Full wwPDB EM Validation Report ⓘ

Dec 3, 2022 – 12:29 PM EST

PDB ID	:	8E99
EMDB ID	:	EMD-27961
Title	:	Human GluN1a-GluN2A-GluN2C triheteromeric NMDA receptor in complex with Nb-4
Authors	:	Chou, T.-H.; Furukawa, H.
Deposited on	:	2022-08-26
Resolution	:	4.24 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:

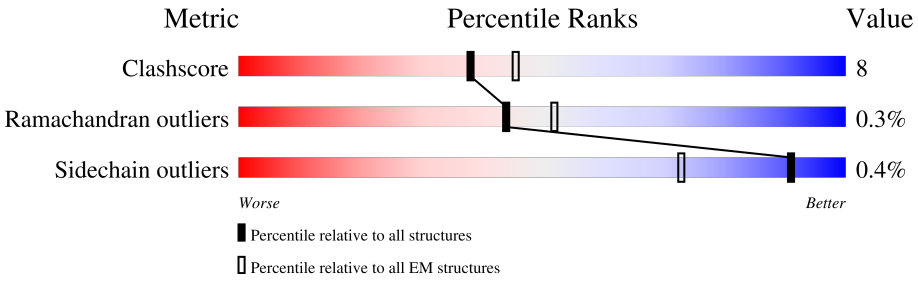
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.24 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	847	68% 9% 23%
1	C	847	65% 12% 23%
2	B	875	60% 14% 26%
3	D	880	62% 10% 28%
4	E	163	64% 7% 28%
5	F	2	50% 50%
5	G	2	100%
5	H	2	50% 50%

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Mol	Chain	Length	Quality of chain
5	I	2	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17583 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 Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	655	Total	C	N	O	S	0	0
			4134	2646	703	774	11		
1	C	653	Total	C	N	O	S	0	0
			4197	2690	727	768	12		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	HIS	ARG	conflict	UNP Q05586
A	9	PHE	LEU	conflict	UNP Q05586
A	17	PHE	VAL	conflict	UNP Q05586
A	22	SER	CYS	conflict	UNP Q05586
A	844	ASN	-	expression tag	UNP Q05586
A	845	GLY	-	expression tag	UNP Q05586
A	846	ALA	-	expression tag	UNP Q05586
A	847	GLN	-	expression tag	UNP Q05586
C	5	HIS	ARG	conflict	UNP Q05586
C	9	PHE	LEU	conflict	UNP Q05586
C	17	PHE	VAL	conflict	UNP Q05586
C	22	SER	CYS	conflict	UNP Q05586
C	844	ASN	-	expression tag	UNP Q05586
C	845	GLY	-	expression tag	UNP Q05586
C	846	ALA	-	expression tag	UNP Q05586
C	847	GLN	-	expression tag	UNP Q05586

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	648	Total	C	N	O	S	0	0
			4283	2771	710	791	11		

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	GLY	-	expression tag	UNP Q12879
B	-13	SER	-	expression tag	UNP Q12879
B	-12	GLY	-	expression tag	UNP Q12879
B	-11	ALA	-	expression tag	UNP Q12879
B	-10	THR	-	expression tag	UNP Q12879
B	-9	ASN	-	expression tag	UNP Q12879
B	-8	PHE	-	expression tag	UNP Q12879
B	-7	SER	-	expression tag	UNP Q12879
B	-6	LEU	-	expression tag	UNP Q12879
B	-5	LEU	-	expression tag	UNP Q12879
B	-4	LYS	-	expression tag	UNP Q12879
B	-3	GLN	-	expression tag	UNP Q12879
B	-2	ALA	-	expression tag	UNP Q12879
B	-1	GLY	-	expression tag	UNP Q12879
B	0	ASP	-	expression tag	UNP Q12879
B	1	VAL	-	expression tag	UNP Q12879
B	2	GLU	-	expression tag	UNP Q12879
B	3	GLU	-	expression tag	UNP Q12879
B	4	ASN	-	expression tag	UNP Q12879
B	5	PRO	-	expression tag	UNP Q12879
B	6	GLY	-	expression tag	UNP Q12879
B	7	PRO	-	expression tag	UNP Q12879
B	8	MET	-	expression tag	UNP Q12879
B	9	GLY	-	expression tag	UNP Q12879
B	10	THR	-	expression tag	UNP Q12879
B	11	MET	-	expression tag	UNP Q12879
B	12	ARG	-	expression tag	UNP Q12879
B	13	LEU	-	expression tag	UNP Q12879
B	14	PHE	-	expression tag	UNP Q12879
B	15	LEU	-	expression tag	UNP Q12879
B	16	LEU	-	expression tag	UNP Q12879
B	17	ALA	-	expression tag	UNP Q12879
B	18	VAL	-	expression tag	UNP Q12879
B	19	LEU	-	expression tag	UNP Q12879
B	20	PHE	-	expression tag	UNP Q12879
B	21	LEU	-	expression tag	UNP Q12879
B	22	PHE	-	expression tag	UNP Q12879
B	23	SER	-	expression tag	UNP Q12879
B	24	PHE	-	expression tag	UNP Q12879
B	25	ALA	-	expression tag	UNP Q12879
B	26	ARG	-	expression tag	UNP Q12879
B	27	ALA	-	expression tag	UNP Q12879
B	28	THR	-	expression tag	UNP Q12879

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Chain	Residue	Modelled	Actual	Comment	Reference
B	29	GLY	-	expression tag	UNP Q12879
B	231	SER	CYS	conflict	UNP Q12879
B	399	SER	CYS	conflict	UNP Q12879
B	460	SER	CYS	conflict	UNP Q12879
B	848	SER	CYS	conflict	UNP Q12879
B	852	THR	-	expression tag	UNP Q12879
B	853	GLU	-	expression tag	UNP Q12879
B	854	THR	-	expression tag	UNP Q12879
B	855	SER	-	expression tag	UNP Q12879
B	856	GLN	-	expression tag	UNP Q12879
B	857	VAL	-	expression tag	UNP Q12879
B	858	ALA	-	expression tag	UNP Q12879
B	859	PRO	-	expression tag	UNP Q12879
B	860	ALA	-	expression tag	UNP Q12879

- Molecule 3 is a protein called Glutamate receptor ionotropic, NMDA 2C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	637	Total	C	N	O	S	0	0
			4135	2695	683	745	12		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-30	MET	-	expression tag	UNP Q14957
D	-29	GLY	-	expression tag	UNP Q14957
D	-28	THR	-	expression tag	UNP Q14957
D	-27	MET	-	expression tag	UNP Q14957
D	-26	ARG	-	expression tag	UNP Q14957
D	-25	LEU	-	expression tag	UNP Q14957
D	-24	PHE	-	expression tag	UNP Q14957
D	-23	LEU	-	expression tag	UNP Q14957
D	-22	LEU	-	expression tag	UNP Q14957
D	-21	ALA	-	expression tag	UNP Q14957
D	-20	VAL	-	expression tag	UNP Q14957
D	-19	LEU	-	expression tag	UNP Q14957
D	-18	PHE	-	expression tag	UNP Q14957
D	-17	LEU	-	expression tag	UNP Q14957
D	-16	PHE	-	expression tag	UNP Q14957
D	-15	SER	-	expression tag	UNP Q14957
D	-14	PHE	-	expression tag	UNP Q14957
D	-13	ALA	-	expression tag	UNP Q14957

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	ARG	-	expression tag	UNP Q14957
D	-11	ALA	-	expression tag	UNP Q14957
D	-10	THR	-	expression tag	UNP Q14957
D	-9	GLY	-	expression tag	UNP Q14957
D	-8	TRP	-	expression tag	UNP Q14957
D	-7	SER	-	expression tag	UNP Q14957
D	-6	HIS	-	expression tag	UNP Q14957
D	-5	PRO	-	expression tag	UNP Q14957
D	-4	GLN	-	expression tag	UNP Q14957
D	-3	PHE	-	expression tag	UNP Q14957
D	-2	GLU	-	expression tag	UNP Q14957
D	-1	LYS	-	expression tag	UNP Q14957
D	0	GLY	-	expression tag	UNP Q14957
D	1	GLY	-	expression tag	UNP Q14957
D	2	GLY	-	expression tag	UNP Q14957
D	3	SER	-	expression tag	UNP Q14957
D	4	GLY	-	expression tag	UNP Q14957
D	5	GLY	-	expression tag	UNP Q14957
D	6	GLY	-	expression tag	UNP Q14957
D	7	SER	-	expression tag	UNP Q14957
D	8	GLY	-	expression tag	UNP Q14957
D	9	GLY	-	expression tag	UNP Q14957
D	10	SER	-	expression tag	UNP Q14957
D	11	ALA	-	expression tag	UNP Q14957
D	12	TRP	-	expression tag	UNP Q14957
D	13	SER	-	expression tag	UNP Q14957
D	14	HIS	-	expression tag	UNP Q14957
D	15	PRO	-	expression tag	UNP Q14957
D	16	GLN	-	expression tag	UNP Q14957
D	17	PHE	-	expression tag	UNP Q14957
D	18	GLU	-	expression tag	UNP Q14957
D	19	LYS	-	expression tag	UNP Q14957
D	20	GLY	-	expression tag	UNP Q14957
D	21	ALA	-	expression tag	UNP Q14957
D	22	LEU	-	expression tag	UNP Q14957
D	23	VAL	-	expression tag	UNP Q14957
D	24	PRO	-	expression tag	UNP Q14957
D	25	ARG	-	expression tag	UNP Q14957

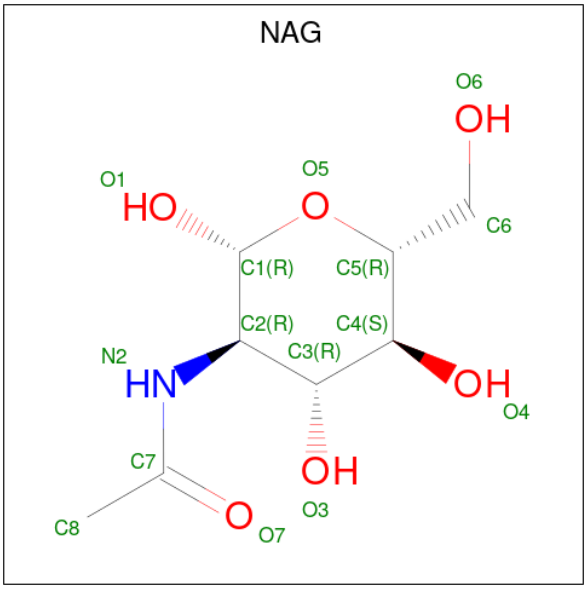
- Molecule 4 is a protein called Nanobody 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	117	Total	C	N	O	S	0	0
			694	434	125	133	2		

- 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	F	2	Total	C	N	O	0	0
			28	16	2	10		
5	G	2	Total	C	N	O	0	0
			28	16	2	10		
5	H	2	Total	C	N	O	0	0
			28	16	2	10		
5	I	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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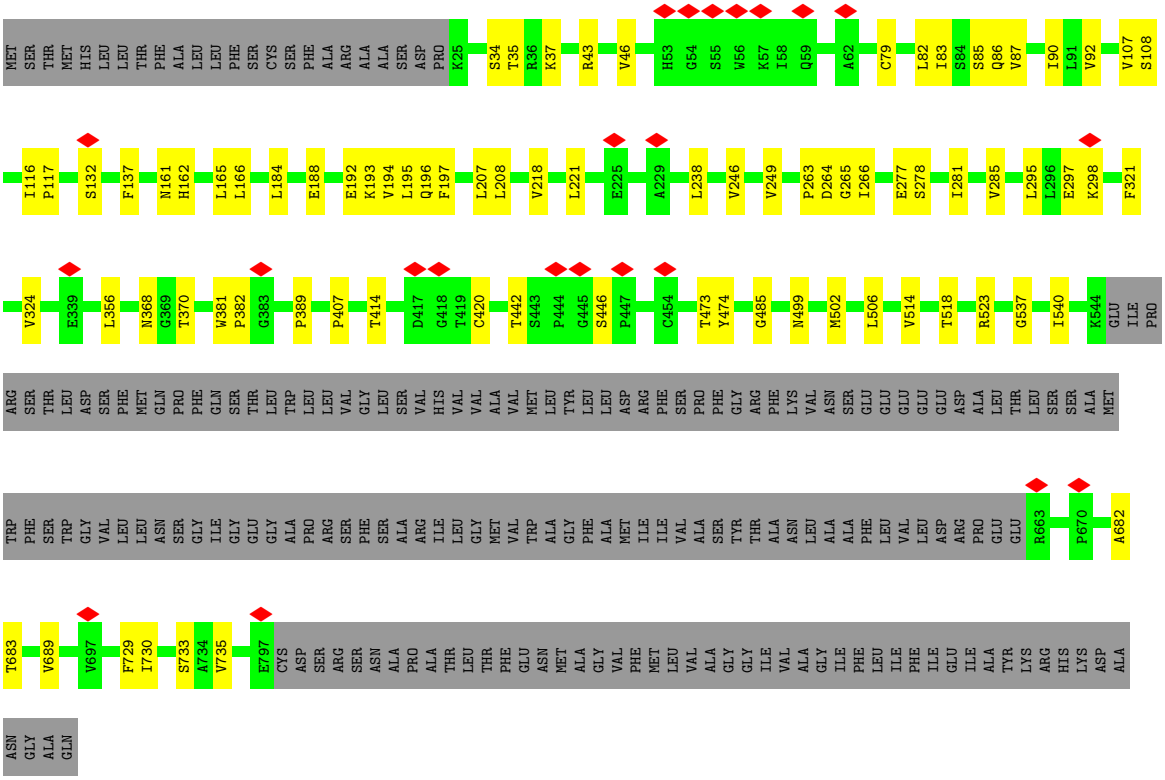
Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			14	8	1	5	

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.

