



## wwPDB EM Validation Summary Report ⓘ

Nov 7, 2022 – 09:11 AM JST

PDB ID : 5GJV  
EMDB ID : EMD-9513  
Title : Structure of the mammalian voltage-gated calcium channel Cav1.1 complex at near atomic resolution  
Authors : Wu, J.P.; Yan, Z.; Li, Z.Q.; Zhou, Q.; Yan, N.  
Deposited on : 2016-07-02  
Resolution : 3.60 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

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

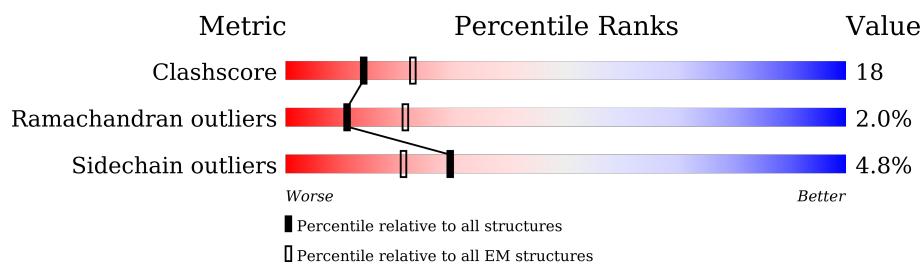
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1873	<div> <div>27%</div> <div>48% 17% 32%</div> </div>
2	B	106	<div> <div>94%</div> <div>88% 5% 6%</div> </div>
3	C	199	<div> <div>89%</div> <div>82% 7% 11%</div> </div>
4	E	222	<div> <div>52%</div> <div>62% 9% 25%</div> </div>
5	F	1106	<div> <div>12%</div> <div>55% 24% 6% 15%</div> </div>
6	D	2	<div> <div>100%</div> <div>50% 50%</div> </div>
6	G	2	<div> <div>100%</div> <div>100%</div> </div>
6	J	2	<div> <div>50%</div> <div>50% 50%</div> </div>

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Mol	Chain	Length	Quality of chain
6	K	2	 50% 100%
7	H	3	 33% 67% 67%
7	I	3	 67% 33%
8	L	3	 33% 67% 67%

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 21904 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 Voltage-dependent L-type calcium channel subunit alpha-1S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1276	Total	C	N	O	S	4	0
			10183	6699	1673	1742	69		

- Molecule 2 is a protein called Voltage-dependent L-type calcium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	100	Total	C	N	O	S	0	0
			710	455	125	129	1		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	69	SER	-	expression tag	UNP P19517
B	70	LEU	-	expression tag	UNP P19517
B	71	GLU	-	expression tag	UNP P19517
B	72	VAL	-	expression tag	UNP P19517
B	73	LEU	-	expression tag	UNP P19517
B	74	PHE	-	expression tag	UNP P19517
B	75	GLN	-	expression tag	UNP P19517
B	76	GLY	-	expression tag	UNP P19517
B	77	PRO	-	expression tag	UNP P19517
B	78	HIS	-	expression tag	UNP P19517
B	79	MET	-	expression tag	UNP P19517

- Molecule 3 is a protein called Voltage-dependent L-type calcium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	178	Total	C	N	O	S	0	0
			1367	876	232	254	5		

- Molecule 4 is a protein called Voltage-dependent calcium channel gamma-1 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	166	Total	C	N	O	S	0	0
			1304	860	213	213	18		

- Molecule 5 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	942	Total	C	N	O	S	1	0
			7567	4809	1277	1451	30		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	1075	ETA	GLY	conflict	UNP P13806

- 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	D	2	Total	C	N	O	0	0
			28	16	2	10		
6	G	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-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



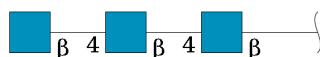
Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	3	Total	C	N	O	0	0
			39	22	2	15		

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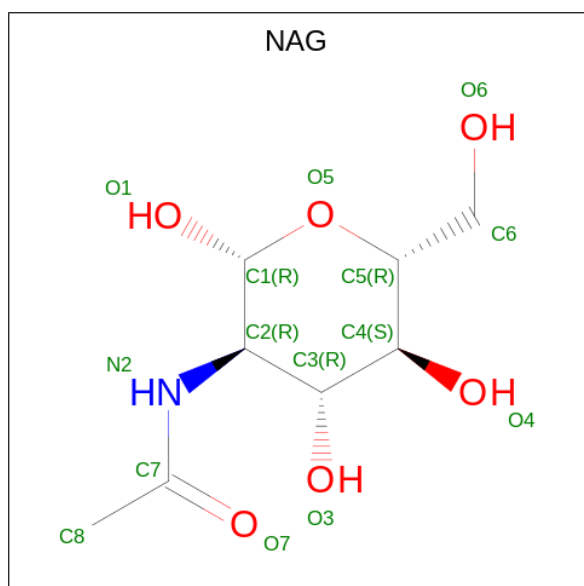
Mol	Chain	Residues	Atoms				AltConf	Trace
7	I	3	Total	C	N	O	0	0
			39	22	2	15		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
8	L	3	Total	C	N	O	0	0
			42	24	3	15		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



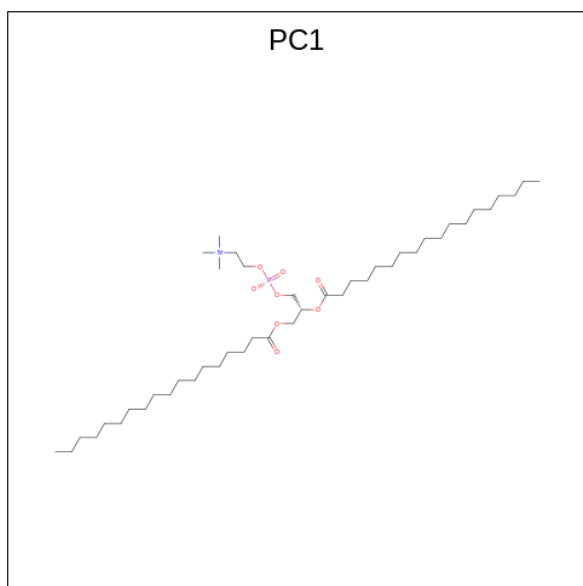
Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	F	1	Total	C	N	O	0
			98	56	7	35	
9	F	1	Total	C	N	O	0
			98	56	7	35	
9	F	1	Total	C	N	O	0
			98	56	7	35	

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Mol	Chain	Residues	Atoms				AltConf
9	F	1	Total	C	N	O	0
			98	56	7	35	
9	F	1	Total	C	N	O	0
			98	56	7	35	
9	F	1	Total	C	N	O	0
			98	56	7	35	
9	F	1	Total	C	N	O	0
			98	56	7	35	

- Molecule 10 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	O	P	0
			426	356	7	56	7	
10	A	1	Total	C	N	O	P	0
			426	356	7	56	7	
10	A	1	Total	C	N	O	P	0
			426	356	7	56	7	
10	A	1	Total	C	N	O	P	0
			426	356	7	56	7	
10	A	1	Total	C	N	O	P	0
			426	356	7	56	7	
10	A	1	Total	C	N	O	P	0
			426	356	7	56	7	

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Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	O	P	0
			426	356	7	56	7	
10	A	1	Total	C	N	O	P	0
			426	356	7	56	7	
10	A	1	Total	C	N	O	P	0
			426	356	7	56	7	
10	A	1	Total	C	N	O	P	0
			426	356	7	56	7	
10	A	1	Total	C	N	O	P	0
			426	356	7	56	7	
10	A	1	Total	C	N	O	P	0
			426	356	7	56	7	

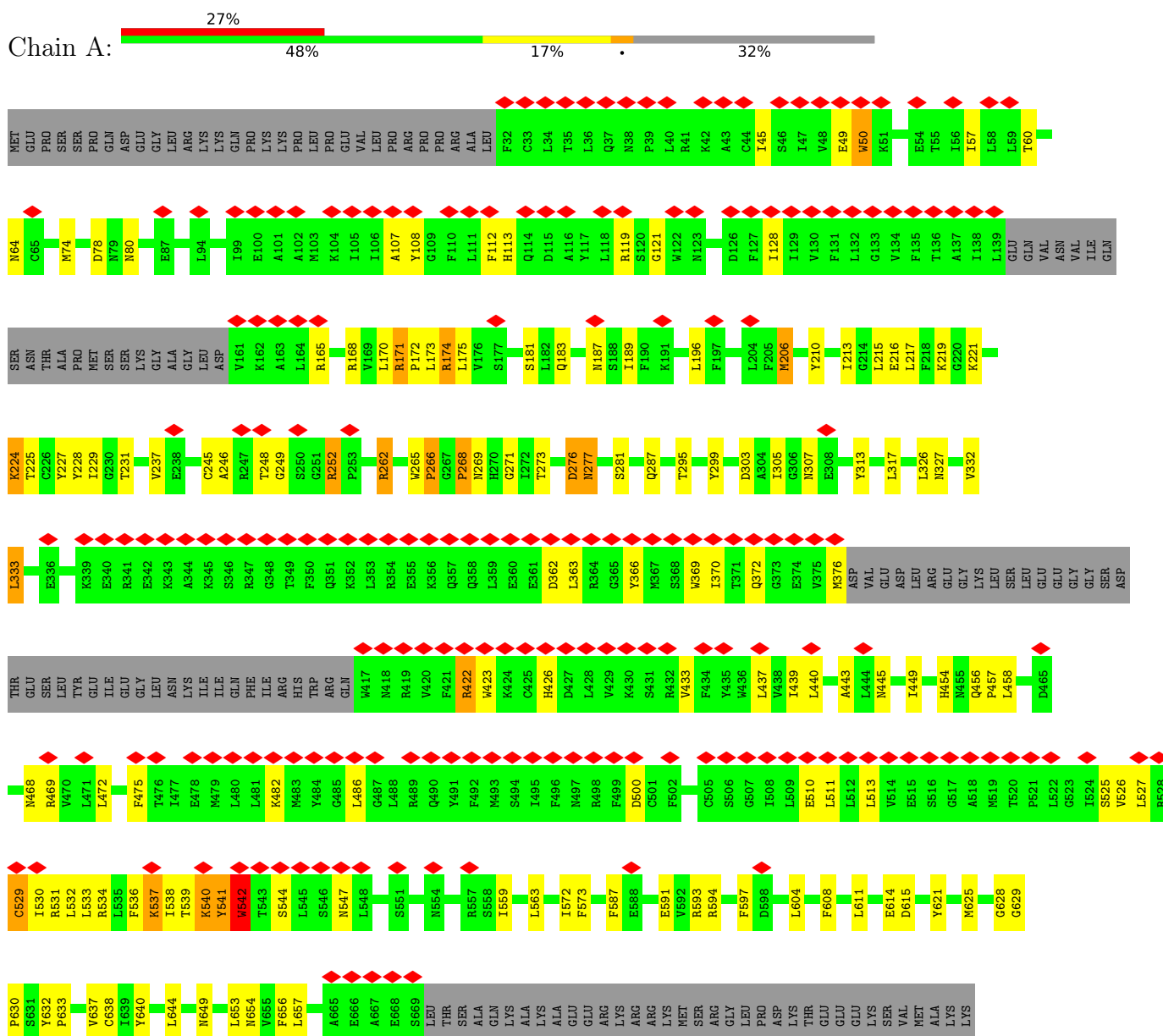
- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
11	A	2	Total	Ca	0
			2	2	
11	F	1	Total	Ca	0
			1	1	

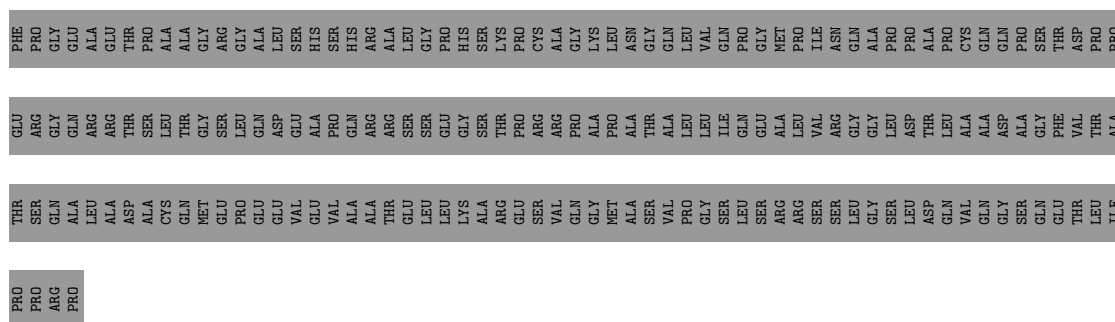
### 3 Residue-property plots

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.

