



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:33 PM UTC

PDB ID : 8WFS / pdb_00008wfs
EMDB ID : EMD-37498
Title : Cryo-EM structure of GPIb-IX Complex
Authors : Shu, Z.M.; Duan, J.S.; Zhou, A.W.
Deposited on : 2023-09-20
Resolution : 3.36 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

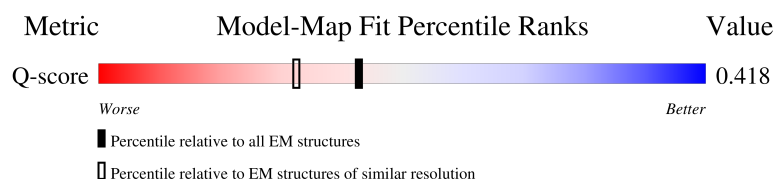
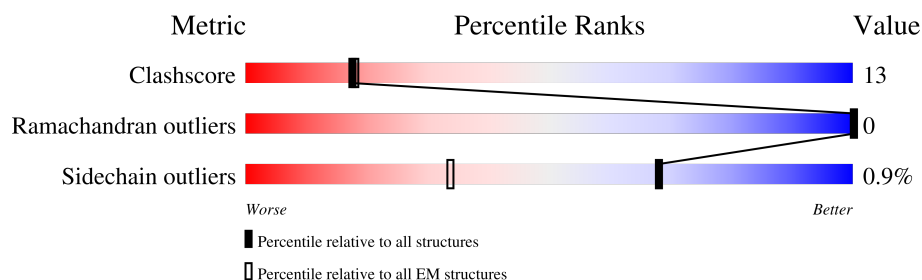
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

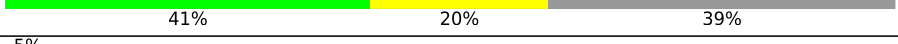
The reported resolution of this entry is 3.36 Å.

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



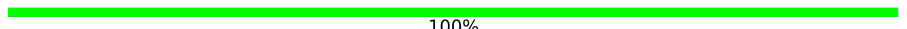
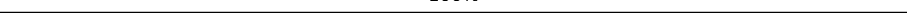
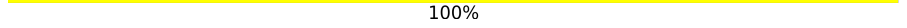
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14332 (2.86 - 3.86)

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	B	192	 55% 18% 27%
1	C	192	 41% 20% 39%
1	b	192	 5% 51% 21% 27%
1	c	192	 42% 19% 39%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	191	
2	X	191	
3	a	140	
4	A	2	
4	D	2	
4	H	2	
4	I	2	
5	F	3	
5	G	3	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6274 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 Platelet glycoprotein Ib beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	c	118	Total	C	N	O	S	0	0
			884	558	165	153	8		
1	C	117	Total	C	N	O	S	1	0
			882	556	165	153	8		
1	B	140	Total	C	N	O	S	0	0
			1035	659	191	176	9		
1	b	140	Total	C	N	O	S	0	0
			1035	659	191	176	9		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	148	SER	CYS	engineered mutation	UNP P13224
c	182	GLY	-	expression tag	UNP P13224
c	183	SER	-	expression tag	UNP P13224
c	184	GLY	-	expression tag	UNP P13224
c	185	ASP	-	expression tag	UNP P13224
c	186	TYR	-	expression tag	UNP P13224
c	187	LYS	-	expression tag	UNP P13224
c	188	ASP	-	expression tag	UNP P13224
c	189	ASP	-	expression tag	UNP P13224
c	190	ASP	-	expression tag	UNP P13224
c	191	ASP	-	expression tag	UNP P13224
c	192	LYS	-	expression tag	UNP P13224
C	148	SER	CYS	engineered mutation	UNP P13224
C	182	GLY	-	expression tag	UNP P13224
C	183	SER	-	expression tag	UNP P13224
C	184	GLY	-	expression tag	UNP P13224
C	185	ASP	-	expression tag	UNP P13224
C	186	TYR	-	expression tag	UNP P13224
C	187	LYS	-	expression tag	UNP P13224
C	188	ASP	-	expression tag	UNP P13224
C	189	ASP	-	expression tag	UNP P13224
C	190	ASP	-	expression tag	UNP P13224

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	191	ASP	-	expression tag	UNP P13224
C	192	LYS	-	expression tag	UNP P13224
B	148	SER	CYS	engineered mutation	UNP P13224
B	182	GLY	-	expression tag	UNP P13224
B	183	SER	-	expression tag	UNP P13224
B	184	GLY	-	expression tag	UNP P13224
B	185	ASP	-	expression tag	UNP P13224
B	186	TYR	-	expression tag	UNP P13224
B	187	LYS	-	expression tag	UNP P13224
B	188	ASP	-	expression tag	UNP P13224
B	189	ASP	-	expression tag	UNP P13224
B	190	ASP	-	expression tag	UNP P13224
B	191	ASP	-	expression tag	UNP P13224
B	192	LYS	-	expression tag	UNP P13224
b	148	SER	CYS	engineered mutation	UNP P13224
b	182	GLY	-	expression tag	UNP P13224
b	183	SER	-	expression tag	UNP P13224
b	184	GLY	-	expression tag	UNP P13224
b	185	ASP	-	expression tag	UNP P13224
b	186	TYR	-	expression tag	UNP P13224
b	187	LYS	-	expression tag	UNP P13224
b	188	ASP	-	expression tag	UNP P13224
b	189	ASP	-	expression tag	UNP P13224
b	190	ASP	-	expression tag	UNP P13224
b	191	ASP	-	expression tag	UNP P13224
b	192	LYS	-	expression tag	UNP P13224

- Molecule 2 is a protein called Platelet glycoprotein IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	125	Total	C	N	O	S	0	0
			957	600	175	173	9		
2	X	146	Total	C	N	O	S	0	0
			1112	705	201	197	9		

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	154	SER	CYS	engineered mutation	UNP P14770
E	162	SER	-	expression tag	UNP P14770
E	163	ALA	-	expression tag	UNP P14770
E	164	TRP	-	expression tag	UNP P14770

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	165	SER	-	expression tag	UNP P14770
E	166	HIS	-	expression tag	UNP P14770
E	167	PRO	-	expression tag	UNP P14770
E	168	GLN	-	expression tag	UNP P14770
E	169	PHE	-	expression tag	UNP P14770
E	170	GLU	-	expression tag	UNP P14770
E	171	LYS	-	expression tag	UNP P14770
E	172	GLY	-	expression tag	UNP P14770
E	173	GLY	-	expression tag	UNP P14770
E	174	GLY	-	expression tag	UNP P14770
E	175	SER	-	expression tag	UNP P14770
E	176	GLY	-	expression tag	UNP P14770
E	177	GLY	-	expression tag	UNP P14770
E	178	GLY	-	expression tag	UNP P14770
E	179	SER	-	expression tag	UNP P14770
E	180	GLY	-	expression tag	UNP P14770
E	181	GLY	-	expression tag	UNP P14770
E	182	SER	-	expression tag	UNP P14770
E	183	ALA	-	expression tag	UNP P14770
E	184	TRP	-	expression tag	UNP P14770
E	185	SER	-	expression tag	UNP P14770
E	186	HIS	-	expression tag	UNP P14770
E	187	PRO	-	expression tag	UNP P14770
E	188	GLN	-	expression tag	UNP P14770
E	189	PHE	-	expression tag	UNP P14770
E	190	GLU	-	expression tag	UNP P14770
E	191	LYS	-	expression tag	UNP P14770
X	154	SER	CYS	engineered mutation	UNP P14770
X	162	SER	-	expression tag	UNP P14770
X	163	ALA	-	expression tag	UNP P14770
X	164	TRP	-	expression tag	UNP P14770
X	165	SER	-	expression tag	UNP P14770
X	166	HIS	-	expression tag	UNP P14770
X	167	PRO	-	expression tag	UNP P14770
X	168	GLN	-	expression tag	UNP P14770
X	169	PHE	-	expression tag	UNP P14770
X	170	GLU	-	expression tag	UNP P14770
X	171	LYS	-	expression tag	UNP P14770
X	172	GLY	-	expression tag	UNP P14770
X	173	GLY	-	expression tag	UNP P14770
X	174	GLY	-	expression tag	UNP P14770
X	175	SER	-	expression tag	UNP P14770

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
X	176	GLY	-	expression tag	UNP P14770
X	177	GLY	-	expression tag	UNP P14770
X	178	GLY	-	expression tag	UNP P14770
X	179	SER	-	expression tag	UNP P14770
X	180	GLY	-	expression tag	UNP P14770
X	181	GLY	-	expression tag	UNP P14770
X	182	SER	-	expression tag	UNP P14770
X	183	ALA	-	expression tag	UNP P14770
X	184	TRP	-	expression tag	UNP P14770
X	185	SER	-	expression tag	UNP P14770
X	186	HIS	-	expression tag	UNP P14770
X	187	PRO	-	expression tag	UNP P14770
X	188	GLN	-	expression tag	UNP P14770
X	189	PHE	-	expression tag	UNP P14770
X	190	GLU	-	expression tag	UNP P14770
X	191	LYS	-	expression tag	UNP P14770

- Molecule 3 is a protein called Platelet glycoprotein Ib alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	22	Total	C	N	O	S	0	0
			179	128	23	26	2		

There are 12 discrepancies between the modelled and reference sequences:

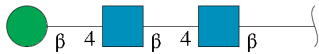
Chain	Residue	Modelled	Actual	Comment	Reference
a	559	GLU	SER	engineered mutation	UNP P07359
a	609	GLU	SER	engineered mutation	UNP P07359
a	611	GLY	-	expression tag	UNP P07359
a	612	GLY	-	expression tag	UNP P07359
a	613	HIS	-	expression tag	UNP P07359
a	614	HIS	-	expression tag	UNP P07359
a	615	HIS	-	expression tag	UNP P07359
a	616	HIS	-	expression tag	UNP P07359
a	617	HIS	-	expression tag	UNP P07359
a	618	HIS	-	expression tag	UNP P07359
a	619	HIS	-	expression tag	UNP P07359
a	620	HIS	-	expression tag	UNP P07359

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	H	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		

- 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.

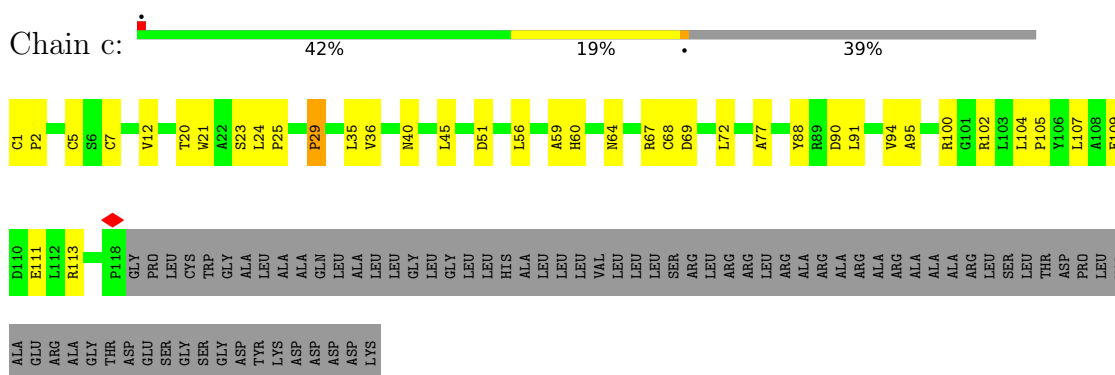


Mol	Chain	Residues	Atoms				AltConf	Trace
5	F	3	Total	C	N	O	0	0
			39	22	2	15		
5	G	3	Total	C	N	O	0	0
			39	22	2	15		

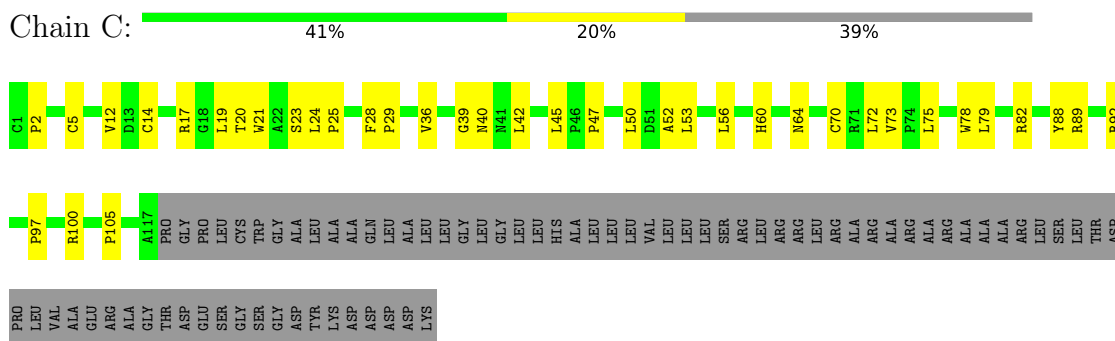
3 Residue-property plots

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.

