



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 02:00 PM UTC

PDB ID : 3H32 / pdb_00003h32
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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

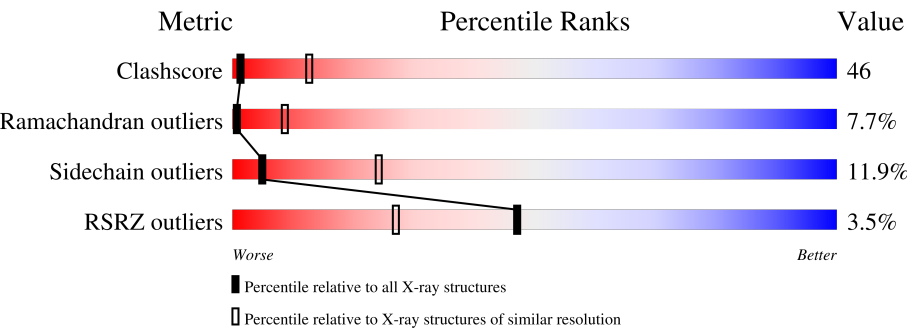
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (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 ≥ 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	4% 11% 19% 7% • 62%
1	D	197	2% 12% 20% • • 62%
2	B	458	2% 23% 36% 6% • 33%
2	E	458	2% 22% 37% 8% 33%
3	C	317	3% 32% 45% 15% • 5%
3	F	317	4% 28% 49% 15% • 7%
4	M	5	40% 60%

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Mol	Chain	Length	Quality of chain
4	N	5	 60%40%
5	G	8	 75%25%
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	NAG	G	5	X	-	-	-
5	MAN	G	8	X	-	-	-
5	NAG	H	2	X	-	-	-
5	NAG	H	5	X	-	-	-
5	SIA	H	7	X	-	-	-

2 Entry composition

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
1	A	74	Total	C	N	O	S	0	0	0
			608	377	115	113	3			
1	D	74	Total	C	N	O	S	0	0	0
			608	377	115	113	3			

- Molecule 2 is a protein called Fibrinogen beta chain.

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

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

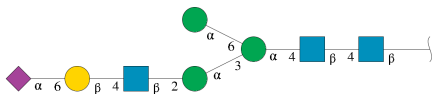
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	301	Total	C	N	O	S	0	0	0
			2404	1523	405	465	11			
3	F	296	Total	C	N	O	S	0	0	0
			2372	1504	400	457	11			

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

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

- 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.



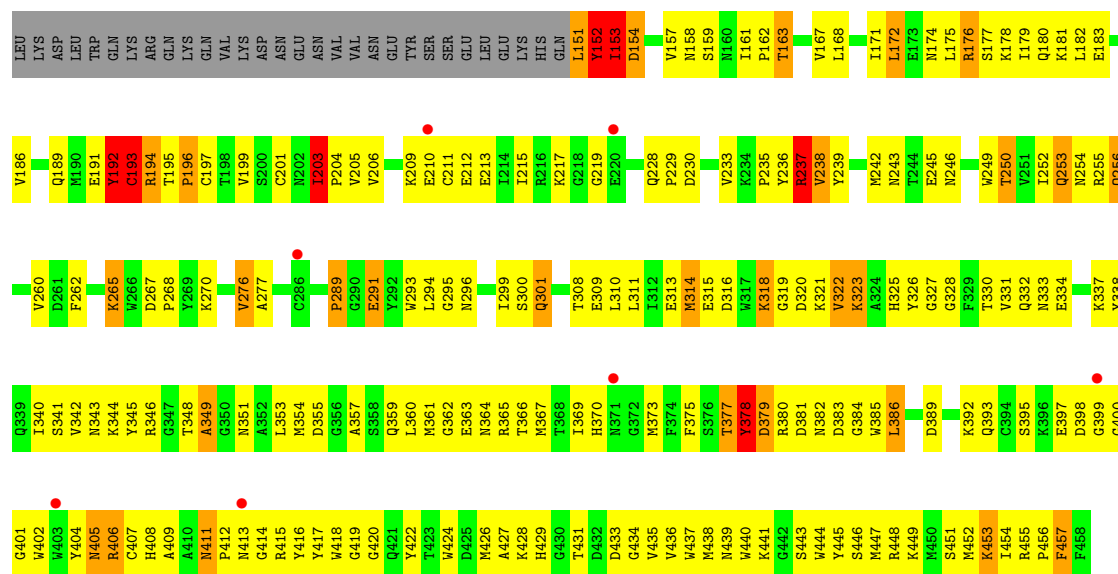
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	8	Total	C	N	O	0	0	0
			106	59	4	43			
5	H	8	Total	C	N	O	0	0	0
			106	59	4	43			

