



wwPDB EM Validation Summary Report ⓘ

May 31, 2022 – 07:20 pm BST

PDB ID : 7R4I
EMDB ID : EMD-14313
Title : The SARS-CoV-2 spike in complex with the 2.15 neutralizing nanobody
Authors : Casasnovas, J.M.; Melero, R.; Arranz, R.; Fernandez, L.A.
Deposited on : 2022-02-08
Resolution : 3.20 Å (reported)
Based on initial models : 6ZXN, 6DBA

This is a wwPDB EM Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev8
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

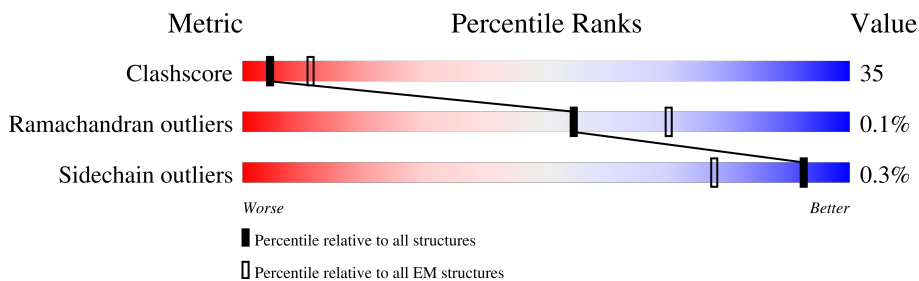
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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.



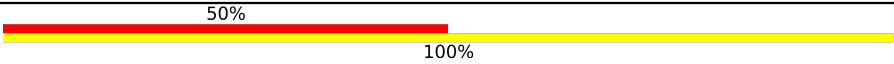
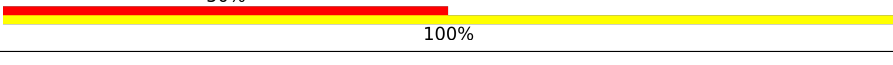
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1264	
1	B	1264	
1	C	1264	
2	D	130	
2	E	130	
3	F	2	
3	G	2	
3	H	2	

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Mol	Chain	Length	Quality of chain
3	I	2	 50% 100%
3	J	2	 50% 100%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 52010 atoms, of which 24685 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	1057	16320	5278	8045	1380	1579	38	2	0
1	B	1056	16302	5277	8034	1380	1573	38	3	0
1	C	1060	16361	5292	8069	1382	1580	38	1	0

There are 186 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	SER	-	expression tag	UNP P0DTC2
A	1213	GLY	-	expression tag	UNP P0DTC2
A	1214	TYR	-	expression tag	UNP P0DTC2
A	1215	ILE	-	expression tag	UNP P0DTC2
A	1216	PRO	-	expression tag	UNP P0DTC2
A	1217	GLU	-	expression tag	UNP P0DTC2
A	1218	ALA	-	expression tag	UNP P0DTC2
A	1219	PRO	-	expression tag	UNP P0DTC2
A	1220	ARG	-	expression tag	UNP P0DTC2
A	1221	ASP	-	expression tag	UNP P0DTC2
A	1222	GLY	-	expression tag	UNP P0DTC2
A	1223	GLN	-	expression tag	UNP P0DTC2
A	1224	ALA	-	expression tag	UNP P0DTC2
A	1225	TYR	-	expression tag	UNP P0DTC2
A	1226	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1227	ARG	-	expression tag	UNP P0DTC2
A	1228	LYS	-	expression tag	UNP P0DTC2
A	1229	ASP	-	expression tag	UNP P0DTC2
A	1230	GLY	-	expression tag	UNP P0DTC2
A	1231	GLU	-	expression tag	UNP P0DTC2
A	1232	TRP	-	expression tag	UNP P0DTC2
A	1233	VAL	-	expression tag	UNP P0DTC2
A	1234	LEU	-	expression tag	UNP P0DTC2
A	1235	LEU	-	expression tag	UNP P0DTC2
A	1236	SER	-	expression tag	UNP P0DTC2
A	1237	THR	-	expression tag	UNP P0DTC2
A	1238	PHE	-	expression tag	UNP P0DTC2
A	1239	LEU	-	expression tag	UNP P0DTC2
A	1240	GLY	-	expression tag	UNP P0DTC2
A	1241	THR	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	ASN	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	TYR	-	expression tag	UNP P0DTC2
A	1246	PHE	-	expression tag	UNP P0DTC2
A	1247	GLN	-	expression tag	UNP P0DTC2
A	1248	GLY	-	expression tag	UNP P0DTC2
A	1249	ASP	-	expression tag	UNP P0DTC2
A	1250	TYR	-	expression tag	UNP P0DTC2
A	1251	LYS	-	expression tag	UNP P0DTC2
A	1252	ASP	-	expression tag	UNP P0DTC2
A	1253	ASP	-	expression tag	UNP P0DTC2
A	1254	ASP	-	expression tag	UNP P0DTC2
A	1255	ASP	-	expression tag	UNP P0DTC2
A	1256	LYS	-	expression tag	UNP P0DTC2
A	1257	GLY	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
A	1260	HIS	-	expression tag	UNP P0DTC2
A	1261	HIS	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	HIS	-	expression tag	UNP P0DTC2
A	1264	HIS	-	expression tag	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	SER	-	expression tag	UNP P0DTC2
B	1213	GLY	-	expression tag	UNP P0DTC2
B	1214	TYR	-	expression tag	UNP P0DTC2
B	1215	ILE	-	expression tag	UNP P0DTC2
B	1216	PRO	-	expression tag	UNP P0DTC2
B	1217	GLU	-	expression tag	UNP P0DTC2
B	1218	ALA	-	expression tag	UNP P0DTC2
B	1219	PRO	-	expression tag	UNP P0DTC2
B	1220	ARG	-	expression tag	UNP P0DTC2
B	1221	ASP	-	expression tag	UNP P0DTC2
B	1222	GLY	-	expression tag	UNP P0DTC2
B	1223	GLN	-	expression tag	UNP P0DTC2
B	1224	ALA	-	expression tag	UNP P0DTC2
B	1225	TYR	-	expression tag	UNP P0DTC2
B	1226	VAL	-	expression tag	UNP P0DTC2
B	1227	ARG	-	expression tag	UNP P0DTC2
B	1228	LYS	-	expression tag	UNP P0DTC2
B	1229	ASP	-	expression tag	UNP P0DTC2
B	1230	GLY	-	expression tag	UNP P0DTC2
B	1231	GLU	-	expression tag	UNP P0DTC2
B	1232	TRP	-	expression tag	UNP P0DTC2
B	1233	VAL	-	expression tag	UNP P0DTC2
B	1234	LEU	-	expression tag	UNP P0DTC2
B	1235	LEU	-	expression tag	UNP P0DTC2
B	1236	SER	-	expression tag	UNP P0DTC2
B	1237	THR	-	expression tag	UNP P0DTC2
B	1238	PHE	-	expression tag	UNP P0DTC2
B	1239	LEU	-	expression tag	UNP P0DTC2
B	1240	GLY	-	expression tag	UNP P0DTC2
B	1241	THR	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	ASN	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	TYR	-	expression tag	UNP P0DTC2
B	1246	PHE	-	expression tag	UNP P0DTC2
B	1247	GLN	-	expression tag	UNP P0DTC2
B	1248	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1249	ASP	-	expression tag	UNP P0DTC2
B	1250	TYR	-	expression tag	UNP P0DTC2
B	1251	LYS	-	expression tag	UNP P0DTC2
B	1252	ASP	-	expression tag	UNP P0DTC2
B	1253	ASP	-	expression tag	UNP P0DTC2
B	1254	ASP	-	expression tag	UNP P0DTC2
B	1255	ASP	-	expression tag	UNP P0DTC2
B	1256	LYS	-	expression tag	UNP P0DTC2
B	1257	GLY	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
B	1260	HIS	-	expression tag	UNP P0DTC2
B	1261	HIS	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	HIS	-	expression tag	UNP P0DTC2
B	1264	HIS	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	SER	-	expression tag	UNP P0DTC2
C	1213	GLY	-	expression tag	UNP P0DTC2
C	1214	TYR	-	expression tag	UNP P0DTC2
C	1215	ILE	-	expression tag	UNP P0DTC2
C	1216	PRO	-	expression tag	UNP P0DTC2
C	1217	GLU	-	expression tag	UNP P0DTC2
C	1218	ALA	-	expression tag	UNP P0DTC2
C	1219	PRO	-	expression tag	UNP P0DTC2
C	1220	ARG	-	expression tag	UNP P0DTC2
C	1221	ASP	-	expression tag	UNP P0DTC2
C	1222	GLY	-	expression tag	UNP P0DTC2
C	1223	GLN	-	expression tag	UNP P0DTC2
C	1224	ALA	-	expression tag	UNP P0DTC2
C	1225	TYR	-	expression tag	UNP P0DTC2
C	1226	VAL	-	expression tag	UNP P0DTC2
C	1227	ARG	-	expression tag	UNP P0DTC2
C	1228	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1229	ASP	-	expression tag	UNP P0DTC2
C	1230	GLY	-	expression tag	UNP P0DTC2
C	1231	GLU	-	expression tag	UNP P0DTC2
C	1232	TRP	-	expression tag	UNP P0DTC2
C	1233	VAL	-	expression tag	UNP P0DTC2
C	1234	LEU	-	expression tag	UNP P0DTC2
C	1235	LEU	-	expression tag	UNP P0DTC2
C	1236	SER	-	expression tag	UNP P0DTC2
C	1237	THR	-	expression tag	UNP P0DTC2
C	1238	PHE	-	expression tag	UNP P0DTC2
C	1239	LEU	-	expression tag	UNP P0DTC2
C	1240	GLY	-	expression tag	UNP P0DTC2
C	1241	THR	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	ASN	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	TYR	-	expression tag	UNP P0DTC2
C	1246	PHE	-	expression tag	UNP P0DTC2
C	1247	GLN	-	expression tag	UNP P0DTC2
C	1248	GLY	-	expression tag	UNP P0DTC2
C	1249	ASP	-	expression tag	UNP P0DTC2
C	1250	TYR	-	expression tag	UNP P0DTC2
C	1251	LYS	-	expression tag	UNP P0DTC2
C	1252	ASP	-	expression tag	UNP P0DTC2
C	1253	ASP	-	expression tag	UNP P0DTC2
C	1254	ASP	-	expression tag	UNP P0DTC2
C	1255	ASP	-	expression tag	UNP P0DTC2
C	1256	LYS	-	expression tag	UNP P0DTC2
C	1257	GLY	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	HIS	-	expression tag	UNP P0DTC2
C	1260	HIS	-	expression tag	UNP P0DTC2
C	1261	HIS	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	HIS	-	expression tag	UNP P0DTC2
C	1264	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Camel-derived nanobody 2.15.

