



Full wwPDB EM Validation Report ⓘ

Apr 28, 2026 – 02:18 PM JST

PDB ID : 9L23 / pdb_00009L23
EMDB ID : EMD-62767
Title : cryo-EM structure of Vitamin K-dependent gamma-carboxylase complexed with Osteocalcin
Authors : Yao, D.; Wu, K.; Lan, P.
Deposited on : 2024-12-16
Resolution : 2.62 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

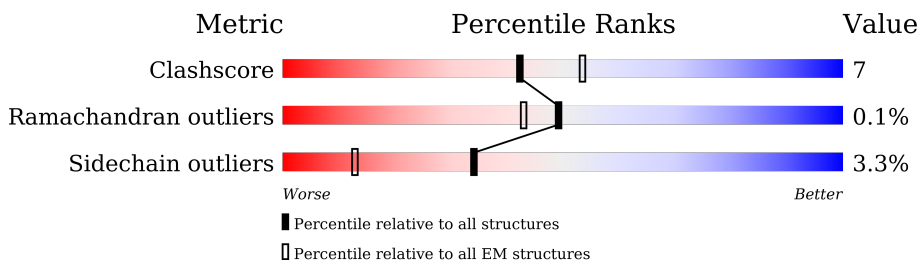
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.62 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	68	
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
10	BCT	A	809	-	-	X	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 6258 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	674	Total	C	N	O	S	0	0
			5577	3640	947	963	27		

- Molecule 2 is a protein called Osteocalcin.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	42	Total	C	N	O	0	0
			333	212	57	64		

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



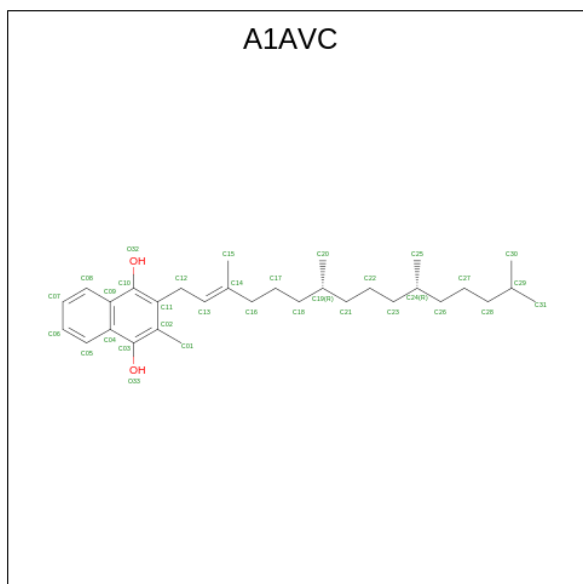
Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		

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



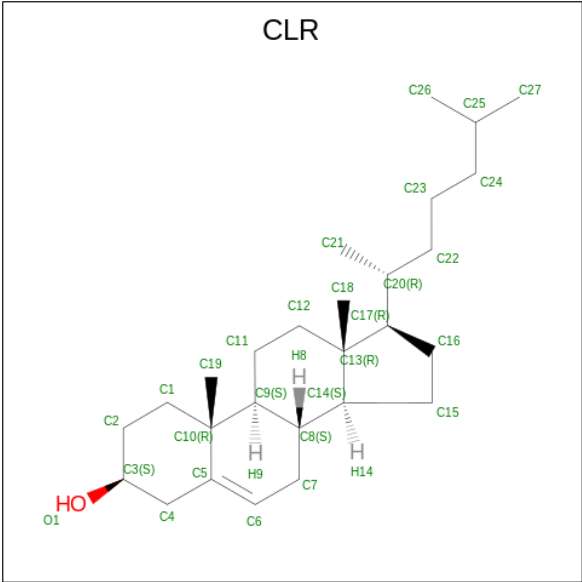
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 5 is vitamin K1 hydroquinone (CCD ID: A1AVC) (formula: $C_{31}H_{48}O_2$) (labeled as "Ligand of Interest" by depositor).



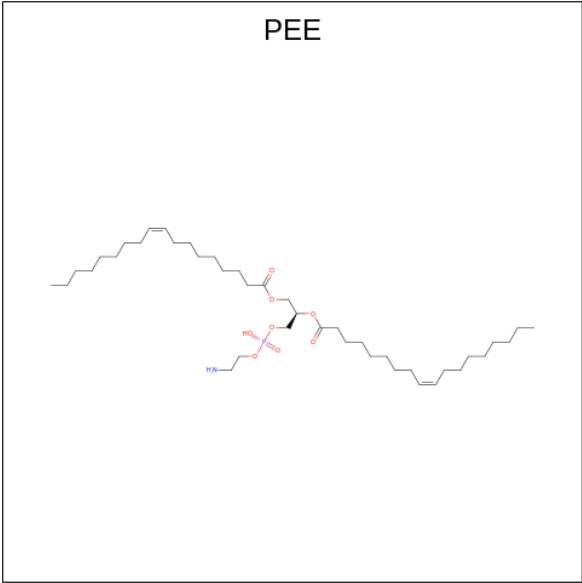
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			33	31	2	

- 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	

Continued on next page...

