Full wwPDB EM Validation Report (i)

Jul 17, 2024 – 06:08 pm BST

PDB ID	:	7NYD
EMDB ID	:	EMD-12651
Title	:	cryoEM structure of 2C9-sMAC
Authors	:	Menny, A.; Couves, E.C.; Bubeck, D.
Deposited on	:	2021-03-22
Resolution	:	3.27 Å(reported)
Based on initial models	:	2WCY, 6H03, 6H04, 4A5W, 6CXO

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:

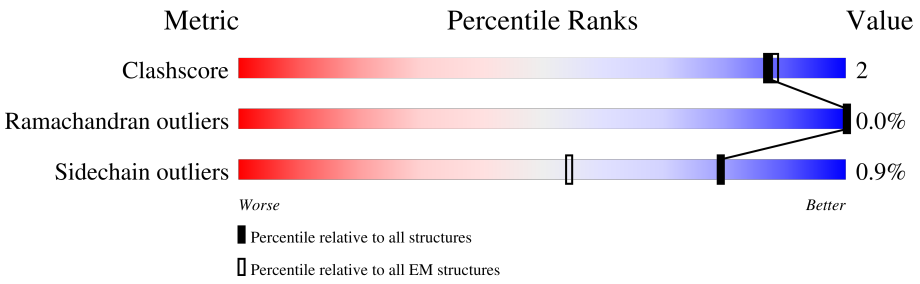
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.27 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	D	537	85% 5% • 9%
2	E	554	6% 82% 5% 13%
3	G	538	7% 73% • 23%
3	H	538	5% 55% • • 41%
4	C	821	19% 93% 5% ••
5	B	913	74% • 21%
6	F	182	88% • 8%
7	A	1658	5% 90% • 7%

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Mol	Chain	Length	Quality of chain
8	I	3	100%
9	J	2	50% 50%
10	K	5	40% 40% 20% 40%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	MAN	D	602	X	-	-	-
13	NAG	H	601	-	-	X	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 38430 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 Complement component C8 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	D	487	3914	2434	702	743	35	0	0

- Molecule 2 is a protein called Complement component C8 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	484	3819	2363	673	746	37	0	0

- Molecule 3 is a protein called Complement component C9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	413	3259	2036	561	633	29	0	0
3	H	319	2517	1578	427	496	16	0	0

- Molecule 4 is a protein called Complement component C7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	809	5977	3696	1054	1179	48	0	0

- Molecule 5 is a protein called Complement component C6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	718	5631	3479	993	1109	50	0	0

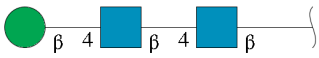
- Molecule 6 is a protein called Complement component C8 gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	168	1319	841	230	244	4	0	0

- Molecule 7 is a protein called Complement C5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	A	1542	11744	7507	1949	2251	37	0	0

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

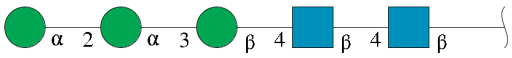


Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	I	3	39	22	2	15	0	0

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

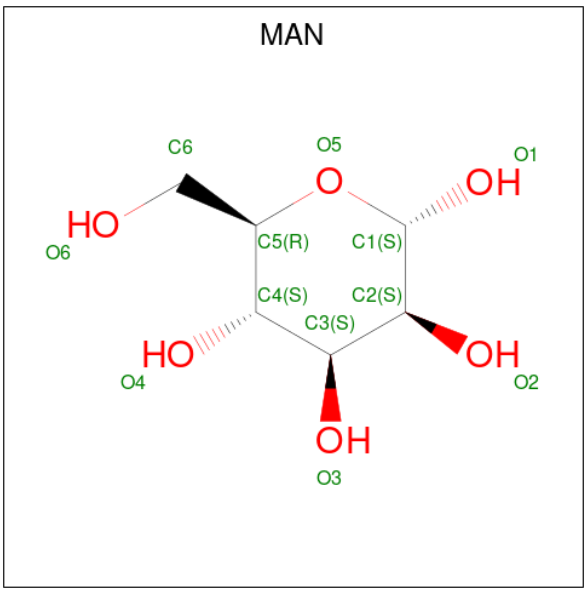
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	J	2	28	16	2	10	0	0

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-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		
10	K	5	61	34	2	25	0	0

- Molecule 11 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



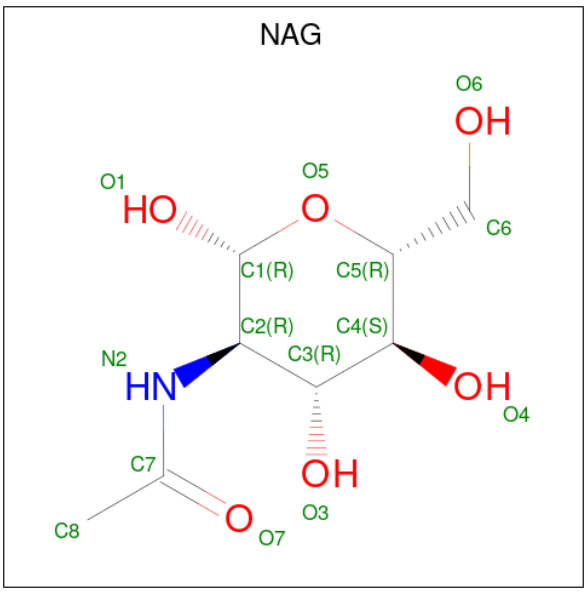
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
11	D	1	11	6	5	0
			Total	C	O	
11	D	1	11	6	5	0
			Total	C	O	
11	E	1	11	6	5	0
			Total	C	O	
11	E	1	11	6	5	0
			Total	C	O	
11	G	1	11	6	5	0
			Total	C	O	
11	C	1	11	6	5	0

- Molecule 12 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
12	D	1	1	1	0
			Total	Ca	
12	E	1	1	1	0
			Total	Ca	
12	G	1	1	1	0
			Total	Ca	
12	H	1	1	1	0

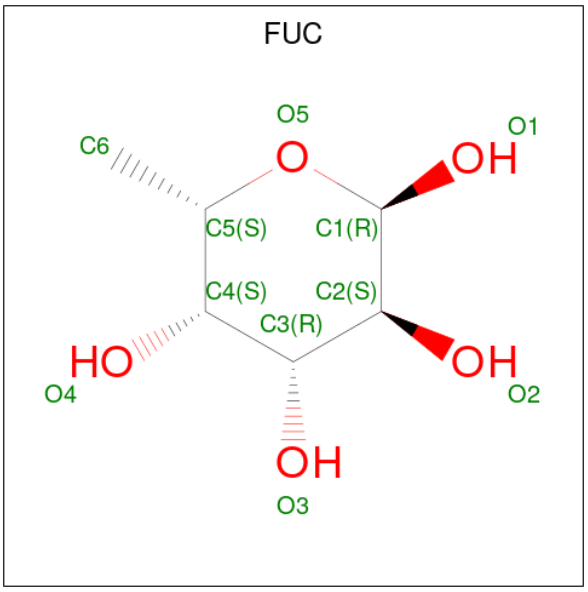
- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG)

(formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
13	G	1	14	8	1	5	0
13	B	1	14	8	1	5	0
13	H	1	14	8	1	5	0

- Molecule 14 is alpha-L-fucopyranose (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



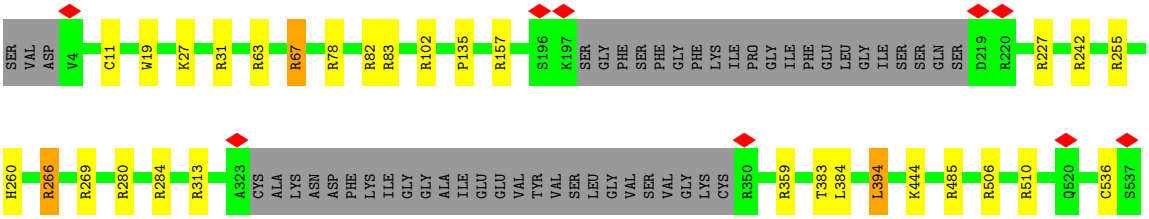
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
14	B	1	10	6	4	0

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.

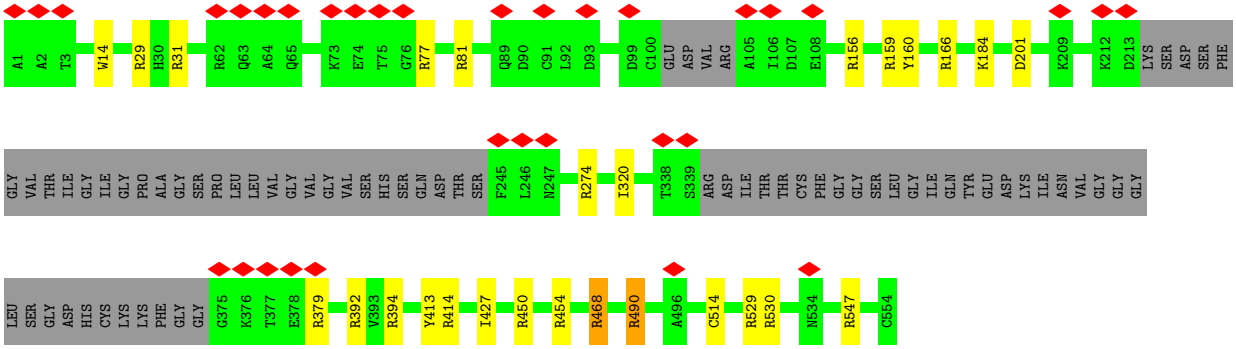
- Molecule 1: Complement component C8 beta chain

Chain D:



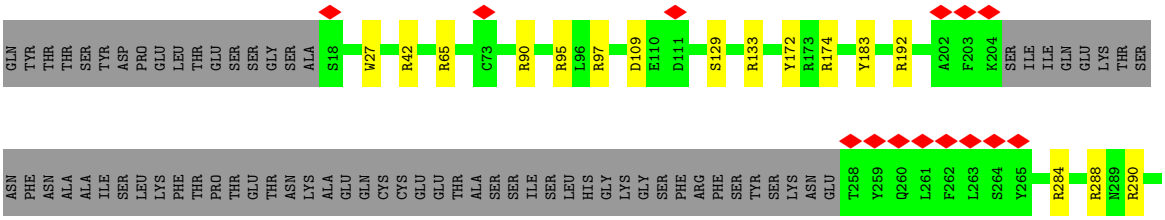
- Molecule 2: Complement component C8 alpha chain

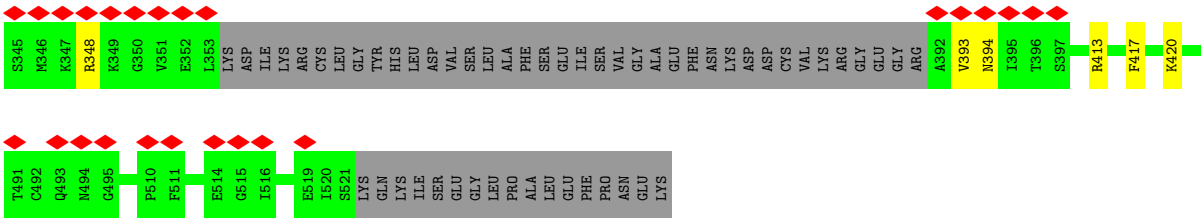
Chain E:



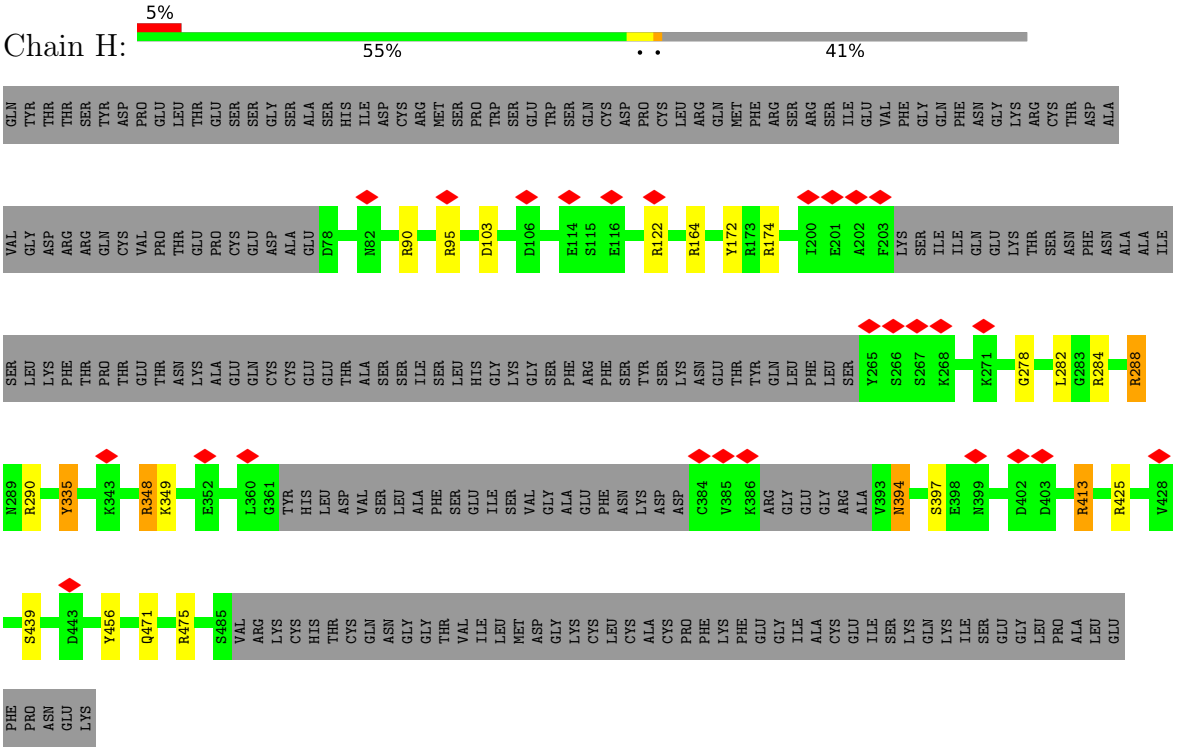
- Molecule 3: Complement component C9

Chain G:

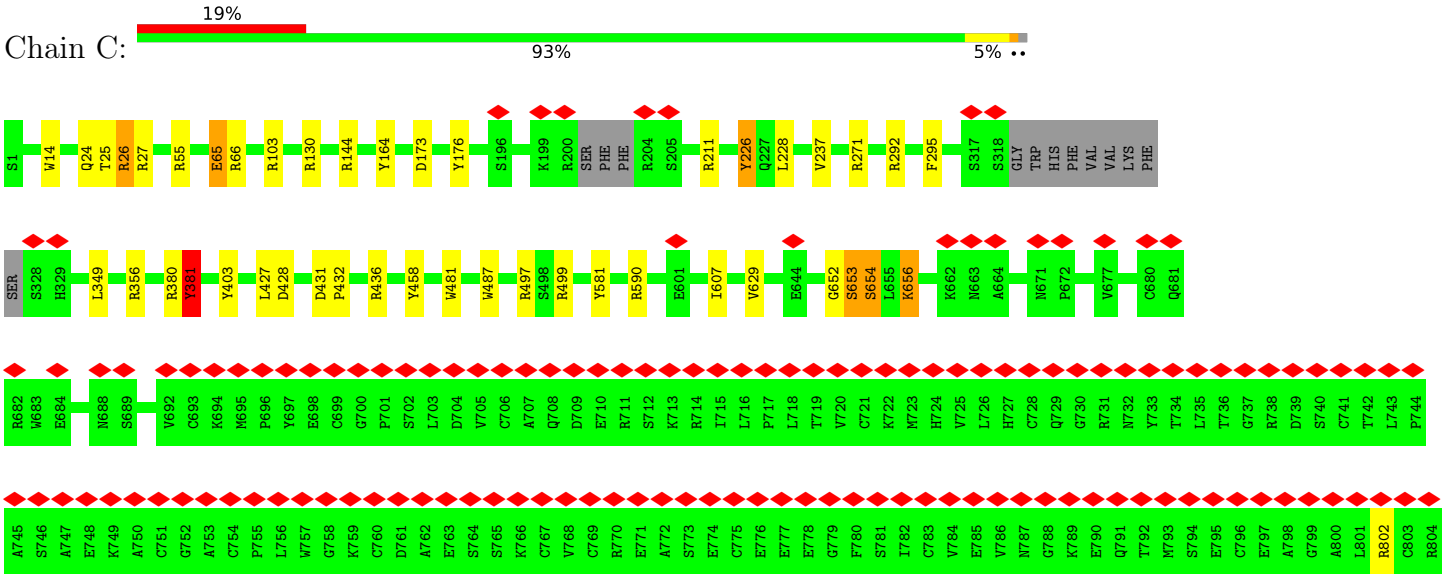


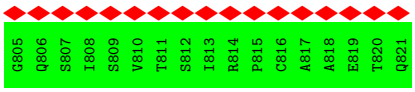


• Molecule 3: Complement component C9

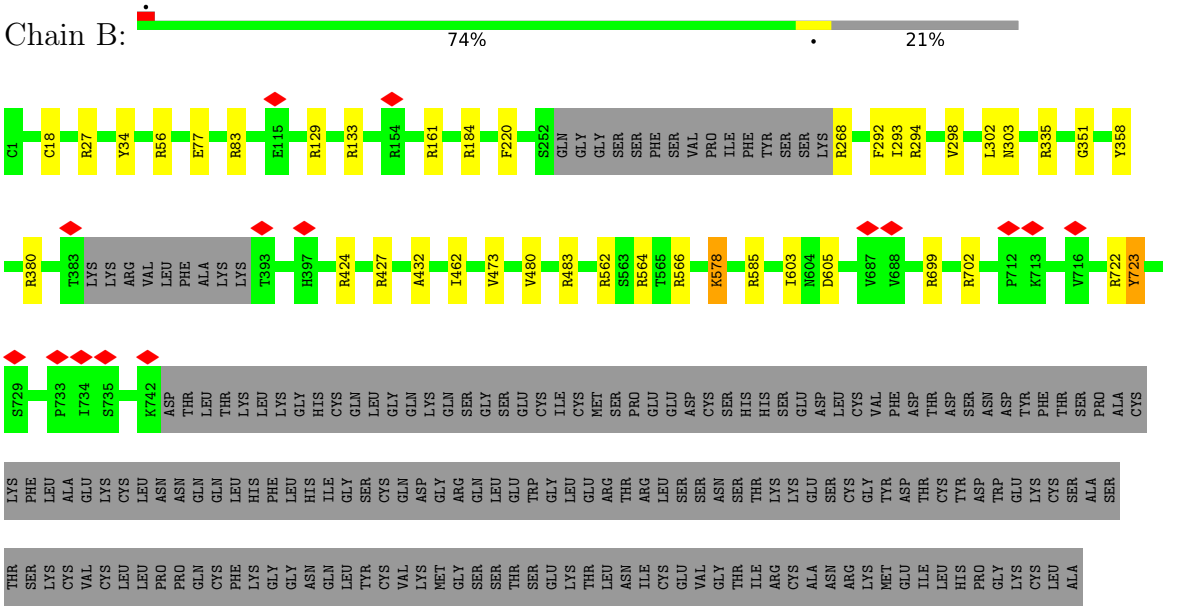


• Molecule 4: Complement component C7

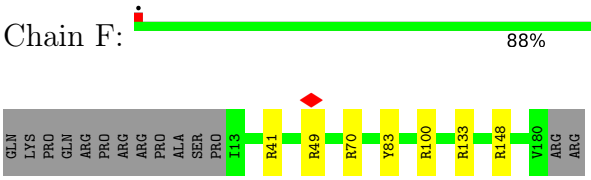




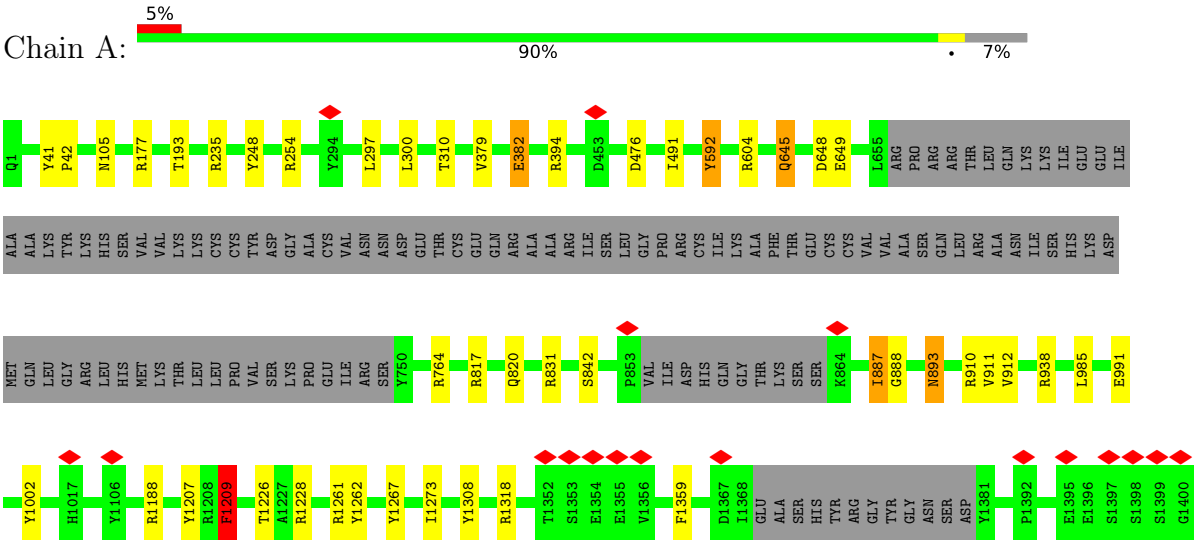
• Molecule 5: Complement component C6

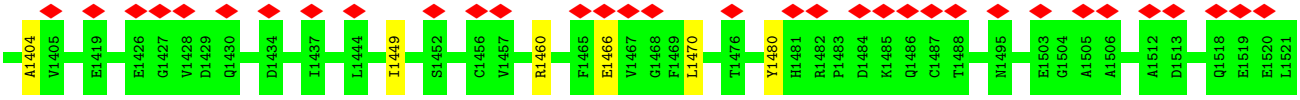


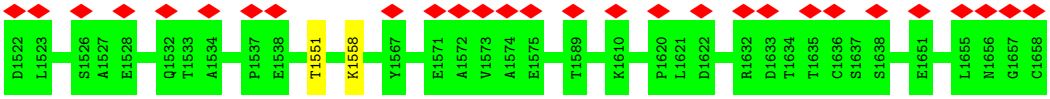
• Molecule 6: Complement component C8 gamma chain



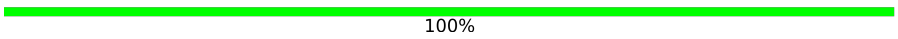
• Molecule 7: Complement C5







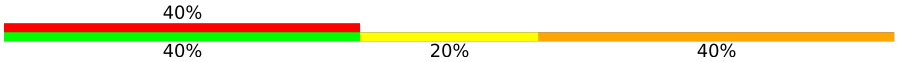
• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

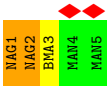
Chain I: 

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	142499	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	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	2.098	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	418.80002, 418.80002, 418.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.047, 1.047, 1.047	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, CA, NAG, FUC, MAN

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	D	0.69	0/4004	1.05	19/5409 (0.4%)
2	E	0.67	0/3896	1.05	20/5249 (0.4%)
3	G	0.67	0/3322	1.01	13/4485 (0.3%)
3	H	0.68	0/2562	1.01	10/3457 (0.3%)
4	C	0.66	0/6109	0.99	18/8290 (0.2%)
5	B	0.66	0/5750	1.02	24/7770 (0.3%)
6	F	0.69	0/1348	1.05	7/1829 (0.4%)
7	A	0.64	0/11993	0.95	19/16320 (0.1%)
All	All	0.66	0/38984	1.00	130/52809 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
2	E	0	2
3	G	0	2
3	H	0	4
4	C	0	4
5	B	0	1
7	A	0	7
All	All	0	21

There are no bond length outliers.

