



Full wwPDB EM Validation Report ⓘ

Nov 9, 2022 – 04:04 AM JST

PDB ID : 6IDF
EMDB ID : EMD-9648
Title : Cryo-EM structure of gamma secretase in complex with a Notch fragment
Authors : Yang, G.; Zhou, R.; Zhou, Q.; Guo, X.; Yan, C.; Ke, M.; Lei, J.; Shi, Y.
Deposited on : 2018-09-09
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:

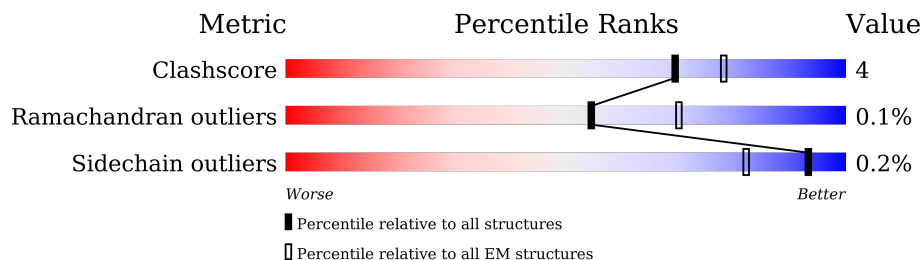
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 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.




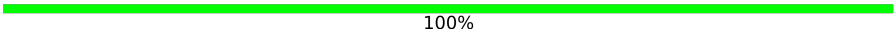

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	709	
2	B	467	
3	C	265	
4	D	101	
5	E	129	
6	F	2	
6	H	2	
6	I	2	

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Mol	Chain	Length	Quality of chain
6	J	2	 50% 50%
6	K	2	 100%
7	G	5	 40% 60% 40%

2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 11188 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 Nicastrin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	667	5235	3321	890	1003	21	0	0

- Molecule 2 is a protein called Presenilin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	312	2414	1635	372	391	16	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	112	CYS	GLN	engineered mutation	UNP P49768
B	385	ALA	ASP	engineered mutation	UNP P49768

- Molecule 3 is a protein called Gamma-secretase subunit APH-1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	243	1872	1254	299	315	4	0	0

- Molecule 4 is a protein called Gamma-secretase subunit PEN-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	100	850	580	134	135	1	0	0

- Molecule 5 is a protein called Notch1.

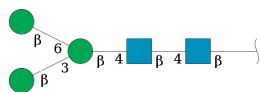
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	41	263	167	45	49	2	0	0

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



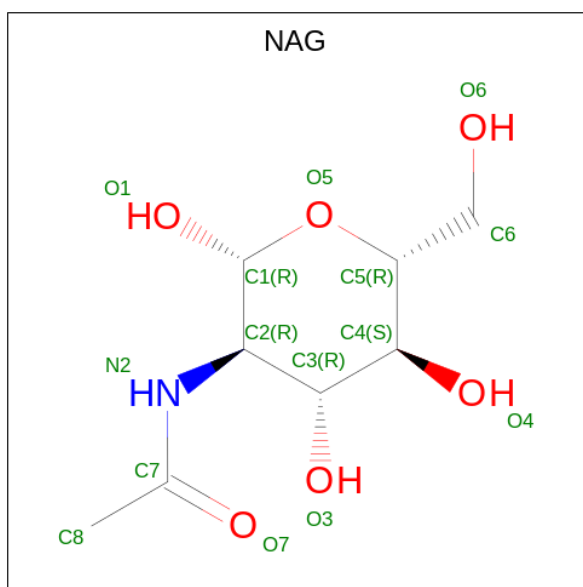
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	F	2	28	16	2	10	0	0
6	H	2	28	16	2	10	0	0
6	I	2	28	16	2	10	0	0
6	J	2	28	16	2	10	0	0
6	K	2	28	16	2	10	0	0

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-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.



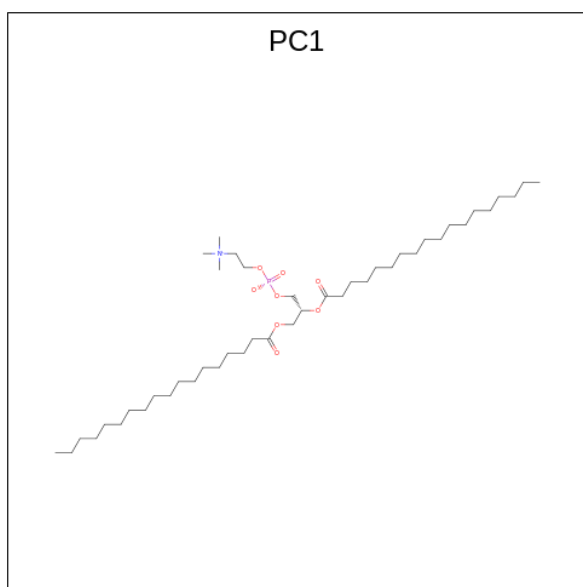
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	G	5	61	34	2	25	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



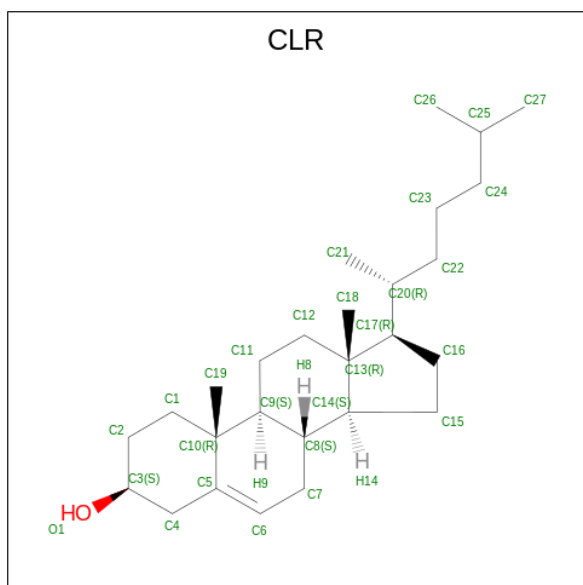
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
8	A	1	Total	C	N	O	0
			85	48	6	31	
8	A	1	Total	C	N	O	0
			85	48	6	31	
8	A	1	Total	C	N	O	0
			85	48	6	31	
8	A	1	Total	C	N	O	0
			85	48	6	31	
8	A	1	Total	C	N	O	0
			85	48	6	31	

- Molecule 9 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		
9	B	1	Total	95	75	2	16	2	0
9	B	1	Total	95	75	2	16	2	0
9	C	1	Total	50	40	1	8	1	0
9	D	1	Total	39	29	1	8	1	0

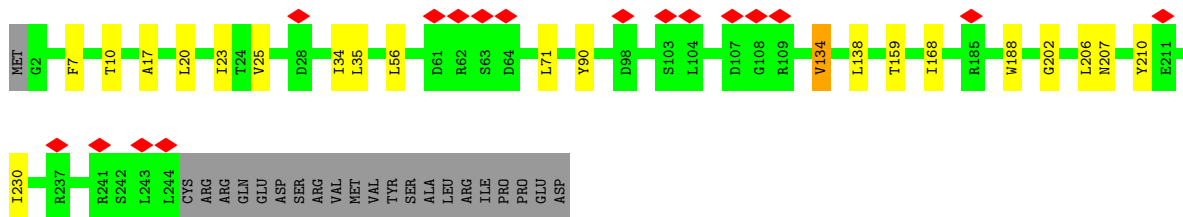
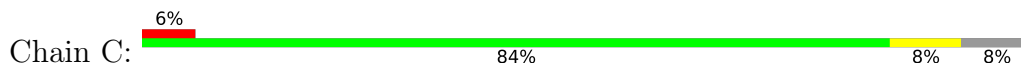
- Molecule 10 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



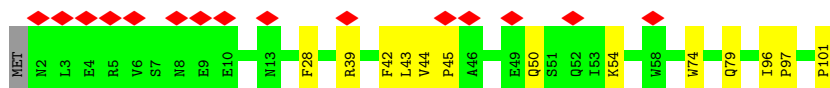
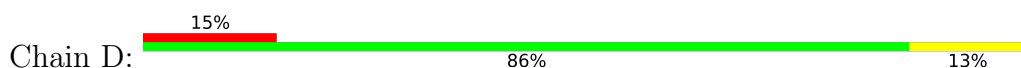
Mol	Chain	Residues	Atoms			AltConf
10	C	1	Total 84	C 81	O 3	0
10	C	1	Total 84	C 81	O 3	0
10	C	1	Total 84	C 81	O 3	0



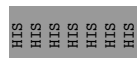
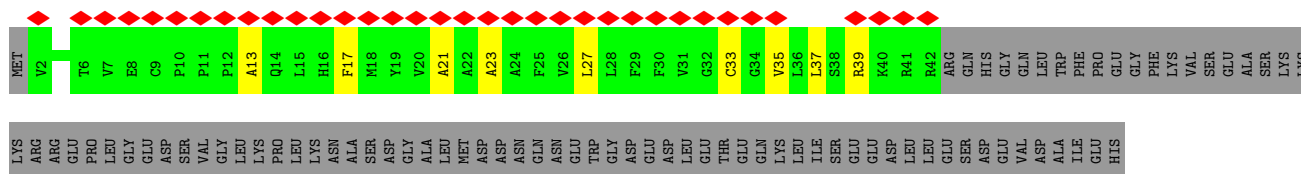
- Molecule 3: Gamma-secretase subunit APH-1A



- Molecule 4: Gamma-secretase subunit PEN-2



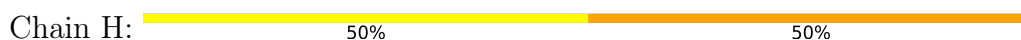
- Molecule 5: Notch1



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



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



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

Chain I:  50% 50%

MAG1
MAG2

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

Chain J:  50% 50%


MAG1
MAG2

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

Chain K:  100%

MAG1
MAG2

- Molecule 7: beta-D-mannopyranose-(1-3)-[beta-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:  40% 60% 40%

MAG1
MAG2
BMA3
BMA4
BMA5

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	476853	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.5625	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.376	Depositor
Minimum map value	-0.191	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.05	Depositor
Map size (\AA)	349.12, 349.12, 349.12	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.091, 1.091, 1.091	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, BMA, NAG, CLR

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	0.30	0/5358	0.58	0/7302
2	B	0.29	0/2474	0.56	1/3378 (0.0%)
3	C	0.30	0/1924	0.57	0/2624
4	D	0.29	0/883	0.51	0/1205
5	E	0.28	0/264	0.55	0/361
All	All	0.30	0/10903	0.57	1/14870 (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	2
3	C	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	117	PRO	N-CA-CB	6.41	110.99	103.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	PHE	Peptide
1	A	91	ASN	Peptide

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Mol	Chain	Res	Type	Group
3	C	206	LEU	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	5235	0	5127	33	0
2	B	2414	0	2511	30	0
3	C	1872	0	1911	13	0
4	D	850	0	840	10	0
5	E	263	0	228	8	0
6	F	28	0	25	0	0
6	H	28	0	25	1	0
6	I	28	0	25	0	0
6	J	28	0	25	0	0
6	K	28	0	25	0	0
7	G	61	0	52	0	0
8	A	85	0	80	0	0
9	B	95	0	141	2	0
9	C	50	0	74	2	0
9	D	39	0	52	0	0
10	C	84	0	136	5	0
All	All	11188	0	11277	84	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 4.

