



Full wwPDB EM Validation Report ⓘ

Apr 16, 2026 – 12:36 PM JST

PDB ID : 9L6S / pdb_00009l6s
EMDB ID : EMD-62864
Title : double-mutant (K217A & K218A) Vitamin K-dependent gamma-carboxylase
in complex with coagulation factors X and vitamin K
Authors : Hang, J.; Chen, D.D.; Zhong, Q.H.
Deposited on : 2024-12-25
Resolution : 2.58 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

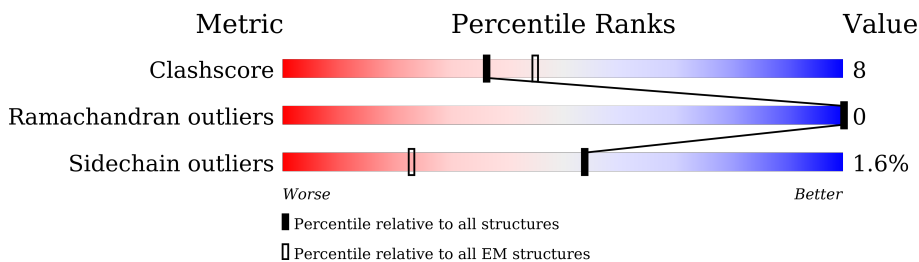
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

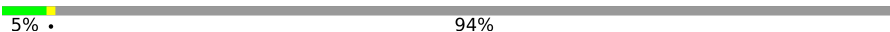
The reported resolution of this entry is 2.58 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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

Mol	Chain	Length	Quality of chain
1	C	488	
2	A	758	
3	B	3	
3	E	3	
4	D	2	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5876 atoms, of which 42 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Coagulation factor X.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	27	Total	C	N	O	S	0	0
			218	138	42	37	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	668	Total	C	N	O	S	0	0
			5339	3497	887	928	27		

There are 2 discrepancies between the modelled and reference sequences:

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

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



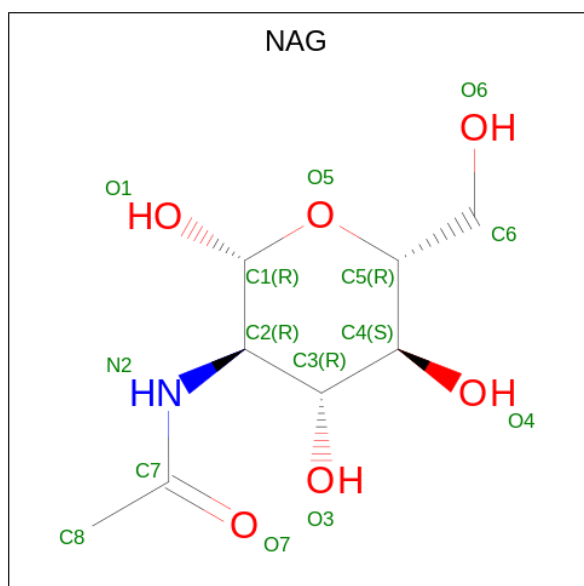
Mol	Chain	Residues	Atoms				AltConf	Trace
3	B	3	Total	C	N	O	0	0
			39	22	2	15		
3	E	3	Total	C	N	O	0	0
			39	22	2	15		

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



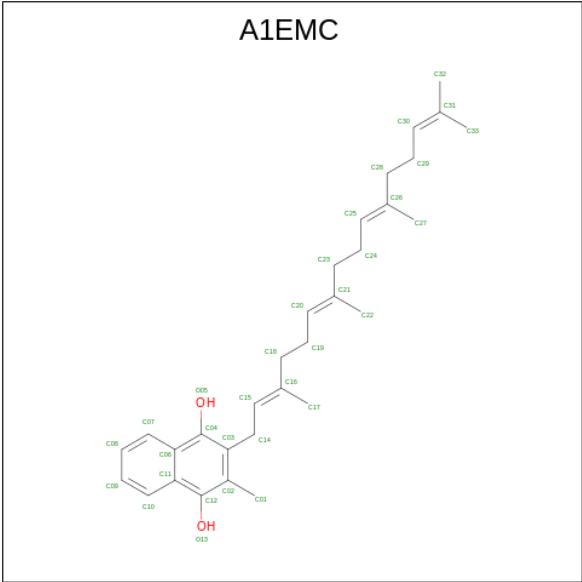
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



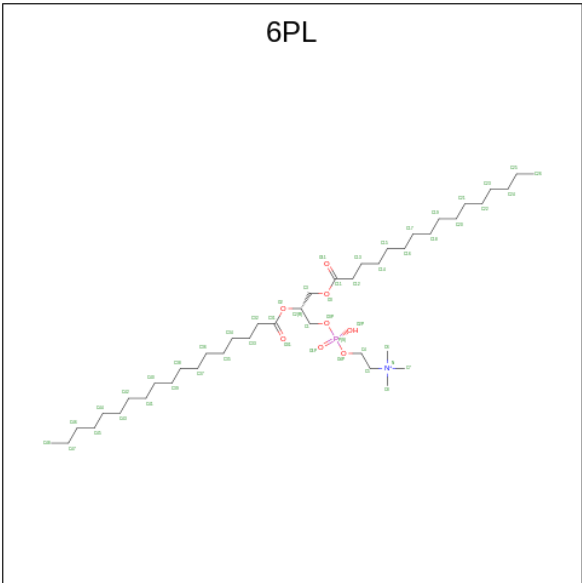
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 6 is 2-methyl-3-[(2 {E},6 {E},10 {E})-3,7,11,15-tetramethylhexadeca-2,6,10,14-tetraenyl]naphthalene-1,4-diol (CCD ID: A1EMC) (formula: $C_{31}H_{42}O_2$) (labeled as "Ligand of Interest" by depositor).



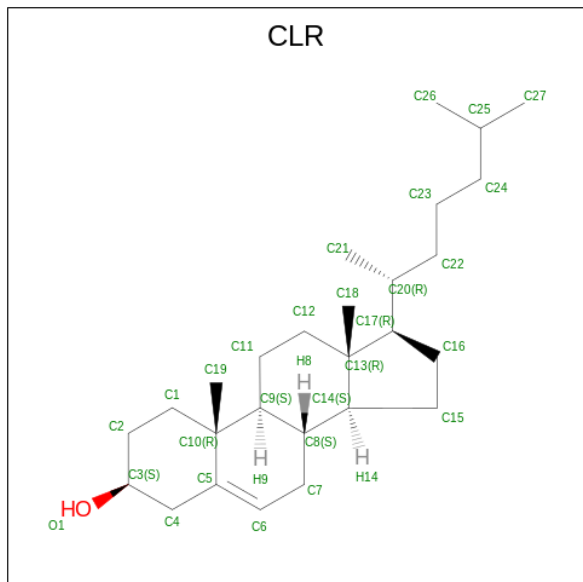
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
6	A	1	75	31	42	2	0

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



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

- Molecule 8 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).

