wwPDB X-ray Structure Validation Summary Report (i)

Sep 25, 2023 – 07:16 AM EDT

PDB ID	:	5W1K
Title	:	JUNV GP1 CR1-10 Fab CR1-28 Fab complex
Authors	:	Raymond, D.D.; Clark, L.E.; Abraham, J.
Deposited on	:	2017-06-03
Resolution	:	3.99 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 (i) 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 (1)) were used in the production of this report:

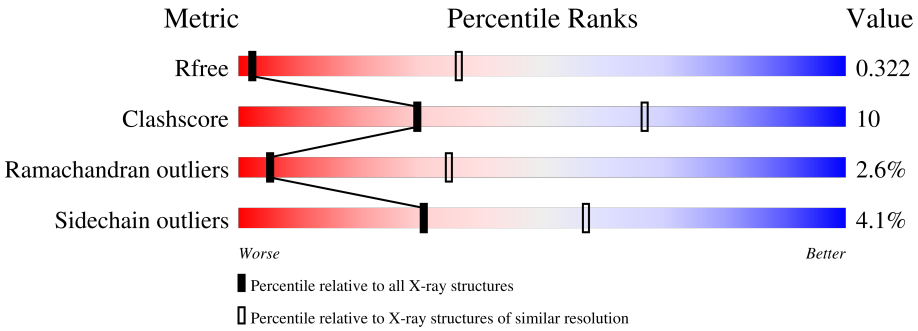
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.99 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	206	81% 18% .
1	F	206	80% 17% .
1	K	206	75% 23% .
1	S	206	77% 21% ..
2	B	226	73% 25% .
2	G	226	71% 25% .
2	L	226	72% 26% .

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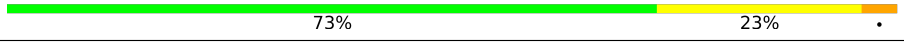
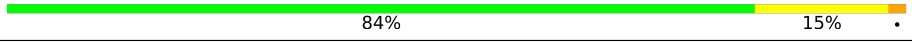
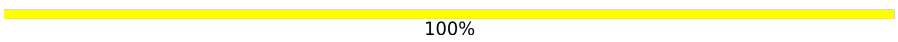
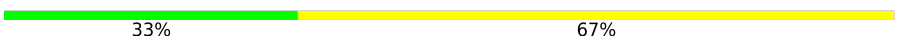
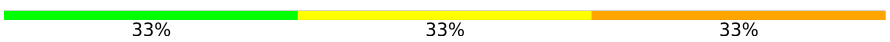
Mol	Chain	Length	Quality of chain
2	T	226	
3	C	213	
3	H	213	
3	M	213	
3	N	213	
4	D	225	
4	I	225	
4	O	225	
4	Q	225	
5	E	142	
5	J	142	
5	P	142	
5	R	142	
6	U	3	
6	W	3	
6	X	3	
7	V	2	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 31130 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 CR1-28 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1590	994	272	319	5			
1	F	206	Total	C	N	O	S	0	0	0
			1590	994	272	319	5			
1	K	206	Total	C	N	O	S	0	0	0
			1590	994	272	319	5			
1	S	206	Total	C	N	O	S	0	0	0
			1590	994	272	319	5			

- Molecule 2 is a protein called CR1-28 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	226	Total	C	N	O	S	0	0	0
			1703	1074	286	337	6			
2	G	226	Total	C	N	O	S	0	0	0
			1703	1074	286	337	6			
2	L	226	Total	C	N	O	S	0	0	0
			1703	1074	286	337	6			
2	T	226	Total	C	N	O	S	0	0	0
			1703	1074	286	337	6			

- Molecule 3 is a protein called CR1-10 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	213	Total	C	N	O	S	0	0	0
			1629	1019	276	330	4			
3	H	213	Total	C	N	O	S	0	0	0
			1629	1019	276	330	4			
3	M	213	Total	C	N	O	S	0	0	0
			1629	1019	276	330	4			
3	N	211	Total	C	N	O	S	0	0	0
			1616	1012	274	326	4			

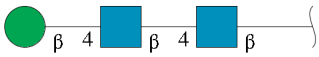
- Molecule 4 is a protein called CR1-10 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	225	Total	C	N	O	S	0	0	0
			1673	1053	283	330	7			
4	I	225	Total	C	N	O	S	0	0	0
			1673	1053	283	330	7			
4	O	225	Total	C	N	O	S	0	0	0
			1673	1053	283	330	7			
4	Q	225	Total	C	N	O	S	0	0	0
			1673	1053	283	330	7			

- Molecule 5 is a protein called Pre-glycoprotein polyprotein GP complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	142	Total	C	N	O	S	0	0	0
			1153	745	190	208	10			
5	J	141	Total	C	N	O	S	0	0	0
			1145	741	189	205	10			
5	P	142	Total	C	N	O	S	0	0	0
			1153	745	190	208	10			
5	R	142	Total	C	N	O	S	0	0	0
			1153	745	190	208	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.

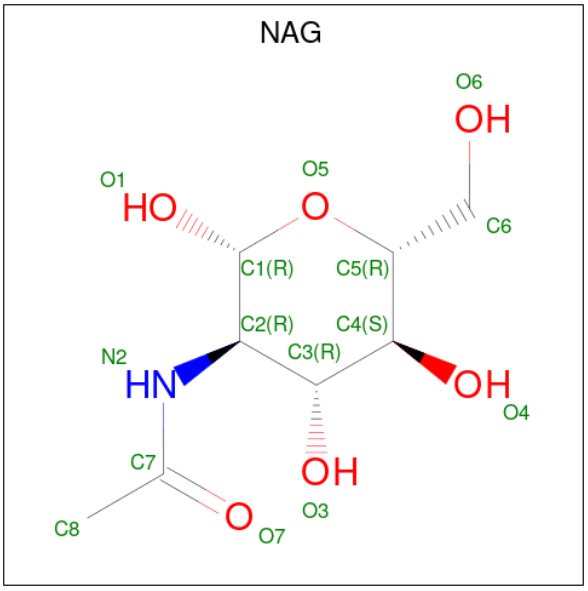


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	U	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	W	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	X	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	V	2	Total C N O 28 16 2 10	0	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



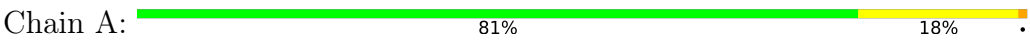
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	P	1	Total C N O 14 8 1 5	0	0

3 Residue-property plots (i)

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. 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. 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.

