



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 12:35 PM BST

PDB ID : 4Z7I
Title : Crystal structure of insulin regulated aminopeptidase in complex with ligand
Authors : Mpakali, A.; Saridakis, E.; Harlos, K.; Zhao, Y.; Stratikos, E.
Deposited on : 2015-04-07
Resolution : 3.31 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) : 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

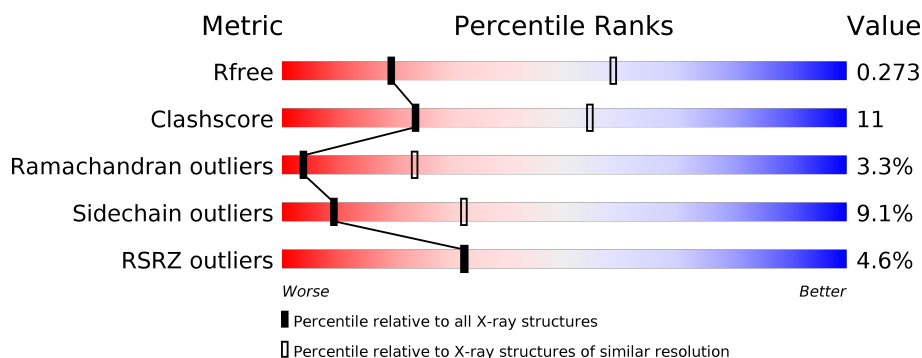
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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.




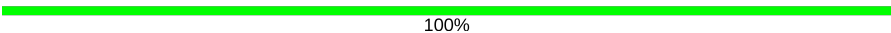

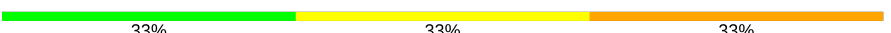
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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	912	<div> <div>3%</div> <div> <div>65%</div> <div>24%</div> <div>• • 6%</div> </div> </div>
1	B	912	<div> <div>6%</div> <div> <div>61%</div> <div>28%</div> <div>• 7%</div> </div> </div>
2	C	10	<div> <div>60%</div> <div>30%</div> <div>10%</div> </div>
2	D	10	<div> <div>10%</div> <div> <div>10%</div> <div>30%</div> <div>10%</div> <div>50%</div> </div> </div>
3	E	2	<div> <div>100%</div> </div>
3	F	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	H	2	 50% 50%
3	I	2	 100%
3	J	2	 50% 50%
4	G	3	 33% 33% 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
6	NAG	A	1110	-	-	-	X
6	NAG	B	1113	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14358 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 Leucyl-cystinyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	859	Total	C	N	O	S	0	0	0
			6947	4496	1132	1293	26			
1	B	852	Total	C	N	O	S	0	0	0
			6874	4448	1117	1284	25			

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	MET	-	initiating methionine	UNP Q9UIQ6
A	125	GLY	-	expression tag	UNP Q9UIQ6
A	126	ILE	-	expression tag	UNP Q9UIQ6
A	127	LEU	-	expression tag	UNP Q9UIQ6
A	128	PRO	-	expression tag	UNP Q9UIQ6
A	129	SER	-	expression tag	UNP Q9UIQ6
A	130	PRO	-	expression tag	UNP Q9UIQ6
A	131	GLY	-	expression tag	UNP Q9UIQ6
A	132	MET	-	expression tag	UNP Q9UIQ6
A	133	PRO	-	expression tag	UNP Q9UIQ6
A	134	ALA	-	expression tag	UNP Q9UIQ6
A	135	LEU	-	expression tag	UNP Q9UIQ6
A	136	LEU	-	expression tag	UNP Q9UIQ6
A	137	SER	-	expression tag	UNP Q9UIQ6
A	138	LEU	-	expression tag	UNP Q9UIQ6
A	139	VAL	-	expression tag	UNP Q9UIQ6
A	140	SER	-	expression tag	UNP Q9UIQ6
A	141	LEU	-	expression tag	UNP Q9UIQ6
A	142	LEU	-	expression tag	UNP Q9UIQ6
A	143	SER	-	expression tag	UNP Q9UIQ6
A	144	VAL	-	expression tag	UNP Q9UIQ6
A	145	LEU	-	expression tag	UNP Q9UIQ6
A	146	LEU	-	expression tag	UNP Q9UIQ6
A	147	MET	-	expression tag	UNP Q9UIQ6
A	148	GLY	-	expression tag	UNP Q9UIQ6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	149	CYS	-	expression tag	UNP Q9UIQ6
A	150	VAL	-	expression tag	UNP Q9UIQ6
A	151	ALA	-	expression tag	UNP Q9UIQ6
A	152	GLU	-	expression tag	UNP Q9UIQ6
A	153	THR	-	expression tag	UNP Q9UIQ6
A	154	GLY	-	expression tag	UNP Q9UIQ6
A	1026	ARG	-	expression tag	UNP Q9UIQ6
A	1027	THR	-	expression tag	UNP Q9UIQ6
A	1028	GLU	-	expression tag	UNP Q9UIQ6
A	1029	THR	-	expression tag	UNP Q9UIQ6
A	1030	SER	-	expression tag	UNP Q9UIQ6
A	1031	GLN	-	expression tag	UNP Q9UIQ6
A	1032	VAL	-	expression tag	UNP Q9UIQ6
A	1033	ALA	-	expression tag	UNP Q9UIQ6
A	1034	PRO	-	expression tag	UNP Q9UIQ6
A	1035	ALA	-	expression tag	UNP Q9UIQ6
B	124	MET	-	initiating methionine	UNP Q9UIQ6
B	125	GLY	-	expression tag	UNP Q9UIQ6
B	126	ILE	-	expression tag	UNP Q9UIQ6
B	127	LEU	-	expression tag	UNP Q9UIQ6
B	128	PRO	-	expression tag	UNP Q9UIQ6
B	129	SER	-	expression tag	UNP Q9UIQ6
B	130	PRO	-	expression tag	UNP Q9UIQ6
B	131	GLY	-	expression tag	UNP Q9UIQ6
B	132	MET	-	expression tag	UNP Q9UIQ6
B	133	PRO	-	expression tag	UNP Q9UIQ6
B	134	ALA	-	expression tag	UNP Q9UIQ6
B	135	LEU	-	expression tag	UNP Q9UIQ6
B	136	LEU	-	expression tag	UNP Q9UIQ6
B	137	SER	-	expression tag	UNP Q9UIQ6
B	138	LEU	-	expression tag	UNP Q9UIQ6
B	139	VAL	-	expression tag	UNP Q9UIQ6
B	140	SER	-	expression tag	UNP Q9UIQ6
B	141	LEU	-	expression tag	UNP Q9UIQ6
B	142	LEU	-	expression tag	UNP Q9UIQ6
B	143	SER	-	expression tag	UNP Q9UIQ6
B	144	VAL	-	expression tag	UNP Q9UIQ6
B	145	LEU	-	expression tag	UNP Q9UIQ6
B	146	LEU	-	expression tag	UNP Q9UIQ6
B	147	MET	-	expression tag	UNP Q9UIQ6
B	148	GLY	-	expression tag	UNP Q9UIQ6
B	149	CYS	-	expression tag	UNP Q9UIQ6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	150	VAL	-	expression tag	UNP Q9UIQ6
B	151	ALA	-	expression tag	UNP Q9UIQ6
B	152	GLU	-	expression tag	UNP Q9UIQ6
B	153	THR	-	expression tag	UNP Q9UIQ6
B	154	GLY	-	expression tag	UNP Q9UIQ6
B	1026	ARG	-	expression tag	UNP Q9UIQ6
B	1027	THR	-	expression tag	UNP Q9UIQ6
B	1028	GLU	-	expression tag	UNP Q9UIQ6
B	1029	THR	-	expression tag	UNP Q9UIQ6
B	1030	SER	-	expression tag	UNP Q9UIQ6
B	1031	GLN	-	expression tag	UNP Q9UIQ6
B	1032	VAL	-	expression tag	UNP Q9UIQ6
B	1033	ALA	-	expression tag	UNP Q9UIQ6
B	1034	PRO	-	expression tag	UNP Q9UIQ6
B	1035	ALA	-	expression tag	UNP Q9UIQ6

- Molecule 2 is a protein called DG025 transition-state analogue enzyme inhibitor.

