



Full wwPDB EM Validation Report ⓘ

Nov 15, 2022 – 02:06 AM EST

PDB ID : 6W5R
EMDB ID : EMD-21545
Title : NPC1 structure in Nanodisc
Authors : Yan, N.; Qian, H.W.; Wu, X.L.
Deposited on : 2020-03-13
Resolution : 3.60 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
buster-report : 1.1.7 (2018)
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

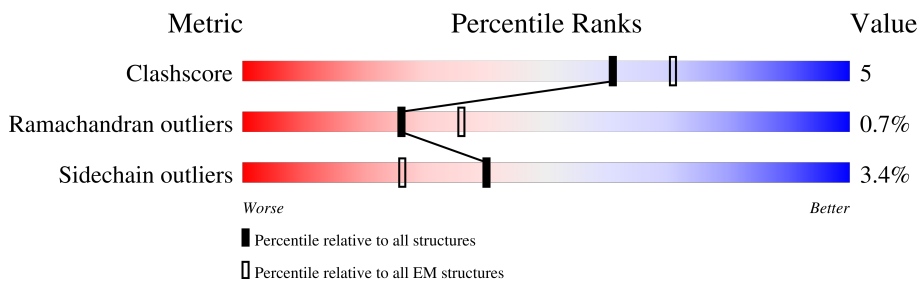
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	A	1311	
2	B	2	
2	C	2	
3	D	3	
4	E	3	

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
4	NAG	E	2	X	-	-	-

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 9629 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 NPC intracellular cholesterol transporter 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1194	9341	6048	1508	1710	75	0	0

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1279	LEU	-	expression tag	UNP O15118
A	1280	GLU	-	expression tag	UNP O15118
A	1281	GLY	-	expression tag	UNP O15118
A	1282	SER	-	expression tag	UNP O15118
A	1283	ASP	-	expression tag	UNP O15118
A	1284	GLU	-	expression tag	UNP O15118
A	1285	VAL	-	expression tag	UNP O15118
A	1286	ASP	-	expression tag	UNP O15118
A	1287	ALA	-	expression tag	UNP O15118
A	1288	GLY	-	expression tag	UNP O15118
A	1289	SER	-	expression tag	UNP O15118
A	1290	HIS	-	expression tag	UNP O15118
A	1291	HIS	-	expression tag	UNP O15118
A	1292	HIS	-	expression tag	UNP O15118
A	1293	HIS	-	expression tag	UNP O15118
A	1294	HIS	-	expression tag	UNP O15118
A	1295	HIS	-	expression tag	UNP O15118
A	1296	HIS	-	expression tag	UNP O15118
A	1297	HIS	-	expression tag	UNP O15118
A	1298	HIS	-	expression tag	UNP O15118
A	1299	HIS	-	expression tag	UNP O15118
A	1300	GLY	-	expression tag	UNP O15118
A	1301	SER	-	expression tag	UNP O15118
A	1302	VAL	-	expression tag	UNP O15118
A	1303	GLU	-	expression tag	UNP O15118
A	1304	ASP	-	expression tag	UNP O15118
A	1305	TYR	-	expression tag	UNP O15118
A	1306	LYS	-	expression tag	UNP O15118

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1307	ASP	-	expression tag	UNP O15118
A	1308	ASP	-	expression tag	UNP O15118
A	1309	ASP	-	expression tag	UNP O15118
A	1310	ASP	-	expression tag	UNP O15118
A	1311	LYS	-	expression tag	UNP O15118

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



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

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



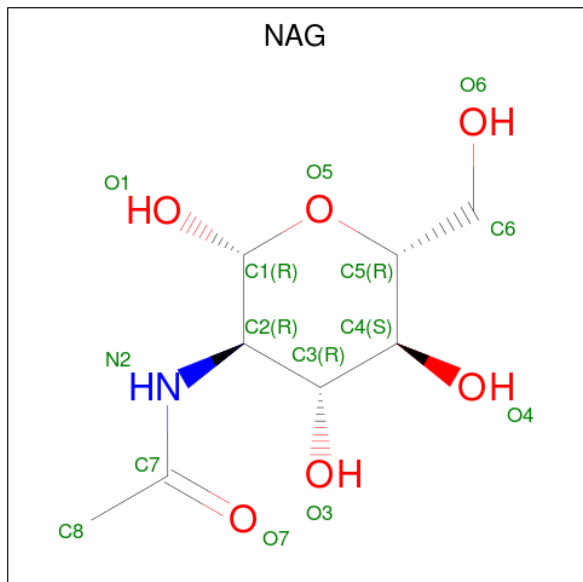
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	D	3	39	22	2	15	0	0

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



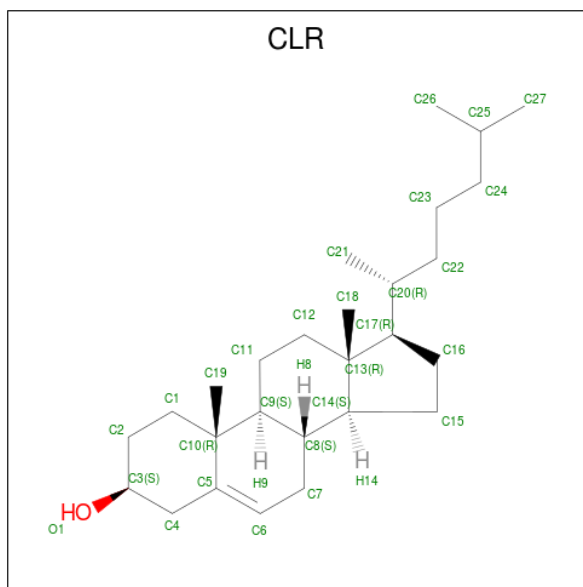
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	E	3	39	22	2	15	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	Total	C	N	O	0
			126	72	9	45	
5	A	1	Total	C	N	O	0
			126	72	9	45	
5	A	1	Total	C	N	O	0
			126	72	9	45	
5	A	1	Total	C	N	O	0
			126	72	9	45	
5	A	1	Total	C	N	O	0
			126	72	9	45	
5	A	1	Total	C	N	O	0
			126	72	9	45	
5	A	1	Total	C	N	O	0
			126	72	9	45	

- Molecule 6 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).

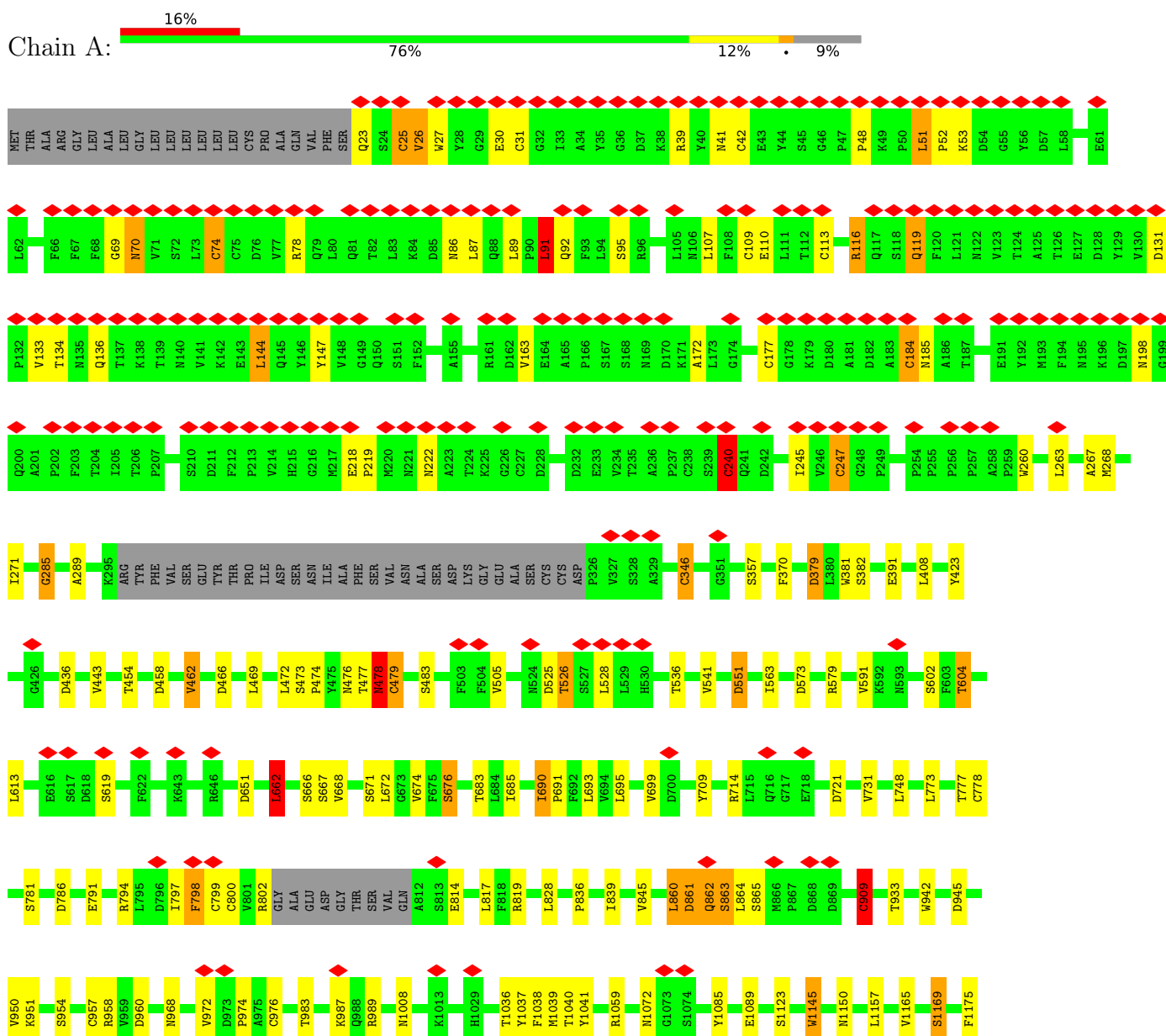


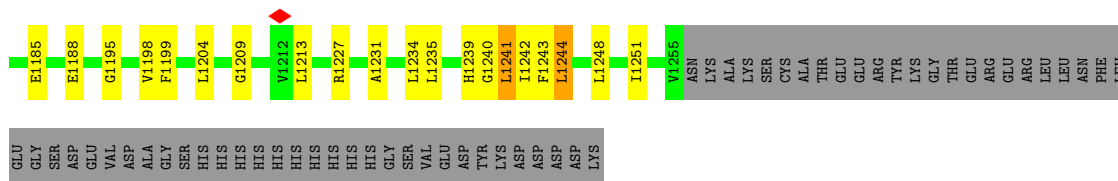
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			28	27	1	