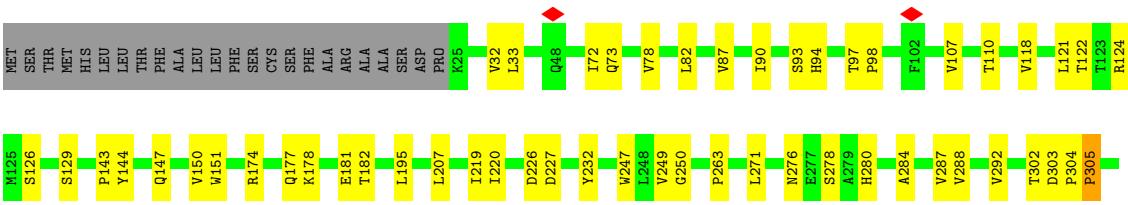
• Molecule 1: Glutamate receptor ionotropic, NMDA 1

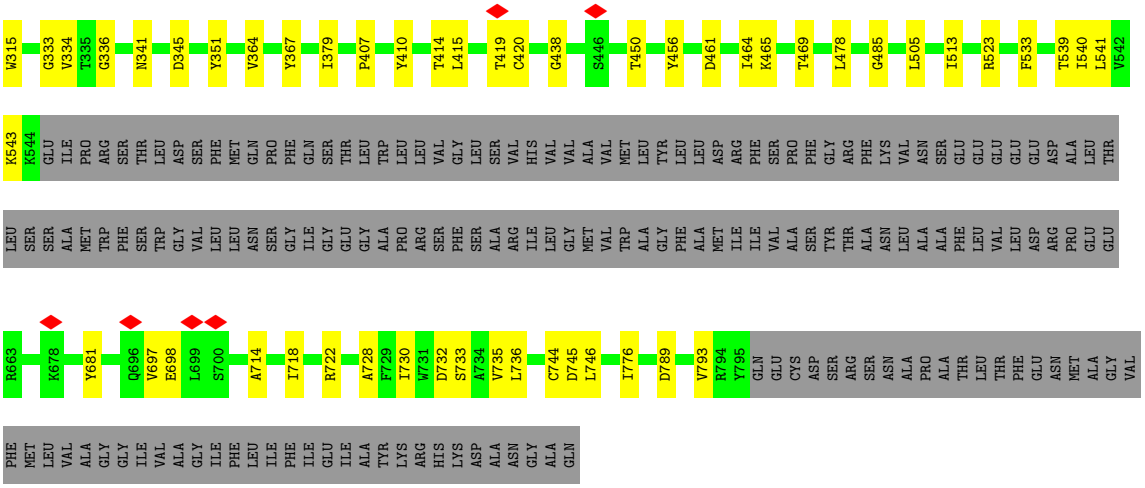
Chain A:



• Molecule 1: Glutamate receptor ionotropic, NMDA 1

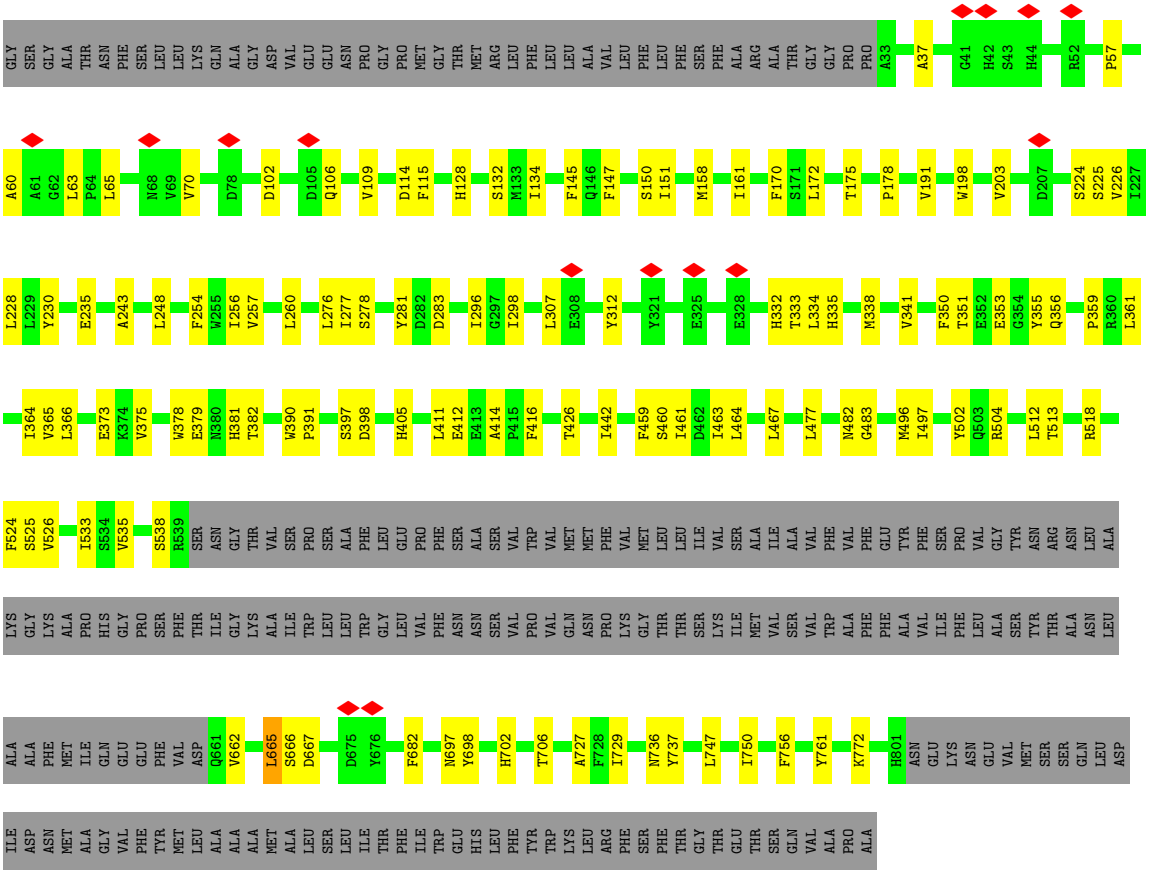
Chain C:





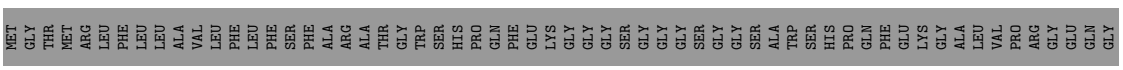
• Molecule 2: Glutamate receptor ionotropic, NMDA 2A

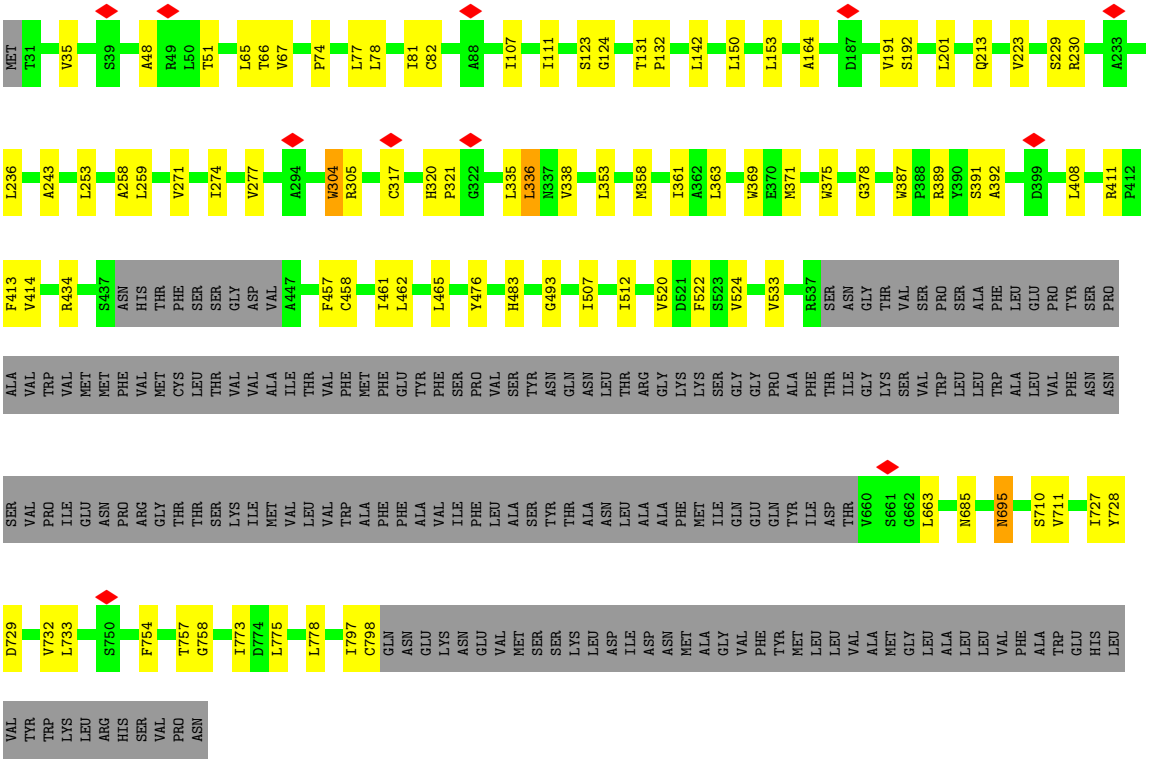
Chain B:



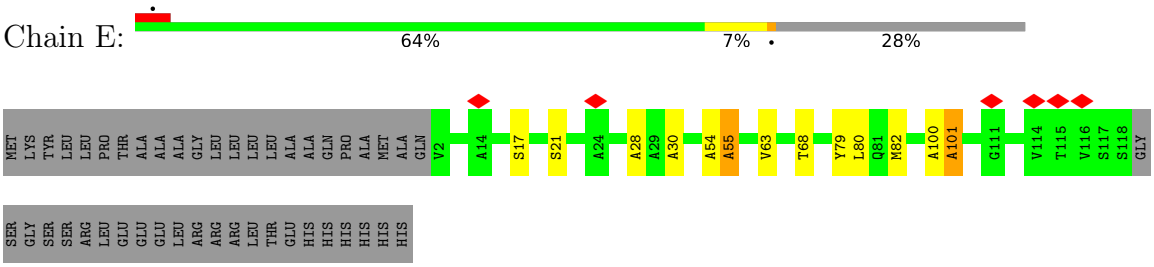
• Molecule 3: Glutamate receptor ionotropic, NMDA 2C

Chain D:





• Molecule 4: Nanobody 4



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

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

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

Chain H:

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

Chain I:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	375086	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	57.6	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	17.970	Depositor
Minimum map value	-8.984	Depositor
Average map value	0.031	Depositor
Map value standard deviation	0.707	Depositor
Recommended contour level	3.05	Depositor
Map size (Å)	342.4, 342.4, 342.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.856, 0.856, 0.856	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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.27	0/4219	0.49	0/5852
1	C	0.26	0/4290	0.49	0/5944
2	B	0.29	0/4381	0.50	0/6061
3	D	0.27	0/4236	0.50	0/5877
4	E	0.32	0/704	0.53	0/973
All	All	0.28	0/17830	0.50	0/24707

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
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	60	ALA	Mainchain

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	4134	0	3354	48	0
1	C	4197	0	3455	65	0
2	B	4283	0	3645	75	0
3	D	4135	0	3619	58	0
4	E	694	0	597	10	0
5	F	28	0	25	1	0
5	G	28	0	25	0	0
5	H	28	0	25	1	0
5	I	28	0	25	2	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
All	All	17583	0	14796	258	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 8.

