



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 09:03 AM BST

PDB ID : 2XWB
Title : Crystal Structure of Complement C3b in complex with Factors B and D
Authors : Forneris, F.; Ricklin, D.; Wu, J.; Tzekou, A.; Wallace, R.S.; Lambris, J.D.; Gros, P.
Deposited on : 2010-11-01
Resolution : 3.49 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

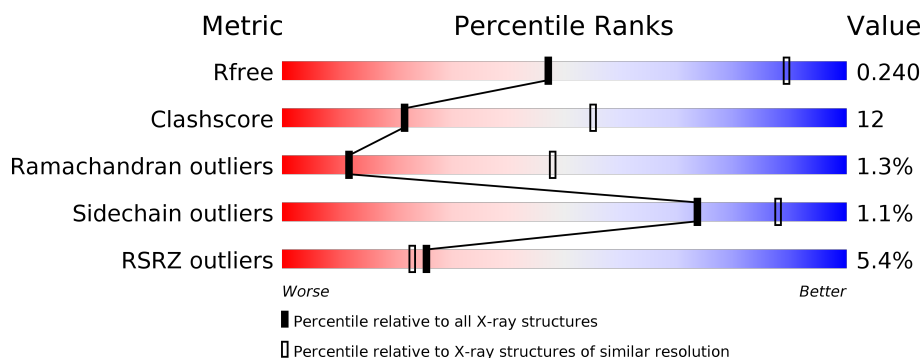
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	642	<div> <div>7%</div> <div> <div></div> <div>70%</div> <div>28%</div> <div>.</div> </div> </div>
1	C	642	<div> <div>13%</div> <div> <div></div> <div>70%</div> <div>28%</div> <div>.</div> </div> </div>
2	B	912	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>27%</div> <div>..</div> </div> </div>
2	D	912	<div> <div>9%</div> <div> <div></div> <div>70%</div> <div>28%</div> <div>..</div> </div> </div>
3	F	732	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>23%</div> <div>..</div> </div> </div>
3	H	732	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>21%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	I	228	 80% 19%
4	J	228	 78% 21%
5	E	2	 50% 50%
5	G	2	 50% 50%
5	K	2	 100%
6	L	3	 33% 67%
6	M	3	 100%

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	K	1	-	-	X	-
8	NAG	F	1747	X	-	-	-
9	GOL	J	1229	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 39285 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 COMPLEMENT C3B BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	640	Total	C	N	O	S	0	0	0
			4992	3179	846	952	15			
1	C	640	Total	C	N	O	S	0	0	0
			4992	3179	846	952	15			

- Molecule 2 is a protein called COMPLEMENT C3B ALPHA' CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	901	Total	C	N	O	S	0	0	0
			7197	4563	1210	1386	38			
2	D	901	Total	C	N	O	S	0	0	0
			7197	4563	1210	1386	38			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	991	GLU	GLN	SEE REMARK 999	UNP P01024
D	991	GLU	GLN	SEE REMARK 999	UNP P01024

- Molecule 3 is a protein called COMPLEMENT FACTOR B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	714	Total	C	N	O	S	0	0	0
			5627	3536	979	1079	33			
3	H	711	Total	C	N	O	S	0	0	0
			5608	3523	976	1076	33			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	254	GLY	ASP	engineered mutation	UNP P00751
F	260	ASP	ASN	engineered mutation	UNP P00751

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Chain	Residue	Modelled	Actual	Comment	Reference
F	740	ALA	-	expression tag	UNP P00751
F	741	ALA	-	expression tag	UNP P00751
H	254	GLY	ASP	engineered mutation	UNP P00751
H	260	ASP	ASN	engineered mutation	UNP P00751
H	740	ALA	-	expression tag	UNP P00751
H	741	ALA	-	expression tag	UNP P00751

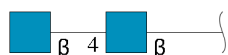
- Molecule 4 is a protein called COMPLEMENT FACTOR D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	228	Total	C	N	O	S	0	0	0
			1710	1058	325	317	10			
4	J	228	Total	C	N	O	S	0	0	0
			1710	1058	325	317	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	183	ALA	SER	engineered mutation	UNP P00746
J	183	ALA	SER	engineered mutation	UNP P00746

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



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

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

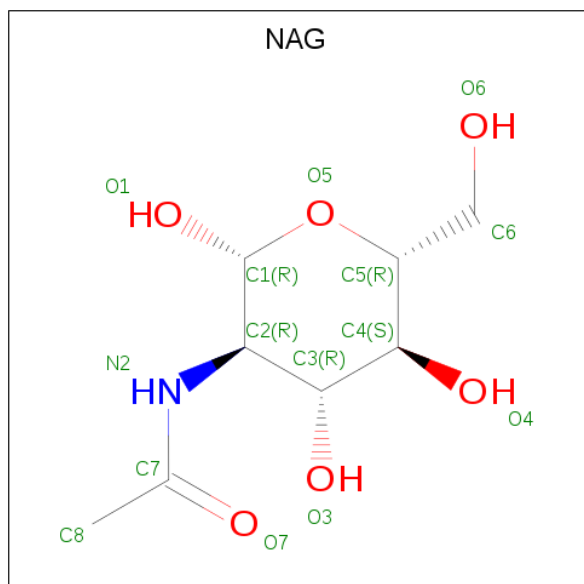


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	L	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	M	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	1	Total	Mg	0	0
			1	1		
7	A	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		
7	F	1	Total	Mg	0	0
			1	1		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



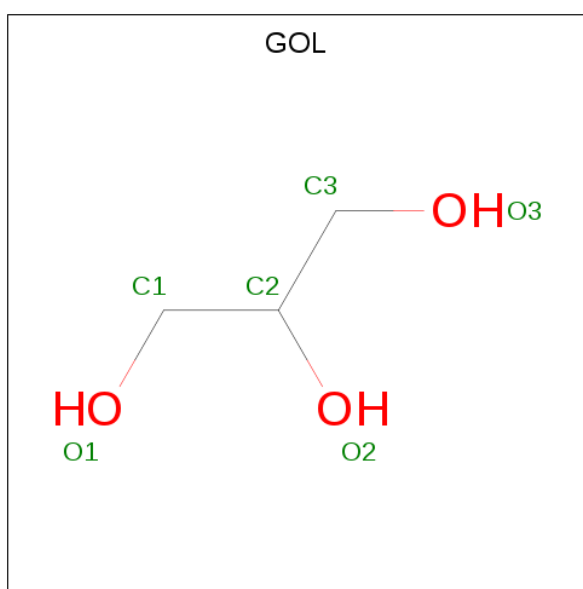
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	D	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	I	1	Total	C	O	0	0
			6	3	3		
9	J	1	Total	C	O	0	0
			6	3	3		

