



Full wwPDB EM Validation Report ⓘ

Jun 24, 2025 – 04:43 pm BST

PDB ID : 9FAU / pdb_00009fau
EMDB ID : EMD-50282
Title : CryoEM structure of human full-length beta3gamma2 GABA(A) receptor in complex with GARLH4, the TMD of Neuroligin2 and Megabody25, in a closed state (StateC1)
Authors : Kasaragod, V.B.; Aricescu, A.R.
Deposited on : 2024-05-10
Resolution : 3.10 Å (reported)
Based on initial model : 7QNB

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.dev118
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.44

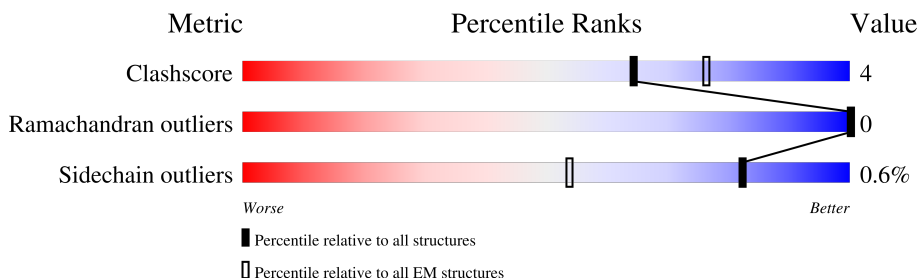
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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.





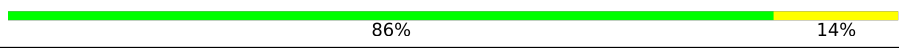
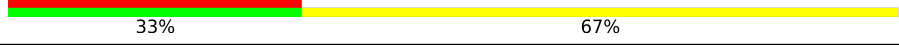
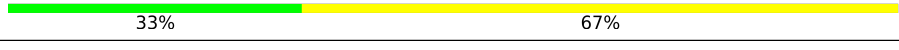
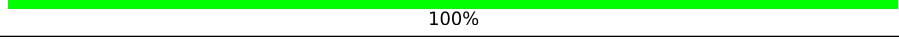

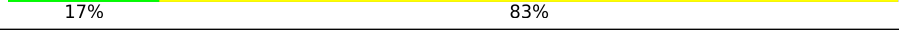
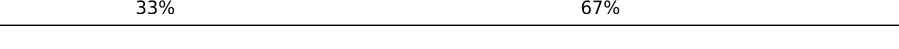
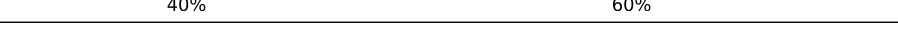
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	439	
1	B	439	
1	D	439	
1	E	439	
2	C	404	
3	H	33	
4	L	188	
5	F	522	

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Mol	Chain	Length	Quality of chain
5	K	522	 21% 78%
5	O	522	 20% 78%
6	G	7	 86% 14%
7	I	3	 33% 67%
7	P	3	 33% 67%
8	J	2	 100%
8	Q	2	 50% 50%
9	M	6	 17% 83%
9	N	6	 33% 67%
10	R	5	 40% 60%

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 19115 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 Gamma-aminobutyric acid receptor subunit beta-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	330	Total	C	N	O	S	0	0
			2712	1777	442	477	16		
1	E	331	Total	C	N	O	S	3	0
			2745	1805	444	480	16		
1	A	330	Total	C	N	O	S	2	0
			2731	1792	446	477	16		
1	D	330	Total	C	N	O	S	2	0
			2732	1795	443	478	16		

- Molecule 2 is a protein called Isoform 2 of Gamma-aminobutyric acid receptor subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	350	Total	C	N	O	S	3	0
			2949	1937	478	514	20		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	429	GLY	-	expression tag	UNP P18507

- Molecule 3 is a protein called Neuroligin-2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	H	33	Total	C	N	O	0	0
			255	168	38	49		

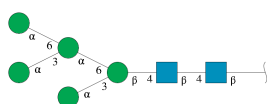
- Molecule 4 is a protein called LHFPL tetraspan subfamily member 4 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	188	Total	C	N	O	S	1	0
			1455	966	229	244	16		

- Molecule 5 is a protein called Megabody25.

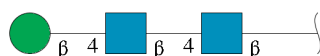
Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	117	Total	C	N	O	S	0	0
			912	575	156	177	4		
5	O	115	Total	C	N	O	S	0	0
			902	570	154	174	4		
5	F	117	Total	C	N	O	S	0	0
			912	575	156	177	4		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
6	G	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 7 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.



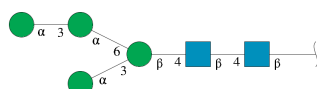
Mol	Chain	Residues	Atoms				AltConf	Trace
7	I	3	Total	C	N	O	0	0
			39	22	2	15		
7	P	3	Total	C	N	O	0	0
			39	22	2	15		

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



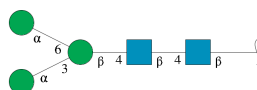
Mol	Chain	Residues	Atoms				AltConf	Trace
8	J	2	Total	C	N	O	0	0
			28	16	2	10		
8	Q	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



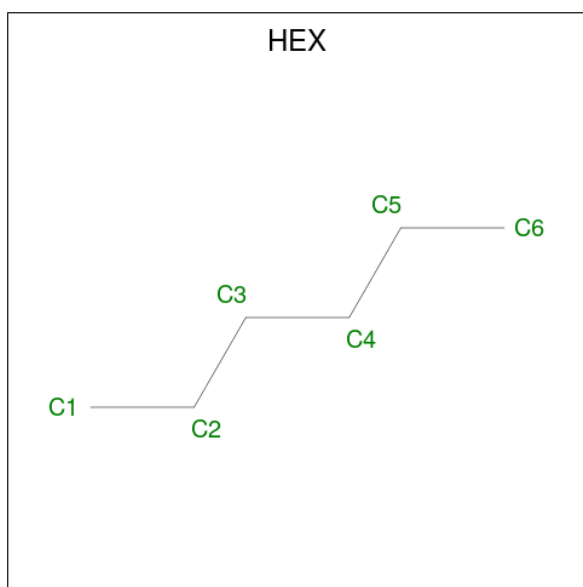
Mol	Chain	Residues	Atoms				AltConf	Trace
9	M	6	Total	C	N	O	0	0
			72	40	2	30		
9	N	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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.



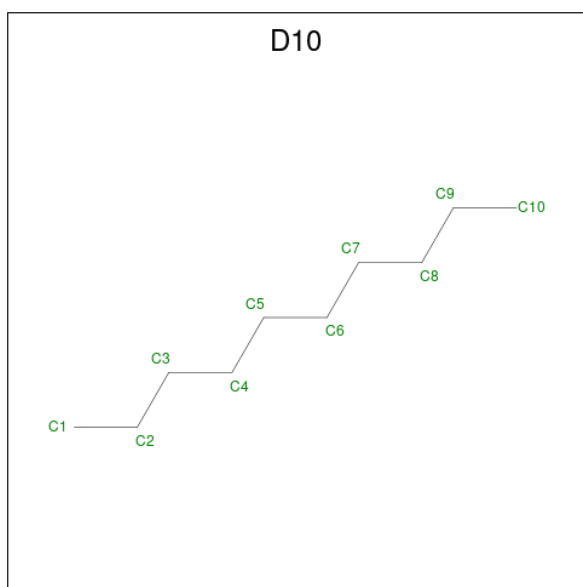
Mol	Chain	Residues	Atoms				AltConf	Trace
10	R	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 11 is HEXANE (CCD ID: HEX) (formula: C₆H₁₄).



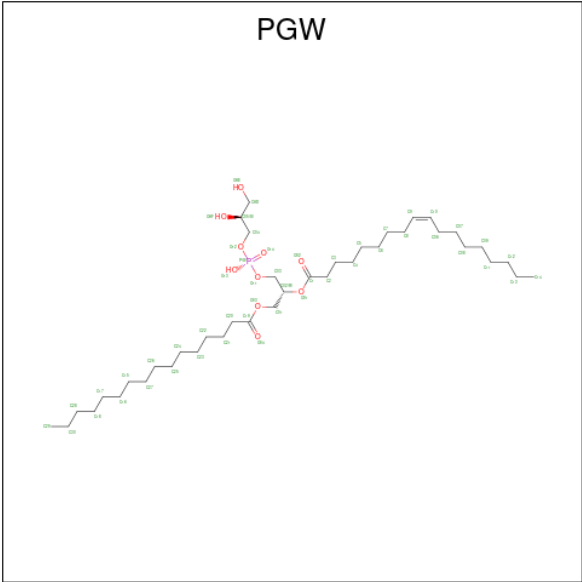
Mol	Chain	Residues	Atoms		AltConf
11	B	1	Total	C	0
			6	6	
11	B	1	Total	C	0
			6	6	
11	E	1	Total	C	0
			6	6	
11	E	1	Total	C	0
			6	6	
11	A	1	Total	C	0
			6	6	
11	A	1	Total	C	0
			6	6	

- Molecule 12 is DECANE (CCD ID: D10) (formula: $C_{10}H_{22}$).



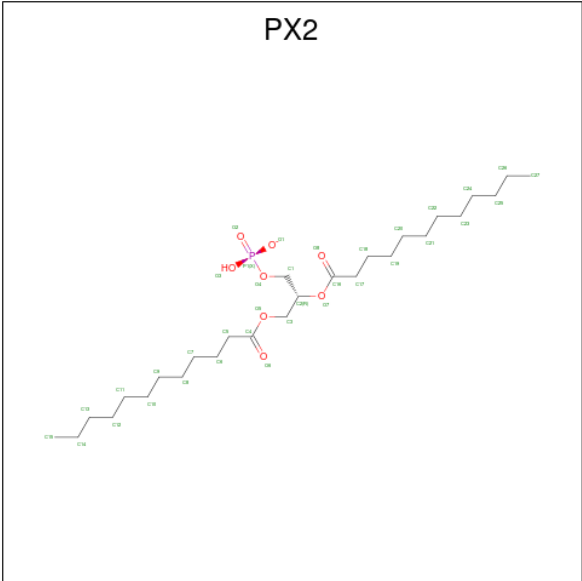
Mol	Chain	Residues	Atoms	AltConf
12	B	1	Total C 10 10	0
12	E	1	Total C 10 10	0
12	A	1	Total C 10 10	0
12	D	1	Total C 10 10	0
12	D	1	Total C 10 10	0
12	L	1	Total C 10 10	0

- Molecule 13 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (CCD ID: PGW) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
13	B	1	Total	C	O	P	0
			51	40	10	1	
13	L	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 14 is 1,2-DILAUROYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: PX2) (formula: $C_{27}H_{52}O_8P$).



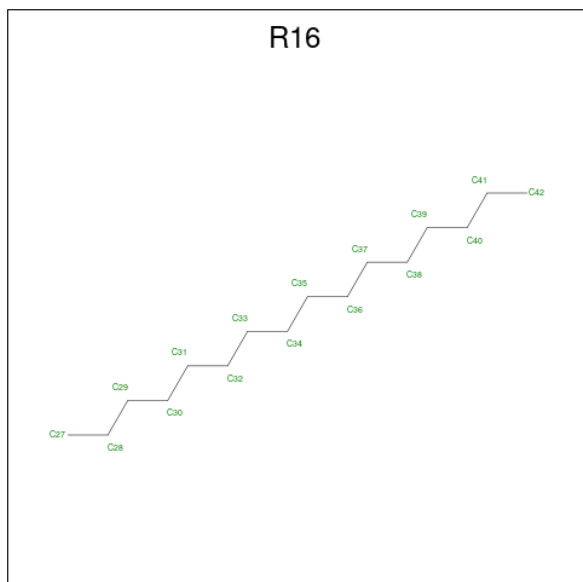
Mol	Chain	Residues	Atoms				AltConf
14	C	1	Total	C	O	P	0
			36	27	8	1	

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



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

- Molecule 16 is HEXADECANE (CCD ID: R16) (formula: $C_{16}H_{34}$).



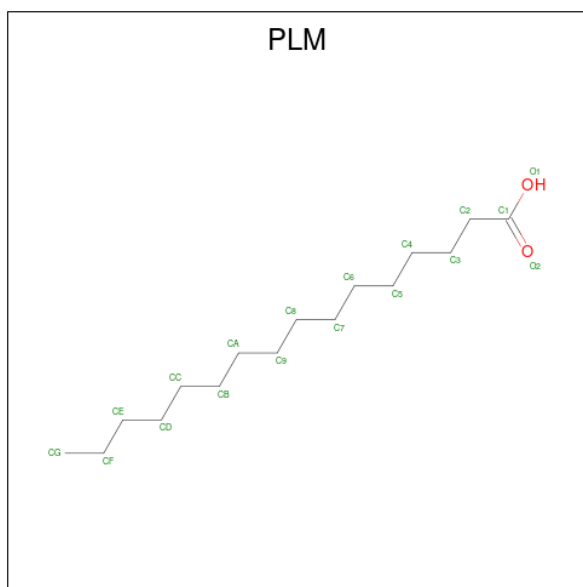
Mol	Chain	Residues	Atoms		AltConf
16	C	1	Total	C	0
			16	16	

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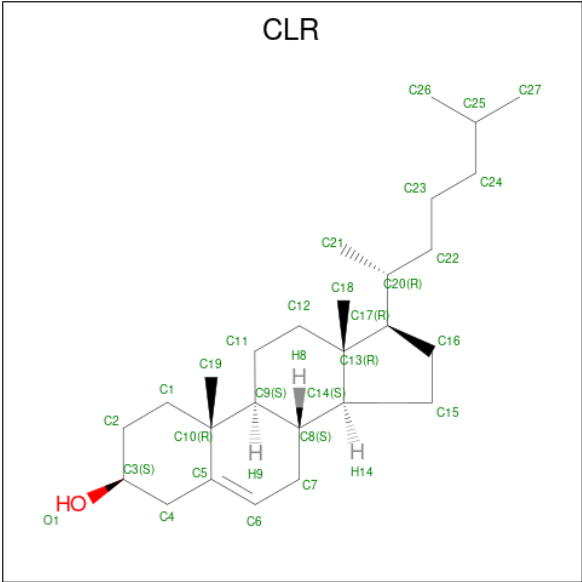
Mol	Chain	Residues	Atoms	AltConf
16	C	1	Total C 16 16	0
16	C	1	Total C 16 16	0

- Molecule 17 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms	AltConf
17	C	1	Total C O 18 16 2	0
17	C	1	Total C O 18 16 2	0

- Molecule 18 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).

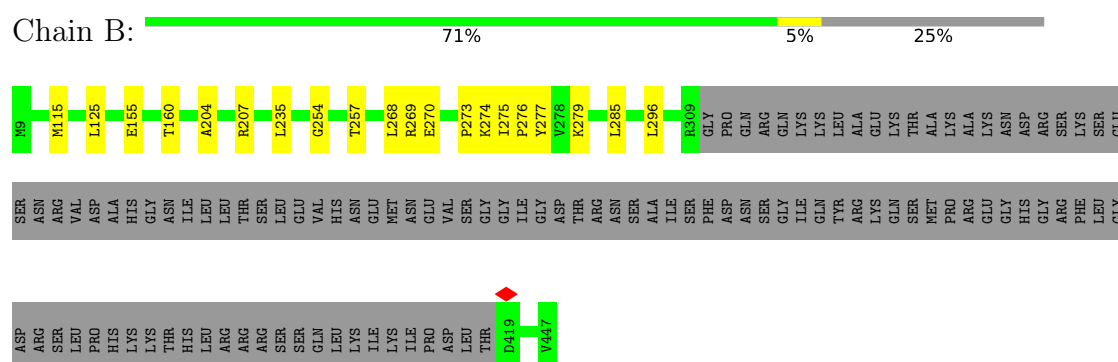


Mol	Chain	Residues	Atoms			AltConf
18	C	1	Total	C	O	0
			28	27	1	
18	L	1	Total	C	O	0
			28	27	1	

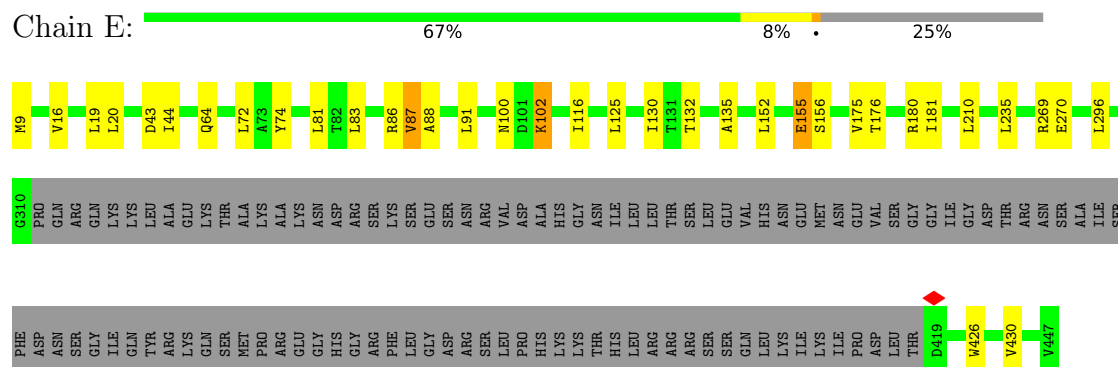
3 Residue-property plots [i](#)

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.

