



Full wwPDB EM Validation Report ⓘ

Nov 2, 2022 – 10:45 PM EDT

PDB ID : 5UJZ
EMDB ID : EMD-8561
Title : CryoEM structure of an influenza virus receptor-binding site antibody-antigen interface - Class 1
Authors : Liu, Y.; Pan, J.; Caradonna, T.; Jenni, S.; Raymond, D.D.; Schmidt, A.G.; Harrison, S.C.; Grigorieff, N.
Deposited on : 2017-01-19
Resolution : 4.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

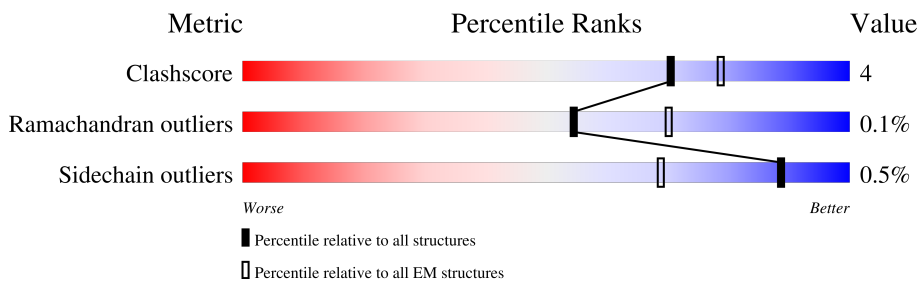
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	323	
1	C	323	
1	E	323	
2	B	173	
2	D	173	
2	F	173	
3	G	266	
3	H	266	

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Mol	Chain	Length	Quality of chain
3	I	266	
4	J	3	
4	L	3	
4	N	3	
5	K	2	
5	M	2	
5	O	2	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 34389 atoms, of which 16842 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 Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	323	4973	1597	2438	441	486	11	0	0
1	C	323	4973	1597	2438	441	486	11	0	0
1	E	323	4973	1597	2438	441	486	11	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLU	-	expression tag	UNP A7UPX0
C	4	GLU	-	expression tag	UNP A7UPX0
E	4	GLU	-	expression tag	UNP A7UPX0

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	B	173	2716	874	1322	238	275	7	0	0
2	D	173	2716	874	1322	238	275	7	0	0
2	F	173	2716	874	1322	238	275	7	0	0

- Molecule 3 is a protein called scFv.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	G	236	3476	1111	1707	306	345	7	0	0
3	H	236	3476	1111	1707	306	345	7	0	0
3	I	236	3476	1111	1707	306	345	7	0	0

- Molecule 4 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
			Total	C	H	N	O		
4	J	3	75	22	36	2	15	0	0
4	L	3	75	22	36	2	15	0	0
4	N	3	75	22	36	2	15	0	0

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



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
5	K	2	55	16	27	2	10	0	0
5	M	2	55	16	27	2	10	0	0
5	O	2	55	16	27	2	10	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
6	A	1	Total	C	H	N	O	0
			140	40	70	5	25	
6	A	1	Total	C	H	N	O	0
			140	40	70	5	25	
6	A	1	Total	C	H	N	O	0
			140	40	70	5	25	
6	A	1	Total	C	H	N	O	0
			140	40	70	5	25	
6	A	1	Total	C	H	N	O	0
			140	40	70	5	25	
6	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	C	1	Total	C	H	N	O	0
			140	40	70	5	25	
6	C	1	Total	C	H	N	O	0
			140	40	70	5	25	
6	C	1	Total	C	H	N	O	0
			140	40	70	5	25	
6	C	1	Total	C	H	N	O	0
			140	40	70	5	25	
6	D	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	E	1	Total	C	H	N	O	0
			140	40	70	5	25	
6	E	1	Total	C	H	N	O	0
			140	40	70	5	25	

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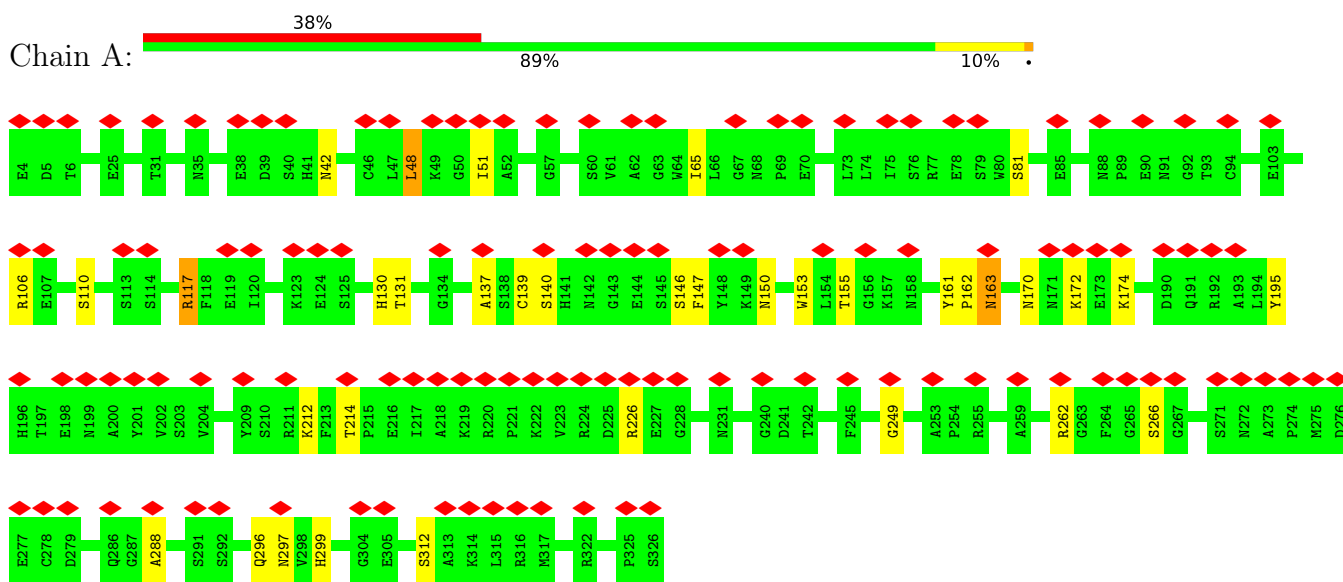
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
6	E	1	Total 140	40	70	5	25	0
6	E	1	Total 140	40	70	5	25	0
6	E	1	Total 140	40	70	5	25	0
6	F	1	Total 28	8	14	1	5	0

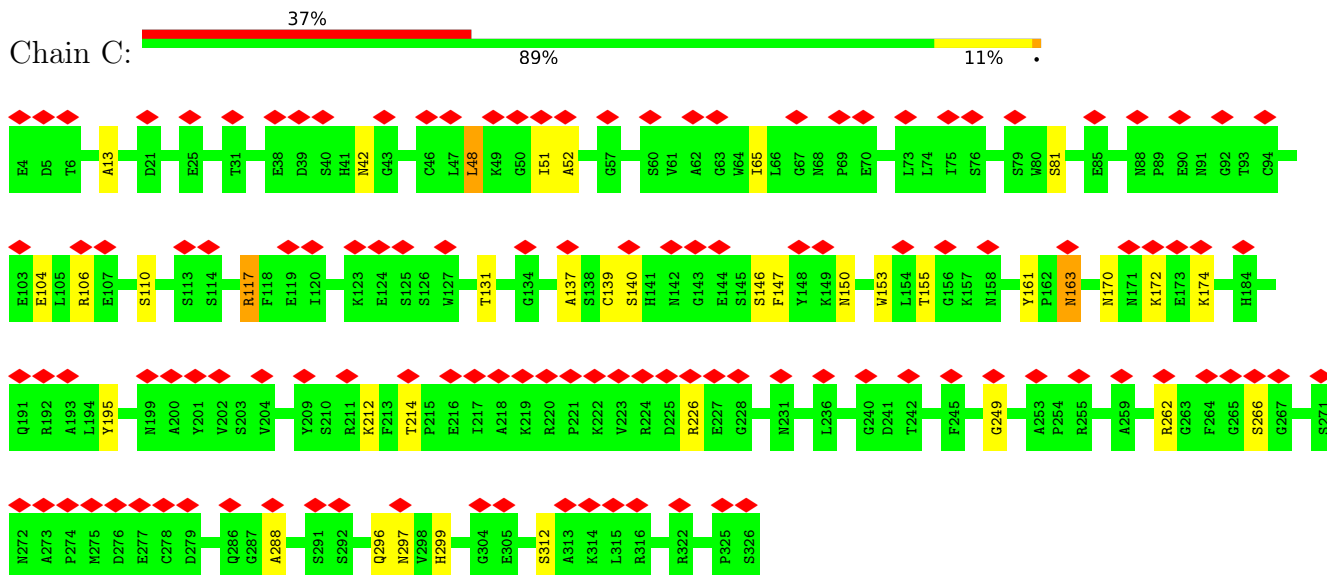
3 Residue-property plots

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.