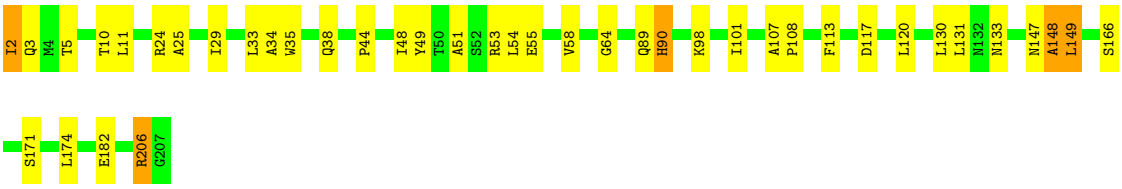
- Molecule 1: CR1-28 Fab light chain

Chain A:



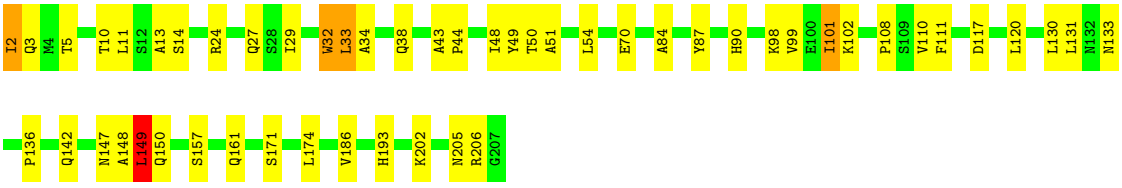
- Molecule 1: CR1-28 Fab light chain

Chain F:



- Molecule 1: CR1-28 Fab light chain

Chain K:

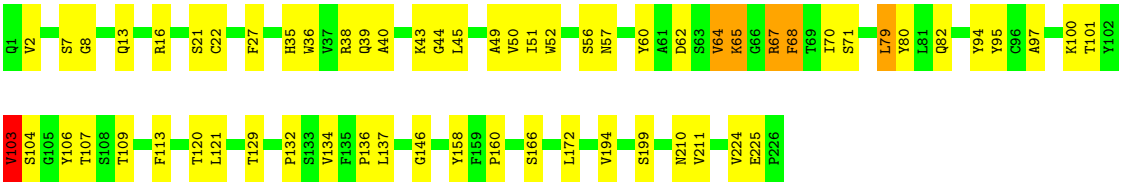


- Molecule 1: CR1-28 Fab light chain

Chain S:

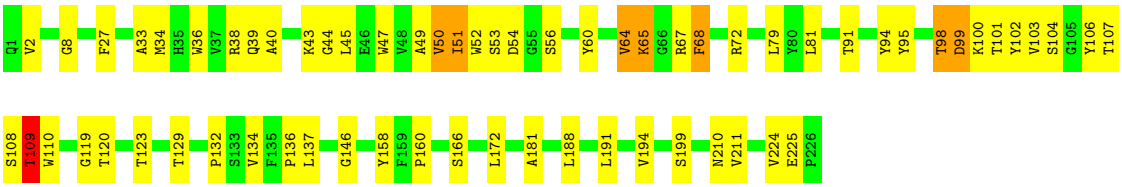
• Molecule 2: CR1-28 Fab heavy chain

Chain B:



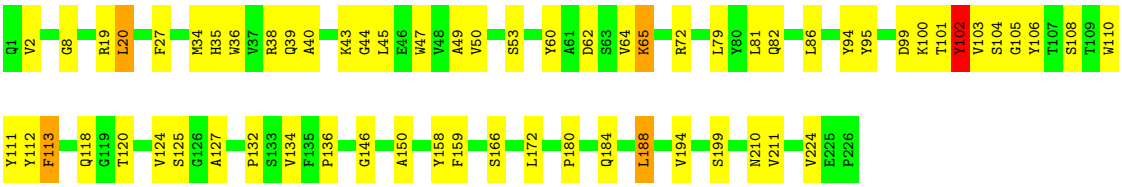
• Molecule 2: CR1-28 Fab heavy chain

Chain G:



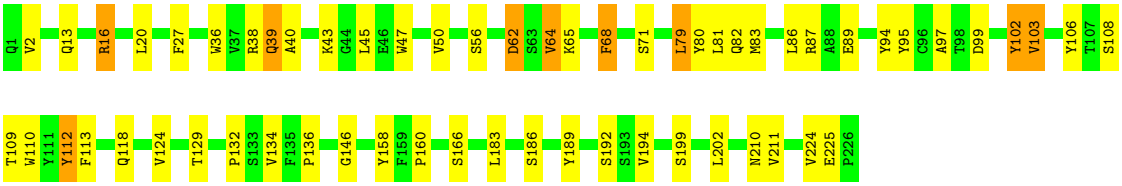
• Molecule 2: CR1-28 Fab heavy chain

Chain L:



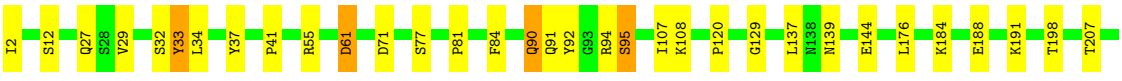
• Molecule 2: CR1-28 Fab heavy chain

Chain T:



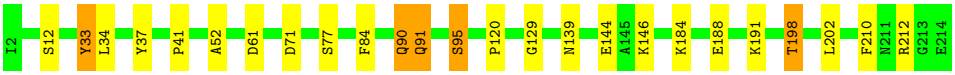
• Molecule 3: CR1-10 Fab light chain

Chain C:



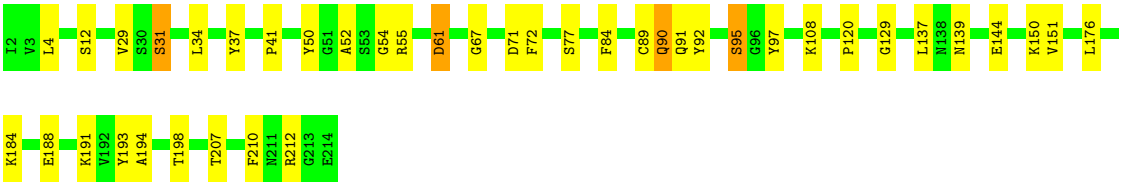
• Molecule 3: CR1-10 Fab light chain

Chain H:



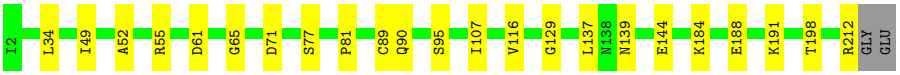
• Molecule 3: CR1-10 Fab light chain

Chain M:



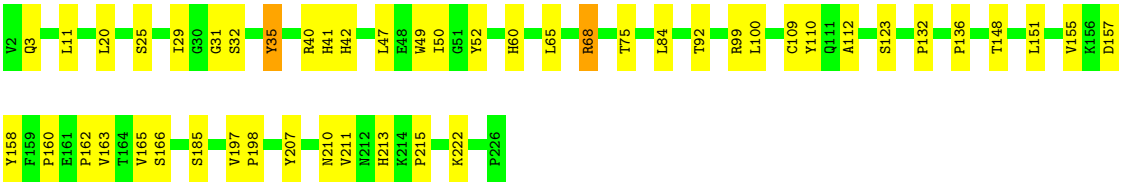
• Molecule 3: CR1-10 Fab light chain

Chain N:



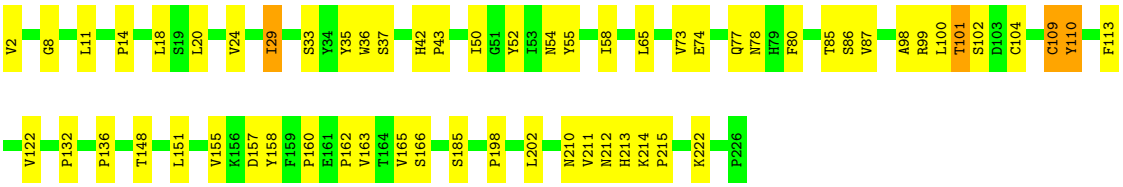
• Molecule 4: CR1-10 Fab heavy chain

Chain D:



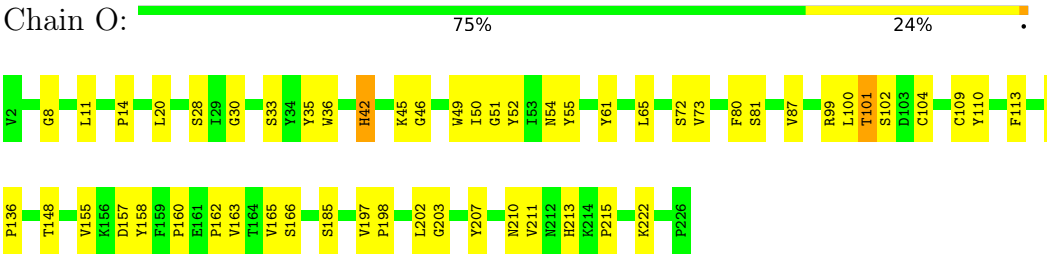
• Molecule 4: CR1-10 Fab heavy chain

Chain I:



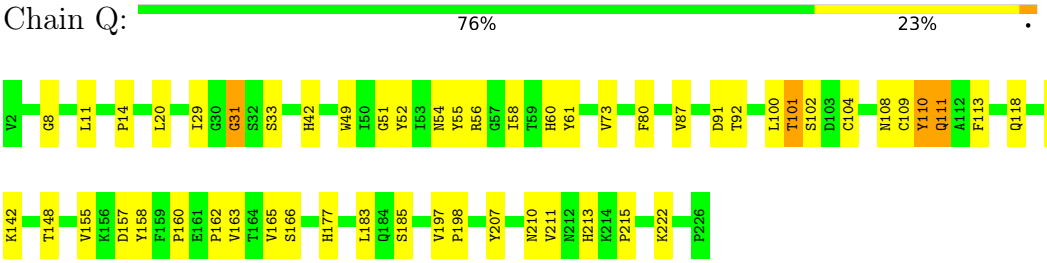
• Molecule 4: CR1-10 Fab heavy chain

Chain O:



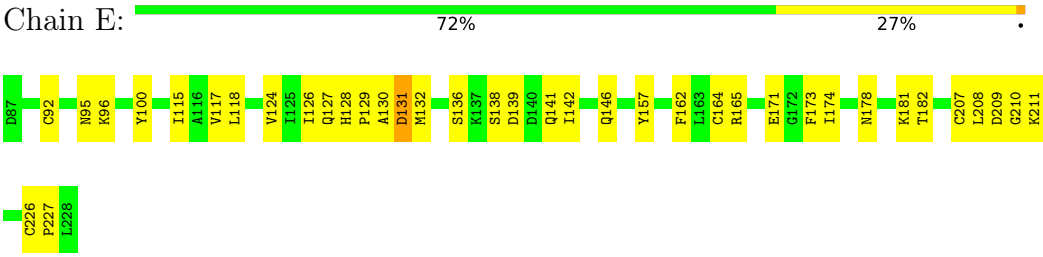
• Molecule 4: CR1-10 Fab heavy chain

Chain Q:



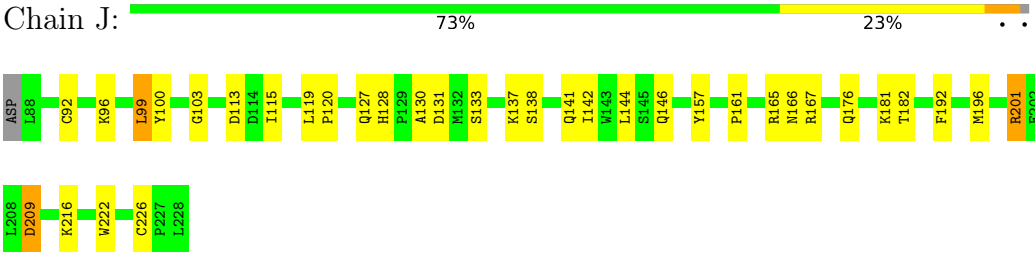
• Molecule 5: Pre-glycoprotein polyprotein GP complex

Chain E:



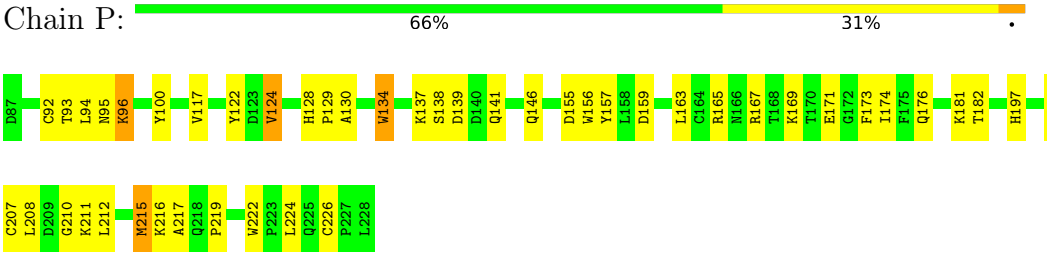
• Molecule 5: Pre-glycoprotein polyprotein GP complex

Chain J:



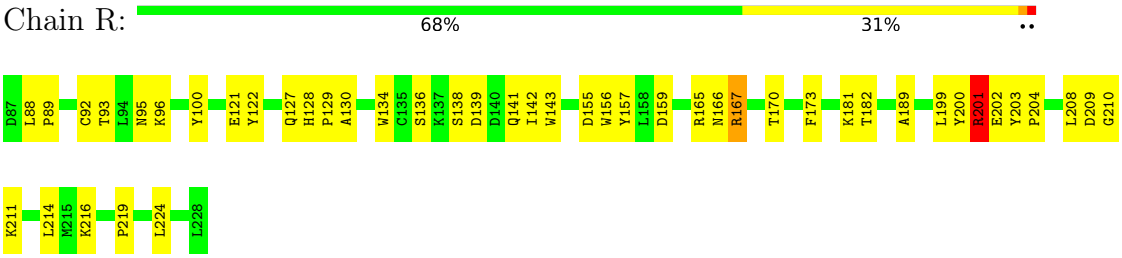
• Molecule 5: Pre-glycoprotein polyprotein GP complex