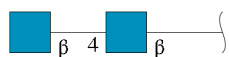
Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			S
2	D	125	944	589	164	186	5	0	0

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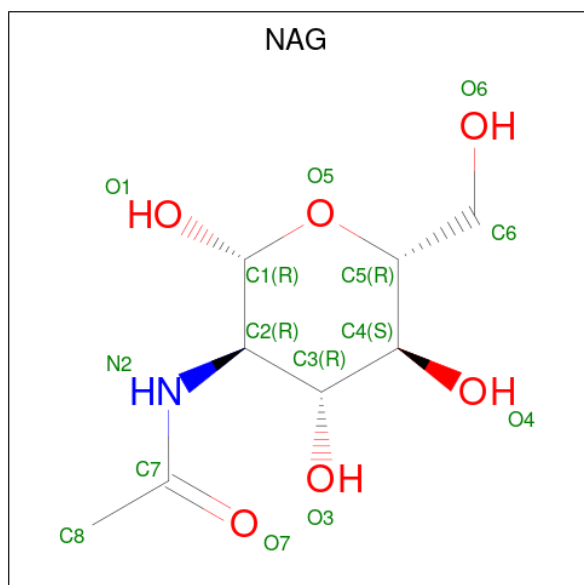
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	125	944	589	164	186	5	0	0

- Molecule 3 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		
3	F	2	53	16	25	2	10	0	0
3	G	2	53	16	25	2	10	0	0
3	H	2	53	16	25	2	10	0	0
3	I	2	53	16	25	2	10	0	0
3	J	2	53	16	25	2	10	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

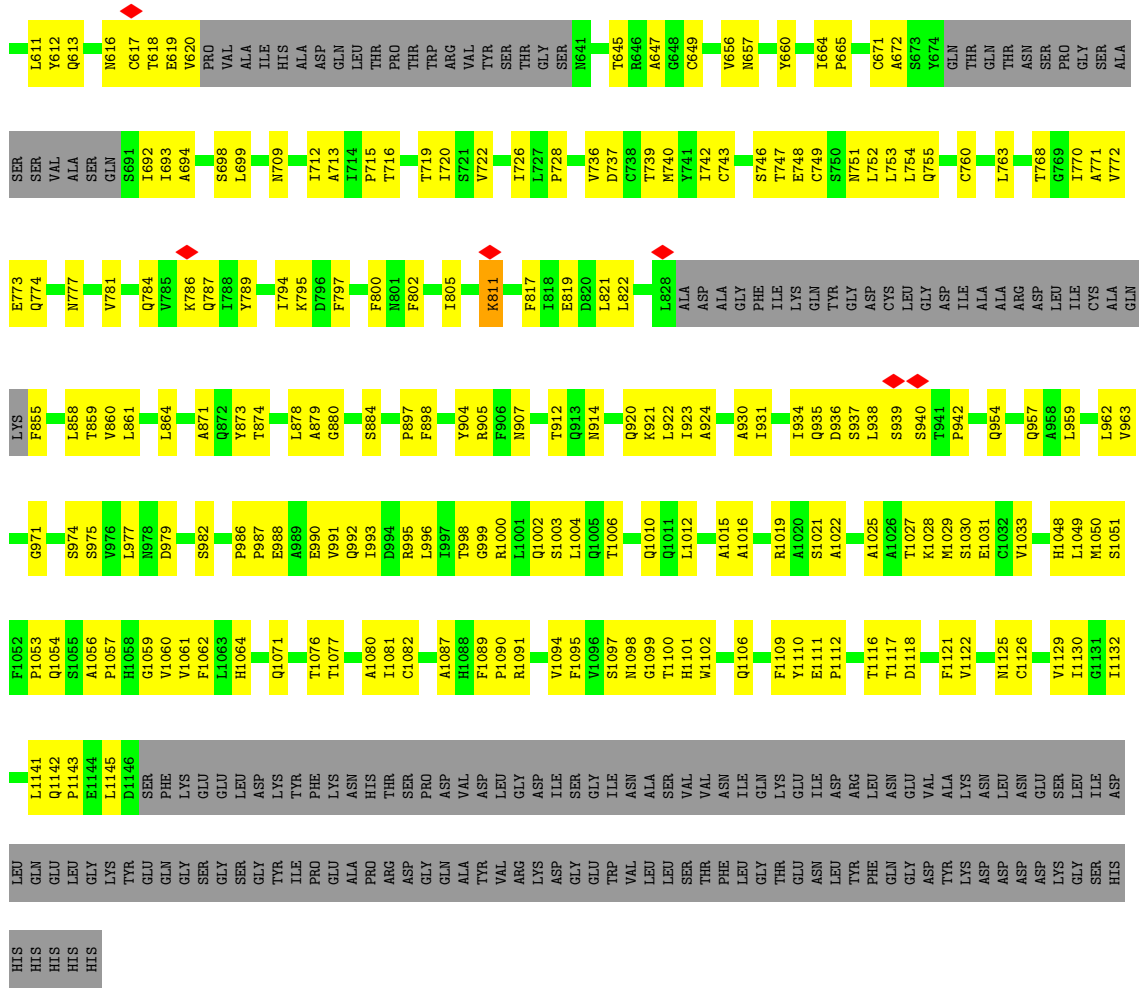


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	A	1	Total 377	C 112	H 181	N 14	O 70	0
4	B	1	Total 349	C 104	H 167	N 13	O 65	0
4	B	1	Total 349	C 104	H 167	N 13	O 65	0
4	B	1	Total 349	C 104	H 167	N 13	O 65	0
4	B	1	Total 349	C 104	H 167	N 13	O 65	0
4	B	1	Total 349	C 104	H 167	N 13	O 65	0
4	B	1	Total 349	C 104	H 167	N 13	O 65	0
4	B	1	Total 349	C 104	H 167	N 13	O 65	0
4	B	1	Total 349	C 104	H 167	N 13	O 65	0
4	B	1	Total 349	C 104	H 167	N 13	O 65	0

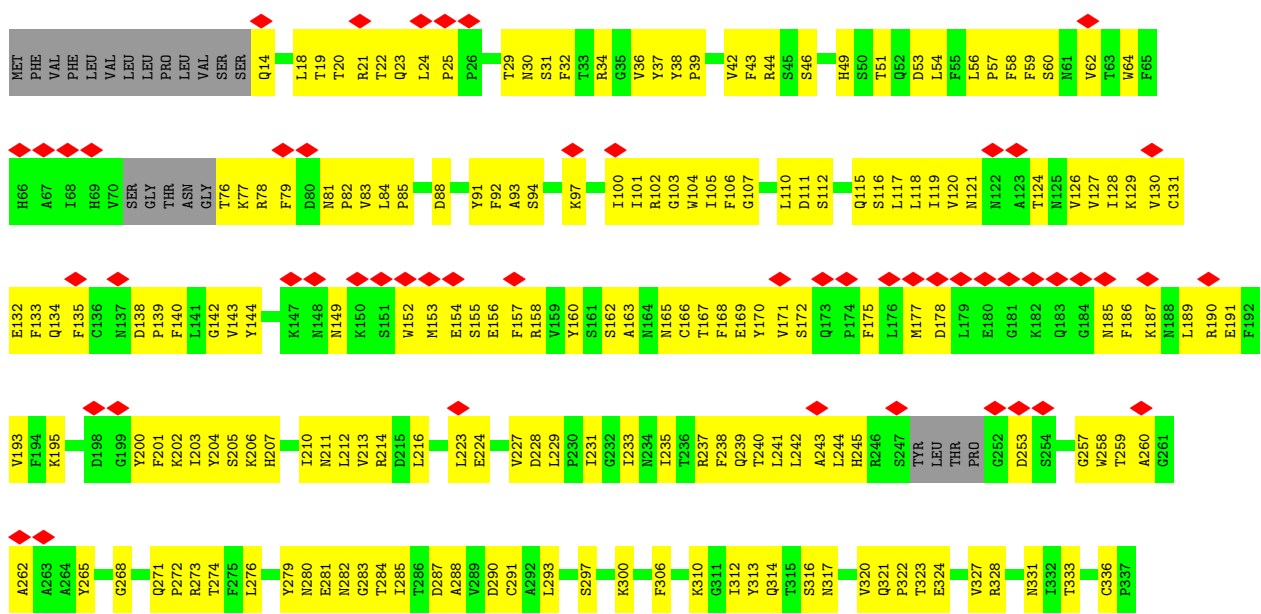
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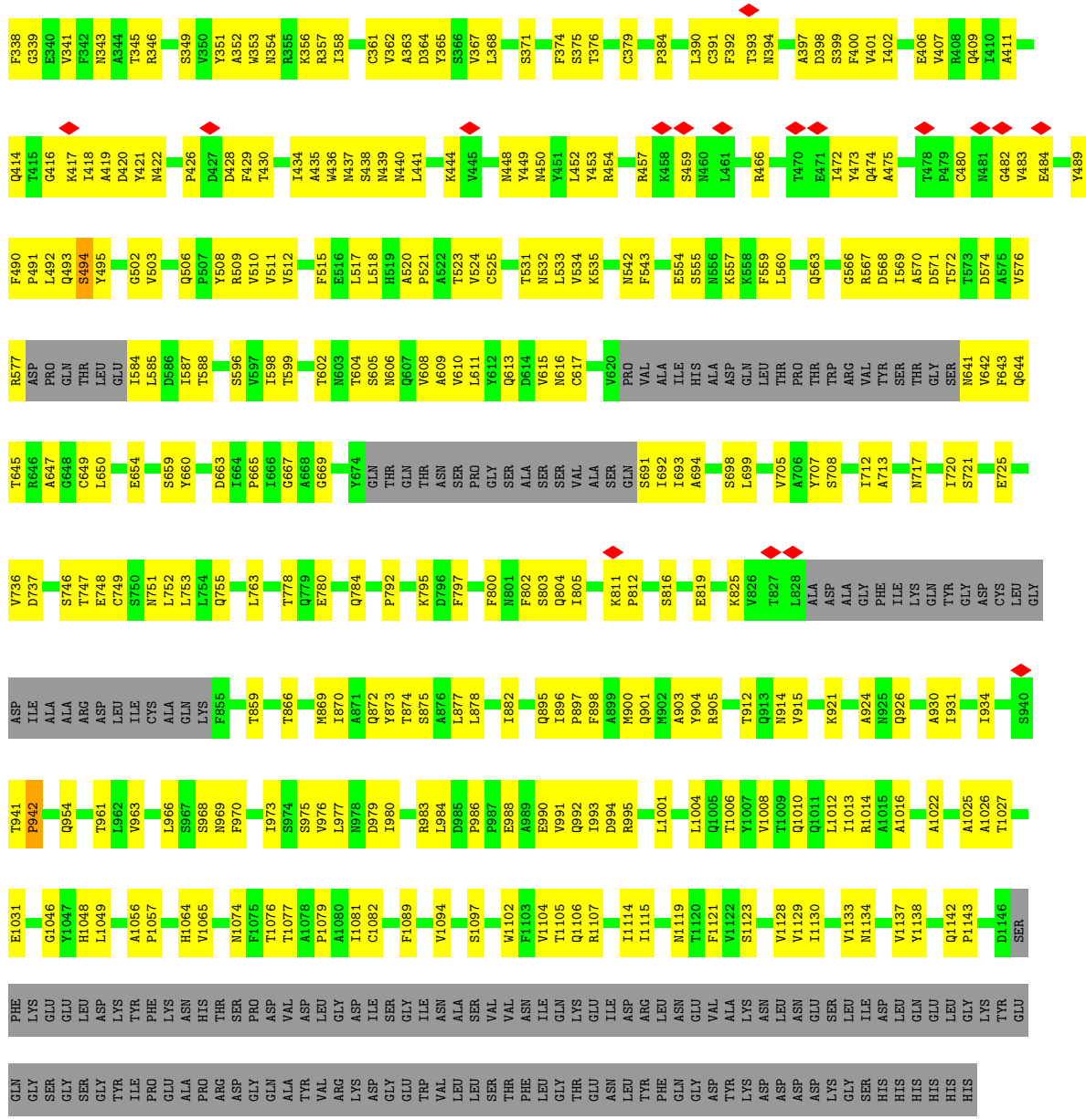
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Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	H	N	O	0
			349	104	167	13	65	
4	B	1	Total	C	H	N	O	0
			349	104	167	13	65	
4	B	1	Total	C	H	N	O	0
			349	104	167	13	65	
4	B	1	Total	C	H	N	O	0
			349	104	167	13	65	
4	C	1	Total	C	H	N	O	0
			148	48	64	6	30	
4	C	1	Total	C	H	N	O	0
			148	48	64	6	30	
4	C	1	Total	C	H	N	O	0
			148	48	64	6	30	
4	C	1	Total	C	H	N	O	0
			148	48	64	6	30	
4	C	1	Total	C	H	N	O	0
			148	48	64	6	30	

