



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:30 AM UTC

PDB ID : 1CRL / pdb_00001crl
Title : INSIGHTS INTO INTERFACIAL ACTIVATION FROM AN 'OPEN'
STRUCTURE OF CANDIDA RUGOSA LIPASE
Authors : Grochulski, P.; Cygler, M.
Deposited on : 1993-03-02
Resolution : 2.06 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
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

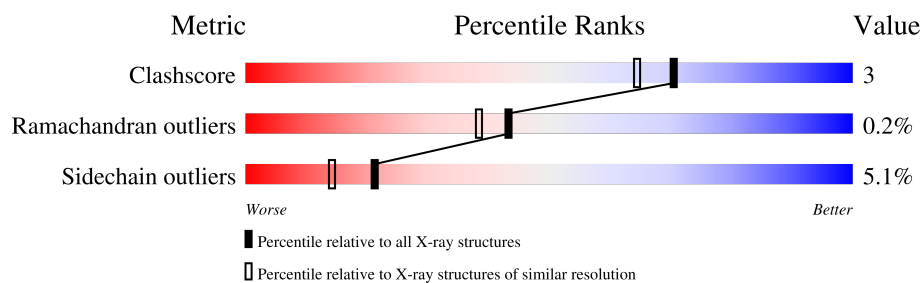
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)

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	
2	B	2	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4374 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 LIPASE.

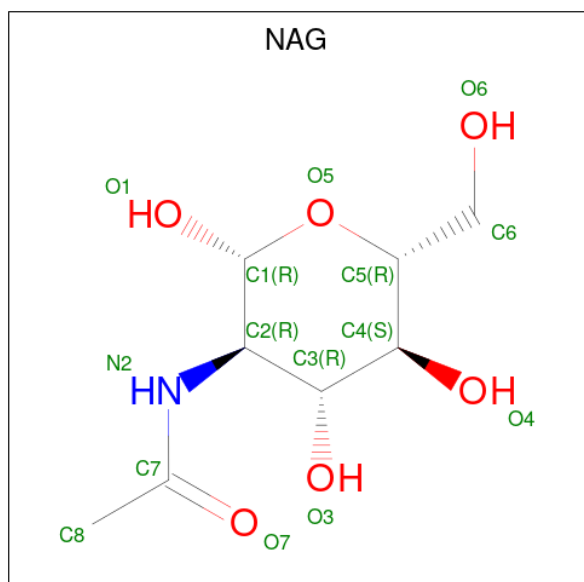
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	0	0	0
			4022	2556	659	788	19			

- 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	B	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: $C_8H_{15}NO_6$).



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

- Molecule 4 is water.

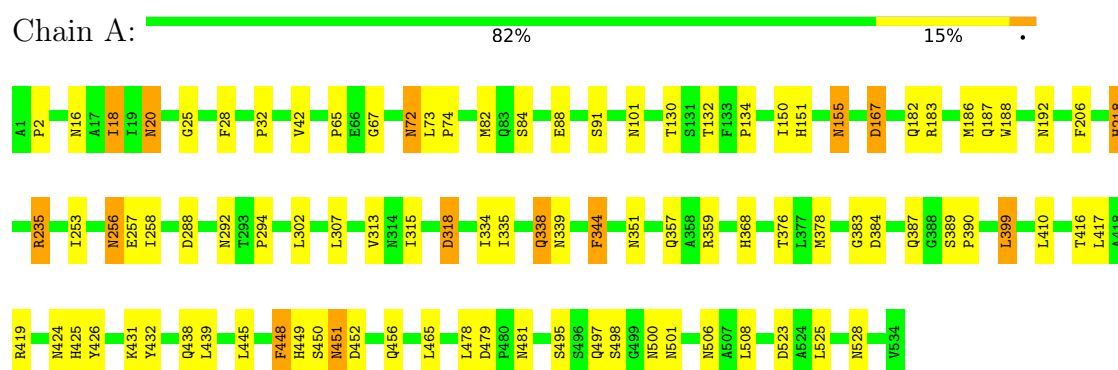
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	310	Total	O	0	0
			310	310		

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: LIPASE



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



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	64.90Å 97.50Å 175.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.06	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.06)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.134 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4374	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

