Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 07:04 pm GMT

PDB ID	:	6ENY
EMDB ID	:	EMD-3906
Title	:	Structure of the human PLC editing module
Authors	:	Trowitzsch, S.; Januliene, D.; Blees, A.; Moeller, A.; Tampe, R.
Deposited on	:	2017-10-07
Resolution	:	5.80 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:

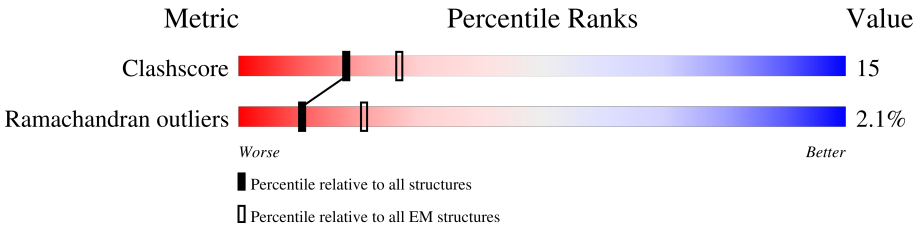
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance

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

The reported resolution of this entry is 5.80 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

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	B	99	22% 71% 28%
2	C	428	32% 65% 18% 15%
3	D	481	31% 88% 8%
4	F	341	26% 72% 9% 20%
5	G	400	64% 83% 8% 9%
6	A	2	50% 50% 50%
7	E	4	50% 75% 25%

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
6	NAG	A	1	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7778 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 Beta-2-microglobulin.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	B	99	Total	C	N	O	0	0
			492	294	99	99		

- Molecule 2 is a protein called Tapasin.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	364	Total	C	N	O	0	0
			1788	1060	364	364		

- Molecule 3 is a protein called Protein disulfide-isomerase A3.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	461	Total	C	N	O	0	0
			2276	1354	461	461		

- Molecule 4 is a protein called HLA class I histocompatibility antigen, A-3 alpha chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	274	Total	C	N	O	0	0
			1349	801	274	274		

- Molecule 5 is a protein called Calreticulin.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	365	Total	C	N	O	0	0
			1799	1069	365	365		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	163	SER	CYS	conflict	UNP P27797

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	A	2	Total	C	N	O	0	0
			29	16	2	11		

- Molecule 7 is an oligosaccharide called beta-D-glucopyranose-(1-3)-alpha-D-mannopyranose -(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose.

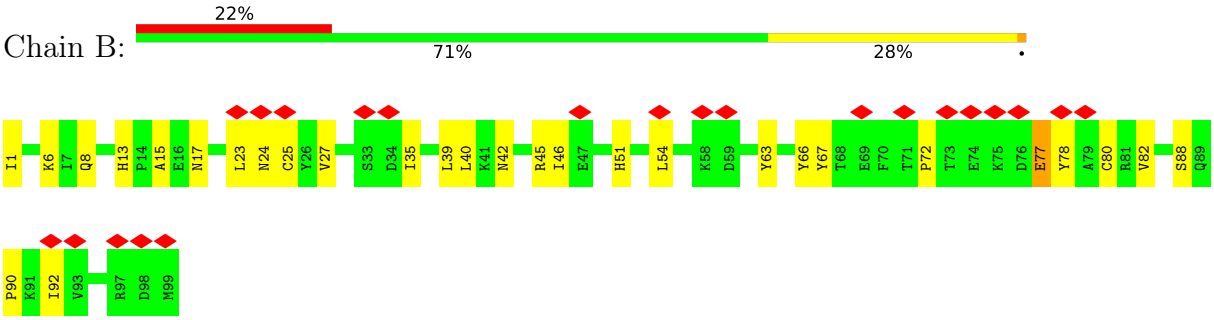
Mol	Chain	Residues	Atoms			AltConf	Trace
7	E	4	Total	C	O	0	0
			45	24	21		

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.

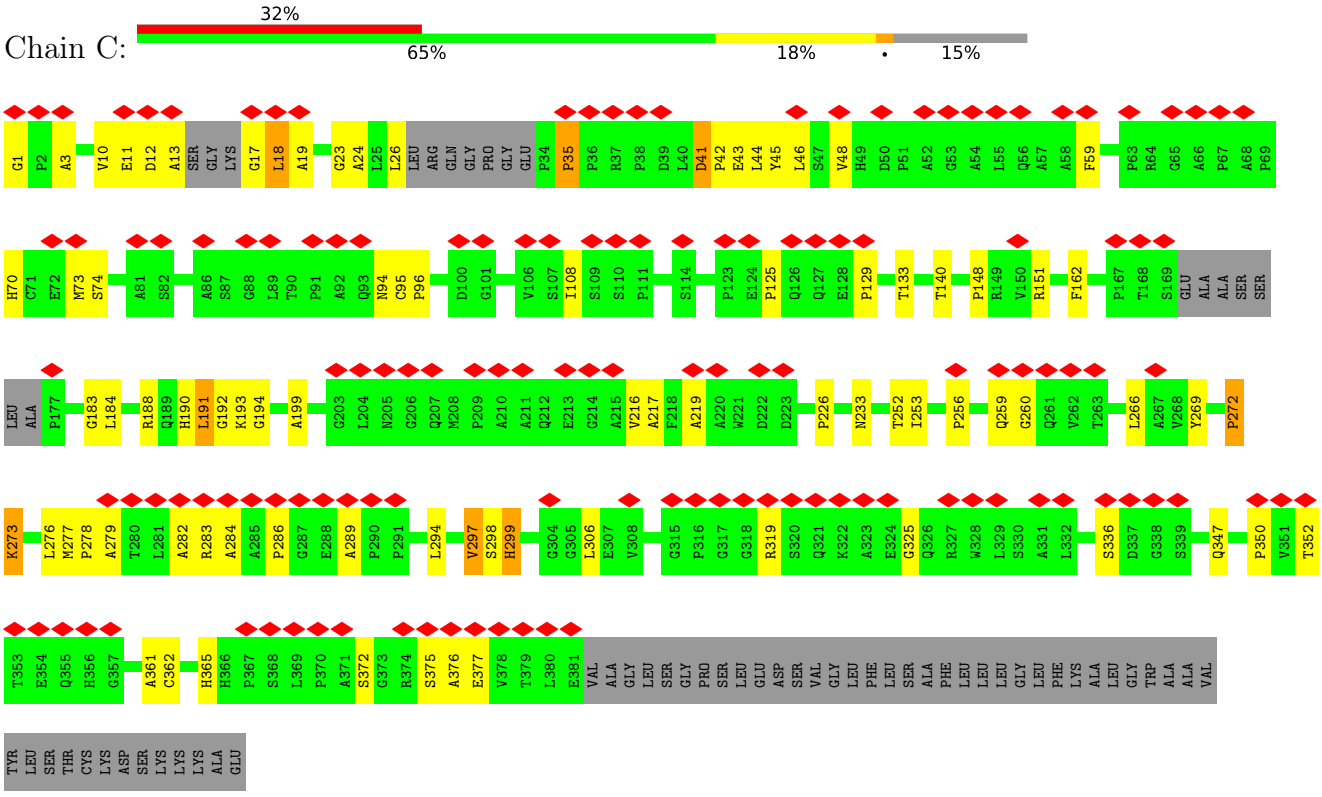
- Molecule 1: Beta-2-microglobulin

Chain B:



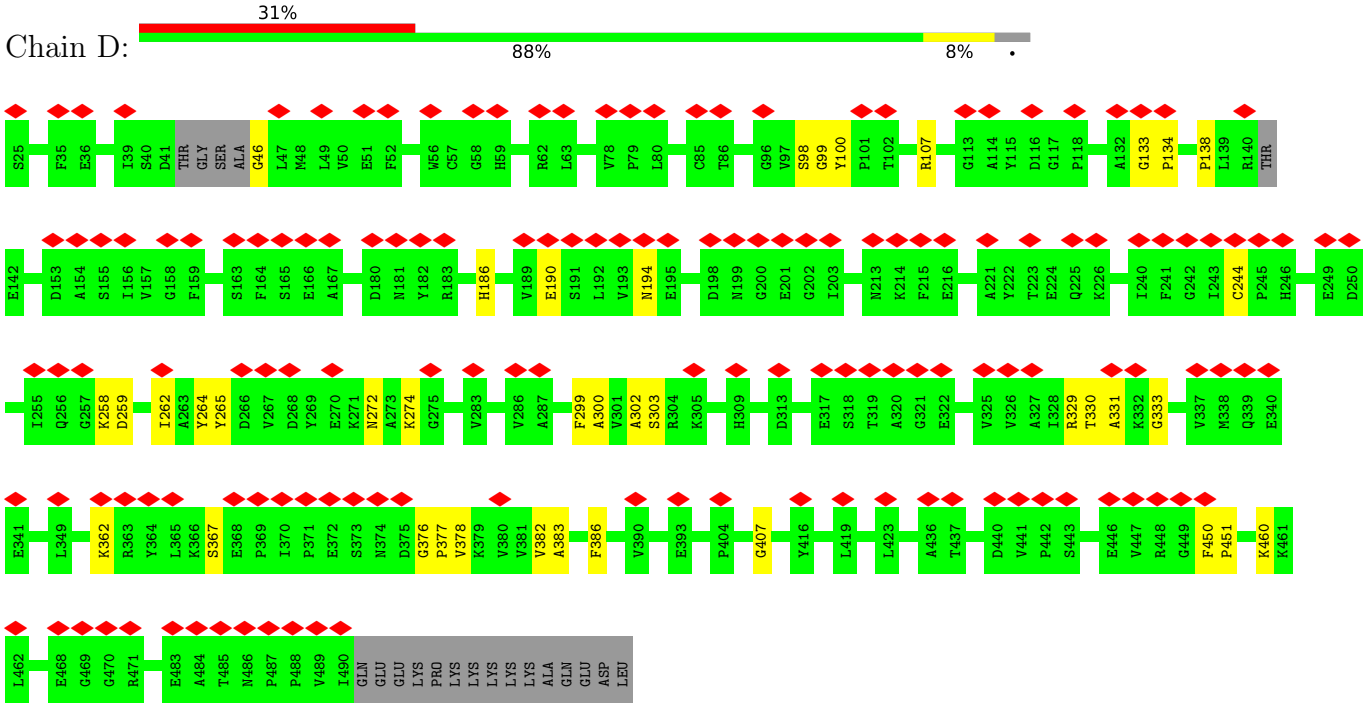
- Molecule 2: Tapasin

Chain C:



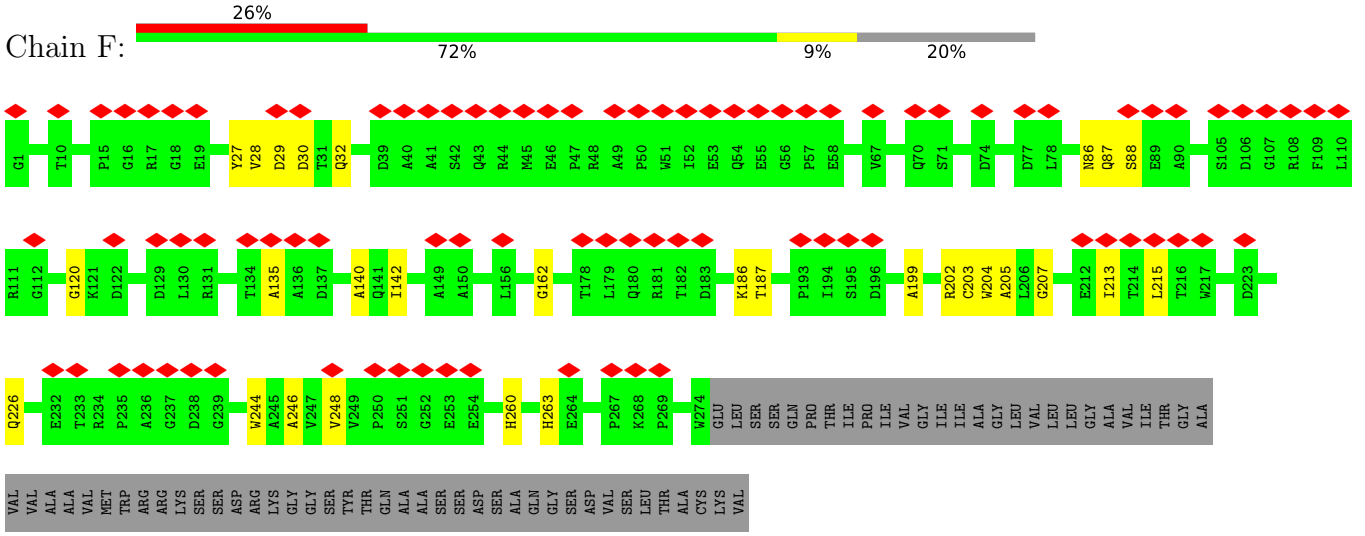
- Molecule 3: Protein disulfide-isomerase A3

Chain D:



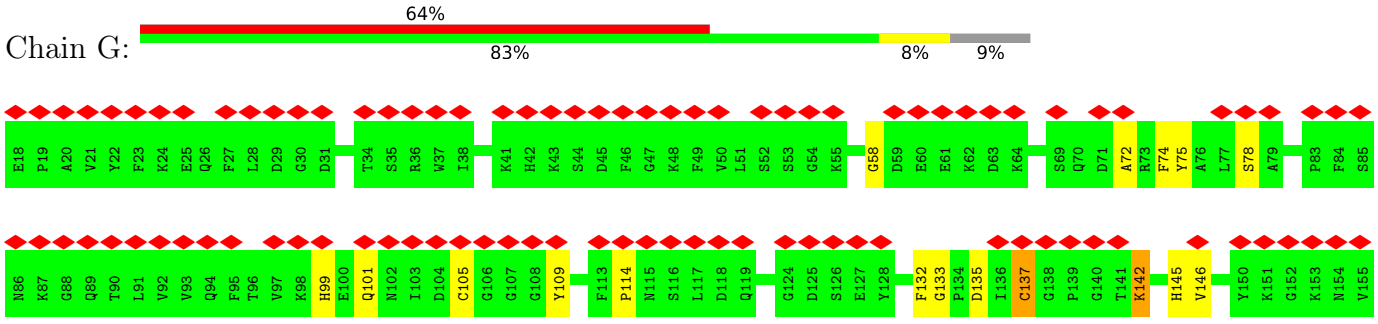
• Molecule 4: HLA class I histocompatibility antigen, A-3 alpha chain

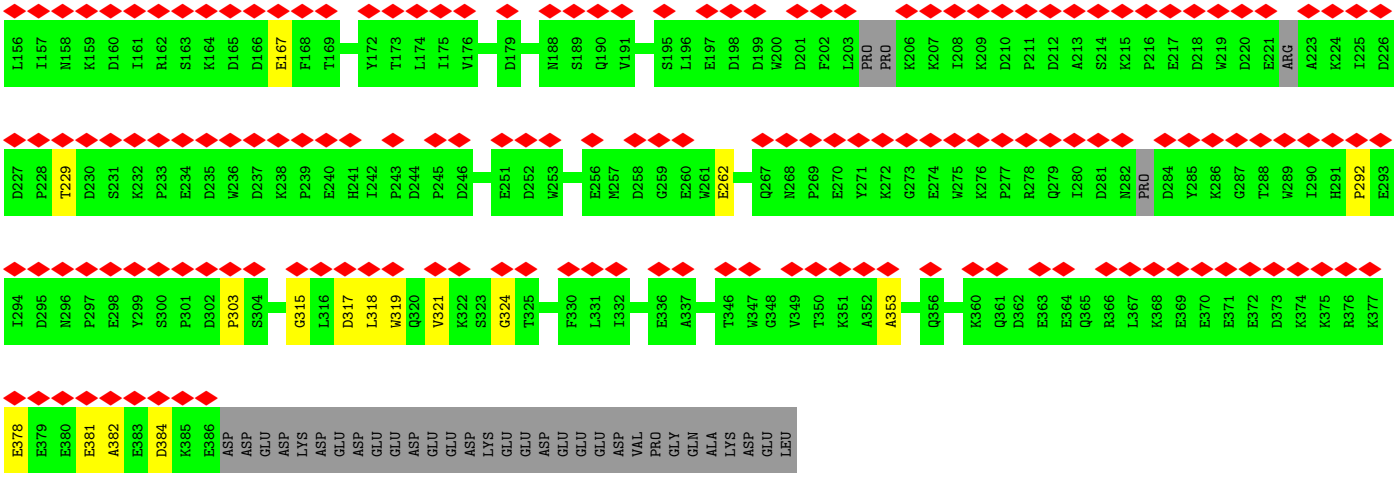
Chain F:



• Molecule 5: Calreticulin

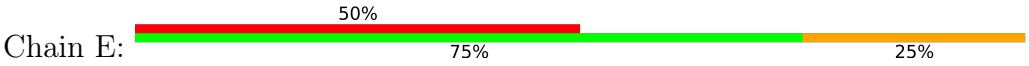
Chain G:





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

• Molecule 7: beta-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	141078	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTF correction was performed internally in Relion and Frealign	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	55	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	0.069	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.032	Depositor
Map size (Å)	215.40001, 215.40001, 215.40001	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.077, 1.077, 1.077	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, MAN, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	B	0.23	0/491	0.39	0/684
2	C	0.26	0/1784	0.42	0/2472
3	D	0.24	0/2274	0.41	0/3163
4	F	0.24	0/1348	0.41	0/1873
5	G	0.24	0/1794	0.47	2/2488 (0.1%)
All	All	0.24	0/7691	0.43	2/10680 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	292	PRO	N-CA-CB	5.94	110.43	103.30
5	G	303	PRO	N-CA-CB	5.64	110.07	103.30

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	B	492	0	204	17	0
2	C	1788	0	836	84	0
3	D	2276	0	1031	41	0
4	F	1349	0	624	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	1799	0	765	27	0
6	A	29	0	27	21	0
7	E	45	0	39	5	0
All	All	7778	0	3526	170	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 15.