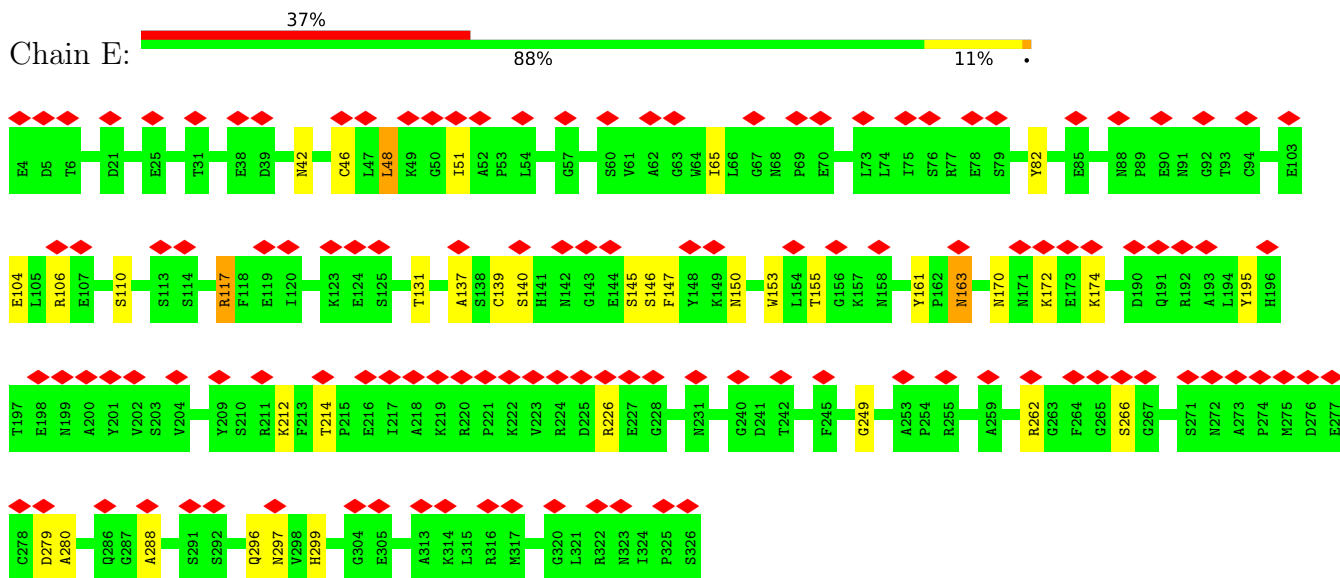
- Molecule 1: Hemagglutinin HA1



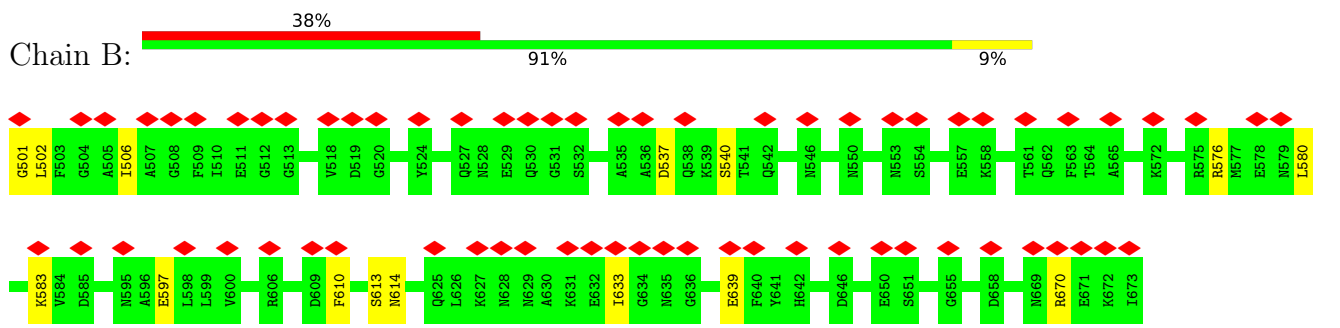
- Molecule 1: Hemagglutinin HA1



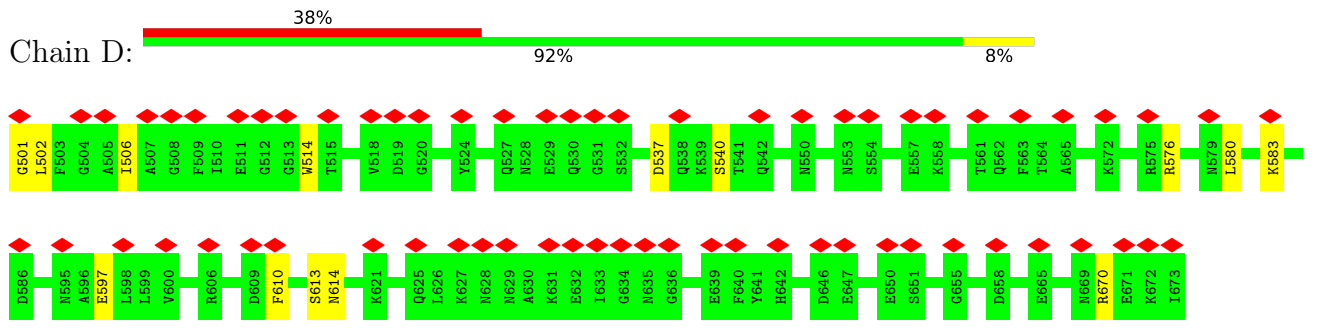
- Molecule 1: Hemagglutinin HA1



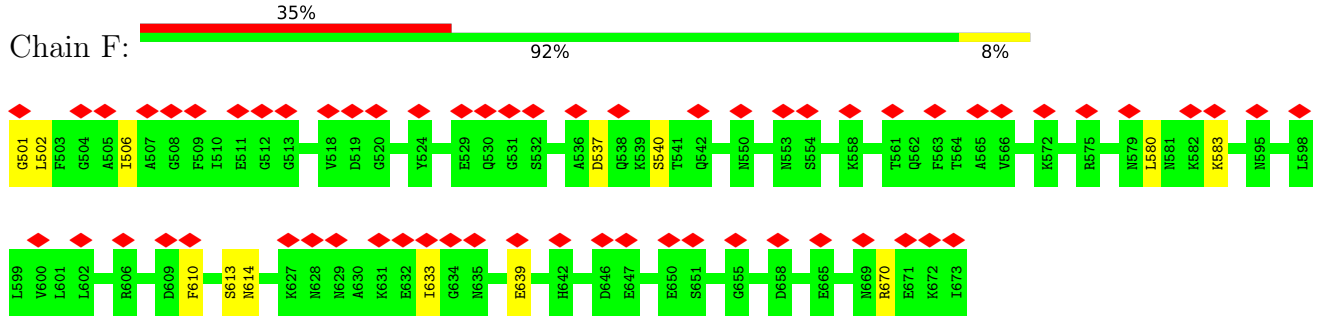
• Molecule 2: Hemagglutinin HA2



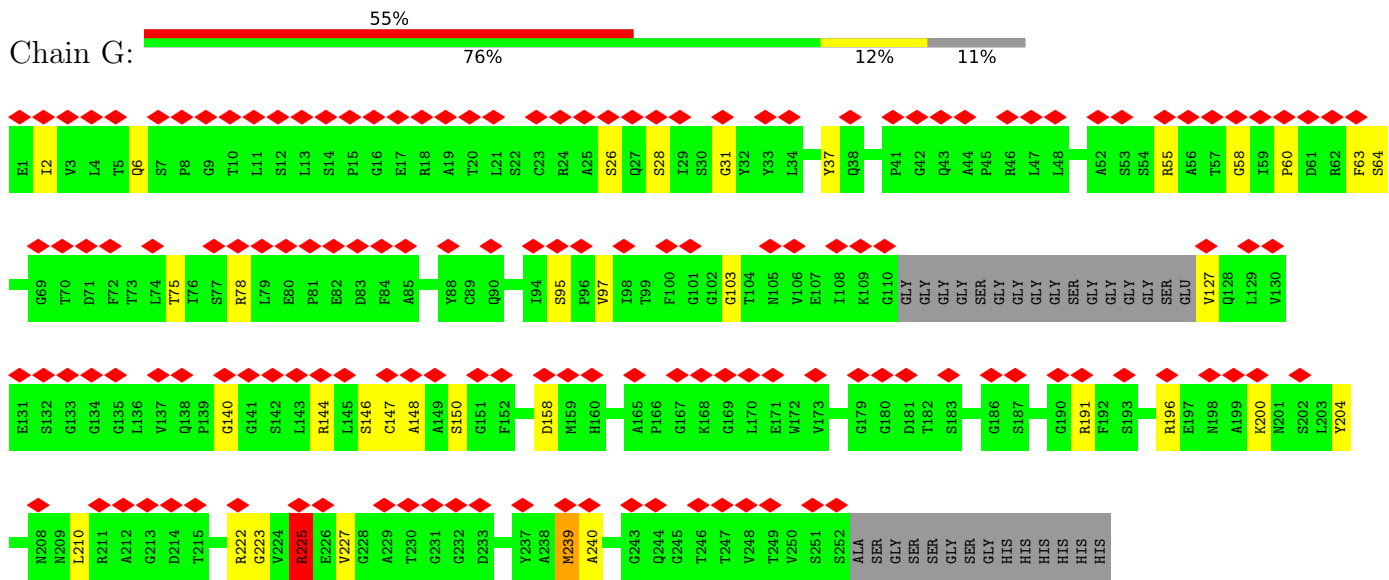
• Molecule 2: Hemagglutinin HA2



• Molecule 2: Hemagglutinin HA2



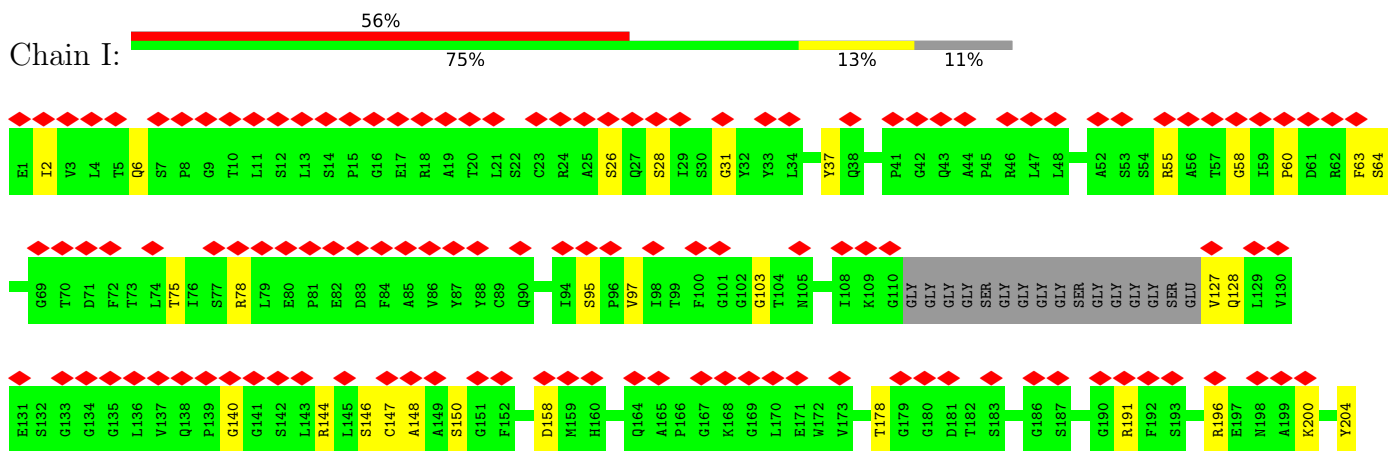
• Molecule 3: scFv

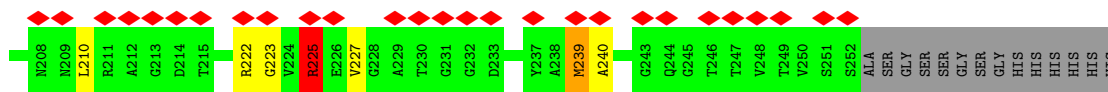


• Molecule 3: scFv



• Molecule 3: scFv





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



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



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



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



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	142314	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)	1000	Depositor
Maximum defocus (nm)	9000	Depositor
Magnification	30444	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	7.246	Depositor
Minimum map value	-3.359	Depositor
Average map value	0.071	Depositor
Map value standard deviation	0.427	Depositor
Recommended contour level	2.3	Depositor
Map size (Å)	196.8, 196.8, 196.8	wwPDB
Map dimensions	120, 120, 120	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.64, 1.64, 1.64	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: 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	A	0.46	0/2601	0.79	5/3540 (0.1%)
1	C	0.46	0/2601	0.79	5/3540 (0.1%)
1	E	0.46	0/2601	0.79	5/3540 (0.1%)
2	B	0.45	0/1421	0.71	1/1909 (0.1%)
2	D	0.45	0/1421	0.71	1/1909 (0.1%)
2	F	0.45	0/1421	0.71	1/1909 (0.1%)
3	G	0.51	0/1808	0.94	6/2452 (0.2%)
3	H	0.50	0/1808	0.94	6/2452 (0.2%)
3	I	0.50	0/1808	0.94	6/2452 (0.2%)
All	All	0.47	0/17490	0.82	36/23703 (0.2%)

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	A	0	2
1	C	0	2
1	E	0	2
3	G	0	3
3	H	0	3
3	I	0	3
All	All	0	15

