



Full wwPDB EM Validation Report ⓘ

Apr 28, 2026 – 02:24 PM JST

PDB ID : 9L21 / pdb_00009L21
EMDB ID : EMD-62765
Title : cryo-EM structure of Vitamin K-dependent gamma-carboxylase complexed with factor IX
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

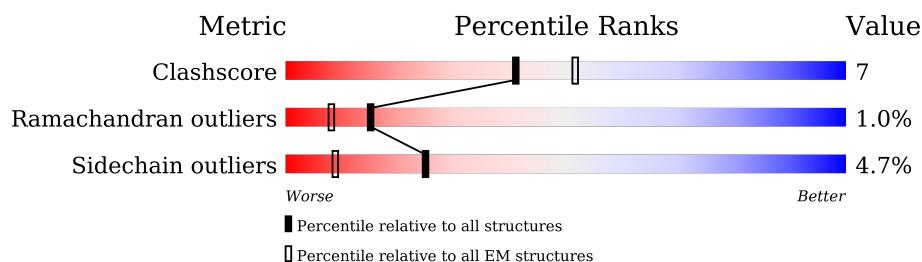
1 Overall quality at a glance

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	28	
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
6	BCT	A	803	-	-	X	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 6162 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 Coagulation factor IX.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	28	Total	C	N	O	0	0
			235	149	43	43		

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



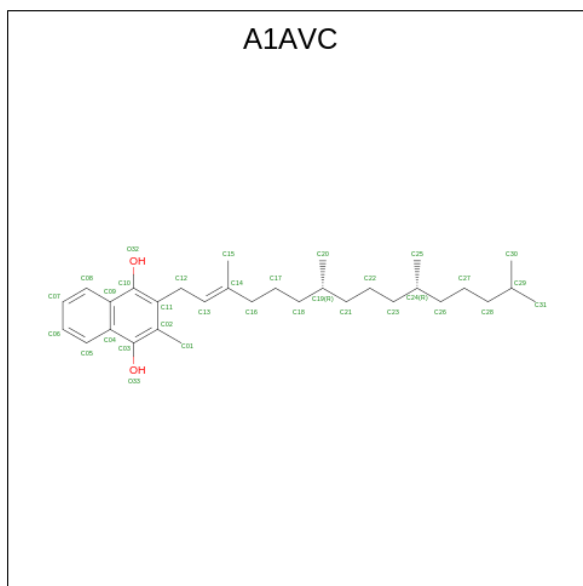
Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		

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



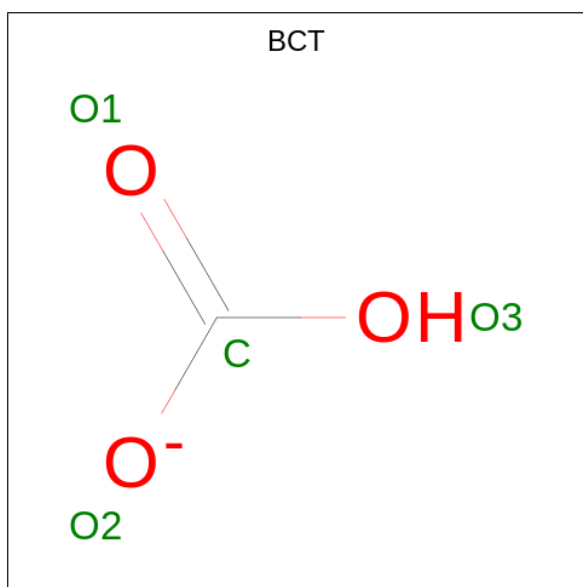
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	

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



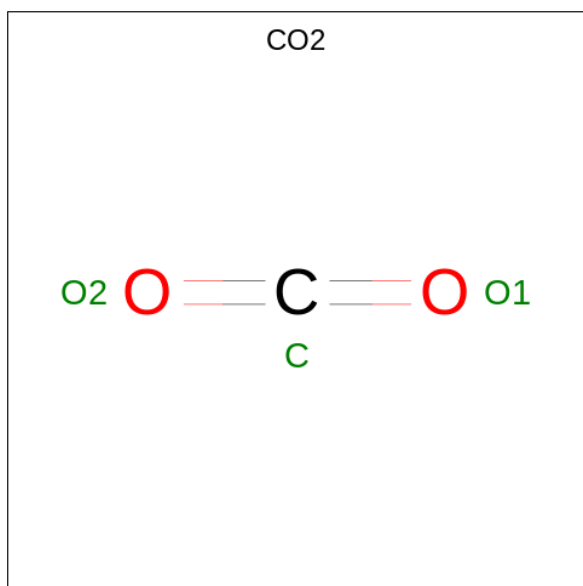
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O		0
			33	31	2		

- Molecule 6 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



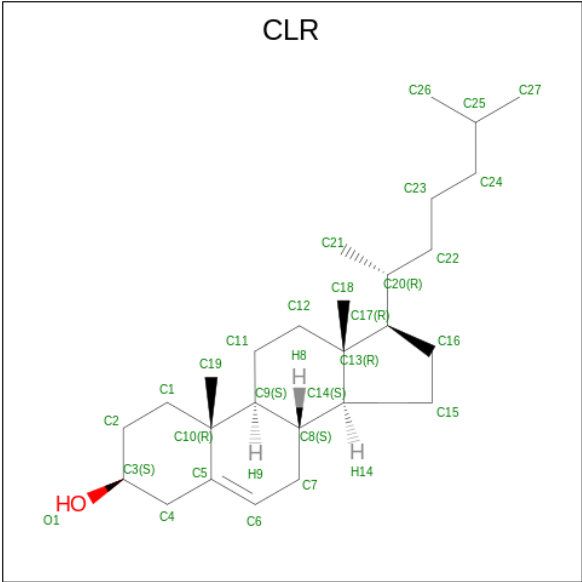
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			4	1	3	

- Molecule 7 is CARBON DIOXIDE (CCD ID: CO2) (formula: CO₂).



