



wwPDB EM Validation Summary Report ⓘ

Sep 28, 2024 – 10:15 pm BST

PDB ID : 7QNA
EMDB ID : EMD-14072
Title : Cryo-EM structure of human full-length alpha4beta3gamma2 GABA(A)R in complex with GABA and nanobody Nb25
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 : 3.00 Å(reported)

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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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

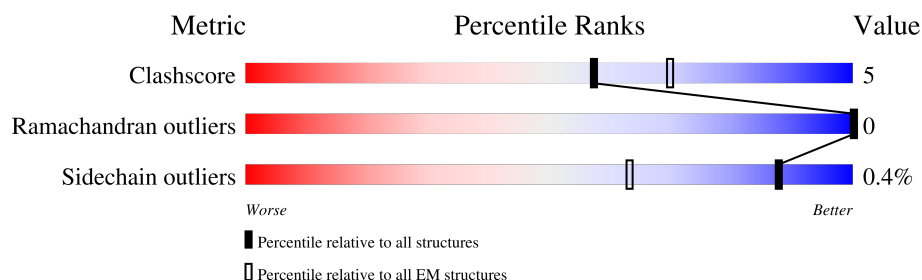
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
2	B	473	
2	D	473	
2	E	473	
3	C	487	
4	N	121	
5	F	5	
5	G	5	

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Mol	Chain	Length	Quality of chain
5	H	5	<div><div></div><div>80%</div><div>20%</div></div>
5	a	5	<div><div></div><div>100%</div></div>
6	b	2	<div><div></div><div>100%</div></div>
6	d	2	<div><div></div><div>100%</div></div>
6	e	2	<div><div></div><div>100%</div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14777 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	327	Total	C	N	O	S	1	0
			2691	1767	436	472	16		
2	D	327	Total	C	N	O	S	1	0
			2698	1771	437	474	16		
2	E	327	Total	C	N	O	S	1	0
			2691	1767	436	472	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	328	Total	C	N	O	S	0	0
			2701	1766	443	477	15		

There are 133 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-30	MET	-	initiating methionine	UNP A0A1W2PQX1
C	-29	GLY	-	expression tag	UNP A0A1W2PQX1
C	-28	ILE	-	expression tag	UNP A0A1W2PQX1
C	-27	LEU	-	expression tag	UNP A0A1W2PQX1
C	-26	PRO	-	expression tag	UNP A0A1W2PQX1
C	-25	SER	-	expression tag	UNP A0A1W2PQX1
C	-24	PRO	-	expression tag	UNP A0A1W2PQX1
C	-23	GLY	-	expression tag	UNP A0A1W2PQX1
C	-22	MET	VAL	conflict	UNP A0A1W2PQX1
C	-21	PRO	TRP	conflict	UNP A0A1W2PQX1
C	-20	ALA	ILE	conflict	UNP A0A1W2PQX1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	SER	-	insertion	UNP A0A1W2PQX1
C	-16	LEU	-	insertion	UNP A0A1W2PQX1
C	-15	VAL	-	insertion	UNP A0A1W2PQX1
C	-14	SER	-	insertion	UNP A0A1W2PQX1
C	-10	VAL	-	insertion	UNP A0A1W2PQX1
C	-8	LEU	TYR	conflict	UNP A0A1W2PQX1
C	-7	MET	PRO	conflict	UNP A0A1W2PQX1
C	-5	CYS	-	insertion	UNP A0A1W2PQX1
C	-4	VAL	-	insertion	UNP A0A1W2PQX1
C	-3	ALA	-	insertion	UNP A0A1W2PQX1
C	-2	GLU	PHE	conflict	UNP A0A1W2PQX1
C	0	GLY	SER	conflict	UNP A0A1W2PQX1
C	11	THR	ALA	conflict	UNP A0A1W2PQX1
C	338	LEU	-	insertion	UNP A0A1W2PQX1
C	339	LEU	-	insertion	UNP A0A1W2PQX1
C	340	ARG	-	insertion	UNP A0A1W2PQX1
C	341	MET	-	insertion	UNP A0A1W2PQX1
C	342	PHE	-	insertion	UNP A0A1W2PQX1
C	343	SER	LYS	conflict	UNP A0A1W2PQX1
C	344	PHE	VAL	conflict	UNP A0A1W2PQX1
C	345	LYS	VAL	conflict	UNP A0A1W2PQX1
C	346	ALA	LEU	conflict	UNP A0A1W2PQX1
C	347	PRO	LEU	conflict	UNP A0A1W2PQX1
C	348	THR	ARG	conflict	UNP A0A1W2PQX1
C	349	ILE	VAL	conflict	UNP A0A1W2PQX1
C	350	ASP	GLY	conflict	UNP A0A1W2PQX1
C	352	ARG	LEU	conflict	UNP A0A1W2PQX1
C	354	ARG	ALA	conflict	UNP A0A1W2PQX1
C	356	ALA	TYR	conflict	UNP A0A1W2PQX1
C	357	THR	ASN	conflict	UNP A0A1W2PQX1
C	358	ILE	LYS	conflict	UNP A0A1W2PQX1
C	359	GLN	ASP	conflict	UNP A0A1W2PQX1
C	361	ASN	-	insertion	UNP A0A1W2PQX1
C	362	ASN	ARG	conflict	UNP A0A1W2PQX1
C	363	ALA	THR	conflict	UNP A0A1W2PQX1
C	364	THR	GLY	conflict	UNP A0A1W2PQX1
C	365	HIS	PHE	conflict	UNP A0A1W2PQX1
C	366	LEU	GLN	conflict	UNP A0A1W2PQX1
C	367	GLN	THR	conflict	UNP A0A1W2PQX1
C	368	GLU	SER	conflict	UNP A0A1W2PQX1
C	369	ARG	SER	conflict	UNP A0A1W2PQX1
C	372	GLU	SER	conflict	UNP A0A1W2PQX1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	373	TYR	PHE	conflict	UNP A0A1W2PQX1
C	375	TYR	LYS	conflict	UNP A0A1W2PQX1
C	376	GLU	SER	conflict	UNP A0A1W2PQX1
C	377	CYS	PRO	conflict	UNP A0A1W2PQX1
C	379	ASP	-	insertion	UNP A0A1W2PQX1
C	380	GLY	-	insertion	UNP A0A1W2PQX1
C	381	LYS	ALA	conflict	UNP A0A1W2PQX1
C	382	ASP	LEU	conflict	UNP A0A1W2PQX1
C	383	CYS	SER	conflict	UNP A0A1W2PQX1
C	384	ALA	VAL	conflict	UNP A0A1W2PQX1
C	386	PHE	-	insertion	UNP A0A1W2PQX1
C	387	PHE	TYR	conflict	UNP A0A1W2PQX1
C	388	CYS	ALA	conflict	UNP A0A1W2PQX1
C	389	CYS	ILE	conflict	UNP A0A1W2PQX1
C	390	PHE	ALA	conflict	UNP A0A1W2PQX1
C	392	ASP	-	expression tag	UNP A0A1W2PQX1
C	393	CYS	-	expression tag	UNP A0A1W2PQX1
C	394	ARG	-	expression tag	UNP A0A1W2PQX1
C	395	THR	-	expression tag	UNP A0A1W2PQX1
C	396	GLY	-	expression tag	UNP A0A1W2PQX1
C	397	ALA	-	expression tag	UNP A0A1W2PQX1
C	398	TRP	-	expression tag	UNP A0A1W2PQX1
C	399	ARG	-	expression tag	UNP A0A1W2PQX1
C	400	HIS	-	expression tag	UNP A0A1W2PQX1
C	401	GLY	-	expression tag	UNP A0A1W2PQX1
C	402	ARG	-	expression tag	UNP A0A1W2PQX1
C	403	ILE	-	expression tag	UNP A0A1W2PQX1
C	404	HIS	-	expression tag	UNP A0A1W2PQX1
C	405	ILE	-	expression tag	UNP A0A1W2PQX1
C	406	ARG	-	expression tag	UNP A0A1W2PQX1
C	407	ILE	-	expression tag	UNP A0A1W2PQX1
C	408	ALA	-	expression tag	UNP A0A1W2PQX1
C	409	LYS	-	expression tag	UNP A0A1W2PQX1
C	410	MET	-	expression tag	UNP A0A1W2PQX1
C	411	ASP	-	expression tag	UNP A0A1W2PQX1
C	412	SER	-	expression tag	UNP A0A1W2PQX1
C	413	TYR	-	expression tag	UNP A0A1W2PQX1
C	414	ALA	-	expression tag	UNP A0A1W2PQX1
C	415	ARG	-	expression tag	UNP A0A1W2PQX1
C	416	ILE	-	expression tag	UNP A0A1W2PQX1
C	417	PHE	-	expression tag	UNP A0A1W2PQX1
C	418	PHE	-	expression tag	UNP A0A1W2PQX1

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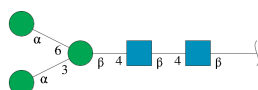
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Chain	Residue	Modelled	Actual	Comment	Reference
C	419	PRO	-	expression tag	UNP A0A1W2PQX1
C	420	THR	-	expression tag	UNP A0A1W2PQX1
C	421	ALA	-	expression tag	UNP A0A1W2PQX1
C	422	PHE	-	expression tag	UNP A0A1W2PQX1
C	423	CYS	-	expression tag	UNP A0A1W2PQX1
C	424	LEU	-	expression tag	UNP A0A1W2PQX1
C	425	PHE	-	expression tag	UNP A0A1W2PQX1
C	426	ASN	-	expression tag	UNP A0A1W2PQX1
C	427	LEU	-	expression tag	UNP A0A1W2PQX1
C	428	VAL	-	expression tag	UNP A0A1W2PQX1
C	429	TYR	-	expression tag	UNP A0A1W2PQX1
C	430	TRP	-	expression tag	UNP A0A1W2PQX1
C	431	VAL	-	expression tag	UNP A0A1W2PQX1
C	432	SER	-	expression tag	UNP A0A1W2PQX1
C	433	TYR	-	expression tag	UNP A0A1W2PQX1
C	434	LEU	-	expression tag	UNP A0A1W2PQX1
C	435	TYR	-	expression tag	UNP A0A1W2PQX1
C	436	LEU	-	expression tag	UNP A0A1W2PQX1
C	437	GLY	-	expression tag	UNP A0A1W2PQX1
C	438	THR	-	expression tag	UNP A0A1W2PQX1
C	439	GLY	-	expression tag	UNP A0A1W2PQX1
C	440	GLY	-	expression tag	UNP A0A1W2PQX1
C	441	SER	-	expression tag	UNP A0A1W2PQX1
C	442	GLY	-	expression tag	UNP A0A1W2PQX1
C	443	GLY	-	expression tag	UNP A0A1W2PQX1
C	444	SER	-	expression tag	UNP A0A1W2PQX1
C	445	GLY	-	expression tag	UNP A0A1W2PQX1
C	446	GLY	-	expression tag	UNP A0A1W2PQX1
C	447	SER	-	expression tag	UNP A0A1W2PQX1
C	448	THR	-	expression tag	UNP A0A1W2PQX1
C	449	GLU	-	expression tag	UNP A0A1W2PQX1
C	450	THR	-	expression tag	UNP A0A1W2PQX1
C	451	SER	-	expression tag	UNP A0A1W2PQX1
C	452	GLN	-	expression tag	UNP A0A1W2PQX1
C	453	VAL	-	expression tag	UNP A0A1W2PQX1
C	454	ALA	-	expression tag	UNP A0A1W2PQX1
C	455	PRO	-	expression tag	UNP A0A1W2PQX1
C	456	ALA	-	expression tag	UNP A0A1W2PQX1

- Molecule 4 is a protein called Nanobody Nb25.