3 Residue-property plots

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: NPC intracellular cholesterol transporter 1





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



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



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



- Molecule 4: alpha-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	284427	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 ($e^-/\text{\AA}^2$)	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	0.175	Depositor
Minimum map value	-0.087	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	267.36, 267.36, 267.36	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.114, 1.114, 1.114	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: CLR, NAG, MAN, BMA

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	A	0.67	12/9585 (0.1%)	1.08	65/13053 (0.5%)

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	A	0	7

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	423	TYR	C-N	7.84	1.49	1.34
1	A	479	CYS	CB-SG	-6.76	1.70	1.82
1	A	909	CYS	CB-SG	-5.88	1.72	1.81
1	A	602	SER	CA-CB	-5.79	1.44	1.52
1	A	668	VAL	CB-CG2	-5.56	1.41	1.52
1	A	983	THR	C-N	5.55	1.44	1.34
1	A	1244	LEU	C-N	5.45	1.44	1.34
1	A	346	CYS	CB-SG	-5.16	1.73	1.81
1	A	699	VAL	CB-CG1	-5.16	1.42	1.52
1	A	957	CYS	CB-SG	-5.15	1.73	1.81
1	A	74	CYS	CA-C	5.14	1.66	1.52
1	A	541	VAL	CB-CG1	-5.11	1.42	1.52

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	ASN	N-CA-C	-11.38	80.27	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	458	ASP	CB-CG-OD1	11.13	128.31	118.30
1	A	91	LEU	CA-CB-CG	9.92	138.11	115.30
1	A	177	CYS	CA-CB-SG	9.78	131.61	114.00
1	A	613	LEU	CA-CB-CG	9.26	136.61	115.30
1	A	263	LEU	CA-CB-CG	9.18	136.41	115.30
1	A	74	CYS	CA-CB-SG	8.56	129.41	114.00
1	A	1234	LEU	CA-CB-CG	7.99	133.67	115.30
1	A	247	CYS	CA-CB-SG	7.90	128.22	114.00
1	A	690	ILE	CG1-CB-CG2	-7.71	94.43	111.40
1	A	89	LEU	CA-CB-CG	7.67	132.95	115.30
1	A	1039	MET	CA-CB-CG	7.23	125.59	113.30
1	A	472	LEU	CA-CB-CG	7.08	131.57	115.30
1	A	573	ASP	CB-CG-OD1	6.89	124.50	118.30
1	A	443	VAL	CG1-CB-CG2	-6.83	99.97	110.90
1	A	144	LEU	CA-CB-CG	6.80	130.95	115.30
1	A	960	ASP	CB-CG-OD1	6.79	124.42	118.30
1	A	116	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	A	184	CYS	CA-CB-SG	6.70	126.06	114.00
1	A	240	CYS	CA-CB-SG	6.65	125.96	114.00
1	A	370	PHE	CB-CG-CD1	6.58	125.40	120.80
1	A	528	LEU	CA-CB-CG	6.47	130.18	115.30
1	A	864	LEU	CB-CG-CD2	6.40	121.87	111.00
1	A	699	VAL	CG1-CB-CG2	-6.37	100.70	110.90
1	A	976	CYS	CA-CB-SG	6.30	125.34	114.00
1	A	693	LEU	CB-CG-CD2	6.20	121.53	111.00
1	A	1038	PHE	CB-CG-CD1	6.17	125.12	120.80
1	A	525	ASP	CB-CG-OD1	6.15	123.84	118.30
1	A	662	LEU	CA-CB-CG	6.15	129.45	115.30
1	A	786	ASP	CB-CG-OD1	6.13	123.82	118.30
1	A	87	LEU	CB-CG-CD1	6.07	121.32	111.00
1	A	469	LEU	CA-CB-CG	6.03	129.17	115.30
1	A	370	PHE	CB-CG-CD2	-5.99	116.61	120.80
1	A	651	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	1242	ILE	CG1-CB-CG2	-5.92	98.38	111.40
1	A	674	VAL	CG1-CB-CG2	-5.83	101.57	110.90
1	A	113	CYS	CA-CB-SG	5.82	124.48	114.00
1	A	1038	PHE	CB-CG-CD2	-5.81	116.73	120.80
1	A	845	VAL	CG1-CB-CG2	-5.72	101.75	110.90
1	A	408	LEU	CA-CB-CG	5.71	128.44	115.30
1	A	828	LEU	CA-CB-CG	5.53	128.03	115.30
1	A	147	TYR	CA-CB-CG	5.53	123.90	113.40
1	A	1175	PHE	CB-CG-CD2	-5.51	116.95	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	LYS	CA-CB-CG	5.49	125.48	113.40
1	A	551	ASP	C-N-CA	5.46	135.34	121.70
1	A	1241	LEU	CA-CB-CG	5.44	127.82	115.30
1	A	662	LEU	CB-CG-CD1	-5.44	101.75	111.00
1	A	604	THR	CA-CB-CG2	5.43	120.01	112.40
1	A	1037	TYR	CA-CB-CG	5.40	123.65	113.40
1	A	860	LEU	CA-CB-CG	5.32	127.54	115.30
1	A	591	VAL	CG1-CB-CG2	-5.32	102.39	110.90
1	A	798	PHE	C-N-CA	5.32	134.99	121.70
1	A	1175	PHE	CB-CG-CD1	5.30	124.51	120.80
1	A	683	THR	CA-CB-CG2	5.26	119.76	112.40
1	A	709	TYR	CB-CG-CD1	-5.24	117.86	121.00
1	A	144	LEU	CB-CG-CD2	5.23	119.89	111.00
1	A	462	VAL	CA-CB-CG1	5.20	118.70	110.90
1	A	458	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	A	721	ASP	CB-CG-OD1	5.16	122.95	118.30
1	A	48	PRO	C-N-CA	5.16	134.59	121.70
1	A	1157	LEU	CB-CG-CD2	-5.14	102.26	111.00
1	A	479	CYS	N-CA-CB	5.07	119.72	110.60
1	A	693	LEU	CA-CB-CG	5.06	126.93	115.30
1	A	74	CYS	O-C-N	-5.05	114.62	122.70
1	A	662	LEU	CB-CG-CD2	5.04	119.57	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	LEU	Mainchain
1	A	285	GLY	Mainchain
1	A	473	SER	Peptide
1	A	478	ASN	Peptide
1	A	69	GLY	Mainchain
1	A	799	CYS	Peptide
1	A	909	CYS	Peptide

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	A	9341	0	9119	85	0
2	B	28	0	25	0	0
2	C	28	0	25	1	0
3	D	39	0	34	0	0
4	E	39	0	34	2	0
5	A	126	0	117	0	0
6	A	28	0	46	3	0
All	All	9629	0	9400	88	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 5.