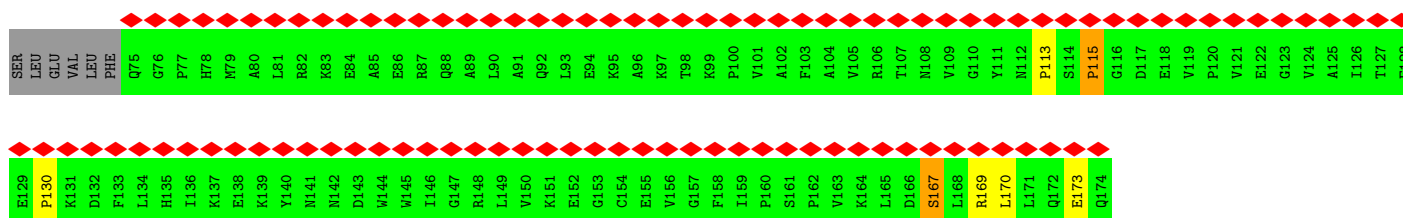
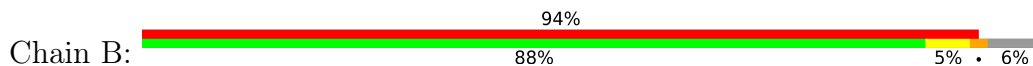
- Molecule 1: Voltage-dependent L-type calcium channel subunit alpha-1S



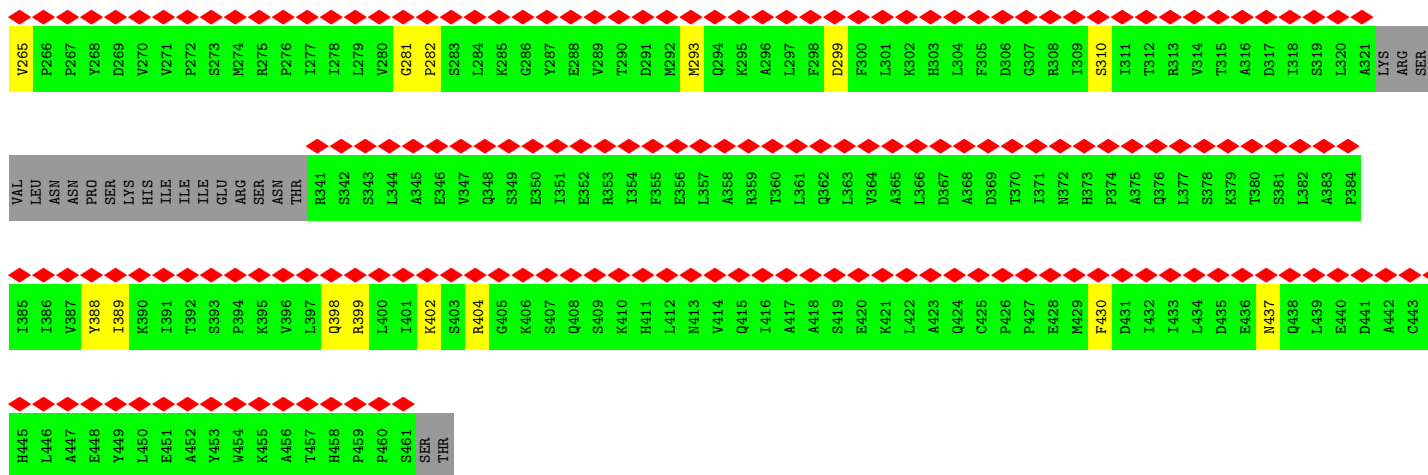
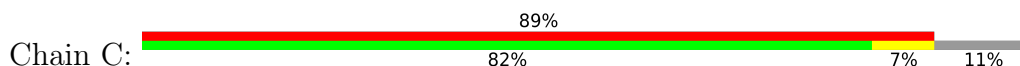
[illegible]



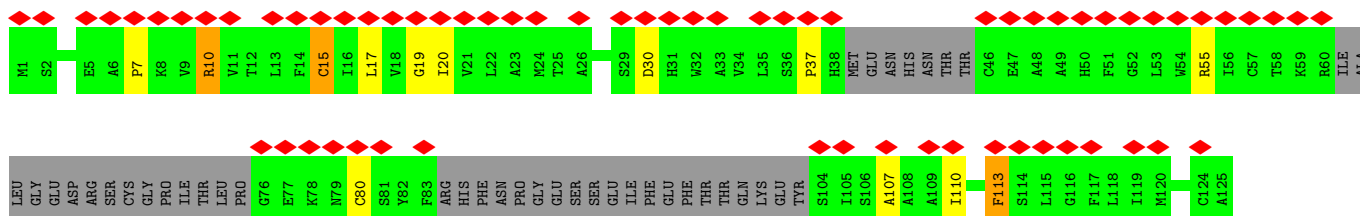
- Molecule 2: Voltage-dependent L-type calcium channel subunit beta-1

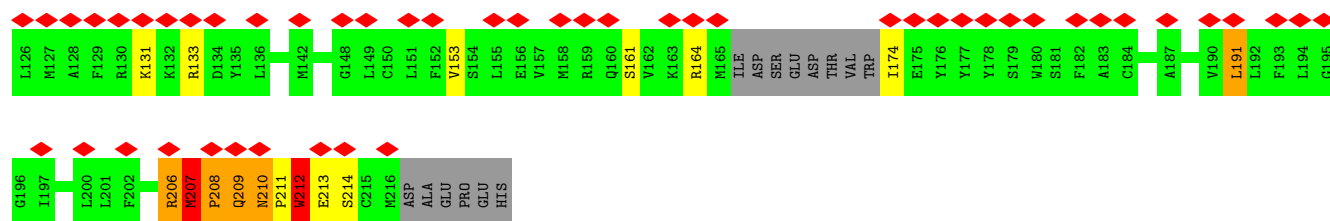


- Molecule 3: Voltage-dependent L-type calcium channel subunit beta-1

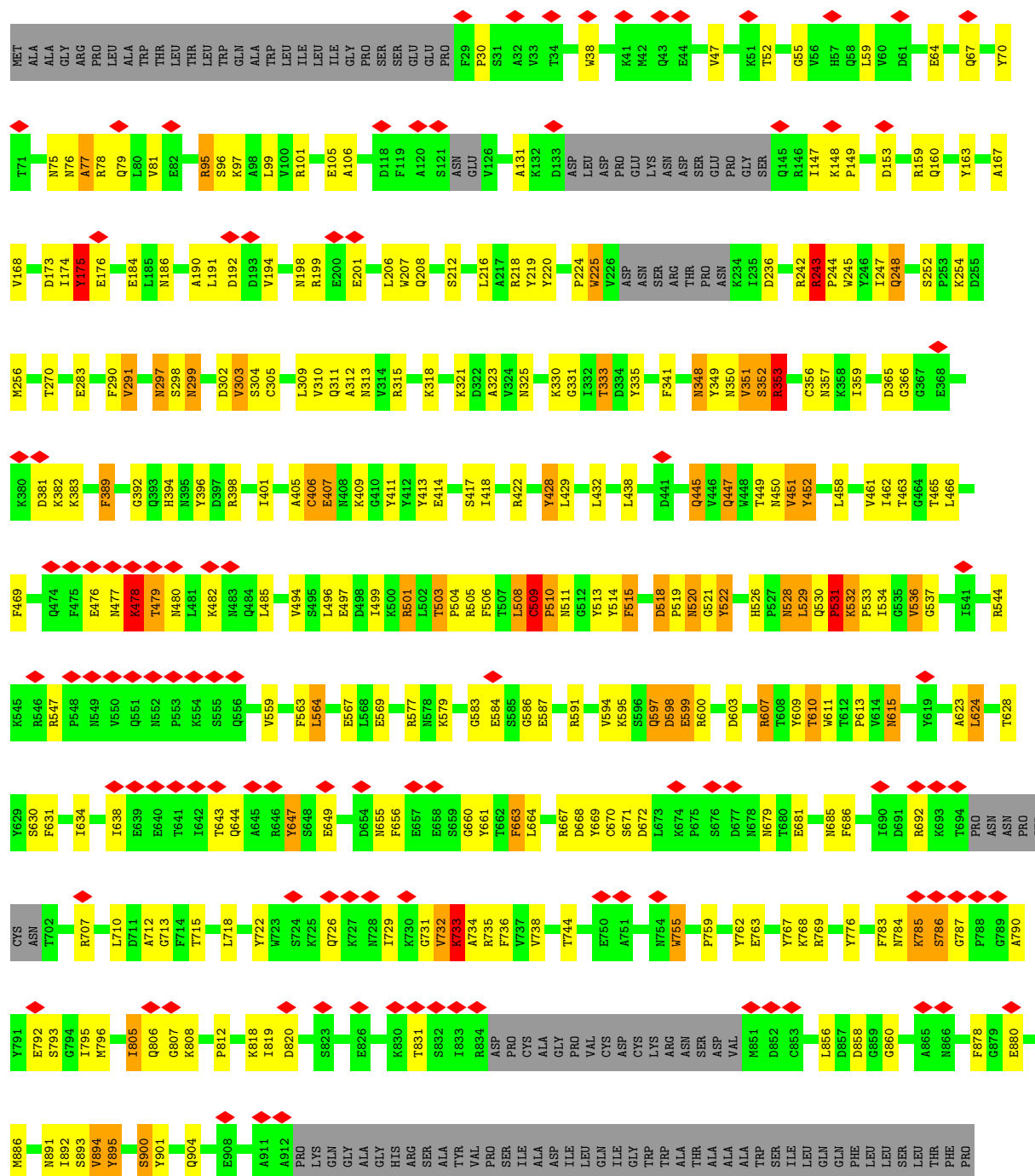


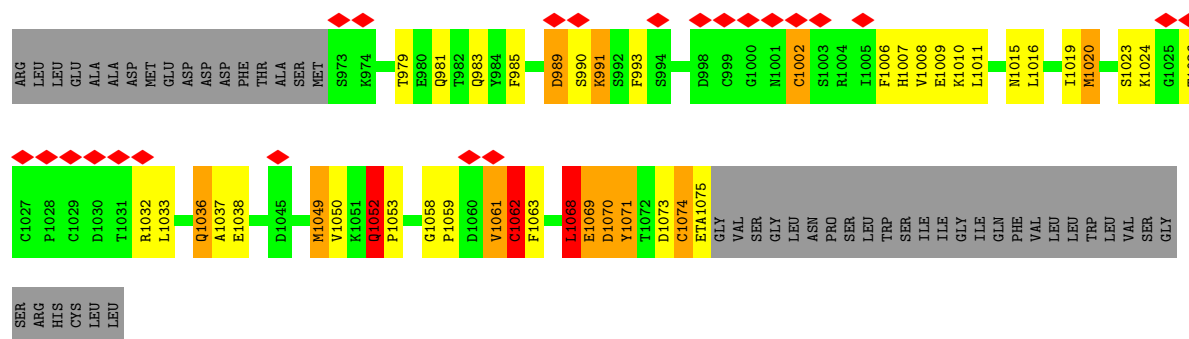
- Molecule 4: Voltage-dependent calcium channel gamma-1 subunit





• Molecule 5: Voltage-dependent calcium channel subunit alpha-2/delta-1





- 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



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





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



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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	527833	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1.3	Depositor
Maximum defocus (nm)	2.9	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.294	Depositor
Minimum map value	-0.187	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.044	Depositor
Map size (Å)	337.92, 337.92, 337.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	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: CA, NAG, PC1, BMA, ETA

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	0.56	2/10431 (0.0%)	0.73	24/14157 (0.2%)
2	B	0.43	1/723 (0.1%)	0.65	3/979 (0.3%)
3	C	0.34	0/1394	0.50	0/1892
4	E	0.42	1/1336 (0.1%)	0.58	2/1802 (0.1%)
5	F	0.68	13/7721 (0.2%)	0.85	32/10463 (0.3%)
All	All	0.58	17/21605 (0.1%)	0.76	61/29293 (0.2%)

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	11
3	C	0	2
5	F	0	14
All	All	0	27

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171	ARG	C-O	13.19	1.48	1.23
5	F	647	TYR	C-N	10.24	1.57	1.34
5	F	312	ALA	C-O	7.40	1.37	1.23
2	B	167	SER	CB-OG	6.12	1.50	1.42
5	F	526	HIS	C-N	-6.02	1.22	1.34

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	518	ASP	CB-CA-C	-10.92	88.55	110.40
5	F	469	PHE	CB-CA-C	-9.64	91.12	110.40
5	F	445	GLN	CB-CA-C	9.59	129.57	110.40
1	A	1174	ALA	CB-CA-C	-8.28	97.69	110.10
5	F	175	TYR	N-CA-C	8.25	133.27	111.00

There are no chirality outliers.

5 of 27 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	228	TYR	Peptide
1	A	229	ILE	Peptide
1	A	237	VAL	Peptide
1	A	266	PRO	Peptide
1	A	268	PRO	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	10183	0	10143	394	0
2	B	710	0	633	1	0
3	C	1367	0	1343	9	0
4	E	1304	0	1330	66	0
5	F	7567	0	7404	316	0
6	D	28	0	25	0	0
6	G	28	0	25	5	0
6	J	28	0	25	1	0
6	K	28	0	25	0	0
7	H	39	0	34	0	0
7	I	39	0	34	0	0
8	L	42	0	37	0	0
9	A	14	0	13	0	0
9	F	98	0	91	0	0
10	A	426	0	675	20	0
11	A	2	0	0	0	0
11	F	1	0	0	0	0
All	All	21904	0	21837	768	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 18.

