



Full wwPDB EM Validation Report ⓘ

Apr 16, 2026 – 12:37 PM JST

PDB ID : 9L6Q / pdb_00009l6q
EMDB ID : EMD-62862
Title : Vitamin K-dependent gamma-carboxylase in complex with Coagulation factor IX and vitamin K
Authors : Hang, J.; Chen, D.D.; Zhong, Q.H.
Deposited on : 2024-12-25
Resolution : 2.78 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

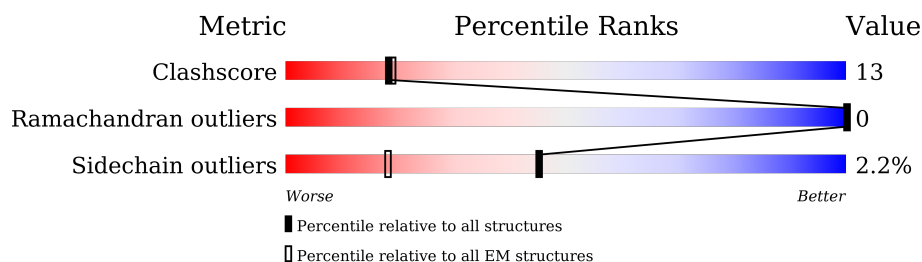
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.78 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	758	64% 23% 12%
2	C	461	5% 93%
3	B	2	100%
3	D	2	100%
4	E	3	100%

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
7	1L3	A	804	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5893 atoms, of which 40 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	665	Total	C	N	O	S	0	0
			5363	3510	897	930	26		

- Molecule 2 is a protein called Coagulation factor IX.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	32	Total	C	N	O	0	0
			238	148	42	48		

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



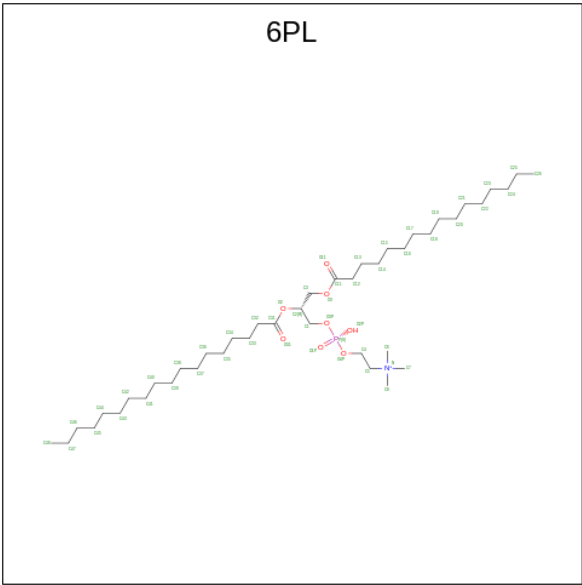
Mol	Chain	Residues	Atoms				AltConf	Trace
3	B	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		

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



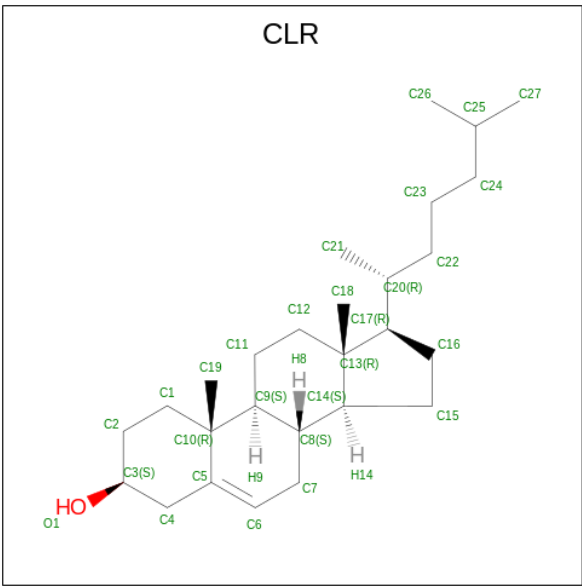
Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 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).



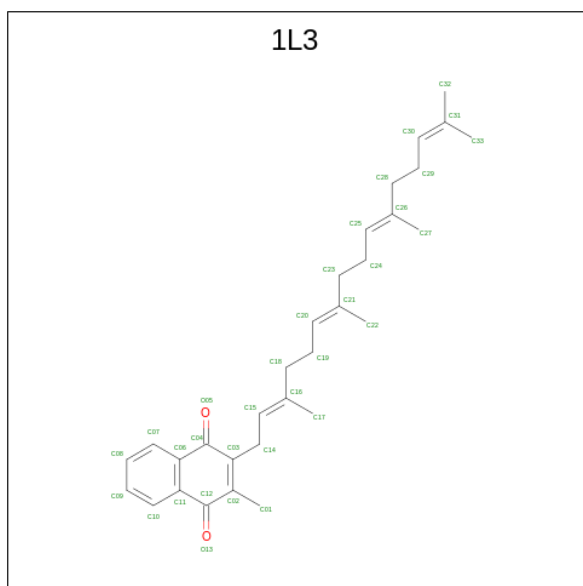
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			50	40	1	8	1	
5	A	1	Total	C	N	O	P	0
			46	36	1	8	1	

- Molecule 6 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is Menaquinone-4 (CCD ID: 1L3) (formula: $C_{31}H_{40}O_2$) (labeled as "Ligand of Interest" by depositor).

