



Full wwPDB EM Validation Report ⓘ

Mar 31, 2025 – 05:43 PM JST

PDB ID : 6IYC / pdb_00006iyc
EMDB ID : EMD-9751
Title : Recognition of the Amyloid Precursor Protein by Human gamma-secretase
Authors : Zhou, R.; Yang, G.; Guo, X.; Zhou, Q.; Lei, J.; Shi, Y.
Deposited on : 2018-12-14
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.42

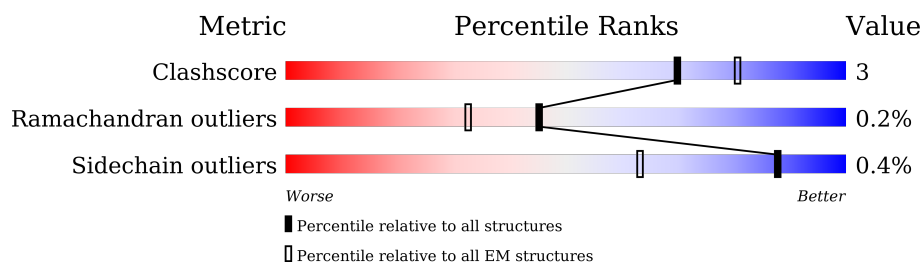
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 Å.

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






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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 $\leq 5\%$. 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	 12% 83% 11% 6%
2	B	467	 12% 61% 5% 33%
3	C	265	 7% 84% 8% 8%
4	D	101	 7% 91% 8%
5	E	104	 15% 31% 54%
6	F	2	 50% 50%
6	H	2	 100%
6	I	2	 50% 50%

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

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 11037 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
1	A	667	Total	C	N	O	S	0	0
			5235	3321	890	1003	21		

- Molecule 2 is a protein called Presenilin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	311	Total	C	N	O	S	0	0
			2407	1630	369	393	15		

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

- Molecule 5 is a protein called Amyloid-beta A4 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	34	Total	C	N	O	S	0	0
			226	150	36	38	2		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	MET	-	initiating methionine	UNP P05067
E	8	CYS	VAL	engineered mutation	UNP P05067
E	84	GLU	-	expression tag	UNP P05067
E	85	GLN	-	expression tag	UNP P05067
E	86	LYS	-	expression tag	UNP P05067
E	87	LEU	-	expression tag	UNP P05067
E	88	ILE	-	expression tag	UNP P05067
E	89	SER	-	expression tag	UNP P05067
E	90	GLU	-	expression tag	UNP P05067
E	91	GLU	-	expression tag	UNP P05067
E	92	ASP	-	expression tag	UNP P05067
E	93	LEU	-	expression tag	UNP P05067
E	94	LEU	-	expression tag	UNP P05067
E	95	GLU	-	expression tag	UNP P05067
E	96	HIS	-	expression tag	UNP P05067
E	97	HIS	-	expression tag	UNP P05067
E	98	HIS	-	expression tag	UNP P05067
E	99	HIS	-	expression tag	UNP P05067
E	100	HIS	-	expression tag	UNP P05067
E	101	HIS	-	expression tag	UNP P05067
E	102	HIS	-	expression tag	UNP P05067
E	103	HIS	-	expression tag	UNP P05067

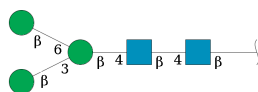
- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

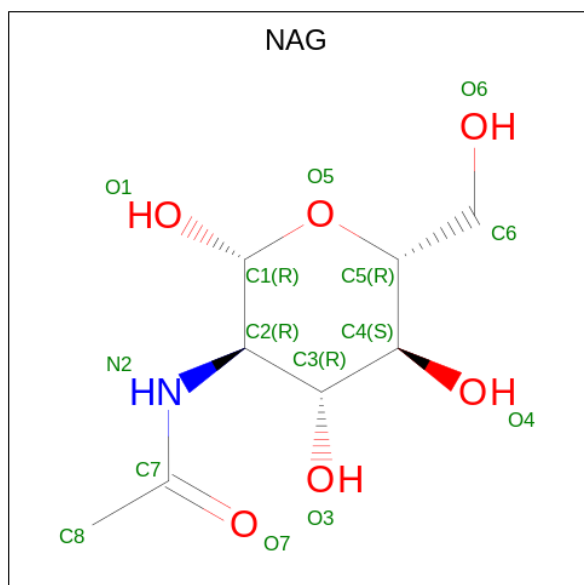
- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranos

e-(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
7	G	5	Total	C	N	O	0	0
			61	34	2	25		

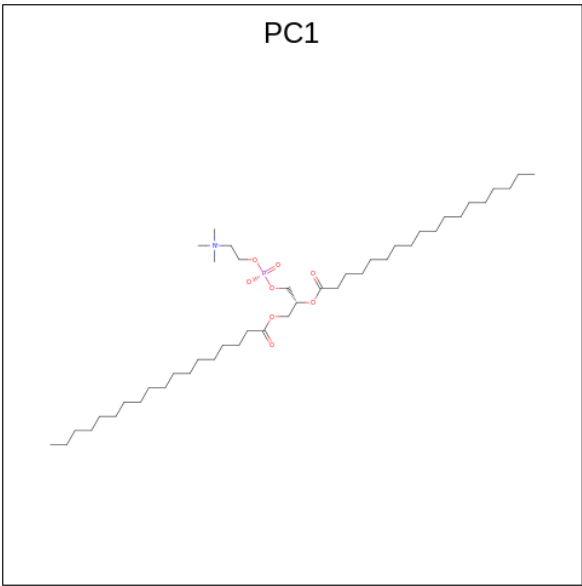
- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

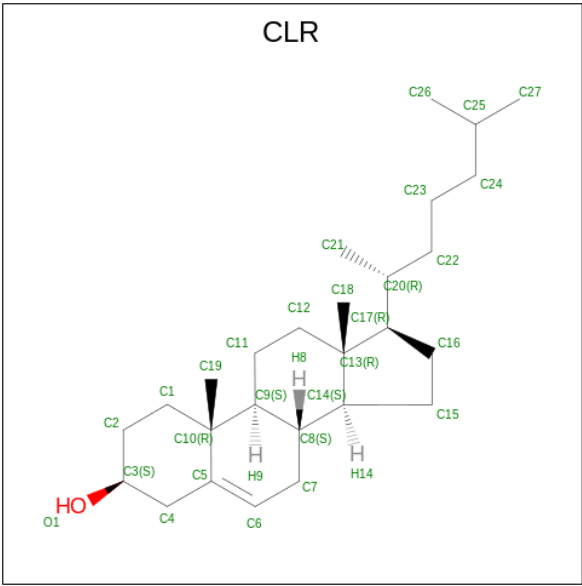
- Molecule 9 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1)

(formula: C₄₄H₈₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
9	B	1	Total	C	N	O	P	0
			37	27	1	8	1	
9	C	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 10 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



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

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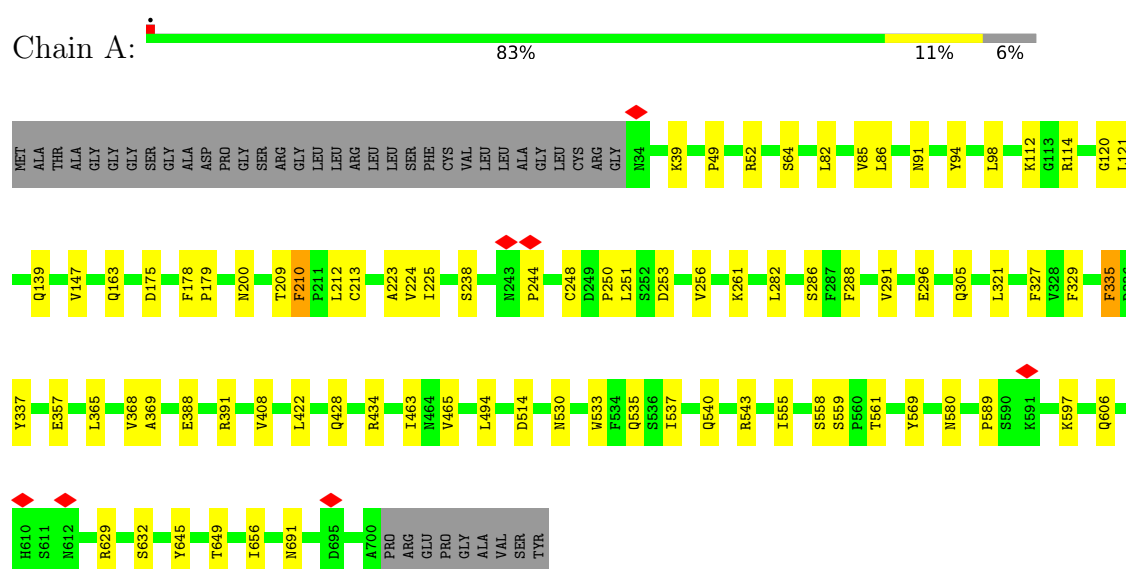
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Mol	Chain	Residues	Atoms			AltConf
10	C	1	Total	C	O	0
			28	27	1	
10	C	1	Total	C	O	0
			28	27	1	