The worst 5 of 768 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:A:1389:ARG:HD2	1:A:1391:TRP:CE3	1.43	1.51
5:F:669:TYR:HD1	5:F:670:CYS:N	1.28	1.29
4:E:208:PRO:CG	4:E:214:SER:HA	1.64	1.26
1:A:1203:ASP:OD2	1:A:1229:ARG:HD2	1.15	1.24
1:A:1389:ARG:HB2	1:A:1391:TRP:CZ3	1.71	1.24

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	1268/1873 (68%)	1103 (87%)	143 (11%)	22 (2%)	9	45
2	B	98/106 (92%)	90 (92%)	8 (8%)	0	100	100
3	C	174/199 (87%)	171 (98%)	3 (2%)	0	100	100
4	E	156/222 (70%)	142 (91%)	12 (8%)	2 (1%)	12	50
5	F	929/1106 (84%)	764 (82%)	137 (15%)	28 (3%)	4	33
All	All	2625/3506 (75%)	2270 (86%)	303 (12%)	52 (2%)	11	41

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	TRP
1	A	977	ASP
1	A	1174	ALA
1	A	1391	TRP
1	A	1441	HIS

### 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	1073/1628 (66%)	1020 (95%)	53 (5%)	25	59
2	B	59/91 (65%)	56 (95%)	3 (5%)	24	58
3	C	143/179 (80%)	141 (99%)	2 (1%)	67	85
4	E	141/192 (73%)	134 (95%)	7 (5%)	24	59
5	F	837/974 (86%)	793 (95%)	44 (5%)	22	58
All	All	2253/3064 (74%)	2144 (95%)	109 (5%)	29	60

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	310	SER
5	F	299	ASN
5	F	991	LYS
4	E	15	CYS
5	F	95	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1311	GLN
5	F	685	ASN
5	F	76	ASN
5	F	1052	GLN
5	F	556	GLN

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	ETA	F	1075	5	3,3,3	0.43	0	2,2,2	0.53	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
5	ETA	F	1075	5	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	1075	ETA	N-CA-CB-O

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1075	ETA	1	0

## 5.5 Carbohydrates ⓘ

17 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	D	1	6,5	14,14,15	0.61	1 (7%)	17,19,21	0.92	1 (5%)
6	NAG	D	2	6	14,14,15	0.47	0	17,19,21	0.42	0
6	NAG	G	1	6,5	14,14,15	0.30	0	17,19,21	0.61	0
6	NAG	G	2	6	14,14,15	0.30	0	17,19,21	0.61	0
7	NAG	H	1	7,5	14,14,15	0.65	1 (7%)	17,19,21	0.58	0
7	NAG	H	2	7	14,14,15	0.26	0	17,19,21	0.80	1 (5%)
7	BMA	H	3	7	11,11,12	0.87	0	15,15,17	0.81	0
7	NAG	I	1	7,5	14,14,15	0.31	0	17,19,21	0.77	0
7	NAG	I	2	7	14,14,15	0.31	0	17,19,21	0.57	0
7	BMA	I	3	7	11,11,12	0.61	0	15,15,17	0.93	2 (13%)
6	NAG	J	1	6,5	14,14,15	0.26	0	17,19,21	0.50	0
6	NAG	J	2	6	14,14,15	0.28	0	17,19,21	0.50	0
6	NAG	K	1	6,5	14,14,15	0.58	0	17,19,21	0.95	1 (5%)
6	NAG	K	2	6	14,14,15	0.58	0	17,19,21	1.02	1 (5%)
8	NAG	L	1	8,5	14,14,15	0.35	0	17,19,21	0.63	0
8	NAG	L	2	8	14,14,15	0.32	0	17,19,21	0.86	1 (5%)
8	NAG	L	3	8	14,14,15	0.43	0	17,19,21	0.67	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	D	1	6,5	-	3/6/23/26	0/1/1/1
6	NAG	D	2	6	-	2/6/23/26	0/1/1/1
6	NAG	G	1	6,5	-	2/6/23/26	0/1/1/1
6	NAG	G	2	6	-	4/6/23/26	0/1/1/1
7	NAG	H	1	7,5	-	2/6/23/26	0/1/1/1
7	NAG	H	2	7	-	2/6/23/26	0/1/1/1
7	BMA	H	3	7	-	0/2/19/22	0/1/1/1
7	NAG	I	1	7,5	-	2/6/23/26	0/1/1/1

*Continued on next page...*

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	I	2	7	-	2/6/23/26	0/1/1/1
7	BMA	I	3	7	-	2/2/19/22	0/1/1/1
6	NAG	J	1	6,5	-	1/6/23/26	0/1/1/1
6	NAG	J	2	6	-	2/6/23/26	0/1/1/1
6	NAG	K	1	6,5	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	3/6/23/26	0/1/1/1
8	NAG	L	1	8,5	-	1/6/23/26	0/1/1/1
8	NAG	L	2	8	-	2/6/23/26	0/1/1/1
8	NAG	L	3	8	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1	NAG	C1-C2	2.14	1.55	1.52
7	H	1	NAG	O5-C1	-2.02	1.40	1.43

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	1	NAG	C1-O5-C5	3.39	116.79	112.19
6	K	2	NAG	C2-N2-C7	3.03	127.21	122.90
8	L	2	NAG	C1-O5-C5	2.89	116.11	112.19
6	D	1	NAG	C2-N2-C7	2.77	126.85	122.90
7	H	2	NAG	C1-O5-C5	2.66	115.80	112.19

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

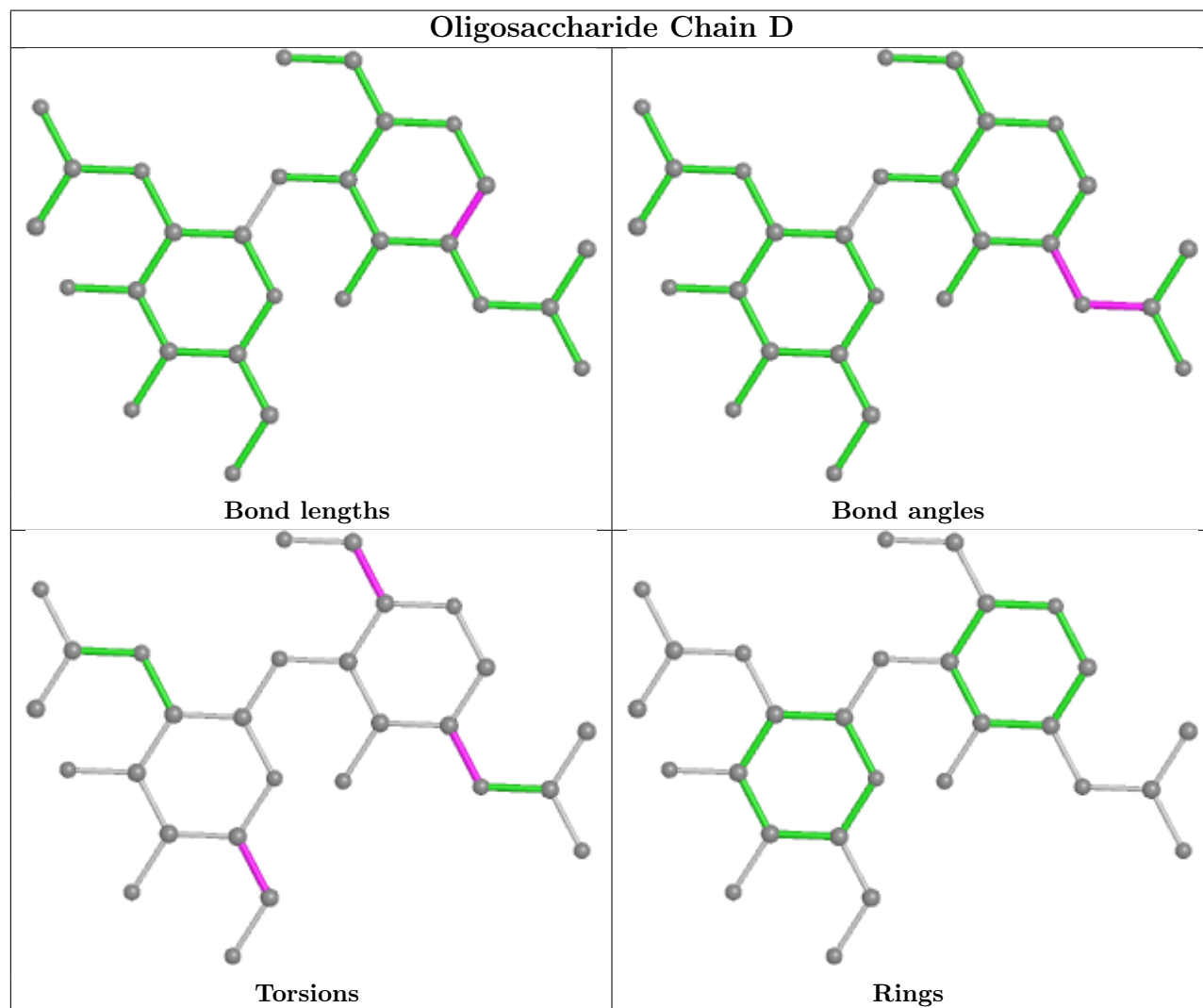
Mol	Chain	Res	Type	Atoms
8	L	2	NAG	O5-C5-C6-O6
8	L	3	NAG	O5-C5-C6-O6
7	I	3	BMA	O5-C5-C6-O6
7	I	3	BMA	C4-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6

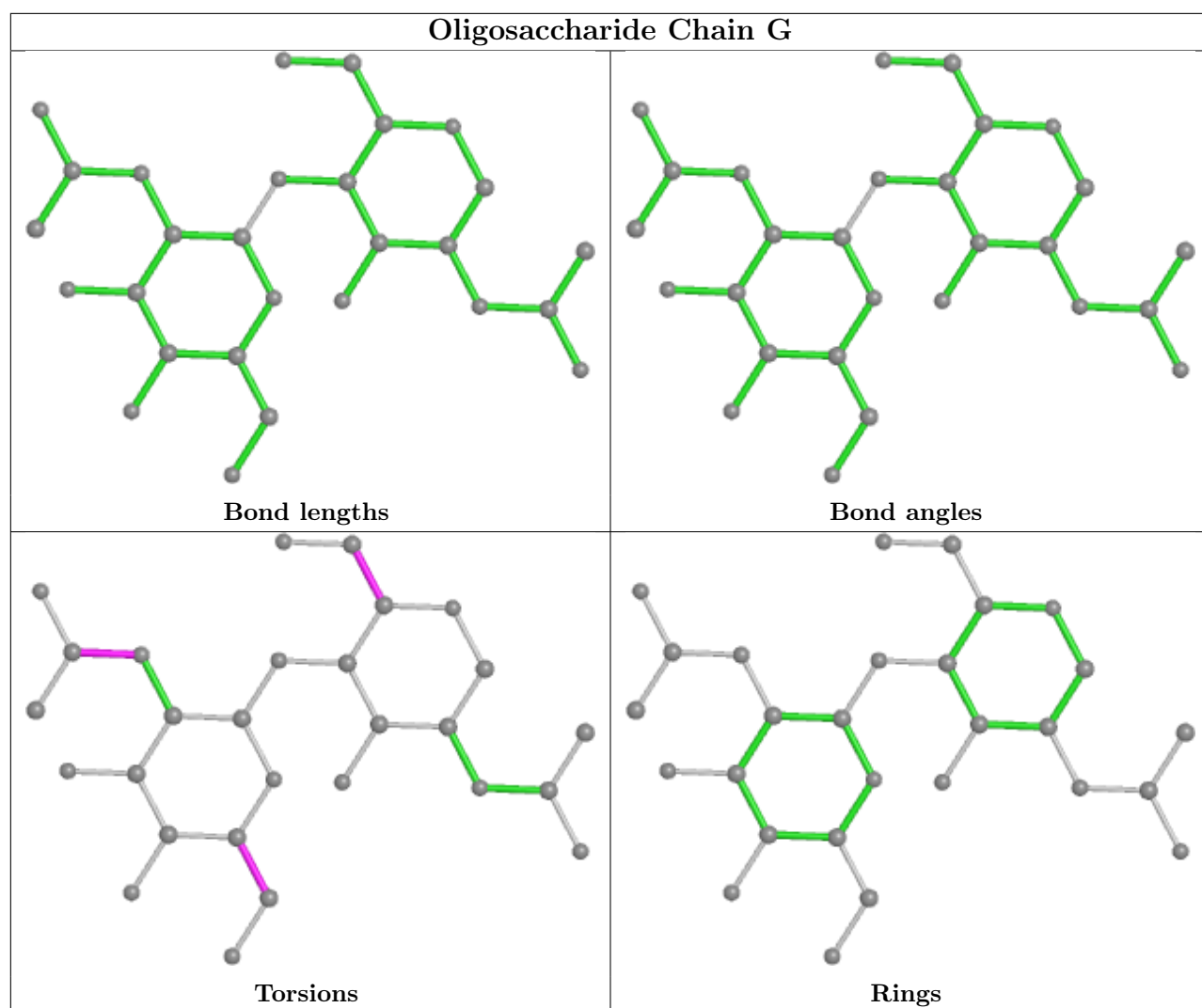
There are no ring outliers.