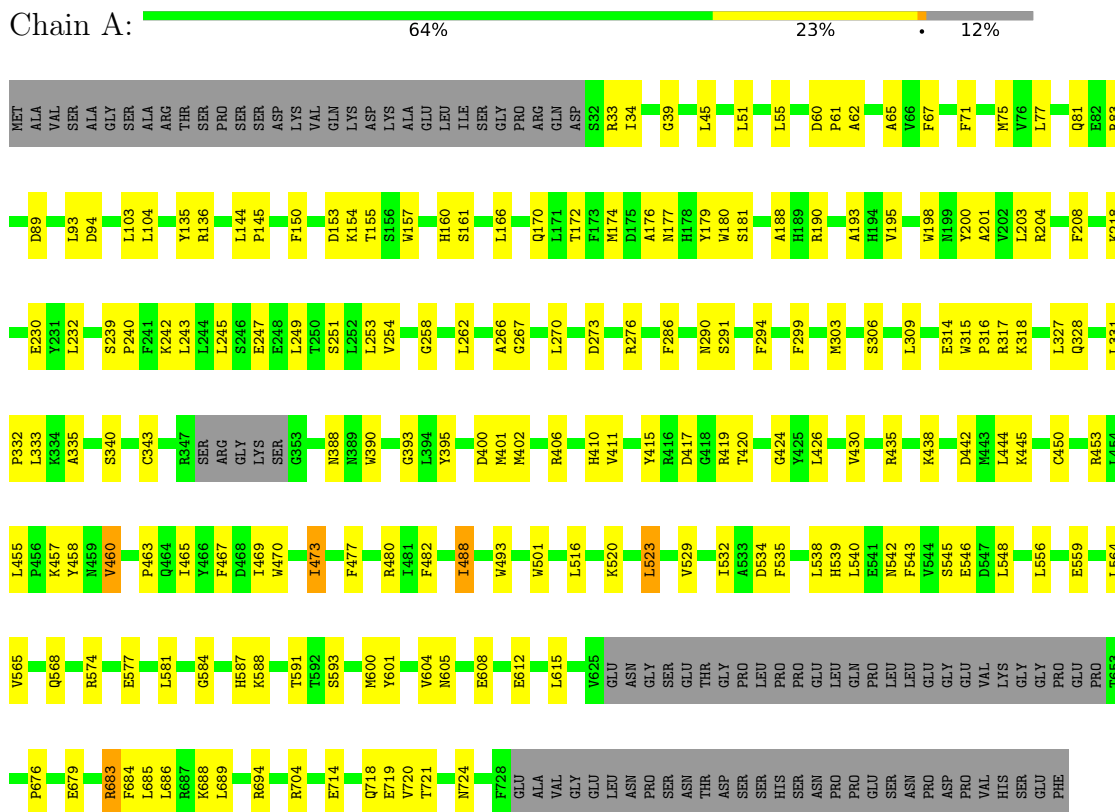


Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	H	O	0
			73	31	40	2	

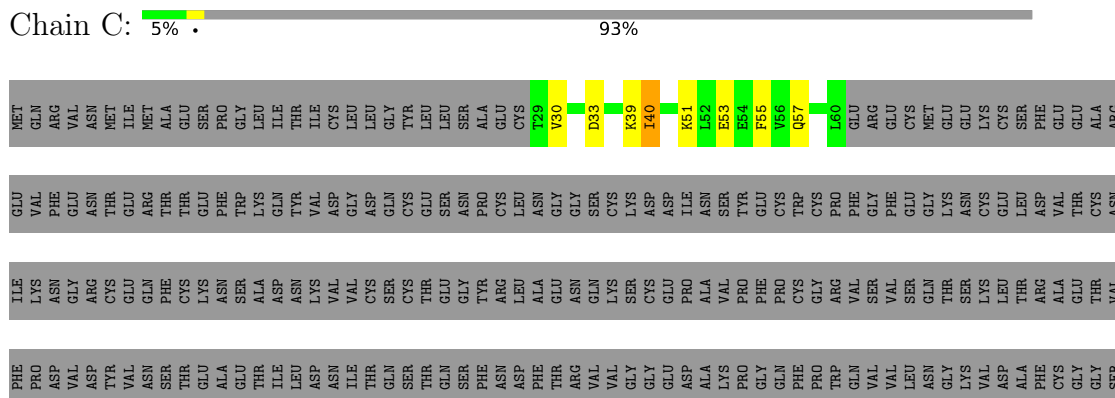
3 Residue-property plots

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



ILE	VAL	ASN	GLU	LYS	TRP	ILE	VAL	THR	ALA	ALA	HIS	CYS	CYS	VAL	GLU	THR	GLY	VAL	GLY	ILE	THR	VAL	VAL	VAL	ALA	GLY	GLU	HIS	THR	ILE	ILE	GLU	GLY	ASN	ASN	GLY	GLU	GLU	THR	THR	GLN	LYS	ARG	ASN	ASN	VAL	TRP	VAL	ILE	ARG	VAL	ILE	PRO	HIS	HIS	ASN	TYR	ASN	ASN	ALA	VAL	ILE	GLN	ASN	LYS	TYR	ASN	VAL	HIS	ASP
ILE	ALA	ASN	LEU	GLY	LEU	GLU	ASP	GLU	PRO	THR	VAL	THR	VAL	TYR	ASN	SER	THR	VAL	THR	GLY	ASN	THR	VAL	THR	ASP	LYS	GLU	TYR	THR	ASN	ASN	ILE	PHE	GLU	LEU	LYS	LYS	PHE	GLN	THR	GLY	THR	GLY	TRP	GLY	VAL	THR	GLY	VAL	PHE	HIS	LYS	GLY	ARG	SER	ALA	LEU	VAL	ILE	LEU	GLN	TYR	LEU	ARG	VAL	PRO	CYS			
ALA	MET	LYS	GLY	LYS	TYR	GLY	ILE	TYR	THR	LYS	VAL	SER	ARG	TYR	VAL	VAL	ASN	ASN	TRP	ILE	ILE	LYS	GLU	LYS	THR	LYS	LEU	THR	GLY	GLY	GLY	ARG	ASP	SER	CYS	GLN	GLY	THR	GLY	PRO	HIS	VAL	THR	GLU	VAL	VAL	GLU	GLY	THR	SER	PHE	LEU	THR	GLY	ILE	LEU	SER	TRP	GLY	GLU	GLU	CYS								

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

Chain B: 100%

NAG1	NAG2
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- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 100%

NAG1	NAG2
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- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 100%

NAG1	NAG2	EM13
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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	331914	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 1L3, 6PL, BMA, CLR

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	0.25	0/5520	0.39	0/7515
2	C	0.30	0/241	0.42	0/326
All	All	0.25	0/5761	0.39	0/7841

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 [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	5363	0	5204	144	0
2	C	238	0	212	9	0
3	B	28	0	25	1	0
3	D	28	0	25	0	0
4	E	39	0	34	0	0
5	A	96	0	143	15	0
6	A	28	0	46	0	0
7	A	33	40	0	22	0
All	All	5853	40	5689	151	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 13.