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	49	ARG	NE-CZ-NH1	9.06	124.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	483	ARG	NE-CZ-NH1	8.63	124.61	120.30
2	E	454	ARG	NE-CZ-NH1	8.57	124.58	120.30
2	E	77	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	D	266	ARG	NE-CZ-NH2	8.56	124.58	120.30
5	B	294	ARG	NE-CZ-NH2	8.53	124.56	120.30
4	C	271	ARG	NE-CZ-NH2	8.34	124.47	120.30
5	B	427	ARG	NE-CZ-NH2	8.32	124.46	120.30
5	B	564	ARG	NE-CZ-NH1	8.13	124.36	120.30
4	C	356	ARG	NE-CZ-NH2	-8.11	116.25	120.30
5	B	184	ARG	NE-CZ-NH1	8.11	124.35	120.30
7	A	592	TYR	CB-CG-CD2	-7.89	116.26	121.00
1	D	510	ARG	NE-CZ-NH2	7.78	124.19	120.30
7	A	938	ARG	NE-CZ-NH1	7.61	124.11	120.30
3	H	90	ARG	NE-CZ-NH1	7.55	124.07	120.30
2	E	31	ARG	NE-CZ-NH1	7.53	124.06	120.30
3	H	122	ARG	NE-CZ-NH2	7.36	123.98	120.30
4	C	356	ARG	NE-CZ-NH1	7.36	123.98	120.30
5	B	566	ARG	NE-CZ-NH2	7.33	123.97	120.30
1	D	359	ARG	NE-CZ-NH2	7.27	123.93	120.30
1	D	102	ARG	NE-CZ-NH1	7.21	123.91	120.30
5	B	427	ARG	NE-CZ-NH1	-7.17	116.71	120.30
1	D	83	ARG	NE-CZ-NH1	7.14	123.87	120.30
7	A	604	ARG	NE-CZ-NH1	7.13	123.87	120.30
2	E	274	ARG	NE-CZ-NH1	7.12	123.86	120.30
2	E	468	ARG	NE-CZ-NH1	7.00	123.80	120.30
5	B	161	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	D	280	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	D	269	ARG	NE-CZ-NH1	6.95	123.77	120.30
5	B	129	ARG	NE-CZ-NH1	6.91	123.75	120.30
3	G	133	ARG	NE-CZ-NH2	6.89	123.74	120.30
2	E	379	ARG	NE-CZ-NH2	6.88	123.74	120.30
4	C	130	ARG	NE-CZ-NH2	6.86	123.73	120.30
4	C	381	TYR	CB-CG-CD2	-6.80	116.92	121.00
3	H	290	ARG	NE-CZ-NH2	6.77	123.69	120.30
1	D	485	ARG	NE-CZ-NH1	6.74	123.67	120.30
7	A	910	ARG	NE-CZ-NH1	6.73	123.67	120.30
7	A	1460	ARG	NE-CZ-NH1	6.72	123.66	120.30
3	G	65	ARG	NE-CZ-NH2	6.66	123.63	120.30
7	A	1209	PHE	CB-CG-CD1	6.65	125.45	120.80
7	A	1318	ARG	NE-CZ-NH1	6.65	123.62	120.30
2	E	159	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	D	227	ARG	NE-CZ-NH1	6.64	123.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	235	ARG	NE-CZ-NH1	6.57	123.58	120.30
5	B	424	ARG	NE-CZ-NH2	6.56	123.58	120.30
3	H	425	ARG	NE-CZ-NH1	6.53	123.56	120.30
3	H	348	ARG	CB-CA-C	6.52	123.45	110.40
7	A	1228	ARG	NE-CZ-NH1	6.52	123.56	120.30
5	B	380	ARG	NE-CZ-NH2	6.51	123.56	120.30
3	G	95	ARG	NE-CZ-NH2	6.49	123.54	120.30
7	A	254	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	D	313	ARG	NE-CZ-NH2	6.45	123.53	120.30
7	A	1209	PHE	CB-CG-CD2	-6.44	116.29	120.80
2	E	392	ARG	NE-CZ-NH1	6.42	123.51	120.30
5	B	56	ARG	NE-CZ-NH1	6.41	123.50	120.30
3	H	284	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	D	242	ARG	NE-CZ-NH1	6.38	123.49	120.30
2	E	547	ARG	NE-CZ-NH1	6.37	123.48	120.30
3	H	475	ARG	NE-CZ-NH2	6.37	123.48	120.30
3	G	90	ARG	NE-CZ-NH1	6.33	123.47	120.30
6	F	41	ARG	NE-CZ-NH1	6.31	123.45	120.30
3	G	174	ARG	NE-CZ-NH1	6.30	123.45	120.30
3	H	288	ARG	NE-CZ-NH1	6.29	123.44	120.30
4	C	380	ARG	NE-CZ-NH1	6.28	123.44	120.30
4	C	590	ARG	NE-CZ-NH2	6.27	123.44	120.30
3	H	174	ARG	NE-CZ-NH1	6.26	123.43	120.30
4	C	55	ARG	NE-CZ-NH2	6.26	123.43	120.30
6	F	100	ARG	NE-CZ-NH1	6.24	123.42	120.30
2	E	81	ARG	NE-CZ-NH1	6.20	123.40	120.30
7	A	394	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	D	485	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	D	284	ARG	NE-CZ-NH2	6.04	123.32	120.30
4	C	292	ARG	NE-CZ-NH1	6.04	123.32	120.30
5	B	585	ARG	NE-CZ-NH1	6.01	123.30	120.30
5	B	722	ARG	NE-CZ-NH2	6.01	123.30	120.30
2	E	529	ARG	NE-CZ-NH1	5.96	123.28	120.30
6	F	148	ARG	NE-CZ-NH1	5.94	123.27	120.30
5	B	268	ARG	NE-CZ-NH2	5.88	123.24	120.30
4	C	103	ARG	NE-CZ-NH1	5.86	123.23	120.30
7	A	893	ASN	CB-CA-C	-5.86	98.68	110.40
3	H	413	ARG	NE-CZ-NH1	5.84	123.22	120.30
4	C	211	ARG	NE-CZ-NH2	5.84	123.22	120.30
4	C	26	ARG	NE-CZ-NH1	5.83	123.21	120.30
3	G	284	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	D	157	ARG	NE-CZ-NH1	5.78	123.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	450	ARG	NE-CZ-NH1	5.78	123.19	120.30
4	C	27	ARG	NE-CZ-NH2	5.77	123.19	120.30
3	G	192	ARG	NE-CZ-NH1	5.70	123.15	120.30
5	B	562	ARG	NE-CZ-NH1	5.70	123.15	120.30
7	A	817	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	D	82	ARG	NE-CZ-NH1	5.66	123.13	120.30
2	E	29	ARG	NE-CZ-NH1	5.65	123.13	120.30
4	C	436	ARG	NE-CZ-NH2	5.63	123.11	120.30
2	E	530	ARG	NE-CZ-NH1	5.62	123.11	120.30
4	C	66	ARG	NE-CZ-NH1	5.62	123.11	120.30
2	E	166	ARG	NE-CZ-NH1	5.61	123.10	120.30
7	A	764	ARG	NE-CZ-NH2	5.59	123.09	120.30
5	B	702	ARG	NE-CZ-NH1	5.58	123.09	120.30
5	B	335	ARG	NE-CZ-NH1	5.57	123.09	120.30
7	A	1188	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	D	78	ARG	NE-CZ-NH1	5.52	123.06	120.30
2	E	156	ARG	NE-CZ-NH1	5.51	123.05	120.30
7	A	177	ARG	NE-CZ-NH1	5.50	123.05	120.30
3	G	97	ARG	NE-CZ-NH2	5.46	123.03	120.30
2	E	160	TYR	CB-CG-CD1	-5.45	117.73	121.00
2	E	490	ARG	NE-CZ-NH1	5.44	123.02	120.30
7	A	831	ARG	NE-CZ-NH1	5.42	123.01	120.30
5	B	27	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	D	506	ARG	NE-CZ-NH1	5.40	123.00	120.30
5	B	83	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	D	255	ARG	NE-CZ-NH1	5.38	122.99	120.30
4	C	497	ARG	NE-CZ-NH2	5.36	122.98	120.30
7	A	248	TYR	CB-CG-CD2	-5.36	117.79	121.00
5	B	723	TYR	CB-CG-CD2	-5.34	117.80	121.00
3	G	288	ARG	NE-CZ-NH1	5.32	122.96	120.30
3	G	90	ARG	NH1-CZ-NH2	-5.26	113.62	119.40
3	G	284	ARG	NE-CZ-NH2	-5.22	117.69	120.30
5	B	699	ARG	NE-CZ-NH1	5.20	122.90	120.30
2	E	394	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	D	31	ARG	NE-CZ-NH1	5.18	122.89	120.30
6	F	133	ARG	NE-CZ-NH1	5.18	122.89	120.30
6	F	70	ARG	NE-CZ-NH1	5.17	122.88	120.30
4	C	802	ARG	NE-CZ-NH1	5.12	122.86	120.30
3	G	348	ARG	NE-CZ-NH2	5.11	122.85	120.30
5	B	133	ARG	NE-CZ-NH1	5.09	122.85	120.30
6	F	83	TYR	CB-CG-CD2	-5.09	117.94	121.00
2	E	392	ARG	NE-CZ-NH2	-5.07	117.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	427	ARG	CD-NE-CZ	5.07	130.69	123.60
4	C	144	ARG	NE-CZ-NH1	5.04	122.82	120.30
3	G	90	ARG	NE-CZ-NH2	5.03	122.81	120.30

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	A	1207	TYR	Sidechain
7	A	1209	PHE	Peptide
7	A	1262	TYR	Sidechain
7	A	1308	TYR	Sidechain
7	A	592	TYR	Sidechain
7	A	985	LEU	Peptide
7	A	991	GLU	Peptide
5	B	34	TYR	Sidechain
4	C	226	TYR	Sidechain
4	C	381	TYR	Sidechain
4	C	403	TYR	Sidechain
4	C	581	TYR	Sidechain
1	D	266	ARG	Sidechain
2	E	413	TYR	Sidechain
2	E	468	ARG	Sidechain
3	G	183	TYR	Sidechain
3	G	290	ARG	Sidechain
3	H	172	TYR	Sidechain
3	H	288	ARG	Sidechain
3	H	335	TYR	Sidechain
3	H	456	TYR	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	D	3914	0	3735	16	0
2	E	3819	0	3601	4	0
3	G	3259	0	3101	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	2517	0	2385	23	0
4	C	5977	0	5400	39	0
5	B	5631	0	5332	20	0
6	F	1319	0	1282	0	0
7	A	11744	0	11282	31	0
8	I	39	0	34	0	0
9	J	28	0	25	1	0
10	K	61	0	52	5	0
11	C	11	0	10	3	0
11	D	22	0	19	3	0
11	E	22	0	20	2	0
11	G	11	0	10	4	0
12	D	1	0	0	0	0
12	E	1	0	0	0	0
12	G	1	0	0	0	0
12	H	1	0	0	0	0
13	B	14	0	13	4	0
13	G	14	0	13	3	0
13	H	14	0	13	10	0
14	B	10	0	10	2	0
All	All	38430	0	36337	148	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 2.

