



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 12, 2024 – 11:41 PM EDT

PDB ID : 1WHS
Title : STRUCTURE OF THE COMPLEX OF L-BENZYL SUCCINATE WITH
WHEAT SERINE CARBOXYPEPTIDASE II AT 2.0 ANGSTROMS RES-
OLUTION
Authors : Bullock, T.L.; Remington, S.J.
Deposited on : 1994-03-07
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

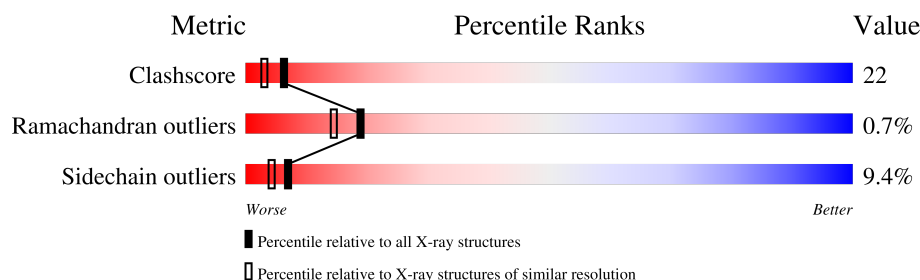
1 Overall quality at a glance

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	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (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	255	
2	B	153	
3	C	3	
4	D	2	

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
3	NAG	C	3	X	-	-	-
4	NAG	D	1	-	-	X	-
4	NAG	D	2	X	-	-	-
5	NAG	A	1131	X	-	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 3683 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.

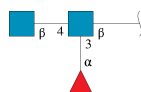
- Molecule 1 is a protein called SERINE CARBOXYPEPTIDASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			1999	1280	334	378	7			

- Molecule 2 is a protein called SERINE CARBOXYPEPTIDASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	153	Total	C	N	O	S	0	0	0
			1207	774	208	219	6			

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



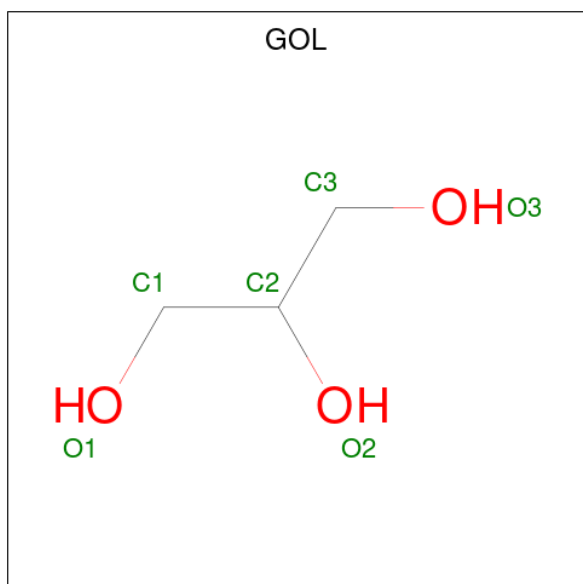
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



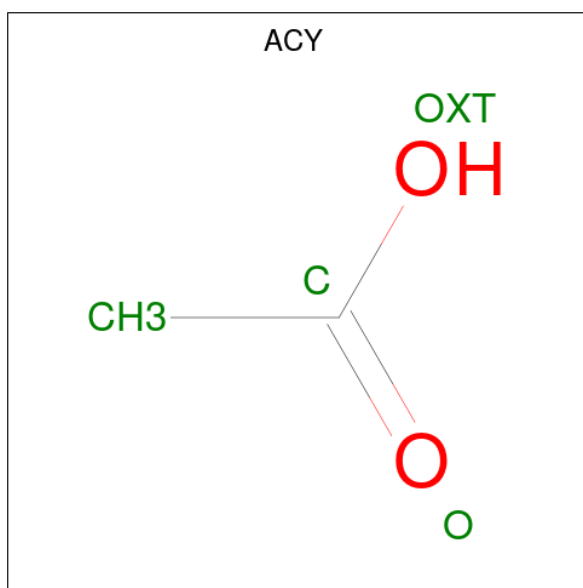
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is ACETIC ACID (three-letter code: ACY) (formula: $\text{C}_2\text{H}_4\text{O}_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0

- Molecule 8 is water.