All (88) 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)
1:A:357:SER:CB	1:A:778:CYS:SG	2.63	0.86
1:A:357:SER:HB2	1:A:778:CYS:SG	2.20	0.81
1:A:1145:TRP:CZ3	1:A:1227:ARG:HG2	2.20	0.76
1:A:861:ASP:O	1:A:862:GLN:HG3	1.86	0.76
1:A:245:ILE:N	1:A:245:ILE:HD12	2.02	0.74
4:E:2:NAG:O4	4:E:2:NAG:O7	2.05	0.72
1:A:30:GLU:OE1	1:A:39:ARG:HD2	1.91	0.71
1:A:30:GLU:CD	1:A:78:ARG:HG3	2.10	0.71
1:A:1145:TRP:CE3	1:A:1227:ARG:HG2	2.30	0.67
1:A:1239:HIS:O	1:A:1243:PHE:HB3	1.94	0.66
1:A:1231:ALA:O	1:A:1235:LEU:HB2	1.96	0.64
1:A:357:SER:OG	1:A:778:CYS:SG	2.57	0.62
1:A:30:GLU:CD	1:A:78:ARG:CG	2.69	0.61
1:A:245:ILE:HD12	1:A:245:ILE:H	1.66	0.60
1:A:381:TRP:HH2	1:A:685:ILE:HD11	1.67	0.60
1:A:662:LEU:O	1:A:666:SER:HB2	2.03	0.59
1:A:861:ASP:O	1:A:862:GLN:CG	2.52	0.58
1:A:245:ILE:HG22	1:A:245:ILE:O	2.03	0.58
1:A:30:GLU:CD	1:A:39:ARG:HD2	2.24	0.57
1:A:1195:GLY:HA2	1:A:1198:VAL:HG12	1.87	0.57
1:A:30:GLU:O	1:A:30:GLU:HG3	2.04	0.57
1:A:260:TRP:HB2	1:A:267:ALA:HB2	1.87	0.56
1:A:31:CYS:N	1:A:42:CYS:SG	2.79	0.55
1:A:1240:GLY:HA2	1:A:1244:LEU:HD23	1.88	0.55
1:A:30:GLU:OE2	1:A:78:ARG:CG	2.54	0.55
1:A:379:ASP:OD1	1:A:379:ASP:N	2.37	0.55
1:A:1251:ILE:HD12	1:A:1251:ILE:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:GLU:O	1:A:819:ARG:NH1	2.41	0.53
1:A:25:CYS:SG	1:A:26:VAL:N	2.82	0.53
1:A:381:TRP:CH2	1:A:685:ILE:HD11	2.44	0.53
1:A:951:LYS:NZ	1:A:954:SER:OG	2.39	0.53
1:A:1165:VAL:O	1:A:1169:SER:HB3	2.09	0.52
1:A:268:MET:HA	1:A:271:ILE:HG22	1.92	0.51
1:A:714:ARG:NH2	1:A:791:GLU:OE1	2.44	0.51
1:A:972:VAL:HG23	1:A:974:PRO:HD3	1.92	0.51
1:A:942:TRP:HE1	1:A:1036:THR:HG1	1.56	0.51
1:A:1209:GLY:O	1:A:1213:LEU:HB2	2.10	0.51
1:A:116:ARG:NH2	1:A:222:ASN:OD1	2.44	0.50
1:A:773:LEU:O	1:A:777:THR:HG23	2.12	0.50
1:A:462:VAL:HG21	1:A:579:ARG:HB3	1.94	0.49
1:A:1150:ASN:N	1:A:1150:ASN:OD1	2.43	0.49
1:A:285:GLY:O	1:A:289:ALA:HB2	2.12	0.49
1:A:91:LEU:O	1:A:95:SER:HB3	2.13	0.48
1:A:91:LEU:O	1:A:95:SER:CB	2.61	0.48
1:A:198:ASN:HD22	6:A:1420:CLR:H273	1.77	0.47
1:A:109:CYS:SG	1:A:110:GLU:N	2.88	0.47
1:A:691:PRO:O	1:A:695:LEU:HB2	2.14	0.47
4:E:1:NAG:H4	4:E:2:NAG:H2	1.53	0.46
1:A:133:VAL:HG13	1:A:134:THR:HG22	1.96	0.46
1:A:346:CYS:SG	1:A:781:SER:OG	2.74	0.46
1:A:23:GLN:OE1	1:A:119:GLN:NE2	2.47	0.46
1:A:863:SER:C	1:A:865:SER:N	2.70	0.45
1:A:551:ASP:N	1:A:551:ASP:OD1	2.47	0.45
1:A:240:CYS:HB2	1:A:247:CYS:HB3	1.59	0.45
1:A:1145:TRP:CH2	1:A:1227:ARG:HG2	2.52	0.44
1:A:1199:PHE:HB2	1:A:1241:LEU:HD21	1.99	0.44
1:A:163:VAL:HG13	1:A:172:ALA:HB3	2.00	0.44
1:A:476:ASN:ND2	2:C:1:NAG:O6	2.50	0.44
1:A:92:GLN:HE22	1:A:526:THR:HG21	1.83	0.44
1:A:1248:LEU:HD23	1:A:1248:LEU:HA	1.92	0.44
1:A:51:LEU:HD13	1:A:52:PRO:HD2	2.00	0.43
1:A:667:SER:O	1:A:671:SER:OG	2.36	0.43
1:A:483:SER:HB3	1:A:563:ILE:HG23	2.01	0.42
1:A:478:ASN:HD22	1:A:536:THR:HB	1.84	0.42
1:A:391:GLU:OE2	1:A:1059:ARG:NH2	2.52	0.42
1:A:131:ASP:OD2	1:A:136:GLN:N	2.52	0.42
1:A:1085:TYR:O	1:A:1089:GLU:HB2	2.19	0.42
1:A:30:GLU:OE2	1:A:78:ARG:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:GLY:O	1:A:289:ALA:CB	2.68	0.42
1:A:794:ARG:HA	1:A:802:ARG:HA	2.02	0.42
1:A:1185:GLU:HA	1:A:1188:GLU:HG2	2.02	0.42
1:A:672:LEU:O	1:A:676:SER:HB2	2.20	0.42
1:A:860:LEU:HD22	1:A:1150:ASN:HD22	1.85	0.42
1:A:1040:THR:OG1	1:A:1041:TYR:N	2.52	0.42
1:A:86:ASN:HB3	6:A:1420:CLR:H212	2.01	0.41
1:A:958:ARG:HH11	1:A:958:ARG:HD3	1.74	0.41
1:A:1204:LEU:HD23	1:A:1204:LEU:HA	1.92	0.41
1:A:748:LEU:HD12	1:A:748:LEU:HA	1.85	0.41
1:A:968:ASN:OD1	1:A:1008:ASN:ND2	2.54	0.41
1:A:41:ASN:N	1:A:41:ASN:HD22	2.18	0.41
1:A:862:GLN:HG3	1:A:862:GLN:O	2.19	0.41
1:A:357:SER:HG	1:A:778:CYS:HG	1.64	0.41
1:A:817:LEU:HD23	1:A:817:LEU:HA	1.95	0.41
1:A:987:LYS:HE2	1:A:987:LYS:HB3	1.95	0.41
1:A:836:PRO:HA	1:A:839:ILE:HG22	2.03	0.41
1:A:218:GLU:HA	1:A:219:PRO:HD3	1.87	0.40
1:A:466:ASP:OD2	1:A:579:ARG:NH2	2.53	0.40
6:A:1420:CLR:H211	6:A:1420:CLR:H231	1.88	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	A	1188/1311 (91%)	1100 (93%)	80 (7%)	8 (1%)	22 61

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	ASN

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Mol	Chain	Res	Type
1	A	478	ASN
1	A	479	CYS
1	A	474	PRO
1	A	798	PHE
1	A	863	SER
1	A	800	CYS
1	A	797	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1035/1138 (91%)	1000 (97%)	35 (3%)	37 69

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	CYS
1	A	26	VAL
1	A	27	TRP
1	A	51	LEU
1	A	74	CYS
1	A	91	LEU
1	A	119	GLN
1	A	144	LEU
1	A	184	CYS
1	A	185	ASN
1	A	240	CYS
1	A	379	ASP
1	A	382	SER
1	A	436	ASP
1	A	454	THR
1	A	477	THR
1	A	505	VAL
1	A	526	THR
1	A	604	THR

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Mol	Chain	Res	Type
1	A	619	SER
1	A	662	LEU
1	A	676	SER
1	A	690	ILE
1	A	731	VAL
1	A	861	ASP
1	A	862	GLN
1	A	909	CYS
1	A	933	THR
1	A	945	ASP
1	A	950	VAL
1	A	989	ARG
1	A	1072	ASN
1	A	1123	SER
1	A	1145	TRP
1	A	1169	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	41	ASN
1	A	92	GLN
1	A	119	GLN
1	A	145	GLN
1	A	185	ASN
1	A	476	ASN
1	A	701	ASN
1	A	707	GLN
1	A	775	GLN
1	A	906	ASN
1	A	925	ASN
1	A	1016	HIS
1	A	1137	ASN

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](#)

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
2	NAG	B	1	2,1	14,14,15	0.97	1 (7%)	17,19,21	0.74	0
2	NAG	B	2	2	14,14,15	1.27	1 (7%)	17,19,21	0.87	1 (5%)
2	NAG	C	1	2,1	14,14,15	0.72	0	17,19,21	1.49	2 (11%)
2	NAG	C	2	2	14,14,15	0.39	0	17,19,21	1.32	2 (11%)
3	NAG	D	1	1,3	14,14,15	0.90	1 (7%)	17,19,21	0.63	0
3	NAG	D	2	3	14,14,15	0.94	1 (7%)	17,19,21	0.55	0
3	BMA	D	3	3	11,11,12	1.72	3 (27%)	15,15,17	1.14	1 (6%)
4	NAG	E	1	4,1	14,14,15	2.44	1 (7%)	17,19,21	1.71	3 (17%)
4	NAG	E	2	4	14,14,15	0.37	0	17,19,21	1.14	3 (17%)
4	MAN	E	3	4	11,11,12	0.25	0	15,15,17	0.68	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
2	NAG	B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1
2	NAG	C	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	1/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	E	2	4	1/1/5/7	3/6/23/26	0/1/1/1
4	MAN	E	3	4	-	1/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1	NAG	O5-C1	8.71	1.57	1.43
2	B	2	NAG	O5-C1	4.05	1.50	1.43
3	D	3	BMA	C1-C2	3.30	1.59	1.52
3	D	3	BMA	C2-C3	2.95	1.56	1.52
3	D	2	NAG	O5-C1	2.79	1.48	1.43
3	D	1	NAG	O5-C1	2.72	1.48	1.43
3	D	3	BMA	O5-C5	2.71	1.48	1.43
2	B	1	NAG	C1-C2	2.54	1.56	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C2-N2-C7	5.00	130.02	122.90
4	E	1	NAG	C1-O5-C5	4.74	118.62	112.19
4	E	1	NAG	O5-C5-C6	3.62	112.87	107.20
2	C	2	NAG	O5-C1-C2	3.34	116.56	111.29
2	C	2	NAG	C1-O5-C5	-3.20	107.85	112.19
4	E	1	NAG	C6-C5-C4	3.15	120.38	113.00
3	D	3	BMA	C1-O5-C5	2.98	116.22	112.19
2	B	2	NAG	C2-N2-C7	2.81	126.90	122.90
4	E	2	NAG	C3-C4-C5	2.72	115.08	110.24
2	C	1	NAG	C1-C2-N2	2.49	114.74	110.49
4	E	2	NAG	C4-C3-C2	2.38	114.51	111.02
4	E	2	NAG	O5-C1-C2	-2.38	107.53	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	2	NAG	C1

