Full wwPDB EM Validation Report ⓘ

Jun 12, 2025 – 05:40 PM EDT

PDB ID	:	9EF2 / pdb_00009ef2
EMDB ID	:	EMD-47968
Title	:	Cryo-EM structure of alpha5beta1 integrin in complex with NeoNectin candidate 2, open conformation
Authors	:	Werther, R.; Nguyen, A.; Estrada Alamo, K.A.; Wang, X.; Campbell, M.G.
Deposited on	:	2024-11-19
Resolution	:	3.36 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:

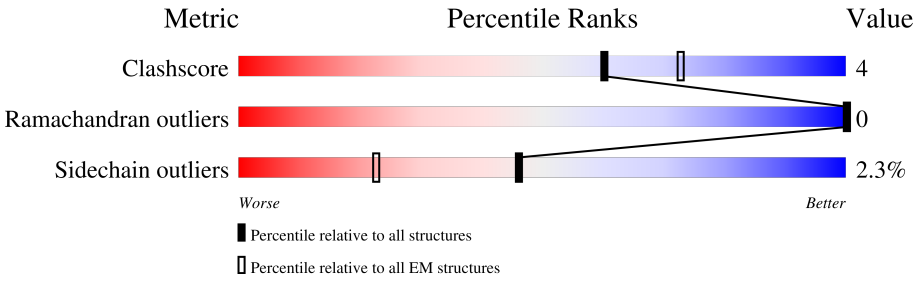
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.36 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=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	1005	39% 5% 56%
2	B	738	29% · 67%
3	C	99	49% 10% · 38%
4	D	2	50% 50%
4	E	2	50% 50%
4	F	2	100%
5	G	6	17% 83%
6	H	3	33% 67%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5756 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 Integrin alpha-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	443	Total	C	N	O	S	0	0
			3227	2069	534	616	8		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	956	THR	-	expression tag	UNP P08648
A	957	GLY	-	expression tag	UNP P08648
A	958	GLY	-	expression tag	UNP P08648
A	959	LEU	-	expression tag	UNP P08648
A	960	GLU	-	expression tag	UNP P08648
A	961	VAL	-	expression tag	UNP P08648
A	962	LEU	-	expression tag	UNP P08648
A	963	PHE	-	expression tag	UNP P08648
A	964	GLN	-	expression tag	UNP P08648

- Molecule 2 is a protein called Integrin beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	240	Total	C	N	O	S	0	0
			1861	1182	307	360	12		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	709	ASP	-	expression tag	UNP P05556
B	710	THR	-	expression tag	UNP P05556
B	711	SER	-	expression tag	UNP P05556
B	712	GLY	-	expression tag	UNP P05556
B	713	LEU	-	expression tag	UNP P05556
B	714	GLU	-	expression tag	UNP P05556
B	715	VAL	-	expression tag	UNP P05556
B	716	LEU	-	expression tag	UNP P05556

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Chain	Residue	Modelled	Actual	Comment	Reference
B	717	PHE	-	expression tag	UNP P05556
B	718	GLN	-	expression tag	UNP P05556

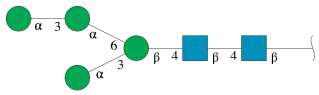
- Molecule 3 is a protein called NeoNectin candidate 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	61	Total	C	N	O	0	0
			426	273	78	75		

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

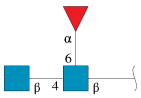
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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	G	6	Total	C	N	O	0	0
			72	40	2	30		

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

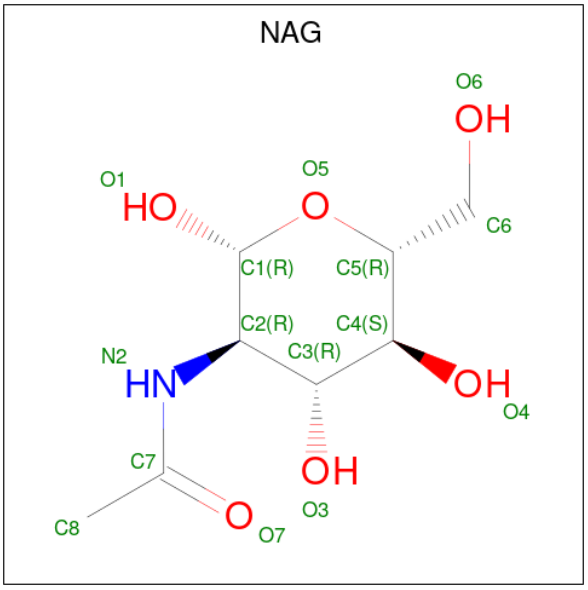


Mol	Chain	Residues	Atoms				AltConf	Trace
6	H	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 9 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

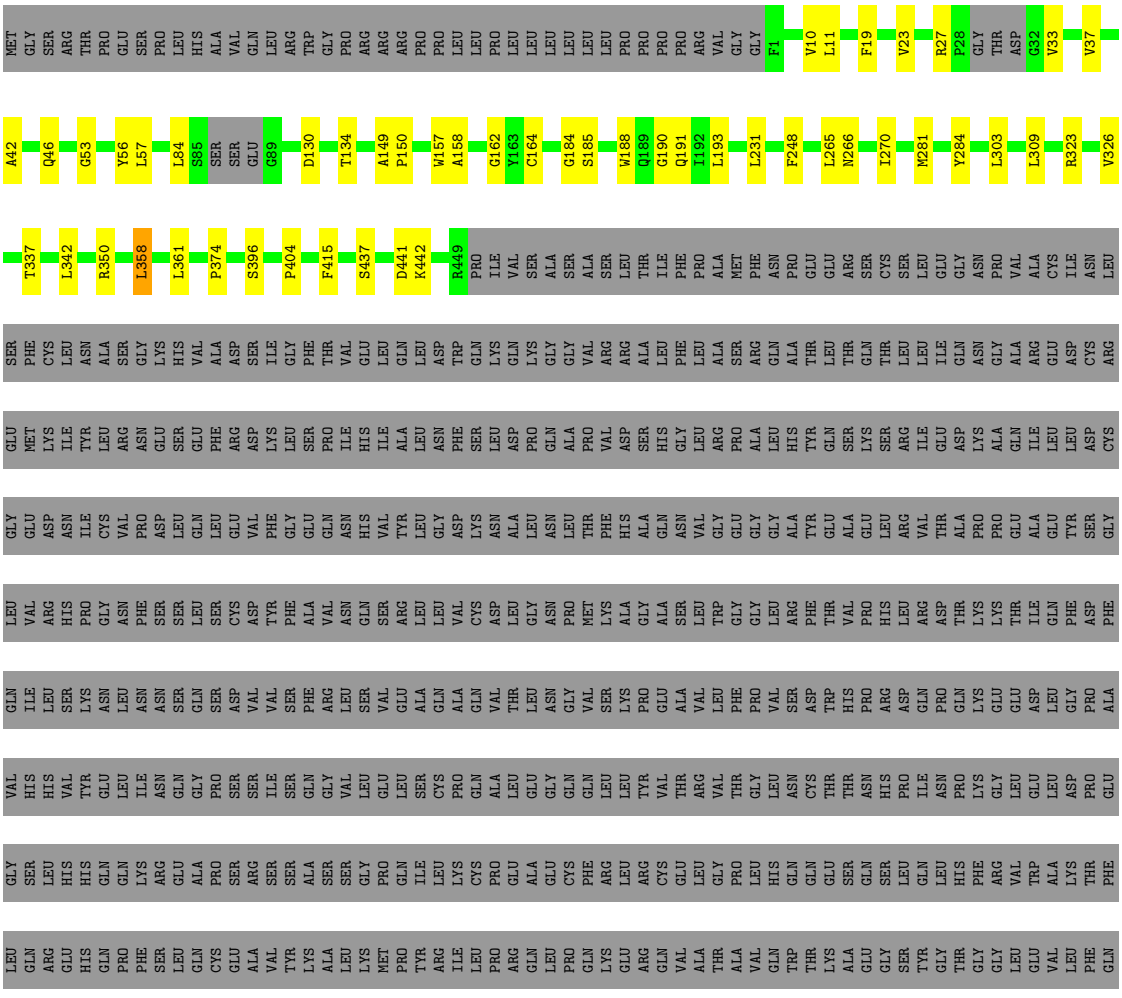
Mol	Chain	Residues	Atoms		AltConf
			Total	Mn	
9	B	3	3	3	0

3 Residue-property plots (i)

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: Integrin alpha-5

Chain A:

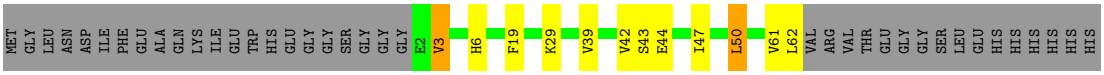


- Molecule 2: Integrin beta-1

Chain B:

• Molecule 3: NeoNectin candidate 2

Chain C:



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

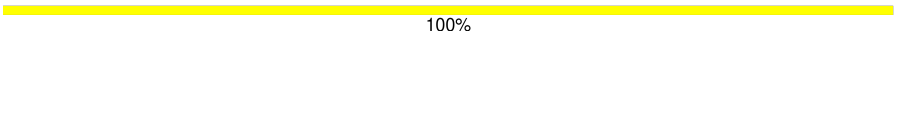
Chain D:

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

Chain E:

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

Chain F:



• Molecule 5: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63256	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	36000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.517	Depositor
Minimum map value	-0.677	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	394.944, 394.944, 394.944	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.122, 1.122, 1.122	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, MN, CA, FUC, 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	0.18	0/3317	0.35	1/4533 (0.0%)
2	B	0.19	0/1899	0.35	0/2575
3	C	0.23	0/431	0.50	0/588
All	All	0.18	0/5647	0.37	1/7696 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	266	ASN	CA-CB-CG	7.21	119.81	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	3227	0	2992	26	0
2	B	1861	0	1815	14	0
3	C	426	0	407	9	0
4	D	28	0	25	0	0
4	E	28	0	25	0	0
4	F	28	0	25	0	0
5	G	72	0	61	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	38	0	34	0	0
7	A	3	0	0	0	0
8	B	42	0	39	0	0
9	B	3	0	0	0	0
All	All	5756	0	5423	48	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 (48) 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:42:VAL:HG23	3:C:43:SER:H	1.53	0.73
1:A:150:PRO:HB2	1:A:193:LEU:HD22	1.76	0.66
1:A:265:LEU:HD13	1:A:270:ILE:HG23	1.75	0.66
1:A:23:VAL:HG12	1:A:37:VAL:HG12	1.81	0.63
2:B:164:PHE:CE2	2:B:202:VAL:HG11	2.35	0.61
1:A:437:SER:HB3	1:A:442:LYS:HB2	1.84	0.59
2:B:258:THR:HG23	2:B:317:VAL:HG23	1.85	0.58
3:C:3:VAL:HB	3:C:47:ILE:HD11	1.86	0.58
2:B:232:PHE:HB3	2:B:297:PRO:HG2	1.87	0.57
3:C:44:GLU:O	3:C:47:ILE:HG22	2.08	0.53
1:A:134:THR:HG22	1:A:149:ALA:HB2	1.92	0.51
1:A:358:LEU:HD23	1:A:361:LEU:HD22	1.92	0.51
2:B:145:LEU:HD13	2:B:344:SER:HB2	1.94	0.50
2:B:139:LEU:HG	2:B:143:LYS:HE3	1.92	0.50
3:C:42:VAL:HG23	3:C:43:SER:N	2.23	0.49
2:B:229:GLU:HG2	2:B:260:ALA:HB3	1.95	0.48
1:A:248:PHE:HB2	1:A:265:LEU:HD12	1.95	0.48
1:A:190:GLY:HA3	1:A:231:LEU:HB3	1.95	0.48
1:A:404:PRO:HG3	1:A:415:PHE:CG	2.48	0.48
1:A:27:ARG:HB2	1:A:33:VAL:HG23	1.94	0.48
2:B:123:ILE:HG22	2:B:157:THR:HG21	1.95	0.48
1:A:337:THR:HG23	1:A:337:THR:O	2.15	0.46
3:C:50:LEU:HD13	3:C:50:LEU:HA	1.83	0.46
1:A:19:PHE:CZ	1:A:37:VAL:HG21	2.51	0.45
1:A:46:GLN:H	1:A:46:GLN:HG2	1.63	0.45
3:C:19:PHE:CE2	3:C:50:LEU:HD12	2.52	0.45
2:B:122:PRO:HG2	2:B:250:VAL:HG23	1.98	0.44
1:A:185:SER:OG	1:A:191:GLN:HB2	2.18	0.44
1:A:281:MET:HE1	2:B:324:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:PHE:HB3	1:A:441:ASP:HB3	2.00	0.43
1:A:342:LEU:HD11	1:A:396:SER:HA	2.01	0.43
1:A:303:LEU:HG	1:A:326:VAL:HG22	2.00	0.43
3:C:29:LYS:O	3:C:39:VAL:HG13	2.19	0.43
1:A:130:ASP:OD2	1:A:162:GLY:CA	2.68	0.42
1:A:130:ASP:O	1:A:130:ASP:OD1	2.38	0.42
1:A:157:TRP:CG	1:A:158:ALA:H	2.37	0.42
2:B:275:LEU:HD12	2:B:275:LEU:H	1.84	0.42
3:C:6:HIS:CD2	3:C:62:LEU:HD23	2.54	0.42
1:A:184:GLY:HA2	1:A:188:TRP:HA	2.02	0.42
2:B:302:LEU:HD23	2:B:302:LEU:HA	1.89	0.42
1:A:37:VAL:HG23	1:A:56:TYR:HB2	2.02	0.41
1:A:350:ARG:HB2	1:A:374:PRO:HD2	2.02	0.41
2:B:260:ALA:HA	2:B:321:PHE:CE2	2.55	0.41
2:B:326:LYS:O	2:B:329:LYS:HB3	2.21	0.41
1:A:42:ALA:HB3	1:A:53:GLY:HA2	2.03	0.41
2:B:125:LEU:HB3	2:B:162:ILE:HG22	2.02	0.41
3:C:19:PHE:CZ	3:C:50:LEU:HD12	2.56	0.41
1:A:309:LEU:HD22	1:A:323:ARG:HB2	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	437/1005 (44%)	418 (96%)	19 (4%)	0	100	100
2	B	238/738 (32%)	228 (96%)	10 (4%)	0	100	100
3	C	59/99 (60%)	53 (90%)	6 (10%)	0	100	100
All	All	734/1842 (40%)	699 (95%)	35 (5%)	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	319/836 (38%)	312 (98%)	7 (2%)	47 68
2	B	209/656 (32%)	206 (99%)	3 (1%)	62 78
3	C	39/83 (47%)	36 (92%)	3 (8%)	10 34
All	All	567/1575 (36%)	554 (98%)	13 (2%)	46 68

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	11	LEU
1	A	57	LEU
1	A	84	LEU
1	A	164	CYS
1	A	284	TYR
1	A	358	LEU
2	B	150	MET
2	B	183	LEU
2	B	324	VAL
3	C	3	VAL
3	C	50	LEU
3	C	61	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	GLN
1	A	380	GLN
1	A	381	GLN
2	B	201	ASN
2	B	237	GLN
3	C	6	HIS

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

15 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	0.70	0	17,19,21	0.98	1 (5%)
4	NAG	D	2	4	14,14,15	0.71	0	17,19,21	0.84	0
4	NAG	E	1	1,4	14,14,15	0.75	0	17,19,21	0.81	0
4	NAG	E	2	4	14,14,15	0.69	0	17,19,21	0.88	1 (5%)
4	NAG	F	1	1,4	14,14,15	0.50	0	17,19,21	1.13	1 (5%)
4	NAG	F	2	4	14,14,15	0.41	0	17,19,21	0.99	2 (11%)
5	NAG	G	1	1,5	14,14,15	0.78	0	17,19,21	0.84	0
5	NAG	G	2	5	14,14,15	0.77	0	17,19,21	0.98	2 (11%)
5	BMA	G	3	5	11,11,12	0.84	0	15,15,17	1.88	3 (20%)
5	MAN	G	4	5	11,11,12	0.79	0	15,15,17	1.18	1 (6%)
5	MAN	G	5	5	11,11,12	0.71	0	15,15,17	1.11	1 (6%)
5	MAN	G	6	5	11,11,12	0.72	0	15,15,17	1.07	1 (6%)
6	NAG	H	1	1,6	14,14,15	0.75	0	17,19,21	1.31	2 (11%)
6	NAG	H	2	6	14,14,15	0.78	0	17,19,21	0.93	1 (5%)
6	FUC	H	3	6	10,10,11	0.79	0	14,14,16	1.03	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
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
5	NAG	G	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	2/2/19/22	0/1/1/1
5	MAN	G	4	5	-	1/2/19/22	0/1/1/1
5	MAN	G	5	5	-	2/2/19/22	1/1/1/1
5	MAN	G	6	5	-	2/2/19/22	1/1/1/1
6	NAG	H	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	H	2	6	-	0/6/23/26	0/1/1/1
6	FUC	H	3	6	-	-	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	3	BMA	C1-O5-C5	5.37	119.39	112.19
4	F	1	NAG	C1-O5-C5	3.89	117.40	112.19
5	G	5	MAN	C1-O5-C5	3.14	116.40	112.19
5	G	4	MAN	C1-O5-C5	2.98	116.18	112.19
5	G	6	MAN	C1-O5-C5	2.95	116.13	112.19
6	H	1	NAG	O4-C4-C3	-2.91	103.51	110.38
6	H	2	NAG	O5-C1-C2	-2.52	107.40	111.29
4	E	2	NAG	O5-C1-C2	-2.42	107.55	111.29
6	H	1	NAG	O5-C1-C2	-2.37	107.62	111.29
5	G	2	NAG	O4-C4-C3	-2.21	105.17	110.38
5	G	2	NAG	O5-C1-C2	-2.18	107.91	111.29
4	F	2	NAG	C2-N2-C7	-2.15	120.02	122.90
5	G	3	BMA	C3-C4-C5	2.08	114.00	110.23
4	F	2	NAG	C4-C3-C2	-2.02	108.05	111.02
4	D	1	NAG	C1-O5-C5	2.02	114.89	112.19
5	G	3	BMA	C2-C3-C4	2.00	114.38	110.86

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
5	G	5	MAN	O5-C5-C6-O6
5	G	5	MAN	C4-C5-C6-O6
5	G	3	BMA	O5-C5-C6-O6
5	G	6	MAN	O5-C5-C6-O6
5	G	3	BMA	C4-C5-C6-O6
5	G	6	MAN	C4-C5-C6-O6
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
6	H	1	NAG	C8-C7-N2-C2
6	H	1	NAG	O7-C7-N2-C2
5	G	1	NAG	O5-C5-C6-O6
5	G	4	MAN	O5-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6

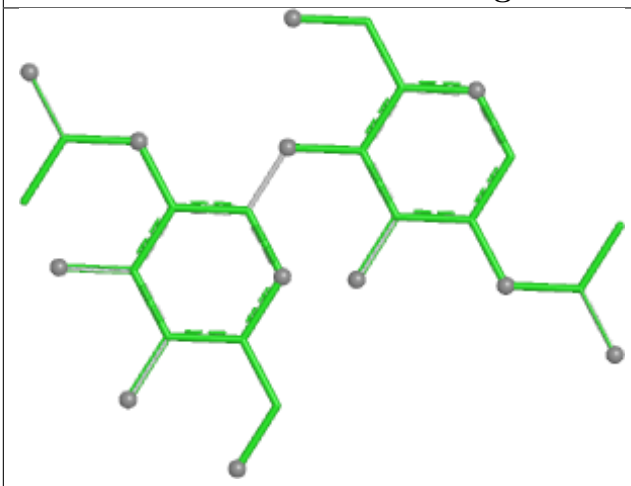
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	6	MAN	C1-C2-C3-C4-C5-O5
5	G	5	MAN	C1-C2-C3-C4-C5-O5

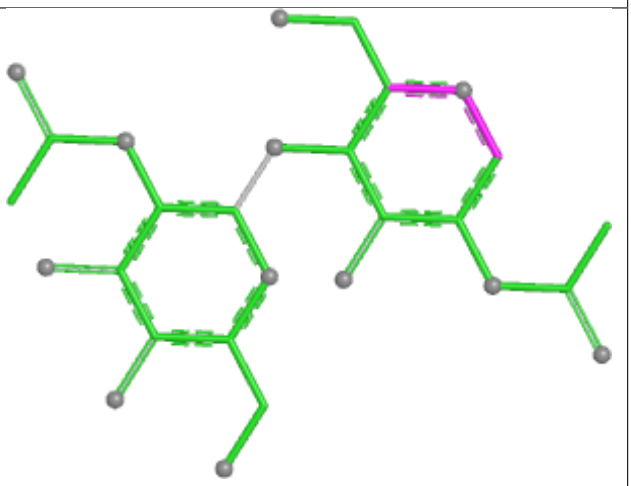
No monomer is involved in short contacts.

