



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:54 PM UTC

PDB ID : 7QN9 / pdb_00007qn9
EMDB ID : EMD-14071
Title : Cryo-EM structure of human full-length extrasynaptic alpha4beta3delta GABA(A)R in complex with GABA, histamine and nanobody Nb25 in a pre-open/closed state
Authors : Sente, A.; Desai, R.; Naydenova, K.; Malinauskas, T.; Jounaidi, Y.; Miehl, J.; Zhou, X.; Masiulis, S.; Hardwick, S.W.; Chirgadze, D.Y.; Miller, K.W.; Aricescu, A.R.
Deposited on : 2021-12-20
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

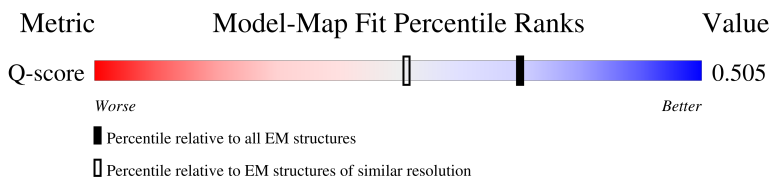
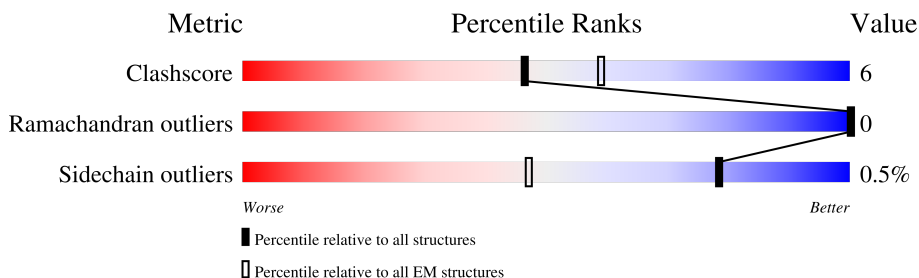
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

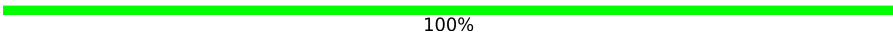
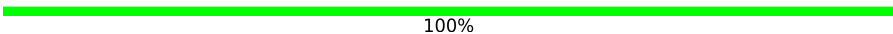
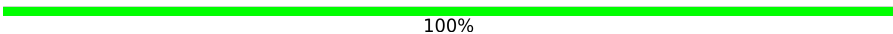
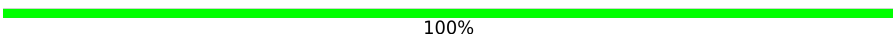
The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	554	 49% 11% 40%
2	B	473	 60% 10% 30%
2	C	473	 60% 10% 30%

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Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	D	473	
3	E	472	
4	L	121	
4	M	121	
5	a	3	
6	b	2	
6	c	2	
6	d	2	
7	F	5	
7	G	5	
7	H	5	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 15696 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 Gamma-aminobutyric acid receptor subunit alpha-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	333	Total	C	N	O	S	0	0
			2693	1758	432	481	22		

- Molecule 2 is a protein called Gamma-aminobutyric acid receptor subunit beta-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	331	Total	C	N	O	S	0	0
			2720	1781	444	479	16		
2	C	331	Total	C	N	O	S	0	0
			2720	1781	444	479	16		
2	D	331	Total	C	N	O	S	0	0
			2720	1781	444	479	16		

- Molecule 3 is a protein called Gamma-aminobutyric acid receptor subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	321	Total	C	N	O	S	2	0
			2579	1678	422	466	13		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	453	GLY	-	expression tag	UNP O14764
E	454	GLY	-	expression tag	UNP O14764
E	455	SER	-	expression tag	UNP O14764
E	456	GLY	-	expression tag	UNP O14764
E	457	GLY	-	expression tag	UNP O14764
E	458	SER	-	expression tag	UNP O14764
E	459	GLY	-	expression tag	UNP O14764
E	460	GLY	-	expression tag	UNP O14764
E	461	SER	-	expression tag	UNP O14764
E	462	GLY	-	expression tag	UNP O14764
E	463	LYS	-	expression tag	UNP O14764

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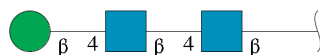
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Chain	Residue	Modelled	Actual	Comment	Reference
E	464	THR	-	expression tag	UNP O14764
E	465	GLU	-	expression tag	UNP O14764
E	466	THR	-	expression tag	UNP O14764
E	467	SER	-	expression tag	UNP O14764
E	468	GLN	-	expression tag	UNP O14764
E	469	VAL	-	expression tag	UNP O14764
E	470	ALA	-	expression tag	UNP O14764
E	471	PRO	-	expression tag	UNP O14764
E	472	ALA	-	expression tag	UNP O14764

- Molecule 4 is a protein called Nanobody Nb25.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	121	Total	C	N	O	S	0	0
			940	593	161	182	4		
4	M	121	Total	C	N	O	S	0	0
			940	593	161	182	4		

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



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

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



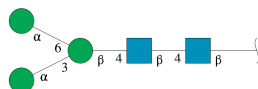
Mol	Chain	Residues	Atoms				AltConf	Trace
6	b	2	Total	C	N	O	0	0
			28	16	2	10		
6	c	2	Total	C	N	O	0	0
			28	16	2	10		

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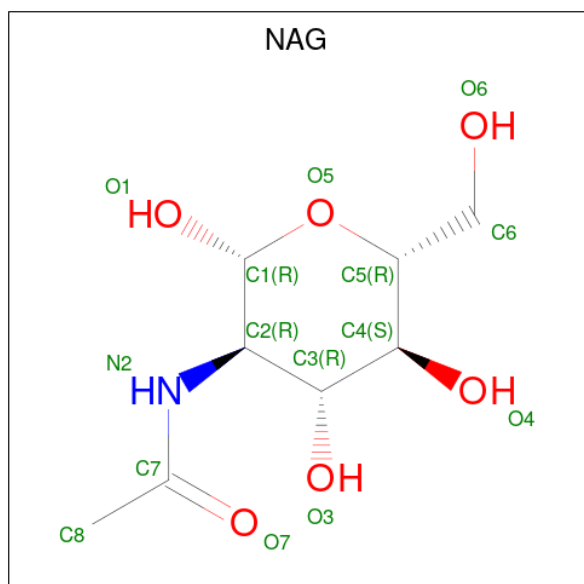
Mol	Chain	Residues	Atoms				AltConf	Trace
6	d	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



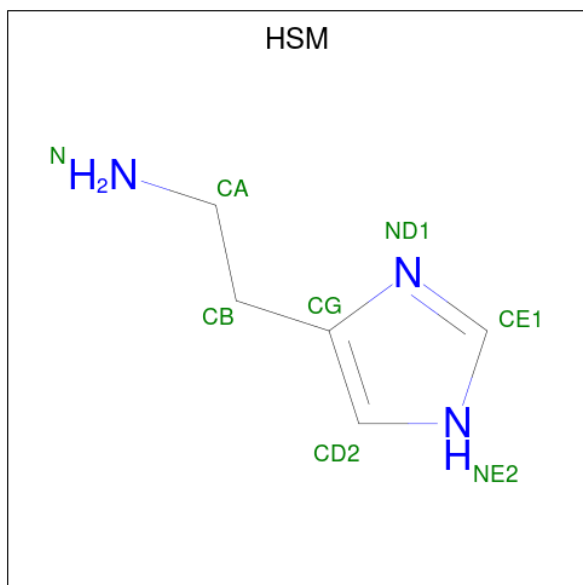
Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			14	8	1	5	

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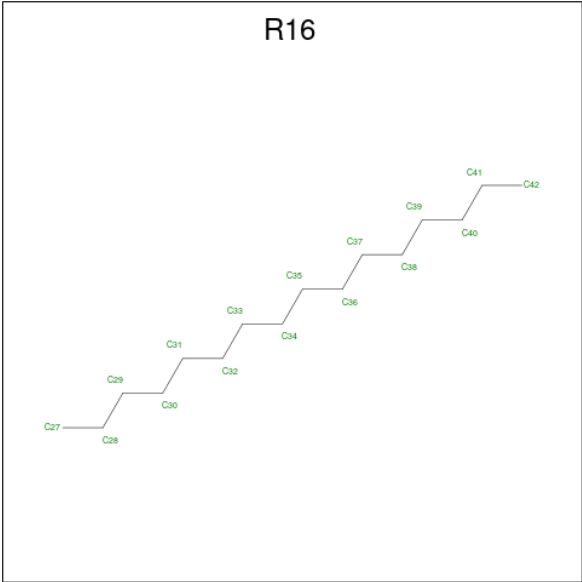
Mol	Chain	Residues	Atoms				AltConf
8	E	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 9 is HISTAMINE (CCD ID: HSM) (formula: $C_5H_9N_3$) (labeled as "Ligand of Interest" by depositor).



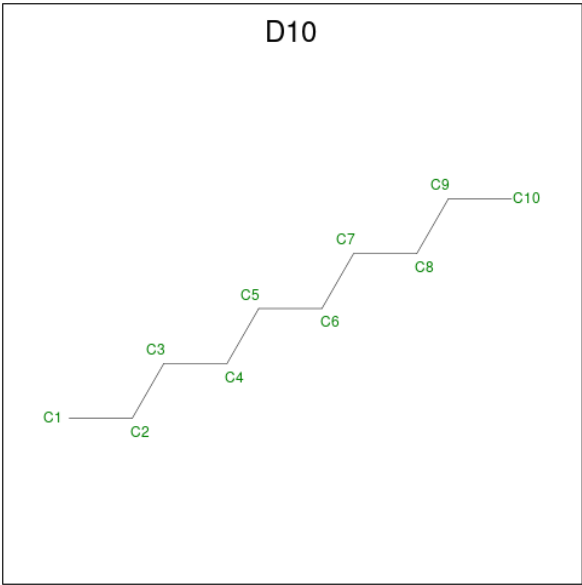
Mol	Chain	Residues	Atoms			AltConf
9	B	1	Total	C	N	0
			8	5	3	
9	C	1	Total	C	N	0
			8	5	3	
9	D	1	Total	C	N	0
			8	5	3	

- Molecule 10 is HEXADECANE (CCD ID: R16) (formula: $C_{16}H_{34}$).



Mol	Chain	Residues	Atoms		AltConf
10	B	1	Total	C	0
			16	16	

- Molecule 11 is DECANE (CCD ID: D10) (formula: C₁₀H₂₂).

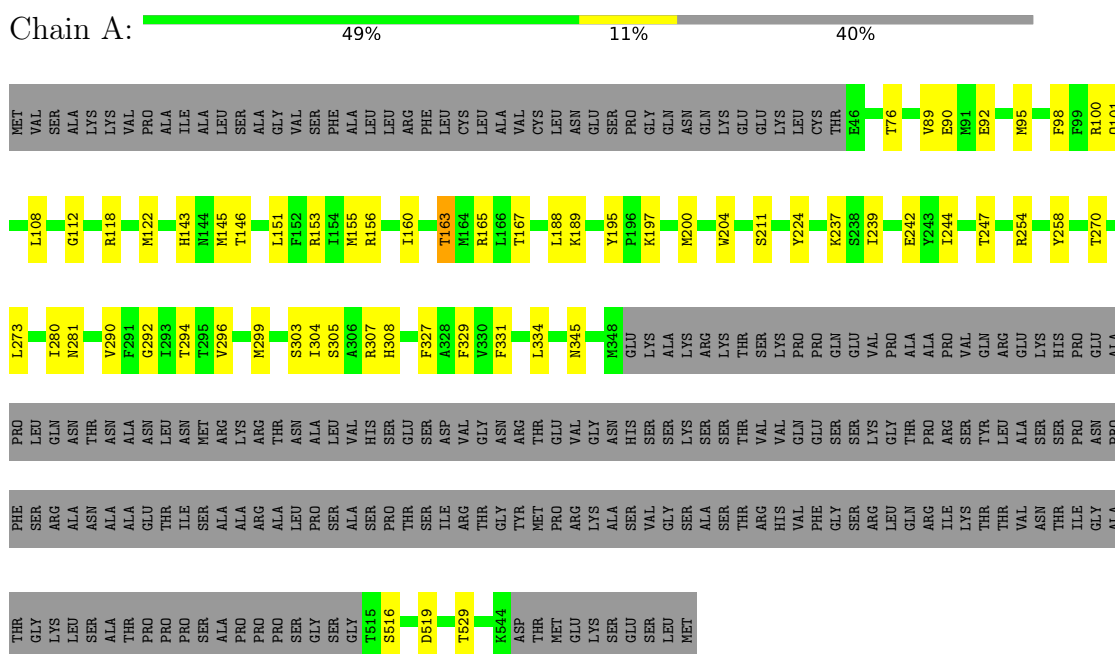


Mol	Chain	Residues	Atoms		AltConf
11	D	1	Total	C	0
			10	10	

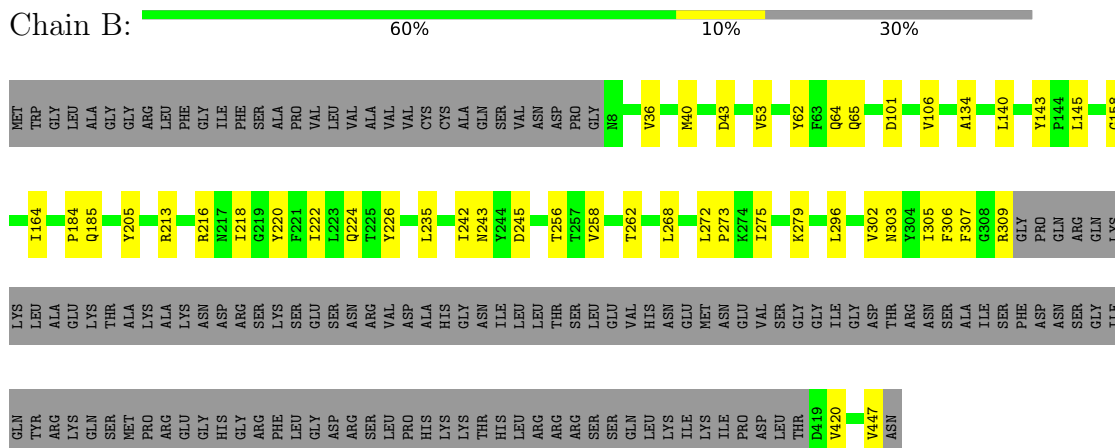
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Gamma-aminobutyric acid receptor subunit alpha-4



