



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 05:32 AM BST

PDB ID : 5ISM  
Title : Human DPP4 in complex with a novel 5,5,6-tricyclic pyrrolidine inhibitor  
Authors : Scapin, G.  
Deposited on : 2016-03-15  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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.

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

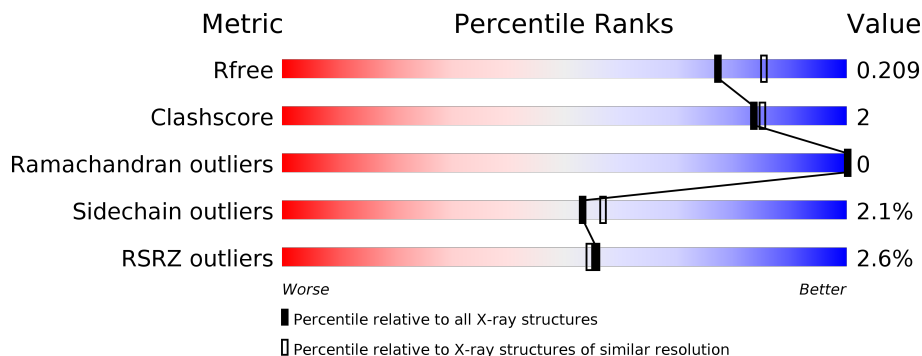
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : 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 2.00 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.



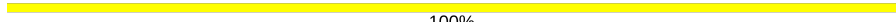
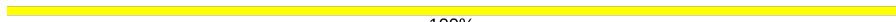
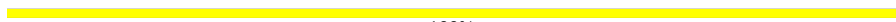
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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	728	2% 94% 5%
1	B	728	3% 94% 6%
2	C	2	100%
2	D	2	100%
2	E	2	100%
2	F	2	100%

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	D	2	-	-	-	X
2	NAG	E	2	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 14031 atoms, of which 14 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	728	6012	3848	996	1141	27	0	18	0
1	B	728	6006	3849	987	1142	28	0	15	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	THR	SER	engineered mutation	UNP P27487
B	39	THR	SER	engineered mutation	UNP P27487

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



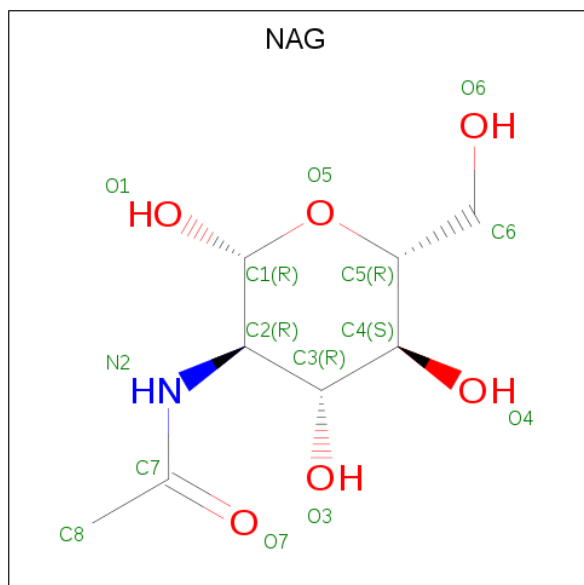
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0
2	D	2	42	16	14	2	10	0	0
2	E	2	28	16	2	10	0	0	0
2	F	2	28	16	2	10	0	0	0
2	G	2	28	16	2	10	0	0	0
2	H	2	28	16	2	10	0	0	0

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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

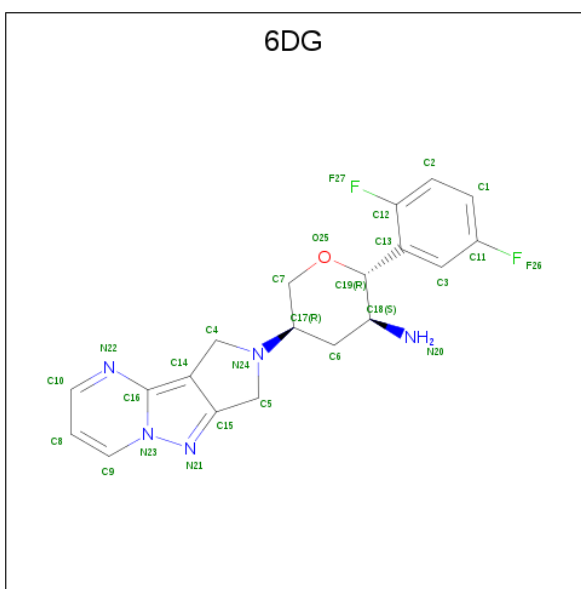


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	14	8	1	5	0	0
3	A	1	14	8	1	5	0	0
3	A	1	14	8	1	5	0	0
3	B	1	14	8	1	5	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0

- Molecule 5 is (2R,3S,5R)-2-(2,5-difluorophenyl)-5-(7H-pyrrolo[3',4':3,4]pyrazolo[1,5-a]pyrimidin-8(9H)-yl)oxan-3-amine (three-letter code: 6DG) (formula: C<sub>19</sub>H<sub>19</sub>F<sub>2</sub>N<sub>5</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
5	A	1	27	19	2	5	1	0	0
5	B	1	54	38	4	10	2	0	1

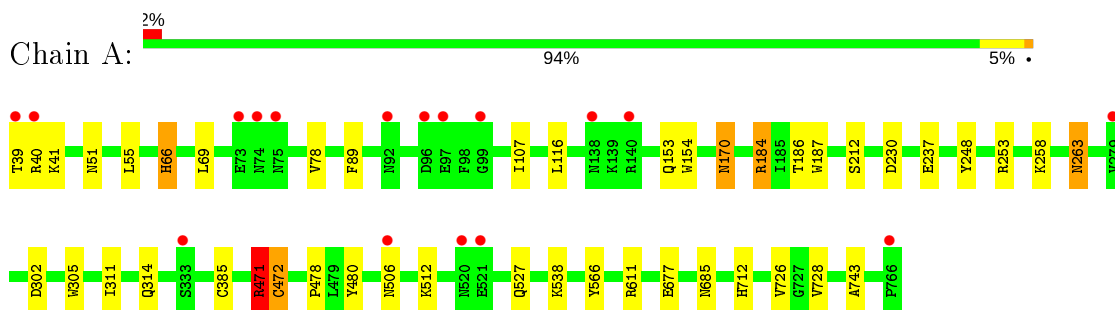
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	832	832	832	0	0
6	B	833	833	833	0	0

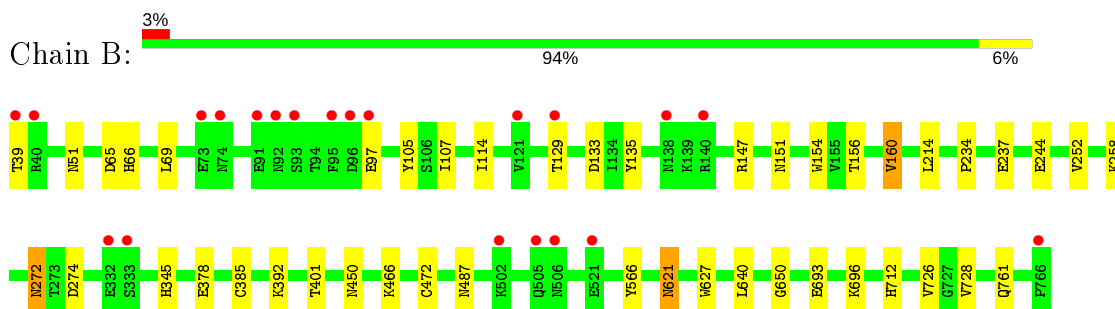
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

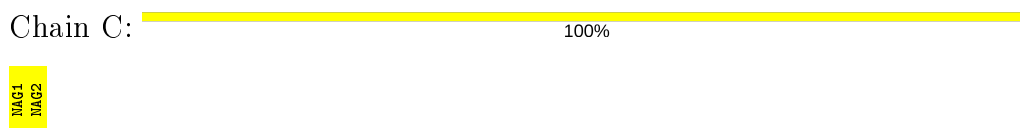
- Molecule 1: Dipeptidyl peptidase 4



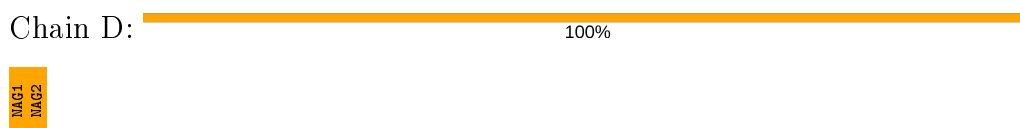
- Molecule 1: Dipeptidyl peptidase 4



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



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



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

Chain E:  100%

■ MAG1  
■ MAG2

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

Chain F:  100%


■ MAG1  
■ MAG2

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

Chain G:  100%

■ MAG1  
■ MAG2

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

Chain H:  100%

■ MAG1  
■ MAG2

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

Chain I:  100%

■ MAG1  
■ MAG2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.27Å 126.03Å 137.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.93 – 2.00 29.87 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.93-2.00) 99.8 (29.87-2.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.12 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.165 , 0.201 0.175 , 0.209	Depositor DCC
$R_{free}$ test set	6939 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.0	Xtrriage
Anisotropy	0.028	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 54.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14031	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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: NA, NAG, 6DG

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	0.48	0/6282	0.70	5/8539 (0.1%)
1	B	0.46	0/6254	0.68	2/8507 (0.0%)
All	All	0.47	0/12536	0.69	7/17046 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	B	160[A]	VAL	CG1-CB-CG2	6.95	122.02	110.90
1	B	160[B]	VAL	CG1-CB-CG2	6.95	122.02	110.90
1	A	471[A]	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	471[B]	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	611	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	611	ARG	NE-CZ-NH1	5.07	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6012	0	5720	30	0
1	B	6006	0	5722	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	28	0	25	0	0
2	D	28	14	25	1	0
2	E	28	0	25	0	0
2	F	28	0	25	1	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
3	A	42	0	39	0	0
3	B	14	0	13	0	0
4	A	1	0	0	0	0
5	A	27	0	0	0	0
5	B	54	0	0	0	0
6	A	832	0	0	7	0
6	B	833	0	0	8	0
All	All	14017	14	11669	58	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 2.

