Full wwPDB EM Validation Report

Aug 18, 2022 – 04:21 pm BST

PDB ID	:	7Z14
EMDB ID	:	EMD-14440
Title	:	Cryo-EM structure of Torpedo nicotinic acetylcholine receptor in complex with a short-chain neurotoxin.
Authors	:	Nys, M.A.E.M.; Zarkadas, E.; Ulens, C.; Nury, H.
Deposited on	:	2022-02-24
Resolution	:	3.15 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

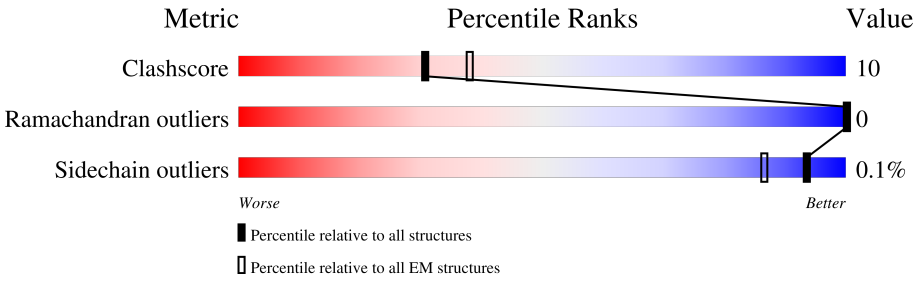
EMDB validation analysis	:	0.0.1.dev8
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.15 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	437	60% 21% 19%
1	D	437	56% 19% 25%
2	B	469	61% 18% 20%
3	C	501	55% 19% 25%
4	E	489	56% 18% 26%
5	F	60	73% 27%
5	G	60	72% 28%
6	H	9	33% 67%

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Mol	Chain	Length	Quality of chain
6	K	9	33% 67%
7	I	2	100%
7	J	2	100%
8	L	5	40% 60%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15856 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 Acetylcholine receptor subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	355	Total	C	N	O	S	0	0
			2892	1907	462	503	20		
1	D	328	Total	C	N	O	S	0	0
			2669	1759	424	468	18		

- Molecule 2 is a protein called Acetylcholine receptor subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	373	Total	C	N	O	S	0	0
			3018	1979	482	543	14		

- Molecule 3 is a protein called Acetylcholine receptor subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	376	Total	C	N	O	S	0	0
			3046	1991	490	550	15		

- Molecule 4 is a protein called Acetylcholine receptor subunit gamma.

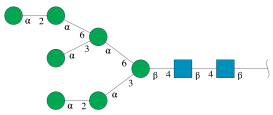
Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	361	Total	C	N	O	S	0	0
			2945	1941	465	529	10		

- Molecule 5 is a protein called Consensus short-chain short-chain alpha-neurotoxin ScNtx.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	60	Total	C	N	O	S	0	0
			471	284	90	88	9		
5	G	60	Total	C	N	O	S	0	0
			471	284	90	88	9		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyr

anose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deox y-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

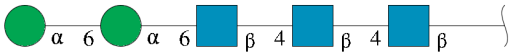


Mol	Chain	Residues	Atoms				AltConf	Trace
6	H	9	Total	C	N	O	0	0
			105	58	2	45		
6	K	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.

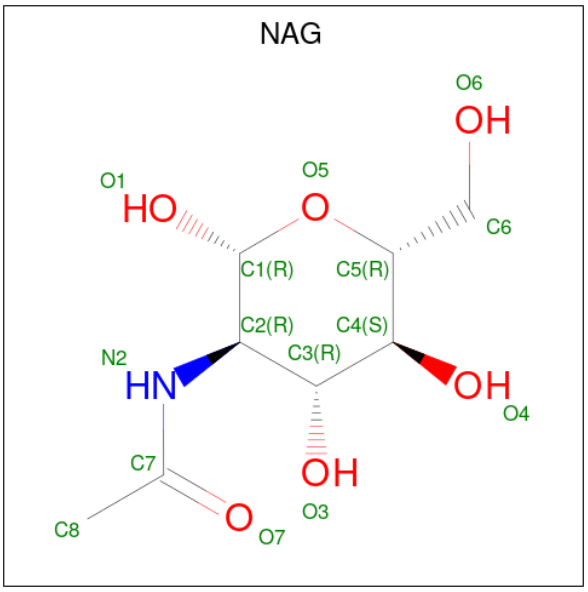
Mol	Chain	Residues	Atoms				AltConf	Trace
7	I	2	Total	C	N	O	0	0
			28	16	2	10		
7	J	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyran ose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glu copyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
8	L	5	Total	C	N	O	0	0
			64	36	3	25		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



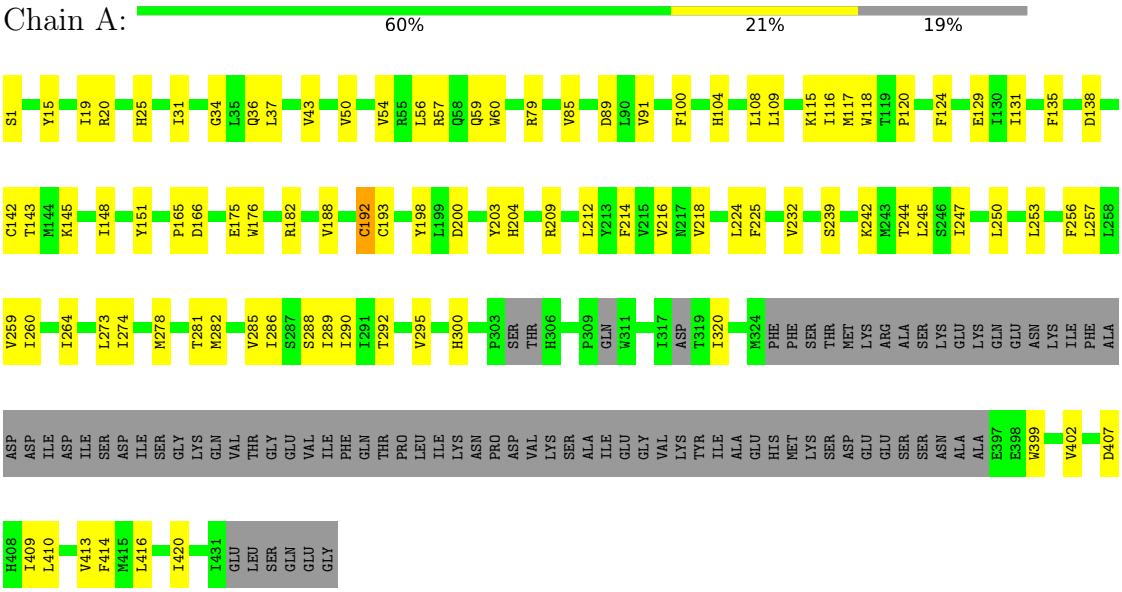
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	C	1	14	8	1	5	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

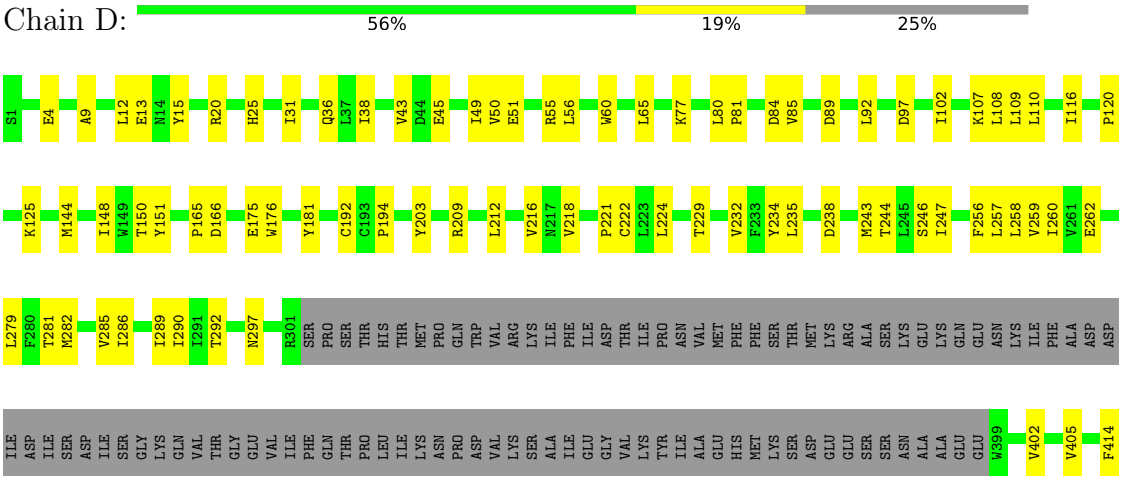
• Molecule 1: Acetylcholine receptor subunit alpha

Chain A:



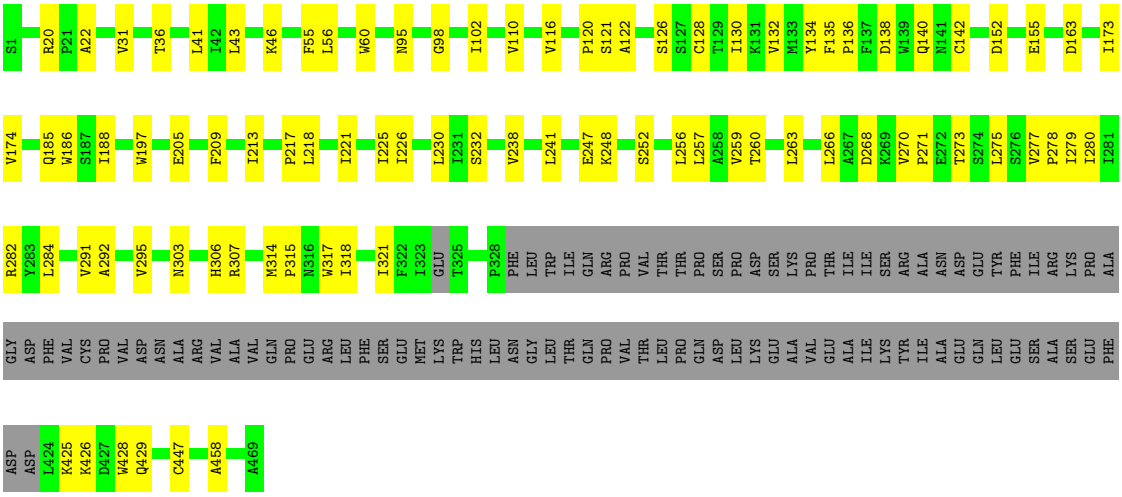
• Molecule 1: Acetylcholine receptor subunit alpha

Chain D:



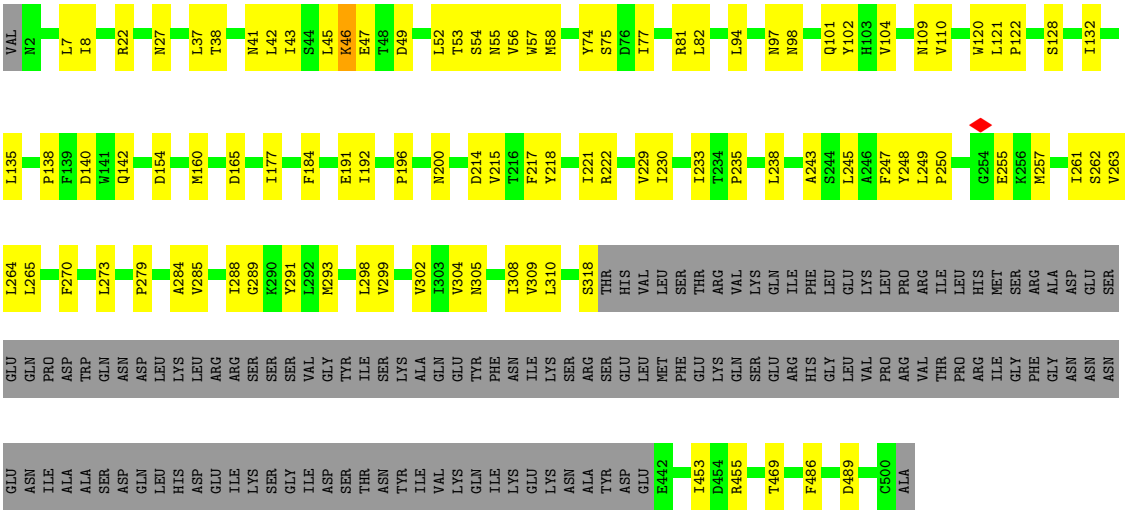
• Molecule 2: Acetylcholine receptor subunit beta