• Molecule 2: Gamma-aminobutyric acid receptor subunit beta-3



Chain C:

60% 10% 30%

MET TRP GLY LEU ALA GLY GLY ARG ARG LEU PHE PHE ILE PHE ALA PRO VAL LEU VAL ALA VAL VAL CYS CYS ALA ALA GLN SER SER ASN ASP PRO GLY H8 V36 M40 D43 V53 Y62 F63 Q64 Q65 D101 A134 L140 Y143 P144 L145 I164 P190

LYS LEU LEU ARG ALA GLY LYS THR ALA MET PRO PRO ARG GLY HIS ASP GLY HIS ASP GLY ARG ASP GLY LYS PHE LYS SER GLY SER ASP ARG ARG LEU LEU PRO ASP ALA HIS LYS THR ASN ILE LEU LEU ARG ARG THR SER LEU GLU VAL HIS ASN GLN ILE THR L262 R269 E270 T271 L272 P273 K274 L275 P276 K279 G279 L296 V302 N303 V304 I305 F306 A307 G308 R309 GLY PRO ASN GLN GLN

GLN TYR ARG ALA GLN SER MET PRO ARG GLY HIS ASP GLY HIS ASP GLY ARG ARG ASP ARG ARG LEU LEU PRO ASP HIS LYS THR ASN HIS ILE ARG ARG ARG SER SER GLN GLN THR D419 V420 V447 ASN

Chain D:

Amino Acid	Percentage
MET	60%
TRP	60%
GLY	60%
LEU	60%
ALA	60%
GLY	60%
GLY	60%
ARG	60%
LEU	60%
PHE	60%
GLY	60%
ILE	60%
PHE	60%
SER	60%
ALA	60%
PRO	60%
VAL	60%
LEU	60%
VAL	60%
ALA	60%
VAL	60%
VAL	60%
CYS	60%
CYS	60%
GLN	60%
SER	60%
ASN	60%
ASP	60%
PRO	60%
GLY	60%
H8	60%
M9	60%
V36	60%
M40	60%
D43	60%
V53	60%
Y62	60%
F63	60%
Q64	60%
Q65	60%
D101	60%
R117	60%
A134	60%
L140	60%
Y143	60%
P144	60%
L145	60%
I164	60%
Q185	60%
R216	60%
R217	60%
I218	60%
G219	60%
Y220	60%
F221	60%
I222	60%
L223	60%
T225	60%
Y226	60%
I230	60%
L236	60%
D245	60%
A251	60%
I255	60%
V258	60%
T262	60%
L268	60%
L272	60%
P273	60%
K274	60%
M275	60%
P276	60%
K279	60%
F293	60%
L296	60%
V302	60%
N303	60%
Y304	60%
A305	60%
F306	60%
F307	60%
G308	60%
R309	60%
GLY	60%
PRO	60%
ASN	60%
GLN	60%
ARG	60%
GLN	60%
LYS	60%
LYS	60%
TYR	60%
LEU	60%
ARG	60%
I385	60%

Chain E:

56% 12% 32%

Sequence logo for Chain E, showing amino acid conservation across three regions. The top bar indicates overall conservation: 56% (green), 12% (yellow), and 32% (grey). The logo consists of three rows of amino acid single-letter codes. The first row (top) has a grey background and shows high conservation with large letters for MET, ASP, ALA, PRO, ARG, LEU, ALA, PRO, LEU, LEU, LEU, CYS, ALA, GLN, GLN, LEU, ARG, THR, THR, ARG, ALA, MET, ASN, ASP, ASP, ILE, ILE, GLY, ASP, TYR, VAL, GLY, SER, SER, ASN, LEU, LEU, ILE, SER, TRP, LEU, PRO, ASN. The second row (middle) has a yellow background and shows moderate conservation with letters like Y85, T86, M280, M87, V89, P90, S94, L100, V127, K142, R145, I152, L153, I156, P172, D181, V193, S197, Q200, I203, F221, A231, S234, S236, L239, Y250, T251, T252, Q253, S254, Y255, L260, L261, V262, A265, M264, S268, S272. The third row (bottom) has a grey background and shows low conservation with small letters like R279, T289, M290, T291, T292, L293, M294, R298, L301, L310, D311, W315, V321, F322, A323, A324, L325, V326, D336, T337, ARG, LYS, LYS, GLN, LYS, ALA, LYS, VAL, LYS, VAL, VAL, SER, ARG, PRO, ARG, GLY, GLY, ALA, GLU, MET, ASP, VAL, ARG, ALA, ARG, LEU, ARG, LEU, ILE, ASP, A454, A451, MET, GLY, GLY, VAL.

GLY
GLY
SER
GLY
SER
GLY
LYS
THR
THR
SER
GLN
VAL
ALA
PRO
ALA

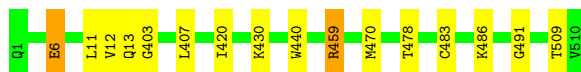
• Molecule 4: Nanobody Nb25

Chain L:  85% 13%



• Molecule 4: Nanobody Nb25

Chain M:  87% 12%

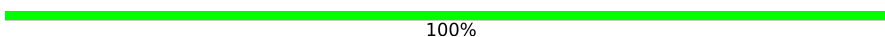


• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  33% 67% 33%

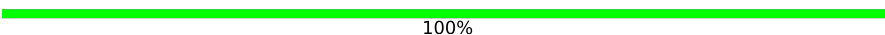


• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  100%

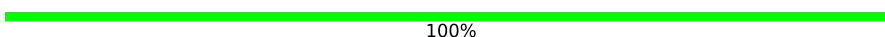


• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  100%



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

Chain d:  100%



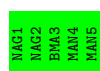
- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  80% 20%

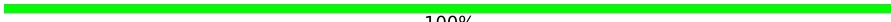


- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%



- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	92694	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.086	Depositor
Minimum map value	-0.031	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	259.84, 259.84, 259.84	wwPDB
Map dimensions	290, 290, 290	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.89599997, 0.89599997, 0.89599997	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: R16, HSM, BMA, MAN, D10, 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	0.08	0/2764	0.20	0/3749
2	B	0.12	0/2792	0.41	0/3798
2	C	0.12	0/2792	0.41	0/3798
2	D	0.12	0/2792	0.41	0/3798
3	E	0.08	0/2655	0.21	0/3620
4	L	0.11	0/963	0.40	0/1304
4	M	0.11	0/963	0.40	0/1304
All	All	0.11	0/15721	0.35	0/21371

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2693	0	2703	42	0
2	B	2720	0	2711	39	0
2	C	2720	0	2711	47	0
2	D	2720	0	2711	42	0
3	E	2579	0	2531	40	0
4	L	940	0	887	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	940	0	887	11	0
5	a	39	0	34	1	0
6	b	28	0	25	0	0
6	c	28	0	25	0	0
6	d	28	0	25	0	0
7	F	61	0	52	1	0
7	G	61	0	52	0	0
7	H	61	0	52	0	0
8	A	14	0	13	0	0
8	E	14	0	13	1	0
9	B	8	0	9	1	0
9	C	8	0	9	0	0
9	D	8	0	9	0	0
10	B	16	0	34	1	0
11	D	10	0	22	1	0
All	All	15696	0	15515	191	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 6.