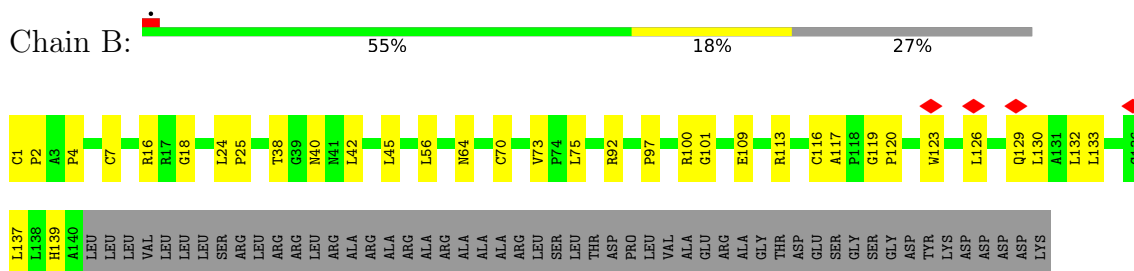
- Molecule 1: Platelet glycoprotein Ib beta chain



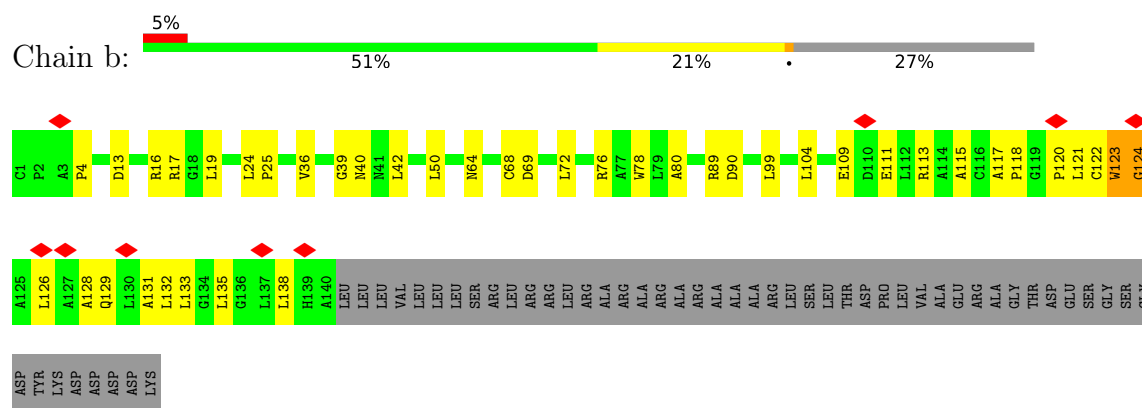
- Molecule 1: Platelet glycoprotein Ib beta chain



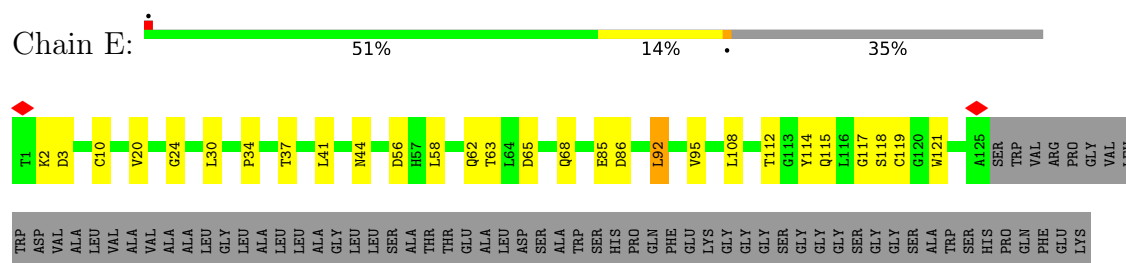
- Molecule 1: Platelet glycoprotein Ib beta chain



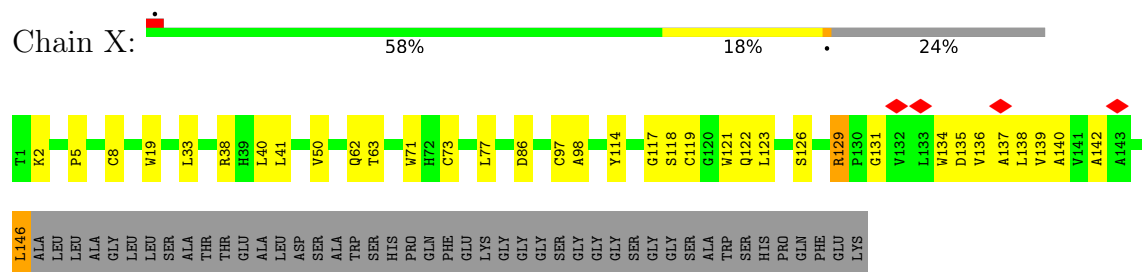
- Molecule 1: Platelet glycoprotein Ib beta chain



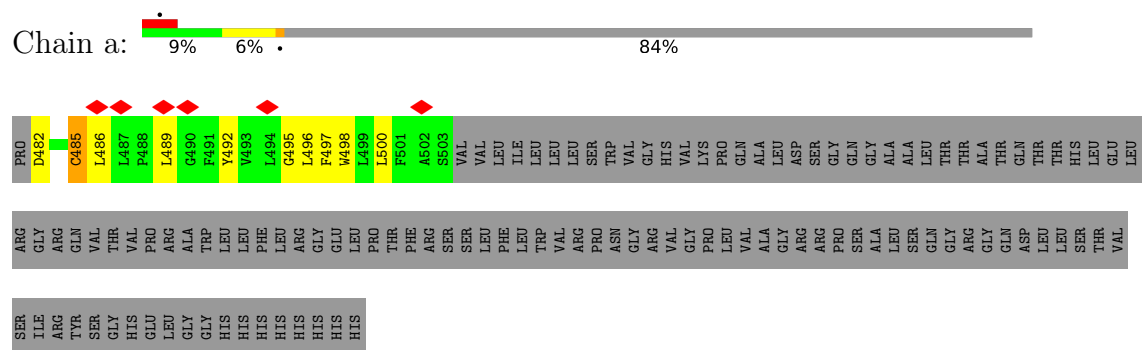
- Molecule 2: Platelet glycoprotein IX



- Molecule 2: Platelet glycoprotein IX



- Molecule 3: Platelet glycoprotein Ib alpha chain



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





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

Chain D:  100%



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

Chain H:  100%



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

Chain I:  50% 50%



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

Chain F:  33% 67%



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

Chain G:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	180680	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 ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.133	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.0457	Depositor
Map size (Å)	386.712, 386.712, 386.712	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality

5.1 Standard geometry

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

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	B	0.17	0/1063	0.43	0/1462
1	C	0.18	0/905	0.39	0/1244
1	b	0.16	0/1063	0.43	1/1462 (0.1%)
1	c	0.20	0/908	0.50	1/1249 (0.1%)
2	E	0.15	0/983	0.34	0/1347
2	X	0.15	0/1143	0.37	0/1570
3	a	0.18	0/186	0.51	0/253
All	All	0.17	0/6251	0.41	2/8587 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	b	0	1
2	X	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	29	PRO	CA-N-CD	-9.33	98.94	112.00
1	b	124	GLY	N-CA-C	-6.58	105.40	115.66

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	X	129	ARG	Peptide
1	b	123	TRP	Peptide

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	B	1035	0	1054	23	0
1	C	882	0	890	28	0
1	b	1035	0	1054	40	0
1	c	884	0	893	27	0
2	E	957	0	938	20	0
2	X	1112	0	1102	32	0
3	a	179	0	175	15	0
4	A	28	0	25	0	0
4	D	28	0	25	0	0
4	H	28	0	25	1	0
4	I	28	0	25	1	0
5	F	39	0	34	2	0
5	G	39	0	34	0	0
All	All	6274	0	6274	169	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 13.