All (258) 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:295:LEU:O	1:A:297:GLU:N	2.03	0.91
2:B:662:VAL:O	2:B:750:ILE:HD11	1.71	0.90
4:E:54:ALA:O	4:E:55:ALA:CB	2.25	0.83
2:B:147:PHE:HA	2:B:356:GLN:HE22	1.43	0.82
3:D:757:THR:HG22	3:D:758:GLY:H	1.51	0.74
2:B:524:PHE:O	2:B:772:LYS:NZ	2.23	0.72
4:E:54:ALA:O	4:E:55:ALA:HB3	1.92	0.69
2:B:298:ILE:HG23	2:B:341:VAL:HG21	1.73	0.69
1:A:161:ASN:OD1	1:A:162:HIS:N	2.26	0.68
3:D:336:LEU:HD12	3:D:336:LEU:C	2.13	0.68
3:D:685:ASN:OD1	5:H:1:NAG:N2	2.27	0.68
1:A:117:PRO:HG2	1:A:321:PHE:HD2	1.58	0.68
1:C:744:CYS:SG	1:C:745:ASP:N	2.68	0.67
1:A:196:GLN:NE2	1:A:197:PHE:O	2.28	0.67
1:C:541:LEU:HG	1:C:736:LEU:HD23	1.75	0.67
1:C:351:TYR:H	1:C:367:TYR:HB3	1.58	0.67
1:C:540:ILE:HG12	1:C:730:ILE:HG22	1.77	0.66
4:E:100:ALA:O	4:E:101:ALA:HB3	1.93	0.66
3:D:35:VAL:HG12	3:D:67:VAL:HB	1.78	0.65
3:D:524:VAL:HG11	3:D:778:LEU:HD21	1.77	0.65
2:B:226:VAL:HG12	2:B:254:PHE:HB2	1.78	0.65
2:B:191:VAL:HG23	2:B:198:TRP:HB3	1.77	0.65
2:B:414:ALA:O	2:B:416:PHE:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:ILE:HG12	1:A:730:ILE:HG22	1.76	0.65
2:B:333:THR:HG23	2:B:335:HIS:H	1.61	0.65
3:D:271:VAL:HA	3:D:363:LEU:HD23	1.79	0.65
3:D:533:VAL:HG12	3:D:727:ILE:HG22	1.80	0.64
2:B:502:TYR:O	2:B:504:ARG:NH1	2.30	0.64
4:E:100:ALA:O	4:E:101:ALA:CB	2.47	0.63
2:B:224:SER:OG	2:B:225:SER:N	2.29	0.63
5:I:1:NAG:O7	5:I:1:NAG:O3	2.14	0.63
3:D:213:GLN:HE22	3:D:243:ALA:HB2	1.64	0.62
1:C:121:LEU:HD22	1:C:280:HIS:HB3	1.82	0.62
1:A:192:GLU:HG2	1:A:193:LYS:HG2	1.82	0.62
2:B:276:LEU:HB3	2:B:366:LEU:HD23	1.82	0.62
1:A:221:LEU:HB2	1:A:249:VAL:HG12	1.82	0.62
1:A:264:ASP:HA	1:A:356:LEU:HD23	1.82	0.62
2:B:405:HIS:O	2:B:405:HIS:ND1	2.33	0.61
3:D:164:ALA:HB3	3:D:223:VAL:HB	1.83	0.61
1:C:681:TYR:HA	1:C:728:ALA:HB3	1.82	0.61
2:B:257:VAL:HG23	2:B:278:SER:HB2	1.82	0.61
1:C:414:THR:HA	1:C:420:CYS:HB3	1.82	0.61
1:C:438:GLY:HA2	1:C:478:LEU:HB2	1.82	0.60
2:B:63:LEU:O	2:B:65:LEU:N	2.31	0.60
1:A:381:TRP:CZ3	1:A:389:PRO:HD3	2.37	0.60
1:A:184:LEU:O	1:A:188:GLU:N	2.34	0.59
2:B:114:ASP:OD1	2:B:115:PHE:N	2.36	0.59
1:C:151:TRP:CD2	1:C:220:ILE:HD11	2.38	0.59
1:A:117:PRO:HG2	1:A:321:PHE:CD2	2.39	0.58
1:A:192:GLU:N	1:A:192:GLU:OE2	2.37	0.58
2:B:230:TYR:HE1	2:B:260:LEU:HD21	1.68	0.58
1:C:461:ASP:HA	1:C:464:ILE:HG12	1.86	0.58
2:B:411:LEU:HD12	2:B:412:GLU:H	1.69	0.57
2:B:513:THR:O	2:B:518:ARG:NH1	2.37	0.57
2:B:504:ARG:NE	2:B:504:ARG:HA	2.20	0.56
1:C:94:HIS:N	1:C:122:THR:OG1	2.39	0.56
1:A:165:LEU:HD21	1:A:194:VAL:HG12	1.86	0.56
1:A:473:THR:HG22	1:A:474:TYR:H	1.69	0.56
1:A:195:LEU:HD12	1:A:207:LEU:HD12	1.87	0.56
3:D:150:LEU:HD12	3:D:153:LEU:HD13	1.88	0.56
3:D:371:MET:SD	3:D:371:MET:N	2.79	0.55
1:A:414:THR:HA	1:A:420:CYS:HB3	1.87	0.55
2:B:411:LEU:HD12	2:B:412:GLU:N	2.22	0.55
2:B:150:SER:HB3	2:B:355:TYR:CG	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:ILE:HD13	2:B:277:ILE:HB	1.88	0.55
4:E:54:ALA:O	4:E:55:ALA:HB2	2.04	0.55
2:B:736:ASN:OD1	2:B:737:TYR:N	2.40	0.55
1:A:132:SER:HA	2:B:178:PRO:HB3	1.89	0.54
2:B:497:ILE:HD11	2:B:512:LEU:HD11	1.90	0.54
1:C:226:ASP:OD1	1:C:227:ASP:N	2.40	0.54
1:C:302:THR:O	1:C:315:TRP:NE1	2.35	0.54
1:C:697:VAL:HG23	1:C:698:GLU:H	1.73	0.54
3:D:361:ILE:HD11	3:D:369:TRP:HB3	1.88	0.54
1:A:82:LEU:HA	1:A:87:VAL:HG21	1.89	0.54
2:B:662:VAL:O	2:B:750:ILE:CD1	2.52	0.54
2:B:134:ILE:HG21	2:B:151:ILE:HD11	1.90	0.54
1:C:276:ASN:OD1	1:C:278:SER:OG	2.20	0.54
2:B:665:LEU:CD1	2:B:665:LEU:N	2.71	0.53
2:B:461:ILE:HD13	2:B:477:LEU:HD21	1.90	0.53
1:C:789:ASP:O	1:C:793:VAL:HG12	2.08	0.53
3:D:258:ALA:O	3:D:259:LEU:HG	2.08	0.53
2:B:175:THR:HG21	2:B:235:GLU:HG2	1.90	0.53
1:C:465:LYS:O	1:C:469:THR:HG23	2.09	0.53
1:C:126:SER:O	1:C:129:SER:OG	2.24	0.52
1:C:288:VAL:O	1:C:292:VAL:HG13	2.09	0.52
3:D:408:LEU:O	3:D:414:VAL:HG11	2.09	0.52
3:D:304:TRP:CD1	3:D:304:TRP:C	2.82	0.52
1:A:278:SER:HA	1:A:281:ILE:HG12	1.92	0.52
1:A:518:THR:O	1:A:523:ARG:NH2	2.41	0.52
1:C:533:PHE:HB3	1:C:776:ILE:HD11	1.92	0.51
1:C:232:TYR:CE2	1:C:263:PRO:HA	2.45	0.51
1:A:79:CYS:O	1:A:83:ILE:HG23	2.10	0.51
1:C:407:PRO:HG3	1:C:735:VAL:HA	1.92	0.51
2:B:460:SER:O	2:B:463:ILE:HG22	2.09	0.51
1:C:124:ARG:NH2	1:C:271:LEU:HD12	2.25	0.51
1:A:485:GLY:HA2	1:A:499:ASN:O	2.11	0.51
3:D:695:ASN:O	3:D:695:ASN:ND2	2.43	0.51
2:B:416:PHE:HA	2:B:459:PHE:HB3	1.92	0.50
2:B:496:MET:SD	2:B:496:MET:N	2.81	0.50
1:C:271:LEU:HD21	1:C:351:TYR:HE1	1.77	0.50
2:B:298:ILE:HA	2:B:341:VAL:HG11	1.93	0.50
3:D:123:SER:OG	3:D:124:GLY:N	2.45	0.50
1:C:485:GLY:O	1:C:523:ARG:NH2	2.36	0.50
1:C:78:VAL:O	1:C:82:LEU:HG	2.11	0.50
3:D:728:TYR:HB3	3:D:733:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:732:ASP:O	1:C:736:LEU:HD13	2.13	0.49
3:D:663:LEU:HB2	3:D:754:PHE:CE2	2.47	0.49
3:D:520:VAL:HG13	3:D:522:PHE:CE1	2.48	0.49
1:C:415:LEU:H	1:C:420:CYS:HA	1.76	0.49
3:D:142:LEU:HB2	3:D:353:LEU:HD23	1.95	0.49
2:B:682:PHE:HA	2:B:727:ALA:O	2.13	0.49
3:D:229:SER:OG	3:D:230:ARG:N	2.45	0.49
2:B:697:ASN:OD1	2:B:698:TYR:N	2.45	0.49
1:C:333:GLY:O	1:C:336:GLY:N	2.46	0.49
1:C:147:GLN:HA	1:C:150:VAL:HG12	1.95	0.49
1:C:174:ARG:O	1:C:177:GLN:HG3	2.13	0.48
1:C:415:LEU:N	1:C:419:THR:O	2.45	0.48
3:D:512:ILE:HD12	3:D:512:ILE:H	1.78	0.48
2:B:312:TYR:OH	2:B:332:HIS:N	2.47	0.48
3:D:78:LEU:HD13	3:D:111:ILE:HD11	1.94	0.48
3:D:775:LEU:HA	3:D:778:LEU:HD12	1.95	0.48
3:D:107:ILE:O	3:D:111:ILE:HG12	2.14	0.48
2:B:390:TRP:CD2	2:B:391:PRO:HD2	2.49	0.48
1:C:72:ILE:HG13	1:C:73:GLN:N	2.28	0.48
4:E:63:VAL:HG12	4:E:63:VAL:O	2.14	0.48
2:B:359:PRO:HB2	2:B:361:LEU:HD12	1.96	0.48
1:A:682:ALA:O	1:A:729:PHE:HB2	2.13	0.48
1:A:683:THR:HG21	1:A:689:VAL:HG11	1.96	0.48
3:D:201:LEU:HD11	3:D:236:LEU:HD11	1.96	0.47
3:D:304:TRP:HD1	3:D:305:ARG:N	2.12	0.47
3:D:757:THR:HG22	3:D:758:GLY:N	2.26	0.47
2:B:170:PHE:CB	2:B:224:SER:OG	2.62	0.47
2:B:128:HIS:O	2:B:132:SER:N	2.44	0.47
3:D:483:HIS:O	3:D:493:GLY:HA3	2.14	0.47
1:C:304:PRO:N	1:C:305:PRO:HD2	2.29	0.47
3:D:153:LEU:H	3:D:153:LEU:HD12	1.79	0.47
1:C:414:THR:OG1	1:C:419:THR:O	2.27	0.47
3:D:411:ARG:O	3:D:413:PHE:N	2.48	0.47
1:C:303:ASP:C	1:C:305:PRO:HD2	2.35	0.47
3:D:710:SER:OG	3:D:711:VAL:N	2.47	0.47
3:D:65:LEU:HD12	3:D:66:THR:H	1.80	0.47
2:B:461:ILE:CD1	2:B:477:LEU:HD21	2.44	0.47
3:D:434:ARG:HE	3:D:476:TYR:HB2	1.80	0.47
1:C:249:VAL:HG22	1:C:250:GLY:H	1.78	0.47
1:C:714:ALA:O	1:C:718:ILE:HG13	2.14	0.46
2:B:513:THR:HG22	2:B:761:TYR:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:535:VAL:HG12	2:B:729:ILE:HG12	1.97	0.46
1:C:94:HIS:H	1:C:122:THR:HG1	1.63	0.46
1:A:108:SER:HB2	1:A:137:PHE:CZ	2.50	0.46
1:C:178:LYS:O	1:C:182:THR:HG23	2.16	0.46
3:D:131:THR:HB	3:D:132:PRO:HD3	1.96	0.46
3:D:277:VAL:O	3:D:358:MET:HB2	2.15	0.46
2:B:334:LEU:O	2:B:338:MET:N	2.49	0.46
1:C:124:ARG:HD2	1:C:144:TYR:CE1	2.51	0.46
2:B:158:MET:O	2:B:161:ILE:HG22	2.15	0.46
1:A:407:PRO:HG2	1:A:735:VAL:HA	1.97	0.46
2:B:482:ASN:OD1	2:B:483:GLY:N	2.49	0.46
1:C:697:VAL:HG23	1:C:698:GLU:N	2.31	0.46
3:D:413:PHE:HA	3:D:457:PHE:HB3	1.99	0.45
3:D:729:ASP:O	3:D:733:LEU:HD23	2.16	0.45
1:A:381:TRP:HB3	1:A:382:PRO:HD2	1.97	0.45
1:C:177:GLN:O	1:C:181:GLU:OE1	2.35	0.45
1:C:543:LYS:HA	1:C:746:LEU:HD13	1.98	0.45
1:C:107:VAL:HA	1:C:110:THR:HG22	1.98	0.45
1:C:195:LEU:HD12	1:C:207:LEU:HD12	1.99	0.45
3:D:458:CYS:HA	3:D:461:ILE:HG22	1.98	0.45
1:C:90:ILE:HB	1:C:118:VAL:HG23	1.98	0.45
1:C:341:ASN:N	1:C:345:ASP:O	2.38	0.45
1:A:85:SER:OG	1:A:86:GLN:N	2.49	0.45
2:B:533:ILE:HD11	2:B:756:PHE:HD2	1.81	0.45
1:A:34:SER:O	1:A:34:SER:OG	2.25	0.45
1:A:407:PRO:HG2	1:A:735:VAL:HG12	1.97	0.45
2:B:665:LEU:N	2:B:665:LEU:HD13	2.31	0.45
3:D:335:LEU:HD23	3:D:335:LEU:O	2.16	0.45
2:B:379:GLU:O	2:B:382:THR:HG22	2.16	0.45
1:A:166:LEU:HD23	1:A:221:LEU:HD11	1.99	0.45
1:C:124:ARG:HG2	1:C:143:PRO:HA	1.99	0.45
2:B:351:THR:HG23	2:B:353:GLU:H	1.82	0.44
2:B:702:HIS:O	2:B:706:THR:HG23	2.17	0.44
3:D:465:LEU:HD21	3:D:773:ILE:HD12	1.99	0.44
5:I:2:NAG:H3	5:I:2:NAG:H82	1.99	0.44
2:B:378:TRP:CZ2	2:B:381:HIS:HA	2.53	0.44
3:D:77:LEU:O	3:D:81:ILE:HG22	2.17	0.44
4:E:21:SER:HA	4:E:79:TYR:HA	2.00	0.44
3:D:274:ILE:HD11	3:D:387:TRP:CZ2	2.52	0.44
2:B:172:LEU:HA	2:B:228:LEU:O	2.18	0.44
2:B:172:LEU:HB2	2:B:203:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:82:CYS:HB2	3:D:317:CYS:HB2	1.78	0.43
3:D:48:ALA:O	3:D:51:THR:OG1	2.35	0.43
1:A:514:VAL:O	1:A:514:VAL:HG13	2.19	0.43
2:B:243:ALA:HB1	2:B:248:LEU:HB2	2.00	0.43
3:D:74:PRO:O	3:D:78:LEU:HD23	2.18	0.43
2:B:461:ILE:HD12	2:B:464:LEU:HD21	2.01	0.43
1:C:271:LEU:CD2	1:C:351:TYR:CE1	3.01	0.43
1:C:539:THR:HG23	1:C:733:SER:OG	2.19	0.43
5:F:1:NAG:H4	5:F:2:NAG:H2	1.89	0.43
2:B:145:PHE:HB3	2:B:350:PHE:CE2	2.54	0.43
2:B:102:ASP:O	2:B:128:HIS:ND1	2.52	0.43
2:B:416:PHE:O	2:B:459:PHE:N	2.52	0.43
3:D:191:VAL:HG12	3:D:192:SER:N	2.34	0.43
1:A:537:GLY:H	1:A:733:SER:HB3	1.83	0.43
1:C:32:VAL:C	1:C:33:LEU:HD12	2.39	0.43
4:E:17:SER:OG	4:E:82:MET:O	2.36	0.43
2:B:426:THR:O	2:B:426:THR:HG22	2.19	0.43
1:A:195:LEU:HD23	1:A:195:LEU:H	1.82	0.42
1:A:368:ASN:O	1:A:370:THR:N	2.48	0.42
2:B:525:SER:OG	2:B:526:VAL:N	2.52	0.42
1:C:284:ALA:HA	1:C:287:VAL:HG12	2.00	0.42
3:D:336:LEU:HD12	3:D:336:LEU:O	2.19	0.42
3:D:391:SER:OG	3:D:392:ALA:N	2.52	0.42
2:B:397:SER:OG	2:B:398:ASP:N	2.53	0.42
2:B:134:ILE:HD12	2:B:134:ILE:HA	1.93	0.42
1:C:364:VAL:HG21	1:C:379:ILE:HG12	2.00	0.42
1:A:208:LEU:HG	1:A:238:LEU:HD23	2.00	0.42
1:A:442:THR:HG23	1:A:446:SER:HB3	2.01	0.42
2:B:307:LEU:HA	2:B:312:TYR:HB3	2.00	0.42
1:C:93:SER:OG	1:C:94:HIS:N	2.53	0.42
1:C:410:TYR:HD2	1:C:456:TYR:CE2	2.38	0.42
1:C:722:ARG:HG2	1:C:746:LEU:HD21	2.02	0.42
3:D:153:LEU:HD23	3:D:253:LEU:HD13	2.02	0.42
1:C:789:ASP:C	1:C:793:VAL:HG12	2.41	0.42
3:D:458:CYS:HB3	3:D:507:ILE:HG12	2.01	0.42
3:D:320:HIS:N	3:D:321:PRO:HD3	2.35	0.41
1:A:218:VAL:HA	1:A:246:VAL:O	2.20	0.41
2:B:390:TRP:CG	2:B:391:PRO:HD2	2.55	0.41
1:C:219:ILE:HD11	1:C:247:TRP:CZ3	2.54	0.41
1:A:92:VAL:HG11	1:A:107:VAL:HG11	2.02	0.41
1:C:271:LEU:CD2	1:C:351:TYR:HE1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:PRO:O	1:A:266:ILE:HG13	2.20	0.41
2:B:281:TYR:O	2:B:283:ASP:N	2.53	0.41
1:C:249:VAL:HG22	1:C:250:GLY:N	2.35	0.41
2:B:365:VAL:HG13	2:B:375:VAL:HG21	2.02	0.41
1:C:82:LEU:HD22	1:C:87:VAL:HG11	2.01	0.41
4:E:28:ALA:O	4:E:30:ALA:N	2.54	0.41
1:A:502:MET:O	1:A:506:LEU:HD23	2.21	0.41
2:B:364:ILE:HG13	2:B:373:GLU:O	2.21	0.41
3:D:732:VAL:HG23	3:D:733:LEU:HD22	2.01	0.41
1:A:35:THR:C	1:A:37:LYS:H	2.24	0.41
1:A:43:ARG:O	1:A:46:VAL:HG12	2.21	0.41
1:A:90:ILE:HD11	1:A:116:ILE:HD12	2.03	0.41
1:A:295:LEU:HD13	1:A:324:VAL:HG11	2.03	0.41
2:B:37:ALA:HA	2:B:70:VAL:O	2.21	0.41
2:B:106:GLN:O	2:B:109:VAL:HG22	2.21	0.41
1:C:505:LEU:HD22	1:C:513:ILE:HG23	2.01	0.41
3:D:458:CYS:O	3:D:461:ILE:HG22	2.20	0.40
3:D:797:ILE:HG13	3:D:798:CYS:N	2.36	0.40
1:C:151:TRP:CE3	1:C:220:ILE:HD11	2.57	0.40
1:A:281:ILE:O	1:A:285:VAL:HG23	2.21	0.40
2:B:57:PRO:HG3	2:B:296:ILE:HG21	2.04	0.40
2:B:464:LEU:HA	2:B:467:LEU:HB3	2.03	0.40
4:E:68:THR:O	4:E:80:LEU:HD12	2.21	0.40
1:A:263:PRO:HD2	1:A:266:ILE:HD11	2.04	0.40
2:B:538:SER:HA	2:B:747:LEU:HD13	2.04	0.40
2:B:666:SER:O	2:B:667:ASP:C	2.57	0.40
3:D:375:TRP:CZ2	3:D:378:GLY:HA2	2.57	0.40
1:A:265:GLY:H	1:A:356:LEU:HB3	1.85	0.40
1:C:97:THR:HA	1:C:98:PRO:HD3	1.98	0.40
3:D:462:LEU:HD12	3:D:462:LEU:HA	1.94	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	651/847 (77%)	601 (92%)	48 (7%)	2 (0%)	41 76
1	C	649/847 (77%)	613 (94%)	33 (5%)	3 (0%)	29 68
2	B	644/875 (74%)	588 (91%)	55 (8%)	1 (0%)	47 81
3	D	631/880 (72%)	575 (91%)	55 (9%)	1 (0%)	47 81
4	E	115/163 (71%)	104 (90%)	9 (8%)	2 (2%)	9 44
All	All	2690/3612 (74%)	2481 (92%)	200 (7%)	9 (0%)	44 76

