Full wwPDB EM Validation Report

Oct 6, 2024 – 06:28 AM EDT

PDB ID	:	8F6Z
EMDB ID	:	EMD-28893
Title	:	Cryo-EM structure of Torpedo nicotinic acetylcholine receptor in complex with succinylcholine, desensitized-like state
Authors	:	Goswami, U.; Rahman, M.M.; Teng, J.; Hibbs, R.E.
Deposited on	:	2022-11-17
Resolution	:	2.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

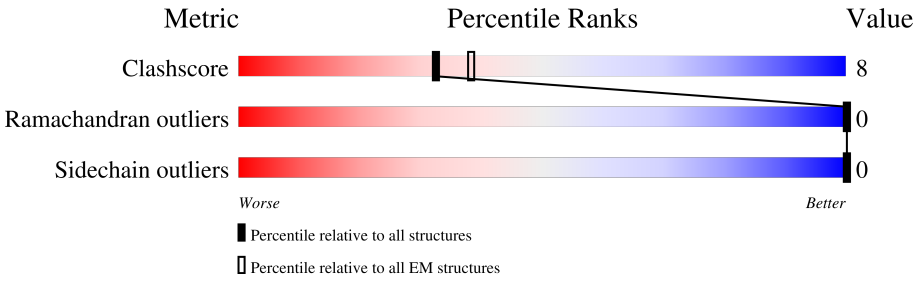
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	433	71% 18% 11%
1	D	433	68% 21% 10%
2	B	500	71% 14% 15%
3	C	469	72% 14% 13%
4	E	489	70% 14% 16%
5	F	5	40% 60%
5	J	5	40% 60%
5	K	5	40% 60%

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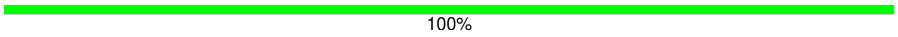
Mol	Chain	Length	Quality of chain
6	G	4	
7	H	2	
8	I	3	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 16997 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	387	Total	C	N	O	S	0	0
			3140	2059	499	560	22		
1	D	388	Total	C	N	O	S	0	0
			3151	2065	503	561	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	425	Total	C	N	O	S	0	0
			3456	2251	564	626	15		

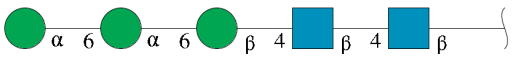
- Molecule 3 is a protein called Acetylcholine receptor subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	406	Total	C	N	O	S	0	0
			3294	2156	524	600	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	409	Total	C	N	O	S	0	0
			3317	2173	527	605	12		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	F	5	Total 61	C 34	N 2	O 25	0	0
5	J	5	Total 61	C 34	N 2	O 25	0	0
5	K	5	Total 61	C 34	N 2	O 25	0	0

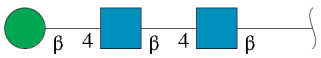
- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	G	4	Total 50	C 28	N 2	O 20	0	0

- Molecule 7 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
7	H	2	Total 28	C 16	N 2	O 10	0	0

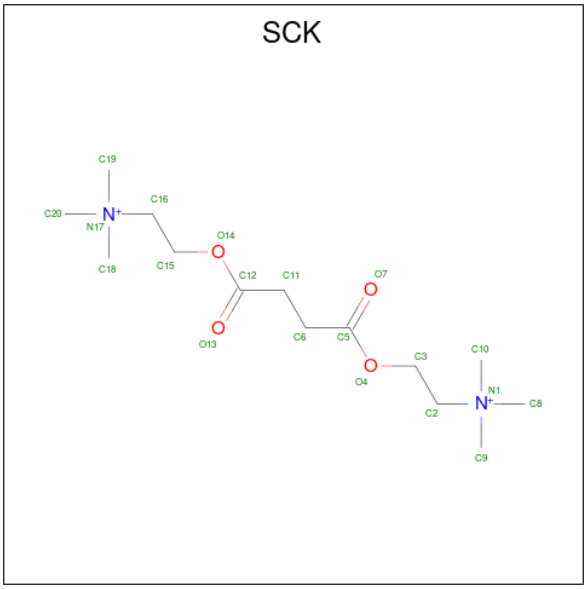
- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

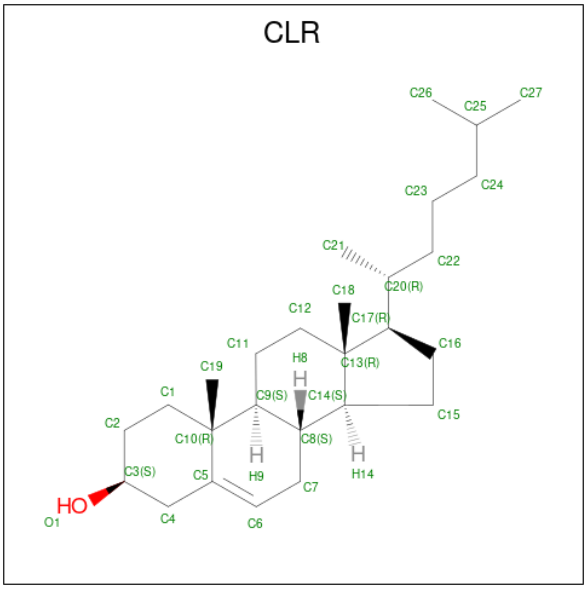
- Molecule 9 is 2,2'-[(1,4-DIOXOBUTANE-1,4-DIYL)BIS(OXY)]BIS(N,N,N-TRIMETHYLE

THANAMINIUM) (three-letter code: SCK) (formula: $C_{14}H_{30}N_2O_4$) (labeled as "Ligand of Interest" by depositor).



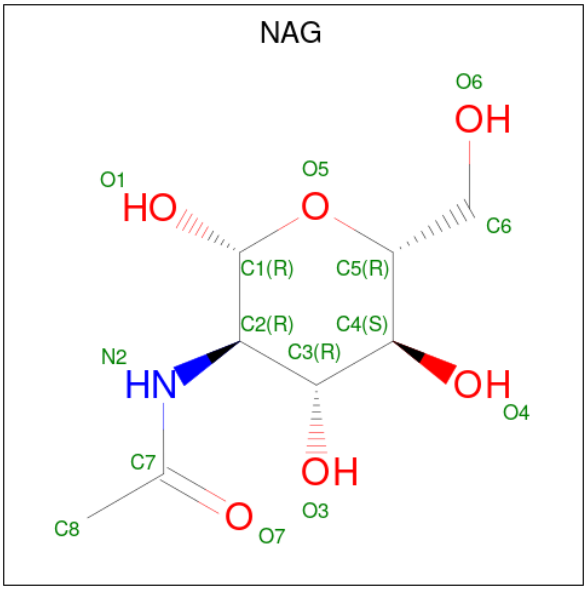
Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	N	O	0
			20	14	2	4	
9	D	1	Total	C	N	O	0
			20	14	2	4	

- Molecule 10 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



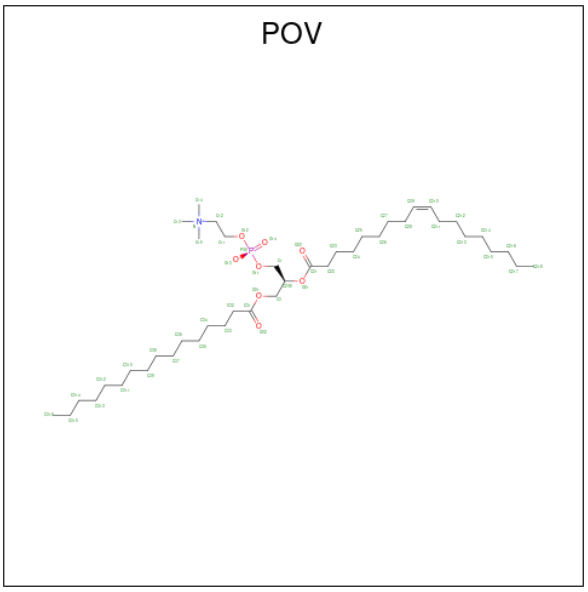
Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total C O 28 27 1	0
10	C	1	Total C O 28 27 1	0
10	D	1	Total C O 28 27 1	0

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



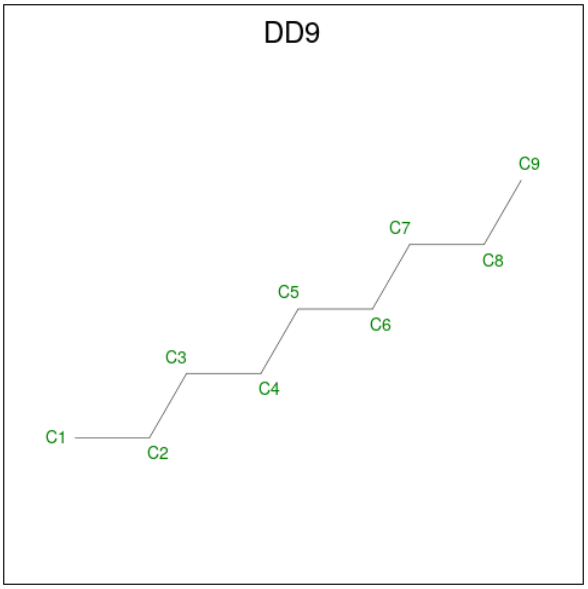
Mol	Chain	Residues	Atoms	AltConf
11	B	1	Total C N O 14 8 1 5	0
11	E	1	Total C N O 14 8 1 5	0

- Molecule 12 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: $C_{42}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total	C	N	O	P	0
			37	27	1	8	1	
12	C	1	Total	C	N	O	P	0
			35	25	1	8	1	
12	C	1	Total	C	N	O	P	0
			35	25	1	8	1	
12	D	1	Total	C	N	O	P	0
			35	25	1	8	1	
12	E	1	Total	C	N	O	P	0
			31	21	1	8	1	

- Molecule 13 is nonane (three-letter code: DD9) (formula: C_9H_{20}).



Mol	Chain	Residues	Atoms	AltConf
13	B	1	Total C 9 9	0

- Molecule 14 is water.

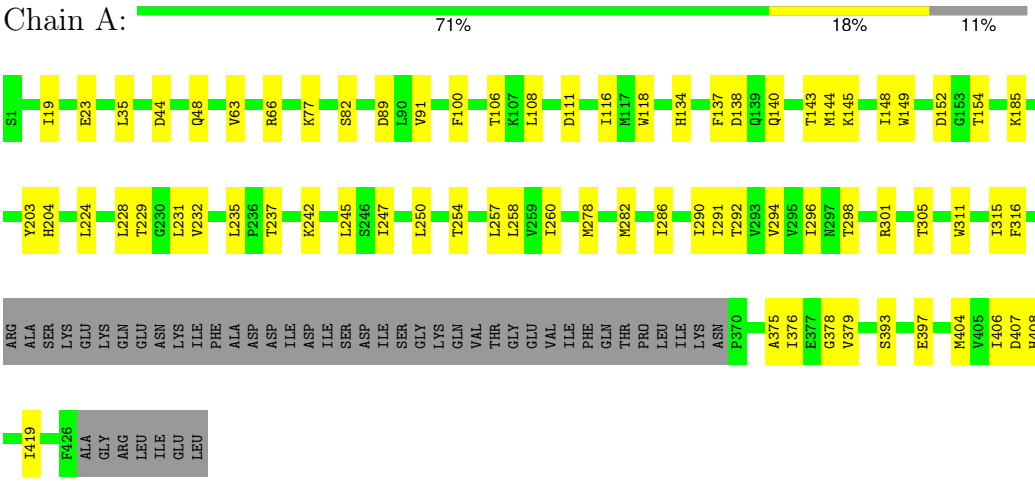
Mol	Chain	Residues	Atoms	AltConf
14	B	2	Total O 2 2	0
14	D	2	Total O 2 2	0
14	E	1	Total O 1 1	0

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.

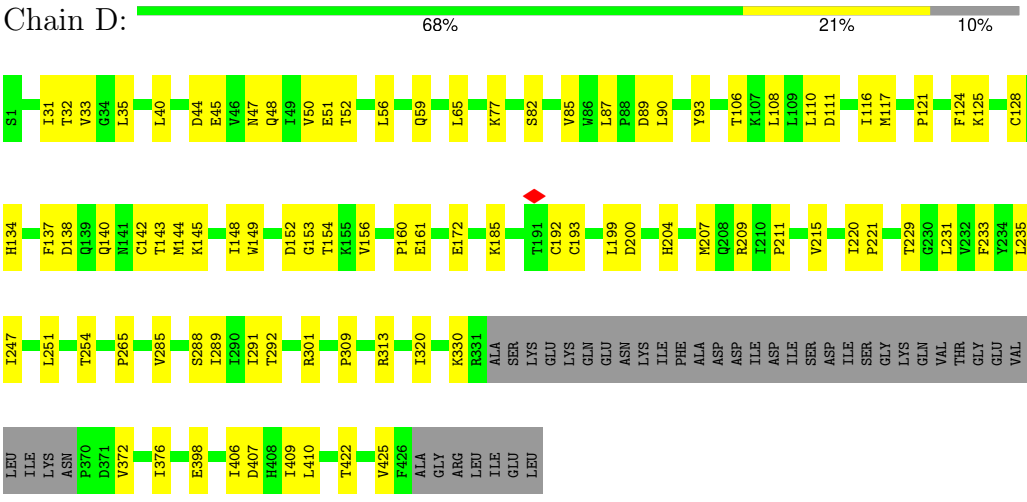
• Molecule 1: Acetylcholine receptor subunit alpha

Chain A:



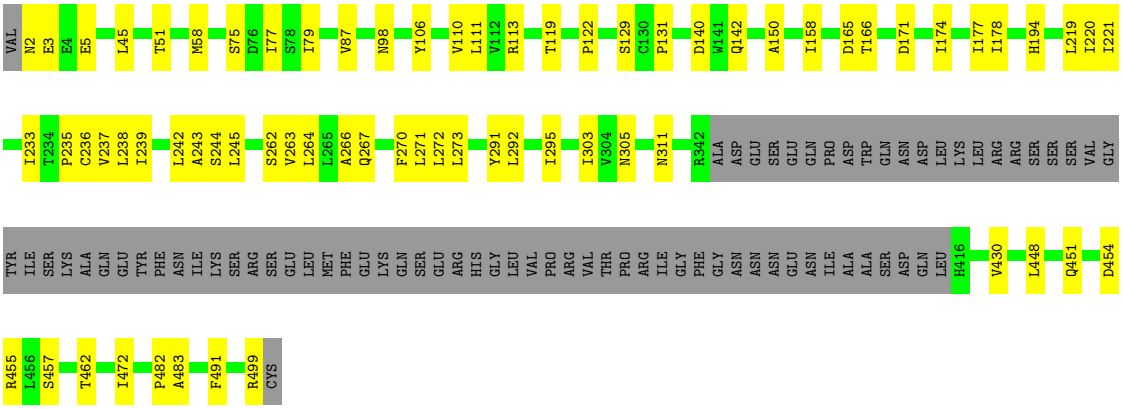
• Molecule 1: Acetylcholine receptor subunit alpha

Chain D:



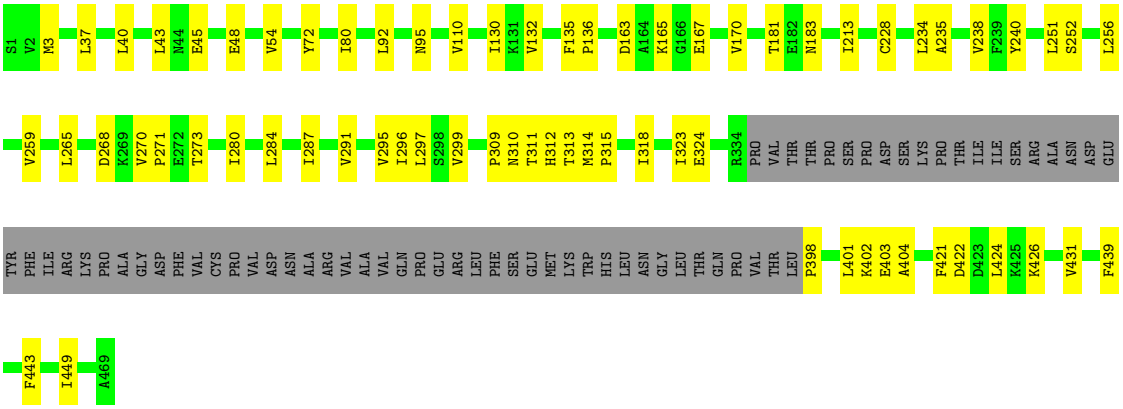
• Molecule 2: Acetylcholine receptor subunit delta

Chain B:



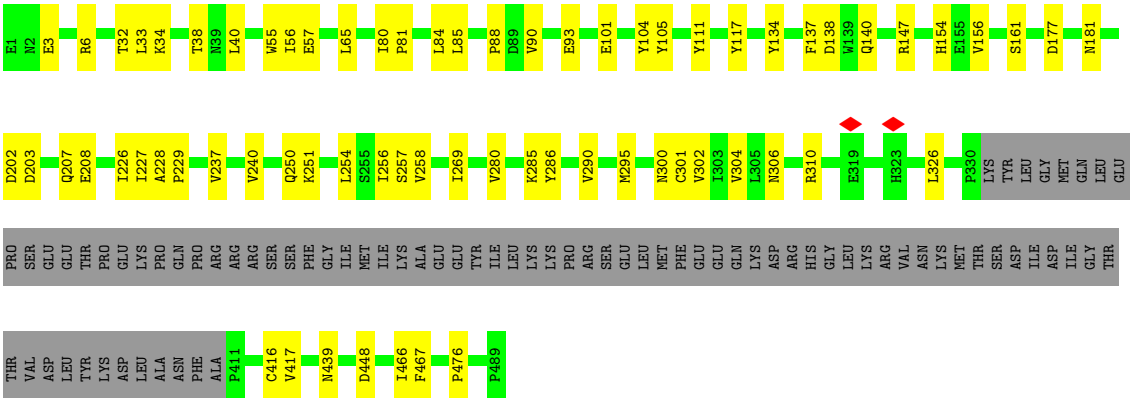
• Molecule 3: Acetylcholine receptor subunit beta

Chain C:



• Molecule 4: Acetylcholine receptor subunit gamma

Chain E:

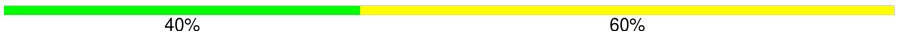


• Molecule 5: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

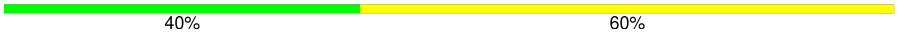
• Molecule 5: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



• Molecule 5: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



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

Chain G:

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

Chain H:

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

Chain I:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	123104	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.094	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0154	Depositor
Map size (Å)	307.98718, 307.98718, 307.98718	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0694, 1.0694, 1.0694	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, POV, SCK, CLR, DD9, NAG, 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	0.33	0/3226	0.48	0/4400
1	D	0.34	0/3237	0.48	0/4414
2	B	0.34	0/3552	0.48	0/4848
3	C	0.35	0/3381	0.47	0/4617
4	E	0.35	0/3404	0.47	0/4645
All	All	0.34	0/16800	0.48	0/22924

There are no bond length outliers.

