



# wwPDB X-ray Structure Validation Summary Report

Mar 9, 2026 – 01:09 AM UTC

PDB ID : 7PFS / pdb\_00007pfs  
Title : Crystal structure of ERAP2 aminopeptidase in complex with phosphinic pseudotriptide ((1R)-1-Amino-3-phenylpropyl){2-([1,1:3,1-terphenyl]-5-ylmethyl)-3-[(2S)-1-amino-1-oxo-3-phenylpropan-2-yl)-amino]-3-oxopropyl}phosphinic acid  
Authors : Giastas, P.; Stratikos, E.; Mpakali, A.  
Deposited on : 2021-08-12  
Resolution : 2.70 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references](#) ①) were used in the production of this report:

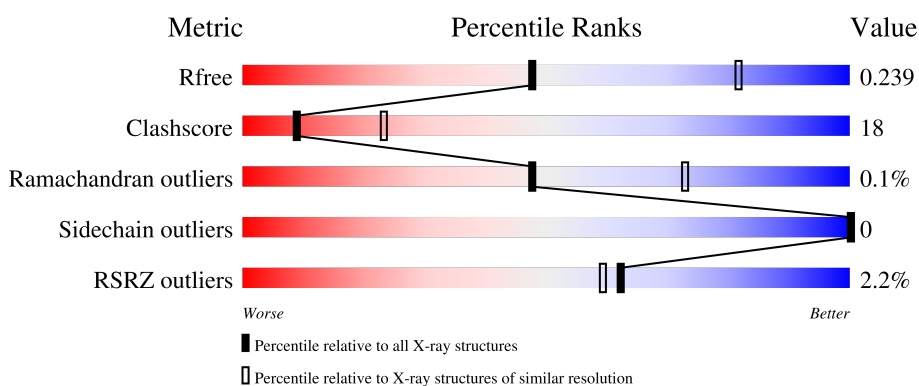
MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 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 2.70 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.



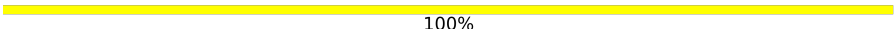

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	963	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 67%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 28%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">67% 28% 5%</p>
1	B	963	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 55%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 35%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">55% 35% 9%</p>
2	C	3	<div style="display: flex; align-items: center;"> <div style="width: 33%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 67%; height: 10px; background-color: yellow; margin-right: 2px;"></div> </div> <p style="margin-left: 20px;">33% 67%</p>
2	D	3	<div style="display: flex; align-items: center;"> <div style="width: 33%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 67%; height: 10px; background-color: yellow; margin-right: 2px;"></div> </div> <p style="margin-left: 20px;">33% 67%</p>
2	E	3	<div style="display: flex; align-items: center;"> <div style="width: 67%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 2px;"></div> </div> <p style="margin-left: 20px;">67% 33%</p>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	F	2	 100%
3	H	2	 50% 50%
3	I	2	 100%
3	J	2	 50% 50%
3	K	2	 100%
4	G	5	 20% 80%

## 2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 14867 atoms, of which 88 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.

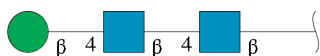
- Molecule 1 is a protein called Endoplasmic reticulum aminopeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	916	Total 7360	C 4743	N 1224	O 1360	S 33	0	2	0
1	B	872	Total 6800	C 4399	N 1132	O 1243	S 26	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

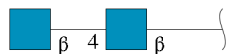
Chain	Residue	Modelled	Actual	Comment	Reference
A	392	ASN	LYS	variant	UNP Q6P179
A	961	ARG	-	expression tag	UNP Q6P179
A	962	HIS	-	expression tag	UNP Q6P179
A	963	HIS	-	expression tag	UNP Q6P179
B	392	ASN	LYS	variant	UNP Q6P179
B	961	ARG	-	expression tag	UNP Q6P179
B	962	HIS	-	expression tag	UNP Q6P179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

- Molecule 2 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.



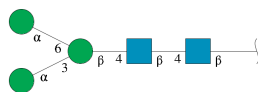
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	3	Total 39	C 22	N 2	O 15	0	0	0
2	D	3	Total 39	C 22	N 2	O 15	0	0	0
2	E	3	Total 39	C 22	N 2	O 15	0	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



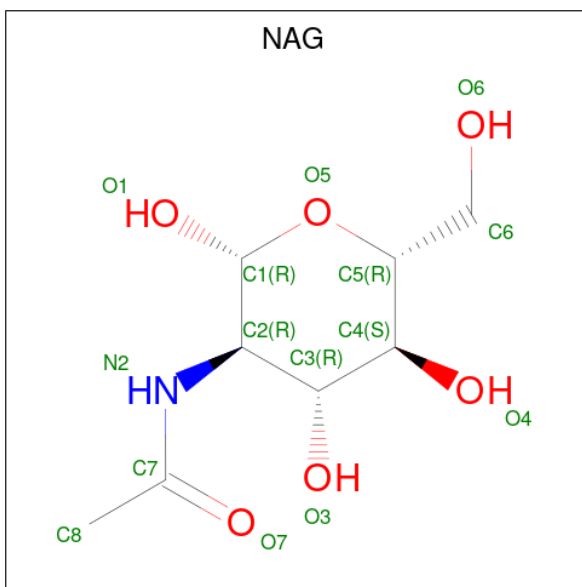
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	F	2	28	16	2	10	0	0	0
3	H	2	28	16	2	10	0	0	0
3	I	2	28	16	2	10	0	0	0
3	J	2	28	16	2	10	0	0	0
3	K	2	28	16	2	10	0	0	0

- 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.



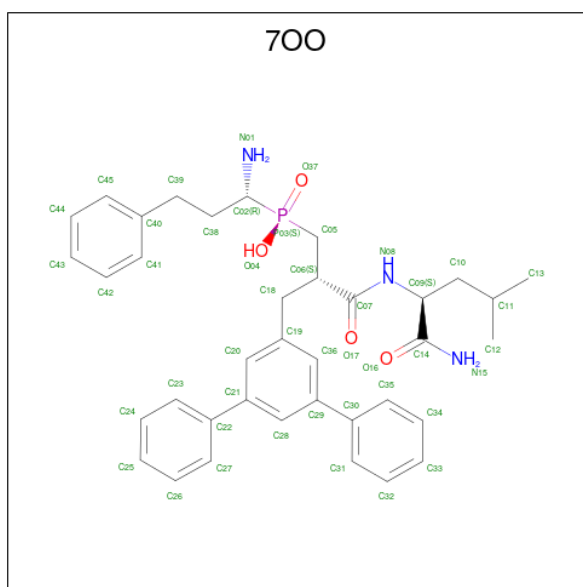
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	G	5	61	34	2	25	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



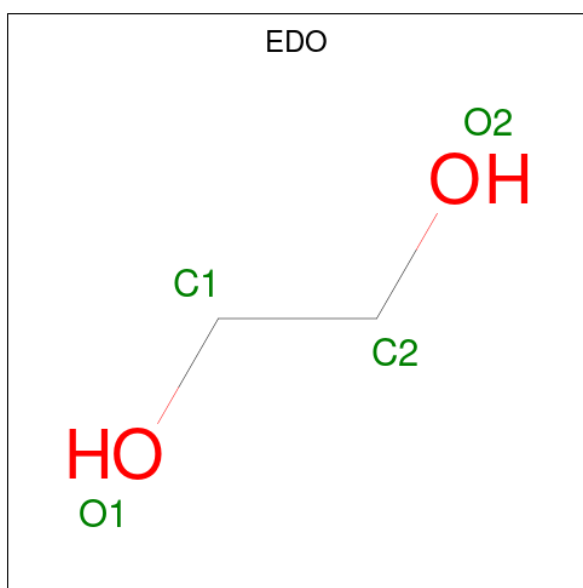
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
5	A	1	14	8	1	5	0	0
5	A	1	14	8	1	5	0	0
5	A	1	14	8	1	5	0	0
5	A	1	14	8	1	5	0	0
5	B	1	14	8	1	5	0	0
5	B	1	14	8	1	5	0	0
5	B	1	14	8	1	5	0	0

- Molecule 6 is [(2 {S})-3-[(2 {S})-1-azanyl-4-methyl-1-oxidanylidene-pentan-2-yl]amino]-2-[(3,5-diphenylphenyl)methyl]-3-oxidanylidene-propyl]-[(1 {R})-1-azanyl-3-phenyl-propyl]phosphinic acid (CCD ID: 700) (formula: C<sub>37</sub>H<sub>44</sub>N<sub>3</sub>O<sub>4</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
6	A	1	89	37	44	3	4	1	0	0
6	B	1	89	37	44	3	4	1	0	0

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



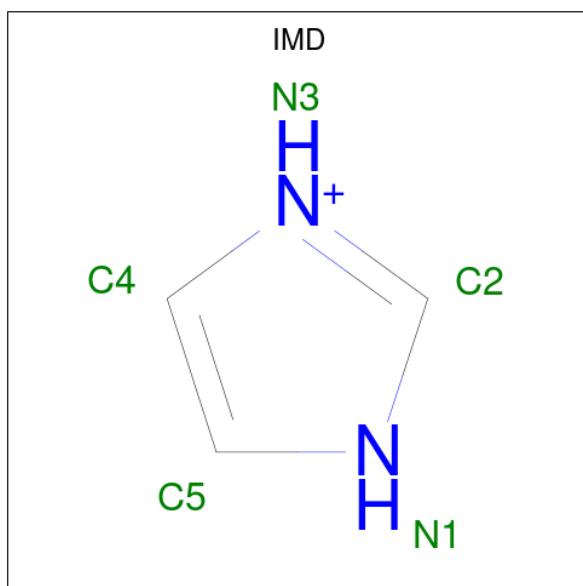
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C O		
7	A	1	4	2 2	0	0
7	A	1	4	2 2	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is IMIDAZOLE (CCD ID: IMD) (formula:  $C_3H_5N_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	N	0	0
			5	3	2		

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

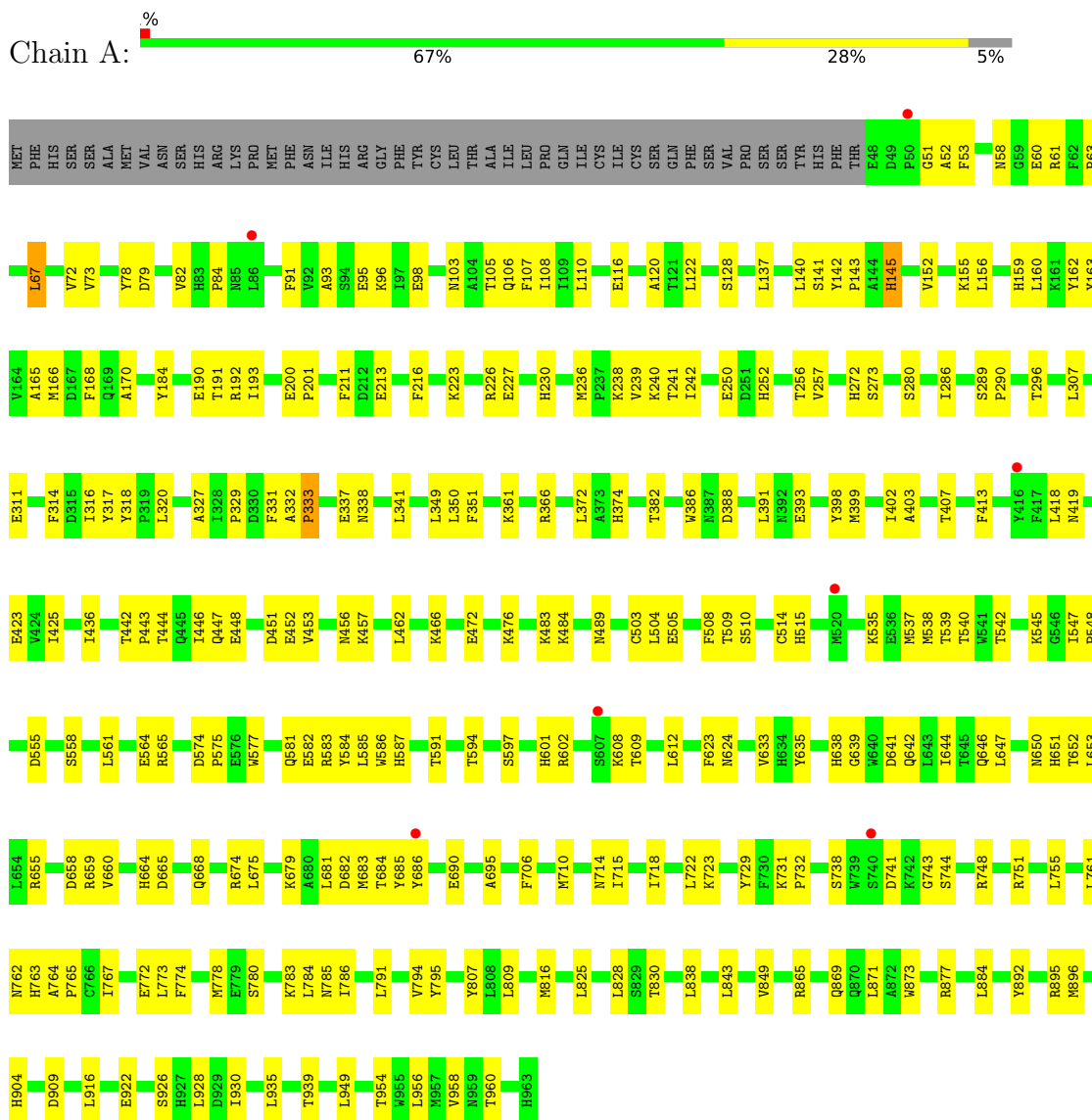
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	55	Total	O	0	0
			55	55		
10	B	25	Total	O	0	0
			25	25		

