



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 10:38 AM UTC

PDB ID : 4GXU / pdb_00004gxu
Title : Crystal structure of antibody 1F1 bound to the 1918 influenza hemagglutinin
Authors : Ekiert, D.C.; Wilson, I.A.
Deposited on : 2012-09-04
Resolution : 3.29 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

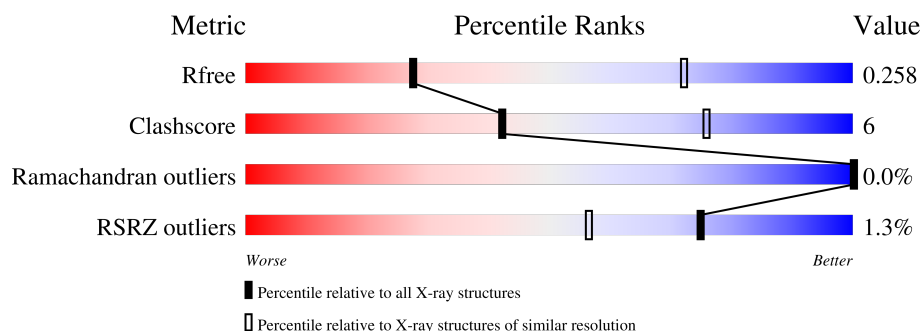
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.29 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.



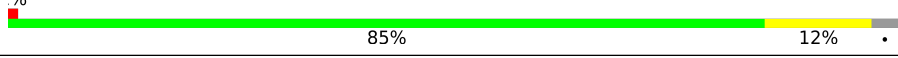
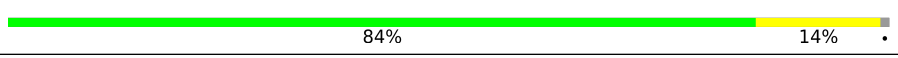
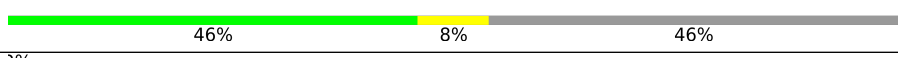
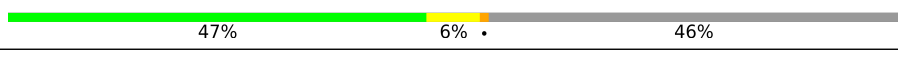
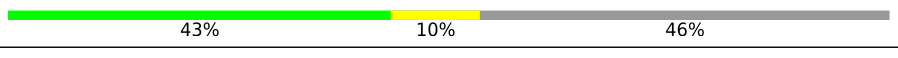
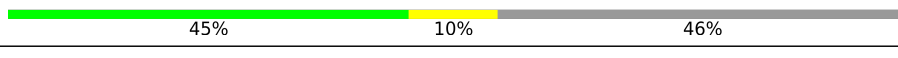
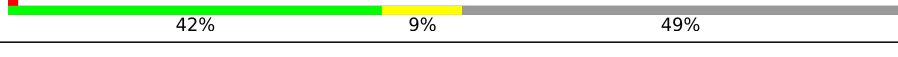
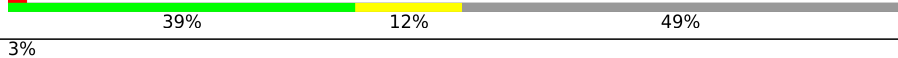
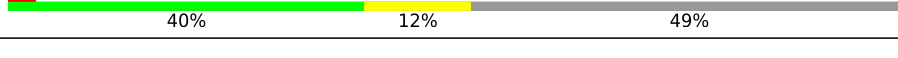
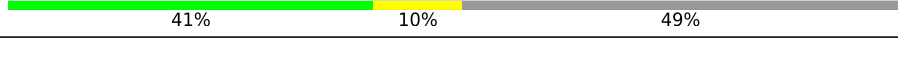
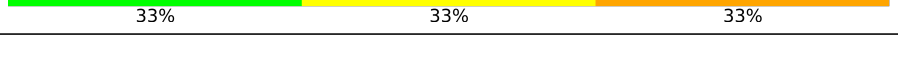
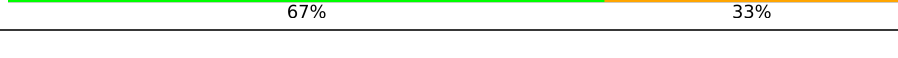
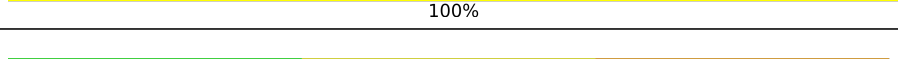
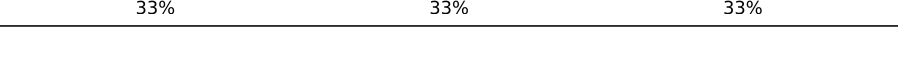
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	331	2% 83% 15% .
1	C	331	2% 79% 18% ..
1	E	331	2% 78% 19% ..
1	G	331	86% 12% .
1	I	331	% 84% 14% .
1	K	331	% 87% 11% .