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	442	ILE
1	C	305	PRO
4	E	55	ALA
4	E	101	ALA
1	A	298	LYS
1	C	334	VAL
1	A	277	GLU
3	D	389	ARG
1	C	450	THR

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	304/728 (42%)	304 (100%)	0	100 100
1	C	316/728 (43%)	316 (100%)	0	100 100
2	B	355/757 (47%)	354 (100%)	1 (0%)	92 95
3	D	339/735 (46%)	335 (99%)	4 (1%)	71 84
4	E	37/102 (36%)	37 (100%)	0	100 100
All	All	1351/3050 (44%)	1346 (100%)	5 (0%)	91 94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	665	LEU
3	D	304	TRP
3	D	336	LEU
3	D	338	VAL
3	D	695	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	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 (i)

8 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	F	1	1,5	14,14,15	0.21	0	17,19,21	0.47	0
5	NAG	F	2	5	14,14,15	0.61	1 (7%)	17,19,21	0.45	0
5	NAG	G	1	1,5	14,14,15	0.17	0	17,19,21	0.55	0
5	NAG	G	2	5	14,14,15	0.24	0	17,19,21	0.45	0
5	NAG	H	1	3,5	14,14,15	1.06	1 (7%)	17,19,21	0.94	1 (5%)
5	NAG	H	2	5	14,14,15	0.49	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	I	1	3,5	14,14,15	0.55	0	17,19,21	1.08	1 (5%)
5	NAG	I	2	5	14,14,15	0.50	0	17,19,21	1.27	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
5	NAG	F	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	F	2	5	-	1/6/23/26	0/1/1/1
5	NAG	G	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	NAG	H	1	3,5	-	1/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
5	NAG	I	1	3,5	-	6/6/23/26	0/1/1/1
5	NAG	I	2	5	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	1	NAG	O5-C1	-3.73	1.37	1.43
5	F	2	NAG	C1-C2	2.03	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	2	NAG	C2-N2-C7	-3.04	118.58	122.90
5	I	1	NAG	O5-C1-C2	-2.89	106.73	111.29
5	H	1	NAG	C4-C3-C2	2.57	114.78	111.02
5	I	2	NAG	O5-C5-C6	2.37	110.93	107.20
5	I	2	NAG	C1-C2-N2	-2.09	106.91	110.49

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	1	NAG	C8-C7-N2-C2
5	I	1	NAG	O7-C7-N2-C2
5	I	2	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	I	2	NAG	O7-C7-N2-C2
5	F	1	NAG	O5-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
5	I	2	NAG	C1-C2-N2-C7
5	I	1	NAG	C4-C5-C6-O6
5	I	1	NAG	C1-C2-N2-C7
5	G	1	NAG	O5-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
5	I	1	NAG	C3-C2-N2-C7
5	F	2	NAG	O5-C5-C6-O6
5	H	1	NAG	C3-C2-N2-C7
5	H	2	NAG	C3-C2-N2-C7
5	H	2	NAG	C1-C2-N2-C7

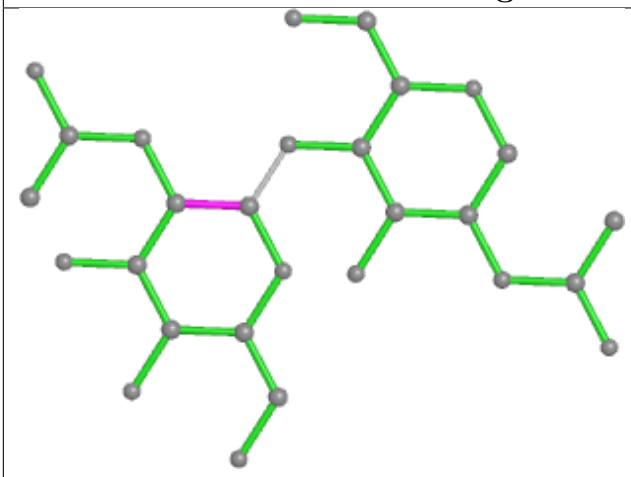
There are no ring outliers.

