



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 03:33 PM BST

PDB ID : 5J6S
Title : Crystal structure of Endoplasmic Reticulum Aminopeptidase 2 (ERAP2) in complex with a hydroxamic derivative ligand
Authors : Saridakis, E.; Giastas, P.; Mpakali, A.; Deprez-Poulain, R.; Stratikos, E.
Deposited on : 2016-04-05
Resolution : 2.80 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
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)	:	2.13.1

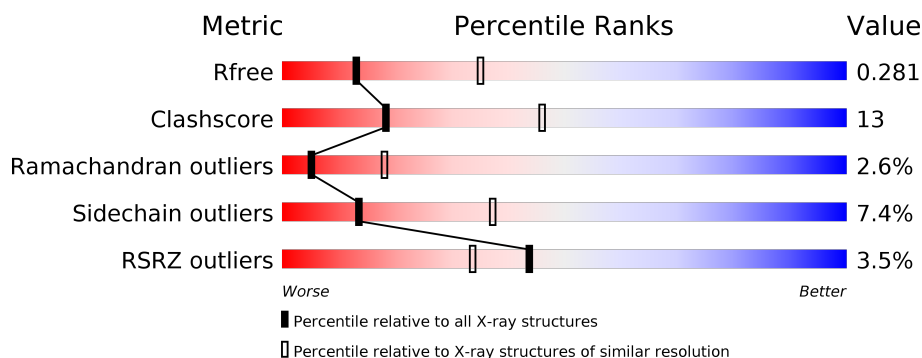
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



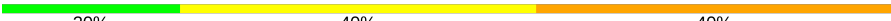
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	967	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>27%</div> <div>• 6%</div> </div> </div>
1	B	967	<div> <div>5%</div> <div> <div></div> <div>56%</div> <div>31%</div> <div>• 9%</div> </div> </div>
2	C	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
2	E	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
3	D	3	<div> <div></div> <div> <div>67%</div> <div>33%</div> </div> </div>
3	G	3	<div> <div></div> <div> <div>33%</div> <div>33%</div> <div>33%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	F	5	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: green (20%), yellow (40%), and orange (40%).

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15067 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 Endoplasmic reticulum aminopeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	910	Total	C	N	O	S	0	2	0
			7413	4777	1229	1375	32			
1	B	880	Total	C	N	O	S	0	1	0
			7185	4633	1197	1327	28			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	392	ASN	LYS	variant	UNP Q6P179
A	961	ARG	-	expression tag	UNP Q6P179
A	962	HIS	-	expression tag	UNP Q6P179
A	963	HIS	-	expression tag	UNP Q6P179
A	964	HIS	-	expression tag	UNP Q6P179
A	965	HIS	-	expression tag	UNP Q6P179
A	966	HIS	-	expression tag	UNP Q6P179
A	967	HIS	-	expression tag	UNP Q6P179
B	392	ASN	LYS	variant	UNP Q6P179
B	961	ARG	-	expression tag	UNP Q6P179
B	962	HIS	-	expression tag	UNP Q6P179
B	963	HIS	-	expression tag	UNP Q6P179
B	964	HIS	-	expression tag	UNP Q6P179
B	965	HIS	-	expression tag	UNP Q6P179
B	966	HIS	-	expression tag	UNP Q6P179
B	967	HIS	-	expression tag	UNP Q6P179

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



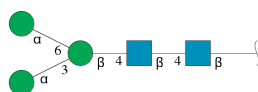
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called beta-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
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

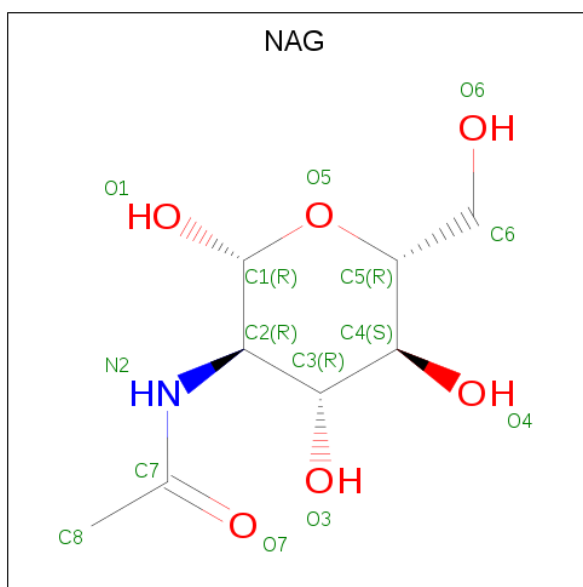


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	5	Total	C	N	O	0	0	0
			61	34	2	25			

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

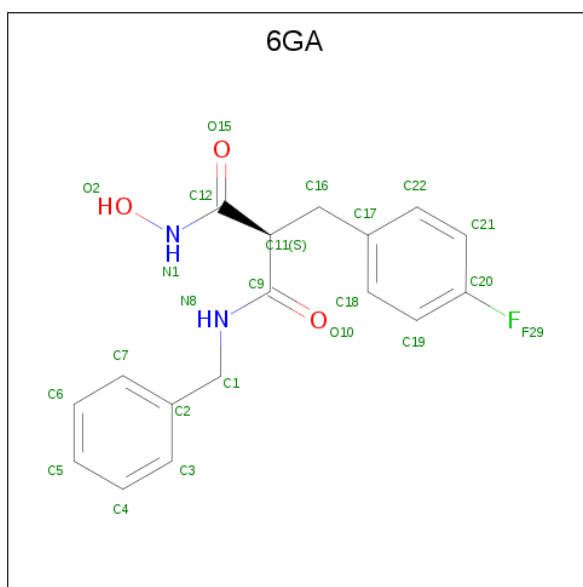
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		
5	A	1	Total	Zn	0	0
			1	1		

- 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		
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		

- Molecule 7 is (2S)-N 1 -benzyl-2-[(4-fluorophenyl)methyl]-N 3 -hydroxypropanediamide (three-letter code: 6GA) (formula: C₁₇H₁₇FN₂O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	F	N	O	0	1
			46	34	2	4	6		
7	B	1	Total	C	F	N	O	0	0
			23	17	1	2	3		

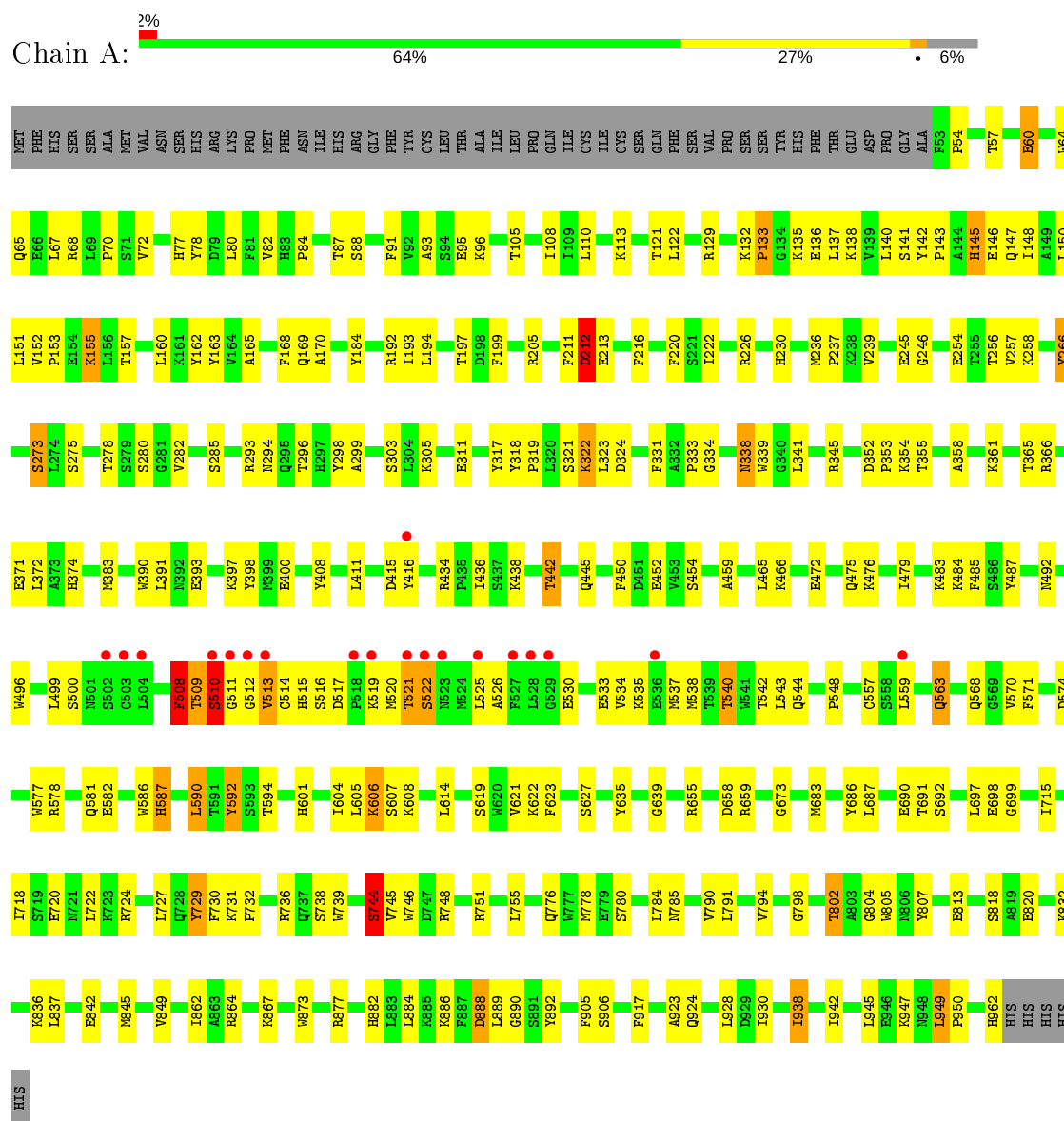
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	34	Total	O	0	0
			34	34		
8	B	15	Total	O	0	0
			15	15		