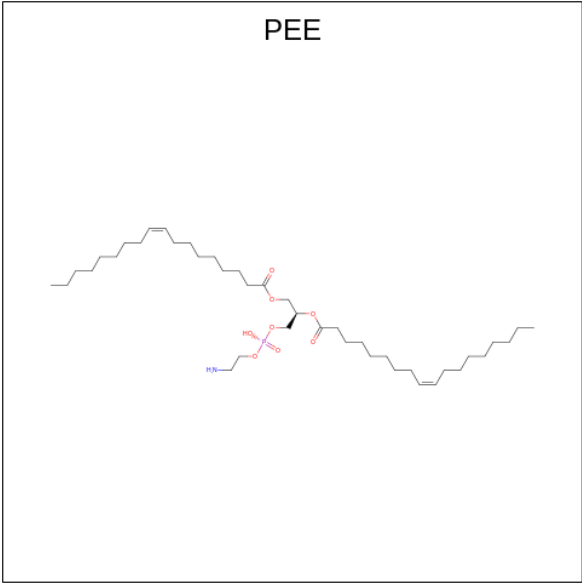
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			3	1	2	

- Molecule 8 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



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

- Molecule 9 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



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

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

- # Y01

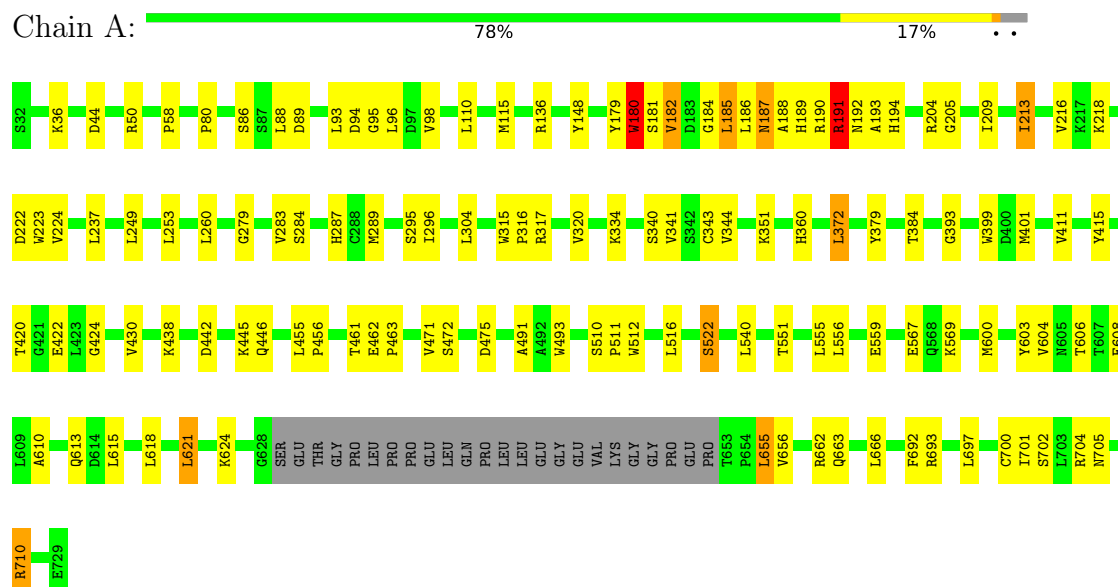
Mol	Chain	Residues	Atoms			AltConf
10	A	1	Total	C	O	0
			35	31	4	

- | Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|------------------|---------|
| 11 | A | 23 | Total O
23 23 | 0 |
| 11 | B | 1 | Total O
1 1 | 0 |

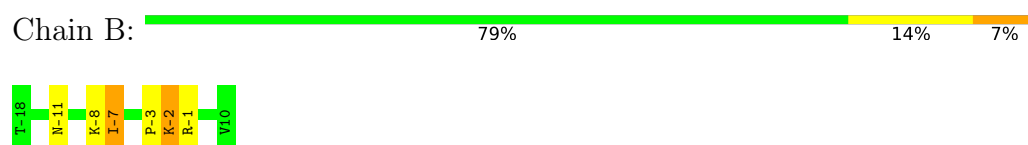
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

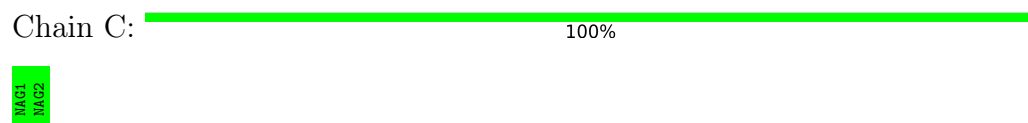
- Molecule 1: Vitamin K-dependent gamma-carboxylase



- Molecule 2: Coagulation factor IX



- 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



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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	680930	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: A1AVC, CO2, CLR, NAG, PEE, Y01, 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	0.31	2/5739 (0.0%)	0.49	9/7791 (0.1%)
2	B	0.16	0/239	0.42	0/320
All	All	0.30	2/5978 (0.0%)	0.49	9/8111 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	TRP	C-O	-7.58	1.14	1.24
1	A	182	VAL	C-O	-6.49	1.17	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	VAL	N-CA-C	-9.66	102.12	113.42
1	A	179	TYR	CA-C-O	-7.62	112.98	121.51
1	A	187	ASN	CB-CA-C	6.63	120.67	111.51
1	A	179	TYR	N-CA-C	-5.60	100.80	109.14
1	A	180	TRP	CB-CA-C	5.59	121.54	110.42
1	A	191	ARG	CA-C-O	-5.32	114.53	120.54
1	A	180	TRP	N-CA-C	5.10	121.67	110.80
1	A	191	ARG	CB-CA-C	5.04	118.07	109.80
1	A	180	TRP	CA-CB-CG	5.00	123.11	113.60