All (148) 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)
5:B:303:ASN:HD22	13:B:1001:NAG:C1	0.92	1.53
2:E:14:TRP:HD1	11:E:601:MAN:C1	0.84	1.49
5:B:303:ASN:ND2	13:B:1001:NAG:C1	1.76	1.43
4:C:629:VAL:HG13	4:C:652:GLY:O	1.22	1.32
7:A:887:ILE:HG22	7:A:911:VAL:O	1.32	1.28
3:H:397:SER:HB3	13:H:601:NAG:O5	1.39	1.21
4:C:629:VAL:HG21	4:C:653:SER:O	1.40	1.20
7:A:887:ILE:CG2	7:A:911:VAL:O	1.91	1.18
1:D:67:ARG:HD2	7:A:476:ASP:OD2	1.53	1.09
4:C:656:LYS:HE3	4:C:656:LYS:HA	1.34	1.09
3:G:413:ARG:HD3	3:H:439:SER:HA	1.35	1.06
1:D:384:LEU:HG	1:D:394:LEU:HD11	1.39	1.03
4:C:65:GLU:HB3	7:A:645:GLN:HG2	1.44	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:431:ASP:OD2	11:C:901:MAN:H3	1.64	0.97
3:H:397:SER:HA	13:H:601:NAG:O6	1.65	0.96
4:C:629:VAL:CG1	4:C:652:GLY:O	2.13	0.95
4:C:14:TRP:CE3	4:C:25:THR:C	2.39	0.95
3:H:394:ASN:OD1	13:H:601:NAG:C2	2.04	0.94
4:C:14:TRP:HZ3	4:C:25:THR:HA	1.32	0.94
3:G:413:ARG:HH11	3:G:413:ARG:HG3	1.33	0.94
3:H:397:SER:HB3	13:H:601:NAG:C1	1.99	0.92
4:C:629:VAL:CG2	4:C:653:SER:O	2.19	0.91
3:H:397:SER:CB	13:H:601:NAG:O5	2.18	0.91
7:A:379:VAL:O	7:A:382:GLU:HB3	1.72	0.89
13:G:601:NAG:C1	13:G:601:NAG:H82	2.04	0.88
11:G:602:MAN:O3	3:H:471:GLN:NE2	2.08	0.87
5:B:293:ILE:HG23	5:B:358:TYR:HB3	1.55	0.86
3:H:394:ASN:ND2	3:H:397:SER:H	1.74	0.86
1:D:67:ARG:CD	7:A:476:ASP:OD2	2.26	0.83
7:A:887:ILE:HG23	7:A:911:VAL:C	2.00	0.82
4:C:428:ASP:HA	11:C:901:MAN:O3	1.80	0.82
4:C:14:TRP:CZ3	4:C:25:THR:HA	2.15	0.81
4:C:656:LYS:HE3	4:C:656:LYS:CA	2.10	0.81
7:A:842:SER:HB3	7:A:893:ASN:HB2	1.61	0.80
4:C:14:TRP:CZ3	4:C:25:THR:CA	2.64	0.79
2:E:14:TRP:CD1	11:E:601:MAN:C2	2.64	0.79
4:C:14:TRP:HE3	4:C:25:THR:C	1.85	0.78
7:A:887:ILE:HG23	7:A:911:VAL:O	1.84	0.77
7:A:645:GLN:OE1	7:A:645:GLN:HA	1.84	0.76
4:C:14:TRP:CZ3	4:C:24:GLN:O	2.39	0.75
1:D:67:ARG:HG2	1:D:67:ARG:HH11	1.50	0.75
3:H:394:ASN:OD1	13:H:601:NAG:H2	1.86	0.75
4:C:656:LYS:HA	4:C:656:LYS:CE	2.04	0.74
4:C:14:TRP:HZ3	4:C:25:THR:CA	2.01	0.73
5:B:578:LYS:H	5:B:578:LYS:CE	2.02	0.72
1:D:384:LEU:CG	1:D:394:LEU:HD11	2.19	0.72
10:K:2:NAG:H83	10:K:2:NAG:C3	2.18	0.72
7:A:887:ILE:CG2	7:A:911:VAL:C	2.57	0.72
3:H:394:ASN:OD1	13:H:601:NAG:N2	2.22	0.71
5:B:578:LYS:N	5:B:578:LYS:HE3	2.05	0.71
5:B:578:LYS:H	5:B:578:LYS:HE3	1.58	0.68
3:G:27:TRP:NE1	11:G:602:MAN:O2	2.25	0.68
1:D:383:THR:HG23	1:D:394:LEU:HD22	1.74	0.67
13:G:601:NAG:C1	13:G:601:NAG:C8	2.73	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:14:TRP:CE3	4:C:25:THR:CA	2.77	0.66
3:H:394:ASN:ND2	3:H:397:SER:HB3	2.09	0.66
4:C:607:ILE:HG23	4:C:654:SER:HB2	1.77	0.64
7:A:648:ASP:N	7:A:648:ASP:OD1	2.27	0.64
10:K:2:NAG:H83	10:K:2:NAG:H3	1.78	0.64
3:G:413:ARG:HH21	3:H:282:LEU:HD13	1.63	0.64
3:G:413:ARG:NH2	3:H:282:LEU:HD13	2.14	0.63
3:H:394:ASN:HD22	3:H:397:SER:H	1.43	0.63
3:H:397:SER:HA	13:H:601:NAG:HO6	1.63	0.63
4:C:654:SER:OG	4:C:654:SER:O	2.15	0.62
3:H:394:ASN:ND2	3:H:397:SER:CB	2.62	0.62
3:G:413:ARG:HG3	3:G:413:ARG:NH1	2.08	0.61
5:B:293:ILE:HG22	5:B:358:TYR:HD2	1.65	0.61
5:B:293:ILE:CG2	5:B:358:TYR:HD2	2.15	0.60
5:B:220:PHE:CE2	5:B:302:LEU:HD13	2.37	0.59
3:G:413:ARG:CD	3:H:439:SER:HA	2.23	0.59
4:C:14:TRP:CZ3	4:C:25:THR:C	2.76	0.58
4:C:65:GLU:CB	7:A:645:GLN:HG2	2.28	0.58
10:K:2:NAG:H83	10:K:2:NAG:O3	2.03	0.57
3:G:413:ARG:HH11	3:G:413:ARG:CG	2.12	0.57
5:B:18:CYS:SG	14:B:1002:FUC:O2	2.62	0.56
1:D:394:LEU:C	1:D:394:LEU:HD12	2.27	0.55
5:B:473:VAL:HG23	5:B:473:VAL:O	2.05	0.55
4:C:14:TRP:CE3	4:C:26:ARG:N	2.74	0.55
4:C:14:TRP:CE3	4:C:25:THR:N	2.75	0.54
3:H:394:ASN:HD22	3:H:394:ASN:C	2.11	0.54
1:D:67:ARG:NE	7:A:476:ASP:OD2	2.40	0.54
1:D:444:LYS:NZ	11:D:601:MAN:H2	2.23	0.54
1:D:67:ARG:HH11	1:D:67:ARG:CG	2.16	0.53
5:B:293:ILE:CG2	5:B:358:TYR:HB3	2.33	0.53
4:C:14:TRP:CZ3	4:C:24:GLN:C	2.81	0.53
5:B:298:VAL:HG13	5:B:462:ILE:HD13	1.90	0.53
13:G:601:NAG:H3	13:G:601:NAG:H83	1.91	0.53
5:B:77:GLU:O	5:B:77:GLU:HG3	2.09	0.52
3:G:417:PHE:CD2	3:G:420:LYS:HE2	2.45	0.52
1:D:444:LYS:HZ3	11:D:601:MAN:H2	1.74	0.52
3:G:413:ARG:NH1	3:G:413:ARG:CG	2.72	0.52
1:D:394:LEU:HD12	1:D:394:LEU:O	2.11	0.50
14:B:1002:FUC:O2	14:B:1002:FUC:H5	2.11	0.50
7:A:887:ILE:HG23	7:A:912:VAL:N	2.26	0.50
4:C:164:TYR:CE1	4:C:237:VAL:HG11	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:397:SER:CA	13:H:601:NAG:O5	2.59	0.49
1:D:67:ARG:CG	1:D:67:ARG:NH1	2.75	0.49
3:H:394:ASN:ND2	3:H:397:SER:N	2.53	0.49
4:C:431:ASP:OD1	4:C:432:PRO:HD2	2.13	0.49
2:E:320:ILE:HD11	2:E:427:ILE:HG23	1.95	0.48
7:A:887:ILE:CG2	7:A:912:VAL:HA	2.43	0.48
7:A:887:ILE:HG21	7:A:912:VAL:HA	1.94	0.48
5:B:293:ILE:CG2	5:B:358:TYR:CD2	2.97	0.48
4:C:295:PHE:CE1	4:C:349:LEU:HD21	2.49	0.48
13:H:601:NAG:O3	13:H:601:NAG:H82	2.14	0.47
10:K:2:NAG:C3	10:K:2:NAG:C8	2.85	0.47
4:C:164:TYR:CZ	4:C:237:VAL:HG11	2.50	0.47
4:C:14:TRP:CZ3	4:C:26:ARG:N	2.83	0.47
7:A:310:THR:HG21	7:A:1466:GLU:HG2	1.97	0.46
11:G:602:MAN:HO3	3:H:471:GLN:NE2	2.10	0.46
7:A:310:THR:HG21	7:A:1466:GLU:CG	2.45	0.46
4:C:14:TRP:CE3	4:C:24:GLN:C	2.89	0.46
7:A:1226:THR:HG23	7:A:1261:ARG:HB3	1.97	0.46
7:A:1551:THR:CB	7:A:1558:LYS:H	2.29	0.46
10:K:1:NAG:HO6	10:K:2:NAG:HN2	1.63	0.45
7:A:887:ILE:HA	7:A:911:VAL:HB	1.98	0.45
4:C:14:TRP:HE3	4:C:25:THR:O	1.98	0.45
7:A:105:ASN:H	7:A:193:THR:CG2	2.28	0.45
5:B:480:VAL:HB	5:B:603:ILE:HG13	1.98	0.45
3:G:394:ASN:OD1	3:G:394:ASN:C	2.56	0.44
2:E:414:ARG:HH11	2:E:414:ARG:HG2	1.82	0.44
5:B:303:ASN:ND2	13:B:1001:NAG:O5	2.42	0.44
3:G:27:TRP:CE2	11:G:602:MAN:C2	3.00	0.43
7:A:1404:ALA:HA	7:A:1480:TYR:H	1.84	0.43
1:D:19:TRP:HE1	11:D:602:MAN:H4	1.83	0.43
3:G:129:SER:HB2	3:G:172:TYR:CD1	2.52	0.43
4:C:14:TRP:HE3	4:C:25:THR:N	2.16	0.43
5:B:351:GLY:HA3	5:B:462:ILE:HD12	2.00	0.43
7:A:41:TYR:CD1	7:A:42:PRO:HA	2.54	0.43
5:B:578:LYS:H	5:B:578:LYS:NZ	2.15	0.43
4:C:458:TYR:CD1	4:C:458:TYR:N	2.86	0.42
13:B:1001:NAG:O3	13:B:1001:NAG:C7	2.68	0.42
7:A:1359:PHE:CE1	7:A:1449:ILE:HG21	2.53	0.42
1:D:383:THR:HG23	1:D:394:LEU:CD2	2.46	0.42
4:C:176:TYR:CD1	4:C:228:LEU:HD22	2.55	0.42
7:A:1470:LEU:H	7:A:1470:LEU:HD23	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:381:TYR:CE2	5:B:432:ALA:HB1	2.56	0.41
7:A:649:GLU:N	7:A:649:GLU:OE1	2.53	0.41
1:D:135:PRO:HG2	1:D:260:HIS:CD2	2.55	0.41
4:C:427:LEU:C	11:C:901:MAN:O4	2.58	0.41
3:H:278:GLY:HA3	3:H:335:TYR:CE1	2.56	0.41
7:A:1002:TYR:CZ	7:A:1273:ILE:HG23	2.56	0.41
4:C:481:TRP:CE3	4:C:499:ARG:HD3	2.56	0.41
9:J:1:NAG:HO3	9:J:1:NAG:C7	2.34	0.41
3:H:348:ARG:HA	3:H:348:ARG:HD3	1.15	0.40
7:A:887:ILE:HG22	7:A:888:GLY:H	1.87	0.40
4:C:14:TRP:HZ3	4:C:24:GLN:O	2.00	0.40
7:A:297:LEU:H	7:A:300:LEU:HD12	1.86	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	D	481/537 (90%)	464 (96%)	17 (4%)	0	100	100
2	E	476/554 (86%)	459 (96%)	17 (4%)	0	100	100
3	G	407/538 (76%)	385 (95%)	22 (5%)	0	100	100
3	H	311/538 (58%)	291 (94%)	20 (6%)	0	100	100
4	C	803/821 (98%)	774 (96%)	28 (4%)	1 (0%)	51	82
5	B	712/913 (78%)	684 (96%)	28 (4%)	0	100	100
6	F	166/182 (91%)	162 (98%)	4 (2%)	0	100	100
7	A	1534/1658 (92%)	1434 (94%)	100 (6%)	0	100	100
All	All	4890/5741 (85%)	4653 (95%)	236 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	654	SER

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	D	433/473 (92%)	427 (99%)	6 (1%)	67	82
2	E	411/466 (88%)	407 (99%)	4 (1%)	76	85
3	G	359/477 (75%)	356 (99%)	3 (1%)	81	89
3	H	273/477 (57%)	267 (98%)	6 (2%)	52	74
4	C	615/714 (86%)	609 (99%)	6 (1%)	76	85
5	B	630/810 (78%)	626 (99%)	4 (1%)	86	91
6	F	136/149 (91%)	136 (100%)	0	100	100
7	A	1234/1470 (84%)	1227 (99%)	7 (1%)	86	91
All	All	4091/5036 (81%)	4055 (99%)	36 (1%)	79	87

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	11	CYS
1	D	27	LYS
1	D	63	ARG
1	D	67	ARG
1	D	394	LEU
1	D	536	CYS
2	E	184	LYS
2	E	201	ASP
2	E	490	ARG
2	E	514	CYS
3	G	42	ARG
3	G	109	ASP
3	G	393	VAL
4	C	65	GLU
4	C	173	ASP

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Mol	Chain	Res	Type
4	C	226	TYR
4	C	487	TRP
4	C	653	SER
4	C	656	LYS
5	B	292	PHE
5	B	578	LYS
5	B	605	ASP
5	B	723	TYR
3	H	95	ARG
3	H	103	ASP
3	H	164	ARG
3	H	349	LYS
3	H	394	ASN
3	H	413	ARG
7	A	382	GLU
7	A	491	ILE
7	A	645	GLN
7	A	820	GLN
7	A	887	ILE
7	A	1209	PHE
7	A	1267	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	240	HIS
1	D	260	HIS
1	D	380	HIS
2	E	24	GLN
5	B	303	ASN
3	H	471	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)

10 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	NAG	I	1	1,8	14,14,15	0.28	0	17,19,21	0.75	0
8	NAG	I	2	8	14,14,15	0.26	0	17,19,21	0.63	0
8	BMA	I	3	8	11,11,12	0.25	0	15,15,17	0.86	0
9	NAG	J	1	2,9	14,14,15	0.27	0	17,19,21	0.65	0
9	NAG	J	2	9	14,14,15	0.27	0	17,19,21	0.72	0
10	NAG	K	1	7,10	14,14,15	2.08	5 (35%)	17,19,21	2.11	8 (47%)
10	NAG	K	2	10	14,14,15	1.02	1 (7%)	17,19,21	1.46	3 (17%)
10	BMA	K	3	10	11,11,12	0.22	0	15,15,17	1.62	3 (20%)
10	MAN	K	4	10	11,11,12	0.31	0	15,15,17	0.84	0
10	MAN	K	5	10	11,11,12	0.27	0	15,15,17	0.96	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	I	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	I	2	8	-	0/6/23/26	0/1/1/1
8	BMA	I	3	8	-	0/2/19/22	0/1/1/1
9	NAG	J	1	2,9	-	5/6/23/26	0/1/1/1
9	NAG	J	2	9	-	3/6/23/26	0/1/1/1
10	NAG	K	1	7,10	-	4/6/23/26	0/1/1/1
10	NAG	K	2	10	-	3/6/23/26	0/1/1/1
10	BMA	K	3	10	-	2/2/19/22	0/1/1/1
10	MAN	K	4	10	-	0/2/19/22	0/1/1/1
10	MAN	K	5	10	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	K	1	NAG	O5-C1	-3.67	1.37	1.43
10	K	1	NAG	C1-C2	-3.64	1.46	1.52
10	K	1	NAG	C2-N2	-3.14	1.41	1.46
10	K	1	NAG	C4-C5	-2.73	1.47	1.53
10	K	2	NAG	O5-C1	-2.59	1.39	1.43
10	K	1	NAG	O5-C5	-2.13	1.39	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	K	1	NAG	O5-C1-C2	-3.96	105.04	111.29
10	K	3	BMA	O5-C1-C2	-3.83	104.86	110.77
10	K	1	NAG	C3-C4-C5	-3.50	104.00	110.24
10	K	2	NAG	C1-C2-N2	-3.38	104.72	110.49
10	K	1	NAG	C6-C5-C4	-2.91	106.18	113.00
10	K	3	BMA	O5-C5-C6	2.67	111.38	107.20
10	K	1	NAG	O7-C7-N2	-2.64	117.10	121.95
10	K	2	NAG	O4-C4-C5	-2.46	103.19	109.30
10	K	1	NAG	O6-C6-C5	-2.41	103.03	111.29
10	K	1	NAG	C1-C2-N2	-2.29	106.57	110.49
10	K	1	NAG	O5-C5-C6	2.23	110.70	107.20
10	K	1	NAG	O4-C4-C5	-2.19	103.86	109.30
10	K	3	BMA	C3-C4-C5	-2.13	106.43	110.24
10	K	2	NAG	C6-C5-C4	-2.07	108.15	113.00