All (191) 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)
2:C:220:TYR:HB2	2:D:276:PRO:HA	1.56	0.85
2:D:272:LEU:HD13	2:D:279:LYS:HE3	1.59	0.85
2:B:272:LEU:HD13	2:B:279:LYS:HE3	1.59	0.85
2:D:305:ILE:HG23	2:D:309:ARG:HD2	1.59	0.84
2:C:272:LEU:HD13	2:C:279:LYS:HE3	1.59	0.84
2:C:305:ILE:HG23	2:C:309:ARG:HD2	1.59	0.83
2:B:305:ILE:HG23	2:B:309:ARG:HD2	1.59	0.82
2:C:256:THR:OG1	2:D:255:ILE:HG12	1.80	0.82
4:L:440:TRP:O	4:L:459:ARG:NH1	2.16	0.78
4:M:440:TRP:O	4:M:459:ARG:NH1	2.16	0.78
2:D:53:VAL:HA	2:D:273:PRO:HB3	1.72	0.71
2:B:53:VAL:HA	2:B:273:PRO:HB3	1.72	0.69
3:E:172:PRO:HD3	3:E:310:LEU:HB2	1.72	0.69
2:C:53:VAL:HA	2:C:273:PRO:HB3	1.72	0.69
2:C:184:PRO:O	2:D:276:PRO:HG3	1.94	0.68
3:E:145:ARG:HB2	3:E:153:LEU:HB3	1.76	0.68
2:C:243:ASN:HD21	2:D:307:PHE:HB3	1.59	0.67
3:E:68[A]:LEU:HD12	3:E:237:LEU:HD12	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:THR:OG1	2:C:255:ILE:HG12	1.96	0.66
4:M:12:VAL:HG11	4:M:403:GLY:HA3	1.79	0.65
4:L:12:VAL:HG11	4:L:403:GLY:HA3	1.79	0.64
1:A:305:SER:O	1:A:308:HIS:ND1	2.27	0.64
2:C:235:LEU:HB2	2:D:293:PHE:CE1	2.33	0.63
2:B:220:TYR:HB2	2:C:276:PRO:HA	1.81	0.63
2:D:9:MET:HG2	3:E:59:ILE:HG22	1.82	0.62
2:D:117:ARG:HH22	3:E:231:ALA:HB1	1.65	0.61
3:E:142:LYS:HG2	3:E:156:ILE:HG22	1.82	0.61
1:A:145:MET:HE1	2:B:106:VAL:HG23	1.81	0.61
3:E:52:ALA:HB1	3:E:55:PHE:HD2	1.66	0.61
3:E:294:MET:HB3	3:E:298:ARG:HH21	1.67	0.60
2:B:275:ILE:HD11	2:B:279:LYS:HG3	1.84	0.60
2:C:275:ILE:HD11	2:C:279:LYS:HG3	1.84	0.60
2:C:271:THR:HB	2:D:274:LYS:NZ	2.16	0.59
2:D:275:ILE:HD11	2:D:279:LYS:HG3	1.84	0.58
2:B:235:LEU:HD11	2:C:296:LEU:HD23	1.85	0.57
4:L:12:VAL:HG12	4:L:13:GLN:H	1.68	0.57
4:M:12:VAL:HG12	4:M:13:GLN:H	1.68	0.57
3:E:67:ALA:HB3	3:E:94:SER:HB3	1.87	0.56
4:M:478:THR:HG23	4:M:509:THR:HA	1.88	0.56
1:A:151:LEU:HD12	2:B:158:GLY:HA2	1.88	0.56
1:A:197:LYS:HG2	1:A:244:ILE:HG12	1.88	0.55
1:A:95:MET:HE1	1:A:188:LEU:HD22	1.88	0.55
2:B:235:LEU:HD11	2:C:296:LEU:CD2	2.37	0.55
4:L:478:THR:HG23	4:L:509:THR:HA	1.88	0.55
3:E:72:VAL:HA	3:E:89:VAL:HG12	1.88	0.55
3:E:298:ARG:NH1	3:E:311:ASP:OD1	2.40	0.55
2:C:271:THR:HB	2:D:274:LYS:HZ3	1.71	0.54
3:E:85:TYR:HE2	3:E:87:MET:HE3	1.72	0.54
2:C:235:LEU:HD11	2:D:296:LEU:HD23	1.88	0.54
3:E:71:GLU:HB2	3:E:90:PHE:HB2	1.90	0.54
1:A:237:LYS:HG2	1:A:242:GLU:HG3	1.90	0.54
2:B:243:ASN:HD21	2:C:307:PHE:HB3	1.72	0.54
1:A:270:THR:HB	1:A:299:MET:HE2	1.90	0.54
2:C:242:ILE:HA	2:D:303:ASN:ND2	2.23	0.53
3:E:56:ARG:HH21	3:E:64:VAL:HG23	1.73	0.53
2:D:220:TYR:CE1	2:D:224:GLN:HG3	2.44	0.53
2:B:220:TYR:CE1	2:B:224:GLN:HG3	2.44	0.53
1:A:189:LYS:HG2	1:A:247:THR:HG22	1.89	0.53
1:A:100:ARG:HE	9:B:501:HSM:HE2	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:235:LEU:HB2	2:D:293:PHE:HE1	1.73	0.53
2:C:220:TYR:CE1	2:C:224:GLN:HG3	2.44	0.52
1:A:296:VAL:HG11	3:E:264:MET:HE1	1.90	0.52
2:B:143:TYR:CD1	2:B:279:LYS:HD2	2.45	0.52
2:C:143:TYR:CD1	2:C:279:LYS:HD2	2.45	0.52
2:D:143:TYR:CD1	2:D:279:LYS:HD2	2.45	0.52
2:C:220:TYR:CB	2:D:276:PRO:HA	2.36	0.51
2:B:218:ILE:HG21	10:B:502:R16:H281	1.93	0.51
1:A:224:TYR:OH	1:A:254:ARG:NH2	2.44	0.51
2:B:36:VAL:HG13	2:B:164:ILE:HG13	1.93	0.51
1:A:327:PHE:HE1	3:E:260:LEU:HD11	1.76	0.50
3:E:291:THR:HA	3:E:294:MET:HE2	1.93	0.50
1:A:153:ARG:NH2	2:B:205:TYR:OH	2.45	0.50
2:D:306:PHE:CD1	2:D:420:VAL:HG21	2.47	0.50
2:B:306:PHE:CD1	2:B:420:VAL:HG21	2.47	0.50
1:A:290:VAL:O	1:A:294:THR:OG1	2.26	0.50
2:C:36:VAL:HG13	2:C:164:ILE:HG13	1.93	0.50
3:E:70:LEU:N	3:E:200:GLN:OE1	2.44	0.50
4:L:12:VAL:HG12	4:L:13:GLN:N	2.27	0.50
2:B:184:PRO:O	2:C:276:PRO:HG3	2.12	0.49
2:D:36:VAL:HG13	2:D:164:ILE:HG13	1.93	0.49
1:A:112:GLY:O	1:A:156:ARG:NH1	2.35	0.49
2:D:230:ILE:HD13	11:D:501:D10:H22	1.94	0.49
2:C:143:TYR:CZ	2:C:272:LEU:HD21	2.47	0.49
2:C:306:PHE:CD1	2:C:420:VAL:HG21	2.47	0.49
2:B:143:TYR:CZ	2:B:272:LEU:HD21	2.47	0.49
1:A:89:VAL:HG23	1:A:90:GLU:HG2	1.94	0.49
1:A:98:PHE:HE1	1:A:165:ARG:HD2	1.78	0.49
2:D:143:TYR:CZ	2:D:272:LEU:HD21	2.47	0.49
1:A:304:ILE:HA	1:A:307:ARG:HD2	1.95	0.48
4:M:12:VAL:HG12	4:M:13:GLN:N	2.27	0.48
1:A:143:HIS:NE2	1:A:167:THR:OG1	2.44	0.48
1:A:280:ILE:HA	2:B:303:ASN:ND2	2.28	0.48
2:D:145:LEU:HD22	2:D:447:VAL:HG22	1.96	0.48
1:A:118:ARG:HG2	1:A:153:ARG:HG2	1.96	0.48
1:A:516:SER:HB3	1:A:519:ASP:HB2	1.95	0.47
1:A:331:PHE:HD1	3:E:264:MET:HE2	1.79	0.47
1:A:76:THR:HG22	1:A:101:GLN:HG2	1.96	0.47
2:C:145:LEU:HD22	2:C:447:VAL:HG22	1.96	0.47
2:C:243:ASN:ND2	2:D:307:PHE:HB3	2.29	0.47
2:D:185:GLN:OE1	2:D:216:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:ARG:HB2	7:F:1:NAG:H81	1.96	0.47
2:C:235:LEU:HD11	2:D:296:LEU:CD2	2.45	0.47
3:E:67:ALA:HB1	3:E:197:SER:HB3	1.96	0.47
3:E:251:ILE:O	3:E:255:TYR:N	2.34	0.47
4:L:430:LYS:H	4:L:430:LYS:HD2	1.79	0.47
1:A:329:PHE:HE1	1:A:529:THR:HG23	1.80	0.47
2:B:145:LEU:HD22	2:B:447:VAL:HG22	1.96	0.47
3:E:294:MET:O	3:E:298:ARG:NE	2.48	0.47
4:M:430:LYS:H	4:M:430:LYS:HD2	1.79	0.47
1:A:90:GLU:HB2	1:A:92:GLU:HG2	1.96	0.46
1:A:273:LEU:HD11	2:B:296:LEU:HD23	1.97	0.46
2:C:185:GLN:OE1	2:C:216:ARG:NH1	2.48	0.46
1:A:108:LEU:HD12	1:A:160:ILE:HD11	1.96	0.46
4:M:420:ILE:HB	4:M:486:LYS:HB3	1.96	0.46
4:L:420:ILE:HB	4:L:486:LYS:HB3	1.96	0.46
2:B:101:ASP:HA	2:B:134:ALA:HA	1.98	0.46
2:D:302:VAL:HG13	2:D:420:VAL:HG13	1.98	0.46
1:A:327:PHE:CE1	3:E:260:LEU:HD11	2.51	0.46
1:A:281:ASN:H	2:B:303:ASN:HD21	1.63	0.45
2:B:302:VAL:HG13	2:B:420:VAL:HG13	1.98	0.45
3:E:268:SER:OG	3:E:279:ARG:NE	2.38	0.45
2:B:185:GLN:OE1	2:B:216:ARG:NH1	2.48	0.45
1:A:197:LYS:HE3	1:A:244:ILE:HD11	1.98	0.45
3:E:262:VAL:HG12	3:E:321:VAL:HG13	1.98	0.45
2:B:224:GLN:OE1	2:C:269:ARG:NE	2.48	0.45
1:A:204:TRP:HB3	1:A:211:SER:OG	2.16	0.45
2:C:101:ASP:HA	2:C:134:ALA:HA	1.98	0.45
2:D:306:PHE:HD2	2:D:307:PHE:CE1	2.36	0.44
4:L:460:ASP:OD2	4:L:463:LYS:NZ	2.27	0.44
1:A:303:SER:HB2	1:A:307:ARG:HH12	1.83	0.44
2:C:302:VAL:HG13	2:C:420:VAL:HG13	1.98	0.44
2:B:222:ILE:HA	2:B:226:TYR:HB2	1.99	0.44
1:A:292:GLY:HA3	1:A:334:LEU:HD13	1.99	0.44
2:C:40:MET:SD	2:C:65:GLN:HG2	2.58	0.44
2:D:101:ASP:HA	2:D:134:ALA:HA	1.98	0.44
3:E:200:GLN:O	3:E:200:GLN:NE2	2.51	0.44
2:C:222:ILE:HA	2:C:226:TYR:HB2	2.00	0.44
3:E:100:LEU:HD12	3:E:152:ILE:HD11	2.00	0.44
1:A:145:MET:HA	1:A:146:THR:HA	1.73	0.44
3:E:311:ASP:O	3:E:315:TRP:HE3	2.01	0.44
4:M:407:LEU:HD13	4:M:470:MET:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:306:PHE:HD2	2:B:307:PHE:CE1	2.36	0.43
2:D:222:ILE:HA	2:D:226:TYR:HB2	1.99	0.43
2:D:40:MET:SD	2:D:65:GLN:HG2	2.58	0.43
2:D:258:VAL:O	2:D:262:THR:HG23	2.18	0.43
4:L:407:LEU:HD13	4:L:470:MET:HE2	1.99	0.43
2:C:306:PHE:HD2	2:C:307:PHE:CE1	2.36	0.43
4:M:6:GLU:HG2	4:M:483:CYS:HB2	2.01	0.43
2:B:40:MET:SD	2:B:65:GLN:HG2	2.58	0.43
2:C:258:VAL:O	2:C:262:THR:HG23	2.18	0.43
2:D:235:LEU:HD11	3:E:325:LEU:HD23	2.01	0.43
2:B:258:VAL:O	2:B:262:THR:HG23	2.18	0.43
2:C:200:PHE:CE1	4:L:491:GLY:HA2	2.54	0.43
2:C:43:ASP:HB3	2:C:62:TYR:HB2	2.01	0.43
2:B:43:ASP:HB3	2:B:62:TYR:HB2	2.01	0.42
4:L:6:GLU:HG2	4:L:483:CYS:HB2	2.01	0.42
1:A:239:ILE:HG23	3:E:203:ILE:HG21	2.00	0.42
3:E:301:LEU:HD11	3:E:310:LEU:HD23	2.00	0.42
2:D:140:LEU:O	2:D:279:LYS:HG2	2.20	0.42
1:A:155:MET:SD	1:A:155:MET:N	2.92	0.42
2:C:245:ASP:HA	2:C:307:PHE:HZ	1.85	0.42
1:A:195:TYR:HB2	1:A:200:MET:HE2	2.02	0.42
2:B:245:ASP:HA	2:B:307:PHE:HZ	1.84	0.42
3:E:127:VAL:HB	3:E:181:ASP:HB2	2.01	0.42
1:A:151:LEU:HD22	1:A:163:THR:HG23	2.01	0.41
3:E:193:VAL:HG11	8:E:501:NAG:H62	2.01	0.41
2:C:242:ILE:HA	2:D:303:ASN:HD21	1.83	0.41
1:A:258:TYR:HB2	2:B:275:ILE:O	2.19	0.41
2:D:245:ASP:HA	2:D:307:PHE:HZ	1.85	0.41
2:B:268:LEU:HD23	2:B:268:LEU:HA	1.75	0.41
2:B:140:LEU:O	2:B:279:LYS:HG2	2.20	0.41
2:D:43:ASP:HB3	2:D:62:TYR:HB2	2.01	0.41
2:C:180:ARG:NH2	4:M:491:GLY:O	2.50	0.41
2:C:241:TRP:HD1	2:D:304:TYR:CE1	2.38	0.41
3:E:52:ALA:HB1	3:E:55:PHE:CD2	2.51	0.41
3:E:250:TYR:O	3:E:253:GLN:HB3	2.20	0.41
2:C:140:LEU:O	2:C:279:LYS:HG2	2.20	0.41
2:C:218:ILE:HG12	2:C:222:ILE:HG12	2.03	0.41
3:E:221:PHE:CE2	3:E:239:LEU:HD13	2.56	0.41
4:M:11:LEU:HD12	4:M:509:THR:O	2.21	0.41
1:A:345:ASN:HD22	3:E:272:SER:HB2	1.86	0.40
3:E:323:ALA:HA	3:E:326:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:11:LEU:HD12	4:L:509:THR:O	2.21	0.40
2:C:241:TRP:HD1	2:D:304:TYR:CD1	2.39	0.40
3:E:261:LEU:HD23	3:E:261:LEU:HA	1.96	0.40
3:E:289:THR:O	3:E:292:THR:OG1	2.37	0.40
1:A:122:MET:HG2	5:a:2:NAG:H82	2.04	0.40
2:B:218:ILE:HG12	2:B:222:ILE:HG12	2.03	0.40
2:B:242:ILE:HA	2:C:303:ASN:ND2	2.36	0.40
2:D:218:ILE:HG12	2:D:222:ILE:HG12	2.03	0.40
2:D:268:LEU:HD23	2:D:268:LEU:HA	1.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	329/554 (59%)	323 (98%)	6 (2%)	0	100	100
2	B	327/473 (69%)	322 (98%)	5 (2%)	0	100	100
2	C	327/473 (69%)	322 (98%)	5 (2%)	0	100	100
2	D	327/473 (69%)	322 (98%)	5 (2%)	0	100	100
3	E	319/472 (68%)	313 (98%)	6 (2%)	0	100	100
4	L	117/121 (97%)	111 (95%)	6 (5%)	0	100	100
4	M	117/121 (97%)	111 (95%)	6 (5%)	0	100	100
All	All	1863/2687 (69%)	1824 (98%)	39 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	302/486 (62%)	301 (100%)	1 (0%)	86	96
2	B	298/417 (72%)	297 (100%)	1 (0%)	86	96
2	C	298/417 (72%)	297 (100%)	1 (0%)	86	96
2	D	298/417 (72%)	297 (100%)	1 (0%)	86	96
3	E	276/389 (71%)	276 (100%)	0	100	100
4	L	97/97 (100%)	95 (98%)	2 (2%)	47	77
4	M	97/97 (100%)	95 (98%)	2 (2%)	47	77
All	All	1666/2320 (72%)	1658 (100%)	8 (0%)	78	93

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	THR
2	B	64	GLN
2	C	64	GLN
2	D	64	GLN
4	L	6	GLU
4	L	459	ARG
4	M	6	GLU
4	M	459	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	243	ASN
2	B	267	HIS
2	B	303	ASN
2	C	191	HIS
2	C	243	ASN
2	C	267	HIS
2	C	303	ASN

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Mol	Chain	Res	Type
2	D	267	HIS
2	D	303	ASN
3	E	141	ASN
3	E	213	GLN
3	E	233	GLN
3	E	273	GLN
4	L	1	GLN
4	M	1	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](#)