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

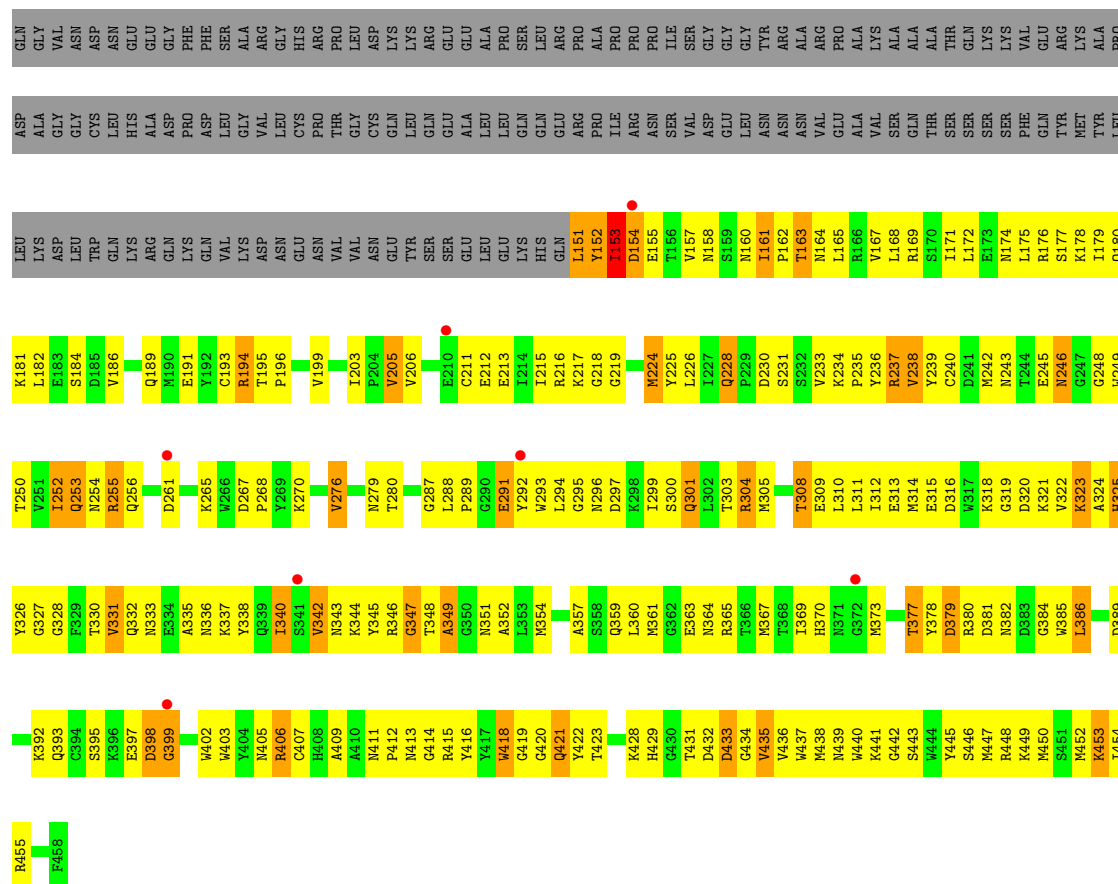
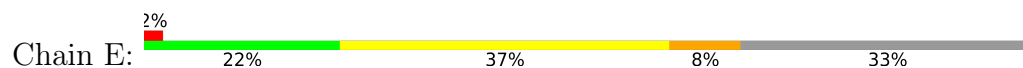
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	C	1	Total	Ca	0	0
			1	1		
6	E	1	Total	Ca	0	0
			1	1		
6	F	1	Total	Ca	0	0
			1	1		

