



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2022 – 12:08 PM EDT

PDB ID : 8DGG
Title : Structure of glycosylated LAG-3 homodimer
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Deposited on : 2022-06-23
Resolution : 3.78 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.29
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

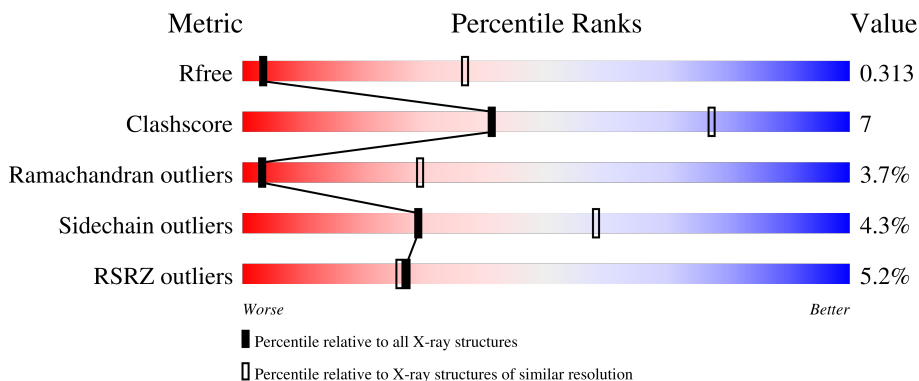
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.78 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}	130704	1038 (3.96-3.60)
Clashscore	141614	1100 (3.96-3.60)
Ramachandran outliers	138981	1062 (3.96-3.60)
Sidechain outliers	138945	1058 (3.96-3.60)
RSRZ outliers	127900	1009 (3.98-3.58)

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	425	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 69%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: grey;"></div> </div>
1	B	425	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 46%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 35%; height: 10px; background-color: grey;"></div> </div>
2	C	3	<div style="display: flex; align-items: center;"> <div style="width: 67%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: orange;"></div> </div>
2	E	3	<div style="display: flex; align-items: center;"> <div style="width: 33%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: orange;"></div> </div>
3	D	2	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background-color: yellow;"></div> </div>

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	NAG	B	502	-	-	-	X

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 5049 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.

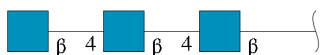
- Molecule 1 is a protein called Lymphocyte activation gene 3 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	354	2729	1743	495	481	10	0	0	0
1	B	277	2130	1363	385	375	7	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	443	HIS	-	expression tag	UNP Q61790
A	444	HIS	-	expression tag	UNP Q61790
A	445	HIS	-	expression tag	UNP Q61790
A	446	HIS	-	expression tag	UNP Q61790
A	447	HIS	-	expression tag	UNP Q61790
A	448	HIS	-	expression tag	UNP Q61790
B	443	HIS	-	expression tag	UNP Q61790
B	444	HIS	-	expression tag	UNP Q61790
B	445	HIS	-	expression tag	UNP Q61790
B	446	HIS	-	expression tag	UNP Q61790
B	447	HIS	-	expression tag	UNP Q61790
B	448	HIS	-	expression tag	UNP Q61790

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	3	42	24	3	15	0	0	0

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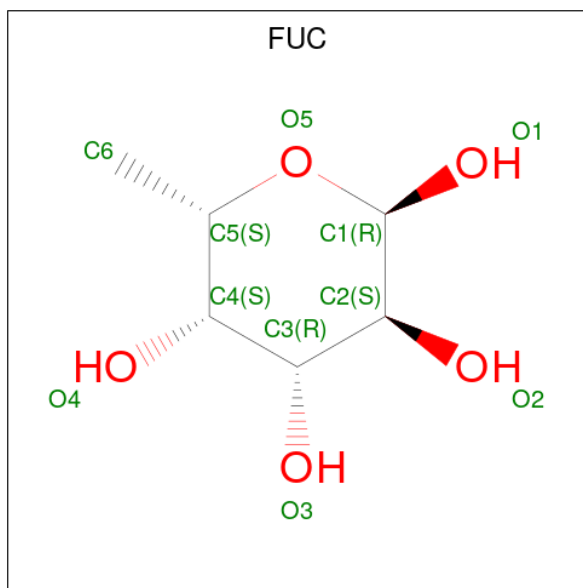
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	N				O
2	E	3	42	24	3	15	0	0	0

- Molecule 3 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	
			Total	C	N				O
3	D	2	28	16	2	10	0	0	0

- Molecule 4 is alpha-L-fucopyranose (three-letter code: FUC) (formula: C₆H₁₂O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	11	6	5	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

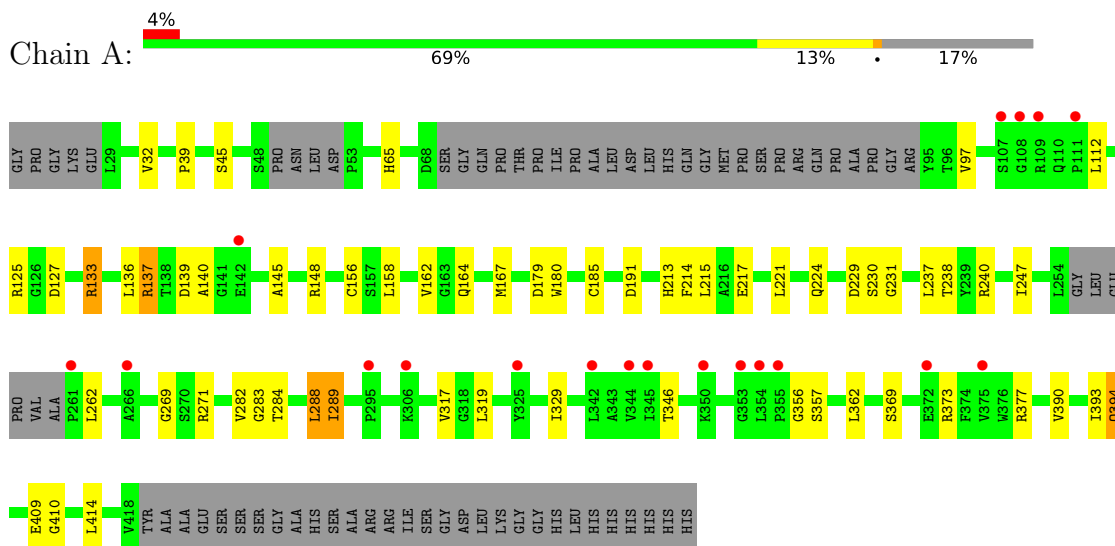
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	5	5	5	0	0
6	B	6	6	6	0	0

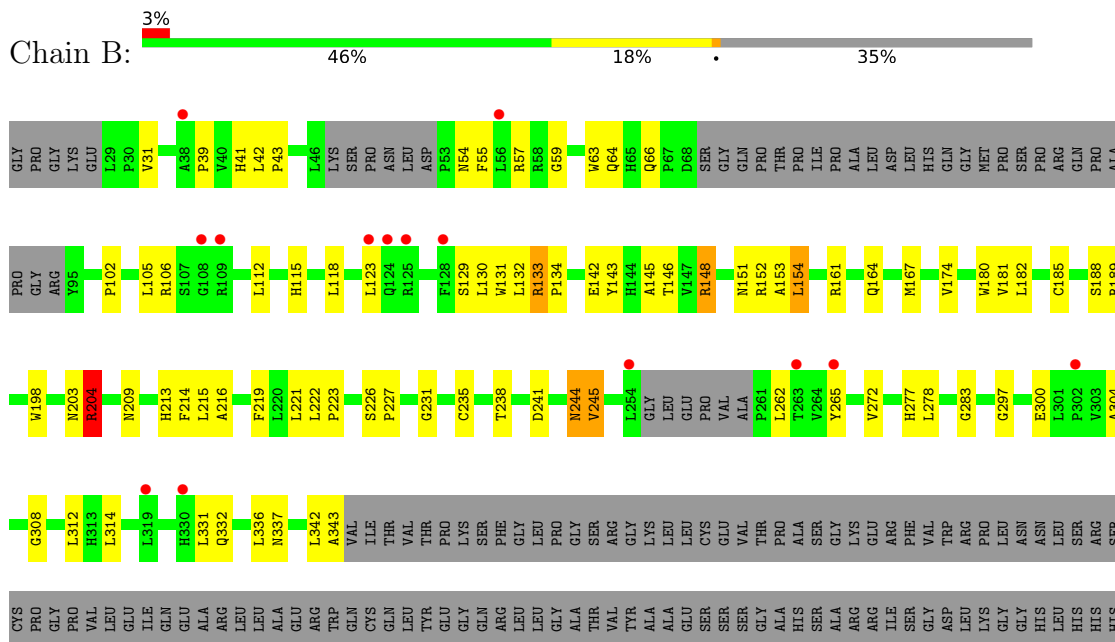
3 Residue-property plots [i](#)

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: Lymphocyte activation gene 3 protein

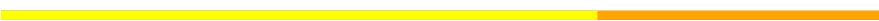


- Molecule 1: Lymphocyte activation gene 3 protein



HIS
HIS
HIS

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

Chain C:  67% 33%


MAG1
MAG2
MAG3

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

Chain E:  33% 33% 33%

MAG1
MAG2
MAG3

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.69Å 97.67Å 174.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.32 – 3.78 39.32 – 3.78	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.32-3.78) 100.0 (39.32-3.78)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 3.76Å)	Xtrriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.255 , 0.315 0.259 , 0.313	Depositor DCC
R_{free} test set	640 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	204.0	Xtrriage
Anisotropy	0.034	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 196.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5049	wwPDB-VP
Average B, all atoms (Å ²)	240.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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: FUC, 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	0.29	0/2803	0.52	0/3825
1	B	0.30	0/2191	0.54	0/2995
All	All	0.30	0/4994	0.53	0/6820

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	ARG	Sidechain
1	A	377	ARG	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	2729	0	2742	27	0
1	B	2130	0	2122	44	0
2	C	42	0	37	1	0
2	E	42	0	37	1	0
3	D	28	0	25	1	0
4	A	11	0	12	0	0
5	A	28	0	26	0	0
5	B	28	0	26	1	0
6	A	5	0	0	0	0
6	B	6	0	0	0	0
All	All	5049	0	5027	71	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 7.