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	5577	0	5549	79	0
2	B	235	0	236	5	0
3	C	28	0	25	0	0
3	D	28	0	25	0	0
4	A	14	0	13	1	0
5	A	33	0	0	0	0
6	A	4	0	0	2	0
7	A	3	0	0	0	0
8	A	28	0	46	1	0
9	A	153	0	246	5	0
10	A	35	0	49	5	0
11	A	23	0	0	1	0
11	B	1	0	0	1	0
All	All	6162	0	6189	85	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 (85) 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:213:ILE:HG21	1:A:399:TRP:HD1	1.30	0.96
1:A:218:LYS:NZ	6:A:803:BCT:O1	1.99	0.96
1:A:213:ILE:HG21	1:A:399:TRP:CD1	2.08	0.86
1:A:218:LYS:HE3	1:A:223:TRP:CZ2	2.16	0.81
1:A:693:ARG:HG3	10:A:808:Y01:HAE2	1.63	0.80
1:A:213:ILE:HG22	1:A:399:TRP:HB2	1.69	0.74
1:A:615:LEU:HD12	1:A:655:LEU:HB2	1.81	0.63
1:A:445:LYS:NZ	1:A:491:ALA:O	2.29	0.63
1:A:393:GLY:HA2	11:A:918:HOH:O	2.01	0.61
1:A:446:GLN:HG3	9:A:809:PEE:H9	1.83	0.60
1:A:704:ARG:NH1	1:A:705:ASN:OD1	2.35	0.60
1:A:693:ARG:HD2	10:A:808:Y01:HAC1	1.84	0.59
1:A:44:ASP:OD1	1:A:50:ARG:NH2	2.37	0.57
1:A:216:VAL:CG1	1:A:379:TYR:OH	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:GLY:O	1:A:283:VAL:HG22	2.04	0.56
1:A:205:GLY:O	1:A:209:ILE:HG13	2.05	0.56
1:A:193:ALA:HB1	1:A:340:SER:HB2	1.87	0.56
1:A:522:SER:O	1:A:522:SER:OG	2.22	0.55
1:A:401:MET:HE3	6:A:803:BCT:O2	2.07	0.54
1:A:693:ARG:HG3	10:A:808:Y01:CAE	2.36	0.54
1:A:663:GLN:HA	1:A:666:LEU:HD12	1.90	0.54
1:A:216:VAL:HG12	1:A:379:TYR:OH	2.07	0.54
1:A:567:GLU:OE2	1:A:569:LYS:NZ	2.41	0.54
1:A:317:ARG:HB3	1:A:334:LYS:HD2	1.90	0.53
1:A:608:GLU:HG3	4:A:801:NAG:H82	1.90	0.53
1:A:655:LEU:HD12	1:A:656:VAL:H	1.73	0.53
1:A:461:THR:HG22	1:A:462:GLU:H	1.75	0.52
1:A:58:PRO:HD3	1:A:344:VAL:O	2.10	0.52
1:A:697:LEU:O	1:A:701:ILE:HG13	2.10	0.51
1:A:213:ILE:CG2	1:A:399:TRP:HB2	2.41	0.51
1:A:287:HIS:HB2	1:A:304:LEU:HD13	1.92	0.51
1:A:58:PRO:HB2	1:A:194:HIS:ND1	2.27	0.50
2:B:-1:ARG:NH2	11:B:101:HOH:O	2.43	0.50
1:A:295:SER:O	1:A:295:SER:OG	2.30	0.50
2:B:-3:PRO:O	2:B:-2:LYS:HB3	2.10	0.49
1:A:93:LEU:HB3	1:A:96:LEU:HD22	1.93	0.49
1:A:411:VAL:HG21	1:A:438:LYS:HD3	1.94	0.49
1:A:556:LEU:HD21	1:A:600:MET:HE2	1.96	0.48
1:A:249:LEU:O	1:A:253:LEU:HB2	2.14	0.48
1:A:461:THR:HG22	1:A:462:GLU:N	2.29	0.48
1:A:693:ARG:HD2	10:A:808:Y01:CAC	2.44	0.47
1:A:621:LEU:HD12	1:A:621:LEU:HA	1.79	0.47
2:B:-2:LYS:HG3	2:B:-1:ARG:N	2.30	0.47
1:A:610:ALA:O	1:A:613:GLN:HG3	2.14	0.47
1:A:540:LEU:HD11	2:B:-7:ILE:HD12	1.96	0.47
1:A:420:THR:OG1	1:A:422:GLU:HG2	2.14	0.46
1:A:218:LYS:HB3	1:A:260:LEU:HD13	1.97	0.46
1:A:80:PRO:HG2	1:A:692:PHE:CE1	2.50	0.46
9:A:806:PEE:H57	9:A:806:PEE:H63	1.75	0.46
1:A:693:ARG:CG	10:A:808:Y01:HAE2	2.42	0.46
1:A:662:ARG:HH21	1:A:666:LEU:HG	1.81	0.46
2:B:-11:ASN:HA	2:B:-8:LYS:HD2	1.98	0.46
1:A:89:ASP:N	1:A:89:ASP:OD1	2.47	0.45
1:A:551:THR:HG23	1:A:603:TYR:HB3	1.99	0.45
1:A:96:LEU:HG	1:A:98:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ASP:HB3	1:A:493:TRP:CZ2	2.52	0.45
1:A:512:TRP:O	1:A:516:LEU:HG	2.17	0.45
1:A:110:LEU:H	1:A:115:MET:HE3	1.82	0.45
1:A:555:LEU:HD21	1:A:559:GLU:HA	1.98	0.45
1:A:710:ARG:H	1:A:710:ARG:HG2	1.41	0.44
1:A:315:TRP:CG	1:A:316:PRO:HD3	2.53	0.44
1:A:148:TYR:HB2	8:A:805:CLR:H272	1.99	0.44
1:A:237:LEU:HD13	1:A:289:MET:SD	2.57	0.44
1:A:115:MET:HE1	1:A:148:TYR:HE2	1.83	0.44
1:A:185:LEU:HD12	1:A:191:ARG:HH12	1.81	0.44
1:A:455:LEU:N	1:A:456:PRO:HD2	2.33	0.44
1:A:36:LYS:HB3	1:A:36:LYS:HE3	1.75	0.44
9:A:806:PEE:H25	9:A:806:PEE:H20	1.60	0.43
1:A:94:ASP:OD1	1:A:95:GLY:N	2.51	0.43
1:A:415:TYR:CZ	1:A:424:GLY:HA3	2.52	0.43
1:A:284:SER:HA	1:A:304:LEU:HD11	2.01	0.43
1:A:184:GLY:C	1:A:186:LEU:H	2.26	0.43
1:A:304:LEU:HD12	1:A:304:LEU:HA	1.87	0.43
1:A:344:VAL:HB	1:A:360:HIS:CD2	2.55	0.42
1:A:213:ILE:CG2	1:A:399:TRP:CD1	2.93	0.42
1:A:655:LEU:HD12	1:A:656:VAL:N	2.34	0.42
1:A:462:GLU:HA	1:A:463:PRO:HD3	1.85	0.42
1:A:216:VAL:HG11	1:A:379:TYR:OH	2.19	0.42
1:A:372:LEU:HD21	9:A:806:PEE:H41	2.02	0.41
1:A:204:ARG:HB3	9:A:806:PEE:H53	2.03	0.41
1:A:88:LEU:HD12	1:A:88:LEU:HA	1.91	0.40
1:A:510:SER:N	1:A:511:PRO:HD2	2.35	0.40
1:A:93:LEU:HD12	1:A:93:LEU:HA	1.89	0.40
1:A:624:LYS:HA	1:A:624:LYS:HD2	1.91	0.40
1:A:224:VAL:O	1:A:224:VAL:HG12	2.22	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%)	640 (96%)	24 (4%)	6 (1%)	14	28
2	B	26/28 (93%)	21 (81%)	4 (15%)	1 (4%)	2	3
All	All	696/726 (96%)	661 (95%)	28 (4%)	7 (1%)	15	26

