



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 11, 2021 – 01:21 PM EDT

PDB ID : 2GD4  
Title : Crystal Structure of the Antithrombin-S195A Factor Xa-Pentasaccharide Complex  
Authors : Johnson, D.J.; Li, W.; Adams, T.E.; Huntington, J.A.  
Deposited on : 2006-03-15  
Resolution : 3.30 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	:	2.23.2
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)	:	2.23.2

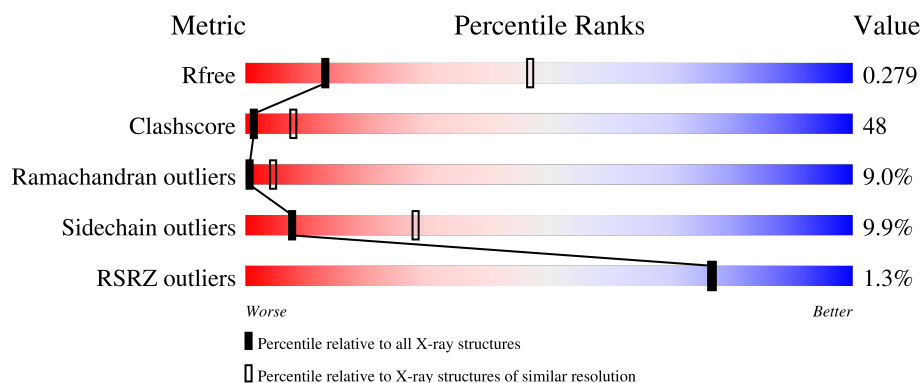
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	58	<div> <div>2%</div> <div> <div></div> <div>48%</div> <div>34%</div> <div>7%</div> <div>10%</div> </div> </div>
1	L	58	<div> <div>52%</div> <div>31%</div> <div>10%</div> <div>7%</div> </div>
2	B	241	<div> <div>32%</div> <div>55%</div> <div>10%</div> <div>..</div> </div>
2	H	241	<div> <div>33%</div> <div>55%</div> <div>8%</div> <div>..</div> </div>
3	C	443	<div> <div>2%</div> <div>30%</div> <div>51%</div> <div>11%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
3	I	443	
4	D	6	
5	E	2	
6	F	5	
6	G	5	

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
4	MAN	D	4	-	-	-	X
8	NAG	C	701	-	-	-	X
8	NAG	I	701	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11165 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 Coagulation factor X, Stuart factor, Stuart-Prower factor, Contains: Factor X light chain; Factor X heavy chain; Activated factor Xa heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	54	Total	C	N	O	S	0	0	0
			366	219	67	73	7			
1	A	52	Total	C	N	O	S	6	0	0
			349	209	62	71	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	85	MET	-	cloning artifact	UNP P00742
A	85	MET	-	cloning artifact	UNP P00742

- Molecule 2 is a protein called Coagulation factor, Stuart factor, Stuart-Prower factor, Contains: Factor X light chain; Factor X heavy chain; Activated factor Xa heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	234	Total	C	N	O	S	0	0	0
			1811	1143	312	342	14			
2	B	239	Total	C	N	O	S	3	0	0
			1840	1162	319	345	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	104	ALA	SER	engineered mutation	UNP P00742
B	104	ALA	SER	engineered mutation	UNP P00742

- Molecule 3 is a protein called Antithrombin-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	417	Total	C	N	O	S	14	0	0
			3197	2045	537	599	16			

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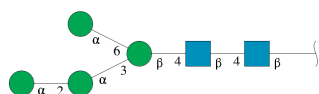
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	418	Total	C	N	O	S	20	0	0
			3200	2048	538	597	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	137	ALA	SER	engineered mutation	UNP P01008
I	347	ALA	GLU	engineered mutation	UNP P01008
I	348	ALA	LYS	engineered mutation	UNP P01008
I	350	ALA	LYS	engineered mutation	UNP P01008
C	137	ALA	SER	engineered mutation	UNP P01008
C	347	ALA	GLU	engineered mutation	UNP P01008
C	348	ALA	LYS	engineered mutation	UNP P01008
C	350	ALA	LYS	engineered mutation	UNP P01008

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	6	Total	C	N	O	0	0	0
			71	40	2	29			

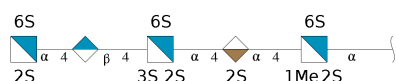
- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 6 is an oligosaccharide called 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-2-deoxy-3,6-di-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-methyl 2-deoxy-6-O-sulf

o-2-(sulfoamino)-alpha-D-glucopyranoside.

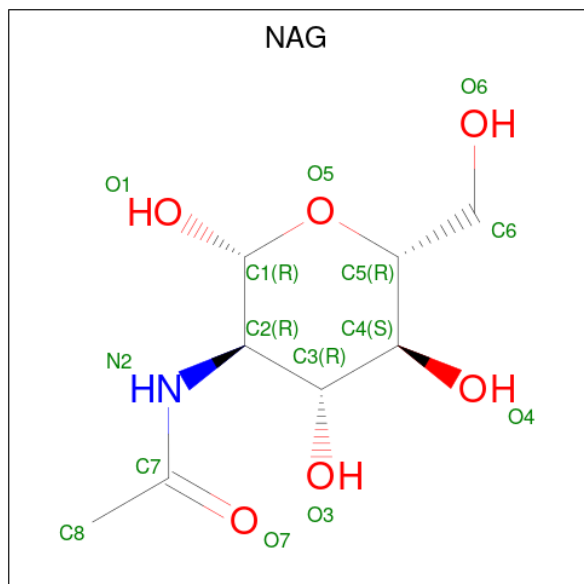


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	5	Total	C	N	O	S	0	0	0
			91	31	3	49	8			
6	G	5	Total	C	N	O	S	0	0	0
			91	31	3	49	8			

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		

- Molecule 8 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
8	I	1	Total	C	N	O	0	0
			14	8	1	5		
8	I	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	3	Total	O	0	0
			3	3		
9	H	10	Total	O	0	0
			10	10		
9	I	22	Total	O	0	0
			22	22		
9	A	2	Total	O	0	0
			2	2		
9	B	9	Total	O	0	0
			9	9		
9	C	17	Total	O	0	0
			17	17		

