



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2025 – 12:17 am GMT

PDB ID : 9H8U  
Title : FAD-dependent oxidase sorD with sorbicillin bound  
Authors : Tjallinks, G.; Mattevi, A.  
Deposited on : 2024-10-29  
Resolution : 3.00 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>.

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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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

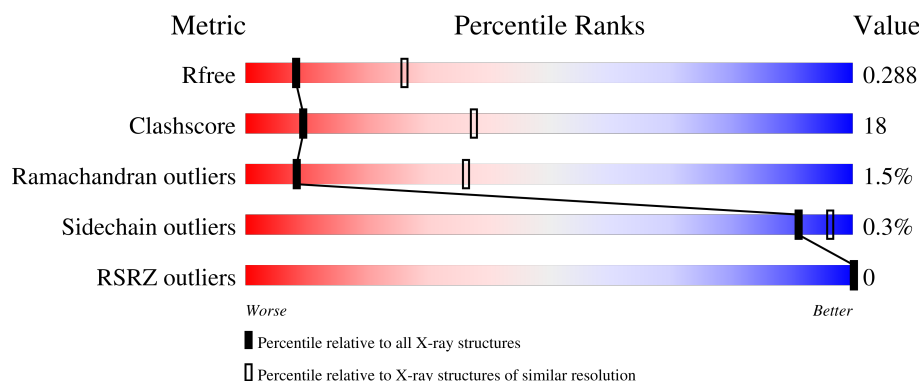
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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.




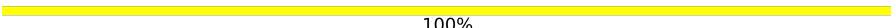
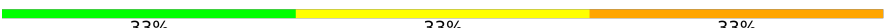
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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 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	471	<div> <div style="width: 72%; background-color: green;"></div> <div style="width: 27%; background-color: yellow;"></div> <div style="width: 1%; background-color: grey;"></div> </div> <div>72% 27% ..</div>
1	B	471	<div> <div style="width: 61%; background-color: green;"></div> <div style="width: 36%; background-color: yellow;"></div> <div style="width: 3%; background-color: grey;"></div> </div> <div>61% 36% ..</div>
2	C	5	<div> <div style="width: 40%; background-color: yellow;"></div> <div style="width: 60%; background-color: orange;"></div> </div> <div>40% 60%</div>
3	D	5	<div> <div style="width: 80%; background-color: yellow;"></div> <div style="width: 20%; background-color: orange;"></div> </div> <div>80% 20%</div>
4	E	4	<div> <div style="width: 50%; background-color: yellow;"></div> <div style="width: 50%; background-color: orange;"></div> </div> <div>50% 50%</div>

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Mol	Chain	Length	Quality of chain
5	F	3	 67% 33%
5	G	3	 100%
5	H	3	 33% 33% 33%

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7514 atoms, of which 23 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 FAD-linked oxidoreductase sorD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	0
			3501	2211	588	694	8			
1	B	467	Total	C	N	O	S	0	0	0
			3501	2211	583	699	8			

There are 8 discrepancies between the modelled and reference sequences:

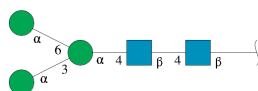
Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ASN	ASP	conflict	UNP B6HNC6
A	291	THR	ALA	conflict	UNP B6HNC6
A	432	PRO	SER	conflict	UNP B6HNC6
A	435	GLU	LYS	conflict	UNP B6HNC6
B	103	ASN	ASP	conflict	UNP B6HNC6
B	291	THR	ALA	conflict	UNP B6HNC6
B	432	PRO	SER	conflict	UNP B6HNC6
B	435	GLU	LYS	conflict	UNP B6HNC6

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



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

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



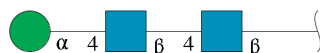
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	5	Total	C	H	N	O	0	0	0
			72	34	11	2	25			

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



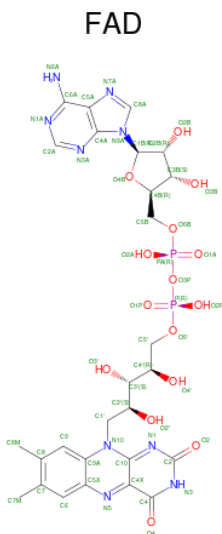
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	4	Total	C	H	N	O	0	0	0
			63	28	12	2	21			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



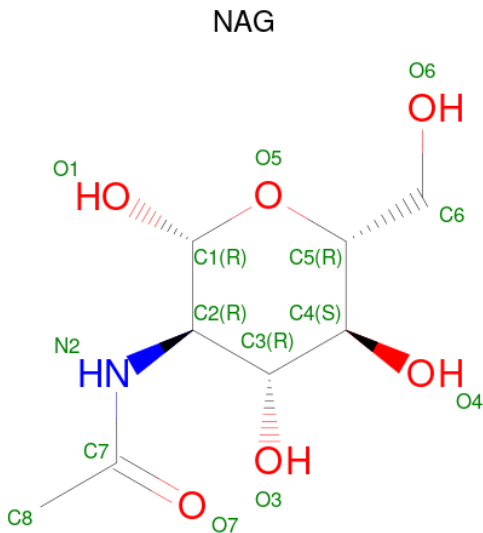
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	H	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
6	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $\text{C}_8\text{H}_{15}\text{NO}_6$ ).



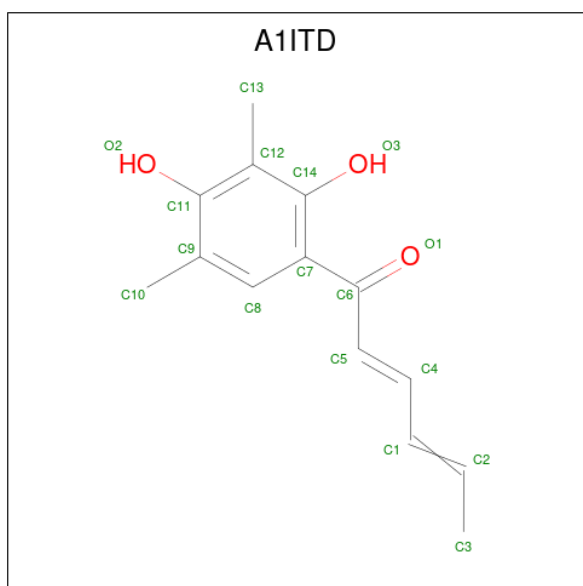
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 8 is (2 {Z})-1-[3,5-dimethyl-2,4-bis(oxidanyl)phenyl]hexa-2,4-dien-1-one (three-letter code: A1ITD) (formula: C<sub>14</sub>H<sub>16</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			13	10	3		
8	B	1	Total	C	O	0	0
			15	12	3		

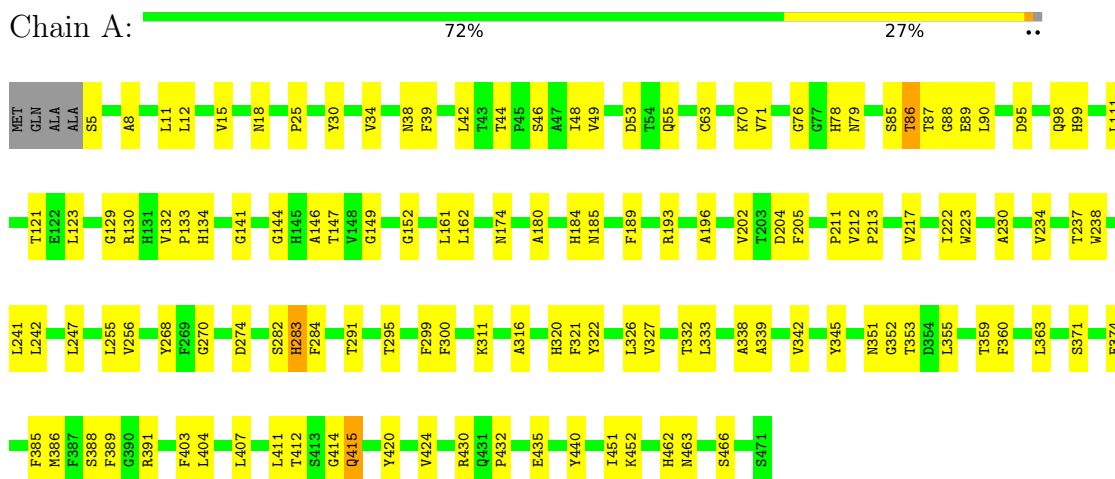
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	8	Total	O	0	0
			8	8		
9	B	1	Total	O	0	0
			1	1		

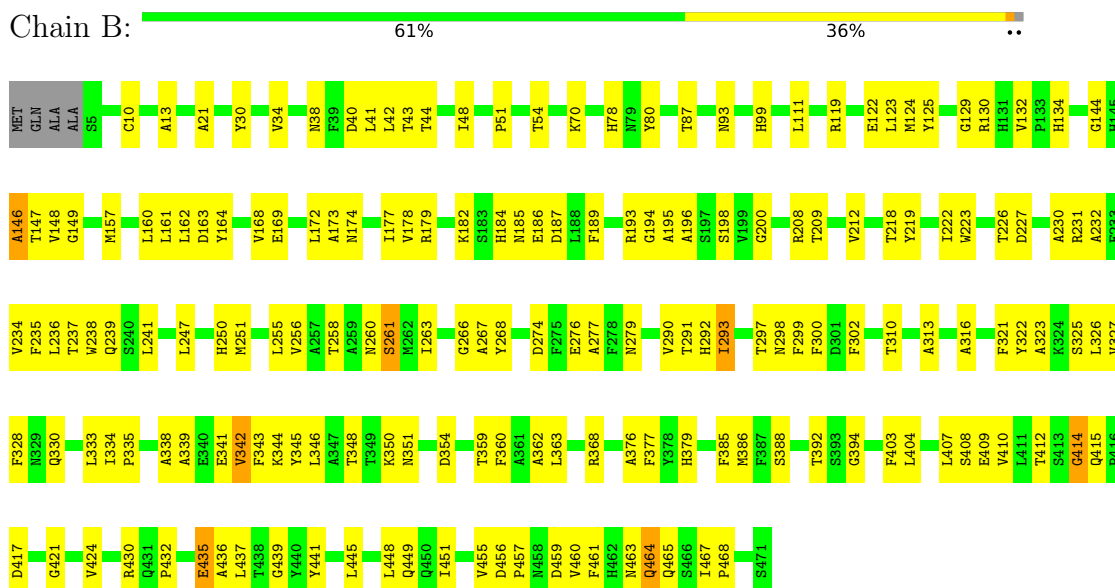
### 3 Residue-property plots

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: FAD-linked oxidoreductase sorD



