9	A	1006	NAG	C2-N2-C7	2.92	127.06	122.90
9	A	1006	NAG	C3-C4-C5	-2.53	105.73	110.24
9	A	1006	NAG	O5-C1-C2	2.11	114.62	111.29

There are no chirality outliers.

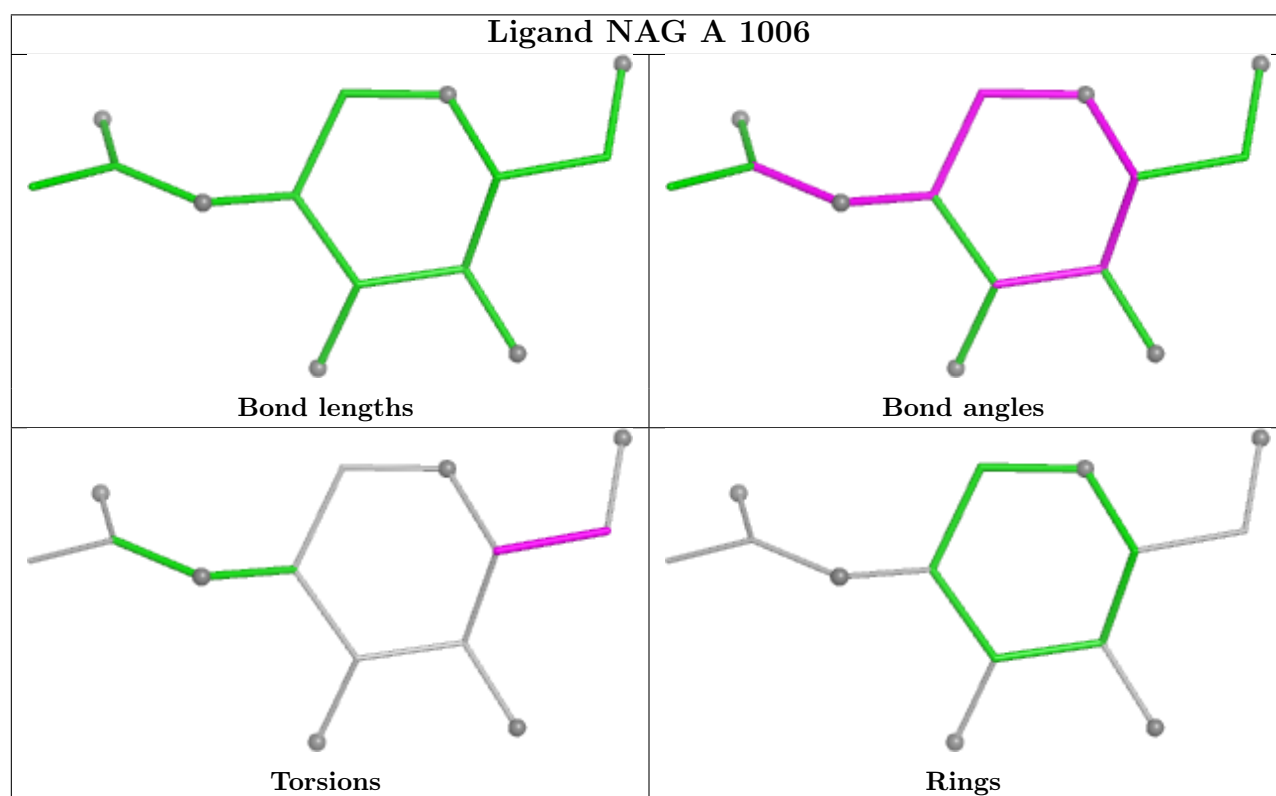
All (3) torsion outliers are listed below:

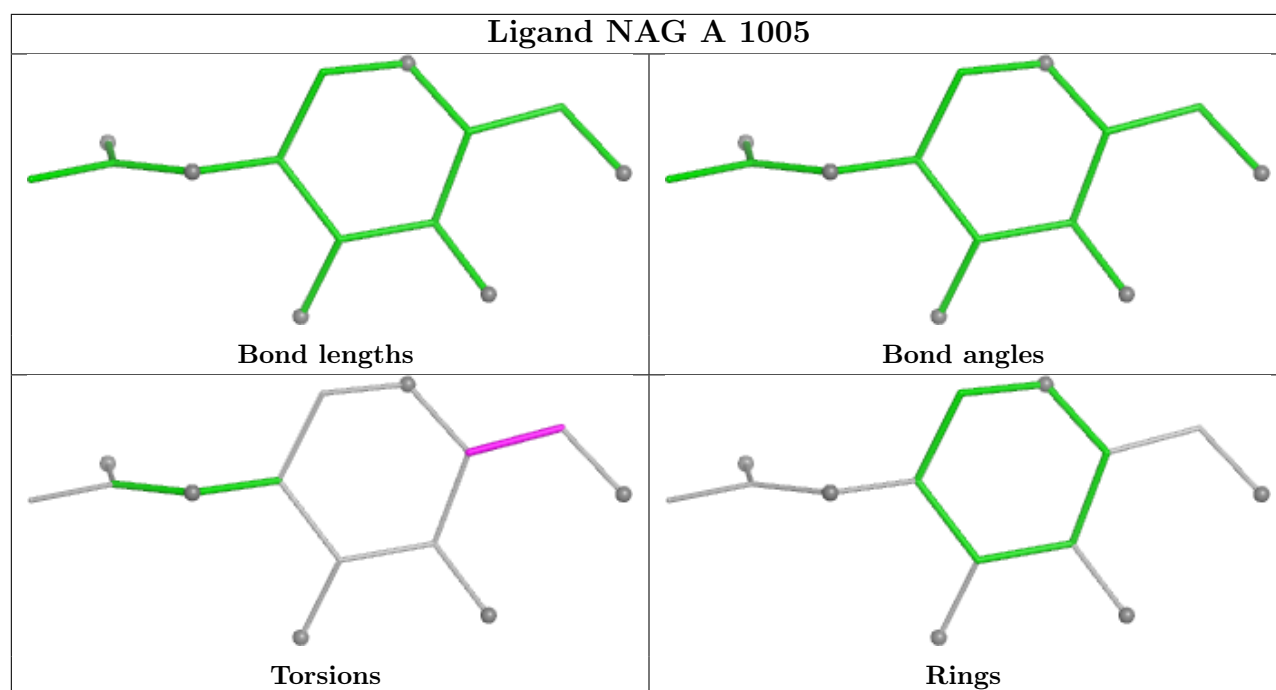
Mol	Chain	Res	Type	Atoms
9	A	1006	NAG	O5-C5-C6-O6
9	A	1006	NAG	C4-C5-C6-O6
9	A	1005	NAG	O5-C5-C6-O6

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.