- Molecule 1: Fibrinogen alpha chain



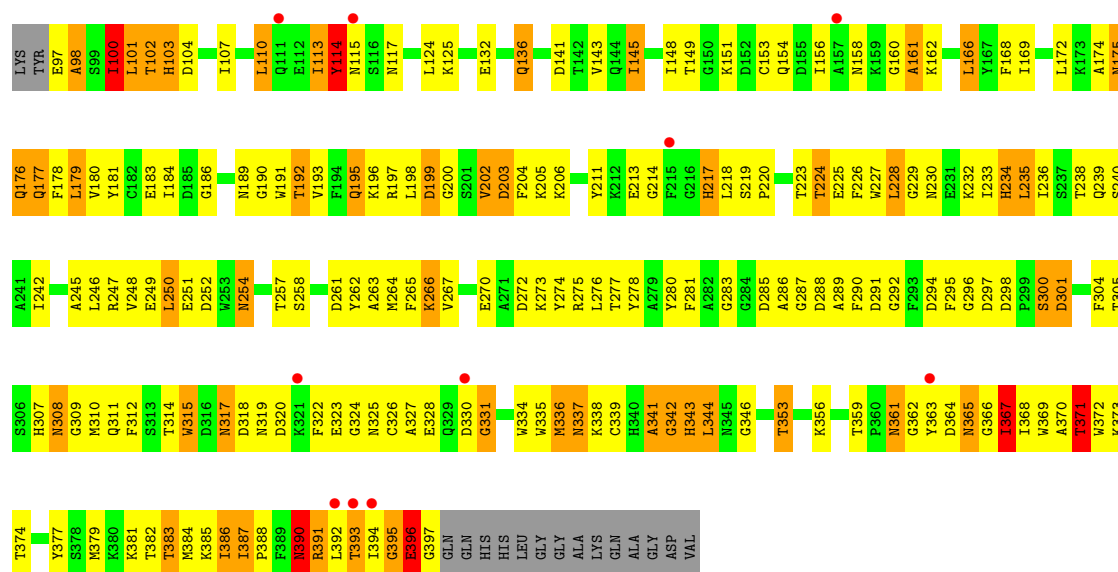


• Molecule 2: Fibrinogen beta chain

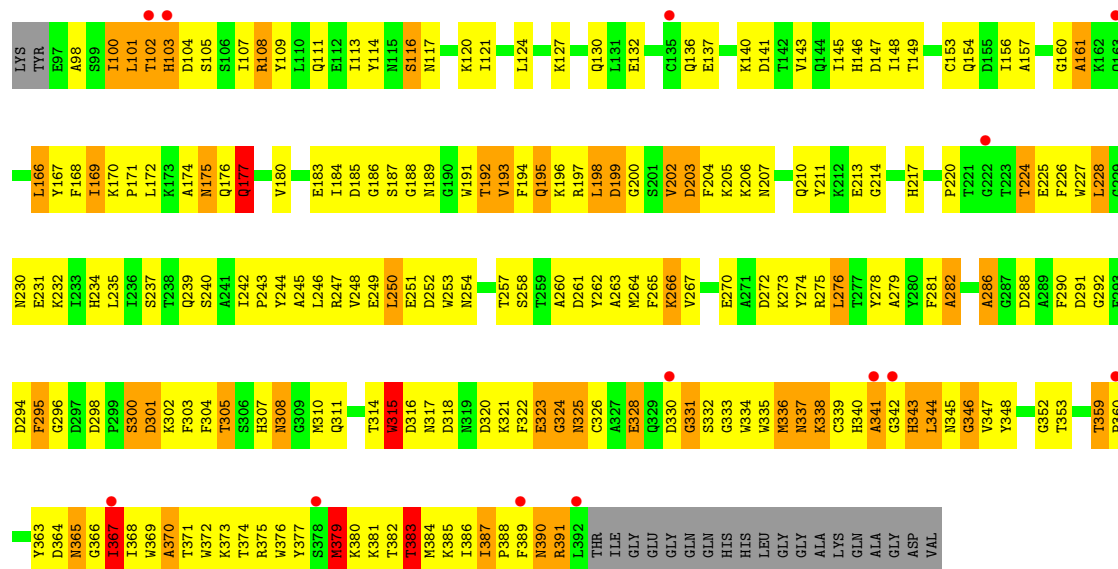


• Molecule 3: Fibrinogen gamma chain, isoform gamma-A





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



• Molecule 4: Fibrin B knob pentapeptide



• Molecule 4: Fibrin B knob pentapeptide



- 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:  75% 25%

NAG1	NAG2	MAN3	MAN4	NAG5	GAL6	ST17	MAN8
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- 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%

NAG1	NAG2	MAN3	MAN4	NAG5	GAL6	ST17	MAN8
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	264.72Å 97.32Å 132.49Å 90.00° 122.78° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 50.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	75.5 (50.00-3.60) 75.6 (50.00-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	30.66 (at 3.55Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.263 , 0.320 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	89.3	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 12.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11246	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CA, GAL, MAN, SIA

