



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 08:47 AM BST

PDB ID : 6ATK
Title : Crystal structure of the human coronavirus 229E spike protein receptor binding domain in complex with human aminopeptidase N
Authors : Wong, A.H.; Rini, J.M.
Deposited on : 2017-08-29
Resolution : 3.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

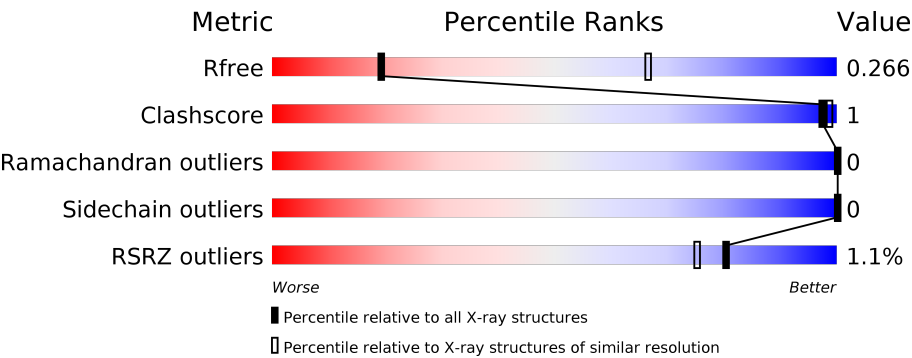
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

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 3.50 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.








Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 $\leq 5\%$. 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	905	<div><div></div><div>97%</div><div>..</div></div>
1	B	905	<div><div>%</div><div>96%</div><div>..</div></div>
1	C	905	<div><div>2%</div><div>95%</div><div>..</div></div>
2	D	146	<div><div>4%</div><div>51%</div><div>47%</div><div>.</div></div>
2	E	146	<div><div>2%</div><div>90%</div><div>8%</div><div>.</div></div>
2	F	146	<div><div>8%</div><div>92%</div></div>

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Mol	Chain	Length	Quality of chain
3	G	2	 100%
3	H	2	 100%
3	I	2	 100%
3	J	2	 100%
3	K	2	 100%

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
4	NAG	C	1007	-	-	-	X
4	NAG	D	1001	-	-	-	X
4	NAG	E	1002	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23660 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 Aminopeptidase N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	892	Total	C	N	O	S	0	0	0
			7206	4593	1217	1372	24			
1	B	892	Total	C	N	O	S	0	0	0
			7206	4593	1217	1372	24			
1	C	891	Total	C	N	O	S	0	0	0
			7198	4589	1216	1369	24			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	GLY	-	expression tag	UNP P15144
A	64	ARG	-	expression tag	UNP P15144
A	65	PRO	-	expression tag	UNP P15144
B	63	GLY	-	expression tag	UNP P15144
B	64	ARG	-	expression tag	UNP P15144
B	65	PRO	-	expression tag	UNP P15144
C	63	GLY	-	expression tag	UNP P15144
C	64	ARG	-	expression tag	UNP P15144
C	65	PRO	-	expression tag	UNP P15144

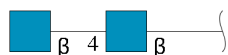
- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	134	Total	C	N	O	S	0	0	0
			1025	667	165	185	8			
2	D	78	Total	C	N	O	S	0	0	0
			598	390	96	106	6			
2	F	11	Total	C	N	O	S	0	0	0
			74	44	14	14	2			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	290	GLY	-	expression tag	UNP P15423
E	291	ARG	-	expression tag	UNP P15423
E	292	PRO	-	expression tag	UNP P15423
E	300	MET	THR	conflict	UNP P15423
E	414	THR	SER	conflict	UNP P15423
D	290	GLY	-	expression tag	UNP P15423
D	291	ARG	-	expression tag	UNP P15423
D	292	PRO	-	expression tag	UNP P15423
D	300	MET	THR	conflict	UNP P15423
D	414	THR	SER	conflict	UNP P15423
F	290	GLY	-	expression tag	UNP P15423
F	291	ARG	-	expression tag	UNP P15423
F	292	PRO	-	expression tag	UNP P15423
F	300	MET	THR	conflict	UNP P15423
F	414	THR	SER	conflict	UNP P15423

- 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
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		
5	A	1	Total	Zn	0	0
			1	1		
5	C	1	Total	Zn	0	0
			1	1		

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 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.

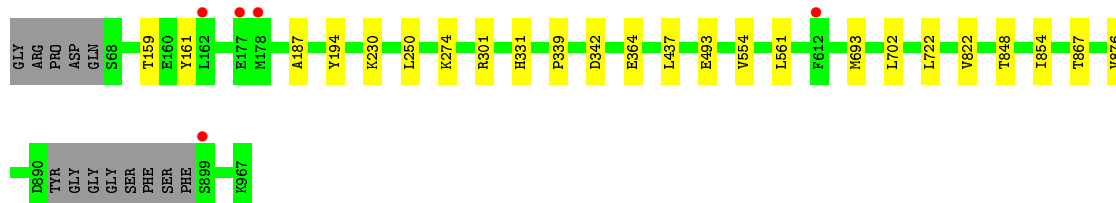
- Molecule 1: Aminopeptidase N

Chain A:  97%



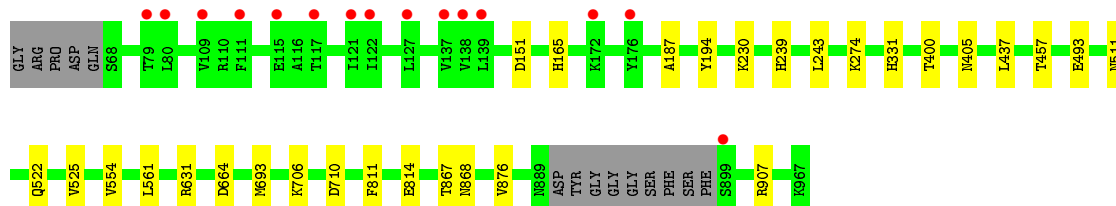
- Molecule 1: Aminopeptidase N

Chain B:  96%




- Molecule 1: Aminopeptidase N

Chain C:  95%



- Molecule 2: Spike glycoprotein

Chain E:  90% 8%



- Molecule 2: Spike glycoprotein

Mol
196
Mag

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

Chain K:

100%

Mol
196
Mag

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	153.82Å 153.82Å 322.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.80 – 3.50 49.79 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.80-3.50) 99.6 (49.79-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.12 _2829	Depositor
R, R_{free}	0.244 , 0.267 0.244 , 0.266	Depositor DCC
R_{free} test set	1991 reflections (3.56%)	wwPDB-VP
Wilson B-factor (Å ²)	94.7	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 30.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	23660	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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: ZN, 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	0.26	0/7390	0.48	0/10065
1	B	0.27	0/7390	0.48	0/10065
1	C	0.26	0/7382	0.48	0/10054
2	D	0.26	0/614	0.40	0/832
2	E	0.29	0/1058	0.44	0/1441
2	F	0.26	0/75	0.37	0/97
All	All	0.27	0/23909	0.47	0/32554

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	7206	0	6980	5	0
1	B	7206	0	6982	13	0
1	C	7198	0	6978	15	0
2	D	598	0	566	2	0
2	E	1025	0	980	2	0
2	F	74	0	65	0	0
3	G	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
4	A	70	0	65	0	0
4	B	42	0	39	0	0
4	C	56	0	52	0	0
4	D	14	0	13	0	0
4	E	28	0	26	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
All	All	23660	0	22871	37	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 1.

All (37) 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:C:554:VAL:HG22	1:C:561:LEU:HD22	1.96	0.47
1:B:187:ALA:O	1:B:194:TYR:HB2	2.15	0.47
2:E:364:ILE:HG13	2:E:364:ILE:O	2.16	0.46
1:A:554:VAL:HG22	1:A:561:LEU:HD22	1.98	0.45
1:B:437:LEU:N	1:B:437:LEU:HD12	2.30	0.45
1:B:301:ARG:HB2	1:B:342:ASP:OD1	2.16	0.45
1:A:864:ILE:O	1:A:867:THR:HG22	2.16	0.45
1:B:867:THR:CG2	1:B:876:VAL:HG11	2.47	0.45
1:B:554:VAL:HG22	1:B:561:LEU:HD22	2.00	0.44
1:B:250:LEU:CD1	1:B:339:PRO:HG2	2.47	0.44
1:C:230:LYS:HB3	1:C:274:LYS:HG2	2.00	0.44
1:A:187:ALA:O	1:A:194:TYR:HB2	2.17	0.44
1:C:811:PHE:O	1:C:814:GLU:HG2	2.17	0.44
1:C:706:LYS:O	1:C:710:ASP:HB2	2.16	0.44
1:C:331:HIS:NE2	1:C:493:GLU:OE2	2.49	0.44
1:C:522:GLN:O	1:C:525:VAL:HG22	2.17	0.44
1:C:868:ASN:OD1	1:C:907:ARG:NH2	2.43	0.44
2:D:308:PHE:HA	2:D:324:GLY:O	2.17	0.43
1:C:239:HIS:ND1	1:C:243:LEU:O	2.51	0.43
1:C:437:LEU:HD11	1:C:693:MET:HG3	2.01	0.43
2:E:364:ILE:HG22	2:E:400:ILE:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:HIS:NE2	1:B:493:GLU:OE2	2.50	0.42
2:D:311:GLN:CG	2:D:323:ALA:HB2	2.50	0.42
1:A:507:PHE:CE2	1:A:516:ASN:HB3	2.56	0.41
1:B:364:GLU:HB2	1:B:822:VAL:HG21	2.03	0.41
1:C:400:THR:O	1:C:511:ASN:HA	2.21	0.41
1:C:405:ASN:HB2	1:C:457:THR:O	2.21	0.40
1:B:437:LEU:HD11	1:B:693:MET:CG	2.51	0.40
1:C:151:ASP:HB3	1:C:165:HIS:O	2.21	0.40
1:B:159:THR:HB	1:B:161:TYR:CE2	2.57	0.40
1:C:631:ARG:NH1	1:C:664:ASP:OD1	2.50	0.40
1:B:702:LEU:HD13	1:B:722:LEU:HD21	2.02	0.40
1:B:848:THR:HA	1:B:854:ILE:HD12	2.03	0.40
1:C:867:THR:CG2	1:C:876:VAL:HG11	2.52	0.40
1:A:591:ILE:HG22	1:A:596:GLN:HA	2.03	0.40
1:B:230:LYS:HB3	1:B:274:LYS:HG2	2.04	0.40
1:C:187:ALA:O	1:C:194:TYR:HB2	2.20	0.40

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	888/905 (98%)	868 (98%)	20 (2%)	0	100	100
1	B	888/905 (98%)	866 (98%)	22 (2%)	0	100	100
1	C	887/905 (98%)	866 (98%)	21 (2%)	0	100	100
2	D	68/146 (47%)	62 (91%)	6 (9%)	0	100	100
2	E	132/146 (90%)	114 (86%)	18 (14%)	0	100	100
2	F	9/146 (6%)	9 (100%)	0	0	100	100
All	All	2872/3153 (91%)	2785 (97%)	87 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	793/802 (99%)	793 (100%)	0	100	100
1	B	793/802 (99%)	793 (100%)	0	100	100
1	C	792/802 (99%)	792 (100%)	0	100	100
2	D	64/121 (53%)	64 (100%)	0	100	100
2	E	111/121 (92%)	111 (100%)	0	100	100
2	F	8/121 (7%)	8 (100%)	0	100	100
All	All	2561/2769 (92%)	2561 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

10 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	G	1	1,3	14,14,15	0.23	0	17,19,21	0.57	0
3	NAG	G	2	3	14,14,15	0.27	0	17,19,21	0.48	0
3	NAG	H	1	1,3	14,14,15	0.25	0	17,19,21	0.46	0
3	NAG	H	2	3	14,14,15	0.21	0	17,19,21	0.38	0
3	NAG	I	1	1,3	14,14,15	0.24	0	17,19,21	0.46	0
3	NAG	I	2	3	14,14,15	0.27	0	17,19,21	0.40	0
3	NAG	J	1	1,3	14,14,15	0.24	0	17,19,21	0.46	0
3	NAG	J	2	3	14,14,15	0.18	0	17,19,21	0.45	0
3	NAG	K	1	1,3	14,14,15	0.25	0	17,19,21	0.49	0
3	NAG	K	2	3	14,14,15	0.25	0	17,19,21	0.45	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
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	1/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6