#### • Molecule 1: FAD-linked oxidoreductase sorD




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



Chain C:  40% 60%

NAG1  
NAG2  
MAN3  
MAN4  
MAN5

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

Chain D:  80% 20%

NAG1  
NAG2  
MAN3  
MAN4  
MAN5

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

Chain E:  50% 50%

NAG1  
NAG2  
MAN3  
MAN4

- Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  67% 33%

NAG1  
NAG2  
MAN3

- Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%

NAG1  
NAG2  
MAN3

- Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  33% 33% 33%

NAG1  
NAG2  
MAN3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.56Å 90.56Å 290.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.85 – 3.00 76.85 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.6 (76.85-3.00) 96.6 (76.85-3.00)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.20_4459, PHENIX 1.20_4459	Depositor
R, $R_{free}$	0.206 , 0.286 0.210 , 0.288	Depositor DCC
$R_{free}$ test set	1276 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	77.6	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 42.4	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	0.94	EDS
Total number of atoms	7514	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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: MAN, NAG, FAD, A1ITD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.54	0/3589	0.74	0/4904
1	B	0.55	1/3589 (0.0%)	0.73	2/4905 (0.0%)
All	All	0.55	1/7178 (0.0%)	0.73	2/9809 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	435	GLU	CG-CD	5.74	1.60	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	163	ASP	CB-CG-OD1	5.39	123.15	118.30
1	B	437	LEU	CA-CB-CG	-5.38	102.93	115.30

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	3501	0	3284	93	0
1	B	3501	0	3276	155	0
2	C	61	0	52	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	61	11	52	1	0
4	E	51	12	44	4	0
5	F	39	0	34	1	0
5	G	39	0	34	1	0
5	H	39	0	34	2	0
6	A	53	0	30	7	0
6	B	53	0	30	6	0
7	A	28	0	26	1	0
7	B	28	0	26	0	0
8	A	13	0	0	0	0
8	B	15	0	0	0	0
9	A	8	0	0	1	0
9	B	1	0	0	1	0
All	All	7491	23	6922	253	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 18.

The worst 5 of 253 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:194:GLY:HA3	1:B:376:ALA:HB3	1.30	1.13
1:A:256:VAL:HG22	1:A:359:THR:HG23	1.40	1.03
1:B:70:LYS:NZ	1:B:459:ASP:O	2.06	0.87
1:B:344:LYS:O	1:B:348:THR:OG1	1.91	0.87
1:A:86:THR:HG22	1:A:89:GLU:HG3	1.57	0.85

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	465/471 (99%)	426 (92%)	34 (7%)	5 (1%)	12	44
1	B	465/471 (99%)	389 (84%)	67 (14%)	9 (2%)	6	31
All	All	930/942 (99%)	815 (88%)	101 (11%)	14 (2%)	8	36

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	41	LEU
1	B	464	GLN
1	A	18	ASN
1	B	185	ASN
1	B	350	LYS

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	366/376 (97%)	364 (100%)	2 (0%)	86	94
1	B	367/376 (98%)	367 (100%)	0	100	100
All	All	733/752 (98%)	731 (100%)	2 (0%)	91	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	204	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	450	GLN
1	B	27	GLN
1	B	260	ASN

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Mol	Chain	Res	Type
1	B	464	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

23 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	0.91	1 (7%)	17,19,21	1.16	1 (5%)
2	NAG	C	2	2	14,14,15	1.45	1 (7%)	17,19,21	1.28	1 (5%)
2	MAN	C	3	2	11,11,12	1.56	1 (9%)	15,15,17	1.81	4 (26%)
2	MAN	C	4	2	11,11,12	1.31	2 (18%)	15,15,17	2.61	4 (26%)
2	MAN	C	5	2	11,11,12	2.16	4 (36%)	15,15,17	1.69	2 (13%)
3	NAG	D	1	1,3	14,14,15	1.53	1 (7%)	17,19,21	0.83	0
3	NAG	D	2	3	14,14,15	1.16	1 (7%)	17,19,21	0.79	0
3	MAN	D	3	3	11,11,12	1.23	1 (9%)	15,15,17	1.07	1 (6%)
3	MAN	D	4	3	11,11,12	1.55	2 (18%)	15,15,17	1.18	1 (6%)
3	MAN	D	5	3	11,11,12	3.33	9 (81%)	15,15,17	1.61	3 (20%)
4	NAG	E	1	1,4	14,14,15	0.40	0	17,19,21	0.93	1 (5%)
4	NAG	E	2	4	14,14,15	1.35	1 (7%)	17,19,21	2.16	2 (11%)
4	MAN	E	3	4	11,11,12	1.13	1 (9%)	15,15,17	1.41	2 (13%)
4	MAN	E	4	4	12,12,12	3.24	9 (75%)	17,17,17	2.71	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	F	1	1,5	14,14,15	0.46	0	17,19,21	1.52	1 (5%)
5	NAG	F	2	5	14,14,15	1.34	2 (14%)	17,19,21	0.92	1 (5%)
5	MAN	F	3	5	11,11,12	2.53	6 (54%)	15,15,17	1.34	3 (20%)
5	NAG	G	1	1,5	14,14,15	0.57	0	17,19,21	0.47	0
5	NAG	G	2	5	14,14,15	0.93	1 (7%)	17,19,21	0.62	0
5	MAN	G	3	5	11,11,12	1.66	4 (36%)	15,15,17	1.17	2 (13%)
5	NAG	H	1	1,5	14,14,15	0.29	0	17,19,21	0.90	1 (5%)
5	NAG	H	2	5	14,14,15	0.59	0	17,19,21	0.60	0
5	MAN	H	3	5	11,11,12	1.04	1 (9%)	15,15,17	1.53	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
2	MAN	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
2	MAN	C	5	2	-	2/2/19/22	1/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	1/6/23/26	0/1/1/1
3	MAN	D	3	3	-	2/2/19/22	0/1/1/1
3	MAN	D	4	3	-	1/2/19/22	0/1/1/1
3	MAN	D	5	3	-	2/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	4/6/23/26	0/1/1/1
4	MAN	E	3	4	-	0/2/19/22	1/1/1/1
4	MAN	E	4	4	-	2/2/22/22	0/1/1/1
5	NAG	F	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1
5	MAN	F	3	5	-	1/2/19/22	0/1/1/1
5	NAG	G	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	MAN	G	3	5	-	2/2/19/22	0/1/1/1
5	NAG	H	1	1,5	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
5	MAN	H	3	5	-	2/2/19/22	1/1/1/1

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	5	MAN	O5-C1	6.54	1.54	1.43
4	E	4	MAN	C1-C2	5.52	1.65	1.52
4	E	4	MAN	O5-C5	5.44	1.57	1.44
3	D	1	NAG	O5-C1	-5.33	1.35	1.43
2	C	2	NAG	O5-C1	5.32	1.52	1.43

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	4	MAN	O1-C1-O5	9.20	137.98	110.38
4	E	2	NAG	C1-O5-C5	7.76	122.71	112.19
2	C	4	MAN	C1-C2-C3	-7.19	100.82	109.67
5	F	1	NAG	C1-O5-C5	5.46	119.58	112.19
2	C	5	MAN	C1-O5-C5	5.00	118.97	112.19

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	2	NAG	C3-C2-N2-C7
2	C	2	NAG	C4-C5-C6-O6
5	H	3	MAN	C4-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6

All (3) ring outliers are listed below:

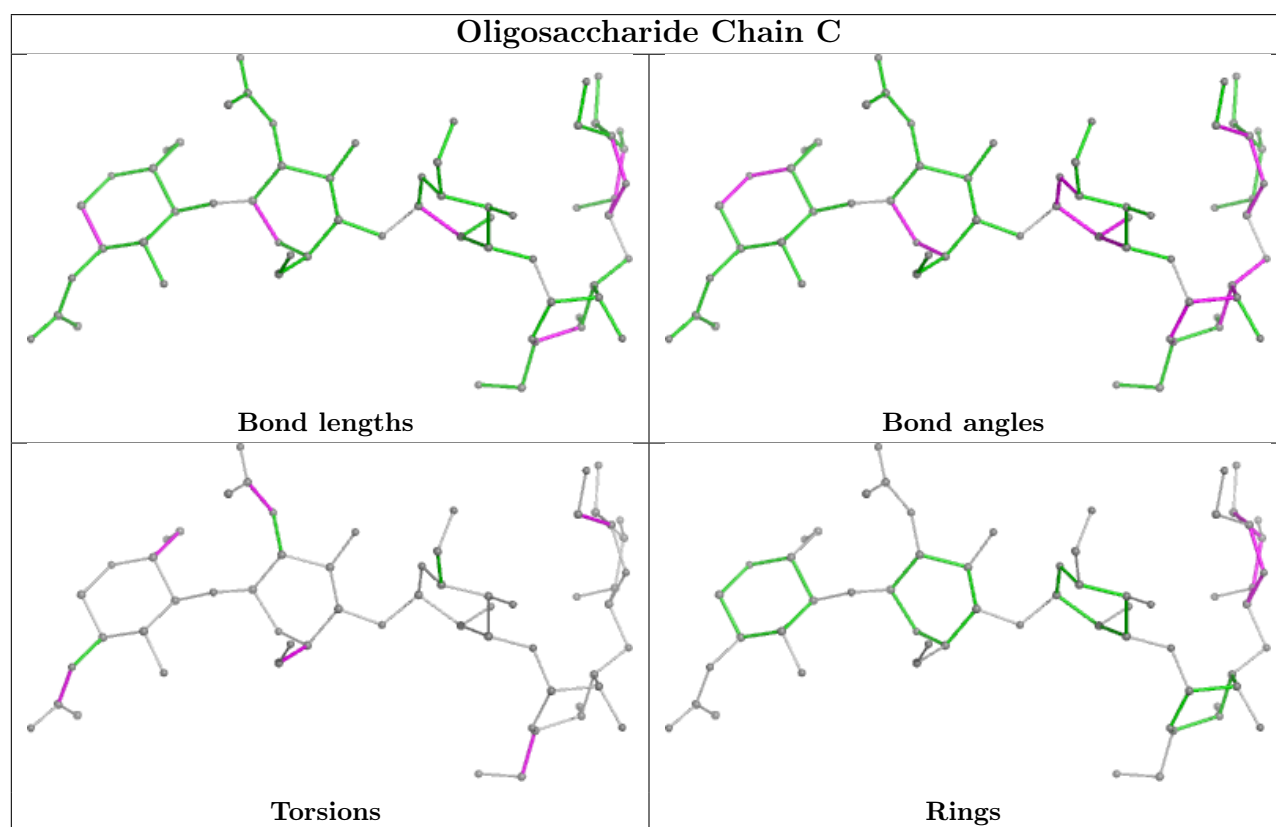
Mol	Chain	Res	Type	Atoms
2	C	5	MAN	C1-C2-C3-C4-C5-O5
4	E	3	MAN	C1-C2-C3-C4-C5-O5
5	H	3	MAN	C1-C2-C3-C4-C5-O5