24 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	$\# Z > 2$
7	NAG	F	1	2,7	14,14,15	0.24	0	17,19,21	0.44	0
7	NAG	F	2	7	14,14,15	0.24	0	17,19,21	0.49	0
7	BMA	F	3	7	11,11,12	0.60	0	15,15,17	0.73	0
7	MAN	F	4	7	11,11,12	0.20	0	15,15,17	0.22	0
7	MAN	F	5	7	11,11,12	0.18	0	15,15,17	0.23	0
7	NAG	G	1	2,7	14,14,15	0.23	0	17,19,21	0.41	0
7	NAG	G	2	7	14,14,15	0.23	0	17,19,21	0.49	0
7	BMA	G	3	7	11,11,12	0.58	0	15,15,17	0.79	0
7	MAN	G	4	7	11,11,12	0.21	0	15,15,17	0.23	0
7	MAN	G	5	7	11,11,12	0.19	0	15,15,17	0.23	0
7	NAG	H	1	2,7	14,14,15	0.25	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	H	2	7	14,14,15	0.23	0	17,19,21	0.52	0
7	BMA	H	3	7	11,11,12	0.57	0	15,15,17	0.83	0
7	MAN	H	4	7	11,11,12	0.20	0	15,15,17	0.23	0
7	MAN	H	5	7	11,11,12	0.21	0	15,15,17	0.23	0
5	NAG	a	1	1,5	14,14,15	0.24	0	17,19,21	0.45	0
5	NAG	a	2	5	14,14,15	0.22	0	17,19,21	0.44	0
5	BMA	a	3	5	11,11,12	0.54	0	15,15,17	0.72	0
6	NAG	b	1	6,2	14,14,15	0.24	0	17,19,21	0.43	0
6	NAG	b	2	6	14,14,15	0.24	0	17,19,21	0.44	0
6	NAG	c	1	6,2	14,14,15	0.23	0	17,19,21	0.41	0
6	NAG	c	2	6	14,14,15	0.22	0	17,19,21	0.44	0
6	NAG	d	1	6,2	14,14,15	0.23	0	17,19,21	0.39	0
6	NAG	d	2	6	14,14,15	0.22	0	17,19,21	0.44	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
7	NAG	F	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	F	2	7	-	0/6/23/26	0/1/1/1
7	BMA	F	3	7	-	0/2/19/22	0/1/1/1
7	MAN	F	4	7	-	0/2/19/22	0/1/1/1
7	MAN	F	5	7	-	0/2/19/22	0/1/1/1
7	NAG	G	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	G	2	7	-	0/6/23/26	0/1/1/1
7	BMA	G	3	7	-	2/2/19/22	0/1/1/1
7	MAN	G	4	7	-	0/2/19/22	0/1/1/1
7	MAN	G	5	7	-	0/2/19/22	0/1/1/1
7	NAG	H	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	H	2	7	-	0/6/23/26	0/1/1/1
7	BMA	H	3	7	-	2/2/19/22	0/1/1/1
7	MAN	H	4	7	-	0/2/19/22	0/1/1/1
7	MAN	H	5	7	-	0/2/19/22	0/1/1/1
5	NAG	a	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	a	2	5	-	0/6/23/26	0/1/1/1
5	BMA	a	3	5	-	0/2/19/22	0/1/1/1
6	NAG	b	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	b	2	6	-	0/6/23/26	0/1/1/1
6	NAG	c	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	c	2	6	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	d	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	d	2	6	-	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 (5) torsion outliers are listed below:

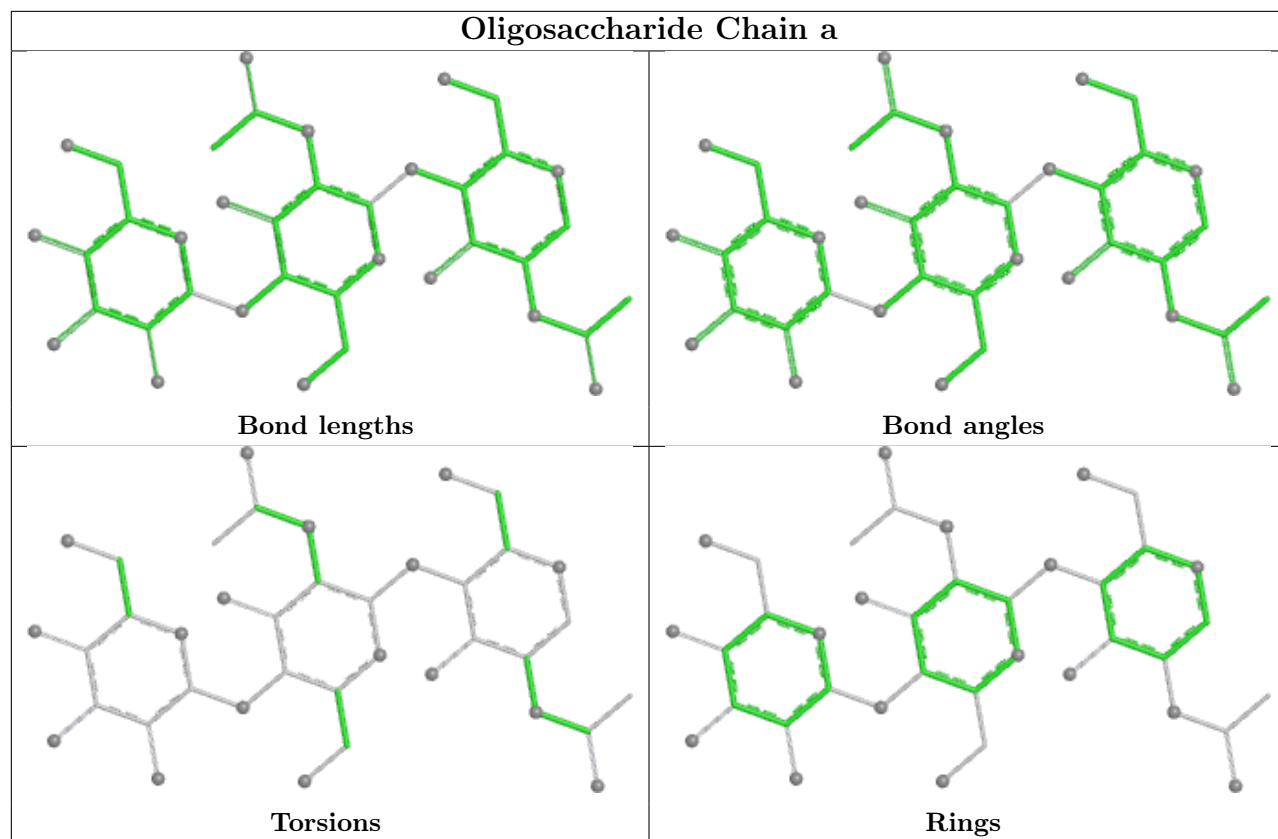
Mol	Chain	Res	Type	Atoms
7	H	3	BMA	C4-C5-C6-O6
7	H	3	BMA	O5-C5-C6-O6
7	G	3	BMA	C4-C5-C6-O6
7	G	3	BMA	O5-C5-C6-O6
6	c	2	NAG	C1-C2-N2-C7

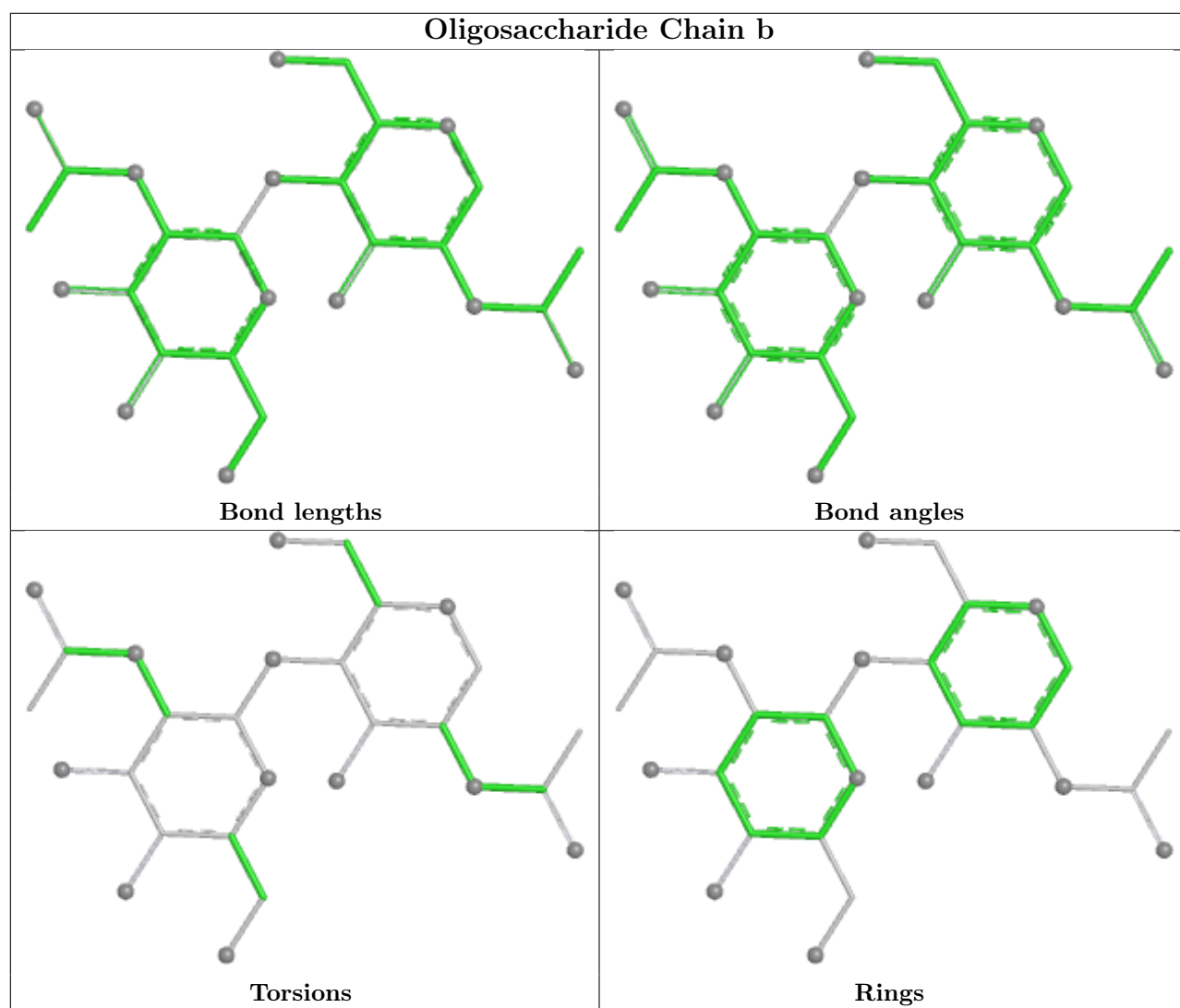
There are no ring outliers.

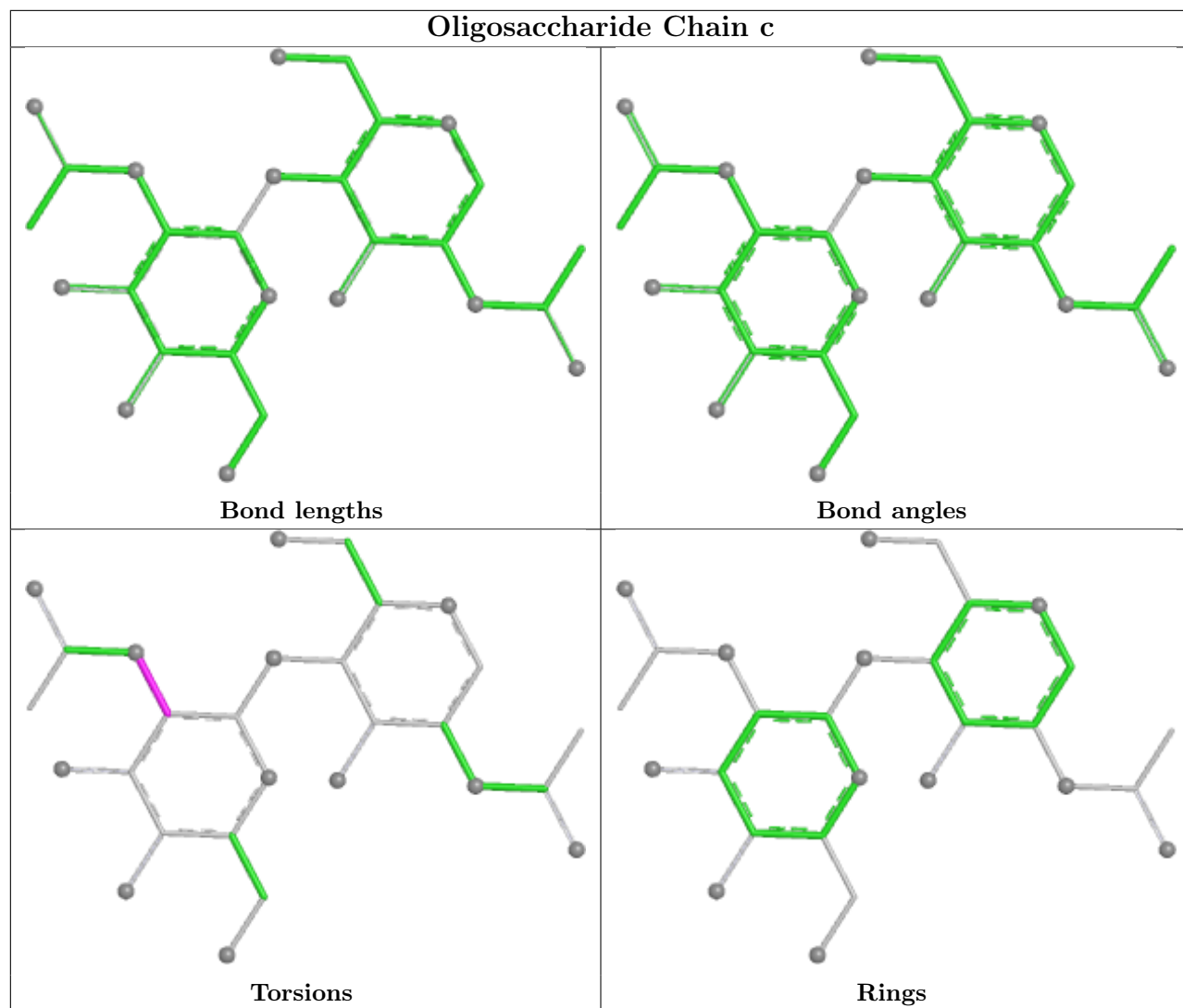
2 monomers are involved in 2 short contacts:

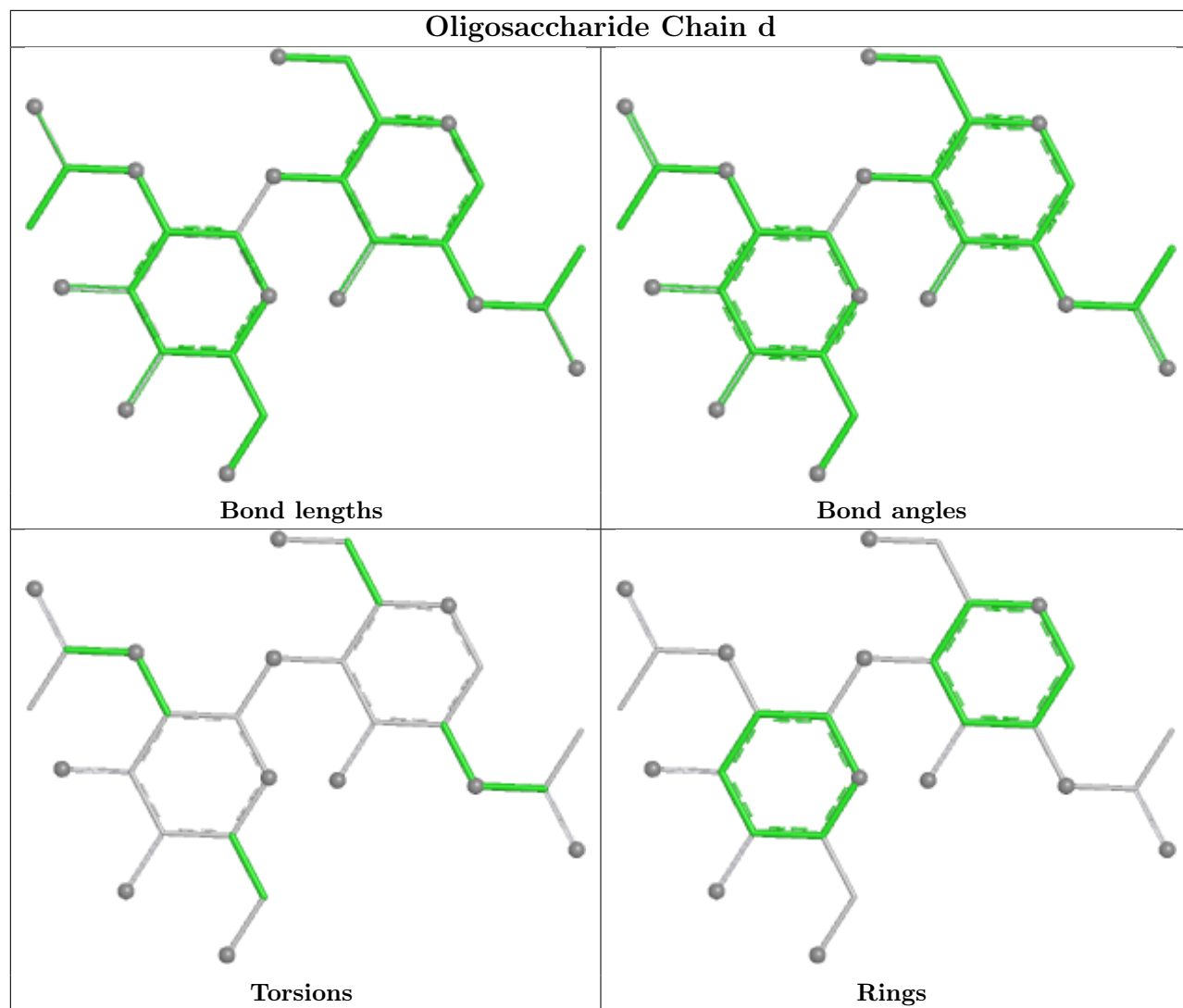
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	1	NAG	1	0
5	a	2	NAG	1	0

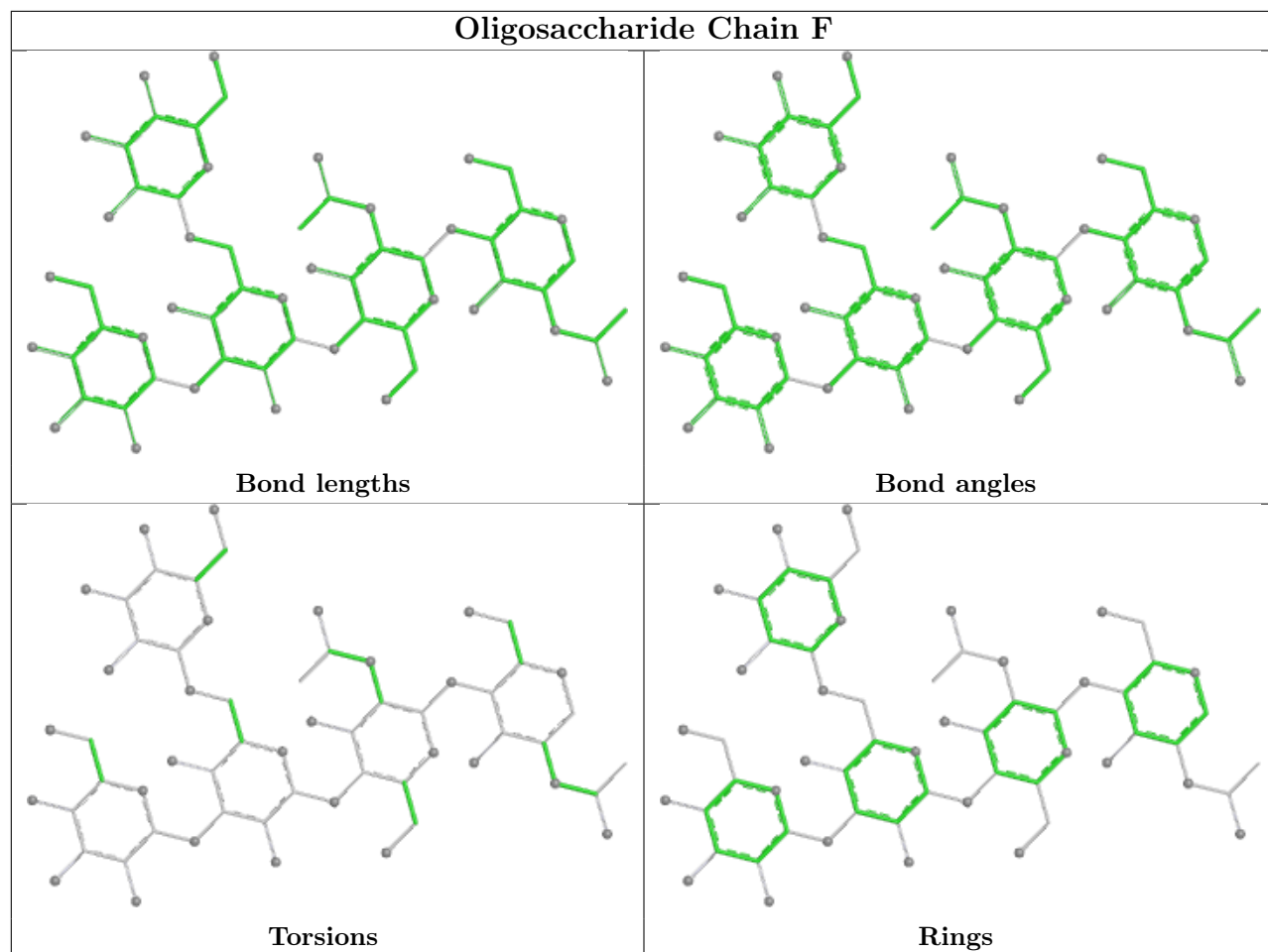
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