3 Residue-property plots

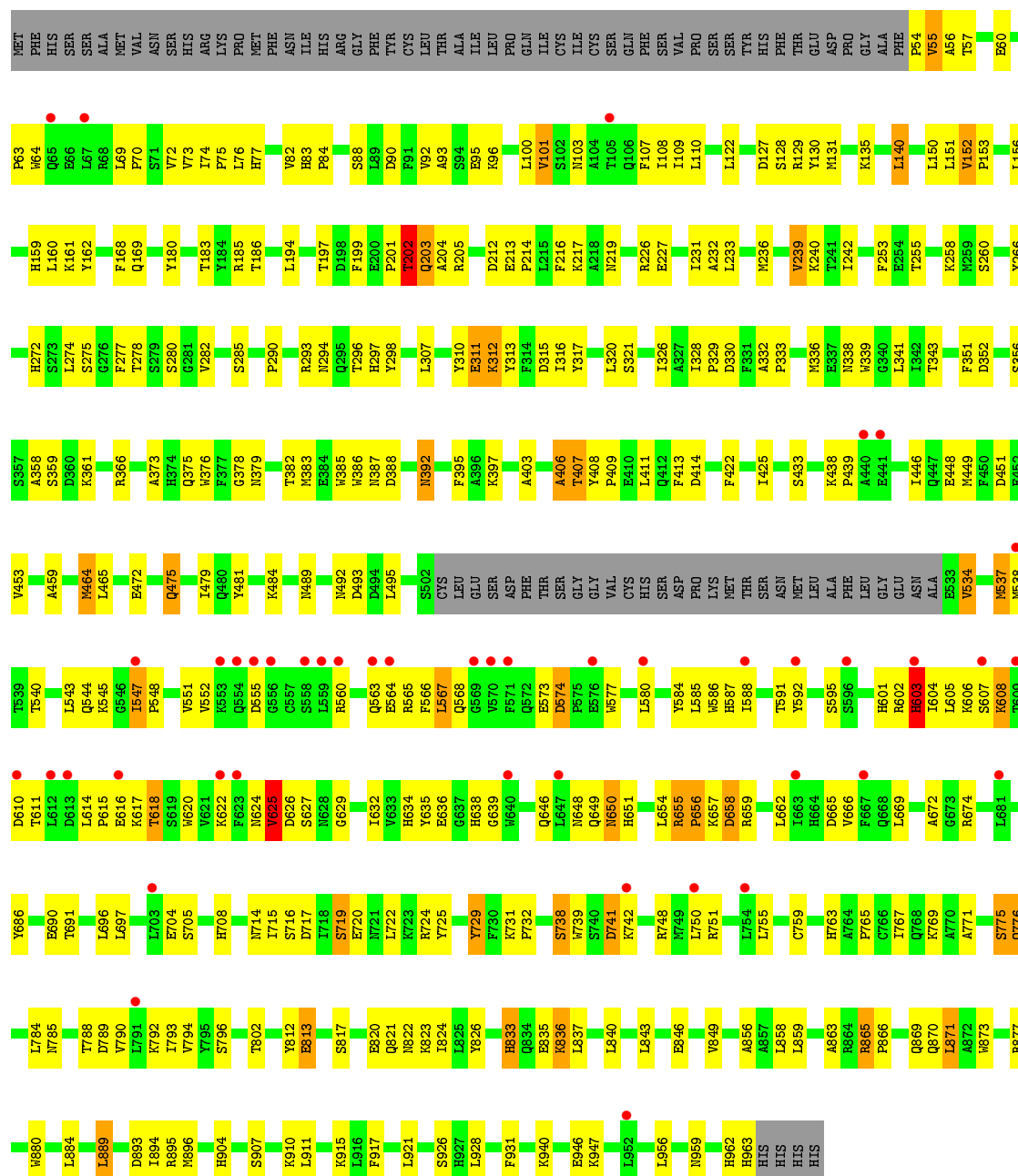
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Endoplasmic reticulum aminopeptidase 2



• Molecule 1: Endoplasmic reticulum aminopeptidase 2





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

Chain C: 50% 50%

MAG1
MAG2

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

Chain E: 50% 50%



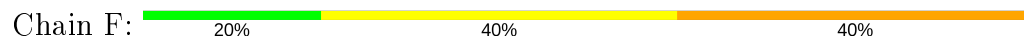
- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.54Å 134.33Å 127.58Å 90.00° 91.71° 90.00°	Depositor
Resolution (Å)	73.51 – 2.80 73.51 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (73.51-2.80) 99.5 (73.51-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.205 , 0.276 0.223 , 0.281	Depositor DCC
R_{free} test set	3075 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	75.8	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15067	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: MAN, ZN, BMA, NAG, 6GA

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	0.54	0/7605	0.67	0/10307
1	B	0.43	0/7365	0.61	0/9981
All	All	0.49	0/14970	0.64	0/20288

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	889	LEU	Peptide

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	7413	0	7339	185	0
1	B	7185	0	7127	205	0
2	C	28	0	25	0	0
2	E	28	0	25	0	0
3	D	39	0	34	1	0
3	G	39	0	34	1	0
4	F	61	0	52	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	84	0	78	1	0
6	B	70	0	65	1	0
7	A	46	0	0	2	0
7	B	23	0	0	0	0
8	A	34	0	0	7	0
8	B	15	0	0	6	0
All	All	15067	0	14779	395	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 13.

The worst 5 of 395 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)
6:A:1010:NAG:O4	8:A:1101:HOH:O	1.88	0.91
1:A:88:SER:OG	8:A:1102:HOH:O	1.92	0.88
1:B:72:VAL:HG23	1:B:73:VAL:HG23	1.57	0.85
1:A:273:SER:O	4:F:5:MAN:O4	1.95	0.84
1:A:278:THR:HG22	1:A:280:SER:H	1.43	0.84

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	910/967 (94%)	798 (88%)	90 (10%)	22 (2%)	6	20
1	B	877/967 (91%)	748 (85%)	105 (12%)	24 (3%)	5	17
All	All	1787/1934 (92%)	1546 (86%)	195 (11%)	46 (3%)	5	18

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	ASP
1	A	416	TYR
1	A	513	VAL
1	A	888	ASP
1	A	924	GLN

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	820/870 (94%)	766 (93%)	54 (7%)	16	44
1	B	793/870 (91%)	728 (92%)	65 (8%)	11	33
All	All	1613/1740 (93%)	1494 (93%)	119 (7%)	13	37

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	949	LEU
1	B	274	LEU
1	B	813	GLU
1	B	101	VAL
1	B	183	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	515	HIS

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Mol	Chain	Res	Type
1	B	375	GLN

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 ⓘ

15 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	1,2	14,14,15	0.69	1 (7%)	17,19,21	0.44	0
2	NAG	C	2	2	14,14,15	0.37	0	17,19,21	0.41	0
3	NAG	D	1	1,3	14,14,15	0.58	0	17,19,21	0.69	0
3	NAG	D	2	3	14,14,15	1.17	1 (7%)	17,19,21	1.30	1 (5%)
3	BMA	D	3	3	11,11,12	1.12	2 (18%)	15,15,17	2.15	5 (33%)
2	NAG	E	1	1,2	14,14,15	0.69	1 (7%)	17,19,21	0.64	0
2	NAG	E	2	2	14,14,15	0.48	0	17,19,21	0.37	0
4	NAG	F	1	1,4	14,14,15	0.62	0	17,19,21	0.38	0
4	NAG	F	2	4	14,14,15	0.70	1 (7%)	17,19,21	0.69	0
4	BMA	F	3	4	11,11,12	1.41	2 (18%)	15,15,17	0.73	0
4	MAN	F	4	4	11,11,12	1.35	2 (18%)	15,15,17	1.04	1 (6%)
4	MAN	F	5	4	11,11,12	1.77	3 (27%)	15,15,17	1.75	3 (20%)
3	NAG	G	1	1,3	14,14,15	0.43	0	17,19,21	0.57	0
3	NAG	G	2	3	14,14,15	0.39	0	17,19,21	1.44	2 (11%)
3	BMA	G	3	3	11,11,12	1.43	2 (18%)	15,15,17	2.09	4 (26%)

