



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 10:21 PM BST

PDB ID : 3GHG
Title : Crystal Structure of Human Fibrinogen
Authors : Doolittle, R.F.; Kollman, J.M.; Sawaya, M.R.; Pandi, L.; Riley, M.
Deposited on : 2009-03-03
Resolution : 2.90 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 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 : 2.13.1
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) : 2.13.1

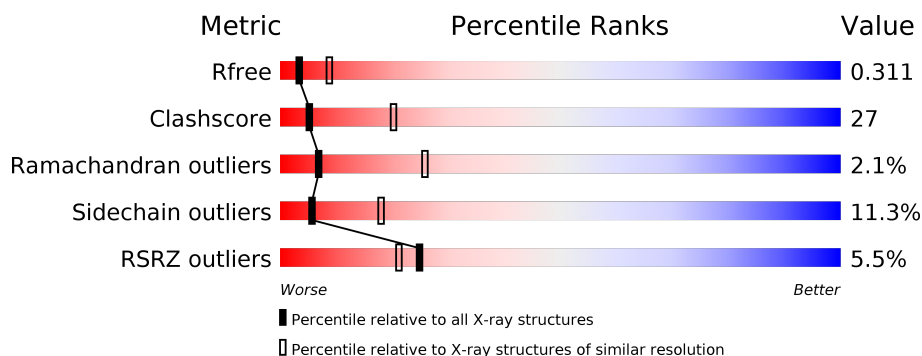
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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	562	<div> <div>18% 12% 69%</div> <div>18% 12% 69%</div> </div>
1	D	562	<div> <div>6% 18% 12% 69%</div> <div>18% 12% 69%</div> </div>
1	G	562	<div> <div>2% 20% 10% 69%</div> <div>20% 10% 69%</div> </div>
1	J	562	<div> <div>4% 16% 15% 67%</div> <div>16% 15% 67%</div> </div>
2	B	461	<div> <div>46% 34% 6% 13%</div> <div>46% 34% 6% 13%</div> </div>
2	E	461	<div> <div>8% 46% 35% 6% 13%</div> <div>46% 35% 6% 13%</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	461	
2	K	461	
3	C	411	
3	F	411	
3	I	411	
3	L	411	
4	M	4	
4	N	4	
4	Q	4	
4	R	4	
5	O	4	
5	P	4	
5	S	4	
5	T	4	
6	U	11	
6	V	11	
6	X	11	
7	W	5	
8	Y	2	

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
6	NAG	U	1	-	-	X	-
6	GAL	U	10	-	-	-	X
6	SIA	U	11	-	-	-	X
6	MAN	U	4	-	-	-	X
6	NDG	U	5	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GAL	U	6	X	-	-	-
6	SIA	U	7	-	-	-	X
6	MAN	U	8	-	-	-	X
6	NDG	U	9	-	-	-	X
6	NAG	V	1	X	-	-	-
6	GAL	V	10	-	-	-	X
6	SIA	V	11	-	-	-	X
6	MAN	V	4	-	-	-	X
6	NDG	V	5	-	-	-	X
6	GAL	V	6	X	-	-	X
6	MAN	V	8	-	-	-	X
6	NDG	V	9	-	-	-	X
6	NAG	X	1	-	-	X	-
6	GAL	X	10	-	-	-	X
6	SIA	X	11	-	-	-	X
6	NDG	X	2	-	-	-	X
6	BMA	X	3	-	-	-	X
6	MAN	X	4	-	-	-	X
6	NDG	X	5	-	-	-	X
6	GAL	X	6	X	-	-	X
6	SIA	X	7	-	-	-	X
6	NDG	X	9	-	-	-	X
7	NAG	W	1	X	-	-	-
7	MAN	W	4	-	-	-	X
7	MAN	W	5	-	-	-	X
8	NAG	Y	1	-	-	X	X
8	NAG	Y	2	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 31833 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	174	Total	C	N	O	S	0	0	0
			1431	876	268	278	9			
1	D	174	Total	C	N	O	S	0	0	0
			1431	876	268	278	9			
1	G	174	Total	C	N	O	S	0	0	0
			1431	876	268	278	9			
1	J	186	Total	C	N	O	S	0	0	0
			1527	941	284	292	10			

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	401	Total	C	N	O	S	0	0	0
			3209	1995	564	624	26			
2	E	401	Total	C	N	O	S	0	0	0
			3209	1995	564	624	26			
2	H	401	Total	C	N	O	S	0	0	0
			3209	1995	564	624	26			
2	K	401	Total	C	N	O	S	0	0	0
			3209	1995	564	624	26			

- Molecule 3 is a protein called Fibrinogen gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	381	Total	C	N	O	S	0	0	0
			3050	1931	510	593	16			
3	F	382	Total	C	N	O	S	0	0	0
			3054	1933	511	594	16			
3	I	394	Total	C	N	O	S	0	0	0
			3145	1986	527	614	18			
3	L	391	Total	C	N	O	S	0	0	0
			3126	1974	524	610	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	408	ALA	-	SEE REMARK 999	UNP P02679
C	409	GLY	-	SEE REMARK 999	UNP P02679
C	410	ASP	-	SEE REMARK 999	UNP P02679
F	408	ALA	-	SEE REMARK 999	UNP P02679
F	409	GLY	-	SEE REMARK 999	UNP P02679
F	410	ASP	-	SEE REMARK 999	UNP P02679
I	408	ALA	-	SEE REMARK 999	UNP P02679
I	409	GLY	-	SEE REMARK 999	UNP P02679
I	410	ASP	-	SEE REMARK 999	UNP P02679
L	408	ALA	-	SEE REMARK 999	UNP P02679
L	409	GLY	-	SEE REMARK 999	UNP P02679
L	410	ASP	-	SEE REMARK 999	UNP P02679

- Molecule 4 is a protein called A knob.

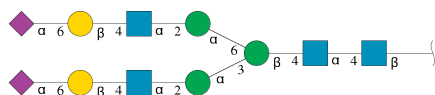
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	4	Total	C	N	O	0	0	0
			30	18	7	5			
4	N	4	Total	C	N	O	0	0	0
			30	18	7	5			
4	Q	4	Total	C	N	O	0	0	0
			30	18	7	5			
4	R	4	Total	C	N	O	0	0	0
			30	18	7	5			

- Molecule 5 is a protein called B knob.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	O	4	Total	C	N	O	0	0	0
			33	19	9	5			
5	P	4	Total	C	N	O	0	0	0
			33	19	9	5			
5	S	4	Total	C	N	O	0	0	0
			33	19	9	5			
5	T	4	Total	C	N	O	0	0	0
			33	19	9	5			

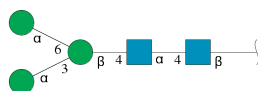
- Molecule 6 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyran

ose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	U	11	Total	C	N	O	0	0	0
			151	84	6	61			
6	V	11	Total	C	N	O	0	0	0
			151	84	6	61			
6	X	11	Total	C	N	O	0	0	0
			151	84	6	61			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 8 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
8	Y	2	Total	C	N	O	0	0	0
			28	16	2	10			

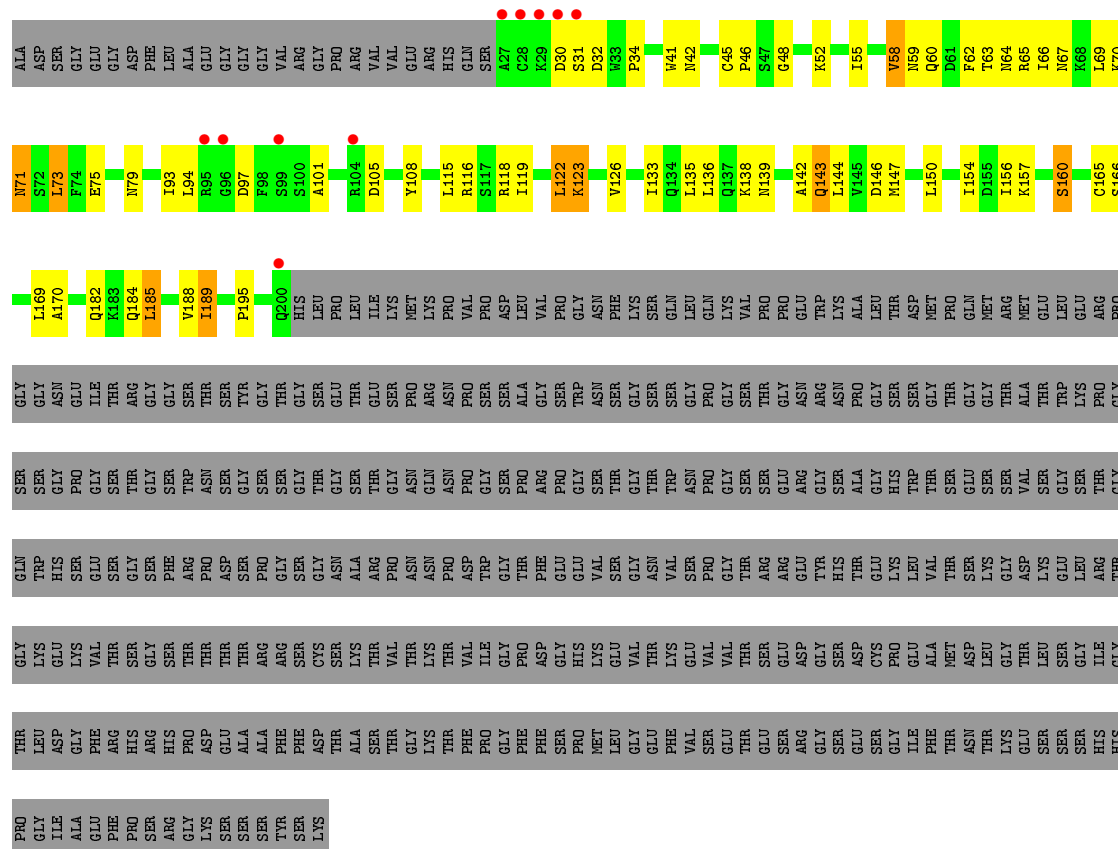
- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	K	1	Total	Ca	0	0
			1	1		

