



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 11:54 PM UTC

PDB ID : 1IGR / pdb_00001igr
Title : Type 1 Insulin-like growth factor receptor (DOMAINS 1-3)
Authors : Garrett, T.P.J.; Mckern, N.M.; Lou, M.; Frenkel, M.J.; Bentley, J.D.; Lovrecz, G.O.; Elleman, T.C.; Cosgrove, L.J.; Ward, C.W.
Deposited on : 1998-09-28
Resolution : 2.60 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (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

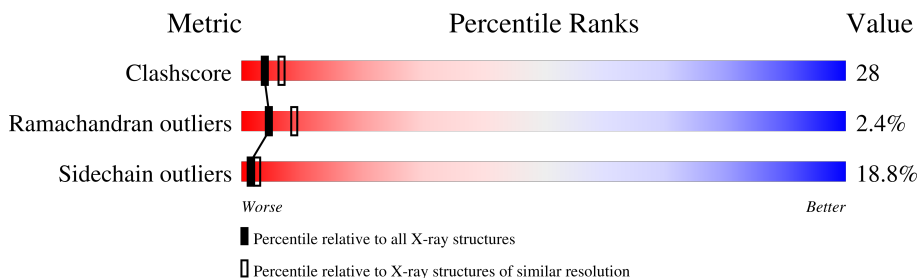
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	478	
2	B	3	
3	C	5	

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
2	NAG	B	2	-	-	X	-
2	FUC	B	3	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	2	X	-	-	-
4	NAG	A	479(A)	X	-	-	-
5	SO4	A	493	-	-	X	-
5	SO4	A	497	-	-	X	-

2 Entry composition [i](#)

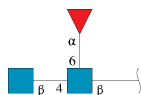
There are 6 unique types of molecules in this entry. The entry contains 3900 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 INSULIN-LIKE GROWTH FACTOR RECEPTOR 1.

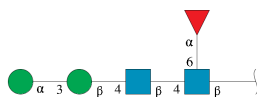
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	471	3686	2312	633	701	40	0	0	0

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	5	60	34	2	24	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is SULFATE ION (CCD ID: SO₄) (formula: O₄S).



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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	48	Total	O	0	0
			48	48		