All (71) 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:288:LEU:HD22	1:A:329:ILE:HD11	1.74	0.68
2:C:2:NAG:H83	2:C:3:NAG:H82	1.76	0.67
1:B:42:LEU:HD12	1:B:130:LEU:HD22	1.76	0.67
1:A:229:ASP:O	1:A:231:GLY:N	2.30	0.65
1:B:244:ASN:O	1:B:245:VAL:HB	2.01	0.61
1:B:180:TRP:HB3	1:B:223:PRO:O	2.01	0.60
1:A:319:LEU:HD13	1:A:346:THR:HG21	1.84	0.60
1:A:140:ALA:HB2	1:A:162:VAL:HG22	1.83	0.60
1:A:221:LEU:HD21	1:B:221:LEU:HD22	1.83	0.59
1:A:409:GLU:HB2	1:A:414:LEU:HD11	1.85	0.58
1:B:59:GLY:O	1:B:102:PRO:HA	2.03	0.58
1:B:278:LEU:HD21	1:B:336:LEU:HD22	1.88	0.56
1:A:373:ARG:NH2	1:A:410:GLY:O	2.40	0.54
1:B:216:ALA:HB3	1:B:219:PHE:CZ	2.42	0.54
1:B:198:TRP:CD1	1:B:215:LEU:HD23	2.43	0.53
1:B:203:ASN:O	1:B:204:ARG:C	2.46	0.53
1:A:214:PHE:CZ	1:B:182:LEU:HD22	2.44	0.53
1:A:393:ILE:HD11	1:A:394:GLN:HE21	1.74	0.53
1:A:45:SER:HA	1:A:127:ASP:HA	1.91	0.52
1:B:272:VAL:HG21	1:B:342:LEU:HD13	1.92	0.52
1:A:215:LEU:N	1:A:215:LEU:HD12	2.27	0.50
1:B:238:THR:HA	1:B:244:ASN:HA	1.92	0.50
1:A:362:LEU:HD13	1:A:390:VAL:HG22	1.94	0.50
1:B:64:GLN:O	1:B:143:TYR:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:TRP:CZ2	1:B:214:PHE:CG	2.99	0.49
1:A:185:CYS:SG	1:A:237:LEU:HD21	2.51	0.49
1:B:204:ARG:HH11	1:B:204:ARG:HB3	1.76	0.49
1:B:118:LEU:HD21	1:B:123:LEU:HD21	1.95	0.49
1:A:137:ARG:NE	1:A:164:GLN:HE21	2.11	0.48
1:A:112:LEU:O	1:A:112:LEU:HD23	2.13	0.48
1:B:226:SER:HB2	1:B:227:PRO:HD2	1.96	0.48
1:B:182:LEU:HD23	1:B:182:LEU:O	2.14	0.48
1:B:215:LEU:HD12	1:B:215:LEU:N	2.28	0.48
1:A:39:PRO:HB3	1:A:133:ARG:HD3	1.97	0.47
3:D:1:NAG:H82	3:D:2:NAG:H82	1.97	0.47
1:B:216:ALA:HB3	1:B:219:PHE:CE2	2.51	0.46
1:B:66:GLN:HB3	1:B:142:GLU:HB3	1.96	0.46
1:A:217:GLU:HG2	2:E:2:NAG:H82	1.97	0.46
1:A:145:ALA:HB3	1:A:156:CYS:HB2	1.98	0.46
1:A:32:VAL:HG21	1:A:158:LEU:HD13	1.97	0.46
1:B:54:ASN:HA	1:B:57:ARG:HD3	1.97	0.46
1:A:269:GLY:N	1:A:317:VAL:O	2.49	0.45
1:B:43:PRO:HA	1:B:129:SER:OG	2.17	0.44
1:B:244:ASN:O	1:B:245:VAL:CB	2.65	0.44
1:B:331:LEU:HG	1:B:332:GLN:HE21	1.83	0.44
1:B:312:LEU:HD11	1:B:314:LEU:HD12	1.99	0.44
1:B:151:ASN:OD1	1:B:152:ARG:N	2.51	0.43
1:B:181:VAL:HG12	1:B:222:LEU:HB2	2.01	0.43
1:B:265:TYR:CD1	1:B:343:ALA:HB3	2.53	0.43
1:B:167:MET:HE2	1:B:185:CYS:HB3	2.00	0.43
1:B:39:PRO:HA	1:B:132:LEU:O	2.19	0.43
1:A:139:ASP:O	1:A:140:ALA:C	2.57	0.43
1:B:181:VAL:CG1	1:B:222:LEU:HD12	2.48	0.43
1:A:224:GLN:HE21	1:A:224:GLN:HA	1.84	0.42
1:A:289:ILE:HD12	1:A:289:ILE:N	2.34	0.42
1:B:41:HIS:HB2	1:B:131:TRP:CH2	2.55	0.42
1:B:31:VAL:HG13	1:B:161:ARG:HG2	2.01	0.42
5:B:502:NAG:HO3	5:B:502:NAG:C7	2.33	0.42
1:B:54:ASN:O	1:B:55:PHE:C	2.58	0.41
1:B:153:ALA:O	1:B:154:LEU:C	2.58	0.41
1:B:164:GLN:HG2	1:B:188:SER:OG	2.20	0.41
1:A:282:VAL:O	1:A:284:THR:HG23	2.19	0.41
1:B:133:ARG:HA	1:B:134:PRO:HA	1.84	0.41
1:B:39:PRO:HB3	1:B:133:ARG:HB3	2.03	0.41
1:B:105:LEU:HD23	1:B:106:ARG:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:VAL:HG13	1:B:161:ARG:CG	2.51	0.41
1:A:393:ILE:O	1:A:394:GLN:O	2.39	0.40
1:B:63:TRP:CD2	1:B:145:ALA:HB2	2.55	0.40
1:B:278:LEU:CD2	1:B:336:LEU:HD13	2.51	0.40
1:A:65:HIS:NE2	1:A:139:ASP:O	2.54	0.40
1:B:189:ARG:HH22	1:B:241:ASP:CG	2.24	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	346/425 (81%)	292 (84%)	44 (13%)	10 (3%)	4	34
1	B	269/425 (63%)	218 (81%)	38 (14%)	13 (5%)	2	23
All	All	615/850 (72%)	510 (83%)	82 (13%)	23 (4%)	3	29

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	394	GLN
1	B	204	ARG
1	A	125	ARG
1	A	230	SER
1	A	283	GLY
1	B	174	VAL
1	B	209	ASN
1	B	231	GLY
1	B	283	GLY
1	A	356	GLY
1	B	148	ARG
1	B	154	LEU

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Mol	Chain	Res	Type
1	B	262	LEU
1	B	304	ALA
1	B	308	GLY
1	A	369	SER
1	B	245	VAL
1	A	262	LEU
1	A	271	ARG
1	A	357	SER
1	B	112	LEU
1	A	238	THR
1	B	297	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	298/352 (85%)	286 (96%)	12 (4%)	31	60
1	B	232/352 (66%)	221 (95%)	11 (5%)	26	56
All	All	530/704 (75%)	507 (96%)	23 (4%)	29	58

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	VAL
1	A	133	ARG
1	A	136	LEU
1	A	137	ARG
1	A	148	ARG
1	A	167	MET
1	A	179	ASP
1	A	191	ASP
1	A	213	HIS
1	A	247	ILE
1	A	288	LEU
1	A	289	ILE

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Mol	Chain	Res	Type
1	B	115	HIS
1	B	133	ARG
1	B	146	THR
1	B	148	ARG
1	B	204	ARG
1	B	213	HIS
1	B	235	CYS
1	B	244	ASN
1	B	277	HIS
1	B	300	GLU
1	B	337	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	GLN
1	A	335	GLN
1	A	380	ASN
1	A	394	GLN
1	B	164	GLN