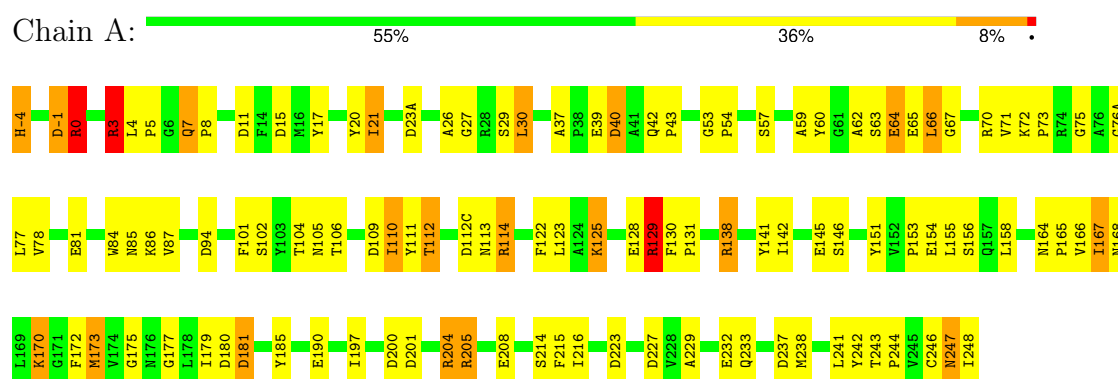
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	231	Total O 231 231	0	0
8	B	152	Total O 152 152	0	0

3 Residue-property plots

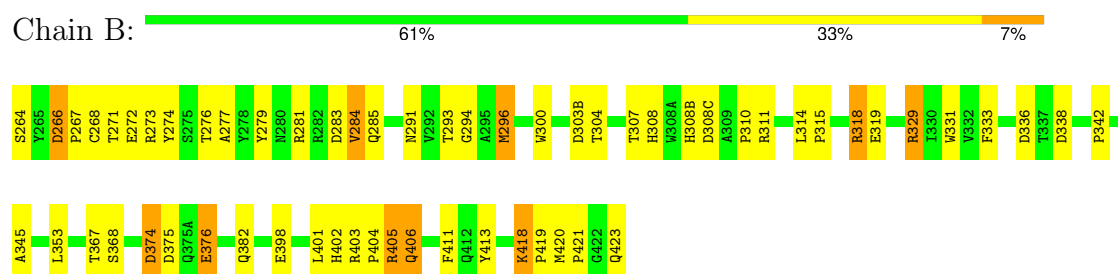
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

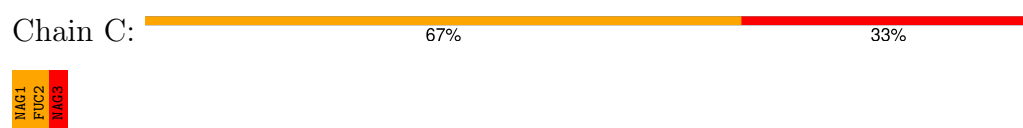
• Molecule 1: SERINE CARBOXYPEPTIDASE II



• Molecule 2: SERINE CARBOXYPEPTIDASE II



• Molecule 3: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 4: 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	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	95.60Å 95.60Å 208.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.175 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3683	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

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: FUC, NAG, GOL, ACY

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	0.97	9/2062 (0.4%)	1.38	37/2814 (1.3%)
2	B	0.90	4/1247 (0.3%)	1.33	15/1709 (0.9%)
All	All	0.95	13/3309 (0.4%)	1.36	52/4523 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	1	0

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	GLU	CD-OE1	7.47	1.33	1.25
1	A	208	GLU	CD-OE1	7.34	1.33	1.25
2	B	376	GLU	CD-OE1	6.78	1.33	1.25
1	A	39	GLU	CD-OE2	6.64	1.32	1.25
1	A	128	GLU	CD-OE2	6.33	1.32	1.25

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	A	151	TYR	CB-CG-CD1	8.80	126.28	121.00
2	B	405	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	A	151	TYR	CB-CG-CD2	-8.38	115.97	121.00
1	A	23(A)	ASP	CB-CG-OD2	-7.73	111.35	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	423	GLN	CA

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	1999	0	1854	88	0
2	B	1207	0	1142	53	0
3	C	38	0	34	10	0
4	D	28	0	24	8	0
5	A	14	0	13	3	0
6	A	6	0	8	0	0
7	A	4	0	3	0	0
7	B	4	0	3	1	0
8	A	231	0	0	11	0
8	B	152	0	0	6	0
All	All	3683	0	3081	139	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 22.

