



Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 08:33 PM EST

PDB ID : 6NIJ
EMDB ID : EMD-9378
Title : PGT145 Fab in complex with full length AMC011 HIV-1 Env
Authors : Cottrell, C.A.; Torrents de la Pena, A.; Rantalainen, K.; Torres, J.L.; Ward, A.B.
Deposited on : 2018-12-29
Resolution : 5.70 Å(reported)

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

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

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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

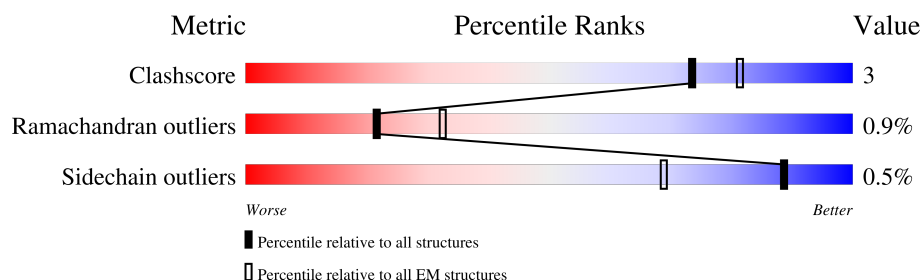
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



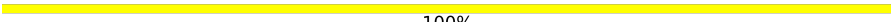
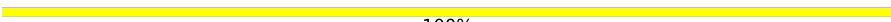
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	H	140	
2	L	113	
3	A	473	
3	C	473	
3	E	473	
4	B	345	
4	D	345	
4	F	345	

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Mol	Chain	Length	Quality of chain
5	G	2	 100%
6	I	3	 100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15939 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 PGT145 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	140	Total	C	N	O	S	0	0
			1095	685	191	214	5		

- Molecule 2 is a protein called PGT145 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	112	Total	C	N	O	S	0	0
			860	542	153	161	4		

- Molecule 3 is a protein called AMC011 Glycoprotein 120.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	449	Total	C	N	O	S	0	0
			3535	2229	618	662	26		
3	C	445	Total	C	N	O	S	0	0
			3507	2214	612	655	26		
3	E	444	Total	C	N	O	S	0	0
			3495	2205	612	652	26		

- Molecule 4 is a protein called AMC011 Glycoprotein 41.

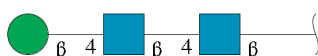
Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	140	Total	C	N	O	S	0	0
			1124	714	191	213	6		
4	D	133	Total	C	N	O	S	0	0
			1067	676	180	205	6		
4	F	139	Total	C	N	O	S	0	0
			1119	711	190	212	6		

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



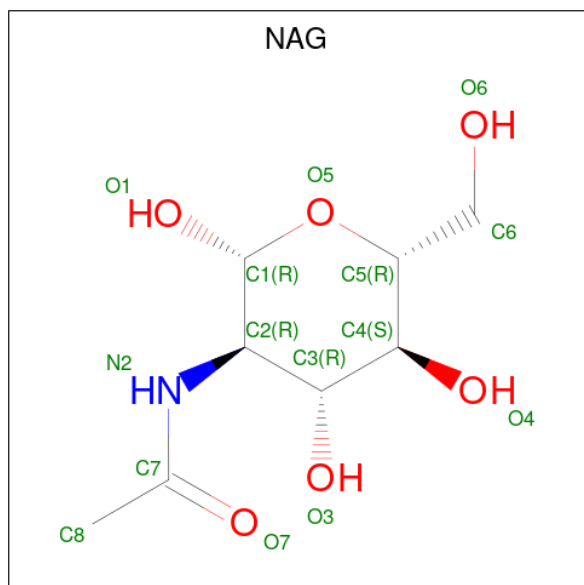
Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 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
6	I	3	Total	C	N	O	0	0
			39	22	2	15		

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



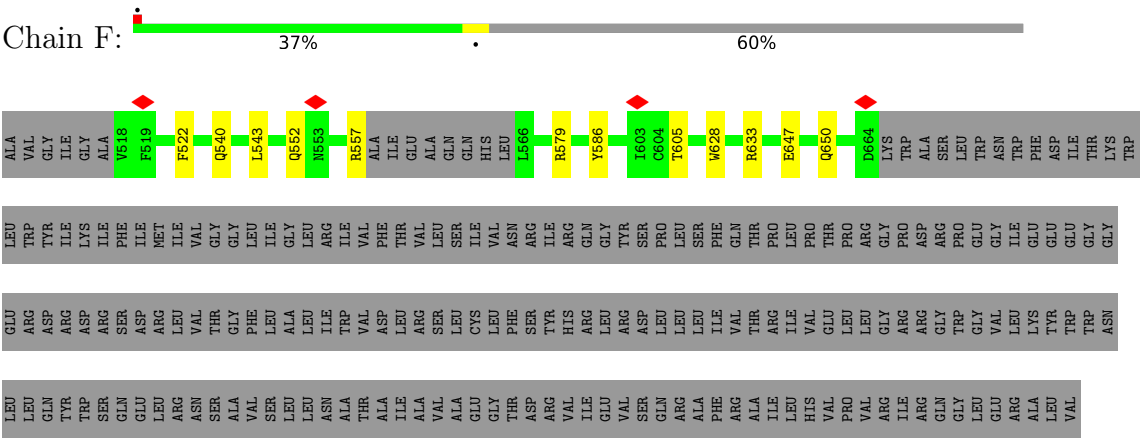
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			42	24	3	15	

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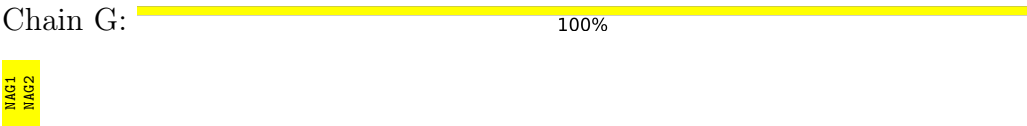
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Mol	Chain	Residues	Atoms				AltConf
7	C	1	Total	C	N	O	0
			42	24	3	15	
7	C	1	Total	C	N	O	0
			42	24	3	15	
7	E	1	Total	C	N	O	0
			14	8	1	5	

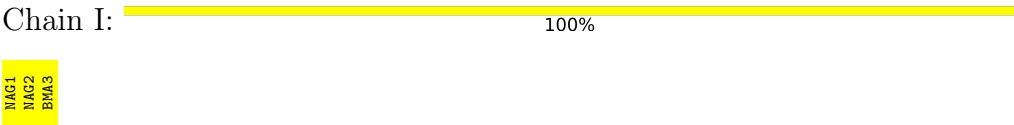
● Molecule 4: AMC011 Glycoprotein 41



● Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



● Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	51588	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.533	Depositor
Minimum map value	-0.505	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	368.0, 368.0, 368.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	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, 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	H	1.17	5/1122 (0.4%)	1.11	12/1519 (0.8%)
2	L	1.06	4/883 (0.5%)	1.03	2/1199 (0.2%)
3	A	0.98	6/3609 (0.2%)	0.95	5/4899 (0.1%)
3	C	0.97	7/3581 (0.2%)	1.08	10/4860 (0.2%)
3	E	0.96	2/3567 (0.1%)	0.99	11/4839 (0.2%)
4	B	1.00	1/1143 (0.1%)	0.89	1/1551 (0.1%)
4	D	1.04	4/1086 (0.4%)	0.90	2/1474 (0.1%)
4	F	1.07	2/1138 (0.2%)	0.95	4/1544 (0.3%)
All	All	1.00	31/16129 (0.2%)	1.00	47/21885 (0.2%)