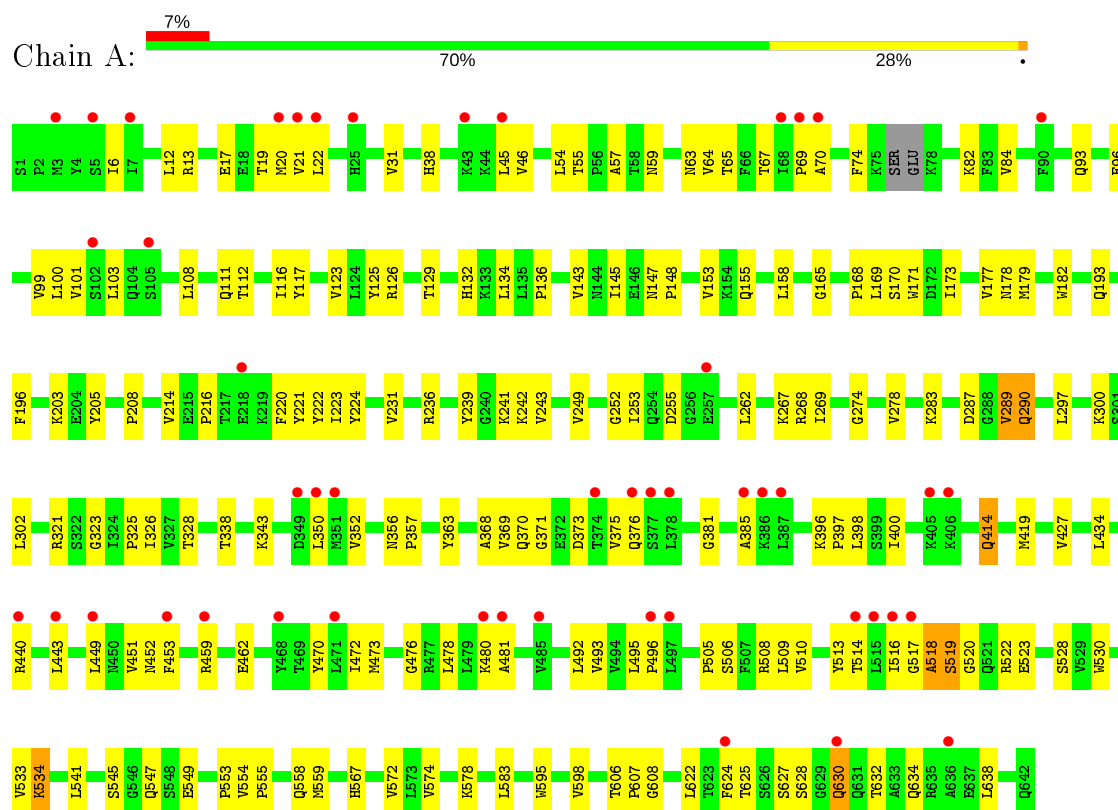
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	F	2	Total	O	0	0
			2	2		
10	H	2	Total	O	0	0
			2	2		

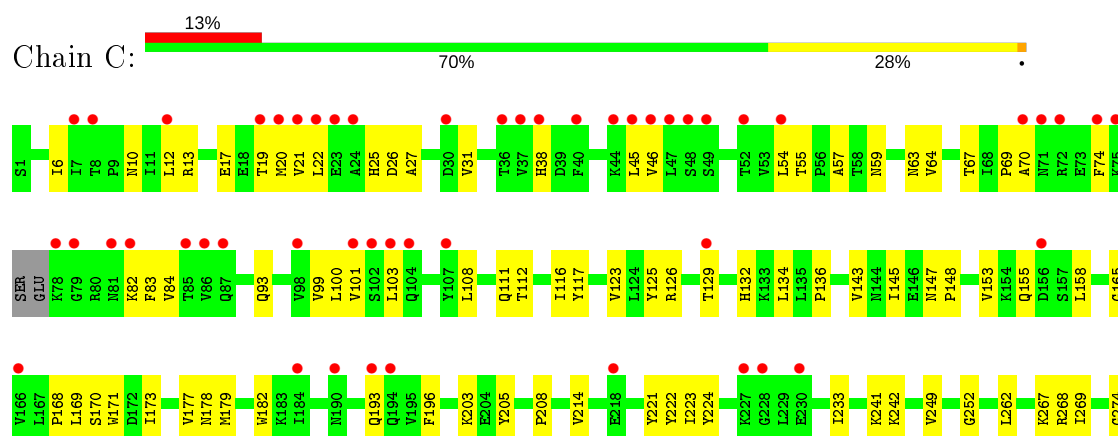
3 Residue-property plots

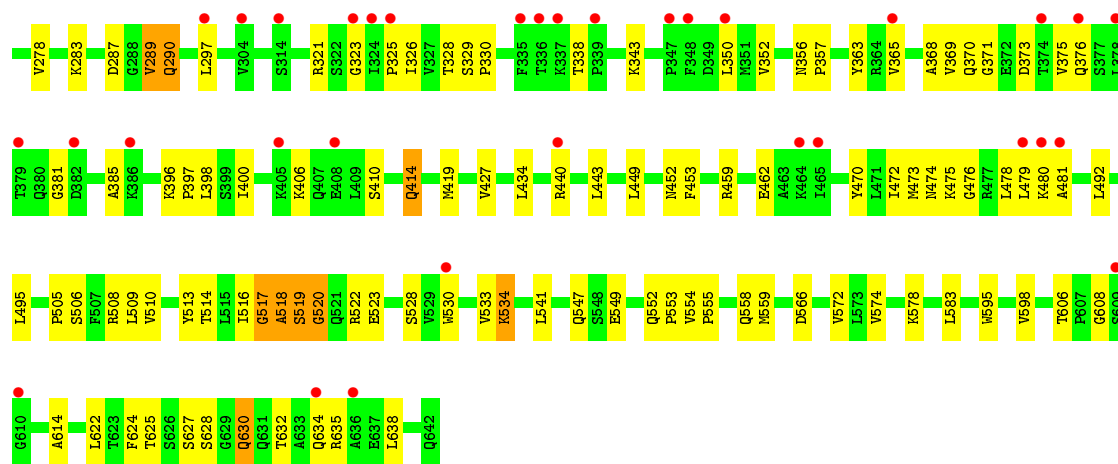
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: COMPLEMENT C3B BETA CHAIN

