



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 12, 2021 – 10:22 AM EDT

PDB ID : 2B5T  
Title : 2.1 Angstrom structure of a nonproductive complex between antithrombin, synthetic heparin mimetic SR123781 and two S195A thrombin molecules  
Authors : Johnson, D.J.; Li, W.; Luis, S.A.; Carrell, R.W.; Huntington, J.A.  
Deposited on : 2005-09-29  
Resolution : 2.10 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

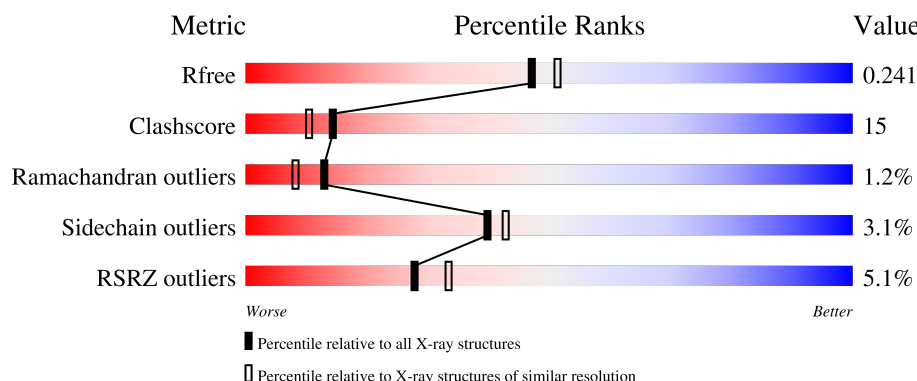
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	49	<div> <div>2%</div> <div>65%</div> <div>31%</div> <div>.</div> </div>
1	C	49	<div> <div>6%</div> <div>80%</div> <div>14%</div> <div>6%</div> </div>
2	B	259	<div> <div>2%</div> <div>75%</div> <div>20%</div> <div>.</div> <div>.</div> </div>
2	D	259	<div> <div>4%</div> <div>78%</div> <div>19%</div> <div>.</div> </div>
3	I	432	<div> <div>8%</div> <div>60%</div> <div>33%</div> <div>.</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
4	E	2	 50% 50%
4	F	2	 50% 50%
5	G	16	 44% 56%
6	H	7	 57% 14% 29%
7	J	2	 50% 50%

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	NAG	E	1	-	-	X	-
4	FUC	E	2	-	-	X	X
4	NAG	F	1	X	-	-	-
4	FUC	F	2	-	-	-	X
5	GU8	G	10	-	-	-	X
5	GU8	G	12	-	-	X	-
5	GU6	G	15	X	-	-	-
6	NAG	H	1	X	-	-	-
6	NAG	H	2	-	-	-	X
6	MAN	H	6	-	-	-	X
7	NAG	J	2	-	-	-	X
8	GOL	A	1102	-	-	X	-
8	GOL	B	1103	-	-	X	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 9026 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 Thrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	47	Total	C	N	O	S	0	1	0
			394	245	65	83	1			
1	C	46	Total	C	N	O	S	0	0	0
			372	233	60	78	1			

- Molecule 2 is a protein called Thrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	252	Total	C	N	O	S	0	3	0
			2065	1317	368	366	14			
2	D	252	Total	C	N	O	S	0	0	0
			2022	1290	353	365	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	195	ALA	SER	engineered mutation	UNP P00734
D	195	ALA	SER	engineered mutation	UNP P00734

- Molecule 3 is a protein called Antithrombin-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	415	Total	C	N	O	S	0	0	0
			3233	2065	540	609	19			

There are 3 discrepancies between the modelled and reference sequences:

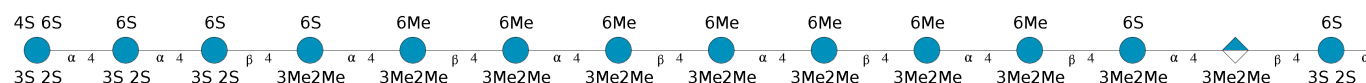
Chain	Residue	Modelled	Actual	Comment	Reference
I	137	ALA	SER	engineered mutation	UNP P01008
I	317	CYS	VAL	engineered mutation	UNP P01008
I	401	CYS	THR	engineered mutation	UNP P01008

- Molecule 4 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



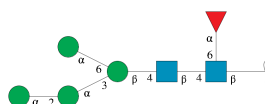
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	0	0	0
			24	14	1	9			
4	F	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 5 is an oligosaccharide called 2,3,4,6-tetra-O-sulfonato-alpha-D-glucopyranose-(1-4)-2,3,6-tri-O-sulfo-alpha-D-glucopyranose-(1-4)-2,3,6-tri-O-sulfonato-beta-D-glucopyranose-(1-4)-2,3-di-O-methyl-6-O-sulfonato-alpha-D-glucopyranose-(1-4)-2,3,6-tri-O-methyl-beta-D-glucopyranose-(1-4)-2,3,6-tri-O-methyl-alpha-D-glucopyranose-(1-4)-2,3,6-tri-O-methyl-beta-D-glucopyranose-(1-4)-2,3,6-tri-O-methyl-alpha-D-glucopyranose-(1-4)-2,3,6-tri-O-methyl-beta-D-glucopyranose-(1-4)-2,3-di-O-methyl-6-O-sulfonato-alpha-D-glucopyranose-(1-4)-2,3-di-O-methyl-beta-D-glucopyranuronic acid-(1-4)-2,3,6-tri-O-sulfo-alpha-D-glucopyranose-(1-4)-2,3-di-O-methyl-alpha-L-idopyranuronic acid-(1-4)-methyl 3-O-methyl-2,6-di-O-sulfo-alpha-D-glucopyranoside.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	16	Total	C	O	S	0	0	0
			278	127	134	17			

- Molecule 6 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



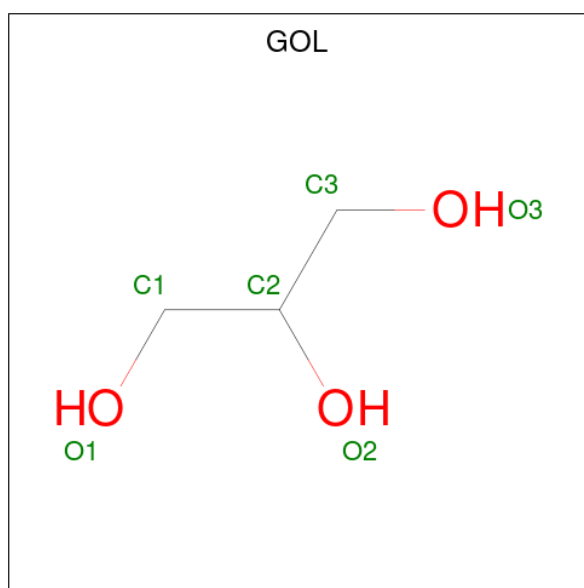
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	H	7	Total	C	N	O	0	0	0
			81	46	2	33			

