



Full wwPDB EM Validation Report ⓘ

Apr 28, 2026 – 02:19 PM JST

PDB ID : 9L20 / pdb_00009L20
EMDB ID : EMD-62764
Title : cryo-EM structure of Vitamin K-dependent gamma-carboxylase complexed with anisindione
Authors : Yao, D.; Wu, K.; Lan, P.
Deposited on : 2024-12-16
Resolution : 2.82 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

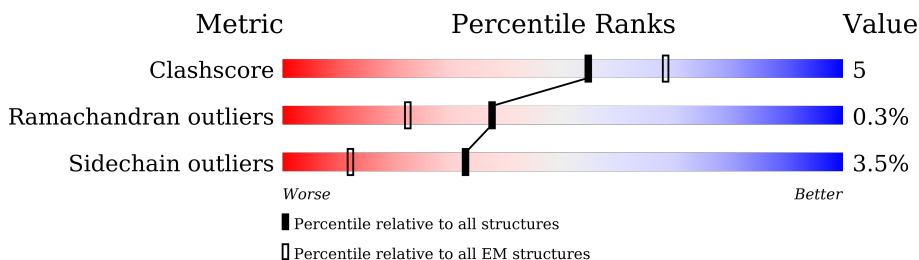
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.82 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	26	
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 6041 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.

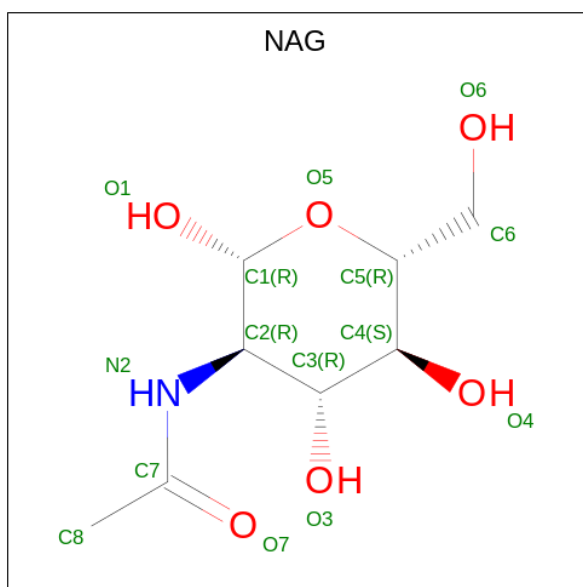
Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	21	Total	C	N	O	0	0
			162	101	27	34		

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



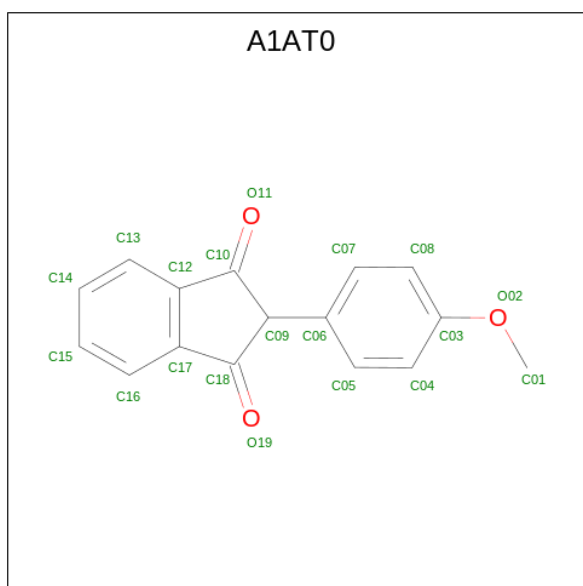
Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		

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



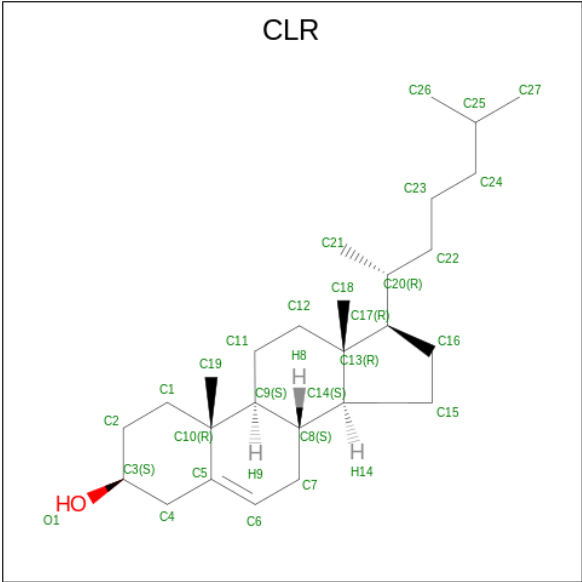
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 5 is anisindione (CCD ID: A1AT0) (formula: $C_{16}H_{12}O_3$) (labeled as "Ligand of Interest" by depositor).



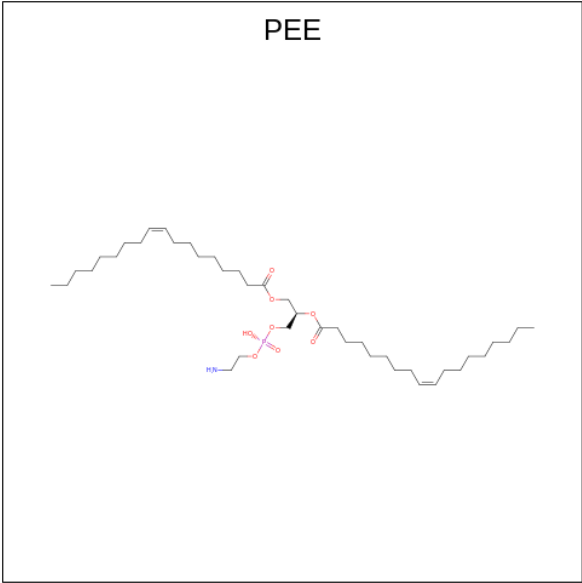
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			19	16	3	