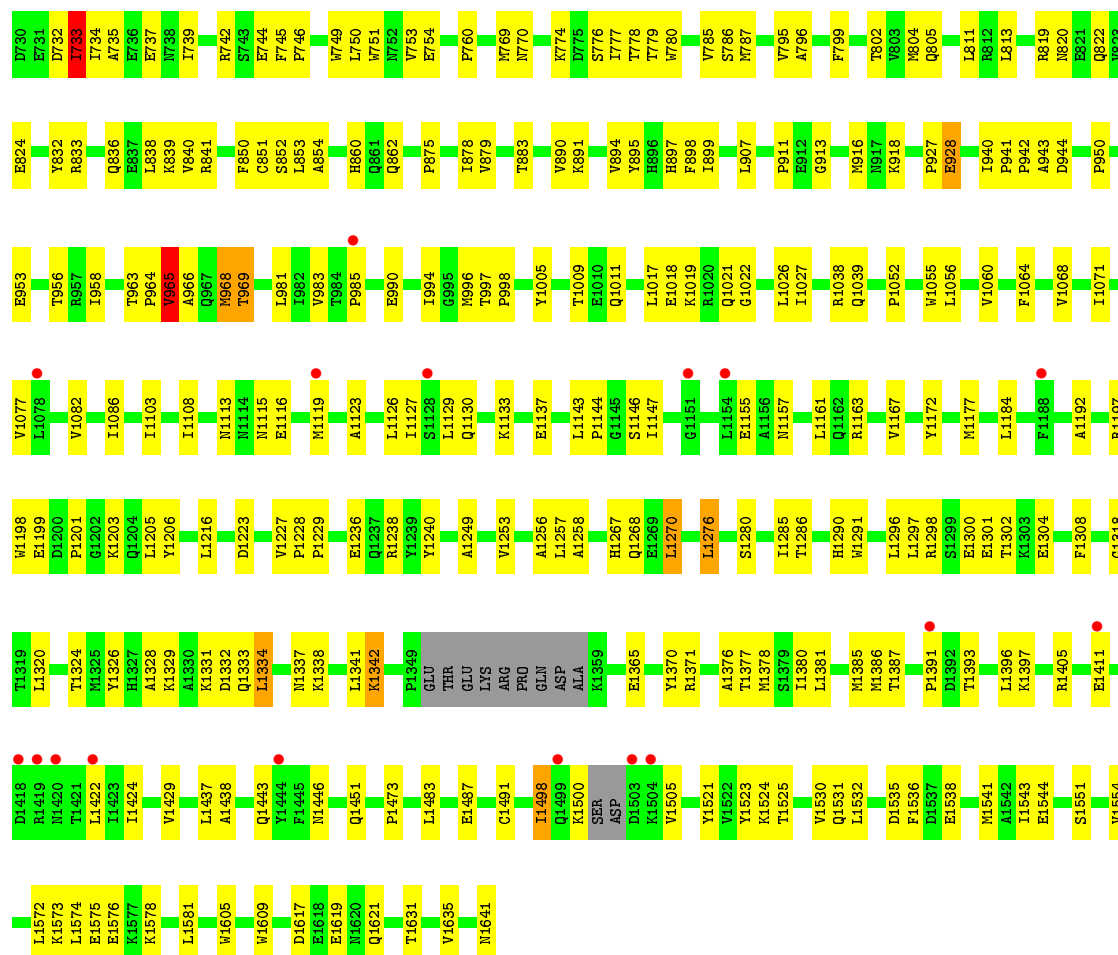


• Molecule 1: COMPLEMENT C3B BETA CHAIN



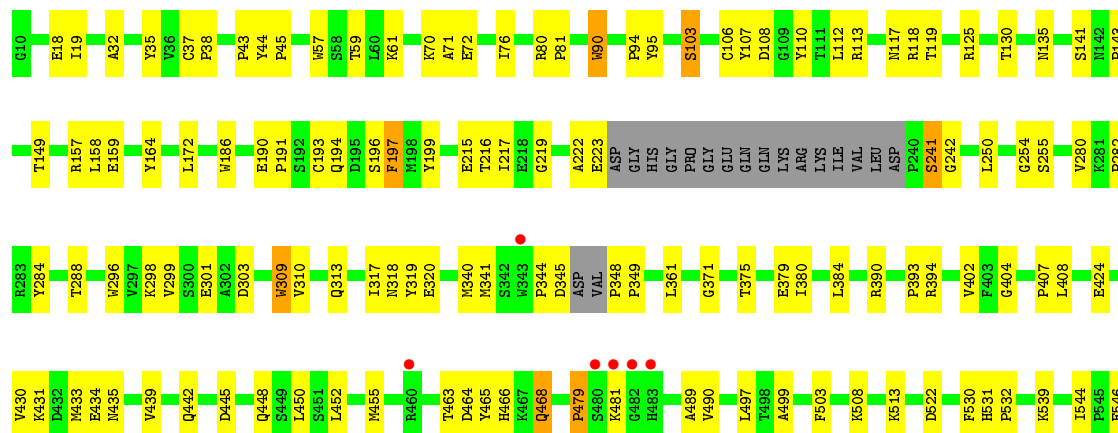


• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

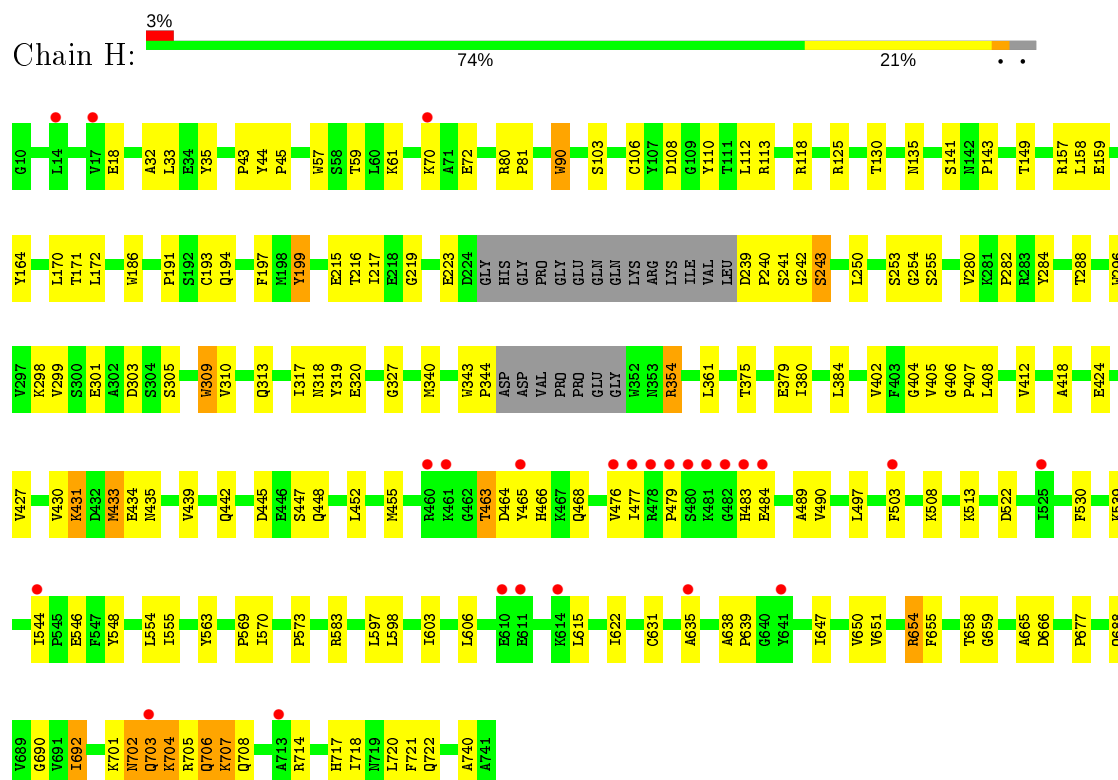


• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

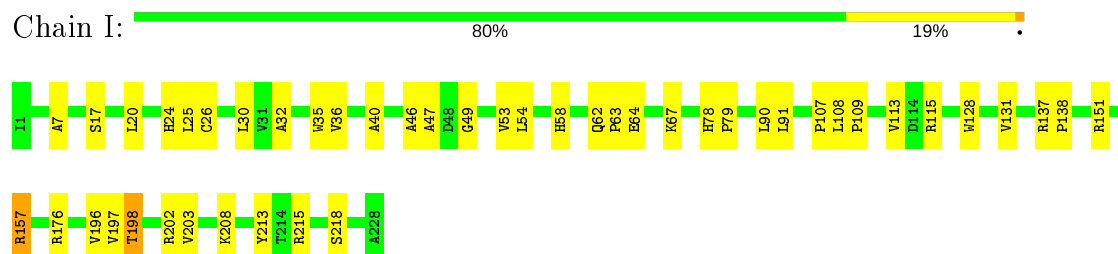




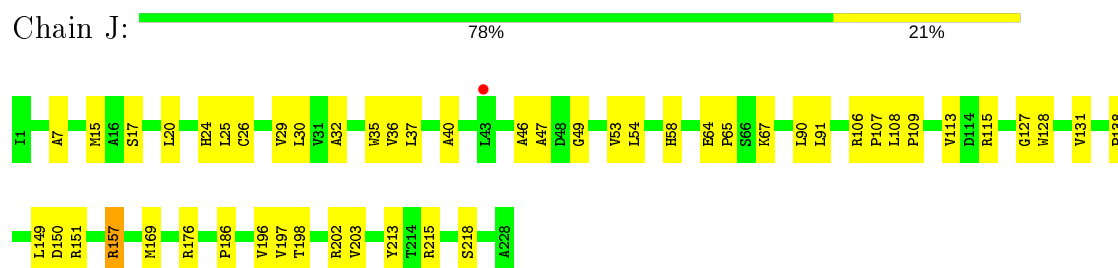
- Molecule 3: COMPLEMENT FACTOR B



- Molecule 4: COMPLEMENT FACTOR D



- Molecule 4: COMPLEMENT FACTOR D



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

Chain E:  50% 50%

UAG1
UAG2

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

Chain G:  50% 50%

UAG1
UAG2

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

Chain K:  100%

UAG1
UAG2

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  33% 67%

UAG1
UAG2
BMA3

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%

UAG1
UAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	108.28Å 135.78Å 149.97Å 95.47° 110.69° 113.39°	Depositor
Resolution (Å)	65.95 – 3.49 67.46 – 3.49	Depositor EDS
% Data completeness (in resolution range)	98.6 (65.95-3.49) 91.0 (67.46-3.49)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 3.49Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.5_2)	Depositor
R, R_{free}	0.189 , 0.244 0.186 , 0.240	Depositor DCC
