



## Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 02:01 PM JST

PDB ID : 7WPE  
EMDB ID : EMD-32684  
Title : SARS-CoV-2 Omicron Variant S Trimer complexed with two JMB2002 Fab  
Authors : Yin, W.; Xu, Y.; Xu, P.; Cao, X.; Wu, C.; Gu, C.; He, X.; Wang, X.; Huang, S.; Yuan, Q.; Wu, K.; Hu, W.; Huang, Z.; Liu, J.; Wang, Z.; Jia, F.; Xia, K.; Liu, P.; Wang, X.; Song, B.; Zheng, J.; Jiang, H.; Cheng, X.; Jiang, Y.; Deng, S.J.; Xu, H.E.  
Deposited on : 2022-01-23  
Resolution : 2.69 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](mailto: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>.

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

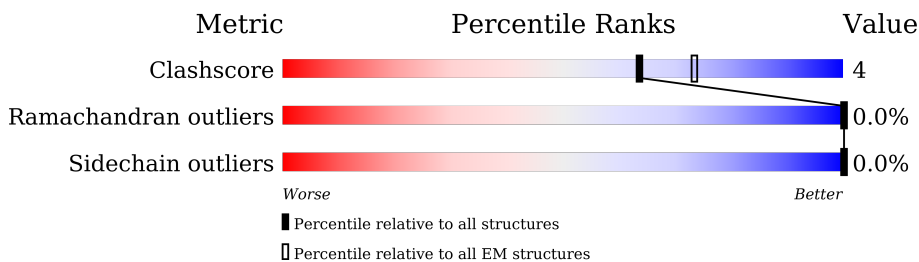
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.69 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  $\geq 3$ , 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	1205	
1	B	1205	
1	C	1205	
2	U	237	
2	X	237	
3	V	215	
3	Y	215	
4	W	133	

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Mol	Chain	Length	Quality of chain
4	Z	133	<p>62% 72% 17% 10%</p>
5	D	2	<p>50% 100%</p>
5	E	2	<p>100%</p>

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 32038 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1021	7701	4958	1277	1431	35	0	0
1	B	1024	7681	4922	1278	1447	34	0	0
1	C	1024	7642	4912	1267	1429	34	0	0

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	212	ILE	LEU	variant	UNP P0DTC2
A	215	GLU	-	insertion	UNP P0DTC2
A	216	PRO	-	insertion	UNP P0DTC2
A	217	GLU	-	insertion	UNP P0DTC2
A	342	ASP	GLY	variant	UNP P0DTC2
A	374	LEU	SER	variant	UNP P0DTC2
A	376	PRO	SER	variant	UNP P0DTC2
A	378	PHE	SER	variant	UNP P0DTC2
A	420	ASN	LYS	variant	UNP P0DTC2
A	443	LYS	ASN	variant	UNP P0DTC2
A	449	SER	GLY	variant	UNP P0DTC2
A	480	ASN	SER	variant	UNP P0DTC2
A	481	LYS	THR	variant	UNP P0DTC2
A	487	ALA	GLU	variant	UNP P0DTC2
A	496	ARG	GLN	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	499	SER	GLY	variant	UNP P0DTC2
A	501	ARG	GLN	variant	UNP P0DTC2
A	504	TYR	ASN	variant	UNP P0DTC2
A	508	HIS	TYR	variant	UNP P0DTC2
A	550	LYS	THR	variant	UNP P0DTC2
A	617	GLY	ASP	variant	UNP P0DTC2
A	658	TYR	HIS	variant	UNP P0DTC2
A	682	LYS	ASN	variant	UNP P0DTC2
A	684	HIS	PRO	variant	UNP P0DTC2
A	685	GLY	ARG	engineered mutation	UNP P0DTC2
A	686	SER	ARG	engineered mutation	UNP P0DTC2
A	688	SER	ARG	engineered mutation	UNP P0DTC2
A	767	LYS	ASN	variant	UNP P0DTC2
A	799	TYR	ASP	variant	UNP P0DTC2
A	859	LYS	ASN	variant	UNP P0DTC2
A	957	HIS	GLN	variant	UNP P0DTC2
A	972	LYS	ASN	variant	UNP P0DTC2
A	984	PHE	LEU	variant	UNP P0DTC2
A	989	PRO	LYS	engineered mutation	UNP P0DTC2
A	990	PRO	VAL	engineered mutation	UNP P0DTC2
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	212	ILE	LEU	variant	UNP P0DTC2
B	215	GLU	-	insertion	UNP P0DTC2
B	216	PRO	-	insertion	UNP P0DTC2
B	217	GLU	-	insertion	UNP P0DTC2
B	342	ASP	GLY	variant	UNP P0DTC2
B	374	LEU	SER	variant	UNP P0DTC2
B	376	PRO	SER	variant	UNP P0DTC2
B	378	PHE	SER	variant	UNP P0DTC2
B	420	ASN	LYS	variant	UNP P0DTC2
B	443	LYS	ASN	variant	UNP P0DTC2
B	449	SER	GLY	variant	UNP P0DTC2
B	480	ASN	SER	variant	UNP P0DTC2
B	481	LYS	THR	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	487	ALA	GLU	variant	UNP P0DTC2
B	496	ARG	GLN	engineered mutation	UNP P0DTC2
B	499	SER	GLY	variant	UNP P0DTC2
B	501	ARG	GLN	variant	UNP P0DTC2
B	504	TYR	ASN	variant	UNP P0DTC2
B	508	HIS	TYR	variant	UNP P0DTC2
B	550	LYS	THR	variant	UNP P0DTC2
B	617	GLY	ASP	variant	UNP P0DTC2
B	658	TYR	HIS	variant	UNP P0DTC2
B	682	LYS	ASN	variant	UNP P0DTC2
B	684	HIS	PRO	variant	UNP P0DTC2
B	685	GLY	ARG	engineered mutation	UNP P0DTC2
B	686	SER	ARG	engineered mutation	UNP P0DTC2
B	688	SER	ARG	engineered mutation	UNP P0DTC2
B	767	LYS	ASN	variant	UNP P0DTC2
B	799	TYR	ASP	variant	UNP P0DTC2
B	859	LYS	ASN	variant	UNP P0DTC2
B	957	HIS	GLN	variant	UNP P0DTC2
B	972	LYS	ASN	variant	UNP P0DTC2
B	984	PHE	LEU	variant	UNP P0DTC2
B	989	PRO	LYS	engineered mutation	UNP P0DTC2
B	990	PRO	VAL	engineered mutation	UNP P0DTC2
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	212	ILE	LEU	variant	UNP P0DTC2
C	215	GLU	-	insertion	UNP P0DTC2
C	216	PRO	-	insertion	UNP P0DTC2
C	217	GLU	-	insertion	UNP P0DTC2
C	342	ASP	GLY	variant	UNP P0DTC2
C	374	LEU	SER	variant	UNP P0DTC2
C	376	PRO	SER	variant	UNP P0DTC2
C	378	PHE	SER	variant	UNP P0DTC2
C	420	ASN	LYS	variant	UNP P0DTC2
C	443	LYS	ASN	variant	UNP P0DTC2
C	449	SER	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	480	ASN	SER	variant	UNP P0DTC2
C	481	LYS	THR	variant	UNP P0DTC2
C	487	ALA	GLU	variant	UNP P0DTC2
C	496	ARG	GLN	engineered mutation	UNP P0DTC2
C	499	SER	GLY	variant	UNP P0DTC2
C	501	ARG	GLN	variant	UNP P0DTC2
C	504	TYR	ASN	variant	UNP P0DTC2
C	508	HIS	TYR	variant	UNP P0DTC2
C	550	LYS	THR	variant	UNP P0DTC2
C	617	GLY	ASP	variant	UNP P0DTC2
C	658	TYR	HIS	variant	UNP P0DTC2
C	682	LYS	ASN	variant	UNP P0DTC2
C	684	HIS	PRO	variant	UNP P0DTC2
C	685	GLY	ARG	engineered mutation	UNP P0DTC2
C	686	SER	ARG	engineered mutation	UNP P0DTC2
C	688	SER	ARG	engineered mutation	UNP P0DTC2
C	767	LYS	ASN	variant	UNP P0DTC2
C	799	TYR	ASP	variant	UNP P0DTC2
C	859	LYS	ASN	variant	UNP P0DTC2
C	957	HIS	GLN	variant	UNP P0DTC2
C	972	LYS	ASN	variant	UNP P0DTC2
C	984	PHE	LEU	variant	UNP P0DTC2
C	989	PRO	LYS	engineered mutation	UNP P0DTC2
C	990	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called JMB2002 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	X	225	Total	C	N	O	S	0	0
			1665	1050	274	334	7		
2	U	225	Total	C	N	O	S	0	0
			1665	1050	274	334	7		

- Molecule 3 is a protein called JMB2002 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Y	214	Total	C	N	O	S	0	0
			1637	1024	273	335	5		
3	V	214	Total	C	N	O	S	0	0
			1637	1024	273	335	5		

- Molecule 4 is a protein called Anti-Fab nanobody.

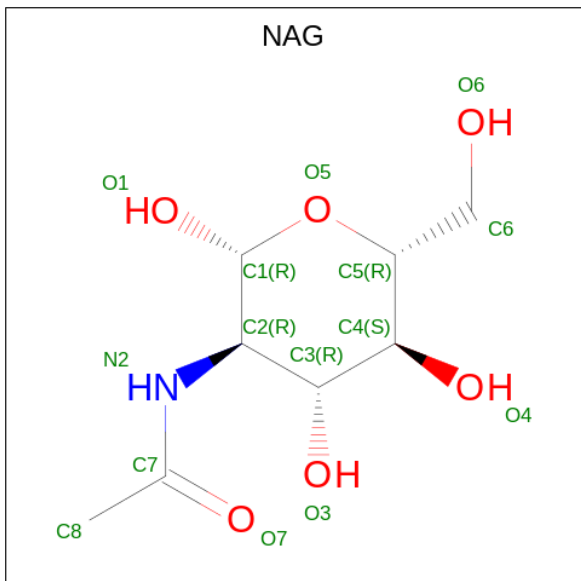
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	Z	120	Total 925	C 574	N 163	O 184	S 4	0	0
4	W	120	Total 925	C 574	N 163	O 184	S 4	0	0

- 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	N	O		
5	D	2	Total 28	C 16	N 2	O 10	0	0
5	E	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	A	1	Total 168	C 96	N 12	O 60	0
6	A	1	Total 168	C 96	N 12	O 60	0