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	C	1	2,1	14,14,15	0.40	0	17,19,21	0.83	1 (5%)
2	NAG	C	2	2	14,14,15	0.41	0	17,19,21	0.97	0
2	NAG	C	3	2	14,14,15	0.50	0	17,19,21	2.10	2 (11%)
3	NAG	D	1	3,1	14,14,15	0.45	0	17,19,21	0.52	0
3	NAG	D	2	3	14,14,15	0.39	0	17,19,21	0.61	0
2	NAG	E	1	2,1	14,14,15	0.44	0	17,19,21	1.71	4 (23%)
2	NAG	E	2	2	14,14,15	0.52	0	17,19,21	1.59	2 (11%)
2	NAG	E	3	2	14,14,15	0.46	0	17,19,21	0.75	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	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
2	NAG	C	3	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	1/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
2	NAG	E	3	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	NAG	O5-C1-C2	7.45	123.05	111.29
2	E	2	NAG	C4-C3-C2	4.59	117.74	111.02
2	E	1	NAG	O5-C1-C2	4.45	118.31	111.29
2	E	2	NAG	O5-C1-C2	3.77	117.25	111.29
2	C	3	NAG	C1-O5-C5	3.55	117.00	112.19
2	E	1	NAG	C1-O5-C5	3.34	116.71	112.19
2	E	1	NAG	O4-C4-C3	2.55	116.24	110.35
2	E	1	NAG	C4-C3-C2	-2.29	107.66	111.02
2	C	1	NAG	C1-C2-N2	2.06	114.01	110.49

There are no chirality outliers.

All (16) torsion outliers are listed below:

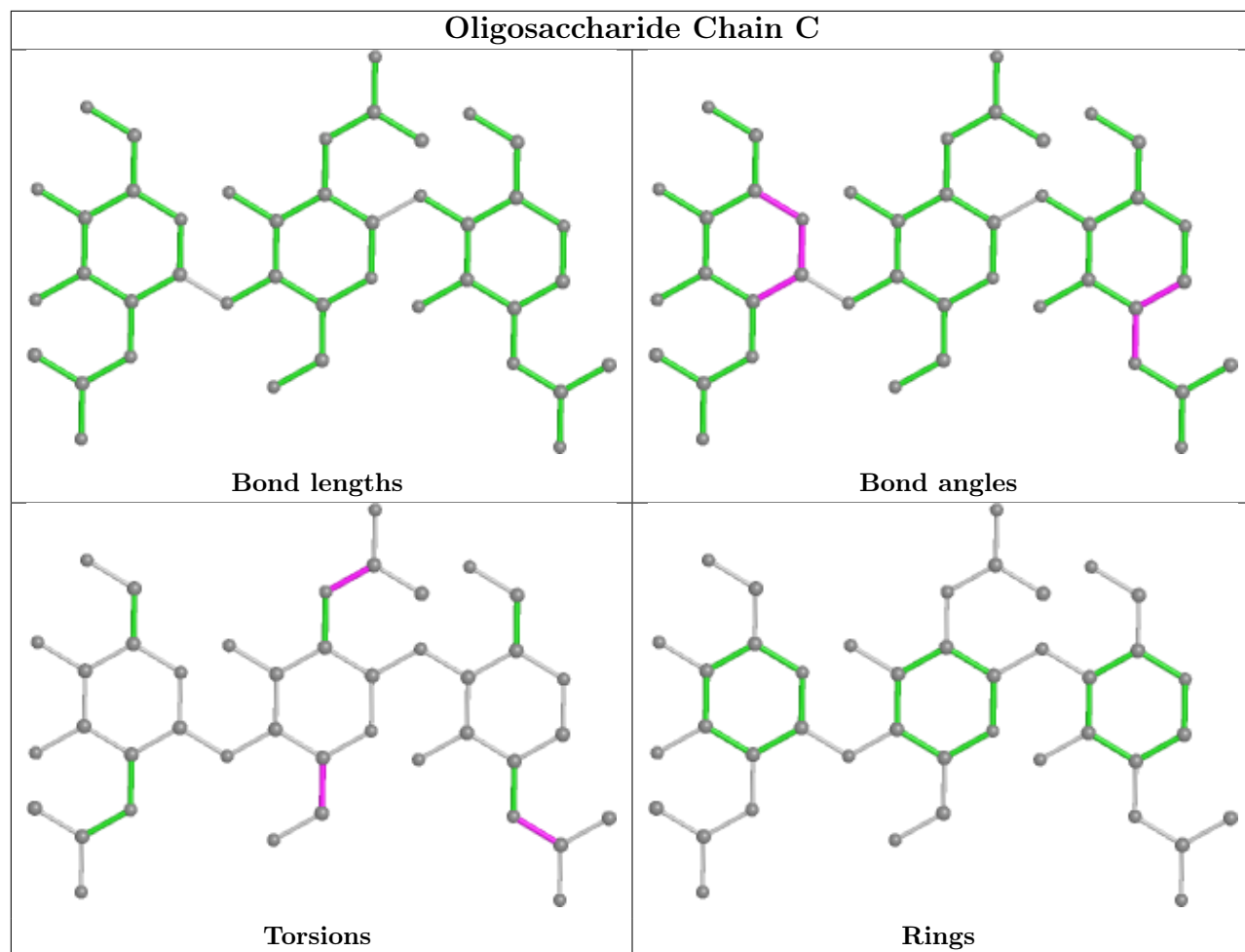
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	E	3	NAG	C3-C2-N2-C7
2	E	3	NAG	C8-C7-N2-C2
2	E	3	NAG	O7-C7-N2-C2
2	E	2	NAG	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
3	D	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O7-C7-N2-C2

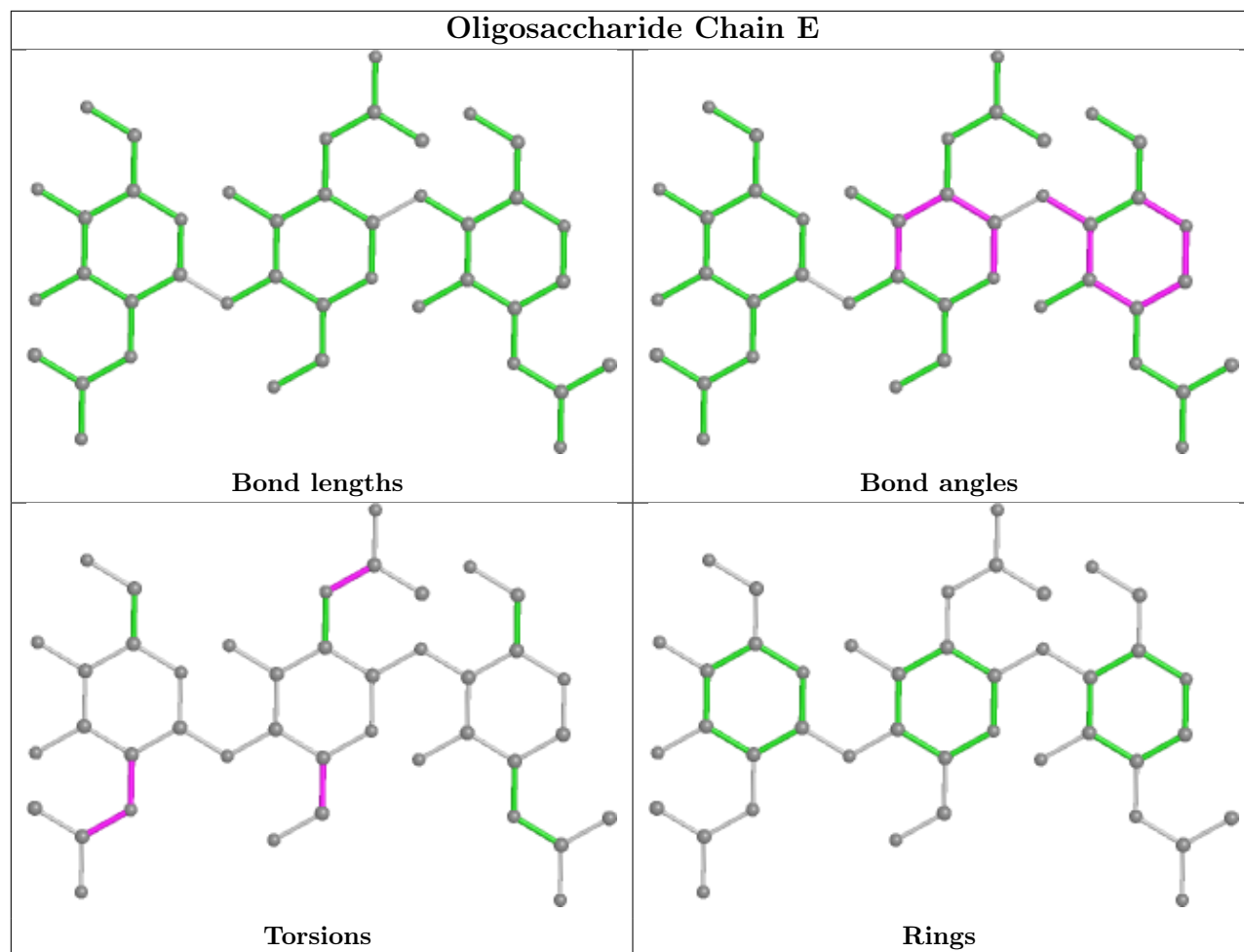
There are no ring outliers.

