Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 01:40 pm GMT

PDB ID	:	6QD7
EMDB ID	:	EMD-4520
Title	:	EM structure of a EBOV-GP bound to 3T0331 neutralizing antibody
Authors	:	Diskin, R.; Cohen-Dvashi, H.
Deposited on	:	2019-01-01
Resolution	:	3.10 Å(reported)
Based on initial models	:	5JQ3, 6QCU

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 (i) 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 (i)) were used in the production of this report:

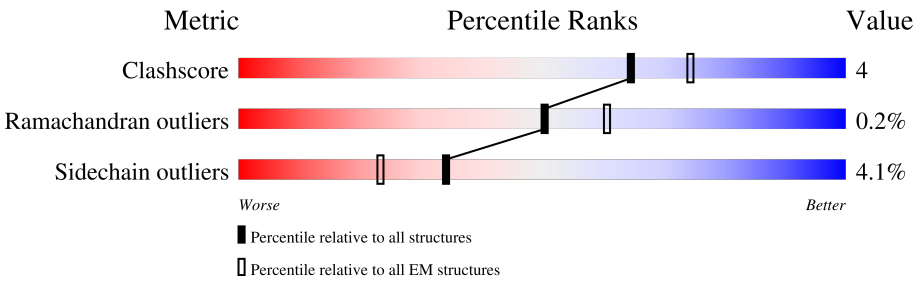
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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 <=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	L	214	45% 5% 50%
1	P	214	44% 6% 50%
1	Z	214	44% 6% 50%
2	H	224	52% • 46%
2	U	224	52% • 46%
2	X	224	52% • 46%
3	A	322	22% 65% 12% • • 20%
3	C	322	22% 65% 12% • • 20%

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Mol	Chain	Length	Quality of chain
3	E	322	22% 66% 11% 20%
4	B	168	61% 15% 23%
4	D	168	63% 14% 23%
4	F	168	5% 64% 12% 23%
5	G	4	25% 75%
5	I	4	25% 75%
5	J	4	25% 75%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 14445 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 Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	L	108	827	520	143	162	2	1	0
1	Z	108	827	520	143	162	2	1	0
1	P	108	827	520	143	162	2	1	0

- Molecule 2 is a protein called Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	120	909	566	164	175	4	0	0
2	X	120	909	566	164	175	4	0	0
2	U	120	909	566	164	175	4	0	0

- Molecule 3 is a protein called Envelope glycoprotein,Virion spike glycoprotein,EBOV-GP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	256	1972	1254	334	379	5	0	0
3	C	256	1972	1254	334	379	5	0	0
3	E	256	1972	1254	334	379	5	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	GLY	-	expression tag	UNP Q05320
A	30	SER	-	expression tag	UNP Q05320
A	31	ARG	-	expression tag	UNP Q05320

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Chain	Residue	Modelled	Actual	Comment	Reference
A	42	ALA	THR	conflict	UNP Q05320
C	29	GLY	-	expression tag	UNP Q05320
C	30	SER	-	expression tag	UNP Q05320
C	31	ARG	-	expression tag	UNP Q05320
C	42	ALA	THR	conflict	UNP Q05320
E	29	GLY	-	expression tag	UNP Q05320
E	30	SER	-	expression tag	UNP Q05320
E	31	ARG	-	expression tag	UNP Q05320
E	42	ALA	THR	conflict	UNP Q05320

- Molecule 4 is a protein called Envelope glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	130	1032	659	178	189	6	0	0
4	D	130	1032	659	178	189	6	0	0
4	F	130	1032	659	178	189	6	0	0

There are 111 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	633	GLY	-	expression tag	UNP Q05320
B	634	SER	-	expression tag	UNP Q05320
B	635	GLY	-	expression tag	UNP Q05320
B	636	TYR	-	expression tag	UNP Q05320
B	637	ILE	-	expression tag	UNP Q05320
B	638	PRO	-	expression tag	UNP Q05320
B	639	GLU	-	expression tag	UNP Q05320
B	640	ALA	-	expression tag	UNP Q05320
B	641	PRO	-	expression tag	UNP Q05320
B	642	ARG	-	expression tag	UNP Q05320
B	643	ASP	-	expression tag	UNP Q05320
B	644	GLY	-	expression tag	UNP Q05320
B	645	GLN	-	expression tag	UNP Q05320
B	646	ALA	-	expression tag	UNP Q05320
B	647	TYR	-	expression tag	UNP Q05320
B	648	VAL	-	expression tag	UNP Q05320
B	649	ARG	-	expression tag	UNP Q05320
B	650	LYS	-	expression tag	UNP Q05320
B	651	ASP	-	expression tag	UNP Q05320

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Chain	Residue	Modelled	Actual	Comment	Reference
B	652	GLY	-	expression tag	UNP Q05320
B	653	GLU	-	expression tag	UNP Q05320
B	654	TRP	-	expression tag	UNP Q05320
B	655	VAL	-	expression tag	UNP Q05320
B	656	LEU	-	expression tag	UNP Q05320
B	657	LEU	-	expression tag	UNP Q05320
B	658	SER	-	expression tag	UNP Q05320
B	659	THR	-	expression tag	UNP Q05320
B	660	PHE	-	expression tag	UNP Q05320
B	661	LEU	-	expression tag	UNP Q05320
B	662	GLY	-	expression tag	UNP Q05320
B	663	THR	-	expression tag	UNP Q05320
B	664	HIS	-	expression tag	UNP Q05320
B	665	HIS	-	expression tag	UNP Q05320
B	666	HIS	-	expression tag	UNP Q05320
B	667	HIS	-	expression tag	UNP Q05320
B	668	HIS	-	expression tag	UNP Q05320
B	669	HIS	-	expression tag	UNP Q05320
D	633	GLY	-	expression tag	UNP Q05320
D	634	SER	-	expression tag	UNP Q05320
D	635	GLY	-	expression tag	UNP Q05320
D	636	TYR	-	expression tag	UNP Q05320
D	637	ILE	-	expression tag	UNP Q05320
D	638	PRO	-	expression tag	UNP Q05320
D	639	GLU	-	expression tag	UNP Q05320
D	640	ALA	-	expression tag	UNP Q05320
D	641	PRO	-	expression tag	UNP Q05320
D	642	ARG	-	expression tag	UNP Q05320
D	643	ASP	-	expression tag	UNP Q05320
D	644	GLY	-	expression tag	UNP Q05320
D	645	GLN	-	expression tag	UNP Q05320
D	646	ALA	-	expression tag	UNP Q05320
D	647	TYR	-	expression tag	UNP Q05320
D	648	VAL	-	expression tag	UNP Q05320
D	649	ARG	-	expression tag	UNP Q05320
D	650	LYS	-	expression tag	UNP Q05320
D	651	ASP	-	expression tag	UNP Q05320
D	652	GLY	-	expression tag	UNP Q05320
D	653	GLU	-	expression tag	UNP Q05320
D	654	TRP	-	expression tag	UNP Q05320
D	655	VAL	-	expression tag	UNP Q05320
D	656	LEU	-	expression tag	UNP Q05320

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Chain	Residue	Modelled	Actual	Comment	Reference
D	657	LEU	-	expression tag	UNP Q05320
D	658	SER	-	expression tag	UNP Q05320
D	659	THR	-	expression tag	UNP Q05320
D	660	PHE	-	expression tag	UNP Q05320
D	661	LEU	-	expression tag	UNP Q05320
D	662	GLY	-	expression tag	UNP Q05320
D	663	THR	-	expression tag	UNP Q05320
D	664	HIS	-	expression tag	UNP Q05320
D	665	HIS	-	expression tag	UNP Q05320
D	666	HIS	-	expression tag	UNP Q05320
D	667	HIS	-	expression tag	UNP Q05320
D	668	HIS	-	expression tag	UNP Q05320
D	669	HIS	-	expression tag	UNP Q05320
F	633	GLY	-	expression tag	UNP Q05320
F	634	SER	-	expression tag	UNP Q05320
F	635	GLY	-	expression tag	UNP Q05320
F	636	TYR	-	expression tag	UNP Q05320
F	637	ILE	-	expression tag	UNP Q05320
F	638	PRO	-	expression tag	UNP Q05320
F	639	GLU	-	expression tag	UNP Q05320
F	640	ALA	-	expression tag	UNP Q05320
F	641	PRO	-	expression tag	UNP Q05320
F	642	ARG	-	expression tag	UNP Q05320
F	643	ASP	-	expression tag	UNP Q05320
F	644	GLY	-	expression tag	UNP Q05320
F	645	GLN	-	expression tag	UNP Q05320
F	646	ALA	-	expression tag	UNP Q05320
F	647	TYR	-	expression tag	UNP Q05320
F	648	VAL	-	expression tag	UNP Q05320
F	649	ARG	-	expression tag	UNP Q05320
F	650	LYS	-	expression tag	UNP Q05320
F	651	ASP	-	expression tag	UNP Q05320
F	652	GLY	-	expression tag	UNP Q05320
F	653	GLU	-	expression tag	UNP Q05320
F	654	TRP	-	expression tag	UNP Q05320
F	655	VAL	-	expression tag	UNP Q05320
F	656	LEU	-	expression tag	UNP Q05320
F	657	LEU	-	expression tag	UNP Q05320
F	658	SER	-	expression tag	UNP Q05320
F	659	THR	-	expression tag	UNP Q05320
F	660	PHE	-	expression tag	UNP Q05320
F	661	LEU	-	expression tag	UNP Q05320

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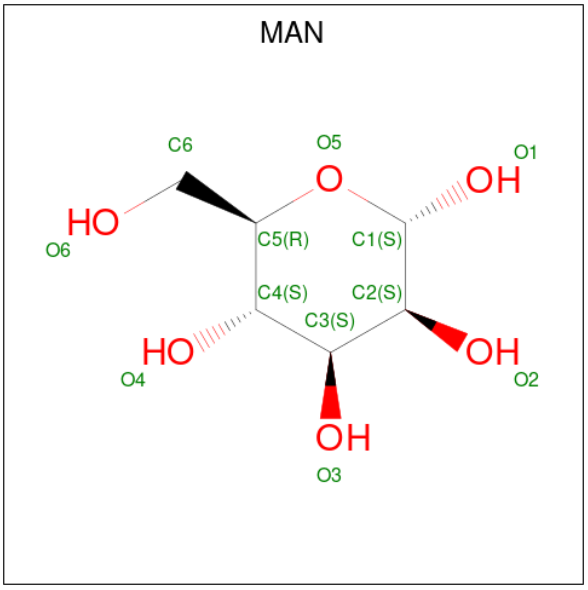
Chain	Residue	Modelled	Actual	Comment	Reference
F	662	GLY	-	expression tag	UNP Q05320
F	663	THR	-	expression tag	UNP Q05320
F	664	HIS	-	expression tag	UNP Q05320
F	665	HIS	-	expression tag	UNP Q05320
F	666	HIS	-	expression tag	UNP Q05320
F	667	HIS	-	expression tag	UNP Q05320
F	668	HIS	-	expression tag	UNP Q05320
F	669	HIS	-	expression tag	UNP Q05320

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

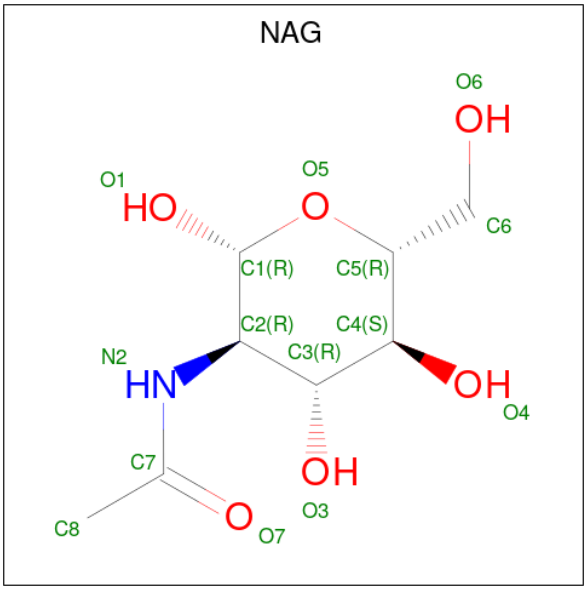
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	G	4	50	28	2	20	0	0
			Total	C	N	O		
5	I	4	50	28	2	20	0	0
			Total	C	N	O		
5	J	4	50	28	2	20	0	0

- Molecule 6 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	O		0
			11	6	5		
6	C	1	Total	C	O		0
			11	6	5		
6	E	1	Total	C	O		0
			11	6	5		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



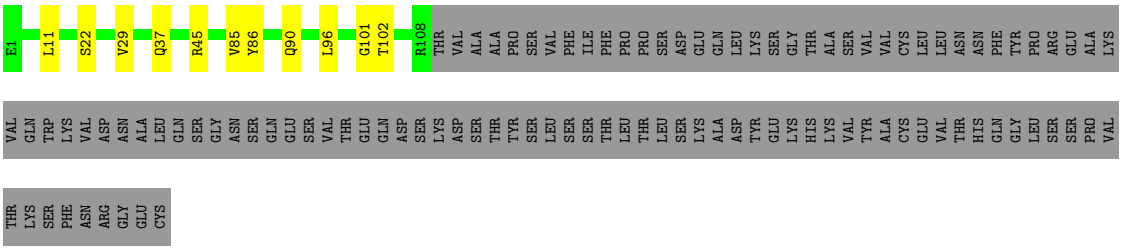
Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	D	1	Total	C	N	O	0
			14	8	1	5	
7	F	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots (i)

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.