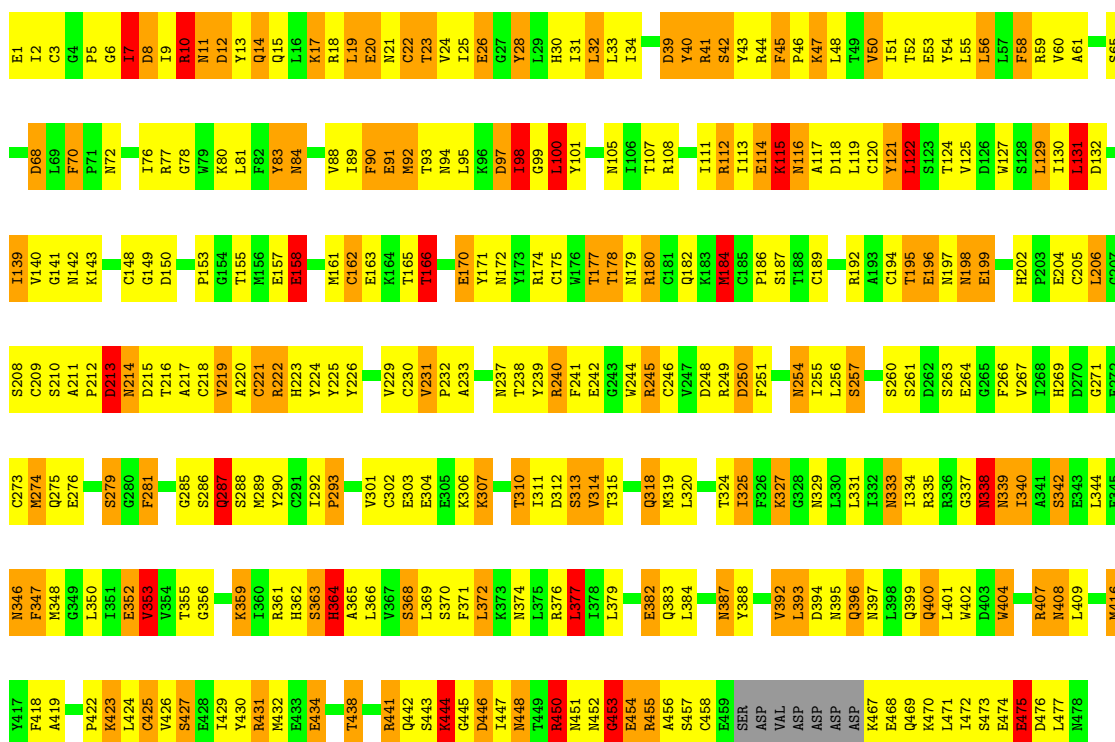
3 Residue-property plots

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: INSULIN-LIKE GROWTH FACTOR RECEPTOR 1

Chain A: 



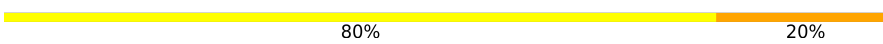
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 

MAG1
MAG2
FUC3

- Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



MAG1
MAG2
BGA3
MAN4
FUC5

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.39Å 99.72Å 120.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.60	Depositor
% Data completeness (in resolution range)	97.0 (7.00-2.60)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.237 , 0.304	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3900	wwPDB-VP
Average B, all atoms (Å ²)	53.0	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, SO4, MAN, NAG, BMA

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	1.09	1/3756 (0.0%)	2.34	228/5082 (4.5%)

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
1	A	0	17

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	LEU	N-CA	-5.25	1.40	1.46

The worst 5 of 228 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	387	ASN	OD1-CG-ND2	-13.53	109.07	122.60
1	A	451	ASN	OD1-CG-ND2	11.32	133.92	122.60
1	A	431	ARG	NE-CZ-NH2	11.23	129.31	119.20
1	A	59	ARG	CD-NE-CZ	11.05	139.87	124.40
1	A	214	ASN	OD1-CG-ND2	-10.84	111.76	122.60

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	LEU	Mainchain

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Mol	Chain	Res	Type	Group
1	A	19	LEU	Mainchain
1	A	45	PHE	Mainchain
1	A	50	VAL	Mainchain
1	A	8	ASP	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3686	0	3545	198	0
2	B	38	0	34	23	0
3	C	60	0	50	1	0
4	A	28	0	26	1	0
5	A	40	0	0	5	0
6	A	48	0	0	5	0
All	All	3900	0	3655	212	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 28.

The worst 5 of 212 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:222:ARG:HD3	2:B:3:FUC:H61	1.36	1.07
2:B:2:NAG:H3	2:B:3:FUC:H3	1.39	1.02
1:A:143:LYS:HG2	1:A:148:CYS:SG	2.07	0.94
2:B:2:NAG:N2	2:B:3:FUC:H3	1.88	0.89
2:B:2:NAG:HN2	2:B:3:FUC:H3	1.39	0.86

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	467/478 (98%)	396 (85%)	60 (13%)	11 (2%)	4 9

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	LEU
1	A	158	GLU
1	A	213	ASP
1	A	41	ARG
1	A	338	ASN

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	405/426 (95%)	329 (81%)	76 (19%)	1 2