- 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	
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	

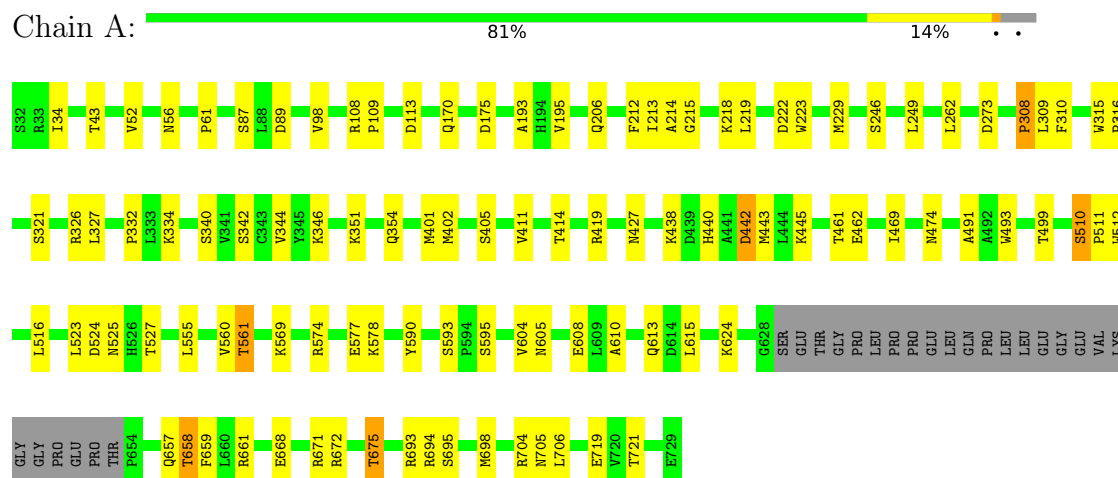
- BCT
-
- The diagram shows the chemical structure of Bicarbonate (BCT). A central carbon atom (C) is bonded to three oxygen atoms and one hydrogen atom. One oxygen atom (O1) is double-bonded to the carbon. Another oxygen atom (O2) is single-bonded to the carbon and carries a negative charge (O⁻). The third oxygen atom (O3) is single-bonded to the carbon and is part of a hydroxyl group (OH). The hydrogen atom is also single-bonded to the carbon. The atoms are color-coded: carbon is green, oxygen is red, and hydrogen is green. The labels O1, O2, and O3 are in green, while the 'C' and 'H' are in red.
- [O-]C(=O)O

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

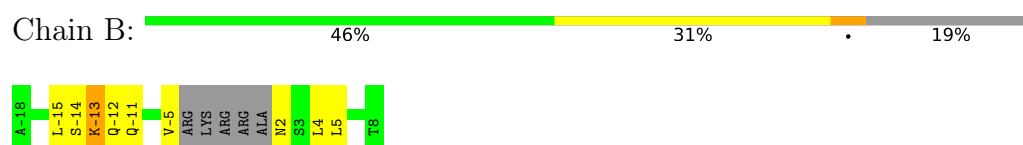
3 Residue-property plots [i](#)

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



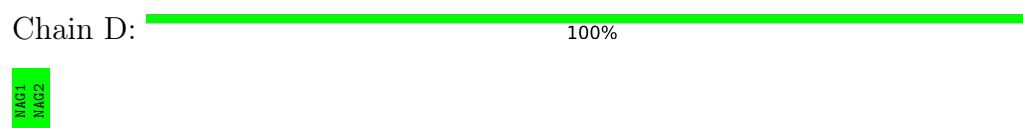
- Molecule 2: Vitamin K-dependent protein S



- 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	469550	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CLR, Y01, PEE, A1AT0, BCT

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	0.32	5/5732 (0.1%)	0.43	5/7780 (0.1%)
2	B	0.60	0/161	0.93	2/215 (0.9%)
All	All	0.34	5/5893 (0.1%)	0.45	7/7995 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	214	ALA	C-O	-7.04	1.14	1.24
1	A	215	GLY	C-O	-6.58	1.16	1.24
1	A	212	PHE	C-O	-6.41	1.16	1.24
1	A	308	PRO	C-O	-5.84	1.16	1.24
1	A	213	ILE	C-O	-5.70	1.15	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	PHE	N-CA-C	-7.43	104.24	113.38
1	A	219	LEU	N-CA-C	-6.42	103.53	112.25
1	A	214	ALA	N-CA-C	-6.06	104.96	112.90
1	A	309	LEU	N-CA-C	-6.05	104.53	113.61
2	B	-12	GLN	N-CA-C	-5.59	105.05	112.94
1	A	212	PHE	CA-C-O	-5.58	114.63	120.55
2	B	-11	GLN	N-CA-C	-5.40	106.56	114.39