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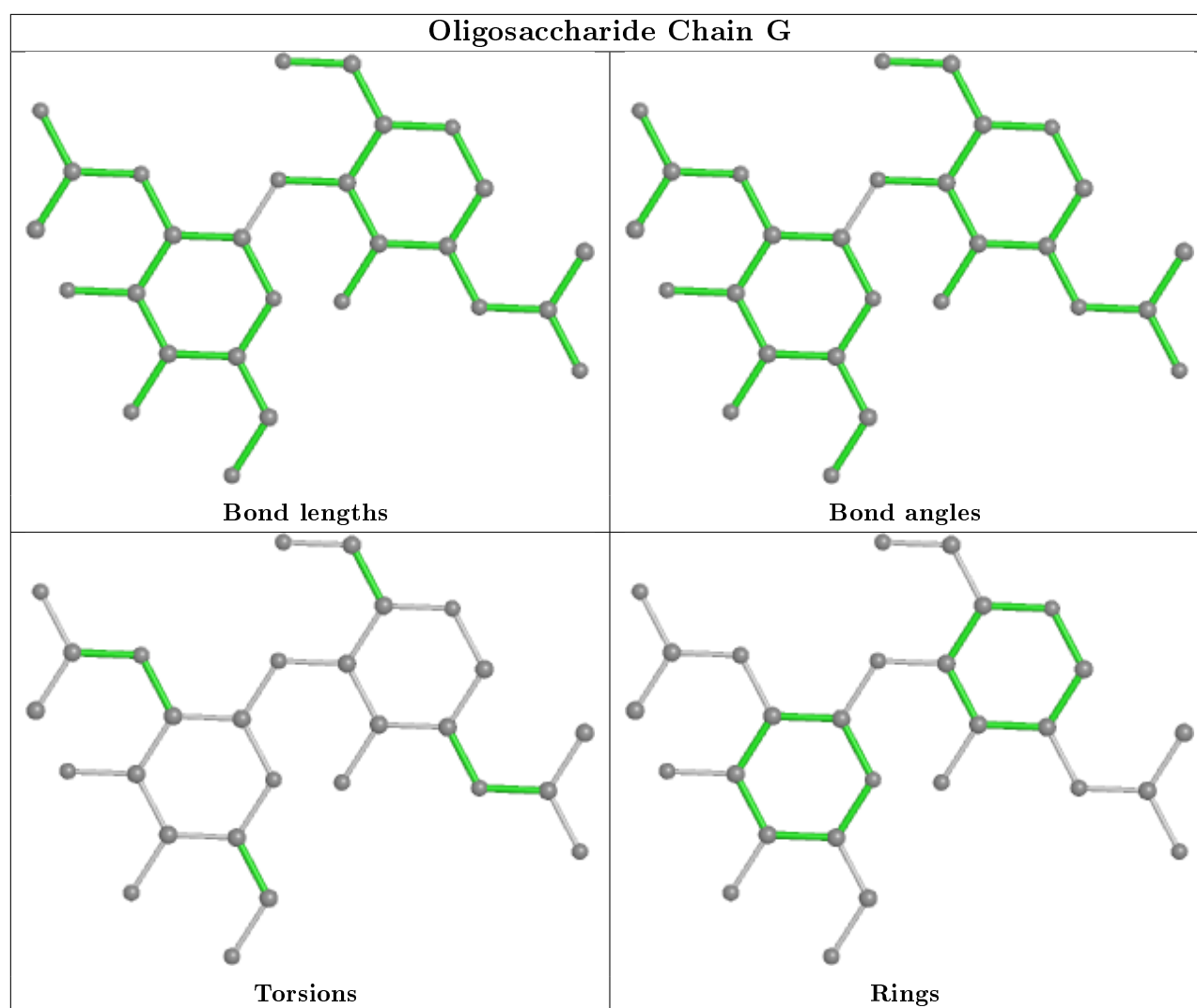
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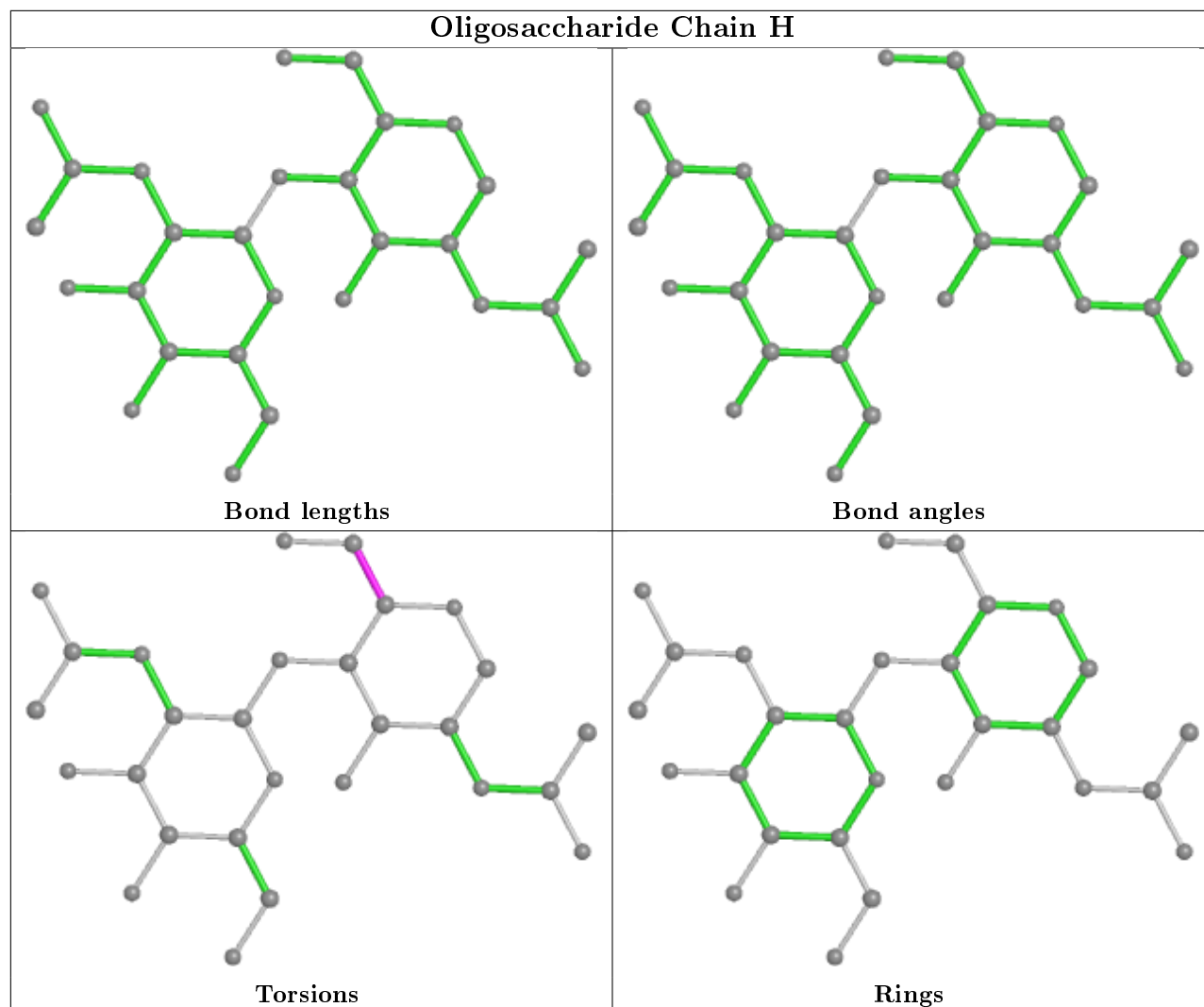
Mol	Chain	Res	Type	Atoms
3	J	2	NAG	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6

