



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 27, 2023 – 11:41 AM EDT

PDB ID : 3H32  
Title : Crystal structure of D-dimer from human fibrin complexed with Gly-His-Arg-Pro-Tyr-amide  
Authors : Doolittle, R.F.; Pandi, L.  
Deposited on : 2009-04-15  
Resolution : 3.60 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

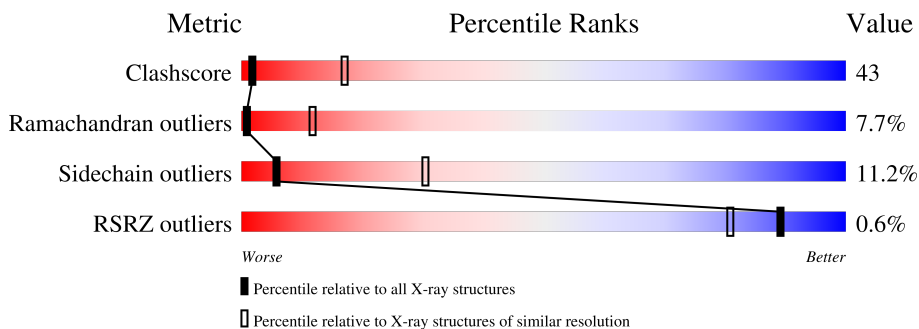
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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))
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	197	
1	D	197	
2	B	458	
2	E	458	
3	C	317	
3	F	317	
4	M	5	

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Mol	Chain	Length	Quality of chain
4	N	5	 60% 40%
5	G	8	 62% 38%
5	H	8	 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
5	NAG	G	2	X	-	-	-
5	MAN	G	4	-	-	-	X
5	NAG	G	5	X	-	-	X
5	SIA	G	7	-	-	-	X
5	MAN	G	8	X	-	-	X
5	NAG	H	2	X	-	-	-
5	MAN	H	3	-	-	-	X
5	MAN	H	4	-	-	-	X
5	NAG	H	5	X	-	-	X
5	SIA	H	7	X	-	-	X
5	MAN	H	8	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11246 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 Fibrinogen alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	74	Total 608	C 377	N 115	O 113	S 3	0	0	0
1	D	74	Total 608	C 377	N 115	O 113	S 3	0	0	0

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	308	Total 2474	C 1544	N 434	O 474	S 22	0	0	0
2	E	308	Total 2474	C 1544	N 434	O 474	S 22	0	0	0

- Molecule 3 is a protein called Fibrinogen gamma chain, isoform gamma-A.

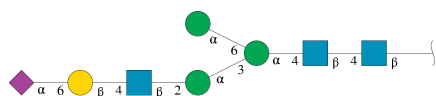
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	301	Total 2404	C 1523	N 405	O 465	S 11	0	0	0
3	F	296	Total 2372	C 1504	N 400	O 457	S 11	0	0	0

- Molecule 4 is a protein called Fibrin B knob pentapeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	M	5	Total 45	C 28	N 10	O 7	0	0	0
4	N	5	Total 45	C 28	N 10	O 7	0	0	0

- Molecule 5 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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.

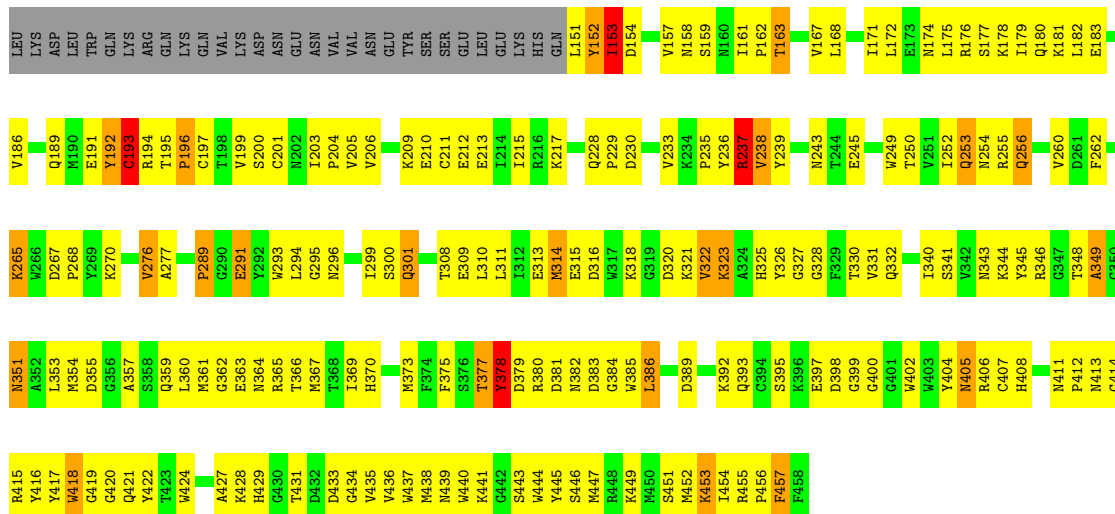


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
5	G	8	Total	C	N	O	0	0	0
			106	59	4	43			
5	H	8	Total	C	N	O	0	0	0
			106	59	4	43			