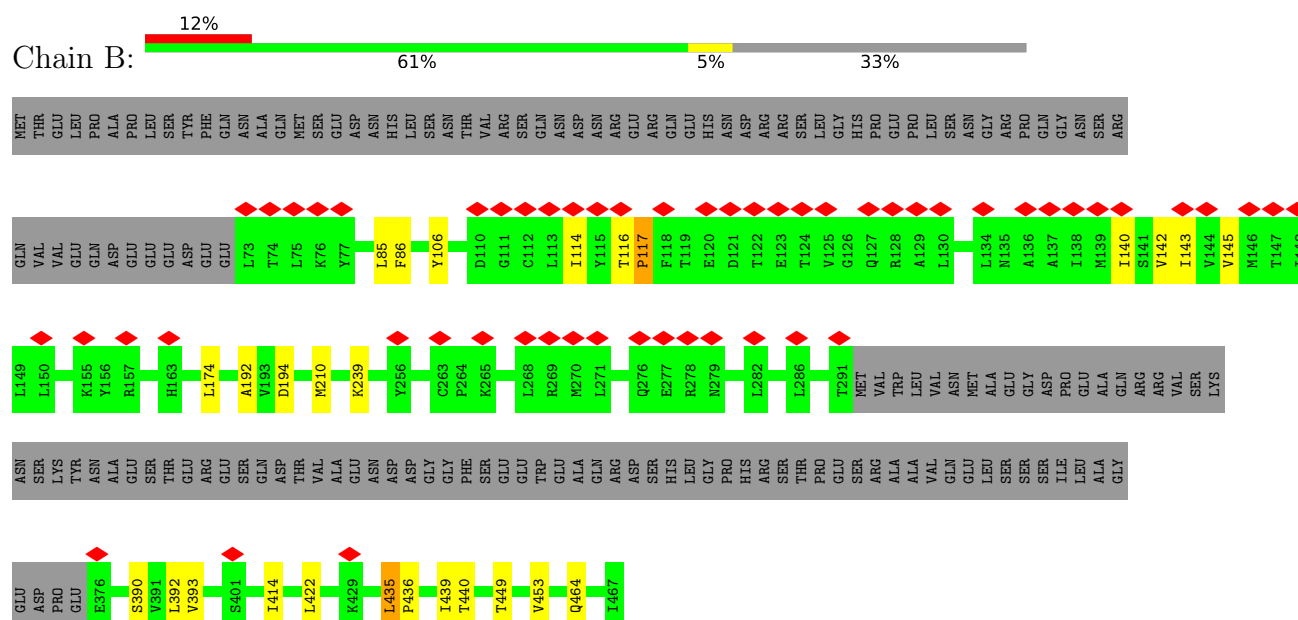
3 Residue-property plots

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

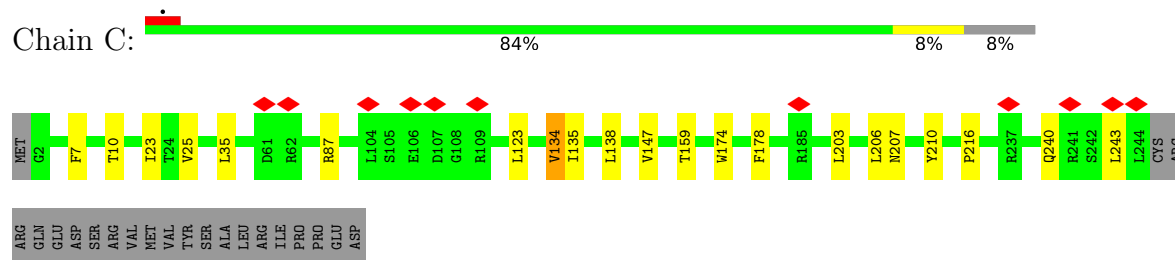
• Molecule 1: Nicastrin



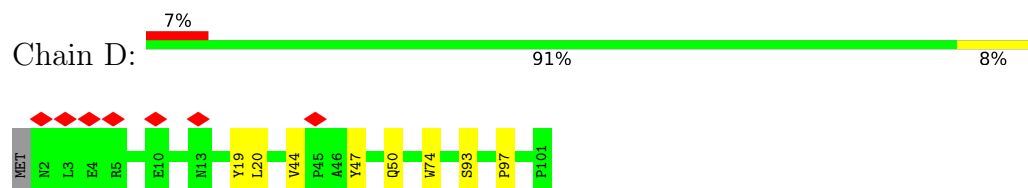
• Molecule 2: Presenilin-1



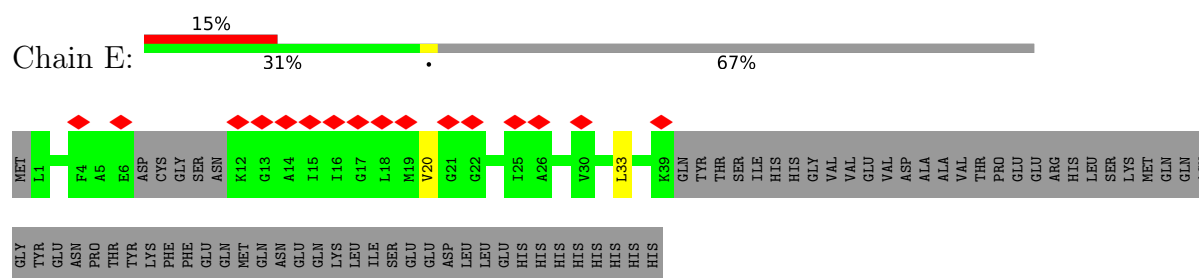
- Molecule 3: Gamma-secretase subunit APH-1A



- Molecule 4: Gamma-secretase subunit PEN-2



- Molecule 5: Amyloid-beta A4 protein



- 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



- 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:  50% 50%

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%

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	502450	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	0.184	Depositor
Minimum map value	-0.072	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.024	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: CLR, PC1, 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	0.58	1/5358 (0.0%)	0.69	2/7302 (0.0%)
2	B	0.42	0/2467	0.61	1/3370 (0.0%)
3	C	0.50	0/1924	0.65	1/2624 (0.0%)
4	D	0.47	0/883	0.57	0/1205
5	E	0.32	0/224	0.63	0/302
All	All	0.52	1/10856 (0.0%)	0.66	4/14803 (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	6
2	B	0	1
3	C	0	2
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	248	CYS	CB-SG	-7.31	1.69	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	117	PRO	N-CA-CB	6.84	111.51	103.30
1	A	251	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	98	LEU	CA-CB-CG	5.15	127.15	115.30
3	C	123	LEU	CA-CB-CG	5.08	126.98	115.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	209	THR	Peptide
1	A	224	VAL	Peptide
1	A	288	PHE	Peptide
1	A	335	PHE	Peptide
1	A	558	SER	Peptide
1	A	91	ASN	Peptide
2	B	435	LEU	Peptide
3	C	134	VAL	Peptide
3	C	206	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5235	0	5126	40	0
2	B	2407	0	2497	17	0
3	C	1872	0	1911	12	0
4	D	850	0	840	6	0
5	E	226	0	253	2	0
6	F	28	0	25	0	0
6	H	28	0	25	0	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	84	0	78	2	0
9	B	37	0	48	4	0
9	C	41	0	56	0	0
10	C	84	0	133	1	0
All	All	11037	0	11119	75	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 3.

All (75) 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)
9:B:501:PC1:H362	3:C:135:ILE:HD11	1.54	0.88
8:A:810:NAG:O7	8:A:810:NAG:O3	2.05	0.71
9:B:501:PC1:O14	9:B:501:PC1:H133	1.98	0.64
1:A:200:ASN:ND2	1:A:213:CYS:SG	2.71	0.64
1:A:49:PRO:HG3	1:A:656:ILE:HD13	1.82	0.61
1:A:530:ASN:OD1	1:A:535:GLN:NE2	2.31	0.60
1:A:632:SER:OG	1:A:645:TYR:O	2.20	0.60
2:B:464:GLN:O	3:C:207:ASN:ND2	2.29	0.60
2:B:85:LEU:HD12	2:B:422:LEU:HD21	1.83	0.59
1:A:388:GLU:OE1	1:A:391:ARG:NH2	2.36	0.58
1:A:253:ASP:OD1	1:A:561:THR:OG1	2.22	0.57
9:B:501:PC1:O13	9:B:501:PC1:H132	2.05	0.57
8:A:810:NAG:HO3	8:A:810:NAG:C7	2.11	0.57
2:B:194:ASP:OD2	4:D:74:TRP:NE1	2.38	0.56
1:A:86:LEU:HD12	1:A:114:ARG:HD2	1.88	0.56
2:B:106:TYR:HA	2:B:239:LYS:HD3	1.89	0.54
1:A:543:ARG:HD3	1:A:606:GLN:HE22	1.70	0.54
3:C:134:VAL:HG13	3:C:138:LEU:HD13	1.89	0.54
2:B:192:ALA:HB2	4:D:97:PRO:HD3	1.89	0.54
1:A:559:SER:HB2	1:A:629:ARG:HH12	1.73	0.53
1:A:261:LYS:NZ	1:A:321:LEU:O	2.42	0.53
1:A:256:VAL:HG13	1:A:329:PHE:HB2	1.91	0.52
3:C:203:LEU:HD13	3:C:216:PRO:HB2	1.92	0.52
1:A:282:LEU:HD13	1:A:329:PHE:HB3	1.92	0.52
1:A:296:GLU:HG2	1:A:369:ALA:HB3	1.90	0.52
2:B:392:LEU:HD22	2:B:414:ILE:HD11	1.93	0.51
2:B:194:ASP:HA	4:D:93:SER:HA	1.92	0.51
1:A:335:PHE:O	1:A:337:TYR:N	2.44	0.50
3:C:7:PHE:HA	3:C:10:THR:HG22	1.94	0.50
3:C:87:ARG:HH12	3:C:174:TRP:HB3	1.75	0.50
3:C:240:GLN:HA	3:C:243:LEU:HG	1.94	0.50
1:A:514:ASP:OD1	1:A:514:ASP:N	2.46	0.49
2:B:114:ILE:HG12	5:E:20:VAL:HG22	1.95	0.48
2:B:194:ASP:OD1	2:B:194:ASP:N	2.38	0.48
1:A:52:ARG:NH1	1:A:223:ALA:O	2.42	0.48
2:B:142:VAL:HA	2:B:145:VAL:HG12	1.96	0.48
1:A:112:LYS:NZ	1:A:175:ASP:O	2.40	0.48
9:B:501:PC1:H32	9:B:501:PC1:H321	1.75	0.47
3:C:25:VAL:HG11	3:C:35:LEU:HD13	1.95	0.47
1:A:85:VAL:HG23	1:A:94:TYR:HB2	1.97	0.46
3:C:159:THR:HG21	3:C:210:TYR:CD1	2.51	0.45
1:A:82:LEU:O	1:A:86:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:LEU:HD21	1:A:494:LEU:HG	1.99	0.45
3:C:174:TRP:O	3:C:178:PHE:HB2	2.17	0.45
1:A:357:GLU:HG2	1:A:434:ARG:HH12	1.81	0.44
1:A:365:LEU:HD12	1:A:368:VAL:HG11	2.00	0.44
1:A:537:ILE:HG22	1:A:569:TYR:HB3	2.00	0.44
2:B:435:LEU:HB3	2:B:439:ILE:HD12	1.99	0.43
1:A:139:GLN:HG2	1:A:163:GLN:HE21	1.82	0.43
1:A:286:SER:OG	1:A:291:VAL:O	2.28	0.43
1:A:463:ILE:HG13	1:A:465:VAL:HG23	2.01	0.43
1:A:691:ASN:HD22	3:C:23:ILE:HG22	1.84	0.43
1:A:39:LYS:HB3	3:C:147:VAL:HG13	1.99	0.43
2:B:436:PRO:O	2:B:440:THR:OG1	2.32	0.43
4:D:19:TYR:HD2	4:D:20:LEU:HD12	1.83	0.43
1:A:210:PHE:O	1:A:212:LEU:N	2.52	0.42
1:A:238:SER:HA	1:A:244:PRO:HB3	2.02	0.42
1:A:422:LEU:HD23	1:A:428:GLN:HG2	2.01	0.42
4:D:44:VAL:O	4:D:50:GLN:NE2	2.37	0.42
1:A:253:ASP:HB2	1:A:555:ILE:HG13	2.03	0.41
1:A:305:GLN:HE21	1:A:327:PHE:HD1	1.68	0.41
1:A:64:SER:HB2	1:A:179:PRO:HG3	2.03	0.41
1:A:580:ASN:O	1:A:580:ASN:OD1	2.38	0.41
2:B:435:LEU:HG	5:E:33:LEU:HD13	2.03	0.41
10:C:303:CLR:H222	10:C:303:CLR:H162	1.62	0.41
1:A:540:GLN:HG3	1:A:606:GLN:HE21	1.85	0.41
2:B:140:ILE:HA	2:B:143:ILE:HG22	2.02	0.41
2:B:174:LEU:HD12	2:B:210:MET:HE1	2.03	0.41
1:A:120:GLY:H	1:A:178:PHE:HB2	1.86	0.41
2:B:390:SER:HA	2:B:393:VAL:HG12	2.04	0.40
1:A:589:PRO:HG2	1:A:597:LYS:HB2	2.03	0.40
2:B:449:THR:HA	2:B:453:VAL:HB	2.03	0.40
4:D:47:TYR:HD2	4:D:50:GLN:HG3	1.86	0.40
1:A:250:PRO:HA	1:A:649:THR:HG22	2.03	0.40
1:A:533:TRP:O	1:A:537:ILE:HG12	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	603 (91%)	61 (9%)	1 (0%)	44	66
2	B	307/467 (66%)	284 (92%)	21 (7%)	2 (1%)	19	38
3	C	241/265 (91%)	231 (96%)	10 (4%)	0	100	100
4	D	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
5	E	30/104 (29%)	27 (90%)	3 (10%)	0	100	100
All	All	1341/1646 (82%)	1238 (92%)	100 (8%)	3 (0%)	45	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	116	THR
2	B	117	PRO
1	A	225	ILE

5.3.2 Protein sidechains

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%)	580 (99%)	4 (1%)	81	93
2	B	253/408 (62%)	252 (100%)	1 (0%)	89	96
3	C	193/214 (90%)	193 (100%)	0	100	100
4	D	88/89 (99%)	88 (100%)	0	100	100
5	E	22/92 (24%)	22 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1140/1415 (81%)	1135 (100%)	5 (0%)	88 96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	LEU
1	A	147	VAL
1	A	210	PHE
1	A	408	VAL
2	B	86	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	158	HIS
1	A	163	GLN
1	A	200	ASN
1	A	358	ASN
1	A	454	GLN
1	A	531	ASN
1	A	606	GLN
1	A	691	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

