



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 09:05 AM BST

PDB ID : 5ZSA  
Title : Crystal structure of monkey TLR7 in complex with IMDQ and UUUUUU  
Authors : Zhang, Z.; Ohto, U.; Shimizu, T.  
Deposited on : 2018-04-28  
Resolution : 2.50 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.

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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

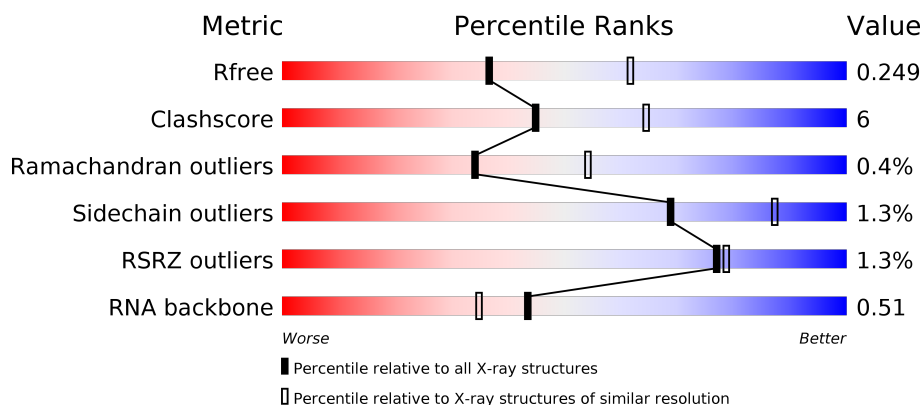
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





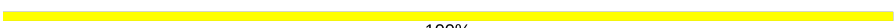
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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	823	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>6%</div> </div> </div>
1	B	823	<div> <div>82%</div> <div>12%</div> <div>6%</div> </div>
2	C	6	<div> <div>33%</div> <div>33%</div> <div>33%</div> </div>
2	D	6	<div> <div>50%</div> <div>17%</div> <div>33%</div> </div>

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Mol	Chain	Length	Quality of chain
3	E	2	 50% 50%
3	F	2	 50% 50%
3	G	2	 50% 50%
3	H	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
6	SO4	A	1013	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13272 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 Toll-like receptor 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	775	Total	C	N	O	S	0	1	0
			6292	4033	1075	1154	30			
1	A	773	Total	C	N	O	S	0	0	0
			6261	4012	1068	1151	30			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	23	ARG	-	expression tag	UNP B3Y653
B	24	SER	-	expression tag	UNP B3Y653
B	25	PRO	-	expression tag	UNP B3Y653
B	26	TRP	-	expression tag	UNP B3Y653
B	167	GLN	ASN	engineered mutation	UNP B3Y653
B	389	GLN	ASN	engineered mutation	UNP B3Y653
B	440	LEU	SER	see sequence details	UNP B3Y653
B	441	VAL	GLU	see sequence details	UNP B3Y653
B	442	PRO	VAL	see sequence details	UNP B3Y653
B	443	ARG	GLY	see sequence details	UNP B3Y653
B	444	GLY	PHE	see sequence details	UNP B3Y653
B	445	SER	CYS	see sequence details	UNP B3Y653
B	488	GLN	ASN	engineered mutation	UNP B3Y653
B	799	GLN	ASN	engineered mutation	UNP B3Y653
B	840	GLU	-	expression tag	UNP B3Y653
B	841	PHE	-	expression tag	UNP B3Y653
B	842	LEU	-	expression tag	UNP B3Y653
B	843	VAL	-	expression tag	UNP B3Y653
B	844	PRO	-	expression tag	UNP B3Y653
B	845	ARG	-	expression tag	UNP B3Y653
A	23	ARG	-	expression tag	UNP B3Y653
A	24	SER	-	expression tag	UNP B3Y653
A	25	PRO	-	expression tag	UNP B3Y653
A	26	TRP	-	expression tag	UNP B3Y653
A	167	GLN	ASN	engineered mutation	UNP B3Y653

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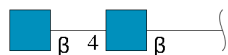
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Chain	Residue	Modelled	Actual	Comment	Reference
A	389	GLN	ASN	engineered mutation	UNP B3Y653
A	440	LEU	SER	see sequence details	UNP B3Y653
A	441	VAL	GLU	see sequence details	UNP B3Y653
A	442	PRO	VAL	see sequence details	UNP B3Y653
A	443	ARG	GLY	see sequence details	UNP B3Y653
A	444	GLY	PHE	see sequence details	UNP B3Y653
A	445	SER	CYS	see sequence details	UNP B3Y653
A	488	GLN	ASN	engineered mutation	UNP B3Y653
A	799	GLN	ASN	engineered mutation	UNP B3Y653
A	840	GLU	-	expression tag	UNP B3Y653
A	841	PHE	-	expression tag	UNP B3Y653
A	842	LEU	-	expression tag	UNP B3Y653
A	843	VAL	-	expression tag	UNP B3Y653
A	844	PRO	-	expression tag	UNP B3Y653
A	845	ARG	-	expression tag	UNP B3Y653

- Molecule 2 is a RNA chain called RNA (5'-R(P\*UP\*UP\*UP\*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	P	0	0	0
			64	27	6	27	4			
2	D	4	Total	C	N	O	P	0	0	0
			64	27	6	27	4			

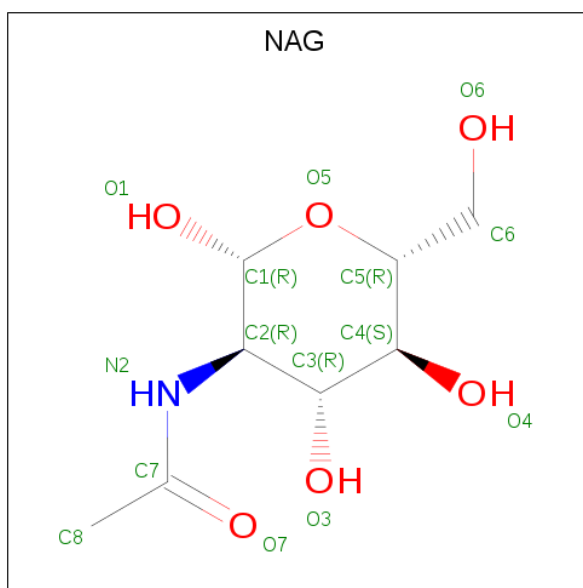
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

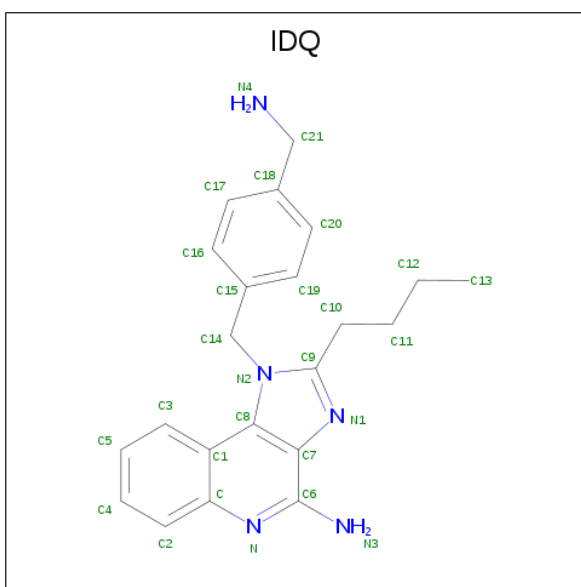
- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



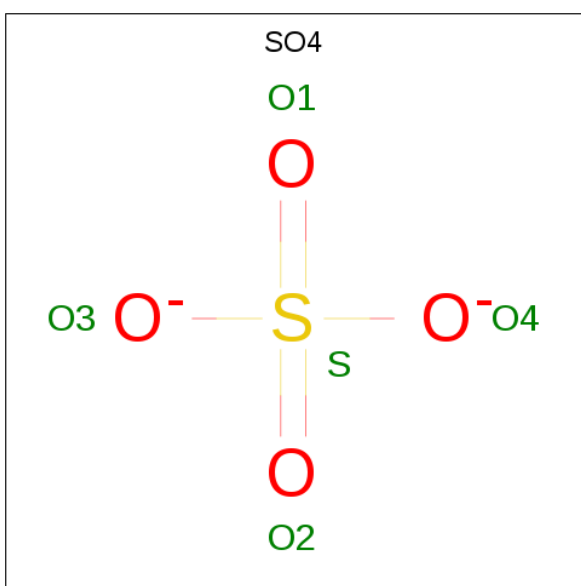
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1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