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	191	ARG	NE-CZ-NH1	6.62	123.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	191	ARG	NE-CZ-NH1	6.60	123.60	120.30
3	I	191	ARG	NE-CZ-NH1	6.47	123.53	120.30
2	D	670	ARG	NE-CZ-NH1	5.86	123.23	120.30
2	B	670	ARG	NE-CZ-NH1	5.83	123.22	120.30
3	H	78	ARG	NE-CZ-NH1	5.80	123.20	120.30
2	F	670	ARG	NE-CZ-NH1	5.79	123.19	120.30
3	G	78	ARG	NE-CZ-NH1	5.79	123.19	120.30
3	I	78	ARG	NE-CZ-NH1	5.75	123.18	120.30
3	I	196	ARG	NE-CZ-NH1	5.68	123.14	120.30
3	H	31	GLY	N-CA-C	5.59	127.08	113.10
3	G	196	ARG	NE-CZ-NH1	5.58	123.09	120.30
3	I	31	GLY	N-CA-C	5.58	127.04	113.10
1	E	262	ARG	NE-CZ-NH1	5.57	123.08	120.30
3	H	196	ARG	NE-CZ-NH1	5.56	123.08	120.30
3	G	31	GLY	N-CA-C	5.55	126.97	113.10
3	H	158	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	262	ARG	NE-CZ-NH1	5.51	123.06	120.30
3	I	158	ASP	CB-CG-OD1	5.49	123.24	118.30
3	G	158	ASP	CB-CG-OD1	5.47	123.22	118.30
1	C	262	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	117	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	E	106	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	C	106	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	E	117	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	E	117	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	117	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	106	ARG	NE-CZ-NH1	5.22	122.91	120.30
3	H	225	ARG	NE-CZ-NH1	5.20	122.90	120.30
3	G	225	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	C	117	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	C	226	ARG	NE-CZ-NH1	5.18	122.89	120.30
3	I	225	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	C	117	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	226	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	E	226	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	297	ASN	Peptide
1	A	48	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	C	297	ASN	Peptide
1	C	48	LEU	Peptide
1	E	297	ASN	Peptide
1	E	48	LEU	Peptide
3	G	223	GLY	Peptide
3	G	28	SER	Peptide
3	G	58	GLY	Peptide
3	H	223	GLY	Peptide
3	H	28	SER	Peptide
3	H	58	GLY	Peptide
3	I	223	GLY	Peptide
3	I	28	SER	Peptide
3	I	58	GLY	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	A	2535	2438	2438	22	0
1	C	2535	2438	2438	24	0
1	E	2535	2438	2438	23	0
2	B	1394	1322	1322	9	0
2	D	1394	1322	1322	9	0
2	F	1394	1322	1322	7	0
3	G	1769	1707	1711	13	0
3	H	1769	1707	1711	12	0
3	I	1769	1707	1711	15	0
4	J	39	36	34	0	0
4	L	39	36	34	0	0
4	N	39	36	34	0	0
5	K	28	27	25	0	0
5	M	28	27	25	0	0
5	O	28	27	25	0	0
6	A	70	70	65	0	0
6	B	14	14	13	0	0
6	C	70	70	65	0	0
6	D	14	14	13	0	0
6	E	70	70	65	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	14	14	13	0	0
All	All	17547	16842	16824	122	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (122) 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:B:576:ARG:NE	1:C:104:GLU:OE2	2.22	0.73
2:D:502:LEU:O	2:F:613:SER:OG	2.07	0.71
3:G:55:ARG:NH1	3:G:63:PHE:O	2.24	0.71
3:H:55:ARG:NH1	3:H:63:PHE:O	2.24	0.71
1:C:296:GLN:NE2	1:C:299:HIS:O	2.24	0.70
1:E:296:GLN:NE2	1:E:299:HIS:O	2.24	0.70
3:I:55:ARG:NH1	3:I:63:PHE:O	2.24	0.70
1:A:296:GLN:NE2	1:A:299:HIS:O	2.24	0.70
3:I:64:SER:O	3:I:75:THR:OG1	2.10	0.69
3:H:144:ARG:NH1	3:H:146:SER:OG	2.26	0.69
3:I:144:ARG:NH1	3:I:146:SER:OG	2.26	0.68
1:C:137:ALA:O	1:C:140:SER:OG	2.12	0.68
1:A:137:ALA:O	1:A:140:SER:OG	2.12	0.67
3:G:144:ARG:NH1	3:G:146:SER:OG	2.26	0.67
1:C:110:SER:OG	1:C:266:SER:O	2.13	0.67
1:E:137:ALA:O	1:E:140:SER:OG	2.12	0.67
1:A:110:SER:OG	1:A:266:SER:O	2.13	0.66
1:E:110:SER:OG	1:E:266:SER:O	2.13	0.66
1:A:42:ASN:HD21	1:A:288:ALA:HB3	1.61	0.65
1:E:42:ASN:HD21	1:E:288:ALA:HB3	1.61	0.65
2:B:501:GLY:N	2:B:506:ILE:O	2.31	0.64
1:C:42:ASN:HD21	1:C:288:ALA:HB3	1.61	0.64
2:F:501:GLY:N	2:F:506:ILE:O	2.31	0.64
2:D:501:GLY:N	2:D:506:ILE:O	2.31	0.64
2:D:576:ARG:NE	1:E:104:GLU:OE2	2.27	0.63
3:H:127:VAL:N	3:H:150:SER:O	2.32	0.63
1:C:131:THR:N	1:C:155:THR:O	2.32	0.63
3:G:127:VAL:N	3:G:150:SER:O	2.32	0.63
1:A:131:THR:N	1:A:155:THR:O	2.32	0.62
1:C:312:SER:OG	2:D:597:GLU:OE2	2.15	0.62
3:I:127:VAL:N	3:I:150:SER:O	2.32	0.62
3:G:64:SER:O	3:G:75:THR:OG1	2.10	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:THR:N	1:E:155:THR:O	2.32	0.61
3:I:225:ARG:NE	3:I:227:VAL:O	2.34	0.61
2:B:613:SER:OG	2:F:502:LEU:O	2.19	0.61
3:H:225:ARG:NE	3:H:227:VAL:O	2.34	0.61
3:G:225:ARG:NE	3:G:227:VAL:O	2.34	0.60
3:I:200:LYS:NZ	3:I:204:TYR:OH	2.28	0.58
2:F:537:ASP:OD2	2:F:540:SER:OG	2.16	0.58
1:E:65:ILE:O	1:E:150:ASN:ND2	2.37	0.58
1:A:81:SER:O	1:A:266:SER:OG	2.16	0.57
1:C:13:ALA:N	2:D:514:TRP:O	2.36	0.57
1:A:65:ILE:O	1:A:150:ASN:ND2	2.37	0.57
1:C:65:ILE:O	1:C:150:ASN:ND2	2.37	0.57
1:E:170:ASN:OD1	1:E:172:LYS:N	2.38	0.57
1:A:312:SER:OG	2:B:597:GLU:OE2	2.18	0.56
1:A:170:ASN:OD1	1:A:172:LYS:N	2.38	0.56
1:C:170:ASN:OD1	1:C:172:LYS:N	2.38	0.56
3:H:64:SER:O	3:H:75:THR:OG1	2.10	0.56
2:B:502:LEU:O	2:D:613:SER:OG	2.24	0.55
1:C:81:SER:O	1:C:266:SER:OG	2.16	0.55
3:G:200:LYS:NZ	3:G:204:TYR:OH	2.28	0.55
2:D:610:PHE:O	2:D:614:ASN:ND2	2.40	0.55
1:A:163:ASN:N	1:A:163:ASN:OD1	2.40	0.55
2:B:610:PHE:O	2:B:614:ASN:ND2	2.40	0.55
3:H:200:LYS:NZ	3:H:204:TYR:OH	2.28	0.55
1:A:139:CYS:O	1:A:146:SER:N	2.40	0.55
2:F:610:PHE:O	2:F:614:ASN:ND2	2.40	0.55
1:C:214:THR:O	1:E:212:LYS:NZ	2.38	0.54
1:C:139:CYS:O	1:C:146:SER:N	2.40	0.54
1:E:139:CYS:O	1:E:146:SER:N	2.40	0.54
1:A:48:LEU:O	1:A:51:ILE:N	2.41	0.54
1:E:163:ASN:N	1:E:163:ASN:OD1	2.40	0.54
3:H:37:TYR:OH	3:H:239:MET:SD	2.55	0.54
1:C:48:LEU:O	1:C:51:ILE:N	2.41	0.53
1:C:163:ASN:OD1	1:C:163:ASN:N	2.40	0.53
1:E:48:LEU:O	1:E:51:ILE:N	2.41	0.52
1:A:214:THR:O	1:C:212:LYS:NZ	2.43	0.51
3:H:95:SER:O	3:H:97:VAL:N	2.44	0.51
3:I:95:SER:O	3:I:97:VAL:N	2.44	0.51
3:G:95:SER:O	3:G:97:VAL:N	2.44	0.51
2:B:537:ASP:OD2	2:B:540:SER:OG	2.16	0.50
3:I:147:CYS:SG	3:I:148:ALA:N	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:ASN:ND2	1:E:288:ALA:HB3	2.27	0.49
3:G:147:CYS:SG	3:G:148:ALA:N	2.85	0.49
2:D:580:LEU:O	2:D:583:LYS:N	2.46	0.48
3:I:37:TYR:OH	3:I:239:MET:SD	2.55	0.48
3:H:147:CYS:SG	3:H:148:ALA:N	2.86	0.48
2:B:580:LEU:O	2:B:583:LYS:N	2.46	0.48
2:F:580:LEU:O	2:F:583:LYS:N	2.46	0.48
1:A:42:ASN:ND2	1:A:288:ALA:HB3	2.27	0.48
1:C:42:ASN:OD1	1:C:288:ALA:N	2.46	0.48
1:E:146:SER:OG	1:E:147:PHE:N	2.47	0.48
1:C:146:SER:OG	1:C:147:PHE:N	2.47	0.48
3:G:222:ARG:HG3	3:G:240:ALA:HB3	1.96	0.48
1:A:146:SER:OG	1:A:147:PHE:N	2.47	0.47
1:C:42:ASN:ND2	1:C:288:ALA:HB3	2.27	0.47
1:A:212:LYS:NZ	1:E:214:THR:O	2.47	0.47
1:E:170:ASN:ND2	1:E:174:LYS:O	2.48	0.47
1:E:42:ASN:OD1	1:E:288:ALA:N	2.46	0.47
1:A:170:ASN:ND2	1:A:174:LYS:O	2.48	0.47
3:I:222:ARG:HG3	3:I:240:ALA:HB3	1.96	0.47
1:C:170:ASN:ND2	1:C:174:LYS:O	2.48	0.46
3:H:222:ARG:HG3	3:H:240:ALA:HB3	1.96	0.46
1:A:42:ASN:OD1	1:A:288:ALA:N	2.46	0.46
3:I:128:GLN:O	3:I:150:SER:OG	2.35	0.44
1:E:117:ARG:NE	1:E:150:ASN:OD1	2.47	0.43
2:D:537:ASP:OD2	2:D:540:SER:OG	2.16	0.43
3:H:2:ILE:HG23	3:H:26:SER:HB3	2.01	0.43
3:H:6:GLN:OE1	3:H:103:GLY:N	2.52	0.43
1:E:46:CYS:O	1:E:82:TYR:OH	2.30	0.42
3:G:6:GLN:OE1	3:G:103:GLY:N	2.52	0.42
3:G:140:GLY:N	3:G:210:LEU:O	2.48	0.42
1:A:117:ARG:NE	1:A:150:ASN:OD1	2.47	0.42
3:G:2:ILE:HG23	3:G:26:SER:HB3	2.01	0.42
3:I:6:GLN:OE1	3:I:103:GLY:N	2.52	0.42
1:A:161:TYR:OH	1:A:249:GLY:N	2.53	0.42
3:I:2:ILE:HG23	3:I:26:SER:HB3	2.01	0.41
1:C:117:ARG:NE	1:C:150:ASN:OD1	2.47	0.41
1:C:161:TYR:OH	1:C:249:GLY:N	2.53	0.41
1:E:145:SER:N	3:I:178:THR:O	2.51	0.41
1:E:161:TYR:OH	1:E:249:GLY:N	2.53	0.41
1:A:153:TRP:CZ2	1:A:195:TYR:OH	2.74	0.41
1:A:130:HIS:NE2	1:A:162:PRO:O	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:37:TYR:OH	3:G:239:MET:SD	2.55	0.41
1:E:153:TRP:CZ2	1:E:195:TYR:OH	2.74	0.41
1:E:279:ASP:OD1	1:E:280:ALA:N	2.54	0.41
1:C:153:TRP:CZ2	1:C:195:TYR:OH	2.74	0.41
3:I:140:GLY:N	3:I:210:LEU:O	2.48	0.41
1:C:52:ALA:O	1:C:81:SER:N	2.52	0.40
2:B:633:ILE:HG21	2:B:639:GLU:HB2	2.04	0.40
2:F:633:ILE:HG21	2:F:639:GLU:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	321/323 (99%)	303 (94%)	18 (6%)	0	100	100
1	C	321/323 (99%)	303 (94%)	18 (6%)	0	100	100
1	E	321/323 (99%)	303 (94%)	18 (6%)	0	100	100
2	B	171/173 (99%)	157 (92%)	14 (8%)	0	100	100
2	D	171/173 (99%)	157 (92%)	14 (8%)	0	100	100
2	F	171/173 (99%)	157 (92%)	14 (8%)	0	100	100
3	G	232/266 (87%)	208 (90%)	23 (10%)	1 (0%)	34	72
3	H	232/266 (87%)	208 (90%)	23 (10%)	1 (0%)	34	72
3	I	232/266 (87%)	208 (90%)	23 (10%)	1 (0%)	34	72
All	All	2172/2286 (95%)	2004 (92%)	165 (8%)	3 (0%)	54	85

