



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 05:59 PM UTC

PDB ID : 7NYD / pdb_00007nyd
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 : 6H04, 6CXO, 4A5W, 2WCY, 6H03

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

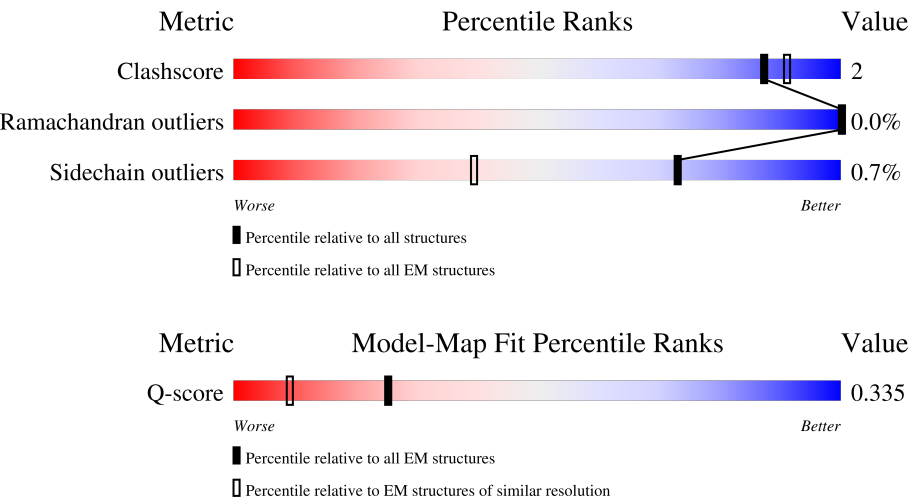
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14508 (2.77 - 3.77)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	D	537	6%87%9%
2	E	554	6%85%13%
3	G	538	7%75%23%
3	H	538	5%56%41%

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Mol	Chain	Length	Quality of chain
4	C	821	
5	B	913	
6	F	182	
7	A	1658	
8	I	3	
9	J	2	
10	K	5	

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	-	-	-
11	MAN	G	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
1	D	487	Total	C	N	O	S	0	0
			3914	2434	702	743	35		

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

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

- Molecule 3 is a protein called Complement component C9.

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

- Molecule 4 is a protein called Complement component C7.

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

- Molecule 5 is a protein called Complement component C6.

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

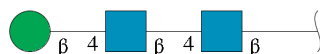
- Molecule 6 is a protein called Complement component C8 gamma chain.

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

- Molecule 7 is a protein called Complement C5.

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

- 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
8	I	3	Total	C	N	O	0	0
			39	22	2	15		

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



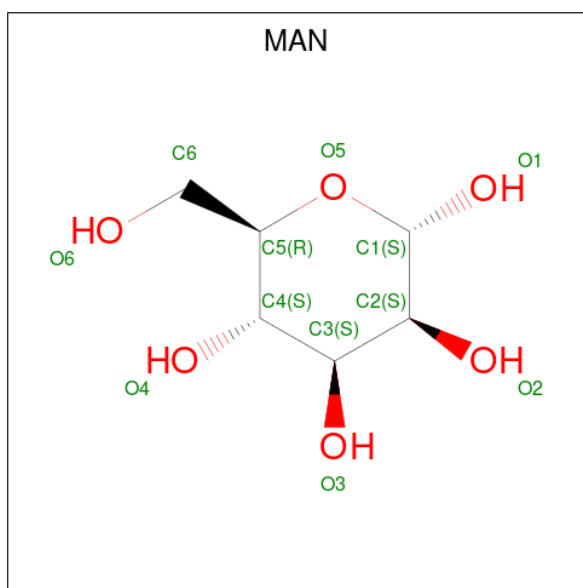
Mol	Chain	Residues	Atoms				AltConf	Trace
9	J	2	Total	C	N	O	0	0
			28	16	2	10		

- 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
10	K	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 11 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$).



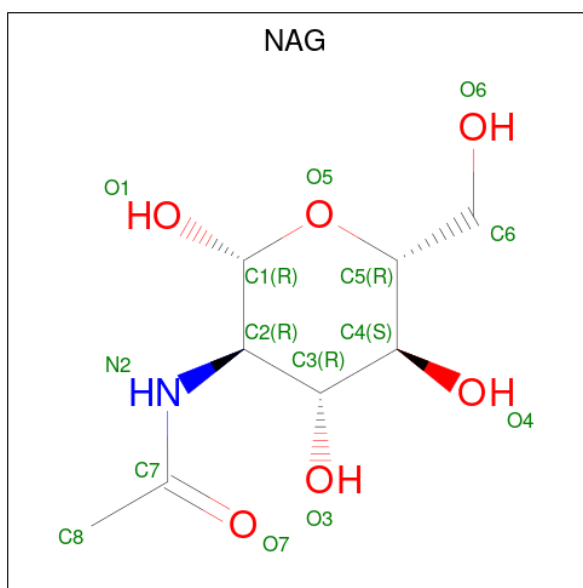
Mol	Chain	Residues	Atoms			AltConf
11	D	1	Total	C	O	0
			11	6	5	
11	D	1	Total	C	O	0
			11	6	5	
11	E	1	Total	C	O	0
			11	6	5	
11	E	1	Total	C	O	0
			11	6	5	
11	G	1	Total	C	O	0
			11	6	5	
11	C	1	Total	C	O	0
			11	6	5	

- Molecule 12 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

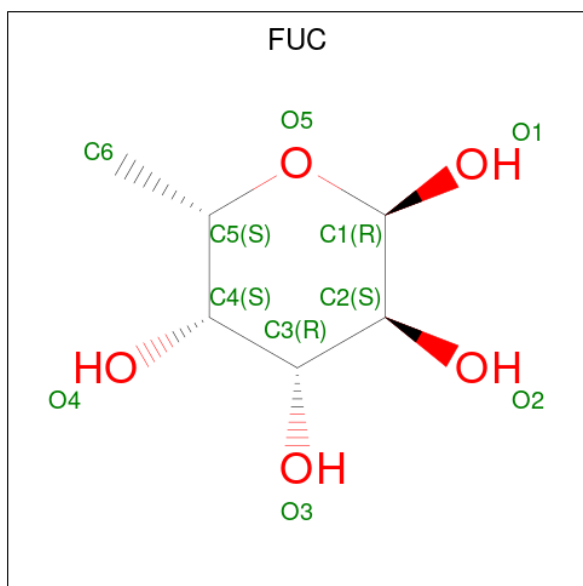
- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C₈H₁₅NO₆).



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

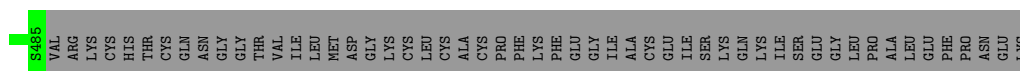
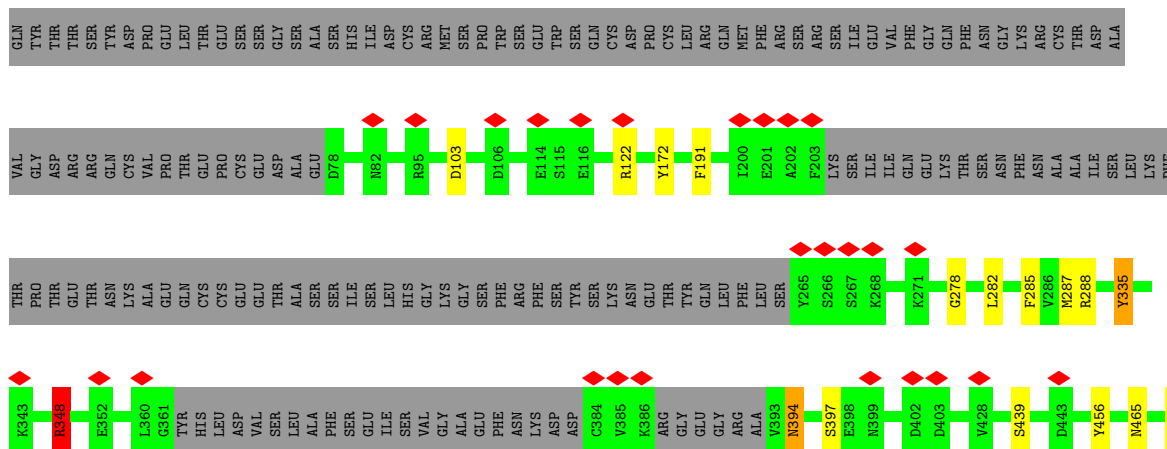
- Molecule 14 is alpha-L-fucopyranose (CCD ID: FUC) (formula: C₆H₁₂O₅).



