



Full wwPDB EM Validation Report ⓘ

Apr 28, 2026 – 02:21 PM JST

PDB ID : 9L54 / pdb_00009L54
EMDB ID : EMD-62822
Title : cryo-EM structure of Vitamin K-dependent gamma-carboxylase complexed with Vitamin K1 2,3-epoxide
Authors : Yao, D.; Wu, K.; Lan, P.
Deposited on : 2024-12-22
Resolution : 3.04 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

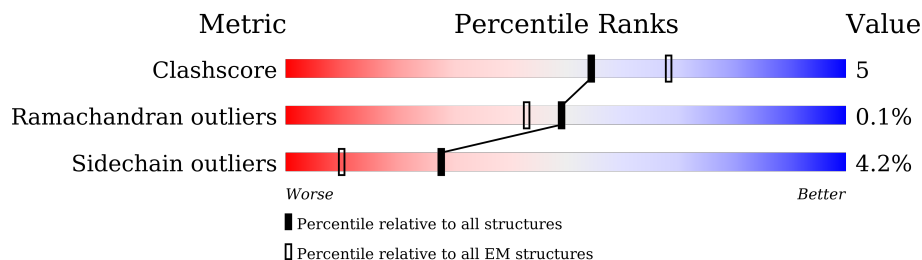
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.04 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	A	698	
2	B	27	
3	C	2	
3	D	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	BCT	A	808	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6054 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 Vitamin K-dependent gamma-carboxylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	673	Total	C	N	O	S	0	0
			5570	3636	946	961	27		

- Molecule 2 is a protein called Vitamin K-dependent protein S.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	21	Total	C	N	O	0	0
			160	100	26	34		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	3	ALA	LEU	conflict	UNP P07225
B	7	GLU	-	expression tag	UNP P07225
B	8	VAL	-	expression tag	UNP P07225

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



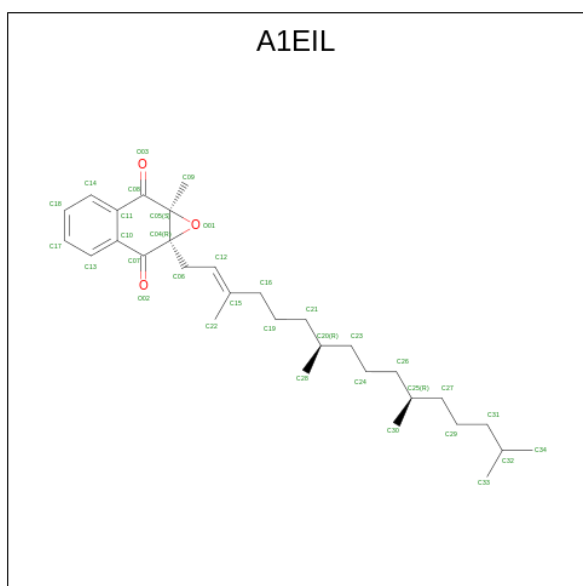
Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



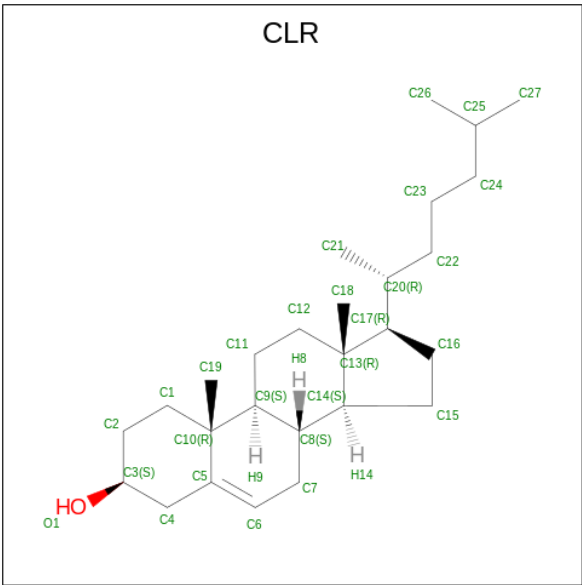
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 5 is (1 {a} {R},7 {a} {S})-7 {a}-methyl-1 {a}-[({E},7 {R},11 {R})-3,7,11,15-tetramethylhexadec-2-enyl]naphtho[2,3-b]oxirene-2,7-dione (CCD ID: A1EIL) (formula: $C_{31}H_{46}O_3$) (labeled as "Ligand of Interest" by depositor).



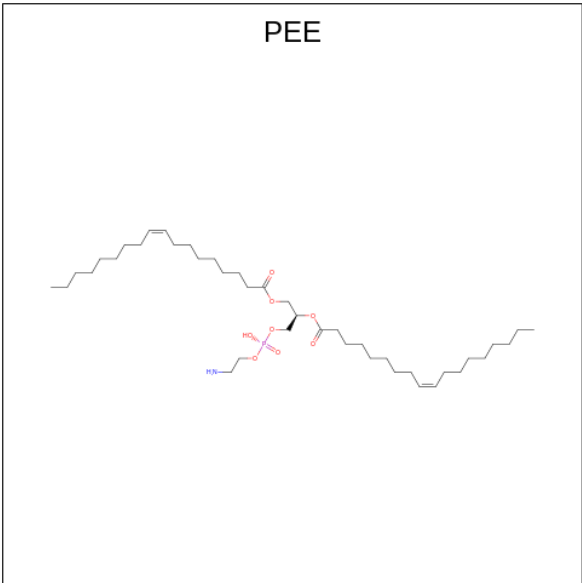
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O		0
			34	31	3		

- Molecule 6 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



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

- Molecule 7 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



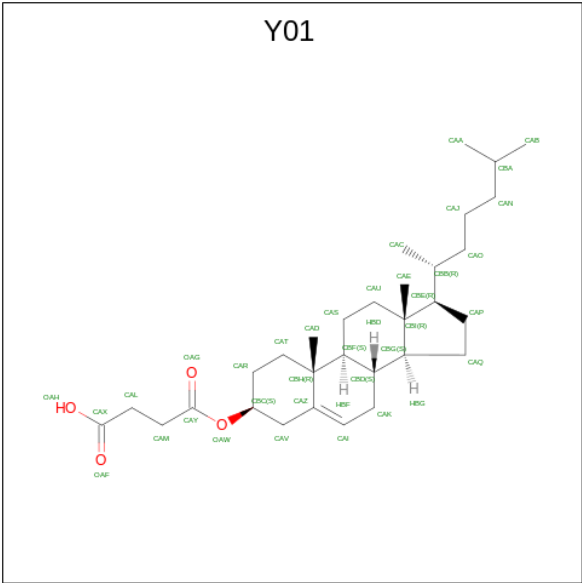
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
7	A	1	Total	C	N	O	P	0
			51	41	1	8	1	