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	2	NAG	C3-C2-N2-C7

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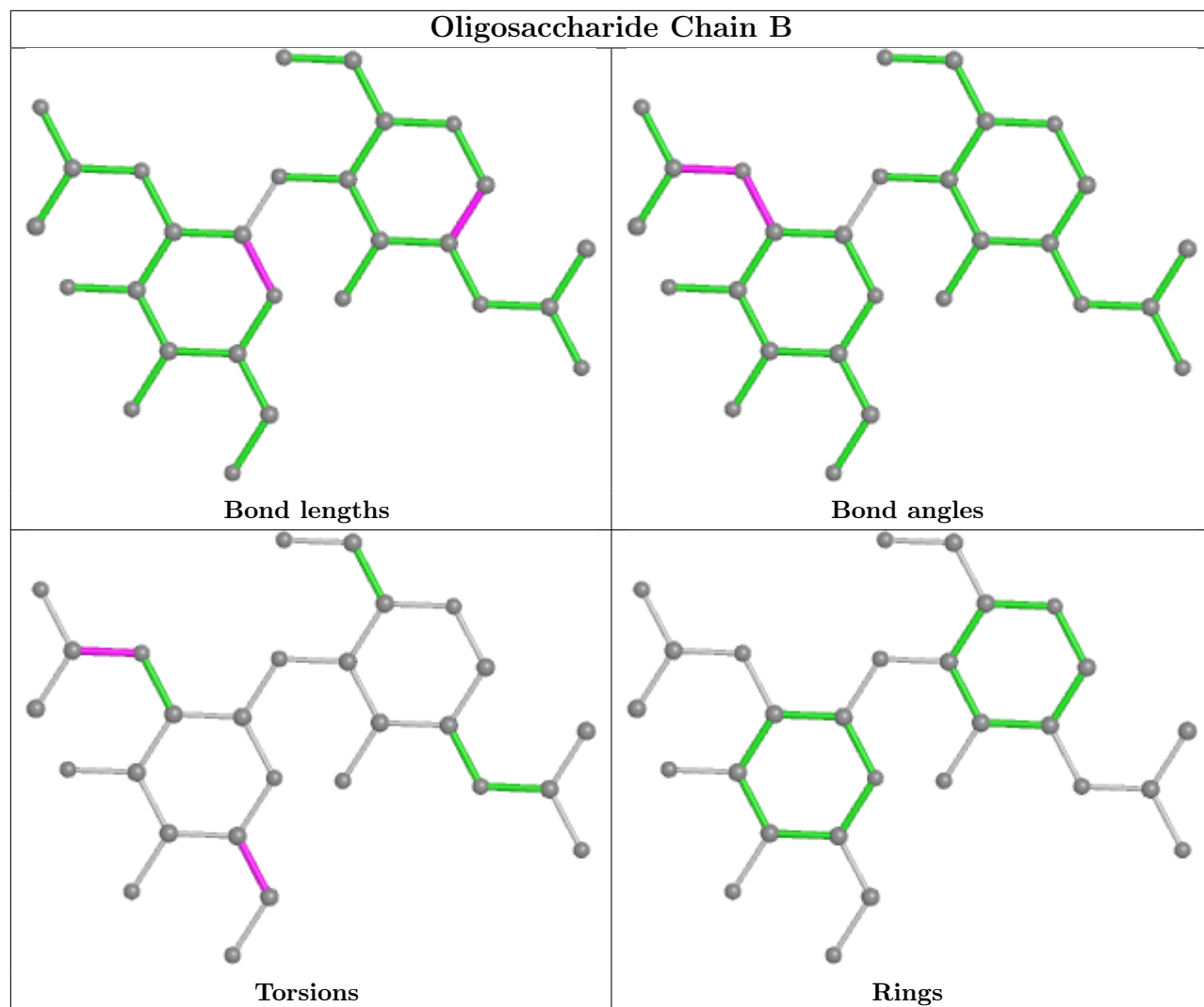
Mol	Chain	Res	Type	Atoms
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
2	B	2	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	C	1	NAG	C4-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
4	E	3	MAN	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6
2	C	1	NAG	C3-C2-N2-C7

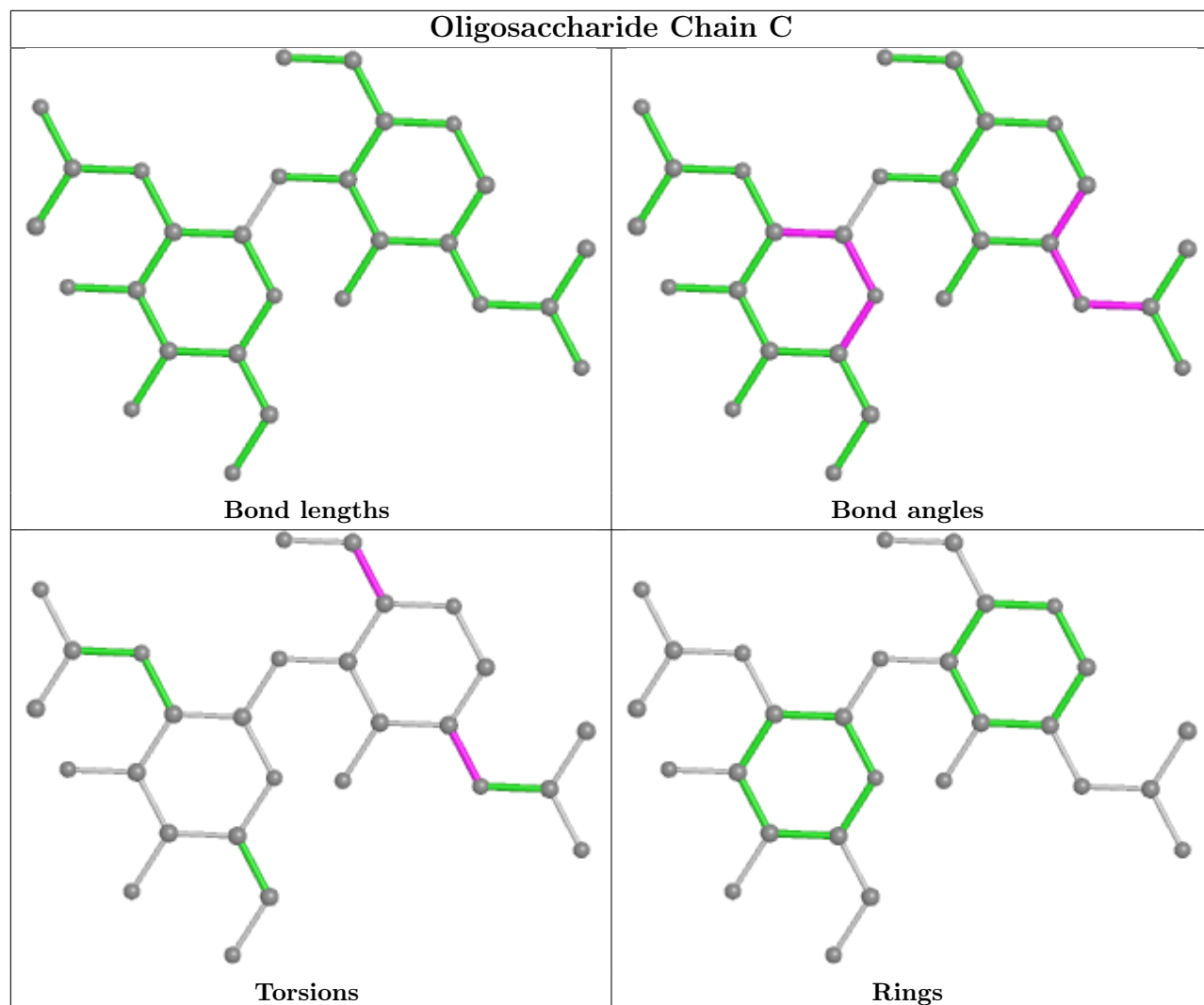
There are no ring outliers.

