



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:44 AM UTC

PDB ID : 1CLE / pdb_00001cle
Title : STRUCTURE OF UNCOMPLEXED AND LINOLEATE-BOUND CANDIDA CYLINDRACEA CHOLESTEROL ESTERASE
Authors : Ghosh, D.
Deposited on : 1995-02-08
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

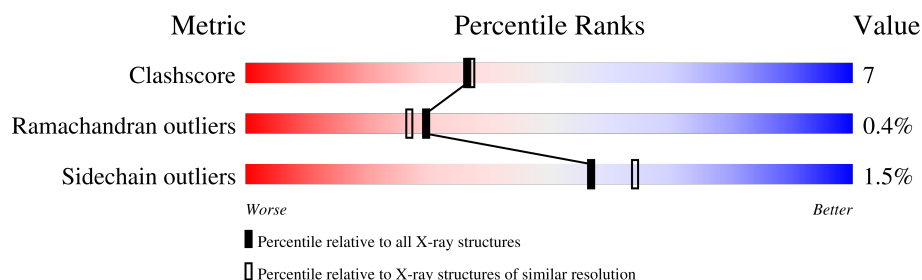
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	534	
1	B	534	
2	C	2	
2	D	2	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8738 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 CHOLESTEROL ESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	0	0	0
			4036	2571	670	775	20			
1	B	534	Total	C	N	O	S	0	0	0
			4036	2571	670	775	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	344	VAL	ILE	conflict	UNP P32947
B	344	VAL	ILE	conflict	UNP P32947

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



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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



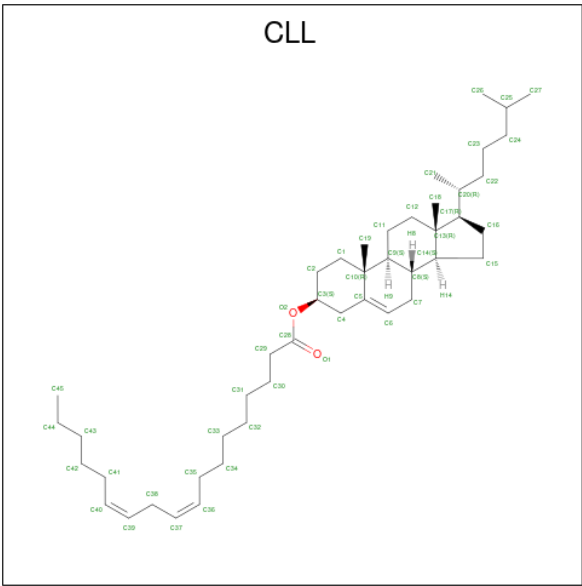
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is CHOLESTERYL LINOLEATE (CCD ID: CLL) (formula: C₄₅H₇₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			47	45	2		
5	B	1	Total	C	O	0	0
			47	45	2		

- Molecule 6 is water.

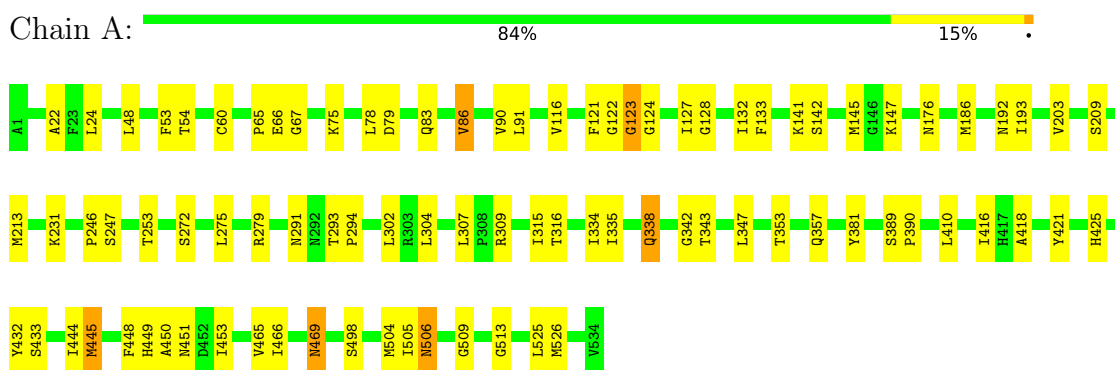
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	241	Total	O	0	0
			241	241		
6	B	237	Total	O	0	0
			237	237		

3 Residue-property plots

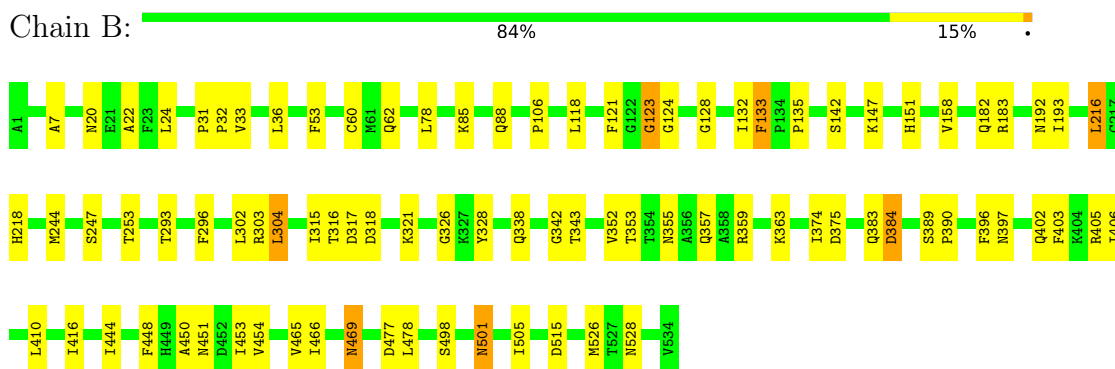
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

Note EDS was not executed.