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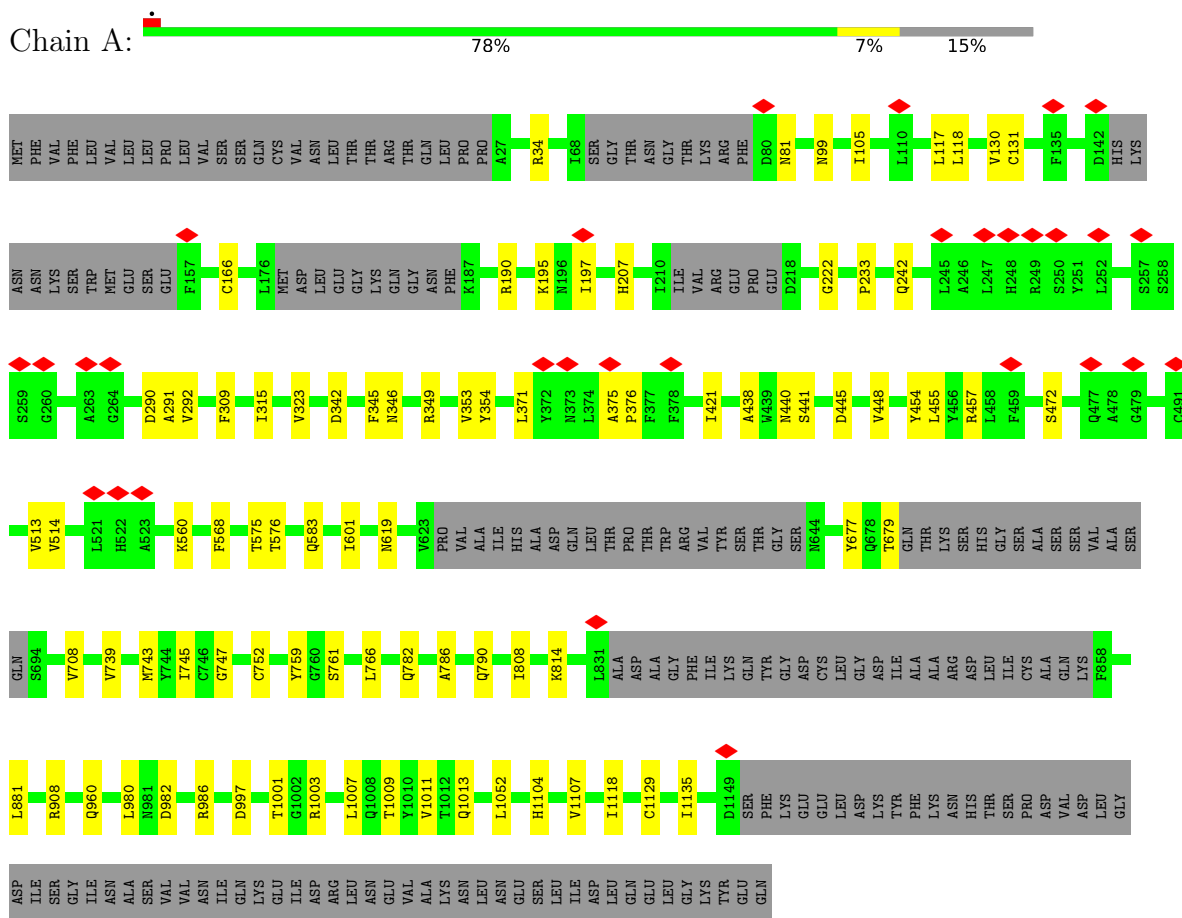
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	B	1	Total 168	C 96	N 12	O 60	0
6	C	1	Total 168	C 96	N 12	O 60	0
6	C	1	Total 168	C 96	N 12	O 60	0
6	C	1	Total 168	C 96	N 12	O 60	0
6	C	1	Total 168	C 96	N 12	O 60	0
6	C	1	Total 168	C 96	N 12	O 60	0
6	C	1	Total 168	C 96	N 12	O 60	0
6	C	1	Total 168	C 96	N 12	O 60	0
6	C	1	Total 168	C 96	N 12	O 60	0
6	C	1	Total 168	C 96	N 12	O 60	0
6	C	1	Total 168	C 96	N 12	O 60	0
6	C	1	Total 168	C 96	N 12	O 60	0
6	C	1	Total 168	C 96	N 12	O 60	0
6	C	1	Total 168	C 96	N 12	O 60	0

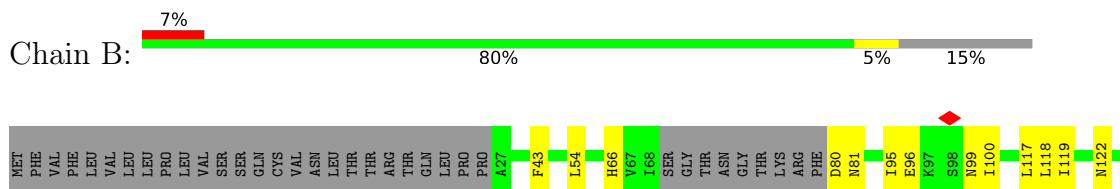
### 3 Residue-property plots

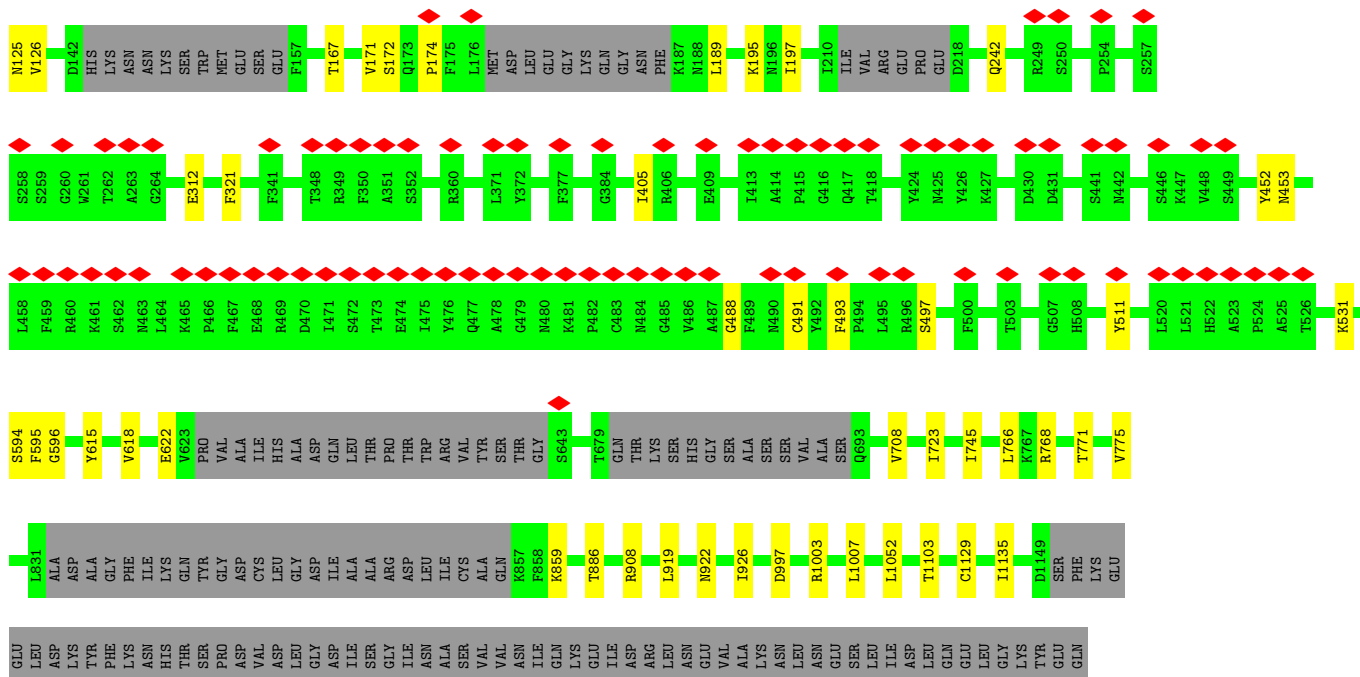
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Spike glycoprotein

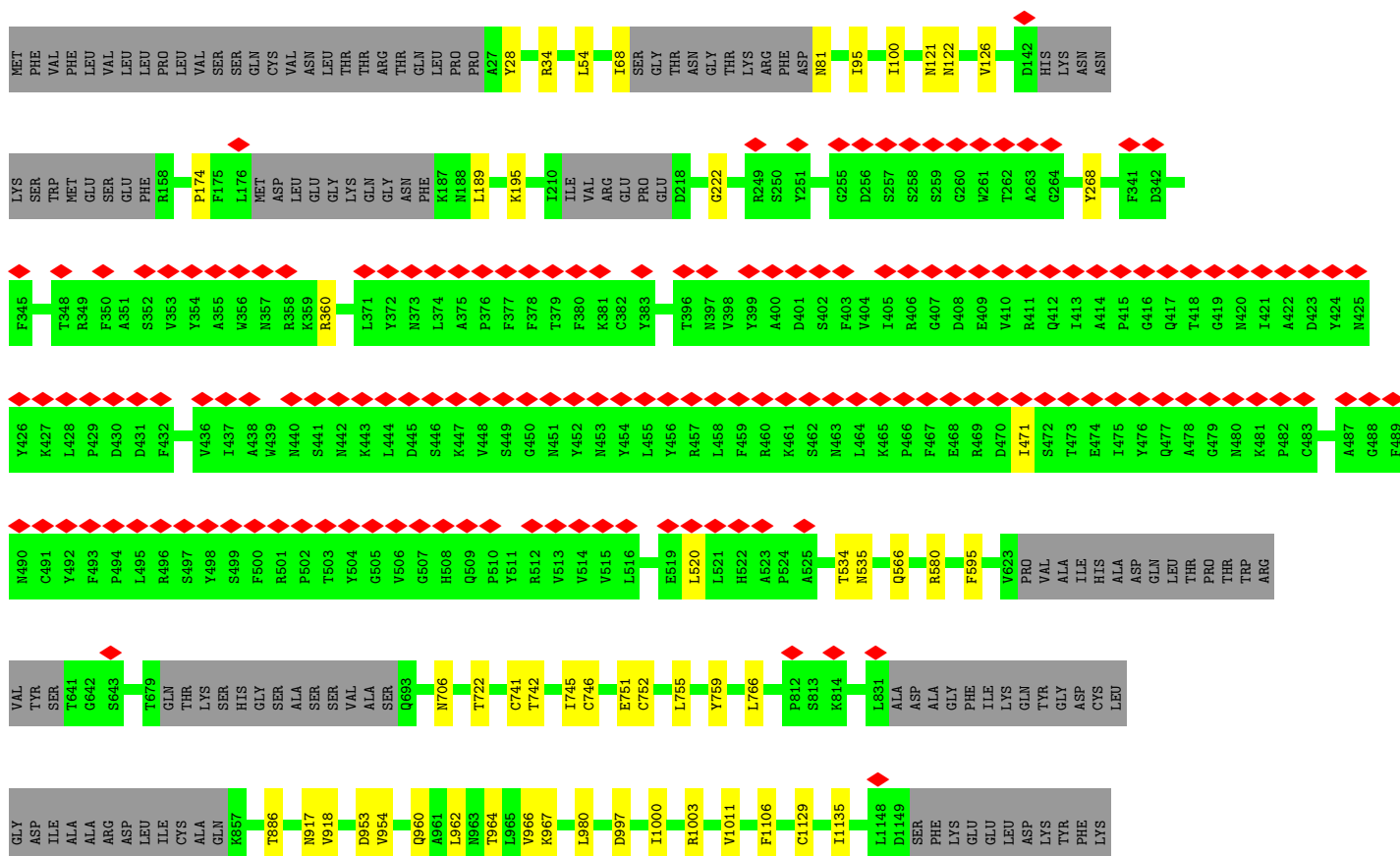
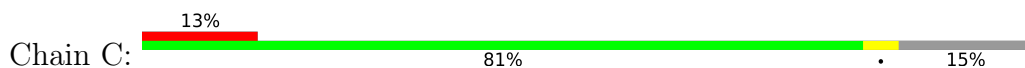


- Molecule 1: Spike glycoprotein



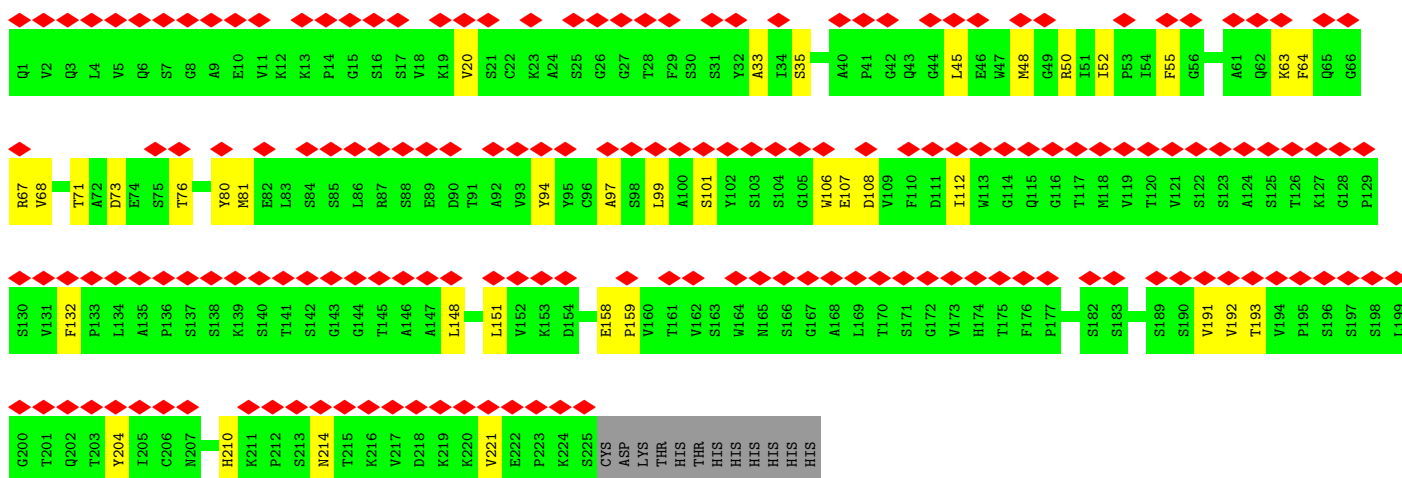
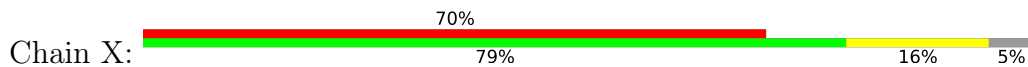