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Mol	Chain	Length	Quality of chain
2	B	176	
2	D	176	
2	F	176	
2	H	176	
2	J	176	
2	L	176	
3	M	231	
3	O	231	
3	Q	231	
3	S	231	
3	U	231	
3	W	231	
4	N	217	
4	P	217	
4	R	217	
4	T	217	
4	V	217	
4	X	217	
5	Y	3	
5	Z	3	
5	a	3	
5	b	3	
5	c	3	
5	d	3	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 38412 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	7	0
			2568	1619	440	498	11			
1	C	325	Total	C	N	O	S	0	8	0
			2576	1623	442	500	11			
1	E	325	Total	C	N	O	S	0	8	0
			2576	1623	442	500	11			
1	G	325	Total	C	N	O	S	0	8	0
			2576	1623	442	500	11			
1	I	325	Total	C	N	O	S	0	8	0
			2576	1623	442	500	11			
1	K	325	Total	C	N	O	S	0	8	0
			2576	1623	442	500	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP Q9WFX3
A	8	ASP	-	expression tag	UNP Q9WFX3
A	9	PRO	-	expression tag	UNP Q9WFX3
A	10	GLY	-	expression tag	UNP Q9WFX3
C	7	ALA	-	expression tag	UNP Q9WFX3
C	8	ASP	-	expression tag	UNP Q9WFX3
C	9	PRO	-	expression tag	UNP Q9WFX3
C	10	GLY	-	expression tag	UNP Q9WFX3
E	7	ALA	-	expression tag	UNP Q9WFX3
E	8	ASP	-	expression tag	UNP Q9WFX3
E	9	PRO	-	expression tag	UNP Q9WFX3
E	10	GLY	-	expression tag	UNP Q9WFX3
G	7	ALA	-	expression tag	UNP Q9WFX3
G	8	ASP	-	expression tag	UNP Q9WFX3
G	9	PRO	-	expression tag	UNP Q9WFX3
G	10	GLY	-	expression tag	UNP Q9WFX3
I	7	ALA	-	expression tag	UNP Q9WFX3

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Chain	Residue	Modelled	Actual	Comment	Reference
I	8	ASP	-	expression tag	UNP Q9WFX3
I	9	PRO	-	expression tag	UNP Q9WFX3
I	10	GLY	-	expression tag	UNP Q9WFX3
K	7	ALA	-	expression tag	UNP Q9WFX3
K	8	ASP	-	expression tag	UNP Q9WFX3
K	9	PRO	-	expression tag	UNP Q9WFX3
K	10	GLY	-	expression tag	UNP Q9WFX3