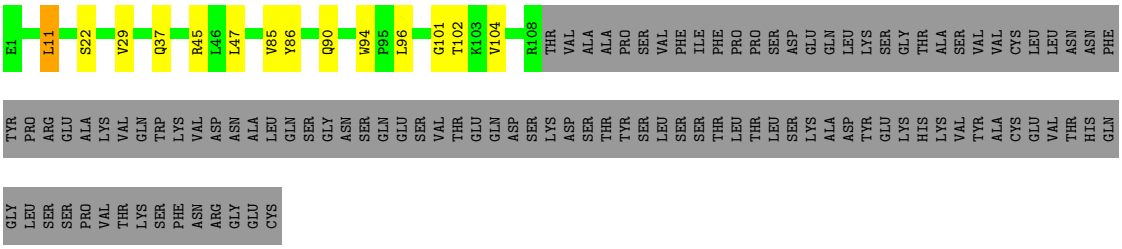
• Molecule 1: Light chain

Chain L: 45% 5% 50%



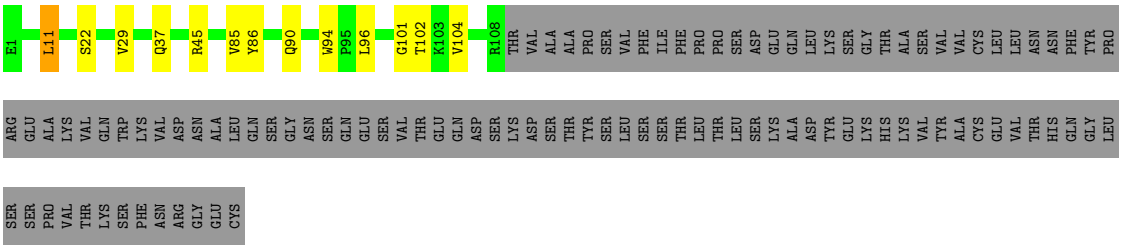
• Molecule 1: Light chain

Chain Z: 44% 6% 50%



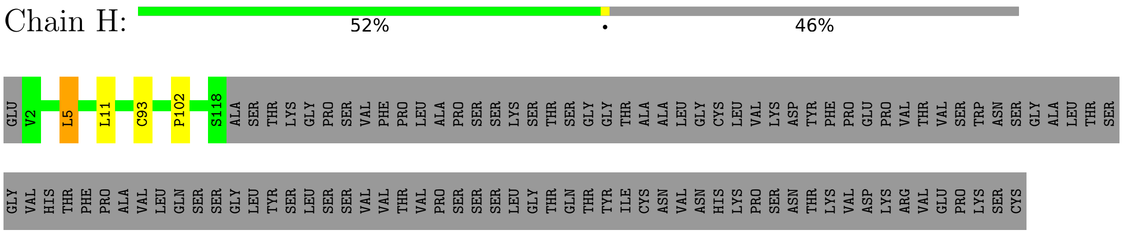
• Molecule 1: Light chain

Chain P: 44% 6% 50%



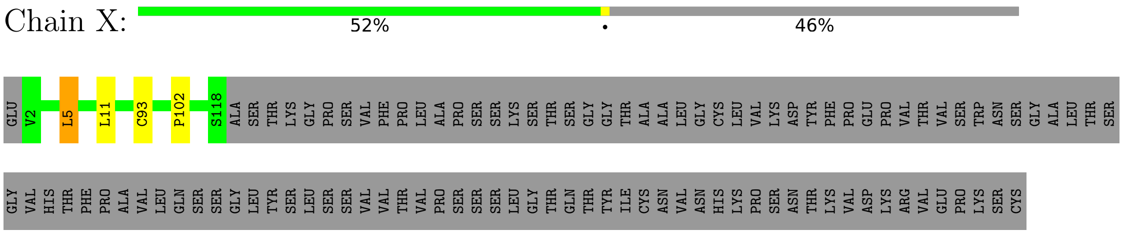
• Molecule 2: Heavy chain

Chain H:



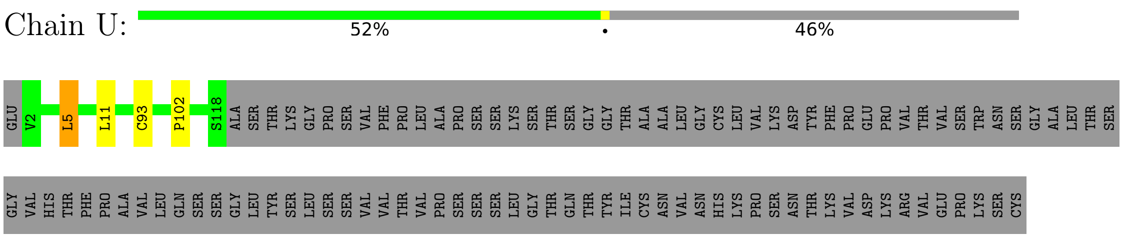
• Molecule 2: Heavy chain

Chain X:



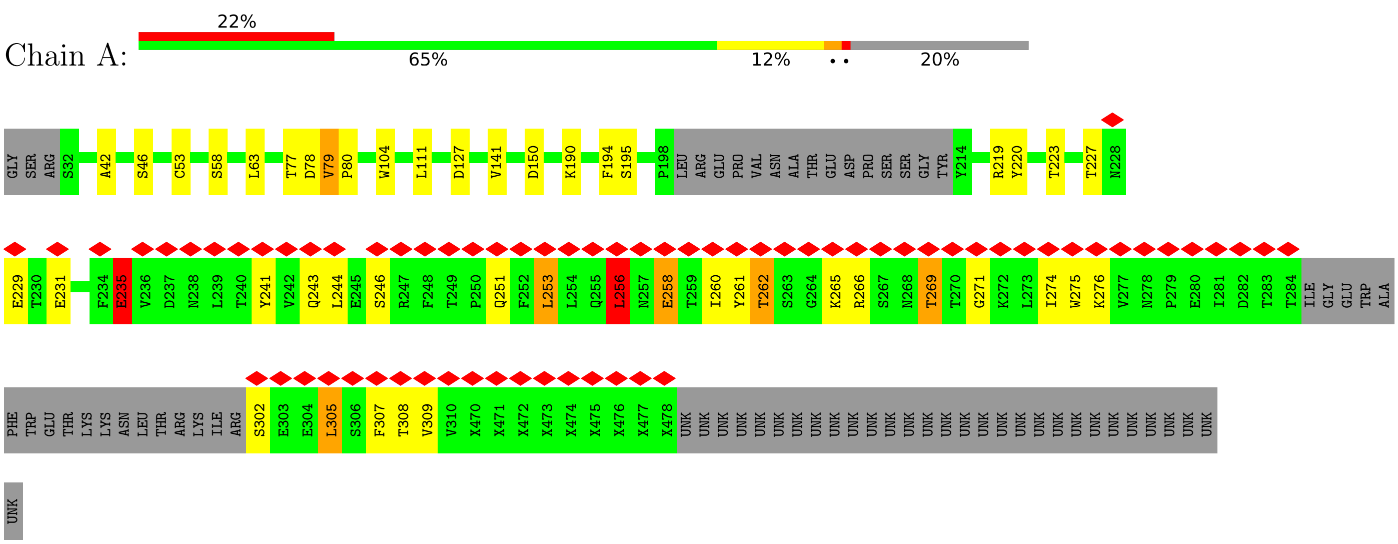
• Molecule 2: Heavy chain

Chain U:



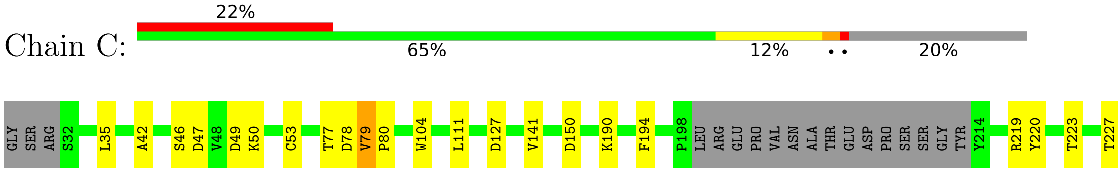
• Molecule 3: Envelope glycoprotein,Virion spike glycoprotein,EBOV-GP1

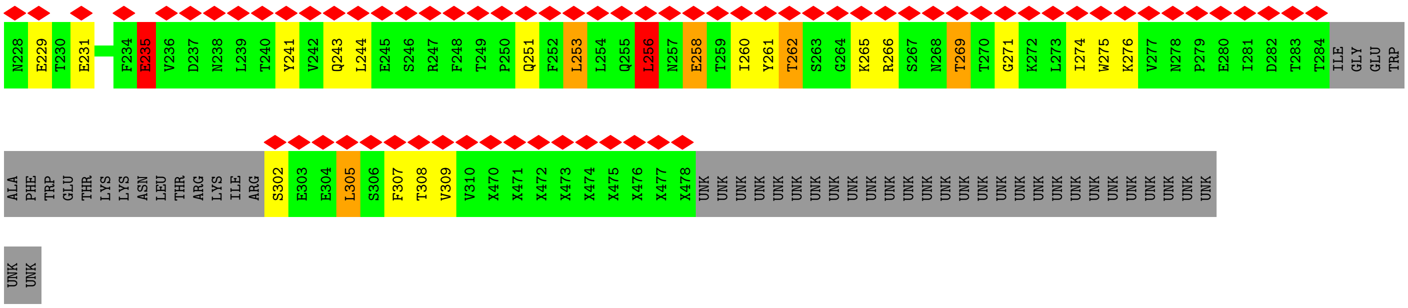
Chain A:



• Molecule 3: Envelope glycoprotein,Virion spike glycoprotein,EBOV-GP1

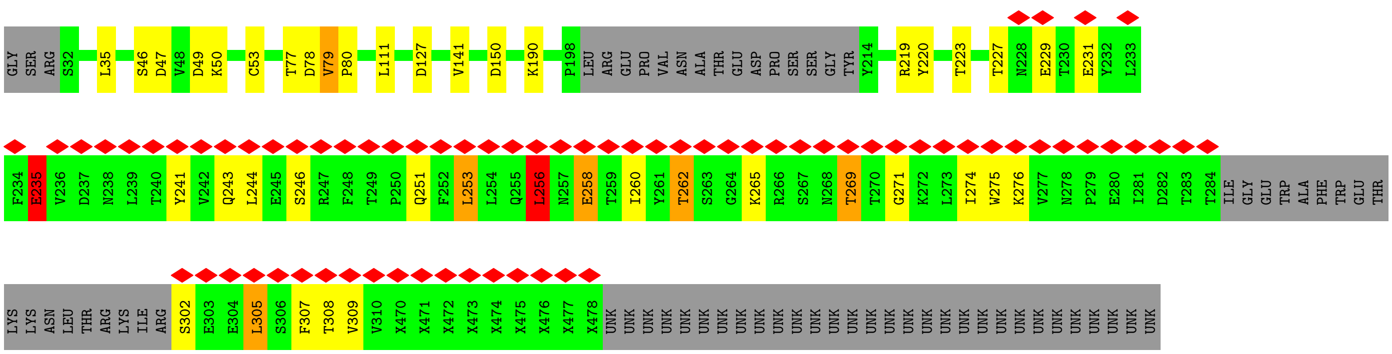
Chain C:





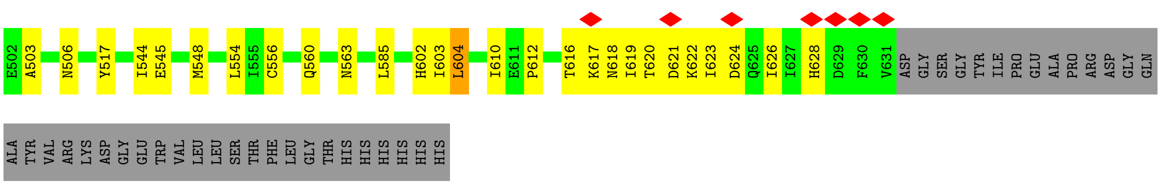
• Molecule 3: Envelope glycoprotein,Virion spike glycoprotein,EBOV-GP1

Chain E:



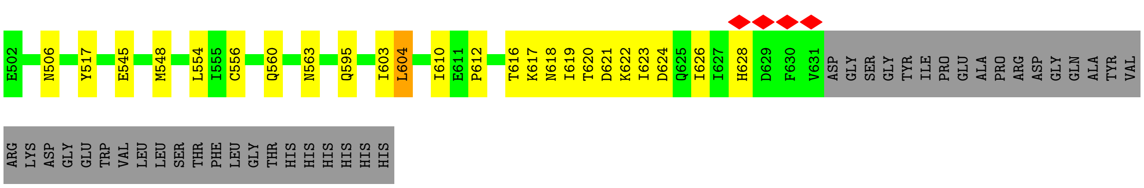
• Molecule 4: Envelope glycoprotein

Chain B:



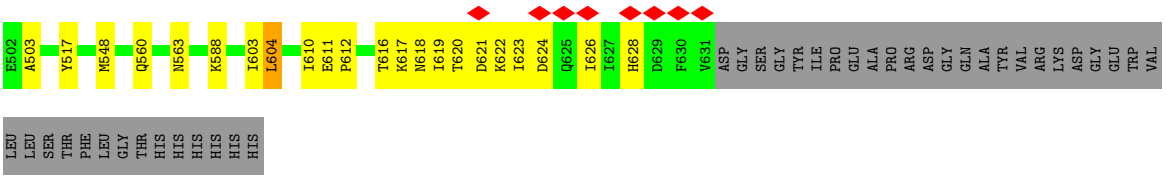
• Molecule 4: Envelope glycoprotein

Chain D:

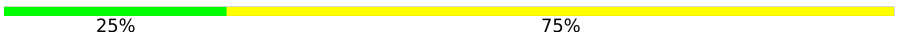


• Molecule 4: Envelope glycoprotein

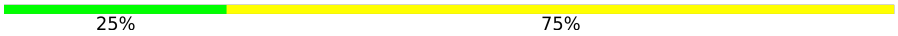
Chain F:



• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 

• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 

• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	109407	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	6.873	Depositor
Minimum map value	-4.651	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.103	Depositor
Recommended contour level	0.108	Depositor
Map size (Å)	306.0, 306.0, 306.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	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: BMA, MAN, 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	L	0.41	0/849	0.82	1/1156 (0.1%)
1	P	0.42	0/849	0.78	1/1156 (0.1%)
1	Z	0.39	0/849	0.76	2/1156 (0.2%)
2	H	0.38	0/927	0.78	3/1255 (0.2%)
2	U	0.38	0/927	0.78	3/1255 (0.2%)
2	X	0.38	0/927	0.78	3/1255 (0.2%)
3	A	0.45	0/1973	0.95	7/2680 (0.3%)
3	C	0.45	0/1973	0.95	7/2680 (0.3%)
3	E	0.45	0/1973	0.95	7/2680 (0.3%)
4	B	0.40	0/1058	0.82	3/1442 (0.2%)
4	D	0.40	0/1058	0.82	3/1442 (0.2%)
4	F	0.40	0/1058	0.82	3/1442 (0.2%)
All	All	0.42	0/14421	0.86	43/19599 (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
3	A	0	1
3	C	0	1
3	E	0	1
All	All	0	3

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	256	LEU	CA-CB-CG	9.67	137.53	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	256	LEU	CA-CB-CG	9.66	137.53	115.30
3	C	256	LEU	CA-CB-CG	9.64	137.48	115.30
4	B	604	LEU	CA-CB-CG	8.08	133.89	115.30
4	F	604	LEU	CA-CB-CG	8.08	133.88	115.30
4	D	604	LEU	CA-CB-CG	8.06	133.84	115.30
1	L	11	LEU	CA-CB-CG	7.75	133.14	115.30
3	A	305	LEU	CA-CB-CG	7.59	132.75	115.30
3	C	305	LEU	CA-CB-CG	7.59	132.75	115.30
3	E	305	LEU	CA-CB-CG	7.58	132.73	115.30
1	P	11	LEU	CA-CB-CG	7.43	132.38	115.30
1	Z	11	LEU	CA-CB-CG	6.96	131.31	115.30
3	C	235	GLU	OE1-CD-OE2	-6.82	115.11	123.30
3	E	235	GLU	OE1-CD-OE2	-6.81	115.13	123.30
3	A	235	GLU	OE1-CD-OE2	-6.79	115.15	123.30
3	A	253	LEU	CA-CB-CG	6.67	130.65	115.30
3	E	253	LEU	CA-CB-CG	6.65	130.59	115.30
3	C	253	LEU	CA-CB-CG	6.64	130.58	115.30
2	U	5	LEU	CA-CB-CG	6.40	130.02	115.30
2	H	5	LEU	CA-CB-CG	6.40	130.01	115.30
2	X	5	LEU	CA-CB-CG	6.38	129.98	115.30
2	U	93	CYS	CA-CB-SG	6.02	124.83	114.00
2	X	93	CYS	CA-CB-SG	6.00	124.80	114.00
2	H	93	CYS	CA-CB-SG	6.00	124.79	114.00
3	A	305	LEU	CB-CG-CD1	5.89	121.01	111.00
3	C	305	LEU	CB-CG-CD1	5.89	121.01	111.00
3	E	305	LEU	CB-CG-CD1	5.89	121.01	111.00
3	A	111	LEU	CA-CB-CG	5.78	128.58	115.30
3	C	111	LEU	CA-CB-CG	5.75	128.51	115.30
3	E	111	LEU	CA-CB-CG	5.74	128.51	115.30
3	A	229	GLU	CA-CB-CG	5.58	125.69	113.40
3	C	229	GLU	CA-CB-CG	5.57	125.65	113.40
3	E	229	GLU	CA-CB-CG	5.55	125.61	113.40
4	B	621	ASP	CB-CG-OD2	5.44	123.20	118.30
2	U	11	LEU	CA-CB-CG	5.41	127.74	115.30
4	F	621	ASP	CB-CG-OD2	5.40	123.16	118.30
2	X	11	LEU	CA-CB-CG	5.40	127.72	115.30
2	H	11	LEU	CA-CB-CG	5.40	127.71	115.30
4	D	621	ASP	CB-CG-OD2	5.38	123.14	118.30
1	Z	47	LEU	CB-CG-CD1	-5.32	101.96	111.00
4	D	617	LYS	CA-CB-CG	5.28	125.00	113.40
4	B	617	LYS	CA-CB-CG	5.27	124.99	113.40
4	F	617	LYS	CA-CB-CG	5.25	124.95	113.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	235	GLU	Sidechain
3	C	235	GLU	Sidechain
3	E	235	GLU	Sidechain