### 3 Residue-property plots

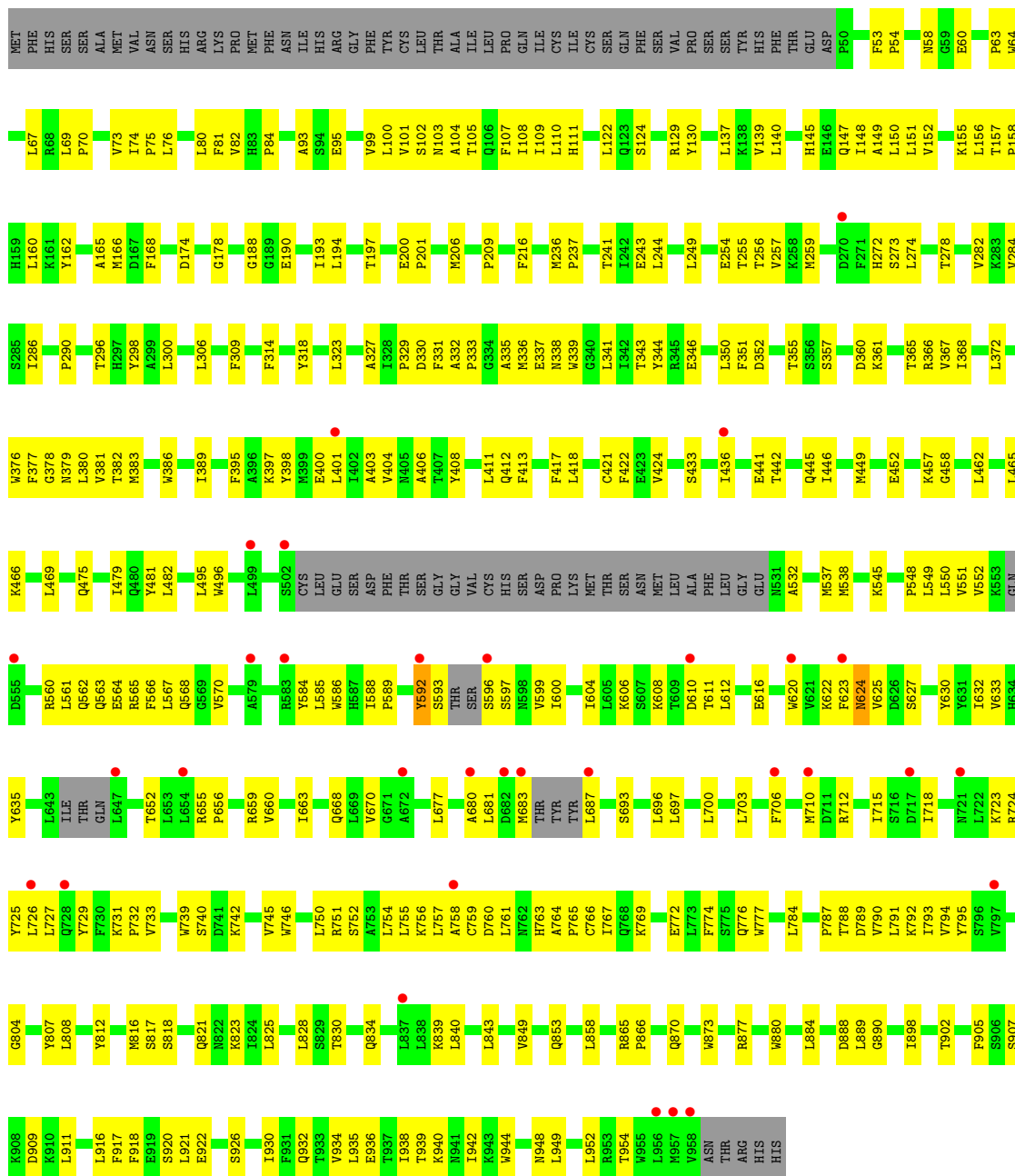
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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





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

Chain E: 67% 33%



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

Chain K: 100%



- 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

Chain G:  20% 80%

MAG1
MAG2
MAN3
MAN4
MAN5

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.14Å 133.82Å 128.70Å 90.00° 90.28° 90.00°	Depositor
Resolution (Å)	65.03 – 2.70 65.03 – 2.70	Depositor EDS
% Data completeness (in resolution range)	88.6 (65.03-2.70) 88.6 (65.03-2.70)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.14_3219, PHENIX 1.14_3219	Depositor
R, $R_{free}$	0.188 , 0.238 0.190 , 0.239	Depositor DCC
$R_{free}$ test set	3103 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.4	Xtrriage
Anisotropy	0.019	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 70.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.018 for -h,-l,-k 0.000 for -h,l,k 0.029 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14867	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NAG, BMA, 7OO, ZN, EDO, MAN, IMD

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	1/7552 (0.0%)	0.80	14/10251 (0.1%)
1	B	0.51	3/6976 (0.0%)	0.76	6/9492 (0.1%)
All	All	0.52	4/14528 (0.0%)	0.78	20/19743 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	103	ASN	CG-ND2	-10.85	1.10	1.33
1	B	103	ASN	CG-OD1	-6.41	1.11	1.23
1	B	206	MET	SD-CE	-5.29	1.66	1.79
1	A	896	MET	CB-CG	-5.18	1.36	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	LEU	CD1-CG-CD2	13.28	140.02	110.80
1	A	67	LEU	CB-CG-CD2	-11.15	77.24	110.70
1	B	616	GLU	CA-C-N	-6.59	111.44	122.64
1	B	616	GLU	C-N-CA	-6.59	111.44	122.64
1	A	333	PRO	CA-C-N	-6.18	109.29	121.41

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	684	THR	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	7360	0	7201	223	1
1	B	6800	0	6452	311	0
2	C	39	0	34	1	0
2	D	39	0	34	1	0
2	E	39	0	34	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	2	0
3	K	28	0	25	0	0
4	G	61	0	52	0	0
5	A	70	0	65	2	0
5	B	42	0	39	0	0
6	A	45	44	0	2	0
6	B	45	44	0	2	0
7	A	12	0	18	0	0
8	A	5	0	5	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	55	0	0	1	0
10	B	25	0	0	2	0
All	All	14779	88	14059	532	1

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 18.

The worst 5 of 532 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:594:THR:HG23	1:A:597:SER:H	1.15	1.08

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:VAL:HG21	1:A:108:ILE:HD13	1.36	1.04
1:A:436:ILE:HD11	1:A:457:LYS:HG2	1.40	1.04
1:B:756:LYS:HA	1:B:793:ILE:HD11	1.37	1.03
1:B:917:PHE:HA	1:B:920:SER:HB3	1.38	1.02

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:SER:OG	1:A:909:ASP:OD1[2_555]	2.17	0.03

## 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	916/963 (95%)	861 (94%)	54 (6%)	1 (0%)	48 73
1	B	861/963 (89%)	797 (93%)	63 (7%)	1 (0%)	48 73
All	All	1777/1926 (92%)	1658 (93%)	117 (7%)	2 (0%)	48 73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	624	ASN
1	A	583	ARG

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	799/866 (92%)	799 (100%)	0	100	100
1	B	695/866 (80%)	695 (100%)	0	100	100
All	All	1494/1732 (86%)	1494 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	668	GLN
1	B	821	GLN
1	B	854	ASN
1	B	776	GLN
1	A	904	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

24 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	C	1	2,1	14,14,15	0.47	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	C	2	2	14,14,15	0.55	0	17,19,21	0.43	0
2	BMA	C	3	2	11,11,12	0.85	1 (9%)	15,15,17	1.13	1 (6%)
2	NAG	D	1	2,1	14,14,15	0.37	0	17,19,21	0.64	0
2	NAG	D	2	2	14,14,15	0.85	1 (7%)	17,19,21	0.73	0
2	BMA	D	3	2	11,11,12	0.70	0	15,15,17	0.71	0
2	NAG	E	1	2,1	14,14,15	0.53	0	17,19,21	0.72	0
2	NAG	E	2	2	14,14,15	0.35	0	17,19,21	0.44	0
2	BMA	E	3	2	11,11,12	1.20	2 (18%)	15,15,17	0.89	1 (6%)
3	NAG	F	1	1,3	14,14,15	0.28	0	17,19,21	0.43	0
3	NAG	F	2	3	14,14,15	0.27	0	17,19,21	0.51	0
4	NAG	G	1	4,1	14,14,15	0.75	1 (7%)	17,19,21	0.58	0
4	NAG	G	2	4	14,14,15	0.71	0	17,19,21	0.57	0
4	BMA	G	3	4	11,11,12	0.95	1 (9%)	15,15,17	0.78	0
4	MAN	G	4	4	11,11,12	1.20	1 (9%)	15,15,17	1.02	0
4	MAN	G	5	4	11,11,12	1.22	2 (18%)	15,15,17	1.15	2 (13%)
3	NAG	H	1	1,3	14,14,15	0.41	0	17,19,21	0.45	0
3	NAG	H	2	3	14,14,15	0.98	1 (7%)	17,19,21	0.55	0
3	NAG	I	1	1,3	14,14,15	0.71	1 (7%)	17,19,21	0.73	1 (5%)
3	NAG	I	2	3	14,14,15	0.94	1 (7%)	17,19,21	0.79	1 (5%)
3	NAG	J	1	1,3	14,14,15	2.39	3 (21%)	17,19,21	2.00	5 (29%)
3	NAG	J	2	3	14,14,15	1.42	2 (14%)	17,19,21	0.97	2 (11%)
3	NAG	K	1	1,3	14,14,15	0.55	0	17,19,21	0.69	0
3	NAG	K	2	3	14,14,15	0.60	0	17,19,21	0.79	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	1/2/19/22	0/1/1/1
4	MAN	G	5	4	-	0/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	I	2	3	-	3/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	4/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1	NAG	O5-C1	-7.96	1.30	1.43
3	J	2	NAG	O5-C1	-4.43	1.36	1.43
3	H	2	NAG	O5-C1	-3.46	1.37	1.43
3	I	2	NAG	C1-C2	3.33	1.56	1.52
4	G	5	MAN	O5-C5	2.91	1.49	1.43

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1	NAG	C4-C3-C2	-4.11	105.00	111.02
3	J	1	NAG	C1-C2-N2	4.09	116.88	110.43
3	J	1	NAG	C2-N2-C7	3.56	127.67	122.90
3	J	2	NAG	C4-C3-C2	2.68	114.94	111.02
4	G	5	MAN	O2-C2-C3	-2.65	104.67	110.15

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	2	NAG	C1-C2-N2-C7
3	J	1	NAG	C1-C2-N2-C7

Continued on next page...