All (84) 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)
2:B:149:LEU:O	2:B:153:LEU:HB2	1.92	0.68
2:B:435:LEU:HD23	5:E:35:VAL:HG13	1.78	0.64
1:A:559:SER:HB2	1:A:629:ARG:HH12	1.63	0.63
4:D:44:VAL:O	4:D:50:GLN:NE2	2.35	0.60
1:A:54:LEU:HD11	1:A:223:ALA:HB1	1.85	0.58
3:C:134:VAL:HG13	3:C:138:LEU:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:230:ILE:HG21	10:C:303:CLR:H213	1.86	0.57
1:A:530:ASN:OD1	1:A:535:GLN:NE2	2.37	0.57
1:A:256:VAL:HG22	1:A:329:PHE:HB2	1.87	0.57
2:B:275:ALA:HB2	2:B:282:LEU:HD13	1.86	0.55
2:B:106:TYR:HA	2:B:239:LYS:HD3	1.89	0.55
1:A:289:TRP:NE1	1:A:650:GLU:OE2	2.40	0.54
1:A:52:ARG:NH2	1:A:63:GLN:OE1	2.40	0.53
9:B:501:PC1:H2C1	9:B:501:PC1:H3C1	1.90	0.53
2:B:381:LEU:HD13	5:E:37:LEU:HD12	1.91	0.52
2:B:392:LEU:HD22	2:B:414:ILE:HD11	1.91	0.52
1:A:285:ARG:HG2	1:A:454:GLN:HE21	1.73	0.52
1:A:383:VAL:O	6:H:1:NAG:O6	2.28	0.52
3:C:7:PHE:HA	3:C:10:THR:HG22	1.92	0.52
2:B:114:ILE:HD11	5:E:21:ALA:HA	1.92	0.51
1:A:543:ARG:HD3	1:A:606:GLN:HE22	1.76	0.51
1:A:112:LYS:NZ	1:A:175:ASP:O	2.44	0.50
2:B:194:ASP:OD2	4:D:74:TRP:NE1	2.43	0.50
1:A:64:SER:HB2	1:A:179:PRO:HG3	1.93	0.50
1:A:85:VAL:HG23	1:A:94:TYR:HB2	1.94	0.49
2:B:125:VAL:HA	2:B:128:ARG:HE	1.76	0.49
1:A:691:ASN:HD22	3:C:23:ILE:HG22	1.77	0.49
1:A:225:ILE:HD11	4:D:101:PRO:HB3	1.95	0.49
1:A:355:GLN:H	1:A:358:ASN:HD22	1.61	0.49
2:B:429:LYS:HG2	5:E:39:ARG:HH22	1.78	0.49
3:C:202:GLY:HA3	10:C:302:CLR:H42	1.94	0.49
3:C:188:TRP:HH2	10:C:303:CLR:H151	1.78	0.48
2:B:226:LEU:HD23	2:B:383:LEU:HD21	1.95	0.48
5:E:13:ALA:HB3	5:E:17:PHE:H	1.79	0.48
2:B:173:LEU:HD13	5:E:27:LEU:HD11	1.96	0.48
2:B:172:LEU:HD21	5:E:23:ALA:HB1	1.95	0.48
4:D:39:ARG:HD2	4:D:43:LEU:HD21	1.95	0.48
1:A:261:LYS:NZ	1:A:321:LEU:O	2.47	0.47
1:A:82:LEU:O	1:A:86:LEU:HB2	2.15	0.47
2:B:101:LYS:NZ	2:B:403:ASP:OD1	2.48	0.47
1:A:305:GLN:HE21	1:A:327:PHE:HD1	1.63	0.47
3:C:25:VAL:HG11	3:C:35:LEU:HD13	1.97	0.46
3:C:17:ALA:HB2	3:C:168:ILE:HG21	1.98	0.46
10:C:302:CLR:H222	10:C:302:CLR:H162	1.63	0.46
10:C:303:CLR:H211	10:C:303:CLR:H232	1.82	0.45
2:B:96:VAL:HG21	2:B:390:SER:HB3	1.99	0.45
1:A:48:ALA:HB3	1:A:182:LEU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:390:SER:HA	2:B:393:VAL:HG12	1.99	0.44
2:B:286:LEU:HD22	5:E:33:CYS:HB2	1.99	0.44
1:A:257:TRP:NE1	1:A:326:MET:SD	2.73	0.43
1:A:276:VAL:HG13	1:A:361:SER:HB2	2.00	0.43
1:A:282:LEU:HD23	1:A:331:GLN:HG2	1.99	0.43
2:B:449:THR:HA	2:B:453:VAL:HB	2.01	0.43
2:B:142:VAL:HA	2:B:145:VAL:HG12	2.01	0.43
1:A:233:ARG:HD3	4:D:96:ILE:HG21	2.00	0.43
2:B:192:ALA:HB2	4:D:97:PRO:HD3	2.01	0.42
2:B:256:TYR:HA	2:B:259:VAL:HG12	2.01	0.42
2:B:211:ILE:HG23	2:B:215:TRP:HE3	1.84	0.42
1:A:632:SER:HB2	1:A:635:PHE:HD2	1.84	0.42
1:A:86:LEU:HD12	1:A:114:ARG:HD2	2.01	0.41
1:A:105:ARG:HH12	1:A:174:GLU:HG3	1.85	0.41
2:B:121:ASP:HA	2:B:128:ARG:HD3	2.00	0.41
1:A:141:PRO:HG2	1:A:424:PRO:HG3	2.02	0.41
2:B:208:VAL:HG21	4:D:28:PHE:HD2	1.85	0.41
2:B:435:LEU:HD12	2:B:439:ILE:HD11	2.01	0.41
1:A:460:ALA:HB1	1:A:465:VAL:HB	2.01	0.41
1:A:524:GLY:HA2	1:A:531:ASN:HD21	1.85	0.41
1:A:275:VAL:HG12	1:A:324:ASN:HB3	2.01	0.41
9:C:301:PC1:H111	9:C:301:PC1:H132	1.84	0.41
4:D:45:PRO:HA	4:D:50:GLN:HE22	1.86	0.41
2:B:85:LEU:HD12	2:B:422:LEU:HD21	2.02	0.41
2:B:192:ALA:O	4:D:79:GLN:NE2	2.35	0.41
2:B:421:THR:HG21	2:B:434:ALA:HA	2.03	0.41
2:B:464:GLN:O	3:C:207:ASN:ND2	2.42	0.41
9:B:502:PC1:H392	9:B:502:PC1:H362	1.84	0.41
1:A:265:THR:HG23	1:A:353:PRO:HG3	2.02	0.40
1:A:142:ASN:ND2	1:A:335:PHE:O	2.51	0.40
3:C:159:THR:HG21	3:C:210:TYR:CD1	2.57	0.40
1:A:208:PRO:HB2	1:A:212:LEU:HD21	2.03	0.40
3:C:20:LEU:HD21	9:C:301:PC1:H3A2	2.03	0.40
2:B:161:VAL:O	2:B:165:TRP:N	2.54	0.40
3:C:34:ILE:O	3:C:90:TYR:OH	2.37	0.40
3:C:56:LEU:HB3	3:C:71:LEU:HD23	2.02	0.40
4:D:42:PHE:HE1	4:D:54:LYS:HG2	1.85	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	665/709 (94%)	617 (93%)	48 (7%)	0	100	100
2	B	308/467 (66%)	282 (92%)	24 (8%)	2 (1%)	25	50
3	C	241/265 (91%)	232 (96%)	9 (4%)	0	100	100
4	D	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
5	E	39/129 (30%)	33 (85%)	6 (15%)	0	100	100
All	All	1351/1671 (81%)	1257 (93%)	92 (7%)	2 (0%)	54	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	116	THR
2	B	117	PRO

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	584/612 (95%)	584 (100%)	0	100	100
2	B	253/407 (62%)	252 (100%)	1 (0%)	91	97
3	C	193/214 (90%)	192 (100%)	1 (0%)	88	96
4	D	88/89 (99%)	88 (100%)	0	100	100
5	E	21/112 (19%)	21 (100%)	0	100	100
All	All	1139/1434 (79%)	1137 (100%)	2 (0%)	93	98

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

Mol	Chain	Res	Type
2	B	148	ILE
3	C	134	VAL

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	358	ASN
1	A	454	GLN
1	A	531	ASN
1	A	606	GLN
1	A	691	ASN
2	B	81	HIS
4	D	50	GLN

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](#)

15 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	F	1	1,6	14,14,15	0.23	0	17,19,21	0.43	0
6	NAG	F	2	6	14,14,15	0.28	0	17,19,21	0.61	0
7	NAG	G	1	7,1	14,14,15	0.19	0	17,19,21	0.54	0
7	NAG	G	2	7	14,14,15	0.29	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BMA	G	3	7	11,11,12	0.84	0	15,15,17	0.68	0
7	BMA	G	4	7	11,11,12	0.68	0	15,15,17	0.93	1 (6%)
7	BMA	G	5	7	11,11,12	1.70	3 (27%)	15,15,17	1.86	4 (26%)
6	NAG	H	1	1,6	14,14,15	0.31	0	17,19,21	1.18	2 (11%)
6	NAG	H	2	6	14,14,15	0.68	0	17,19,21	1.10	2 (11%)
6	NAG	I	1	1,6	14,14,15	0.76	1 (7%)	17,19,21	0.75	1 (5%)
6	NAG	I	2	6	14,14,15	0.69	0	17,19,21	0.52	0
6	NAG	J	1	1,6	14,14,15	0.29	0	17,19,21	0.48	0
6	NAG	J	2	6	14,14,15	1.32	2 (14%)	17,19,21	2.38	4 (23%)
6	NAG	K	1	1,6	14,14,15	0.38	0	17,19,21	0.53	0
6	NAG	K	2	6	14,14,15	0.34	0	17,19,21	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	F	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	4/6/23/26	0/1/1/1
7	NAG	G	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	G	2	7	-	2/6/23/26	0/1/1/1
7	BMA	G	3	7	-	2/2/19/22	0/1/1/1
7	BMA	G	4	7	-	2/2/19/22	0/1/1/1
7	BMA	G	5	7	-	0/2/19/22	0/1/1/1
6	NAG	H	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	H	2	6	-	2/6/23/26	0/1/1/1
6	NAG	I	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	I	2	6	-	3/6/23/26	0/1/1/1
6	NAG	J	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	J	2	6	-	5/6/23/26	0/1/1/1
6	NAG	K	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	5	BMA	C2-C3	3.29	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	2	NAG	O5-C1	-3.25	1.38	1.43
7	G	5	BMA	C1-C2	3.07	1.59	1.52
6	J	2	NAG	C1-C2	2.84	1.56	1.52
6	I	1	NAG	O5-C1	-2.41	1.39	1.43
7	G	5	BMA	O5-C1	2.26	1.47	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	2	NAG	C2-N2-C7	7.49	133.57	122.90
7	G	5	BMA	C1-O5-C5	5.08	119.07	112.19
6	J	2	NAG	C1-C2-N2	3.75	116.89	110.49
6	J	2	NAG	C4-C3-C2	3.23	115.76	111.02
6	H	1	NAG	C2-N2-C7	3.20	127.46	122.90
6	H	2	NAG	C3-C4-C5	2.79	115.22	110.24
7	G	5	BMA	C1-C2-C3	2.76	113.06	109.67
7	G	4	BMA	C1-O5-C5	2.73	115.89	112.19
7	G	5	BMA	O5-C1-C2	2.69	114.93	110.77
6	H	2	NAG	C4-C3-C2	2.62	114.86	111.02
6	H	1	NAG	C1-O5-C5	2.53	115.61	112.19
6	J	2	NAG	C3-C4-C5	2.49	114.68	110.24
7	G	5	BMA	C2-C3-C4	2.15	114.62	110.89
6	I	1	NAG	O4-C4-C3	-2.08	105.55	110.35

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	3	BMA	C4-C5-C6-O6
7	G	3	BMA	O5-C5-C6-O6
7	G	2	NAG	O5-C5-C6-O6
6	J	1	NAG	O5-C5-C6-O6
7	G	4	BMA	C4-C5-C6-O6
6	F	1	NAG	C4-C5-C6-O6
6	J	1	NAG	C4-C5-C6-O6
6	F	1	NAG	O5-C5-C6-O6
6	F	2	NAG	O5-C5-C6-O6
7	G	2	NAG	C4-C5-C6-O6
7	G	4	BMA	O5-C5-C6-O6
6	F	2	NAG	C4-C5-C6-O6
6	F	2	NAG	C8-C7-N2-C2
6	F	2	NAG	O7-C7-N2-C2

