wwPDB EM Validation Summary Report (i)

Oct 16, 2024 – 12:35 AM JST

PDB ID	:	8KCO
EMDB ID	:	EMD-37106
Title	:	Cryo-EM structure of human gamma-secretase in complex with RO4929097
Authors	:	Guo, X.; Li, H.; Kai, U.; Yan, C.; Lei, J.; Zhou, R.; Shi, Y.
Deposited on	:	2023-08-08
Resolution	:	2.80 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.80 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	Percentile Ranks	Value
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		0.5%

Worse   *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures
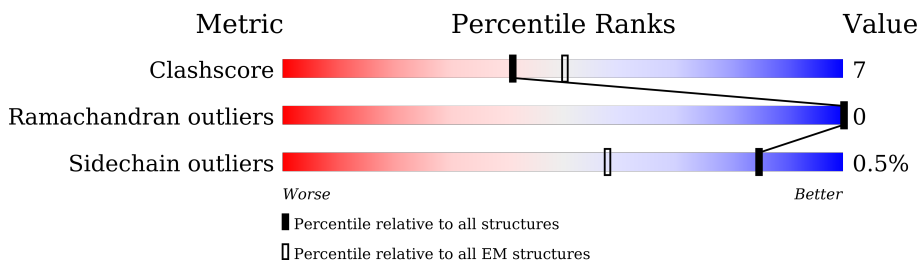
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	701	83% 12% 5%
2	B	467	55% 10% • 34%
3	C	265	80% 11% 8%
4	D	101	86% 9% 5%
5	E	2	100%
5	G	2	50% 50%
5	H	2	50% 50%
5	I	2	50% 50%
5	J	2	50% 50%

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Mol	Chain	Length	Quality of chain
6	F	5	80% 20%

2   Entry composition ⓘ

There are 10 unique types of molecules in this entry. The entry contains 10837 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Nicastrin.

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

- Molecule 2 is a protein called Presenilin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	307	Total 2436	C 1649	N 370	O 403	S 14	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	96	Total 814	C 559	N 126	O 128	S 1	0	0

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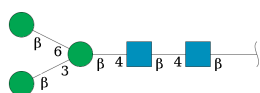

Mol	Chain	Residues	Atoms			AltConf	Trace
5	E	2	Total 28	C 16	N 2 O 10	0	0
5	G	2	Total 28	C 16	N 2 O 10	0	0

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

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

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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
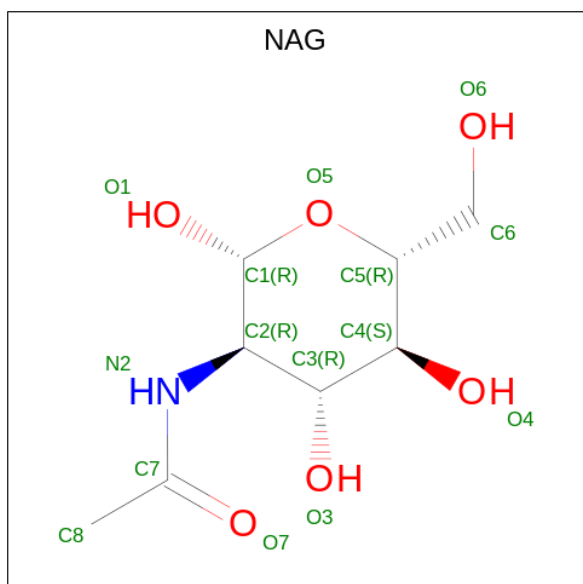
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	1	5	

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

- Molecule 8 is 2,2-dimethyl-N-[(7S)-6-oxo-5,7-dihydrobenzo[d][1]benzazepin-7-yl]-N'-(2,2,3 ,3,3-pentafluoropropyl)propanediamide (three-letter code: N60) (formula: $C_{22}H_{20}F_5N_3O_3$) (labeled as "Ligand of Interest" by depositor).
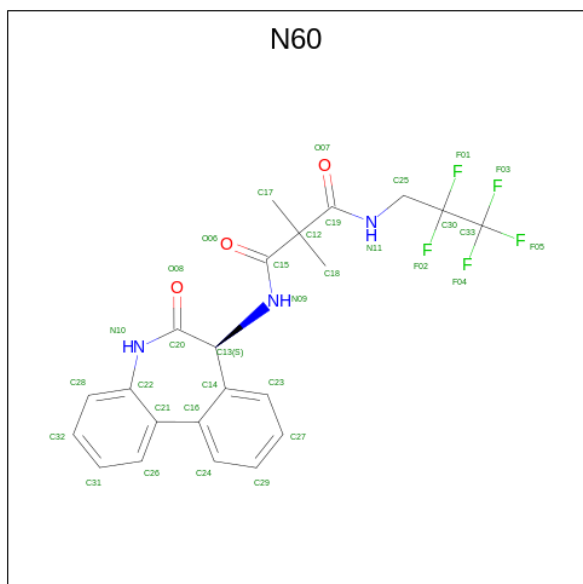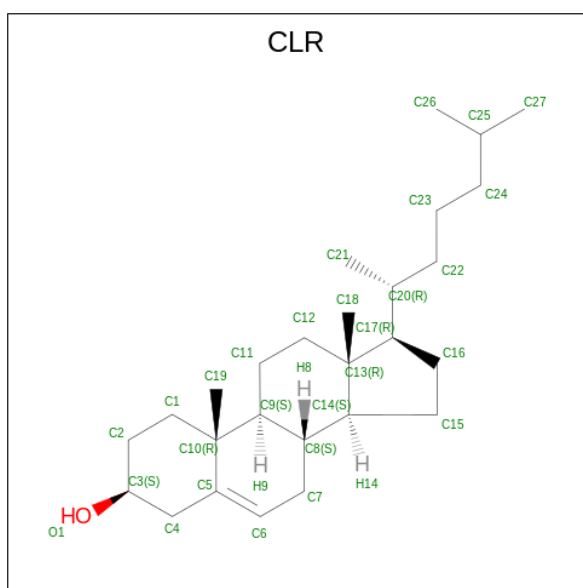

