



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 11:37 PM EDT

PDB ID : 1LLF / pdb_00001llf
Title : Cholesterol Esterase (Candida Cyldracea) Crystal Structure at 1.4A resolution
Authors : Pletnev, V.; Addlagatta, A.; Wawrzak, Z.; Duax, W.
Deposited on : 2002-04-28
Resolution : 1.40 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

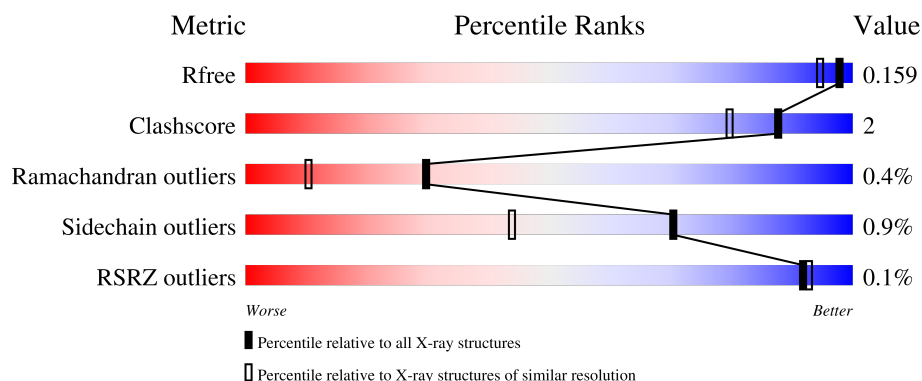
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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))
R_{free}	180053	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	534	93% 7%
1	B	534	91% 7% .
2	C	2	100%
2	D	2	100%
2	E	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	2	 100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17493 atoms, of which 8136 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 Lipase 3.

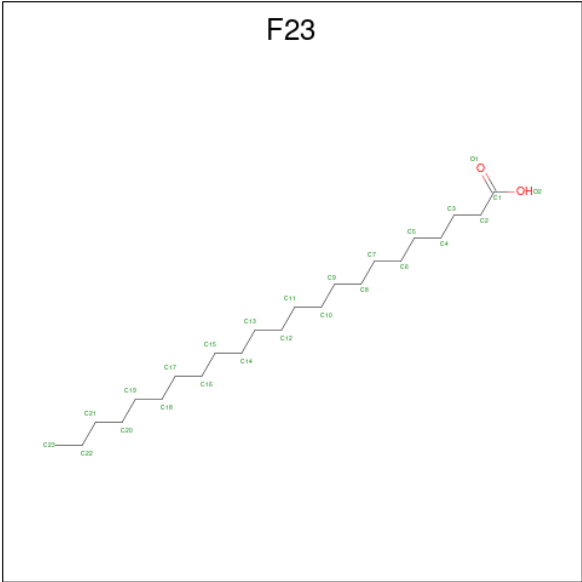
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	534	Total	C	H	N	O	S	0	6	0
			8020	2583	3965	673	778	21			
1	B	534	Total	C	H	N	O	S	0	8	0
			8043	2589	3981	674	778	21			

- 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	H	N	O	0	0	0
			55	16	27	2	10			
2	D	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
2	E	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
2	F	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			

- Molecule 3 is TRICOSANOIC ACID (CCD ID: F23) (formula: C₂₃H₄₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			66	23	41	2		
3	B	1	Total	C	H	O	0	0
			66	23	41	2		

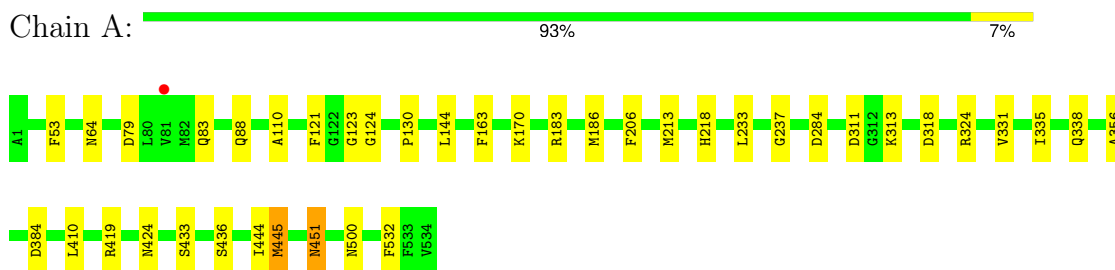
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	540	Total	O	0	0
			540	540		
4	B	538	Total	O	0	0
			538	538		

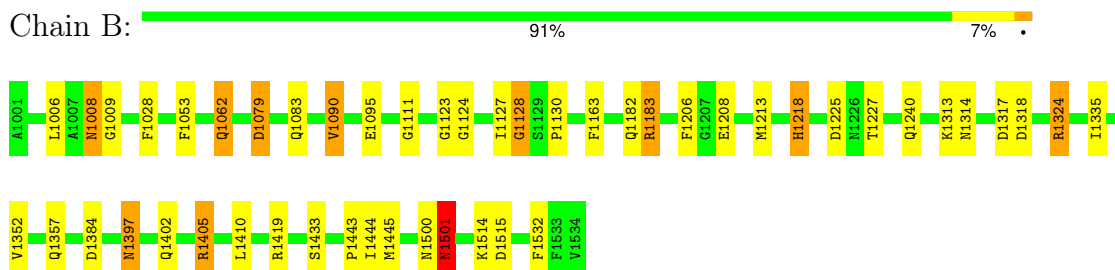
3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Lipase 3



- Molecule 1: Lipase 3



- 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



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

Chain E:  100%

MAG1
MAG2

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

Chain F:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	58.46Å 58.48Å 89.52Å 92.71° 97.48° 109.38°	Depositor
Resolution (Å)	30.00 – 1.40 30.00 – 1.40	Depositor EDS
% Data completeness (in resolution range)	90.2 (30.00-1.40) 94.3 (30.00-1.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.37 (at 1.40Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.136 , 0.169 0.128 , 0.159	Depositor DCC
R_{free} test set	10364 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	12.0	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17493	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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, F23

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	0.65	0/4179	1.27	27/5678 (0.5%)
1	B	0.70	2/4195 (0.0%)	1.35	46/5699 (0.8%)
All	All	0.67	2/8374 (0.0%)	1.31	73/11377 (0.6%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1218	HIS	CD2-NE2	-7.88	1.29	1.37
1	B	1128	GLY	N-CA	-5.84	1.39	1.45