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	TRP
1	A	189	HIS
1	A	192	ASN
1	A	351	LYS
2	B	-2	LYS
1	A	188	ALA
1	A	185	LEU

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%)	580 (95%)	29 (5%)	23	45
2	B	26/26 (100%)	25 (96%)	1 (4%)	29	54
All	All	635/655 (97%)	605 (95%)	30 (5%)	25	46

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	SER
1	A	136	ARG
1	A	180	TRP
1	A	181	SER
1	A	182	VAL
1	A	187	ASN

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Mol	Chain	Res	Type
1	A	190	ARG
1	A	191	ARG
1	A	213	ILE
1	A	222	ASP
1	A	296	ILE
1	A	320	VAL
1	A	341	VAL
1	A	343	CYS
1	A	372	LEU
1	A	384	THR
1	A	430	VAL
1	A	471	VAL
1	A	472	SER
1	A	475	ASP
1	A	522	SER
1	A	604	VAL
1	A	606	THR
1	A	618	LEU
1	A	621	LEU
1	A	655	LEU
1	A	700	CYS
1	A	702	SER
1	A	710	ARG
2	B	-7	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	178	HIS
1	A	192	ASN
1	A	381	HIS
1	A	410	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

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	0.20	0	17,19,21	0.47	0
3	NAG	C	2	3	14,14,15	0.27	0	17,19,21	0.61	0
3	NAG	D	1	1,3	14,14,15	0.26	0	17,19,21	0.40	0
3	NAG	D	2	3	14,14,15	0.23	0	17,19,21	0.44	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	-	2/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	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	C	1	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6

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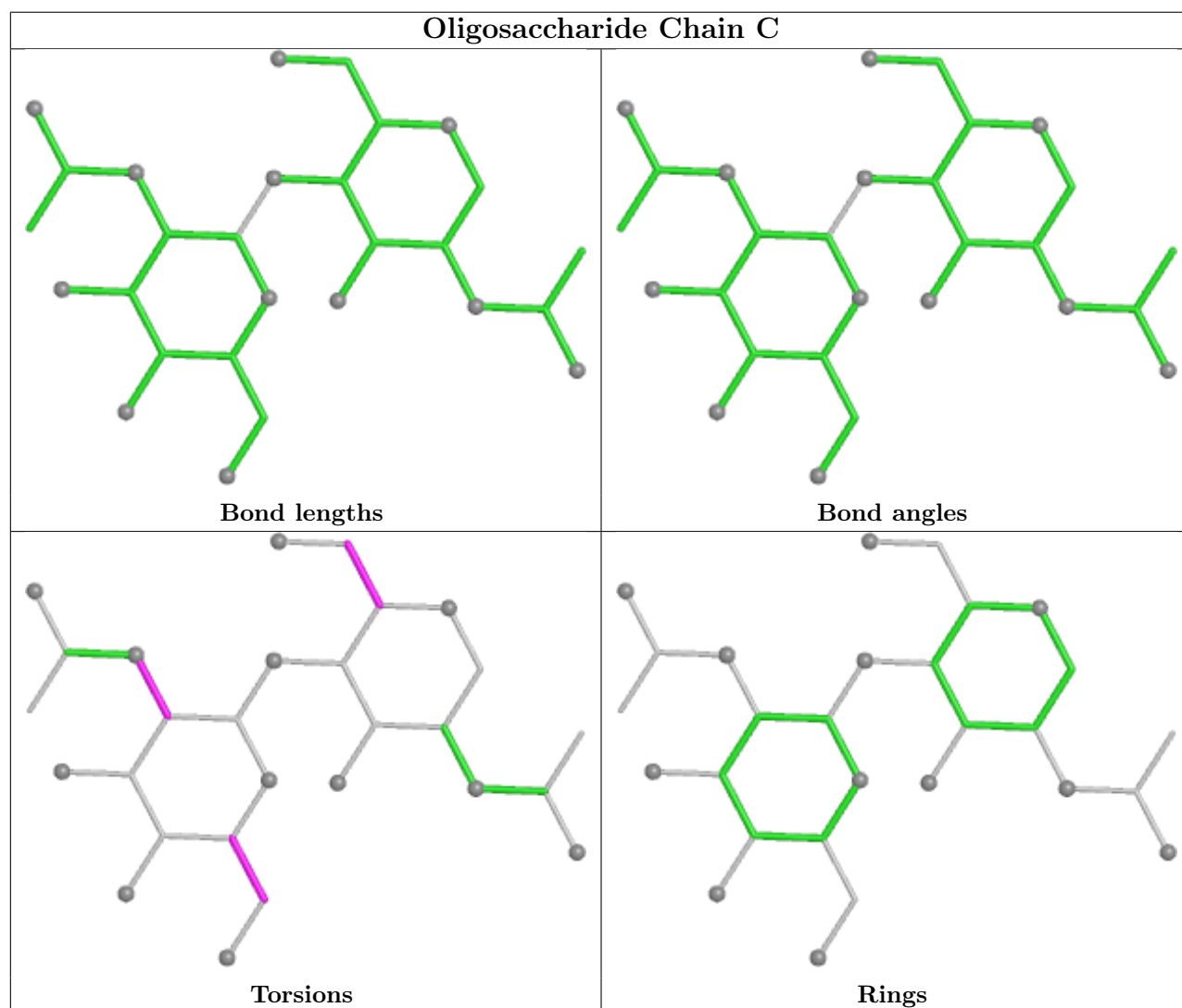
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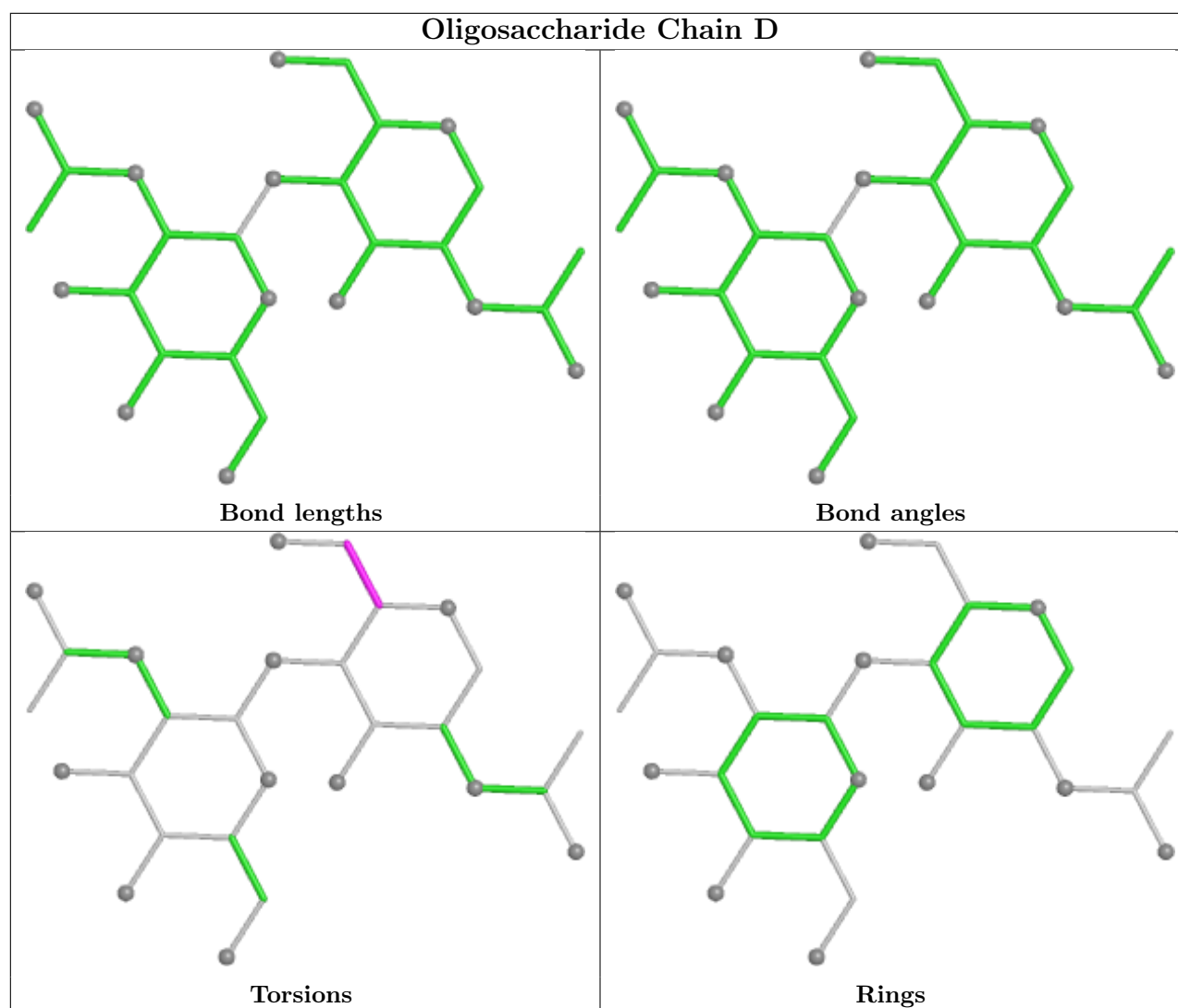
Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	C	2	NAG	C3-C2-N2-C7