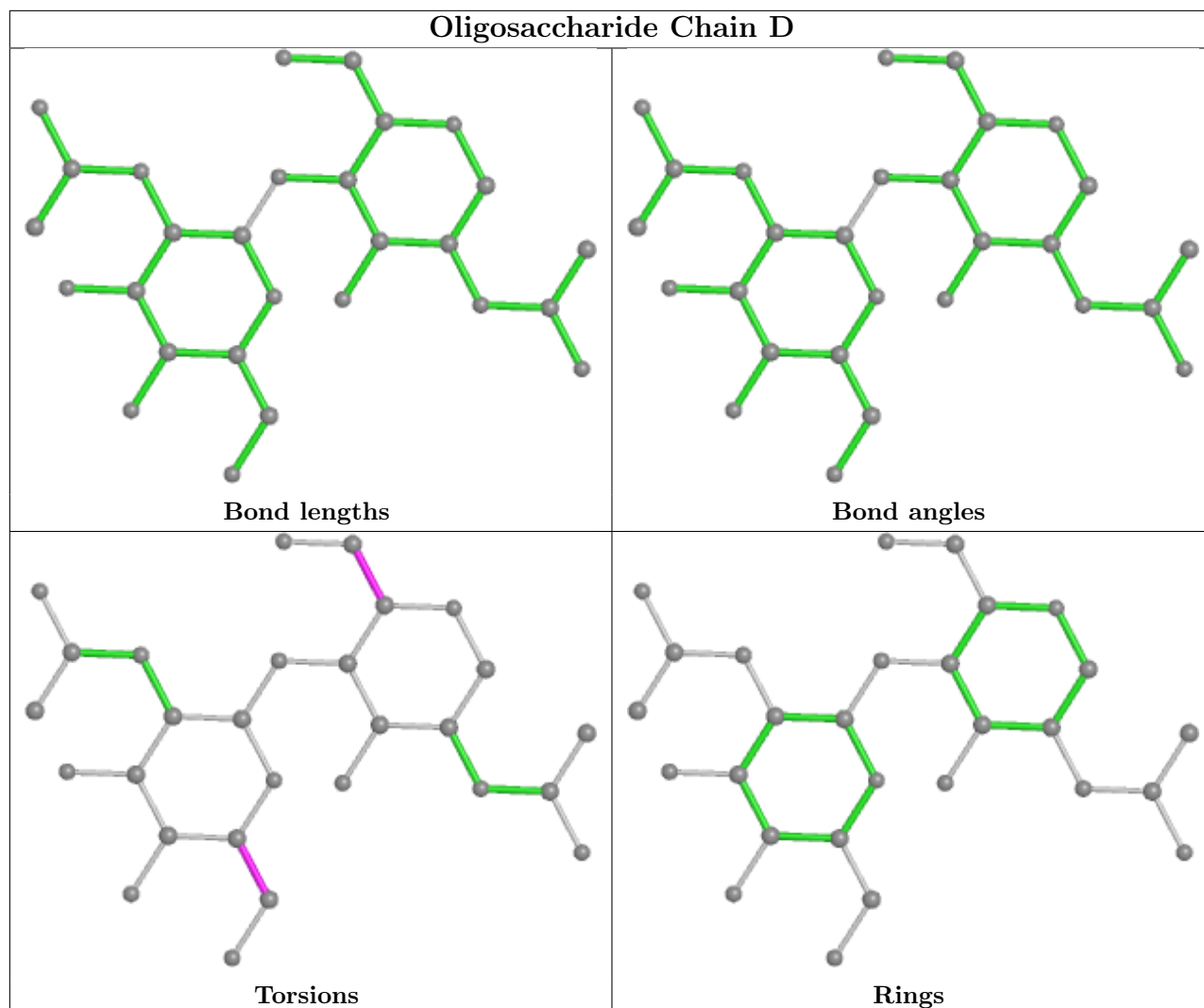
5 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	1	0
3	D	1	NAG	1	0
3	D	2	NAG	1	0
2	C	3	NAG	1	0
2	C	2	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](#)

5 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	NAG	B	501	1	14,14,15	0.44	0	17,19,21	0.75	0
5	NAG	A	503	1	14,14,15	0.41	0	17,19,21	0.84	1 (5%)
5	NAG	A	502	1	14,14,15	0.42	0	17,19,21	0.95	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	502	1	14,14,15	0.45	0	17,19,21	0.63	0
4	FUC	A	501	-	11,11,11	0.51	0	15,16,16	0.63	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
5	NAG	B	501	1	-	3/6/23/26	0/1/1/1
5	NAG	A	503	1	-	4/6/23/26	0/1/1/1
5	NAG	A	502	1	-	6/6/23/26	0/1/1/1
5	NAG	B	502	1	-	6/6/23/26	0/1/1/1
4	FUC	A	501	-	-	-	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(°)
5	A	502	NAG	C1-O5-C5	3.50	116.93	112.19
5	A	503	NAG	C1-C2-N2	2.57	114.88	110.49

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	502	NAG	C8-C7-N2-C2
5	A	502	NAG	O7-C7-N2-C2
5	A	503	NAG	C8-C7-N2-C2
5	B	501	NAG	C8-C7-N2-C2
5	B	501	NAG	O7-C7-N2-C2
5	A	502	NAG	C4-C5-C6-O6
5	A	503	NAG	O7-C7-N2-C2
5	B	502	NAG	C1-C2-N2-C7
5	A	502	NAG	O5-C5-C6-O6
5	B	502	NAG	C8-C7-N2-C2
5	B	502	NAG	C4-C5-C6-O6
5	A	502	NAG	C1-C2-N2-C7
5	A	503	NAG	O5-C5-C6-O6
5	B	502	NAG	O7-C7-N2-C2