All (169) 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:c:24:LEU:HD12	1:c:25:PRO:HD2	1.51	0.92
2:E:41:LEU:HD22	2:E:65:ASP:HB2	1.54	0.89
1:B:132:LEU:HG	2:X:138:LEU:HB3	1.64	0.79
2:X:114:TYR:HA	2:X:118:SER:HB2	1.65	0.77
3:a:489:LEU:HD23	3:a:492:TYR:HE2	1.50	0.77
1:c:95:ALA:HA	1:c:100:ARG:HH12	1.51	0.75
1:b:135:LEU:HD12	1:b:138:LEU:HD22	1.70	0.74
1:c:102:ARG:NH1	1:c:111:GLU:OE2	2.26	0.69
2:E:44:ASN:H	2:E:68:GLN:HB2	1.60	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:67:ARG:NH1	1:c:69:ASP:OD2	2.27	0.67
3:a:492:TYR:O	3:a:496:LEU:HB2	1.94	0.67
1:b:132:LEU:HD13	2:X:138:LEU:HD21	1.77	0.67
2:X:135:ASP:HA	2:X:138:LEU:HD12	1.77	0.66
2:X:71:TRP:HB2	2:X:97:CYS:HA	1.78	0.65
1:C:45:LEU:HD13	1:C:50:LEU:HD21	1.78	0.65
1:c:20:THR:H	1:c:23:SER:HB3	1.63	0.64
1:B:117:ALA:HB1	1:B:120:PRO:HD2	1.80	0.64
1:c:29:PRO:HD2	1:c:29:PRO:O	1.98	0.64
1:b:76:ARG:HH12	1:b:80:ALA:HB2	1.64	0.64
1:c:2:PRO:HG2	1:c:5:CYS:HB2	1.80	0.63
1:b:132:LEU:HD21	3:a:492:TYR:HB3	1.82	0.62
1:B:73:VAL:HG12	2:X:123:LEU:HD11	1.80	0.62
2:X:71:TRP:O	2:X:98:ALA:N	2.33	0.61
1:C:89:ARG:NH1	2:E:86:ASP:OD1	2.32	0.60
1:c:56:LEU:HD21	1:c:59:ALA:HB2	1.85	0.59
1:c:72:LEU:HD21	1:c:104:LEU:HD11	1.84	0.59
1:c:109:GLU:OE1	1:c:113:ARG:NH2	2.35	0.59
1:B:109:GLU:CD	1:b:113:ARG:HH12	2.11	0.58
2:E:114:TYR:HA	2:E:118:SER:HB2	1.85	0.58
1:c:94:VAL:O	1:c:100:ARG:NH1	2.36	0.58
2:X:135:ASP:O	2:X:138:LEU:HB2	2.03	0.58
1:C:2:PRO:HD2	1:C:29:PRO:HD3	1.85	0.58
2:E:24:GLY:HA3	5:F:1:NAG:H83	1.86	0.58
1:b:42:LEU:HB2	1:b:64:ASN:HD22	1.68	0.57
1:b:19:LEU:HD23	1:b:42:LEU:HD21	1.86	0.57
2:X:38:ARG:NH2	2:X:62:GLN:OE1	2.37	0.57
1:b:128:ALA:O	1:b:132:LEU:HG	2.04	0.56
1:C:39:GLY:C	1:C:40:ASN:HD22	2.13	0.56
1:C:97:PRO:HA	1:C:100:ARG:HG2	1.88	0.56
2:X:5:PRO:HB2	2:X:8:CYS:HB2	1.88	0.56
1:b:89:ARG:NH1	2:X:86:ASP:OD2	2.38	0.56
1:b:19:LEU:H	1:b:40:ASN:HD22	1.54	0.55
1:b:135:LEU:HG	3:a:496:LEU:HD21	1.88	0.55
1:b:122:CYS:O	1:b:124:GLY:N	2.33	0.55
1:B:45:LEU:HD12	1:B:75:LEU:HD13	1.87	0.55
1:c:88:TYR:HD1	1:c:91:LEU:HD11	1.71	0.55
1:B:113:ARG:HA	1:B:116:CYS:HB3	1.88	0.54
1:b:109:GLU:HG3	2:X:121:TRP:HE1	1.72	0.54
1:b:122:CYS:O	3:a:482:ASP:N	2.40	0.54
1:c:24:LEU:HD21	1:c:45:LEU:HD23	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:4:PRO:O	1:b:17:ARG:NH1	2.40	0.54
1:C:92:ARG:NH2	2:E:56:ASP:O	2.42	0.53
1:C:40:ASN:HB2	1:C:64:ASN:HD21	1.73	0.53
1:b:69:ASP:HA	1:b:115:ALA:HB3	1.91	0.53
3:a:495:GLY:HA2	3:a:498:TRP:HE3	1.73	0.53
2:E:62:GLN:HG3	2:E:63:THR:HG23	1.90	0.53
1:B:97:PRO:HA	1:B:100:ARG:HG2	1.91	0.53
1:C:5:CYS:HB2	1:C:14:CYS:HA	1.90	0.53
1:b:72:LEU:HD21	1:b:104:LEU:HD11	1.90	0.52
3:a:482:ASP:N	3:a:485:CYS:SG	2.83	0.52
2:E:37:THR:HB	2:E:58:LEU:HD13	1.92	0.51
1:b:40:ASN:HB2	1:b:64:ASN:HD21	1.75	0.51
2:X:126:SER:O	2:X:126:SER:OG	2.29	0.51
2:X:139:VAL:O	2:X:142:ALA:HB3	2.10	0.51
2:X:131:GLY:O	2:X:135:ASP:N	2.38	0.51
3:a:486:LEU:HD23	3:a:489:LEU:HD12	1.93	0.51
1:C:42:LEU:HB2	1:C:64:ASN:HD22	1.77	0.50
1:b:129:GLN:HB3	2:X:134:TRP:CE2	2.47	0.50
2:X:19:TRP:HE1	2:X:41:LEU:HD11	1.76	0.50
1:b:123:TRP:HB2	1:b:126:LEU:HB2	1.94	0.49
1:B:2:PRO:HB2	1:B:4:PRO:HD2	1.95	0.49
1:B:123:TRP:HA	1:B:126:LEU:HB3	1.95	0.49
1:b:117:ALA:HB1	1:b:120:PRO:HD2	1.95	0.49
1:b:117:ALA:O	1:b:121:LEU:HB2	2.11	0.49
3:a:489:LEU:HD23	3:a:492:TYR:CE2	2.40	0.49
1:b:113:ARG:HG2	1:b:113:ARG:HH11	1.76	0.49
1:B:24:LEU:HD12	1:B:25:PRO:HD2	1.95	0.48
1:b:99:LEU:HD21	1:b:111:GLU:HB3	1.95	0.48
2:X:122:GLN:H	2:X:122:GLN:CD	2.20	0.48
1:B:16:ARG:N	1:B:38:THR:O	2.47	0.48
2:X:136:VAL:O	2:X:139:VAL:HG22	2.13	0.48
3:a:489:LEU:HA	3:a:492:TYR:CE2	2.48	0.48
1:c:20:THR:OG1	1:c:21:TRP:N	2.45	0.48
1:c:51:ASP:OD1	1:c:51:ASP:N	2.42	0.48
2:X:129:ARG:O	2:X:131:GLY:N	2.47	0.48
1:c:90:ASP:N	1:c:90:ASP:OD1	2.45	0.47
1:b:118:PRO:HB2	2:X:129:ARG:HD2	1.96	0.47
1:C:72:LEU:HD11	1:C:75:LEU:HD23	1.97	0.47
2:E:24:GLY:N	2:E:44:ASN:HB3	2.29	0.47
1:b:16:ARG:HD3	1:b:39:GLY:HA3	1.97	0.47
1:C:53:LEU:HD12	1:C:56:LEU:HD22	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:30:LEU:HD23	2:E:30:LEU:HA	1.77	0.47
1:b:68:CYS:HA	1:b:72:LEU:HD13	1.97	0.47
5:F:1:NAG:H62	5:F:2:NAG:H82	1.98	0.46
1:c:36:VAL:HG12	1:c:60:HIS:HB2	1.96	0.46
1:C:82:ARG:HD2	1:C:88:TYR:HE2	1.81	0.46
1:C:78:TRP:NE1	1:C:82:ARG:HH21	2.14	0.46
4:H:1:NAG:H62	4:H:2:NAG:HN2	1.80	0.46
2:E:95:VAL:HG13	2:E:108:LEU:HB2	1.98	0.45
1:b:132:LEU:HD12	2:X:134:TRP:CD1	2.52	0.45
1:B:1:CYS:HB3	1:B:7:CYS:HB3	1.86	0.45
1:c:1:CYS:HB3	1:c:7:CYS:HB3	1.67	0.45
1:b:24:LEU:HD23	1:b:25:PRO:HD2	1.99	0.45
4:I:1:NAG:O3	4:I:2:NAG:N2	2.49	0.45
1:b:13:ASP:HA	1:b:36:VAL:HG22	1.99	0.45
1:c:102:ARG:NH1	1:C:47:PRO:HB2	2.32	0.45
2:X:123:LEU:HD23	2:X:123:LEU:HA	1.87	0.44
1:C:20:THR:OG1	1:C:21:TRP:N	2.50	0.44
2:E:117:GLY:O	2:E:119:CYS:N	2.50	0.44
3:a:497:PHE:HA	3:a:500:LEU:HG	1.99	0.44
1:b:50:LEU:HD12	1:b:78:TRP:CE2	2.52	0.44
1:b:120:PRO:HA	1:b:123:TRP:CE2	2.52	0.44
1:C:88:TYR:O	1:C:105:PRO:HG3	2.17	0.44
2:X:50:VAL:HG23	2:X:71:TRP:HH2	1.82	0.44
1:C:82:ARG:HD2	1:C:88:TYR:CE2	2.52	0.44
1:B:56:LEU:HD12	1:B:56:LEU:HA	1.81	0.44
1:b:135:LEU:HA	1:b:138:LEU:HB3	2.00	0.44
1:c:88:TYR:O	1:c:105:PRO:HG3	2.17	0.44
1:C:45:LEU:HD12	1:C:75:LEU:HD22	1.99	0.44
2:X:33:LEU:HD22	2:X:40:LEU:HD11	2.00	0.44
1:C:2:PRO:HG2	1:C:28:PHE:CD1	2.53	0.43
1:b:120:PRO:HA	1:b:123:TRP:NE1	2.33	0.43
1:c:68:CYS:HB3	1:c:72:LEU:HD22	2.00	0.43
1:C:79:LEU:HD23	1:C:79:LEU:HA	1.85	0.43
1:c:104:LEU:HD12	1:c:104:LEU:HA	1.70	0.43
1:C:24:LEU:HD13	1:C:42:LEU:HD21	2.00	0.43
2:E:112:THR:H	2:E:115:GLN:HE21	1.66	0.43
1:b:135:LEU:CG	3:a:496:LEU:HD21	2.49	0.43
1:B:42:LEU:HB2	1:B:64:ASN:HD22	1.83	0.43
1:b:113:ARG:HG2	1:b:113:ARG:NH1	2.33	0.43
2:X:137:ALA:O	2:X:140:ALA:HB3	2.19	0.43
2:X:117:GLY:O	2:X:119:CYS:N	2.51	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:LEU:HD22	1:C:24:LEU:HA	2.00	0.42
1:c:77:ALA:HB1	2:E:121:TRP:HB2	2.01	0.42
1:c:107:LEU:HD23	1:c:107:LEU:HA	1.84	0.42
1:C:5:CYS:HB2	1:C:17:ARG:HD2	2.00	0.42
2:E:112:THR:HG23	2:E:115:GLN:NE2	2.33	0.42
1:B:139:HIS:CD2	2:X:146:LEU:HB2	2.55	0.42
1:b:133:LEU:HD23	1:b:133:LEU:HA	1.79	0.42
2:E:10:CYS:SG	2:E:20:VAL:HG12	2.59	0.42
1:c:40:ASN:HB2	1:c:64:ASN:HD21	1.84	0.42
1:B:100:ARG:HA	1:B:100:ARG:HD2	1.76	0.42
1:B:92:ARG:HG3	1:B:101:GLY:HA2	2.01	0.42
1:B:119:GLY:N	1:B:120:PRO:CD	2.83	0.42
1:C:36:VAL:HG23	1:C:60:HIS:HB2	2.02	0.42
1:c:12:VAL:HG13	1:c:35:LEU:HB2	2.02	0.41
2:X:73:CYS:HB3	2:X:97:CYS:HB3	1.86	0.41
2:X:2:LYS:HA	2:X:2:LYS:HD2	1.87	0.41
2:E:108:LEU:HD12	2:E:108:LEU:HA	1.93	0.41
2:E:85:GLU:HG3	2:E:92:LEU:HD21	2.02	0.41
1:b:90:ASP:N	1:b:90:ASP:OD1	2.52	0.41
1:b:121:LEU:HD23	1:b:121:LEU:HA	1.89	0.41
1:B:123:TRP:HE3	1:B:123:TRP:H	1.69	0.41
1:B:137:LEU:HD23	1:B:137:LEU:HA	1.90	0.41
1:b:131:ALA:HB1	3:a:496:LEU:HD11	2.02	0.41
2:E:2:LYS:HD2	2:E:2:LYS:HA	1.85	0.41
2:E:3:ASP:O	2:E:34:PRO:HG3	2.21	0.41
1:c:59:ALA:HB3	1:c:88:TYR:OH	2.21	0.41
2:X:62:GLN:HG3	2:X:63:THR:HG23	2.03	0.41
1:C:70:CYS:O	1:C:73:VAL:HG12	2.21	0.40
1:C:24:LEU:HD12	1:C:25:PRO:HD2	2.03	0.40
1:C:52:ALA:C	1:C:53:LEU:HD23	2.45	0.40
1:B:18:GLY:N	1:B:40:ASN:HD22	2.19	0.40
3:a:485:CYS:O	3:a:489:LEU:N	2.54	0.40
1:B:130:LEU:O	1:B:133:LEU:HG	2.21	0.40
1:C:20:THR:HG23	1:C:23:SER:H	1.85	0.40
1:B:42:LEU:HD23	1:B:42:LEU:HA	1.89	0.40
2:X:73:CYS:HA	2:X:77:LEU:HD22	2.03	0.40
3:a:486:LEU:HA	3:a:489:LEU:HG	2.04	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	b	65/192 (34%)	61 (94%)	4 (6%)	0	100	100
2	E	9/191 (5%)	9 (100%)	0	0	100	100
2	X	144/191 (75%)	131 (91%)	13 (9%)	0	100	100
3	a	20/140 (14%)	20 (100%)	0	0	100	100
All	All	238/714 (33%)	221 (93%)	17 (7%)	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	B	105/146 (72%)	103 (98%)	2 (2%)	50	66
1	C	91/146 (62%)	90 (99%)	1 (1%)	65	73
1	b	105/146 (72%)	105 (100%)	0	100	100
1	c	92/146 (63%)	92 (100%)	0	100	100
2	E	105/150 (70%)	104 (99%)	1 (1%)	68	74
2	X	120/150 (80%)	119 (99%)	1 (1%)	73	76
3	a	19/117 (16%)	18 (95%)	1 (5%)	20	48
All	All	637/1001 (64%)	631 (99%)	6 (1%)	68	75