All (58) 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:472:CYS:SG	6:A:1374:HOH:O	1.91	1.28
1:A:184:ARG:HD2	1:A:186:THR:O	1.87	0.75
1:A:506[B]:ASN:ND2	6:A:902:HOH:O	2.28	0.67
1:A:78:VAL:HG23	1:A:89:PHE:HB2	1.78	0.66
1:B:272:ASN:C	1:B:272:ASN:HD22	2.01	0.64
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.80	0.63
1:A:69:LEU:HD23	1:A:78:VAL:HG22	1.81	0.63
1:A:471[A]:ARG:HG2	1:A:480:TYR:CE2	2.35	0.62
1:A:66[B]:HIS:HB2	6:A:1418:HOH:O	2.00	0.61
1:A:184:ARG:HG2	1:A:187:TRP:CE2	2.36	0.61
1:A:258:LYS:NZ	1:A:712:HIS:HD2	2.01	0.59
1:A:538:LYS:HE2	6:A:1137:HOH:O	2.03	0.58
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.86	0.57
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.87	0.56
1:A:743:ALA:HB3	6:A:1361:HOH:O	2.04	0.56
1:B:761:GLN:NE2	6:B:910:HOH:O	2.38	0.54
1:A:69:LEU:HD13	1:A:107:ILE:HD12	1.89	0.54
1:A:69:LEU:CD2	1:A:78:VAL:HG22	2.38	0.54
1:B:129:THR:HB	6:B:1183:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:LYS:NZ	1:B:712:HIS:HD2	2.07	0.53
1:A:685[A]:ASN:ND2	6:A:910:HOH:O	2.42	0.53
1:B:151:ASN:N	6:B:902:HOH:O	2.42	0.52
1:A:153:GLN:HE22	1:A:170:ASN:ND2	2.07	0.52
1:A:258:LYS:HZ3	1:A:712:HIS:HD2	1.58	0.51
1:B:392:LYS:NZ	6:B:918:HOH:O	2.44	0.51
1:B:66[A]:HIS:HB2	6:B:1437:HOH:O	2.11	0.50
1:B:696:LYS:HG3	1:B:728:VAL:HG22	1.92	0.50
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.93	0.50
1:B:69:LEU:HD11	1:B:107:ILE:HD13	1.94	0.50
1:A:51:ASN:HB3	6:A:1304:HOH:O	2.11	0.49
1:B:154:TRP:HE1	1:B:156[B]:THR:HG1	1.60	0.49
1:A:237:GLU:OE1	1:A:253[B]:ARG:HD2	2.11	0.49
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.95	0.48
1:B:272:ASN:HD21	1:B:274:ASP:HB2	1.79	0.48
1:B:693:GLU:OE2	6:B:901:HOH:O	2.20	0.47
1:B:258:LYS:HZ3	1:B:712:HIS:HD2	1.63	0.46
2:D:1:NAG:H62	2:D:2:NAG:O5	2.17	0.45
1:B:154:TRP:NE1	1:B:156[B]:THR:OG1	2.48	0.44
1:B:345:HIS:HD2	6:B:1001:HOH:O	2.00	0.43
1:A:154:TRP:CE2	1:A:212[B]:SER:HB3	2.54	0.43
1:A:154:TRP:CE2	1:A:212[A]:SER:HB3	2.54	0.43
2:F:1:NAG:O3	2:F:2:NAG:H2	2.18	0.43
1:A:302:ASP:HB3	1:A:314:GLN:HB2	2.01	0.42
1:A:305:TRP:CE2	1:A:311:ILE:HD12	2.55	0.42
1:B:65:ASP:OD2	1:B:466:LYS:HB2	2.19	0.42
1:B:401:THR:HG21	6:B:1286:HOH:O	2.19	0.42
1:B:69:LEU:CD1	1:B:107:ILE:HD13	2.49	0.42
1:A:258:LYS:HZ3	1:A:712:HIS:CD2	2.38	0.41
1:A:512:LYS:HE3	1:A:527:GLN:OE1	2.20	0.41
1:B:237:GLU:HA	1:B:252:VAL:O	2.21	0.41
1:A:184:ARG:HG2	1:A:187:TRP:CZ2	2.56	0.41
1:B:133:ASP:OD2	1:B:147:ARG:NH1	2.54	0.41
1:A:263:ASN:HA	1:A:263:ASN:HD22	1.65	0.41
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.56	0.41
1:A:472:CYS:O	1:A:478:PRO:HA	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	744/728 (102%)	723 (97%)	21 (3%)	0	100	100
1	B	741/728 (102%)	717 (97%)	24 (3%)	0	100	100
All	All	1485/1456 (102%)	1440 (97%)	45 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	671/653 (103%)	656 (98%)	15 (2%)	52	55
1	B	668/653 (102%)	648 (97%)	20 (3%)	41	41
All	All	1339/1306 (102%)	1304 (97%)	35 (3%)	53	48

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	THR
1	A	41	LYS
1	A	55	LEU
1	A	66[A]	HIS
1	A	66[B]	HIS
1	A	116	LEU
1	A	170	ASN
1	A	230	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	263	ASN
1	A	385	CYS
1	A	471[A]	ARG
1	A	471[B]	ARG
1	A	472	CYS
1	A	566	TYR
1	A	677	GLU
1	B	39	THR
1	B	51[A]	ASN
1	B	51[B]	ASN
1	B	97	GLU
1	B	160[A]	VAL
1	B	160[B]	VAL
1	B	244	GLU
1	B	272	ASN
1	B	378[A]	GLU
1	B	378[B]	GLU
1	B	385[A]	CYS
1	B	385[B]	CYS
1	B	450[A]	ASN
1	B	450[B]	ASN
1	B	472	CYS
1	B	487	ASN
1	B	566	TYR
1	B	621[A]	ASN
1	B	621[B]	ASN
1	B	627	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	169	ASN
1	A	170	ASN
1	A	263	ASN
1	A	388	GLN
1	A	435	GLN
1	A	505	GLN
1	A	572	ASN
1	A	694	ASN
1	A	712	HIS
1	B	150	ASN
1	B	169	ASN

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Mol	Chain	Res	Type
1	B	272	ASN
1	B	345	HIS
1	B	487	ASN
1	B	572	ASN
1	B	694	ASN
1	B	712	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](#)

14 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	0.67	0	17,19,21	1.28	2 (11%)
2	NAG	C	2	2	14,14,15	0.50	0	17,19,21	1.54	1 (5%)
2	NAG	D	1	1,2	14,14,15	1.54	3 (21%)	17,19,21	2.58	4 (23%)
2	NAG	D	2	2	14,14,15	1.32	2 (14%)	17,19,21	2.40	7 (41%)
2	NAG	E	1	1,2	14,14,15	0.74	0	17,19,21	1.38	2 (11%)
2	NAG	E	2	2	14,14,15	0.47	0	17,19,21	2.15	5 (29%)
2	NAG	F	1	1,2	14,14,15	0.53	0	17,19,21	1.23	3 (17%)
2	NAG	F	2	2	14,14,15	1.02	1 (7%)	17,19,21	1.58	3 (17%)
2	NAG	G	1	1,2	14,14,15	0.64	0	17,19,21	1.15	2 (11%)
2	NAG	G	2	2	14,14,15	0.57	0	17,19,21	1.28	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	H	1	1,2	14,14,15	0.67	0	17,19,21	1.42	3 (17%)
2	NAG	H	2	2	14,14,15	0.49	0	17,19,21	1.18	1 (5%)
2	NAG	I	1	1,2	14,14,15	0.80	0	17,19,21	1.22	2 (11%)
2	NAG	I	2	2	14,14,15	0.56	0	17,19,21	1.44	3 (17%)

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	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	NAG	C2-N2	-2.77	1.41	1.46
2	D	2	NAG	O5-C1	-2.43	1.39	1.43
2	D	1	NAG	O4-C4	-2.40	1.37	1.43
2	F	2	NAG	C1-C2	2.39	1.55	1.52
2	D	2	NAG	C1-C2	-2.33	1.48	1.52
2	D	1	NAG	O5-C5	-2.10	1.39	1.43

All (39) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	O4-C4-C3	-8.10	91.63	110.35
2	C	2	NAG	C1-O5-C5	5.20	119.23	112.19
2	D	2	NAG	O5-C1-C2	-5.15	103.15	111.29
2	E	2	NAG	O5-C5-C6	4.80	114.73	107.20
2	E	2	NAG	C1-O5-C5	4.69	118.55	112.19
2	D	1	NAG	C1-O5-C5	4.64	118.47	112.19
2	D	2	NAG	C6-C5-C4	4.30	123.07	113.00
2	F	2	NAG	C4-C3-C2	4.22	117.20	111.02
2	G	2	NAG	C1-O5-C5	3.68	117.17	112.19
2	D	2	NAG	C4-C3-C2	3.67	116.40	111.02
2	E	2	NAG	C8-C7-N2	3.66	122.29	116.10
2	I	2	NAG	O5-C5-C6	3.55	112.77	107.20
2	H	1	NAG	C1-O5-C5	3.52	116.96	112.19
2	H	2	NAG	C1-O5-C5	3.43	116.83	112.19
2	C	1	NAG	C1-O5-C5	-3.42	107.56	112.19
2	E	1	NAG	C1-O5-C5	3.20	116.53	112.19
2	D	2	NAG	O5-C5-C6	-3.18	102.21	107.20
2	E	1	NAG	O4-C4-C5	-3.00	101.84	109.30
2	F	1	NAG	C4-C3-C2	2.97	115.37	111.02
2	I	1	NAG	C4-C3-C2	-2.94	106.71	111.02
2	E	2	NAG	O7-C7-C8	-2.80	116.85	122.06
2	I	2	NAG	O7-C7-C8	-2.66	117.12	122.06
2	D	1	NAG	C6-C5-C4	-2.54	107.05	113.00
2	D	2	NAG	C3-C4-C5	2.44	114.60	110.24
2	G	1	NAG	C1-O5-C5	-2.44	108.88	112.19
2	F	2	NAG	C2-N2-C7	2.33	126.22	122.90
2	H	1	NAG	C1-C2-N2	2.32	114.45	110.49
2	I	1	NAG	O5-C1-C2	-2.32	107.63	111.29
2	C	1	NAG	C1-C2-N2	-2.31	106.55	110.49
2	E	2	NAG	C2-N2-C7	2.27	126.14	122.90
2	H	1	NAG	C6-C5-C4	-2.19	107.88	113.00
2	D	1	NAG	O3-C3-C2	2.15	113.92	109.47
2	F	1	NAG	O4-C4-C3	-2.13	105.42	110.35
2	D	2	NAG	O5-C5-C4	-2.13	105.65	110.83
2	F	2	NAG	O5-C5-C4	-2.09	105.75	110.83
2	D	2	NAG	O4-C4-C3	-2.09	105.52	110.35
2	G	1	NAG	O4-C4-C3	-2.08	105.53	110.35
2	F	1	NAG	C1-O5-C5	2.08	115.01	112.19
2	I	2	NAG	C1-O5-C5	2.05	114.98	112.19

There are no chirality outliers.