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	60	PRO
3	H	60	PRO
3	I	60	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	283/283 (100%)	282 (100%)	1 (0%)	91	94
1	C	283/283 (100%)	282 (100%)	1 (0%)	91	94
1	E	283/283 (100%)	282 (100%)	1 (0%)	91	94
2	B	149/149 (100%)	149 (100%)	0	100	100
2	D	149/149 (100%)	149 (100%)	0	100	100
2	F	149/149 (100%)	149 (100%)	0	100	100
3	G	186/200 (93%)	184 (99%)	2 (1%)	73	85
3	H	186/200 (93%)	184 (99%)	2 (1%)	73	85
3	I	186/200 (93%)	184 (99%)	2 (1%)	73	85
All	All	1854/1896 (98%)	1845 (100%)	9 (0%)	89	93

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	ASN
1	C	163	ASN
1	E	163	ASN
3	G	225	ARG
3	G	239	MET
3	H	225	ARG
3	H	239	MET
3	I	225	ARG
3	I	239	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	550	ASN
2	B	614	ASN
2	D	614	ASN
2	F	614	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](#)

15 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	J	1	4,1	14,14,15	0.36	0	17,19,21	0.66	0
4	NAG	J	2	4	14,14,15	0.27	0	17,19,21	0.57	0
4	BMA	J	3	4	11,11,12	0.86	1 (9%)	15,15,17	0.86	0
5	NAG	K	1	5,1	14,14,15	0.45	0	17,19,21	0.62	0
5	NAG	K	2	5	14,14,15	0.20	0	17,19,21	0.56	0
4	NAG	L	1	4,1	14,14,15	0.41	0	17,19,21	0.64	0
4	NAG	L	2	4	14,14,15	0.28	0	17,19,21	0.55	0
4	BMA	L	3	4	11,11,12	0.91	1 (9%)	15,15,17	0.89	0
5	NAG	M	1	5,1	14,14,15	0.43	0	17,19,21	0.61	0
5	NAG	M	2	5	14,14,15	0.22	0	17,19,21	0.56	0
4	NAG	N	1	4,1	14,14,15	0.38	0	17,19,21	0.64	0
4	NAG	N	2	4	14,14,15	0.28	0	17,19,21	0.58	0
4	BMA	N	3	4	11,11,12	0.85	1 (9%)	15,15,17	0.88	0
5	NAG	O	1	5,1	14,14,15	0.41	0	17,19,21	0.62	0
5	NAG	O	2	5	14,14,15	0.20	0	17,19,21	0.57	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	J	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	1/6/23/26	0/1/1/1
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1
5	NAG	K	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
4	NAG	L	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	1/6/23/26	0/1/1/1
4	BMA	L	3	4	-	0/2/19/22	0/1/1/1
5	NAG	M	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
4	NAG	N	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	1/6/23/26	0/1/1/1
4	BMA	N	3	4	-	0/2/19/22	0/1/1/1
5	NAG	O	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	3	BMA	O5-C1	-2.44	1.39	1.43
4	J	3	BMA	O5-C1	-2.29	1.40	1.43
4	N	3	BMA	O5-C1	-2.22	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

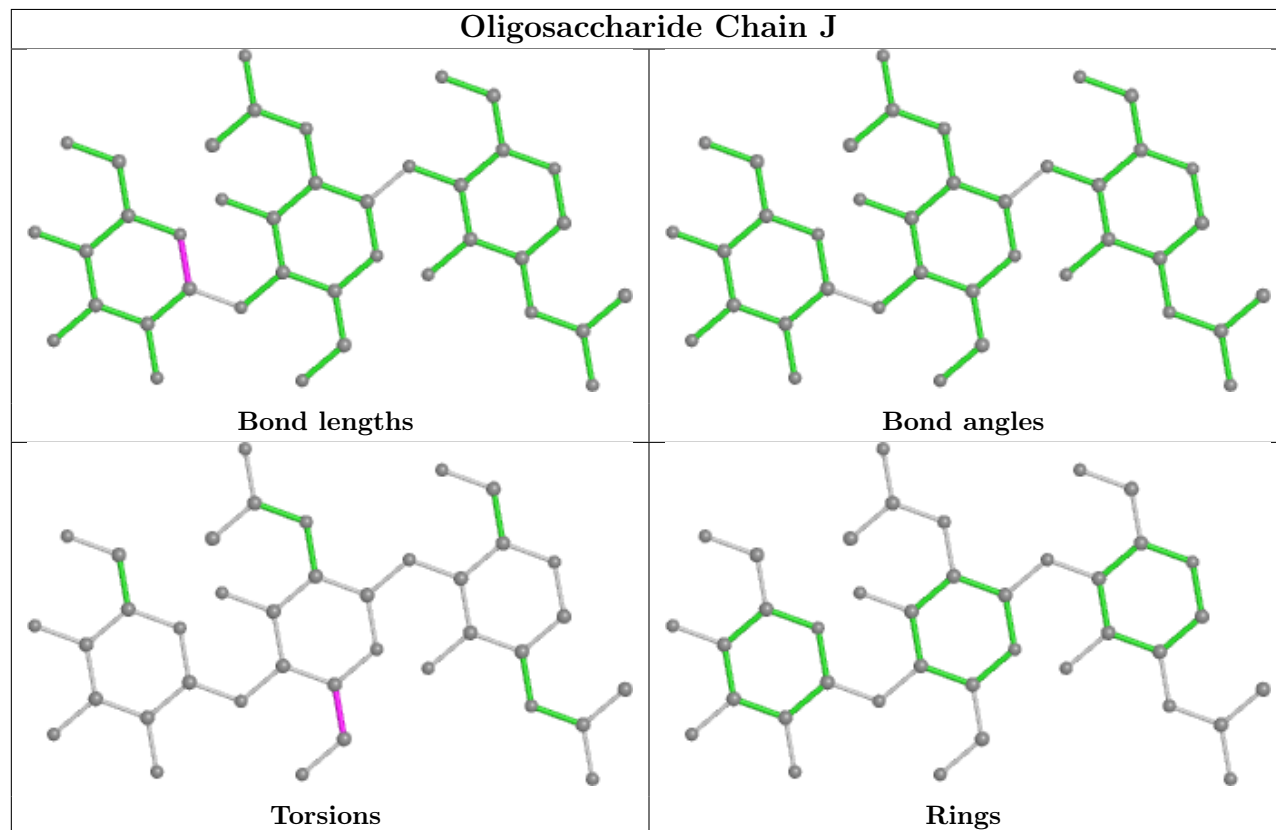
All (9) torsion outliers are listed below:

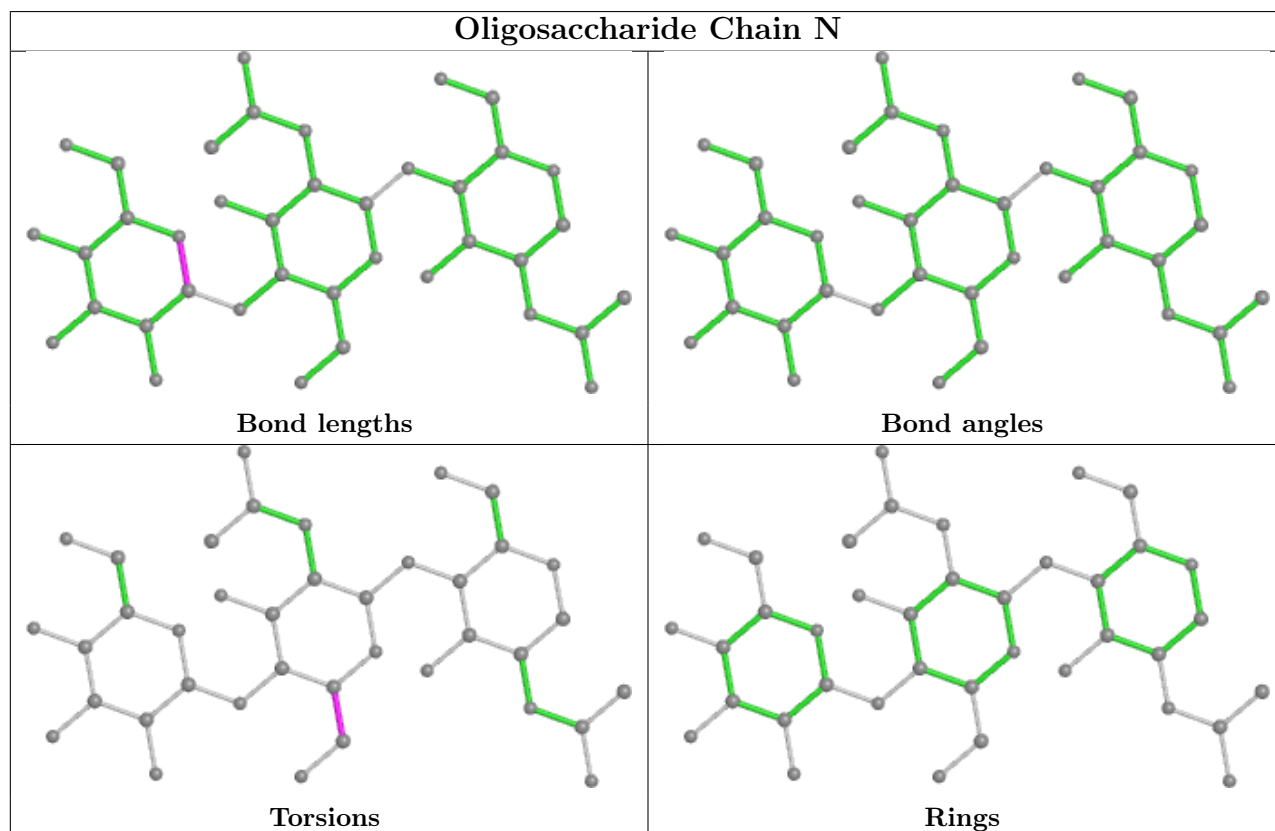
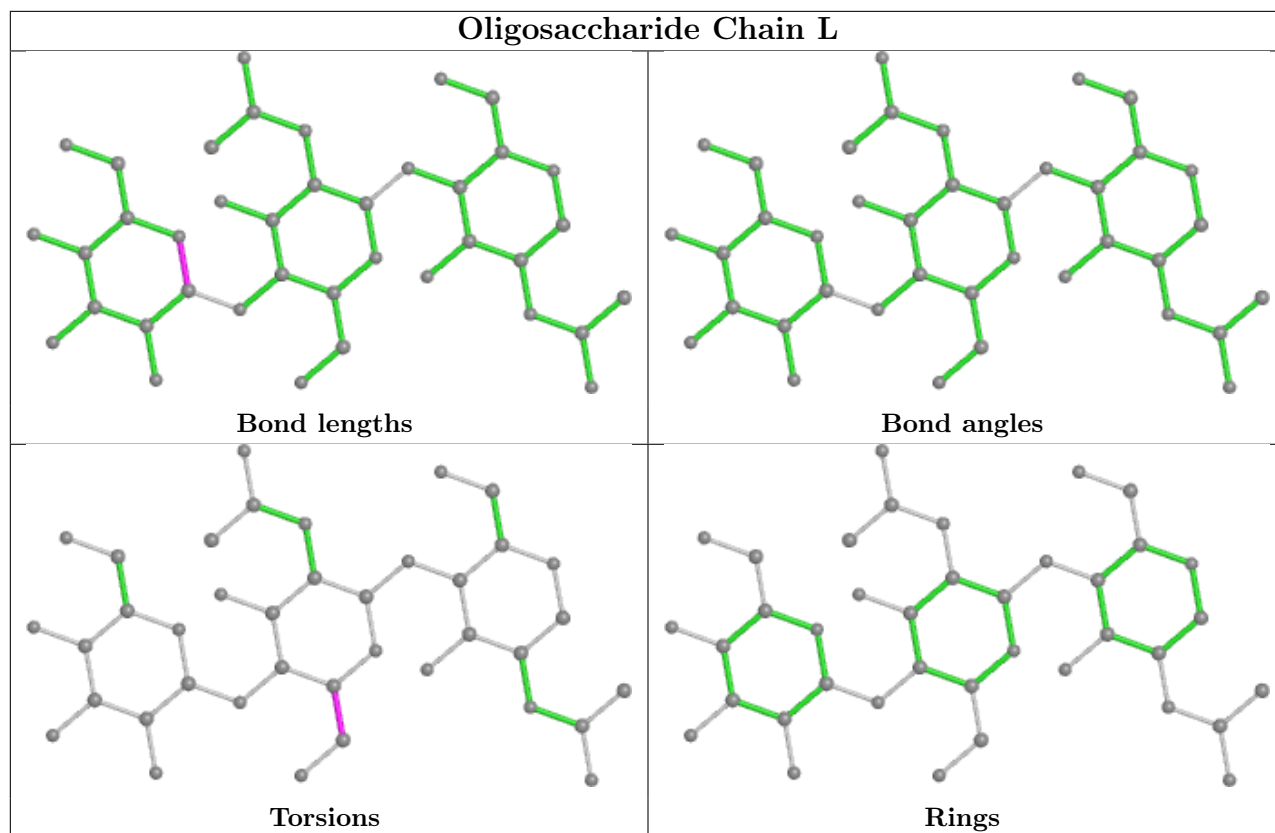
Mol	Chain	Res	Type	Atoms
5	O	1	NAG	O5-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
5	O	1	NAG	C4-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6