There are no bond angle outliers.

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	A	3140	0	3164	75	0
1	D	3151	0	3177	82	0
2	B	3456	0	3432	55	0
3	C	3294	0	3307	50	0
4	E	3317	0	3316	52	0
5	F	61	0	52	1	0
5	J	61	0	52	1	0
5	K	61	0	52	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	50	0	43	0	0
7	H	28	0	25	0	0
8	I	39	0	34	0	0
9	A	20	0	30	5	0
9	D	20	0	30	5	0
10	A	28	0	46	2	0
10	C	28	0	46	2	0
10	D	28	0	46	12	0
11	B	14	0	13	0	0
11	E	14	0	13	0	0
12	B	37	0	48	4	0
12	C	70	0	88	1	0
12	D	35	0	44	2	0
12	E	31	0	36	1	0
13	B	9	0	20	0	0
14	B	2	0	0	0	0
14	D	2	0	0	0	0
14	E	1	0	0	0	0
All	All	16997	0	17114	284	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 8.

All (284) 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:145:LYS:HE3	1:D:200:ASP:OD2	1.65	0.94
1:A:245:LEU:HD13	4:E:256:ILE:HD11	1.58	0.85
4:E:237:VAL:HG13	4:E:258:VAL:HG11	1.59	0.84
1:D:45:GLU:OE2	1:D:209:ARG:NH2	2.11	0.83
1:D:138:ASP:OD2	1:D:140:GLN:NE2	2.11	0.82
3:C:449:ILE:HD11	12:C:502:POV:H39	1.62	0.82
1:A:138:ASP:OD2	1:A:140:GLN:NE2	2.14	0.80
2:B:244:SER:OG	2:B:462:THR:OG1	1.91	0.80
1:D:211:PRO:O	1:D:215:VAL:HG23	1.82	0.79
3:C:40:LEU:O	3:C:183:ASN:ND2	2.16	0.79
2:B:236:CYS:SG	2:B:267:GLN:OE1	2.41	0.77
1:D:143:THR:HG21	5:J:1:NAG:H62	1.65	0.77
2:B:98:ASN:OD1	2:B:129:SER:OG	2.03	0.76
4:E:40:LEU:O	4:E:181:ASN:ND2	2.18	0.76
2:B:51:THR:OG1	2:B:98:ASN:ND2	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:235:ALA:O	3:C:238:VAL:HG12	1.86	0.76
1:A:145:LYS:HE3	1:A:200:ASP:OD2	1.87	0.74
1:D:44:ASP:OD2	1:D:47:ASN:ND2	2.23	0.72
1:D:320:ILE:HG21	1:D:409:ILE:HD11	1.72	0.71
3:C:313:THR:OG1	1:D:330:LYS:HG2	1.90	0.71
1:A:152:ASP:OD2	1:A:154:THR:OG1	2.07	0.71
3:C:311:THR:HG23	3:C:312:HIS:ND1	2.08	0.69
4:E:3:GLU:OE2	4:E:6:ARG:NH2	2.24	0.69
1:A:258:LEU:HD13	2:B:273:LEU:CD2	2.23	0.69
1:D:244:THR:OG1	4:E:250:GLN:NE2	2.25	0.69
1:A:82:SER:OG	1:A:106:THR:O	2.08	0.68
2:B:140:ASP:OD2	2:B:142:GLN:NE2	2.26	0.68
1:A:185:LYS:HE3	1:A:199:LEU:HD23	1.76	0.68
1:A:286:ILE:HD13	2:B:238:LEU:HB3	1.76	0.67
4:E:147:ARG:NH2	4:E:208:GLU:OE1	2.26	0.67
1:A:260:ILE:HD12	1:A:278:MET:CE	2.25	0.67
1:D:192:CYS:O	9:D:501:SCK:H83	1.94	0.67
1:A:254:THR:HG21	2:B:239:ILE:HD11	1.77	0.67
3:C:92:LEU:O	3:C:95:ASN:ND2	2.28	0.67
1:D:185:LYS:HE3	1:D:199:LEU:HD23	1.78	0.66
3:C:310:ASN:OD1	3:C:421:PHE:CE2	2.49	0.66
1:A:254:THR:HG22	1:A:282:MET:CE	2.27	0.65
3:C:422:ASP:O	3:C:426:LYS:HG2	1.96	0.65
1:D:108:LEU:HD13	1:D:116:ILE:HG23	1.79	0.64
1:A:229:THR:O	1:A:232:VAL:HG12	1.98	0.64
1:D:301:ARG:HH22	10:D:503:CLR:H42	1.62	0.64
1:A:224:LEU:HD22	4:E:295:MET:SD	2.38	0.63
1:D:138:ASP:OD1	1:D:209:ARG:NH1	2.30	0.63
2:B:3:GLU:OE1	2:B:75:SER:N	2.31	0.63
2:B:305:ASN:ND2	2:B:457:SER:OG	2.32	0.63
2:B:454:ASP:OD1	2:B:455:ARG:N	2.31	0.63
12:B:602:POV:H3A	12:B:602:POV:H36	1.81	0.62
2:B:243:ALA:HB2	2:B:263:VAL:HG11	1.80	0.62
3:C:299:VAL:HG22	1:D:235:LEU:HD13	1.81	0.62
9:D:501:SCK:H32	4:E:117:TYR:CE1	2.35	0.62
1:A:258:LEU:HD13	2:B:273:LEU:HD22	1.80	0.61
4:E:101:GLU:OE1	4:E:105:TYR:OH	2.16	0.61
1:A:232:VAL:O	1:A:242:LYS:NZ	2.26	0.61
1:A:143:THR:HG22	1:A:204:HIS:CB	2.31	0.60
3:C:398:PRO:HB2	3:C:401:LEU:HD13	1.83	0.60
3:C:132:VAL:HG12	3:C:271:PRO:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:439:PHE:HZ	10:C:501:CLR:H181	1.66	0.60
9:A:501:SCK:H31	2:B:113:ARG:HH22	1.65	0.60
2:B:113:ARG:NH1	2:B:119:THR:OG1	2.35	0.59
1:D:143:THR:HG22	1:D:204:HIS:CB	2.31	0.59
3:C:404:ALA:HB2	1:D:376:ILE:HG23	1.83	0.59
1:A:260:ILE:HD12	1:A:278:MET:HE1	1.85	0.59
1:D:301:ARG:HH12	10:D:503:CLR:H42	1.68	0.59
1:D:132:VAL:HG11	1:D:265:PRO:HD2	1.83	0.59
3:C:256:LEU:O	3:C:259:VAL:HG12	2.04	0.58
2:B:491:PHE:HB2	2:B:499:ARG:HH21	1.69	0.58
1:A:143:THR:HG22	1:A:204:HIS:HB2	1.86	0.57
4:E:138:ASP:OD2	4:E:140:GLN:NE2	2.35	0.57
1:A:294:VAL:HG11	10:A:502:CLR:H182	1.87	0.57
4:E:88:PRO:O	4:E:90:VAL:N	2.37	0.57
4:E:280:VAL:O	4:E:285:LYS:NZ	2.38	0.57
4:E:304:VAL:HG21	4:E:448:ASP:OD1	2.06	0.56
1:A:254:THR:HG22	1:A:282:MET:HE1	1.87	0.56
1:D:143:THR:HG22	1:D:204:HIS:HB3	1.87	0.56
1:A:305:THR:HG21	2:B:448:LEU:HD21	1.87	0.56
1:D:152:ASP:OD2	1:D:154:THR:OG1	2.17	0.56
1:D:301:ARG:NH2	10:D:503:CLR:H42	2.19	0.55
4:E:65:LEU:HD11	4:E:85:LEU:HD22	1.89	0.55
2:B:174:ILE:HG21	2:B:178:ILE:HD11	1.87	0.55
1:D:40:LEU:HD12	1:D:52:THR:HG22	1.88	0.55
1:A:77:LYS:NZ	1:A:111:ASP:OD1	2.34	0.55
1:D:247:ILE:HG21	4:E:257:SER:CB	2.37	0.55
4:E:476:PRO:HG2	5:K:1:NAG:H81	1.87	0.55
4:E:228:ALA:HB3	4:E:229:PRO:HD3	1.89	0.54
9:A:501:SCK:H92	2:B:113:ARG:NH2	2.22	0.54
1:D:93:TYR:CD2	1:D:145:LYS:HE2	2.43	0.54
1:A:250:LEU:O	1:A:254:THR:HG23	2.08	0.54
1:A:257:LEU:HD22	1:A:282:MET:SD	2.47	0.54
2:B:291:TYR:HB2	2:B:472:ILE:HG21	1.89	0.54
1:A:254:THR:HG22	1:A:282:MET:HE3	1.91	0.53
2:B:45:LEU:CD1	2:B:221:ILE:HD11	2.39	0.53
12:D:502:POV:H25A	10:D:503:CLR:H183	1.91	0.53
9:D:501:SCK:H92	4:E:111:TYR:OH	2.09	0.53
4:E:33:LEU:HD11	4:E:56:ILE:HD11	1.89	0.53
2:B:166:THR:OG1	2:B:171:ASP:OD1	2.16	0.53
1:D:309:PRO:HG2	10:D:503:CLR:H3	1.91	0.53
1:A:407:ASP:OD1	1:A:408:HIS:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:ILE:HD11	2:B:111:LEU:HD23	1.91	0.53
12:B:602:POV:H25	12:B:602:POV:H36A	1.91	0.53
1:A:185:LYS:CE	1:A:199:LEU:HD23	2.40	0.52
1:A:143:THR:HB	1:A:203:TYR:O	2.09	0.52
3:C:314:MET:HE3	3:C:431:VAL:HG21	1.92	0.52
2:B:311:ASN:ND2	3:C:240:TYR:O	2.41	0.52
1:A:108:LEU:HD13	1:A:116:ILE:HG23	1.93	0.51
2:B:177:ILE:HD12	2:B:219:LEU:HD13	1.91	0.51
1:D:301:ARG:NH1	10:D:503:CLR:H42	2.24	0.51
1:A:242:LYS:HE3	1:A:292:THR:HG23	1.93	0.51
3:C:228:CYS:SG	3:C:284:LEU:HD21	2.51	0.51
1:D:51:GLU:HG2	1:D:125:LYS:HG2	1.93	0.51
1:D:59:GLN:HG2	1:D:117:MET:SD	2.51	0.51
4:E:32:THR:HG23	4:E:161:SER:HA	1.92	0.50
1:A:315:ILE:HG23	1:A:316:PHE:N	2.27	0.50
3:C:296:ILE:HA	1:D:231:LEU:HD21	1.94	0.50
3:C:310:ASN:OD1	3:C:421:PHE:HE2	1.92	0.50
1:D:247:ILE:HD11	4:E:254:LEU:HD13	1.94	0.50
1:A:305:THR:HG21	2:B:448:LEU:CD2	2.42	0.50
1:D:149:TRP:O	9:D:501:SCK:H152	2.12	0.50
2:B:233:ILE:O	2:B:237:VAL:HG23	2.12	0.49
1:D:40:LEU:HD21	1:D:207:MET:CE	2.42	0.49
1:D:40:LEU:CD1	1:D:52:THR:HG22	2.41	0.49
4:E:237:VAL:O	4:E:240:VAL:HG22	2.12	0.49
1:D:124:PHE:HD2	1:D:144:MET:SD	2.35	0.49
3:C:252:SER:HB2	3:C:295:VAL:HG22	1.93	0.49
3:C:313:THR:OG1	1:D:330:LYS:CG	2.60	0.49
1:D:40:LEU:HD21	1:D:207:MET:HE1	1.95	0.49
1:D:56:LEU:HD21	1:D:90:LEU:HD23	1.94	0.49
1:A:260:ILE:HD12	1:A:278:MET:HE3	1.94	0.49
4:E:286:TYR:HB2	4:E:466:ILE:HG21	1.95	0.49
4:E:227:ILE:HG23	4:E:467:PHE:CZ	2.48	0.49
1:A:393:SER:O	1:A:397:GLU:OE1	2.30	0.48
1:D:130:ILE:HG22	1:D:132:VAL:HG13	1.94	0.48
4:E:154:HIS:ND1	4:E:202:ASP:OD1	2.46	0.48
4:E:93:GLU:HG3	4:E:147:ARG:CD	2.43	0.48
1:A:19:ILE:HG13	2:B:5:GLU:OE1	2.12	0.48
4:E:81:PRO:HG2	4:E:84:LEU:HD12	1.95	0.48
1:A:35:LEU:HD21	1:A:144:MET:SD	2.53	0.48
1:A:406:ILE:O	1:A:410:LEU:HD23	2.13	0.48
3:C:136:PRO:HD3	3:C:280:ILE:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:ASP:O	1:D:48:GLN:N	2.46	0.48
1:D:406:ILE:HD11	10:D:503:CLR:H151	1.95	0.48
1:A:63:VAL:HG12	1:A:66:ARG:NH2	2.28	0.48
1:A:378:GLY:HA3	2:B:430:VAL:HG21	1.94	0.48
1:A:149:TRP:O	9:A:501:SCK:H203	2.12	0.48
1:D:35:LEU:HD21	1:D:144:MET:HE1	1.96	0.48
1:D:410:LEU:HD21	10:D:503:CLR:H242	1.95	0.48
3:C:165:LYS:O	3:C:167:GLU:N	2.43	0.48
1:A:235:LEU:O	1:A:242:LYS:NZ	2.37	0.47
1:A:143:THR:HG21	5:F:1:NAG:H62	1.96	0.47
1:D:185:LYS:CE	1:D:199:LEU:HD23	2.45	0.47
1:A:315:ILE:O	1:A:320:ILE:HD12	2.14	0.47
3:C:268:ASP:OD1	3:C:268:ASP:O	2.32	0.47
1:A:224:LEU:CD2	4:E:295:MET:SD	3.02	0.47
1:D:33:VAL:O	1:D:160:PRO:HA	2.15	0.47
1:A:44:ASP:O	1:A:48:GLN:N	2.48	0.47
2:B:482:PRO:O	2:B:483:ALA:HB3	2.15	0.47
3:C:287:ILE:O	3:C:291:VAL:HG23	2.14	0.47
12:B:602:POV:H2	12:B:602:POV:H34	1.97	0.46
3:C:163:ASP:N	3:C:163:ASP:OD1	2.48	0.46
1:D:89:ASP:HB2	4:E:104:TYR:OH	2.15	0.46
4:E:56:ILE:HG23	4:E:56:ILE:O	2.15	0.46
1:A:228:LEU:HA	1:A:231:LEU:HD13	1.97	0.46
1:A:375:ALA:O	1:A:379:VAL:HG23	2.15	0.46
2:B:235:PRO:HB2	2:B:270:PHE:CZ	2.51	0.46
1:D:247:ILE:HG21	4:E:257:SER:HB2	1.97	0.46
1:D:313:ARG:NH1	1:D:398:GLU:OE1	2.48	0.46
2:B:150:ALA:HB1	2:B:158:ILE:HD11	1.98	0.46
1:A:311:TRP:O	1:A:315:ILE:HG22	2.14	0.46
1:D:35:LEU:HD21	1:D:144:MET:CE	2.46	0.46
3:C:314:MET:CE	3:C:431:VAL:HG21	2.45	0.46
3:C:309:PRO:O	1:D:330:LYS:HD3	2.16	0.45
4:E:80:ILE:HB	4:E:85:LEU:HD11	1.97	0.45
1:A:245:LEU:HD13	4:E:256:ILE:CD1	2.37	0.45
1:A:286:ILE:HD13	2:B:238:LEU:CB	2.46	0.45
2:B:303:ILE:HG21	3:C:234:LEU:HD22	1.98	0.45
3:C:43:LEU:HD22	3:C:213:ILE:HD11	1.99	0.45
1:D:289:ILE:HA	1:D:292:THR:HG22	1.99	0.45
1:A:89:ASP:HB2	2:B:106:TYR:OH	2.16	0.45
1:A:231:LEU:HB3	4:E:302:VAL:HG21	1.99	0.45
2:B:239:ILE:HG21	2:B:266:ALA:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:48:GLU:OE2	3:C:273:THR:HG21	2.16	0.45
1:D:50:VAL:HG23	1:D:128:CYS:CB	2.46	0.45
3:C:309:PRO:O	1:D:330:LYS:CD	2.65	0.45
2:B:58:MET:O	2:B:122:PRO:HD2	2.16	0.45
3:C:43:LEU:HD11	3:C:130:ILE:HD11	1.99	0.45
1:D:233:PHE:CA	1:D:407:ASP:OD1	2.65	0.45
3:C:45:GLU:HB3	3:C:271:PRO:HG3	1.99	0.44
1:D:242:LYS:NZ	1:D:407:ASP:OD2	2.49	0.44
1:D:372:VAL:HG22	4:E:417:VAL:HG21	1.99	0.44
1:D:106:THR:HG21	1:D:121:PRO:HD3	1.99	0.44
2:B:165:ASP:OD1	2:B:166:THR:N	2.50	0.44
1:D:301:ARG:HH22	10:D:503:CLR:H192	1.83	0.44
1:A:254:THR:CG2	2:B:239:ILE:HD11	2.47	0.44
3:C:170:VAL:O	3:C:170:VAL:HG13	2.17	0.44
1:D:134:HIS:O	1:D:137:PHE:N	2.48	0.44
1:D:233:PHE:HB3	1:D:407:ASP:OD1	2.18	0.44
1:D:406:ILE:O	1:D:410:LEU:HD23	2.18	0.44
4:E:32:THR:HG23	4:E:161:SER:CA	2.48	0.44
4:E:286:TYR:CZ	4:E:290:VAL:HG11	2.52	0.44
1:A:397:GLU:OE1	1:A:397:GLU:N	2.50	0.44
4:E:306:ASN:O	4:E:310:ARG:HG3	2.18	0.44
1:A:89:ASP:OD1	1:A:148:ILE:HG23	2.17	0.43
3:C:80:ILE:HD12	3:C:110:VAL:HG21	2.00	0.43
1:D:89:ASP:OD1	1:D:148:ILE:HG23	2.18	0.43
1:A:91:VAL:HG13	1:A:100:PHE:HB3	2.00	0.43
3:C:3:MET:SD	3:C:72:TYR:HA	2.58	0.43
10:C:501:CLR:H222	10:C:501:CLR:H162	1.91	0.43
4:E:300:ASN:ND2	12:E:502:POV:H37	2.33	0.43
4:E:240:VAL:HG21	4:E:301:CYS:SG	2.58	0.43
4:E:251:LYS:HG2	4:E:301:CYS:SG	2.58	0.43
3:C:309:PRO:HG3	3:C:424:LEU:HB3	2.01	0.43
1:D:65:LEU:HB3	1:D:110:LEU:HD21	2.01	0.43
1:D:233:PHE:O	1:D:407:ASP:OD1	2.37	0.43
10:D:503:CLR:H221	10:D:503:CLR:H162	1.30	0.43
1:A:290:ILE:HA	2:B:245:LEU:HD21	2.00	0.43
2:B:271:LEU:HA	2:B:292:LEU:HD13	2.01	0.43
3:C:315:PRO:CG	3:C:318:ILE:HD12	2.48	0.43
1:D:82:SER:HB2	1:D:87:LEU:HD11	2.01	0.43
1:D:233:PHE:HA	1:D:407:ASP:OD1	2.18	0.43
1:D:291:ILE:HG21	1:D:410:LEU:HG	1.99	0.43
2:B:264:LEU:HD22	3:C:234:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:ILE:HG21	2:B:266:ALA:CB	2.48	0.43
4:E:202:ASP:O	4:E:203:ASP:HB2	2.19	0.43
3:C:323:ILE:HD11	3:C:431:VAL:HG23	2.01	0.43
3:C:403:GLU:OE1	3:C:403:GLU:HA	2.19	0.43
1:D:172:GLU:OE1	1:D:172:GLU:HA	2.18	0.43
2:B:272:LEU:HD13	3:C:265:LEU:HD22	2.00	0.43
2:B:491:PHE:HB2	2:B:499:ARG:NH2	2.32	0.43
1:A:108:LEU:O	1:A:108:LEU:HD12	2.19	0.42
1:D:153:GLY:CA	1:D:199:LEU:HD13	2.49	0.42
12:D:502:POV:H31A	12:D:502:POV:H37A	1.48	0.42
4:E:38:THR:HG21	4:E:55:TRP:CE2	2.54	0.42
1:A:291:ILE:HD13	1:A:410:LEU:HD11	1.99	0.42
2:B:292:LEU:HA	2:B:295:ILE:HG22	2.01	0.42
1:D:77:LYS:NZ	1:D:111:ASP:OD1	2.45	0.42
4:E:226:ILE:HG21	4:E:269:ILE:HD11	2.00	0.42
3:C:238:VAL:HA	3:C:251:LEU:HD23	2.00	0.42
1:D:193:CYS:SG	9:D:501:SCK:H22	2.59	0.42
1:D:406:ILE:CD1	10:D:503:CLR:H151	2.49	0.42
1:A:237:THR:HG23	1:A:296:ILE:HG12	2.02	0.42
1:A:376:ILE:HG23	4:E:416:CYS:HB2	2.00	0.42
1:A:404:MET:O	1:A:407:ASP:OD1	2.37	0.42
1:A:406:ILE:HD11	10:A:502:CLR:H72	2.01	0.42
1:D:32:THR:HG22	1:D:161:GLU:HG3	2.01	0.42
1:A:298:THR:HA	1:A:301:ARG:HG2	2.02	0.42
1:A:63:VAL:HG12	1:A:66:ARG:HH22	1.85	0.42
12:B:602:POV:H25A	12:B:602:POV:H22	1.71	0.42
1:D:85:VAL:CG2	1:D:108:LEU:HD21	2.49	0.42
3:C:324:GLU:OE1	3:C:324:GLU:N	2.53	0.42
1:D:220:ILE:HB	1:D:221:PRO:HD3	2.02	0.42
1:A:415:MET:O	1:A:419:ILE:HG12	2.20	0.42
1:A:23:GLU:O	2:B:2:ASN:N	2.53	0.41
1:A:247:ILE:HG21	2:B:262:SER:CB	2.50	0.41
3:C:37:LEU:HD12	3:C:54:VAL:HG12	2.03	0.41
3:C:135:PHE:CE1	3:C:270:VAL:HG12	2.55	0.41
1:D:233:PHE:O	1:D:407:ASP:CG	2.58	0.41
1:A:134:HIS:O	1:A:137:PHE:N	2.53	0.41
2:B:87:VAL:HG21	2:B:110:VAL:HG21	2.02	0.41
3:C:398:PRO:O	3:C:402:LYS:HD3	2.20	0.41
1:D:229:THR:CG2	1:D:285:VAL:HG22	2.50	0.41
4:E:55:TRP:CZ2	4:E:177:ASP:OD2	2.73	0.41
1:A:82:SER:OG	1:A:118:TRP:NE1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ILE:HG12	2:B:242:LEU:HD11	2.02	0.41
1:A:320:ILE:N	1:A:321:PRO:CD	2.84	0.41
2:B:454:ASP:OD1	2:B:454:ASP:C	2.59	0.41
3:C:297:LEU:HD12	3:C:443:PHE:CE1	2.55	0.41
1:D:31:ILE:HD12	1:D:156:VAL:CG1	2.51	0.41
1:A:192:CYS:O	9:A:501:SCK:H83	2.21	0.41
2:B:194:HIS:HB2	2:B:220:ILE:HD13	2.02	0.41
2:B:75:SER:O	2:B:77:ILE:HG13	2.21	0.41
1:D:251:LEU:O	1:D:254:THR:HG22	2.20	0.41
1:D:288:SER:O	1:D:292:THR:HG22	2.21	0.41
4:E:34:LYS:HB3	4:E:57:GLU:HB3	2.03	0.41
10:D:503:CLR:H183	10:D:503:CLR:H20	1.99	0.41
2:B:131:PRO:HG3	3:C:181:THR:HG21	2.03	0.40
4:E:3:GLU:OE2	4:E:6:ARG:NE	2.54	0.40
1:A:407:ASP:OD1	1:A:407:ASP:C	2.60	0.40
4:E:304:VAL:HG11	4:E:448:ASP:OD1	2.21	0.40
4:E:326:LEU:HD11	4:E:439:ASN:OD1	2.22	0.40
1:D:50:VAL:HG21	1:D:142:CYS:SG	2.61	0.40
1:D:422:THR:O	1:D:425:VAL:HG12	2.22	0.40
4:E:134:TYR:O	4:E:137:PHE:N	2.53	0.40
1:A:192:CYS:SG	9:A:501:SCK:H193	2.61	0.40
2:B:451:GLN:O	2:B:454:ASP:OD1	2.39	0.40
4:E:156:VAL:O	4:E:207:GLN:NE2	2.49	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	383/433 (88%)	373 (97%)	10 (3%)	0	100	100
1	D	384/433 (89%)	376 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	421/500 (84%)	409 (97%)	12 (3%)	0	100	100
3	C	402/469 (86%)	386 (96%)	16 (4%)	0	100	100
4	E	405/489 (83%)	392 (97%)	13 (3%)	0	100	100
All	All	1995/2324 (86%)	1936 (97%)	59 (3%)	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	362/402 (90%)	362 (100%)	0	100	100
1	D	363/402 (90%)	363 (100%)	0	100	100
2	B	391/458 (85%)	391 (100%)	0	100	100
3	C	374/431 (87%)	374 (100%)	0	100	100
4	E	373/446 (84%)	373 (100%)	0	100	100
All	All	1863/2139 (87%)	1863 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
2	B	305	ASN
1	D	204	HIS
1	D	385	HIS
4	E	250	GLN
4	E	300	ASN
4	E	437	ASN