All (151) 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:294:PHE:CE2	7:A:804:1L3:C01	2.21	1.24
1:A:254:VAL:HG13	7:A:804:1L3:C27	1.86	1.04
1:A:402:MET:SD	7:A:804:1L3:C01	2.57	0.92
1:A:254:VAL:HG12	7:A:804:1L3:C22	2.02	0.90
1:A:467:PHE:CE1	1:A:488:ILE:HG21	2.06	0.90
1:A:67:PHE:HB2	1:A:309:LEU:HD11	1.59	0.83
1:A:218:LYS:HE3	7:A:804:1L3:O05	1.80	0.81
1:A:294:PHE:CZ	7:A:804:1L3:C01	2.64	0.81
1:A:254:VAL:CG1	7:A:804:1L3:C22	2.58	0.81
1:A:286:PHE:CE1	7:A:804:1L3:C19	2.66	0.79
1:A:208:PHE:HD2	1:A:267:GLY:HA3	1.47	0.78
1:A:406:ARG:HG2	1:A:473:ILE:HG12	1.66	0.77
1:A:39:GLY:HA3	5:A:802:6PL:H42	1.68	0.76
1:A:286:PHE:HE1	7:A:804:1L3:C19	1.99	0.75
1:A:467:PHE:HE1	1:A:488:ILE:HG21	1.54	0.71
1:A:45:LEU:HD22	5:A:802:6PL:H391	1.73	0.70
1:A:254:VAL:HG22	7:A:804:1L3:C27	2.22	0.70
1:A:455:LEU:HB3	1:A:460:VAL:HG13	1.75	0.69
1:A:410:HIS:CD2	2:C:40:ILE:HD13	2.28	0.68
1:A:294:PHE:HE2	7:A:804:1L3:C01	1.99	0.65
1:A:411:VAL:HG13	1:A:469:ILE:HG12	1.79	0.65
1:A:488:ILE:HD13	1:A:501:TRP:CH2	2.31	0.65
1:A:254:VAL:CG1	7:A:804:1L3:C27	2.72	0.64
1:A:465:ILE:O	1:A:488:ILE:HG22	1.99	0.63
1:A:208:PHE:CD2	1:A:267:GLY:HA3	2.30	0.63
1:A:286:PHE:HZ	7:A:804:1L3:C04	2.11	0.62
1:A:426:LEU:HD11	1:A:455:LEU:HD11	1.81	0.62
2:C:55:PHE:O	2:C:57:GLN:NE2	2.33	0.62
1:A:685:LEU:HB3	5:A:801:6PL:H202	1.81	0.62
1:A:467:PHE:CD1	1:A:488:ILE:HG21	2.35	0.61
1:A:411:VAL:HG22	1:A:469:ILE:HG23	1.83	0.60
1:A:170:GLN:HB3	1:A:174:MET:HE3	1.85	0.58
1:A:435:ARG:HB3	1:A:438:LYS:HE2	1.86	0.57
1:A:411:VAL:HG21	1:A:438:LYS:HD3	1.87	0.56
1:A:685:LEU:HD13	5:A:801:6PL:H202	1.88	0.56
1:A:174:MET:HE1	1:A:203:LEU:HG	1.89	0.55
1:A:523:LEU:HD21	1:A:529:VAL:HB	1.89	0.55
1:A:103:LEU:HA	1:A:154:LYS:HD3	1.88	0.54
1:A:564:LEU:O	1:A:568:GLN:N	2.41	0.54
1:A:714:GLU:O	1:A:718:GLN:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ASP:OD2	1:A:155:THR:OG1	2.26	0.54
1:A:245:LEU:HD22	1:A:249:LEU:HD23	1.91	0.53
1:A:480:ARG:NH1	1:A:534:ASP:OD1	2.42	0.53
1:A:480:ARG:NH2	1:A:539:HIS:O	2.38	0.53
1:A:160:HIS:HB3	1:A:299:PHE:CG	2.44	0.53
1:A:419:ARG:NH1	1:A:420:THR:OG1	2.42	0.52
1:A:67:PHE:CB	1:A:309:LEU:HD11	2.35	0.52
1:A:180:TRP:CD1	1:A:332:PRO:HG3	2.44	0.52
1:A:314:GLU:HG2	1:A:318:LYS:HE3	1.90	0.52
1:A:328:GLN:HA	1:A:331:LEU:HD12	1.92	0.52
1:A:242:LYS:HE2	1:A:247:GLU:HA	1.91	0.52
1:A:430:VAL:HG21	2:C:30:VAL:HA	1.91	0.51
1:A:542:ASN:HD22	1:A:587:HIS:CE1	2.28	0.51
1:A:545:SER:HB3	2:C:39:LYS:HD3	1.93	0.51
1:A:203:LEU:HB3	1:A:309:LEU:HD23	1.92	0.51
1:A:61:PRO:HB3	1:A:195:VAL:HG13	1.94	0.50
1:A:299:PHE:CE2	7:A:804:1L3:C09	2.95	0.50
1:A:39:GLY:HA3	5:A:802:6PL:C4	2.41	0.49
1:A:315:TRP:CG	1:A:316:PRO:HD3	2.48	0.49
1:A:534:ASP:HB3	1:A:591:THR:OG1	2.12	0.49
1:A:286:PHE:CD1	7:A:804:1L3:C19	2.95	0.49
1:A:144:LEU:HB2	1:A:145:PRO:HD3	1.95	0.49
1:A:529:VAL:HA	1:A:601:TYR:O	2.13	0.49
1:A:240:PRO:O	1:A:243:LEU:HB3	2.12	0.49
1:A:445:LYS:HA	1:A:488:ILE:HD11	1.94	0.49
1:A:306:SER:HA	1:A:309:LEU:HD13	1.95	0.49
1:A:543:PHE:HD2	2:C:39:LYS:HE2	1.78	0.48
1:A:511:LEU:HD22	5:A:802:6PL:H412	1.94	0.48
1:A:218:LYS:CE	7:A:804:1L3:O05	2.59	0.48
1:A:684:PHE:HZ	5:A:801:6PL:H2	1.78	0.48
1:A:390:TRP:CE3	1:A:473:ILE:HG13	2.49	0.48
1:A:290:ASN:ND2	7:A:804:1L3:C12	2.76	0.48
1:A:559:GLU:HG2	1:A:593:SER:HB3	1.95	0.47
1:A:388:ASN:HA	1:A:393:GLY:H	1.80	0.47
1:A:477:PHE:CZ	1:A:516:LEU:HD11	2.48	0.47
1:A:55:LEU:O	1:A:198:TRP:N	2.46	0.47
1:A:467:PHE:HE1	1:A:488:ILE:CG2	2.26	0.46
1:A:60:ASP:O	1:A:200:TYR:OH	2.27	0.46
1:A:676:PRO:HG2	1:A:679:GLU:HB2	1.97	0.46