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	L	827	0	815	5	0
1	P	827	0	815	7	0
1	Z	827	0	815	7	0
2	H	909	0	888	1	0
2	U	909	0	888	1	0
2	X	909	0	888	1	0
3	A	1972	0	1885	24	0
3	C	1972	0	1885	24	0
3	E	1972	0	1885	20	0
4	B	1032	0	998	17	0
4	D	1032	0	998	15	0
4	F	1032	0	998	13	0
5	G	50	0	43	0	0
5	I	50	0	43	0	0
5	J	50	0	43	0	0
6	A	11	0	10	0	0
6	C	11	0	10	0	0
6	E	11	0	10	0	0
7	B	14	0	13	1	0
7	D	14	0	13	1	0
7	F	14	0	13	1	0
All	All	14445	0	13956	120	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 (120) 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)
4:B:622:LYS:NZ	7:B:701:NAG:O7	2.31	0.63
4:D:622:LYS:NZ	7:D:701:NAG:O7	2.31	0.62
4:F:622:LYS:NZ	7:F:701:NAG:O7	2.31	0.62
4:B:602:HIS:ND1	4:F:611:GLU:OE2	2.32	0.62
3:A:79:VAL:HG13	3:A:80:PRO:HD3	1.83	0.60
3:E:79:VAL:HG13	3:E:80:PRO:HD3	1.82	0.60
3:C:79:VAL:HG13	3:C:80:PRO:HD3	1.83	0.60
3:A:253:LEU:HA	3:A:256:LEU:HG	1.86	0.56
3:A:269:THR:HG23	3:A:271:GLY:H	1.70	0.56
3:C:253:LEU:HA	3:C:256:LEU:HG	1.86	0.56
3:C:141:VAL:HG12	3:C:220:TYR:HB2	1.88	0.56
3:C:274:ILE:HG13	3:C:276:LYS:HZ1	1.70	0.56
3:E:269:THR:HG23	3:E:271:GLY:H	1.70	0.56
3:E:274:ILE:HG13	3:E:276:LYS:HZ1	1.70	0.56
3:E:253:LEU:HA	3:E:256:LEU:HG	1.86	0.55
3:C:269:THR:HG23	3:C:271:GLY:H	1.70	0.55
3:C:104:TRP:HE1	4:D:545:GLU:HG2	1.71	0.55
3:E:141:VAL:HG12	3:E:220:TYR:HB2	1.88	0.55
1:P:29:VAL:HG21	1:P:90:GLN:HB2	1.89	0.54
3:A:141:VAL:HG12	3:A:220:TYR:HB2	1.88	0.54
3:A:275:TRP:O	3:A:276:LYS:NZ	2.42	0.53
3:C:275:TRP:O	3:C:276:LYS:NZ	2.41	0.53
1:L:29:VAL:HG21	1:L:90:GLN:HB2	1.91	0.52
3:E:235:GLU:HG2	3:E:241:TYR:CE1	2.44	0.52
3:C:235:GLU:HG2	3:C:241:TYR:CE1	2.44	0.52
2:U:102:PRO:HB2	1:P:96:LEU:HD11	1.91	0.52
4:B:517:TYR:HE2	4:B:548:MET:HG3	1.75	0.52
3:A:235:GLU:HG2	3:A:241:TYR:CE1	2.44	0.51
4:B:612:PRO:O	4:B:616:THR:N	2.43	0.51
4:F:517:TYR:HE2	4:F:548:MET:HG3	1.75	0.51
3:E:243:GLN:HE21	3:E:274:ILE:HG12	1.75	0.51
3:C:219:ARG:HB3	3:C:235:GLU:OE1	2.10	0.51
3:C:256:LEU:O	3:C:260:ILE:HG12	2.11	0.51
3:E:219:ARG:HB3	3:E:235:GLU:OE1	2.10	0.51
3:A:219:ARG:HB3	3:A:235:GLU:OE1	2.10	0.51
3:C:243:GLN:HE21	3:C:274:ILE:HG12	1.75	0.51
3:E:256:LEU:O	3:E:260:ILE:HG12	2.11	0.51
3:C:243:GLN:HG2	3:C:274:ILE:HD11	1.93	0.51
3:A:243:GLN:HE21	3:A:274:ILE:HG12	1.75	0.51
3:A:256:LEU:O	3:A:260:ILE:HG12	2.11	0.51
3:A:243:GLN:HG2	3:A:274:ILE:HD11	1.93	0.51
1:Z:29:VAL:HG21	1:Z:90:GLN:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:96:LEU:HD11	2:H:102:PRO:HB2	1.93	0.50
4:D:517:TYR:HE2	4:D:548:MET:HG3	1.75	0.50
3:E:243:GLN:HG2	3:E:274:ILE:HD11	1.93	0.50
2:X:102:PRO:HB2	1:Z:96:LEU:HD11	1.94	0.50
4:D:612:PRO:O	4:D:616:THR:N	2.43	0.50
3:E:275:TRP:O	3:E:276:LYS:NZ	2.41	0.49
4:B:624:ASP:OD1	4:B:628:HIS:NE2	2.46	0.49
4:F:612:PRO:O	4:F:616:THR:N	2.43	0.49
3:A:78:ASP:OD1	3:A:246:SER:OG	2.23	0.49
4:D:624:ASP:OD1	4:D:628:HIS:NE2	2.46	0.49
4:B:619:ILE:HG23	4:B:622:LYS:HE2	1.95	0.48
3:C:235:GLU:HA	3:C:241:TYR:HD1	1.78	0.48
4:F:619:ILE:HG23	4:F:622:LYS:HE2	1.95	0.48
3:E:235:GLU:HA	3:E:241:TYR:HD1	1.78	0.48
4:F:517:TYR:CE2	4:F:548:MET:HG3	2.49	0.48
4:F:624:ASP:OD1	4:F:628:HIS:NE2	2.46	0.48
4:D:619:ILE:HG23	4:D:622:LYS:HE2	1.95	0.47
1:Z:37:GLN:OE1	1:Z:45:ARG:NH2	2.47	0.47
4:D:517:TYR:CE2	4:D:548:MET:HG3	2.49	0.47
4:B:517:TYR:CE2	4:B:548:MET:HG3	2.49	0.47
1:Z:85:VAL:HA	1:Z:102:THR:O	2.14	0.47
3:A:235:GLU:HA	3:A:241:TYR:HD1	1.78	0.47
4:D:560:GLN:O	4:D:563:ASN:HB3	2.15	0.47
3:C:42:ALA:HA	4:D:554:LEU:HD21	1.96	0.47
4:F:603:ILE:HD13	4:F:610:ILE:HG23	1.97	0.47
1:P:37:GLN:OE1	1:P:45:ARG:NH2	2.48	0.47
3:A:223:THR:HB	3:A:231:GLU:HG3	1.97	0.46
3:C:78:ASP:OD2	3:C:78:ASP:N	2.49	0.46
3:A:42:ALA:HA	4:B:554:LEU:HD21	1.96	0.46
3:E:78:ASP:OD1	3:E:246:SER:OG	2.23	0.46
1:L:37:GLN:OE1	1:L:45:ARG:NH2	2.48	0.46
3:C:265:LYS:HE3	3:C:307:PHE:HB2	1.98	0.46
3:A:265:LYS:HE3	3:A:307:PHE:HB2	1.98	0.46
3:A:195:SER:HB2	4:B:544:ILE:HD12	1.97	0.46
4:D:603:ILE:HD13	4:D:610:ILE:HG23	1.97	0.46
3:A:78:ASP:OD2	3:A:78:ASP:N	2.49	0.46
4:B:560:GLN:O	4:B:563:ASN:HB3	2.15	0.46
4:F:560:GLN:O	4:F:563:ASN:HB3	2.15	0.46
3:A:194:PHE:HB3	4:B:517:TYR:CE1	2.51	0.45
1:P:85:VAL:HA	1:P:102:THR:O	2.16	0.45
3:C:223:THR:HB	3:C:231:GLU:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:265:LYS:HE3	3:E:307:PHE:HB2	1.98	0.45
4:B:603:ILE:HD13	4:B:610:ILE:HG23	1.97	0.45
3:E:223:THR:HB	3:E:231:GLU:HG3	1.97	0.45
1:Z:86:TYR:O	1:Z:101:GLY:HA2	2.17	0.45
3:E:78:ASP:OD2	3:E:78:ASP:N	2.49	0.45
3:A:58:SER:O	4:D:595:GLN:NE2	2.50	0.45
3:C:194:PHE:HB3	4:D:517:TYR:CE1	2.52	0.45
3:A:220:TYR:HE2	3:A:244:LEU:HD22	1.82	0.45
3:A:63:LEU:HD13	4:B:585:LEU:HB3	1.98	0.44
3:C:220:TYR:HE2	3:C:244:LEU:HD22	1.82	0.44
1:L:85:VAL:HA	1:L:102:THR:O	2.18	0.44
4:B:506:ASN:ND2	4:B:556:CYS:O	2.35	0.44
4:F:588:LYS:HE2	4:F:588:LYS:HB2	1.80	0.44
4:B:503:ALA:HB1	1:P:94:TRP:CE2	2.54	0.43
3:E:220:TYR:HE2	3:E:244:LEU:HD22	1.82	0.43
4:D:506:ASN:ND2	4:D:556:CYS:O	2.35	0.43
3:A:258:GLU:O	3:A:262:THR:HG22	2.19	0.43
3:A:104:TRP:HE1	4:B:545:GLU:HG2	1.84	0.42
3:C:258:GLU:O	3:C:262:THR:HG22	2.19	0.42
4:D:620:THR:HA	4:D:623:ILE:HG12	2.01	0.42
4:F:620:THR:HA	4:F:623:ILE:HG12	2.02	0.42
3:E:35:LEU:HD23	3:E:50:LYS:HZ1	1.85	0.42
4:F:610:ILE:HD12	4:F:610:ILE:HA	1.91	0.42
3:C:269:THR:HG23	3:C:271:GLY:N	2.35	0.42
1:P:11:LEU:HD22	1:P:104:VAL:HG12	2.02	0.42
4:D:610:ILE:HD12	4:D:610:ILE:HA	1.91	0.42
1:L:86:TYR:O	1:L:101:GLY:HA2	2.20	0.41
3:C:35:LEU:HD23	3:C:50:LYS:HZ1	1.85	0.41
3:E:258:GLU:O	3:E:262:THR:HG22	2.19	0.41
1:P:86:TYR:O	1:P:101:GLY:HA2	2.20	0.41
1:Z:11:LEU:HD22	1:Z:104:VAL:HG12	2.03	0.41
4:F:503:ALA:HB1	1:Z:94:TRP:CE2	2.55	0.41
3:C:261:TYR:HD2	3:C:266:ARG:HH12	1.69	0.41
4:B:620:THR:HA	4:B:623:ILE:HG12	2.02	0.40
3:E:47:ASP:O	3:E:49:ASP:N	2.53	0.40
3:C:47:ASP:O	3:C:49:ASP:N	2.53	0.40
3:A:261:TYR:HD2	3:A:266:ARG:HH12	1.70	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	L	107/214 (50%)	103 (96%)	4 (4%)	0	100	100
1	P	107/214 (50%)	103 (96%)	4 (4%)	0	100	100
1	Z	107/214 (50%)	103 (96%)	4 (4%)	0	100	100
2	H	118/224 (53%)	117 (99%)	1 (1%)	0	100	100
2	U	118/224 (53%)	117 (99%)	1 (1%)	0	100	100
2	X	118/224 (53%)	117 (99%)	1 (1%)	0	100	100
3	A	241/322 (75%)	224 (93%)	16 (7%)	1 (0%)	34	69
3	C	241/322 (75%)	224 (93%)	16 (7%)	1 (0%)	34	69
3	E	241/322 (75%)	224 (93%)	16 (7%)	1 (0%)	34	69
4	B	128/168 (76%)	121 (94%)	7 (6%)	0	100	100
4	D	128/168 (76%)	121 (94%)	7 (6%)	0	100	100
4	F	128/168 (76%)	121 (94%)	7 (6%)	0	100	100
All	All	1782/2784 (64%)	1695 (95%)	84 (5%)	3 (0%)	50	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	190	LYS
3	C	190	LYS
3	E	190	LYS

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	L	90/184 (49%)	88 (98%)	2 (2%)	52	78
1	P	90/184 (49%)	88 (98%)	2 (2%)	52	78
1	Z	90/184 (49%)	88 (98%)	2 (2%)	52	78
2	H	98/188 (52%)	97 (99%)	1 (1%)	76	90
2	U	98/188 (52%)	97 (99%)	1 (1%)	76	90
2	X	98/188 (52%)	97 (99%)	1 (1%)	76	90
3	A	211/243 (87%)	195 (92%)	16 (8%)	13	41
3	C	211/243 (87%)	195 (92%)	16 (8%)	13	41
3	E	211/243 (87%)	195 (92%)	16 (8%)	13	41
4	B	109/140 (78%)	106 (97%)	3 (3%)	43	73
4	D	109/140 (78%)	106 (97%)	3 (3%)	43	73
4	F	109/140 (78%)	106 (97%)	3 (3%)	43	73
All	All	1524/2265 (67%)	1458 (96%)	66 (4%)	34	62

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	22[A]	SER
1	L	22[B]	SER
2	H	5	LEU
3	A	46	SER
3	A	53	CYS
3	A	77	THR
3	A	79	VAL
3	A	127	ASP
3	A	150	ASP
3	A	227	THR
3	A	251	GLN
3	A	256	LEU
3	A	258	GLU
3	A	262	THR
3	A	269	THR
3	A	302	SER
3	A	305	LEU
3	A	308	THR
3	A	309	VAL
4	B	604	LEU
4	B	618	ASN
4	B	626	ILE

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Mol	Chain	Res	Type
3	C	46	SER
3	C	53	CYS
3	C	77	THR
3	C	79	VAL
3	C	127	ASP
3	C	150	ASP
3	C	227	THR
3	C	251	GLN
3	C	256	LEU
3	C	258	GLU
3	C	262	THR
3	C	269	THR
3	C	302	SER
3	C	305	LEU
3	C	308	THR
3	C	309	VAL
3	E	46	SER
3	E	53	CYS
3	E	77	THR
3	E	79	VAL
3	E	127	ASP
3	E	150	ASP
3	E	227	THR
3	E	251	GLN
3	E	256	LEU
3	E	258	GLU
3	E	262	THR
3	E	269	THR
3	E	302	SER
3	E	305	LEU
3	E	308	THR
3	E	309	VAL
4	D	604	LEU
4	D	618	ASN
4	D	626	ILE
4	F	604	LEU
4	F	618	ASN
4	F	626	ILE
2	X	5	LEU
2	U	5	LEU
1	Z	22[A]	SER
1	Z	22[B]	SER

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Mol	Chain	Res	Type
1	P	22[A]	SER
1	P	22[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	82	GLN
3	A	61	ASN
3	A	243	GLN
3	A	257	ASN
3	C	61	ASN
3	C	243	GLN
3	C	257	ASN
3	E	61	ASN
3	E	243	GLN
3	E	257	ASN
4	D	595	GLN
2	X	82	GLN
2	U	82	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)

12 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	G	1	4,5	14,14,15	0.44	0	17,19,21	0.85	1 (5%)
5	NAG	G	2	5	14,14,15	0.24	0	17,19,21	0.60	0
5	BMA	G	3	5	11,11,12	1.00	0	15,15,17	1.09	2 (13%)
5	MAN	G	4	5	11,11,12	1.52	3 (27%)	15,15,17	1.60	2 (13%)
5	NAG	I	1	4,5	14,14,15	0.44	0	17,19,21	0.86	1 (5%)
5	NAG	I	2	5	14,14,15	0.25	0	17,19,21	0.60	0
5	BMA	I	3	5	11,11,12	0.99	0	15,15,17	1.09	2 (13%)
5	MAN	I	4	5	11,11,12	1.51	3 (27%)	15,15,17	1.61	2 (13%)
5	NAG	J	1	4,5	14,14,15	0.44	0	17,19,21	0.86	1 (5%)
5	NAG	J	2	5	14,14,15	0.24	0	17,19,21	0.60	0
5	BMA	J	3	5	11,11,12	0.99	0	15,15,17	1.08	2 (13%)
5	MAN	J	4	5	11,11,12	1.52	3 (27%)	15,15,17	1.61	2 (13%)