Mol	Chain	Residues	Atoms					AltConf
8	B	1	Total 33	C 22	F 5	N 3	O 3	0

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

PC1
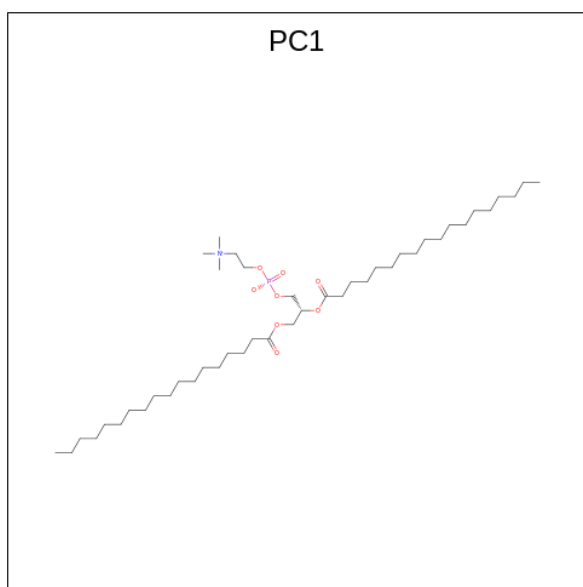
Mol	Chain	Residues	Atoms					AltConf
9	B	1	Total	C	N	O	P	0
			37	27	1	8	1	
9	C	1	Total	C	N	O	P	0
			41	31	1	8	1	

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

CLR

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

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

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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
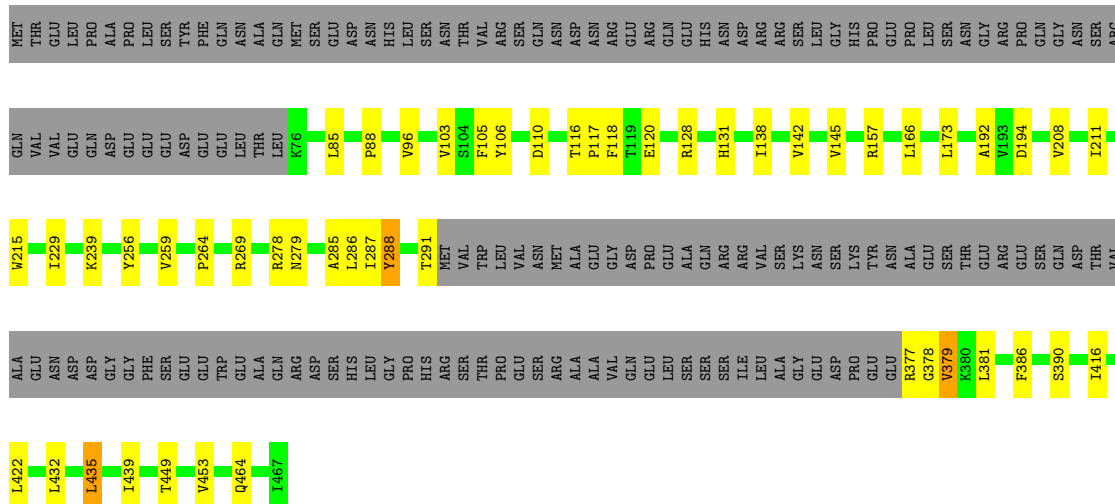
- Molecule 1: Nicastrin

Chain A:
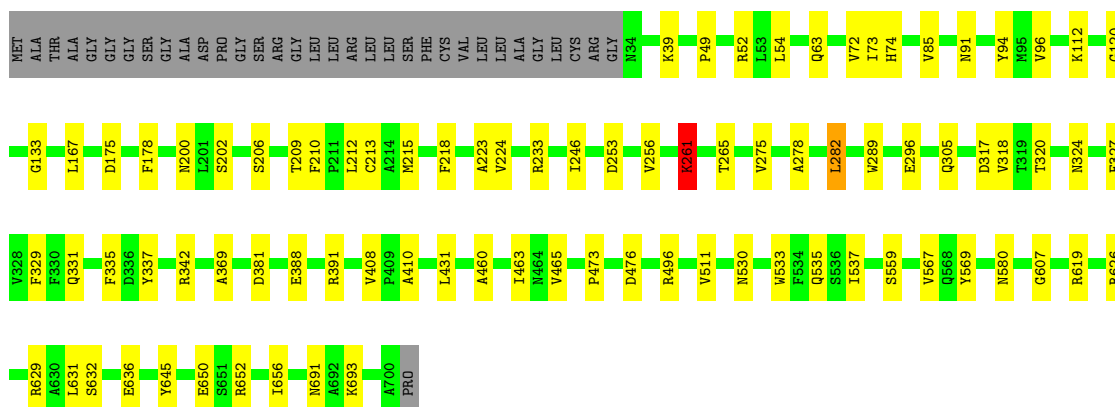
- Molecule 2: Presenilin-1

Chain B:

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

Chain C:
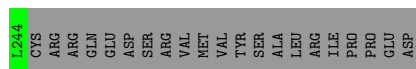
• Molecule 4: Gamma-secretase subunit PEN-2
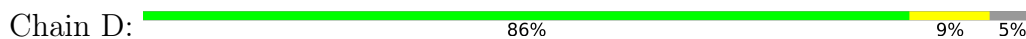
Chain D:

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

Chain E:

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

Chain G:

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

Chain H:

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

Chain I:

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

Chain J:

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

Chain F:

80%   20%

NAG1 NAG2 BMA3 BMA4 BMA5

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5551418	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 $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, NAG, BMA, PC1, N60

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	0.42	1/5358 (0.0%)	0.60	1/7302 (0.0%)
2	B	0.40	0/2499	0.61	1/3410 (0.0%)
3	C	0.43	0/1924	0.61	0/2624
4	D	0.42	0/847	0.53	0/1157
All	All	0.41	1/10628 (0.0%)	0.60	2/14493 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	2
3	C	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	261	LYS	C-N	9.04	1.51	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	286	LEU	CA-CB-CG	6.86	131.08	115.30
1	A	282	LEU	CA-CB-CG	6.09	129.31	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	209	THR	Peptide
1	A	91	ASN	Peptide
2	B	279	ASN	Peptide
2	B	435	LEU	Peptide
3	C	206	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5235	0	5126	54	0
2	B	2436	0	2558	46	0
3	C	1872	0	1911	34	0
4	D	814	0	804	7	0
5	E	28	0	25	0	0
5	G	28	0	25	0	0
5	H	28	0	25	0	0
5	I	28	0	25	0	0
5	J	28	0	25	0	0
6	F	61	0	52	0	0
7	A	84	0	78	0	0
8	B	33	0	0	1	0
9	B	37	0	48	1	0
9	C	41	0	56	1	0
10	C	84	0	138	17	0
All	All	10837	0	10896	146	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 7.

