



Full wwPDB EM Validation Report ⓘ

Apr 16, 2026 – 12:36 PM JST

PDB ID : 9L6R / pdb_00009l6r
EMDB ID : EMD-62863
Title : double-mutant (K217A & K218A) Vitamin K-dependent gamma-carboxylase
in complex with Coagulation factor IX and vitamin K
Authors : Hang, J.; Chen, D.D.; Zhong, Q.H.
Deposited on : 2024-12-25
Resolution : 2.59 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

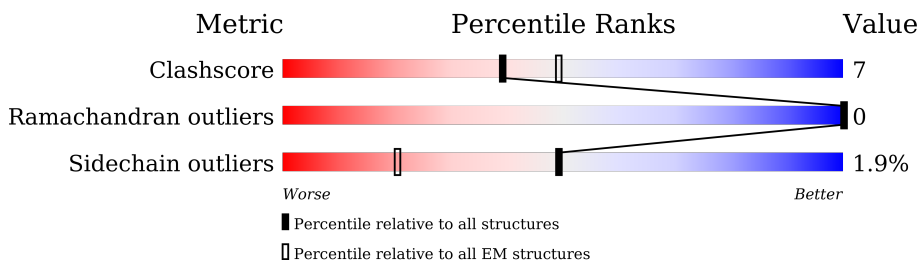
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.59 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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

Mol	Chain	Length	Quality of chain
1	C	461	 5% • 94%
2	A	758	 75% 16% 9%
3	B	3	 100%
3	E	3	 67% 33%
4	D	2	 100%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6124 atoms, of which 42 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 Coagulation factor IX.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	C	29	Total	C	N	O	0	0
			224	141	40	43		

- Molecule 2 is a protein called Vitamin K-dependent gamma-carboxylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	690	Total	C	N	O	S	0	0
			5595	3659	929	980	27		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	217	ALA	LYS	engineered mutation	UNP P38435
A	218	ALA	LYS	engineered mutation	UNP P38435

- Molecule 3 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.



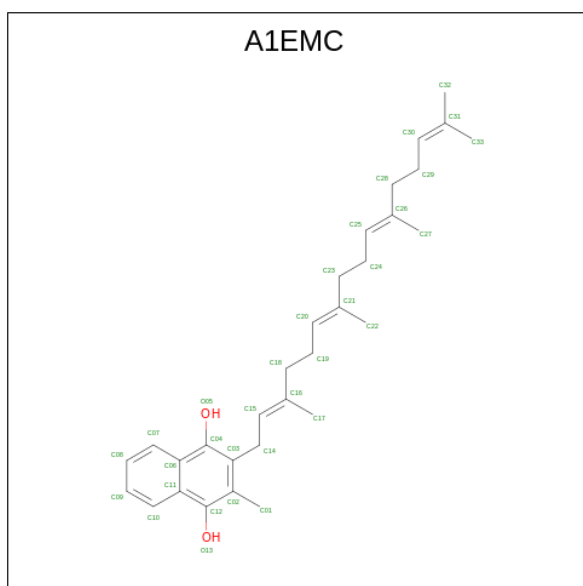
Mol	Chain	Residues	Atoms				AltConf	Trace
3	B	3	Total	C	N	O	0	0
			39	22	2	15		
3	E	3	Total	C	N	O	0	0
			39	22	2	15		

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



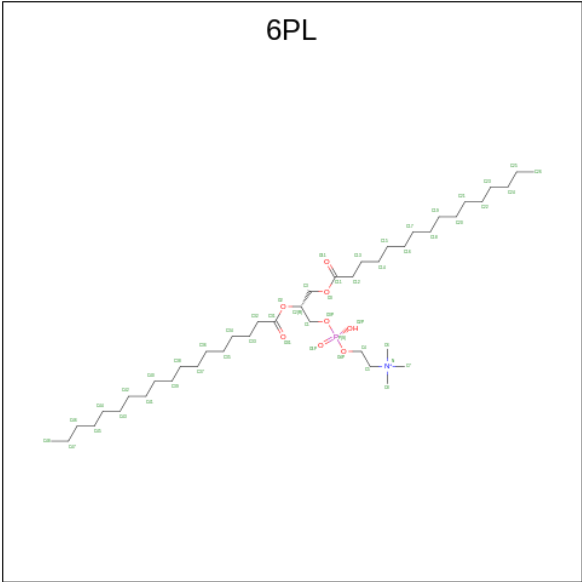
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-methyl-3-[(2 {E},6 {E},10 {E})-3,7,11,15-tetramethylhexadeca-2,6,10,14-tetraenyl]naphthalene-1,4-diol (CCD ID: A1EMC) (formula: C₃₁H₄₂O₂).