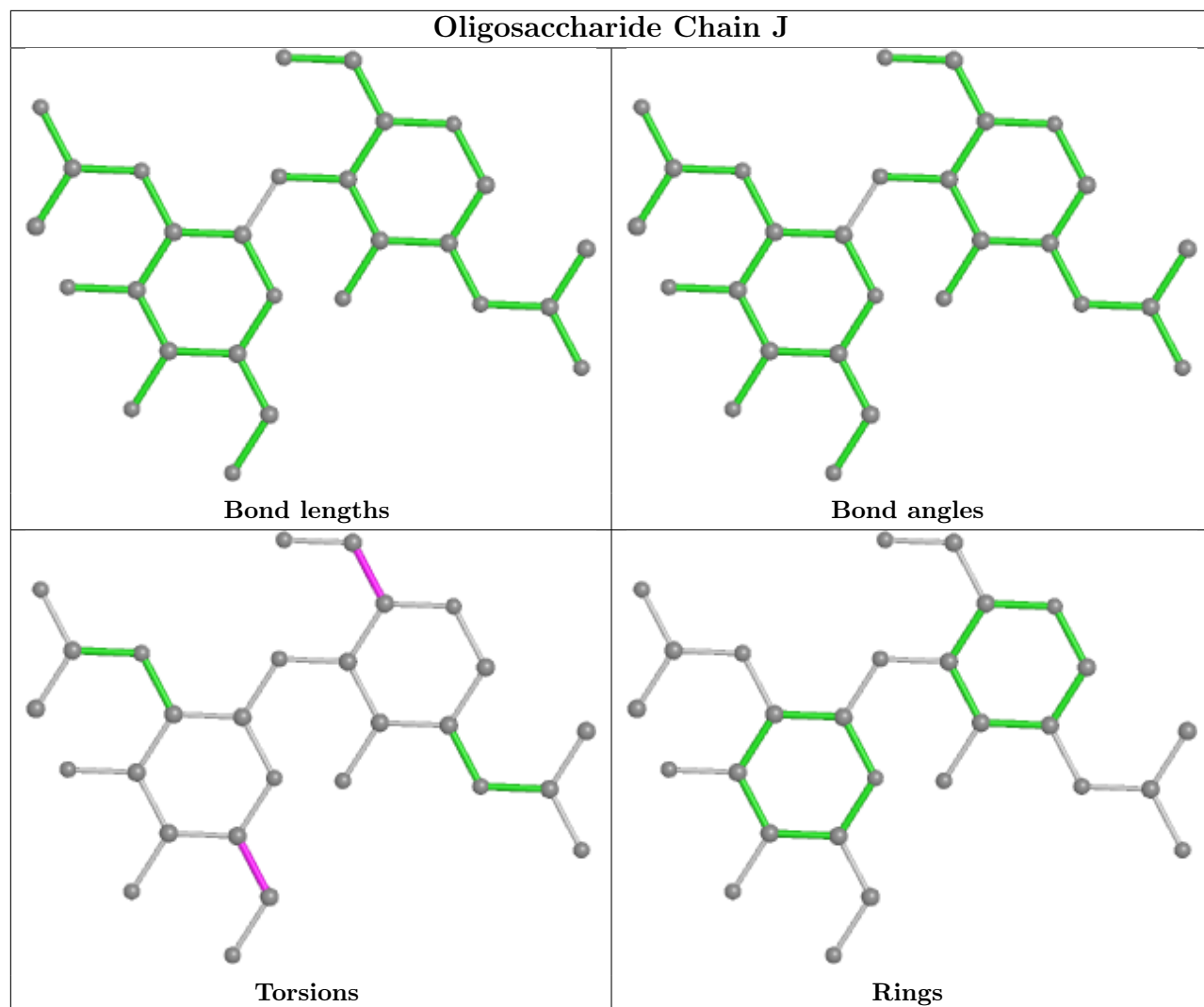
3 monomers are involved in 6 short contacts:

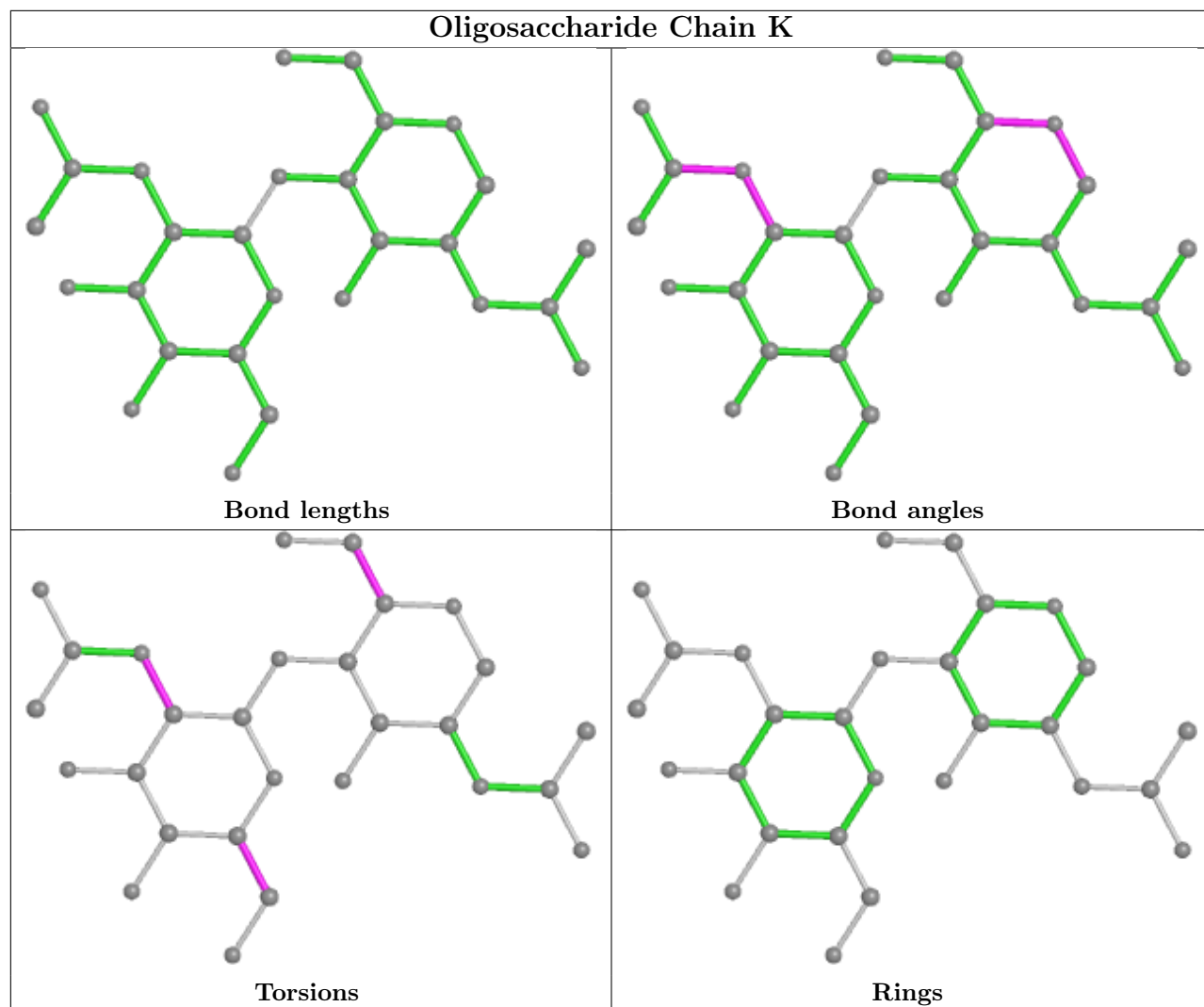
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	1	NAG	1	0
6	G	1	NAG	5	0
6	G	2	NAG	4	0

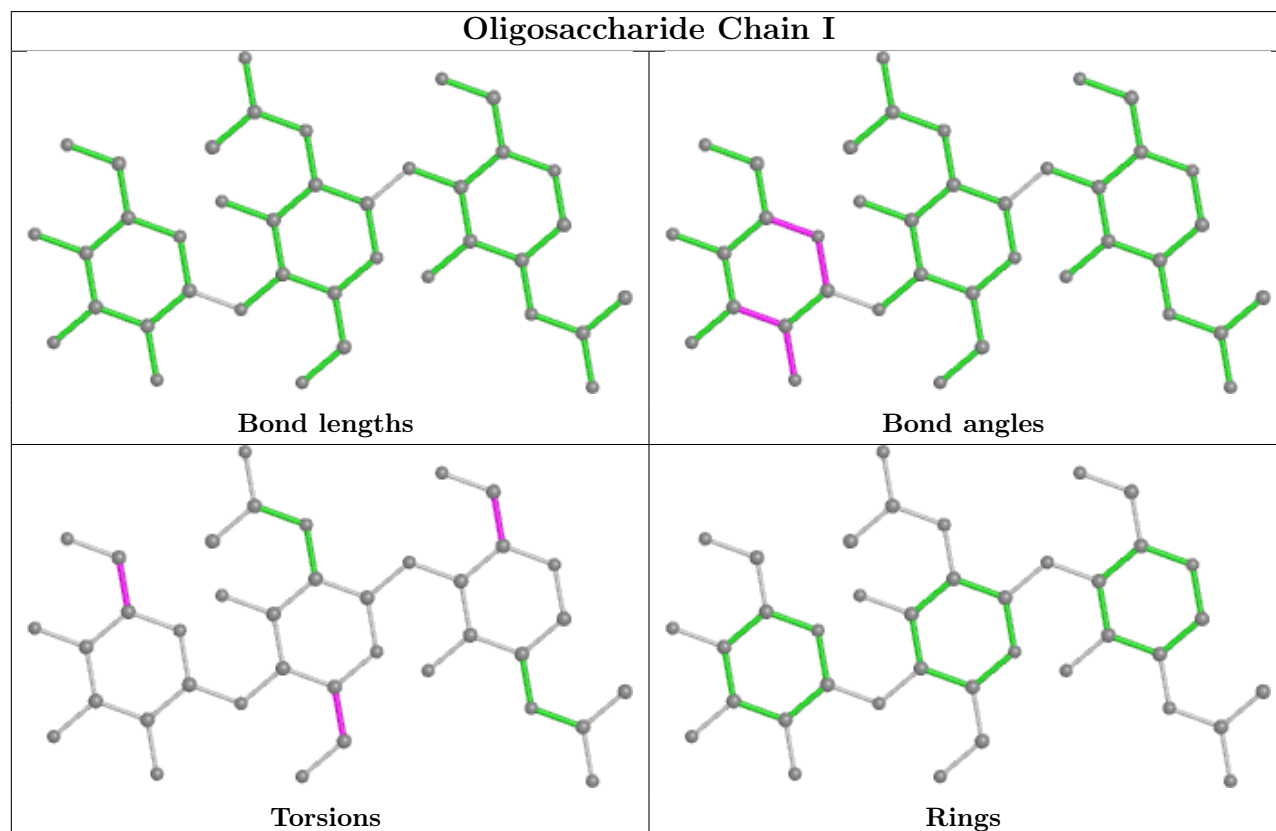
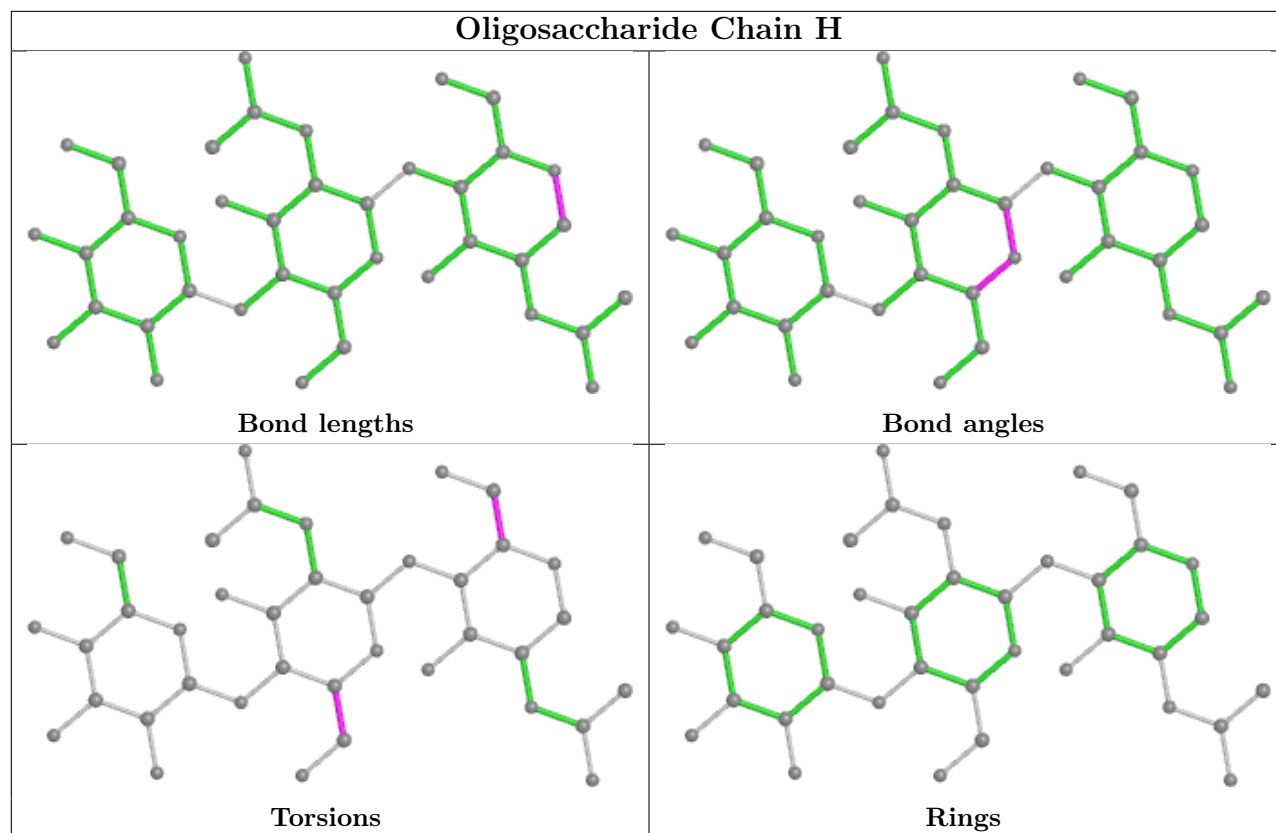
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