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	93	CYS	CB-SG	-9.51	1.66	1.82
1	H	37	VAL	CB-CG1	-9.47	1.32	1.52
4	D	631	TRP	CB-CG	-7.60	1.36	1.50
4	F	628	TRP	CB-CG	-7.48	1.36	1.50
3	A	74	CYS	CB-SG	-7.31	1.69	1.82
1	H	108	TRP	CB-CG	7.21	1.63	1.50
3	A	239	CYS	CB-SG	-6.37	1.71	1.82
2	L	103	PHE	CB-CG	-6.21	1.40	1.51
3	E	84	VAL	CB-CG1	-5.99	1.40	1.52
1	H	100(P)	TRP	CB-CG	-5.93	1.39	1.50
4	B	631	TRP	CB-CG	-5.90	1.39	1.50
3	C	36	VAL	CB-CG2	-5.81	1.40	1.52
3	A	457	ASP	CB-CG	5.77	1.63	1.51
3	C	381	GLU	CD-OE1	-5.70	1.19	1.25
3	E	370	GLU	CD-OE1	-5.54	1.19	1.25
2	L	76	PHE	CB-CG	-5.54	1.42	1.51
3	C	191	TYR	CB-CG	-5.52	1.43	1.51
3	C	91	GLU	CD-OE1	-5.46	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	69	TRP	CB-CG	-5.40	1.40	1.50
4	D	632	GLU	CD-OE2	-5.38	1.19	1.25
3	C	153	GLU	CD-OE1	-5.34	1.19	1.25
3	A	35	TRP	CG-CD1	-5.27	1.29	1.36
1	H	36	TRP	CZ3-CH2	-5.26	1.31	1.40
4	D	632	GLU	CD-OE1	-5.19	1.20	1.25
3	A	172	GLU	CD-OE2	-5.15	1.20	1.25
4	F	628	TRP	CD2-CE2	-5.12	1.35	1.41
1	H	100(M)	TYR	CD1-CE1	-5.08	1.31	1.39
2	L	23	CYS	CB-SG	-5.06	1.73	1.81
3	A	89	VAL	CB-CG2	-5.05	1.42	1.52
3	C	75	VAL	CB-CG2	-5.02	1.42	1.52
4	D	657	GLU	CD-OE1	-5.01	1.20	1.25

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	440	LYS	O-C-N	22.83	162.01	123.20
3	C	440	LYS	CA-C-O	-18.81	80.59	120.10
3	C	440	LYS	CA-C-N	-17.35	81.50	116.20
1	H	64	ARG	NE-CZ-NH2	-10.67	114.97	120.30
3	E	480	ARG	NE-CZ-NH2	-10.13	115.24	120.30
2	L	59	ARG	NE-CZ-NH1	8.93	124.76	120.30
4	F	557	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	H	100(M)	TYR	CB-CG-CD1	-8.30	116.02	121.00
3	E	273	ARG	NE-CZ-NH2	-7.75	116.42	120.30
4	F	633	ARG	NE-CZ-NH2	-7.45	116.57	120.30
3	C	298	ARG	NE-CZ-NH2	-7.27	116.67	120.30
3	E	191	TYR	CB-CG-CD2	-7.19	116.69	121.00
3	A	273	ARG	NE-CZ-NH2	-7.08	116.76	120.30
3	E	476	ARG	NE-CZ-NH2	-6.92	116.84	120.30
3	A	475	MET	CG-SD-CE	6.78	111.05	100.20
4	D	579	ARG	NE-CZ-NH2	-6.62	116.99	120.30
3	C	504	ARG	NE-CZ-NH1	6.58	123.59	120.30
4	B	636	ASP	CB-CG-OD1	6.56	124.20	118.30
1	H	64	ARG	NE-CZ-NH1	6.33	123.46	120.30
3	E	480	ARG	NE-CZ-NH1	6.30	123.45	120.30
4	F	579	ARG	NE-CZ-NH1	6.20	123.40	120.30
3	E	39	TYR	CB-CG-CD2	-6.18	117.29	121.00
1	H	37	VAL	CB-CA-C	-6.13	99.76	111.40
3	E	318	TYR	CB-CG-CD2	-5.99	117.41	121.00
3	E	42	VAL	N-CA-C	-5.99	94.84	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	252	ARG	NE-CZ-NH2	-5.81	117.40	120.30
3	E	444	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	H	100(F)	TYR	CB-CG-CD2	-5.68	117.59	121.00
3	A	456	ARG	NE-CZ-NH2	-5.65	117.47	120.30
2	L	76	PHE	CB-CG-CD1	-5.64	116.85	120.80
3	C	273	ARG	NE-CZ-NH2	-5.60	117.50	120.30
3	E	273	ARG	NE-CZ-NH1	5.55	123.08	120.30
3	A	98	ASN	N-CA-C	5.49	125.82	111.00
1	H	106	ASP	N-CA-C	5.43	125.66	111.00
3	C	456	ARG	NE-CZ-NH2	5.32	122.96	120.30
4	F	586	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	H	38	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	H	79	TYR	CB-CG-CD1	-5.30	117.82	121.00
3	A	273	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	H	101	TYR	CB-CG-CD2	-5.26	117.84	121.00
3	C	298	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	H	100(A)	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	H	100(M)	TYR	CB-CG-CD2	5.21	124.12	121.00
3	C	469	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	H	91	TYR	CB-CG-CD2	-5.15	117.91	121.00
4	D	579	ARG	NE-CZ-NH1	5.12	122.86	120.30
3	C	307	ILE	CB-CA-C	-5.09	101.43	111.60

There are no chirality outliers.

There are no planarity outliers.

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	H	1095	0	1033	5	0
2	L	860	0	841	2	0
3	A	3535	0	3500	15	0
3	C	3507	0	3475	19	0
3	E	3495	0	3468	28	0
4	B	1124	0	1114	5	0
4	D	1067	0	1044	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	1119	0	1109	28	0
5	G	28	0	25	0	0
6	I	39	0	33	0	0
7	A	14	0	13	0	0
7	C	42	0	39	1	0
7	E	14	0	13	0	0
All	All	15939	0	15707	104	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 3.