Chain P:



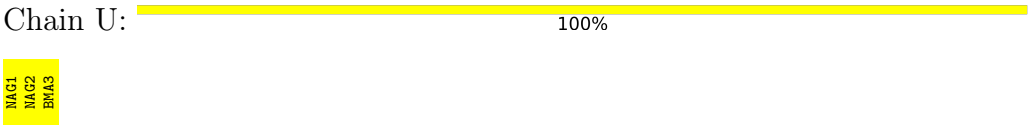
• Molecule 5: Pre-glycoprotein polyprotein GP complex

Chain R:



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

Chain U:

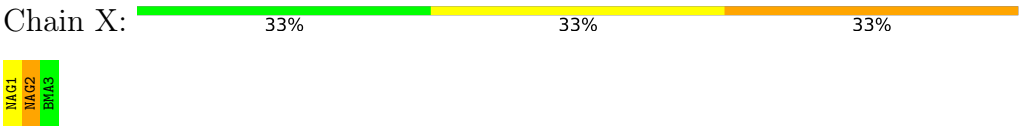


• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:

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

Chain X:



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

Chain V:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	154.84Å 132.23Å 167.42Å 90.00° 92.47° 90.00°	Depositor
Resolution (Å)	49.35 – 3.99 49.35 – 3.99	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.35-3.99) 87.6 (49.35-3.99)	Depositor EDS
R_{merge}	0.72	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 4.00Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.237 , 0.288 0.300 , 0.322	Depositor DCC
R_{free} test set	2860 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	65.5	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 53.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	0.086 for h,-k,-l	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	31130	wwPDB-VP
Average B, all atoms (Å^2)	69.0	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 37.32 % 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 4.3700e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, BMA

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	0.44	0/1624	0.70	0/2204
1	F	0.42	0/1624	0.72	0/2204
1	K	0.44	0/1624	0.70	0/2204
1	S	0.44	0/1624	0.71	0/2204
2	B	0.44	0/1747	0.73	1/2383 (0.0%)
2	G	0.45	0/1747	0.77	1/2383 (0.0%)
2	L	0.43	0/1747	0.73	0/2383
2	T	0.43	0/1747	0.71	0/2383
3	C	0.41	0/1664	0.65	0/2258
3	H	0.41	0/1664	0.67	0/2258
3	M	0.40	0/1664	0.65	0/2258
3	N	0.42	0/1651	0.65	0/2241
4	D	0.41	0/1717	0.71	0/2344
4	I	0.41	0/1717	0.68	0/2344
4	O	0.40	0/1717	0.70	0/2344
4	Q	0.40	0/1717	0.70	0/2344
5	E	0.45	0/1189	0.69	0/1615
5	J	0.48	0/1181	0.71	0/1604
5	P	0.43	0/1189	0.66	0/1615
5	R	0.45	0/1189	0.71	0/1615
All	All	0.43	0/31743	0.70	2/43188 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	98	THR	C-N-CA	5.88	136.41	121.70
2	B	103	VAL	C-N-CA	5.22	134.75	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1590	0	1552	31	0
1	F	1590	0	1552	29	0
1	K	1590	0	1552	37	0
1	S	1590	0	1552	26	0
2	B	1703	0	1646	48	0
2	G	1703	0	1646	58	0
2	L	1703	0	1646	61	0
2	T	1703	0	1646	31	0
3	C	1629	0	1580	24	0
3	H	1629	0	1580	15	0
3	M	1629	0	1580	22	0
3	N	1616	0	1571	11	0
4	D	1673	0	1616	32	0
4	I	1673	0	1616	32	0
4	O	1673	0	1616	31	0
4	Q	1673	0	1616	31	0
5	E	1153	0	1113	32	0
5	J	1145	0	1109	37	0
5	P	1153	0	1112	30	0
5	R	1153	0	1113	45	0
6	U	39	0	34	0	0
6	W	39	0	34	0	0
6	X	39	0	34	2	0
7	V	28	0	25	1	0
8	P	14	0	13	0	0
All	All	31130	0	30154	584	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 10.

The worst 5 of 584 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:A:53:ARG:HH22	2:B:103:VAL:HB	1.17	1.05
4:Q:110:TYR:CE2	5:R:134:TRP:HB3	1.98	0.99
2:G:33:ALA:CB	2:G:100:LYS:NZ	2.26	0.99
1:F:149:LEU:HD21	1:F:174:LEU:HD11	1.42	0.98
4:O:109:CYS:HB2	5:P:134:TRP:CE3	2.01	0.95

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	204/206 (99%)	175 (86%)	23 (11%)	6 (3%)	4	32
1	F	204/206 (99%)	172 (84%)	24 (12%)	8 (4%)	3	26
1	K	204/206 (99%)	176 (86%)	22 (11%)	6 (3%)	4	32
1	S	204/206 (99%)	172 (84%)	24 (12%)	8 (4%)	3	26
2	B	224/226 (99%)	183 (82%)	35 (16%)	6 (3%)	5	34
2	G	224/226 (99%)	186 (83%)	28 (12%)	10 (4%)	2	24
2	L	224/226 (99%)	187 (84%)	29 (13%)	8 (4%)	3	28
2	T	224/226 (99%)	189 (84%)	28 (12%)	7 (3%)	4	31
3	C	211/213 (99%)	192 (91%)	14 (7%)	5 (2%)	6	36
3	H	211/213 (99%)	193 (92%)	13 (6%)	5 (2%)	6	36
3	M	211/213 (99%)	195 (92%)	12 (6%)	4 (2%)	8	40
3	N	209/213 (98%)	191 (91%)	15 (7%)	3 (1%)	11	46
4	D	223/225 (99%)	196 (88%)	24 (11%)	3 (1%)	12	48
4	I	223/225 (99%)	199 (89%)	18 (8%)	6 (3%)	5	34
4	O	223/225 (99%)	201 (90%)	18 (8%)	4 (2%)	8	41
4	Q	223/225 (99%)	198 (89%)	20 (9%)	5 (2%)	6	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	140/142 (99%)	125 (89%)	13 (9%)	2 (1%)	11	46
5	J	139/142 (98%)	114 (82%)	23 (16%)	2 (1%)	11	46
5	P	140/142 (99%)	125 (89%)	13 (9%)	2 (1%)	11	46
5	R	140/142 (99%)	118 (84%)	17 (12%)	5 (4%)	3	28
All	All	4005/4048 (99%)	3487 (87%)	413 (10%)	105 (3%)	5	34