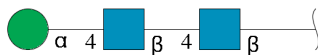
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	P	0	0	0
			87	58	15	13	1			
2	D	5	Total	C	N	O	P	0	0	0
			45	31	7	6	1			

- 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	E	2	Total	C	N	O		0	0	0
			28	16	2	10				
3	F	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				

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

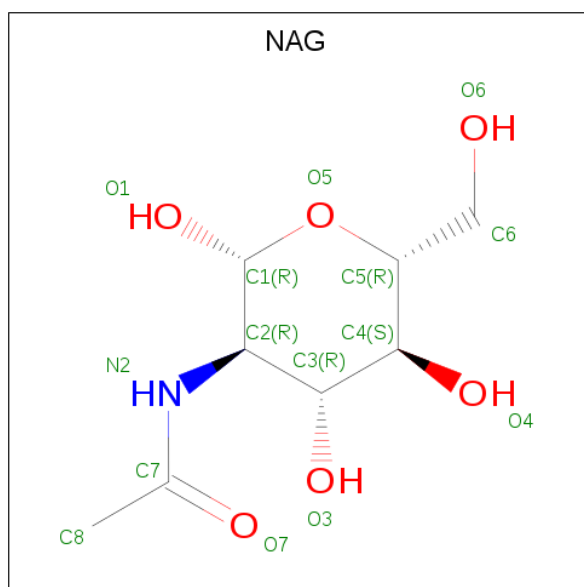


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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

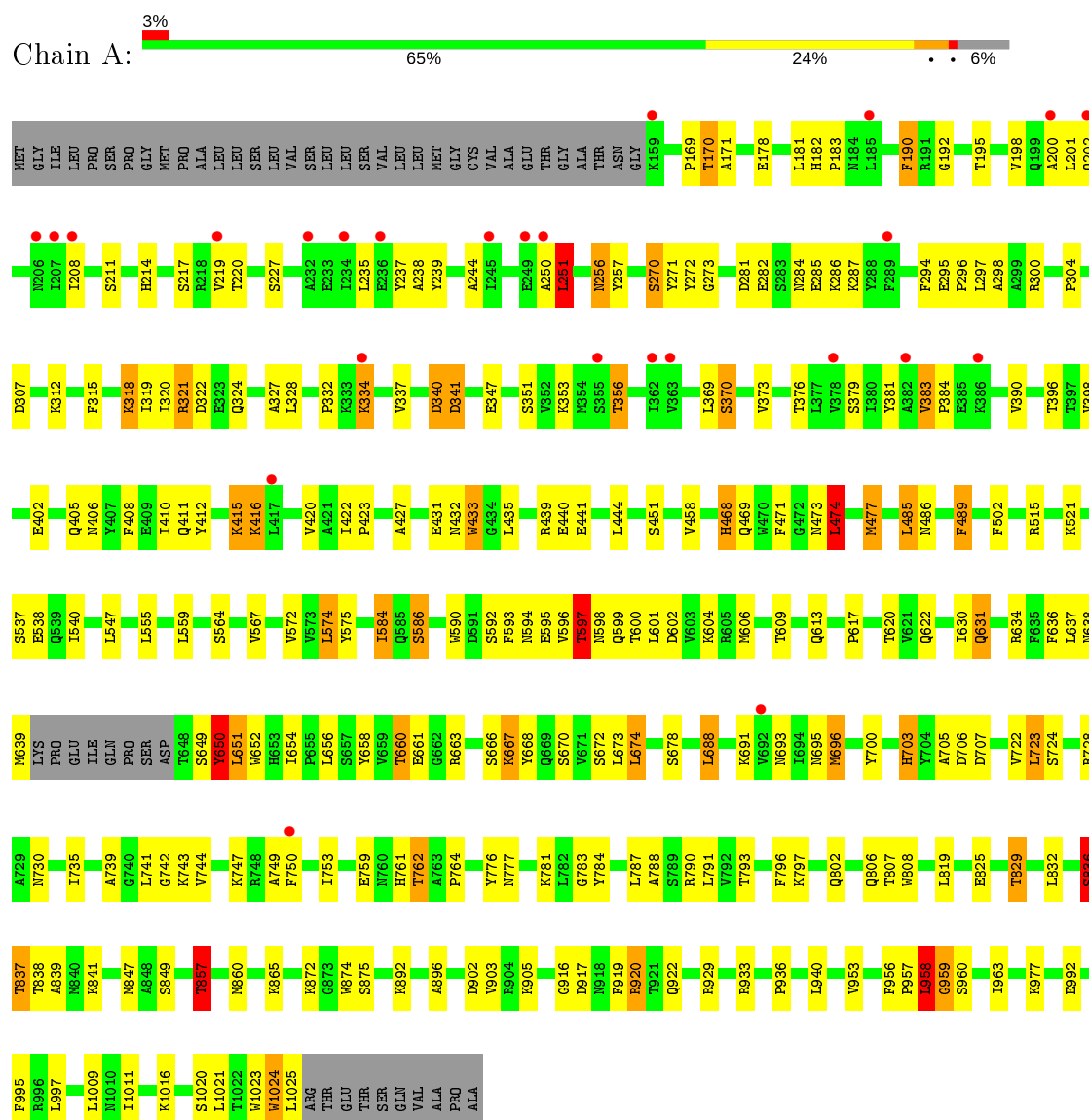
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	7	Total	O	0	0
			7	7		
7	B	6	Total	O	0	0
			6	6		
7	C	1	Total	O	0	0
			1	1		

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: Leucyl-cystinyl aminopeptidase



• Molecule 1: Leucyl-cystinyl aminopeptidase



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

Chain E:  100%



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

Chain F:  100%



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

Chain H:  50% 50%



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

Chain I:  100%



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

Chain J:  50% 50%



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

Chain G:  33% 33% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.52Å 256.35Å 73.06Å 90.00° 111.58° 90.00°	Depositor
Resolution (Å)	128.18 – 3.31 128.17 – 3.31	Depositor EDS
% Data completeness (in resolution range)	99.9 (128.18-3.31) 99.9 (128.17-3.31)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.211 , 0.270 0.212 , 0.273	Depositor DCC
R_{free} test set	1676 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	127.3	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 85.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14358	wwPDB-VP
Average B, all atoms (Å ²)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: 2X0, ZN, 4L8, NAG, 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	0.26	0/7117	0.49	1/9654 (0.0%)
1	B	0.26	0/7038	0.52	1/9543 (0.0%)
2	C	0.27	0/68	0.69	0/87
2	D	0.19	0/24	0.25	0/30
All	All	0.26	0/14247	0.50	2/19314 (0.0%)

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.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	339	LEU	CA-CB-CG	7.86	133.38	115.30
1	A	251	LEU	CA-CB-CG	6.00	129.09	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	596	VAL	Peptide
1	A	598	ASN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6947	0	6829	149	0
1	B	6874	0	6745	164	0
2	C	87	0	83	2	0
2	D	45	0	44	5	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	1	0
4	G	39	0	34	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	98	0	91	1	0
6	B	112	0	104	4	0
7	A	7	0	0	0	0
7	B	6	0	0	0	0
7	C	1	0	0	0	0
All	All	14358	0	14055	318	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 11.