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	407	ARG
1	A	470	LYS
1	A	416	MET
1	A	444	LYS
1	A	475	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	400	GLN
1	A	408	ASN
1	A	237	ASN
1	A	318	GLN
1	A	333	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	B	1	2,1	14,14,15	2.48	6 (42%)	17,19,21	2.85	8 (47%)
2	NAG	B	2	2	14,14,15	2.09	3 (21%)	17,19,21	1.88	2 (11%)
2	FUC	B	3	2	10,10,11	1.22	1 (10%)	14,14,16	2.24	4 (28%)
3	NAG	C	1	3,1	14,14,15	1.42	2 (14%)	17,19,21	1.67	4 (23%)
3	NAG	C	2	3	14,14,15	1.92	4 (28%)	17,19,21	3.00	6 (35%)
3	BMA	C	3	3	11,11,12	1.71	1 (9%)	15,15,17	1.52	1 (6%)
3	MAN	C	4	3	11,11,12	0.98	1 (9%)	15,15,17	1.39	1 (6%)
3	FUC	C	5	3	10,10,11	0.63	0	14,14,16	1.24	2 (14%)

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	2,1	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	1/6/23/26	0/1/1/1
2	FUC	B	3	2	-	-	0/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	1/1/5/7	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	FUC	C	5	3	-	-	0/1/1/1

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	C1-C2	6.40	1.61	1.52
2	B	2	NAG	C1-C2	-5.40	1.45	1.52
3	C	2	NAG	C1-C2	-5.04	1.45	1.52
3	C	3	BMA	C4-C5	-4.45	1.43	1.53
2	B	2	NAG	O5-C1	-4.24	1.36	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	C1-C2-N2	8.19	123.33	110.43
2	B	1	NAG	C8-C7-N2	6.21	126.42	116.12
2	B	1	NAG	C1-O5-C5	5.89	120.08	112.19
2	B	3	FUC	C1-C2-C3	5.20	117.21	109.64
2	B	2	NAG	C2-N2-C7	-4.82	116.45	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	2	NAG	C2

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6

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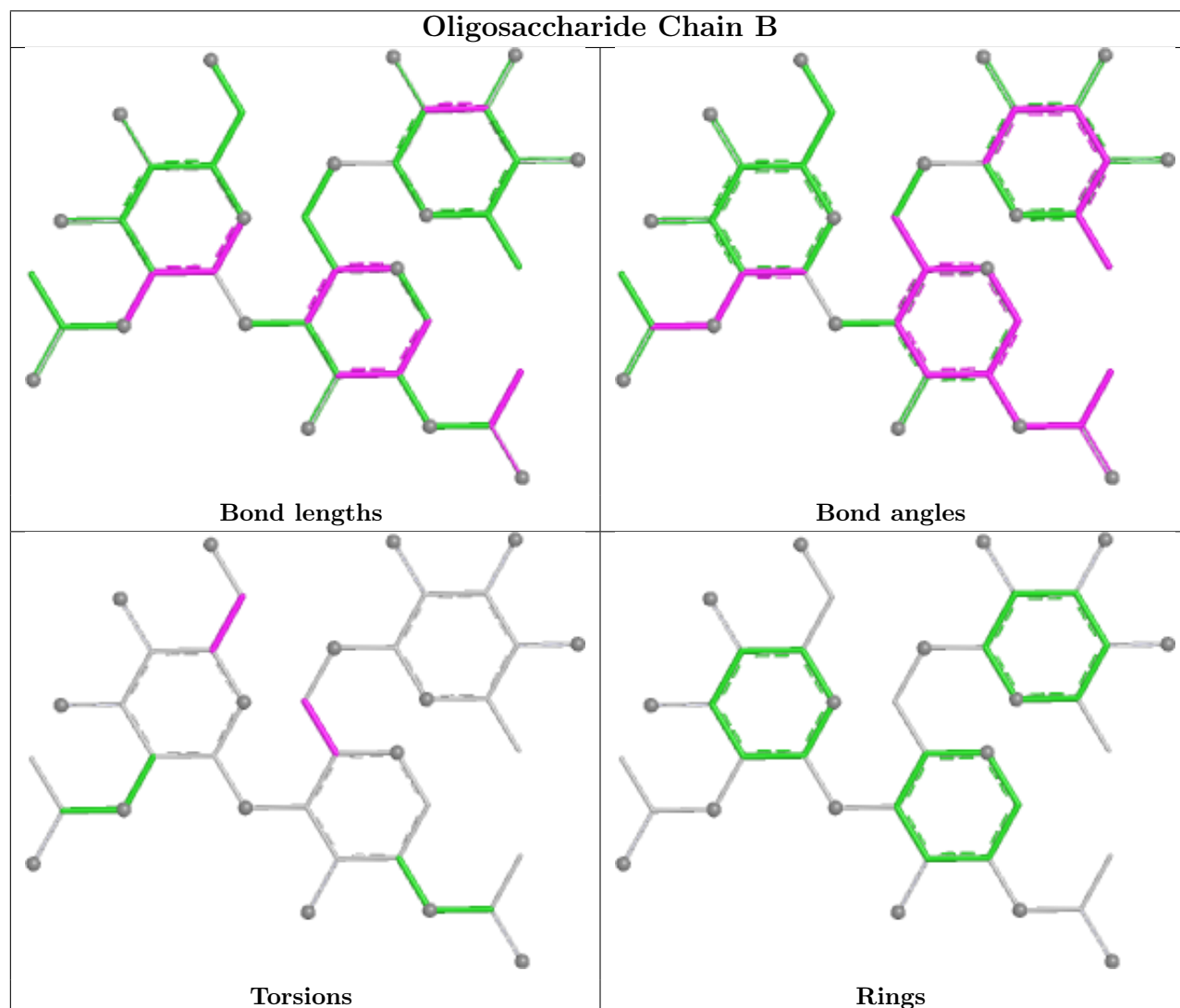
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	O5-C5-C6-O6