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	1.04	4/609 (0.7%)	1.29	5/811 (0.6%)
1	D	0.91	2/609 (0.3%)	1.27	5/811 (0.6%)
2	B	0.73	1/2536 (0.0%)	1.08	13/3425 (0.4%)
2	E	0.78	2/2536 (0.1%)	1.07	16/3425 (0.5%)
3	C	0.73	2/2469 (0.1%)	1.01	7/3339 (0.2%)
3	F	0.68	1/2437 (0.0%)	1.02	10/3296 (0.3%)
4	M	0.58	0/47	0.95	0/61
4	N	0.65	0/47	0.88	0/61
All	All	0.76	12/11290 (0.1%)	1.07	56/15229 (0.4%)

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

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	359	THR	CA-CB	7.34	1.63	1.53
1	D	126	VAL	CA-CB	7.30	1.64	1.54
1	A	127	ILE	CA-CB	6.99	1.64	1.54
1	A	126	VAL	CA-CB	6.91	1.63	1.54
2	E	361	MET	SD-CE	6.18	1.95	1.79

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	ARG	N-CA-C	12.84	124.81	111.07
1	D	124	ARG	N-CA-C	11.65	123.67	110.97
1	A	121	VAL	N-CA-C	10.45	121.27	110.72
2	B	154	ASP	N-CA-C	9.60	122.75	111.71
2	E	409	ALA	N-CA-C	-9.33	102.27	114.31

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

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	66	0
1	D	608	0	649	63	0
2	B	2474	0	2336	211	0
2	E	2474	0	2336	243	0
3	C	2404	0	2249	245	0
3	F	2372	0	2219	260	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	1006	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 46.

The worst 5 of 1006 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%)	1	14
1	D	72/197 (36%)	62 (86%)	7 (10%)	3 (4%)	2	19
2	B	306/458 (67%)	230 (75%)	57 (19%)	19 (6%)	1	12
2	E	306/458 (67%)	226 (74%)	63 (21%)	17 (6%)	1	14
3	C	299/317 (94%)	199 (67%)	67 (22%)	33 (11%)	0	5
3	F	294/317 (93%)	211 (72%)	54 (18%)	29 (10%)	0	6
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	9

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 ⓘ

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%)	59 (86%)	10 (14%)	3	18
1	D	69/179 (38%)	58 (84%)	11 (16%)	2	15
2	B	266/393 (68%)	236 (89%)	30 (11%)	5	26
2	E	266/393 (68%)	237 (89%)	29 (11%)	6	27
3	C	252/263 (96%)	221 (88%)	31 (12%)	4	23
3	F	249/263 (95%)	220 (88%)	29 (12%)	5	25
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%)	1039 (88%)	140 (12%)	5	24

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	169	ILE
3	F	195	GLN
3	F	343	HIS
3	C	177	GLN
3	C	175	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	117	ASN
3	F	177	GLN
3	F	308	ASN
3	C	119	GLN
3	C	117	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 ⓘ

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	1.04	1 (5%)
5	NAG	G	2	5	14,14,15	1.05	1 (7%)	17,19,21	1.27	2 (11%)
5	MAN	G	3	5	11,11,12	0.96	0	15,15,17	1.35	2 (13%)
5	MAN	G	4	5	11,11,12	1.15	0	15,15,17	0.78	0
5	NAG	G	5	5	14,14,15	1.44	1 (7%)	17,19,21	1.75	3 (17%)
5	GAL	G	6	5	11,11,12	1.10	0	15,15,17	0.73	0
5	SIA	G	7	5	20,20,21	1.63	4 (20%)	21,28,31	1.16	2 (9%)
5	MAN	G	8	5	11,11,12	0.74	0	15,15,17	0.98	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	1.33	2 (11%)
5	MAN	H	3	5	11,11,12	1.23	0	15,15,17	0.73	0
5	MAN	H	4	5	11,11,12	1.66	1 (9%)	15,15,17	1.52	3 (20%)
5	NAG	H	5	5	14,14,15	1.67	2 (14%)	17,19,21	0.89	1 (5%)
5	GAL	H	6	5	11,11,12	1.04	1 (9%)	15,15,17	0.68	0
5	SIA	H	7	5	20,20,21	2.65	7 (35%)	21,28,31	1.77	3 (14%)
5	MAN	H	8	5	11,11,12	0.91	0	15,15,17	1.00	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