Chain B:



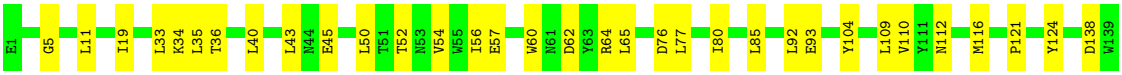
• Molecule 3: Acetylcholine receptor subunit delta

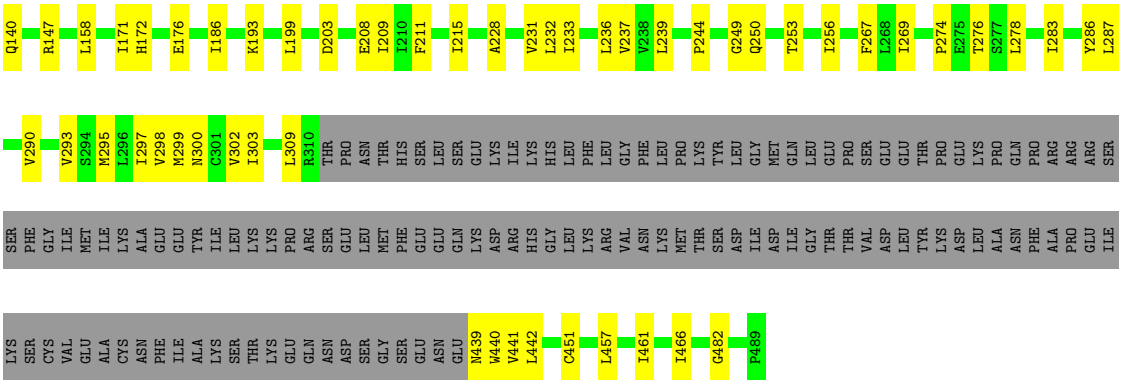
Chain C:



• Molecule 4: Acetylcholine receptor subunit gamma

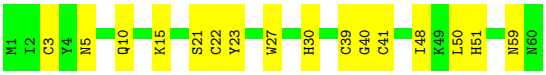
Chain E:





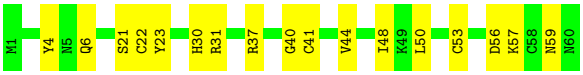
• Molecule 5: Consensus short-chain short-chain alpha-neurotoxin ScNtx

Chain F:



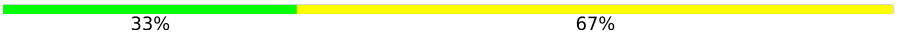
• Molecule 5: Consensus short-chain short-chain alpha-neurotoxin ScNtx

Chain G:



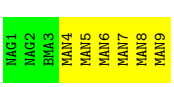
• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



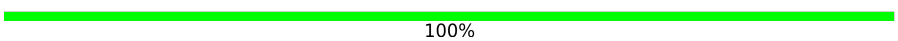
• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

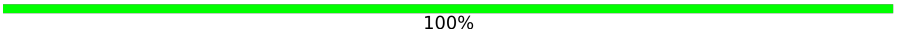


• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

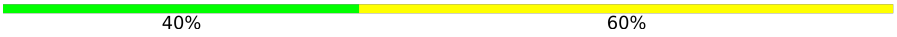
Chain I:



• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 

• Molecule 8: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L: 

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	26581	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.778	Depositor
Minimum map value	-1.041	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.115	Depositor
Map size (Å)	293.12, 293.12, 293.12	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.145, 1.145, 1.145	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	A	0.37	2/2970 (0.1%)	0.60	3/4052 (0.1%)
1	D	0.27	0/2742	0.50	0/3746
2	B	0.25	0/3098	0.48	0/4233
3	C	0.25	0/3135	0.47	0/4288
4	E	0.26	0/3024	0.47	0/4133
5	F	0.25	0/480	0.56	0/643
5	G	0.24	0/480	0.59	0/643
All	All	0.28	2/15929 (0.0%)	0.51	3/21738 (0.0%)

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	1
1	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	192	CYS	CB-SG	-10.84	1.63	1.82
1	A	193	CYS	CB-SG	9.65	1.98	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	192	CYS	CA-CB-SG	18.41	147.14	114.00
1	A	193	CYS	CA-CB-SG	7.27	127.08	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	192	CYS	CB-CA-C	-6.53	97.35	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	192	CYS	Peptide
1	D	192	CYS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2892	0	2935	65	0
1	D	2669	0	2707	72	0
2	B	3018	0	3045	59	0
3	C	3046	0	3007	75	0
4	E	2945	0	2954	61	0
5	F	471	0	463	11	0
5	G	471	0	463	11	0
6	H	105	0	88	0	0
6	K	105	0	88	0	0
7	I	28	0	25	0	0
7	J	28	0	25	0	0
8	L	64	0	55	1	0
9	C	14	0	13	0	0
All	All	15856	0	15868	311	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 10.