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	J	2	NAG	C8-C7-N2-C2
9	J	2	NAG	O7-C7-N2-C2
10	K	1	NAG	C8-C7-N2-C2
10	K	1	NAG	O7-C7-N2-C2
10	K	2	NAG	C3-C2-N2-C7
10	K	2	NAG	C8-C7-N2-C2
10	K	2	NAG	O7-C7-N2-C2
9	J	1	NAG	C1-C2-N2-C7
10	K	1	NAG	O5-C5-C6-O6
10	K	3	BMA	C4-C5-C6-O6
10	K	1	NAG	C4-C5-C6-O6
9	J	1	NAG	O5-C5-C6-O6
9	J	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	J	1	NAG	C8-C7-N2-C2
10	K	3	BMA	O5-C5-C6-O6
8	I	1	NAG	C8-C7-N2-C2
9	J	1	NAG	O7-C7-N2-C2
8	I	1	NAG	O7-C7-N2-C2
9	J	1	NAG	C3-C2-N2-C7

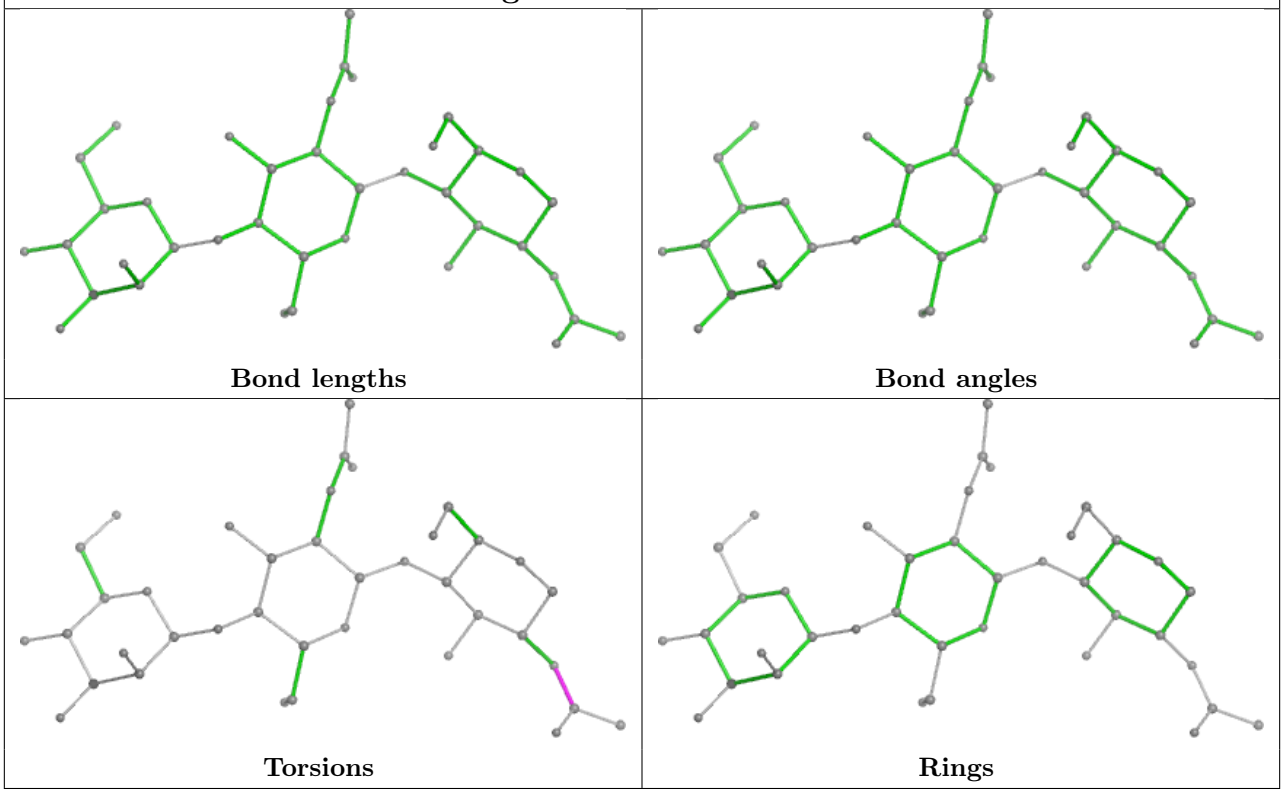
There are no ring outliers.

3 monomers are involved in 6 short contacts:

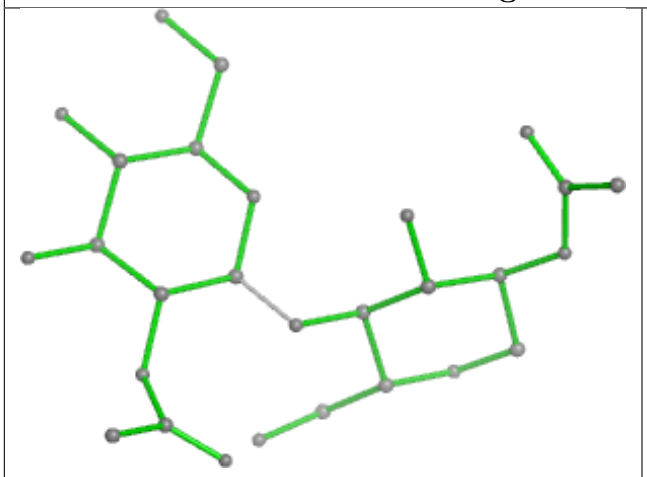
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	K	2	NAG	5	0
10	K	1	NAG	1	0
9	J	1	NAG	1	0

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

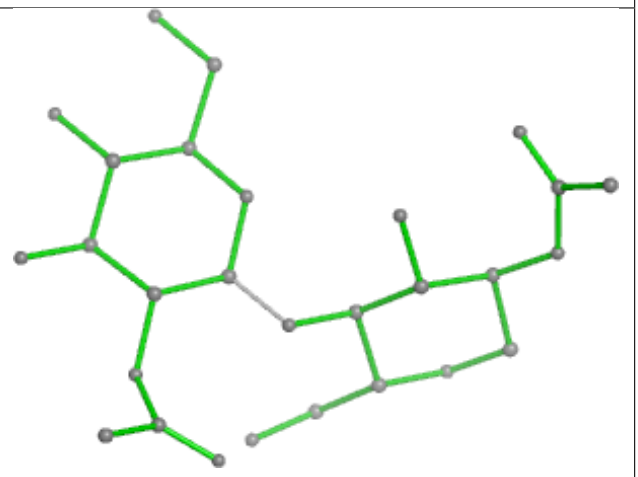
Oligosaccharide Chain I



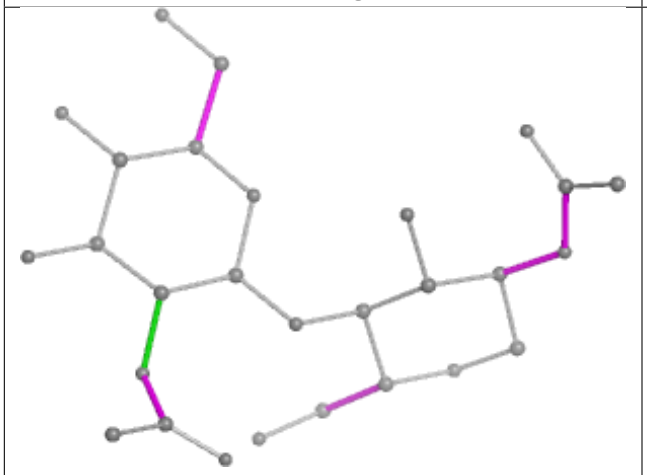
Oligosaccharide Chain J



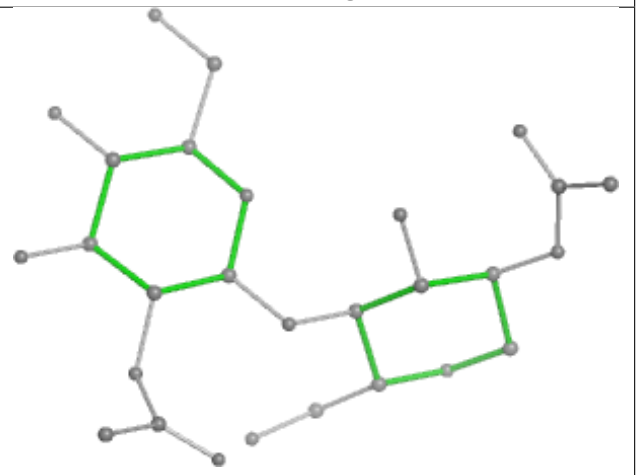
Bond lengths



Bond angles

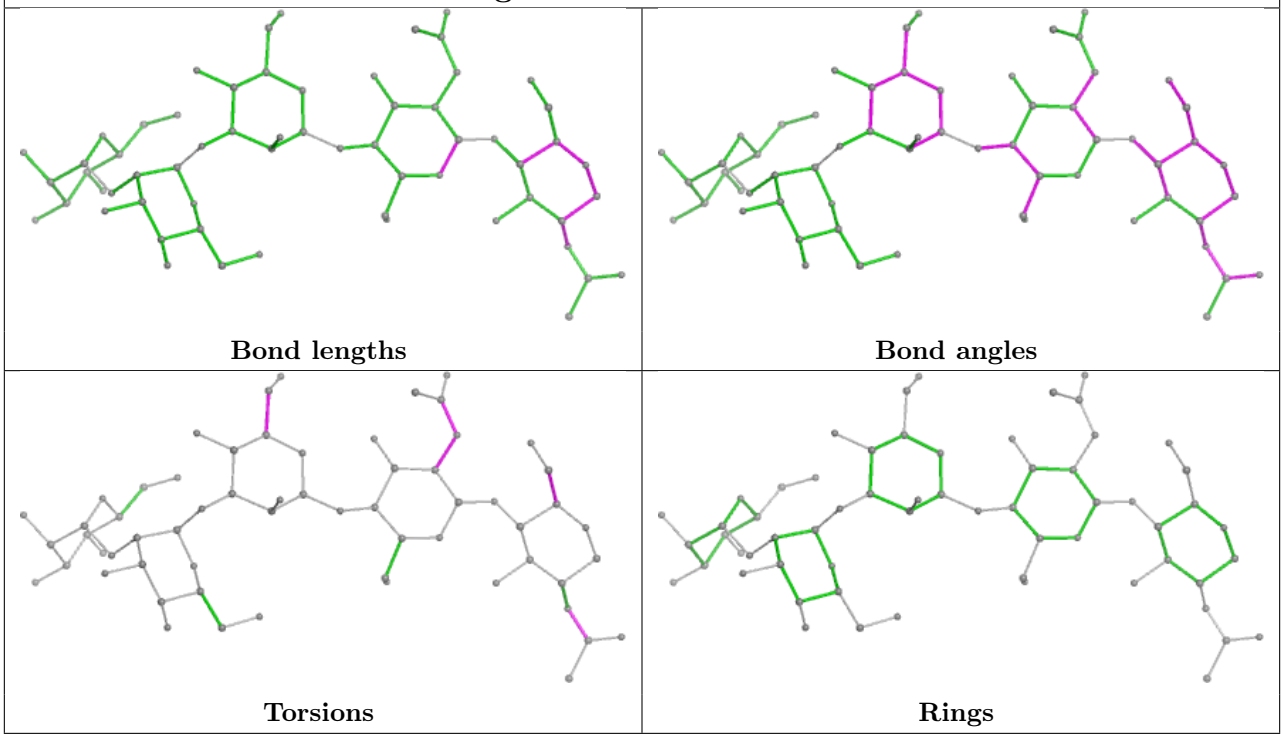


Torsions



Rings

Oligosaccharide Chain K



5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 for Mogul analysis.

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	$\#\|Z\| > 2$
14	FUC	B	1002	5	10,10,11	0.62	0	14,14,16	1.88	5 (35%)
11	MAN	D	601	1	11,11,12	1.29	1 (9%)	15,15,17	1.29	2 (13%)
13	NAG	H	601	3	14,14,15	1.36	2 (14%)	17,19,21	2.54	5 (29%)
11	MAN	E	602	2	11,11,12	1.19	1 (9%)	15,15,17	2.53	4 (26%)
13	NAG	B	1001	-	14,14,15	0.45	0	17,19,21	1.52	2 (11%)
13	NAG	G	601	3	14,14,15	0.33	0	17,19,21	0.80	1 (5%)
11	MAN	E	601	2	11,11,12	0.80	0	15,15,17	2.19	5 (33%)
11	MAN	C	901	4	11,11,12	0.43	0	15,15,17	2.40	5 (33%)
11	MAN	D	602	1	11,11,12	0.31	0	15,15,17	1.37	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	MAN	G	602	3	11,11,12	1.06	1 (9%)	15,15,17	2.10	6 (40%)

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
14	FUC	B	1002	5	-	-	0/1/1/1
11	MAN	D	601	1	-	2/2/19/22	0/1/1/1
13	NAG	H	601	3	-	3/6/23/26	0/1/1/1
11	MAN	E	602	2	-	1/2/19/22	0/1/1/1
13	NAG	B	1001	-	-	5/6/23/26	0/1/1/1
13	NAG	G	601	3	-	3/6/23/26	0/1/1/1
11	MAN	E	601	2	-	2/2/19/22	0/1/1/1
11	MAN	C	901	4	-	2/2/19/22	0/1/1/1
11	MAN	D	602	1	1/1/4/5	1/2/19/22	0/1/1/1
11	MAN	G	602	3	-	2/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	601	MAN	O2-C2	-3.64	1.35	1.43
13	H	601	NAG	O5-C1	3.56	1.49	1.43
13	H	601	NAG	C1-C2	3.26	1.57	1.52
11	E	602	MAN	C2-C3	2.87	1.56	1.52
11	G	602	MAN	O5-C1	-2.65	1.39	1.43