• Molecule 1: Spike glycoprotein

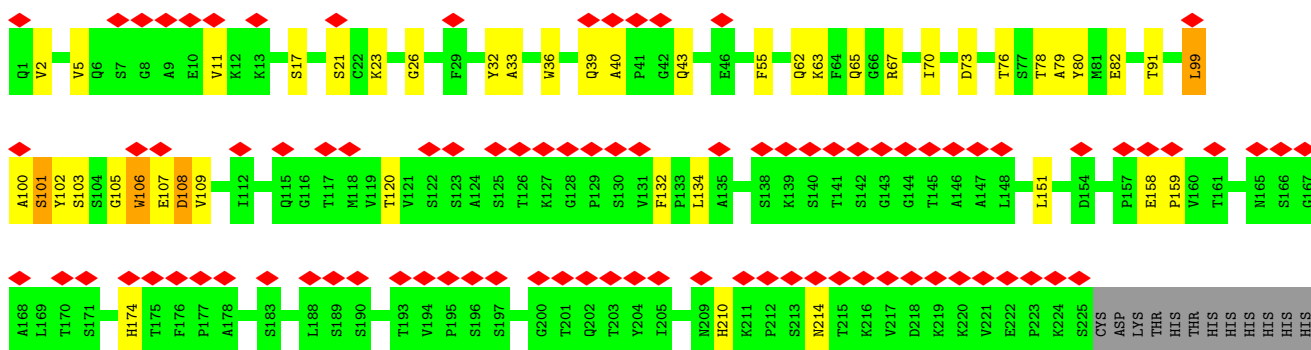
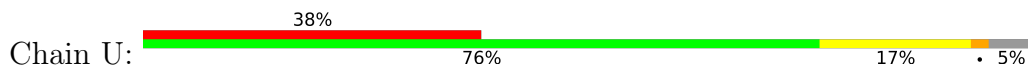


ASN HIS THR SER PRO ASP VAL LEU ASP ASP SER GLY ILE ILE ILE ASN ALA VAL VAL ASN ASN GLN LYS LYS ILE ASP ARG LEU LEU ASN ASN GLU VAL VAL ALA LYS ASN LEU LEU LEU SER LEU ILE ASP GLN GLU GLU GLY LYS LYS TVR GLU GLN

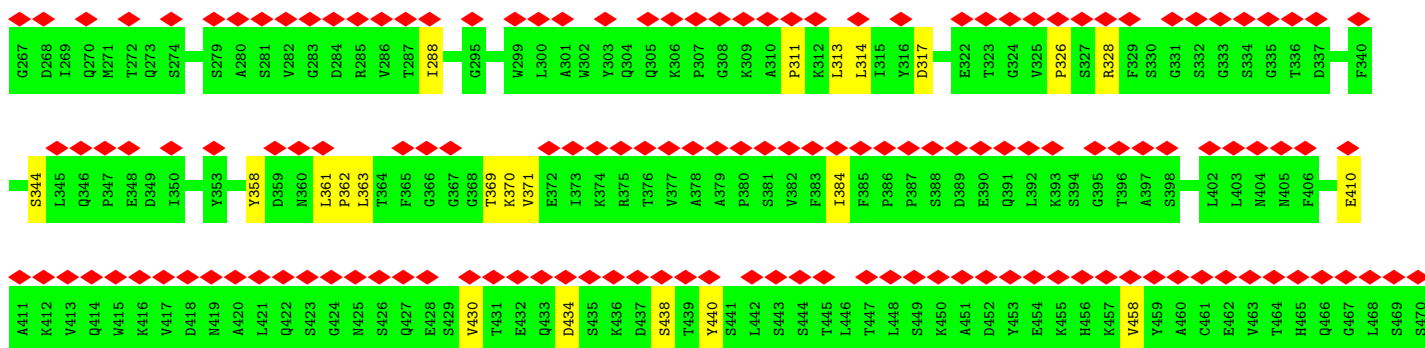
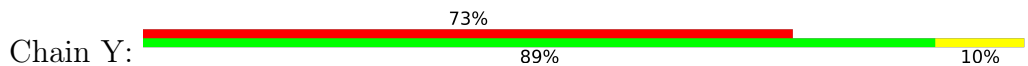
• Molecule 2: JMB2002 Fab heavy chain

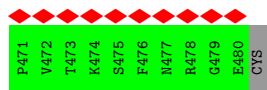


• Molecule 2: JMB2002 Fab heavy chain

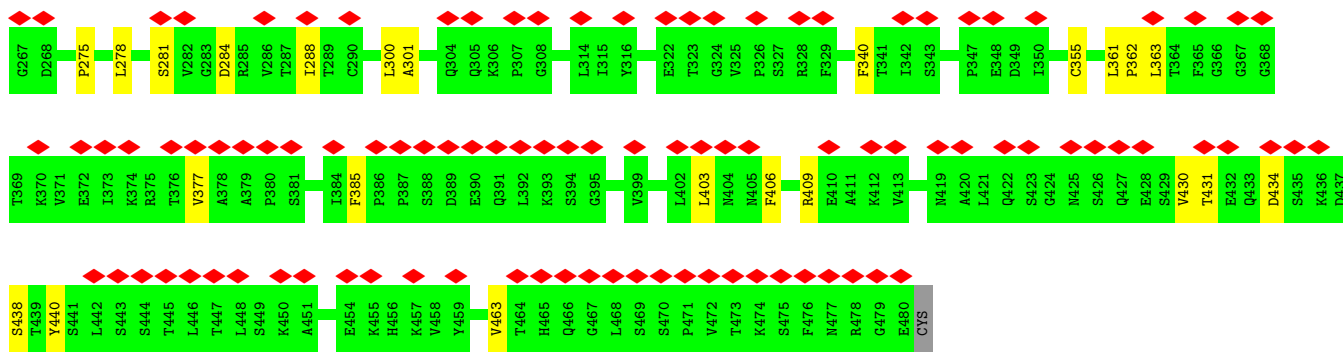
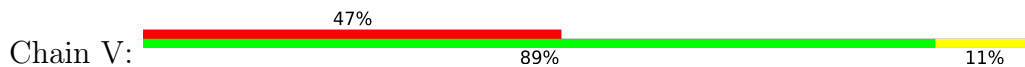


• Molecule 3: JMB2002 Fab light chain

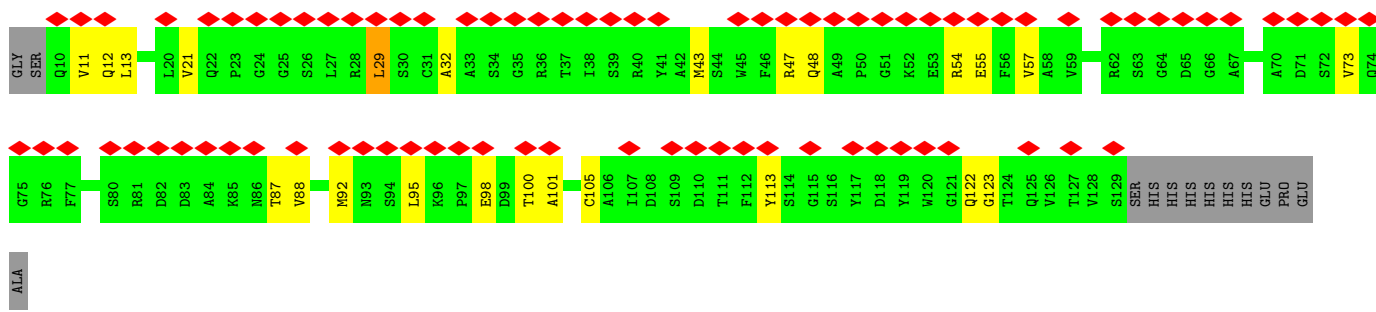




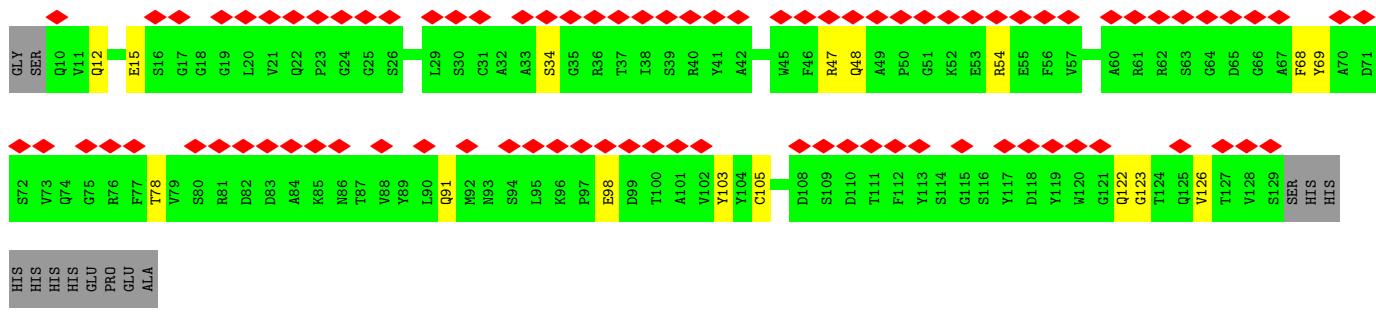
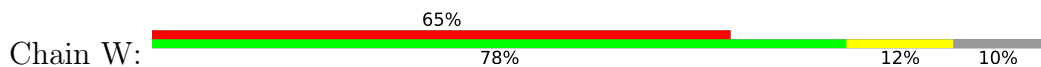
• Molecule 3: JMB2002 Fab light chain