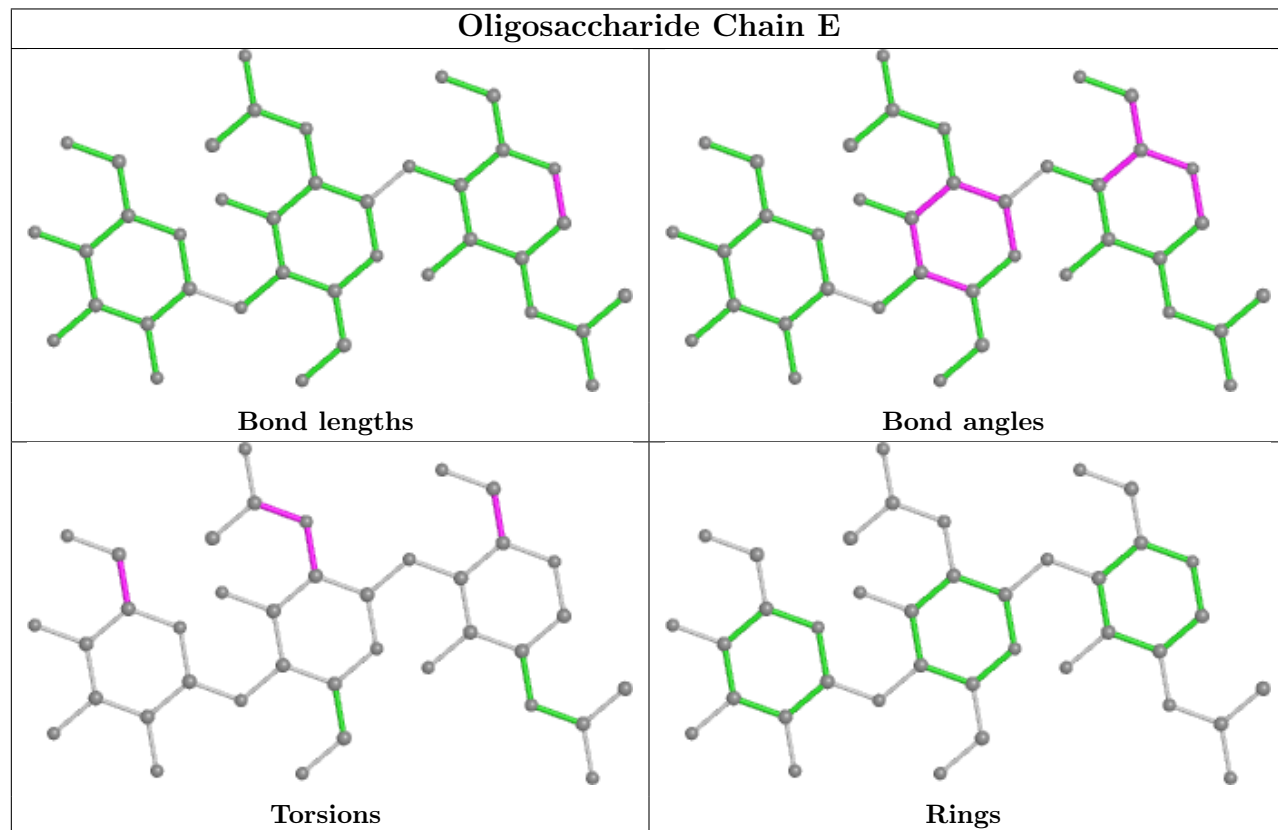
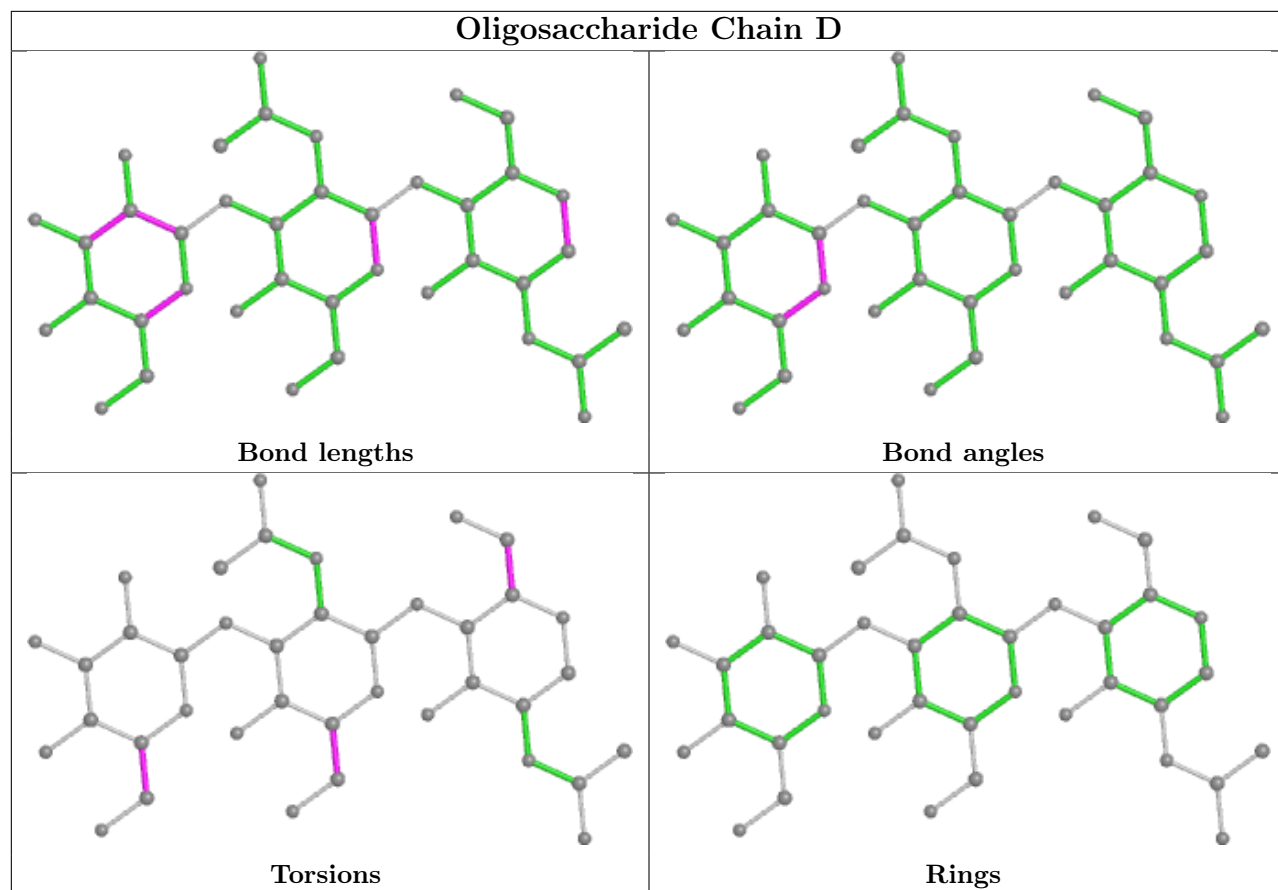
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0
4	E	1	NAG	1	0
4	E	2	NAG	2	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

10 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
5	NAG	A	1418	1	14,14,15	1.15	1 (7%)	17,19,21	0.91	1 (5%)
5	NAG	A	1417	1	14,14,15	0.98	1 (7%)	17,19,21	0.56	0
5	NAG	A	1412	1	14,14,15	1.11	1 (7%)	17,19,21	2.99	4 (23%)
5	NAG	A	1408	1	14,14,15	1.89	3 (21%)	17,19,21	1.26	1 (5%)
6	CLR	A	1420	-	31,31,31	0.92	1 (3%)	48,48,48	1.59	6 (12%)
5	NAG	A	1413	1	14,14,15	2.26	2 (14%)	17,19,21	1.58	3 (17%)
5	NAG	A	1403	1	14,14,15	0.99	1 (7%)	17,19,21	0.90	1 (5%)
5	NAG	A	1405	1	14,14,15	1.34	2 (14%)	17,19,21	0.42	0
5	NAG	A	1404	1	14,14,15	1.26	2 (14%)	17,19,21	2.95	3 (17%)
5	NAG	A	1419	1	14,14,15	0.95	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
5	NAG	A	1418	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1417	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1412	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1408	1	-	1/6/23/26	0/1/1/1
6	CLR	A	1420	-	-	3/10/68/68	0/4/4/4
5	NAG	A	1413	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1403	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1405	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1404	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1419	1	-	4/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1413	NAG	O5-C1	8.02	1.56	1.43
5	A	1408	NAG	O5-C1	5.46	1.52	1.43
5	A	1405	NAG	O5-C1	4.18	1.50	1.43
5	A	1418	NAG	O5-C1	3.86	1.49	1.43
5	A	1408	NAG	C1-C2	3.46	1.57	1.52
5	A	1403	NAG	O5-C1	3.22	1.48	1.43
5	A	1417	NAG	O5-C1	3.08	1.48	1.43
5	A	1419	NAG	O5-C1	2.95	1.48	1.43
5	A	1404	NAG	O5-C1	2.57	1.47	1.43
5	A	1404	NAG	C1-C2	2.55	1.56	1.52
6	A	1420	CLR	C20-C17	2.53	1.58	1.54
5	A	1412	NAG	C1-C2	2.41	1.55	1.52
5	A	1405	NAG	C1-C2	2.34	1.55	1.52
5	A	1408	NAG	C3-C2	2.27	1.57	1.52
5	A	1413	NAG	C1-C2	2.11	1.55	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1404	NAG	C2-N2-C7	10.41	137.72	122.90
5	A	1412	NAG	C2-N2-C7	10.20	137.43	122.90
5	A	1412	NAG	C1-C2-N2	5.28	119.50	110.49
5	A	1413	NAG	C1-O5-C5	5.10	119.10	112.19
5	A	1404	NAG	C1-C2-N2	4.91	118.87	110.49
6	A	1420	CLR	C18-C13-C17	-4.86	102.65	111.71
6	A	1420	CLR	C17-C13-C14	4.49	105.39	100.07
5	A	1408	NAG	C1-O5-C5	4.10	117.75	112.19
6	A	1420	CLR	C13-C17-C20	3.87	125.55	119.49
5	A	1419	NAG	C2-N2-C7	3.10	127.31	122.90
5	A	1418	NAG	C2-N2-C7	2.96	127.12	122.90
5	A	1404	NAG	C8-C7-N2	2.92	121.03	116.10
5	A	1413	NAG	O5-C5-C6	2.91	111.77	107.20
5	A	1412	NAG	C8-C7-N2	2.83	120.89	116.10
5	A	1403	NAG	C2-N2-C7	2.73	126.79	122.90
6	A	1420	CLR	C4-C5-C6	-2.47	117.05	120.61
6	A	1420	CLR	C15-C16-C17	2.20	109.50	105.13
5	A	1412	NAG	C1-O5-C5	2.18	115.14	112.19
5	A	1413	NAG	C6-C5-C4	2.08	117.88	113.00
6	A	1420	CLR	C22-C20-C17	2.06	114.53	110.28