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	500	ASN	OD1-CG-ND2	-11.72	110.88	122.60
1	B	1062	GLN	OE1-CD-NE2	10.65	133.25	122.60
1	A	206	PHE	CA-CB-CG	9.30	123.10	113.80
1	B	1218	HIS	CG-CD2-NE2	9.09	116.29	107.20
1	B	1127	ILE	CA-C-N	8.94	137.27	122.43
1	B	1127	ILE	C-N-CA	8.94	137.27	122.43
1	B	1130	PRO	CA-C-N	8.78	132.41	120.38
1	B	1130	PRO	C-N-CA	8.78	132.41	120.38
1	B	1206	PHE	CA-CB-CG	8.64	122.44	113.80
1	B	1062	GLN	CG-CD-NE2	-8.35	103.88	116.40
1	B	1183	ARG	NH1-CZ-NH2	-7.74	109.24	119.30
1	B	1352	VAL	O-C-N	-7.50	113.85	122.62
1	B	1127	ILE	O-C-N	-7.43	114.88	122.75
1	A	318	ASP	CA-CB-CG	7.18	119.78	112.60
1	A	130	PRO	CA-C-N	7.17	129.89	120.28
1	A	130	PRO	C-N-CA	7.17	129.89	120.28
1	B	1318	ASP	CA-CB-CG	7.04	119.64	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1218	HIS	CE1-NE2-CD2	-6.92	102.08	109.00
1	A	331	VAL	O-C-N	6.77	125.96	121.69
1	B	1514	LYS	CA-C-N	6.73	134.72	122.27
1	B	1514	LYS	C-N-CA	6.73	134.72	122.27
1	B	1357	GLN	OE1-CD-NE2	-6.72	115.88	122.60
1	B	1006	LEU	CA-C-N	6.58	129.09	120.28
1	B	1006	LEU	C-N-CA	6.58	129.09	120.28
1	B	1419	ARG	CG-CD-NE	-6.54	97.62	112.00
1	A	183	ARG	NE-CZ-NH2	6.52	125.07	119.20
1	A	424	ASN	OD1-CG-ND2	6.48	129.08	122.60
1	A	284	ASP	CA-C-N	6.36	128.71	120.44
1	A	284	ASP	C-N-CA	6.36	128.71	120.44
1	B	1405	ARG	NH1-CZ-NH2	-6.30	111.10	119.30
1	A	64	ASN	CA-CB-CG	6.18	118.78	112.60
1	B	1501	ASN	CA-CB-CG	6.13	118.73	112.60
1	A	110	ALA	CA-C-N	-6.03	114.06	122.86
1	A	110	ALA	C-N-CA	-6.03	114.06	122.86
1	A	284	ASP	O-C-N	-5.92	115.85	122.12
1	B	1008	ASN	CA-CB-CG	5.81	118.41	112.60
1	A	53	PHE	CA-CB-CG	-5.74	108.06	113.80
1	A	451	ASN	OD1-CG-ND2	5.71	128.31	122.60
1	A	500	ASN	CB-CG-ND2	5.67	124.91	116.40
1	B	1079	ASP	CA-CB-CG	-5.62	106.98	112.60
1	B	1130	PRO	O-C-N	-5.60	115.00	122.22
1	B	1357	GLN	CB-CG-CD	5.58	122.09	112.60
1	B	1111	GLY	CA-C-O	5.57	125.18	119.10
1	B	1183	ARG	NE-CZ-NH2	5.57	124.21	119.20
1	B	1009	GLY	CA-C-N	5.55	128.65	120.82
1	B	1009	GLY	C-N-CA	5.55	128.65	120.82
1	B	1405	ARG	NE-CZ-NH2	5.55	124.19	119.20
1	A	532	PHE	CA-CB-CG	-5.46	108.34	113.80
1	A	419	ARG	CG-CD-NE	-5.45	100.01	112.00
1	B	1163	PHE	CA-CB-CG	-5.40	108.40	113.80
1	B	1514	LYS	O-C-N	-5.36	116.23	123.19
1	A	237	GLY	CA-C-O	-5.25	116.74	121.47
1	B	1053	PHE	CA-CB-CG	-5.20	108.60	113.80
1	B	1324[A]	ARG	NE-CZ-NH2	5.17	123.86	119.20
1	B	1324[B]	ARG	NE-CZ-NH2	5.17	123.86	119.20
1	B	1532	PHE	CA-CB-CG	-5.12	108.68	113.80
1	A	218	HIS	ND1-CE1-NE2	-5.12	103.28	108.40
1	B	1095	GLU	CA-C-N	5.11	130.43	122.26
1	B	1095	GLU	C-N-CA	5.11	130.43	122.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1397	ASN	OD1-CG-ND2	5.11	127.71	122.60
1	A	88	GLN	OE1-CD-NE2	-5.10	117.50	122.60
1	B	1443	PRO	CA-C-N	5.10	131.15	121.97
1	B	1443	PRO	C-N-CA	5.10	131.15	121.97
1	A	356	ALA	CA-C-N	5.08	127.50	120.29
1	A	356	ALA	C-N-CA	5.08	127.50	120.29
1	B	1500	ASN	OD1-CG-ND2	-5.07	117.53	122.60
1	B	1218	HIS	CA-CB-CG	-5.07	108.73	113.80
1	B	1028	PHE	CA-CB-CG	5.07	118.86	113.80
1	A	183	ARG	NH1-CZ-NH2	-5.05	112.73	119.30
1	A	121	PHE	CA-CB-CG	5.04	118.84	113.80
1	A	163	PHE	CA-CB-CG	-5.02	108.78	113.80
1	B	1183	ARG	NE-CZ-NH1	5.01	126.51	121.50
1	B	1317	ASP	CA-CB-CG	5.00	117.60	112.60

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	4055	3965	3955	13	0
1	B	4062	3981	3966	17	0
2	C	28	27	25	0	0
2	D	28	27	25	0	0
2	E	28	27	25	0	0
2	F	28	27	25	0	0
3	A	25	41	45	5	0
3	B	25	41	45	4	0
4	A	540	0	0	3	0
4	B	538	0	0	4	0
All	All	9357	8136	8111	32	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 2.