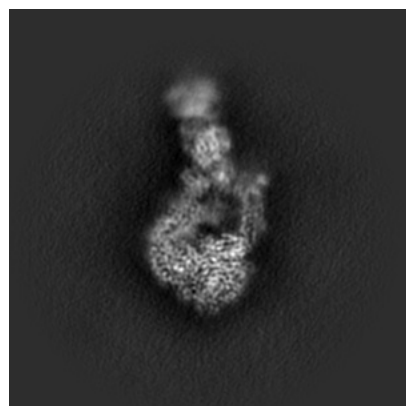
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55800. These allow visual inspection of the internal detail of the map and identification of artifacts.

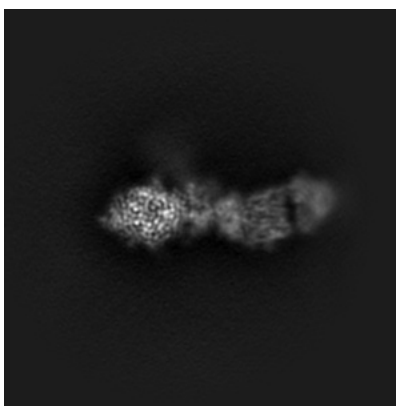
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

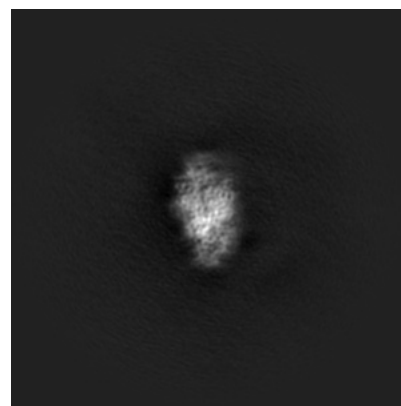
6.1.1 Primary map



X

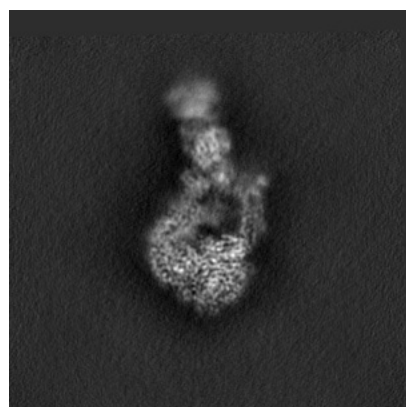


Y

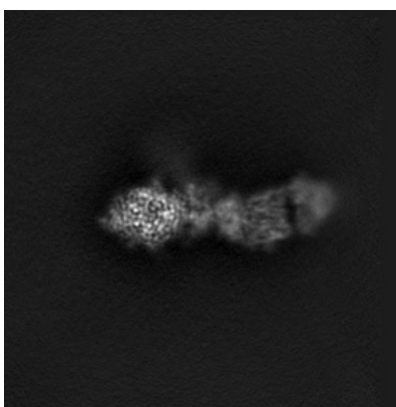


Z

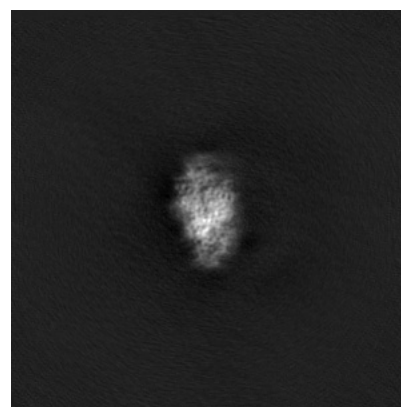
6.1.2 Raw map



X



Y

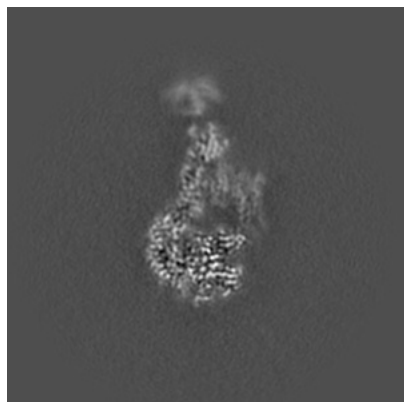


Z

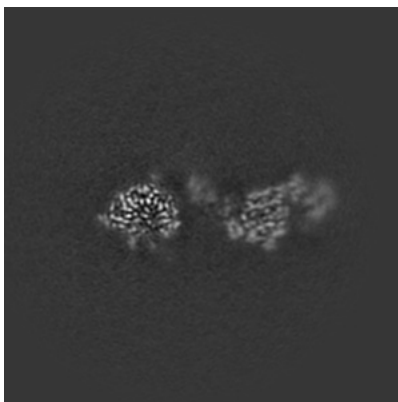
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