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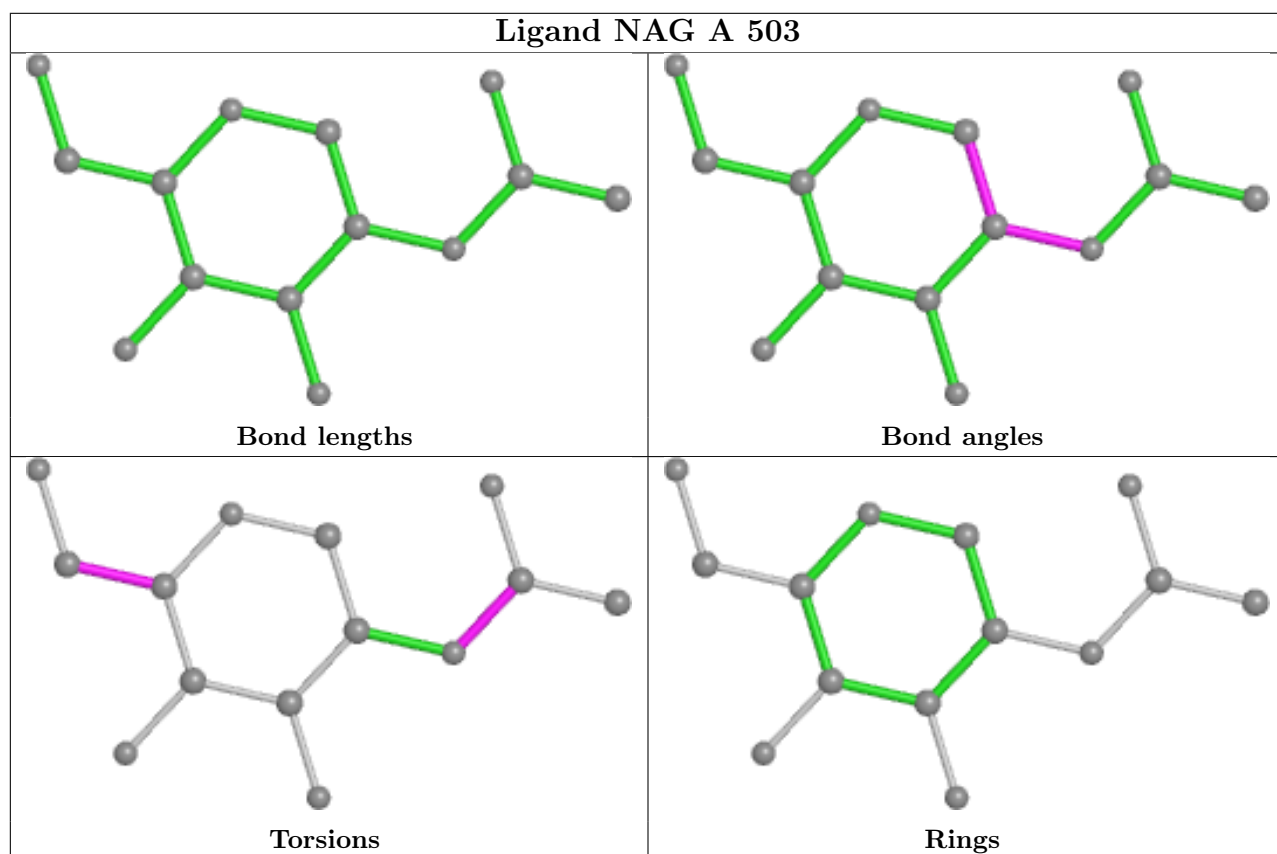
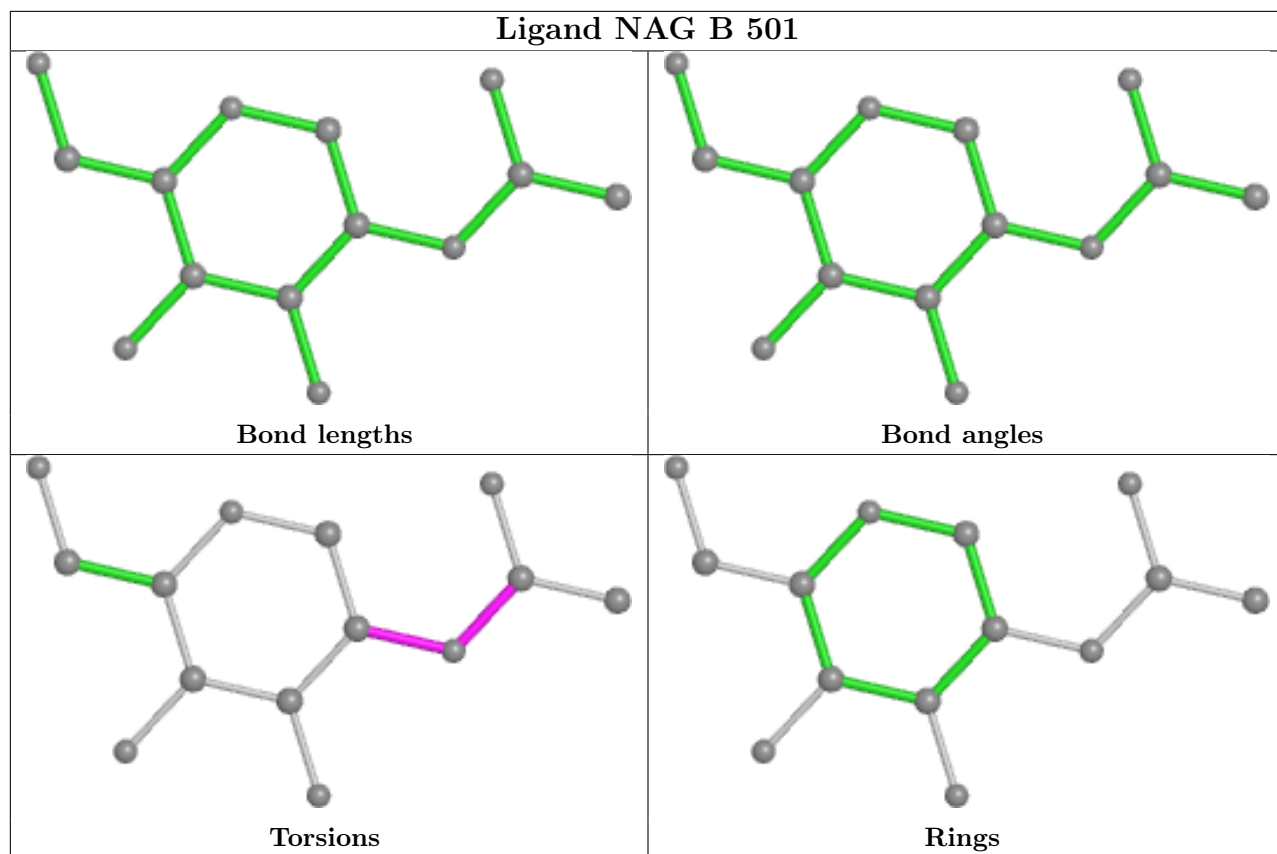
Mol	Chain	Res	Type	Atoms
5	B	501	NAG	C3-C2-N2-C7
5	B	502	NAG	O5-C5-C6-O6
5	A	502	NAG	C3-C2-N2-C7
5	B	502	NAG	C3-C2-N2-C7
5	A	503	NAG	C4-C5-C6-O6

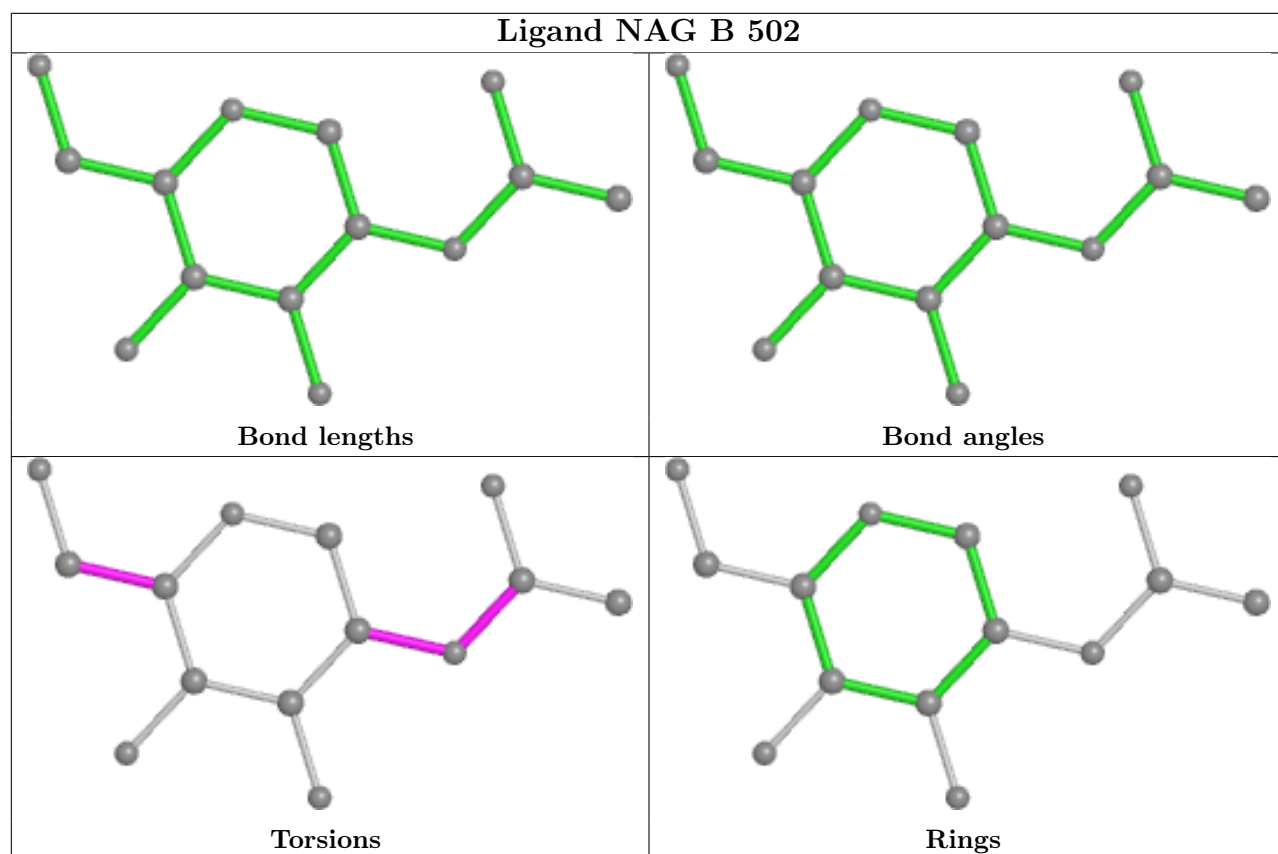
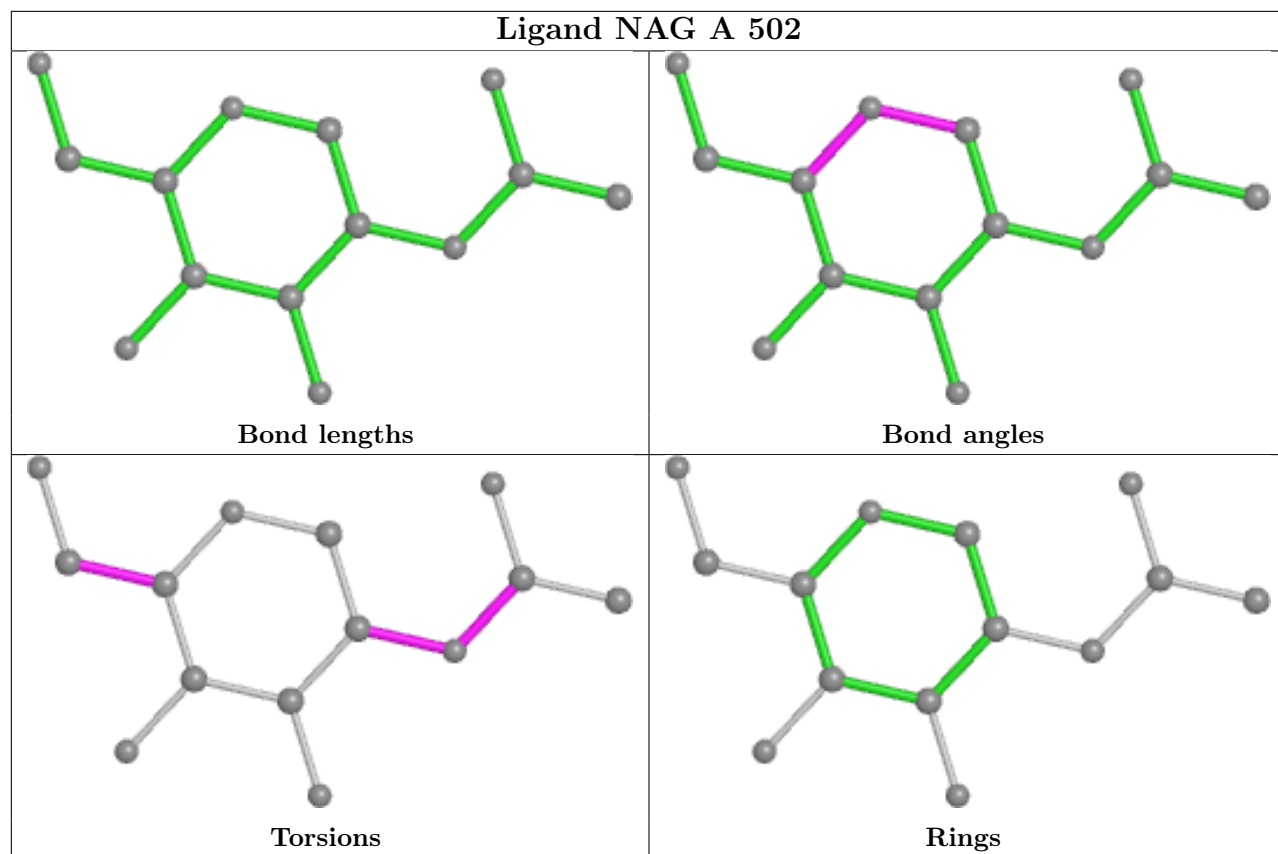
There are no ring outliers.