All (104) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:522:PHE:CD2	4:F:543:LEU:HD21	1.27	1.70
4:F:522:PHE:CD2	4:F:543:LEU:CD2	1.91	1.51
4:D:605:THR:HG22	3:E:37:THR:CG2	1.41	1.50
4:F:540:GLN:CD	4:F:543:LEU:HD12	1.46	1.36
4:F:540:GLN:NE2	4:F:543:LEU:CD1	2.06	1.19
4:F:540:GLN:OE1	4:F:543:LEU:HD12	1.42	1.17
4:F:522:PHE:CG	4:F:543:LEU:HD21	1.82	1.14
4:D:605:THR:CG2	3:E:37:THR:HG22	1.78	1.12
4:F:540:GLN:HE22	4:F:543:LEU:HD11	1.13	1.09
4:F:540:GLN:NE2	4:F:543:LEU:HD11	1.65	1.09
4:D:605:THR:CG2	3:E:37:THR:CG2	2.30	1.08
4:D:605:THR:HG22	3:E:37:THR:HG23	1.40	1.01
4:F:540:GLN:CD	4:F:543:LEU:CD1	2.24	1.01
4:D:605:THR:HG22	3:E:37:THR:HG22	1.03	0.99
4:F:540:GLN:OE1	4:F:543:LEU:CD1	2.13	0.96
4:F:522:PHE:CE2	4:F:543:LEU:CD2	2.48	0.96
4:F:540:GLN:HE22	4:F:543:LEU:CD1	1.71	0.96
4:F:522:PHE:CD2	4:F:543:LEU:HD23	2.03	0.93
4:F:522:PHE:HD2	4:F:543:LEU:HD21	1.13	0.90
4:F:522:PHE:CD2	4:F:543:LEU:CG	2.57	0.87
4:F:540:GLN:NE2	4:F:543:LEU:HD12	1.80	0.87
4:F:522:PHE:CE2	4:F:543:LEU:HD23	2.08	0.86
4:F:522:PHE:HD2	4:F:543:LEU:CG	1.94	0.80
4:F:522:PHE:HD2	4:F:543:LEU:CD2	1.70	0.64
3:A:160:ASN:N	3:A:160:ASN:OD1	2.32	0.63
4:F:522:PHE:CD2	4:F:543:LEU:HG	2.35	0.61
3:A:66:HIS:NE2	3:A:115:SER:HB2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:35:TRP:CD2	4:B:605:THR:HG23	2.40	0.57
3:A:35:TRP:CE3	4:B:605:THR:HG23	2.40	0.56
1:H:100(A):ARG:HB3	1:H:100(P):TRP:HB3	1.88	0.56
3:A:66:HIS:CE1	3:A:115:SER:HB2	2.42	0.55
4:F:522:PHE:CE2	4:F:543:LEU:HG	2.43	0.53
3:E:231:LYS:NZ	3:E:267:GLU:OE1	2.41	0.53
3:E:167:ASP:OD2	3:E:168:LYS:NZ	2.42	0.53
3:E:289:ASN:N	3:E:289:ASN:OD1	2.40	0.52
3:C:123:THR:N	3:C:124:PRO:HD2	2.25	0.52
3:A:63:THR:OG1	3:A:64:GLU:N	2.44	0.51
4:B:519:PHE:CD2	4:B:543:LEU:HD21	2.45	0.51
4:D:553:ASN:O	4:D:554:ASN:C	2.48	0.51
4:F:522:PHE:CB	4:F:543:LEU:HD21	2.37	0.51
3:C:197:ASN:OD1	3:C:197:ASN:N	2.43	0.51
4:D:546:SER:OG	4:D:547:GLY:N	2.43	0.50
4:F:522:PHE:CE2	4:F:543:LEU:CG	2.91	0.50
3:C:163:THR:OG1	3:C:164:SER:N	2.43	0.49
3:E:123:THR:N	3:E:124:PRO:CD	2.76	0.49
4:F:605:THR:O	4:F:605:THR:HG23	2.12	0.49
3:E:474:ASP:OD1	3:E:475:MET:N	2.45	0.49
4:F:540:GLN:HA	4:F:543:LEU:HD12	1.93	0.49
3:E:225:ILE:HB	3:E:245:VAL:HB	1.94	0.48
3:E:56:SER:OG	3:E:57:ASP:N	2.46	0.48
1:H:16:SER:OG	1:H:17:SER:N	2.47	0.48
3:E:303:THR:OG1	3:E:304:ARG:N	2.46	0.48
2:L:112:LYS:NZ	2:L:113:ARG:OXT	2.40	0.47
3:C:199:SER:OG	3:C:200:VAL:N	2.47	0.47
3:C:370:GLU:OE2	3:C:421:LYS:NZ	2.47	0.47
4:B:622:ILE:O	4:B:626:MET:N	2.47	0.47
3:A:198:THR:OG1	3:A:199:SER:N	2.47	0.47
3:C:62:ASP:O	3:C:66:HIS:CD2	2.68	0.47
3:E:257:THR:OG1	3:E:258:GLN:N	2.46	0.47
3:E:66:HIS:NE2	3:E:207:LYS:HE2	2.30	0.47
3:C:198:THR:HB	7:C:603:NAG:H82	1.97	0.46
3:E:95:MET:HB3	3:E:484:TYR:CD2	2.50	0.46
3:A:77:THR:OG1	3:A:78:ASP:N	2.47	0.46
3:C:77:THR:OG1	3:C:78:ASP:N	2.48	0.46
3:C:160:ASN:N	3:C:160:ASN:OD1	2.48	0.46
3:E:99:ASN:OD1	3:E:99:ASN:N	2.47	0.46
3:C:162:THR:OG1	3:C:163:THR:N	2.47	0.46
4:D:614:TRP:CG	4:D:615:SER:N	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:540:GLN:OE1	4:F:543:LEU:HD13	2.13	0.45
4:B:557:ARG:O	4:B:558:ALA:C	2.53	0.45
3:A:283:ILE:HG12	3:A:454:LEU:HB3	1.99	0.45
4:D:611:ASN:OD1	4:D:611:ASN:N	2.50	0.45
3:E:258:GLN:NE2	3:E:372:VAL:O	2.50	0.45
3:C:358:THR:OG1	3:C:464(A):ASN:O	2.34	0.44
3:E:77:THR:OG1	3:E:78:ASP:N	2.50	0.44
3:C:229:ASN:ND2	3:C:243:SER:OG	2.50	0.44
3:E:123:THR:N	3:E:124:PRO:HD2	2.33	0.43
3:C:62:ASP:OD1	3:C:62:ASP:N	2.50	0.43
1:H:100(J):GLY:N	1:H:100(K):PRO:CD	2.81	0.43
3:A:362:ASN:HB3	3:A:467:ILE:HG23	2.01	0.43
4:F:647:GLU:O	4:F:650:GLN:HG2	2.20	0.42
3:E:480:ARG:HB3	3:E:484:TYR:CE2	2.54	0.42
3:E:234:ASN:N	3:E:234:ASN:OD1	2.52	0.42
2:L:40:TRP:HE1	2:L:91:TYR:HB3	1.84	0.42
3:C:280:ASN:OD1	3:C:280:ASN:N	2.47	0.42
4:D:603:ILE:HB	3:E:39:TYR:CZ	2.54	0.42
3:C:393:SER:OG	3:C:394:THR:N	2.53	0.42
4:D:524:GLY:H	3:E:86:LEU:HD23	1.84	0.42
3:E:186:ASN:OD1	3:E:186:ASN:N	2.53	0.42
1:H:108:TRP:CG	1:H:109:GLY:N	2.87	0.41
3:A:36:VAL:O	3:A:37:THR:CB	2.68	0.41
3:C:319:THR:OG1	3:C:320:THR:N	2.53	0.41
3:E:86:LEU:HB3	3:E:89:VAL:HB	2.02	0.41
1:H:93:LEU:HD12	1:H:106:ASP:HB3	2.02	0.41
3:A:123:THR:N	3:A:124:PRO:CD	2.84	0.41
4:F:552:GLN:OE1	4:F:552:GLN:N	2.48	0.41
3:E:50:THR:OG1	3:E:51:THR:N	2.53	0.41
3:E:218:CYS:HB3	3:E:247:CYS:HA	2.02	0.41
3:C:358:THR:HG1	3:C:359:ILE:H	1.67	0.41
3:C:164:SER:O	3:C:165:MET:CB	2.69	0.40
3:A:133:ASP:OD1	3:A:155:LYS:NZ	2.53	0.40
3:A:211:GLU:HA	3:A:212:PRO:HD3	1.96	0.40
3:A:469:ARG:HB2	3:A:470:PRO:HD2	2.03	0.40
3:C:257:THR:OG1	3:C:258:GLN:N	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	H	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
2	L	110/113 (97%)	102 (93%)	7 (6%)	1 (1%)	17	56
3	A	443/473 (94%)	419 (95%)	18 (4%)	6 (1%)	11	46
3	C	439/473 (93%)	413 (94%)	19 (4%)	7 (2%)	9	43
3	E	436/473 (92%)	415 (95%)	18 (4%)	3 (1%)	22	62
4	B	136/345 (39%)	133 (98%)	3 (2%)	0	100	100
4	D	129/345 (37%)	122 (95%)	6 (5%)	1 (1%)	19	60
4	F	135/345 (39%)	130 (96%)	5 (4%)	0	100	100
All	All	1966/2707 (73%)	1868 (95%)	80 (4%)	18 (1%)	21	56