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	G	1	4,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
5	MAN	G	4	5	-	0/2/19/22	1/1/1/1
5	NAG	I	1	4,5	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
5	MAN	I	4	5	-	0/2/19/22	1/1/1/1
5	NAG	J	1	4,5	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
5	BMA	J	3	5	-	0/2/19/22	0/1/1/1
5	MAN	J	4	5	-	0/2/19/22	1/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	4	MAN	O5-C5	3.08	1.49	1.43
5	G	4	MAN	O5-C5	3.06	1.49	1.43
5	I	4	MAN	O5-C5	3.05	1.49	1.43
5	G	4	MAN	C2-C3	2.64	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	4	MAN	C2-C3	2.63	1.56	1.52
5	J	4	MAN	C2-C3	2.61	1.56	1.52
5	G	4	MAN	C4-C3	2.25	1.58	1.52
5	J	4	MAN	C4-C3	2.22	1.58	1.52
5	I	4	MAN	C4-C3	2.22	1.58	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	4	MAN	C1-O5-C5	5.14	119.15	112.19
5	J	4	MAN	C1-O5-C5	5.13	119.14	112.19
5	G	4	MAN	C1-O5-C5	5.10	119.10	112.19
5	G	3	BMA	C1-O5-C5	2.42	115.47	112.19
5	J	3	BMA	C1-O5-C5	2.41	115.46	112.19
5	I	3	BMA	C1-O5-C5	2.40	115.44	112.19
5	J	1	NAG	O4-C4-C5	-2.18	103.88	109.30
5	I	1	NAG	O4-C4-C5	-2.17	103.90	109.30
5	G	4	MAN	O2-C2-C3	-2.17	105.79	110.14
5	J	4	MAN	O2-C2-C3	-2.16	105.82	110.14
5	G	1	NAG	O4-C4-C5	-2.15	103.95	109.30
5	I	4	MAN	O2-C2-C3	-2.14	105.85	110.14
5	I	3	BMA	O2-C2-C3	-2.11	105.91	110.14
5	G	3	BMA	O2-C2-C3	-2.09	105.95	110.14
5	J	3	BMA	O2-C2-C3	-2.06	106.01	110.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	2	NAG	O5-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
5	I	2	NAG	C4-C5-C6-O6
5	J	2	NAG	C4-C5-C6-O6

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	4	MAN	C1-C2-C3-C4-C5-O5
5	G	4	MAN	C1-C2-C3-C4-C5-O5

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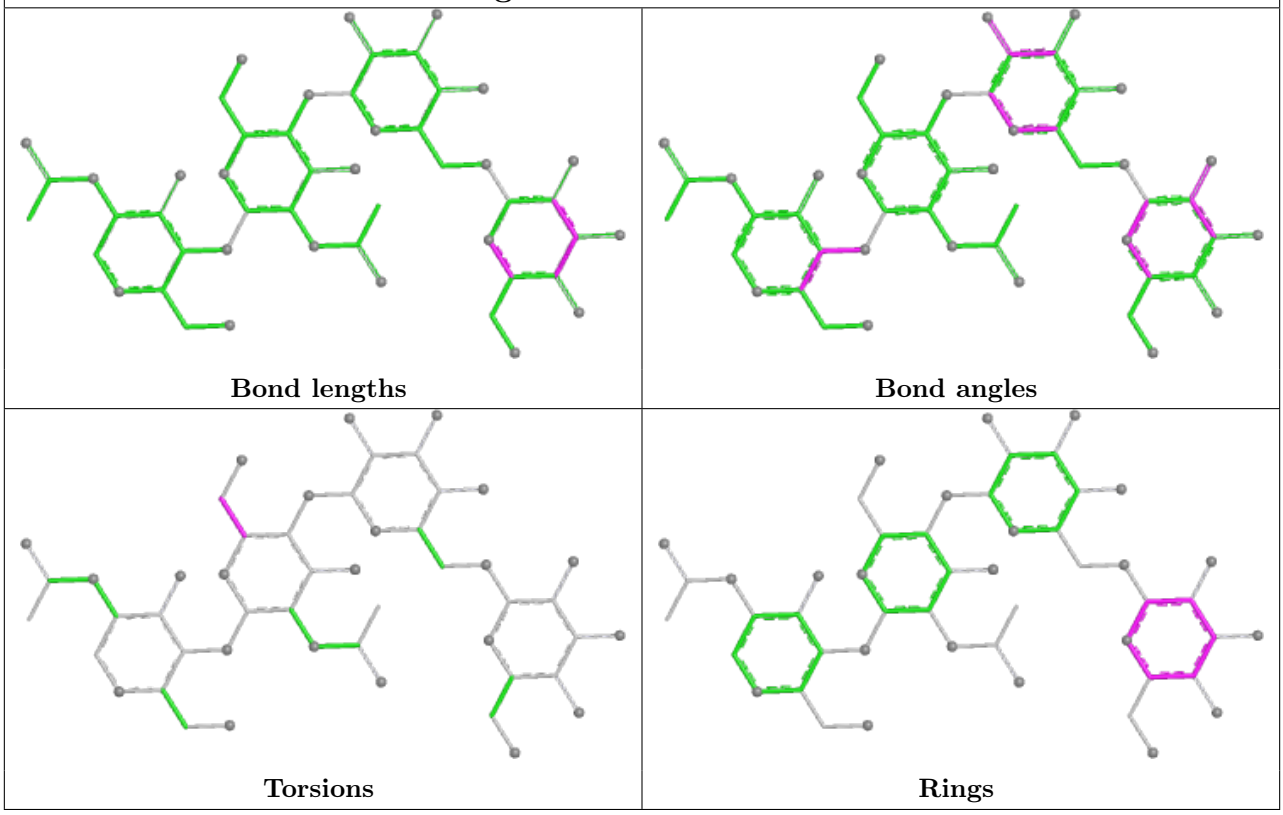
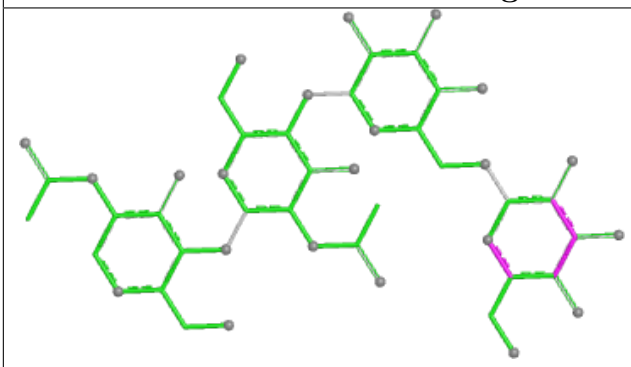
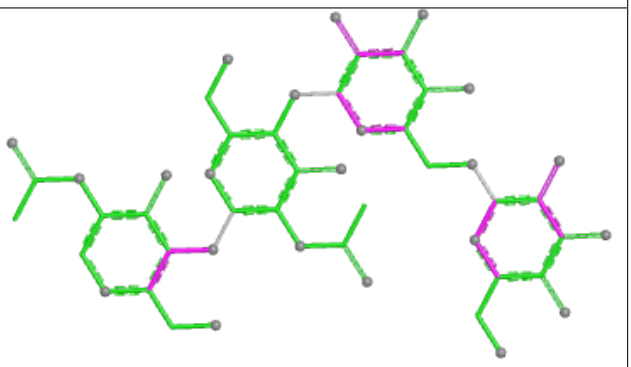
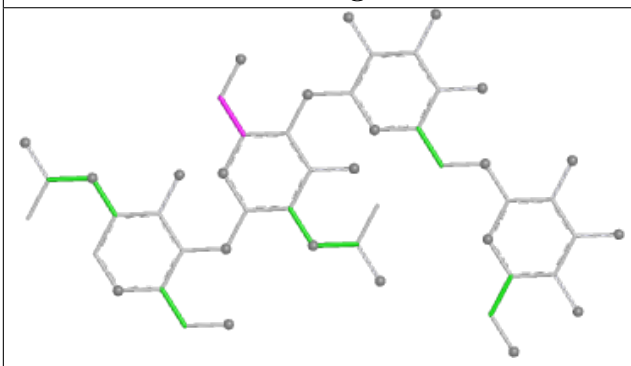
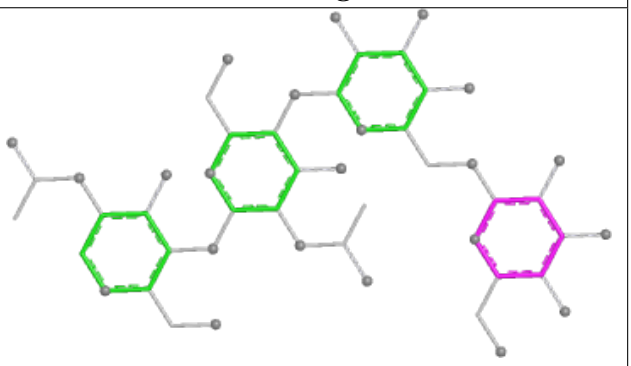
Mol	Chain	Res	Type	Atoms
5	I	4	MAN	C1-C2-C3-C4-C5-O5

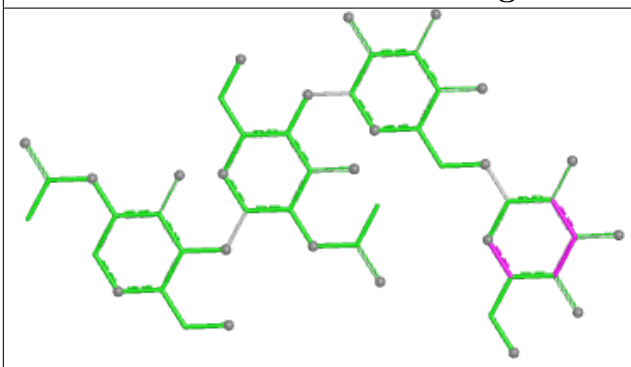
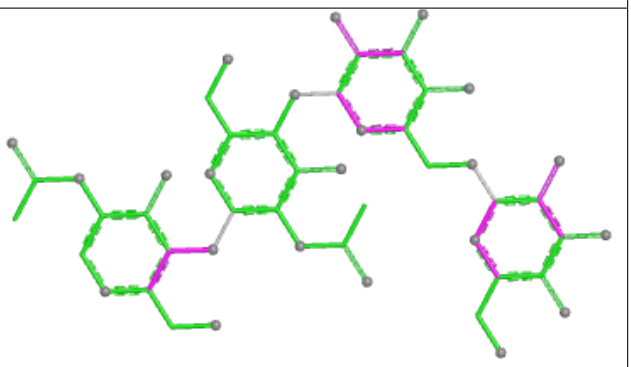
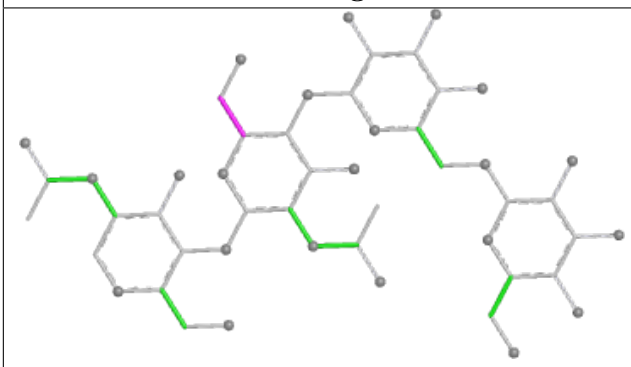
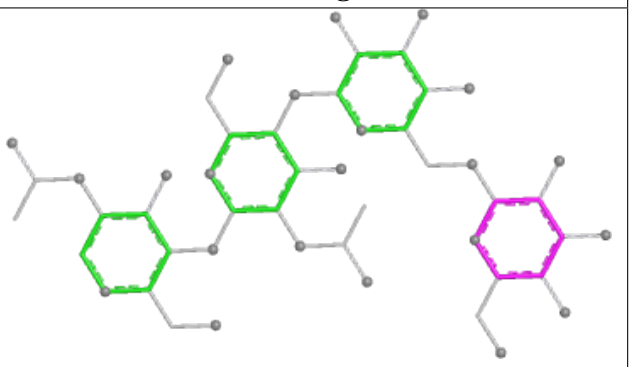
No monomer is involved in short contacts.