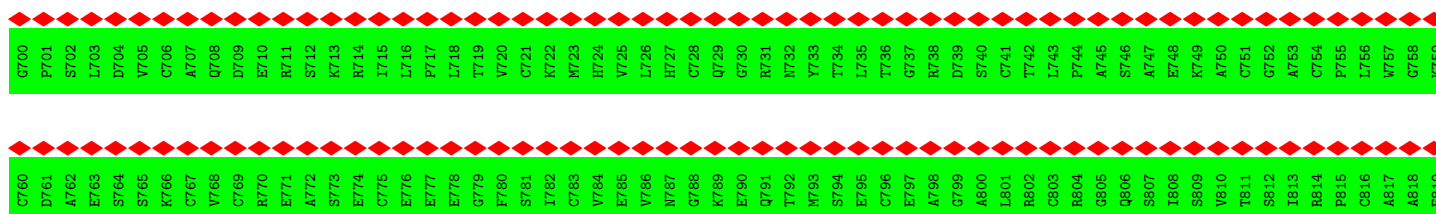
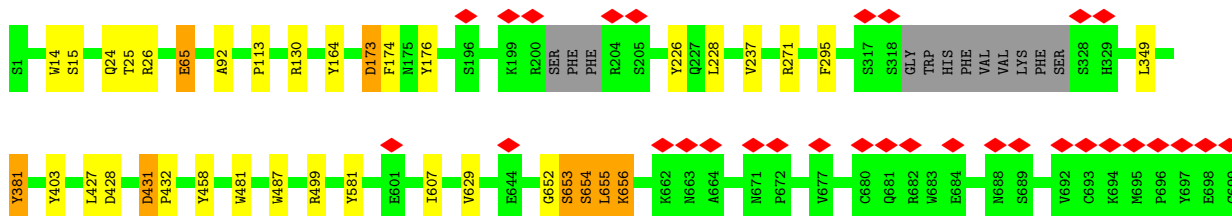
Mol	Chain	Residues	Atoms			AltConf
14	B	1	Total	C	O	0
			10	6	4	



• Molecule 3: Complement component C9

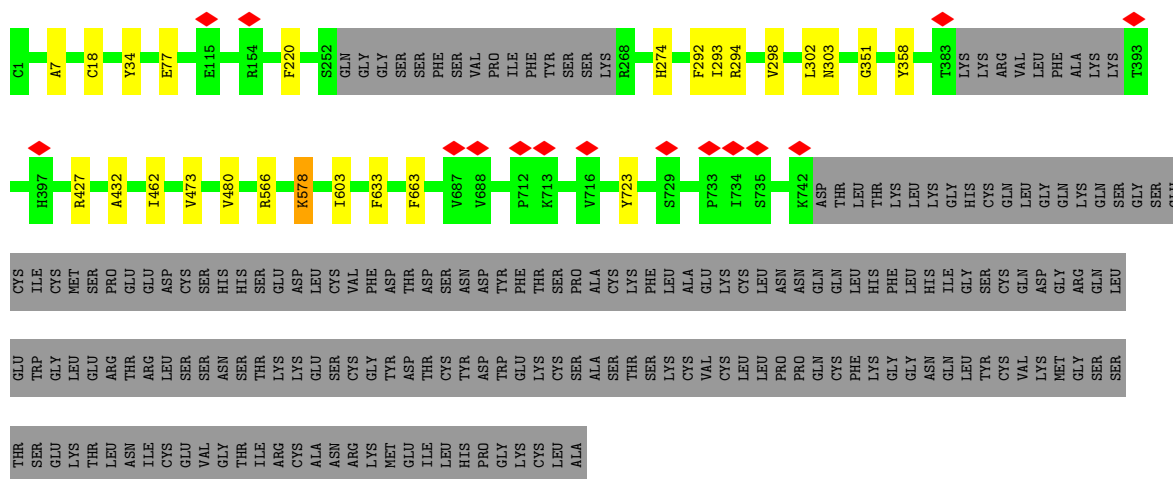


• Molecule 4: Complement component C7



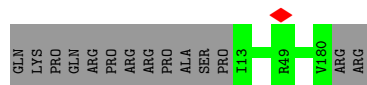
• Molecule 5: Complement component C6

Chain B:  76% 21%

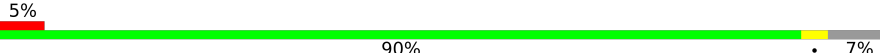


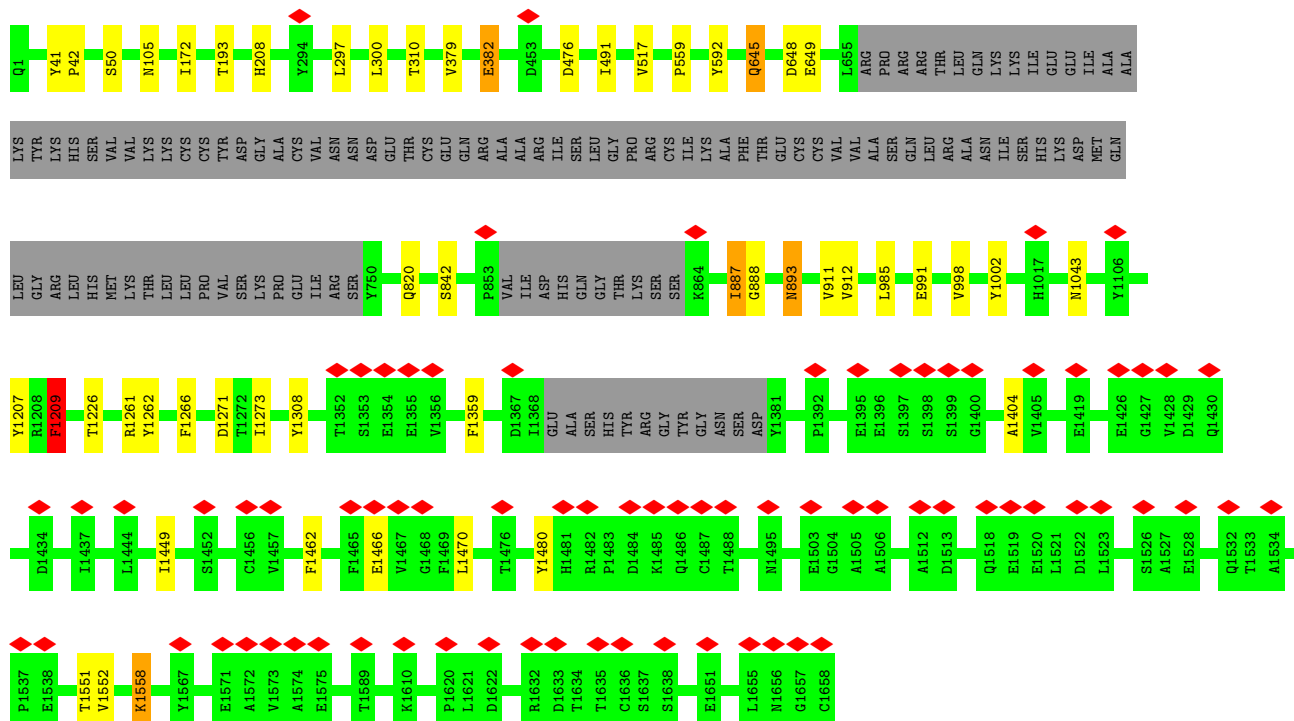
• Molecule 6: Complement component C8 gamma chain

Chain F:  92% 8%



• Molecule 7: Complement C5

Chain A:  5% 90% 7%



- 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:  100%

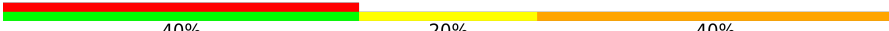
NAG1
NAG2
BMA3

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

Chain J:  100%

NAG1
NAG2

- 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:  40% 40% 20% 40%

NAG1
NAG2
BMA3
MAN4
MAN5

4 Experimental information

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 ($e^-/\text{\AA}^2$)	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, CA, BMA, FUC, 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	D	0.76	0/4004	1.30	12/5409 (0.2%)
2	E	0.74	0/3896	1.29	7/5249 (0.1%)
3	G	0.75	0/3322	1.27	1/4485 (0.0%)
3	H	0.76	0/2562	1.29	4/3457 (0.1%)
4	C	0.78	2/6109 (0.0%)	1.31	9/8290 (0.1%)
5	B	0.75	0/5750	1.27	7/7770 (0.1%)
6	F	0.77	0/1348	1.29	0/1829
7	A	0.73	0/11993	1.27	17/16320 (0.1%)
All	All	0.75	2/38984 (0.0%)	1.29	57/52809 (0.1%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	173	ASP	C-O	-5.45	1.17	1.23
4	C	15	SER	CA-C	-5.19	1.45	1.53

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1209	PHE	CA-CB-CG	11.79	125.59	113.80
1	D	518	PRO	N-CA-C	8.62	121.22	110.70
2	E	201	ASP	CA-CB-CG	7.91	120.51	112.60
5	B	633	PHE	CA-CB-CG	7.75	121.55	113.80
3	H	465	ASN	CA-CB-CG	7.06	119.66	112.60
7	A	893	ASN	CB-CA-C	-7.02	98.68	110.19
5	B	663	PHE	CA-CB-CG	6.97	120.77	113.80
3	H	348	ARG	CB-CA-C	6.86	123.45	109.67
4	C	174	PHE	CA-CB-CG	6.74	120.54	113.80
4	C	92	ALA	CA-C-N	6.01	129.16	120.38
4	C	92	ALA	C-N-CA	6.01	129.16	120.38
1	D	266	ARG	NE-CZ-NH2	5.98	124.58	119.20
5	B	294	ARG	NE-CZ-NH2	5.96	124.56	119.20
7	A	1558	LYS	N-CA-C	5.89	118.65	111.82
5	B	7	ALA	N-CA-C	5.86	118.77	110.50
4	C	271	ARG	NE-CZ-NH2	5.85	124.47	119.20
5	B	427	ARG	NE-CZ-NH2	5.84	124.46	119.20
2	E	512	TRP	N-CA-C	5.62	118.63	110.42
1	D	97	ASP	CA-CB-CG	5.59	118.19	112.60
2	E	199	PHE	CA-CB-CG	5.54	119.34	113.80
1	D	510	ARG	NE-CZ-NH2	5.54	124.19	119.20
7	A	998	VAL	N-CA-CB	5.54	113.99	110.50
7	A	559	PRO	N-CA-CB	5.54	106.42	102.65
7	A	1462	PHE	CA-CB-CG	5.53	119.33	113.80
7	A	50	SER	CA-C-N	5.52	125.86	121.61
7	A	50	SER	C-N-CA	5.52	125.86	121.61
7	A	1266	PHE	CA-CB-CG	5.48	119.28	113.80
2	E	170	GLY	N-CA-C	5.47	120.55	113.27
7	A	517	VAL	N-CA-C	5.47	120.70	108.88
1	D	320	ASN	CA-CB-CG	5.46	118.06	112.60
7	A	208	HIS	CB-CG-CD2	-5.45	124.12	131.20
7	A	1552	VAL	N-CA-CB	-5.41	104.49	111.90
5	B	274	HIS	CA-CB-CG	5.33	119.12	113.80
3	H	122	ARG	NE-CZ-NH2	5.31	123.98	119.20
5	B	566	ARG	NE-CZ-NH2	5.30	123.97	119.20
2	E	41	GLY	CA-C-N	5.28	128.21	120.71
2	E	41	GLY	C-N-CA	5.28	128.21	120.71
1	D	359	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	D	517	PRO	N-CA-C	5.25	117.11	110.70
7	A	1552	VAL	N-CA-C	5.25	116.53	112.12
1	D	521	ASN	CA-C-N	5.24	125.08	120.10
1	D	521	ASN	C-N-CA	5.24	125.08	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	431	ASP	CA-CB-CG	5.23	117.83	112.60
7	A	1271	ASP	CA-CB-CG	5.12	117.72	112.60
3	H	191	PHE	CA-CB-CG	5.12	118.92	113.80
4	C	821	GLN	OE1-CD-NE2	-5.09	117.51	122.60
4	C	15	SER	CA-C-O	-5.09	115.72	121.72
7	A	1043	ASN	CA-CB-CG	5.08	117.68	112.60
7	A	172	ILE	CA-C-N	5.07	125.06	119.89
7	A	172	ILE	C-N-CA	5.07	125.06	119.89
3	G	133	ARG	NE-CZ-NH2	5.05	123.74	119.20
2	E	379	ARG	NE-CZ-NH2	5.05	123.74	119.20
1	D	188	ARG	N-CA-C	5.04	115.64	107.32
1	D	313	ARG	CA-C-N	5.04	125.07	121.65
1	D	313	ARG	C-N-CA	5.04	125.07	121.65
4	C	130	ARG	NE-CZ-NH2	5.03	123.73	119.20
4	C	113	PRO	N-CA-C	5.03	120.21	114.03