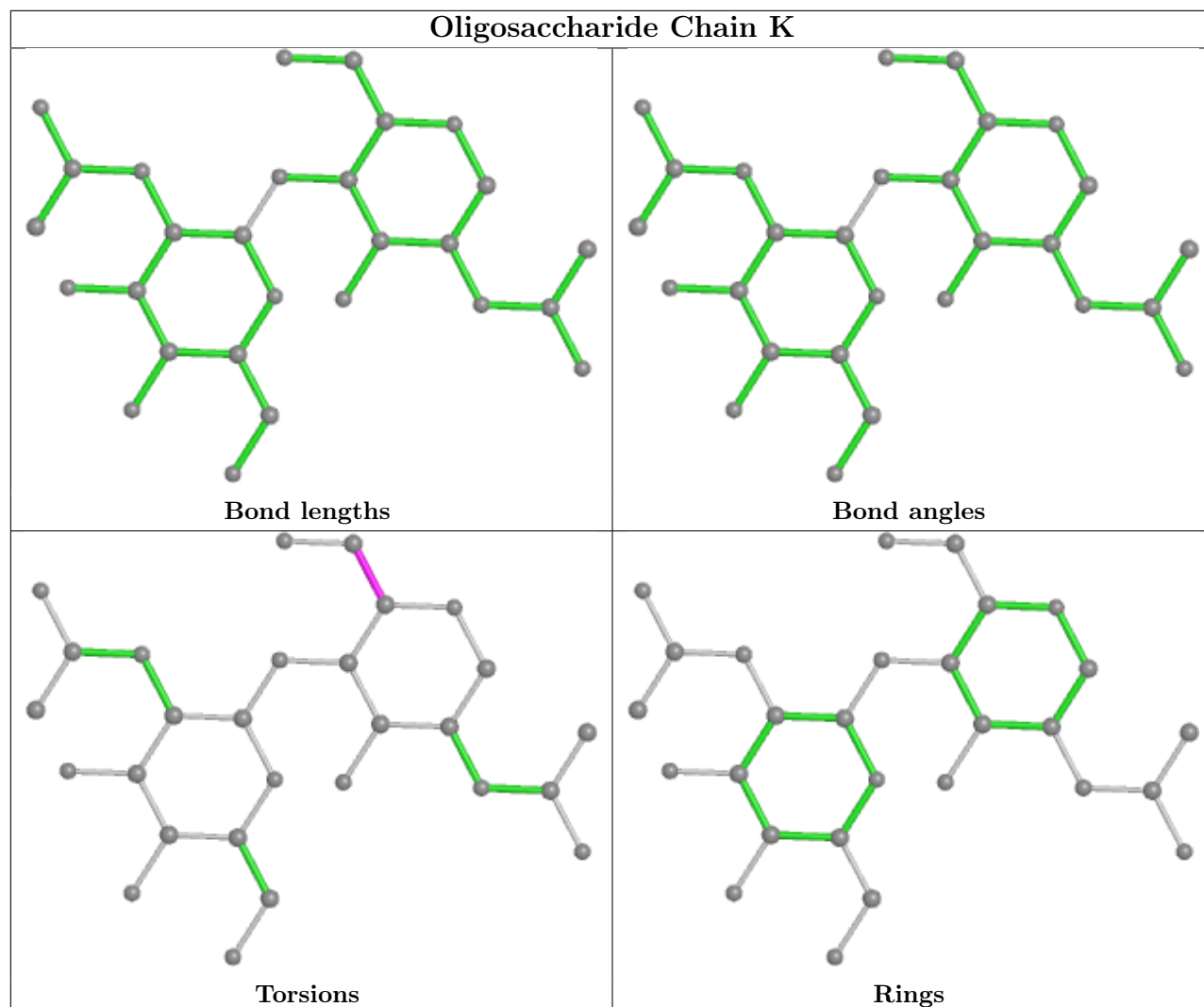
There are no ring outliers.

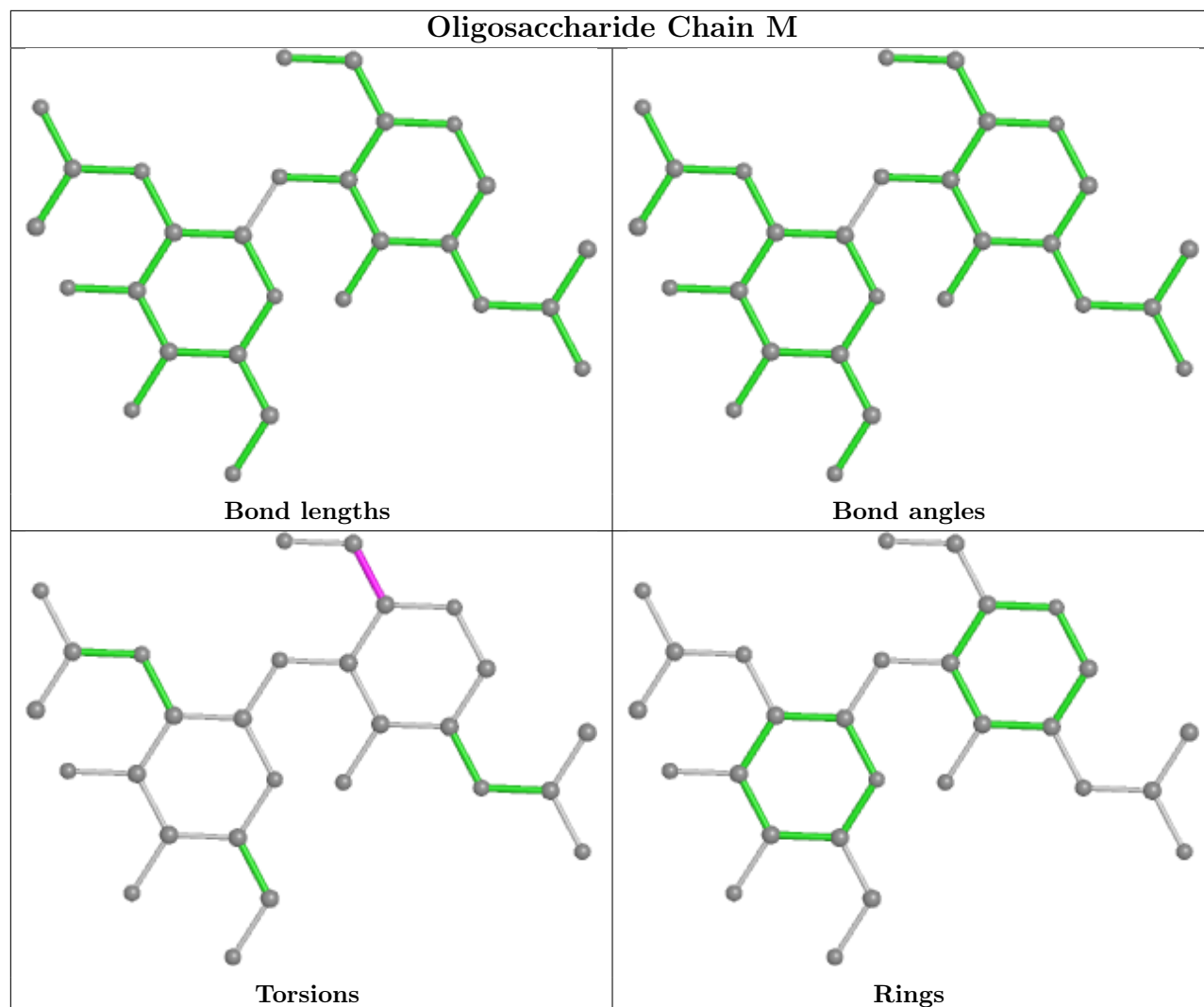
No monomer is involved in short contacts.