All (18) torsion outliers are listed below:

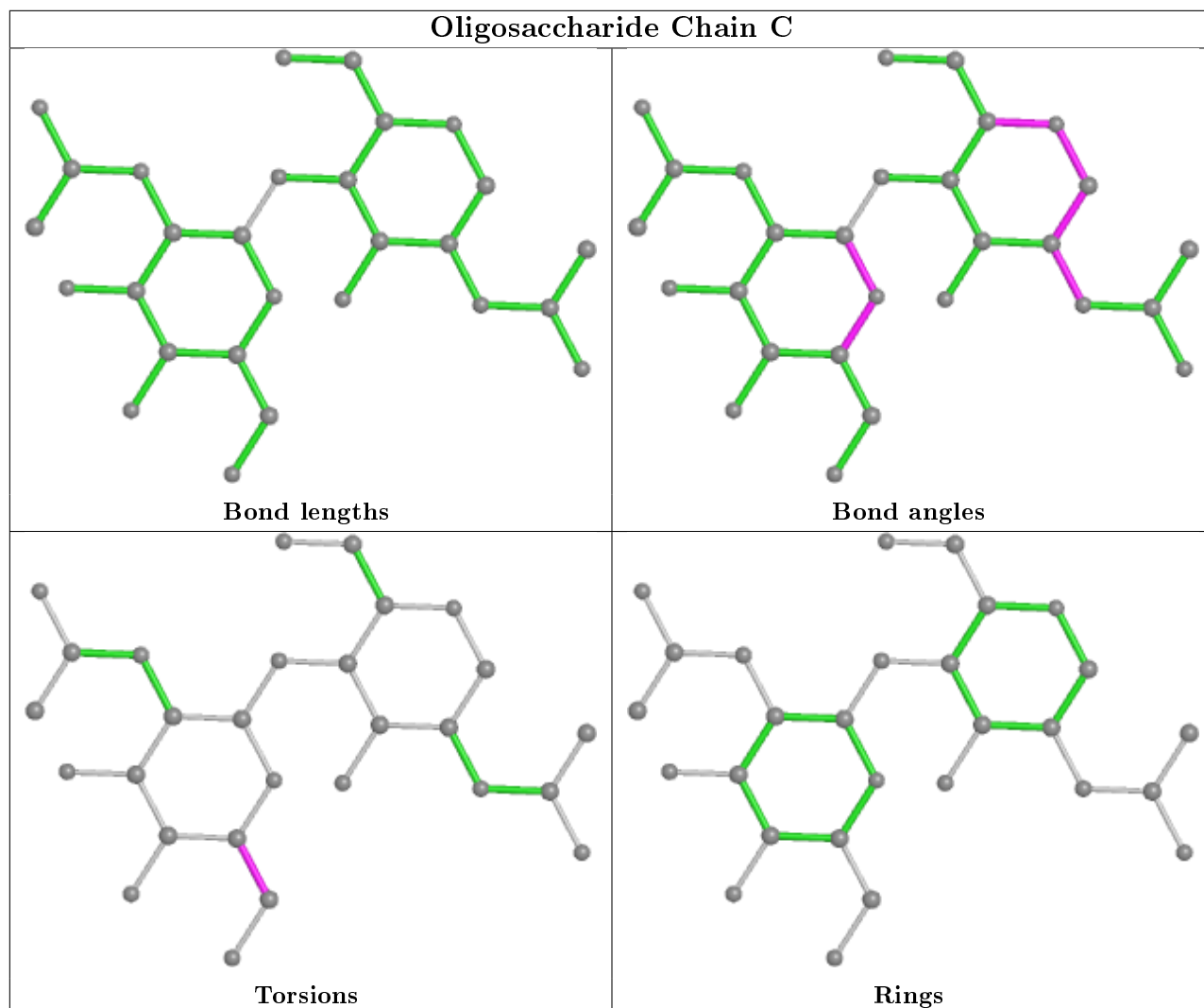
Mol	Chain	Res	Type	Atoms
2	I	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C1-C2-N2-C7
2	C	2	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	G	2	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C3-C2-N2-C7
2	F	1	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6

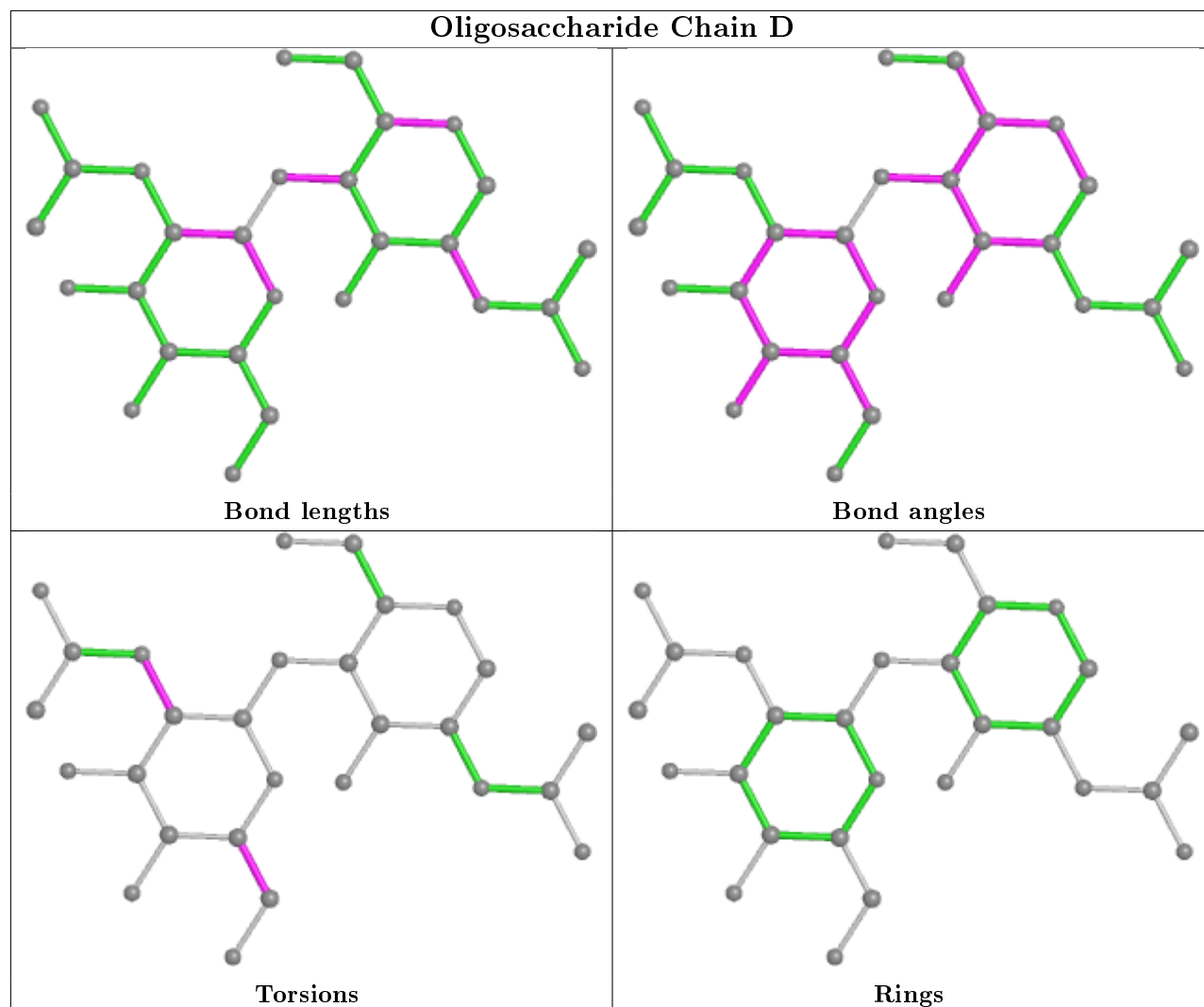
There are no ring outliers.

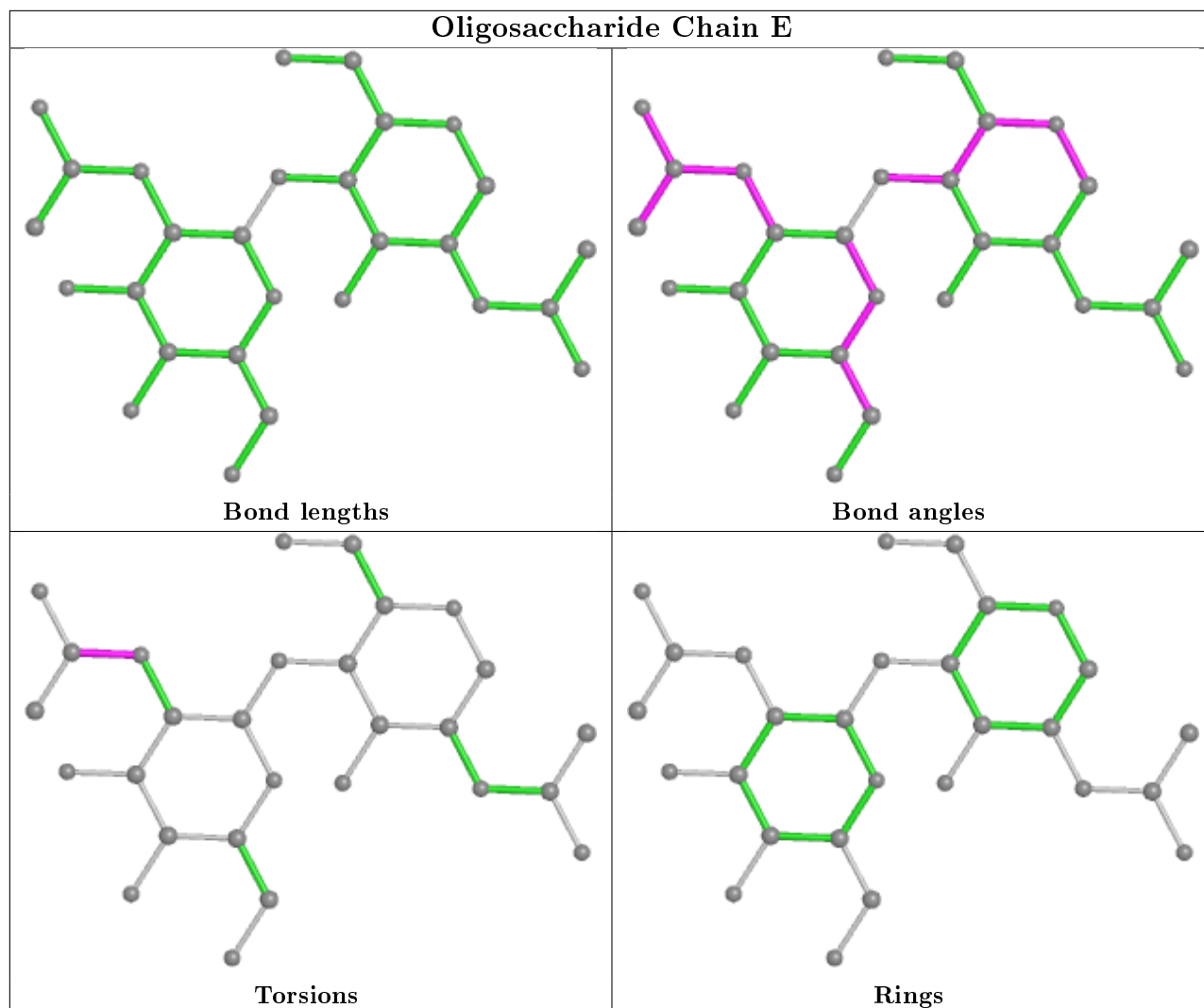
4 monomers are involved in 2 short contacts:

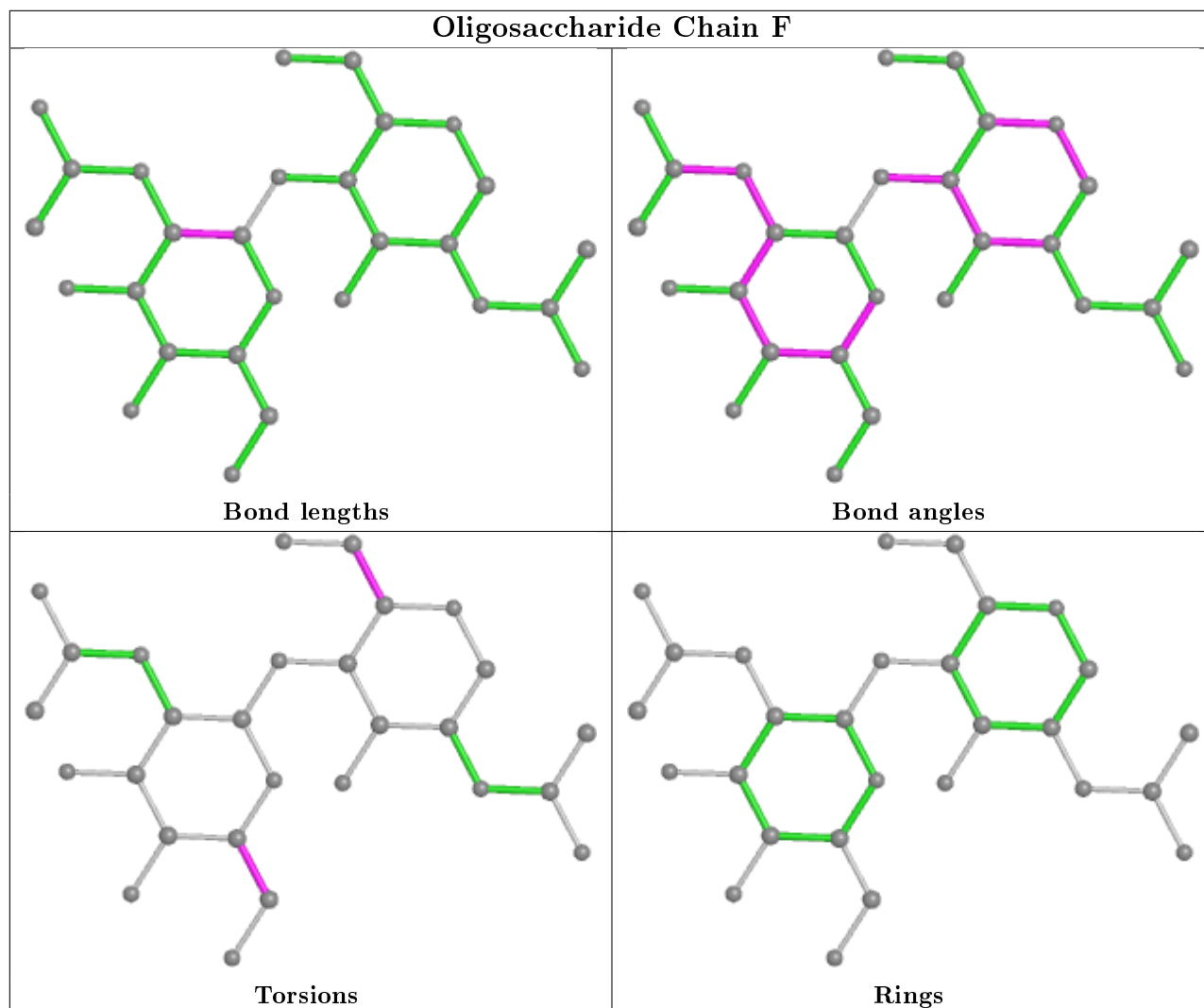
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	1	0
2	F	2	NAG	1	0
2	D	2	NAG	1	0
2	F	1	NAG	1	0

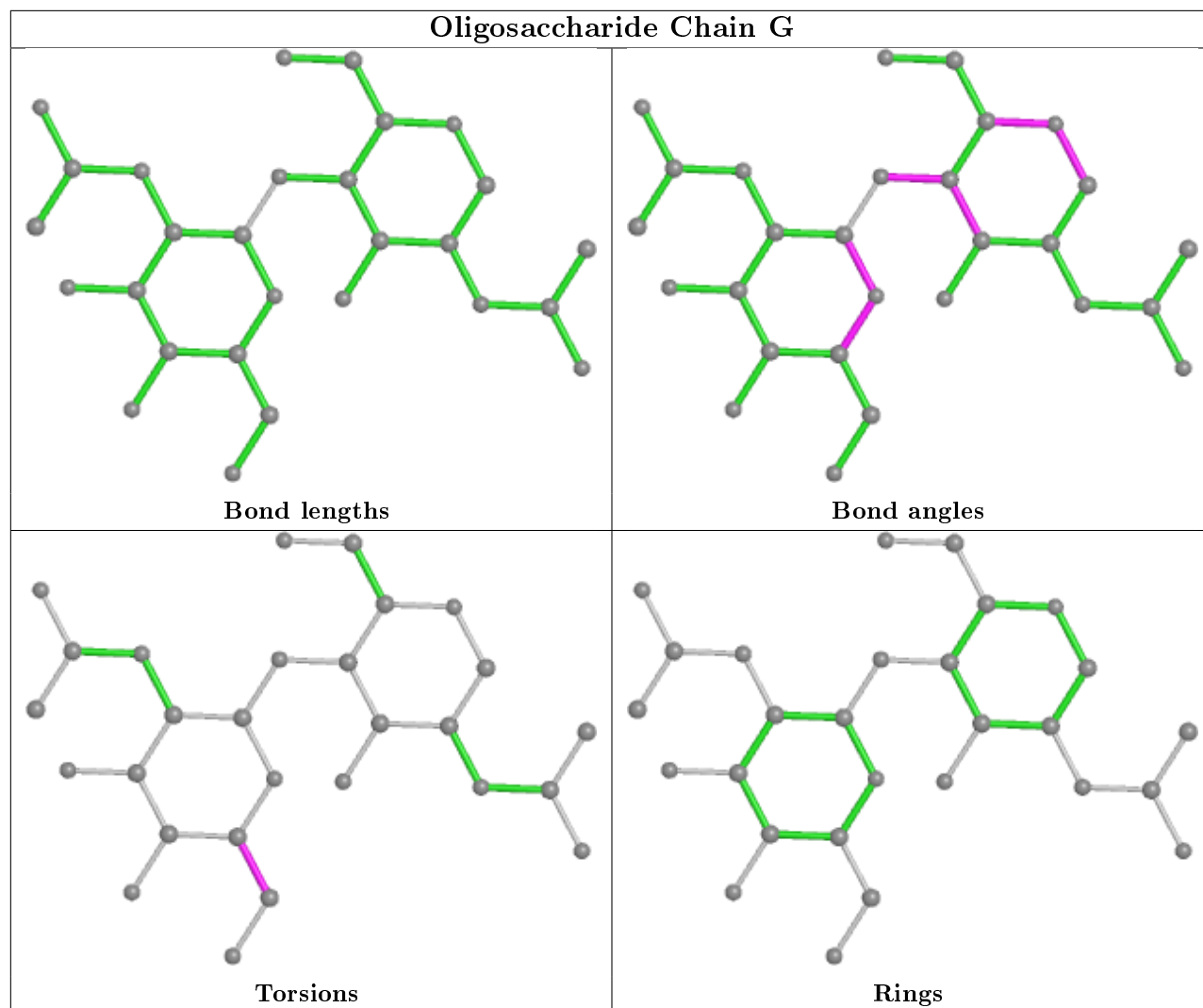
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