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	100	PRO
3	A	37	THR
3	A	501	ALA
3	C	163	THR
3	C	165	MET
3	A	98	ASN
3	A	305	LYS
3	A	205	CYS
3	C	72	HIS
3	C	361	PHE
3	A	230	ASP
3	C	429	GLU
3	E	84	VAL
3	E	302	ASN
3	C	51	THR
4	D	548	ILE
3	E	181	VAL

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Mol	Chain	Res	Type
3	C	120	VAL

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	H	115/115 (100%)	114 (99%)	1 (1%)	78	87
2	L	95/96 (99%)	95 (100%)	0	100	100
3	A	400/420 (95%)	397 (99%)	3 (1%)	81	89
3	C	397/420 (94%)	395 (100%)	2 (0%)	88	93
3	E	396/420 (94%)	393 (99%)	3 (1%)	81	89
4	B	122/298 (41%)	122 (100%)	0	100	100
4	D	116/298 (39%)	116 (100%)	0	100	100
4	F	122/298 (41%)	122 (100%)	0	100	100
All	All	1763/2365 (74%)	1754 (100%)	9 (0%)	89	93

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	48	MET
3	A	160	ASN
3	A	298	ARG
3	A	434	MET
3	C	160	ASN
3	C	426	MET
3	E	298	ARG
3	E	456	ARG
3	E	469	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	31	HIS
3	C	66	HIS
3	C	229	ASN
3	E	114	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 ⓘ

5 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	G	1	5,3	14,14,15	2.21	3 (21%)	17,19,21	1.08	0
5	NAG	G	2	5	14,14,15	2.15	1 (7%)	17,19,21	0.95	0
6	NAG	I	1	6,3	14,14,15	2.13	2 (14%)	17,19,21	0.80	1 (5%)
6	NAG	I	2	6	14,14,15	2.15	3 (21%)	17,19,21	0.79	0
6	BMA	I	3	6	11,11,12	1.78	2 (18%)	15,15,17	1.03	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	I	1	6,3	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	1/6/23/26	0/1/1/1
6	BMA	I	3	6	-	1/2/19/22	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	1	NAG	O5-C1	7.29	1.55	1.43
5	G	2	NAG	O5-C1	7.24	1.55	1.43
6	I	1	NAG	O5-C1	6.91	1.54	1.43
6	I	2	NAG	O5-C1	6.76	1.54	1.43
6	I	3	BMA	O2-C2	-4.13	1.34	1.43
5	G	1	NAG	C3-C2	-2.48	1.47	1.52
6	I	1	NAG	C3-C2	-2.32	1.47	1.52
6	I	2	NAG	C4-C3	2.29	1.58	1.52
6	I	3	BMA	C2-C3	-2.11	1.49	1.52
5	G	1	NAG	C4-C3	2.08	1.57	1.52
6	I	2	NAG	C3-C2	-2.01	1.48	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	3	BMA	C2-C3-C4	-2.42	106.71	110.89
6	I	1	NAG	C3-C4-C5	-2.21	106.30	110.24

There are no chirality outliers.

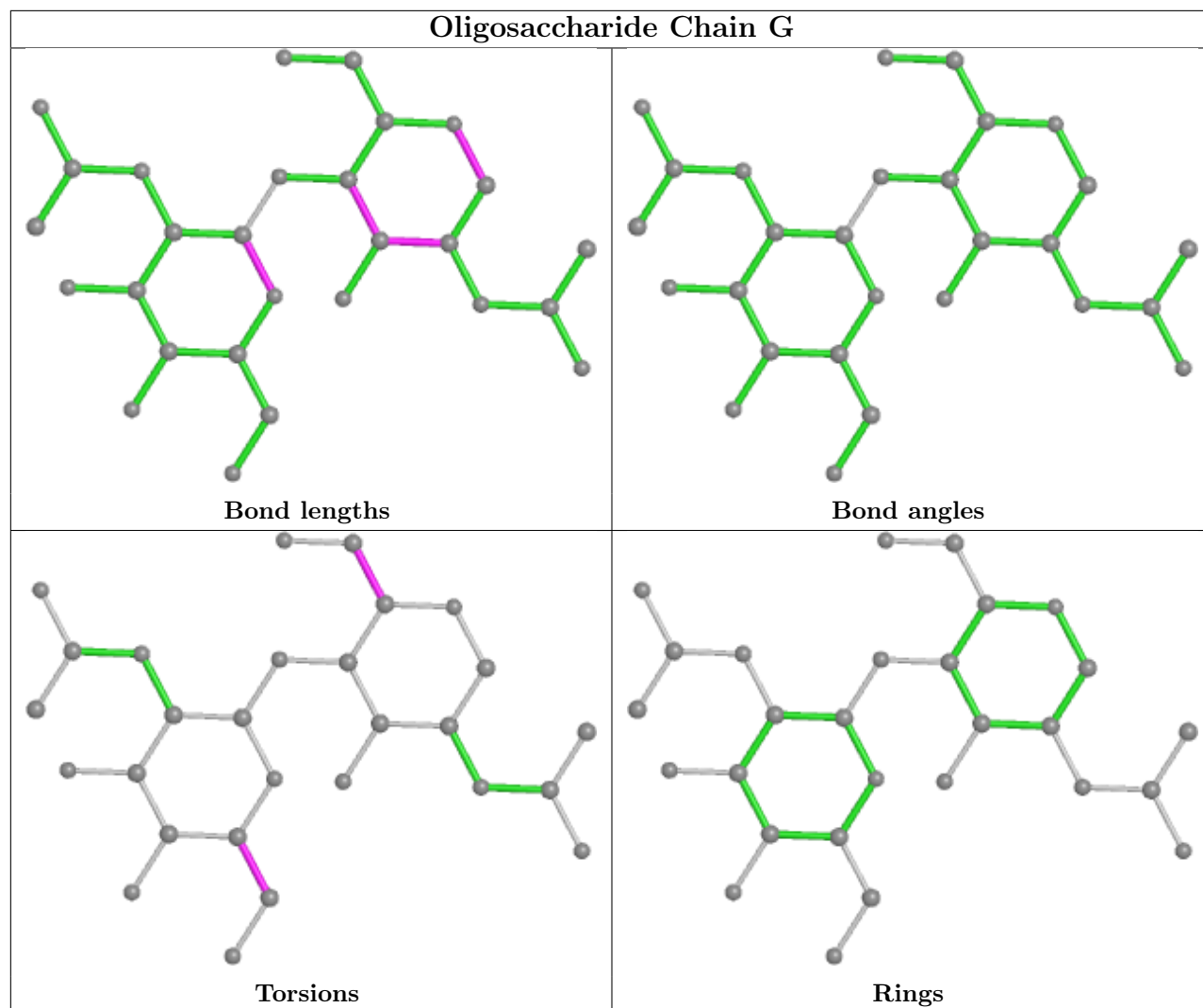
All (5) torsion outliers are listed below:

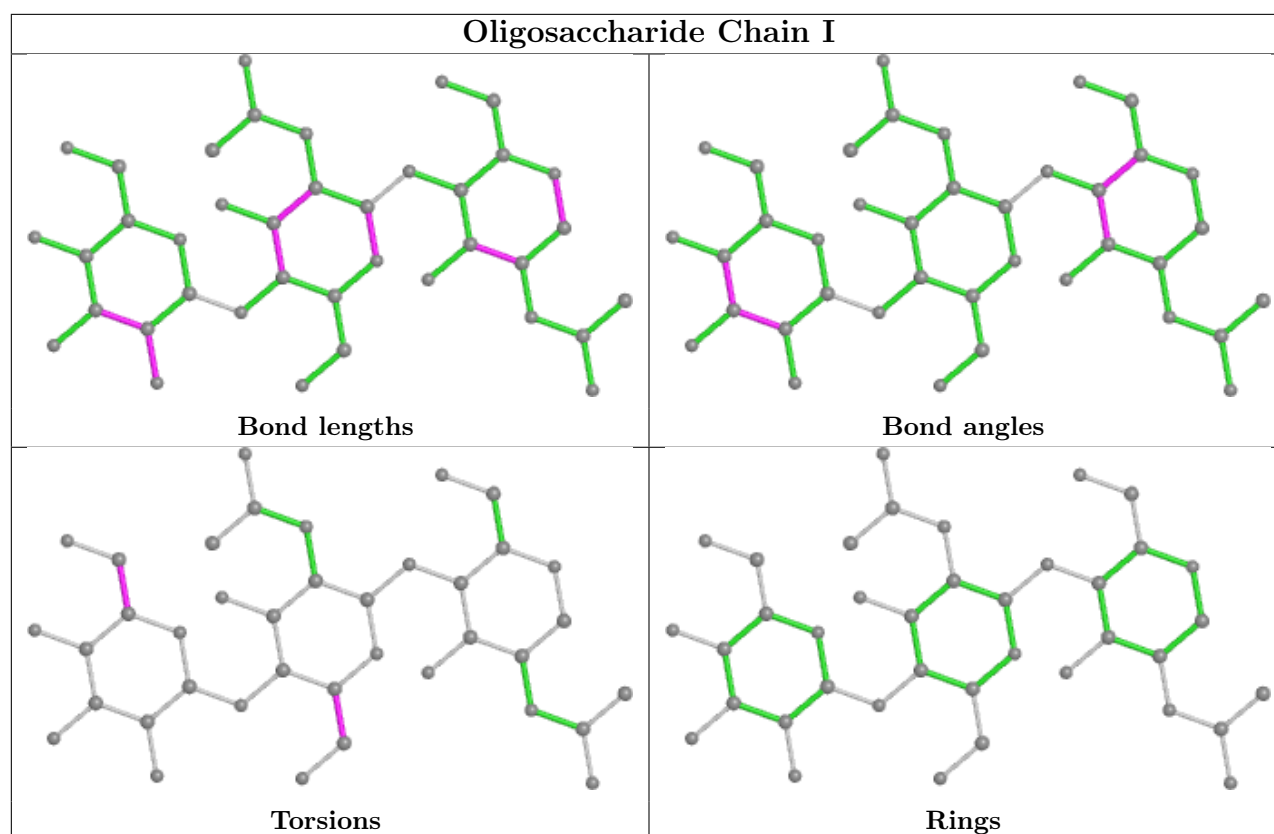
Mol	Chain	Res	Type	Atoms
5	G	2	NAG	O5-C5-C6-O6
6	I	3	BMA	O5-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	E	604	3	14,14,15	2.16	2 (14%)	17,19,21	0.86	1 (5%)
7	NAG	C	603	3	14,14,15	2.18	2 (14%)	17,19,21	0.85	1 (5%)
7	NAG	A	603	3	14,14,15	2.13	2 (14%)	17,19,21	1.11	1 (5%)
7	NAG	C	601	3	14,14,15	2.13	2 (14%)	17,19,21	1.12	2 (11%)
7	NAG	C	602	3	14,14,15	2.15	1 (7%)	17,19,21	1.00	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	E	604	3	-	2/6/23/26	0/1/1/1
7	NAG	C	603	3	-	1/6/23/26	0/1/1/1
7	NAG	A	603	3	-	4/6/23/26	0/1/1/1
7	NAG	C	601	3	-	1/6/23/26	0/1/1/1
7	NAG	C	602	3	-	1/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	602	NAG	O5-C1	7.21	1.55	1.43
7	C	603	NAG	O5-C1	7.14	1.55	1.43
7	E	604	NAG	O5-C1	7.12	1.55	1.43
7	A	603	NAG	O5-C1	7.08	1.55	1.43
7	C	601	NAG	O5-C1	6.84	1.54	1.43
7	E	604	NAG	C3-C2	-2.24	1.47	1.52
7	A	603	NAG	C3-C2	-2.16	1.47	1.52
7	C	603	NAG	C3-C2	-2.15	1.47	1.52
7	C	601	NAG	C4-C3	2.02	1.57	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	601	NAG	C1-O5-C5	-3.21	107.84	112.19
7	A	603	NAG	C8-C7-N2	2.89	121.00	116.10
7	C	601	NAG	C4-C3-C2	-2.64	107.15	111.02
7	C	603	NAG	C4-C3-C2	-2.36	107.55	111.02
7	E	604	NAG	C4-C3-C2	-2.34	107.59	111.02
7	C	602	NAG	C3-C4-C5	-2.02	106.64	110.24

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	E	604	NAG	O5-C5-C6-O6
7	A	603	NAG	O5-C5-C6-O6
7	A	603	NAG	C8-C7-N2-C2
7	A	603	NAG	O7-C7-N2-C2
7	C	603	NAG	O5-C5-C6-O6
7	C	602	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	C	601	NAG	O5-C5-C6-O6
7	E	604	NAG	C4-C5-C6-O6
7	A	603	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	603	NAG	1	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.

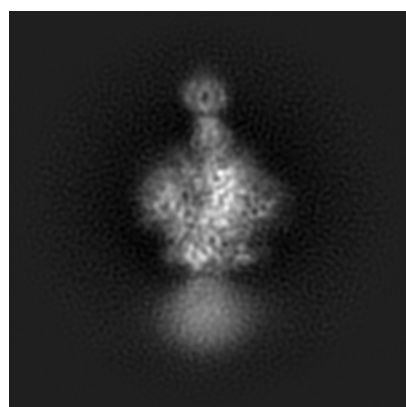
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9378. These allow visual inspection of the internal detail of the map and identification of artifacts.

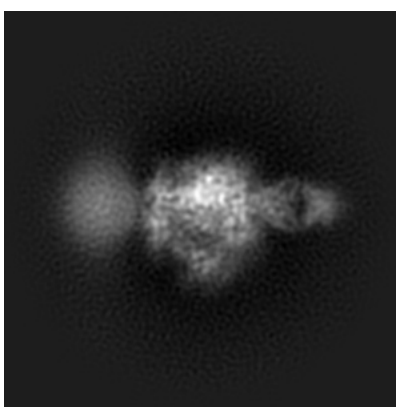
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

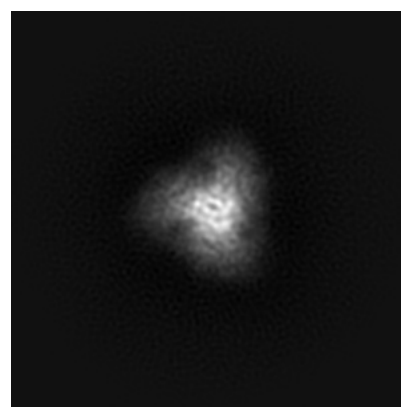
6.1.1 Primary map



X



Y

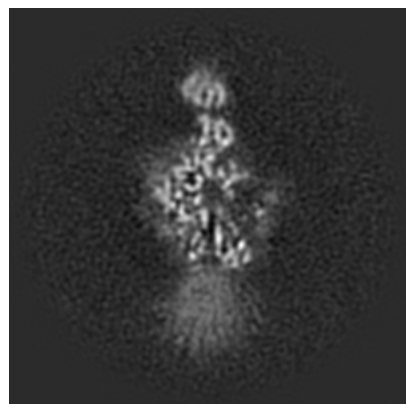


Z

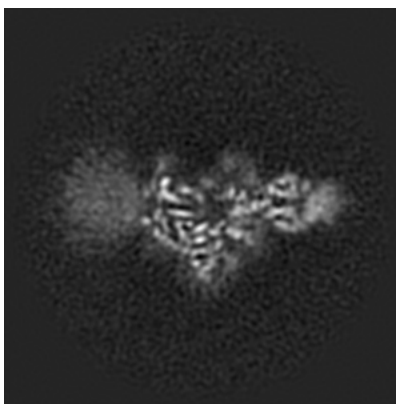
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 160