• Molecule 1: CHOLESTEROL ESTERASE



• Molecule 1: CHOLESTEROL ESTERASE



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



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



MAG1
MAG2

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	58.79Å 90.92Å 58.79Å 93.39° 105.74° 97.22°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.149 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8738	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CLL, PO4

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	0.62	1/4134 (0.0%)	1.05	21/5619 (0.4%)
1	B	0.59	0/4134	1.06	22/5619 (0.4%)
All	All	0.61	1/8268 (0.0%)	1.06	43/11238 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	MET	SD-CE	-7.20	1.61	1.79

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	416	ILE	N-CA-C	10.18	120.19	110.42
1	B	416	ILE	N-CA-C	9.33	119.38	110.42
1	B	498	SER	N-CA-C	8.21	120.31	111.36
1	B	316	THR	N-CA-C	7.65	121.71	112.38
1	A	343	THR	N-CA-C	7.50	119.45	111.28
1	B	193	ILE	N-CA-C	7.26	120.13	111.05
1	A	448	PHE	N-CA-C	7.16	119.80	110.43
1	B	448	PHE	N-CA-C	7.03	119.81	110.53
1	A	193	ILE	N-CA-C	6.81	119.56	111.05
1	B	342	GLY	N-CA-C	6.71	122.98	114.66
1	A	381	TYR	CA-C-N	6.70	126.66	120.03
1	A	381	TYR	C-N-CA	6.70	126.66	120.03
1	A	342	GLY	N-CA-C	6.62	124.00	115.32
1	A	60	CYS	N-CA-C	-6.54	101.89	110.33
1	A	316	THR	N-CA-C	6.37	120.65	113.01
1	B	315	ILE	N-CA-C	-6.23	97.75	106.53
1	A	418	ALA	N-CA-C	-6.02	104.80	111.36
1	B	304	LEU	N-CA-C	5.90	119.01	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	60	CYS	N-CA-C	-5.83	103.24	110.41
1	A	293	THR	N-CA-C	-5.82	102.08	110.40
1	A	304	LEU	N-CA-C	5.80	118.64	110.23
1	A	338	GLN	N-CA-C	-5.78	100.27	109.76
1	B	403	PHE	N-CA-C	5.68	117.93	111.11
1	A	128	GLY	N-CA-C	5.64	117.30	111.95
1	B	343	THR	N-CA-C	5.60	118.11	111.33
1	A	315	ILE	N-CA-C	-5.57	98.67	106.53
1	B	293	THR	N-CA-C	-5.55	103.12	110.40
1	B	133	PHE	CA-C-N	5.53	126.07	120.38
1	B	133	PHE	C-N-CA	5.53	126.07	120.38
1	A	253	THR	N-CA-C	5.46	117.69	111.02
1	B	528	ASN	CA-C-N	5.44	125.52	119.32
1	B	528	ASN	C-N-CA	5.44	125.52	119.32
1	B	526	MET	N-CA-C	5.39	119.55	112.92
1	B	338	GLN	N-CA-C	-5.38	100.94	109.76
1	A	272	SER	N-CA-C	-5.36	105.88	112.90
1	A	247	SER	N-CA-C	5.33	117.93	109.50
1	A	469	ASN	N-CA-C	5.17	117.33	111.02
1	B	451	ASN	N-CA-C	-5.16	105.84	111.82
1	B	303	ARG	N-CA-C	-5.13	99.59	108.52
1	A	192	ASN	N-CA-C	5.10	120.50	113.97
1	A	54	THR	N-CA-C	5.06	119.41	112.88
1	B	253	THR	N-CA-C	5.05	116.47	110.97
1	B	247	SER	N-CA-C	5.00	117.41	109.50