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

- Molecule 5 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.



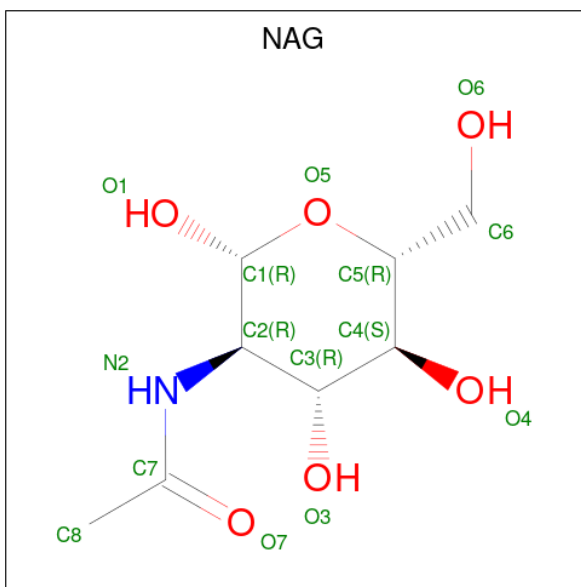
Mol	Chain	Residues	Atoms					AltConf	Trace
5	a	5	Total	C	N	O		0	0
			61	34	2	25			
5	F	5	Total	C	N	O		0	0
			61	34	2	25			
5	G	5	Total	C	N	O		0	0
			61	34	2	25			
5	H	5	Total	C	N	O		0	0
			61	34	2	25			

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



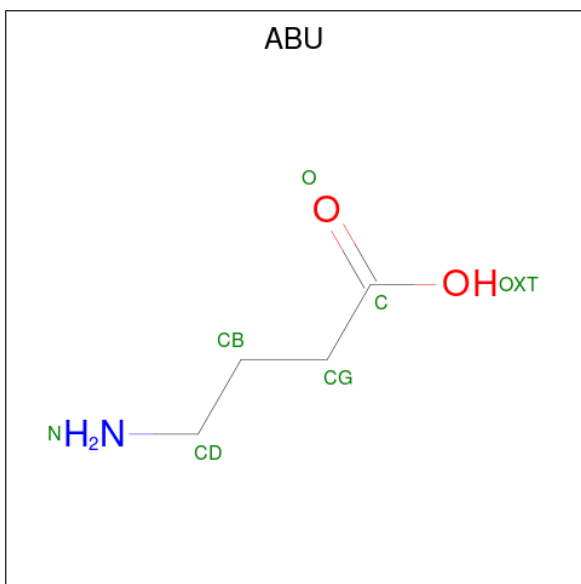
Mol	Chain	Residues	Atoms					AltConf	Trace
6	b	2	Total	C	N	O		0	0
			28	16	2	10			
6	d	2	Total	C	N	O		0	0
			28	16	2	10			
6	e	2	Total	C	N	O		0	0
			28	16	2	10			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 8 is GAMMA-AMINO-BUTANOIC ACID (three-letter code: ABU) (formula: $C_4H_9NO_2$) (labeled as "Ligand of Interest" by depositor).

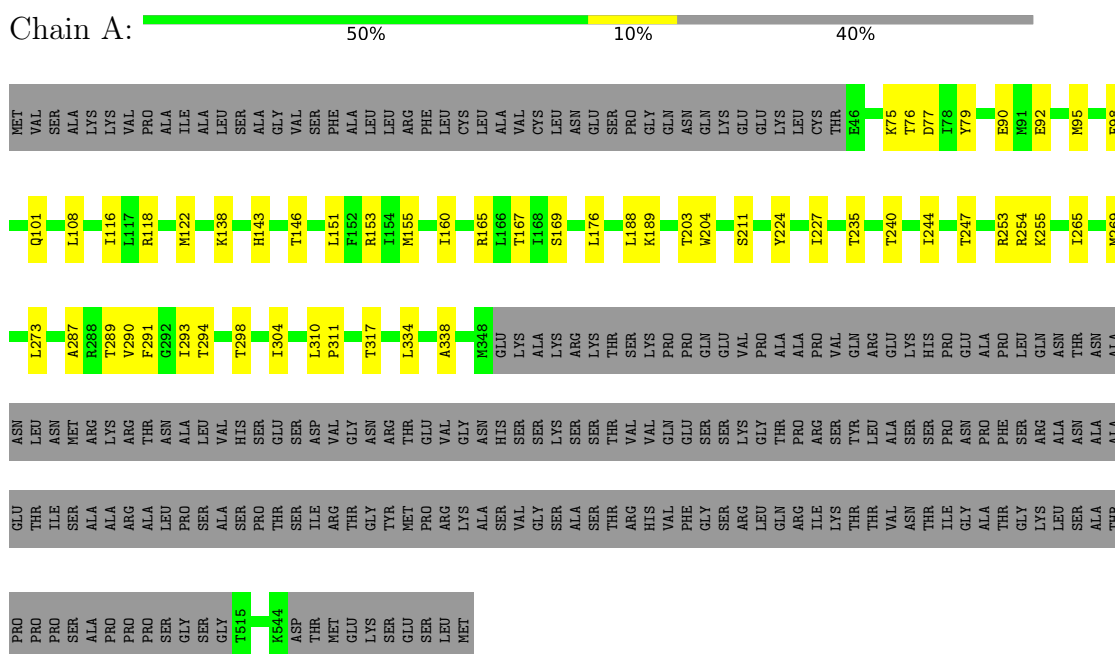


Mol	Chain	Residues	Atoms				AltConf
8	B	1	Total	C	N	O	0
			7	4	1	2	

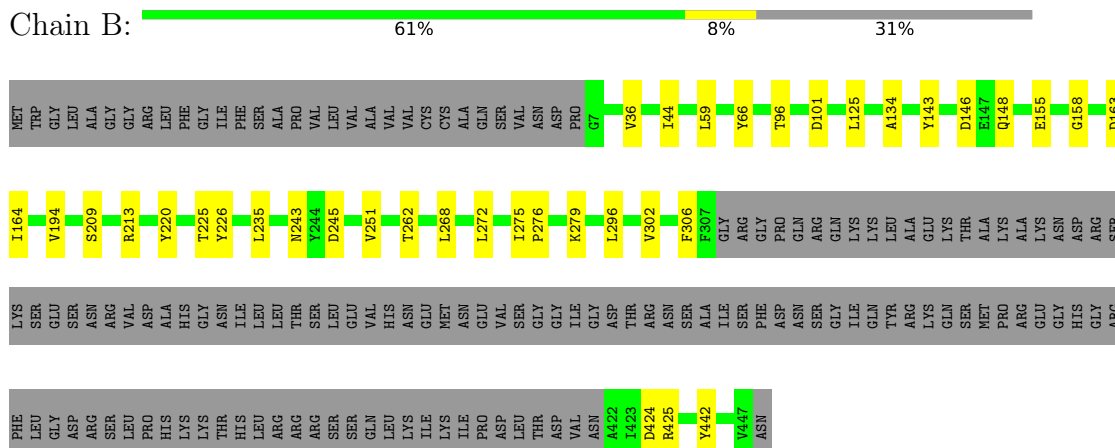
3 Residue-property plots


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 N:  77% 23%




- Molecule 5: 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 a:  100%



- Molecule 5: 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 5: 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 5: 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:  80% 20%



- 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 d:  100%

3AG1
3AG2

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

Chain e:  100%

3AG1
3AG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55567	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 ($e^-/\text{\AA}^2$)	47.46	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	0.095	Depositor
Minimum map value	-0.041	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.005	Depositor
Map size (\AA)	259.84, 259.84, 259.84	wwPDB
Map dimensions	290, 290, 290	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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: MAN, BMA, NAG, ABU

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	0.26	0/2764	0.45	0/3749
2	B	0.25	0/2766	0.46	0/3763
2	D	0.25	0/2771	0.46	0/3770
2	E	0.25	0/2766	0.46	0/3763
3	C	0.25	0/2775	0.46	0/3779
4	N	0.25	0/963	0.47	0/1304
All	All	0.25	0/14805	0.46	0/20128

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	36	0
2	B	2691	0	2690	26	0
2	D	2698	0	2687	30	0
2	E	2691	0	2690	29	0
3	C	2701	0	2693	28	0
4	N	940	0	887	16	0
5	F	61	0	52	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	61	0	52	0	0
5	H	61	0	52	2	0
5	a	61	0	52	0	0
6	b	28	0	25	0	0
6	d	28	0	25	0	0
6	e	28	0	25	0	0
7	A	14	0	13	0	0
7	C	14	0	13	0	0
8	B	7	0	0	1	0
All	All	14777	0	14659	135	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 5.