5.3.3 RNA (i)

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)

24 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	F	1	1,5	14,14,15	0.41	0	17,19,21	0.41	0
5	NAG	F	2	5	14,14,15	0.25	0	17,19,21	0.49	0
5	BMA	F	3	5	11,11,12	0.43	0	15,15,17	0.73	0
5	MAN	F	4	5	11,11,12	0.57	0	15,15,17	0.93	1 (6%)
5	MAN	F	5	5	11,11,12	0.79	1 (9%)	15,15,17	1.18	2 (13%)
6	NAG	G	1	6,2	14,14,15	0.31	0	17,19,21	0.49	0
6	NAG	G	2	6	14,14,15	0.17	0	17,19,21	0.49	0
6	BMA	G	3	6	11,11,12	0.49	0	15,15,17	0.73	0
6	MAN	G	4	6	11,11,12	0.65	0	15,15,17	1.06	2 (13%)
7	NAG	H	1	2,7	14,14,15	0.34	0	17,19,21	0.64	1 (5%)
7	NAG	H	2	7	14,14,15	0.23	0	17,19,21	0.39	0
8	NAG	I	1	8,3	14,14,15	0.52	0	17,19,21	0.41	0
8	NAG	I	2	8	14,14,15	0.20	0	17,19,21	0.50	0
8	BMA	I	3	8	11,11,12	0.53	0	15,15,17	0.62	0
5	NAG	J	1	1,5	14,14,15	0.56	0	17,19,21	0.41	0
5	NAG	J	2	5	14,14,15	0.42	0	17,19,21	0.49	0
5	BMA	J	3	5	11,11,12	0.55	0	15,15,17	0.67	0
5	MAN	J	4	5	11,11,12	0.54	0	15,15,17	0.96	2 (13%)
5	MAN	J	5	5	11,11,12	0.77	1 (9%)	15,15,17	1.01	1 (6%)
5	NAG	K	1	4,5	14,14,15	0.47	0	17,19,21	0.49	0
5	NAG	K	2	5	14,14,15	0.31	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	BMA	K	3	5	11,11,12	0.47	0	15,15,17	0.82	0
5	MAN	K	4	5	11,11,12	0.85	1 (9%)	15,15,17	1.09	1 (6%)
5	MAN	K	5	5	11,11,12	1.02	1 (9%)	15,15,17	1.29	3 (20%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	5	MAN	C1-C2	2.98	1.59	1.52
5	F	5	MAN	C1-C2	2.37	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	4	MAN	C1-C2	2.20	1.57	1.52
5	J	5	MAN	C1-C2	2.01	1.57	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	4	MAN	C1-O5-C5	2.59	115.66	112.19
5	J	5	MAN	O2-C2-C3	-2.45	105.07	110.15
5	K	5	MAN	C1-O5-C5	2.41	115.41	112.19
5	F	5	MAN	C1-O5-C5	2.34	115.33	112.19
5	K	5	MAN	C1-C2-C3	2.33	113.04	109.64
5	F	4	MAN	O2-C2-C3	-2.31	105.36	110.15
5	J	4	MAN	C1-O5-C5	2.30	115.28	112.19
5	K	5	MAN	O2-C2-C3	-2.30	105.38	110.15
5	F	5	MAN	O2-C2-C3	-2.30	105.38	110.15
5	K	4	MAN	O2-C2-C3	-2.26	105.48	110.15
5	J	4	MAN	O2-C2-C3	-2.20	105.59	110.15
6	G	4	MAN	O2-C2-C3	-2.19	105.62	110.15
7	H	1	NAG	C1-O5-C5	2.11	115.01	112.19

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	2	NAG	C1-C2-N2-C7
8	I	1	NAG	O5-C5-C6-O6
5	F	1	NAG	O5-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
8	I	1	NAG	C4-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
5	J	5	MAN	O5-C5-C6-O6
5	J	5	MAN	C4-C5-C6-O6
6	G	1	NAG	O5-C5-C6-O6
5	K	3	BMA	O5-C5-C6-O6
5	K	3	BMA	C4-C5-C6-O6
7	H	1	NAG	O5-C5-C6-O6
7	H	1	NAG	C4-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
6	G	1	NAG	C4-C5-C6-O6
5	K	5	MAN	O5-C5-C6-O6
7	H	2	NAG	C4-C5-C6-O6

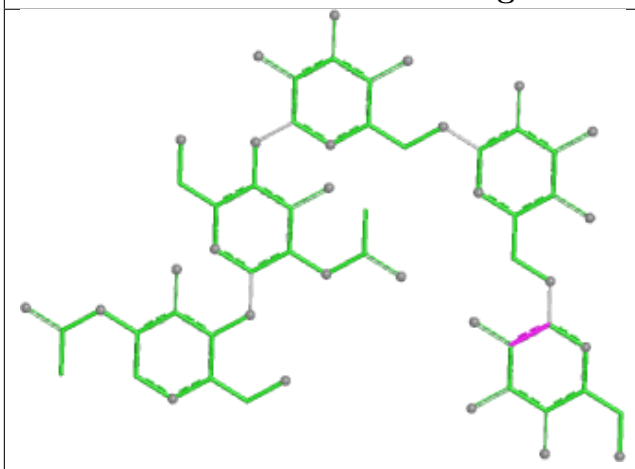
There are no ring outliers.

3 monomers are involved in 3 short contacts:

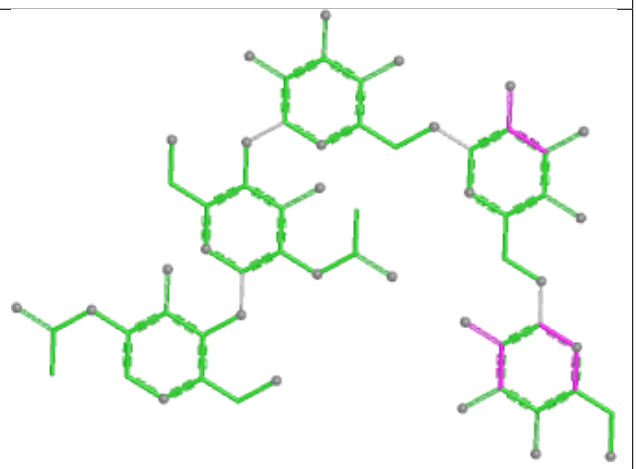
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	1	NAG	1	0
5	K	1	NAG	1	0
5	F	1	NAG	1	0