5 monomers are involved in 4 short contacts:

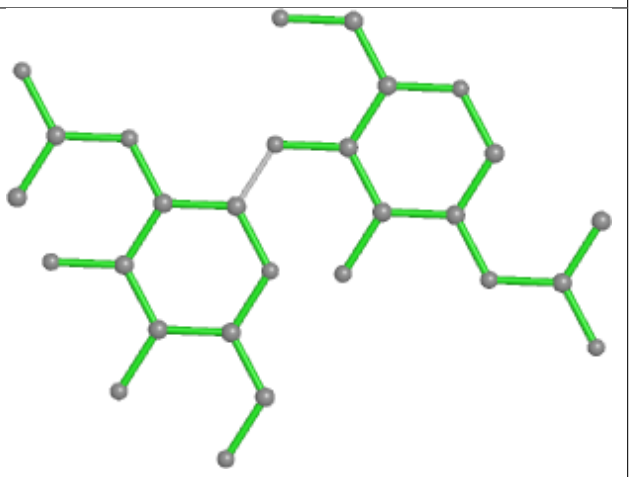
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1	NAG	1	0
5	I	2	NAG	1	0
5	I	1	NAG	1	0
5	F	2	NAG	1	0
5	F	1	NAG	1	0

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

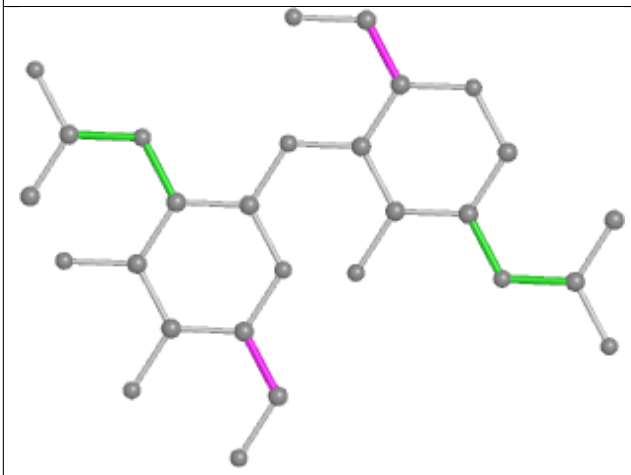
Oligosaccharide Chain F



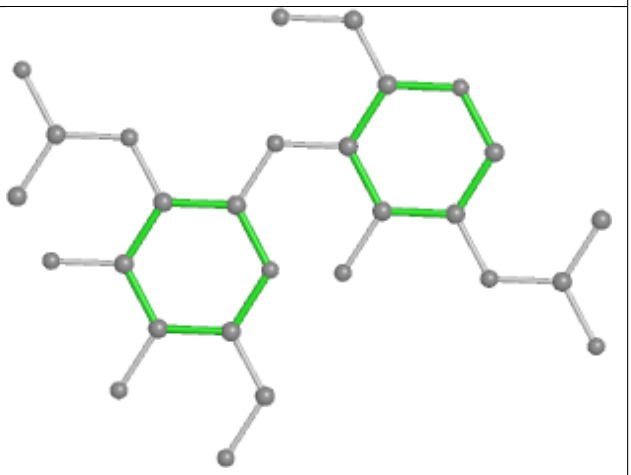
Bond lengths



Bond angles

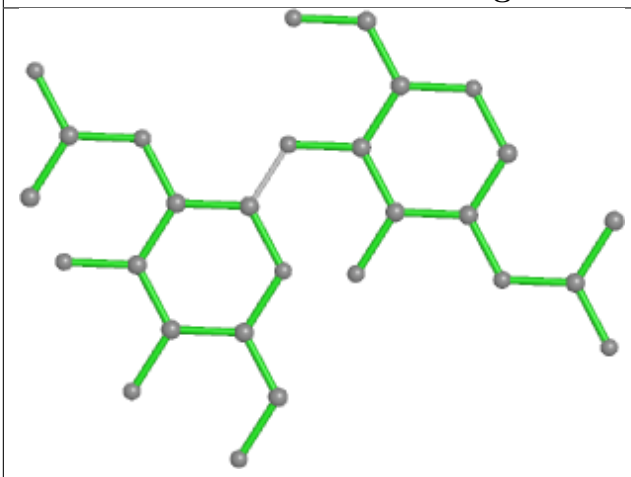


Torsions

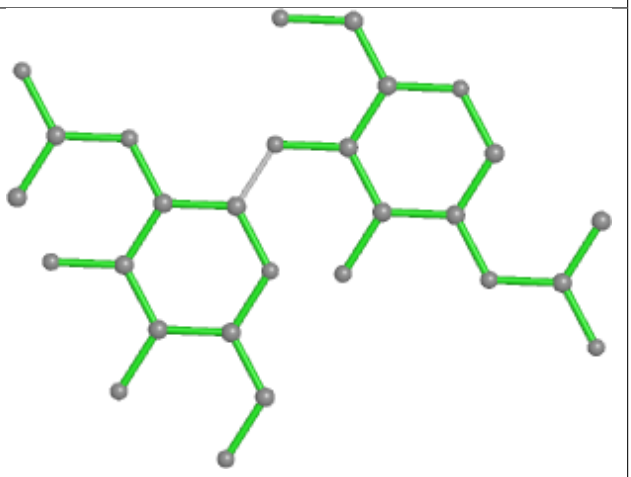


Rings

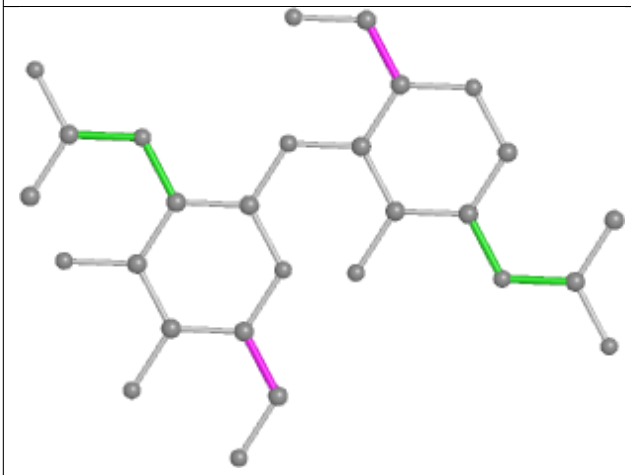
Oligosaccharide Chain G



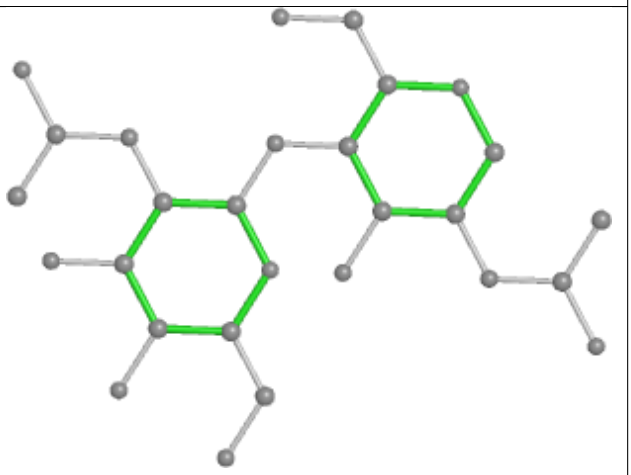
Bond lengths



Bond angles

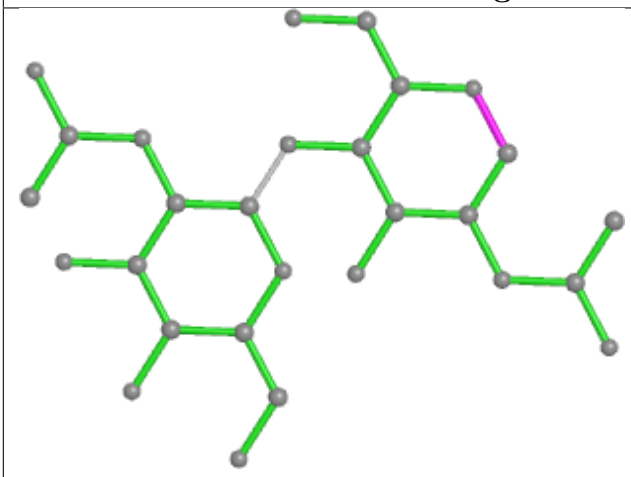


Torsions

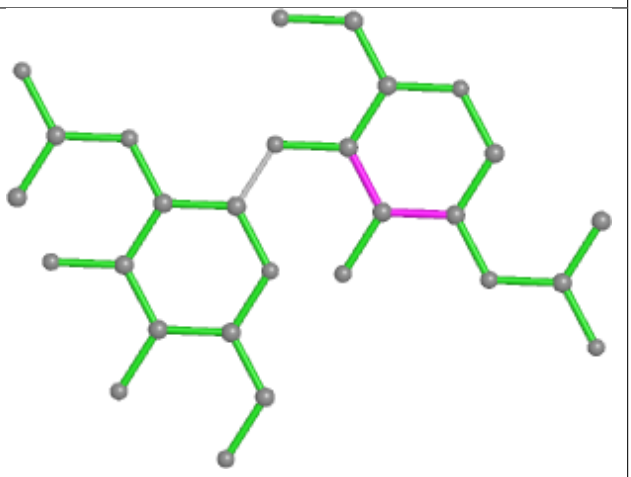


Rings

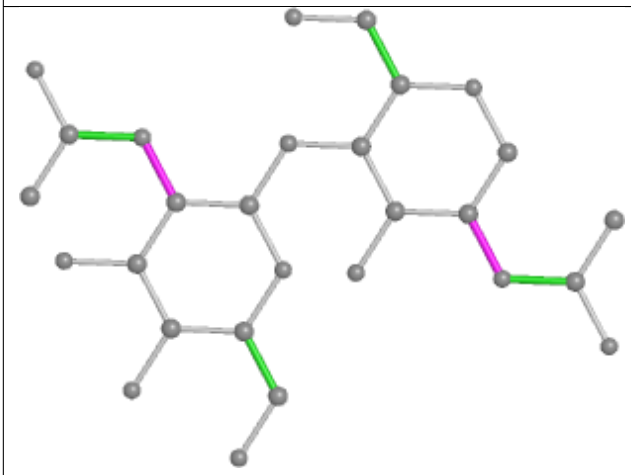
Oligosaccharide Chain H



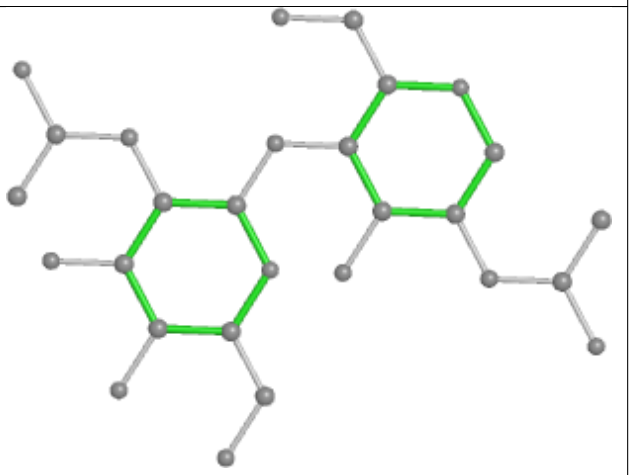
Bond lengths



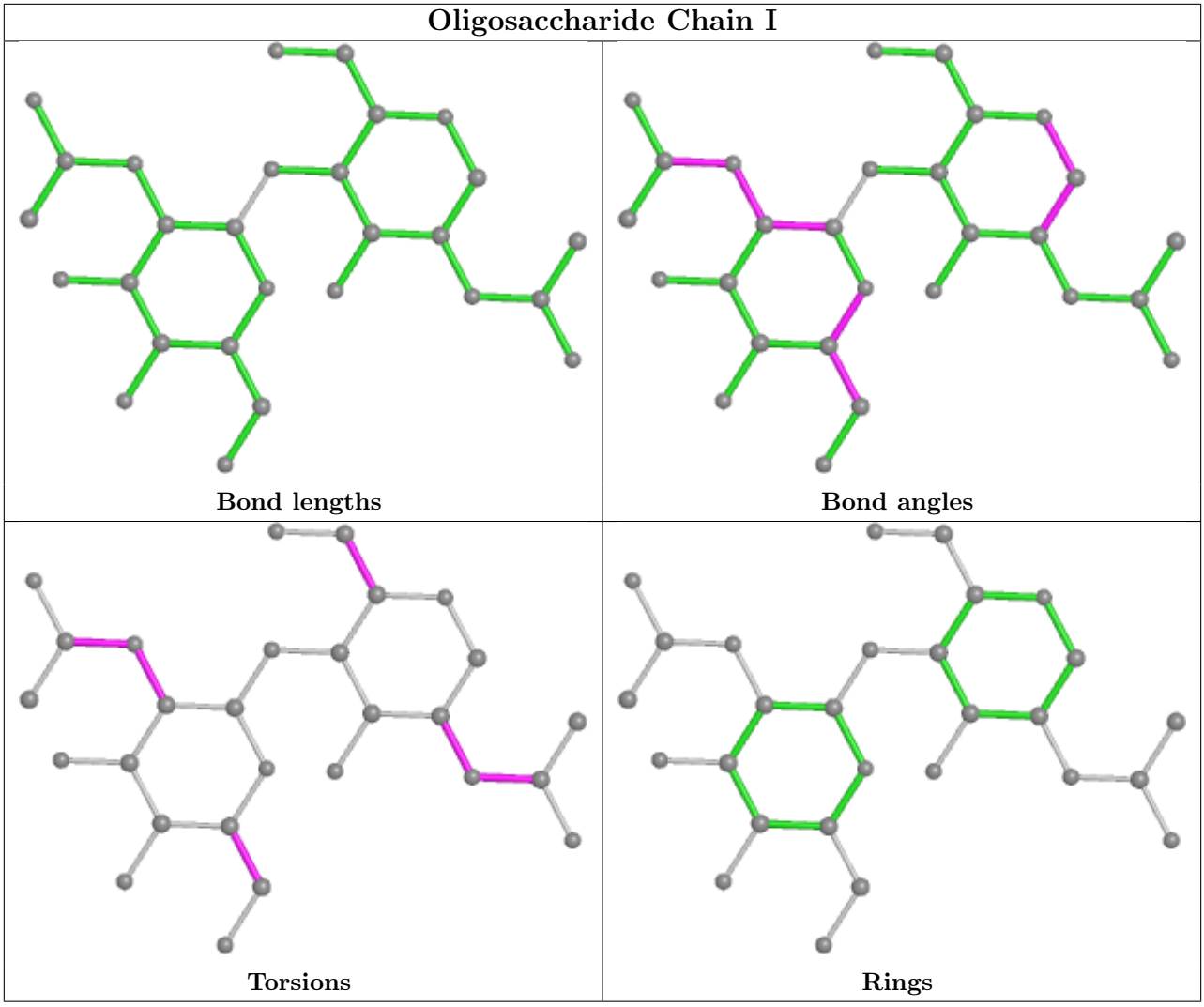
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

2 ligands 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	$\#\|Z\| > 2$
6	NAG	A	901	1	14,14,15	0.37	0	17,19,21	0.54	0
6	NAG	B	901	2	14,14,15	0.19	0	17,19,21	0.35	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
6	NAG	A	901	1	-	1/6/23/26	0/1/1/1
6	NAG	B	901	2	-	3/6/23/26	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
6	B	901	NAG	C8-C7-N2-C2
6	B	901	NAG	O7-C7-N2-C2
6	A	901	NAG	O5-C5-C6-O6
6	B	901	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.