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	12	VAL
2	E	92	LEU
1	B	70	CYS
1	B	129	GLN
2	X	146	LEU
3	a	485	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	c	64	ASN
1	C	40	ASN
1	C	64	ASN
2	E	115	GLN
1	B	64	ASN
1	b	40	ASN
1	b	64	ASN

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](#)

14 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	1	4,1	14,14,15	0.23	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	2	4	14,14,15	0.20	0	17,19,21	0.44	0
4	NAG	D	1	4,1	14,14,15	0.29	0	17,19,21	0.40	0
4	NAG	D	2	4	14,14,15	0.22	0	17,19,21	0.47	0
5	NAG	F	1	5,2	14,14,15	0.45	0	17,19,21	0.42	0
5	NAG	F	2	5	14,14,15	0.24	0	17,19,21	0.40	0
5	BMA	F	3	5	11,11,12	0.49	0	15,15,17	0.73	0
5	NAG	G	1	5,1	14,14,15	0.19	0	17,19,21	0.44	0
5	NAG	G	2	5	14,14,15	0.22	0	17,19,21	0.45	0
5	BMA	G	3	5	11,11,12	0.51	0	15,15,17	0.90	0
4	NAG	H	1	4,1	14,14,15	0.25	0	17,19,21	0.42	0
4	NAG	H	2	4	14,14,15	0.22	0	17,19,21	0.45	0
4	NAG	I	1	4,2	14,14,15	0.31	0	17,19,21	0.87	1 (5%)
4	NAG	I	2	4	14,14,15	0.25	0	17,19,21	0.43	0

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	I	1	NAG	O4-C4-C3	2.02	115.14	110.38

There are no chirality outliers.

All (26) torsion outliers are listed below:

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

There are no ring outliers.

6 monomers are involved in 4 short contacts:

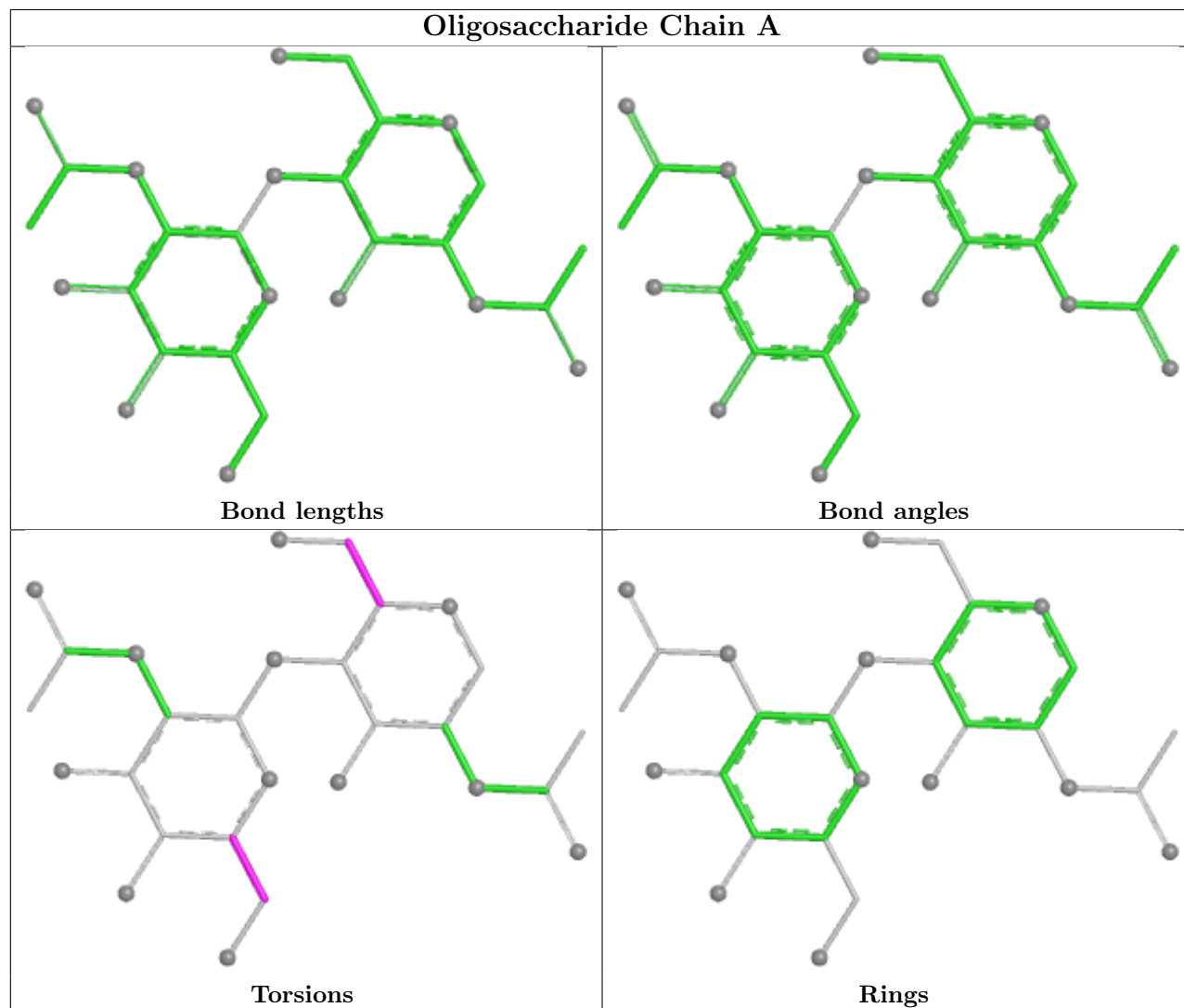
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	2	NAG	1	0
5	F	1	NAG	2	0
4	I	2	NAG	1	0
4	H	1	NAG	1	0
5	F	2	NAG	1	0

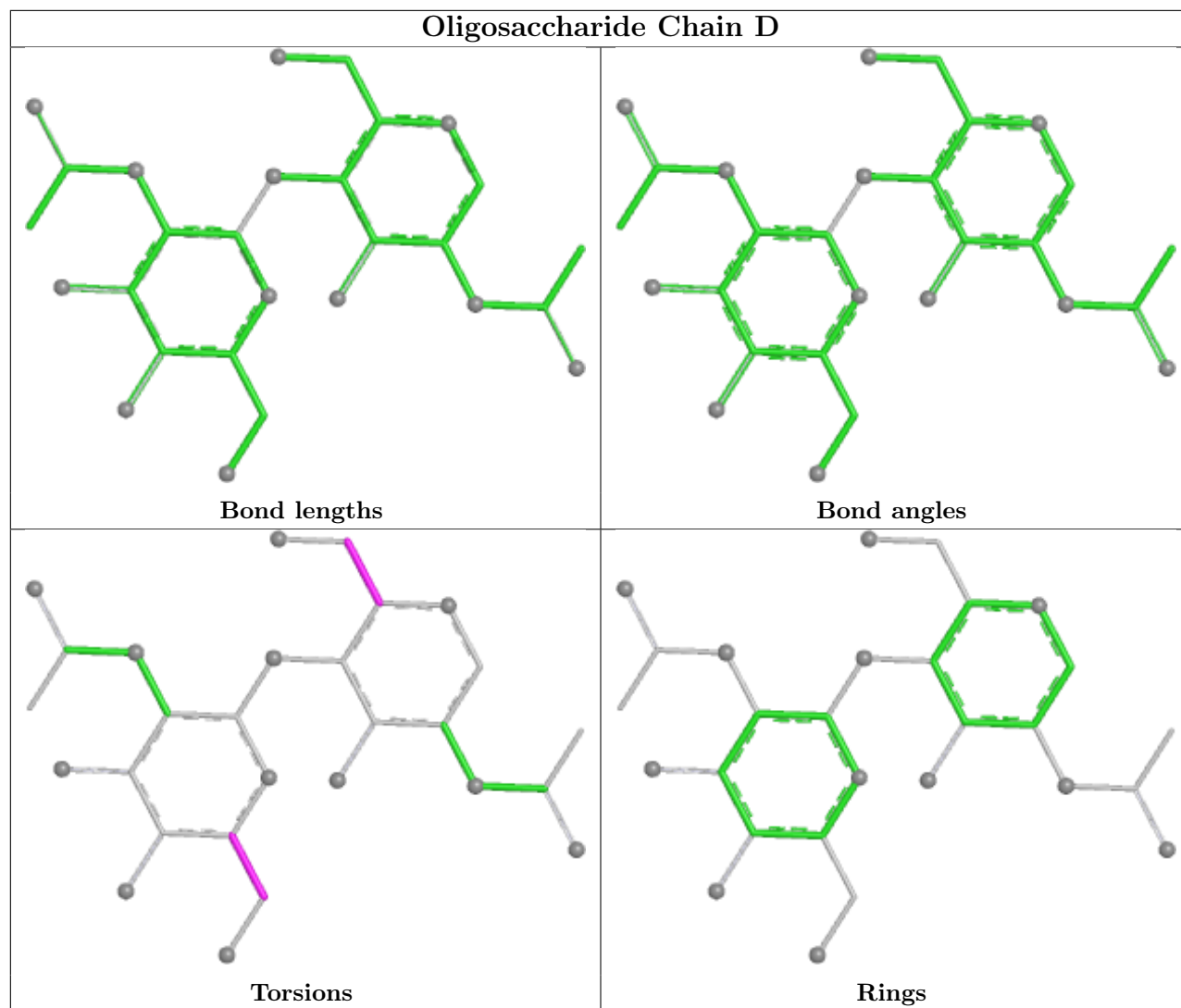
Continued on next page...

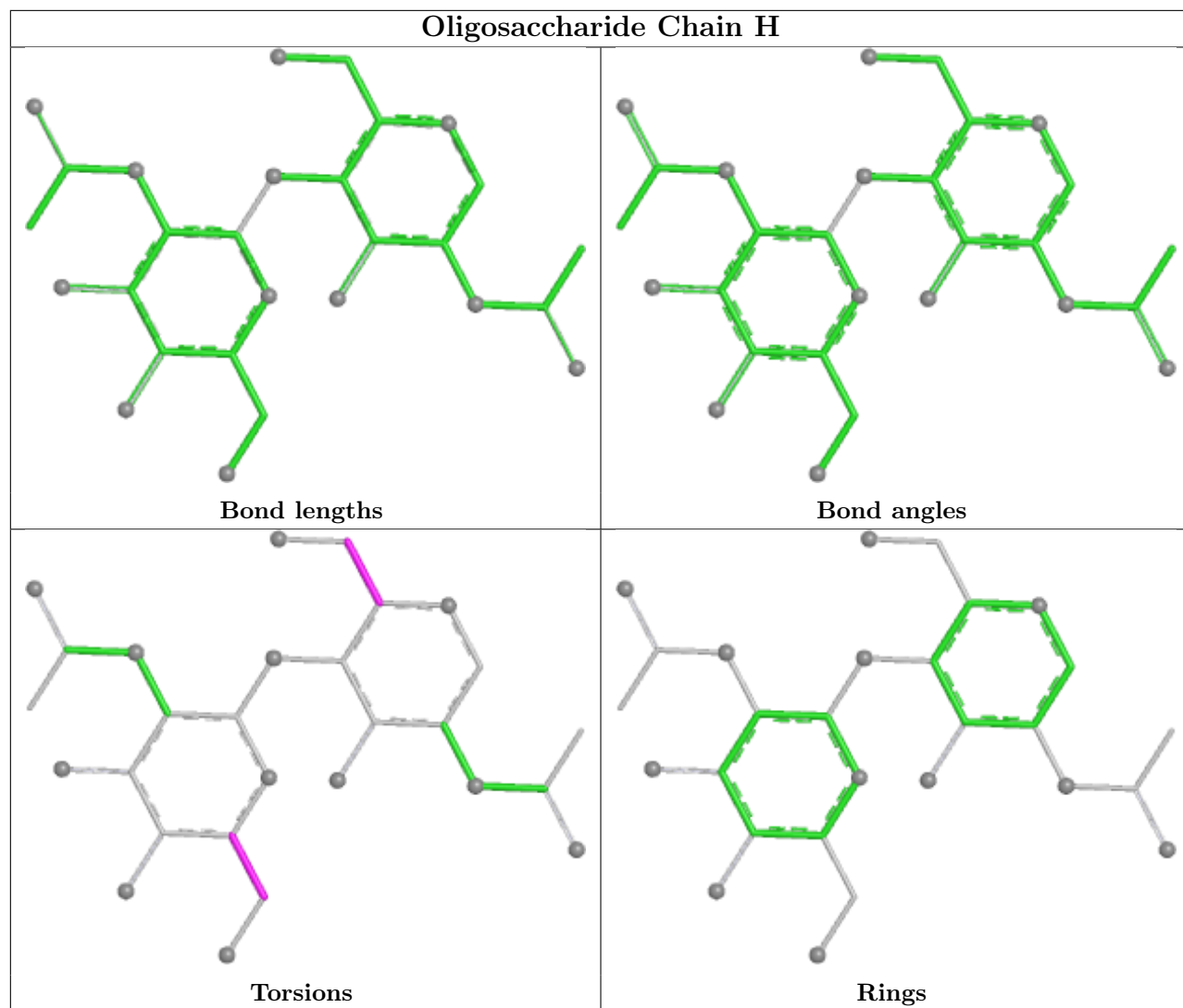
Continued from previous page...