All (311) 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:D:229:THR:HG21	1:D:285:VAL:HG22	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:243:ALA:HB2	3:C:263:VAL:HG11	1.62	0.82
4:E:147:ARG:NH2	4:E:208:GLU:OE1	2.14	0.79
2:B:257:LEU:HD22	3:C:265:LEU:HD11	1.65	0.79
3:C:81:ARG:HB3	3:C:109:ASN:HD21	1.49	0.78
3:C:248:TYR:O	1:D:297:ASN:ND2	2.13	0.77
2:B:102:ILE:HG21	2:B:120:PRO:HB2	1.69	0.74
2:B:425:LYS:HG2	2:B:429:GLN:HE22	1.53	0.73
4:E:300:ASN:ND2	4:E:451:CYS:SG	2.59	0.73
3:C:230:ILE:HD12	1:D:279:LEU:HD11	1.71	0.72
2:B:218:LEU:HD21	3:C:285:VAL:HG22	1.71	0.71
1:A:320:ILE:HG21	1:A:409:ILE:HD11	1.73	0.70
4:E:199:LEU:HD21	4:E:203:ASP:HB2	1.72	0.70
1:A:109:LEU:HB3	1:A:117:MET:HB3	1.72	0.70
4:E:33:LEU:HD12	4:E:56:ILE:HD11	1.73	0.70
4:E:482:GLY:HA3	8:L:3:NAG:H81	1.74	0.70
1:A:239:SER:OG	2:B:306:HIS:NE2	2.24	0.69
2:B:277:VAL:O	2:B:282:ARG:NH2	2.25	0.69
1:D:194:PRO:O	5:F:10:GLN:NE2	2.25	0.69
1:A:290:ILE:HG13	4:E:239:LEU:HD11	1.74	0.69
2:B:110:VAL:HG12	2:B:116:VAL:HG22	1.75	0.67
2:B:252:SER:HB3	2:B:295:VAL:HG22	1.77	0.67
1:D:246:SER:HB3	1:D:289:ILE:HD13	1.77	0.67
2:B:128:CYS:HB2	2:B:142:CYS:HA	1.76	0.66
3:C:138:PRO:HD3	3:C:288:ILE:HD11	1.75	0.66
4:E:43:LEU:HD12	4:E:50:LEU:HD12	1.77	0.66
1:A:129:GLU:H	1:A:142:CYS:HB3	1.60	0.66
3:C:8:ILE:HD12	3:C:82:LEU:HD21	1.78	0.66
5:F:41:CYS:HB2	5:F:50:LEU:HD21	1.77	0.65
3:C:43:ILE:HB	3:C:53:THR:HG23	1.77	0.64
1:A:43:VAL:HG22	1:A:50:VAL:HG23	1.79	0.64
2:B:173:ILE:HD11	2:B:209:PHE:HB3	1.80	0.64
4:E:40:LEU:HA	4:E:52:THR:HG22	1.79	0.64
4:E:171:ILE:HD11	4:E:211:PHE:HB3	1.80	0.64
1:D:414:PHE:HA	1:D:417:ILE:HG12	1.80	0.63
1:D:45:GLU:OE2	1:D:209:ARG:NH2	2.32	0.62
4:E:33:LEU:HD21	4:E:209:ILE:HG13	1.81	0.61
3:C:45:LEU:HD13	3:C:221:ILE:HD11	1.82	0.61
1:D:20:ARG:NH2	1:D:25:HIS:O	2.33	0.61
2:B:136:PRO:HD3	2:B:280:ILE:HB	1.83	0.61
2:B:102:ILE:HG23	2:B:122:ALA:HB2	1.83	0.60
1:A:91:VAL:HG13	1:A:100:PHE:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:GLU:HG3	1:D:125:LYS:HG2	1.83	0.60
4:E:138:ASP:OD2	4:E:140:GLN:NE2	2.34	0.60
4:E:35:LEU:HD11	4:E:54:VAL:HB	1.83	0.59
1:D:282:MET:HE3	1:D:286:ILE:HD11	1.84	0.59
1:D:285:VAL:O	1:D:289:ILE:HG12	2.03	0.58
2:B:263:LEU:HD23	2:B:284:LEU:HD13	1.85	0.58
3:C:249:LEU:HD12	3:C:250:PRO:HD2	1.83	0.58
3:C:140:ASP:OD2	3:C:142:GLN:NE2	2.36	0.58
3:C:196:PRO:HG2	3:C:218:TYR:HB2	1.85	0.58
3:C:97:ASN:HA	3:C:128:SER:HA	1.85	0.58
2:B:197:TRP:NE1	2:B:205:GLU:OE1	2.37	0.58
1:D:224:LEU:HD11	4:E:295:MET:HG3	1.87	0.57
2:B:132:VAL:HG11	2:B:271:PRO:HG3	1.85	0.57
2:B:241:LEU:O	2:B:248:LYS:NZ	2.28	0.57
1:D:281:THR:O	1:D:285:VAL:HG23	2.04	0.57
4:E:440:TRP:NE1	4:E:442:LEU:HD13	2.20	0.57
3:C:81:ARG:HB3	3:C:109:ASN:ND2	2.19	0.56
1:D:65:LEU:HD13	1:D:110:LEU:HD11	1.87	0.56
1:D:247:ILE:HD13	1:D:289:ILE:HD12	1.87	0.56
2:B:188:ILE:HA	2:B:213:ILE:HG22	1.86	0.56
5:G:56:ASP:OD1	5:G:57:LYS:HG2	2.05	0.56
3:C:41:ASN:HA	3:C:184:PHE:HE1	1.71	0.56
2:B:232:SER:OG	2:B:447:CYS:SG	2.60	0.56
3:C:82:LEU:O	3:C:110:VAL:HG22	2.05	0.56
2:B:217:PRO:HG2	2:B:221:ILE:HD11	1.88	0.55
1:A:256:PHE:HA	1:A:259:VAL:HG12	1.87	0.55
5:G:44:VAL:HG11	5:G:50:LEU:HD21	1.87	0.55
1:A:410:LEU:HA	1:A:413:VAL:HG12	1.88	0.55
3:C:38:THR:HB	3:C:57:TRP:HB2	1.87	0.55
5:G:23:TYR:HB3	5:G:41:CYS:HB3	1.88	0.55
1:A:286:ILE:O	1:A:290:ILE:HD12	2.07	0.55
5:F:5:ASN:HD22	5:F:15:LYS:HD3	1.71	0.55
5:F:50:LEU:HD23	5:F:51:HIS:N	2.22	0.55
2:B:46:LYS:NZ	2:B:268:ASP:O	2.35	0.55
1:A:242:LYS:HE3	1:A:292:THR:HG23	1.89	0.55
2:B:41:LEU:HD21	3:C:98:ASN:HA	1.89	0.55
1:A:15:TYR:HE2	1:A:85:VAL:HA	1.72	0.54
2:B:36:THR:OG1	2:B:55:PHE:HB2	2.08	0.54
1:A:56:LEU:HD23	1:A:124:PHE:HZ	1.73	0.54
4:E:244:PRO:HG2	4:E:249:GLY:HA2	1.89	0.54
1:A:36:GLN:HG2	1:A:166:ASP:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:ILE:HD13	1:D:120:PRO:HG2	1.90	0.54
2:B:134:TYR:HA	2:B:279:ILE:HG12	1.90	0.54
1:D:38:ILE:HD11	1:D:55:ARG:HE	1.72	0.54
4:E:93:GLU:HG3	4:E:147:ARG:HH11	1.72	0.54
4:E:36:THR:HG22	4:E:172:HIS:HB3	1.89	0.53
1:D:417:ILE:HA	1:D:420:ILE:HG12	1.89	0.53
4:E:60:TRP:CZ3	4:E:62:ASP:HB2	2.42	0.53
4:E:92:LEU:HD22	4:E:124:TYR:HB3	1.90	0.53
2:B:247:GLU:CD	3:C:257:MET:HB2	2.29	0.53
1:D:262:GLU:HG2	4:E:267:PHE:HE1	1.74	0.53
1:A:143:THR:HG22	1:A:204:HIS:HB3	1.90	0.53
2:B:135:PHE:HB3	2:B:278:PRO:HB3	1.91	0.53
5:F:21:SER:O	5:F:40:GLY:N	2.38	0.53
2:B:43:LEU:HD13	2:B:213:ILE:HD11	1.91	0.53
4:E:286:TYR:HB2	4:E:466:ILE:HG21	1.90	0.52
3:C:200:ASN:HB2	3:C:214:ASP:HB3	1.91	0.52
3:C:264:LEU:HD12	3:C:299:VAL:HG12	1.90	0.52
4:E:299:MET:O	4:E:303:ILE:HD12	2.09	0.52
1:D:238:ASP:HB2	4:E:309:LEU:HD13	1.91	0.52
1:A:188:VAL:HG23	1:A:198:TYR:HB2	1.91	0.52
3:C:45:LEU:HD12	3:C:52:LEU:HD12	1.90	0.51
4:E:293:VAL:O	4:E:297:ILE:HG12	2.10	0.51
4:E:11:LEU:HB3	4:E:65:LEU:HD23	1.93	0.51
3:C:249:LEU:HD21	1:D:243:MET:HG3	1.93	0.51
1:D:234:TYR:HD2	4:E:302:VAL:HG12	1.76	0.51
1:A:224:LEU:HD21	2:B:292:ALA:HB2	1.91	0.50
1:A:253:LEU:HD11	1:A:281:THR:HG22	1.93	0.50
1:A:37:LEU:HD12	1:A:54:VAL:HG12	1.93	0.50
1:A:104:HIS:NE2	2:B:98:GLY:O	2.45	0.50
3:C:247:PHE:CE1	3:C:302:VAL:HG13	2.46	0.50
3:C:47:GLU:HB3	3:C:279:PRO:HD3	1.93	0.50
4:E:104:TYR:HB3	4:E:121:PRO:HG2	1.92	0.50
1:A:257:LEU:HA	1:A:260:ILE:HG22	1.94	0.50
1:A:257:LEU:O	1:A:260:ILE:HG22	2.12	0.50
3:C:110:VAL:HG12	3:C:120:TRP:CD1	2.47	0.50
1:D:108:LEU:HD13	1:D:116:ILE:HG23	1.93	0.50
3:C:298:LEU:O	3:C:302:VAL:HG23	2.12	0.50
1:D:222:CYS:SG	1:D:256:PHE:HE2	2.34	0.50
3:C:109:ASN:HB3	1:D:150:THR:HG21	1.93	0.50
1:D:81:PRO:HA	1:D:107:LYS:HG2	1.94	0.50
1:D:12:LEU:HD21	1:D:84:ASP:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:3:CYS:HB2	5:F:59:ASN:HD21	1.76	0.49
1:A:148:ILE:HG21	1:A:151:TYR:HB2	1.95	0.49
3:C:273:LEU:HG	1:D:258:LEU:HD12	1.94	0.49
1:A:108:LEU:HD13	1:A:116:ILE:HG23	1.93	0.49
1:A:135:PHE:HE2	1:A:264:ILE:HD12	1.77	0.49
4:E:441:VAL:HG13	4:E:442:LEU:HD12	1.93	0.49
3:C:214:ASP:OD1	3:C:215:VAL:N	2.45	0.49
1:D:224:LEU:HD11	4:E:295:MET:CG	2.43	0.49
1:A:282:MET:O	1:A:286:ILE:HG12	2.13	0.49
3:C:235:PRO:HB2	3:C:270:PHE:CZ	2.47	0.49
5:G:22:CYS:HB3	5:G:59:ASN:ND2	2.28	0.49
1:A:79:ARG:CZ	1:A:109:LEU:HD13	2.43	0.48
3:C:191:GLU:OE1	3:C:222:ARG:NH2	2.46	0.48
3:C:104:VAL:HG11	3:C:122:PRO:HG2	1.95	0.48
4:E:176:GLU:HB2	5:G:48:ILE:HD11	1.95	0.48
2:B:138:ASP:OD2	2:B:140:GLN:NE2	2.47	0.48
2:B:314:MET:HG3	2:B:318:ILE:HD11	1.94	0.48
1:A:286:ILE:HG23	4:E:236:LEU:HD21	1.95	0.48
3:C:135:LEU:HD13	3:C:284:ALA:HB1	1.95	0.48
3:C:304:VAL:O	3:C:308:ILE:HG12	2.13	0.48
2:B:121:SER:HG	3:C:102:TYR:HH	1.60	0.48
1:D:256:PHE:O	1:D:260:ILE:HG13	2.14	0.48
5:F:15:LYS:NZ	5:F:39:CYS:SG	2.81	0.48
3:C:257:MET:O	3:C:261:ILE:HG12	2.14	0.48
1:A:182:ARG:HB3	1:A:204:HIS:NE2	2.29	0.48
2:B:56:LEU:O	2:B:120:PRO:HD2	2.14	0.48
4:E:76:ASP:HB2	4:E:112:ASN:HB2	1.96	0.48
1:D:148:ILE:HG21	1:D:151:TYR:HB2	1.95	0.47
1:D:165:PRO:HD2	1:D:181:TYR:HD2	1.79	0.47
4:E:237:VAL:HB	4:E:297:ILE:HG13	1.96	0.47
1:A:19:ILE:HG12	4:E:5:GLY:HA2	1.95	0.47
2:B:318:ILE:HA	2:B:321:ILE:HG22	1.95	0.47
3:C:230:ILE:HG23	1:D:279:LEU:HD21	1.95	0.47
3:C:255:GLU:OE1	1:D:244:THR:N	2.47	0.47
3:C:262:SER:OG	1:D:247:ILE:HG21	2.13	0.47
1:A:175:GLU:HG3	1:A:176:TRP:CD1	2.49	0.47
3:C:46:LYS:HZ1	3:C:49:ASP:HB2	1.78	0.47
4:E:110:VAL:HG12	4:E:116:MET:SD	2.54	0.47
1:A:300:HIS:ND1	4:E:244:PRO:HG3	2.30	0.47
1:D:43:VAL:HG22	1:D:50:VAL:HG22	1.96	0.47
2:B:303:ASN:O	2:B:307:ARG:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:235:PRO:HB2	3:C:270:PHE:HZ	1.79	0.47
3:C:291:TYR:HE1	3:C:469:THR:HG22	1.80	0.47
1:D:243:MET:HE1	1:D:292:THR:HG23	1.96	0.47
1:D:244:THR:HG21	4:E:253:THR:HB	1.97	0.47
4:E:19:ILE:HB	4:E:64:ARG:HH12	1.79	0.47
5:G:21:SER:O	5:G:40:GLY:N	2.30	0.47
2:B:266:LEU:HG	2:B:270:VAL:HG13	1.96	0.47
1:A:59:GLN:HB3	1:A:115:LYS:HE2	1.97	0.47
1:A:100:PHE:CZ	4:E:121:PRO:HB2	2.50	0.47
1:A:20:ARG:NH2	1:A:25:HIS:O	2.42	0.47
1:D:31:ILE:HG12	1:D:60:TRP:HB3	1.96	0.47
1:D:56:LEU:O	1:D:120:PRO:HD2	2.15	0.46
4:E:80:ILE:HB	4:E:85:LEU:HD11	1.97	0.46
2:B:425:LYS:O	2:B:428:TRP:N	2.48	0.46
1:A:138:ASP:OD2	1:A:209:ARG:NH2	2.44	0.46
1:D:9:ALA:O	1:D:13:GLU:HG2	2.16	0.46
1:A:34:GLY:O	1:A:57:ARG:N	2.34	0.46
2:B:221:ILE:O	2:B:225:ILE:HB	2.16	0.46
2:B:55:PHE:CE1	2:B:121:SER:HB2	2.51	0.46
2:B:130:ILE:HG22	2:B:132:VAL:HG13	1.97	0.46
3:C:97:ASN:ND2	3:C:101:GLN:O	2.48	0.46
1:D:175:GLU:N	1:D:175:GLU:OE1	2.49	0.46
1:D:256:PHE:HA	1:D:259:VAL:HG12	1.97	0.46
4:E:457:LEU:O	4:E:461:ILE:HG12	2.16	0.46
3:C:45:LEU:HD23	3:C:45:LEU:O	2.15	0.46
3:C:309:VAL:HG22	3:C:453:ILE:HG23	1.98	0.46
1:D:257:LEU:HA	1:D:260:ILE:HD12	1.97	0.46
1:A:260:ILE:HG21	1:A:278:MET:HE2	1.98	0.46
1:A:31:ILE:HG12	1:A:60:TRP:HB3	1.98	0.45
3:C:47:GLU:HG3	3:C:132:ILE:HD13	1.98	0.45
1:D:218:VAL:HA	1:D:256:PHE:HZ	1.80	0.45
1:A:285:VAL:O	1:A:288:SER:OG	2.25	0.45
5:F:27:TRP:HB3	5:F:48:ILE:HG23	1.97	0.45
3:C:58:MET:O	3:C:122:PRO:HD2	2.17	0.45
3:C:238:LEU:HD13	1:D:286:ILE:HG13	1.98	0.45
4:E:34:LYS:HG2	4:E:57:GLU:HG2	1.99	0.45
5:F:23:TYR:HB3	5:F:41:CYS:HB3	1.97	0.45
1:D:282:MET:O	1:D:286:ILE:HG12	2.16	0.45
5:G:6:GLN:HG3	5:G:37:ARG:HH11	1.82	0.45
5:G:30:HIS:CD2	5:G:31:ARG:HG3	2.52	0.45
3:C:192:ILE:HA	3:C:221:ILE:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:276:THR:HG22	4:E:278:LEU:H	1.82	0.45
5:G:4:TYR:HB2	5:G:59:ASN:OD1	2.17	0.45
1:D:232:VAL:HA	1:D:235:LEU:HD13	1.99	0.45
1:A:165:PRO:HG3	1:A:203:TYR:CD1	2.52	0.45
1:A:214:PHE:O	1:A:218:VAL:HB	2.16	0.45
2:B:43:LEU:HD23	2:B:43:LEU:O	2.17	0.45
1:D:4:GLU:HG2	4:E:19:ILE:HD12	1.99	0.45
1:A:416:LEU:O	1:A:420:ILE:HG12	2.17	0.44
3:C:255:GLU:OE1	1:D:243:MET:HB2	2.17	0.44
1:A:85:VAL:HG21	1:A:108:LEU:HD21	1.99	0.44
1:A:247:ILE:HD12	1:A:250:LEU:HD23	1.98	0.44
4:E:253:THR:HA	4:E:256:ILE:HG22	1.98	0.44
2:B:238:VAL:HG21	2:B:252:SER:OG	2.17	0.44
1:A:56:LEU:O	1:A:120:PRO:HD2	2.18	0.44
2:B:20:ARG:NH1	2:B:155:GLU:O	2.50	0.44
2:B:256:LEU:O	2:B:259:VAL:HG12	2.16	0.44
3:C:41:ASN:OD1	3:C:55:ASN:HB3	2.18	0.44
4:E:45:GLU:HB3	4:E:274:PRO:HG3	2.00	0.44
1:A:131:ILE:O	1:A:131:ILE:HG13	2.18	0.44
1:D:80:LEU:HD12	1:D:110:LEU:HD13	1.99	0.44
2:B:163:ASP:OD1	2:B:163:ASP:N	2.49	0.44
3:C:257:MET:HE3	3:C:310:LEU:HD12	1.99	0.44
1:A:285:VAL:O	1:A:289:ILE:HG12	2.17	0.44
2:B:36:THR:HG22	2:B:174:VAL:HG13	2.00	0.44
3:C:42:LEU:HD12	3:C:54:SER:HB3	2.00	0.44
3:C:165:ASP:OD1	3:C:165:ASP:N	2.50	0.44
3:C:38:THR:HG21	5:F:30:HIS:HB3	2.00	0.44
4:E:298:VAL:O	4:E:302:VAL:HG23	2.16	0.44
2:B:279:ILE:HG21	2:B:458:ALA:HB2	2.00	0.43
4:E:158:LEU:O	4:E:193:LYS:HE2	2.18	0.43
1:D:175:GLU:HG2	1:D:176:TRP:CD1	2.53	0.43
1:D:243:MET:CE	1:D:292:THR:HG23	2.48	0.43
4:E:287:LEU:HA	4:E:290:VAL:HG12	2.00	0.43
3:C:273:LEU:HD11	1:D:258:LEU:HA	1.99	0.43
1:D:77:LYS:HD2	1:D:109:LEU:HD11	2.00	0.43
1:A:15:TYR:CE2	1:A:85:VAL:HA	2.53	0.43
1:A:108:LEU:HB3	1:A:118:TRP:CD1	2.54	0.43
1:A:145:LYS:HE3	1:A:200:ASP:OD2	2.18	0.43
3:C:43:ILE:HG23	1:D:49:ILE:HD11	2.01	0.43
3:C:247:PHE:CZ	3:C:302:VAL:HG13	2.54	0.43
1:D:15:TYR:CE1	1:D:85:VAL:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:269:ILE:HD11	4:E:283:ILE:HG23	2.01	0.43
3:C:229:VAL:HA	3:C:233:ILE:HB	2.01	0.43
1:A:218:VAL:HG11	1:A:274:ILE:HD13	2.00	0.43
3:C:245:LEU:HD13	1:D:290:ILE:HG12	2.00	0.43
2:B:273:THR:HG22	2:B:275:LEU:H	1.83	0.43
1:A:225:PHE:HZ	2:B:260:THR:HG21	1.84	0.42
1:D:85:VAL:HG21	1:D:108:LEU:HD21	2.01	0.42
1:D:221:PRO:HB2	1:D:256:PHE:CZ	2.54	0.42
1:D:235:LEU:HD11	4:E:302:VAL:HG22	2.02	0.42
2:B:185:GLN:HG3	2:B:186:TRP:CD1	2.55	0.42
2:B:426:LYS:NZ	3:C:318:SER:HB3	2.35	0.42
3:C:154:ASP:OD1	3:C:154:ASP:N	2.49	0.42
2:B:95:ASN:HA	2:B:126:SER:HA	2.00	0.42
1:A:232:VAL:HG23	1:A:245:LEU:HD23	2.01	0.42
2:B:291:VAL:O	2:B:295:VAL:HG23	2.20	0.42
1:D:36:GLN:HA	1:D:166:ASP:HB3	2.01	0.42
1:D:402:VAL:HA	1:D:405:VAL:HG22	2.00	0.42
1:A:1:SER:HB2	2:B:22:ALA:HB3	2.02	0.42
3:C:7:LEU:HD13	3:C:74:TYR:CE2	2.55	0.42
4:E:80:ILE:HG21	4:E:85:LEU:HD21	2.02	0.42
1:A:244:THR:HB	4:E:250:GLN:NE2	2.35	0.42
3:C:177:ILE:HD11	3:C:217:PHE:HB3	2.01	0.42
3:C:289:GLY:O	3:C:293:MET:HG2	2.20	0.42
4:E:186:ILE:HA	4:E:215:ILE:HG22	2.02	0.42
4:E:228:ALA:HA	4:E:231:VAL:HG12	2.02	0.42
2:B:315:PRO:HG2	2:B:318:ILE:HG12	2.01	0.42
1:D:246:SER:HB3	1:D:289:ILE:CD1	2.45	0.42
1:A:282:MET:HE1	4:E:233:ILE:HD11	2.02	0.42
1:A:399:TRP:HA	1:A:402:VAL:HG12	2.02	0.42
3:C:57:TRP:HB3	3:C:121:LEU:HD21	2.01	0.42
2:B:102:ILE:HD12	2:B:102:ILE:H	1.85	0.41
4:E:232:LEU:HD23	4:E:232:LEU:HA	1.91	0.41
1:D:256:PHE:CD2	1:D:260:ILE:HD11	2.55	0.41
4:E:77:LEU:HD21	4:E:109:LEU:HD23	2.01	0.41
1:D:165:PRO:HG3	1:D:203:TYR:CD1	2.55	0.41
1:A:89:ASP:OD1	1:A:89:ASP:N	2.46	0.41
1:A:286:ILE:HD12	4:E:236:LEU:HD11	2.02	0.41
1:D:77:LYS:HB3	1:D:109:LEU:HD11	2.01	0.41
1:D:256:PHE:O	1:D:259:VAL:HG12	2.21	0.41
3:C:486:PHE:O	3:C:489:ASP:N	2.54	0.41
2:B:226:ILE:O	2:B:230:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:GLU:H	1:A:142:CYS:CB	2.31	0.41
3:C:37:LEU:HD11	3:C:56:VAL:HB	2.03	0.41
4:E:439:ASN:HB3	4:E:440:TRP:H	1.67	0.41
5:G:22:CYS:HB2	5:G:53:CYS:SG	2.61	0.41
1:A:295:VAL:HG11	1:A:407:ASP:OD1	2.22	0.40
3:C:94:LEU:HD23	3:C:97:ASN:HB3	2.04	0.40
3:C:160:MET:HB2	3:C:160:MET:HE2	1.83	0.40
1:D:212:LEU:O	1:D:216:VAL:HG22	2.20	0.40
3:C:455:ARG:HA	3:C:455:ARG:HD2	1.91	0.40
1:D:92:LEU:HD21	1:D:144:MET:HB2	2.03	0.40
5:G:44:VAL:HG21	5:G:50:LEU:HD23	2.03	0.40
3:C:75:SER:O	3:C:77:ILE:N	2.49	0.40
1:D:97:ASP:OD1	1:D:125:LYS:HD2	2.22	0.40
4:E:60:TRP:CE2	4:E:116:MET:HG3	2.57	0.40
5:F:22:CYS:HB3	5:F:59:ASN:ND2	2.35	0.40
1:A:212:LEU:O	1:A:216:VAL:HG22	2.22	0.40
1:A:273:LEU:HD12	1:A:273:LEU:HA	1.98	0.40
2:B:315:PRO:HB2	2:B:317:TRP:CD1	2.57	0.40
3:C:22:ARG:NH1	3:C:27:ASN:OD1	2.38	0.40
1:A:410:LEU:O	1:A:414:PHE:HB2	2.22	0.40
2:B:31:VAL:HG22	2:B:60:TRP:HB3	2.03	0.40
2:B:152:ASP:OD1	2:B:155:GLU:HG3	2.22	0.40
1:D:89:ASP:OD1	1:D:89:ASP:N	2.52	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	345/437 (79%)	328 (95%)	17 (5%)	0	100	100
1	D	324/437 (74%)	310 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	367/469 (78%)	349 (95%)	18 (5%)	0	100	100
3	C	372/501 (74%)	355 (95%)	17 (5%)	0	100	100
4	E	357/489 (73%)	348 (98%)	9 (2%)	0	100	100
5	F	58/60 (97%)	55 (95%)	3 (5%)	0	100	100
5	G	58/60 (97%)	53 (91%)	5 (9%)	0	100	100
All	All	1881/2453 (77%)	1798 (96%)	83 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	333/405 (82%)	333 (100%)	0	100	100
1	D	308/405 (76%)	308 (100%)	0	100	100
2	B	345/431 (80%)	345 (100%)	0	100	100
3	C	344/458 (75%)	342 (99%)	2 (1%)	86	94
4	E	329/446 (74%)	329 (100%)	0	100	100
5	F	56/56 (100%)	56 (100%)	0	100	100
5	G	56/56 (100%)	56 (100%)	0	100	100
All	All	1771/2257 (78%)	1769 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	46	LYS
3	C	305	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	60	HIS
4	E	300	ASN