R_{free} test set	4098 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	83.1	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 90.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.045 for h,-h-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	39285	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.21% 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: GOL, MG, BMA, NAG

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	0.20	0/5092	0.37	0/6917
1	C	0.21	0/5092	0.39	0/6917
2	B	0.20	0/7340	0.36	0/9936
2	D	0.20	0/7340	0.36	0/9936
3	F	0.21	0/5754	0.37	0/7786
3	H	0.22	0/5733	0.37	0/7758
4	I	0.19	0/1745	0.36	0/2376
4	J	0.18	0/1745	0.36	0/2376
All	All	0.21	0/39841	0.37	0/54002

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	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	964	PRO	Peptide

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	4992	0	5055	137	0
1	C	4992	0	5056	144	0
2	B	7197	0	7124	199	0
2	D	7197	0	7124	189	0
3	F	5627	0	5476	124	0
3	H	5608	0	5456	119	0
4	I	1710	0	1698	30	0
4	J	1710	0	1698	32	0
5	E	28	0	25	2	0
5	G	28	0	25	1	0
5	K	28	0	25	10	0
6	L	39	0	34	1	0
6	M	39	0	34	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
7	F	1	0	0	0	0
7	H	1	0	0	0	0
8	D	14	0	13	0	0
8	F	28	0	26	1	0
8	H	28	0	26	0	0
9	I	6	0	8	3	0
9	J	6	0	8	4	0
10	F	2	0	0	0	0
10	H	2	0	0	1	0
All	All	39285	0	38911	932	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 12.