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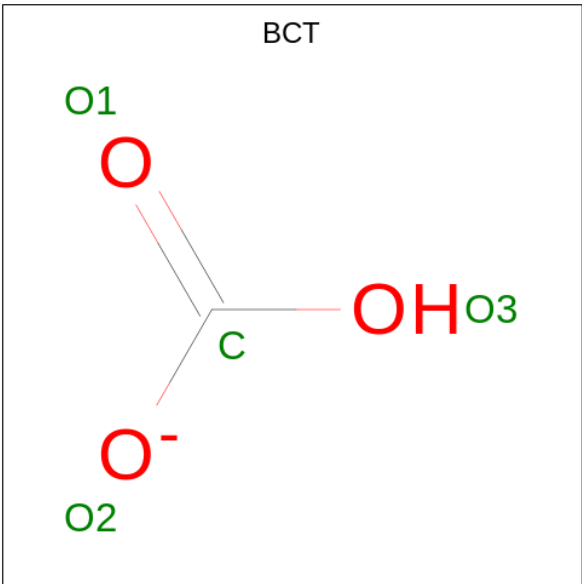
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	A	1	51	41	1	8	1	0

- Molecule 8 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C₃₁H₅₀O₄).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
8	A	1	35	31	4	0

- Molecule 9 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).

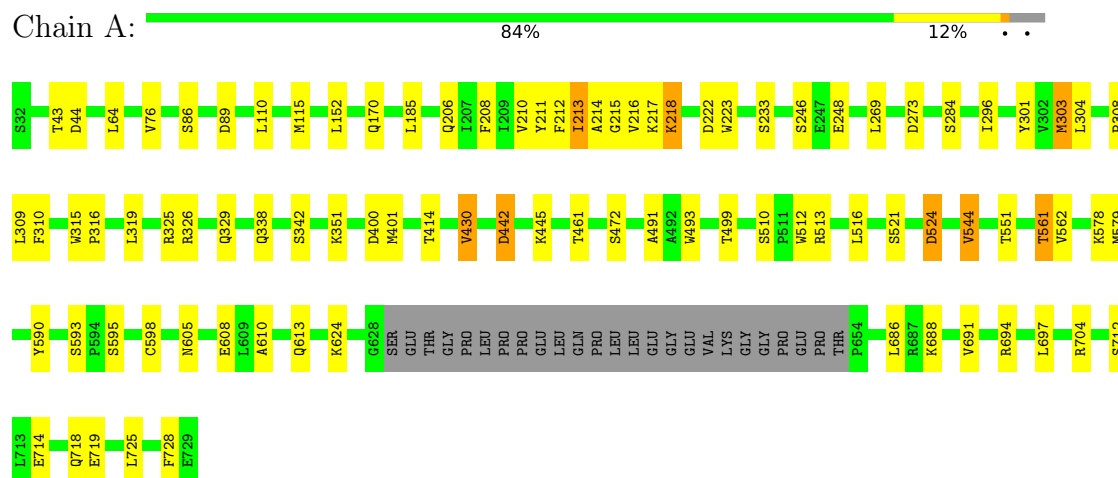


Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			4	1	3	

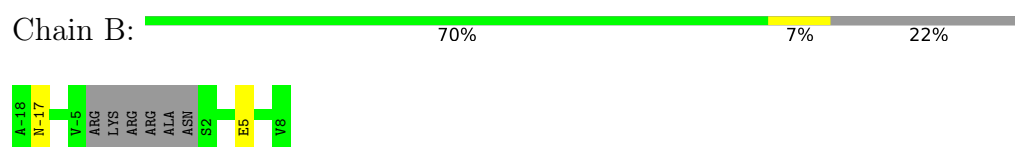
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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: Vitamin K-dependent gamma-carboxylase



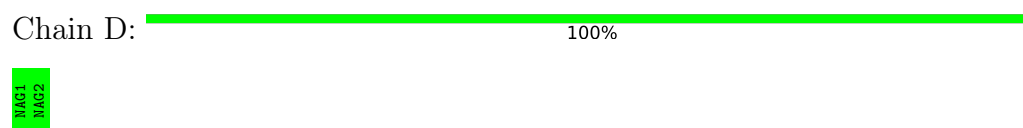
- Molecule 2: Vitamin K-dependent protein S



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



- Molecule 3: 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, Not provided	
Number of particles used	319391	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI/PHILIPS CM300FEG/T	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	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: BCT, NAG, Y01, A1EIL, CLR, PEE

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	0.39	8/5732 (0.1%)	0.47	9/7780 (0.1%)
2	B	0.12	0/159	0.31	0/212
All	All	0.38	8/5891 (0.1%)	0.46	9/7992 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	213	ILE	C-O	-7.37	1.15	1.24
1	A	214	ALA	C-O	-7.07	1.15	1.23
1	A	308	PRO	C-O	-6.86	1.15	1.24
1	A	214	ALA	CA-CB	-6.23	1.45	1.54
1	A	211	TYR	C-O	-6.14	1.17	1.24
1	A	215	GLY	C-O	-6.03	1.15	1.23
1	A	210	VAL	C-O	-5.54	1.17	1.24
1	A	208	PHE	C-O	-5.36	1.17	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	PHE	N-CA-C	-6.99	105.02	113.97
1	A	210	VAL	CA-C-N	6.07	128.70	120.44
1	A	210	VAL	C-N-CA	6.07	128.70	120.44
1	A	309	LEU	N-CA-C	-5.84	105.73	112.92
1	A	217	LYS	N-CA-C	-5.77	106.22	113.72
1	A	210	VAL	CA-C-O	-5.65	113.72	120.78
1	A	216	VAL	N-CA-C	-5.42	107.47	112.83
1	A	218	LYS	N-CA-C	-5.17	106.83	112.72
1	A	212	PHE	CA-C-O	-5.10	113.22	120.51

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5570	0	5543	43	0
2	B	160	0	161	1	0
3	C	28	0	25	0	0
3	D	28	0	25	0	0
4	A	14	0	13	1	0
5	A	34	0	0	0	0
6	A	28	0	46	0	0
7	A	153	0	246	18	0
8	A	35	0	49	13	0
9	A	4	0	0	5	0
All	All	6054	0	6108	62	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 5.