The worst 5 of 135 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:D:223:LEU:HD11	2:E:286:MET:HG3	1.60	0.81
2:E:272:LEU:HD13	2:E:279:LYS:HE3	1.65	0.79
2:D:272:LEU:HD13	2:D:279:LYS:HE3	1.65	0.79
2:B:272:LEU:HD13	2:B:279:LYS:HE3	1.65	0.76
2:B:243:ASN:ND2	2:B:245:ASP:OD2	2.27	0.67

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	329/554 (59%)	324 (98%)	5 (2%)	0	100	100
2	B	324/473 (68%)	322 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	324/473 (68%)	323 (100%)	1 (0%)	0	100	100
2	E	324/473 (68%)	322 (99%)	2 (1%)	0	100	100
3	C	324/487 (66%)	315 (97%)	9 (3%)	0	100	100
4	N	117/121 (97%)	116 (99%)	1 (1%)	0	100	100
All	All	1742/2581 (68%)	1722 (99%)	20 (1%)	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%)	300 (99%)	2 (1%)	81	91
2	B	295/417 (71%)	294 (100%)	1 (0%)	91	96
2	D	295/417 (71%)	294 (100%)	1 (0%)	91	96
2	E	295/417 (71%)	294 (100%)	1 (0%)	91	96
3	C	303/437 (69%)	303 (100%)	0	100	100
4	N	97/97 (100%)	96 (99%)	1 (1%)	73	88
All	All	1587/2271 (70%)	1581 (100%)	6 (0%)	88	95

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	424	ASP
2	E	424	ASP
4	N	459	ARG
1	A	291	PHE
1	A	122	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	303	ASN
2	E	267	HIS
2	D	267	HIS
3	C	323	ASN
2	D	303	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

26 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	5,2	14,14,15	0.24	0	17,19,21	0.41	0
5	NAG	F	2	5	14,14,15	0.23	0	17,19,21	0.45	0
5	BMA	F	3	5	11,11,12	0.61	0	15,15,17	0.76	0
5	MAN	F	4	5	11,11,12	0.20	0	15,15,17	0.26	0
5	MAN	F	5	5	11,11,12	0.20	0	15,15,17	0.25	0
5	NAG	G	1	5,2	14,14,15	0.25	0	17,19,21	0.46	0
5	NAG	G	2	5	14,14,15	0.23	0	17,19,21	0.51	0
5	BMA	G	3	5	11,11,12	0.67	0	15,15,17	0.86	0
5	MAN	G	4	5	11,11,12	0.21	0	15,15,17	0.25	0
5	MAN	G	5	5	11,11,12	0.20	0	15,15,17	0.24	0
5	NAG	H	1	5,2	14,14,15	0.25	0	17,19,21	0.42	0
5	NAG	H	2	5	14,14,15	0.24	0	17,19,21	0.49	0
5	BMA	H	3	5	11,11,12	0.65	0	15,15,17	0.88	0
5	MAN	H	4	5	11,11,12	0.21	0	15,15,17	0.26	0
5	MAN	H	5	5	11,11,12	0.20	0	15,15,17	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	a	1	5,1	14,14,15	0.24	0	17,19,21	0.40	0
5	NAG	a	2	5	14,14,15	0.22	0	17,19,21	0.42	0
5	BMA	a	3	5	11,11,12	0.58	0	15,15,17	0.77	0
5	MAN	a	4	5	11,11,12	0.20	0	15,15,17	0.23	0
5	MAN	a	5	5	11,11,12	0.21	0	15,15,17	0.23	0
6	NAG	b	1	2,6	14,14,15	0.23	0	17,19,21	0.41	0
6	NAG	b	2	6	14,14,15	0.24	0	17,19,21	0.43	0
6	NAG	d	1	2,6	14,14,15	0.24	0	17,19,21	0.39	0
6	NAG	d	2	6	14,14,15	0.23	0	17,19,21	0.41	0
6	NAG	e	1	2,6	14,14,15	0.24	0	17,19,21	0.39	0
6	NAG	e	2	6	14,14,15	0.24	0	17,19,21	0.40	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
5	NAG	F	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1
5	MAN	F	4	5	-	0/2/19/22	0/1/1/1
5	MAN	F	5	5	-	0/2/19/22	0/1/1/1
5	NAG	G	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	2/2/19/22	0/1/1/1
5	MAN	G	4	5	-	0/2/19/22	0/1/1/1
5	MAN	G	5	5	-	0/2/19/22	0/1/1/1
5	NAG	H	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	BMA	H	3	5	-	1/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	MAN	H	5	5	-	0/2/19/22	0/1/1/1
5	NAG	a	1	5,1	-	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
5	MAN	a	4	5	-	0/2/19/22	0/1/1/1
5	MAN	a	5	5	-	0/2/19/22	0/1/1/1
6	NAG	b	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	b	2	6	-	0/6/23/26	0/1/1/1
6	NAG	d	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	d	2	6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	e	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	e	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 (3) torsion outliers are listed below:

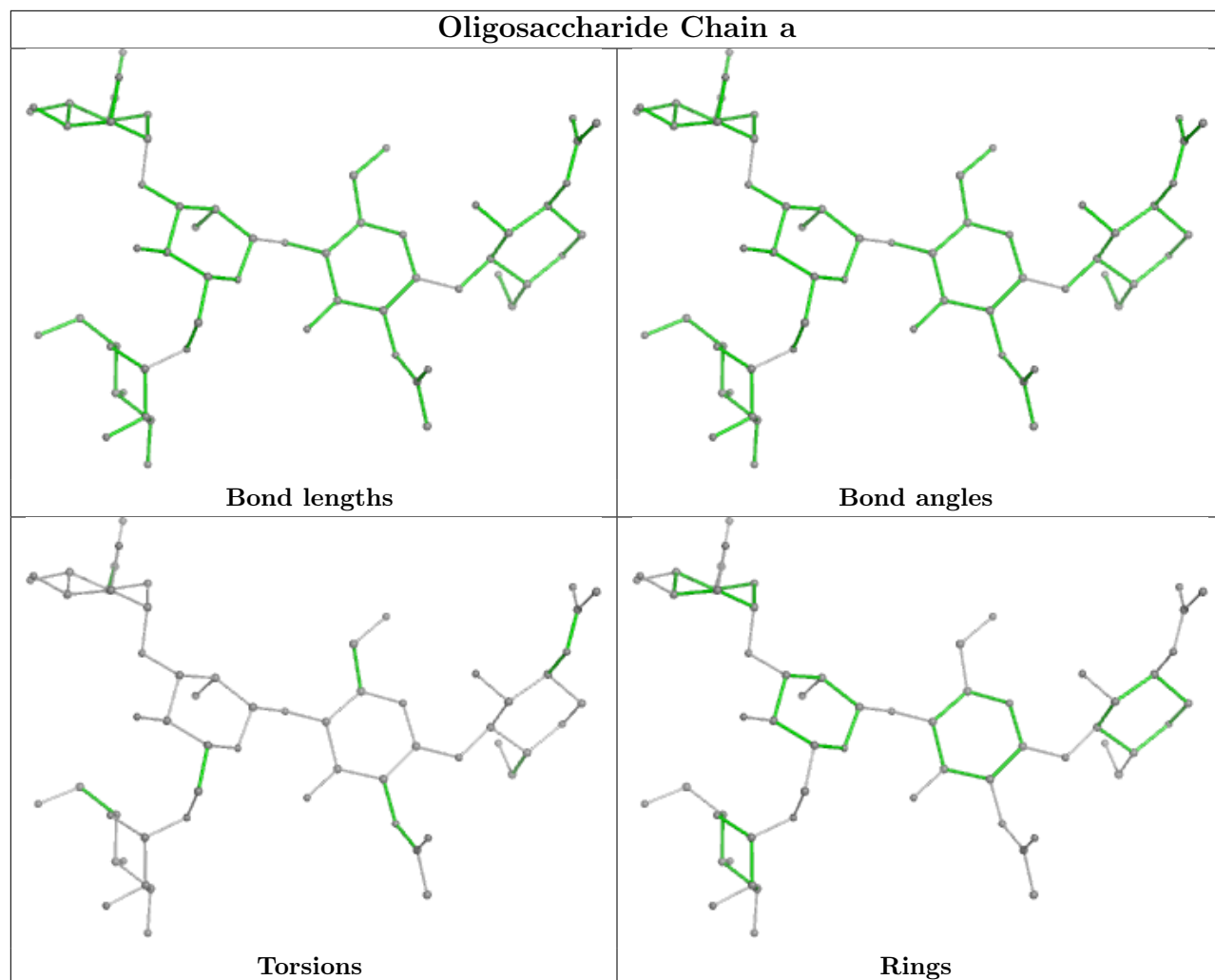
Mol	Chain	Res	Type	Atoms
5	G	3	BMA	C4-C5-C6-O6
5	G	3	BMA	O5-C5-C6-O6
5	H	3	BMA	C4-C5-C6-O6

There are no ring outliers.

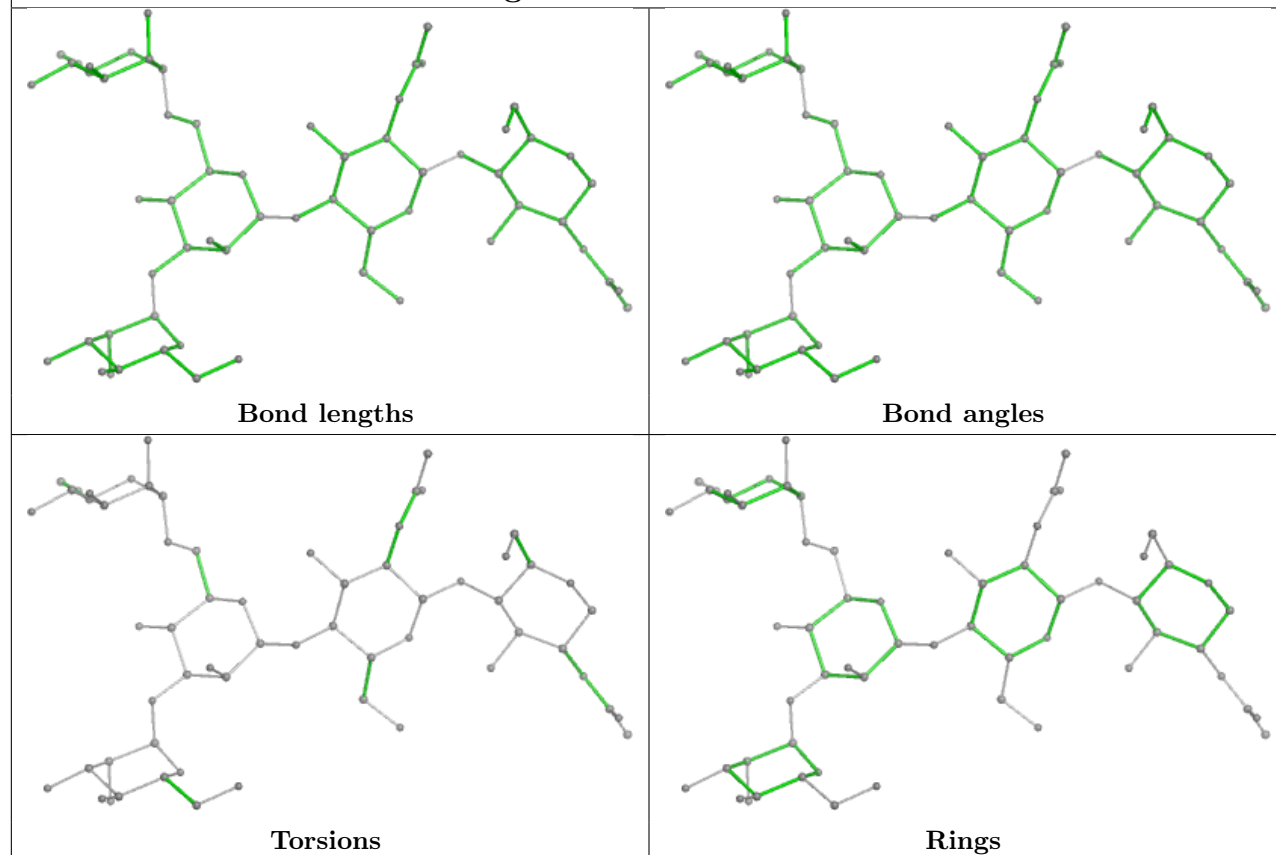
2 monomers are involved in 3 short contacts:

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

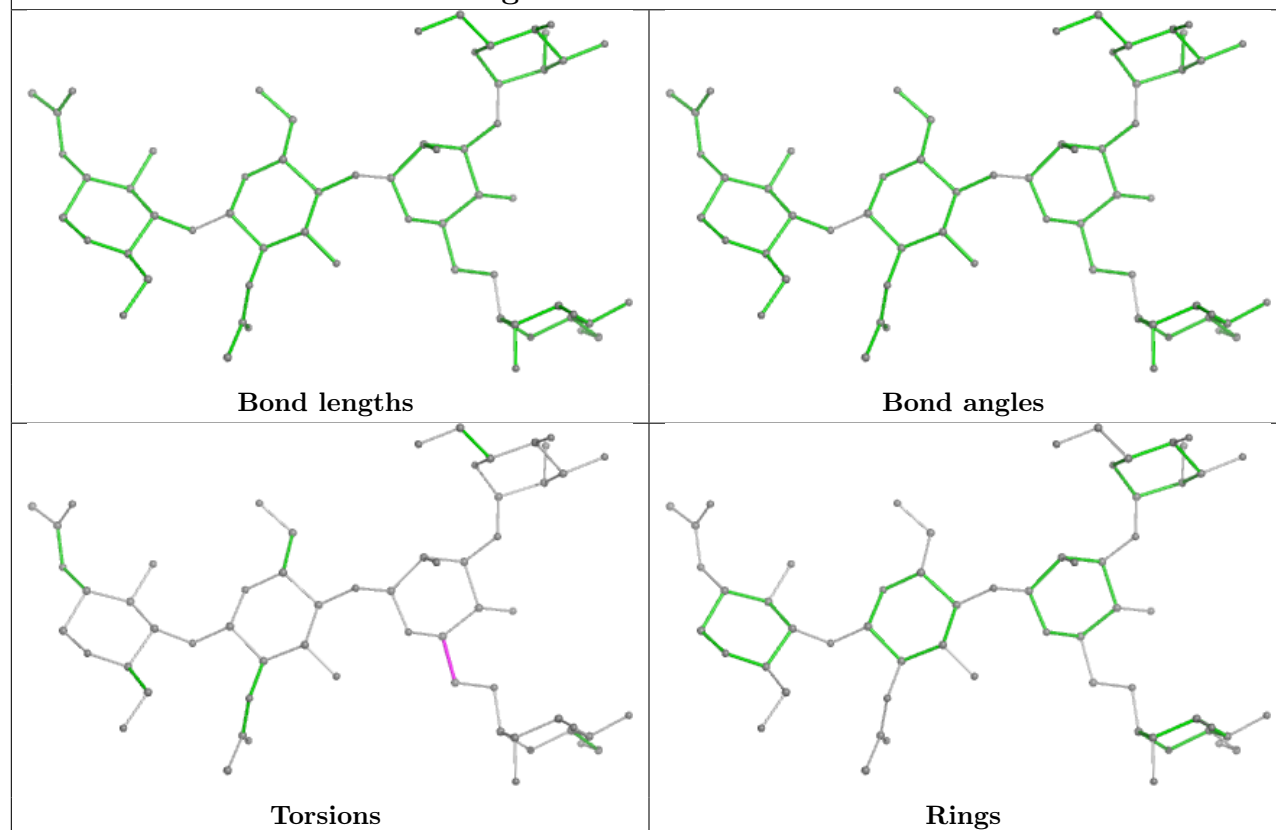
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

