wwPDB EM Validation Summary Report (i)

Jun 11, 2024 – 08:12 PM JST

PDB ID	:	8X52
EMDB ID	:	EMD-38059
Title	:	Cryo-EM structure of human gamma-secretase in complex with Abeta49
Authors	:	Guo, X.; Yan, C.; Lei, J.; Zhou, R.; Shi, Y.
Deposited on	:	2023-11-16
Resolution	:	2.90 Å(reported)

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

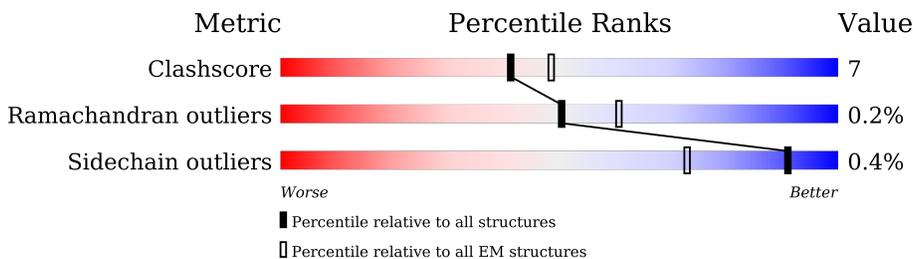|		
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.90 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.
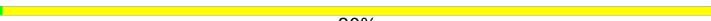
Metric	Percentile Ranks	Value
Clashscore		7
Ramachandran outliers		0.2%
Sidechain outliers		0.4%

Worse *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures

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

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

Mol	Chain	Length	Quality of chain
1	E	120	8% 10% • 82%
2	A	709	83% 11% 6%
3	B	467	52% 12% • 34%
4	C	265	84% 8% 8%
5	D	101	84% 11% 5%
6	F	2	100%
6	H	2	50% 50%
6	I	2	100%
6	J	2	50% 50%

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Mol	Chain	Length	Quality of chain
6	K	2	100%
7	G	5	20%　　　　80%

2 Entry composition ⓘ

There are 10 unique types of molecules in this entry. The entry contains 10907 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 Amyloid-beta precursor protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	E	22	145	97	22	24	2	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	28	CYS	LYS	conflict	UNP P05067
E	100	GLU	-	expression tag	UNP P05067
E	101	GLN	-	expression tag	UNP P05067
E	102	LYS	-	expression tag	UNP P05067
E	103	LEU	-	expression tag	UNP P05067
E	104	ILE	-	expression tag	UNP P05067
E	105	SER	-	expression tag	UNP P05067
E	106	GLU	-	expression tag	UNP P05067
E	107	GLU	-	expression tag	UNP P05067
E	108	ASP	-	expression tag	UNP P05067
E	109	LEU	-	expression tag	UNP P05067
E	110	LEU	-	expression tag	UNP P05067
E	111	GLU	-	expression tag	UNP P05067
E	112	HIS	-	expression tag	UNP P05067
E	113	HIS	-	expression tag	UNP P05067
E	114	HIS	-	expression tag	UNP P05067
E	115	HIS	-	expression tag	UNP P05067
E	116	HIS	-	expression tag	UNP P05067
E	117	HIS	-	expression tag	UNP P05067
E	118	HIS	-	expression tag	UNP P05067
E	119	HIS	-	expression tag	UNP P05067

- Molecule 2 is a protein called Nicastrin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	667	5233	3318	890	1003	22	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	242	CYS	ILE	conflict	UNP Q92542

- Molecule 3 is a protein called Presenilin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	306	Total 2424	C 1640	N 370	O 400	S 14	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	385	ASN	ASP	conflict	UNP P49768

- Molecule 4 is a protein called Gamma-secretase subunit APH-1A.

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

- Molecule 5 is a protein called Gamma-secretase subunit PEN-2.

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

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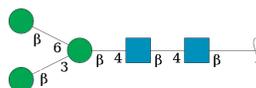

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	2	Total 28	C 16	N 2	O 10	0	0
6	H	2	Total 28	C 16	N 2	O 10	0	0
6	I	2	Total 28	C 16	N 2	O 10	0	0

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

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-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
7	G	5	Total	C	N	O	0	0
			61	34	2	25		

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

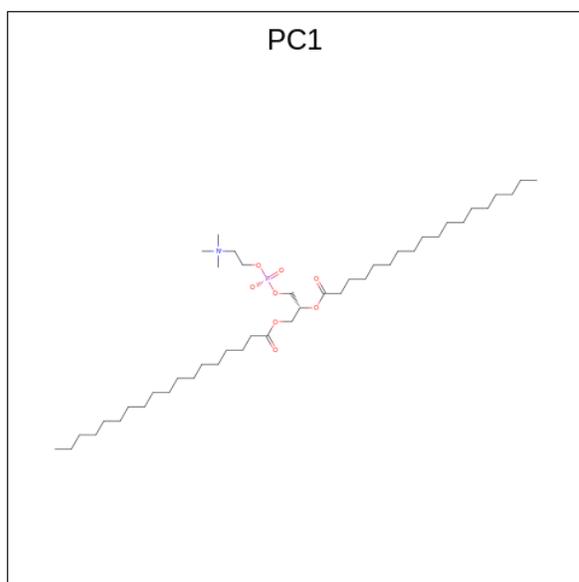| Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	

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

- Molecule 9 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).