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	171	Total	C	N	O	S	0	3	0
			1399	873	241	279	6			
2	D	171	Total	C	N	O	S	0	3	0
			1399	873	241	279	6			
2	F	171	Total	C	N	O	S	0	3	0
			1399	873	241	279	6			
2	H	171	Total	C	N	O	S	0	3	0
			1399	873	241	279	6			
2	J	171	Total	C	N	O	S	0	3	0
			1399	873	241	279	6			
2	L	171	Total	C	N	O	S	0	3	0
			1399	873	241	279	6			

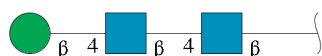
- Molecule 3 is a protein called Antibody 1F1, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	228	Total	C	N	O	S	0	4	0
			1758	1106	304	339	9			
3	O	125	Total	C	N	O	S	0	2	0
			1003	632	178	187	6			
3	Q	228	Total	C	N	O	S	0	5	0
			1766	1111	305	340	10			
3	S	125	Total	C	N	O	S	0	2	0
			1003	632	178	187	6			
3	U	125	Total	C	N	O	S	0	2	0
			1003	632	178	187	6			
3	W	125	Total	C	N	O	S	0	2	0
			1003	632	178	187	6			

- Molecule 4 is a protein called Antibody 1F1, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	214	Total	C	N	O	S	0	7	0
			1620	1019	268	329	4			
4	P	111	Total	C	N	O	S	0	7	0
			848	534	140	172	2			
4	R	214	Total	C	N	O	S	0	7	0
			1620	1019	268	329	4			
4	T	111	Total	C	N	O	S	0	7	0
			848	534	140	172	2			
4	V	111	Total	C	N	O	S	0	7	0
			848	534	140	172	2			
4	X	111	Total	C	N	O	S	0	7	0
			848	534	140	172	2			

- Molecule 5 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
5	Y	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	Z	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	a	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	b	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	c	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	d	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

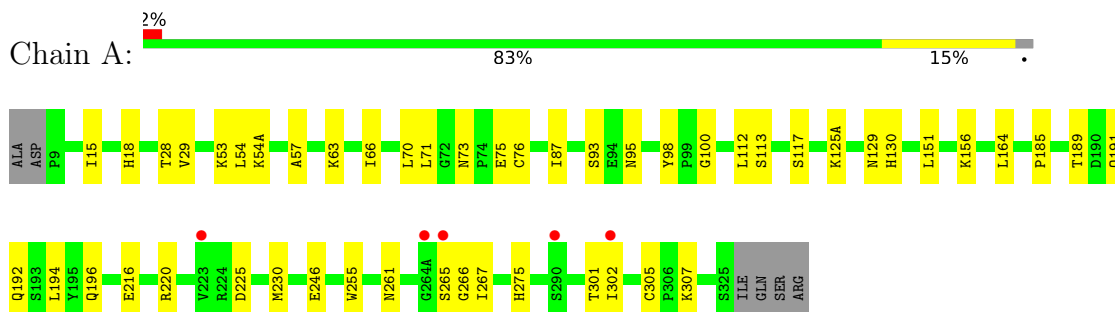


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	F	1	Total	C	N	O	0	0
			14	8	1	5		
6	G	1	Total	C	N	O	0	0
			14	8	1	5		
6	H	1	Total	C	N	O	0	0
			14	8	1	5		
6	I	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	K	1	Total	C	N	O	0	0
			14	8	1	5		
6	L	1	Total	C	N	O	0	0
			14	8	1	5		