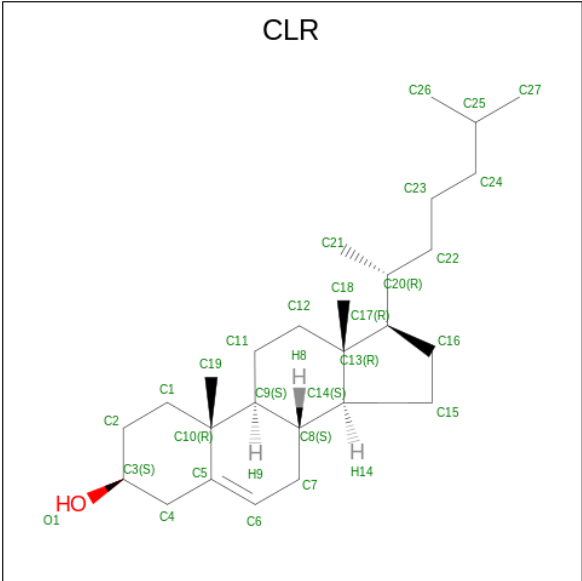
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	H	O	0
			75	31	42	2	

- Molecule 6 is (4S,7R)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (CCD ID: 6PL) (formula: C₄₂H₈₅NO₈P) (labeled as "Ligand of Interest" by depositor).

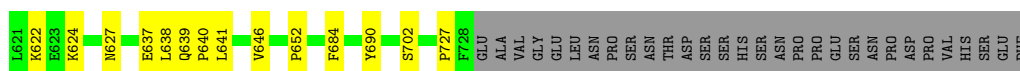


Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
6	A	1	Total	C	N	O	P	0
			50	40	1	8	1	

- Molecule 7 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O) (labeled as "Ligand of Interest" by depositor).



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



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  100%



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  67%  33%



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

Chain D:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	95734	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (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: NAG, 6PL, CLR, BMA, A1EMC

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	C	0.11	0/227	0.23	0/306
2	A	0.07	0/5761	0.20	0/7845
All	All	0.08	0/5988	0.20	0/8151

There are no bond length outliers.

There are no bond angle outliers.

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	C	224	0	208	10	0
2	A	5595	0	5490	80	0
3	B	39	0	34	0	0
3	E	39	0	34	0	0
4	D	28	0	25	0	0
5	A	33	42	0	2	0
6	A	96	0	143	4	0
7	A	28	0	46	1	0
All	All	6082	42	5980	87	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.