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	0.90	5/4118 (0.1%)	1.69	57/5601 (1.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	368	HIS	CD2-NE2	-7.26	1.29	1.37
1	A	218	HIS	CD2-NE2	-5.99	1.31	1.37
1	A	151	HIS	CD2-NE2	-5.97	1.31	1.37
1	A	425	HIS	CD2-NE2	-5.53	1.31	1.37
1	A	449	HIS	CD2-NE2	-5.03	1.32	1.37

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	ASP	CA-CB-CG	11.70	124.30	112.60
1	A	344	PHE	CA-CB-CG	-10.12	103.68	113.80
1	A	182	GLN	OE1-CD-NE2	-9.29	113.31	122.60
1	A	384	ASP	CA-CB-CG	9.27	121.87	112.60
1	A	72	ASN	CA-CB-CG	9.09	121.69	112.60
1	A	206	PHE	CA-CB-CG	8.99	122.79	113.80
1	A	452	ASP	CA-CB-CG	8.48	121.08	112.60
1	A	456	GLN	OE1-CD-NE2	-8.06	114.54	122.60
1	A	292	ASN	OD1-CG-ND2	-7.98	114.62	122.60
1	A	72	ASN	OD1-CG-ND2	-7.53	115.07	122.60
1	A	187	GLN	OE1-CD-NE2	-7.29	115.31	122.60
1	A	351	ASN	CA-CB-CG	7.21	119.81	112.60
1	A	20	ASN	CA-CB-CG	7.19	119.79	112.60
1	A	338	GLN	N-CA-C	-7.14	98.67	110.17
1	A	167	ASP	N-CA-C	6.96	118.87	111.28
1	A	528	ASN	CA-CB-CG	-6.78	105.83	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	523	ASP	CA-CB-CG	-6.66	105.94	112.60
1	A	155	ASN	OD1-CG-ND2	-6.59	116.01	122.60
1	A	450	SER	CA-CB-OG	6.33	123.77	111.10
1	A	307	LEU	CA-C-N	6.25	126.62	119.93
1	A	307	LEU	C-N-CA	6.25	126.62	119.93
1	A	479	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	72	ASN	CB-CG-ND2	6.13	125.60	116.40
1	A	438	GLN	OE1-CD-NE2	-6.13	116.47	122.60
1	A	368	HIS	CB-CG-CD2	-6.11	123.26	131.20
1	A	417	LEU	N-CA-C	-6.09	106.01	113.50
1	A	32	PRO	CA-C-O	6.07	125.80	121.31
1	A	151	HIS	CB-CG-CD2	-5.94	123.48	131.20
1	A	500	ASN	OD1-CG-ND2	-5.90	116.70	122.60
1	A	416	THR	N-CA-C	5.84	117.73	111.36
1	A	357	GLN	OE1-CD-NE2	-5.78	116.82	122.60
1	A	315	ILE	N-CA-C	-5.77	97.55	106.72
1	A	20	ASN	OD1-CG-ND2	-5.76	116.84	122.60
1	A	501	ASN	CA-CB-CG	5.75	118.34	112.60
1	A	448	PHE	N-CA-C	5.69	118.23	110.55
1	A	188	TRP	CG-CD2-CE3	5.68	139.58	133.90
1	A	506	ASN	CA-CB-CG	5.65	118.25	112.60
1	A	187	GLN	CG-CD-NE2	5.60	124.80	116.40
1	A	16	ASN	OD1-CG-ND2	-5.60	117.00	122.60
1	A	500	ASN	CB-CG-ND2	5.56	124.74	116.40
1	A	256	ASN	CA-CB-CG	-5.54	107.06	112.60
1	A	481	ASN	OD1-CG-ND2	-5.51	117.09	122.60
1	A	42	VAL	N-CA-C	-5.46	101.94	107.89
1	A	155	ASN	CA-CB-CG	5.45	118.05	112.60
1	A	497	GLN	OE1-CD-NE2	-5.44	117.16	122.60
1	A	188	TRP	CB-CG-CD1	-5.43	118.75	126.90
1	A	451	ASN	OD1-CG-ND2	-5.39	117.21	122.60
1	A	451	ASN	CA-CB-CG	5.36	117.95	112.60
1	A	218	HIS	CA-CB-CG	-5.29	108.50	113.80
1	A	257	GLU	CB-CA-C	-5.26	102.63	110.88
1	A	134	PRO	CA-C-N	5.20	125.66	120.04
1	A	134	PRO	C-N-CA	5.20	125.66	120.04
1	A	218	HIS	CB-CG-CD2	-5.17	124.48	131.20
1	A	339	ASN	CB-CG-ND2	5.11	124.07	116.40
1	A	192	ASN	OD1-CG-ND2	-5.07	117.53	122.60
1	A	399	LEU	N-CA-C	-5.03	105.79	111.28
1	A	28	PHE	CA-CB-CG	5.01	118.81	113.80

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	4022	0	3893	26	0
2	B	28	0	25	1	0
3	A	14	0	13	0	0
4	A	310	0	0	4	0
All	All	4374	0	3931	27	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 3.