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

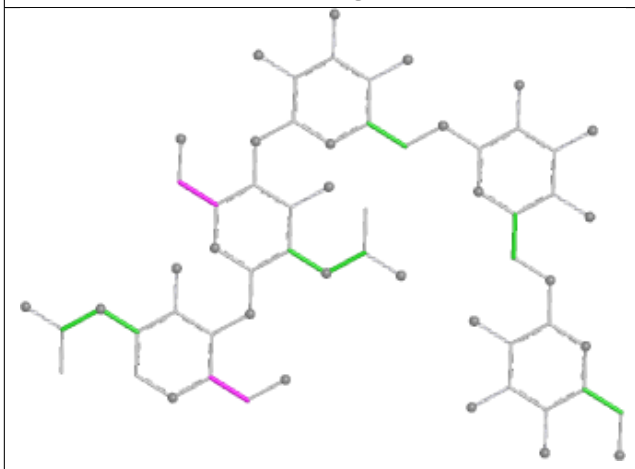
Oligosaccharide Chain F



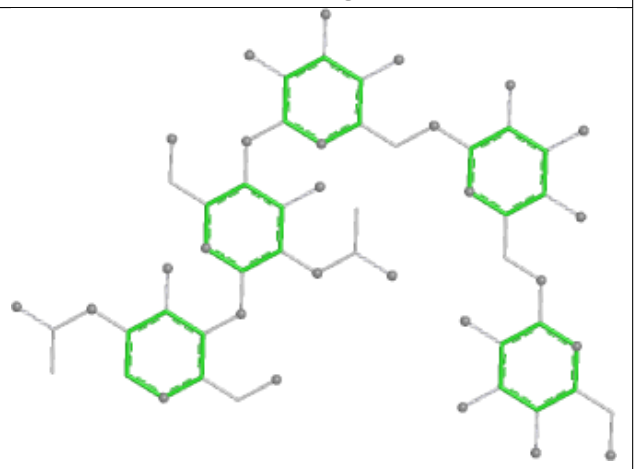
Bond lengths



Bond angles

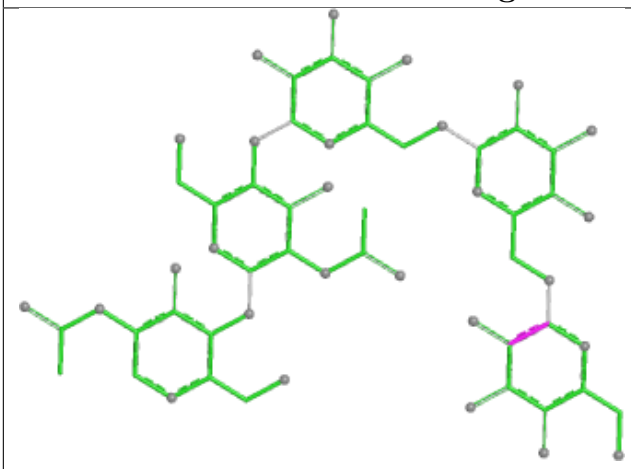


Torsions

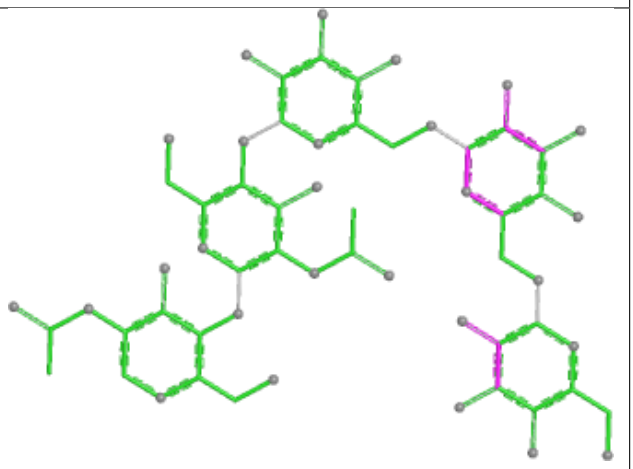


Rings

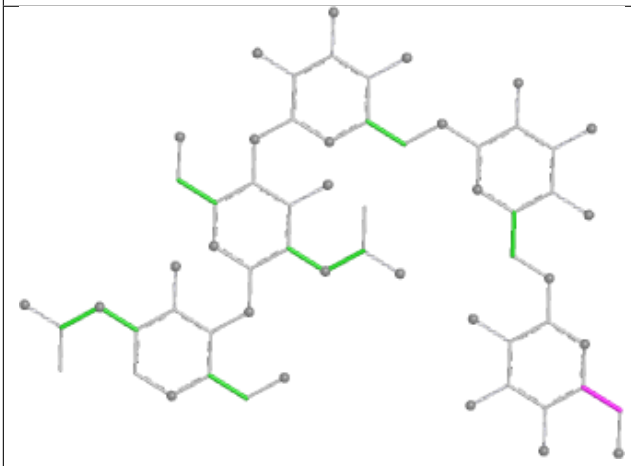
Oligosaccharide Chain J



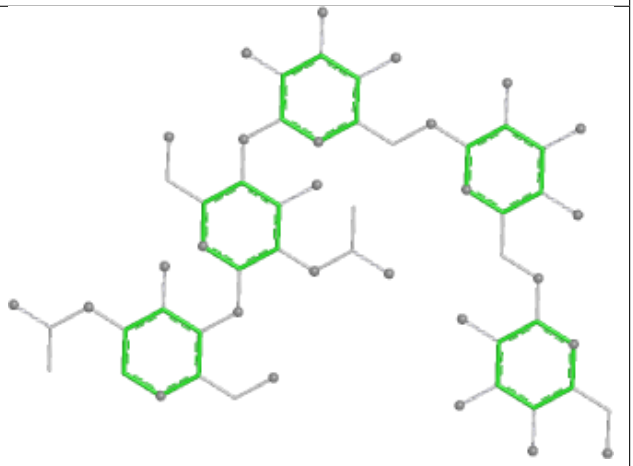
Bond lengths



Bond angles

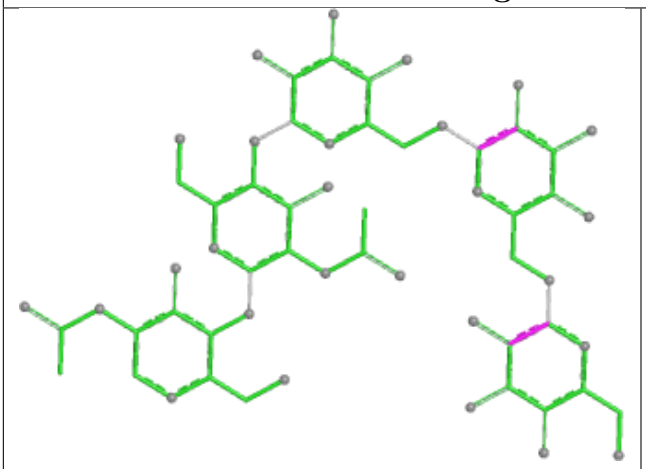


Torsions

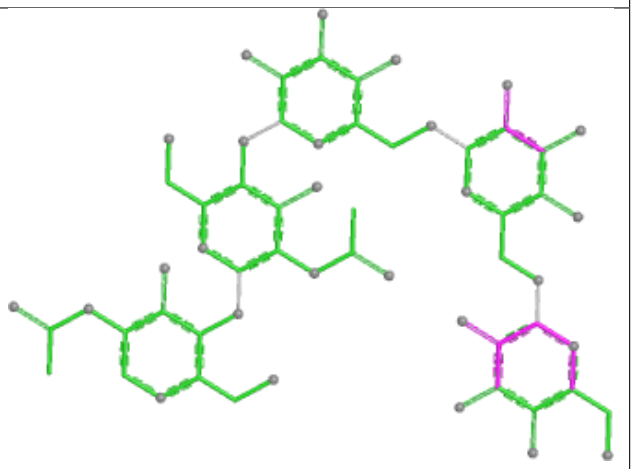


Rings

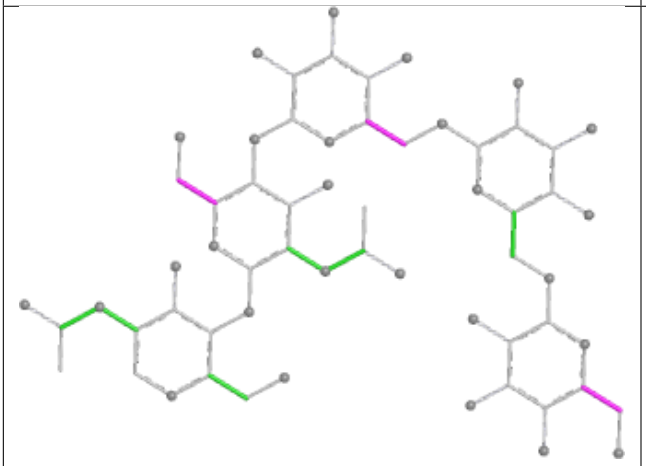
Oligosaccharide Chain K



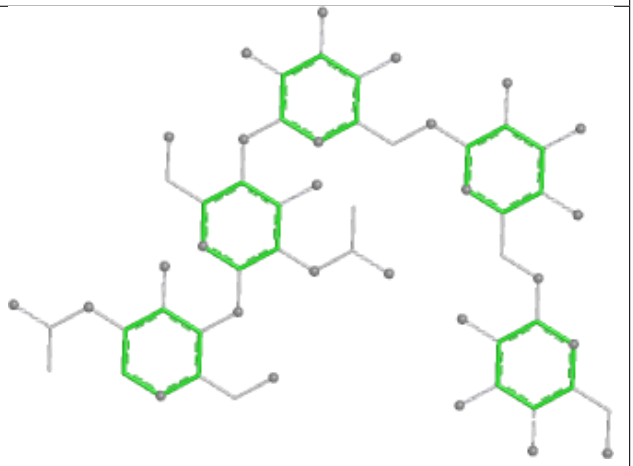
Bond lengths



Bond angles

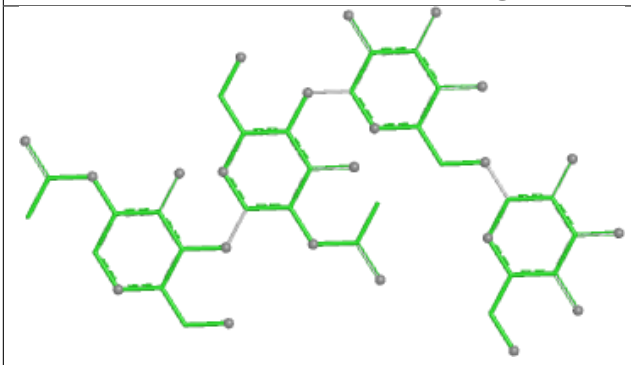


Torsions

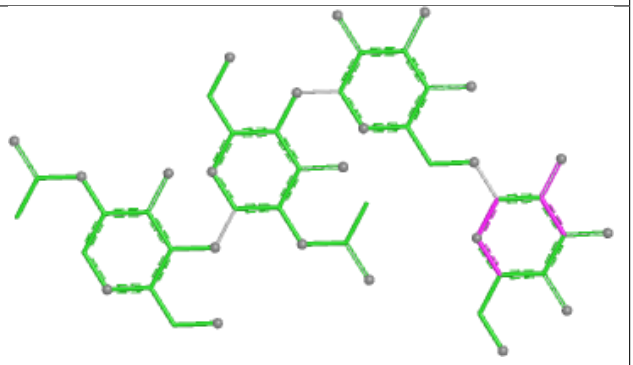


Rings

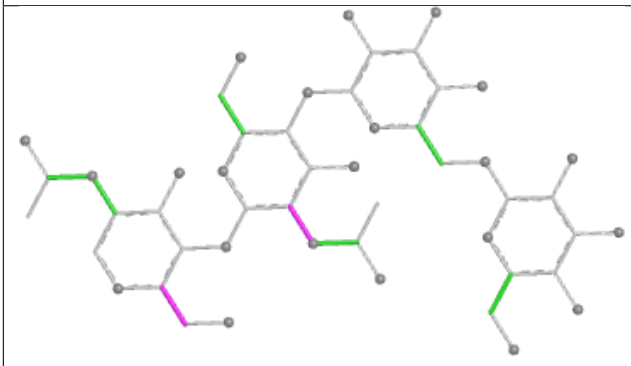
Oligosaccharide Chain G



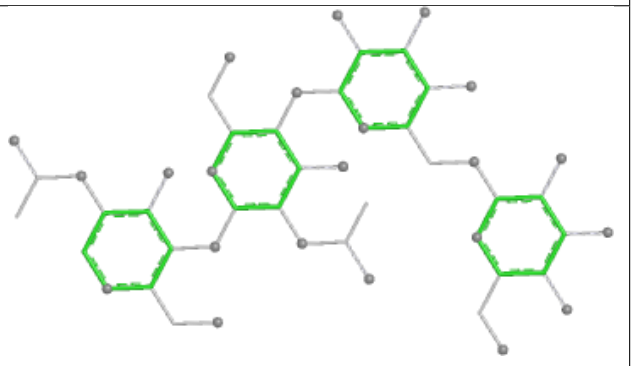
Bond lengths



Bond angles

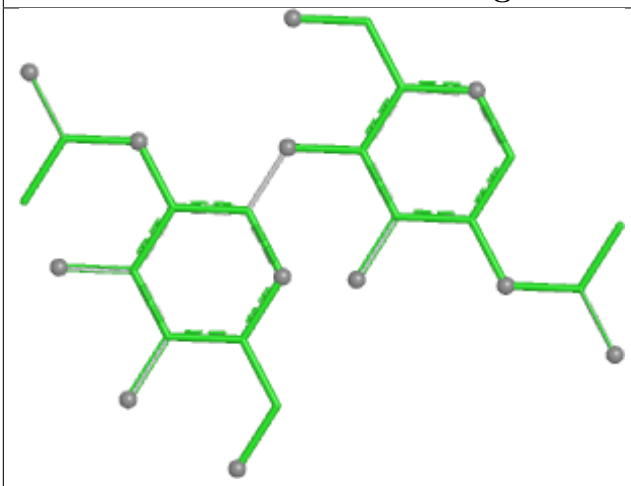


Torsions

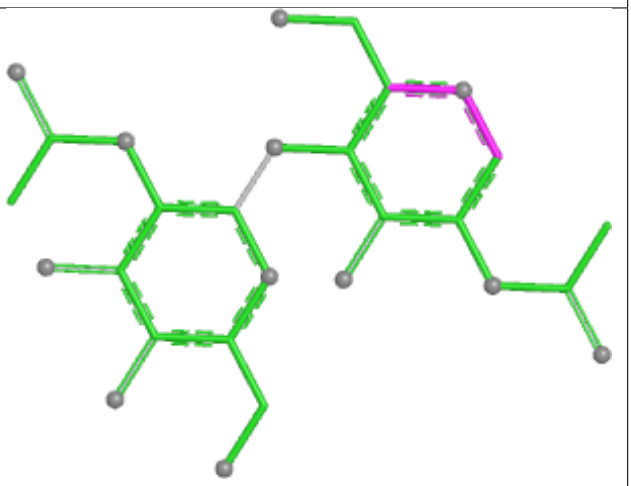


Rings

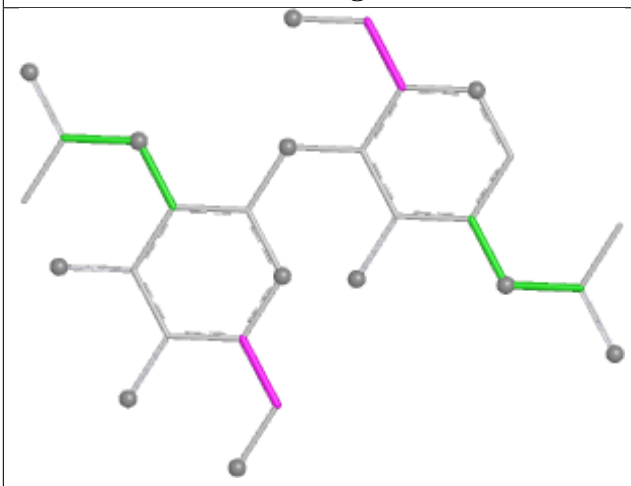
Oligosaccharide Chain H



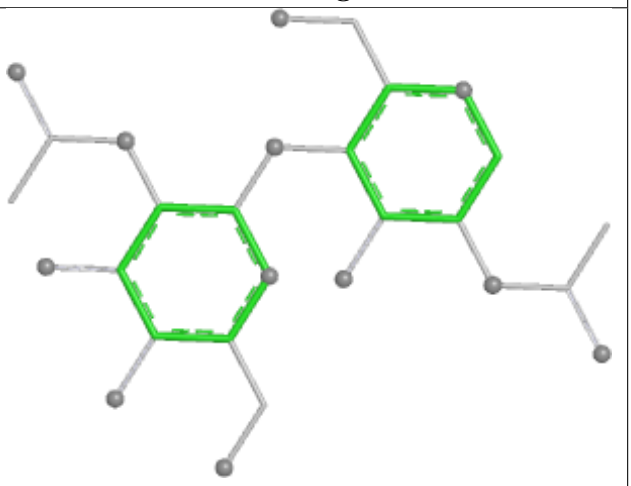
Bond lengths



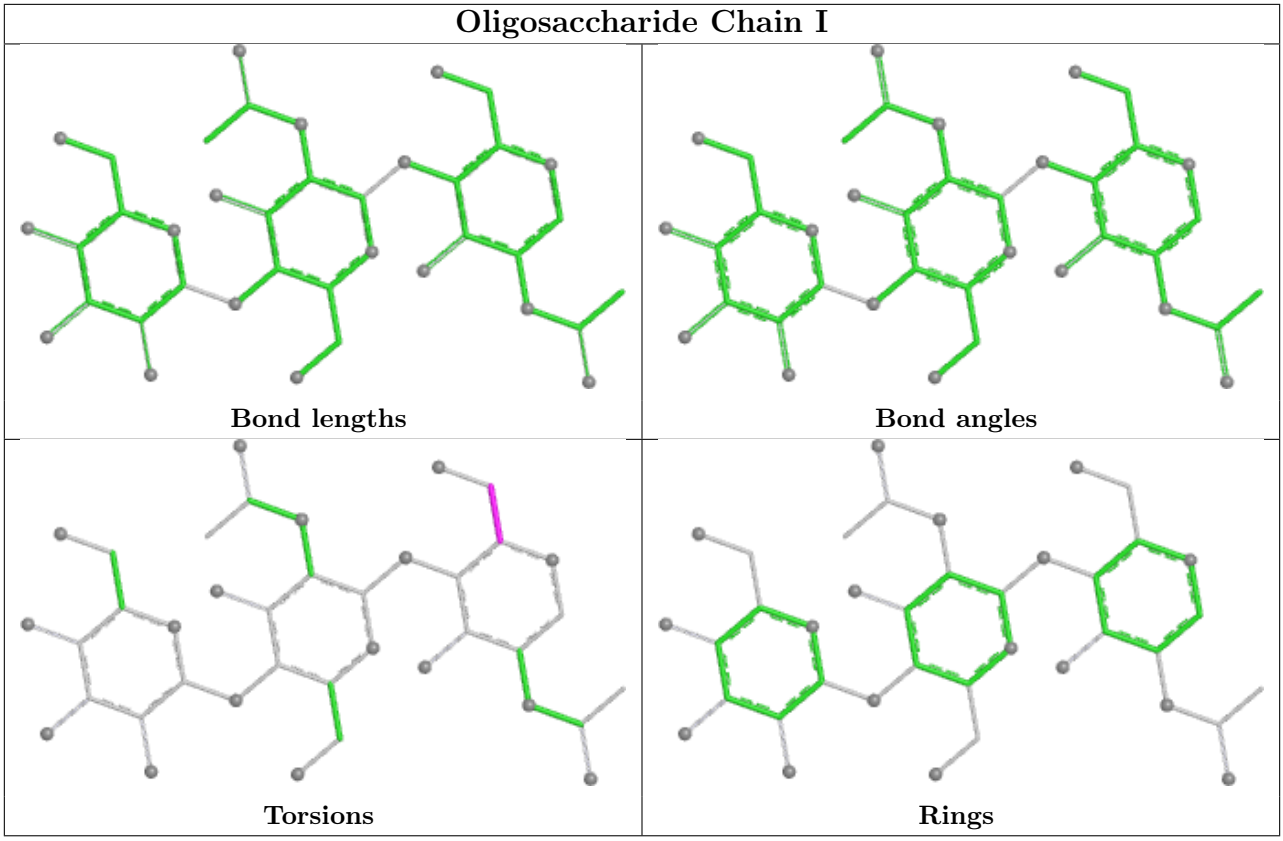
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