Y Index: 160

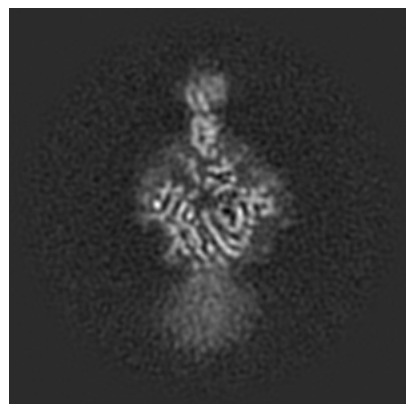


Z Index: 160

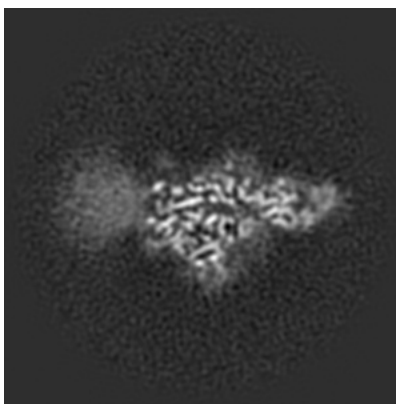
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

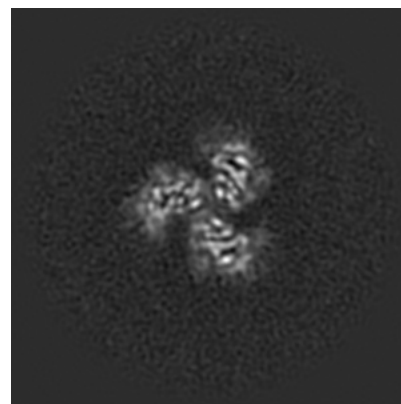
6.3.1 Primary map



X Index: 172



Y Index: 165



Z Index: 162

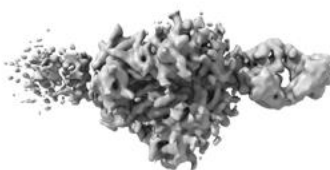
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

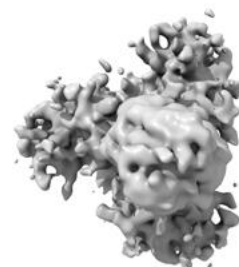
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