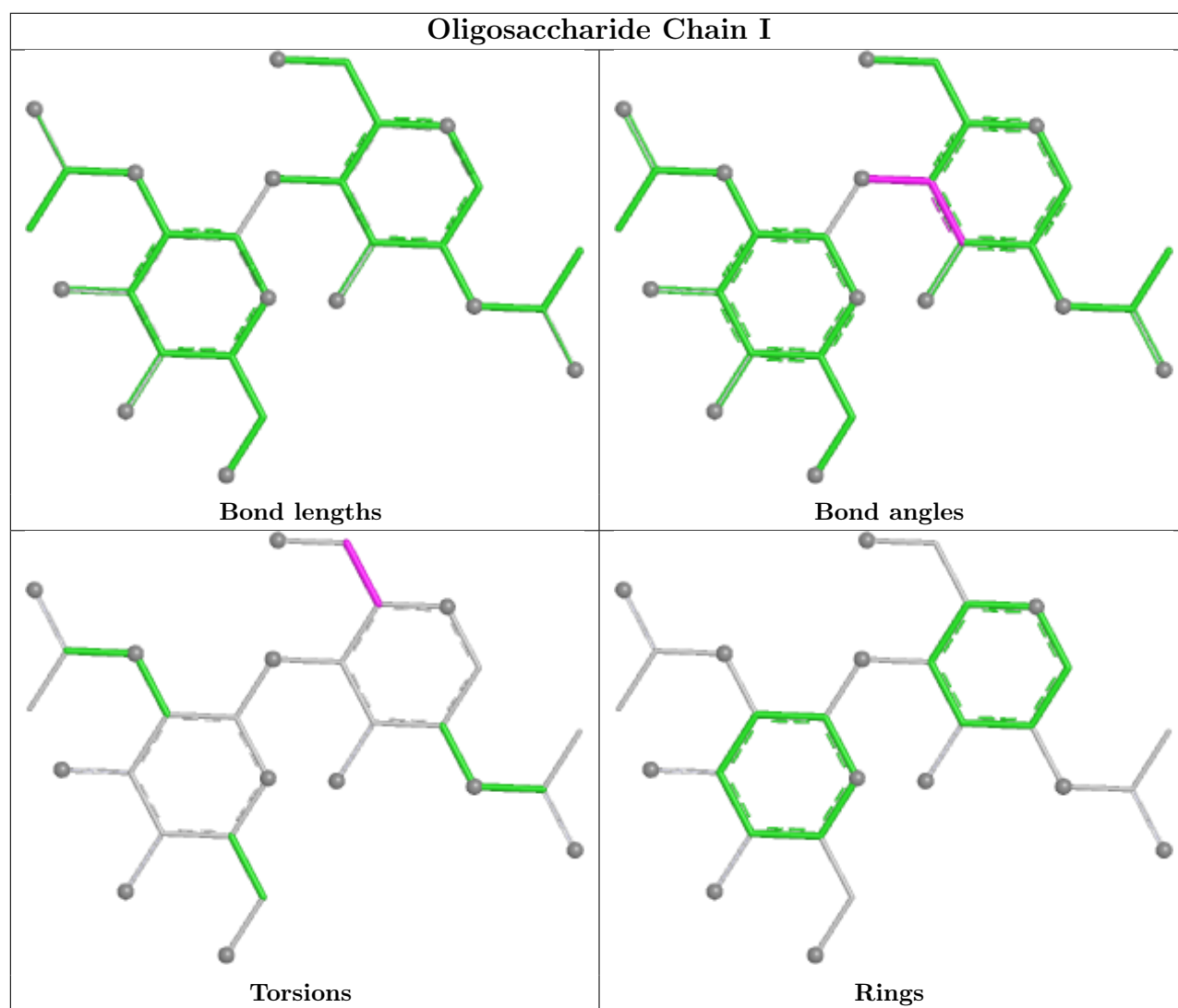
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	1	0

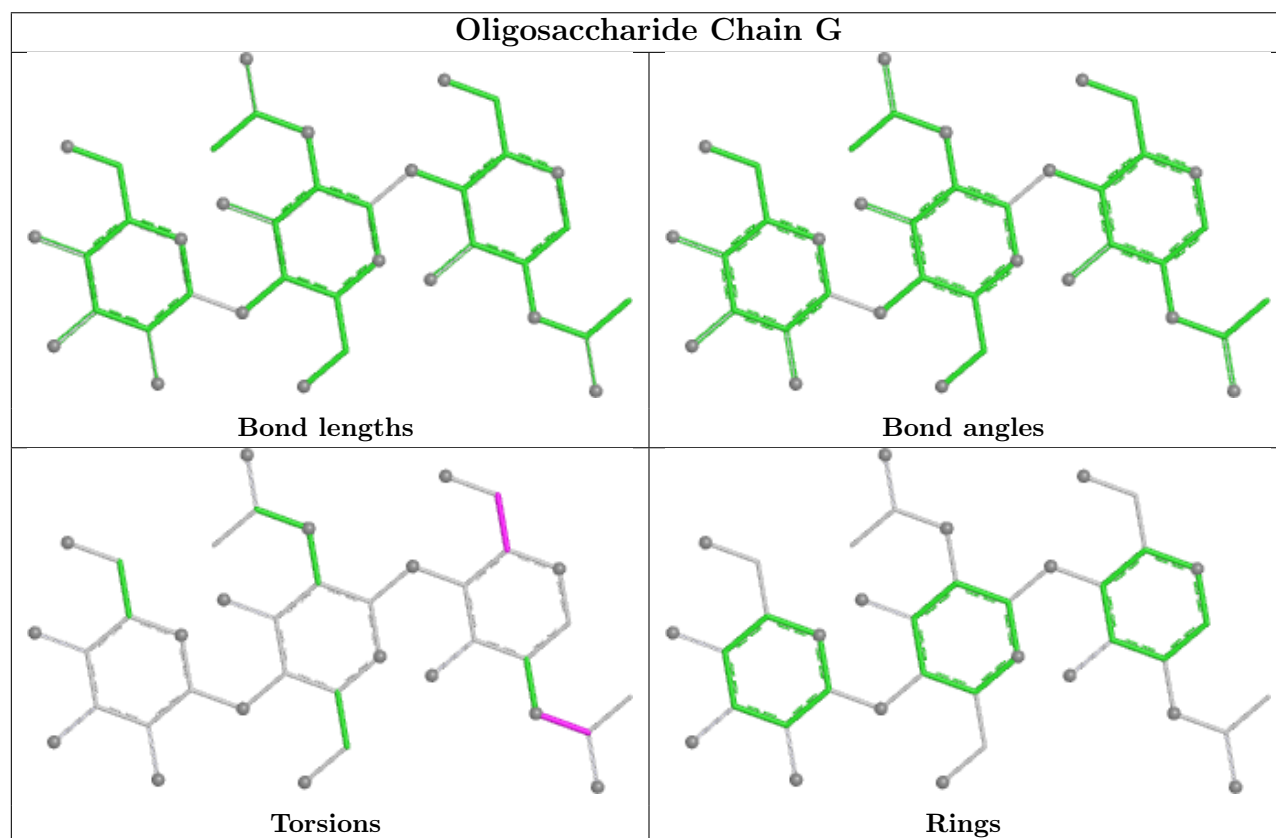
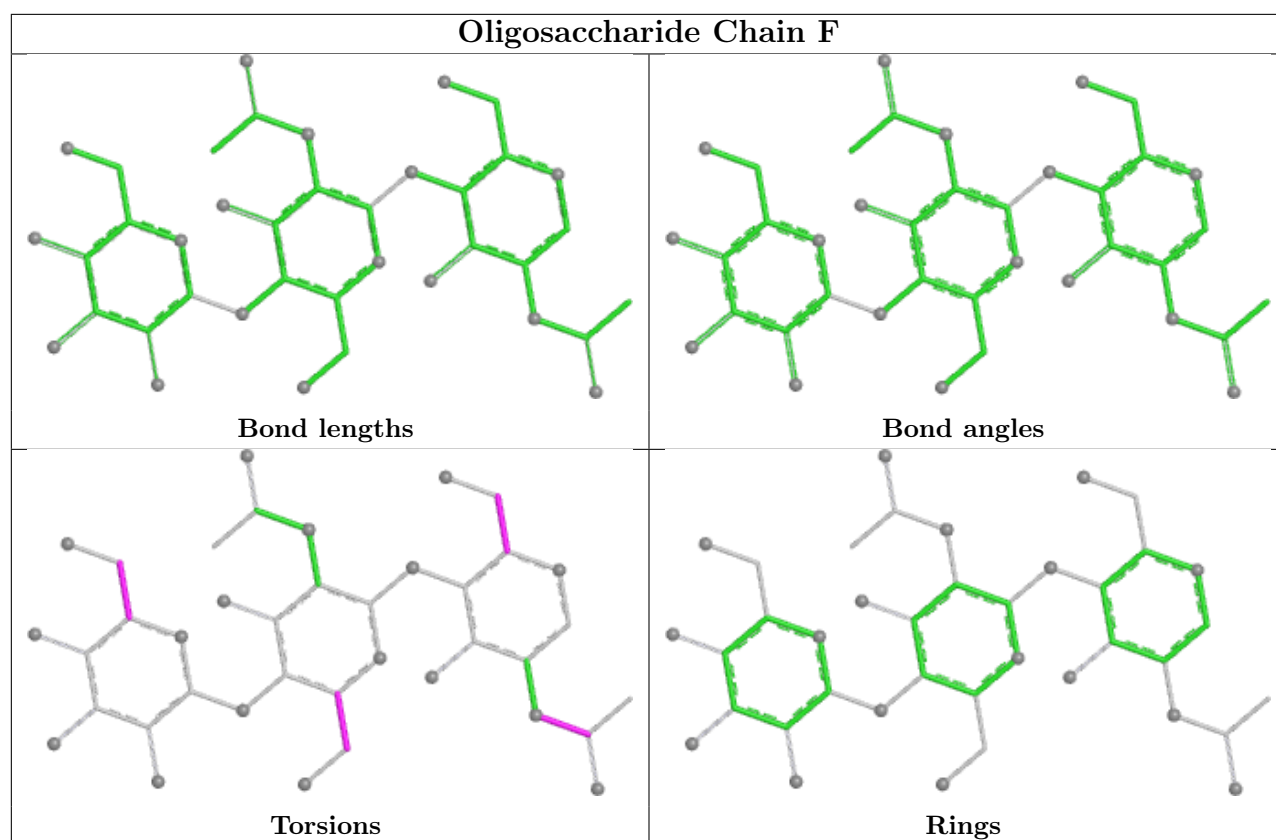
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