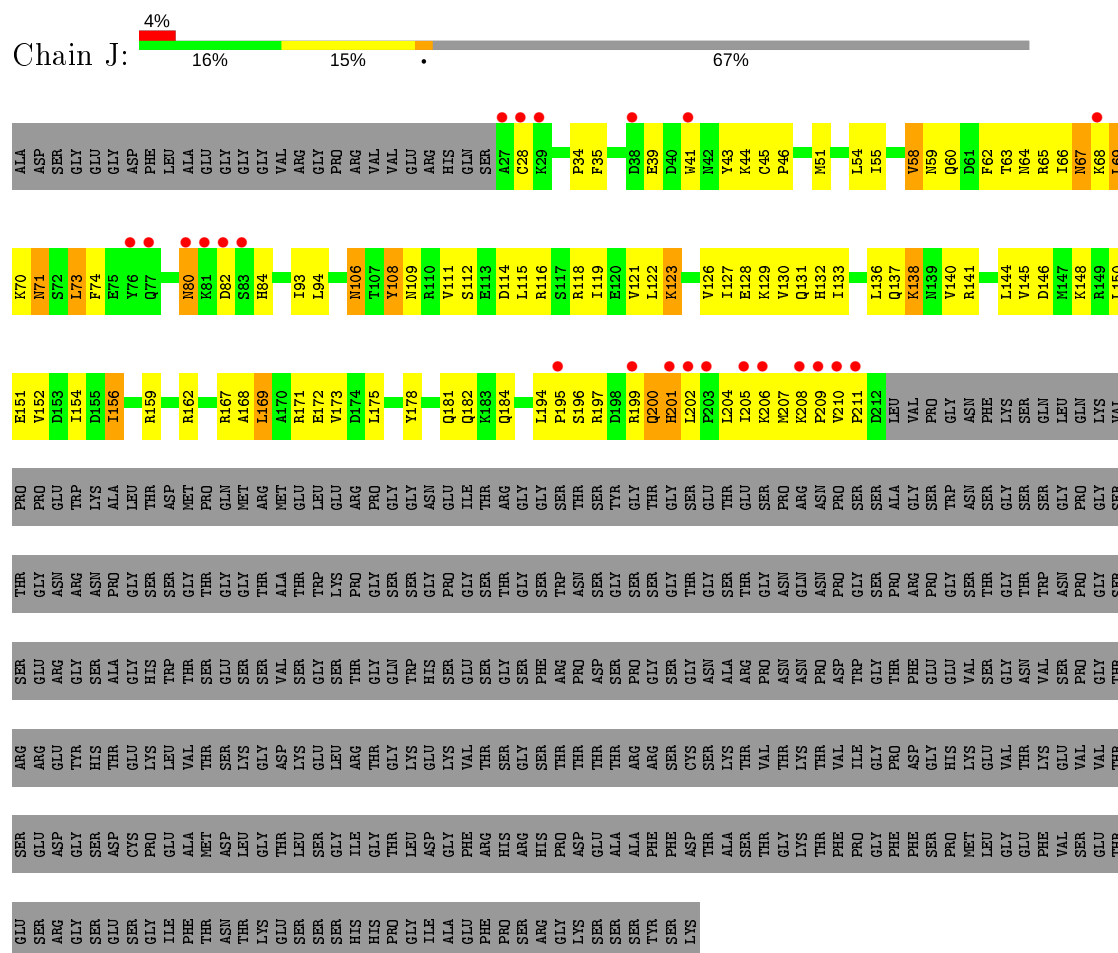
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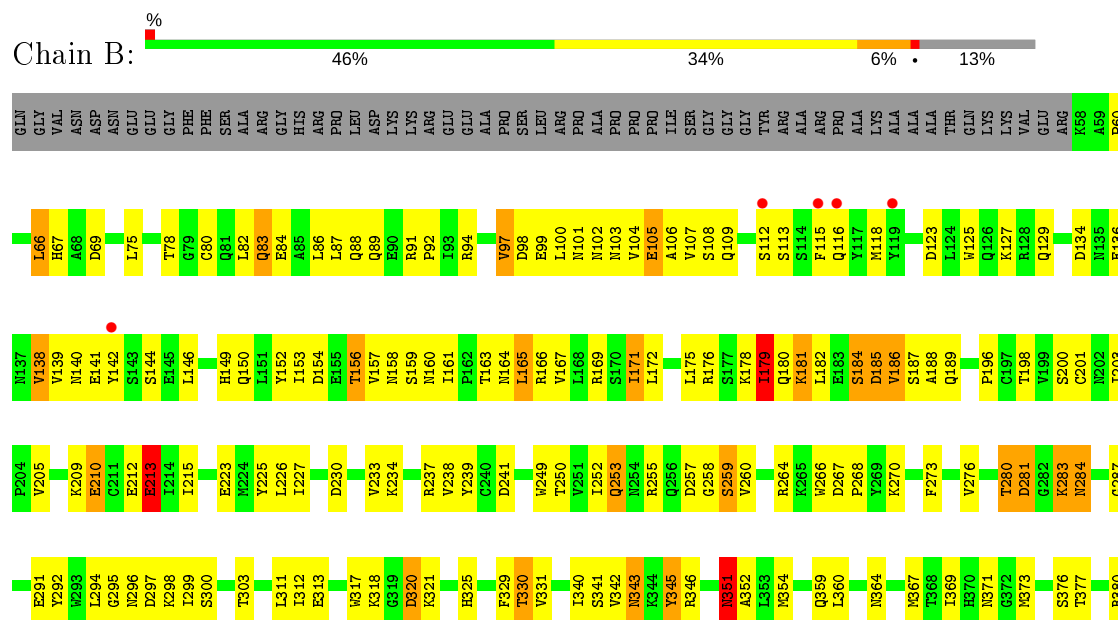
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	E	1	Total 1	Ca 1	0	0
9	H	1	Total 1	Ca 1	0	0
9	B	1	Total 1	Ca 1	0	0
9	I	1	Total 1	Ca 1	0	0
9	C	1	Total 1	Ca 1	0	0
9	L	1	Total 1	Ca 1	0	0
9	F	1	Total 1	Ca 1	0	0