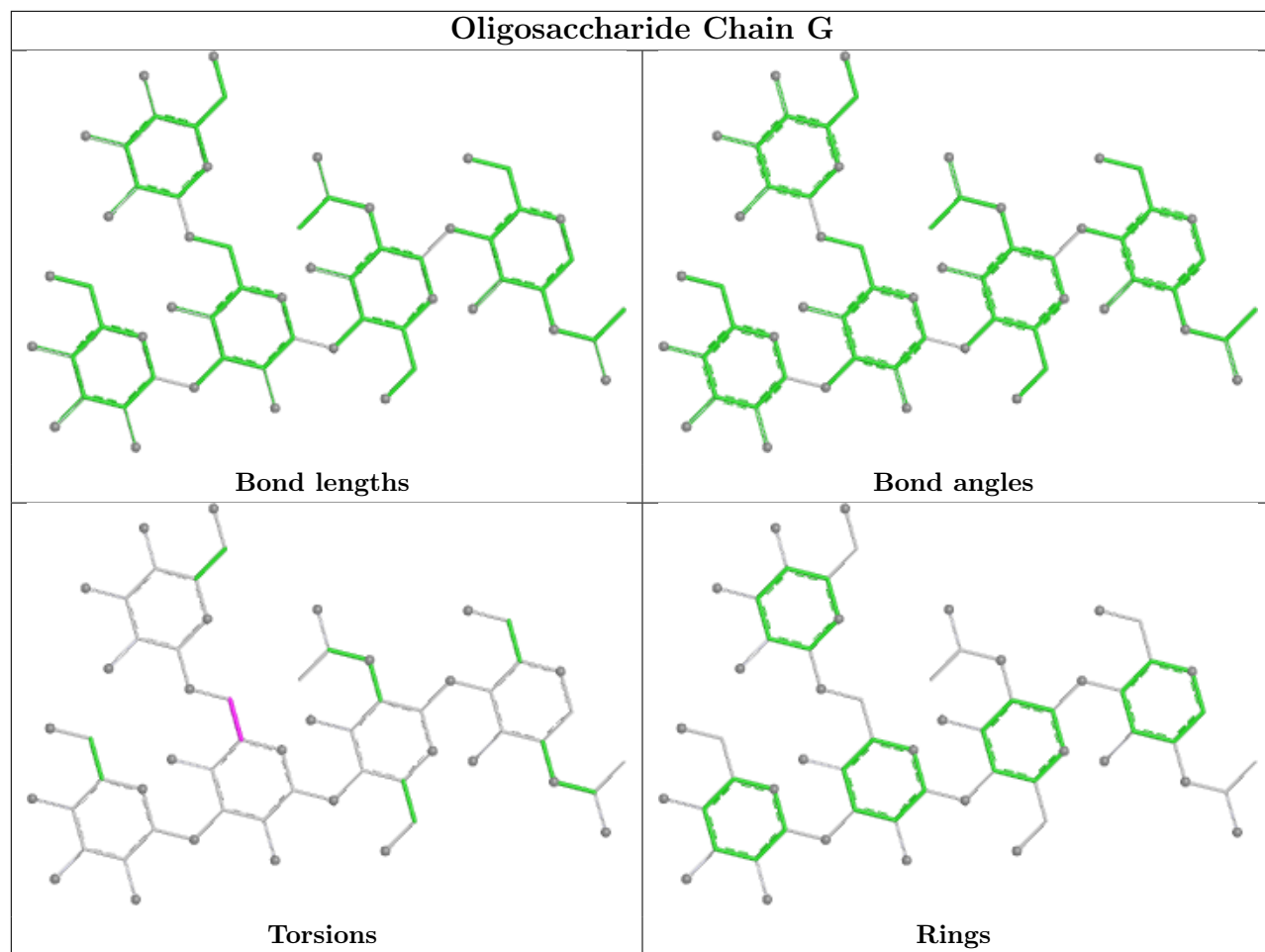


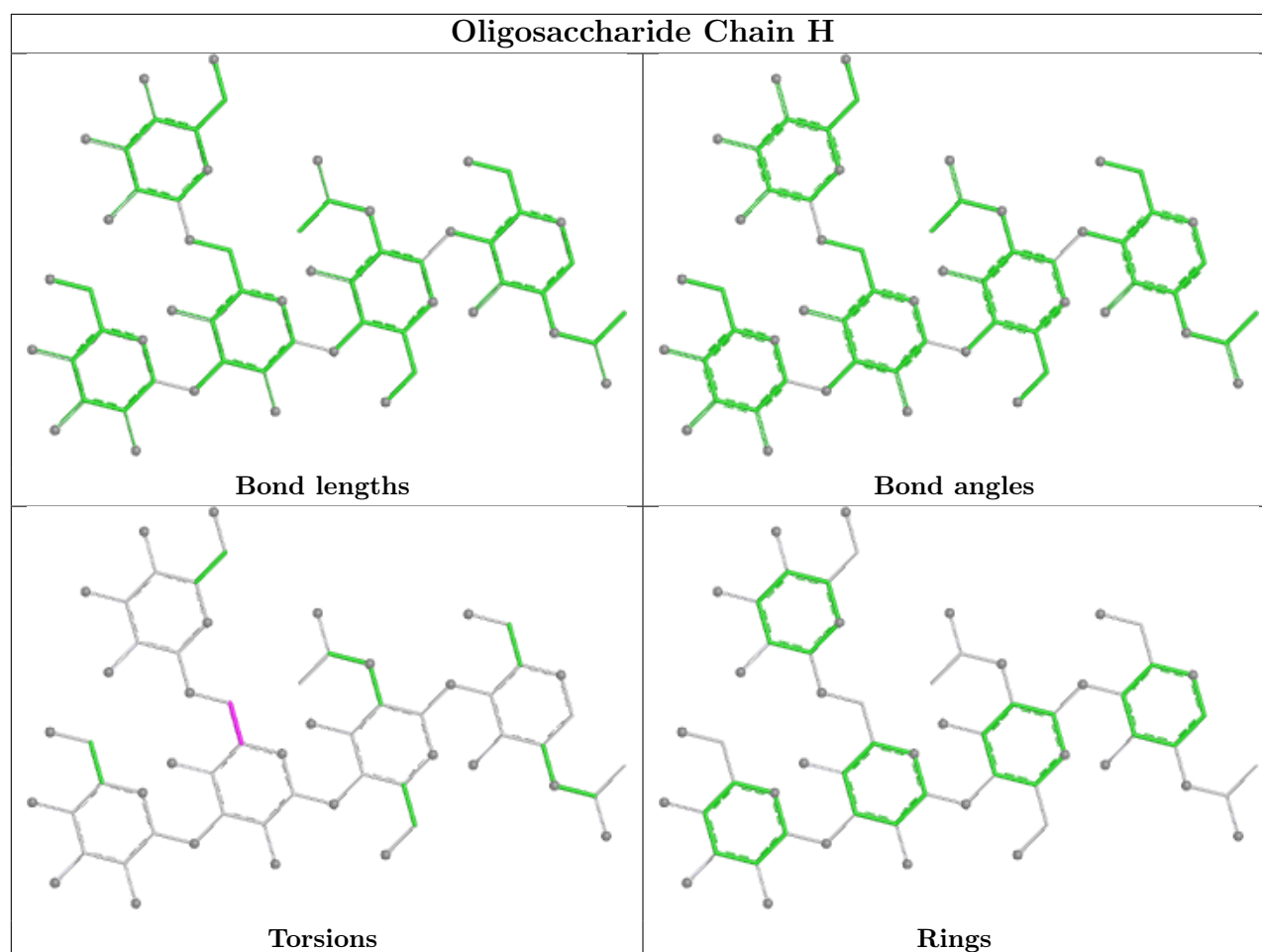












5.6 Ligand geometry [i](#)

7 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	$\# Z > 2$
9	HSM	B	501	-	8,8,8	0.23	0	9,9,9	0.34	0
10	R16	B	502	-	15,15,15	0.12	0	14,14,14	0.11	0
9	HSM	C	501	-	8,8,8	0.24	0	9,9,9	0.33	0
11	D10	D	501	-	9,9,9	0.12	0	8,8,8	0.09	0
8	NAG	A	601	1	14,14,15	0.23	0	17,19,21	0.45	0
9	HSM	D	502	-	8,8,8	0.24	0	9,9,9	0.33	0
8	NAG	E	501	3	14,14,15	0.23	0	17,19,21	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	HSM	B	501	-	-	0/3/3/3	0/1/1/1
10	R16	B	502	-	-	0/13/13/13	-
9	HSM	C	501	-	-	2/3/3/3	0/1/1/1
11	D10	D	501	-	-	0/7/7/7	-
8	NAG	A	601	1	-	1/6/23/26	0/1/1/1
9	HSM	D	502	-	-	2/3/3/3	0/1/1/1
8	NAG	E	501	3	-	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 (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	501	HSM	CA-CB-CG-ND1
9	C	501	HSM	CA-CB-CG-CD2
9	D	502	HSM	CA-CB-CG-ND1
9	D	502	HSM	CA-CB-CG-CD2
8	A	601	NAG	O5-C5-C6-O6

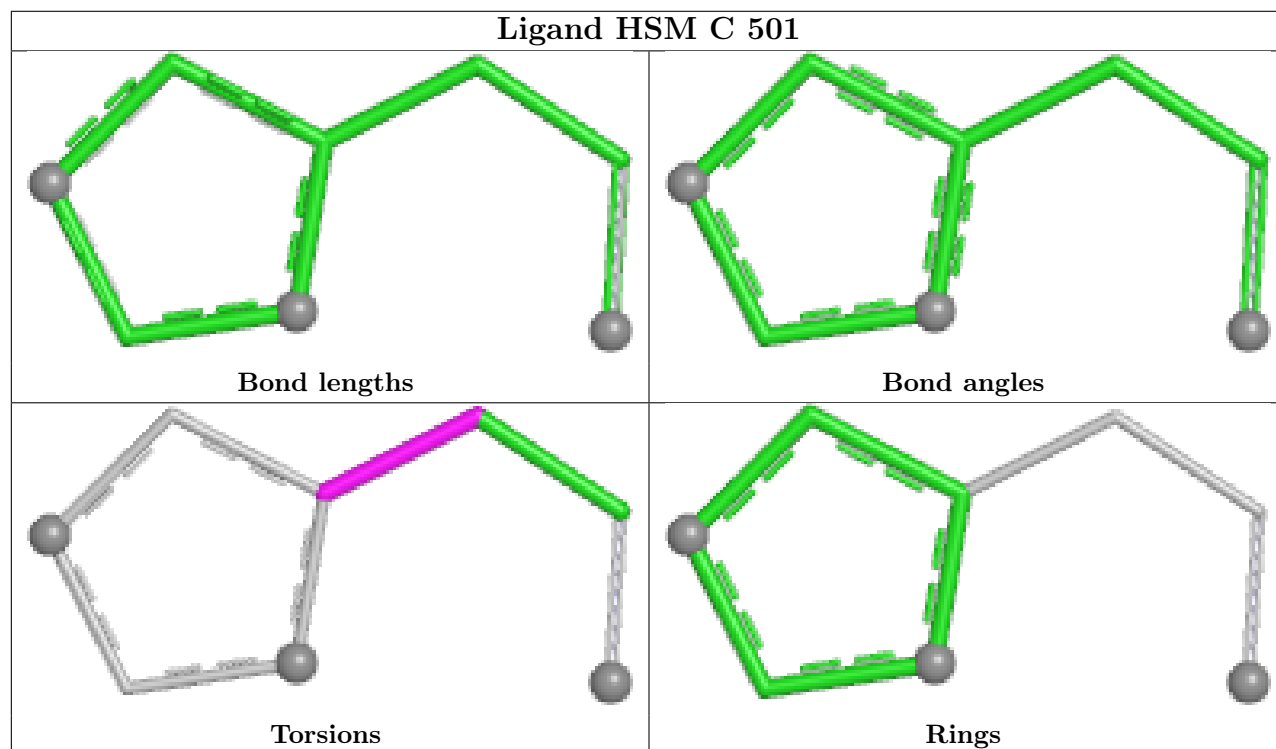
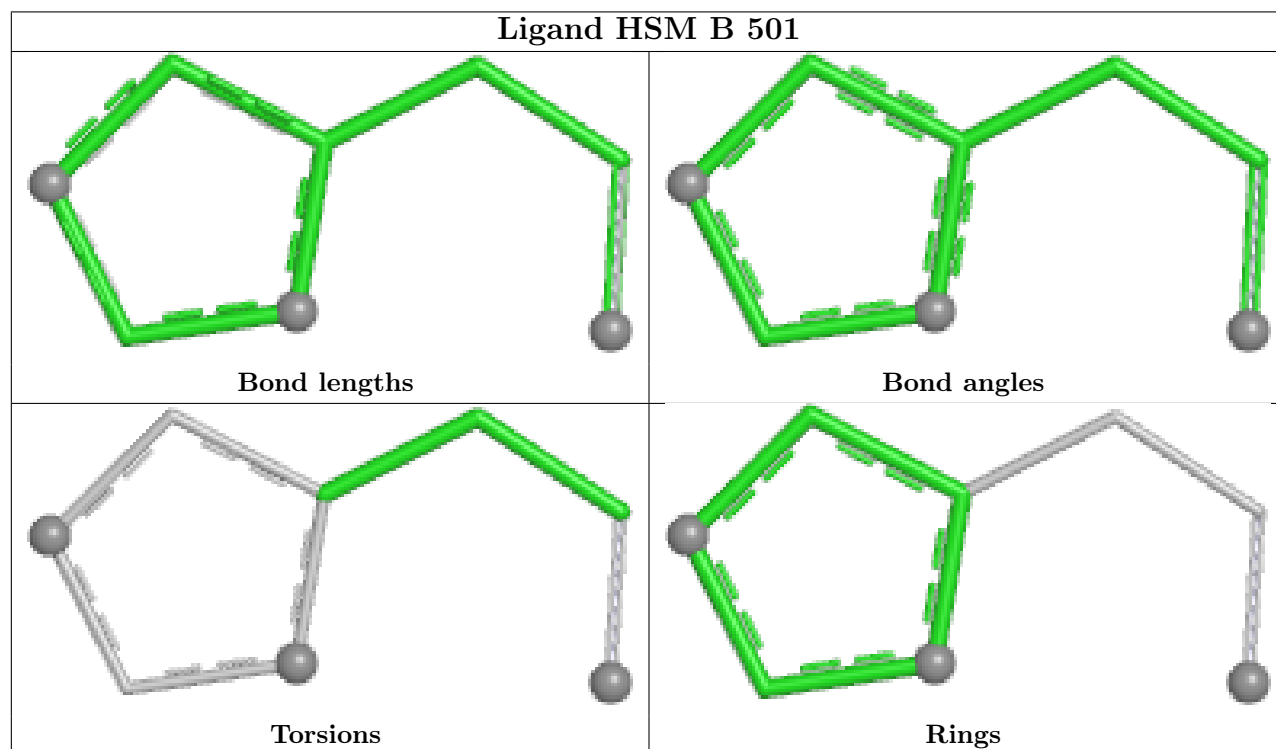
There are no ring outliers.

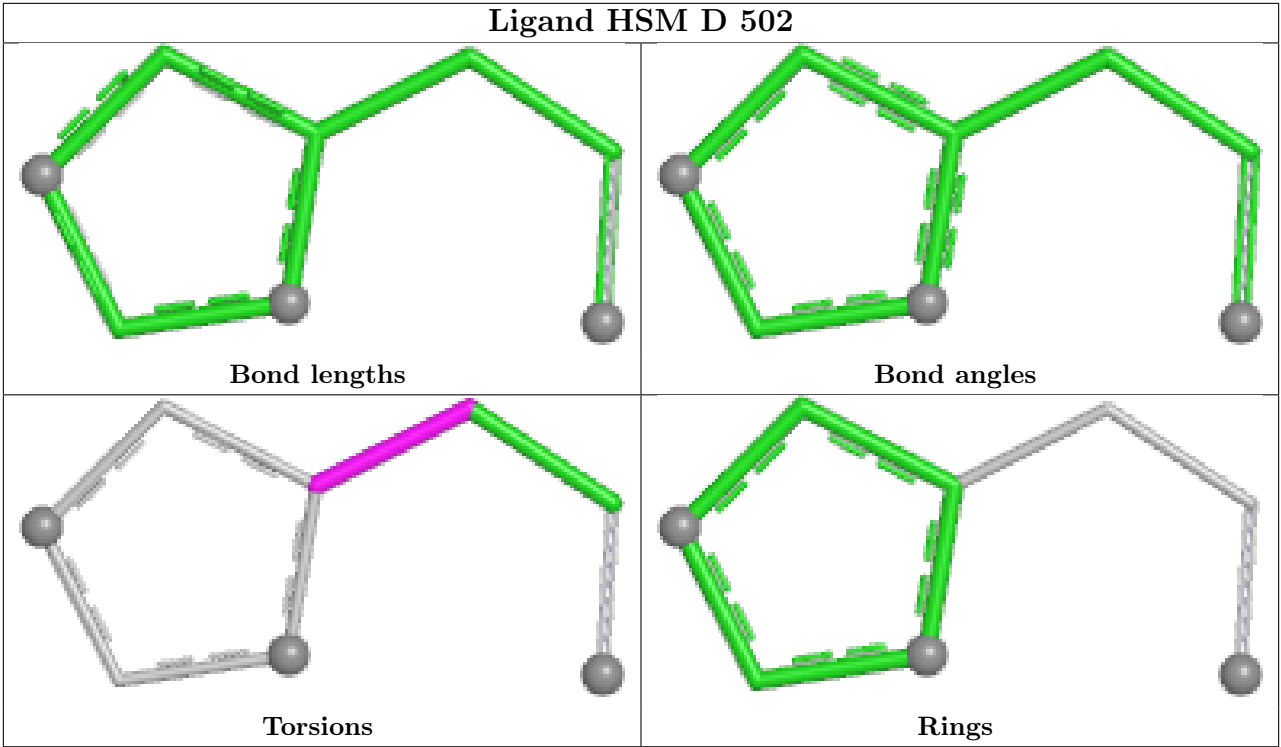
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	501	HSM	1	0
10	B	502	R16	1	0
11	D	501	D10	1	0
8	E	501	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	L	1
4	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	13:GLN	C	403:GLY	N	7.34
1	M	13:GLN	C	403:GLY	N	7.34

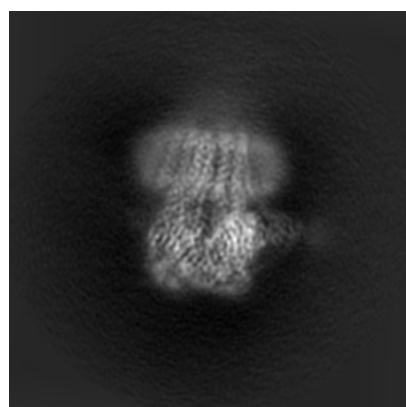
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14071. These allow visual inspection of the internal detail of the map and identification of artifacts.