1:A:89:ASP:OD1	1:A:694:ARG:NH2	2.48	0.46
1:A:299:PHE:CE2	7:A:804:1L3:C10	2.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:MET:HB3	1:A:402:MET:HE3	1.97	0.46
1:A:581:LEU:HD13	1:A:587:HIS:CE1	2.50	0.46
1:A:177:ASN:O	1:A:181:SER:OG	2.25	0.46
1:A:540:LEU:HD11	2:C:40:ILE:HG13	1.98	0.46
1:A:303:MET:HE3	1:A:303:MET:HB3	1.79	0.45
1:A:198:TRP:HA	1:A:201:ALA:HB3	1.99	0.45
1:A:230:GLU:HA	1:A:251:SER:OG	2.16	0.45
1:A:417:ASP:OD1	1:A:419:ARG:N	2.50	0.45
1:A:470:TRP:CZ2	1:A:540:LEU:HD13	2.51	0.45
1:A:179:TYR:OH	1:A:333:LEU:O	2.33	0.44
1:A:608:GLU:O	1:A:612:GLU:HG2	2.17	0.44
1:A:135:TYR:CZ	1:A:176:ALA:HB3	2.53	0.44
1:A:535:PHE:HB2	1:A:538:LEU:HD12	1.99	0.44
3:B:1:NAG:H61	3:B:2:NAG:C7	2.48	0.44
1:A:546:GLU:HG2	1:A:584:GLY:HA3	1.99	0.44
5:A:802:6PL:O31	5:A:802:6PL:H12	2.17	0.44
1:A:166:LEU:O	1:A:170:GLN:HG3	2.18	0.44
1:A:720:VAL:O	1:A:724:ASN:ND2	2.51	0.44
1:A:442:ASP:HB3	1:A:493:TRP:CZ2	2.54	0.43
1:A:488:ILE:HD13	1:A:501:TRP:CZ2	2.53	0.43
1:A:273:ASP:OD2	1:A:276:ARG:NH2	2.52	0.43
1:A:150:PHE:O	1:A:157:TRP:NE1	2.41	0.43
1:A:327:LEU:H	1:A:327:LEU:HD23	1.83	0.43
1:A:83:ARG:NH2	1:A:161:SER:OG	2.51	0.43
1:A:136:ARG:NH1	1:A:172:THR:O	2.52	0.43
1:A:254:VAL:HG13	7:A:804:1L3:C22	2.42	0.43
1:A:688:LYS:HB3	5:A:801:6PL:H132	2.00	0.43
1:A:270:LEU:O	1:A:276:ARG:HD3	2.18	0.42
1:A:704:ARG:NH2	1:A:719:GLU:OE1	2.48	0.42
5:A:801:6PL:H372	5:A:801:6PL:H401	1.79	0.42
1:A:574:ARG:H	1:A:577:GLU:HG3	1.84	0.42
1:A:565:VAL:HG22	1:A:588:LYS:HE2	2.02	0.42
1:A:62:ALA:HA	1:A:179:TYR:CD2	2.54	0.42
1:A:65:ALA:HB2	1:A:179:TYR:HB3	2.02	0.42
1:A:400:ASP:OD1	1:A:400:ASP:N	2.50	0.42
1:A:683:ARG:HA	1:A:683:ARG:HD3	1.75	0.42
1:A:689:LEU:HD12	5:A:801:6PL:H181	2.01	0.42
1:A:395:TYR:OH	2:C:53:GLU:HB2	2.20	0.41
1:A:444:LEU:HD22	1:A:482:PHE:CD2	2.55	0.41
1:A:51:LEU:HD22	5:A:802:6PL:H431	2.02	0.41
1:A:204:ARG:HH12	5:A:802:6PL:P	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LEU:HD12	1:A:94:ASP:N	2.35	0.41
1:A:188:ALA:C	1:A:190:ARG:H	2.28	0.41
1:A:291:SER:O	5:A:801:6PL:H63	2.20	0.41
1:A:299:PHE:CZ	7:A:804:1L3:C09	3.03	0.41
1:A:460:VAL:HG22	1:A:463:PRO:HG3	2.02	0.41
5:A:802:6PL:H31	5:A:802:6PL:H121	1.37	0.41
1:A:77:LEU:O	1:A:81:GLN:NE2	2.50	0.41
1:A:232:LEU:CD2	7:A:804:1L3:C17	2.98	0.41
1:A:306:SER:O	1:A:309:LEU:HB2	2.19	0.41
2:C:33:ASP:N	2:C:33:ASP:OD1	2.37	0.41
1:A:253:LEU:O	1:A:258:GLY:N	2.52	0.41
1:A:450:CYS:O	1:A:453:ARG:HG2	2.20	0.41
1:A:415:TYR:CZ	1:A:424:GLY:HA3	2.56	0.41
1:A:71:PHE:O	1:A:75:MET:HG2	2.21	0.41
1:A:548:LEU:HD23	1:A:605:ASN:HA	2.03	0.41
1:A:604:VAL:O	1:A:605:ASN:HB3	2.21	0.41
1:A:239:SER:N	1:A:240:PRO:HD2	2.36	0.41
1:A:457:LYS:HD2	1:A:458:TYR:CE1	2.56	0.41
1:A:520:LYS:HB2	1:A:520:LYS:HE2	1.86	0.41
1:A:262:LEU:O	1:A:266:ALA:HB2	2.20	0.40
1:A:33:ARG:HD3	1:A:33:ARG:HA	1.87	0.40
1:A:193:ALA:HB1	1:A:340:SER:HB2	2.02	0.40
1:A:556:LEU:HD21	1:A:600:MET:SD	2.61	0.40
2:C:40:ILE:H	2:C:40:ILE:HG12	1.71	0.40
1:A:254:VAL:CG2	7:A:804:1L3:C27	2.97	0.40
1:A:317:ARG:NH1	1:A:335:ALA:O	2.55	0.40
1:A:328:GLN:HA	1:A:331:LEU:HB2	2.03	0.40
1:A:470:TRP:CZ3	1:A:532:ILE:HG23	2.56	0.40
1:A:694:ARG:NH1	1:A:724:ASN:OD1	2.50	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	659/758 (87%)	650 (99%)	9 (1%)	0	100	100
2	C	30/461 (6%)	28 (93%)	2 (7%)	0	100	100
All	All	689/1219 (56%)	678 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	566/681 (83%)	555 (98%)	11 (2%)	50	78
2	C	24/403 (6%)	22 (92%)	2 (8%)	10	29
All	All	590/1084 (54%)	577 (98%)	13 (2%)	45	75