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1417	NAG	O5-C5-C6-O6
5	A	1413	NAG	O5-C5-C6-O6
5	A	1413	NAG	C4-C5-C6-O6
5	A	1417	NAG	C4-C5-C6-O6
6	A	1420	CLR	C21-C20-C22-C23
5	A	1419	NAG	O5-C5-C6-O6
5	A	1403	NAG	C8-C7-N2-C2
5	A	1403	NAG	O7-C7-N2-C2
5	A	1404	NAG	C8-C7-N2-C2
5	A	1404	NAG	O7-C7-N2-C2
5	A	1412	NAG	C8-C7-N2-C2
5	A	1412	NAG	O7-C7-N2-C2
5	A	1418	NAG	C8-C7-N2-C2
5	A	1418	NAG	O7-C7-N2-C2
5	A	1419	NAG	C8-C7-N2-C2
5	A	1419	NAG	O7-C7-N2-C2
5	A	1419	NAG	C4-C5-C6-O6
6	A	1420	CLR	C22-C23-C24-C25
5	A	1408	NAG	O5-C5-C6-O6
5	A	1404	NAG	O5-C5-C6-O6
6	A	1420	CLR	C20-C22-C23-C24
5	A	1418	NAG	C4-C5-C6-O6
5	A	1418	NAG	O5-C5-C6-O6
5	A	1405	NAG	C4-C5-C6-O6
5	A	1404	NAG	C3-C2-N2-C7
5	A	1412	NAG	C3-C2-N2-C7

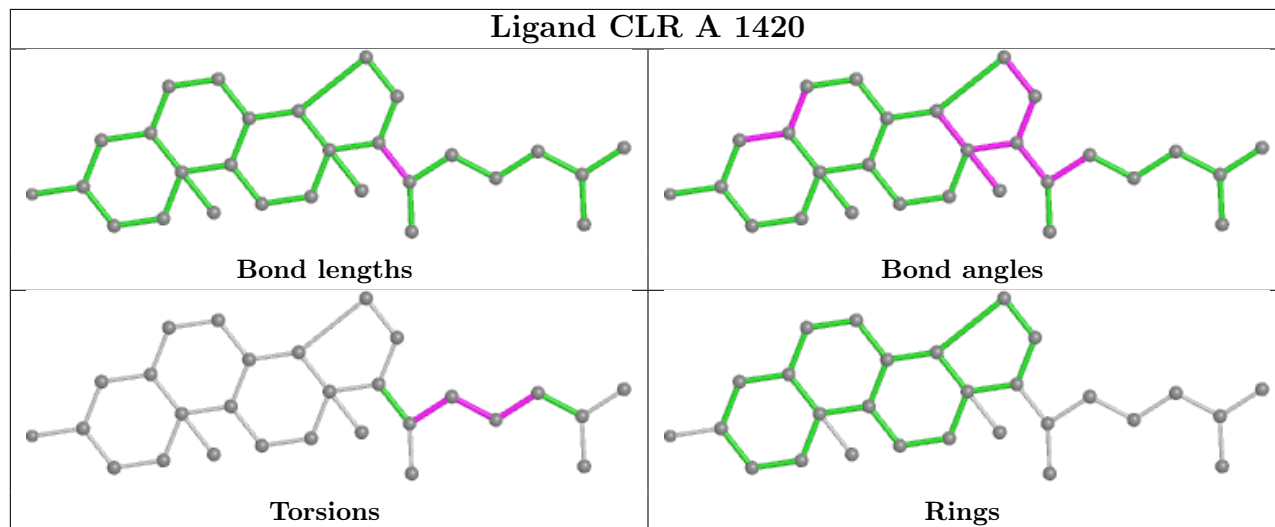
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1420	CLR	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

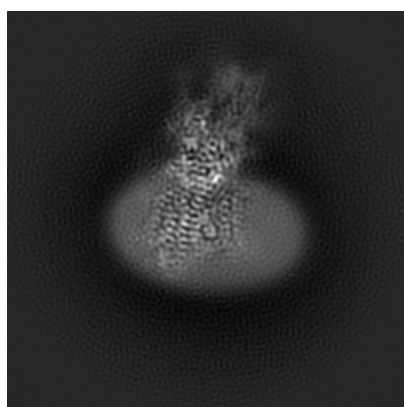
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21545. These allow visual inspection of the internal detail of the map and identification of artifacts.

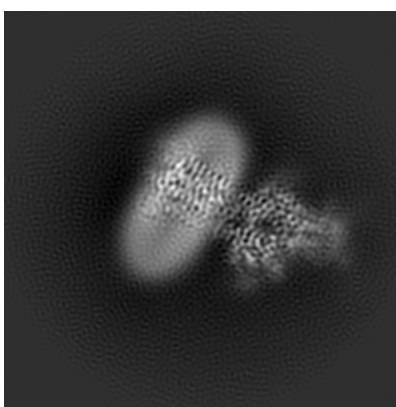
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

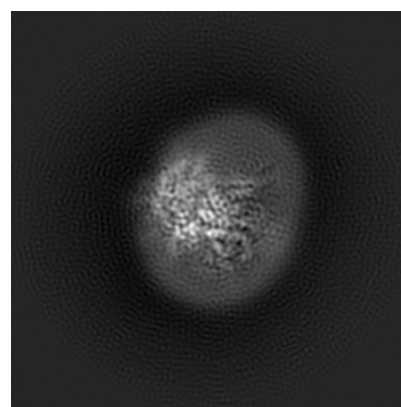
6.1.1 Primary map



X



Y

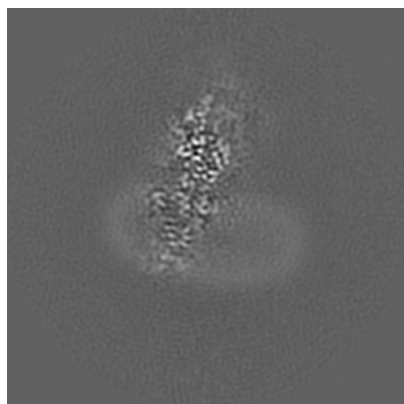


Z

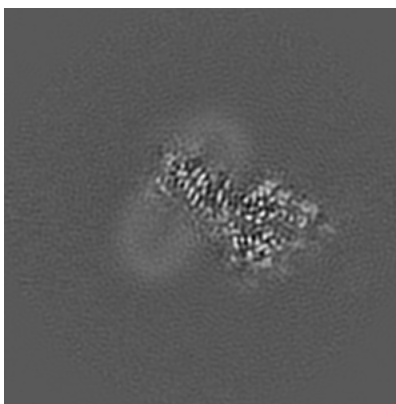
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

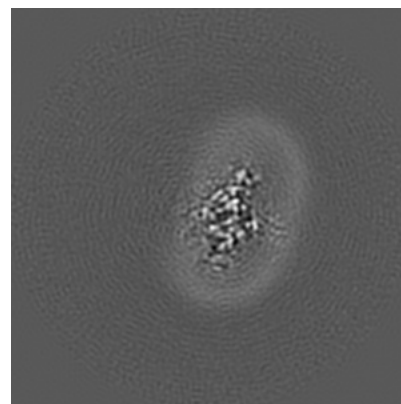
6.2.1 Primary map



X Index: 120



Y Index: 120

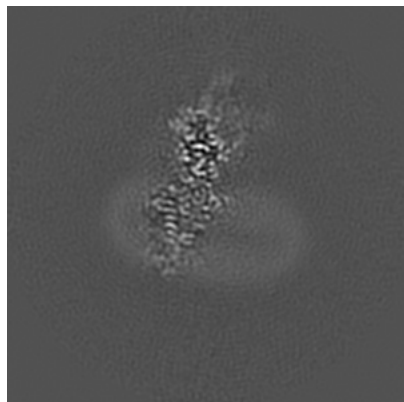


Z Index: 120

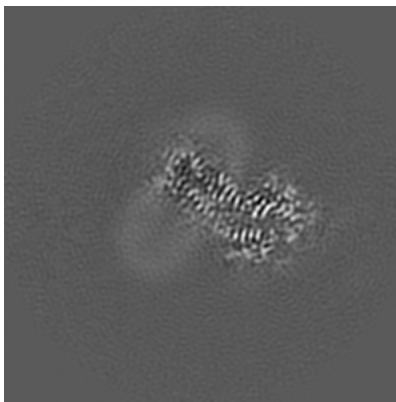
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

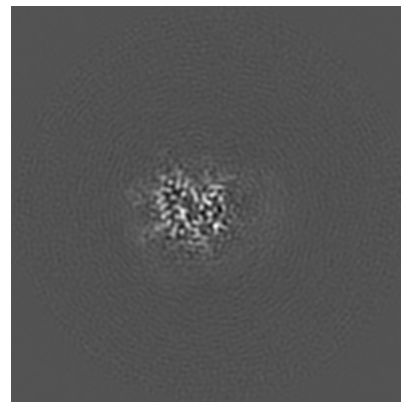
6.3.1 Primary map



X Index: 122



Y Index: 117



Z Index: 148

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 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