### 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.

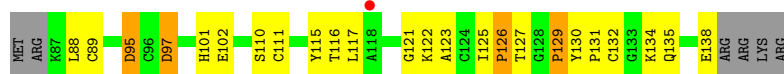
- Molecule 1: Coagulation factor X, Stuart factor, Stuart-Prower factor, Contains: Factor X light chain; Factor X heavy chain; Activated factor Xa heavy chain

Chain L: 



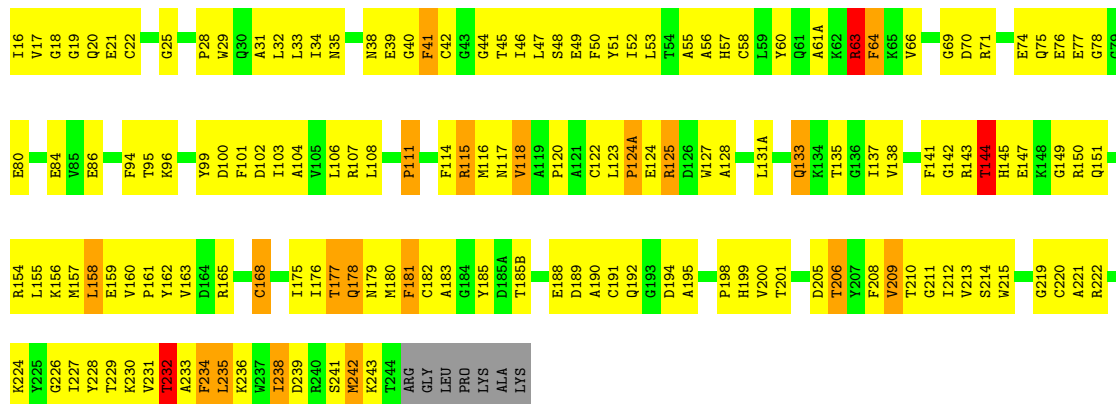
- Molecule 1: Coagulation factor X, Stuart factor, Stuart-Prower factor, Contains: Factor X light chain; Factor X heavy chain; Activated factor Xa heavy chain

Chain A: 



- Molecule 2: Coagulation factor, Stuart factor, Stuart-Prower factor, Contains: Factor X light chain; Factor X heavy chain; Activated factor Xa heavy chain

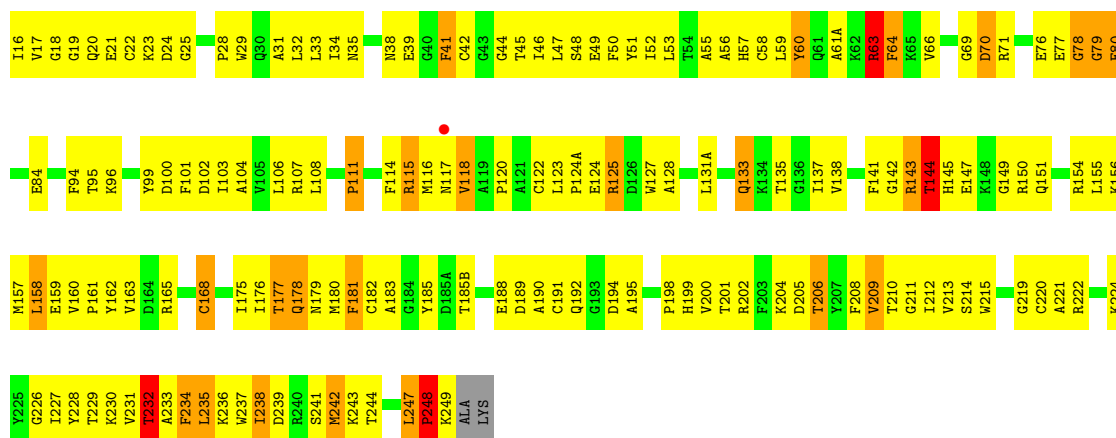
Chain H: 



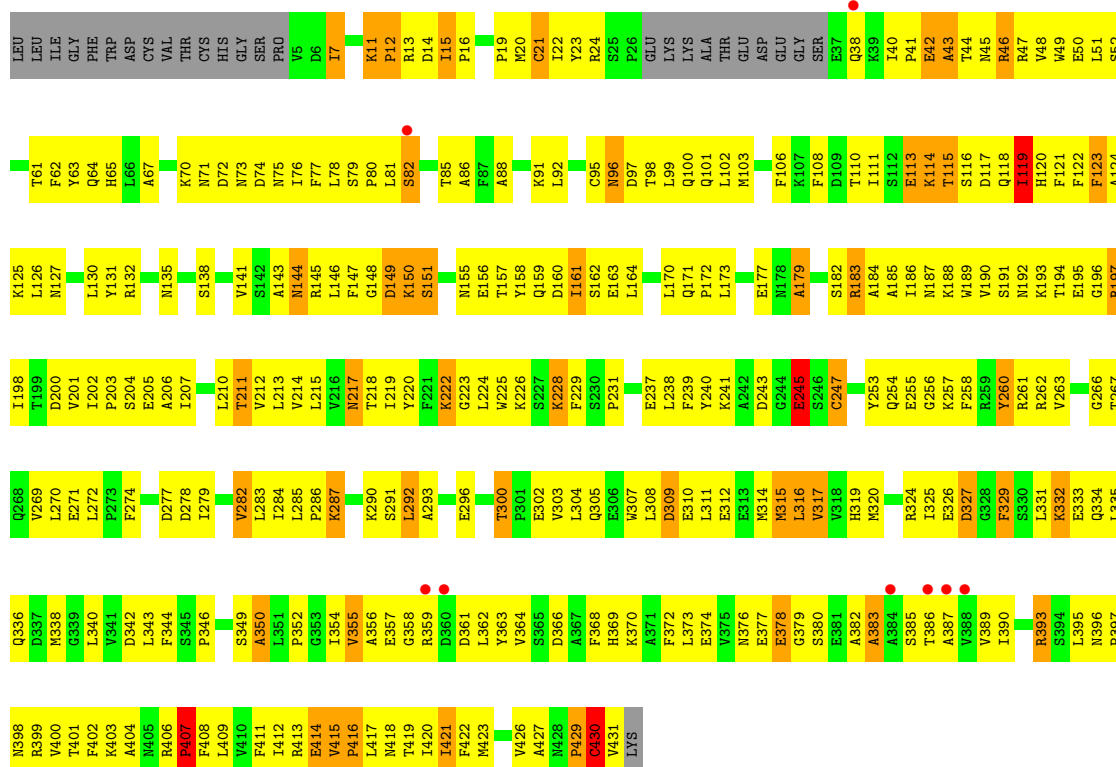
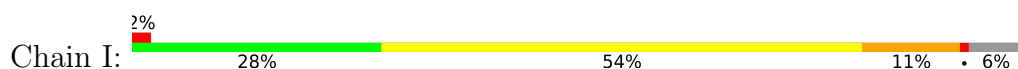
- Molecule 2: Coagulation factor, Stuart factor, Stuart-Prower factor, Contains: Factor X light chain; Factor X heavy chain; Activated factor Xa heavy chain