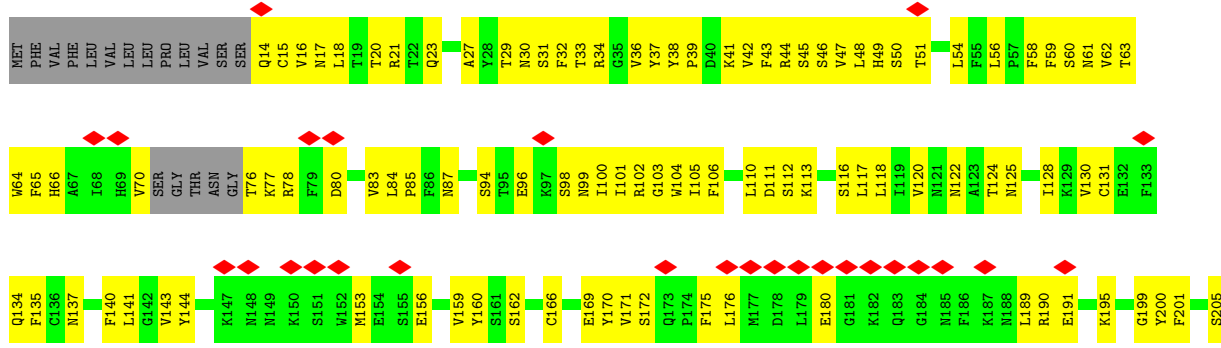


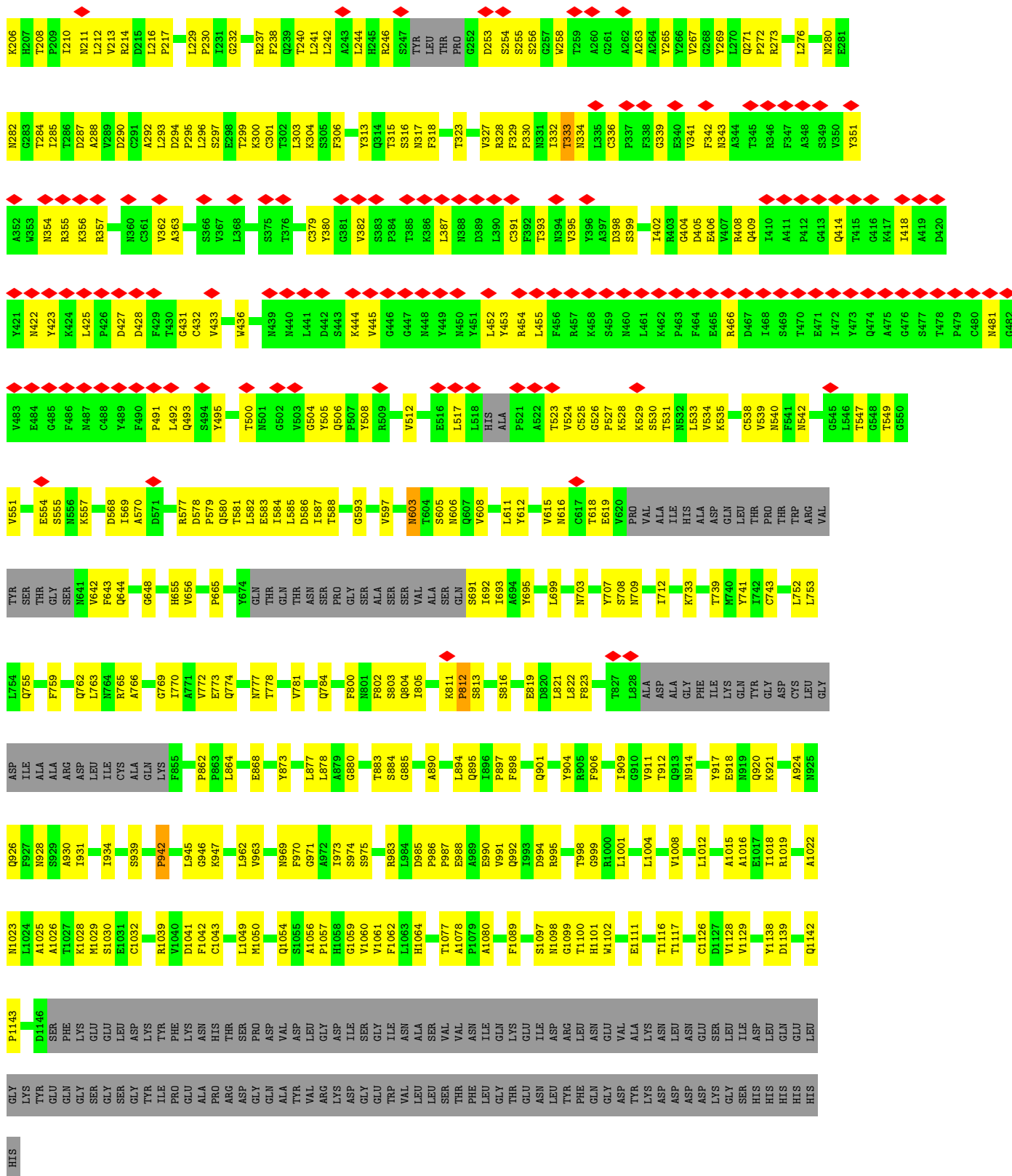
• Molecule 1: Spike glycoprotein





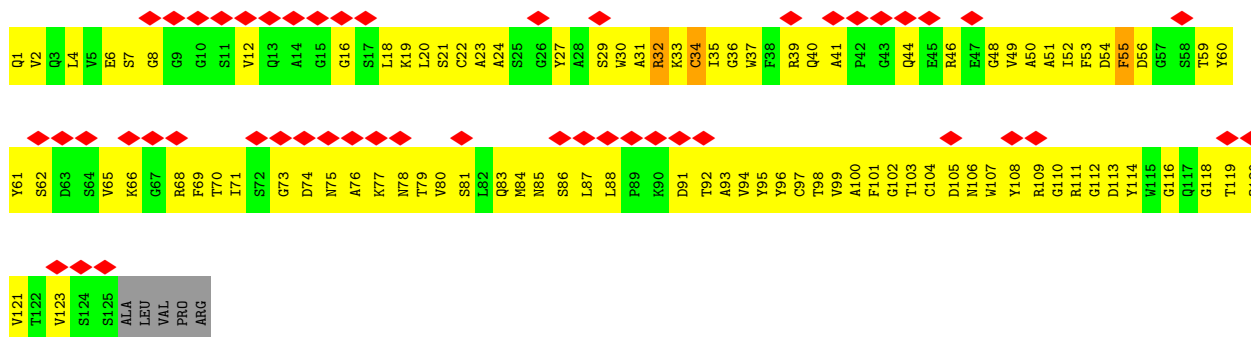
● Molecule 1: Spike glycoprotein



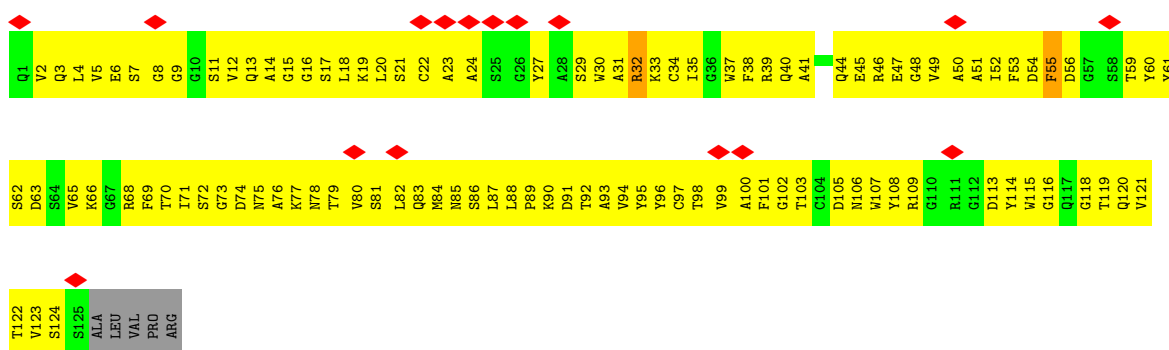


- Molecule 2: Camel-derived nanobody 2.15





• Molecule 2: Camel-derived nanobody 2.15



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucofuranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucofuranose-(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	40000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.973	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.025	Depositor
Map size (\AA)	420.66, 420.66, 420.66	wwPDB
Map dimensions	492, 492, 492	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.855, 0.855, 0.855	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