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	4036	0	3935	54	0
1	B	4036	0	3935	63	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	5	0	0	1	0
4	B	5	0	0	1	0
5	A	47	0	75	19	0
5	B	47	0	75	19	0
6	A	241	0	0	1	0
6	B	237	0	0	1	0
All	All	8738	0	8096	118	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 (118) 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:B:123:GLY:HA2	5:B:802:CLL:H41	1.32	1.09
1:A:123:GLY:HA2	5:A:801:CLL:H42	1.44	0.98
1:B:363:LYS:HG2	1:B:374:ILE:HD13	1.56	0.85
1:B:62:GLN:HE22	1:B:128:GLY:H	1.26	0.82
1:A:246:PRO:HG2	5:A:801:CLL:H39	1.64	0.80
1:A:444:ILE:HG22	1:A:445:MET:HE3	1.66	0.76
1:B:469:ASN:H	1:B:469:ASN:HD22	1.32	0.76
1:A:353:THR:H	1:A:357:GLN:NE2	1.85	0.74
1:A:338:GLN:HE21	1:A:451:ASN:HD21	1.35	0.72
1:B:216:LEU:HD22	1:B:244:MET:HA	1.72	0.71
1:B:410:LEU:HD21	5:B:802:CLL:H452	1.74	0.69
1:B:397:ASN:ND2	1:B:444:ILE:H	1.89	0.69
1:B:353:THR:H	1:B:357:GLN:NE2	1.90	0.69
1:B:402:GLN:HE22	1:B:405:ARG:HH11	1.41	0.68
1:B:124:GLY:CA	5:B:802:CLL:H291	2.23	0.67
1:A:209:SER:OG	5:A:801:CLL:H311	1.95	0.66
1:B:132:ILE:HD12	5:B:802:CLL:H151	1.77	0.65
1:A:141:LYS:O	1:A:145:MET:HG2	1.98	0.63
1:A:132:ILE:HD12	5:A:801:CLL:H152	1.81	0.63
1:B:183:ARG:HH11	1:B:218:HIS:HD2	1.47	0.63
1:A:122:GLY:O	5:A:801:CLL:H192	1.99	0.62
1:B:124:GLY:N	5:B:802:CLL:H291	2.15	0.62
1:B:7:ALA:H	1:B:192:ASN:HD22	1.49	0.60
1:B:453:ILE:HG21	5:B:802:CLL:C18	2.31	0.60
1:A:353:THR:H	1:A:357:GLN:HE21	1.47	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:GLN:OE1	1:B:218:HIS:HE1	1.85	0.59
1:A:466:ILE:HG13	1:A:505:ILE:HD11	1.85	0.59
1:A:142:SER:HB2	1:A:147:LYS:O	2.02	0.59
1:A:338:GLN:NE2	1:A:451:ASN:HD21	2.00	0.58
1:B:450:ALA:HB1	5:B:802:CLL:H193	1.84	0.58
1:A:22:ALA:HB2	4:A:601:PO4:O4	2.02	0.58
1:A:133:PHE:HZ	5:A:801:CLL:C19	2.16	0.58
1:B:302:LEU:HB3	5:B:802:CLL:H382	1.85	0.58
1:B:355:ASN:ND2	1:B:405:ARG:HH12	2.03	0.57
1:B:450:ALA:CB	5:B:802:CLL:H193	2.34	0.57
1:A:176:ASN:HD21	1:A:309:ARG:H	1.51	0.57
1:A:65:PRO:HD2	1:A:78:LEU:HD13	1.87	0.56
1:B:85:LYS:HA	1:B:88:GLN:HE21	1.71	0.56
1:A:506:ASN:ND2	1:A:509:GLY:H	2.03	0.55
1:A:410:LEU:HD22	5:A:801:CLL:H421	1.89	0.55
1:B:7:ALA:H	1:B:192:ASN:ND2	2.04	0.55
1:A:421:TYR:O	1:A:425:HIS:HD2	1.90	0.54
1:B:454:VAL:HG22	5:B:802:CLL:H211	1.88	0.54
1:B:302:LEU:O	5:B:802:CLL:H381	2.06	0.54
1:A:66:GLU:HG2	1:A:78:LEU:HD12	1.89	0.54
1:B:183:ARG:HH11	1:B:218:HIS:CD2	2.27	0.54
1:A:275:LEU:O	1:A:279:ARG:HG3	2.08	0.53
1:A:347:LEU:HD11	1:A:445:MET:HE1	1.89	0.53
1:B:389:SER:HA	1:B:390:PRO:C	2.34	0.53
1:A:525:LEU:HB3	1:A:526:MET:HE2	1.90	0.52
1:A:445:MET:HE2	1:A:445:MET:HA	1.92	0.52
1:A:506:ASN:HD22	1:A:509:GLY:H	1.56	0.52
1:A:506:ASN:HD22	1:A:506:ASN:C	2.18	0.51
1:B:469:ASN:HD22	1:B:469:ASN:N	2.06	0.51
1:A:389:SER:HA	1:A:390:PRO:C	2.36	0.51
1:A:453:ILE:HG21	5:A:801:CLL:H183	1.92	0.50