9 monomers are involved in 11 short contacts:

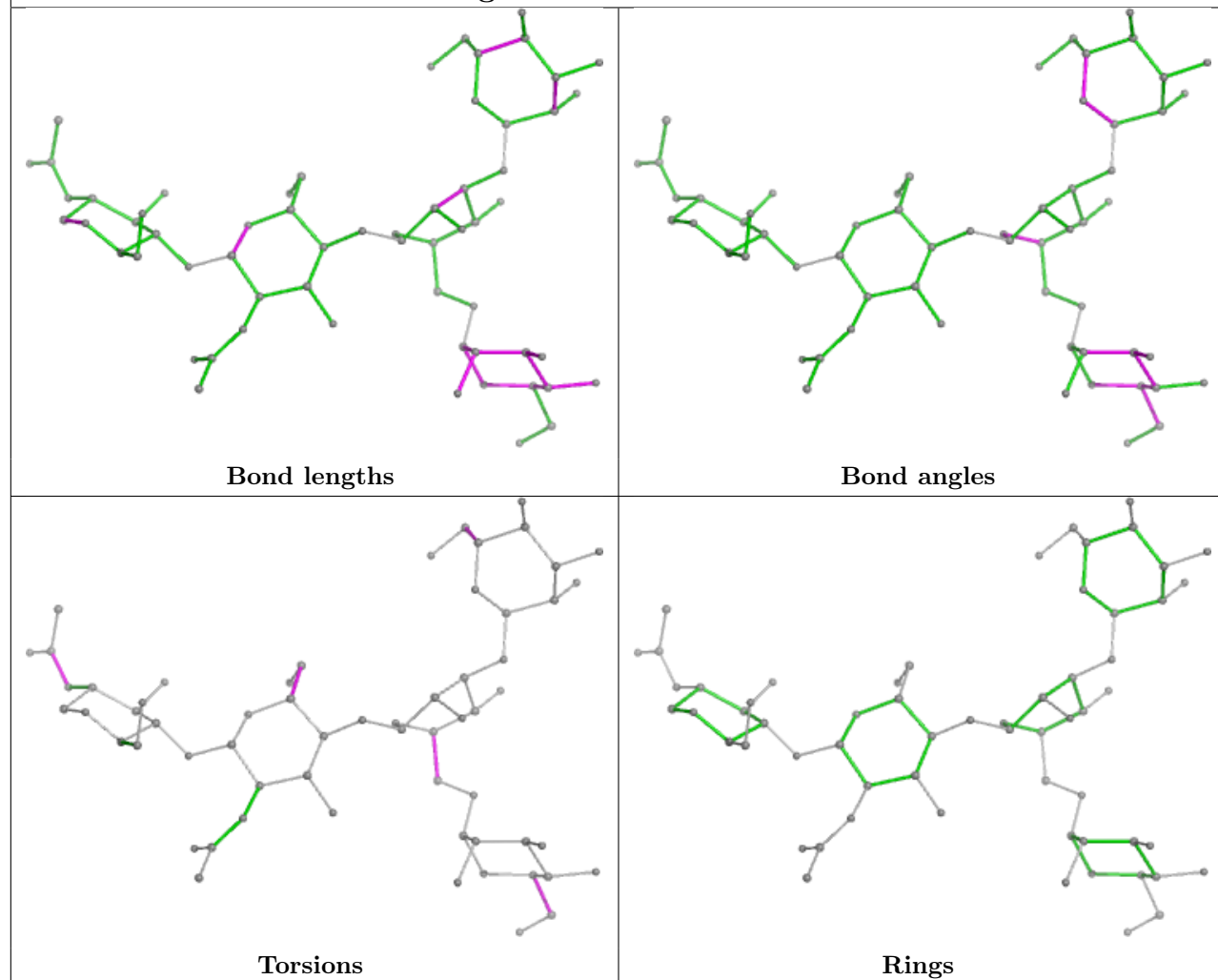


Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1	NAG	1	0
4	E	1	NAG	4	0
5	H	1	NAG	2	0
2	C	3	MAN	1	0
4	E	2	NAG	1	0
2	C	1	NAG	1	0
5	G	1	NAG	1	0
3	D	1	NAG	1	0
2	C	2	NAG	2	0

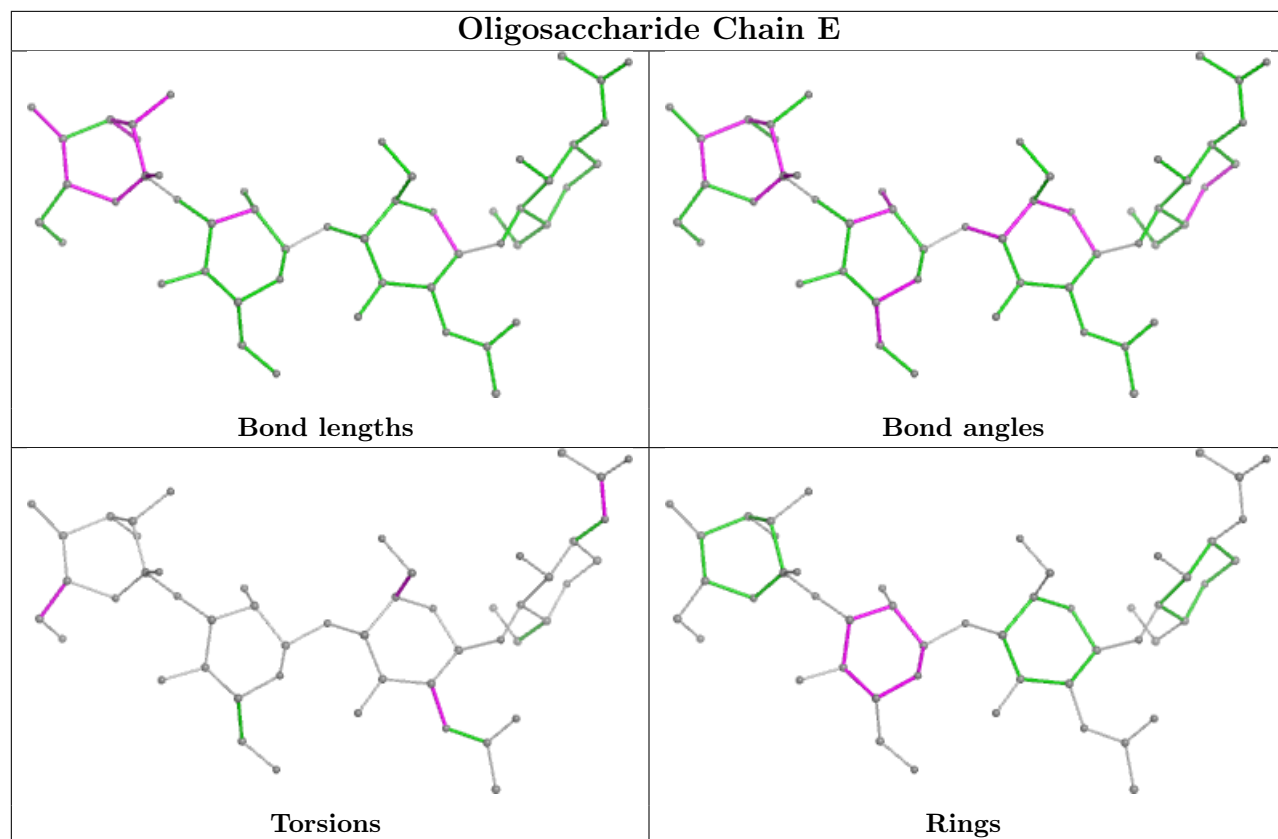
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