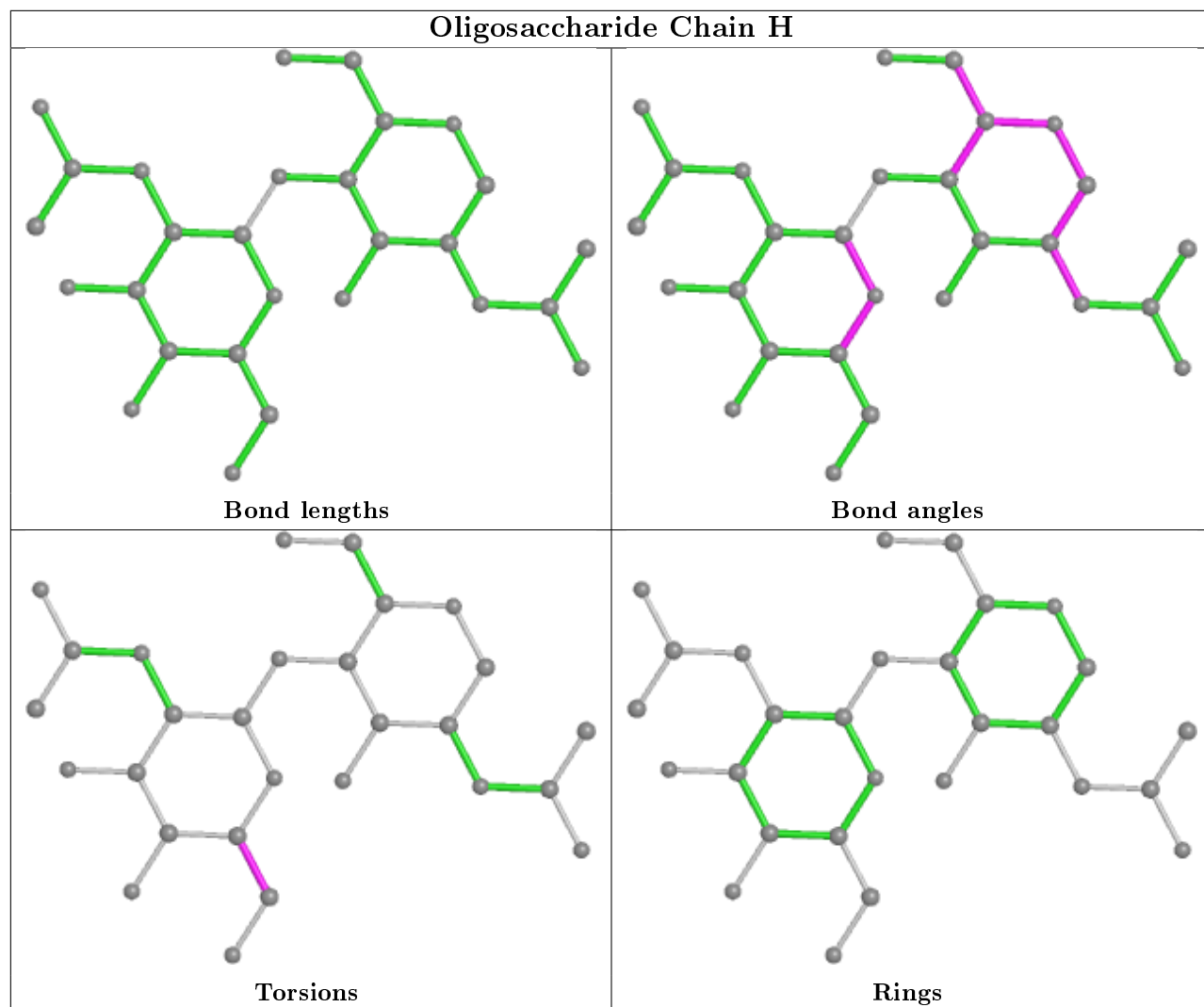




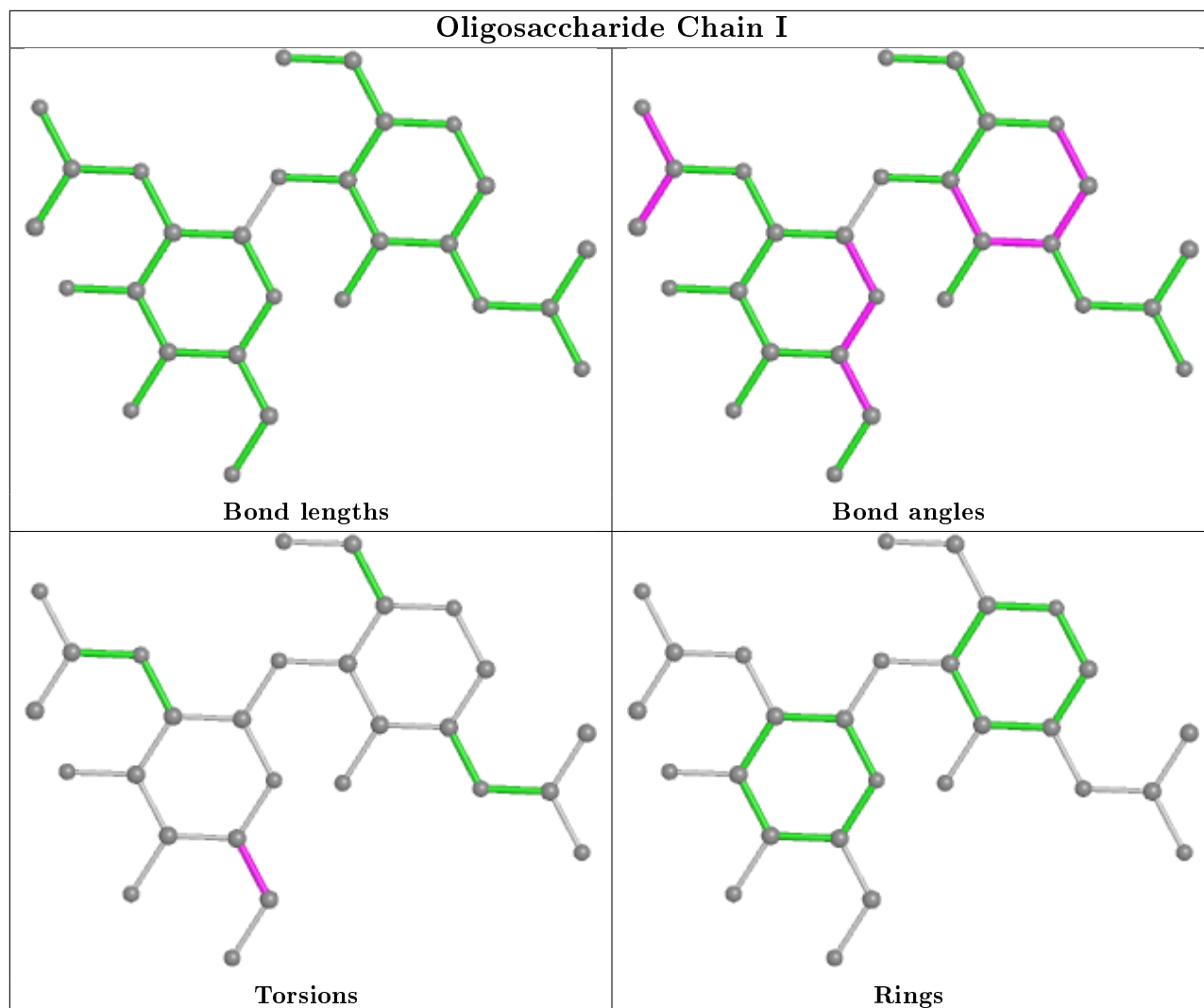












## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	6DG	B	810[A]	-	24,31,31	1.64	5 (20%)	24,46,46	1.71	5 (20%)
3	NAG	A	807	1	14,14,15	0.52	0	17,19,21	1.41	2 (11%)
3	NAG	A	801	1	14,14,15	0.54	0	17,19,21	1.96	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	6DG	B	810[B]	-	24,31,31	1.51	5 (20%)	24,46,46	1.49	4 (16%)
3	NAG	A	802	1	14,14,15	0.29	0	17,19,21	0.61	0
3	NAG	B	809	1	14,14,15	0.49	0	17,19,21	1.79	3 (17%)
5	6DG	A	811	-	24,31,31	1.66	6 (25%)	24,46,46	1.41	4 (16%)

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	6DG	B	810[A]	-	-	4/8/29/29	0/5/5/5
3	NAG	A	807	1	-	1/6/23/26	0/1/1/1
3	NAG	A	801	1	-	0/6/23/26	0/1/1/1
5	6DG	B	810[B]	-	-	0/8/29/29	0/5/5/5
3	NAG	A	802	1	-	0/6/23/26	0/1/1/1
3	NAG	B	809	1	-	0/6/23/26	0/1/1/1
5	6DG	A	811	-	-	0/8/29/29	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	811	6DG	C7-C17	3.52	1.58	1.51
5	B	810[A]	6DG	C14-C15	3.41	1.44	1.39
5	B	810[B]	6DG	C16-N22	3.23	1.40	1.35
5	A	811	6DG	C19-C18	3.10	1.57	1.53
5	B	810[A]	6DG	C19-C18	2.89	1.57	1.53
5	B	810[A]	6DG	C4-C14	-2.66	1.47	1.50
5	B	810[A]	6DG	C16-N22	2.65	1.39	1.35
5	B	810[B]	6DG	C14-C15	2.52	1.43	1.39
5	A	811	6DG	C8-C10	2.51	1.45	1.37
5	A	811	6DG	C3-C11	2.50	1.41	1.37
5	A	811	6DG	C15-N21	2.41	1.37	1.34
5	A	811	6DG	C16-N22	2.37	1.38	1.35
5	B	810[A]	6DG	C7-C17	2.35	1.56	1.51
5	B	810[B]	6DG	C7-C17	2.20	1.55	1.51
5	B	810[B]	6DG	C4-C14	-2.13	1.48	1.50
5	B	810[B]	6DG	C8-C10	2.06	1.43	1.37

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	809	NAG	C1-O5-C5	5.27	119.33	112.19
3	A	801	NAG	C1-O5-C5	4.87	118.79	112.19
5	B	810[A]	6DG	O25-C7-C17	-4.38	104.80	111.47
3	A	807	NAG	C1-O5-C5	4.09	117.73	112.19
5	A	811	6DG	C15-N21-N23	-3.79	101.57	105.59
5	B	810[B]	6DG	C15-N21-N23	-3.37	102.01	105.59
5	B	810[A]	6DG	C15-N21-N23	-3.35	102.03	105.59
3	B	809	NAG	O5-C1-C2	-3.31	106.06	111.29
5	B	810[A]	6DG	C3-C13-C12	3.31	119.23	116.48
3	A	801	NAG	C4-C3-C2	-3.21	106.32	111.02
3	A	801	NAG	O4-C4-C3	3.09	117.49	110.35
3	A	807	NAG	O5-C5-C6	2.72	111.47	107.20
5	B	810[A]	6DG	C2-C12-C13	-2.70	120.71	123.72
5	B	810[B]	6DG	C3-C13-C12	2.63	118.67	116.48
5	B	810[B]	6DG	O25-C19-C18	-2.60	106.92	110.65
5	B	810[B]	6DG	C9-C8-C10	2.54	120.50	117.27
5	B	810[A]	6DG	C9-C8-C10	2.40	120.32	117.27
5	A	811	6DG	O25-C19-C18	-2.37	107.24	110.65
5	A	811	6DG	C3-C13-C12	2.27	118.37	116.48
5	A	811	6DG	C9-C8-C10	2.16	120.03	117.27
3	A	801	NAG	C3-C4-C5	-2.16	106.39	110.24
3	B	809	NAG	O7-C7-C8	-2.14	118.09	122.06

There are no chirality outliers.

All (5) torsion outliers are listed below:

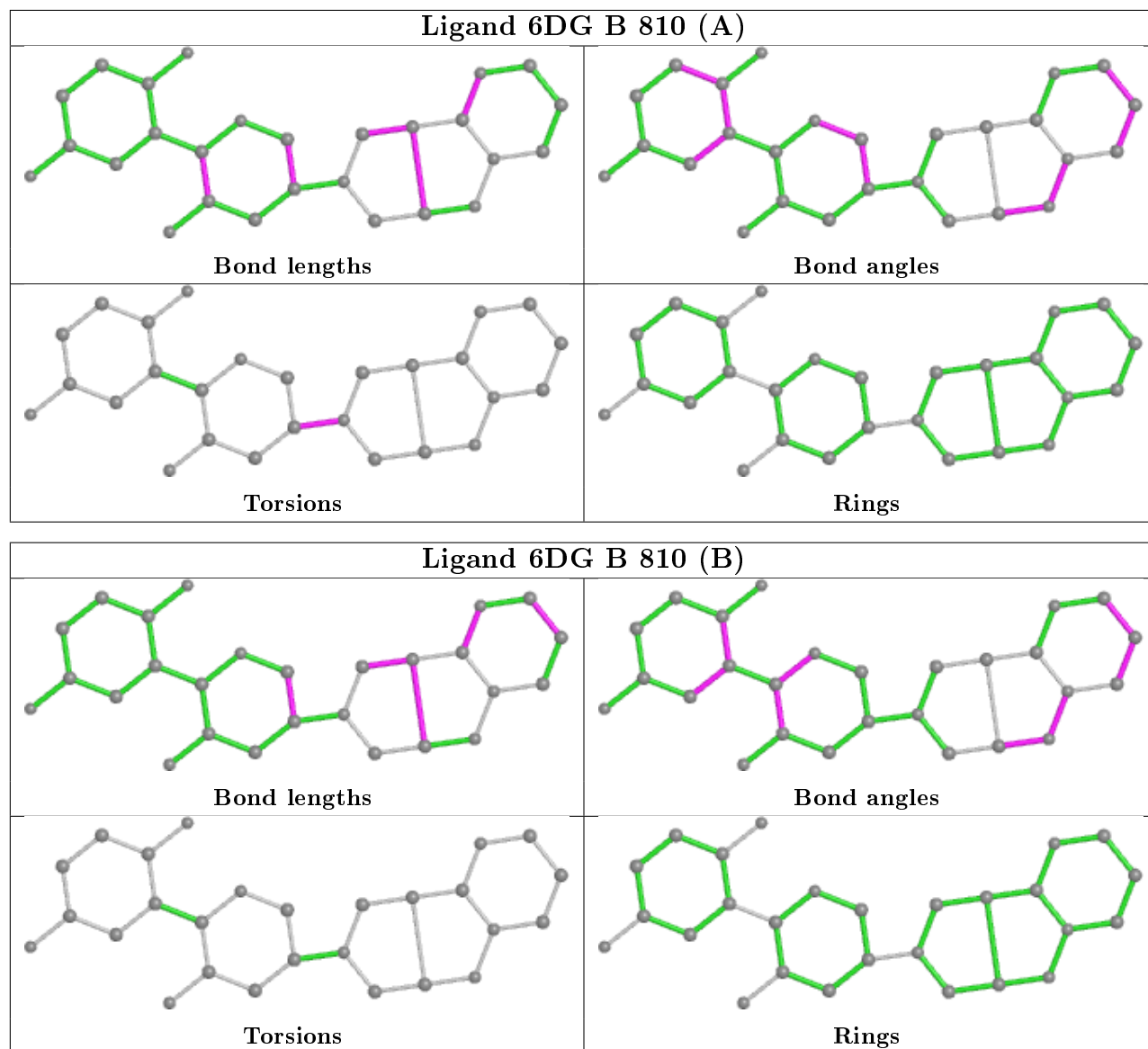
Mol	Chain	Res	Type	Atoms
5	B	810[A]	6DG	C6-C17-N24-C5
5	B	810[A]	6DG	C6-C17-N24-C4
5	B	810[A]	6DG	C7-C17-N24-C5
5	B	810[A]	6DG	C7-C17-N24-C4
3	A	807	NAG	C4-C5-C6-O6