All (87) 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:A:646:VAL:HG11	2:A:652:PRO:HD3	1.72	0.71
2:A:61:PRO:HG3	2:A:193:ALA:O	1.90	0.70
7:A:803:CLR:H183	7:A:803:CLR:H212	1.75	0.69
2:A:524:ASP:OD1	2:A:525:ASN:N	2.26	0.68
2:A:637:GLU:O	2:A:640:PRO:HD2	1.94	0.68
6:A:802:6PL:H52	6:A:802:6PL:O2P	1.93	0.68
2:A:609:LEU:O	2:A:613:GLN:HG3	1.95	0.67
2:A:228:SER:O	2:A:256:HIS:NE2	2.24	0.64
2:A:624:LYS:HA	2:A:627:ASN:HD21	1.62	0.64
2:A:646:VAL:HG21	2:A:652:PRO:HG3	1.78	0.63
2:A:415:TYR:HA	2:A:464:GLN:O	1.98	0.63
2:A:255:VAL:HA	5:A:801:A1EMC:C22	2.27	0.63
2:A:305:ALA:O	2:A:308:PRO:HD2	1.98	0.63
2:A:529:VAL:HA	2:A:601:TYR:O	2.00	0.60
2:A:315:TRP:CG	2:A:316:PRO:HD3	2.38	0.59
2:A:624:LYS:HA	2:A:627:ASN:ND2	2.19	0.58
2:A:227:TYR:O	2:A:230:GLU:HG2	2.04	0.57
2:A:622:LYS:O	2:A:622:LYS:HD3	2.03	0.57
2:A:357:GLY:O	2:A:361:GLN:HG3	2.05	0.57
2:A:245:LEU:HD22	2:A:249:LEU:HD23	1.86	0.56
2:A:445:LYS:NZ	2:A:491:ALA:O	2.37	0.55
2:A:75:MET:HE2	2:A:75:MET:HA	1.90	0.54
2:A:454:LEU:O	2:A:457:LYS:HG2	2.09	0.53
2:A:331:LEU:HB3	2:A:332:PRO:HD2	1.90	0.53
2:A:470:TRP:CZ2	2:A:540:LEU:HD13	2.45	0.51
1:C:51:LYS:HZ3	2:A:405:SER:HB2	1.76	0.51
1:C:40:ILE:HD13	2:A:410:HIS:CD2	2.45	0.51
2:A:245:LEU:CD2	2:A:249:LEU:HD23	2.40	0.51
1:C:39:LYS:HG2	1:C:42:ASN:CG	2.36	0.50
1:C:29:THR:HG22	1:C:31:PHE:O	2.12	0.50
2:A:61:PRO:HB3	2:A:195:VAL:HG13	1.93	0.50
2:A:546:GLU:O	2:A:546:GLU:OE2	2.30	0.50
2:A:456:PRO:HA	2:A:460:VAL:O	2.12	0.50
2:A:388:ASN:OD1	2:A:393:GLY:N	2.43	0.49
2:A:684:PHE:HZ	6:A:804:6PL:H12	1.77	0.49
1:C:51:LYS:NZ	2:A:405:SER:HB2	2.28	0.48
2:A:638:LEU:HG	2:A:641:LEU:HD12	1.94	0.48
1:C:33:ASP:N	1:C:33:ASP:OD1	2.46	0.48
2:A:135:TYR:CZ	2:A:176:ALA:HB3	2.49	0.47
2:A:315:TRP:CD1	2:A:316:PRO:HD3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:55:LEU:HD13	2:A:367:THR:HG21	1.97	0.47
2:A:82:GLU:O	2:A:82:GLU:HG3	2.14	0.47
2:A:108:ARG:H	2:A:108:ARG:HD2	1.80	0.47
2:A:108:ARG:HD2	2:A:108:ARG:O	2.15	0.46
1:C:29:THR:O	2:A:427:ASN:HB2	2.14	0.46
2:A:228:SER:C	2:A:229:MET:HG3	2.41	0.46
2:A:512:TRP:O	2:A:516:LEU:HG	2.15	0.46
2:A:551:THR:HG23	2:A:603:TYR:HB3	1.97	0.46
2:A:229:MET:HE1	5:A:801:A1EMC:C17	2.46	0.46
2:A:190:ARG:HG3	2:A:190:ARG:HH11	1.81	0.46
2:A:162:TYR:CE2	2:A:166:LEU:HD11	2.49	0.46
2:A:461:THR:HG22	2:A:462:GLU:HG2	1.98	0.46
2:A:430:VAL:HG13	2:A:431:PHE:CD2	2.51	0.45
2:A:239:SER:N	2:A:240:PRO:HD2	2.31	0.45
2:A:411:VAL:HG21	2:A:438:LYS:HD3	1.98	0.45
2:A:192:ASN:O	2:A:338:GLN:HG2	2.17	0.45
2:A:68:ARG:HD3	2:A:129:MET:O	2.17	0.44
2:A:442:ASP:HB3	2:A:493:TRP:CZ2	2.52	0.44
1:C:49:SER:HB2	2:A:405:SER:OG	2.18	0.44
1:C:51:LYS:HE3	1:C:51:LYS:HA	1.99	0.44
2:A:80:PRO:HA	2:A:85:LEU:HB3	1.99	0.44
2:A:192:ASN:OD1	2:A:317:ARG:NH2	2.50	0.44
2:A:305:ALA:HA	6:A:804:6PL:H441	1.98	0.44
2:A:136:ARG:HH11	2:A:136:ARG:HG2	1.83	0.44
2:A:208:PHE:HD1	2:A:267:GLY:HA3	1.81	0.43
2:A:324:PRO:O	2:A:328:GLN:HG3	2.18	0.43
2:A:279:GLY:O	2:A:283:VAL:HG22	2.18	0.43
2:A:37:LEU:O	6:A:802:6PL:H83	2.18	0.43
2:A:377:LEU:N	2:A:378:PRO:HD2	2.33	0.43
2:A:690:TYR:HB2	2:A:727:PRO:CG	2.48	0.43
1:C:39:LYS:HB2	1:C:39:LYS:HE3	1.42	0.42
2:A:591:THR:HG23	2:A:597:SER:OG	2.18	0.42
2:A:223:TRP:CH2	2:A:229:MET:HE1	2.55	0.42
2:A:620:GLU:HG2	2:A:624:LYS:HE3	2.01	0.42
2:A:401:MET:HE2	2:A:401:MET:HB2	1.88	0.42
2:A:639:GLN:HB2	2:A:640:PRO:HD3	2.02	0.42
2:A:96:LEU:HG	2:A:98:VAL:HG23	2.01	0.42
2:A:690:TYR:HB2	2:A:727:PRO:HD3	2.02	0.42
2:A:262:LEU:HD12	2:A:262:LEU:HA	1.85	0.42
2:A:477:PHE:CE1	2:A:531:PHE:HB3	2.55	0.41
2:A:90:ARG:HH11	2:A:90:ARG:HG3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:455:LEU:HD23	2:A:455:LEU:HA	1.93	0.41
2:A:481:ILE:HG23	2:A:482:PHE:CD2	2.56	0.41
2:A:473:ILE:O	2:A:473:ILE:HG23	2.21	0.41
2:A:155:THR:HG22	2:A:436:ARG:HB3	2.02	0.40
2:A:174:MET:HE1	2:A:203:LEU:HG	2.04	0.40
2:A:273:ASP:OD1	2:A:273:ASP:N	2.38	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	27/461 (6%)	26 (96%)	1 (4%)	0	100	100
2	A	686/758 (90%)	675 (98%)	11 (2%)	0	100	100
All	All	713/1219 (58%)	701 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	C	23/403 (6%)	23 (100%)	0	100	100
2	A	603/679 (89%)	591 (98%)	12 (2%)	48	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	626/1082 (58%)	614 (98%)	12 (2%)	49 75