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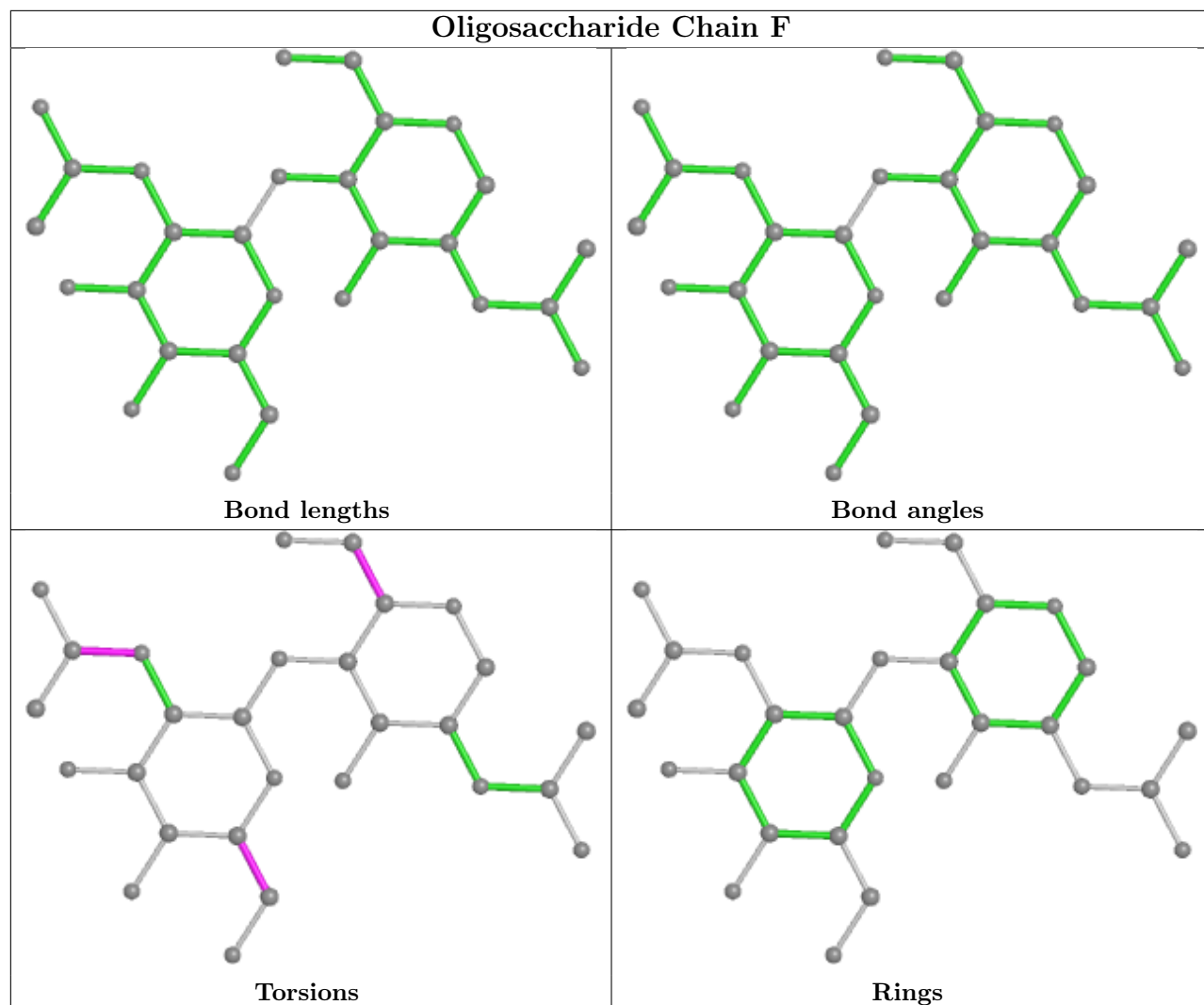
Mol	Chain	Res	Type	Atoms
6	H	2	NAG	C8-C7-N2-C2
6	H	2	NAG	O7-C7-N2-C2
6	I	2	NAG	C8-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
6	J	2	NAG	C8-C7-N2-C2
6	J	2	NAG	O7-C7-N2-C2
7	G	1	NAG	C8-C7-N2-C2
7	G	1	NAG	O7-C7-N2-C2
6	H	1	NAG	C4-C5-C6-O6
6	J	2	NAG	O5-C5-C6-O6
6	J	2	NAG	C4-C5-C6-O6
6	H	1	NAG	O5-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6
6	I	1	NAG	O5-C5-C6-O6
6	I	2	NAG	C4-C5-C6-O6
6	H	1	NAG	C3-C2-N2-C7
6	J	2	NAG	C3-C2-N2-C7
6	K	1	NAG	C4-C5-C6-O6

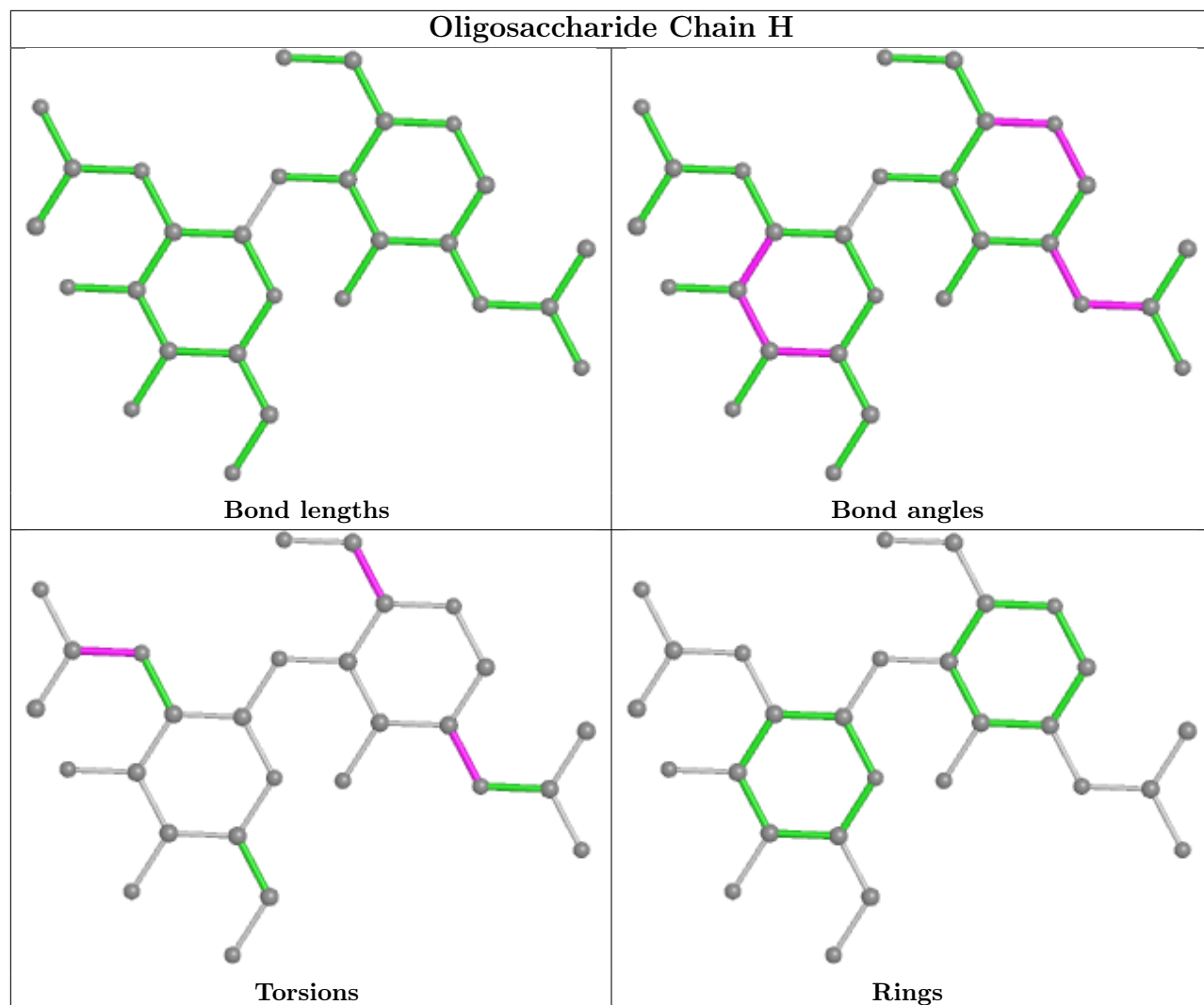
There are no ring outliers.

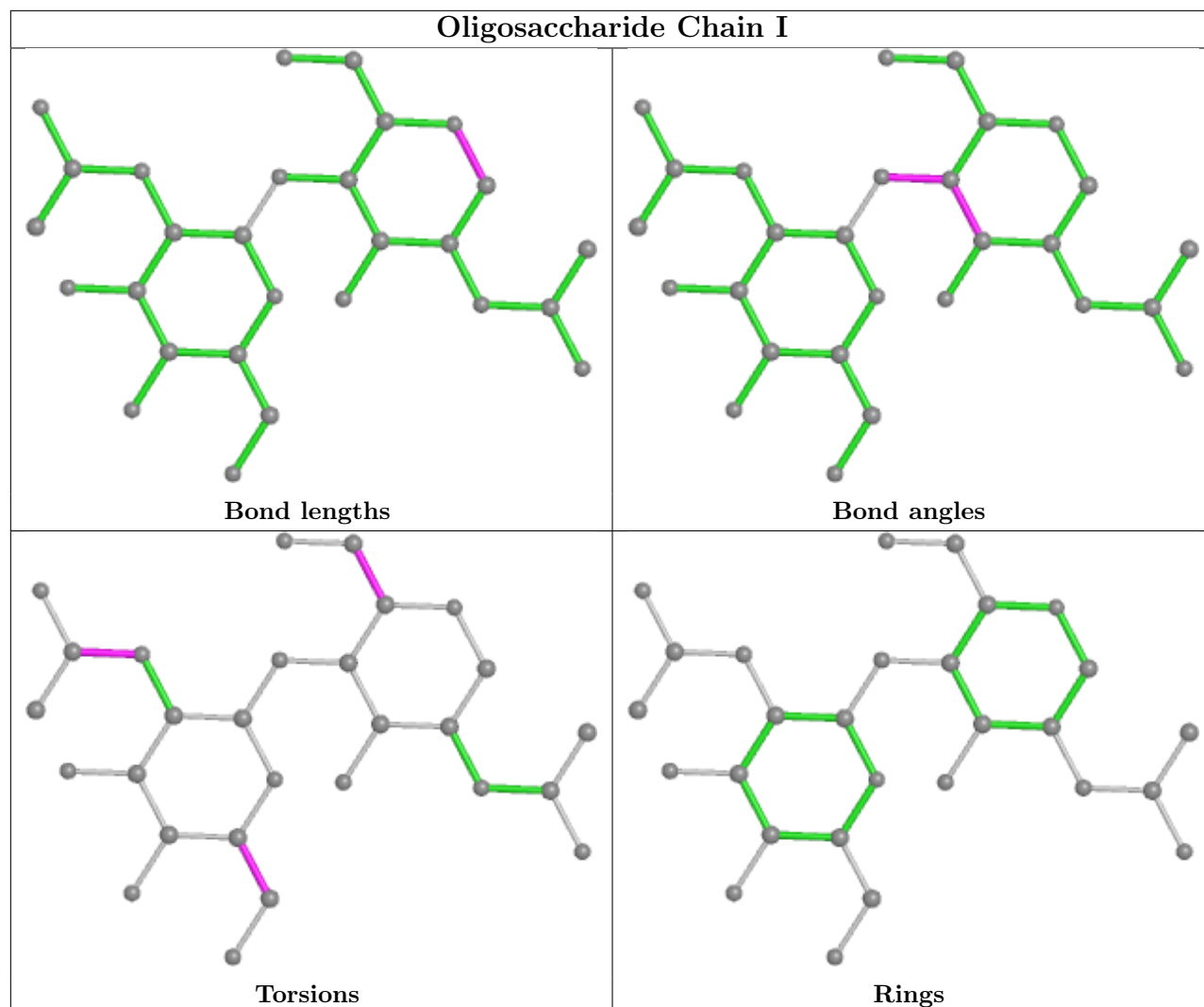
1 monomer is involved in 1 short contact:

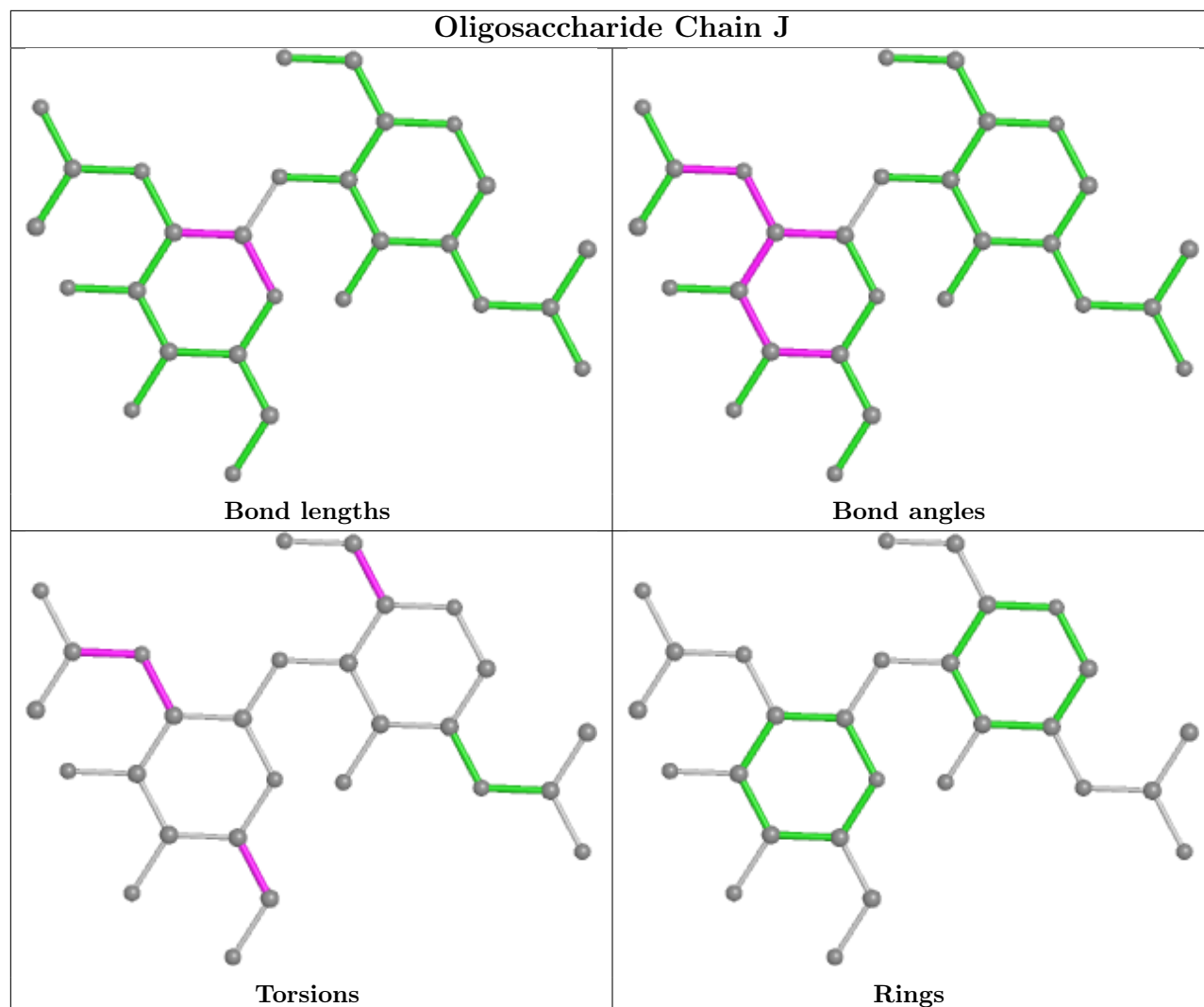
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	1	NAG	1	0

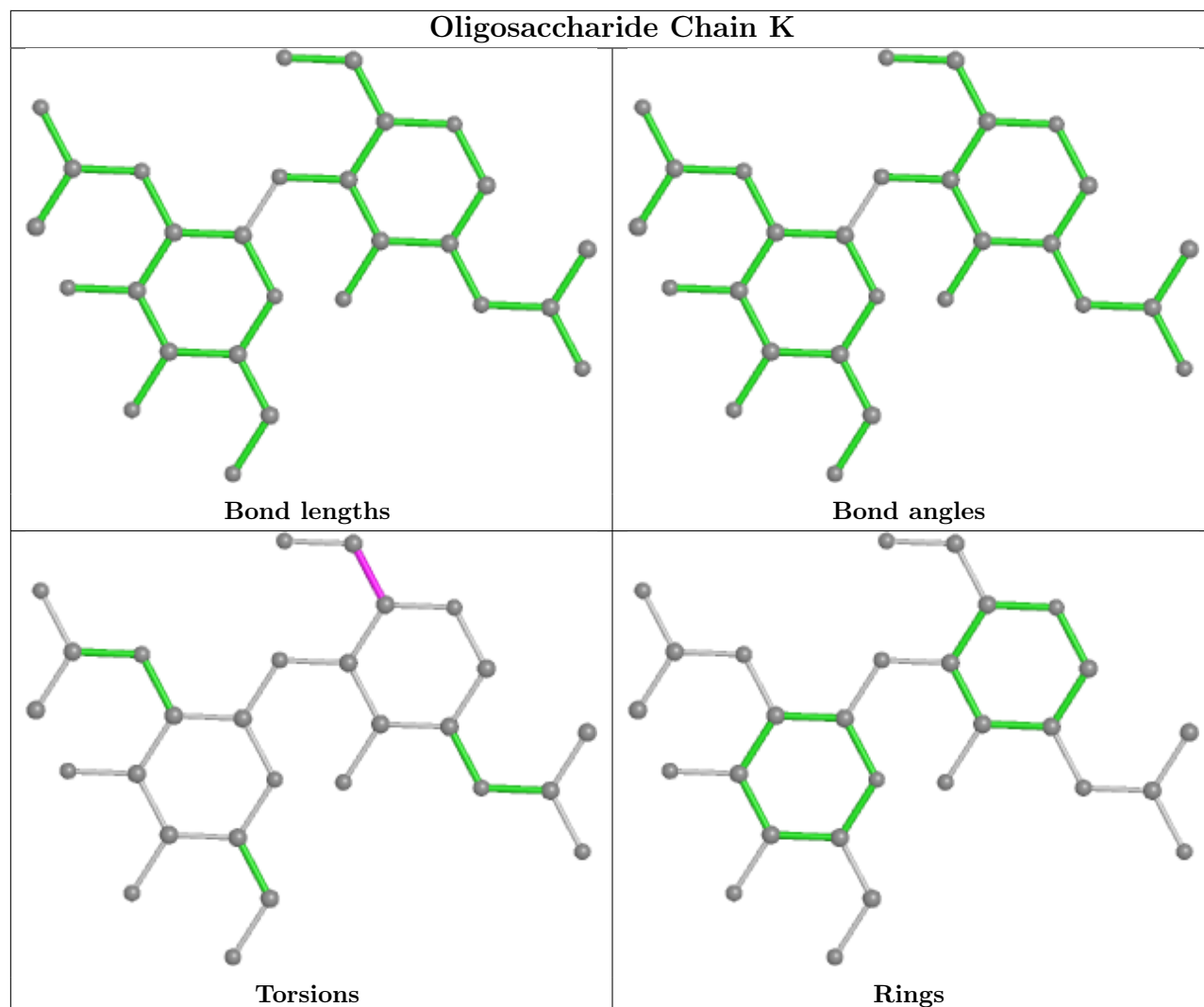
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

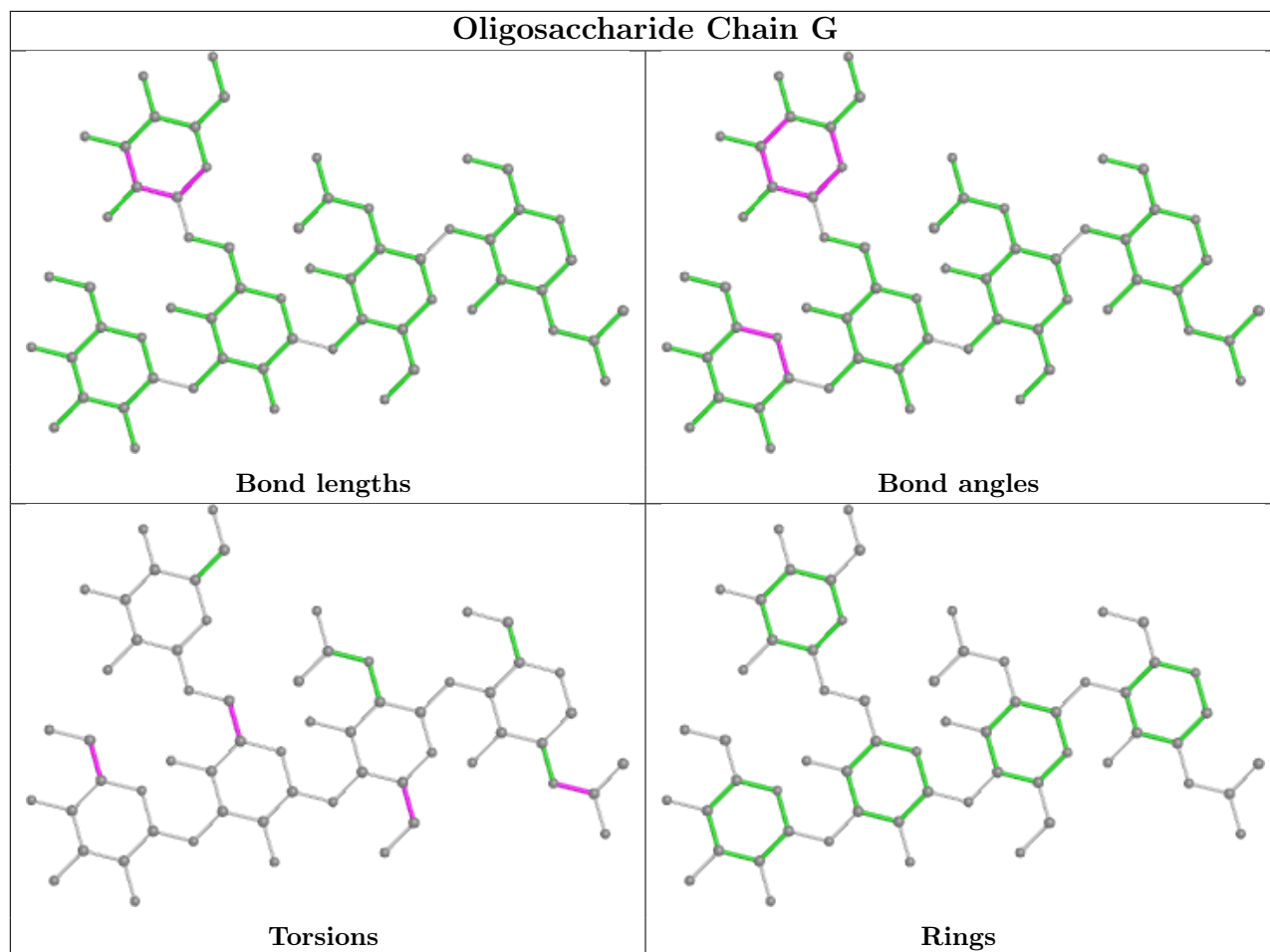












5.6 Ligand geometry [i](#)

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	$\# Z > 2$
8	NAG	A	810	1	14,14,15	0.33	0	17,19,21	0.48	0
9	PC1	B	501	-	51,51,53	1.31	6 (11%)	57,59,61	1.12	3 (5%)
9	PC1	C	301	-	49,49,53	1.34	6 (12%)	55,57,61	1.12	3 (5%)
8	NAG	A	818	1	14,14,15	0.40	0	17,19,21	0.46	0
10	CLR	C	302	3	31,31,31	0.34	0	48,48,48	0.55	0
10	CLR	C	303	-	31,31,31	0.34	0	48,48,48	0.56	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLR	C	304	-	31,31,31	0.35	0	48,48,48	0.59	1 (2%)
8	NAG	A	817	1	14,14,15	0.68	1 (7%)	17,19,21	0.99	1 (5%)
8	NAG	A	819	1	14,14,15	0.60	0	17,19,21	0.55	0
8	NAG	A	820	1	14,14,15	0.33	0	17,19,21	0.50	0
9	PC1	D	201	-	38,38,53	1.46	6 (15%)	44,46,61	1.13	3 (6%)
9	PC1	B	502	-	42,42,53	1.42	6 (14%)	48,50,61	1.12	3 (6%)
8	NAG	A	821	-	15,15,15	0.20	0	21,21,21	0.15	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
8	NAG	A	810	1	-	1/6/23/26	0/1/1/1
9	PC1	B	501	-	-	30/55/55/57	-
9	PC1	C	301	-	-	26/53/53/57	-
8	NAG	A	818	1	-	2/6/23/26	0/1/1/1
10	CLR	C	302	3	-	4/10/68/68	0/4/4/4
10	CLR	C	303	-	-	1/10/68/68	0/4/4/4
10	CLR	C	304	-	-	1/10/68/68	0/4/4/4
8	NAG	A	817	1	-	3/6/23/26	0/1/1/1
8	NAG	A	819	1	-	2/6/23/26	0/1/1/1
8	NAG	A	820	1	-	2/6/23/26	0/1/1/1
9	PC1	D	201	-	-	20/42/42/57	-
9	PC1	B	502	-	-	18/46/46/57	-
8	NAG	A	821	-	-	2/6/26/26	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	502	PC1	O31-C31	3.34	1.43	1.33
9	D	201	PC1	O31-C31	3.33	1.43	1.33
9	B	501	PC1	O31-C31	3.32	1.43	1.33
9	C	301	PC1	O31-C31	3.27	1.42	1.33
9	C	301	PC1	C2A-C29	-2.93	1.35	1.51
9	B	502	PC1	O21-C21	2.92	1.42	1.34
9	B	501	PC1	C2A-C29	-2.91	1.35	1.51
9	B	502	PC1	C2A-C29	-2.90	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	201	PC1	C2A-C29	-2.89	1.35	1.51
9	D	201	PC1	O21-C21	2.85	1.42	1.34
9	B	501	PC1	O21-C21	2.84	1.42	1.34
9	C	301	PC1	O21-C21	2.84	1.42	1.34
9	D	201	PC1	O21-C2	-2.50	1.40	1.46
9	C	301	PC1	O21-C2	-2.49	1.40	1.46
9	B	501	PC1	O21-C2	-2.49	1.40	1.46
9	B	502	PC1	O21-C2	-2.44	1.40	1.46
9	D	201	PC1	P-O11	2.31	1.68	1.59
9	B	501	PC1	P-O11	2.31	1.68	1.59
9	C	301	PC1	P-O11	2.28	1.68	1.59
9	B	502	PC1	P-O11	2.28	1.68	1.59
8	A	817	NAG	C1-C2	2.14	1.55	1.52
9	C	301	PC1	P-O13	2.14	1.67	1.59
9	B	502	PC1	P-O13	2.05	1.67	1.59
9	B	501	PC1	P-O13	2.04	1.67	1.59
9	D	201	PC1	P-O13	2.04	1.67	1.59