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

Oligosaccharide Chain G



Oligosaccharide Chain I	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain J	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
7	NAG	B	701	4	14,14,15	1.79	2 (14%)	17,19,21	1.53	1 (5%)
6	MAN	E	601	-	11,11,12	0.90	0	15,15,17	0.89	1 (6%)
7	NAG	F	701	4	14,14,15	1.80	2 (14%)	17,19,21	1.53	1 (5%)
6	MAN	C	601	-	11,11,12	0.89	0	15,15,17	0.88	1 (6%)
6	MAN	A	601	-	11,11,12	0.90	0	15,15,17	0.88	1 (6%)
7	NAG	D	701	4	14,14,15	1.80	2 (14%)	17,19,21	1.53	1 (5%)

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
7	NAG	B	701	4	-	2/6/23/26	0/1/1/1
6	MAN	E	601	-	-	2/2/19/22	0/1/1/1
7	NAG	F	701	4	-	2/6/23/26	0/1/1/1
6	MAN	C	601	-	-	2/2/19/22	0/1/1/1
6	MAN	A	601	-	-	2/2/19/22	0/1/1/1
7	NAG	D	701	4	-	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	701	NAG	O5-C1	5.60	1.52	1.43
7	F	701	NAG	O5-C1	5.60	1.52	1.43
7	B	701	NAG	O5-C1	5.57	1.52	1.43
7	F	701	NAG	C1-C2	3.43	1.57	1.52
7	B	701	NAG	C1-C2	3.42	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	701	NAG	C1-C2	3.40	1.57	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	701	NAG	C1-O5-C5	6.04	120.38	112.19
7	D	701	NAG	C1-O5-C5	6.04	120.37	112.19
7	F	701	NAG	C1-O5-C5	6.03	120.37	112.19
6	E	601	MAN	O2-C2-C3	-2.14	105.84	110.14
6	A	601	MAN	O2-C2-C3	-2.13	105.86	110.14
6	C	601	MAN	O2-C2-C3	-2.12	105.89	110.14

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	601	MAN	O5-C5-C6-O6
6	C	601	MAN	O5-C5-C6-O6
6	E	601	MAN	O5-C5-C6-O6
7	B	701	NAG	O5-C5-C6-O6
7	D	701	NAG	O5-C5-C6-O6
7	F	701	NAG	O5-C5-C6-O6
6	A	601	MAN	C4-C5-C6-O6
6	C	601	MAN	C4-C5-C6-O6
6	E	601	MAN	C4-C5-C6-O6
7	B	701	NAG	C4-C5-C6-O6
7	D	701	NAG	C4-C5-C6-O6
7	F	701	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	701	NAG	1	0
7	F	701	NAG	1	0
7	D	701	NAG	1	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
3	A	1
3	C	1
3	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	310:VAL	C	470:UNK	N	12.79
1	C	310:VAL	C	470:UNK	N	12.79
1	E	310:VAL	C	470:UNK	N	12.79

6 Map visualisation (i)

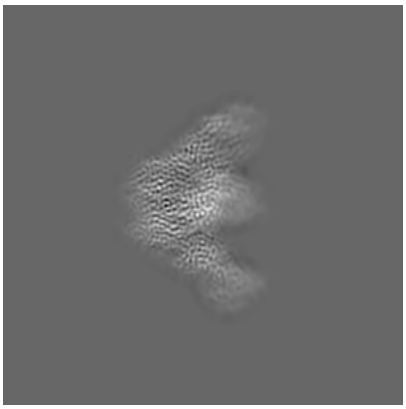
This section contains visualisations of the EMDB entry EMD-4520. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

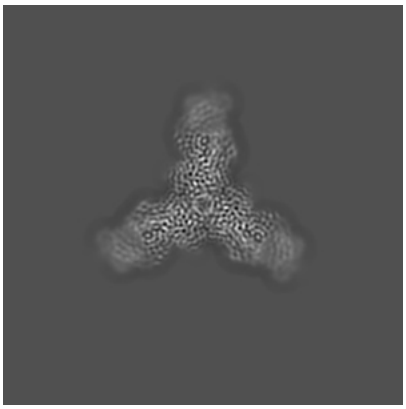
6.1 Orthogonal projections (i)

6.1.1 Primary map

X

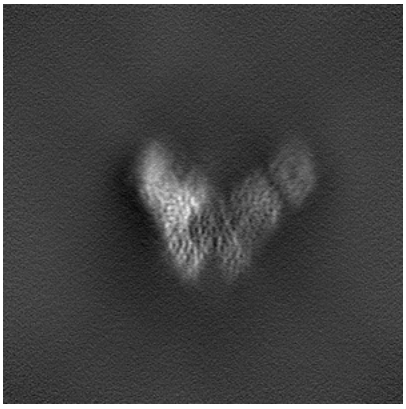


Y

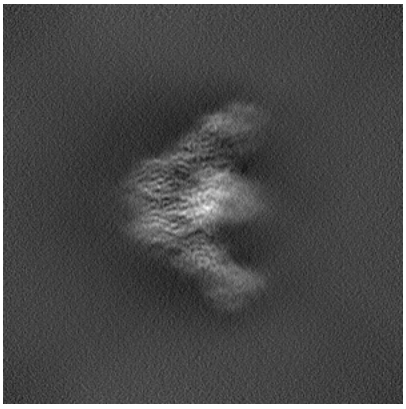


Z

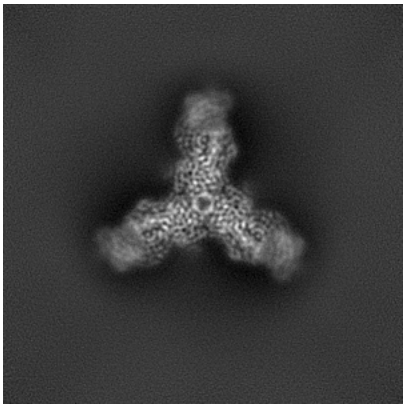
6.1.2 Raw map



X



Y



Z

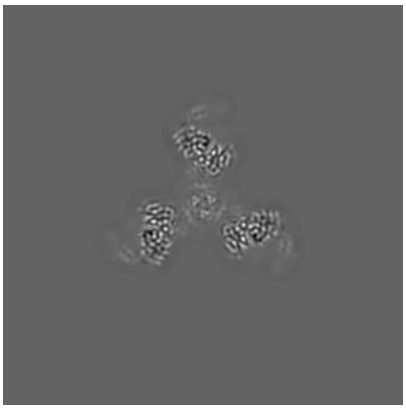
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

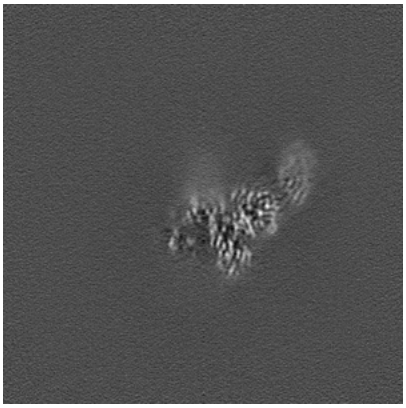
6.2.1 Primary map

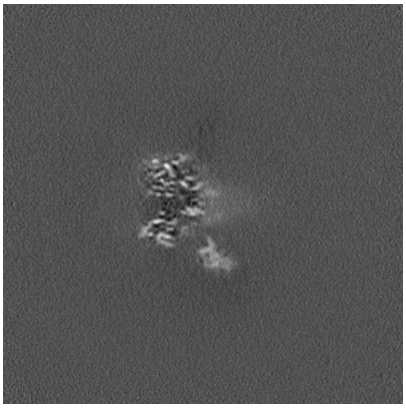
X Index: 180

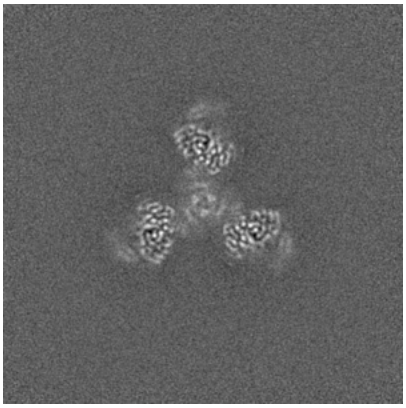
Y Index: 180


Z Index: 180

6.2.2 Raw map


X Index: 180


Y Index: 180


Z Index: 180

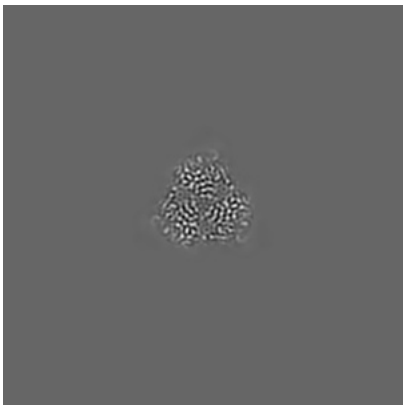
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

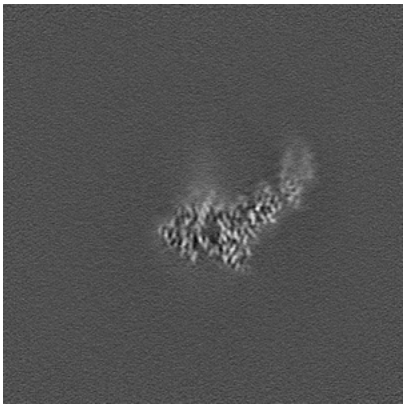
X Index: 172

Y Index: 165

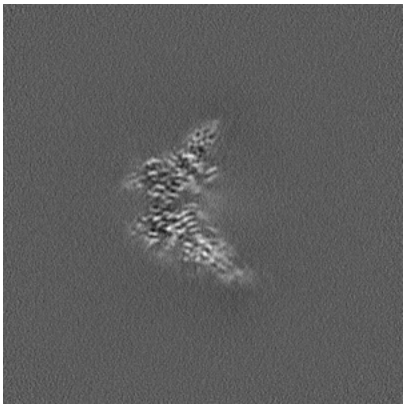


Z Index: 143

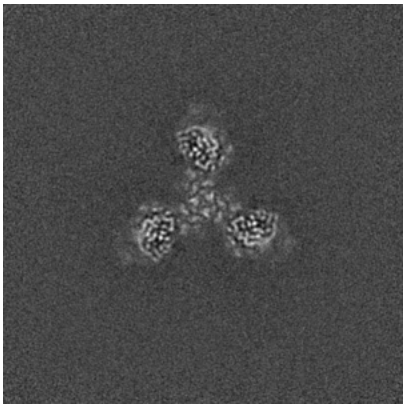
6.3.2 Raw map



X Index: 172



Y Index: 165

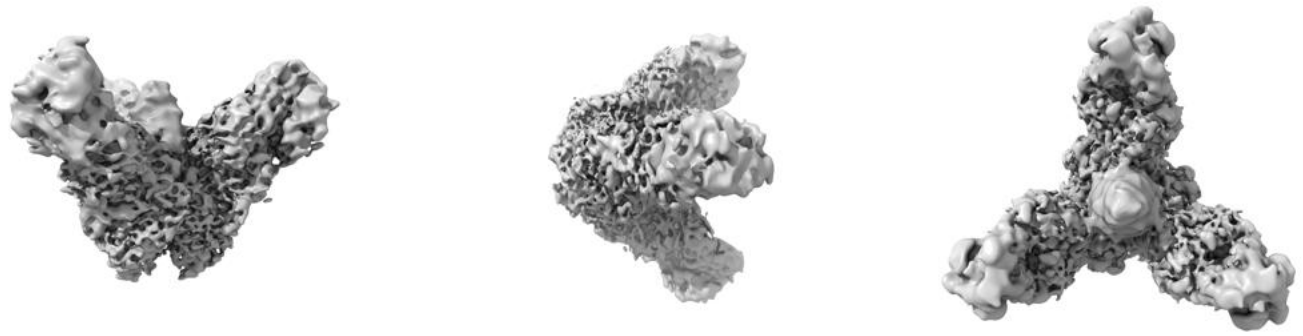


Z Index: 176

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

6.4 Orthogonal surface views (i)

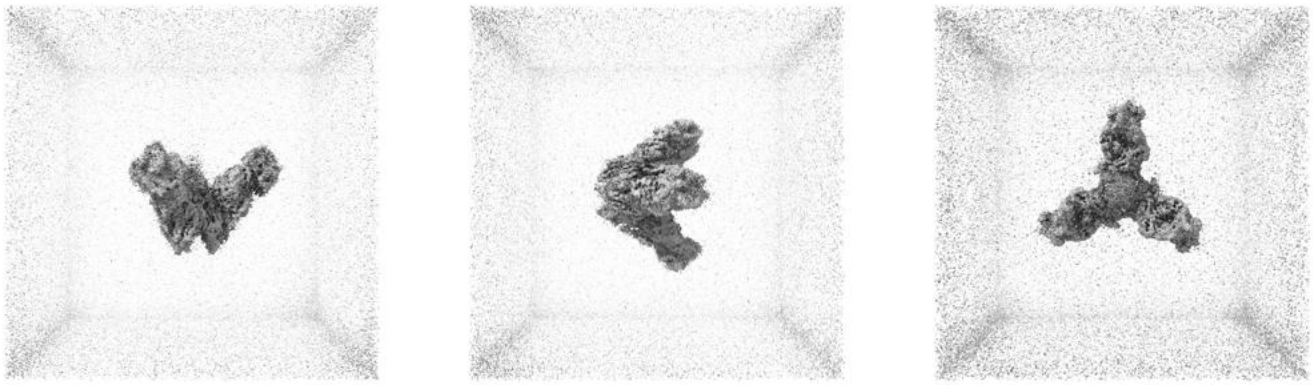
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.108. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