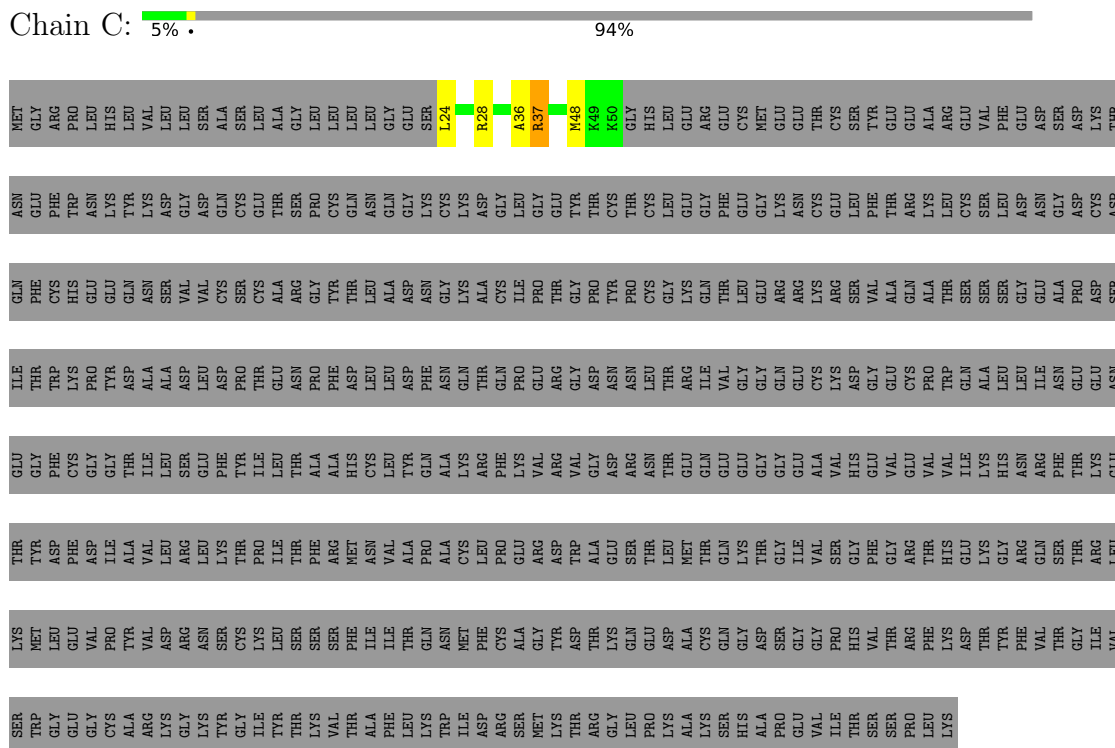


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
8	A	1	28	27	1	0

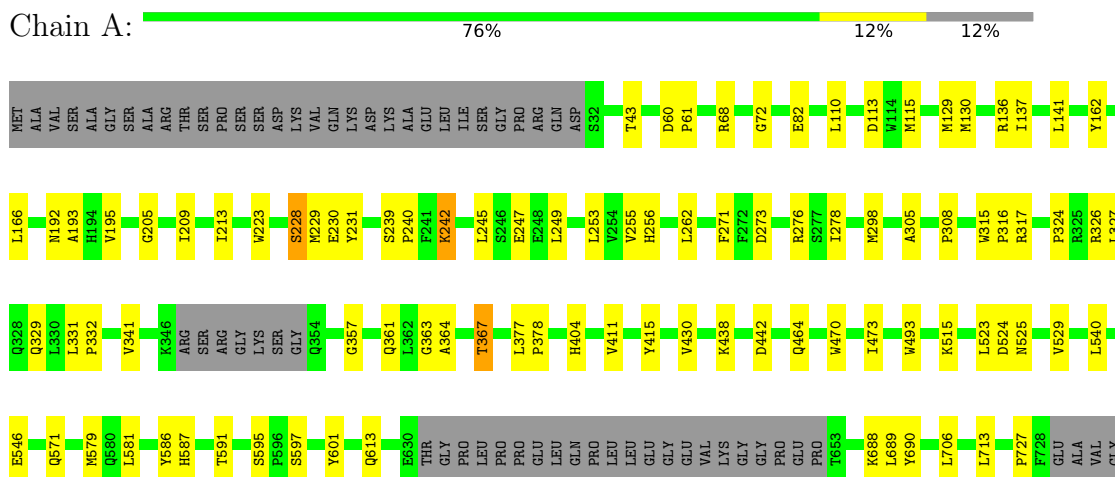
3 Residue-property plots

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: Coagulation factor X



- Molecule 2: Vitamin K-dependent gamma-carboxylase



GLU
LEU
ASN
PRO
SER
ASN
THR
ASP
SER
HIS
SER
ASN
PRO
GLU
SER
ASN
PRO
ASP
VAL
HIS
SER
GLU
PHE

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

Chain B:  67% 33%

NAG1
NAG2
BMA3

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

Chain E:  67% 33%

NAG1
NAG2
BMA3

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

Chain D:  50% 50%

NAG1
NAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64570	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1EMC, NAG, CLR, 6PL, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	C	0.13	0/219	0.26	0/291
2	A	0.30	0/5496	0.44	0/7490
All	All	0.29	0/5715	0.43	0/7781

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	218	0	220	5	0
2	A	5339	0	5147	75	0
3	B	39	0	34	1	0
3	E	39	0	34	0	0
4	D	28	0	25	0	0
5	A	14	0	13	0	0
6	A	33	42	0	8	0
7	A	96	0	143	16	0
8	A	28	0	46	1	0
All	All	5834	42	5662	88	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 8.