PC1

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

- Molecule 10 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).
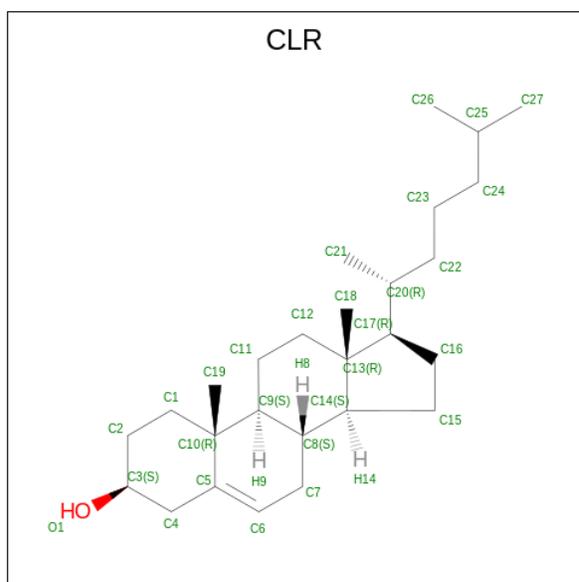
Mol	Chain	Residues	Atoms			AltConf
10	C	1	Total 28	C 27	O 1	0
10	C	1	Total 28	C 27	O 1	0

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: Amyloid-beta precursor protein

Chain E:

- Molecule 2: Nicastrin

Chain A:

- Molecule 3: Presenilin-1

Chain B:

GLU GLU R377 K380 L383 G384 N385 F386 I387 F388 Y389 S390 V391 L392 I414 L432 P433 A434 L435 P436 I437 S438 I439 Q464 I467

• Molecule 4: Gamma-secretase subunit APH-1A

Chain C: 84%   8%   8%

MET G2 L20 I23 T24 R31 V80 I137 G143 V147 G148 I149 H150 T159 S160 L192 H197 T204 N207 Y210 L214 V220 G233 L244 CYS ARG ARG GLN GLU ASP SER ARG VAL MET VAL TYR SER ALA LEU ARG ILE PRO PRO

GLU ASP
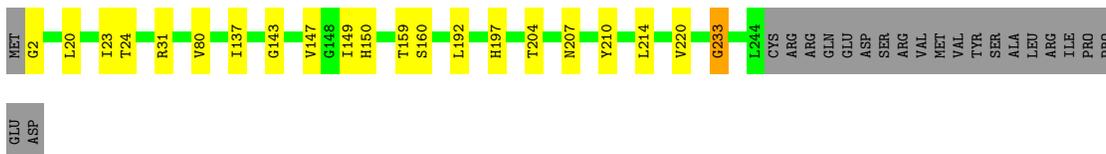
• Molecule 5: Gamma-secretase subunit PEN-2

Chain D: 84%   11%   5%
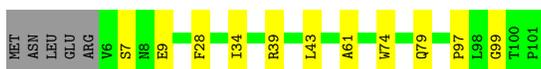
MET ASN LEU GLU ARG V6 S7 N8 E9 F28 I34 R39 L43 A61 W74 Q79 P97 L98 G99 T100 P101

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

Chain F: 100%

NAG1 NAG2

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

Chain H: 50%   50%

NAG1 NAG2

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

Chain I: 100%

NAG1 NAG2

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

Chain J: 50%   50%

NAG1 NAG2

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

Chain K:

• Molecule 7: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose
-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyrano
se

Chain G:

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	463727	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, PC1, NAG, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	E	0.55	0/144	0.98	2/196 (1.0%)
2	A	0.37	0/5356	0.54	0/7299
3	B	0.68	6/2486 (0.2%)	0.71	7/3392 (0.2%)
4	C	0.39	0/1924	0.61	1/2624 (0.0%)
5	D	0.35	0/847	0.48	0/1157
All	All	0.46	6/10757 (0.1%)	0.60	10/14668 (0.1%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	433	PRO	N-CA	12.78	1.69	1.47
3	B	384	GLY	C-O	-8.86	1.09	1.23
3	B	435	LEU	C-N	8.59	1.50	1.34
3	B	433	PRO	C-O	-7.40	1.08	1.23
3	B	386	PHE	C-O	-5.33	1.13	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	233	GLY	N-CA-C	12.39	144.07	113.10
3	B	433	PRO	CA-N-CD	-8.15	100.09	111.50
3	B	112	GLN	CB-CA-C	-6.85	96.70	110.40
3	B	386	PHE	CB-CA-C	-6.40	97.59	110.40
1	E	48	THR	N-CA-C	-5.93	95.00	111.00

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	E	145	0	171	40	0
2	A	5233	0	5121	48	0
3	B	2424	0	2551	91	0
4	C	1872	0	1911	20	0
5	D	814	0	804	9	0
6	F	28	0	25	0	0
6	H	28	0	25	0	0
6	I	28	0	25	0	0
6	J	28	0	25	0	0
6	K	28	0	25	0	0
7	G	61	0	52	0	0
8	A	84	0	78	1	0
9	B	37	0	48	1	0
9	C	41	0	56	3	0
10	C	56	0	92	4	0
All	All	10907	0	11009	162	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 162 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:E:28:CYS:SG	2:A:242:CYS:SG	1.47	1.46
3:B:433:PRO:CA	3:B:433:PRO:N	1.69	1.37
1:E:37:GLY:HA3	3:B:115:TYR:OH	1.49	1.10
3:B:286:LEU:O	3:B:383:LEU:HB2	1.56	1.06
3:B:286:LEU:HD12	3:B:287:ILE:HG13	1.44	0.99