All (27) 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:65:PRO:HD2	1:A:82:MET:HE1	1.61	0.83
1:A:338:GLN:HE21	1:A:451:ASN:HD21	1.32	0.75
1:A:424:ASN:HD21	1:A:495:SER:H	1.41	0.68
1:A:338:GLN:NE2	1:A:451:ASN:HD21	2.00	0.60
1:A:426:TYR:HD2	1:A:431:LYS:HD2	1.69	0.56
1:A:183:ARG:HH11	1:A:218:HIS:HD1	1.51	0.56
1:A:335:ILE:HG12	1:A:419:ARG:HG3	1.88	0.55
1:A:383:GLY:HA3	4:A:836:HOH:O	2.07	0.54
1:A:84:SER:O	1:A:88:GLU:HG2	2.08	0.54
1:A:167:ASP:H	1:A:256:ASN:HD21	1.58	0.50
1:A:235:ARG:HD3	1:A:478:LEU:HD21	1.94	0.49
4:A:848:HOH:O	2:B:1:NAG:H83	2.13	0.49
1:A:359:ARG:HE	1:A:378:MET:HE1	1.79	0.47
1:A:25:GLY:H	1:A:101:ASN:HD22	1.63	0.47
1:A:235:ARG:HD2	4:A:604:HOH:O	2.13	0.47
1:A:25:GLY:H	1:A:101:ASN:ND2	2.13	0.45
1:A:389:SER:HA	1:A:390:PRO:C	2.42	0.45
1:A:67:GLY:O	1:A:294:PRO:HA	2.17	0.45
1:A:445:LEU:HB3	1:A:448:PHE:HB3	1.99	0.44
1:A:73:LEU:HB3	1:A:74:PRO:HD3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:GLN:HE21	1:A:451:ASN:ND2	2.08	0.44
1:A:334:ILE:HG12	1:A:432:TYR:HB2	1.98	0.43
1:A:424:ASN:ND2	1:A:495:SER:H	2.11	0.42
1:A:186:MET:HE1	1:A:218:HIS:CD2	2.55	0.42
1:A:376:THR:HB	4:A:671:HOH:O	2.20	0.42
1:A:258:ILE:HA	1:A:258:ILE:HD13	1.80	0.41
1:A:130:THR:HG23	1:A:155:ASN:HD22	1.86	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	532/534 (100%)	509 (96%)	22 (4%)	1 (0%)	43 38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ILE

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 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	431/431 (100%)	409 (95%)	22 (5%)	21 14

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	PRO
1	A	18	ILE
1	A	20	ASN
1	A	72	ASN
1	A	91	SER
1	A	132	THR
1	A	150	ILE
1	A	235	ARG
1	A	253	ILE
1	A	288	ASP
1	A	302	LEU
1	A	313	VAL
1	A	318	ASP
1	A	344	PHE
1	A	387	GLN
1	A	399	LEU
1	A	410	LEU
1	A	439	LEU
1	A	465	LEU
1	A	498	SER
1	A	508	LEU
1	A	525	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	72	ASN
1	A	101	ASN
1	A	155	ASN
1	A	182	GLN
1	A	240	GLN
1	A	256	ASN
1	A	338	GLN
1	A	387	GLN
1	A	424	ASN
1	A	451	ASN
1	A	456	GLN
1	A	500	ASN
1	A	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 ⓘ

2 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	B	1	1,2	14,14,15	0.56	0	17,19,21	0.89	1 (5%)
2	NAG	B	2	2	14,14,15	0.38	0	17,19,21	1.08	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	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	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(°)
2	B	1	NAG	C1-C2-N2	-2.65	106.26	110.43
2	B	2	NAG	O3-C3-C2	2.44	114.48	109.40

There are no chirality outliers.