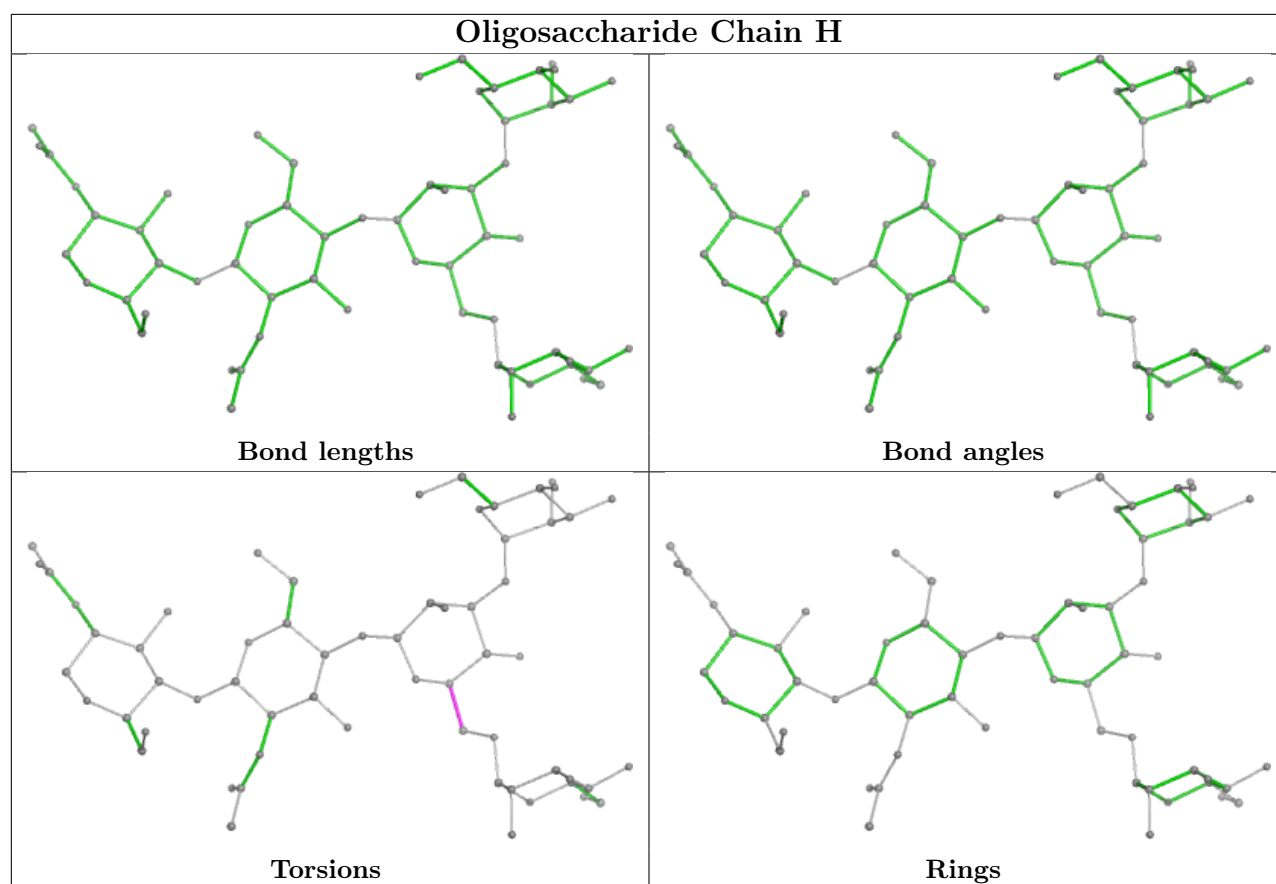


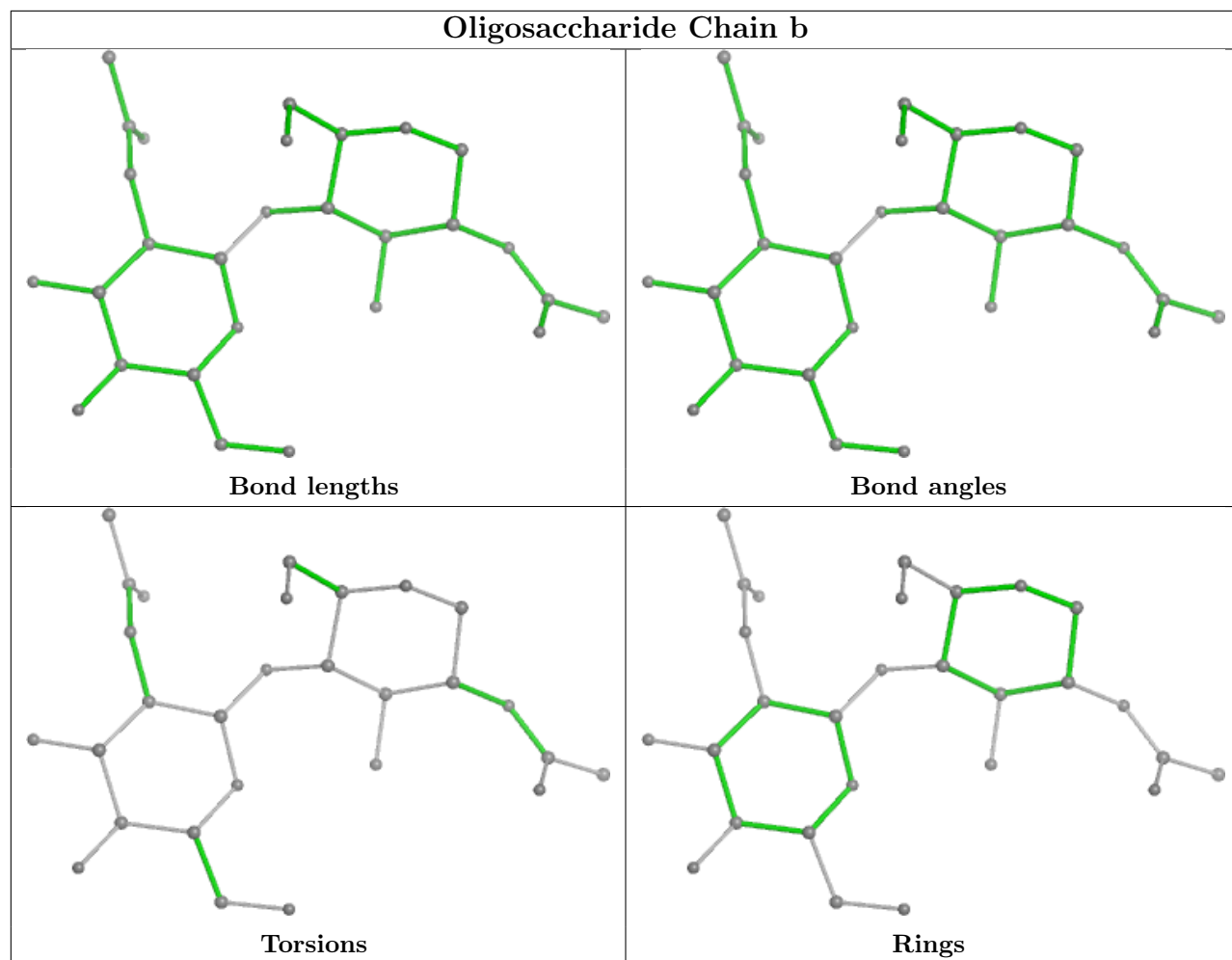
Oligosaccharide Chain F

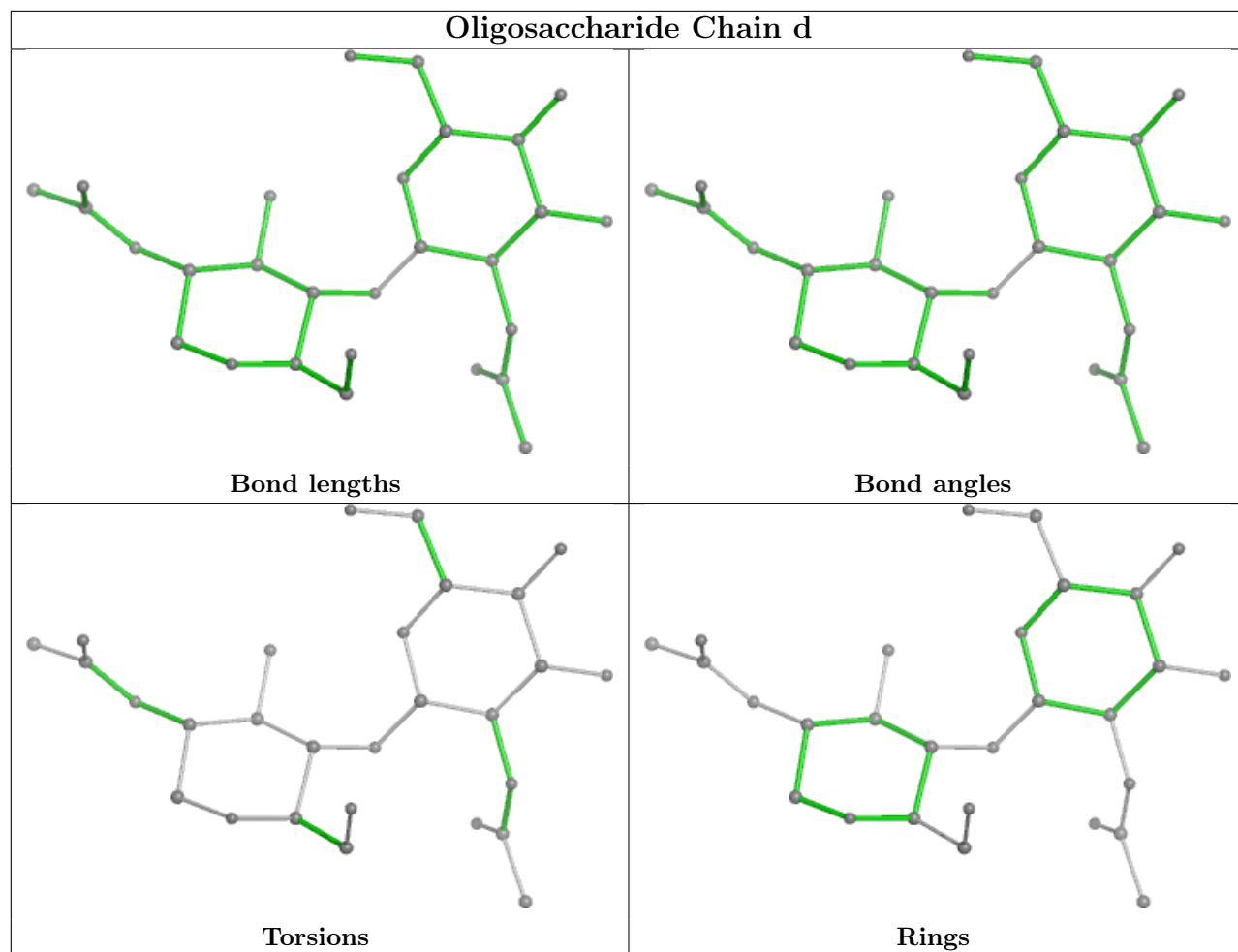


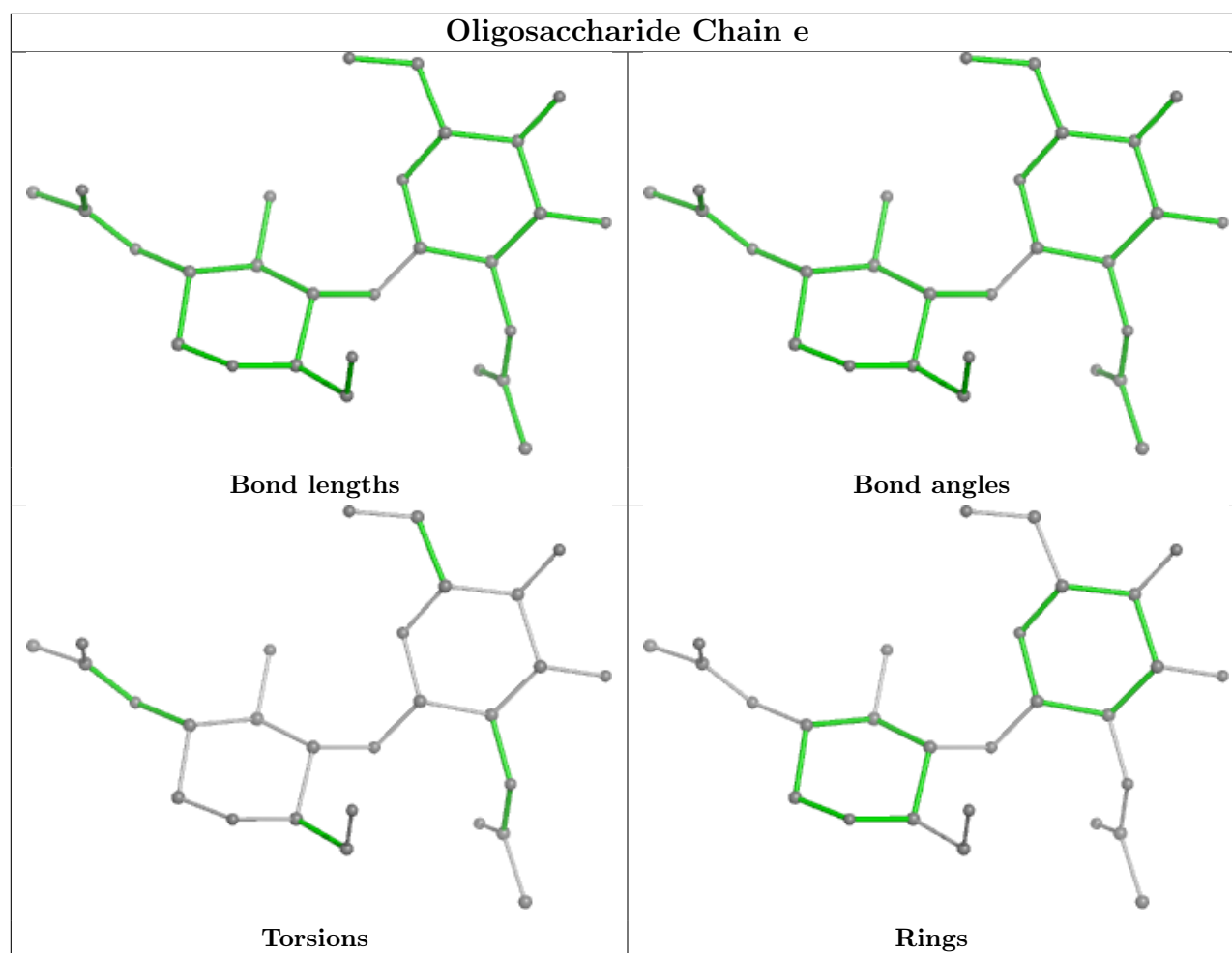
Oligosaccharide Chain G











5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
8	ABU	B	501	-	6,6,6	0.77	0	6,6,6	1.70	2 (33%)
7	NAG	C	501	3	14,14,15	0.22	0	17,19,21	0.44	0
7	NAG	A	601	1	14,14,15	0.23	0	17,19,21	0.47	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ABU	B	501	-	-	2/4/4/4	-
7	NAG	C	501	3	-	1/6/23/26	0/1/1/1
7	NAG	A	601	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	501	ABU	O-C-CG	-3.03	113.35	123.08
8	B	501	ABU	OXT-C-CG	2.84	123.15	114.03

There are no chirality outliers.