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	6,1	14,14,15	0.33	0	17,19,21	0.47	0
6	NAG	F	2	6	14,14,15	0.22	0	17,19,21	0.72	1 (5%)
7	NAG	G	1	1,7	14,14,15	0.42	0	17,19,21	0.73	0
7	NAG	G	2	7	14,14,15	0.54	0	17,19,21	0.57	0
7	BMA	G	3	7	11,11,12	0.74	0	15,15,17	0.87	1 (6%)
7	BMA	G	4	7	11,11,12	0.89	0	15,15,17	0.98	1 (6%)
7	BMA	G	5	7	11,11,12	1.50	3 (27%)	15,15,17	1.66	2 (13%)
6	NAG	H	1	6,1	14,14,15	0.67	1 (7%)	17,19,21	1.25	3 (17%)
6	NAG	H	2	6	14,14,15	0.60	0	17,19,21	0.93	1 (5%)
6	NAG	I	1	6,1	14,14,15	0.69	1 (7%)	17,19,21	0.58	0
6	NAG	I	2	6	14,14,15	0.27	0	17,19,21	0.54	0
6	NAG	J	1	6,1	14,14,15	0.42	0	17,19,21	0.62	0
6	NAG	J	2	6	14,14,15	1.24	2 (14%)	17,19,21	2.40	5 (29%)
6	NAG	K	1	6,1	14,14,15	0.36	0	17,19,21	0.62	0
6	NAG	K	2	6	14,14,15	0.21	0	17,19,21	0.71	1 (5%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	J	2	6	-	4/6/23/26	0/1/1/1
6	NAG	K	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	2	NAG	O5-C1	-3.35	1.38	1.43
7	G	5	BMA	C1-C2	2.62	1.58	1.52
6	I	1	NAG	O5-C1	-2.46	1.39	1.43
6	J	2	NAG	C1-C2	2.27	1.55	1.52
6	H	1	NAG	O5-C1	-2.26	1.40	1.43
7	G	5	BMA	O5-C1	2.22	1.47	1.43
7	G	5	BMA	C2-C3	2.21	1.55	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	2	NAG	C2-N2-C7	7.53	133.62	122.90
7	G	5	BMA	C1-O5-C5	4.71	118.57	112.19
6	J	2	NAG	C1-C2-N2	3.60	116.64	110.49
6	H	1	NAG	C2-N2-C7	3.23	127.50	122.90
6	J	2	NAG	C4-C3-C2	3.08	115.53	111.02
6	J	2	NAG	C3-C4-C5	2.73	115.11	110.24
6	K	2	NAG	C1-O5-C5	2.51	115.60	112.19
6	H	1	NAG	C1-O5-C5	2.31	115.33	112.19
6	H	2	NAG	C4-C3-C2	2.26	114.33	111.02
6	F	2	NAG	C1-O5-C5	2.25	115.24	112.19
7	G	5	BMA	C2-C3-C4	2.22	114.74	110.89
6	H	1	NAG	C1-C2-N2	2.13	114.12	110.49
7	G	3	BMA	O2-C2-C3	-2.12	105.88	110.14
6	J	2	NAG	C8-C7-N2	2.06	119.58	116.10
7	G	4	BMA	O5-C1-C2	-2.06	107.60	110.77

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	2	NAG	O5-C5-C6-O6
6	H	1	NAG	O5-C5-C6-O6
6	F	2	NAG	C4-C5-C6-O6

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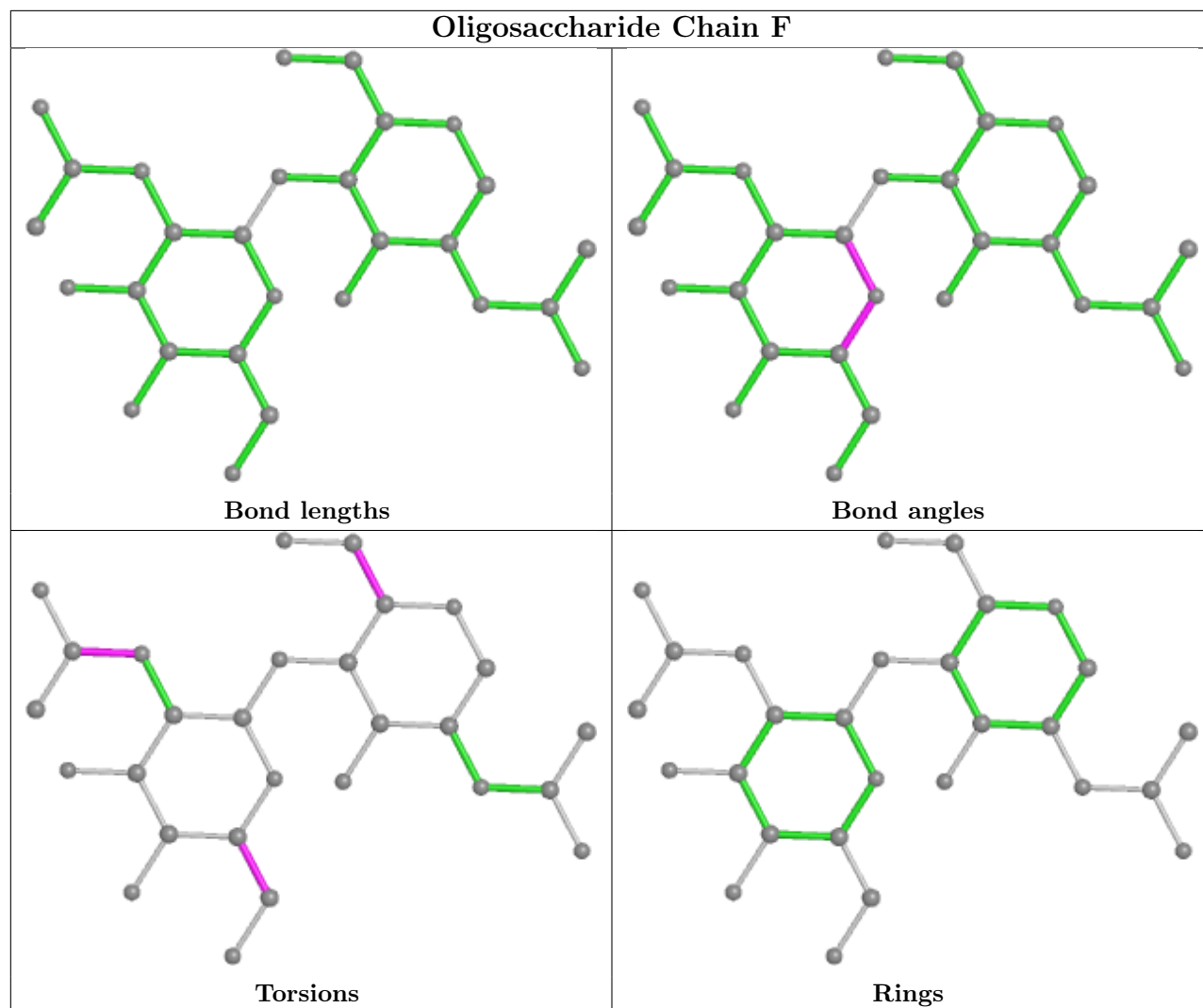
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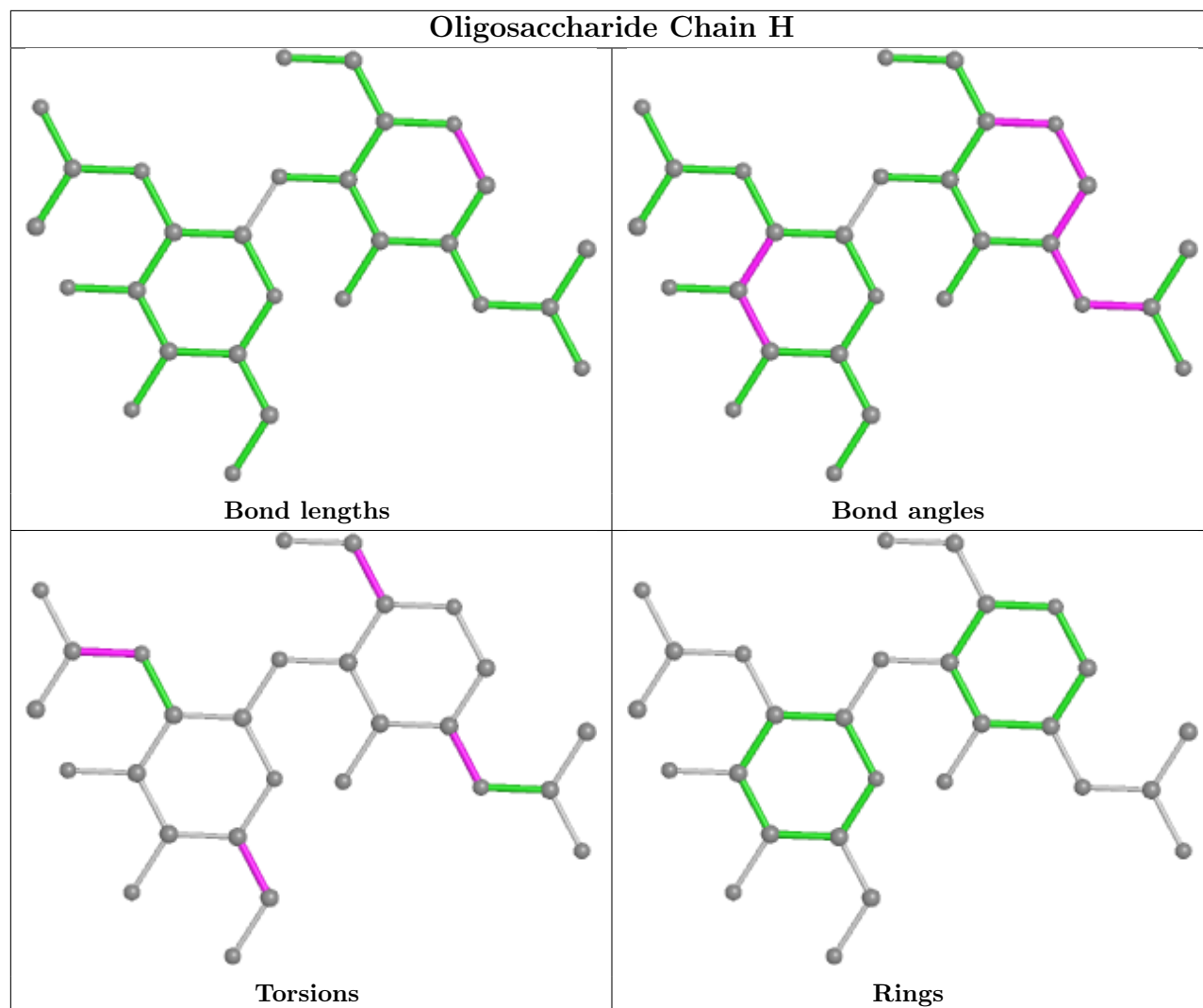
Mol	Chain	Res	Type	Atoms
6	H	1	NAG	C4-C5-C6-O6
6	I	2	NAG	C4-C5-C6-O6
6	F	1	NAG	C4-C5-C6-O6
6	F	2	NAG	C8-C7-N2-C2
6	F	2	NAG	O7-C7-N2-C2
6	H	2	NAG	C8-C7-N2-C2
6	H	2	NAG	O7-C7-N2-C2
6	I	2	NAG	C8-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
6	J	2	NAG	C8-C7-N2-C2
6	J	2	NAG	O7-C7-N2-C2
7	G	1	NAG	C8-C7-N2-C2
7	G	1	NAG	O7-C7-N2-C2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