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	E	20/120 (17%)	16 (80%)	3 (15%)	1 (5%)	2	7
2	A	665/709 (94%)	624 (94%)	41 (6%)	0	100	100
3	B	302/467 (65%)	294 (97%)	7 (2%)	1 (0%)	41	71
4	C	241/265 (91%)	234 (97%)	7 (3%)	0	100	100
5	D	94/101 (93%)	90 (96%)	4 (4%)	0	100	100
All	All	1322/1662 (80%)	1258 (95%)	62 (5%)	2 (0%)	50	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	46	VAL
3	B	117	PRO

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	E	16/106 (15%)	16 (100%)	0	100	100
2	A	584/612 (95%)	584 (100%)	0	100	100
3	B	264/408 (65%)	260 (98%)	4 (2%)	65	87
4	C	193/214 (90%)	193 (100%)	0	100	100
5	D	84/89 (94%)	84 (100%)	0	100	100
All	All	1141/1429 (80%)	1137 (100%)	4 (0%)	91	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	139	MET
3	B	163	HIS
3	B	261	VAL
3	B	435	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	691	ASN
3	B	464	GLN
3	B	81	HIS
4	C	207	ASN
3	B	405	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	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
6	NAG	F	1	2,6	14,14,15	0.26	0	17,19,21	0.42	0
6	NAG	F	2	6	14,14,15	0.24	0	17,19,21	0.59	0
7	NAG	G	1	2,7	14,14,15	0.26	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
7	NAG	G	2	7	14,14,15	0.21	0	17,19,21	0.64	1 (5%)
7	BMA	G	3	7	11,11,12	0.67	0	15,15,17	0.89	1 (6%)
7	BMA	G	4	7	11,11,12	0.67	0	15,15,17	0.92	1 (6%)
7	BMA	G	5	7	11,11,12	1.59	3 (27%)	15,15,17	1.90	4 (26%)
6	NAG	H	1	2,6	14,14,15	0.34	0	17,19,21	1.06	1 (5%)
6	NAG	H	2	6	14,14,15	0.39	0	17,19,21	0.50	0
6	NAG	I	1	6	14,14,15	0.23	0	17,19,21	0.47	0
6	NAG	I	2	6	14,14,15	0.22	0	17,19,21	0.56	0
6	NAG	J	1	2,6	14,14,15	0.23	0	17,19,21	0.51	0
6	NAG	J	2	6	14,14,15	0.72	1 (7%)	17,19,21	2.23	3 (17%)
6	NAG	K	1	2,6	14,14,15	0.33	0	17,19,21	0.53	0
6	NAG	K	2	6	14,14,15	0.26	0	17,19,21	0.49	0

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	5	BMA	C2-C3	3.11	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	5	BMA	C1-C2	2.94	1.58	1.52
7	G	5	BMA	O5-C1	2.07	1.47	1.43
6	J	2	NAG	C1-C2	2.01	1.55	1.52

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	2	NAG	C2-N2-C7	7.76	133.96	122.90
7	G	5	BMA	C1-O5-C5	5.02	119.00	112.19
6	J	2	NAG	C1-C2-N2	3.68	116.77	110.49
6	H	1	NAG	C2-N2-C7	3.19	127.44	122.90
7	G	5	BMA	C1-C2-C3	3.02	113.38	109.67

There are no chirality outliers.

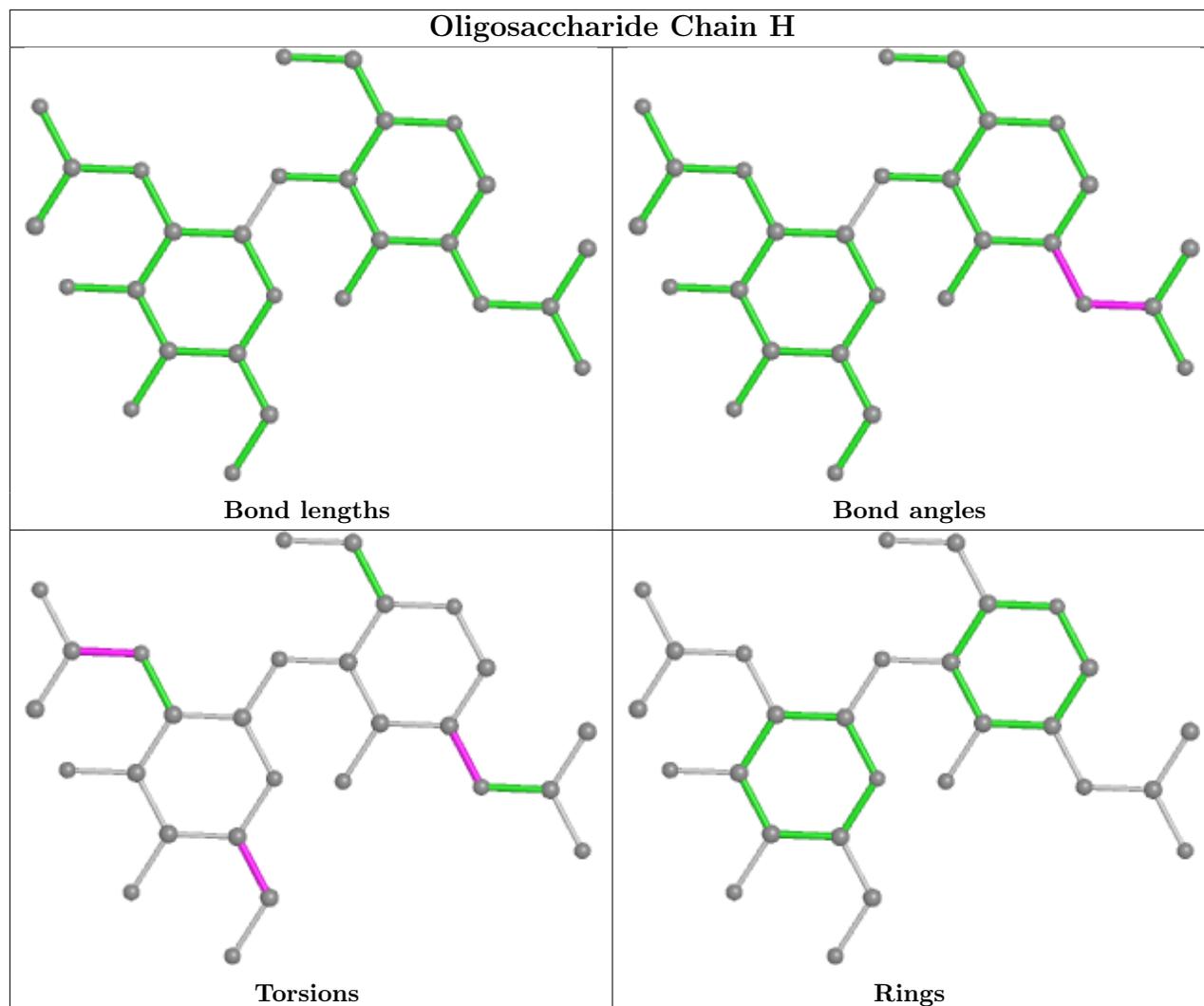5 of 28 torsion outliers are listed below:

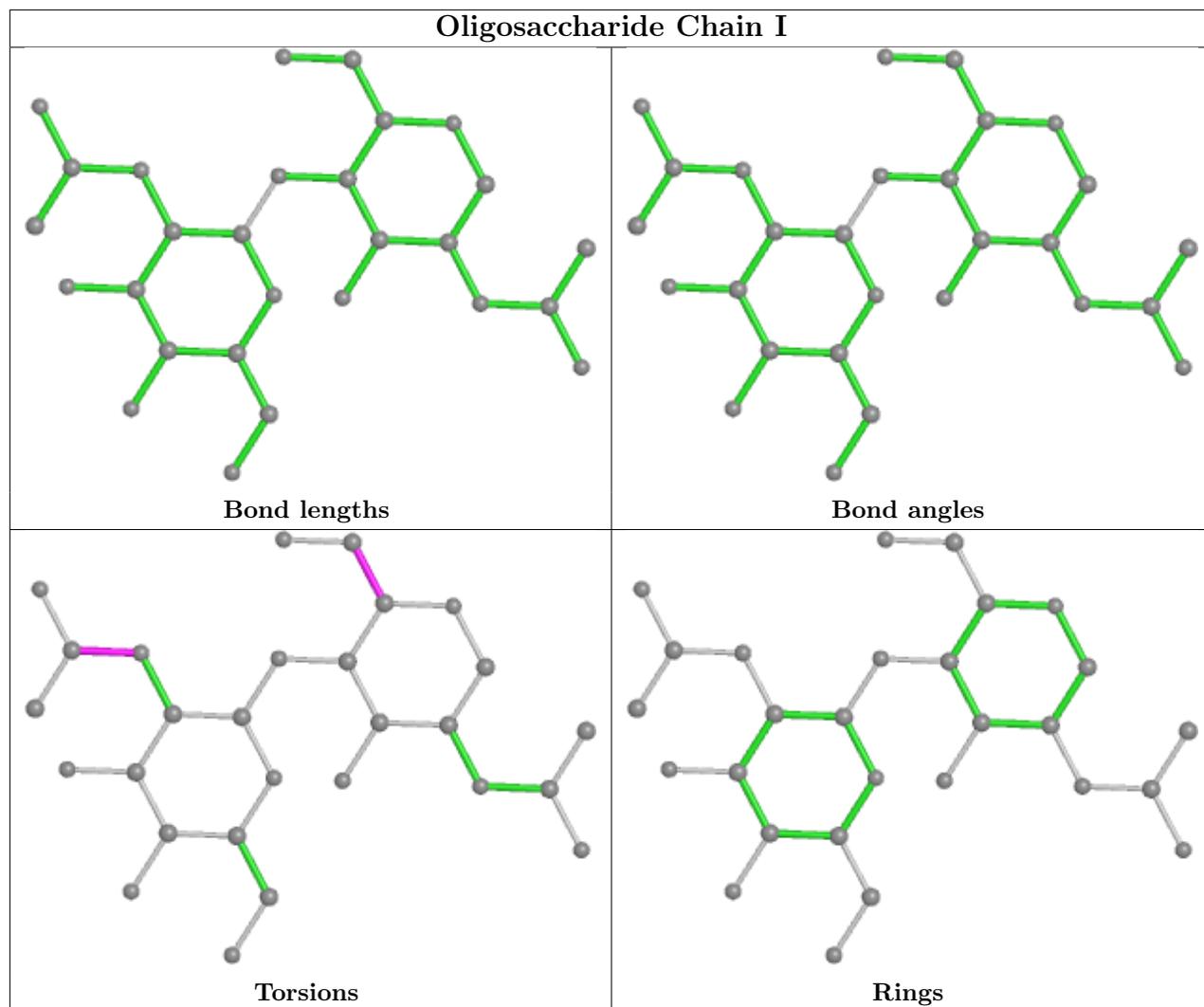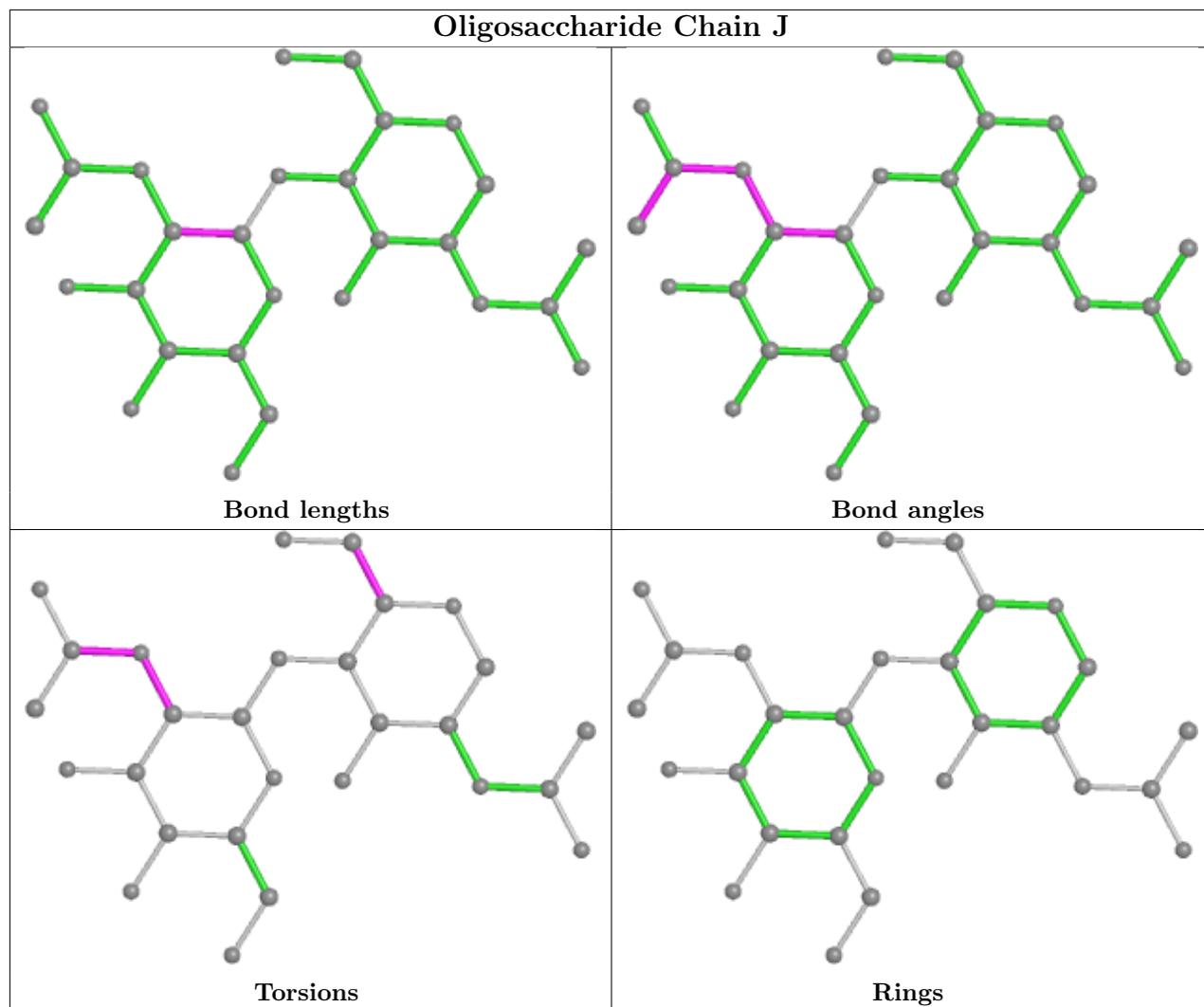| Mol	Chain	Res	Type	Atoms
6	J	1	NAG	O5-C5-C6-O6
7	G	3	BMA	C4-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
6	J	1	NAG	C4-C5-C6-O6
7	G	3	BMA	O5-C5-C6-O6