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	301	PC1	O21-C21-C22	4.11	120.36	111.50
9	B	502	PC1	O21-C21-C22	4.00	120.13	111.50
9	D	201	PC1	O21-C21-C22	3.97	120.06	111.50
9	B	501	PC1	O21-C21-C22	3.64	119.35	111.50
8	A	817	NAG	C2-N2-C7	2.96	127.12	122.90
9	B	501	PC1	O31-C31-C32	2.70	120.38	111.91
9	C	301	PC1	O31-C31-C32	2.57	119.97	111.91
9	C	301	PC1	O12-P-O14	-2.44	100.19	112.24
9	B	502	PC1	O31-C31-C32	2.43	119.54	111.91
9	D	201	PC1	O31-C31-C32	2.36	119.32	111.91
9	B	501	PC1	O12-P-O14	-2.26	101.07	112.24
9	D	201	PC1	O12-P-O14	-2.25	101.14	112.24
9	B	502	PC1	O12-P-O14	-2.24	101.17	112.24
10	C	303	CLR	C13-C17-C20	2.04	122.69	119.49
10	C	304	CLR	C13-C17-C20	2.02	122.64	119.49

There are no chirality outliers.

All (112) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	501	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
9	B	501	PC1	C1-O11-P-O12
9	B	501	PC1	O13-C11-C12-N
9	B	502	PC1	O13-C11-C12-N
9	B	502	PC1	C22-C21-O21-C2
9	C	301	PC1	C11-O13-P-O12
9	C	301	PC1	C11-O13-P-O14
9	C	301	PC1	O22-C21-O21-C2
9	D	201	PC1	C11-O13-P-O12
9	D	201	PC1	C11-O13-P-O14
9	C	301	PC1	C22-C21-O21-C2
9	C	301	PC1	O32-C31-O31-C3
8	A	821	NAG	O5-C5-C6-O6
9	B	501	PC1	C28-C29-C2A-C2B
9	B	502	PC1	C28-C29-C2A-C2B
9	D	201	PC1	C28-C29-C2A-C2B
9	C	301	PC1	C32-C31-O31-C3
8	A	820	NAG	O5-C5-C6-O6
9	B	502	PC1	O22-C21-O21-C2
8	A	817	NAG	O5-C5-C6-O6
8	A	820	NAG	C4-C5-C6-O6
8	A	821	NAG	C4-C5-C6-O6
8	A	817	NAG	C4-C5-C6-O6
9	B	502	PC1	C32-C31-O31-C3
8	A	819	NAG	O5-C5-C6-O6
9	C	301	PC1	C21-C22-C23-C24
9	B	502	PC1	O32-C31-O31-C3
8	A	819	NAG	C4-C5-C6-O6
9	B	501	PC1	C22-C21-O21-C2
10	C	303	CLR	C20-C22-C23-C24
9	B	501	PC1	C21-C22-C23-C24
9	B	501	PC1	C1-O11-P-O13
9	B	502	PC1	C11-O13-P-O11
9	C	301	PC1	C11-O13-P-O11
9	D	201	PC1	C11-O13-P-O11
9	B	501	PC1	O22-C21-O21-C2
9	D	201	PC1	C33-C34-C35-C36
9	B	501	PC1	C36-C37-C38-C39
9	B	501	PC1	C39-C3A-C3B-C3C
9	C	301	PC1	C31-C32-C33-C34
9	D	201	PC1	C21-C22-C23-C24
9	C	301	PC1	C24-C25-C26-C27
9	C	301	PC1	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
9	D	201	PC1	C22-C23-C24-C25
9	B	501	PC1	C26-C27-C28-C29
8	A	818	NAG	O5-C5-C6-O6
9	C	301	PC1	C22-C23-C24-C25
9	B	502	PC1	C35-C36-C37-C38
9	B	501	PC1	C2E-C2F-C2G-C2H
9	C	301	PC1	C3A-C3B-C3C-C3D
9	C	301	PC1	C33-C34-C35-C36
9	C	301	PC1	C32-C33-C34-C35
9	C	301	PC1	C37-C38-C39-C3A
9	D	201	PC1	O22-C21-O21-C2
9	D	201	PC1	C22-C21-O21-C2
9	D	201	PC1	C29-C2A-C2B-C2C
9	C	301	PC1	C2D-C2E-C2F-C2G
9	B	502	PC1	C29-C2A-C2B-C2C
9	D	201	PC1	C32-C33-C34-C35
9	B	501	PC1	C32-C33-C34-C35
9	B	501	PC1	C1-C2-C3-O31
8	A	810	NAG	O5-C5-C6-O6
9	C	301	PC1	C35-C36-C37-C38
9	B	501	PC1	C3A-C3B-C3C-C3D
9	B	501	PC1	C32-C31-O31-C3
10	C	302	CLR	C16-C17-C20-C22
9	B	501	PC1	O11-C1-C2-C3
10	C	304	CLR	C20-C22-C23-C24
9	B	502	PC1	C1-C2-C3-O31
9	D	201	PC1	C1-O11-P-O13
9	B	501	PC1	C24-C25-C26-C27
9	B	501	PC1	C2-C1-O11-P
9	B	501	PC1	O21-C21-C22-C23
10	C	302	CLR	C13-C17-C20-C22
9	B	502	PC1	O11-C1-C2-C3
9	C	301	PC1	C2-C1-O11-P
9	B	501	PC1	O32-C31-O31-C3
9	B	501	PC1	O11-C1-C2-O21
9	C	301	PC1	O11-C1-C2-O21
9	B	502	PC1	C1-O11-P-O13
9	B	501	PC1	C1-O11-P-O14
9	B	502	PC1	C11-O13-P-O12
9	D	201	PC1	C1-O11-P-O12
9	C	301	PC1	O11-C1-C2-C3
10	C	302	CLR	C16-C17-C20-C21

Continued on next page...

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Mol	Chain	Res	Type	Atoms
9	C	301	PC1	C12-C11-O13-P
9	B	502	PC1	O11-C1-C2-O21
9	B	501	PC1	C2D-C2E-C2F-C2G
9	B	501	PC1	C33-C34-C35-C36
9	C	301	PC1	O13-C11-C12-N
9	D	201	PC1	O13-C11-C12-N
9	B	501	PC1	O21-C2-C3-O31
9	C	301	PC1	O21-C2-C3-O31
9	B	501	PC1	C25-C26-C27-C28
10	C	302	CLR	C13-C17-C20-C21
9	B	502	PC1	O21-C2-C3-O31
9	D	201	PC1	C2-C1-O11-P
9	B	502	PC1	C24-C25-C26-C27
9	D	201	PC1	O31-C31-C32-C33
9	D	201	PC1	C2A-C2B-C2C-C2D
9	B	501	PC1	C2F-C2G-C2H-C2I
8	A	818	NAG	C4-C5-C6-O6
9	B	501	PC1	C35-C36-C37-C38
9	D	201	PC1	C23-C24-C25-C26
9	C	301	PC1	C1-C2-C3-O31
9	D	201	PC1	O11-C1-C2-O21
9	D	201	PC1	C35-C36-C37-C38
9	B	502	PC1	C2B-C2C-C2D-C2E
8	A	817	NAG	C3-C2-N2-C7
9	C	301	PC1	C2B-C2C-C2D-C2E
9	B	501	PC1	O22-C21-C22-C23
9	B	502	PC1	C32-C33-C34-C35

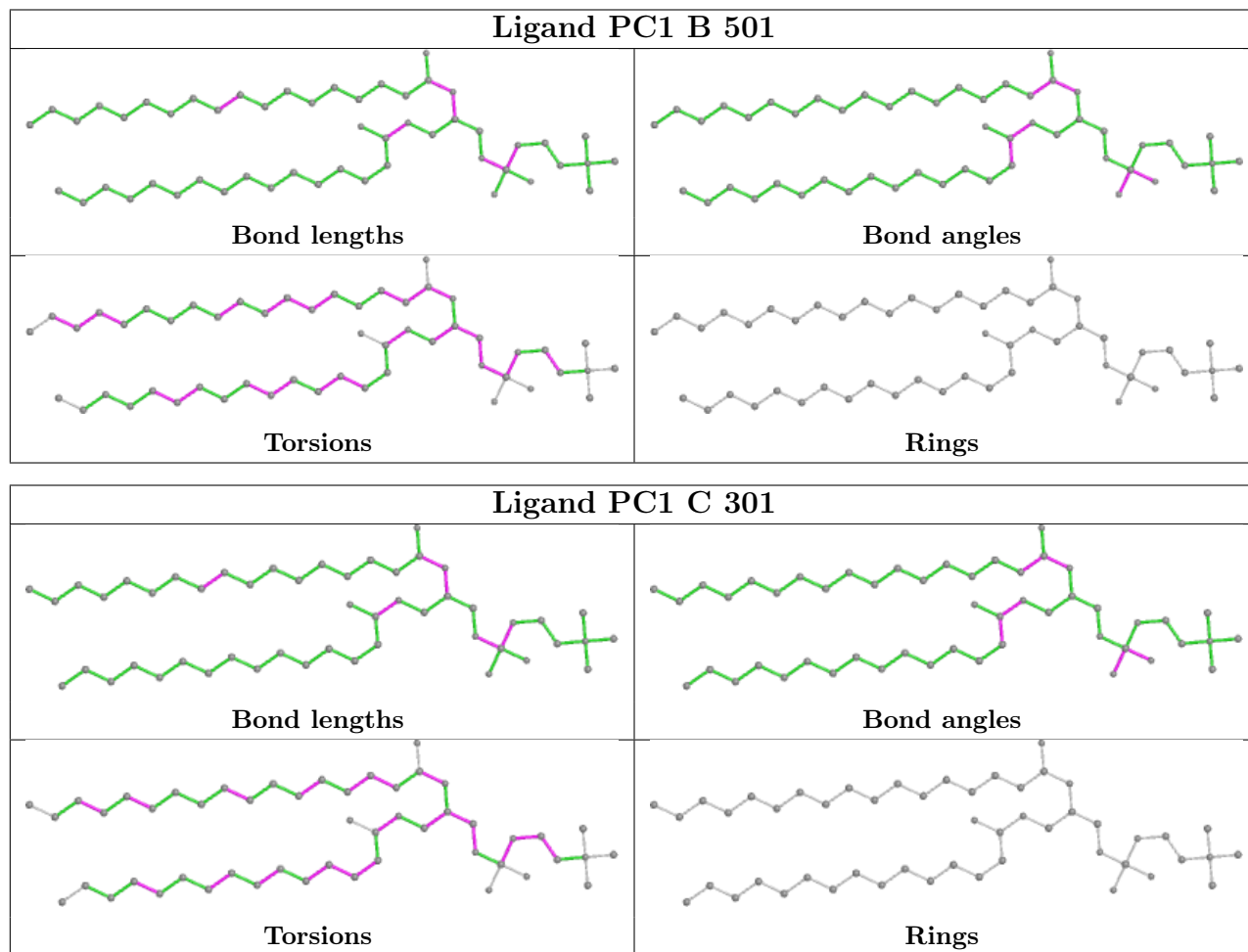
There are no ring outliers.