- Molecule 5 is 1-[[4-(aminomethyl)phenyl]methyl]-2-butyl-imidazo[4,5-c]quinolin-4-amine (three-letter code: IDQ) (formula: C<sub>22</sub>H<sub>25</sub>N<sub>5</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	N	0	0
			27	22	5		
5	A	1	Total	C	N	0	0
			27	22	5		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

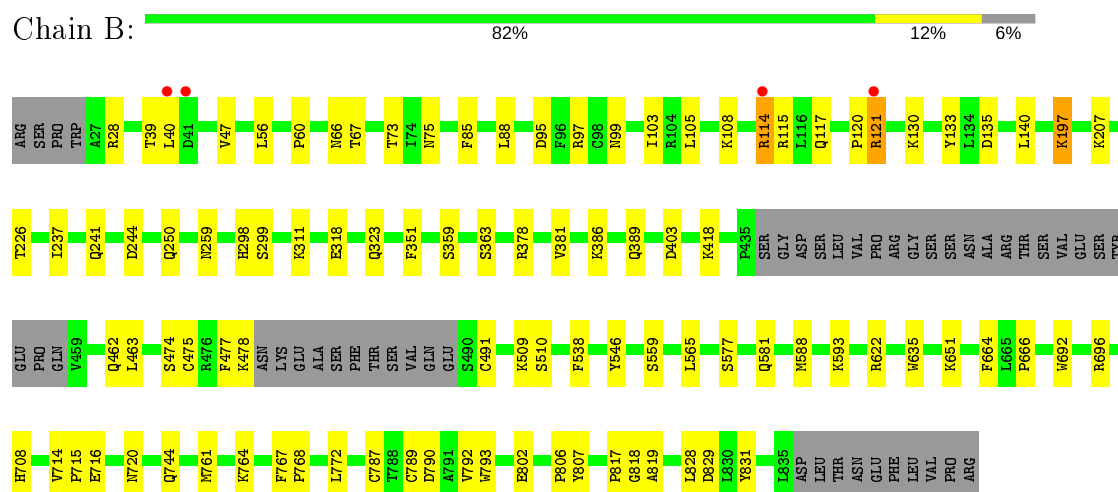
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	142	Total	O	0	0
			142	142		
7	A	73	Total	O	0	0
			73	73		
7	C	1	Total	O	0	0
			1	1		



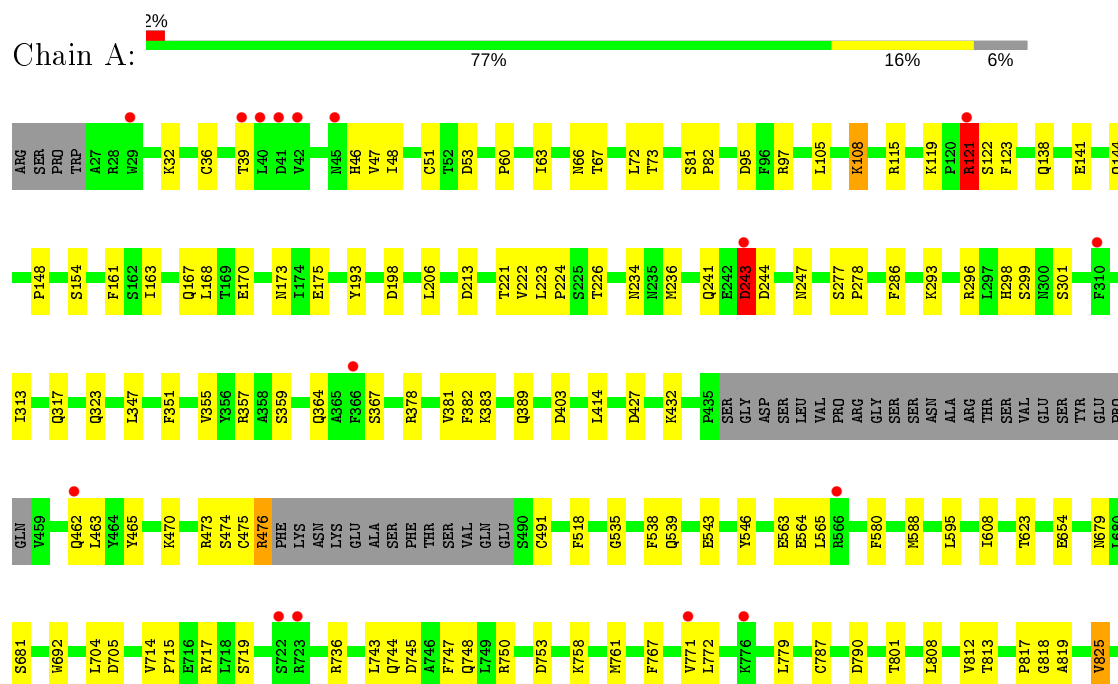
### 3 Residue-property plots [i](#)

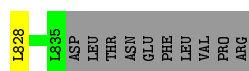
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: Toll-like receptor 7

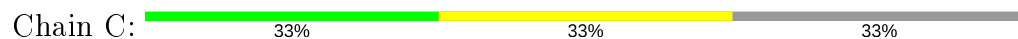


#### • Molecule 1: Toll-like receptor 7

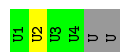




- Molecule 2: RNA (5'-R(P\*UP\*UP\*UP\*U)-3')



- Molecule 2: RNA (5'-R(P\*UP\*UP\*UP\*U)-3')



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



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



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



- Molecule 3: 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 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.18Å 139.73Å 150.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.18 – 2.50 47.18 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.18-2.50) 99.9 (47.18-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, $R_{free}$	0.199 , 0.249 0.199 , 0.249	Depositor DCC
$R_{free}$ test set	3584 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.9	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13272	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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: IDQ, SO4, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.43	1/6392 (0.0%)	0.67	5/8660 (0.1%)
1	B	0.48	2/6424 (0.0%)	0.78	8/8701 (0.1%)
2	C	0.57	0/69	0.90	0/105
2	D	0.55	0/69	0.91	0/105
All	All	0.46	3/12954 (0.0%)	0.73	13/17571 (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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	121	ARG	CB-CG	5.65	1.67	1.52
1	B	114	ARG	CG-CD	5.57	1.65	1.51
1	A	243	ASP	CG-OD2	5.06	1.36	1.25

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	114	ARG	NE-CZ-NH2	-22.67	108.97	120.30
1	B	114	ARG	NE-CZ-NH1	21.62	131.11	120.30
1	B	114	ARG	CD-NE-CZ	12.46	141.04	123.60
1	B	114	ARG	CG-CD-NE	-11.98	86.64	111.80
1	A	121	ARG	NE-CZ-NH1	-10.93	114.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	ASP	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6261	0	6311	95	0
1	B	6292	0	6342	70	0
2	C	64	0	30	2	0
2	D	64	0	30	2	0
3	E	28	0	25	1	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
4	A	56	0	52	1	0
4	B	98	0	91	5	0
5	A	27	0	23	1	0
5	B	27	0	24	1	0
6	A	35	0	0	2	0
6	B	20	0	0	0	0
7	A	73	0	0	17	0
7	B	142	0	0	8	0
7	C	1	0	0	1	0
All	All	13272	0	13003	168	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 6.