Chain B: 

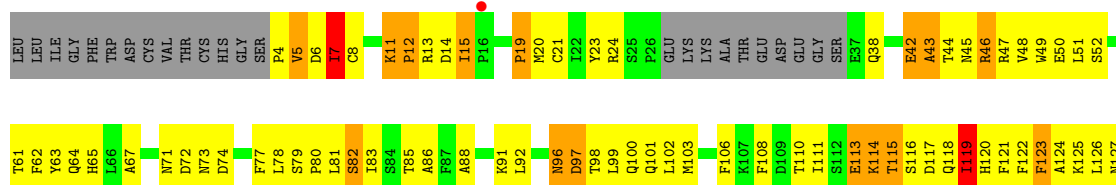


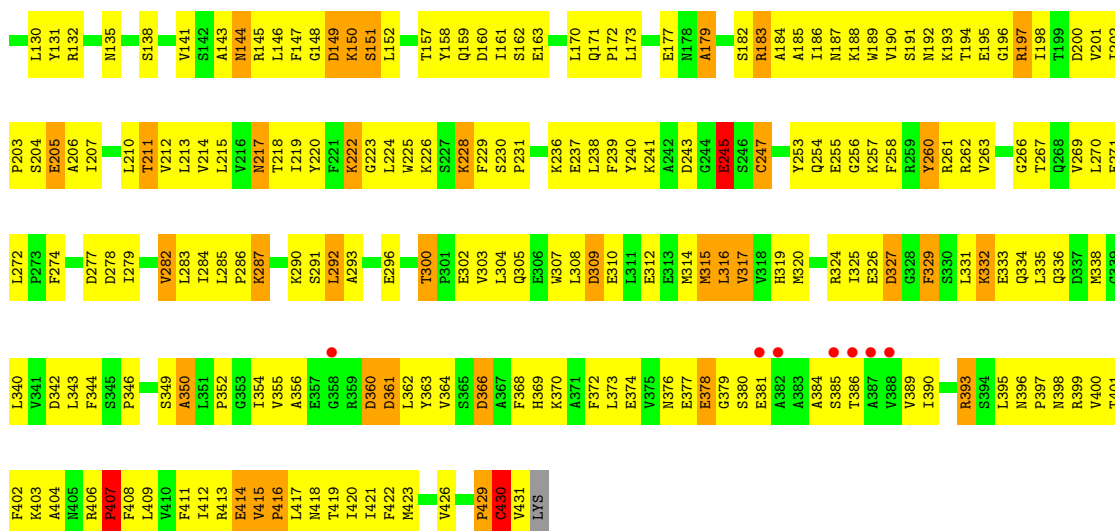


### • Molecule 3: Antithrombin-III



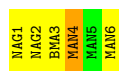
### • Molecule 3: Antithrombin-III





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

Chain D: 17% 67% 17%



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

Chain E: 100%



- Molecule 6: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-2-deoxy-3,6-di-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-methyl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside

Chain F: 60% 40%



- Molecule 6: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-2-deoxy-3,6-di-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-methyl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside

Chain G: 60% 40%

ZD01
IDS2
SUS3
BDF4
SGN5

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	220.26Å 60.59Å 156.17Å 90.00° 113.14° 90.00°	Depositor
Resolution (Å)	36.90 – 3.30 36.92 – 3.20	Depositor EDS
% Data completeness (in resolution range)	93.7 (36.90-3.30) 93.7 (36.92-3.20)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 3.18Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.247 , 0.298 0.235 , 0.279	Depositor DCC
$R_{free}$ test set	1202 reflections (4.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.4	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 69.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	11165	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.87% 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: BMA, NAG, BDP, SUS, ZDO, IDS, SGN, MAN, CA

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	0.31	0/355	0.61	0/484
1	L	0.31	0/372	0.65	0/506
2	B	0.50	0/1879	0.78	1/2541 (0.0%)
2	H	0.50	0/1849	0.76	1/2500 (0.0%)
3	C	0.43	0/3267	0.72	0/4440
3	I	0.44	0/3263	0.71	0/4435
All	All	0.45	0/10985	0.73	2/14906 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	168	CYS	CA-CB-SG	5.41	123.75	114.00
2	B	168	CYS	CA-CB-SG	5.26	123.47	114.00

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	349	0	279	30	0
1	L	366	0	296	31	0
2	B	1840	0	1752	183	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1811	0	1727	176	0
3	C	3200	0	3073	317	0
3	I	3197	0	3072	323	0
4	D	71	0	59	9	0
5	E	28	0	25	8	0
6	F	91	0	27	2	0
6	G	91	0	27	2	0
7	B	1	0	0	0	0
7	H	1	0	0	0	0
8	C	28	0	26	1	0
8	I	28	0	26	1	0
9	A	2	0	0	1	0
9	B	9	0	0	0	0
9	C	17	0	0	2	0
9	H	10	0	0	1	0
9	I	22	0	0	0	0
9	L	3	0	0	0	0
All	All	11165	0	10389	1033	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 48.

