W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 10:16 PM BST

PDB ID	:	1FRT
Title	:	CRYSTAL STRUCTURE OF THE COMPLEX OF RAT NEONATAL FC RECEPTOR WITH FC
Authors	:	Burmeister, W.P.; Bjorkman, P.J.
Deposited on	:	1994-11-11
Resolution	:	4.50 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 following versions of software and data (see references ⓘ) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 4.50 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.

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
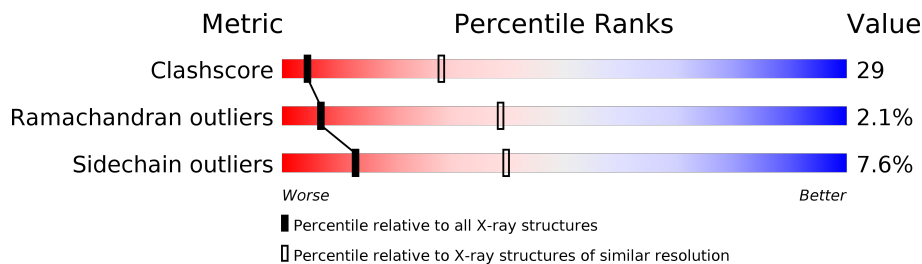
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)

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 on 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	269	70% 26% ··
2	B	99	72% 22% 6%
3	C	205	49% 43% 8%
4	D	2	100%
5	E	9	67% 33%

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
5	FUC	E	9	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4756 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 NEONATAL FC RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2138	1354	370	404	10			

- Molecule 2 is a protein called BETA 2-MICROGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			821	528	137	152	4			

- Molecule 3 is a protein called IGG FC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	205	Total	C	N	O	S	0	0	0
			1649	1049	280	313	7			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	272	GLN	GLU	conflict	GB 243866
C	283	GLN	GLU	conflict	GB 243866
C	294	GLN	GLU	conflict	GB 243866
C	312	ASN	ASP	conflict	GB 243866
C	315	ASP	ASN	conflict	GB 243866
C	356	GLU	ASP	conflict	GB 243866
C	358	MET	LEU	conflict	GB 243866

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total 24	C 14	N 1	O 9	0	0	0

- Molecule 5 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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.
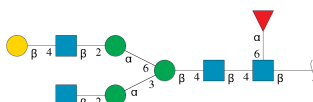
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	9	Total 110	C 62	N 4	O 44	0	0	0

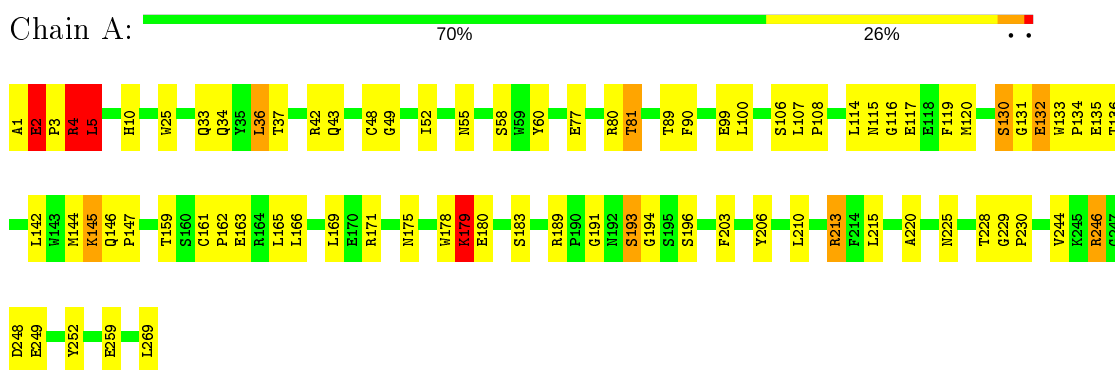- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
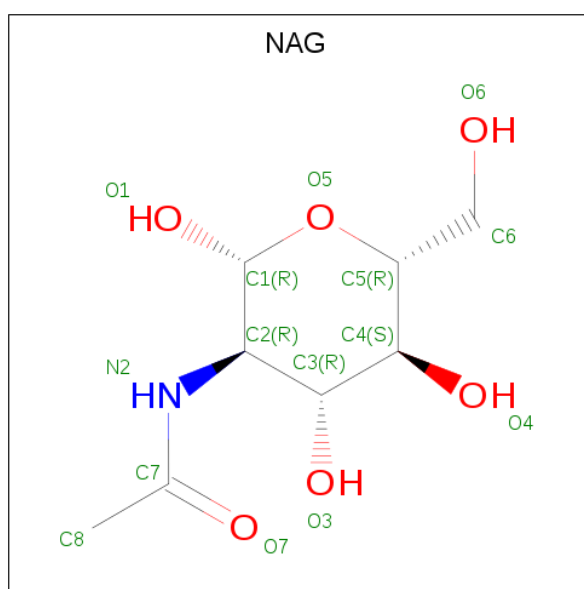
| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 14	C 8	N 1	O 5	0	0