13 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	$\#\|Z\| > 2$
10	CLR	A	502	-	31,31,31	0.96	0	48,48,48	0.81	0
10	CLR	C	501	-	31,31,31	0.98	0	48,48,48	1.11	4 (8%)
11	NAG	B	601	2	14,14,15	0.19	0	17,19,21	0.47	0
9	SCK	A	501	-	19,19,19	0.25	0	26,26,26	0.34	0
13	DD9	B	603	-	8,8,8	0.29	0	7,7,7	0.83	0
10	CLR	D	503	-	31,31,31	0.95	0	48,48,48	0.98	2 (4%)
12	POV	C	502	-	34,34,51	1.17	3 (8%)	40,42,59	1.15	2 (5%)
12	POV	C	503	-	34,34,51	1.17	4 (11%)	40,42,59	1.11	2 (5%)
11	NAG	E	501	4	14,14,15	0.22	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	SCK	D	501	-	19,19,19	0.24	0	26,26,26	0.28	0
12	POV	B	602	-	36,36,51	1.14	4 (11%)	42,44,59	1.12	2 (4%)
12	POV	E	502	-	30,30,51	1.25	4 (13%)	36,38,59	1.25	3 (8%)
12	POV	D	502	-	34,34,51	1.19	4 (11%)	40,42,59	1.07	2 (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
10	CLR	A	502	-	-	0/10/68/68	0/4/4/4
10	CLR	C	501	-	-	8/10/68/68	0/4/4/4
11	NAG	B	601	2	-	2/6/23/26	0/1/1/1
9	SCK	A	501	-	-	5/19/19/19	-
13	DD9	B	603	-	-	0/6/6/6	-
10	CLR	D	503	-	-	6/10/68/68	0/4/4/4
12	POV	C	502	-	-	14/38/38/55	-
12	POV	C	503	-	-	20/38/38/55	-
11	NAG	E	501	4	-	4/6/23/26	0/1/1/1
9	SCK	D	501	-	-	10/19/19/19	-
12	POV	B	602	-	-	15/40/40/55	-
12	POV	E	502	-	-	9/34/34/55	-
12	POV	D	502	-	-	17/38/38/55	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	502	POV	O21-C2	-2.80	1.40	1.46
12	E	502	POV	O21-C2	-2.68	1.40	1.46
12	C	503	POV	O21-C2	-2.67	1.40	1.46
12	C	502	POV	O21-C2	-2.61	1.40	1.46
12	B	602	POV	O21-C2	-2.57	1.40	1.46
12	B	602	POV	O31-C31	2.51	1.40	1.33
12	C	503	POV	O31-C31	2.44	1.40	1.33
12	C	502	POV	O31-C31	2.42	1.40	1.33
12	D	502	POV	O31-C3	-2.38	1.39	1.45
12	E	502	POV	O31-C31	2.35	1.40	1.33
12	D	502	POV	O31-C31	2.28	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	E	502	POV	O31-C3	-2.25	1.40	1.45
12	C	503	POV	O21-C21	2.22	1.40	1.34
12	B	602	POV	O21-C21	2.20	1.40	1.34
12	C	503	POV	O31-C3	-2.15	1.40	1.45
12	C	502	POV	O21-C21	2.11	1.40	1.34
12	D	502	POV	O21-C21	2.11	1.40	1.34
12	E	502	POV	O21-C21	2.08	1.40	1.34
12	B	602	POV	O31-C3	-2.05	1.40	1.45

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	E	502	POV	O21-C21-C22	4.48	121.17	111.48
12	C	502	POV	O21-C21-C22	4.33	120.84	111.48
12	B	602	POV	O21-C21-C22	4.14	120.43	111.48
12	C	503	POV	O21-C21-C22	3.90	119.91	111.48
12	D	502	POV	O21-C21-C22	3.84	119.79	111.48
10	C	501	CLR	C14-C8-C9	-3.23	104.86	109.09
12	B	602	POV	O31-C31-C32	2.93	120.77	111.83
10	C	501	CLR	C7-C8-C9	2.93	113.11	109.72
12	C	502	POV	O31-C31-C32	2.90	120.67	111.83
12	C	503	POV	O31-C31-C32	2.85	120.53	111.83
12	E	502	POV	O31-C31-C32	2.64	119.88	111.83
12	D	502	POV	O31-C31-C32	2.50	119.47	111.83
10	D	503	CLR	C15-C14-C13	-2.29	101.15	103.84
10	C	501	CLR	C16-C17-C13	2.23	106.46	103.84
10	C	501	CLR	C16-C15-C14	-2.14	100.95	105.14
10	D	503	CLR	C17-C13-C14	2.06	102.47	100.10
12	E	502	POV	C2-O21-C21	-2.00	113.00	117.80

There are no chirality outliers.

All (110) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	D	503	CLR	C13-C17-C20-C21
10	D	503	CLR	C16-C17-C20-C22
12	B	602	POV	C11-O12-P-O11
12	B	602	POV	C11-O12-P-O13
12	B	602	POV	O12-C11-C12-N
12	C	502	POV	C1-O11-P-O12
12	C	502	POV	C1-O11-P-O13
12	C	502	POV	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
12	C	502	POV	C11-O12-P-O11
12	C	503	POV	C1-O11-P-O12
12	C	503	POV	C1-O11-P-O13
12	C	503	POV	C1-O11-P-O14
12	C	503	POV	C11-O12-P-O11
12	C	503	POV	C11-O12-P-O13
12	C	503	POV	C11-O12-P-O14
12	D	502	POV	C1-O11-P-O12
12	D	502	POV	C1-O11-P-O13
12	D	502	POV	C1-O11-P-O14
12	D	502	POV	C11-O12-P-O11
12	D	502	POV	C11-O12-P-O13
12	D	502	POV	C11-O12-P-O14
12	E	502	POV	C1-O11-P-O12
12	B	602	POV	O32-C31-O31-C3
12	B	602	POV	C32-C31-O31-C3
10	D	503	CLR	C16-C17-C20-C21
10	D	503	CLR	C13-C17-C20-C22
10	D	503	CLR	C21-C20-C22-C23
11	E	501	NAG	O5-C5-C6-O6
9	D	501	SCK	C6-C5-O4-C3
12	C	503	POV	C32-C31-O31-C3
11	B	601	NAG	O5-C5-C6-O6
11	E	501	NAG	C4-C5-C6-O6
12	E	502	POV	C31-C32-C33-C34
10	C	501	CLR	C21-C20-C22-C23
12	D	502	POV	O11-C1-C2-O21
11	B	601	NAG	C4-C5-C6-O6
10	D	503	CLR	C17-C20-C22-C23
12	D	502	POV	C32-C31-O31-C3
9	D	501	SCK	O7-C5-O4-C3
12	C	503	POV	O32-C31-O31-C3
12	C	503	POV	C31-C32-C33-C34
9	D	501	SCK	C12-C11-C6-C5
12	D	502	POV	C37-C38-C39-C310
12	B	602	POV	C22-C23-C24-C25
12	D	502	POV	C36-C37-C38-C39
12	D	502	POV	O32-C31-O31-C3
12	B	602	POV	C33-C34-C35-C36
12	C	502	POV	C36-C37-C38-C39
10	C	501	CLR	C23-C24-C25-C26
12	E	502	POV	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
12	B	602	POV	C35-C36-C37-C38
12	C	502	POV	O21-C2-C3-O31
12	E	502	POV	O22-C21-O21-C2
12	C	502	POV	C1-C2-C3-O31
12	B	602	POV	C37-C38-C39-C310
12	B	602	POV	C23-C24-C25-C26
10	C	501	CLR	C16-C17-C20-C21
9	A	501	SCK	C12-C11-C6-C5
12	C	503	POV	O21-C2-C3-O31
9	D	501	SCK	C6-C11-C12-O14
10	C	501	CLR	C23-C24-C25-C27
12	C	503	POV	C35-C36-C37-C38
12	C	502	POV	O11-C1-C2-C3
12	D	502	POV	O11-C1-C2-C3
12	C	503	POV	C33-C34-C35-C36
12	C	502	POV	O11-C1-C2-O21
12	E	502	POV	O11-C1-C2-O21
10	C	501	CLR	C16-C17-C20-C22
12	D	502	POV	O21-C2-C3-O31
11	E	501	NAG	C1-C2-N2-C7
12	B	602	POV	C32-C33-C34-C35
10	C	501	CLR	C13-C17-C20-C22
9	D	501	SCK	O13-C12-O14-C15
12	C	502	POV	O12-C11-C12-N
12	C	503	POV	O12-C11-C12-N
12	D	502	POV	O12-C11-C12-N
12	E	502	POV	O12-C11-C12-N
9	D	501	SCK	C11-C12-O14-C15
12	C	503	POV	C34-C35-C36-C37
12	E	502	POV	O11-C1-C2-C3
12	D	502	POV	C32-C33-C34-C35
10	C	501	CLR	C13-C17-C20-C21
12	C	503	POV	C1-C2-C3-O31
11	E	501	NAG	C3-C2-N2-C7
12	B	602	POV	C11-O12-P-O14
12	E	502	POV	C2-C1-O11-P
12	C	503	POV	C23-C24-C25-C26
12	C	502	POV	C34-C35-C36-C37
12	E	502	POV	C34-C35-C36-C37
9	A	501	SCK	C6-C5-O4-C3
12	D	502	POV	C311-C310-C39-C38
10	C	501	CLR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
9	D	501	SCK	C6-C11-C12-O13
9	A	501	SCK	N1-C2-C3-O4
9	D	501	SCK	N1-C2-C3-O4
12	B	602	POV	O11-C1-C2-O21
12	D	502	POV	C1-C2-C3-O31
9	D	501	SCK	O4-C5-C6-C11
12	C	502	POV	O31-C31-C32-C33
12	C	503	POV	O21-C21-C22-C23
12	B	602	POV	O11-C1-C2-C3
12	C	503	POV	O31-C31-C32-C33
9	A	501	SCK	O7-C5-O4-C3
9	D	501	SCK	O7-C5-C6-C11
12	C	502	POV	O32-C31-C32-C33
9	A	501	SCK	C6-C11-C12-O14
12	B	602	POV	C21-C22-C23-C24
12	C	502	POV	C35-C36-C37-C38
12	C	503	POV	O22-C21-C22-C23
12	C	503	POV	O32-C31-C32-C33

There are no ring outliers.

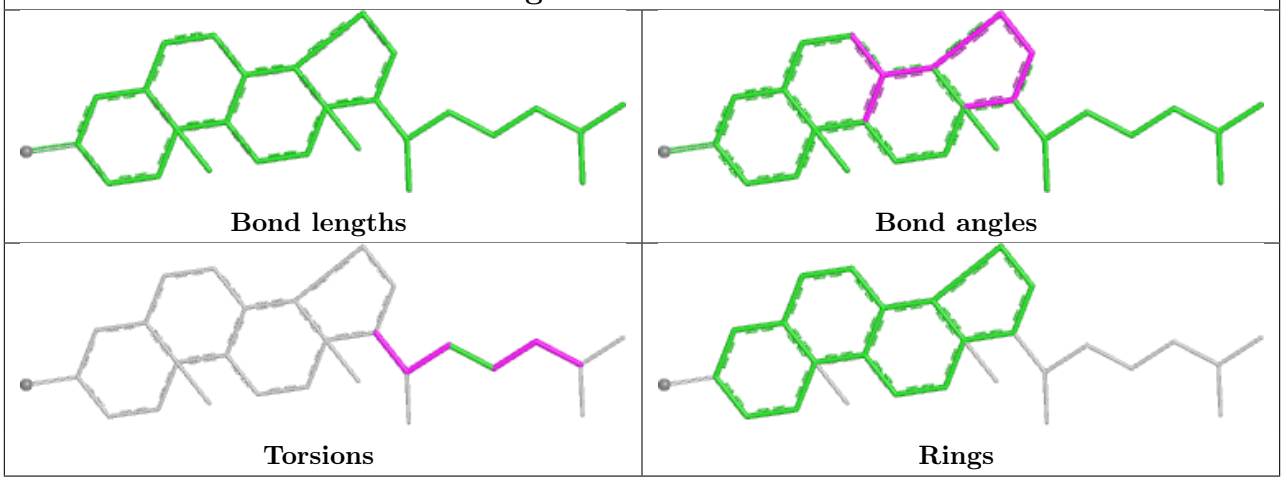
9 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	502	CLR	2	0
10	C	501	CLR	2	0
9	A	501	SCK	5	0
10	D	503	CLR	12	0
12	C	502	POV	1	0
9	D	501	SCK	5	0
12	B	602	POV	4	0
12	E	502	POV	1	0
12	D	502	POV	2	0

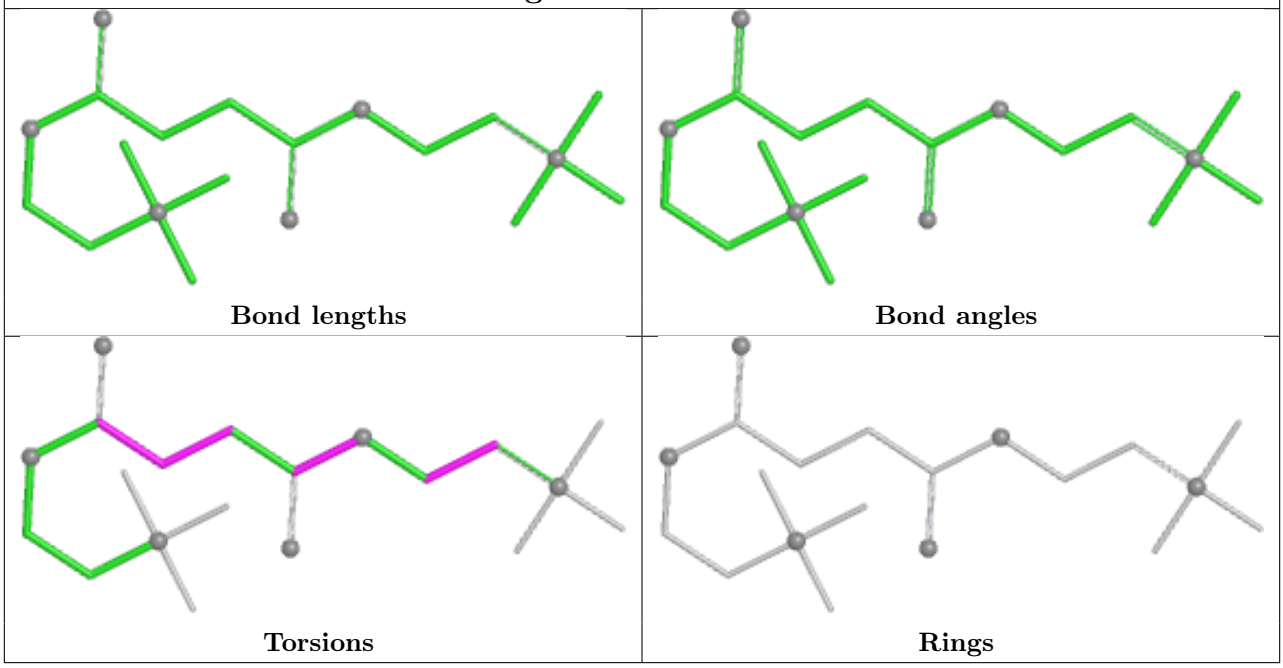
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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

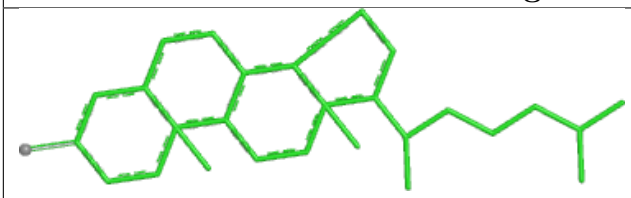
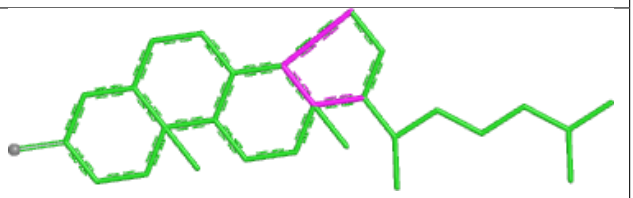
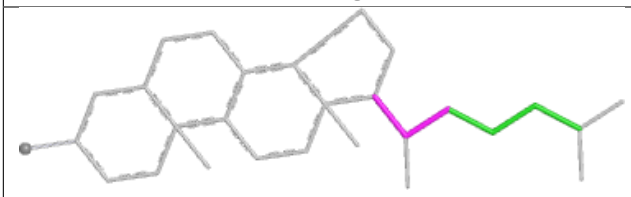
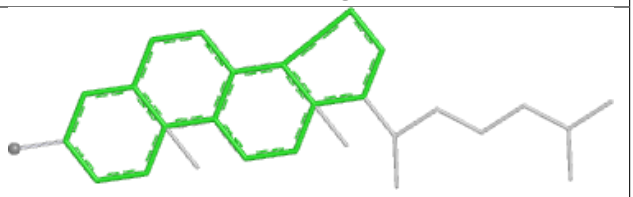
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand CLR C 501



Ligand SCK A 501



Ligand CLR D 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

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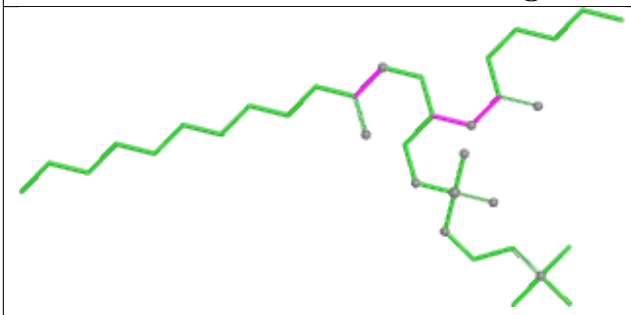
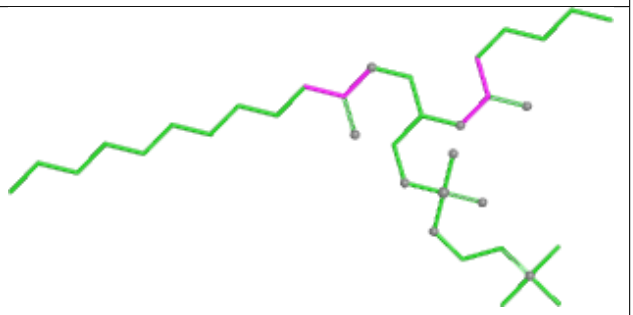
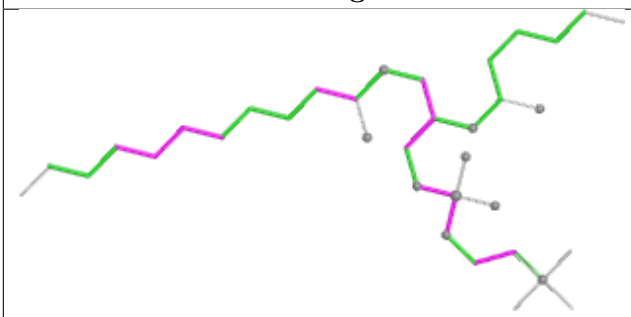
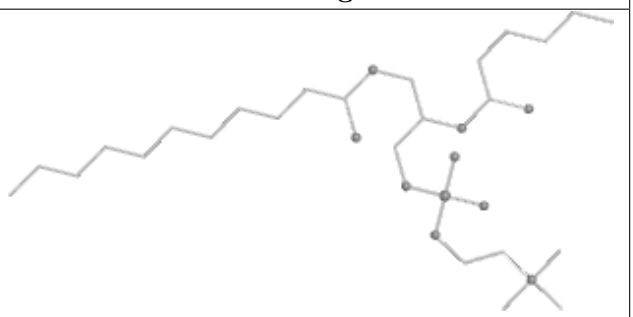
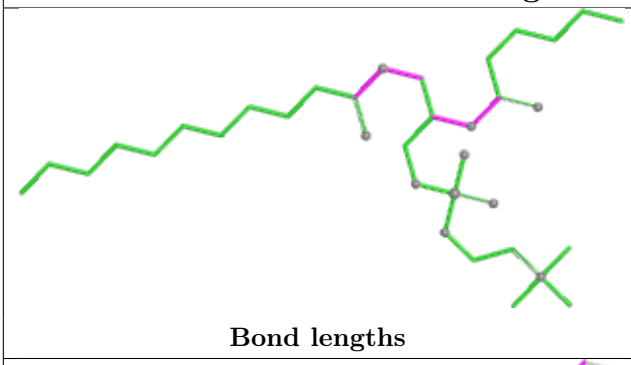
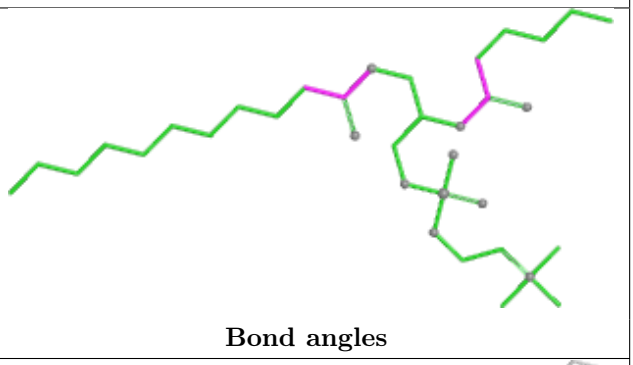
 Bond lengths	 Bond angles
 Torsions	 Rings