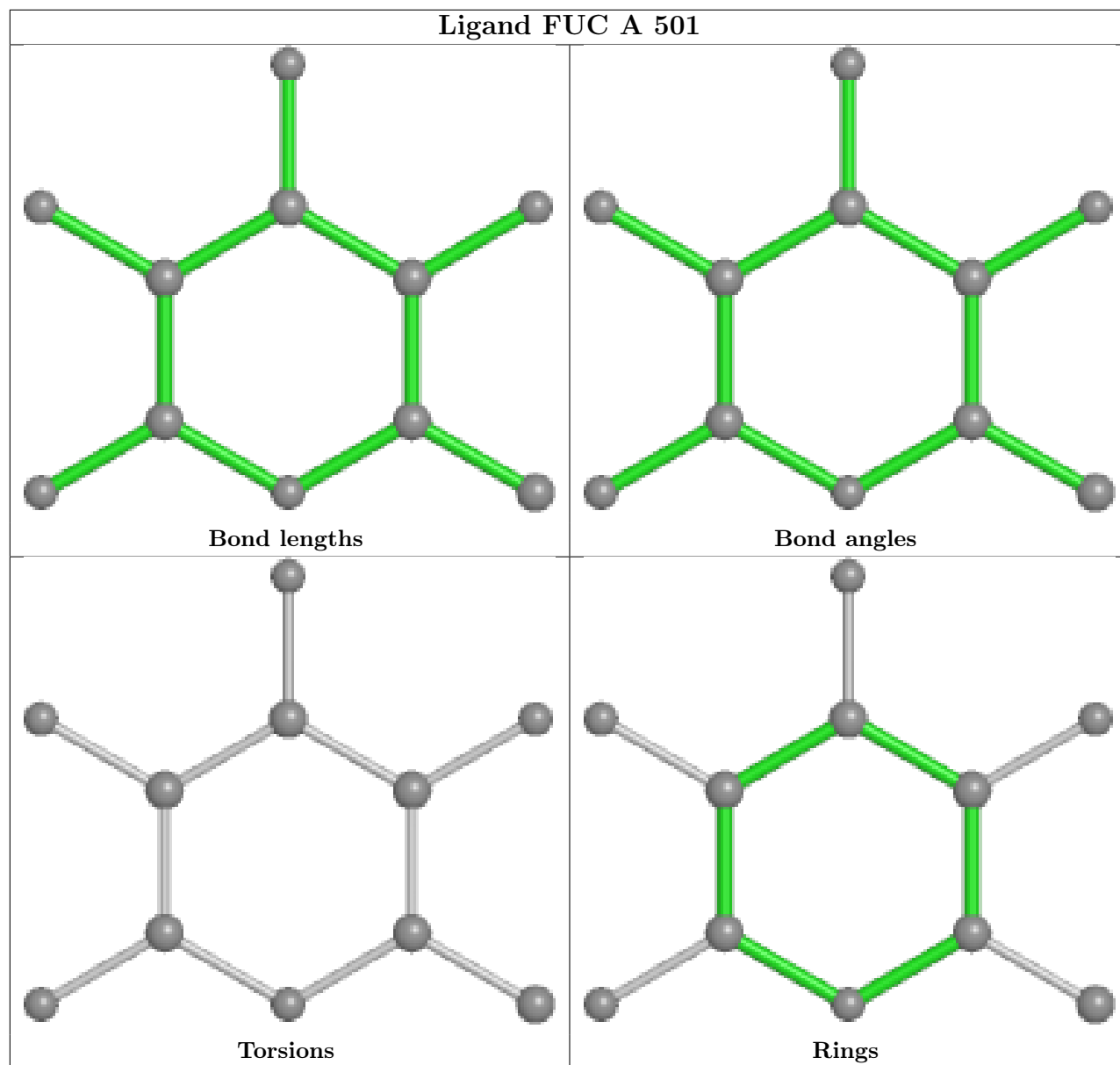
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	502	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 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 [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

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	354/425 (83%)	0.20	19 (5%) 25 23	180, 235, 311, 356	0
1	B	277/425 (65%)	0.25	14 (5%) 28 26	165, 224, 326, 374	0
All	All	631/850 (74%)	0.22	33 (5%) 27 26	165, 231, 317, 374	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	108	GLY	9.4
1	B	124	GLN	7.8
1	B	123	LEU	5.2
1	A	108	GLY	4.8
1	A	261	PRO	4.5
1	A	107	SER	3.9
1	B	265	TYR	3.7
1	A	350	LYS	3.4
1	A	109	ARG	2.9
1	B	125	ARG	2.9
1	B	302	PRO	2.9
1	A	295	PRO	2.8
1	A	353	GLY	2.7
1	A	344	VAL	2.6
1	B	319	LEU	2.5
1	B	330	HIS	2.4
1	A	325	TYR	2.4
1	B	56	LEU	2.4
1	A	266	ALA	2.4
1	A	342	LEU	2.4
1	B	263	THR	2.3
1	A	306	LYS	2.3
1	B	109	ARG	2.3
1	A	355	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	372	GLU	2.2
1	B	254	LEU	2.2
1	A	142	GLU	2.1
1	B	38	ALA	2.1
1	A	111	PRO	2.1
1	A	354	LEU	2.1
1	B	128	PHE	2.1
1	A	345	ILE	2.0
1	A	375	VAL	2.0

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 [\(i\)](#)

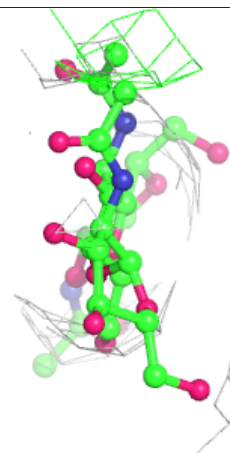
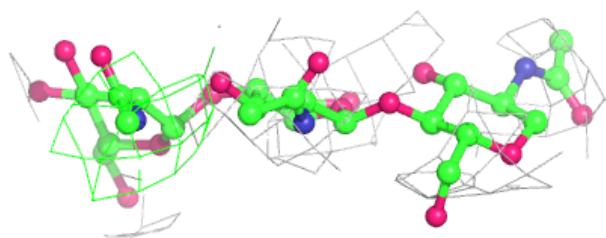
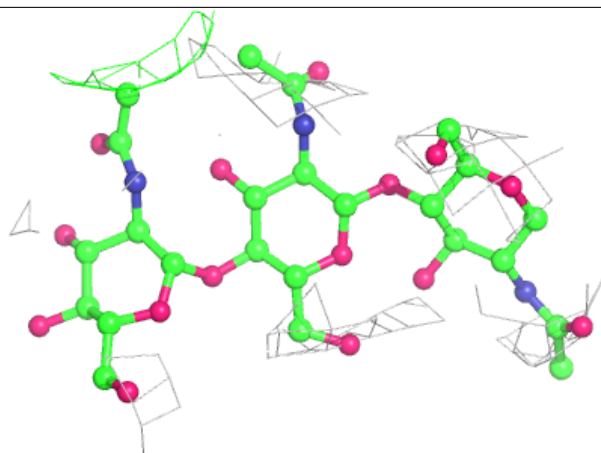
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	D	2	14/15	0.75	0.20	235,292,322,352	0
2	NAG	C	3	14/15	0.78	0.15	222,262,286,303	0
3	NAG	D	1	14/15	0.90	0.28	229,268,299,310	0
2	NAG	C	1	14/15	0.93	0.24	174,230,241,246	0
2	NAG	E	1	14/15	0.93	0.36	209,242,262,262	0
2	NAG	E	2	14/15	0.94	0.32	230,261,285,296	0
2	NAG	E	3	14/15	0.94	0.34	257,274,280,283	0
2	NAG	C	2	14/15	0.95	0.14	229,250,286,301	0