All (88) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:229:MET:HE1	6:A:802:A1EMC:C17	1.75	1.15
7:A:803:6PL:H11	7:A:803:6PL:C4	1.83	1.09
2:A:262:LEU:HD12	6:A:802:A1EMC:C27	1.91	1.00
7:A:803:6PL:H42	7:A:803:6PL:C1	1.91	0.99
7:A:803:6PL:H11	7:A:803:6PL:H42	0.99	0.98
2:A:524:ASP:OD1	2:A:525:ASN:N	2.04	0.90
2:A:262:LEU:CD1	6:A:802:A1EMC:C27	2.52	0.87
2:A:229:MET:CE	6:A:802:A1EMC:C17	2.52	0.87
2:A:110:LEU:H	2:A:115:MET:HE3	1.41	0.85
2:A:255:VAL:HA	6:A:802:A1EMC:C22	2.07	0.84
2:A:271:PHE:HE1	7:A:803:6PL:H121	1.46	0.78
2:A:271:PHE:CE1	7:A:803:6PL:H121	2.22	0.73
2:A:363:GLY:O	2:A:367:THR:HG22	1.91	0.71
2:A:298:MET:HE1	7:A:804:6PL:O31	1.92	0.69
2:A:205:GLY:O	2:A:209:ILE:HG13	1.95	0.67
7:A:803:6PL:C4	7:A:803:6PL:C1	2.63	0.66
2:A:326:ARG:HA	2:A:329:GLN:NE2	2.15	0.62
2:A:688:LYS:HB3	7:A:804:6PL:H162	1.81	0.62
2:A:415:TYR:HA	2:A:464:GLN:O	2.02	0.60
2:A:229:MET:SD	6:A:802:A1EMC:C17	2.90	0.59
2:A:242:LYS:NZ	2:A:247:GLU:OE1	2.24	0.58
2:A:61:PRO:HG3	2:A:193:ALA:O	2.03	0.58
2:A:228:SER:O	2:A:256:HIS:NE2	2.23	0.58
2:A:137:ILE:O	2:A:141:LEU:HG	2.03	0.58
2:A:110:LEU:HB2	2:A:115:MET:HE2	1.87	0.57
2:A:571:GLN:OE1	2:A:579:MET:HE3	2.05	0.56
2:A:529:VAL:HA	2:A:601:TYR:O	2.04	0.56
1:C:48:MET:O	1:C:48:MET:HG3	2.06	0.55
2:A:245:LEU:HD22	2:A:249:LEU:HD23	1.87	0.55
2:A:209:ILE:O	2:A:213:ILE:HG12	2.07	0.54
2:A:262:LEU:HD11	6:A:802:A1EMC:C27	2.35	0.54
2:A:357:GLY:O	2:A:361:GLN:HG3	2.08	0.53
2:A:442:ASP:HB3	2:A:493:TRP:CZ2	2.44	0.53
2:A:245:LEU:CD2	2:A:249:LEU:HD23	2.39	0.53
7:A:803:6PL:H73	7:A:803:6PL:O4P	2.09	0.53
2:A:315:TRP:CG	2:A:316:PRO:HD3	2.44	0.53
2:A:591:THR:HG23	2:A:597:SER:OG	2.10	0.52
2:A:581:LEU:HD13	2:A:587:HIS:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:60:ASP:OD2	2:A:317:ARG:NH1	2.43	0.51
2:A:223:TRP:CH2	2:A:229:MET:HE2	2.46	0.51
2:A:68:ARG:HD3	2:A:129:MET:O	2.11	0.51
2:A:411:VAL:HG21	2:A:438:LYS:HD3	1.92	0.51
2:A:515:LYS:O	2:A:515:LYS:HD3	2.12	0.50
2:A:230:GLU:HG3	2:A:231:TYR:CE1	2.46	0.50
2:A:223:TRP:CZ3	2:A:229:MET:HE2	2.48	0.48
2:A:136:ARG:HH11	2:A:136:ARG:HG2	1.78	0.48
2:A:364:ALA:HA	2:A:367:THR:CG2	2.43	0.48
1:C:36:ALA:O	1:C:37:ARG:HG3	2.13	0.48
2:A:110:LEU:H	2:A:115:MET:CE	2.21	0.48
1:C:24:LEU:HD12	2:A:430:VAL:HG21	1.95	0.48
2:A:273:ASP:OD1	2:A:273:ASP:C	2.57	0.47
2:A:364:ALA:O	2:A:367:THR:HG23	2.14	0.47
2:A:404:HIS:HB3	2:A:473:ILE:HD11	1.97	0.47
2:A:324:PRO:HD2	2:A:327:LEU:HD23	1.97	0.46
2:A:72:GLY:HA3	2:A:130:MET:HB2	1.97	0.46
7:A:804:6PL:H222	7:A:804:6PL:H192	1.38	0.46
2:A:546:GLU:OE1	2:A:546:GLU:N	2.29	0.46
2:A:523:LEU:HD22	3:B:2:NAG:H81	1.97	0.46
1:C:24:LEU:CD1	2:A:430:VAL:HG21	2.46	0.46
1:C:28:ARG:HD3	2:A:586:TYR:OH	2.16	0.45
2:A:524:ASP:OD1	2:A:524:ASP:C	2.59	0.45
2:A:239:SER:N	2:A:240:PRO:HD2	2.31	0.45
2:A:331:LEU:HB3	2:A:332:PRO:HD2	1.98	0.45
2:A:713:LEU:C	2:A:713:LEU:HD23	2.41	0.45
2:A:249:LEU:HG	2:A:253:LEU:HD13	1.98	0.45
2:A:113:ASP:HB3	2:A:706:LEU:HG	1.98	0.45
2:A:298:MET:CE	7:A:804:6PL:O31	2.64	0.44
2:A:223:TRP:HH2	6:A:802:A1EMC:C17	2.30	0.44
2:A:82:GLU:O	2:A:82:GLU:HG3	2.17	0.43
2:A:524:ASP:OD1	2:A:525:ASN:OD1	2.37	0.43
2:A:689:LEU:HD13	7:A:804:6PL:H232	2.00	0.43
2:A:273:ASP:HB3	2:A:276:ARG:HH22	1.83	0.43
7:A:804:6PL:H211	7:A:804:6PL:H242	1.85	0.43
2:A:110:LEU:N	2:A:115:MET:HE3	2.20	0.43
2:A:249:LEU:HG	2:A:253:LEU:CD1	2.48	0.43
2:A:305:ALA:O	2:A:308:PRO:HD2	2.19	0.42
2:A:230:GLU:H	2:A:230:GLU:HG2	1.63	0.41
7:A:804:6PL:H411	7:A:804:6PL:H441	1.65	0.41
2:A:546:GLU:H	2:A:546:GLU:CD	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:804:6PL:H191	7:A:804:6PL:H161	1.34	0.41
2:A:192:ASN:OD1	2:A:317:ARG:NH2	2.53	0.41
2:A:377:LEU:N	2:A:378:PRO:HD2	2.35	0.41
2:A:690:TYR:HB2	2:A:727:PRO:CG	2.50	0.41
8:A:805:CLR:H232	8:A:805:CLR:H211	1.85	0.41
2:A:470:TRP:CZ2	2:A:540:LEU:HD13	2.56	0.41
2:A:61:PRO:HB3	2:A:195:VAL:HG13	2.02	0.40
7:A:803:6PL:H212	7:A:803:6PL:H161	2.02	0.40
2:A:162:TYR:CE2	2:A:166:LEU:HD11	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	C	25/488 (5%)	22 (88%)	3 (12%)	0	100	100
2	A	662/758 (87%)	642 (97%)	20 (3%)	0	100	100
All	All	687/1246 (55%)	664 (97%)	23 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	21/419 (5%)	20 (95%)	1 (5%)	23	45
2	A	558/679 (82%)	550 (99%)	8 (1%)	59	79
All	All	579/1098 (53%)	570 (98%)	9 (2%)	54	77