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ILE
1	A	104	LEU
1	A	343	CYS
1	A	460	VAL
1	A	473	ILE
1	A	488	ILE
1	A	523	LEU
1	A	615	LEU
1	A	683	ARG
1	A	686	LEU
1	A	721	THR
2	C	40	ILE
2	C	51	LYS

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

Mol	Chain	Res	Type
1	A	290	ASN
1	A	338	GLN
1	A	478	GLN
1	A	542	ASN
1	A	554	GLN
1	A	718	GLN
2	C	48	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

7 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	1,3	14,14,15	0.25	0	17,19,21	0.44	0
3	NAG	B	2	3	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	D	1	1,3	14,14,15	0.24	0	17,19,21	0.41	0
3	NAG	D	2	3	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	E	1	1,4	14,14,15	0.28	0	17,19,21	0.56	0
4	NAG	E	2	4	14,14,15	0.24	0	17,19,21	0.52	0
4	BMA	E	3	4	11,11,12	0.91	0	15,15,17	0.93	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	1,3	-	2/6/23/26	0/1/1/1
3	NAG	B	2	3	-	4/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	4/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

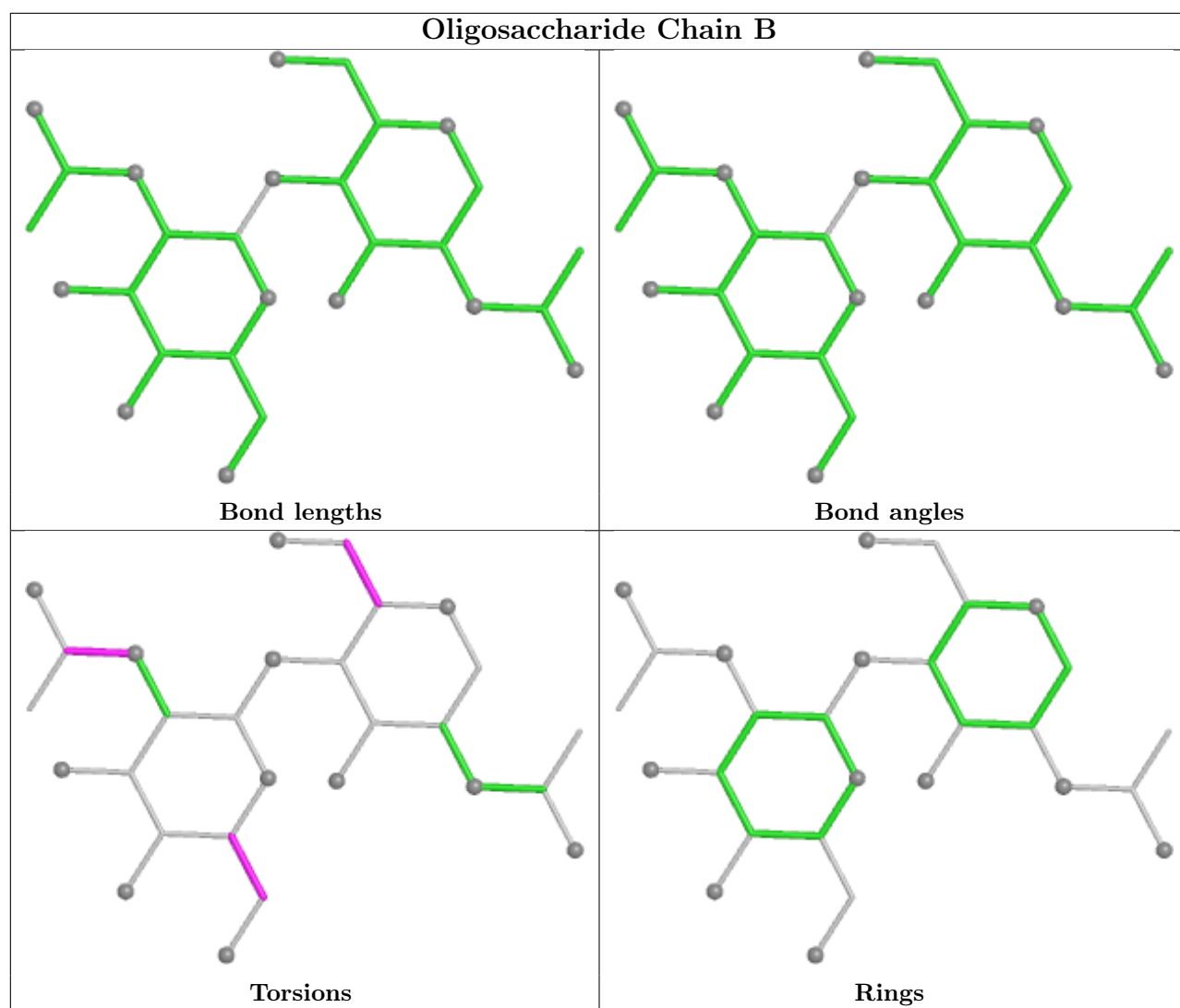
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
3	B	2	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	B	2	NAG	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	B	2	NAG	C8-C7-N2-C2
3	B	2	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	D	2	NAG	O5-C5-C6-O6
3	B	1	NAG	C4-C5-C6-O6
3	B	1	NAG	O5-C5-C6-O6
4	E	2	NAG	C3-C2-N2-C7
4	E	2	NAG	O5-C5-C6-O6