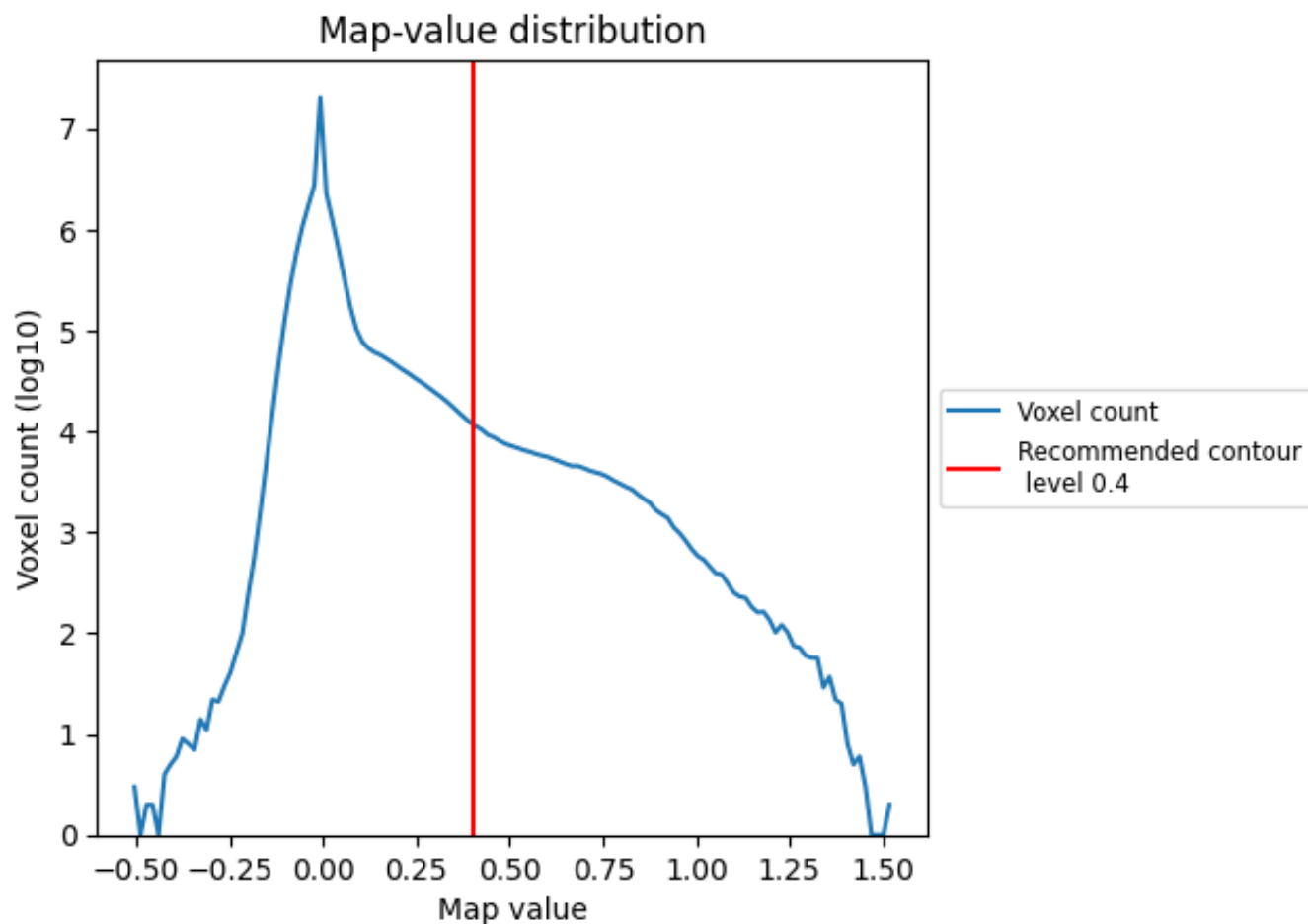
6.5 Mask visualisation

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

7 Map analysis [i](#)

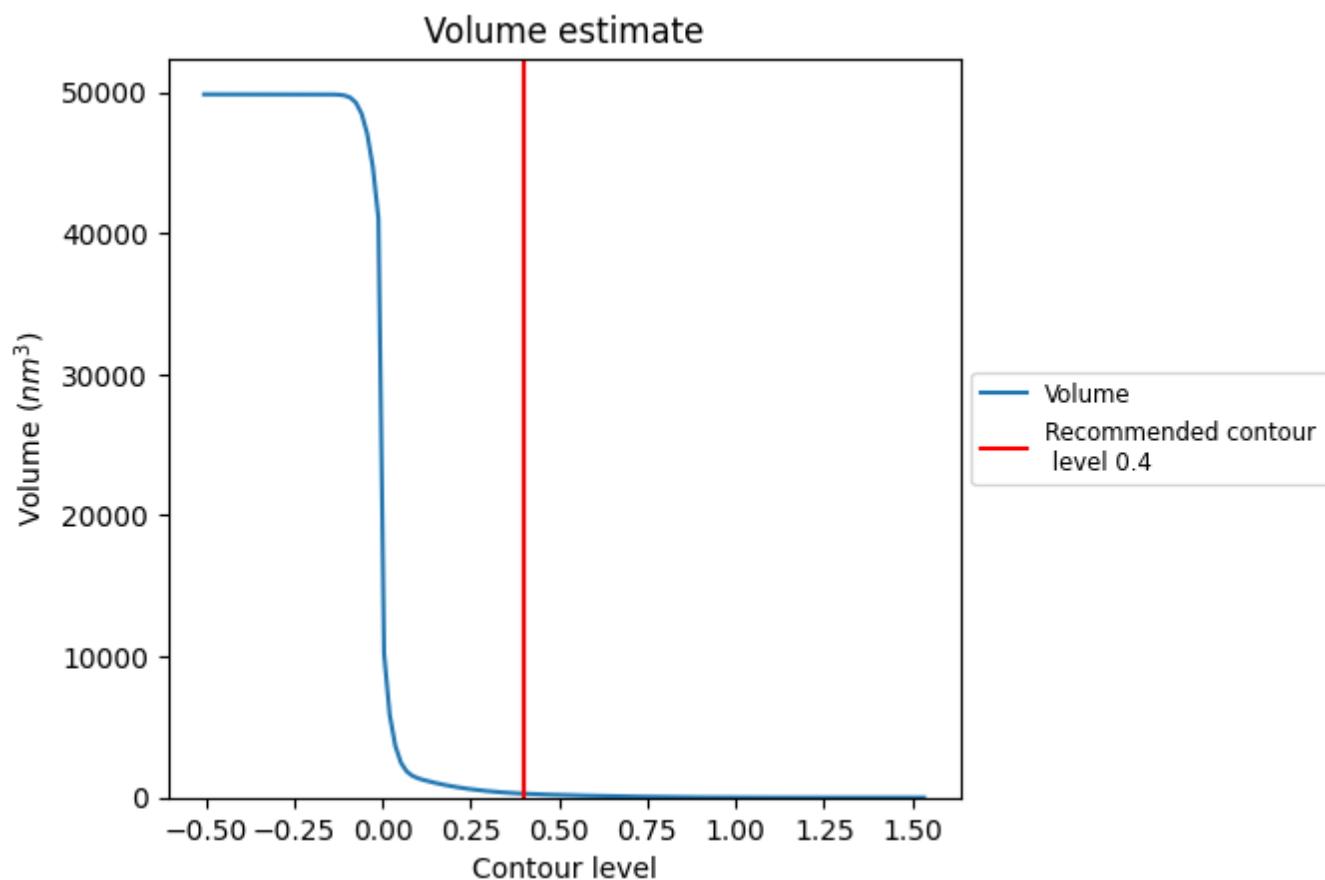
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

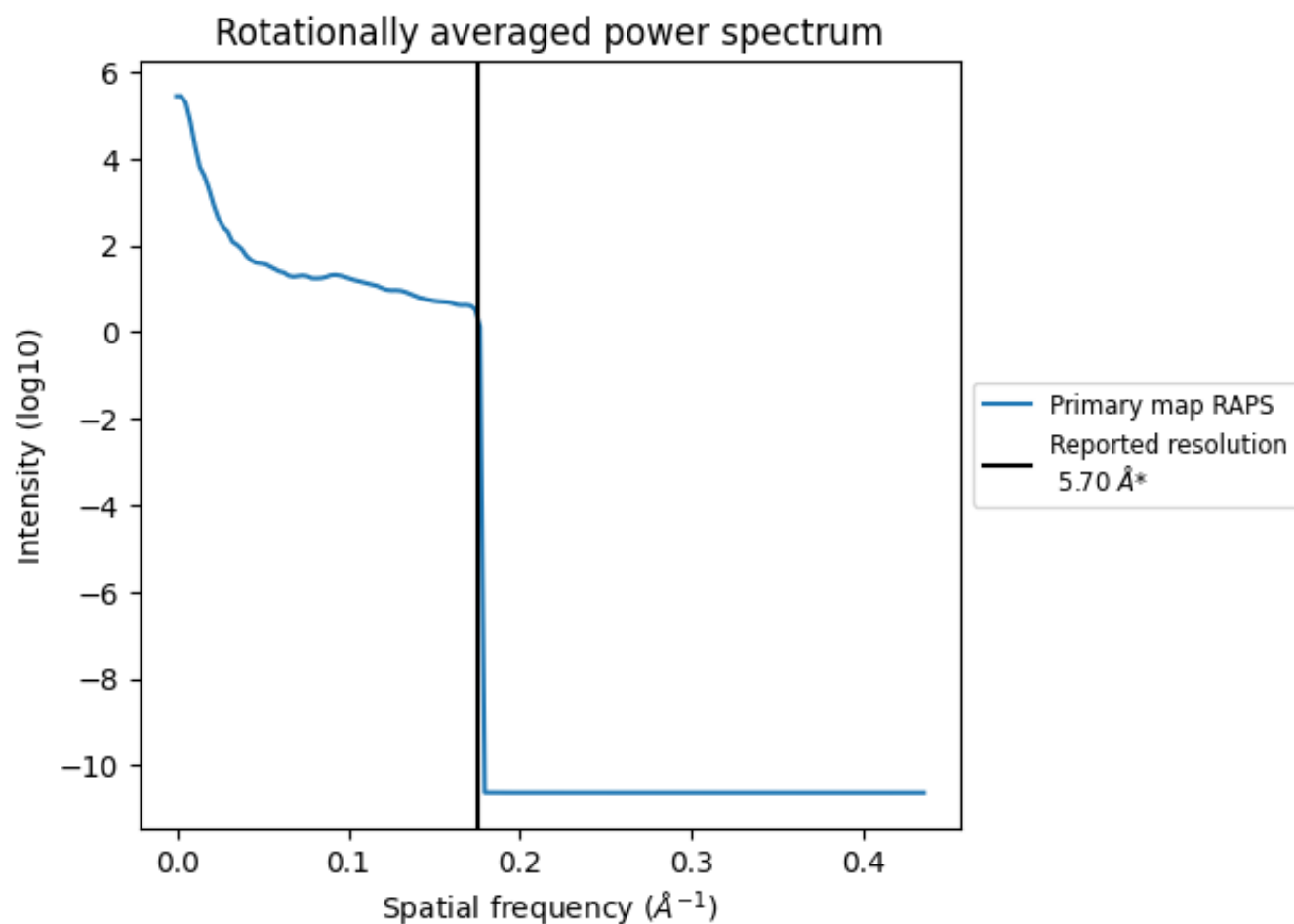
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 276 nm³; this corresponds to an approximate mass of 250 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 0.175 Å⁻¹