• Molecule 4: Anti-Fab nanobody



• Molecule 4: Anti-Fab nanobody



• 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-glucofuranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	906588	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.798	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.0428	Depositor
Map size ( $\text{\AA}$ )	395.52, 395.52, 395.52	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.824, 0.824, 0.824	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	0.25	0/7885	0.47	0/10767
1	B	0.25	0/7861	0.47	0/10741
1	C	0.25	0/7823	0.47	0/10700
2	U	0.30	0/1704	0.50	0/2321
2	X	0.26	0/1704	0.62	2/2321 (0.1%)
3	V	0.25	0/1672	0.44	0/2271
3	Y	0.27	0/1672	0.54	3/2271 (0.1%)
4	W	0.25	0/944	0.47	0/1276
4	Z	0.26	0/944	0.56	2/1276 (0.2%)
All	All	0.26	0/32209	0.48	7/43944 (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
2	U	0	1
2	X	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	191	VAL	CG1-CB-CG2	6.84	121.85	110.90
3	Y	458	VAL	CG1-CB-CG2	6.82	121.81	110.90
3	Y	384	ILE	CG1-CB-CG2	6.76	126.27	111.40
2	X	112	ILE	CG1-CB-CG2	6.50	125.71	111.40
4	Z	29	LEU	CB-CG-CD2	6.21	121.56	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	326	PRO	CA-N-CD	-5.38	103.96	111.50
4	Z	29	LEU	CB-CG-CD1	5.23	119.90	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	U	99	LEU	Mainchain
2	X	106	TRP	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7701	0	7278	70	0
1	B	7681	0	7202	62	0
1	C	7642	0	7169	40	0
2	U	1665	0	1635	37	0
2	X	1665	0	1635	31	0
3	V	1637	0	1584	17	0
3	Y	1637	0	1584	14	0
4	W	925	0	870	9	0
4	Z	925	0	870	16	0
5	D	28	0	25	0	0
5	E	28	0	25	0	0
6	A	168	0	156	3	0
6	B	168	0	156	2	0
6	C	168	0	156	2	0
All	All	32038	0	30345	267	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 (267) 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:X:63:LYS:O	2:X:67:ARG:NH2	1.98	0.97
1:A:190:ARG:HG3	1:A:207:HIS:CD2	2.02	0.93
1:C:95:ILE:HG22	1:C:95:ILE:O	1.72	0.89
2:U:17:SER:OG	2:U:82:GLU:OE2	1.89	0.89
4:W:47:ARG:NH1	4:W:98:GLU:O	2.08	0.86
2:U:100:ALA:HB1	2:U:107:GLU:O	1.76	0.83
2:U:63:LYS:O	2:U:67:ARG:NH1	2.12	0.83
2:U:101:SER:HB3	2:U:108:ASP:N	1.95	0.82
4:W:12:GLN:NE2	4:W:34:SER:O	2.14	0.81
2:U:103:SER:HB2	2:U:106:TRP:CD1	2.16	0.80
1:A:759:TYR:OH	1:A:997:ASP:OD1	1.99	0.80
1:A:195:LYS:CE	1:A:197:ILE:HD11	2.13	0.79
3:Y:328:ARG:NH2	3:Y:344:SER:O	2.16	0.78
1:B:195:LYS:HD2	1:B:197:ILE:CD1	2.15	0.76
1:B:321:PHE:CE2	1:B:615:TYR:HD1	2.03	0.76
4:W:48:GLN:OE1	4:W:54:ARG:NH2	2.19	0.76
3:V:281:SER:OG	3:V:284:ASP:OD2	2.04	0.74
1:B:453:ASN:ND2	2:X:107:GLU:OE1	2.20	0.73
1:A:195:LYS:HE2	1:A:197:ILE:HD11	1.71	0.73
1:A:195:LYS:CE	1:A:197:ILE:CD1	2.65	0.73
1:B:96:GLU:N	1:B:96:GLU:OE1	2.22	0.73
1:B:195:LYS:CD	1:B:197:ILE:HD13	2.20	0.71
4:W:122:GLN:NE2	4:W:123:GLY:O	2.23	0.71
2:U:91:THR:HG23	2:U:120:THR:HA	1.71	0.71
4:Z:29:LEU:HG	4:Z:92:MET:HE1	1.74	0.70
1:A:195:LYS:HE2	1:A:197:ILE:CD1	2.23	0.68
2:X:45:LEU:HD11	3:Y:311:PRO:HG2	1.73	0.68
1:A:290:ASP:OD1	1:A:291:ALA:N	2.27	0.67
1:A:233:PRO:O	1:C:360:ARG:NH1	2.28	0.67
1:B:81:ASN:O	1:B:81:ASN:OD1	2.13	0.67
1:C:917:ASN:OD1	1:C:918:VAL:N	2.27	0.67
3:V:409:ARG:HH22	3:V:430:VAL:HG11	1.61	0.66
2:X:45:LEU:HD11	3:Y:311:PRO:CG	2.26	0.66
1:C:953:ASP:OD1	1:C:954:VAL:N	2.28	0.66
2:U:40:ALA:HB3	2:U:43:GLN:NE2	2.11	0.65
1:B:126:VAL:HG23	1:B:174:PRO:HA	1.77	0.65
1:A:131:CYS:HA	1:A:166:CYS:CB	2.27	0.65
1:A:195:LYS:HE3	1:A:197:ILE:HD13	1.79	0.64
1:B:321:PHE:CZ	1:B:618:VAL:HG21	2.33	0.64
1:A:34:ARG:NH1	1:A:222:GLY:O	2.31	0.64
2:X:192:VAL:HG11	2:X:204:TYR:CZ	2.33	0.64
2:U:55:PHE:CE2	2:U:102:TYR:HE1	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Z:122:GLN:NE2	4:Z:123:GLY:O	2.30	0.63
2:X:33:ALA:O	2:X:99:LEU:N	2.31	0.63
1:A:195:LYS:HE3	1:A:197:ILE:CD1	2.28	0.63
1:B:312:GLU:OE1	1:B:312:GLU:N	2.31	0.63
1:B:195:LYS:HD3	1:B:197:ILE:HD13	1.80	0.63
1:A:619:ASN:OD1	6:A:1309:NAG:N2	2.32	0.62
1:C:95:ILE:O	1:C:95:ILE:CG2	2.45	0.62
3:Y:434:ASP:O	3:Y:438:SER:N	2.33	0.62
3:V:300:LEU:HD12	3:V:301:ALA:H	1.65	0.61
1:B:723:ILE:CD1	1:B:926:ILE:HG23	2.31	0.61
1:C:121:ASN:ND2	1:C:122:ASN:O	2.34	0.61
1:A:457:ARG:NH2	1:A:472:SER:O	2.34	0.60
2:X:35:SER:N	2:X:97:ALA:O	2.34	0.60
4:Z:29:LEU:HG	4:Z:92:MET:CE	2.30	0.60
2:X:50:ARG:NH2	2:X:52:ILE:HD11	2.16	0.60
2:U:62:GLN:OE1	2:U:65:GLN:NE2	2.34	0.60
1:B:723:ILE:HD12	1:B:926:ILE:HG23	1.84	0.60
2:U:101:SER:HB3	2:U:108:ASP:CA	2.31	0.60
1:C:745:ILE:O	1:C:1003:ARG:NH1	2.30	0.59
1:A:342:ASP:OD1	1:A:346:ASN:ND2	2.33	0.59
2:U:103:SER:HB2	2:U:106:TRP:NE1	2.18	0.59
1:B:195:LYS:CD	1:B:197:ILE:CD1	2.81	0.59
1:B:493:PHE:CE2	2:X:55:PHE:HE1	2.20	0.59
1:A:117:LEU:HD13	1:A:118:LEU:N	2.17	0.59
1:B:493:PHE:CE2	2:X:55:PHE:CE1	2.90	0.59
1:A:583:GLN:O	6:A:1302:NAG:H82	2.02	0.59
1:A:1129:CYS:HB2	1:A:1135:ILE:HD13	1.85	0.58
1:A:790:GLN:OE1	1:C:706:ASN:ND2	2.36	0.58
2:X:20:VAL:HG21	2:X:94:TYR:CE2	2.39	0.58
2:X:101:SER:OG	2:X:108:ASP:N	2.36	0.58
1:A:438:ALA:HB2	1:A:513:VAL:HG22	1.85	0.58
2:U:107:GLU:C	2:U:109:VAL:H	2.07	0.58
2:X:148:LEU:HD13	2:X:221:VAL:HG21	1.85	0.58
1:A:440:ASN:OD1	1:A:441:SER:N	2.36	0.58
2:X:73:ASP:OD1	2:X:76:THR:OG1	2.22	0.57
1:C:81:ASN:HA	1:C:268:TYR:OH	2.04	0.57
4:Z:100:THR:HG23	4:Z:100:THR:O	2.04	0.57
1:C:1106:PHE:HZ	6:C:1309:NAG:H82	1.70	0.57
1:A:131:CYS:HA	1:A:166:CYS:HB2	1.87	0.56
1:A:349:ARG:HH22	2:U:107:GLU:HB2	1.70	0.56
1:A:982:ASP:OD1	1:A:986:ARG:NE	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ASN:OD1	1:B:99:ASN:O	2.23	0.56
1:C:34:ARG:NH1	1:C:222:GLY:O	2.38	0.56
3:Y:317:ASP:OD1	3:Y:358:TYR:OH	2.23	0.56
1:A:349:ARG:HH22	2:U:107:GLU:CA	2.19	0.56
3:Y:288:ILE:HD13	3:Y:369:THR:HG21	1.87	0.56
1:B:1129:CYS:CB	1:B:1135:ILE:HD13	2.35	0.56
1:B:100:ILE:N	1:B:100:ILE:HD12	2.21	0.55
2:U:210:HIS:O	2:U:214:ASN:N	2.39	0.55
1:A:292:VAL:HG23	1:A:309:PHE:CZ	2.41	0.55
1:B:919:LEU:HD12	1:B:926:ILE:HD12	1.87	0.55
2:X:20:VAL:HG21	2:X:94:TYR:HE2	1.71	0.55
1:A:766:LEU:HD22	1:A:1011:VAL:HG21	1.87	0.55
3:V:361:LEU:O	3:V:363:LEU:N	2.40	0.54
2:U:5:VAL:O	2:U:23:LYS:N	2.40	0.54
1:B:167:THR:CG2	6:B:1311:NAG:H81	2.37	0.54
1:B:488:GLY:N	1:B:491:CYS:SG	2.78	0.54
1:C:745:ILE:CG2	1:C:1000:ILE:HD13	2.37	0.54
1:B:766:LEU:HD21	1:B:1007:LEU:HB3	1.91	0.54
1:B:745:ILE:O	1:B:1003:ARG:NH1	2.39	0.53
1:A:997:ASP:O	1:A:1001:THR:HG23	2.09	0.53
1:B:493:PHE:CD2	2:X:55:PHE:CE1	2.97	0.53
1:C:1106:PHE:CZ	6:C:1309:NAG:H82	2.43	0.53
1:A:190:ARG:CG	1:A:207:HIS:CD2	2.86	0.53
2:U:134:LEU:HD13	3:V:385:PHE:CD2	2.43	0.53
1:A:808:ILE:HD12	1:A:881:LEU:HD11	1.90	0.53
1:B:117:LEU:HD23	1:B:118:LEU:N	2.23	0.53
1:C:566:GLN:O	1:C:580:ARG:NH1	2.42	0.52
2:U:33:ALA:HB3	2:U:99:LEU:HB3	1.91	0.52
1:A:743:MET:O	1:A:747:GLY:N	2.41	0.52
1:A:349:ARG:HH22	2:U:107:GLU:CB	2.23	0.52
1:C:54:LEU:HD12	1:C:195:LYS:HE3	1.92	0.52
2:U:101:SER:HA	2:U:106:TRP:O	2.10	0.51
1:B:405:ILE:O	1:B:511:TYR:N	2.40	0.51
1:A:752:CYS:SG	1:A:980:LEU:HD13	2.50	0.51
1:B:452:TYR:HE2	3:Y:361:LEU:HD11	1.75	0.51
1:C:100:ILE:HD12	1:C:100:ILE:N	2.26	0.51
4:Z:48:GLN:OE1	4:Z:54:ARG:NH2	2.44	0.51