- Molecule 7 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
7	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



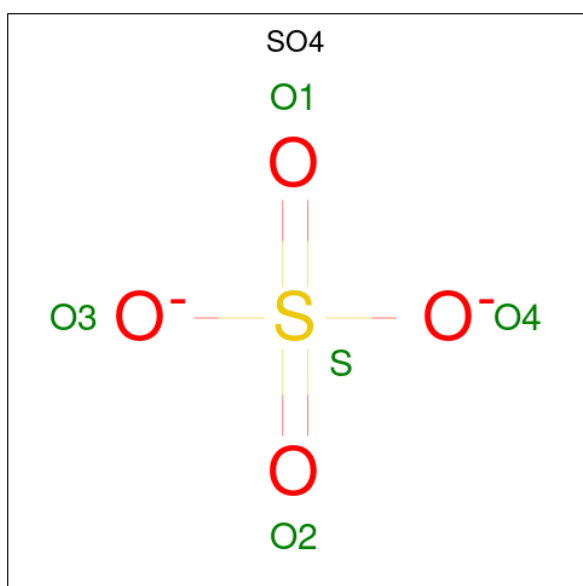
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

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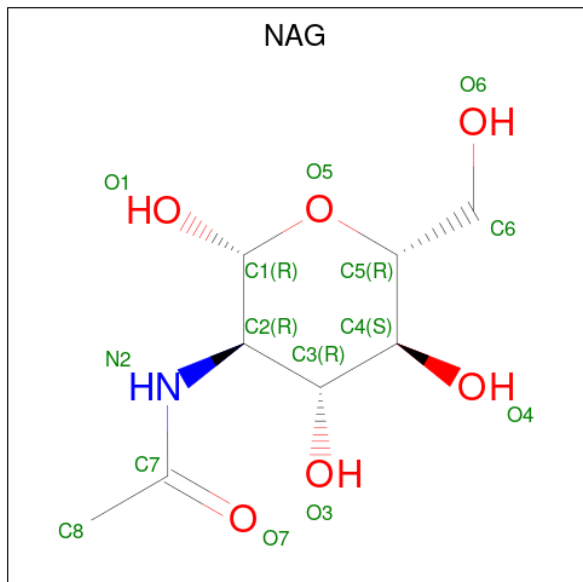
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		
8	I	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	I	1	Total	O	S	0	0
			5	4	1		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



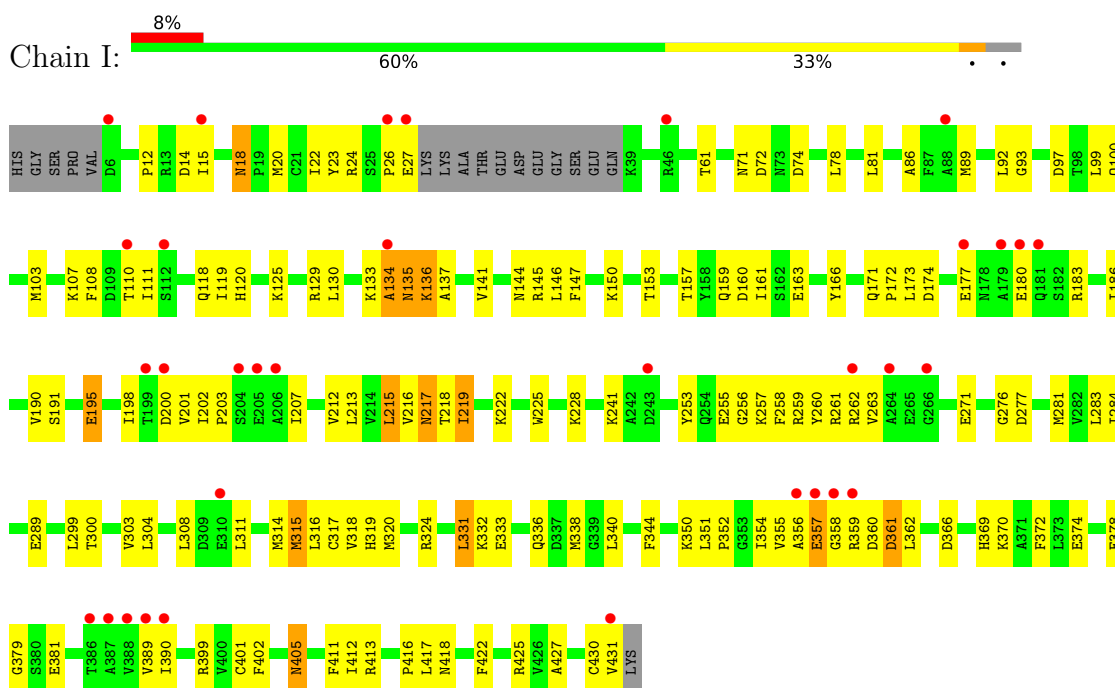
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	I	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	29	Total	O	0	0
			29	29		
11	B	132	Total	O	0	0
			132	132		
11	C	24	Total	O	0	0
			24	24		
11	D	117	Total	O	0	0
			117	117		
11	I	87	Total	O	0	0
			87	87		







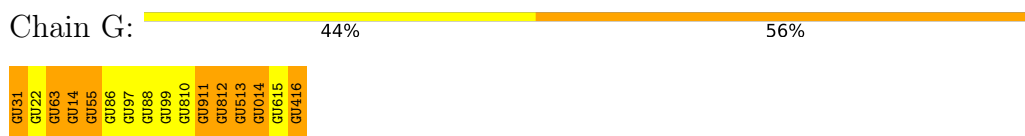
- Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose




- Molecule 5: 2,3,4,6-tetra-O-sulfonato-alpha-D-glucopyranose-(1-4)-2,3,6-tri-O-sulfo-alpha-D-glucopyranose-(1-4)-2,3,6-tri-O-sulfonato-beta-D-glucopyranose-(1-4)-2,3-di-O-methyl-6-O-sulfonato-alpha-D-glucopyranose-(1-4)-2,3,6-tri-O-methyl-beta-D-glucopyranose-(1-4)-2,3,6-tri-O-methyl-alpha-D-glucopyranose-(1-4)-2,3,6-tri-O-methyl-beta-D-glucopyranose-(1-4)-2,3,6-tri-O-methyl-alpha-D-glucopyranose-(1-4)-2,3,6-tri-O-methyl-beta-D-glucopyranose-(1-4)-2,3-di-O-methyl-6-O-sulfonato-alpha-D-glucopyranose-(1-4)-2,3-di-O-methyl-beta-D-glucopyranuronic acid-(1-4)-2,3,6-tri-O-sulfo-alpha-D-glucopyranose-(1-4)-2,3-di-O-methyl-alpha-L-idopyranuronic acid-(1-4)-methyl 3-O-methyl-2,6-di-O-sulfo-alpha-D-glucopyranoside