All (62) 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:401:MET:HE3	9:A:808:BCT:O2	1.45	1.14
7:A:805:PEE:H73	8:A:806:Y01:HAS1	1.43	0.99
1:A:218:LYS:NZ	9:A:808:BCT:O1	2.05	0.89
7:A:805:PEE:C43	8:A:806:Y01:HAS1	2.05	0.87
7:A:805:PEE:H75	8:A:806:Y01:HAS1	1.58	0.84
7:A:805:PEE:C44	8:A:806:Y01:HAS1	2.09	0.83
7:A:805:PEE:H75	8:A:806:Y01:CAT	2.11	0.79
7:A:805:PEE:H75	8:A:806:Y01:HAT2	1.66	0.76
1:A:605:ASN:HB3	1:A:608:GLU:HB3	1.70	0.72
7:A:805:PEE:H73	8:A:806:Y01:CAS	2.23	0.67
7:A:805:PEE:C44	8:A:806:Y01:HAT2	2.27	0.65
1:A:89:ASP:OD2	1:A:694:ARG:NH2	2.33	0.62
1:A:110:LEU:H	1:A:115:MET:HE3	1.66	0.59
1:A:430:VAL:HG11	2:B:-17:ASN:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:GLU:O	1:A:718:GLN:HG2	2.05	0.55
7:A:805:PEE:H75	8:A:806:Y01:CAS	2.34	0.55
1:A:401:MET:CE	9:A:808:BCT:O2	2.37	0.53
7:A:805:PEE:H75	8:A:806:Y01:HAT1	1.91	0.52
1:A:510:SER:HB3	1:A:513:ARG:HH21	1.73	0.52
1:A:170:GLN:OE1	1:A:206:GLN:NE2	2.35	0.51
1:A:248:GLU:OE2	1:A:248:GLU:N	2.37	0.51
1:A:273:ASP:OD1	1:A:273:ASP:N	2.35	0.51
1:A:284:SER:HA	1:A:304:LEU:HD21	1.92	0.51
1:A:593:SER:OG	1:A:595:SER:O	2.30	0.50
1:A:442:ASP:HB3	1:A:493:TRP:CZ2	2.47	0.49
1:A:401:MET:H	9:A:808:BCT:C	2.26	0.49
1:A:325:ARG:O	1:A:329:GLN:NE2	2.39	0.48
1:A:524:ASP:OD1	1:A:524:ASP:N	2.45	0.48
1:A:218:LYS:HE3	1:A:223:TRP:CZ2	2.49	0.47
1:A:315:TRP:CG	1:A:316:PRO:HD3	2.51	0.45
1:A:319:LEU:HD12	1:A:319:LEU:HA	1.83	0.45
1:A:610:ALA:O	1:A:613:GLN:HG3	2.16	0.45
8:A:806:Y01:HAM1	8:A:806:Y01:HBC	1.57	0.45
1:A:562:VAL:HB	1:A:579:MET:HE1	1.99	0.45
7:A:807:PEE:H67	7:A:807:PEE:H72	1.61	0.45
7:A:805:PEE:C44	8:A:806:Y01:CAT	2.88	0.44
1:A:445:LYS:NZ	1:A:491:ALA:O	2.51	0.44
1:A:303:MET:HB3	1:A:303:MET:HE3	1.62	0.44
7:A:804:PEE:H82	7:A:804:PEE:H74	1.83	0.44
1:A:725:LEU:HD23	1:A:725:LEU:HA	1.84	0.44
1:A:561:THR:HG23	1:A:590:TYR:HB2	1.98	0.43
1:A:152:LEU:HD12	1:A:152:LEU:HA	1.87	0.43
7:A:804:PEE:H52	7:A:804:PEE:H58	1.87	0.43
1:A:304:LEU:HD23	1:A:304:LEU:HA	1.85	0.43
8:A:806:Y01:HAE2	8:A:806:Y01:HAC1	2.01	0.43
7:A:807:PEE:H57	7:A:807:PEE:H51	1.77	0.43
1:A:578:LYS:HB3	1:A:578:LYS:HE2	1.78	0.43
7:A:804:PEE:H57	7:A:804:PEE:H62	1.81	0.42
7:A:804:PEE:H29	7:A:804:PEE:H39	2.01	0.42
1:A:400:ASP:HA	9:A:808:BCT:O3	2.20	0.42
1:A:704:ARG:NH2	1:A:719:GLU:OE1	2.50	0.42
1:A:608:GLU:HB2	4:A:801:NAG:H82	2.01	0.41
1:A:512:TRP:O	1:A:516:LEU:HG	2.19	0.41
1:A:544:VAL:HG11	1:A:551:THR:HG21	2.02	0.41
1:A:712:SER:OG	1:A:714:GLU:OE1	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:TYR:CE2	7:A:805:PEE:H13	2.56	0.41
1:A:686:LEU:HD11	1:A:728:PHE:HB2	2.01	0.41
1:A:624:LYS:HE2	1:A:624:LYS:HB2	1.87	0.41
1:A:64:LEU:HD12	1:A:64:LEU:HA	1.94	0.40
1:A:269:LEU:HD23	1:A:269:LEU:HA	1.92	0.40
1:A:688:LYS:O	1:A:691:VAL:HG12	2.21	0.40
1:A:44:ASP:OD1	1:A:44:ASP:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	669/698 (96%)	642 (96%)	26 (4%)	1 (0%)	48	78
2	B	17/27 (63%)	17 (100%)	0	0	100	100
All	All	686/725 (95%)	659 (96%)	26 (4%)	1 (0%)	49	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	351	LYS

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	A	608/629 (97%)	583 (96%)	25 (4%)	27	58
2	B	18/23 (78%)	17 (94%)	1 (6%)	19	49
All	All	626/652 (96%)	600 (96%)	26 (4%)	28	58

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	THR
1	A	76	VAL
1	A	86	SER
1	A	185	LEU
1	A	213	ILE
1	A	222	ASP
1	A	233	SER
1	A	246	SER
1	A	296	ILE
1	A	303	MET
1	A	326	ARG
1	A	338	GLN
1	A	342	SER
1	A	414	THR
1	A	430	VAL
1	A	442	ASP
1	A	461	THR
1	A	472	SER
1	A	499	THR
1	A	521	SER
1	A	524	ASP
1	A	544	VAL
1	A	561	THR
1	A	598	CYS
1	A	697	LEU
2	B	5	GLU

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	56	ASN

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 ⓘ

4 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	C	1	1,3	14,14,15	0.44	0	17,19,21	0.90	1 (5%)
3	NAG	C	2	3	14,14,15	0.25	0	17,19,21	0.62	0
3	NAG	D	1	1,3	14,14,15	0.18	0	17,19,21	0.41	0
3	NAG	D	2	3	14,14,15	0.23	0	17,19,21	0.41	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	C	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	1/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	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	C	1	NAG	C1-O5-C5	2.99	116.25	112.19

There are no chirality outliers.