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	0.53	1/8472 (0.0%)	0.53	5/11525 (0.0%)
1	B	0.55	1/8469 (0.0%)	0.53	5/11521 (0.0%)
1	C	0.41	0/8490	0.51	1/11550 (0.0%)
2	D	2.77	6/965 (0.6%)	0.52	1/1306 (0.1%)
2	E	2.78	6/965 (0.6%)	0.53	0/1306
All	All	0.88	14/27361 (0.1%)	0.53	12/37208 (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	A	0	1
1	C	0	1
All	All	0	2

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	55	PHE	CD1-CE1	42.86	2.25	1.39
2	D	55	PHE	CD2-CE2	41.02	2.21	1.39
2	E	55	PHE	CE2-CZ	40.74	2.14	1.37
2	D	55	PHE	CE1-CZ	39.99	2.13	1.37
2	D	55	PHE	CE2-CZ	39.32	2.12	1.37

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	942	PRO	CA-N-CD	-8.13	100.12	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	942	PRO	CA-N-CD	-8.08	100.18	111.50
1	A	942	PRO	CA-N-CD	-8.05	100.23	111.50
1	A	494	SER	N-CA-CB	7.73	122.10	110.50
1	B	494	SER	CA-CB-OG	7.61	131.74	111.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	811	LYS	Peptide
1	C	812	PRO	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	8275	8045	8048	492	0
1	B	8268	8034	8055	503	0
1	C	8292	8069	8075	383	0
2	D	944	0	887	259	0
2	E	944	0	887	364	0
3	F	28	25	25	1	0
3	G	28	25	25	0	0
3	H	28	25	25	3	0
3	I	28	25	25	2	0
3	J	28	25	25	1	0
4	A	196	181	182	8	0
4	B	182	167	169	13	0
4	C	84	64	78	5	0
All	All	27325	24685	26506	1865	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 35.

The worst 5 of 1865 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:55:PHE:CD2	2:D:55:PHE:CG	1.75	1.68
2:E:55:PHE:CD2	2:E:55:PHE:CG	1.76	1.65
1:A:494:SER:HB2	2:D:55:PHE:CD1	1.48	1.46
1:B:494:SER:HA	2:E:55:PHE:CZ	1.48	1.44
2:E:55:PHE:CZ	2:E:55:PHE:CE1	2.05	1.43

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	1042/1264 (82%)	914 (88%)	128 (12%)	0	100	100
1	B	1043/1264 (82%)	896 (86%)	146 (14%)	1 (0%)	51	83
1	C	1045/1264 (83%)	906 (87%)	138 (13%)	1 (0%)	51	83
2	D	123/130 (95%)	111 (90%)	12 (10%)	0	100	100
2	E	123/130 (95%)	107 (87%)	16 (13%)	0	100	100
All	All	3376/4052 (83%)	2934 (87%)	440 (13%)	2 (0%)	54	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	333	THR
1	B	942	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	927/1100 (84%)	924 (100%)	3 (0%)	92	96
1	B	926/1100 (84%)	925 (100%)	1 (0%)	93	98
1	C	929/1100 (84%)	926 (100%)	3 (0%)	92	96
2	D	97/101 (96%)	95 (98%)	2 (2%)	53	79
2	E	97/101 (96%)	96 (99%)	1 (1%)	76	90
All	All	2976/3502 (85%)	2966 (100%)	10 (0%)	92	96

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	32	ARG
2	D	34	CYS
2	E	32	ARG
1	B	444	LYS
1	C	61	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	703	ASN
1	C	164	ASN
2	E	106	ASN
1	C	1088	HIS
1	B	717	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](#)

10 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
3	NAG	F	1	3	14,14,15	0.37	0	17,19,21	0.44	0
3	NAG	F	2	3	14,14,15	0.24	0	17,19,21	0.40	0
3	NAG	G	1	3	14,14,15	0.25	0	17,19,21	0.47	0
3	NAG	G	2	3	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	H	1	3,1	14,14,15	0.44	0	17,19,21	0.55	0
3	NAG	H	2	3	14,14,15	0.21	0	17,19,21	0.48	0
3	NAG	I	1	3,1	14,14,15	0.28	0	17,19,21	0.49	0
3	NAG	I	2	3	14,14,15	0.21	0	17,19,21	0.34	0
3	NAG	J	1	3,1	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	J	2	3	14,14,15	0.21	0	17,19,21	0.38	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
3	NAG	F	1	3	-	4/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	3	-	4/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

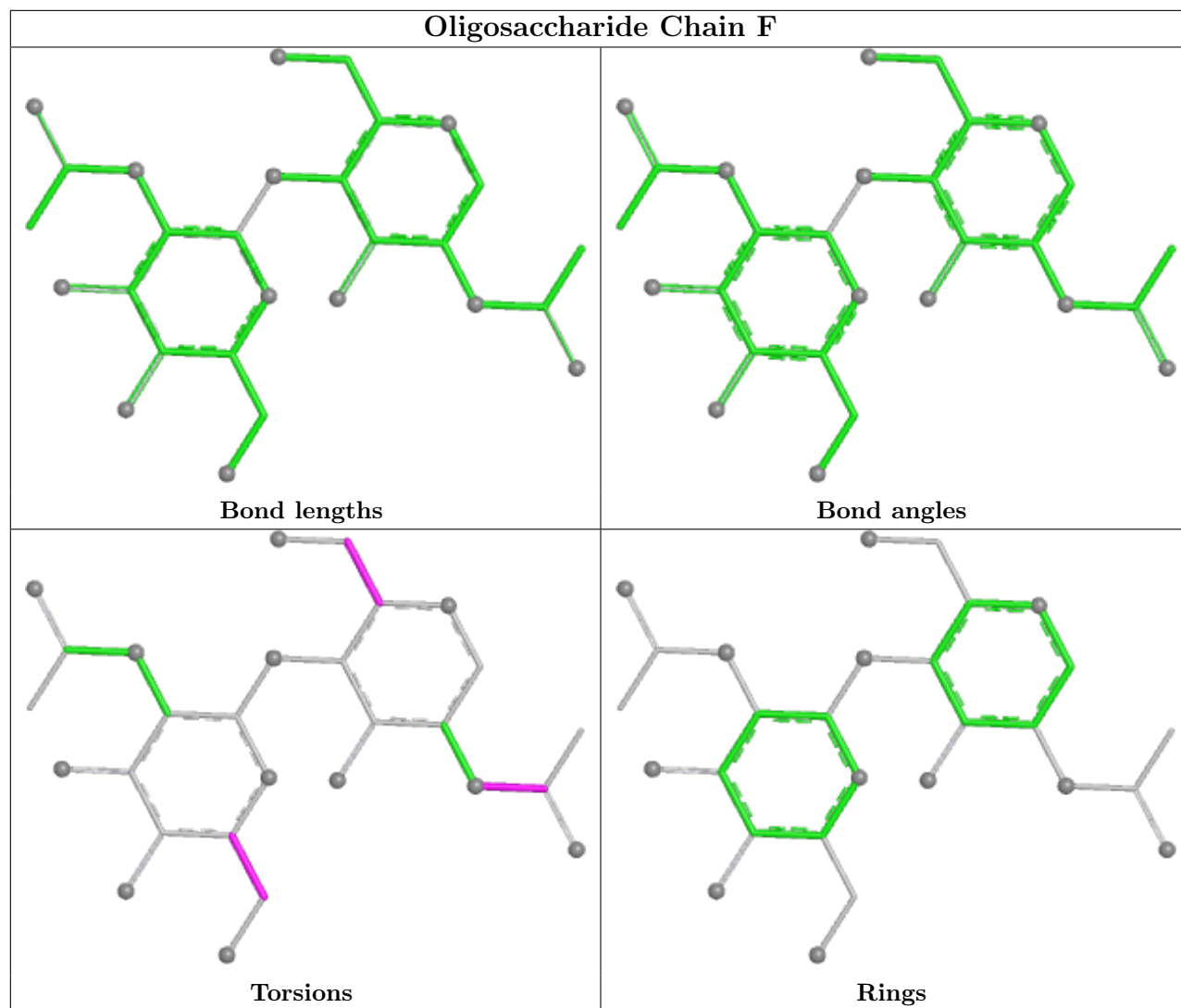
Mol	Chain	Res	Type	Atoms
3	F	2	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6