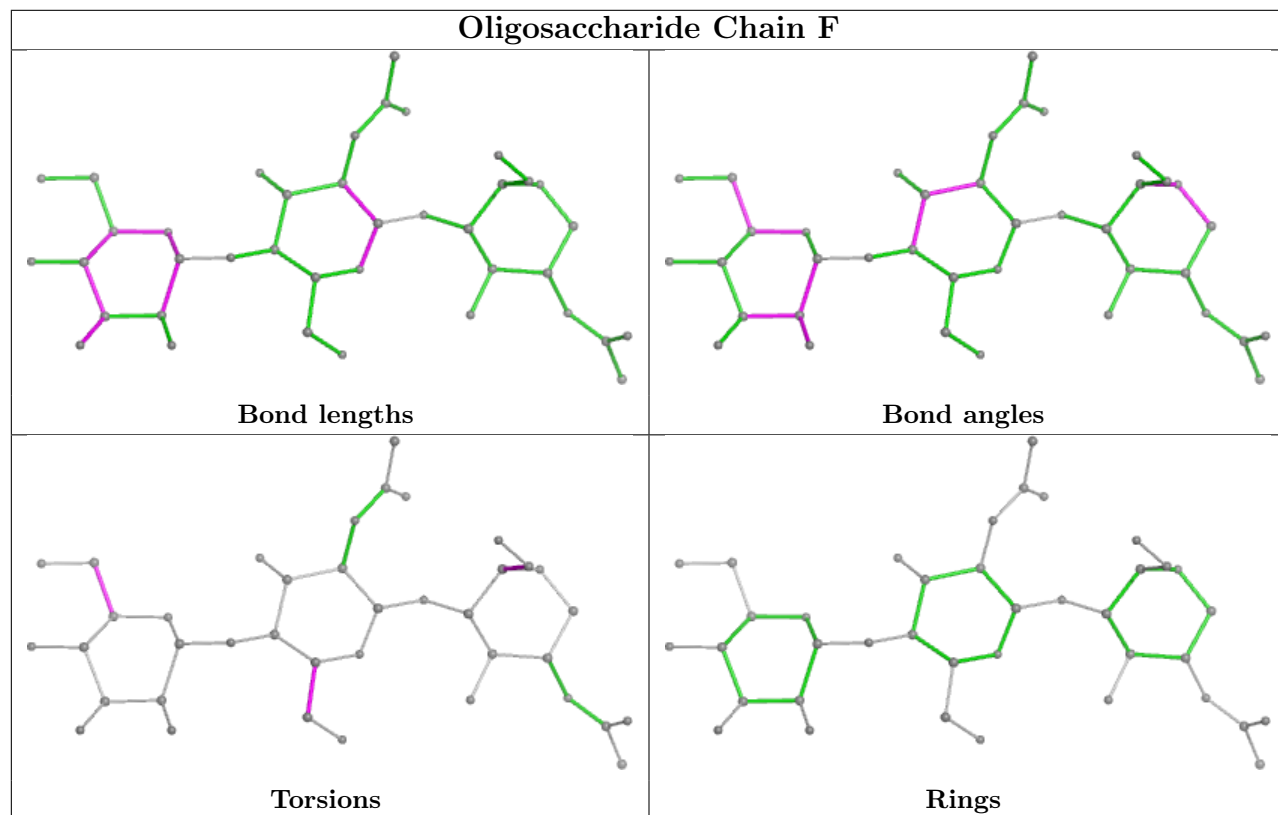
## Oligosaccharide Chain D



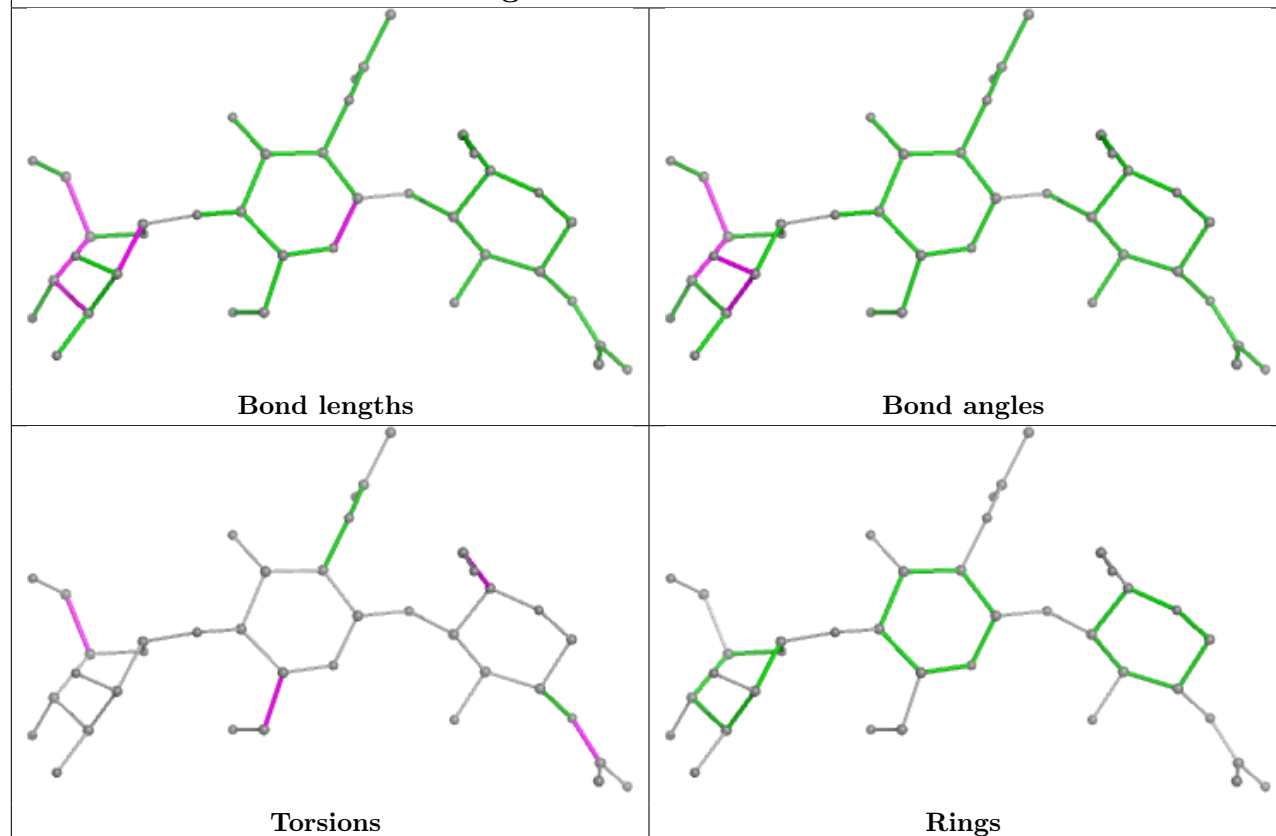
## Oligosaccharide Chain E



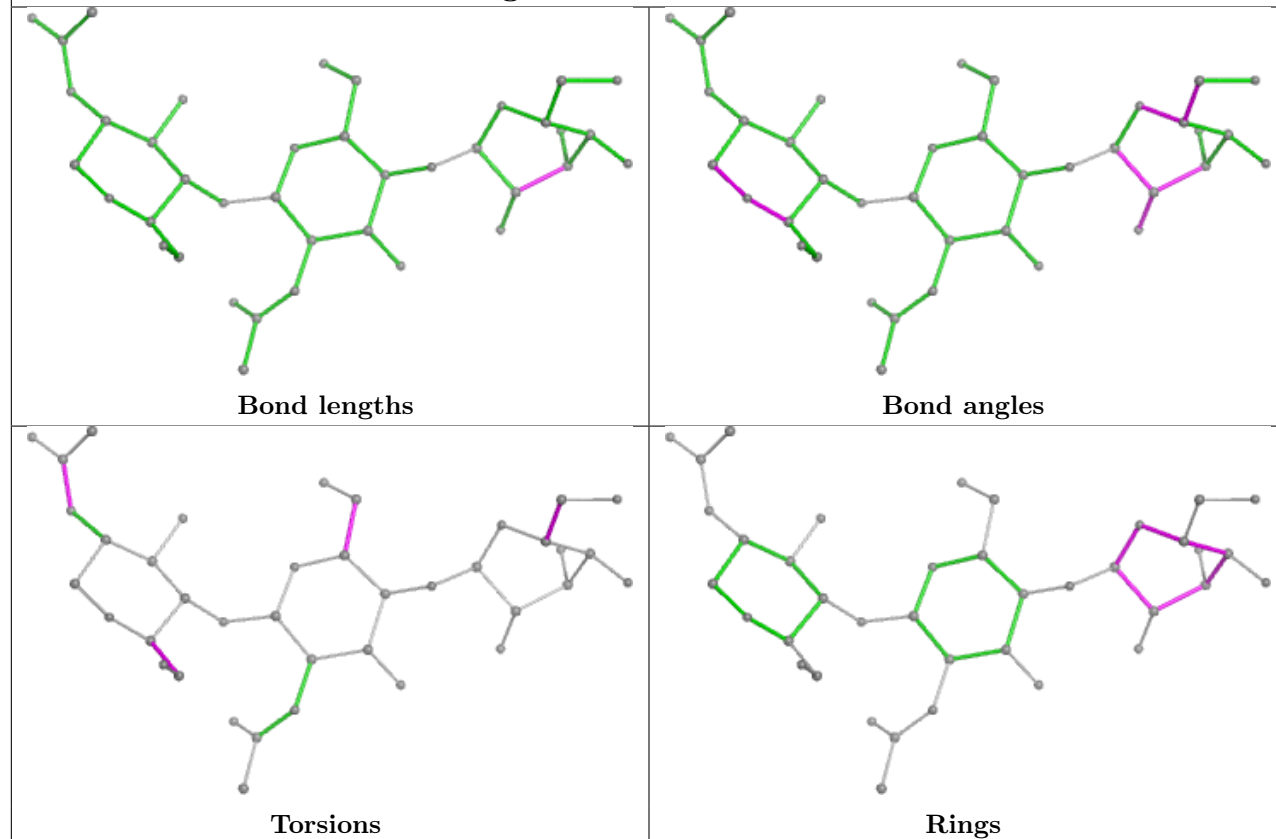
## Oligosaccharide Chain F



## Oligosaccharide Chain G



## Oligosaccharide Chain H



## 5.6 Ligand geometry

8 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
7	NAG	B	503	1	14,14,15	0.70	0	17,19,21	0.56	0
7	NAG	B	504	1	14,14,15	1.27	2 (14%)	17,19,21	1.53	1 (5%)
7	NAG	A	502	1	14,14,15	0.24	0	17,19,21	0.82	1 (5%)
8	A1ITD	A	503	-	13,13,17	0.65	0	18,19,23	0.55	0
7	NAG	A	504	1	14,14,15	0.59	0	17,19,21	0.54	0
6	FAD	B	501	-	53,58,58	0.48	0	68,89,89	0.70	1 (1%)
6	FAD	A	501	-	53,58,58	0.66	1 (1%)	68,89,89	0.69	2 (2%)
8	A1ITD	B	502	-	15,15,17	0.89	1 (6%)	20,21,23	0.68	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
7	NAG	B	503	1	-	3/6/23/26	0/1/1/1
7	NAG	B	504	1	-	0/6/23/26	0/1/1/1
7	NAG	A	502	1	-	4/6/23/26	0/1/1/1
8	A1ITD	A	503	-	-	0/4/4/9	0/1/1/1
7	NAG	A	504	1	-	2/6/23/26	0/1/1/1
6	FAD	B	501	-	-	11/30/50/50	0/6/6/6
6	FAD	A	501	-	-	4/30/50/50	0/6/6/6
8	A1ITD	B	502	-	-	0/7/7/9	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	504	NAG	O5-C1	3.69	1.49	1.43
7	B	504	NAG	C1-C2	2.79	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	501	FAD	P-O1P	-2.53	1.41	1.50
8	B	502	A1ITD	C1-C4	-2.03	1.41	1.49