There are no ring outliers.
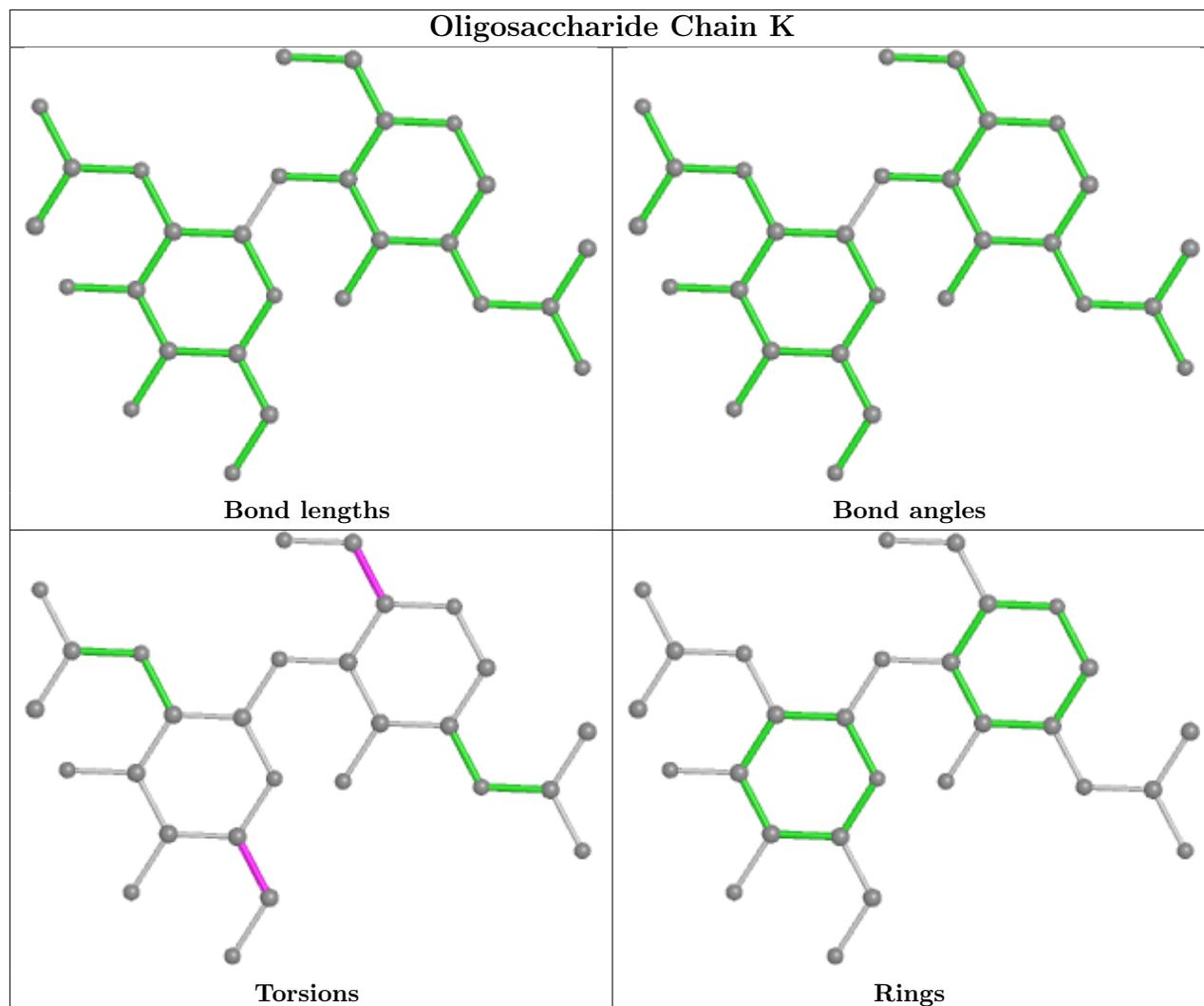
No monomer is involved in short contacts.