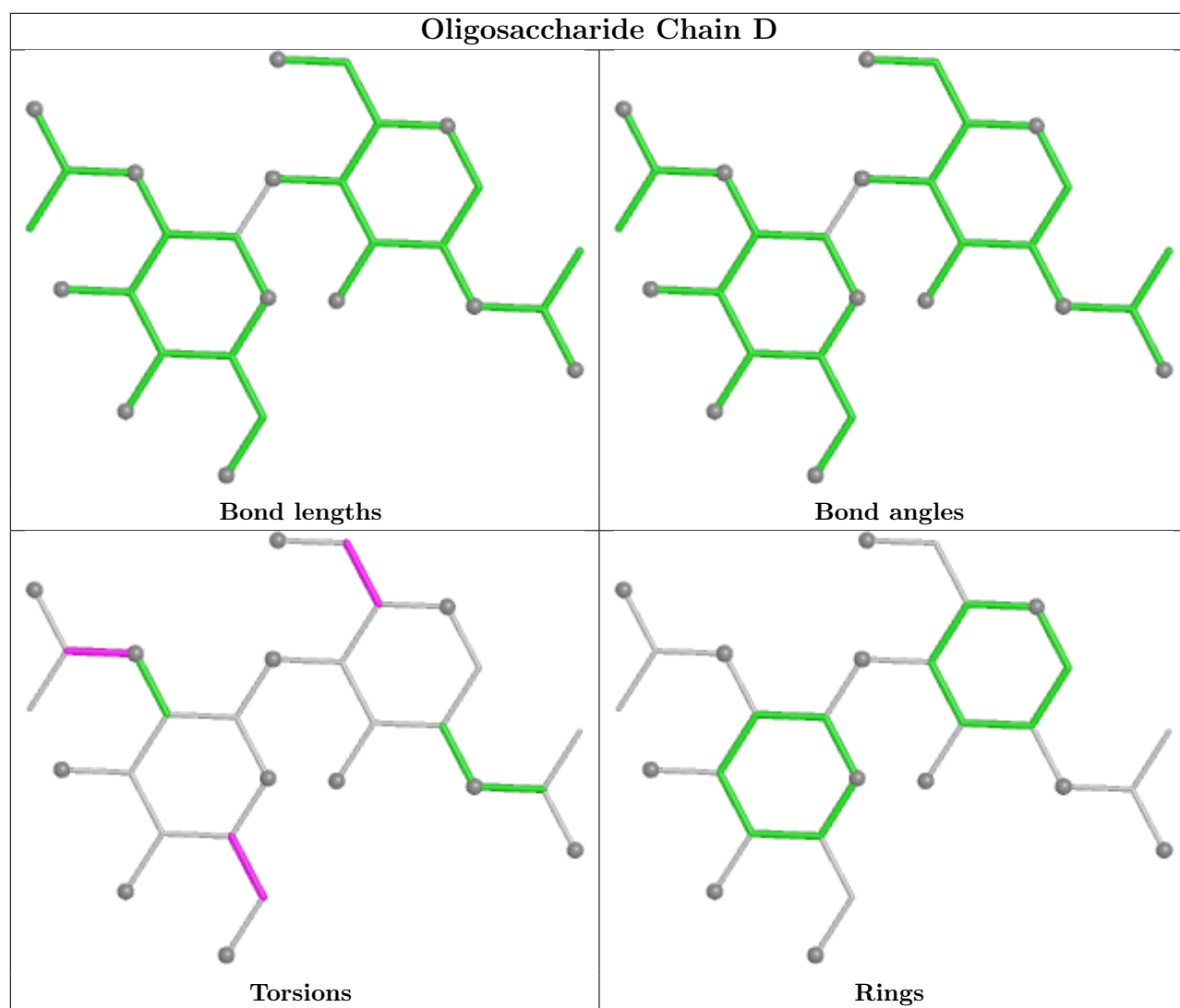
There are no ring outliers.

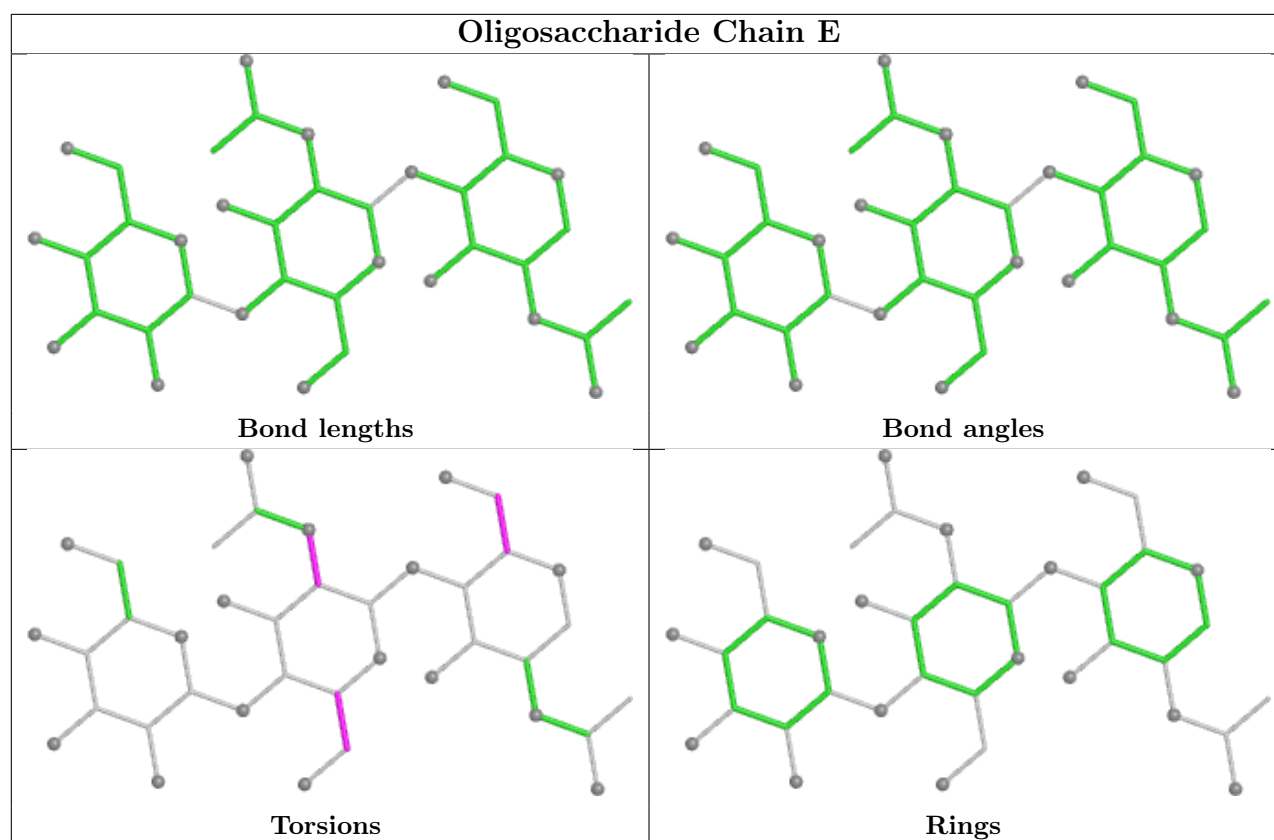
2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1	NAG	1	0
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](#)