The worst 5 of 318 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:790:ARG:HD3	1:A:1025:LEU:HD22	1.52	0.89
1:B:655:PRO:HA	1:B:656:LEU:HB2	1.61	0.82
1:B:331:MET:HG3	1:B:351:SER:HA	1.65	0.78
1:A:597:THR:H	1:A:599:GLN:H	1.35	0.75
1:B:691:LYS:HE2	1:B:731:LEU:HG	1.68	0.74

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	855/912 (94%)	762 (89%)	71 (8%)	22 (3%)	5	28
1	B	842/912 (92%)	723 (86%)	87 (10%)	32 (4%)	3	20
2	C	7/10 (70%)	1 (14%)	3 (43%)	3 (43%)	0	0
2	D	2/10 (20%)	1 (50%)	1 (50%)	0	100	100
All	All	1706/1844 (92%)	1487 (87%)	162 (10%)	57 (3%)	4	23

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	ALA
1	A	217	SER
1	A	238	ALA
1	A	663	ARG
1	A	836	SER

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	761/813 (94%)	692 (91%)	69 (9%)	9	32
1	B	752/813 (92%)	684 (91%)	68 (9%)	9	33
2	C	6/7 (86%)	6 (100%)	0	100	100
2	D	2/7 (29%)	1 (50%)	1 (50%)	0	0
All	All	1521/1640 (93%)	1383 (91%)	138 (9%)	9	32

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	857	THR
1	B	220	THR
1	B	829	THR
1	A	917	ASP
1	B	165	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	631	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	4L8	D	2	2	7,7,9	0.89	0	7,8,11	1.00	0
2	4L8	C	2	2	7,7,9	0.87	0	7,8,11	1.05	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	4L8	D	2	2	-	2/5/6/10	-
2	4L8	C	2	2	-	2/5/6/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	4L8	C1-CA-CB-CG
2	D	2	4L8	C-CA-CB-CG
2	C	2	4L8	C1-CA-CB-CG
2	C	2	4L8	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	4L8	1	0
2	C	2	4L8	1	0

5.5 Carbohydrates ⓘ

13 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	E	1	1,3	14,14,15	0.57	0	17,19,21	0.53	0
3	NAG	E	2	3	14,14,15	0.22	0	17,19,21	0.38	0
3	NAG	F	1	1,3	14,14,15	0.34	0	17,19,21	0.55	0
3	NAG	F	2	3	14,14,15	0.24	0	17,19,21	0.38	0
4	NAG	G	1	1,4	14,14,15	0.55	0	17,19,21	0.67	0
4	NAG	G	2	4	14,14,15	0.31	0	17,19,21	0.51	0
4	MAN	G	3	4	11,11,12	0.68	0	15,15,17	1.10	2 (13%)
3	NAG	H	1	1,3	14,14,15	0.36	0	17,19,21	0.66	1 (5%)
3	NAG	H	2	3	14,14,15	0.23	0	17,19,21	0.38	0
3	NAG	I	1	1,3	14,14,15	0.36	0	17,19,21	0.52	0
3	NAG	I	2	3	14,14,15	0.27	0	17,19,21	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	J	1	1,3	14,14,15	0.45	0	17,19,21	0.75	1 (5%)
3	NAG	J	2	3	14,14,15	0.26	0	17,19,21	0.41	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	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/23/26	0/1/1/1
4	MAN	G	3	4	-	0/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	1/6/23/26	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	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1	NAG	C1-O5-C5	2.49	115.57	112.19
4	G	3	MAN	C1-O5-C5	2.44	115.49	112.19
4	G	3	MAN	O2-C2-C3	-2.08	105.98	110.14
3	H	1	NAG	O5-C1-C2	-2.02	108.09	111.29

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

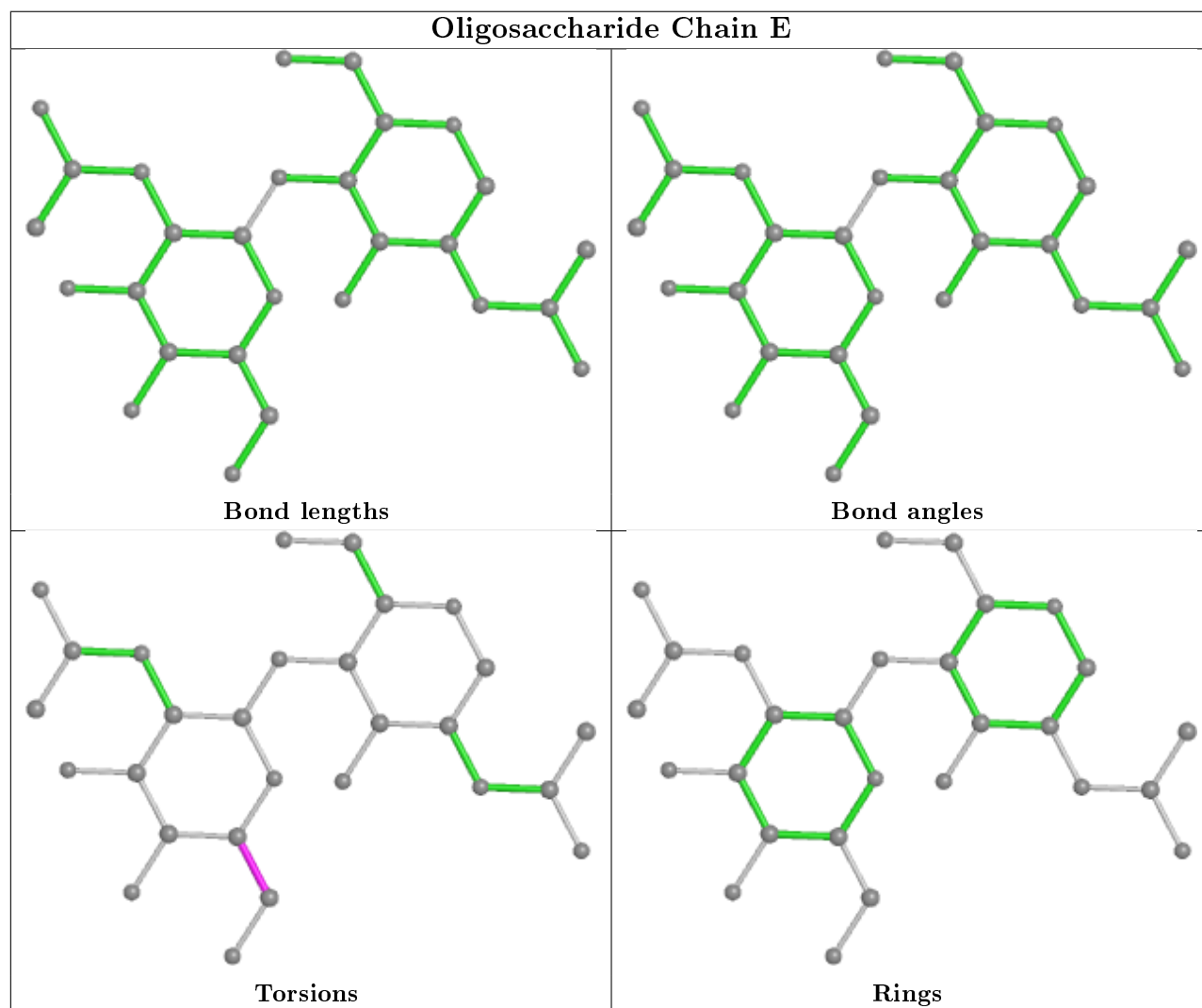
Mol	Chain	Res	Type	Atoms
3	I	1	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6