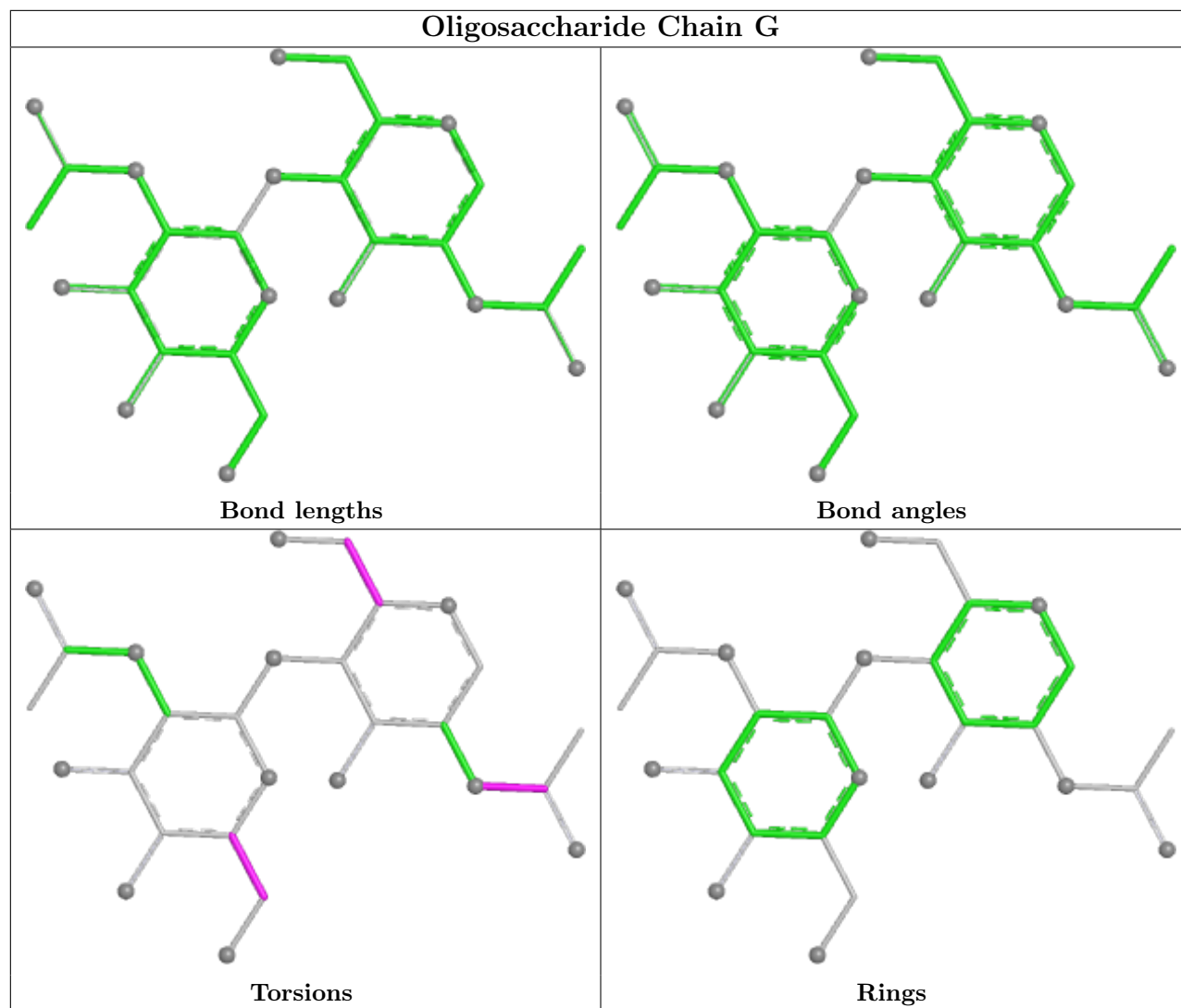
There are no ring outliers.

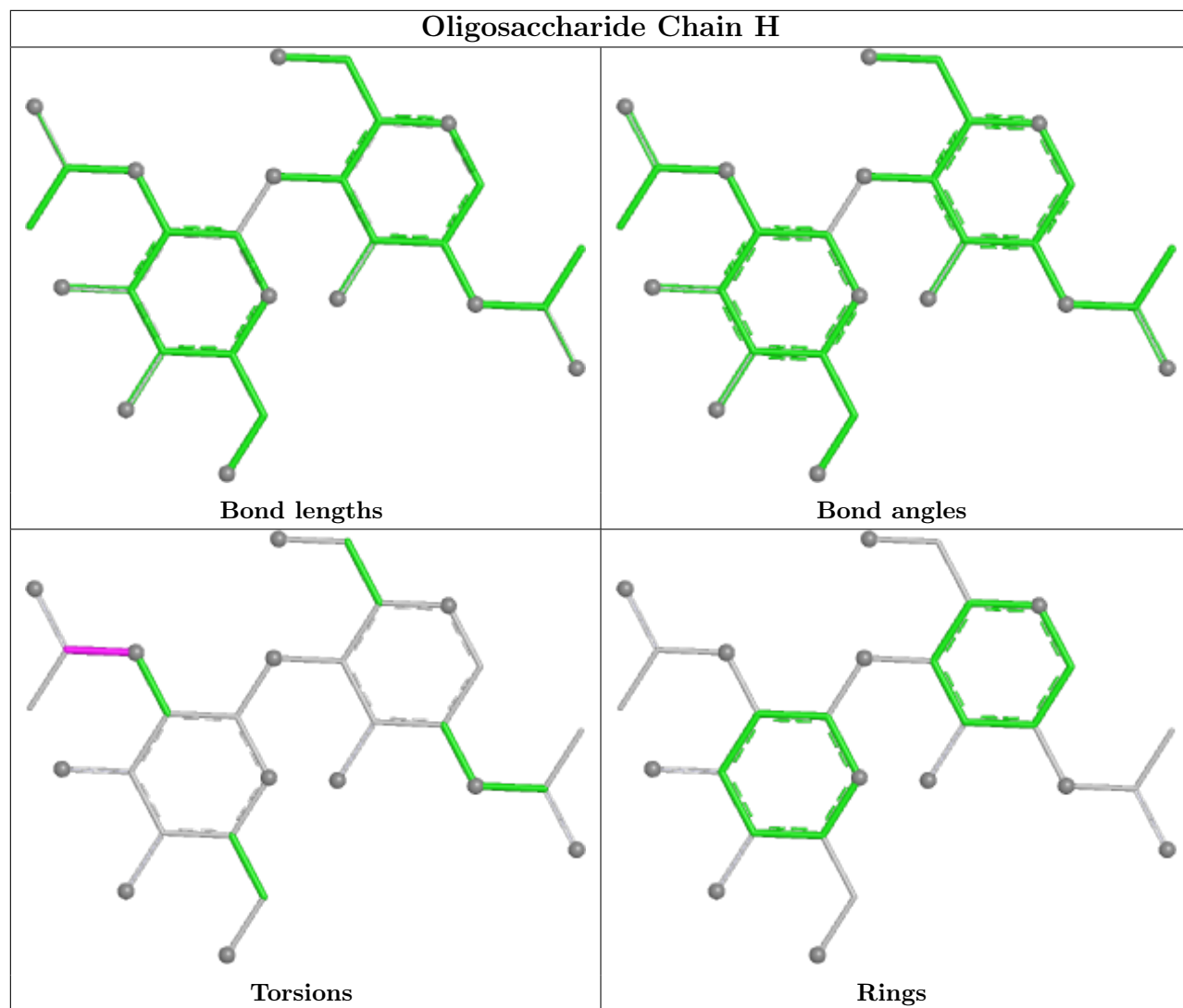
6 monomers are involved in 7 short contacts:

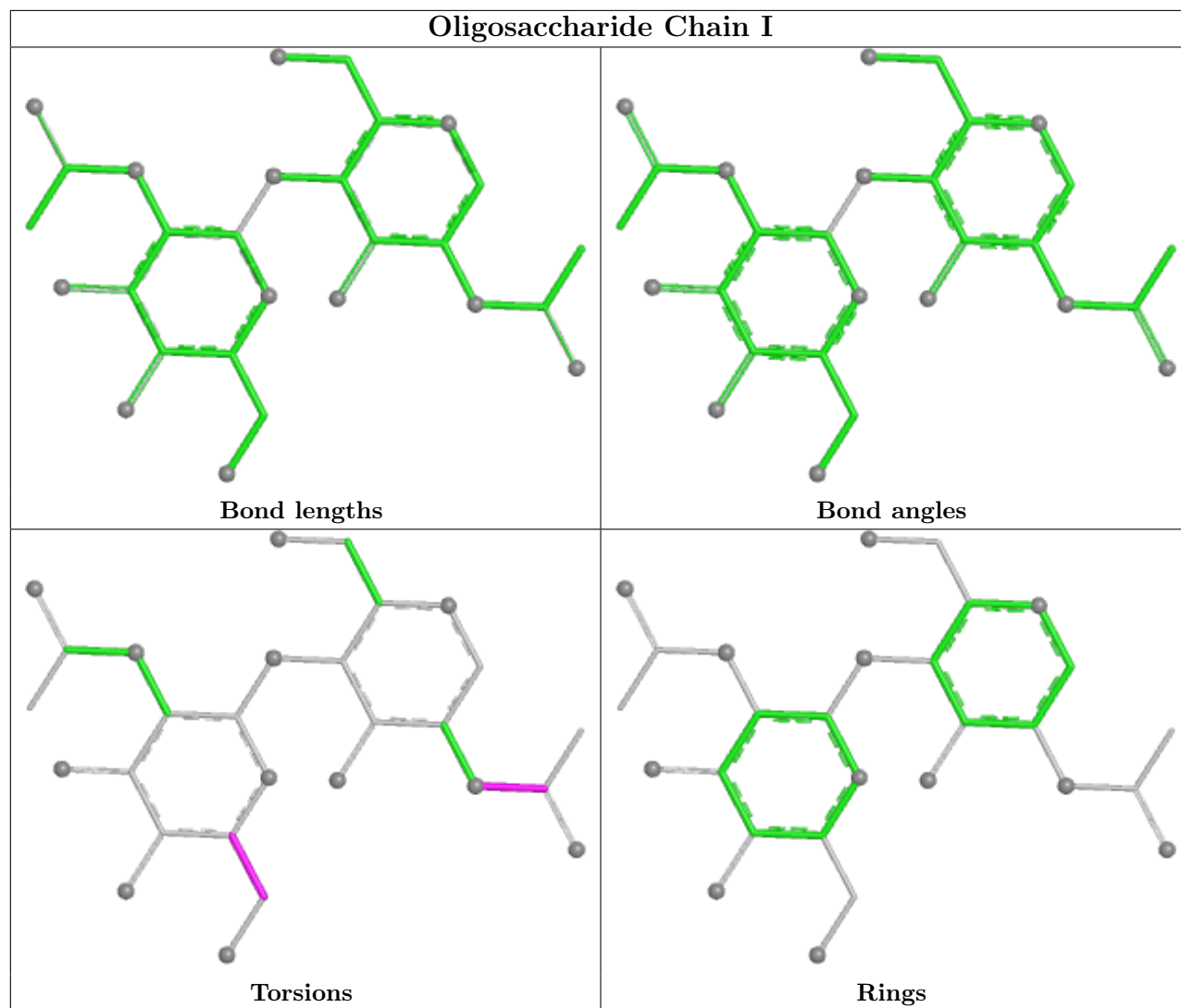
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	1	NAG	2	0
3	H	1	NAG	3	0
3	J	2	NAG	1	0
3	I	2	NAG	1	0
3	F	1	NAG	1	0
3	J	1	NAG	1	0