- Molecule 6: 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)-[alpha-L-

fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  57% 14% 29%

 MAG1  
MAG2  
BFA3  
MAN4  
MAN5  
MAN6  
FUC7

● Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%

 MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.28Å 59.53Å 108.41Å 77.55° 78.94° 68.08°	Depositor
Resolution (Å)	35.70 – 2.10 35.72 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.4 (35.70-2.10) 92.5 (35.72-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 2.10Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.209 , 0.247 0.199 , 0.241	Depositor DCC
$R_{free}$ test set	2937 reflections (4.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.6	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 61.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9026	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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: GU0, MAN, GU9, GU5, GU6, GU2, GU4, GU1, BMA, GOL, NAG, FUC, GU8, GU3, SO4

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	0.40	0/401	0.66	0/535
1	C	0.42	0/379	0.66	0/506
2	B	0.36	0/2118	0.66	0/2859
2	D	0.35	0/2074	0.64	0/2805
3	I	0.39	0/3299	0.65	2/4470 (0.0%)
All	All	0.38	0/8271	0.65	2/11175 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	402	PHE	N-CA-C	-5.51	96.14	111.00
3	I	360	ASP	N-CA-C	-5.47	96.24	111.00

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	394	0	369	15	0
1	C	372	0	346	5	0
2	B	2065	0	2030	52	0
2	D	2022	0	1965	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	3233	0	3143	122	0
4	E	24	0	22	8	0
4	F	24	0	22	4	0
5	G	278	0	192	26	0
6	H	81	0	68	6	0
7	J	28	0	25	1	0
8	A	12	0	16	5	0
8	B	30	0	40	4	0
8	D	24	0	32	4	0
8	I	6	0	8	2	0
9	B	20	0	0	2	0
9	D	5	0	0	0	0
9	I	5	0	0	0	0
10	I	14	0	13	0	0
11	A	29	0	0	0	0
11	B	132	0	0	0	0
11	C	24	0	0	0	0
11	D	117	0	0	1	0
11	I	87	0	0	4	0
All	All	9026	0	8291	262	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 15.

The worst 5 of 262 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)
2:B:93[A]:ARG:HH11	2:B:93[A]:ARG:HB3	1.09	1.14
3:I:129:ARG:HD3	3:I:417:LEU:HD11	1.35	1.03
3:I:358:GLY:HA2	3:I:361:ASP:OD1	1.66	0.94
2:D:18:GLU:HG3	2:D:187:ARG:HG3	1.50	0.94
3:I:361:ASP:HB3	11:I:2052:HOH:O	1.68	0.92

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
1	C	44/49 (90%)	42 (96%)	2 (4%)	0	100	100
2	B	251/259 (97%)	244 (97%)	7 (3%)	0	100	100
2	D	248/259 (96%)	239 (96%)	9 (4%)	0	100	100
3	I	411/432 (95%)	378 (92%)	21 (5%)	12 (3%)	4	1
All	All	1000/1048 (95%)	948 (95%)	40 (4%)	12 (1%)	13	8

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	134	ALA
3	I	136	LYS
3	I	195	GLU
3	I	241	LYS
3	I	357	GLU

### 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	43/43 (100%)	43 (100%)	0	100	100
1	C	40/43 (93%)	39 (98%)	1 (2%)	47	52
2	B	220/224 (98%)	210 (96%)	10 (4%)	27	27
2	D	214/224 (96%)	210 (98%)	4 (2%)	57	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	345/382 (90%)	331 (96%)	14 (4%)	30	31
All	All	862/916 (94%)	833 (97%)	29 (3%)	40	39

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	101	ARG
3	I	405	ASN
3	I	141	VAL
3	I	333	GLU
3	I	97	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
3	I	217	ASN
3	I	405	ASN
3	I	319	HIS
2	D	205	ASN
3	I	181	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 ⓘ

29 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	E	1	2,4	14,14,15	0.66	0	17,19,21	0.95	1 (5%)
4	FUC	E	2	4	10,10,11	0.61	0	14,14,16	0.71	0
4	NAG	F	1	2,4	14,14,15	0.71	0	17,19,21	0.86	1 (5%)
4	FUC	F	2	4	10,10,11	0.58	0	14,14,16	0.74	0
5	GU3	G	1	5	22,22,22	1.68	3 (13%)	28,33,33	1.11	1 (3%)
5	GU8	G	10	5	14,14,15	0.40	0	18,18,20	0.63	0
5	GU9	G	11	5	14,14,15	0.49	0	18,18,20	1.74	2 (11%)
5	GU8	G	12	5	14,14,15	0.39	0	18,18,20	0.88	1 (5%)
5	GU5	G	13	5	17,17,18	1.33	1 (5%)	22,24,26	0.76	0
5	GU0	G	14	5	23,23,24	1.91	4 (17%)	25,36,38	0.97	2 (8%)
5	GU6	G	15	5	23,23,24	3.31	10 (43%)	25,36,38	4.05	9 (36%)
5	GU4	G	16	5	27,27,28	2.00	5 (18%)	29,43,45	1.09	2 (6%)
5	GU2	G	2	5	11,14,15	0.44	0	13,19,21	0.74	0
5	GU6	G	3	5	23,23,24	1.93	4 (17%)	25,36,38	1.36	3 (12%)
5	GU1	G	4	5	11,14,15	0.43	0	13,19,21	0.84	1 (7%)
5	GU5	G	5	5	17,17,18	1.33	1 (5%)	22,24,26	1.24	2 (9%)
5	GU8	G	6	5	14,14,15	0.40	0	18,18,20	0.62	0
5	GU9	G	7	5	14,14,15	0.42	0	18,18,20	0.68	0
5	GU8	G	8	5	14,14,15	0.42	0	18,18,20	0.62	0
5	GU9	G	9	5	14,14,15	0.39	0	18,18,20	0.69	0
6	NAG	H	1	6,3	14,14,15	0.67	0	17,19,21	0.84	1 (5%)
6	NAG	H	2	6	14,14,15	0.58	0	17,19,21	0.80	1 (5%)
6	BMA	H	3	6	11,11,12	0.61	0	15,15,17	0.47	0
6	MAN	H	4	6	11,11,12	0.69	0	15,15,17	0.68	0
6	MAN	H	5	6	10,10,12	0.54	0	13,13,17	0.58	0
6	MAN	H	6	6	11,11,12	0.58	0	15,15,17	0.73	0
6	FUC	H	7	6	10,10,11	0.56	0	14,14,16	0.73	0
7	NAG	J	1	7,3	14,14,15	0.64	0	17,19,21	0.91	1 (5%)
7	NAG	J	2	7	14,14,15	0.55	0	17,19,21	0.60	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	E	1	2,4	-	4/6/23/26	0/1/1/1
4	FUC	E	2	4	-	-	0/1/1/1
4	NAG	F	1	2,4	1/1/5/7	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUC	F	2	4	-	-	0/1/1/1
5	GU3	G	1	5	-	2/15/35/35	0/1/1/1
5	GU8	G	10	5	-	2/7/24/27	0/1/1/1
5	GU9	G	11	5	-	2/7/24/27	0/1/1/1
5	GU8	G	12	5	-	2/7/24/27	0/1/1/1
5	GU5	G	13	5	-	3/10/27/30	0/1/1/1
5	GU0	G	14	5	-	3/16/33/36	0/1/1/1
5	GU6	G	15	5	1/1/7/8	6/16/33/36	0/1/1/1
5	GU4	G	16	5	-	0/21/38/41	0/1/1/1
5	GU2	G	2	5	-	2/4/25/28	0/1/1/1
5	GU6	G	3	5	-	0/16/33/36	0/1/1/1
5	GU1	G	4	5	-	0/4/25/28	0/1/1/1
5	GU5	G	5	5	-	0/10/27/30	0/1/1/1
5	GU8	G	6	5	-	2/7/24/27	0/1/1/1
5	GU9	G	7	5	-	1/7/24/27	0/1/1/1
5	GU8	G	8	5	-	2/7/24/27	0/1/1/1
5	GU9	G	9	5	-	0/7/24/27	0/1/1/1
6	NAG	H	1	6,3	1/1/5/7	3/6/23/26	0/1/1/1
6	NAG	H	2	6	-	4/6/23/26	0/1/1/1
6	BMA	H	3	6	-	2/2/19/22	0/1/1/1
6	MAN	H	4	6	-	0/2/19/22	0/1/1/1
6	MAN	H	5	6	-	0/2/16/22	0/1/1/1
6	MAN	H	6	6	-	2/2/19/22	0/1/1/1
6	FUC	H	7	6	-	-	0/1/1/1
7	NAG	J	1	7,3	-	4/6/23/26	0/1/1/1
7	NAG	J	2	7	-	5/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	15	GU6	O2-C2	-6.72	1.36	1.47
5	G	15	GU6	C4-C5	-6.41	1.39	1.53
5	G	15	GU6	O6-S6	-5.13	1.43	1.56
5	G	13	GU5	O6-S6	-4.97	1.43	1.56
5	G	1	GU3	O6-S6	-4.97	1.43	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	15	GU6	O2-C2-C3	16.09	124.46	106.65
5	G	11	GU9	O4-C4-C3	-6.54	92.60	109.94
5	G	15	GU6	O4-C4-C3	6.49	127.14	109.94
5	G	15	GU6	C6-C5-C4	5.53	123.63	112.09
5	G	15	GU6	O5-C5-C6	4.83	118.31	107.61