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

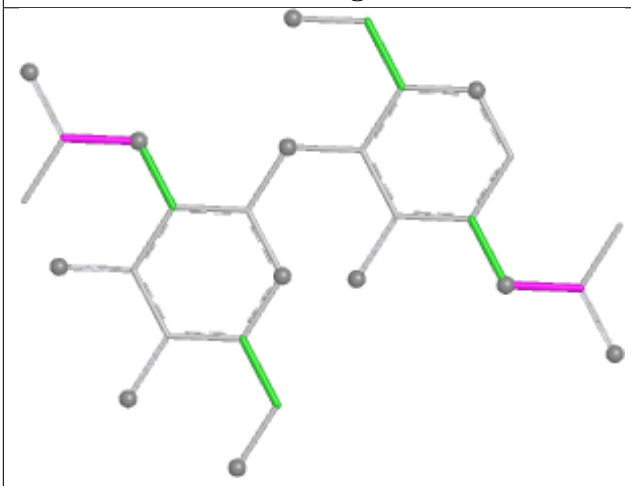
Oligosaccharide Chain D



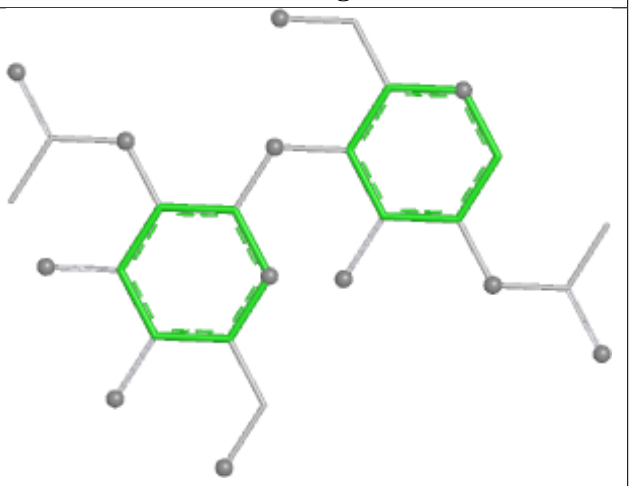
Bond lengths



Bond angles

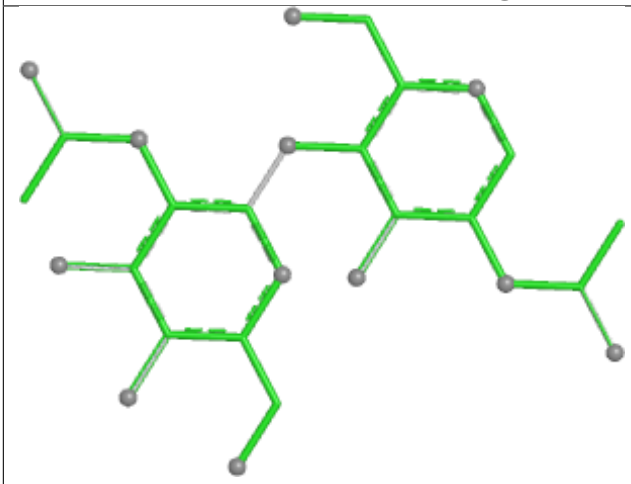


Torsions

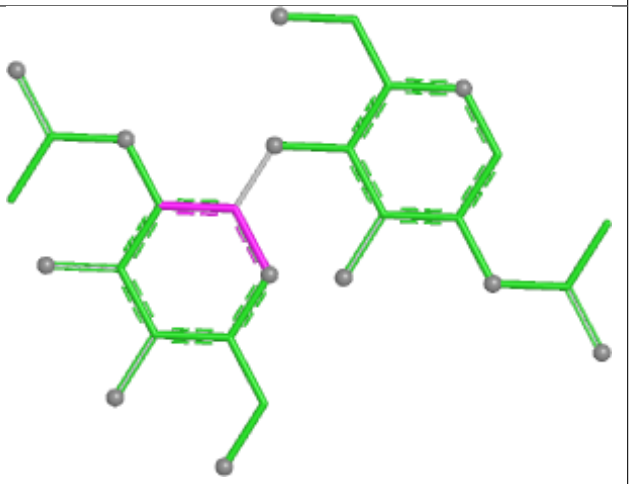


Rings

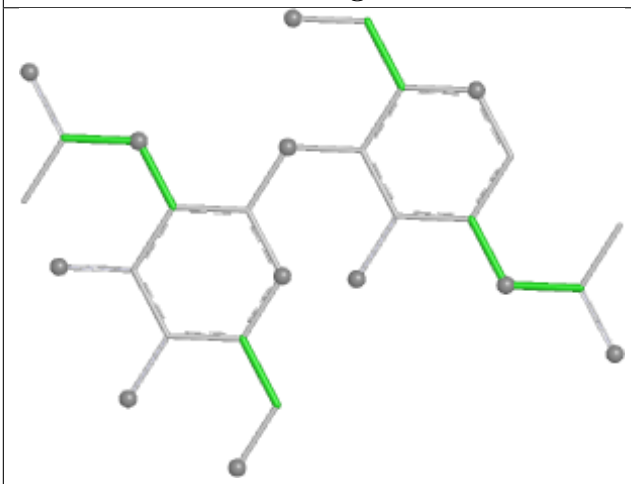
Oligosaccharide Chain E



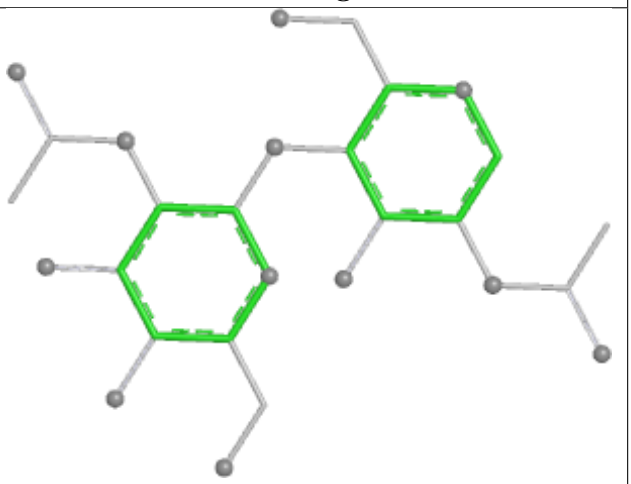
Bond lengths



Bond angles

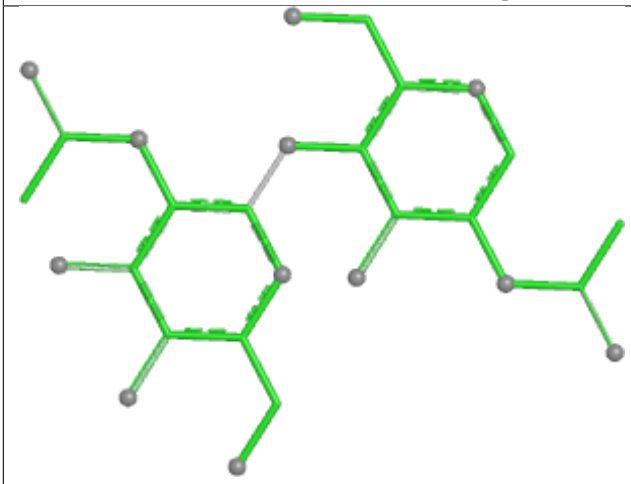


Torsions

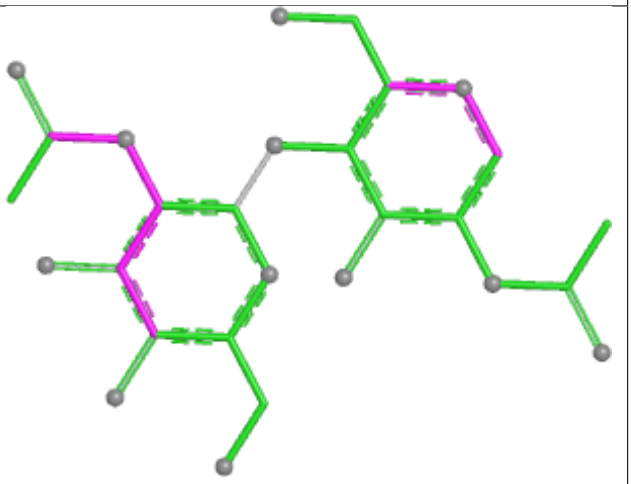


Rings

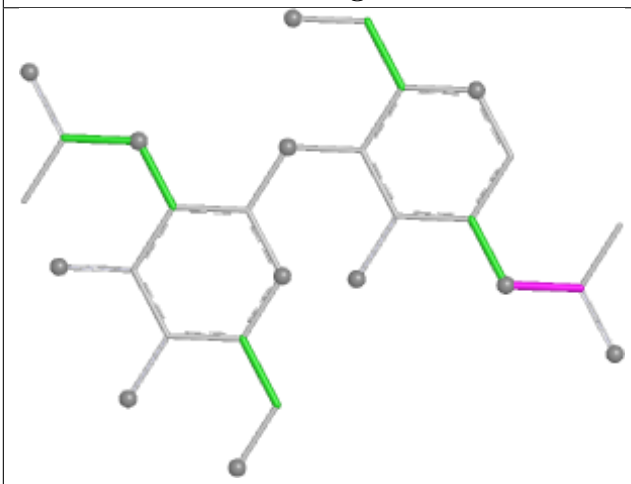
Oligosaccharide Chain F



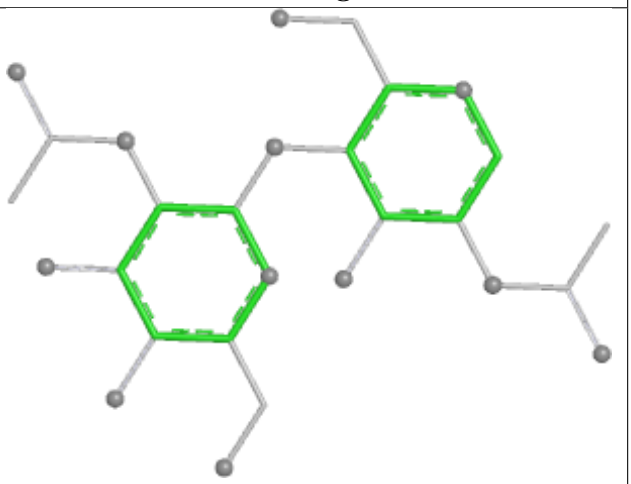
Bond lengths



Bond angles

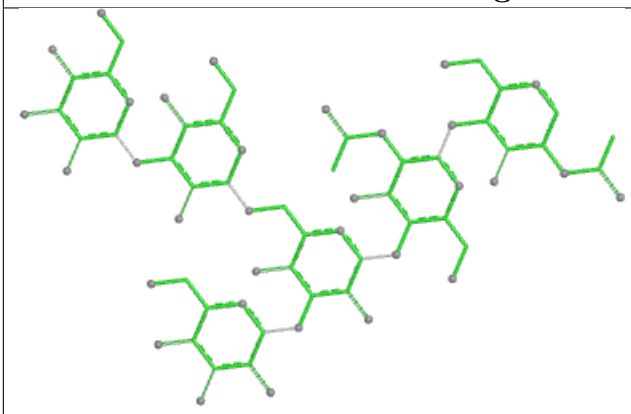


Torsions

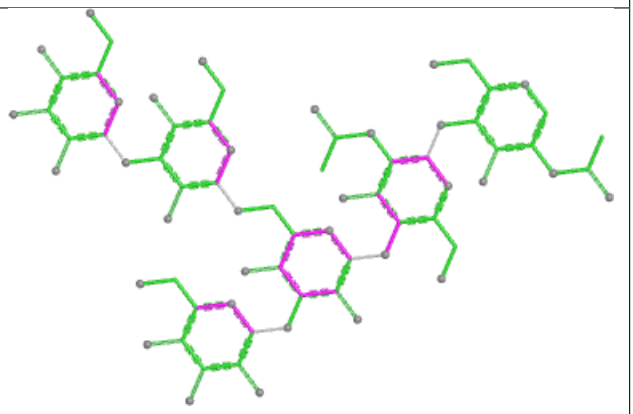


Rings

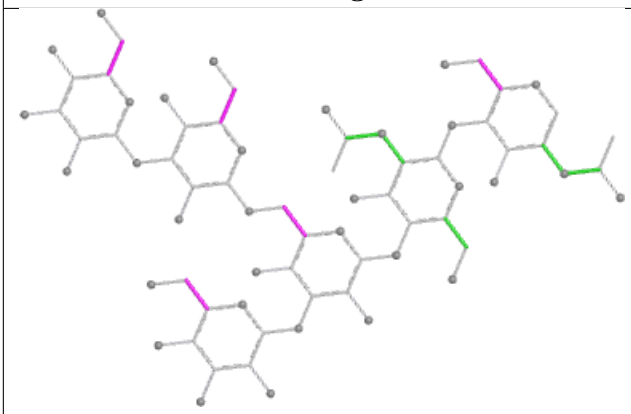
Oligosaccharide Chain G