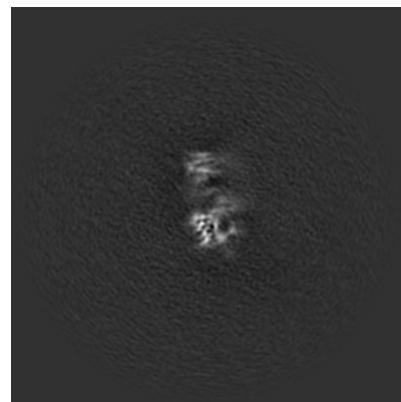
6.2.1 Primary map



X Index: 150

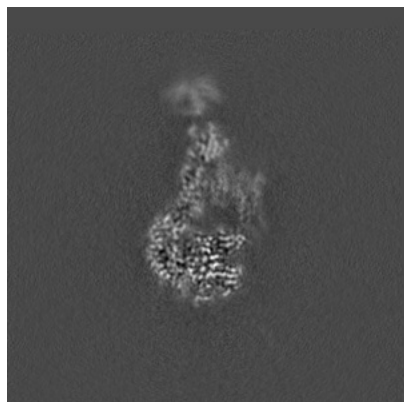


Y Index: 150

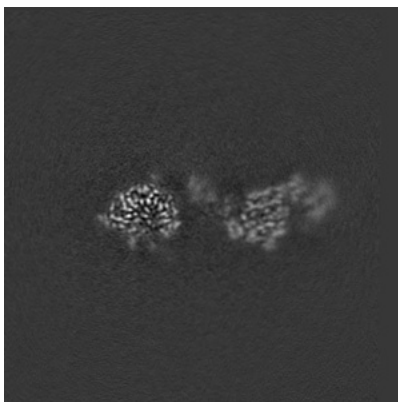


Z Index: 150

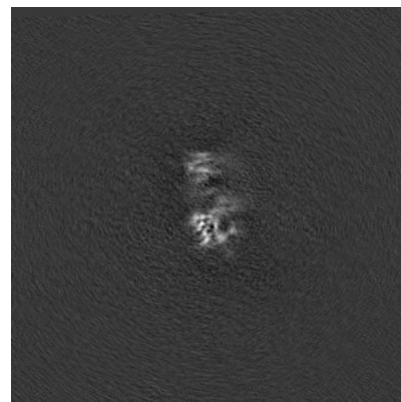
6.2.2 Raw map



X Index: 150



Y Index: 150

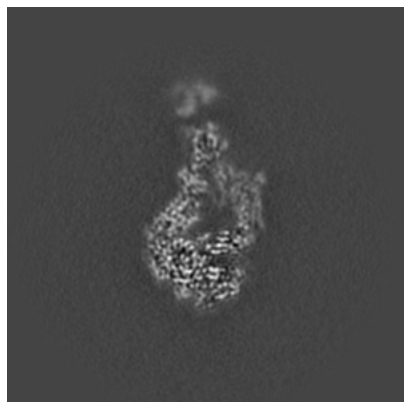


Z Index: 150

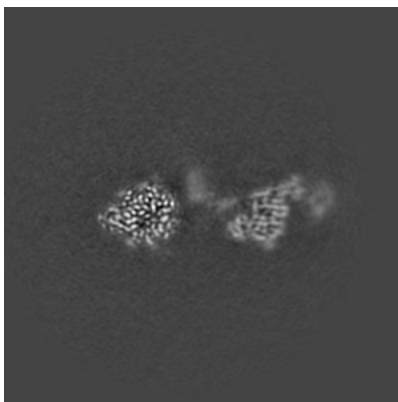
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

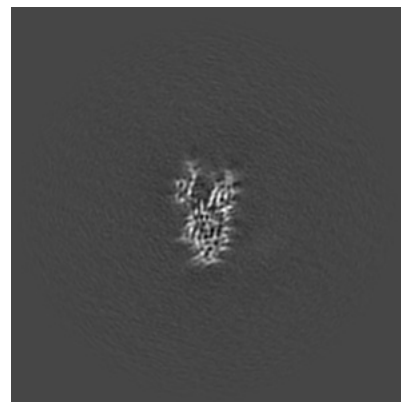
6.3.1 Primary map



X Index: 145



Y Index: 153

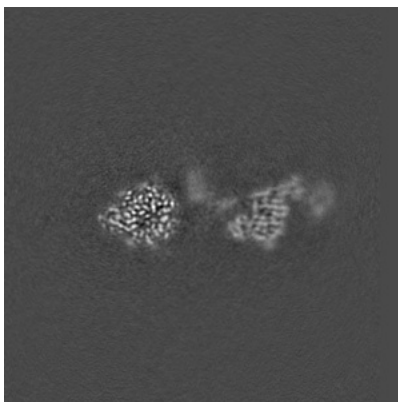


Z Index: 106

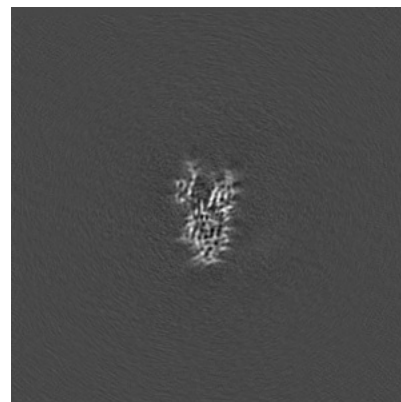
6.3.2 Raw map



X Index: 146



Y Index: 153

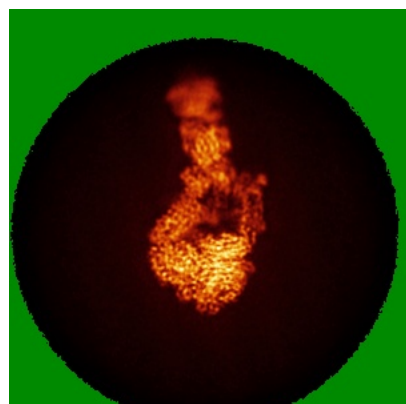


Z Index: 106

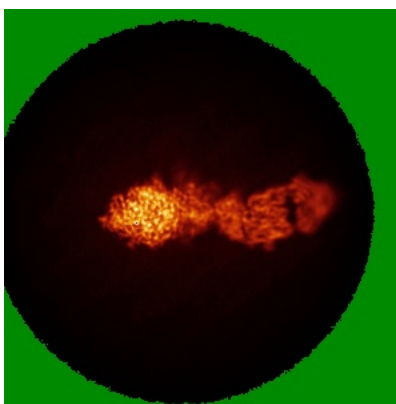
The images above show the largest variance slices of the map in three orthogonal directions.