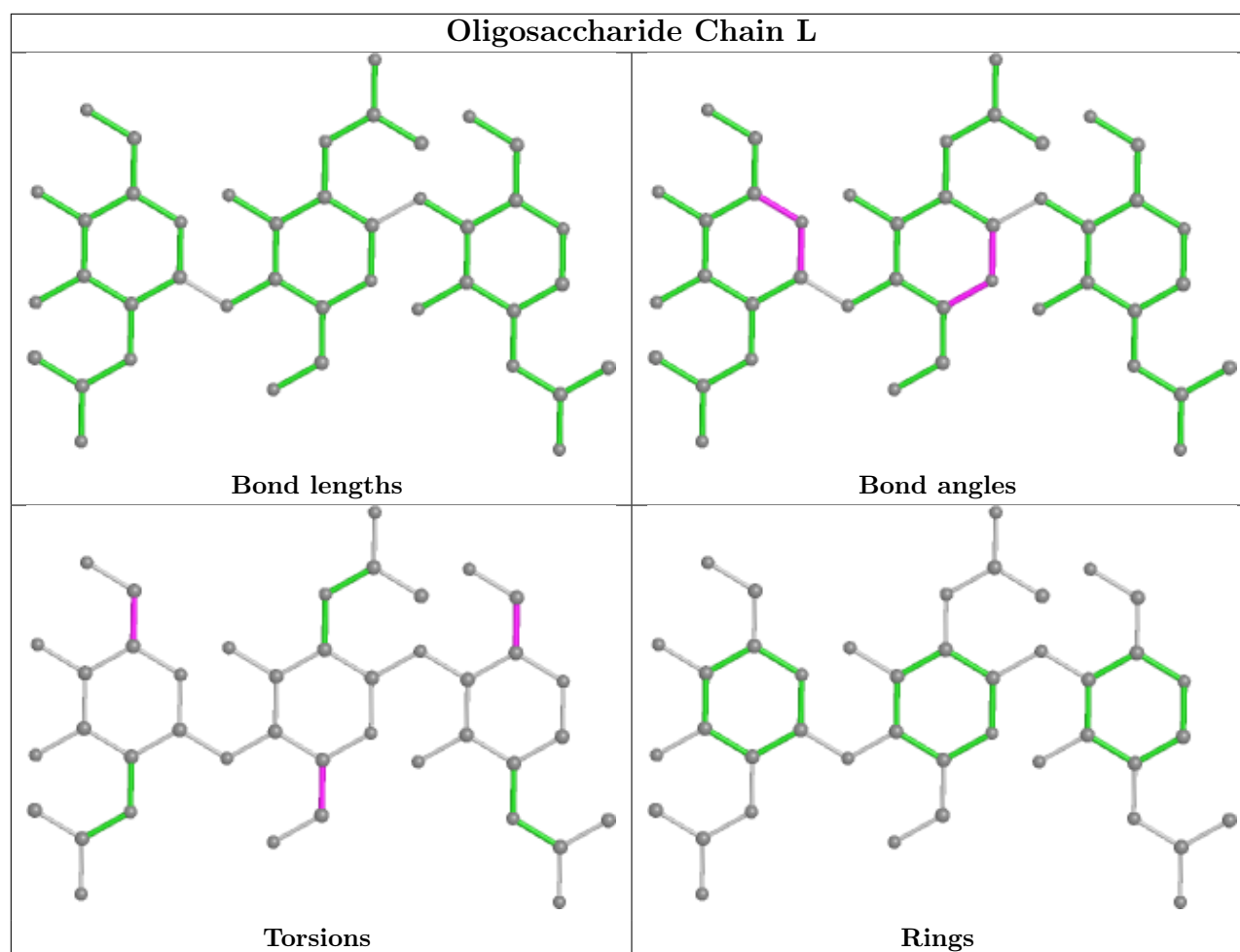












## 5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 3 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
9	NAG	F	1221	5	14,14,15	0.59	1 (7%)	17,19,21	0.60	0
10	PC1	A	1911	-	47,47,53	1.08	3 (6%)	53,55,61	1.10	4 (7%)
10	PC1	A	1906	-	17,17,53	0.69	0	16,16,61	0.48	0
10	PC1	A	1905	-	37,37,53	1.23	2 (5%)	43,45,61	1.14	3 (6%)
9	NAG	F	1214	5	14,14,15	0.64	0	17,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	F	1203	5	14,14,15	0.30	0	17,19,21	0.47	0
10	PC1	A	1908	-	11,11,53	0.61	0	10,10,61	0.33	0
9	NAG	F	1219	5	14,14,15	0.38	0	17,19,21	0.45	0
9	NAG	A	1901	1	14,14,15	0.39	0	17,19,21	0.55	0
9	NAG	F	1213	5	14,14,15	0.45	0	17,19,21	0.69	1 (5%)
10	PC1	A	1902	-	43,43,53	1.18	5 (11%)	49,51,61	1.19	3 (6%)
10	PC1	A	1914	-	13,13,53	0.57	0	12,12,61	0.49	0
10	PC1	A	1907	-	11,11,53	0.70	0	10,10,61	0.37	0
10	PC1	A	1909	-	14,14,53	0.62	0	13,13,61	0.44	0
10	PC1	A	1910	-	17,17,53	0.77	0	16,16,61	0.38	0
9	NAG	F	1220	5	14,14,15	0.81	1 (7%)	17,19,21	1.05	1 (5%)
10	PC1	A	1913	-	17,17,53	0.72	0	16,16,61	0.39	0
10	PC1	A	1904	-	41,41,53	1.22	3 (7%)	47,49,61	1.19	4 (8%)
9	NAG	F	1206	5	14,14,15	0.50	0	17,19,21	0.38	0
10	PC1	A	1915	-	47,47,53	1.17	3 (6%)	53,55,61	1.21	4 (7%)
10	PC1	A	1903	-	53,53,53	1.09	3 (5%)	59,61,61	1.02	3 (5%)
10	PC1	A	1912	-	44,44,53	1.18	3 (6%)	50,52,61	1.10	3 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	F	1221	5	-	1/6/23/26	0/1/1/1
10	PC1	A	1911	-	-	30/51/51/57	-
10	PC1	A	1906	-	-	9/15/15/57	-
10	PC1	A	1905	-	-	29/41/41/57	-
9	NAG	F	1214	5	-	0/6/23/26	0/1/1/1
9	NAG	F	1203	5	-	0/6/23/26	0/1/1/1
10	PC1	A	1908	-	-	5/9/9/57	-
9	NAG	F	1219	5	-	2/6/23/26	0/1/1/1
9	NAG	A	1901	1	-	2/6/23/26	0/1/1/1
9	NAG	F	1213	5	-	2/6/23/26	0/1/1/1
10	PC1	A	1902	-	-	23/47/47/57	-
10	PC1	A	1914	-	-	6/11/11/57	-
10	PC1	A	1907	-	-	4/9/9/57	-
10	PC1	A	1909	-	-	7/12/12/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PC1	A	1910	-	-	9/15/15/57	-
9	NAG	F	1220	5	-	0/6/23/26	0/1/1/1
10	PC1	A	1913	-	-	4/15/15/57	-
10	PC1	A	1904	-	-	19/45/45/57	-
9	NAG	F	1206	5	-	0/6/23/26	0/1/1/1
10	PC1	A	1915	-	-	29/51/51/57	-
10	PC1	A	1903	-	-	27/57/57/57	-
10	PC1	A	1912	-	-	25/48/48/57	-

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1904	PC1	O31-C31	3.29	1.43	1.33
10	A	1902	PC1	O21-C21	3.24	1.43	1.34
10	A	1912	PC1	O31-C31	3.22	1.42	1.33
10	A	1903	PC1	O31-C31	3.22	1.42	1.33
10	A	1915	PC1	O31-C31	3.19	1.42	1.33

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1915	PC1	O21-C21-C22	5.40	123.15	111.50
10	A	1902	PC1	O21-C21-C22	5.05	122.38	111.50
10	A	1912	PC1	O21-C21-C22	4.37	120.91	111.50
10	A	1904	PC1	O21-C21-C22	4.07	120.28	111.50
10	A	1904	PC1	C15-N-C13	4.02	119.32	108.97

There are no chirality outliers.

5 of 233 torsion outliers are listed below:

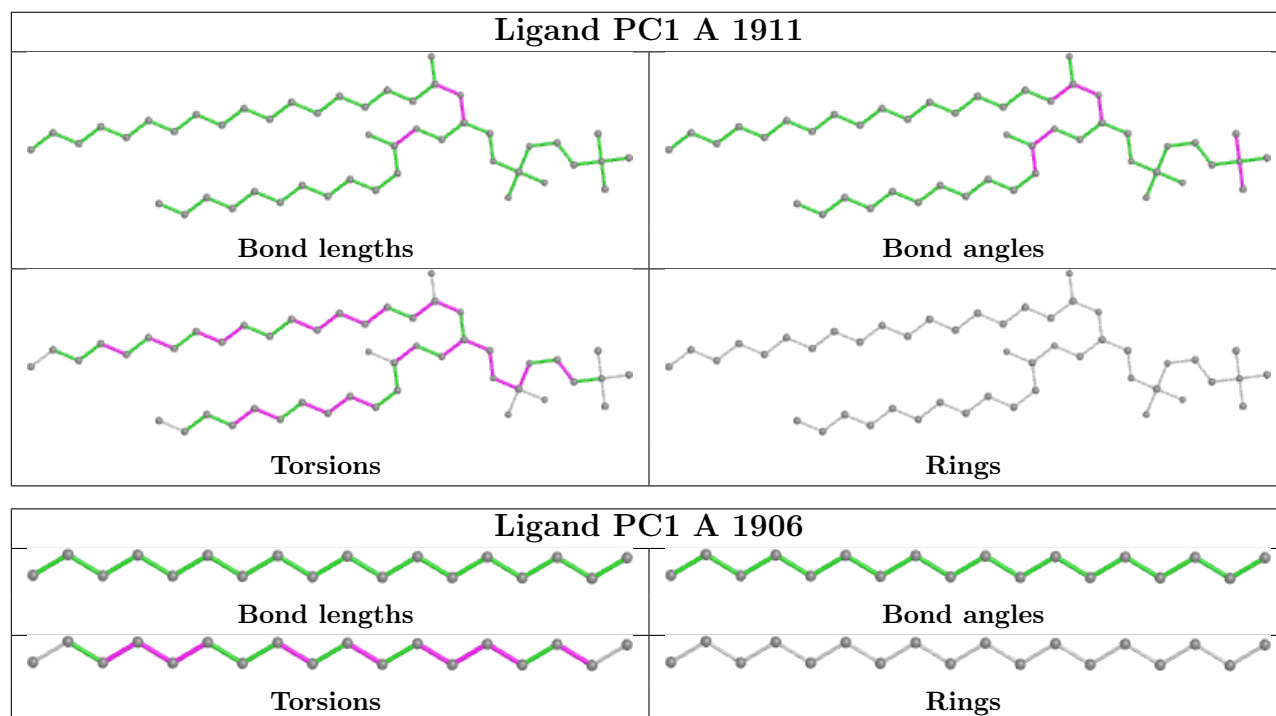
Mol	Chain	Res	Type	Atoms
10	A	1902	PC1	C1-O11-P-O12
10	A	1902	PC1	O13-C11-C12-N
10	A	1903	PC1	C11-O13-P-O14
10	A	1903	PC1	C22-C21-O21-C2
10	A	1904	PC1	C11-O13-P-O12