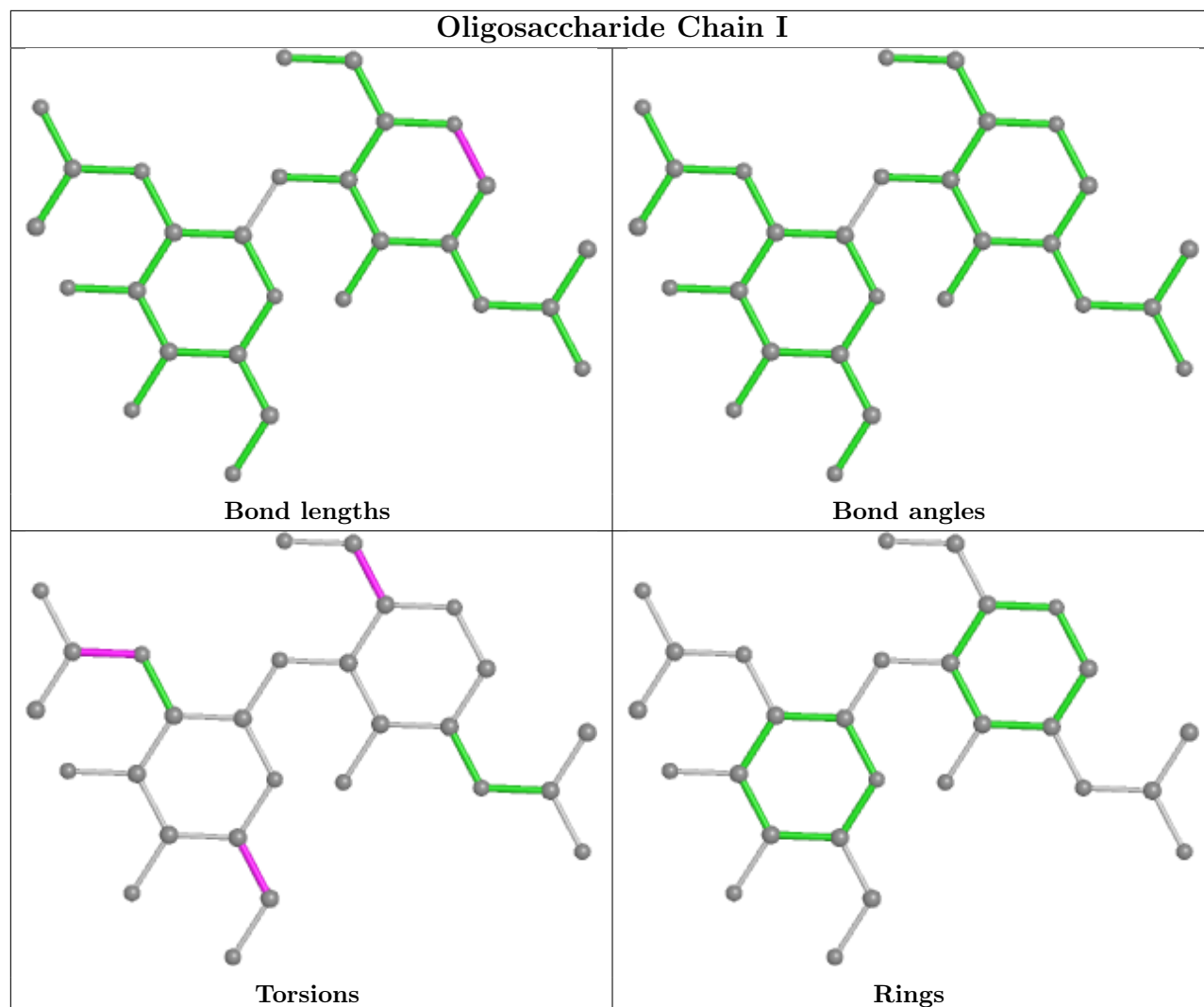
There are no ring outliers.

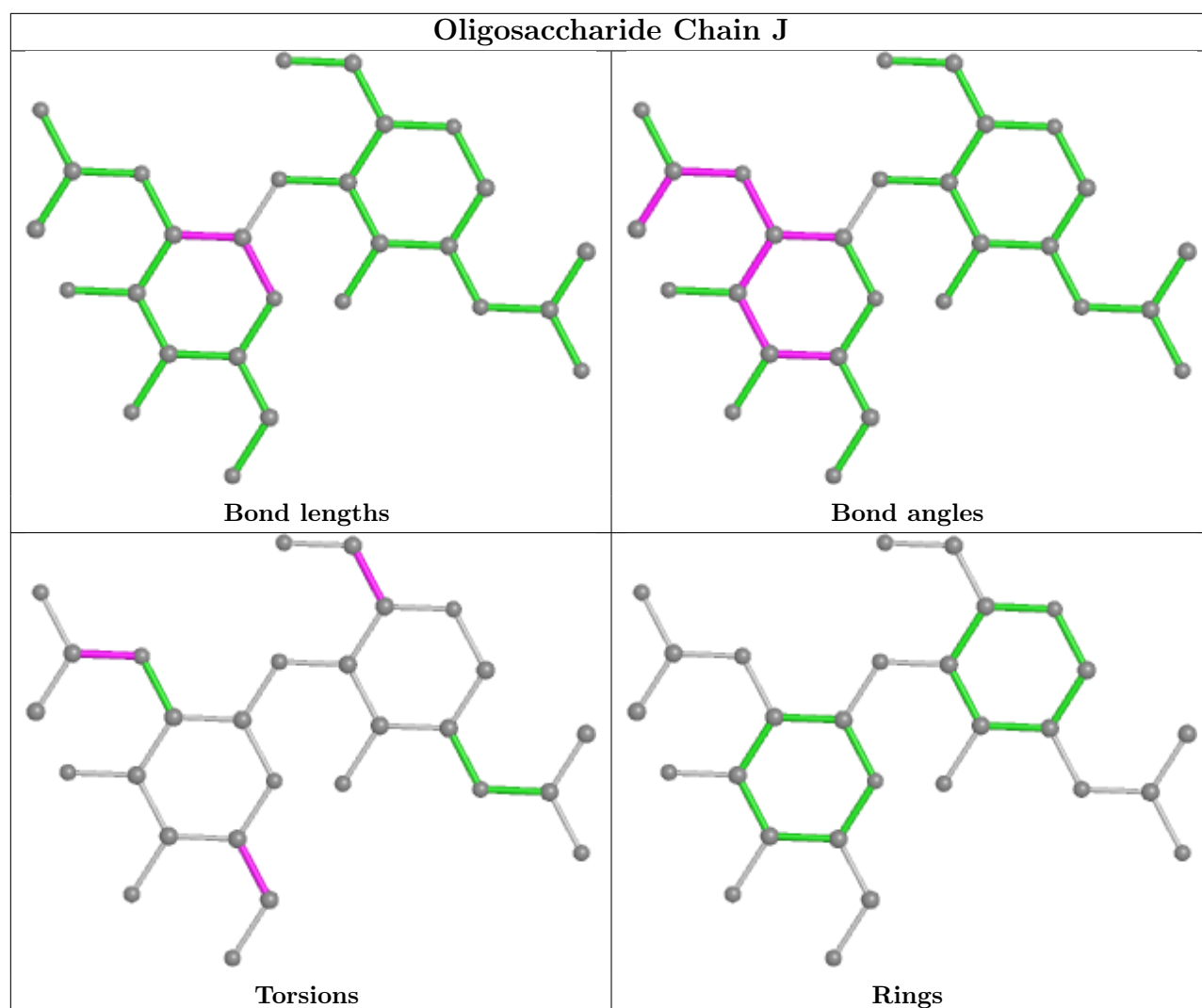
No monomer is involved in short contacts.

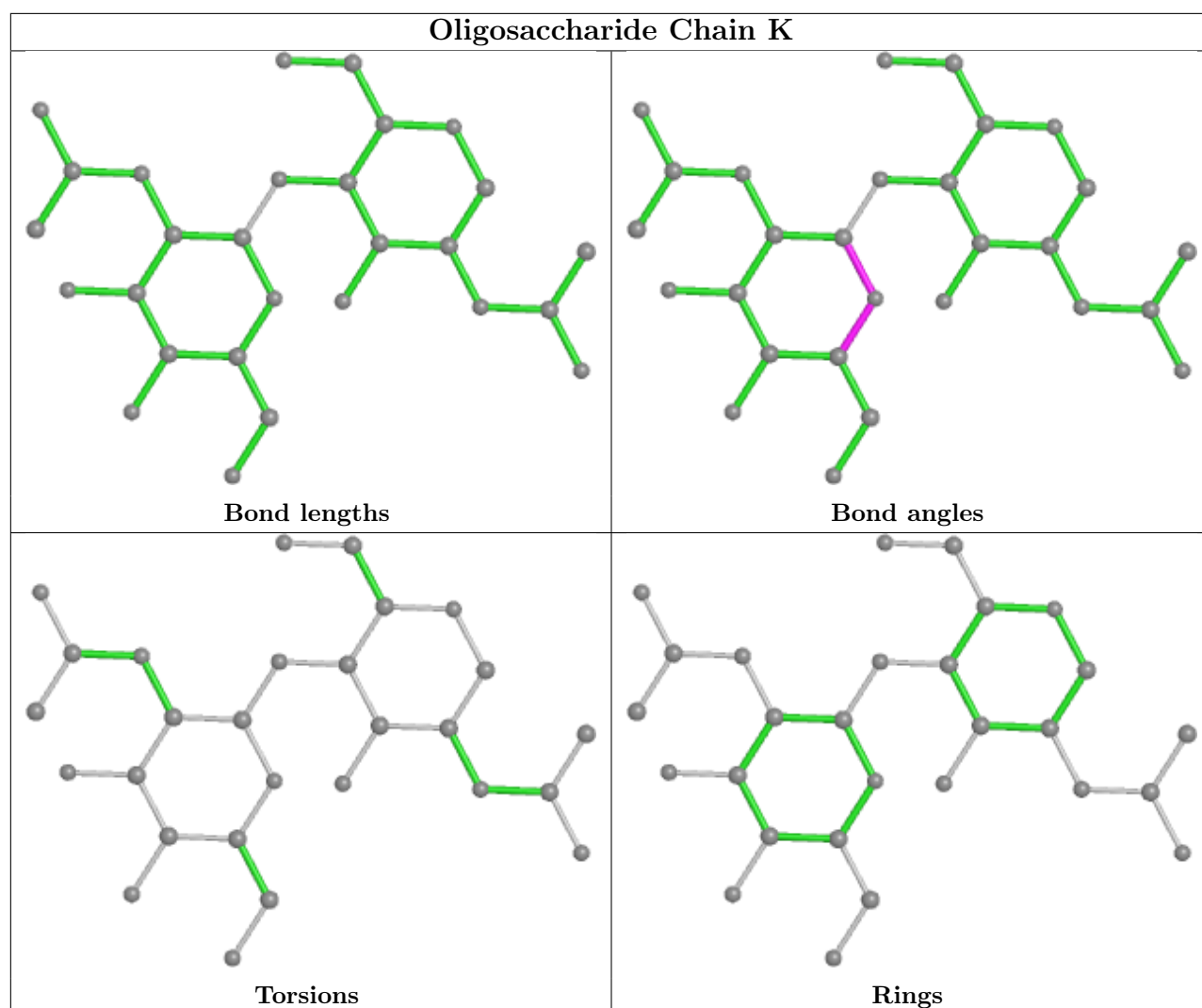
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