4 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	$\# Z > 2$
7	1L3	A	804	-	34,34,34	2.75	12 (35%)	42,45,45	7.51	11 (26%)
5	6PL	A	801	-	49,49,51	0.31	0	55,57,59	0.34	0
6	CLR	A	803	-	31,31,31	0.38	0	48,48,48	0.60	0
5	6PL	A	802	-	45,45,51	0.28	0	51,53,59	0.34	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
7	1L3	A	804	-	-	8/23/43/43	0/2/2/2
5	6PL	A	801	-	-	16/53/53/55	-
6	CLR	A	803	-	-	4/10/68/68	0/4/4/4
5	6PL	A	802	-	-	12/49/49/55	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	804	1L3	C03-C02	8.44	1.50	1.35
7	A	804	1L3	C06-C04	4.94	1.57	1.48
7	A	804	1L3	C18-C16	4.73	1.61	1.51
7	A	804	1L3	C11-C12	4.63	1.57	1.48
7	A	804	1L3	C23-C21	4.11	1.59	1.51
7	A	804	1L3	C28-C26	3.71	1.59	1.51
7	A	804	1L3	C14-C15	3.46	1.55	1.50
7	A	804	1L3	C14-C03	2.99	1.56	1.51
7	A	804	1L3	C27-C26	2.26	1.56	1.50
7	A	804	1L3	C19-C20	2.11	1.57	1.50
7	A	804	1L3	O05-C04	-2.09	1.18	1.23
7	A	804	1L3	O13-C12	-2.07	1.18	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	804	1L3	C18-C16-C15	22.11	165.87	121.12
7	A	804	1L3	C17-C16-C18	-20.94	80.05	115.27
7	A	804	1L3	C22-C21-C20	17.23	167.89	123.68
7	A	804	1L3	C27-C26-C25	16.67	166.45	123.68
7	A	804	1L3	C27-C26-C28	-15.04	89.97	115.27
7	A	804	1L3	C22-C21-C23	-14.85	90.29	115.27
7	A	804	1L3	C17-C16-C15	-14.75	85.84	123.68
7	A	804	1L3	C23-C21-C20	-9.68	101.52	121.12
7	A	804	1L3	C28-C26-C25	-8.78	103.36	121.12
7	A	804	1L3	C19-C18-C16	-2.20	105.72	112.98
7	A	804	1L3	C01-C02-C03	-2.15	120.88	124.40

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	802	6PL	C12-C11-O3-C3

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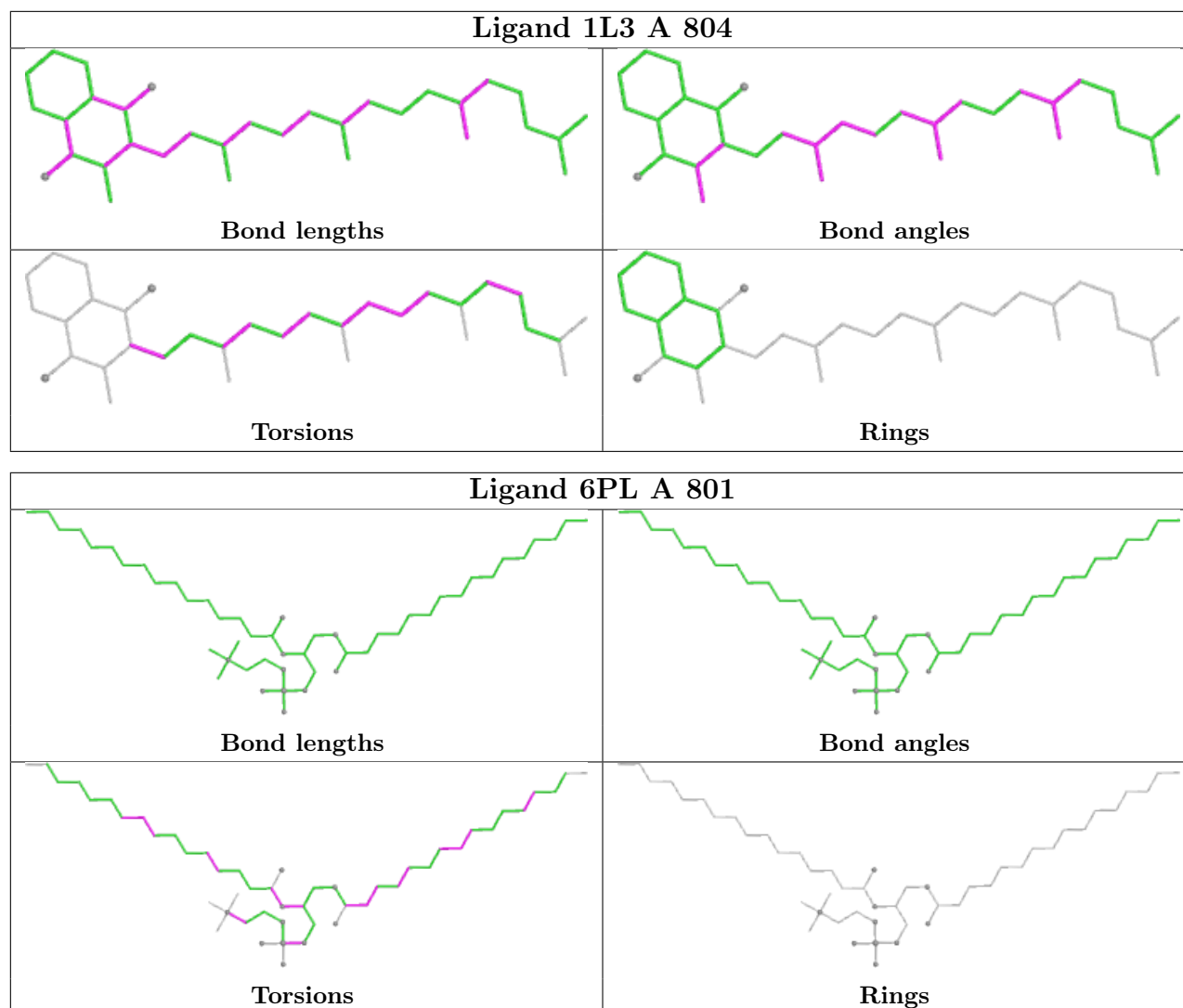
Mol	Chain	Res	Type	Atoms
5	A	802	6PL	O11-C11-O3-C3
7	A	804	1L3	C18-C19-C20-C21
7	A	804	1L3	C04-C03-C14-C15
7	A	804	1L3	C15-C16-C18-C19
7	A	804	1L3	C21-C23-C24-C25
6	A	803	CLR	C22-C23-C24-C25
6	A	803	CLR	C20-C22-C23-C24
5	A	802	6PL	C11-C12-C13-C14
5	A	801	6PL	C32-C31-O2-C2
5	A	801	6PL	O31-C31-O2-C2
6	A	803	CLR	C23-C24-C25-C27
6	A	803	CLR	C23-C24-C25-C26
5	A	802	6PL	O31-C31-O2-C2
5	A	802	6PL	C32-C31-O2-C2
7	A	804	1L3	C02-C03-C14-C15
5	A	801	6PL	C3-C2-O2-C31
5	A	801	6PL	C11-C12-C13-C14
5	A	801	6PL	C38-C39-C40-C41
5	A	801	6PL	C33-C34-C35-C36
5	A	802	6PL	C38-C39-C40-C41
5	A	801	6PL	C21-C22-C23-C24
5	A	801	6PL	C17-C18-C19-C20
5	A	802	6PL	C3-C2-O2-C31
5	A	802	6PL	C4-C5-N-C7
7	A	804	1L3	C23-C24-C25-C26
7	A	804	1L3	C26-C28-C29-C30
5	A	802	6PL	O3P-C1-C2-C3
5	A	802	6PL	C39-C40-C41-C42
7	A	804	1L3	C22-C21-C23-C24
5	A	801	6PL	C4-C5-N-C7
5	A	802	6PL	C4-C5-N-C8
5	A	801	6PL	C37-C38-C39-C40
5	A	801	6PL	C13-C14-C15-C16
5	A	802	6PL	C4-C5-N-C6
5	A	801	6PL	C16-C17-C18-C19
5	A	801	6PL	C1-O3P-P-O1P
5	A	801	6PL	C4-C5-N-C8
5	A	801	6PL	C4-C5-N-C6
5	A	801	6PL	O3-C11-C12-C13