1:B:85:LYS:HD3	1:B:88:GLN:NE2	2.26	0.50
5:A:801:CLL:H212	5:A:801:CLL:H121	1.94	0.50
1:A:121:PHE:HB2	1:A:133:PHE:CE2	2.47	0.50
1:B:410:LEU:CD2	5:B:802:CLL:H452	2.41	0.50
1:A:75:LYS:HE3	1:A:291:ASN:O	2.12	0.50
1:B:465:VAL:O	1:B:469:ASN:HB2	2.12	0.49
1:A:127:ILE:HD11	5:A:801:CLL:H6	1.94	0.49
1:A:133:PHE:HZ	5:A:801:CLL:H193	1.75	0.48
1:B:123:GLY:HA2	5:B:802:CLL:C4	2.22	0.48
1:A:79:ASP:O	1:A:83:GLN:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ASN:ND2	1:B:405:ARG:NH1	2.61	0.48
1:A:246:PRO:CG	5:A:801:CLL:H39	2.39	0.48
1:A:335:ILE:O	1:A:433:SER:HA	2.14	0.48
1:B:501:ASN:HD21	1:B:515:ASP:H	1.61	0.48
1:B:304:LEU:HD11	5:B:802:CLL:H342	1.97	0.47
1:A:66:GLU:CG	1:A:78:LEU:HD12	2.45	0.47
1:A:231:LYS:HE3	6:A:863:HOH:O	2.14	0.47
1:A:133:PHE:CZ	5:A:801:CLL:H193	2.50	0.47
1:A:48:LEU:HD22	1:A:53:PHE:HZ	1.80	0.46
1:A:124:GLY:CA	5:A:801:CLL:H291	2.45	0.46
1:B:359:ARG:O	1:B:363:LYS:HG3	2.16	0.46
1:B:216:LEU:HD22	1:B:244:MET:CA	2.43	0.45
1:B:353:THR:H	1:B:357:GLN:HE22	1.63	0.45
1:A:124:GLY:HA2	5:A:801:CLL:H312	1.99	0.45
1:B:121:PHE:HB2	1:B:133:PHE:CE2	2.51	0.44
1:B:135:PRO:HB3	1:B:151:HIS:CE1	2.52	0.44
1:B:450:ALA:CB	5:B:802:CLL:H11	2.47	0.44
1:B:22:ALA:HB2	4:B:601:PO4:O4	2.17	0.44
1:B:406:ILE:O	1:B:410:LEU:HG	2.17	0.44
1:B:135:PRO:HD2	6:B:900:HOH:O	2.17	0.44
1:B:466:ILE:HG13	1:B:505:ILE:HD11	2.00	0.44
1:B:216:LEU:O	1:B:216:LEU:HG	2.17	0.44
1:A:213:MET:SD	5:A:801:CLL:H341	2.57	0.44
1:B:469:ASN:H	1:B:469:ASN:ND2	2.07	0.44
1:B:317:ASP:OD2	1:B:321:LYS:HD3	2.17	0.43
1:A:353:THR:HG21	1:B:396:PHE:HE2	1.83	0.43
1:A:133:PHE:CE1	5:A:801:CLL:H182	2.54	0.42
1:A:449:HIS:O	1:A:450:ALA:HB3	2.18	0.42
1:B:78:LEU:HD23	1:B:78:LEU:HA	1.77	0.42
1:A:334:ILE:HG12	1:A:432:TYR:HB2	2.01	0.42
1:B:359:ARG:NH1	1:B:375:ASP:OD1	2.53	0.42
1:A:116:VAL:HB	1:A:203:VAL:HG22	2.02	0.42
1:B:326:GLY:HA2	1:B:328:TYR:CE2	2.55	0.42
1:B:142:SER:HB2	1:B:147:LYS:O	2.19	0.42
1:B:296:PHE:CE1	5:B:802:CLL:O1	2.73	0.42
1:B:501:ASN:H	1:B:501:ASN:HD22	1.68	0.42
1:B:450:ALA:HB3	5:B:802:CLL:H11	2.02	0.41
1:B:36:LEU:HD23	1:B:36:LEU:HA	1.89	0.41
1:B:453:ILE:CG2	5:B:802:CLL:C18	2.98	0.41
1:B:477:ASP:O	1:B:478:LEU:HB2	2.20	0.41
1:B:31:PRO:HA	1:B:32:PRO:HD2	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ILE:HD12	5:B:802:CLL:C15	2.46	0.41
1:A:24:LEU:O	1:A:53:PHE:HB3	2.21	0.41
5:A:801:CLL:H331	5:A:801:CLL:H301	1.85	0.41
1:A:302:LEU:HB3	5:A:801:CLL:H381	2.02	0.41
1:A:465:VAL:O	1:A:469:ASN:HB2	2.21	0.41
1:B:20:ASN:HA	1:B:106:PRO:HD3	2.03	0.40
1:A:67:GLY:O	1:A:294:PRO:HA	2.21	0.40
1:A:86:VAL:O	1:A:90:VAL:HG23	2.21	0.40
1:A:504:MET:HE2	1:A:513:GLY:HA3	2.03	0.40
1:B:383:GLN:O	1:B:384:ASP:C	2.64	0.40
1:B:24:LEU:O	1:B:53:PHE:HB3	2.21	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 X-ray entries followed by that with respect to entries of similar resolution.