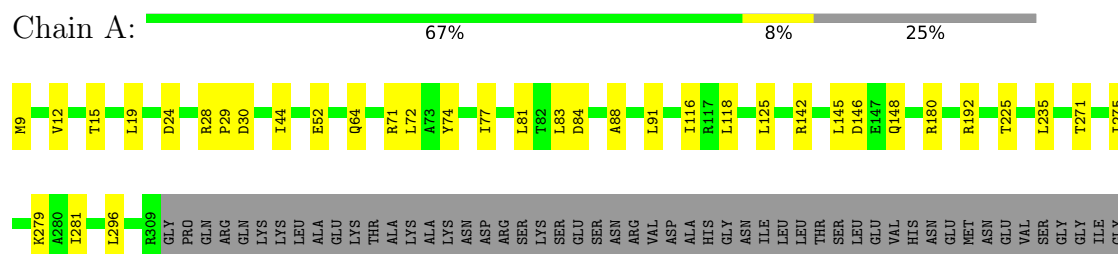
- Molecule 1: Gamma-aminobutyric acid receptor subunit beta-3

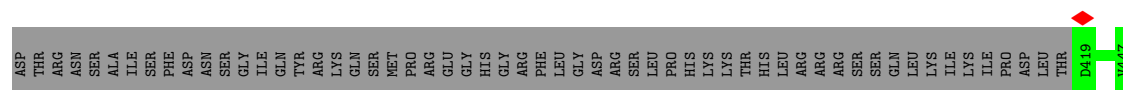


- Molecule 1: Gamma-aminobutyric acid receptor subunit beta-3

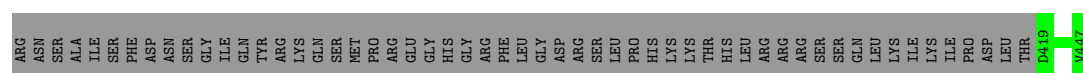
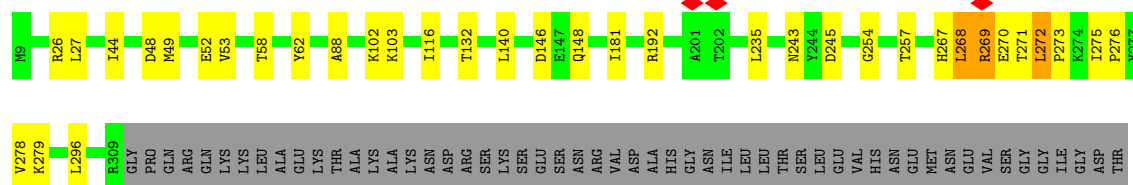


- Molecule 1: Gamma-aminobutyric acid receptor subunit beta-3

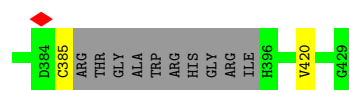
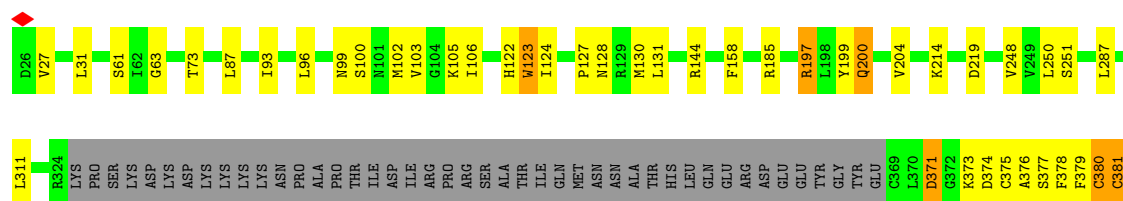
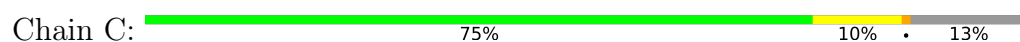




- Molecule 1: Gamma-aminobutyric acid receptor subunit beta-3



- Molecule 2: Isoform 2 of Gamma-aminobutyric acid receptor subunit gamma-2



- Molecule 3: Neuroligin-2

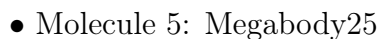


- Molecule 4: LHFPL tetraspan subfamily member 4 protein

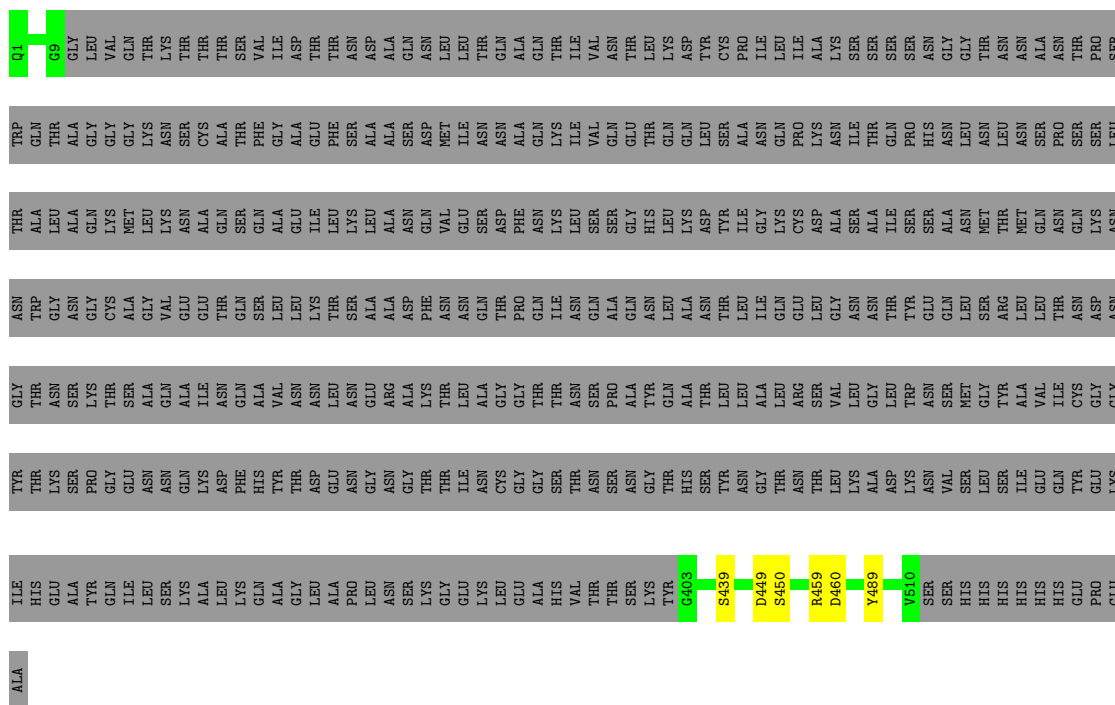


- Molecule 5: Megabody25





Chain F: 21% . 78%



- Molecule 6: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-3)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain G:  86% 14%



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

Chain I:  33% 33% 67%



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

Chain P:  33% 67%



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

Chain J:  100%

MAG1
MAG2

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

Chain Q:  50% 50%

MAG1
MAG2

- Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  17% 83%

MAG1
MAG2
MAN3
MAN4
MAN5
MAN6

- Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  33% 67%

MAG1
MAG2
MAN3
MAN4
MAN5
MAN6

- Molecule 10: alpha-D-mannopyranose-(1-3)-[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 R:  40% 60%

MAG1
MAG2
MAN3
MAN4
MAN5

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	29626	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45.28	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.648	Depositor
Minimum map value	-0.254	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	338.25598, 338.25598, 338.25598	wwPDB
Map dimensions	464, 464, 464	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.729, 0.729, 0.729	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: PX2, PGW, R16, D10, PLM, MAN, NAG, HEX, P1L, CLR, 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	0.18	0/2811	0.41	0/3824
1	B	0.23	0/2784	0.50	3/3787 (0.1%)
1	D	0.44	2/2813 (0.1%)	0.75	10/3828 (0.3%)
1	E	0.27	0/2830	0.51	2/3851 (0.1%)
2	C	0.41	2/2967 (0.1%)	0.67	8/4031 (0.2%)
3	H	0.18	0/259	0.36	0/352
4	L	0.18	0/1497	0.39	0/2034
5	F	0.16	0/935	0.34	0/1266
5	K	0.15	0/935	0.37	0/1266
5	O	0.16	0/925	0.37	0/1253
All	All	0.29	4/18756 (0.0%)	0.54	23/25492 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	123[A]	TRP	C-O	6.96	1.32	1.24
2	C	123[B]	TRP	C-O	6.96	1.32	1.24
1	D	62[A]	TYR	C-O	6.93	1.31	1.23
1	D	62[B]	TYR	C-O	6.93	1.31	1.23

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	268	LEU	N-CA-C	-10.24	101.05	112.72
2	C	123[A]	TRP	CA-C-O	9.65	129.79	118.69
2	C	123[B]	TRP	CA-C-O	9.65	129.79	118.69
1	B	276	PRO	N-CA-CB	-7.26	97.71	102.65
1	D	62[A]	TYR	CA-C-O	6.61	129.23	121.11
1	D	62[B]	TYR	CA-C-O	6.61	129.23	121.11
1	D	272	LEU	CA-C-N	6.44	126.20	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	272	LEU	C-N-CA	6.44	126.20	119.05
1	D	268	LEU	N-CA-CB	6.40	120.24	110.70
1	E	155	GLU	N-CA-CB	-5.97	101.70	111.66
2	C	123[A]	TRP	O-C-N	-5.76	116.26	122.19
2	C	123[B]	TRP	O-C-N	-5.76	116.26	122.19
1	E	102	LYS	N-CA-C	-5.56	107.05	113.88
2	C	371	ASP	CA-CB-CG	5.56	118.16	112.60
1	D	269	ARG	N-CA-C	-5.44	105.75	112.38
1	D	267	HIS	N-CA-C	-5.44	106.43	112.57
1	B	270	GLU	N-CA-C	-5.35	106.52	113.16
1	D	62[A]	TYR	O-C-N	-5.31	116.47	122.84
1	D	62[B]	TYR	O-C-N	-5.31	116.47	122.84
2	C	105	LYS	N-CA-C	-5.17	107.02	113.38
2	C	197	ARG	CA-C-N	-5.06	115.92	123.11
2	C	197	ARG	C-N-CA	-5.06	115.92	123.11
1	B	277	TYR	CA-C-O	-5.03	116.05	121.38

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	2731	0	2728	23	0
1	B	2712	0	2705	15	0
1	D	2732	0	2724	29	0
1	E	2745	0	2736	27	0
2	C	2949	0	2960	37	0
3	H	255	0	256	4	0
4	L	1455	0	1466	15	0
5	F	912	0	856	4	0
5	K	912	0	856	5	0
5	O	902	0	848	8	0
6	G	83	0	70	0	0
7	I	39	0	34	0	0
7	P	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	28	0	25	0	0
8	Q	28	0	25	0	0
9	M	72	0	61	1	0
9	N	72	0	61	1	0
10	R	61	0	52	1	0
11	A	12	0	28	0	0
11	B	12	0	28	0	0
11	E	12	0	28	0	0
12	A	10	0	22	0	0
12	B	10	0	22	0	0
12	D	20	0	44	0	0
12	E	10	0	22	0	0
12	L	10	0	22	1	0
13	B	51	0	76	0	0
13	L	51	0	76	0	0
14	C	36	0	52	0	0
15	C	14	0	13	1	0
16	C	48	0	102	0	0
17	C	36	0	62	0	0
18	C	28	0	46	0	0
18	L	28	0	46	0	0
All	All	19115	0	19186	148	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 (148) 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:269:ARG:HA	1:D:273:PRO:HG2	1.26	1.13
3:H:690:ASN:ND2	4:L:29:PHE:CD2	2.24	1.05
1:D:49:MET:SD	1:D:58:THR:HG23	1.98	1.03
1:E:83:LEU:HD13	1:E:87:VAL:HG21	1.52	0.92
3:H:690:ASN:ND2	4:L:29:PHE:CE2	2.49	0.81
1:E:83:LEU:CD1	1:E:87:VAL:HG21	2.15	0.76
1:B:207:ARG:NH1	5:F:489:TYR:O	2.19	0.75
5:K:439:SER:O	5:K:459:ARG:NH1	2.20	0.74
1:D:49:MET:SD	1:D:58:THR:CG2	2.75	0.74
1:A:88:ALA:HB1	1:A:116:ILE:HD12	1.71	0.72
5:O:465:THR:HG22	5:O:466:VAL:HG13	1.70	0.71
1:D:269:ARG:CA	1:D:273:PRO:HG2	2.14	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:ASP:OD2	1:D:148:GLN:NE2	2.27	0.67
3:H:690:ASN:ND2	4:L:29:PHE:CG	2.56	0.67
2:C:374:ASP:O	2:C:375:CYS:HB3	1.94	0.67
5:K:469:GLU:OE2	5:K:471:ASN:ND2	2.29	0.65
1:D:27:LEU:HD11	2:C:27:VAL:HG21	1.79	0.65
2:C:200:GLN:HE21	2:C:200:GLN:H	1.45	0.64
4:L:136:ALA:O	4:L:140:VAL:HG23	1.97	0.64
2:C:87:LEU:HD11	2:C:106:ILE:HD11	1.80	0.64
1:A:146:ASP:OD2	1:A:148:GLN:NE2	2.30	0.64
1:E:81:LEU:HB3	1:E:83:LEU:HD21	1.79	0.64
2:C:373:LYS:O	2:C:377:SER:OG	2.17	0.63
1:D:44:ILE:HD12	1:D:181:ILE:HD11	1.80	0.62
1:D:275:ILE:HB	2:C:199:TYR:CE2	2.35	0.62
1:E:43:ASP:OD1	1:E:176:THR:OG1	2.16	0.61
1:B:273:PRO:HB2	1:B:275:ILE:HG13	1.83	0.60
1:E:296:LEU:HD23	1:D:235:LEU:HD22	1.82	0.60
1:D:271:THR:C	1:D:273:PRO:HD3	2.27	0.60
1:B:115:MET:HE1	1:B:125:LEU:HD22	1.82	0.60
1:E:44:ILE:HG21	1:E:181:ILE:HD11	1.83	0.60
5:K:456:THR:OG1	5:K:469:GLU:OE1	2.19	0.60
1:A:12:VAL:HG13	1:A:81:LEU:HD11	1.83	0.60
1:D:26:ARG:HD3	2:C:102:MET:HE3	1.84	0.59
5:F:439:SER:O	5:F:459:ARG:NH1	2.36	0.58
1:D:272:LEU:N	1:D:273:PRO:HD3	2.20	0.56
2:C:378:PHE:HD1	2:C:379:PHE:CD1	2.24	0.56
1:D:49:MET:HG3	1:D:58:THR:OG1	2.06	0.56
2:C:380:P1L:O7	2:C:381:P1L:H9C2	2.06	0.55
1:B:274:LYS:O	1:B:275:ILE:C	2.47	0.55
5:O:491:GLY:O	5:O:498:ASN:ND2	2.40	0.55
1:B:155:GLU:OE1	1:B:207:ARG:NH2	2.40	0.54
1:E:426[B]:TRP:CE2	1:E:430:VAL:HG21	2.42	0.53
1:D:296:LEU:HD23	2:C:250:LEU:HD22	1.90	0.53
4:L:120:ASN:ND2	4:L:123:THR:OG1	2.41	0.53
1:E:270:GLU:OE2	1:D:269:ARG:NE	2.42	0.53
1:E:9:MET:SD	1:E:9:MET:N	2.82	0.52
2:C:380:P1L:H9C1	4:L:130:TRP:CE2	2.44	0.52
2:C:63:GLY:N	2:C:73:THR:O	2.40	0.52
1:E:72:LEU:HD13	1:E:91:LEU:HD22	1.92	0.52
2:C:31:LEU:HD21	2:C:96:LEU:HD11	1.92	0.52
1:A:225:THR:HG21	1:A:281:ILE:HD11	1.90	0.52
3:H:697:LEU:HB2	4:L:22:ILE:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ARG:HD2	1:A:271:THR:HG21	1.92	0.51
1:A:72:LEU:HD11	1:A:91:LEU:HD22	1.92	0.51
2:C:122:HIS:CG	2:C:144:ARG:NH1	2.78	0.51
1:E:155:GLU:HG3	1:E:156:SER:N	2.25	0.51
2:C:87:LEU:CD1	2:C:106:ILE:HD11	2.41	0.51
1:A:28:ARG:NH1	1:A:29:PRO:O	2.45	0.50
1:B:235:LEU:HD22	2:C:311:LEU:HD23	1.92	0.50
2:C:103:VAL:O	2:C:106:ILE:HG22	2.12	0.50
1:D:88:ALA:HB2	1:D:116:ILE:HD11	1.93	0.50
4:L:111:THR:O	4:L:114:SER:OG	2.26	0.50
1:D:52:GLU:HG2	1:D:140:LEU:HD21	1.93	0.49
2:C:61:SER:OG	2:C:197:ARG:NH1	2.44	0.49
2:C:123[B]:TRP:CD1	2:C:124:ILE:HG12	2.46	0.49
1:E:235:LEU:HD22	1:A:296:LEU:HD23	1.93	0.49
1:D:48:ASP:HB2	1:D:58:THR:OG1	2.11	0.49
1:E:88:ALA:CA	1:E:116:ILE:HD12	2.42	0.49
1:D:192:ARG:NH2	10:R:1:NAG:O3	2.46	0.49
1:E:19:LEU:HD21	1:E:74:TYR:HB3	1.93	0.49
1:D:44:ILE:CD1	1:D:181:ILE:HD11	2.41	0.49
2:C:106:ILE:HG21	2:C:131:LEU:HD21	1.95	0.49
1:B:296:LEU:HD23	1:A:235:LEU:HD22	1.95	0.48
1:E:64:GLN:OE1	1:E:125:LEU:HD11	2.13	0.48
1:A:84:ASP:OD1	1:A:84:ASP:N	2.46	0.48
1:B:268:LEU:HD22	1:B:285:LEU:HD11	1.96	0.48
1:E:44:ILE:O	1:E:180:ARG:NH1	2.47	0.47
1:E:175:VAL:HG21	1:E:210:LEU:HD13	1.97	0.47
1:B:275:ILE:CG2	1:B:279:LYS:HD3	2.45	0.47
1:B:275:ILE:HG21	1:B:279:LYS:HD3	1.96	0.47
2:C:123[A]:TRP:CE3	2:C:127:PRO:HB3	2.50	0.47
1:B:273:PRO:HB2	1:B:275:ILE:CG1	2.45	0.47
2:C:158:PHE:CD2	2:C:287:LEU:HD11	2.48	0.47
1:A:52:GLU:N	1:A:52:GLU:OE1	2.47	0.47
1:D:269:ARG:O	1:D:273:PRO:HD2	2.15	0.47
1:D:275:ILE:O	1:D:275:ILE:HG13	2.13	0.47
5:K:439:SER:OG	5:K:440:TRP:N	2.43	0.47
1:E:100:ASN:HD21	1:E:152:LEU:HA	1.79	0.47
1:E:426[B]:TRP:NE1	1:E:430:VAL:HG21	2.29	0.47
5:O:439:SER:O	5:O:459:ARG:NE	2.48	0.47
1:E:72:LEU:CD1	1:E:91:LEU:HD22	2.45	0.47
2:C:376:ALA:O	2:C:377:SER:C	2.55	0.47
2:C:380:P1L:O7	4:L:130:TRP:NE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ARG:HG3	9:N:1:NAG:H83	1.98	0.46
4:L:136:ALA:HB1	4:L:188:LEU:HD22	1.98	0.46
4:L:195:PHE:O	4:L:199:ASN:ND2	2.49	0.46
1:A:83:LEU:HD13	1:A:118:LEU:HD13	1.98	0.45
1:A:275:ILE:HG21	1:A:279:LYS:HD3	1.97	0.45
2:C:204:VAL:HG12	2:C:204:VAL:O	2.17	0.45
2:C:378:PHE:HD1	2:C:379:PHE:HD1	1.60	0.45
5:O:421:MET:HE3	5:O:459:ARG:HH22	1.81	0.45
4:L:68:SER:OG	4:L:74:GLU:O	2.29	0.45
1:E:88:ALA:HA	1:E:116:ILE:HD12	1.99	0.45
9:M:1:NAG:O3	9:M:2:NAG:O5	2.33	0.45
2:C:27:VAL:HG12	2:C:93:ILE:HD12	1.98	0.45
1:E:130:ILE:HG22	1:E:132:THR:HG23	1.98	0.44
2:C:374:ASP:O	2:C:376:ALA:N	2.44	0.44
1:B:254:GLY:O	1:B:257:THR:OG1	2.29	0.44
1:E:88:ALA:HA	1:E:116:ILE:CD1	2.48	0.44
1:A:72:LEU:CD1	1:A:91:LEU:HD22	2.46	0.44
4:L:156:ARG:NH1	4:L:163:THR:O	2.51	0.44
5:O:439:SER:OG	5:O:440:TRP:N	2.51	0.44
1:E:102:LYS:HD2	1:E:135:ALA:HB2	2.00	0.43
2:C:248:VAL:O	2:C:251:SER:OG	2.29	0.43
1:D:268:LEU:HD12	1:D:268:LEU:HA	1.64	0.43
1:B:160:THR:OG1	1:B:204:ALA:O	2.34	0.43
5:O:421:MET:HE1	5:O:465:THR:HG21	2.00	0.43
5:F:460:ASP:N	5:F:460:ASP:OD1	2.48	0.43
5:F:449:ASP:OD1	5:F:450:SER:N	2.51	0.43
2:C:420:VAL:HG22	12:L:1001:D10:H71	2.00	0.43
4:L:184:ILE:O	4:L:188:LEU:HD23	2.18	0.43
1:A:9:MET:SD	1:A:9:MET:N	2.91	0.43
5:O:419:PRO:HG2	5:O:420:ILE:HD12	2.00	0.43
1:A:19:LEU:HD11	1:A:74:TYR:CD2	2.54	0.43
2:C:185:ARG:NH2	15:C:502:NAG:O4	2.51	0.42
1:E:269:ARG:NH1	1:D:270:GLU:OE2	2.53	0.42
1:A:64:GLN:NE2	1:A:125:LEU:HD21	2.35	0.42
1:A:44:ILE:O	1:A:180[A]:ARG:NH1	2.53	0.42
1:A:15:THR:HG21	1:A:77:ILE:HD12	2.02	0.42
2:C:122:HIS:CD2	2:C:122:HIS:N	2.88	0.42
5:K:441:SER:O	5:K:441:SER:OG	2.32	0.42
1:E:16:VAL:O	1:E:20:LEU:HD23	2.20	0.41
1:E:88:ALA:HB2	1:E:116:ILE:HD12	2.02	0.41
4:L:17:ARG:NH1	4:L:18:ASN:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ARG:NH1	1:A:30:ASP:O	2.53	0.41
1:D:243:ASN:ND2	1:D:245:ASP:OD1	2.53	0.41
1:D:254:GLY:O	1:D:257:THR:OG1	2.32	0.41
1:D:53:VAL:HG13	1:D:275:ILE:HG23	2.02	0.41
1:D:140:LEU:O	1:D:279:LYS:HG2	2.21	0.41
2:C:214:LYS:NZ	2:C:219:ASP:OD1	2.54	0.41
5:O:469:GLU:OE1	5:O:471:ASN:ND2	2.54	0.41
1:A:24:ASP:O	1:A:71:ARG:NH1	2.54	0.40
1:A:142:ARG:O	1:A:145:LEU:N	2.55	0.40
2:C:130:MET:HE2	2:C:130:MET:HB3	1.96	0.40
1:B:235:LEU:HD22	2:C:311:LEU:CD2	2.51	0.40
1:D:276:PRO:HD2	2:C:200:GLN:HG2	2.02	0.40
2:C:373:LYS:O	2:C:374:ASP:HB3	2.20	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	328/439 (75%)	316 (96%)	12 (4%)	0	100	100
1	B	326/439 (74%)	319 (98%)	7 (2%)	0	100	100
1	D	328/439 (75%)	319 (97%)	9 (3%)	0	100	100
1	E	330/439 (75%)	323 (98%)	7 (2%)	0	100	100
2	C	345/404 (85%)	326 (94%)	19 (6%)	0	100	100
3	H	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
4	L	187/188 (100%)	185 (99%)	2 (1%)	0	100	100
5	F	113/522 (22%)	110 (97%)	3 (3%)	0	100	100
5	K	113/522 (22%)	108 (96%)	5 (4%)	0	100	100
5	O	111/522 (21%)	105 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2212/3947 (56%)	2141 (97%)	71 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	299/392 (76%)	299 (100%)	0	100	100
1	B	297/392 (76%)	297 (100%)	0	100	100
1	D	299/392 (76%)	295 (99%)	4 (1%)	65	82
1	E	300/392 (76%)	298 (99%)	2 (1%)	81	90
2	C	322/366 (88%)	317 (98%)	5 (2%)	58	79
3	H	27/27 (100%)	27 (100%)	0	100	100
4	L	155/154 (101%)	155 (100%)	0	100	100
5	F	94/430 (22%)	94 (100%)	0	100	100
5	K	94/430 (22%)	94 (100%)	0	100	100
5	O	93/430 (22%)	93 (100%)	0	100	100
All	All	1980/3405 (58%)	1969 (99%)	11 (1%)	82	91