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: NEONATAL FC RECEPTOR

Chain A:

• Molecule 2: BETA 2-MICROGLOBULIN

Chain B:
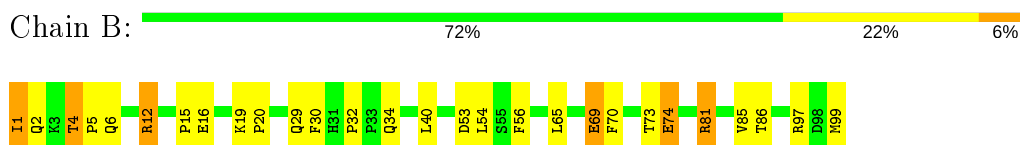
• Molecule 3: IGG FC

Chain C:

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

Chain D:

NAG1
FUC2

• Molecule 5: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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 E: 67%   33%

NAG1 NAG2 BMA3 MAN4 NAG5 GAL6 MAN7 NAG8 FUC9

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	125.00Å 145.00Å 216.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.50	Depositor
% Data completeness (in resolution range)	67.0 (20.00-4.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.423 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4756	wwPDB-VP
Average B, all atoms (Å^2)	199.0	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, GAL, NAG, BMA, MAN

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	0.77	1/2200 (0.0%)	0.98	7/2991 (0.2%)
2	B	0.85	0/846	0.90	0/1149
3	C	1.40	5/1693 (0.3%)	1.26	1/2302 (0.0%)
All	All	1.05	6/4739 (0.1%)	1.08	8/6442 (0.1%)

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
1	A	0	2
3	C	0	13
All	All	0	15

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	443	LEU	C-OXT	38.49	1.96	1.23
3	C	417	TRP	NE1-CE2	-8.12	1.26	1.37
3	C	277	TRP	NE1-CE2	-7.92	1.27	1.37
3	C	381	TRP	NE1-CE2	-7.75	1.27	1.37
3	C	313	TRP	NE1-CE2	-7.68	1.27	1.37

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	179	LYS	O-C-N	-18.23	93.53	122.70
1	A	36	LEU	CA-CB-CG	8.04	133.80	115.30
1	A	4	ARG	N-CA-C	5.71	126.42	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	LEU	N-CA-C	-5.39	96.44	111.00
3	C	367	CYS	N-CA-CB	5.20	119.96	110.60

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	179	LYS	Mainchain
1	A	60	TYR	Sidechain
3	C	252	MET	Mainchain
3	C	276	ASN	Sidechain
3	C	325	ASN	Sidechain

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	2138	0	2032	172	4
2	B	821	0	807	31	4
3	C	1649	0	1620	196	3
4	D	24	0	22	1	1
5	E	110	0	94	3	0
6	A	14	0	13	0	0
All	All	4756	0	4588	267	10

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 29.