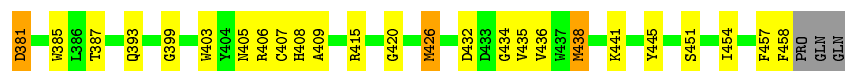


- Molecule 1: Fibrinogen alpha chain

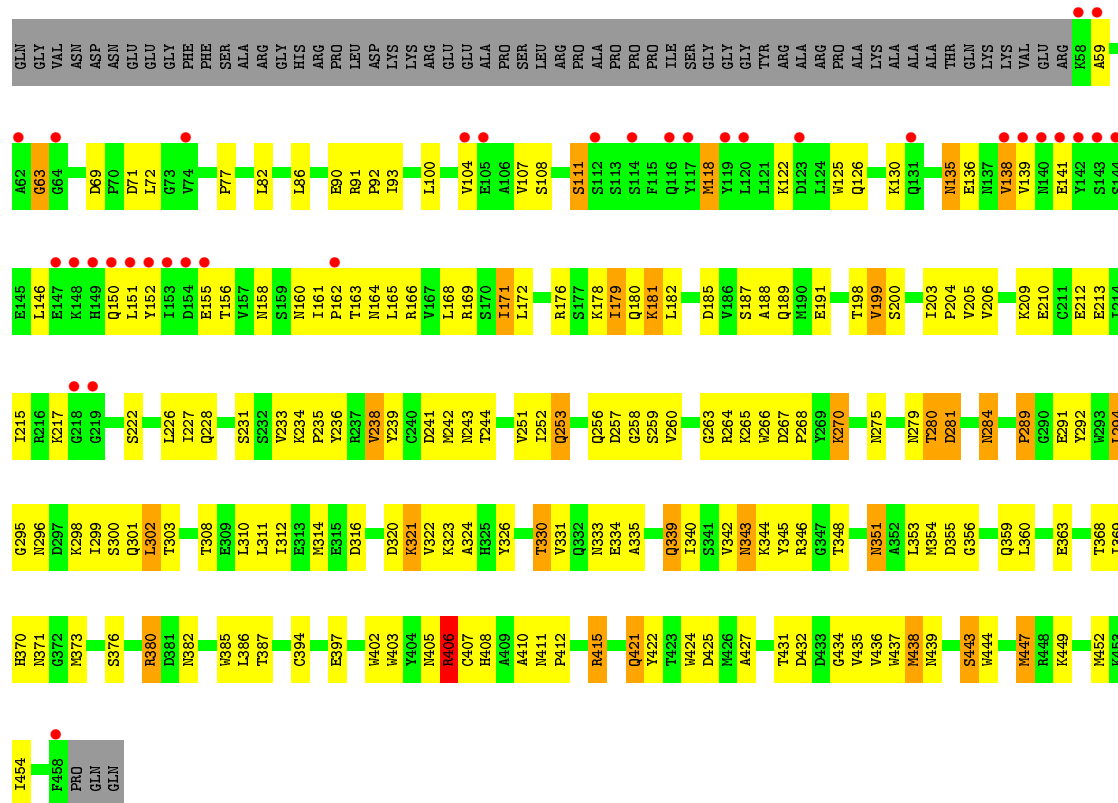


- Molecule 2: Fibrinogen beta chain

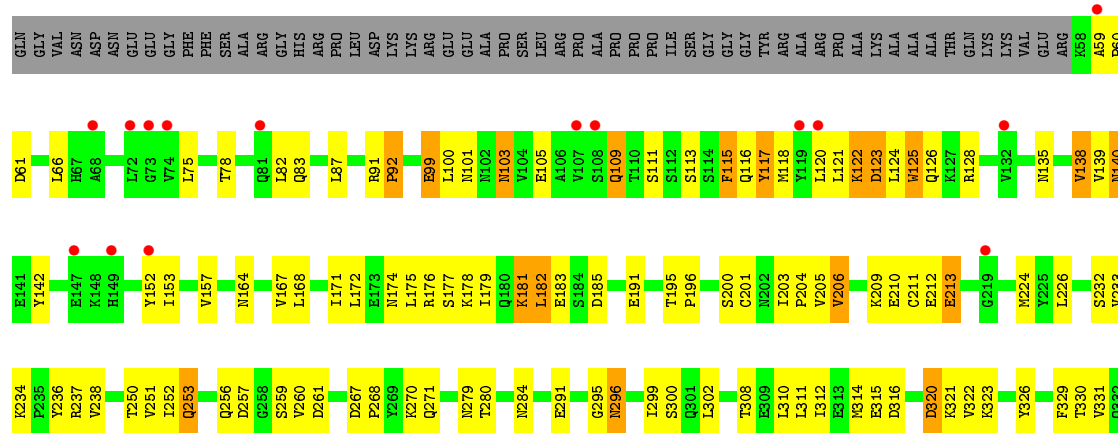




• Molecule 2: Fibrinogen beta chain

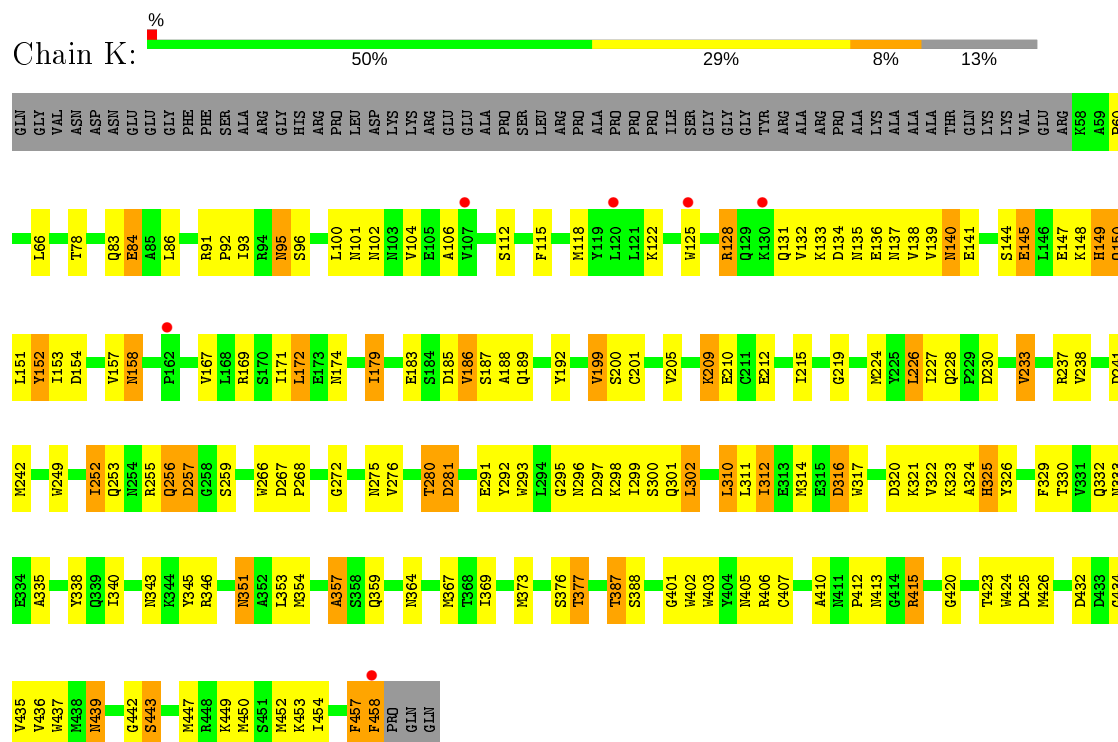


• Molecule 2: Fibrinogen beta chain

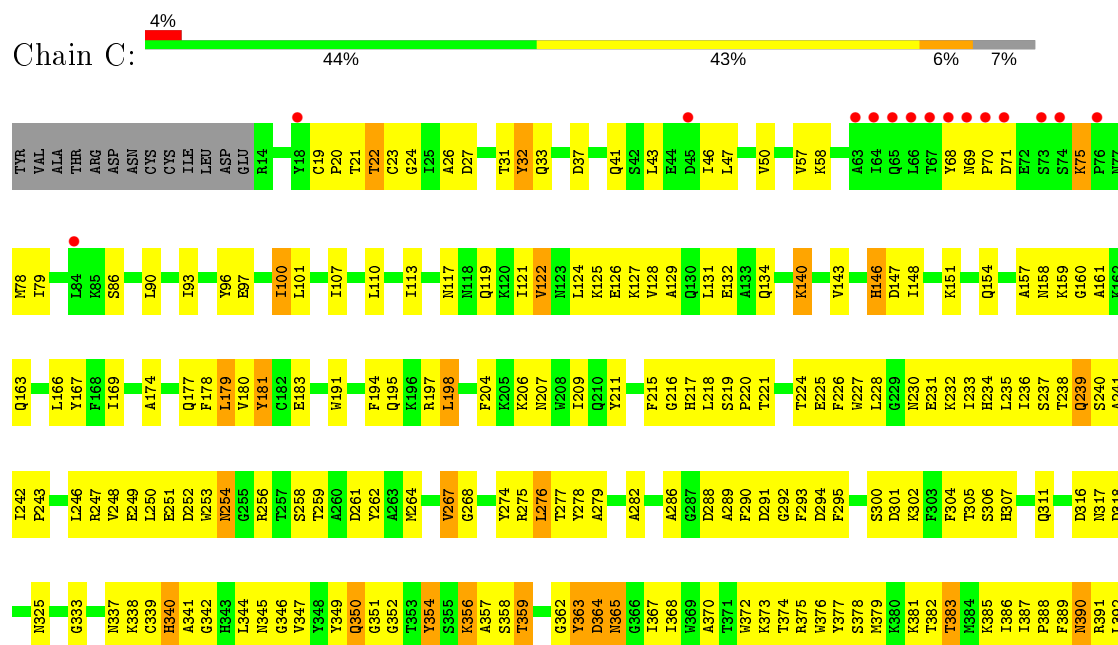




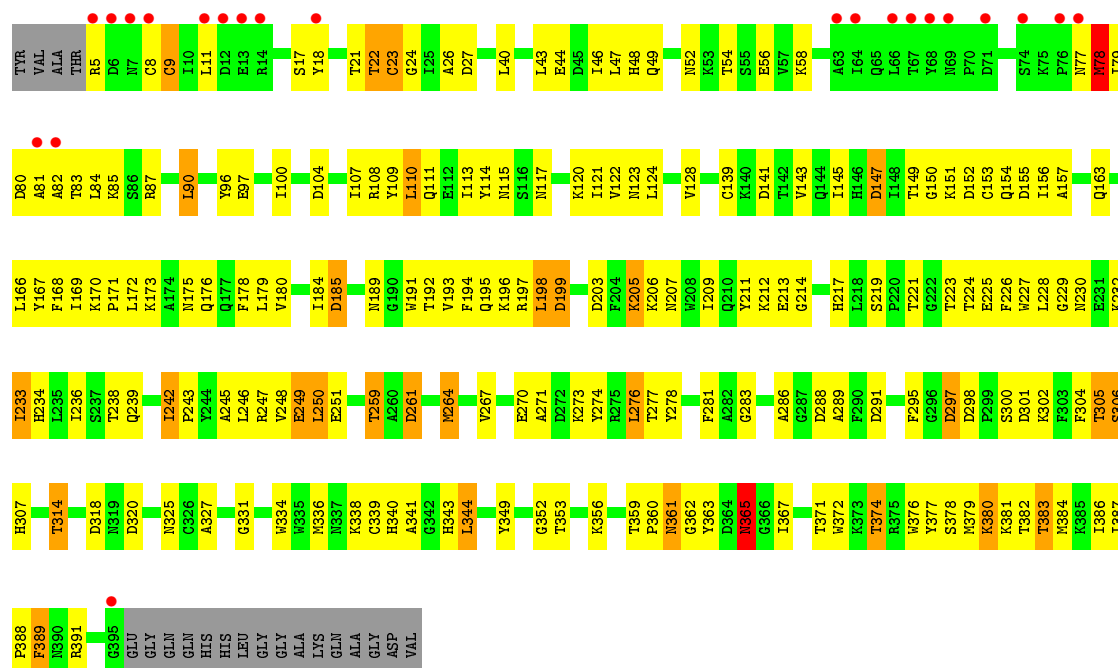
• Molecule 2: Fibrinogen beta chain



• Molecule 3: Fibrinogen gamma chain







- Molecule 4: A knob

Chain M: 25% 50% 25%



- Molecule 4: A knob

Chain N: 75% 25%



- Molecule 4: A knob

Chain Q: 75% 25%



- Molecule 4: A knob

Chain R: 50% 50%



- Molecule 5: B knob

Chain O: 25% 75%



- Molecule 5: B knob

Chain P:  50% 50%

 G1 H2 R3 P4

- Molecule 5: B knob

Chain S:  25% 75%

 G1 H2 R3 P4

- Molecule 5: B knob

Chain T:  50% 50%

 G1 H2 R3 P4

- Molecule 6: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  27% 73%

 MAG1 NDG2 BMA3 MAN4 NDG5 GAL6 SIA7 MAN8 NDG9 GAL10 SIA11

- Molecule 6: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  18% 82%

 MAG1 NDG2 BMA3 MAN4 NDG5 GAL6 SIA7 MAN8 NDG9 GAL10 SIA11

- Molecule 6: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  18% 82%

HA61	NDG2	BYA3	MAN4	NDG5	GAL6	STI7	MAN8	NDG9	GAL10	STI11
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- Molecule 7: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- α -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain W:  20% 20% 60%

HA61	NDG2	BYA3	MAN4	MAN5
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- Molecule 8: 2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain Y:  100%

HA61	HA62
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.24Å 94.87Å 300.81Å 90.00° 94.81° 90.00°	Depositor
Resolution (Å)	19.95 – 2.90 19.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.95-2.90) 69.4 (19.93-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.4.0061	Depositor
R, R_{free}	0.252 , 0.309 0.259 , 0.311	Depositor DCC
R_{free} test set	5820 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	84.4	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 75.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	31833	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2228e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.45	0/1447	0.61	0/1939
1	D	0.44	0/1447	0.56	0/1939
1	G	0.40	0/1447	0.54	0/1939
1	J	0.46	0/1547	0.62	0/2076
2	B	0.59	0/3283	0.73	0/4438
2	E	0.52	0/3283	0.62	0/4438
2	H	0.52	0/3283	0.65	0/4438
2	K	0.51	0/3283	0.65	0/4438
3	C	0.83	2/3125 (0.1%)	0.84	2/4224 (0.0%)
3	F	0.46	0/3129	0.57	1/4229 (0.0%)
3	I	0.53	0/3220	0.63	0/4353
3	L	0.55	0/3201	0.65	0/4326
4	M	0.80	0/31	0.89	0/40
4	N	0.46	0/31	0.62	0/40
4	Q	0.74	0/31	0.62	0/40
4	R	0.74	0/31	0.59	0/40
5	O	0.57	0/34	0.72	0/43
5	P	0.48	0/34	0.67	0/43
5	S	0.47	0/34	0.59	0/43
5	T	0.56	0/34	0.86	0/43
All	All	0.55	2/31955 (0.0%)	0.66	3/43109 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	181	TYR	CG-CD1	-5.83	1.31	1.39
3	C	181	TYR	CG-CD2	-5.10	1.32	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	90	LEU	CA-CB-CG	5.60	128.18	115.30
3	C	364	ASP	CB-CG-OD1	5.47	123.22	118.30
3	C	363	TYR	CA-CB-CG	5.25	123.38	113.40

There are no chirality outliers.