The worst 5 of 168 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:B:114:ARG:HH11	1:B:117:GLN:NE2	1.31	1.28
1:B:114:ARG:NH1	1:B:117:GLN:HE21	1.45	1.12
1:B:114:ARG:NH1	1:B:117:GLN:NE2	2.00	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLU:OE1	7:A:1101:HOH:O	1.81	0.97
1:A:236:MET:SD	7:A:1169:HOH:O	2.30	0.88

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	767/823 (93%)	715 (93%)	48 (6%)	4 (0%)	29	48
1	B	770/823 (94%)	719 (93%)	49 (6%)	2 (0%)	41	61
All	All	1537/1646 (93%)	1434 (93%)	97 (6%)	6 (0%)	34	54

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	818	GLY
1	A	818	GLY
1	A	122	SER
1	B	381	VAL
1	A	121	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	726/774 (94%)	717 (99%)	9 (1%)	71	88
1	B	729/774 (94%)	718 (98%)	11 (2%)	65	85
All	All	1455/1548 (94%)	1435 (99%)	20 (1%)	69	86

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	510	SER
1	B	593	LYS
1	A	476	ARG
1	B	363	SER
1	B	509	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	117	GLN
1	B	644	GLN
1	A	317	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	2/6 (33%)	0	0
2	D	2/6 (33%)	0	0
All	All	4/12 (33%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

## 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 ⓘ

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	E	1	1,3	14,14,15	0.34	0	17,19,21	0.57	0
3	NAG	E	2	3	14,14,15	0.33	0	17,19,21	0.68	0
3	NAG	F	1	1,3	14,14,15	0.56	0	17,19,21	0.50	0
3	NAG	F	2	3	14,14,15	0.53	0	17,19,21	0.77	1 (5%)
3	NAG	G	1	1,3	14,14,15	0.53	0	17,19,21	0.47	0
3	NAG	G	2	3	14,14,15	0.35	0	17,19,21	1.00	1 (5%)
3	NAG	H	1	1,3	14,14,15	0.54	0	17,19,21	0.76	1 (5%)
3	NAG	H	2	3	14,14,15	0.24	0	17,19,21	1.09	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	2	NAG	C1-O5-C5	3.90	117.48	112.19
3	G	2	NAG	C1-O5-C5	3.73	117.25	112.19
3	H	1	NAG	C1-O5-C5	2.40	115.44	112.19
3	F	2	NAG	C1-O5-C5	2.04	114.96	112.19



There are no chirality outliers.

5 of 16 torsion outliers are listed below:

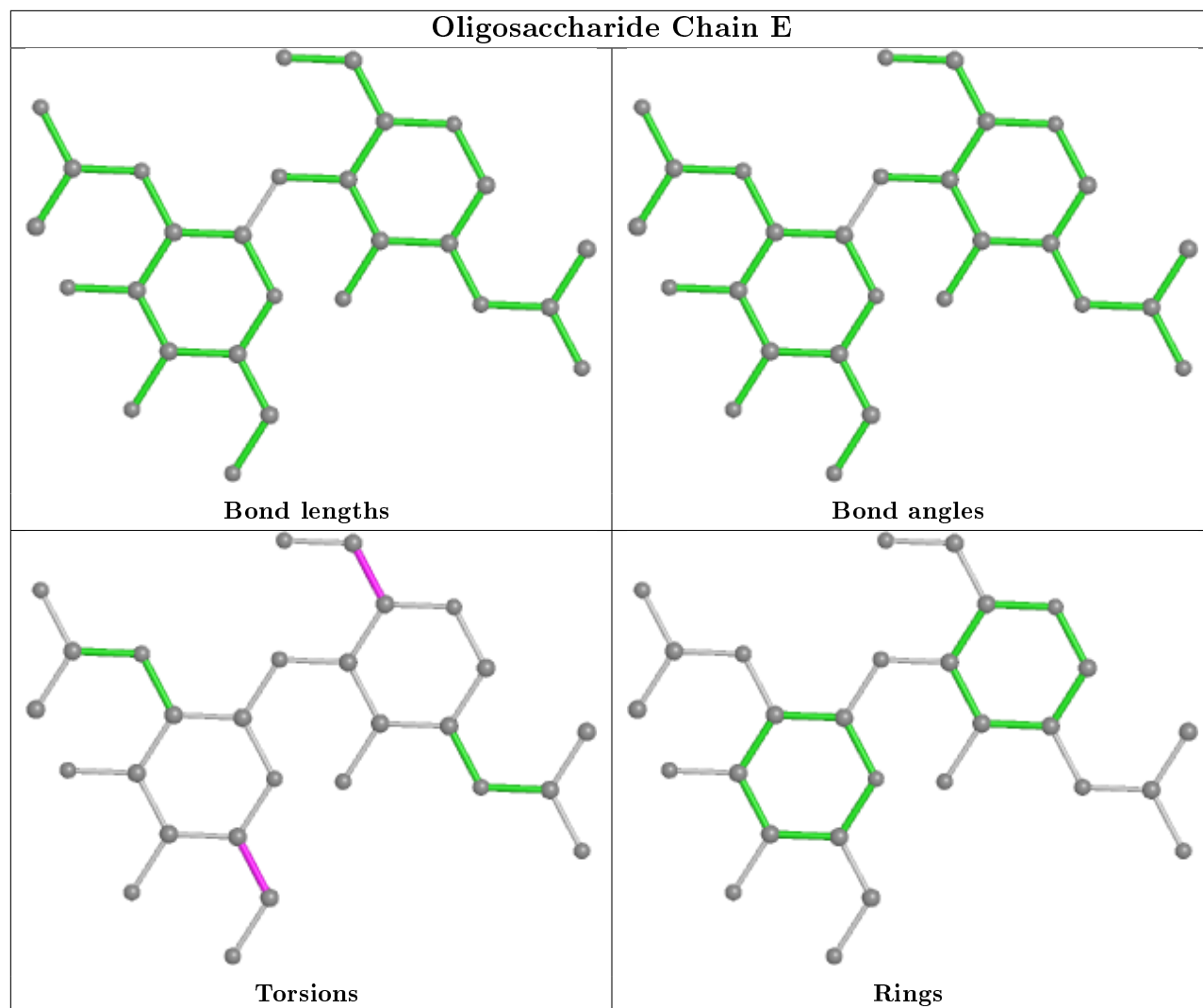
Mol	Chain	Res	Type	Atoms
3	H	2	NAG	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	E	2	NAG	O5-C5-C6-O6

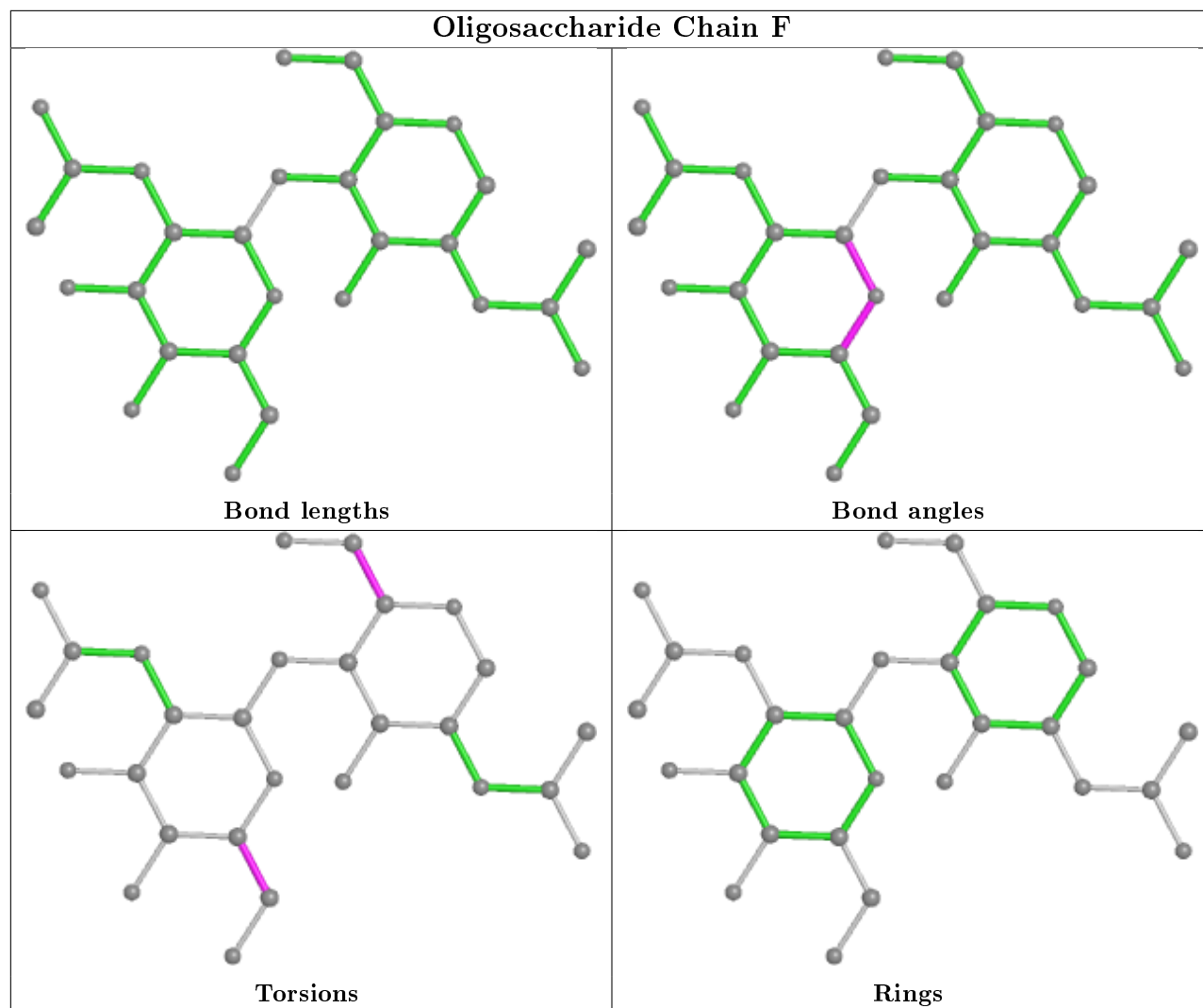
There are no ring outliers.