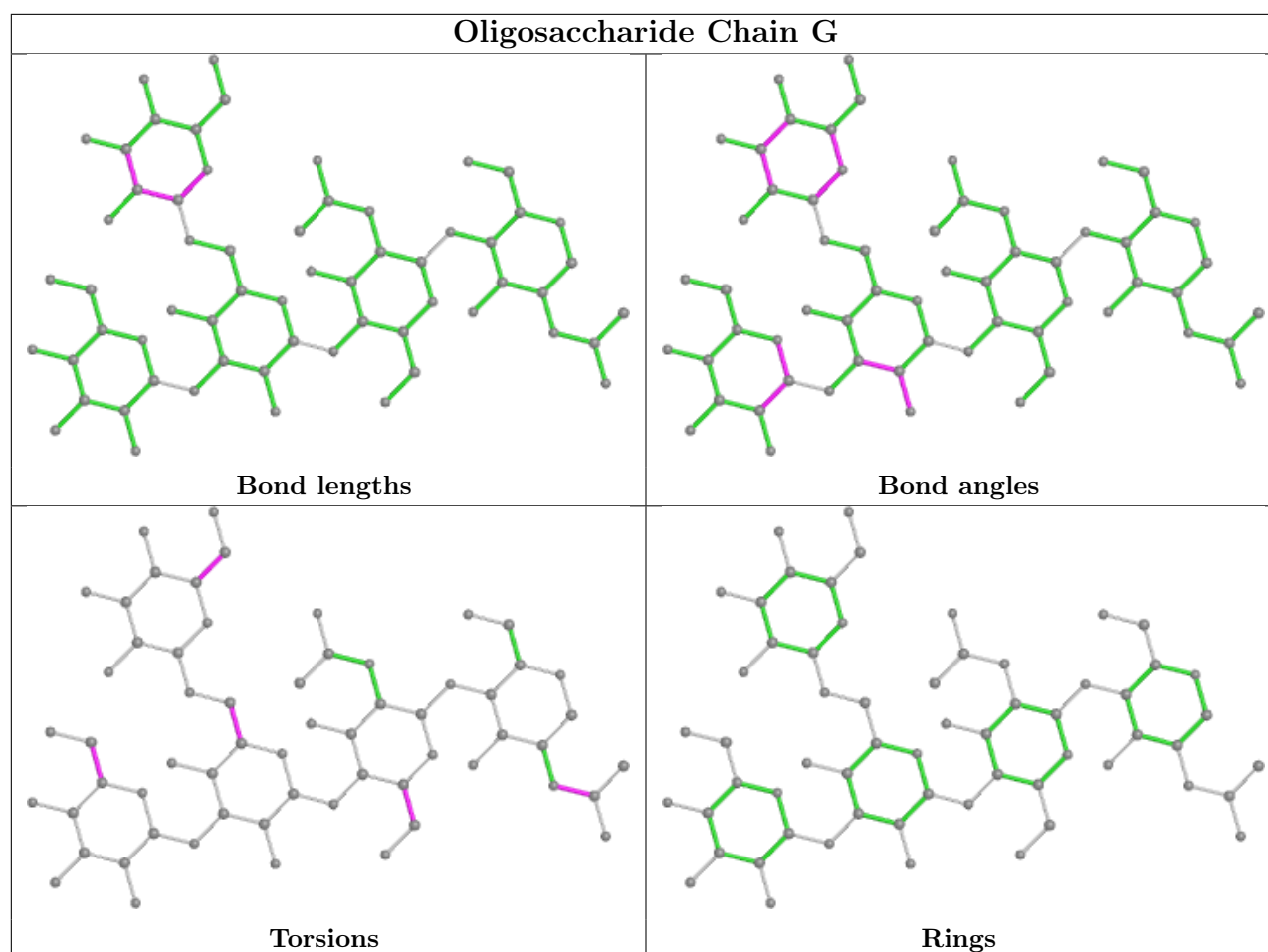












5.6 Ligand geometry [i](#)

11 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	821	1	14,14,15	0.29	0	17,19,21	0.74	1 (5%)
10	CLR	C	301	-	31,31,31	0.31	0	48,48,48	0.65	1 (2%)
10	CLR	C	302	3	31,31,31	0.31	0	48,48,48	0.65	0
8	NAG	A	817	1	14,14,15	0.51	0	17,19,21	1.12	2 (11%)
8	NAG	A	810	1	14,14,15	0.30	0	17,19,21	0.77	0
8	NAG	A	820	1	14,14,15	0.25	0	17,19,21	0.60	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLR	C	303	3	31,31,31	0.36	0	48,48,48	0.67	0
8	NAG	A	818	1	14,14,15	0.50	0	17,19,21	0.49	0
9	PC1	B	501	-	36,36,53	0.32	0	42,44,61	0.34	0
8	NAG	A	819	1	14,14,15	1.01	1 (7%)	17,19,21	2.20	3 (17%)
9	PC1	C	304	-	40,40,53	0.32	0	46,48,61	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	821	1	-	2/6/23/26	0/1/1/1
10	CLR	C	301	-	-	3/10/68/68	0/4/4/4
10	CLR	C	302	3	-	5/10/68/68	0/4/4/4
8	NAG	A	817	1	-	3/6/23/26	0/1/1/1
8	NAG	A	810	1	-	4/6/23/26	0/1/1/1
8	NAG	A	820	1	-	2/6/23/26	0/1/1/1
10	CLR	C	303	3	-	7/10/68/68	0/4/4/4
8	NAG	A	818	1	-	2/6/23/26	0/1/1/1
9	PC1	B	501	-	-	19/40/40/57	-
8	NAG	A	819	1	-	5/6/23/26	0/1/1/1
9	PC1	C	304	-	-	12/44/44/57	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	819	NAG	C1-C2	3.18	1.57	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	819	NAG	C2-N2-C7	7.73	133.91	122.90
8	A	819	NAG	C1-C2-N2	3.57	116.58	110.49
8	A	817	NAG	C2-N2-C7	3.08	127.29	122.90
8	A	821	NAG	C1-O5-C5	2.70	115.85	112.19
8	A	817	NAG	C1-O5-C5	2.42	115.48	112.19
10	C	301	CLR	C10-C9-C8	-2.26	109.34	112.73
8	A	819	NAG	C8-C7-N2	2.15	119.74	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	820	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	501	PC1	C11-O13-P-O14
9	B	501	PC1	C11-O13-P-O11
9	B	501	PC1	C22-C21-O21-C2
9	C	304	PC1	C12-C11-O13-P
9	C	304	PC1	O22-C21-O21-C2
9	B	501	PC1	O32-C31-O31-C3
9	B	501	PC1	C32-C31-O31-C3
9	B	501	PC1	O22-C21-O21-C2
9	C	304	PC1	C22-C21-O21-C2
8	A	817	NAG	O5-C5-C6-O6
8	A	819	NAG	O5-C5-C6-O6
8	A	821	NAG	O5-C5-C6-O6
8	A	817	NAG	C4-C5-C6-O6
8	A	810	NAG	C4-C5-C6-O6
8	A	821	NAG	C4-C5-C6-O6
8	A	810	NAG	C1-C2-N2-C7
8	A	819	NAG	C8-C7-N2-C2
8	A	819	NAG	O7-C7-N2-C2
8	A	810	NAG	O5-C5-C6-O6
10	C	302	CLR	C22-C23-C24-C25
8	A	819	NAG	C4-C5-C6-O6
8	A	820	NAG	C4-C5-C6-O6
9	C	304	PC1	C11-O13-P-O11
10	C	302	CLR	C13-C17-C20-C22
10	C	303	CLR	C23-C24-C25-C27
10	C	302	CLR	C16-C17-C20-C22
8	A	820	NAG	O5-C5-C6-O6
10	C	303	CLR	C23-C24-C25-C26
9	B	501	PC1	C31-C32-C33-C34
9	B	501	PC1	C25-C26-C27-C28
10	C	302	CLR	C16-C17-C20-C21
9	B	501	PC1	C28-C29-C2A-C2B
9	C	304	PC1	C21-C22-C23-C24
10	C	302	CLR	C13-C17-C20-C21
9	B	501	PC1	C22-C23-C24-C25
10	C	303	CLR	C16-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
9	B	501	PC1	C35-C36-C37-C38
10	C	303	CLR	C13-C17-C20-C22
9	C	304	PC1	C23-C24-C25-C26
9	B	501	PC1	O11-C1-C2-O21
9	C	304	PC1	C11-O13-P-O14
9	B	501	PC1	O11-C1-C2-C3
10	C	303	CLR	C16-C17-C20-C21
9	B	501	PC1	C23-C24-C25-C26
9	B	501	PC1	C12-C11-O13-P
10	C	303	CLR	C13-C17-C20-C21
9	C	304	PC1	O13-C11-C12-N
9	B	501	PC1	C3-C2-O21-C21
9	B	501	PC1	C32-C33-C34-C35
10	C	301	CLR	C16-C17-C20-C22
8	A	810	NAG	C3-C2-N2-C7
8	A	817	NAG	C3-C2-N2-C7
8	A	819	NAG	C3-C2-N2-C7
8	A	818	NAG	O5-C5-C6-O6
8	A	818	NAG	C4-C5-C6-O6
9	B	501	PC1	C21-C22-C23-C24
10	C	303	CLR	C22-C23-C24-C25
9	C	304	PC1	C34-C35-C36-C37
9	C	304	PC1	C1-C2-O21-C21
9	C	304	PC1	C36-C37-C38-C39
9	B	501	PC1	C24-C25-C26-C27
10	C	301	CLR	C13-C17-C20-C21
9	C	304	PC1	C3-C2-O21-C21
10	C	301	CLR	C13-C17-C20-C22

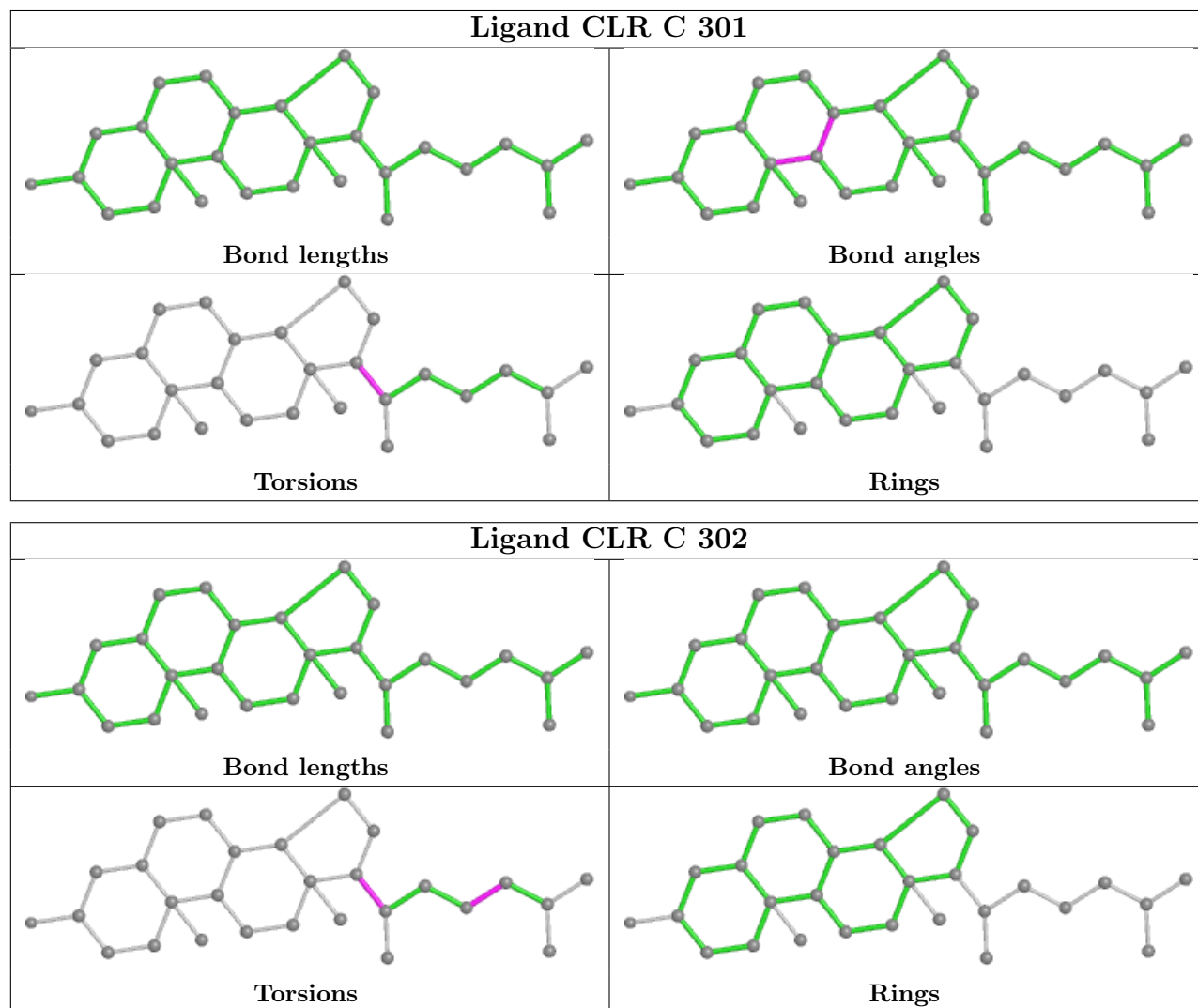
There are no ring outliers.