There are no planarity outliers.

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	1431	0	1424	104	0
1	D	1431	0	1424	72	0
1	G	1431	0	1424	78	0
1	J	1527	0	1533	140	1
2	B	3209	0	3042	210	0
2	E	3209	0	3042	181	0
2	H	3209	0	3041	159	0
2	K	3209	0	3043	192	0
3	C	3050	0	2906	209	0
3	F	3054	0	2909	157	0
3	I	3145	0	2993	186	1
3	L	3126	0	2972	239	0
4	M	30	0	32	2	0
4	N	30	0	32	0	0
4	Q	30	0	32	0	0
4	R	30	0	32	1	0
5	O	33	0	32	3	0
5	P	33	0	32	2	0
5	S	33	0	32	4	0
5	T	33	0	32	4	0
6	U	151	0	123	23	0
6	V	151	0	123	14	0
6	X	151	0	123	16	0
7	W	61	0	51	7	0
8	Y	28	0	25	12	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	E	1	0	0	0	0
9	F	1	0	0	0	0
9	H	1	0	0	0	0
9	I	1	0	0	0	0
9	K	1	0	0	0	0
9	L	1	0	0	0	0
All	All	31833	0	30454	1660	1

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 27.

The worst 5 of 1660 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:K:364:ASN:HD21	6:X:1:NAG:C1	1.17	1.55
2:B:364:ASN:ND2	6:U:1:NAG:C1	1.70	1.52
2:K:364:ASN:ND2	6:X:1:NAG:C1	1.85	1.38
3:L:56:GLU:HB2	8:Y:1:NAG:O3	1.20	1.32
2:H:172:LEU:HD21	3:I:113:ILE:CG2	1.70	1.19

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:72:GLU:OE2	1:J:84:HIS:NE2[1_455]	2.15	0.05

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	172/562 (31%)	150 (87%)	20 (12%)	2 (1%)	13 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	172/562 (31%)	158 (92%)	8 (5%)	6 (4%)	3	14
1	G	172/562 (31%)	150 (87%)	18 (10%)	4 (2%)	6	23
1	J	184/562 (33%)	164 (89%)	18 (10%)	2 (1%)	14	42
2	B	399/461 (87%)	344 (86%)	46 (12%)	9 (2%)	6	23
2	E	399/461 (87%)	337 (84%)	48 (12%)	14 (4%)	3	14
2	H	399/461 (87%)	354 (89%)	38 (10%)	7 (2%)	8	29
2	K	399/461 (87%)	348 (87%)	45 (11%)	6 (2%)	10	34
3	C	379/411 (92%)	322 (85%)	48 (13%)	9 (2%)	6	22
3	F	380/411 (92%)	320 (84%)	54 (14%)	6 (2%)	9	32
3	I	392/411 (95%)	347 (88%)	39 (10%)	6 (2%)	10	34
3	L	389/411 (95%)	338 (87%)	42 (11%)	9 (2%)	6	23
4	M	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
4	N	2/4 (50%)	2 (100%)	0	0	100	100
4	Q	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
4	R	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
5	O	2/4 (50%)	2 (100%)	0	0	100	100
5	P	2/4 (50%)	2 (100%)	0	0	100	100
5	S	2/4 (50%)	2 (100%)	0	0	100	100
5	T	2/4 (50%)	2 (100%)	0	0	100	100
All	All	3852/5768 (67%)	3345 (87%)	427 (11%)	80 (2%)	7	26

5 of 80 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	ASP
1	A	195	PRO
2	B	259	SER
3	C	70	PRO
3	C	350	GLN

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	164/479 (34%)	150 (92%)	14 (8%)	10	31
1	D	164/479 (34%)	150 (92%)	14 (8%)	10	31
1	G	164/479 (34%)	154 (94%)	10 (6%)	18	48
1	J	176/479 (37%)	152 (86%)	24 (14%)	3	11
2	B	350/396 (88%)	306 (87%)	44 (13%)	4	13
2	E	350/396 (88%)	312 (89%)	38 (11%)	6	19
2	H	350/396 (88%)	313 (89%)	37 (11%)	6	20
2	K	350/396 (88%)	309 (88%)	41 (12%)	5	16
3	C	328/350 (94%)	290 (88%)	38 (12%)	5	16
3	F	328/350 (94%)	284 (87%)	44 (13%)	4	11
3	I	339/350 (97%)	303 (89%)	36 (11%)	6	20
3	L	337/350 (96%)	294 (87%)	43 (13%)	4	13
4	M	3/3 (100%)	2 (67%)	1 (33%)	0	0
4	N	3/3 (100%)	2 (67%)	1 (33%)	0	0
4	Q	3/3 (100%)	2 (67%)	1 (33%)	0	0
4	R	3/3 (100%)	2 (67%)	1 (33%)	0	0
5	O	3/3 (100%)	3 (100%)	0	100	100
5	P	3/3 (100%)	3 (100%)	0	100	100
5	S	3/3 (100%)	3 (100%)	0	100	100
5	T	3/3 (100%)	3 (100%)	0	100	100
All	All	3424/4924 (70%)	3037 (89%)	387 (11%)	6	18

5 of 387 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	285	ASP
2	H	140	ASN
3	L	175	ASN
3	F	325	ASN
1	G	122	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 149 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	158	ASN
2	H	89	GLN
3	L	49	GLN
3	F	210	GLN
1	G	59	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 ⓘ

40 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	$\# Z > 2$
6	NAG	U	1	6	14,14,15	0.94	0	17,19,21	1.44	1 (5%)
6	GAL	U	10	6	11,11,12	0.98	0	15,15,17	0.76	0
6	SIA	U	11	6	17,20,21	1.51	2 (11%)	21,28,31	1.39	1 (4%)
6	NDG	U	2	6	14,14,15	0.79	0	17,19,21	1.02	1 (5%)
6	BMA	U	3	6	11,11,12	1.09	1 (9%)	15,15,17	1.20	1 (6%)
6	MAN	U	4	6	11,11,12	1.17	0	15,15,17	0.93	1 (6%)
6	NDG	U	5	6	14,14,15	1.10	1 (7%)	17,19,21	1.03	1 (5%)
6	GAL	U	6	6	11,11,12	0.62	0	15,15,17	0.55	0
6	SIA	U	7	6	17,20,21	1.57	5 (29%)	21,28,31	1.05	1 (4%)
6	MAN	U	8	6	11,11,12	1.65	3 (27%)	15,15,17	1.36	1 (6%)
6	NDG	U	9	6	14,14,15	1.07	1 (7%)	17,19,21	0.87	0
6	NAG	V	1	2,6	14,14,15	0.78	0	17,19,21	1.18	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GAL	V	10	6	11,11,12	1.00	1 (9%)	15,15,17	0.89	1 (6%)
6	SIA	V	11	6	17,20,21	1.09	1 (5%)	21,28,31	0.78	0
6	NDG	V	2	6	14,14,15	0.91	1 (7%)	17,19,21	0.94	0
6	BMA	V	3	6	11,11,12	1.12	1 (9%)	15,15,17	1.38	1 (6%)
6	MAN	V	4	6	11,11,12	1.45	2 (18%)	15,15,17	1.19	3 (20%)
6	NDG	V	5	6	14,14,15	1.24	2 (14%)	17,19,21	0.84	0
6	GAL	V	6	6	11,11,12	1.18	0	15,15,17	0.74	0
6	SIA	V	7	6	17,20,21	0.86	1 (5%)	21,28,31	1.42	3 (14%)
6	MAN	V	8	6	11,11,12	0.97	0	15,15,17	1.64	3 (20%)
6	NDG	V	9	6	14,14,15	1.10	1 (7%)	17,19,21	0.94	0
7	NAG	W	1	2,7	14,14,15	0.68	0	17,19,21	1.14	1 (5%)
7	NDG	W	2	7	14,14,15	0.78	1 (7%)	17,19,21	1.00	1 (5%)
7	BMA	W	3	7	11,11,12	0.76	0	15,15,17	1.18	1 (6%)
7	MAN	W	4	7	11,11,12	1.20	2 (18%)	15,15,17	1.16	1 (6%)
7	MAN	W	5	7	11,11,12	0.65	0	15,15,17	0.69	0
6	NAG	X	1	6	14,14,15	0.99	0	17,19,21	1.29	3 (17%)
6	GAL	X	10	6	11,11,12	1.28	1 (9%)	15,15,17	0.75	0
6	SIA	X	11	6	17,20,21	0.90	0	21,28,31	0.95	1 (4%)
6	NDG	X	2	6	14,14,15	1.24	2 (14%)	17,19,21	1.01	0
6	BMA	X	3	6	11,11,12	1.29	1 (9%)	15,15,17	1.04	2 (13%)
6	MAN	X	4	6	11,11,12	1.06	0	15,15,17	1.31	2 (13%)
6	NDG	X	5	6	14,14,15	1.07	1 (7%)	17,19,21	0.92	0
6	GAL	X	6	6	11,11,12	1.03	0	15,15,17	0.98	2 (13%)
6	SIA	X	7	6	17,20,21	1.38	3 (17%)	21,28,31	1.79	5 (23%)
6	MAN	X	8	6	11,11,12	1.15	2 (18%)	15,15,17	1.39	3 (20%)
6	NDG	X	9	6	14,14,15	1.11	1 (7%)	17,19,21	1.11	2 (11%)
8	NAG	Y	1	8	14,14,15	1.00	0	17,19,21	1.04	1 (5%)
8	NAG	Y	2	8	14,14,15	1.18	2 (14%)	17,19,21	0.87	1 (5%)