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	34	ILE
2	A	37	LEU
2	A	108	ARG
2	A	228	SER
2	A	314	GLU
2	A	319	LEU
2	A	341	VAL
2	A	372	LEU
2	A	471	VAL
2	A	595	SER
2	A	611	LEU
2	A	702	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	170	GLN
2	A	199	ASN
2	A	427	ASN
2	A	440	HIS
2	A	474	ASN
2	A	503	GLN
2	A	517	GLN
2	A	526	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

8 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$
3	NAG	B	1	3,2	14,14,15	0.41	0	17,19,21	0.34	0
3	NAG	B	2	3	14,14,15	0.39	0	17,19,21	0.46	0
3	BMA	B	3	3	11,11,12	0.19	0	15,15,17	0.59	0
4	NAG	D	1	4,2	14,14,15	0.39	0	17,19,21	0.36	0
4	NAG	D	2	4	14,14,15	0.39	0	17,19,21	0.53	0
3	NAG	E	1	3,2	14,14,15	0.38	0	17,19,21	0.45	0
3	NAG	E	2	3	14,14,15	0.39	0	17,19,21	0.68	1 (5%)
3	BMA	E	3	3	11,11,12	0.17	0	15,15,17	0.58	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
3	NAG	B	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	B	2	3	-	2/6/23/26	0/1/1/1
3	BMA	B	3	3	-	1/2/19/22	1/1/1/1
4	NAG	D	1	4,2	-	1/6/23/26	0/1/1/1
4	NAG	D	2	4	-	3/6/23/26	0/1/1/1
3	NAG	E	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	1/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	NAG	C2-N2-C7	2.37	126.28	122.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

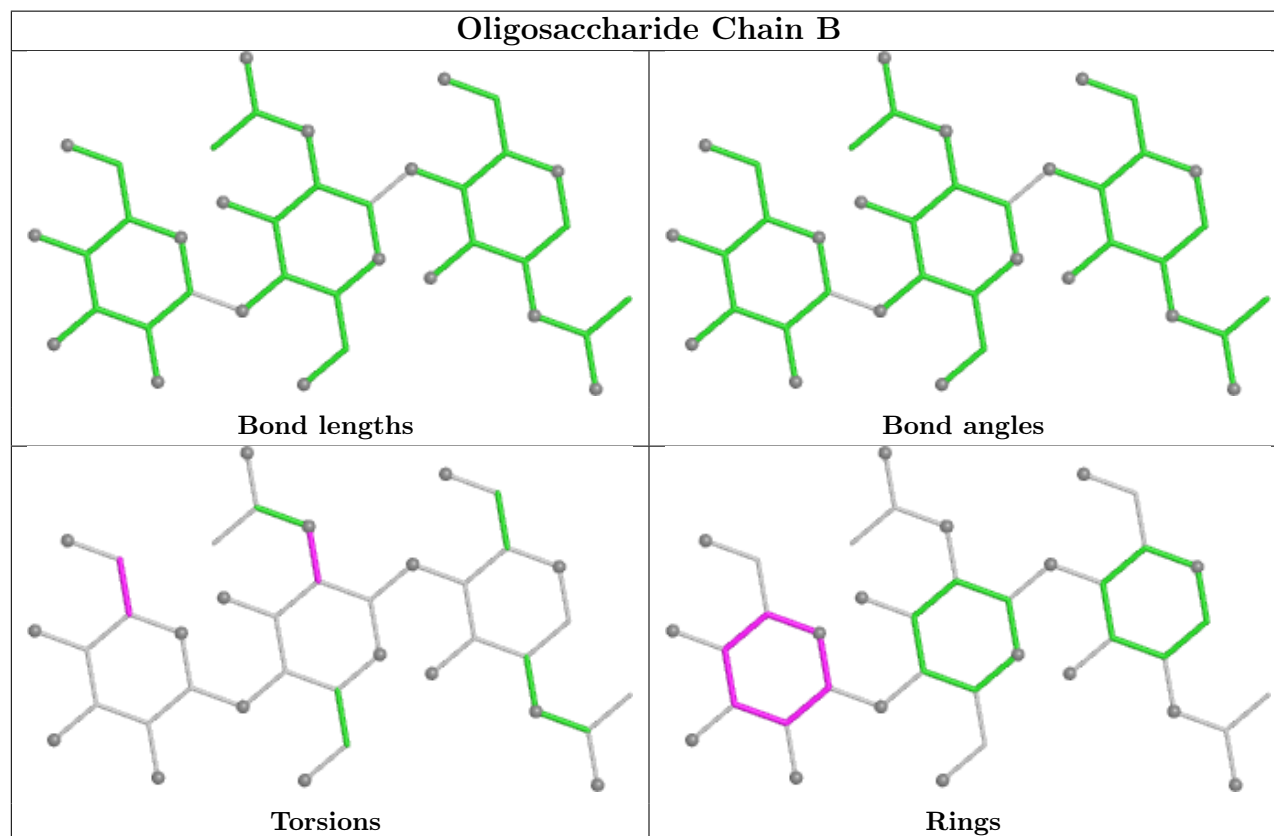
Mol	Chain	Res	Type	Atoms
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
3	B	3	BMA	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
3	B	2	NAG	C1-C2-N2-C7
4	D	2	NAG	C1-C2-N2-C7
3	E	2	NAG	C3-C2-N2-C7
3	B	2	NAG	C3-C2-N2-C7