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	F	1	NAG	C1
5	G	15	GU6	C5
6	H	1	NAG	C1

5 of 55 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	1	GU3	O5-C1-O1-C8
5	G	1	GU3	C2-C1-O1-C8
5	G	7	GU9	C3-C2-O2-C7
5	G	13	GU5	C3-C2-O2-C7
5	G	14	GU0	C3-O3-S3-O26

There are no ring outliers.

24 monomers are involved in 45 short contacts:

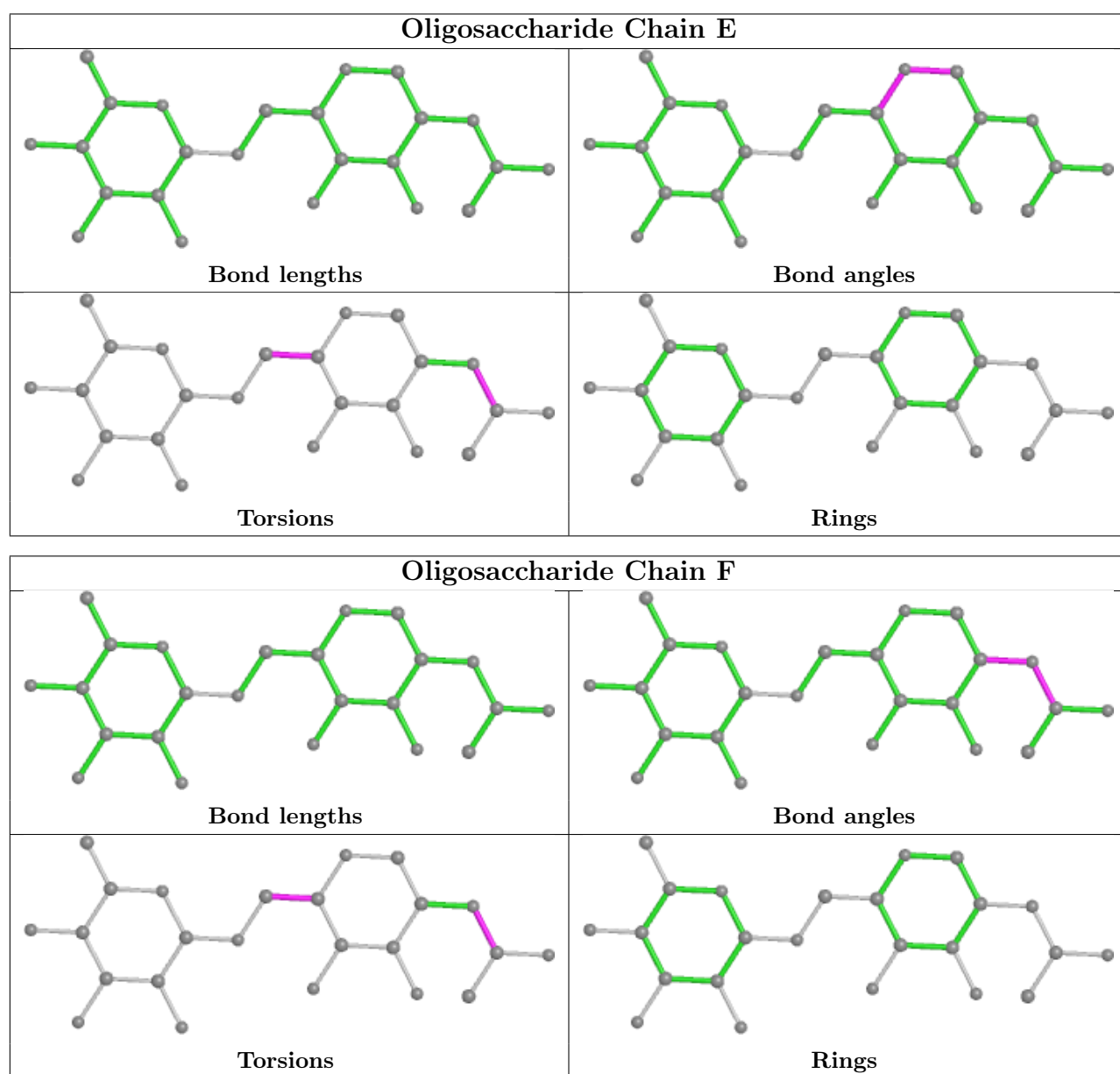
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	14	GU0	1	0
5	G	9	GU9	2	0
5	G	16	GU4	2	0
4	F	2	FUC	4	0
4	E	2	FUC	6	0
7	J	1	NAG	1	0
5	G	4	GU1	3	0
6	H	1	NAG	6	0
6	H	2	NAG	1	0
5	G	5	GU5	2	0
5	G	8	GU8	2	0
5	G	12	GU8	7	0
5	G	6	GU8	1	0
5	G	2	GU2	1	0
4	F	1	NAG	4	0
5	G	7	GU9	4	0
7	J	2	NAG	1	0