The worst 5 of 932 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)
1:C:63:ASN:HD21	5:K:1:NAG:C1	1.35	1.30
1:A:69:PRO:HA	1:A:70:ALA:HB3	1.36	1.06
1:C:69:PRO:HA	1:C:70:ALA:HB3	1.37	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:733:ILE:HD11	2:B:841:ARG:HH21	1.32	0.94
1:A:628:SER:HB2	1:A:630:GLN:HE22	1.32	0.93

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	636/642 (99%)	569 (90%)	59 (9%)	8 (1%)	12	48
1	C	636/642 (99%)	565 (89%)	61 (10%)	10 (2%)	9	43
2	B	895/912 (98%)	802 (90%)	83 (9%)	10 (1%)	14	52
2	D	895/912 (98%)	795 (89%)	92 (10%)	8 (1%)	17	56
3	F	708/732 (97%)	642 (91%)	55 (8%)	11 (2%)	9	43
3	H	705/732 (96%)	637 (90%)	54 (8%)	14 (2%)	7	39
4	I	226/228 (99%)	201 (89%)	23 (10%)	2 (1%)	17	56
4	J	226/228 (99%)	199 (88%)	25 (11%)	2 (1%)	17	56
All	All	4927/5028 (98%)	4410 (90%)	452 (9%)	65 (1%)	12	48

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	VAL
1	A	518	ALA
2	B	733	ILE
2	B	965	VAL
2	B	1498	ILE

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	564/566 (100%)	557 (99%)	7 (1%)	71	87
1	C	564/566 (100%)	558 (99%)	6 (1%)	73	88
2	B	797/807 (99%)	788 (99%)	9 (1%)	73	88
2	D	797/807 (99%)	789 (99%)	8 (1%)	76	88
3	F	620/635 (98%)	612 (99%)	8 (1%)	69	86
3	H	618/635 (97%)	611 (99%)	7 (1%)	73	88
4	I	181/181 (100%)	179 (99%)	2 (1%)	73	88
4	J	181/181 (100%)	180 (99%)	1 (1%)	86	94
All	All	4322/4378 (99%)	4274 (99%)	48 (1%)	73	88

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	634	GLN
2	D	1334	LEU
3	H	654	ARG
2	D	898	PHE
2	D	1270	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	132	HIS
1	C	587	ASN
3	H	357	HIS
1	C	311	HIS
1	C	370	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 ⓘ

12 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	E	1	1,5	14,14,15	0.51	0	17,19,21	1.36	2 (11%)
5	NAG	E	2	5	14,14,15	0.58	0	17,19,21	1.29	2 (11%)
5	NAG	G	1	2,5	14,14,15	0.55	0	17,19,21	0.60	0
5	NAG	G	2	5	14,14,15	0.54	0	17,19,21	0.72	0
5	NAG	K	1	1,5	14,14,15	0.57	0	17,19,21	0.67	0
5	NAG	K	2	5	14,14,15	0.57	0	17,19,21	0.67	0
6	NAG	L	1	3,6	14,14,15	0.61	0	17,19,21	1.41	3 (17%)
6	NAG	L	2	6	14,14,15	0.61	0	17,19,21	1.37	2 (11%)
6	BMA	L	3	6	11,11,12	0.27	0	15,15,17	0.63	0
6	NAG	M	1	3,6	14,14,15	0.47	0	17,19,21	1.91	5 (29%)
6	NAG	M	2	6	14,14,15	0.52	0	17,19,21	1.75	5 (29%)
6	BMA	M	3	6	11,11,12	1.68	2 (18%)	15,15,17	3.70	11 (73%)

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	E	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	NAG	G	1	2,5	-	3/6/23/26	0/1/1/1
5	NAG	G	2	5	-	3/6/23/26	0/1/1/1
5	NAG	K	1	1,5	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
6	NAG	L	1	3,6	-	4/6/23/26	0/1/1/1
6	NAG	L	2	6	-	2/6/23/26	0/1/1/1
6	BMA	L	3	6	-	1/2/19/22	0/1/1/1
6	NAG	M	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	M	2	6	-	2/6/23/26	0/1/1/1
6	BMA	M	3	6	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	3	BMA	C2-C3	3.41	1.57	1.52
6	M	3	BMA	C4-C3	3.11	1.60	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	3	BMA	O5-C5-C6	7.33	118.69	107.20
6	M	3	BMA	O2-C2-C1	5.04	119.47	109.15
6	M	3	BMA	O3-C3-C4	4.79	121.42	110.35
6	M	3	BMA	O4-C4-C5	4.75	121.09	109.30
6	M	3	BMA	O2-C2-C3	4.57	119.29	110.14

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

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

There are no ring outliers.

6 monomers are involved in 14 short contacts:

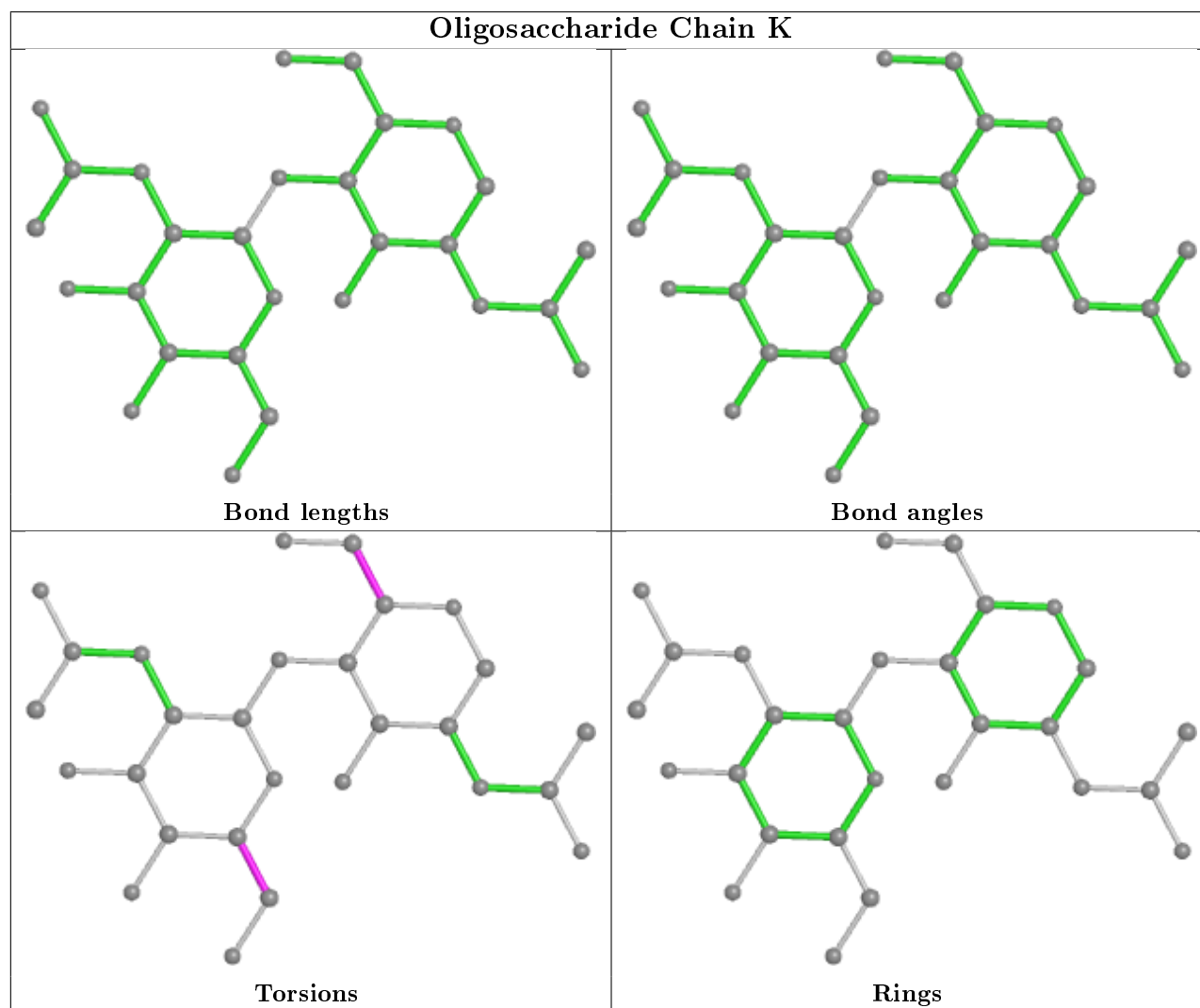
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	2	NAG	2	0
5	K	1	NAG	10	0
5	G	2	NAG	1	0

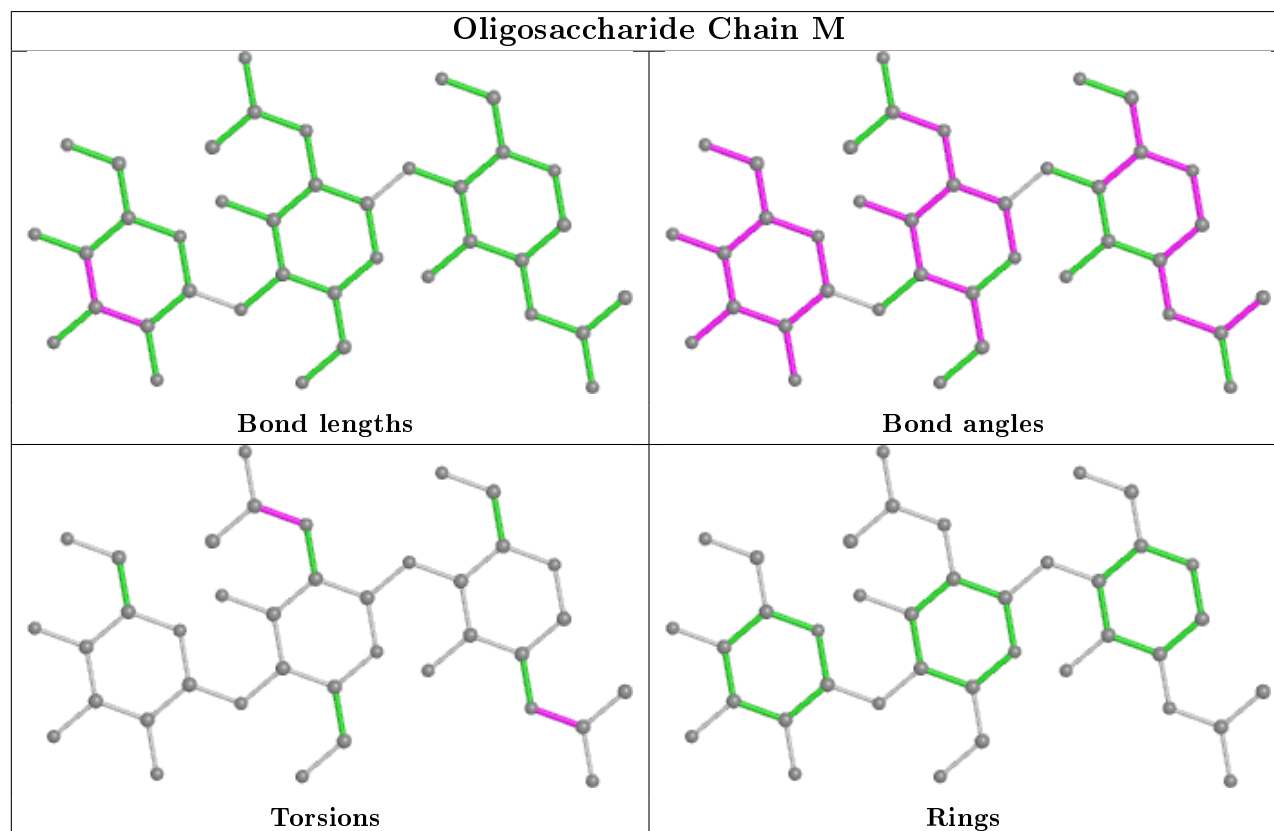
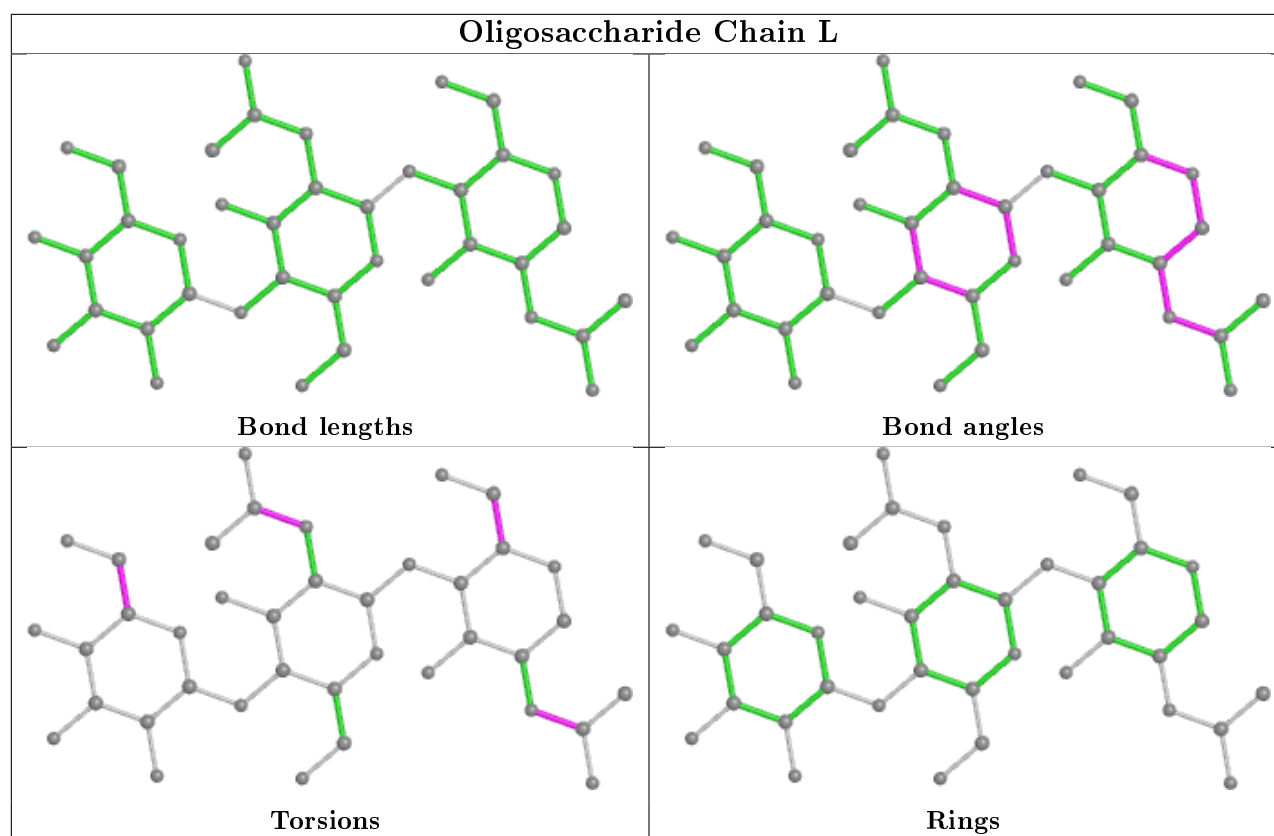
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1	NAG	2	0
6	L	1	NAG	1	0
6	L	2	NAG	1	0