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

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	7	SIA	C7-C6	6.42	1.60	1.52
5	H	7	SIA	C6-C5	4.90	1.60	1.53
5	H	5	NAG	C1-C2	4.81	1.58	1.52
5	H	4	MAN	C2-C3	4.42	1.59	1.52
5	H	7	SIA	C4-C5	4.17	1.57	1.53

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	7	SIA	O6-C2-C3	6.55	119.36	110.56
5	G	5	NAG	C4-C3-C2	5.09	118.47	111.02
5	H	4	MAN	C2-C3-C4	3.96	117.82	110.86
5	G	1	NAG	C2-N2-C7	-3.45	118.28	122.90
5	G	3	MAN	C3-C4-C5	3.34	116.30	110.23

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	G	2	NAG	C1
5	G	5	NAG	C1

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

5 of 50 torsion outliers are listed below:

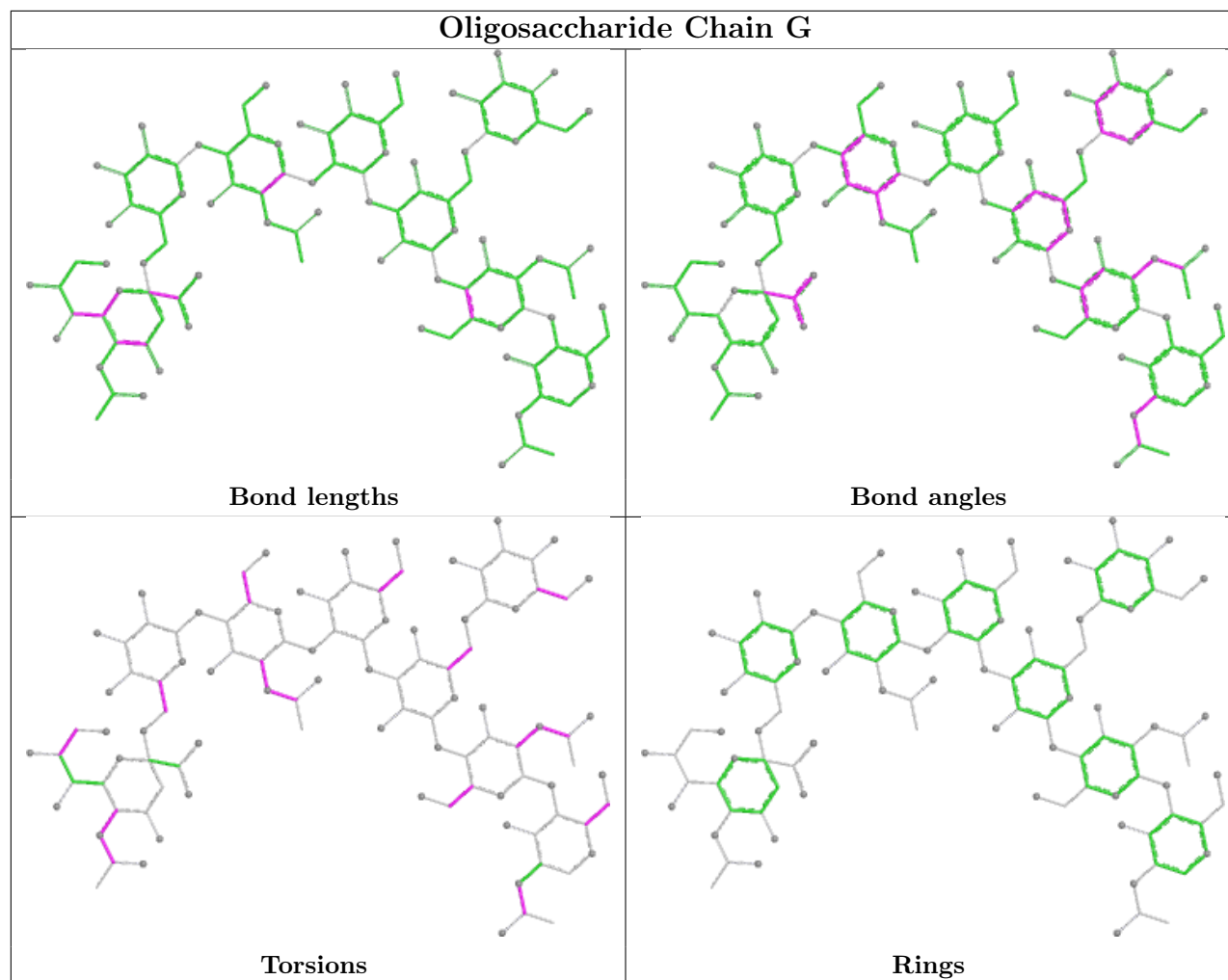
Mol	Chain	Res	Type	Atoms
5	G	1	NAG	C8-C7-N2-C2
5	G	1	NAG	O7-C7-N2-C2
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
5	G	5	NAG	C3-C2-N2-C7