Continued from previous page...

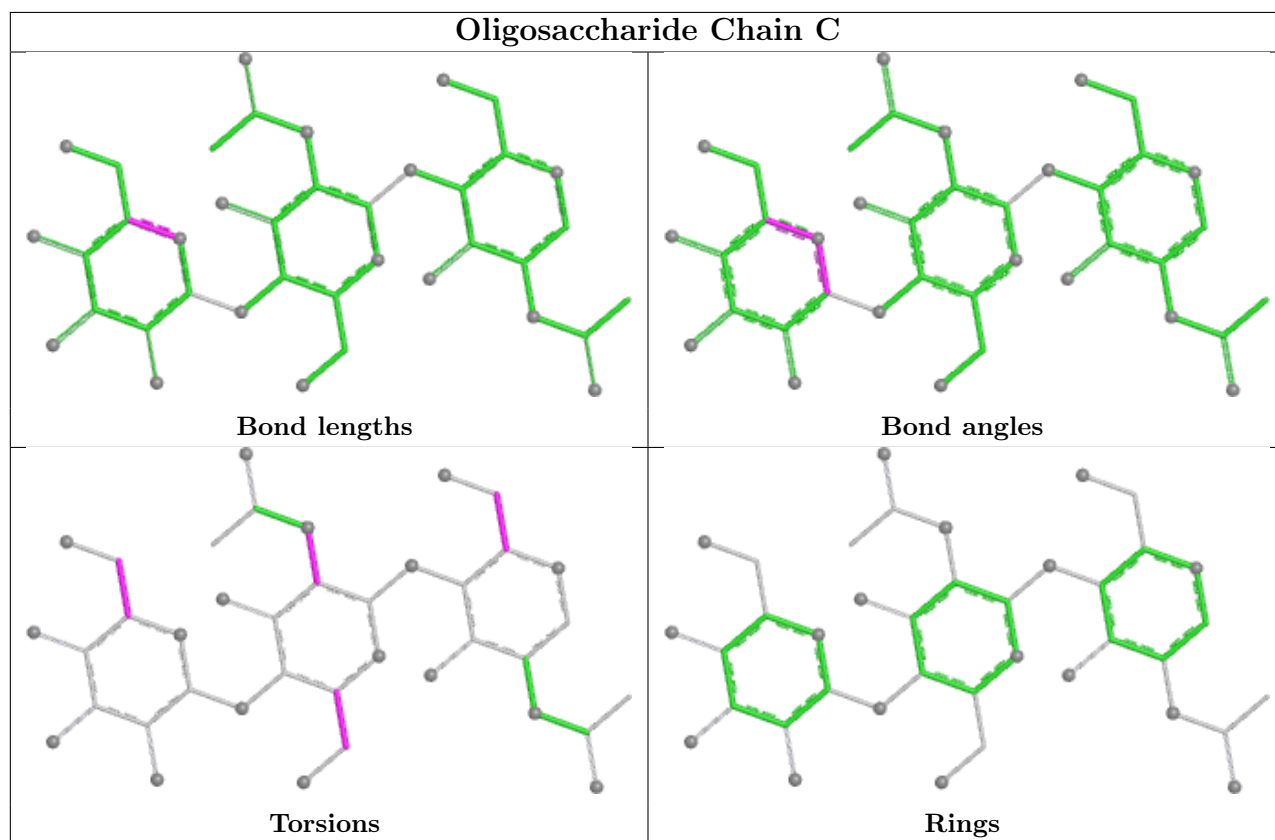
Mol	Chain	Res	Type	Atoms
2	C	3	BMA	C4-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6

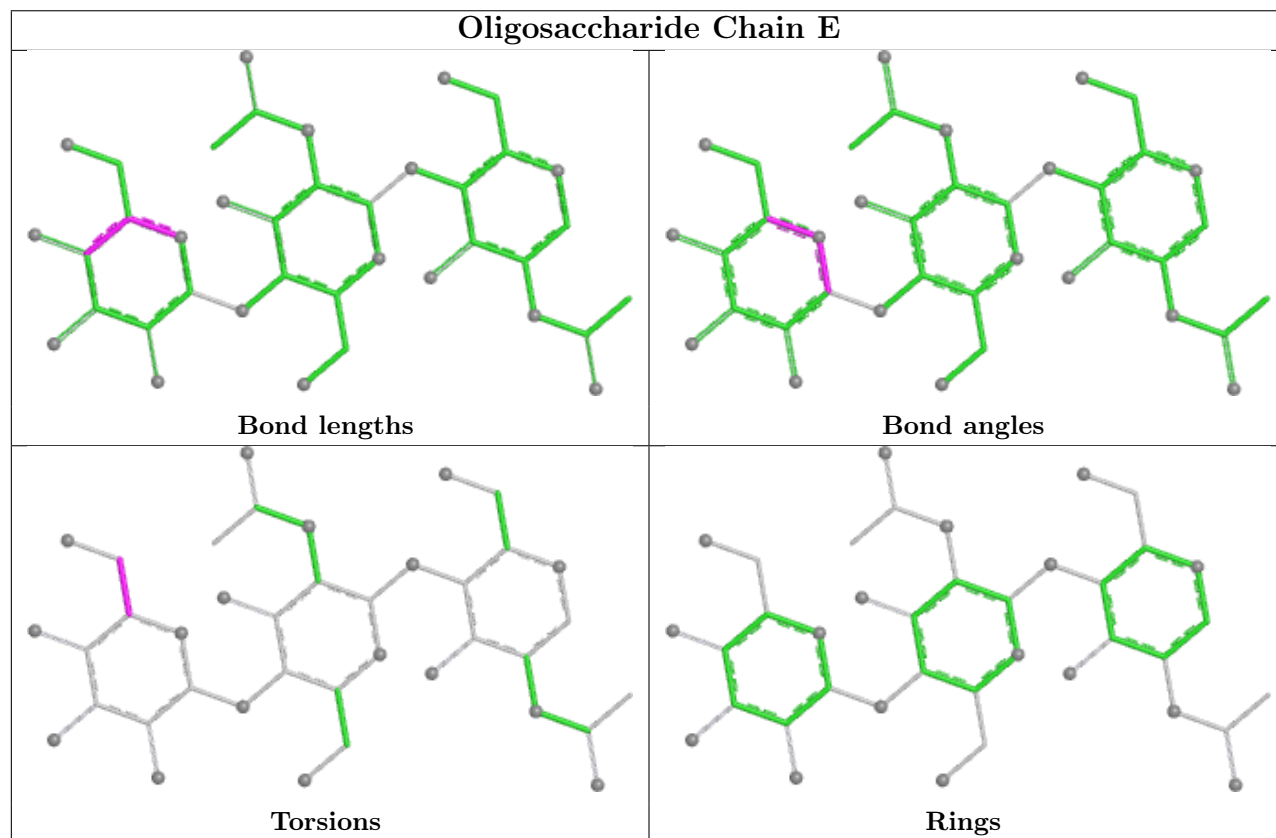
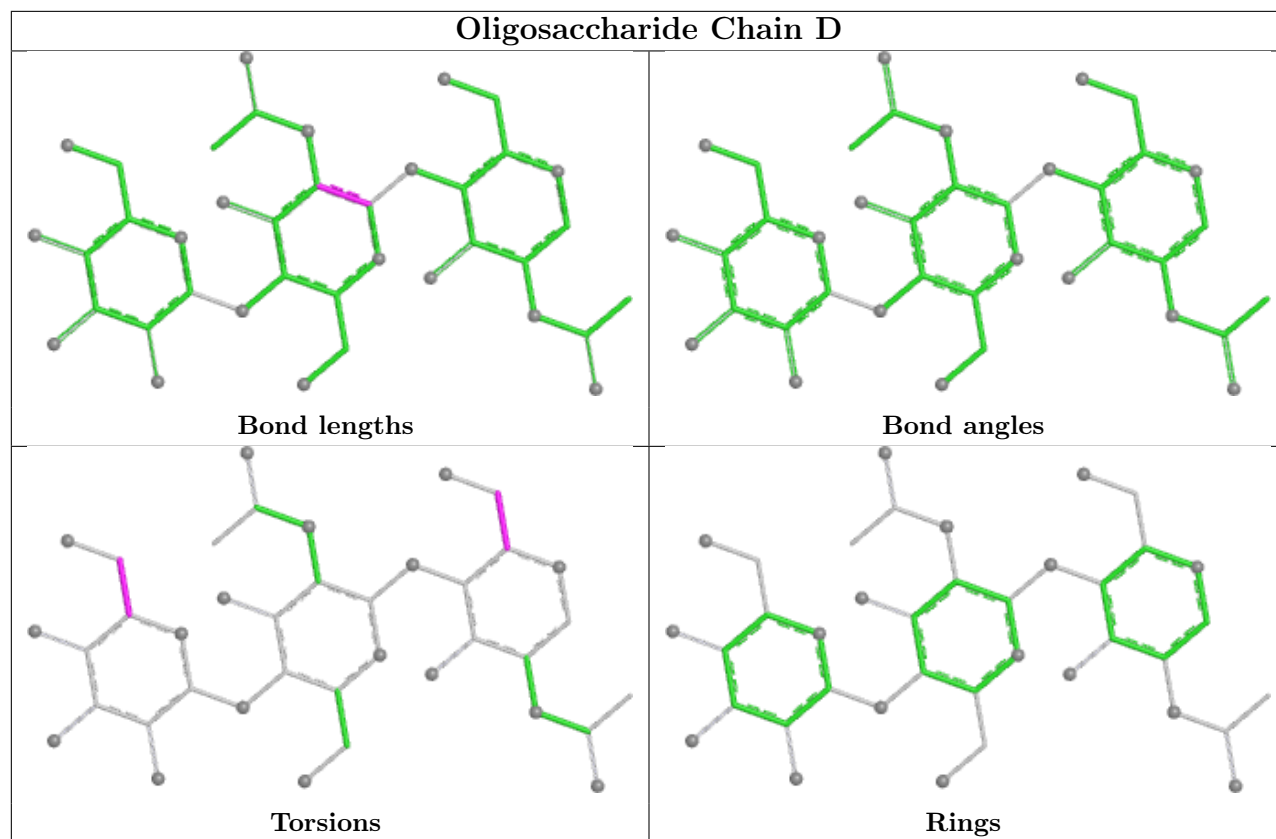
There are no ring outliers.