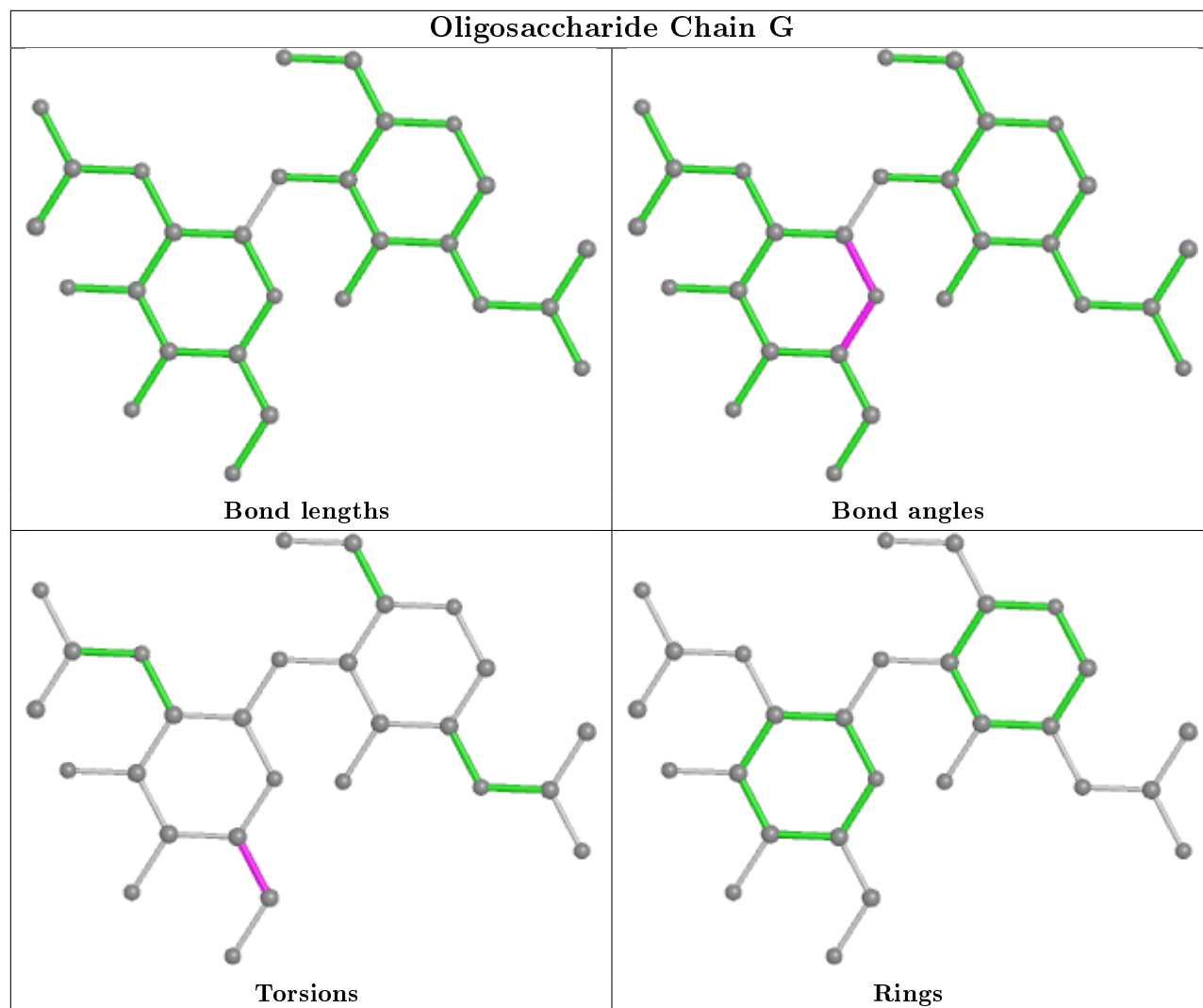
1 monomer is involved in 1 short contact:

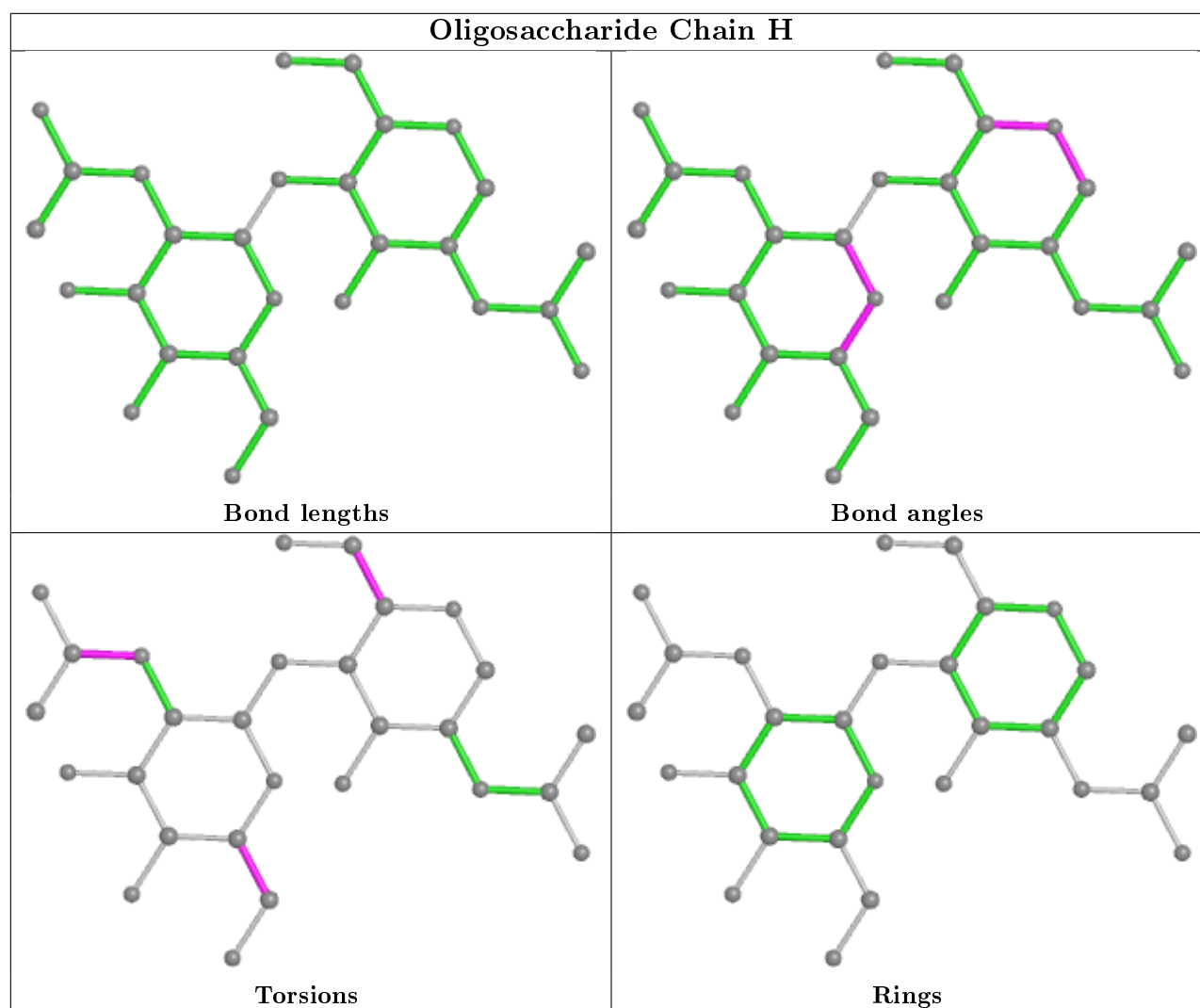
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2	NAG	1	0