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	86	ARG
1	E	87	VAL
1	D	102	LYS
1	D	103	LYS
1	D	132	THR
1	D	278	VAL
2	C	99	ASN
2	C	100	SER
2	C	128	ASN

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Mol	Chain	Res	Type
2	C	200	GLN
2	C	371	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	439	ASN
1	E	85	ASN
1	A	65	GLN
1	D	65	GLN
1	D	90	GLN
2	C	69	ASN
2	C	101	ASN
2	C	200	GLN
3	H	690	ASN
4	L	186	ASN
5	O	507	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	P1L	C	381	2	21,22,23	0.43	0	18,23,25	3.35	1 (5%)
2	P1L	C	385	2	21,22,23	0.31	0	18,23,25	3.26	1 (5%)
2	P1L	C	380	2	21,22,23	0.41	0	18,23,25	2.78	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
2	P1L	C	381	2	-	2/20/22/24	-
2	P1L	C	385	2	-	7/20/22/24	-
2	P1L	C	380	2	-	4/20/22/24	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	381	P1L	CB-SG-C7	14.19	120.69	100.84
2	C	385	P1L	CB-SG-C7	13.79	120.13	100.84
2	C	380	P1L	CB-SG-C7	11.65	117.13	100.84

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	380	P1L	CA-CB-SG-C7
2	C	381	P1L	O7-C7-SG-CB
2	C	381	P1L	C8-C7-SG-CB
2	C	380	P1L	O7-C7-SG-CB
2	C	385	P1L	O7-C7-SG-CB
2	C	385	P1L	SG-C7-C8-C9
2	C	380	P1L	C8-C7-SG-CB
2	C	385	P1L	CA-CB-SG-C7
2	C	385	P1L	C11-C12-C13-C14
2	C	380	P1L	C17-C18-C19-C20
2	C	385	P1L	O7-C7-C8-C9
2	C	385	P1L	C9-C10-C11-C12
2	C	385	P1L	C8-C7-SG-CB

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	381	P1L	1	0
2	C	380	P1L	3	0

5.5 Carbohydrates

34 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	G	1	6,1	14,14,15	0.41	0	17,19,21	1.00	1 (5%)
6	NAG	G	2	6	14,14,15	0.44	0	17,19,21	0.69	0
6	BMA	G	3	6	11,11,12	0.46	0	15,15,17	0.59	0
6	MAN	G	4	6	11,11,12	0.39	0	15,15,17	0.95	0
6	MAN	G	5	6	11,11,12	0.27	0	15,15,17	0.56	0
6	MAN	G	6	6	11,11,12	0.25	0	15,15,17	0.58	0
6	MAN	G	7	6	11,11,12	0.30	0	15,15,17	0.58	0
7	NAG	I	1	7,1	14,14,15	0.39	0	17,19,21	0.93	1 (5%)
7	NAG	I	2	7	14,14,15	0.39	0	17,19,21	0.80	1 (5%)
7	BMA	I	3	7	11,11,12	0.27	0	15,15,17	0.47	0
8	NAG	J	1	8,1	14,14,15	0.20	0	17,19,21	0.43	0
8	NAG	J	2	8	14,14,15	0.22	0	17,19,21	0.40	0
9	NAG	M	1	9,1	14,14,15	0.22	0	17,19,21	0.41	0
9	NAG	M	2	9	14,14,15	0.20	0	17,19,21	0.44	0
9	BMA	M	3	9	11,11,12	0.57	0	15,15,17	0.78	0
9	MAN	M	4	9	11,11,12	0.67	0	15,15,17	1.04	2 (13%)
9	MAN	M	5	9	11,11,12	0.67	0	15,15,17	1.04	2 (13%)
9	MAN	M	6	9	11,11,12	0.66	0	15,15,17	1.06	2 (13%)
9	NAG	N	1	9	14,14,15	0.29	0	17,19,21	0.39	0
9	NAG	N	2	9	14,14,15	0.22	0	17,19,21	0.42	0
9	BMA	N	3	9	11,11,12	0.60	0	15,15,17	0.72	0
9	MAN	N	4	9	11,11,12	0.64	0	15,15,17	1.04	2 (13%)
9	MAN	N	5	9	11,11,12	0.68	0	15,15,17	1.03	2 (13%)
9	MAN	N	6	9	11,11,12	0.68	0	15,15,17	1.06	2 (13%)
7	NAG	P	1	7,1	14,14,15	0.38	0	17,19,21	0.89	1 (5%)
7	NAG	P	2	7	14,14,15	0.39	0	17,19,21	0.94	2 (11%)
7	BMA	P	3	7	11,11,12	0.32	0	15,15,17	0.39	0
8	NAG	Q	1	8,1	14,14,15	0.30	0	17,19,21	0.80	1 (5%)
8	NAG	Q	2	8	14,14,15	0.24	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	R	1	10,1	14,14,15	0.23	0	17,19,21	0.40	0
10	NAG	R	2	10	14,14,15	0.19	0	17,19,21	0.43	0
10	BMA	R	3	10	11,11,12	0.55	0	15,15,17	0.77	0
10	MAN	R	4	10	11,11,12	0.67	0	15,15,17	1.10	2 (13%)
10	MAN	R	5	10	11,11,12	0.68	0	15,15,17	1.07	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	G	1	6,1	-	3/6/23/26	0/1/1/1
6	NAG	G	2	6	-	0/6/23/26	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
6	MAN	G	5	6	-	1/2/19/22	0/1/1/1
6	MAN	G	6	6	-	0/2/19/22	0/1/1/1
6	MAN	G	7	6	-	0/2/19/22	0/1/1/1
7	NAG	I	1	7,1	-	1/6/23/26	0/1/1/1
7	NAG	I	2	7	-	3/6/23/26	0/1/1/1
7	BMA	I	3	7	-	0/2/19/22	0/1/1/1
8	NAG	J	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	J	2	8	-	1/6/23/26	0/1/1/1
9	NAG	M	1	9,1	-	3/6/23/26	0/1/1/1
9	NAG	M	2	9	-	2/6/23/26	0/1/1/1
9	BMA	M	3	9	-	0/2/19/22	0/1/1/1
9	MAN	M	4	9	-	1/2/19/22	0/1/1/1
9	MAN	M	5	9	-	1/2/19/22	0/1/1/1
9	MAN	M	6	9	-	0/2/19/22	0/1/1/1
9	NAG	N	1	9	-	2/6/23/26	0/1/1/1
9	NAG	N	2	9	-	0/6/23/26	0/1/1/1
9	BMA	N	3	9	-	1/2/19/22	0/1/1/1
9	MAN	N	4	9	-	0/2/19/22	0/1/1/1
9	MAN	N	5	9	-	0/2/19/22	0/1/1/1
9	MAN	N	6	9	-	0/2/19/22	0/1/1/1
7	NAG	P	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	P	2	7	-	3/6/23/26	0/1/1/1
7	BMA	P	3	7	-	1/2/19/22	0/1/1/1
8	NAG	Q	1	8,1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	Q	2	8	-	4/6/23/26	0/1/1/1
10	NAG	R	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	R	2	10	-	0/6/23/26	0/1/1/1
10	BMA	R	3	10	-	0/2/19/22	0/1/1/1
10	MAN	R	4	10	-	0/2/19/22	0/1/1/1
10	MAN	R	5	10	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	P	1	NAG	C1-O5-C5	2.71	115.86	112.19
7	P	2	NAG	C1-C2-N2	2.67	115.04	110.49
9	N	4	MAN	C1-O5-C5	2.64	115.77	112.19
8	Q	1	NAG	C2-N2-C7	2.60	126.60	122.90
10	R	4	MAN	C1-O5-C5	2.53	115.61	112.19
6	G	1	NAG	C1-O5-C5	2.44	115.50	112.19
9	M	6	MAN	C1-O5-C5	2.33	115.35	112.19
9	N	6	MAN	C1-O5-C5	2.32	115.33	112.19
9	M	4	MAN	O2-C2-C3	-2.28	105.58	110.14
9	N	5	MAN	O2-C2-C3	-2.27	105.60	110.14
10	R	4	MAN	O2-C2-C3	-2.25	105.63	110.14
9	M	6	MAN	O2-C2-C3	-2.25	105.63	110.14
10	R	5	MAN	C1-O5-C5	2.24	115.23	112.19
10	R	5	MAN	O2-C2-C3	-2.24	105.66	110.14
9	M	5	MAN	O2-C2-C3	-2.23	105.66	110.14
9	M	5	MAN	C1-O5-C5	2.23	115.22	112.19
7	I	1	NAG	C2-N2-C7	2.23	126.08	122.90
9	N	6	MAN	O2-C2-C3	-2.23	105.67	110.14
9	N	5	MAN	C1-O5-C5	2.19	115.15	112.19
9	M	4	MAN	C1-O5-C5	2.09	115.03	112.19
9	N	4	MAN	O2-C2-C3	-2.09	105.94	110.14
7	I	2	NAG	C2-N2-C7	2.07	125.85	122.90
7	P	2	NAG	C2-N2-C7	2.01	125.76	122.90

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	1	NAG	C3-C2-N2-C7
7	I	2	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
7	I	2	NAG	C8-C7-N2-C2
7	I	2	NAG	O7-C7-N2-C2
7	P	1	NAG	O7-C7-N2-C2
7	P	2	NAG	C1-C2-N2-C7
7	P	2	NAG	C8-C7-N2-C2
7	P	2	NAG	O7-C7-N2-C2
9	N	1	NAG	C3-C2-N2-C7
8	Q	1	NAG	C4-C5-C6-O6
9	M	1	NAG	C4-C5-C6-O6
7	P	1	NAG	C8-C7-N2-C2
8	Q	1	NAG	O5-C5-C6-O6
9	M	2	NAG	C4-C5-C6-O6
8	Q	2	NAG	O5-C5-C6-O6
9	M	1	NAG	O5-C5-C6-O6
9	M	2	NAG	O5-C5-C6-O6
8	Q	2	NAG	C4-C5-C6-O6
8	Q	1	NAG	C8-C7-N2-C2
8	Q	1	NAG	O7-C7-N2-C2
9	M	5	MAN	O5-C5-C6-O6
9	N	1	NAG	O5-C5-C6-O6
6	G	1	NAG	O5-C5-C6-O6
7	P	3	BMA	O5-C5-C6-O6
9	N	3	BMA	O5-C5-C6-O6
6	G	5	MAN	O5-C5-C6-O6
9	M	4	MAN	O5-C5-C6-O6
8	J	2	NAG	C3-C2-N2-C7
6	G	1	NAG	C1-C2-N2-C7
7	I	1	NAG	C3-C2-N2-C7
8	Q	2	NAG	C3-C2-N2-C7
9	M	1	NAG	C3-C2-N2-C7
8	Q	2	NAG	C1-C2-N2-C7

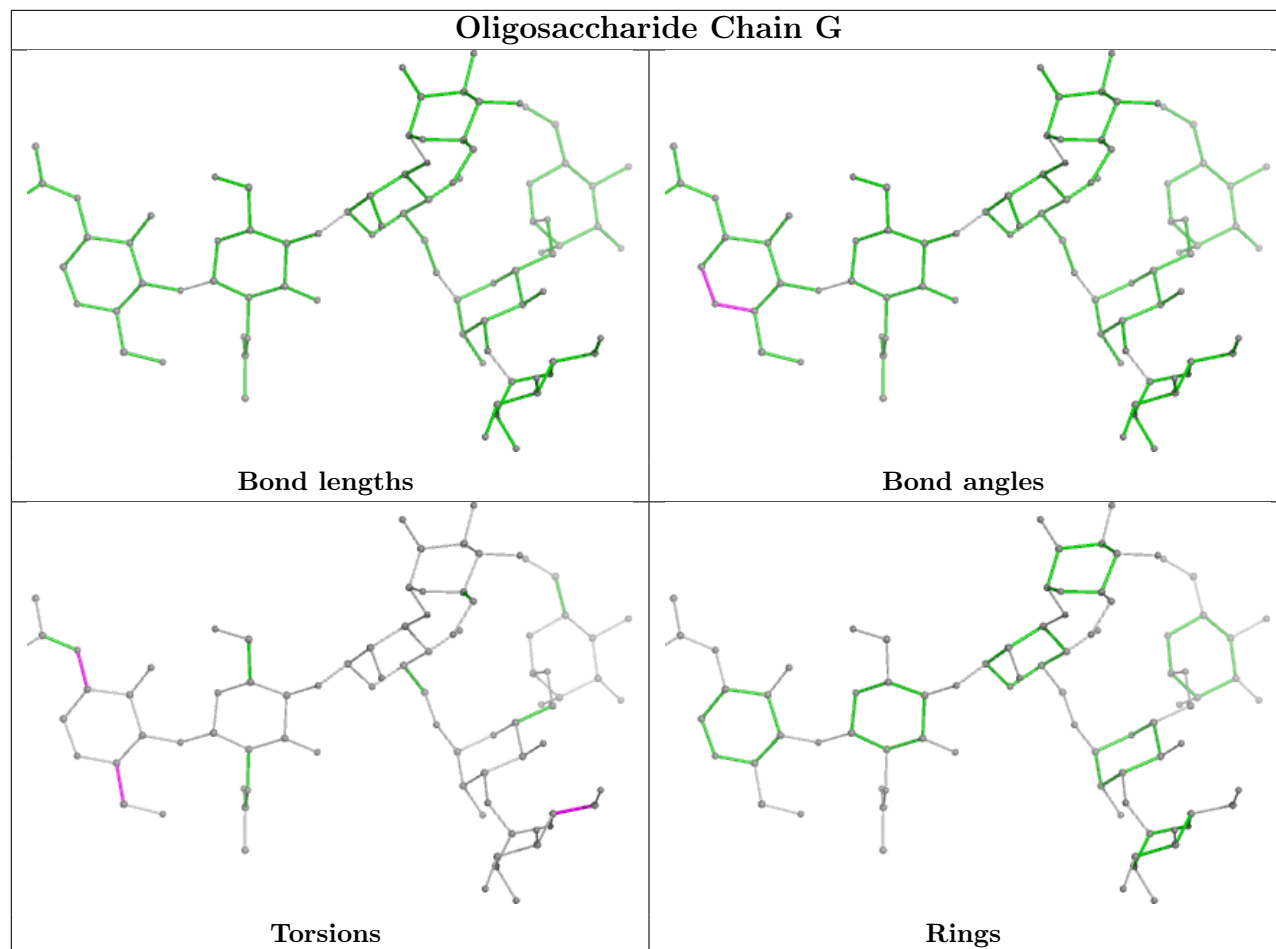
There are no ring outliers.