The worst 5 of 139 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)
3:C:2:FUC:H3	3:C:3:NAG:H61	1.22	1.15
1:A:5:PRO:HG2	2:B:284:VAL:HG12	1.35	1.03
1:A:27:GLY:HA3	1:A:105:ASN:HB2	1.53	0.88
2:B:418:LYS:HE3	2:B:419:PRO:HD2	1.59	0.84
3:C:2:FUC:H3	3:C:3:NAG:C6	2.07	0.83

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	253/255 (99%)	240 (95%)	13 (5%)	0	100	100
2	B	151/153 (99%)	142 (94%)	6 (4%)	3 (2%)	6	2
All	All	404/408 (99%)	382 (95%)	19 (5%)	3 (1%)	19	14

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	375	ASP
2	B	310	PRO
2	B	296	MET

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	205/208 (99%)	179 (87%)	26 (13%)	3	2
2	B	124/128 (97%)	119 (96%)	5 (4%)	27	26
All	All	329/336 (98%)	298 (91%)	31 (9%)	7	4

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	ARG
2	B	284	VAL
1	A	170	LYS

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Mol	Chain	Res	Type
2	B	406	GLN
1	A	247	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	285	GLN
2	B	308	HIS
2	B	412	GLN
1	A	183	HIS
1	A	217	HIS

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 ⓘ

5 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	C	1	3	14,14,15	0.97	0	17,19,21	4.10	4 (23%)
3	FUC	C	2	3	10,10,11	3.08	3 (30%)	14,14,16	3.29	6 (42%)
3	NAG	C	3	3	14,14,15	0.76	0	17,19,21	2.28	6 (35%)
4	NAG	D	1	4	14,14,15	0.92	1 (7%)	17,19,21	1.91	5 (29%)
4	NAG	D	2	4	14,14,15	1.66	2 (14%)	17,19,21	5.04	7 (41%)

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	C	1	3	-	2/6/23/26	0/1/1/1
3	FUC	C	2	3	-	-	0/1/1/1
3	NAG	C	3	3	2/2/5/7	4/6/23/26	0/1/1/1
4	NAG	D	1	4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	2/2/5/7	3/6/23/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	FUC	O5-C1	7.20	1.55	1.43
3	C	2	FUC	O5-C5	5.13	1.53	1.43
4	D	2	NAG	C1-C2	3.83	1.57	1.52
3	C	2	FUC	C4-C3	2.59	1.59	1.52
4	D	1	NAG	O5-C1	-2.18	1.40	1.43

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2	NAG	O6-C6-C5	18.19	173.27	111.33
3	C	1	NAG	O6-C6-C5	14.87	161.98	111.33
3	C	2	FUC	O3-C3-C2	8.57	127.54	110.05
4	D	2	NAG	C1-C2-N2	6.72	121.03	110.43
3	C	2	FUC	C2-C3-C4	-6.16	100.03	110.86

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	3	NAG	C2
3	C	3	NAG	C1
4	D	2	NAG	C2
4	D	2	NAG	C5