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	532/534 (100%)	508 (96%)	22 (4%)	2 (0%)	30	27
1	B	532/534 (100%)	509 (96%)	21 (4%)	2 (0%)	30	27
All	All	1064/1068 (100%)	1017 (96%)	43 (4%)	4 (0%)	30	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLY
1	A	498	SER
1	B	123	GLY
1	B	384	ASP

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 X-ray entries followed by that with respect to entries of similar resolution.

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	432/432 (100%)	427 (99%)	5 (1%)	63	70
1	B	432/432 (100%)	424 (98%)	8 (2%)	50	56
All	All	864/864 (100%)	851 (98%)	13 (2%)	57	64

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

Mol	Chain	Res	Type
1	A	86	VAL
1	A	91	LEU
1	A	307	LEU
1	A	445	MET
1	A	506	ASN
1	B	33	VAL
1	B	118	LEU
1	B	158	VAL
1	B	216	LEU
1	B	318	ASP
1	B	352	VAL
1	B	469	ASN
1	B	501	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	137	GLN
1	A	176	ASN
1	A	187	GLN
1	A	338	GLN
1	A	357	GLN
1	A	425	HIS
1	A	438	GLN
1	A	456	GLN

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Mol	Chain	Res	Type
1	A	468	ASN
1	A	506	ASN
1	A	528	ASN
1	B	51	GLN
1	B	62	GLN
1	B	88	GLN
1	B	113	ASN
1	B	192	ASN
1	B	218	HIS
1	B	292	ASN
1	B	355	ASN
1	B	357	GLN
1	B	383	GLN
1	B	397	ASN
1	B	402	GLN
1	B	438	GLN
1	B	451	ASN
1	B	469	ASN
1	B	501	ASN
1	B	528	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 ⓘ

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
2	NAG	C	1	2,1	14,14,15	0.55	0	17,19,21	0.81	1 (5%)
2	NAG	C	2	2	14,14,15	0.42	0	17,19,21	0.64	0
2	NAG	D	1	2,1	14,14,15	0.64	0	17,19,21	0.98	1 (5%)
2	NAG	D	2	2	14,14,15	0.70	0	17,19,21	1.02	1 (5%)

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
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C2-N2-C7	-2.55	119.48	122.90
2	D	1	NAG	O7-C7-C8	-2.52	117.56	122.05
2	C	1	NAG	O7-C7-C8	-2.04	118.43	122.05

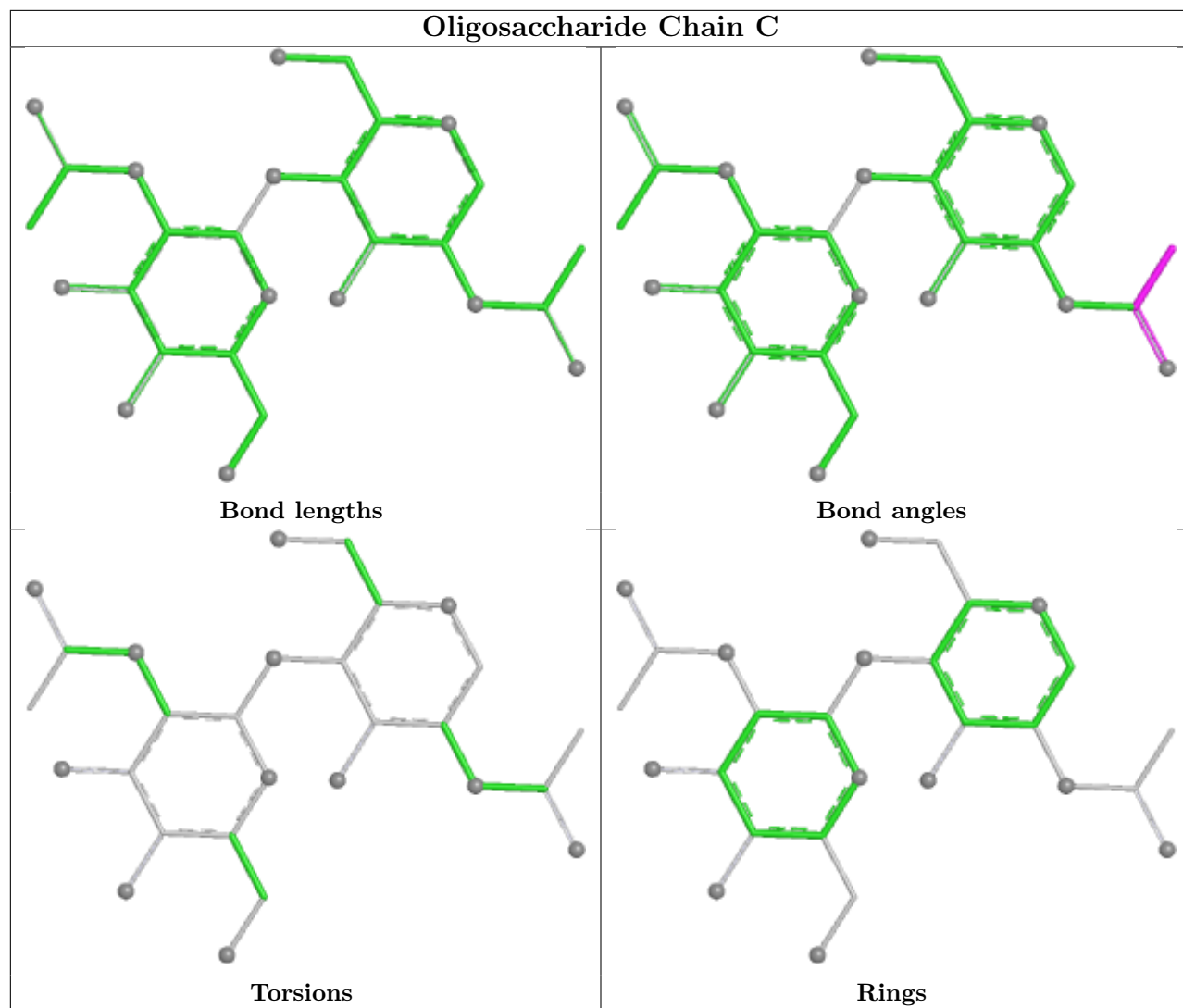
There are no chirality outliers.