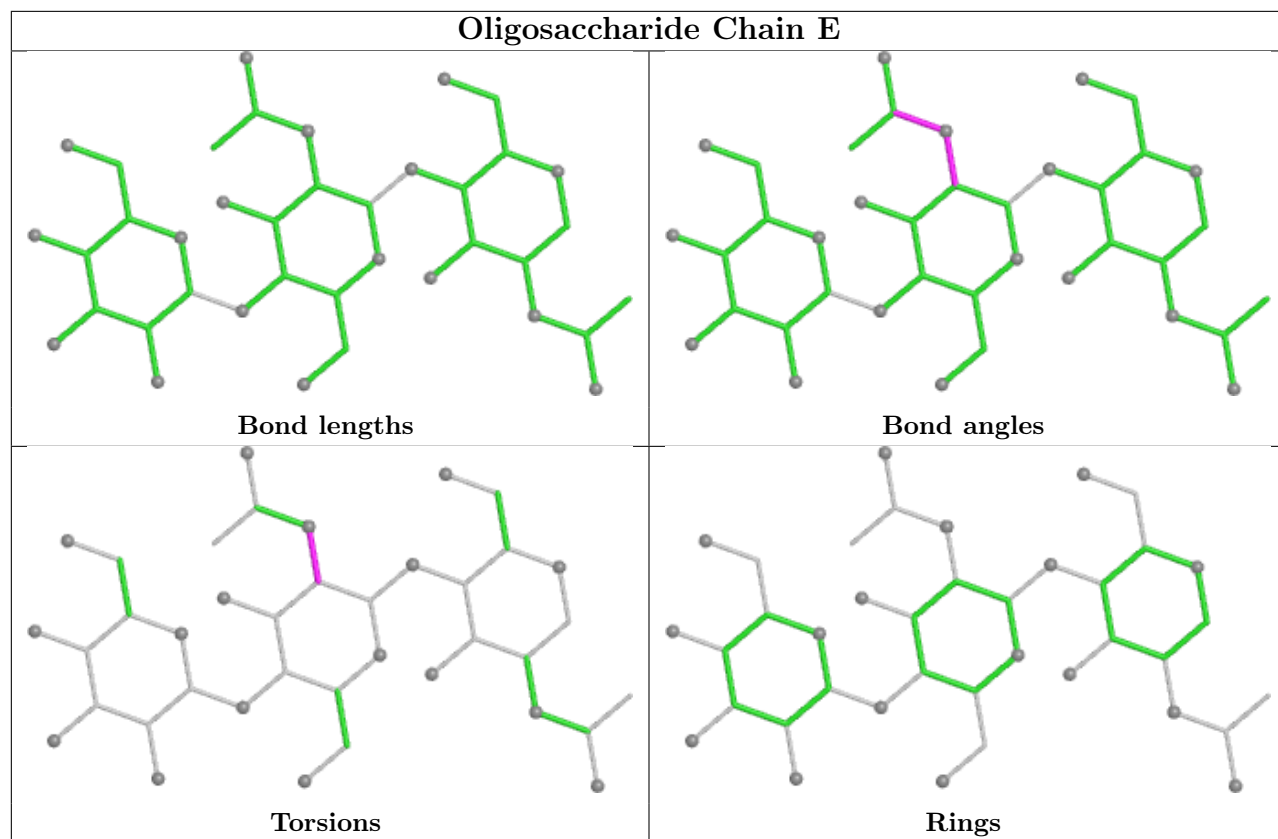
All (1) ring outliers are listed below:

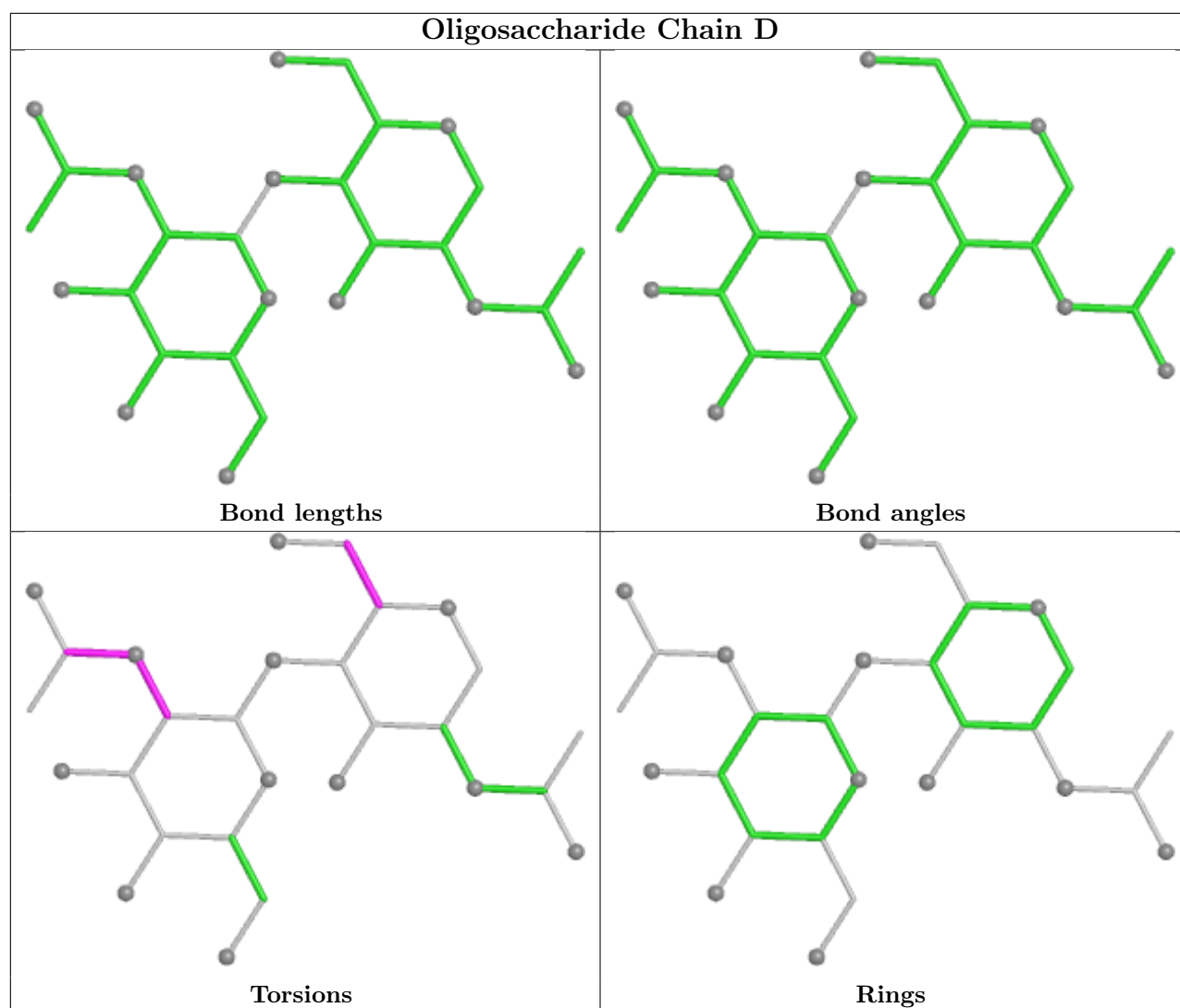
Mol	Chain	Res	Type	Atoms
3	B	3	BMA	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

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







5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
6	6PL	A	802	-	45,45,51	0.51	0	51,53,59	0.45	0
6	6PL	A	804	-	49,49,51	0.49	0	55,57,59	0.43	0
7	CLR	A	803	-	31,31,31	0.36	0	48,48,48	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	A1EMC	A	801	-	34,34,34	1.28	4 (11%)	42,45,45	1.44	8 (19%)

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	6PL	A	802	-	-	17/49/49/55	-
6	6PL	A	804	-	-	21/53/53/55	-
7	CLR	A	803	-	-	7/10/68/68	0/4/4/4
5	A1EMC	A	801	-	-	3/23/23/23	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	801	A1EMC	C11-C06	-3.56	1.36	1.43
5	A	801	A1EMC	C14-C03	2.53	1.54	1.51
5	A	801	A1EMC	C14-C15	2.22	1.55	1.50
5	A	801	A1EMC	C23-C21	2.10	1.55	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	801	A1EMC	C24-C25-C26	-3.05	120.31	127.66
5	A	801	A1EMC	C14-C15-C16	-2.71	123.03	127.24
5	A	801	A1EMC	C19-C20-C21	-2.68	121.20	127.66
5	A	801	A1EMC	C27-C26-C28	2.55	119.56	115.27
5	A	801	A1EMC	C22-C21-C23	2.53	119.53	115.27
5	A	801	A1EMC	C33-C31-C32	2.50	120.13	114.60
5	A	801	A1EMC	C03-C14-C15	-2.37	108.42	112.17
5	A	801	A1EMC	C29-C30-C31	-2.23	120.12	127.75