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
6	NAG	U	1	6	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GAL	U	10	6	-	2/2/19/22	0/1/1/1
6	SIA	U	11	6	-	2/14/34/38	0/1/1/1
6	NDG	U	2	6	-	5/6/23/26	0/1/1/1
6	BMA	U	3	6	-	2/2/19/22	0/1/1/1
6	MAN	U	4	6	-	2/2/19/22	0/1/1/1
6	NDG	U	5	6	-	3/6/23/26	0/1/1/1
6	GAL	U	6	6	1/1/4/5	2/2/19/22	0/1/1/1
6	SIA	U	7	6	-	10/14/34/38	0/1/1/1
6	MAN	U	8	6	-	1/2/19/22	0/1/1/1
6	NDG	U	9	6	-	4/6/23/26	0/1/1/1
6	NAG	V	1	2,6	1/1/5/7	4/6/23/26	0/1/1/1
6	GAL	V	10	6	-	1/2/19/22	0/1/1/1
6	SIA	V	11	6	-	6/14/34/38	0/1/1/1
6	NDG	V	2	6	-	6/6/23/26	0/1/1/1
6	BMA	V	3	6	-	1/2/19/22	0/1/1/1
6	MAN	V	4	6	-	1/2/19/22	0/1/1/1
6	NDG	V	5	6	-	4/6/23/26	0/1/1/1
6	GAL	V	6	6	1/1/4/5	2/2/19/22	0/1/1/1
6	SIA	V	7	6	-	10/14/34/38	0/1/1/1
6	MAN	V	8	6	-	2/2/19/22	0/1/1/1
6	NDG	V	9	6	-	3/6/23/26	0/1/1/1
7	NAG	W	1	2,7	1/1/5/7	4/6/23/26	0/1/1/1
7	NDG	W	2	7	-	4/6/23/26	0/1/1/1
7	BMA	W	3	7	-	1/2/19/22	0/1/1/1
7	MAN	W	4	7	-	1/2/19/22	0/1/1/1
7	MAN	W	5	7	-	2/2/19/22	0/1/1/1
6	NAG	X	1	6	-	4/6/23/26	0/1/1/1
6	GAL	X	10	6	-	2/2/19/22	0/1/1/1
6	SIA	X	11	6	-	8/14/34/38	0/1/1/1
6	NDG	X	2	6	-	3/6/23/26	0/1/1/1
6	BMA	X	3	6	-	2/2/19/22	0/1/1/1
6	MAN	X	4	6	-	2/2/19/22	0/1/1/1
6	NDG	X	5	6	-	4/6/23/26	0/1/1/1
6	GAL	X	6	6	1/1/4/5	2/2/19/22	0/1/1/1
6	SIA	X	7	6	-	10/14/34/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	X	8	6	-	2/2/19/22	0/1/1/1
6	NDG	X	9	6	-	2/6/23/26	0/1/1/1
8	NAG	Y	1	8	-	5/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	6/6/23/26	0/1/1/1

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	U	11	SIA	C3-C2	4.72	1.60	1.52
6	U	8	MAN	C2-C3	4.07	1.58	1.52
6	X	7	SIA	C4-C5	3.70	1.56	1.53
6	U	7	SIA	C4-C5	3.46	1.56	1.53
6	V	3	BMA	C2-C3	3.24	1.57	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	U	11	SIA	C4-C3-C2	5.13	119.01	109.81
6	U	1	NAG	C2-N2-C7	-5.10	115.64	122.90
6	V	8	MAN	C1-C2-C3	4.63	115.36	109.67
6	V	3	BMA	C1-C2-C3	-4.19	104.52	109.67
6	U	8	MAN	C1-C2-C3	3.98	114.56	109.67

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	V	1	NAG	C1
6	U	6	GAL	C1
7	W	1	NAG	C1
6	V	6	GAL	C1
6	X	6	GAL	C1

5 of 139 torsion outliers are listed below:

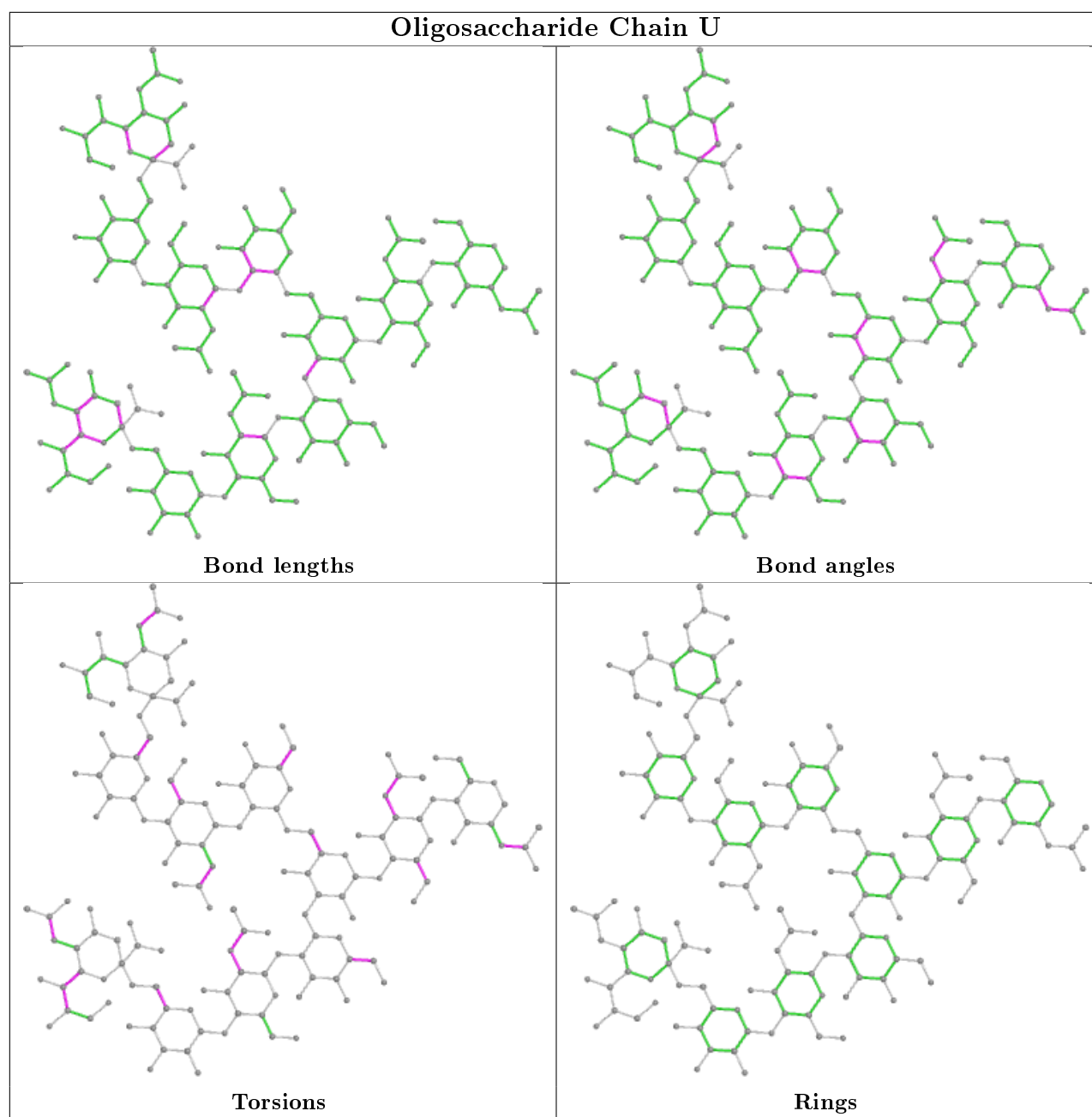
Mol	Chain	Res	Type	Atoms
6	U	7	SIA	C5-C6-C7-C8
6	U	7	SIA	C5-C6-C7-O7
6	U	7	SIA	O6-C6-C7-C8
6	U	7	SIA	O6-C6-C7-O7
6	U	7	SIA	C11-C10-N5-C5

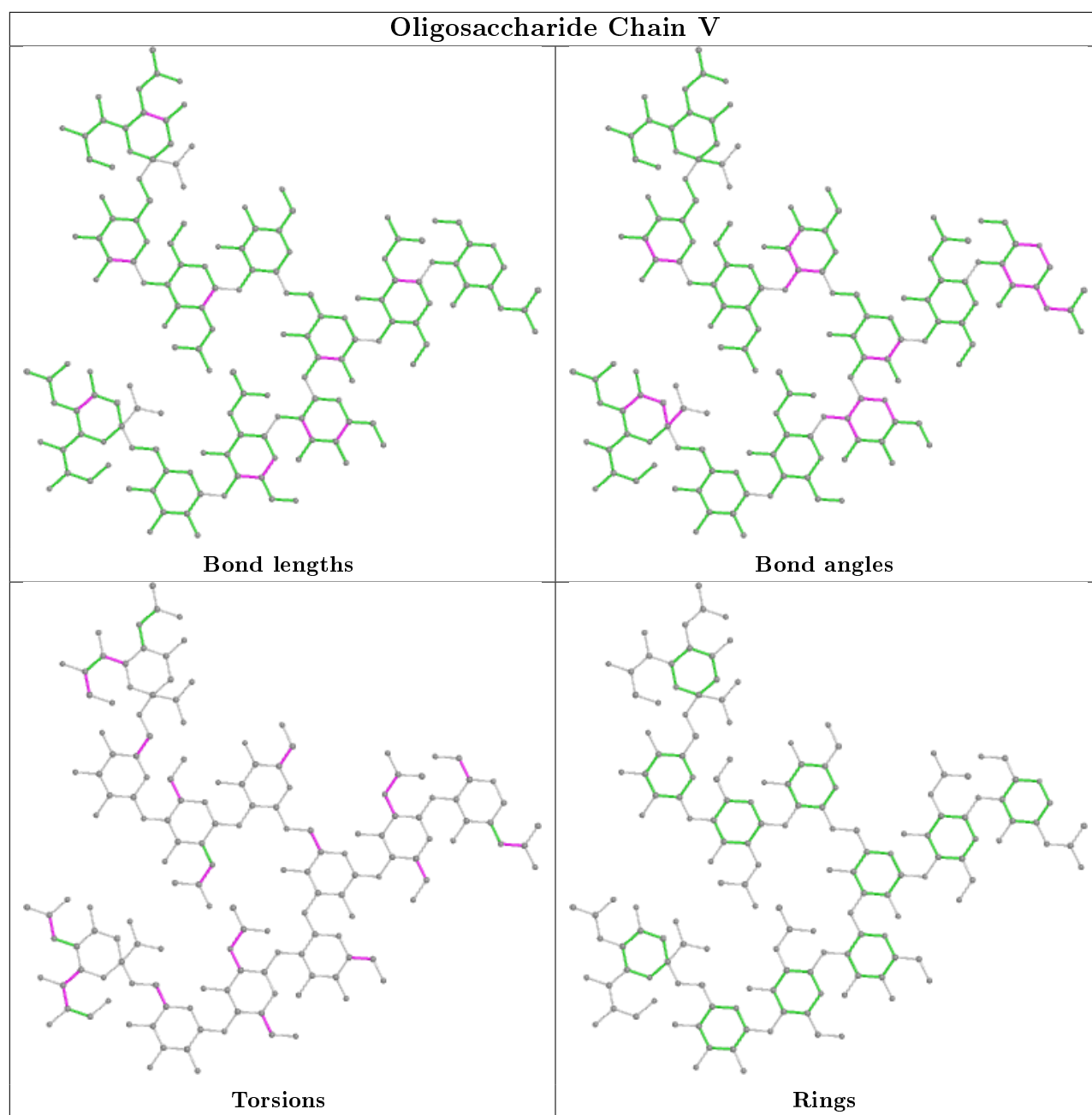
There are no ring outliers.