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	504	NAG	C1-O5-C5	5.76	119.99	112.19
6	A	501	FAD	C4'-C3'-C2'	2.58	118.72	113.36
6	B	501	FAD	C5A-C6A-N6A	2.34	123.90	120.35
7	A	502	NAG	C1-O5-C5	2.25	115.25	112.19
6	A	501	FAD	C5A-C6A-N6A	2.09	123.53	120.35

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	501	FAD	C3'-C4'-C5'-O5'
6	B	501	FAD	O4'-C4'-C5'-O5'
6	B	501	FAD	C5'-O5'-P-O1P
6	B	501	FAD	C5'-O5'-P-O3P
7	A	502	NAG	O5-C5-C6-O6

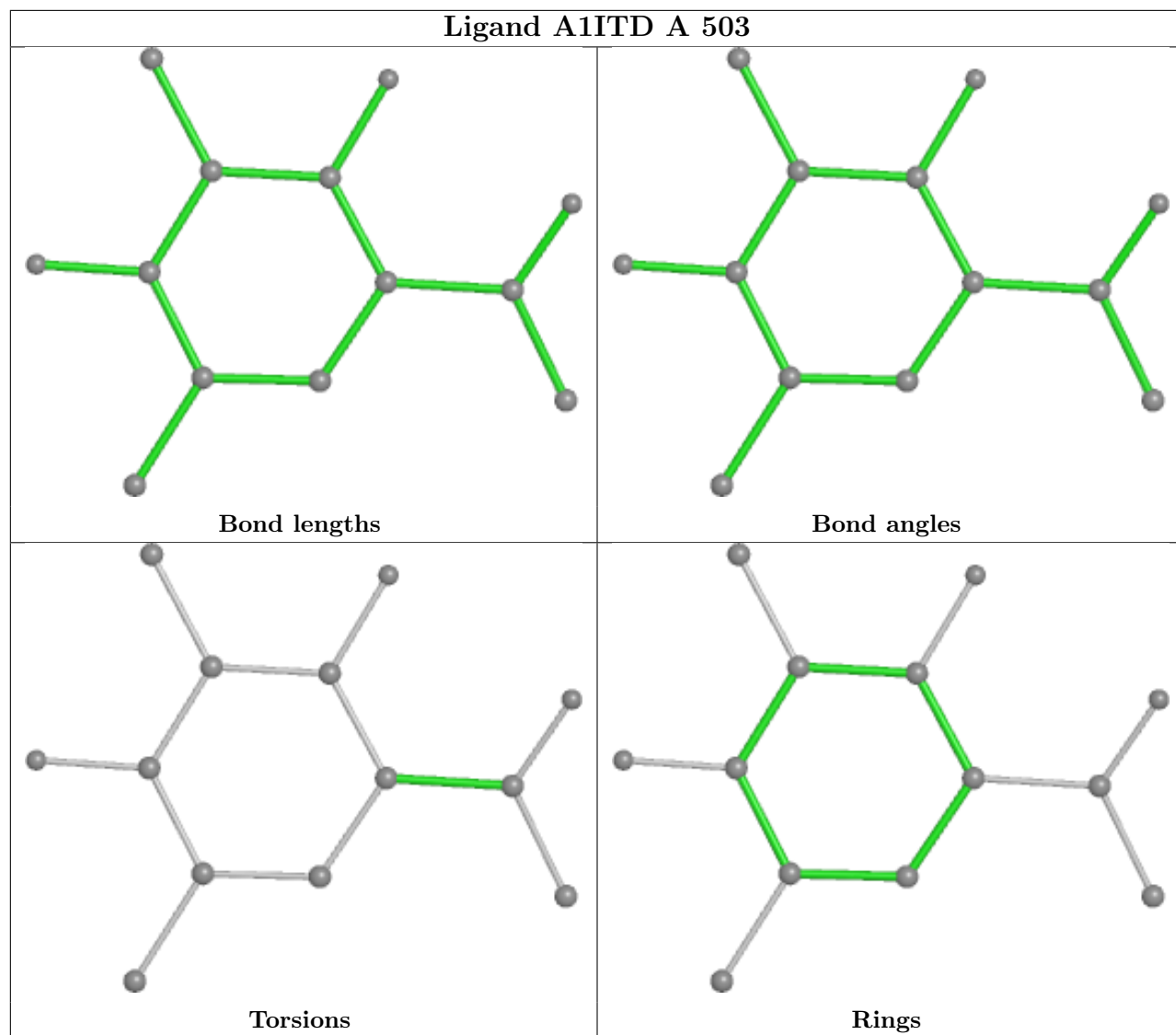
There are no ring outliers.

3 monomers are involved in 14 short contacts:

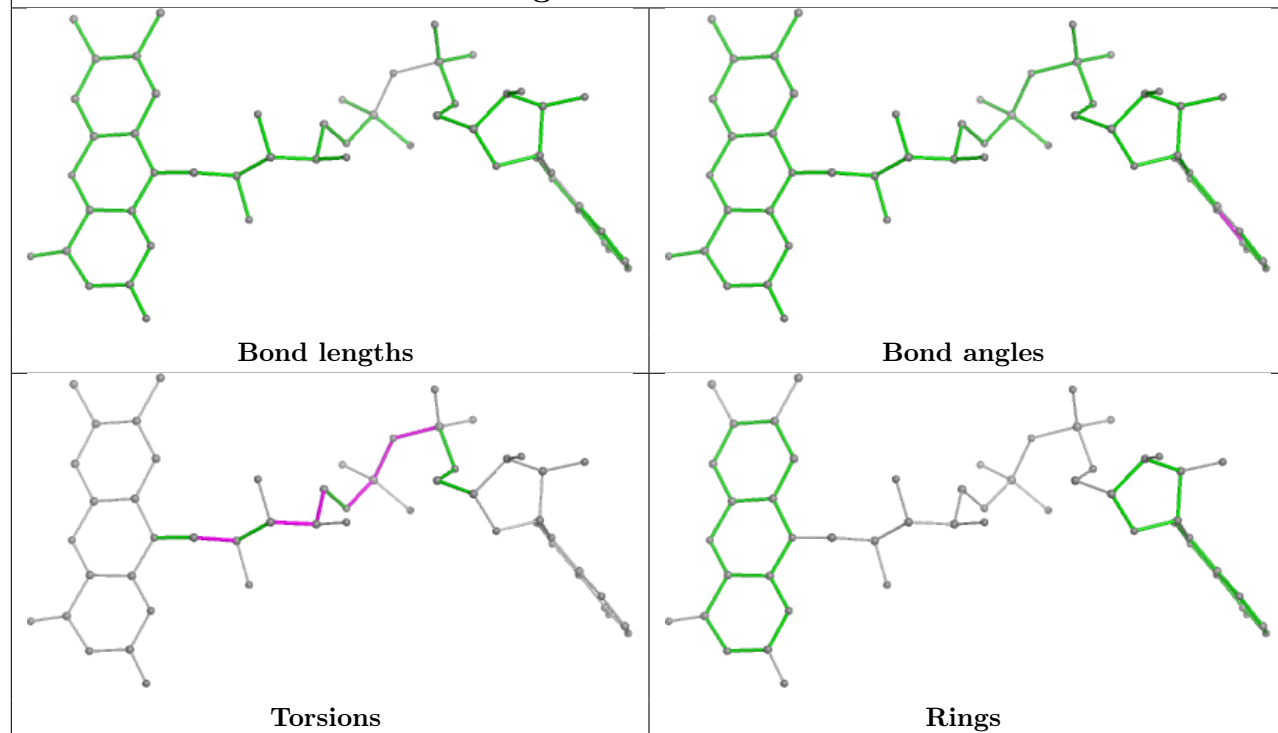
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	502	NAG	1	0
6	B	501	FAD	6	0
6	A	501	FAD	7	0