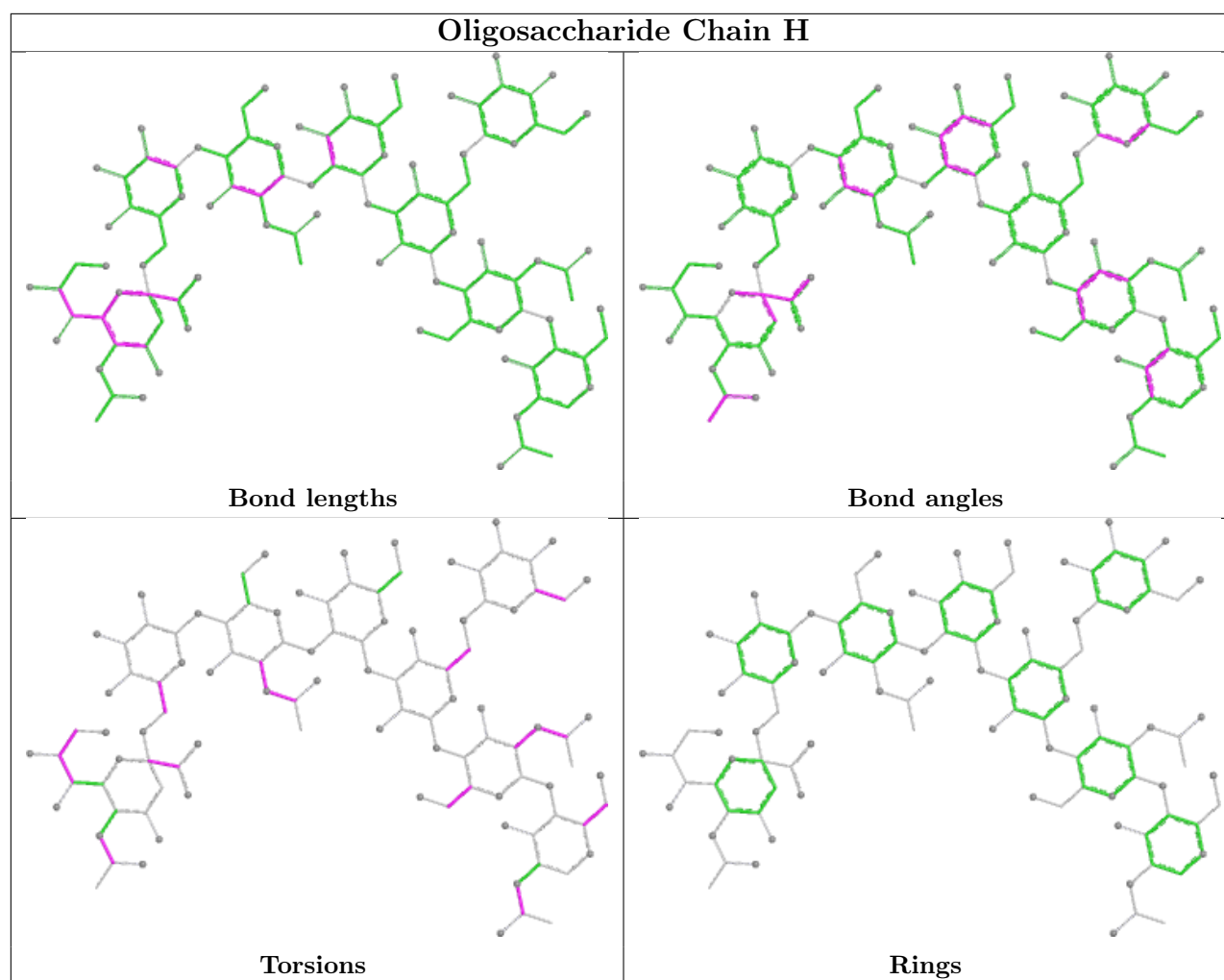
There are no ring outliers.