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

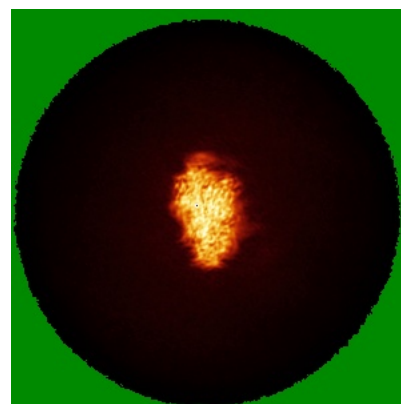
6.4.1 Primary map



X

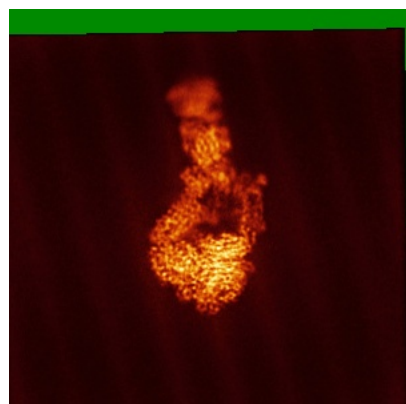


Y

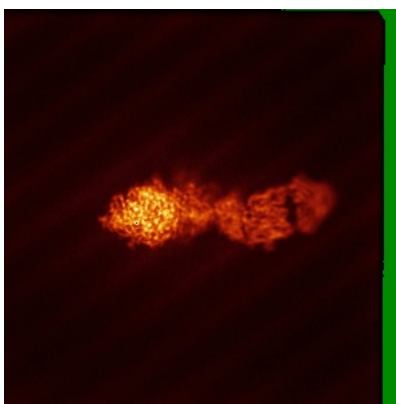


Z

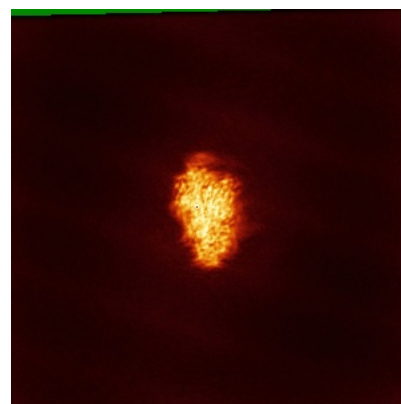
6.4.2 Raw map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.16. 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



X



Y



Z

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.

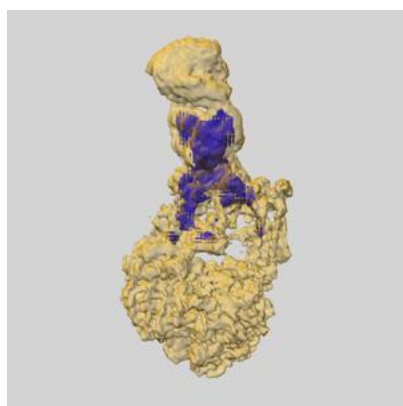
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

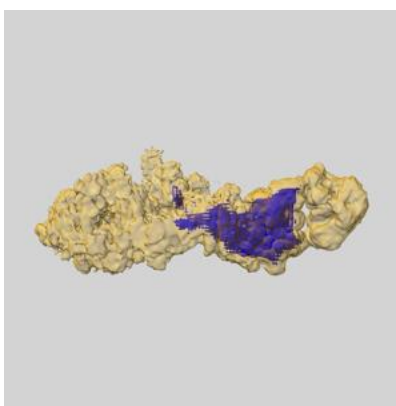
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

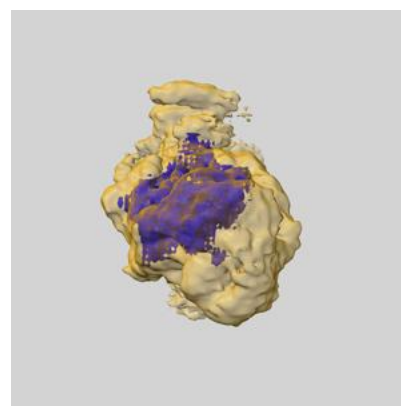
6.6.1 emd_55800_msk_1.map [i](#)