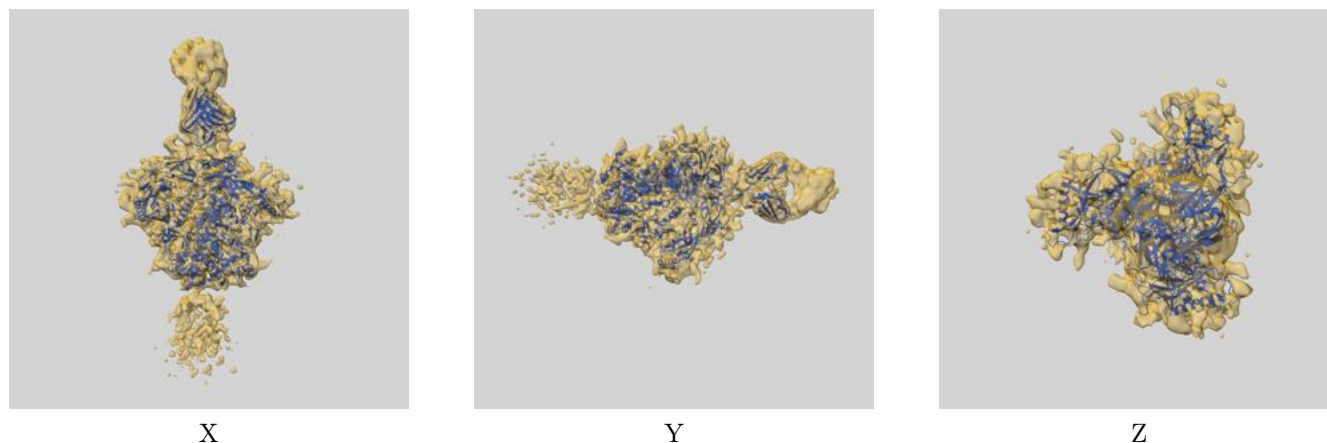
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9378 and PDB model 6NIJ. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



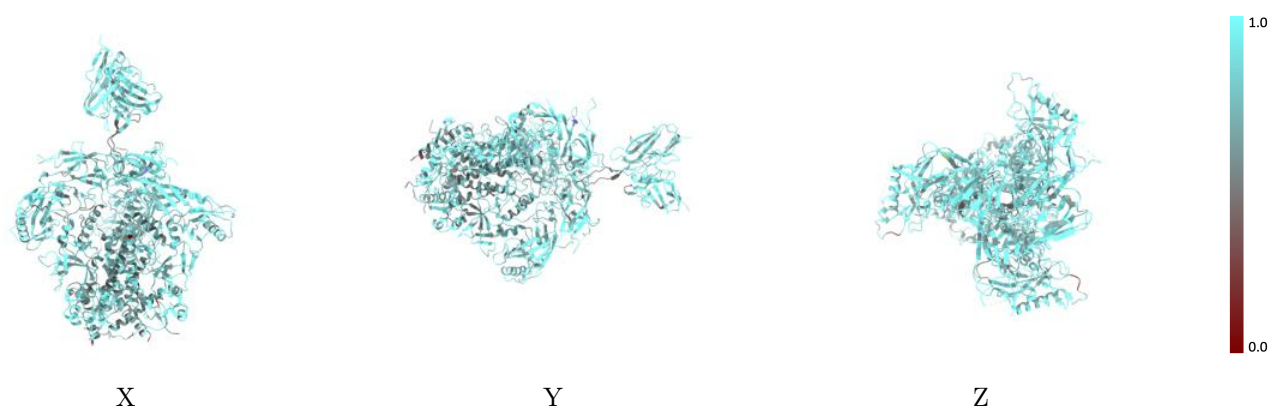
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



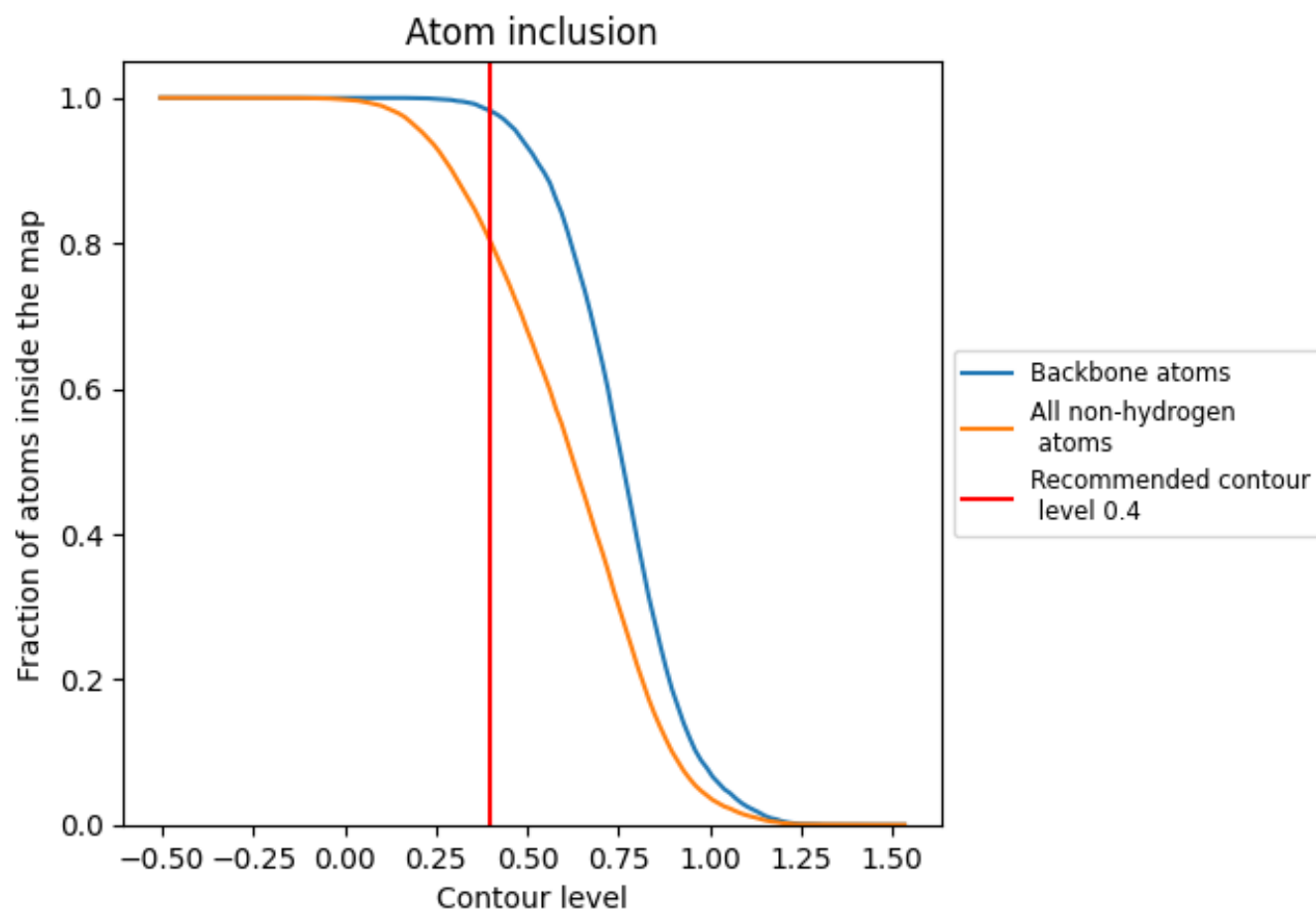
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 80% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8010	<div></div> 0.1800
A	<div></div> 0.8163	<div></div> 0.1900
B	<div></div> 0.7543	<div></div> 0.1560
C	<div></div> 0.8040	<div></div> 0.1830
D	<div></div> 0.7233	<div></div> 0.1610
E	<div></div> 0.8119	<div></div> 0.1860
F	<div></div> 0.7240	<div></div> 0.1620
G	<div></div> 1.0000	<div></div> 0.3190
H	<div></div> 0.8570	<div></div> 0.1720
I	<div></div> 0.9231	<div></div> 0.3560
L	<div></div> 0.8551	<div></div> 0.1750

1.0

0.0

<0.0