1:B:908:ARG:NH1	1:B:1052:LEU:O	2.43	0.51
2:U:11:VAL:HG22	2:U:120:THR:HG22	1.92	0.51
1:B:493:PHE:CD2	2:X:55:PHE:HE1	2.30	0.50
1:B:1129:CYS:HB2	1:B:1135:ILE:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Z:47:ARG:NH1	4:Z:98:GLU:O	2.45	0.50
1:B:771:THR:O	1:B:775:VAL:HG23	2.12	0.49
3:V:406:PHE:O	3:V:440:TYR:N	2.46	0.49
3:V:300:LEU:HD11	3:V:355:CYS:HB2	1.94	0.49
1:A:354:TYR:HE1	1:A:455:LEU:HB2	1.78	0.49
1:A:345:PHE:CE2	1:A:514:VAL:HG11	2.47	0.49
1:B:167:THR:HG22	6:B:1311:NAG:H81	1.93	0.49
3:Y:430:VAL:HG13	3:Y:440:TYR:OH	2.12	0.49
1:C:471:ILE:O	1:C:471:ILE:HG22	2.12	0.49
2:X:132:PHE:CE1	2:X:151:LEU:HD12	2.48	0.48
1:A:130:VAL:HG12	1:A:130:VAL:O	2.13	0.48
4:Z:47:ARG:N	4:Z:55:GLU:O	2.45	0.48
2:U:2:VAL:HG12	2:U:32:TYR:OH	2.13	0.48
3:V:403:LEU:HD21	3:V:463:VAL:HG21	1.94	0.48
4:W:15:GLU:OE1	4:W:105:CYS:N	2.46	0.48
2:U:107:GLU:O	2:U:109:VAL:N	2.41	0.48
1:B:118:LEU:HD23	1:B:119:ILE:N	2.29	0.48
1:C:68:ILE:HG22	1:C:68:ILE:O	2.13	0.48
2:U:36:TRP:CD1	2:U:70:ILE:HD13	2.48	0.48
2:U:101:SER:H	2:U:107:GLU:C	2.16	0.48
4:Z:21:VAL:HG21	4:Z:95:LEU:CD2	2.44	0.48
1:C:759:TYR:OH	1:C:997:ASP:OD1	2.28	0.48
3:V:434:ASP:O	3:V:438:SER:N	2.41	0.48
1:A:117:LEU:HD23	1:A:130:VAL:HG22	1.95	0.47
1:A:190:ARG:HD3	1:A:207:HIS:NE2	2.29	0.47
1:B:54:LEU:HD12	1:B:195:LYS:HD3	1.94	0.47
1:B:594:SER:OG	1:B:622:GLU:OE2	2.32	0.47
1:A:1104:HIS:CD2	6:A:1307:NAG:H5	2.49	0.47
2:U:26:GLY:O	2:U:32:TYR:OH	2.29	0.47
2:U:73:ASP:OD1	2:U:76:THR:OG1	2.32	0.47
1:A:190:ARG:CG	1:A:207:HIS:NE2	2.78	0.47
2:X:52:ILE:HG22	2:X:55:PHE:H	1.80	0.47
1:A:908:ARG:NH1	1:A:1052:LEU:O	2.43	0.47
3:Y:361:LEU:N	3:Y:362:PRO:HD2	2.29	0.47
1:C:766:LEU:HG	1:C:1011:VAL:HG21	1.97	0.47
2:X:158:GLU:HB3	2:X:159:PRO:HA	1.97	0.47
1:B:453:ASN:CG	2:X:107:GLU:OE1	2.53	0.47
1:B:531:LYS:HA	1:B:531:LYS:HE2	1.96	0.47
1:B:195:LYS:HD2	1:B:197:ILE:HG12	1.95	0.47
1:A:349:ARG:NH2	2:U:105:GLY:O	2.48	0.46
1:B:195:LYS:HD2	1:B:197:ILE:CG1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:708:VAL:HB	1:C:886:THR:HG21	1.98	0.46
2:U:39:GLN:NE2	2:U:43:GLN:O	2.46	0.46
1:C:953:ASP:OD1	1:C:954:VAL:HG23	2.15	0.46
3:Y:370:LYS:NZ	3:Y:371:VAL:O	2.48	0.46
3:V:361:LEU:N	3:V:362:PRO:HD2	2.30	0.46
1:C:95:ILE:CG1	1:C:189:LEU:HD13	2.46	0.46
2:X:35:SER:O	2:X:97:ALA:N	2.35	0.46
1:A:448:VAL:HG23	1:A:448:VAL:O	2.15	0.46
4:Z:43:MET:HG2	4:Z:88:VAL:HG11	1.98	0.46
1:A:353:VAL:HG21	1:A:421:ILE:HD12	1.97	0.46
3:Y:410:GLU:O	4:Z:113:TYR:OH	2.30	0.46
2:U:132:PHE:CZ	2:U:151:LEU:HD22	2.51	0.46
2:U:158:GLU:HB3	2:U:159:PRO:HA	1.98	0.46
1:C:746:CYS:HB3	1:C:980:LEU:CD2	2.45	0.45
1:C:960:GLN:O	1:C:964:THR:HG22	2.16	0.45
3:V:275:PRO:HG2	3:V:278:LEU:HD21	1.97	0.45
1:B:321:PHE:HZ	1:B:618:VAL:CG2	2.29	0.45
3:V:275:PRO:CG	3:V:278:LEU:HD21	2.46	0.45
1:B:997:ASP:OD1	1:B:997:ASP:C	2.55	0.45
2:X:192:VAL:HG22	2:X:193:THR:N	2.31	0.45
2:U:174:HIS:NE2	3:V:431:THR:HG21	2.31	0.45
3:V:288:ILE:N	3:V:340:PHE:O	2.44	0.44
1:A:345:PHE:CZ	1:A:514:VAL:HG11	2.52	0.44
1:C:752:CYS:SG	1:C:1000:ILE:HD11	2.58	0.44
1:C:755:LEU:H	1:C:755:LEU:HD12	1.82	0.44
4:Z:13:LEU:HD21	4:Z:105:CYS:SG	2.58	0.44
1:A:568:PHE:CE1	1:A:576:THR:HG23	2.53	0.44
1:A:782:GLN:O	1:A:786:ALA:HB3	2.17	0.44
1:B:66:HIS:O	1:B:80:ASP:N	2.50	0.44
1:B:321:PHE:HZ	1:B:618:VAL:HG21	1.79	0.44
1:A:708:VAL:HG13	1:B:886:THR:HG21	1.99	0.44
1:C:751:GLU:O	1:C:755:LEU:HD12	2.18	0.43
2:X:48:MET:HB3	2:X:68:VAL:HG11	1.99	0.43
1:C:28:TYR:N	1:C:28:TYR:CD1	2.86	0.43
1:A:81:ASN:O	1:A:242:GLN:NE2	2.50	0.43
1:A:190:ARG:HG3	1:A:207:HIS:NE2	2.30	0.43
1:A:323:VAL:O	1:A:323:VAL:HG23	2.19	0.43
4:Z:57:VAL:O	4:Z:73:VAL:HG21	2.19	0.43
1:B:321:PHE:CZ	1:B:618:VAL:CG2	3.00	0.43
1:C:534:THR:HG22	1:C:535:ASN:N	2.33	0.43
1:A:745:ILE:O	1:A:1003:ARG:NH1	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:ILE:N	1:C:100:ILE:CD1	2.82	0.43
2:U:174:HIS:CE1	3:V:431:THR:HG21	2.54	0.43
1:A:677:TYR:CE2	1:A:679:THR:CB	3.02	0.43
1:A:814:LYS:HD3	1:A:814:LYS:N	2.33	0.43
1:B:595:PHE:CD1	1:B:595:PHE:C	2.92	0.43
3:V:300:LEU:HD12	3:V:301:ALA:N	2.31	0.43
4:W:103:TYR:CE2	4:W:126:VAL:HG11	2.54	0.43
1:B:1103:THR:O	1:B:1103:THR:HG22	2.19	0.43
1:A:560:LYS:HD3	1:B:43:PHE:CE2	2.53	0.43
1:A:375:ALA:N	1:A:376:PRO:HD2	2.34	0.42
1:A:960:GLN:OE1	1:B:768:ARG:NE	2.52	0.42
1:B:321:PHE:CE1	1:B:618:VAL:HG21	2.53	0.42
1:B:452:TYR:O	1:B:497:SER:OG	2.20	0.42
1:C:722:THR:O	1:C:722:THR:OG1	2.31	0.42
2:U:107:GLU:C	2:U:109:VAL:N	2.72	0.42
1:B:594:SER:HG	1:B:622:GLU:CD	2.22	0.42
1:A:99:ASN:O	1:A:99:ASN:OD1	2.37	0.42
2:U:21:SER:HG	2:U:80:TYR:HE1	1.62	0.42
1:A:739:VAL:HG21	1:A:1007:LEU:HD11	2.01	0.42
1:C:962:LEU:O	1:C:966:VAL:HG23	2.20	0.42
4:W:78:THR:HB	4:W:91:GLN:HB3	2.02	0.42
2:X:50:ARG:HH21	2:X:52:ILE:HD11	1.84	0.42
3:Y:430:VAL:HG13	3:Y:440:TYR:CE1	2.55	0.42
4:Z:11:VAL:O	4:Z:12:GLN:C	2.57	0.42
1:A:345:PHE:CZ	1:A:371:LEU:HD22	2.55	0.42
1:B:95:ILE:CG1	1:B:189:LEU:HD13	2.50	0.41
1:C:126:VAL:HG23	1:C:174:PRO:HA	2.02	0.41
1:C:741:CYS:O	1:C:742:THR:C	2.59	0.41
2:X:210:HIS:O	2:X:214:ASN:N	2.53	0.41
4:Z:47:ARG:HG2	4:Z:47:ARG:HH21	1.86	0.41
1:A:575:THR:CB	1:B:859:LYS:NZ	2.84	0.41
1:B:81:ASN:O	1:B:242:GLN:NE2	2.43	0.41
1:B:171:VAL:HG12	1:B:172:SER:N	2.35	0.41
1:A:349:ARG:NH2	2:U:107:GLU:HA	2.35	0.41
1:B:122:ASN:N	1:B:125:ASN:O	2.43	0.41
2:X:71:THR:O	2:X:80:TYR:N	2.47	0.41
4:W:69:TYR:OH	4:W:78:THR:HA	2.20	0.41
1:A:986:ARG:NE	1:C:520:LEU:HD13	2.36	0.41
2:X:68:VAL:HG13	2:X:81:MET:SD	2.61	0.41
1:A:986:ARG:CZ	1:C:520:LEU:HD13	2.51	0.41
2:X:64:PHE:HA	2:X:67:ARG:HH21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:192:VAL:HG22	2:X:193:THR:H	1.86	0.41
1:A:445:ASP:OD1	1:A:454:TYR:OH	2.38	0.41
1:A:1009:THR:O	1:A:1013:GLN:HG2	2.21	0.41
1:B:100:ILE:N	1:B:100:ILE:CD1	2.84	0.41
1:B:922:ASN:O	1:B:926:ILE:HG13	2.21	0.41
3:V:377:VAL:HG22	4:W:68:PHE:CZ	2.56	0.41
1:A:105:ILE:HG22	1:A:118:LEU:HD23	2.03	0.41
1:A:761:SER:OG	1:C:967:LYS:HE3	2.21	0.40
1:A:1107:VAL:HG23	1:A:1118:ILE:HG12	2.02	0.40
3:Y:313:LEU:O	3:Y:314:LEU:HD22	2.22	0.40
4:Z:32:ALA:HB2	4:Z:87:THR:HG22	2.01	0.40
2:X:48:MET:HG3	2:X:64:PHE:CG	2.56	0.40
2:U:78:THR:HG22	2:U:79:ALA:N	2.36	0.40
1:B:118:LEU:HD23	1:B:118:LEU:C	2.41	0.40
1:C:1129:CYS:HB3	1:C:1135:ILE:HD13	2.04	0.40
3:Y:361:LEU:O	3:Y:363:LEU:N	2.55	0.40
1:A:315:ILE:HD12	1:A:601:ILE:HD11	2.02	0.40
1:B:321:PHE:CD2	1:B:596:GLY:O	2.75	0.40
1:C:595:PHE:CD1	1:C:595:PHE:C	2.95	0.40
4:Z:48:GLN:O	4:Z:101:ALA:HB1	2.21	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	1005/1205 (83%)	976 (97%)	29 (3%)	0	100	100
1	B	1008/1205 (84%)	981 (97%)	27 (3%)	0	100	100
1	C	1008/1205 (84%)	978 (97%)	30 (3%)	0	100	100
2	U	223/237 (94%)	214 (96%)	7 (3%)	2 (1%)	17	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	X	223/237 (94%)	211 (95%)	12 (5%)	0	100	100
3	V	212/215 (99%)	206 (97%)	6 (3%)	0	100	100
3	Y	212/215 (99%)	204 (96%)	8 (4%)	0	100	100
4	W	118/133 (89%)	113 (96%)	5 (4%)	0	100	100
4	Z	118/133 (89%)	111 (94%)	7 (6%)	0	100	100
All	All	4127/4785 (86%)	3994 (97%)	131 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	U	101	SER
2	U	108	ASP