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

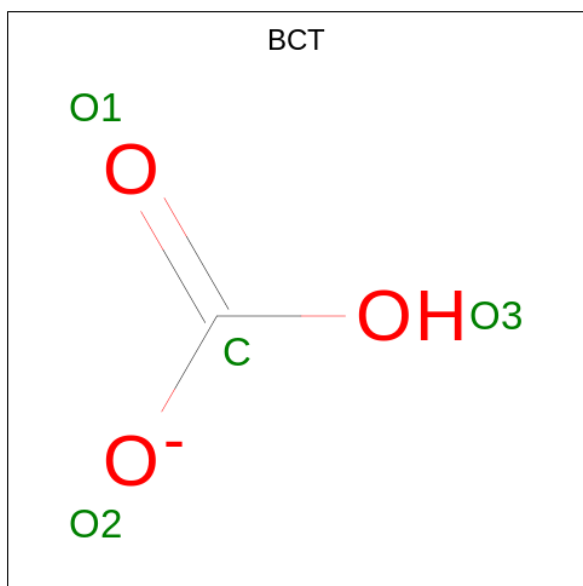
- Y01

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

-
- CO₂
- O O
- C

Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	
			3	1	2	0

- Molecule 10 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



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

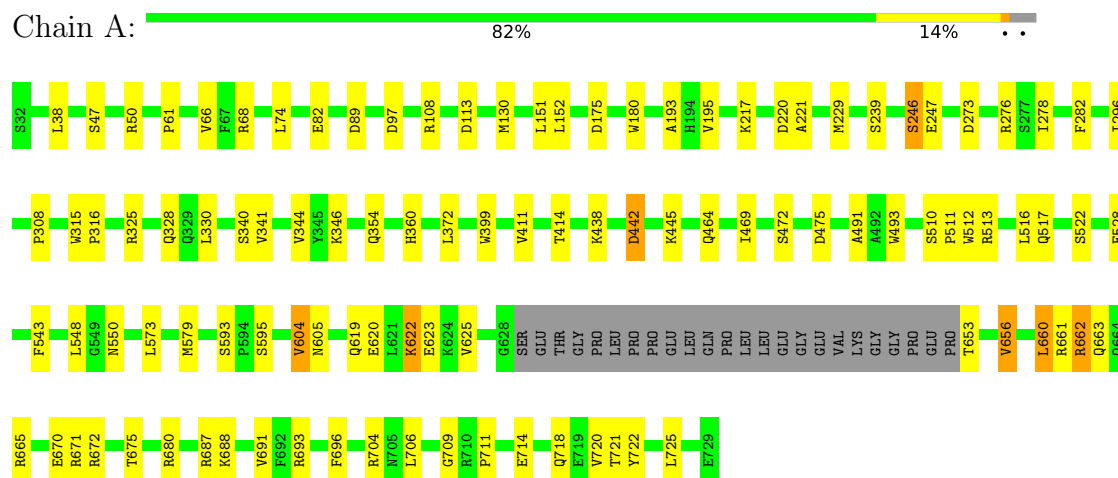
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		AltConf
11	A	20	Total	O	
			20	20	0
11	B	2	Total	O	
			2	2	0

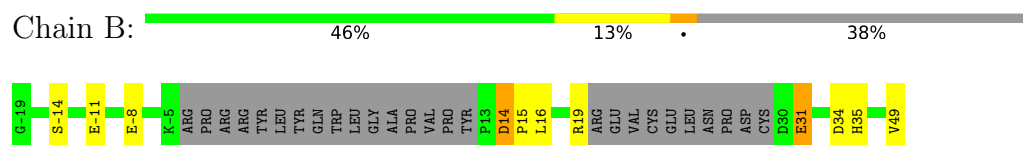
3 Residue-property plots [i](#)

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.

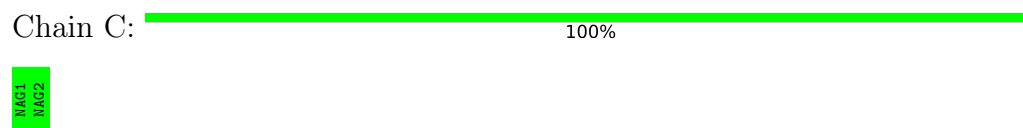
- Molecule 1: Vitamin K-dependent gamma-carboxylase



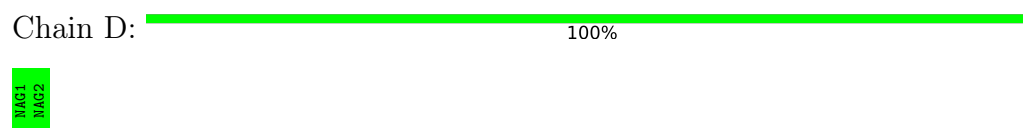
- Molecule 2: Osteocalcin



- 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	994155	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: Y01, CLR, PEE, BCT, NAG, CO2, A1AVC

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	0.12	0/5739	0.31	0/7791
2	B	0.51	0/340	0.85	1/455 (0.2%)
All	All	0.17	0/6079	0.36	1/8246 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	14	ASP	CB-CA-C	5.38	117.67	110.13