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	37	ARG
2	A	43	THR
2	A	228	SER
2	A	242	LYS
2	A	278	ILE
2	A	341	VAL
2	A	367	THR
2	A	595	SER
2	A	613	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	42	ASN
2	A	178	HIS
2	A	199	ASN
2	A	329	GLN
2	A	440	HIS
2	A	474	ASN
2	A	554	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 ⓘ

8 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	B	1	3,2	14,14,15	0.42	0	17,19,21	0.48	0
3	NAG	B	2	3	14,14,15	0.40	0	17,19,21	0.46	0
3	BMA	B	3	3	11,11,12	0.22	0	15,15,17	0.44	0
4	NAG	D	1	4,2	14,14,15	0.39	0	17,19,21	0.63	1 (5%)
4	NAG	D	2	4	14,14,15	0.39	0	17,19,21	0.55	0
3	NAG	E	1	3,2	14,14,15	0.41	0	17,19,21	0.60	0
3	NAG	E	2	3	14,14,15	0.38	0	17,19,21	0.69	1 (5%)
3	BMA	E	3	3	11,11,12	0.18	0	15,15,17	0.61	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	B	2	3	-	0/6/23/26	0/1/1/1
3	BMA	B	3	3	-	0/2/19/22	0/1/1/1
4	NAG	D	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
3	NAG	E	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	1/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	NAG	C2-N2-C7	2.31	126.19	122.90
4	D	1	NAG	O5-C1-C2	2.07	114.56	111.29

There are no chirality outliers.

All (5) torsion outliers are listed below:

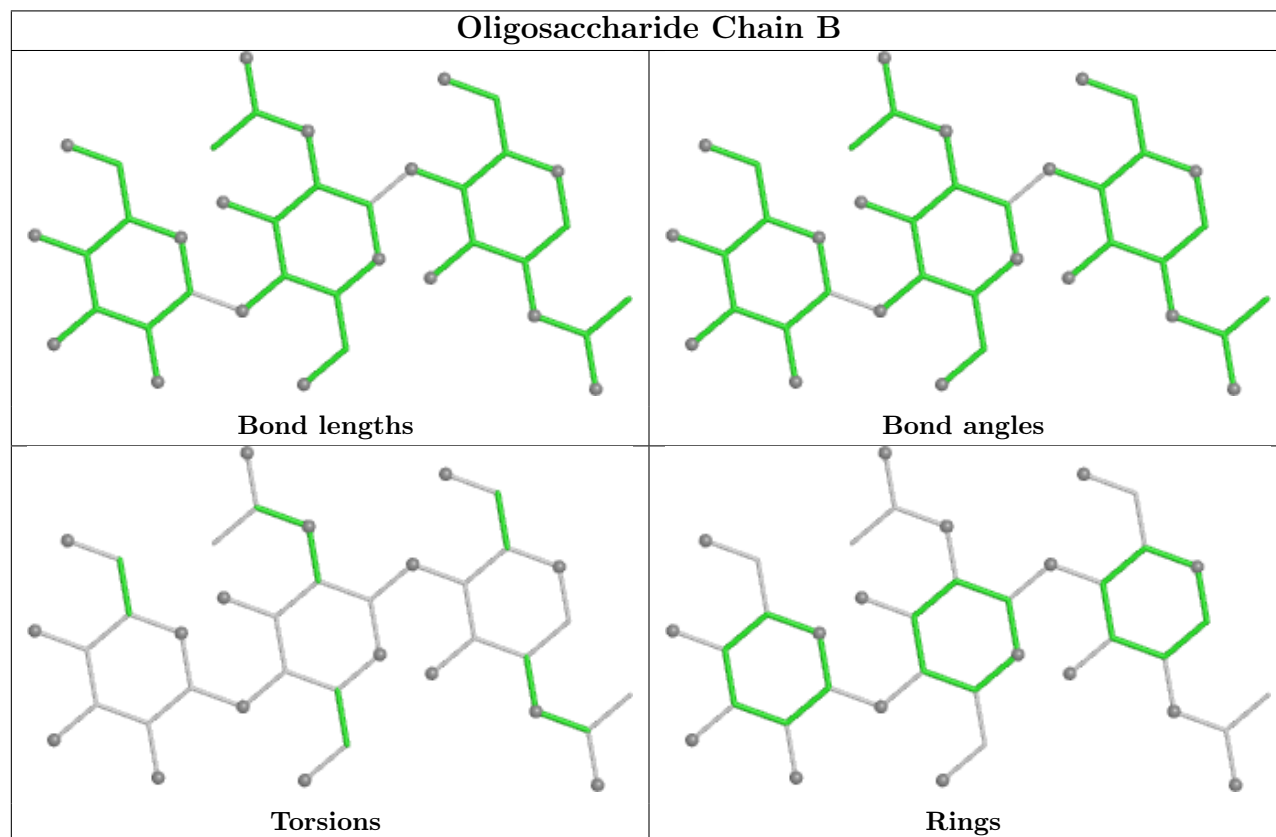
Mol	Chain	Res	Type	Atoms
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
3	E	1	NAG	C1-C2-N2-C7
3	E	2	NAG	C3-C2-N2-C7
3	E	1	NAG	C3-C2-N2-C7