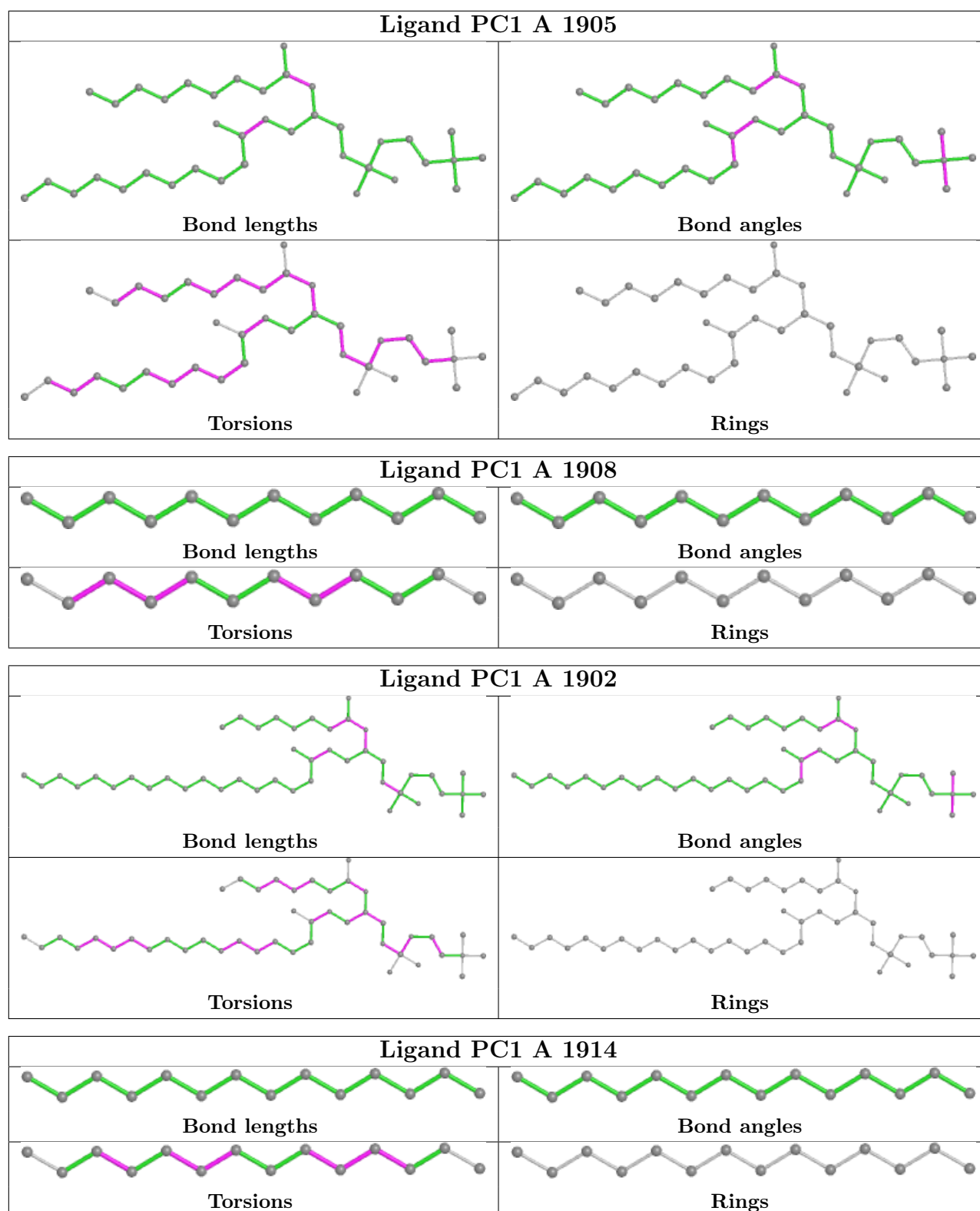
There are no ring outliers.

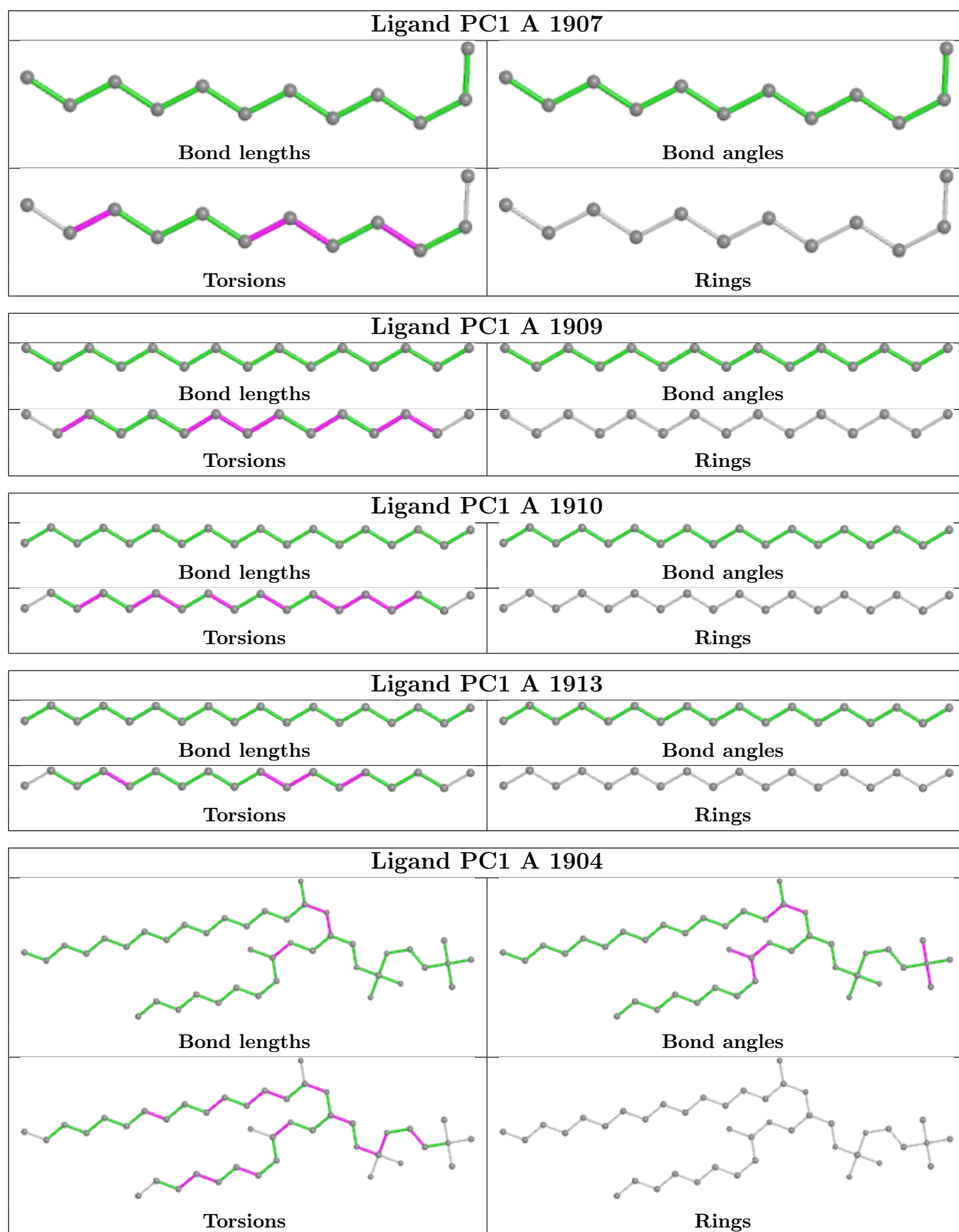
8 monomers are involved in 20 short contacts:

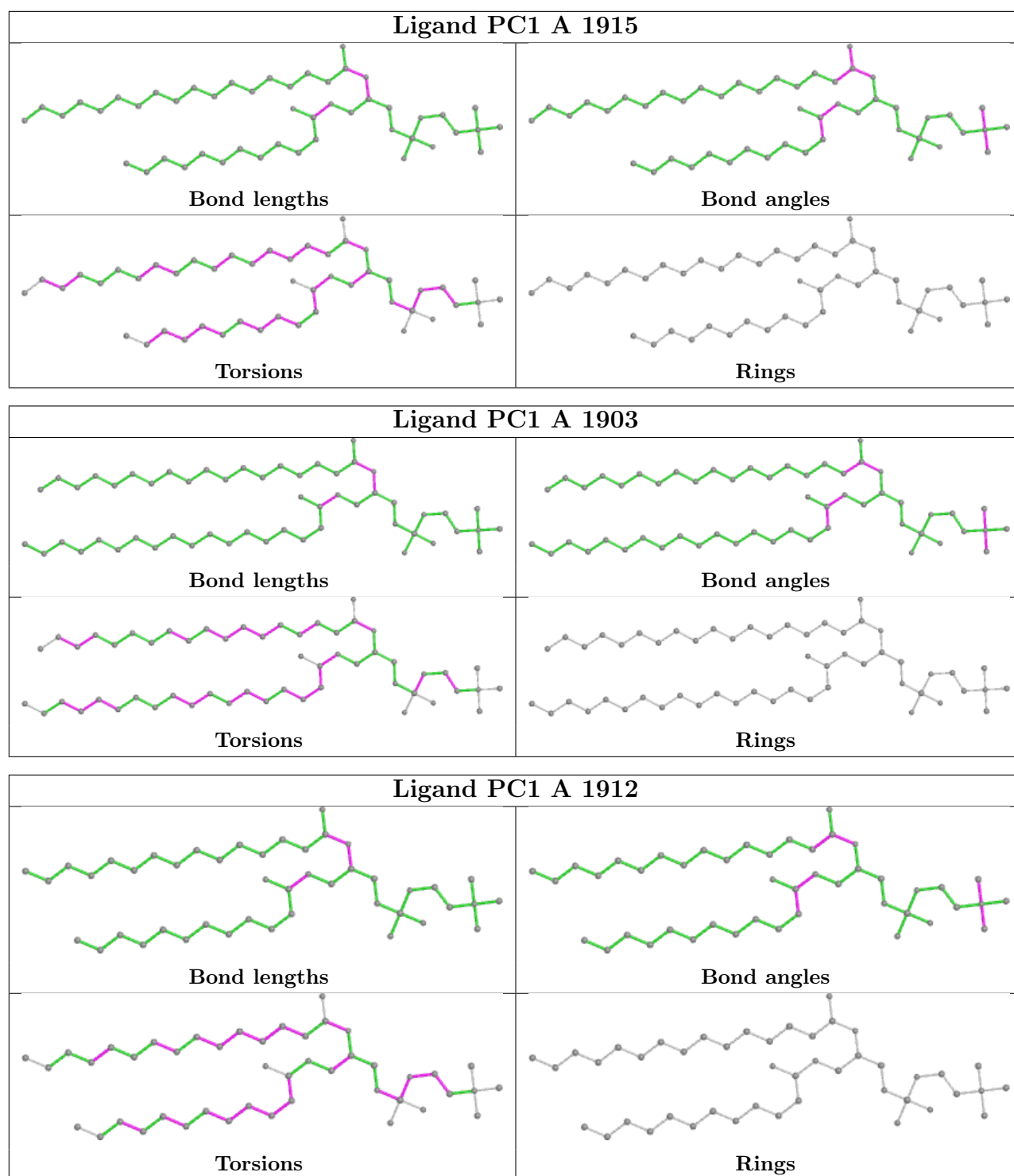
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1911	PC1	2	0
10	A	1902	PC1	2	0
10	A	1914	PC1	4	0
10	A	1909	PC1	2	0
10	A	1904	PC1	4	0
10	A	1915	PC1	1	0
10	A	1903	PC1	2	0
10	A	1912	PC1	3	0

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 ⓘ

There are no chain breaks in this entry.

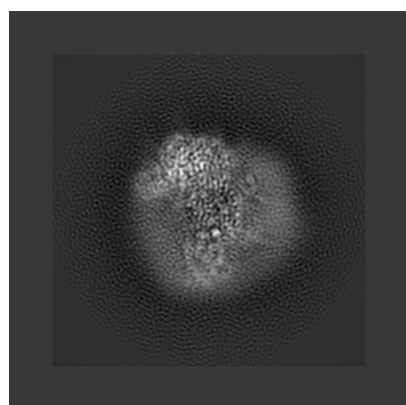
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9513. These allow visual inspection of the internal detail of the map and identification of artifacts.