All (170) 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:88:SER:N	6:A:1:NAG:H81	1.29	1.47
2:C:13:ALA:H	4:F:142:ILE:CB	1.39	1.34
2:C:13:ALA:N	4:F:142:ILE:CB	1.92	1.32
4:F:87:GLN:C	6:A:1:NAG:H81	1.59	1.22
4:F:87:GLN:HA	6:A:1:NAG:C8	1.72	1.20
4:F:86:ASN:O	6:A:1:NAG:O1	1.63	1.16
4:F:87:GLN:CA	6:A:1:NAG:H81	1.76	1.15
4:F:88:SER:N	6:A:1:NAG:C8	2.08	1.15
2:C:94:ASN:CB	3:D:99:GLY:HA3	1.76	1.15
4:F:88:SER:H	6:A:1:NAG:C8	1.59	1.14
1:B:1:ILE:HA	4:F:120:GLY:HA3	1.32	1.11
2:C:12:ASP:CB	4:F:142:ILE:CB	2.29	1.10
2:C:11:GLU:CB	2:C:12:ASP:O	2.01	1.08
2:C:95:CYS:N	3:D:100:TYR:H	1.56	1.03
2:C:306:LEU:HA	2:C:365:HIS:O	1.60	1.00
2:C:362:CYS:O	2:C:375:SER:HA	1.61	1.00
2:C:24:ALA:O	2:C:45:TYR:HA	1.63	0.98
2:C:319:ARG:CB	5:G:378:GLU:O	2.12	0.98
3:D:274:LYS:CB	5:G:262:GLU:O	2.13	0.97
2:C:95:CYS:O	3:D:99:GLY:HA2	1.65	0.97
2:C:94:ASN:CB	3:D:99:GLY:CA	2.43	0.96
4:F:87:GLN:HA	6:A:1:NAG:H81	1.40	0.95
5:G:75:TYR:O	5:G:317:ASP:HA	1.69	0.92
4:F:86:ASN:O	6:A:1:NAG:O7	1.88	0.92
2:C:319:ARG:CB	5:G:381:GLU:CB	2.49	0.90
2:C:95:CYS:H	3:D:100:TYR:H	0.92	0.89
4:F:88:SER:H	6:A:1:NAG:H81	1.07	0.88
1:B:6:LYS:O	1:B:27:VAL:HA	1.75	0.87
5:G:132:PHE:HA	5:G:145:HIS:O	1.74	0.87
1:B:1:ILE:CA	4:F:120:GLY:HA3	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:94:ASN:HA	3:D:100:TYR:O	1.75	0.85
4:F:186:LYS:O	4:F:205:ALA:HA	1.75	0.84
4:F:86:ASN:O	6:A:1:NAG:C7	2.25	0.84
5:G:318:LEU:HA	7:E:3:MAN:H61	1.60	0.83
2:C:361:ALA:HA	2:C:376:ALA:O	1.79	0.82
1:B:54:LEU:HA	1:B:63:TYR:O	1.79	0.82
3:D:274:LYS:CB	5:G:262:GLU:CB	2.59	0.81
2:C:94:ASN:CB	3:D:99:GLY:C	2.49	0.80
2:C:96:PRO:HA	3:D:98:SER:O	1.82	0.80
4:F:87:GLN:HA	6:A:1:NAG:H82	1.61	0.80
4:F:87:GLN:CA	6:A:1:NAG:C8	2.43	0.80
2:C:289:ALA:HA	2:C:350:PRO:HA	1.65	0.79
2:C:95:CYS:H	3:D:100:TYR:N	1.77	0.76
3:D:274:LYS:CB	5:G:262:GLU:C	2.55	0.75
2:C:277:MET:CB	2:C:294:LEU:O	2.36	0.74
2:C:319:ARG:CB	5:G:382:ALA:N	2.49	0.74
2:C:216:VAL:CB	3:D:407:GLY:HA2	2.18	0.74
4:F:203:CYS:O	4:F:244:TRP:HA	1.88	0.74
2:C:11:GLU:N	2:C:12:ASP:HA	2.02	0.74
2:C:190:HIS:C	2:C:192:GLY:HA3	2.09	0.73
1:B:51:HIS:HA	1:B:66:TYR:HA	1.71	0.72
4:F:88:SER:H	6:A:1:NAG:H83	1.53	0.72
5:G:72:ALA:HA	5:G:321:VAL:HA	1.71	0.72
2:C:26:LEU:O	2:C:48:VAL:CB	2.37	0.72
2:C:273:LYS:CB	2:C:298:SER:O	2.38	0.71
2:C:183:GLY:O	2:C:253:ILE:HA	1.89	0.71
3:D:258:LYS:HA	3:D:331:ALA:HB2	1.73	0.71
2:C:13:ALA:HB2	2:C:18:LEU:CB	2.22	0.70
1:B:40:LEU:HA	1:B:45:ARG:HA	1.73	0.70
2:C:372:SER:CB	5:G:384:ASP:CB	2.70	0.69
3:D:274:LYS:HA	5:G:262:GLU:CB	2.22	0.69
2:C:219:ALA:HA	2:C:233:ASN:O	1.92	0.68
3:D:274:LYS:CA	5:G:262:GLU:CB	2.72	0.68
5:G:105:CYS:HA	5:G:137:CYS:HA	1.76	0.68
2:C:11:GLU:CB	2:C:12:ASP:C	2.62	0.68
4:F:86:ASN:CB	6:A:1:NAG:O1	2.43	0.67
2:C:13:ALA:C	4:F:142:ILE:C	2.56	0.64
4:F:87:GLN:C	6:A:1:NAG:C8	2.53	0.63
2:C:184:LEU:O	2:C:199:ALA:HA	1.98	0.63
2:C:319:ARG:CB	5:G:382:ALA:H	2.14	0.61
5:G:318:LEU:CA	7:E:3:MAN:H61	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:202:ARG:HA	4:F:246:ALA:HA	1.82	0.61
2:C:252:THR:HA	2:C:260:GLY:O	2.00	0.61
2:C:361:ALA:HA	2:C:377:GLU:HA	1.82	0.61
2:C:13:ALA:CA	4:F:142:ILE:CB	2.77	0.60
2:C:95:CYS:N	3:D:100:TYR:N	2.40	0.60
1:B:39:LEU:O	1:B:46:ILE:N	2.29	0.59
2:C:273:LYS:O	2:C:297:VAL:HA	2.02	0.59
2:C:276:LEU:CB	2:C:279:ALA:HB2	2.33	0.59
1:B:24:ASN:HA	1:B:66:TYR:O	2.04	0.58
3:D:367:SER:CB	3:D:383:ALA:HB3	2.34	0.58
2:C:190:HIS:O	2:C:192:GLY:HA3	2.04	0.58
5:G:319:TRP:N	7:E:3:MAN:H62	2.20	0.57
2:C:272:PRO:HA	2:C:299:HIS:O	2.05	0.57
4:F:87:GLN:HA	6:A:1:NAG:C7	2.32	0.57
1:B:40:LEU:O	1:B:78:TYR:HA	2.05	0.57
6:A:1:NAG:H62	6:A:2:NAG:C1	2.35	0.56
2:C:13:ALA:C	4:F:142:ILE:CB	2.73	0.56
2:C:191:LEU:N	2:C:192:GLY:HA3	2.20	0.56
2:C:41:ASP:O	2:C:43:GLU:N	2.38	0.56
2:C:188:ARG:O	2:C:194:GLY:HA2	2.06	0.56
2:C:95:CYS:O	3:D:98:SER:O	2.24	0.56
1:B:82:VAL:O	1:B:90:PRO:HA	2.06	0.55
2:C:336:SER:H	4:F:226:GLN:N	2.04	0.55
1:B:42:ASN:N	1:B:77:GLU:O	2.34	0.55
5:G:135:ASP:O	5:G:142:LYS:HA	2.07	0.54
2:C:13:ALA:CB	2:C:18:LEU:CB	2.86	0.54
3:D:264:TYR:HA	3:D:302:ALA:O	2.08	0.54
2:C:24:ALA:HB3	2:C:45:TYR:CB	2.38	0.53
2:C:190:HIS:O	2:C:191:LEU:CB	2.56	0.53
2:C:325:GLY:HA3	2:C:347:GLN:O	2.07	0.53
4:F:135:ALA:HB1	4:F:140:ALA:HB3	1.90	0.53
3:D:382:VAL:O	3:D:386:PHE:N	2.42	0.53
5:G:109:TYR:HA	5:G:133:GLY:HA3	1.91	0.52
2:C:1:GLY:HA3	2:C:59:PHE:O	2.09	0.52
2:C:70:HIS:O	2:C:108:ILE:HA	2.10	0.52
3:D:376:GLY:O	3:D:378:VAL:N	2.43	0.52
2:C:94:ASN:CB	3:D:100:TYR:N	2.72	0.52
5:G:99:HIS:O	5:G:167:GLU:HA	2.10	0.51
2:C:94:ASN:CA	3:D:100:TYR:N	2.73	0.51
4:F:187:THR:HA	4:F:204:TRP:O	2.11	0.51
2:C:286:PRO:HA	2:C:352:THR:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:11:GLU:H	2:C:12:ASP:HA	1.75	0.51
2:C:253:ILE:O	2:C:259:GLN:HA	2.12	0.50
4:F:199:ALA:O	4:F:248:VAL:HA	2.11	0.50
2:C:10:VAL:N	2:C:73:MET:O	2.36	0.50
2:C:361:ALA:CA	2:C:377:GLU:HA	2.42	0.49
2:C:12:ASP:C	4:F:142:ILE:CB	2.73	0.49
2:C:17:GLY:O	2:C:19:ALA:N	2.46	0.49
4:F:213:ILE:HA	4:F:263:HIS:CB	2.42	0.49
5:G:72:ALA:CA	5:G:321:VAL:HA	2.42	0.49
4:F:27:TYR:CB	4:F:32:GLN:HA	2.43	0.49
3:D:138:PRO:HA	3:D:186:HIS:O	2.13	0.49
3:D:258:LYS:HA	3:D:331:ALA:CB	2.43	0.49
2:C:10:VAL:O	2:C:74:SER:HA	2.12	0.48
2:C:95:CYS:O	3:D:99:GLY:CA	2.52	0.48
2:C:151:ARG:HA	2:C:269:TYR:O	2.14	0.48
2:C:13:ALA:O	4:F:142:ILE:O	2.31	0.48
5:G:74:PHE:HA	5:G:318:LEU:O	2.13	0.48
3:D:262:ILE:HA	3:D:300:ALA:O	2.14	0.48
3:D:450:PHE:HA	3:D:451:PRO:HA	1.61	0.48
4:F:28:VAL:O	4:F:30:ASP:N	2.47	0.48
5:G:78:SER:HA	5:G:315:GLY:HA2	1.95	0.48
3:D:244:CYS:HA	3:D:299:PHE:O	2.14	0.47
2:C:95:CYS:C	3:D:99:GLY:HA2	2.34	0.47
2:C:282:ALA:O	2:C:284:ALA:N	2.48	0.47
1:B:8:GLN:O	1:B:25:CYS:HA	2.16	0.46
1:B:17:ASN:HA	1:B:72:PRO:O	2.14	0.46
3:D:265:TYR:O	3:D:303:SER:HA	2.16	0.46
2:C:94:ASN:HA	3:D:100:TYR:C	2.36	0.46
2:C:193:LYS:HA	2:C:194:GLY:HA3	1.51	0.46
4:F:86:ASN:C	6:A:1:NAG:O7	2.54	0.46
5:G:58:GLY:HA2	5:G:353:ALA:HB3	1.98	0.45
3:D:46:GLY:O	3:D:107:ARG:HA	2.16	0.45
2:C:217:ALA:O	3:D:407:GLY:N	2.47	0.44
1:B:23:LEU:O	1:B:67:TYR:HA	2.17	0.44
5:G:318:LEU:C	7:E:3:MAN:H62	2.38	0.44
5:G:101:GLN:CB	5:G:324:GLY:HA3	2.48	0.44
2:C:3:ALA:HB1	2:C:35:PRO:CB	2.48	0.44
2:C:11:GLU:CB	2:C:12:ASP:CA	2.95	0.44
4:F:215:LEU:HA	4:F:260:HIS:O	2.18	0.44
6:A:1:NAG:C7	6:A:1:NAG:HO1	2.31	0.44
2:C:94:ASN:HA	3:D:100:TYR:N	2.33	0.43