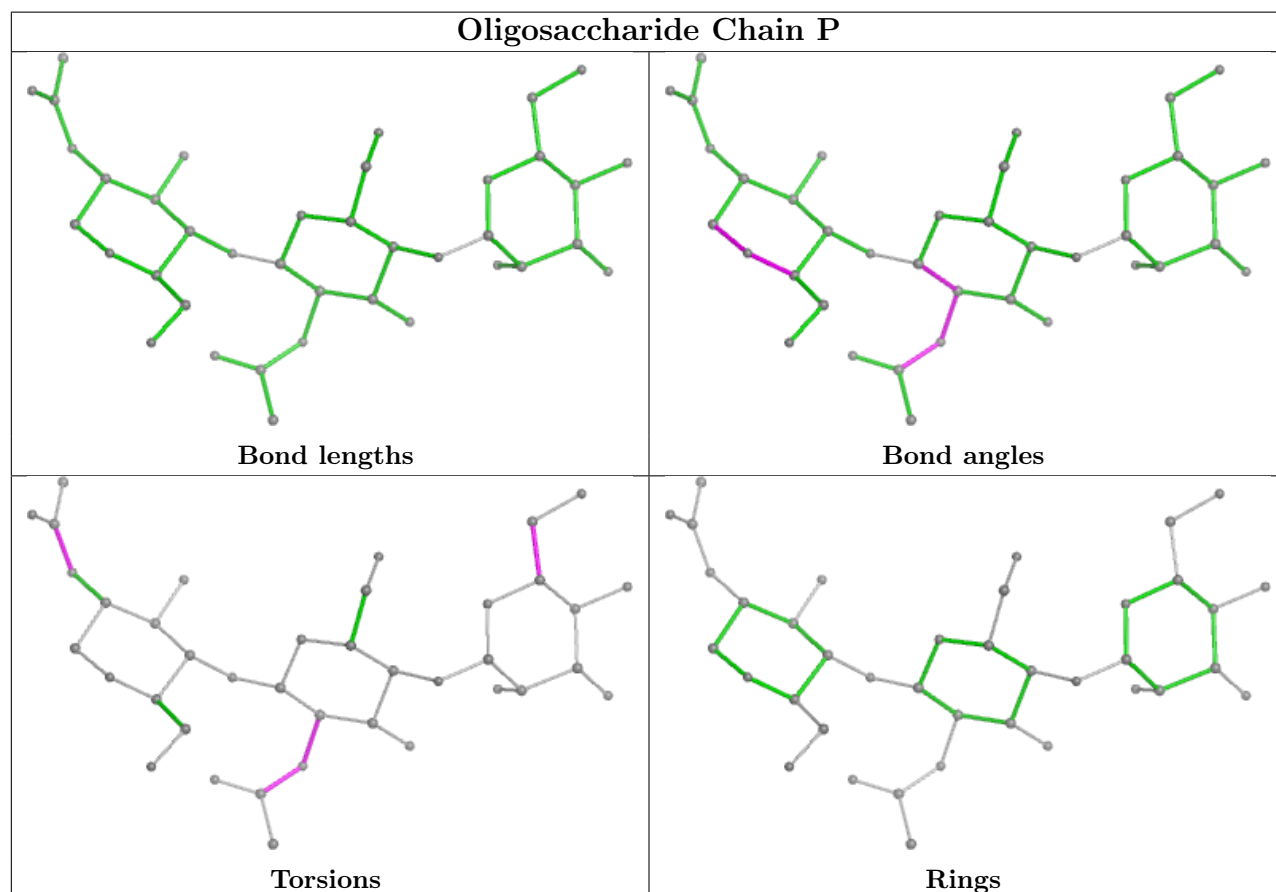
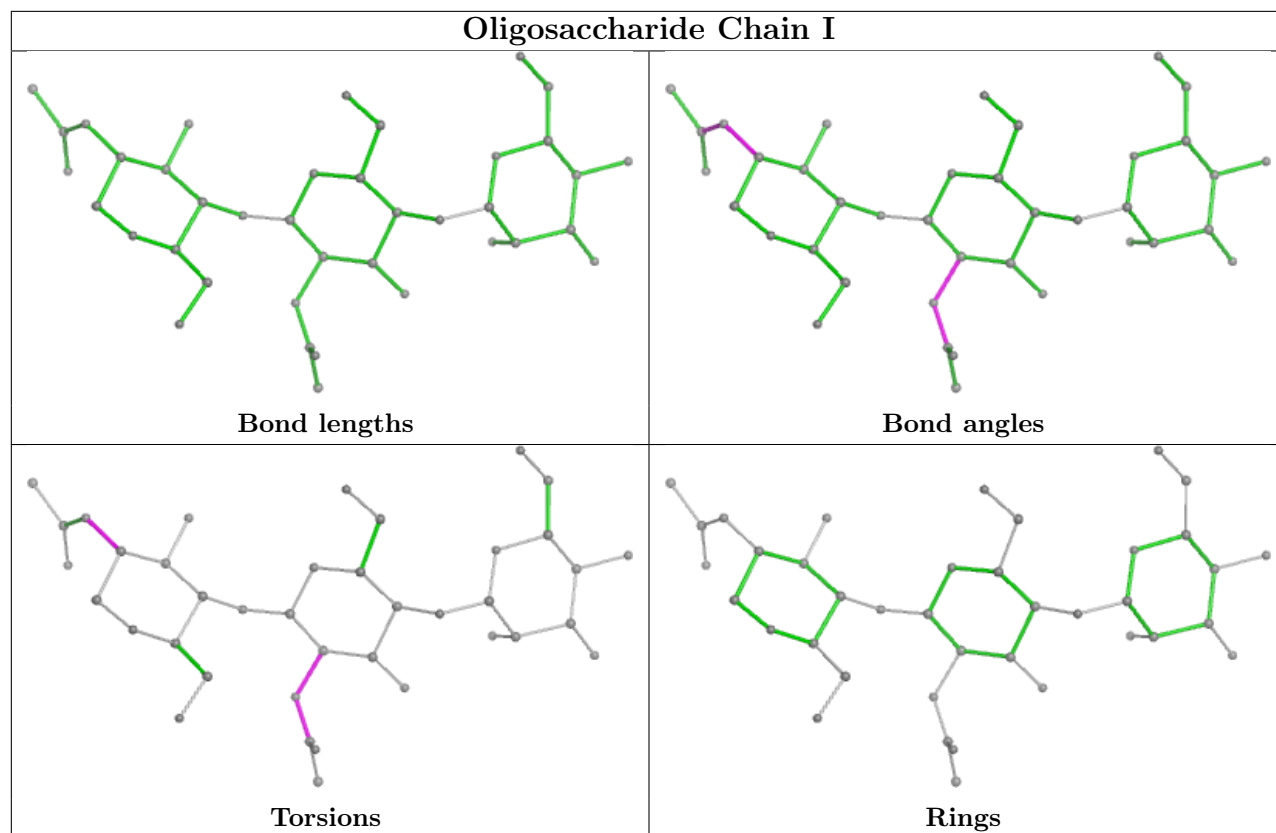
4 monomers are involved in 3 short contacts:

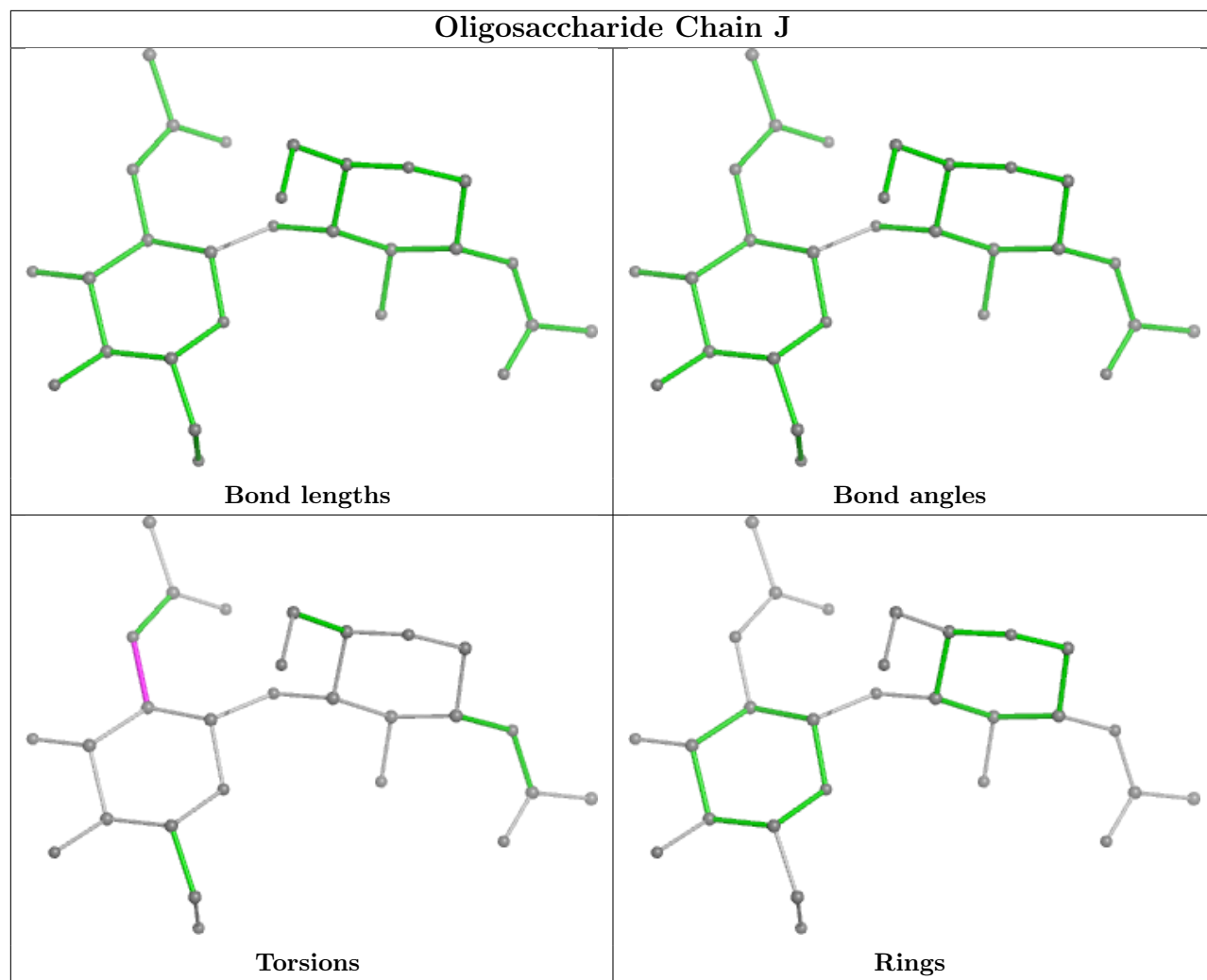
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	M	2	NAG	1	0
9	M	1	NAG	1	0
9	N	1	NAG	1	0
10	R	1	NAG	1	0

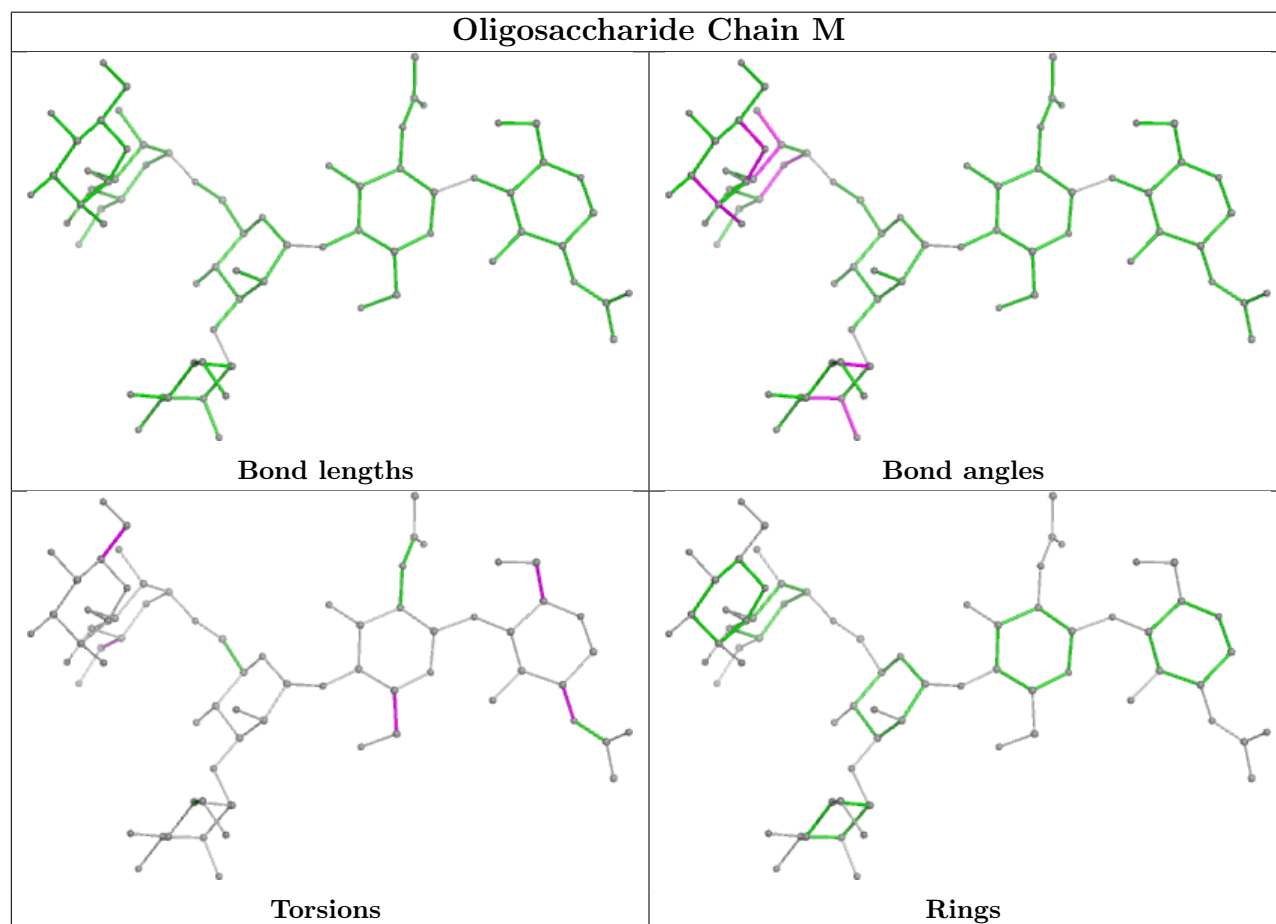
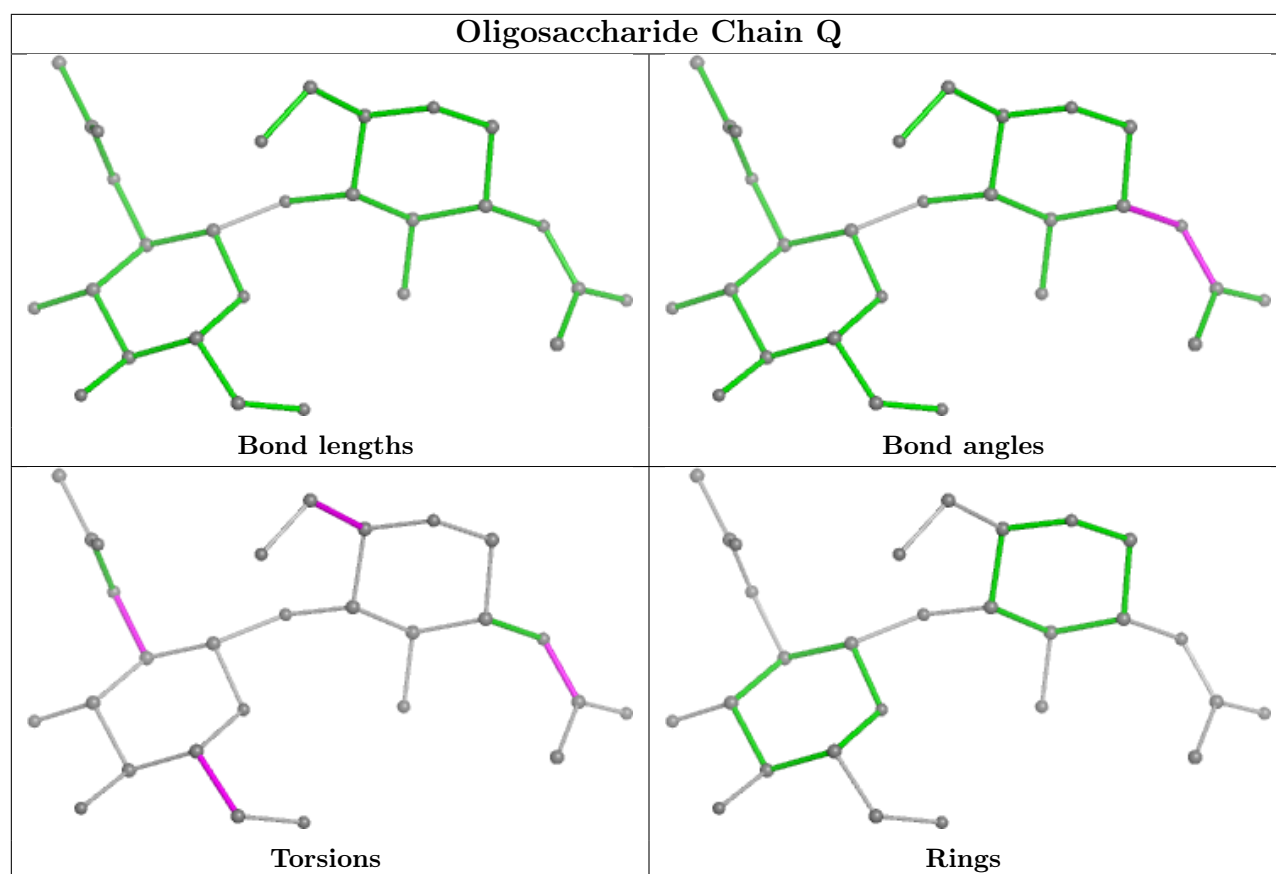
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