The worst 5 of 267 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:134:PRO:CB	3:C:252:MET:HE1	1.26	1.57
1:A:134:PRO:HB2	3:C:252:MET:CE	1.06	1.50
1:A:115:ASN:ND2	3:C:254:SER:HA	1.17	1.47
3:C:251:LEU:HD22	3:C:435:HIS:ND1	1.37	1.37
1:A:115:ASN:HD22	3:C:254:SER:CA	1.35	1.35

The worst 5 of 10 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:356:GLU:OE1	3:C:439:LYS:NZ[8_565]	1.04	1.16
2:B:74:GLU:OE1	2:B:74:GLU:OE1[6_755]	1.54	0.66
2:B:74:GLU:CG	2:B:74:GLU:OE1[6_755]	1.63	0.57
2:B:74:GLU:CD	2:B:74:GLU:OE1[6_755]	1.74	0.46
3:C:356:GLU:CD	3:C:439:LYS:NZ[8_565]	1.97	0.23

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	267/269 (99%)	248 (93%)	13 (5%)	6 (2%)	6	38
2	B	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
3	C	201/205 (98%)	178 (89%)	17 (8%)	6 (3%)	4	31
All	All	565/573 (99%)	517 (92%)	36 (6%)	12 (2%)	7	39

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
3	C	265	ASP
3	C	297	ASN
3	C	339	ALA
1	A	49	GLY

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	227/227 (100%)	208 (92%)	19 (8%)	11	36
2	B	95/95 (100%)	84 (88%)	11 (12%)	5	23
3	C	192/192 (100%)	183 (95%)	9 (5%)	26	52
All	All	514/514 (100%)	475 (92%)	39 (8%)	13	40

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	248	ASP
2	B	6	GLN
3	C	350	THR
1	A	269	LEU
2	B	1	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	276	ASN
3	C	283	GLN
3	C	389	ASN
1	A	251	HIS
3	C	390	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)

11 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	#$|Z| > 2$
4	NAG	D	1	1,4	14,14,15	1.01	1 (7%)	17,19,21	1.15	1 (5%)
4	FUC	D	2	4	10,10,11	1.03	1 (10%)	14,14,16	0.85	1 (7%)
5	NAG	E	1	3,5	14,14,15	0.76	0	17,19,21	1.41	2 (11%)
5	NAG	E	2	5	14,14,15	1.08	1 (7%)	17,19,21	1.43	2 (11%)
5	BMA	E	3	5	11,11,12	0.66	0	15,15,17	1.44	2 (13%)
5	MAN	E	4	5	11,11,12	0.72	0	15,15,17	1.76	2 (13%)
5	NAG	E	5	5	14,14,15	0.75	0	17,19,21	1.54	1 (5%)
5	GAL	E	6	5	11,11,12	0.67	0	15,15,17	1.74	3 (20%)
5	MAN	E	7	5	11,11,12	0.56	0	15,15,17	1.64	1 (6%)
5	NAG	E	8	5	14,14,15	0.74	0	17,19,21	1.56	1 (5%)
5	FUC	E	9	5	10,10,11	0.77	0	14,14,16	1.11	1 (7%)

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	D	1	1,4	-	2/6/23/26	0/1/1/1
4	FUC	D	2	4	-	-	0/1/1/1
5	NAG	E	1	3,5	-	4/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
5	MAN	E	4	5	-	0/2/19/22	0/1/1/1
5	NAG	E	5	5	-	0/6/23/26	0/1/1/1
5	GAL	E	6	5	-	1/2/19/22	0/1/1/1
5	MAN	E	7	5	-	0/2/19/22	0/1/1/1
5	NAG	E	8	5	-	0/6/23/26	0/1/1/1
5	FUC	E	9	5	2/2/4/5	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2	FUC	C1-C2	2.70	1.58	1.52
5	E	2	NAG	C1-C2	2.16	1.55	1.52
4	D	1	NAG	O5-C5	2.04	1.47	1.43

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	8	NAG	C1-O5-C5	5.80	120.04	112.19
5	E	7	MAN	C1-O5-C5	5.63	119.81	112.19
5	E	4	MAN	C1-O5-C5	5.51	119.66	112.19
5	E	6	GAL	C1-O5-C5	5.13	119.14	112.19
5	E	5	NAG	C1-O5-C5	4.91	118.84	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	E	9	FUC	C5
5	E	9	FUC	C1

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
5	E	1	NAG	C8-C7-N2-C2
5	E	1	NAG	O7-C7-N2-C2
5	E	6	GAL	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2	FUC	1	0
5	E	6	GAL	2	0
5	E	1	NAG	1	0
4	D	1	NAG	1	1