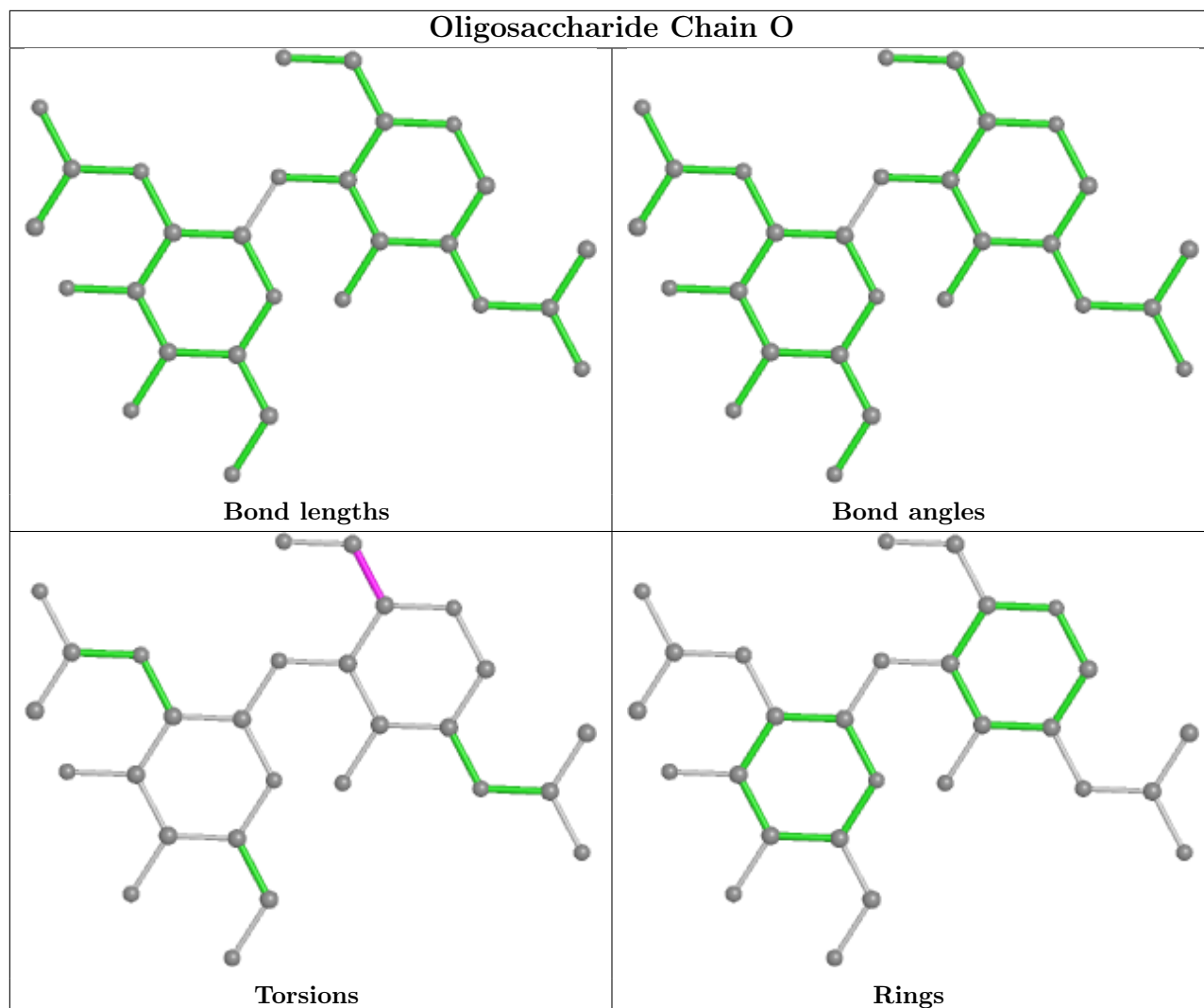
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	NAG	C	407	1	14,14,15	0.19	0	17,19,21	0.53	0
6	NAG	C	410	1	14,14,15	0.62	1 (7%)	17,19,21	0.68	1 (5%)
6	NAG	D	701	2	14,14,15	0.28	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	E	408	1	14,14,15	0.40	0	17,19,21	0.50	0
6	NAG	A	410	1	14,14,15	0.63	1 (7%)	17,19,21	0.67	1 (5%)
6	NAG	A	407	1	14,14,15	0.19	0	17,19,21	0.54	0
6	NAG	A	406	1	14,14,15	0.23	0	17,19,21	0.53	0
6	NAG	E	406	1	14,14,15	0.24	0	17,19,21	0.54	0
6	NAG	E	407	1	14,14,15	0.20	0	17,19,21	0.52	0
6	NAG	E	409	1	14,14,15	0.37	0	17,19,21	0.62	0
6	NAG	C	406	1	14,14,15	0.24	0	17,19,21	0.57	0
6	NAG	F	701	2	14,14,15	0.29	0	17,19,21	0.50	0
6	NAG	B	701	2	14,14,15	0.28	0	17,19,21	0.47	0
6	NAG	C	408	1	14,14,15	0.37	0	17,19,21	0.48	0
6	NAG	C	409	1	14,14,15	0.42	0	17,19,21	0.65	0
6	NAG	E	410	1	14,14,15	0.54	0	17,19,21	0.72	1 (5%)
6	NAG	A	409	1	14,14,15	0.41	0	17,19,21	0.66	0
6	NAG	A	408	1	14,14,15	0.41	0	17,19,21	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	407	1	-	2/6/23/26	0/1/1/1
6	NAG	C	410	1	-	0/6/23/26	0/1/1/1
6	NAG	D	701	2	-	2/6/23/26	0/1/1/1
6	NAG	E	408	1	-	0/6/23/26	0/1/1/1
6	NAG	A	410	1	-	1/6/23/26	0/1/1/1
6	NAG	A	407	1	-	2/6/23/26	0/1/1/1
6	NAG	A	406	1	-	2/6/23/26	0/1/1/1
6	NAG	E	406	1	-	2/6/23/26	0/1/1/1
6	NAG	E	407	1	-	2/6/23/26	0/1/1/1
6	NAG	E	409	1	-	1/6/23/26	0/1/1/1
6	NAG	C	406	1	-	2/6/23/26	0/1/1/1
6	NAG	F	701	2	-	2/6/23/26	0/1/1/1
6	NAG	B	701	2	-	2/6/23/26	0/1/1/1
6	NAG	C	408	1	-	0/6/23/26	0/1/1/1
6	NAG	C	409	1	-	1/6/23/26	0/1/1/1
6	NAG	E	410	1	-	0/6/23/26	0/1/1/1
6	NAG	A	409	1	-	1/6/23/26	0/1/1/1
6	NAG	A	408	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	410	NAG	O5-C1	-2.26	1.40	1.43
6	C	410	NAG	O5-C1	-2.22	1.40	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	410	NAG	C1-O5-C5	2.32	115.34	112.19
6	C	410	NAG	C1-O5-C5	2.08	115.01	112.19
6	A	410	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	407	NAG	C4-C5-C6-O6
6	C	407	NAG	C4-C5-C6-O6
6	E	407	NAG	C4-C5-C6-O6
6	A	406	NAG	O5-C5-C6-O6
6	C	406	NAG	O5-C5-C6-O6
6	E	406	NAG	O5-C5-C6-O6
6	A	407	NAG	O5-C5-C6-O6
6	C	407	NAG	O5-C5-C6-O6
6	E	407	NAG	O5-C5-C6-O6
6	D	701	NAG	O5-C5-C6-O6
6	F	701	NAG	O5-C5-C6-O6
6	B	701	NAG	O5-C5-C6-O6
6	E	409	NAG	O5-C5-C6-O6
6	A	409	NAG	O5-C5-C6-O6
6	C	406	NAG	C4-C5-C6-O6
6	E	406	NAG	C4-C5-C6-O6
6	A	406	NAG	C4-C5-C6-O6
6	C	409	NAG	O5-C5-C6-O6
6	D	701	NAG	C4-C5-C6-O6
6	F	701	NAG	C4-C5-C6-O6
6	B	701	NAG	C4-C5-C6-O6
6	A	410	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

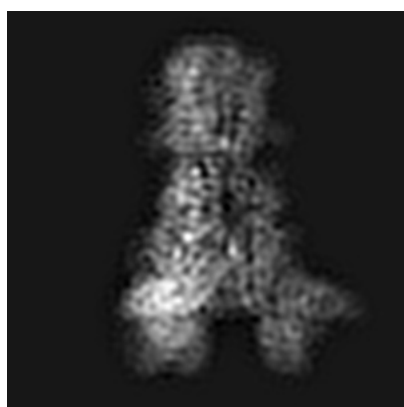
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8561. These allow visual inspection of the internal detail of the map and identification of artifacts.

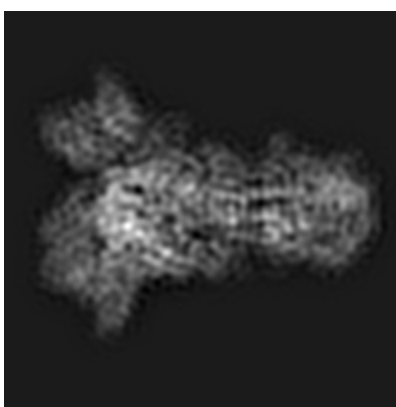
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

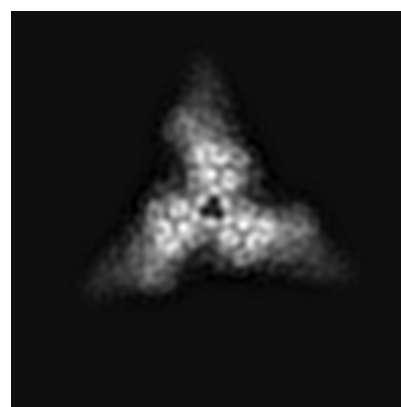
6.1.1 Primary map



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: 60



Y Index: 60

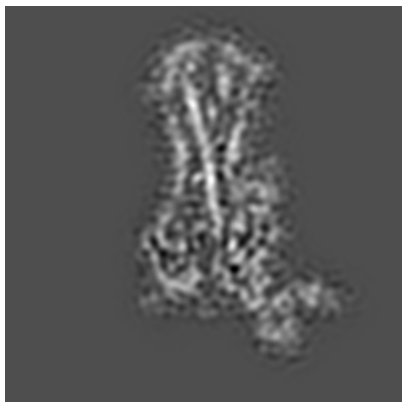


Z Index: 60

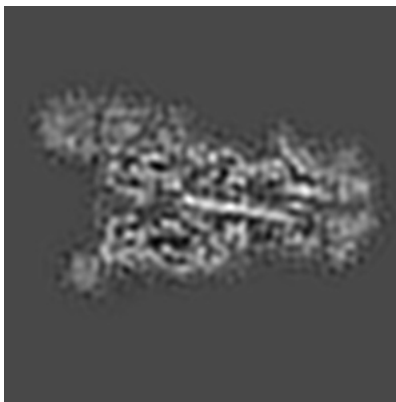
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 64



Y Index: 56



Z Index: 37

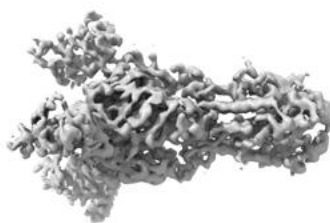
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

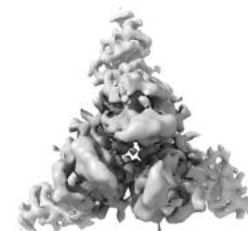
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