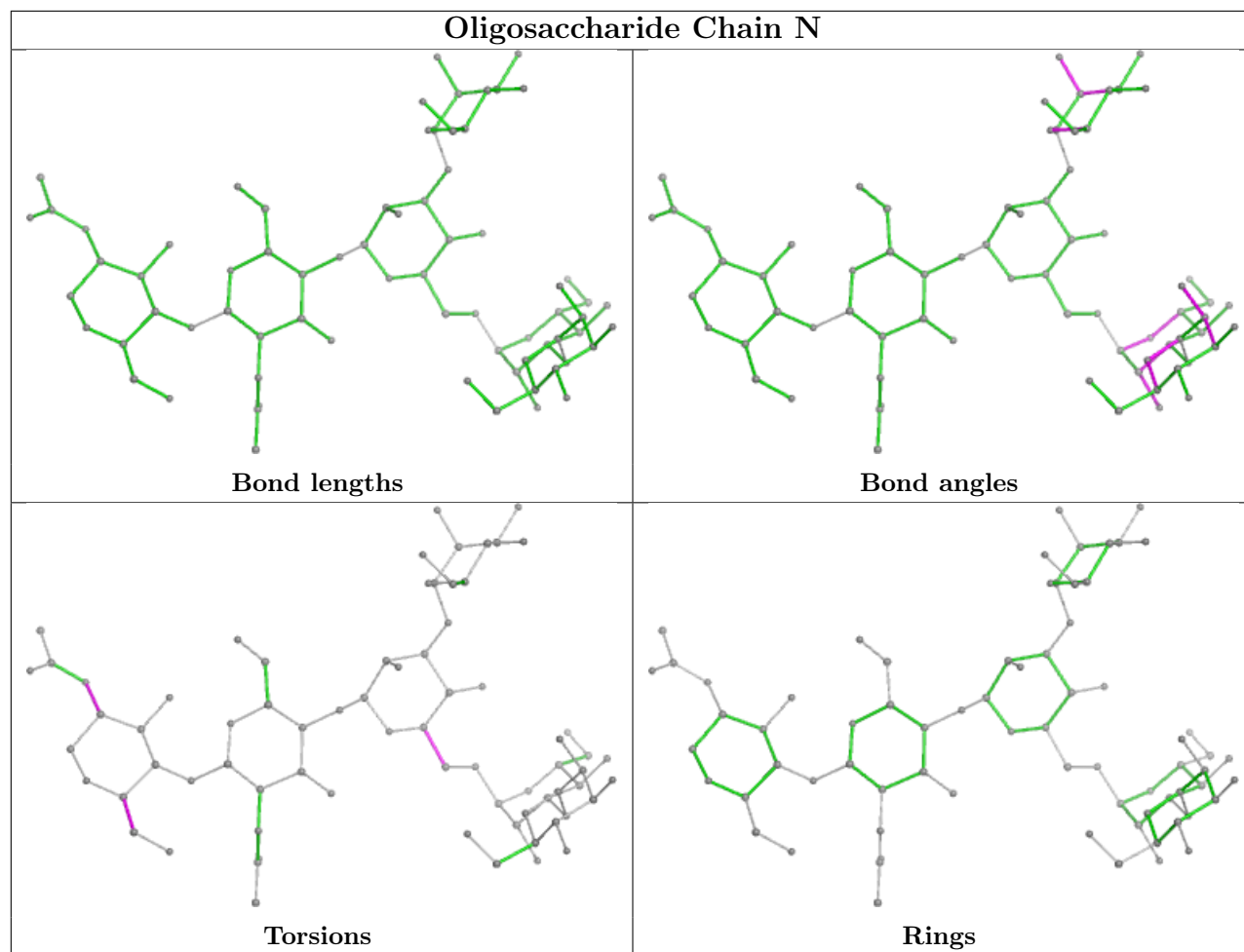
bond angles, torsion angles, and ring geometry for oligosaccharide.

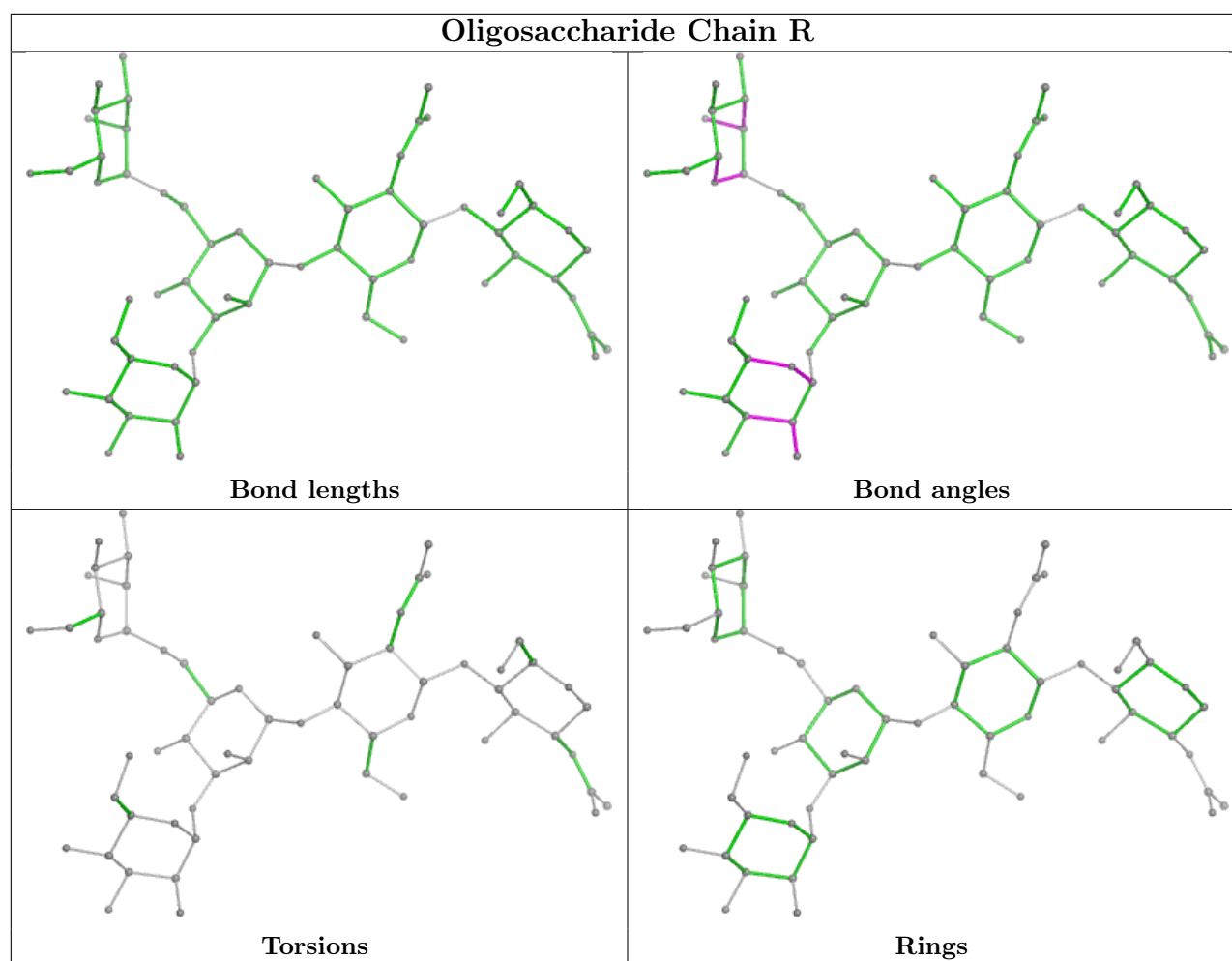












5.6 Ligand geometry [i](#)

23 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	$\# Z > 2$
16	R16	C	506	-	15,15,15	0.32	0	14,14,14	0.72	0
13	PGW	B	504	-	50,50,50	0.98	2 (4%)	53,56,56	0.94	2 (3%)
16	R16	C	503	-	15,15,15	0.33	0	14,14,14	0.67	0
12	D10	A	501	-	9,9,9	0.31	0	8,8,8	0.69	0
17	PLM	C	505	-	17,17,17	0.59	0	17,17,17	1.04	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	NAG	C	502	2	14,14,15	0.20	0	17,19,21	0.45	0
12	D10	D	502	-	9,9,9	0.30	0	8,8,8	0.70	0
13	PGW	L	1002	-	50,50,50	0.97	2 (4%)	53,56,56	1.04	2 (3%)
12	D10	L	1001	-	9,9,9	0.30	0	8,8,8	0.72	0
16	R16	C	504	-	15,15,15	0.32	0	14,14,14	0.79	0
11	HEX	E	501	-	5,5,5	0.31	0	4,4,4	0.57	0
11	HEX	A	503	-	5,5,5	0.31	0	4,4,4	0.56	0
12	D10	E	503	-	9,9,9	0.30	0	8,8,8	0.76	0
14	PX2	C	501	-	35,35,35	0.33	0	39,40,40	0.39	0
18	CLR	C	508	-	31,31,31	0.18	0	48,48,48	0.30	0
12	D10	B	503	-	9,9,9	0.28	0	8,8,8	0.80	0
12	D10	D	501	-	9,9,9	0.32	0	8,8,8	0.64	0
11	HEX	A	502	-	5,5,5	0.31	0	4,4,4	0.57	0
11	HEX	B	501	-	5,5,5	0.30	0	4,4,4	0.57	0
11	HEX	E	502	-	5,5,5	0.31	0	4,4,4	0.56	0
11	HEX	B	502	-	5,5,5	0.31	0	4,4,4	0.57	0
17	PLM	C	507	-	17,17,17	0.59	0	17,17,17	1.04	0
18	CLR	L	1003	-	31,31,31	0.26	0	48,48,48	0.43	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
16	R16	C	506	-	-	2/13/13/13	-
13	PGW	B	504	-	-	25/55/55/55	-
16	R16	C	503	-	-	2/13/13/13	-
12	D10	A	501	-	-	1/7/7/7	-
17	PLM	C	505	-	-	4/15/15/15	-
15	NAG	C	502	2	-	2/6/23/26	0/1/1/1
12	D10	D	502	-	-	2/7/7/7	-
13	PGW	L	1002	-	-	25/55/55/55	-
12	D10	L	1001	-	-	0/7/7/7	-
16	R16	C	504	-	-	1/13/13/13	-
11	HEX	E	501	-	-	0/3/3/3	-
11	HEX	A	503	-	-	0/3/3/3	-
12	D10	E	503	-	-	2/7/7/7	-
14	PX2	C	501	-	-	6/37/37/37	-
18	CLR	C	508	-	-	0/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	D10	B	503	-	-	1/7/7/7	-
12	D10	D	501	-	-	2/7/7/7	-
11	HEX	A	502	-	-	0/3/3/3	-
11	HEX	B	501	-	-	0/3/3/3	-
11	HEX	E	502	-	-	0/3/3/3	-
11	HEX	B	502	-	-	0/3/3/3	-
17	PLM	C	507	-	-	4/15/15/15	-
18	CLR	L	1003	-	-	0/10/68/68	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	504	PGW	O03-C19	2.90	1.41	1.33
13	L	1002	PGW	O03-C19	2.84	1.41	1.33
13	L	1002	PGW	O01-C1	2.73	1.42	1.34
13	B	504	PGW	O01-C1	2.71	1.42	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	1002	PGW	O01-C1-C2	4.08	120.28	111.50
13	B	504	PGW	O01-C1-C2	3.94	120.00	111.50
13	L	1002	PGW	O03-C19-C20	2.98	121.26	111.91
13	B	504	PGW	O03-C19-C20	2.51	119.77	111.91
17	C	505	PLM	C3-C2-C1	-2.11	109.15	114.47

There are no chirality outliers.

All (79) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	B	504	PGW	C04-C05-CAD-OAE
13	B	504	PGW	C03-O11-P-O13
13	B	504	PGW	C03-O11-P-O14
13	L	1002	PGW	C04-O12-P-O14
13	L	1002	PGW	O02-C1-O01-C02
13	L	1002	PGW	O04-C19-O03-C01
13	L	1002	PGW	C2-C1-O01-C02
13	L	1002	PGW	C20-C19-O03-C01
13	B	504	PGW	C20-C19-O03-C01
13	L	1002	PGW	O12-C04-C05-OAF
13	B	504	PGW	O04-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
13	B	504	PGW	C03-O11-P-O12
13	B	504	PGW	C04-O12-P-O11
13	L	1002	PGW	C04-O12-P-O11
13	L	1002	PGW	O12-C04-C05-CAD
13	B	504	PGW	O12-C04-C05-OAF
13	L	1002	PGW	C22-C23-C24-C25
13	B	504	PGW	C27-C15-C16-C17
13	B	504	PGW	C25-C26-C27-C15
13	B	504	PGW	C23-C24-C25-C26
16	C	503	R16	C38-C39-C40-C41
13	B	504	PGW	OAF-C05-CAD-OAE
13	B	504	PGW	C10-C06-C07-C08
13	B	504	PGW	C02-C03-O11-P
13	L	1002	PGW	C08-C09-C11-C12
13	B	504	PGW	C21-C22-C23-C24
13	B	504	PGW	C06-C07-C08-C09
12	E	503	D10	C2-C3-C4-C5
13	B	504	PGW	C2-C3-C4-C5
12	B	503	D10	C7-C8-C9-C10
16	C	506	R16	C34-C35-C36-C37
16	C	503	R16	C28-C29-C30-C31
13	B	504	PGW	C01-C02-C03-O11
13	L	1002	PGW	C06-C07-C08-C09
13	L	1002	PGW	C25-C26-C27-C15
17	C	505	PLM	C7-C8-C9-CA
13	B	504	PGW	O01-C1-C2-C3
16	C	504	R16	C35-C36-C37-C38
13	L	1002	PGW	C01-C02-O01-C1
13	B	504	PGW	O03-C19-C20-C21
13	L	1002	PGW	C11-C12-C13-C14
17	C	505	PLM	C8-C9-CA-CB
13	L	1002	PGW	C3-C4-C5-C6
13	L	1002	PGW	C05-C04-O12-P
13	B	504	PGW	C04-O12-P-O13
13	L	1002	PGW	C27-C15-C16-C17
13	B	504	PGW	O01-C02-C03-O11
14	C	501	PX2	C11-C10-C9-C8
12	D	502	D10	C4-C5-C6-C7
16	C	506	R16	C37-C38-C39-C40
12	A	501	D10	C4-C5-C6-C7
15	C	502	NAG	C3-C2-N2-C7
12	E	503	D10	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	L	1002	PGW	C5-C6-C7-C8
12	D	501	D10	C5-C6-C7-C8
12	D	501	D10	C4-C5-C6-C7
13	L	1002	PGW	O03-C01-C02-O01
13	L	1002	PGW	C17-C18-C28-C30
13	L	1002	PGW	C20-C21-C22-C23
17	C	505	PLM	O1-C1-C2-C3
15	C	502	NAG	C1-C2-N2-C7
17	C	505	PLM	O2-C1-C2-C3
14	C	501	PX2	C23-C24-C25-C26
13	B	504	PGW	C7-C8-C9-C10
13	L	1002	PGW	C7-C8-C9-C10
13	L	1002	PGW	C15-C16-C17-C18
14	C	501	PX2	C12-C13-C14-C15
17	C	507	PLM	O2-C1-C2-C3
13	B	504	PGW	O02-C1-C2-C3
14	C	501	PX2	C24-C25-C26-C27
14	C	501	PX2	C18-C19-C20-C21
13	B	504	PGW	O12-C04-C05-CAD
13	L	1002	PGW	C03-O11-P-O14
17	C	507	PLM	C3-C4-C5-C6
13	L	1002	PGW	O03-C19-C20-C21
14	C	501	PX2	O5-C4-C5-C6
17	C	507	PLM	O1-C1-C2-C3
12	D	502	D10	C7-C8-C9-C10
17	C	507	PLM	C8-C9-CA-CB

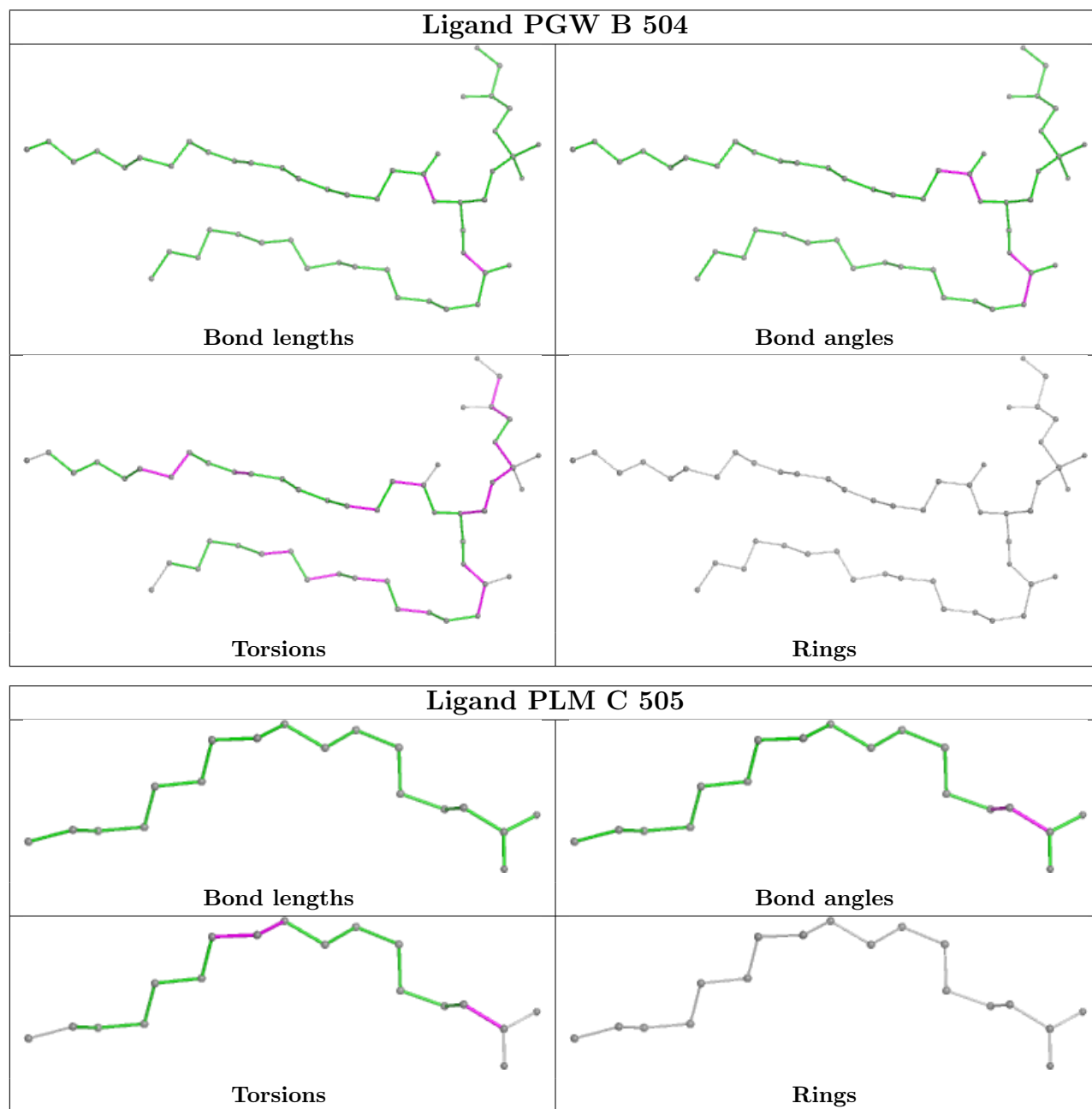
There are no ring outliers.