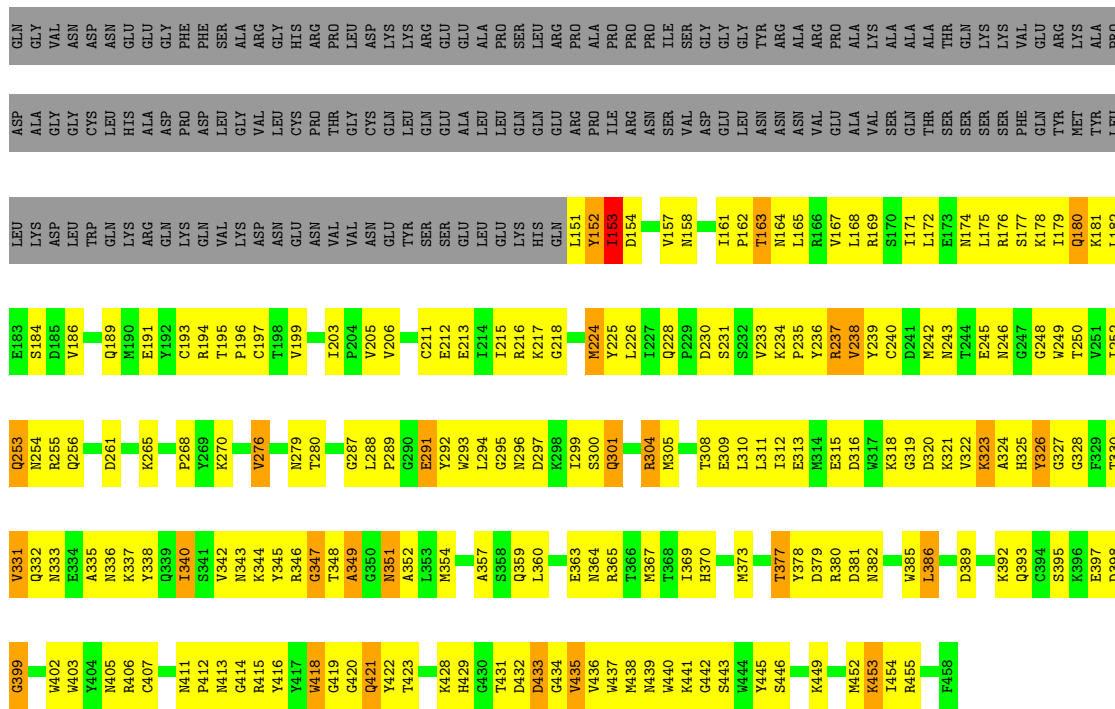
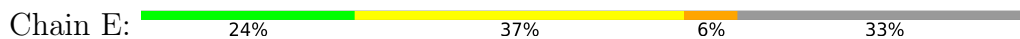
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	C	1	Total	Ca	0	0
			1	1		
6	E	1	Total	Ca	0	0
			1	1		
6	F	1	Total	Ca	0	0
			1	1		

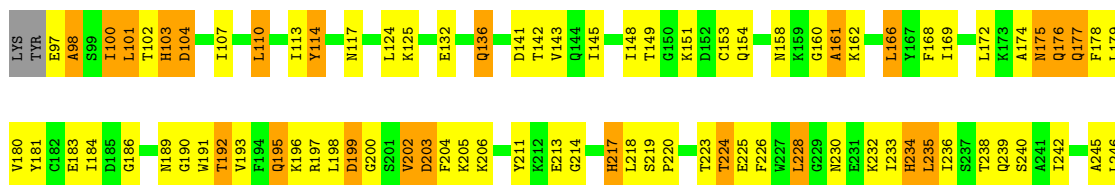
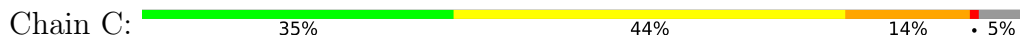