The worst 5 of 1033 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)
4:D:1:NAG:H61	4:D:2:NAG:N2	1.59	1.17
2:B:235:LEU:HD22	2:B:235:LEU:H	1.03	1.14
5:E:1:NAG:H61	5:E:2:NAG:N2	1.59	1.13
2:H:235:LEU:H	2:H:235:LEU:HD22	1.02	1.12
2:B:237:TRP:HD1	2:B:248:PRO:HG2	1.19	1.05

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	50/58 (86%)	36 (72%)	9 (18%)	5 (10%)	0	3
1	L	52/58 (90%)	37 (71%)	10 (19%)	5 (10%)	0	4
2	B	237/241 (98%)	174 (73%)	46 (19%)	17 (7%)	1	7
2	H	232/241 (96%)	174 (75%)	46 (20%)	12 (5%)	2	13
3	C	414/443 (94%)	290 (70%)	79 (19%)	45 (11%)	0	2
3	I	413/443 (93%)	294 (71%)	77 (19%)	42 (10%)	0	3
All	All	1398/1484 (94%)	1005 (72%)	267 (19%)	126 (9%)	1	4

5 of 126 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	87	LYS
1	L	102	GLU
1	L	126	PRO
2	H	125	ARG
2	H	144	THR

### 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	33/50 (66%)	32 (97%)	1 (3%)	41	68
1	L	34/50 (68%)	32 (94%)	2 (6%)	19	49
2	B	189/203 (93%)	168 (89%)	21 (11%)	6	23
2	H	188/203 (93%)	169 (90%)	19 (10%)	7	27
3	C	331/389 (85%)	298 (90%)	33 (10%)	7	27
3	I	332/389 (85%)	298 (90%)	34 (10%)	7	27
All	All	1107/1284 (86%)	997 (90%)	110 (10%)	8	28

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	63	ARG
2	B	205	ASP
3	C	430	CYS
3	C	317	VAL
2	B	70	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	133	GLN
2	B	178	GLN
3	C	305	GLN
3	C	73	ASN
3	C	144	ASN

### 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 ⓘ

18 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	$\# Z  > 2$
4	NAG	D	1	4,3	14,14,15	0.44	0	17,19,21	0.80	0
4	NAG	D	2	4	14,14,15	0.59	0	17,19,21	0.74	0
4	BMA	D	3	4	11,11,12	0.60	0	15,15,17	0.62	0
4	MAN	D	4	4	11,11,12	0.60	0	15,15,17	0.76	1 (6%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MAN	D	5	4	10,10,12	0.62	0	13,13,17	0.52	0
4	MAN	D	6	4	11,11,12	0.64	0	15,15,17	0.76	1 (6%)
5	NAG	E	1	5,3	14,14,15	0.46	0	17,19,21	0.81	0
5	NAG	E	2	5	14,14,15	0.57	0	17,19,21	0.74	0
6	ZDO	F	1	6	20,21,21	2.74	5 (25%)	25,32,32	1.40	3 (12%)
6	IDS	F	2	6	13,16,17	1.57	2 (15%)	15,24,26	1.36	2 (13%)
6	SUS	F	3	6	22,23,24	2.78	5 (22%)	24,36,38	1.67	4 (16%)
6	BDP	F	4	6	9,12,13	0.44	0	12,17,19	0.83	1 (8%)
6	SGN	F	5	6	18,19,20	2.82	4 (22%)	22,29,31	1.41	3 (13%)
6	ZDO	G	1	6	20,21,21	2.75	5 (25%)	25,32,32	1.38	3 (12%)
6	IDS	G	2	6	13,16,17	1.58	2 (15%)	15,24,26	1.36	2 (13%)
6	SUS	G	3	6	22,23,24	2.79	5 (22%)	24,36,38	1.68	4 (16%)
6	BDP	G	4	6	9,12,13	0.46	0	12,17,19	0.83	1 (8%)
6	SGN	G	5	6	18,19,20	2.84	4 (22%)	22,29,31	1.40	3 (13%)

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	D	1	4,3	-	4/6/23/26	0/1/1/1
4	NAG	D	2	4	-	4/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	0/1/1/1
4	MAN	D	4	4	-	1/2/19/22	0/1/1/1
4	MAN	D	5	4	-	0/2/16/22	0/1/1/1
4	MAN	D	6	4	-	2/2/19/22	0/1/1/1
5	NAG	E	1	5,3	-	4/6/23/26	0/1/1/1
5	NAG	E	2	5	-	4/6/23/26	0/1/1/1
6	ZDO	F	1	6	-	4/13/33/33	0/1/1/1
6	IDS	F	2	6	-	0/5/26/29	0/1/1/1
6	SUS	F	3	6	-	8/16/33/36	0/1/1/1
6	BDP	F	4	6	-	0/0/21/24	0/1/1/1
6	SGN	F	5	6	-	2/11/28/31	0/1/1/1
6	ZDO	G	1	6	-	4/13/33/33	0/1/1/1
6	IDS	G	2	6	-	0/5/26/29	0/1/1/1
6	SUS	G	3	6	-	8/16/33/36	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BDP	G	4	6	-	0/0/21/24	0/1/1/1
6	SGN	G	5	6	-	2/11/28/31	0/1/1/1

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	5	SGN	O1S-S1	7.36	1.50	1.42
6	G	5	SGN	O2S-S1	7.35	1.50	1.42
6	G	1	ZDO	OSB-S2	7.32	1.50	1.42
6	F	1	ZDO	OSA-S2	7.31	1.50	1.42
6	F	3	SUS	O1S-S1	7.31	1.50	1.42

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	3	SUS	O3S-S1-O1S	-4.94	108.47	120.16
6	F	3	SUS	O3S-S1-O1S	-4.89	108.61	120.16
6	F	3	SUS	C3-O3-S3	-4.60	109.99	118.88
6	G	3	SUS	C3-O3-S3	-4.58	110.03	118.88
6	F	1	ZDO	OSB-S2-OSA	-4.58	109.34	120.16

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
6	F	1	ZDO	C2-N2-S2-OSA

There are no ring outliers.