X



Y

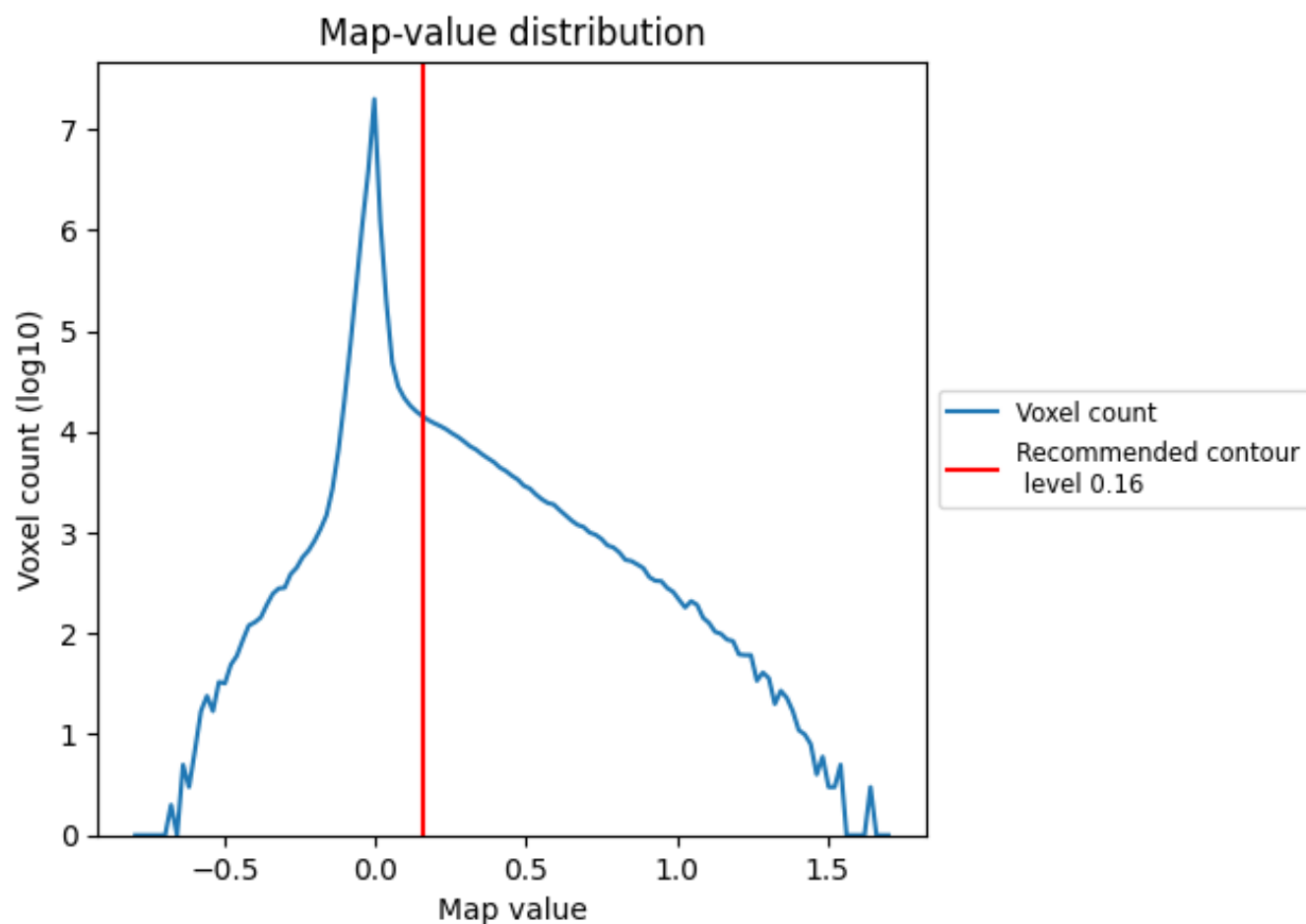


Z

7 Map analysis [i](#)

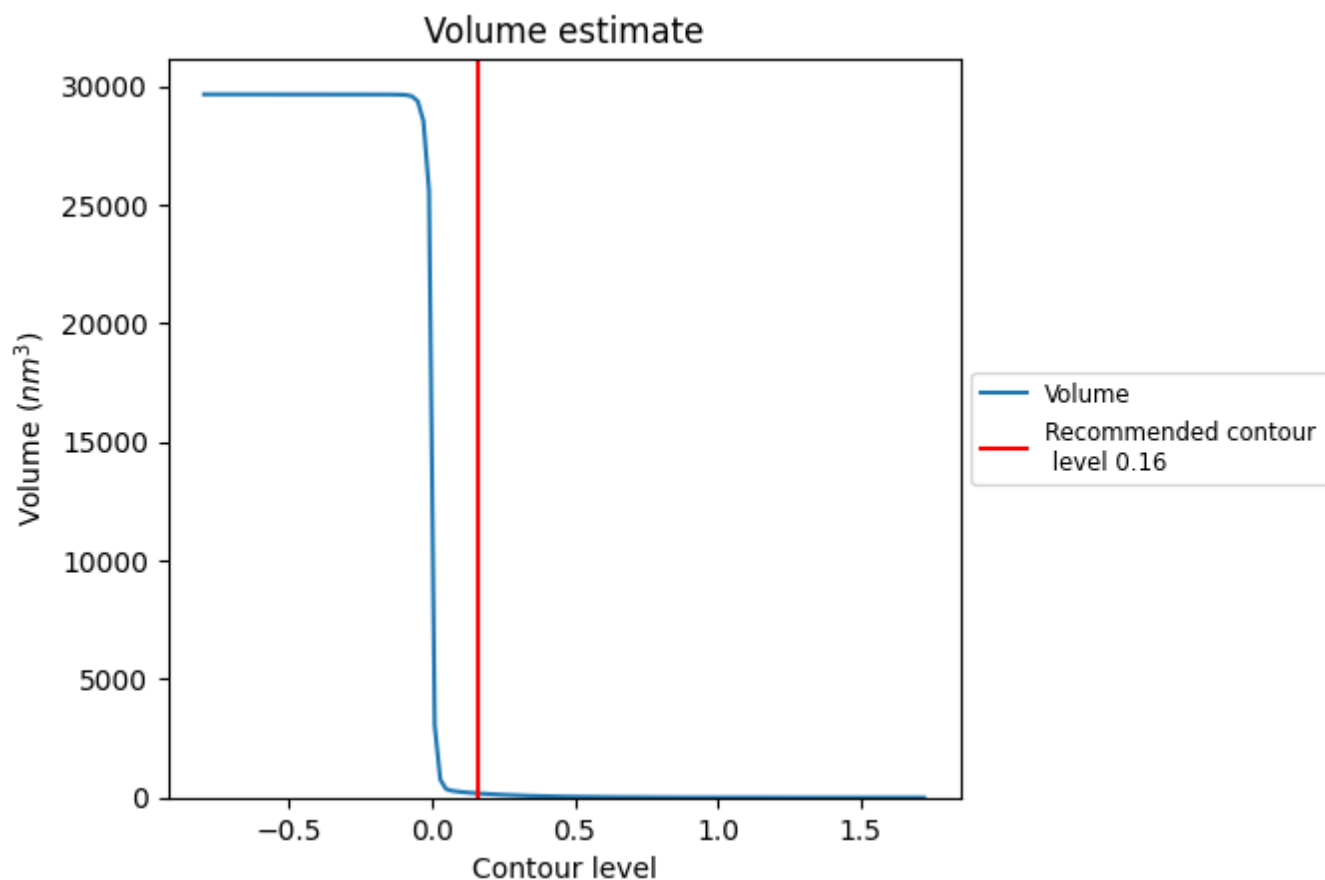
This section contains the results of statistical analysis of the map.