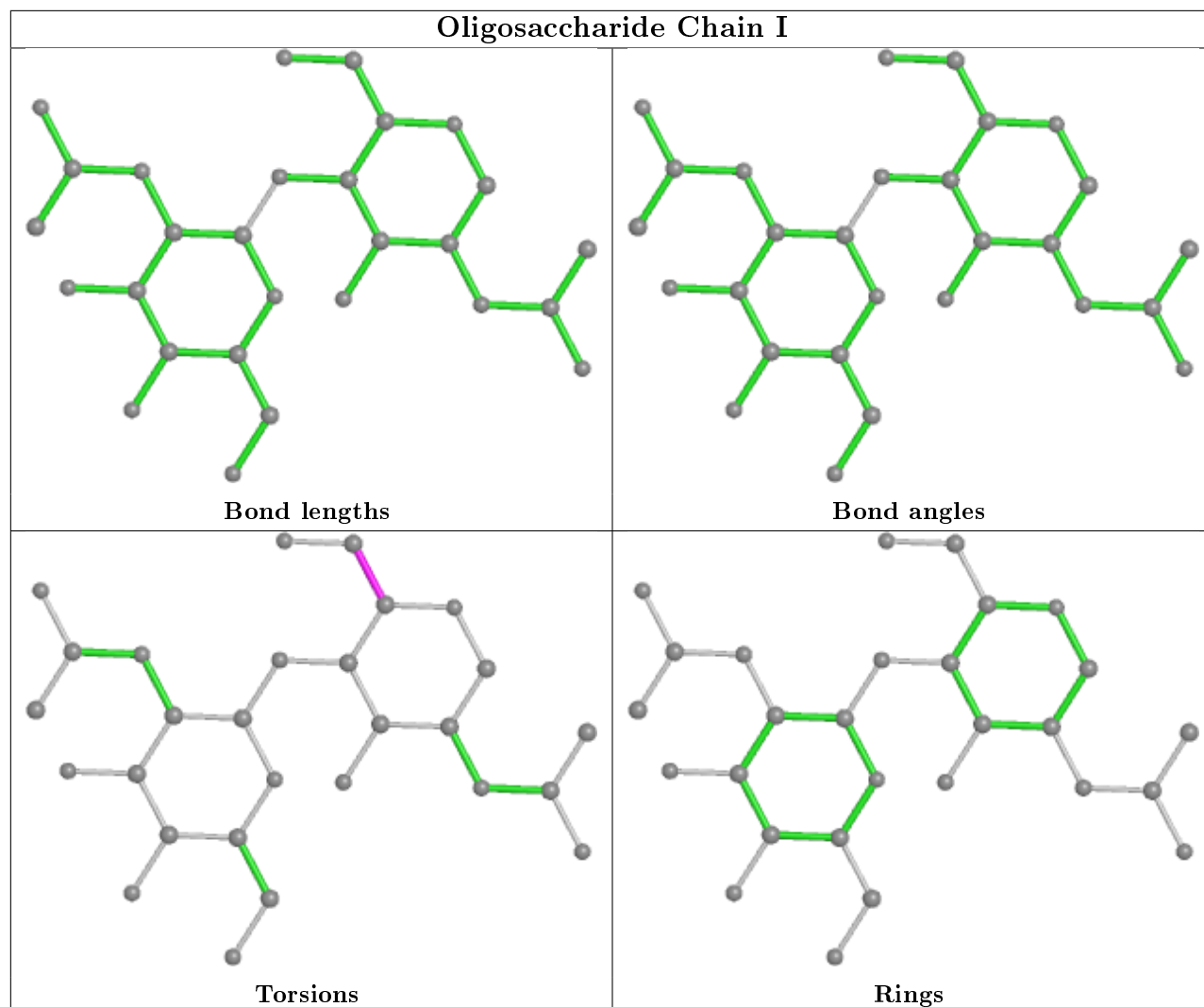
There are no ring outliers.