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	5577	0	5549	78	0
2	B	333	0	315	14	0
3	C	28	0	25	0	0
3	D	28	0	25	0	0
4	A	14	0	13	0	0
5	A	33	0	0	0	0
6	A	28	0	46	0	0
7	A	153	0	246	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	35	0	49	8	0
9	A	3	0	0	0	0
10	A	4	0	0	2	0
11	A	20	0	0	0	0
11	B	2	0	0	0	0
All	All	6258	0	6268	84	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 (84) 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:543:PHE:HD2	2:B:-8:GLU:OE1	1.45	0.99
1:A:543:PHE:CD2	2:B:-8:GLU:OE1	2.17	0.98
1:A:722:TYR:OH	8:A:806:Y01:HAA1	1.74	0.87
1:A:97:ASP:O	2:B:35:HIS:HE1	1.59	0.86
1:A:82:GLU:OE2	2:B:19:ARG:HD2	1.78	0.83
1:A:696:PHE:CD2	8:A:806:Y01:HAQ1	2.16	0.80
1:A:82:GLU:OE2	2:B:19:ARG:CD	2.33	0.77
1:A:82:GLU:CD	2:B:19:ARG:HD2	2.11	0.75
1:A:693:ARG:HG3	8:A:806:Y01:HAE2	1.70	0.73
1:A:672:ARG:O	1:A:680:ARG:NH1	2.23	0.72
1:A:193:ALA:HB1	1:A:340:SER:HB2	1.73	0.69
1:A:445:LYS:NZ	1:A:491:ALA:O	2.30	0.64
1:A:704:ARG:HH12	1:A:711:PRO:HD3	1.62	0.63
1:A:308:PRO:HG2	7:A:805:PEE:H40	1.79	0.63
1:A:671:ARG:O	1:A:675:THR:N	2.33	0.61
1:A:693:ARG:HG3	8:A:806:Y01:CAE	2.30	0.61
1:A:97:ASP:O	2:B:35:HIS:CE1	2.49	0.61
1:A:273:ASP:OD1	1:A:276:ARG:NH2	2.36	0.59
1:A:696:PHE:CE2	8:A:806:Y01:CAQ	2.87	0.58
1:A:151:LEU:HD21	7:A:807:PEE:H74	1.86	0.58
1:A:472:SER:OG	1:A:475:ASP:O	2.21	0.57
1:A:68:ARG:NH1	1:A:130:MET:O	2.36	0.57
1:A:82:GLU:HG3	2:B:19:ARG:HG2	1.85	0.56
1:A:74:LEU:HD21	7:A:805:PEE:H23	1.89	0.54
1:A:522:SER:O	1:A:522:SER:OG	2.25	0.54
1:A:308:PRO:HG2	7:A:805:PEE:H43	1.90	0.53
1:A:82:GLU:OE2	2:B:19:ARG:CG	2.56	0.53
1:A:696:PHE:CE2	8:A:806:Y01:HAQ1	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:PHE:CE2	2:B:-8:GLU:OE1	2.62	0.52
1:A:246:SER:OG	1:A:247:GLU:N	2.43	0.51
1:A:411:VAL:HG21	1:A:438:LYS:HD3	1.91	0.51
2:B:31:GLU:HB3	2:B:34:ASP:OD2	2.10	0.51
1:A:696:PHE:CE2	8:A:806:Y01:HAQ2	2.45	0.51
1:A:68:ARG:NH2	1:A:180:TRP:O	2.44	0.51
1:A:662:ARG:HG3	1:A:663:GLN:N	2.25	0.50
1:A:653:THR:HB	1:A:656:VAL:HG23	1.93	0.49
1:A:619:GLN:O	1:A:623:GLU:HG2	2.12	0.49
1:A:38:LEU:HD23	7:A:804:PEE:H69	1.93	0.48
1:A:704:ARG:NH1	1:A:711:PRO:HD3	2.29	0.47
1:A:220:ASP:OD1	1:A:221:ALA:N	2.47	0.47
1:A:372:LEU:HG	7:A:804:PEE:H35	1.97	0.47
1:A:593:SER:OG	1:A:595:SER:O	2.29	0.46
1:A:722:TYR:HH	8:A:806:Y01:HAA1	1.78	0.46
1:A:411:VAL:HG13	1:A:469:ILE:HG12	1.97	0.46
1:A:113:ASP:HB3	1:A:706:LEU:HG	1.97	0.45
1:A:512:TRP:O	1:A:516:LEU:HG	2.17	0.45
1:A:89:ASP:OD1	1:A:89:ASP:N	2.49	0.45
1:A:725:LEU:HD12	1:A:725:LEU:HA	1.80	0.45
1:A:278:ILE:HG22	1:A:282:PHE:CE2	2.52	0.44
1:A:175:ASP:HB2	1:A:195:VAL:HG12	1.99	0.44
1:A:688:LYS:HG3	7:A:805:PEE:H48	2.00	0.44
1:A:344:VAL:HB	1:A:360:HIS:NE2	2.32	0.44
1:A:548:LEU:HD23	1:A:605:ASN:HA	2.00	0.44
1:A:399:TRP:O	10:A:809:BCT:O2	2.36	0.43
1:A:573:LEU:HD21	1:A:579:MET:HE3	1.99	0.43
7:A:807:PEE:H62	7:A:807:PEE:H57	1.84	0.43
1:A:217:LYS:HB2	10:A:809:BCT:O3	2.18	0.43
1:A:720:VAL:HG12	2:B:49:VAL:HG21	2.00	0.43
1:A:622:LYS:HE3	1:A:622:LYS:HB2	1.85	0.43
1:A:442:ASP:OD1	1:A:442:ASP:N	2.45	0.43
2:B:-14:SER:HB3	2:B:-11:GLU:HG3	2.00	0.43
1:A:442:ASP:HB3	1:A:493:TRP:CZ2	2.53	0.42
1:A:661:ARG:O	1:A:665:ARG:HG2	2.19	0.42
7:A:807:PEE:H72	7:A:807:PEE:H67	1.58	0.42
1:A:517:GLN:HA	1:A:517:GLN:OE1	2.19	0.42
1:A:47:SER:HB3	1:A:50:ARG:HG3	2.01	0.42
1:A:108:ARG:HE	1:A:108:ARG:HB3	1.67	0.42
1:A:346:LYS:NZ	1:A:354:GLN:H	2.17	0.42
1:A:720:VAL:CG1	2:B:49:VAL:HG21	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:ARG:O	1:A:691:VAL:HG13	2.19	0.42
1:A:704:ARG:NH1	1:A:709:GLY:O	2.53	0.42
1:A:660:LEU:HD13	1:A:660:LEU:HA	1.79	0.41
1:A:152:LEU:HD12	1:A:152:LEU:HA	1.88	0.41
1:A:66:VAL:HG12	7:A:805:PEE:H46	2.01	0.41
1:A:550:ASN:HB3	1:A:604:VAL:HG13	2.03	0.41
1:A:330:LEU:HD23	1:A:330:LEU:H	1.86	0.41
1:A:475:ASP:HB3	1:A:513:ARG:HD3	2.02	0.41
7:A:804:PEE:H47	7:A:804:PEE:H39	1.82	0.41
1:A:61:PRO:HG3	1:A:193:ALA:O	2.20	0.40
1:A:714:GLU:O	1:A:718:GLN:HG3	2.21	0.40
7:A:804:PEE:H40	7:A:804:PEE:H33	1.59	0.40
1:A:315:TRP:CG	1:A:316:PRO:HD3	2.56	0.40
1:A:325:ARG:HA	1:A:328:GLN:HG3	2.04	0.40
1:A:510:SER:N	1:A:511:PRO:HD2	2.36	0.40

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	670/698 (96%)	651 (97%)	19 (3%)	0	100	100
2	B	36/68 (53%)	33 (92%)	2 (6%)	1 (3%)	4	6
All	All	706/766 (92%)	684 (97%)	21 (3%)	1 (0%)	49	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	15	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	A	609/629 (97%)	591 (97%)	18 (3%)	36 62
2	B	34/58 (59%)	31 (91%)	3 (9%)	9 19
All	All	643/687 (94%)	622 (97%)	21 (3%)	34 59