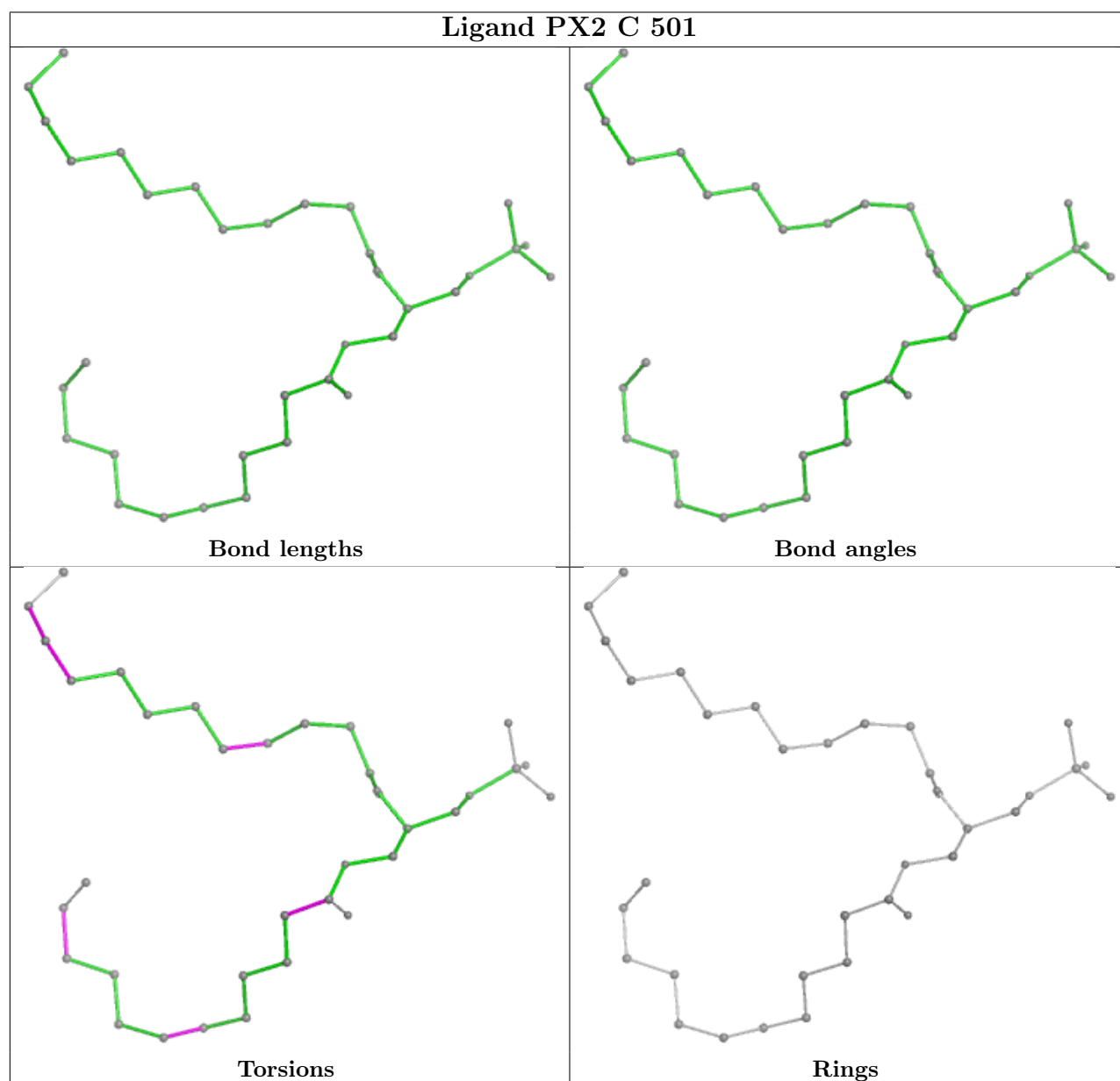
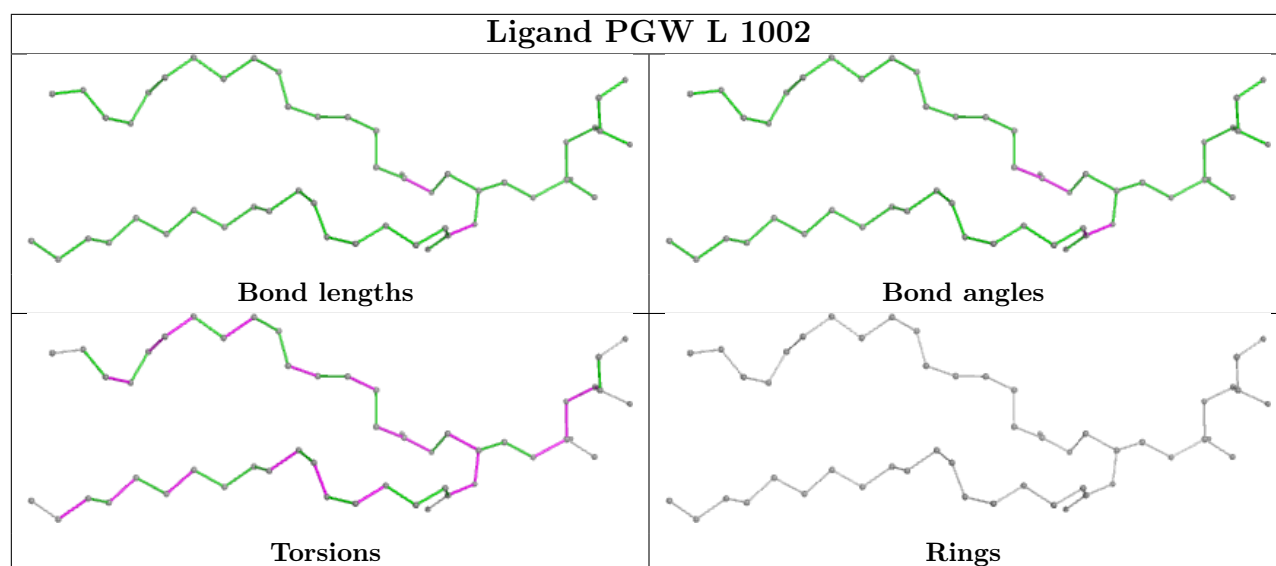
2 monomers are involved in 2 short contacts:

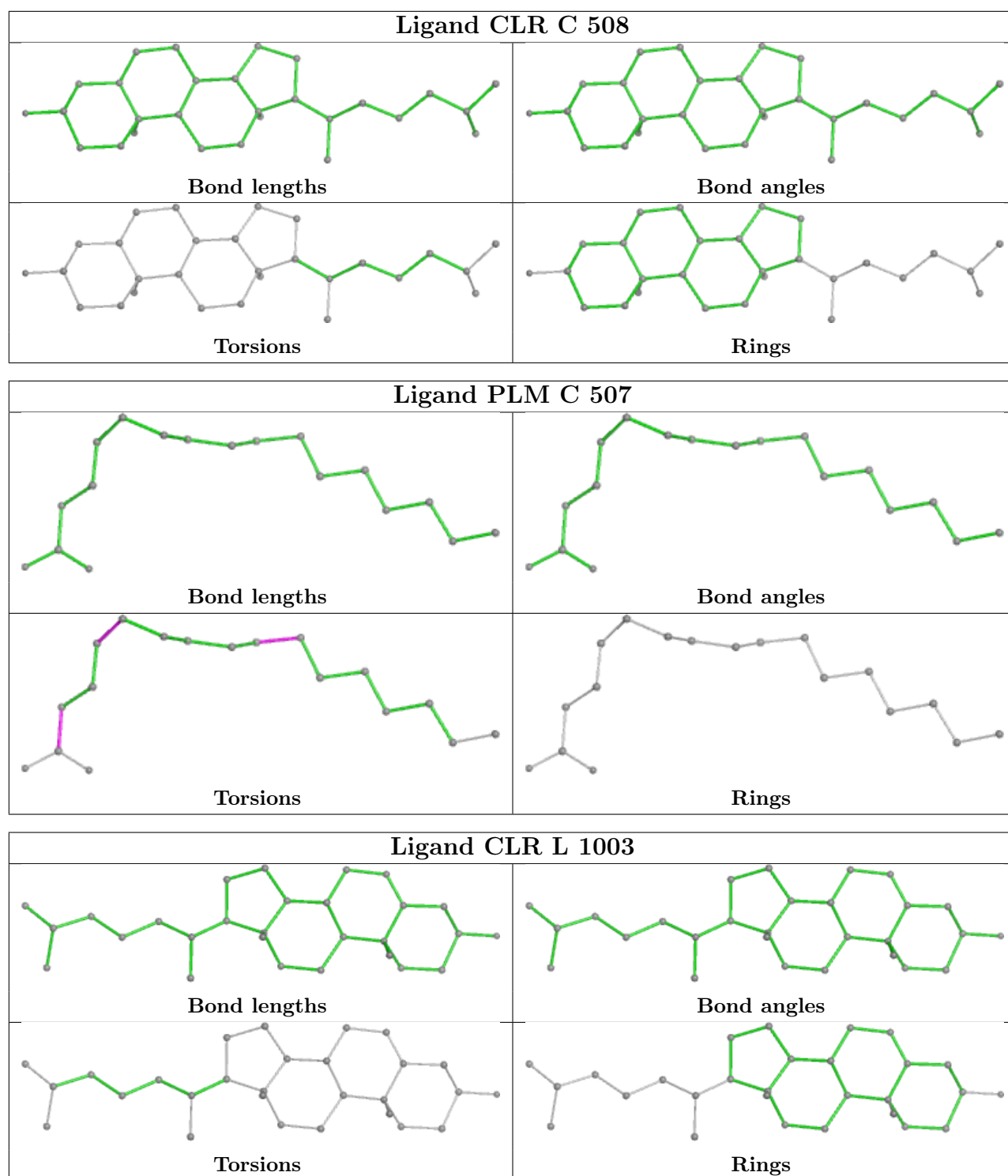
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	502	NAG	1	0
12	L	1001	D10	1	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

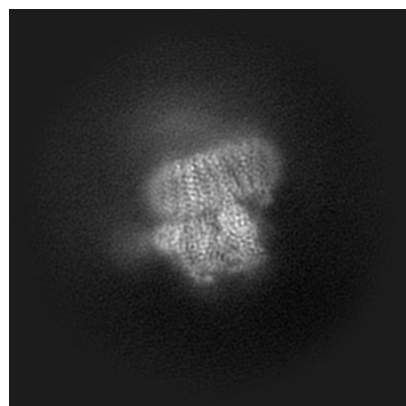
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50282. These allow visual inspection of the internal detail of the map and identification of artifacts.

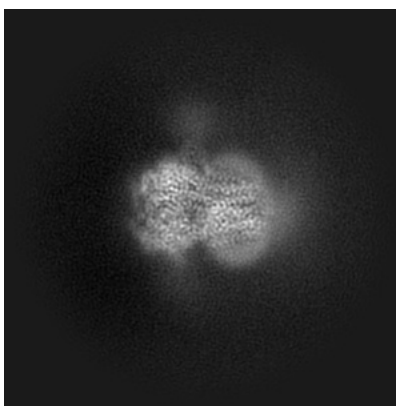
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

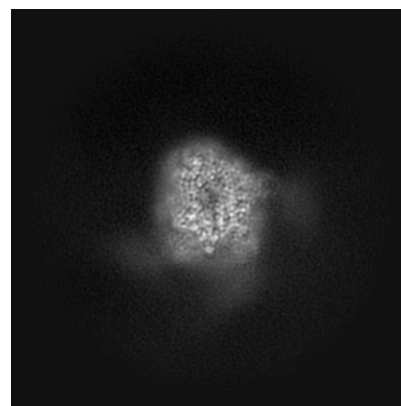
6.1.1 Primary map



X

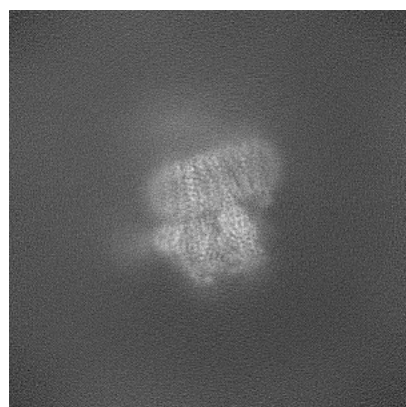


Y

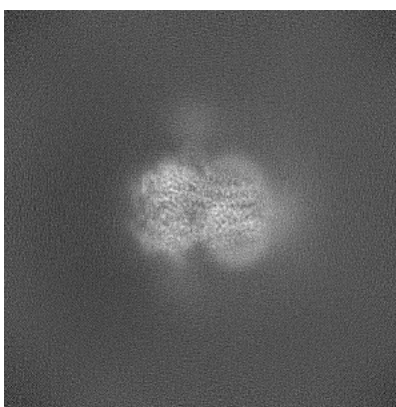


Z

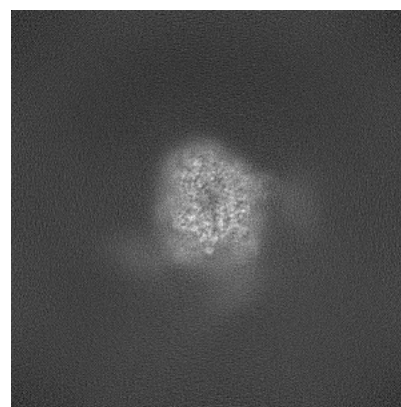
6.1.2 Raw map



X



Y

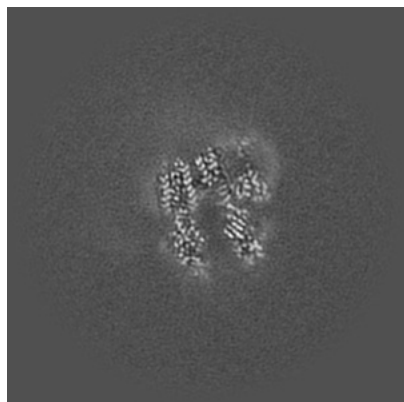


Z

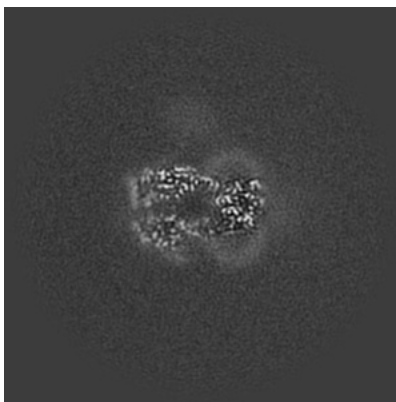
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

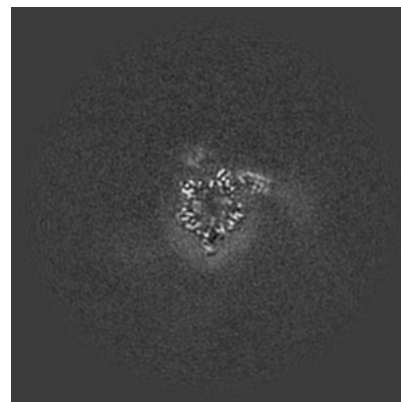
6.2.1 Primary map



X Index: 232

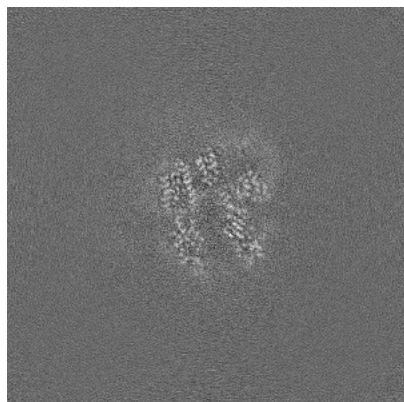


Y Index: 232

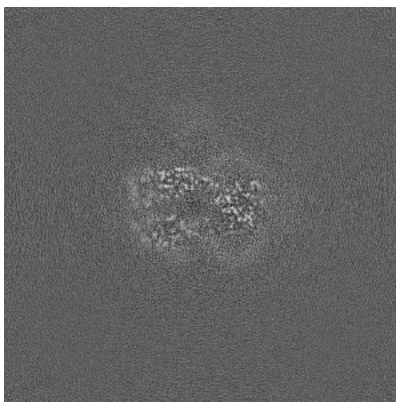


Z Index: 232

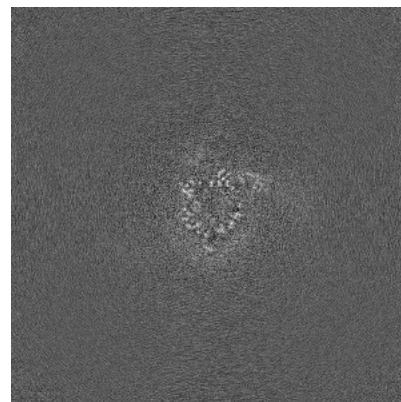
6.2.2 Raw map



X Index: 232



Y Index: 232

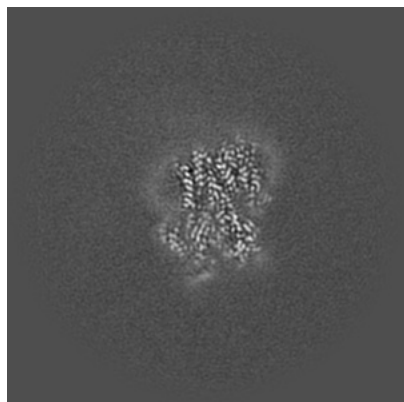


Z Index: 232

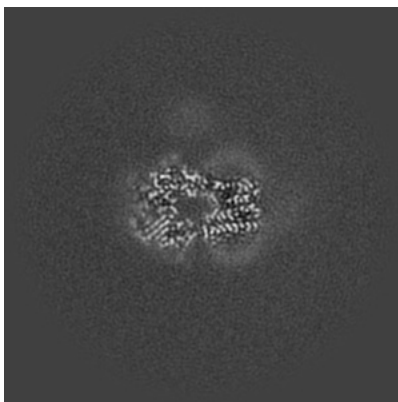
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