10 monomers are involved in 21 short contacts:

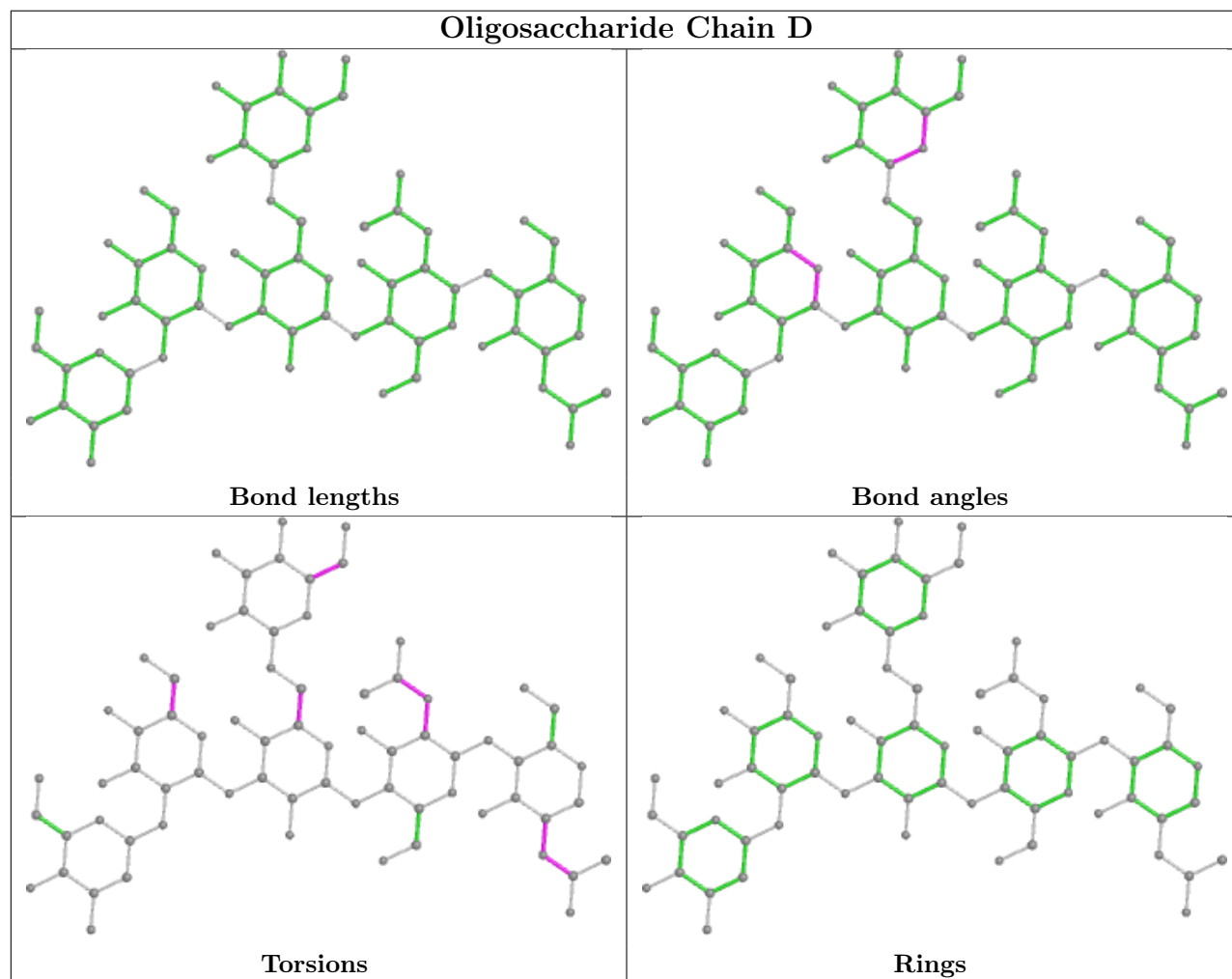
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	1	ZDO	1	0
4	D	2	NAG	4	0
4	D	3	BMA	3	0
6	F	1	ZDO	1	0
6	F	5	SGN	1	0
5	E	2	NAG	6	0