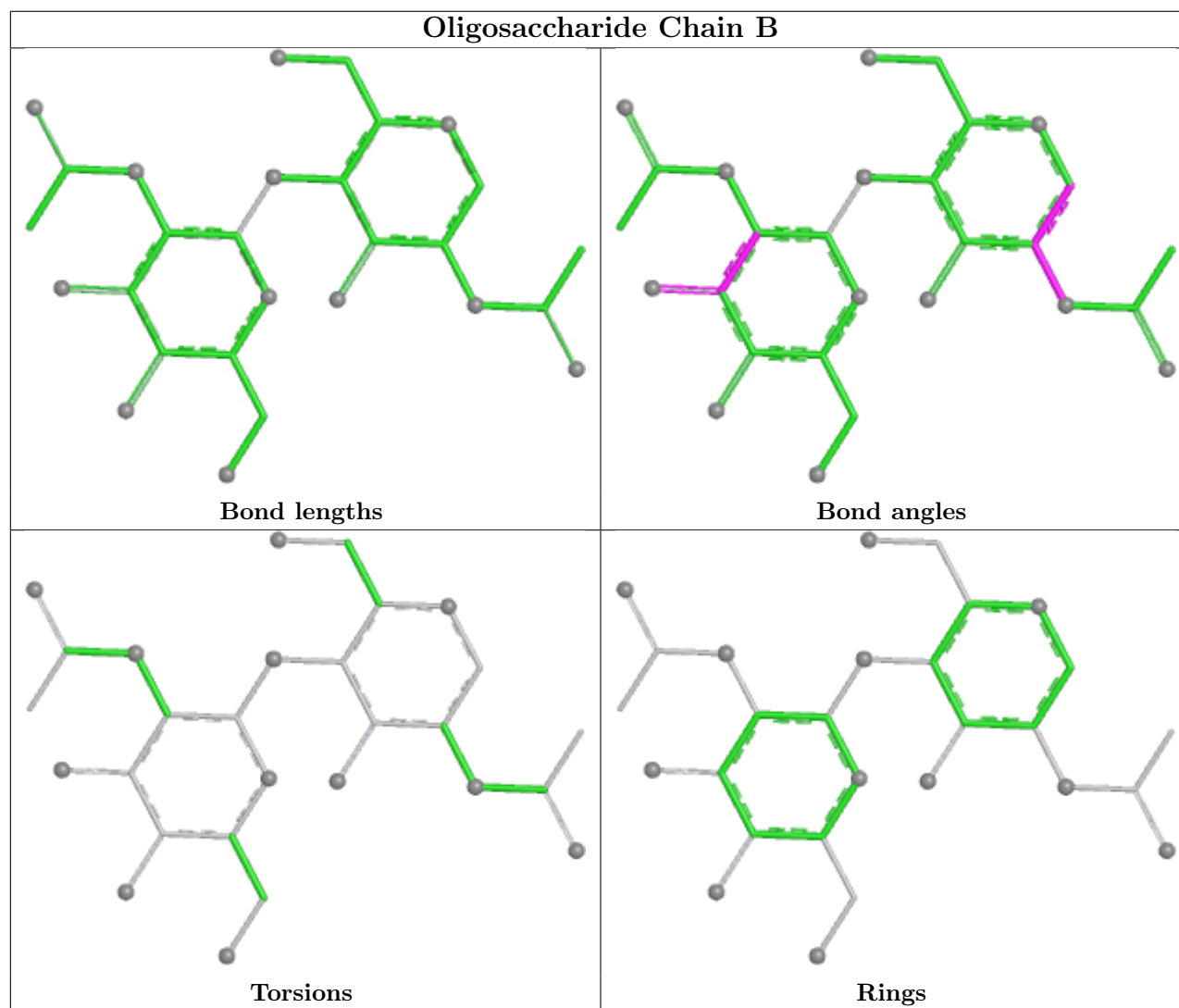
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	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](#)

1 ligand is 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	A	994	1	14,14,15	0.62	0	17,19,21	1.45	4 (23%)

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	A	994	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	994	NAG	C8-C7-N2	3.16	121.36	116.12
3	A	994	NAG	C1-O5-C5	2.73	115.84	112.19
3	A	994	NAG	O7-C7-C8	-2.41	117.76	122.05
3	A	994	NAG	O3-C3-C4	-2.11	105.39	110.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.