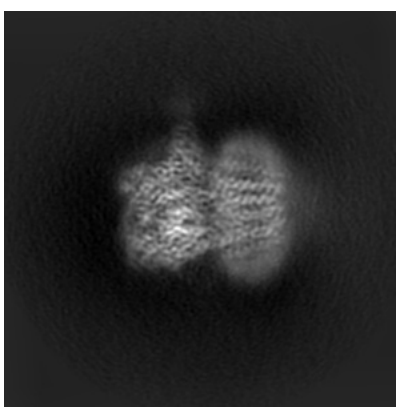
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

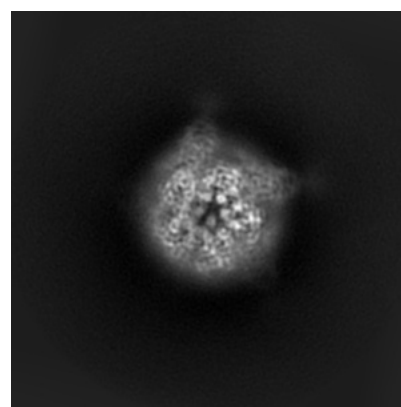
6.1.1 Primary map



X



Y

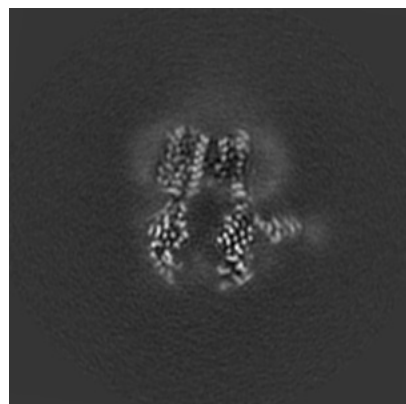


Z

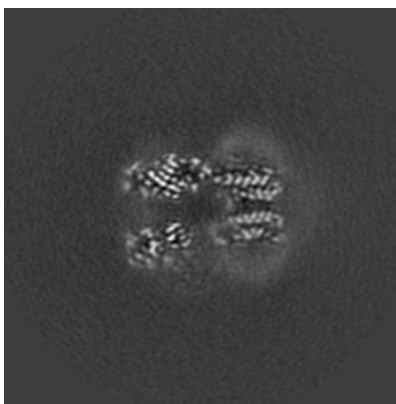
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

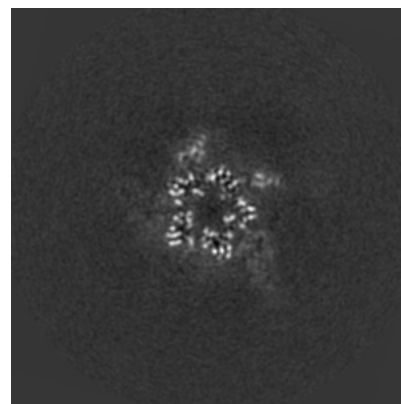
6.2.1 Primary map



X Index: 145



Y Index: 145

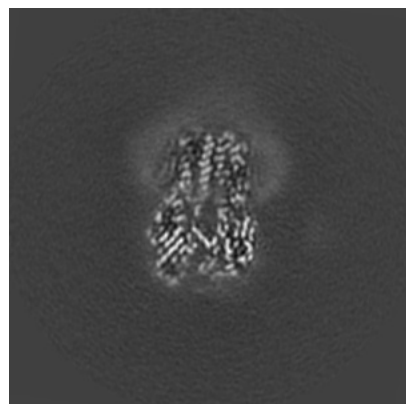


Z Index: 145

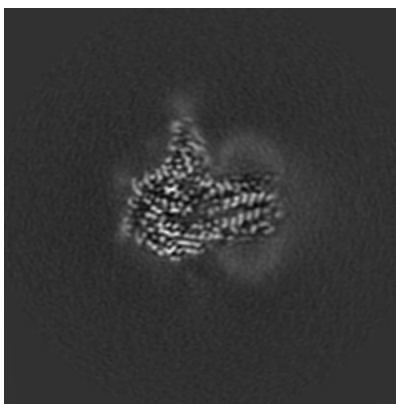
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

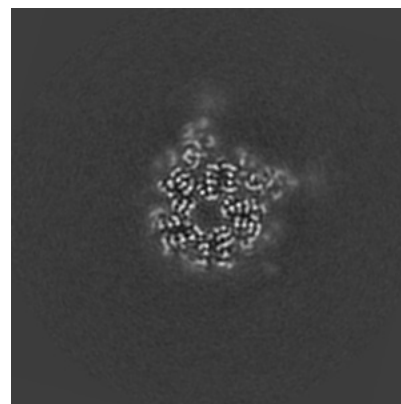
6.3.1 Primary map



X Index: 155



Y Index: 163

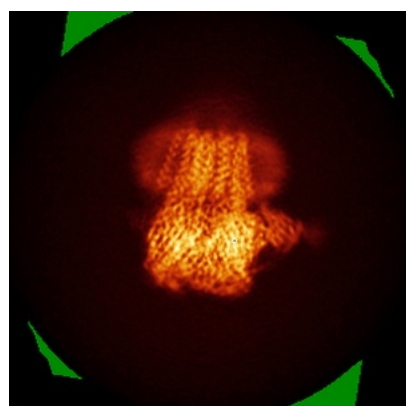


Z Index: 122

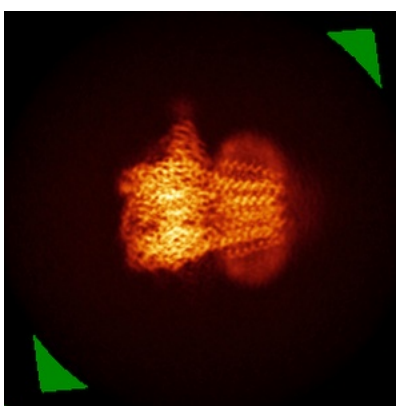
The images above show the largest variance slices of the map in three orthogonal directions.

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

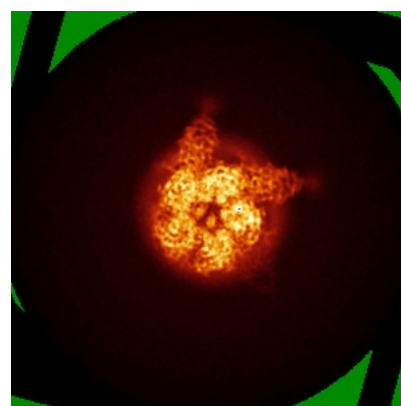
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

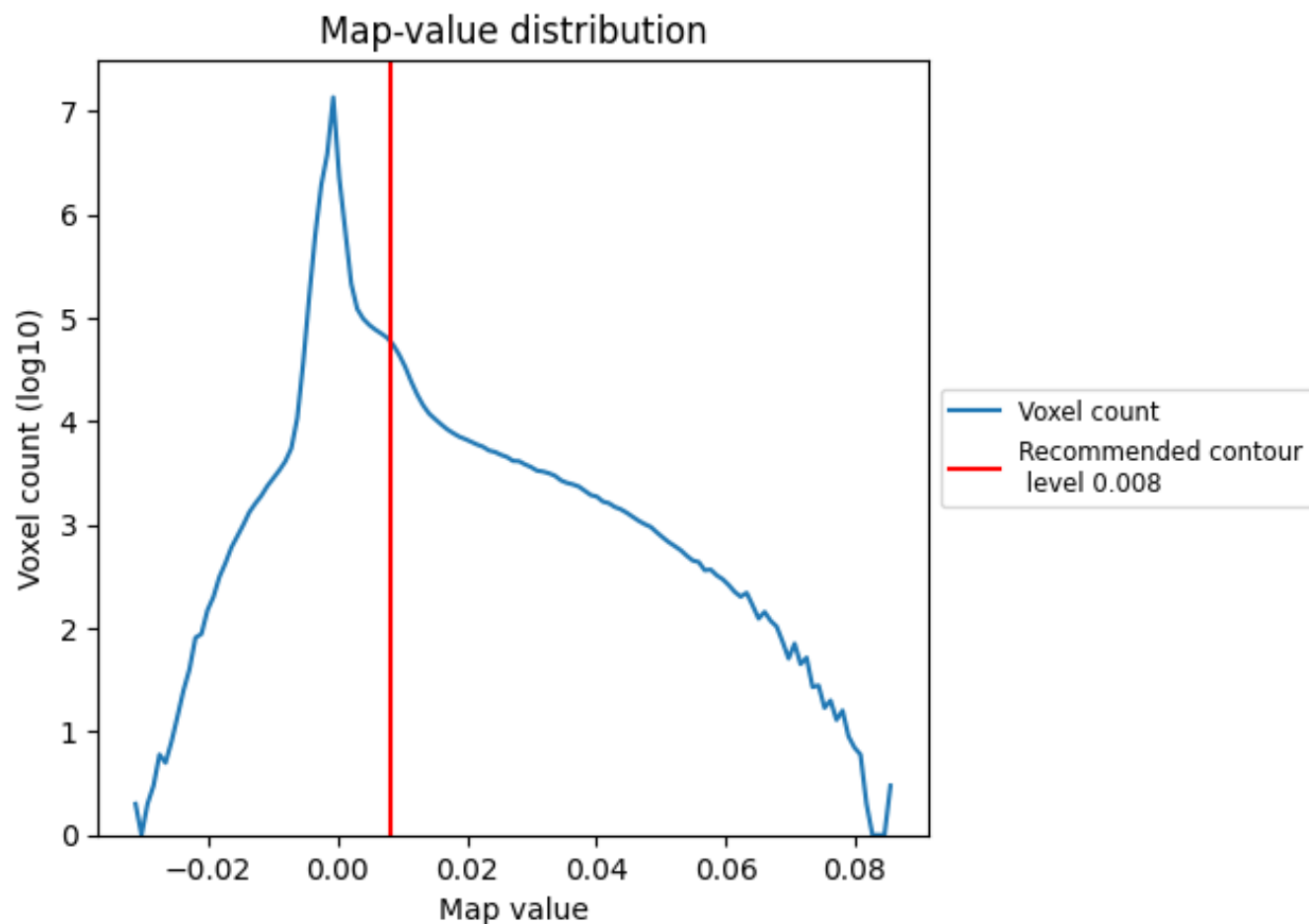
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

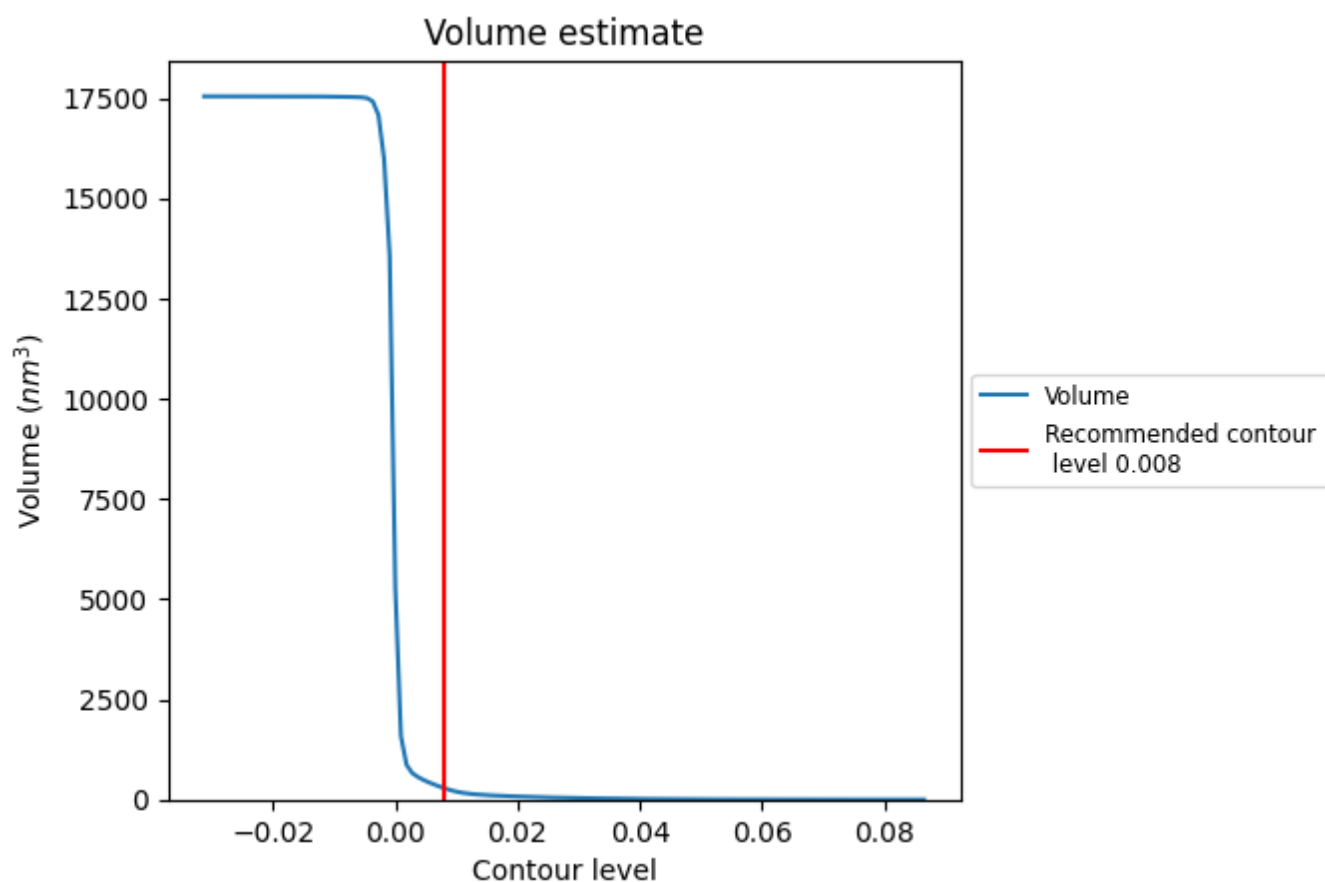
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