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.

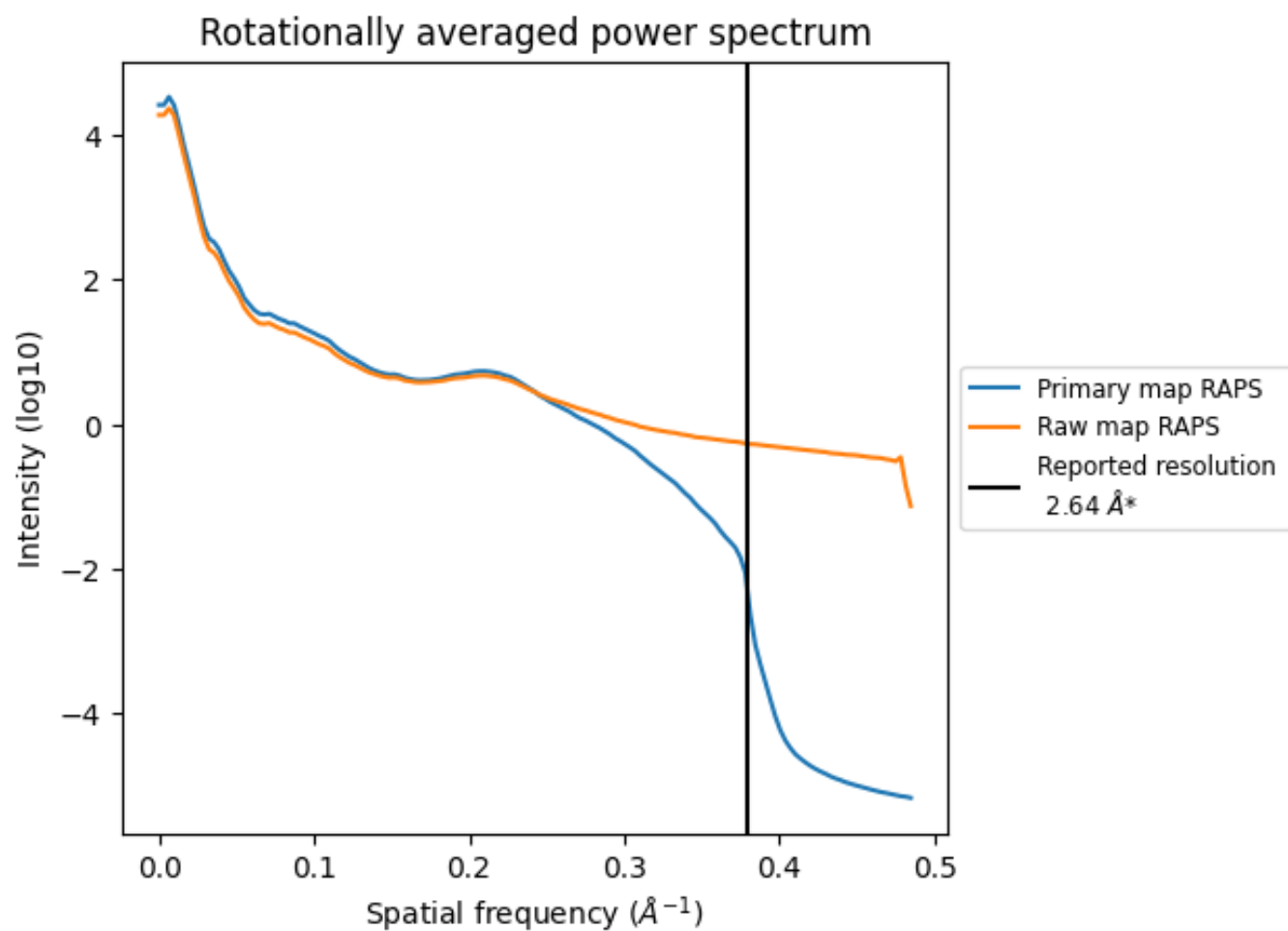
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 177 nm^3 ; this corresponds to an approximate mass of 160 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 ⓘ