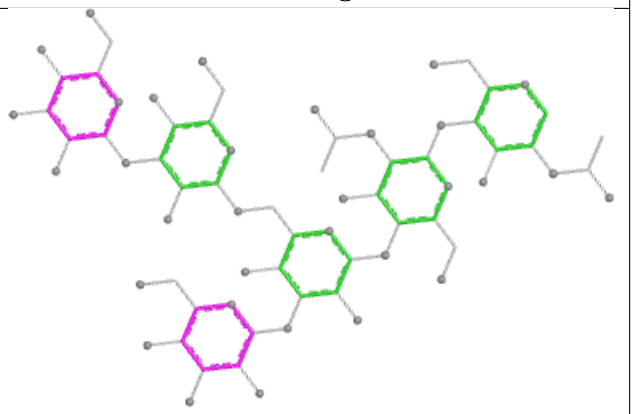
Bond lengths



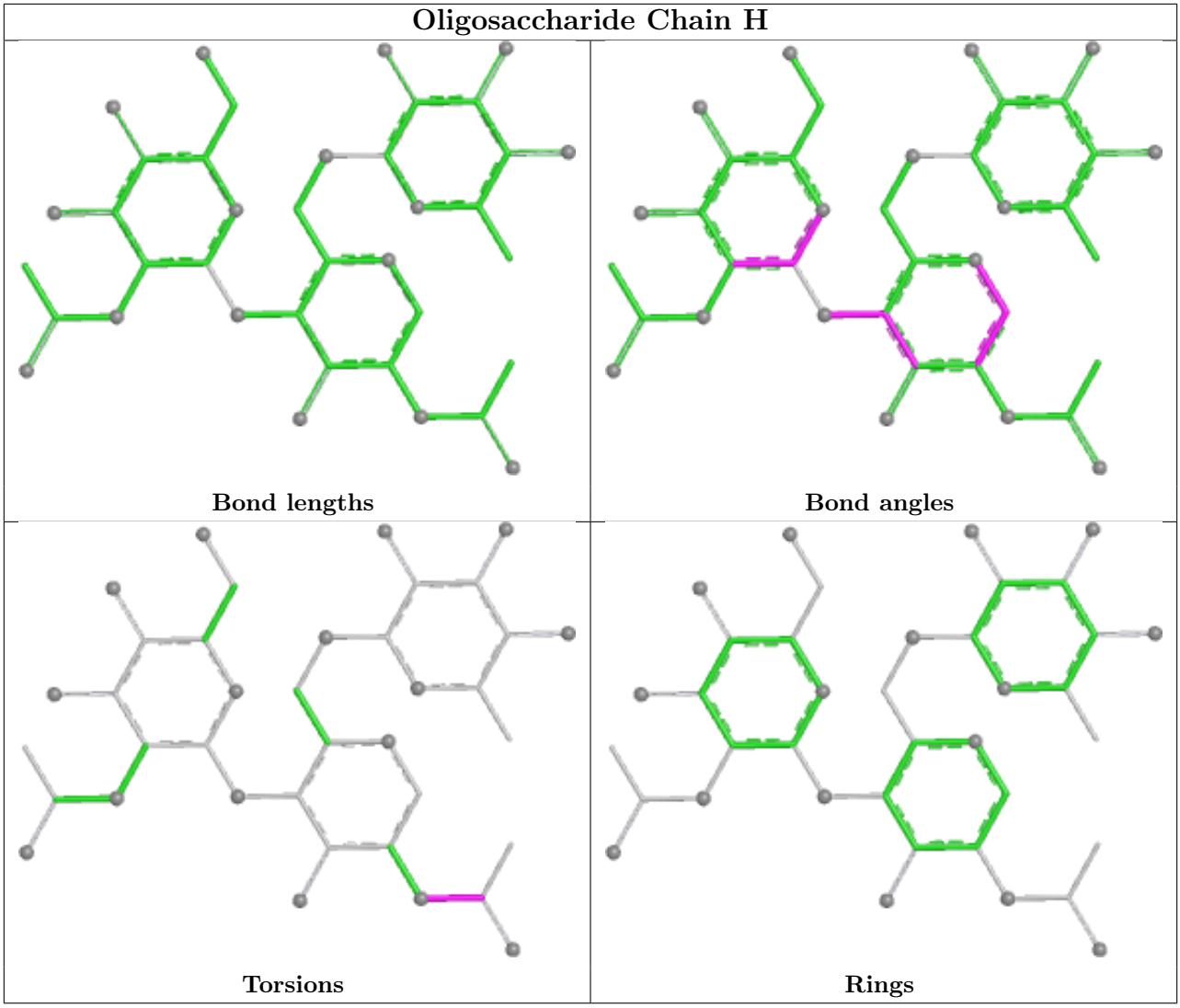
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 6 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	$\#\|Z\| > 2$
8	NAG	B	803	2	14,14,15	0.31	0	17,19,21	0.59	0
8	NAG	B	801	2	14,14,15	0.72	0	17,19,21	0.78	0
8	NAG	B	802	2	14,14,15	0.70	0	17,19,21	0.79	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
8	NAG	B	803	2	-	3/6/23/26	0/1/1/1
8	NAG	B	801	2	-	1/6/23/26	0/1/1/1
8	NAG	B	802	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	803	NAG	C8-C7-N2-C2
8	B	803	NAG	O7-C7-N2-C2
8	B	801	NAG	O5-C5-C6-O6
8	B	803	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.

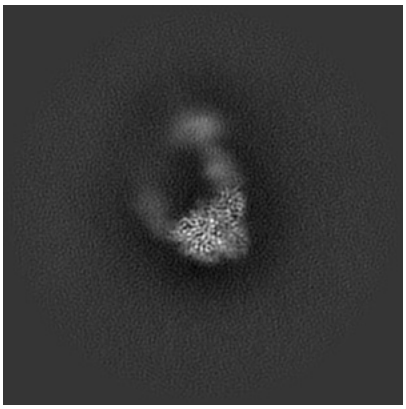
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-47968. These allow visual inspection of the internal detail of the map and identification of artifacts.