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









## 5.6 Ligand geometry ⓘ

24 ligands 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	$\# Z  > 2$
4	NAG	B	1006	1	14,14,15	0.60	0	17,19,21	1.51	2 (11%)
6	SO4	B	1014	-	4,4,4	0.19	0	6,6,6	0.29	0
4	NAG	B	1011	1	14,14,15	0.32	0	17,19,21	1.46	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	B	1010	1	14,14,15	0.53	0	17,19,21	0.99	1 (5%)
6	SO4	A	1010	-	4,4,4	0.19	0	6,6,6	0.29	0
4	NAG	B	1007	1	14,14,15	0.27	0	17,19,21	0.56	0
6	SO4	A	1011	-	4,4,4	0.22	0	6,6,6	0.22	0
5	IDQ	A	1009	6	26,30,30	1.04	1 (3%)	33,42,42	1.61	4 (12%)
6	SO4	A	1012	5	4,4,4	0.61	0	6,6,6	0.75	0
4	NAG	A	1003	1	14,14,15	0.55	0	17,19,21	0.68	0
4	NAG	A	1006	1	14,14,15	0.45	0	17,19,21	0.88	1 (5%)
6	SO4	B	1016	5	4,4,4	0.19	0	6,6,6	0.55	0
4	NAG	B	1003	1	14,14,15	0.50	0	17,19,21	0.61	0
6	SO4	B	1015	-	4,4,4	0.20	0	6,6,6	0.50	0
5	IDQ	B	1012	6	26,30,30	1.15	1 (3%)	33,42,42	1.42	5 (15%)
6	SO4	B	1013	-	4,4,4	0.26	0	6,6,6	0.57	0
4	NAG	B	1009	1	14,14,15	0.59	0	17,19,21	0.63	0
6	SO4	A	1014	-	4,4,4	0.22	0	6,6,6	0.25	0
4	NAG	A	1008	1	14,14,15	1.35	2 (14%)	17,19,21	1.37	2 (11%)
4	NAG	A	1007	1	14,14,15	0.70	1 (7%)	17,19,21	0.74	0
6	SO4	A	1016	-	4,4,4	0.31	0	6,6,6	0.97	0
4	NAG	B	1008	1	14,14,15	0.49	0	17,19,21	0.77	1 (5%)
6	SO4	A	1015	-	4,4,4	0.32	0	6,6,6	0.22	0
6	SO4	A	1013	-	4,4,4	0.28	0	6,6,6	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1006	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1006	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1011	1	-	5/6/23/26	0/1/1/1
4	NAG	B	1009	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1003	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1010	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1008	1	-	0/6/23/26	0/1/1/1
5	IDQ	B	1012	6	-	2/10/10/10	0/4/4/4
4	NAG	B	1007	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1007	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1008	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1003	1	-	2/6/23/26	0/1/1/1
5	IDQ	A	1009	6	-	2/10/10/10	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1012	IDQ	C1-C	4.57	1.50	1.41
5	A	1009	IDQ	C1-C	4.07	1.49	1.41
4	A	1008	NAG	O5-C1	-3.71	1.37	1.43
4	A	1008	NAG	O7-C7	2.23	1.28	1.23
4	A	1007	NAG	O5-C1	-2.07	1.40	1.43

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1009	IDQ	C15-C14-N2	-5.33	104.35	112.63
4	B	1011	NAG	C2-N2-C7	4.26	128.97	122.90
5	A	1009	IDQ	C7-C6-N	-4.24	118.23	121.01
4	B	1006	NAG	C3-C4-C5	3.94	117.26	110.24
5	B	1012	IDQ	C15-C14-N2	-3.89	106.58	112.63

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1007	NAG	C4-C5-C6-O6
4	B	1009	NAG	O5-C5-C6-O6
4	A	1007	NAG	O5-C5-C6-O6
4	B	1009	NAG	C4-C5-C6-O6
4	B	1011	NAG	C8-C7-N2-C2

There are no ring outliers.

8 monomers are involved in 10 short contacts:

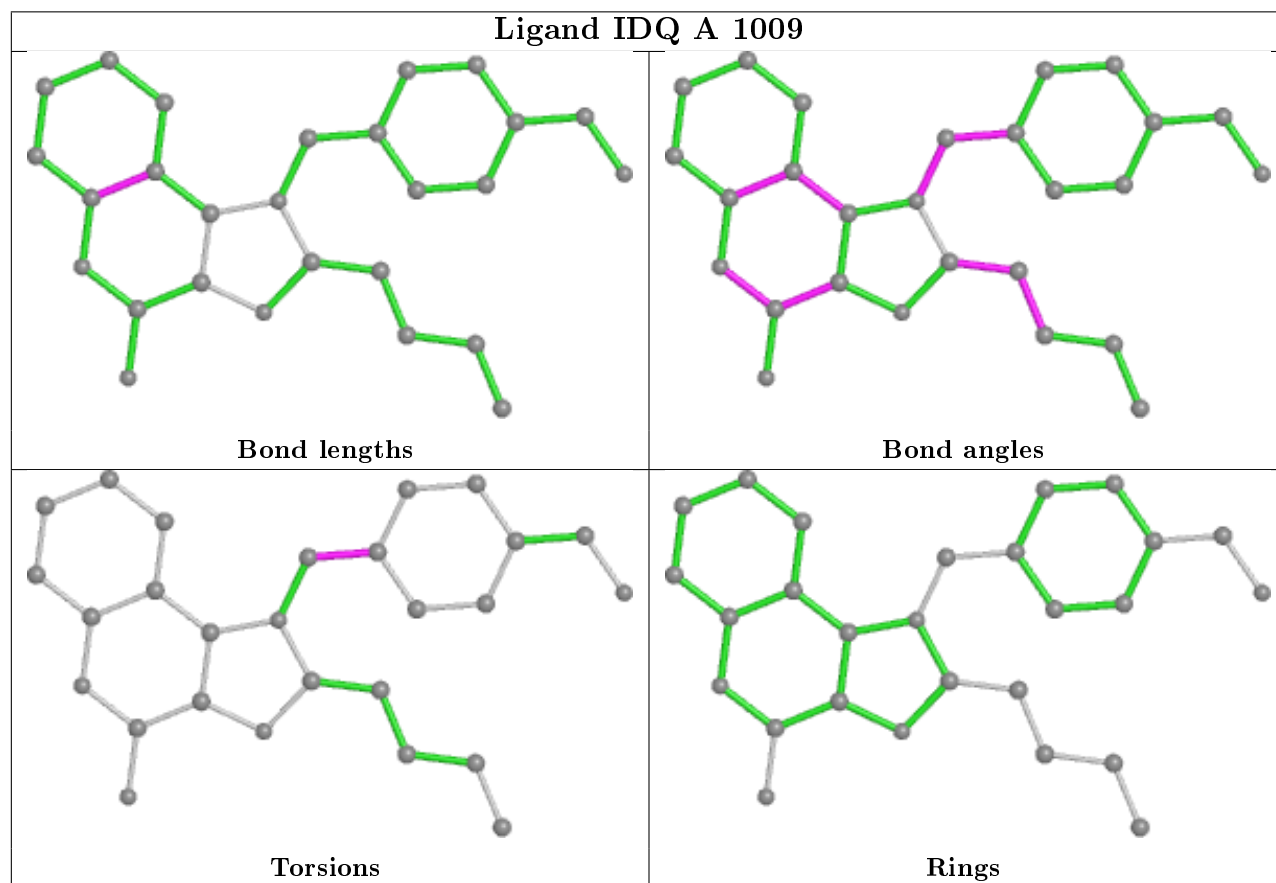
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1006	NAG	2	0
4	B	1011	NAG	1	0
4	B	1007	NAG	1	0
5	A	1009	IDQ	1	0
4	A	1003	NAG	1	0