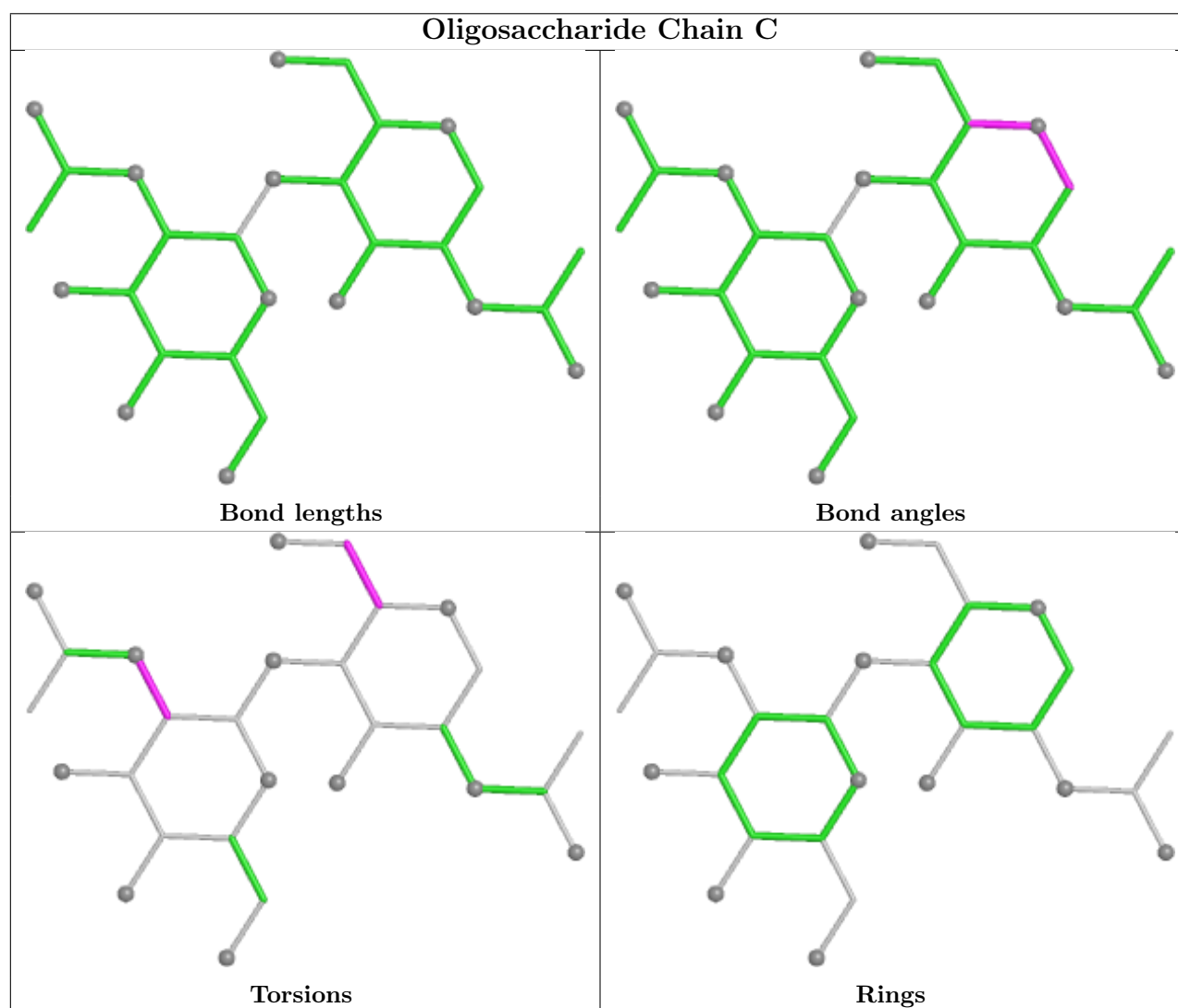
All (4) torsion outliers are listed below:

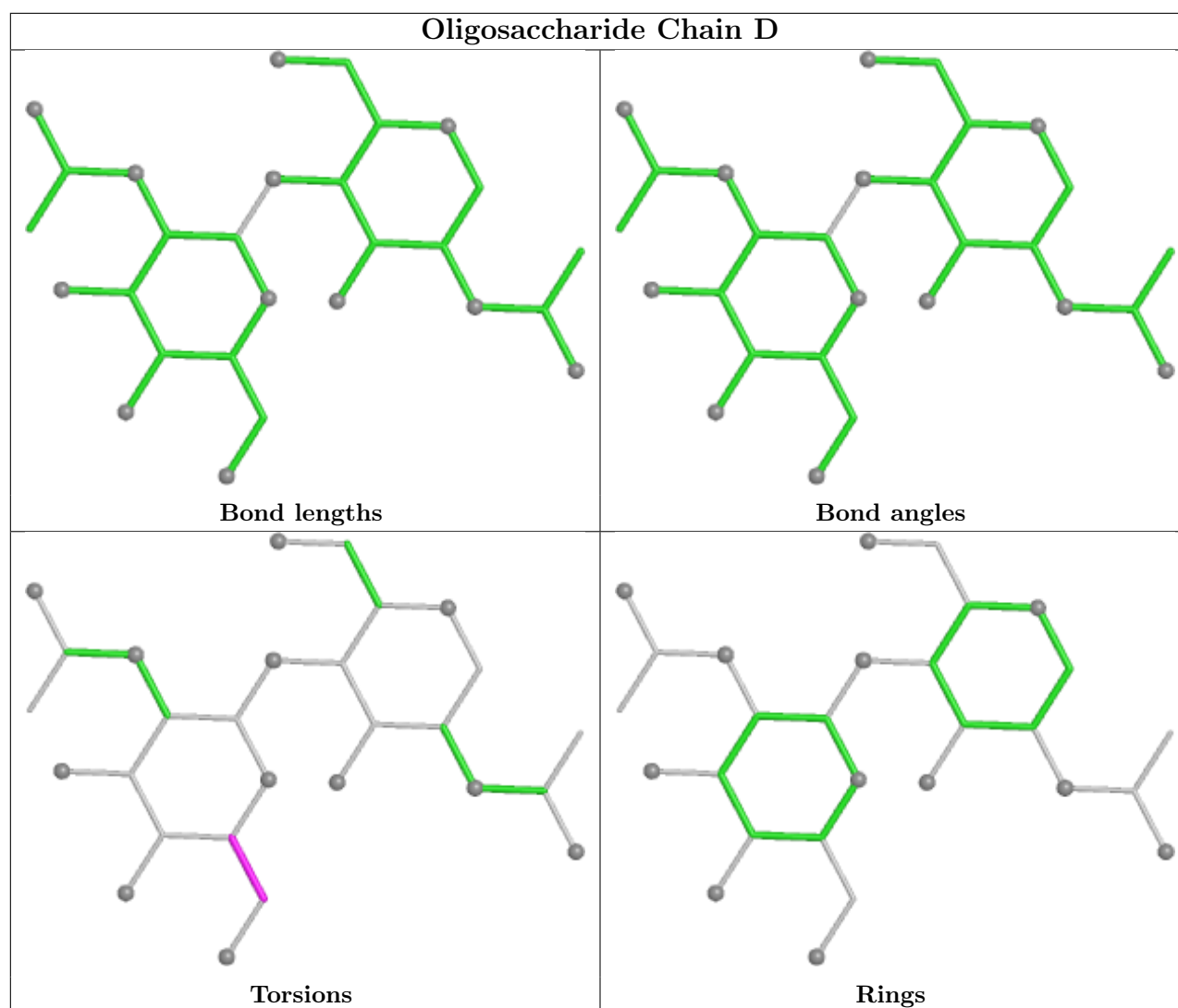
Mol	Chain	Res	Type	Atoms
3	D	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C3-C2-N2-C7
3	C	1	NAG	C4-C5-C6-O6

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.





5.6 Ligand geometry [i](#)

8 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	CLR	A	803	-	31,31,31	1.06	1 (3%)	48,48,48	1.31	6 (12%)
4	NAG	A	801	1	14,14,15	0.29	0	17,19,21	0.39	0
9	BCT	A	808	-	2,3,3	0.97	0	2,3,3	1.67	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	A1EIL	A	802	-	34,36,36	2.87	7 (20%)	41,52,52	2.50	10 (24%)
7	PEE	A	804	-	50,50,50	1.24	4 (8%)	53,55,55	0.96	1 (1%)
8	Y01	A	806	-	38,38,38	1.08	2 (5%)	57,57,57	1.62	5 (8%)
7	PEE	A	805	-	50,50,50	1.26	4 (8%)	53,55,55	0.93	1 (1%)
7	PEE	A	807	-	50,50,50	1.26	4 (8%)	53,55,55	0.93	1 (1%)

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	CLR	A	803	-	-	3/10/68/68	0/4/4/4
4	NAG	A	801	1	-	0/6/23/26	0/1/1/1
5	A1EIL	A	802	-	-	15/24/56/56	0/3/3/3
7	PEE	A	804	-	-	34/54/54/54	-
8	Y01	A	806	-	-	15/19/77/77	0/4/4/4
7	PEE	A	805	-	-	27/54/54/54	-
7	PEE	A	807	-	-	30/54/54/54	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	802	A1EIL	C11-C08	11.28	1.64	1.48
5	A	802	A1EIL	C10-C07	8.70	1.60	1.48
7	A	807	PEE	P-O4P	4.66	1.78	1.59
7	A	805	PEE	P-O4P	4.58	1.77	1.59
7	A	804	PEE	P-O4P	4.49	1.77	1.59
8	A	806	Y01	CAK-CAI	-4.18	1.41	1.50
7	A	805	PEE	C39-C38	3.89	1.54	1.31
7	A	807	PEE	C39-C38	3.83	1.54	1.31
7	A	804	PEE	C39-C38	3.80	1.53	1.31
7	A	804	PEE	C18-C19	3.68	1.53	1.31
7	A	807	PEE	C18-C19	3.66	1.53	1.31
7	A	805	PEE	C18-C19	3.62	1.52	1.31
5	A	802	A1EIL	C14-C11	3.53	1.45	1.39
5	A	802	A1EIL	C13-C10	3.28	1.45	1.39
5	A	802	A1EIL	C06-C04	3.20	1.58	1.52
5	A	802	A1EIL	C16-C15	2.65	1.56	1.51
8	A	806	Y01	CAI-CAZ	2.59	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	803	CLR	C18-C13	-2.23	1.50	1.54
5	A	802	A1EIL	C12-C15	2.13	1.38	1.33
7	A	807	PEE	O4P-C4	-2.02	1.36	1.44
7	A	804	PEE	O3-C3	-2.00	1.40	1.45
7	A	805	PEE	O4P-C4	-2.00	1.36	1.44

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	802	A1EIL	O02-C07-C04	-9.15	108.47	120.32
8	A	806	Y01	CAV-CAZ-CBH	7.56	126.46	116.42
5	A	802	A1EIL	C04-C07-C10	6.03	127.40	116.88
5	A	802	A1EIL	C10-C11-C08	-5.10	115.69	120.98
8	A	806	Y01	CAV-CAZ-CAI	-4.89	113.57	120.61
5	A	802	A1EIL	C14-C11-C08	4.80	125.54	119.39
5	A	802	A1EIL	C05-C08-C11	4.38	124.29	115.80
7	A	804	PEE	O2P-P-O1P	4.30	133.49	112.24
7	A	807	PEE	O2P-P-O1P	4.26	133.30	112.24
7	A	805	PEE	O2P-P-O1P	4.25	133.27	112.24
5	A	802	A1EIL	O03-C08-C05	-3.92	112.56	121.06
5	A	802	A1EIL	O01-C05-C09	-3.50	112.45	117.58
5	A	802	A1EIL	C11-C10-C07	-3.40	117.45	120.98
6	A	803	CLR	C22-C20-C17	-3.20	103.68	110.28
8	A	806	Y01	CBI-CBE-CBB	3.00	124.18	119.49
5	A	802	A1EIL	C13-C10-C07	2.99	123.22	119.39
5	A	802	A1EIL	O01-C04-C07	-2.62	105.47	111.91
6	A	803	CLR	C18-C13-C12	2.42	114.42	110.59
8	A	806	Y01	CAC-CBB-CBE	2.36	116.53	112.92
9	A	808	BCT	O2-C-O1	2.21	125.27	119.55
8	A	806	Y01	CAS-CBF-CBD	-2.18	108.62	111.75
6	A	803	CLR	C7-C8-C14	-2.17	107.75	110.91
6	A	803	CLR	C16-C17-C20	-2.12	108.86	112.15
6	A	803	CLR	C24-C23-C22	-2.07	103.73	113.24
6	A	803	CLR	C10-C5-C6	2.01	125.98	122.90

There are no chirality outliers.