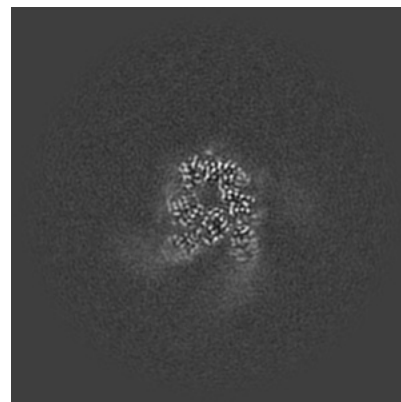
6.3.1 Primary map



X Index: 211

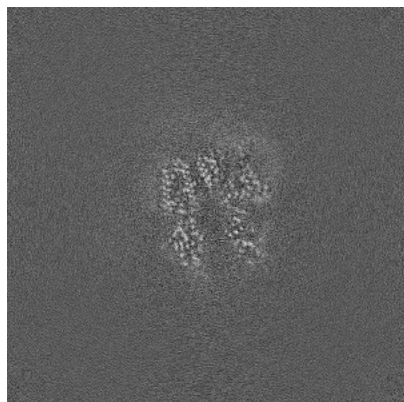


Y Index: 224

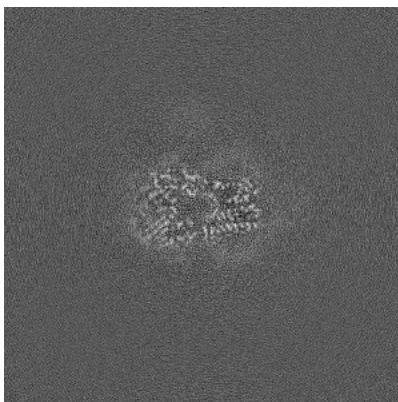


Z Index: 195

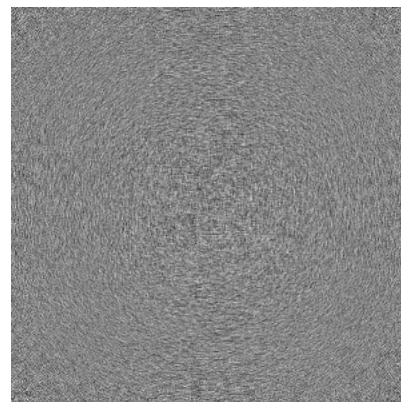
6.3.2 Raw map



X Index: 230



Y Index: 224

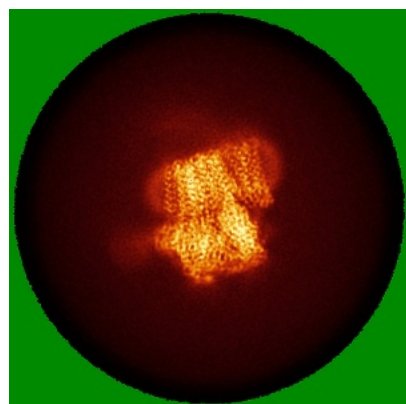


Z Index: 0

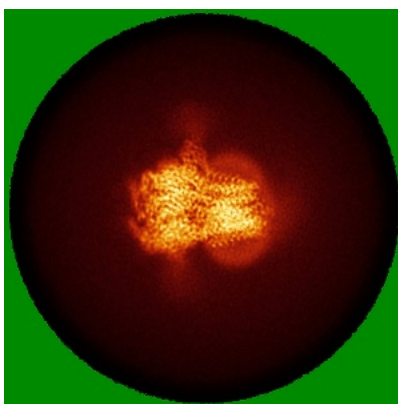
The images above show the largest variance slices of the map in three orthogonal directions.

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

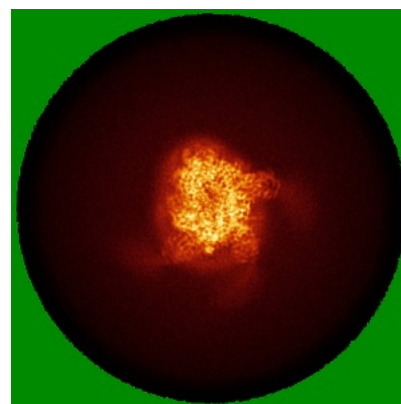
6.4.1 Primary map



X

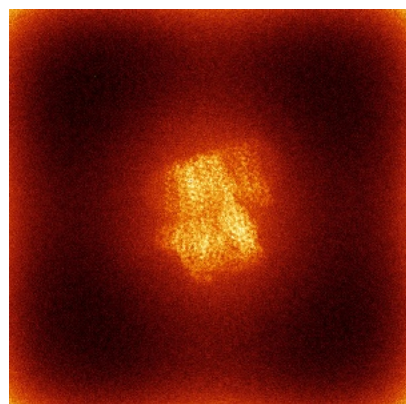


Y

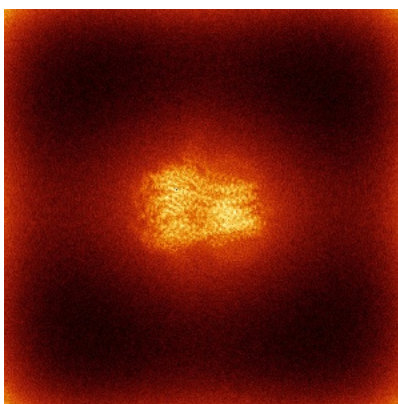


Z

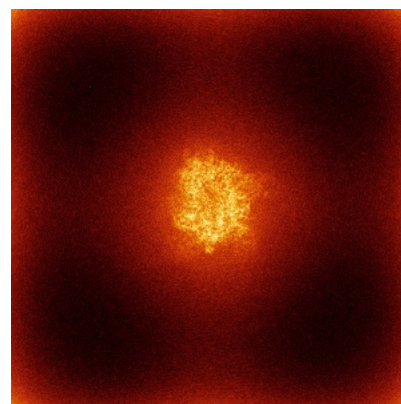
6.4.2 Raw map



X



Y

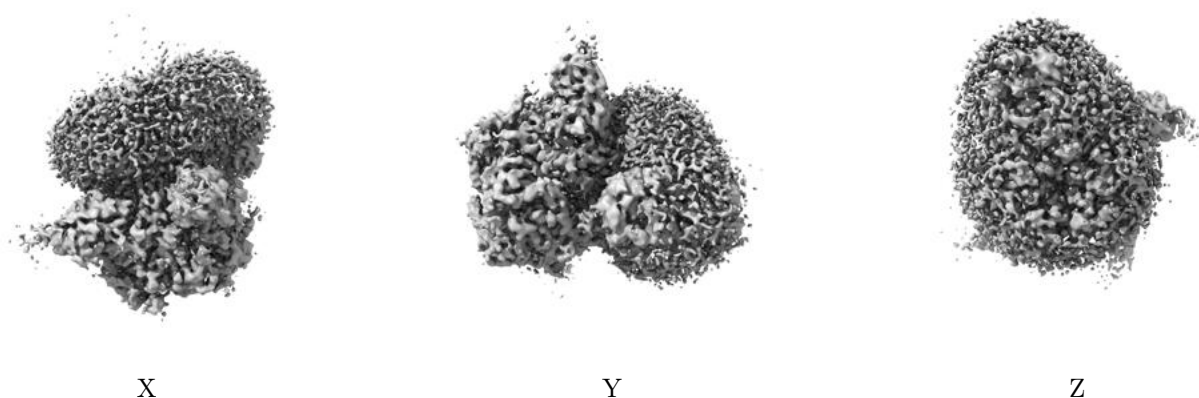


Z

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.

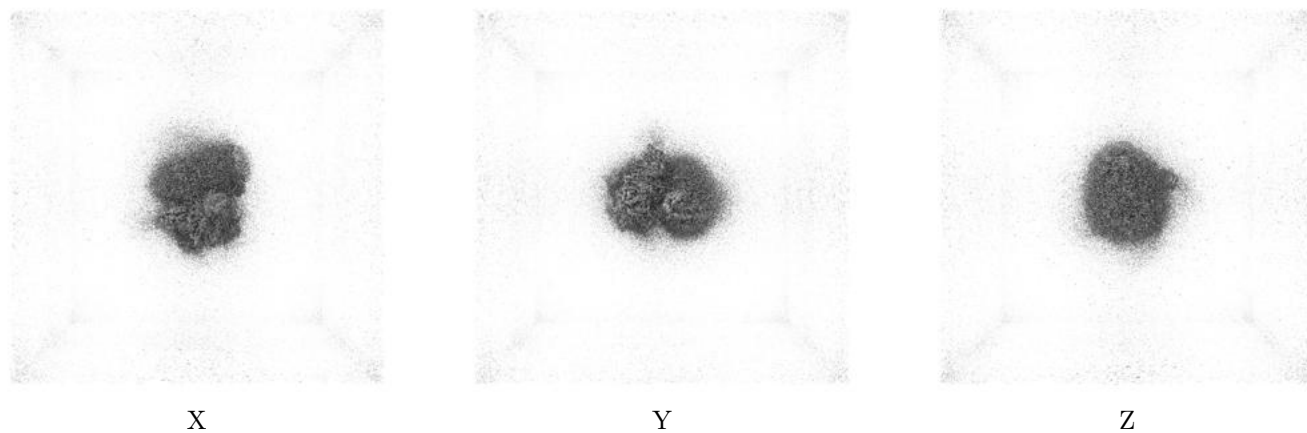
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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



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.

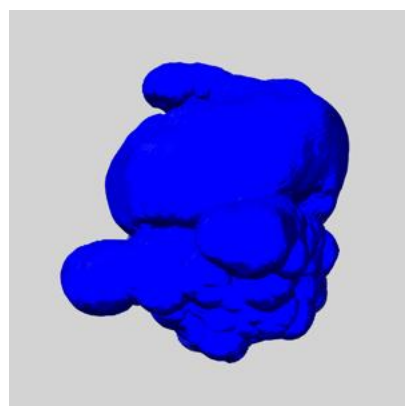
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

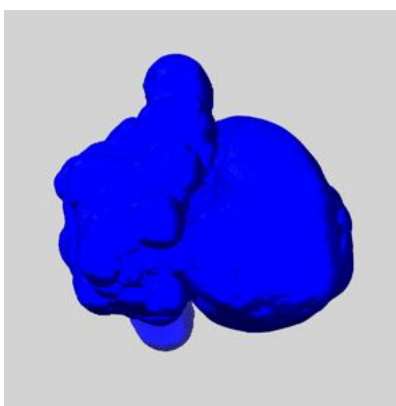
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

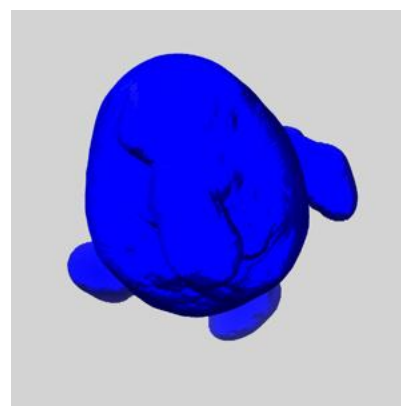
6.6.1 emd_50282_msk_1.map [i](#)



X



Y

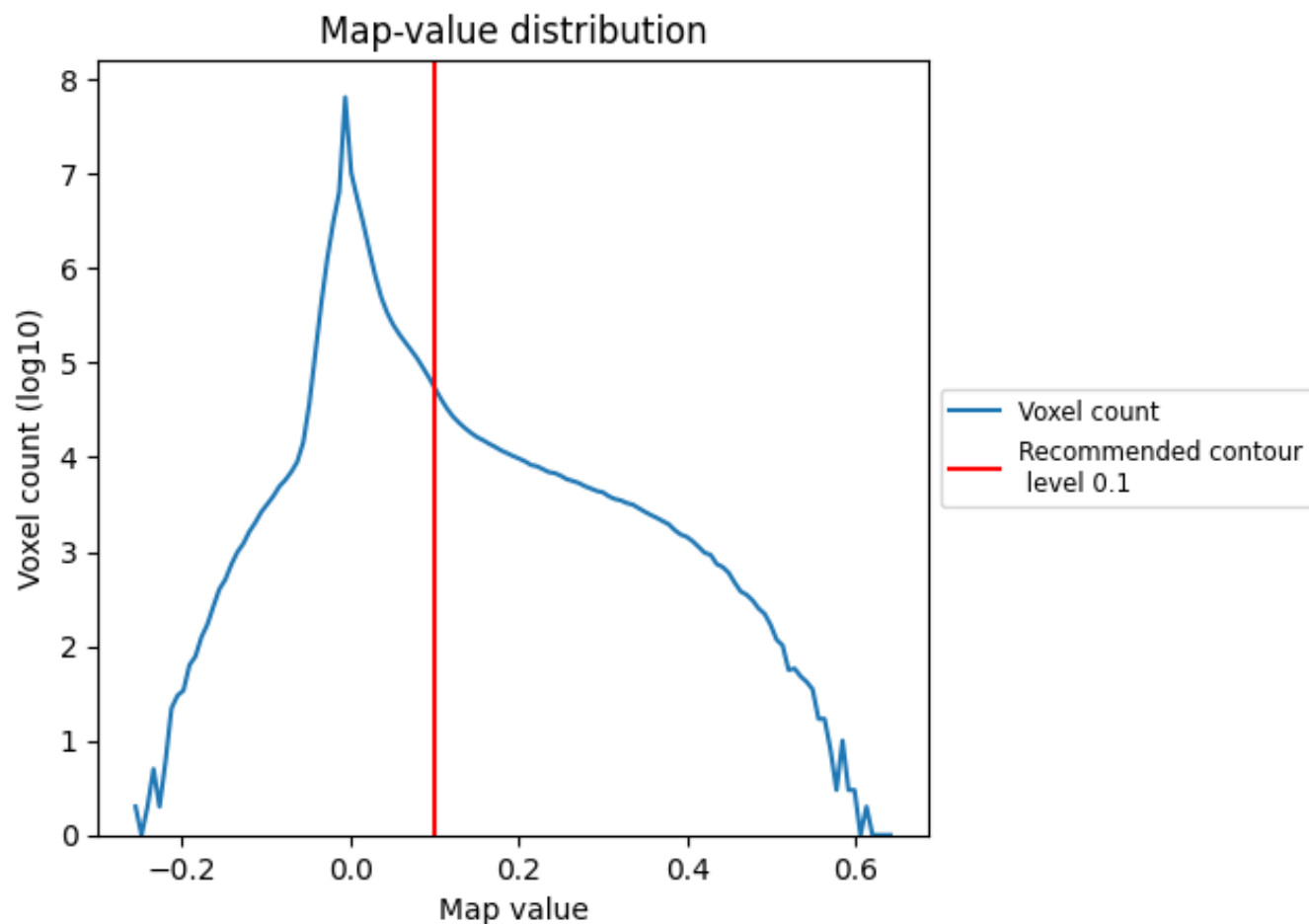


Z

7 Map analysis [i](#)

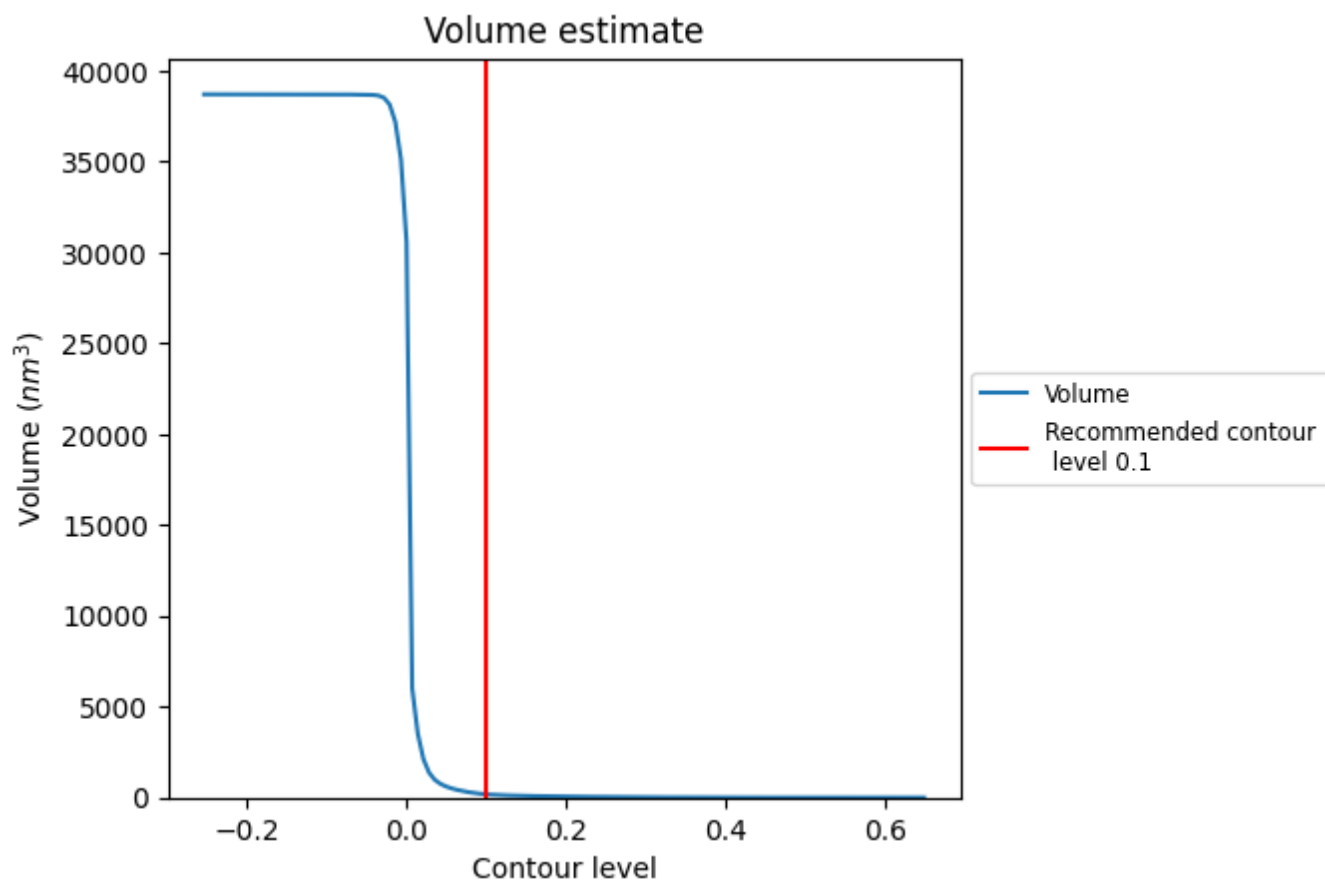
This section contains the results of statistical analysis of the map.