All (4) torsion outliers are listed below:

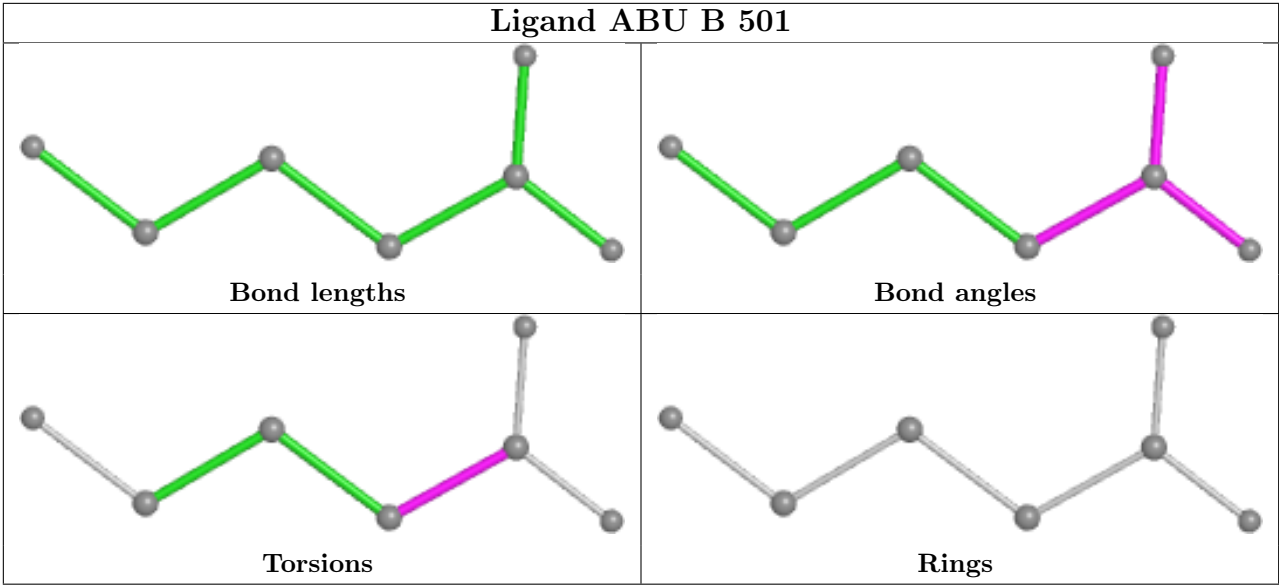
Mol	Chain	Res	Type	Atoms
7	A	601	NAG	O5-C5-C6-O6
7	C	501	NAG	O5-C5-C6-O6
8	B	501	ABU	OXT-C-CG-CB
8	B	501	ABU	O-C-CG-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	501	ABU	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	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	13:GLN	C	403:GLY	N	5.76

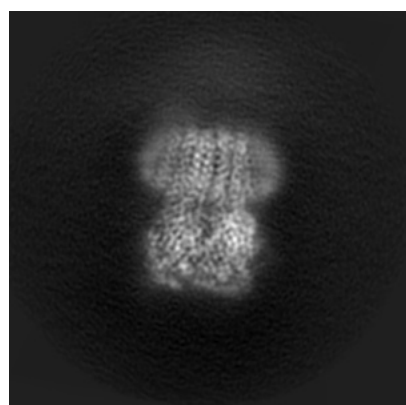
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14072. These allow visual inspection of the internal detail of the map and identification of artifacts.

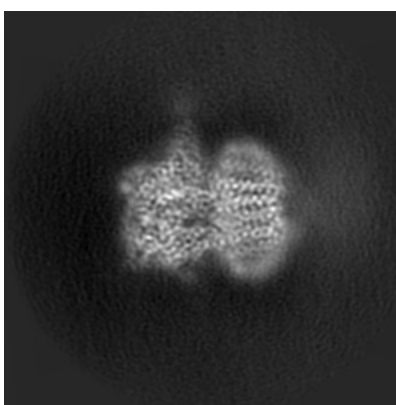
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

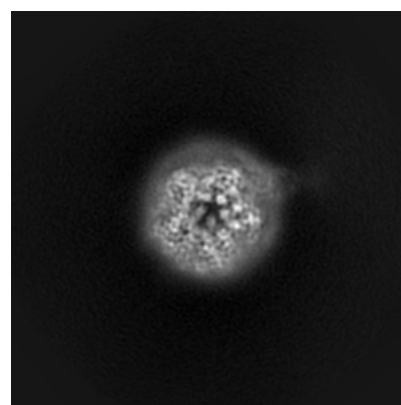
6.1.1 Primary map



X



Y

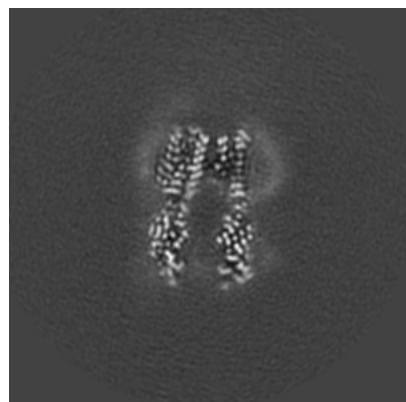


Z

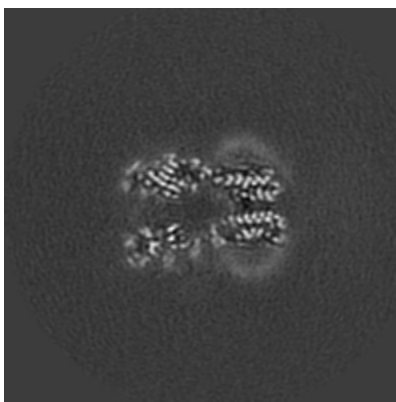
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

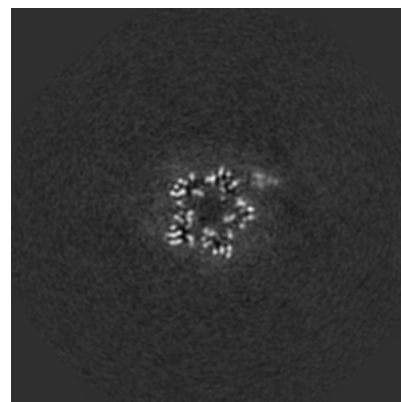
6.2.1 Primary map



X Index: 145



Y Index: 145

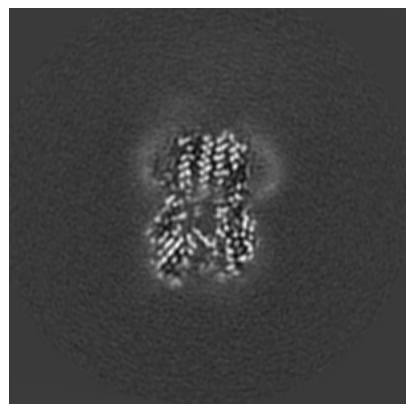


Z Index: 145

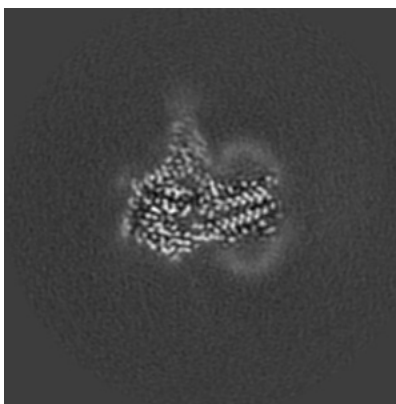
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

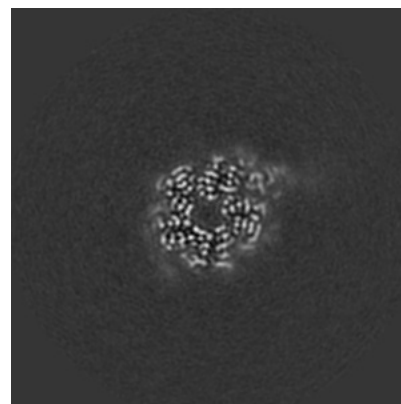
6.3.1 Primary map



X Index: 154



Y Index: 164

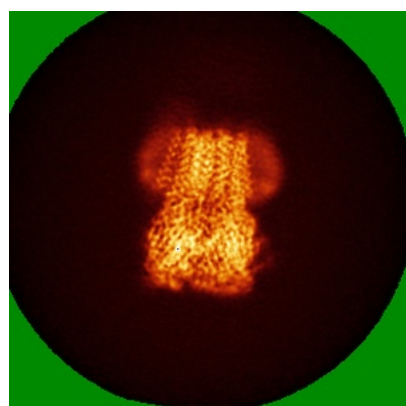


Z Index: 121

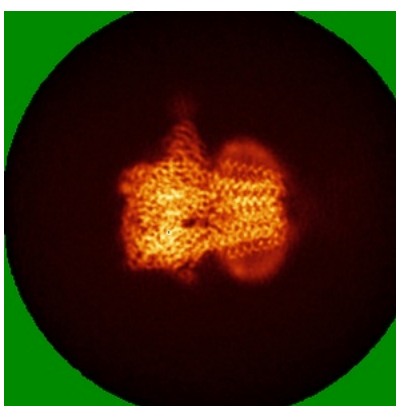
The images above show the largest variance slices of the map in three orthogonal directions.