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	H	601	NAG	C1-O5-C5	7.34	122.14	112.19
11	C	901	MAN	C1-O5-C5	5.89	120.17	112.19
13	H	601	NAG	O5-C1-C2	-5.73	102.24	111.29
11	E	602	MAN	C1-O5-C5	5.69	119.90	112.19
11	E	601	MAN	C1-O5-C5	-5.36	104.93	112.19
11	C	901	MAN	O5-C1-C2	5.28	118.93	110.77
11	E	602	MAN	O3-C3-C2	4.99	119.56	109.99
11	D	602	MAN	C1-C2-C3	3.98	114.56	109.67
13	B	1001	NAG	C1-O5-C5	3.93	117.52	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	G	602	MAN	C1-O5-C5	-3.74	107.12	112.19
11	G	602	MAN	C1-C2-C3	3.74	114.27	109.67
11	E	602	MAN	C1-C2-C3	3.74	114.27	109.67
13	B	1001	NAG	O5-C1-C2	-3.73	105.40	111.29
11	G	602	MAN	O5-C1-C2	-3.53	105.31	110.77
11	E	602	MAN	O4-C4-C3	-3.40	102.49	110.35
11	E	601	MAN	O5-C1-C2	-3.31	105.66	110.77
11	E	601	MAN	O2-C2-C3	-3.16	103.82	110.14
11	G	602	MAN	O5-C5-C6	-3.10	102.34	107.20
11	E	601	MAN	C1-C2-C3	-3.08	105.88	109.67
14	B	1002	FUC	C1-C2-C3	-3.00	105.98	109.67
14	B	1002	FUC	O3-C3-C2	-2.98	104.28	109.99
11	C	901	MAN	C1-C2-C3	2.70	112.98	109.67
14	B	1002	FUC	O5-C1-C2	-2.65	106.67	110.77
13	G	601	NAG	O5-C5-C6	2.59	111.26	107.20
14	B	1002	FUC	O2-C2-C1	2.54	114.34	109.15
11	C	901	MAN	C3-C4-C5	-2.52	105.75	110.24
13	H	601	NAG	O5-C5-C6	2.49	111.11	107.20
11	G	602	MAN	C2-C3-C4	2.47	115.17	110.89
11	D	602	MAN	C1-O5-C5	2.34	115.37	112.19
11	E	601	MAN	C2-C3-C4	-2.24	107.02	110.89
11	C	901	MAN	O5-C5-C6	2.20	110.65	107.20
14	B	1002	FUC	O2-C2-C3	2.14	114.42	110.14
13	H	601	NAG	C4-C3-C2	2.13	114.14	111.02
11	D	601	MAN	C2-C3-C4	-2.12	107.22	110.89
11	G	602	MAN	O4-C4-C5	2.09	114.48	109.30
11	D	601	MAN	C1-O5-C5	-2.02	109.45	112.19
13	H	601	NAG	C2-N2-C7	2.02	125.78	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	D	602	MAN	C1

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	G	601	NAG	C8-C7-N2-C2
13	G	601	NAG	O7-C7-N2-C2
13	B	1001	NAG	C1-C2-N2-C7
13	B	1001	NAG	C8-C7-N2-C2
13	B	1001	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
13	H	601	NAG	C3-C2-N2-C7
13	H	601	NAG	C8-C7-N2-C2
13	H	601	NAG	O7-C7-N2-C2
11	G	602	MAN	O5-C5-C6-O6
11	G	602	MAN	C4-C5-C6-O6
11	E	601	MAN	O5-C5-C6-O6
11	D	601	MAN	O5-C5-C6-O6
11	E	601	MAN	C4-C5-C6-O6
13	G	601	NAG	C1-C2-N2-C7
11	D	601	MAN	C4-C5-C6-O6
11	C	901	MAN	O5-C5-C6-O6
11	D	602	MAN	O5-C5-C6-O6
13	B	1001	NAG	O5-C5-C6-O6
11	C	901	MAN	C4-C5-C6-O6
11	E	602	MAN	C4-C5-C6-O6
13	B	1001	NAG	C3-C2-N2-C7

There are no ring outliers.

9 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	1002	FUC	2	0
11	D	601	MAN	2	0
13	H	601	NAG	10	0
13	B	1001	NAG	4	0
13	G	601	NAG	3	0
11	E	601	MAN	2	0
11	C	901	MAN	3	0
11	D	602	MAN	1	0
11	G	602	MAN	4	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.

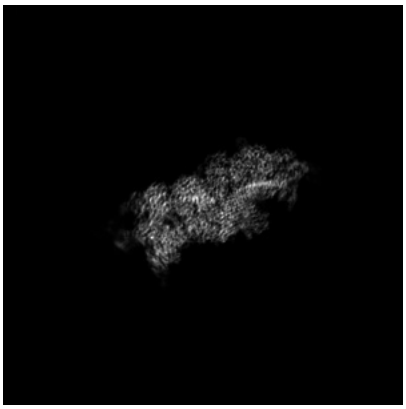
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-12651. These allow visual inspection of the internal detail of the map and identification of artifacts.

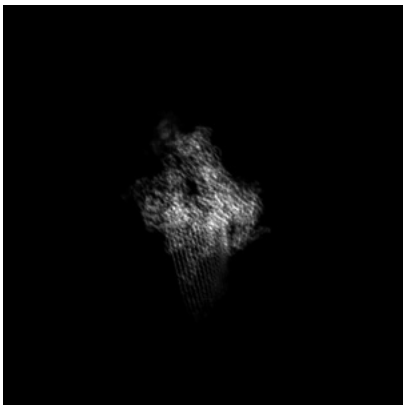
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

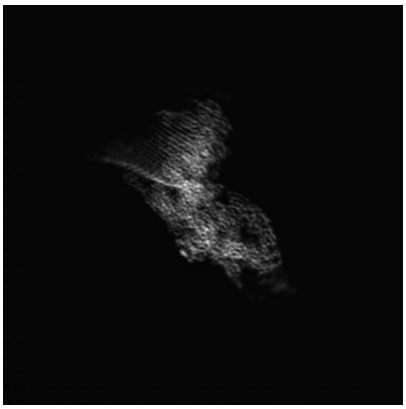
6.1.1 Primary map



X

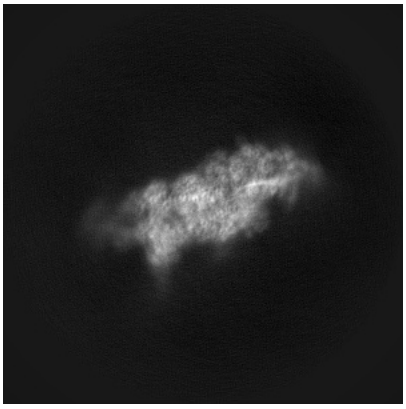


Y

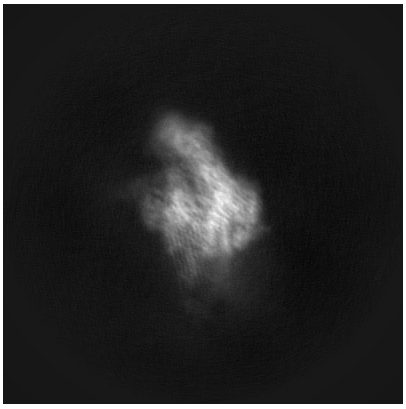


Z

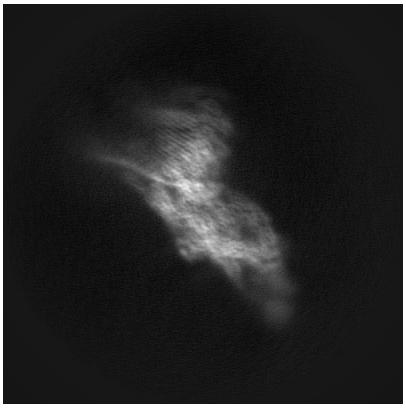
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

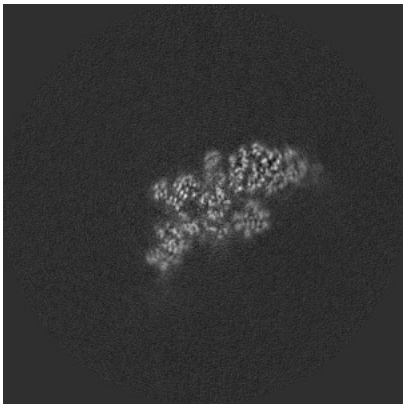
6.2.1 Primary map

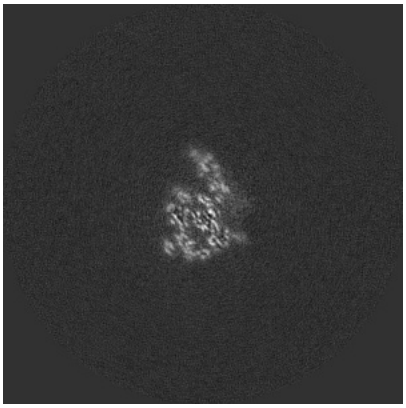
X Index: 200

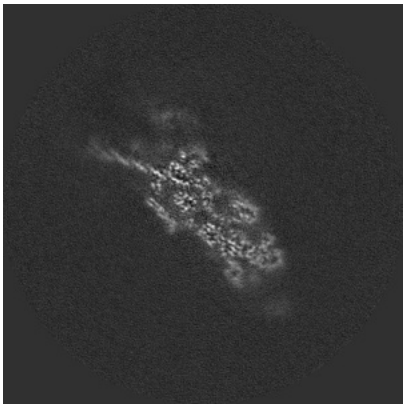
Y Index: 200

Z Index: 200

6.2.2 Raw map


X Index: 200


Y Index: 200

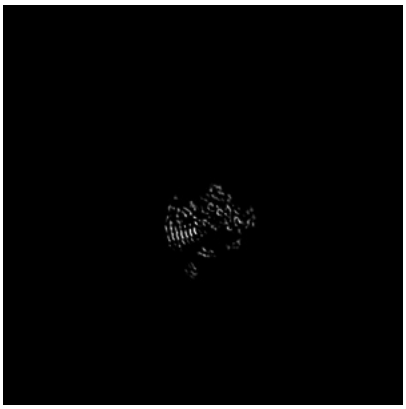

Z Index: 200

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

6.3 Largest variance slices (i)

6.3.1 Primary map

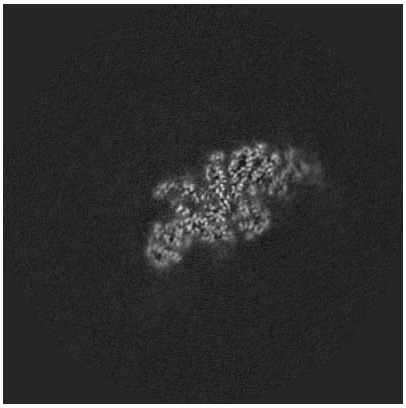
X Index: 186



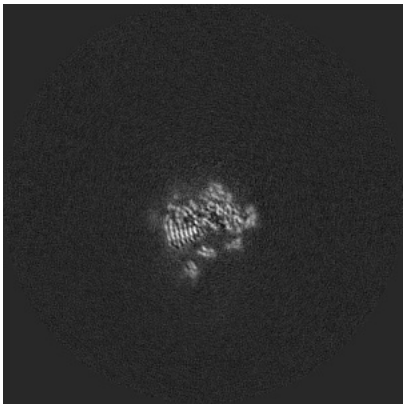
Y Index: 219

Z Index: 207

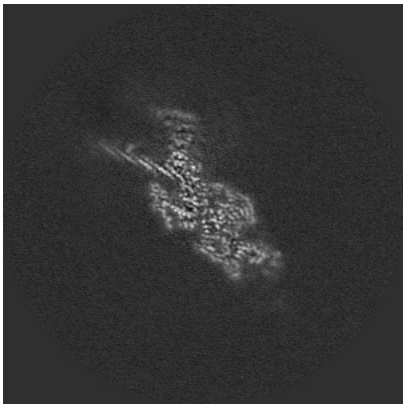
6.3.2 Raw map



X Index: 194



Y Index: 219

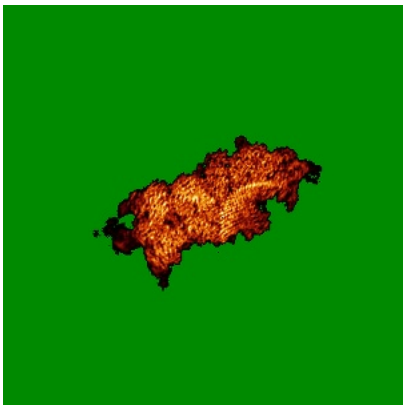


Z Index: 207

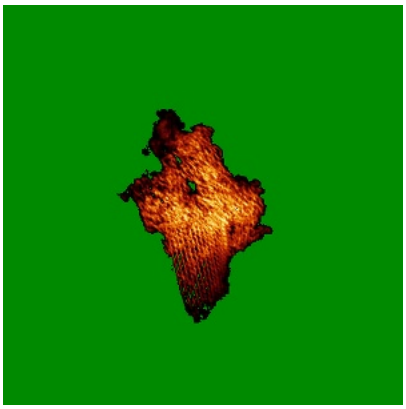
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