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.

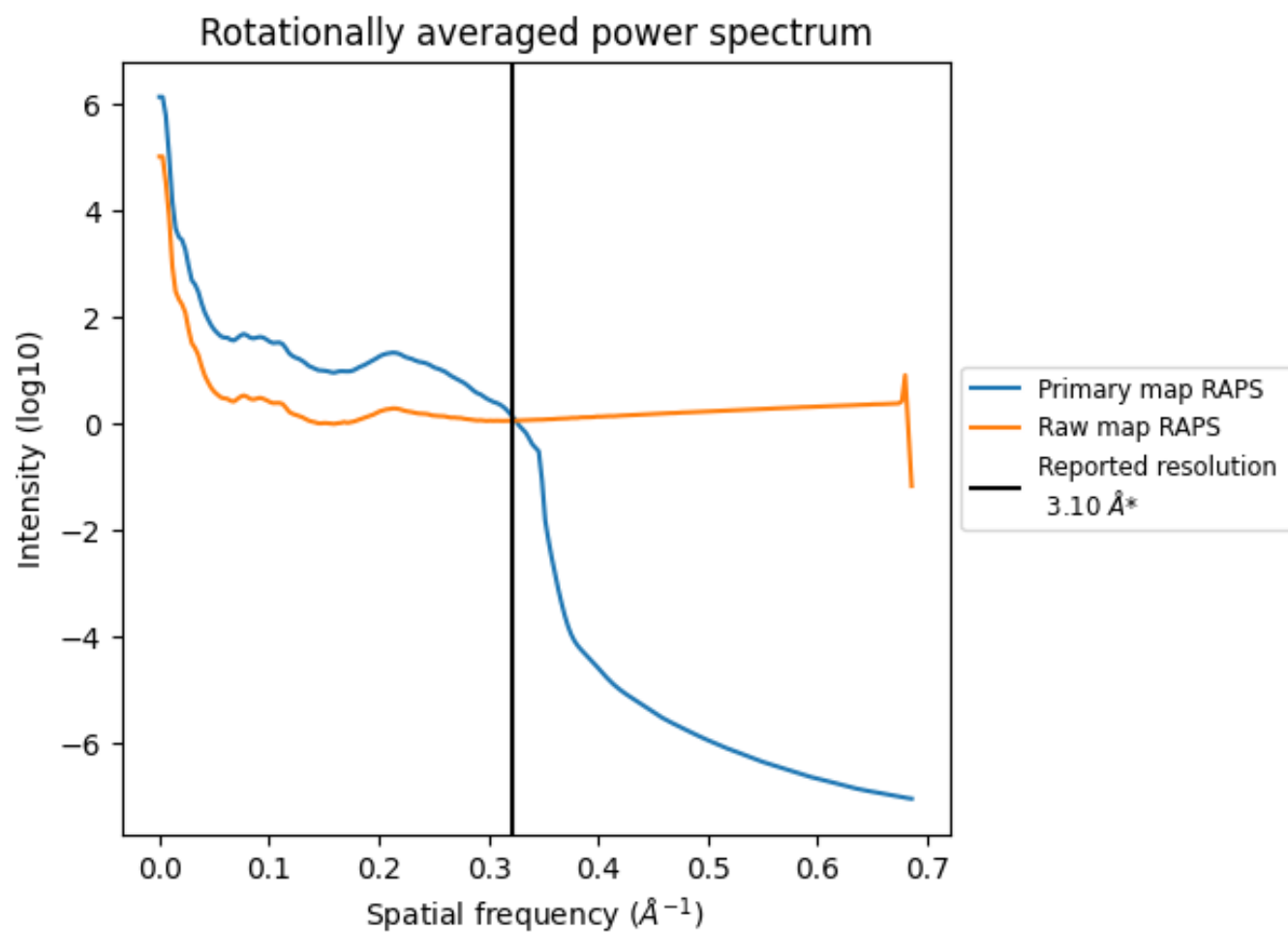
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 179 nm^3 ; this corresponds to an approximate mass of 162 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 ⓘ

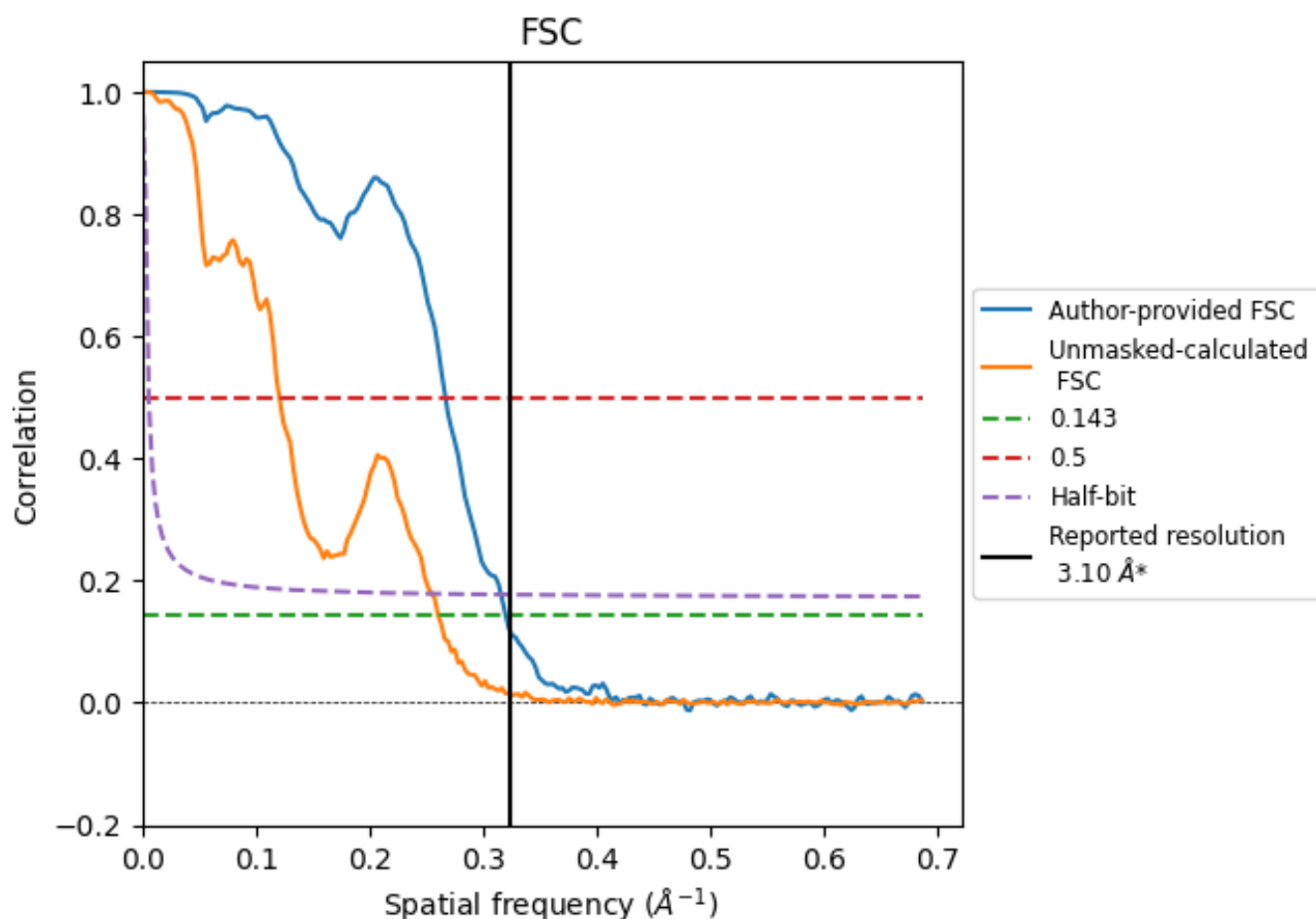


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

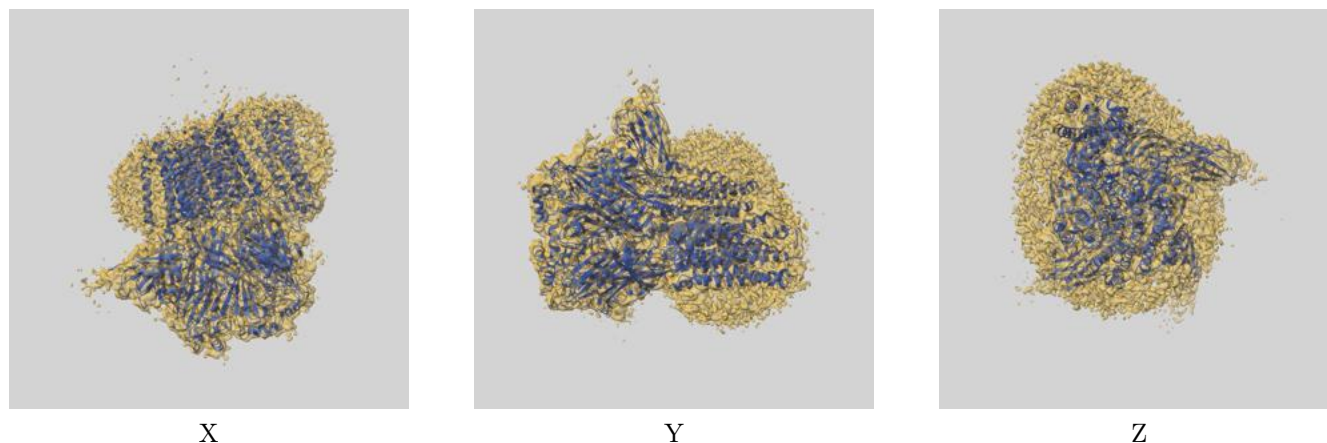
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.13	3.75	3.17
Unmasked-calculated*	3.84	8.29	3.93

*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 3.84 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

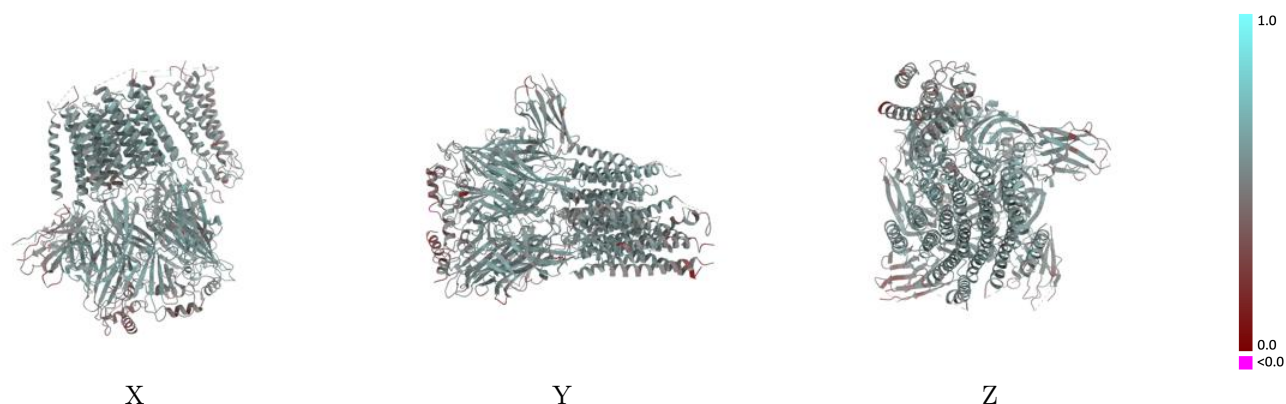
This section contains information regarding the fit between EMDB map EMD-50282 and PDB model 9FAU. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



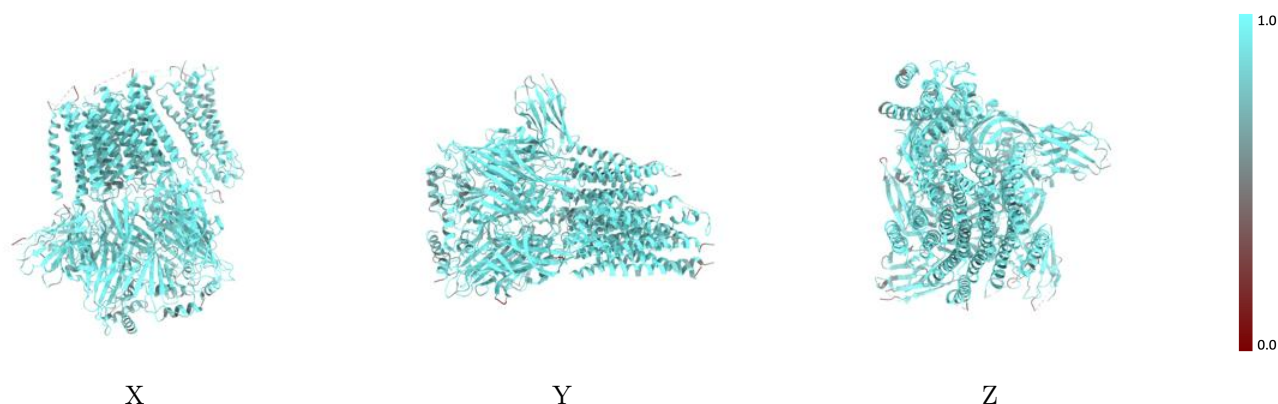
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



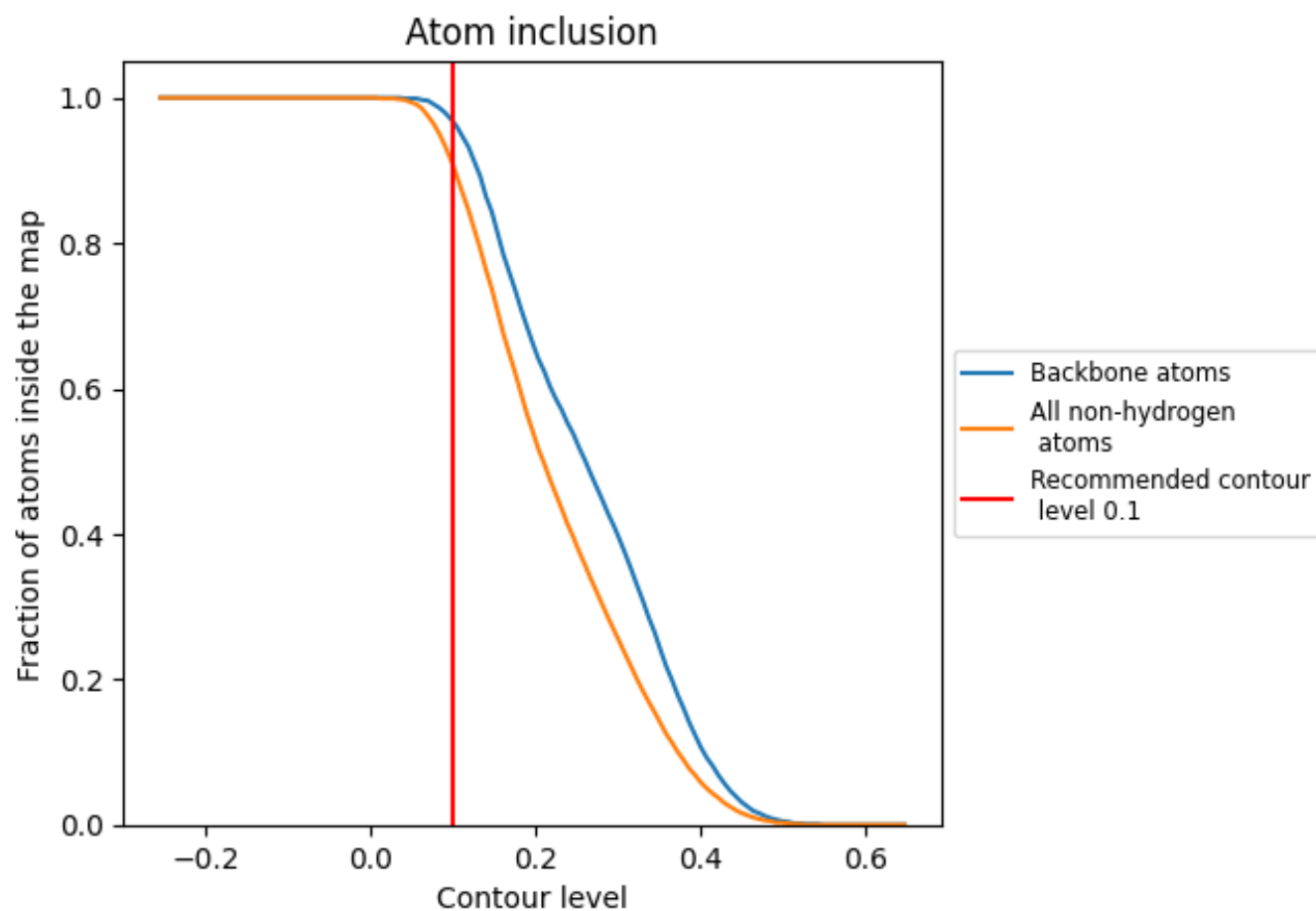
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9090	 0.5270
A	 0.9160	 0.5420
B	 0.9470	 0.5640
C	 0.9200	 0.5420
D	 0.9090	 0.5290
E	 0.9240	 0.5310
F	 0.8860	 0.5130
G	 0.9040	 0.4920
H	 0.8280	 0.4540
I	 0.6410	 0.4400
J	 0.7860	 0.4680
K	 0.8670	 0.4870
L	 0.8870	 0.5040
M	 1.0000	 0.5530
N	 0.9860	 0.5340
O	 0.8240	 0.4430
P	 0.7690	 0.3860
Q	 0.8210	 0.3980
R	 0.8030	 0.5110