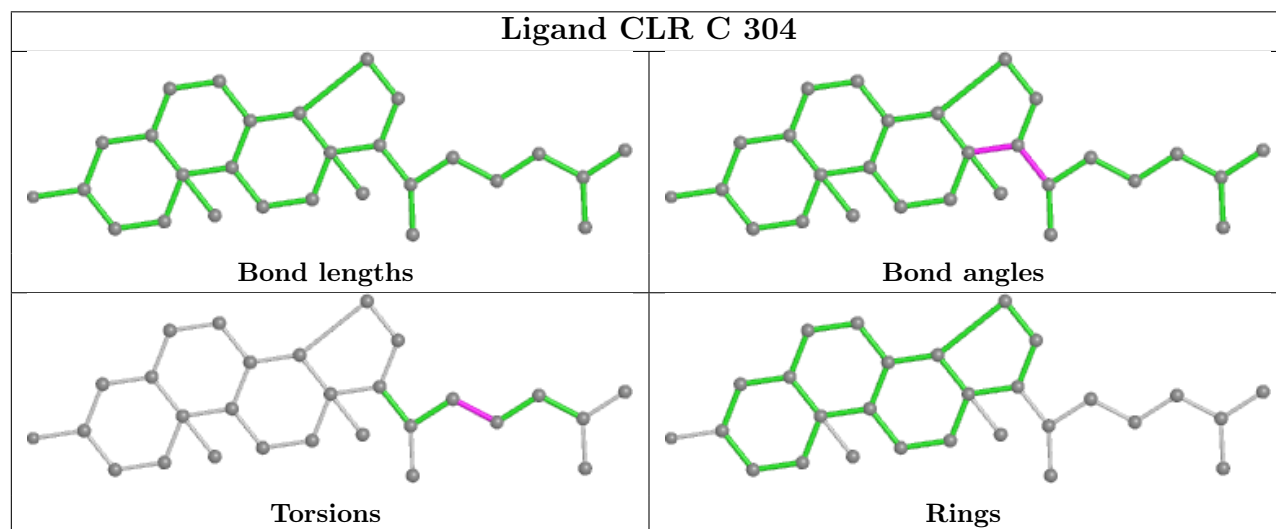
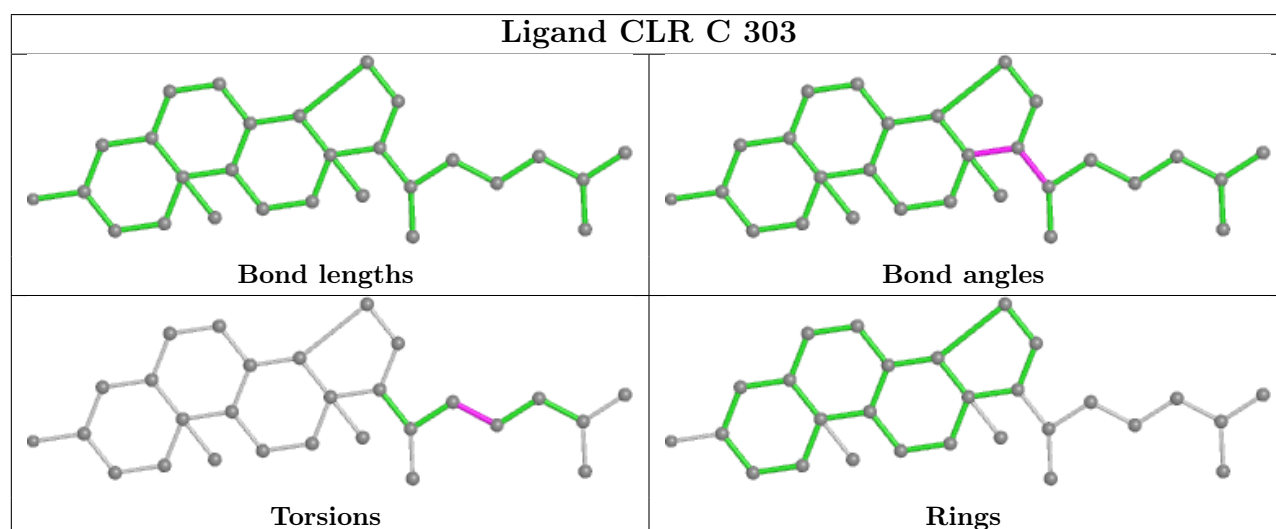
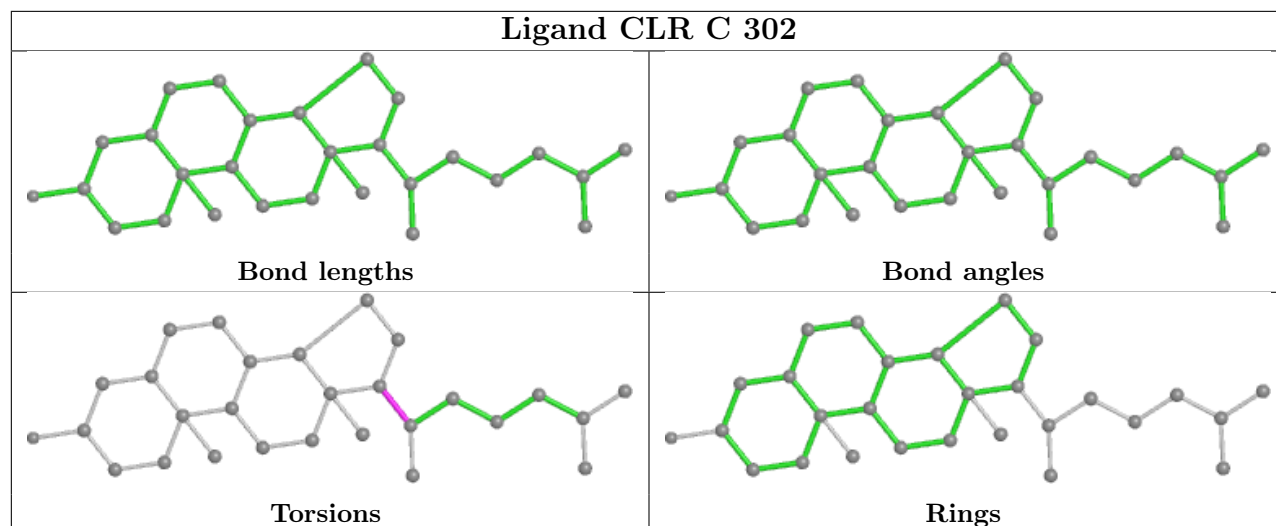
5 monomers are involved in 9 short contacts:

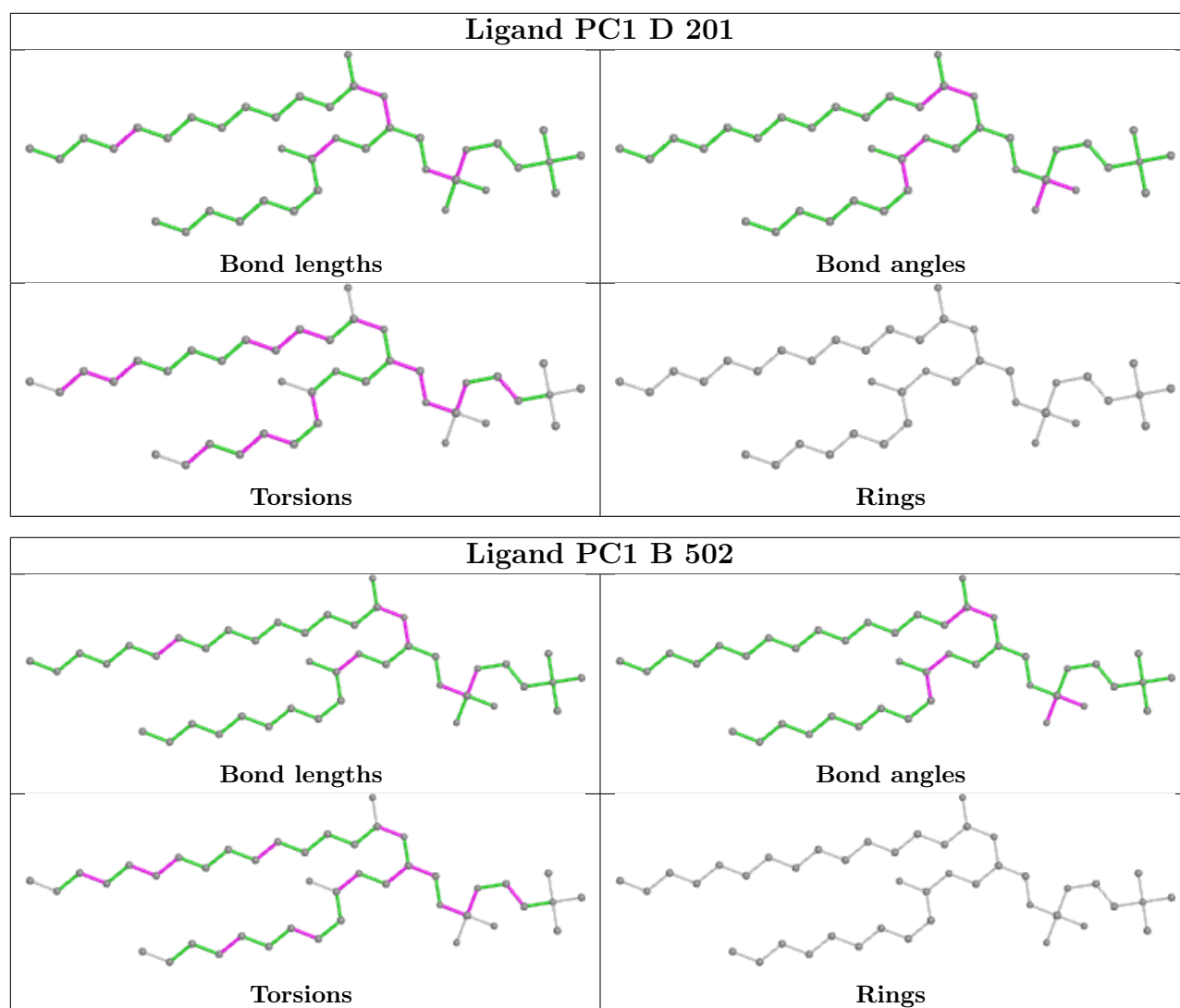
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	501	PC1	1	0
9	C	301	PC1	2	0
10	C	302	CLR	2	0
10	C	303	CLR	3	0
9	B	502	PC1	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

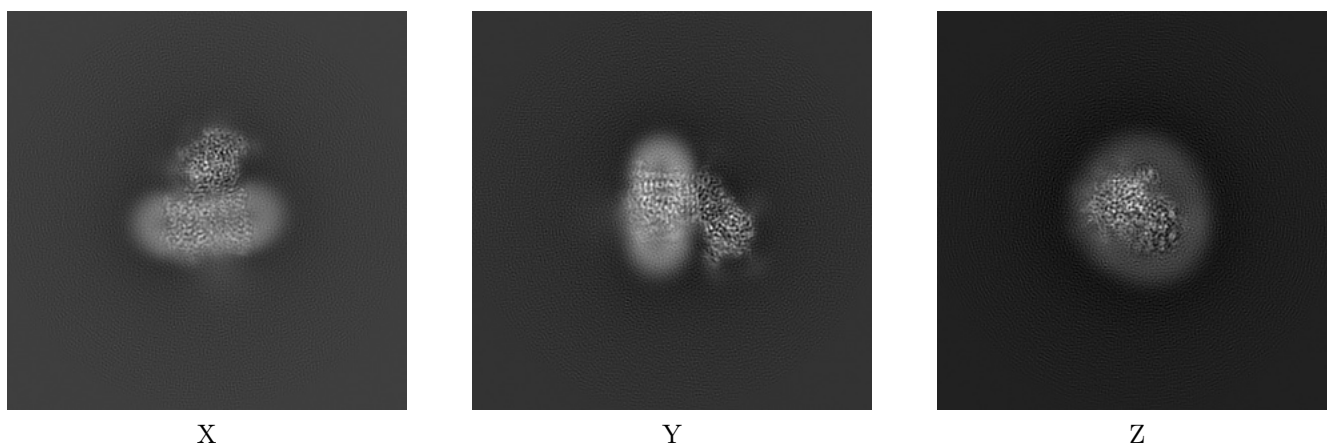
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9648. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