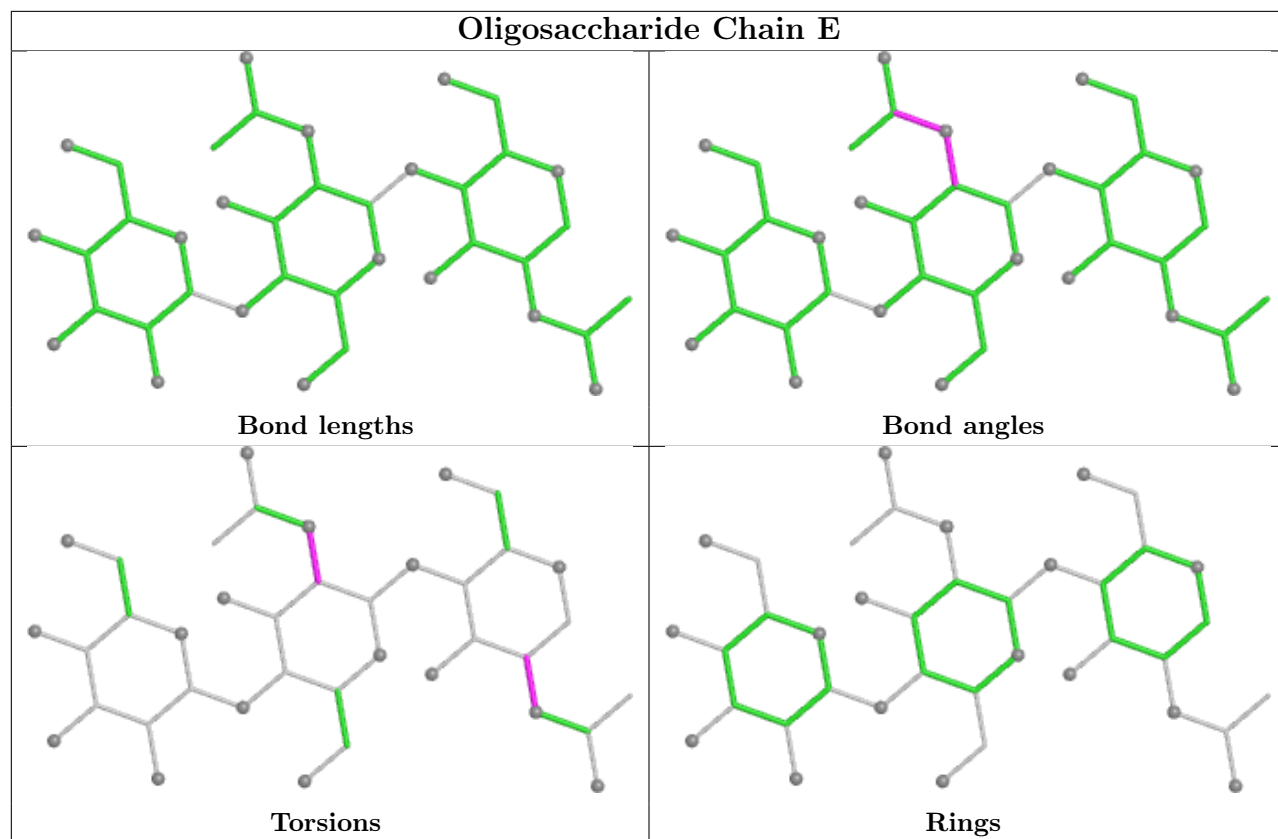
There are no ring outliers.

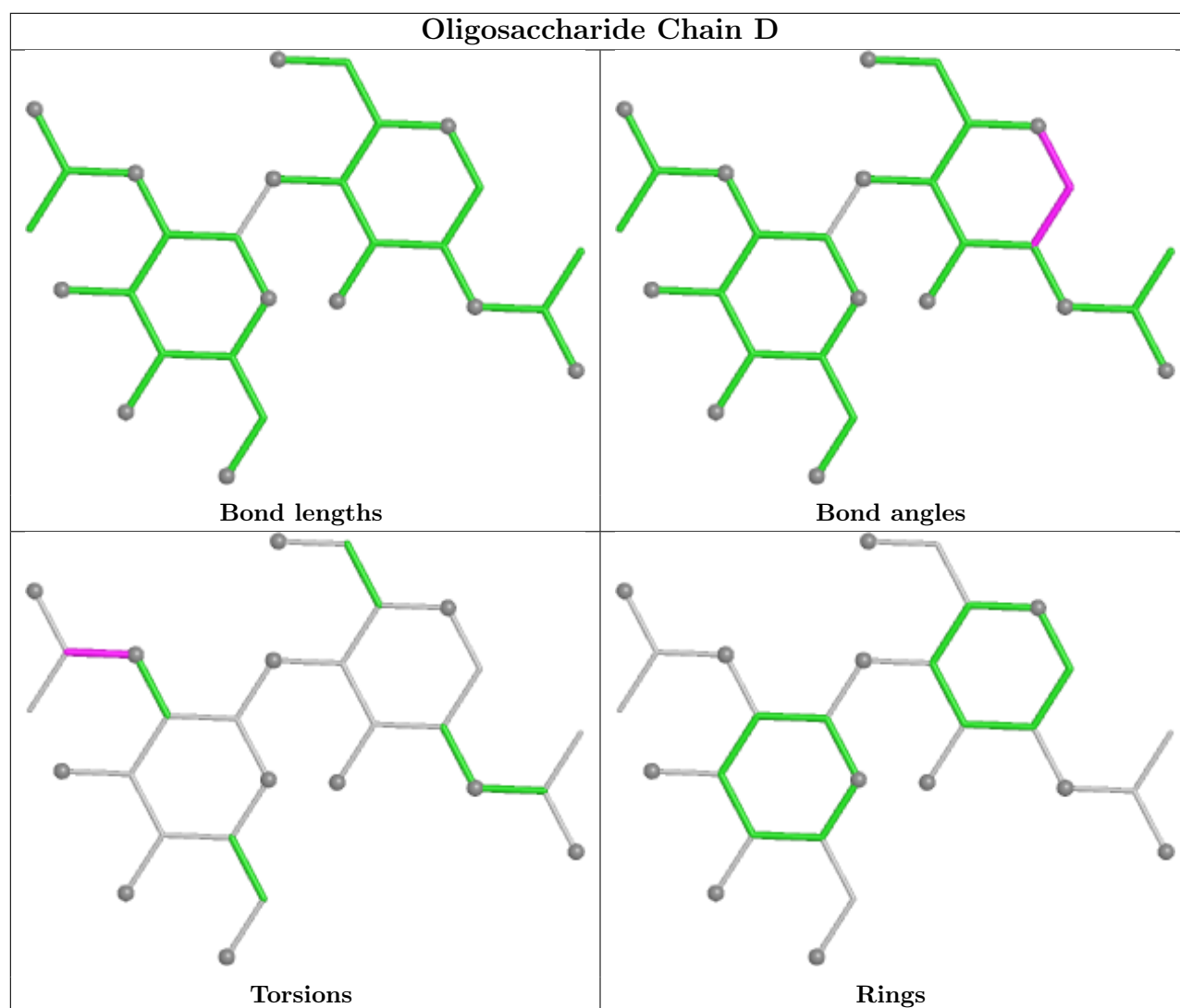
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2	NAG	1	0