All (32) 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:1313[B]:LYS:HE2	4:B:2431:HOH:O	1.93	0.68
1:B:1313[B]:LYS:HE3	1:B:1314:ASN:OD1	1.98	0.62
1:A:144:LEU:HD11	4:A:2851:HOH:O	2.06	0.55
1:B:1182:GLN:OE1	1:B:1218:HIS:HE1	1.90	0.54
1:A:170:LYS:HE3	1:A:311:ASP:O	2.06	0.54
1:A:444:ILE:HG22	1:A:445[A]:MET:HE3	1.89	0.54
1:B:1124:GLY:HA2	3:B:1800:F23:H8B	1.91	0.52
1:B:1397:ASN:ND2	1:B:1444:ILE:H	2.09	0.51
1:A:124:GLY:HA2	3:A:800:F23:H8B	1.93	0.50
1:A:213:MET:HE1	3:A:800:F23:H112	1.93	0.49
1:B:1335:ILE:O	1:B:1433:SER:HA	2.13	0.48
1:A:79:ASP:O	1:A:83:GLN:HG2	2.14	0.47
3:A:800:F23:H5B	4:A:2148:HOH:O	2.14	0.47
1:B:1062:GLN:HE22	1:B:1128:GLY:H	1.63	0.46
1:A:313:LYS:HG3	4:A:3045:HOH:O	2.16	0.45
1:B:1324[B]:ARG:NH1	4:B:2903:HOH:O	2.49	0.45
1:B:1225:ASP:OD1	1:B:1227:THR:HG23	2.16	0.45
1:B:1402:GLN:HE22	1:B:1405:ARG:HH11	1.64	0.45
1:A:335:ILE:O	1:A:433:SER:HA	2.17	0.44
1:B:1410:LEU:HD21	3:B:1800:F23:H222	1.99	0.44
3:B:1800:F23:H5B	4:B:2113:HOH:O	2.17	0.43
1:B:1208:GLU:HA	1:B:1240:GLN:O	2.19	0.43
1:A:213:MET:SD	3:A:800:F23:H101	2.59	0.42
1:B:1183:ARG:HH11	1:B:1218:HIS:HD2	1.66	0.42
1:A:410:LEU:HD21	3:A:800:F23:H222	2.02	0.42
1:B:1213:MET:SD	3:B:1800:F23:H101	2.60	0.42
1:B:1313[B]:LYS:NZ	4:B:3091:HOH:O	2.50	0.42
1:A:338:GLN:HE21	1:A:451:ASN:HD21	1.67	0.41
1:B:1501:ASN:HD21	1:B:1515:ASP:H	1.69	0.41
1:A:338:GLN:NE2	1:A:436:SER:HB3	2.37	0.40
1:A:186:MET:HE2	1:A:233:LEU:HD13	2.03	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 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	538/534 (101%)	516 (96%)	20 (4%)	2 (0%)	30	10
1	B	540/534 (101%)	517 (96%)	21 (4%)	2 (0%)	30	10
All	All	1078/1068 (101%)	1033 (96%)	41 (4%)	4 (0%)	30	10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	384	ASP
1	B	1384	ASP
1	A	123	GLY
1	B	1123	GLY

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	438/432 (101%)	434 (99%)	4 (1%)	70	44
1	B	440/432 (102%)	432 (98%)	8 (2%)	51	20
All	All	878/864 (102%)	866 (99%)	12 (1%)	70	28

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	324[A]	ARG
1	A	324[B]	ARG
1	A	445[A]	MET
1	A	445[B]	MET
1	B	1008	ASN
1	B	1079	ASP
1	B	1083	GLN
1	B	1090[A]	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1090[B]	VAL
1	B	1445[A]	MET
1	B	1445[B]	MET
1	B	1501	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	240	GLN
1	A	338	GLN
1	A	339	ASN
1	A	425	HIS
1	A	438	GLN
1	A	456	GLN
1	A	488	ASN
1	B	1008	ASN
1	B	1051	GLN
1	B	1062	GLN
1	B	1063	GLN
1	B	1192	ASN
1	B	1218	HIS
1	B	1240	GLN
1	B	1355	ASN
1	B	1357	GLN
1	B	1383	GLN
1	B	1397	ASN
1	B	1402	GLN
1	B	1438	GLN
1	B	1451	ASN
1	B	1456	GLN
1	B	1488	ASN
1	B	1501	ASN
1	B	1528	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 ⓘ

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	$\# Z > 2$
2	NAG	C	1	1,2	14,14,15	0.61	0	17,19,21	1.02	1 (5%)
2	NAG	C	2	2	14,14,15	0.61	0	17,19,21	1.27	2 (11%)
2	NAG	D	1	1,2	14,14,15	0.50	0	17,19,21	1.49	2 (11%)
2	NAG	D	2	2	14,14,15	0.80	0	17,19,21	1.10	1 (5%)
2	NAG	E	1	1,2	14,14,15	0.55	0	17,19,21	0.98	2 (11%)
2	NAG	E	2	2	14,14,15	0.76	0	17,19,21	1.11	2 (11%)
2	NAG	F	1	1,2	14,14,15	0.61	0	17,19,21	0.87	0
2	NAG	F	2	2	14,14,15	0.81	0	17,19,21	0.91	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
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C2-N2-C7	-3.65	118.01	122.90
2	D	1	NAG	C1-C2-N2	-3.03	105.66	110.43
2	E	2	NAG	C1-O5-C5	-2.90	108.30	112.19
2	C	2	NAG	C2-N2-C7	-2.60	119.41	122.90
2	E	2	NAG	C3-C4-C5	-2.43	105.83	110.23
2	E	1	NAG	C2-N2-C7	-2.36	119.73	122.90
2	E	1	NAG	C1-O5-C5	-2.22	109.20	112.19
2	D	2	NAG	O5-C5-C6	-2.22	103.34	107.66
2	C	1	NAG	O4-C4-C5	-2.17	103.99	109.32
2	C	2	NAG	C1-O5-C5	-2.15	109.31	112.19

There are no chirality outliers.