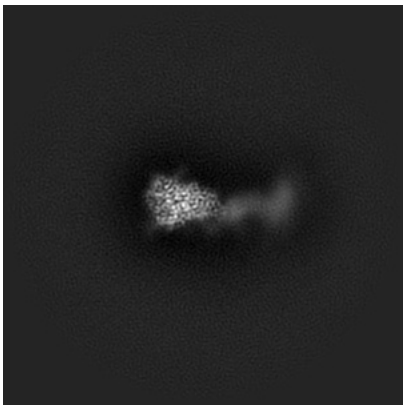
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

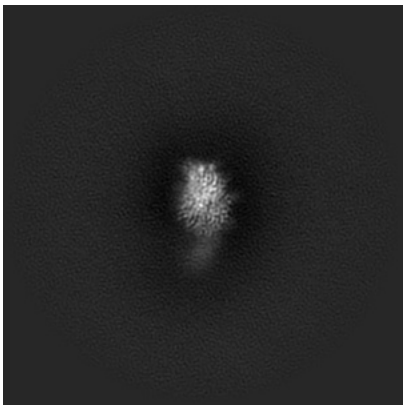
6.1.1 Primary map



X

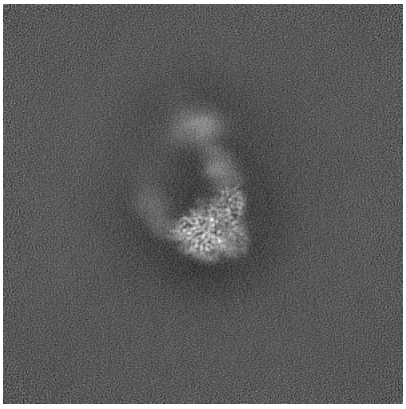


Y

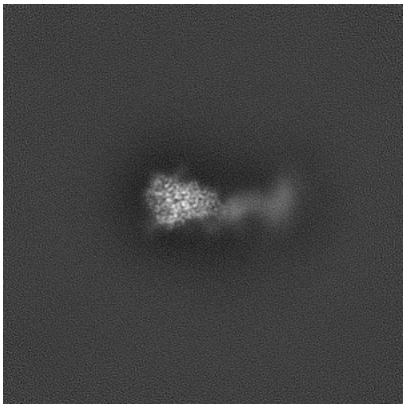


Z

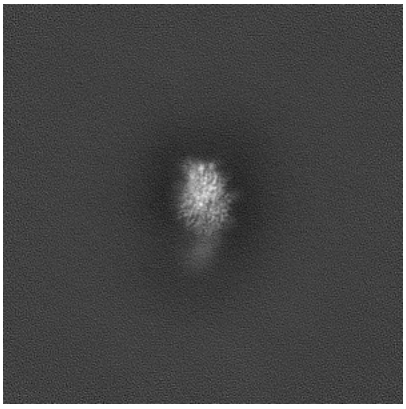
6.1.2 Raw map



X



Y

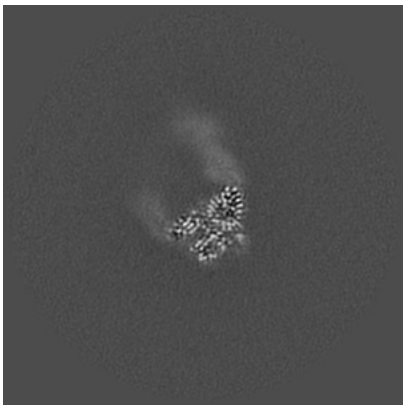


Z

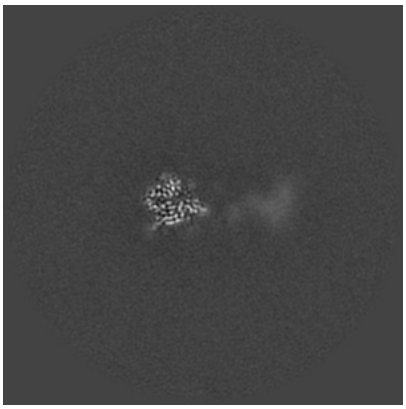
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

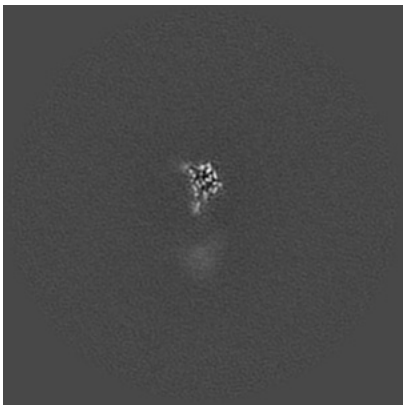
6.2.1 Primary map



X Index: 176

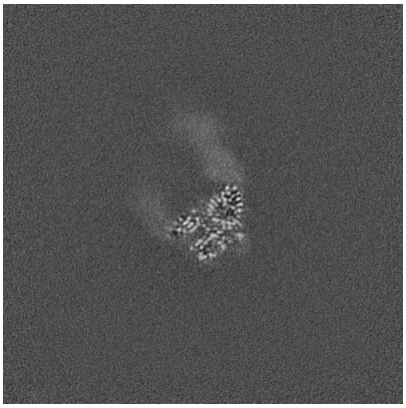


Y Index: 176

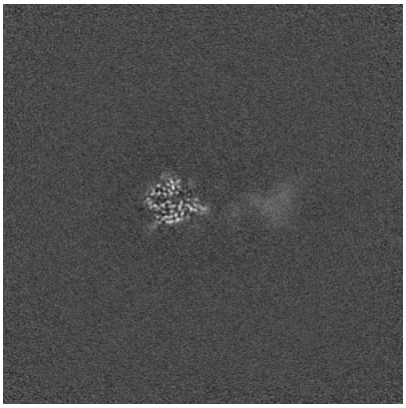


Z Index: 176

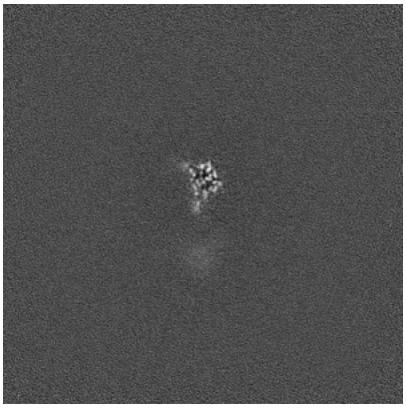
6.2.2 Raw map



X Index: 176



Y Index: 176

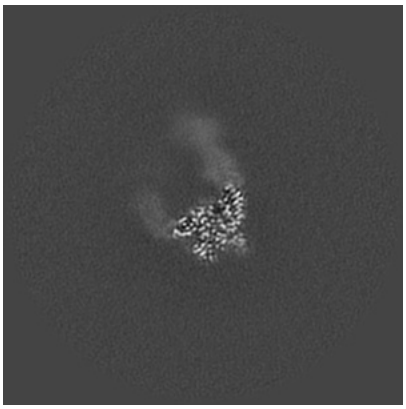


Z Index: 176

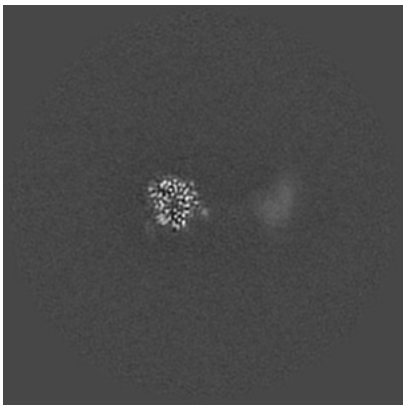
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