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](#)

5 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	A1EMC	A	802	-	34,34,34	1.24	3 (8%)	42,45,45	1.43	8 (19%)
5	NAG	A	801	2	14,14,15	0.39	0	17,19,21	0.38	0
7	6PL	A	804	-	49,49,51	0.28	0	55,57,59	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	CLR	A	805	-	31,31,31	0.30	0	48,48,48	0.37	0
7	6PL	A	803	-	45,45,51	0.30	0	51,53,59	0.32	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
6	A1EMC	A	802	-	-	2/23/23/23	0/2/2/2
5	NAG	A	801	2	-	0/6/23/26	0/1/1/1
7	6PL	A	804	-	-	41/53/53/55	-
8	CLR	A	805	-	-	4/10/68/68	0/4/4/4
7	6PL	A	803	-	-	26/49/49/55	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	802	A1EMC	C11-C06	-3.55	1.36	1.43
6	A	802	A1EMC	C14-C03	2.57	1.54	1.51
6	A	802	A1EMC	C14-C15	2.02	1.55	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	802	A1EMC	C03-C14-C15	-3.76	106.21	112.17
6	A	802	A1EMC	C24-C25-C26	-2.86	120.76	127.66
6	A	802	A1EMC	C14-C15-C16	-2.56	123.27	127.24
6	A	802	A1EMC	C27-C26-C28	2.31	119.15	115.27
6	A	802	A1EMC	C19-C20-C21	-2.30	122.12	127.66
6	A	802	A1EMC	C33-C31-C32	2.22	119.50	114.60
6	A	802	A1EMC	C17-C16-C18	2.18	118.94	115.27
6	A	802	A1EMC	C22-C21-C23	2.15	118.89	115.27

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	802	A1EMC	C21-C23-C24-C25
7	A	803	6PL	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
7	A	803	6PL	C1-O3P-P-O2P
7	A	803	6PL	C1-O3P-P-O4P
7	A	803	6PL	O4P-C4-C5-N
7	A	804	6PL	C1-O3P-P-O1P
7	A	804	6PL	C4-O4P-P-O3P
7	A	804	6PL	C4-O4P-P-O1P
7	A	804	6PL	O31-C31-O2-C2
7	A	804	6PL	C32-C31-O2-C2
7	A	803	6PL	O11-C11-O3-C3
7	A	803	6PL	C12-C11-O3-C3
7	A	804	6PL	C19-C20-C21-C22
7	A	804	6PL	C16-C17-C18-C19
7	A	804	6PL	C41-C42-C43-C44
6	A	802	A1EMC	C16-C18-C19-C20
7	A	804	6PL	C4-C5-N-C7
7	A	804	6PL	C4-C5-N-C6
7	A	804	6PL	C33-C34-C35-C36
8	A	805	CLR	C20-C22-C23-C24
7	A	803	6PL	C11-C12-C13-C14
7	A	804	6PL	C11-C12-C13-C14
7	A	804	6PL	C12-C13-C14-C15
7	A	804	6PL	C21-C22-C23-C24
7	A	803	6PL	C40-C41-C42-C43
7	A	803	6PL	C42-C43-C44-C45
7	A	804	6PL	C15-C16-C17-C18
7	A	803	6PL	C15-C16-C17-C18
7	A	804	6PL	C18-C19-C20-C21
7	A	803	6PL	C31-C32-C33-C34
7	A	804	6PL	C38-C39-C40-C41
7	A	804	6PL	C40-C41-C42-C43
7	A	803	6PL	C41-C42-C43-C44
7	A	804	6PL	C14-C15-C16-C17
7	A	804	6PL	C4-C5-N-C8
8	A	805	CLR	C23-C24-C25-C26
8	A	805	CLR	C23-C24-C25-C27
7	A	803	6PL	C17-C18-C19-C20
7	A	804	6PL	C35-C36-C37-C38
7	A	803	6PL	C33-C34-C35-C36
7	A	804	6PL	C13-C14-C15-C16
7	A	803	6PL	C39-C40-C41-C42
7	A	804	6PL	C12-C11-O3-C3
7	A	804	6PL	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
7	A	803	6PL	C35-C36-C37-C38
7	A	804	6PL	C1-O3P-P-O4P
7	A	804	6PL	O11-C11-O3-C3
7	A	803	6PL	O3P-C1-C2-C3
7	A	804	6PL	C20-C21-C22-C23
7	A	803	6PL	C1-C2-C3-O3
7	A	804	6PL	C34-C35-C36-C37
7	A	804	6PL	C37-C38-C39-C40
7	A	804	6PL	C43-C44-C45-C46
7	A	803	6PL	C43-C44-C45-C46
7	A	803	6PL	C13-C14-C15-C16
7	A	804	6PL	O3P-C1-C2-C3
7	A	804	6PL	C1-C2-C3-O3
7	A	804	6PL	C22-C23-C24-C25
7	A	804	6PL	C23-C24-C25-C26
7	A	804	6PL	O3P-C1-C2-O2
7	A	804	6PL	O2-C2-C3-O3
7	A	804	6PL	C32-C33-C34-C35
7	A	803	6PL	O3P-C1-C2-O2
7	A	804	6PL	C31-C32-C33-C34
7	A	803	6PL	O2-C2-C3-O3
7	A	803	6PL	C16-C17-C18-C19
7	A	804	6PL	C3-C2-O2-C31
7	A	804	6PL	C1-C2-O2-C31
7	A	803	6PL	C38-C39-C40-C41
7	A	803	6PL	C12-C13-C14-C15
8	A	805	CLR	C21-C20-C22-C23
7	A	804	6PL	C1-O3P-P-O2P
7	A	803	6PL	C3-C2-O2-C31