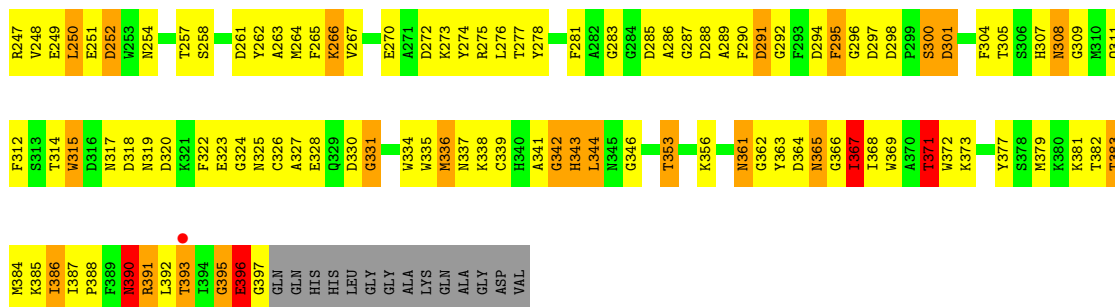


• Molecule 2: Fibrinogen beta chain



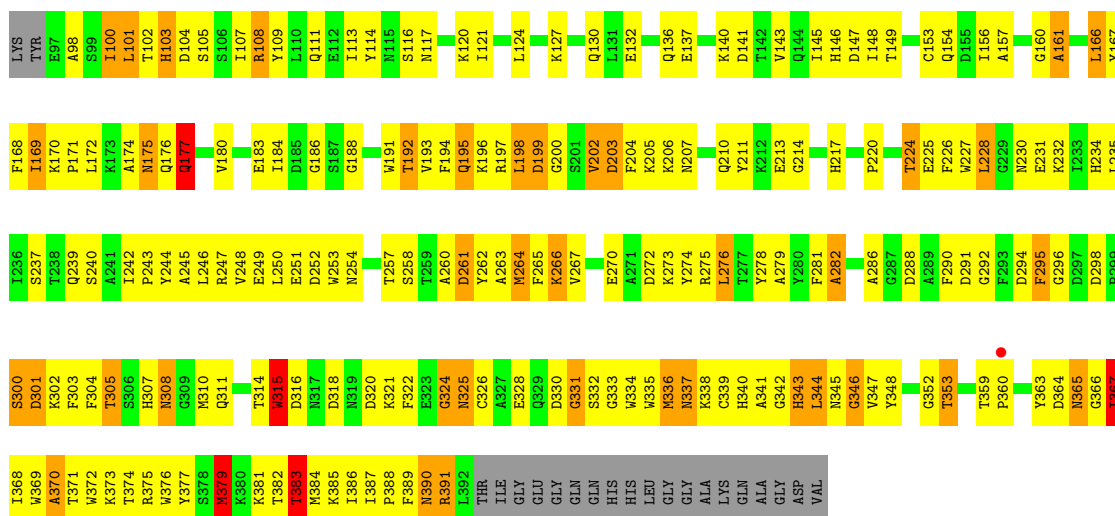
• Molecule 3: Fibrinogen gamma chain, isoform gamma-A





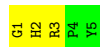
- Molecule 3: Fibrinogen gamma chain, isoform gamma-A

Chain F: 30% 50% 12% 7%



- Molecule 4: Fibrin B knob pentapeptide

Chain M: 40% 60%



- Molecule 4: Fibrin B knob pentapeptide

Chain N: 60% 40%



- Molecule 5: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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 G: 62% 38%





- Molecule 5: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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 H:  50% 50%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	264.72Å 97.32Å 132.49Å 90.00° 122.78° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 29.72 – 3.60	Depositor EDS
% Data completeness (in resolution range)	75.5 (50.00-3.60) 75.7 (29.72-3.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	30.66 (at 3.55Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.263 , 0.320 0.263 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	89.3	Xtrriage
Anisotropy	0.149	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 16.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.016 for -h-2*1,-k,l	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	11246	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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, SIA, GAL, 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	0.72	0/609	0.87	2/811 (0.2%)
1	D	0.64	0/609	0.82	1/811 (0.1%)
2	B	0.58	0/2536	0.71	0/3425
2	E	0.60	0/2536	0.72	1/3425 (0.0%)
3	C	0.59	0/2469	0.69	0/3339
3	F	0.55	0/2437	0.68	0/3296
4	M	0.56	0/47	0.67	0/61
4	N	0.58	0/47	0.50	0/61
All	All	0.59	0/11290	0.72	4/15229 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	CYS	CA-CB-SG	-9.69	96.56	114.00
1	D	161	CYS	CA-CB-SG	6.66	125.98	114.00
2	E	152	TYR	N-CA-C	5.32	125.37	111.00
1	A	124	ARG	N-CA-C	5.11	124.81	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	192	TYR	Sidechain

## 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	608	0	649	62	0
1	D	608	0	649	61	0
2	B	2474	0	2336	196	0
2	E	2474	0	2336	224	0
3	C	2404	0	2249	228	0
3	F	2372	0	2219	251	0
4	M	45	0	41	5	0
4	N	45	0	41	5	0
5	G	106	0	89	5	0
5	H	106	0	89	6	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
All	All	11246	0	10698	941	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 43.