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

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GOL	I	1229	-	5,5,5	0.37	0	5,5,5	0.17	0
8	NAG	D	2642	2	14,14,15	0.56	0	17,19,21	0.66	0
8	NAG	F	1743	3	14,14,15	0.54	0	17,19,21	0.61	0
9	GOL	J	1229	-	5,5,5	0.37	0	5,5,5	0.31	0
8	NAG	F	1747	3	14,14,15	0.58	0	17,19,21	0.67	0
8	NAG	H	1747	3	14,14,15	0.50	0	17,19,21	0.80	0
8	NAG	H	1743	3	14,14,15	0.53	0	17,19,21	0.62	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
9	GOL	I	1229	-	-	2/4/4/4	-
8	NAG	D	2642	2	-	3/6/23/26	0/1/1/1
8	NAG	F	1743	3	-	2/6/23/26	0/1/1/1
9	GOL	J	1229	-	-	2/4/4/4	-
8	NAG	F	1747	3	1/1/5/7	1/6/23/26	0/1/1/1
8	NAG	H	1747	3	-	1/6/23/26	0/1/1/1
8	NAG	H	1743	3	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	F	1747	NAG	C1

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	I	1229	GOL	C1-C2-C3-O3
8	D	2642	NAG	C3-C2-N2-C7
8	D	2642	NAG	C8-C7-N2-C2
8	D	2642	NAG	O7-C7-N2-C2
8	F	1743	NAG	C8-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	I	1229	GOL	3	0
8	F	1743	NAG	1	0
9	J	1229	GOL	4	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, 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	640/642 (99%)	0.40	48 (7%) 14 14	58, 134, 189, 278	0
1	C	640/642 (99%)	0.70	84 (13%) 3 4	67, 134, 189, 281	0
2	B	901/912 (98%)	0.15	17 (1%) 66 61	60, 122, 203, 330	0
2	D	901/912 (98%)	0.34	86 (9%) 8 8	60, 125, 205, 328	0
3	F	714/732 (97%)	0.01	7 (0%) 82 77	37, 82, 154, 272	0
3	H	711/732 (97%)	0.14	25 (3%) 44 39	37, 84, 153, 222	0
4	I	228/228 (100%)	-0.21	0 100 100	46, 79, 125, 218	0
4	J	228/228 (100%)	-0.18	1 (0%) 92 90	42, 79, 125, 220	0
All	All	4963/5028 (98%)	0.23	268 (5%) 25 23	37, 109, 189, 330	0

The worst 5 of 268 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1151	GLY	8.5
2	D	1073	ILE	8.4
3	F	482	GLY	7.6
2	D	1154	LEU	6.9
1	C	636	ALA	6.5