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

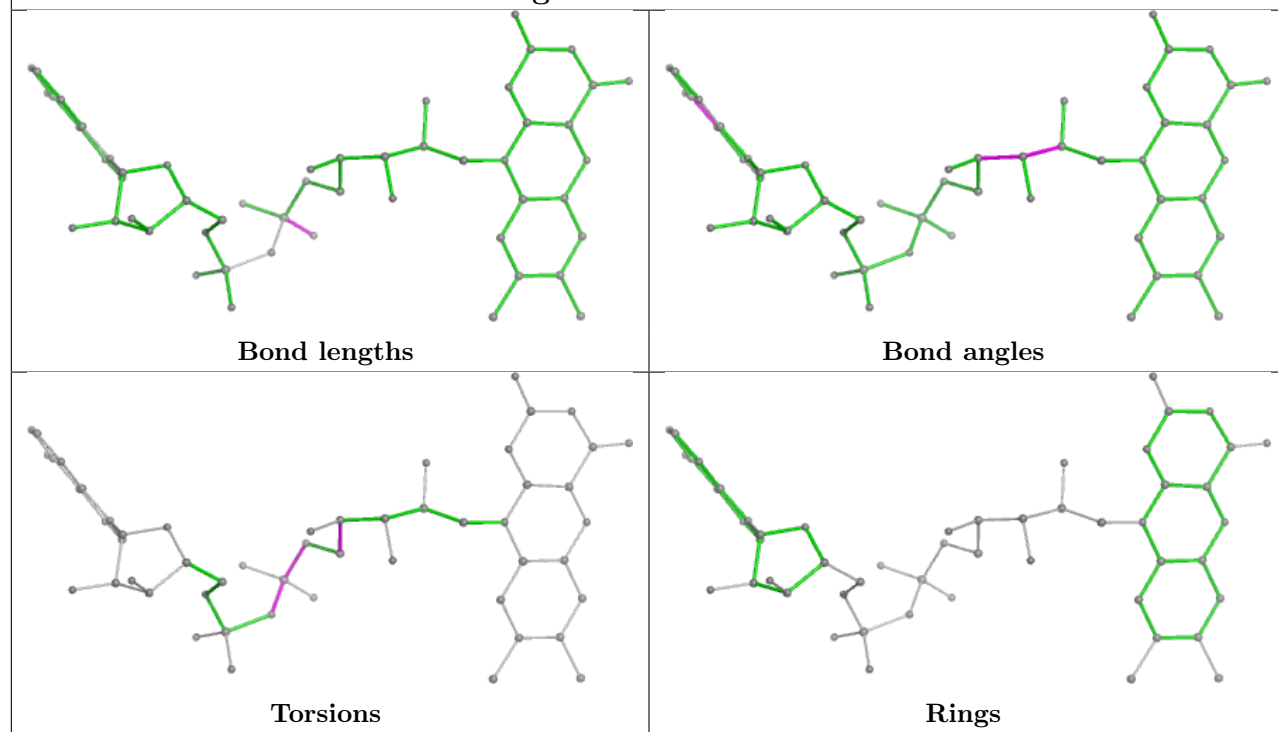
## Ligand A1ITD A 503



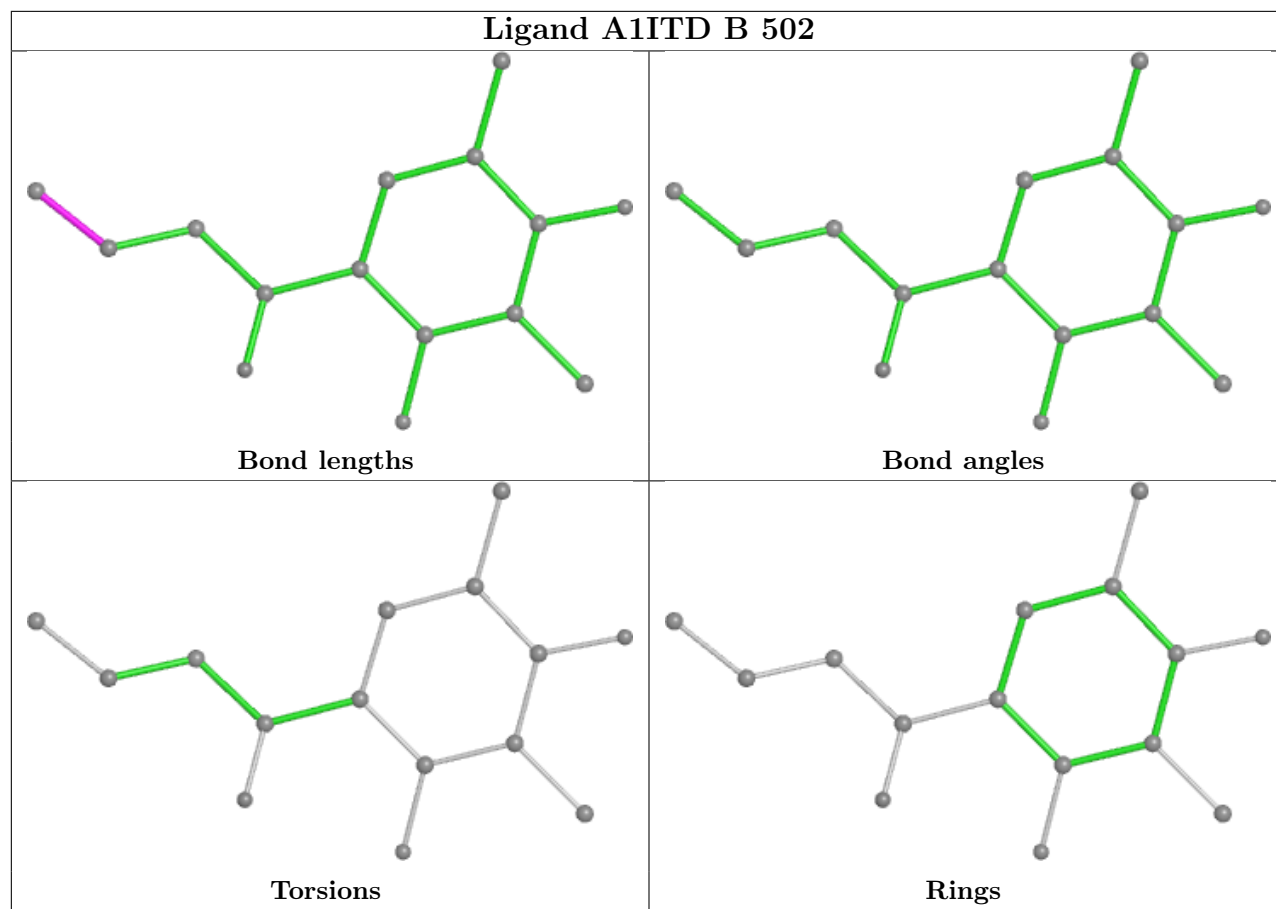
## Ligand FAD B 501



## Ligand FAD A 501







## 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	467/471 (99%)	-0.68	0 100 100	39, 64, 105, 130	0
1	B	467/471 (99%)	-0.40	0 100 100	55, 79, 117, 151	0
All	All	934/942 (99%)	-0.54	0 100 100	39, 73, 110, 151	0

There are no RSRZ outliers to report.

### 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.

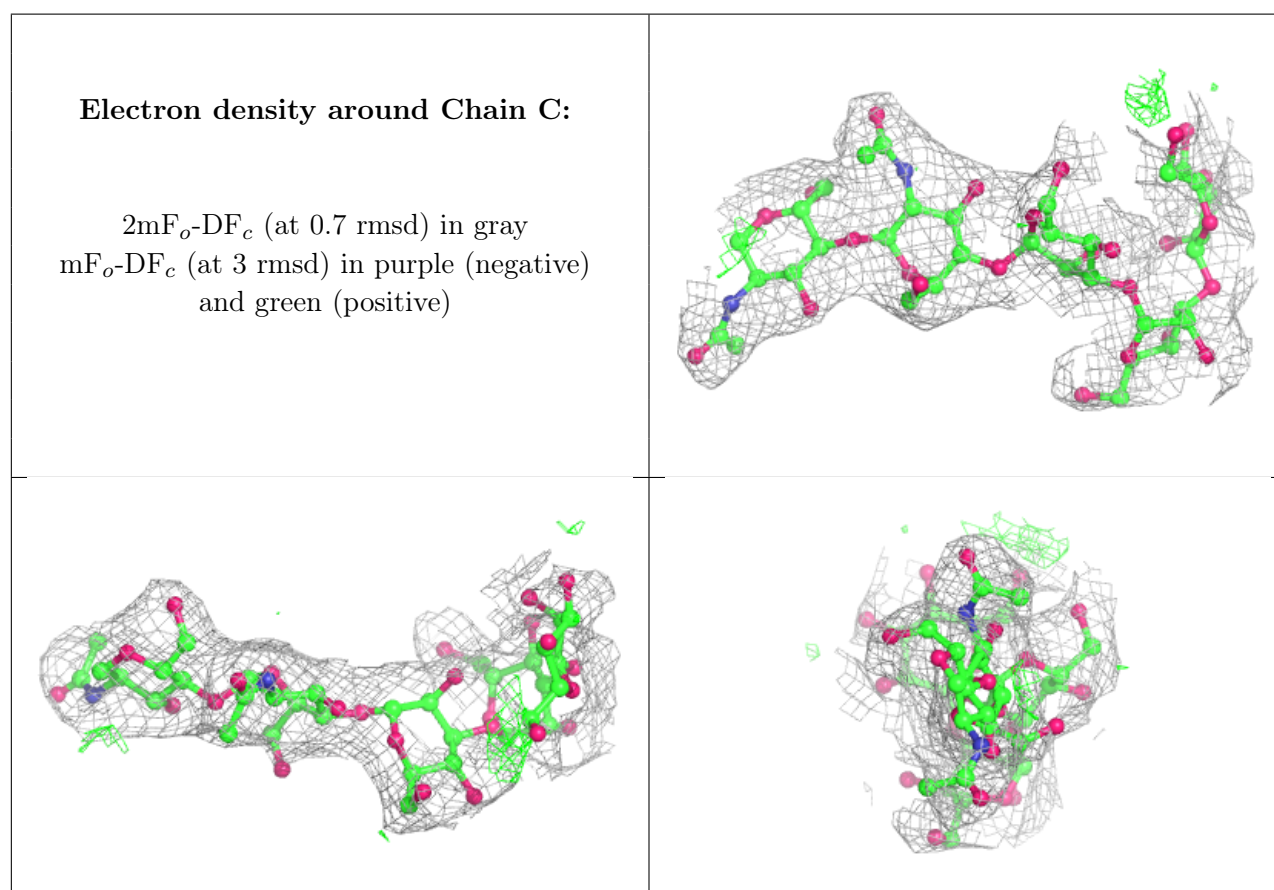
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MAN	D	4	11/12	0.53	0.10	126,141,147,148	0
5	MAN	G	3	11/12	0.57	0.10	114,120,127,127	0
2	MAN	C	5	11/12	0.60	0.14	113,146,158,162	0
5	MAN	H	3	11/12	0.63	0.10	106,113,119,124	0
3	MAN	D	5	11/12	0.64	0.09	95,117,140,143	0
2	MAN	C	4	11/12	0.66	0.10	113,134,141,142	0
5	MAN	F	3	11/12	0.67	0.09	88,106,119,121	0
2	MAN	C	3	11/12	0.71	0.09	98,113,126,134	0
4	NAG	E	1	14/15	0.72	0.10	91,102,109,111	0
4	MAN	E	3	11/12	0.75	0.09	99,103,107,109	0
3	MAN	D	3	11/12	0.79	0.06	103,112,127,139	0