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	55	0
2	B	162	0	165	3	0
3	C	28	0	25	0	0
3	D	28	0	25	0	0
4	A	14	0	13	0	0
5	A	19	0	0	0	0
6	A	28	0	46	2	0
7	A	153	0	246	5	0
8	A	35	0	49	2	0
9	A	4	0	0	2	0
All	All	6041	0	6112	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:218:LYS:NZ	9:A:808:BCT:O1	2.09	0.86
1:A:704:ARG:NH1	1:A:705:ASN:OD1	2.20	0.75
1:A:605:ASN:HB3	1:A:608:GLU:HB3	1.73	0.71
1:A:693:ARG:HG3	8:A:806:Y01:HAE2	1.74	0.69
1:A:445:LYS:NZ	1:A:491:ALA:O	2.26	0.68
1:A:229:MET:HE3	1:A:402:MET:HB3	1.79	0.65
1:A:405:SER:HG	2:B:2:ASN:N	1.97	0.62
1:A:419:ARG:NH1	1:A:461:THR:OG1	2.35	0.59
1:A:527:THR:HG22	1:A:604:VAL:HG22	1.86	0.57
1:A:411:VAL:HG22	1:A:469:ILE:HG23	1.86	0.57
1:A:615:LEU:HD11	1:A:659:PHE:HB2	1.88	0.56
1:A:222:ASP:OD2	1:A:474:ASN:ND2	2.38	0.56
1:A:657:GLN:OE1	1:A:661:ARG:NH2	2.39	0.56
1:A:461:THR:HG22	1:A:462:GLU:H	1.70	0.55
1:A:442:ASP:HB3	1:A:493:TRP:CZ2	2.41	0.55
1:A:401:MET:HE3	9:A:808:BCT:O2	2.07	0.55
1:A:411:VAL:HG21	1:A:438:LYS:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:ARG:HG3	8:A:806:Y01:CAE	2.38	0.54
1:A:332:PRO:O	1:A:334:LYS:NZ	2.27	0.54
1:A:108:ARG:HD3	1:A:109:PRO:HD2	1.88	0.53
1:A:671:ARG:O	1:A:675:THR:OG1	2.26	0.53
1:A:694:ARG:O	1:A:698:MET:HG2	2.09	0.53
1:A:704:ARG:NH2	1:A:719:GLU:OE1	2.41	0.53
1:A:440:HIS:HB2	1:A:443:MET:HG3	1.89	0.52
1:A:402:MET:HA	2:B:4:LEU:HD22	1.92	0.52
1:A:668:GLU:OE1	1:A:672:ARG:NH1	2.43	0.51
2:B:-14:SER:O	2:B:-13:LYS:HB2	2.09	0.51
1:A:52:VAL:O	1:A:56:ASN:ND2	2.34	0.50
1:A:593:SER:OG	1:A:595:SER:O	2.30	0.49
1:A:89:ASP:OD2	1:A:694:ARG:NH2	2.46	0.49
1:A:56:ASN:HB2	1:A:344:VAL:HG12	1.96	0.47
1:A:346:LYS:NZ	1:A:354:GLN:O	2.47	0.47
1:A:578:LYS:HE2	1:A:578:LYS:HB3	1.69	0.47
1:A:113:ASP:HB3	1:A:706:LEU:HG	1.96	0.47
1:A:658:THR:HA	1:A:661:ARG:HG2	1.97	0.46
1:A:574:ARG:N	1:A:577:GLU:OE2	2.45	0.45
6:A:803:CLR:H213	6:A:803:CLR:H231	1.71	0.45
1:A:193:ALA:HB1	1:A:340:SER:HB2	1.98	0.45
1:A:561:THR:HG23	1:A:590:TYR:HB2	2.00	0.44
6:A:803:CLR:H222	6:A:803:CLR:H25	1.76	0.44
7:A:804:PEE:H33	7:A:804:PEE:H40	1.38	0.44
1:A:308:PRO:HG2	7:A:805:PEE:H40	2.00	0.43
7:A:807:PEE:H23	7:A:807:PEE:H30	1.83	0.43
7:A:807:PEE:H67	7:A:807:PEE:H72	1.58	0.43
1:A:170:GLN:NE2	1:A:206:GLN:OE1	2.52	0.43
1:A:523:LEU:HD23	1:A:523:LEU:HA	1.90	0.43
1:A:610:ALA:O	1:A:613:GLN:HG3	2.19	0.43
1:A:512:TRP:O	1:A:516:LEU:HG	2.19	0.42
1:A:524:ASP:OD1	1:A:525:ASN:N	2.51	0.42
1:A:175:ASP:OD1	1:A:195:VAL:HG12	2.18	0.42
7:A:805:PEE:H48	7:A:805:PEE:H55	1.70	0.42
1:A:61:PRO:HG3	1:A:193:ALA:O	2.20	0.41
1:A:555:LEU:HD13	1:A:560:VAL:HG22	2.02	0.41
1:A:668:GLU:O	1:A:672:ARG:HG2	2.21	0.41
1:A:249:LEU:HD23	1:A:249:LEU:HA	1.81	0.41
1:A:315:TRP:CG	1:A:316:PRO:HD3	2.56	0.41
1:A:218:LYS:HE3	1:A:223:TRP:CZ2	2.57	0.40
1:A:427:ASN:OD1	1:A:427:ASN:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:SER:N	1:A:511:PRO:HD2	2.36	0.40
1:A:624:LYS:HB2	1:A:624:LYS:HE2	1.86	0.40
1:A:327:LEU:HD23	1:A:327:LEU:HA	1.94	0.40
1:A:569:LYS:HB2	1:A:569:LYS:HE3	1.93	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%)	645 (96%)	23 (3%)	1 (0%)	48	75
2	B	17/26 (65%)	15 (88%)	1 (6%)	1 (6%)	1	3
All	All	686/724 (95%)	660 (96%)	24 (4%)	2 (0%)	37	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	-13	LYS
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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	608/629 (97%)	589 (97%)	19 (3%)	35	69
2	B	19/23 (83%)	16 (84%)	3 (16%)	2	8
All	All	627/652 (96%)	605 (96%)	22 (4%)	32	65

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ILE
1	A	43	THR
1	A	87	SER
1	A	98	VAL
1	A	246	SER
1	A	262	LEU
1	A	273	ASP
1	A	321	SER
1	A	326	ARG
1	A	342	SER
1	A	414	THR
1	A	442	ASP
1	A	499	THR
1	A	510	SER
1	A	561	THR
1	A	658	THR
1	A	675	THR
1	A	695	SER
1	A	721	THR
2	B	-15	LEU
2	B	-5	VAL
2	B	5	LEU

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	170	GLN
1	A	206	GLN
1	A	292	GLN
1	A	381	HIS
1	A	440	HIS

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Mol	Chain	Res	Type
1	A	718	GLN

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	0.49	0	17,19,21	1.10	1 (5%)
3	NAG	C	2	3	14,14,15	0.23	0	17,19,21	0.65	0
3	NAG	D	1	1,3	14,14,15	0.26	0	17,19,21	0.37	0
3	NAG	D	2	3	14,14,15	0.23	0	17,19,21	0.45	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	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	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	3.48	116.90	112.19

There are no chirality outliers.