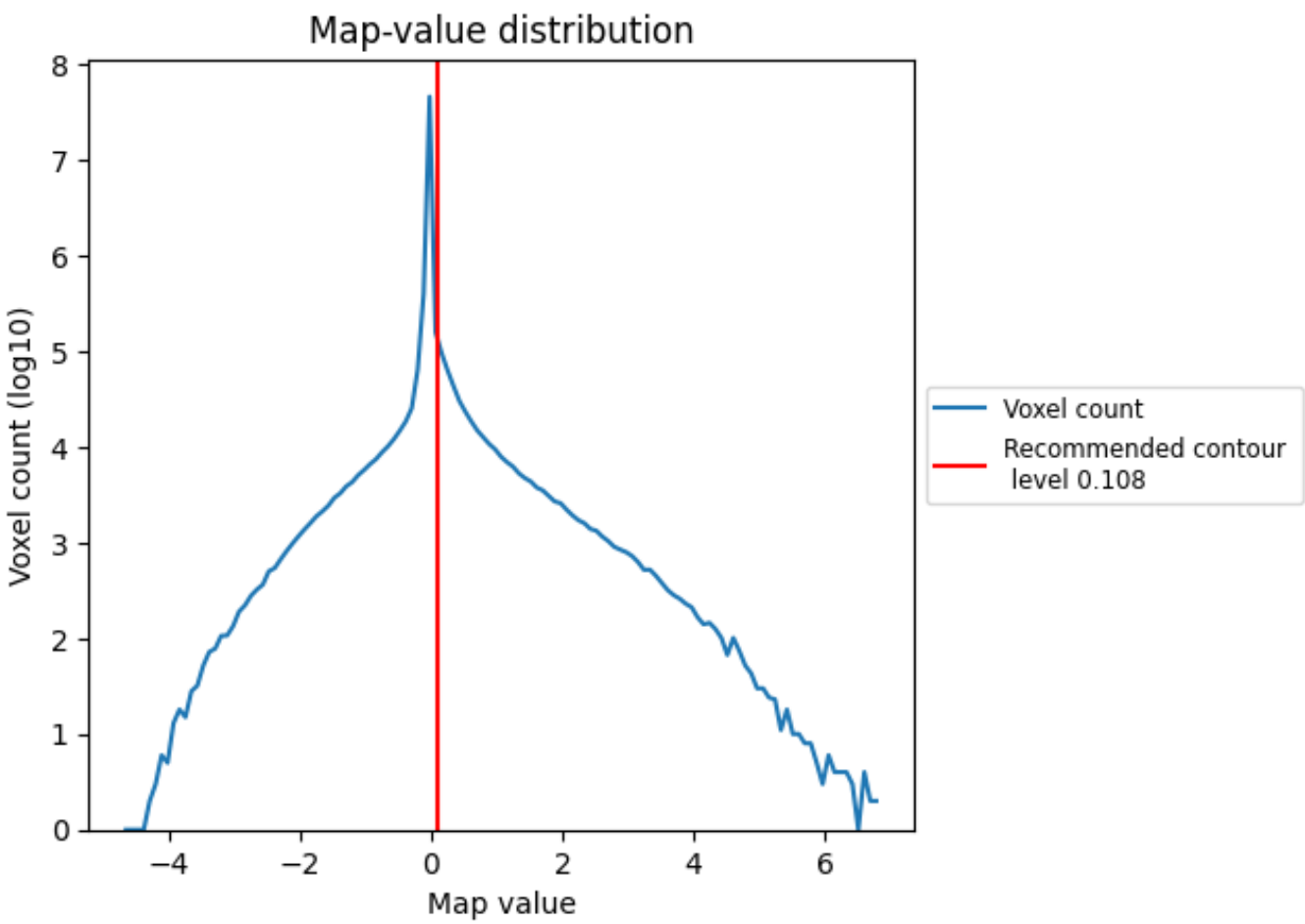
6.5 Mask visualisation (i)

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

7 Map analysis (i)

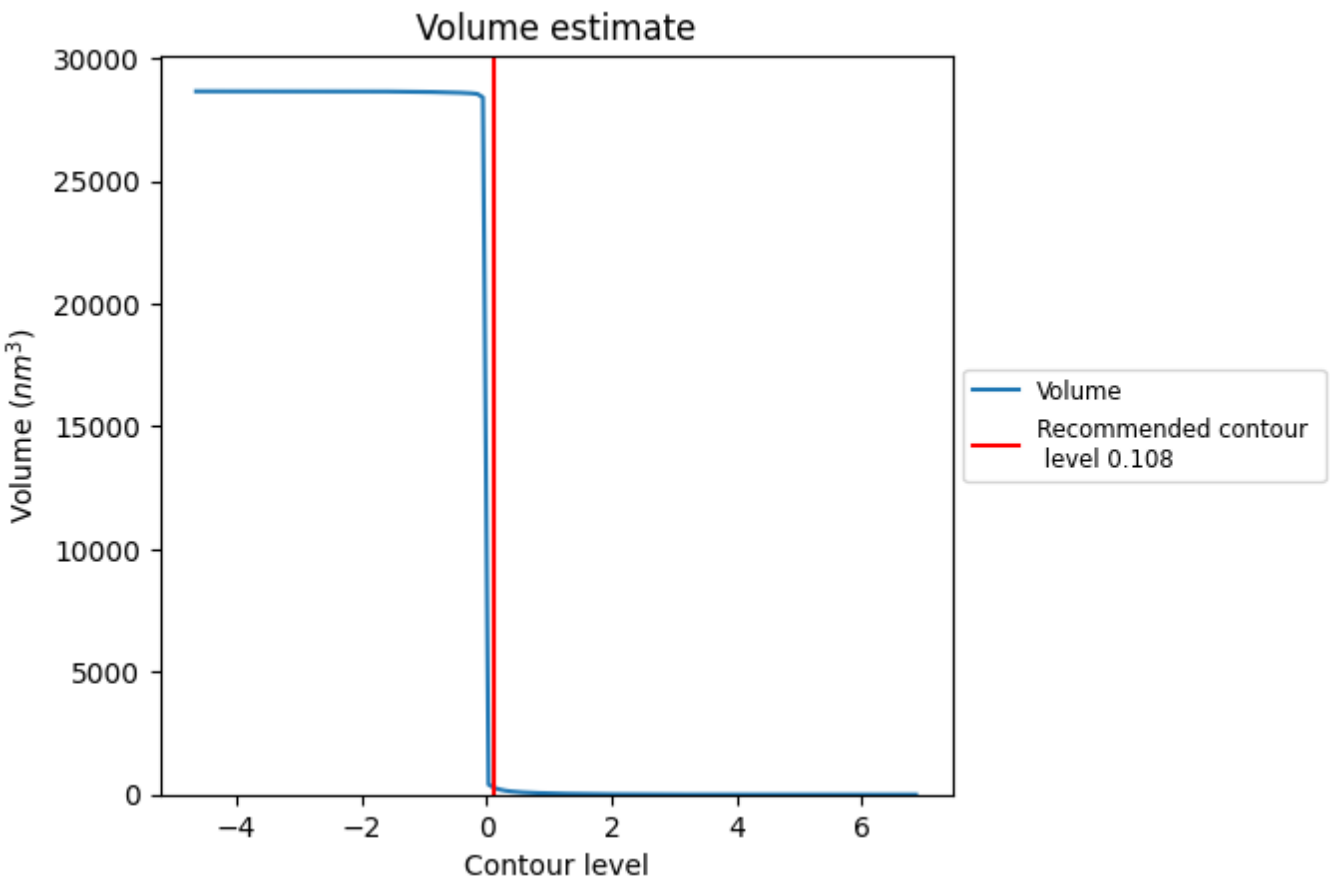
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

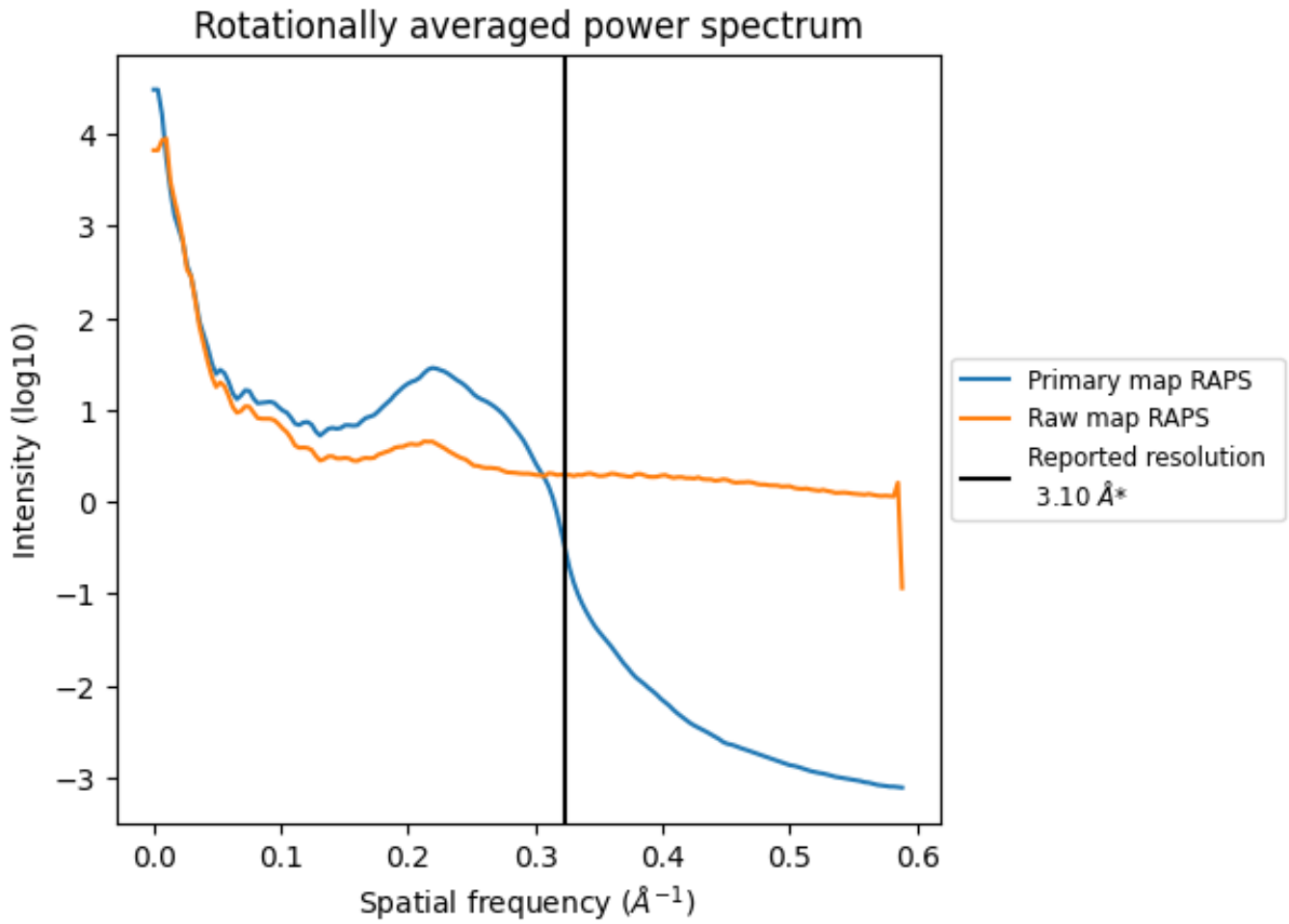
7.2 Volume estimate (i)



The volume at the recommended contour level is 294 nm^3; this corresponds to an approximate mass of 266 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)