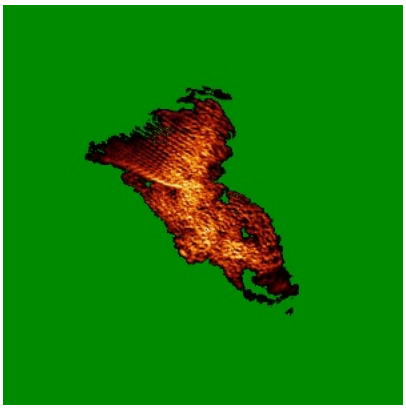
6.4.1 Primary map



X

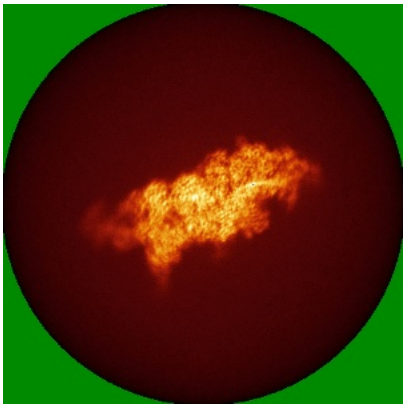


Y

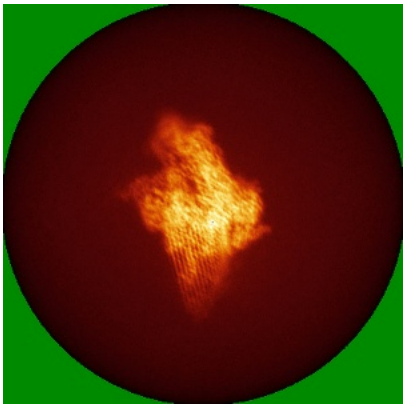


Z

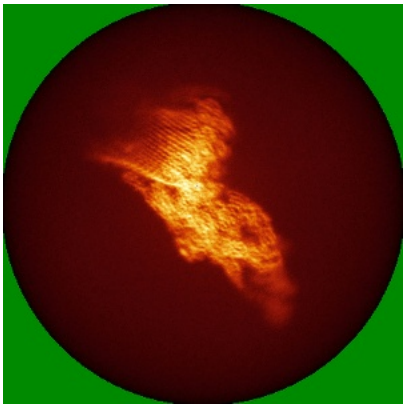
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

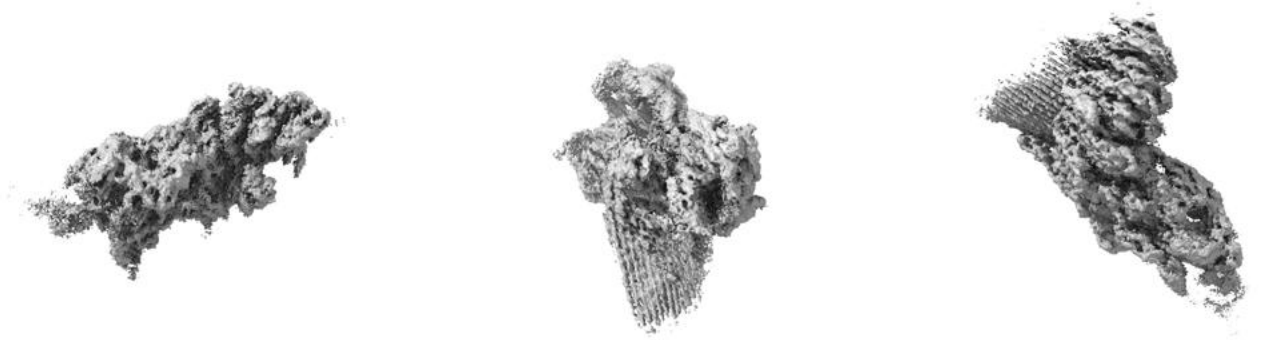
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

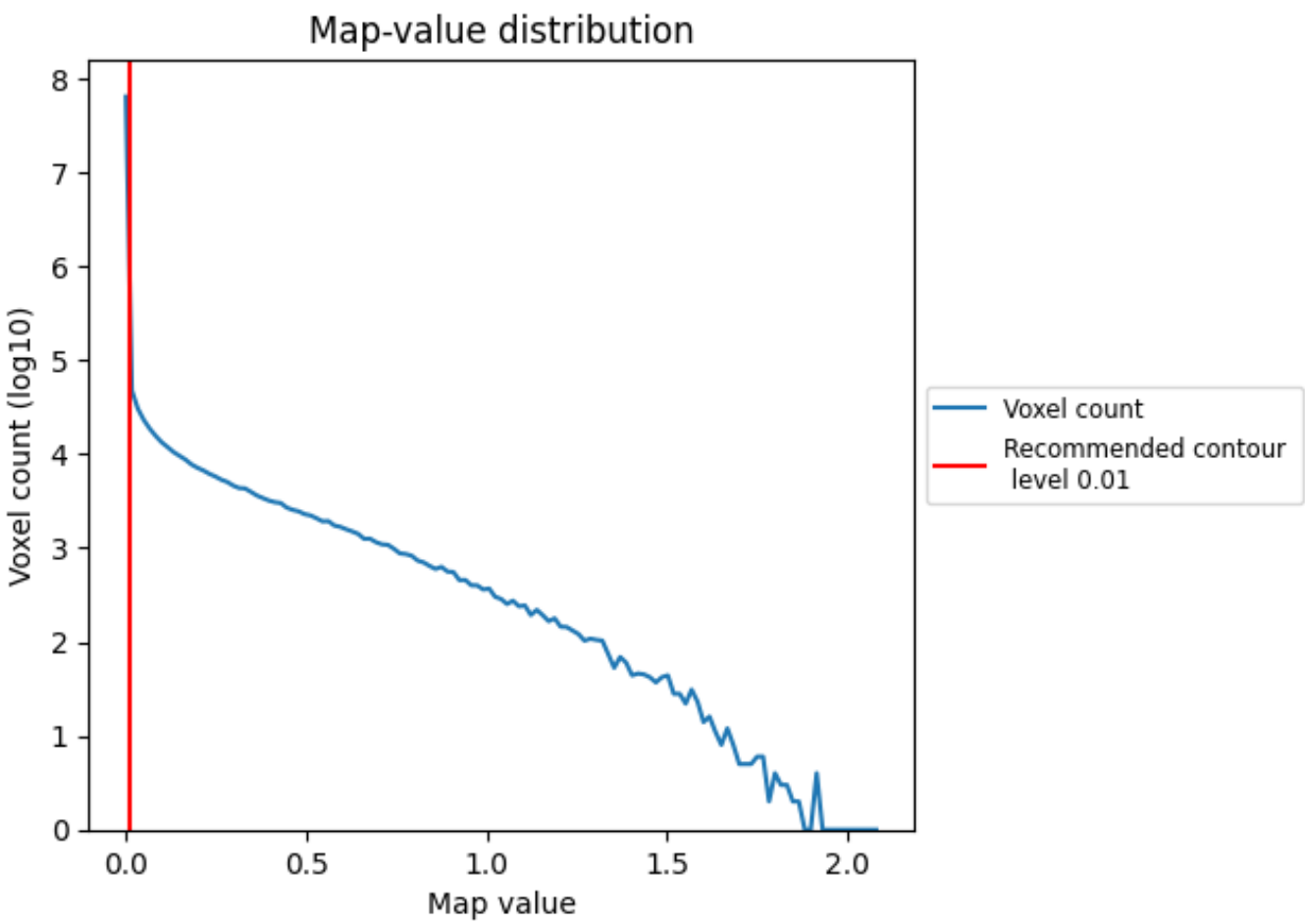
6.6 Mask visualisation (i)

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

7 Map analysis (i)

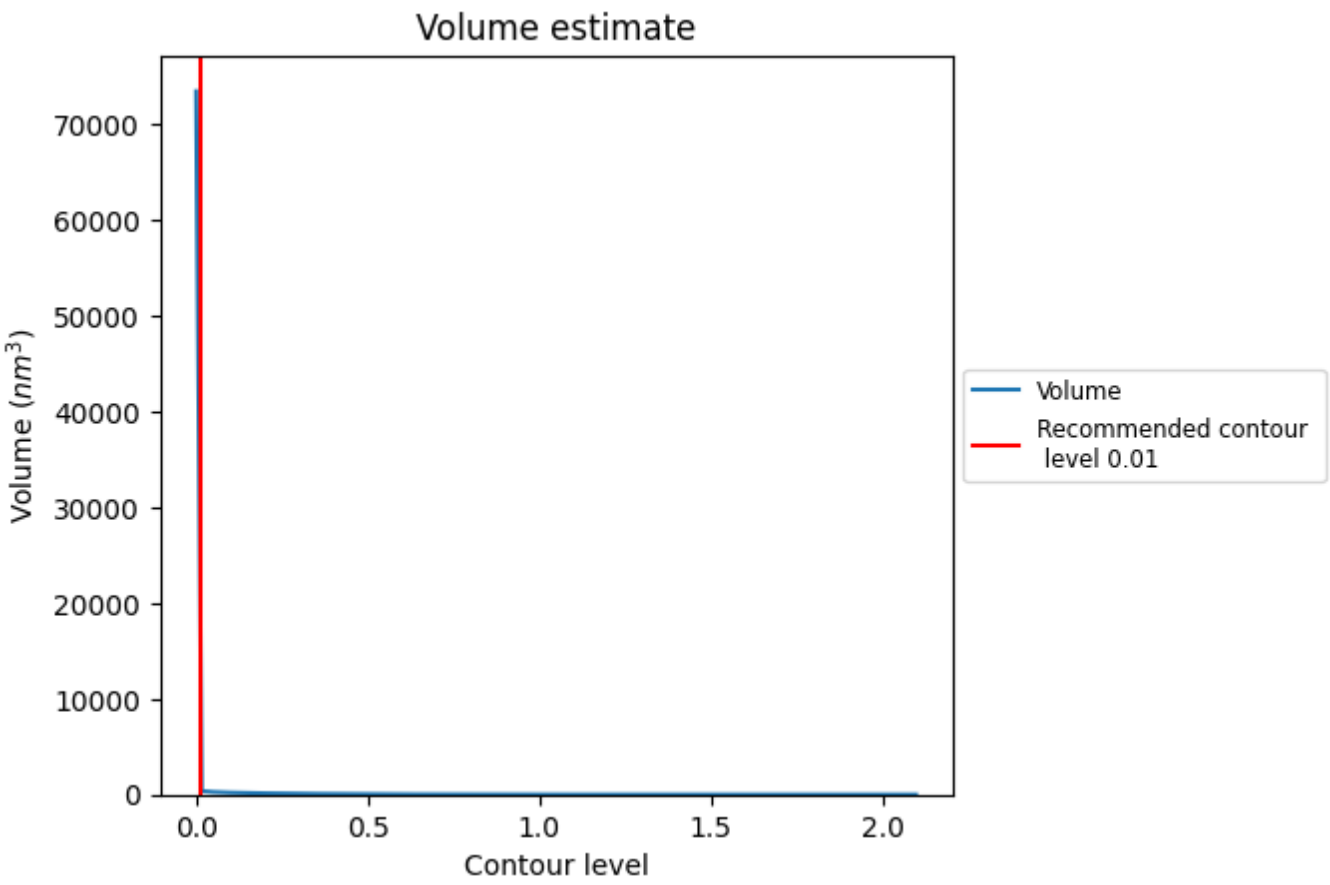
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

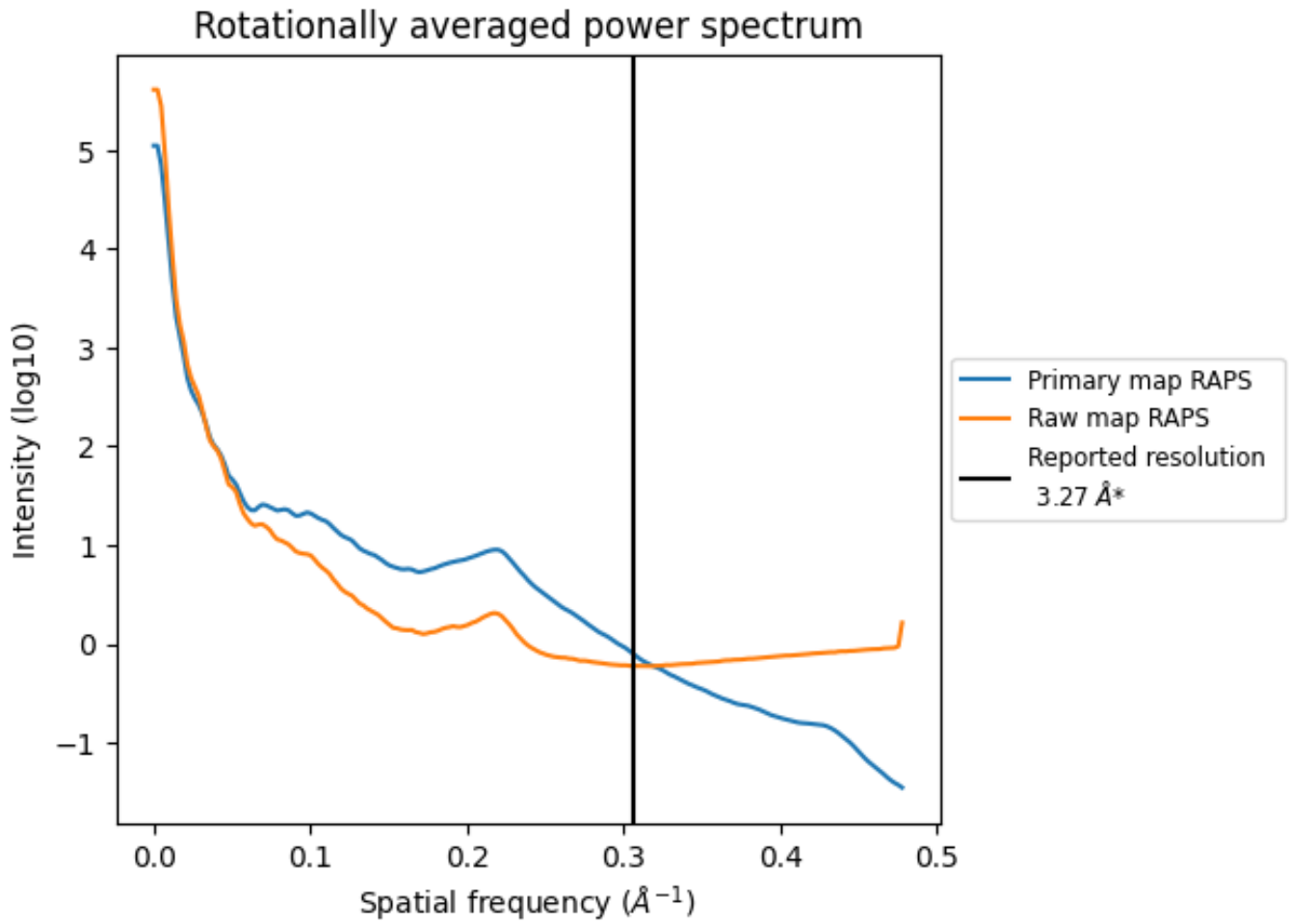
7.2 Volume estimate (i)