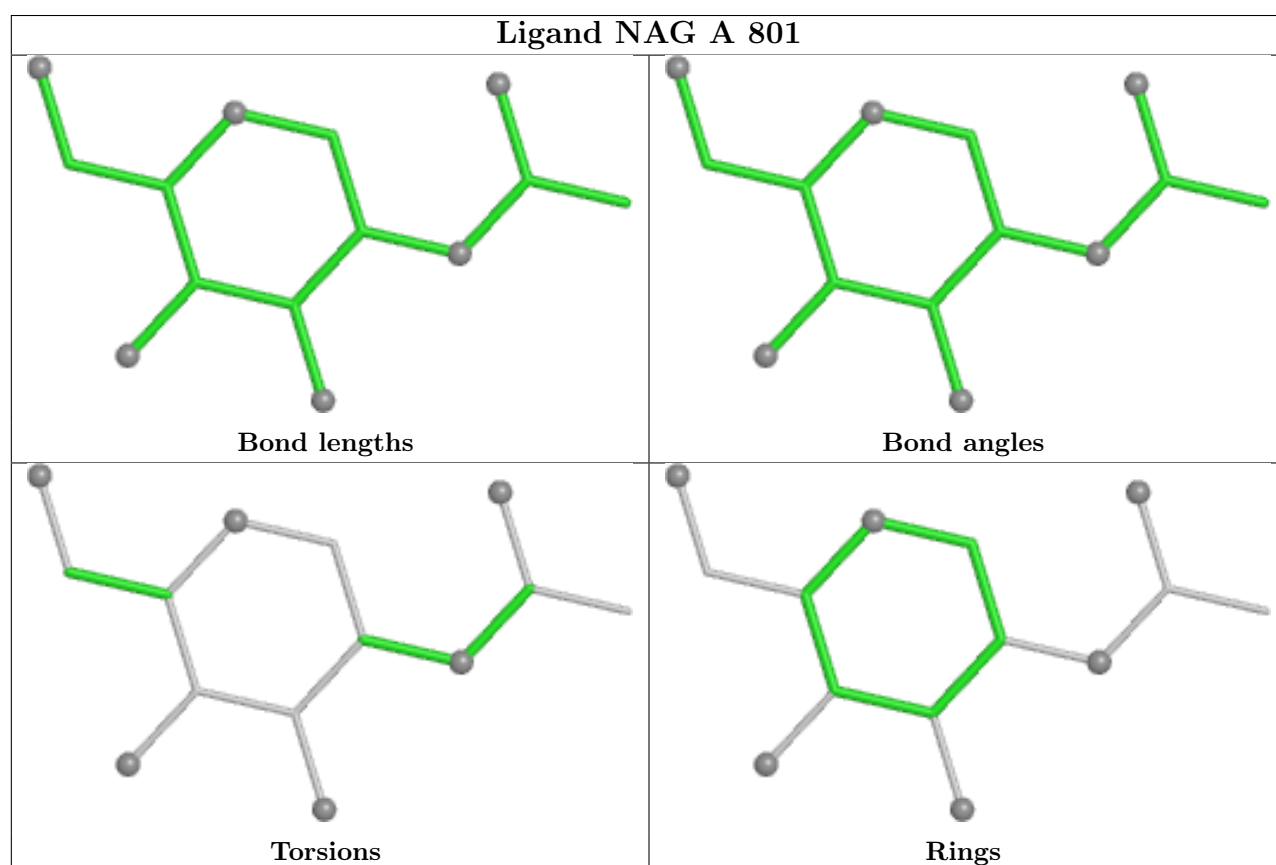
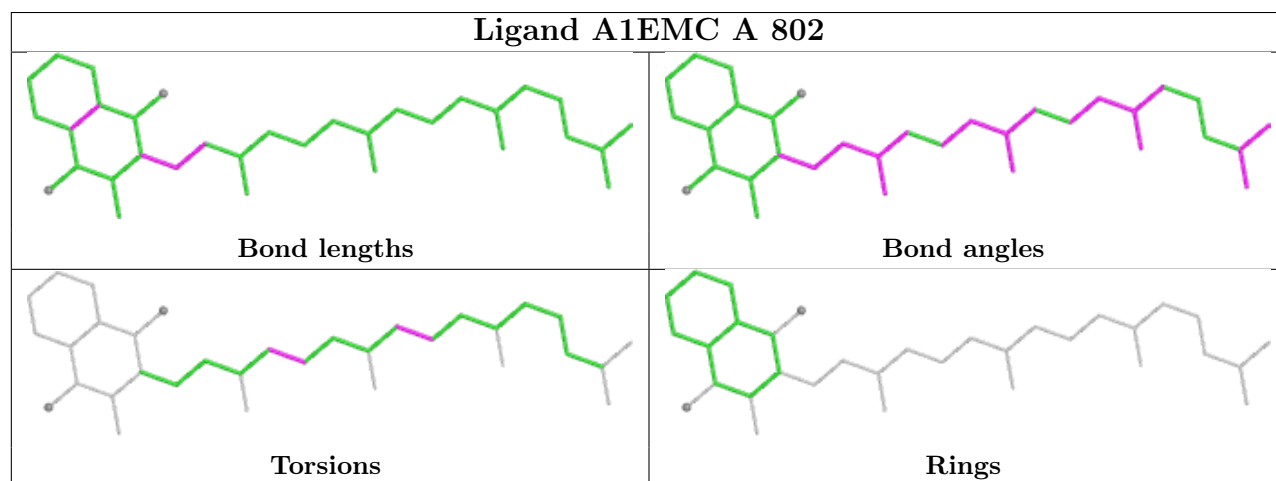
There are no ring outliers.