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	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	BMA	F	3	4	-	1/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	5/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	NAG	O5-C1	4.14	1.50	1.43
4	F	5	MAN	C4-C5	3.71	1.60	1.53
4	F	5	MAN	C1-C2	2.96	1.59	1.52
3	G	3	BMA	C1-C2	2.96	1.58	1.52
4	F	3	BMA	O5-C1	-2.94	1.39	1.43

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	BMA	C1-O5-C5	5.48	119.62	112.19
3	G	3	BMA	C1-O5-C5	5.41	119.52	112.19
3	D	2	NAG	C1-O5-C5	4.66	118.51	112.19
4	F	5	MAN	C1-O5-C5	4.63	118.46	112.19
3	G	2	NAG	C2-N2-C7	4.59	129.44	122.90

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

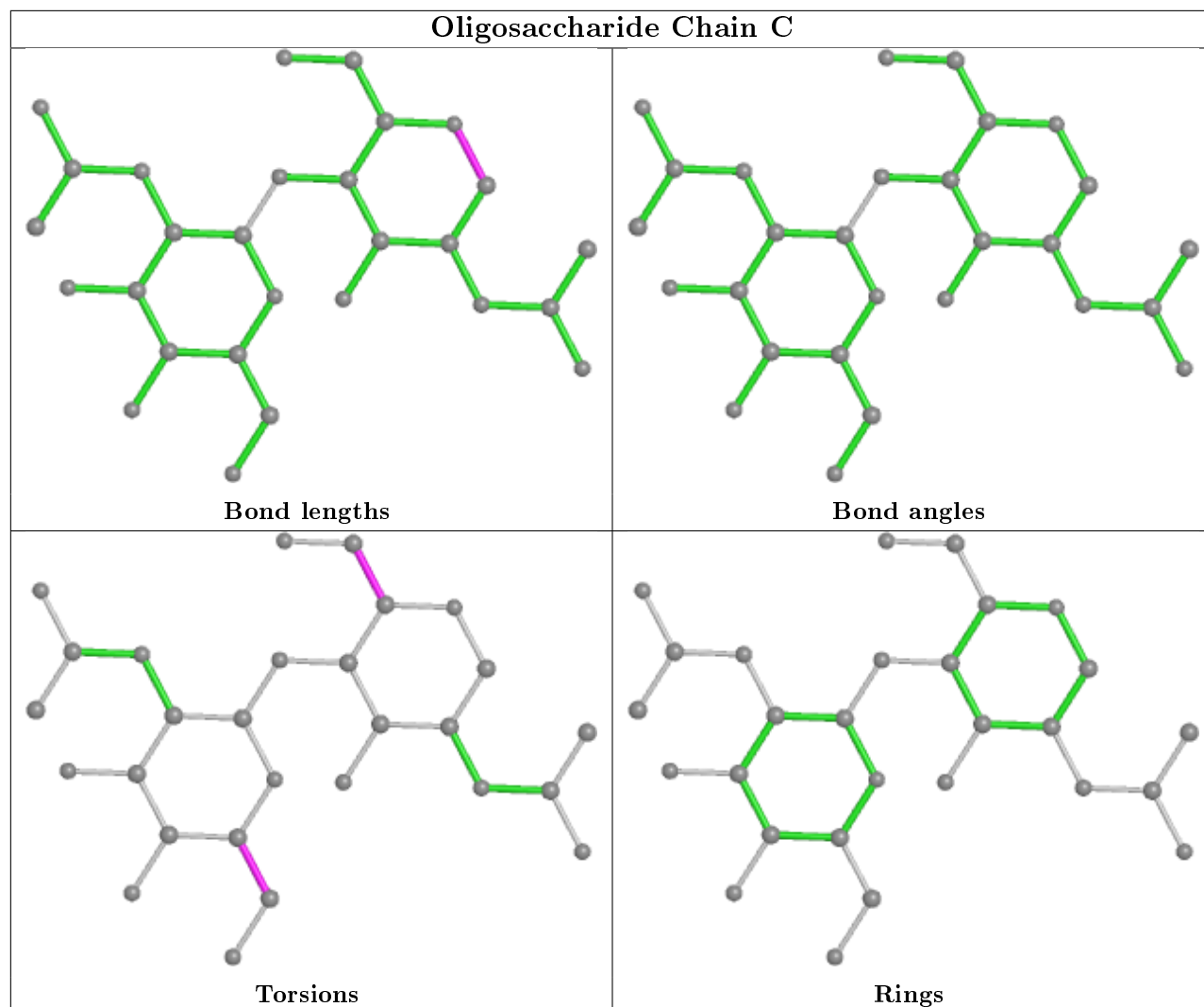
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6

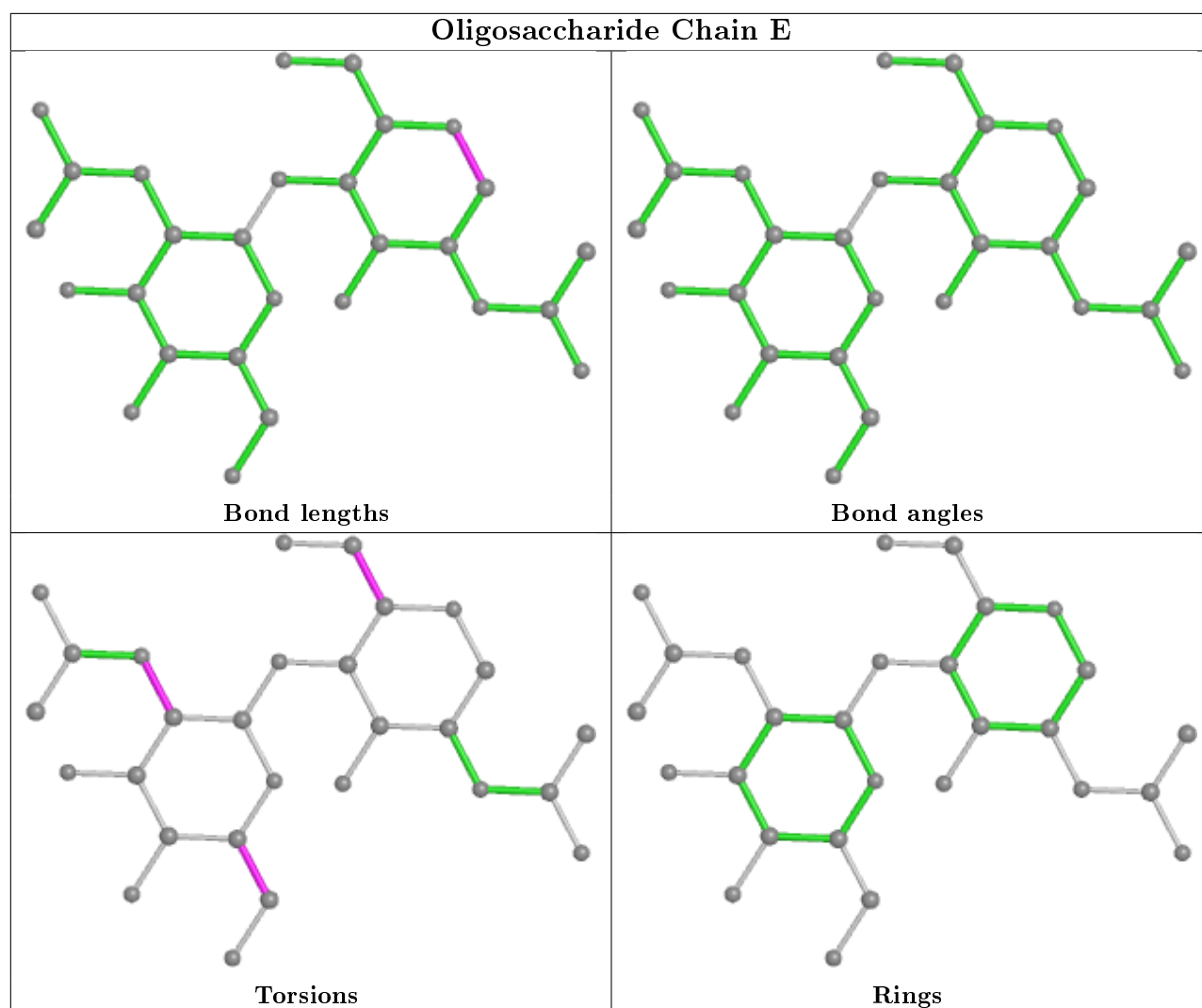
There are no ring outliers.