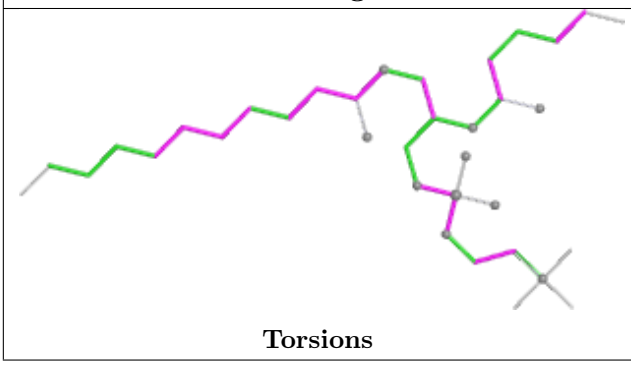
Ligand POV C 503



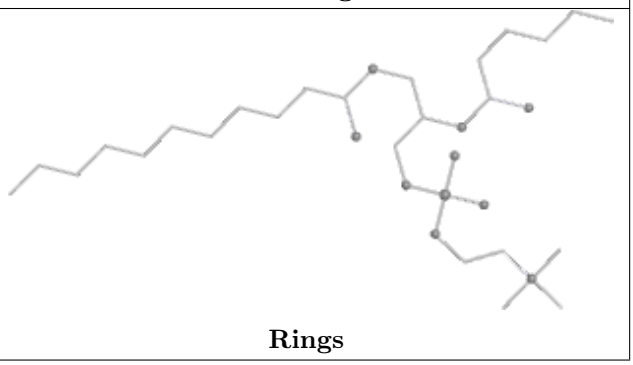
Bond lengths



Bond angles

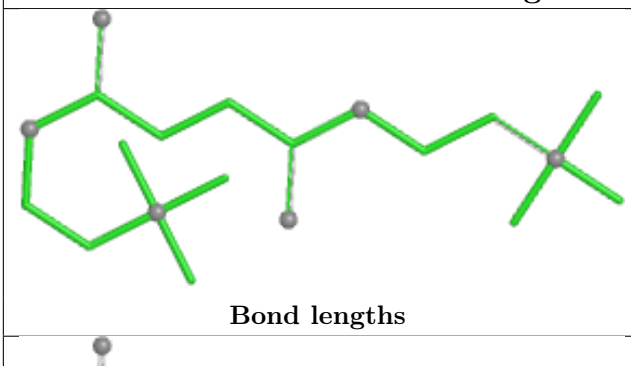


Torsions

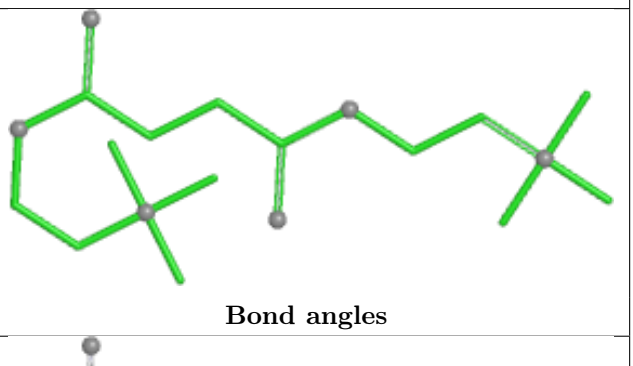


Rings

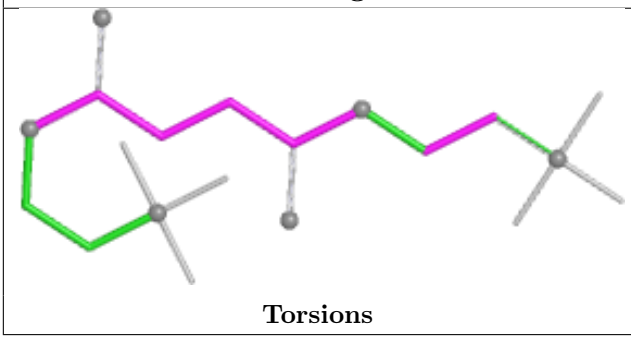
Ligand SCK D 501



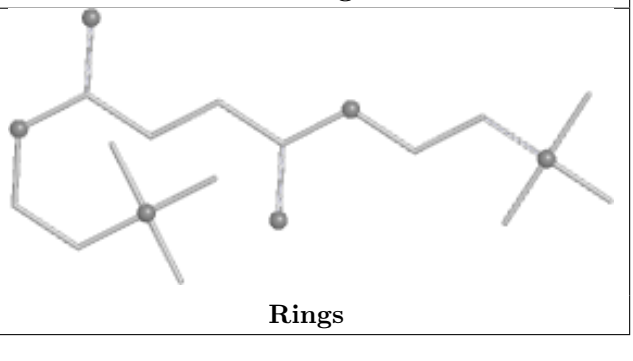
Bond lengths



Bond angles

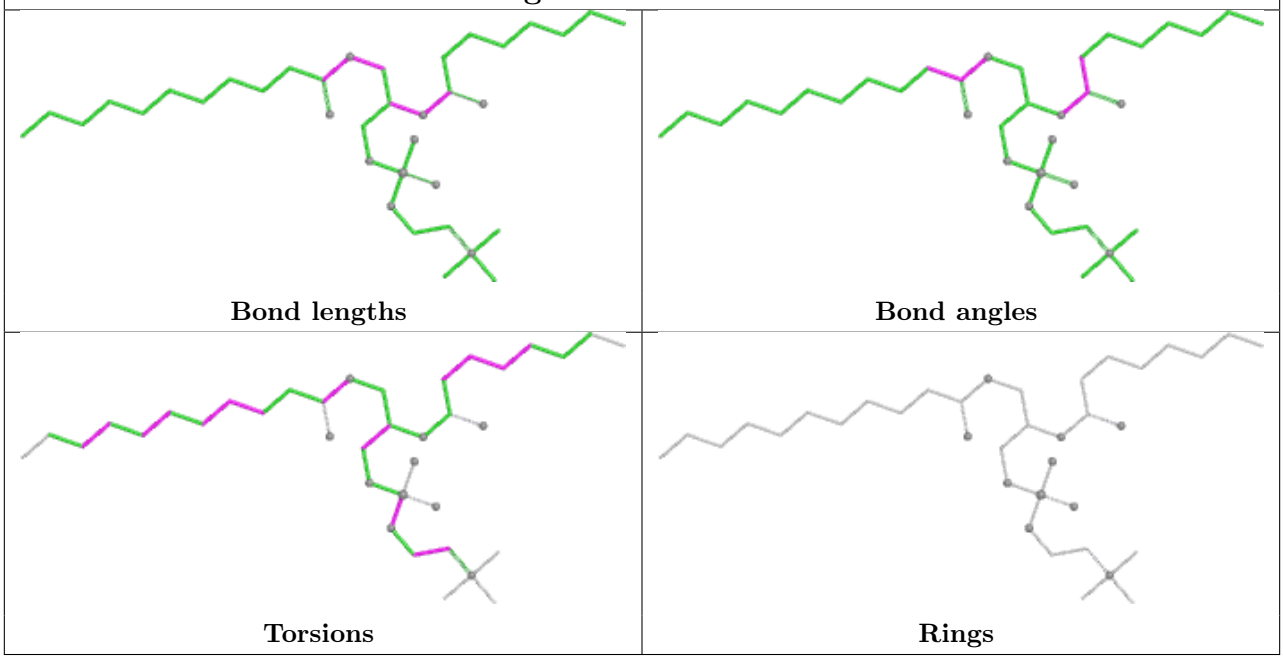


Torsions

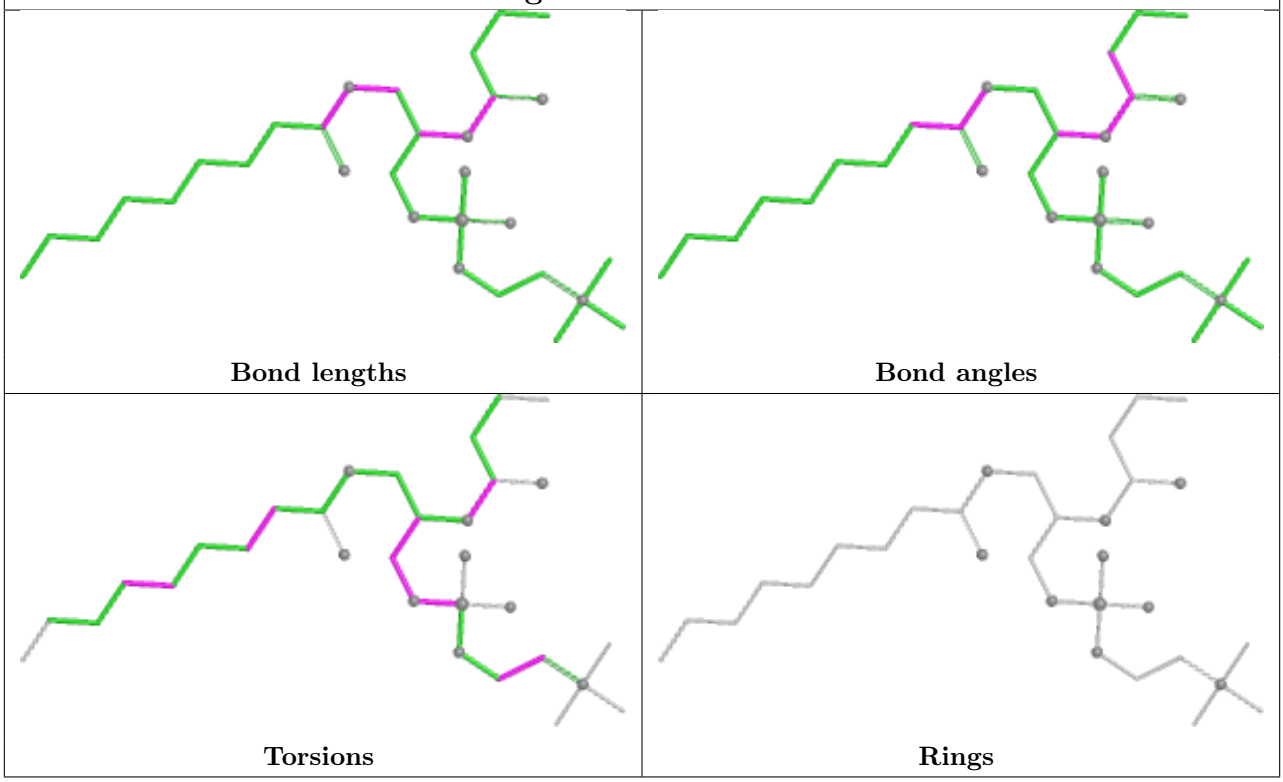


Rings

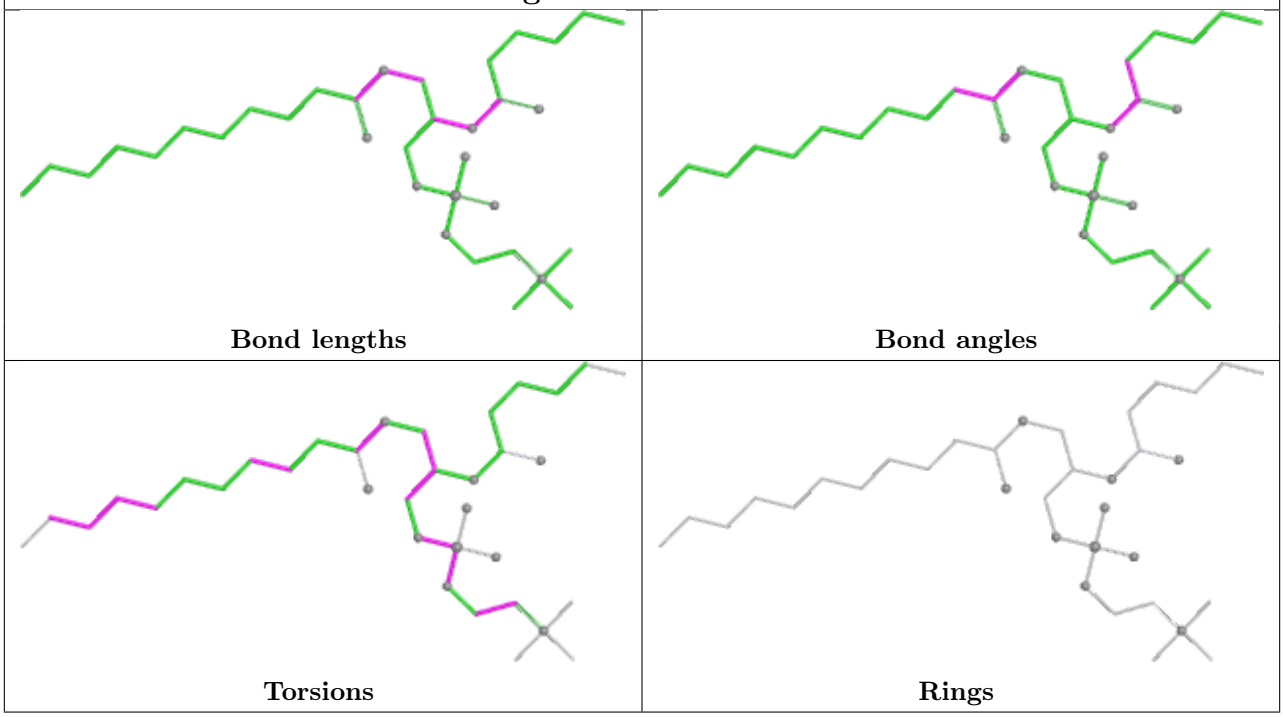
Ligand POV B 602



Ligand POV E 502



Ligand POV D 502



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.

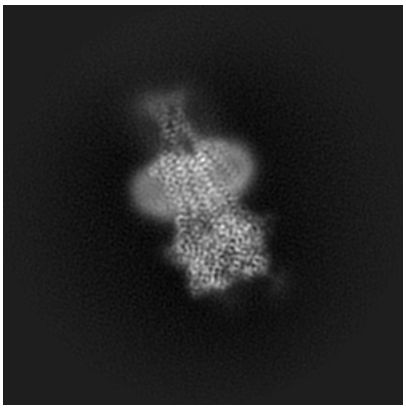
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-28893. These allow visual inspection of the internal detail of the map and identification of artifacts.