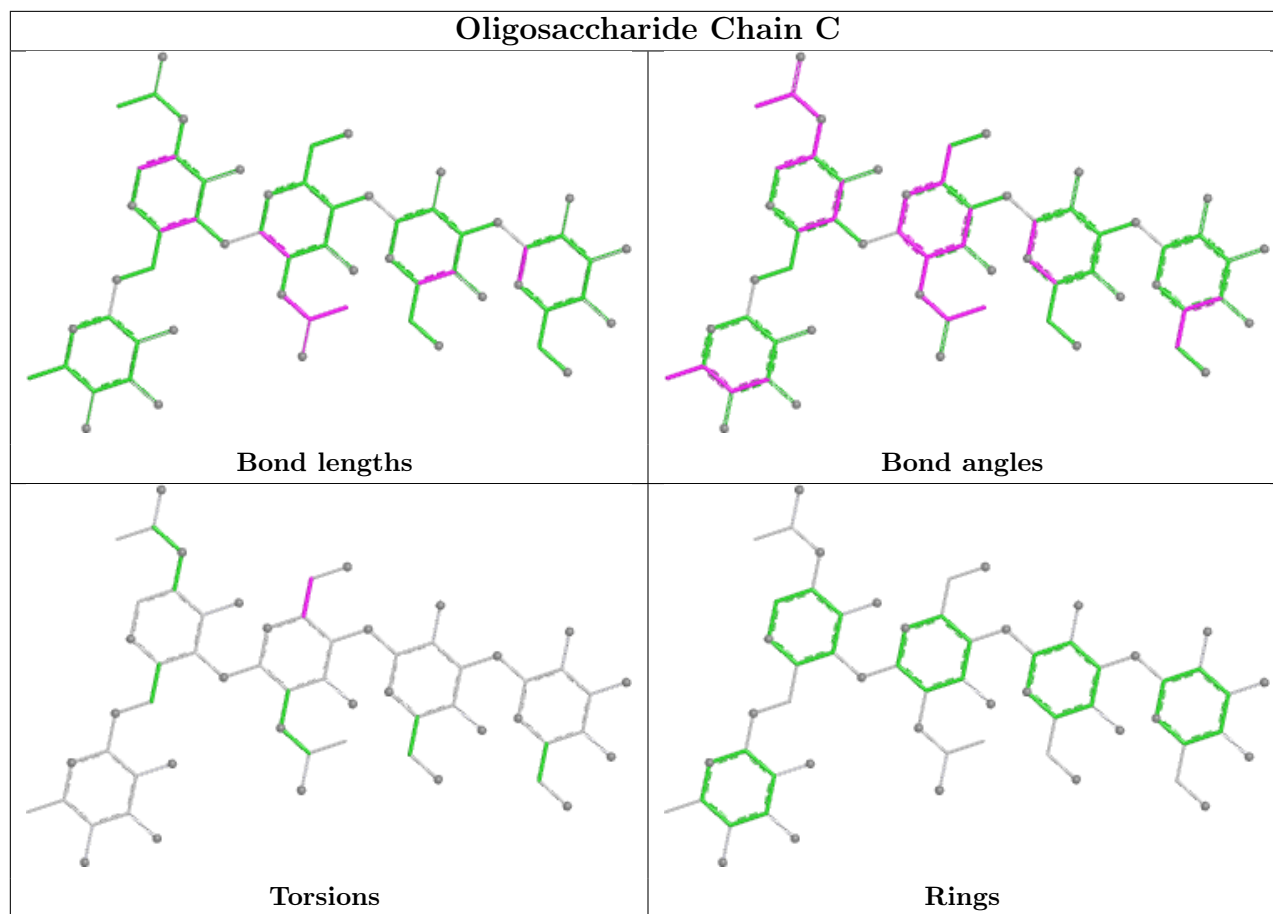
There are no ring outliers.