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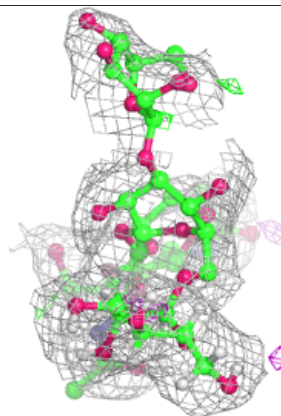
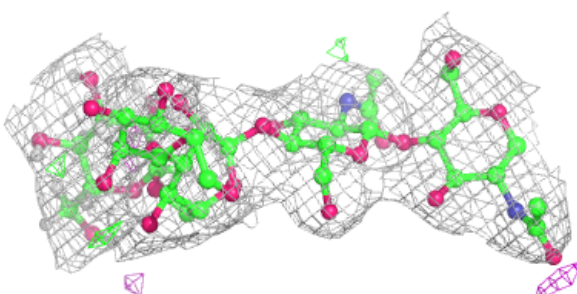
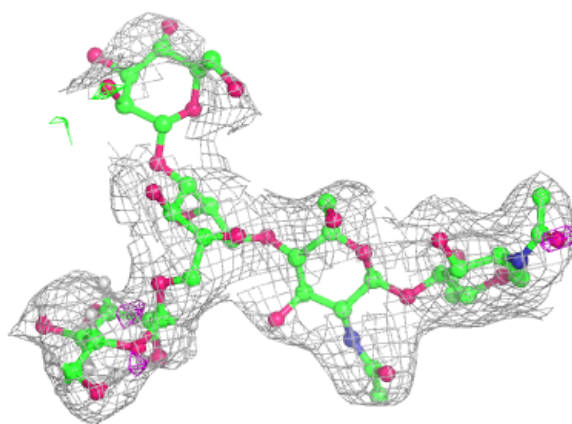
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MAN	E	4	12/12	0.80	0.08	101,119,139,143	0
5	NAG	H	1	14/15	0.82	0.09	86,95,99,100	0
5	NAG	G	1	14/15	0.84	0.09	69,77,85,91	0
4	NAG	E	2	14/15	0.87	0.10	94,102,111,115	0
5	NAG	F	2	14/15	0.88	0.09	76,94,102,103	0
3	NAG	D	1	14/15	0.88	0.07	53,63,75,81	0
5	NAG	H	2	14/15	0.89	0.09	78,91,101,106	0
2	NAG	C	2	14/15	0.89	0.08	68,77,87,90	0
5	NAG	F	1	14/15	0.91	0.07	70,78,87,90	0
2	NAG	C	1	14/15	0.91	0.08	59,68,80,90	0
3	NAG	D	2	14/15	0.92	0.07	59,73,89,92	0
5	NAG	G	2	14/15	0.92	0.09	89,101,121,124	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.

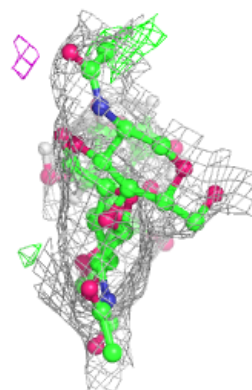
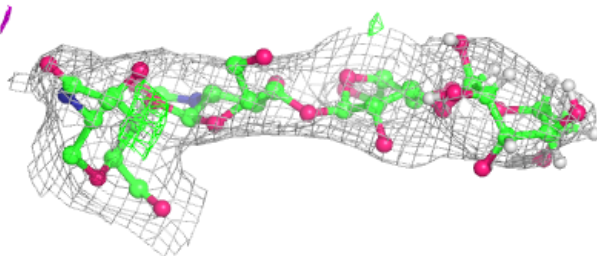
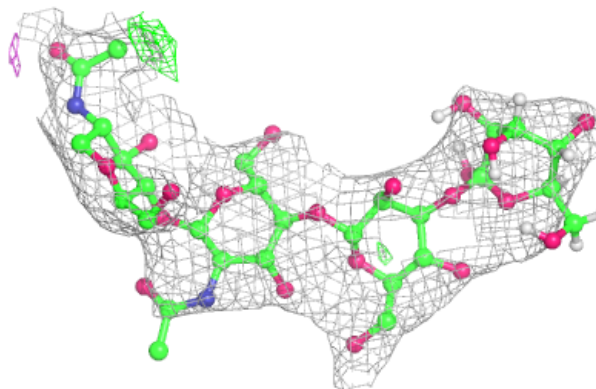


**Electron density around Chain D:**

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

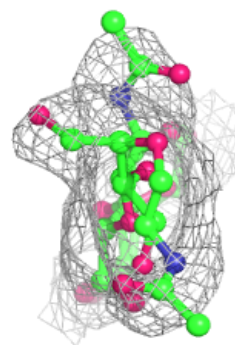
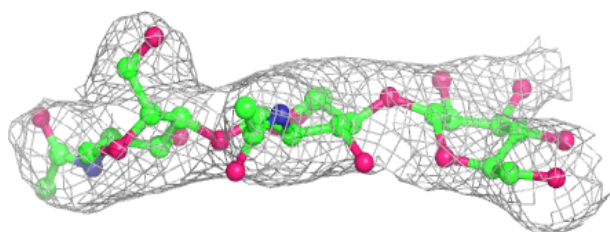
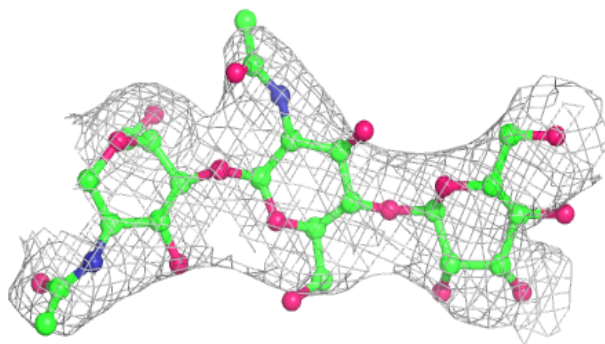
**Electron density around Chain E:**

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

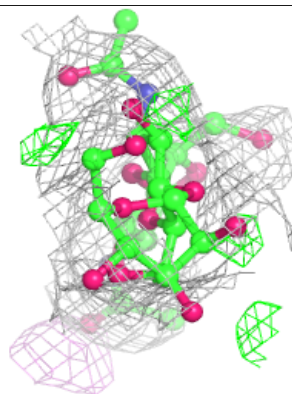
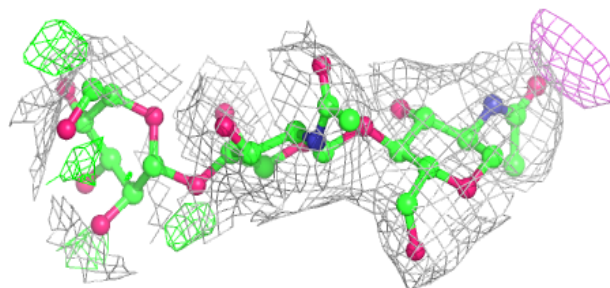
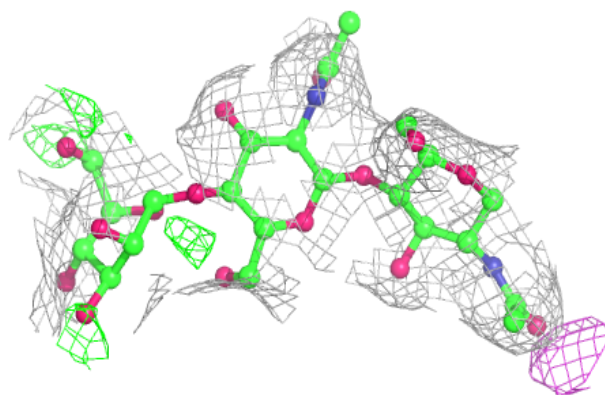