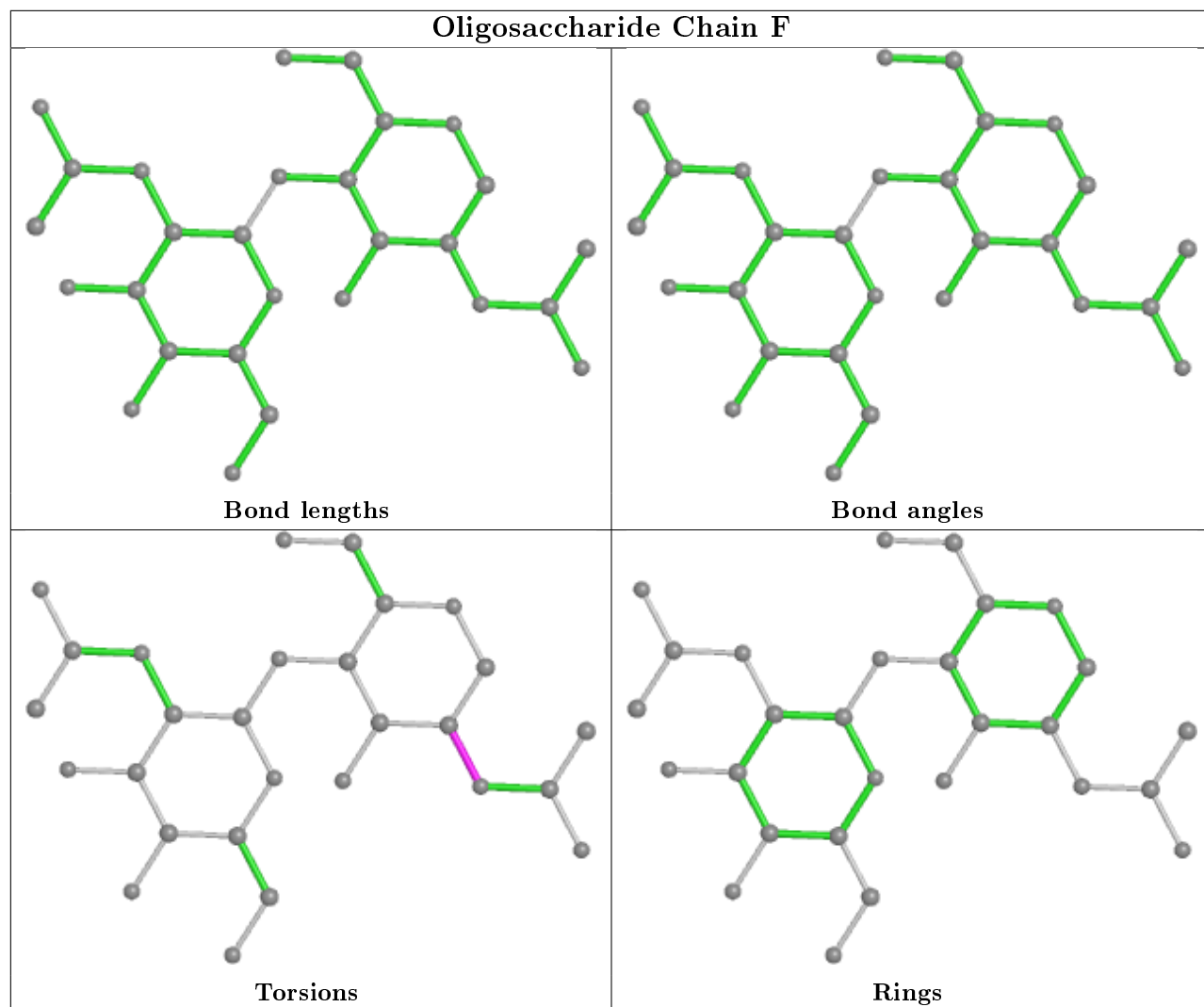
There are no ring outliers.

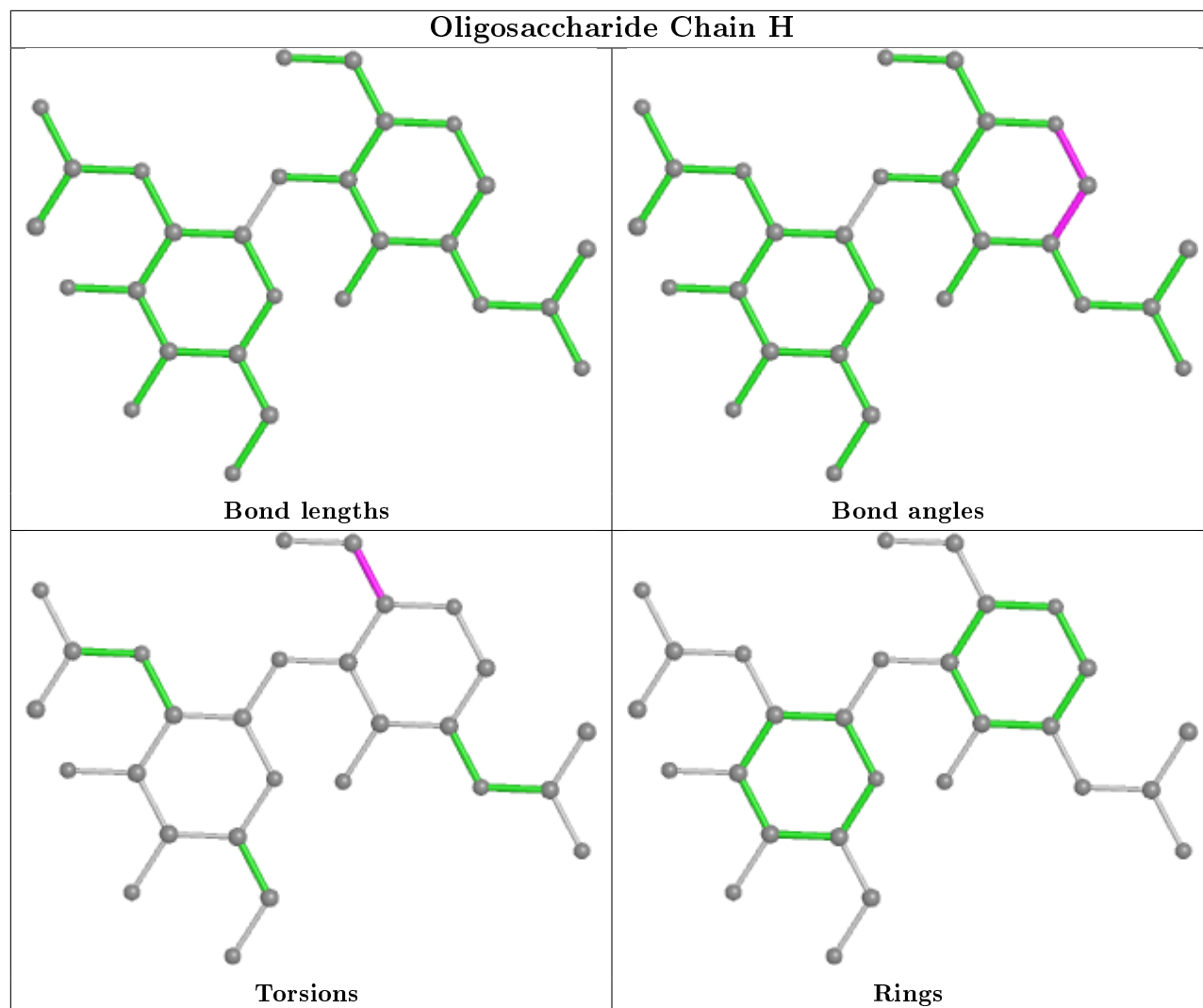
4 monomers are involved in 2 short contacts:

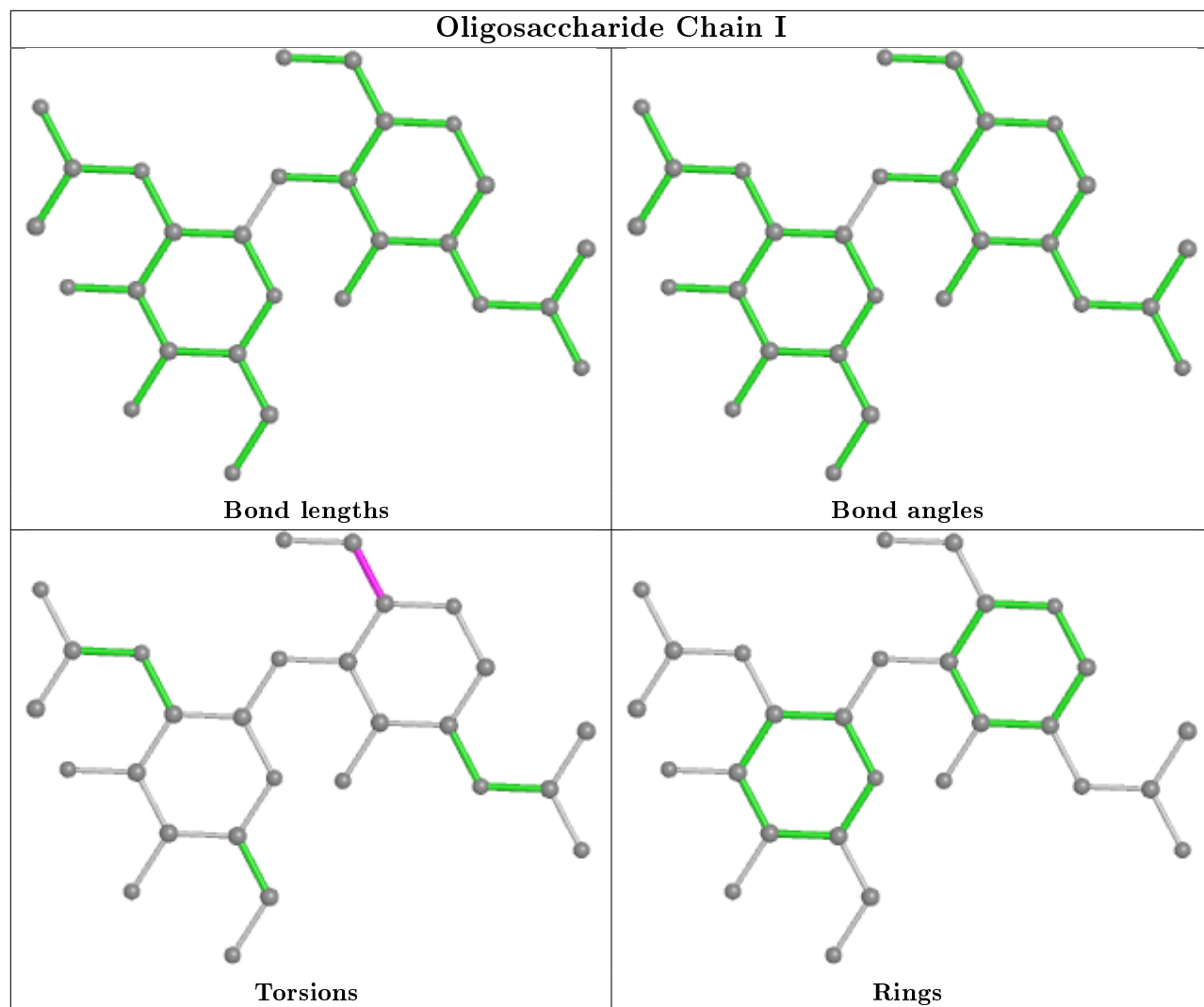
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	2	NAG	1	0
3	J	1	NAG	1	0
4	G	3	MAN	1	0
3	J	2	NAG	1	0

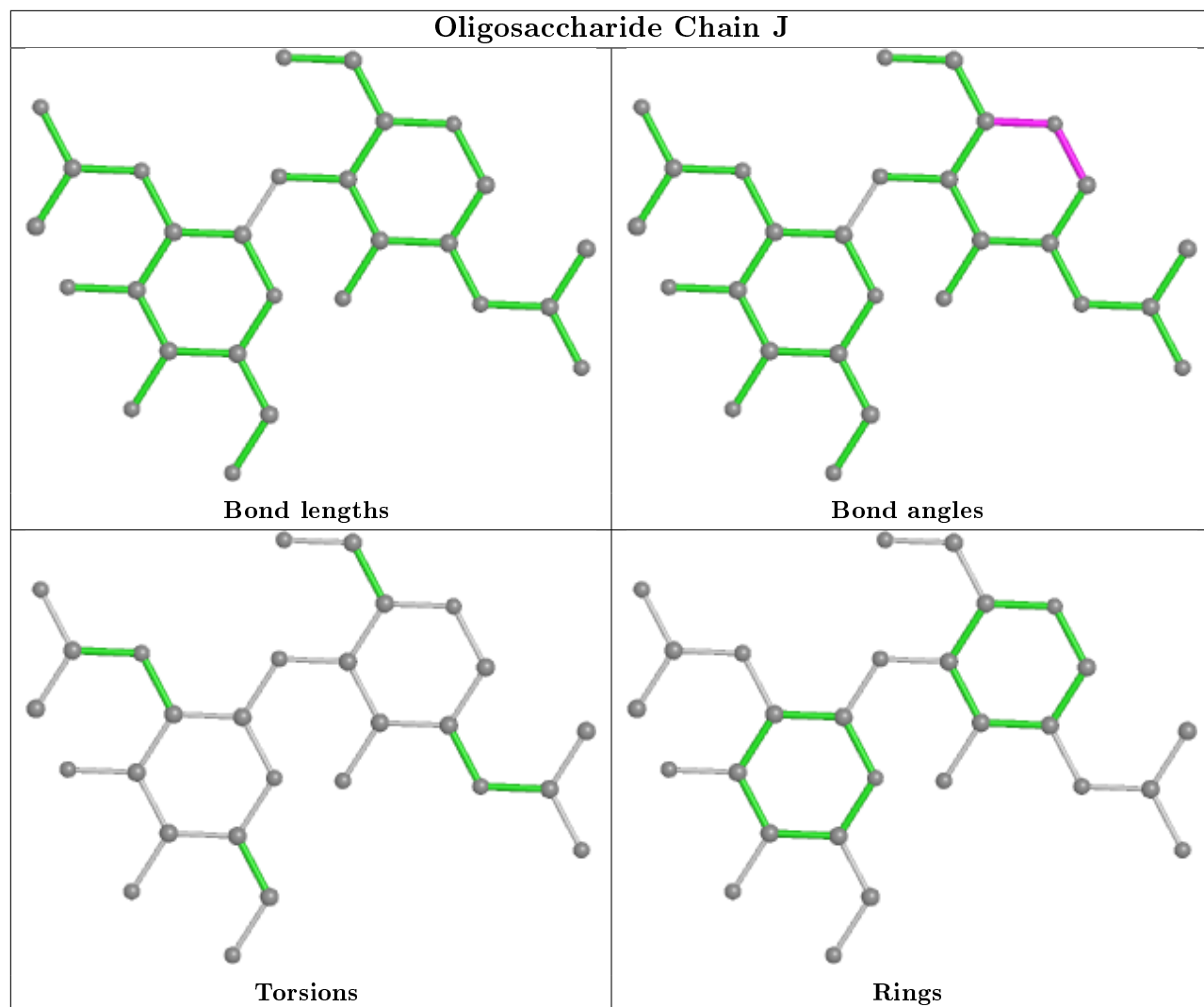
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