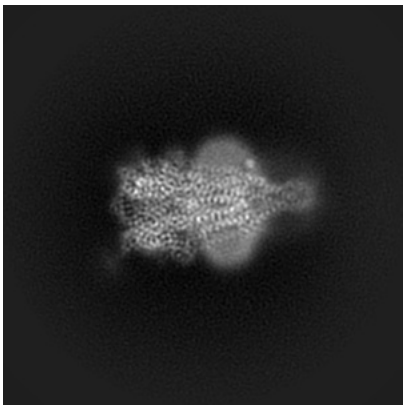
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

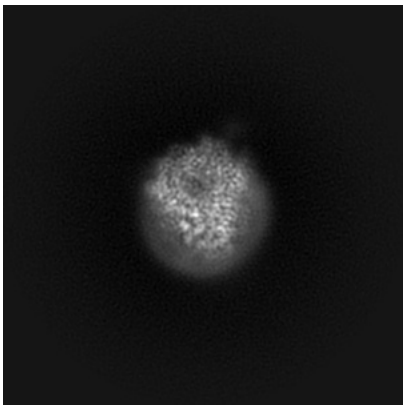
6.1.1 Primary map



X

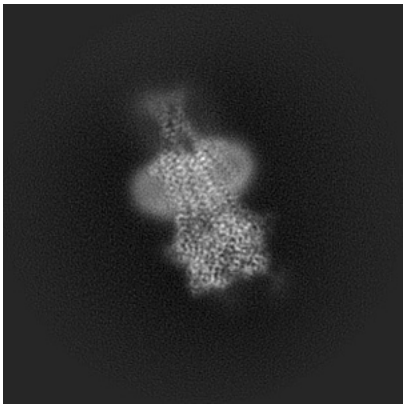


Y



Z

6.1.2 Raw map



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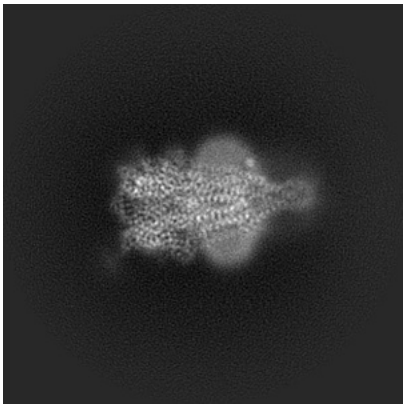

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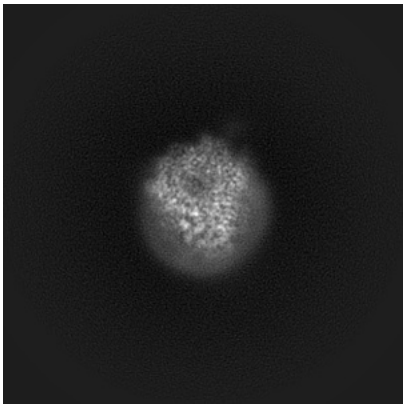
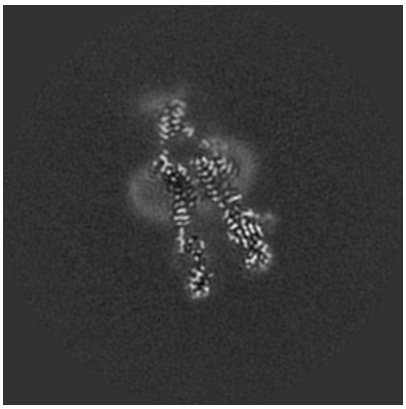


Z

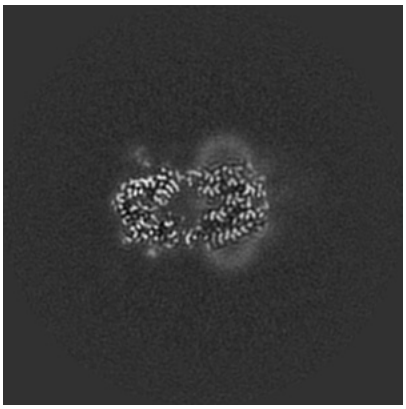
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

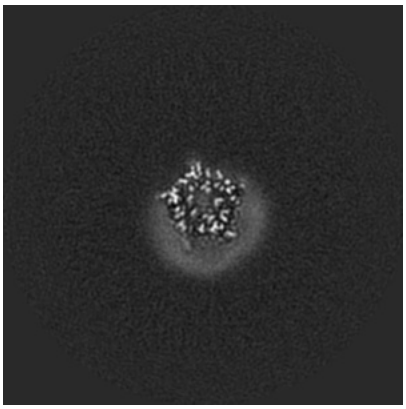
6.2.1 Primary map



X Index: 144

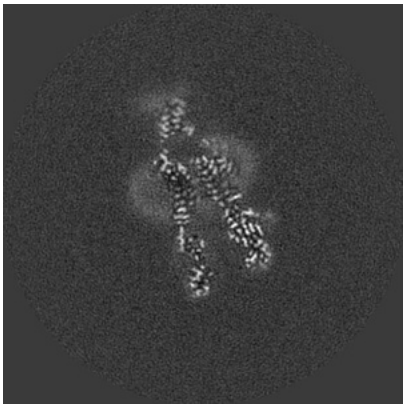


Y Index: 144

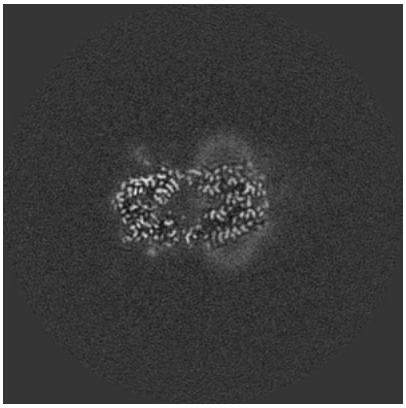


Z Index: 144

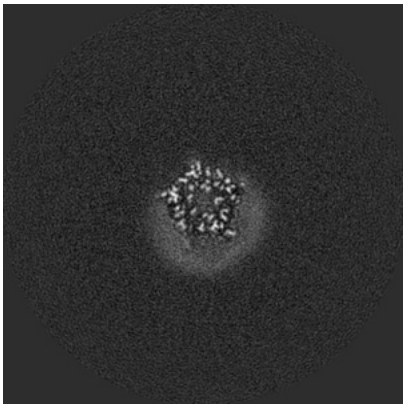
6.2.2 Raw map



X Index: 144



Y Index: 144

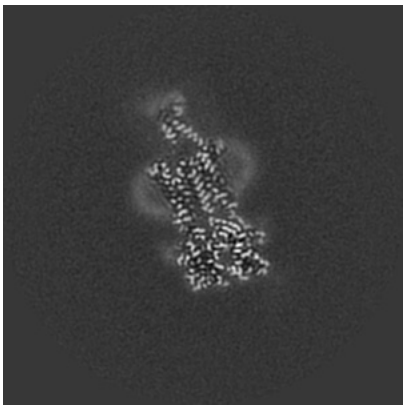


Z Index: 144

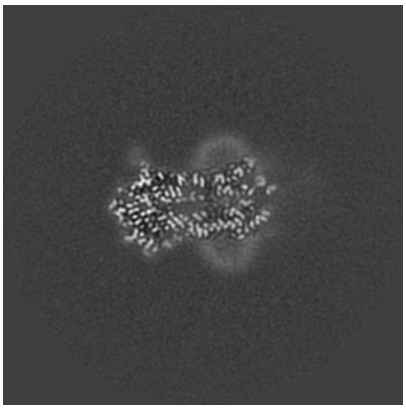
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

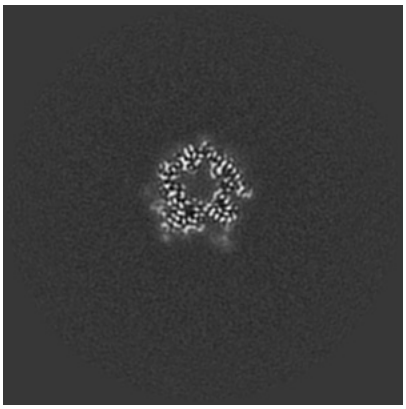
6.3.1 Primary map



X Index: 155

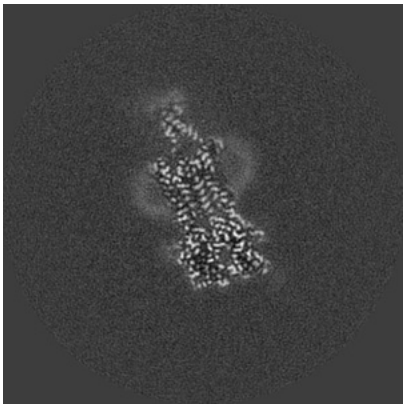


Y Index: 139

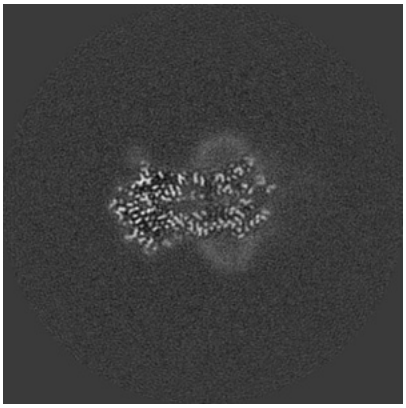


Z Index: 110

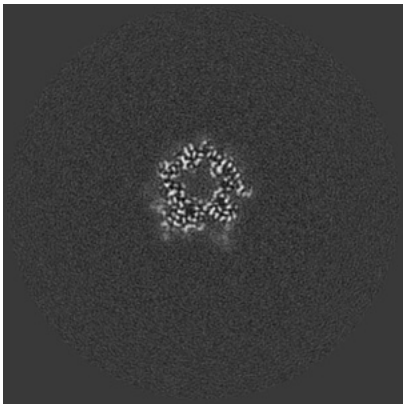
6.3.2 Raw map



X Index: 156



Y Index: 139

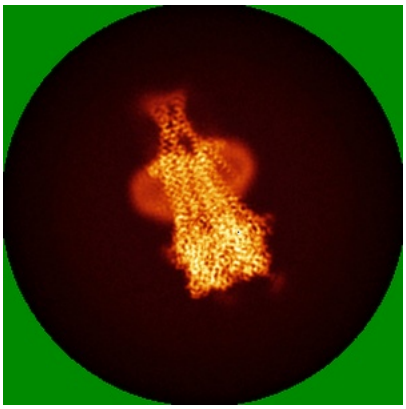


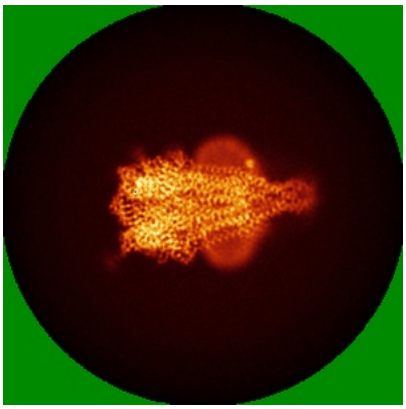
Z Index: 110

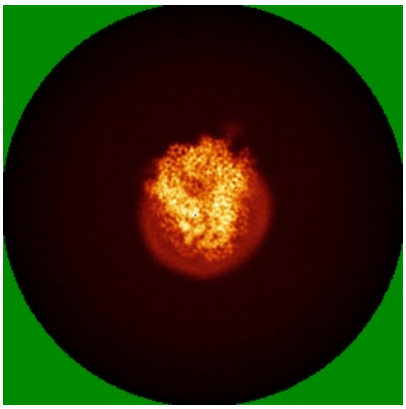
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

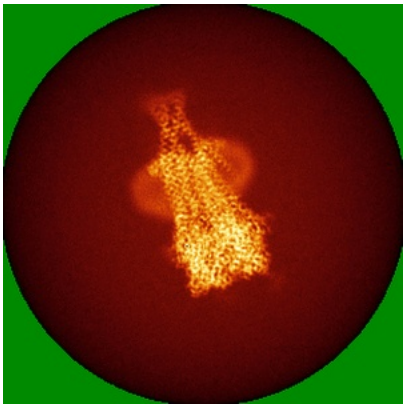
6.4.1 Primary map

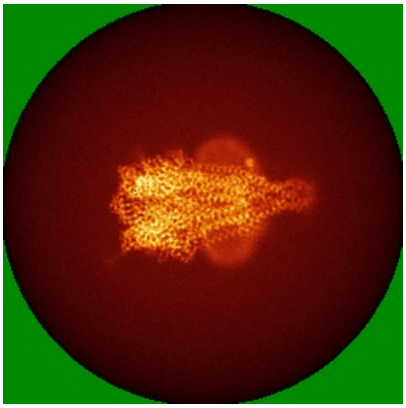

X

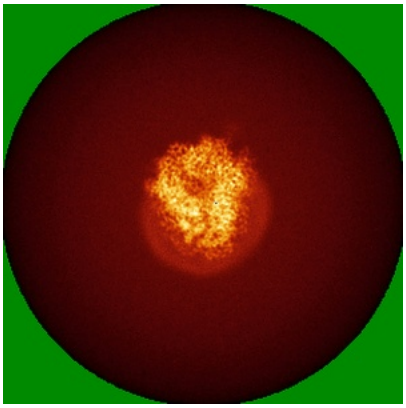

Y


Z

6.4.2 Raw map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

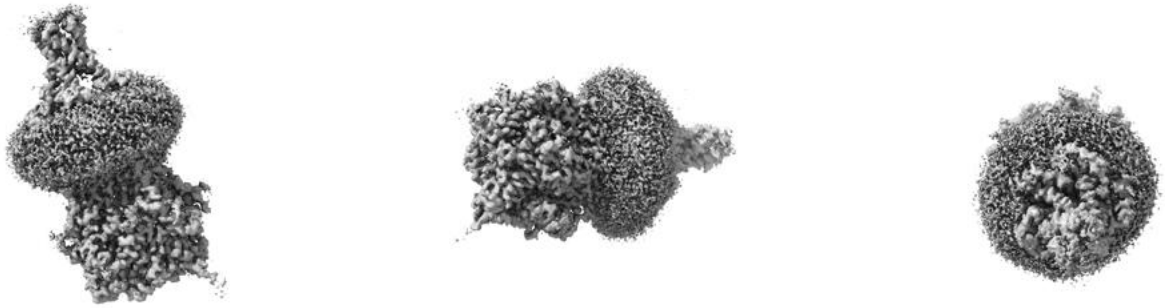
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0154. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

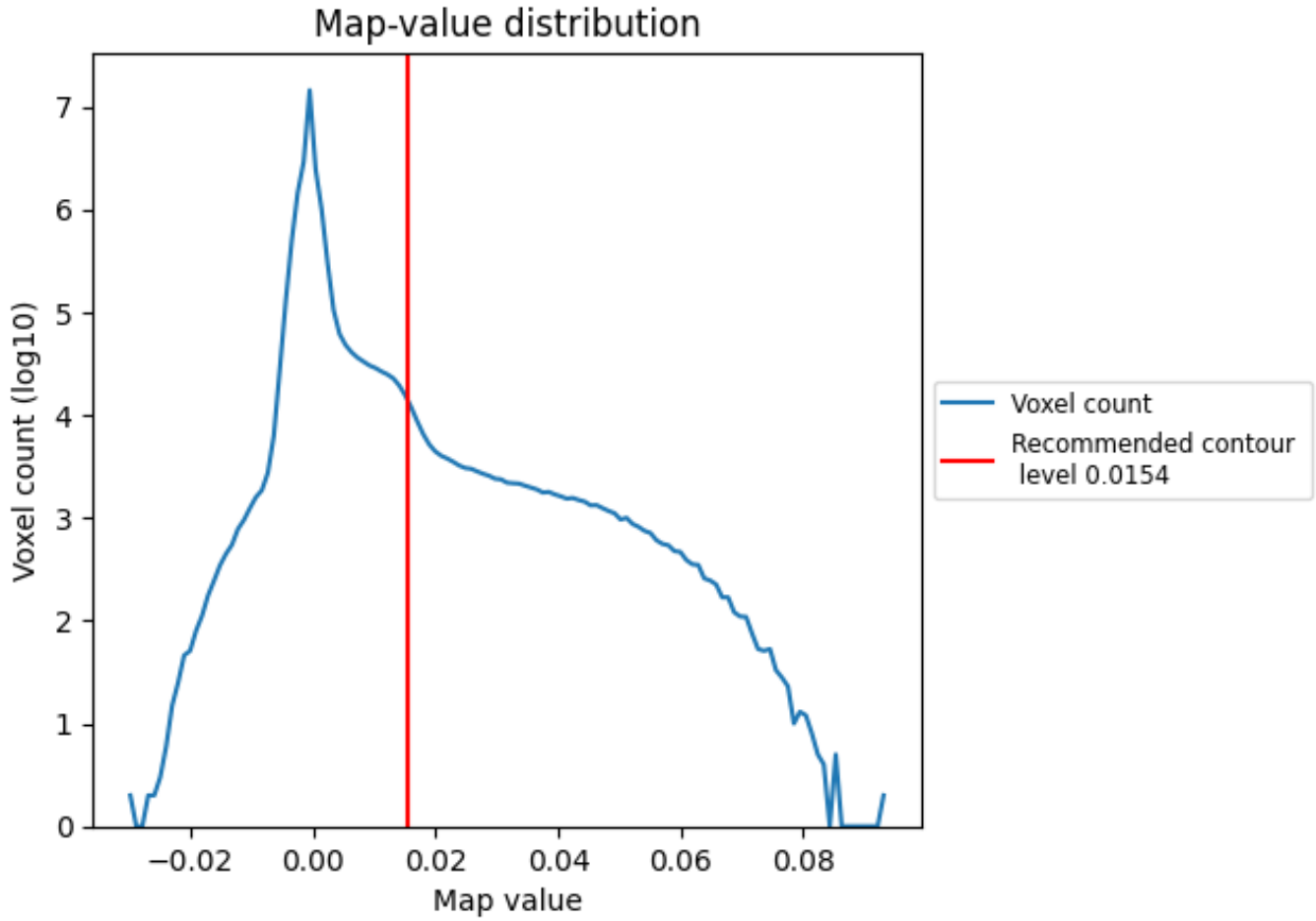
6.6 Mask visualisation (i)

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

7 Map analysis

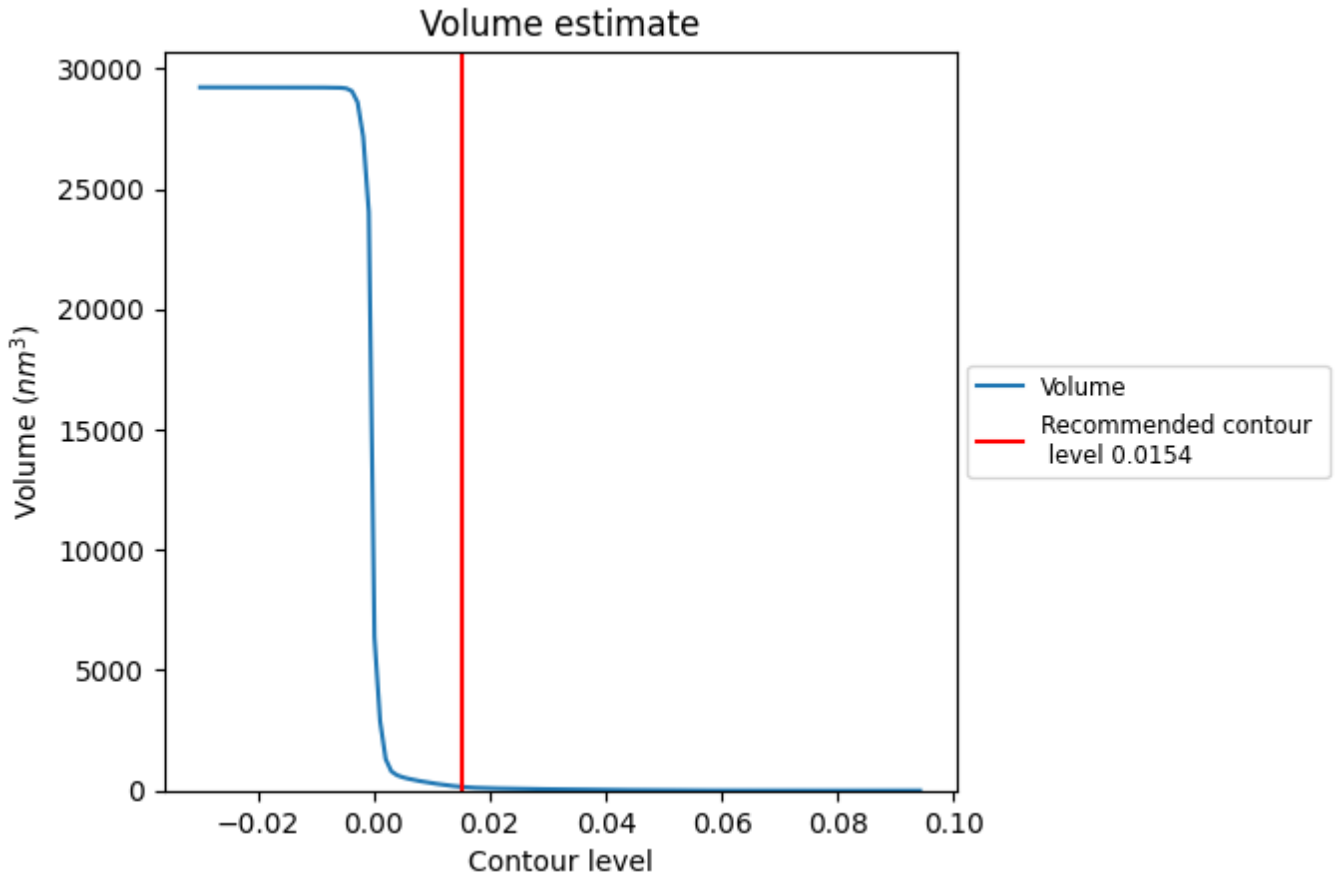
This section contains the results of statistical analysis of the map.