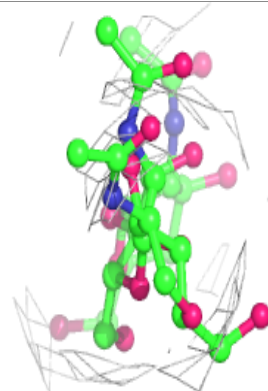
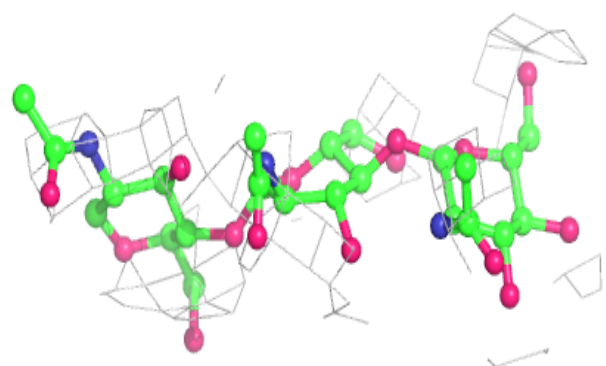
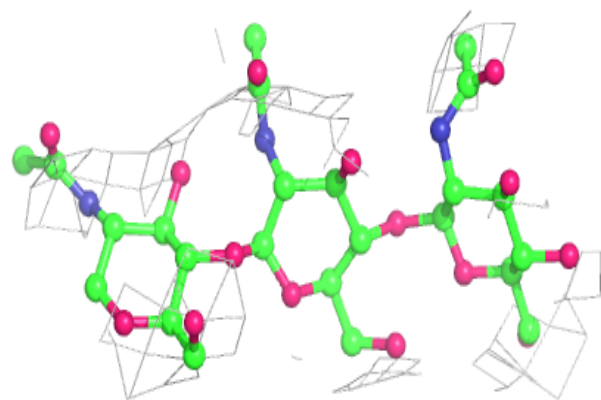
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

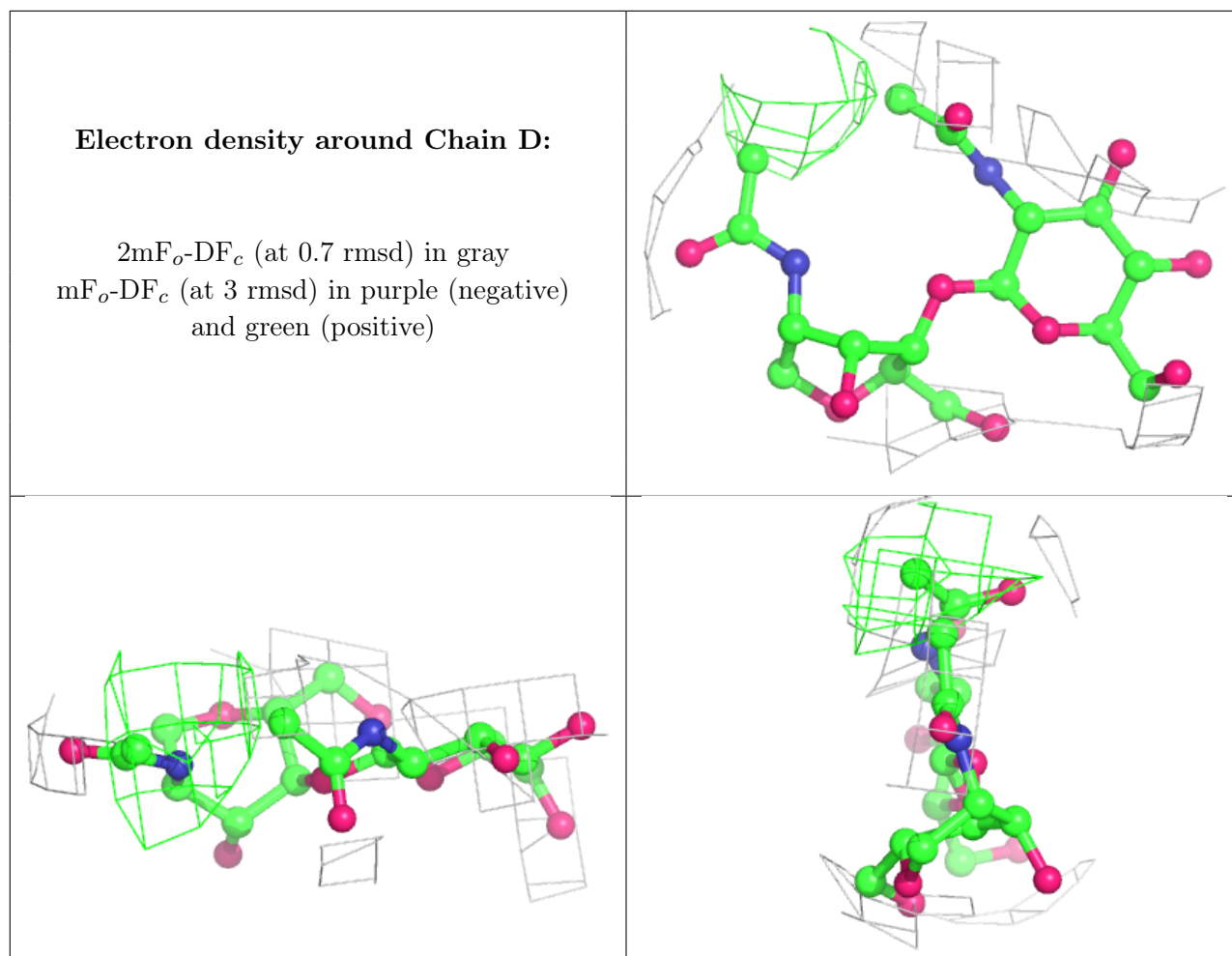
Electron density around Chain C:

$2mF_o-DF_c$ (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](#)

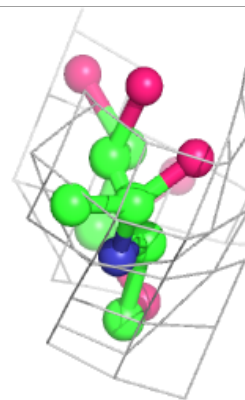
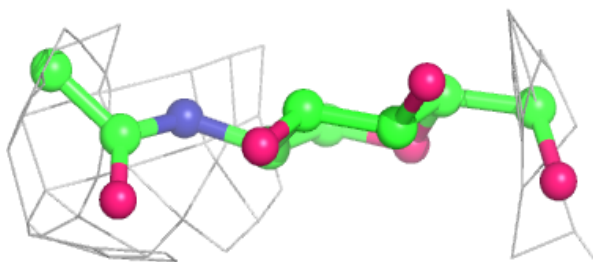
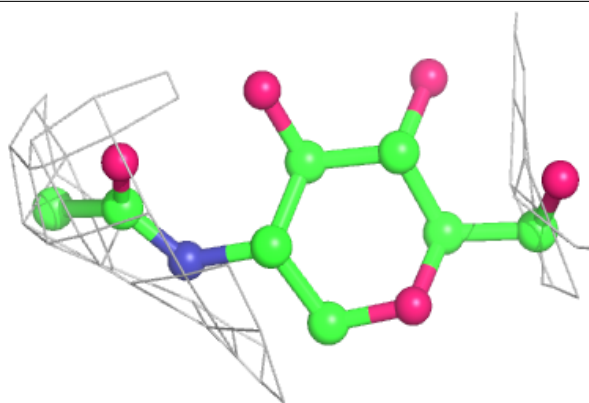
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	B	502	14/15	0.54	0.42	267,316,321,324	0
5	NAG	A	503	14/15	0.70	0.18	279,346,360,363	0
4	FUC	A	501	11/11	0.83	0.13	213,259,275,278	0
5	NAG	A	502	14/15	0.84	0.18	265,293,302,304	0
5	NAG	B	501	14/15	0.92	0.38	251,279,294,304	0