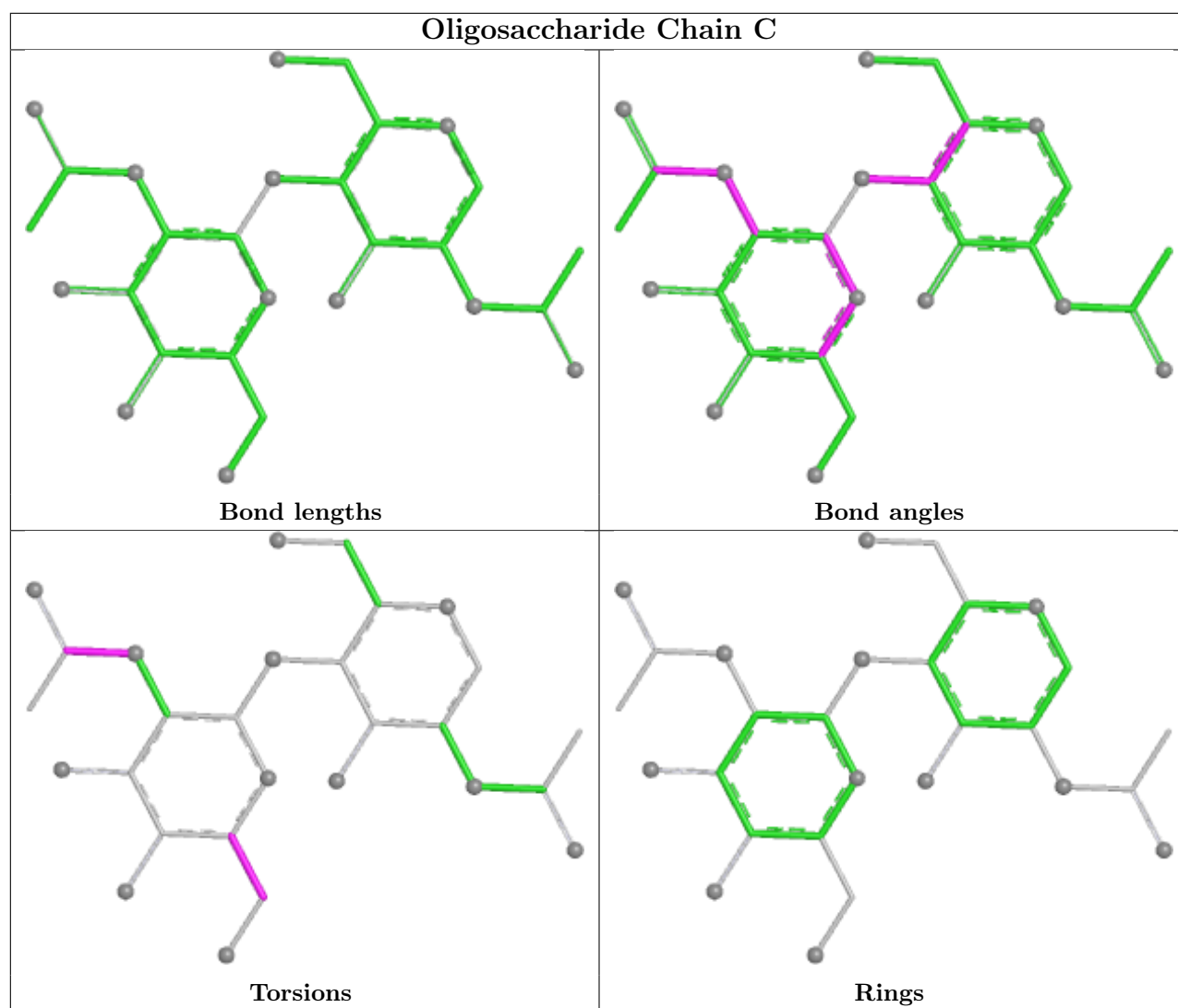
All (5) torsion outliers are listed below:

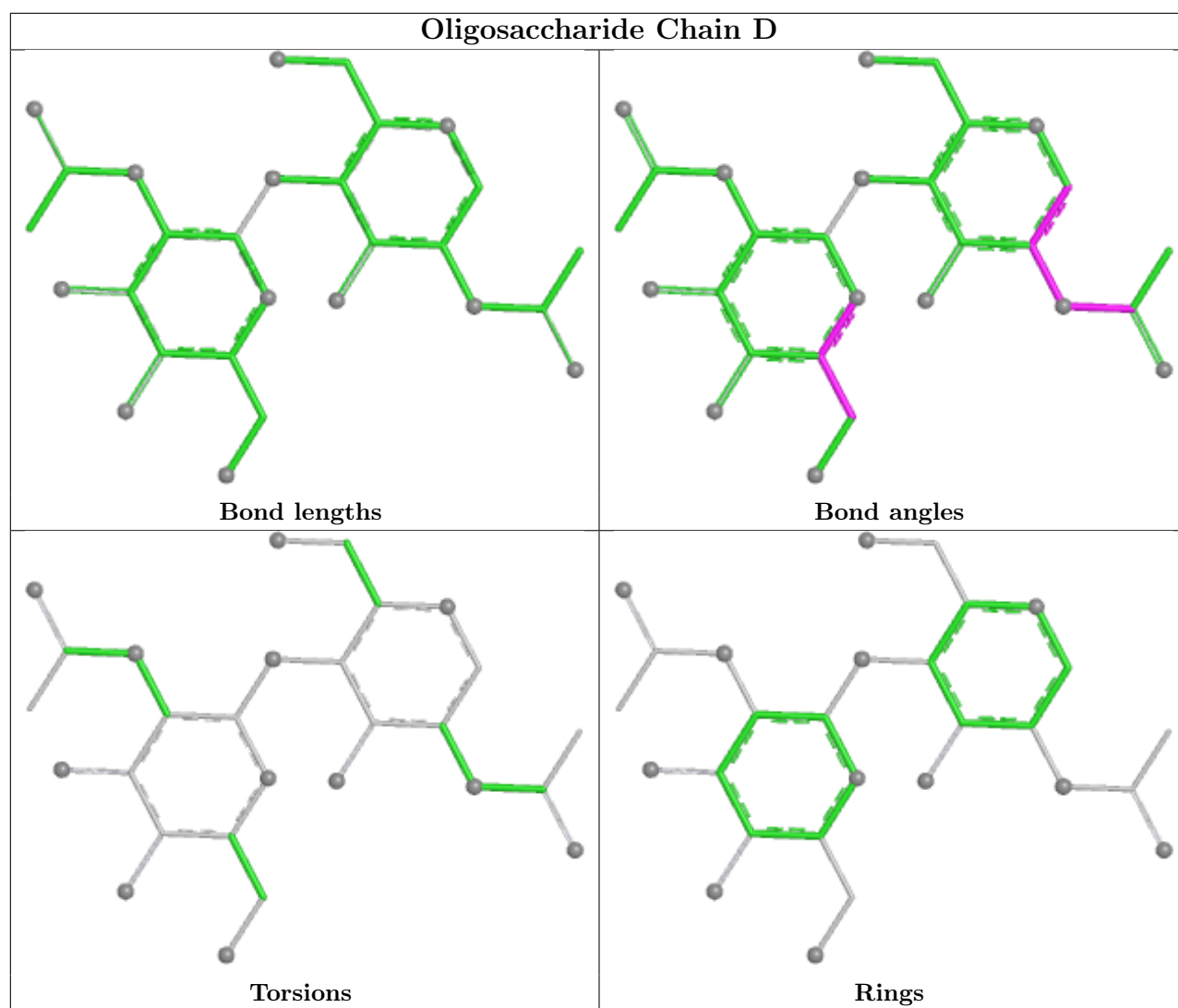
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O7-C7-N2-C2