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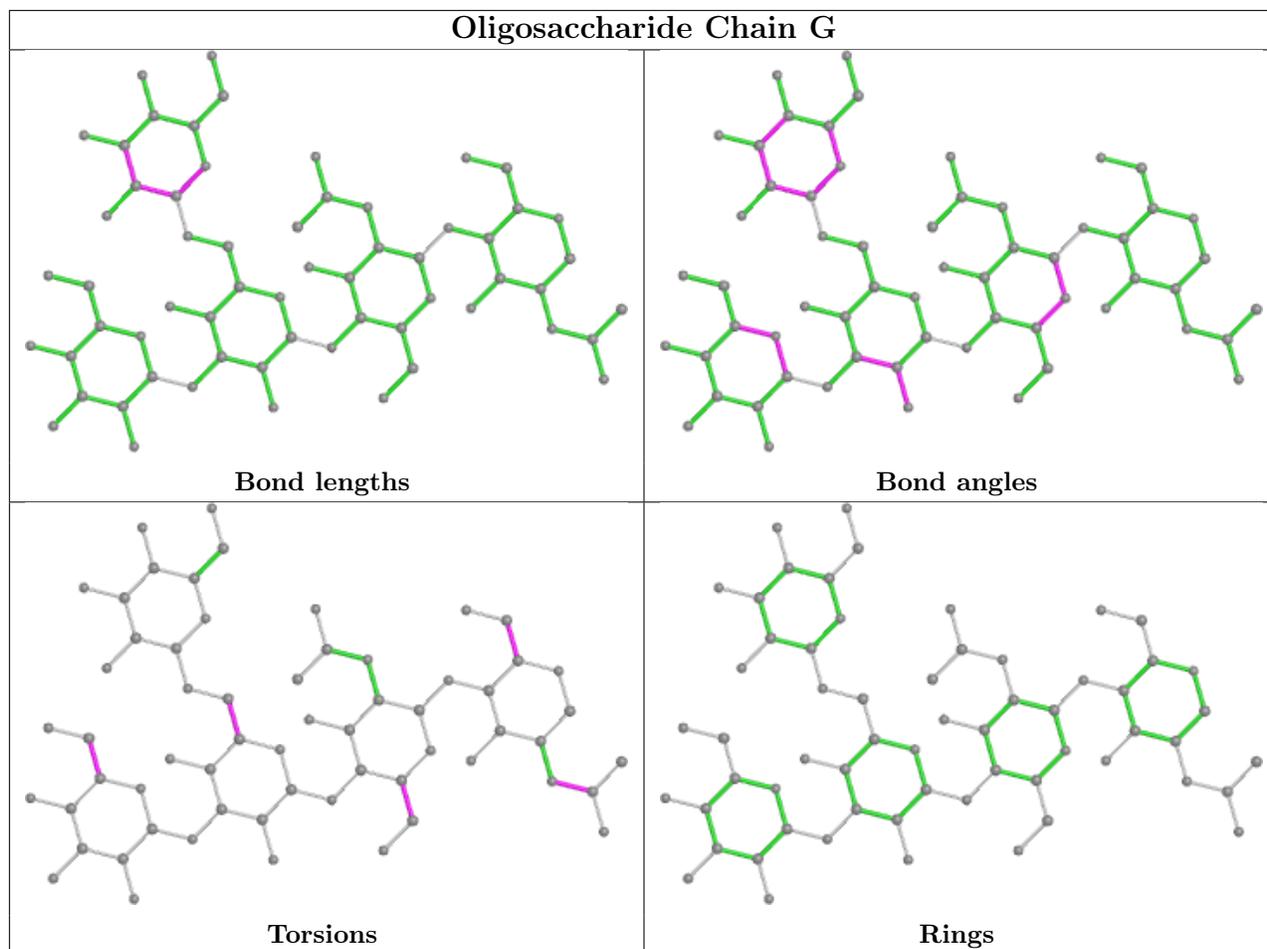
Oligosaccharide Chain F