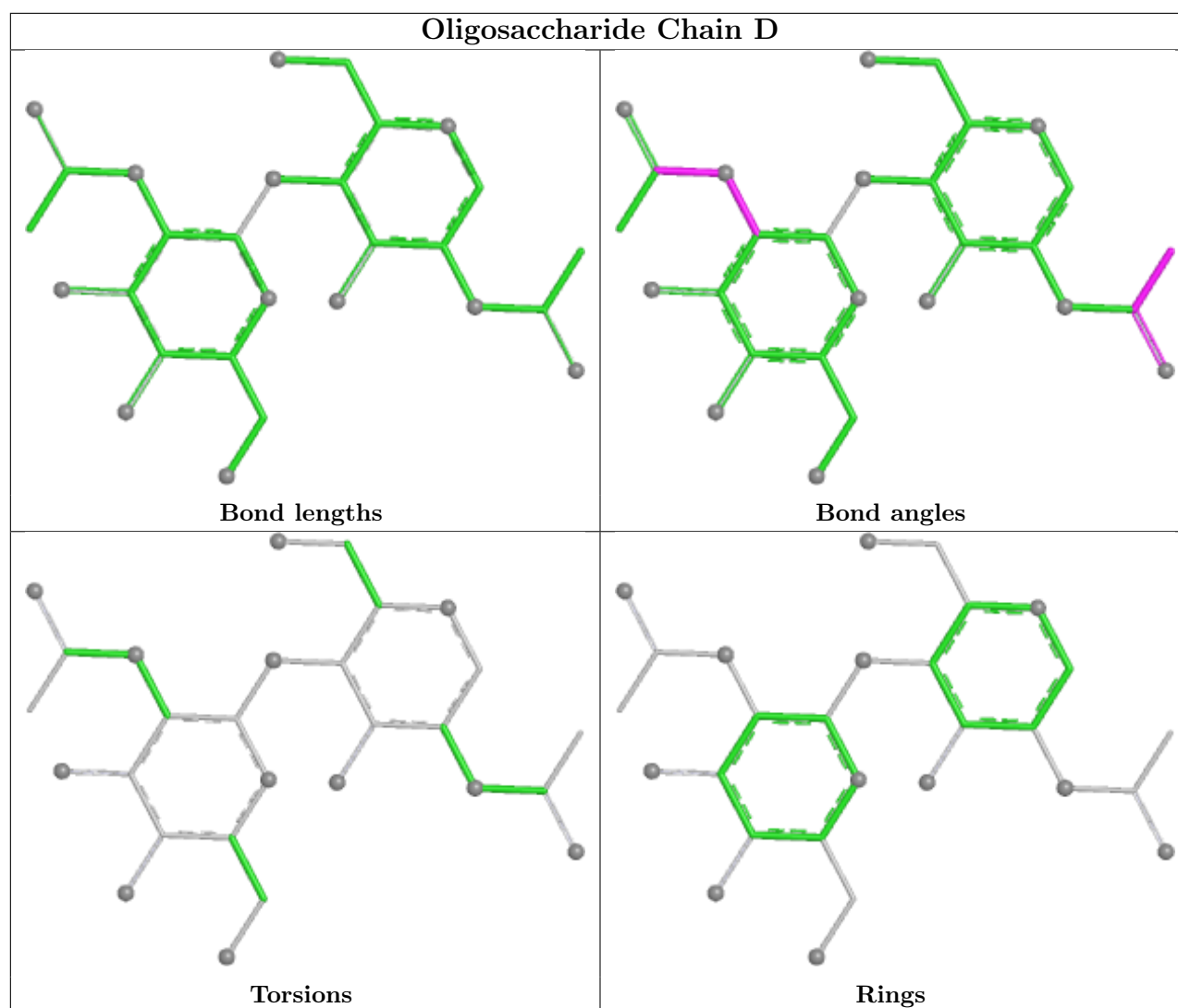
There are no torsion outliers.

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](#)