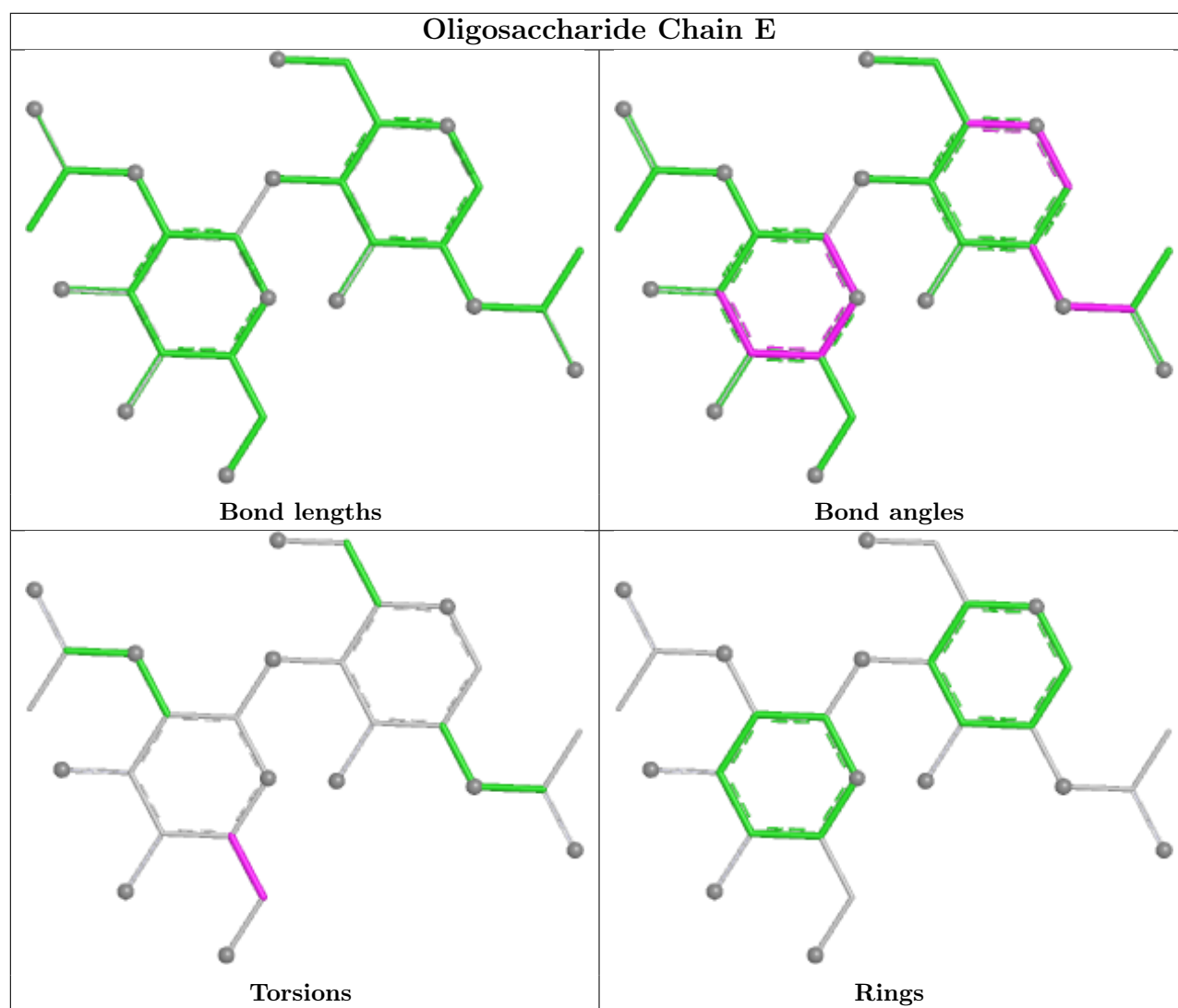
There are no ring outliers.

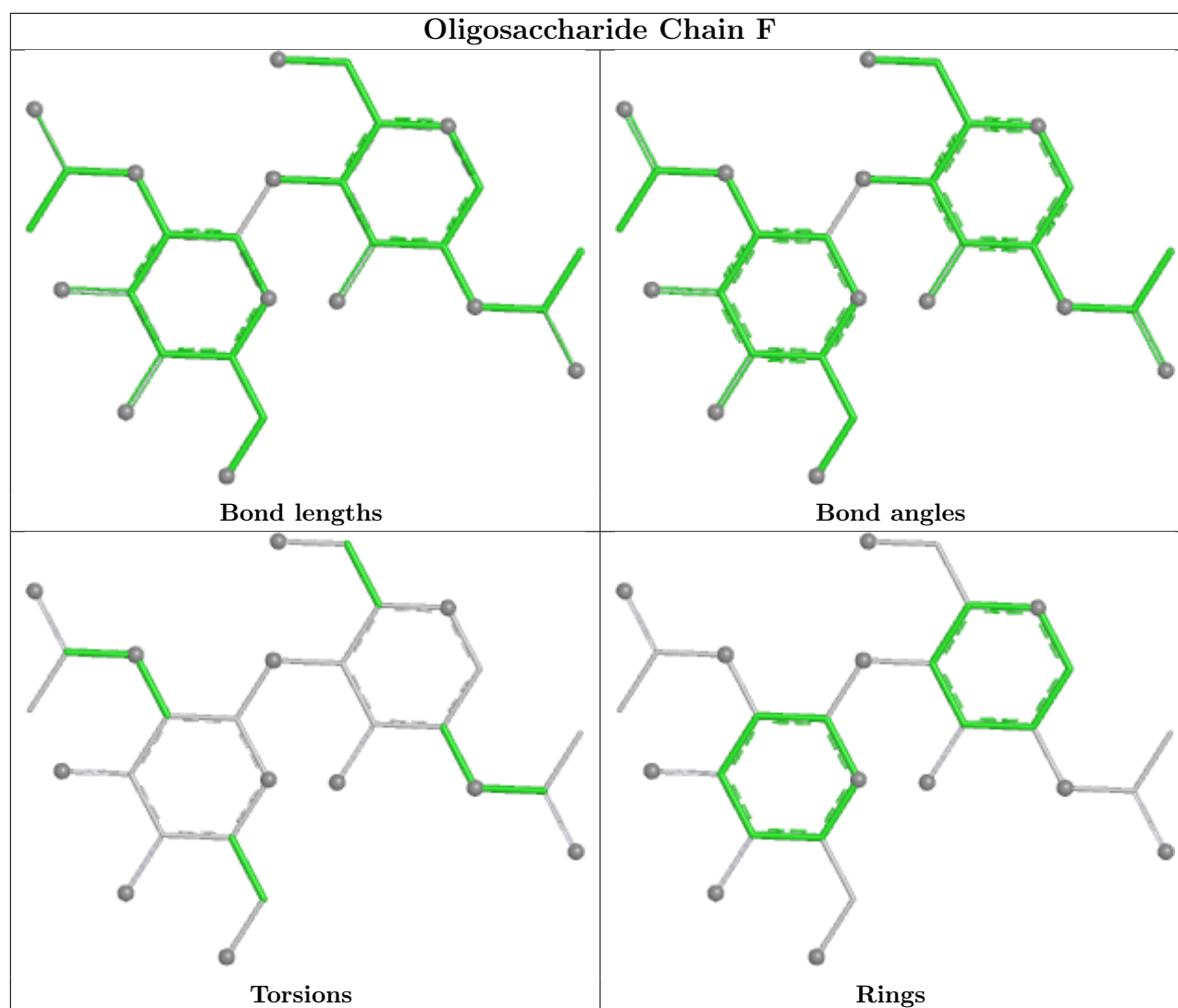
No monomer is involved in short contacts.