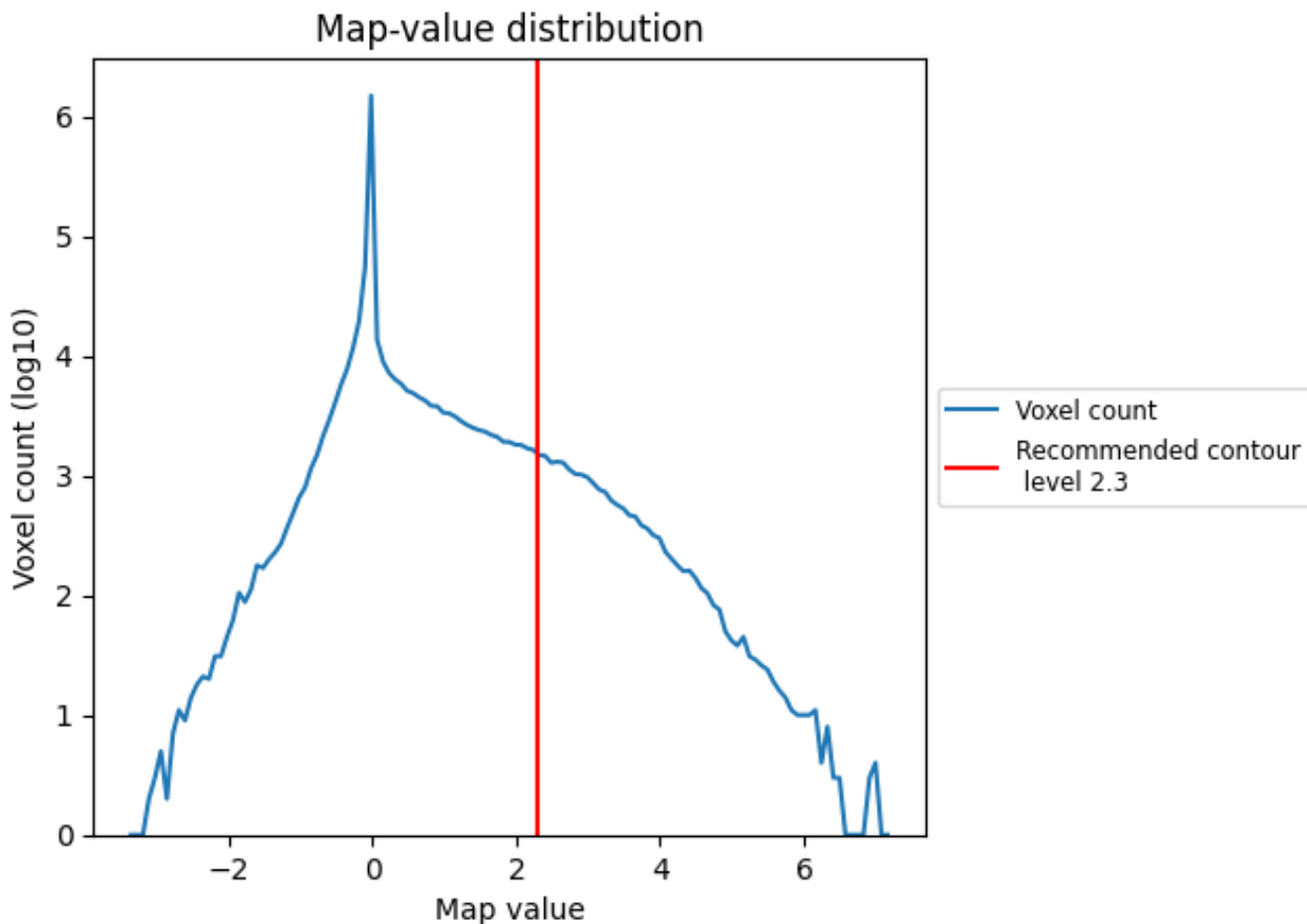
6.5 Mask visualisation

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

7 Map analysis [i](#)

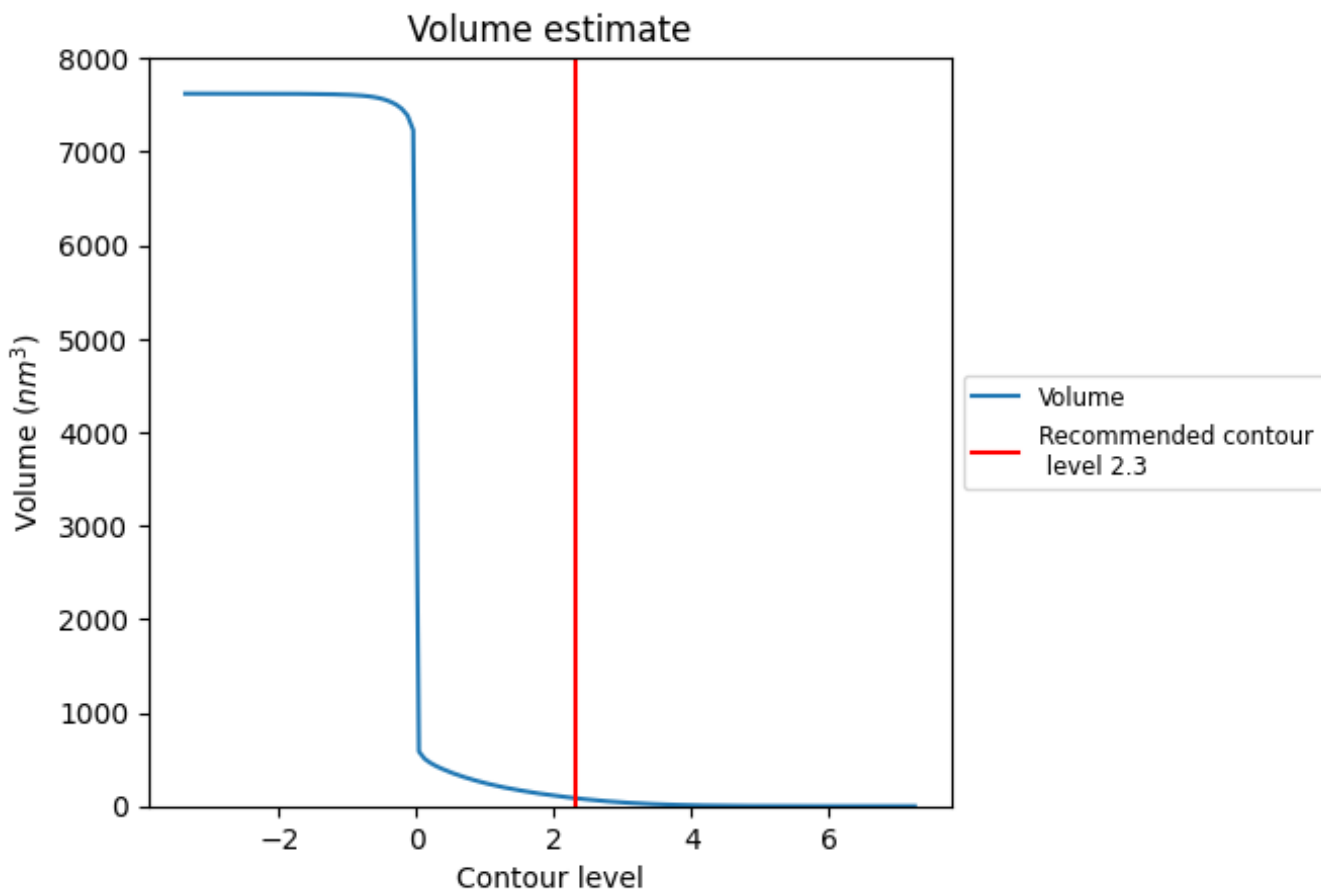
This section contains the results of statistical analysis of the map.

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.

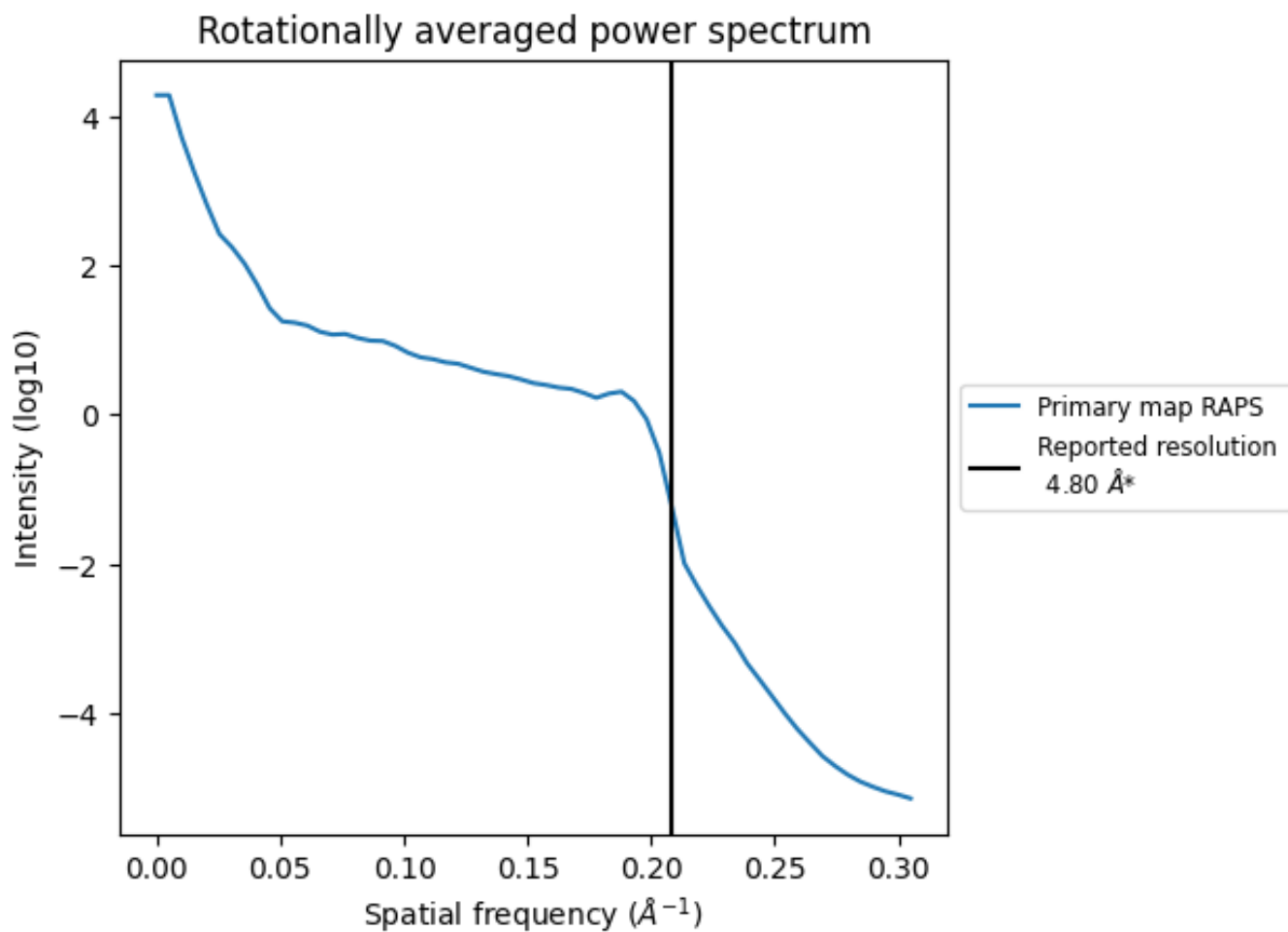
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 86 nm³; this corresponds to an approximate mass of 78 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