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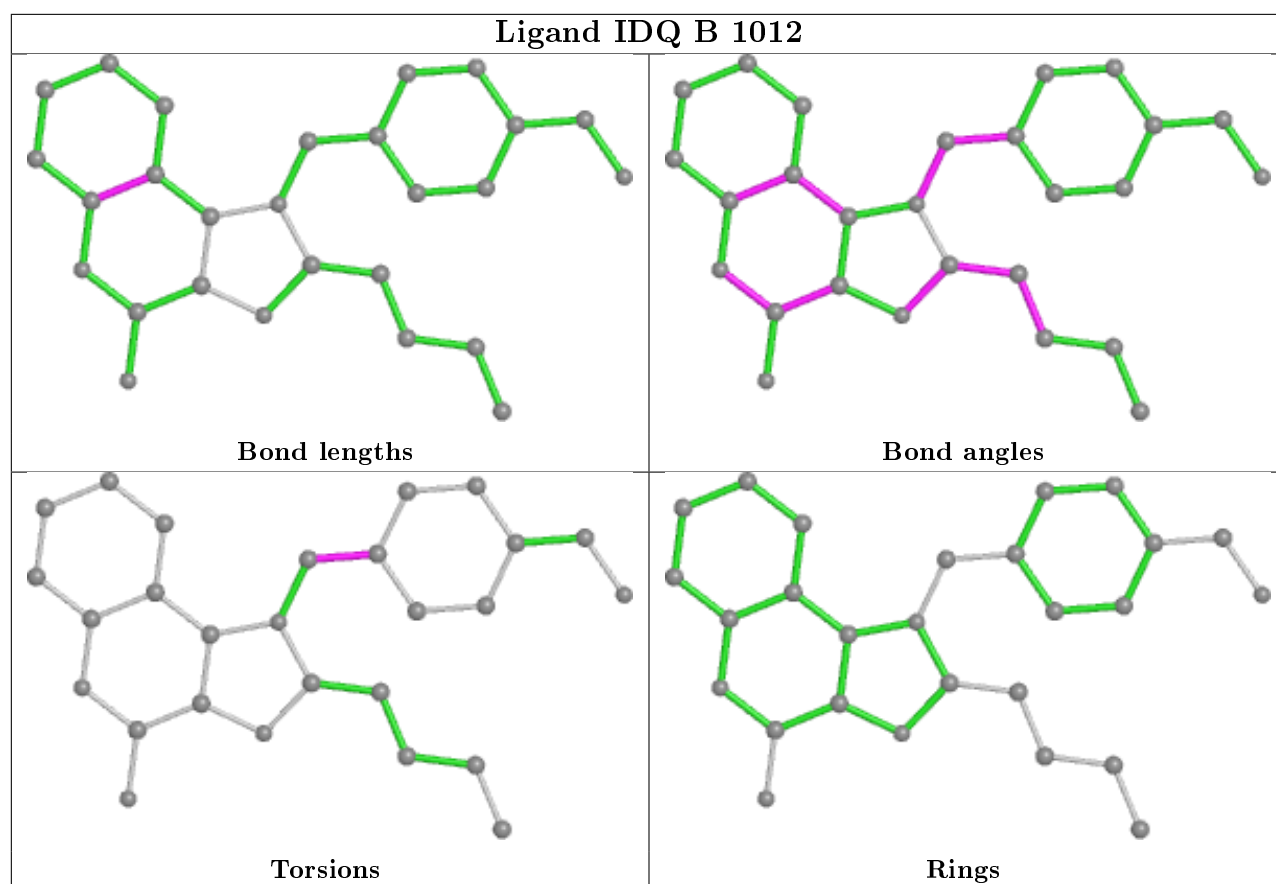
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1003	NAG	1	0
5	B	1012	IDQ	1	0
6	A	1013	SO4	2	0

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	773/823 (93%)	0.17	16 (2%) 63 66	39, 60, 82, 102	0
1	B	775/823 (94%)	-0.06	4 (0%) 91 91	31, 50, 69, 94	0
2	C	4/6 (66%)	-0.28	0 100 100	55, 56, 61, 65	0
2	D	4/6 (66%)	-0.25	0 100 100	57, 64, 65, 67	0
All	All	1556/1658 (93%)	0.05	20 (1%) 77 79	31, 54, 78, 102	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	723	ARG	3.4
1	A	566	ARG	3.3
1	A	40	LEU	3.2
1	A	45	ASN	3.0
1	A	42	VAL	2.9

### 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.

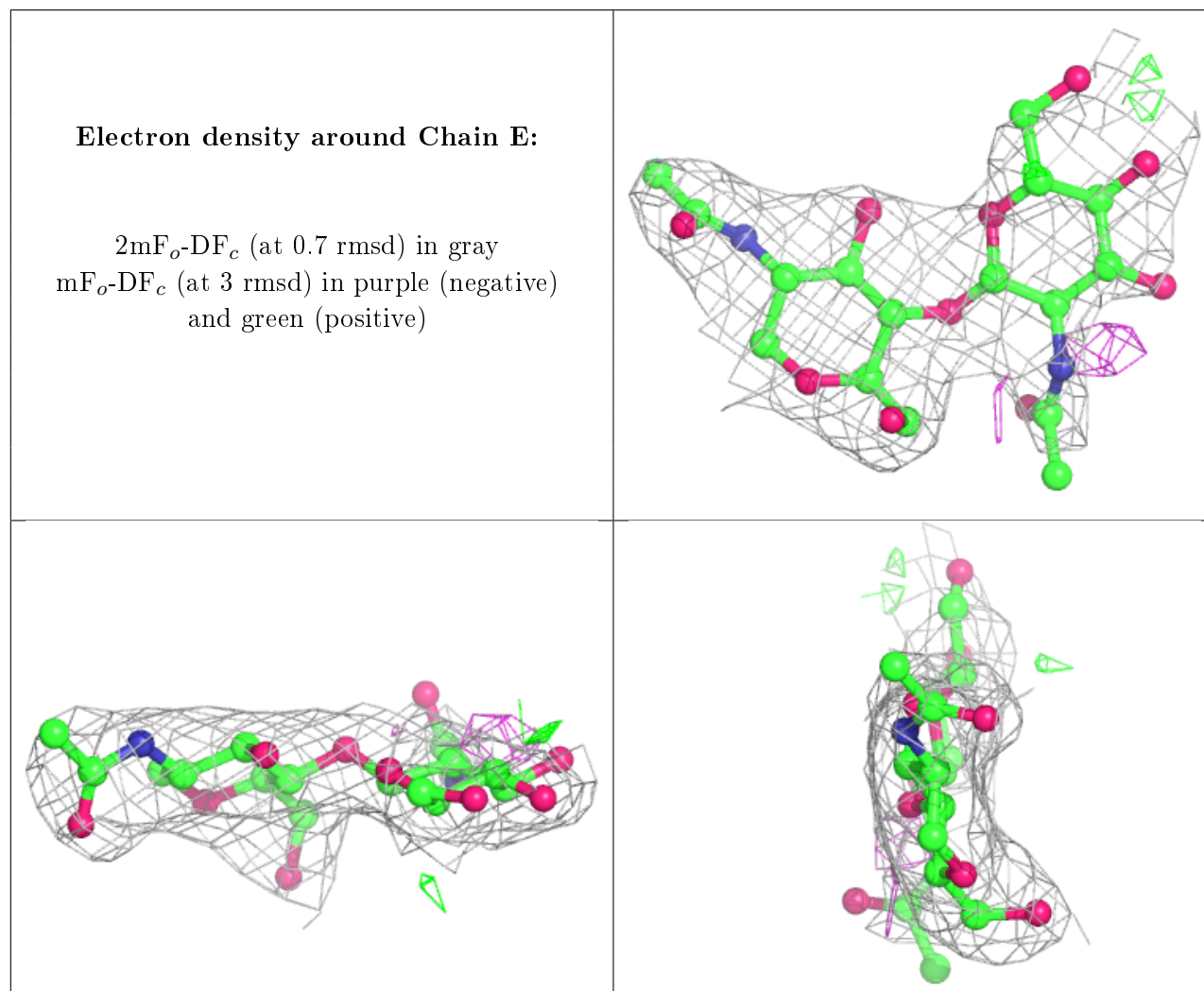
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	E	2	14/15	0.79	0.29	80,95,105,109	0
3	NAG	H	2	14/15	0.81	0.21	88,98,104,107	0