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.

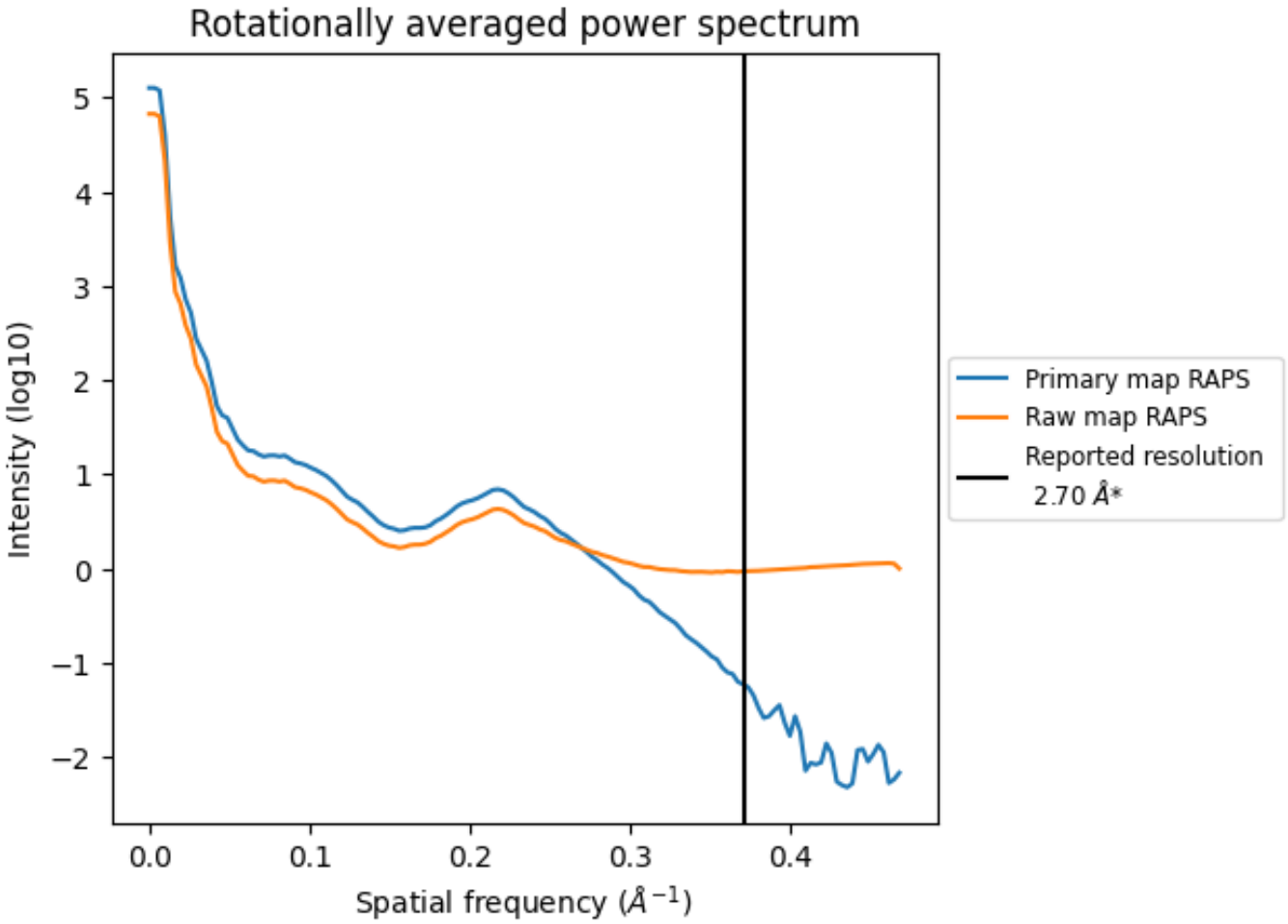
7.2 Volume estimate



The volume at the recommended contour level is 150 nm^3; this corresponds to an approximate mass of 135 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)

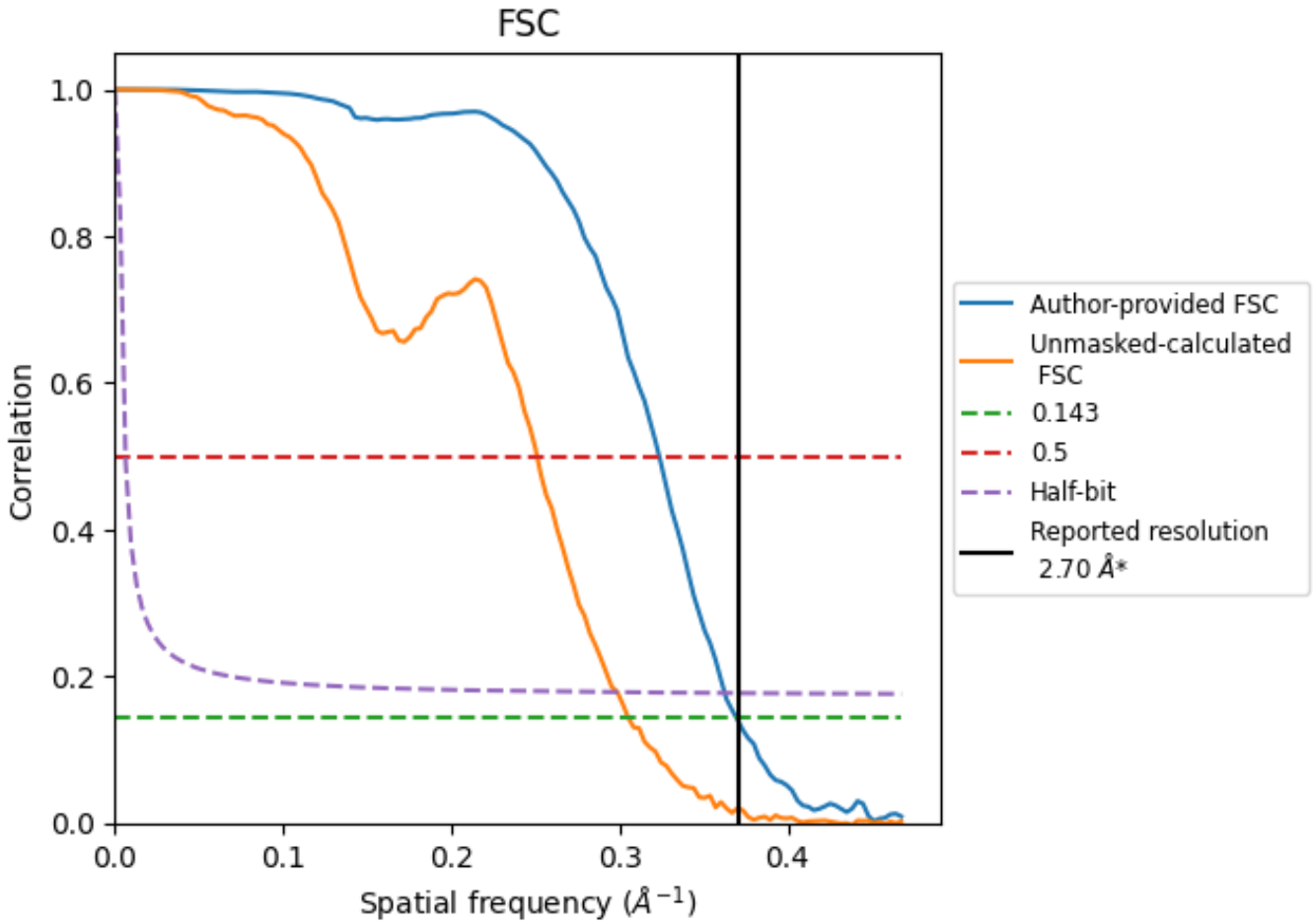


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8.2 Resolution estimates (i)

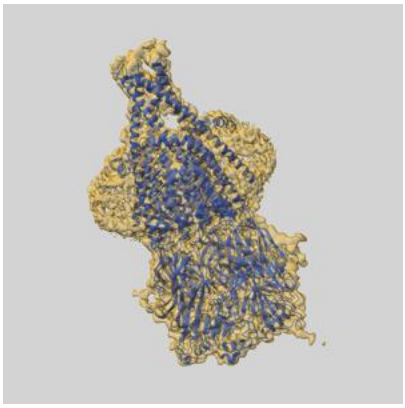
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.71	3.09	2.76
Unmasked-calculated*	3.28	3.98	3.35

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.28 differs from the reported value 2.7 by more than 10 %

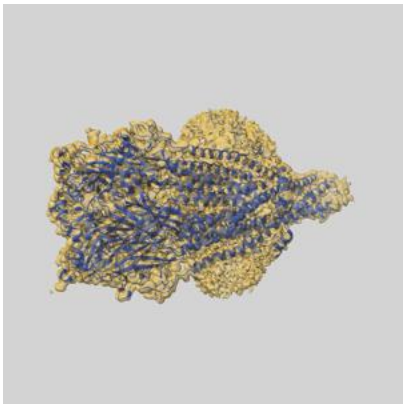
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-28893 and PDB model 8F6Z. Per-residue inclusion information can be found in section 3 on page 10.

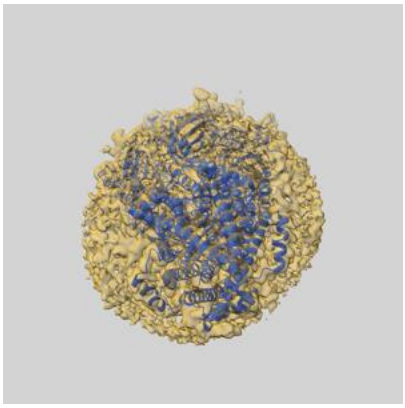
9.1 Map-model overlay



X



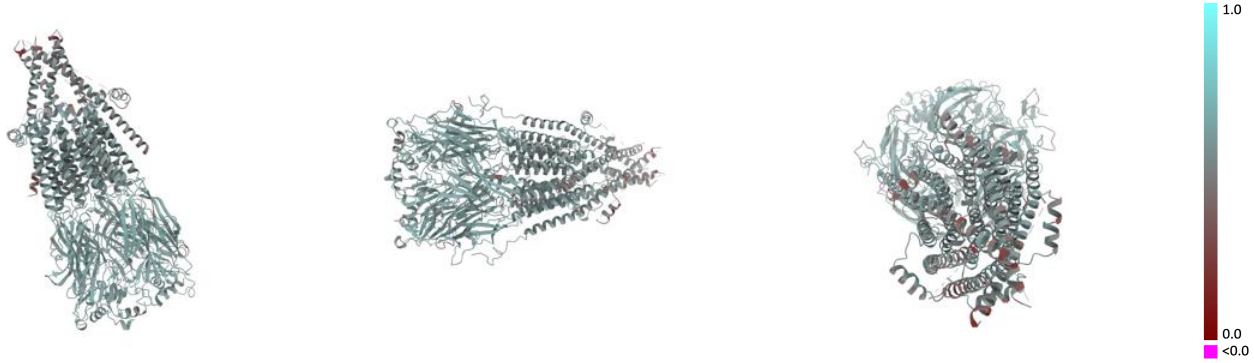
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0154 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.

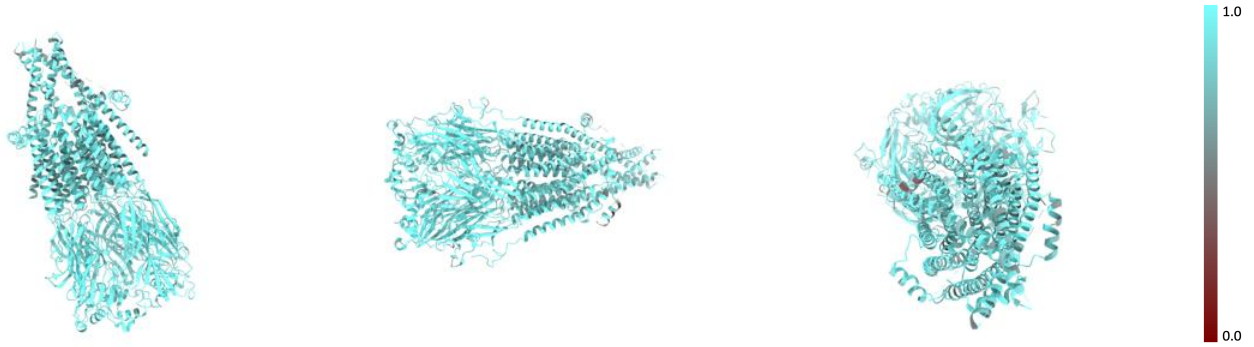
9.2 Q-score mapped to coordinate model (i)



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.

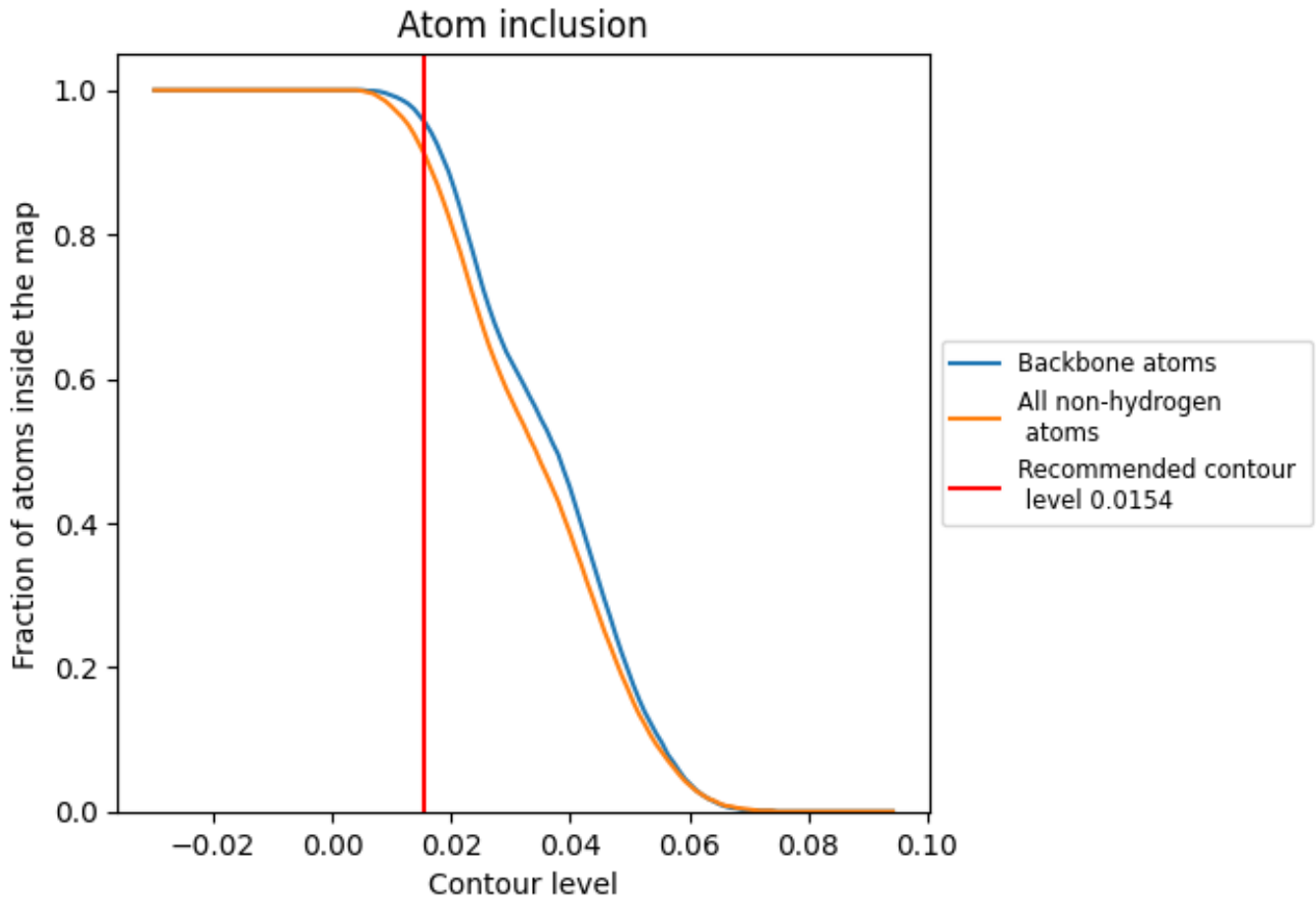
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0154).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 91% 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 (0.0154) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9130	0.5570
A	0.9120	0.5550
B	0.9160	0.5610
C	0.9180	0.5610
D	0.9160	0.5500
E	0.9060	0.5580
F	0.9340	0.5540
G	0.9600	0.5090
H	0.8930	0.5260
I	0.8210	0.5250
J	0.9670	0.5690
K	0.9340	0.5510