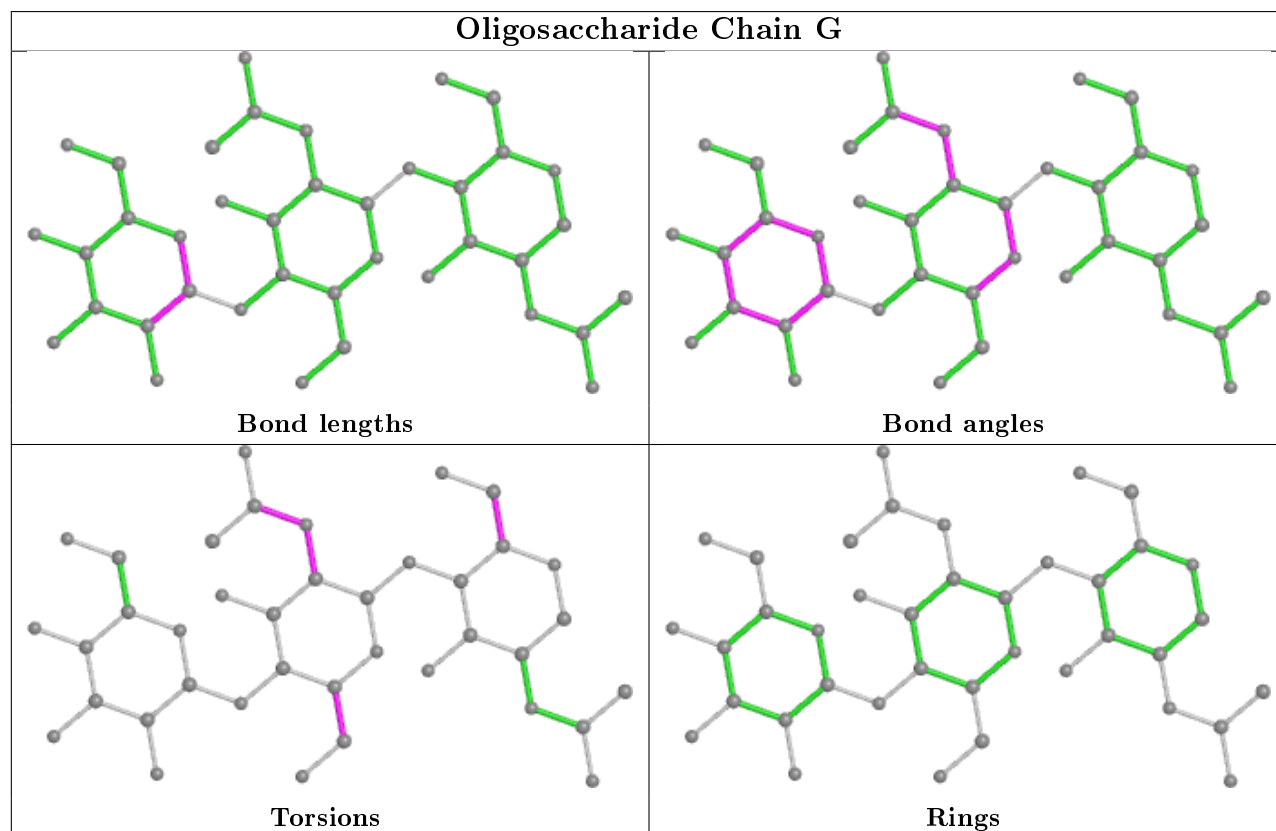
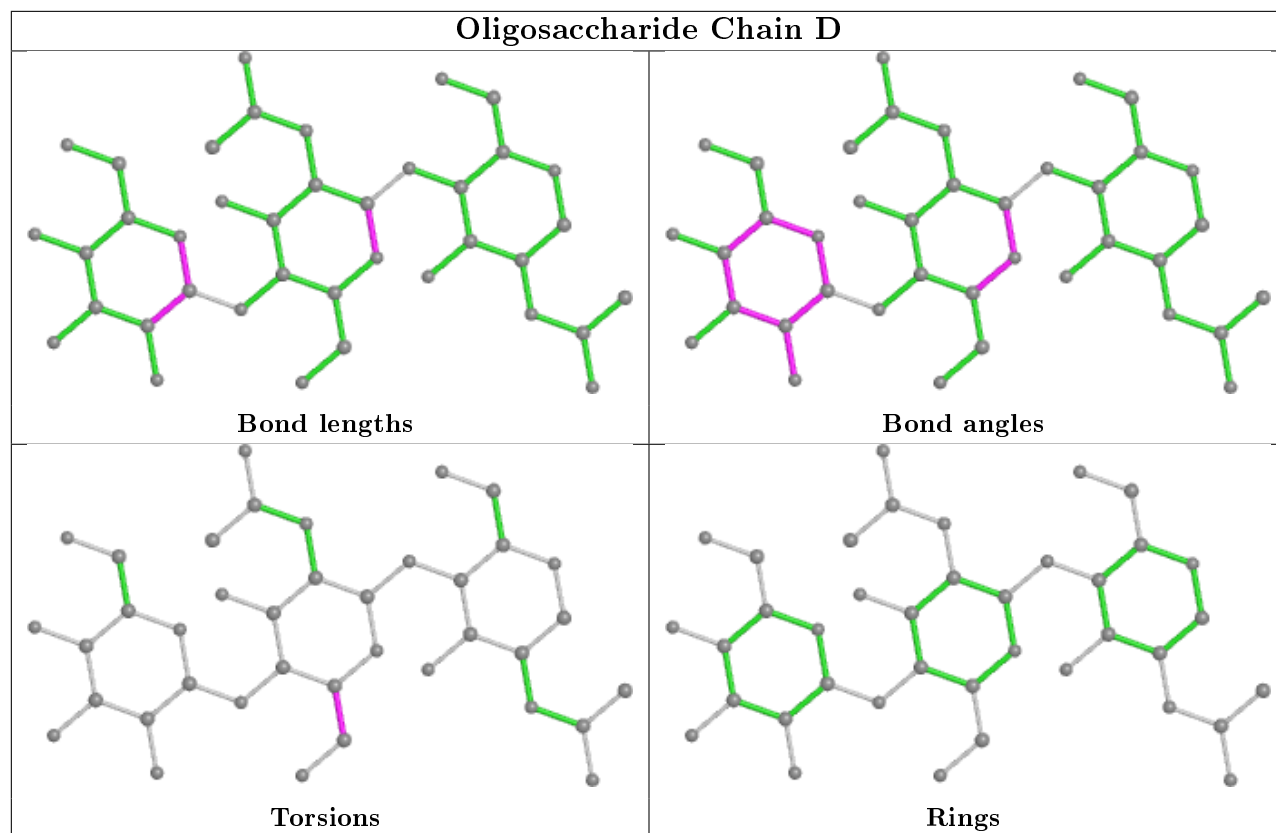
5 monomers are involved in 4 short contacts:

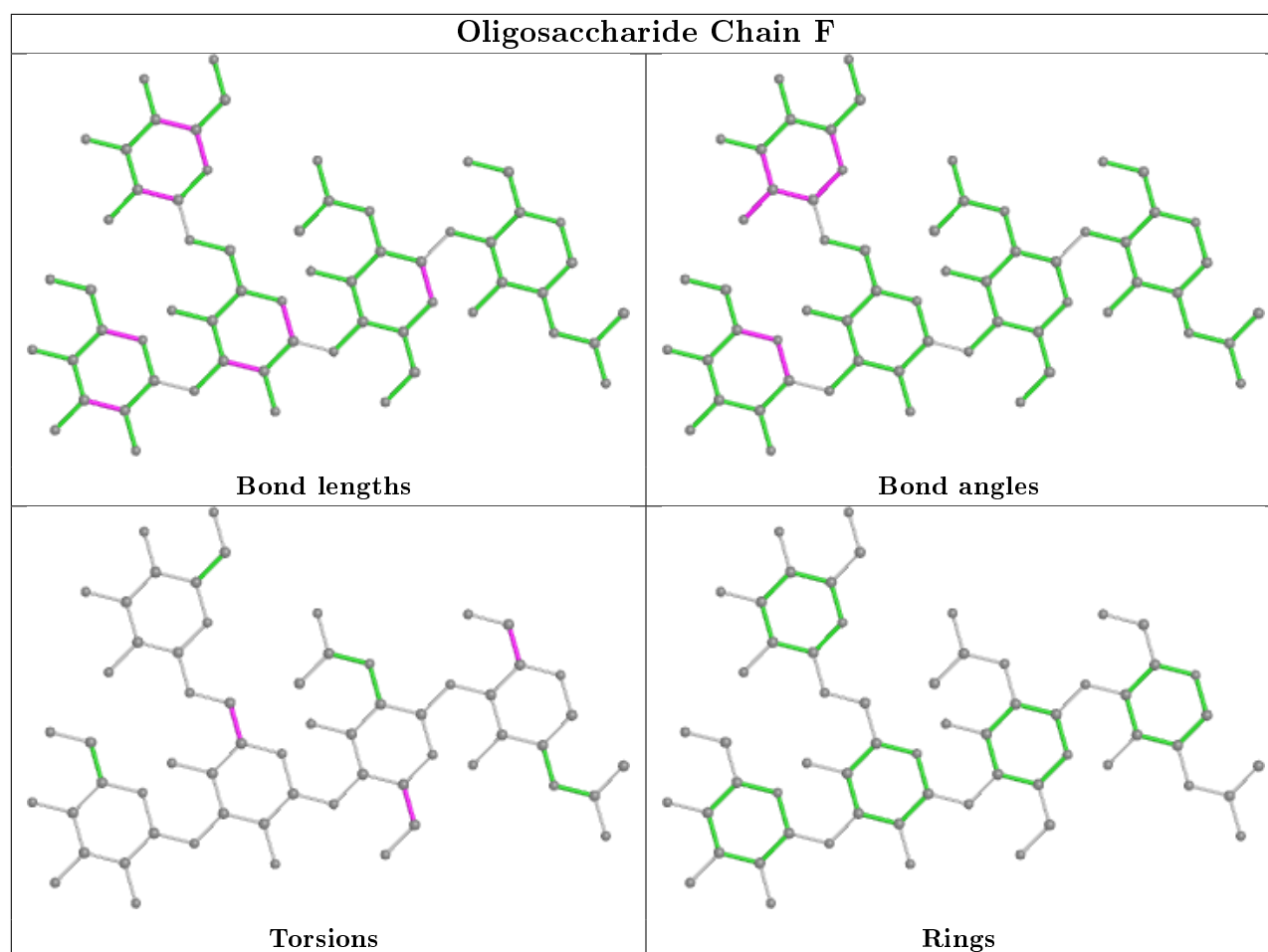
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2	NAG	1	0
4	F	5	MAN	2	0
3	D	2	NAG	1	0
4	F	3	BMA	1	0
3	D	1	NAG	1	0