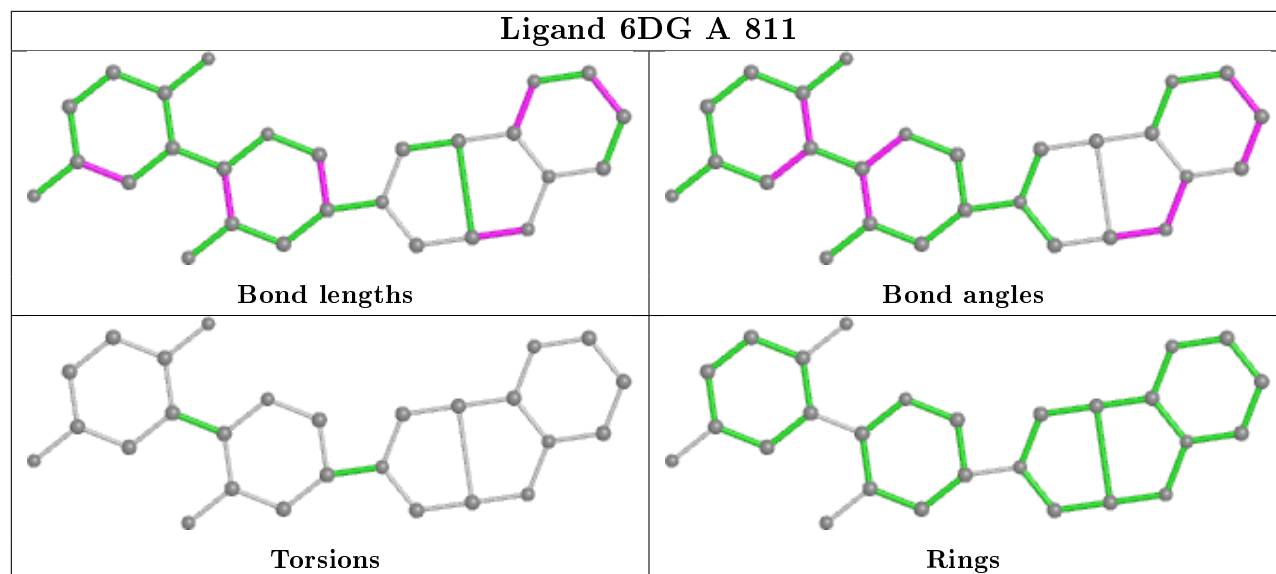
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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	728/728 (100%)	-0.19	17 (2%) 60 59	11, 19, 42, 67	0
1	B	728/728 (100%)	-0.11	21 (2%) 51 50	12, 21, 45, 72	0
All	All	1456/1456 (100%)	-0.15	38 (2%) 56 54	11, 20, 45, 72	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	39	THR	7.8
1	B	766	PRO	7.0
1	A	39	THR	6.3
1	A	73	GLU	5.2
1	A	74	ASN	5.1
1	A	766	PRO	4.4
1	A	99	GLY	3.9
1	A	279	VAL	3.9
1	B	93	SER	3.7
1	B	97	GLU	3.5
1	B	40	ARG	3.4
1	B	73	GLU	3.4
1	B	96	ASP	3.3
1	A	138	ASN	3.2
1	B	333	SER	3.1
1	A	97	GLU	2.9
1	A	333	SER	2.9
1	A	92	ASN	2.8
1	B	140	ARG	2.8
1	A	96	ASP	2.7
1	B	506	ASN	2.6
1	B	521	GLU	2.6
1	B	95	PHE	2.5
1	B	505	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	502	LYS	2.5
1	A	521	GLU	2.5
1	A	75	ASN	2.4
1	B	138	ASN	2.4
1	B	92	ASN	2.4
1	B	121	VAL	2.3
1	B	74	ASN	2.2
1	A	40	ARG	2.2
1	B	91	GLU	2.2
1	B	332	GLU	2.1
1	A	506[A]	ASN	2.1
1	A	520	ASN	2.1
1	A	140	ARG	2.1
1	B	129	THR	2.0

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

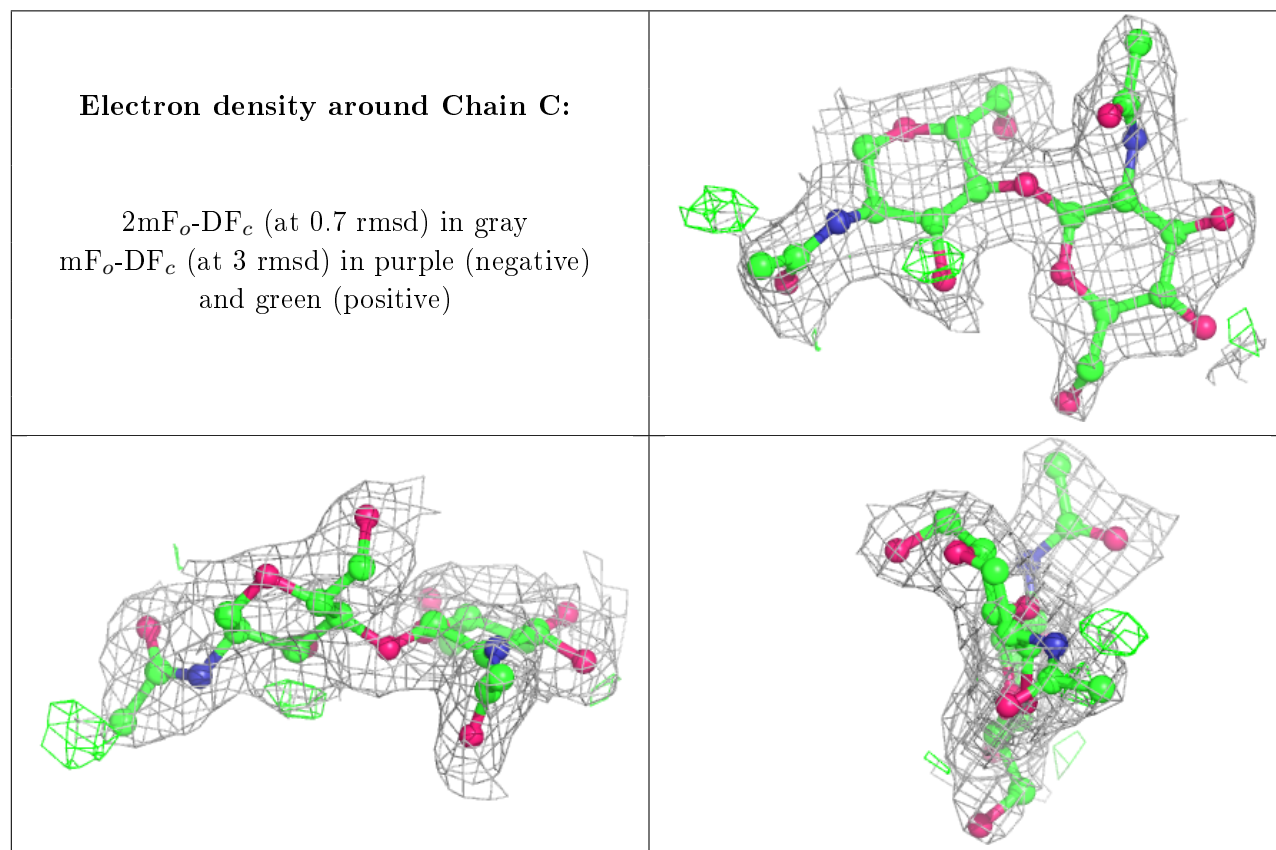
There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	NAG	F	2	14/15	0.44	0.36	58,73,75,77	0
2	NAG	D	2	14/15	0.57	0.51	20,20,20,20	0
2	NAG	E	2	14/15	0.62	0.42	63,66,73,74	0
2	NAG	I	2	14/15	0.69	0.28	45,52,60,62	0
2	NAG	C	2	14/15	0.81	0.30	44,51,59,61	0
2	NAG	E	1	14/15	0.81	0.29	36,41,45,55	0
2	NAG	G	2	14/15	0.83	0.29	42,48,53,56	0
2	NAG	F	1	14/15	0.83	0.18	46,53,63,67	0
2	NAG	H	2	14/15	0.87	0.35	38,44,47,49	0
2	NAG	G	1	14/15	0.91	0.21	29,36,46,46	0
2	NAG	C	1	14/15	0.91	0.19	34,39,44,46	0
2	NAG	H	1	14/15	0.91	0.15	22,25,33,34	0
2	NAG	D	1	14/15	0.91	0.17	27,33,39,44	0
2	NAG	I	1	14/15	0.92	0.13	28,30,37,44	0