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

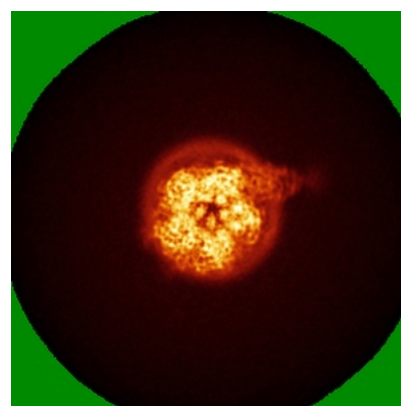
6.4.1 Primary map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

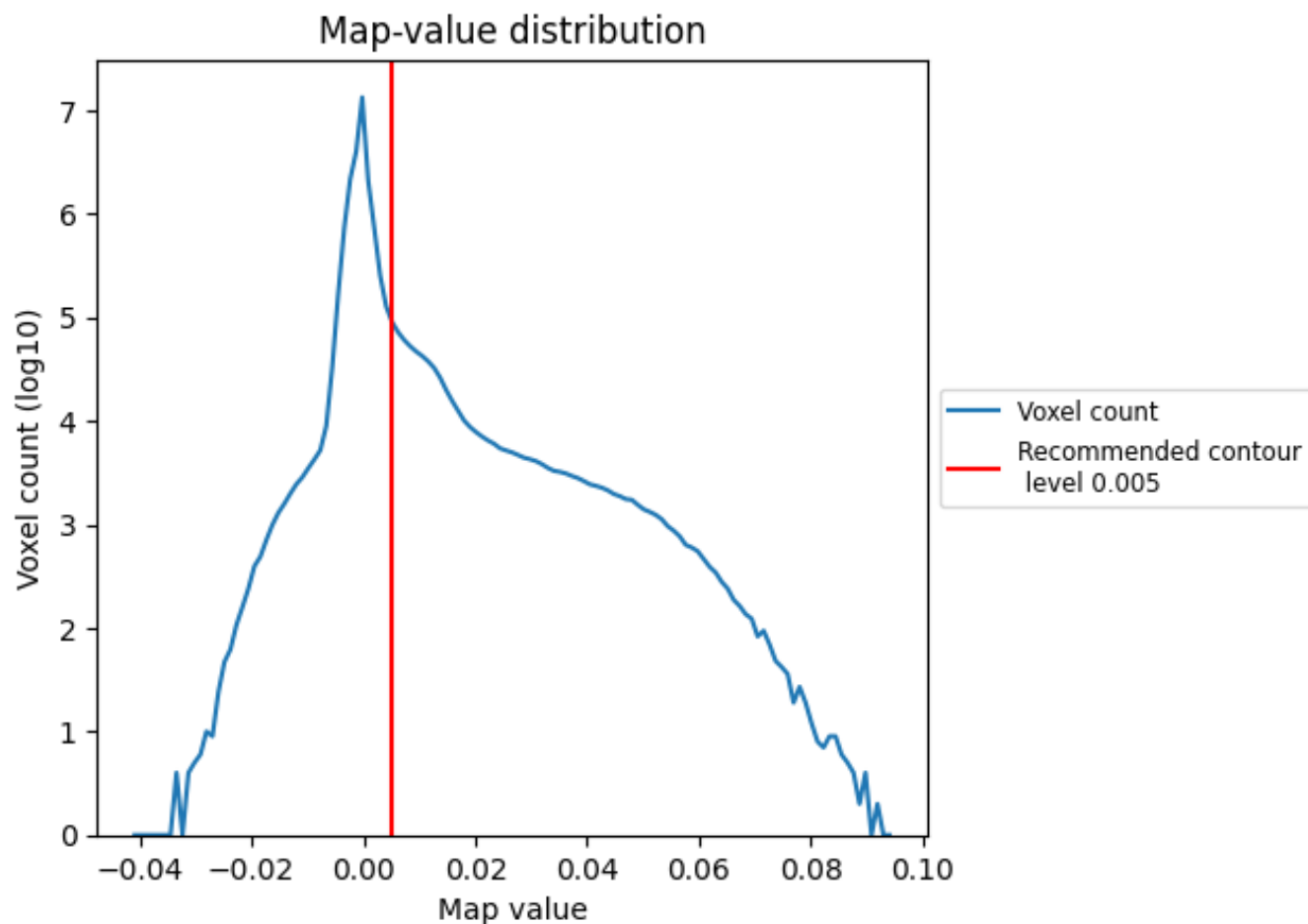
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

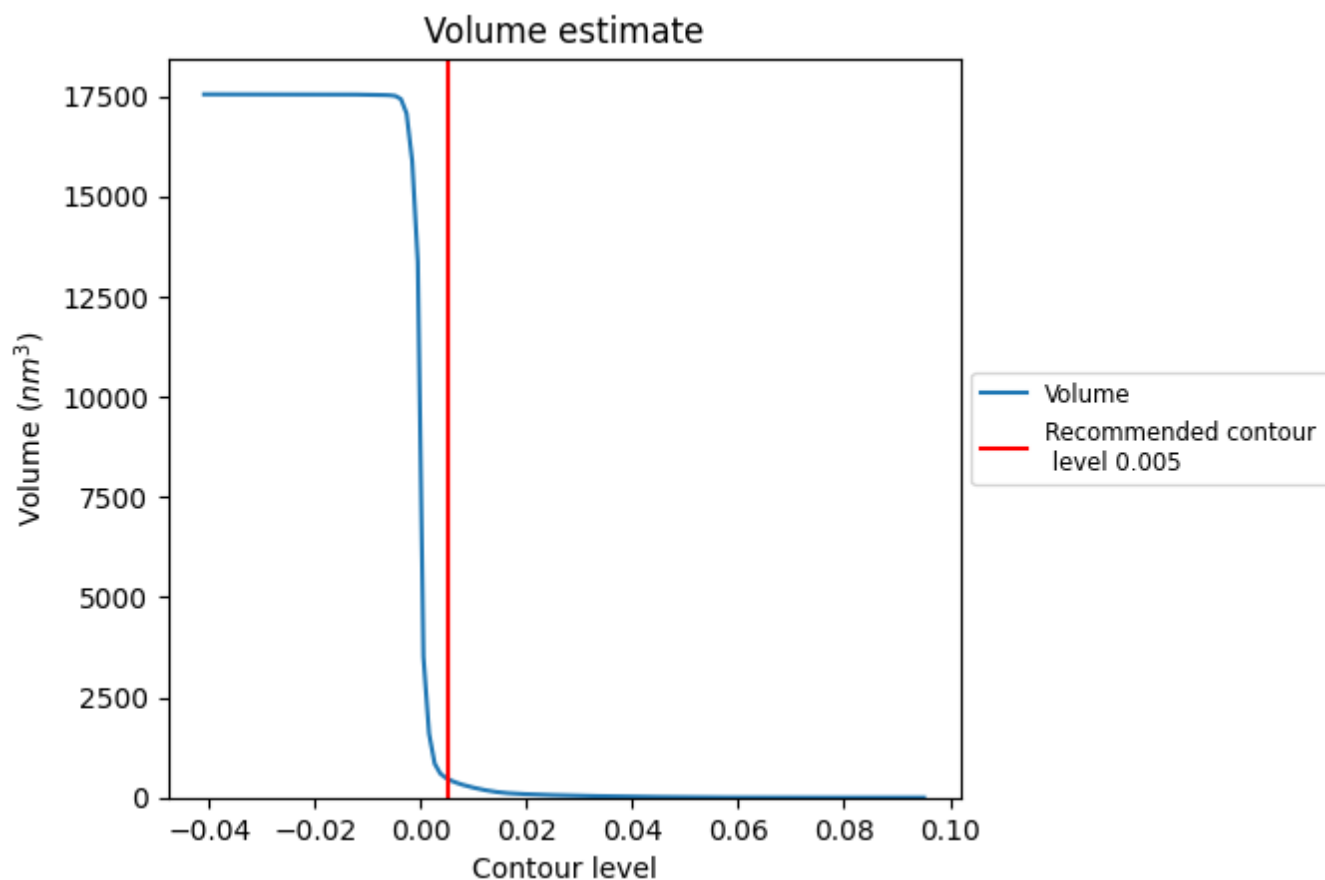
This section contains the results of statistical analysis of the map.

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.

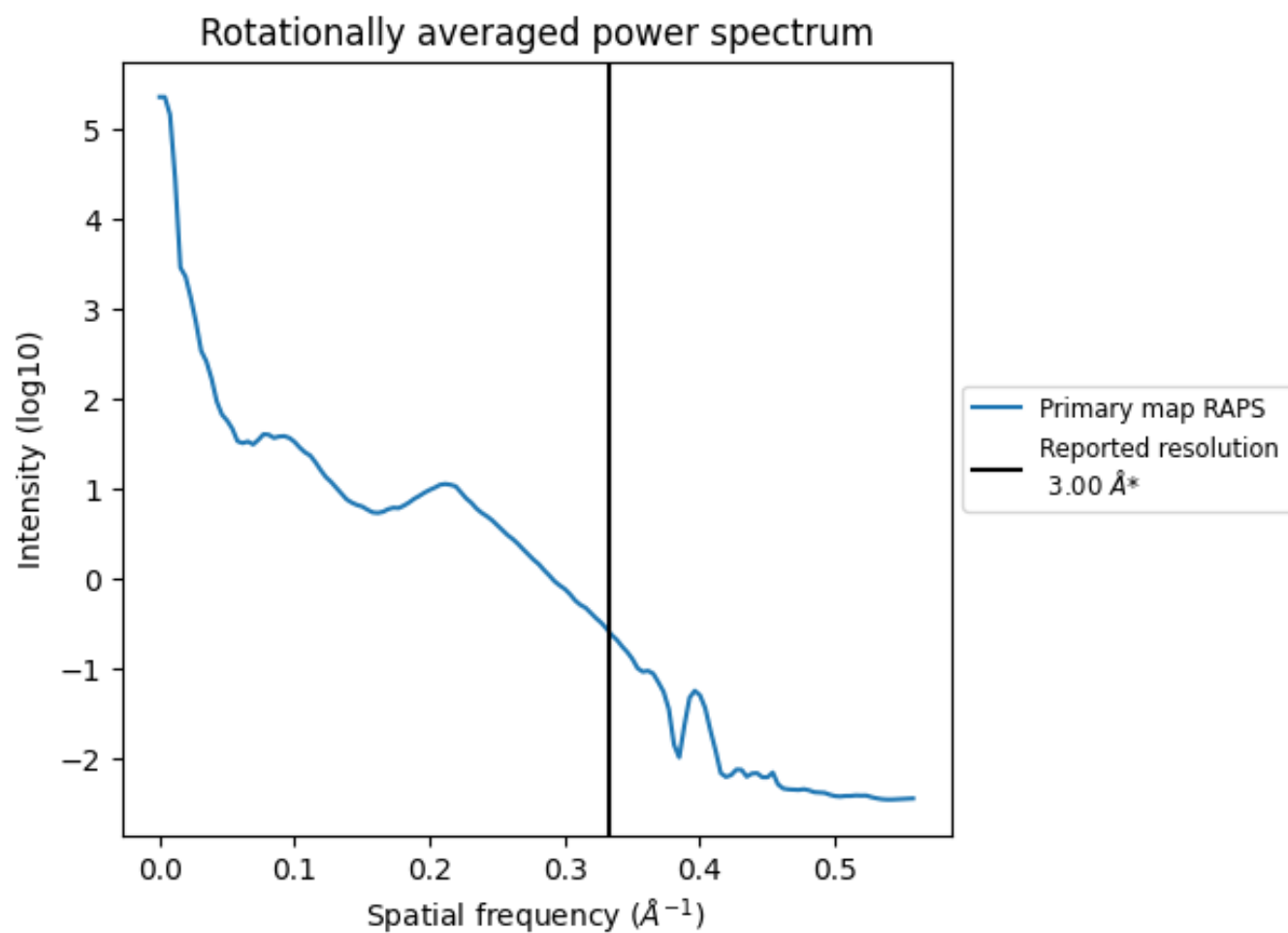
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 474 nm³; this corresponds to an approximate mass of 429 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 0.333 Å⁻¹