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 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	A	1014	1	14,14,15	0.22	0	17,19,21	0.91	1 (5%)
6	NAG	B	1012	1	14,14,15	0.49	0	17,19,21	0.96	1 (5%)
7	6GA	B	1015	5	22,24,24	0.81	0	24,31,31	3.05	5 (20%)
6	NAG	A	1010	1	14,14,15	0.29	0	17,19,21	0.48	0
6	NAG	A	1009	1	14,14,15	0.32	0	17,19,21	0.75	1 (5%)
6	NAG	A	1013	1	14,14,15	0.61	0	17,19,21	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	B	1013	1	14,14,15	0.33	0	17,19,21	0.56	0
6	NAG	A	1012	1	14,14,15	0.43	0	17,19,21	0.57	0
6	NAG	B	1014	1	14,14,15	0.37	0	17,19,21	0.52	0
7	6GA	A	1015[B]	5	22,24,24	0.90	1 (4%)	24,31,31	2.34	7 (29%)
6	NAG	B	1010	1	14,14,15	0.62	1 (7%)	17,19,21	0.53	0
6	NAG	B	1011	1	14,14,15	0.55	0	17,19,21	0.44	0
6	NAG	A	1011	1	14,14,15	0.46	0	17,19,21	0.38	0
7	6GA	A	1015[A]	5	22,24,24	0.88	1 (4%)	24,31,31	1.55	5 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	1014	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1012	1	-	0/6/23/26	0/1/1/1
7	6GA	B	1015	5	-	8/19/19/19	0/2/2/2
6	NAG	A	1010	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1009	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1013	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1013	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1012	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1014	1	-	2/6/23/26	0/1/1/1
7	6GA	A	1015[B]	5	-	6/19/19/19	0/2/2/2
6	NAG	B	1010	1	-	3/6/23/26	0/1/1/1
6	NAG	B	1011	1	-	3/6/23/26	0/1/1/1
6	NAG	A	1011	1	-	2/6/23/26	0/1/1/1
7	6GA	A	1015[A]	5	-	8/19/19/19	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1015[A]	6GA	C9-N8	-2.96	1.27	1.33
7	A	1015[B]	6GA	C9-N8	-2.20	1.28	1.33
6	B	1010	NAG	C1-C2	2.05	1.55	1.52

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
7	B	1015	6GA	C1-N8-C9	12.49	140.31	122.34
7	A	1015[B]	6GA	C1-N8-C9	7.71	133.42	122.34
7	B	1015	6GA	O15-C12-N1	-5.78	115.78	123.27
7	A	1015[B]	6GA	O15-C12-N1	-4.77	117.09	123.27
7	A	1015[B]	6GA	C17-C16-C11	3.63	121.28	113.38

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1015	6GA	C16-C11-C9-O10
7	B	1015	6GA	C16-C11-C9-N8
7	B	1015	6GA	C11-C9-N8-C1
7	B	1015	6GA	C12-C11-C16-C17
7	A	1015[B]	6GA	C16-C11-C9-O10

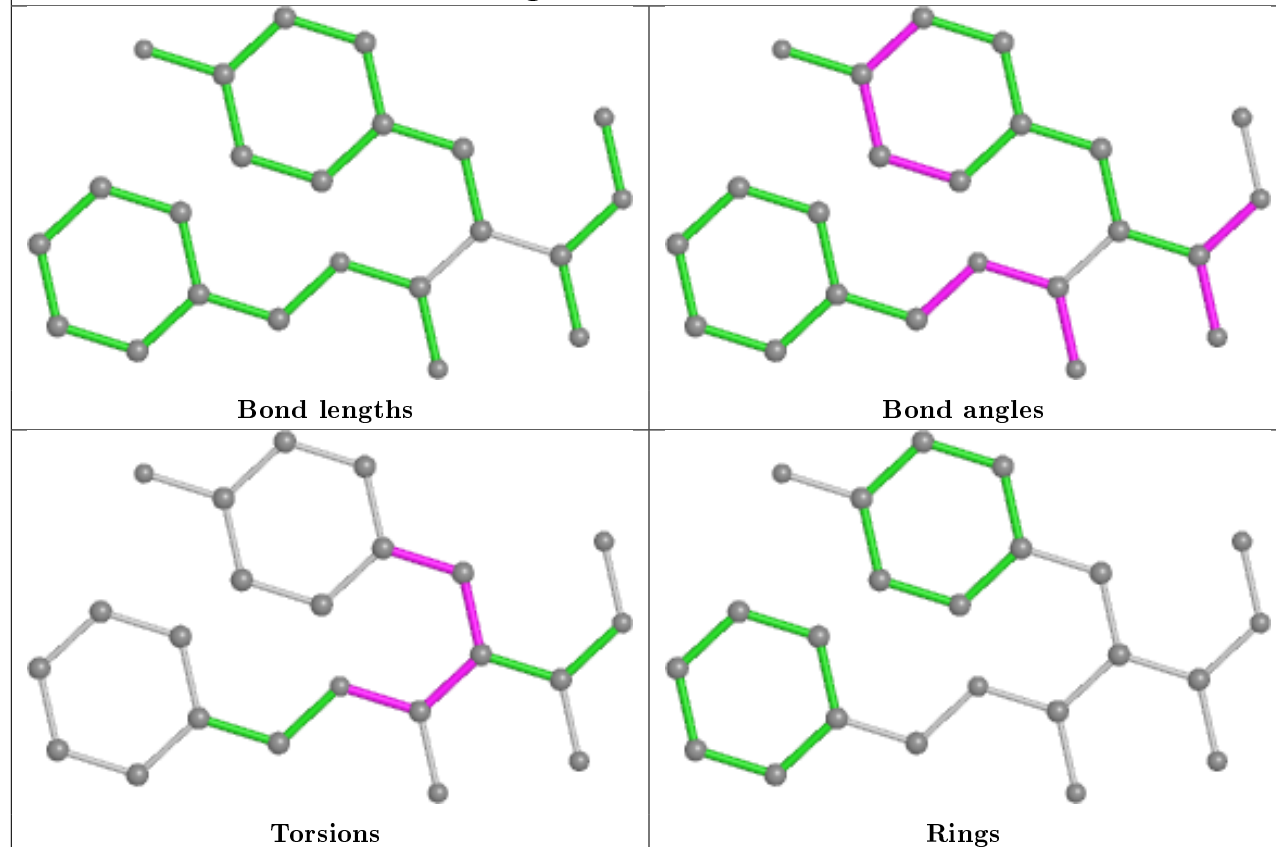
There are no ring outliers.