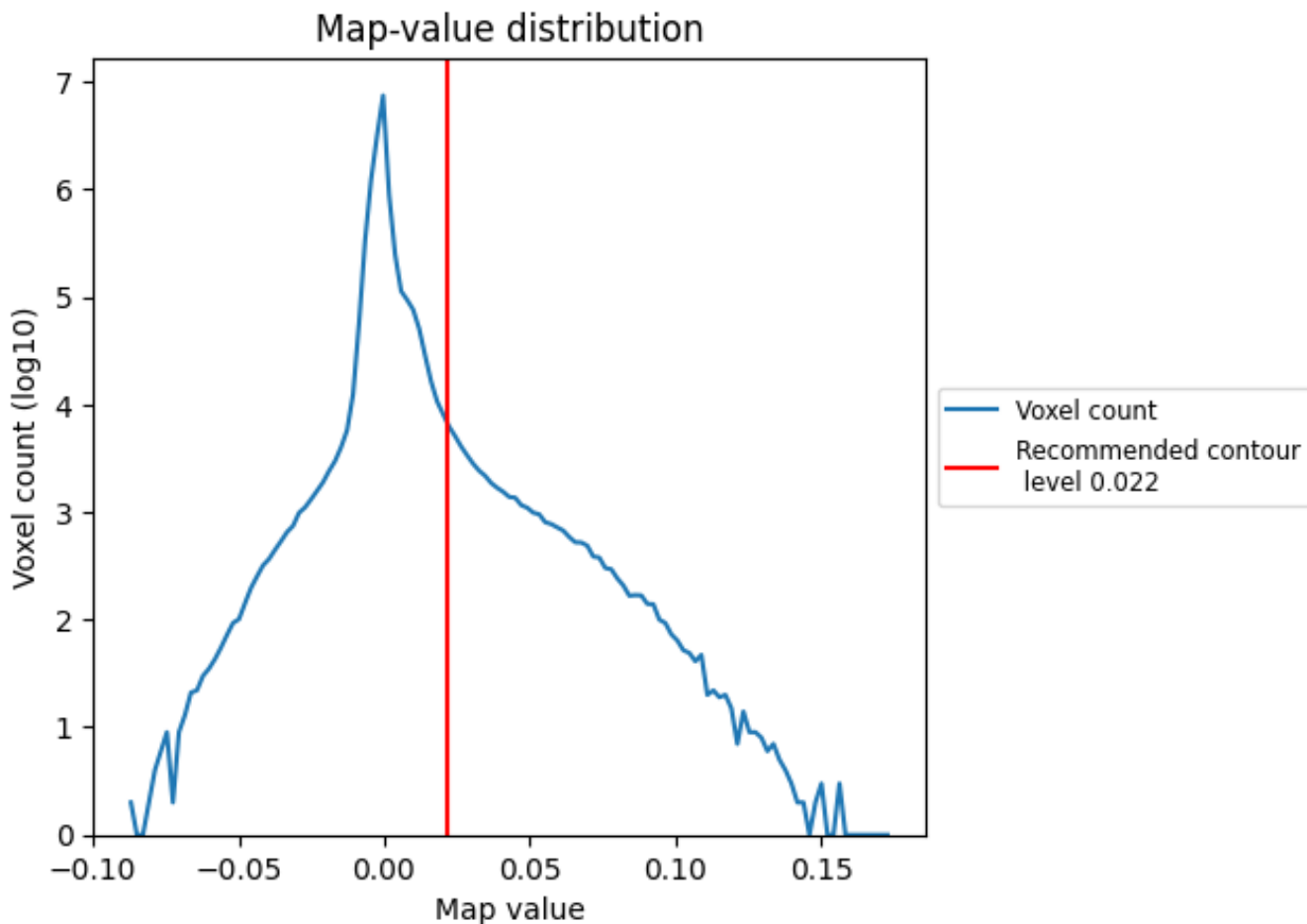
6.5 Mask visualisation

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

7 Map analysis [i](#)

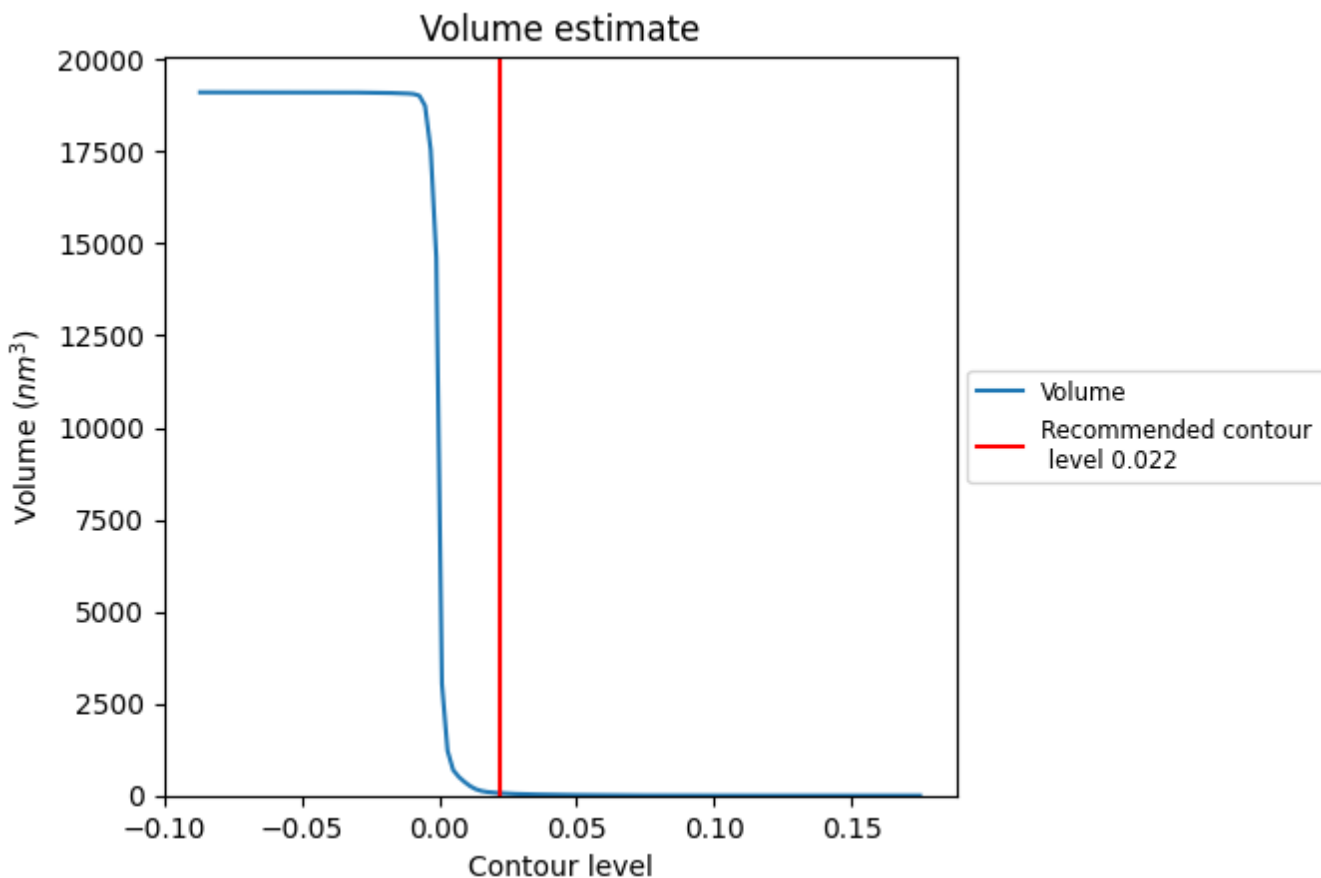
This section contains the results of statistical analysis of the map.

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.

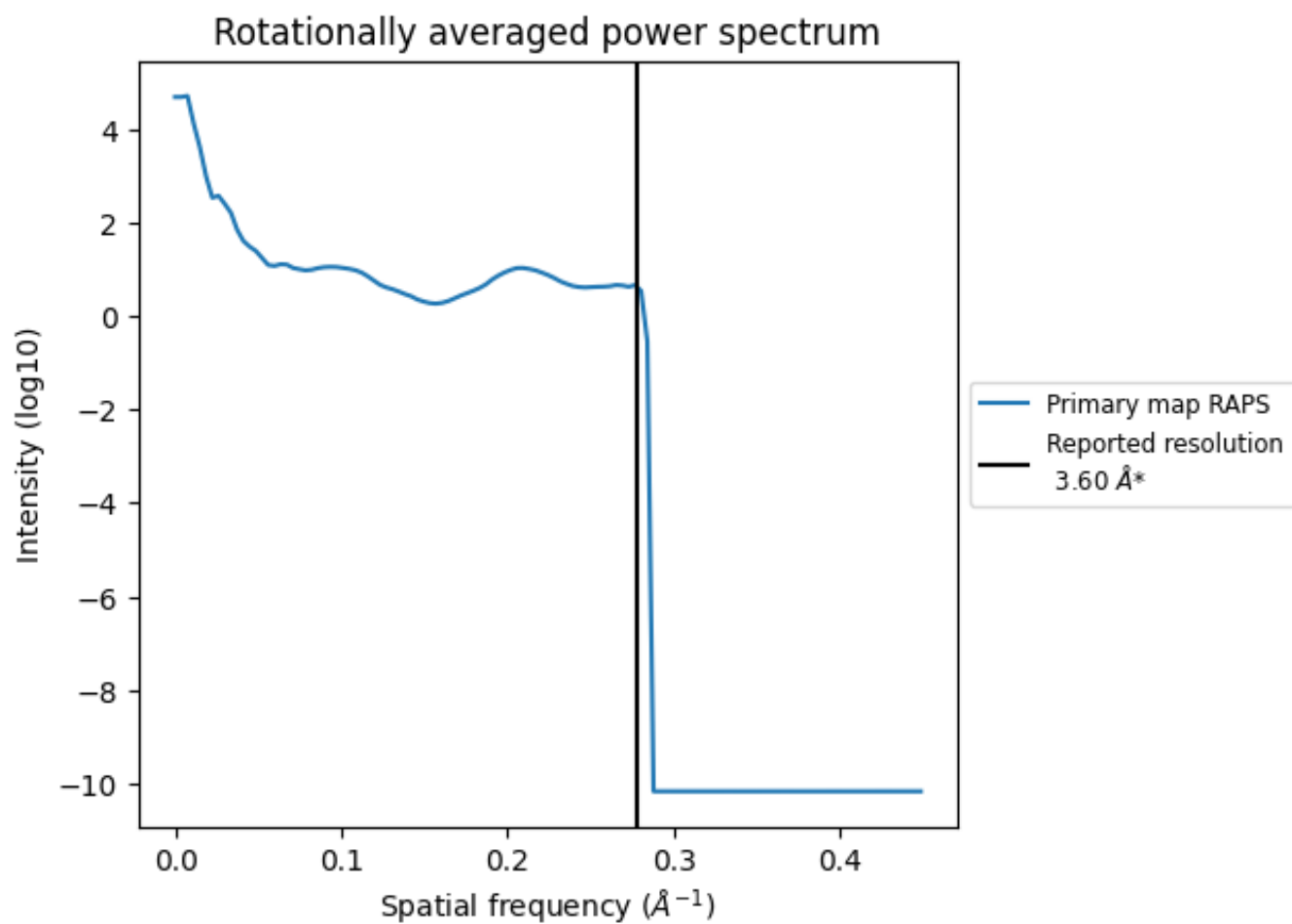
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 66 nm^3 ; this corresponds to an approximate mass of 60 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 0.278 Å⁻¹