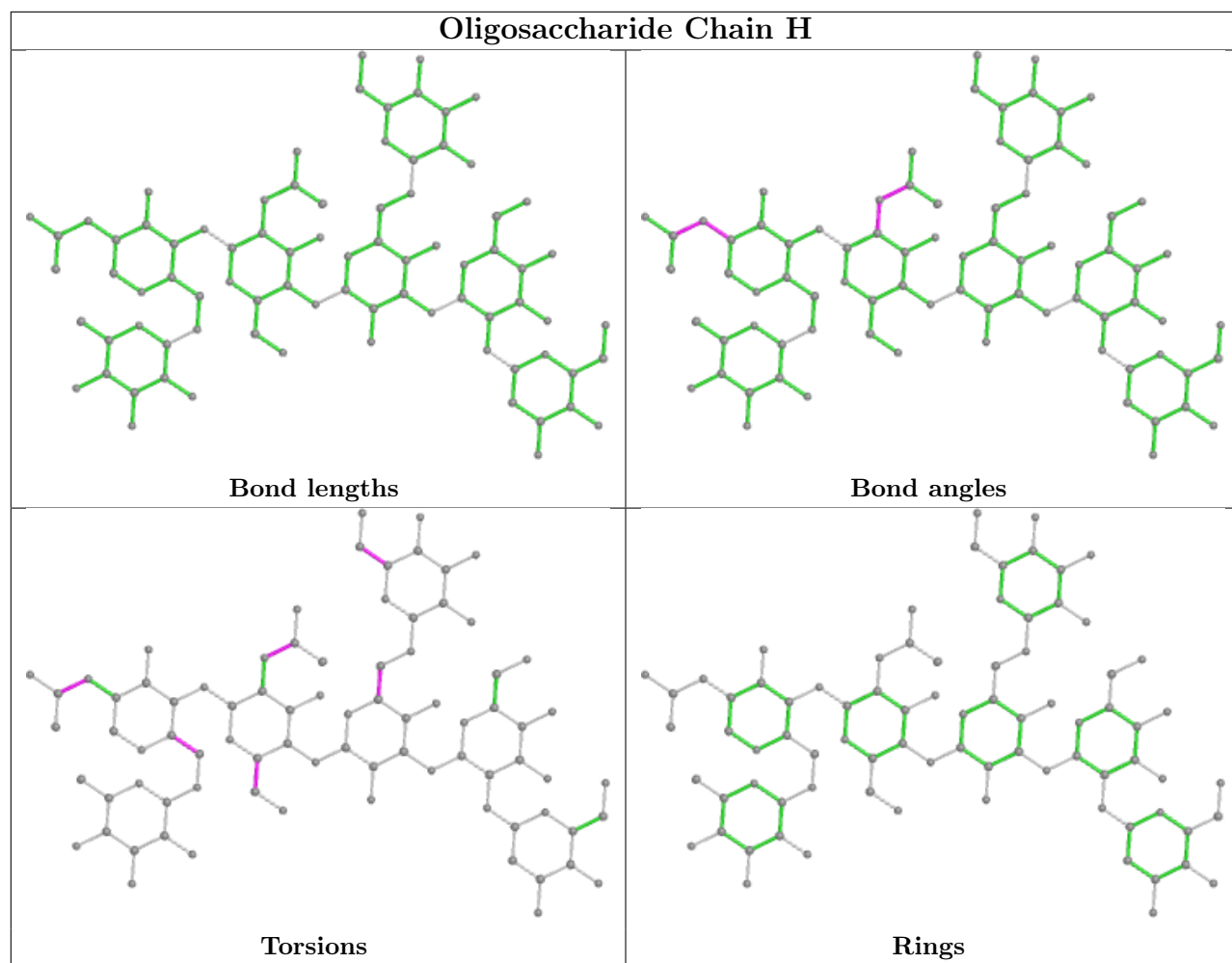
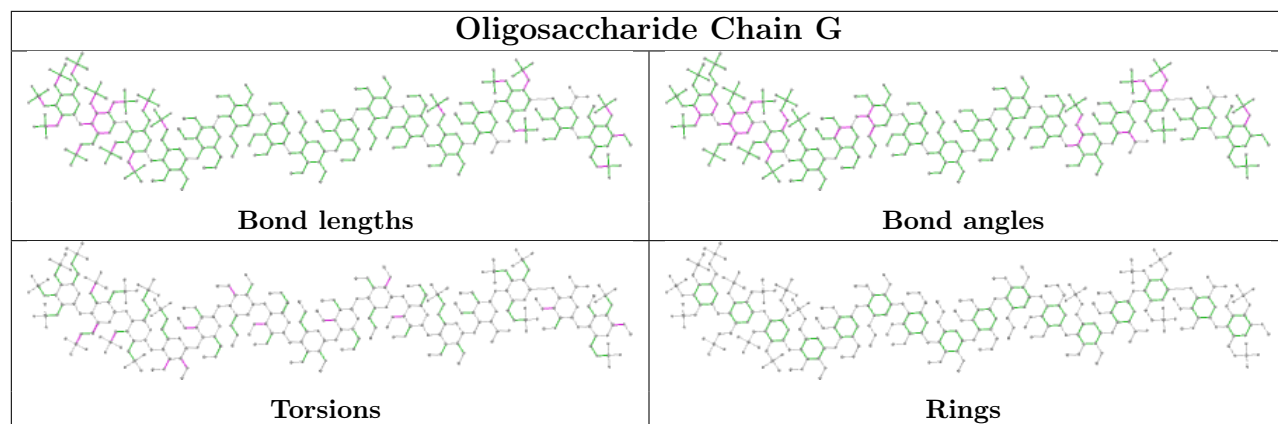
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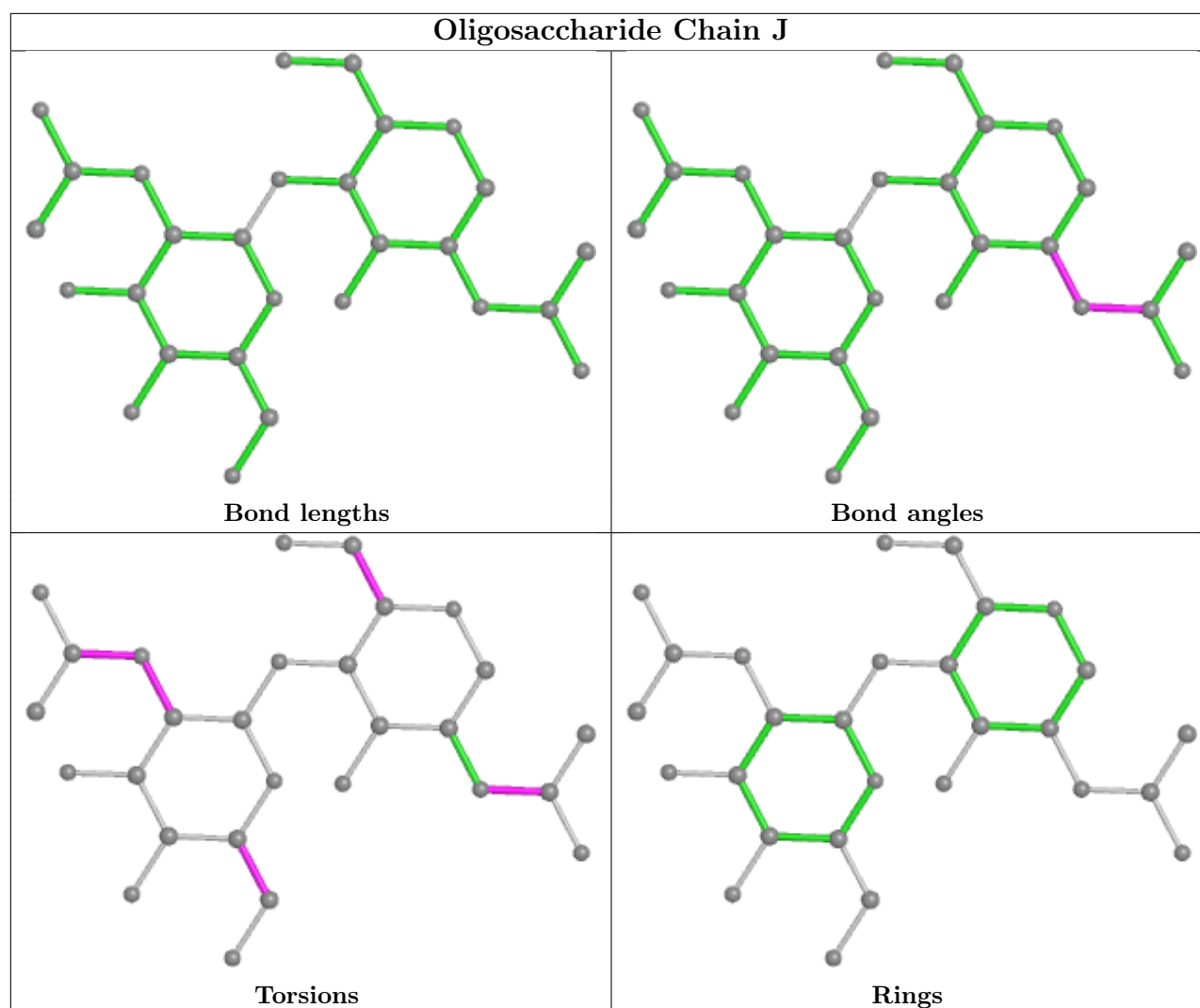
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	11	GU9	2	0
5	G	1	GU3	2	0
5	G	13	GU5	2	0
4	E	1	NAG	8	0
6	H	7	FUC	5	0
5	G	3	GU6	2	0
5	G	10	GU8	1	0