3 monomers are involved in 4 short contacts:

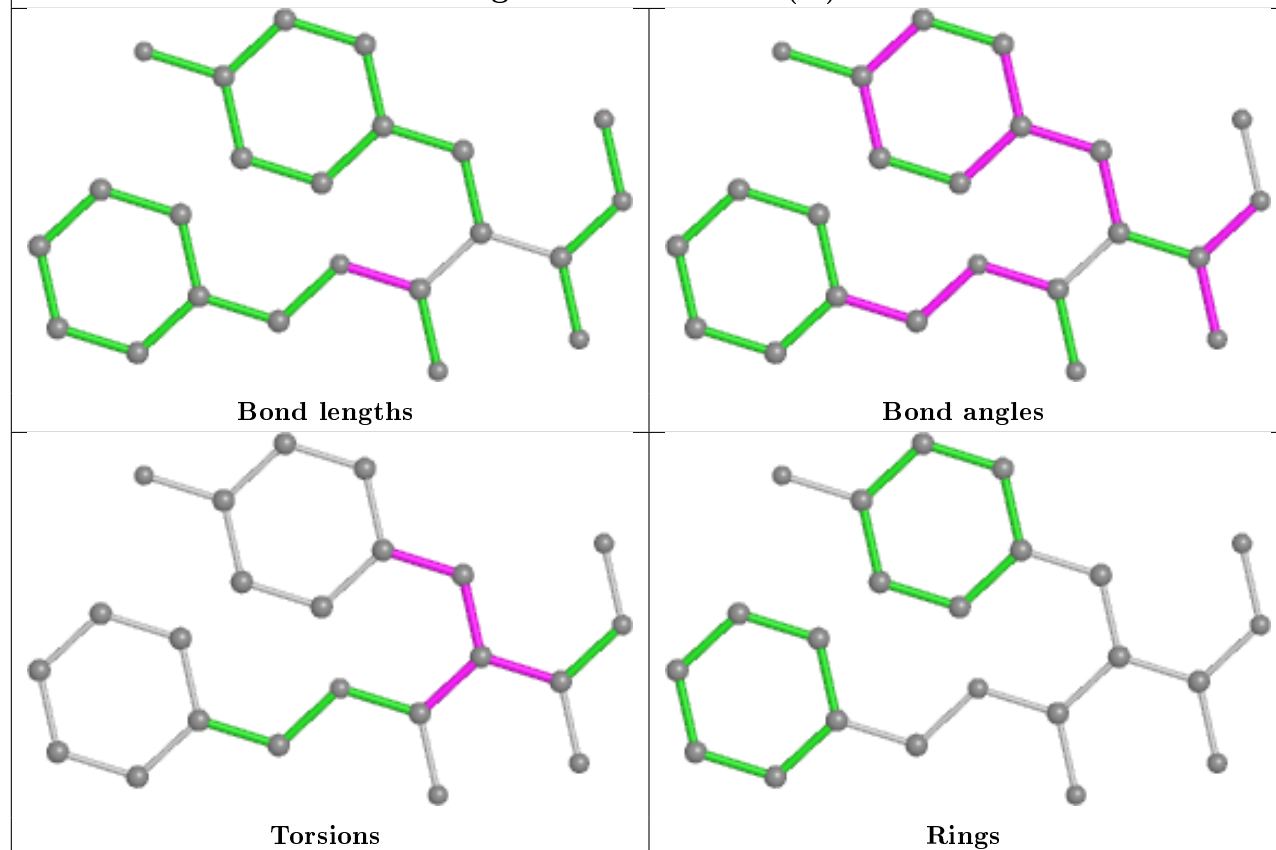
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1010	NAG	1	0
7	A	1015[B]	6GA	2	0
6	B	1010	NAG	1	0

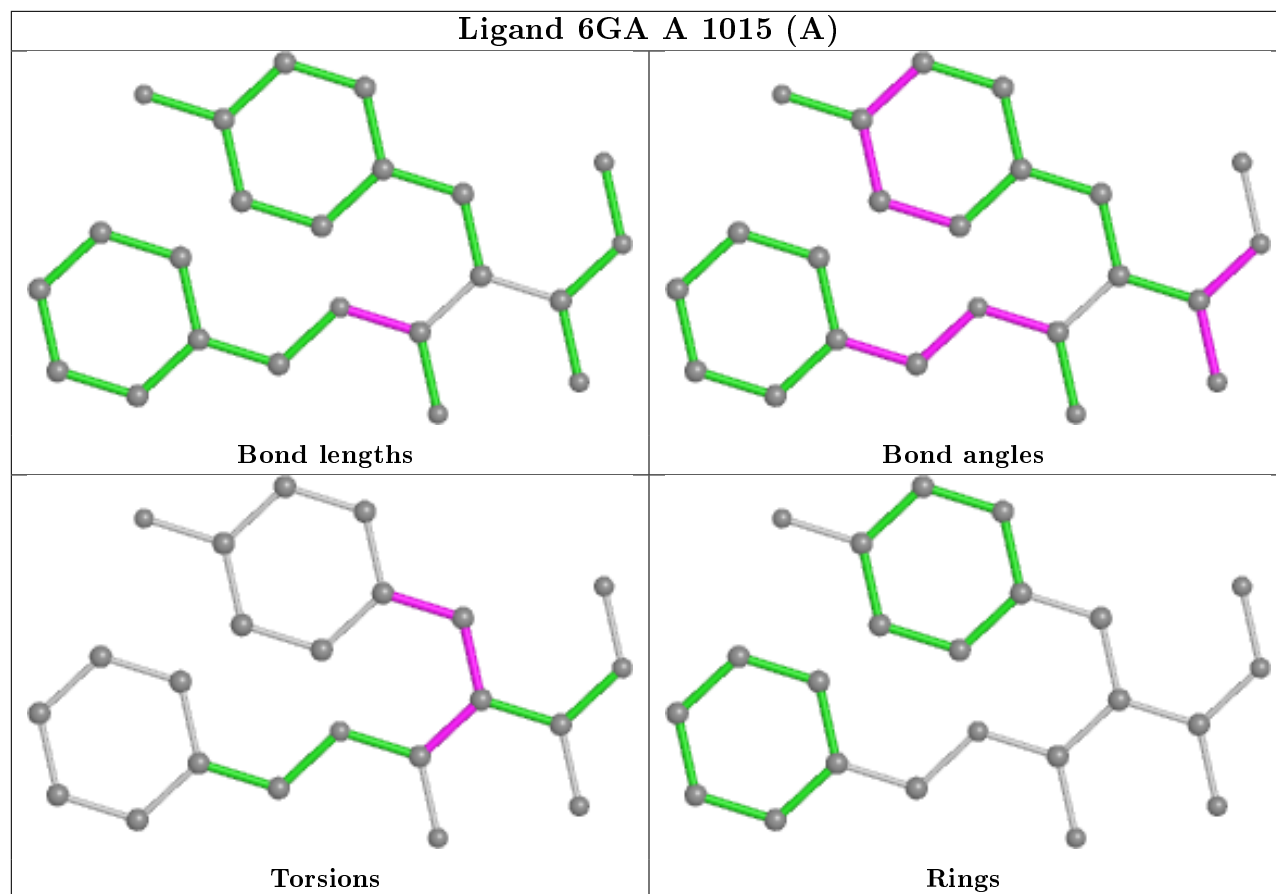
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand 6GA B 1015



Ligand 6GA A 1015 (B)





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	910/967 (94%)	0.02	19 (2%) 63 54	29, 57, 101, 156	0
1	B	880/967 (91%)	0.22	44 (5%) 28 19	37, 82, 132, 164	0
All	All	1790/1934 (92%)	0.12	63 (3%) 44 34	29, 69, 126, 164	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	510	SER	10.6
1	A	511	GLY	8.4
1	B	580	LEU	5.9
1	B	612	LEU	5.7
1	B	613	ASP	5.5

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.