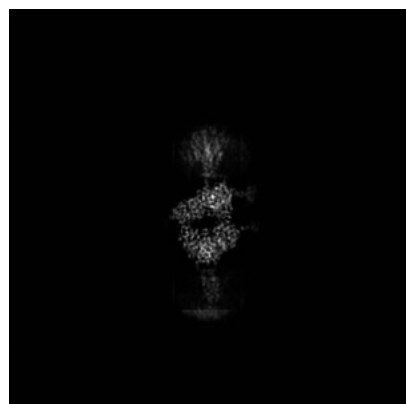
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37498. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

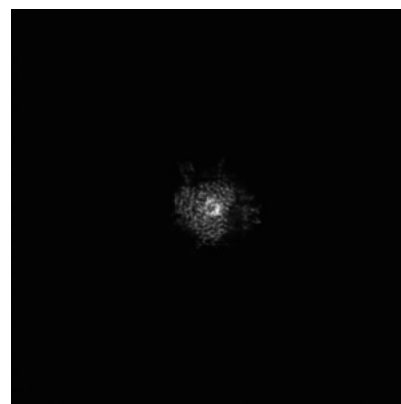
6.1.1 Primary map



X

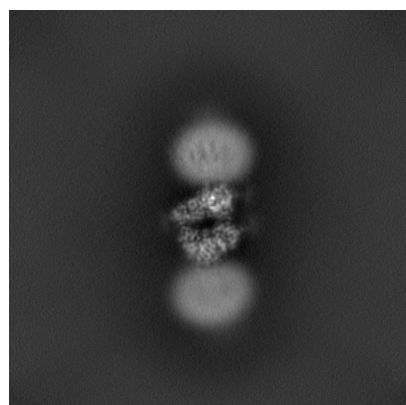


Y

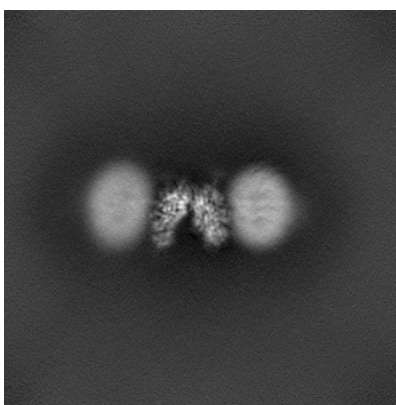


Z

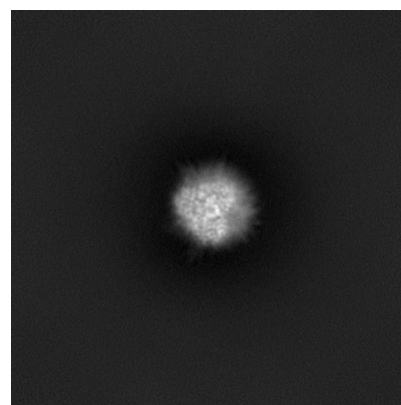
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 180

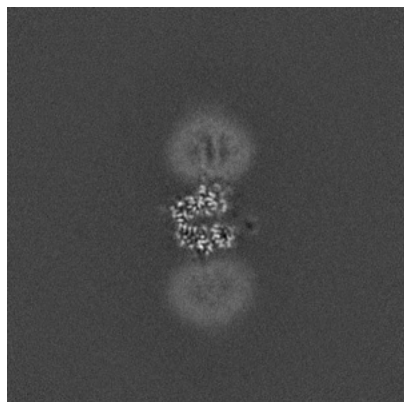


Y Index: 180

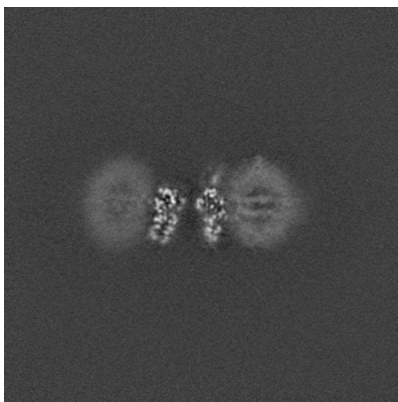


Z Index: 180

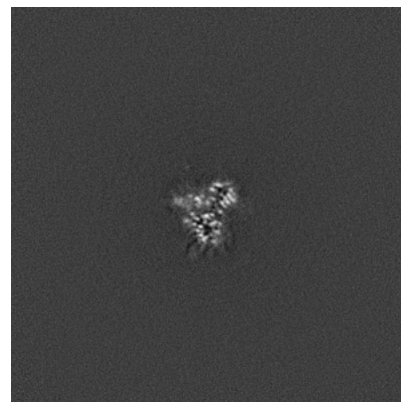
6.2.2 Raw map



X Index: 180



Y Index: 180



Z Index: 180

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: 182

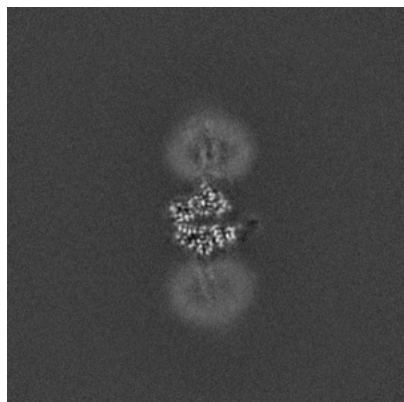


Y Index: 179

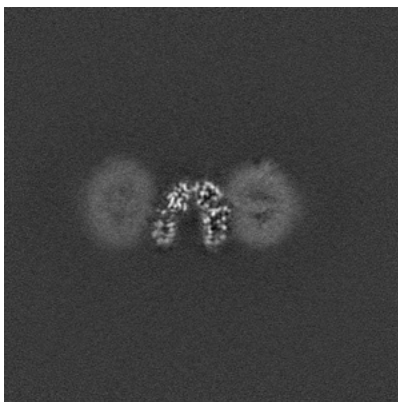


Z Index: 147

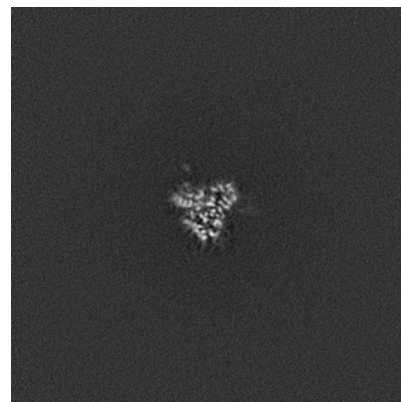
6.3.2 Raw map



X Index: 182



Y Index: 188

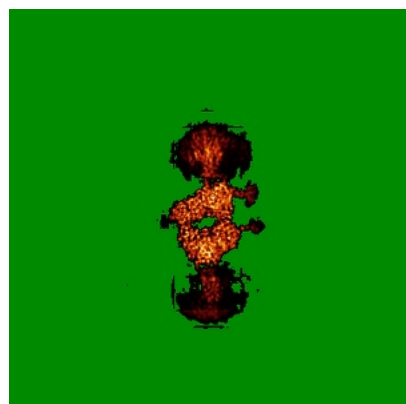


Z Index: 182

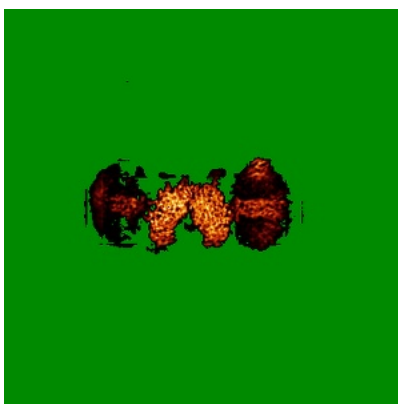
The images above show the largest variance slices of the map in three orthogonal directions.

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

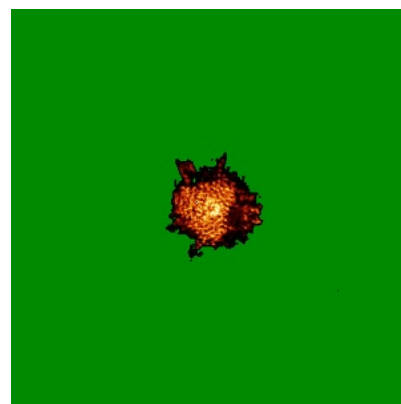
6.4.1 Primary map



X

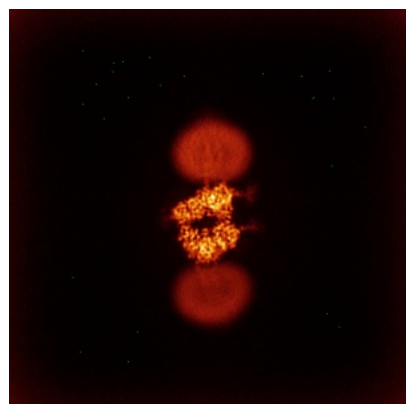


Y

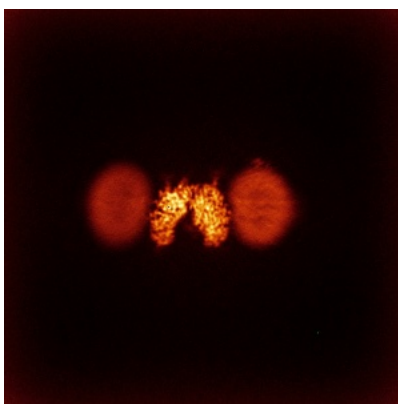


Z

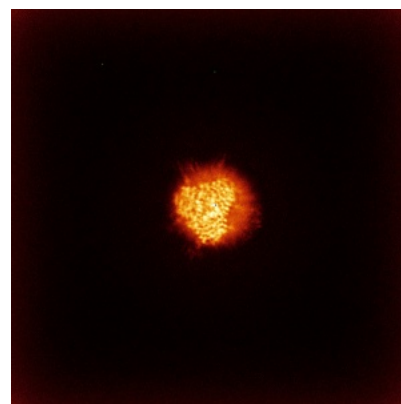
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

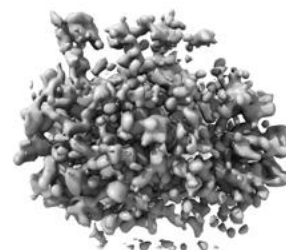
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0457. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