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](#)

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	$\# Z > 2$
4	NAG	A	801	1	14,14,15	0.24	0	17,19,21	0.43	0
10	Y01	A	808	-	38,38,38	1.17	3 (7%)	57,57,57	1.93	9 (15%)
9	PEE	A	806	-	50,50,50	1.27	4 (8%)	53,55,55	0.93	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	CO2	A	804	-	2,2,2	0.39	0	1,1,1	0.52	0
9	PEE	A	809	-	50,50,50	1.30	4 (8%)	53,55,55	0.93	1 (1%)
8	CLR	A	805	-	31,31,31	1.02	2 (6%)	48,48,48	1.46	9 (18%)
6	BCT	A	803	-	2,3,3	0.97	0	2,3,3	1.66	1 (50%)
9	PEE	A	807	-	50,50,50	1.25	4 (8%)	53,55,55	0.93	1 (1%)
5	A1AVC	A	802	-	34,34,34	1.25	4 (11%)	42,45,45	1.83	6 (14%)

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	-	2/6/23/26	0/1/1/1
10	Y01	A	808	-	-	10/19/77/77	0/4/4/4
9	PEE	A	806	-	-	21/54/54/54	-
9	PEE	A	809	-	-	32/54/54/54	-
8	CLR	A	805	-	-	1/10/68/68	0/4/4/4
9	PEE	A	807	-	-	25/54/54/54	-
5	A1AVC	A	802	-	-	7/23/23/23	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	802	A1AVC	C09-C04	-4.88	1.34	1.43
9	A	809	PEE	P-O4P	4.83	1.78	1.59
9	A	806	PEE	P-O4P	4.55	1.77	1.59
9	A	807	PEE	P-O4P	4.40	1.77	1.59
10	A	808	Y01	CAK-CAI	-4.18	1.41	1.50
9	A	807	PEE	C39-C38	3.88	1.54	1.31
9	A	809	PEE	C39-C38	3.88	1.54	1.31
9	A	806	PEE	C39-C38	3.84	1.54	1.31
9	A	806	PEE	C18-C19	3.68	1.53	1.31
9	A	809	PEE	C18-C19	3.68	1.53	1.31
9	A	807	PEE	C18-C19	3.65	1.52	1.31
5	A	802	A1AVC	C12-C13	2.69	1.56	1.50
10	A	808	Y01	CAI-CAZ	2.59	1.38	1.33
5	A	802	A1AVC	C12-C11	2.28	1.54	1.51
9	A	809	PEE	O2-C2	-2.15	1.41	1.46
9	A	806	PEE	O2-C2	-2.09	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	802	A1AVC	C16-C14	2.07	1.55	1.51
9	A	807	PEE	O4P-C4	-2.06	1.36	1.44
8	A	805	CLR	C8-C14	-2.06	1.49	1.53
10	A	808	Y01	CAL-CAX	2.04	1.55	1.50
8	A	805	CLR	C18-C13	-2.02	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	-9.38	97.30	112.17
10	A	808	Y01	CAV-CAZ-CBH	7.57	126.47	116.42
10	A	808	Y01	OAW-CAY-CAM	5.23	122.77	111.50
10	A	808	Y01	OAW-CAY-OAG	-5.09	111.41	123.70
10	A	808	Y01	CAV-CAZ-CAI	-4.89	113.56	120.61
8	A	805	CLR	C22-C20-C17	-4.42	101.16	110.28
9	A	809	PEE	O2P-P-O1P	4.26	133.29	112.24
9	A	806	PEE	O2P-P-O1P	4.23	133.18	112.24
9	A	807	PEE	O2P-P-O1P	4.23	133.15	112.24
5	A	802	A1AVC	O32-C10-C11	3.63	122.83	118.67
8	A	805	CLR	C18-C13-C12	2.68	114.82	110.59
10	A	808	Y01	OAW-CBC-CAV	-2.68	102.64	108.12
8	A	805	CLR	C16-C17-C20	-2.67	108.01	112.15
8	A	805	CLR	C21-C20-C17	2.55	116.83	112.92
8	A	805	CLR	C10-C5-C6	2.36	126.51	122.90
10	A	808	Y01	OAW-CBC-CAR	2.32	113.92	108.33
10	A	808	Y01	CAP-CBE-CBB	-2.31	108.57	112.15
5	A	802	A1AVC	C15-C14-C16	2.30	119.13	115.27
8	A	805	CLR	C12-C13-C14	-2.25	103.77	107.27
8	A	805	CLR	C24-C23-C22	-2.22	103.06	113.24
8	A	805	CLR	C21-C20-C22	-2.19	106.92	110.36
6	A	803	BCT	O2-C-O1	2.19	125.23	119.55