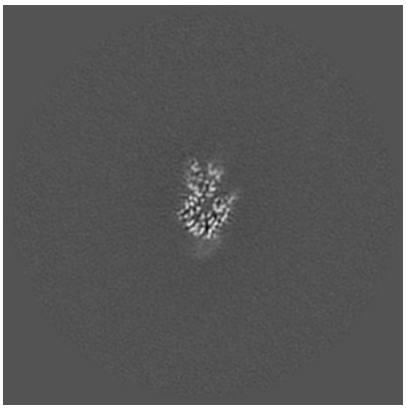
6.3.1 Primary map



X Index: 174

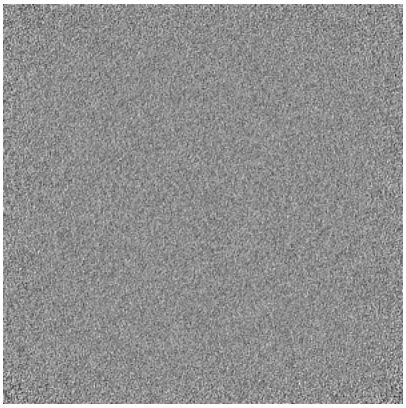


Y Index: 170

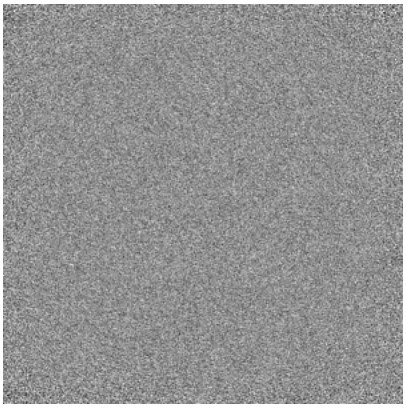


Z Index: 152

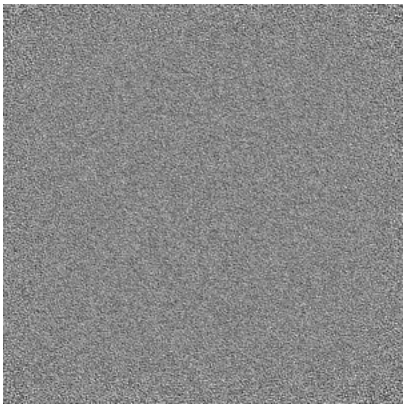
6.3.2 Raw map



X Index: 0



Y Index: 0

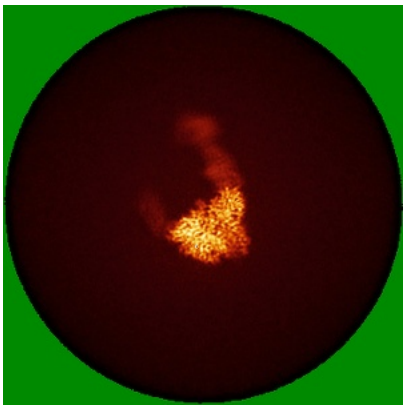


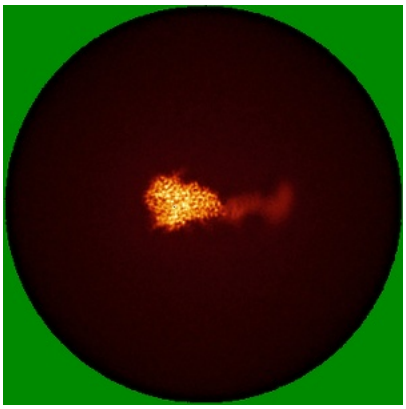
Z Index: 0

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

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

6.4.1 Primary map


X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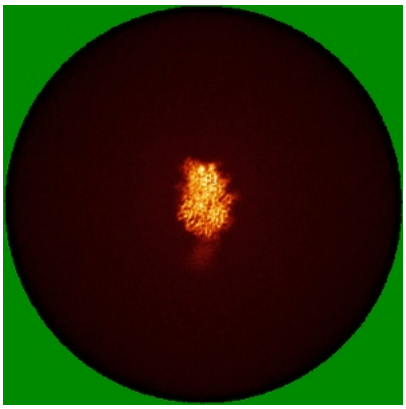
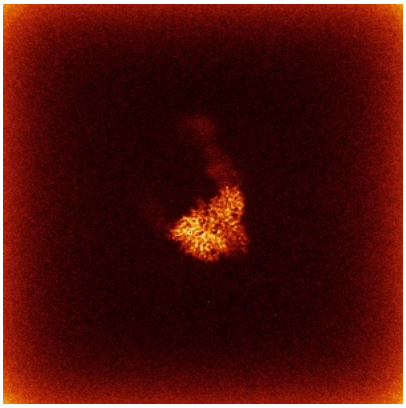
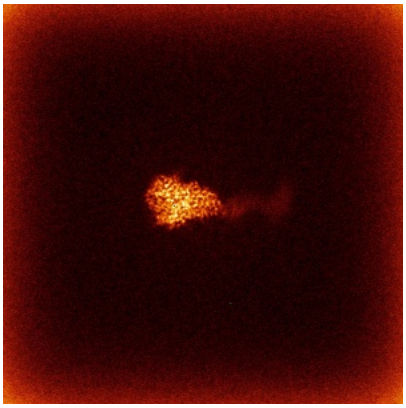
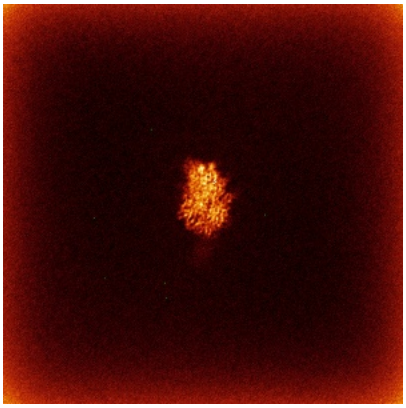

Z

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 0.2. 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.

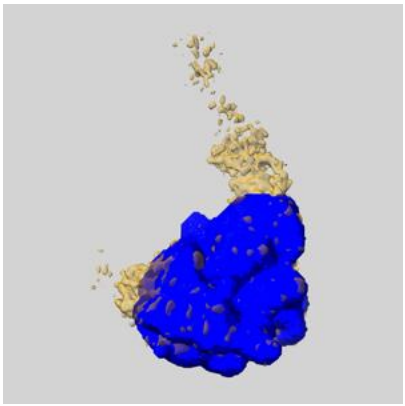
6.6 Mask visualisation (i)

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

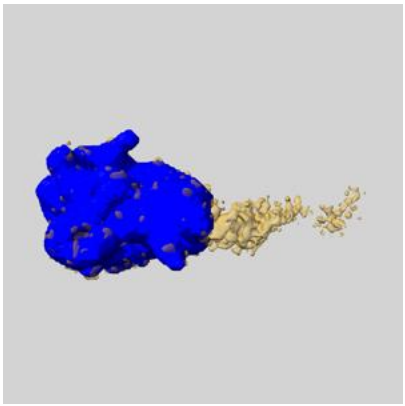
A mask typically either:

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

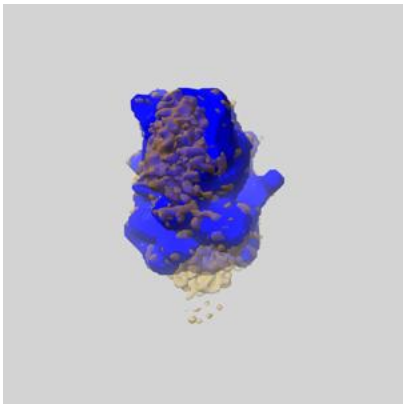
6.6.1 emd_47968_msk_1.map (i)