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	MET
1	A	239	SER
1	A	246	SER
1	A	296	ILE
1	A	341	VAL
1	A	414	THR
1	A	442	ASP
1	A	464	GLN
1	A	528	GLU
1	A	604	VAL
1	A	620	GLU
1	A	622	LYS
1	A	625	VAL
1	A	656	VAL
1	A	660	LEU
1	A	662	ARG
1	A	670	GLU
1	A	721	THR
2	B	14	ASP
2	B	16	LEU
2	B	31	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	381	HIS
1	A	404	HIS
1	A	408	HIS
1	A	503	GLN
2	B	35	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 ⓘ

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	3,1	14,14,15	0.19	0	17,19,21	0.44	0
3	NAG	C	2	3	14,14,15	0.25	0	17,19,21	0.54	0
3	NAG	D	1	3,1	14,14,15	0.19	0	17,19,21	0.42	0
3	NAG	D	2	3	14,14,15	0.24	0	17,19,21	0.43	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	3,1	–	0/6/23/26	0/1/1/1
3	NAG	C	2	3	–	1/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

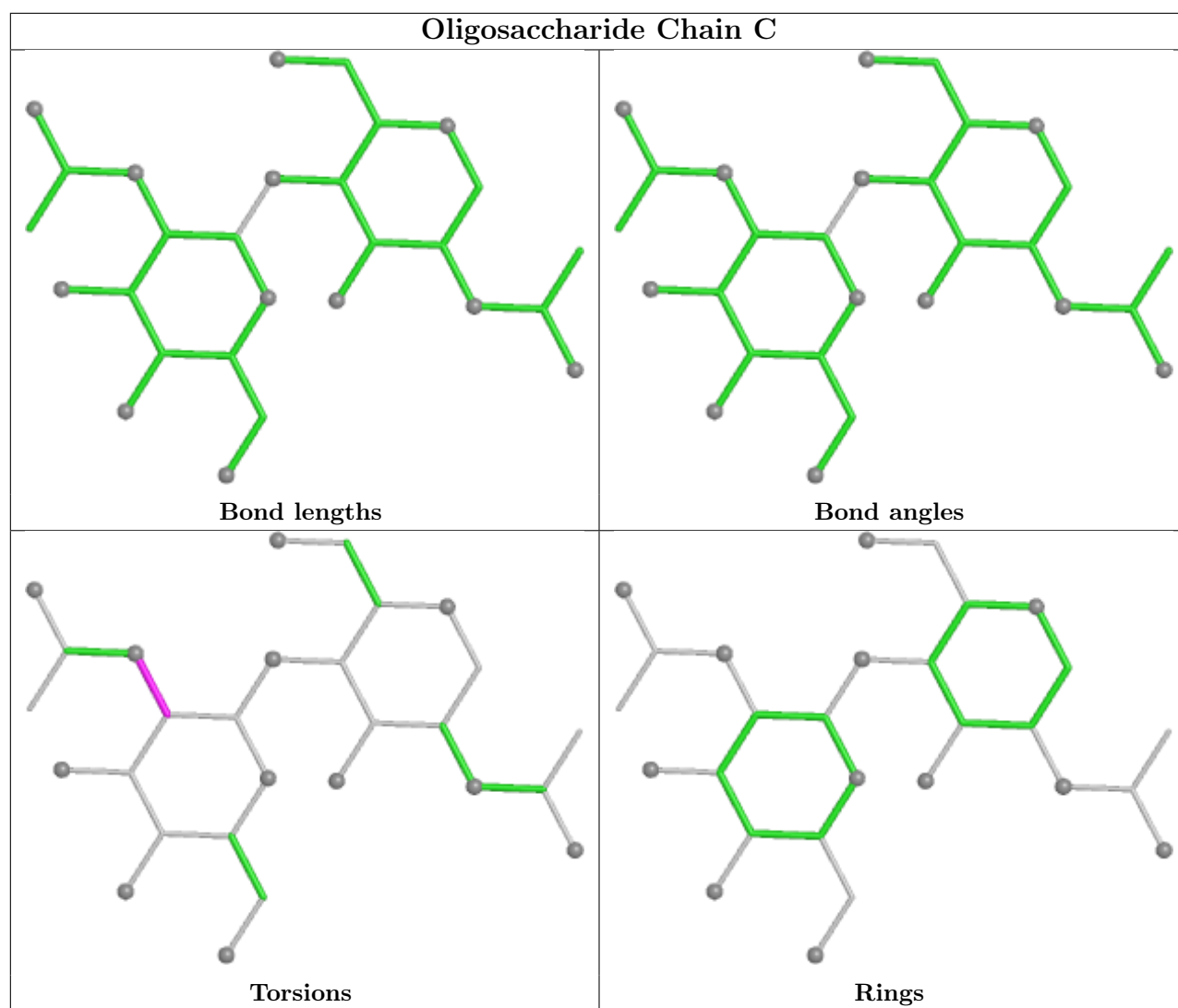
All (5) torsion outliers are listed below:

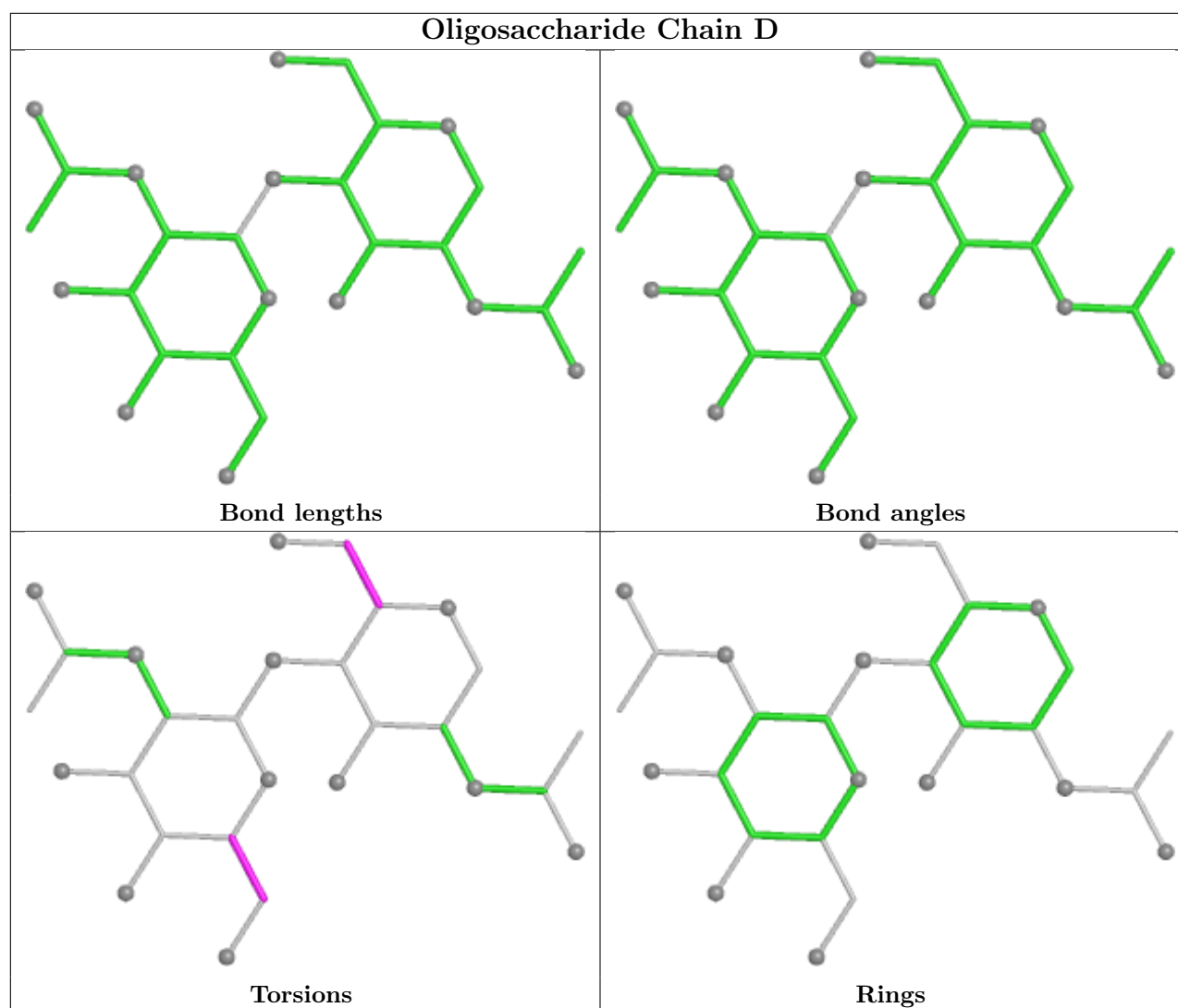
Mol	Chain	Res	Type	Atoms
3	D	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	C	2	NAG	C3-C2-N2-C7
3	D	1	NAG	O5-C5-C6-O6

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.





5.6 Ligand geometry [i](#)

9 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	CO2	A	808	-	2,2,2	0.41	0	1,1,1	0.52	0
7	PEE	A	807	-	50,50,50	1.28	3 (6%)	53,55,55	0.94	1 (1%)
10	BCT	A	809	-	2,3,3	0.98	0	2,3,3	1.66	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	801	1	14,14,15	0.27	0	17,19,21	0.43	0
7	PEE	A	804	-	50,50,50	1.27	3 (6%)	53,55,55	0.93	1 (1%)
5	A1AVC	A	802	-	34,34,34	1.37	4 (11%)	42,45,45	2.04	9 (21%)
7	PEE	A	805	-	50,50,50	1.26	3 (6%)	53,55,55	0.93	1 (1%)
8	Y01	A	806	-	38,38,38	1.18	3 (7%)	57,57,57	1.93	9 (15%)
6	CLR	A	803	-	31,31,31	1.07	1 (3%)	48,48,48	1.33	6 (12%)

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	PEE	A	807	-	-	34/54/54/54	-
4	NAG	A	801	1	-	2/6/23/26	0/1/1/1
7	PEE	A	804	-	-	19/54/54/54	-
5	A1AVC	A	802	-	-	12/23/23/23	0/2/2/2
7	PEE	A	805	-	-	29/54/54/54	-
8	Y01	A	806	-	-	10/19/77/77	0/4/4/4
6	CLR	A	803	-	-	2/10/68/68	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	807	PEE	P-O4P	4.72	1.78	1.59
7	A	804	PEE	P-O4P	4.53	1.77	1.59
7	A	805	PEE	P-O4P	4.51	1.77	1.59
5	A	802	A1AVC	C09-C04	-4.47	1.35	1.43
8	A	806	Y01	CAK-CAI	-4.19	1.41	1.50
7	A	804	PEE	C39-C38	3.96	1.54	1.31
7	A	805	PEE	C39-C38	3.84	1.54	1.31
7	A	807	PEE	C39-C38	3.82	1.53	1.31
7	A	807	PEE	C18-C19	3.65	1.52	1.31
7	A	804	PEE	C18-C19	3.62	1.52	1.31
7	A	805	PEE	C18-C19	3.60	1.52	1.31
5	A	802	A1AVC	C12-C13	3.51	1.58	1.50
5	A	802	A1AVC	C12-C11	2.95	1.54	1.51
8	A	806	Y01	CAI-CAZ	2.61	1.38	1.33
5	A	802	A1AVC	C16-C14	2.59	1.56	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	806	Y01	CAL-CAX	2.03	1.55	1.50
6	A	803	CLR	C18-C13	-2.00	1.50	1.54