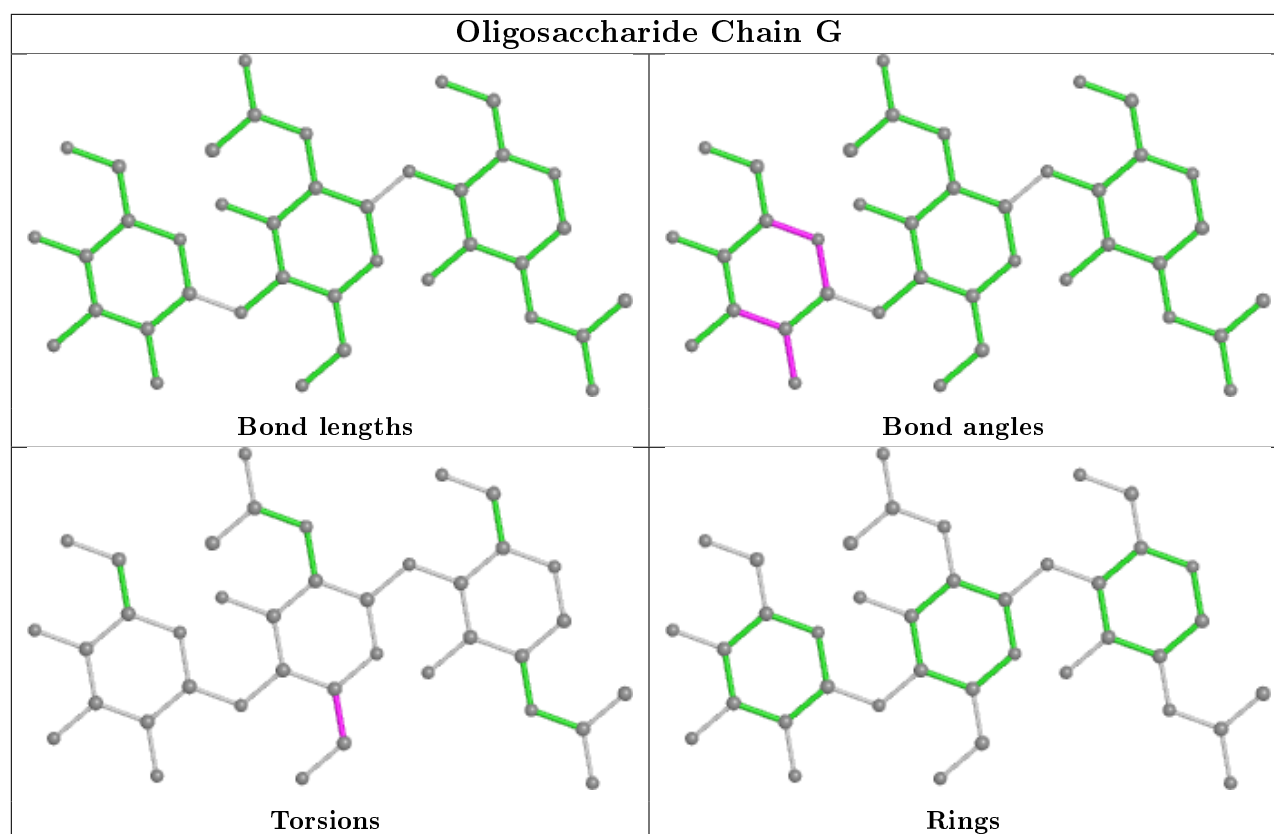












5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 2 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	$\# Z > 2$
6	NAG	B	1108	1	14,14,15	0.64	0	17,19,21	0.92	2 (11%)
6	NAG	A	1105	1	14,14,15	0.32	0	17,19,21	0.47	0
6	NAG	A	1115	1	14,14,15	0.63	0	17,19,21	0.87	2 (11%)
6	NAG	B	1107	1	14,14,15	0.27	0	17,19,21	0.45	0
6	NAG	A	1109	1	14,14,15	0.40	0	17,19,21	0.48	0
6	NAG	B	1113	1	14,14,15	0.28	0	17,19,21	0.43	0
6	NAG	A	1104	1	14,14,15	0.37	0	17,19,21	0.56	0
6	NAG	B	1105	1	14,14,15	0.22	0	17,19,21	0.45	0
6	NAG	A	1108	1	14,14,15	0.29	0	17,19,21	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	B	1109	-	14,14,15	0.23	0	17,19,21	0.38	0
6	NAG	A	1110	1	14,14,15	1.02	2 (14%)	17,19,21	1.01	2 (11%)
6	NAG	B	1102	1	14,14,15	0.20	0	17,19,21	0.42	0
6	NAG	A	1111	1	14,14,15	0.20	0	17,19,21	0.41	0
6	NAG	B	1106	1	14,14,15	0.27	0	17,19,21	0.45	0
6	NAG	B	1110	1	14,14,15	0.87	2 (14%)	17,19,21	0.97	2 (11%)

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	B	1108	1	-	3/6/23/26	0/1/1/1
6	NAG	A	1105	1	-	3/6/23/26	0/1/1/1
6	NAG	A	1115	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1107	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1109	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1113	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1104	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1105	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1108	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1109	-	-	0/6/23/26	0/1/1/1
6	NAG	A	1110	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1102	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1111	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1106	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1110	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)
6	A	1110	NAG	O5-C1	2.94	1.48	1.43
6	B	1110	NAG	O5-C1	2.47	1.47	1.43
6	B	1110	NAG	C1-C2	2.07	1.55	1.52
6	A	1110	NAG	C2-N2	2.02	1.49	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	B	1110	NAG	C1-O5-C5	3.22	116.55	112.19
6	B	1108	NAG	C1-O5-C5	2.81	116.00	112.19
6	A	1110	NAG	O5-C1-C2	-2.73	106.98	111.29
6	A	1110	NAG	C1-O5-C5	2.69	115.84	112.19
6	A	1115	NAG	C1-O5-C5	2.41	115.46	112.19