5 of 105 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	LEU
2	B	103	VAL
2	B	104	SER
2	B	109	THR
3	C	32	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	181/181 (100%)	174 (96%)	7 (4%)	32	58
1	F	181/181 (100%)	177 (98%)	4 (2%)	52	71
1	K	181/181 (100%)	170 (94%)	11 (6%)	18	47
1	S	181/181 (100%)	168 (93%)	13 (7%)	14	42
2	B	190/190 (100%)	184 (97%)	6 (3%)	39	62
2	G	190/190 (100%)	184 (97%)	6 (3%)	39	62
2	L	190/190 (100%)	185 (97%)	5 (3%)	46	67
2	T	190/190 (100%)	176 (93%)	14 (7%)	13	41
3	C	182/182 (100%)	176 (97%)	6 (3%)	38	62
3	H	182/182 (100%)	176 (97%)	6 (3%)	38	62
3	M	182/182 (100%)	176 (97%)	6 (3%)	38	62
3	N	181/182 (100%)	177 (98%)	4 (2%)	52	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	D	189/189 (100%)	180 (95%)	9 (5%)	25 53
4	I	189/189 (100%)	185 (98%)	4 (2%)	53 72
4	O	189/189 (100%)	186 (98%)	3 (2%)	62 79
4	Q	189/189 (100%)	176 (93%)	13 (7%)	15 43
5	E	129/129 (100%)	125 (97%)	4 (3%)	40 63
5	J	128/129 (99%)	123 (96%)	5 (4%)	32 58
5	P	129/129 (100%)	122 (95%)	7 (5%)	22 50
5	R	129/129 (100%)	120 (93%)	9 (7%)	15 43
All	All	3482/3484 (100%)	3340 (96%)	142 (4%)	30 57

5 of 142 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	32	TRP
1	S	101	ILE
2	T	62	ASP
4	I	55	TYR
3	H	202	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
5	J	154	HIS
4	Q	118	GLN
1	K	38	GLN
5	R	146	GLN
4	Q	54	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

11 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	5,6	14,14,15	0.63	0	17,19,21	1.80	3 (17%)
6	NAG	U	2	6	14,14,15	0.83	0	17,19,21	1.12	2 (11%)
6	BMA	U	3	6	11,11,12	0.46	0	15,15,17	1.03	1 (6%)
7	NAG	V	1	5,7	14,14,15	0.54	0	17,19,21	0.97	1 (5%)
7	NAG	V	2	7	14,14,15	0.60	0	17,19,21	1.12	1 (5%)
6	NAG	W	1	5,6	14,14,15	0.48	0	17,19,21	0.86	1 (5%)
6	NAG	W	2	6	14,14,15	0.43	0	17,19,21	1.00	1 (5%)
6	BMA	W	3	6	11,11,12	0.51	0	15,15,17	0.79	0
6	NAG	X	1	5,6	14,14,15	0.43	0	17,19,21	0.84	1 (5%)
6	NAG	X	2	6	14,14,15	0.48	0	17,19,21	0.77	1 (5%)
6	BMA	X	3	6	11,11,12	0.51	0	15,15,17	0.80	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
6	NAG	U	1	5,6	-	3/6/23/26	0/1/1/1
6	NAG	U	2	6	-	4/6/23/26	0/1/1/1
6	BMA	U	3	6	-	1/2/19/22	0/1/1/1
7	NAG	V	1	5,7	-	4/6/23/26	0/1/1/1
7	NAG	V	2	7	-	3/6/23/26	0/1/1/1
6	NAG	W	1	5,6	-	4/6/23/26	0/1/1/1
6	NAG	W	2	6	-	4/6/23/26	0/1/1/1
6	BMA	W	3	6	-	0/2/19/22	0/1/1/1
6	NAG	X	1	5,6	-	1/6/23/26	0/1/1/1
6	NAG	X	2	6	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	X	3	6	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	U	1	NAG	C1-C2-N2	-5.05	101.87	110.49
6	U	1	NAG	C1-O5-C5	-3.52	107.42	112.19
6	W	2	NAG	O5-C1-C2	3.04	116.09	111.29
6	U	3	BMA	C1-O5-C5	3.00	116.25	112.19
7	V	2	NAG	C1-O5-C5	2.97	116.22	112.19

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	U	1	NAG	C3-C2-N2-C7
6	U	1	NAG	C8-C7-N2-C2
6	U	1	NAG	O7-C7-N2-C2
6	U	2	NAG	C8-C7-N2-C2
6	U	2	NAG	O7-C7-N2-C2

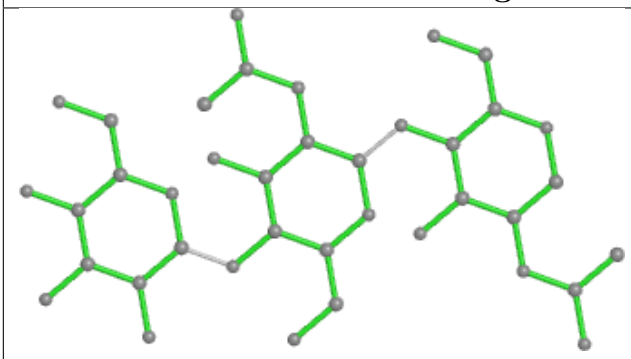
There are no ring outliers.

2 monomers are involved in 3 short contacts:

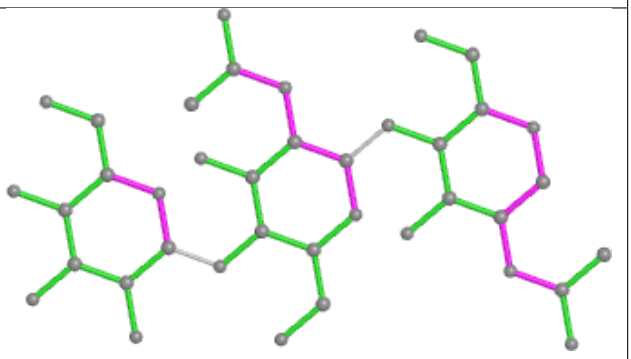
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	X	2	NAG	2	0
7	V	2	NAG	1	0