The worst 5 of 146 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:291:THR:CG2	2:B:378:GLY:HA3	1.48	1.41
2:B:291:THR:HG23	2:B:378:GLY:HA3	1.22	1.12
10:C:302:CLR:H25	10:C:302:CLR:H211	1.18	1.12
2:B:291:THR:CG2	2:B:378:GLY:CA	2.26	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:291:THR:HG21	2:B:378:GLY:CA	1.83	1.08

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	665/701 (95%)	616 (93%)	49 (7%)	0	100	100
2	B	303/467 (65%)	285 (94%)	18 (6%)	0	100	100
3	C	241/265 (91%)	229 (95%)	12 (5%)	0	100	100
4	D	94/101 (93%)	88 (94%)	6 (6%)	0	100	100
All	All	1303/1534 (85%)	1218 (94%)	85 (6%)	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	584/606 (96%)	582 (100%)	2 (0%)	91	97
2	B	265/408 (65%)	262 (99%)	3 (1%)	70	90
3	C	193/214 (90%)	192 (100%)	1 (0%)	86	95
4	D	84/89 (94%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1126/1317 (86%)	1120 (100%)	6 (0%)	85 95

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	377	ARG
2	B	379	VAL
3	C	135	ILE
1	A	691	ASN
1	A	261	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	691	ASN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates (i)

15 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z \rvert > 2$	Counts	RMSZ	$\#\lvert Z \rvert > 2$
5	NAG	E	1	1,5	14,14,15	0.29	0	17,19,21	0.47	0
5	NAG	E	2	5	14,14,15	0.23	0	17,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
6	NAG	F	1	1,6	14,14,15	0.32	0	17,19,21	0.59	0
6	NAG	F	2	6	14,14,15	0.21	0	17,19,21	0.59	0
6	BMA	F	3	6	11,11,12	0.81	0	15,15,17	0.94	0
6	BMA	F	4	6	11,11,12	0.81	0	15,15,17	0.82	0
6	BMA	F	5	6	11,11,12	1.55	2 (18%)	15,15,17	1.99	4 (26%)
5	NAG	G	1	1,5	14,14,15	0.28	0	17,19,21	1.12	2 (11%)
5	NAG	G	2	5	14,14,15	0.45	0	17,19,21	0.57	0
5	NAG	H	1	1,5	14,14,15	0.59	1 (7%)	17,19,21	0.64	0
5	NAG	H	2	5	14,14,15	0.24	0	17,19,21	0.63	0
5	NAG	I	1	1,5	14,14,15	0.19	0	17,19,21	0.56	0
5	NAG	I	2	5	14,14,15	0.86	1 (7%)	17,19,21	2.23	3 (17%)
5	NAG	J	1	1,5	14,14,15	0.46	0	17,19,21	0.48	0
5	NAG	J	2	5	14,14,15	0.19	0	17,19,21	0.63	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
5	NAG	E	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	4/6/23/26	0/1/1/1
6	NAG	F	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	F	2	6	-	2/6/23/26	0/1/1/1
6	BMA	F	3	6	-	2/2/19/22	0/1/1/1
6	BMA	F	4	6	-	2/2/19/22	0/1/1/1
6	BMA	F	5	6	-	2/2/19/22	0/1/1/1
5	NAG	G	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	G	2	5	-	4/6/23/26	0/1/1/1
5	NAG	H	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	H	2	5	-	4/6/23/26	0/1/1/1
5	NAG	I	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	5/6/23/26	0/1/1/1
5	NAG	J	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	5	BMA	C2-C3	3.11	1.57	1.52
6	F	5	BMA	C1-C2	3.08	1.59	1.52
5	I	2	NAG	C1-C2	2.61	1.56	1.52
5	H	1	NAG	O5-C1	-2.05	1.40	1.43

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	2	NAG	C2-N2-C7	7.79	133.99	122.90
6	F	5	BMA	C1-O5-C5	5.17	119.19	112.19
5	I	2	NAG	C1-C2-N2	3.60	116.64	110.49
6	F	5	BMA	C1-C2-C3	3.31	113.73	109.67
5	G	1	NAG	C2-N2-C7	3.10	127.32	122.90

There are no chirality outliers.

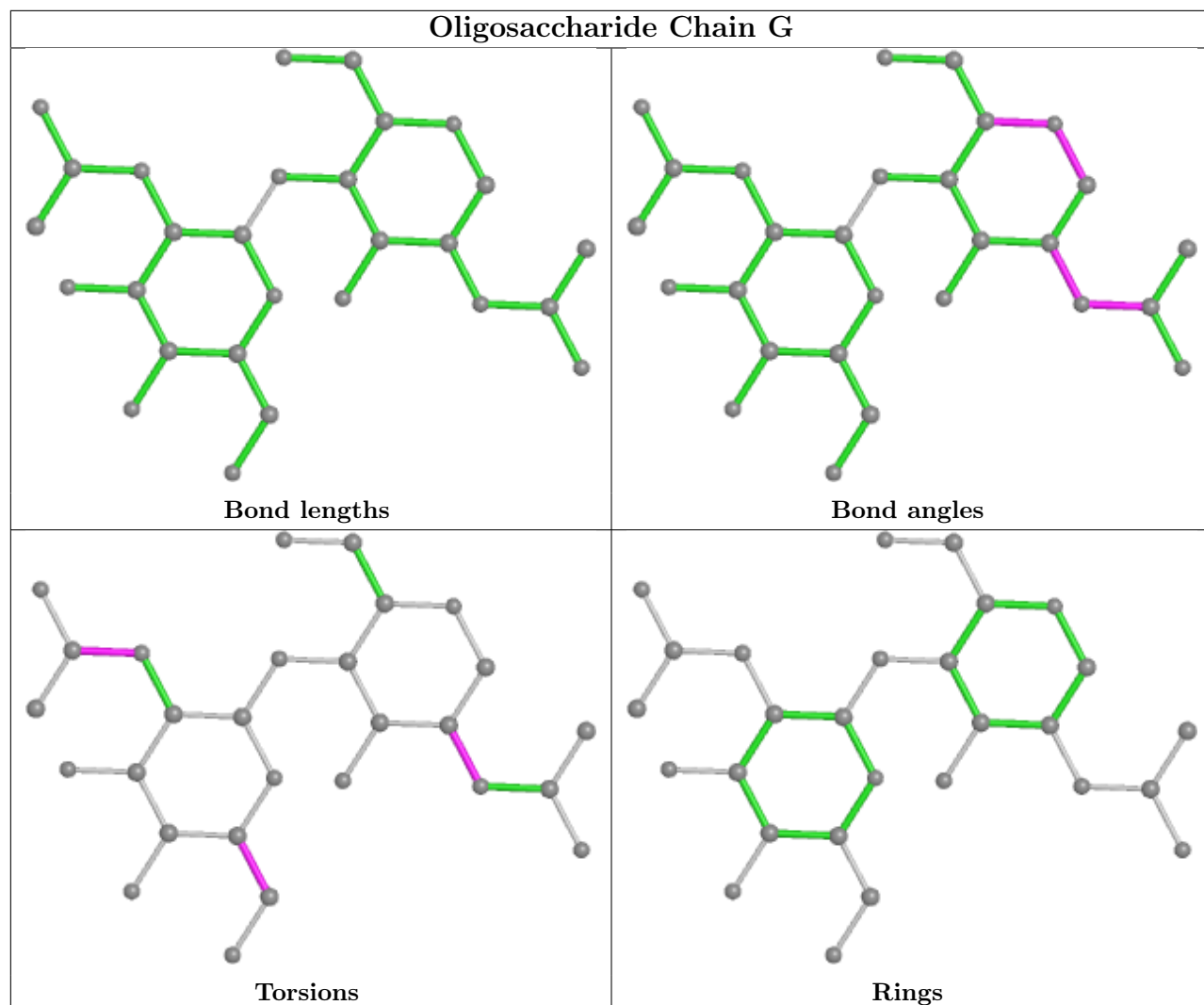5 of 35 torsion outliers are listed below:

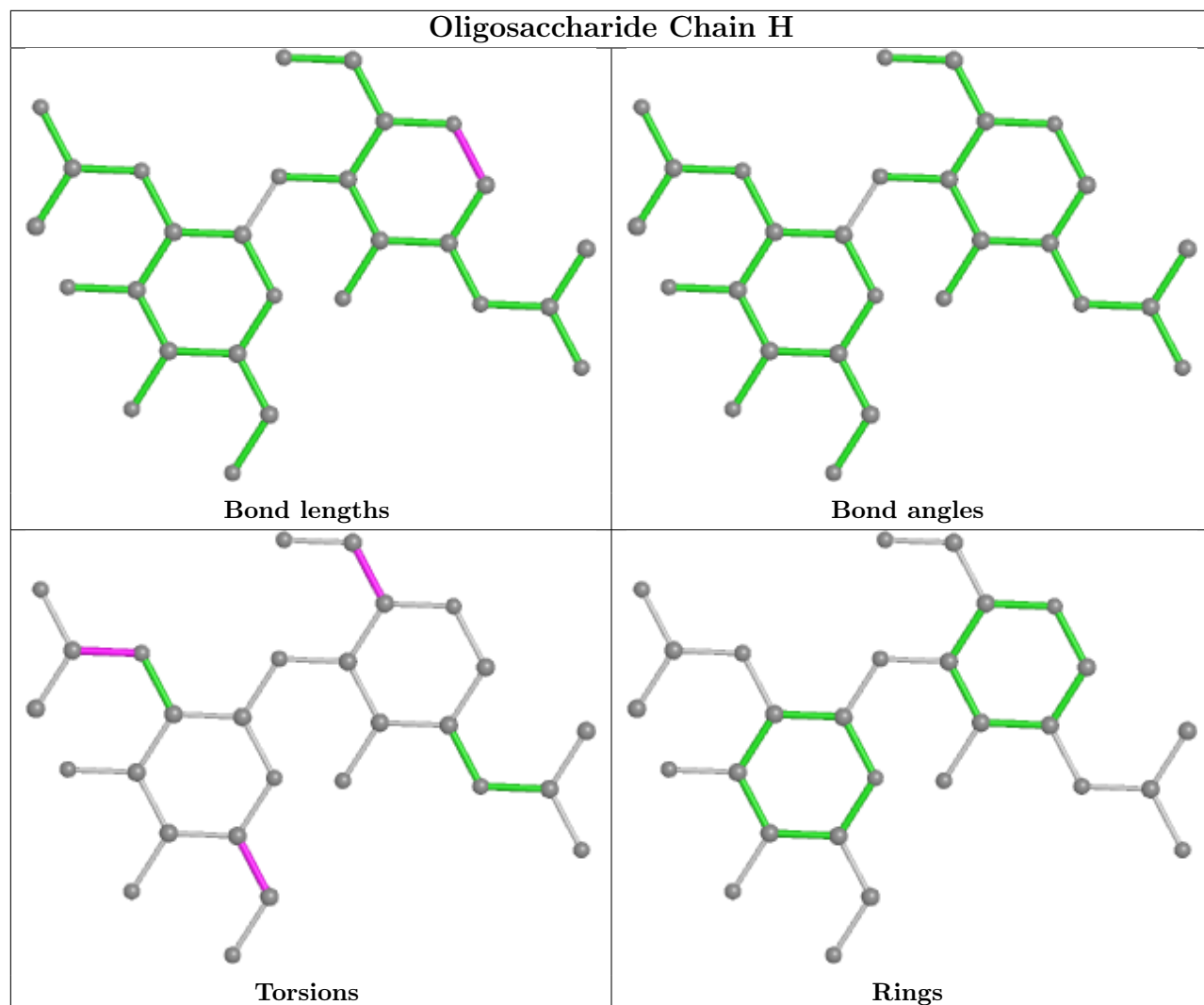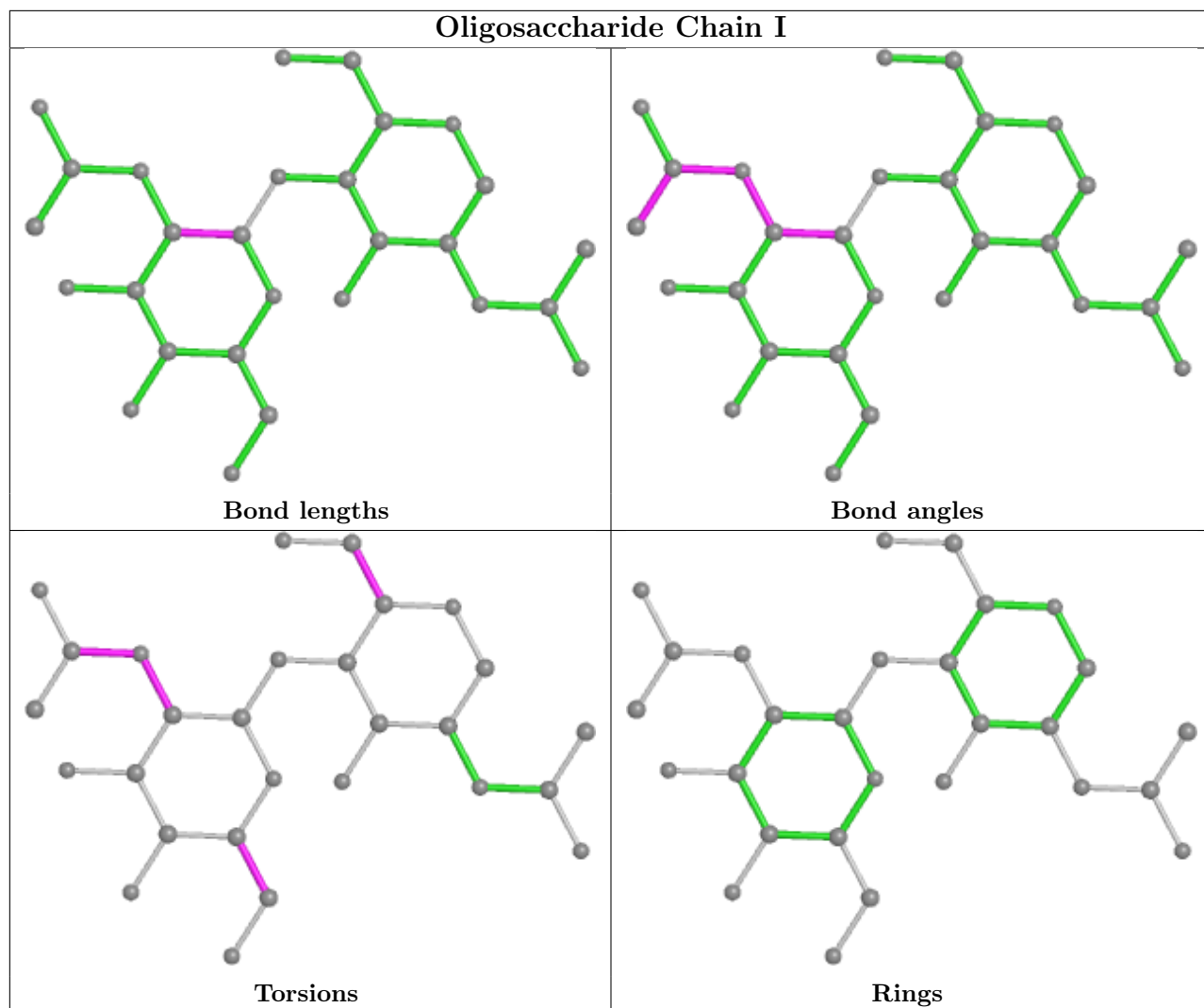| Mol	Chain	Res	Type	Atoms
6	F	3	BMA	C4-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
6	F	3	BMA	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