9 monomers are involved in 11 short contacts:

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

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





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, 95th 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 ²)	Q < 0.9
1	A	74/197 (37%)	0.84	8 (10%) 11 9	77, 91, 103, 108	0
1	D	74/197 (37%)	0.37	3 (4%) 41 23	79, 93, 104, 108	0
2	B	308/458 (67%)	0.39	7 (2%) 61 35	65, 82, 98, 108	0
2	E	308/458 (67%)	0.38	7 (2%) 61 35	64, 83, 97, 106	0
3	C	301/317 (94%)	0.46	10 (3%) 49 28	67, 84, 98, 105	0
3	F	296/317 (93%)	0.45	13 (4%) 39 22	67, 85, 97, 105	0
4	M	5/5 (100%)	0.51	0 100 100	76, 80, 84, 85	0
4	N	5/5 (100%)	0.60	0 100 100	83, 87, 91, 93	0
All	All	1371/1954 (70%)	0.44	48 (3%) 47 27	64, 85, 100, 108	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	127	ILE	5.5
1	A	126	VAL	5.0
1	A	121	VAL	4.6
2	E	399	GLY	3.7
2	E	210	GLU	3.7

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,

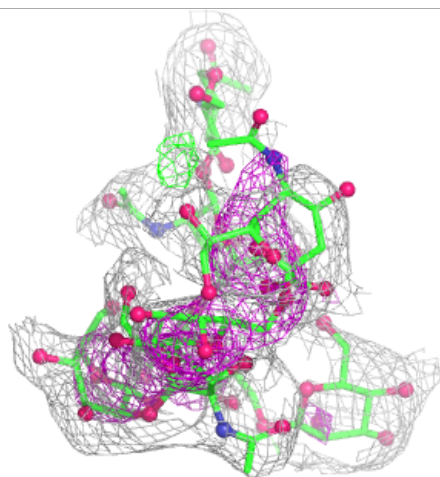
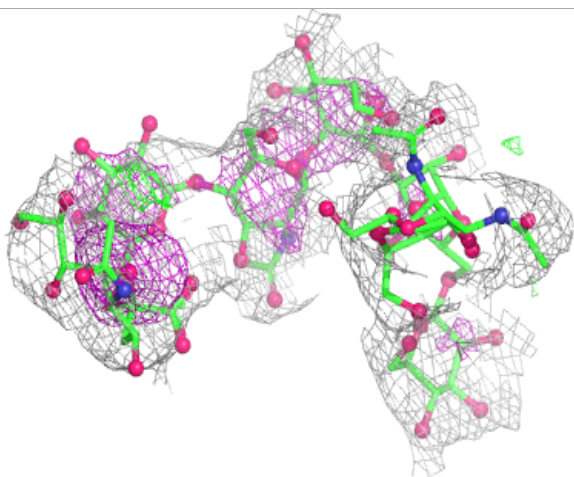
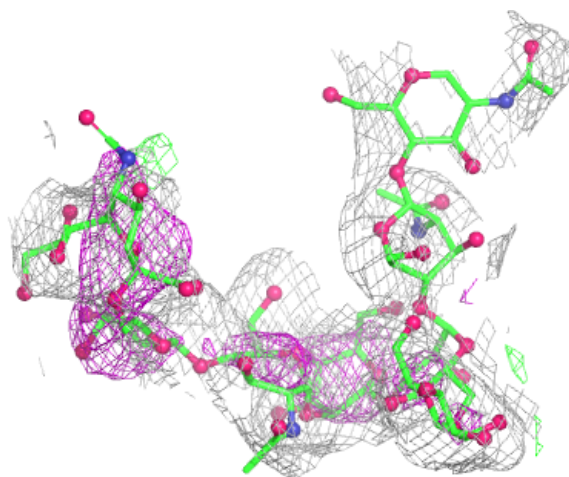
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