X



Y

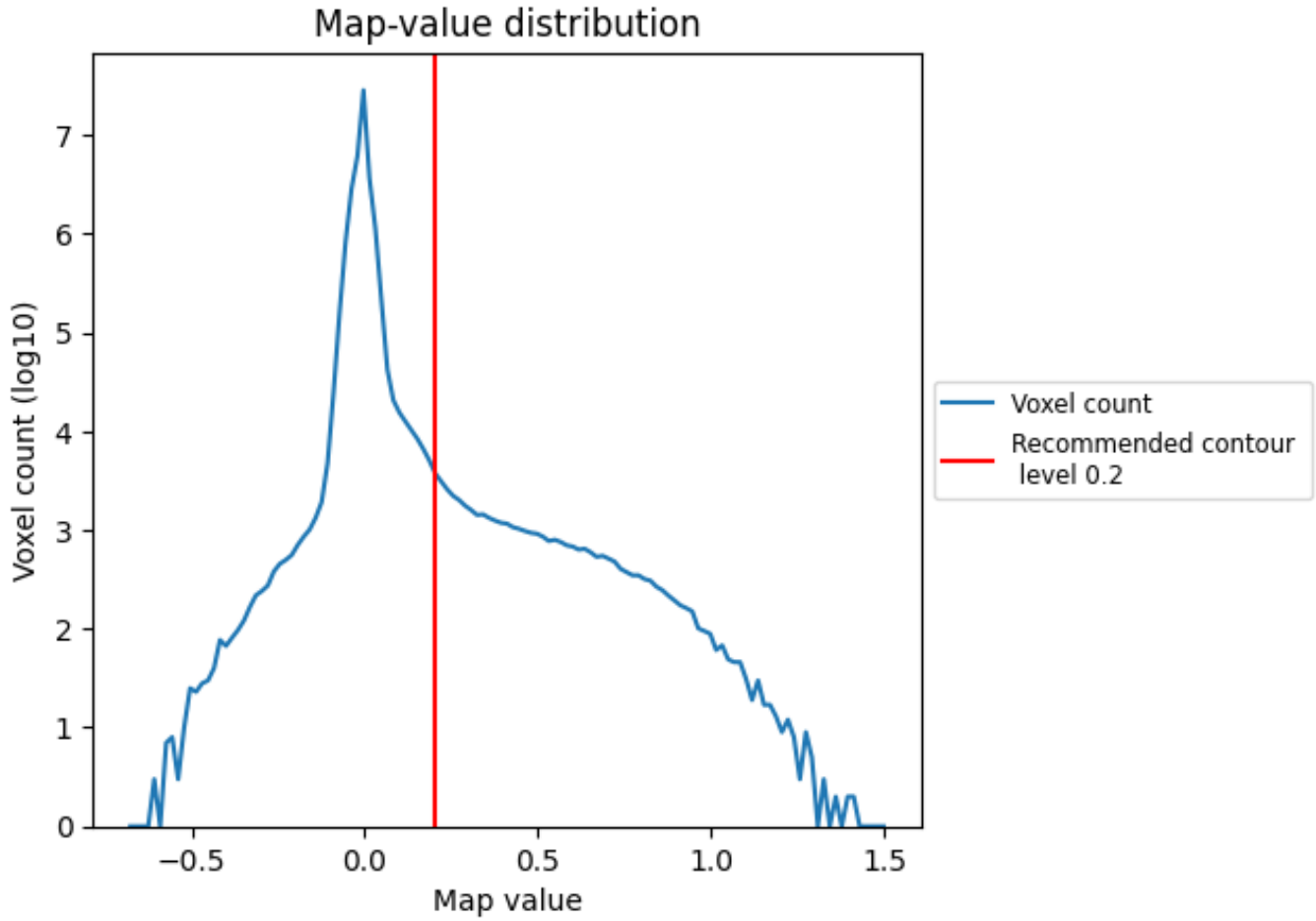


Z

7 Map analysis

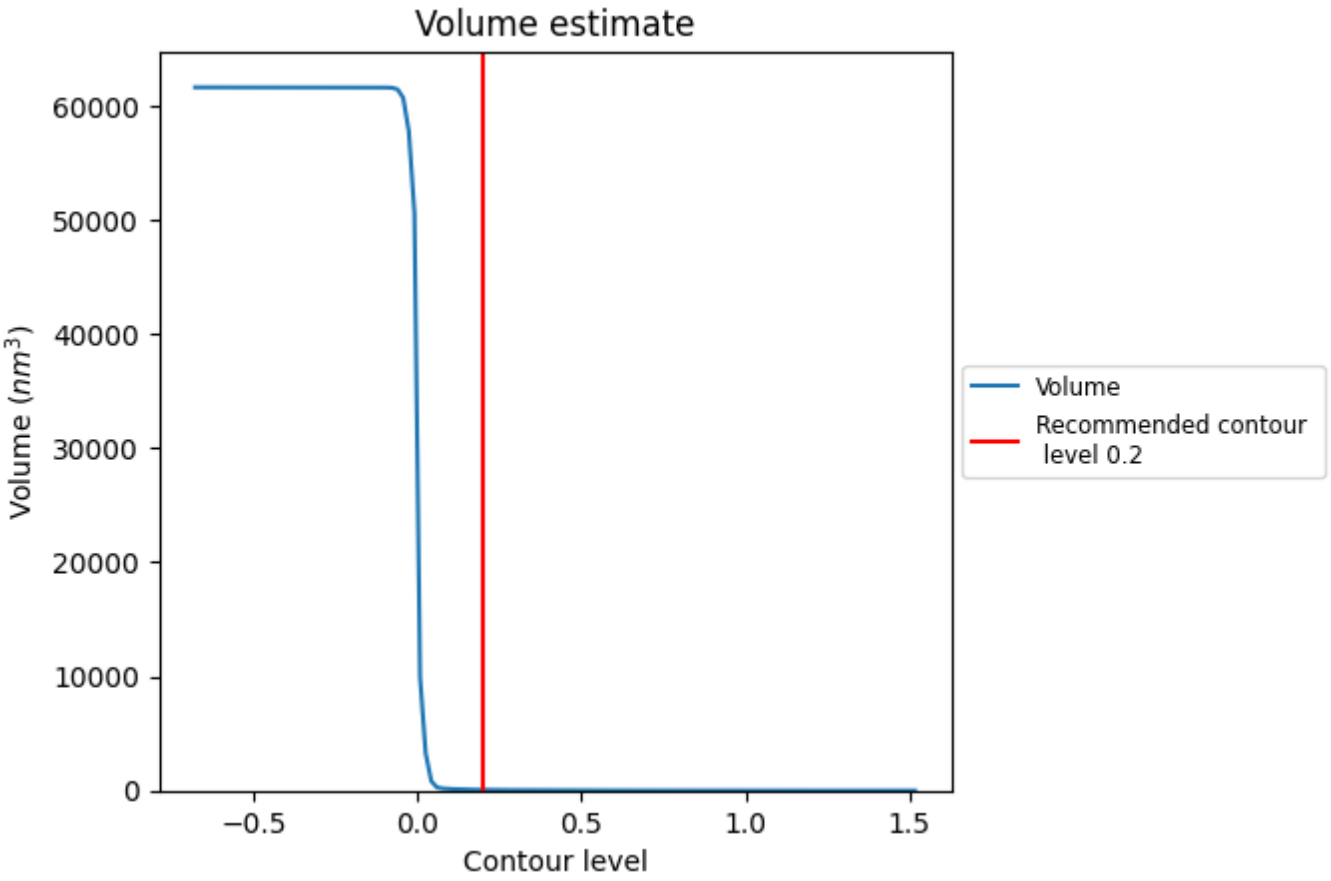
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

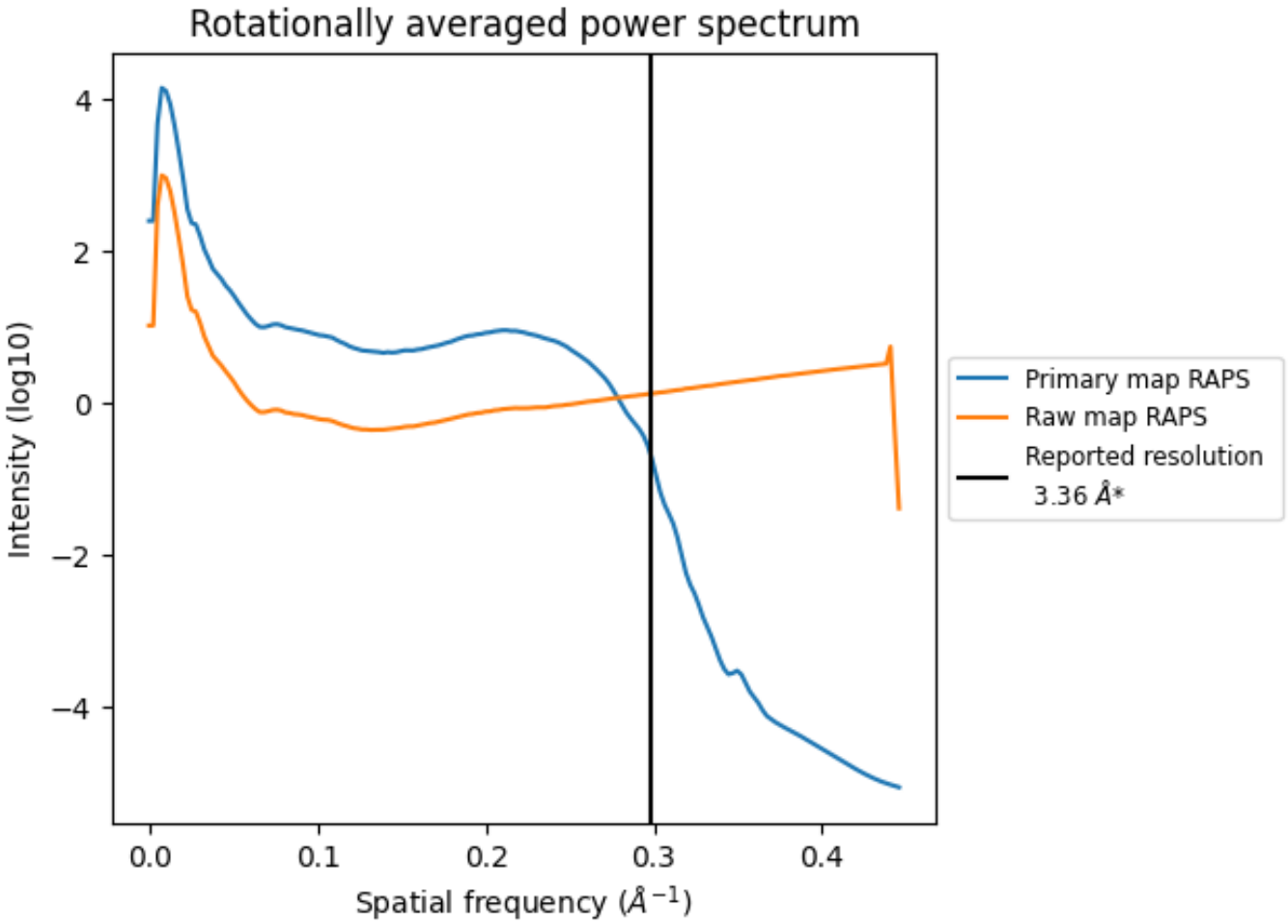
7.2 Volume estimate



The volume at the recommended contour level is 62 nm^3; this corresponds to an approximate mass of 56 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)

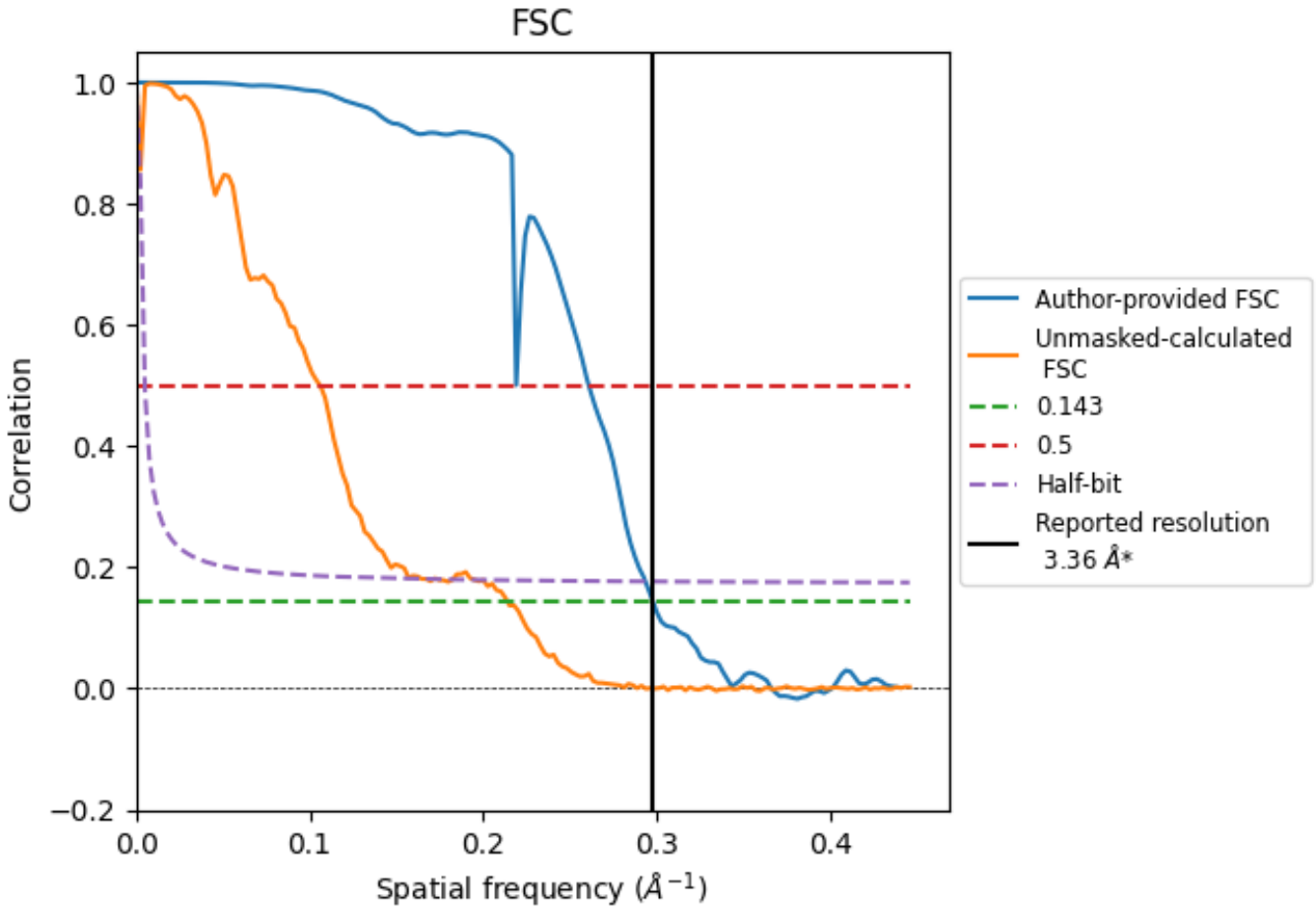


*Reported resolution corresponds to spatial frequency of 0.298 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.298 $Å^{-1}$