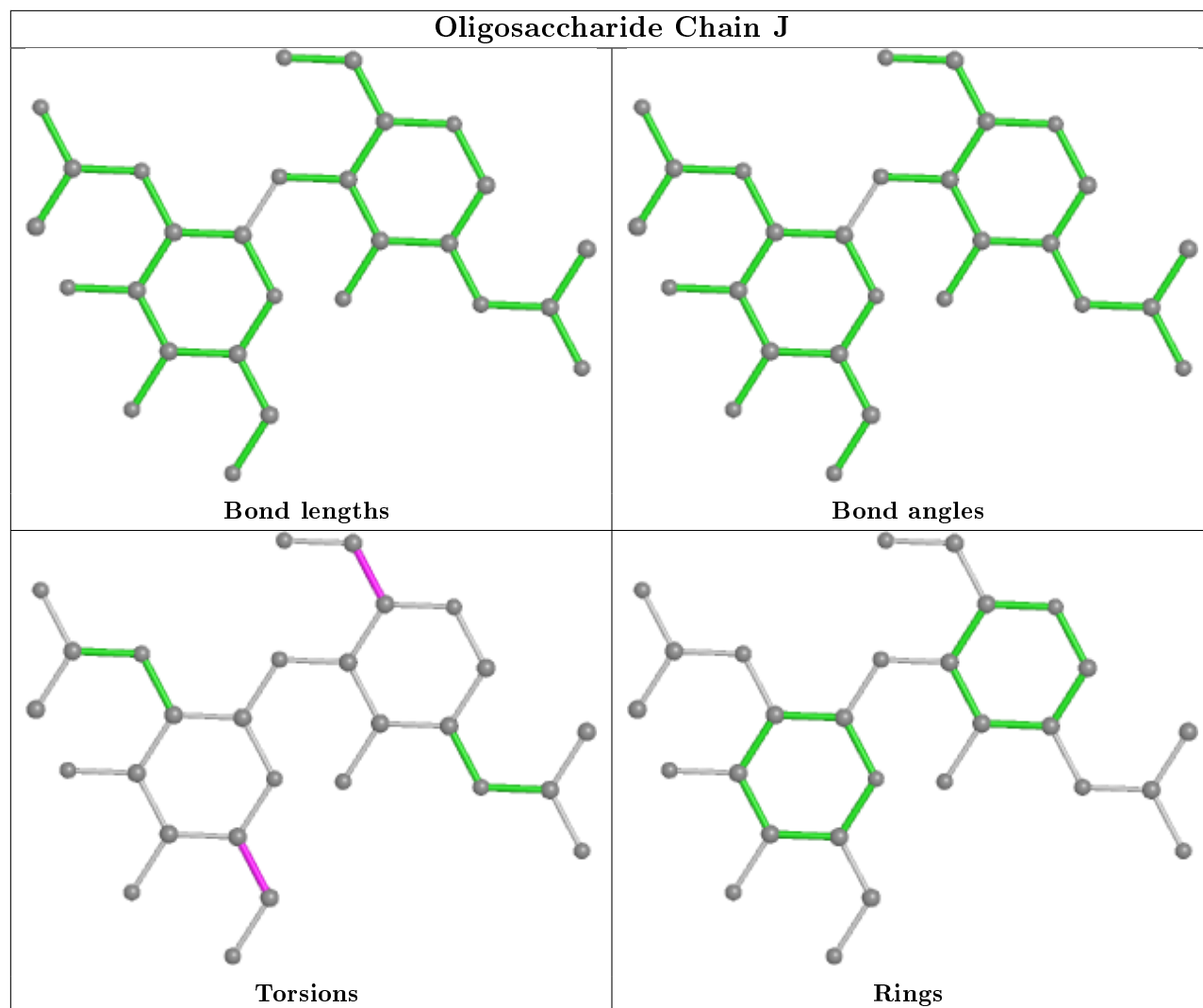
No monomer is involved in short contacts.

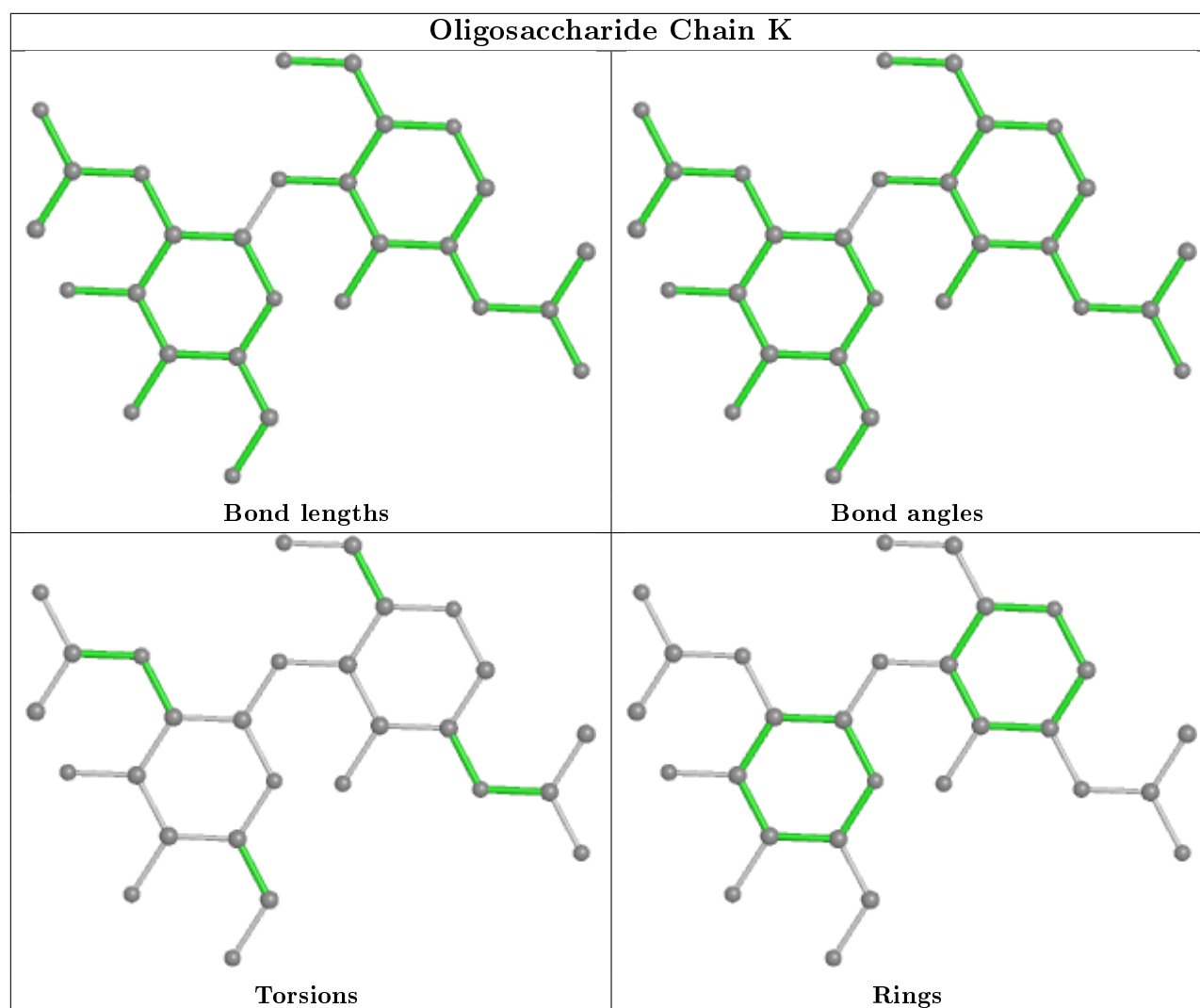
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 3 are monoatomic - leaving 15 for Mogul analysis.