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 ⓘ

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	15	0
2	E	3819	0	3601	4	0
3	G	3259	0	3101	15	0
3	H	2517	0	2385	25	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	0	0
10	K	61	0	52	5	0
11	C	11	0	10	3	0
11	D	22	0	19	2	0
11	E	22	0	20	2	0
11	G	11	0	10	6	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	150	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 (150) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:14:TRP:CE3	4:C:25:THR:C	2.39	0.99
4:C:65:GLU:HB3	7:A:645:GLN:HG2	1.44	0.97
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
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
7:A:887:ILE:HG23	7:A:911:VAL:C	2.00	0.87
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
4:C:14:TRP:HE3	4:C:25:THR:C	1.85	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
3:H:397:SER:HA	13:H:601:NAG:HO6	1.49	0.77
7:A:887:ILE:CG2	7:A:911:VAL:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
7:A:887:ILE:HG23	7:A:911:VAL:O	1.84	0.67
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
4:C:14:TRP:CZ3	4:C:25:THR:C	2.76	0.63
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: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
1:D:394:LEU:C	1:D:394:LEU:HD12	2.27	0.60
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
3:H:394:ASN:HD22	3:H:394:ASN:C	2.11	0.59
4:C:14:TRP:CZ3	4:C:24:GLN:C	2.81	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:H:285:PHE:CD1	3:H:287:MET:HE3	2.39	0.57
5:B:18:CYS:SG	14:B:1002:FUC:O2	2.62	0.57
3:G:413:ARG:HH11	3:G:413:ARG:CG	2.12	0.57
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
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
3:G:27:TRP:NE1	11:G:602:MAN:HO2	2.00	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:G:413:ARG:NH1	3:G:413:ARG:CG	2.72	0.52
3:G:27:TRP:CE2	11:G:602:MAN:O2	2.61	0.51
1:D:394:LEU:HD12	1:D:394:LEU:O	2.11	0.50
4:C:14:TRP:CE3	4:C:24:GLN:C	2.89	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
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
3:G:394:ASN:OD1	3:G:394:ASN:C	2.56	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
10:K:1:NAG:HO6	10:K:2:NAG:HN2	1.62	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
4:C:427:LEU:C	11:C:901:MAN:O4	2.58	0.46
7:A:310:THR:HG21	7:A:1466:GLU:CG	2.45	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
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:H:394:ASN:ND2	3:H:394:ASN:C	2.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:C:655:LEU:C	4:C:656:LYS:HE3	2.45	0.42
7:A:1470:LEU:H	7:A:1470:LEU:HD23	1.84	0.42
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
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	48	76
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 ⓘ

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%)	429 (99%)	4 (1%)	70	78
2	E	411/466 (88%)	409 (100%)	2 (0%)	81	83
3	G	359/477 (75%)	356 (99%)	3 (1%)	73	79
3	H	273/477 (57%)	270 (99%)	3 (1%)	65	76
4	C	615/714 (86%)	609 (99%)	6 (1%)	68	77
5	B	630/810 (78%)	627 (100%)	3 (0%)	81	83
6	F	136/149 (91%)	136 (100%)	0	100	100
7	A	1234/1470 (84%)	1228 (100%)	6 (0%)	81	83
All	All	4091/5036 (81%)	4064 (99%)	27 (1%)	73	80

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	11	CYS

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Mol	Chain	Res	Type
1	D	67	ARG
1	D	394	LEU
1	D	536	CYS
2	E	201	ASP
2	E	514	CYS
3	G	109	ASP
3	G	393	VAL
3	G	413	ARG
4	C	65	GLU
4	C	173	ASP
4	C	487	TRP
4	C	653	SER
4	C	655	LEU
4	C	656	LYS
5	B	292	PHE
5	B	578	LYS
5	B	723	TYR
3	H	103	ASP
3	H	348	ARG
3	H	394	ASN
7	A	382	GLU
7	A	491	ILE
7	A	645	GLN
7	A	820	GLN
7	A	887	ILE
7	A	1209	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	81	ASN
1	D	126	ASN
1	D	240	HIS
1	D	260	HIS
1	D	319	ASN
1	D	380	HIS
2	E	30	HIS
2	E	71	GLN
2	E	89	GLN
2	E	135	GLN
2	E	305	ASN
2	E	423	ASN

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Mol	Chain	Res	Type
2	E	526	GLN
3	G	19	HIS
3	G	66	GLN
3	G	167	ASN
3	G	436	ASN
4	C	24	GLN
4	C	167	GLN
4	C	171	ASN
4	C	175	ASN
4	C	218	ASN
4	C	346	ASN
4	C	347	ASN
4	C	377	ASN
5	B	177	HIS
5	B	273	ASN
5	B	296	HIS
5	B	303	ASN
5	B	408	HIS
5	B	534	GLN
5	B	574	GLN
3	H	471	GLN
6	F	46	GLN
6	F	173	GLN
7	A	1	GLN
7	A	218	ASN
7	A	224	ASN
7	A	271	ASN
7	A	301	ASN
7	A	356	GLN
7	A	363	GLN
7	A	405	ASN
7	A	455	HIS
7	A	493	HIS
7	A	640	ASN
7	A	782	GLN
7	A	891	ASN
7	A	1005	HIS
7	A	1215	GLN
7	A	1242	ASN
7	A	1307	ASN
7	A	1417	ASN
7	A	1436	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

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	0.71	0
8	NAG	I	2	8	14,14,15	0.26	0	17,19,21	0.58	0
8	BMA	I	3	8	11,11,12	0.24	0	15,15,17	0.74	0
9	NAG	J	1	9,2	14,14,15	0.27	0	17,19,21	0.61	0
9	NAG	J	2	9	14,14,15	0.27	0	17,19,21	0.68	0
10	NAG	K	1	10,7	14,14,15	2.11	5 (35%)	17,19,21	2.10	7 (41%)
10	NAG	K	2	10	14,14,15	1.02	2 (14%)	17,19,21	1.49	2 (11%)
10	BMA	K	3	10	11,11,12	0.22	0	15,15,17	1.33	2 (13%)
10	MAN	K	4	10	11,11,12	0.30	0	15,15,17	0.73	0
10	MAN	K	5	10	11,11,12	0.26	0	15,15,17	0.83	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	9,2	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	J	2	9	-	4/6/23/26	0/1/1/1
10	NAG	K	1	10,7	-	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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	K	1	NAG	C1-C2	-4.01	1.46	1.52
10	K	1	NAG	O5-C1	-3.48	1.37	1.43
10	K	1	NAG	C2-N2	-3.19	1.41	1.46
10	K	1	NAG	C4-C5	-2.69	1.47	1.53
10	K	2	NAG	O5-C1	-2.45	1.39	1.43
10	K	1	NAG	O5-C5	-2.20	1.39	1.43
10	K	2	NAG	C1-C2	-2.02	1.49	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	K	1	NAG	O5-C1-C2	-4.04	105.04	111.29
10	K	2	NAG	C1-C2-N2	-3.63	104.72	110.43
10	K	1	NAG	C3-C4-C5	-3.44	104.00	110.23
10	K	1	NAG	C6-C5-C4	-2.78	106.18	113.02
10	K	1	NAG	O7-C7-N2	-2.76	117.10	121.98
10	K	2	NAG	O4-C4-C5	-2.49	103.19	109.32
10	K	3	BMA	O5-C1-C2	-2.49	104.86	110.79
10	K	1	NAG	C1-C2-N2	-2.45	106.57	110.43
10	K	1	NAG	O6-C6-C5	-2.44	103.03	111.33
10	K	1	NAG	O4-C4-C5	-2.22	103.86	109.32
10	K	3	BMA	C3-C4-C5	-2.09	106.43	110.23