### 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	803/1053 (76%)	803 (100%)	0	100	100
1	B	803/1053 (76%)	803 (100%)	0	100	100
1	C	792/1053 (75%)	792 (100%)	0	100	100
2	U	188/200 (94%)	187 (100%)	1 (0%)	88	96
2	X	188/200 (94%)	188 (100%)	0	100	100
3	V	186/187 (100%)	186 (100%)	0	100	100
3	Y	186/187 (100%)	186 (100%)	0	100	100
4	W	96/107 (90%)	96 (100%)	0	100	100
4	Z	96/107 (90%)	96 (100%)	0	100	100
All	All	3338/4147 (80%)	3337 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	U	106	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	790	GLN
1	A	1104	HIS
1	C	121	ASN
1	C	706	ASN
3	Y	346	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

4 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	D	1	1,5	14,14,15	0.22	0	17,19,21	0.44	0
5	NAG	D	2	5	14,14,15	0.20	0	17,19,21	0.43	0
5	NAG	E	1	1,5	14,14,15	0.20	0	17,19,21	0.42	0
5	NAG	E	2	5	14,14,15	0.20	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
5	NAG	D	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	2	5	-	0/6/23/26	0/1/1/1
5	NAG	E	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

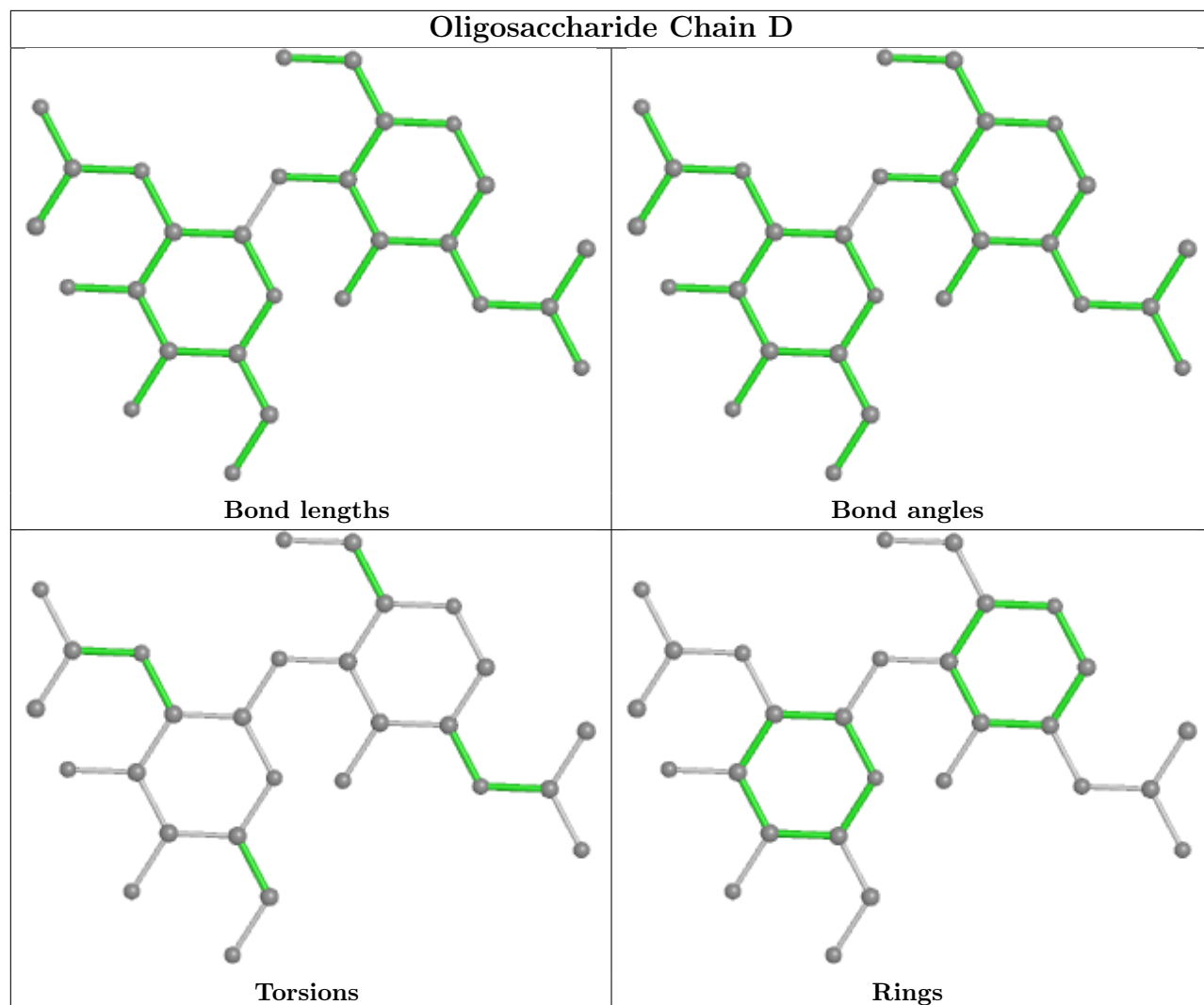
There are no chirality outliers.

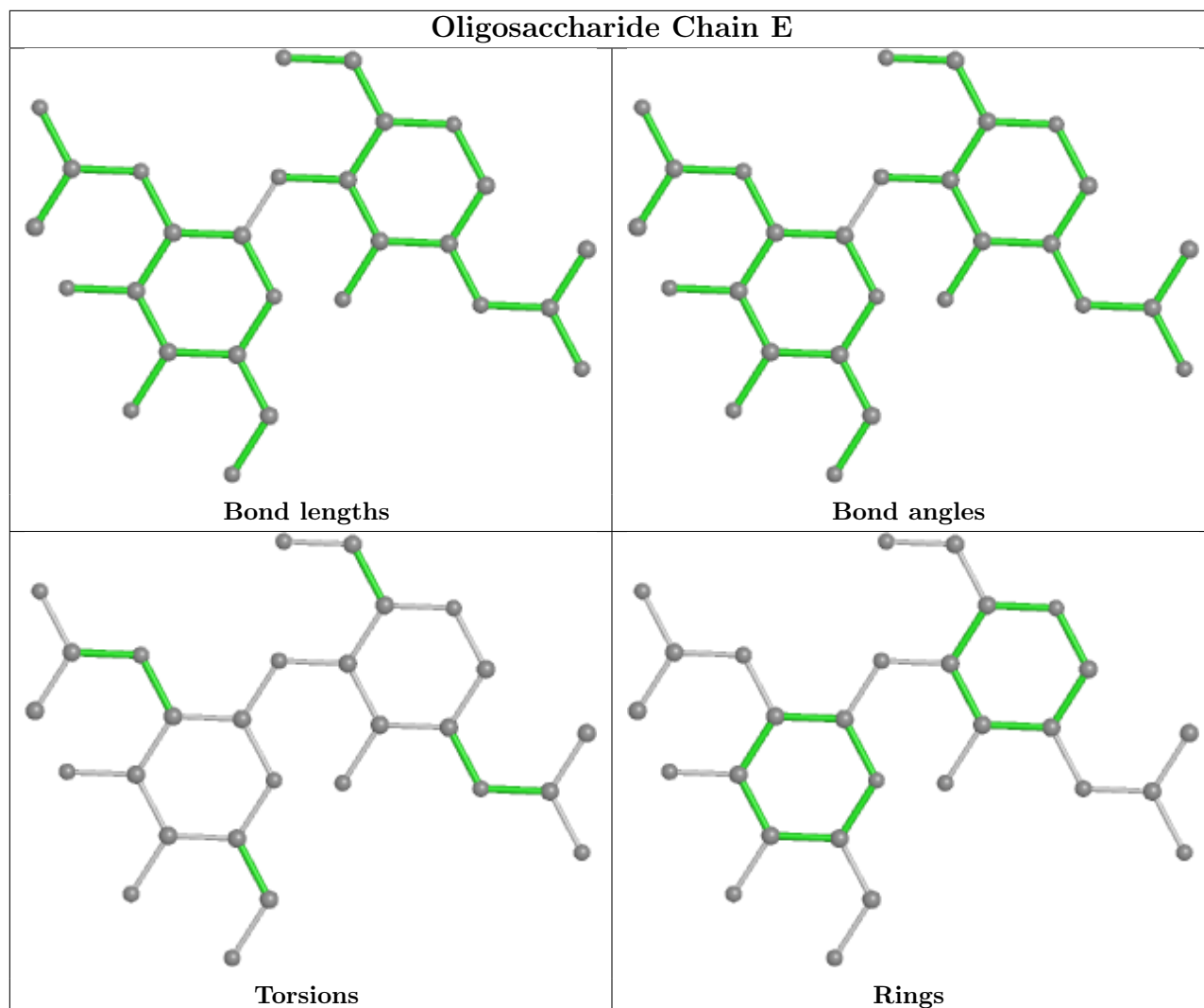
There are no torsion outliers.

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](#)

36 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	B	1311	1	14,14,15	0.18	0	17,19,21	0.40	0
6	NAG	C	1307	1	14,14,15	0.22	0	17,19,21	0.41	0
6	NAG	A	1304	1	14,14,15	0.23	0	17,19,21	0.43	0
6	NAG	A	1311	1	14,14,15	0.22	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	B	1306	1	14,14,15	0.21	0	17,19,21	0.46	0
6	NAG	B	1301	1	14,14,15	0.24	0	17,19,21	0.46	0
6	NAG	C	1304	1	14,14,15	0.21	0	17,19,21	0.42	0
6	NAG	C	1306	1	14,14,15	0.24	0	17,19,21	0.47	0
6	NAG	A	1303	1	14,14,15	0.22	0	17,19,21	0.45	0
6	NAG	A	1302	1	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	C	1312	1	14,14,15	0.24	0	17,19,21	0.51	0
6	NAG	C	1302	1	14,14,15	0.21	0	17,19,21	0.42	0
6	NAG	C	1301	1	14,14,15	0.21	0	17,19,21	0.41	0
6	NAG	A	1307	1	14,14,15	0.21	0	17,19,21	0.46	0
6	NAG	B	1309	1	14,14,15	0.18	0	17,19,21	0.40	0
6	NAG	B	1304	1	14,14,15	0.21	0	17,19,21	0.41	0
6	NAG	B	1307	1	14,14,15	0.18	0	17,19,21	0.35	0
6	NAG	B	1310	1	14,14,15	0.23	0	17,19,21	0.44	0
6	NAG	B	1303	1	14,14,15	0.22	0	17,19,21	0.41	0
6	NAG	B	1312	1	14,14,15	0.42	0	17,19,21	1.16	1 (5%)
6	NAG	C	1303	1	14,14,15	0.20	0	17,19,21	0.42	0
6	NAG	A	1301	1	14,14,15	0.23	0	17,19,21	0.40	0
6	NAG	B	1308	1	14,14,15	0.22	0	17,19,21	0.44	0
6	NAG	A	1309	1	14,14,15	0.44	0	17,19,21	0.57	0
6	NAG	C	1310	1	14,14,15	0.23	0	17,19,21	0.49	0
6	NAG	C	1311	1	14,14,15	0.19	0	17,19,21	0.40	0
6	NAG	A	1308	1	14,14,15	0.23	0	17,19,21	0.47	0
6	NAG	C	1308	1	14,14,15	0.23	0	17,19,21	0.46	0
6	NAG	B	1302	1	14,14,15	0.20	0	17,19,21	0.43	0
6	NAG	A	1312	1	14,14,15	0.20	0	17,19,21	0.39	0
6	NAG	B	1305	1	14,14,15	0.22	0	17,19,21	0.49	0
6	NAG	A	1305	1	14,14,15	0.23	0	17,19,21	0.45	0
6	NAG	C	1309	1	14,14,15	0.26	0	17,19,21	0.49	0
6	NAG	C	1305	1	14,14,15	0.20	0	17,19,21	0.43	0
6	NAG	A	1306	1	14,14,15	0.21	0	17,19,21	0.46	0
6	NAG	A	1310	1	14,14,15	0.21	0	17,19,21	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1311	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1304	1	-	0/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1312	NAG	C8-C7-N2	2.31	120.01	116.10

There are no chirality outliers.