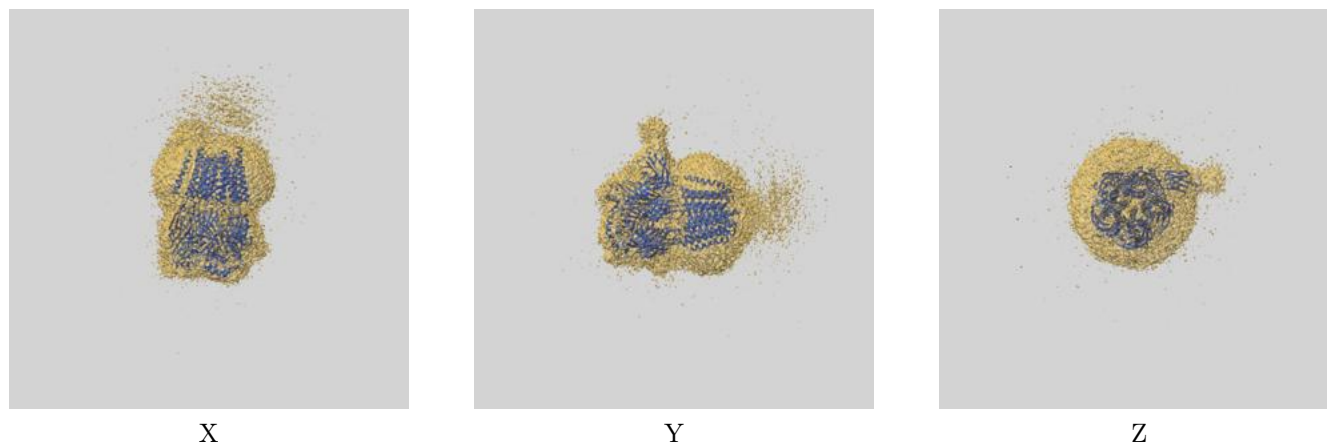
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

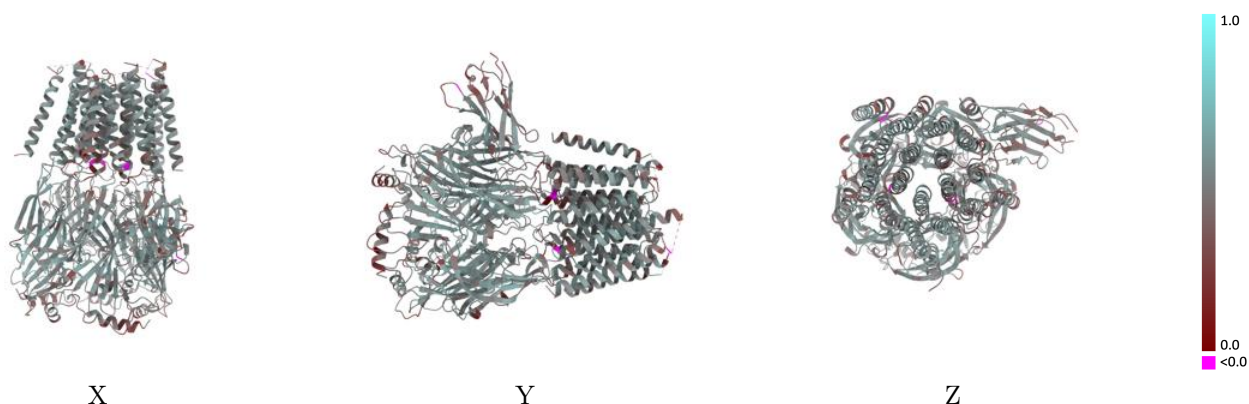
This section contains information regarding the fit between EMDB map EMD-14072 and PDB model 7QNA. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



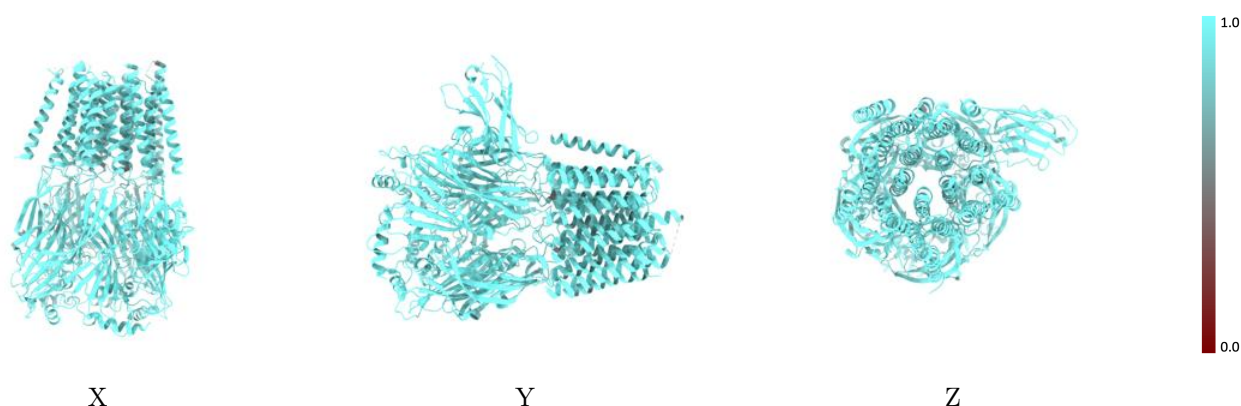
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



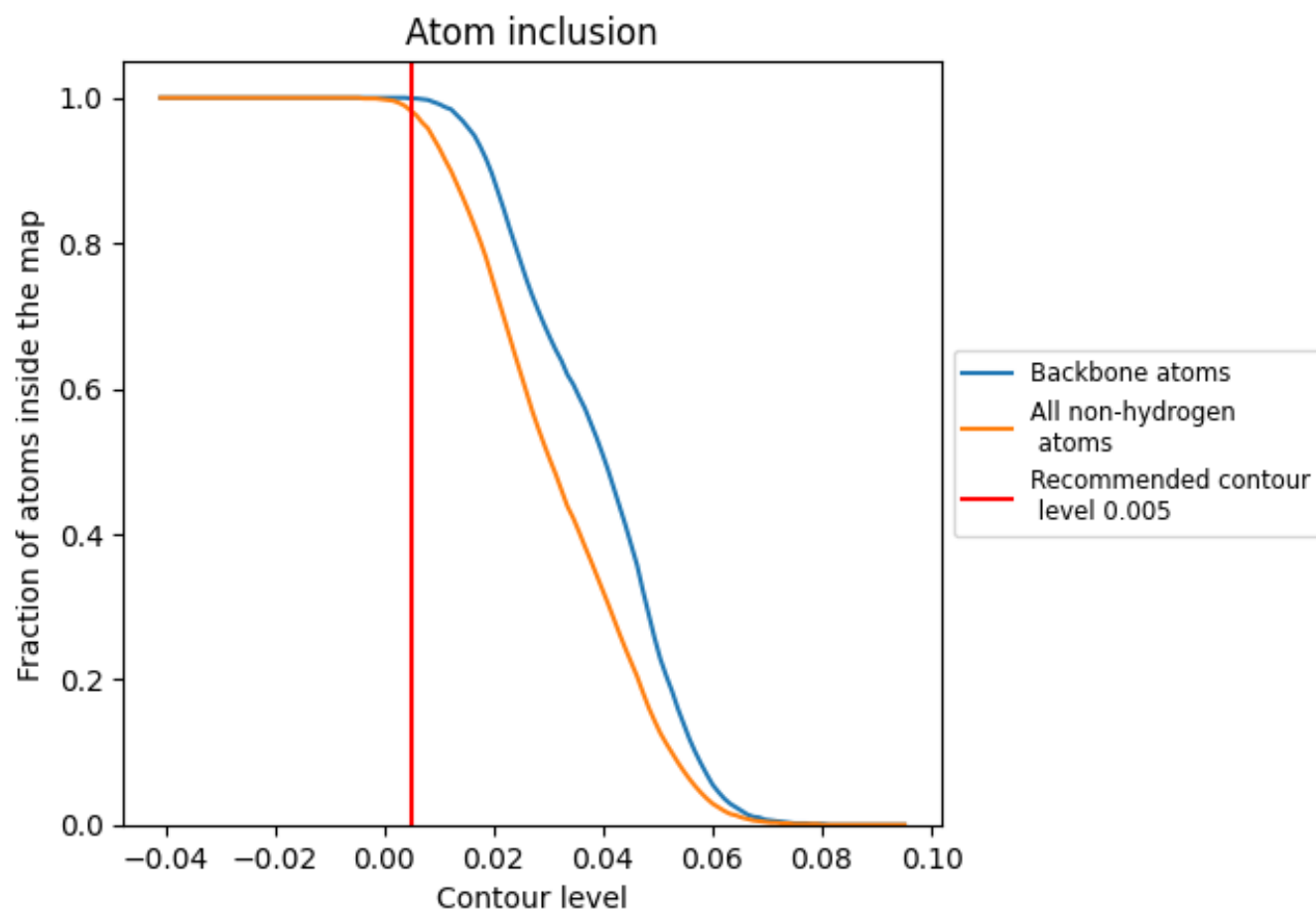
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 98% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9810	 0.4830
A	 0.9730	 0.4950
B	 0.9830	 0.4840
C	 0.9890	 0.5190
D	 0.9790	 0.4630
E	 0.9820	 0.4840
F	 1.0000	 0.4490
G	 0.9840	 0.3120
H	 1.0000	 0.4360
N	 0.9910	 0.4510
a	 0.8850	 0.2350
b	 0.9640	 0.4070
d	 0.8930	 0.2220
e	 0.9640	 0.3310