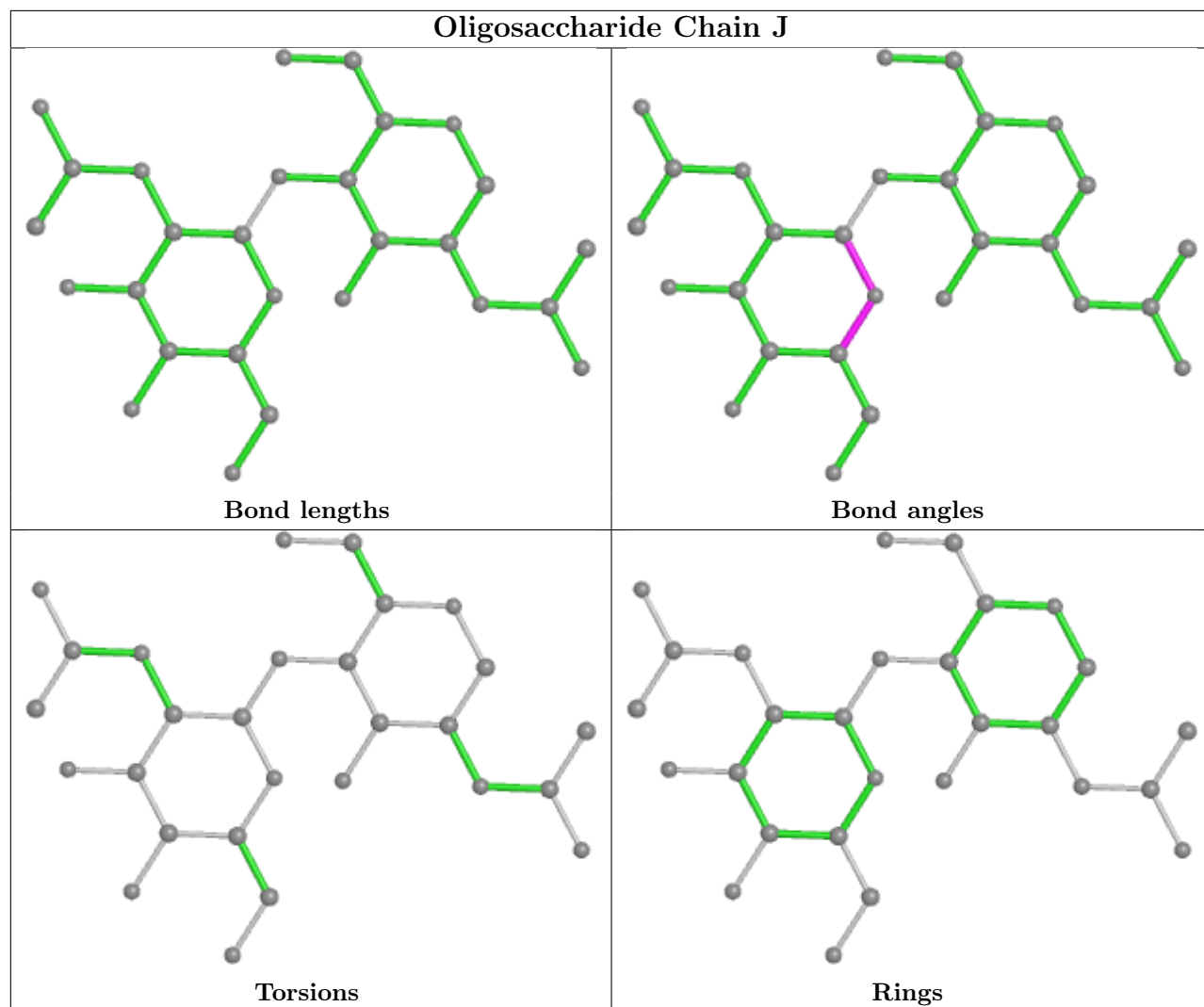The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain J