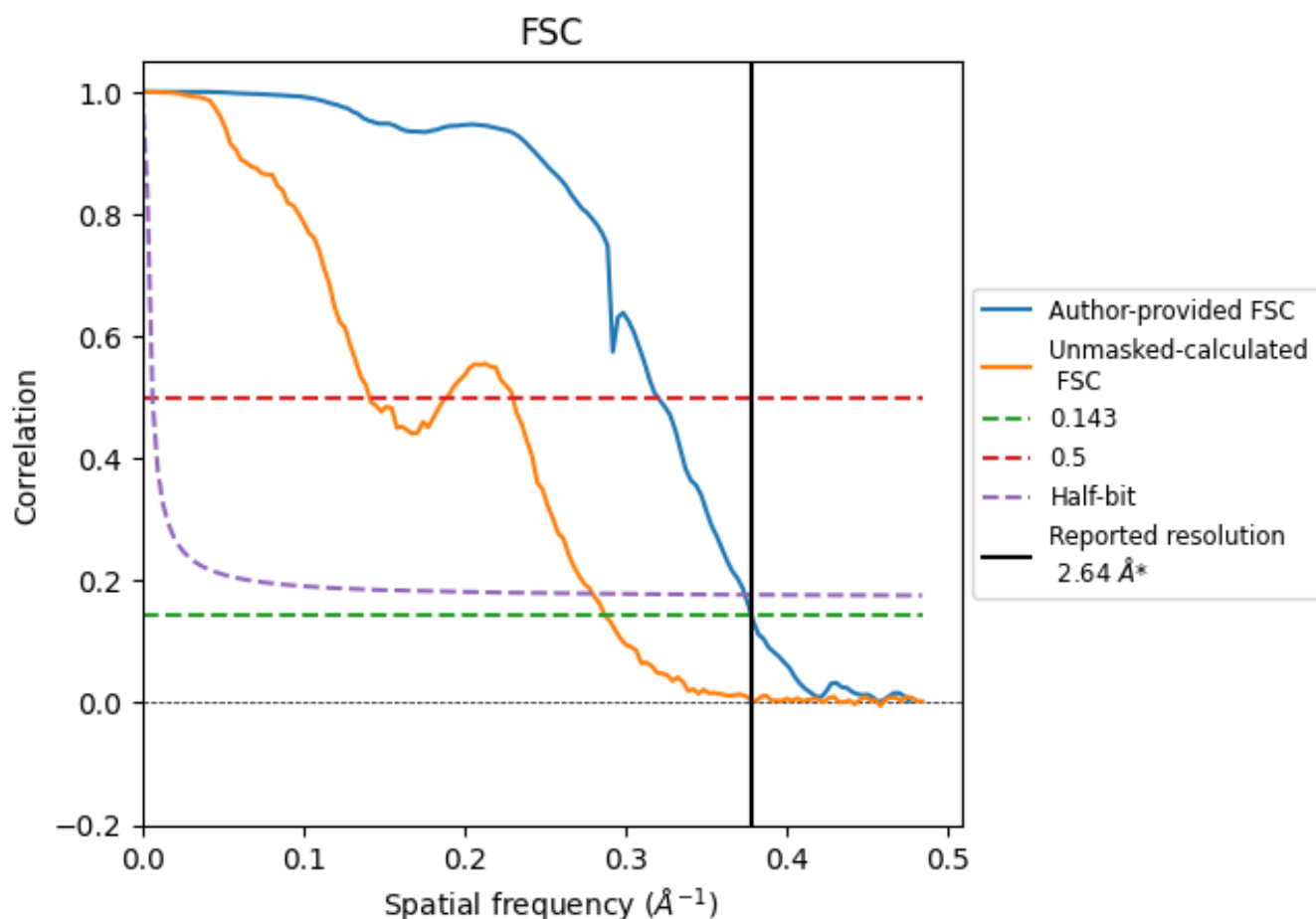


*Reported resolution corresponds to spatial frequency of 0.379 Å⁻¹

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 0.379 Å⁻¹

8.2 Resolution estimates [i](#)

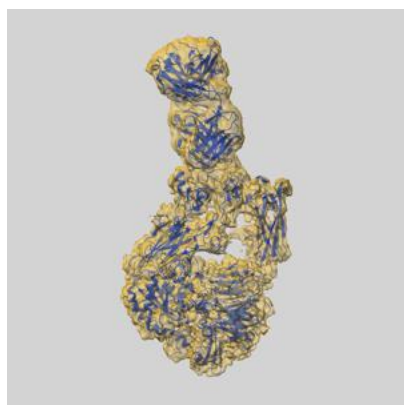
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.64	-	-
Author-provided FSC curve	2.64	3.12	2.67
Unmasked-calculated*	3.48	7.08	3.57

*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 3.48 differs from the reported value 2.64 by more than 10 %

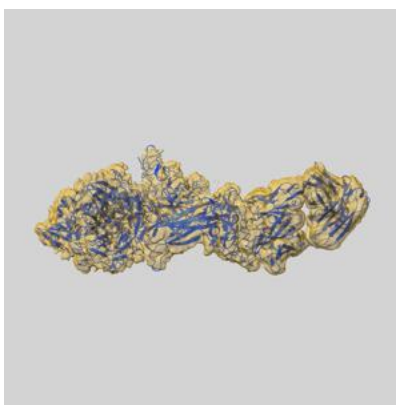
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55800 and PDB model 9TD2. Per-residue inclusion information can be found in section [3](#) on page [9](#).

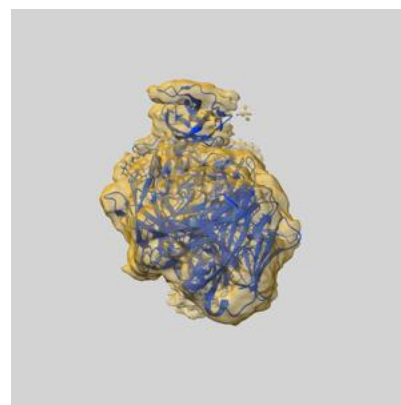
9.1 Map-model overlay [i](#)