All (124) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	802	A1EIL	C04-C06-C12-C15
5	A	802	A1EIL	C12-C15-C16-C19
5	A	802	A1EIL	C22-C15-C16-C19

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Mol	Chain	Res	Type	Atoms
7	A	804	PEE	C1-O3P-P-O2P
7	A	804	PEE	C1-O3P-P-O1P
7	A	804	PEE	C1-O3P-P-O4P
7	A	804	PEE	C4-O4P-P-O1P
7	A	804	PEE	O4P-C4-C5-N
7	A	805	PEE	C1-O3P-P-O1P
7	A	805	PEE	C4-O4P-P-O2P
7	A	807	PEE	O2-C2-C3-O3
7	A	807	PEE	C1-O3P-P-O2P
7	A	807	PEE	C4-O4P-P-O3P
8	A	806	Y01	OAG-CAY-OAW-CBC
8	A	806	Y01	CAM-CAY-OAW-CBC
7	A	807	PEE	O5-C30-O3-C3
7	A	807	PEE	C31-C30-O3-C3
7	A	805	PEE	C42-C43-C44-C45
8	A	806	Y01	CAC-CBB-CBE-CBI
7	A	804	PEE	C42-C43-C44-C45
6	A	803	CLR	C17-C20-C22-C23
7	A	805	PEE	C22-C23-C24-C25
6	A	803	CLR	C21-C20-C22-C23
7	A	804	PEE	C40-C41-C42-C43
8	A	806	Y01	CAN-CAJ-CAO-CBB
5	A	802	A1EIL	C30-C25-C27-C29
7	A	807	PEE	C40-C41-C42-C43
7	A	807	PEE	C17-C18-C19-C20
5	A	802	A1EIL	C16-C19-C21-C20
8	A	806	Y01	CAO-CBB-CBE-CAP
7	A	805	PEE	C10-C11-C12-C13
7	A	804	PEE	C10-C11-C12-C13
8	A	806	Y01	CAO-CAJ-CAN-CBA
8	A	806	Y01	CAX-CAL-CAM-CAY
7	A	805	PEE	C40-C41-C42-C43
6	A	803	CLR	C22-C23-C24-C25
7	A	804	PEE	C4-O4P-P-O3P
7	A	805	PEE	C1-O3P-P-O4P
7	A	805	PEE	C4-O4P-P-O3P
7	A	807	PEE	C1-O3P-P-O4P
7	A	805	PEE	C20-C21-C22-C23
7	A	804	PEE	C22-C23-C24-C25
8	A	806	Y01	CAJ-CAO-CBB-CBE
7	A	804	PEE	C20-C21-C22-C23
7	A	805	PEE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
7	A	805	PEE	C13-C14-C15-C16
7	A	805	PEE	C15-C16-C17-C18
7	A	807	PEE	C39-C40-C41-C42
7	A	804	PEE	C13-C14-C15-C16
7	A	804	PEE	C34-C35-C36-C37
7	A	805	PEE	C34-C35-C36-C37
7	A	807	PEE	C12-C13-C14-C15
7	A	805	PEE	C39-C40-C41-C42
7	A	807	PEE	C20-C21-C22-C23
5	A	802	A1EIL	C27-C29-C31-C32
7	A	807	PEE	C42-C43-C44-C45
7	A	807	PEE	C34-C35-C36-C37
7	A	804	PEE	C17-C18-C19-C20
7	A	804	PEE	C19-C20-C21-C22
7	A	807	PEE	C19-C20-C21-C22
7	A	805	PEE	C33-C34-C35-C36
8	A	806	Y01	CAJ-CAN-CBA-CAB
7	A	804	PEE	C23-C24-C25-C26
7	A	804	PEE	C11-C12-C13-C14
7	A	805	PEE	C35-C36-C37-C38
7	A	805	PEE	C11-C12-C13-C14
7	A	807	PEE	C22-C23-C24-C25
7	A	804	PEE	C38-C39-C40-C41
5	A	802	A1EIL	C25-C27-C29-C31
7	A	807	PEE	C24-C25-C26-C27
7	A	804	PEE	C33-C34-C35-C36
7	A	807	PEE	C1-C2-C3-O3
7	A	805	PEE	C44-C45-C46-C47
8	A	806	Y01	CAC-CBB-CBE-CAP
5	A	802	A1EIL	C26-C25-C27-C29
7	A	807	PEE	C16-C17-C18-C19
7	A	807	PEE	C32-C33-C34-C35
7	A	807	PEE	C41-C42-C43-C44
8	A	806	Y01	CAJ-CAN-CBA-CAA
7	A	804	PEE	C12-C13-C14-C15
5	A	802	A1EIL	C29-C31-C32-C34
7	A	805	PEE	C16-C17-C18-C19
7	A	807	PEE	C11-C12-C13-C14
8	A	806	Y01	CAO-CBB-CBE-CBI
7	A	804	PEE	C1-C2-C3-O3
7	A	807	PEE	C43-C44-C45-C46
8	A	806	Y01	CAJ-CAO-CBB-CAC