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

27 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	H	1	1,6	14,14,15	0.35	0	17,19,21	0.43	0
6	NAG	H	2	6	14,14,15	0.30	0	17,19,21	0.46	0
6	BMA	H	3	6	11,11,12	0.54	0	15,15,17	0.80	0
6	MAN	H	4	6	11,11,12	0.80	1 (9%)	15,15,17	0.92	1 (6%)
6	MAN	H	5	6	11,11,12	0.62	0	15,15,17	1.01	1 (6%)
6	MAN	H	6	6	11,11,12	0.63	0	15,15,17	0.94	2 (13%)
6	MAN	H	7	6	11,11,12	0.85	0	15,15,17	1.10	1 (6%)
6	MAN	H	8	6	11,11,12	0.62	0	15,15,17	0.94	2 (13%)
6	MAN	H	9	6	11,11,12	0.62	0	15,15,17	0.97	2 (13%)
7	NAG	I	1	3,7	14,14,15	0.22	0	17,19,21	0.42	0
7	NAG	I	2	7	14,14,15	0.25	0	17,19,21	0.50	0
7	NAG	J	1	2,7	14,14,15	0.24	0	17,19,21	0.45	0
7	NAG	J	2	7	14,14,15	0.22	0	17,19,21	0.58	0
6	NAG	K	1	1,6	14,14,15	0.35	0	17,19,21	0.46	0
6	NAG	K	2	6	14,14,15	0.24	0	17,19,21	0.49	0
6	BMA	K	3	6	11,11,12	0.52	0	15,15,17	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	MAN	K	4	6	11,11,12	0.55	0	15,15,17	1.04	2 (13%)
6	MAN	K	5	6	11,11,12	0.63	0	15,15,17	1.11	2 (13%)
6	MAN	K	6	6	11,11,12	0.88	0	15,15,17	1.01	1 (6%)
6	MAN	K	7	6	11,11,12	0.62	0	15,15,17	0.92	2 (13%)
6	MAN	K	8	6	11,11,12	0.56	0	15,15,17	1.01	2 (13%)
6	MAN	K	9	6	11,11,12	0.63	0	15,15,17	0.96	2 (13%)
8	NAG	L	1	4,8	14,14,15	0.21	0	17,19,21	0.44	0
8	NAG	L	2	8	14,14,15	0.21	0	17,19,21	0.43	0
8	NAG	L	3	8	14,14,15	0.18	0	17,19,21	0.64	0
8	MAN	L	4	8	11,11,12	0.67	0	15,15,17	1.00	2 (13%)
8	MAN	L	5	8	11,11,12	0.64	0	15,15,17	1.04	2 (13%)