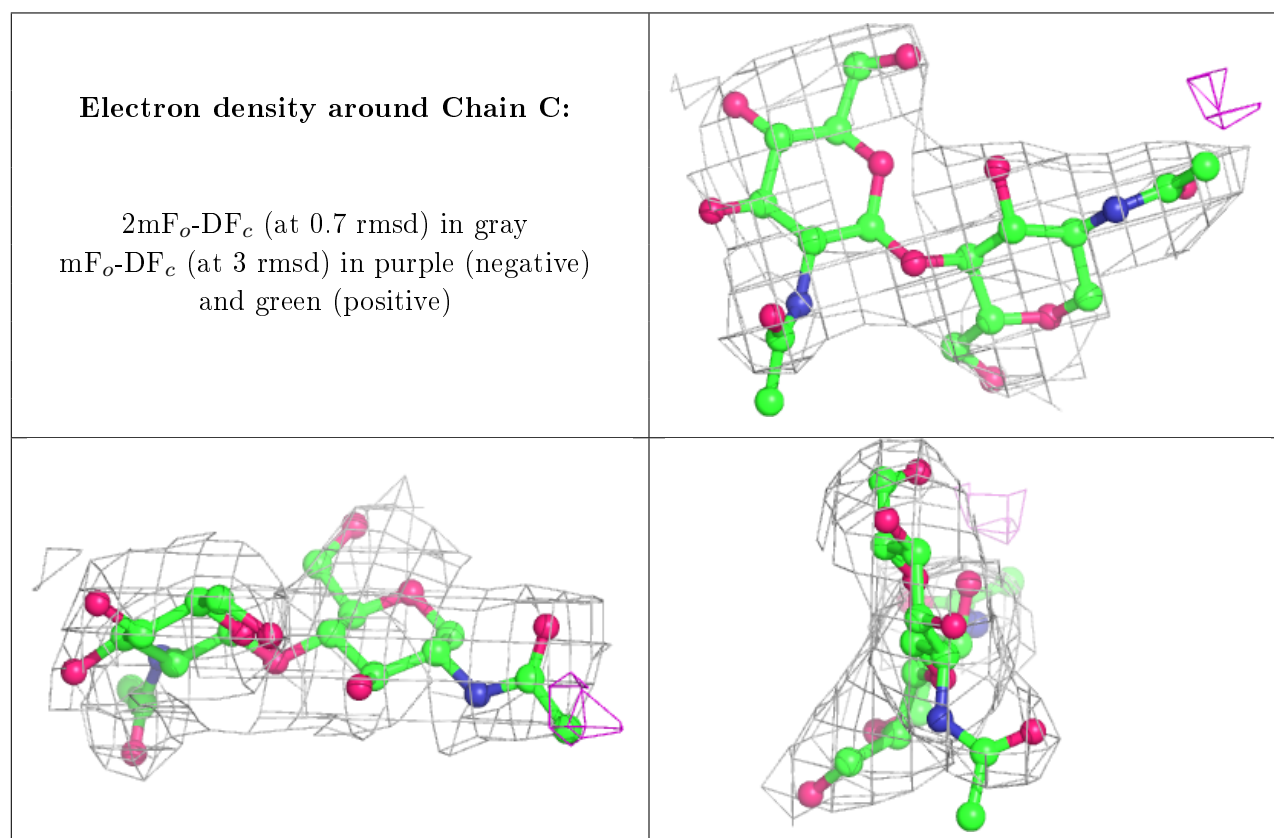
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	G	3	11/12	0.72	0.17	114,119,122,122	0
4	MAN	F	5	11/12	0.76	0.17	72,83,90,94	0
2	NAG	E	2	14/15	0.77	0.24	103,113,121,126	0
3	NAG	G	2	14/15	0.82	0.17	72,102,112,117	0
3	NAG	G	1	14/15	0.84	0.14	73,84,92,102	0

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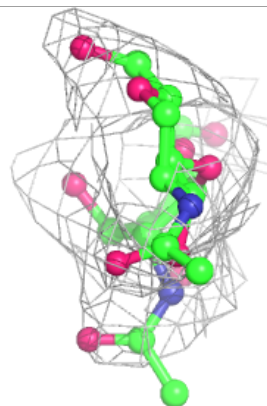
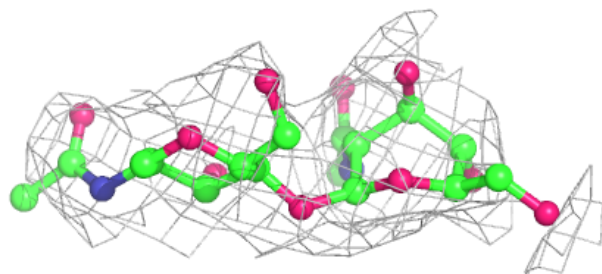
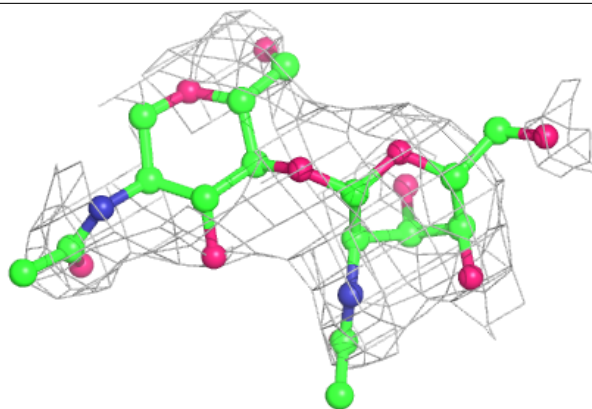
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BMA	D	3	11/12	0.85	0.14	105,111,121,125	0
2	NAG	C	2	14/15	0.86	0.17	86,100,108,117	0
4	MAN	F	4	11/12	0.86	0.15	101,107,116,118	0
2	NAG	E	1	14/15	0.88	0.19	80,93,105,108	0
4	NAG	F	2	14/15	0.90	0.15	48,79,88,90	0
4	BMA	F	3	11/12	0.91	0.10	89,95,102,104	0
4	NAG	F	1	14/15	0.94	0.14	49,61,70,73	0
2	NAG	C	1	14/15	0.94	0.16	52,77,86,86	0
3	NAG	D	2	14/15	0.95	0.09	53,74,93,104	0
3	NAG	D	1	14/15	0.96	0.18	46,57,61,69	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.

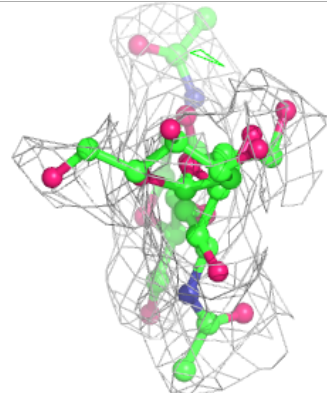
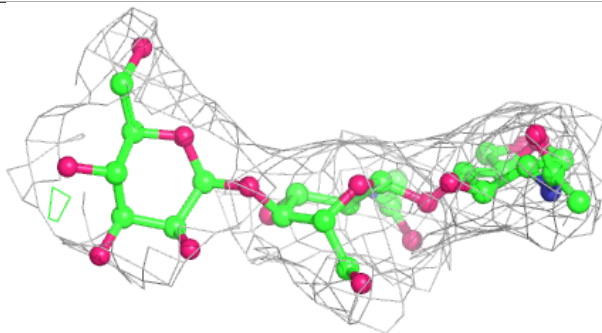
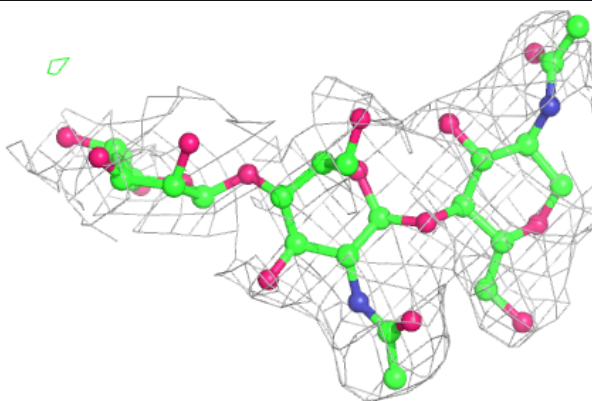


Electron density around Chain E:

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

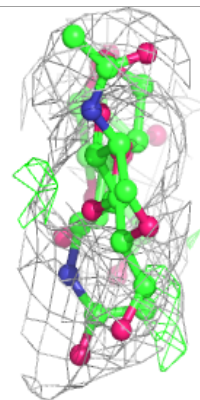
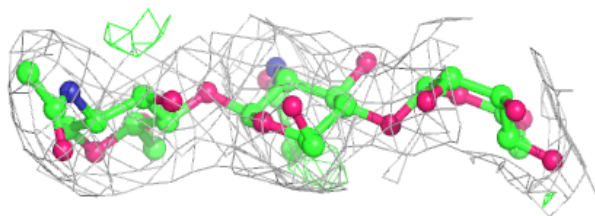
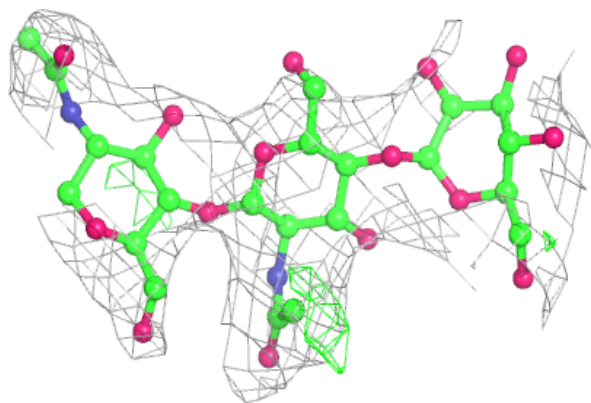
**Electron density around Chain D:**