The worst 5 of 941 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)
3:F:228:LEU:HG	3:F:232:LYS:HD2	1.22	1.15
2:E:415:ARG:H	2:E:434:GLY:HA2	0.98	1.14
3:F:338:LYS:N	3:F:339:CYS:HA	1.70	1.07
3:C:166:LEU:HD12	3:C:166:LEU:H	1.20	1.07
3:C:305:THR:HB	3:C:341:ALA:HB2	1.37	1.07

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	72/197 (36%)	62 (86%)	6 (8%)	4 (6%)	2	19
1	D	72/197 (36%)	62 (86%)	7 (10%)	3 (4%)	3	25
2	B	306/458 (67%)	230 (75%)	57 (19%)	19 (6%)	1	17
2	E	306/458 (67%)	226 (74%)	63 (21%)	17 (6%)	2	19
3	C	299/317 (94%)	199 (67%)	67 (22%)	33 (11%)	0	6
3	F	294/317 (93%)	211 (72%)	54 (18%)	29 (10%)	0	8
4	M	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
4	N	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
All	All	1355/1954 (69%)	994 (73%)	256 (19%)	105 (8%)	1	12

5 of 105 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	153	ILE
2	B	238	VAL
2	B	289	PRO
2	B	349	ALA
3	C	98	ALA

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	69/179 (38%)	58 (84%)	11 (16%)	2	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	69/179 (38%)	58 (84%)	11 (16%)	2	16
2	B	266/393 (68%)	239 (90%)	27 (10%)	7	34
2	E	266/393 (68%)	240 (90%)	26 (10%)	8	36
3	C	252/263 (96%)	223 (88%)	29 (12%)	5	29
3	F	249/263 (95%)	221 (89%)	28 (11%)	6	30
4	M	4/4 (100%)	4 (100%)	0	100	100
4	N	4/4 (100%)	4 (100%)	0	100	100
All	All	1179/1678 (70%)	1047 (89%)	132 (11%)	6	30

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	237	SER
3	F	295	PHE
3	F	390	ASN
3	C	195	GLN
3	C	192	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	118	ASN
3	F	177	GLN
3	F	308	ASN
3	C	177	GLN
3	C	158	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 i

16 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
5	NAG	G	1	5,2	14,14,15	0.63	0	17,19,21	0.99	1 (5%)
5	NAG	G	2	5	14,14,15	1.05	1 (7%)	17,19,21	1.28	2 (11%)
5	MAN	G	3	5	11,11,12	0.96	0	15,15,17	1.39	2 (13%)
5	MAN	G	4	5	11,11,12	1.17	1 (9%)	15,15,17	0.80	1 (6%)
5	NAG	G	5	5	14,14,15	1.40	2 (14%)	17,19,21	1.74	3 (17%)
5	GAL	G	6	5	11,11,12	1.11	0	15,15,17	0.78	0
5	SIA	G	7	5	20,20,21	1.79	5 (25%)	24,28,31	1.28	2 (8%)
5	MAN	G	8	5	11,11,12	0.75	0	15,15,17	1.10	2 (13%)
5	NAG	H	1	5,2	14,14,15	0.67	0	17,19,21	1.05	1 (5%)
5	NAG	H	2	5	14,14,15	1.11	0	17,19,21	1.32	2 (11%)
5	MAN	H	3	5	11,11,12	1.26	0	15,15,17	0.80	0
5	MAN	H	4	5	11,11,12	1.70	1 (9%)	15,15,17	1.59	4 (26%)
5	NAG	H	5	5	14,14,15	1.59	2 (14%)	17,19,21	0.89	1 (5%)
5	GAL	H	6	5	11,11,12	1.07	1 (9%)	15,15,17	0.74	0
5	SIA	H	7	5	20,20,21	2.80	7 (35%)	24,28,31	1.94	4 (16%)
5	MAN	H	8	5	11,11,12	0.92	0	15,15,17	1.04	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	1	5,2	-	4/6/23/26	0/1/1/1
5	NAG	G	2	5	1/1/5/7	4/6/23/26	0/1/1/1
5	MAN	G	3	5	-	2/2/19/22	0/1/1/1
5	MAN	G	4	5	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	5	5	1/1/5/7	6/6/23/26	0/1/1/1
5	GAL	G	6	5	-	2/2/19/22	0/1/1/1
5	SIA	G	7	5	-	6/18/34/38	0/1/1/1
5	MAN	G	8	5	1/1/4/5	2/2/19/22	0/1/1/1
5	NAG	H	1	5,2	-	4/6/23/26	0/1/1/1
5	NAG	H	2	5	1/1/5/7	6/6/23/26	0/1/1/1
5	MAN	H	3	5	-	2/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	NAG	H	5	5	1/1/5/7	4/6/23/26	0/1/1/1
5	GAL	H	6	5	-	2/2/19/22	0/1/1/1
5	SIA	H	7	5	1/1/8/9	4/18/34/38	1/1/1/1
5	MAN	H	8	5	-	1/2/19/22	0/1/1/1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	7	SIA	C7-C6	6.26	1.60	1.53
5	H	7	SIA	C2-C1	5.25	1.57	1.52
5	H	7	SIA	C6-C5	4.72	1.60	1.53
5	H	4	MAN	C2-C3	4.58	1.59	1.52
5	G	7	SIA	C2-C1	4.43	1.56	1.52