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,

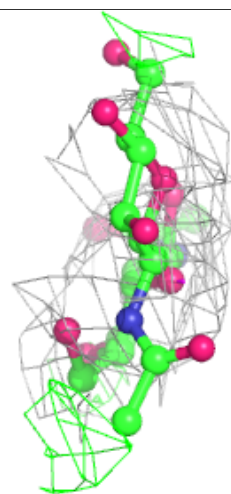
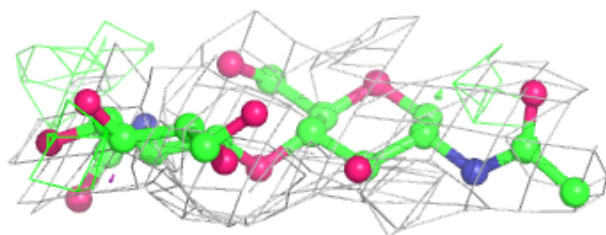
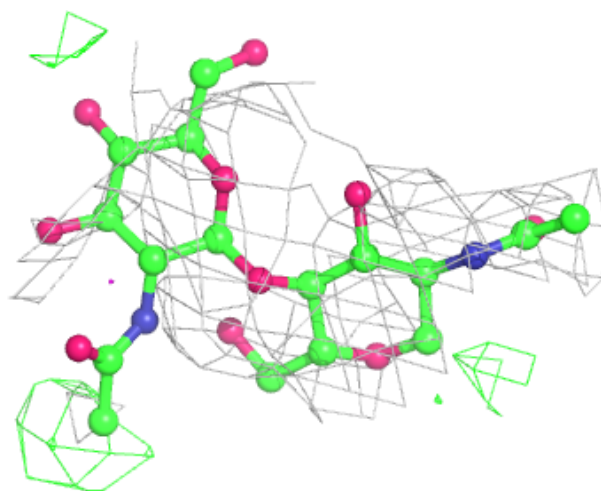
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	K	2	14/15	0.35	0.35	155,202,219,222	0
6	BMA	M	3	11/12	0.59	0.29	132,155,186,196	0
6	NAG	M	2	14/15	0.63	0.32	160,172,206,213	0
6	BMA	L	3	11/12	0.69	0.31	128,162,204,271	0
5	NAG	K	1	14/15	0.75	0.24	123,187,212,212	0
5	NAG	E	2	14/15	0.78	0.17	160,201,217,223	0
6	NAG	L	2	14/15	0.82	0.22	118,138,166,168	0
5	NAG	G	2	14/15	0.86	0.24	114,185,200,200	0
6	NAG	L	1	14/15	0.86	0.21	91,116,131,137	0
5	NAG	E	1	14/15	0.87	0.25	129,188,212,214	0
5	NAG	G	1	14/15	0.89	0.19	102,141,165,192	0
6	NAG	M	1	14/15	0.90	0.23	96,122,150,154	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.

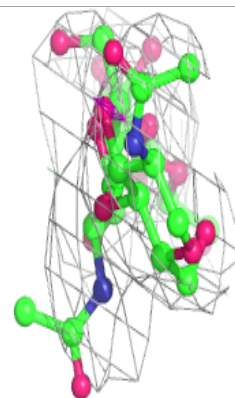
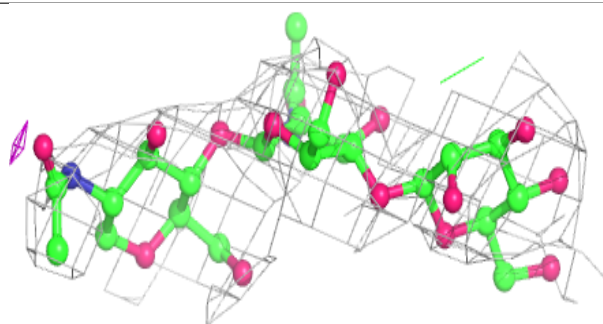
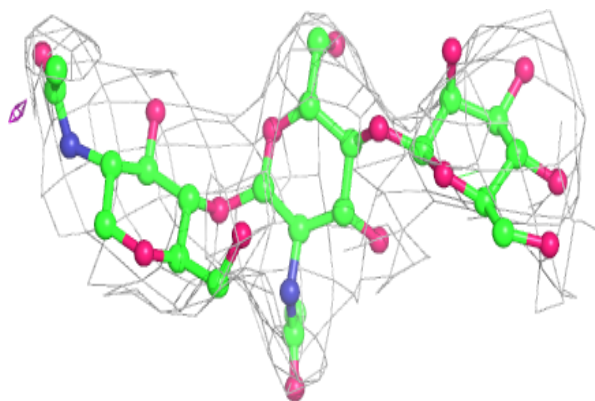
Electron density around Chain K:

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

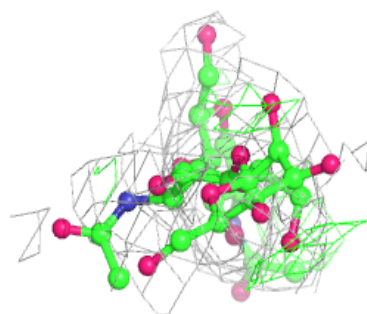
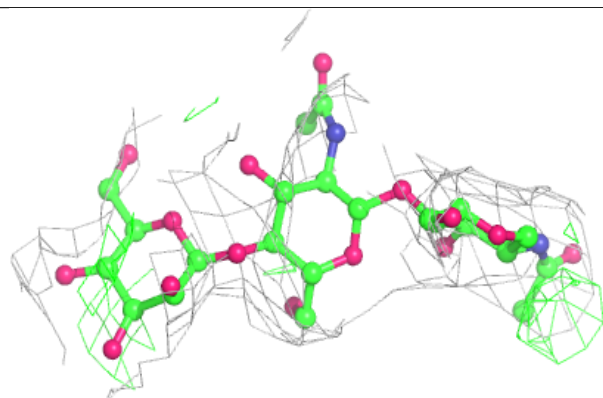
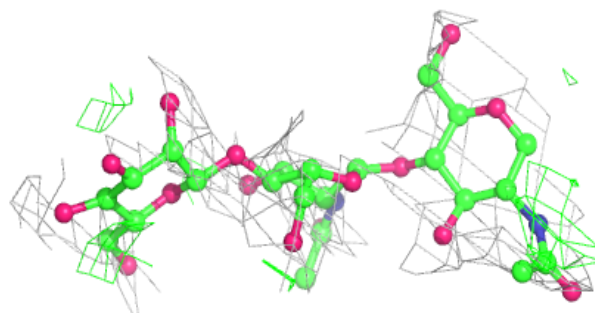


Electron density around Chain L:

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

**Electron density around Chain M:**

$2mF_o-DF_c$ (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
8	NAG	F	1743	14/15	0.73	0.37	97,143,202,215	0
8	NAG	D	2642	14/15	0.81	0.22	104,146,166,179	0
8	NAG	H	1747	14/15	0.81	0.28	118,163,182,198	0
8	NAG	F	1747	14/15	0.85	0.26	135,154,184,195	0
7	MG	H	1742	1/1	0.85	0.30	140,140,140,140	0
8	NAG	H	1743	14/15	0.85	0.27	117,167,189,193	0
7	MG	C	1645	1/1	0.89	0.04	127,127,127,127	0
7	MG	A	1645	1/1	0.92	0.12	108,108,108,108	0
9	GOL	J	1229	6/6	0.95	0.25	58,74,87,95	0
9	GOL	I	1229	6/6	0.96	0.37	73,107,124,127	0
7	MG	F	1742	1/1	0.99	0.20	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.