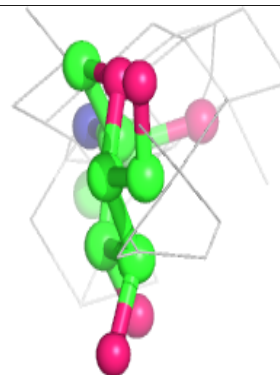
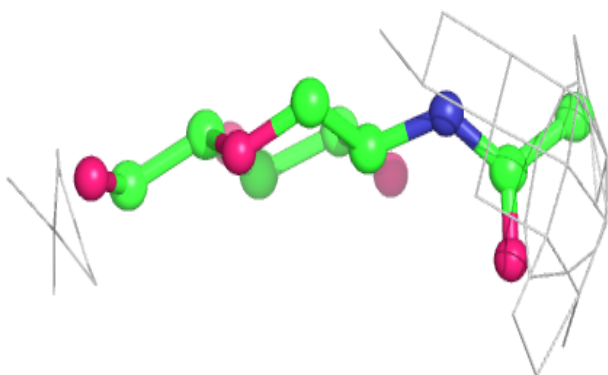
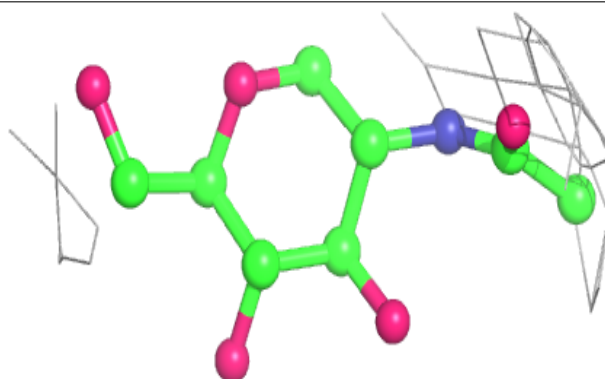
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

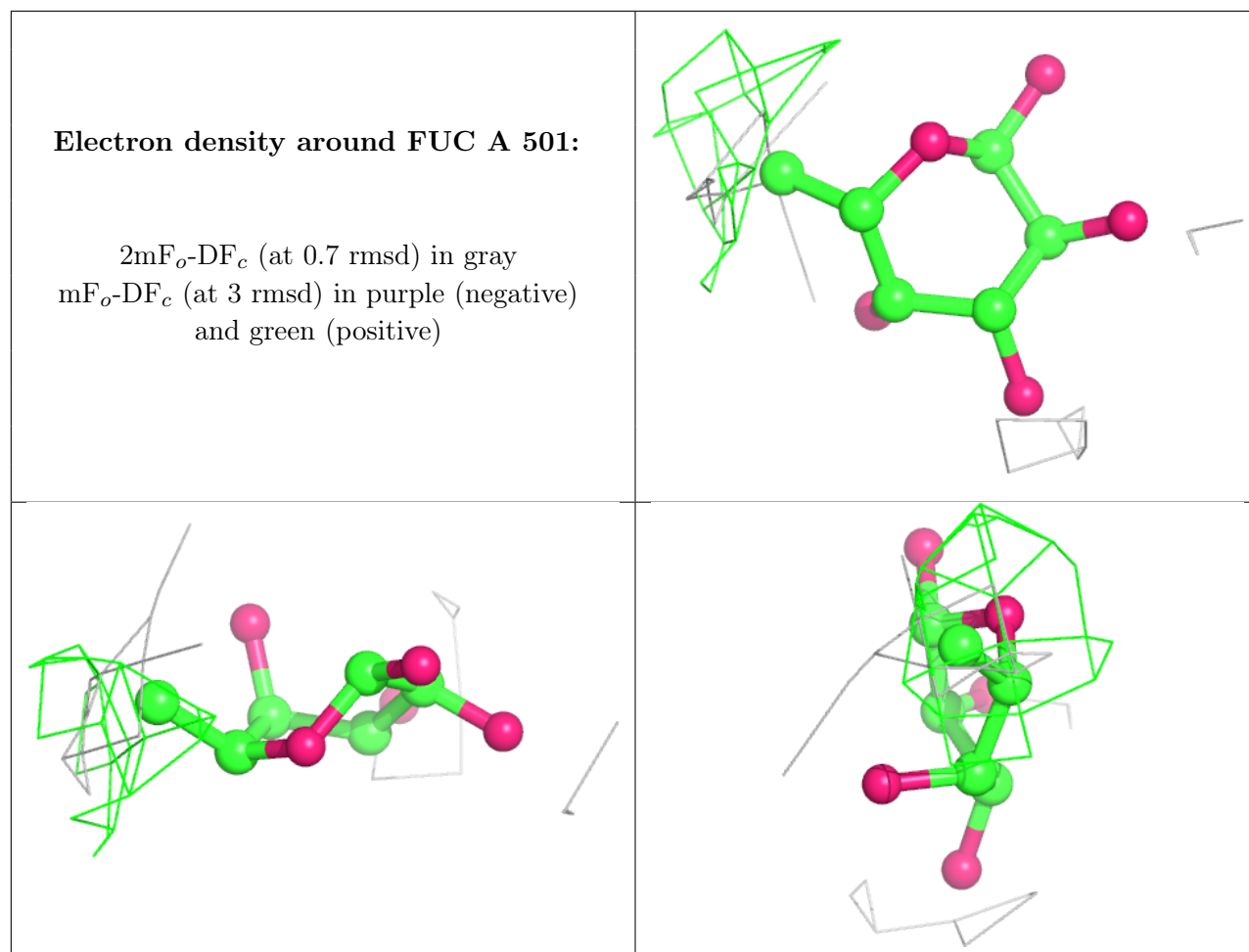
Electron density around NAG B 502:

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

**Electron density around NAG A 503:**

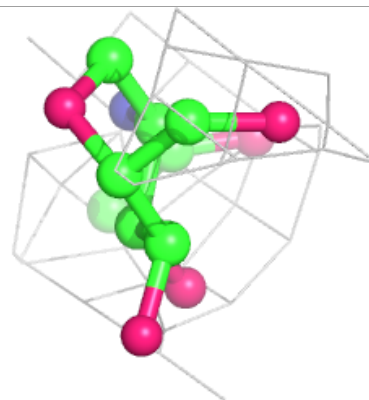
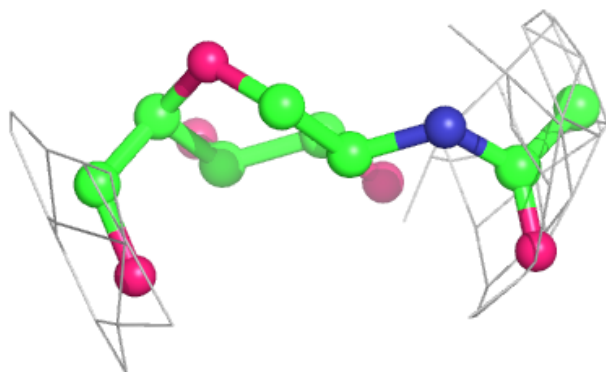
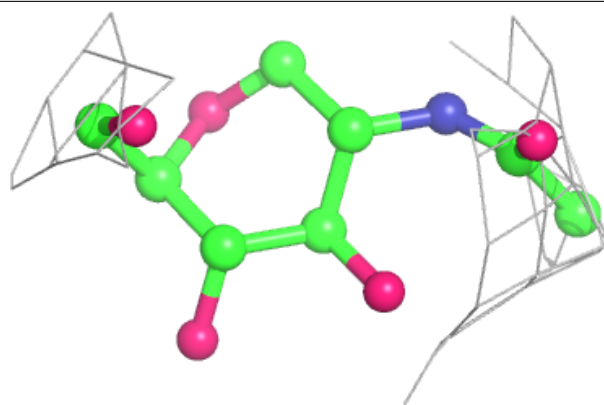
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



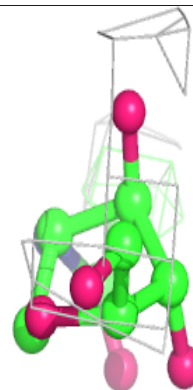
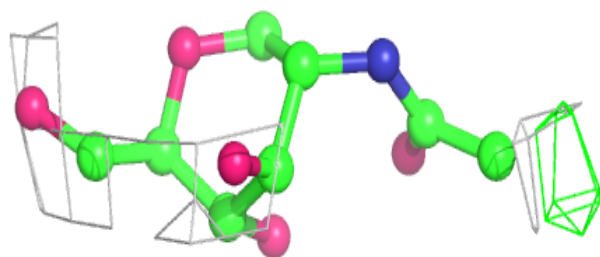
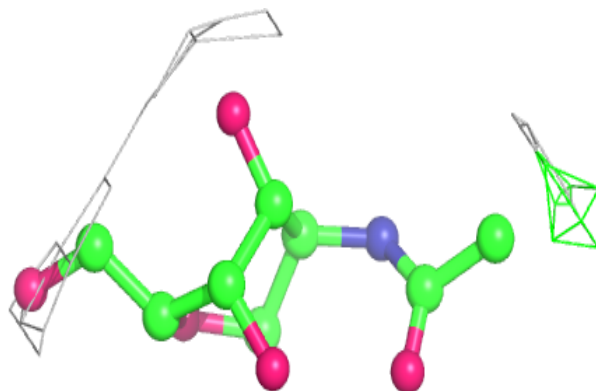


Electron density around NAG A 502:

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

**Electron density around NAG B 501:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.