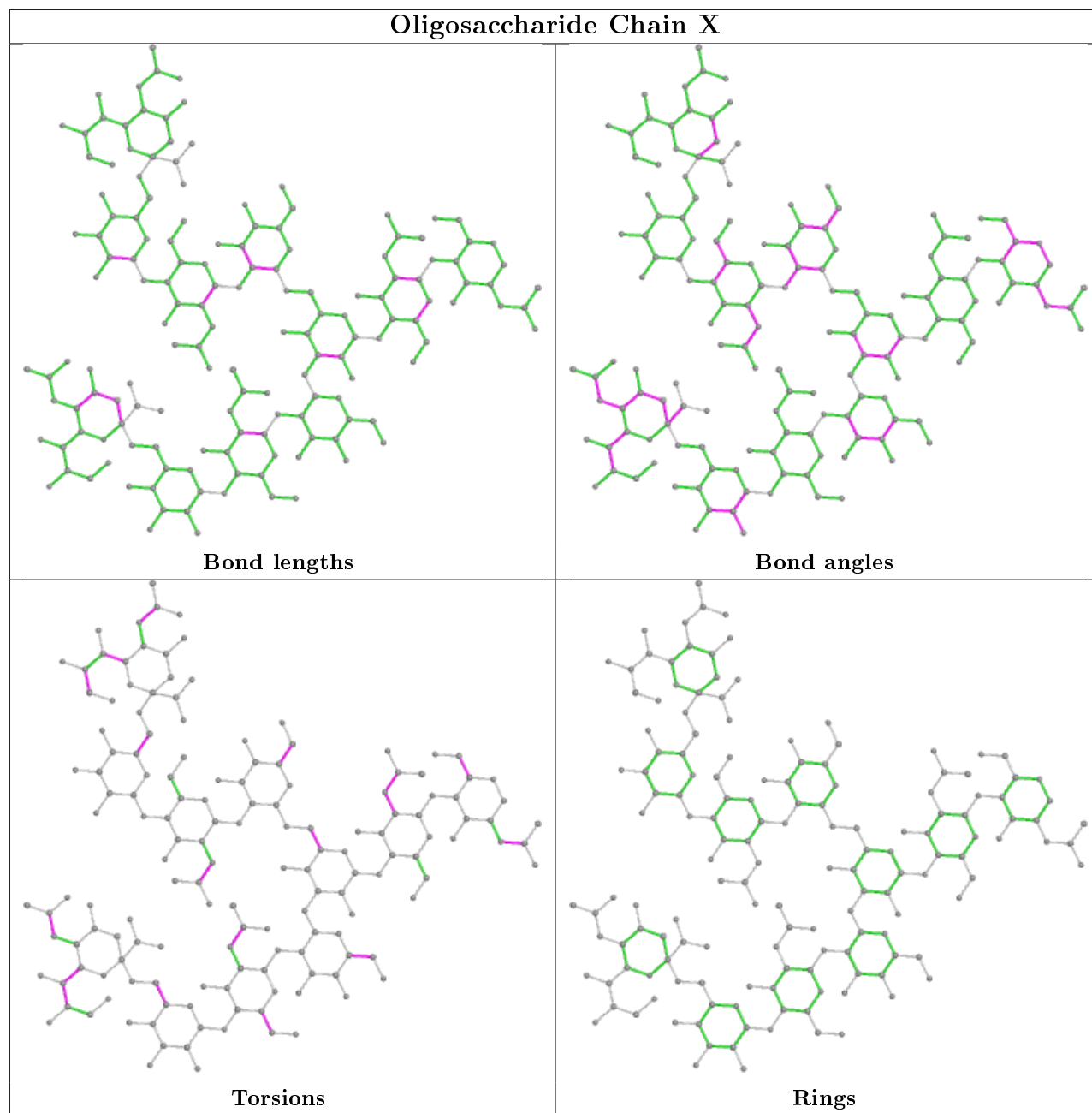
34 monomers are involved in 72 short contacts:

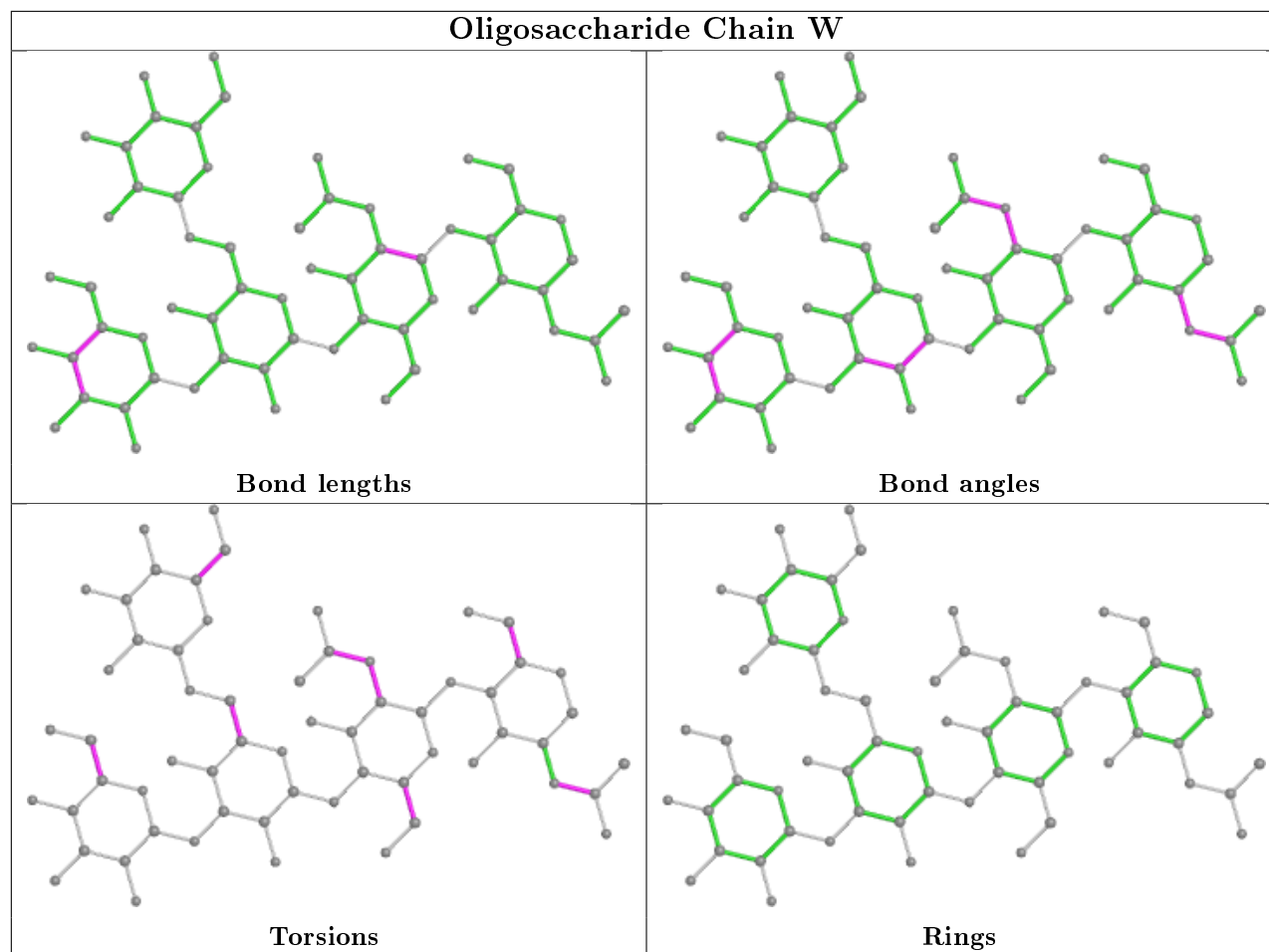
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	X	10	GAL	1	0
6	V	8	MAN	1	0
6	U	7	SIA	5	0
6	U	10	GAL	1	0
8	Y	2	NAG	1	0
6	U	3	BMA	1	0
8	Y	1	NAG	12	0
6	V	1	NAG	2	0
6	X	11	SIA	3	0
6	V	11	SIA	1	0
6	X	8	MAN	2	0
6	V	7	SIA	5	0
6	X	1	NAG	7	0
6	V	5	NDG	3	0
6	X	9	NDG	2	0
6	U	5	NDG	3	0
7	W	2	NDG	3	0
6	U	9	NDG	4	0
6	U	6	GAL	4	0
7	W	1	NAG	5	0
6	X	5	NDG	3	0
6	V	6	GAL	2	0
6	V	2	NDG	2	0
6	V	10	GAL	1	0
6	X	2	NDG	4	0
7	W	3	BMA	1	0
6	X	6	GAL	1	0
6	U	2	NDG	4	0
6	U	11	SIA	1	0
6	U	1	NAG	9	0
6	X	7	SIA	1	0
6	V	4	MAN	2	0
6	V	3	BMA	2	0
6	U	8	MAN	4	0