Continued on next page...

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:362:CYS:O	2:C:375:SER:CA	2.50	0.43
2:C:217:ALA:H	3:D:407:GLY:CA	2.32	0.43
1:B:42:ASN:HA	1:B:77:GLU:CB	2.49	0.43
1:B:80:CYS:O	1:B:92:ILE:HA	2.18	0.43
2:C:13:ALA:C	4:F:142:ILE:O	2.57	0.43
2:C:23:GLY:HA2	2:C:44:LEU:CB	2.49	0.43
6:A:1:NAG:C6	6:A:2:NAG:C1	2.97	0.42
3:D:259:ASP:HA	3:D:330:THR:HA	2.02	0.41
2:C:140:THR:O	2:C:162:PHE:HA	2.21	0.41
3:D:190:GLU:O	3:D:194:ASN:CB	2.68	0.41
5:G:318:LEU:HA	7:E:3:MAN:C6	2.40	0.41
2:C:148:PRO:O	2:C:266:LEU:HA	2.20	0.41
2:C:46:LEU:HA	2:C:133:THR:O	2.21	0.41
3:D:133:GLY:HA2	3:D:134:PRO:HA	1.71	0.41
1:B:54:LEU:CA	1:B:63:TYR:O	2.61	0.40
2:C:191:LEU:CB	2:C:192:GLY:CA	2.99	0.40
3:D:259:ASP:HA	3:D:329:ARG:O	2.22	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	B	97/99 (98%)	75 (77%)	17 (18%)	5 (5%)	2	19
2	C	356/428 (83%)	300 (84%)	41 (12%)	15 (4%)	3	22
3	D	457/481 (95%)	420 (92%)	32 (7%)	5 (1%)	14	51
4	F	272/341 (80%)	252 (93%)	17 (6%)	3 (1%)	14	51
5	G	355/400 (89%)	321 (90%)	29 (8%)	5 (1%)	11	46
All	All	1537/1749 (88%)	1368 (89%)	136 (9%)	33 (2%)	10	36

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	42	PRO
2	C	191	LEU
2	C	278	PRO
3	D	377	PRO
2	C	18	LEU
2	C	129	PRO
2	C	283	ARG
3	D	362	LYS
2	C	35	PRO
2	C	273	LYS
4	F	29	ASP
5	G	137	CYS
5	G	142	LYS
5	G	229	THR
1	B	13	HIS
1	B	15	ALA
1	B	77	GLU
1	B	88	SER
2	C	226	PRO
2	C	297	VAL
2	C	299	HIS
3	D	272	ASN
3	D	460	LYS
4	F	207	GLY
1	B	35	ILE
2	C	41	ASP
5	G	146	VAL
4	F	162	GLY
2	C	256	PRO
2	C	125	PRO
2	C	272	PRO
3	D	333	GLY
5	G	114	PRO

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA

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)

6 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	$\#\|Z\| > 2$
6	NAG	A	1	6	15,15,15	0.49	0	21,21,21	0.92	1 (4%)
6	NAG	A	2	6	14,14,15	0.22	0	17,19,21	0.42	0
7	MAN	E	1	7	11,11,12	0.70	0	13,15,17	0.71	0
7	MAN	E	2	7	11,11,12	0.71	0	13,15,17	0.72	0
7	MAN	E	3	7	11,11,12	0.83	1 (9%)	13,15,17	1.02	0
7	BGC	E	4	7	12,12,12	0.53	0	17,17,17	0.52	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	1	6	-	0/6/26/26	0/1/1/1
6	NAG	A	2	6	-	2/6/23/26	0/1/1/1
7	MAN	E	1	7	-	0/2/18/22	0/1/1/1
7	MAN	E	2	7	-	0/2/18/22	0/1/1/1
7	MAN	E	3	7	-	0/2/18/22	0/1/1/1
7	BGC	E	4	7	-	0/2/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	3	MAN	C1-C2	2.27	1.54	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1	NAG	C8-C7-N2	2.33	120.04	116.10