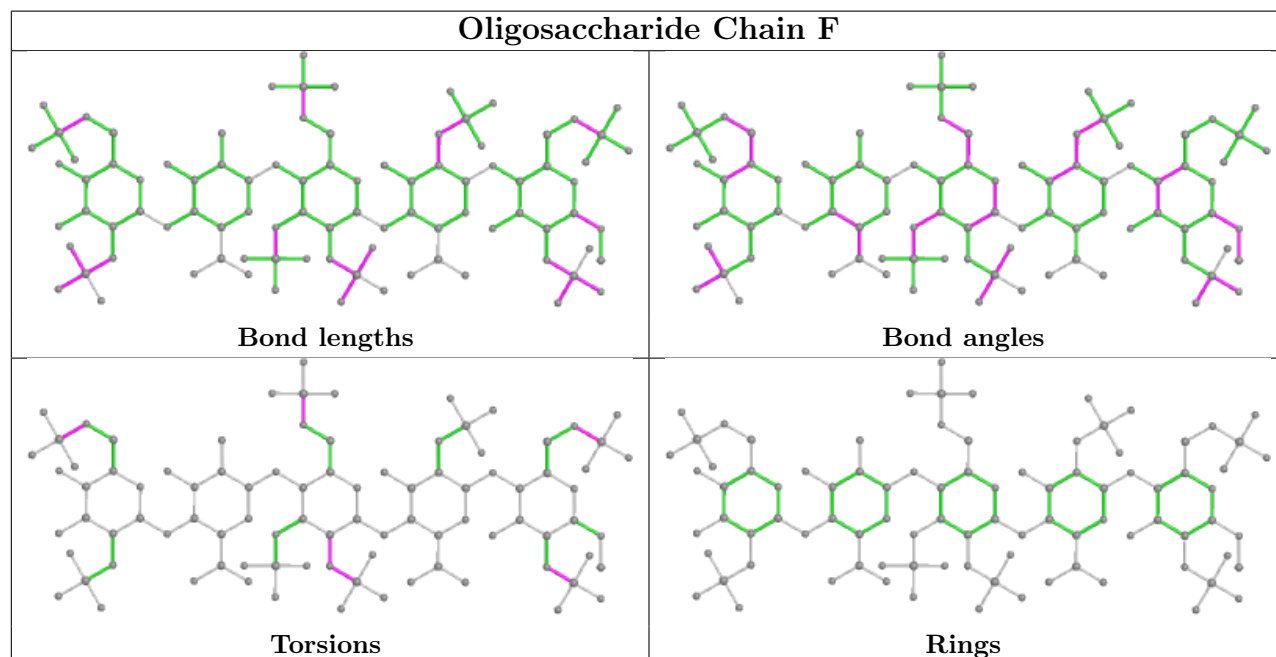
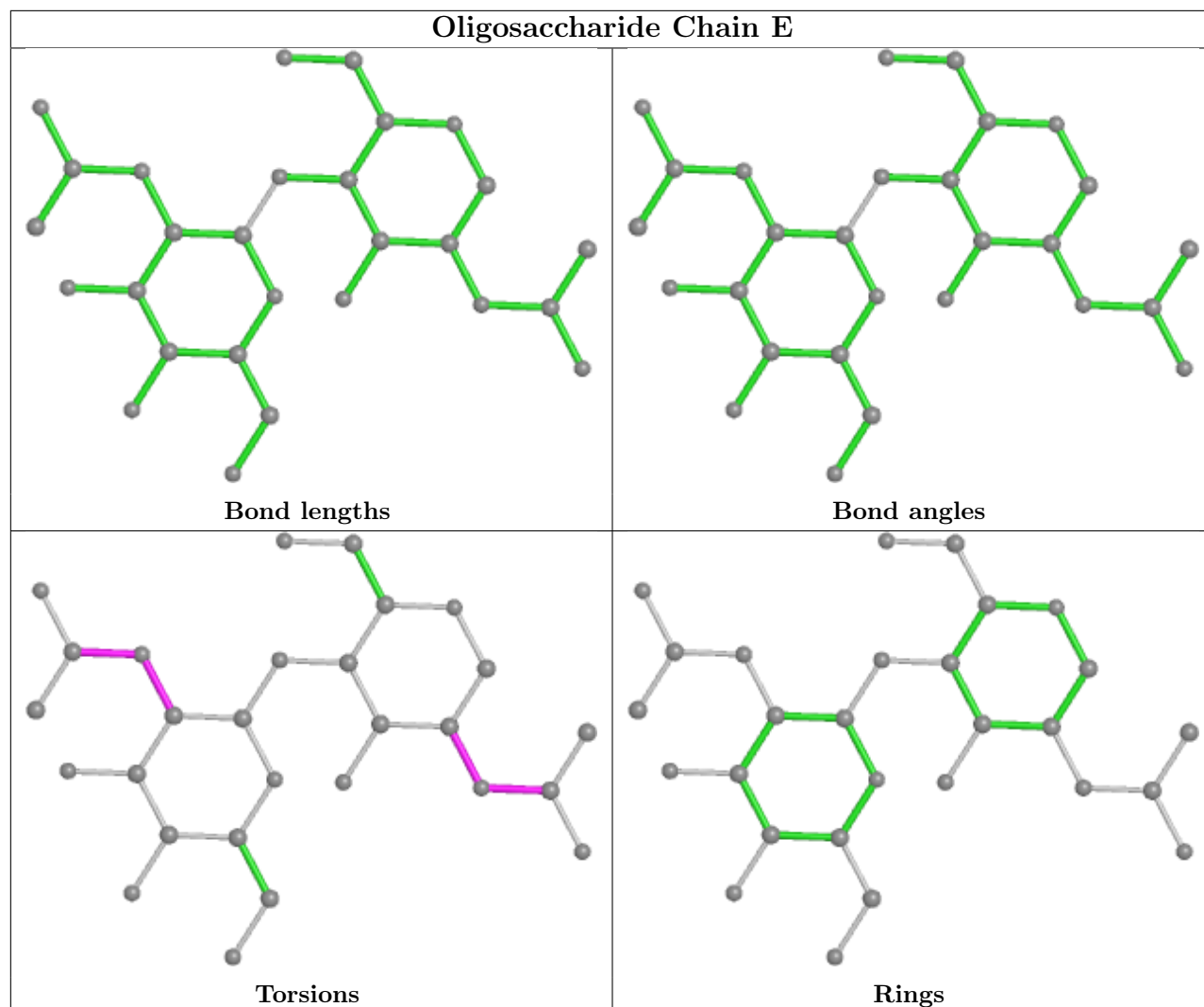
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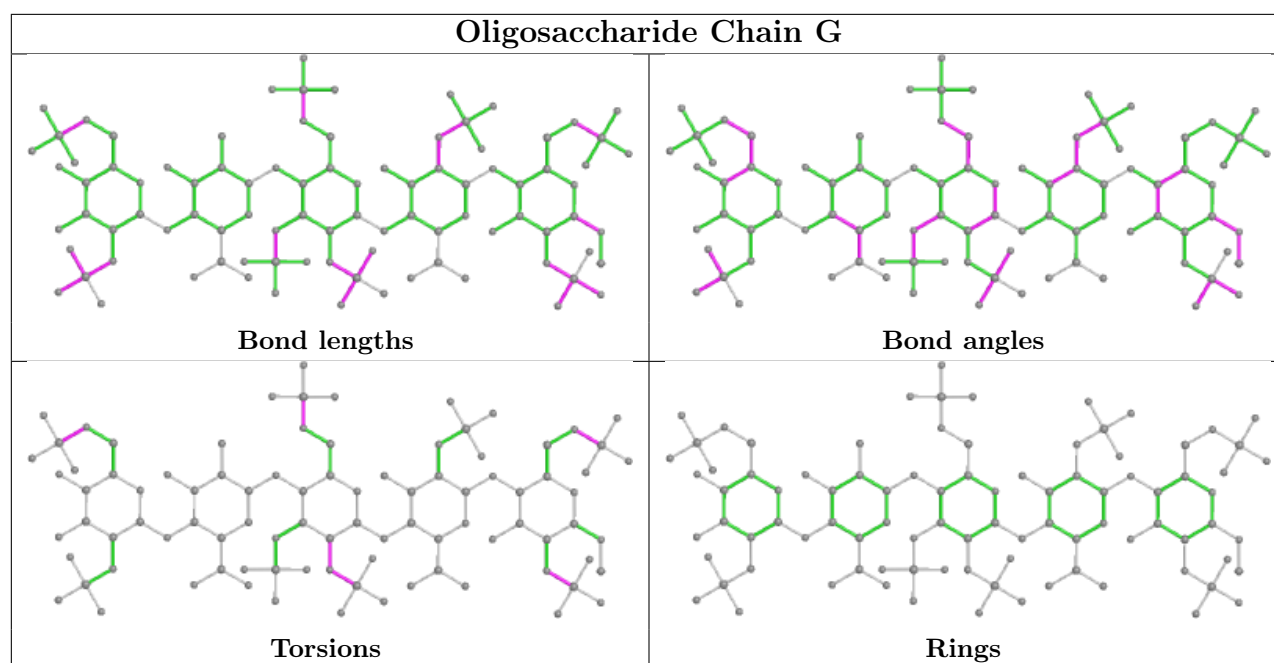
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	5	SGN	1	0
4	D	1	NAG	5	0
4	D	4	MAN	3	0
5	E	1	NAG	5	0