6 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	$\# Z > 2$
3	NAG	B	535	1	14,14,15	0.76	0	17,19,21	0.85	0
5	CLL	B	802	-	50,50,50	3.30	20 (40%)	68,68,68	3.06	24 (35%)
3	NAG	A	535	1	14,14,15	0.55	0	17,19,21	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PO4	B	601	-	4,4,4	0.93	0	6,6,6	0.51	0
5	CLL	A	801	-	50,50,50	3.17	19 (38%)	68,68,68	3.15	24 (35%)
4	PO4	A	601	-	4,4,4	1.02	0	6,6,6	0.53	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
5	CLL	B	802	-	-	9/31/89/89	0/4/4/4
3	NAG	A	535	1	-	0/6/23/26	0/1/1/1
5	CLL	A	801	-	-	11/31/89/89	0/4/4/4
3	NAG	B	535	1	-	0/6/23/26	0/1/1/1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	802	CLL	O2-C28	-14.66	0.92	1.34
5	A	801	CLL	O2-C28	-14.09	0.94	1.34
5	B	802	CLL	C1-C10	7.66	1.68	1.54
5	A	801	CLL	C10-C9	-7.45	1.44	1.56
5	B	802	CLL	C10-C9	-7.37	1.44	1.56
5	A	801	CLL	C1-C10	6.82	1.66	1.54
5	A	801	CLL	C6-C5	-5.43	1.21	1.33
5	B	802	CLL	C6-C5	-5.28	1.22	1.33
5	B	802	CLL	C19-C10	5.26	1.63	1.54
5	B	802	CLL	C11-C9	5.11	1.62	1.53
5	A	801	CLL	C11-C9	4.27	1.60	1.53
5	A	801	CLL	C10-C5	4.01	1.60	1.52
5	B	802	CLL	C10-C5	3.74	1.60	1.52
5	A	801	CLL	C19-C10	3.56	1.60	1.54
5	B	802	CLL	O2-C3	-3.55	1.38	1.46
5	A	801	CLL	C8-C14	3.54	1.60	1.53
5	A	801	CLL	C1-C2	-3.43	1.46	1.53
5	A	801	CLL	C8-C9	3.33	1.59	1.53
5	B	802	CLL	C1-C2	-3.27	1.46	1.53
5	A	801	CLL	C4-C5	3.24	1.58	1.51
5	A	801	CLL	C29-C28	2.95	1.59	1.50
5	B	802	CLL	C40-C39	2.95	1.48	1.31
5	A	801	CLL	O2-C3	-2.90	1.39	1.46
5	B	802	CLL	C8-C9	2.89	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	802	CLL	C8-C14	2.87	1.59	1.53
5	B	802	CLL	C2-C3	-2.68	1.44	1.51
5	A	801	CLL	C40-C39	2.68	1.46	1.31
5	A	801	CLL	C37-C36	2.64	1.46	1.31
5	B	802	CLL	C37-C36	2.62	1.46	1.31
5	A	801	CLL	C2-C3	-2.56	1.44	1.51
5	B	802	CLL	C16-C15	-2.55	1.47	1.54
5	B	802	CLL	C12-C13	-2.45	1.49	1.54
5	B	802	CLL	C4-C5	2.43	1.56	1.51
5	A	801	CLL	C12-C11	2.38	1.58	1.53
5	A	801	CLL	C16-C15	-2.28	1.47	1.54
5	A	801	CLL	C18-C13	2.27	1.58	1.54
5	B	802	CLL	C20-C17	-2.25	1.50	1.54
5	B	802	CLL	C15-C14	-2.09	1.50	1.54
5	B	802	CLL	C4-C3	2.03	1.56	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	801	CLL	C3-O2-C28	13.18	149.34	117.80
5	B	802	CLL	C3-O2-C28	12.71	148.21	117.80
5	B	802	CLL	O2-C28-C29	11.37	136.07	111.48
5	A	801	CLL	O2-C28-C29	11.32	135.97	111.48
5	B	802	CLL	C15-C16-C17	6.85	118.55	105.14
5	A	801	CLL	C15-C16-C17	6.68	118.22	105.14
5	A	801	CLL	C16-C17-C13	-6.60	96.08	103.84
5	B	802	CLL	C16-C17-C13	-5.82	97.00	103.84
5	B	802	CLL	C4-C5-C10	-5.51	109.37	116.42
5	A	801	CLL	C11-C9-C10	5.49	119.85	113.08
5	B	802	CLL	C16-C15-C14	-5.29	94.79	105.14
5	A	801	CLL	C16-C15-C14	-4.75	95.84	105.14
5	A	801	CLL	C16-C17-C20	4.68	119.25	112.18
5	A	801	CLL	O2-C28-O1	-4.62	112.90	123.70
5	B	802	CLL	O2-C28-O1	-4.51	113.15	123.70
5	A	801	CLL	C14-C8-C9	4.38	114.81	109.09
5	B	802	CLL	C14-C8-C9	4.26	114.65	109.09
5	B	802	CLL	C16-C17-C20	4.17	118.49	112.18
5	A	801	CLL	C1-C10-C5	3.89	115.44	108.74
5	B	802	CLL	C11-C9-C10	3.78	117.75	113.08
5	A	801	CLL	C9-C10-C5	-3.62	104.36	109.65
5	B	802	CLL	O1-C28-C29	-3.33	110.78	123.78
5	A	801	CLL	C12-C13-C17	-3.32	111.71	116.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	802	CLL	C10-C5-C6	3.30	127.75	122.93
5	A	801	CLL	O1-C28-C29	-3.24	111.10	123.78
5	B	802	CLL	C12-C13-C17	-3.22	111.85	116.60
5	A	801	CLL	C3-C4-C5	2.83	115.64	111.45
5	A	801	CLL	C8-C7-C6	2.82	116.66	112.76
5	B	802	CLL	C21-C20-C22	2.70	114.52	110.34
5	A	801	CLL	C15-C14-C13	2.65	106.96	103.84
5	A	801	CLL	C21-C20-C22	2.62	114.39	110.34
5	A	801	CLL	C1-C2-C3	2.60	114.58	110.33
5	B	802	CLL	C15-C14-C13	2.59	106.89	103.84
5	A	801	CLL	C23-C22-C20	2.57	122.26	115.08
5	A	801	CLL	C30-C29-C28	2.57	123.10	113.69
5	B	802	CLL	C23-C22-C20	2.43	121.87	115.08
5	B	802	CLL	C2-C3-C4	2.37	114.26	110.97
5	A	801	CLL	C2-C3-C4	2.29	114.16	110.97
5	B	802	CLL	C30-C29-C28	2.22	121.82	113.69
5	B	802	CLL	C1-C2-C3	2.19	113.91	110.33
5	A	801	CLL	C15-C14-C8	2.18	122.58	119.10
5	B	802	CLL	C1-C10-C9	-2.18	105.85	108.74
5	B	802	CLL	C8-C7-C6	2.16	115.75	112.76
5	B	802	CLL	C7-C6-C5	-2.16	121.38	125.02
5	B	802	CLL	C15-C14-C8	2.09	122.43	119.10
5	A	801	CLL	C18-C13-C12	2.08	113.67	110.61
5	B	802	CLL	C1-C10-C5	2.06	112.29	108.74
5	A	801	CLL	C11-C9-C8	-2.02	108.96	111.78