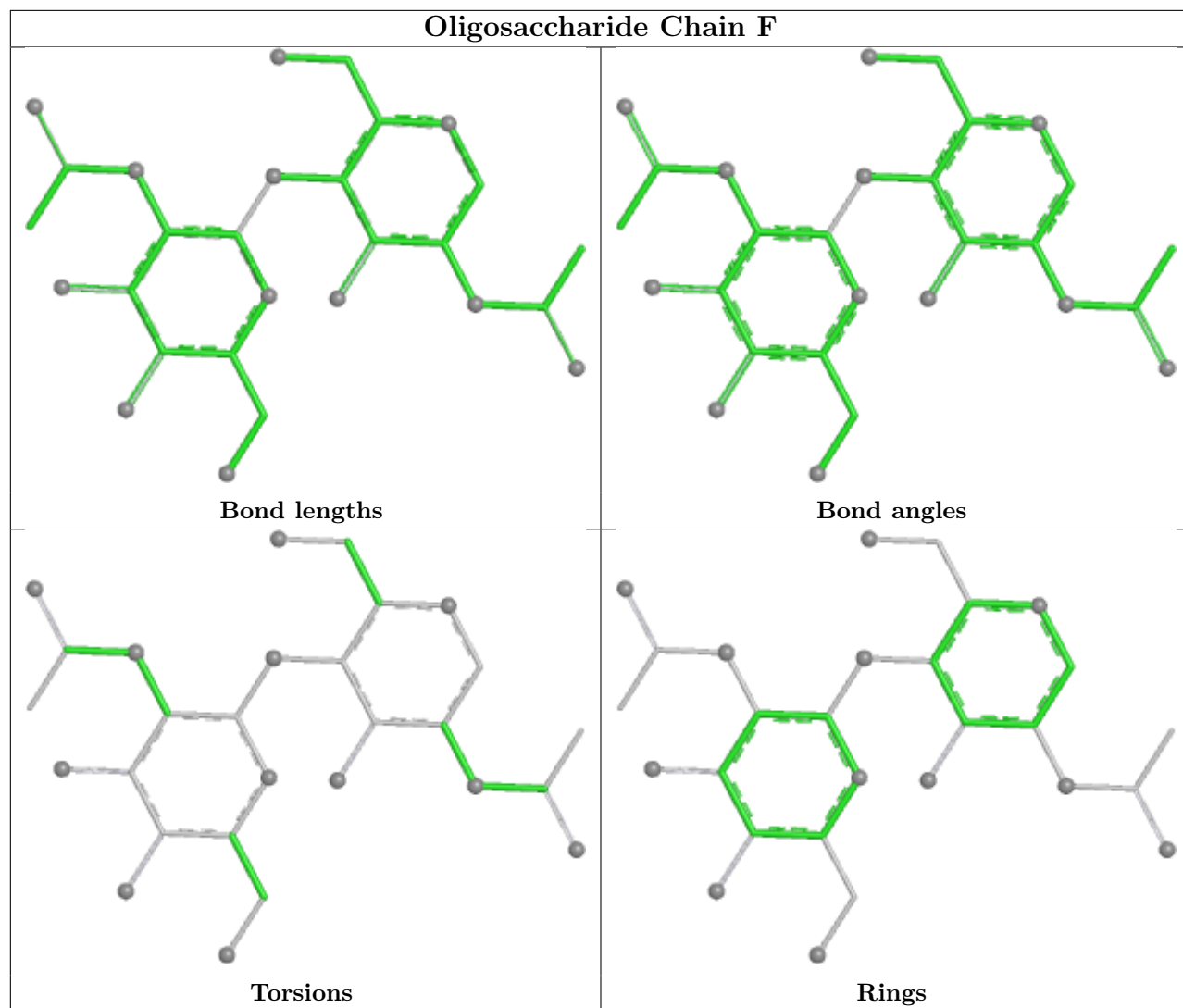
3 monomers are involved in 4 short contacts:

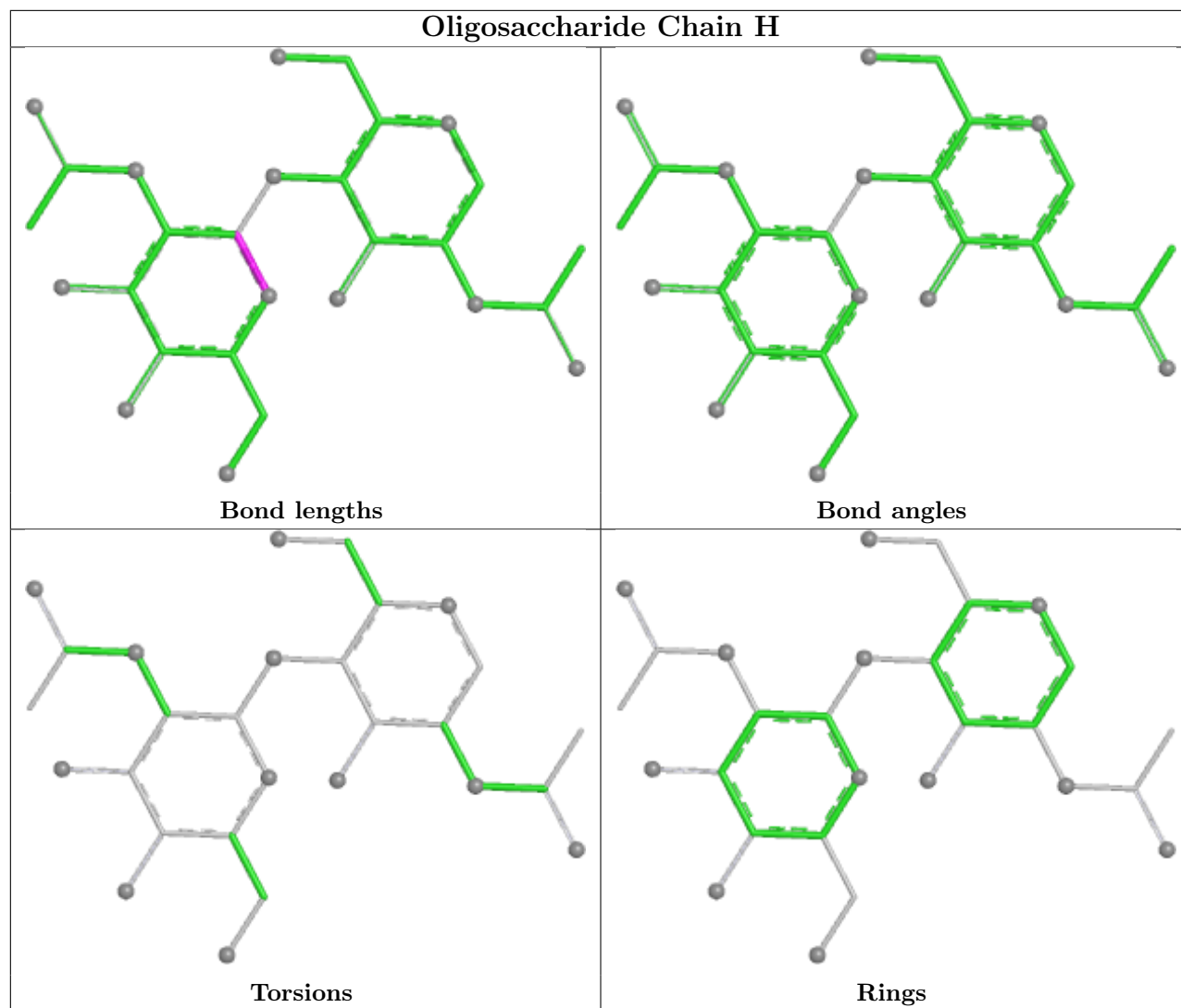
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	1	NAG	2	0
2	C	1	NAG	1	0
2	D	1	NAG	1	0

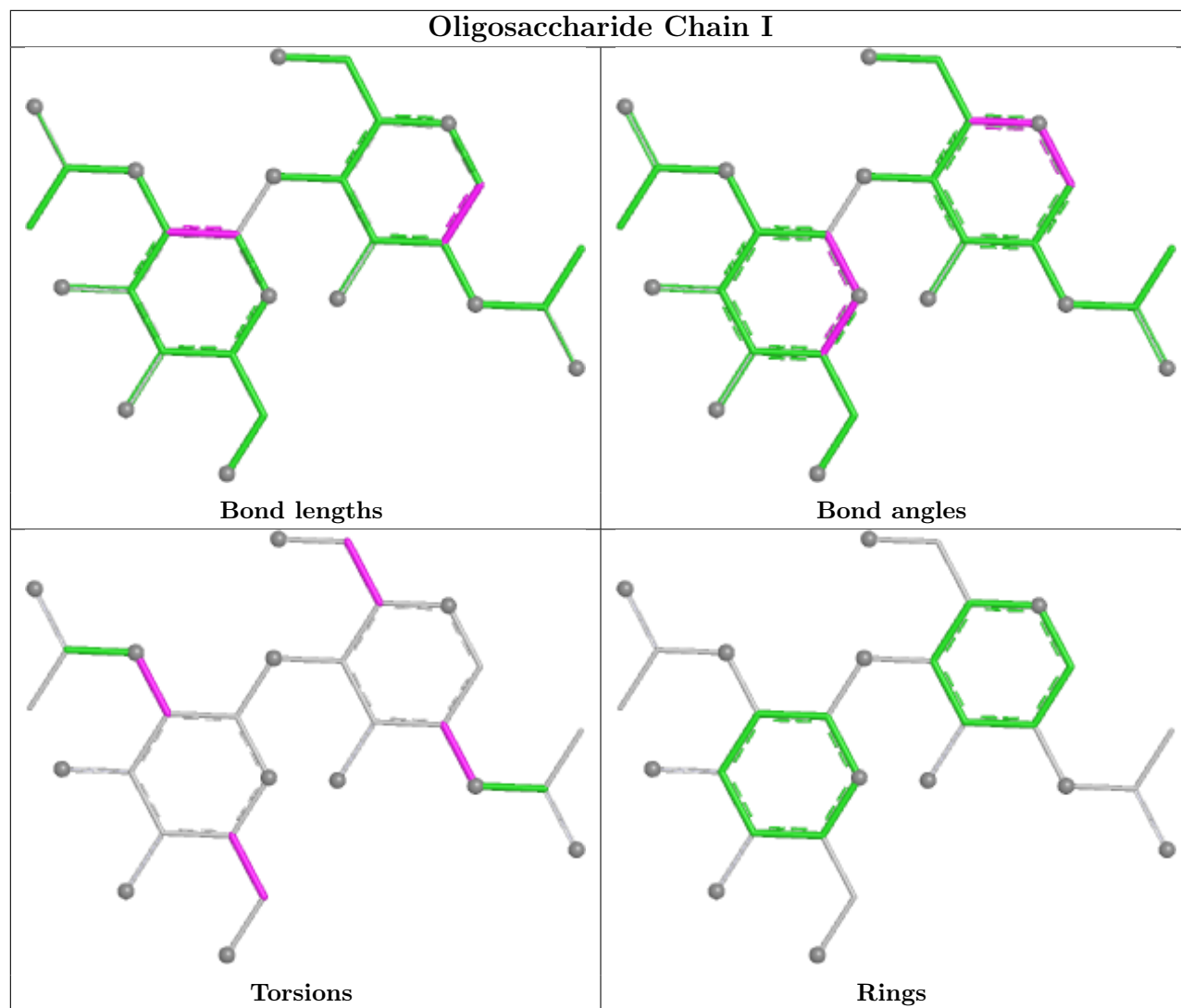
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