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	801	A1EMC	C21-C23-C24-C25
6	A	802	6PL	C1-O3P-P-O2P
6	A	802	6PL	C5-C4-O4P-P

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Mol	Chain	Res	Type	Atoms
6	A	804	6PL	C1-O3P-P-O1P
6	A	804	6PL	C1-O3P-P-O2P
6	A	804	6PL	C1-O3P-P-O4P
6	A	804	6PL	C4-O4P-P-O2P
6	A	804	6PL	O31-C31-O2-C2
6	A	804	6PL	C32-C31-O2-C2
7	A	803	CLR	C13-C17-C20-C21
7	A	803	CLR	C16-C17-C20-C22
5	A	801	A1EMC	C16-C18-C19-C20
6	A	802	6PL	C1-O3P-P-O4P
6	A	804	6PL	C4-O4P-P-O3P
6	A	804	6PL	C14-C15-C16-C17
7	A	803	CLR	C23-C24-C25-C27
6	A	802	6PL	C41-C42-C43-C44
6	A	804	6PL	C37-C38-C39-C40
7	A	803	CLR	C23-C24-C25-C26
6	A	802	6PL	C34-C35-C36-C37
6	A	802	6PL	C33-C34-C35-C36
7	A	803	CLR	C20-C22-C23-C24
6	A	802	6PL	C11-C12-C13-C14
6	A	802	6PL	C13-C14-C15-C16
6	A	804	6PL	C1-C2-C3-O3
6	A	804	6PL	C3-C2-O2-C31
7	A	803	CLR	C16-C17-C20-C21
6	A	802	6PL	O2-C2-C3-O3
6	A	802	6PL	C32-C33-C34-C35
6	A	804	6PL	C16-C17-C18-C19
6	A	802	6PL	C1-C2-C3-O3
6	A	802	6PL	C17-C18-C19-C20
6	A	804	6PL	O2-C2-C3-O3
6	A	804	6PL	C35-C36-C37-C38
6	A	802	6PL	C38-C39-C40-C41
6	A	802	6PL	O3P-C1-C2-C3
6	A	804	6PL	O3P-C1-C2-C3
7	A	803	CLR	C13-C17-C20-C22
6	A	802	6PL	O3P-C1-C2-O2
6	A	804	6PL	O3P-C1-C2-O2
6	A	802	6PL	O4P-C4-C5-N
6	A	804	6PL	O4P-C4-C5-N
6	A	802	6PL	C4-C5-N-C6
6	A	804	6PL	C33-C34-C35-C36
5	A	801	A1EMC	C28-C29-C30-C31

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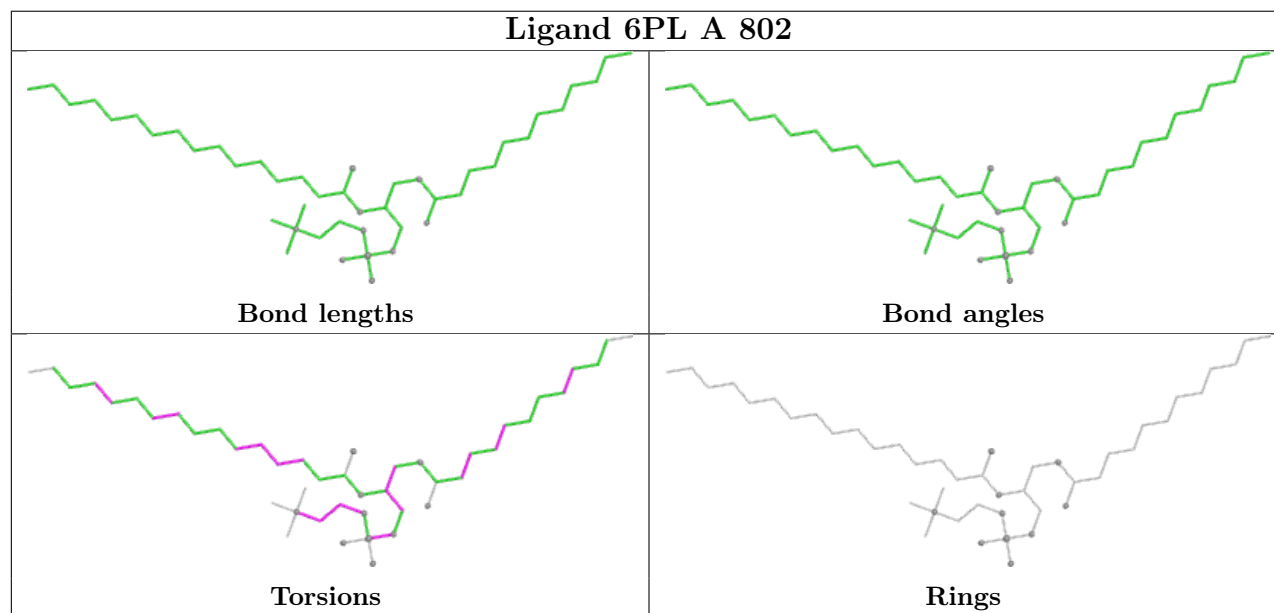
Mol	Chain	Res	Type	Atoms
6	A	804	6PL	C13-C14-C15-C16
6	A	804	6PL	C17-C18-C19-C20
6	A	804	6PL	C12-C13-C14-C15