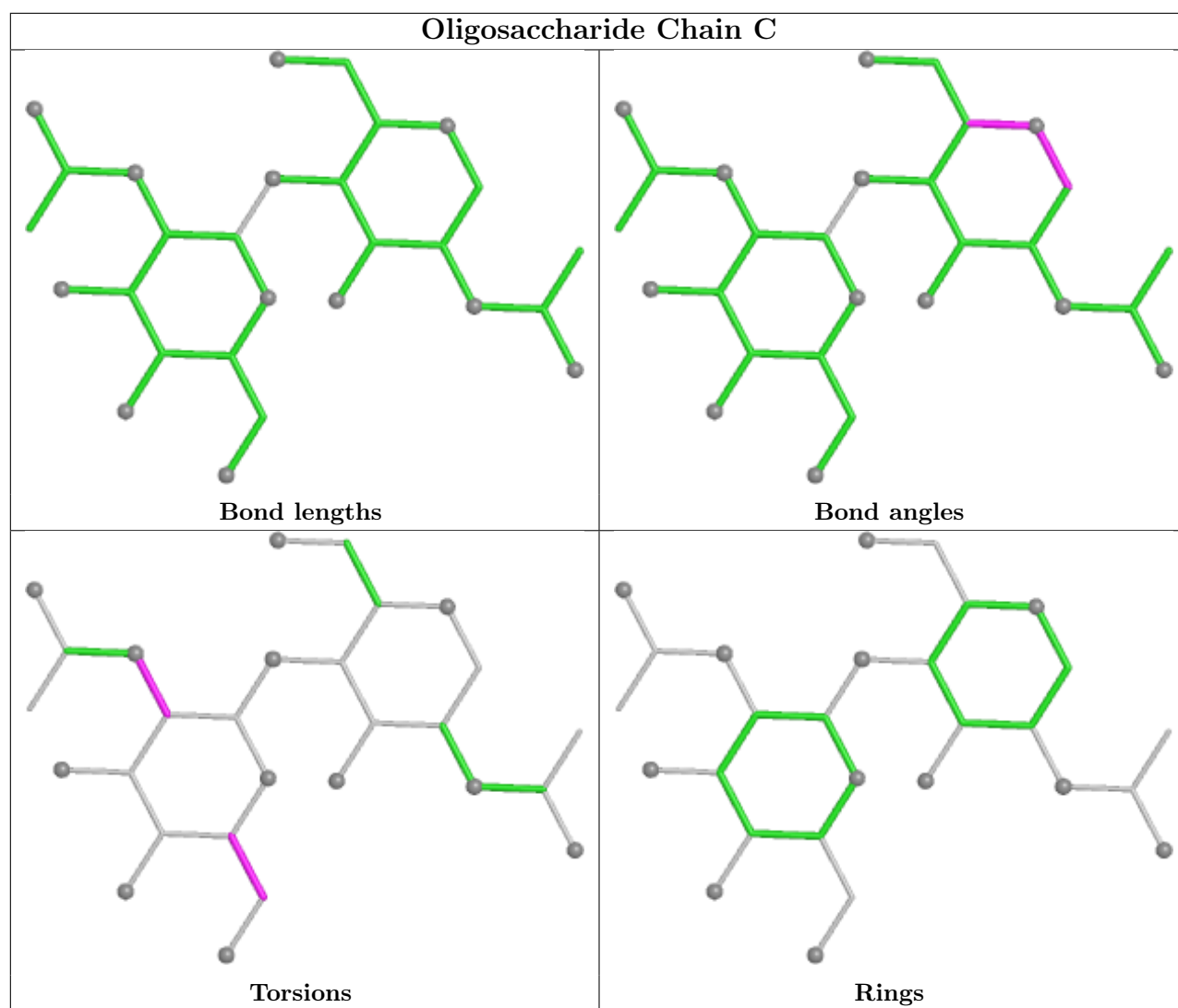
All (5) torsion outliers are listed below:

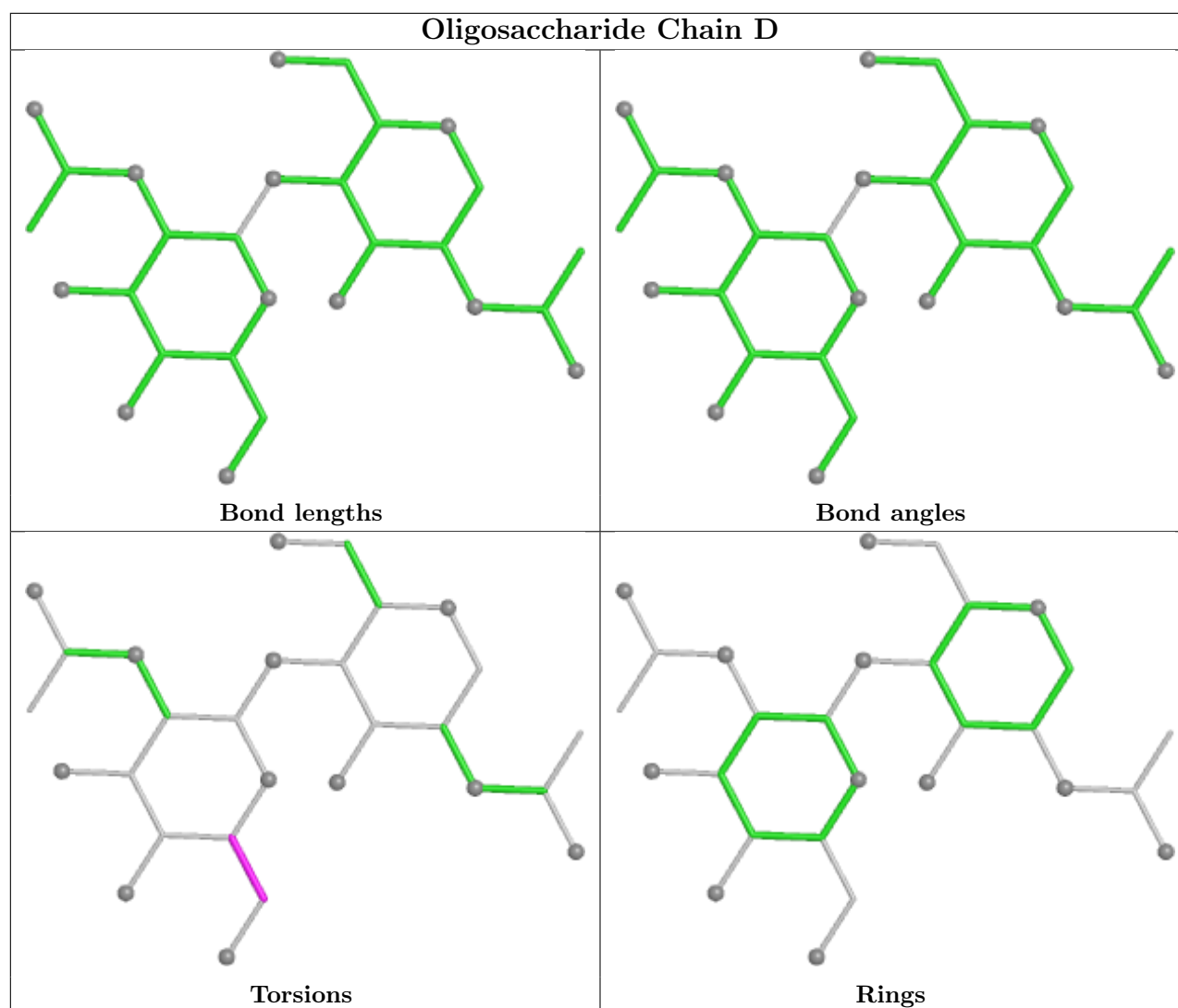
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C3-C2-N2-C7

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	$\# Z > 2$
9	BCT	A	808	-	2,3,3	0.96	0	2,3,3	1.66	1 (50%)
4	NAG	A	801	1	14,14,15	0.33	0	17,19,21	0.40	0
5	A1AT0	A	802	-	21,21,21	1.99	5 (23%)	29,30,30	1.15	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PEE	A	807	-	50,50,50	1.27	5 (10%)	53,55,55	0.94	1 (1%)
7	PEE	A	805	-	50,50,50	1.24	4 (8%)	53,55,55	0.93	1 (1%)
6	CLR	A	803	-	31,31,31	1.04	2 (6%)	48,48,48	1.38	10 (20%)
7	PEE	A	804	-	50,50,50	1.24	5 (10%)	53,55,55	0.95	1 (1%)
8	Y01	A	806	-	38,38,38	1.18	3 (7%)	57,57,57	1.93	9 (15%)

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
4	NAG	A	801	1	-	1/6/23/26	0/1/1/1
5	A1AT0	A	802	-	-	2/6/22/22	0/3/3/3
7	PEE	A	807	-	-	30/54/54/54	-
7	PEE	A	805	-	-	24/54/54/54	-
6	CLR	A	803	-	-	1/10/68/68	0/4/4/4
7	PEE	A	804	-	-	22/54/54/54	-
8	Y01	A	806	-	-	10/19/77/77	0/4/4/4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	807	PEE	P-O4P	4.70	1.78	1.59
7	A	804	PEE	P-O4P	4.34	1.76	1.59
7	A	805	PEE	P-O4P	4.31	1.76	1.59
5	A	802	A1AT0	O11-C10	-4.26	1.16	1.22
5	A	802	A1AT0	C17-C18	4.22	1.53	1.47
8	A	806	Y01	CAK-CAI	-4.22	1.41	1.50
5	A	802	A1AT0	O19-C18	-4.14	1.16	1.22
5	A	802	A1AT0	C12-C10	3.93	1.53	1.47
7	A	804	PEE	C39-C38	3.89	1.54	1.31
7	A	805	PEE	C39-C38	3.87	1.54	1.31
7	A	807	PEE	C39-C38	3.83	1.54	1.31
7	A	807	PEE	C18-C19	3.64	1.52	1.31
7	A	804	PEE	C18-C19	3.61	1.52	1.31
7	A	805	PEE	C18-C19	3.56	1.52	1.31
8	A	806	Y01	CAI-CAZ	2.61	1.38	1.33
5	A	802	A1AT0	C06-C09	2.32	1.56	1.53
6	A	803	CLR	C18-C13	-2.24	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	804	PEE	O2-C2	-2.23	1.41	1.46
7	A	804	PEE	O4P-C4	-2.12	1.36	1.44
6	A	803	CLR	C16-C17	2.10	1.58	1.54
8	A	806	Y01	CAL-CAX	2.07	1.55	1.50
7	A	805	PEE	O4P-C4	-2.04	1.36	1.44
7	A	807	PEE	O2-C2	-2.02	1.41	1.46
7	A	807	PEE	O4P-C4	-2.02	1.36	1.44