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	H	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	H	2	6	-	2/6/23/26	0/1/1/1
6	BMA	H	3	6	-	1/2/19/22	0/1/1/1
6	MAN	H	4	6	-	1/2/19/22	0/1/1/1
6	MAN	H	5	6	-	2/2/19/22	0/1/1/1
6	MAN	H	6	6	-	0/2/19/22	0/1/1/1
6	MAN	H	7	6	-	1/2/19/22	0/1/1/1
6	MAN	H	8	6	-	0/2/19/22	0/1/1/1
6	MAN	H	9	6	-	0/2/19/22	0/1/1/1
7	NAG	I	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	I	2	7	-	3/6/23/26	0/1/1/1
7	NAG	J	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	J	2	7	-	1/6/23/26	0/1/1/1
6	NAG	K	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1
6	BMA	K	3	6	-	0/2/19/22	0/1/1/1
6	MAN	K	4	6	-	0/2/19/22	0/1/1/1
6	MAN	K	5	6	-	2/2/19/22	0/1/1/1
6	MAN	K	6	6	-	0/2/19/22	0/1/1/1
6	MAN	K	7	6	-	1/2/19/22	0/1/1/1
6	MAN	K	8	6	-	2/2/19/22	0/1/1/1

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	4	MAN	O5-C1	-2.24	1.40	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	K	5	MAN	O2-C2-C3	-2.90	104.33	110.14
6	H	5	MAN	O2-C2-C3	-2.79	104.55	110.14
8	L	5	MAN	C1-O5-C5	2.62	115.74	112.19
6	K	4	MAN	C1-O5-C5	2.60	115.71	112.19
6	K	5	MAN	C1-O5-C5	2.58	115.69	112.19
6	H	4	MAN	O2-C2-C3	-2.57	105.00	110.14
6	K	8	MAN	O2-C2-C3	-2.48	105.17	110.14
6	K	8	MAN	C1-O5-C5	2.40	115.44	112.19
6	K	4	MAN	O2-C2-C3	-2.38	105.36	110.14
6	K	6	MAN	O2-C2-C3	-2.28	105.56	110.14
6	H	6	MAN	O2-C2-C3	-2.27	105.58	110.14
6	H	9	MAN	O2-C2-C3	-2.27	105.59	110.14
6	H	7	MAN	O2-C2-C3	-2.27	105.60	110.14
6	H	8	MAN	O2-C2-C3	-2.26	105.61	110.14
6	K	7	MAN	O2-C2-C3	-2.25	105.62	110.14
8	L	5	MAN	O2-C2-C3	-2.25	105.63	110.14
6	H	9	MAN	C1-O5-C5	2.22	115.20	112.19
8	L	4	MAN	O2-C2-C3	-2.21	105.72	110.14
6	K	9	MAN	O2-C2-C3	-2.20	105.72	110.14
6	H	6	MAN	C1-O5-C5	2.15	115.11	112.19
6	K	9	MAN	C1-O5-C5	2.15	115.10	112.19
8	L	4	MAN	C1-O5-C5	2.13	115.08	112.19
6	H	8	MAN	C1-O5-C5	2.07	115.00	112.19
6	K	7	MAN	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	1	NAG	O5-C5-C6-O6
6	H	2	NAG	O5-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
8	L	1	NAG	O5-C5-C6-O6
7	J	1	NAG	O5-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
7	I	2	NAG	C4-C5-C6-O6
6	H	1	NAG	C4-C5-C6-O6
6	H	2	NAG	C4-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6
7	J	1	NAG	C4-C5-C6-O6
8	L	1	NAG	C4-C5-C6-O6
6	K	5	MAN	O5-C5-C6-O6
7	I	1	NAG	O5-C5-C6-O6
8	L	1	NAG	C8-C7-N2-C2
8	L	1	NAG	O7-C7-N2-C2
6	K	7	MAN	O5-C5-C6-O6
6	K	5	MAN	C4-C5-C6-O6
7	I	2	NAG	O5-C5-C6-O6
7	I	1	NAG	C4-C5-C6-O6
6	K	8	MAN	O5-C5-C6-O6
6	H	4	MAN	O5-C5-C6-O6
6	H	7	MAN	O5-C5-C6-O6
6	K	8	MAN	C4-C5-C6-O6
6	H	5	MAN	O5-C5-C6-O6
6	H	5	MAN	C4-C5-C6-O6
7	J	2	NAG	C3-C2-N2-C7
8	L	3	NAG	C3-C2-N2-C7
8	L	2	NAG	C4-C5-C6-O6
7	I	2	NAG	C3-C2-N2-C7
6	H	3	BMA	C4-C5-C6-O6

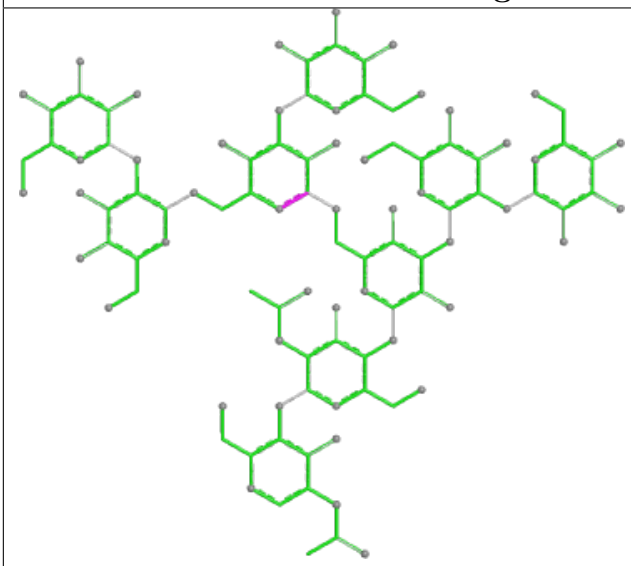
There are no ring outliers.

1 monomer is involved in 1 short contact:

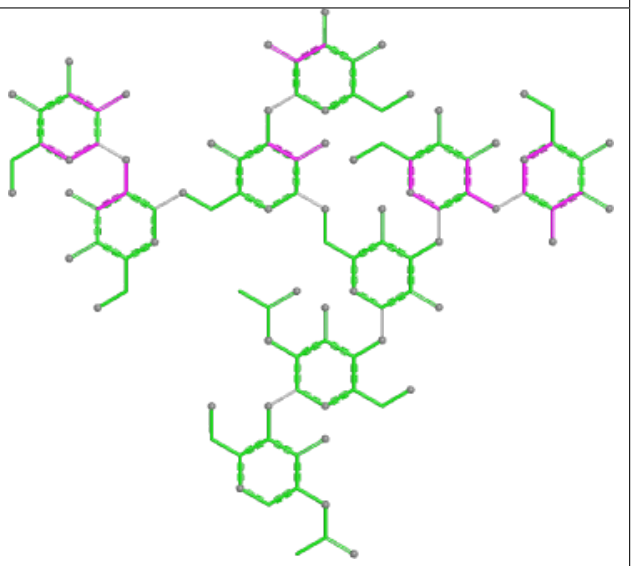
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	3	NAG	1	0