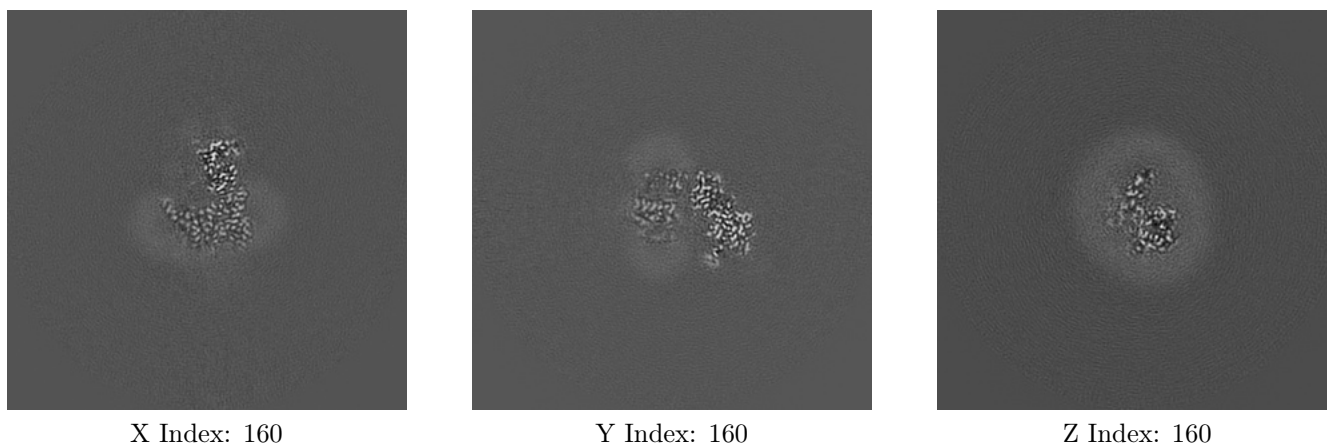
6.1.1 Primary map



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

6.2 Central slices [i](#)

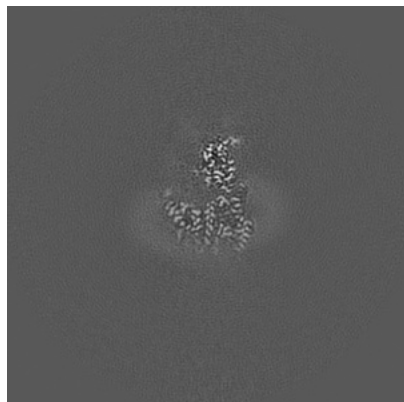
6.2.1 Primary map



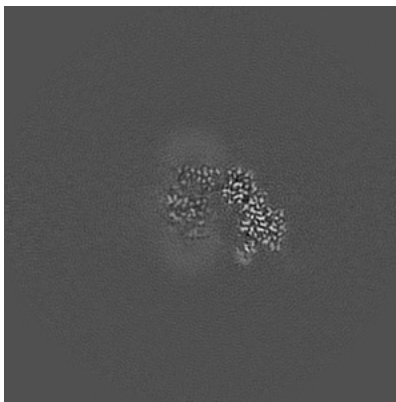
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

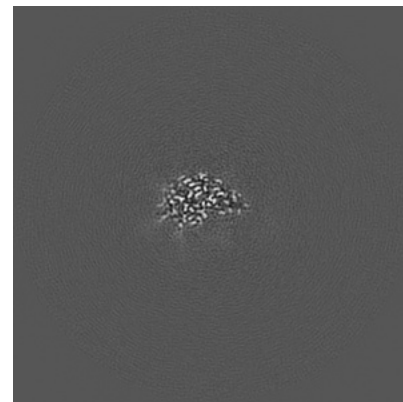
6.3.1 Primary map



X Index: 162



Y Index: 159



Z Index: 196

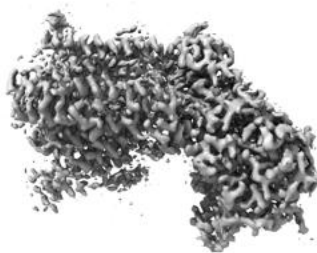
The images above show the largest variance slices of the map in three orthogonal directions.

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

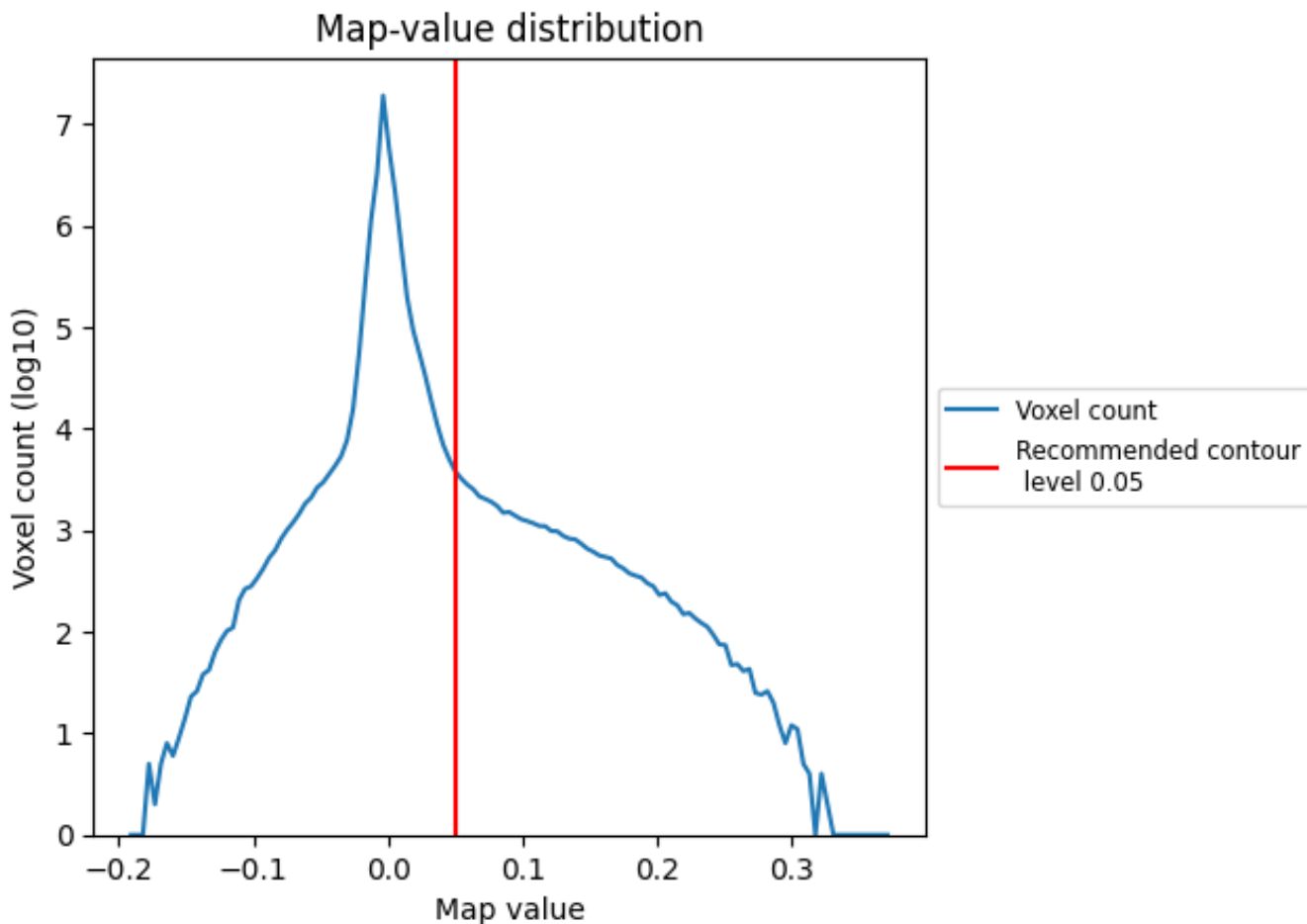
6.5 Mask visualisation

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

7 Map analysis [i](#)

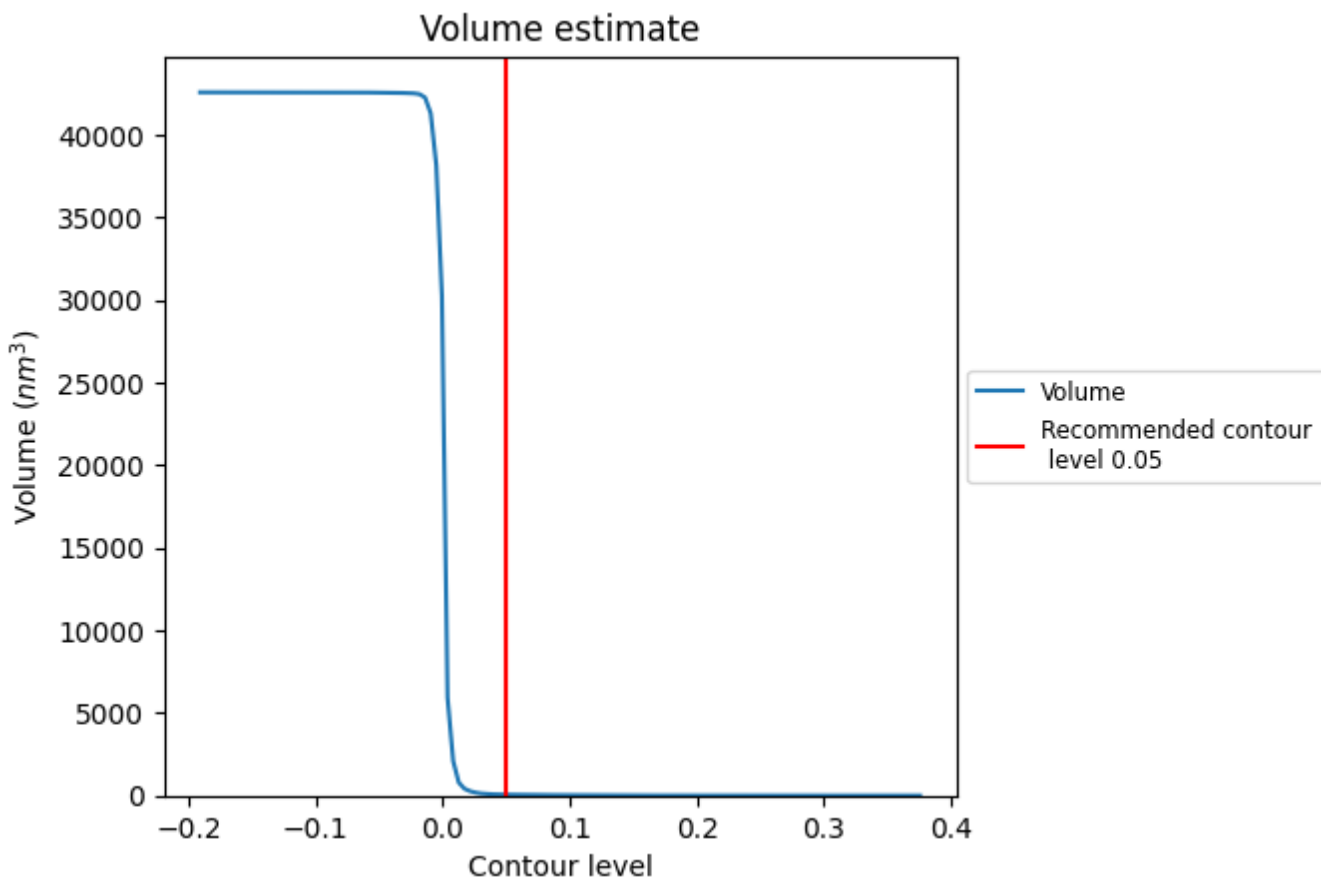
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