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

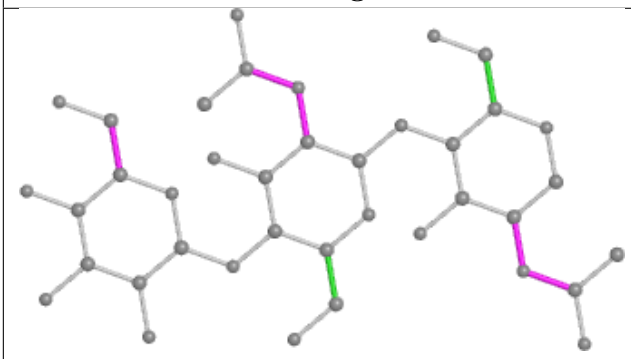
Oligosaccharide Chain U



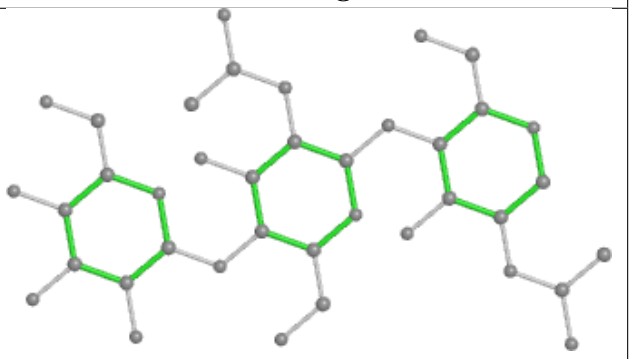
Bond lengths



Bond angles

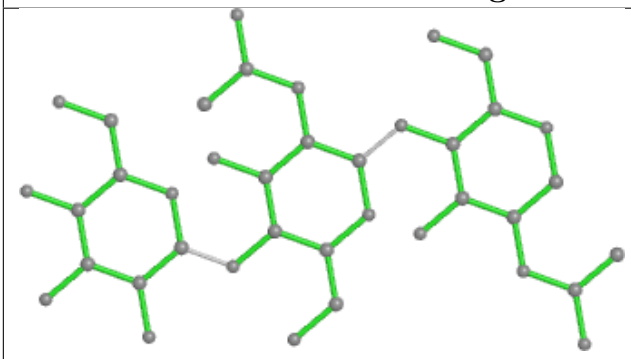


Torsions

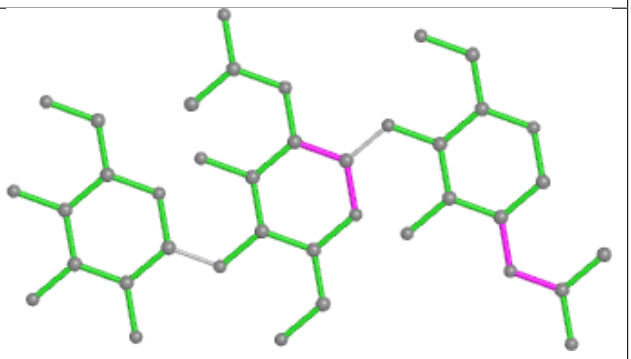


Rings

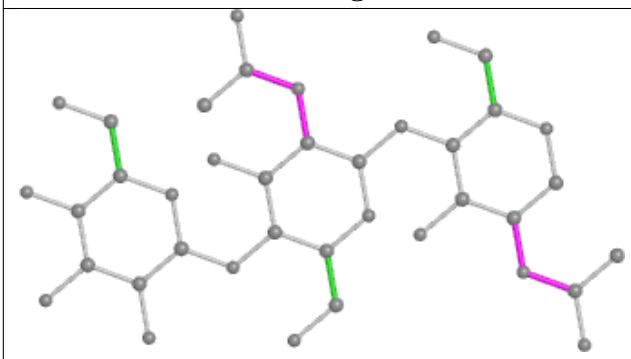
Oligosaccharide Chain W



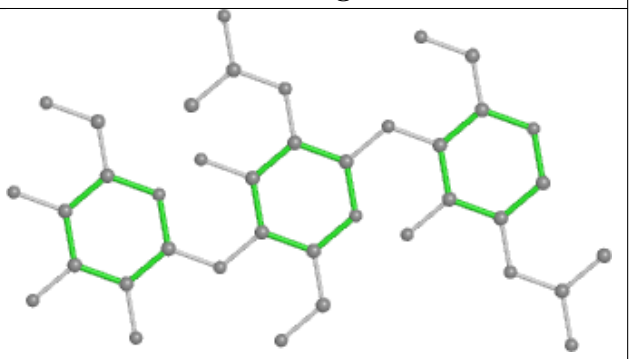
Bond lengths



Bond angles

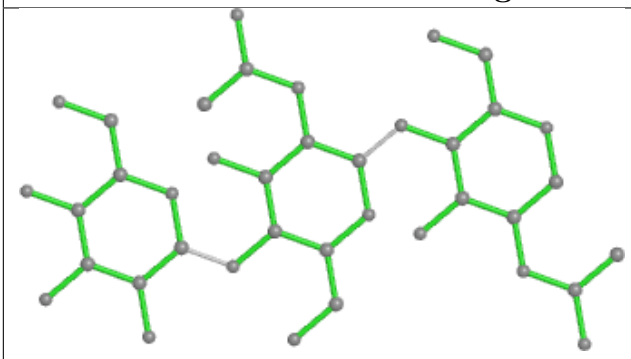


Torsions

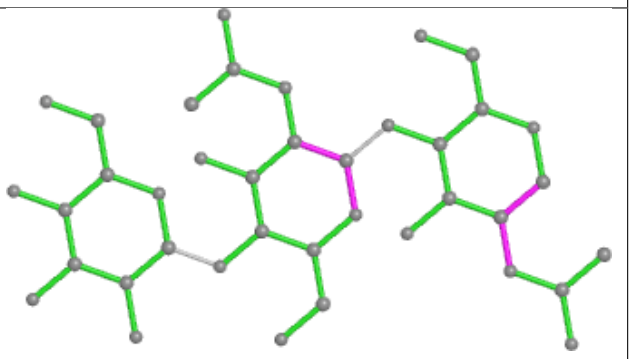


Rings

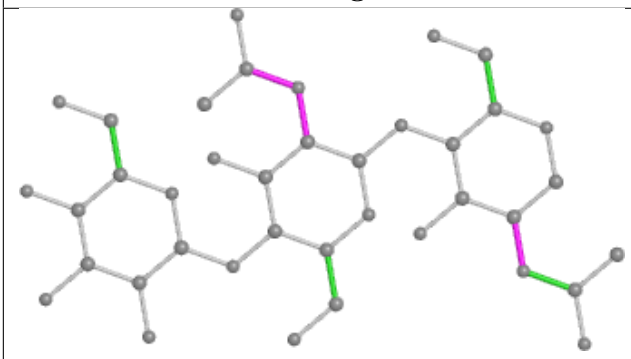
Oligosaccharide Chain X



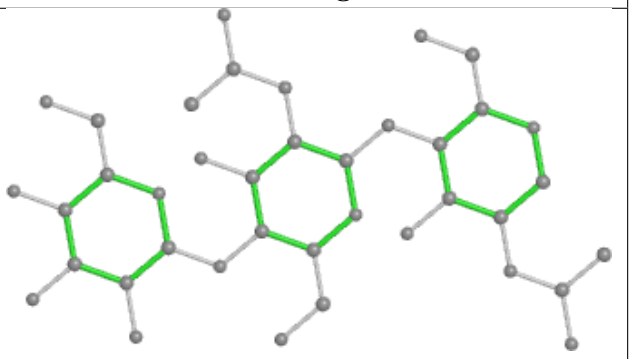
Bond lengths



Bond angles

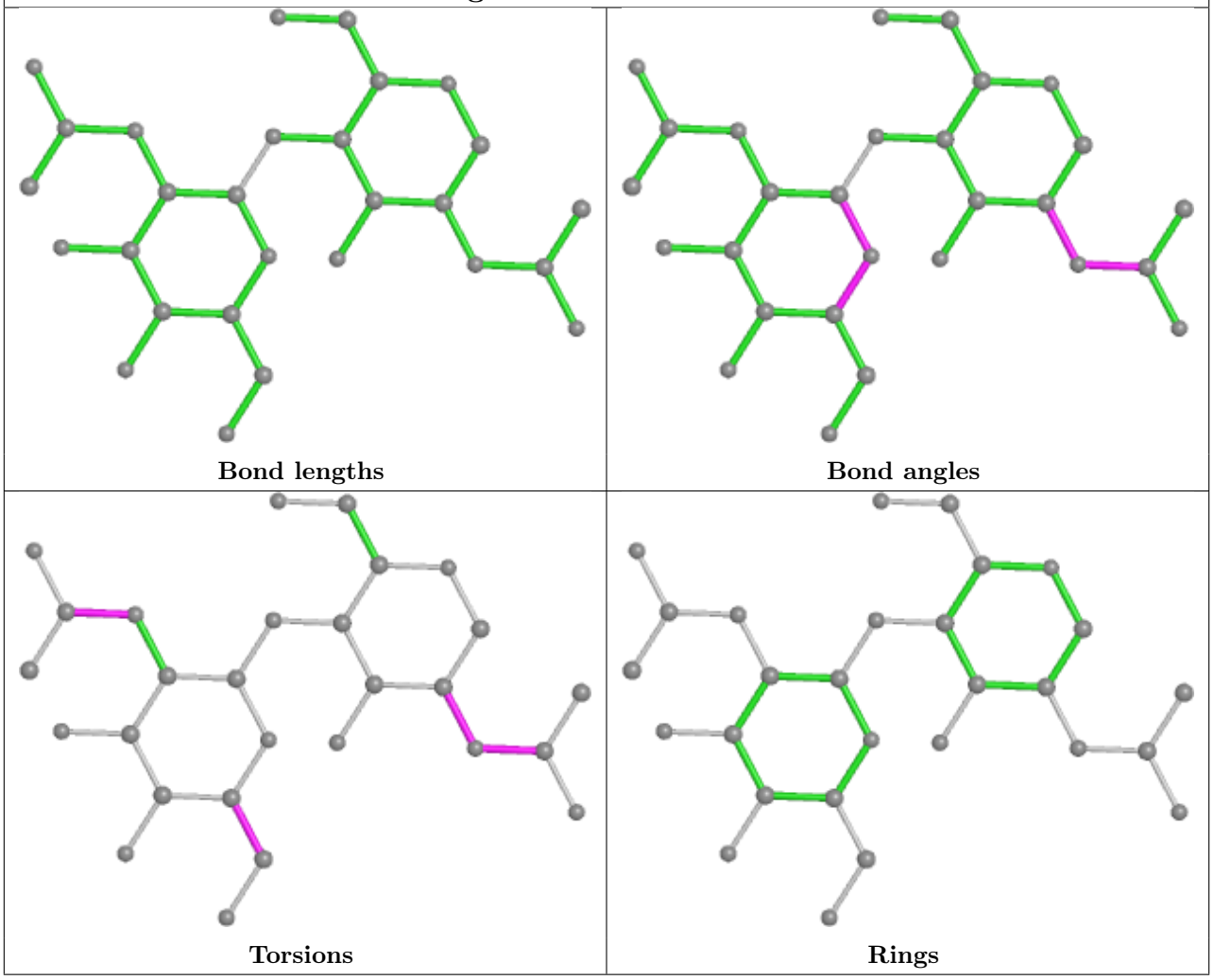


Torsions



Rings

Oligosaccharide Chain V