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







## 5.6 Ligand geometry [i](#)

19 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	$\# Z  > 2$
8	GOL	D	1110	-	5,5,5	0.73	0	5,5,5	0.43	0
9	SO4	D	2004	-	4,4,4	0.24	0	6,6,6	0.09	0
8	GOL	I	1112	-	5,5,5	0.67	0	5,5,5	0.39	0
9	SO4	B	2003	-	4,4,4	0.23	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	GOL	A	1102	-	5,5,5	0.72	0	5,5,5	0.48	0
9	SO4	B	2001	-	4,4,4	0.24	0	6,6,6	0.10	0
8	GOL	B	1105	-	5,5,5	0.68	0	5,5,5	0.41	0
8	GOL	D	1106	-	5,5,5	0.62	0	5,5,5	0.41	0
8	GOL	B	1104	-	5,5,5	0.63	0	5,5,5	0.41	0
8	GOL	B	1101	-	5,5,5	0.81	0	5,5,5	0.43	0
8	GOL	B	1103	-	5,5,5	0.76	0	5,5,5	0.43	0
8	GOL	B	1109	-	5,5,5	0.70	0	5,5,5	0.43	0
10	NAG	I	801	3	14,14,15	0.56	0	17,19,21	0.66	0
9	SO4	B	2002	-	4,4,4	0.25	0	6,6,6	0.07	0
8	GOL	D	1111	-	5,5,5	0.75	0	5,5,5	0.47	0
9	SO4	B	2006	-	4,4,4	0.30	0	6,6,6	0.08	0
9	SO4	I	2005	-	4,4,4	0.30	0	6,6,6	0.11	0
8	GOL	A	1108	-	5,5,5	0.74	0	5,5,5	0.51	0
8	GOL	D	1107	-	5,5,5	0.62	0	5,5,5	0.34	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	GOL	D	1110	-	-	0/4/4/4	-
8	GOL	B	1101	-	-	4/4/4/4	-
8	GOL	D	1111	-	-	2/4/4/4	-
8	GOL	B	1103	-	-	0/4/4/4	-
8	GOL	A	1102	-	-	4/4/4/4	-
8	GOL	B	1105	-	-	1/4/4/4	-
8	GOL	B	1109	-	-	3/4/4/4	-
8	GOL	D	1106	-	-	2/4/4/4	-
8	GOL	I	1112	-	-	2/4/4/4	-
8	GOL	B	1104	-	-	2/4/4/4	-
10	NAG	I	801	3	-	4/6/23/26	0/1/1/1
8	GOL	A	1108	-	-	0/4/4/4	-
8	GOL	D	1107	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.



5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1102	GOL	O1-C1-C2-C3
8	A	1102	GOL	C1-C2-C3-O3
8	A	1102	GOL	O2-C2-C3-O3
8	B	1101	GOL	O1-C1-C2-C3
8	B	1101	GOL	C1-C2-C3-O3

There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	1110	GOL	1	0
8	I	1112	GOL	2	0
8	A	1102	GOL	5	0
8	D	1106	GOL	1	0
8	B	1103	GOL	4	0
9	B	2002	SO4	1	0
8	D	1111	GOL	1	0
9	B	2006	SO4	1	0
8	D	1107	GOL	1	0

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	47/49 (95%)	-0.11	1 (2%) 63 68	22, 34, 47, 66	1 (2%)
1	C	46/49 (93%)	0.03	3 (6%) 18 23	28, 38, 51, 58	0
2	B	252/259 (97%)	0.07	5 (1%) 65 69	14, 31, 50, 63	3 (1%)
2	D	252/259 (97%)	0.14	10 (3%) 38 44	18, 33, 47, 64	0
3	I	415/432 (96%)	0.48	33 (7%) 12 16	34, 51, 77, 89	0
All	All	1012/1048 (96%)	0.25	52 (5%) 28 33	14, 41, 68, 89	4 (0%)