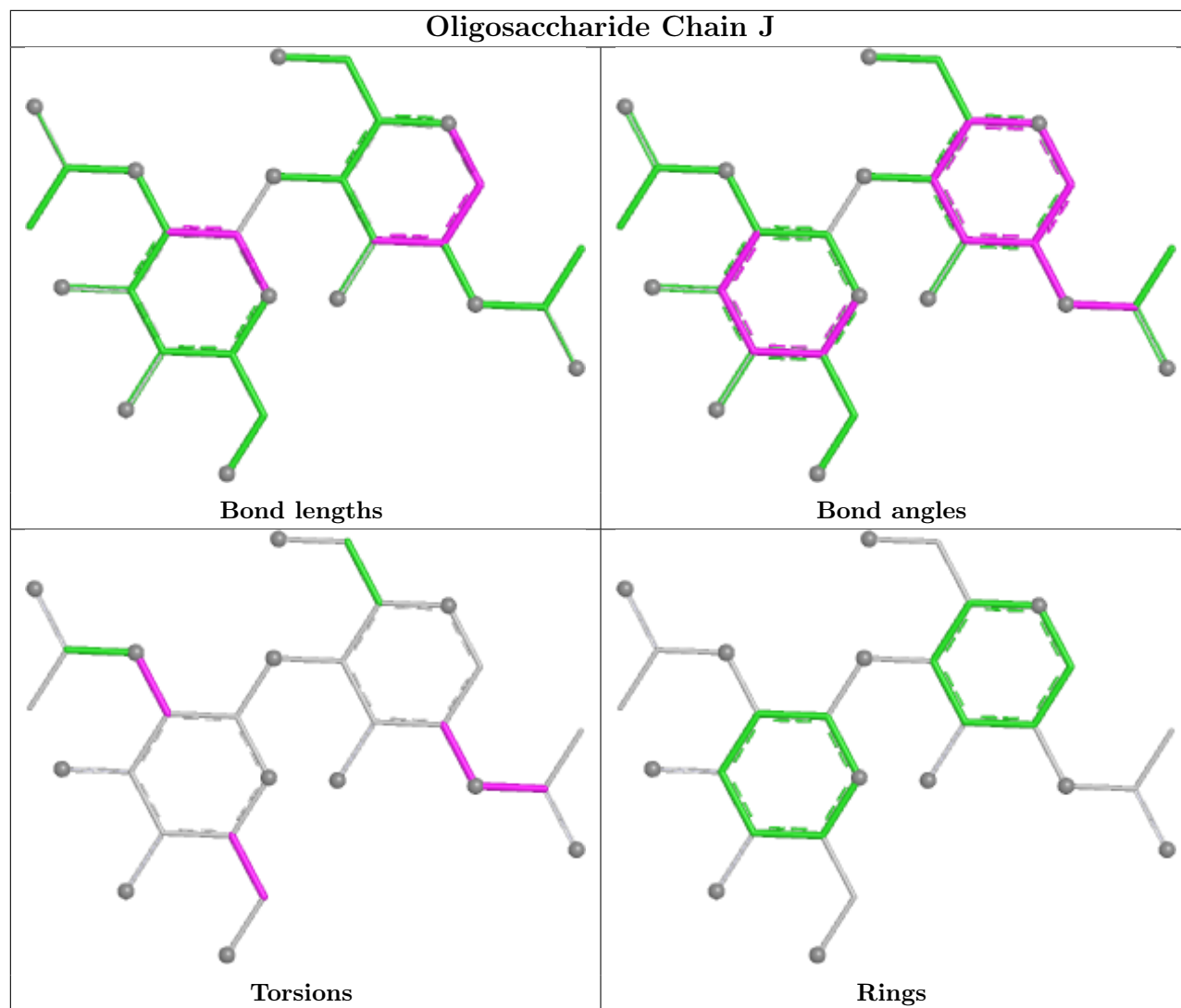


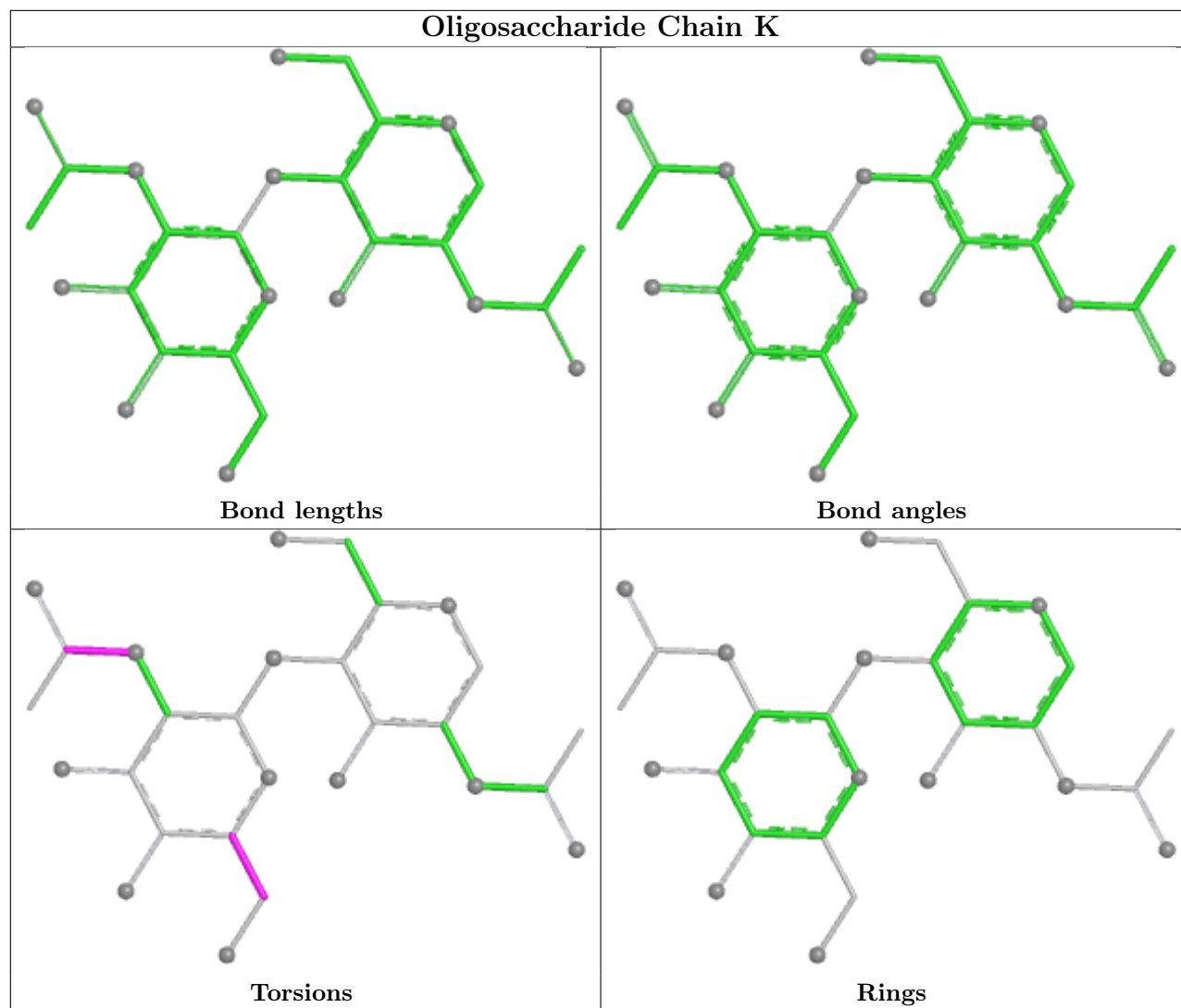


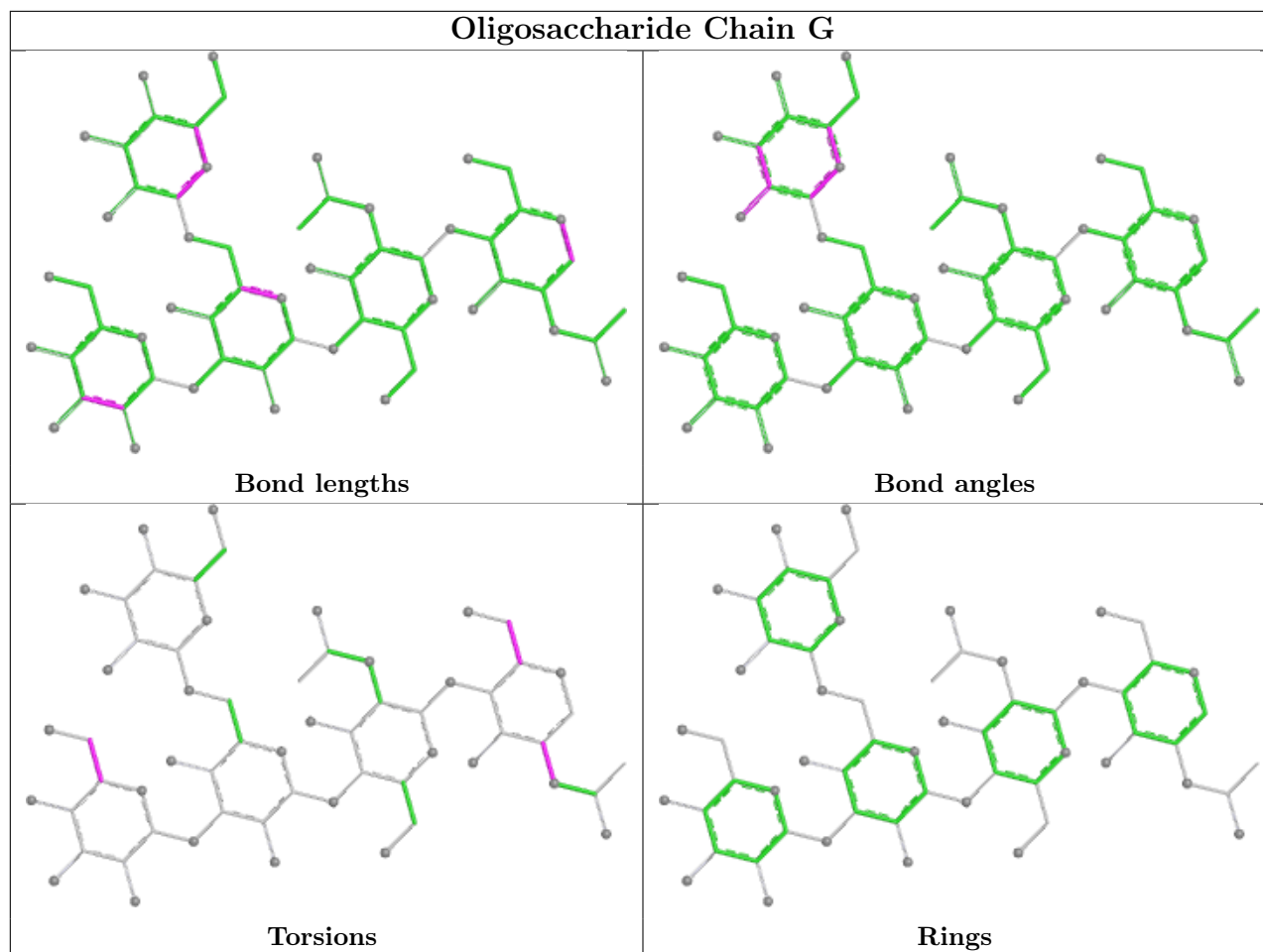












## 5.6 Ligand geometry [i](#)

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$
5	NAG	A	1001	1	14,14,15	0.90	1 (7%)	17,19,21	1.07	1 (5%)
5	NAG	B	2304	1	14,14,15	0.81	1 (7%)	17,19,21	0.94	1 (5%)
5	NAG	A	1005	1	14,14,15	1.41	1 (7%)	17,19,21	3.27	5 (29%)
5	NAG	A	1002	1	14,14,15	0.40	0	17,19,21	0.58	0
6	7OO	B	2301	9	44,48,48	1.91	8 (18%)	54,66,66	1.47	11 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	EDO	A	1007	-	3,3,3	0.44	0	2,2,2	0.28	0
5	NAG	A	1003	1	14,14,15	0.43	0	17,19,21	0.50	0
5	NAG	B	2302	1	14,14,15	0.93	2 (14%)	17,19,21	0.96	1 (5%)
5	NAG	B	2303	1	14,14,15	0.97	1 (7%)	17,19,21	1.06	1 (5%)
6	7OO	A	1006	9	44,48,48	1.93	6 (13%)	54,66,66	1.82	14 (25%)
7	EDO	A	1009	-	3,3,3	0.47	0	2,2,2	0.41	0
7	EDO	A	1008	-	3,3,3	0.51	0	2,2,2	0.53	0
8	IMD	A	1010	-	5,5,5	0.68	0	5,5,5	0.47	0
5	NAG	A	1004	1	14,14,15	0.40	0	17,19,21	1.36	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
5	NAG	B	2304	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1005	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1002	1	-	1/6/23/26	0/1/1/1
6	7OO	B	2301	9	-	7/38/44/44	0/4/4/4
7	EDO	A	1007	-	-	1/1/1/1	-
5	NAG	A	1003	1	-	3/6/23/26	0/1/1/1
5	NAG	B	2302	1	-	4/6/23/26	0/1/1/1
5	NAG	B	2303	1	-	1/6/23/26	0/1/1/1
6	7OO	A	1006	9	-	12/38/44/44	0/4/4/4
7	EDO	A	1009	-	-	0/1/1/1	-
7	EDO	A	1008	-	-	1/1/1/1	-
8	IMD	A	1010	-	-	-	0/1/1/1
5	NAG	A	1004	1	-	2/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	2301	7OO	P03-C05	7.23	1.86	1.79
6	A	1006	7OO	P03-C05	7.20	1.86	1.79
6	B	2301	7OO	C07-N08	5.31	1.45	1.34
6	A	1006	7OO	C07-N08	4.89	1.44	1.34
6	A	1006	7OO	C09-C14	-4.79	1.44	1.52