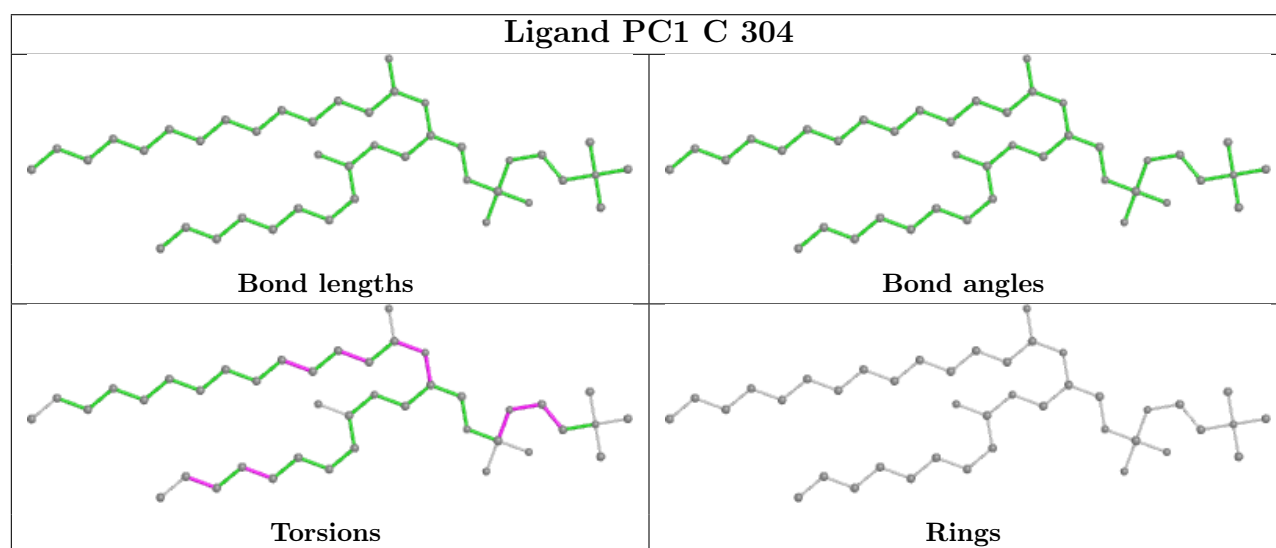
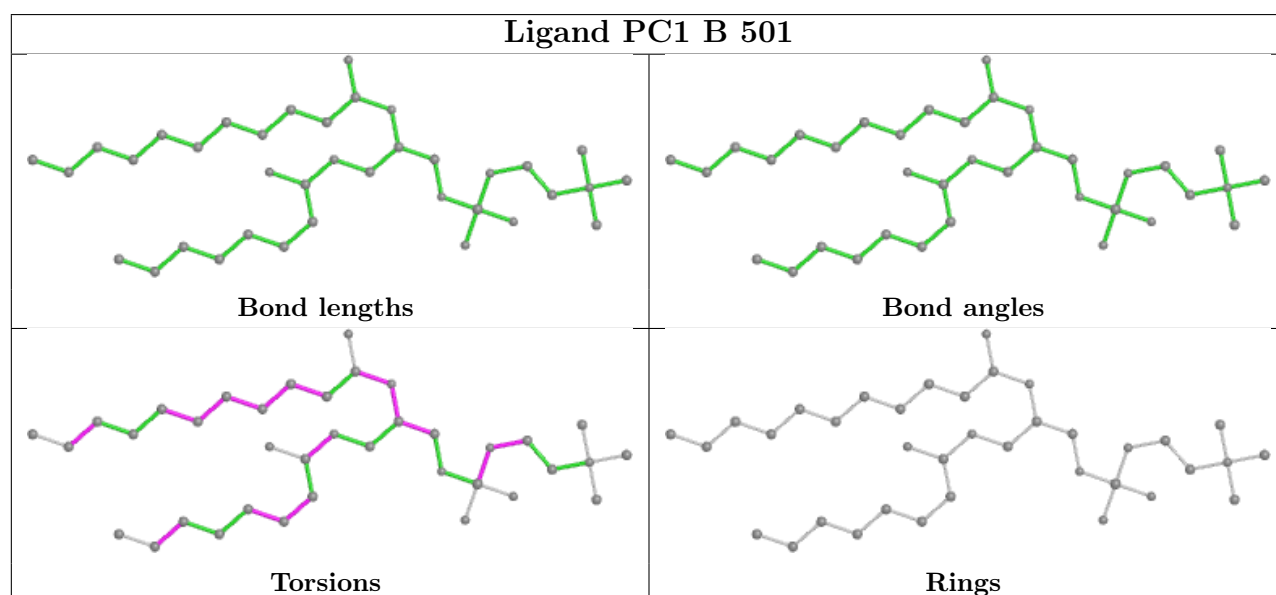
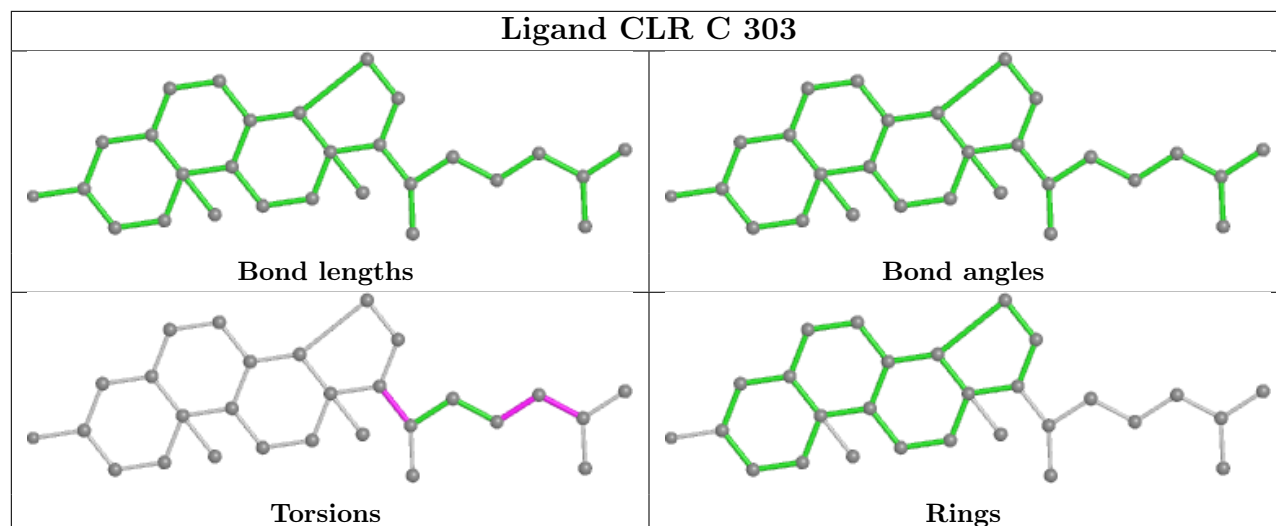
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	810	NAG	2	0
10	C	303	CLR	1	0
9	B	501	PC1	4	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.

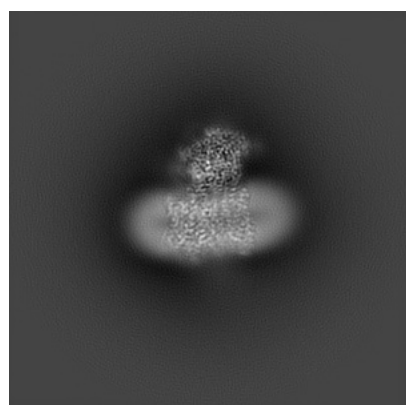
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9751. These allow visual inspection of the internal detail of the map and identification of artifacts.

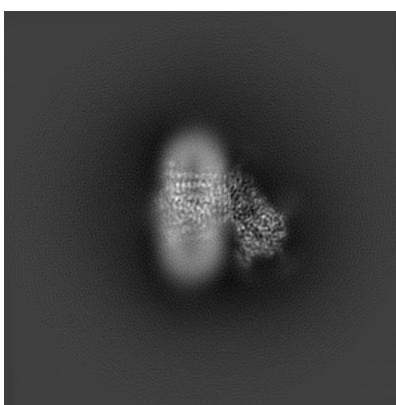
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

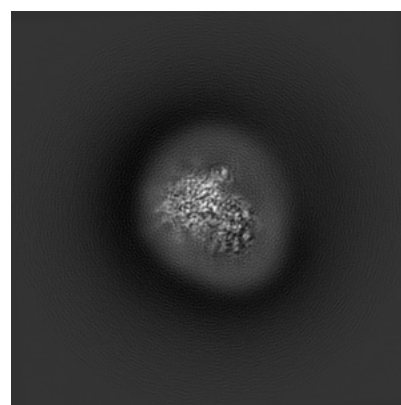
6.1.1 Primary map



X



Y

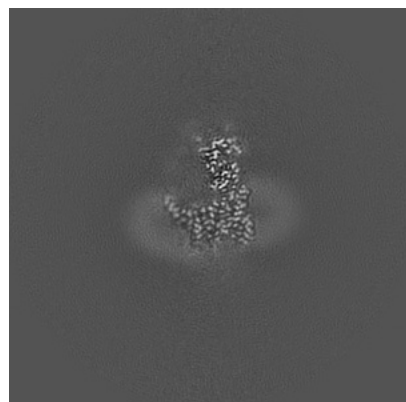


Z

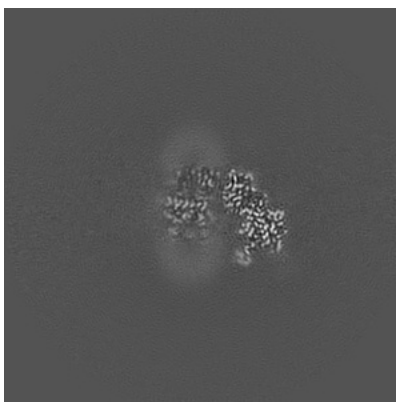
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

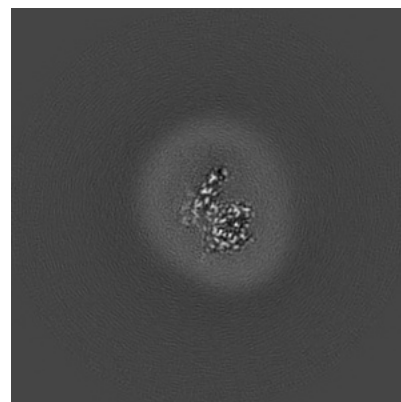
6.2.1 Primary map



X Index: 160



Y Index: 160

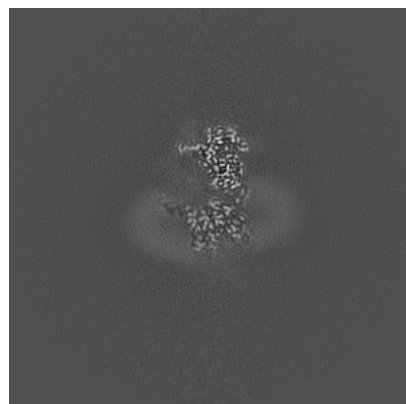


Z Index: 160

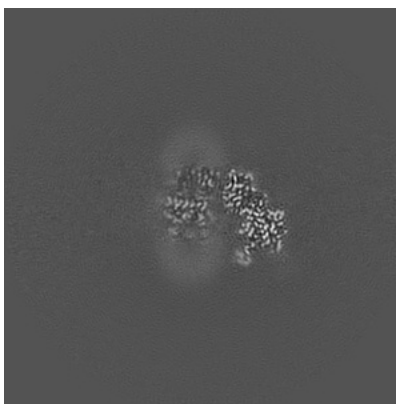
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