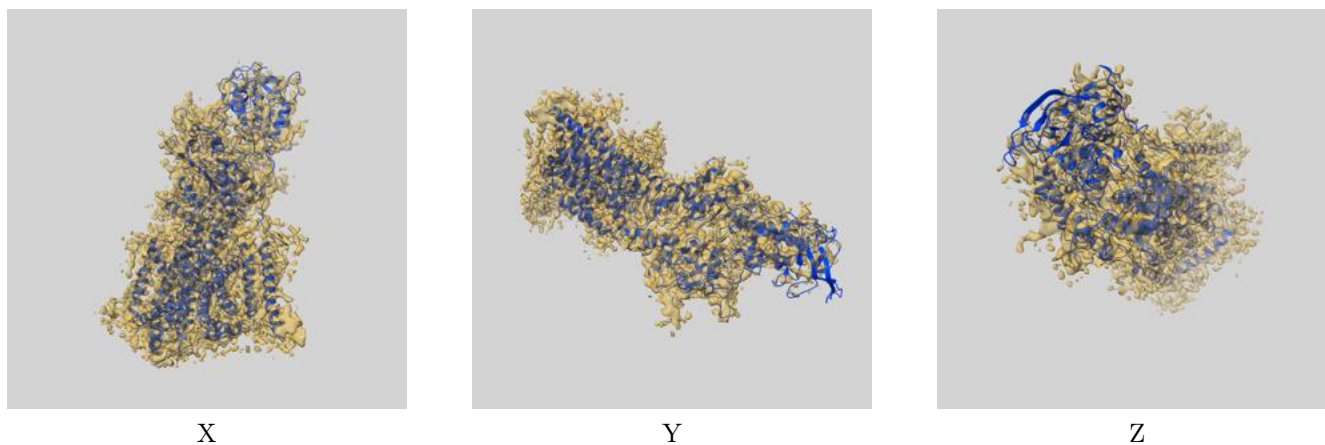
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

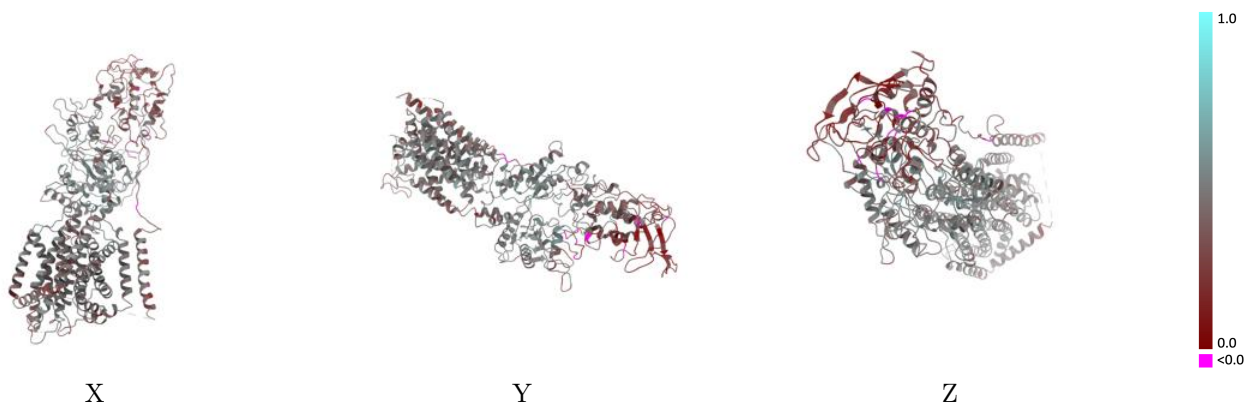
This section contains information regarding the fit between EMDB map EMD-21545 and PDB model 6W5R. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



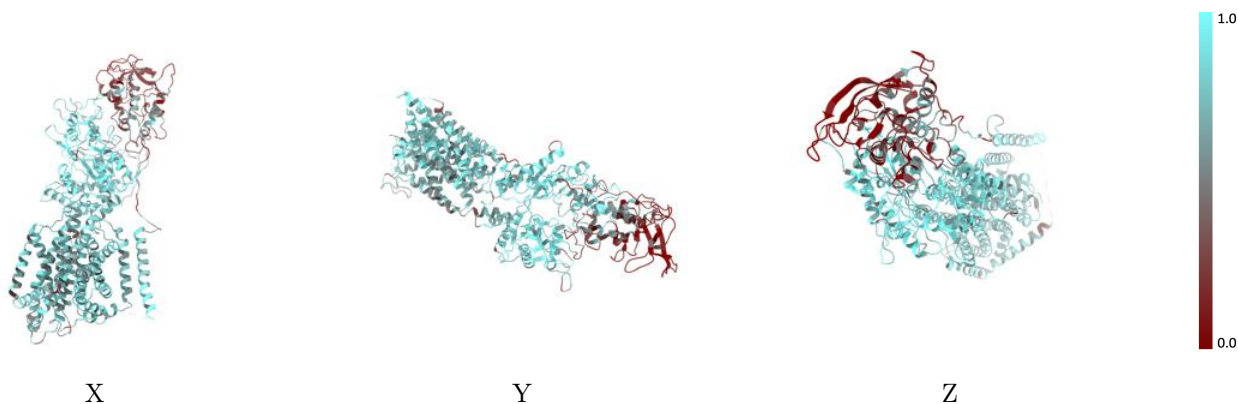
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



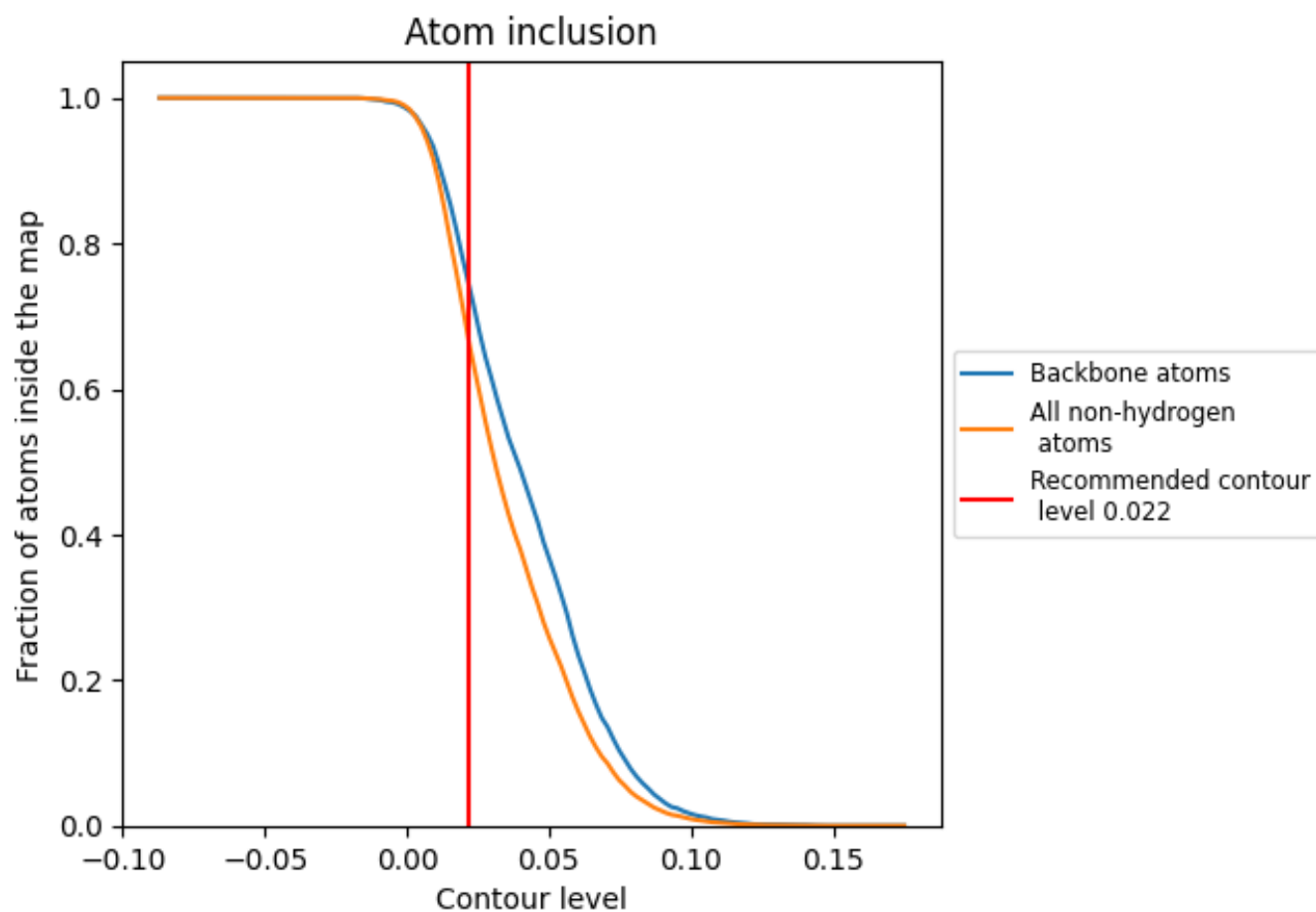
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).













9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 66% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6613	 0.4170
A	 0.6649	 0.4190
B	 0.1071	 0.0900
C	 0.7143	 0.4500
D	 0.7179	 0.4500
E	 0.1026	 0.3080