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1005	NAG	C2-N2-C7	11.79	138.70	122.90
6	A	1006	7OO	C14-C09-N08	5.05	122.66	110.30
6	A	1006	7OO	C13-C11-C10	4.42	126.99	111.08
6	B	2301	7OO	C13-C11-C10	3.65	124.19	111.08
5	B	2302	NAG	C1-O5-C5	3.42	116.77	112.19

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

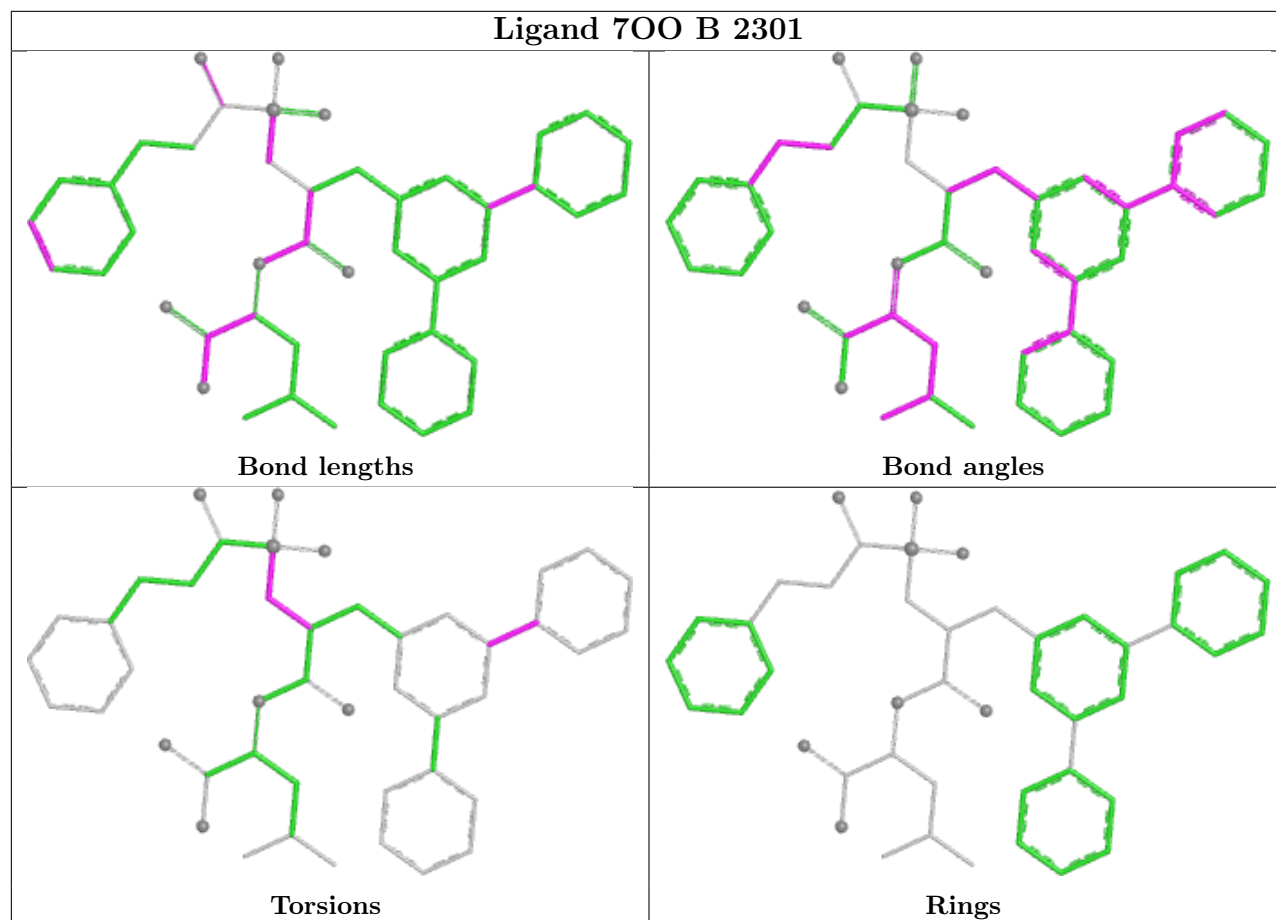
Mol	Chain	Res	Type	Atoms
5	A	1005	NAG	C3-C2-N2-C7
5	A	1005	NAG	C8-C7-N2-C2
6	A	1006	7OO	C06-C05-P03-O04
6	A	1006	7OO	C07-C06-C18-C19
6	B	2301	7OO	C06-C05-P03-O04

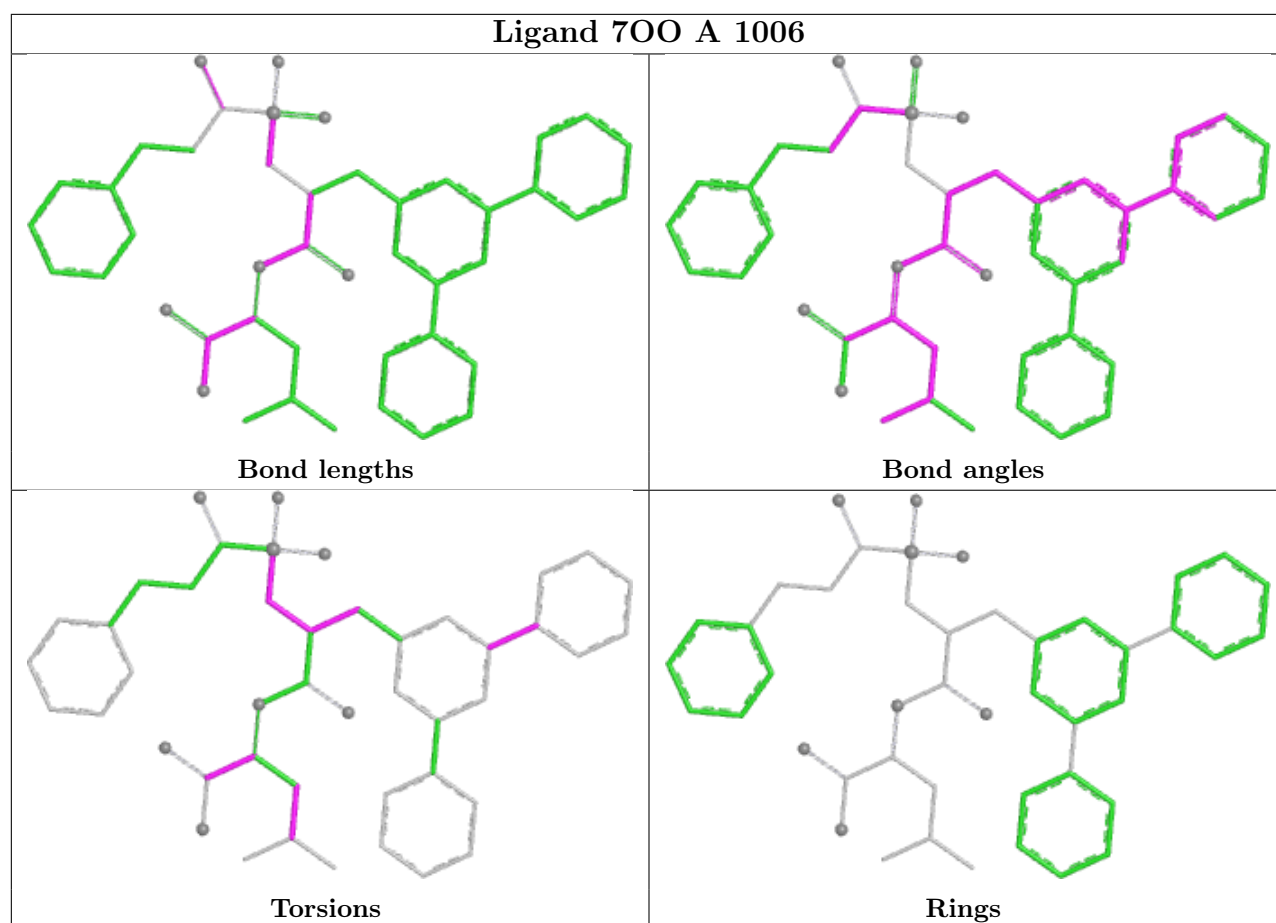
There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	2301	7OO	2	0
5	A	1003	NAG	1	0
6	A	1006	7OO	2	0
5	A	1004	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	916/963 (95%)	-0.11	7 (0%) 82 81	26, 62, 112, 171	2 (0%)
1	B	872/963 (90%)	0.40	32 (3%) 45 41	34, 93, 145, 196	1 (0%)
All	All	1788/1926 (92%)	0.14	39 (2%) 62 59	26, 74, 136, 196	3 (0%)

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	623	PHE	4.3
1	B	680	ALA	4.2
1	B	687	LEU	3.9
1	B	958	VAL	3.8
1	B	837	LEU	3.6

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NAG	J	2	14/15	0.31	0.13	145,182,190,193	0
2	BMA	D	3	11/12	0.38	0.11	122,126,132,133	0
3	NAG	J	1	14/15	0.42	0.12	123,149,172,177	0
3	NAG	K	2	14/15	0.42	0.13	145,167,172,175	0
2	BMA	E	3	11/12	0.59	0.11	105,141,151,154	0

*Continued on next page...*

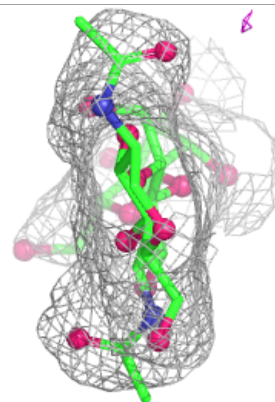
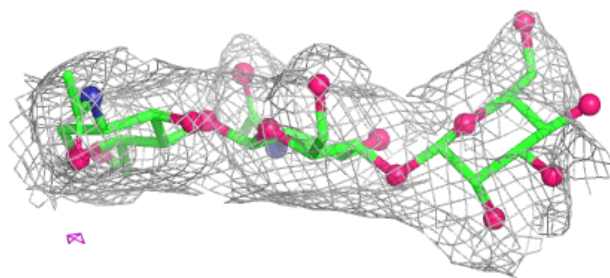
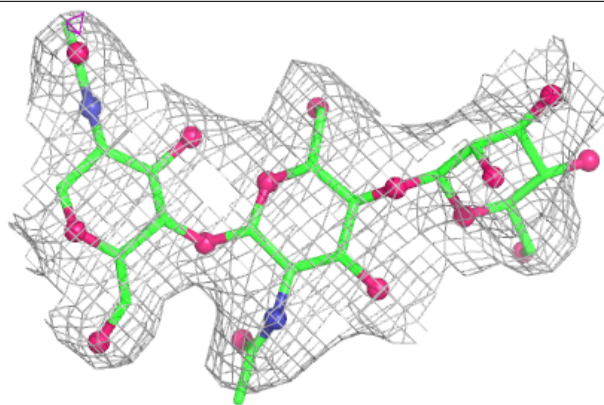
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	F	2	14/15	0.62	0.11	148,167,175,178	0
2	BMA	C	3	11/12	0.64	0.09	113,125,136,139	0
4	MAN	G	4	11/12	0.73	0.09	110,115,132,136	0
3	NAG	I	2	14/15	0.75	0.09	139,162,172,176	0
2	NAG	E	2	14/15	0.79	0.11	115,136,144,151	0
3	NAG	I	1	14/15	0.80	0.10	120,151,171,178	0
3	NAG	H	2	14/15	0.81	0.10	92,103,120,123	0
3	NAG	H	1	14/15	0.84	0.11	63,94,117,118	0
3	NAG	F	1	14/15	0.84	0.10	100,120,131,149	0
4	MAN	G	5	11/12	0.84	0.11	70,86,101,104	0
2	NAG	D	2	14/15	0.85	0.09	88,110,120,122	0
2	NAG	E	1	14/15	0.88	0.11	83,93,106,127	0
4	BMA	G	3	11/12	0.88	0.07	71,77,93,102	0
3	NAG	K	1	14/15	0.89	0.10	99,120,132,154	0
4	NAG	G	2	14/15	0.90	0.09	62,67,77,97	0
2	NAG	D	1	14/15	0.92	0.09	53,84,95,100	0
2	NAG	C	2	14/15	0.93	0.08	71,85,101,109	0
4	NAG	G	1	14/15	0.94	0.08	48,58,79,99	0
2	NAG	C	1	14/15	0.95	0.08	51,60,67,72	0