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F
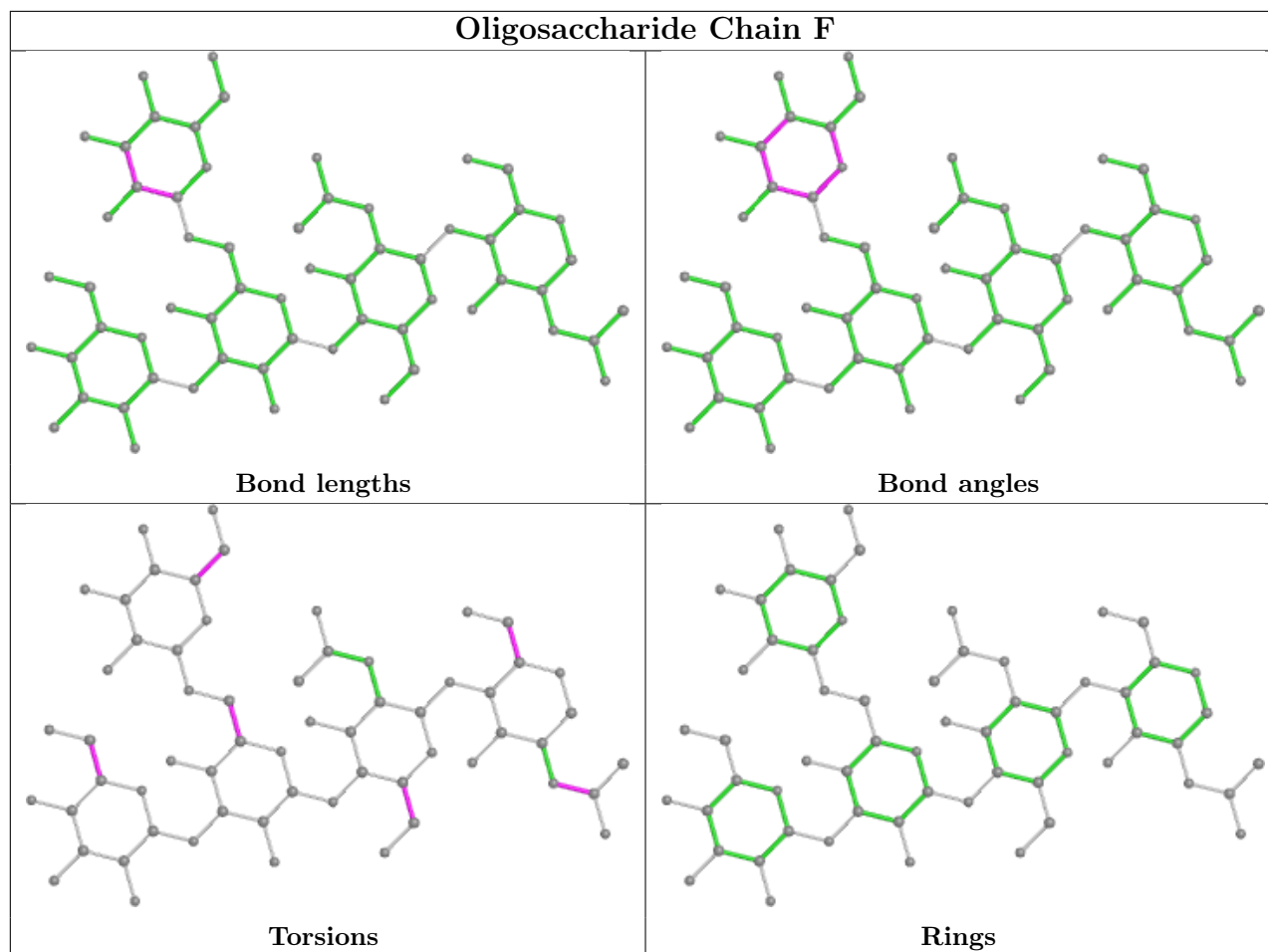

Bond lengths

Bond angles

Torsions

Rings

5.6　Ligand geometry ⓘ

12 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	$\#|Z| > 2$
7	NAG	A	801	1	14,14,15	0.43	0	17,19,21	0.64	1 (5%)
7	NAG	A	805	1	14,14,15	0.35	0	17,19,21	0.53	0
7	NAG	A	803	1	14,14,15	0.43	0	17,19,21	0.45	0
9	PC1	C	304	-	40,40,53	0.30	0	46,48,61	0.40	0
10	CLR	C	303	-	31,31,31	0.57	0	48,48,48	0.88	1 (2%)
7	NAG	A	802	1	14,14,15	0.63	1 (7%)	17,19,21	0.94	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	A	806	1	14,14,15	0.57	0	17,19,21	0.91	1 (5%)
9	PC1	B	502	-	36,36,53	0.32	0	42,44,61	0.44	0
10	CLR	C	301	-	31,31,31	0.65	0	48,48,48	1.25	5 (10%)
10	CLR	C	302	-	31,31,31	0.37	0	48,48,48	1.03	4 (8%)
8	N60	B	501	-	33,35,35	5.26	20 (60%)	47,54,54	1.54	6 (12%)
7	NAG	A	804	1	14,14,15	1.07	1 (7%)	17,19,21	2.22	3 (17%)

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
7	NAG	A	801	1	-	2/6/23/26	0/1/1/1
7	NAG	A	805	1	-	0/6/23/26	0/1/1/1
7	NAG	A	803	1	-	2/6/23/26	0/1/1/1
9	PC1	C	304	-	-	8/44/44/57	-
10	CLR	C	303	-	-	2/10/68/68	0/4/4/4
7	NAG	A	802	1	-	2/6/23/26	0/1/1/1
7	NAG	A	806	1	-	1/6/23/26	0/1/1/1
9	PC1	B	502	-	-	5/40/40/57	-
10	CLR	C	301	-	-	8/10/68/68	0/4/4/4
10	CLR	C	302	-	-	8/10/68/68	0/4/4/4
8	N60	B	501	-	-	0/30/47/47	0/3/3/3
7	NAG	A	804	1	-	5/6/23/26	0/1/1/1