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](#)

2 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	F23	B	1800	-	24,24,24	1.24	2 (8%)	24,24,24	0.92	2 (8%)
3	F23	A	800	-	24,24,24	1.18	2 (8%)	24,24,24	0.93	1 (4%)

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	F23	B	1800	-	-	9/22/22/22	-
3	F23	A	800	-	-	9/22/22/22	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1800	F23	O2-C1	-4.17	1.17	1.30
3	A	800	F23	O2-C1	-4.03	1.17	1.30
3	B	1800	F23	C2-C1	-3.18	1.43	1.50
3	A	800	F23	C2-C1	-2.81	1.44	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800	F23	C9-C8-C7	2.60	127.50	114.37
3	B	1800	F23	C11-C10-C9	-2.05	104.01	114.37
3	B	1800	F23	C9-C8-C7	2.04	124.68	114.37

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	800	F23	C7-C8-C9-C10
3	B	1800	F23	C7-C8-C9-C10
3	B	1800	F23	C2-C3-C4-C5
3	B	1800	F23	C5-C6-C7-C8
3	A	800	F23	C2-C3-C4-C5
3	A	800	F23	C5-C6-C7-C8
3	A	800	F23	C11-C10-C9-C8
3	B	1800	F23	O2-C1-C2-C3
3	A	800	F23	O1-C1-C2-C3
3	B	1800	F23	O1-C1-C2-C3
3	A	800	F23	O2-C1-C2-C3
3	B	1800	F23	C11-C10-C9-C8
3	A	800	F23	C1-C2-C3-C4
3	B	1800	F23	C16-C17-C18-C19
3	B	1800	F23	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

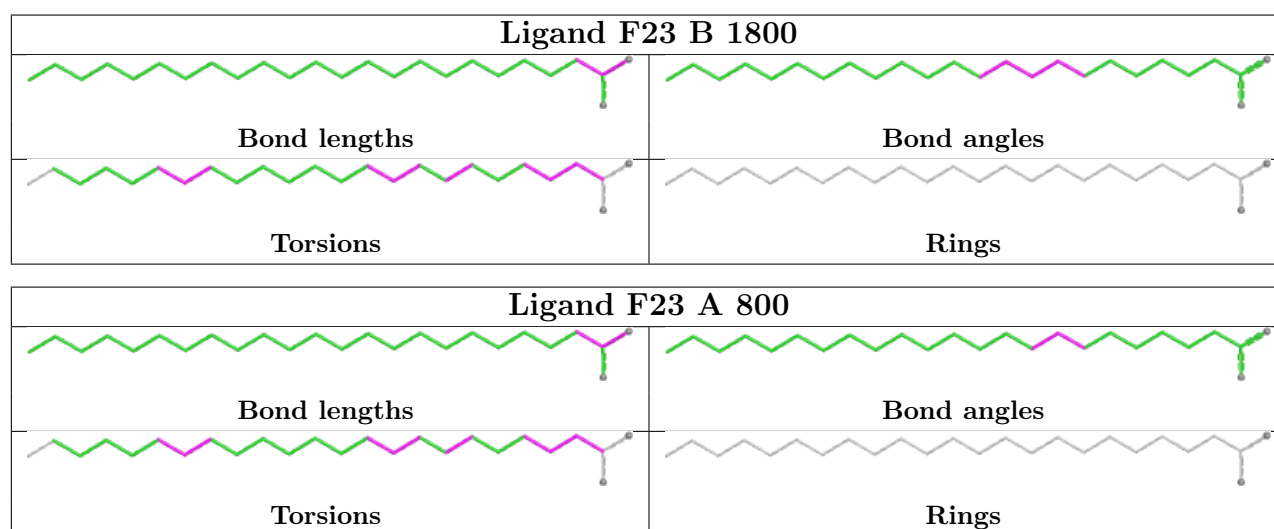
Mol	Chain	Res	Type	Atoms
3	A	800	F23	C15-C16-C17-C18
3	A	800	F23	C16-C17-C18-C19
3	B	1800	F23	C1-C2-C3-C4

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1800	F23	4	0
3	A	800	F23	5	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.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	534/534 (100%)	-0.69	1 (0%) 91 93	10, 14, 30, 57	6 (1%)
1	B	534/534 (100%)	-0.65	0 100 100	10, 15, 29, 56	8 (1%)
All	All	1068/1068 (100%)	-0.67	1 (0%) 92 93	10, 14, 29, 57	14 (1%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	81	VAL	2.1