10	A	808	Y01	CAS-CBF-CBD	-2.17	108.63	111.75
5	A	802	A1AVC	C08-C09-C04	2.17	121.14	118.45
10	A	808	Y01	OAF-CAX-CAL	-2.14	116.21	123.08
5	A	802	A1AVC	C17-C16-C14	-2.13	107.88	113.45
5	A	802	A1AVC	C06-C07-C08	-2.12	117.47	120.44
8	A	805	CLR	C7-C8-C14	-2.02	107.98	110.91

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	806	PEE	C1-O3P-P-O2P
9	A	806	PEE	C4-O4P-P-O3P
9	A	806	PEE	C4-O4P-P-O2P
9	A	807	PEE	C1-O3P-P-O2P
9	A	807	PEE	C1-O3P-P-O4P
9	A	807	PEE	C4-O4P-P-O2P
9	A	807	PEE	O4P-C4-C5-N
9	A	809	PEE	O2-C2-C3-O3
9	A	809	PEE	C1-O3P-P-O2P
9	A	809	PEE	C4-O4P-P-O3P
9	A	809	PEE	C4-O4P-P-O1P
9	A	809	PEE	O4P-C4-C5-N
10	A	808	Y01	OAG-CAY-OAW-CBC
9	A	809	PEE	O5-C30-O3-C3
9	A	809	PEE	C31-C30-O3-C3
10	A	808	Y01	CAM-CAY-OAW-CBC
9	A	809	PEE	C37-C38-C39-C40
9	A	806	PEE	C35-C36-C37-C38
9	A	809	PEE	C22-C23-C24-C25
5	A	802	A1AVC	C26-C27-C28-C29
5	A	802	A1AVC	C25-C24-C26-C27
10	A	808	Y01	CAR-CBC-OAW-CAY
5	A	802	A1AVC	C19-C21-C22-C23
5	A	802	A1AVC	C16-C17-C18-C19
9	A	806	PEE	C10-C11-C12-C13
5	A	802	A1AVC	C24-C26-C27-C28
9	A	806	PEE	C14-C15-C16-C17
5	A	802	A1AVC	C21-C22-C23-C24
9	A	807	PEE	C4-O4P-P-O3P
9	A	809	PEE	C1-O3P-P-O4P
10	A	808	Y01	CAV-CBC-OAW-CAY
9	A	806	PEE	C40-C41-C42-C43
9	A	807	PEE	C21-C22-C23-C24
9	A	809	PEE	C41-C42-C43-C44
9	A	807	PEE	C31-C32-C33-C34
9	A	806	PEE	C13-C14-C15-C16
9	A	806	PEE	C31-C32-C33-C34
4	A	801	NAG	O5-C5-C6-O6
9	A	809	PEE	C32-C33-C34-C35
9	A	806	PEE	C32-C33-C34-C35
9	A	806	PEE	C43-C44-C45-C46
9	A	809	PEE	C13-C14-C15-C16
10	A	808	Y01	CAJ-CAN-CBA-CAB

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Mol	Chain	Res	Type	Atoms
9	A	806	PEE	C20-C21-C22-C23
9	A	807	PEE	C13-C14-C15-C16
9	A	806	PEE	C42-C43-C44-C45
9	A	807	PEE	C20-C21-C22-C23
9	A	806	PEE	C39-C40-C41-C42
9	A	807	PEE	C10-C11-C12-C13
9	A	806	PEE	C22-C23-C24-C25
9	A	809	PEE	C31-C32-C33-C34
9	A	809	PEE	C10-C11-C12-C13
9	A	806	PEE	C19-C20-C21-C22
9	A	807	PEE	C19-C20-C21-C22
9	A	809	PEE	C15-C16-C17-C18
9	A	809	PEE	C39-C40-C41-C42
9	A	809	PEE	C43-C44-C45-C46
9	A	807	PEE	C14-C15-C16-C17
9	A	807	PEE	C1-C2-C3-O3
9	A	809	PEE	C1-C2-C3-O3
9	A	809	PEE	C30-C31-C32-C33
9	A	807	PEE	C35-C36-C37-C38
9	A	807	PEE	C34-C35-C36-C37
9	A	807	PEE	C17-C18-C19-C20
10	A	808	Y01	CAJ-CAN-CBA-CAA
10	A	808	Y01	CAO-CAJ-CAN-CBA
9	A	806	PEE	C17-C18-C19-C20
9	A	807	PEE	C42-C43-C44-C45
9	A	809	PEE	C18-C19-C20-C21
9	A	807	PEE	C43-C44-C45-C46
9	A	809	PEE	C1-O3P-P-O1P
9	A	809	PEE	C4-O4P-P-O2P
9	A	806	PEE	C21-C22-C23-C24
9	A	807	PEE	O2-C2-C3-O3
9	A	809	PEE	C16-C17-C18-C19
5	A	802	A1AVC	C23-C24-C26-C27
9	A	807	PEE	C38-C39-C40-C41
9	A	807	PEE	C24-C25-C26-C27
9	A	806	PEE	C24-C25-C26-C27
9	A	806	PEE	C11-C12-C13-C14
10	A	808	Y01	CAM-CAL-CAX-OAF
10	A	808	Y01	CAM-CAL-CAX-OAH
9	A	807	PEE	C16-C17-C18-C19
4	A	801	NAG	C4-C5-C6-O6
9	A	809	PEE	C12-C13-C14-C15