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	388	VAL	7.1
3	I	358	GLY	6.1
3	I	386	THR	5.6
3	I	431	VAL	5.6
3	I	134	ALA	4.4

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

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

### 6.3 Carbohydrates ⓘ

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
4	NAG	E	1	14/15	0.46	0.38	73,77,84,88	0

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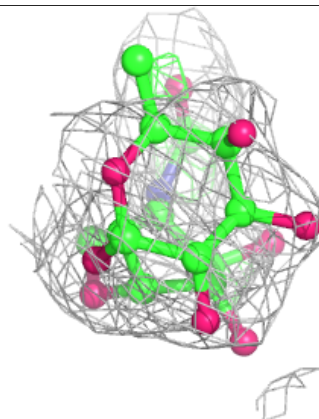
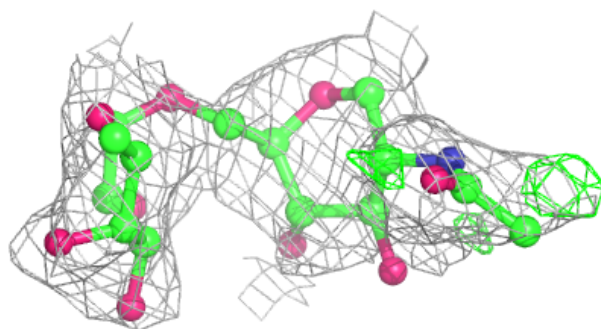
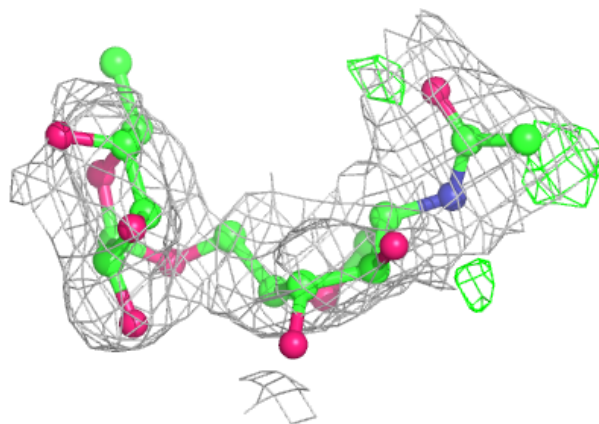
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MAN	H	6	11/12	0.51	0.67	115,116,117,118	0
7	NAG	J	2	14/15	0.58	0.45	102,104,105,106	0
6	MAN	H	5	10/12	0.66	0.34	103,104,105,105	0
6	BMA	H	3	11/12	0.70	0.33	103,105,110,113	0
6	MAN	H	4	11/12	0.71	0.32	99,101,102,103	0
4	FUC	F	2	10/11	0.72	0.47	83,84,85,85	0
7	NAG	J	1	14/15	0.74	0.23	92,94,96,99	0
4	NAG	F	1	14/15	0.74	0.32	59,66,74,80	0
5	GU8	G	10	14/15	0.76	0.50	90,92,93,94	0
5	GU9	G	11	14/15	0.77	0.36	70,86,88,89	0
4	FUC	E	2	10/11	0.80	0.43	90,91,91,91	0
6	NAG	H	2	14/15	0.80	0.42	98,100,101,103	0
6	NAG	H	1	14/15	0.82	0.30	83,88,94,98	0
6	FUC	H	7	10/11	0.84	0.47	101,103,104,104	0
5	GU9	G	7	14/15	0.86	0.24	72,75,80,81	0
5	GU9	G	9	14/15	0.89	0.23	84,84,87,88	0
5	GU8	G	8	14/15	0.90	0.27	81,83,84,85	0
5	GU8	G	12	14/15	0.92	0.21	50,59,63,65	0
5	GU2	G	2	14/15	0.92	0.17	61,64,69,70	0
5	GU8	G	6	14/15	0.94	0.12	60,63,69,69	0
5	GU3	G	1	22/22	0.94	0.14	56,61,66,67	0
5	GU6	G	3	23/24	0.95	0.10	47,61,65,67	0
5	GU1	G	4	14/15	0.96	0.08	51,54,57,57	0
5	GU5	G	5	17/18	0.96	0.10	52,58,59,61	0
5	GU6	G	15	23/24	0.97	0.11	25,30,32,37	0
5	GU5	G	13	17/18	0.98	0.09	34,42,47,47	0
5	GU0	G	14	23/24	0.98	0.10	27,33,41,43	0
5	GU4	G	16	27/28	0.99	0.09	22,26,30,33	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.

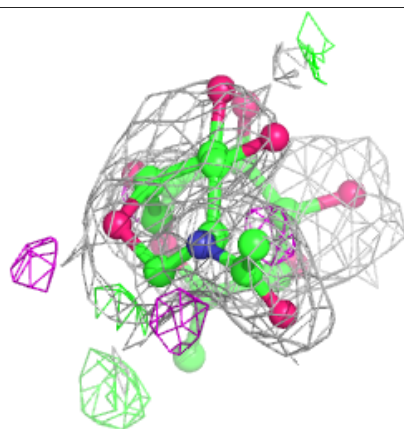
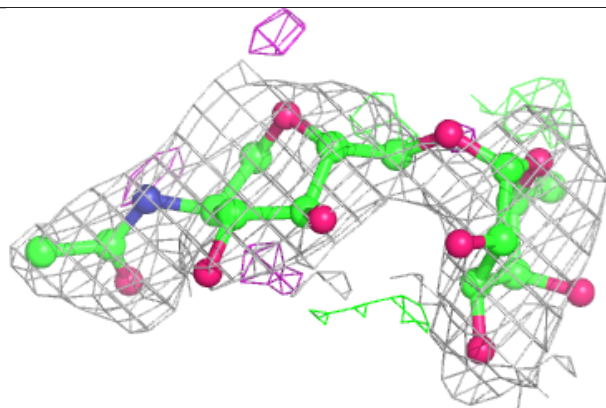
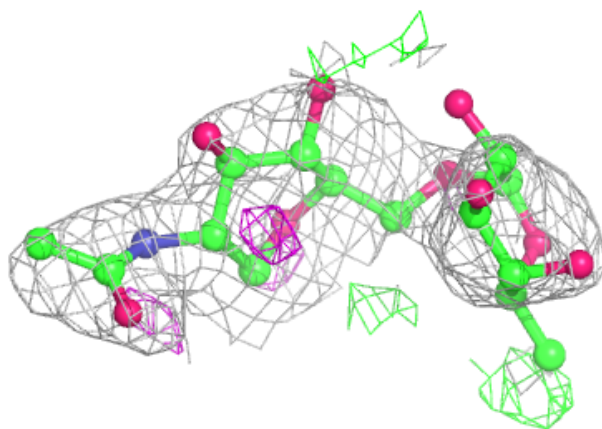
**Electron density around Chain E:**