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2	NAG	O5-C5-C6-O6
6	A	2	NAG	C4-C5-C6-O6

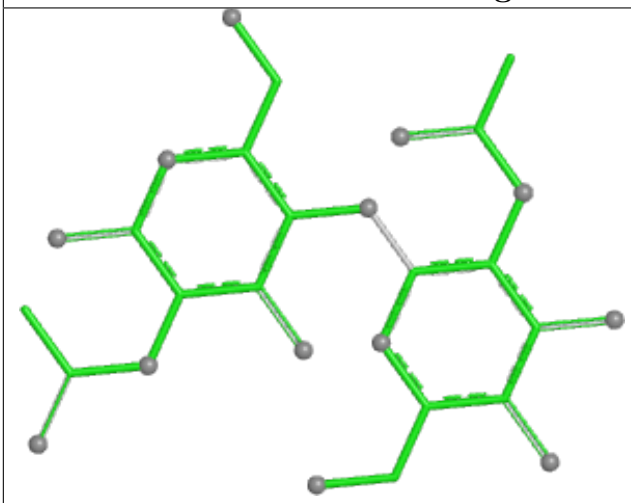
There are no ring outliers.

3 monomers are involved in 26 short contacts:

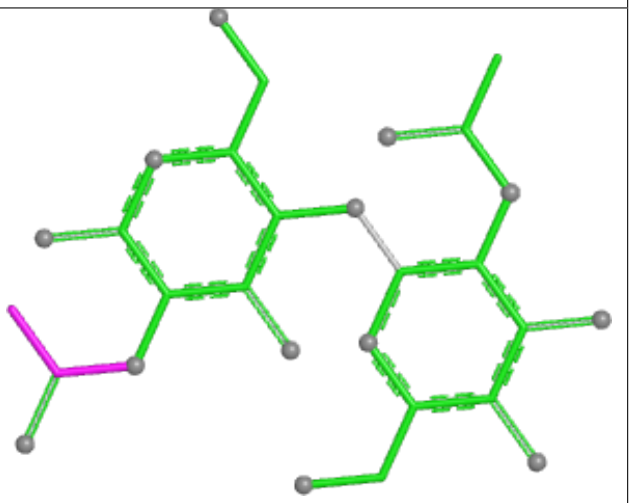
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	3	MAN	5	0
6	A	2	NAG	2	0
6	A	1	NAG	21	0

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

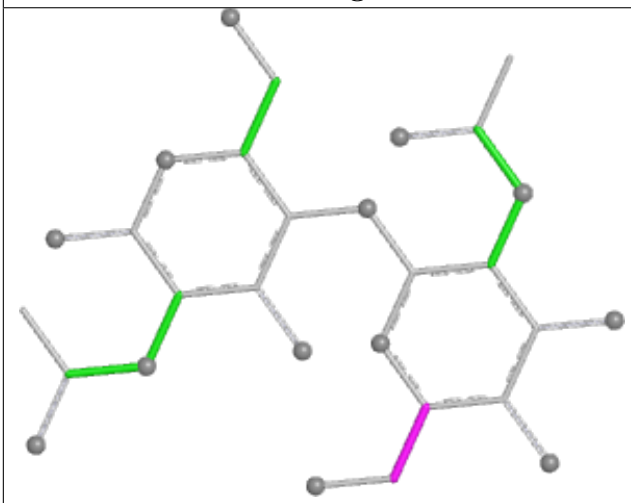
Oligosaccharide Chain A



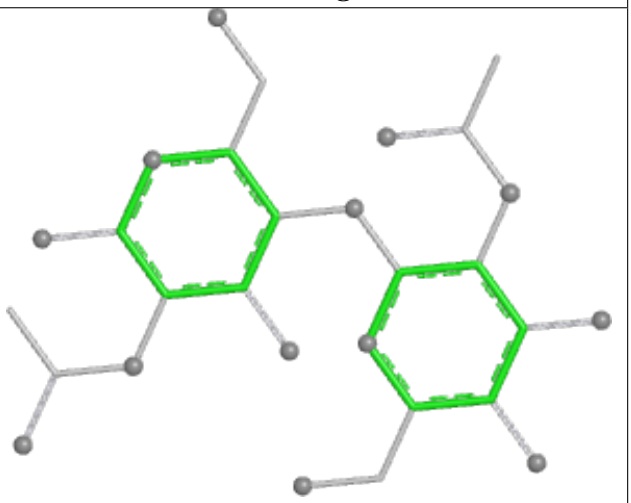
Bond lengths



Bond angles

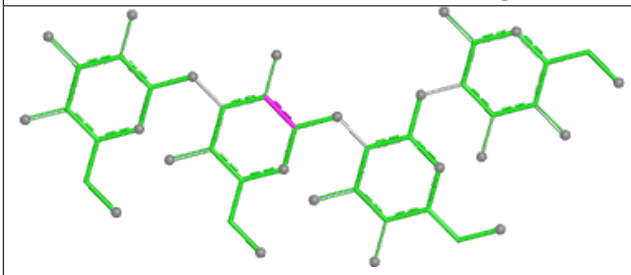


Torsions

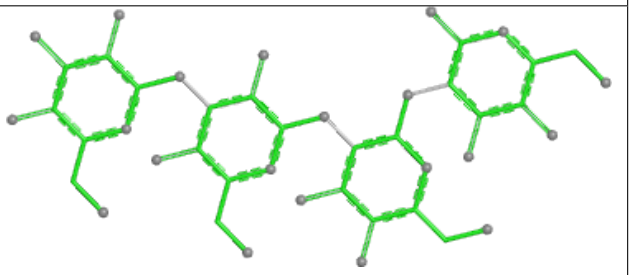


Rings

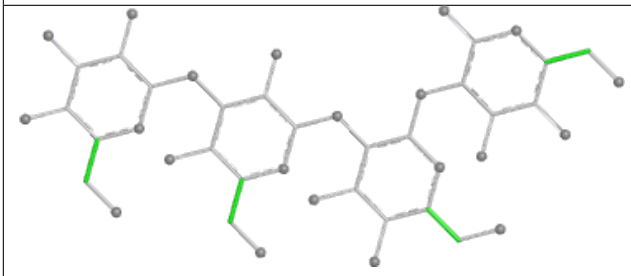
Oligosaccharide Chain E



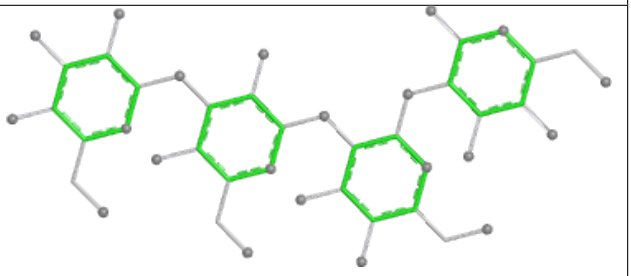
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	300:SER	C	301:PRO	N	3.24

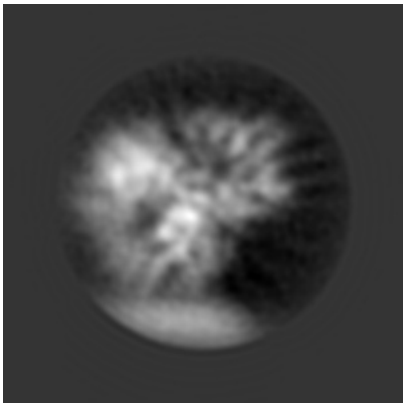
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3906. These allow visual inspection of the internal detail of the map and identification of artifacts.