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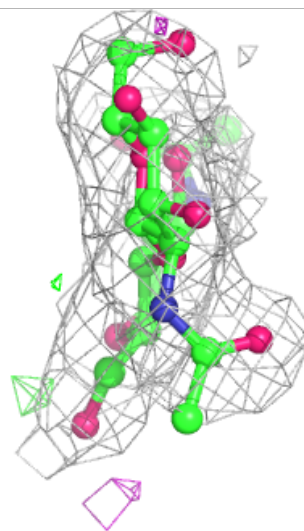
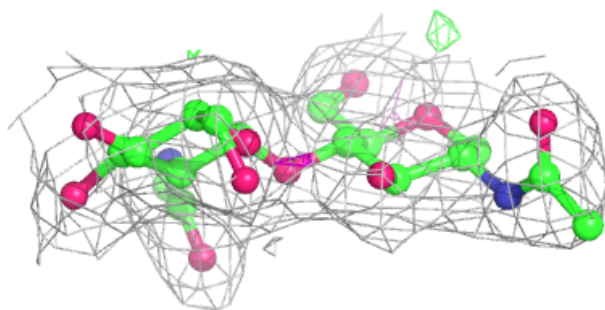
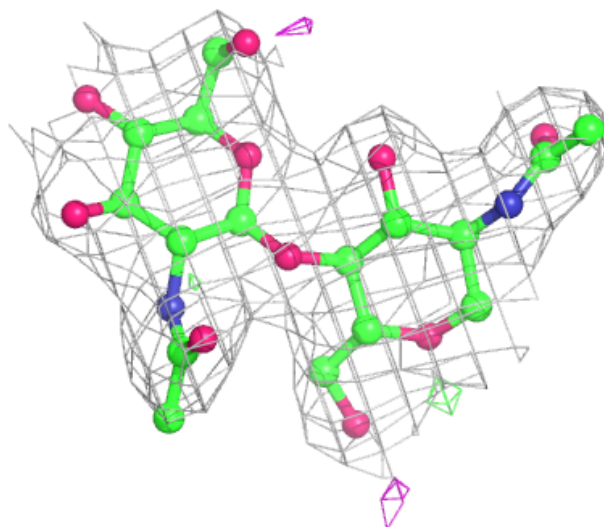
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	G	2	14/15	0.91	0.12	65,73,78,81	0
3	NAG	F	2	14/15	0.93	0.13	61,65,68,71	0
3	NAG	E	1	14/15	0.94	0.14	58,65,72,84	0
3	NAG	H	1	14/15	0.94	0.12	68,73,86,88	0
3	NAG	G	1	14/15	0.97	0.14	55,62,68,68	0
3	NAG	F	1	14/15	0.97	0.12	44,51,60,63	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.



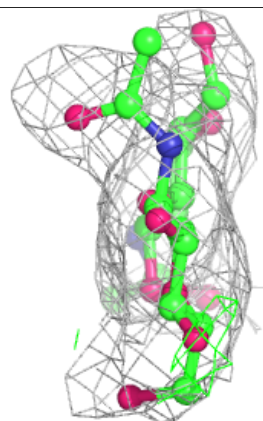
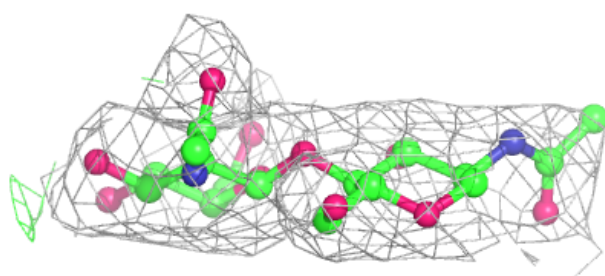
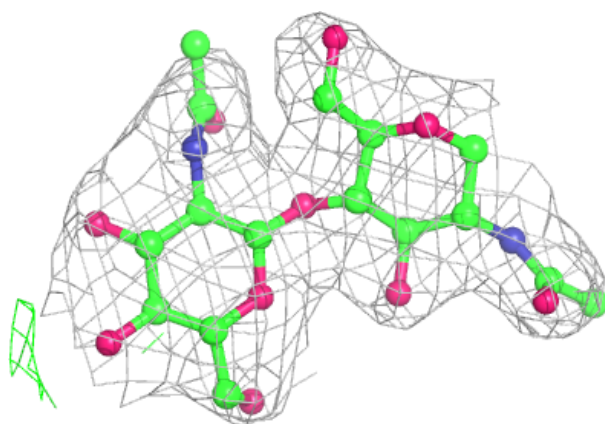
**Electron density around Chain F:**

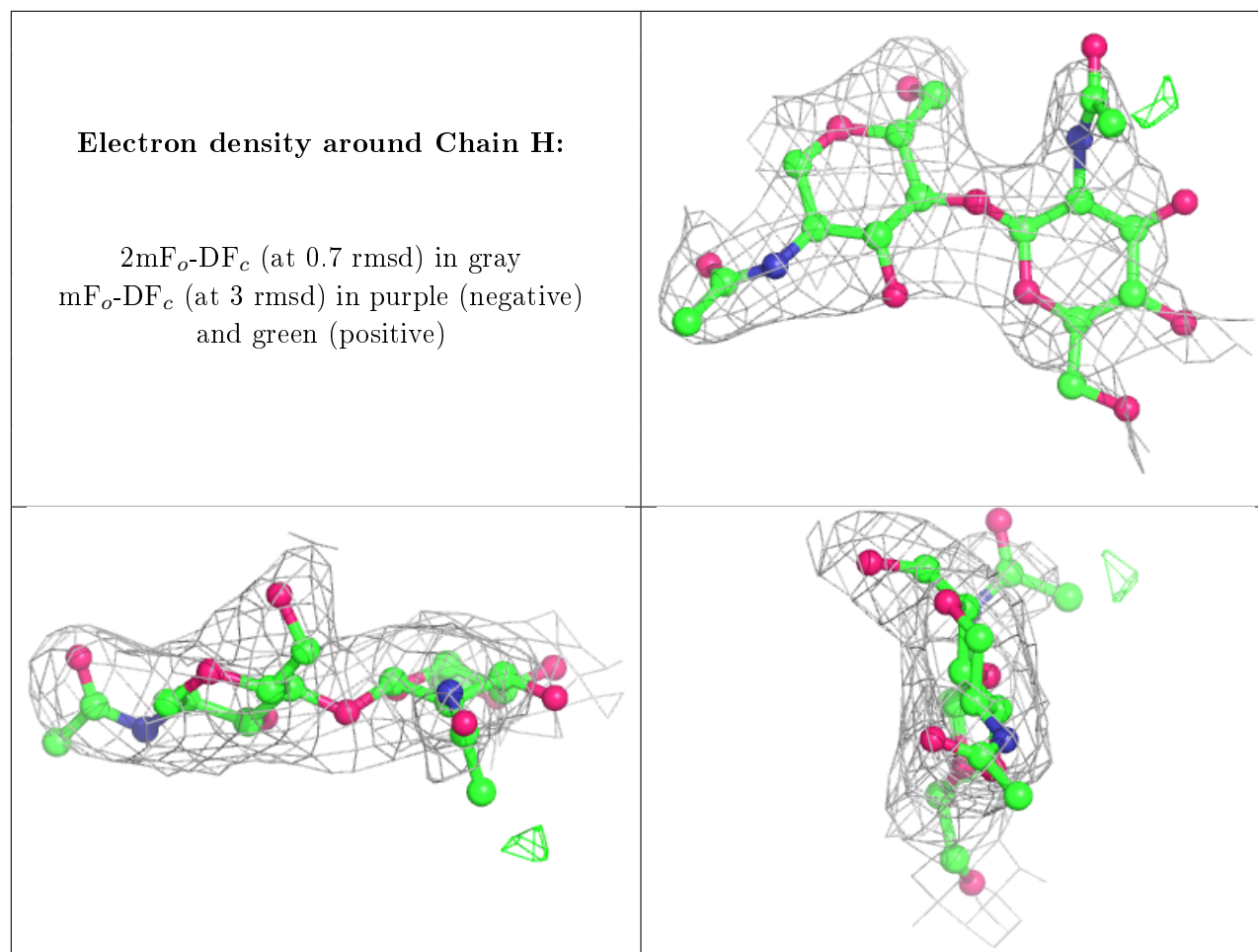
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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)