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings
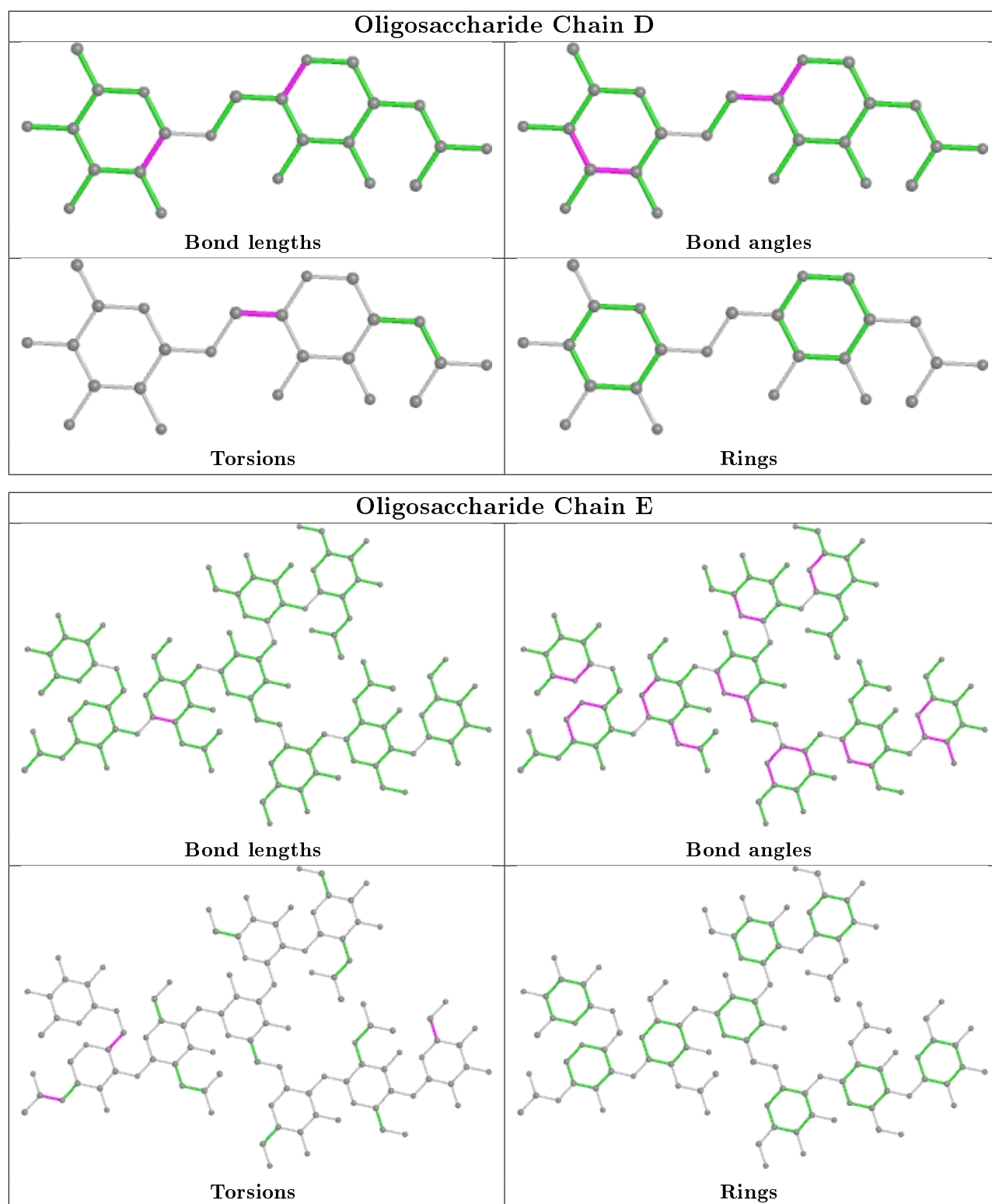
5.6 Ligand geometry (i)

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	$\#|Z| > 2$
6	NAG	A	401	1	14,14,15	0.69	0	17,19,21	1.10	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
6	NAG	A	401	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	401	NAG	C4-C3-C2	-2.96	106.68	111.02

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	341:GLY	C	342:GLN	N	4.64

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.