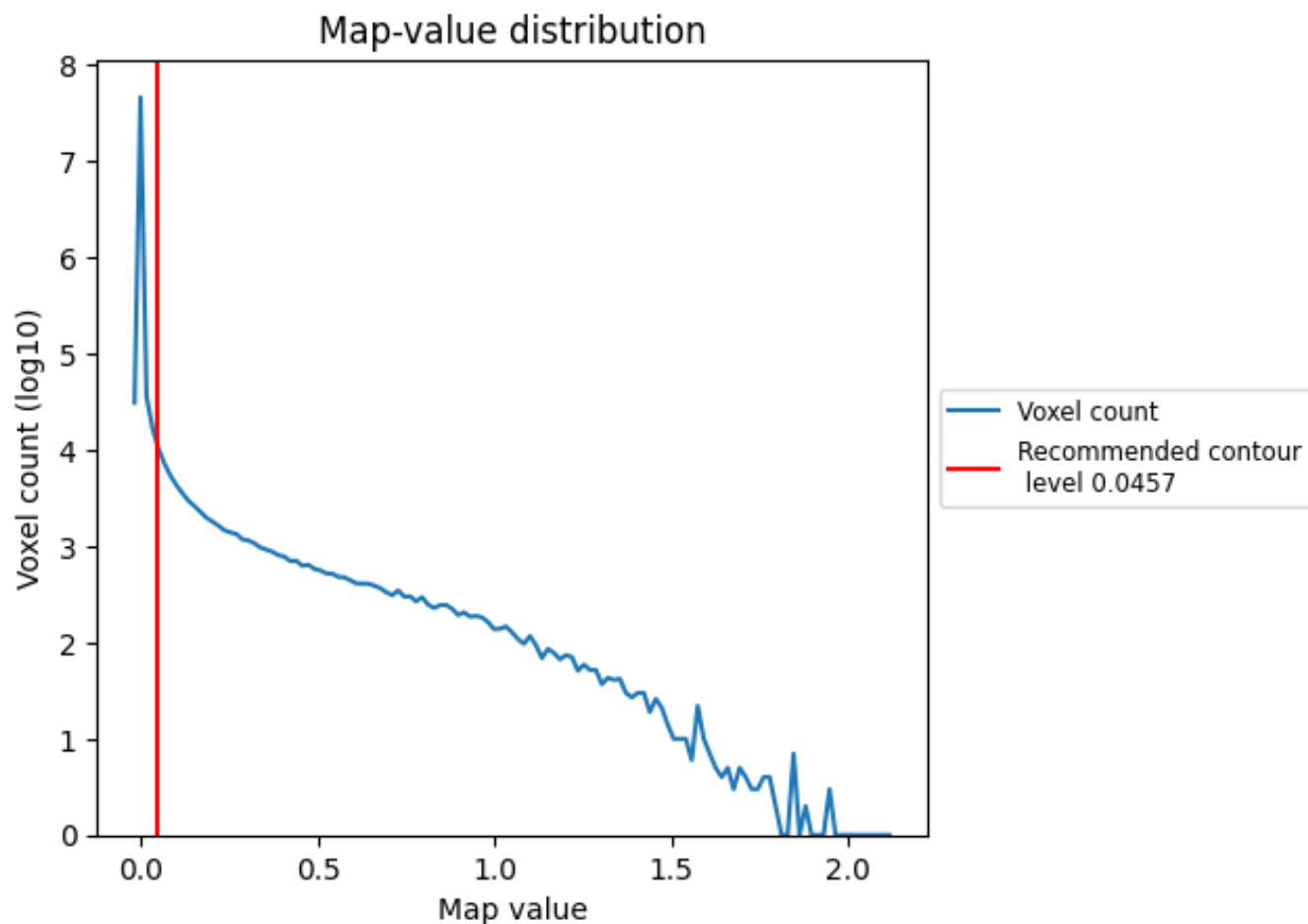
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

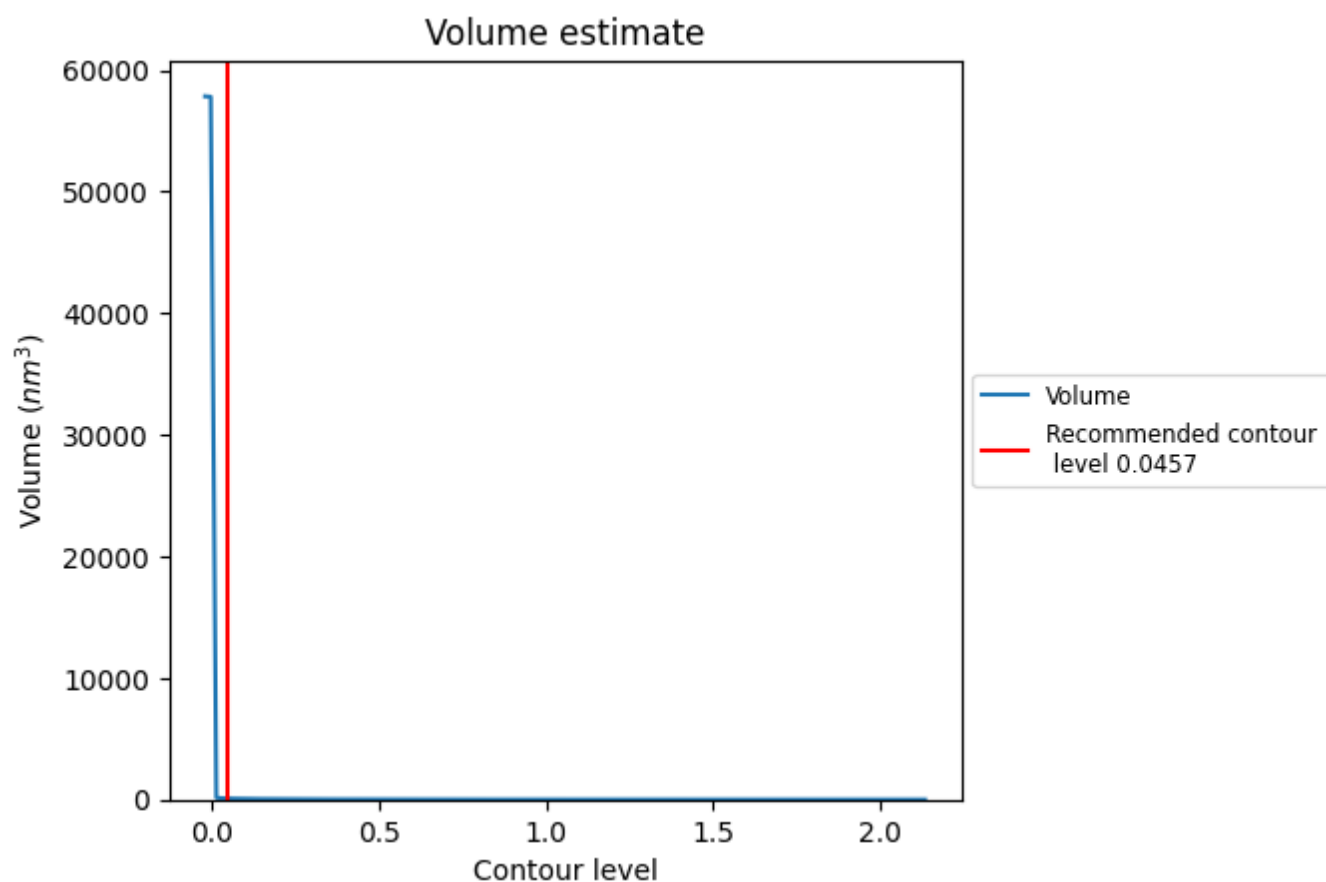
This section contains the results of statistical analysis of the map.

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.

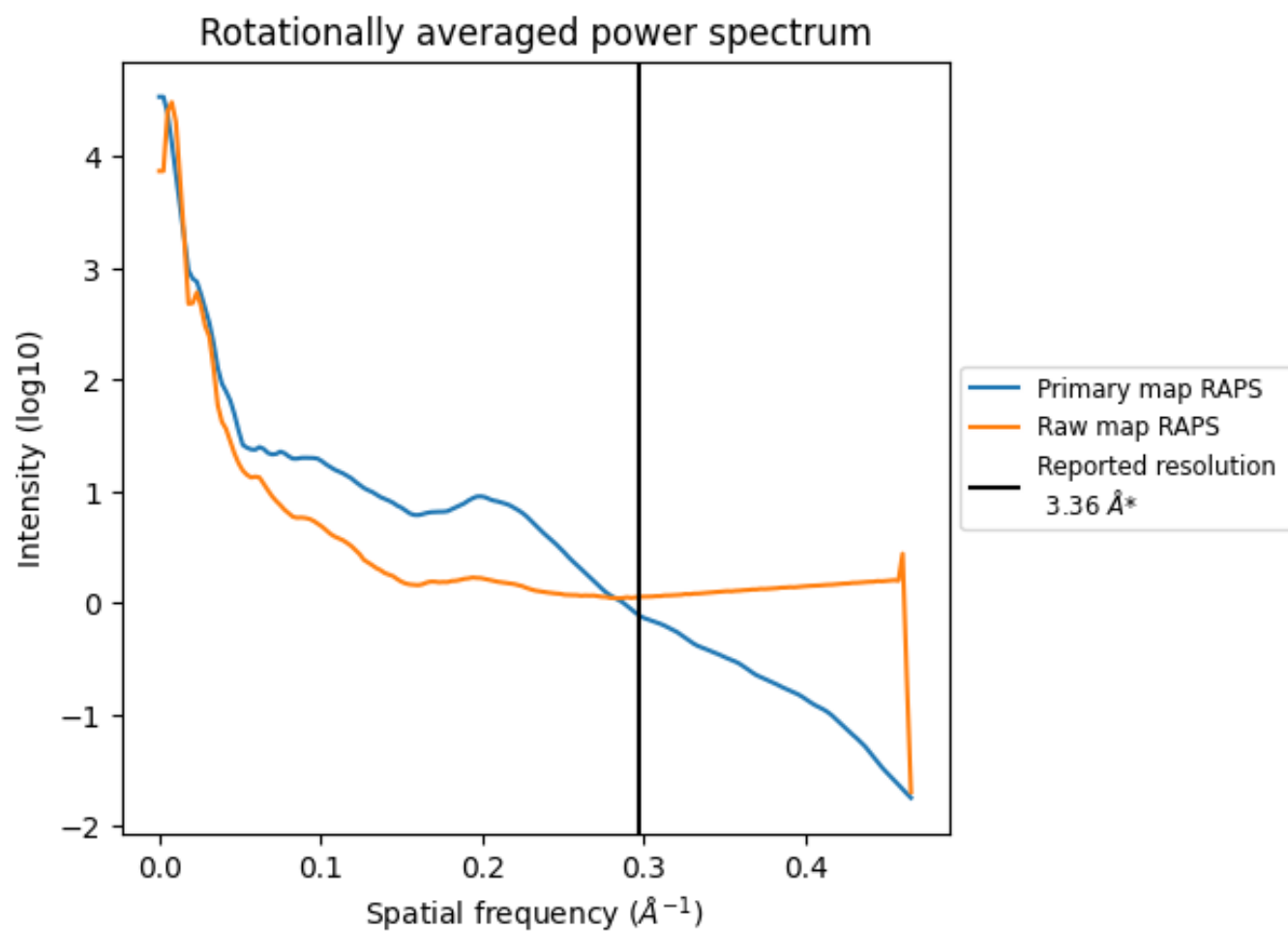
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 92 nm³; this corresponds to an approximate mass of 83 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 ⓘ