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	806	Y01	CAV-CAZ-CBH	7.59	126.50	116.42
8	A	806	Y01	OAW-CAY-CAM	5.24	122.79	111.50
8	A	806	Y01	OAW-CAY-OAG	-5.09	111.41	123.70
8	A	806	Y01	CAV-CAZ-CAI	-4.90	113.54	120.61
7	A	805	PEE	O2P-P-O1P	4.28	133.39	112.24
7	A	804	PEE	O2P-P-O1P	4.26	133.32	112.24
7	A	807	PEE	O2P-P-O1P	4.25	133.26	112.24
6	A	803	CLR	C22-C20-C17	-3.59	102.86	110.28
5	A	802	A1AT0	C07-C06-C05	-2.80	114.80	118.29
5	A	802	A1AT0	C05-C06-C09	2.70	124.38	120.95
8	A	806	Y01	OAW-CBC-CAV	-2.65	102.69	108.12
6	A	803	CLR	C18-C13-C12	2.42	114.40	110.59
6	A	803	CLR	C21-C20-C22	-2.40	106.61	110.36
8	A	806	Y01	OAW-CBC-CAR	2.32	113.93	108.33
6	A	803	CLR	C12-C13-C14	-2.31	103.69	107.27
8	A	806	Y01	CAP-CBE-CBB	-2.30	108.58	112.15
9	A	808	BCT	O2-C-O1	2.19	125.23	119.55
8	A	806	Y01	CAS-CBF-CBD	-2.18	108.62	111.75
6	A	803	CLR	C12-C13-C17	-2.17	113.33	116.57
8	A	806	Y01	OAF-CAX-CAL	-2.15	116.17	123.08
6	A	803	CLR	C13-C17-C20	-2.13	116.15	119.49
6	A	803	CLR	C11-C12-C13	-2.12	109.15	112.78
6	A	803	CLR	C24-C23-C22	-2.08	103.66	113.24
6	A	803	CLR	C10-C5-C6	2.07	126.07	122.90
5	A	802	A1AT0	C08-C07-C06	2.05	123.26	121.20
6	A	803	CLR	C16-C17-C20	-2.04	108.99	112.15

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	804	PEE	C17-C18-C19-C20
7	A	804	PEE	C1-O3P-P-O2P
7	A	804	PEE	C4-O4P-P-O1P
7	A	804	PEE	O4P-C4-C5-N
7	A	805	PEE	C1-O3P-P-O2P
7	A	805	PEE	O4P-C4-C5-N
7	A	807	PEE	C1-O3P-P-O2P
7	A	807	PEE	C4-O4P-P-O1P
7	A	807	PEE	C35-C36-C37-C38
8	A	806	Y01	OAG-CAY-OAW-CBC
7	A	807	PEE	O5-C30-O3-C3
7	A	807	PEE	C31-C30-O3-C3
8	A	806	Y01	CAM-CAY-OAW-CBC
7	A	804	PEE	C21-C22-C23-C24
7	A	807	PEE	C37-C38-C39-C40
8	A	806	Y01	CAR-CBC-OAW-CAY
7	A	807	PEE	O2-C2-C3-O3
7	A	804	PEE	C37-C38-C39-C40
7	A	807	PEE	C40-C41-C42-C43
7	A	804	PEE	C35-C36-C37-C38
7	A	805	PEE	C17-C18-C19-C20
7	A	805	PEE	C1-O3P-P-O4P
7	A	807	PEE	C4-O4P-P-O3P
7	A	807	PEE	C30-C31-C32-C33
8	A	806	Y01	CAV-CBC-OAW-CAY
7	A	805	PEE	C11-C12-C13-C14
7	A	807	PEE	C42-C43-C44-C45
7	A	805	PEE	C23-C24-C25-C26
7	A	807	PEE	C34-C35-C36-C37
7	A	804	PEE	C31-C32-C33-C34
7	A	804	PEE	C13-C14-C15-C16
7	A	807	PEE	C41-C42-C43-C44
7	A	805	PEE	C32-C33-C34-C35
7	A	805	PEE	C40-C41-C42-C43
8	A	806	Y01	CAJ-CAN-CBA-CAB
7	A	804	PEE	C20-C21-C22-C23
7	A	804	PEE	C40-C41-C42-C43
7	A	805	PEE	C13-C14-C15-C16
7	A	804	PEE	C32-C33-C34-C35
7	A	804	PEE	C43-C44-C45-C46
7	A	805	PEE	C22-C23-C24-C25
7	A	804	PEE	C39-C40-C41-C42
7	A	805	PEE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
7	A	805	PEE	C35-C36-C37-C38
7	A	807	PEE	C22-C23-C24-C25
7	A	805	PEE	O3P-C1-C2-C3
7	A	804	PEE	C22-C23-C24-C25
7	A	807	PEE	C13-C14-C15-C16
7	A	807	PEE	C12-C13-C14-C15
7	A	807	PEE	C17-C18-C19-C20
7	A	807	PEE	C43-C44-C45-C46
4	A	801	NAG	O5-C5-C6-O6
5	A	802	A1AT0	C07-C06-C09-C10
7	A	807	PEE	C20-C21-C22-C23
8	A	806	Y01	CAJ-CAN-CBA-CAA
7	A	807	PEE	C1-C2-C3-O3
7	A	804	PEE	C24-C25-C26-C27
7	A	804	PEE	C38-C39-C40-C41
7	A	805	PEE	O2-C2-C3-O3
7	A	807	PEE	C16-C17-C18-C19
8	A	806	Y01	CAO-CAJ-CAN-CBA
7	A	805	PEE	C19-C20-C21-C22
7	A	805	PEE	C16-C17-C18-C19
7	A	805	PEE	O3P-C1-C2-O2
7	A	804	PEE	C42-C43-C44-C45
7	A	807	PEE	C39-C40-C41-C42
7	A	805	PEE	C4-O4P-P-O3P
7	A	805	PEE	C4-O4P-P-O2P
7	A	807	PEE	C4-O4P-P-O2P
7	A	807	PEE	C33-C34-C35-C36
7	A	804	PEE	C11-C12-C13-C14
7	A	805	PEE	C1-C2-C3-O3
7	A	805	PEE	C42-C43-C44-C45
5	A	802	A1AT0	C05-C06-C09-C10
7	A	807	PEE	C24-C25-C26-C27
8	A	806	Y01	CAM-CAL-CAX-OAF
8	A	806	Y01	CAM-CAL-CAX-OAH
7	A	804	PEE	C16-C17-C18-C19
7	A	807	PEE	C19-C20-C21-C22
7	A	807	PEE	C36-C37-C38-C39
7	A	805	PEE	C36-C37-C38-C39
7	A	804	PEE	C12-C13-C14-C15
7	A	804	PEE	C36-C37-C38-C39
7	A	807	PEE	O3P-C1-C2-C3
7	A	807	PEE	C11-C12-C13-C14