All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1309	NAG	O5-C5-C6-O6
6	C	1309	NAG	C4-C5-C6-O6
6	C	1311	NAG	O5-C5-C6-O6
6	B	1301	NAG	O5-C5-C6-O6
6	B	1301	NAG	C4-C5-C6-O6
6	C	1311	NAG	C4-C5-C6-O6
6	A	1307	NAG	O5-C5-C6-O6
6	B	1304	NAG	O5-C5-C6-O6
6	C	1309	NAG	C1-C2-N2-C7
6	C	1308	NAG	C4-C5-C6-O6
6	A	1309	NAG	C3-C2-N2-C7
6	B	1311	NAG	C3-C2-N2-C7
6	B	1311	NAG	C1-C2-N2-C7
6	C	1308	NAG	O5-C5-C6-O6
6	A	1306	NAG	C4-C5-C6-O6
6	C	1309	NAG	C3-C2-N2-C7
6	A	1306	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1311	NAG	2	0
6	A	1302	NAG	1	0
6	A	1307	NAG	1	0
6	A	1309	NAG	1	0
6	C	1309	NAG	2	0

## 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-32684. These allow visual inspection of the internal detail of the map and identification of artifacts.

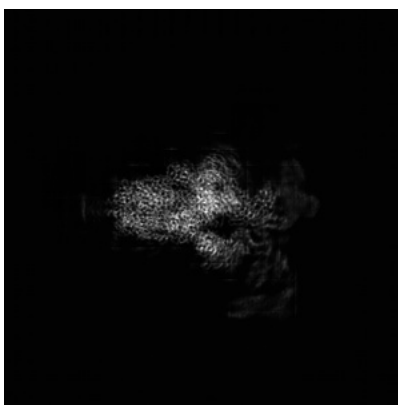
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

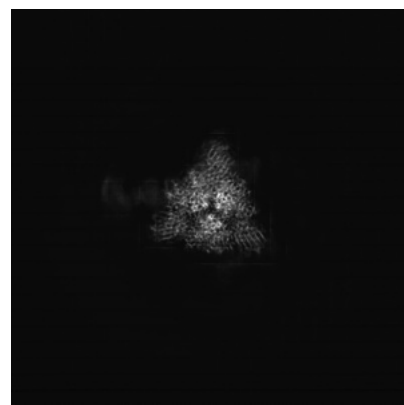
#### 6.1.1 Primary map



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: 240



Y Index: 240



Z Index: 240

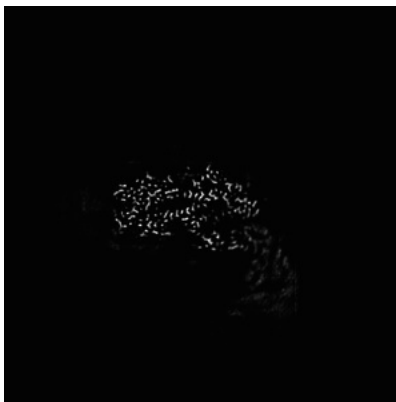
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 249



Y Index: 253



Z Index: 242

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 0.0428. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

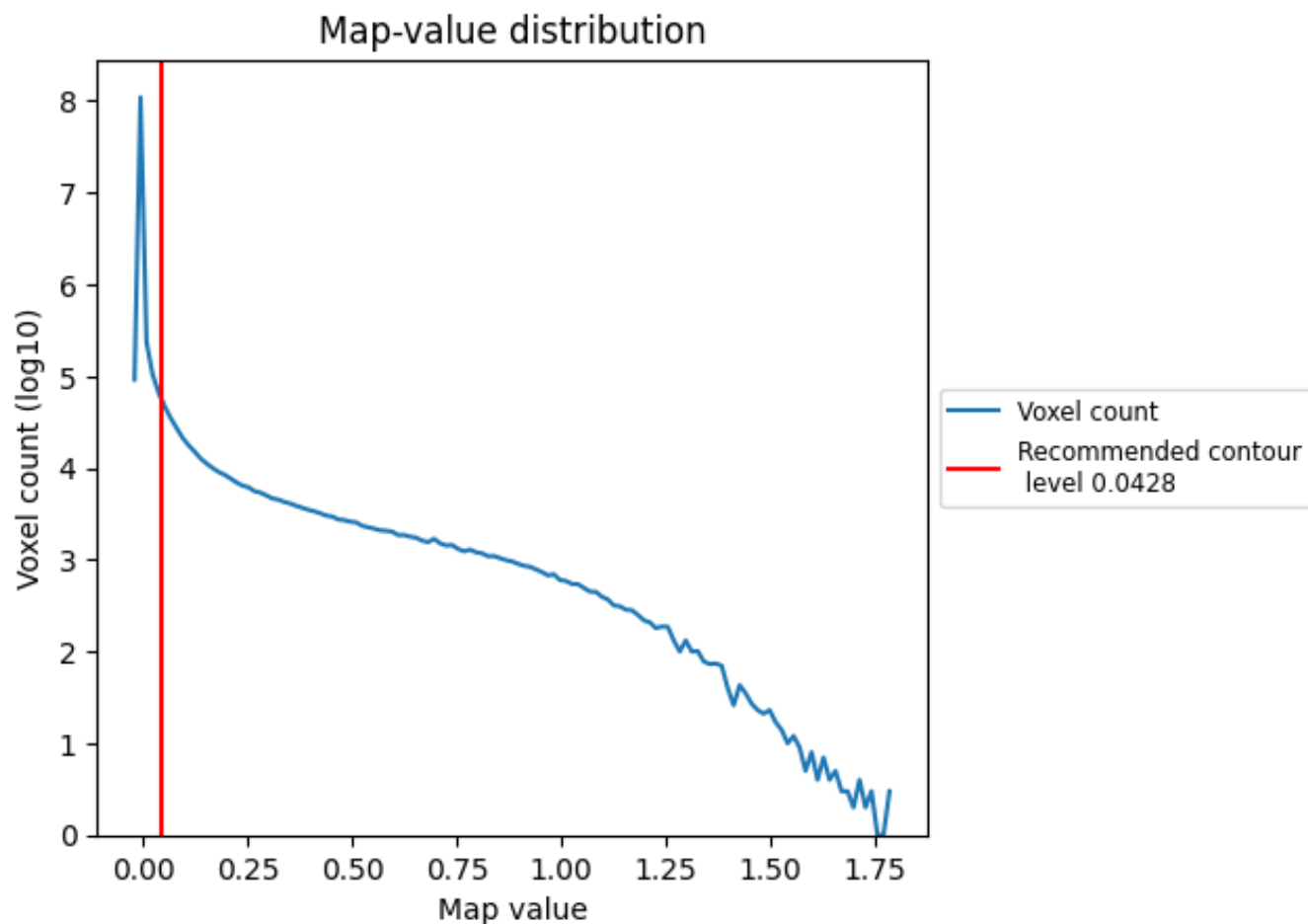
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

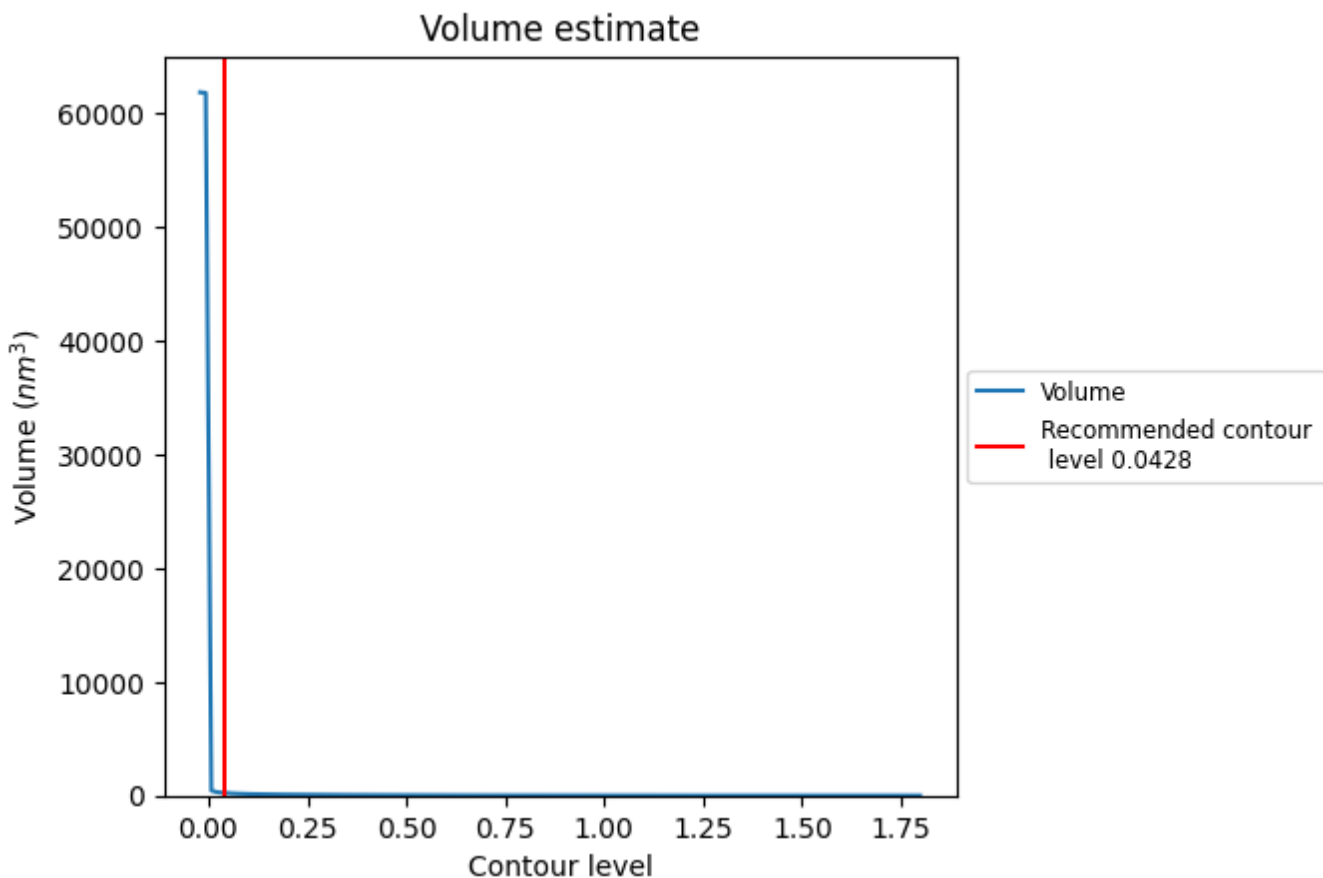
This section contains the results of statistical analysis of the map.