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	501	N60	C23-C14	11.04	1.54	1.39
8	B	501	N60	C26-C21	9.33	1.54	1.40
8	B	501	N60	C28-C22	8.95	1.54	1.39
8	B	501	N60	C24-C16	8.86	1.53	1.40
8	B	501	N60	C16-C14	7.37	1.50	1.40

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	804	NAG	C2-N2-C7	7.69	133.85	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	501	N60	C12-C19-N11	5.60	123.59	116.92
8	B	501	N60	C25-N11-C19	-4.32	117.40	123.24
7	A	804	NAG	C1-C2-N2	3.77	116.94	110.49
10	C	303	CLR	C16-C17-C13	-3.54	99.58	103.84

There are no chirality outliers.
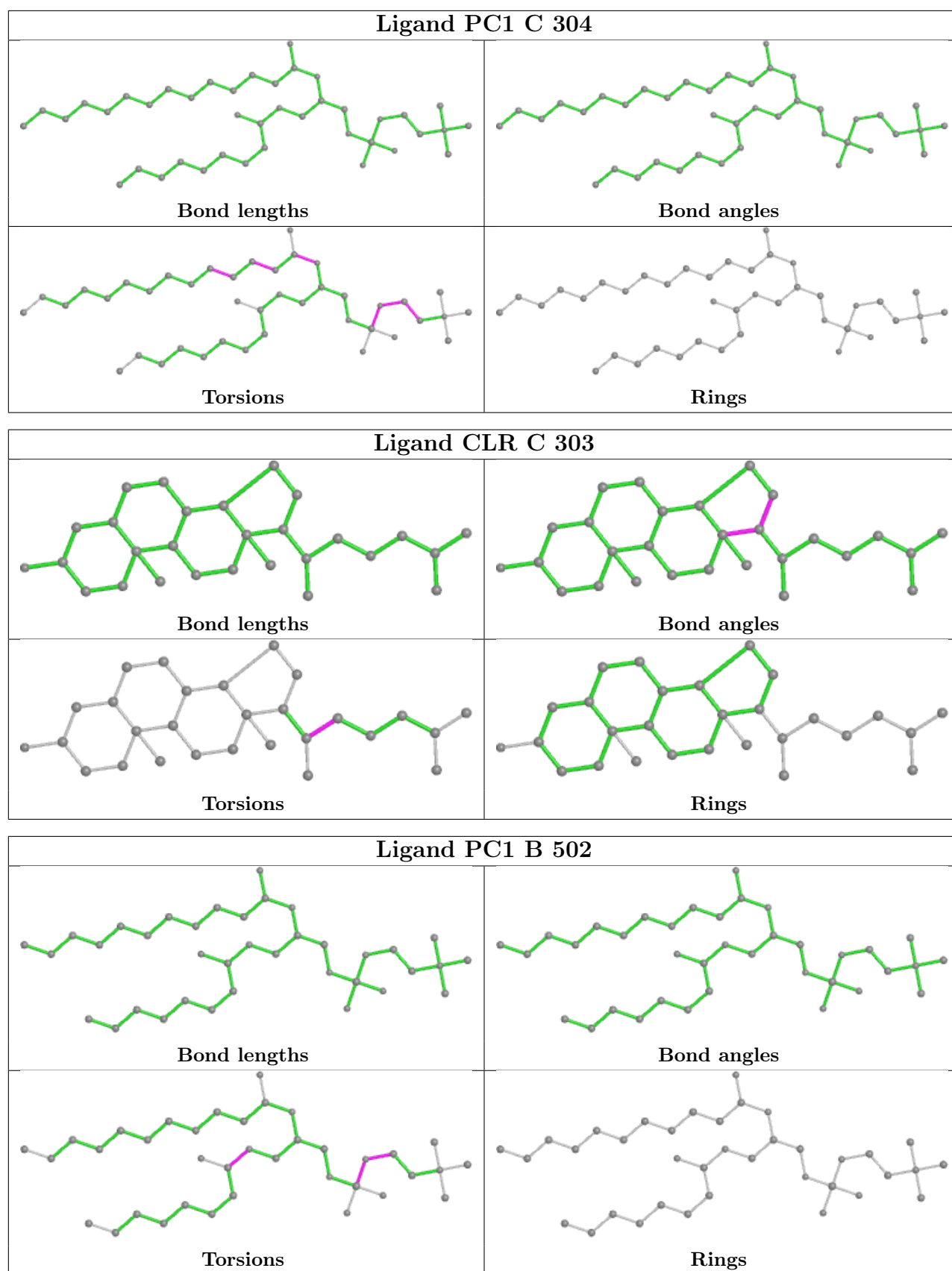
5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	502	PC1	C11-O13-P-O14
9	B	502	PC1	C11-O13-P-O11
9	B	502	PC1	C12-C11-O13-P
9	B	502	PC1	O32-C31-O31-C3
9	B	502	PC1	C32-C31-O31-C3

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	304	PC1	1	0
10	C	303	CLR	1	0
9	B	502	PC1	1	0
10	C	301	CLR	4	0
10	C	302	CLR	12	0
8	B	501	N60	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PC1 C 304