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

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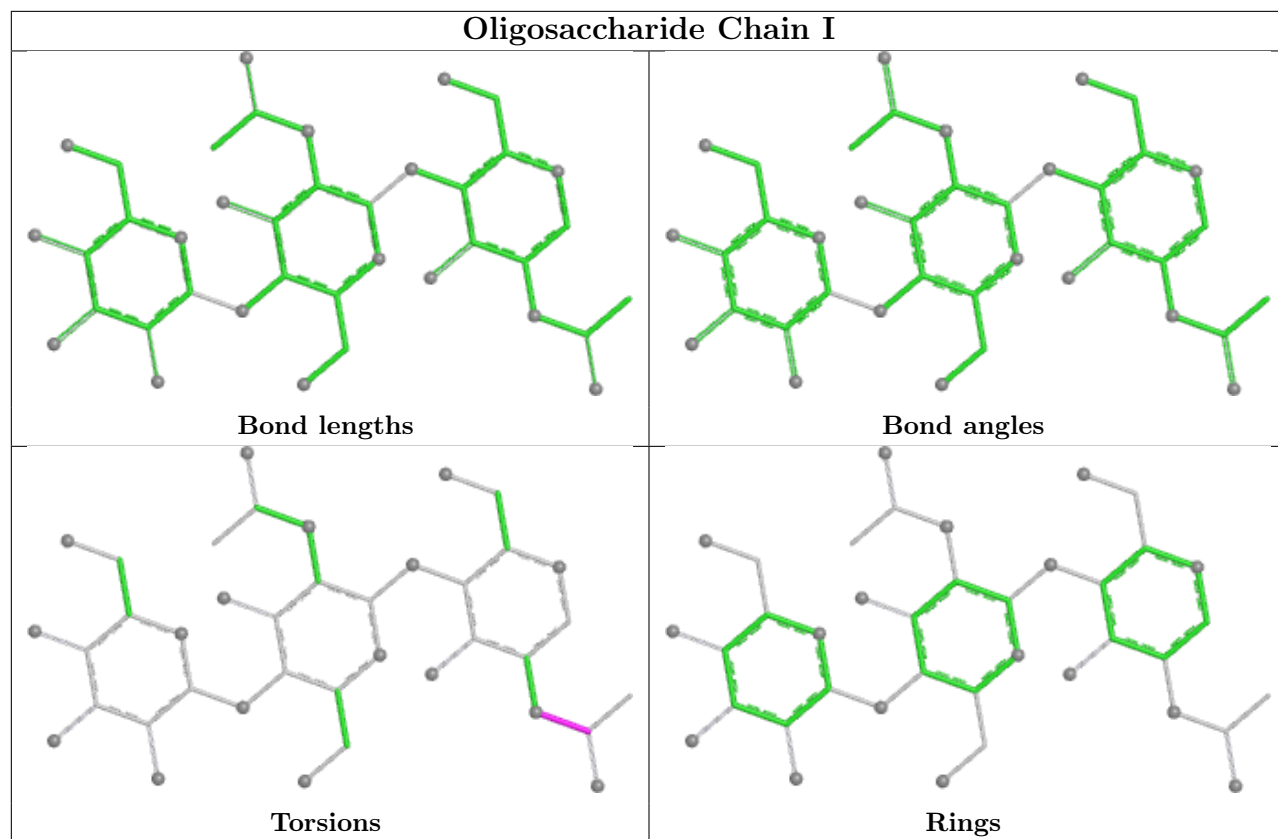
Mol	Chain	Res	Type	Atoms
10	K	1	NAG	O7-C7-N2-C2
10	K	2	NAG	C3-C2-N2-C7
10	K	2	NAG	C8-C7-N2-C2
10	K	2	NAG	O7-C7-N2-C2
10	K	1	NAG	O5-C5-C6-O6
10	K	3	BMA	C4-C5-C6-O6
10	K	1	NAG	C4-C5-C6-O6
9	J	1	NAG	O5-C5-C6-O6
9	J	2	NAG	O5-C5-C6-O6
9	J	1	NAG	C8-C7-N2-C2
10	K	3	BMA	O5-C5-C6-O6
8	I	1	NAG	C8-C7-N2-C2
9	J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

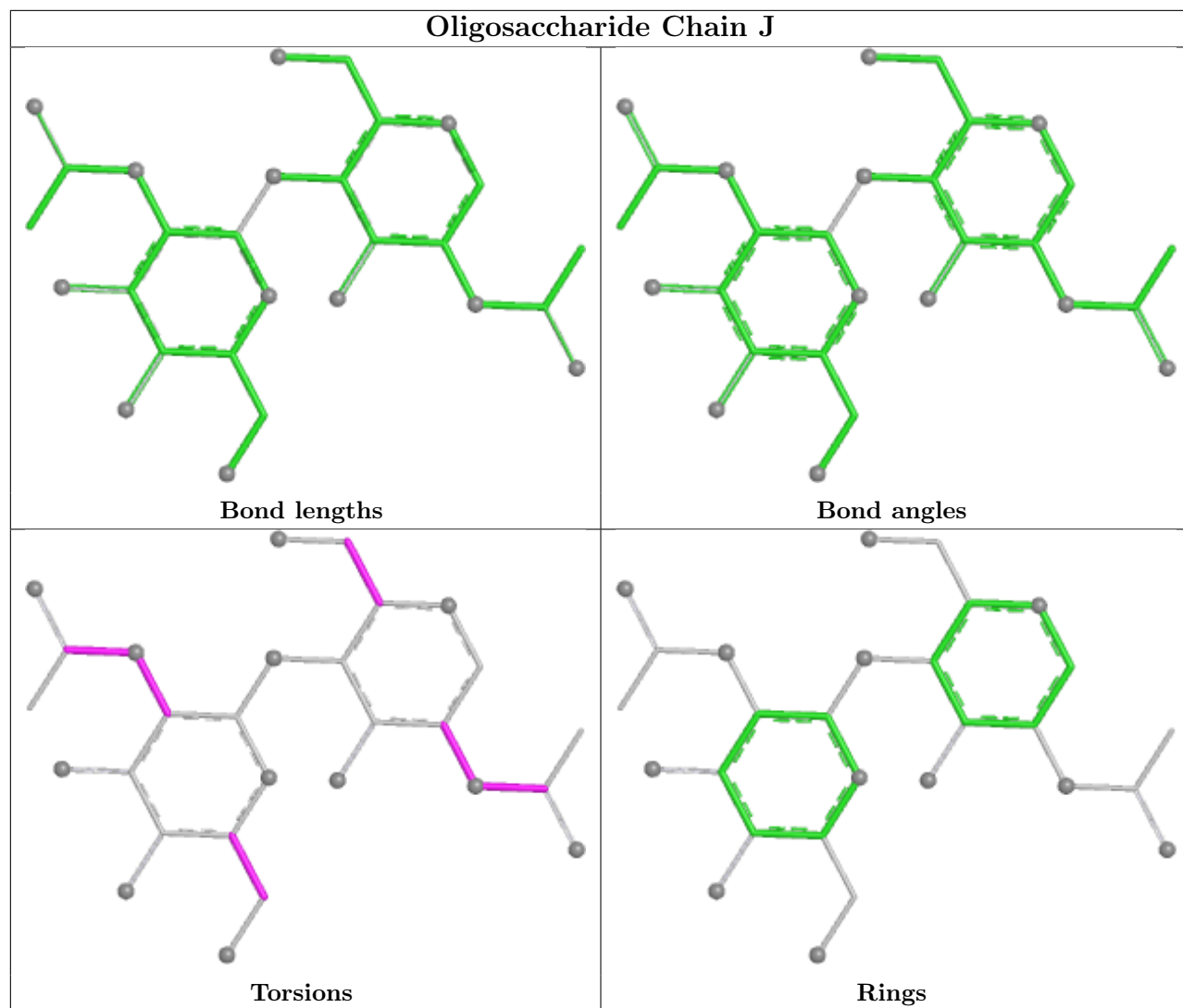
There are no ring outliers.

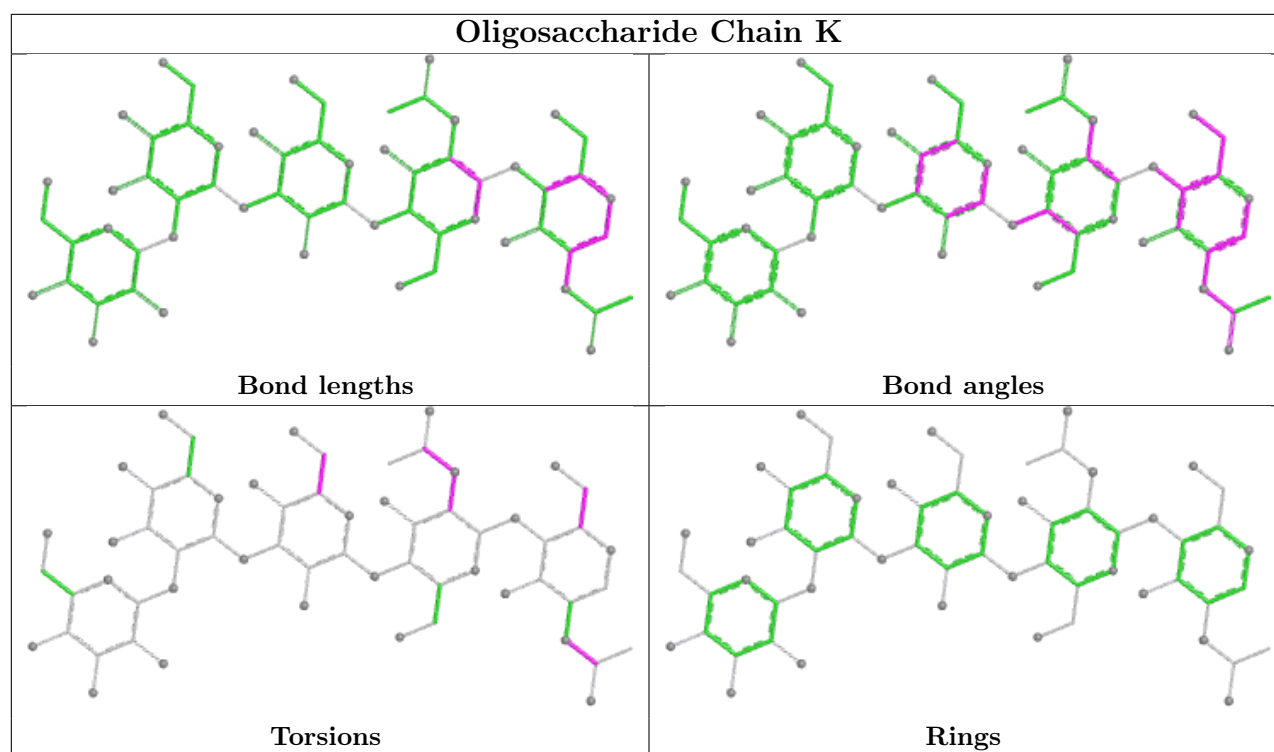
2 monomers are involved in 5 short contacts:

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

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







5.6 Ligand geometry [i](#)

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	0.59	0	14,14,16	1.68	4 (28%)
11	MAN	E	602	2	11,11,12	1.15	1 (9%)	15,15,17	2.40	4 (26%)
11	MAN	D	602	1	11,11,12	0.30	0	15,15,17	1.19	2 (13%)
11	MAN	C	901	4	11,11,12	0.42	0	15,15,17	2.09	4 (26%)
11	MAN	G	602	3	11,11,12	1.03	1 (9%)	15,15,17	1.87	6 (40%)
13	NAG	H	601	3	14,14,15	1.38	2 (14%)	17,19,21	2.54	4 (23%)
13	NAG	B	1001	-	14,14,15	0.47	0	17,19,21	1.53	2 (11%)
13	NAG	G	601	3	14,14,15	0.33	0	17,19,21	0.67	0
11	MAN	D	601	1	11,11,12	1.28	1 (9%)	15,15,17	1.16	2 (13%)
11	MAN	E	601	2	11,11,12	0.78	0	15,15,17	2.01	5 (33%)

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	E	602	2	-	1/2/19/22	0/1/1/1
11	MAN	D	602	1	1/1/4/5	1/2/19/22	0/1/1/1
11	MAN	C	901	4	-	2/2/19/22	0/1/1/1
11	MAN	G	602	3	-	2/2/19/22	0/1/1/1
13	NAG	H	601	3	-	3/6/23/26	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	D	601	1	-	2/2/19/22	0/1/1/1
11	MAN	E	601	2	-	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	-3.67	1.35	1.43
13	H	601	NAG	C1-C2	3.57	1.57	1.52
13	H	601	NAG	O5-C1	3.40	1.49	1.43
11	E	602	MAN	C2-C3	2.77	1.56	1.52
11	G	602	MAN	O5-C1	-2.51	1.39	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	H	601	NAG	C1-O5-C5	7.42	122.14	112.19
11	C	901	MAN	C1-O5-C5	5.95	120.17	112.19
13	H	601	NAG	O5-C1-C2	-5.85	102.24	111.29
11	E	602	MAN	C1-O5-C5	5.75	119.90	112.19
11	E	601	MAN	C1-O5-C5	-5.41	104.93	112.19
11	E	602	MAN	O3-C3-C2	4.66	119.56	110.05
13	B	1001	NAG	C1-O5-C5	3.98	117.52	112.19
13	B	1001	NAG	O5-C1-C2	-3.81	105.40	111.29
11	G	602	MAN	C1-O5-C5	-3.78	107.12	112.19
11	C	901	MAN	O5-C1-C2	3.41	118.93	110.79
11	D	602	MAN	C1-C2-C3	3.38	114.56	109.64
11	E	602	MAN	O4-C4-C3	-3.35	102.49	110.38
11	G	602	MAN	C1-C2-C3	3.17	114.27	109.64
11	E	602	MAN	C1-C2-C3	3.17	114.27	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	E	601	MAN	O2-C2-C3	-3.06	103.82	110.15
14	B	1002	FUC	O3-C3-C2	-2.83	104.28	110.05
11	G	602	MAN	O5-C5-C6	-2.73	102.34	107.66
11	E	601	MAN	C1-C2-C3	-2.58	105.88	109.64
14	B	1002	FUC	C1-C2-C3	-2.52	105.98	109.64
11	C	901	MAN	C3-C4-C5	-2.47	105.75	110.23
11	G	602	MAN	C2-C3-C4	2.45	115.17	110.86
11	D	602	MAN	C1-O5-C5	2.37	115.37	112.19
11	G	602	MAN	O5-C1-C2	-2.29	105.31	110.79
11	C	901	MAN	C1-C2-C3	2.29	112.98	109.64
14	B	1002	FUC	O2-C2-C1	2.23	114.34	109.22
11	E	601	MAN	C2-C3-C4	-2.19	107.02	110.86
13	H	601	NAG	C2-N2-C7	2.15	125.78	122.90
11	E	601	MAN	O5-C1-C2	-2.15	105.66	110.79
13	H	601	NAG	C4-C3-C2	2.13	114.14	111.02
11	G	602	MAN	O4-C4-C5	2.09	114.48	109.32
11	D	601	MAN	C2-C3-C4	-2.07	107.22	110.86
14	B	1002	FUC	O2-C2-C3	2.06	114.42	110.15
11	D	601	MAN	C1-O5-C5	-2.04	109.45	112.19

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	C1-C2-N2-C7
13	G	601	NAG	C8-C7-N2-C2
13	G	601	NAG	O7-C7-N2-C2
13	B	1001	NAG	C8-C7-N2-C2
13	B	1001	NAG	O7-C7-N2-C2
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	E	601	MAN	O5-C5-C6-O6
11	G	602	MAN	C4-C5-C6-O6
11	D	601	MAN	O5-C5-C6-O6
11	E	601	MAN	C4-C5-C6-O6
11	D	601	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
11	C	901	MAN	O5-C5-C6-O6
11	D	602	MAN	O5-C5-C6-O6
13	B	1001	NAG	O5-C5-C6-O6
13	B	1001	NAG	C1-C2-N2-C7
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 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	1002	FUC	2	0
11	D	602	MAN	1	0
11	C	901	MAN	3	0
11	G	602	MAN	6	0
13	H	601	NAG	10	0
13	B	1001	NAG	4	0
13	G	601	NAG	3	0
11	D	601	MAN	1	0
11	E	601	MAN	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

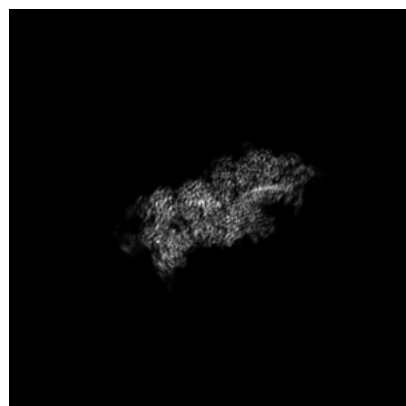
6 Map visualisation [i](#)

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

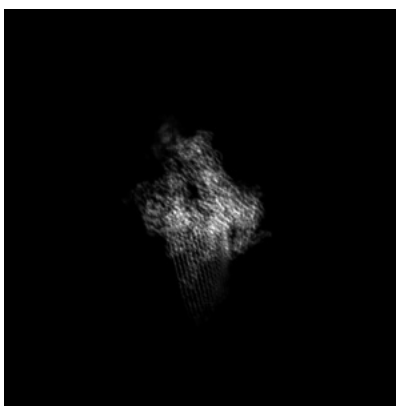
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