## 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.

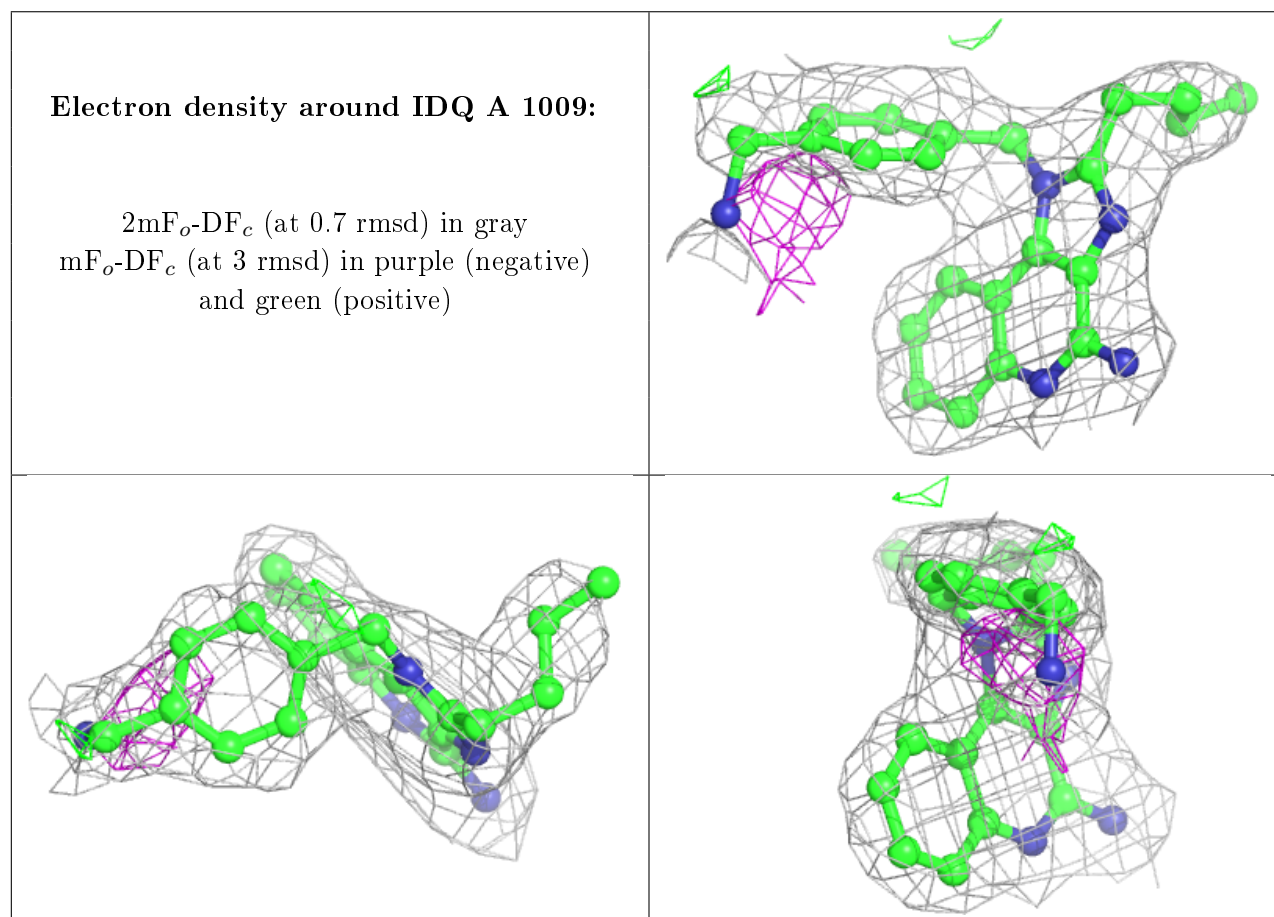
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	SO4	A	1012	5/5	0.82	0.23	79,82,98,105	0
4	NAG	A	1007	14/15	0.82	0.19	77,84,90,95	0
4	NAG	B	1006	14/15	0.85	0.19	63,69,72,79	0
4	NAG	B	1011	14/15	0.86	0.12	78,85,87,91	0
6	SO4	B	1015	5/5	0.86	0.32	61,75,94,101	0
4	NAG	B	1010	14/15	0.86	0.30	62,69,73,79	0
6	SO4	A	1016	5/5	0.86	0.23	67,68,72,96	0
4	NAG	A	1008	14/15	0.87	0.28	73,78,84,86	0
6	SO4	A	1015	5/5	0.87	0.19	71,74,92,99	0
4	NAG	B	1009	14/15	0.88	0.18	63,69,80,81	0
6	SO4	A	1014	5/5	0.88	0.28	80,81,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SO4	B	1016	5/5	0.89	0.26	83,95,103,111	0
4	NAG	A	1006	14/15	0.91	0.16	67,75,79,86	0
4	NAG	B	1008	14/15	0.92	0.13	51,58,64,65	0
6	SO4	A	1011	5/5	0.92	0.19	68,77,87,93	0
6	SO4	B	1013	5/5	0.93	0.12	62,67,80,83	0
4	NAG	B	1007	14/15	0.93	0.15	60,68,74,76	0
6	SO4	B	1014	5/5	0.94	0.25	73,85,90,95	0
6	SO4	A	1010	5/5	0.94	0.11	60,72,77,86	0
5	IDQ	A	1009	27/27	0.94	0.22	43,48,60,84	0
5	IDQ	B	1012	27/27	0.95	0.16	49,57,62,83	0
4	NAG	B	1003	14/15	0.95	0.15	43,47,51,54	0
4	NAG	A	1003	14/15	0.95	0.15	46,52,58,59	0
6	SO4	A	1013	5/5	0.97	0.18	58,60,77,91	0

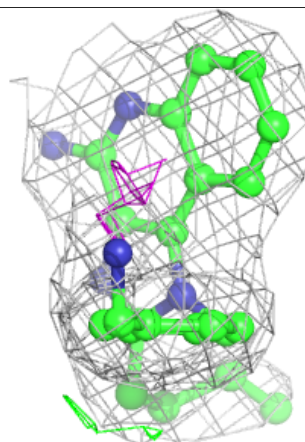
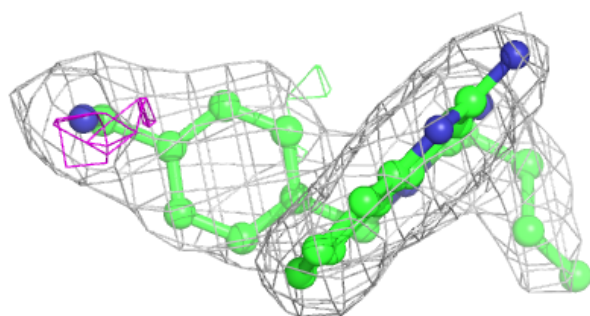
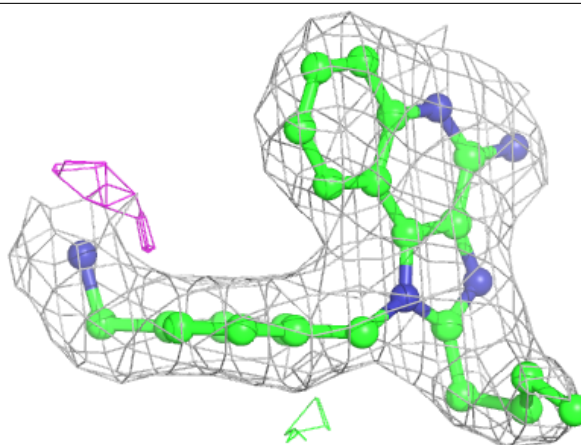
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





**Electron density around IDQ B 1012:**

$2mF_o-DF_c$  (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.