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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$
8	NAG	C	701	3	14,14,15	0.63	0	17,19,21	0.61	0
8	NAG	I	501	3	14,14,15	0.95	1 (7%)	17,19,21	2.15	3 (17%)
8	NAG	C	501	3	14,14,15	0.95	1 (7%)	17,19,21	2.15	3 (17%)
8	NAG	I	701	3	14,14,15	0.63	0	17,19,21	0.61	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
8	NAG	C	701	3	-	6/6/23/26	0/1/1/1
8	NAG	I	501	3	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	C	501	3	-	4/6/23/26	0/1/1/1
8	NAG	I	701	3	-	6/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	501	NAG	O5-C5	2.29	1.48	1.43
8	I	501	NAG	O5-C5	2.11	1.47	1.43

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	501	NAG	C1-O5-C5	6.21	120.61	112.19
8	I	501	NAG	C1-O5-C5	6.13	120.50	112.19
8	C	501	NAG	C4-C3-C2	-4.48	104.45	111.02
8	I	501	NAG	C4-C3-C2	-4.44	104.51	111.02
8	I	501	NAG	O5-C1-C2	3.50	116.82	111.29

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	501	NAG	C8-C7-N2-C2
8	I	501	NAG	O7-C7-N2-C2
8	I	701	NAG	C8-C7-N2-C2
8	I	701	NAG	O7-C7-N2-C2
8	C	501	NAG	C8-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	501	NAG	1	0
8	C	501	NAG	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	52/58 (89%)	0.44	1 (1%) 66 65	29, 65, 82, 83	1 (1%)
1	L	54/58 (93%)	-0.01	0 100 100	29, 65, 81, 83	0
2	B	239/241 (99%)	-0.44	1 (0%) 92 93	1, 19, 45, 80	3 (1%)
2	H	234/241 (97%)	-0.49	0 100 100	1, 19, 38, 53	3 (1%)
3	C	418/443 (94%)	-0.15	8 (1%) 66 65	1, 41, 87, 99	6 (1%)
3	I	417/443 (94%)	-0.14	8 (1%) 66 65	1, 39, 85, 103	3 (0%)
All	All	1414/1484 (95%)	-0.23	18 (1%) 77 77	1, 31, 83, 103	16 (1%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	387	ALA	4.0
3	I	387	ALA	3.8
3	C	388	VAL	3.7
3	C	358	GLY	3.3
3	C	386	THR	3.1

### 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.

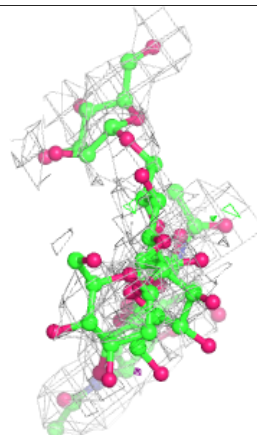
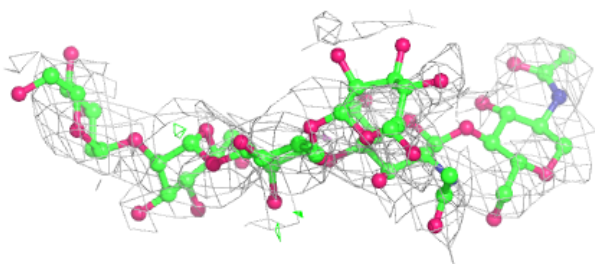
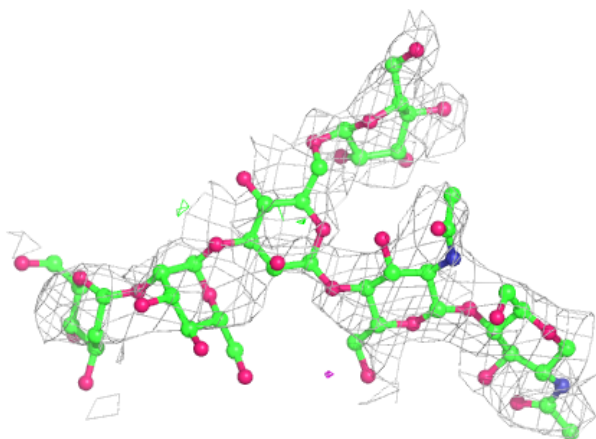


Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MAN	D	6	11/12	0.40	0.34	135,136,137,137	0
4	BMA	D	3	11/12	0.60	0.37	129,134,135,139	0
4	MAN	D	5	10/12	0.66	0.40	148,149,150,150	0
4	NAG	D	2	14/15	0.71	0.32	107,110,117,121	0
4	MAN	D	4	11/12	0.74	0.42	143,145,147,147	0
5	NAG	E	1	14/15	0.82	0.22	85,87,93,100	0
5	NAG	E	2	14/15	0.84	0.30	106,110,114,115	0
6	IDS	G	2	16/17	0.84	0.18	49,55,65,66	0
6	ZDO	G	1	21/21	0.88	0.17	50,54,56,58	0
4	NAG	D	1	14/15	0.89	0.19	84,88,94,101	0
6	IDS	F	2	16/17	0.90	0.15	50,55,65,65	0
6	BDP	G	4	12/13	0.92	0.18	28,32,34,34	0
6	BDP	F	4	12/13	0.93	0.13	27,31,34,34	0
6	ZDO	F	1	21/21	0.93	0.17	50,52,56,59	0
6	SUS	G	3	23/24	0.94	0.14	37,43,49,50	0
6	SUS	F	3	23/24	0.95	0.15	39,43,48,48	0
6	SGN	G	5	19/20	0.95	0.12	28,32,36,36	0
6	SGN	F	5	19/20	0.96	0.13	29,32,36,36	0