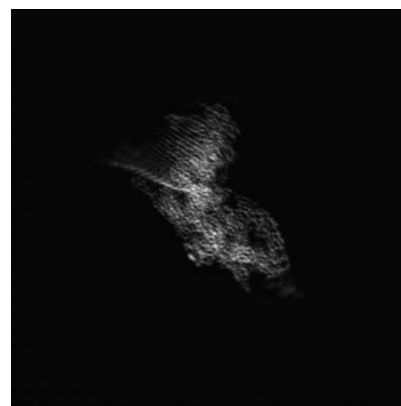
6.1.1 Primary map



X

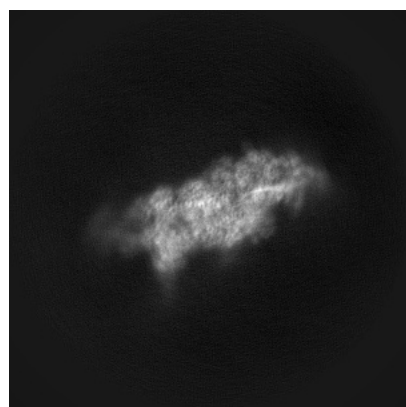


Y

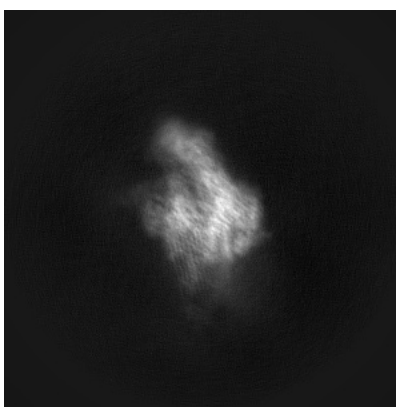


Z

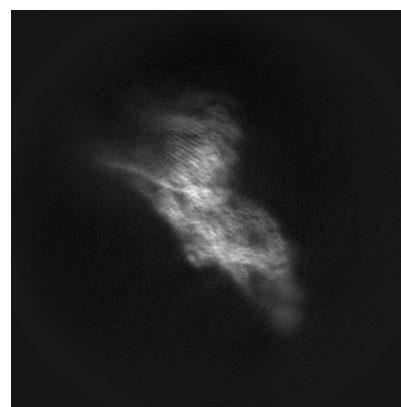
6.1.2 Raw map



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

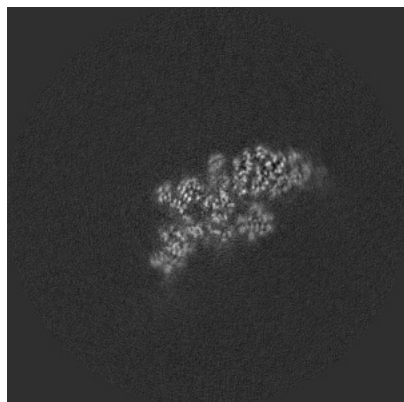


Y Index: 200

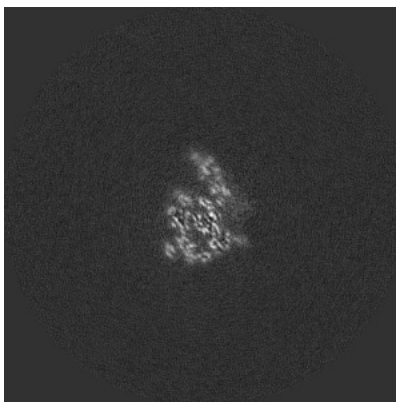


Z Index: 200

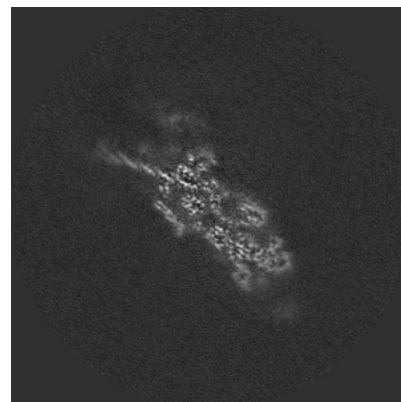
6.2.2 Raw map



X Index: 200



Y Index: 200

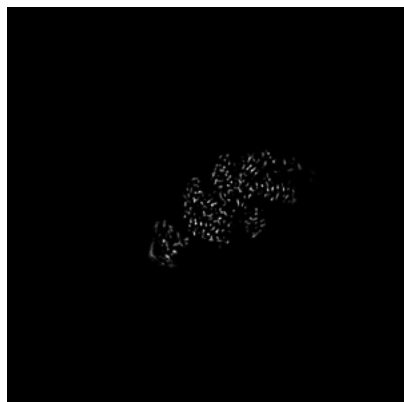


Z Index: 200

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

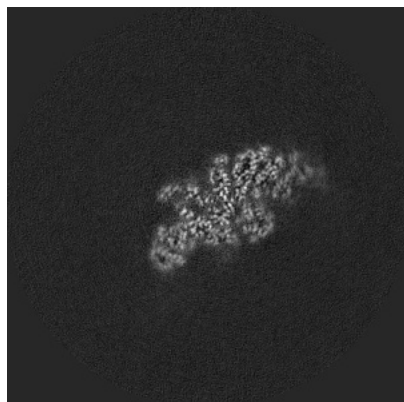


Y Index: 219

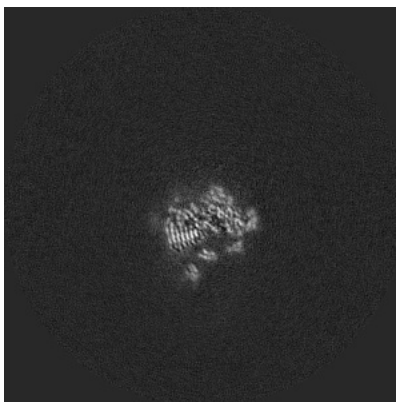


Z Index: 207

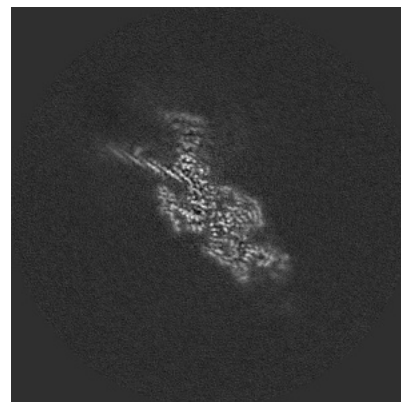
6.3.2 Raw map



X Index: 194



Y Index: 219

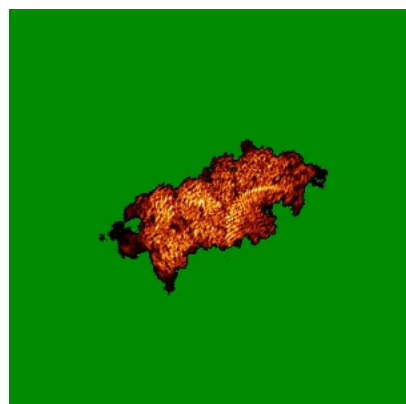


Z Index: 207

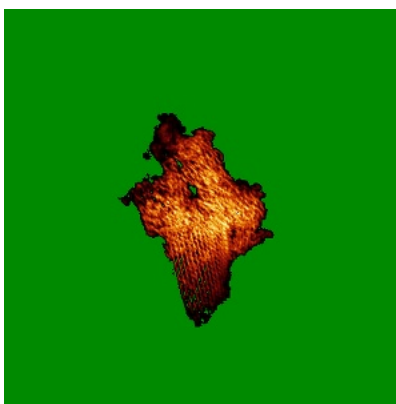
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



X

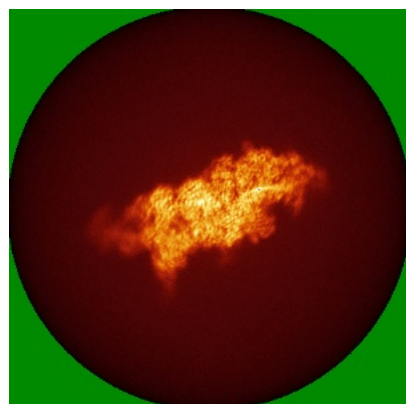


Y

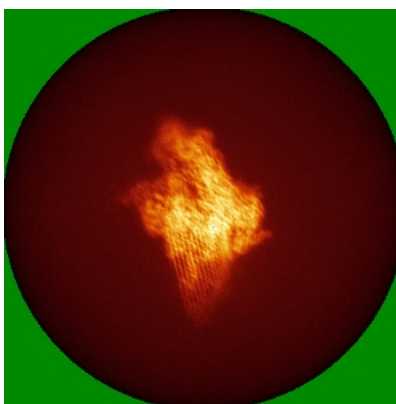


Z

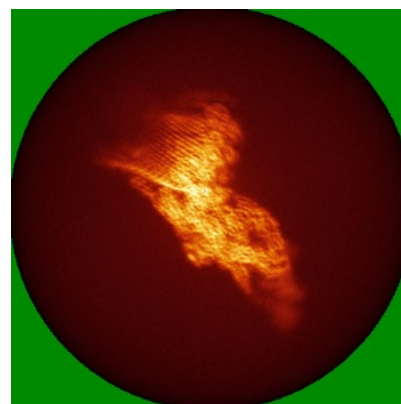
6.4.2 Raw map



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



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



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.

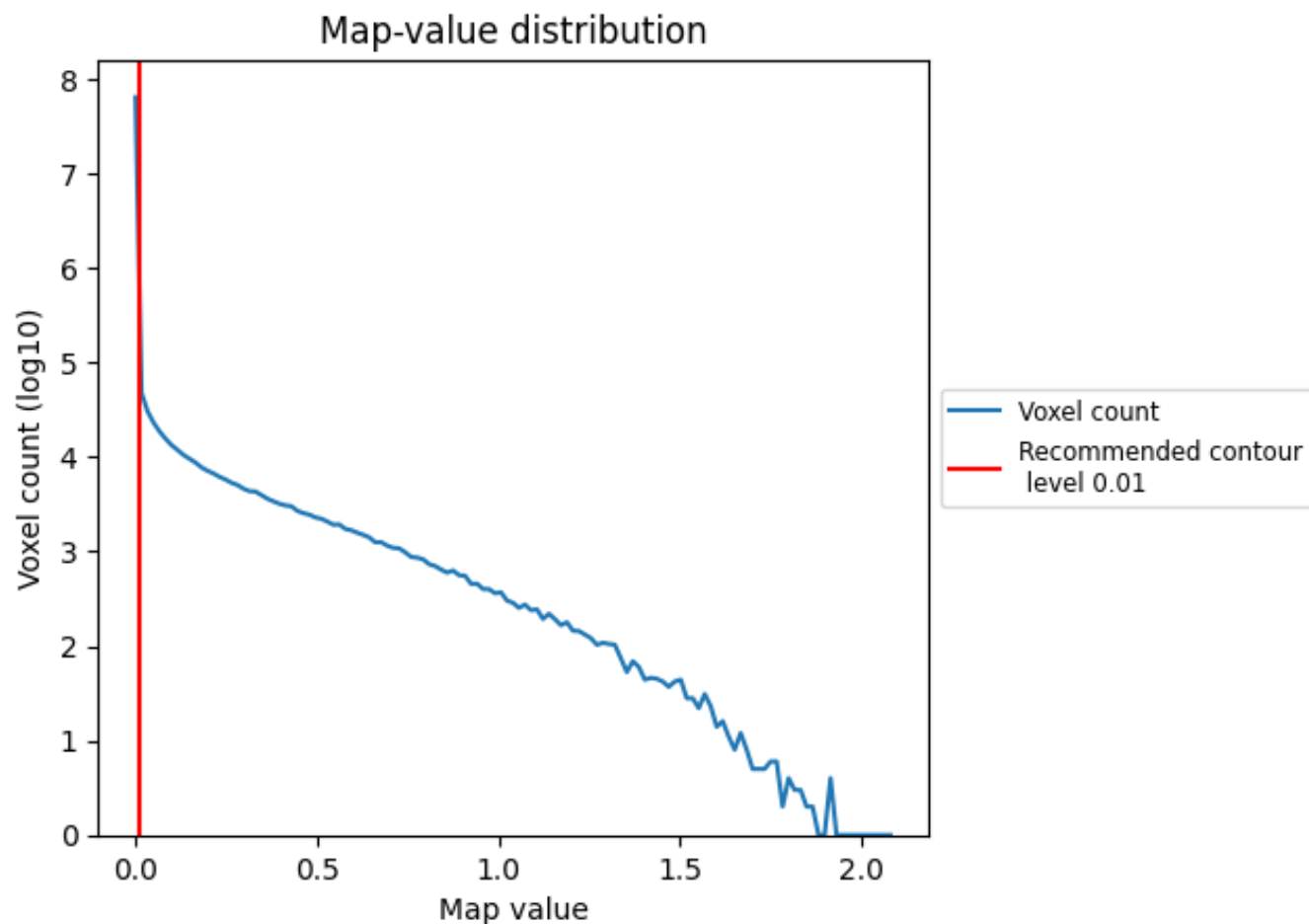
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