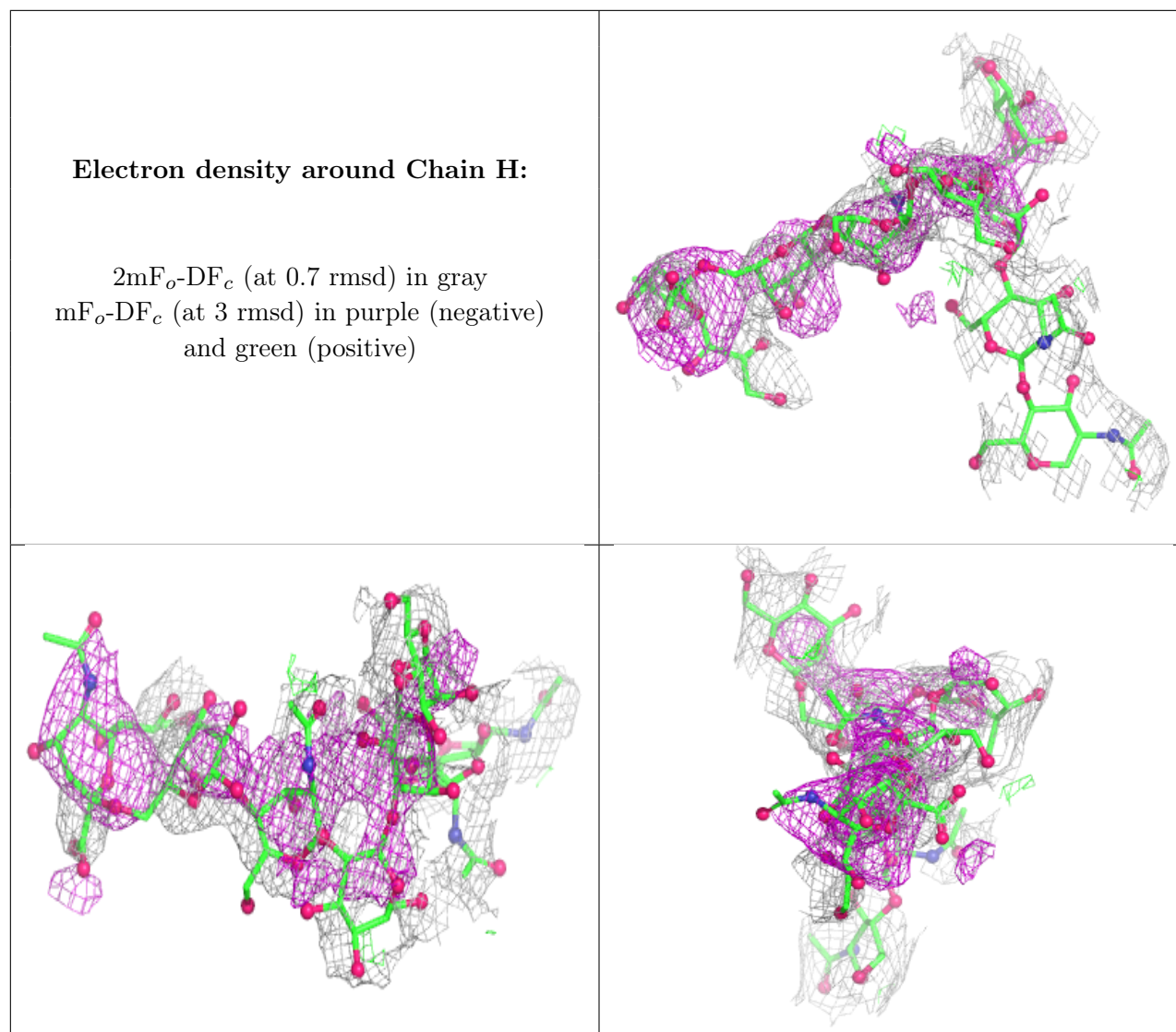
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	G	1	14/15	-	-	85,91,95,99	0
5	NAG	G	2	14/15	-	-	95,105,108,111	0
5	MAN	G	3	11/12	-	-	111,113,114,115	0
5	MAN	G	4	11/12	-	-	115,115,116,116	0
5	NAG	G	5	14/15	-	-	107,114,115,117	0
5	GAL	G	6	11/12	-	-	116,117,118,119	0
5	SIA	G	7	20/21	-	-	107,111,117,118	0
5	MAN	G	8	11/12	-	-	106,110,112,115	0
5	NAG	H	1	14/15	-	-	90,94,97,101	0
5	NAG	H	2	14/15	-	-	104,108,112,114	0
5	MAN	H	3	11/12	-	-	117,118,120,121	0
5	MAN	H	4	11/12	-	-	111,116,119,120	0
5	NAG	H	5	14/15	-	-	103,109,112,112	0
5	GAL	H	6	11/12	-	-	107,110,112,112	0
5	SIA	H	7	20/21	-	-	104,113,114,114	0
5	MAN	H	8	11/12	-	-	114,117,119,122	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, 95th 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 ²)	Q<0.9
6	CA	F	501	1/1	0.88	0.14	108,108,108,108	0
6	CA	B	502	1/1	0.97	0.04	40,40,40,40	0
6	CA	E	502	1/1	0.98	0.09	26,26,26,26	0
6	CA	C	501	1/1	0.99	0.03	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.