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

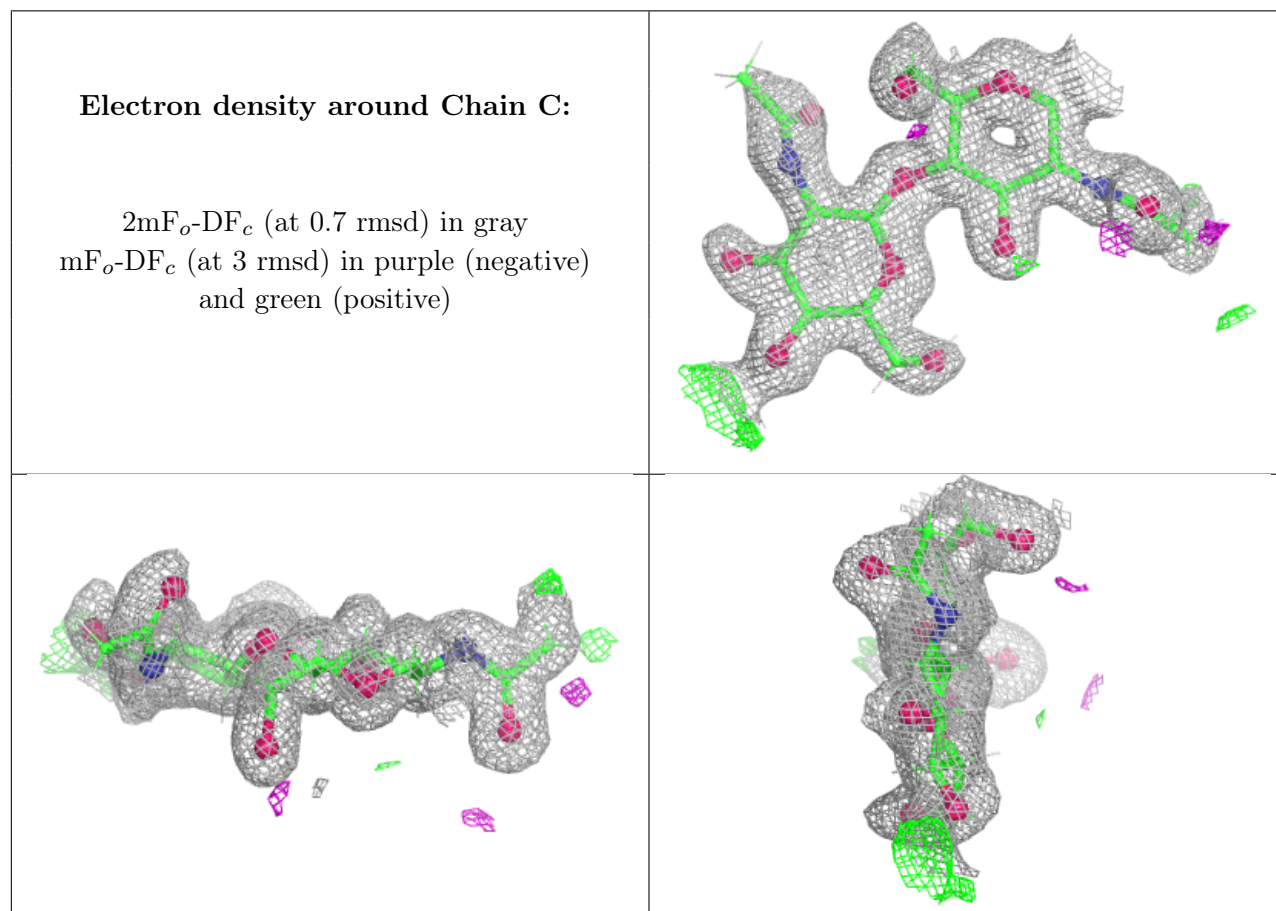
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

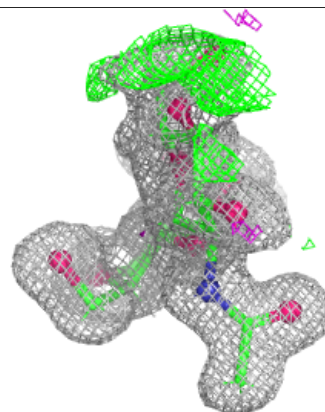
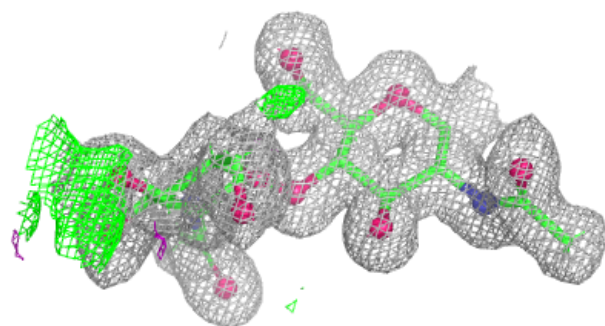
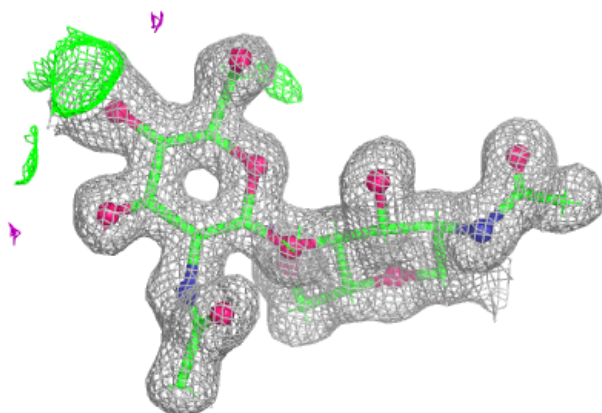
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	E	2	14/15	0.86	0.11	38,52,74,97	0
2	NAG	C	2	14/15	0.88	0.12	29,44,66,92	0
2	NAG	F	2	14/15	0.95	0.06	16,23,33,50	0
2	NAG	E	1	14/15	0.96	0.07	19,26,43,43	0
2	NAG	C	1	14/15	0.96	0.07	15,22,38,39	0
2	NAG	D	2	14/15	0.96	0.07	14,24,40,60	0
2	NAG	F	1	14/15	0.98	0.04	13,18,33,33	0
2	NAG	D	1	14/15	0.98	0.04	12,17,32,32	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

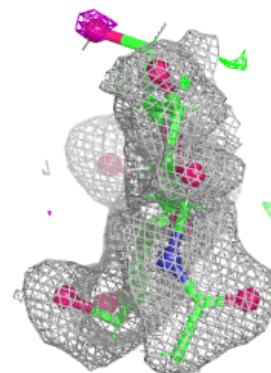
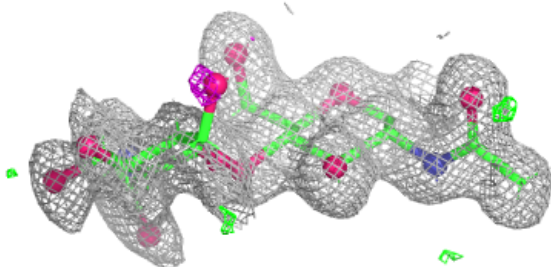
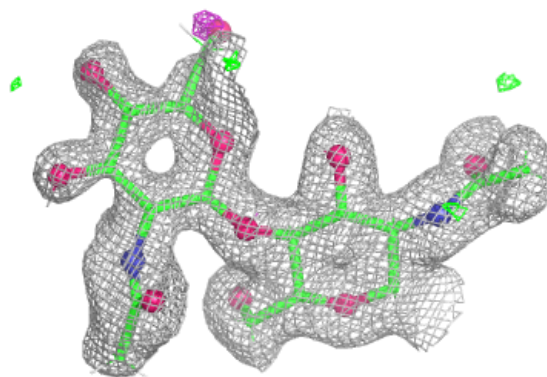