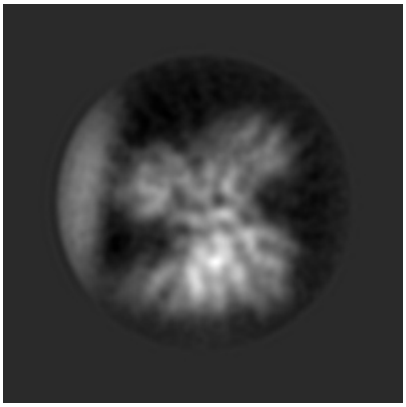
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

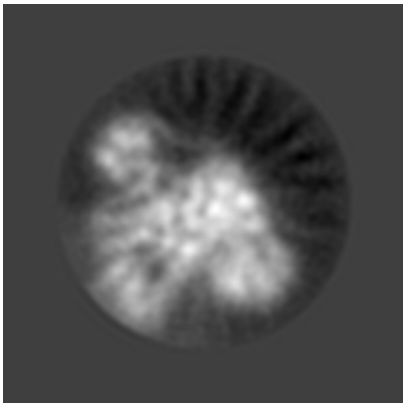
6.1.1 Primary map



X



Y



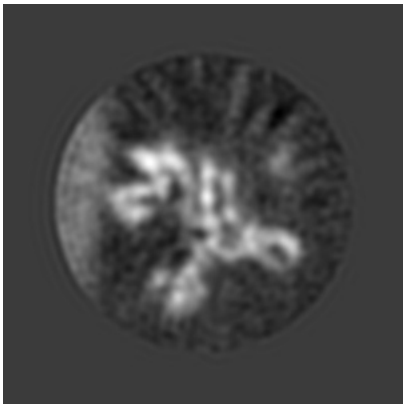
Z

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

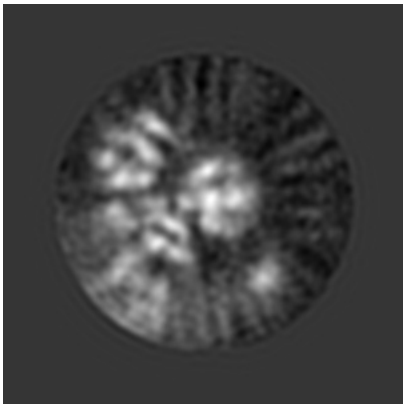
6.2 Central slices

6.2.1 Primary map

X Index: 100



Y Index: 100

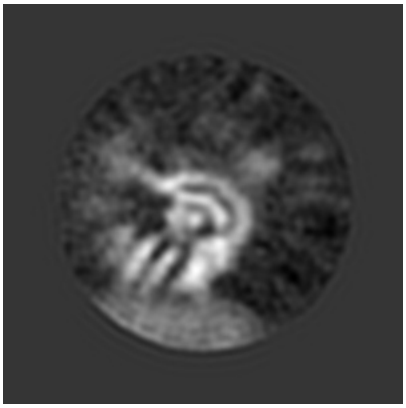


Z Index: 100

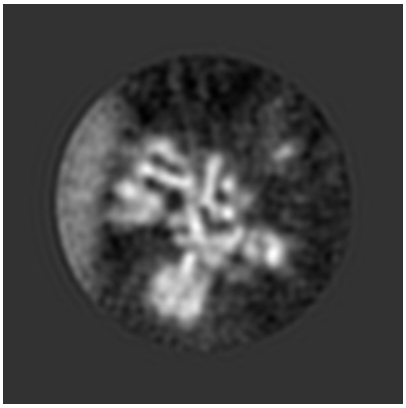
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

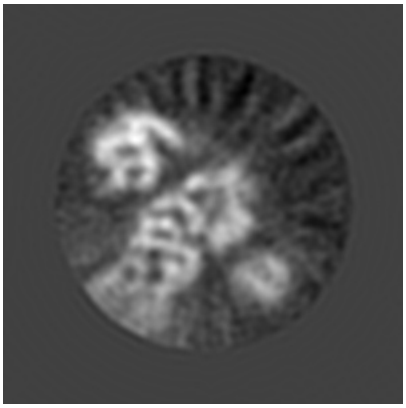
6.3.1 Primary map



X Index: 107



Y Index: 92

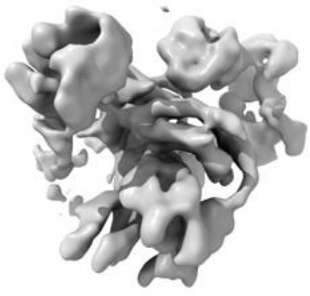


Z Index: 106

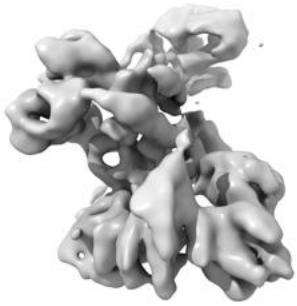
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

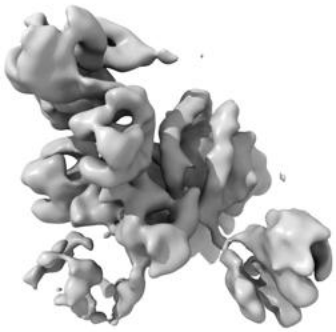
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.032. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

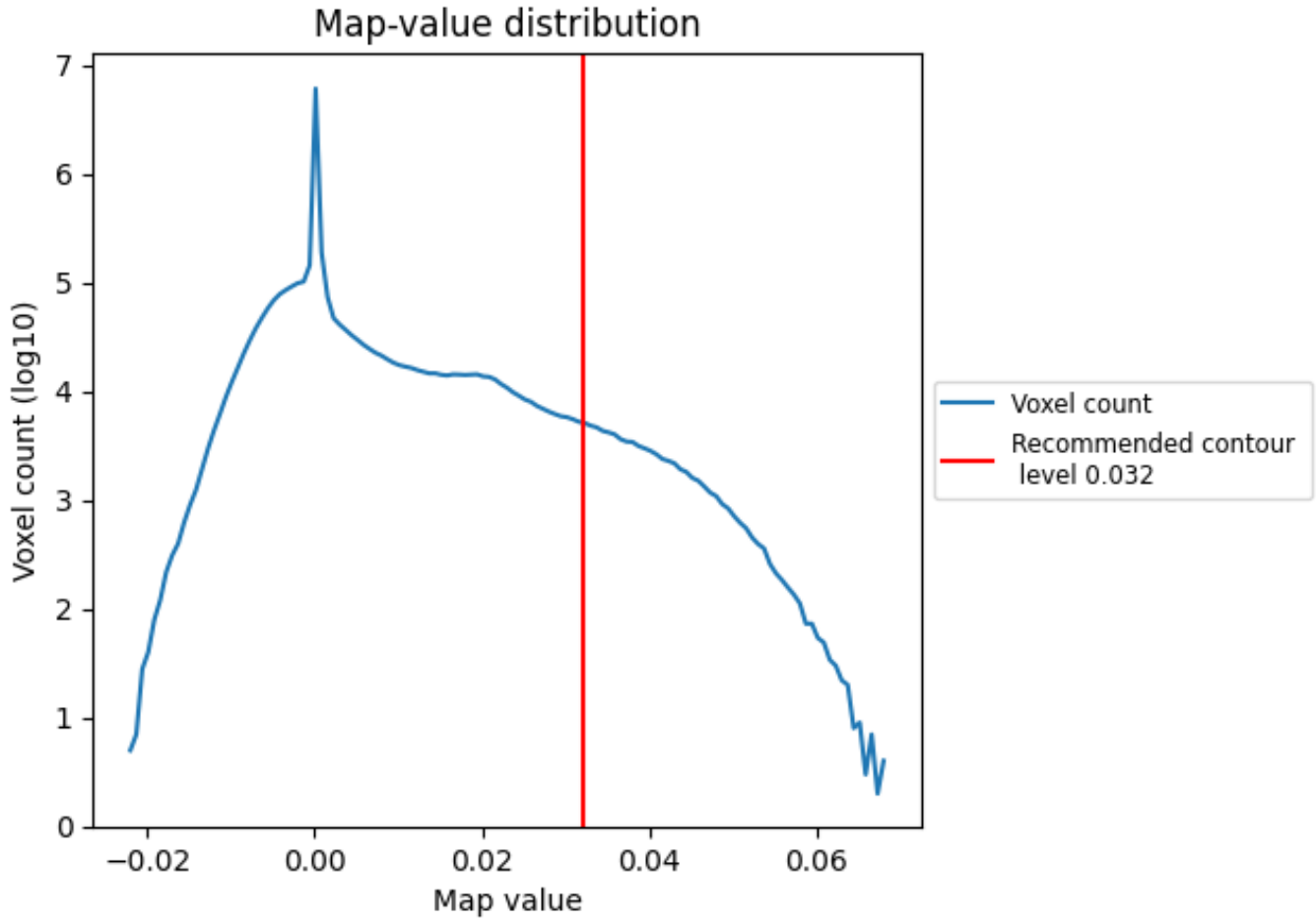
6.5 Mask visualisation (i)