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

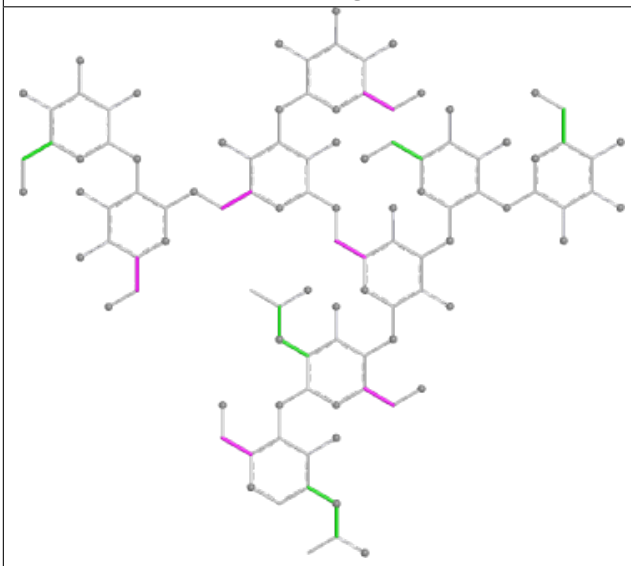
Oligosaccharide Chain H



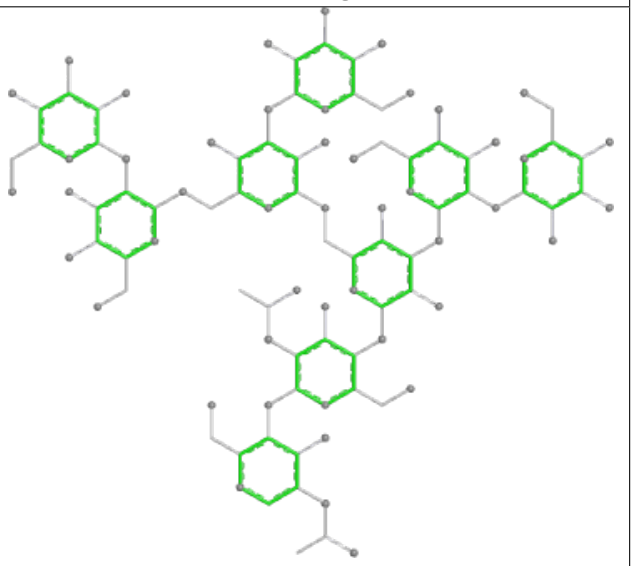
Bond lengths



Bond angles

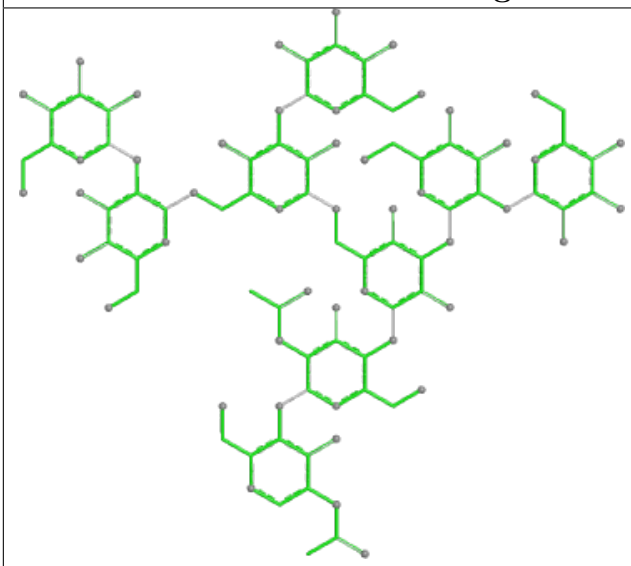


Torsions

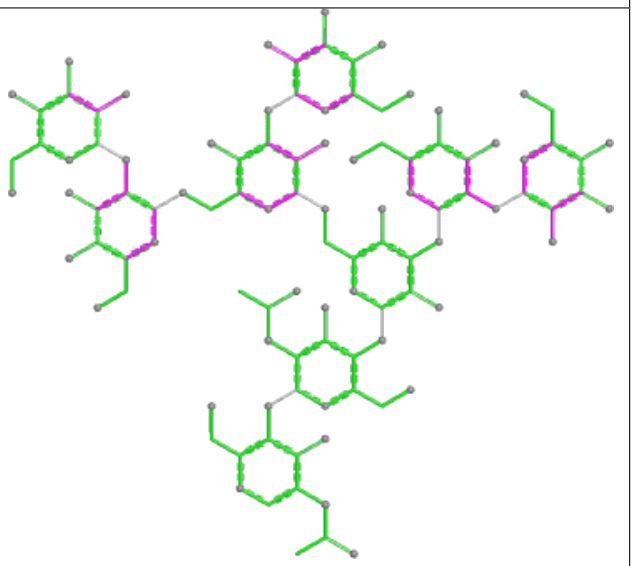


Rings

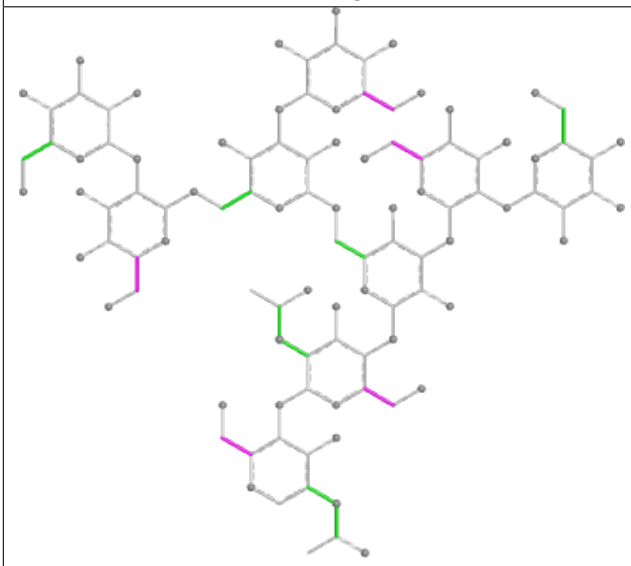
Oligosaccharide Chain K



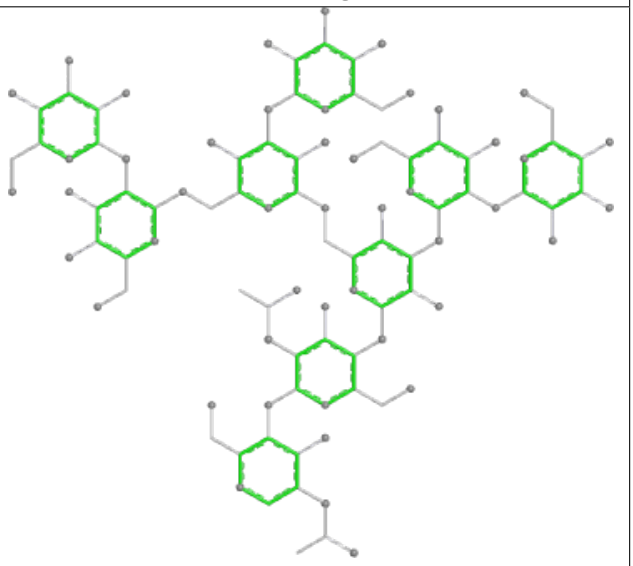
Bond lengths



Bond angles

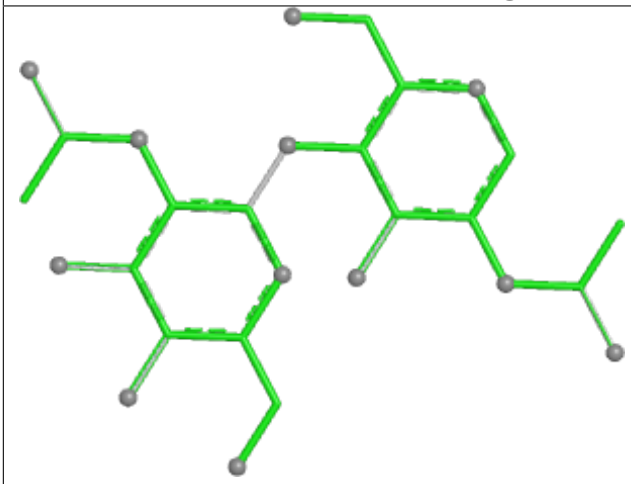


Torsions

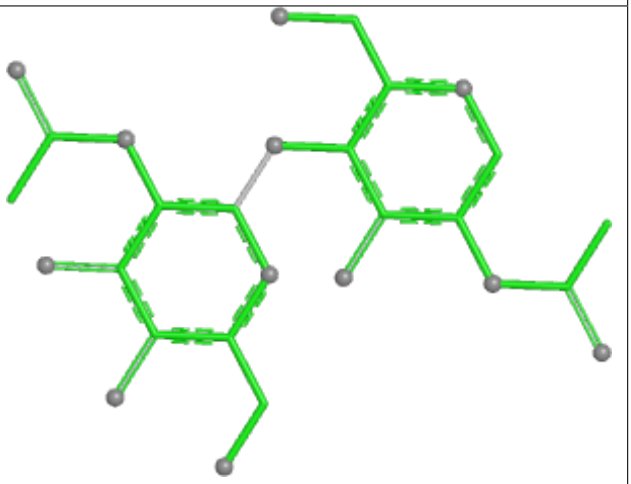


Rings

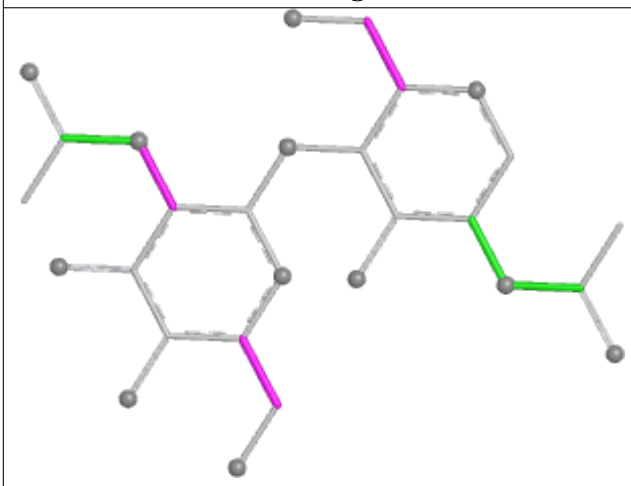
Oligosaccharide Chain I



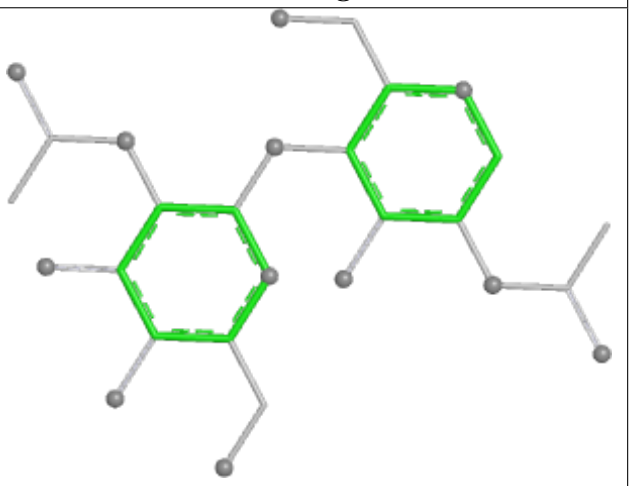
Bond lengths



Bond angles

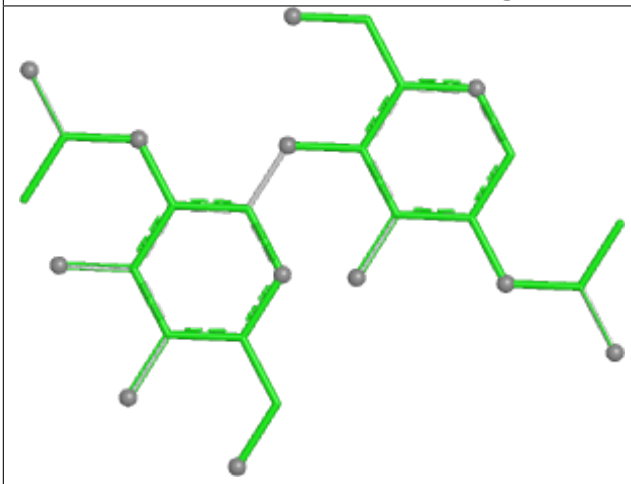


Torsions

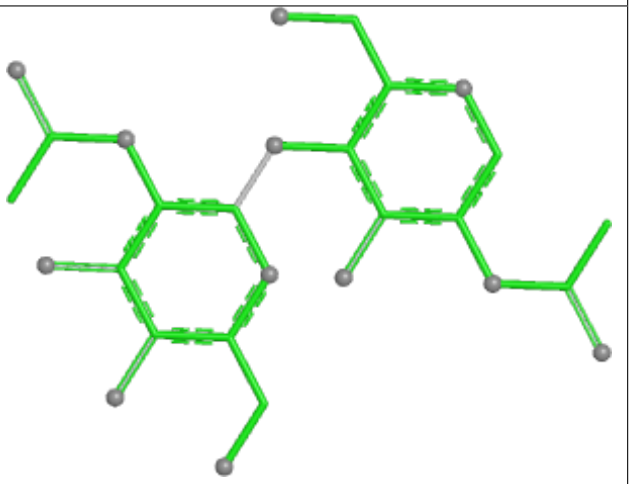


Rings

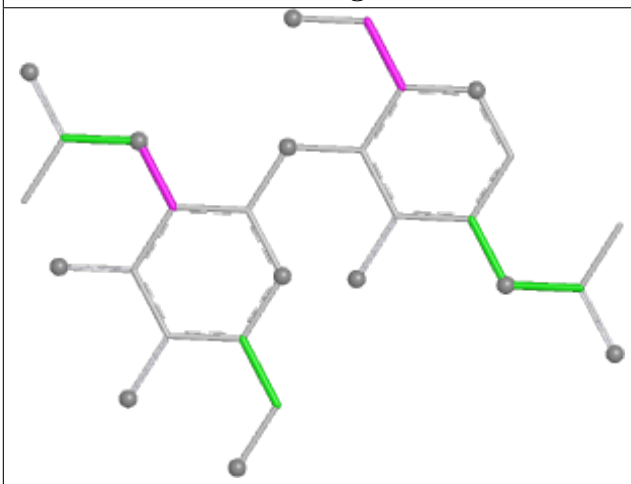
Oligosaccharide Chain J



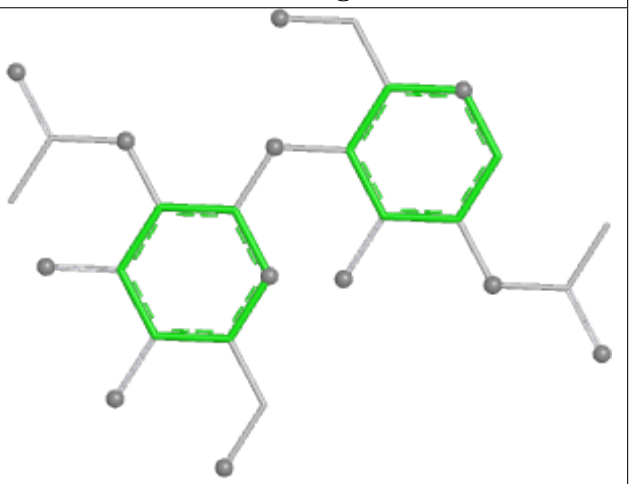
Bond lengths



Bond angles

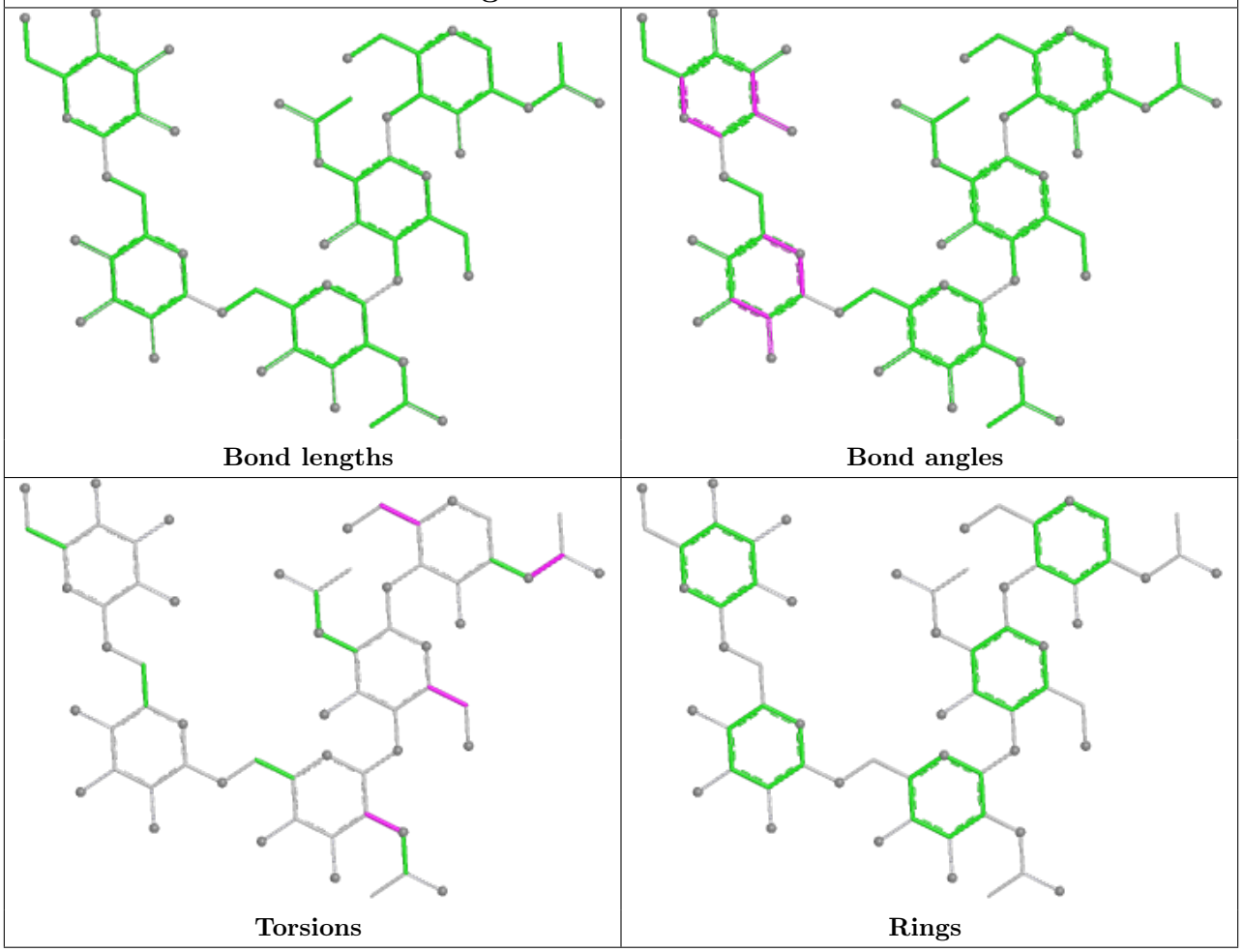


Torsions



Rings

Oligosaccharide Chain L



5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
9	NAG	C	601	3	14,14,15	0.20	0	17,19,21	0.40	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
9	NAG	C	601	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	601	NAG	C4-C5-C6-O6