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	A	1008	1	14,14,15	0.28	0	17,19,21	0.32	0
4	NAG	A	1010	1	14,14,15	0.24	0	17,19,21	0.32	0
4	NAG	A	1005	1	14,14,15	0.19	0	17,19,21	0.36	0
4	NAG	D	1001	2	14,14,15	0.37	0	17,19,21	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1004	1	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	B	1004	1	14,14,15	0.16	0	17,19,21	0.40	0
4	NAG	E	1001	2	14,14,15	0.35	0	17,19,21	0.50	0
4	NAG	B	1003	1	14,14,15	0.33	0	17,19,21	0.32	0
4	NAG	C	1001	1	14,14,15	0.28	0	17,19,21	0.44	0
4	NAG	B	1007	1	14,14,15	0.23	0	17,19,21	0.52	0
4	NAG	C	1005	1	14,14,15	0.24	0	17,19,21	0.55	0
4	NAG	C	1002	1	14,14,15	0.25	0	17,19,21	0.40	0
4	NAG	E	1002	2	14,14,15	0.29	0	17,19,21	0.46	0
4	NAG	A	1001	1	14,14,15	0.23	0	17,19,21	0.40	0
4	NAG	C	1007	1	14,14,15	0.33	0	17,19,21	0.52	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	1008	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1010	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1005	1	-	2/6/23/26	0/1/1/1
4	NAG	D	1001	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1004	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1004	1	-	2/6/23/26	0/1/1/1
4	NAG	E	1001	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1003	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1001	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1007	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1005	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1002	1	-	2/6/23/26	0/1/1/1
4	NAG	E	1002	2	-	4/6/23/26	0/1/1/1
4	NAG	A	1001	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1007	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1007	NAG	O5-C5-C6-O6
4	C	1002	NAG	C4-C5-C6-O6
4	E	1002	NAG	O5-C5-C6-O6
4	C	1007	NAG	O5-C5-C6-O6
4	A	1005	NAG	C4-C5-C6-O6
4	B	1007	NAG	C4-C5-C6-O6
4	C	1007	NAG	C4-C5-C6-O6
4	B	1003	NAG	C4-C5-C6-O6
4	A	1010	NAG	O5-C5-C6-O6
4	B	1003	NAG	O5-C5-C6-O6
4	C	1002	NAG	O5-C5-C6-O6
4	A	1005	NAG	O5-C5-C6-O6
4	A	1004	NAG	C4-C5-C6-O6
4	E	1002	NAG	C4-C5-C6-O6
4	B	1004	NAG	C4-C5-C6-O6
4	A	1010	NAG	C4-C5-C6-O6
4	E	1002	NAG	C8-C7-N2-C2
4	E	1002	NAG	O7-C7-N2-C2
4	A	1004	NAG	O5-C5-C6-O6
4	E	1001	NAG	O5-C5-C6-O6
4	B	1004	NAG	O5-C5-C6-O6
4	D	1001	NAG	O5-C5-C6-O6
4	A	1010	NAG	C1-C2-N2-C7
4	C	1001	NAG	O5-C5-C6-O6
4	E	1001	NAG	C4-C5-C6-O6
4	C	1005	NAG	O5-C5-C6-O6
4	D	1001	NAG	C4-C5-C6-O6
4	C	1005	NAG	C4-C5-C6-O6
4	A	1008	NAG	C1-C2-N2-C7
4	A	1001	NAG	C4-C5-C6-O6
4	A	1001	NAG	O5-C5-C6-O6
4	A	1008	NAG	C3-C2-N2-C7
4	A	1010	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	892/905 (98%)	-0.20	2 (0%) 95 93	59, 84, 109, 127	0
1	B	892/905 (98%)	-0.12	5 (0%) 89 86	60, 88, 125, 147	0
1	C	891/905 (98%)	-0.03	15 (1%) 70 64	86, 107, 149, 166	0
2	D	78/146 (53%)	0.57	6 (7%) 13 13	87, 123, 136, 146	0
2	E	134/146 (91%)	0.05	3 (2%) 62 56	69, 89, 119, 130	0
2	F	11/146 (7%)	0.40	0 100 100	107, 118, 120, 121	0
All	All	2898/3153 (91%)	-0.09	31 (1%) 80 75	59, 95, 131, 166	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	79	THR	3.4
2	D	366	THR	3.3
1	B	178	MET	3.2
1	B	899	SER	3.2
1	A	579	GLU	3.1
1	C	117	THR	3.0
1	C	111	PHE	3.0
2	D	399	PRO	2.7
1	C	139	LEU	2.5
1	C	137	VAL	2.5
1	C	80	LEU	2.4
1	C	115	GLU	2.4
2	D	387	PHE	2.4
1	C	109	VAL	2.4
2	E	426	THR	2.3
2	D	365	ASN	2.3
1	B	162	LEU	2.2
1	C	138	VAL	2.2
1	C	899	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	177	GLU	2.2
1	A	176	TYR	2.2
2	E	356	ASN	2.2
1	C	122	ILE	2.2
1	C	127	LEU	2.2
1	C	176	TYR	2.1
2	D	371	PHE	2.1
1	B	612	PHE	2.1
1	C	121	ILE	2.0
2	D	305	TYR	2.0
1	C	172	LYS	2.0
2	E	375	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