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2

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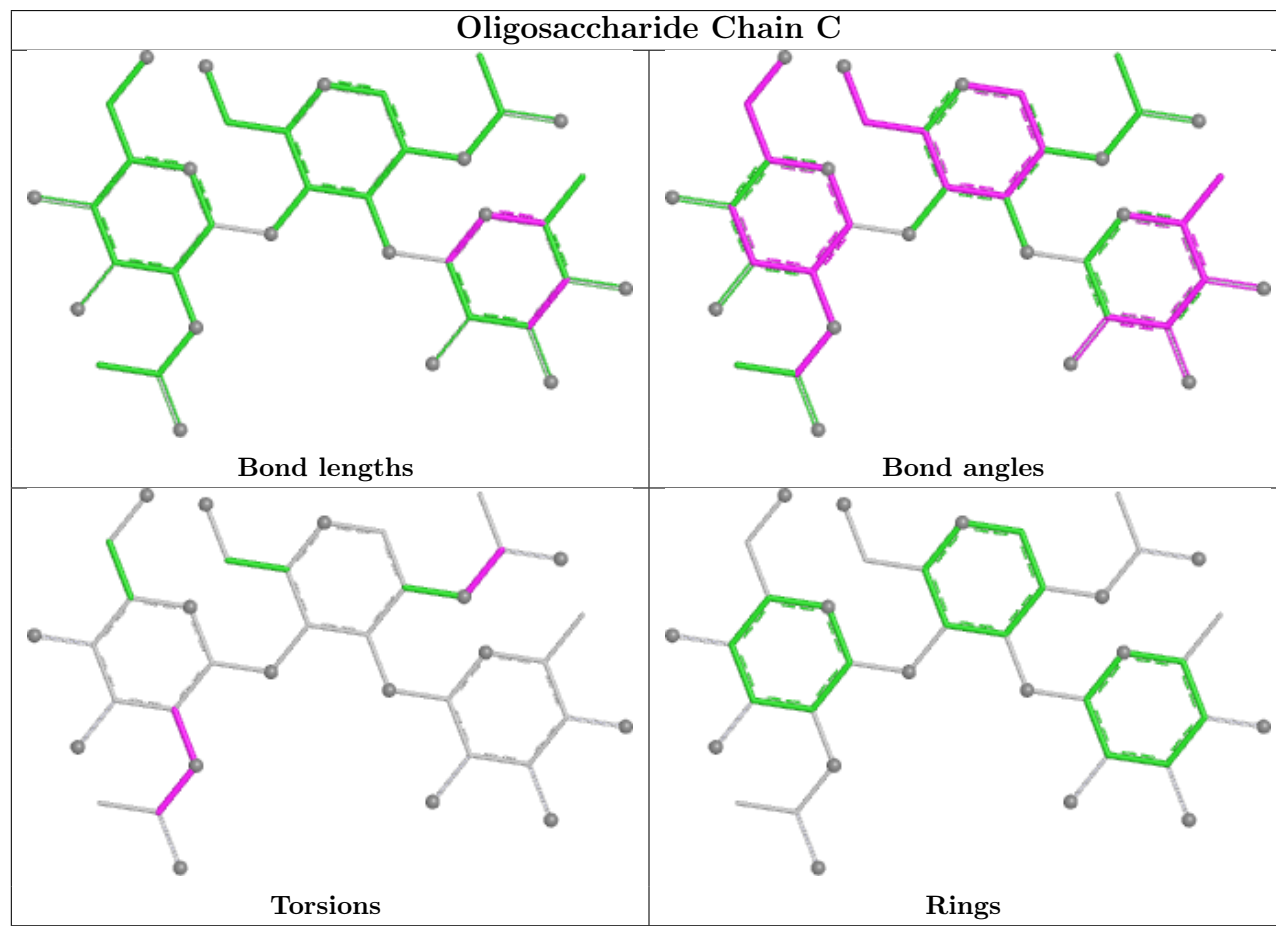
Mol	Chain	Res	Type	Atoms
3	C	3	NAG	C8-C7-N2-C2
3	C	3	NAG	O7-C7-N2-C2
4	D	1	NAG	C8-C7-N2-C2