9	C	601	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.

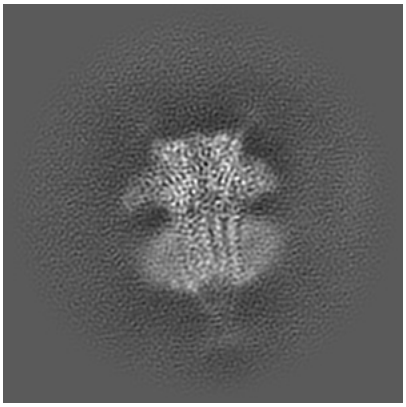
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14440. These allow visual inspection of the internal detail of the map and identification of artifacts.

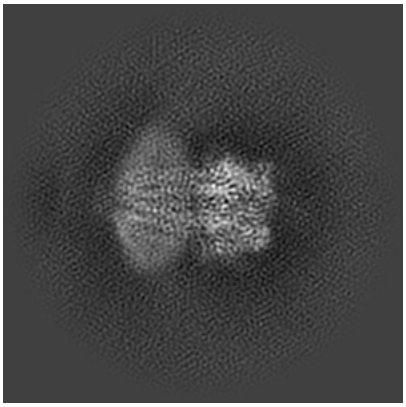
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

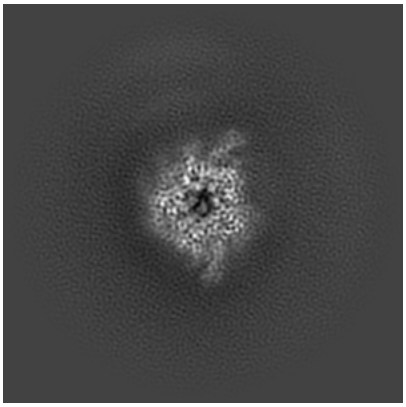
6.1.1 Primary map



X



Y



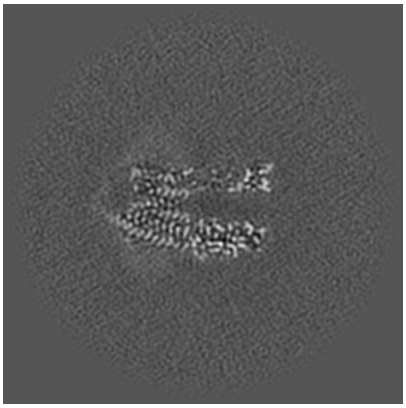
Z

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

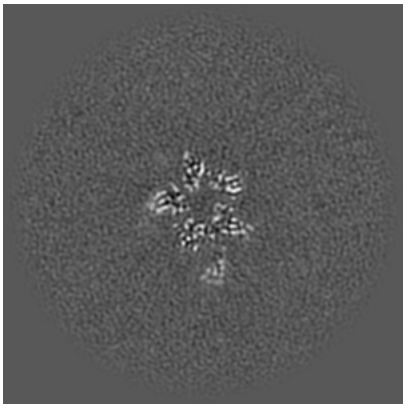
6.2 Central slices

6.2.1 Primary map

X Index: 128



Y Index: 128

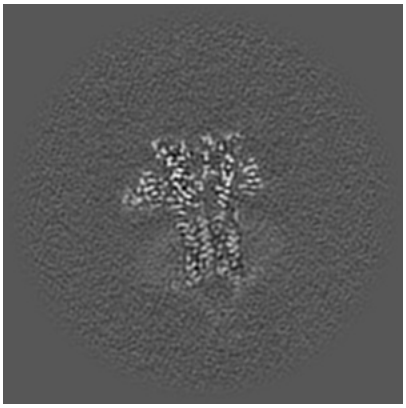


Z Index: 128

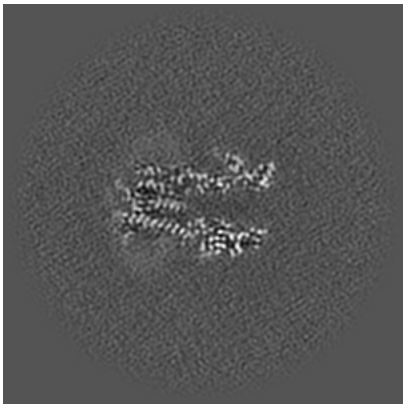
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

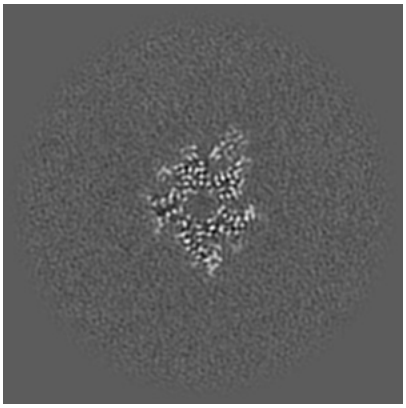
6.3.1 Primary map



X Index: 136



Y Index: 124



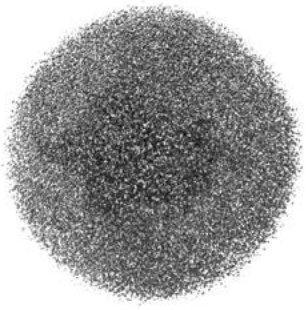
Z Index: 143

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

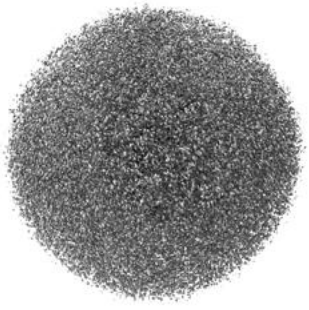
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.115. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

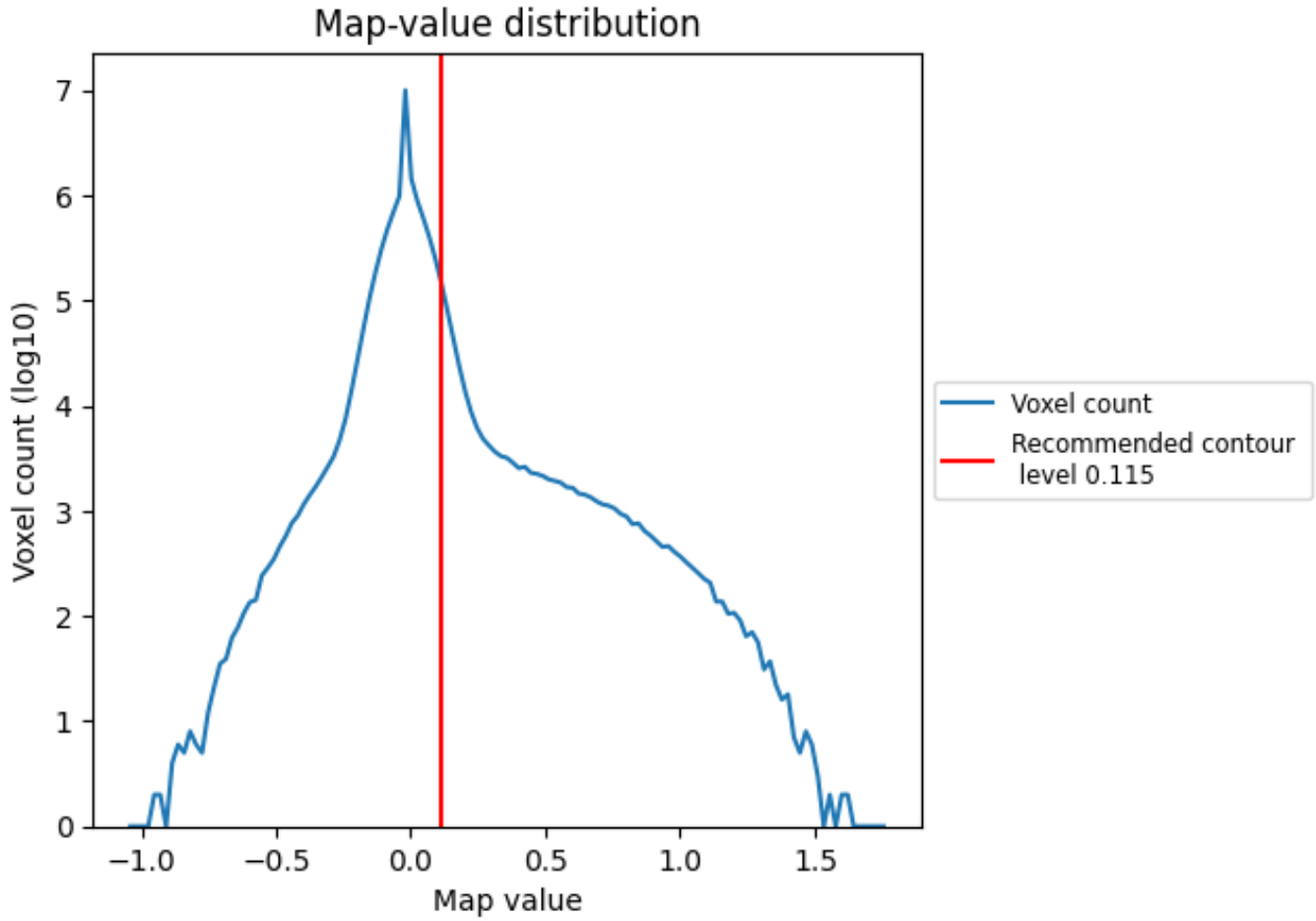
6.5 Mask visualisation (i)