### 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.

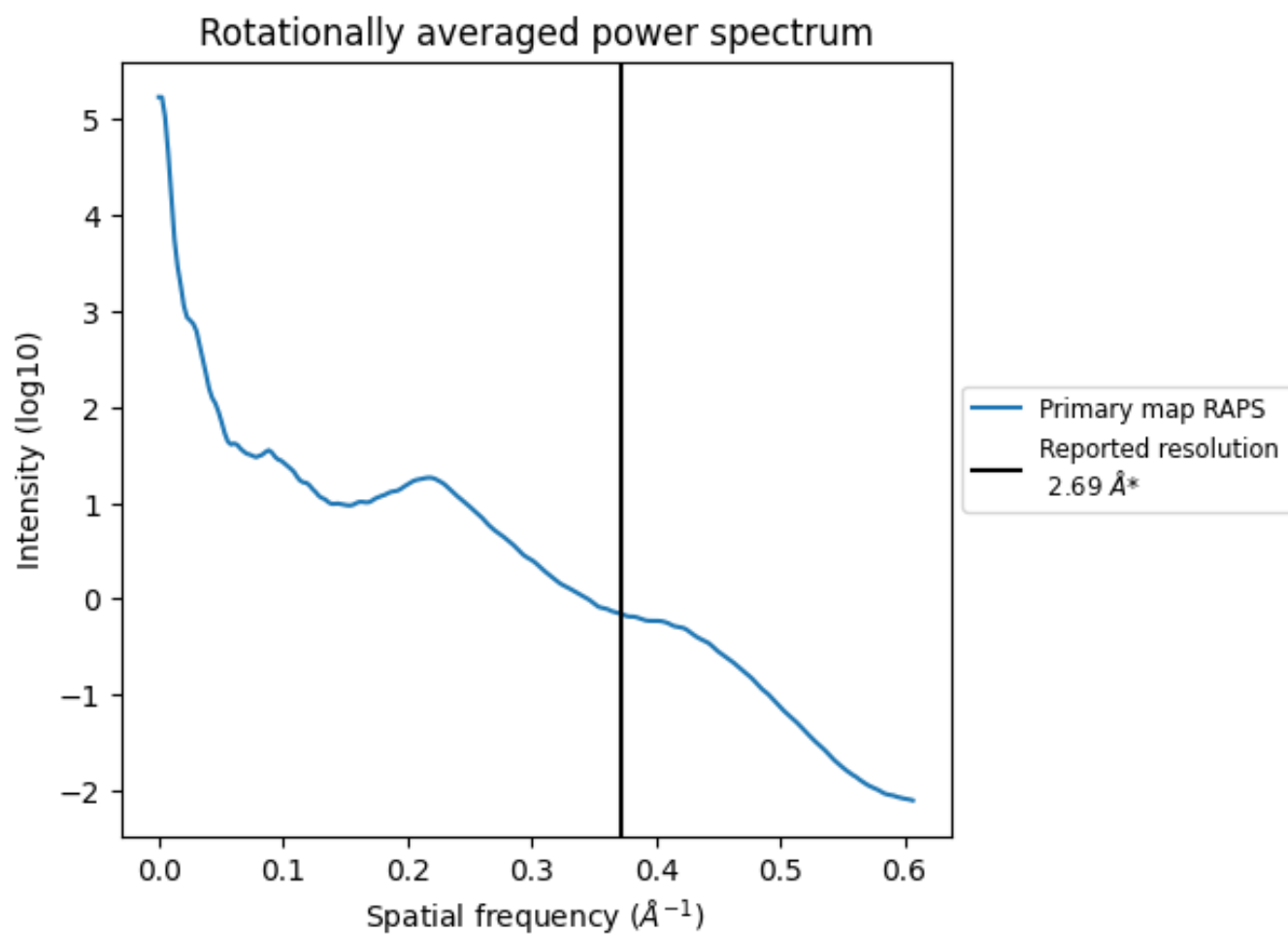
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 225 nm<sup>3</sup>; this corresponds to an approximate mass of 203 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 0.372 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

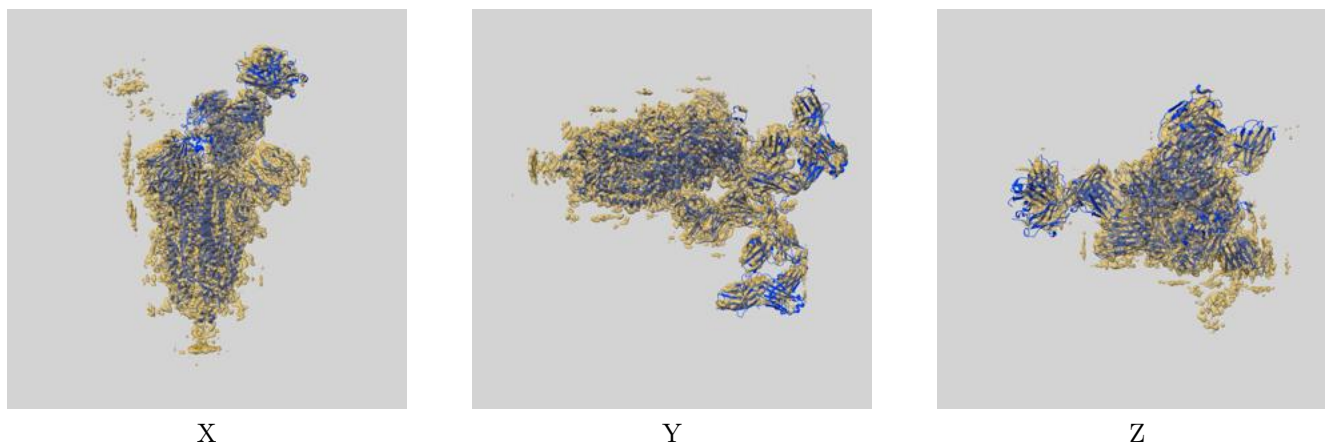
This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit [i](#)

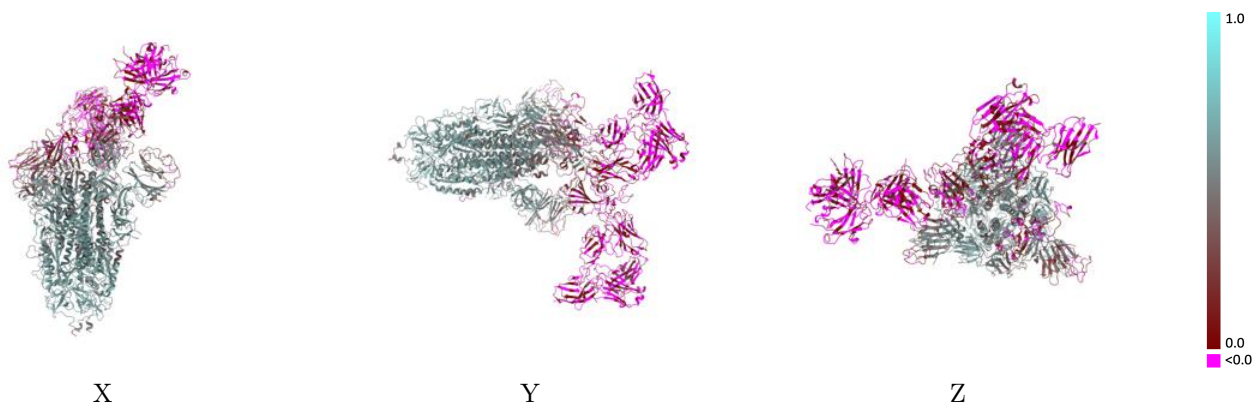
This section contains information regarding the fit between EMDB map EMD-32684 and PDB model 7WPE. Per-residue inclusion information can be found in section [3](#) on page [11](#).

### 9.1 Map-model overlay [i](#)



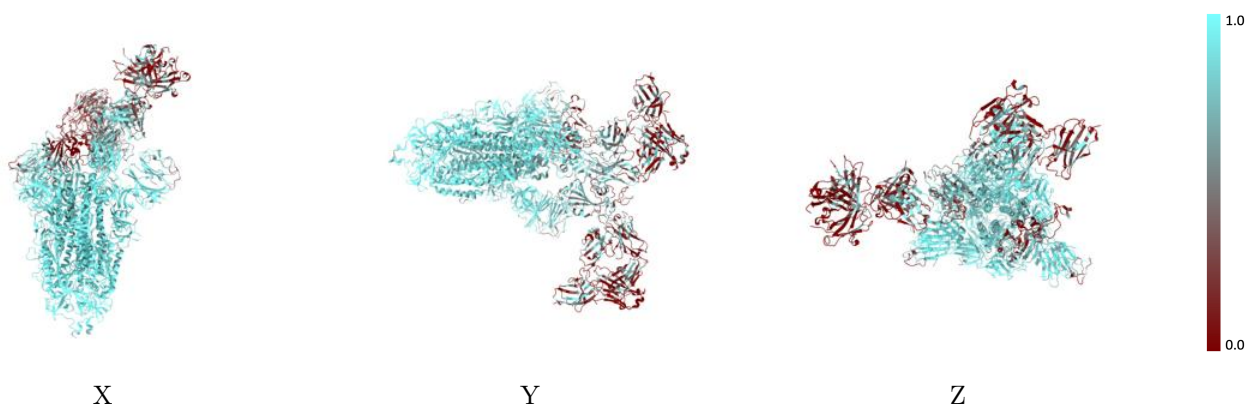
The images above show the 3D surface view of the map at the recommended contour level 0.0428 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



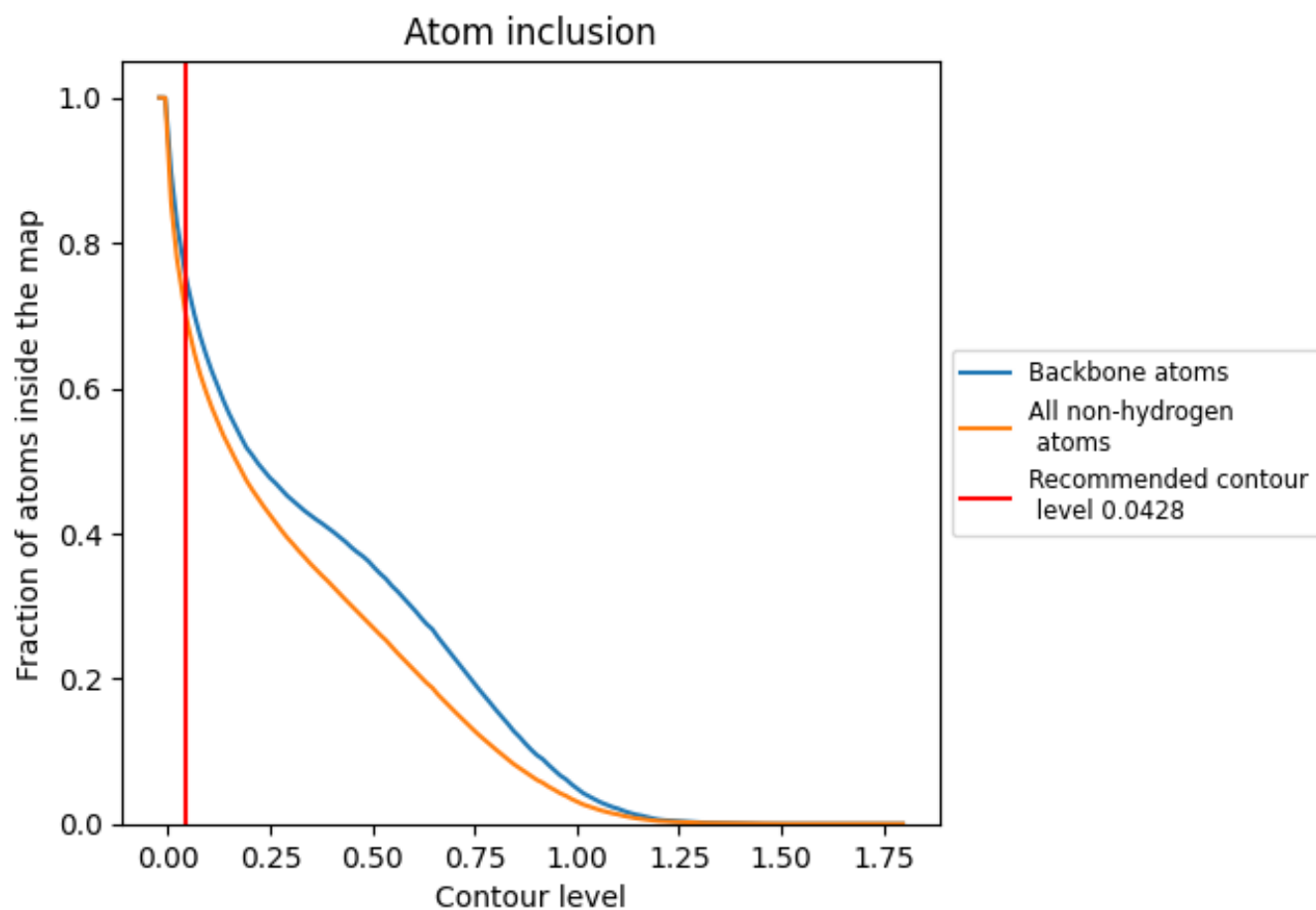
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0428).

























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 70% 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 (0.0428) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7036	 0.3380
A	 0.8907	 0.4890
B	 0.8335	 0.4440
C	 0.7804	 0.4440
D	 0.5000	 0.3990
E	 0.8214	 0.4710
U	 0.4881	 0.0450
V	 0.4507	 -0.0030
W	 0.2508	 -0.0080
X	 0.2538	 -0.0070
Y	 0.2381	 -0.0170
Z	 0.2709	 -0.0150