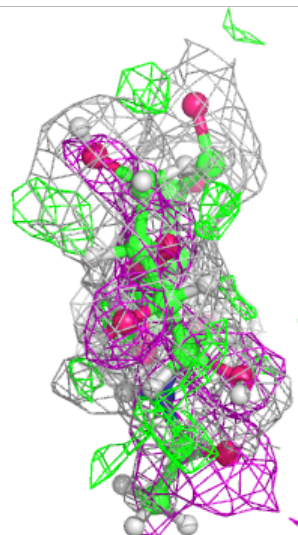
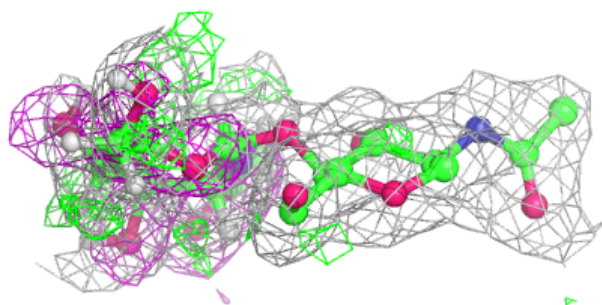
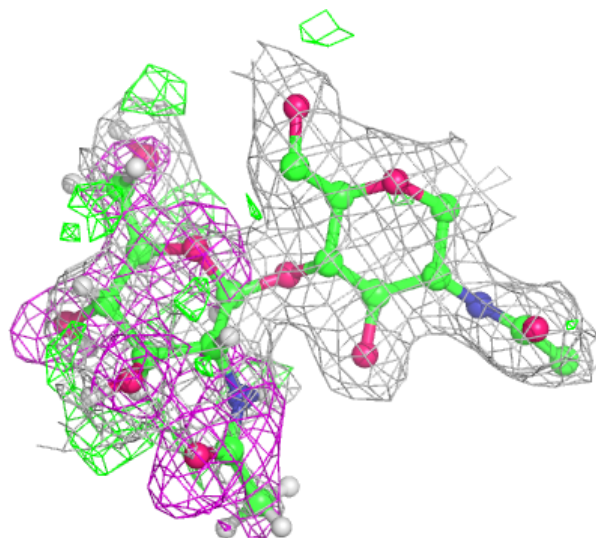
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

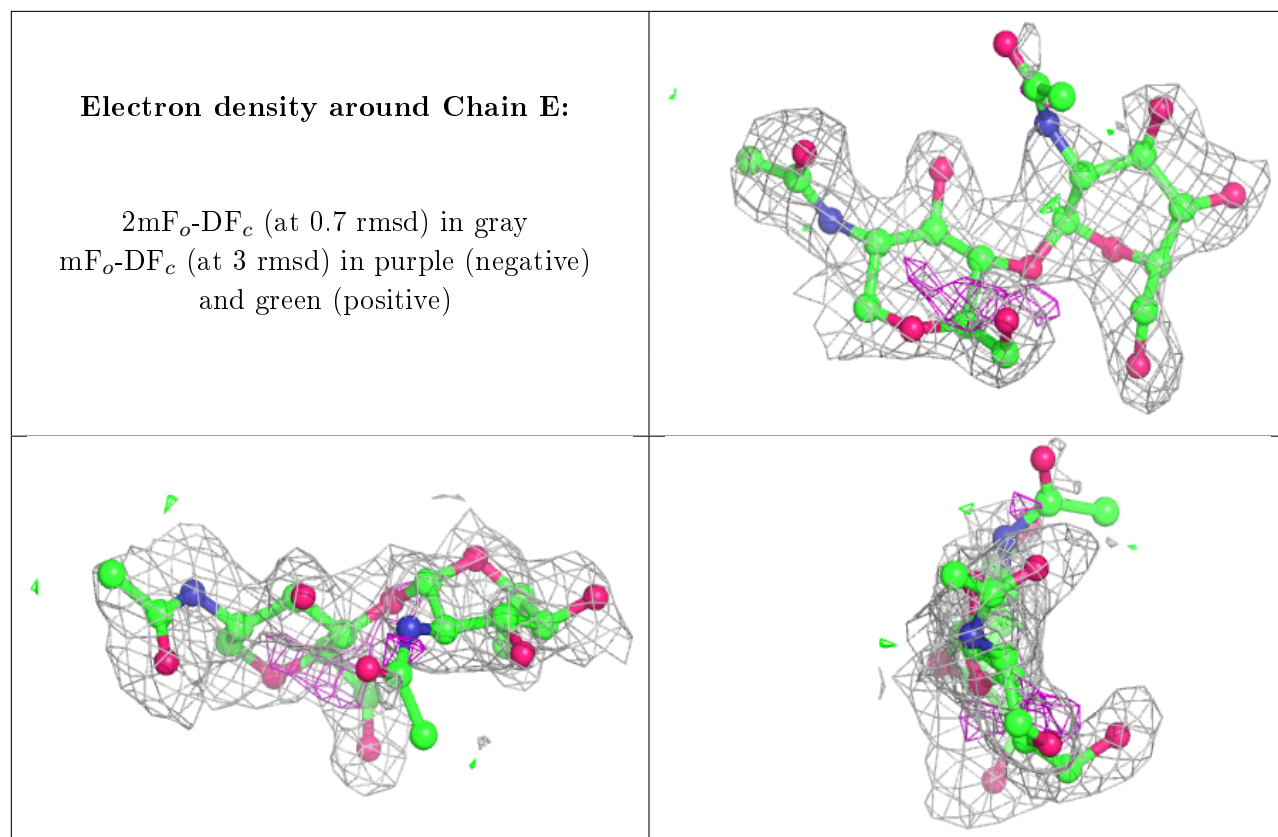




**Electron density around Chain D:**

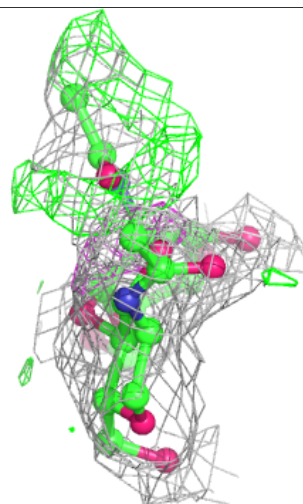
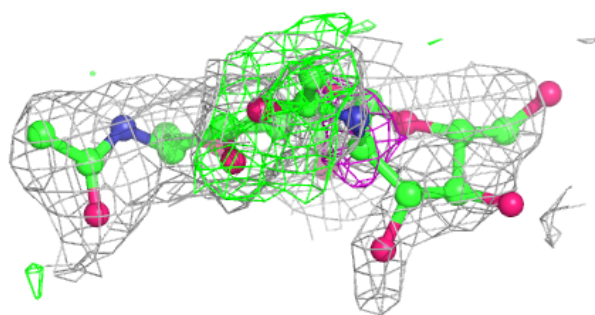
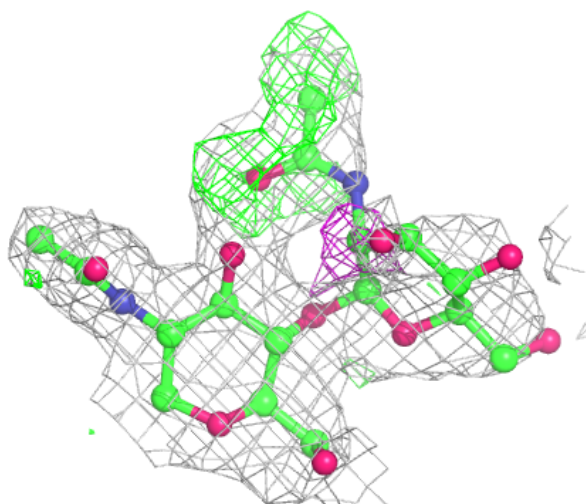
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





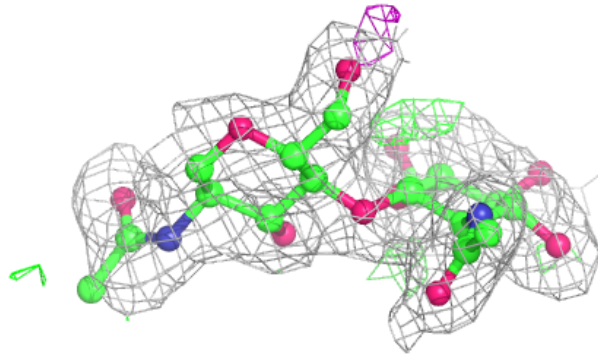
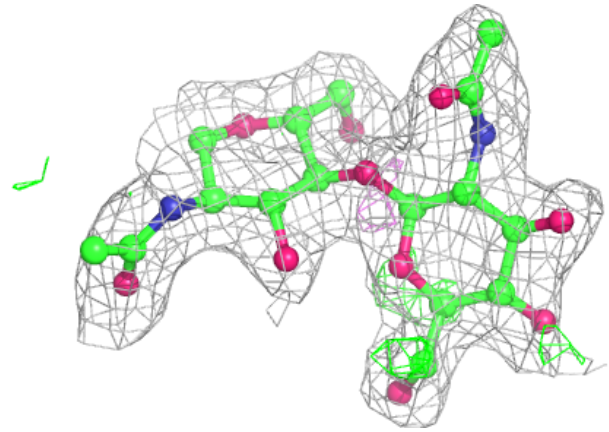
**Electron density around Chain F:**

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



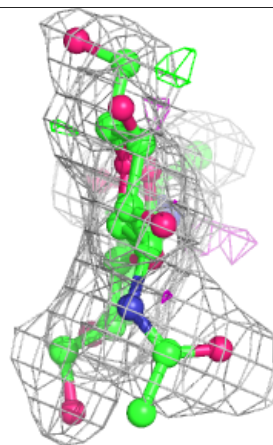
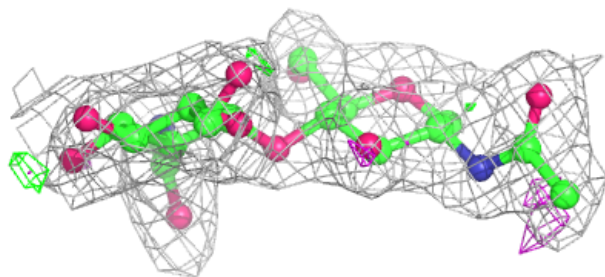
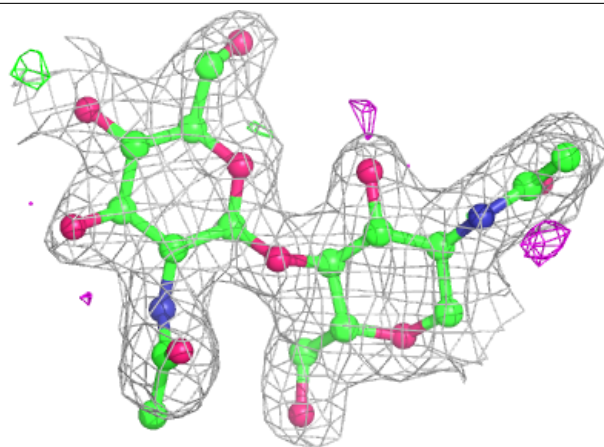
**Electron density around Chain G:**