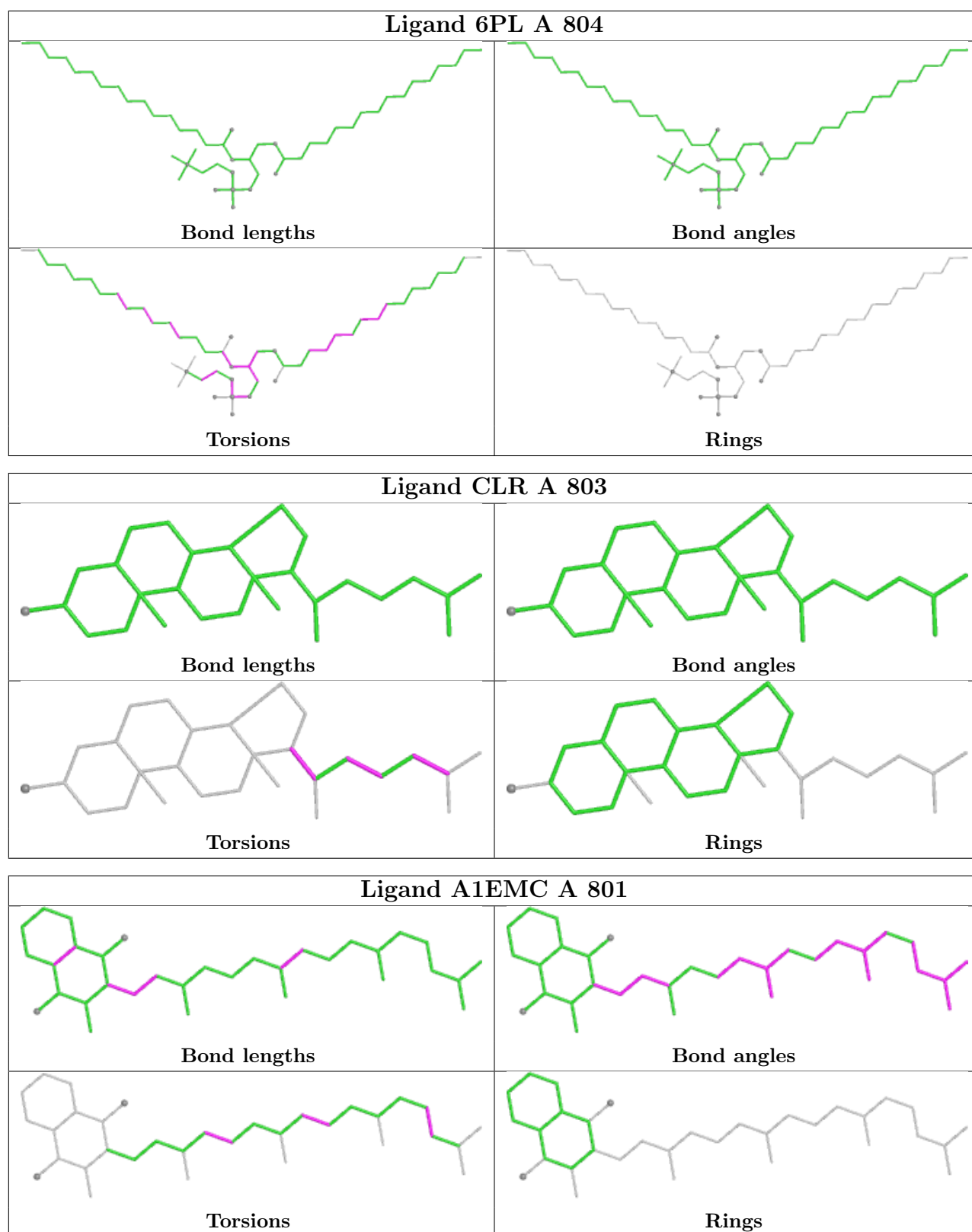
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	802	6PL	2	0
6	A	804	6PL	2	0
7	A	803	CLR	1	0
5	A	801	A1EMC	2	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.