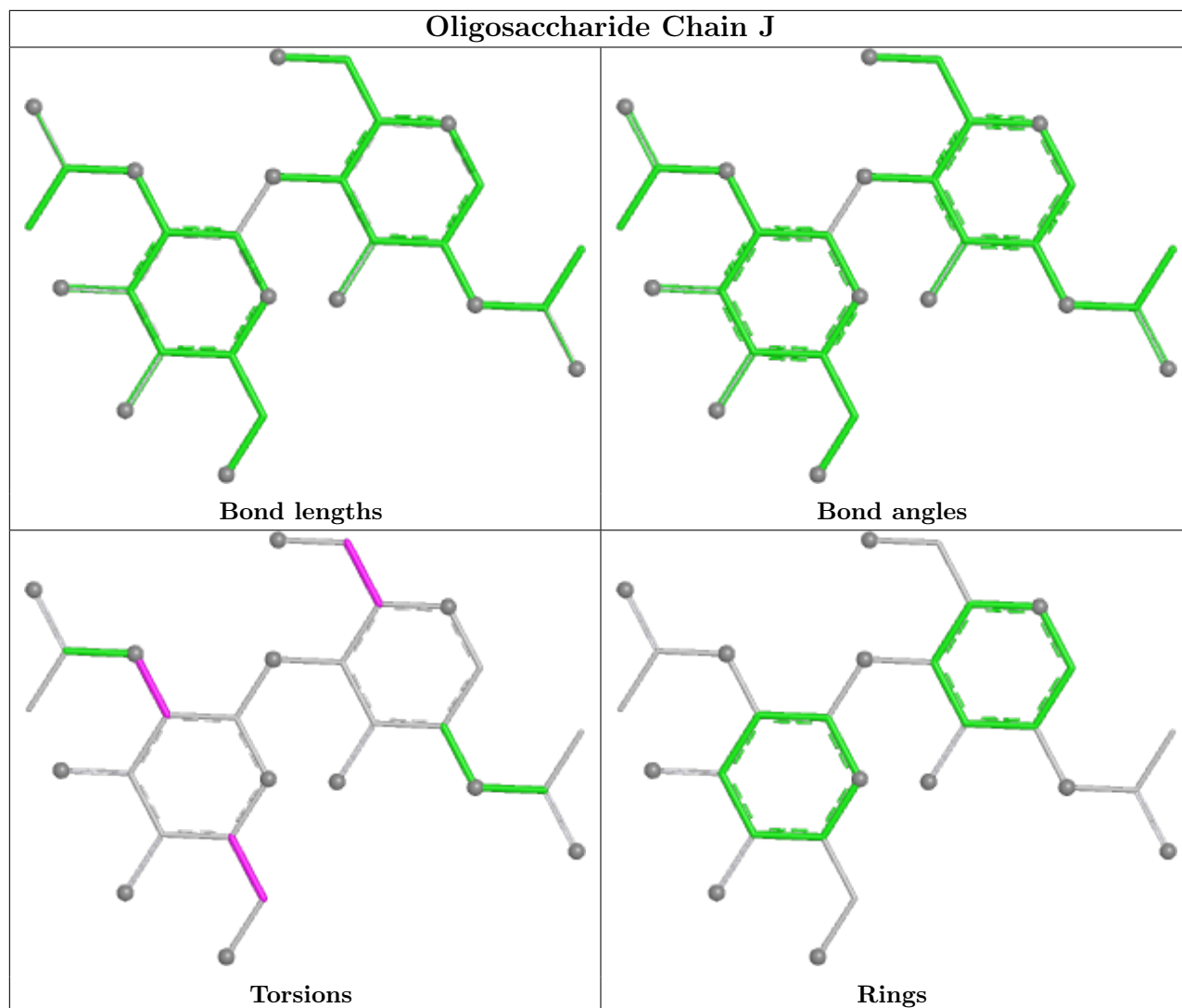
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

33 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	$\# Z > 2$
4	NAG	A	1307	1	14,14,15	0.49	0	17,19,21	0.83	1 (5%)
4	NAG	A	1312	-	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	B	1301	1	14,14,15	0.50	0	17,19,21	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1308	1	14,14,15	0.33	0	17,19,21	0.40	0
4	NAG	B	1312	1	14,14,15	0.23	0	17,19,21	0.49	0
4	NAG	A	1303	-	14,14,15	0.34	0	17,19,21	0.36	0
4	NAG	A	1310	1	14,14,15	0.27	0	17,19,21	0.35	0
4	NAG	A	1309	1	14,14,15	0.31	0	17,19,21	0.53	0
4	NAG	C	1302	1	14,14,15	0.24	0	17,19,21	0.44	0
4	NAG	B	1308	1	14,14,15	0.17	0	17,19,21	0.56	0
4	NAG	A	1304	1	14,14,15	0.29	0	17,19,21	0.37	0
4	NAG	B	1303	-	14,14,15	0.20	0	17,19,21	0.51	0
4	NAG	A	1305	-	14,14,15	0.17	0	17,19,21	0.47	0
4	NAG	B	1304	1	14,14,15	0.19	0	17,19,21	0.88	1 (5%)
4	NAG	A	1306	1	14,14,15	0.20	0	17,19,21	0.39	0
4	NAG	C	1303	1	14,14,15	0.17	0	17,19,21	0.42	0
4	NAG	B	1306	-	14,14,15	0.28	0	17,19,21	0.53	0
4	NAG	A	1301	-	14,14,15	0.21	0	17,19,21	0.46	0
4	NAG	B	1305	-	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	B	1309	1	14,14,15	0.28	0	17,19,21	0.36	0
4	NAG	B	1313	1	14,14,15	0.18	0	17,19,21	0.49	0
4	NAG	C	1305	1	14,14,15	0.29	0	17,19,21	0.61	0
4	NAG	A	1302	-	14,14,15	0.21	0	17,19,21	0.45	0
4	NAG	B	1311	1	14,14,15	0.26	0	17,19,21	0.52	0
4	NAG	B	1310	-	14,14,15	0.27	0	17,19,21	0.50	0
4	NAG	B	1302	-	14,14,15	0.22	0	17,19,21	0.45	0
4	NAG	B	1307	1	14,14,15	0.53	0	17,19,21	0.73	1 (5%)
4	NAG	C	1304	-	14,14,15	0.27	0	17,19,21	0.45	0
4	NAG	A	1313	1	14,14,15	0.16	0	17,19,21	0.61	0
4	NAG	C	1306	1	14,14,15	0.28	0	17,19,21	0.46	0
4	NAG	A	1311	1	14,14,15	0.38	0	17,19,21	0.51	0
4	NAG	A	1314	1	14,14,15	0.25	0	17,19,21	0.63	1 (5%)
4	NAG	C	1301	1	14,14,15	0.33	0	17,19,21	0.42	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	1307	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1312	-	-	3/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1312	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1303	-	-	4/6/23/26	0/1/1/1
4	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1303	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1305	-	-	4/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1306	-	-	1/6/23/26	0/1/1/1
4	NAG	A	1301	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1305	-	-	3/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1313	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1302	-	-	4/6/23/26	0/1/1/1
4	NAG	B	1311	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1310	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1302	-	-	4/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1304	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1313	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1314	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1307	NAG	C1-O5-C5	3.05	116.32	112.19
4	B	1304	NAG	C2-N2-C7	2.64	126.67	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1307	NAG	C1-O5-C5	2.52	115.61	112.19
4	A	1314	NAG	C1-O5-C5	2.07	115.00	112.19

There are no chirality outliers.

5 of 74 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1305	NAG	C3-C2-N2-C7
4	B	1306	NAG	C3-C2-N2-C7
4	C	1306	NAG	C3-C2-N2-C7
4	B	1313	NAG	O5-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6

There are no ring outliers.

15 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1301	NAG	3	0
4	A	1308	NAG	2	0
4	A	1310	NAG	2	0
4	A	1309	NAG	1	0
4	C	1302	NAG	1	0
4	B	1304	NAG	3	0
4	B	1306	NAG	1	0
4	B	1311	NAG	1	0
4	B	1310	NAG	1	0
4	B	1302	NAG	3	0
4	B	1307	NAG	1	0
4	A	1313	NAG	1	0
4	C	1306	NAG	2	0
4	A	1311	NAG	2	0
4	C	1301	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
1	C	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	528:LYS	C	529:LYS	N	5.56
1	A	458:LYS	C	459[B]:SER	N	3.08
1	A	458:LYS	C	459[A]:SER	N	3.03
1	B	481:ASN	C	482:GLY	N	2.95

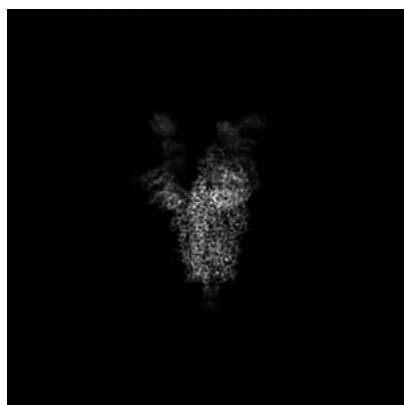
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14313. These allow visual inspection of the internal detail of the map and identification of artifacts.

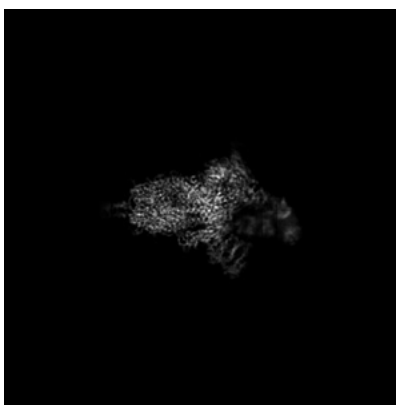
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

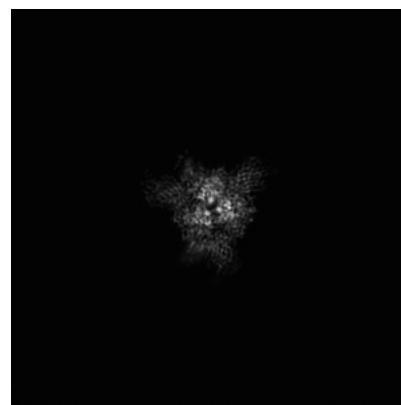
6.1.1 Primary map



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: 246



Y Index: 246



Z Index: 246

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: 243



Y Index: 240

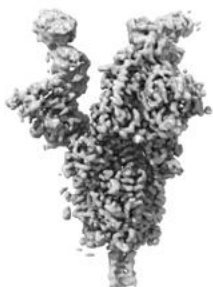


Z Index: 253

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 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