5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	NAG	P	301	5	14,14,15	0.47	0	17,19,21	1.07	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	P	301	5	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	P	301	NAG	C2-N2-C7	2.89	127.01	122.90
8	P	301	NAG	C1-C2-N2	2.21	114.26	110.49

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	P	301	NAG	C3-C2-N2-C7

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 (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

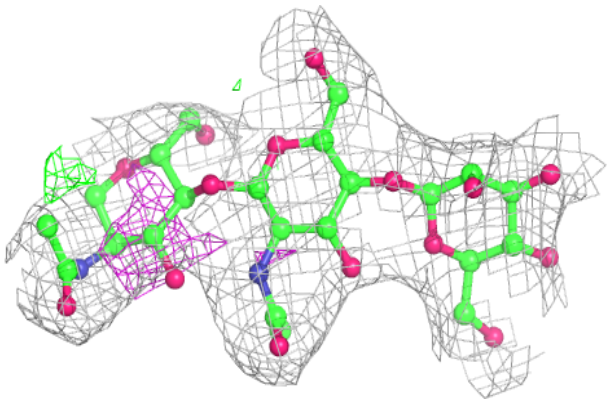
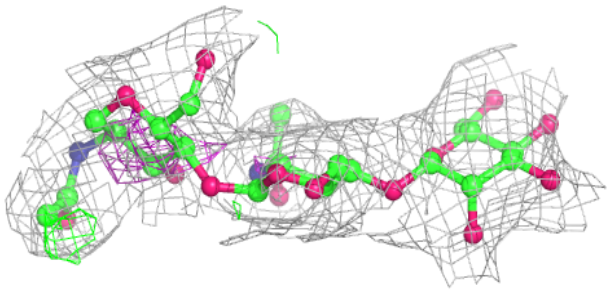
6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

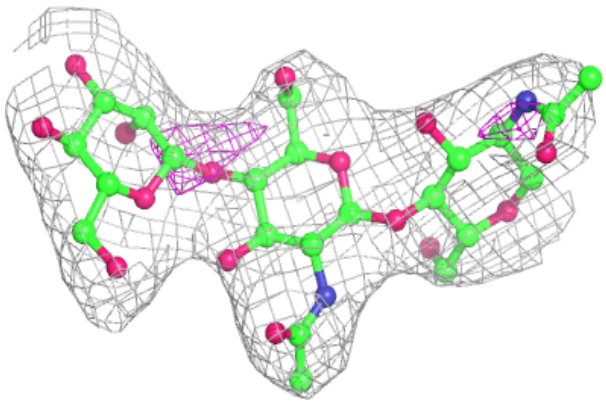
Unable to reproduce the depositors R factor - this section is therefore empty.