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1115	NAG	C4-C5-C6-O6
6	A	1115	NAG	O5-C5-C6-O6
6	B	1110	NAG	O5-C5-C6-O6
6	A	1104	NAG	O5-C5-C6-O6
6	B	1107	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1108	NAG	1	0
6	B	1107	NAG	1	0
6	A	1108	NAG	1	0
6	B	1102	NAG	1	0
6	B	1106	NAG	1	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](#)

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	859/912 (94%)	0.21	25 (2%) 51 51	67, 110, 174, 207	3 (0%)
1	B	852/912 (93%)	0.26	53 (6%) 20 21	73, 147, 195, 229	1 (0%)
2	C	8/10 (80%)	0.08	0 100 100	119, 158, 174, 177	0
2	D	3/10 (30%)	1.46	1 (33%) 0 0	162, 162, 177, 180	0
All	All	1722/1844 (93%)	0.23	79 (4%) 32 32	67, 130, 190, 229	4 (0%)

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	327	ALA	7.0
1	B	221	PHE	6.6
1	B	622	GLN	5.2
1	B	419	LEU	4.3
1	B	220	THR	4.3

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	4L8	D	2	8/10	0.91	0.48	132,140,160,168	0
2	4L8	C	2	8/10	0.95	0.33	104,114,123,131	0

6.3 Carbohydrates ⓘ

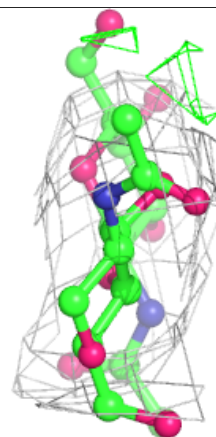
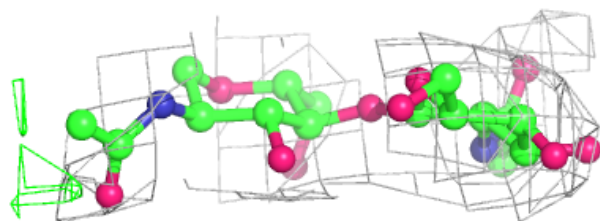
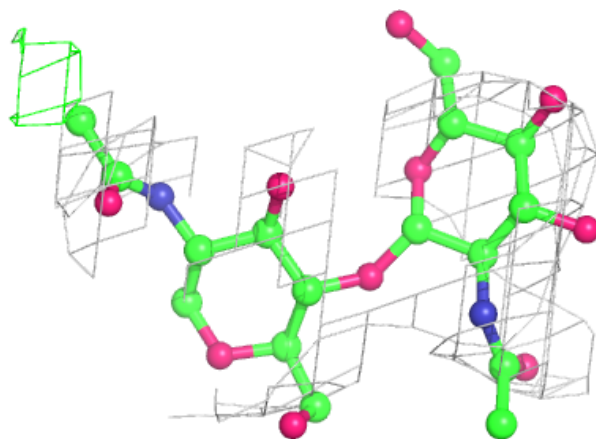
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	H	2	14/15	0.64	0.27	202,211,217,218	0
3	NAG	F	2	14/15	0.67	0.30	179,203,212,213	0
3	NAG	J	1	14/15	0.73	0.24	169,181,188,191	0
3	NAG	J	2	14/15	0.73	0.32	188,194,203,206	0
4	MAN	G	3	11/12	0.77	0.26	175,182,189,211	0
3	NAG	H	1	14/15	0.80	0.17	197,213,217,222	0
3	NAG	I	2	14/15	0.82	0.23	202,208,214,215	0
3	NAG	F	1	14/15	0.83	0.22	167,177,196,196	0
3	NAG	E	2	14/15	0.84	0.23	161,176,182,184	0
4	NAG	G	1	14/15	0.88	0.20	123,135,151,156	0
4	NAG	G	2	14/15	0.89	0.17	137,145,164,165	0
3	NAG	E	1	14/15	0.90	0.17	155,163,177,178	0
3	NAG	I	1	14/15	0.90	0.17	202,206,214,214	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.

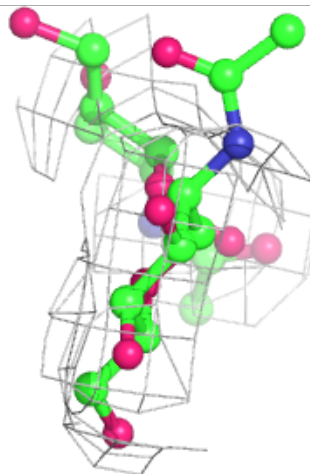
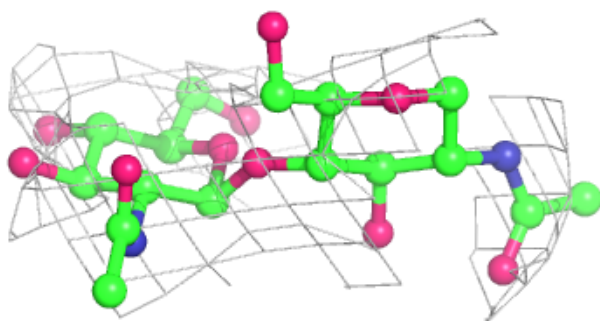
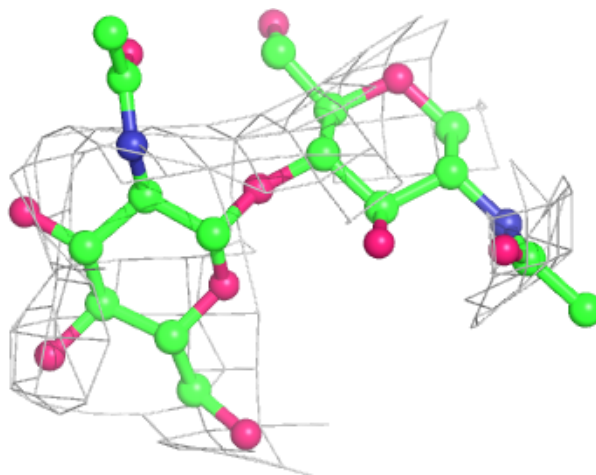
Electron density around Chain E:

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



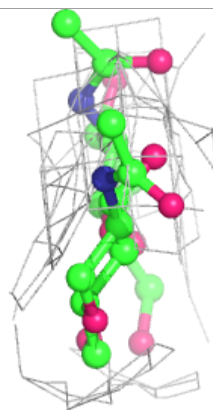
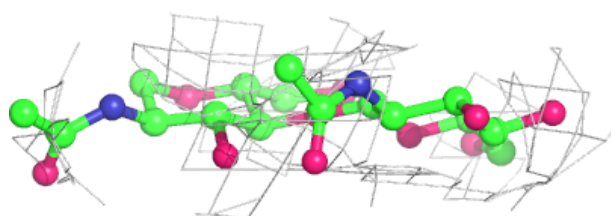
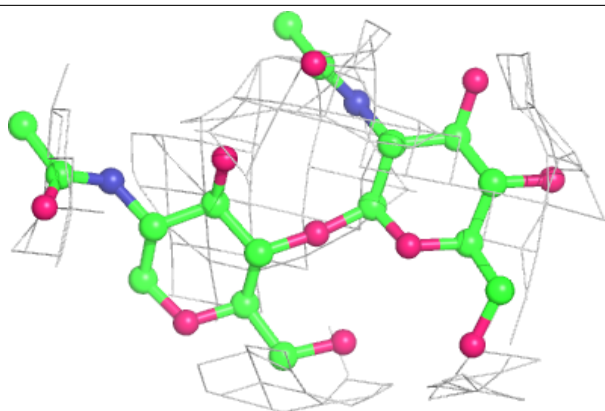
Electron density around Chain F:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