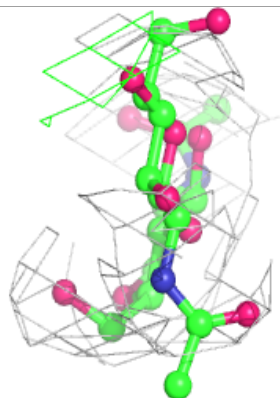
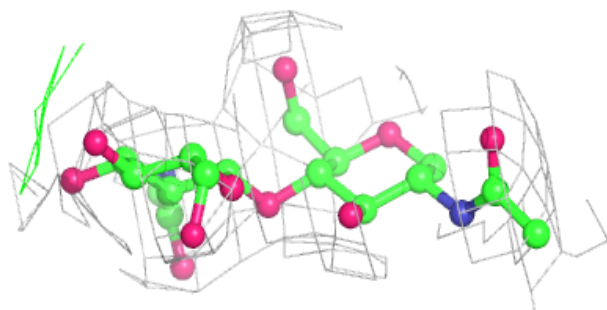
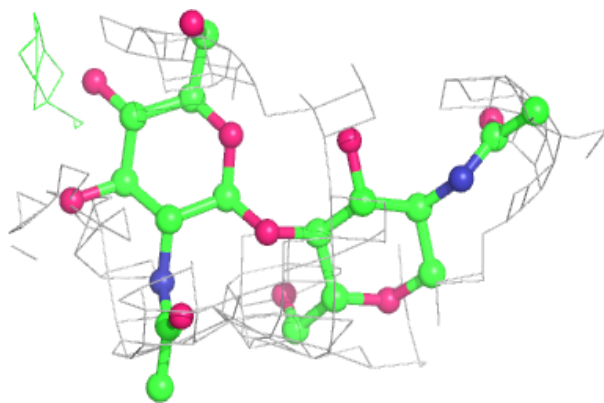
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	K	2	14/15	0.80	0.23	127,135,140,143	0
3	NAG	I	2	14/15	0.80	0.26	102,104,109,114	0
3	NAG	G	2	14/15	0.81	0.28	97,99,104,109	0
3	NAG	J	2	14/15	0.83	0.25	99,107,112,115	0
3	NAG	H	2	14/15	0.83	0.21	109,116,121,124	0
3	NAG	K	1	14/15	0.89	0.24	112,116,122,124	0
3	NAG	I	1	14/15	0.90	0.23	94,98,102,103	0
3	NAG	H	1	14/15	0.91	0.18	97,101,106,108	0
3	NAG	G	1	14/15	0.92	0.12	84,87,91,93	0
3	NAG	J	1	14/15	0.95	0.16	90,95,100,102	0

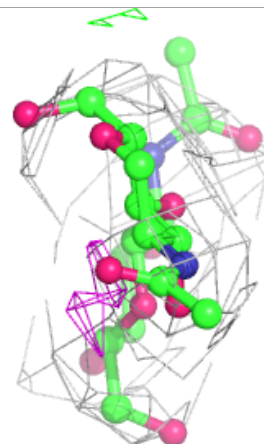
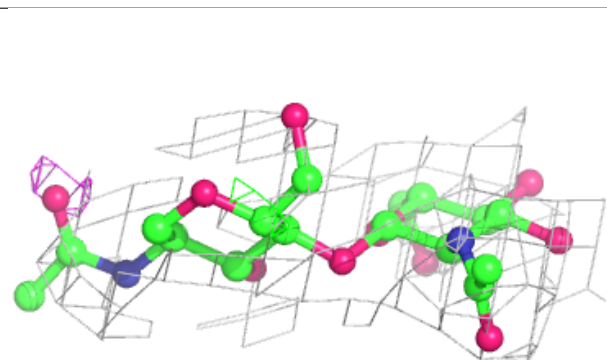
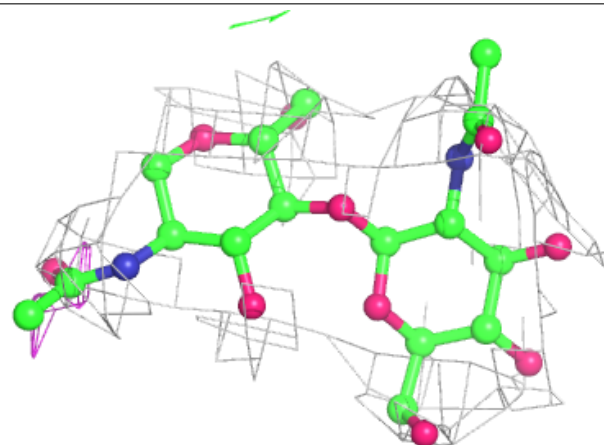
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

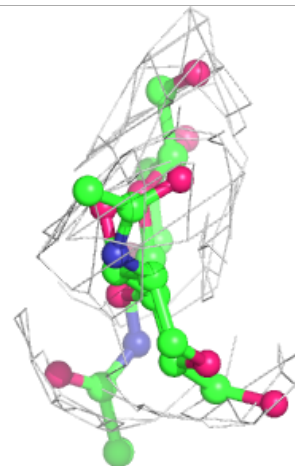
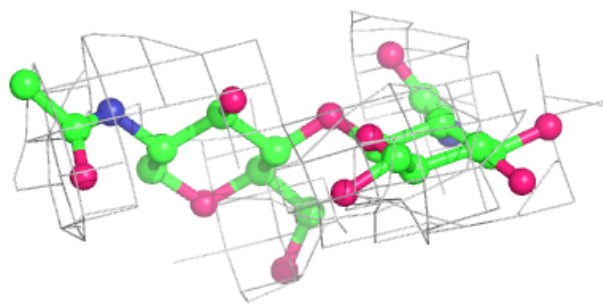
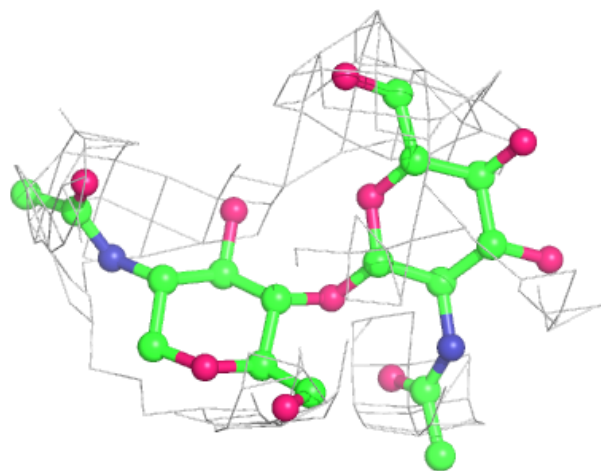
**Electron density around Chain H:**