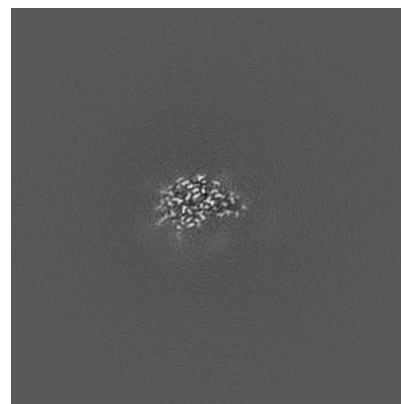
6.3.1 Primary map



X Index: 155



Y Index: 160

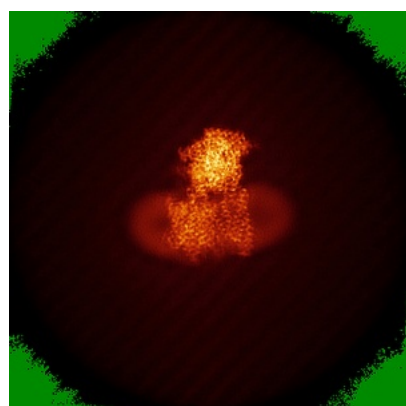


Z Index: 196

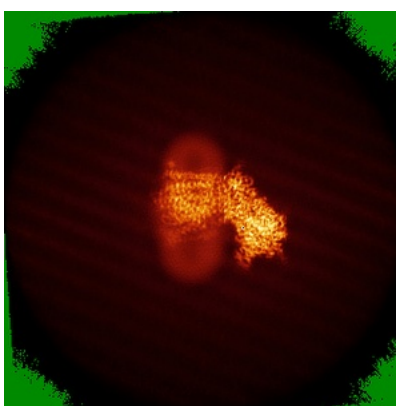
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

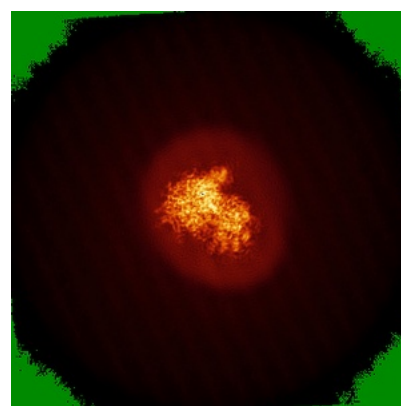
6.4.1 Primary map



X



Y

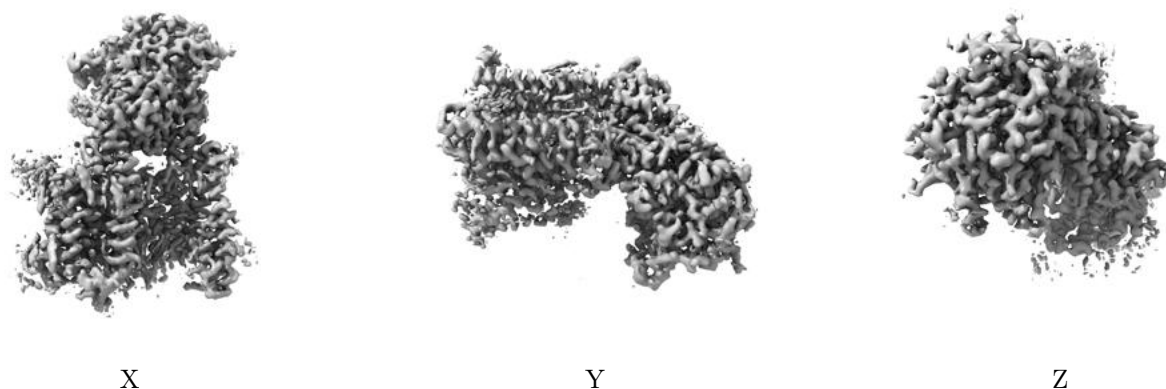


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.024. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

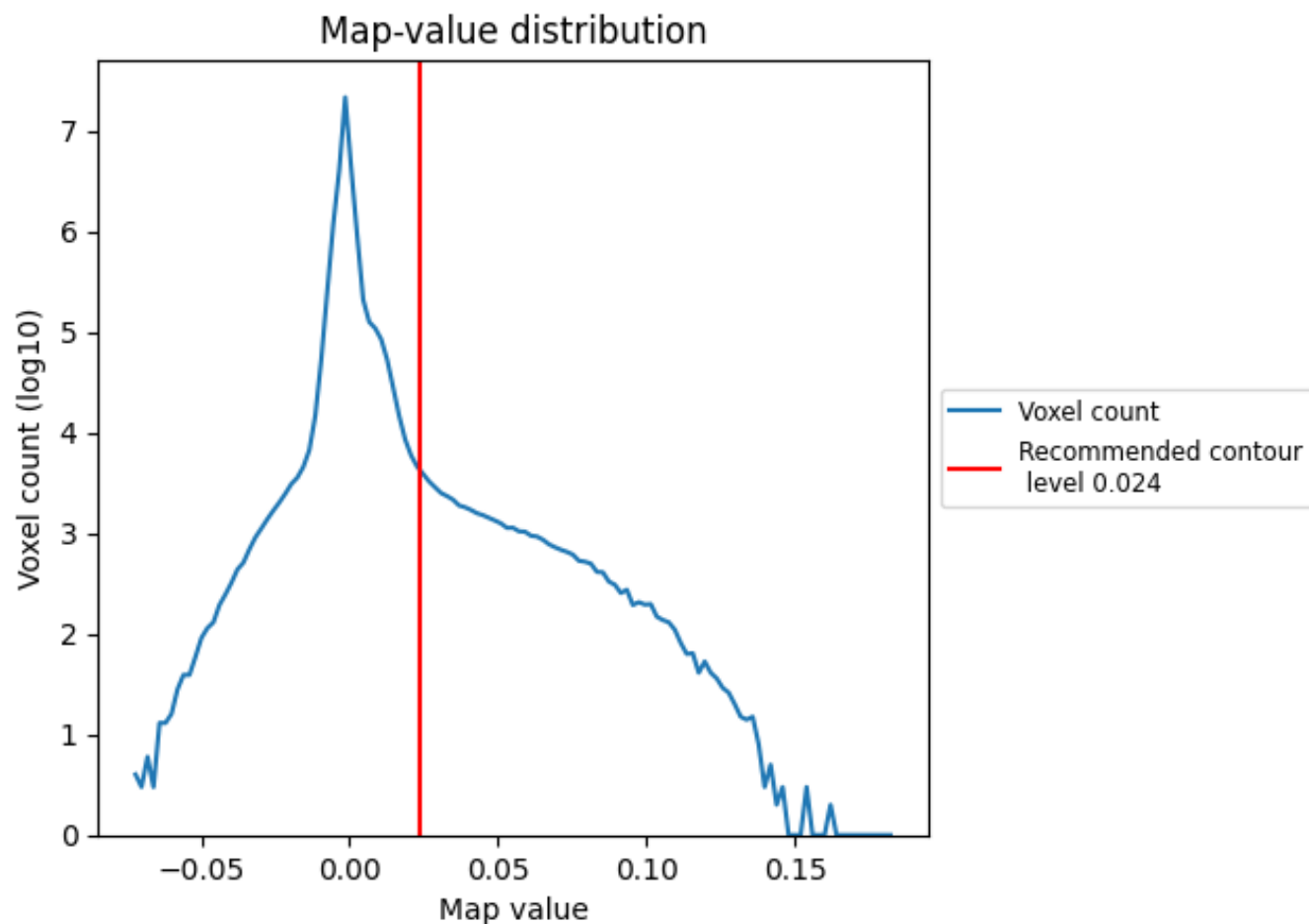
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

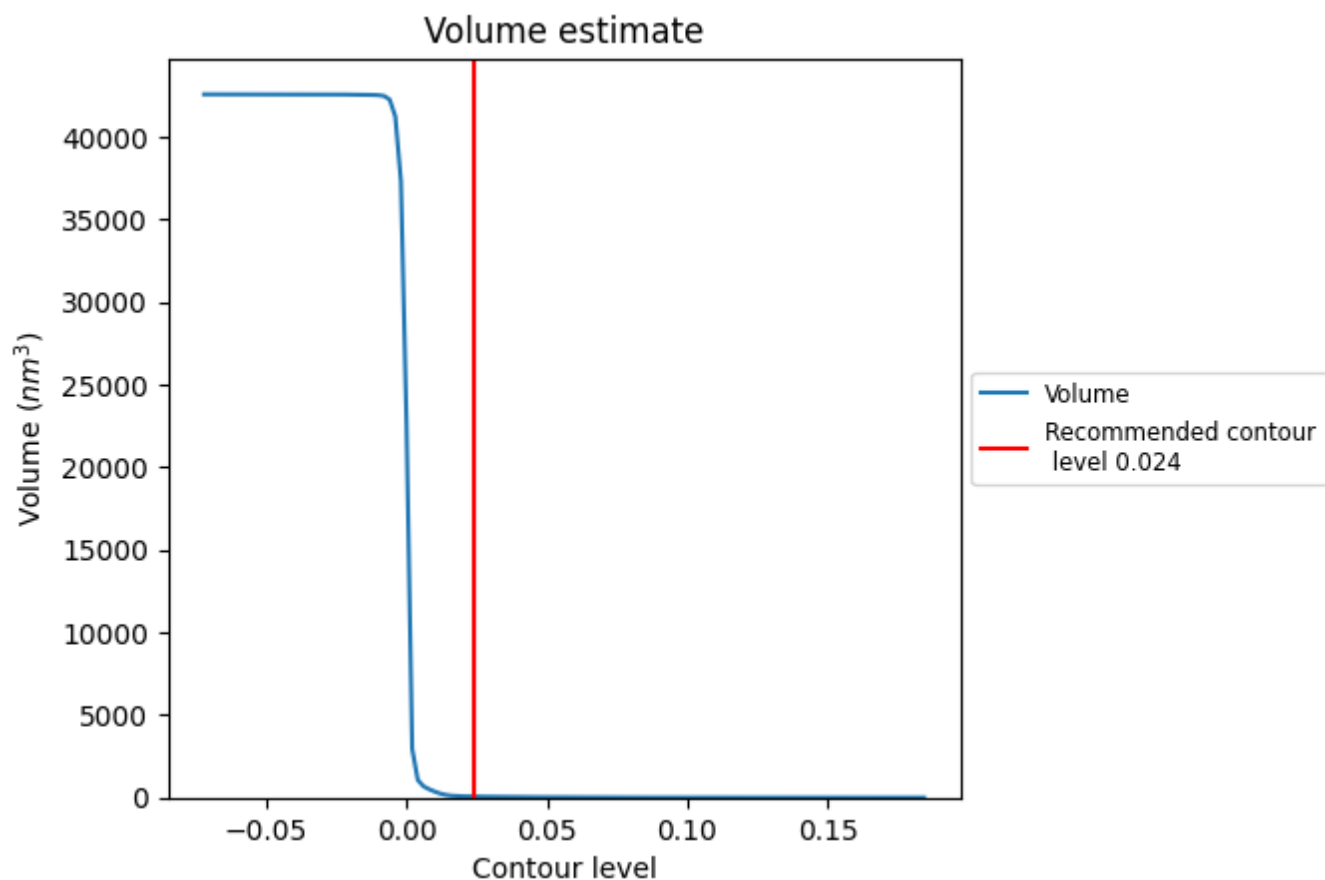
This section contains the results of statistical analysis of the map.

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.