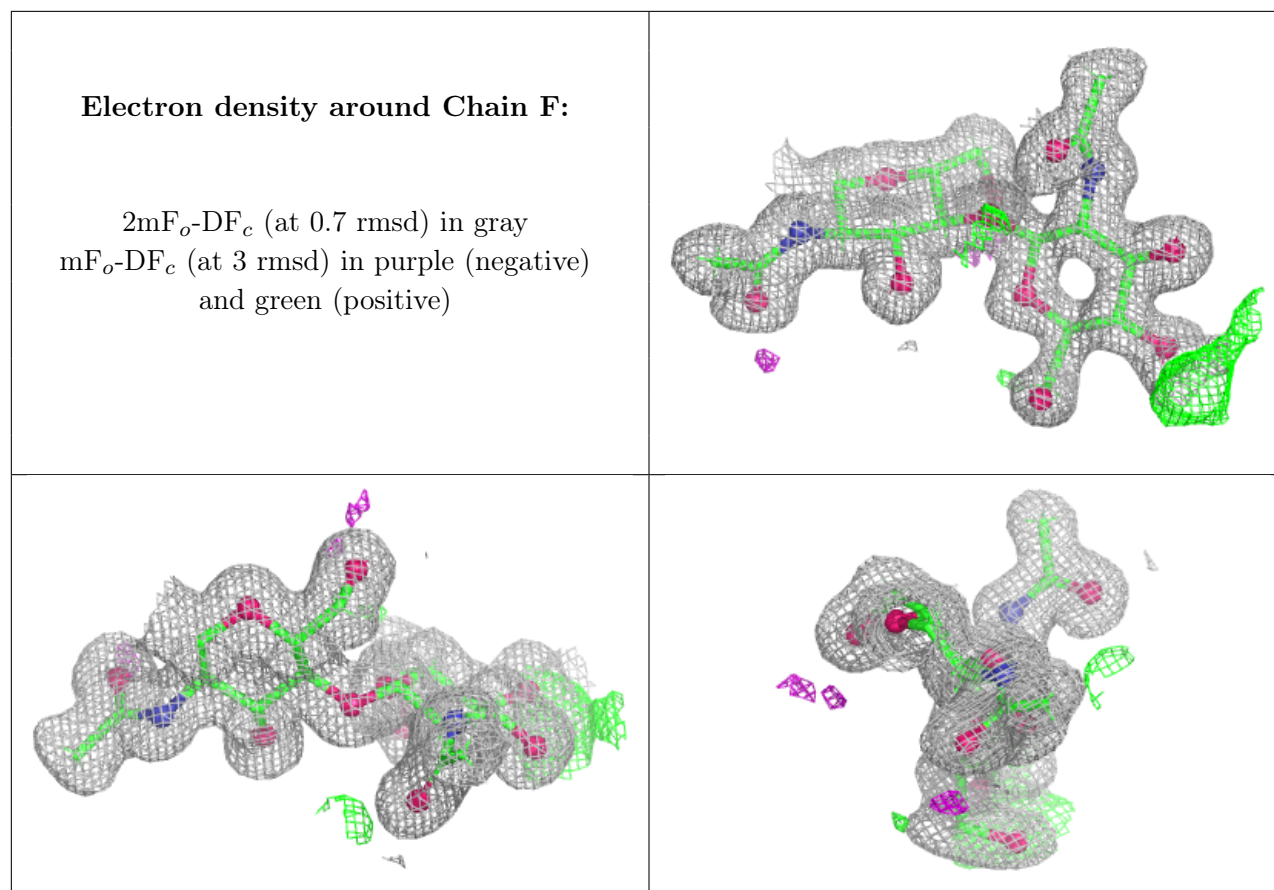
Electron density around Chain D:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain E:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

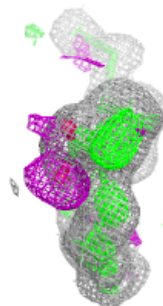
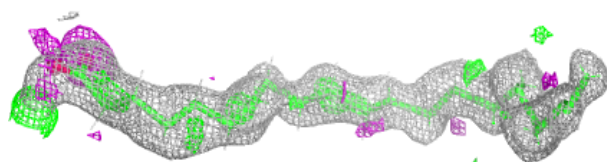
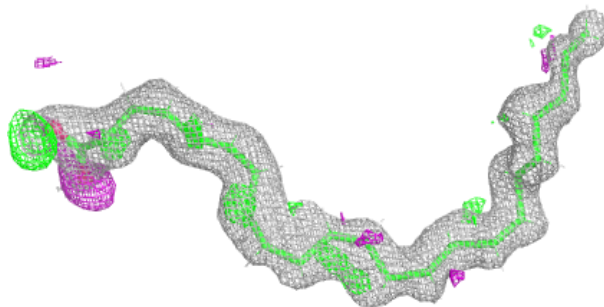
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	F23	B	1800	25/25	0.86	0.14	16,24,33,45	0
3	F23	A	800	25/25	0.90	0.12	16,24,35,40	0

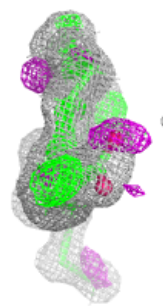
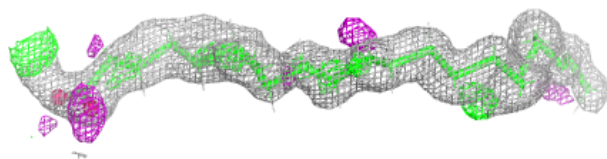
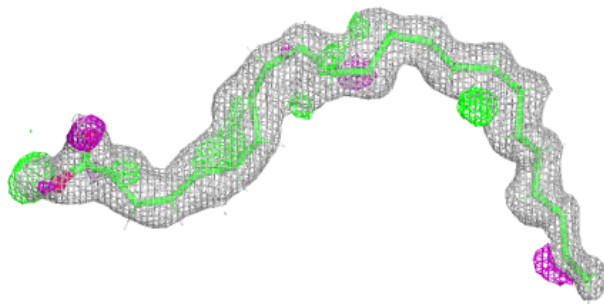
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around F23 B 1800:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around F23 A 800:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.