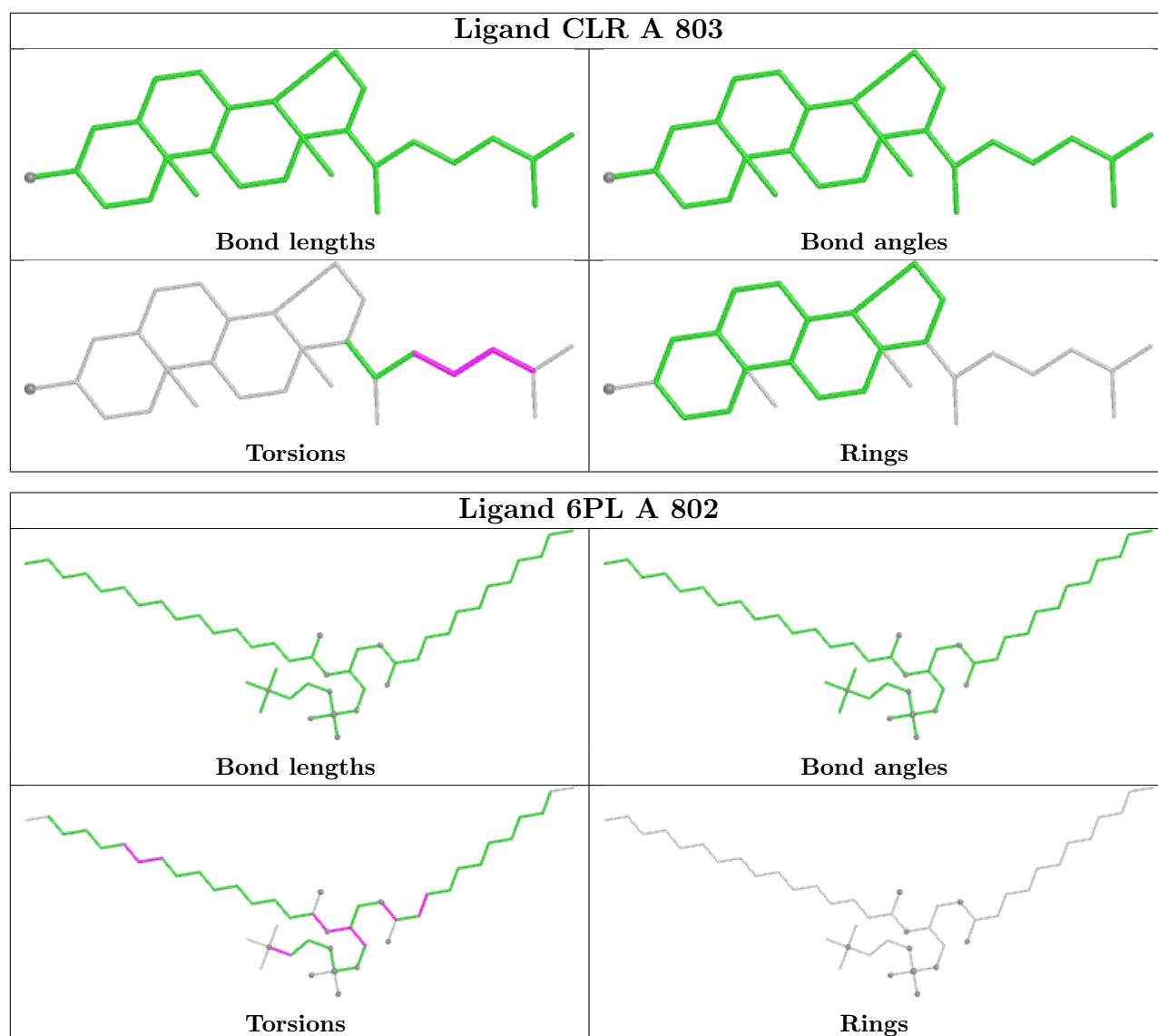
There are no ring outliers.

3 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	804	1L3	22	0
5	A	801	6PL	7	0
5	A	802	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.