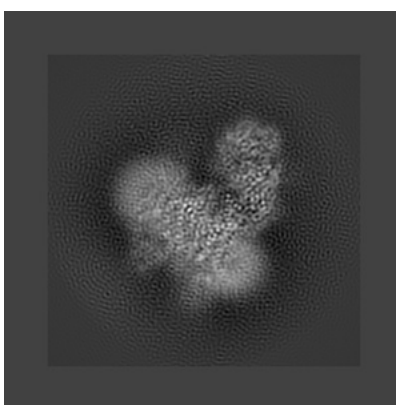
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

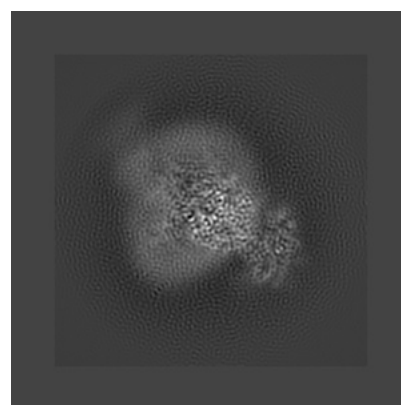
#### 6.1.1 Primary map



X



Y

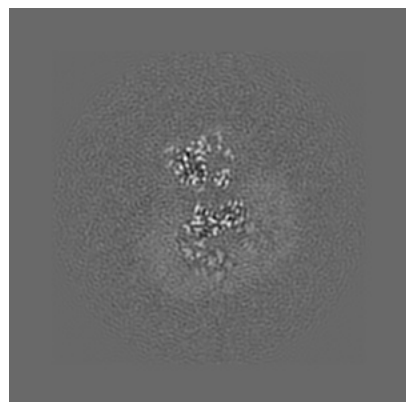


Z

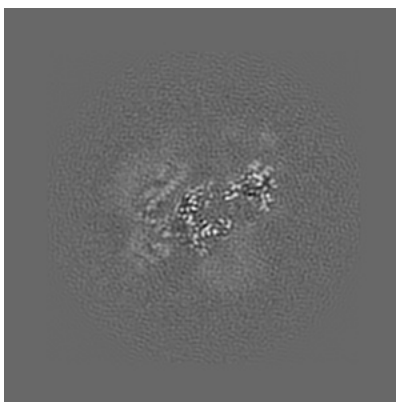
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

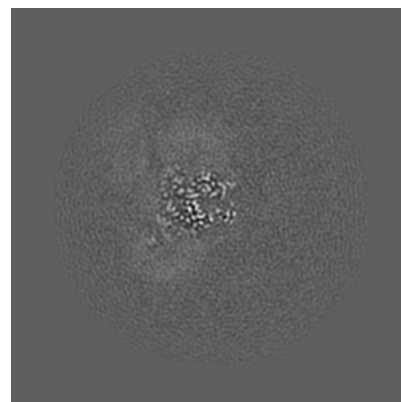
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

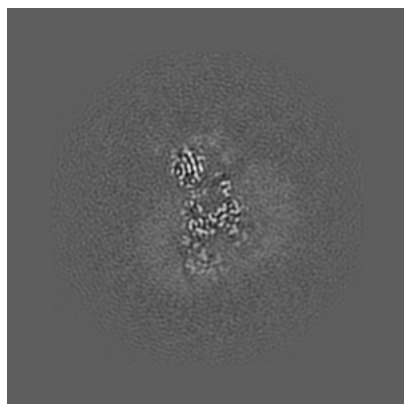


Z Index: 128

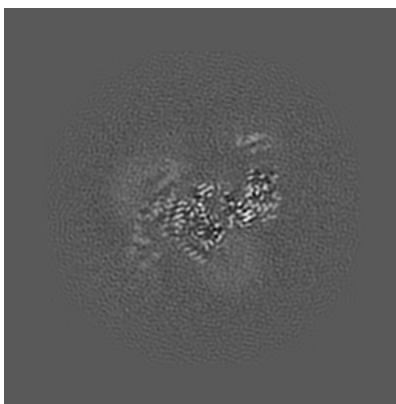
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

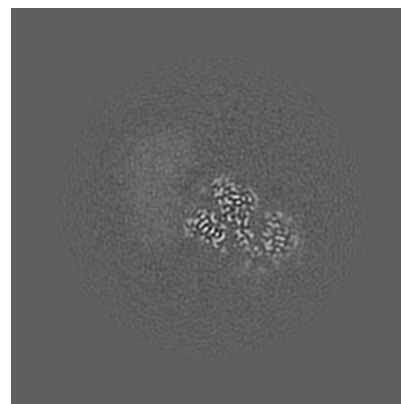
### 6.3.1 Primary map



X Index: 123



Y Index: 123



Z Index: 159

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.044. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

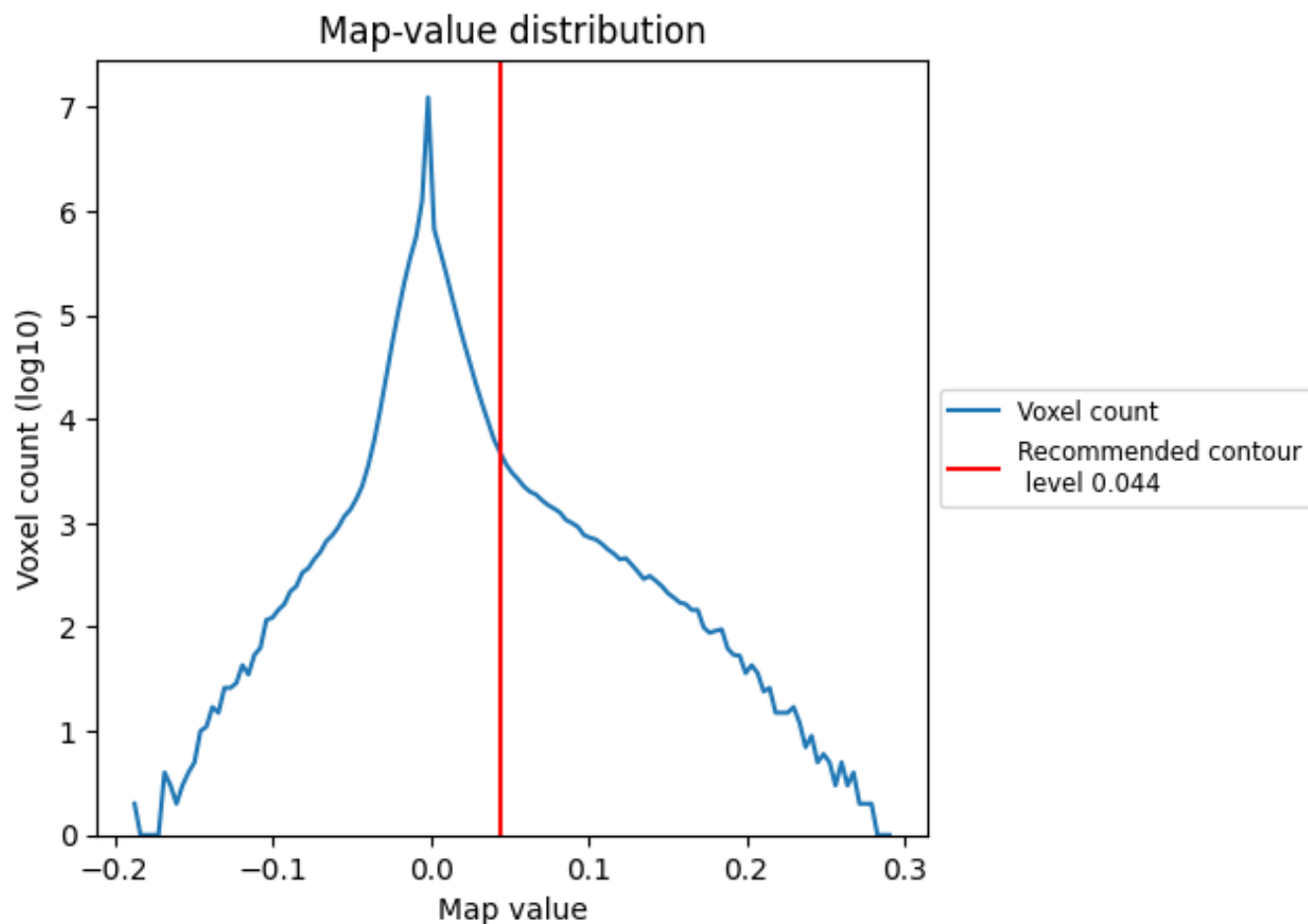
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

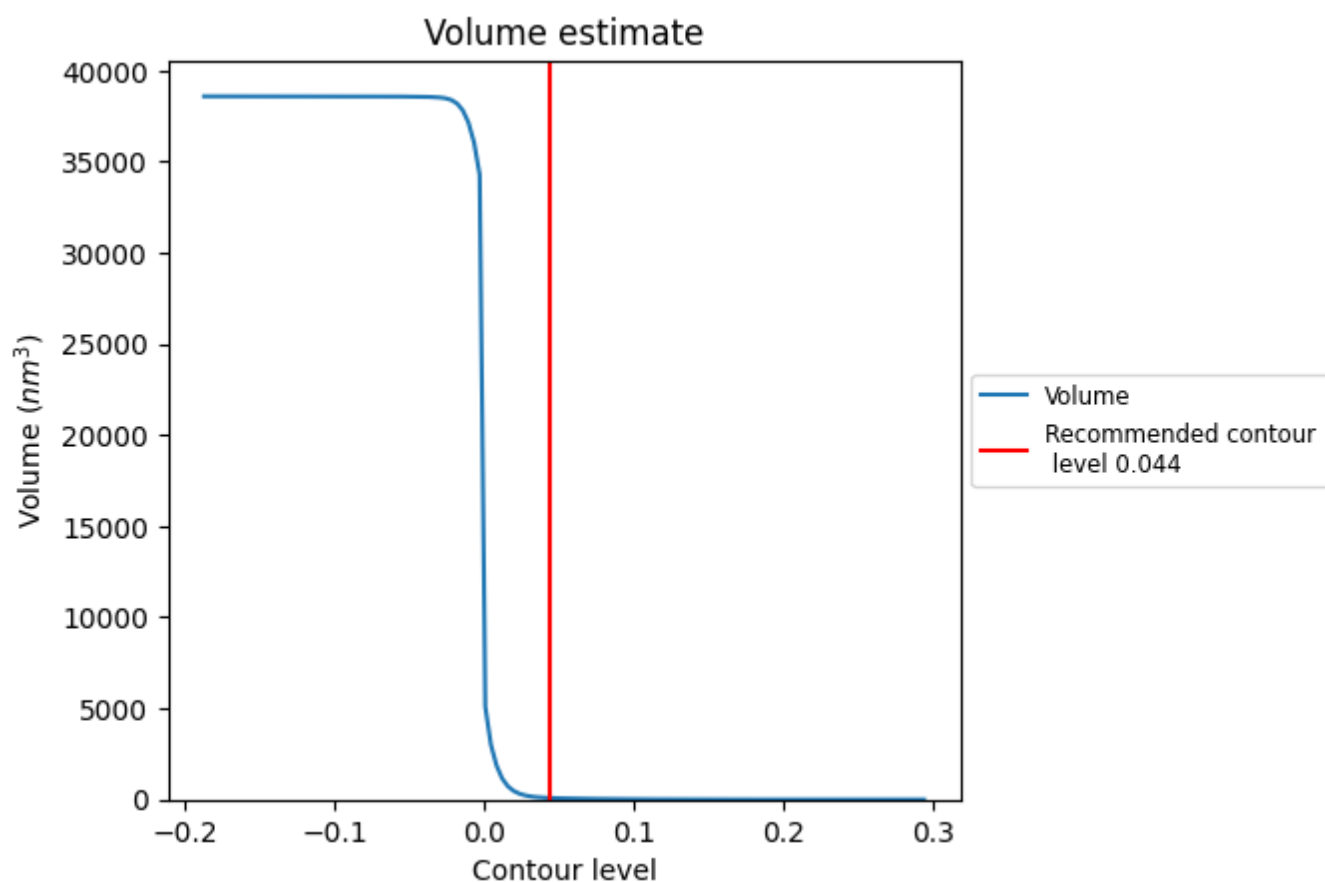
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