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

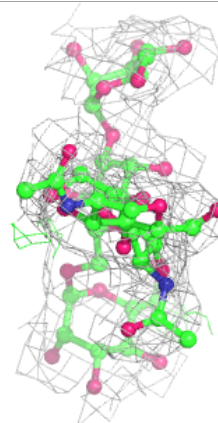
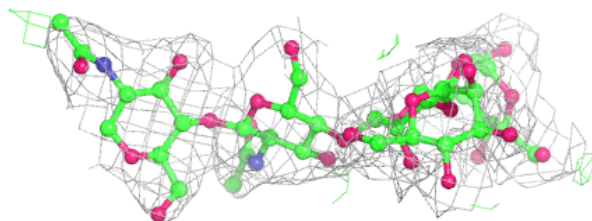
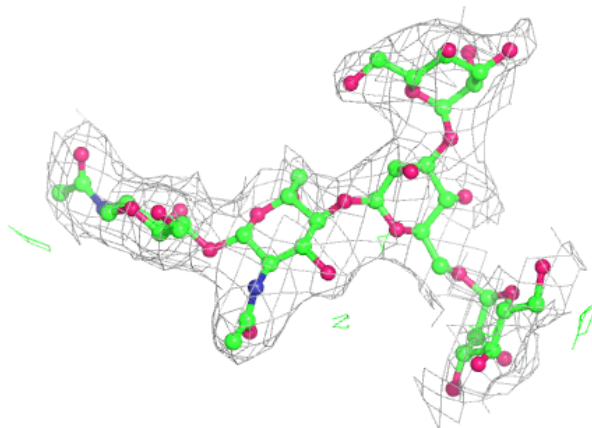


Electron density around Chain G:

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

**Electron density around Chain F:**

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



6.4 Ligands ⓘ

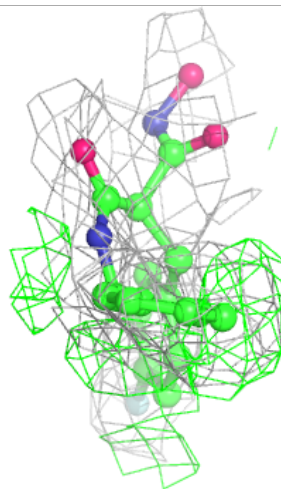
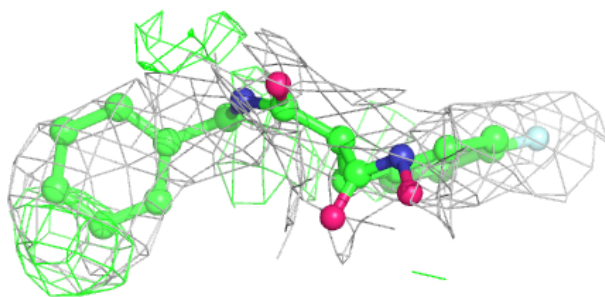
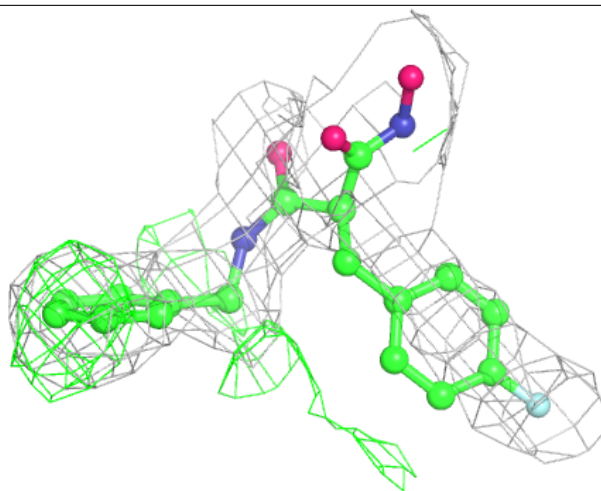
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	1010	14/15	0.76	0.16	137,150,158,163	0
6	NAG	B	1011	14/15	0.76	0.26	113,126,132,133	0
6	NAG	A	1012	14/15	0.78	0.14	83,104,121,124	0
6	NAG	A	1013	14/15	0.82	0.21	80,89,97,99	0
6	NAG	B	1012	14/15	0.82	0.29	92,107,116,117	0
6	NAG	B	1014	14/15	0.83	0.15	95,118,127,129	0
6	NAG	B	1013	14/15	0.84	0.21	107,115,122,122	0
6	NAG	A	1011	14/15	0.84	0.16	99,112,121,122	0
6	NAG	A	1009	14/15	0.88	0.13	83,88,96,97	0
6	NAG	A	1010	14/15	0.89	0.12	102,110,113,116	0
6	NAG	A	1014	14/15	0.89	0.16	84,89,100,102	0
7	6GA	B	1015	23/23	0.89	0.27	65,74,80,83	23
7	6GA	A	1015[B]	23/23	0.91	0.32	44,49,52,57	23
7	6GA	A	1015[A]	23/23	0.91	0.32	41,47,51,51	23
5	ZN	B	1001	1/1	0.99	0.17	54,54,54,54	0
5	ZN	A	1001	1/1	0.99	0.20	37,37,37,37	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.

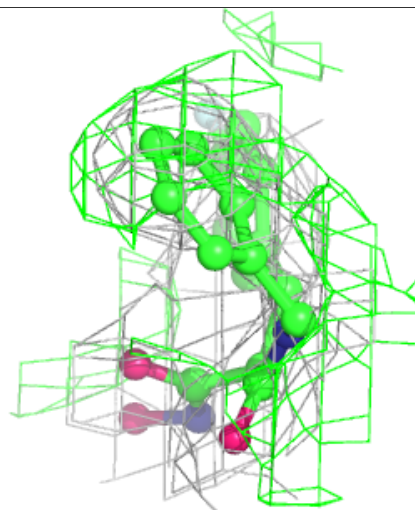
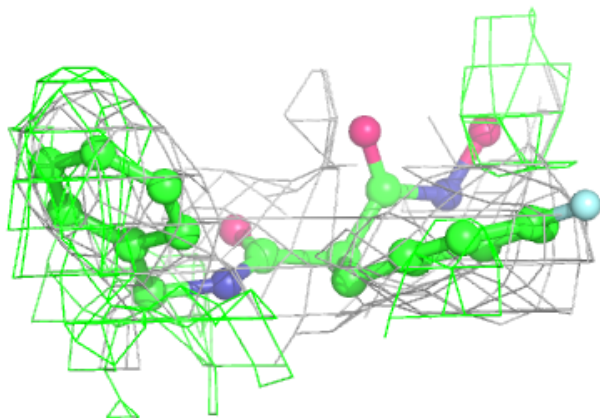
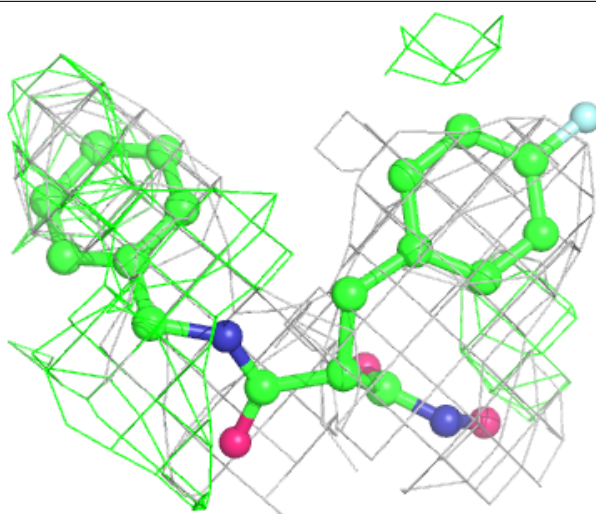
Electron density around 6GA B 1015:

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



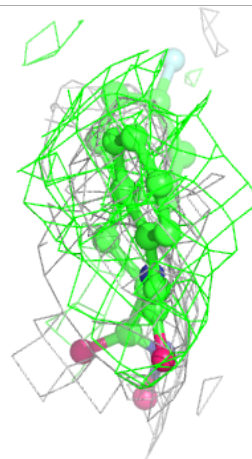
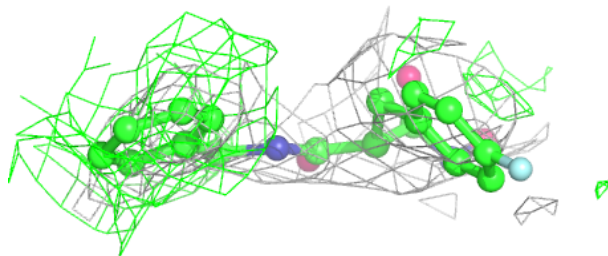
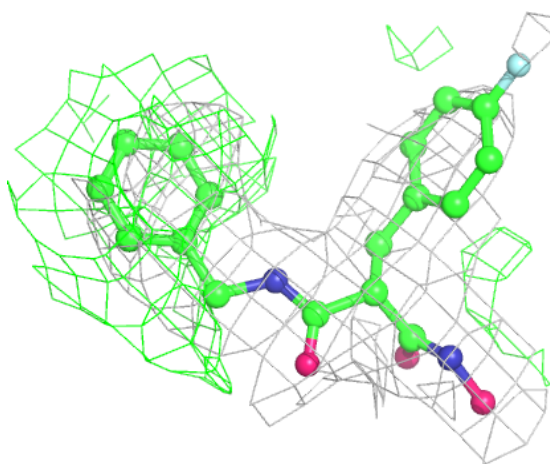
Electron density around 6GA A 1015 (B):

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



Electron density around 6GA A 1015 (A):

$2mF_o-DF_c$ (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.