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	801	CLL	C36-C37-C38-C39
5	A	801	CLL	C30-C31-C32-C33
5	B	802	CLL	C28-C29-C30-C31
5	A	801	CLL	C20-C22-C23-C24
5	B	802	CLL	C29-C30-C31-C32
5	A	801	CLL	C41-C42-C43-C44
5	A	801	CLL	C28-C29-C30-C31
5	B	802	CLL	C32-C33-C34-C35
5	A	801	CLL	C29-C30-C31-C32
5	B	802	CLL	C41-C42-C43-C44
5	B	802	CLL	C30-C31-C32-C33
5	B	802	CLL	C20-C22-C23-C24

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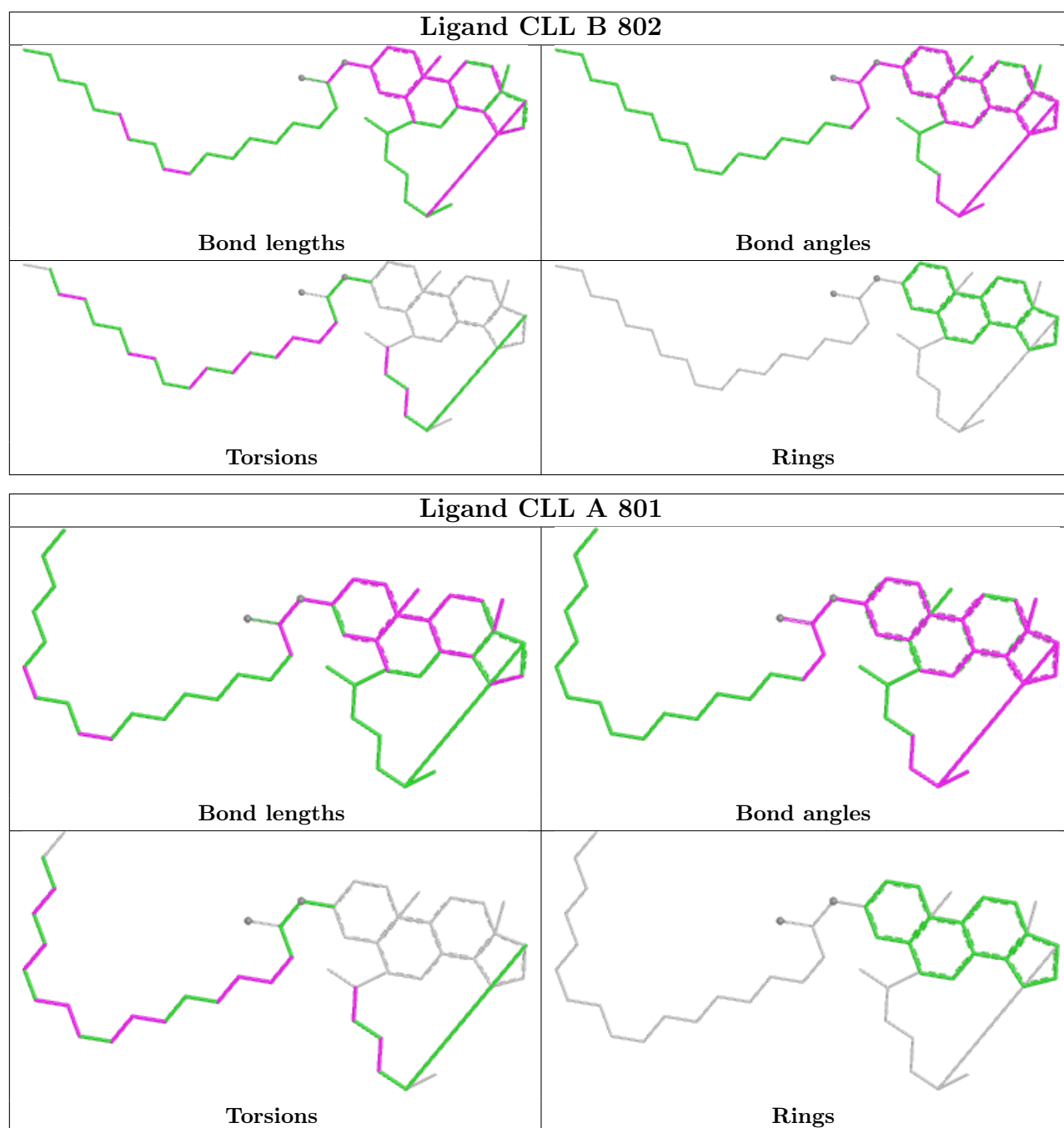
Mol	Chain	Res	Type	Atoms
5	A	801	CLL	C23-C24-C25-C26
5	B	802	CLL	C23-C24-C25-C26
5	A	801	CLL	C34-C35-C36-C37
5	A	801	CLL	C37-C38-C39-C40
5	B	802	CLL	C37-C38-C39-C40
5	B	802	CLL	C34-C35-C36-C37
5	A	801	CLL	C39-C40-C41-C42
5	A	801	CLL	C33-C34-C35-C36

There are no ring outliers.

4 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	802	CLL	19	0
4	B	601	PO4	1	0
5	A	801	CLL	19	0
4	A	601	PO4	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 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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.