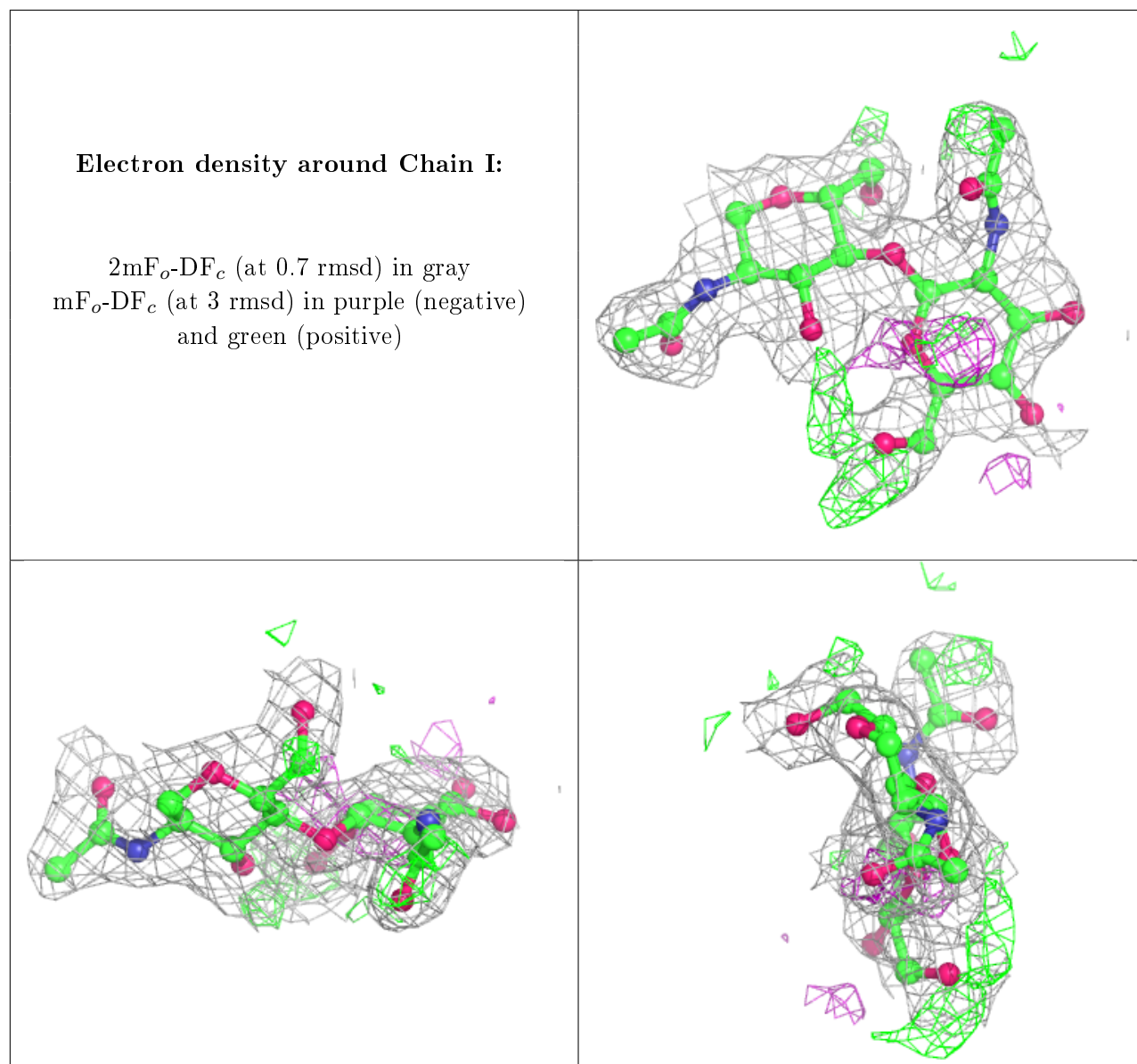
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain H:**

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





## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

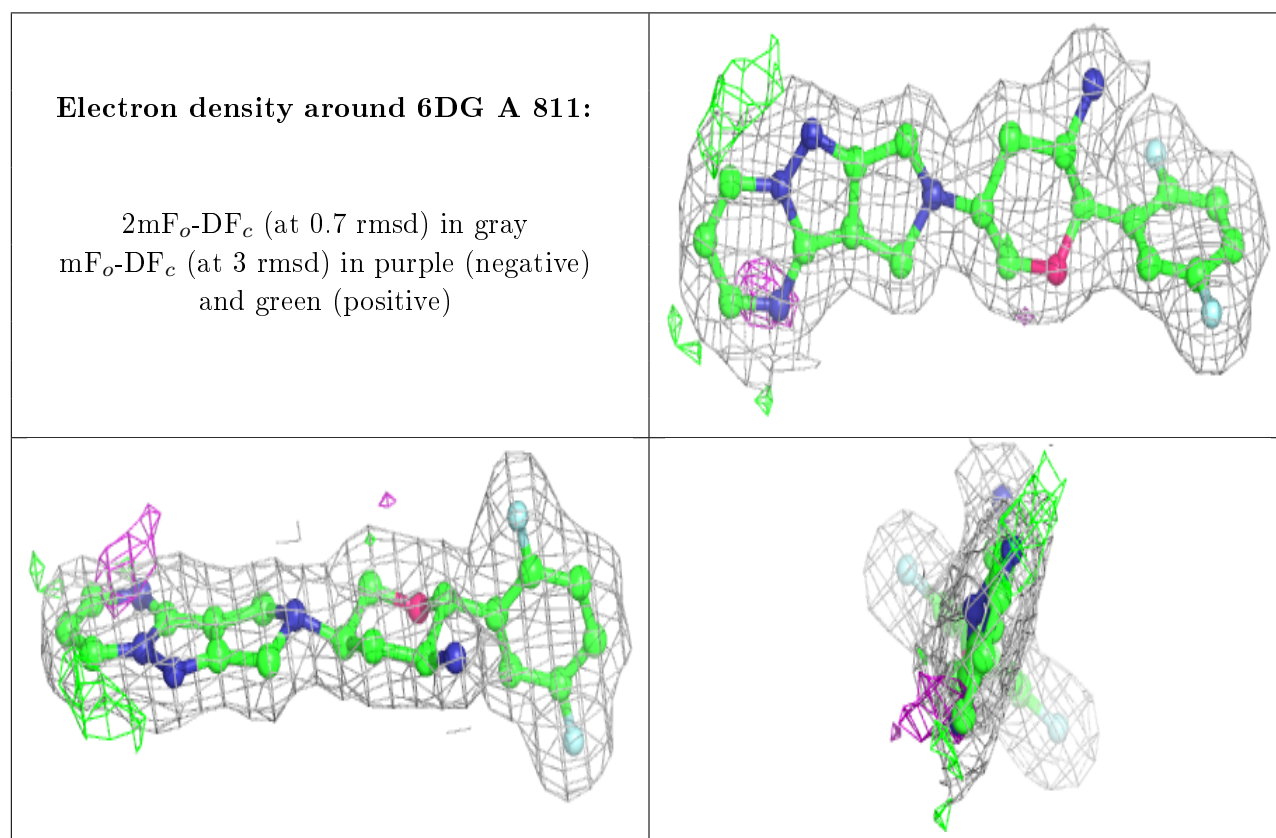
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q < 0.9
3	NAG	A	802	14/15	0.78	0.33	46,52,56,58	0
3	NAG	A	807	14/15	0.83	0.23	37,41,45,46	0
3	NAG	B	809	14/15	0.86	0.28	32,39,41,42	0
3	NAG	A	801	14/15	0.88	0.17	39,44,54,63	0
5	6DG	A	811	27/27	0.95	0.10	13,15,26,27	0

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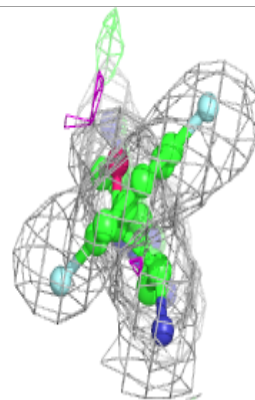
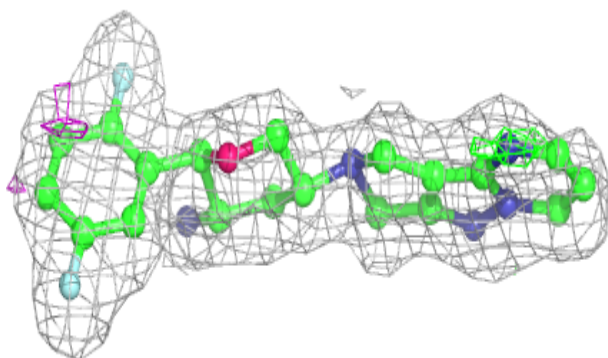
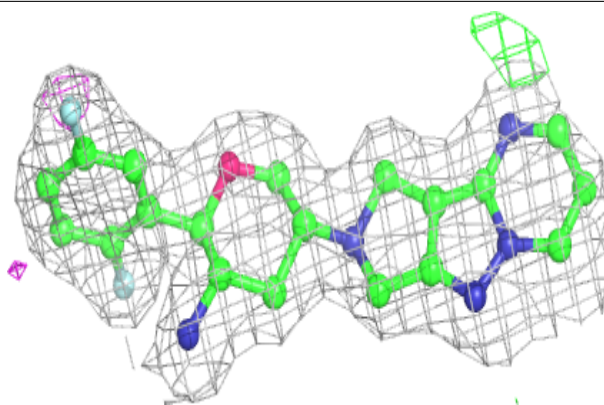
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	6DG	B	810[B]	27/27	0.96	0.11	9,9,9,10	27
5	6DG	B	810[A]	27/27	0.96	0.11	18,20,29,29	27
4	NA	A	810	1/1	0.97	0.07	24,24,24,24	0

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.

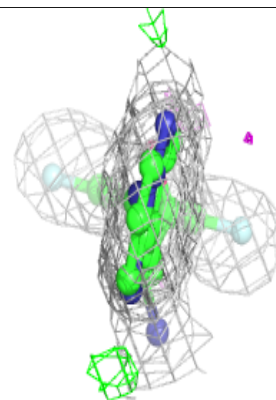
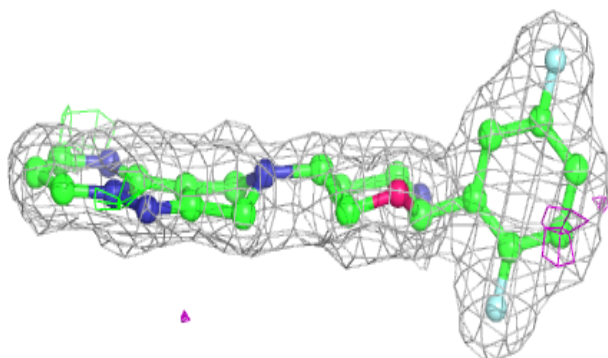
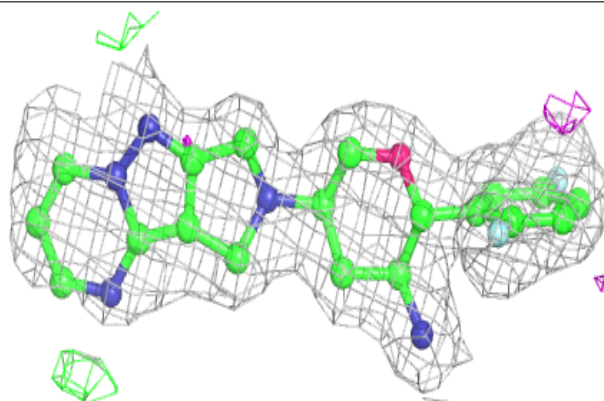


**Electron density around 6DG B 810 (B):**

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

**Electron density around 6DG B 810 (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

There are no such residues in this entry.