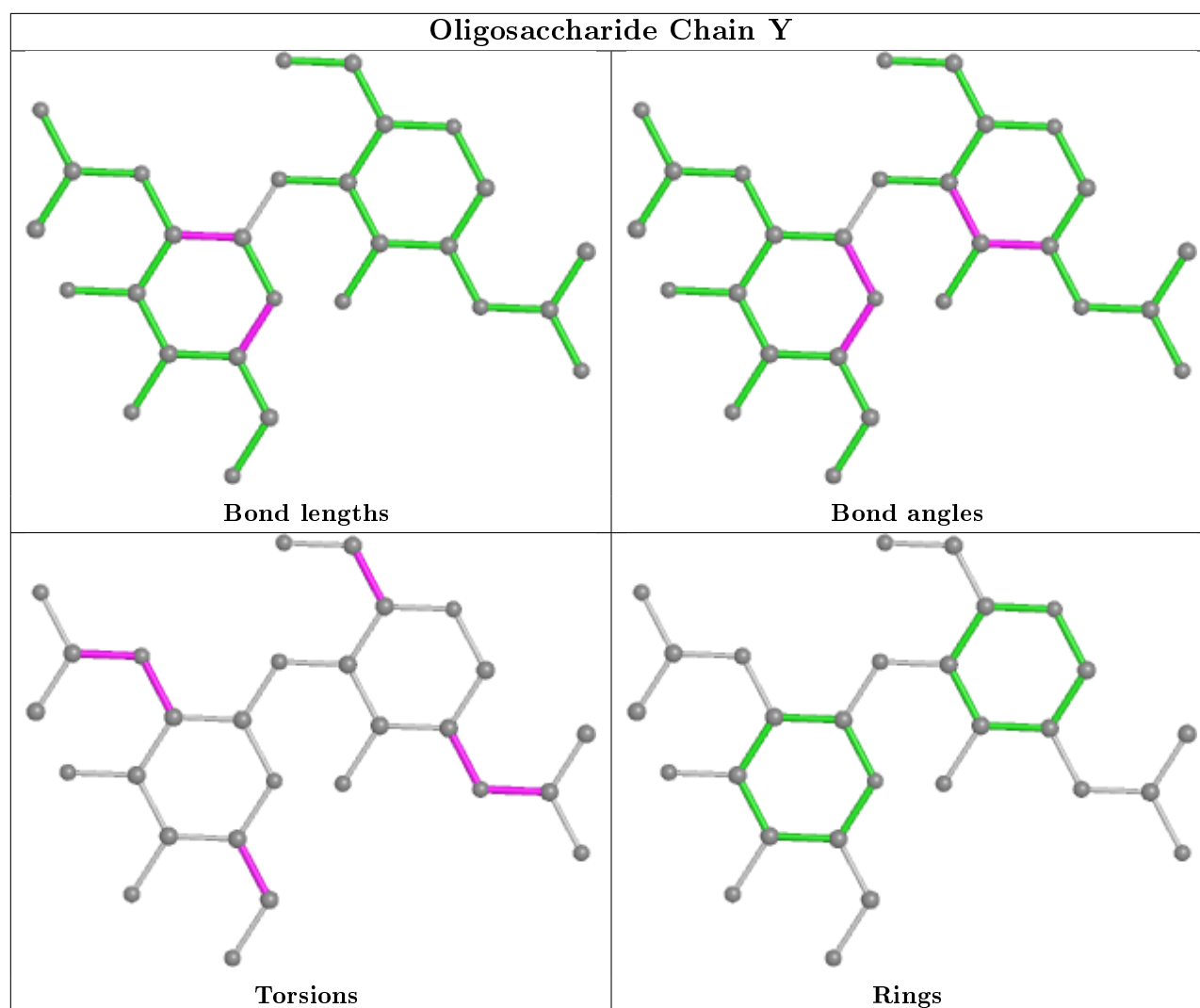
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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 ⓘ

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, 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	174/562 (30%)	0.06	8 (4%) 32 29	21, 106, 173, 187	0
1	D	174/562 (30%)	0.84	33 (18%) 1 0	62, 137, 231, 238	0
1	G	174/562 (30%)	0.11	10 (5%) 23 19	51, 120, 163, 173	0
1	J	186/562 (33%)	0.45	23 (12%) 4 3	64, 135, 224, 246	0
2	B	401/461 (86%)	-0.32	5 (1%) 79 79	21, 53, 151, 184	0
2	E	401/461 (86%)	0.07	35 (8%) 10 7	40, 64, 211, 226	0
2	H	401/461 (86%)	-0.14	15 (3%) 41 37	30, 62, 168, 195	0
2	K	401/461 (86%)	-0.25	6 (1%) 73 73	40, 64, 156, 164	0
3	C	381/411 (92%)	-0.46	15 (3%) 39 35	8, 39, 189, 232	0
3	F	382/411 (92%)	0.13	23 (6%) 21 18	52, 89, 208, 221	0
3	I	394/411 (95%)	-0.17	19 (4%) 30 27	29, 69, 179, 207	0
3	L	391/411 (95%)	-0.10	22 (5%) 24 20	35, 70, 177, 203	0
4	M	4/4 (100%)	0.37	0 100 100	63, 64, 103, 108	0
4	N	4/4 (100%)	0.15	0 100 100	119, 131, 149, 154	0
4	Q	4/4 (100%)	-0.59	0 100 100	78, 89, 90, 115	0
4	R	4/4 (100%)	0.35	0 100 100	92, 105, 106, 118	0
5	O	4/4 (100%)	-0.54	0 100 100	66, 68, 73, 93	0
5	P	4/4 (100%)	-0.21	0 100 100	90, 99, 106, 113	0
5	S	4/4 (100%)	-0.97	0 100 100	58, 69, 75, 95	0
5	T	4/4 (100%)	-0.09	0 100 100	75, 91, 98, 108	0
All	All	3892/5768 (67%)	-0.06	214 (5%) 25 21	8, 75, 189, 246	0

The worst 5 of 214 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	73	GLY	8.6
1	J	206	LYS	7.8
3	I	9	CYS	7.5
2	H	107	VAL	7.5
1	D	117	SER	7.2

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.

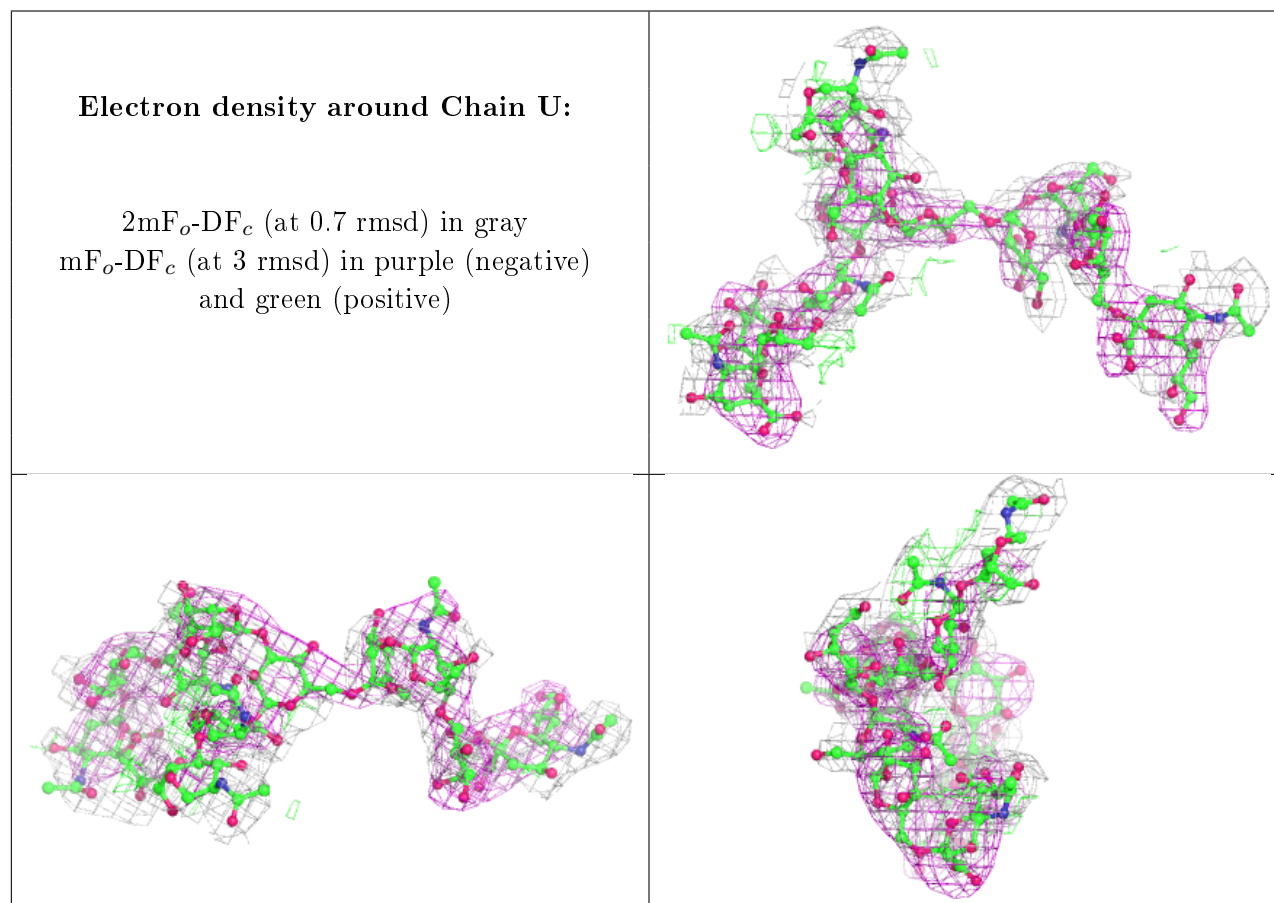
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MAN	W	4	11/12	0.34	0.50	100,103,105,107	0
6	SIA	X	11	20/21	0.45	0.69	105,113,116,116	0
6	SIA	U	7	20/21	0.46	0.52	99,104,108,108	0
6	GAL	X	10	11/12	0.55	0.94	113,116,117,117	0
6	MAN	V	4	11/12	0.55	0.56	106,108,109,112	0
6	SIA	U	11	20/21	0.57	0.60	97,103,109,111	0
6	BMA	X	3	11/12	0.59	0.44	101,104,107,107	0
6	GAL	U	10	11/12	0.59	0.62	106,107,108,112	0
6	SIA	V	11	20/21	0.59	0.67	109,114,119,125	0
6	GAL	V	6	11/12	0.62	0.49	109,112,115,116	0
6	NDG	X	2	14/15	0.62	0.47	97,100,102,104	0
6	SIA	X	7	20/21	0.63	0.42	102,107,109,109	0
6	GAL	X	6	11/12	0.66	0.59	105,110,111,111	0
7	MAN	W	5	11/12	0.67	0.69	104,108,110,110	0
8	NAG	Y	2	14/15	0.68	0.73	105,108,109,109	0
6	MAN	V	8	11/12	0.68	0.76	99,104,107,107	0
6	MAN	U	4	11/12	0.69	0.51	109,111,112,113	0
6	MAN	X	4	11/12	0.69	0.43	93,103,105,105	0
8	NAG	Y	1	14/15	0.69	0.60	106,109,110,111	0
6	BMA	V	3	11/12	0.71	0.35	98,103,106,108	0
6	NDG	V	5	14/15	0.72	0.57	103,110,115,117	0
7	BMA	W	3	11/12	0.73	0.32	100,104,108,110	0
6	GAL	V	10	11/12	0.73	0.48	115,118,118,119	0