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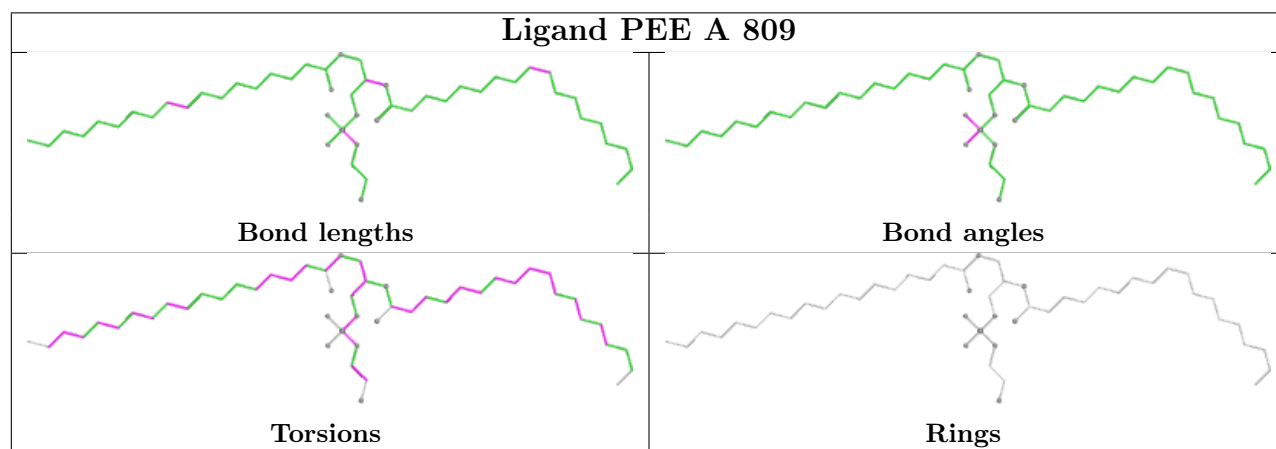
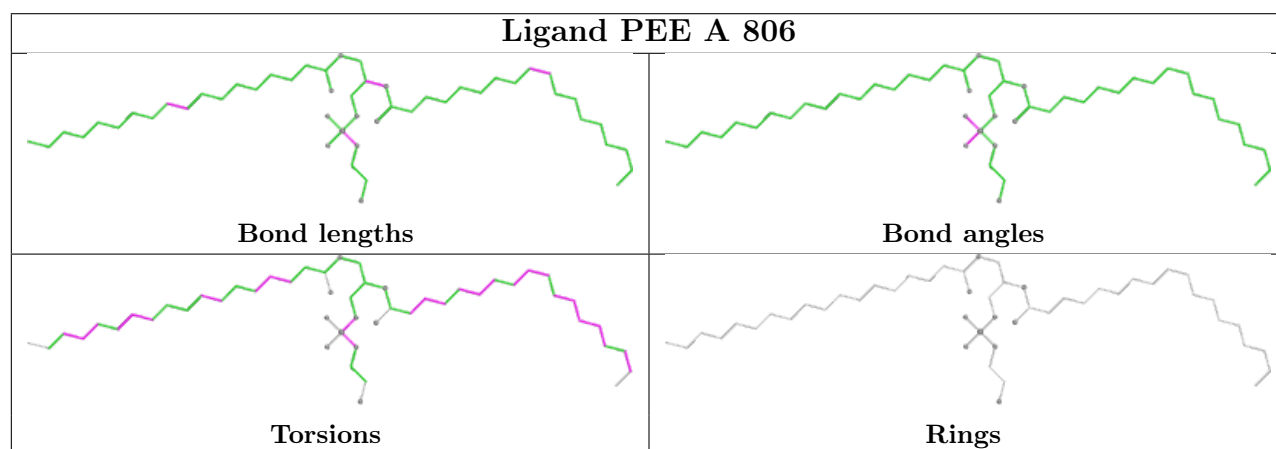
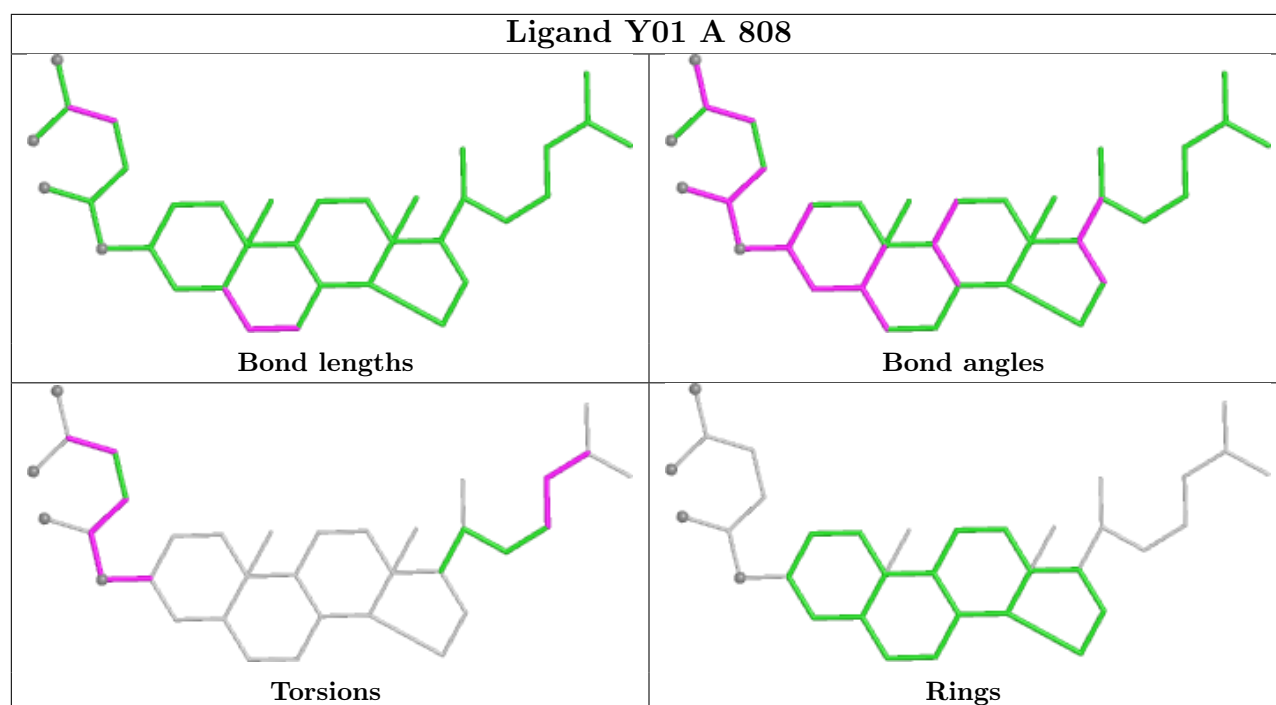
Mol	Chain	Res	Type	Atoms
9	A	809	PEE	C17-C18-C19-C20
9	A	809	PEE	C20-C21-C22-C23
9	A	807	PEE	C36-C37-C38-C39
9	A	809	PEE	O3P-C1-C2-C3
9	A	809	PEE	O2-C10-C11-C12
9	A	807	PEE	C40-C41-C42-C43
9	A	806	PEE	C16-C17-C18-C19
9	A	809	PEE	O3P-C1-C2-O2
9	A	809	PEE	C44-C45-C46-C47
9	A	809	PEE	O4-C10-C11-C12
9	A	807	PEE	C12-C13-C14-C15
8	A	805	CLR	C21-C20-C22-C23
10	A	808	Y01	CAL-CAM-CAY-OAW