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

7 Map analysis

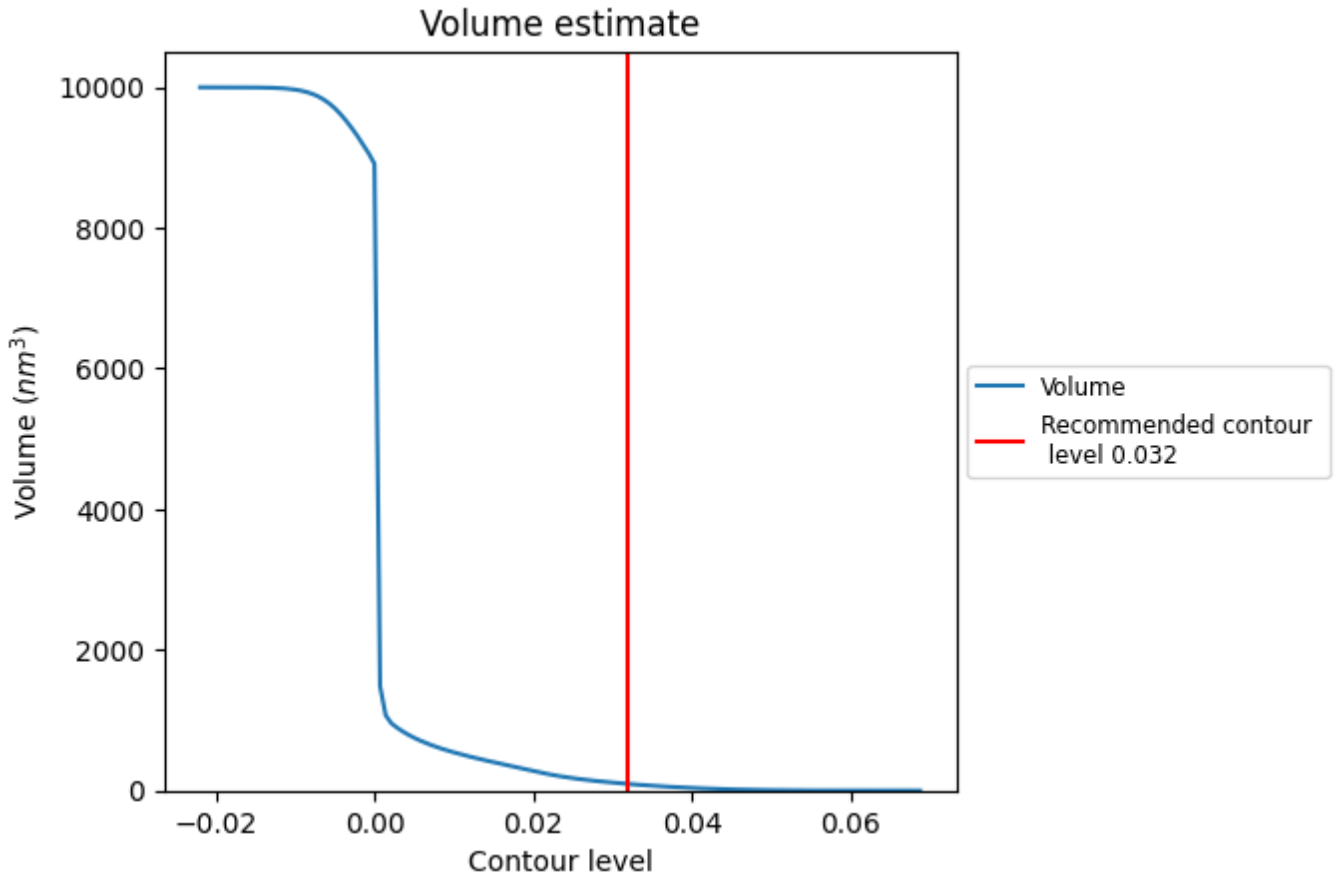
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

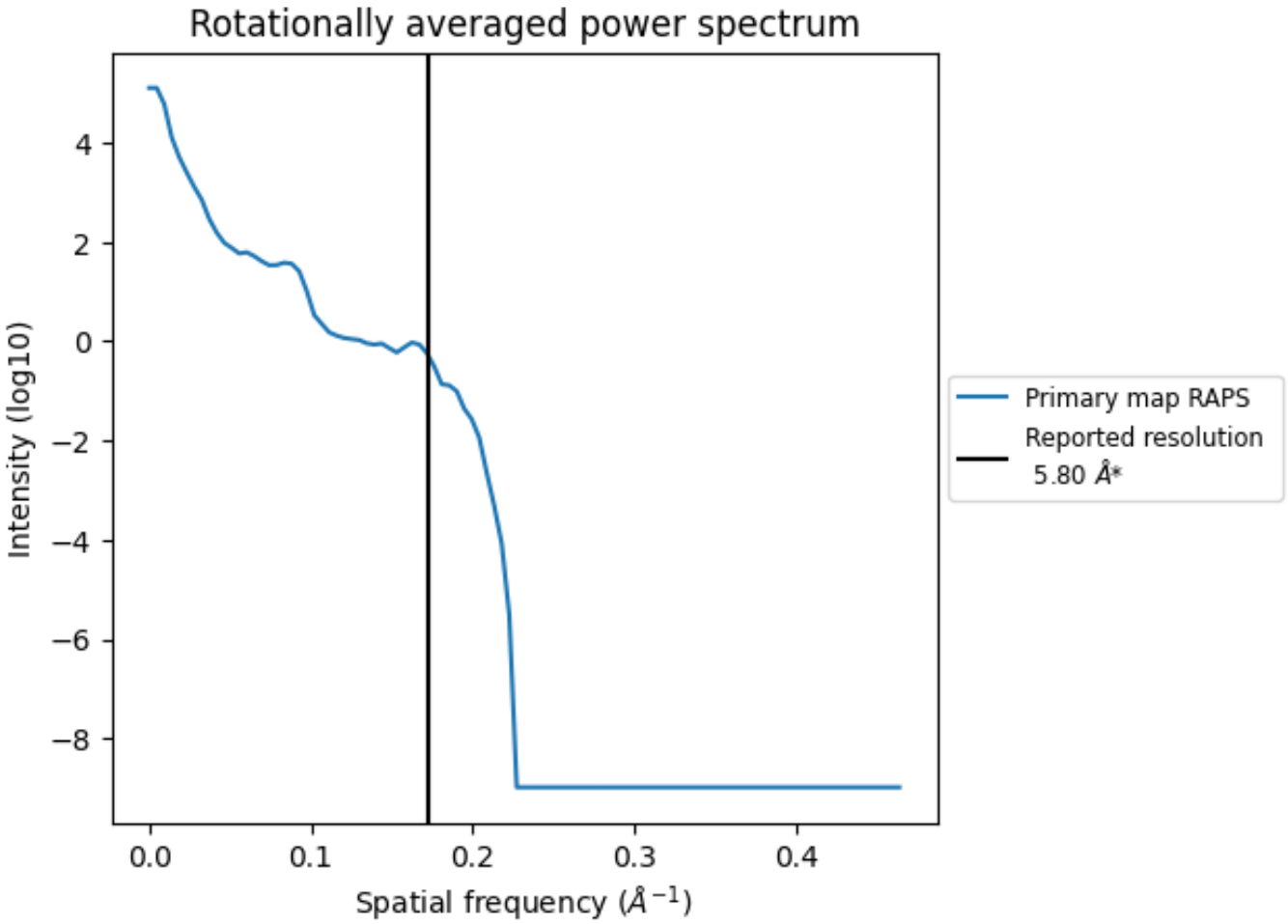
7.2 Volume estimate



The volume at the recommended contour level is 94 nm^3; this corresponds to an approximate mass of 85 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 0.172 Å^{-1}

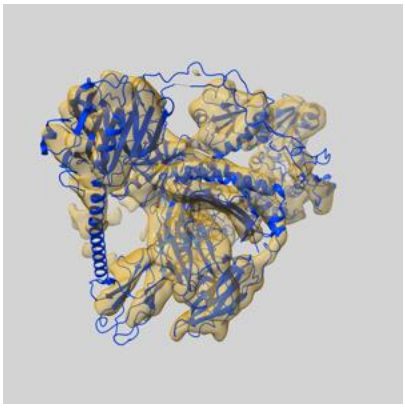
8 Fourier-Shell correlation (i)

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

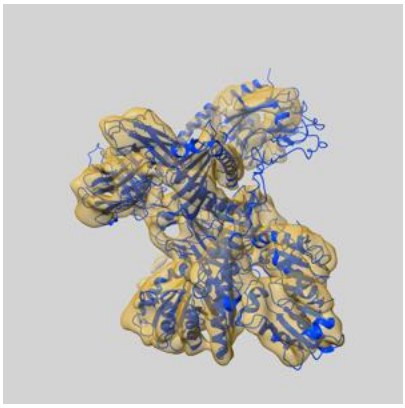
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3906 and PDB model 6ENY. Per-residue inclusion information can be found in section 3 on page 6.