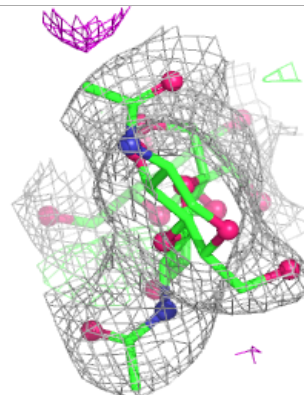
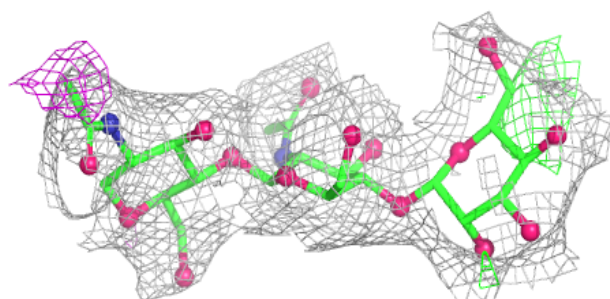
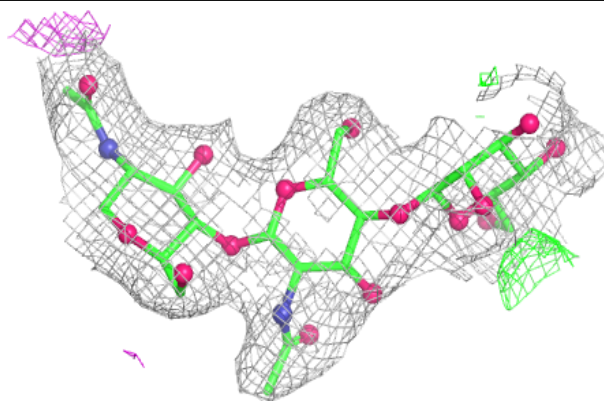
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain C:**

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

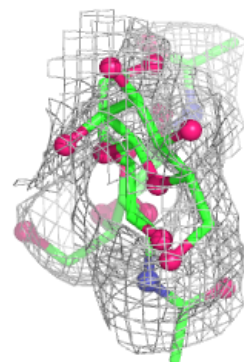
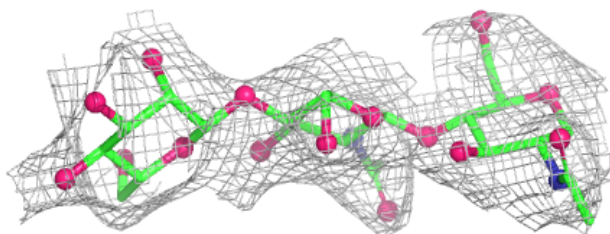
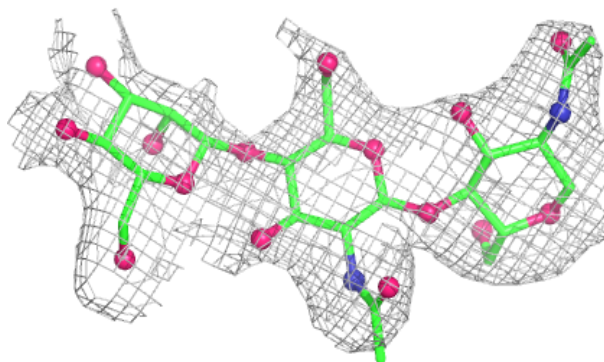
**Electron density around Chain D:**

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

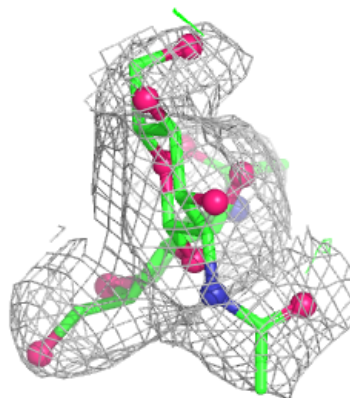
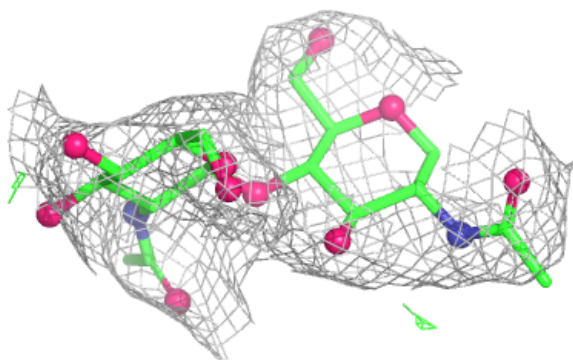
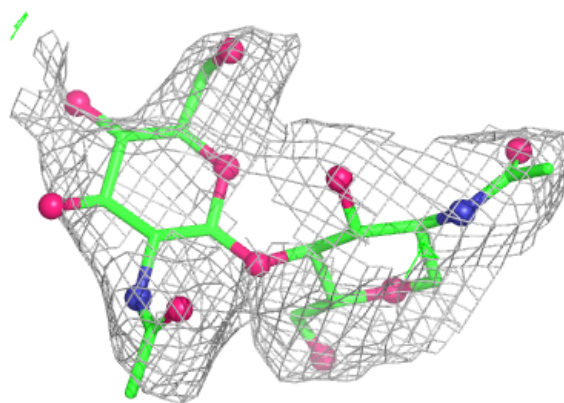


**Electron density around Chain E:**

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

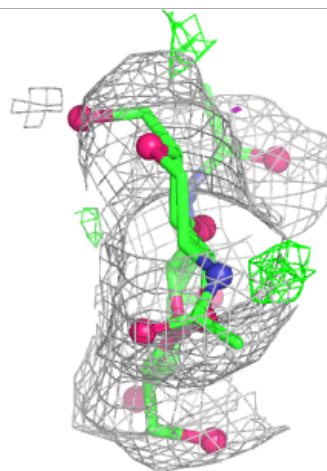
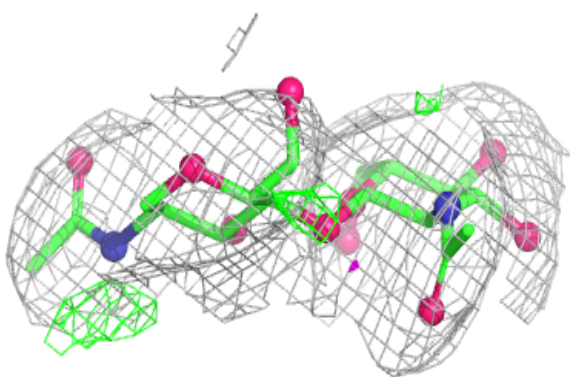
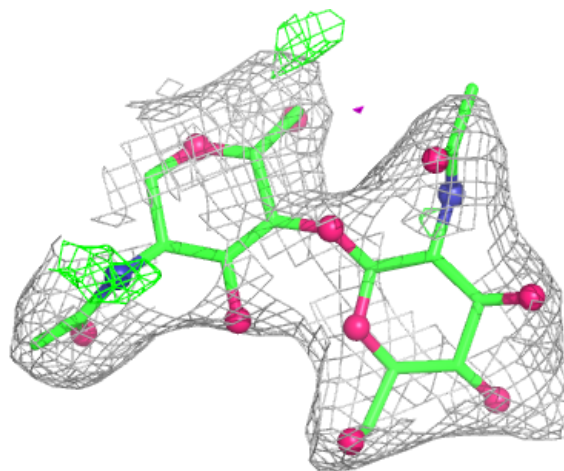
**Electron density around Chain F:**

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



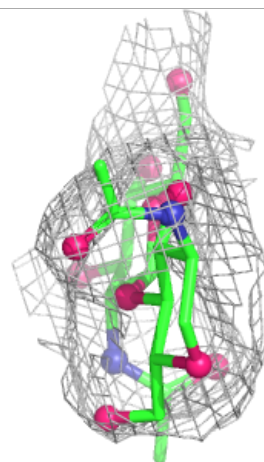
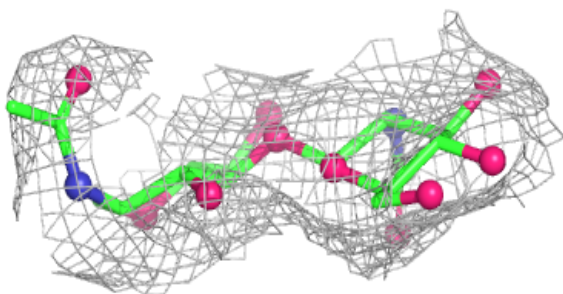
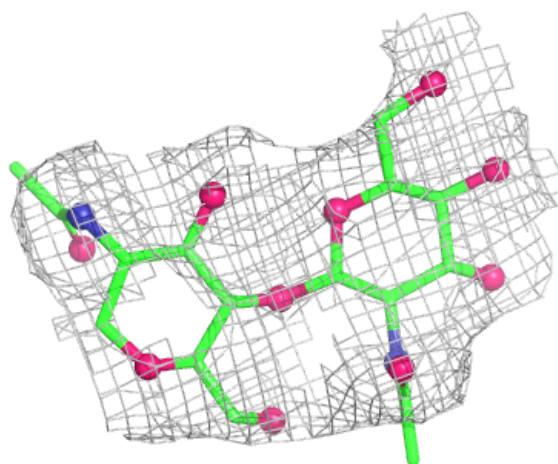
**Electron density around Chain H:**

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



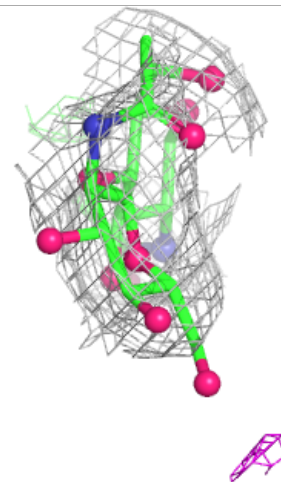
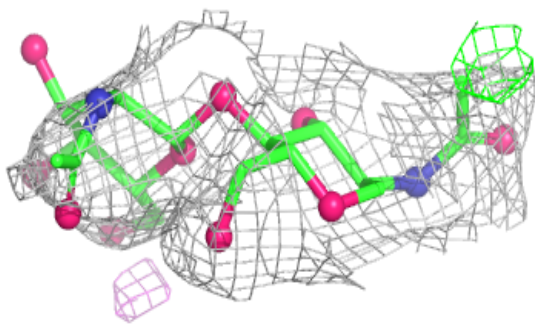
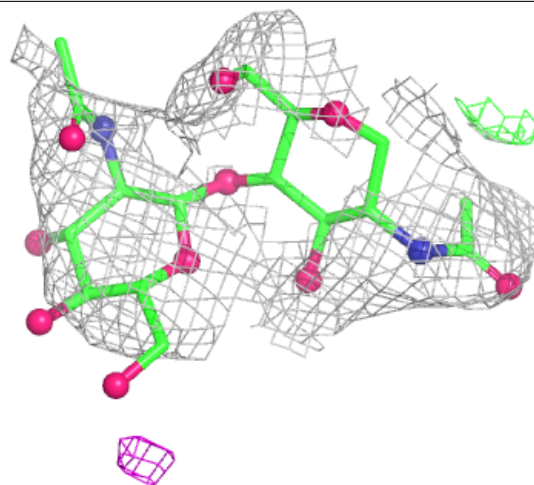
**Electron density around Chain I:**