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 K

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

5.6 Ligand geometry (i)

10 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
9	PC1	B	801	-	36,36,53	0.31	0	42,44,61	0.34	0
8	NAG	A	806	2	14,14,15	0.22	0	17,19,21	0.61	1 (5%)
8	NAG	A	803	2	14,14,15	0.46	0	17,19,21	0.47	0
8	NAG	A	801	2	14,14,15	0.37	0	17,19,21	0.58	1 (5%)
8	NAG	A	805	2	14,14,15	0.26	0	17,19,21	0.47	0
9	PC1	C	403	-	40,40,53	0.30	0	46,48,61	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
8	NAG	A	804	2	14,14,15	0.91	1 (7%)	17,19,21	2.26	3 (17%)
8	NAG	A	802	2	14,14,15	0.51	0	17,19,21	1.01	1 (5%)
10	CLR	C	401	-	31,31,31	0.29	0	48,48,48	0.33	0
10	CLR	C	402	-	31,31,31	0.28	0	48,48,48	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
9	PC1	B	801	-	-	11/40/40/57	-
8	NAG	A	806	2	-	0/6/23/26	0/1/1/1
8	NAG	A	803	2	-	2/6/23/26	0/1/1/1
8	NAG	A	801	2	-	0/6/23/26	0/1/1/1
8	NAG	A	805	2	-	0/6/23/26	0/1/1/1
9	PC1	C	403	-	-	7/44/44/57	-
8	NAG	A	804	2	-	5/6/23/26	0/1/1/1
8	NAG	A	802	2	-	3/6/23/26	0/1/1/1
10	CLR	C	401	-	-	9/10/68/68	0/4/4/4
10	CLR	C	402	-	-	6/10/68/68	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	804	NAG	C1-C2	2.88	1.56	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	804	NAG	C2-N2-C7	7.89	134.13	122.90
8	A	804	NAG	C1-C2-N2	3.71	116.82	110.49
8	A	802	NAG	C2-N2-C7	3.11	127.33	122.90
8	A	804	NAG	C8-C7-N2	2.13	119.71	116.10
8	A	806	NAG	C1-O5-C5	2.12	115.07	112.19

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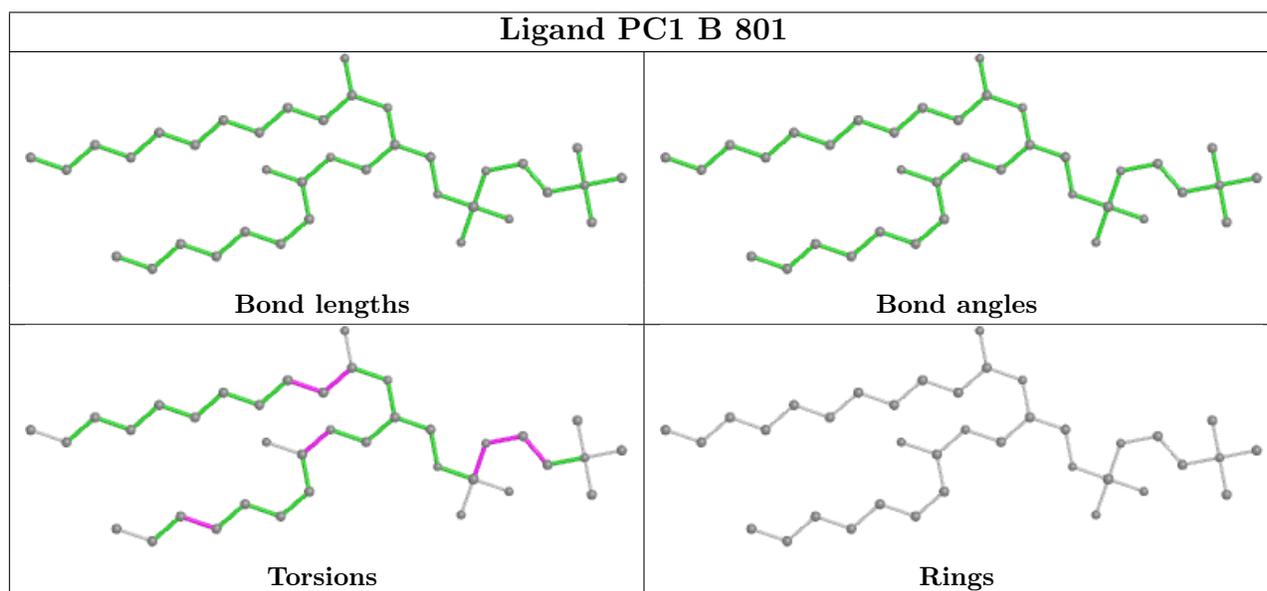
5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	801	PC1	C11-O13-P-O14
9	C	403	PC1	C11-O13-P-O14
9	C	403	PC1	C12-C11-O13-P
9	C	403	PC1	O22-C21-O21-C2
8	A	802	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	801	PC1	1	0
9	C	403	PC1	3	0
8	A	804	NAG	1	0
10	C	401	CLR	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 B 801