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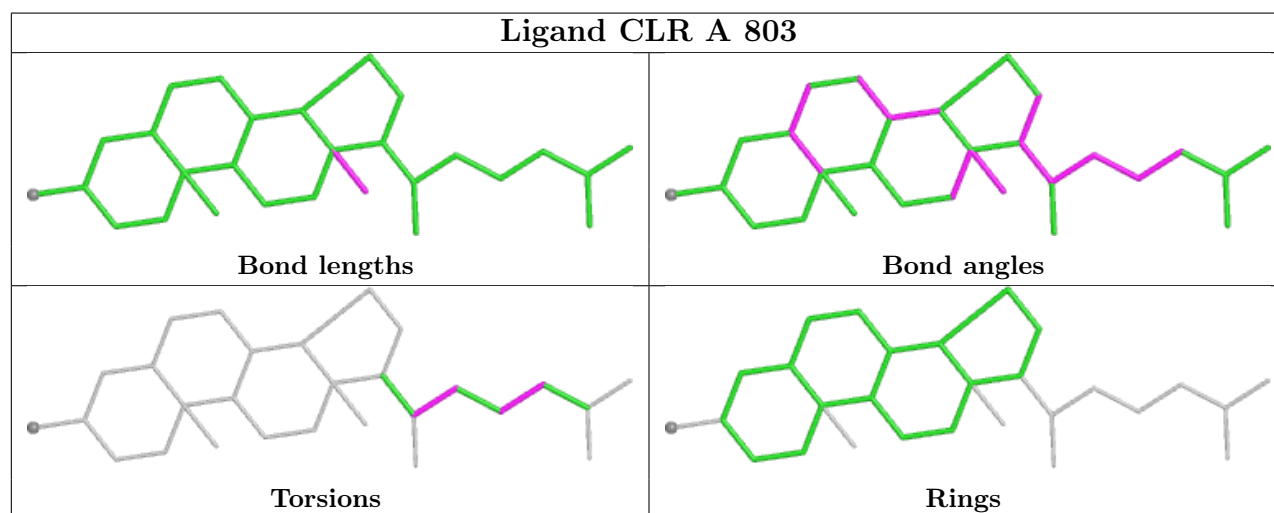
Mol	Chain	Res	Type	Atoms
7	A	804	PEE	C39-C40-C41-C42
7	A	804	PEE	C4-O4P-P-O2P
7	A	807	PEE	C4-O4P-P-O2P
5	A	802	A1EIL	C29-C31-C32-C33
7	A	807	PEE	O3P-C1-C2-C3
5	A	802	A1EIL	C07-C04-C06-C12
5	A	802	A1EIL	C23-C20-C21-C19
7	A	804	PEE	O3P-C1-C2-O2
5	A	802	A1EIL	O01-C04-C06-C12
5	A	802	A1EIL	C28-C20-C21-C19
7	A	807	PEE	O3P-C1-C2-O2
7	A	804	PEE	O2-C2-C3-O3
7	A	805	PEE	C14-C15-C16-C17
7	A	804	PEE	C44-C45-C46-C47
7	A	807	PEE	C35-C36-C37-C38
7	A	805	PEE	O4P-C4-C5-N
7	A	804	PEE	C43-C44-C45-C46
7	A	807	PEE	C31-C32-C33-C34
7	A	805	PEE	C37-C38-C39-C40
7	A	804	PEE	C16-C17-C18-C19
7	A	804	PEE	C14-C15-C16-C17
7	A	805	PEE	C23-C24-C25-C26
7	A	804	PEE	C36-C37-C38-C39
7	A	805	PEE	C38-C39-C40-C41
7	A	804	PEE	O4-C10-O2-C2
8	A	806	Y01	CAM-CAL-CAX-OAH
8	A	806	Y01	CAM-CAL-CAX-OAF
7	A	804	PEE	O3P-C1-C2-C3
7	A	804	PEE	C18-C19-C20-C21
7	A	804	PEE	C11-C10-O2-C2
7	A	805	PEE	C1-O3P-P-O2P
7	A	807	PEE	C1-O3P-P-O1P
7	A	807	PEE	O2-C10-C11-C12
7	A	805	PEE	C12-C13-C14-C15
5	A	802	A1EIL	C28-C20-C23-C24
7	A	805	PEE	C36-C37-C38-C39
7	A	807	PEE	O4-C10-C11-C12

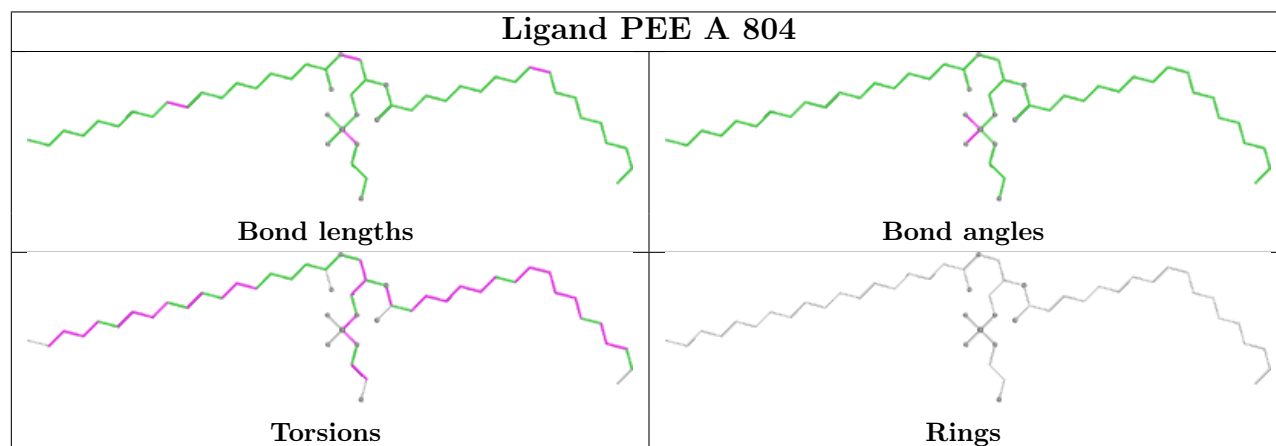
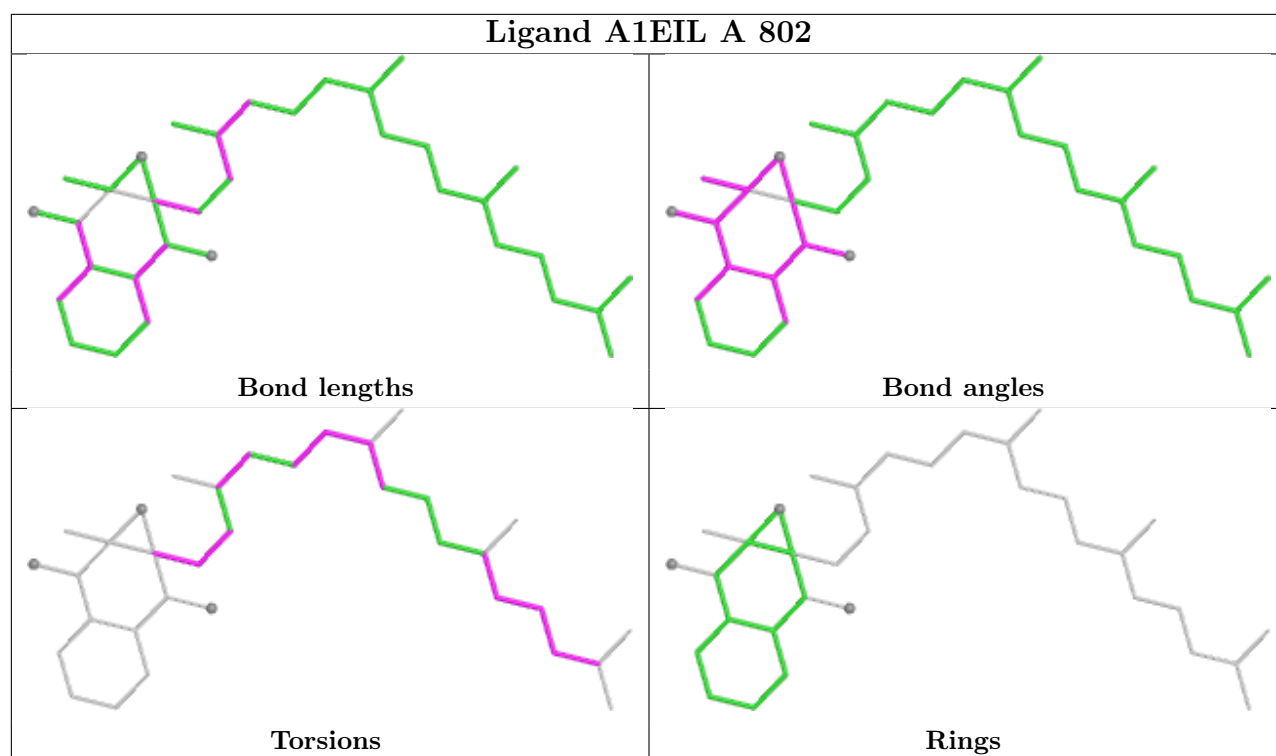
There are no ring outliers.