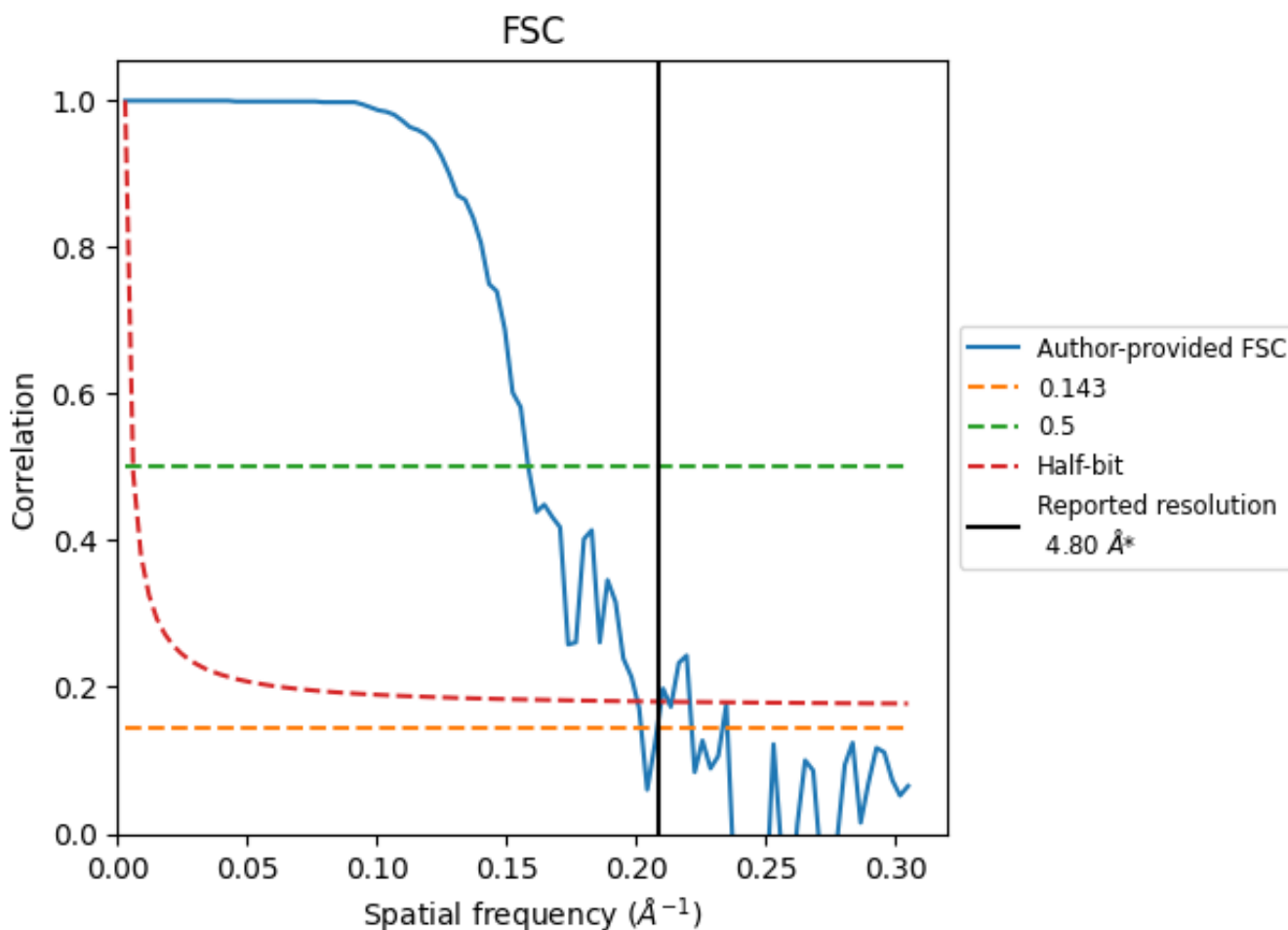


*Reported resolution corresponds to spatial frequency of 0.208\AA^{-1}

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 0.208 Å⁻¹

8.2 Resolution estimates [i](#)

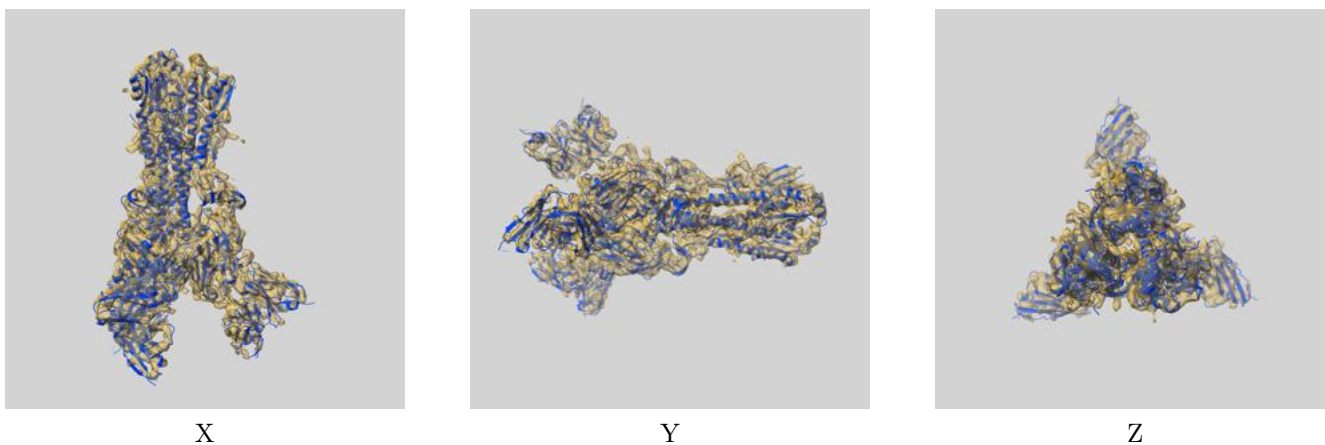
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	4.95	6.31	4.99
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

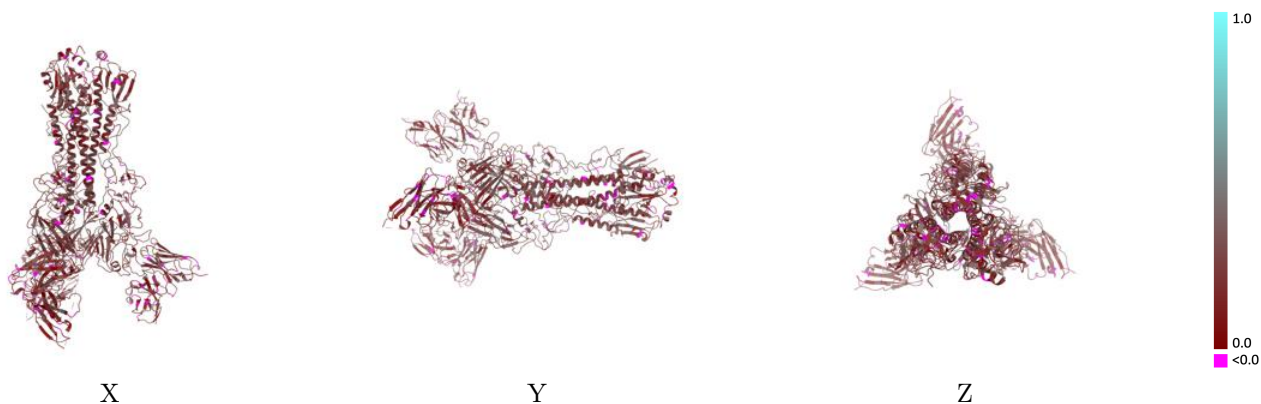
This section contains information regarding the fit between EMDB map EMD-8561 and PDB model 5UJZ. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



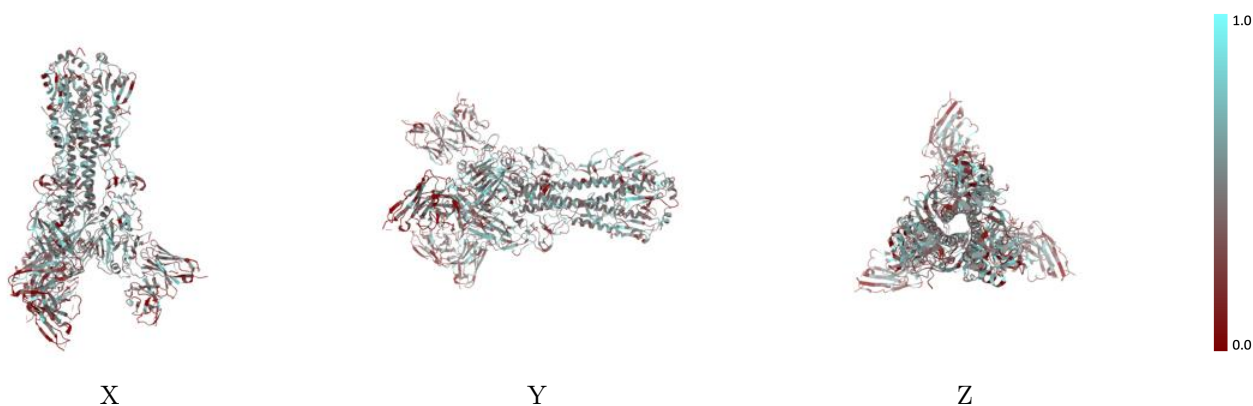
The images above show the 3D surface view of the map at the recommended contour level 2.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



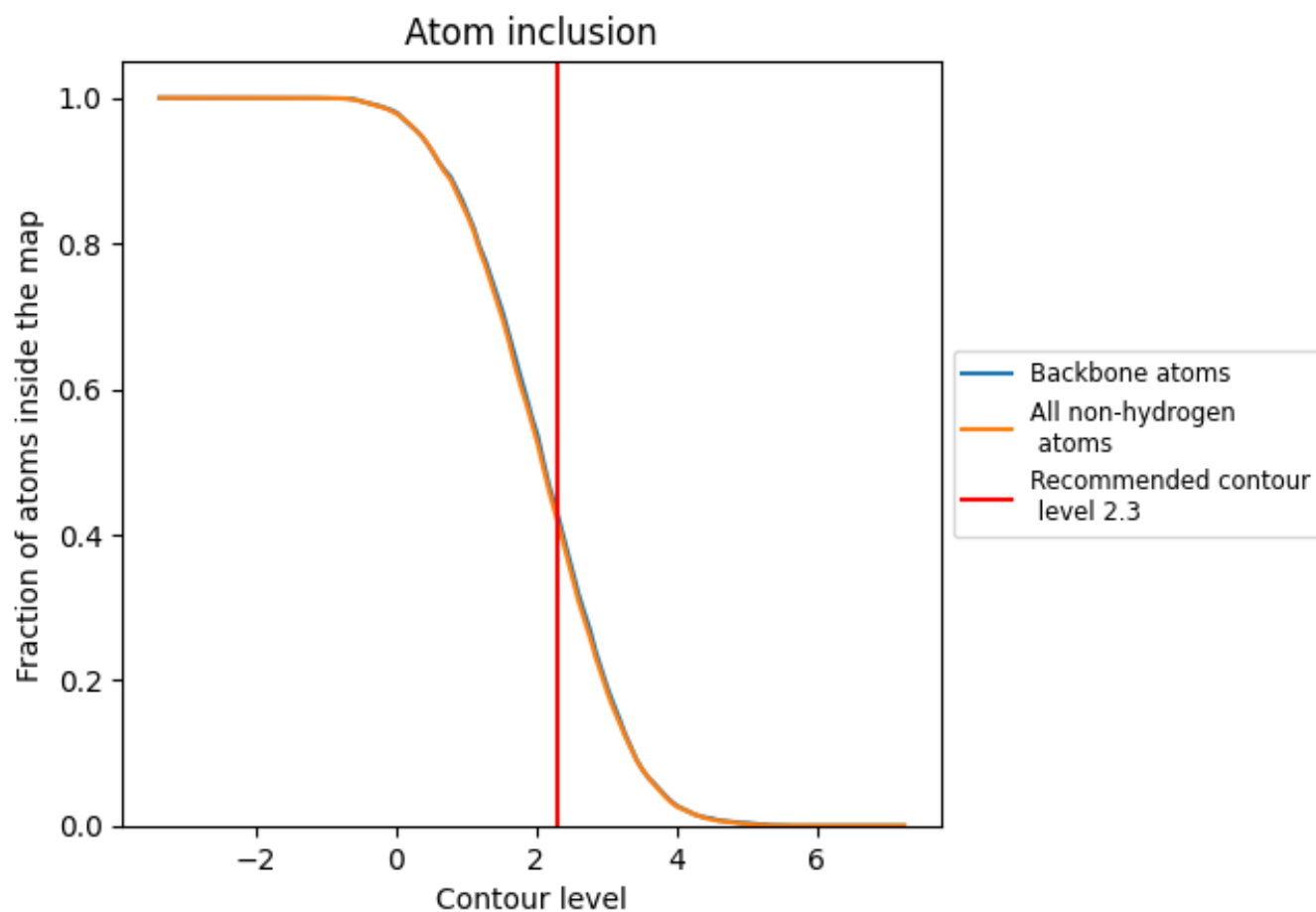
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 43% of all backbone atoms, 42% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (2.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4204	0.2240
A	0.4759	0.2460
B	0.4647	0.2230
C	0.4763	0.2500
D	0.4575	0.2170
E	0.4806	0.2470
F	0.4669	0.2200
G	0.3358	0.1850
H	0.3318	0.1920
I	0.3324	0.1880
J	0.4103	0.3600
K	0.2857	0.3710
L	0.4359	0.3500
M	0.2500	0.3780
N	0.4103	0.3630
O	0.2857	0.3700