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	7	SIA	O6-C2-C3	6.47	119.36	110.46
5	G	5	NAG	C4-C3-C2	5.09	118.47	111.02
5	H	4	MAN	C2-C3-C4	4.00	117.82	110.89
5	G	3	MAN	C3-C4-C5	3.40	116.30	110.24
5	H	7	SIA	C6-O6-C2	3.35	118.50	111.34

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	G	2	NAG	C1
5	G	5	NAG	C1
5	G	8	MAN	C1
5	H	2	NAG	C1
5	H	5	NAG	C1



5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	1	NAG	C8-C7-N2-C2
5	G	1	NAG	O7-C7-N2-C2
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
5	G	5	NAG	C3-C2-N2-C7

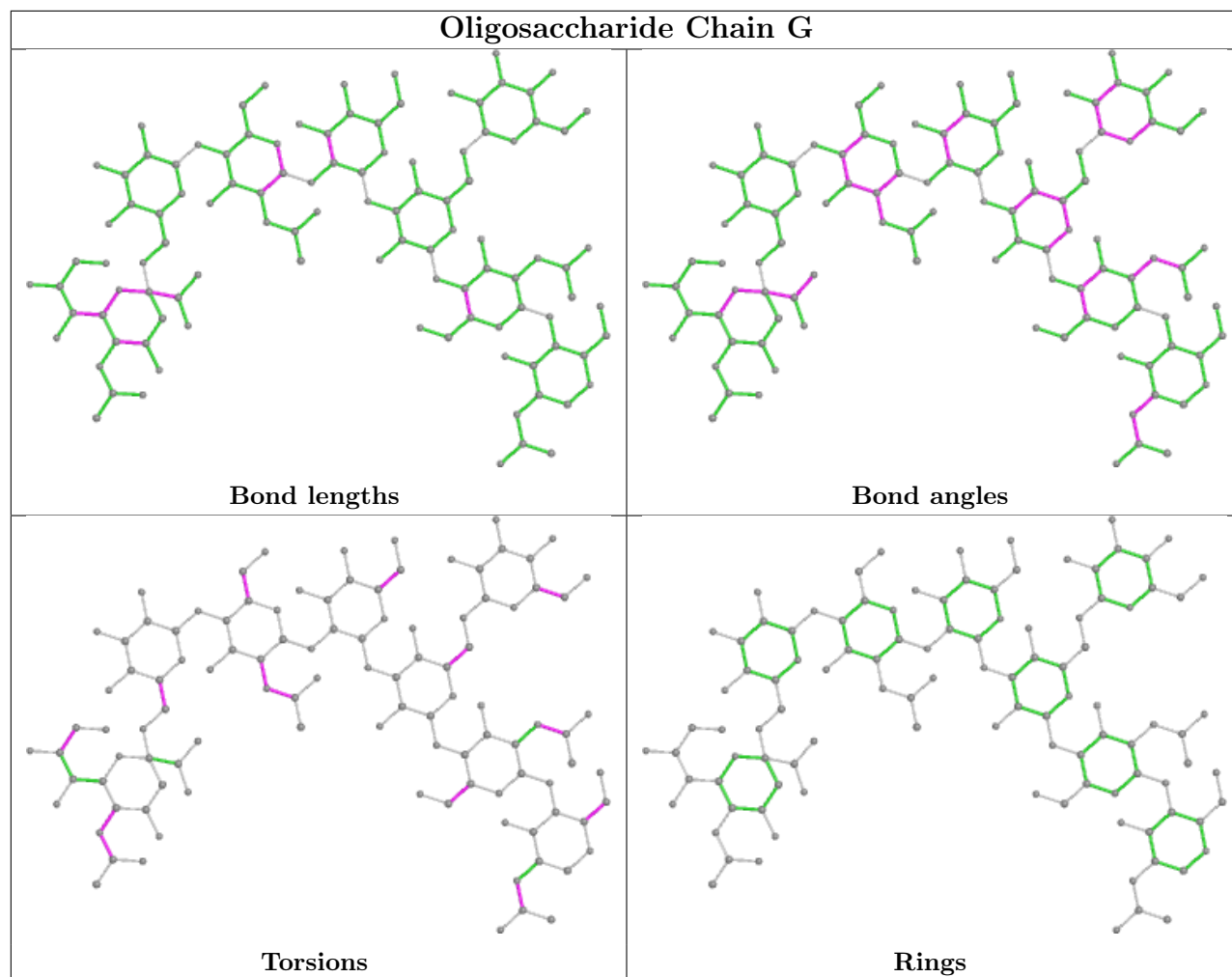
All (1) ring outliers are listed below:

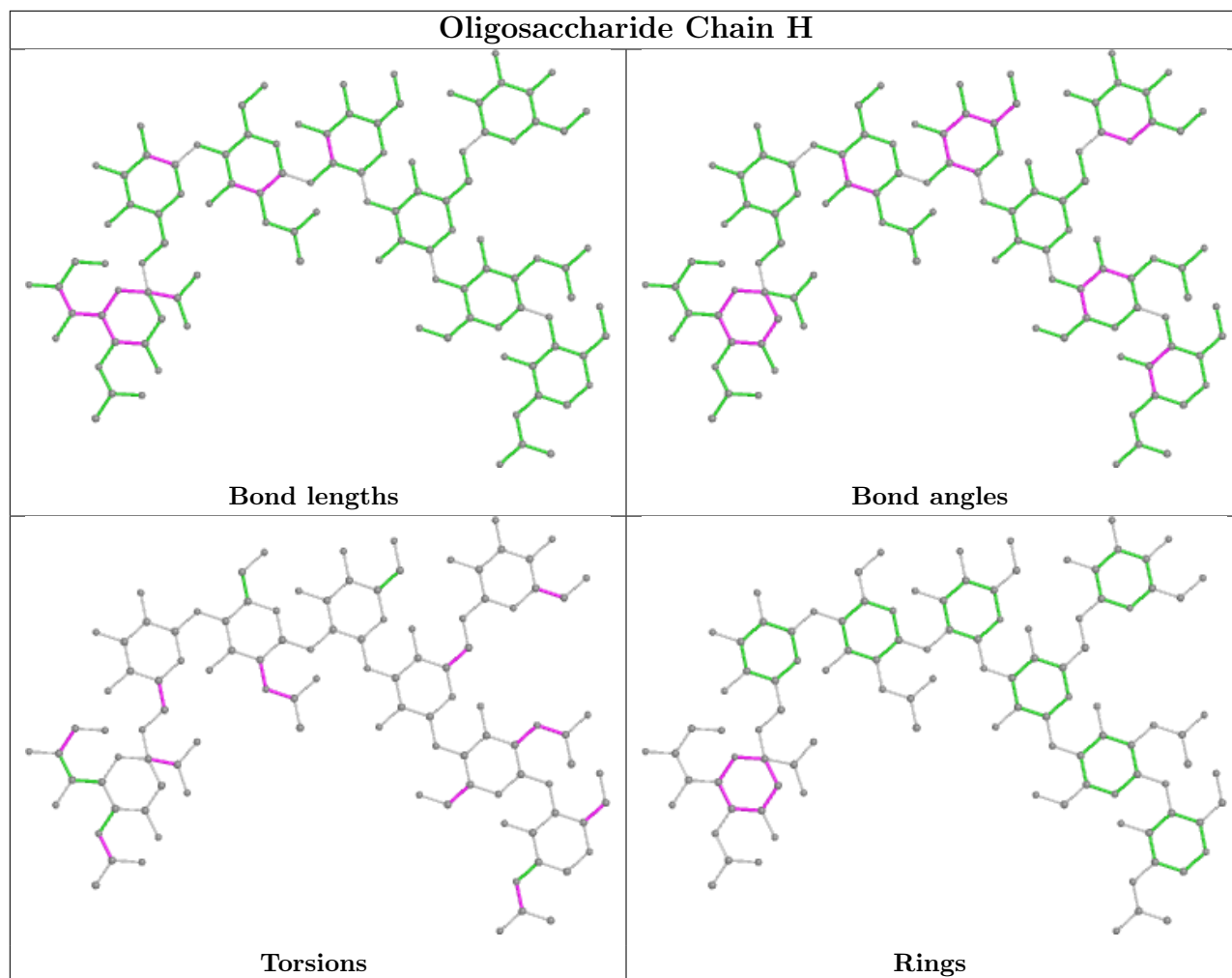
Mol	Chain	Res	Type	Atoms
5	H	7	SIA	C2-C3-C4-C5-C6-O6

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	7	SIA	4	0
5	H	2	NAG	2	0
5	H	3	MAN	2	0
5	G	3	MAN	1	0
5	G	4	MAN	1	0
5	H	7	SIA	2	0
5	H	8	MAN	2	0
5	G	6	GAL	2	0
5	H	6	GAL	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.





## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

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	74/197 (37%)	-0.19	4 (5%) 25 16	77, 91, 103, 108	0
1	D	74/197 (37%)	-0.36	2 (2%) 54 38	79, 93, 104, 108	0
2	B	308/458 (67%)	-0.53	0 100 100	65, 82, 98, 108	0
2	E	308/458 (67%)	-0.53	0 100 100	64, 83, 97, 106	0
3	C	301/317 (94%)	-0.51	1 (0%) 94 88	67, 84, 98, 105	0
3	F	296/317 (93%)	-0.52	1 (0%) 94 88	67, 85, 97, 105	0
4	M	5/5 (100%)	-0.57	0 100 100	76, 80, 84, 85	0
4	N	5/5 (100%)	-0.24	0 100 100	83, 87, 91, 93	0
All	All	1371/1954 (70%)	-0.49	8 (0%) 89 81	64, 85, 100, 108	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	126	VAL	3.2
1	A	127	ILE	3.0
1	A	121	VAL	3.0
1	A	126	VAL	2.8
3	F	360	PRO	2.3

### 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,

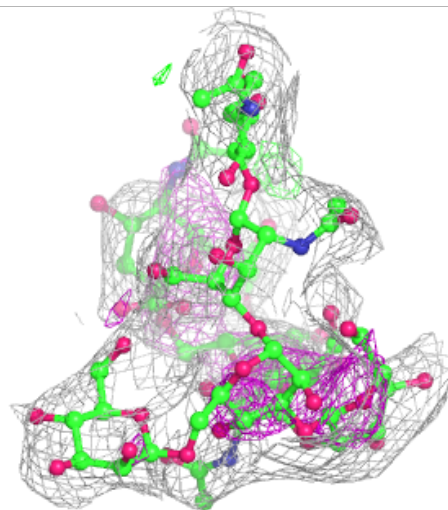
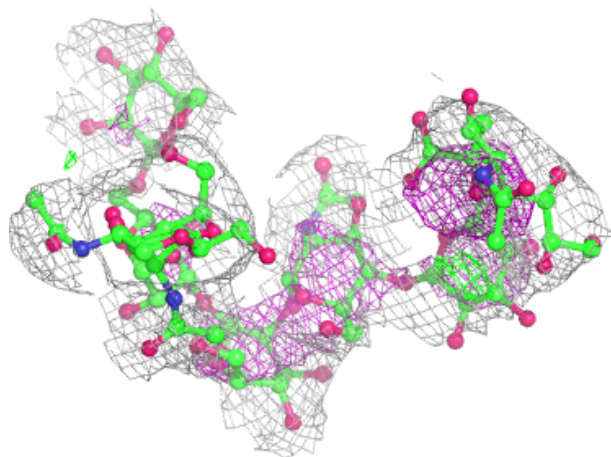
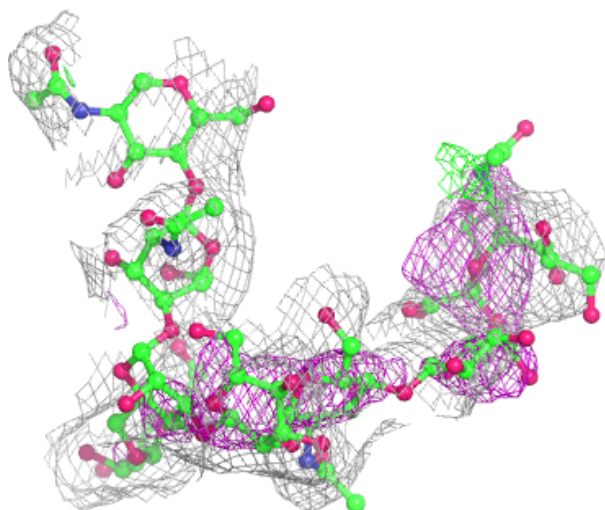
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