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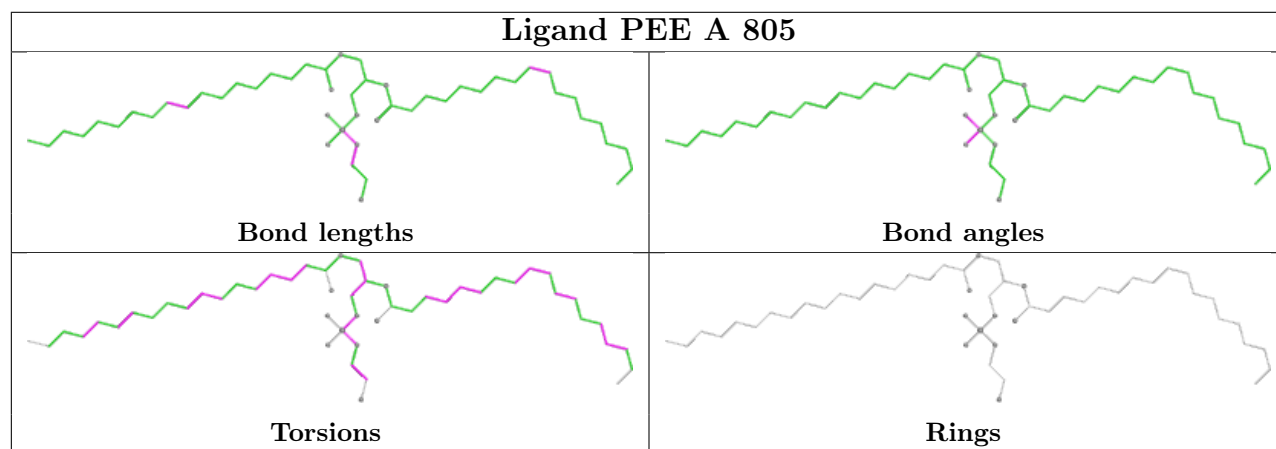
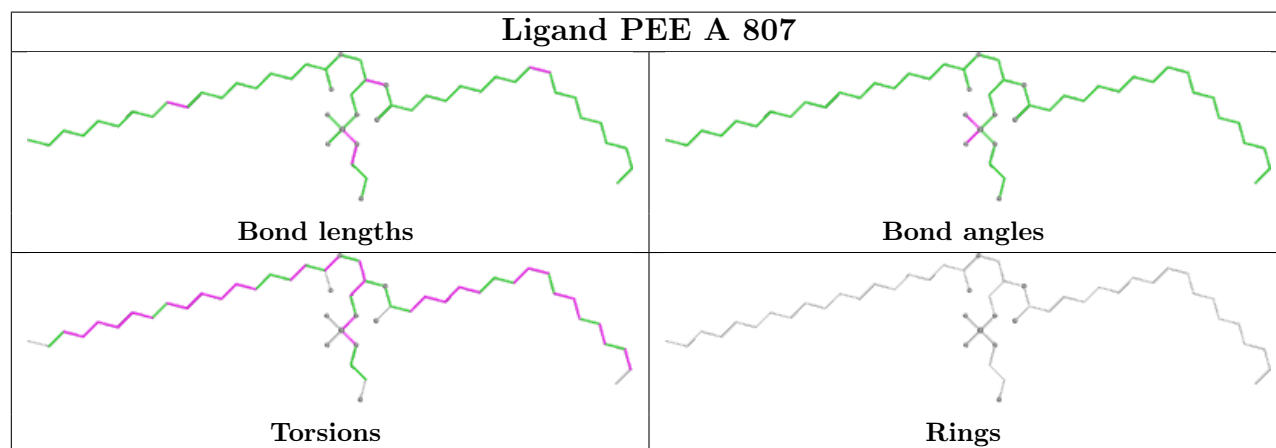
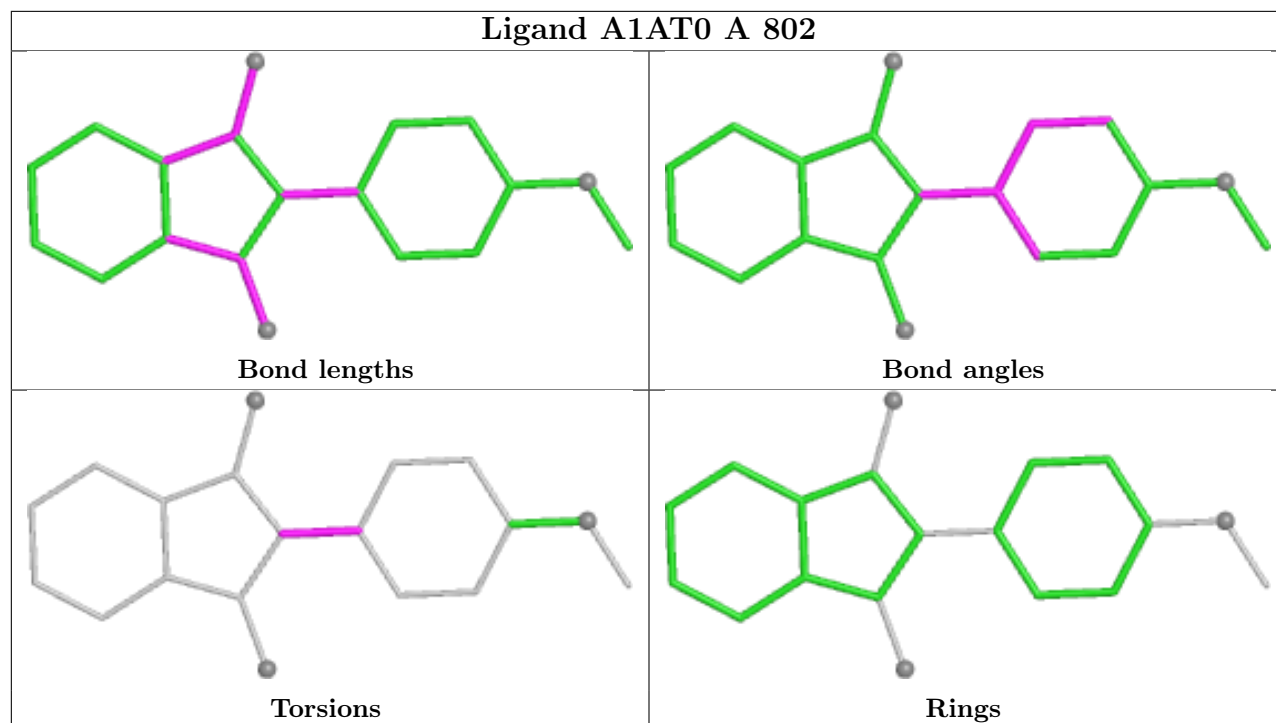
Mol	Chain	Res	Type	Atoms
7	A	805	PEE	C30-C31-C32-C33
6	A	803	CLR	C17-C20-C22-C23
7	A	805	PEE	C12-C13-C14-C15
7	A	807	PEE	C10-C11-C12-C13
8	A	806	Y01	CAL-CAM-CAY-OAW