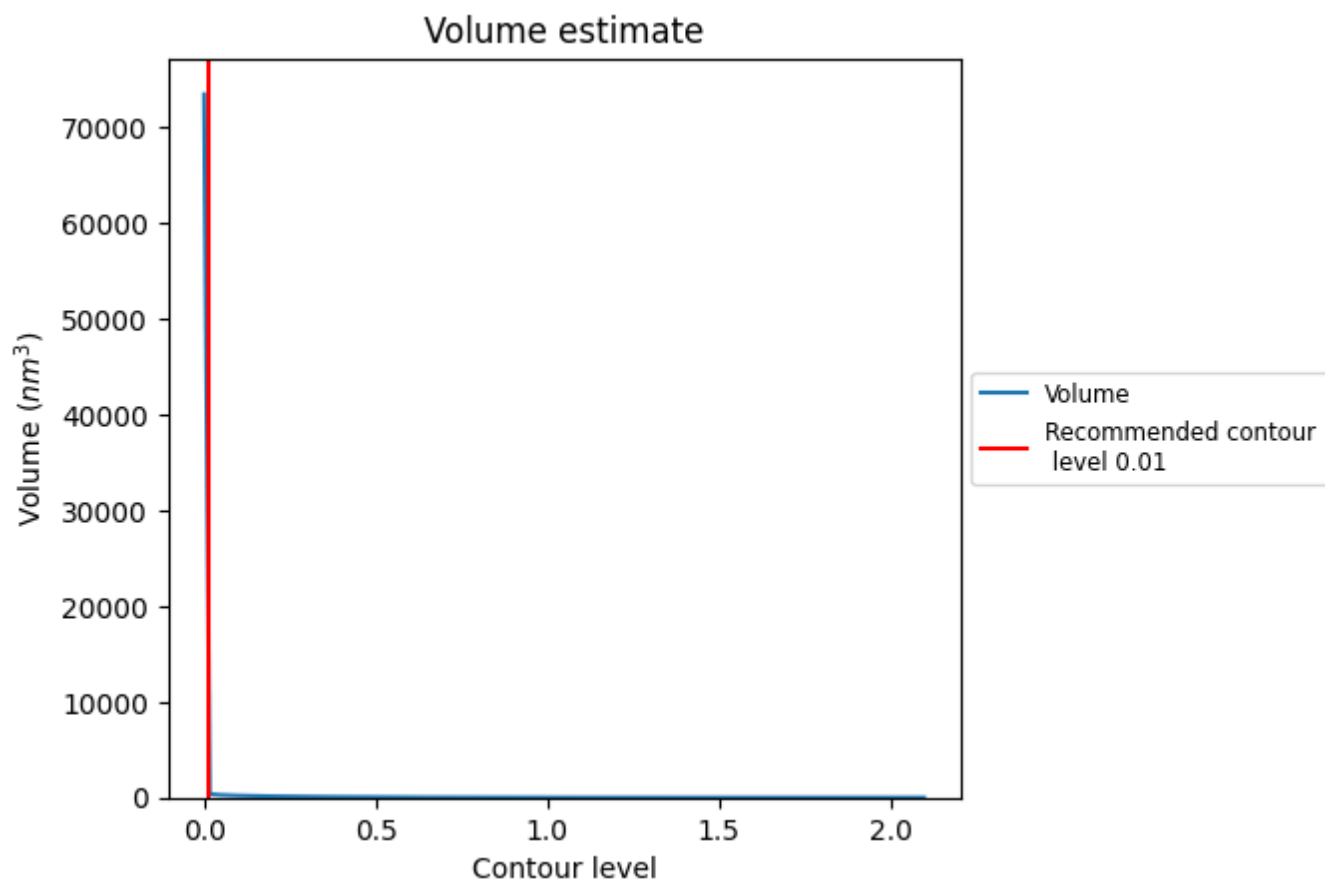
This section contains the results of statistical analysis of the map.

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.

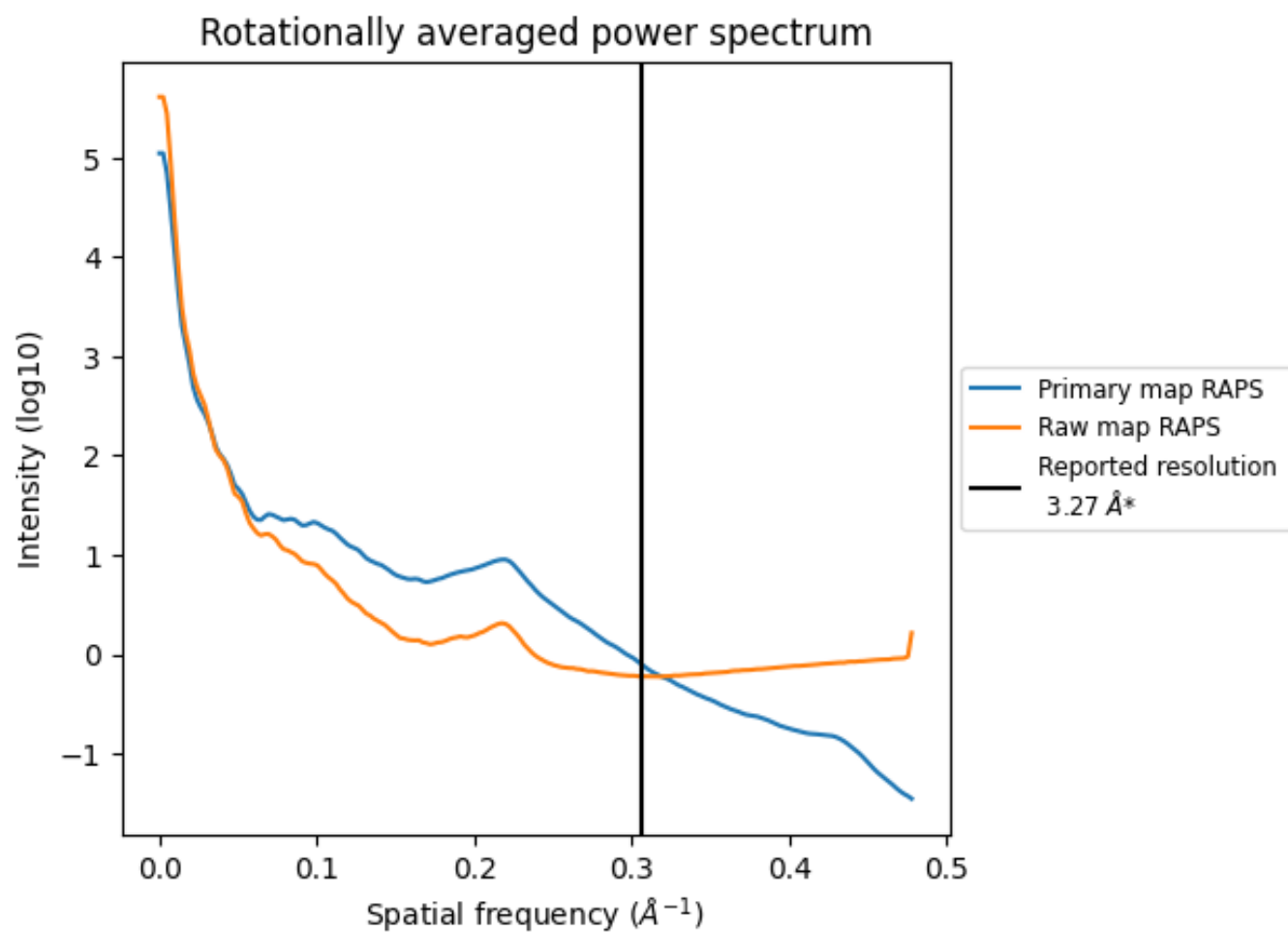
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 20924 nm³; 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 ⓘ

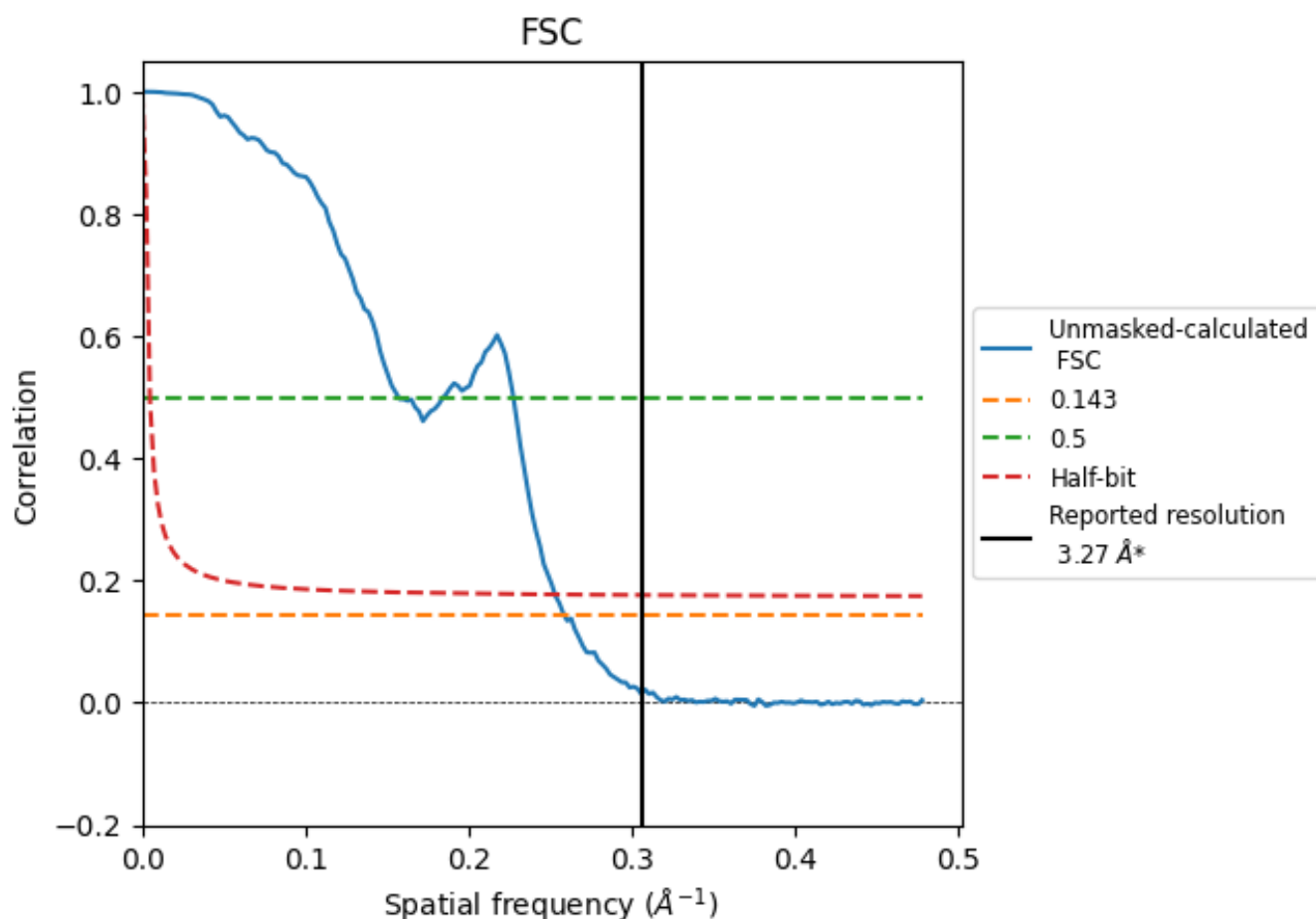


*Reported resolution corresponds to spatial frequency of $0.306 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.306 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