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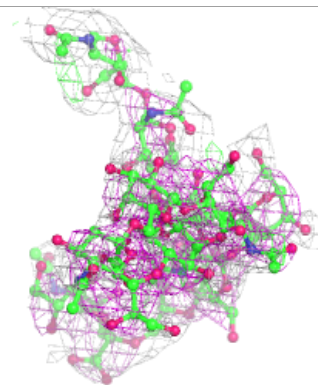
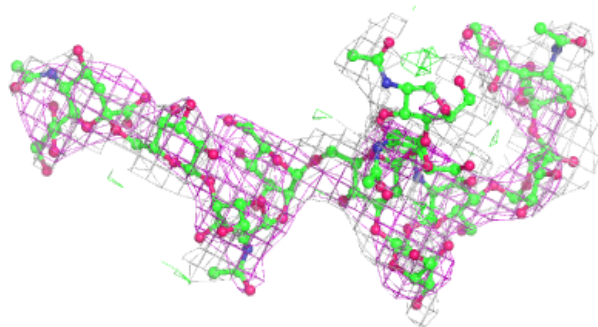
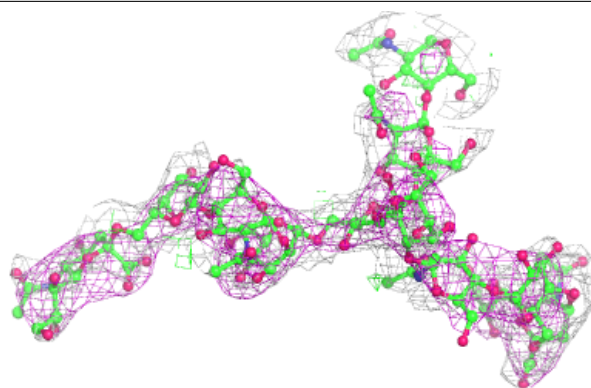
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	NDG	X	5	14/15	0.74	0.55	97,105,107,109	0
6	NDG	X	9	14/15	0.74	0.45	106,111,112,115	0
6	NDG	V	9	14/15	0.74	0.62	105,109,111,115	0
6	NDG	U	5	14/15	0.75	0.47	104,111,112,113	0
6	NDG	U	9	14/15	0.75	0.55	104,107,109,110	0
6	MAN	U	8	11/12	0.76	0.48	104,108,109,109	0
6	MAN	X	8	11/12	0.80	0.33	99,101,106,108	0
6	SIA	V	7	20/21	0.81	0.46	103,107,111,112	0
6	NDG	U	2	14/15	0.81	0.31	96,98,101,102	0
7	NAG	W	1	14/15	0.82	0.20	83,87,91,93	0
6	NAG	X	1	14/15	0.82	0.18	83,87,92,96	0
6	BMA	U	3	11/12	0.82	0.47	99,105,108,109	0
7	NDG	W	2	14/15	0.83	0.28	94,97,102,103	0
6	GAL	U	6	11/12	0.84	0.50	98,104,107,108	0
6	NAG	V	1	14/15	0.84	0.15	80,85,89,92	0
6	NAG	U	1	14/15	0.85	0.18	83,89,92,95	0
6	NDG	V	2	14/15	0.87	0.28	95,97,101,101	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.

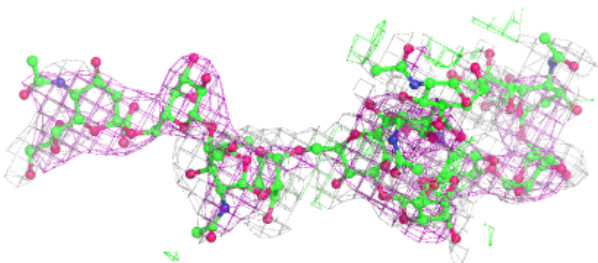
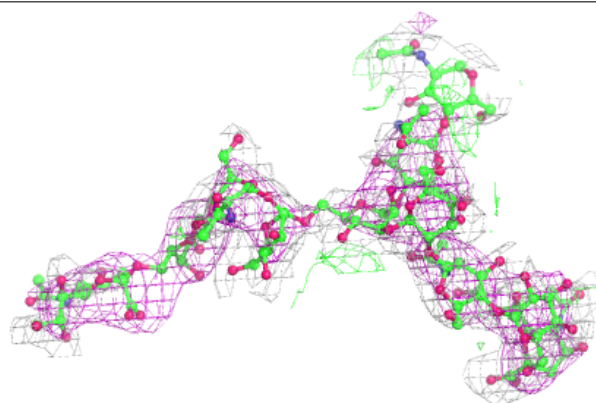


Electron density around Chain V:

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

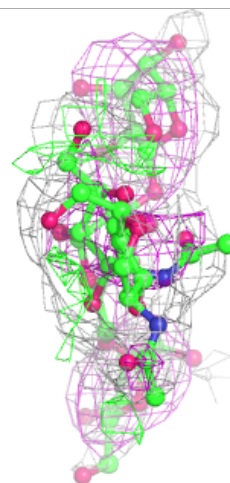
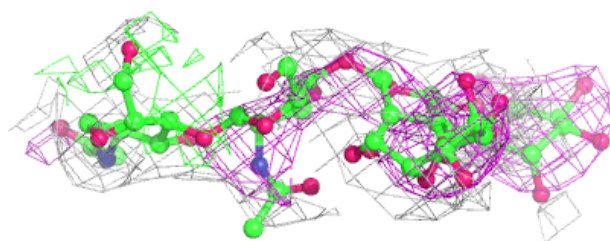
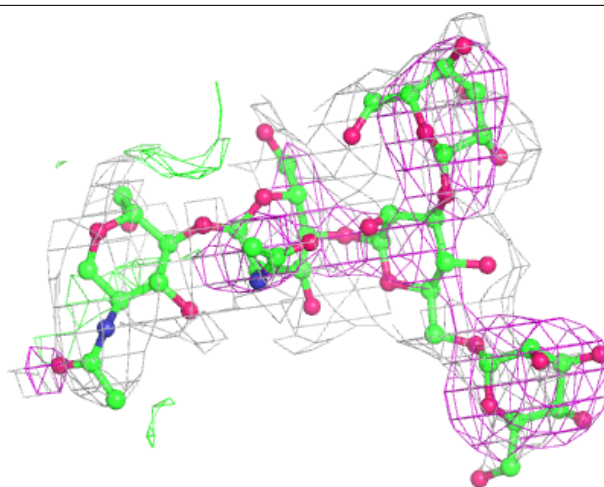
**Electron density around Chain X:**

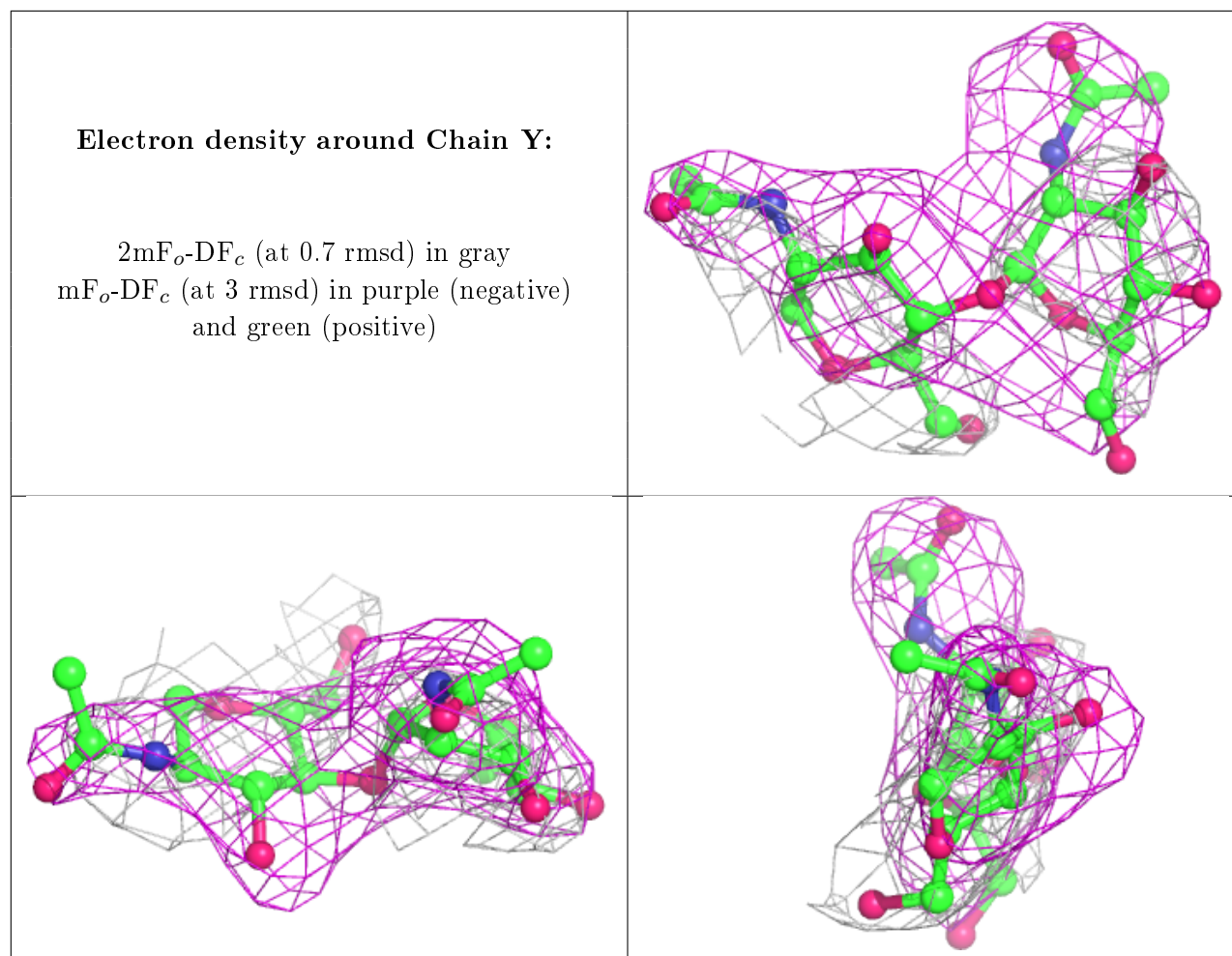
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain W:

$2mF_o-DF_c$ (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(\AA^2)	Q<0.9
9	CA	K	501	1/1	0.91	0.07	68,68,68,68	0
9	CA	E	501	1/1	0.94	0.09	47,47,47,47	0
9	CA	L	601	1/1	0.96	0.07	51,51,51,51	0
9	CA	I	601	1/1	0.97	0.05	56,56,56,56	0
9	CA	C	601	1/1	0.98	0.06	31,31,31,31	0
9	CA	F	601	1/1	0.98	0.05	49,49,49,49	0
9	CA	H	501	1/1	0.99	0.05	51,51,51,51	0
9	CA	B	501	1/1	0.99	0.08	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.