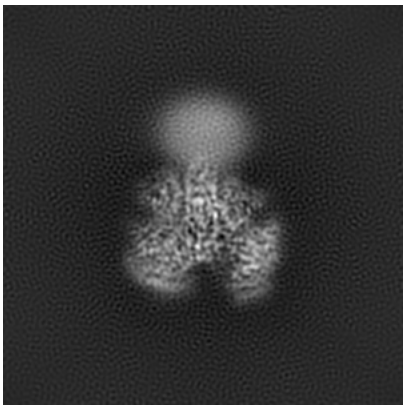
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27961. These allow visual inspection of the internal detail of the map and identification of artifacts.

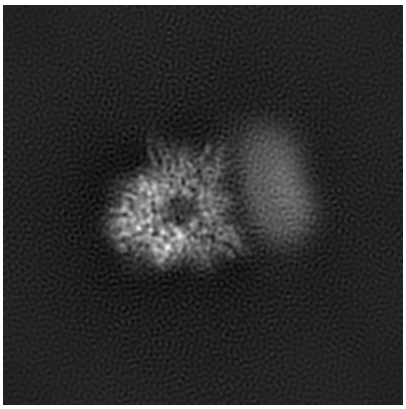
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

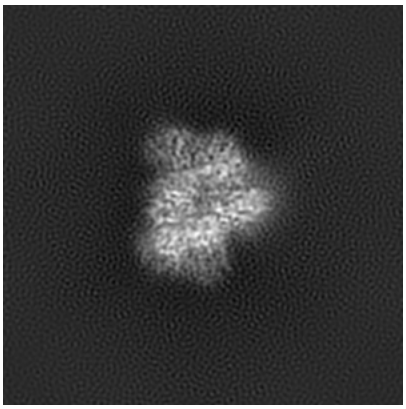
6.1.1 Primary map



X

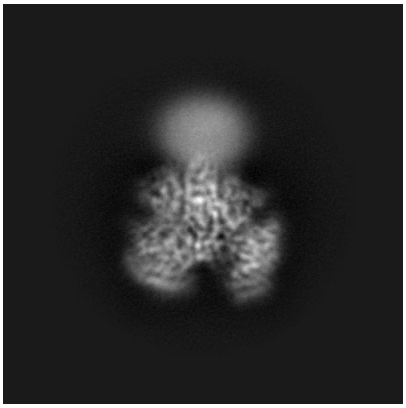


Y

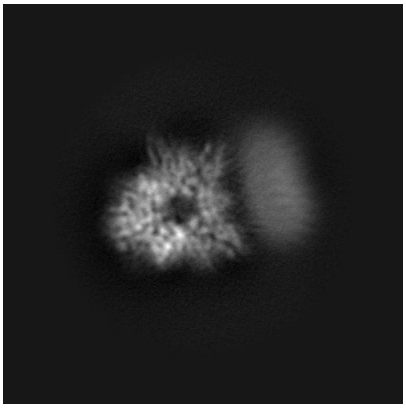


Z

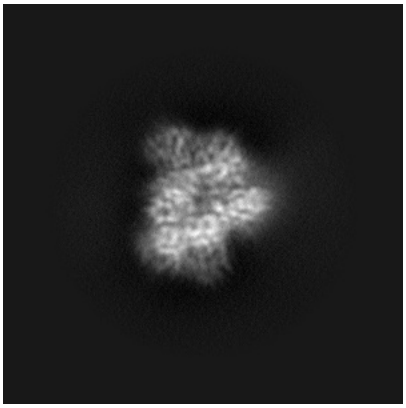
6.1.2 Raw map



X



Y

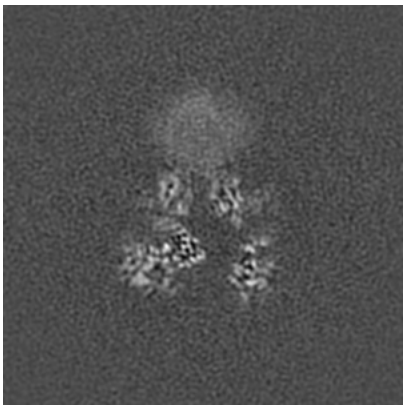


Z

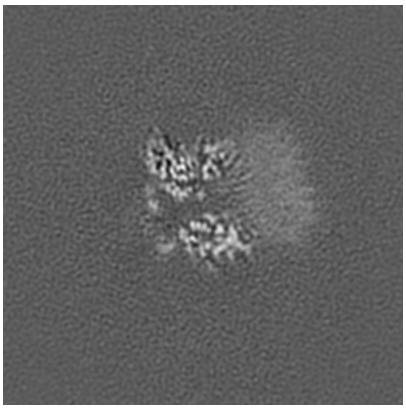
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

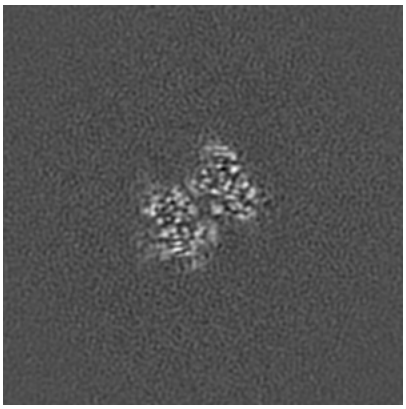
6.2.1 Primary map



X Index: 200

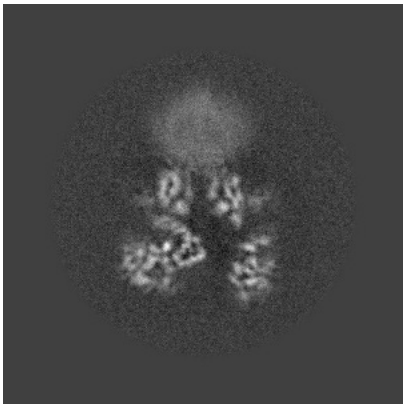


Y Index: 200

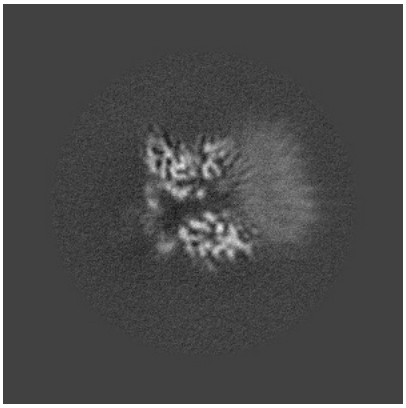


Z Index: 200

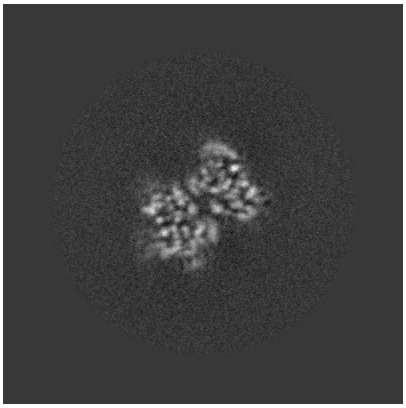
6.2.2 Raw map



X Index: 200



Y Index: 200

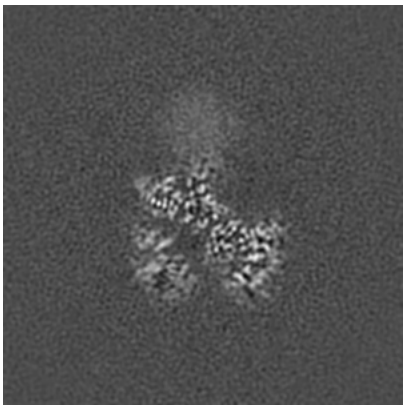


Z Index: 200

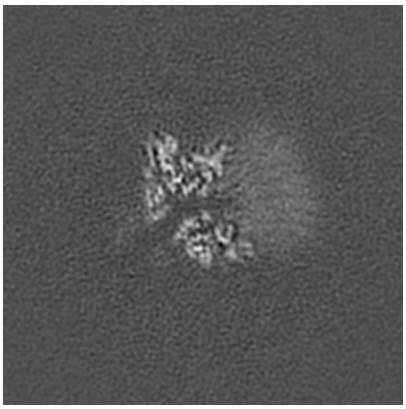
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

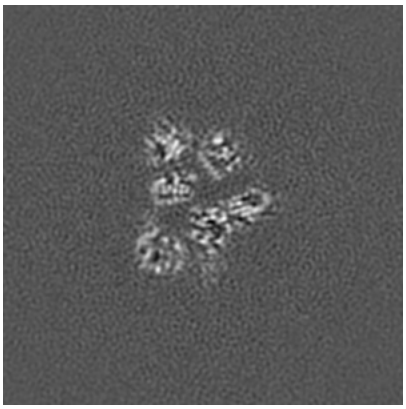
6.3.1 Primary map



X Index: 174

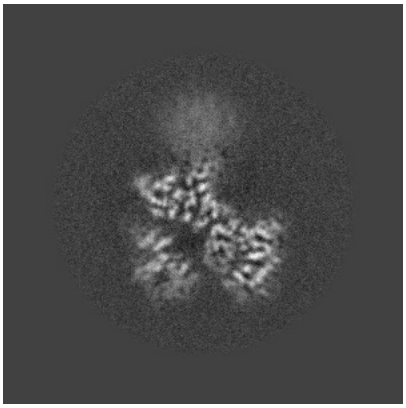


Y Index: 196

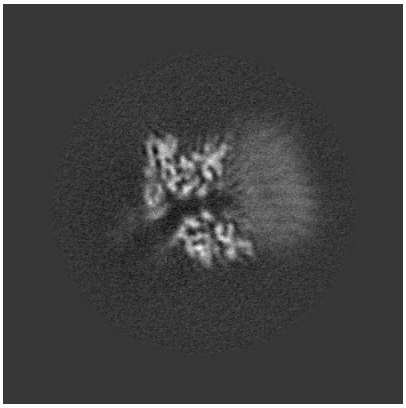


Z Index: 159

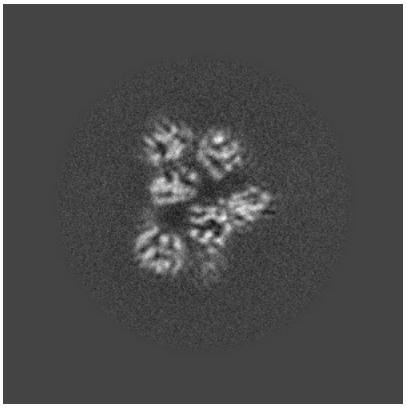
6.3.2 Raw map



X Index: 175



Y Index: 197

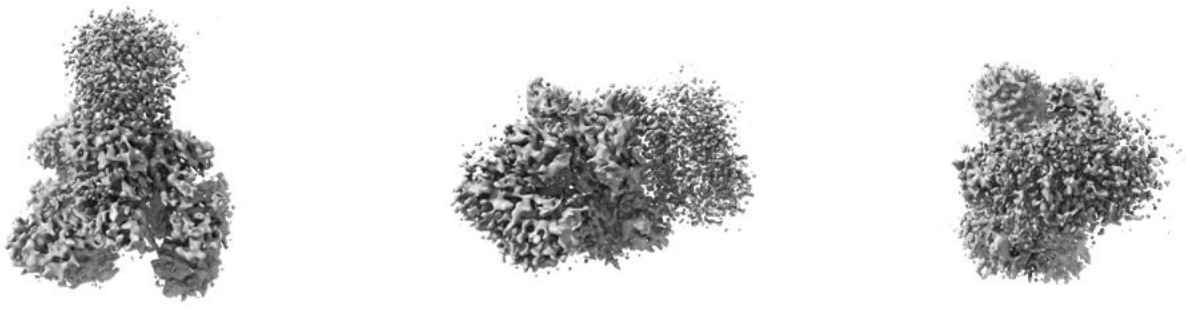


Z Index: 160

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

6.4 Orthogonal surface views (i)

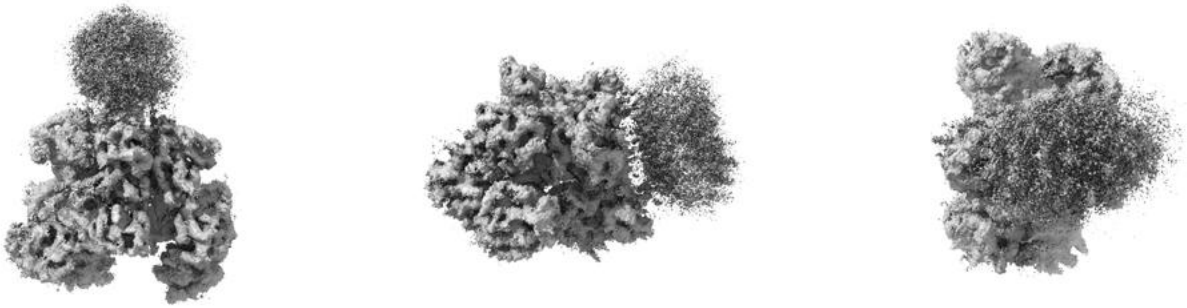
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