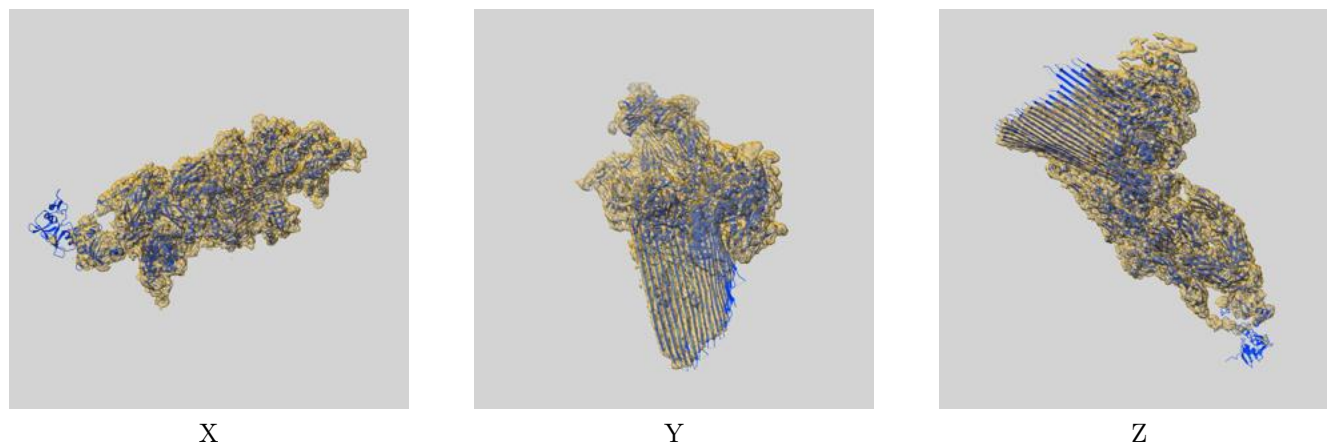
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.27	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.87	6.37	3.96

*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](#)

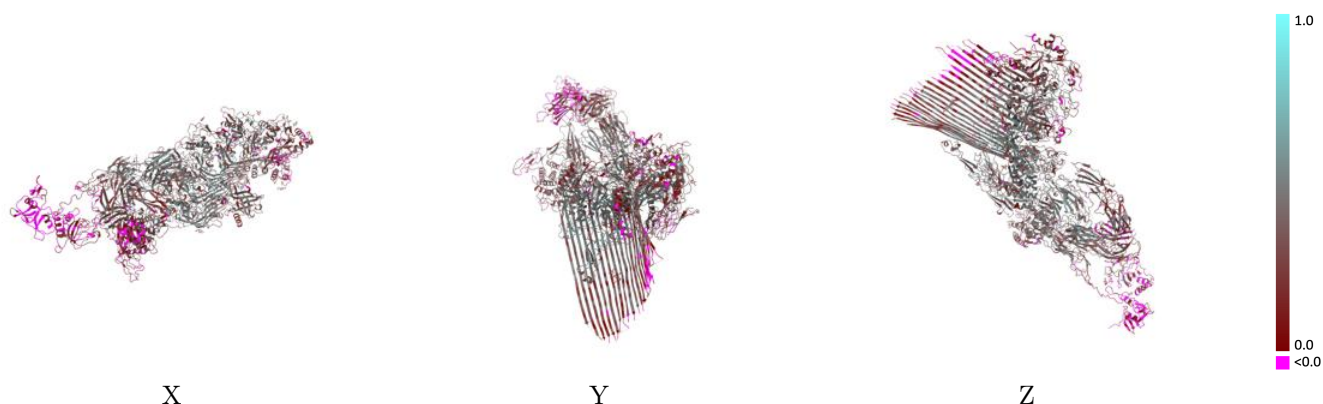
This section contains information regarding the fit between EMDB map EMD-12651 and PDB model 7NYD. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



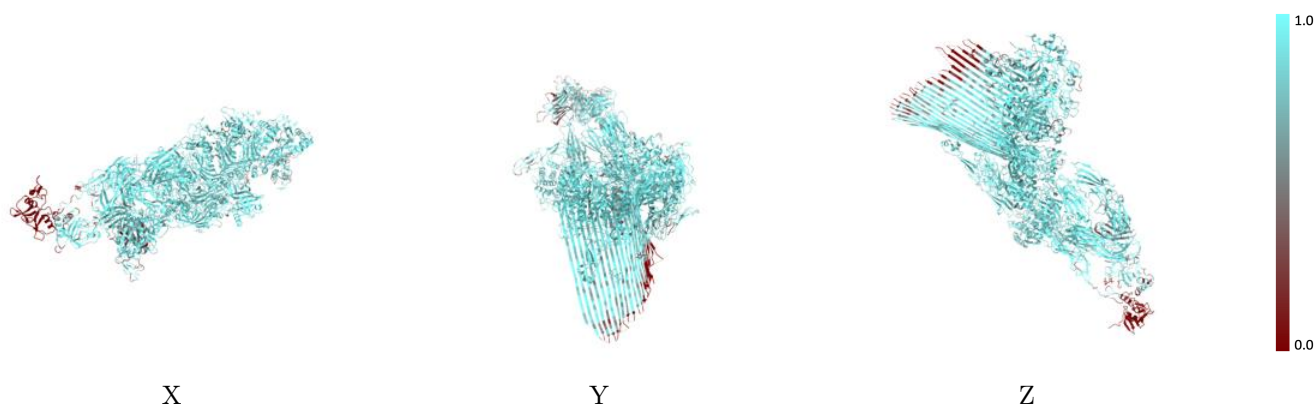
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



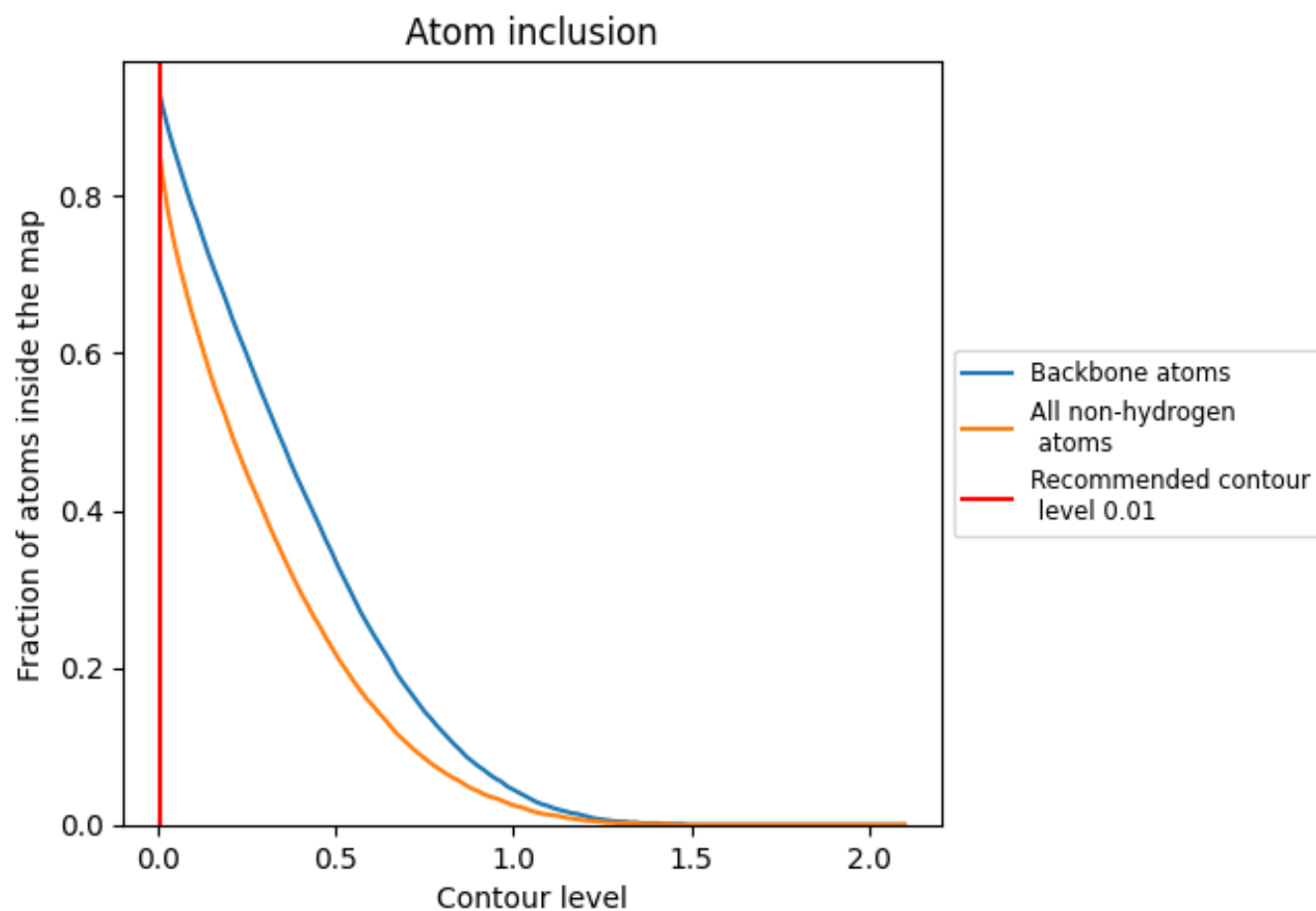
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



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

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

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