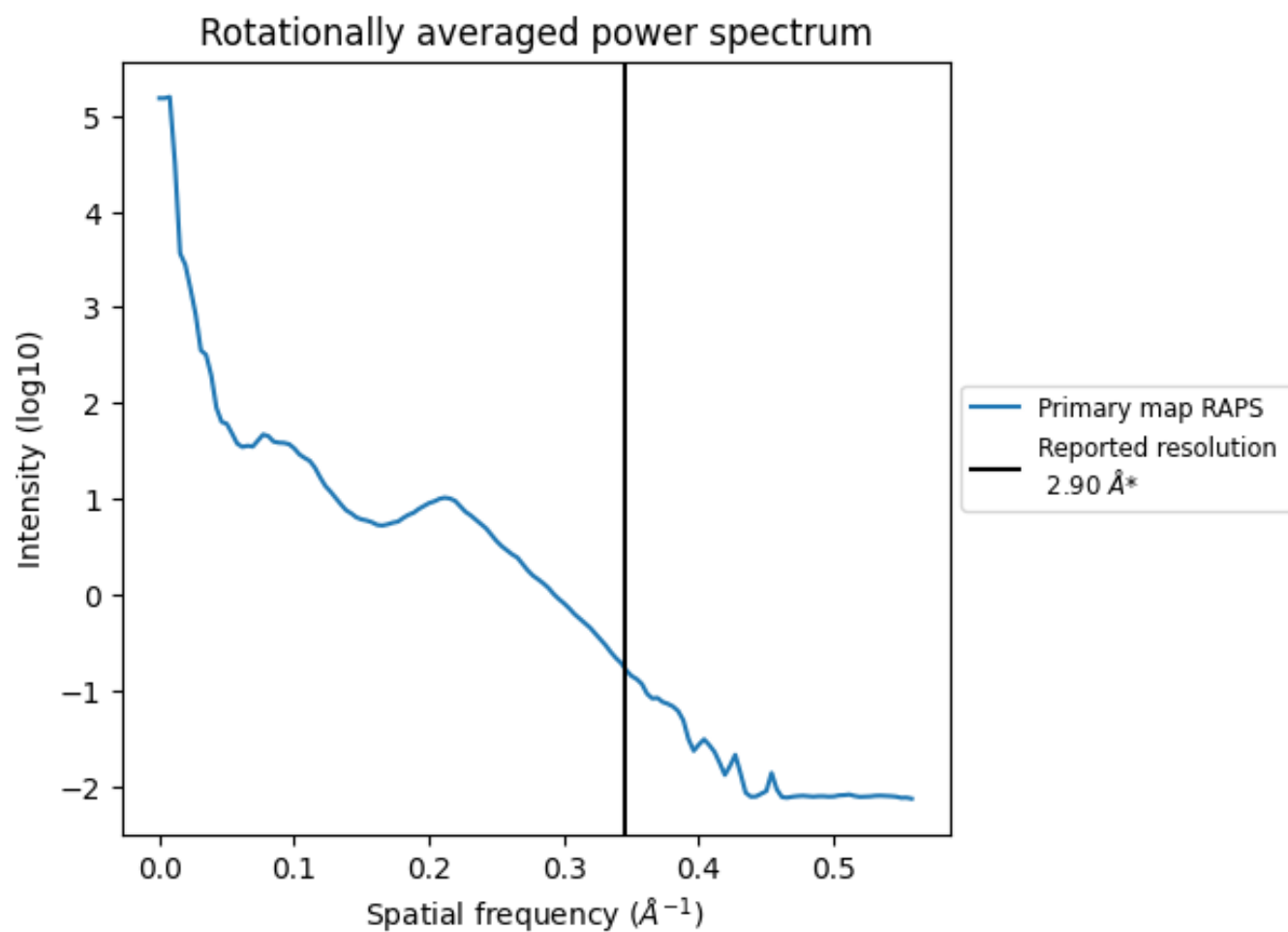
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 283 nm³; this corresponds to an approximate mass of 256 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

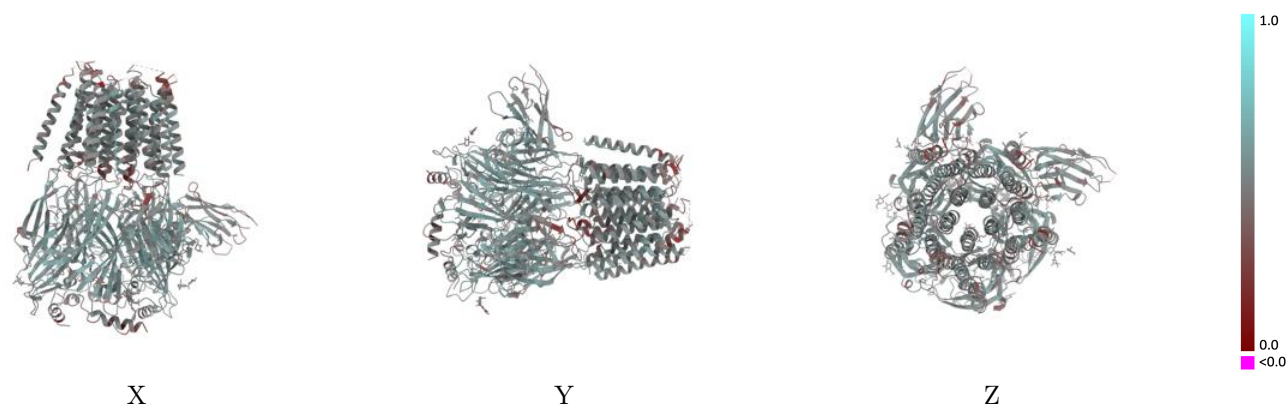


*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8 Fourier-Shell correlation

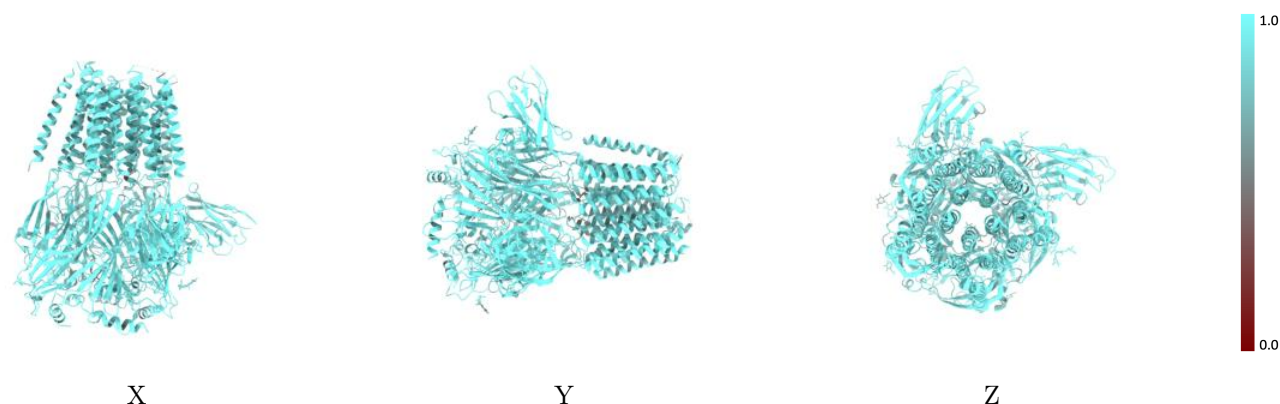
This section was not generated. No FSC curve or half-maps provided.

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



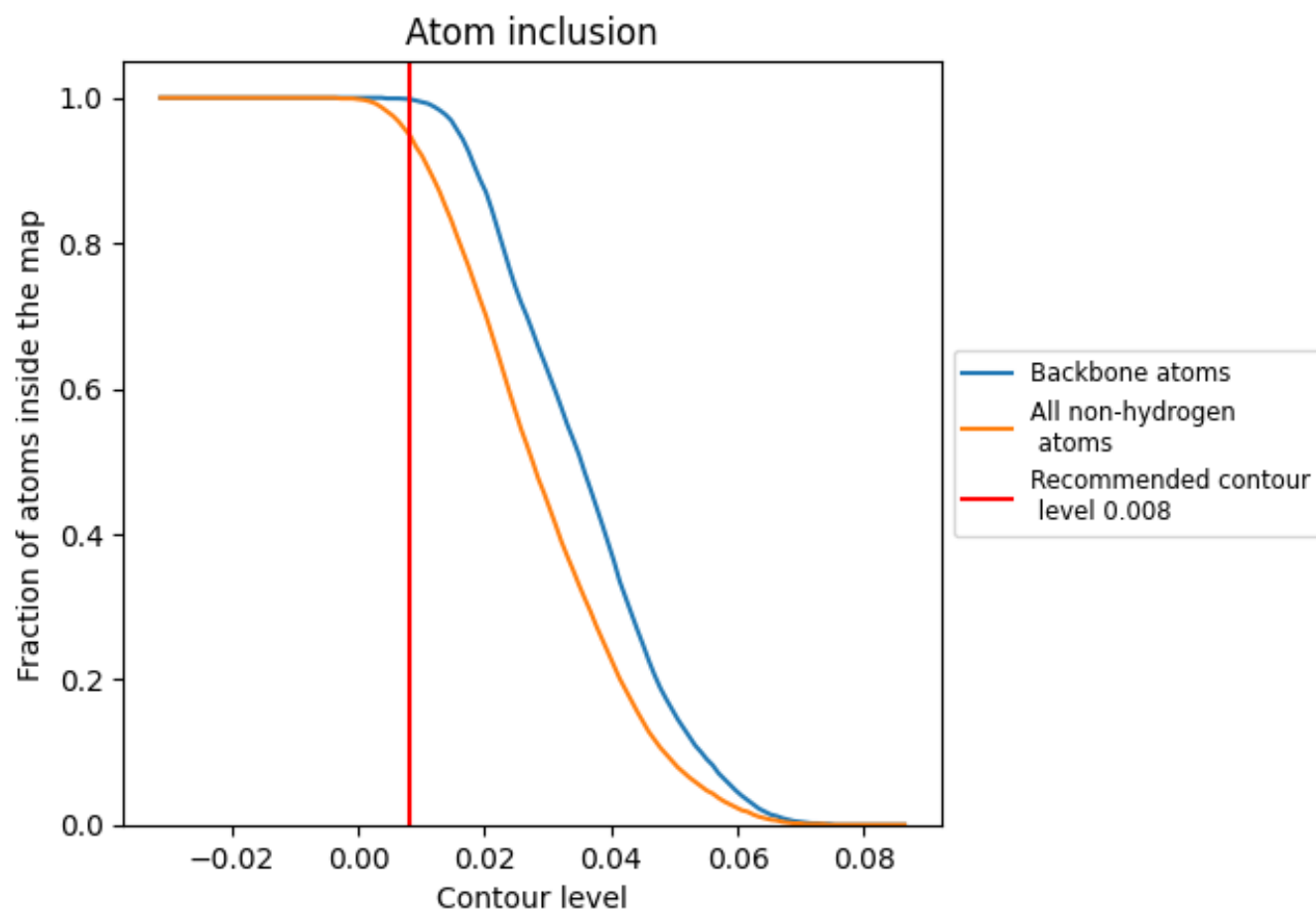
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9500	0.5050
A	0.9440	0.5010
B	0.9540	0.5130
C	0.9550	0.5200
D	0.9460	0.5060
E	0.9450	0.5030
F	1.0000	0.4980
G	0.9840	0.5020
H	0.9670	0.4870
L	0.9630	0.4900
M	0.9660	0.4810
a	0.5640	0.3150
b	0.8210	0.4180
c	0.8930	0.4590
d	0.7860	0.3930