Bond lengths   Bond angles

Torsions   Rings

Ligand PC1 C 403	
Bond lengths	Bond angles
Torsions	Rings

Ligand CLR C 401	
Bond lengths	Bond angles
Torsions	Rings

Ligand CLR C 402	
Bond lengths	Bond angles
Torsions	Rings
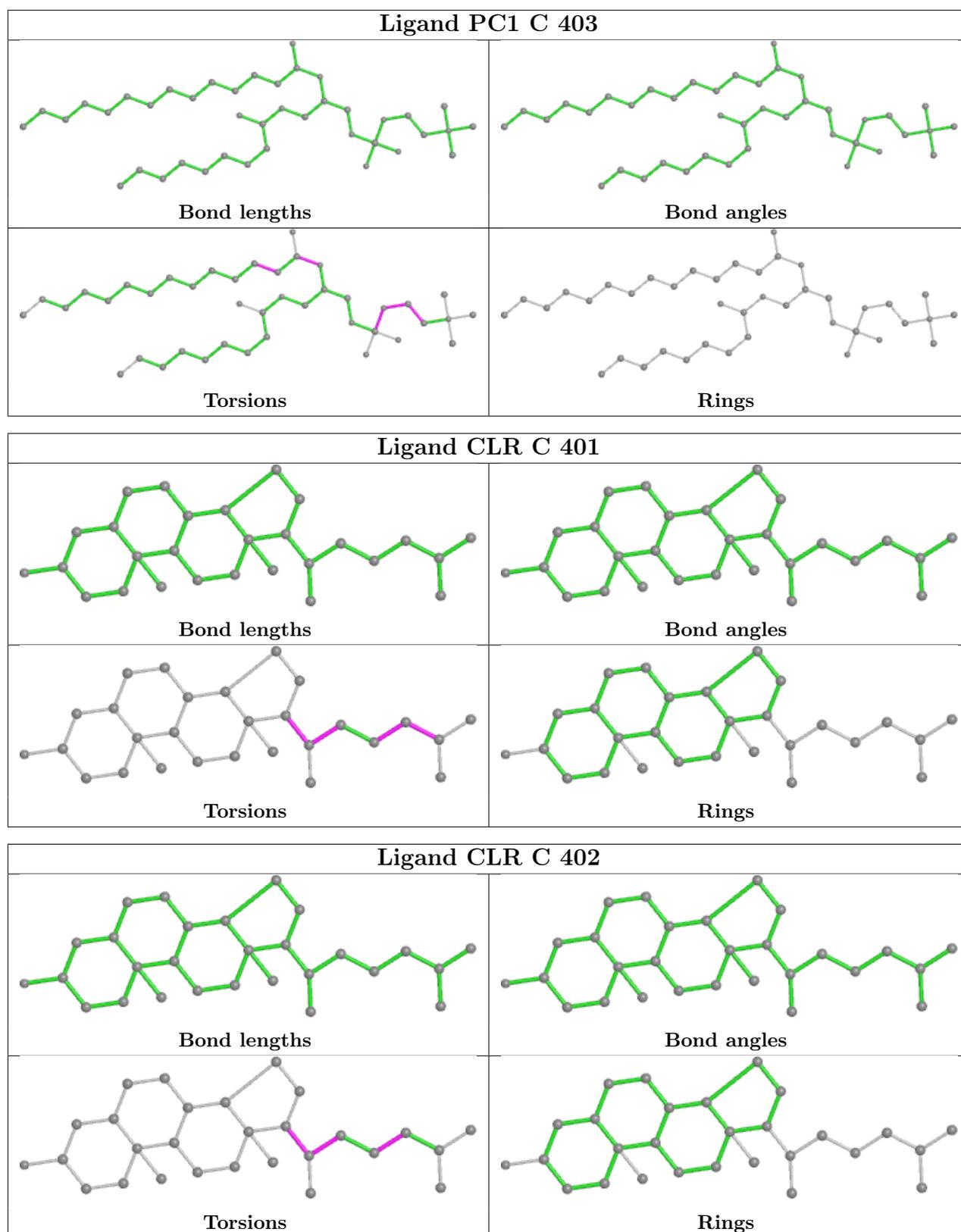
5.7   Other polymers ⓘ

There are no such residues in this entry.

5.8   Polymer linkage issues ⓘ

There are no chain breaks in this entry.