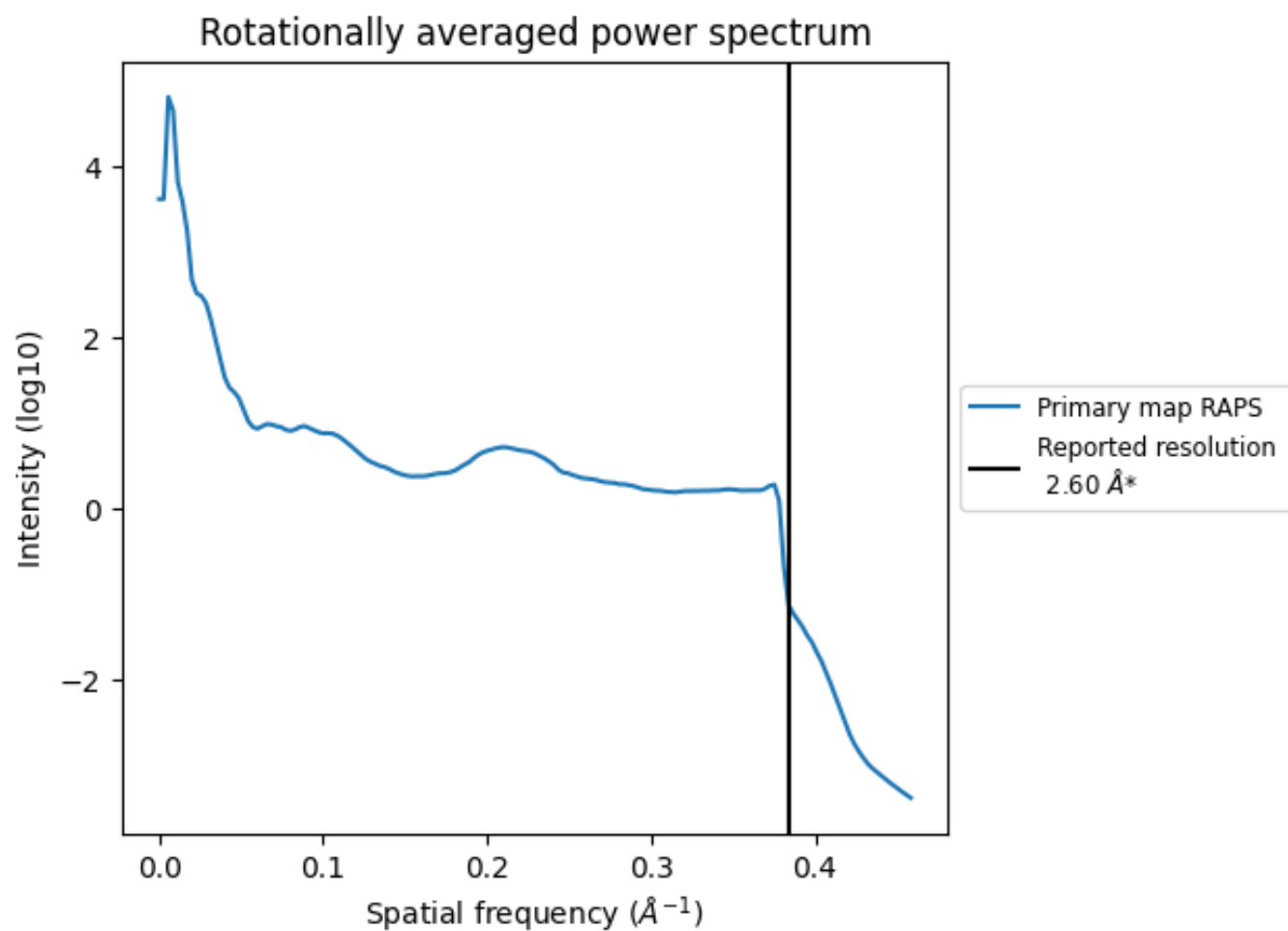
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 61 nm^3 ; this corresponds to an approximate mass of 55 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

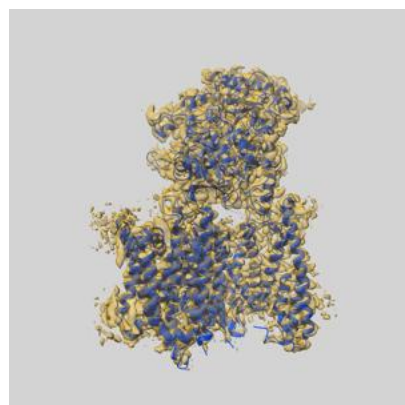
8 Fourier-Shell correlation ⓘ

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

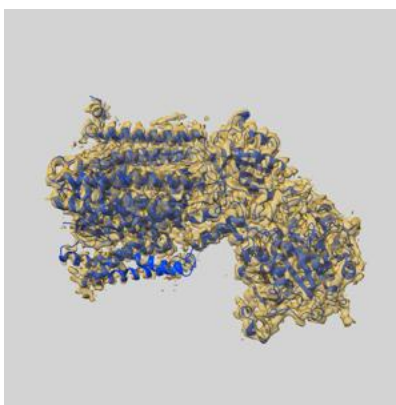
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9751 and PDB model 6IYC. Per-residue inclusion information can be found in section [3](#) on page [9](#).

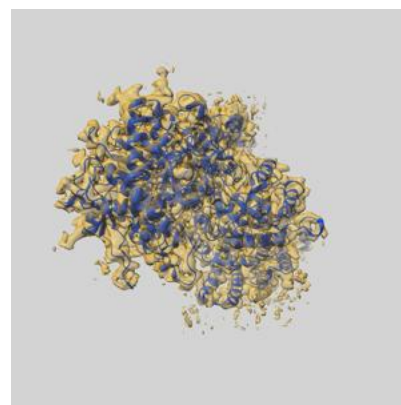
9.1 Map-model overlay [i](#)



X



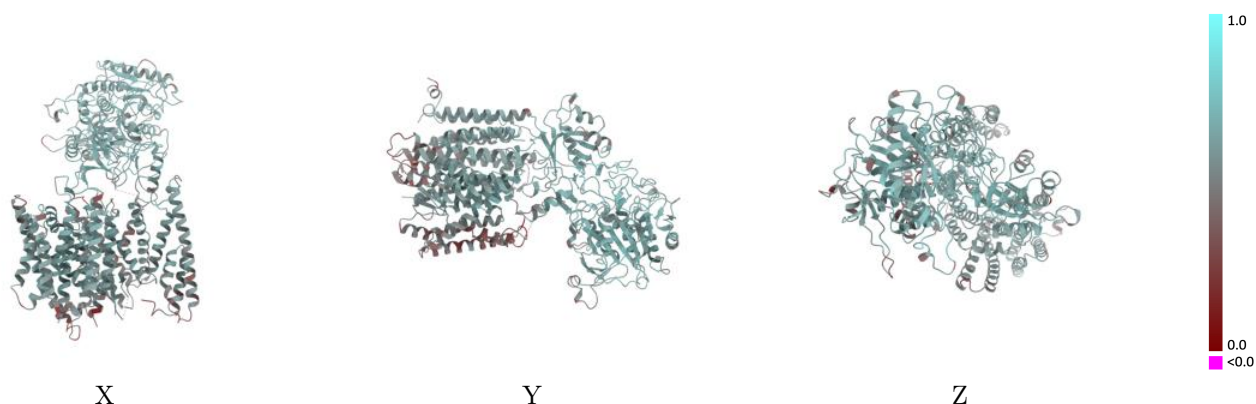
Y



Z

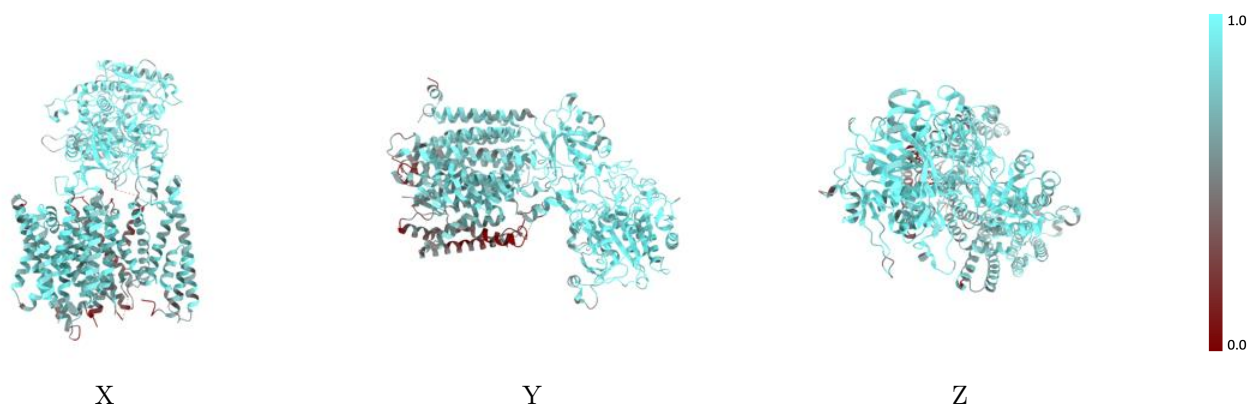
The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



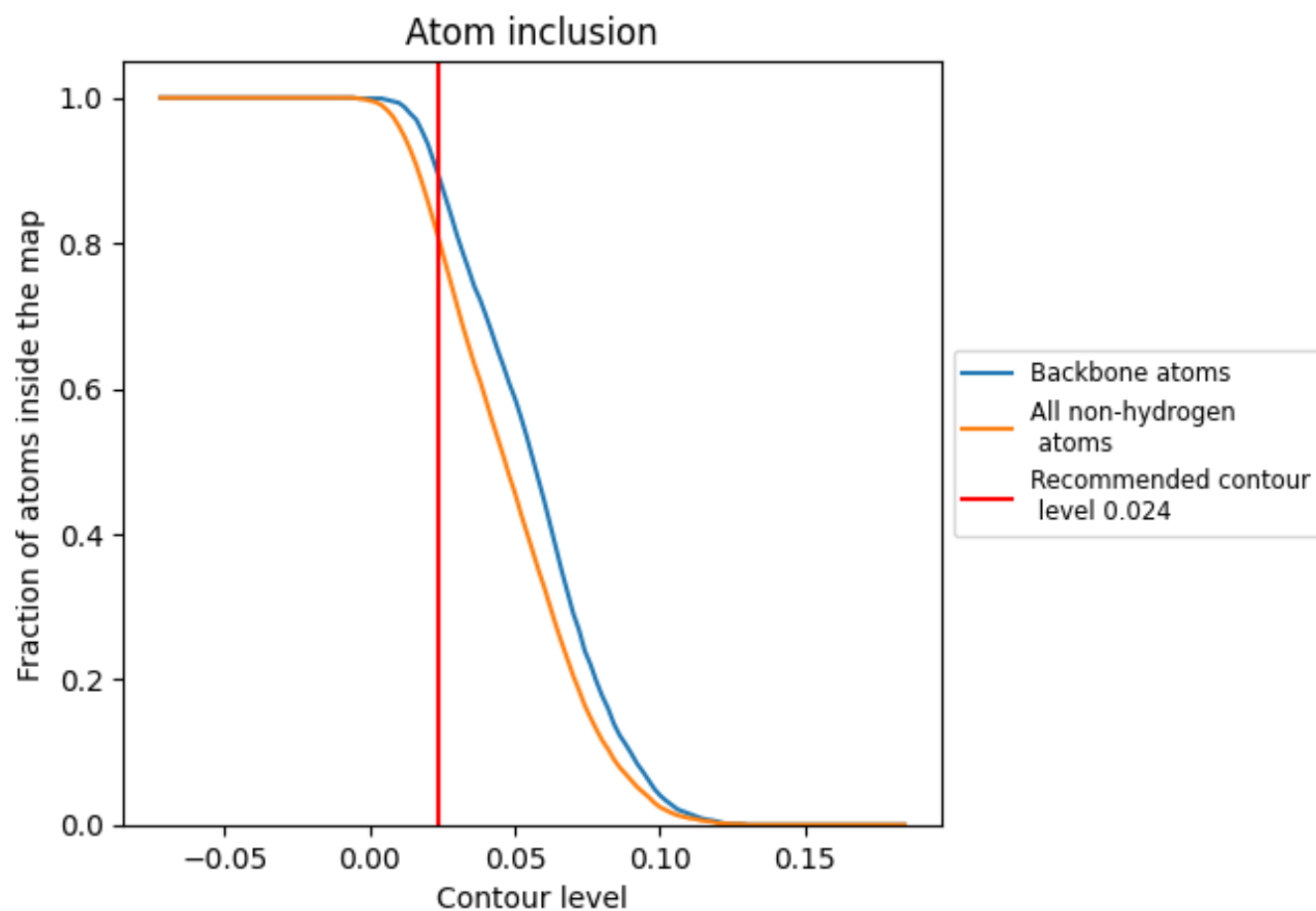
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.024).

























9.4 Atom inclusion ⓘ



At the recommended contour level, 89% of all backbone atoms, 80% 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 (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8030	 0.5670
A	 0.8880	 0.6020
B	 0.6800	 0.5290
C	 0.8090	 0.5550
D	 0.7310	 0.5130
E	 0.3980	 0.4510
F	 0.7500	 0.5850
G	 0.8360	 0.5620
H	 0.8570	 0.5750
I	 0.6790	 0.5180
J	 0.6790	 0.5390
K	 0.8570	 0.5650