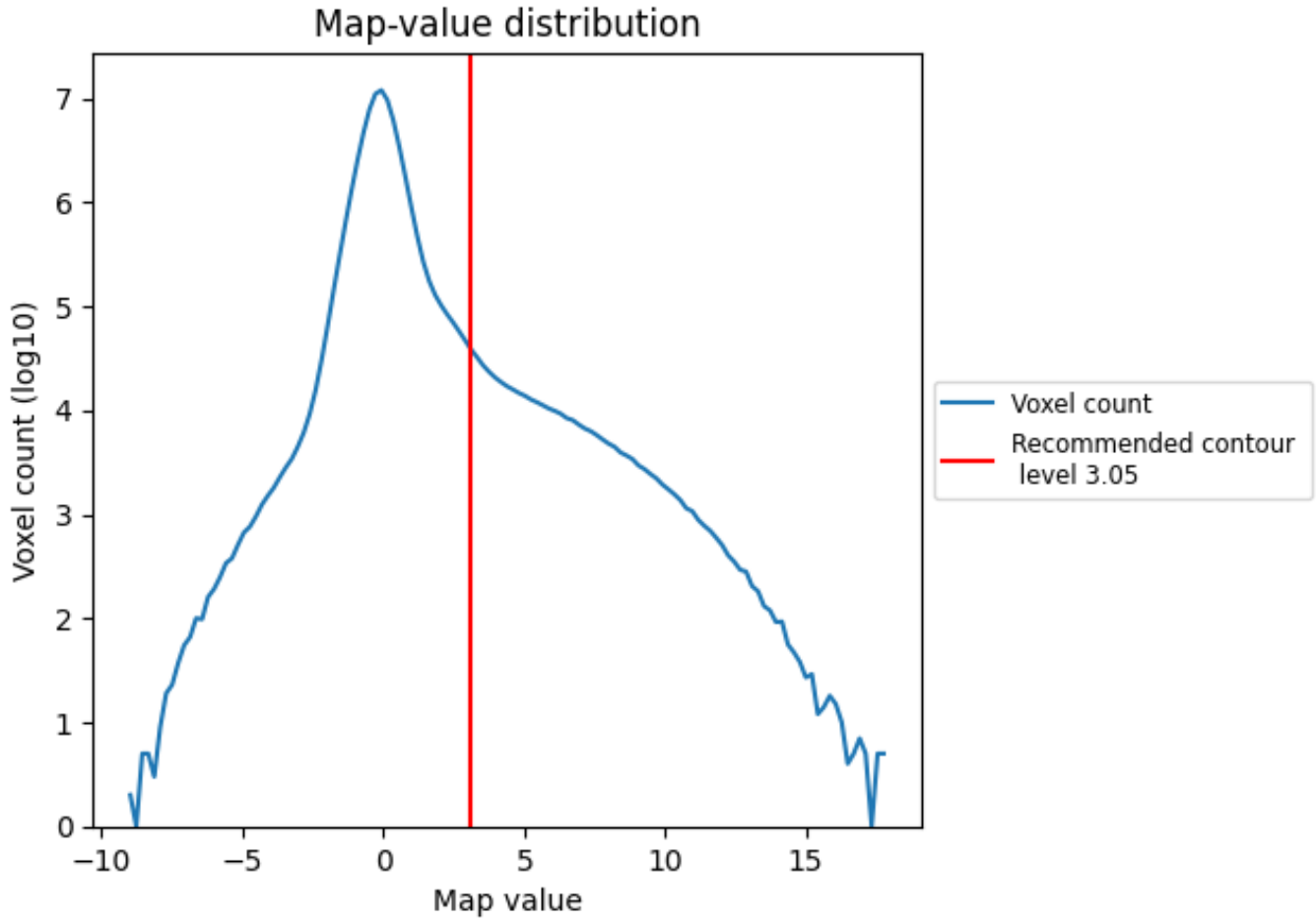
6.5 Mask visualisation (i)

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

7 Map analysis

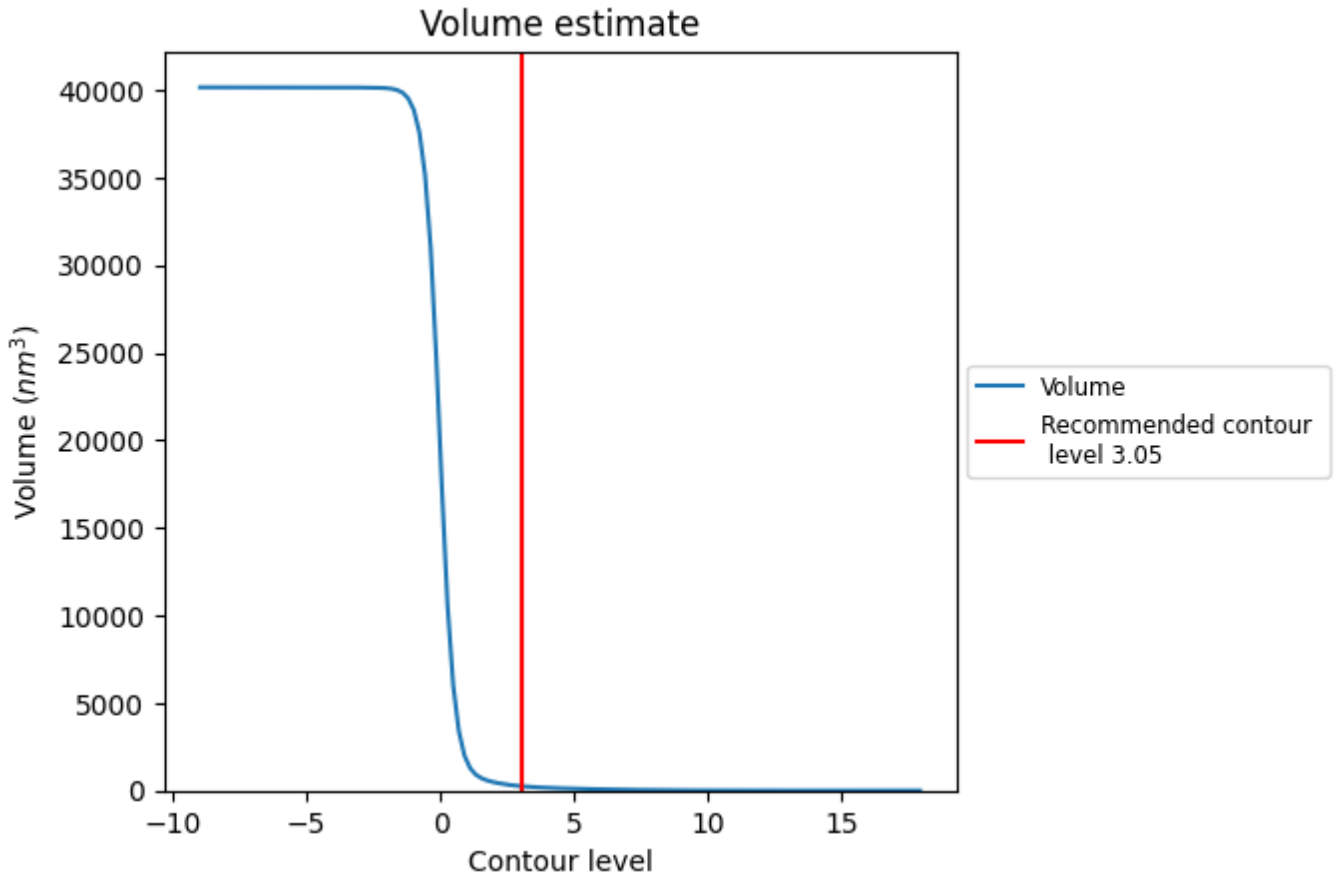
This section contains the results of statistical analysis of the map.

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.

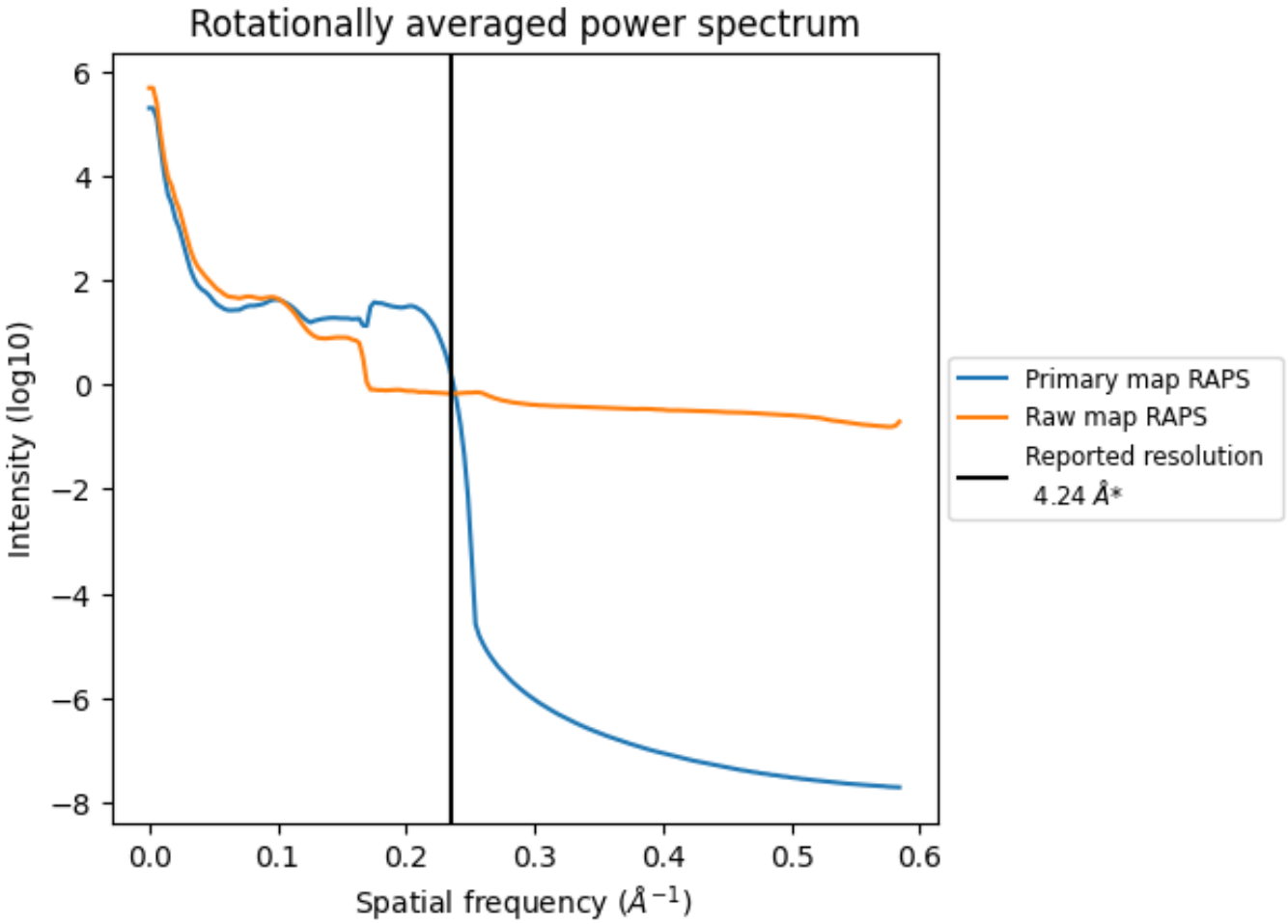
7.2 Volume estimate



The volume at the recommended contour level is 247 nm^3; this corresponds to an approximate mass of 223 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)