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

7 Map analysis

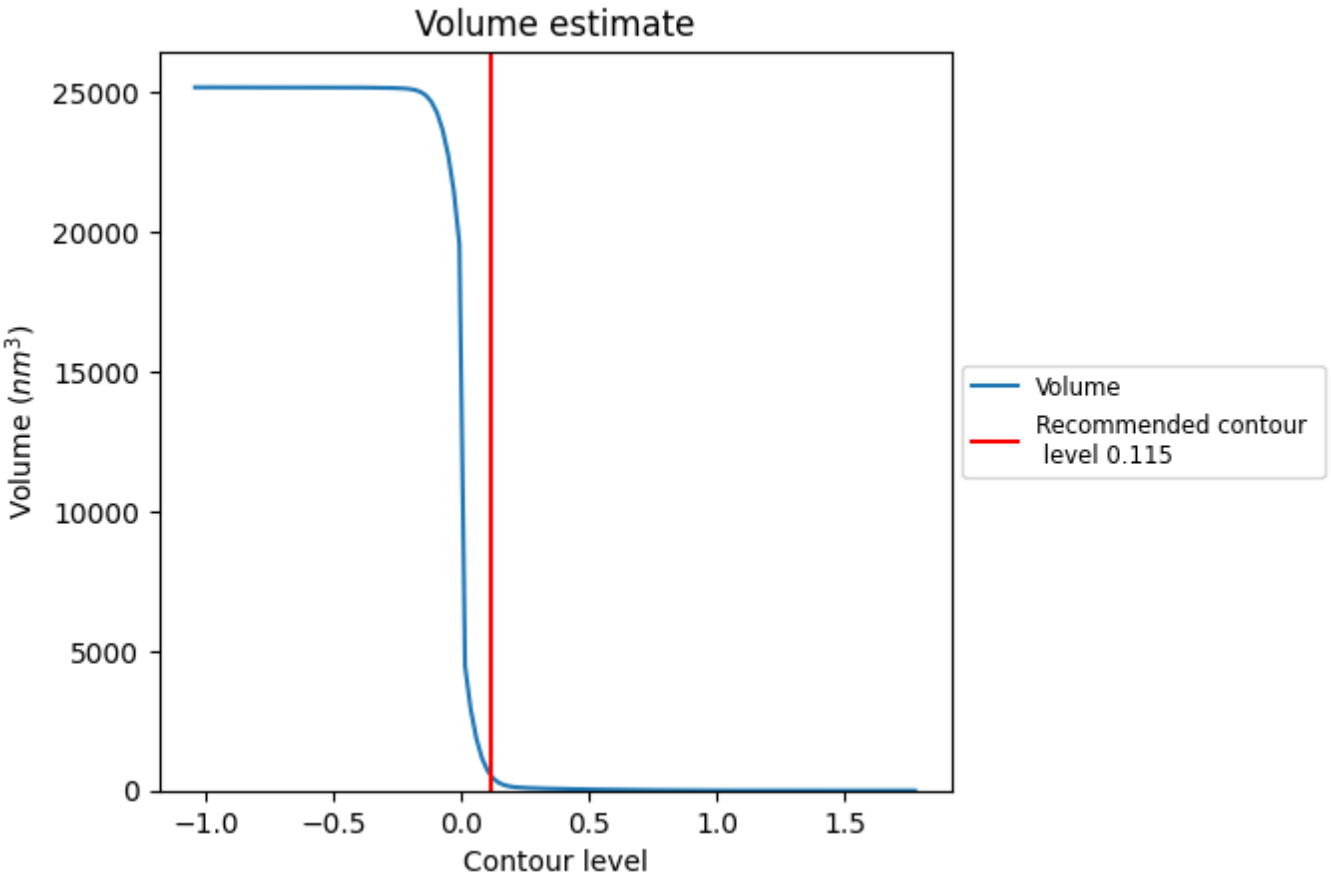
This section contains the results of statistical analysis of the map.

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.

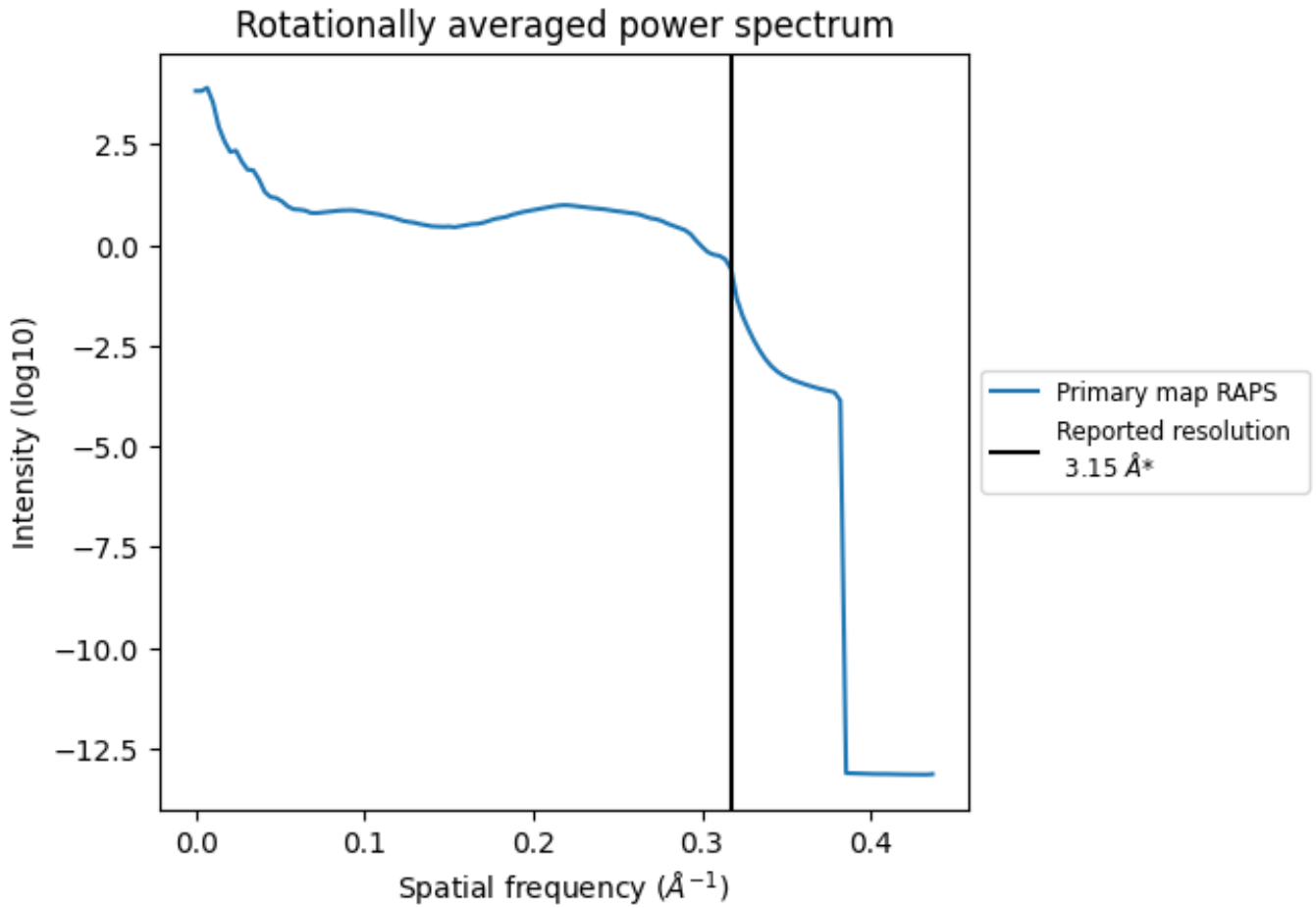
7.2 Volume estimate



The volume at the recommended contour level is 573 nm^3; this corresponds to an approximate mass of 518 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 0.317 $Å^{-1}$

8 Fourier-Shell correlation

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

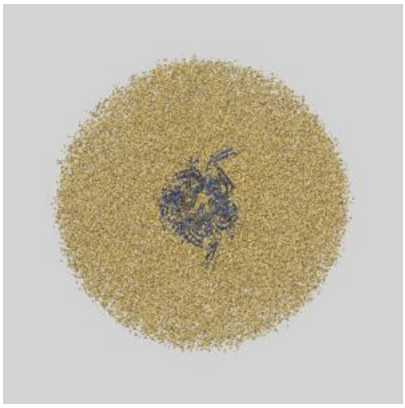
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14440 and PDB model 7Z14. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay

X

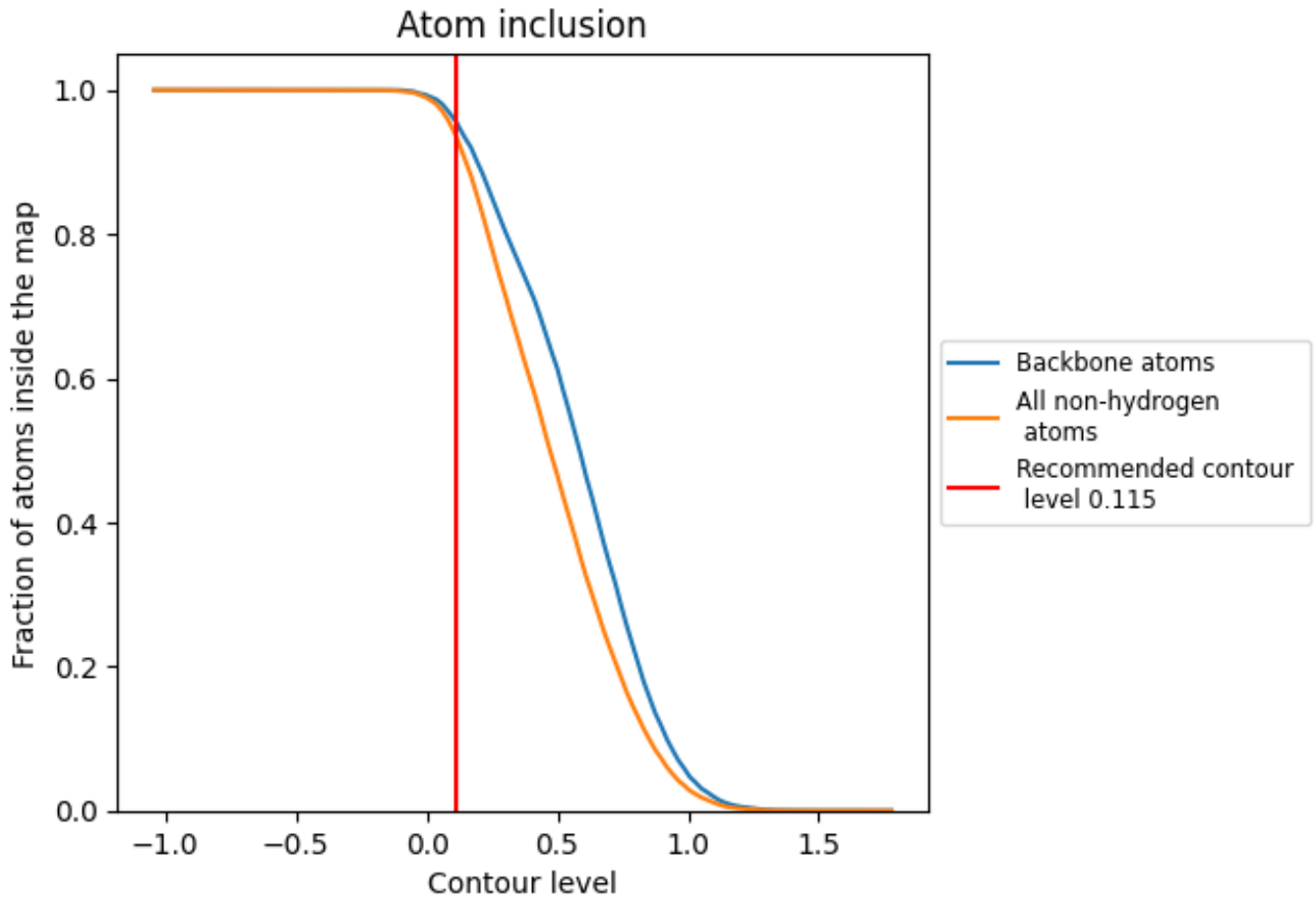
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.115 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 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.