**Electron density around Chain F:**

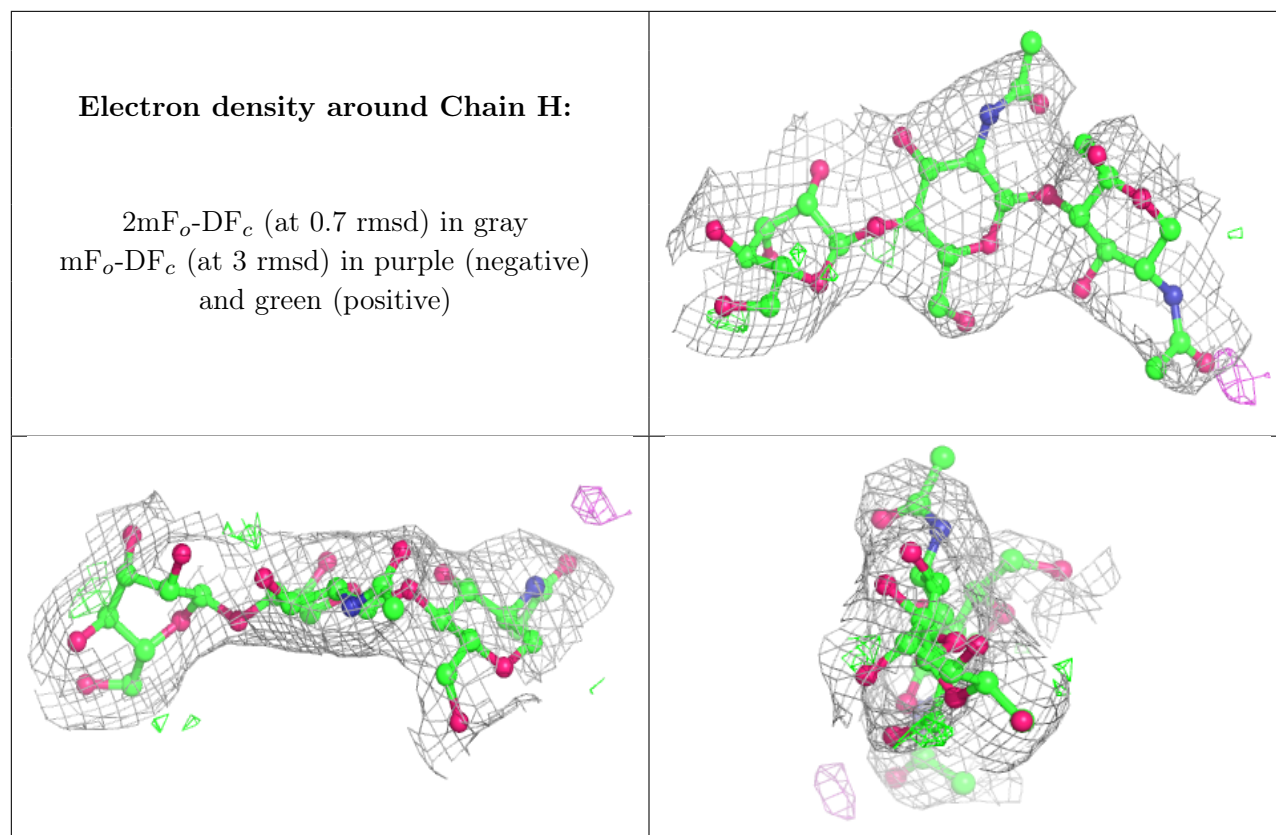
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Chain 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 [i](#)

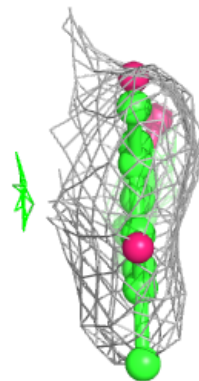
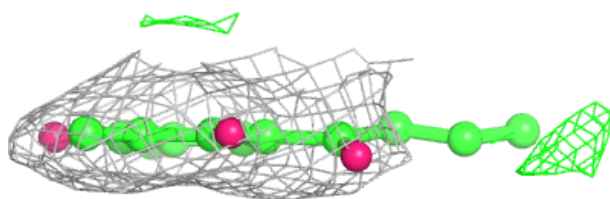
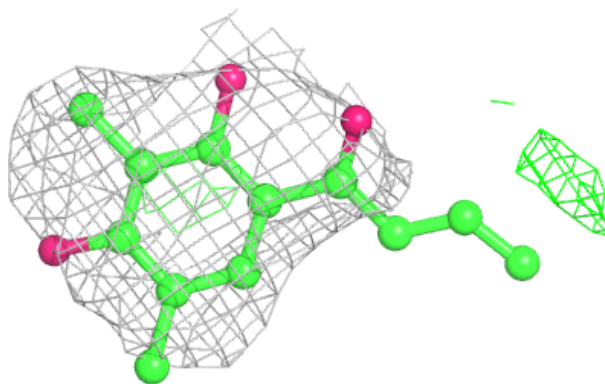
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
7	NAG	A	504	14/15	0.29	0.13	126,159,168,173	0
7	NAG	B	503	14/15	0.72	0.10	129,141,145,151	0
7	NAG	A	502	14/15	0.76	0.11	90,102,108,114	0
8	A1ITD	B	502	15/17	0.82	0.16	70,82,90,93	0
8	A1ITD	A	503	13/17	0.83	0.18	73,89,112,115	0
7	NAG	B	504	14/15	0.89	0.11	114,130,145,162	0
6	FAD	B	501	53/53	0.95	0.08	56,65,75,82	0
6	FAD	A	501	53/53	0.97	0.07	38,47,71,76	0

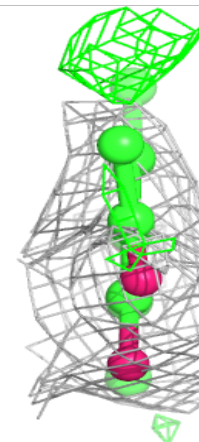
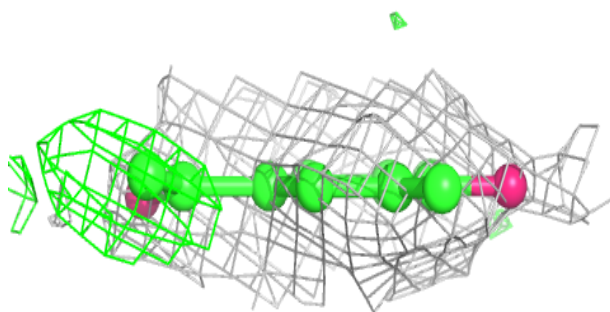
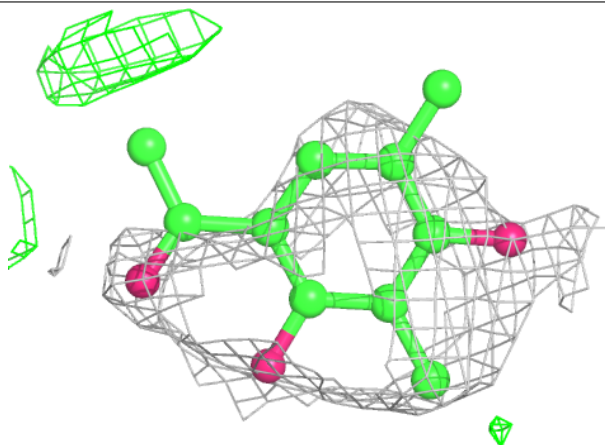
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around A1ITD B 502:**

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

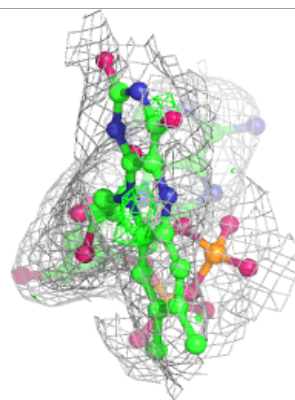
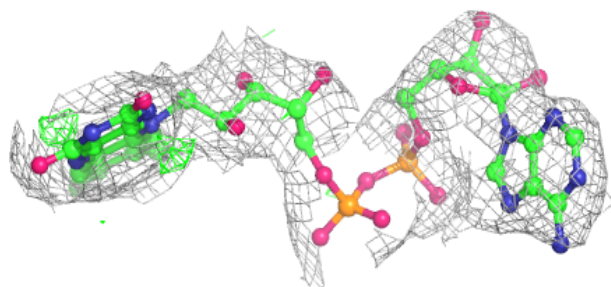
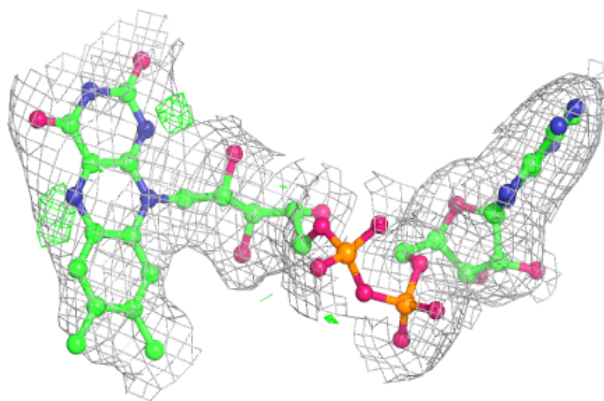
**Electron density around A1ITD A 503:**

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

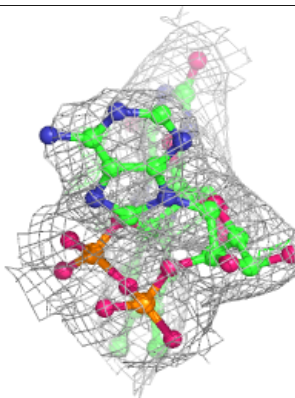
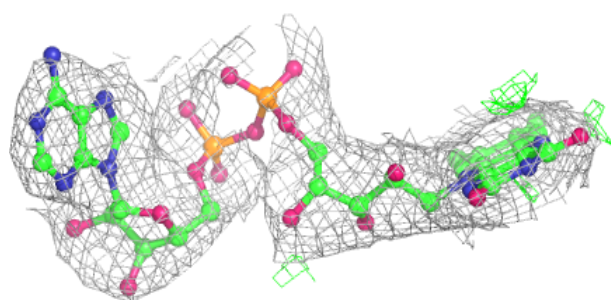
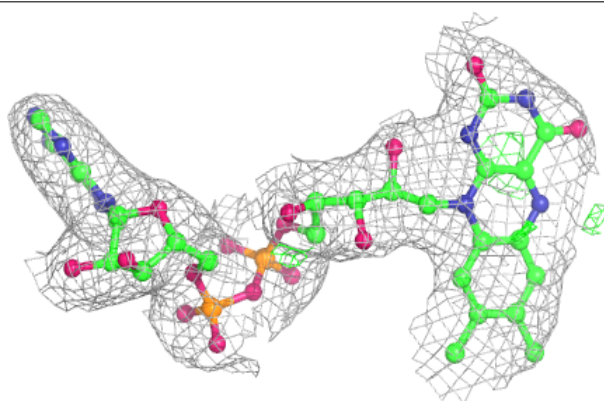


**Electron density around FAD B 501:**

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

**Electron density around FAD A 501:**

$2mF_o-DF_c$  (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.