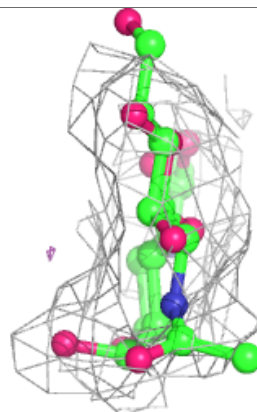
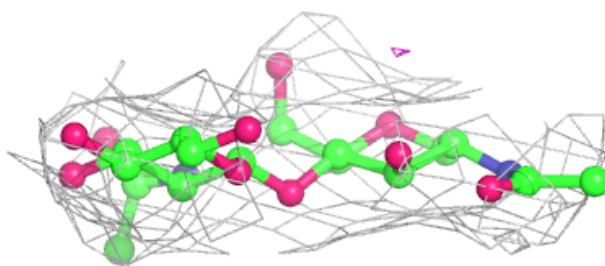
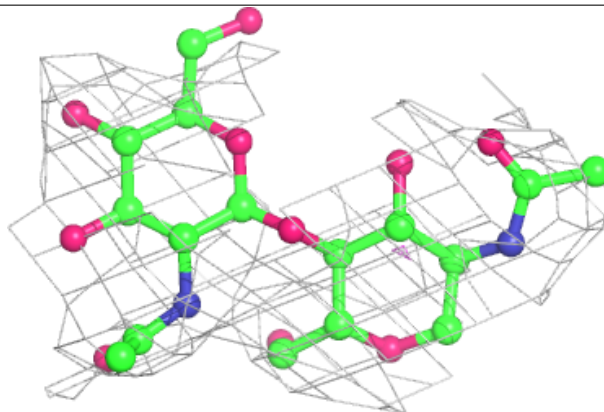
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**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)

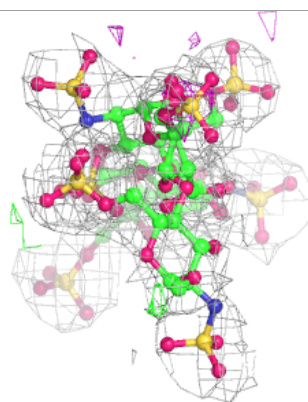
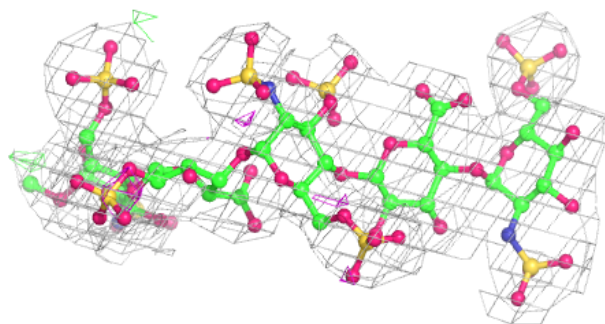
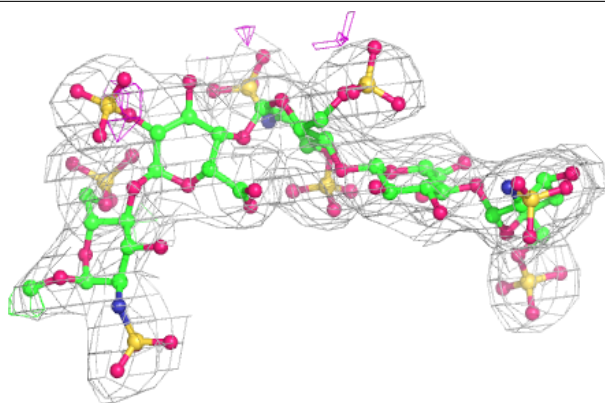
**Electron density around Chain E:**

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

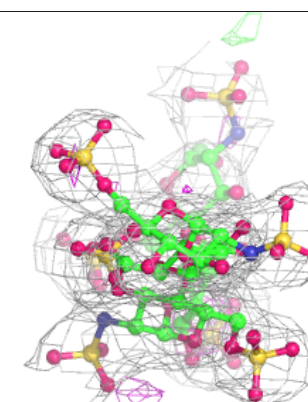
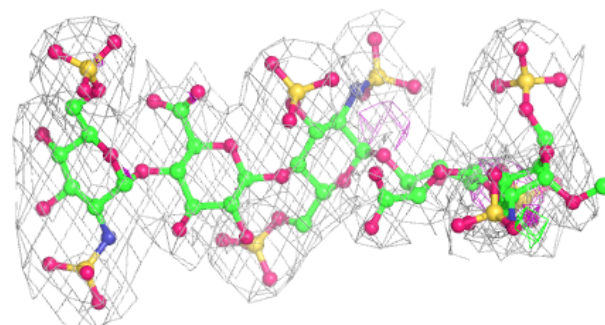
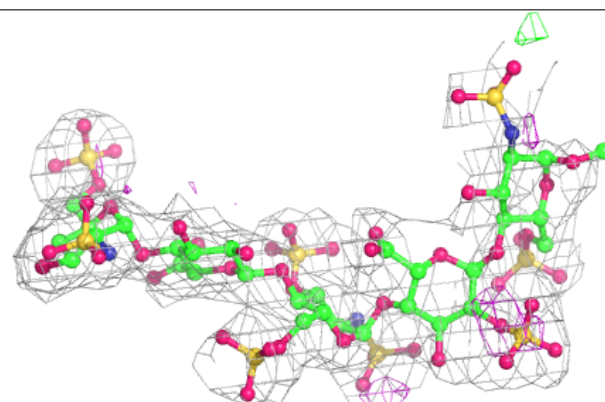


**Electron density around Chain F:**

$2mF_o-DF_c$  (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
8	NAG	I	501	14/15	0.64	0.26	103,108,110,110	0
8	NAG	I	701	14/15	0.64	0.50	92,94,97,97	0
8	NAG	C	501	14/15	0.67	0.26	102,109,110,110	0
8	NAG	C	701	14/15	0.69	0.47	92,94,97,97	0
7	CA	B	401	1/1	0.96	0.04	12,12,12,12	0
7	CA	H	401	1/1	0.98	0.09	19,19,19,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.