Bond lengths

Bond angles

Torsions

Rings

Ligand CLR C 303

Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 B 502

Bond lengths

Bond angles

Torsions

Rings

Ligand CLR C 301

Bond lengths

Bond angles

Torsions

Rings

Ligand CLR C 302

Bond lengths

Bond angles

Torsions

Rings

Ligand N60 B 501

Bond lengths

Bond angles

Torsions

Rings
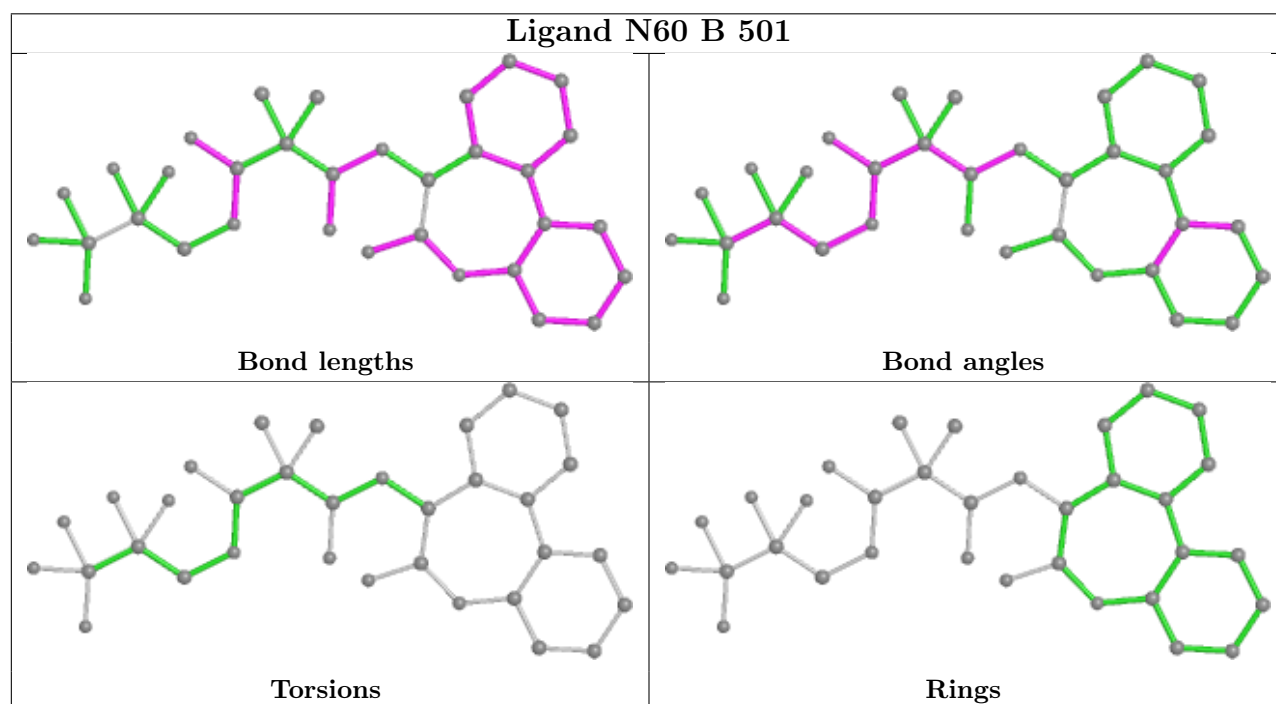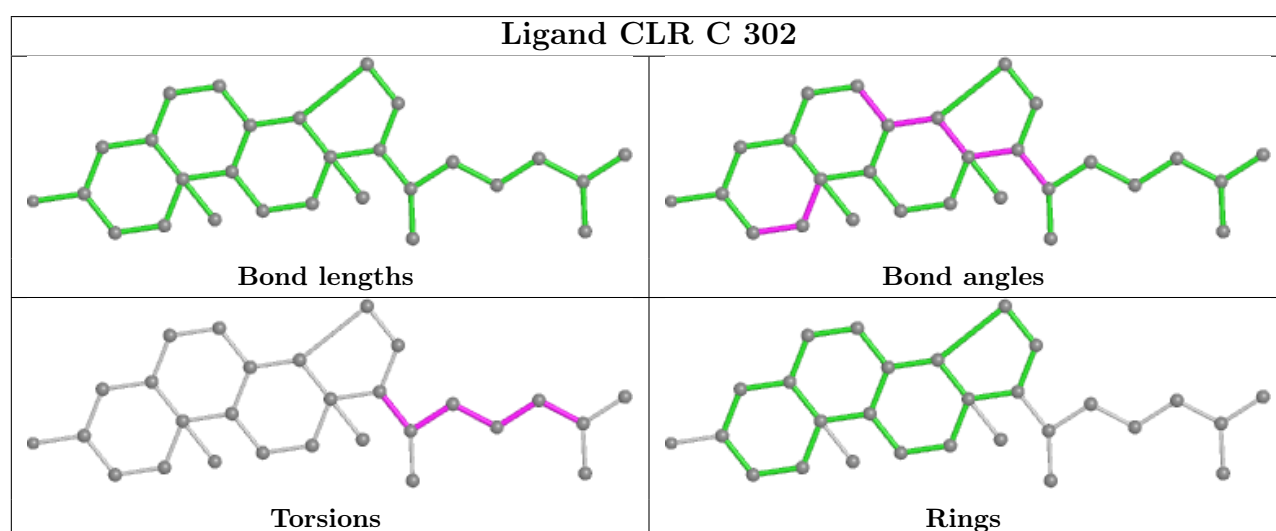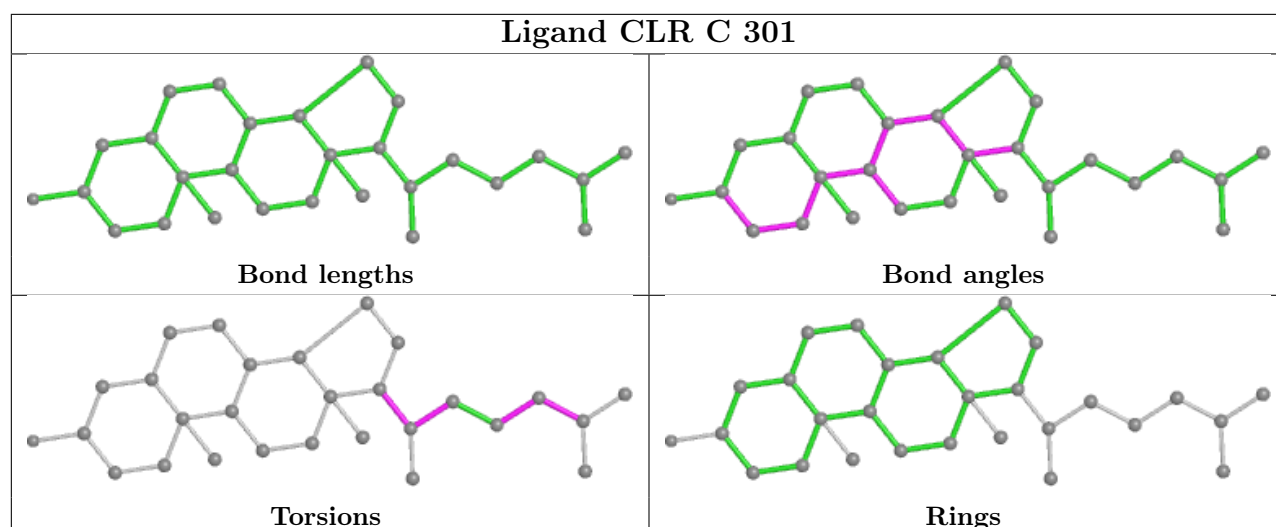
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.