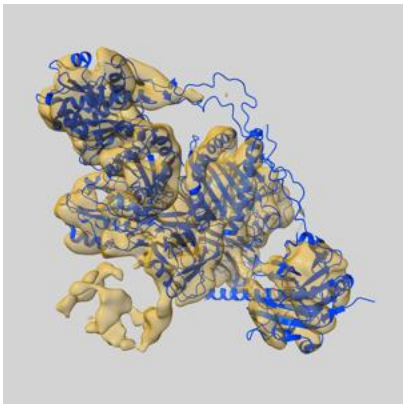
9.1 Map-model overlay



X



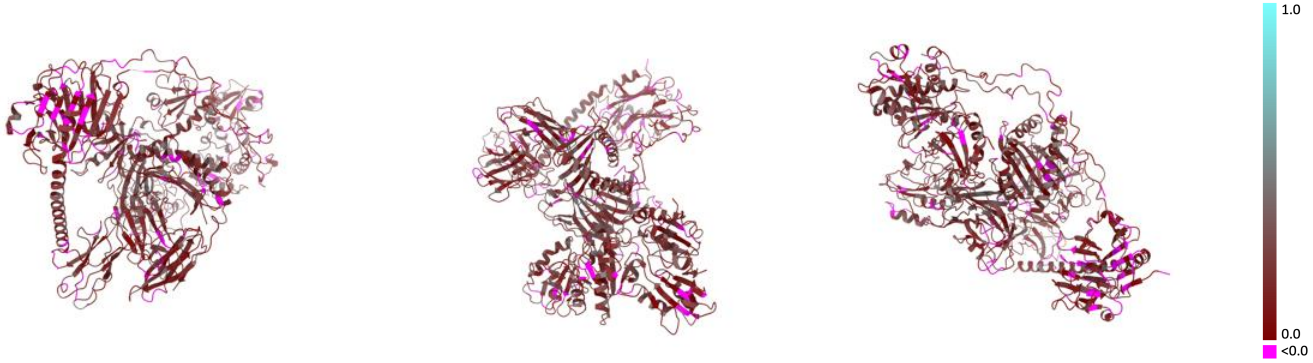
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.032 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.

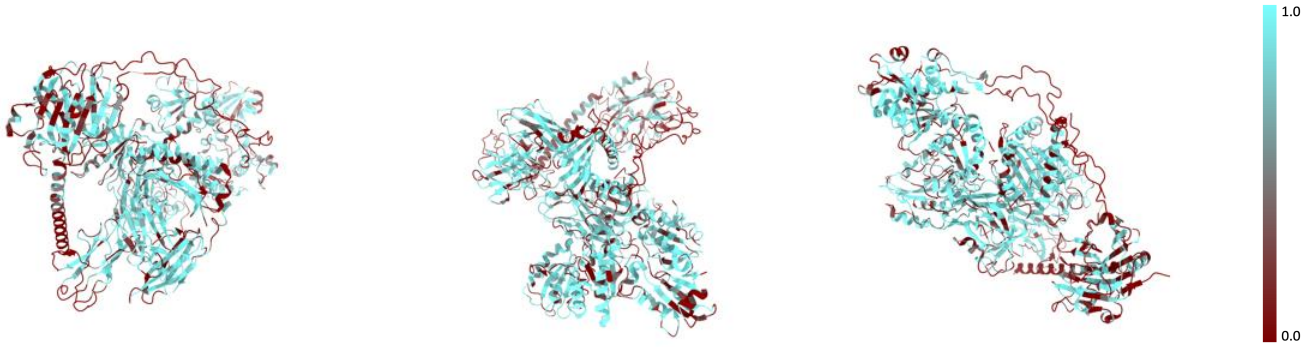
9.2 Q-score mapped to coordinate model



X Y Z

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

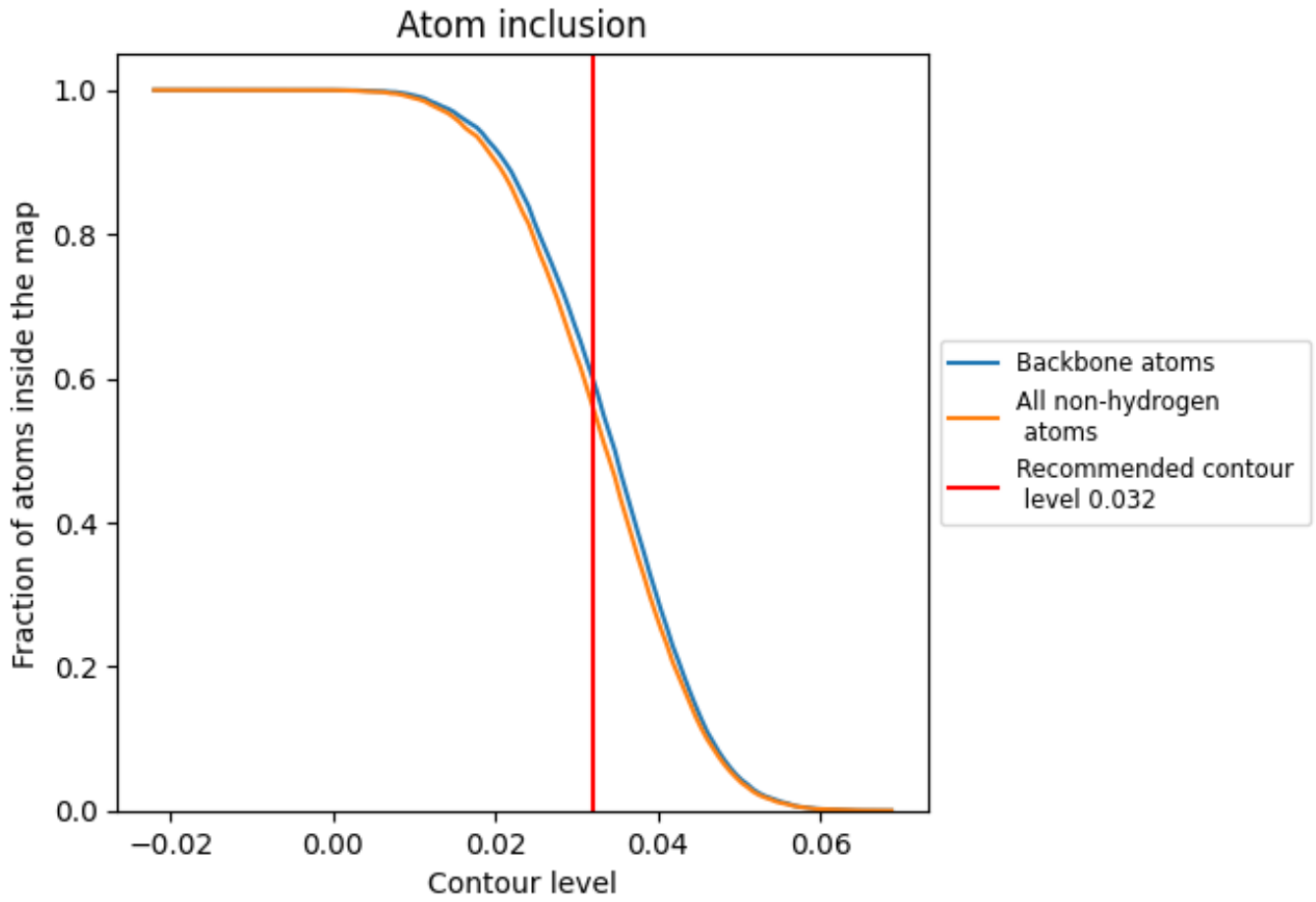
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.032).

9.4 Atom inclusion (i)



At the recommended contour level, 60% of all backbone atoms, 56% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5604	0.1710
A	0.3793	0.1880
B	0.7419	0.1800
C	0.5956	0.1920
D	0.6621	0.1810
E	0.2667	0.1250
F	0.6256	0.1800
G	0.3085	0.1300