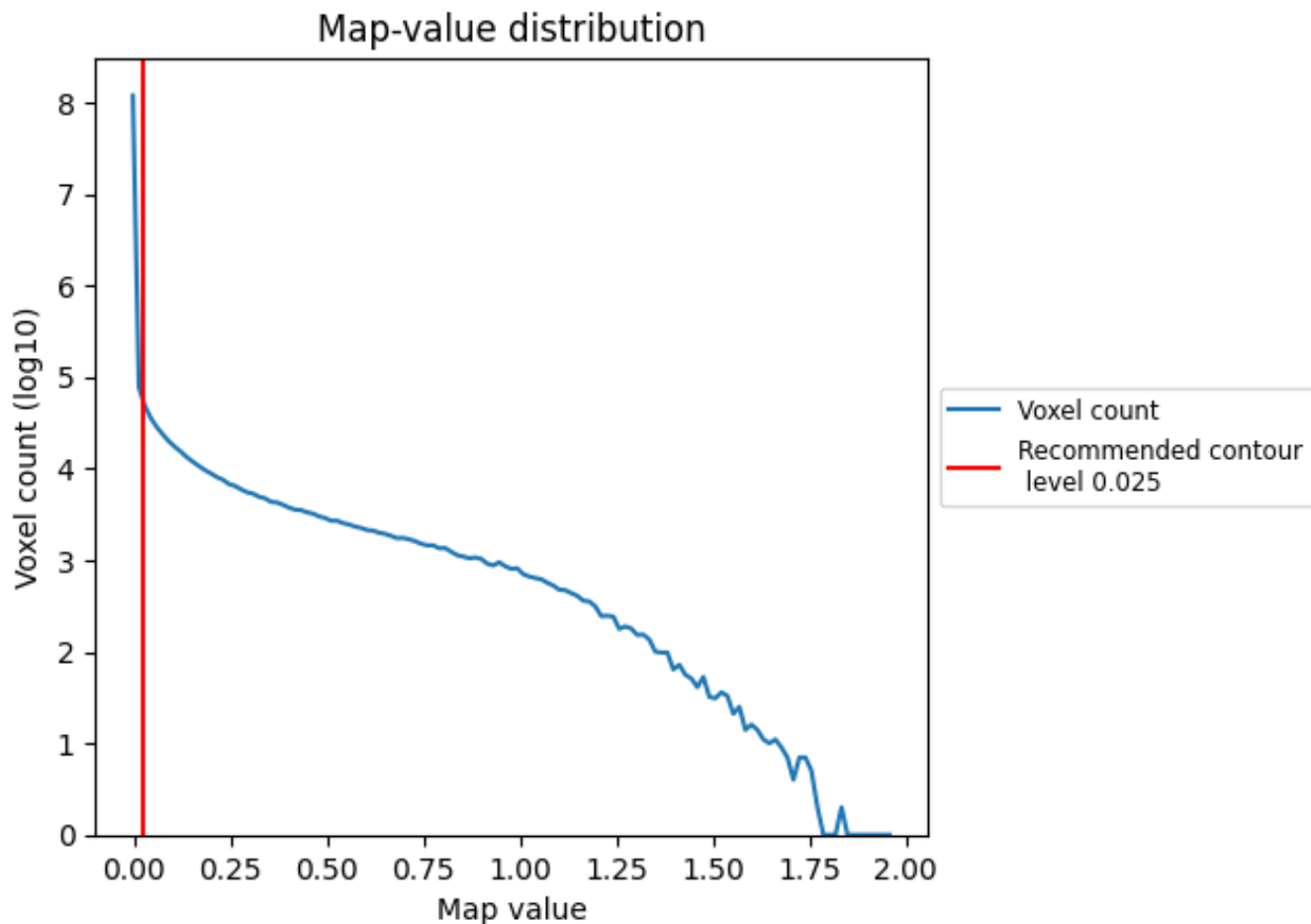
6.5 Mask visualisation

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

7 Map analysis [i](#)

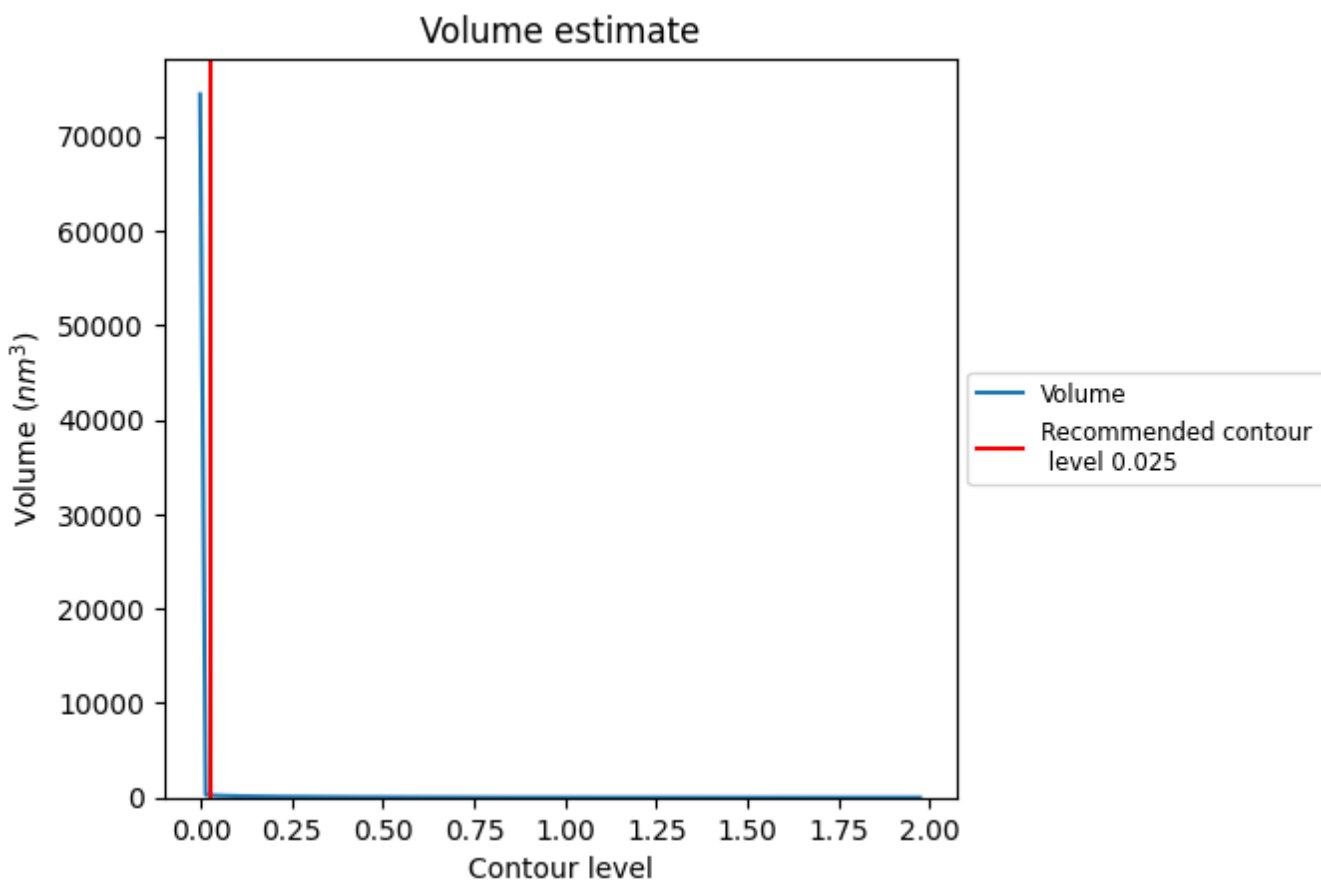
This section contains the results of statistical analysis of the map.

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.

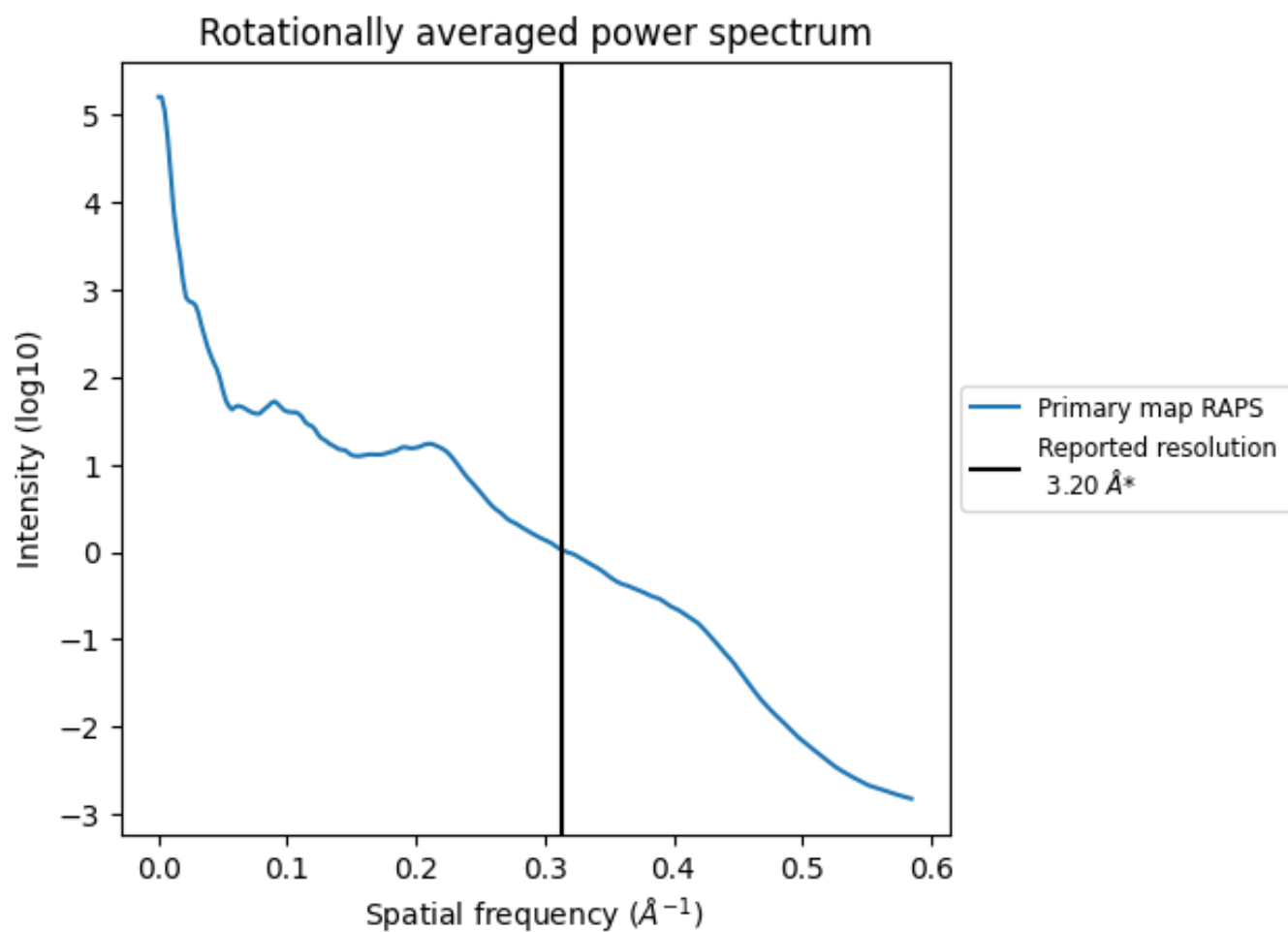
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 259 nm^3 ; this corresponds to an approximate mass of 234 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](#)