X



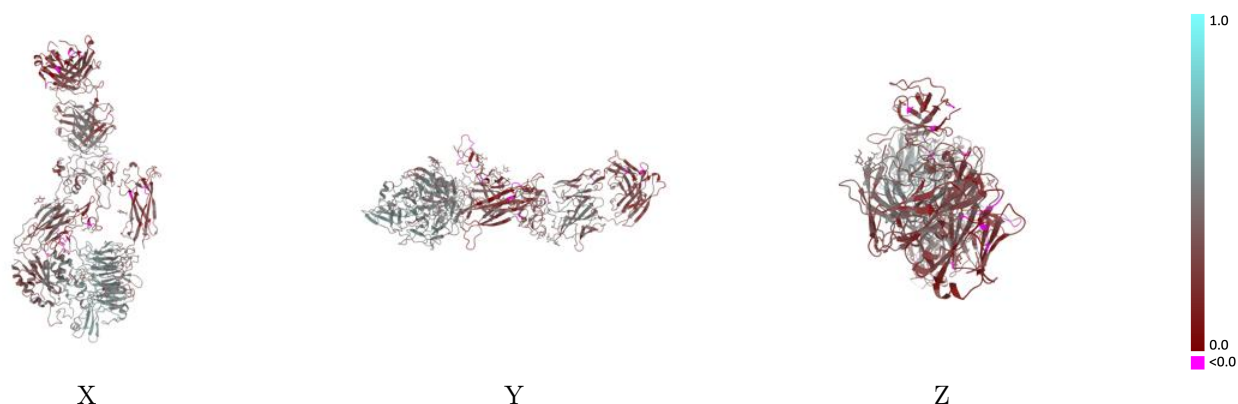
Y



Z

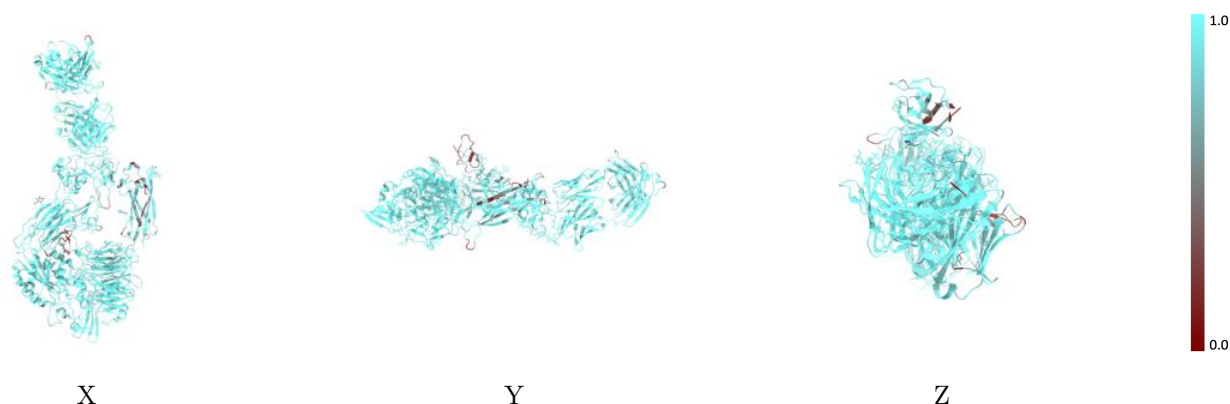
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



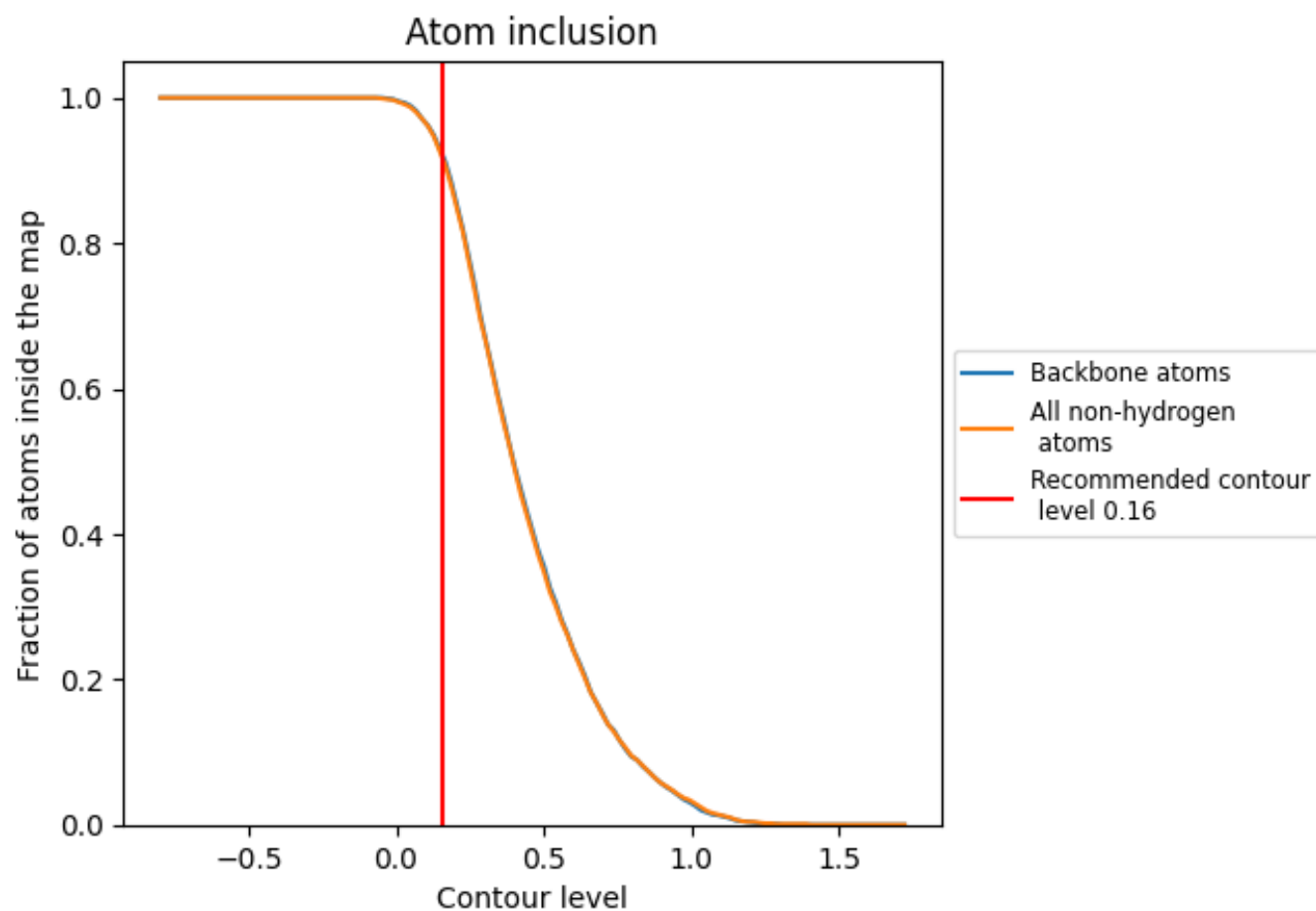
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9140	0.3720
A	0.9170	0.4300
B	0.8960	0.3540
E	0.7500	0.2980
F	0.8600	0.3700
G	0.9740	0.4100
H	0.9530	0.3230
I	0.8210	0.3320
J	0.9230	0.4040
L	0.9290	0.3120

1.0

0.0

<0.0