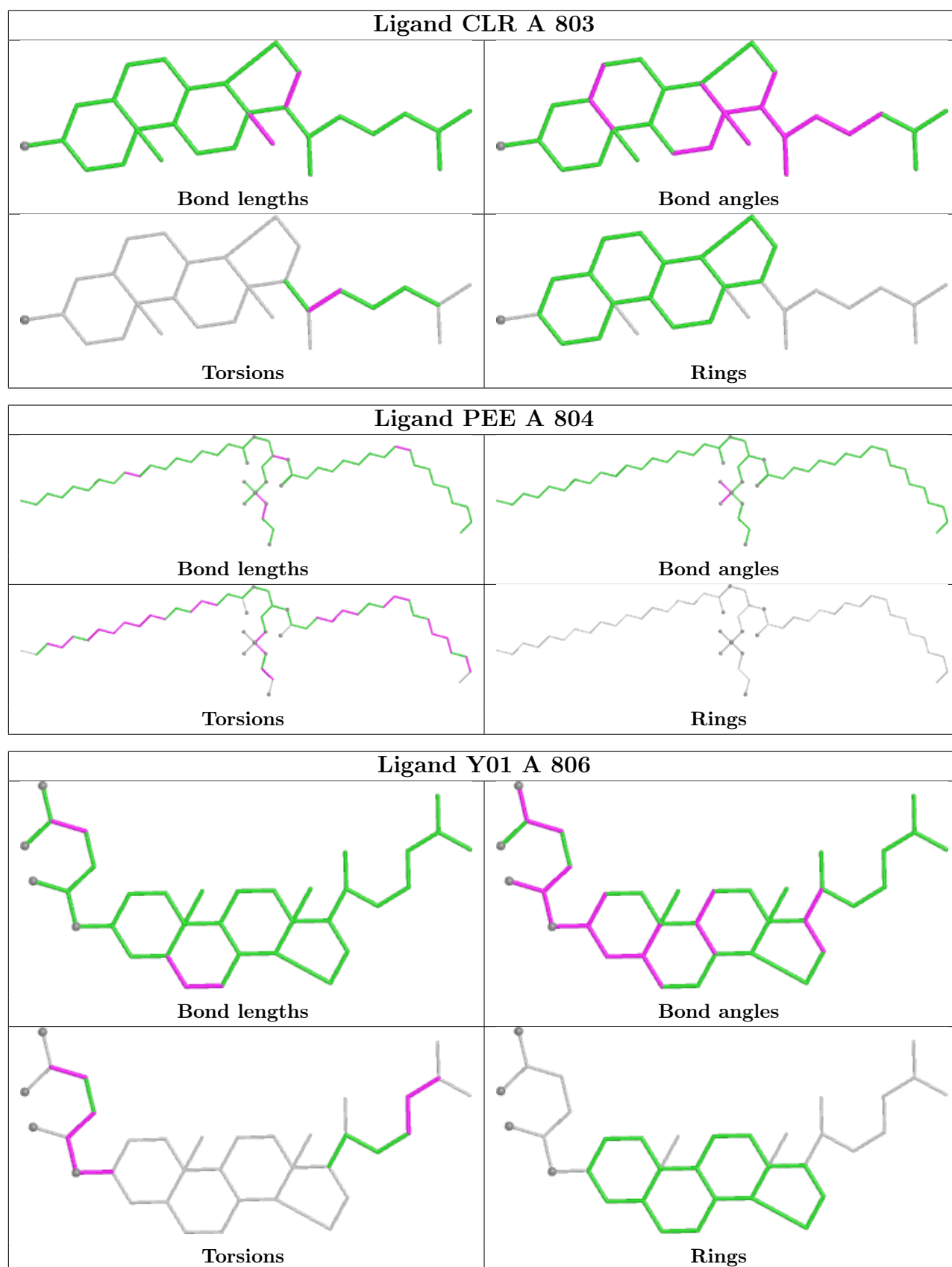
There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	808	BCT	2	0
7	A	807	PEE	2	0
7	A	805	PEE	2	0
6	A	803	CLR	2	0
7	A	804	PEE	1	0
8	A	806	Y01	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 [i](#)

There are no chain breaks in this entry.