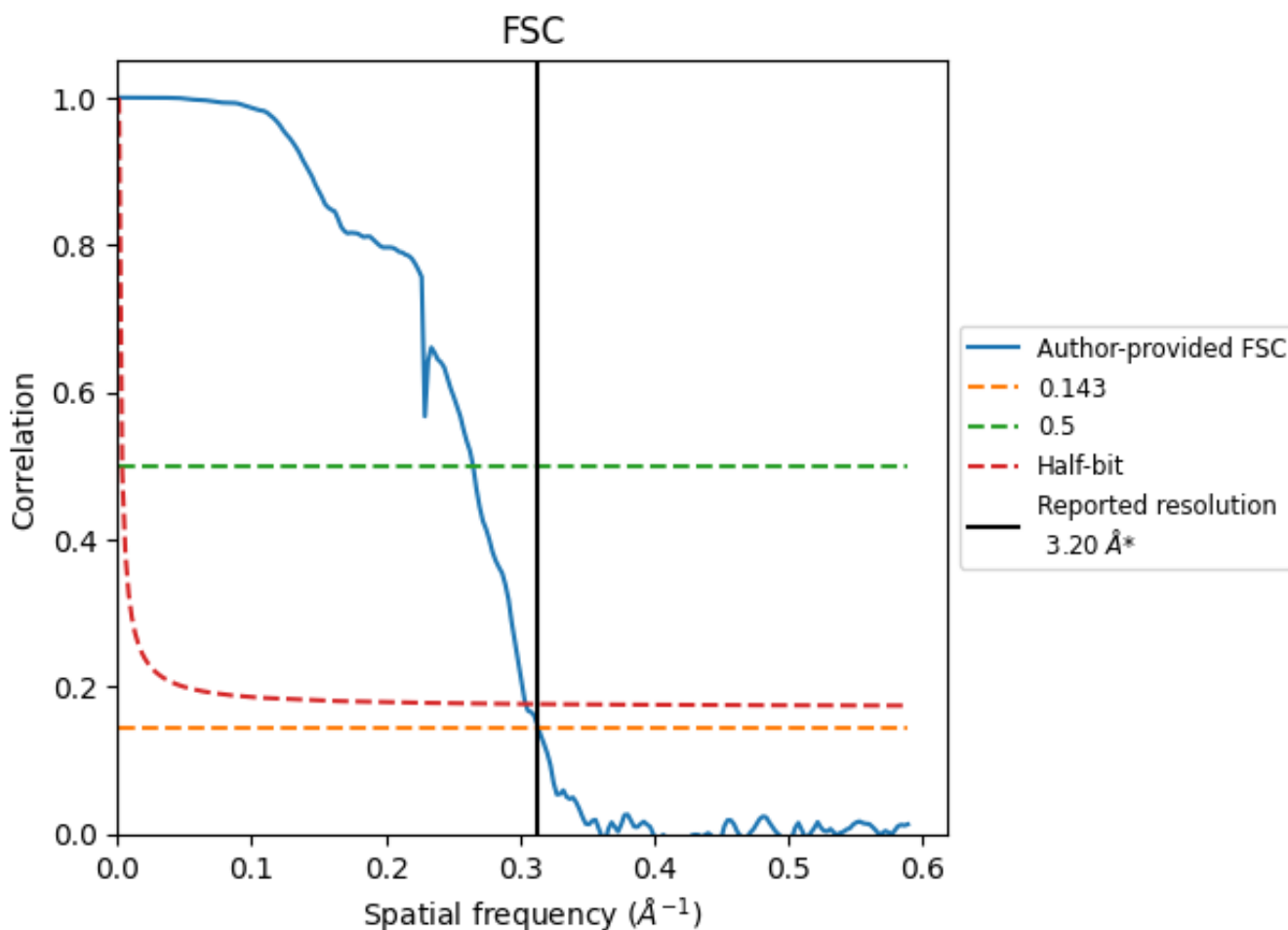


*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

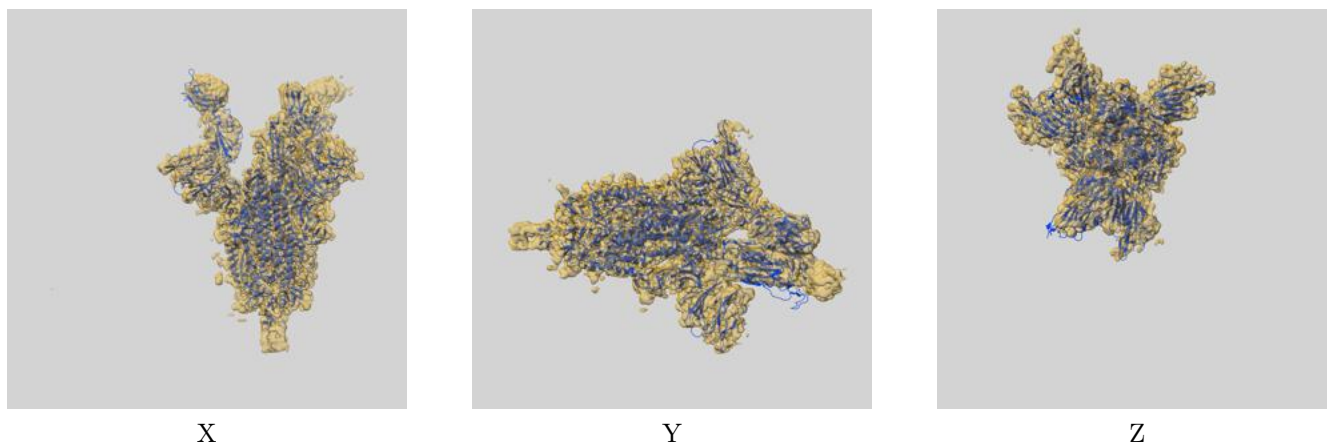
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.19	3.77	3.29
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

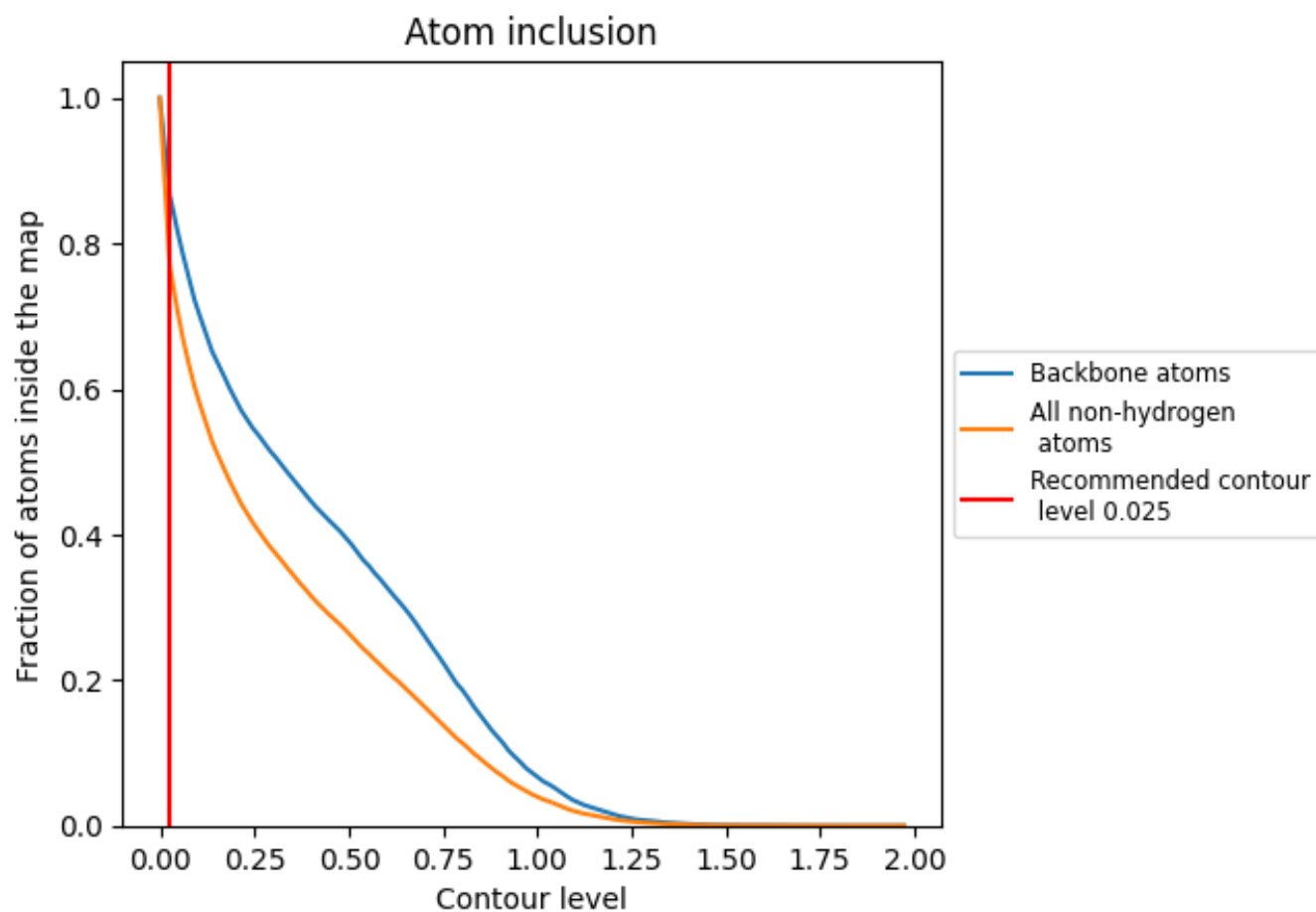
This section contains information regarding the fit between EMDB map EMD-14313 and PDB model 7R4I. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.025 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 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.