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	802	A1AVC	C11-C12-C13	-9.97	96.37	112.17
8	A	806	Y01	CAV-CAZ-CBH	7.58	126.49	116.42
8	A	806	Y01	OAW-CAY-CAM	5.21	122.72	111.50
8	A	806	Y01	OAW-CAY-OAG	-5.05	111.49	123.70
8	A	806	Y01	CAV-CAZ-CAI	-4.90	113.54	120.61
7	A	807	PEE	O2P-P-O1P	4.24	133.18	112.24
7	A	805	PEE	O2P-P-O1P	4.23	133.15	112.24
7	A	804	PEE	O2P-P-O1P	4.23	133.15	112.24
5	A	802	A1AVC	C12-C13-C14	3.74	133.05	127.24
6	A	803	CLR	C22-C20-C17	-3.64	102.76	110.28
5	A	802	A1AVC	O32-C10-C11	3.57	122.75	118.67
5	A	802	A1AVC	C15-C14-C16	2.73	119.86	115.27
8	A	806	Y01	OAW-CBC-CAV	-2.66	102.69	108.12
6	A	803	CLR	C18-C13-C12	2.44	114.45	110.59
5	A	802	A1AVC	C08-C09-C04	2.41	121.44	118.45
6	A	803	CLR	C12-C13-C14	-2.39	103.56	107.27
6	A	803	CLR	C16-C17-C20	-2.39	108.45	112.15
8	A	806	Y01	OAW-CBC-CAR	2.33	113.95	108.33
8	A	806	Y01	CAP-CBE-CBB	-2.31	108.58	112.15
10	A	809	BCT	O2-C-O1	2.18	125.19	119.55
5	A	802	A1AVC	O33-C03-C04	2.18	121.26	116.64
8	A	806	Y01	CAS-CBF-CBD	-2.16	108.64	111.75
8	A	806	Y01	OAF-CAX-CAL	-2.16	116.16	123.08
5	A	802	A1AVC	C22-C23-C24	-2.14	108.99	115.92
5	A	802	A1AVC	C16-C14-C13	-2.11	116.84	121.12
6	A	803	CLR	C24-C23-C22	-2.09	103.62	113.24
6	A	803	CLR	C10-C5-C6	2.08	126.08	122.90
5	A	802	A1AVC	C08-C09-C10	-2.05	118.69	121.42

There are no chirality outliers.

All (108) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	804	PEE	O4P-C4-C5-N
7	A	805	PEE	C1-O3P-P-O1P
7	A	805	PEE	C4-O4P-P-O3P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	805	PEE	C4-O4P-P-O2P
7	A	805	PEE	C4-O4P-P-O1P
7	A	807	PEE	C1-O3P-P-O2P
7	A	807	PEE	C4-O4P-P-O1P
7	A	807	PEE	C35-C36-C37-C38
7	A	807	PEE	C37-C38-C39-C40
8	A	806	Y01	OAG-CAY-OAW-CBC
7	A	807	PEE	O5-C30-O3-C3
5	A	802	A1AVC	C14-C16-C17-C18
7	A	807	PEE	C31-C30-O3-C3
8	A	806	Y01	CAM-CAY-OAW-CBC
6	A	803	CLR	C21-C20-C22-C23
7	A	804	PEE	C37-C38-C39-C40
7	A	805	PEE	C37-C38-C39-C40
7	A	804	PEE	C21-C22-C23-C24
5	A	802	A1AVC	C15-C14-C16-C17
5	A	802	A1AVC	C13-C14-C16-C17
7	A	805	PEE	C20-C21-C22-C23
8	A	806	Y01	CAR-CBC-OAW-CAY
7	A	807	PEE	O2-C2-C3-O3
4	A	801	NAG	O5-C5-C6-O6
5	A	802	A1AVC	C21-C22-C23-C24
6	A	803	CLR	C17-C20-C22-C23
7	A	804	PEE	C17-C18-C19-C20
7	A	805	PEE	C17-C18-C19-C20
7	A	805	PEE	C43-C44-C45-C46
5	A	802	A1AVC	C23-C24-C26-C27
7	A	804	PEE	C35-C36-C37-C38
7	A	807	PEE	C10-C11-C12-C13
7	A	805	PEE	C1-O3P-P-O4P
7	A	807	PEE	C1-O3P-P-O4P
7	A	807	PEE	C4-O4P-P-O3P
8	A	806	Y01	CAV-CBC-OAW-CAY
5	A	802	A1AVC	C27-C28-C29-C30
7	A	804	PEE	C20-C21-C22-C23
7	A	804	PEE	C13-C14-C15-C16
7	A	805	PEE	C41-C42-C43-C44
7	A	804	PEE	C31-C32-C33-C34
7	A	807	PEE	C34-C35-C36-C37
5	A	802	A1AVC	C24-C26-C27-C28
7	A	807	PEE	C42-C43-C44-C45
8	A	806	Y01	CAJ-CAN-CBA-CAB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	807	PEE	C12-C13-C14-C15
7	A	804	PEE	C32-C33-C34-C35
7	A	807	PEE	C20-C21-C22-C23
7	A	805	PEE	C13-C14-C15-C16
7	A	807	PEE	C17-C18-C19-C20
4	A	801	NAG	C4-C5-C6-O6
7	A	807	PEE	C13-C14-C15-C16
7	A	807	PEE	C40-C41-C42-C43
7	A	805	PEE	C33-C34-C35-C36
5	A	802	A1AVC	C17-C18-C19-C21
7	A	807	PEE	C19-C20-C21-C22
7	A	804	PEE	C43-C44-C45-C46
5	A	802	A1AVC	C27-C28-C29-C31
7	A	804	PEE	C39-C40-C41-C42
7	A	807	PEE	C43-C44-C45-C46
7	A	805	PEE	C34-C35-C36-C37
7	A	807	PEE	C22-C23-C24-C25
7	A	807	PEE	C24-C25-C26-C27
7	A	804	PEE	C22-C23-C24-C25
8	A	806	Y01	CAJ-CAN-CBA-CAA
7	A	807	PEE	C1-C2-C3-O3
7	A	804	PEE	C40-C41-C42-C43
7	A	805	PEE	O2-C2-C3-O3
8	A	806	Y01	CAO-CAJ-CAN-CBA
5	A	802	A1AVC	C17-C18-C19-C20
7	A	805	PEE	C39-C40-C41-C42
7	A	805	PEE	C11-C12-C13-C14
7	A	805	PEE	C1-C2-C3-O3
7	A	807	PEE	C16-C17-C18-C19
7	A	807	PEE	C23-C24-C25-C26
7	A	805	PEE	C19-C20-C21-C22
7	A	805	PEE	C1-O3P-P-O2P
7	A	807	PEE	C4-O4P-P-O2P
7	A	807	PEE	C41-C42-C43-C44
7	A	805	PEE	C38-C39-C40-C41
7	A	807	PEE	C32-C33-C34-C35
7	A	805	PEE	C44-C45-C46-C47
5	A	802	A1AVC	C25-C24-C26-C27
7	A	807	PEE	C36-C37-C38-C39
7	A	807	PEE	O3P-C1-C2-C3
7	A	805	PEE	O4-C10-O2-C2
7	A	804	PEE	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	802	A1AVC	C22-C23-C24-C25
7	A	807	PEE	C33-C34-C35-C36
8	A	806	Y01	CAM-CAL-CAX-OAF
7	A	807	PEE	O3P-C1-C2-O2
8	A	806	Y01	CAM-CAL-CAX-OAH
7	A	805	PEE	C16-C17-C18-C19
7	A	805	PEE	C11-C10-O2-C2
7	A	804	PEE	C38-C39-C40-C41
7	A	804	PEE	C24-C25-C26-C27
7	A	807	PEE	C44-C45-C46-C47
7	A	805	PEE	O4P-C4-C5-N
7	A	805	PEE	C30-C31-C32-C33
7	A	805	PEE	C32-C33-C34-C35
7	A	807	PEE	C1-O3P-P-O1P
7	A	804	PEE	O2-C2-C3-O3
7	A	804	PEE	C36-C37-C38-C39
7	A	805	PEE	C5-C4-O4P-P
7	A	805	PEE	C22-C23-C24-C25
7	A	807	PEE	C11-C12-C13-C14
7	A	804	PEE	O2-C10-C11-C12
8	A	806	Y01	CAL-CAM-CAY-OAW