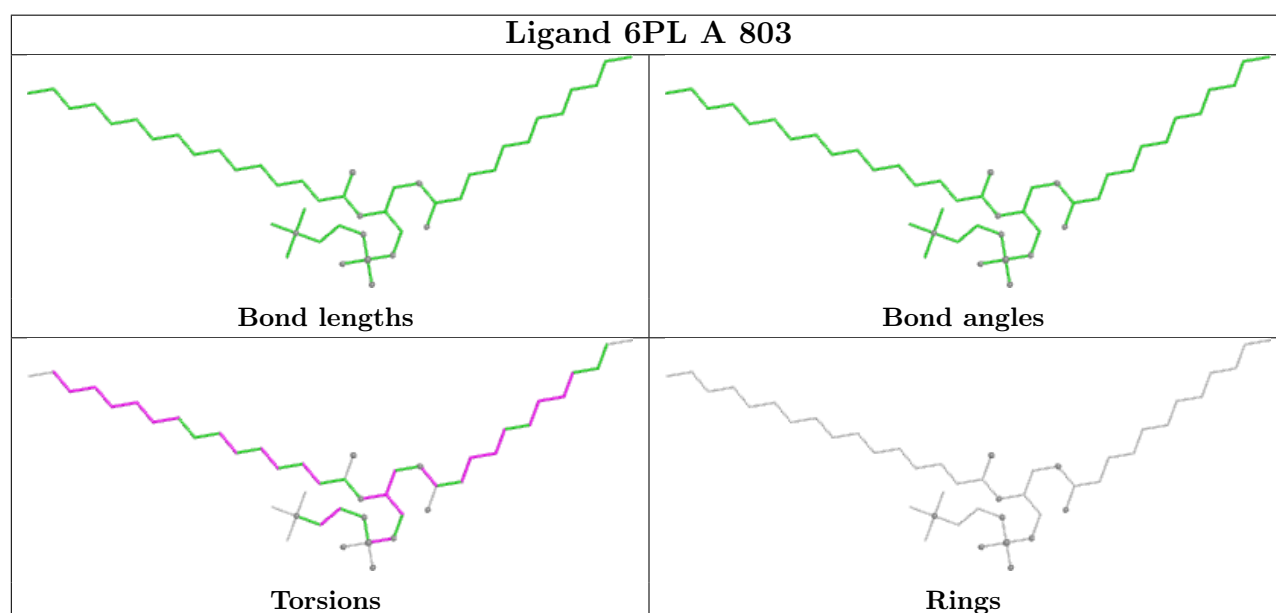
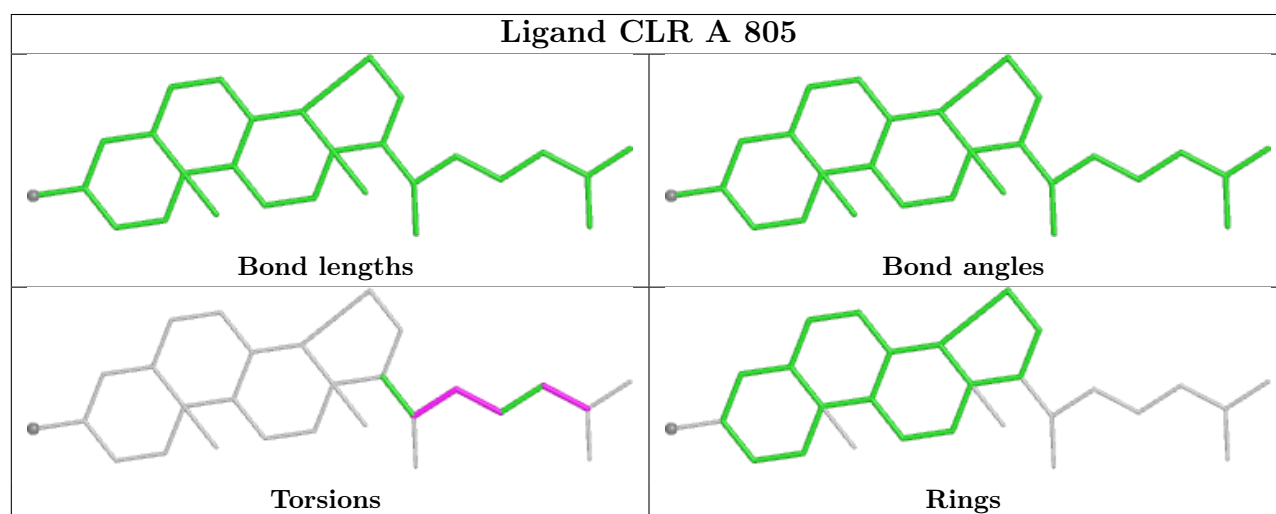
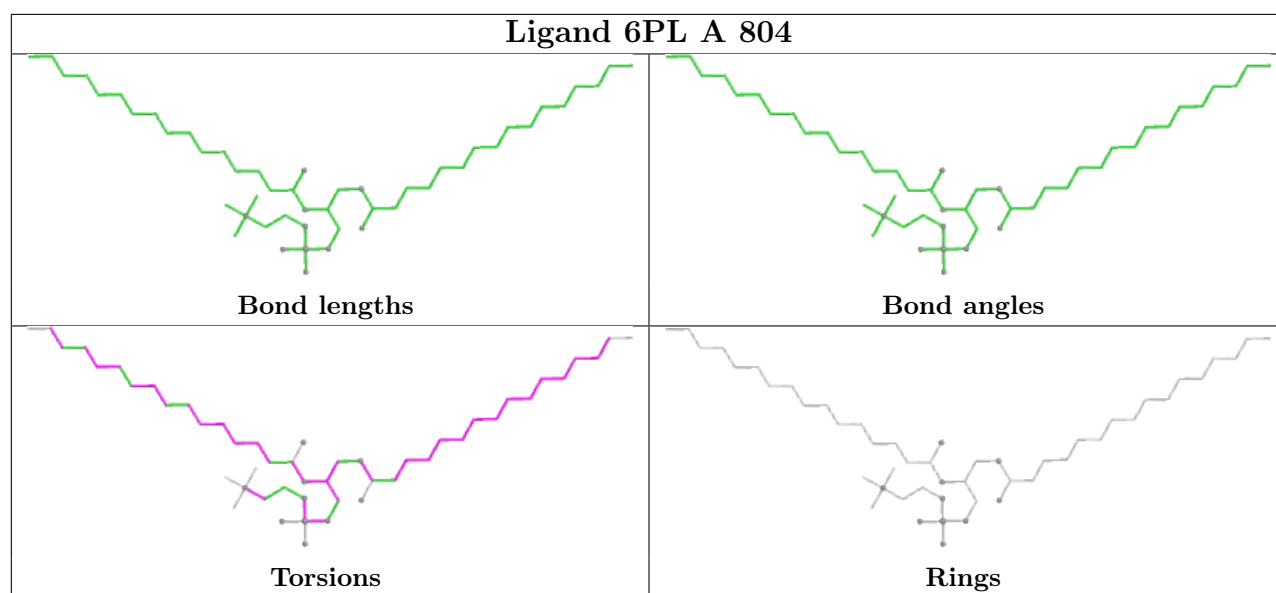
4 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	802	A1EMC	8	0
7	A	804	6PL	8	0
8	A	805	CLR	1	0
7	A	803	6PL	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.