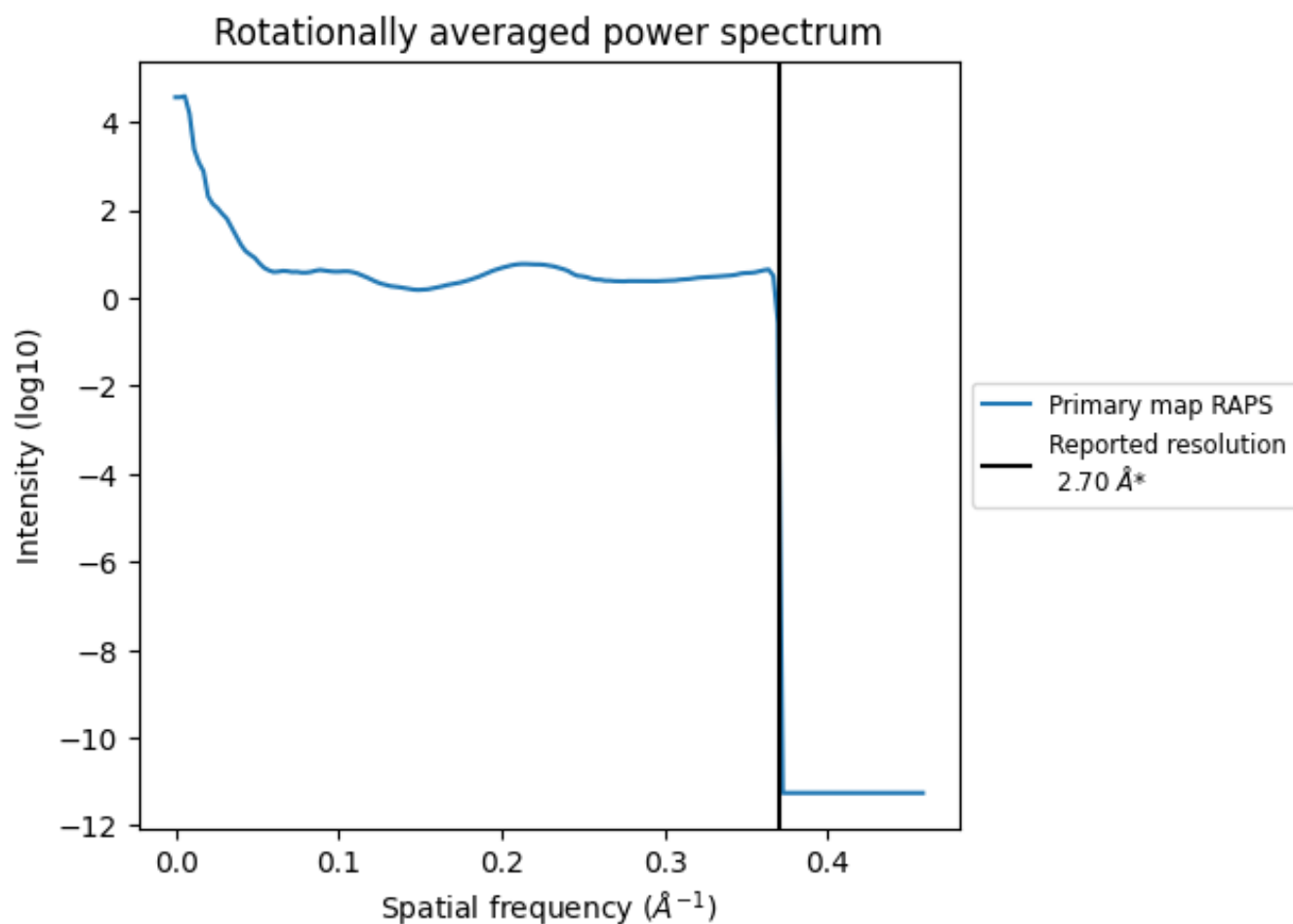
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 56 nm^3 ; this corresponds to an approximate mass of 51 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\AA^{-1}

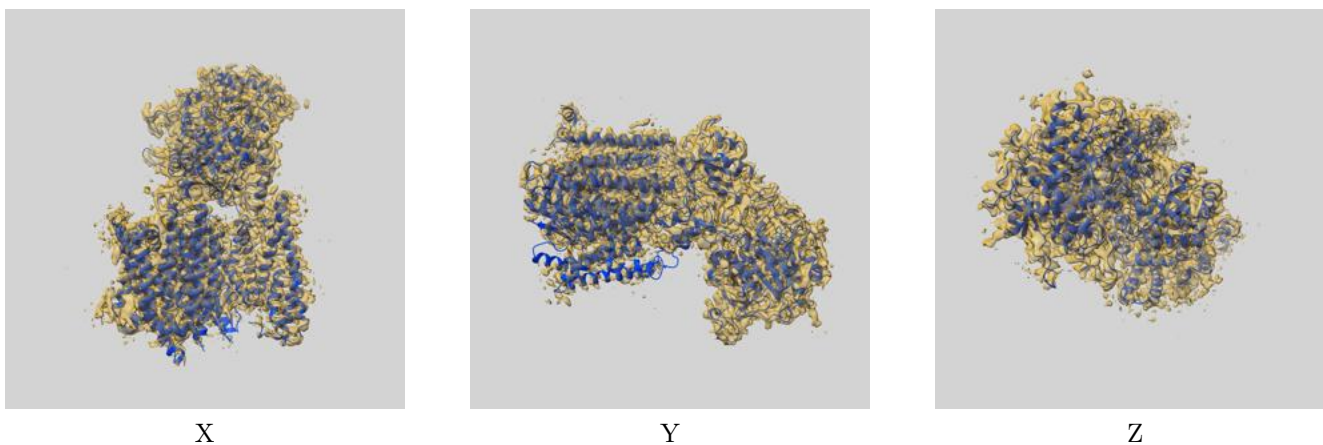
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

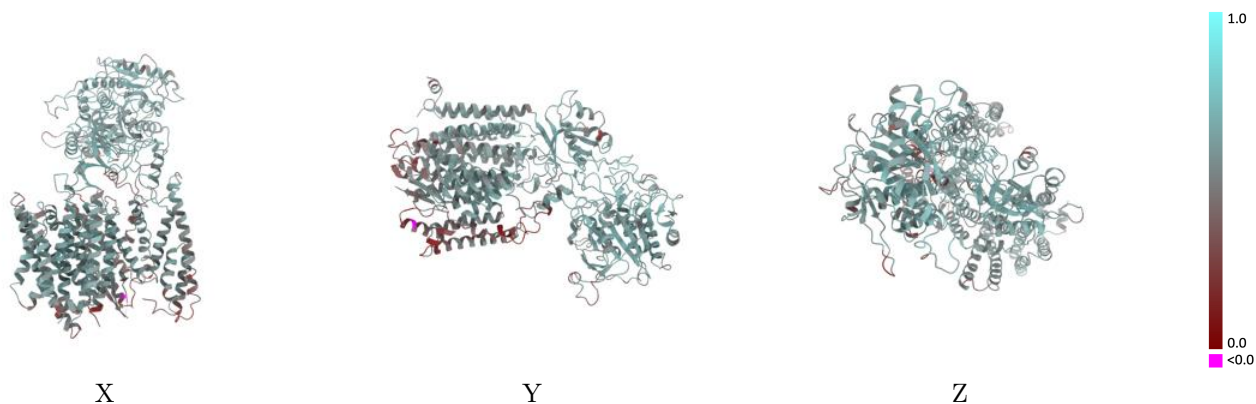
This section contains information regarding the fit between EMDB map EMD-9648 and PDB model 6IDF. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



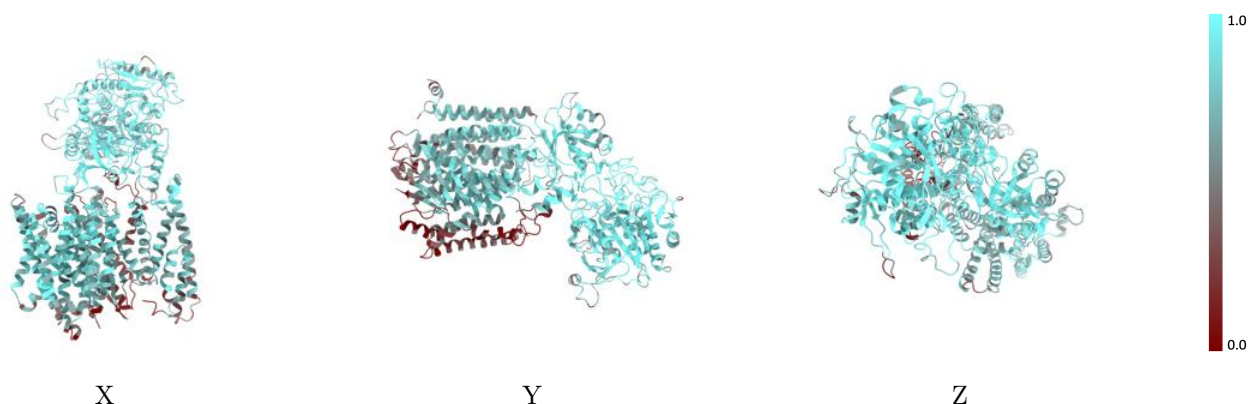
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



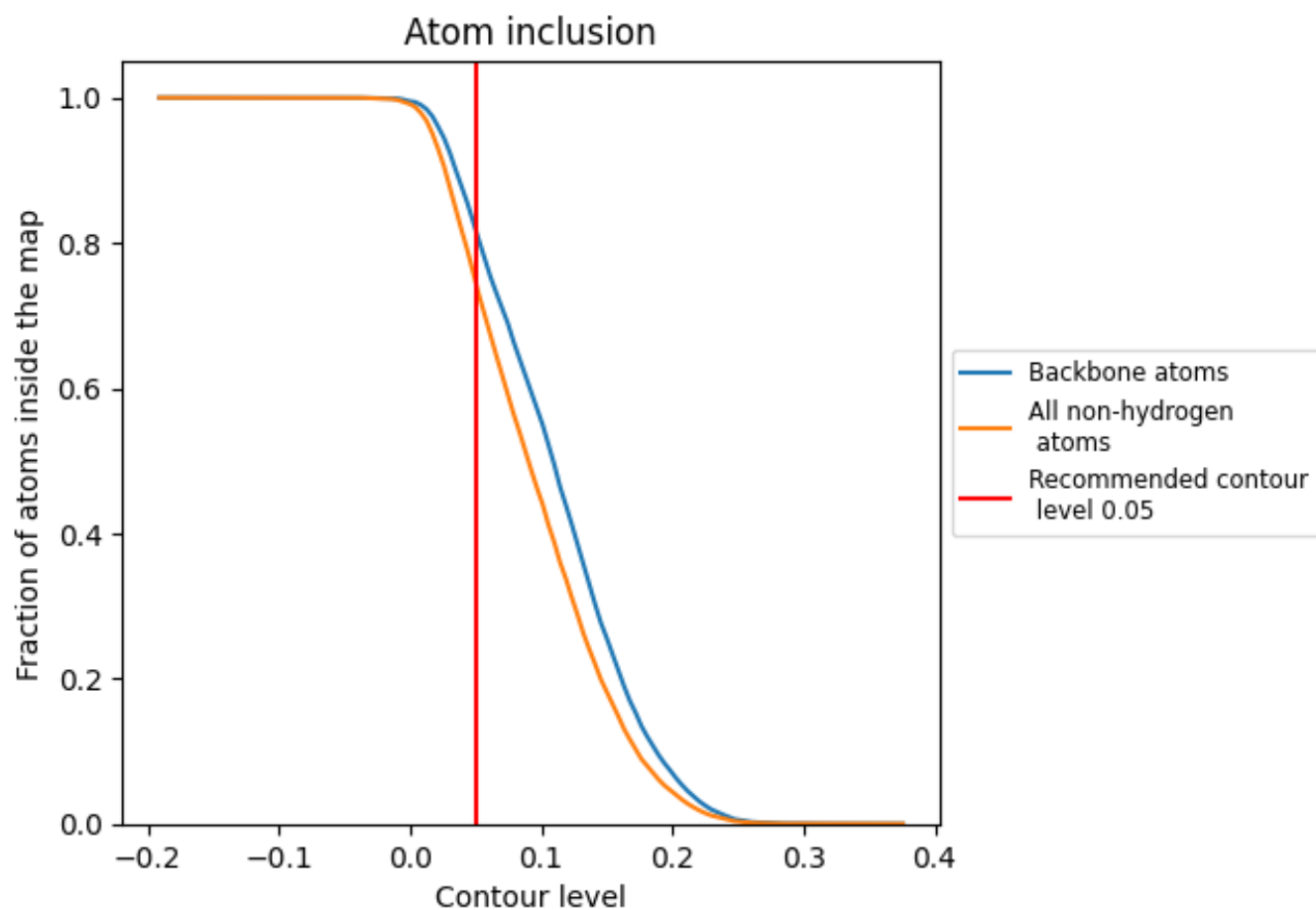
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

























9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 75% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7462	 0.5450
A	 0.8479	 0.5820
B	 0.5963	 0.5020
C	 0.7774	 0.5530
D	 0.6428	 0.4930
E	 0.2682	 0.3370
F	 0.7500	 0.5350
G	 0.7049	 0.5480
H	 0.8571	 0.5630
I	 0.6429	 0.4720
J	 0.5000	 0.5120
K	 0.7857	 0.5580