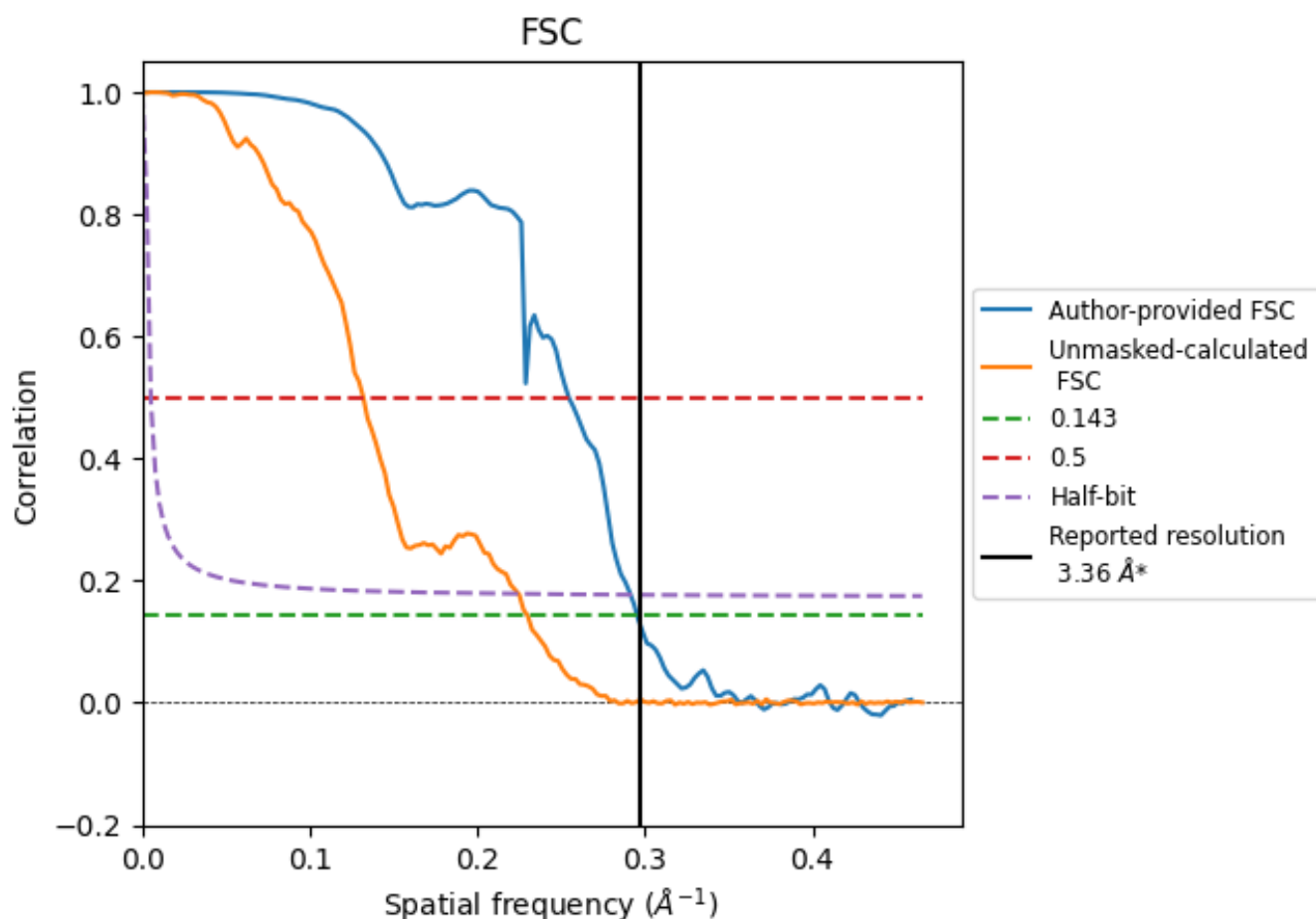


*Reported resolution corresponds to spatial frequency of 0.298 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.298 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

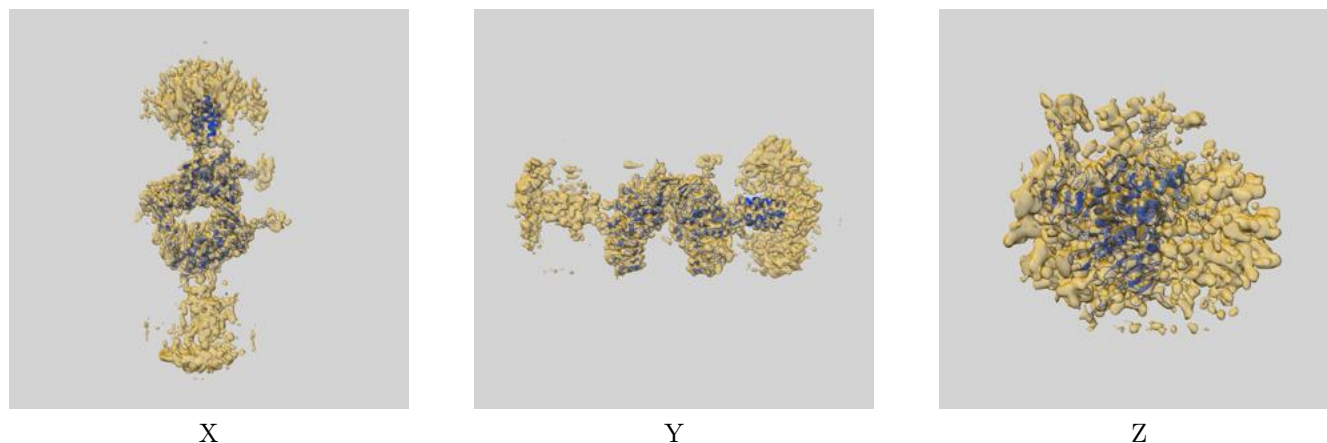
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.36	-	-
Author-provided FSC curve	3.39	3.93	3.43
Unmasked-calculated*	4.35	7.58	4.45

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.35 differs from the reported value 3.36 by more than 10 %

9 Map-model fit [i](#)

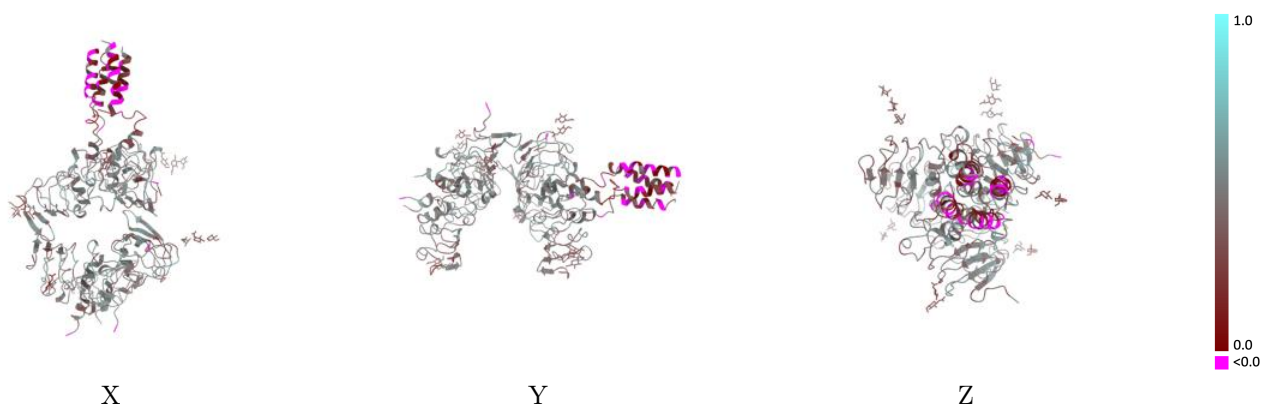
This section contains information regarding the fit between EMDB map EMD-37498 and PDB model 8WFS. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



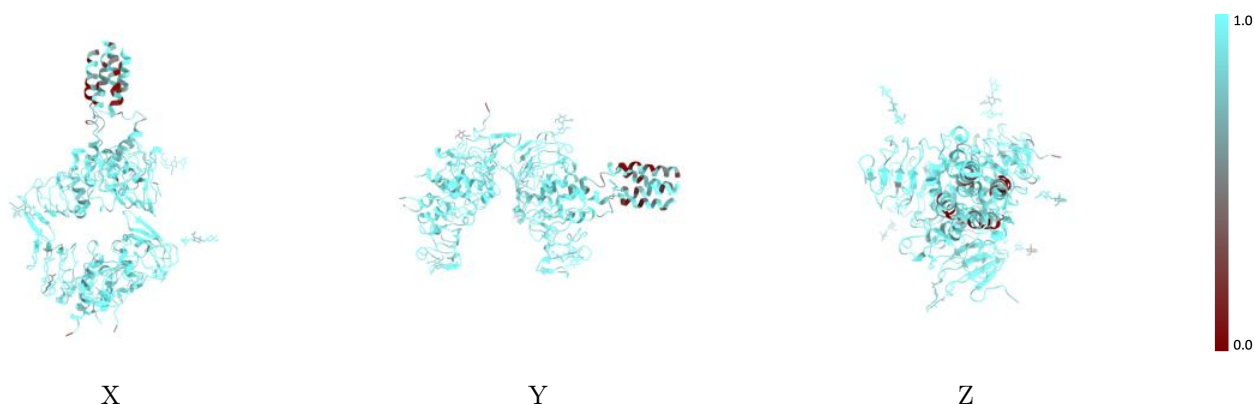
The images above show the 3D surface view of the map at the recommended contour level 0.0457 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



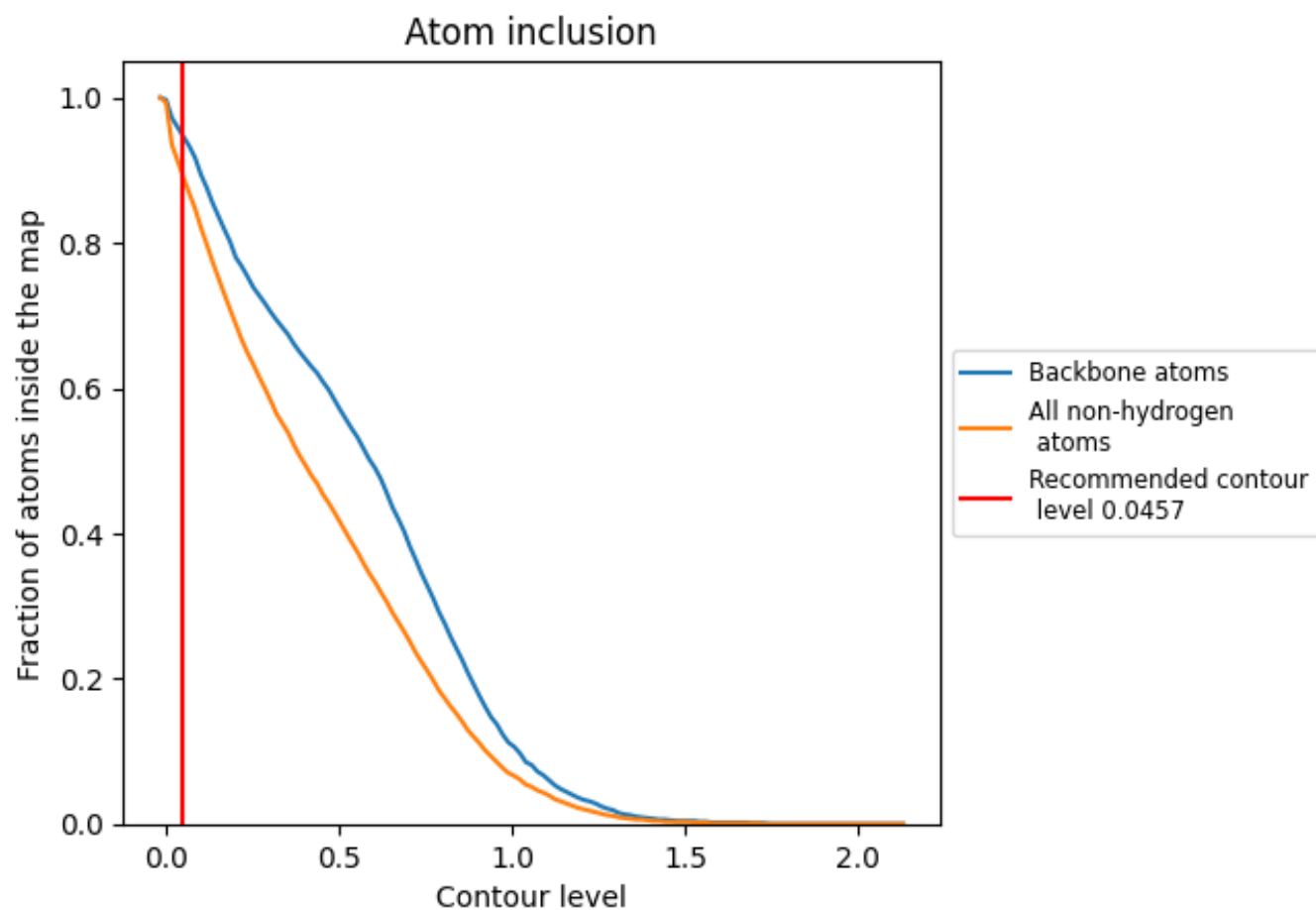
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0457).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 89% 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 (0.0457) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8940	 0.4180
A	 0.7500	 0.3400
B	 0.8880	 0.3980
C	 0.9410	 0.4790
D	 0.6790	 0.2780
E	 0.9280	 0.4630
F	 0.8970	 0.3500
G	 0.8970	 0.3440
H	 0.7860	 0.2780
I	 0.7500	 0.2260
X	 0.8930	 0.4170
a	 0.6160	 0.0980
b	 0.8760	 0.4070
c	 0.9170	 0.4330