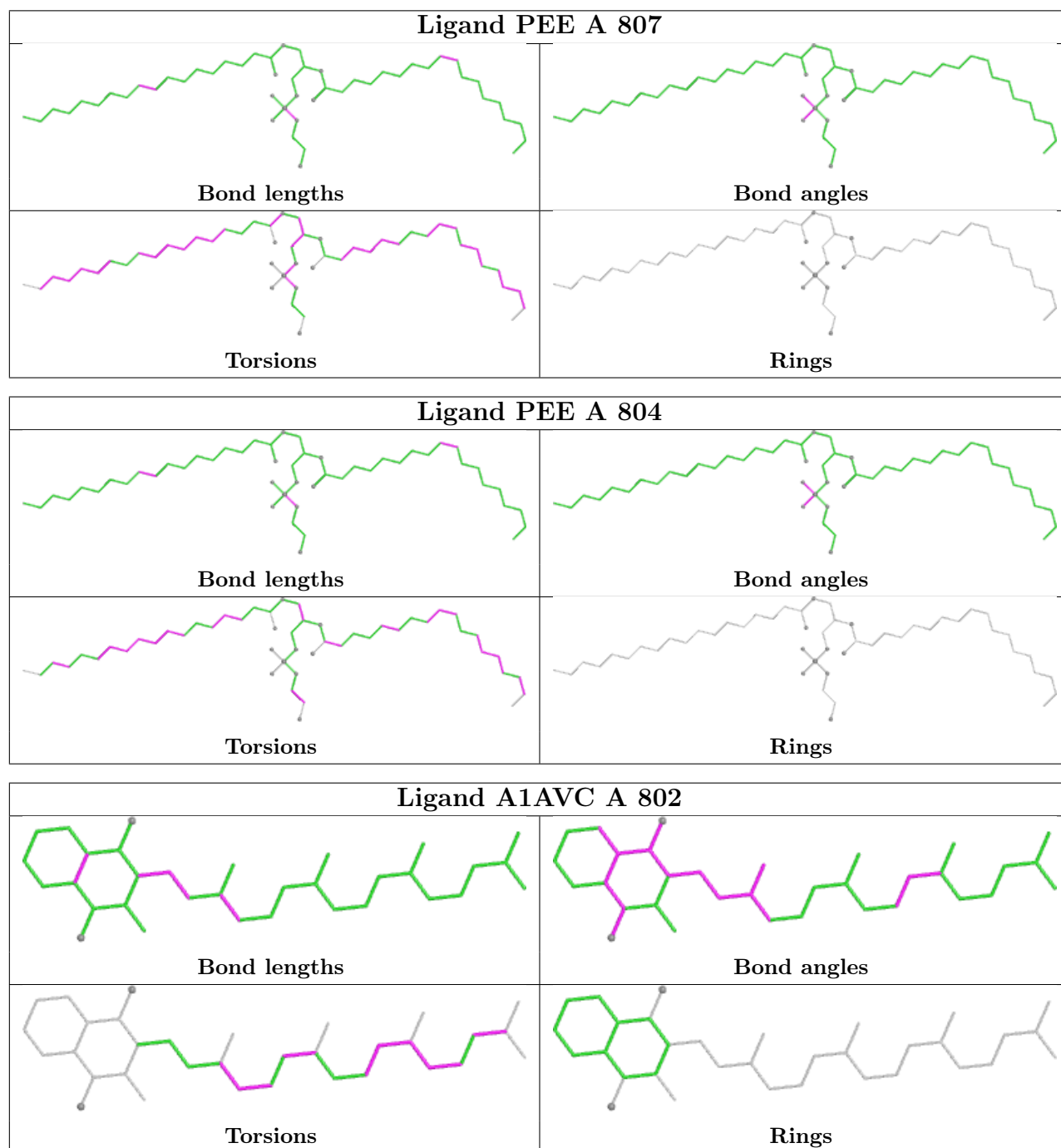
There are no ring outliers.