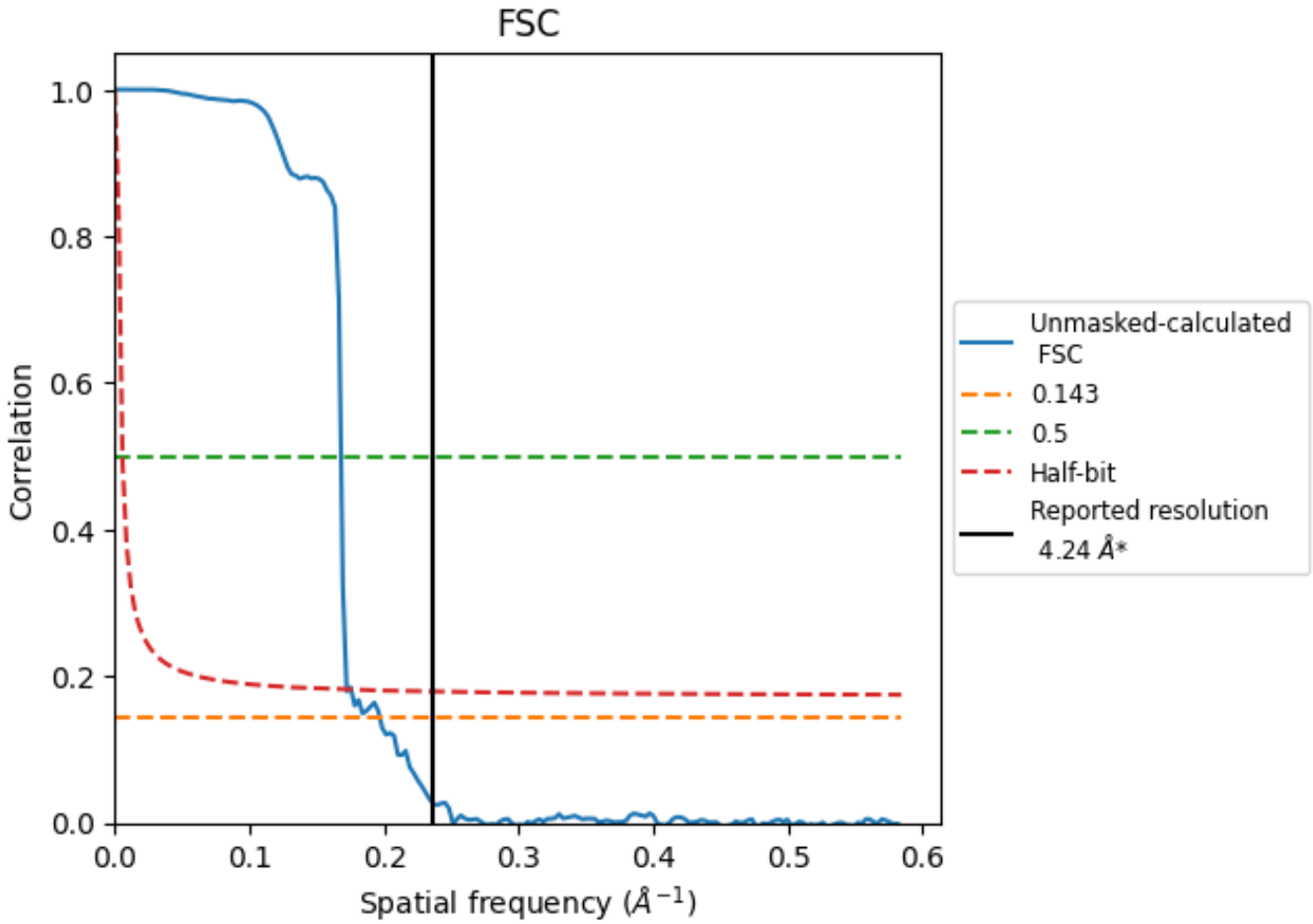


*Reported resolution corresponds to spatial frequency of 0.236 Å^{-1}

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 0.236 Å^{-1}

8.2 Resolution estimates (i)

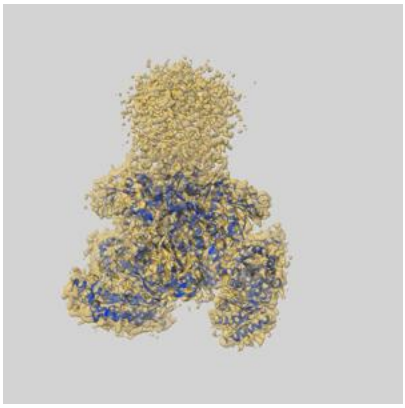
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.24	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.08	5.95	5.80

*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 5.08 differs from the reported value 4.24 by more than 10 %

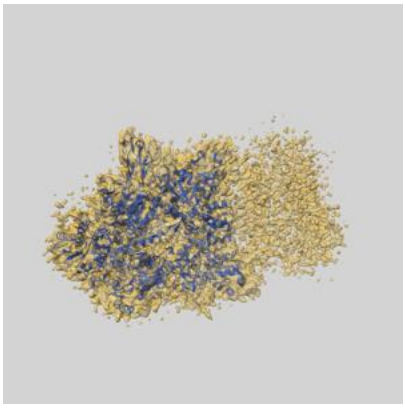
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27961 and PDB model 8E99. Per-residue inclusion information can be found in section 3 on page 10.

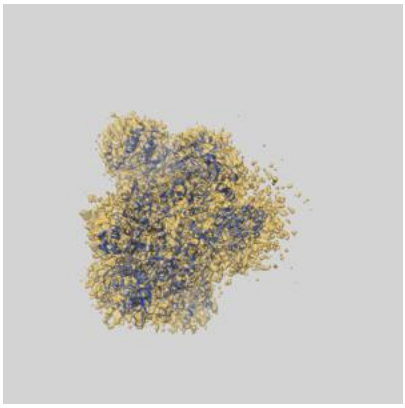
9.1 Map-model overlay



X



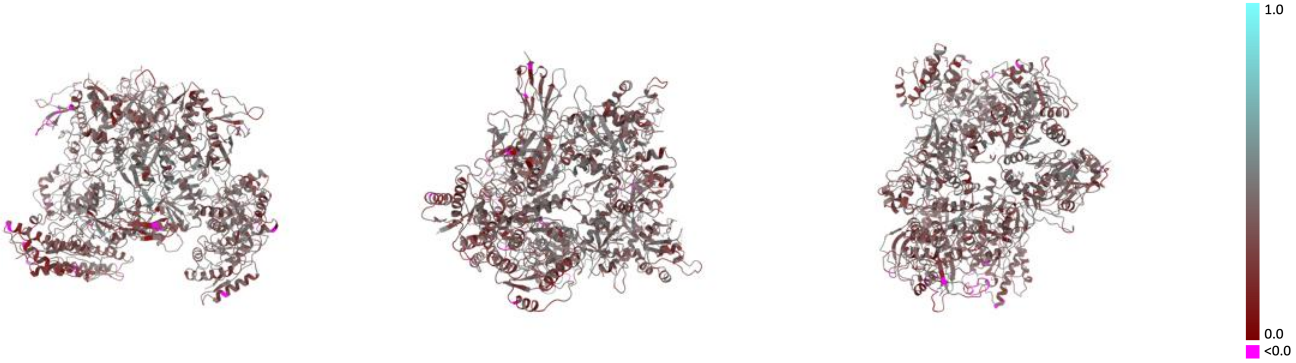
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.05 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.

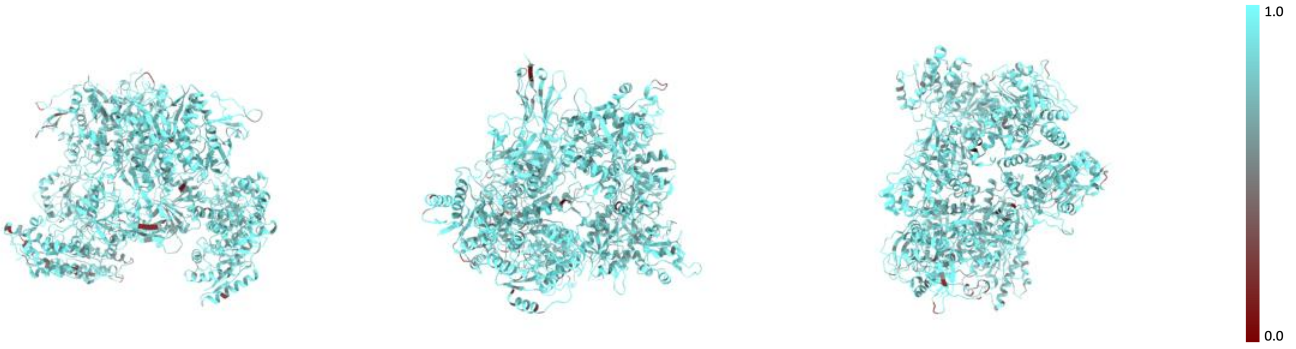
9.2 Q-score mapped to coordinate model



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.

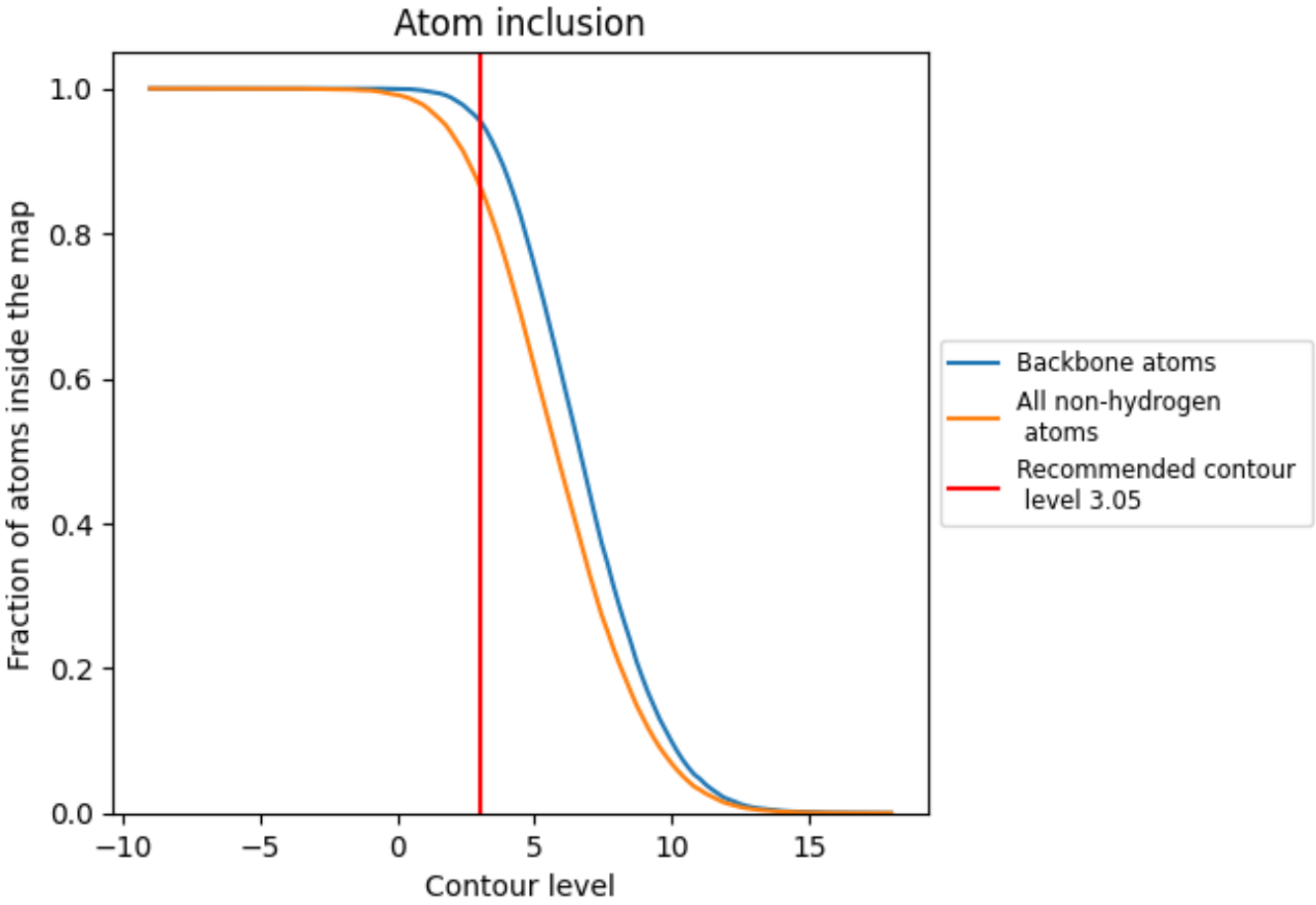
9.3 Atom inclusion mapped to coordinate model



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 (3.05).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 86% 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 (3.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8623	0.3630
A	0.8481	0.3320
B	0.8606	0.3720
C	0.8773	0.3700
D	0.8709	0.3780
E	0.8294	0.3580
F	0.7143	0.3480
G	0.7143	0.3870
H	0.8929	0.3300
I	0.7857	0.4630