4 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	1	0
2	B	2	NAG	14	0
2	B	1	NAG	2	0
2	B	3	FUC	21	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](#)

10 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
5	SO4	A	498	-	4,4,4	0.56	0	6,6,6	1.12	0
4	NAG	A	483(A)	1	14,14,15	1.36	1 (7%)	17,19,21	2.12	3 (17%)
5	SO4	A	496	-	4,4,4	0.72	0	6,6,6	1.35	1 (16%)
5	SO4	A	500	-	4,4,4	0.53	0	6,6,6	0.66	0
4	NAG	A	479(A)	1	14,14,15	1.49	3 (21%)	17,19,21	2.36	6 (35%)
5	SO4	A	495	-	4,4,4	0.80	0	6,6,6	0.72	0
5	SO4	A	497	-	4,4,4	0.57	0	6,6,6	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	A	499	-	4,4,4	0.71	0	6,6,6	0.52	0
5	SO4	A	494	-	4,4,4	0.72	0	6,6,6	0.37	0
5	SO4	A	493	-	4,4,4	0.68	0	6,6,6	0.67	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
4	NAG	A	479(A)	1	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	A	483(A)	1	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	483(A)	NAG	O7-C7	-3.71	1.14	1.23
4	A	479(A)	NAG	O7-C7	-3.40	1.15	1.23
4	A	479(A)	NAG	C2-N2	2.27	1.50	1.46
4	A	479(A)	NAG	C1-C2	-2.02	1.49	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	479(A)	NAG	C2-N2-C7	-6.66	113.97	122.90
4	A	483(A)	NAG	C4-C3-C2	-5.37	103.15	111.02
4	A	483(A)	NAG	C2-N2-C7	-4.18	117.30	122.90
4	A	479(A)	NAG	O3-C3-C4	-2.98	103.36	110.38
4	A	479(A)	NAG	C1-O5-C5	2.92	116.10	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	479(A)	NAG	C1

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	479(A)	NAG	O5-C5-C6-O6
4	A	483(A)	NAG	O5-C5-C6-O6
4	A	479(A)	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	483(A)	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	479(A)	NAG	1	0
5	A	497	SO4	3	0
5	A	493	SO4	2	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 [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.