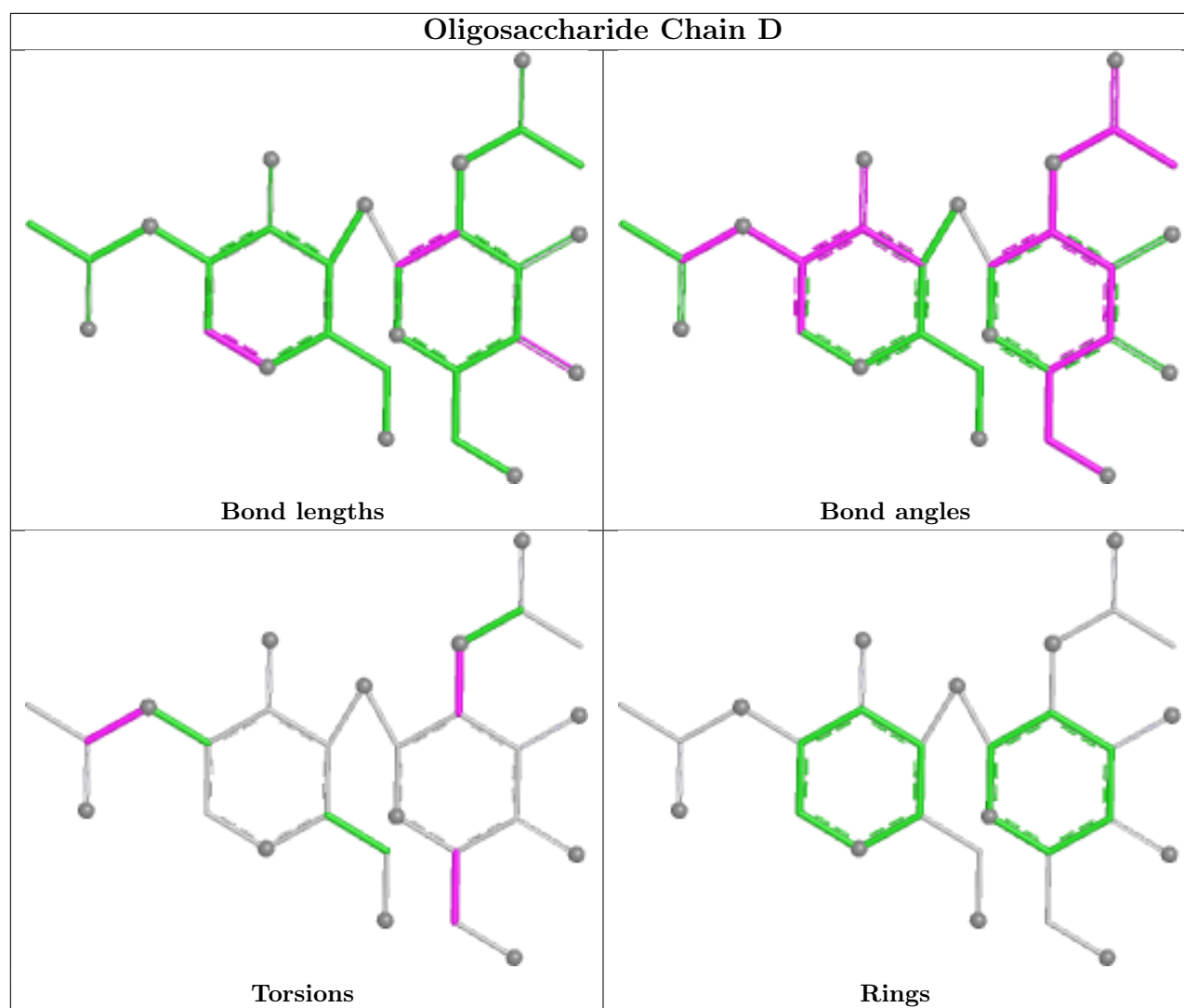
There are no ring outliers.

5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	8	0
4	D	2	NAG	4	0
3	C	2	FUC	4	0
3	C	1	NAG	5	0
3	C	3	NAG	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 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	ACY	B	461	-	3,3,3	0.84	0	3,3,3	0.93	0
6	GOL	A	450	-	5,5,5	0.70	0	5,5,5	0.60	0
5	NAG	A	1131	-	14,14,15	1.08	1 (7%)	17,19,21	1.98	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ACY	A	460	-	3,3,3	0.98	0	3,3,3	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	450	-	-	3/4/4/4	-
5	NAG	A	1131	-	1/1/5/7	5/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1131	NAG	C1-C2	2.53	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1131	NAG	O5-C1-C2	3.72	117.05	111.29
5	A	1131	NAG	O7-C7-C8	-3.47	115.87	122.05
5	A	1131	NAG	C2-N2-C7	3.42	127.48	122.90
5	A	1131	NAG	C8-C7-N2	3.12	121.30	116.12
5	A	1131	NAG	C1-O5-C5	2.67	115.76	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1131	NAG	C2

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1131	NAG	C1-C2-N2-C7
6	A	450	GOL	O1-C1-C2-O2
6	A	450	GOL	O1-C1-C2-C3
5	A	1131	NAG	O5-C5-C6-O6
5	A	1131	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	461	ACY	1	0
5	A	1131	NAG	3	0

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.