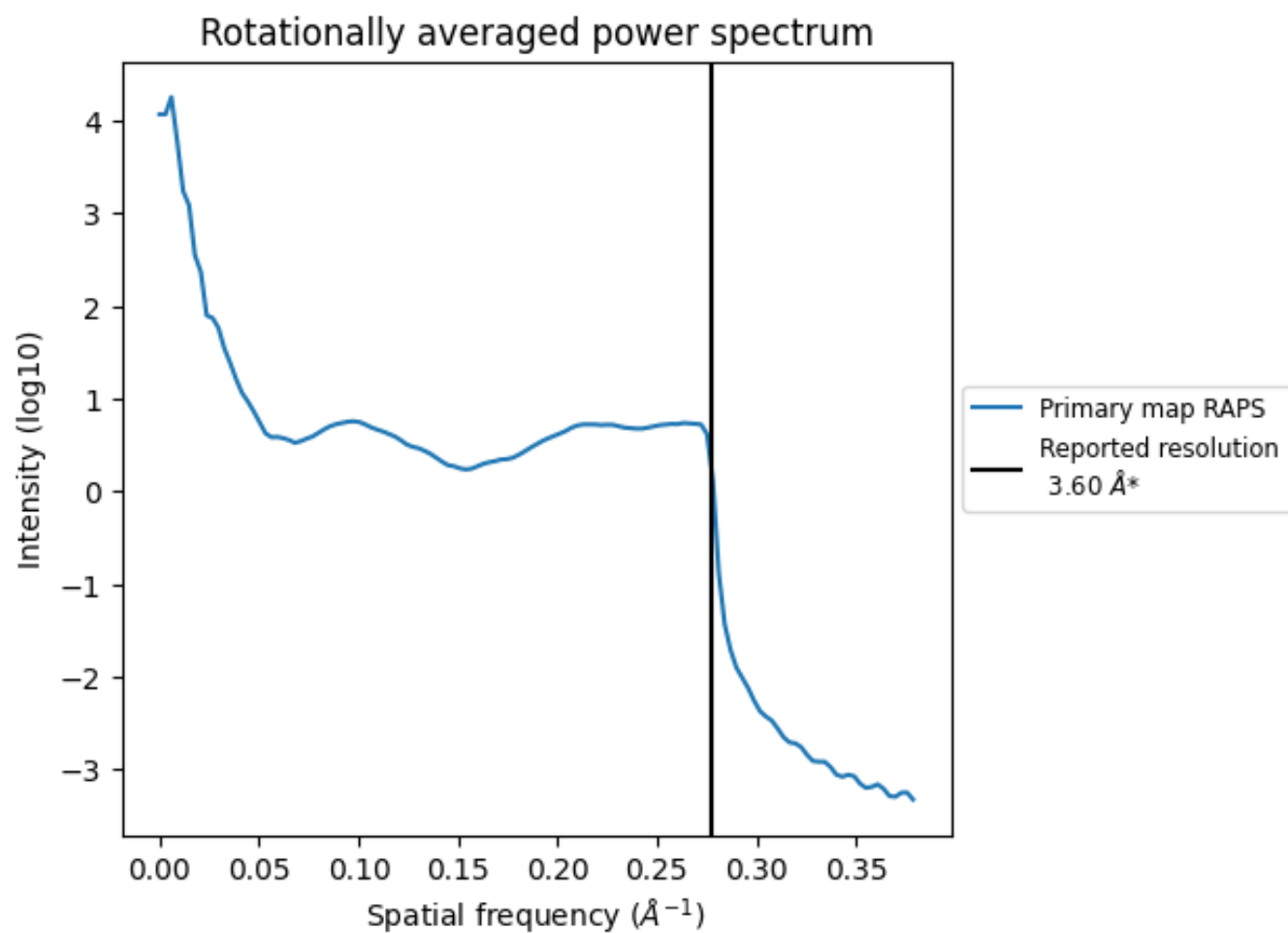
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 87 nm<sup>3</sup>; this corresponds to an approximate mass of 79 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 0.278  $\text{\AA}^{-1}$

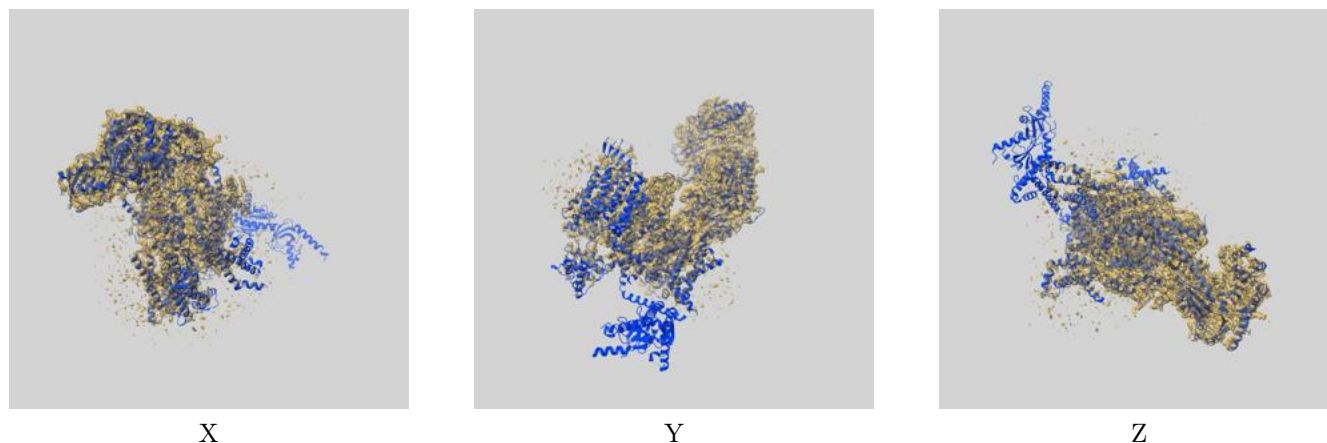
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

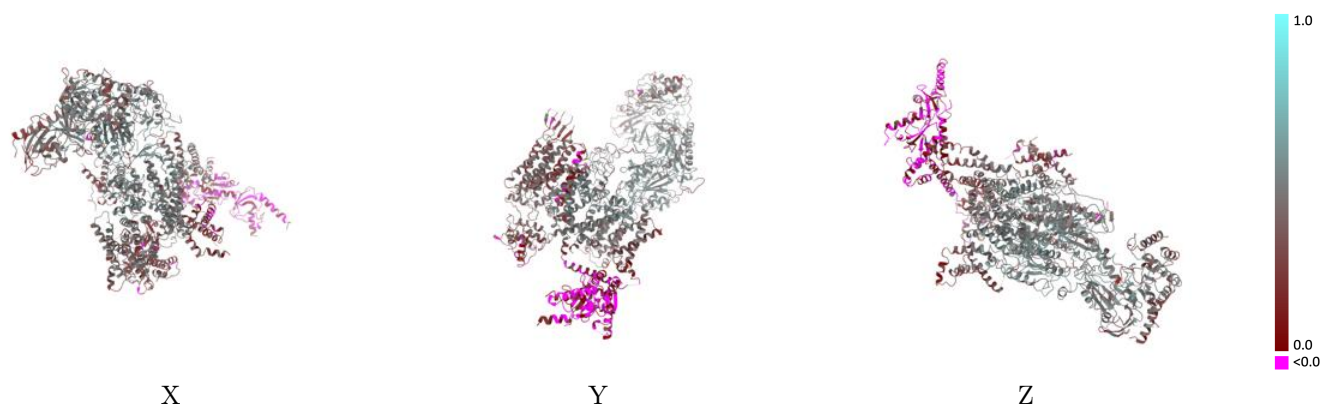
This section contains information regarding the fit between EMDB map EMD-9513 and PDB model 5GJV. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

### 9.1 Map-model overlay [i](#)



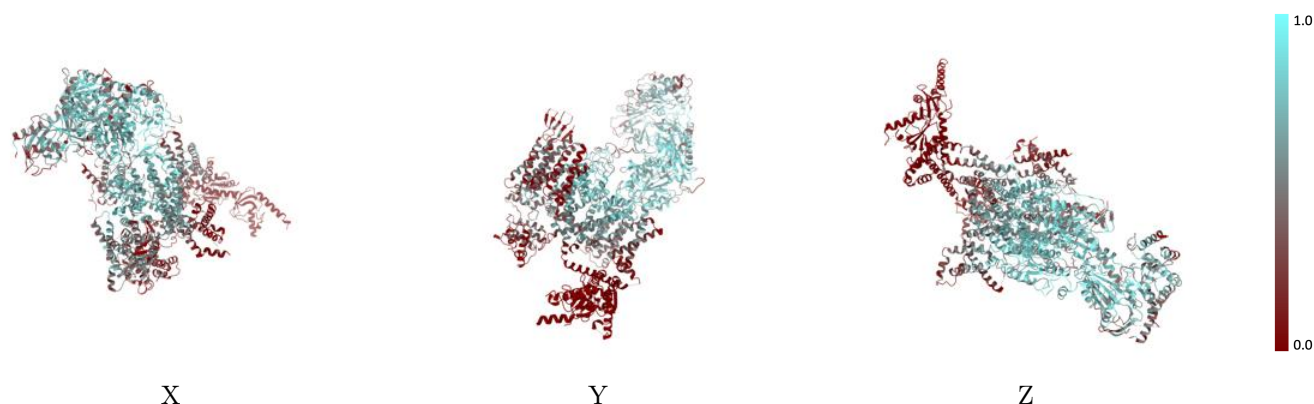
The images above show the 3D surface view of the map at the recommended contour level 0.044 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



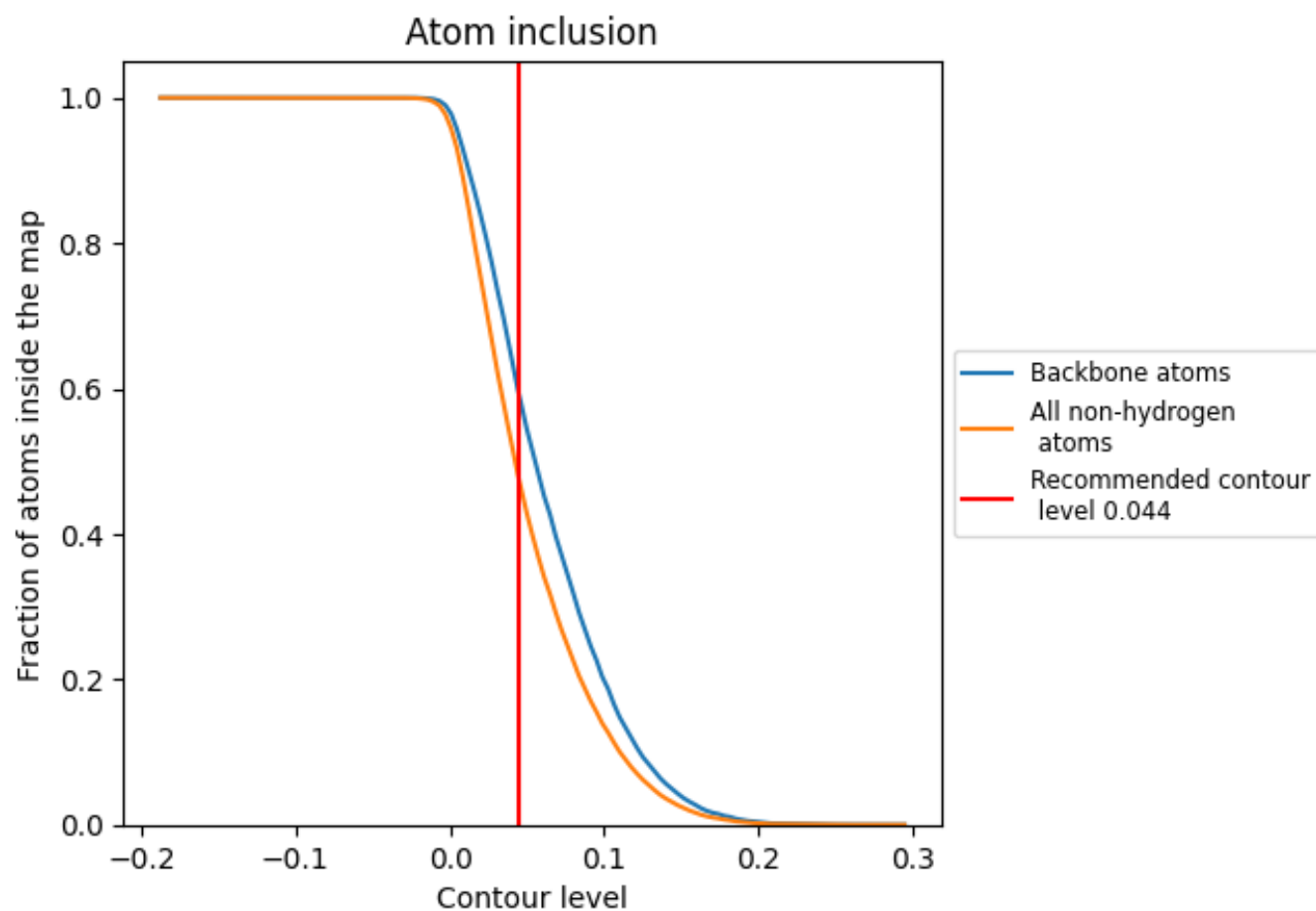
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.044).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 48% 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 (0.044) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4815	<div></div> 0.3850
A	<div></div> 0.4765	<div></div> 0.4090
B	<div></div> 0.0000	<div></div> 0.0240
C	<div></div> 0.0000	<div></div> 0.0110
D	<div></div> 0.0714	<div></div> 0.0690
E	<div></div> 0.3033	<div></div> 0.3470
F	<div></div> 0.6542	<div></div> 0.4590
G	<div></div> 0.1786	<div></div> 0.3640
H	<div></div> 0.3333	<div></div> 0.3700
I	<div></div> 0.6923	<div></div> 0.5200
J	<div></div> 0.5357	<div></div> 0.4920
K	<div></div> 0.2500	<div></div> 0.3890
L	<div></div> 0.2857	<div></div> 0.2870

1.0

0.0

<0.0