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



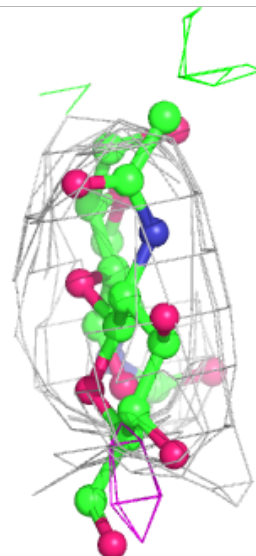
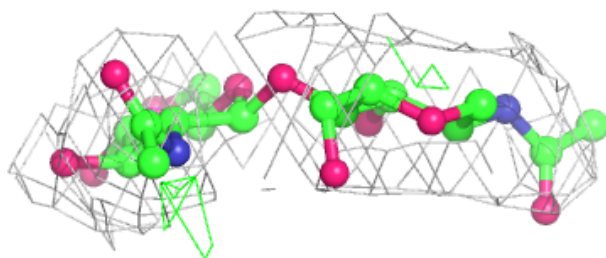
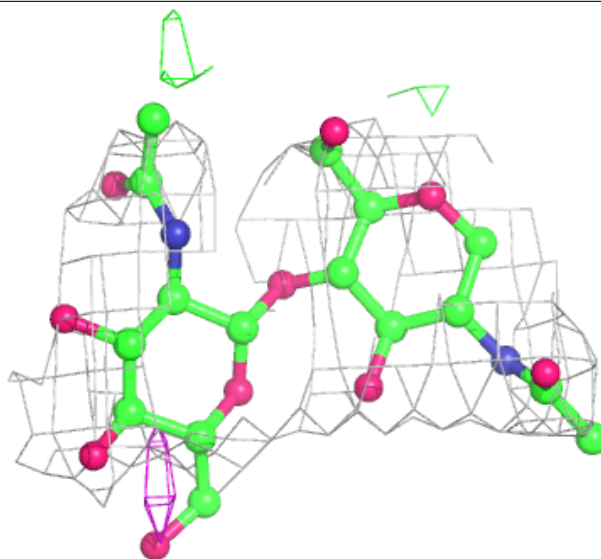
Electron density around Chain I:

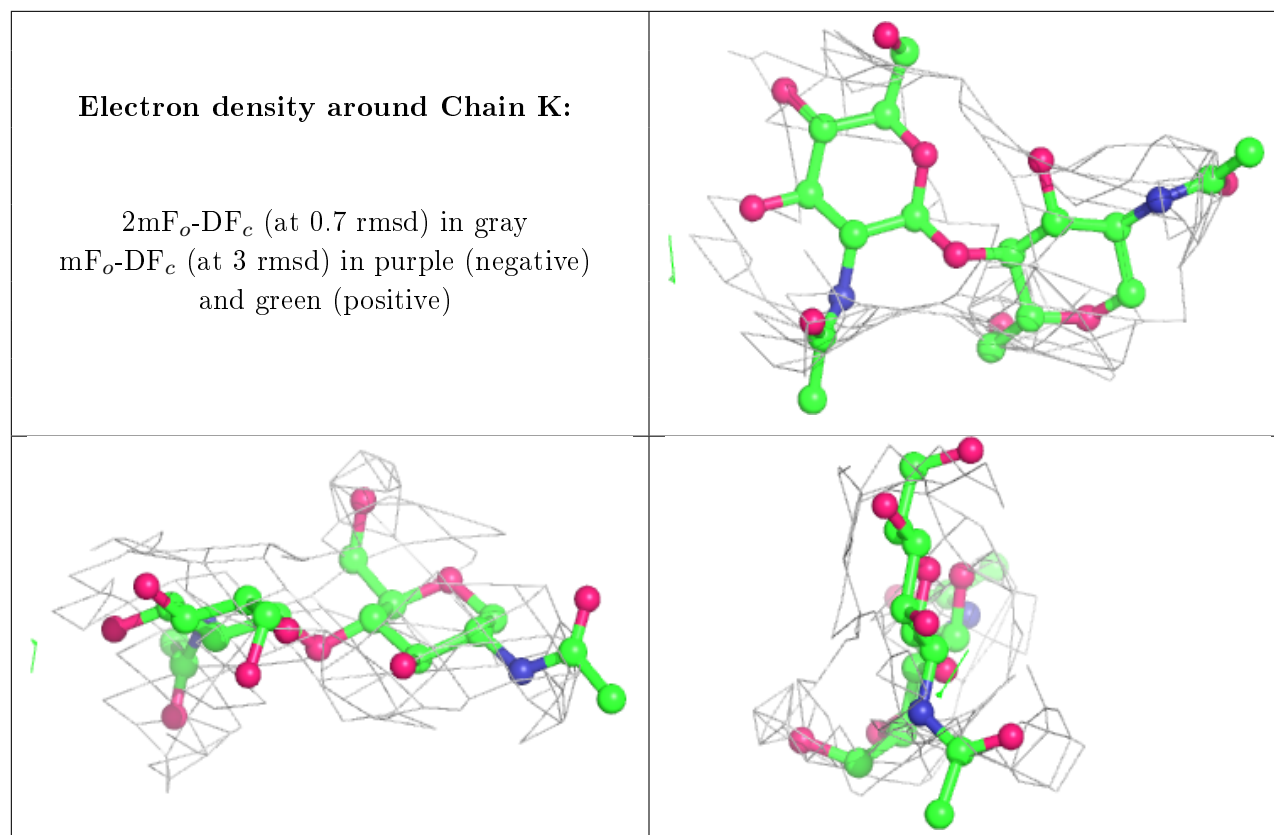
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain J:

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





6.4 Ligands ⓘ

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
4	NAG	D	1001	14/15	0.66	0.46	140,140,140,140	0
4	NAG	E	1002	14/15	0.74	0.54	114,114,114,114	0
4	NAG	C	1001	14/15	0.77	0.23	122,125,129,130	0
4	NAG	C	1007	14/15	0.78	0.46	118,118,118,118	0
4	NAG	C	1002	14/15	0.79	0.18	119,124,127,130	0
4	NAG	A	1010	14/15	0.80	0.38	138,138,138,138	0
4	NAG	A	1004	14/15	0.82	0.26	111,111,111,111	0
4	NAG	A	1005	14/15	0.86	0.18	91,96,99,102	0
4	NAG	B	1003	14/15	0.86	0.20	95,100,103,106	0
4	NAG	A	1008	14/15	0.86	0.19	110,116,123,123	0
4	NAG	A	1001	14/15	0.87	0.27	96,99,107,108	0
4	NAG	B	1007	14/15	0.88	0.22	101,107,113,114	0
4	NAG	C	1005	14/15	0.88	0.33	116,122,129,129	0
4	NAG	B	1004	14/15	0.89	0.15	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	E	1001	14/15	0.89	0.19	73,73,73,73	0
5	ZN	C	1006	1/1	0.96	0.29	87,87,87,87	0
5	ZN	B	1008	1/1	0.97	0.31	67,67,67,67	0
5	ZN	A	1009	1/1	0.98	0.29	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.