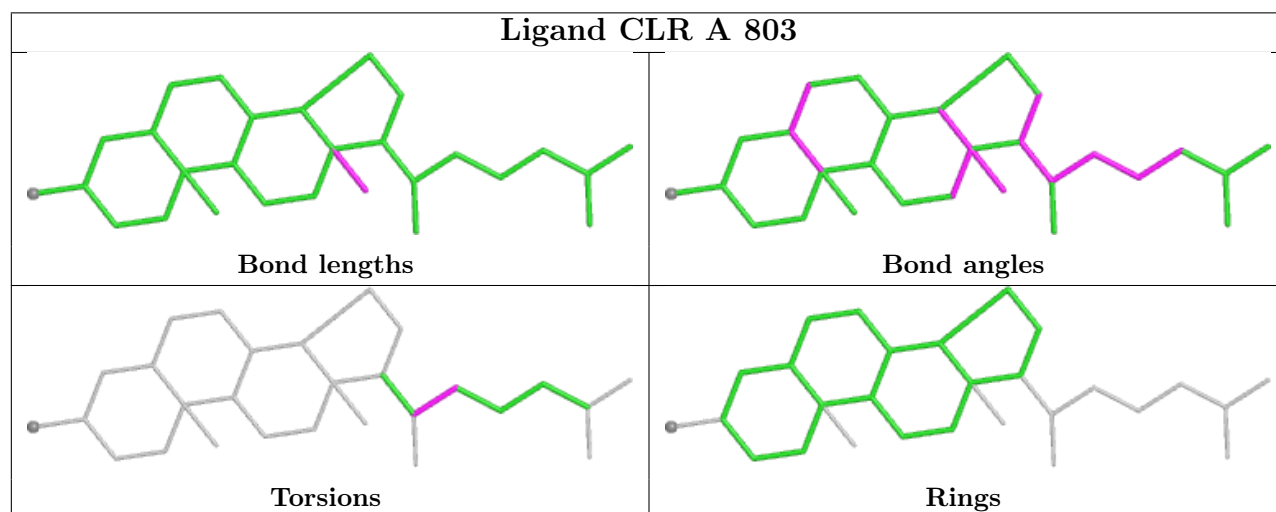
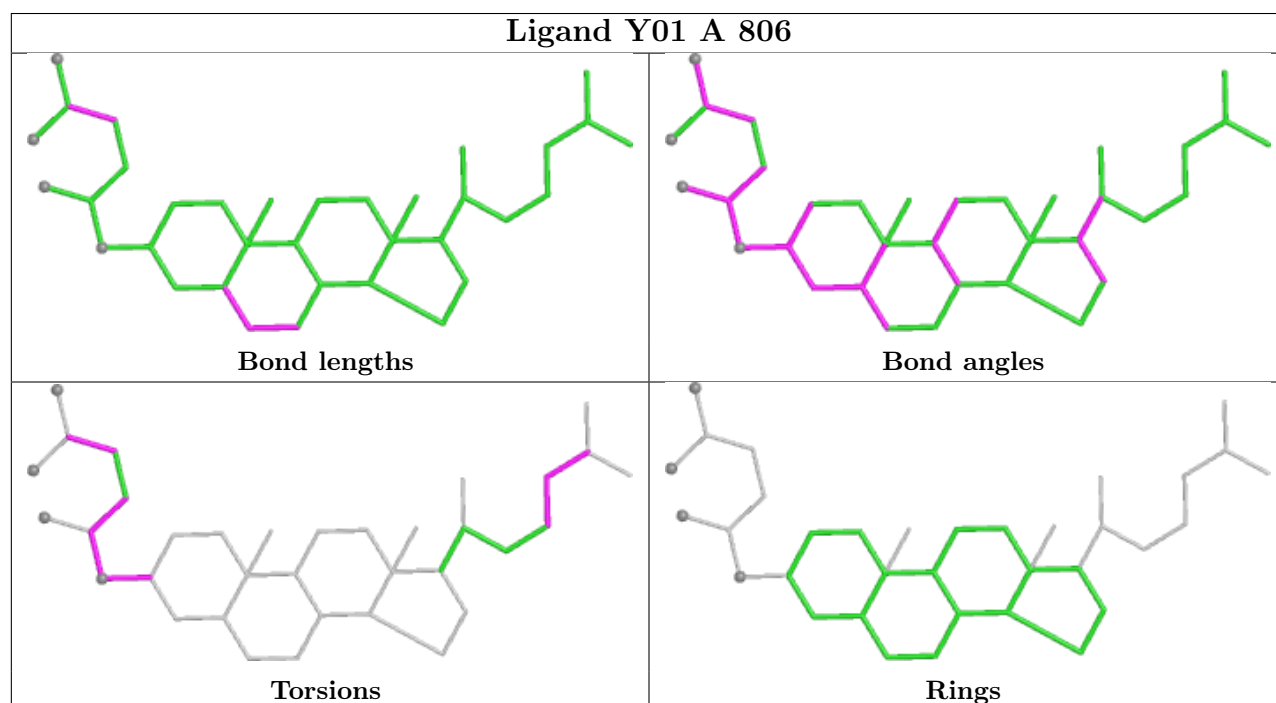
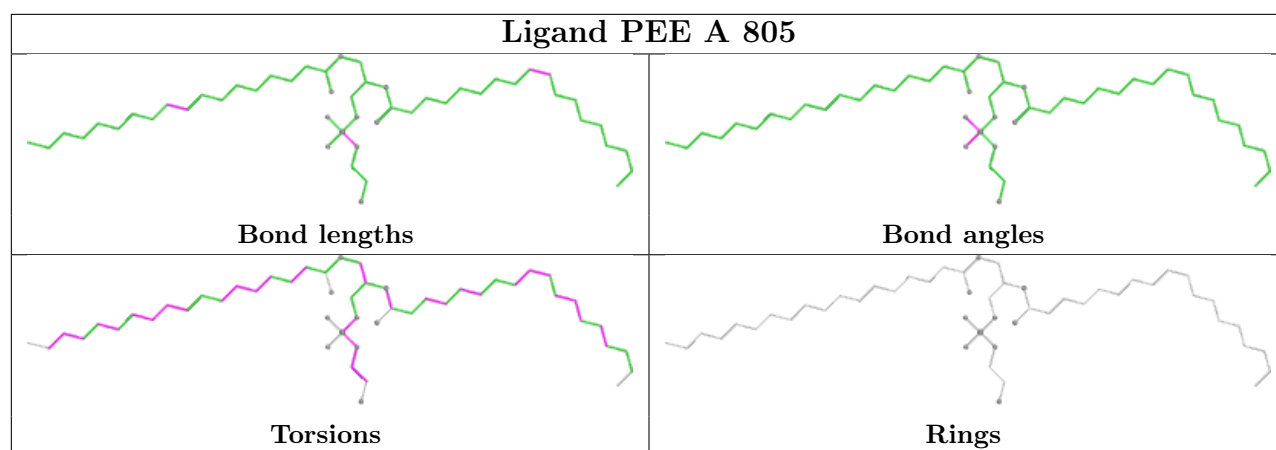
5 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	807	PEE	3	0
10	A	809	BCT	2	0
7	A	804	PEE	4	0
7	A	805	PEE	5	0
8	A	806	Y01	8	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.