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

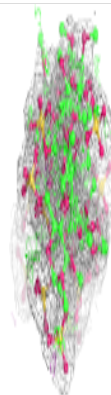
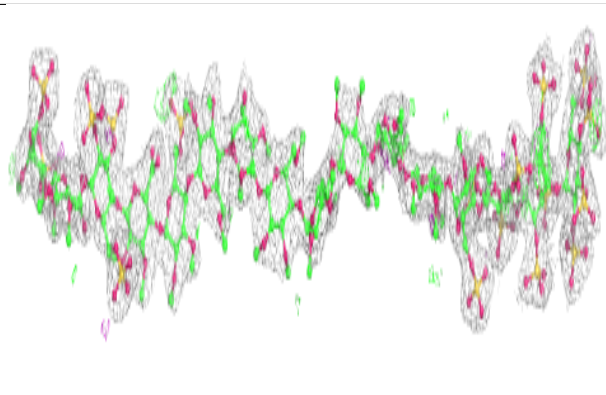
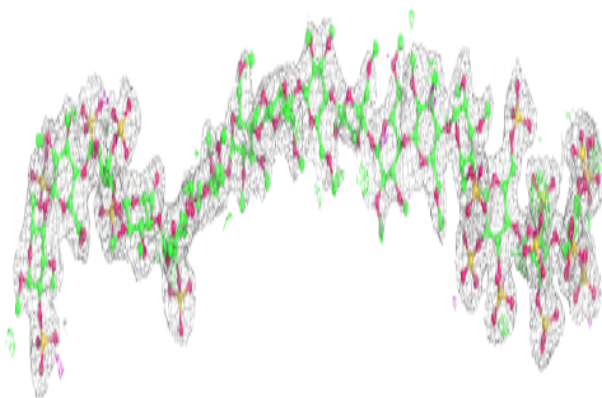


**Electron density around Chain F:**

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and green (positive)

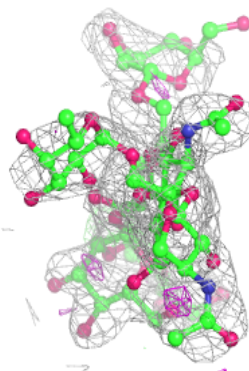
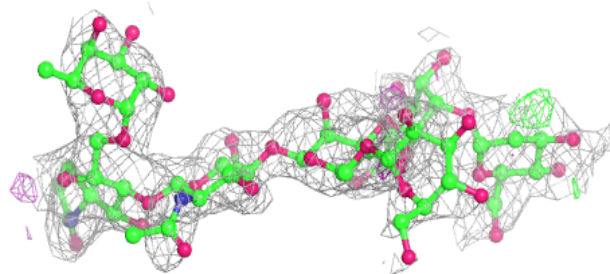
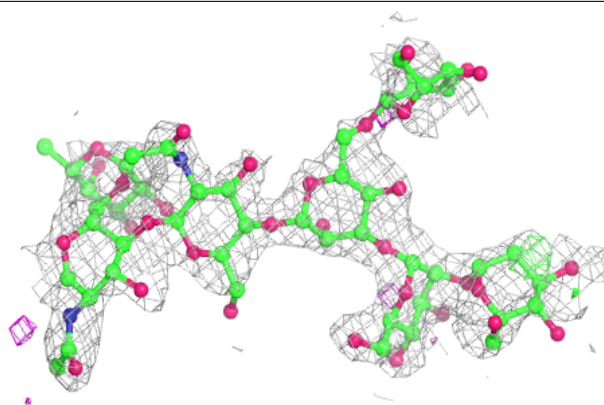
**Electron density around Chain G:**

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

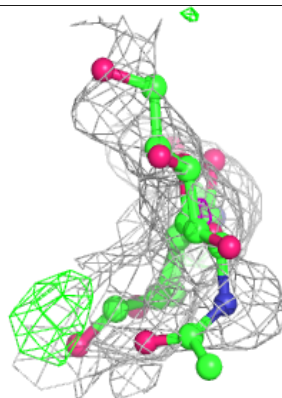
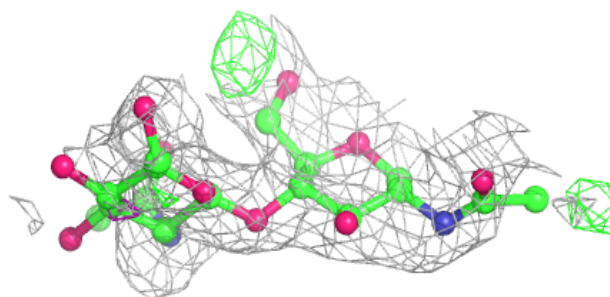
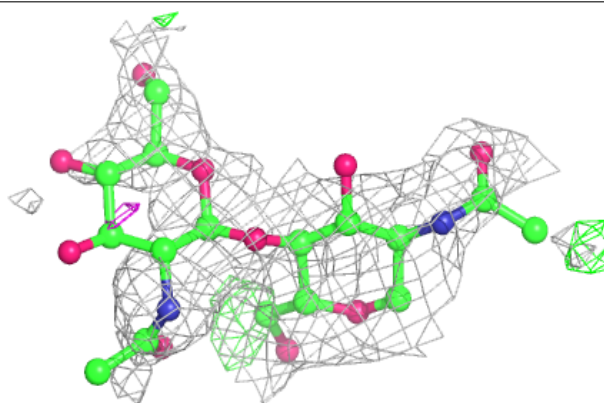


**Electron density around Chain H:**

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

**Electron density around Chain J:**

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





## 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	GOL	B	1101	6/6	0.73	0.35	49,55,57,60	0
8	GOL	I	1112	6/6	0.78	0.27	80,81,81,82	0
8	GOL	B	1103	6/6	0.80	0.20	63,65,65,66	0
8	GOL	D	1110	6/6	0.81	0.23	72,75,76,77	0
8	GOL	B	1105	6/6	0.84	0.25	95,95,95,95	0
8	GOL	A	1108	6/6	0.85	0.26	73,76,77,78	0
8	GOL	B	1109	6/6	0.86	0.17	62,62,64,64	0
8	GOL	D	1111	6/6	0.88	0.26	63,64,64,66	0
8	GOL	D	1106	6/6	0.88	0.13	66,67,67,68	0
8	GOL	A	1102	6/6	0.89	0.27	54,57,58,60	0
9	SO4	B	2003	5/5	0.89	0.21	85,86,87,88	0
10	NAG	I	801	14/15	0.89	0.21	66,68,73,74	0
9	SO4	B	2001	5/5	0.94	0.12	85,85,86,87	0
8	GOL	B	1104	6/6	0.95	0.13	30,35,37,46	0
8	GOL	D	1107	6/6	0.95	0.13	32,41,44,45	0
9	SO4	B	2002	5/5	0.96	0.12	89,89,90,91	0
9	SO4	B	2006	5/5	0.97	0.19	56,56,58,59	0
9	SO4	I	2005	5/5	0.98	0.09	63,63,64,64	0
9	SO4	D	2004	5/5	0.98	0.10	61,63,64,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.