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



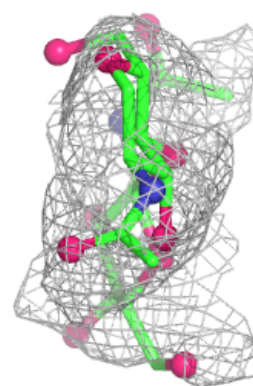
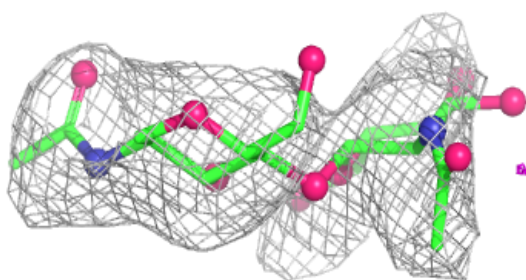
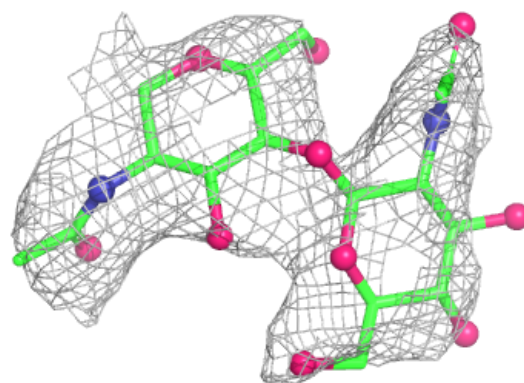
**Electron density around Chain J:**

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

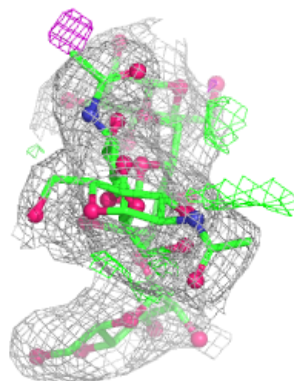
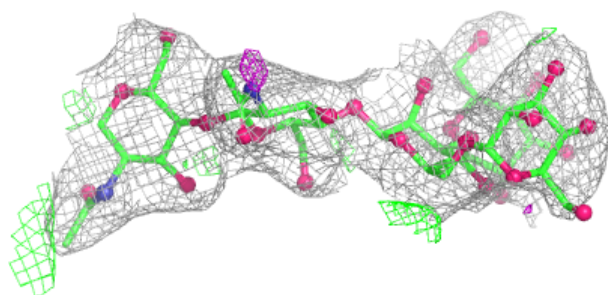
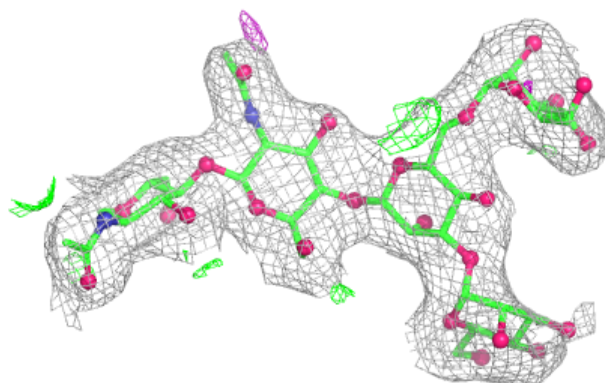


**Electron density around Chain K:**

$2mF_o-DF_c$  (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

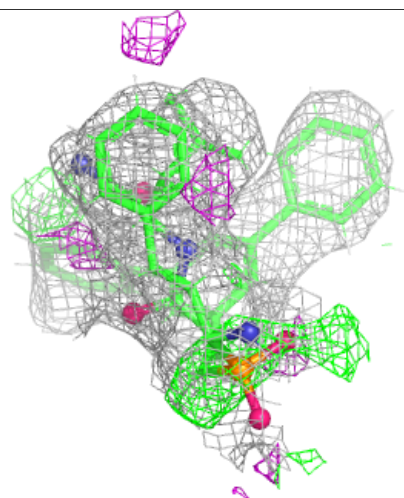
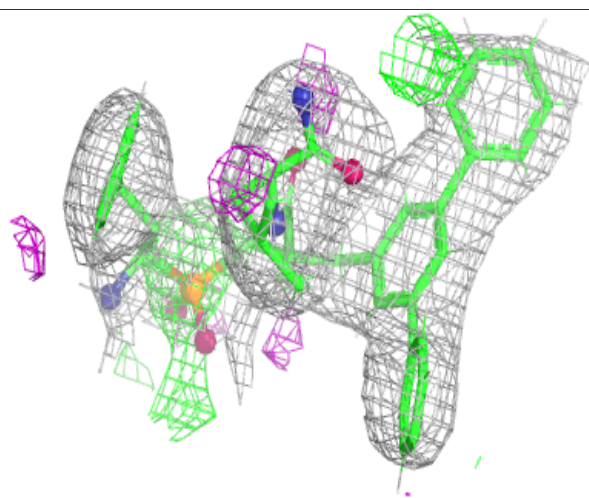
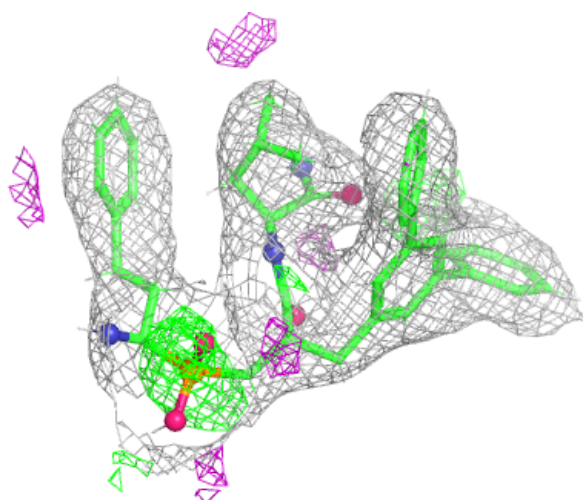
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

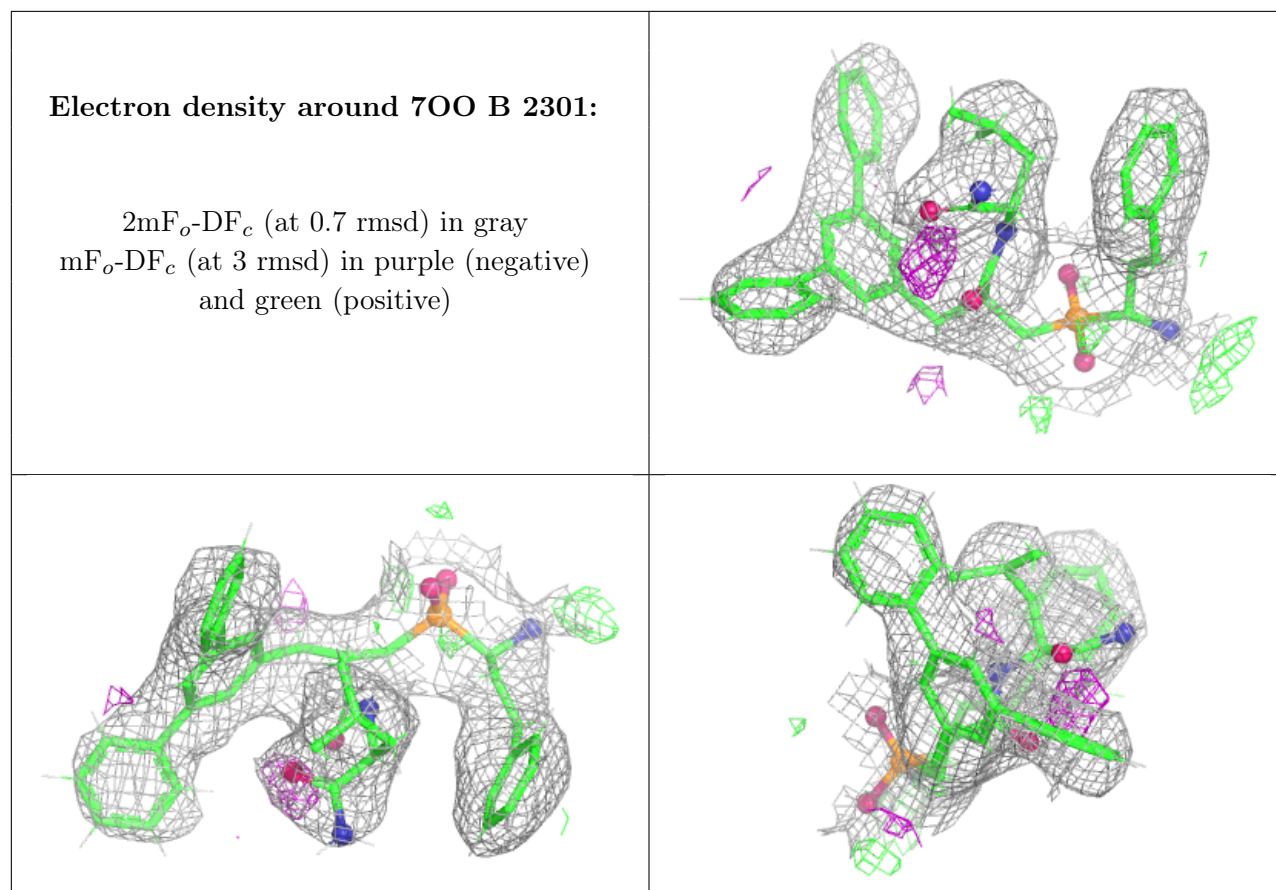
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	B	2304	14/15	0.39	0.13	138,158,168,168	0
5	NAG	B	2303	14/15	0.52	0.12	130,148,163,167	0
5	NAG	B	2302	14/15	0.52	0.13	160,166,174,175	0
5	NAG	A	1005	14/15	0.56	0.15	106,127,136,138	0
5	NAG	A	1003	14/15	0.57	0.13	116,159,174,176	0
5	NAG	A	1002	14/15	0.64	0.11	131,140,149,152	0
5	NAG	A	1004	14/15	0.70	0.11	128,144,149,149	0
5	NAG	A	1001	14/15	0.76	0.10	121,131,137,140	0
7	EDO	A	1007	4/4	0.83	0.14	103,106,106,107	0
7	EDO	A	1008	4/4	0.83	0.11	91,95,96,96	0
7	EDO	A	1009	4/4	0.83	0.12	84,91,92,93	0
8	IMD	A	1010	5/5	0.83	0.15	107,107,108,110	0
6	7OO	A	1006	45/45	0.94	0.11	38,69,97,115	0
6	7OO	B	2301	45/45	0.95	0.10	45,80,106,119	0
9	ZN	A	1011	1/1	0.99	0.04	53,53,53,53	0
9	ZN	B	2305	1/1	0.99	0.04	65,65,65,65	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 7OO A 1006:**

$2mF_o-DF_c$  (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.