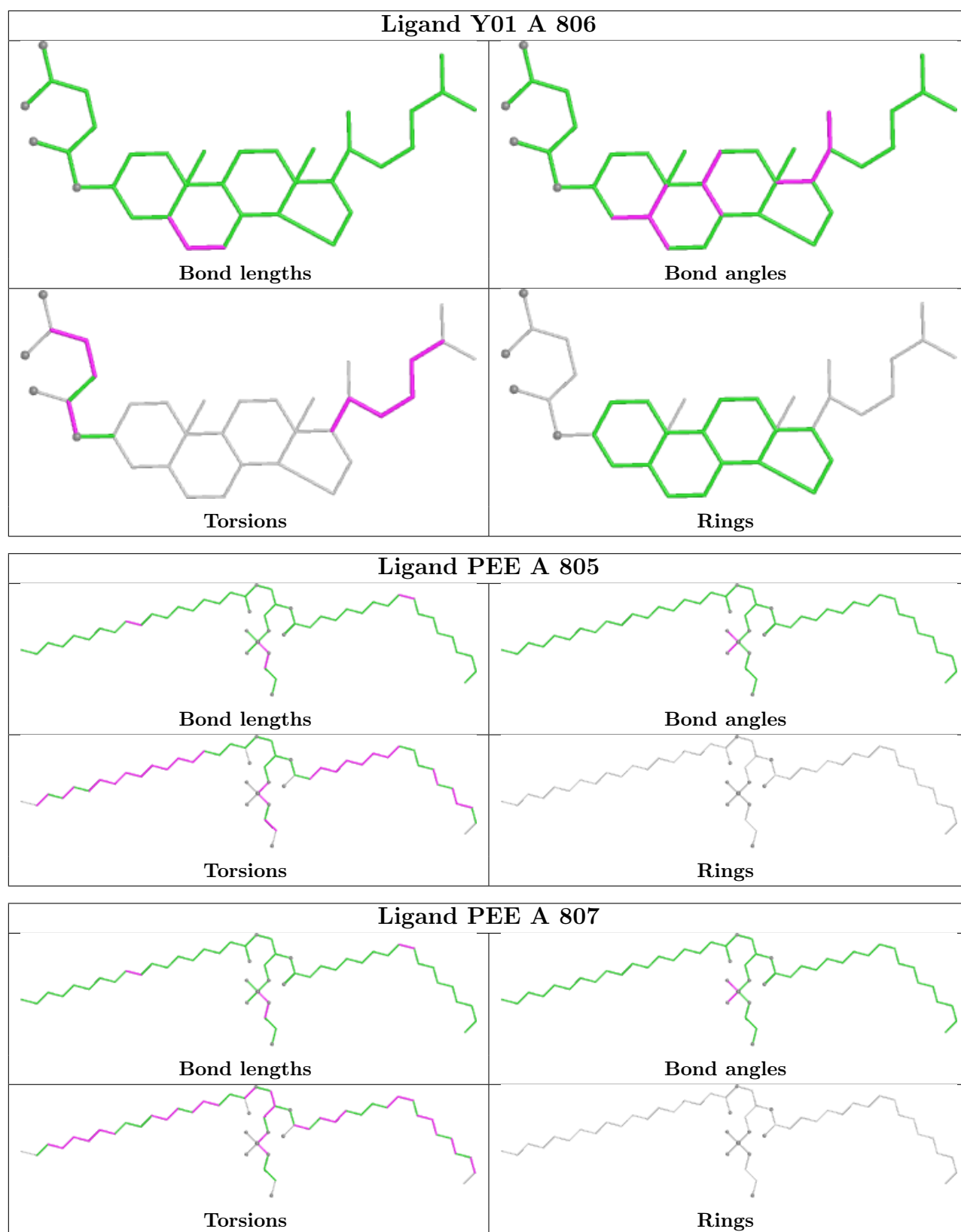
6 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	NAG	1	0
9	A	808	BCT	5	0
7	A	804	PEE	4	0
8	A	806	Y01	13	0
7	A	805	PEE	12	0
7	A	807	PEE	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.