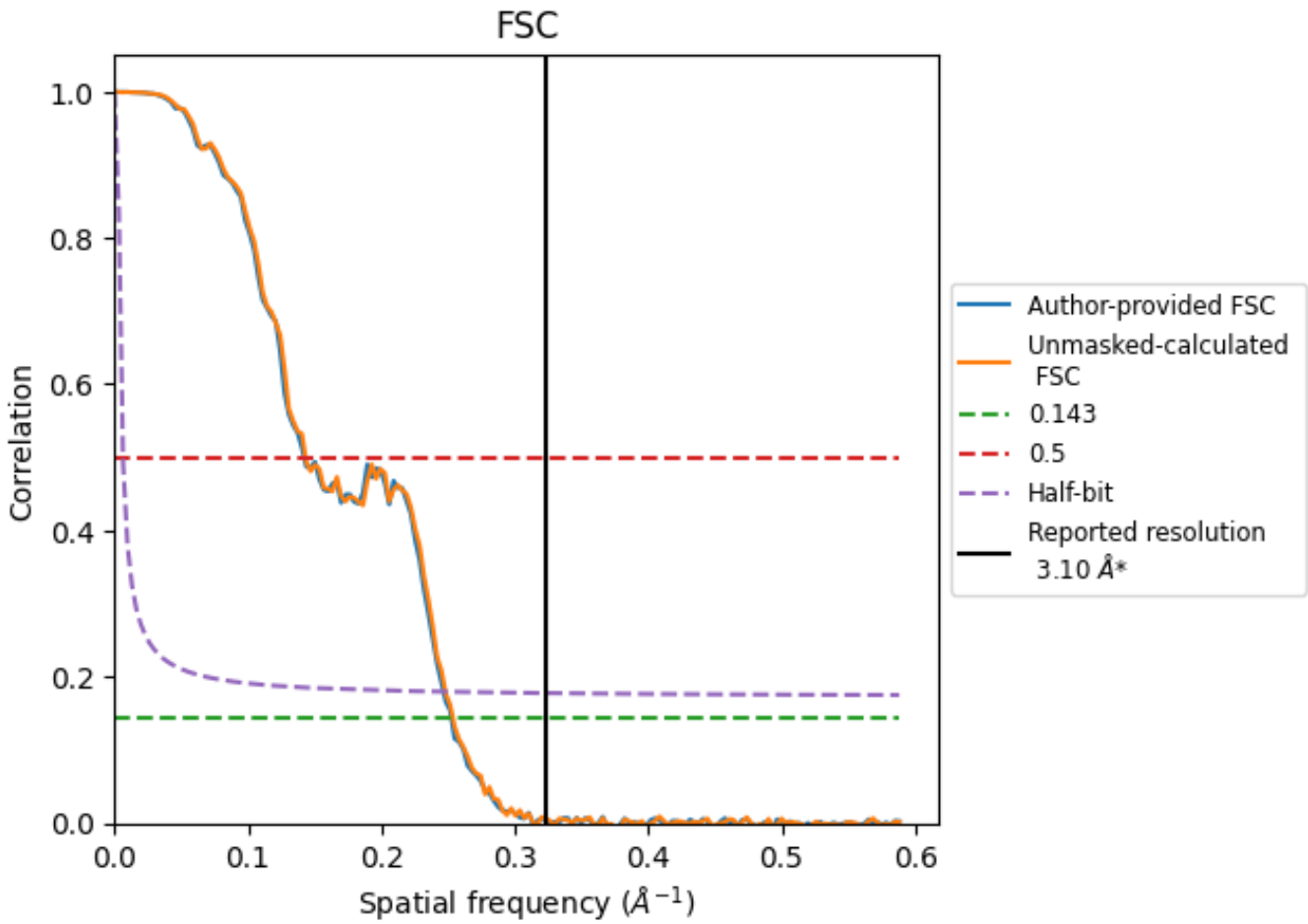


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.96	7.03	4.05
Unmasked-calculated*	3.94	6.98	4.03

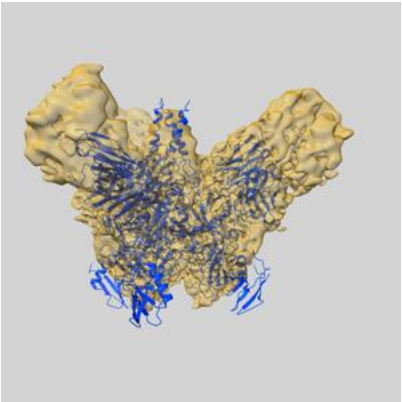
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.96 differs from the reported value 3.1 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.94 differs from the reported value 3.1 by more than 10 %

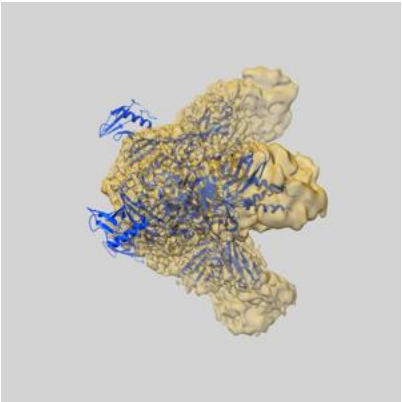
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4520 and PDB model 6QD7. Per-residue inclusion information can be found in section 3 on page 10.

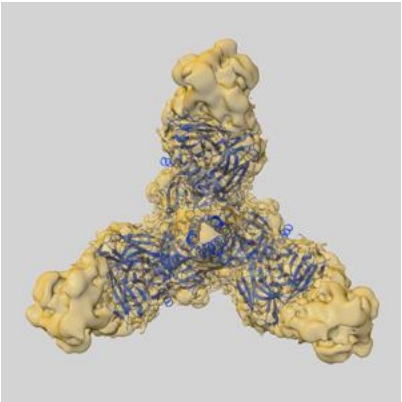
9.1 Map-model overlay (i)



X



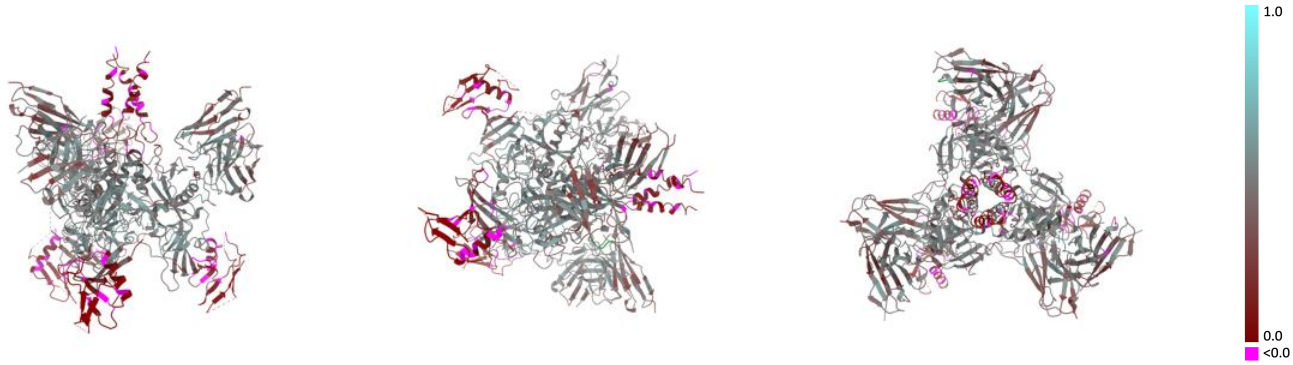
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.108 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.

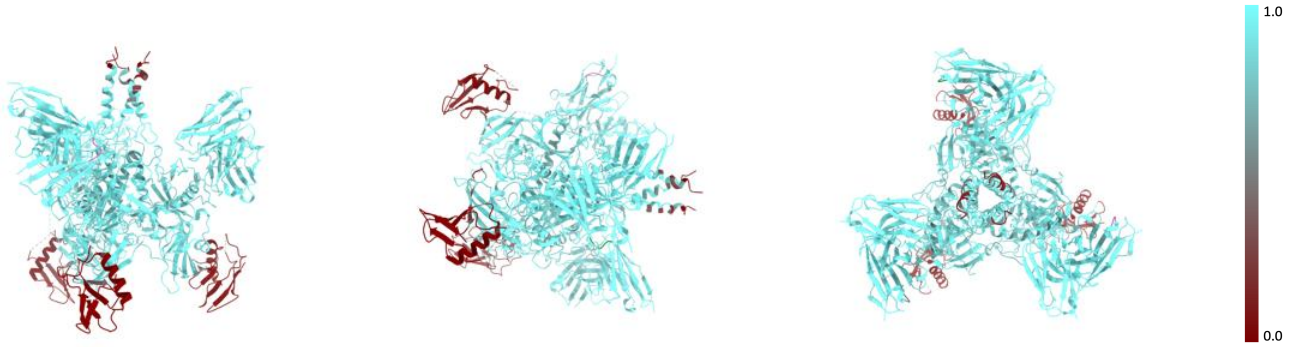
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

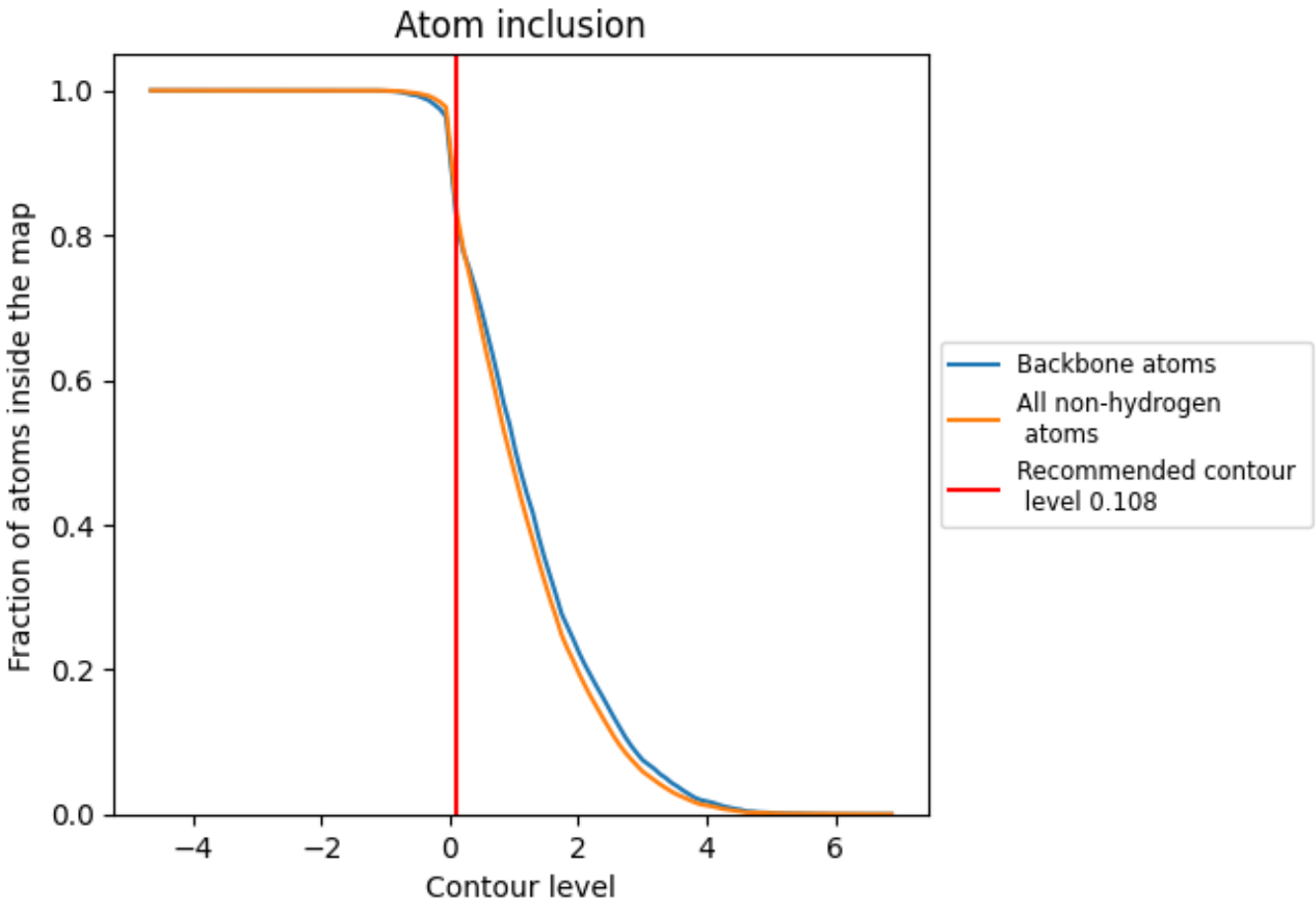
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.108).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 83% 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 (0.108) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8316	0.3860
A	0.6788	0.3370
B	0.8960	0.3860
C	0.6814	0.3350
D	0.8999	0.3810
E	0.6788	0.3390
F	0.8892	0.3780
G	0.9600	0.4680
H	0.9649	0.4490
I	0.9800	0.4750
J	0.9600	0.4620
L	0.9651	0.4370
P	0.9651	0.4380
U	0.9615	0.4490
X	0.9627	0.4470
Z	0.9664	0.4340