8.2 Resolution estimates (i)

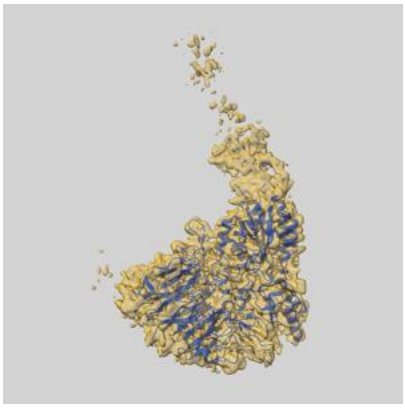
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.36	-	-
Author-provided FSC curve	3.36	3.83	3.41
Unmasked-calculated*	4.67	9.43	5.98

*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 4.67 differs from the reported value 3.36 by more than 10 %

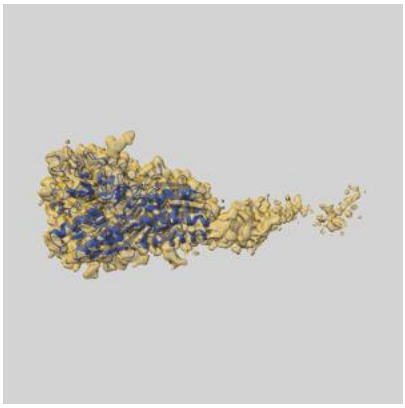
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-47968 and PDB model 9EF2. Per-residue inclusion information can be found in section 3 on page 7.

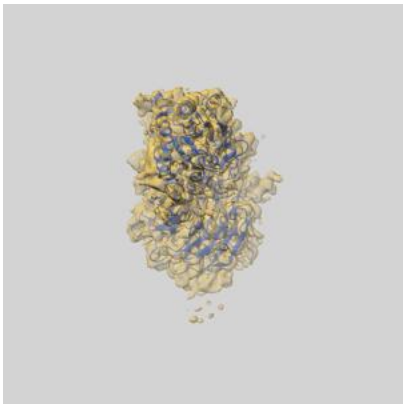
9.1 Map-model overlay



X



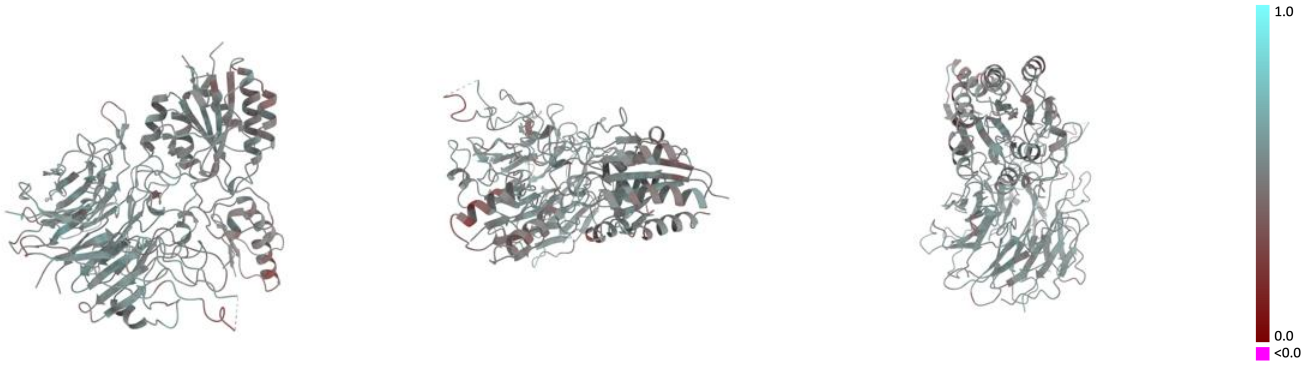
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

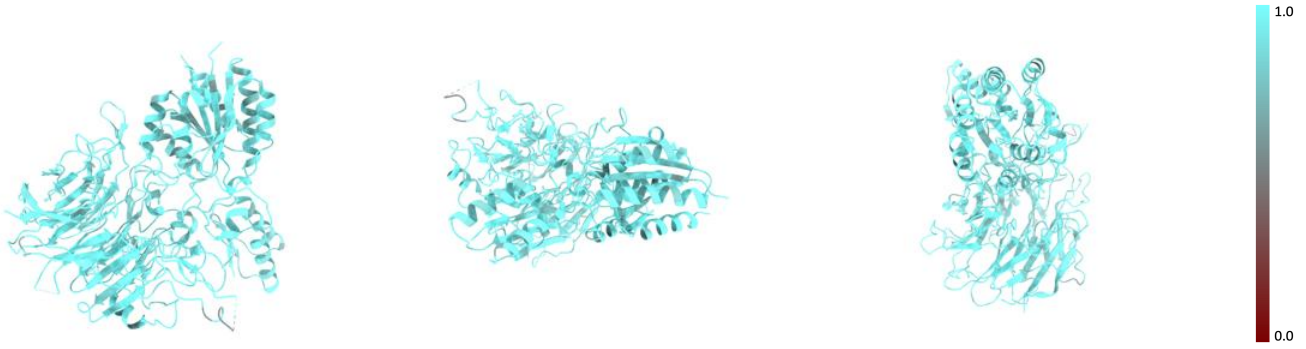
9.2 Q-score mapped to coordinate model



X Y Z

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.

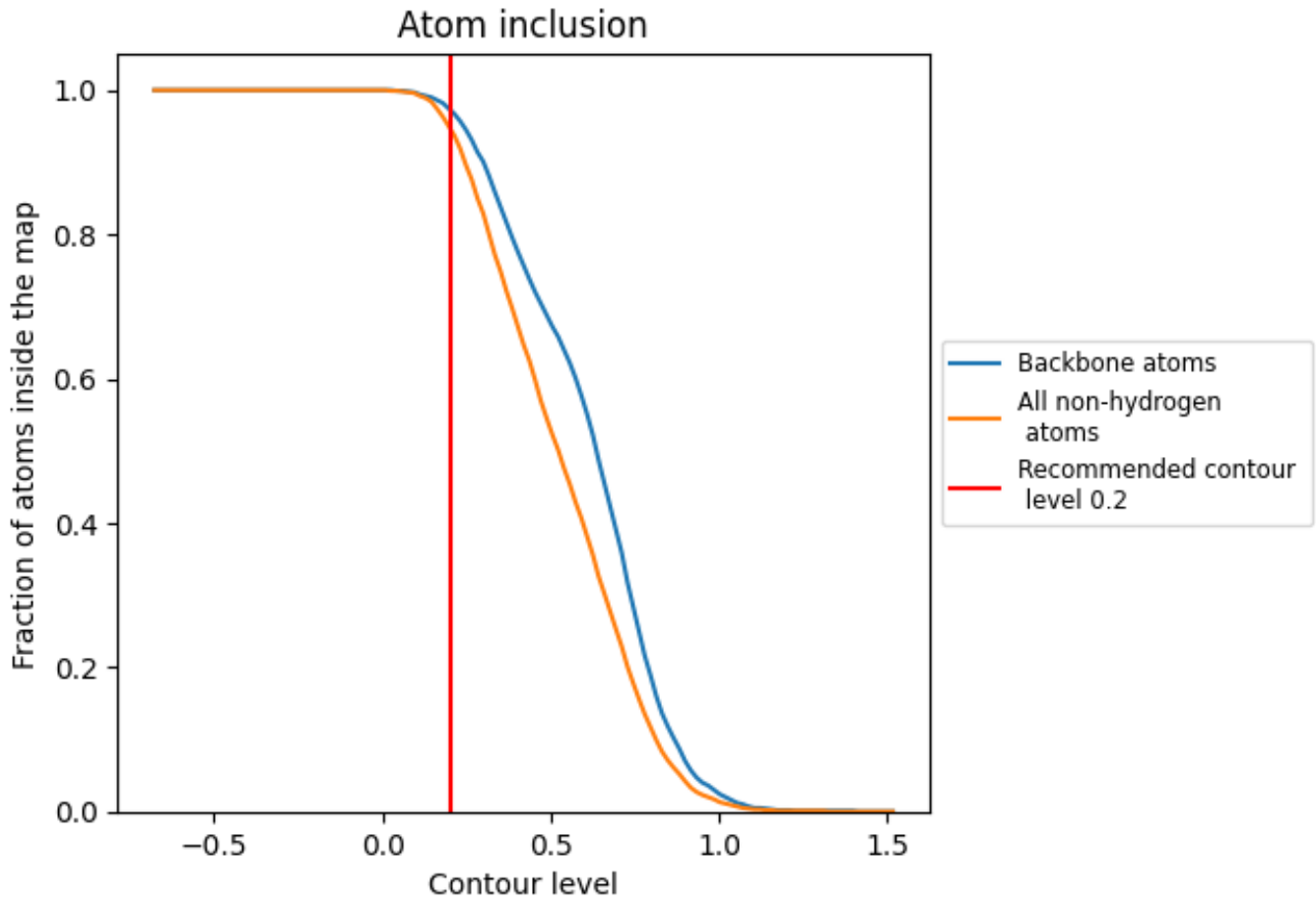
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9480	0.5040
A	0.9640	0.5190
B	0.9390	0.4960
C	0.9190	0.4610
D	0.7860	0.4220
E	0.7500	0.4150
F	0.8210	0.4730
G	0.8470	0.4500
H	0.8680	0.4290