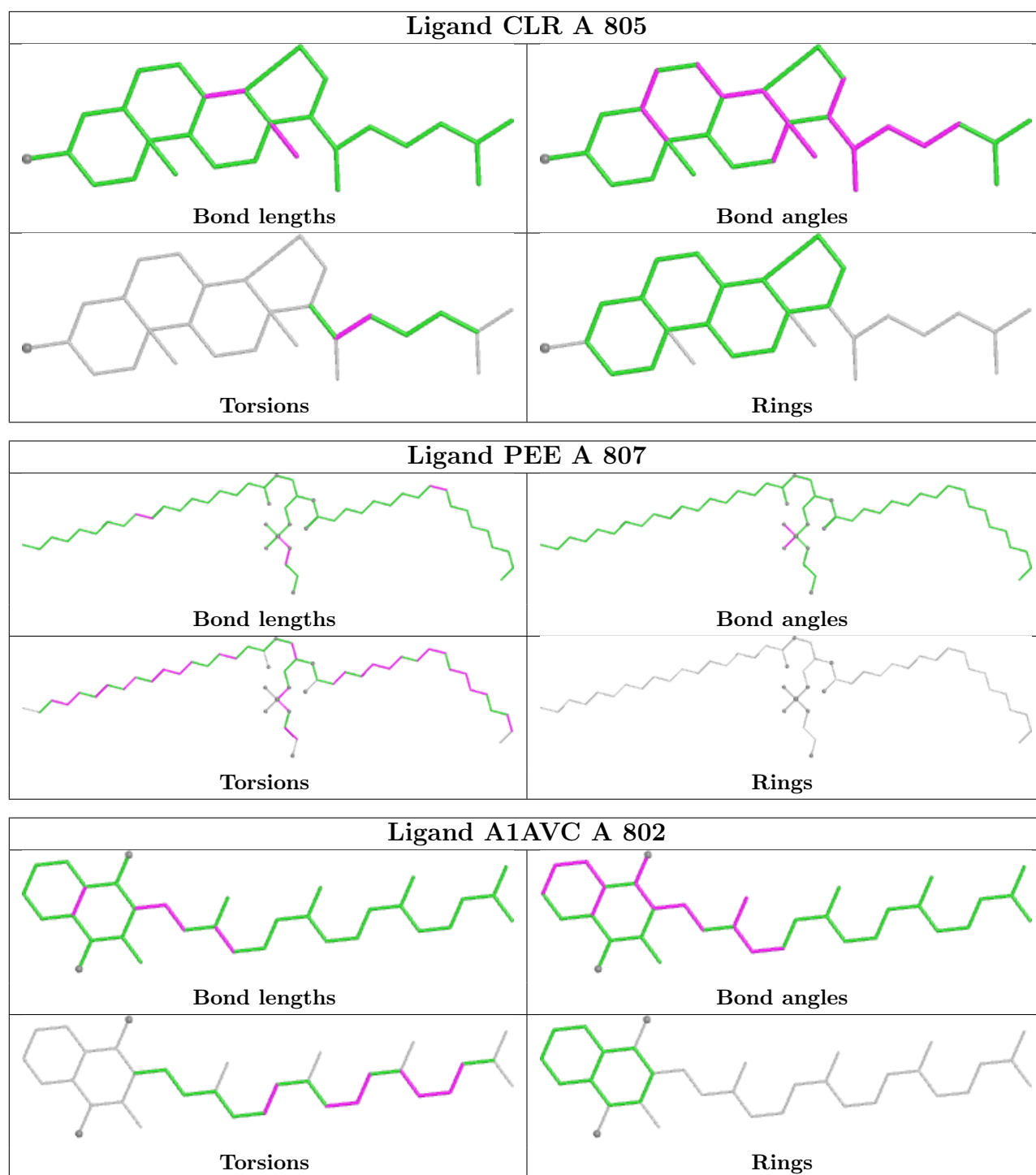
There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	NAG	1	0
10	A	808	Y01	5	0
9	A	806	PEE	4	0
9	A	809	PEE	1	0
8	A	805	CLR	1	0
6	A	803	BCT	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.