The volume at the recommended contour level is 20924 nm^3; this corresponds to an approximate mass of 18901 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)

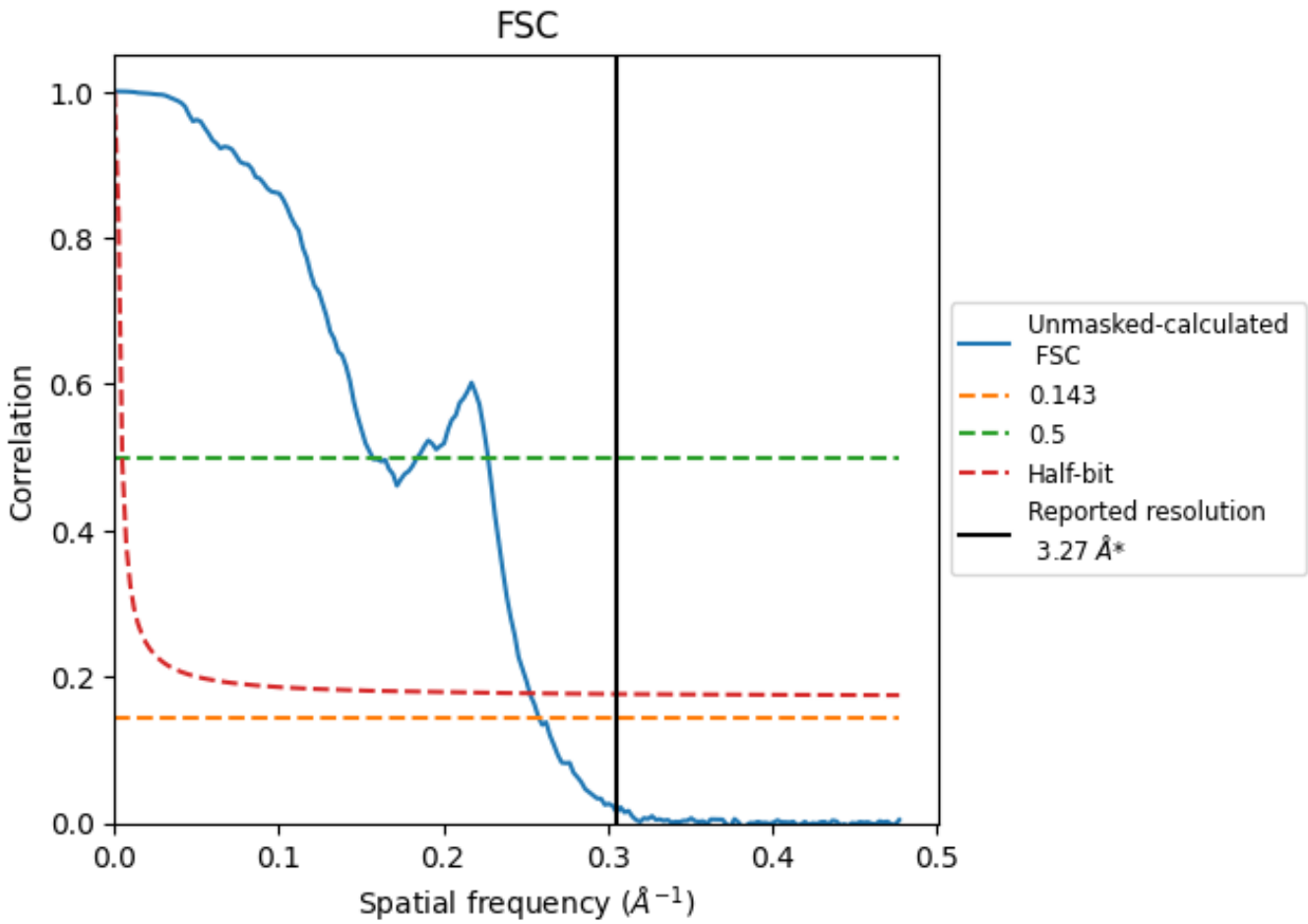


*Reported resolution corresponds to spatial frequency of 0.306 Å^{-1}

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 0.306 Å^{-1}

8.2 Resolution estimates (i)

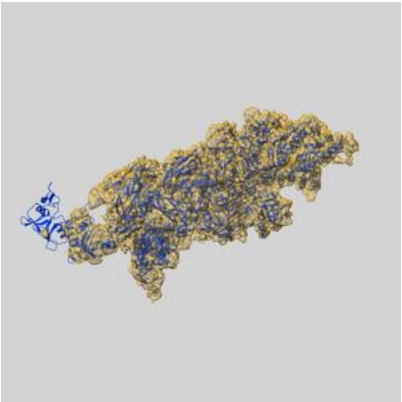
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.27	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.87	6.37	3.96

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.87 differs from the reported value 3.27 by more than 10 %

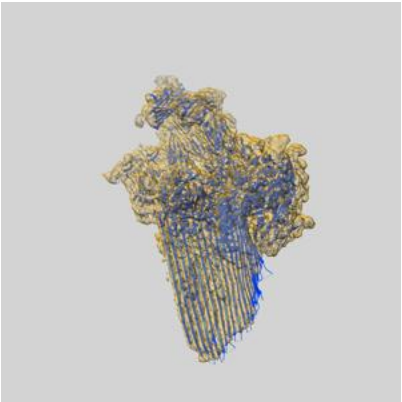
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-12651 and PDB model 7NYD. Per-residue inclusion information can be found in section 3 on page 9.

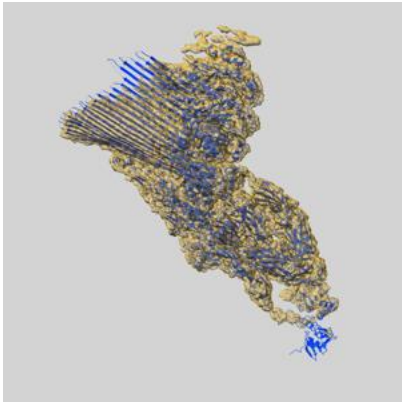
9.1 Map-model overlay (i)



X



Y



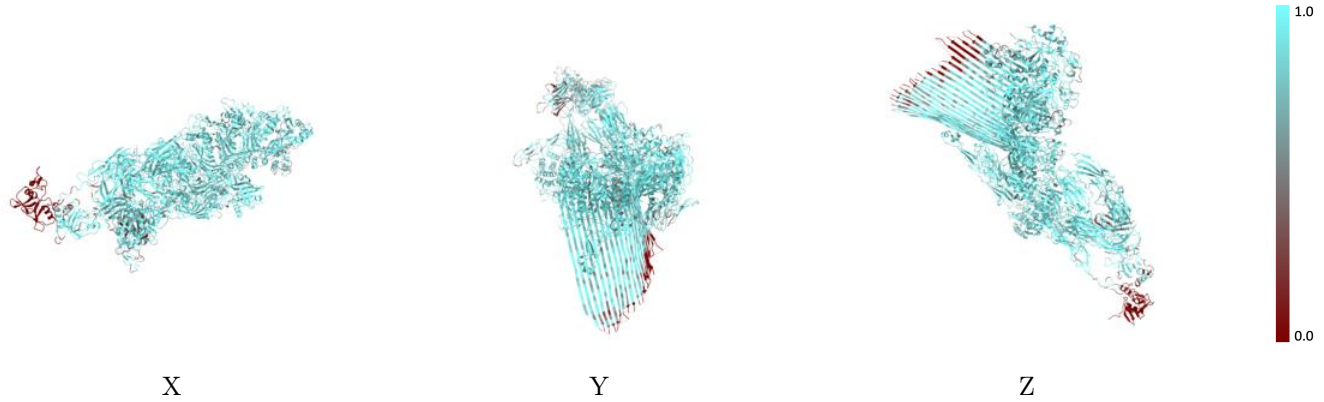
Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

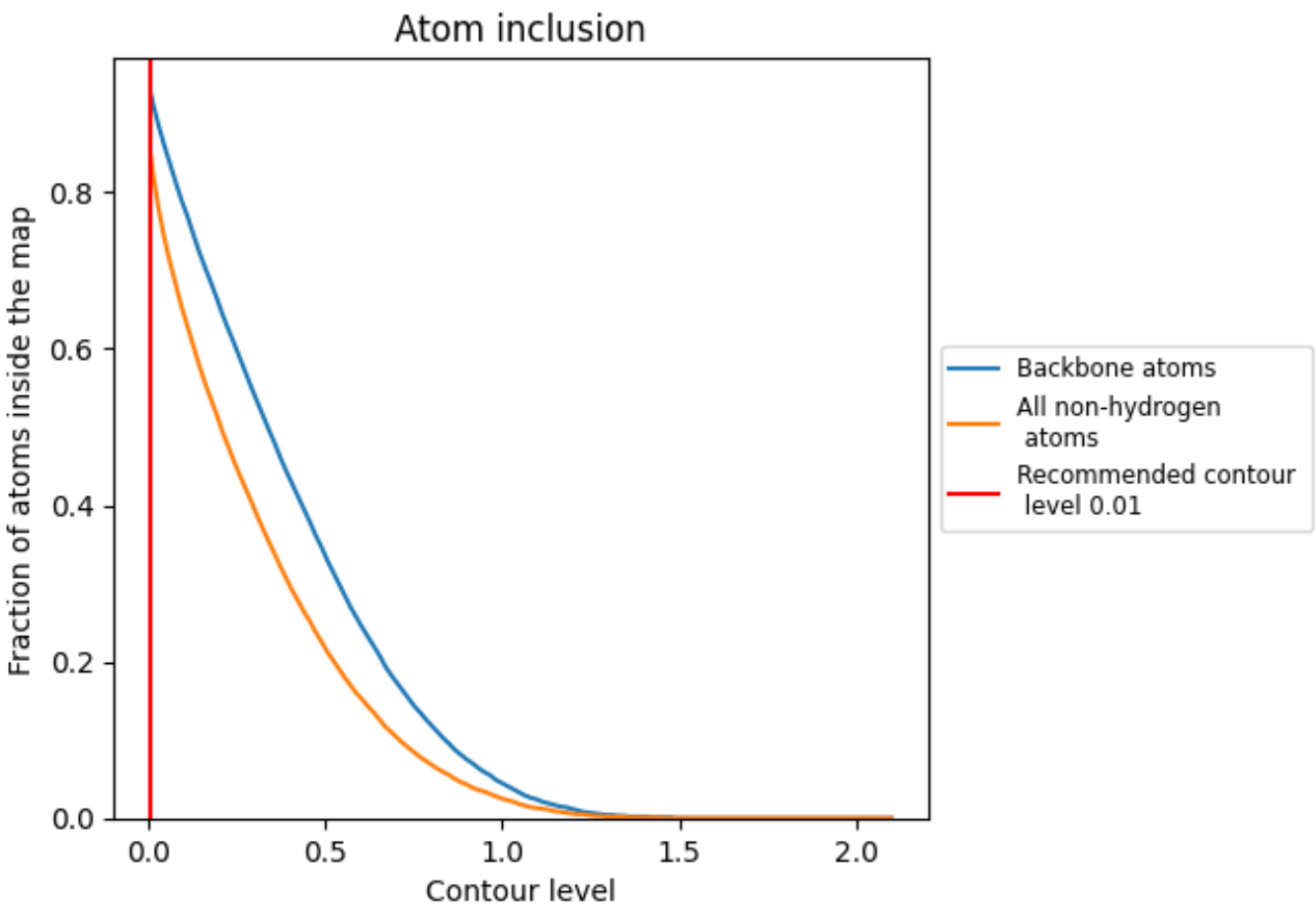
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 84% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8450	0.3350
A	0.8580	0.3070
B	0.8890	0.3840
C	0.7770	0.3450
D	0.8960	0.4040
E	0.8600	0.3640
F	0.8900	0.3270
G	0.8030	0.3050
H	0.7860	0.2300
I	0.7180	0.1840
J	0.5710	0.1580
K	0.5570	0.2480