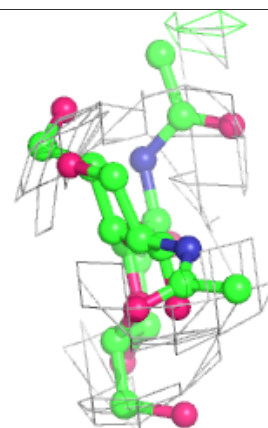
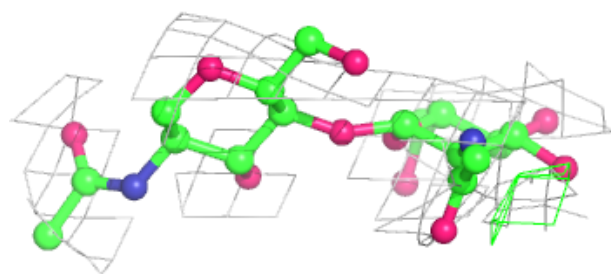
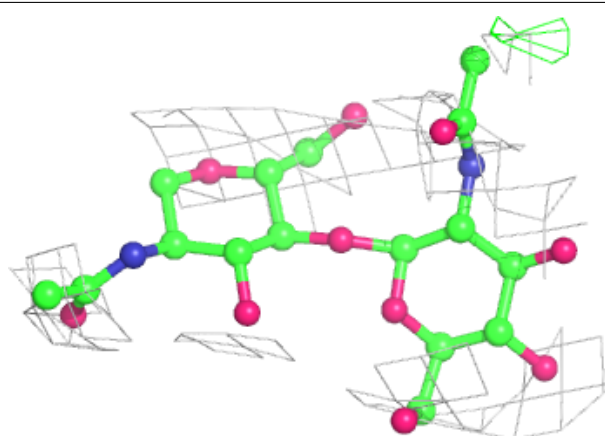


Electron density around Chain H:

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

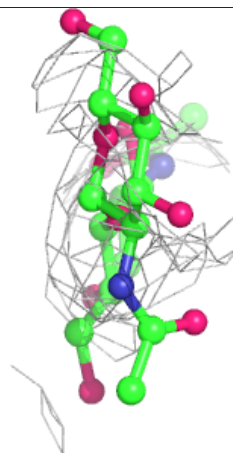
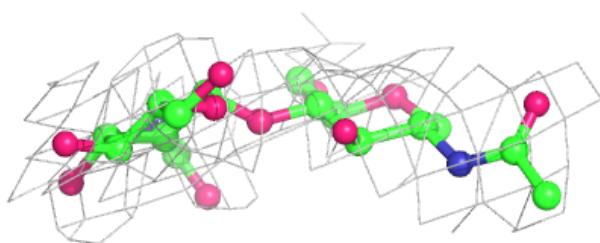
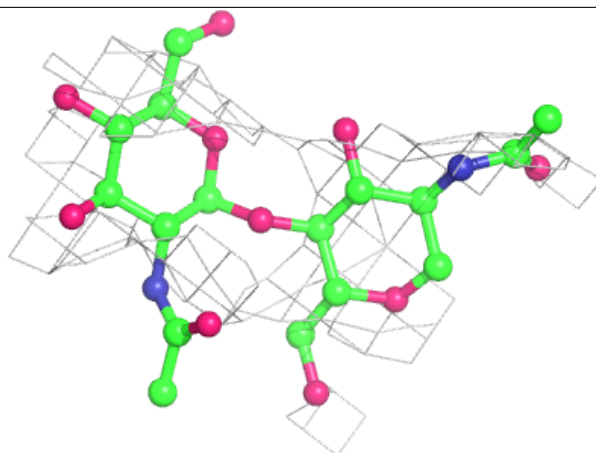
**Electron density around Chain I:**

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

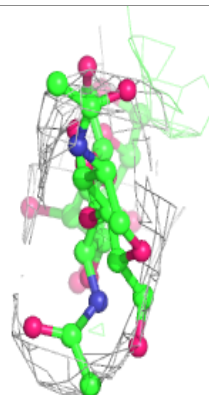
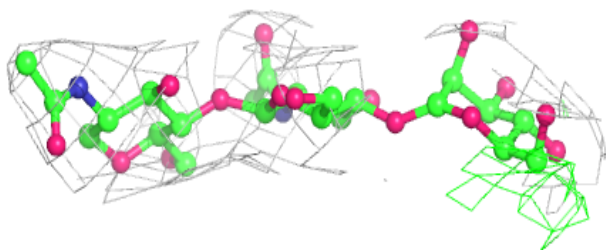
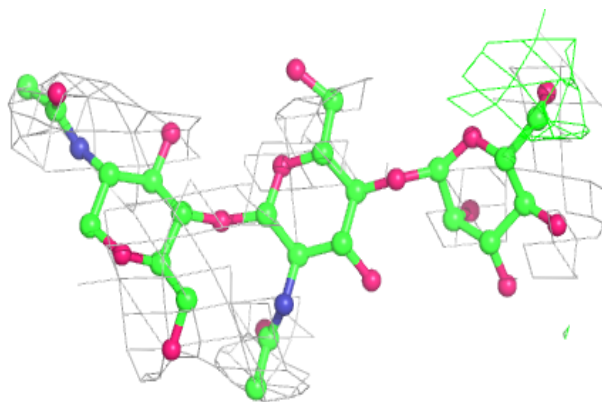


Electron density around Chain J:

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

**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)



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
6	NAG	B	1113	14/15	0.55	0.41	165,177,184,186	0
6	NAG	A	1110	14/15	0.56	0.51	140,159,163,166	0
6	NAG	B	1102	14/15	0.56	0.25	170,182,187,190	0
6	NAG	A	1111	14/15	0.71	0.24	125,143,161,167	0
6	NAG	A	1108	14/15	0.76	0.26	151,156,172,176	0
6	NAG	B	1110	14/15	0.77	0.28	165,180,191,193	0
6	NAG	A	1109	14/15	0.78	0.25	147,182,193,194	0
6	NAG	B	1109	14/15	0.78	0.19	161,173,182,184	0
6	NAG	A	1104	14/15	0.79	0.20	174,182,185,187	0
6	NAG	B	1105	14/15	0.79	0.23	174,186,192,193	0
6	NAG	B	1106	14/15	0.81	0.31	186,197,204,204	0
6	NAG	B	1107	14/15	0.83	0.18	195,199,205,206	0
6	NAG	A	1115	14/15	0.84	0.21	153,169,176,176	0
6	NAG	A	1105	14/15	0.86	0.18	179,190,197,204	0
6	NAG	B	1108	14/15	0.88	0.20	171,178,184,185	0
5	ZN	B	1101	1/1	0.96	0.21	124,124,124,124	0
5	ZN	A	1101	1/1	0.99	0.23	86,86,86,86	0

6.5 Other polymers ⓘ

There are no such residues in this entry.