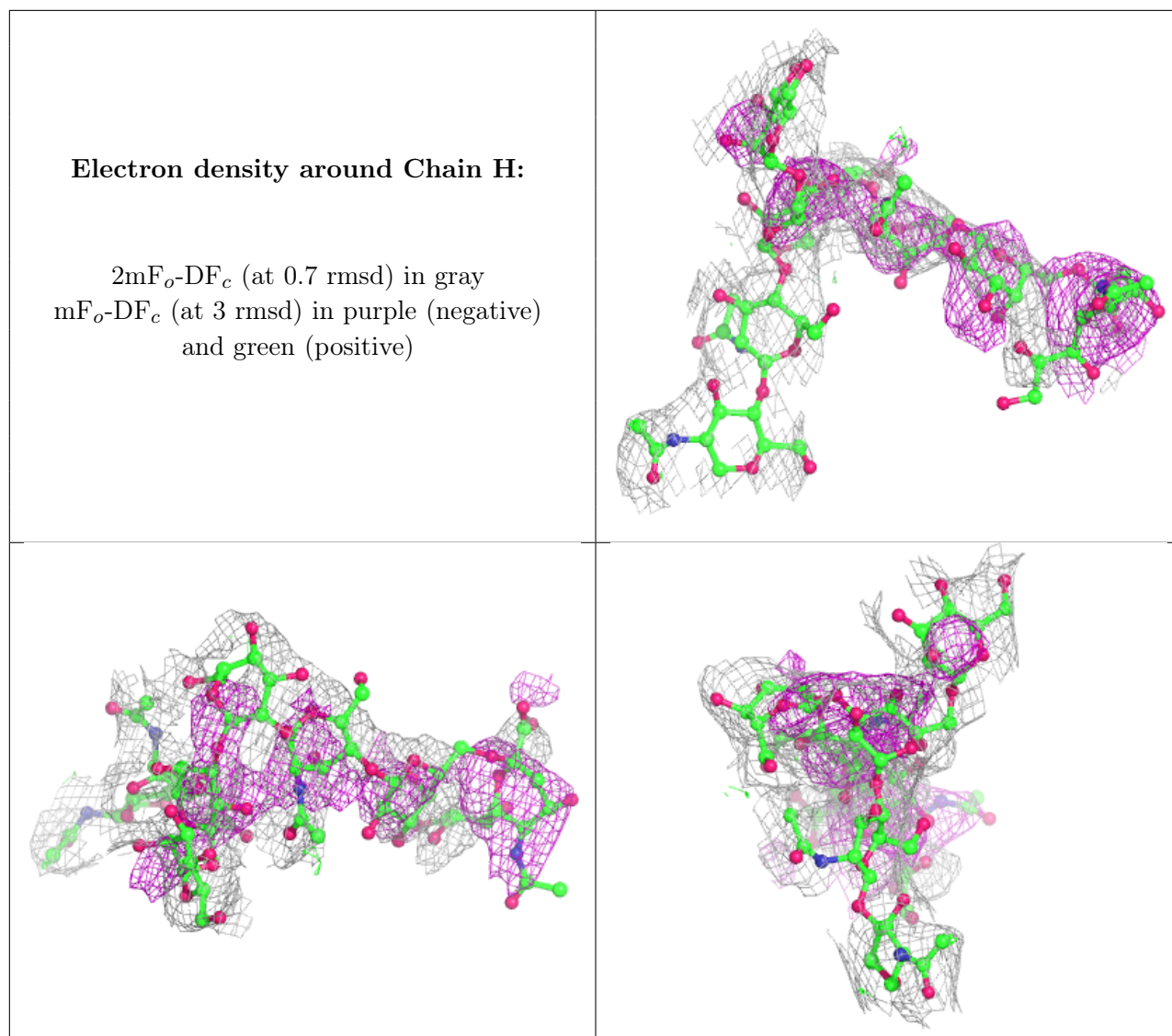
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	MAN	H	8	11/12	0.57	0.51	114,117,119,122	0
5	SIA	H	7	20/21	0.59	0.95	104,113,114,114	0
5	MAN	H	4	11/12	0.69	0.48	111,116,119,120	0
5	MAN	G	3	11/12	0.70	0.35	111,113,114,115	0
5	NAG	G	5	14/15	0.72	0.50	107,114,115,117	0
5	MAN	H	3	11/12	0.73	0.49	117,118,120,121	0
5	NAG	H	2	14/15	0.73	0.38	104,108,112,114	0
5	MAN	G	4	11/12	0.77	0.53	115,115,116,116	0
5	SIA	G	7	20/21	0.78	0.54	107,111,117,118	0
5	MAN	G	8	11/12	0.79	0.44	106,110,112,115	0
5	NAG	H	5	14/15	0.79	0.62	103,109,112,112	0
5	GAL	H	6	11/12	0.82	0.76	107,110,112,112	0
5	GAL	G	6	11/12	0.85	0.60	116,117,118,119	0
5	NAG	G	1	14/15	0.91	0.18	85,91,95,99	0
5	NAG	H	1	14/15	0.92	0.16	90,94,97,101	0
5	NAG	G	2	14/15	0.93	0.23	95,105,108,111	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 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( $\text{\AA}^2$ )	Q<0.9
6	CA	C	501	1/1	0.93	0.07	74,74,74,74	0
6	CA	E	502	1/1	0.95	0.14	26,26,26,26	0
6	CA	F	501	1/1	0.96	0.15	108,108,108,108	0
6	CA	B	502	1/1	0.99	0.07	40,40,40,40	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.