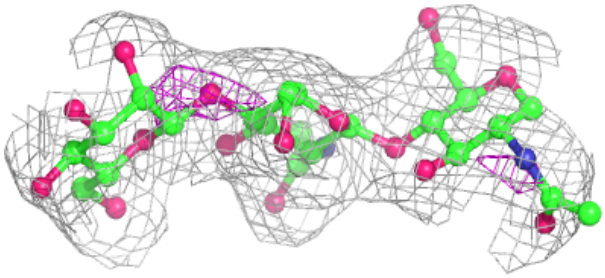
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

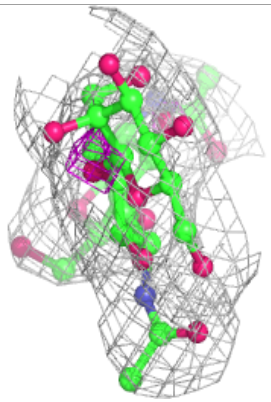
Electron density around Chain U: $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

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)

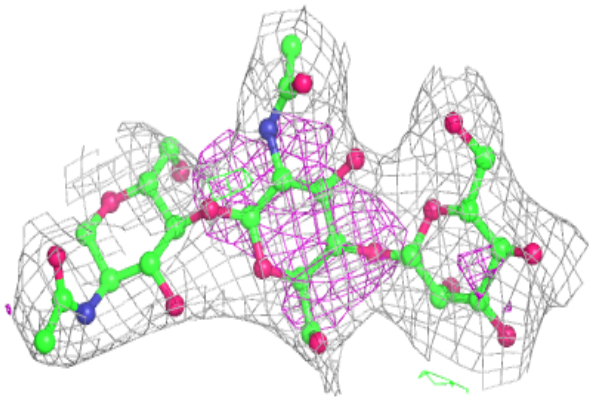


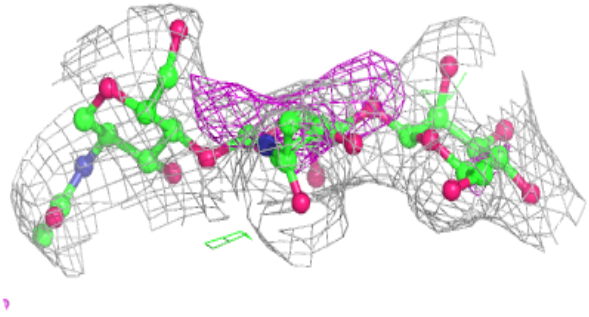


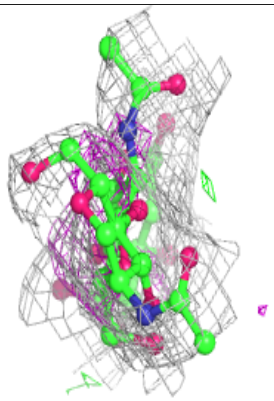


Electron density around Chain X:

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

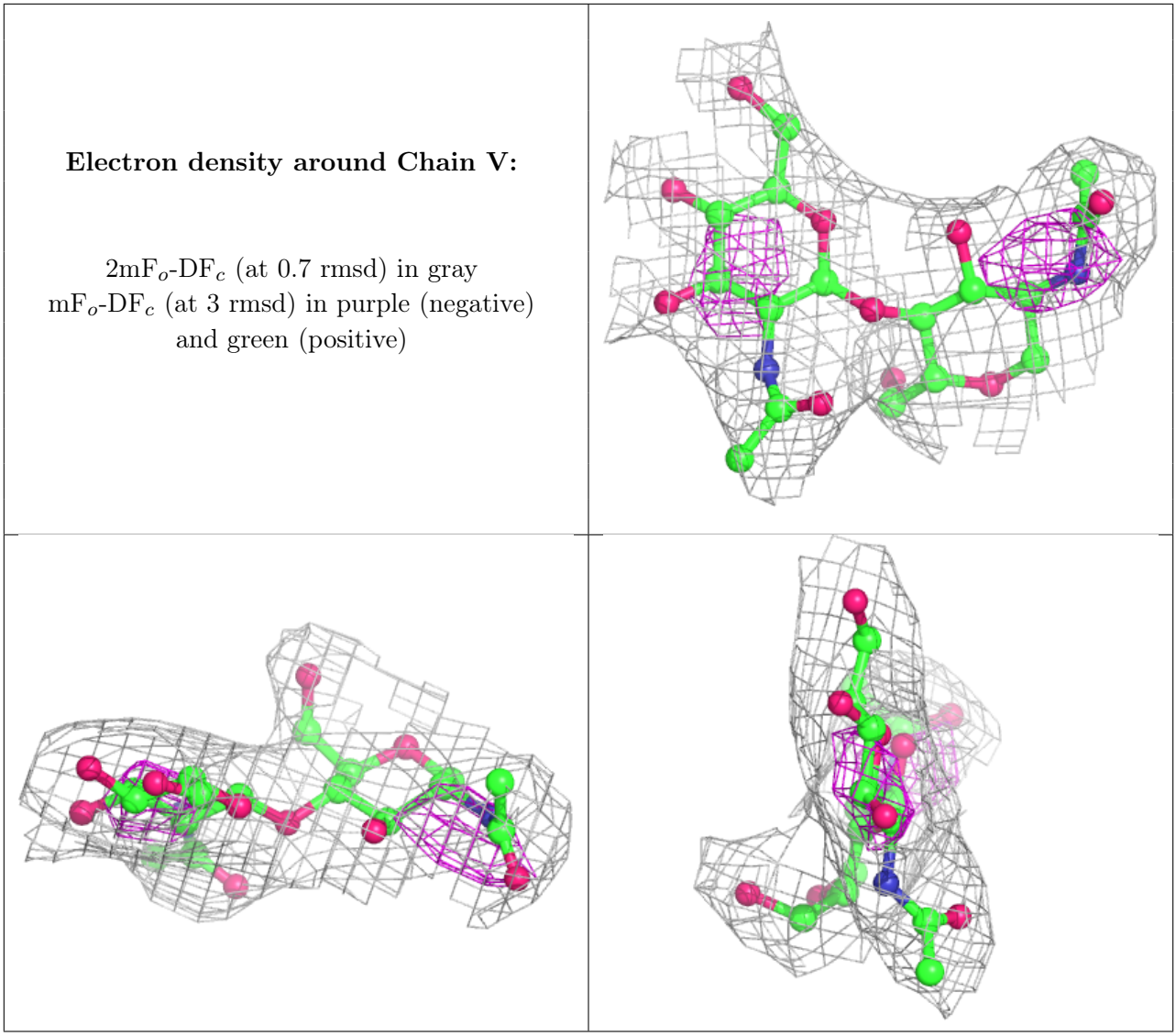






Electron density around Chain V:

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



6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.