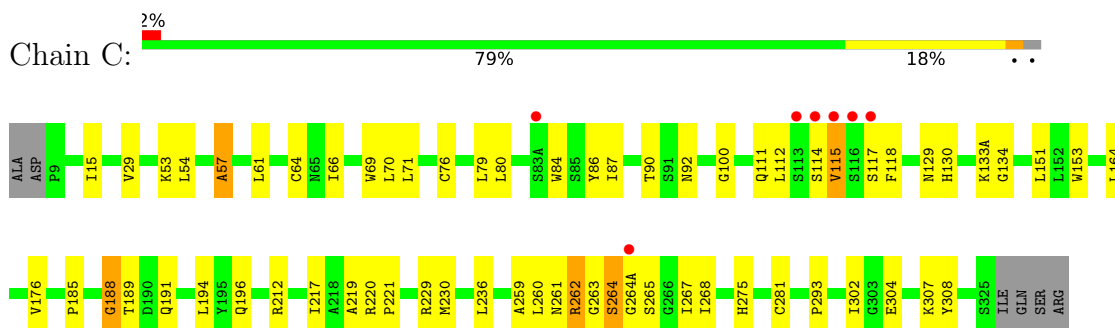
3 Residue-property plots [i](#)

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 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.

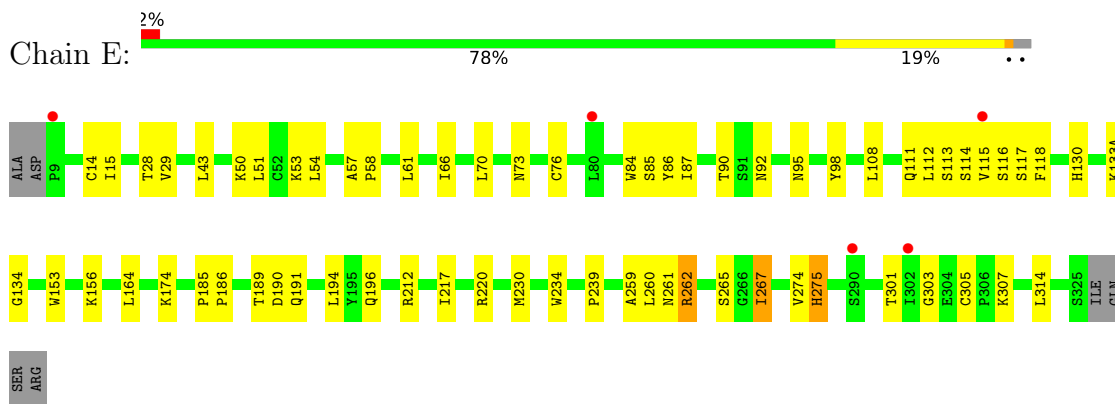
- Molecule 1: Hemagglutinin HA1 chain



- Molecule 1: Hemagglutinin HA1 chain



- Molecule 1: Hemagglutinin HA1 chain



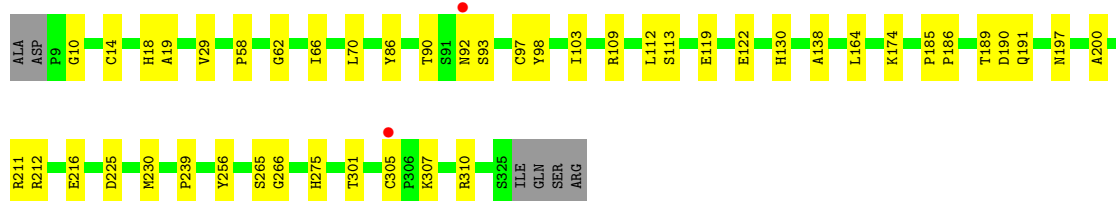
- Molecule 1: Hemagglutinin HA1 chain

Chain G:  86% 12%



- Molecule 1: Hemagglutinin HA1 chain

Chain I:  84% 14%



- Molecule 1: Hemagglutinin HA1 chain

Chain K:  87% 11%



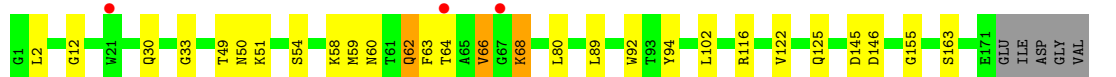
- Molecule 2: Hemagglutinin HA2 chain

Chain B:  81% 16%



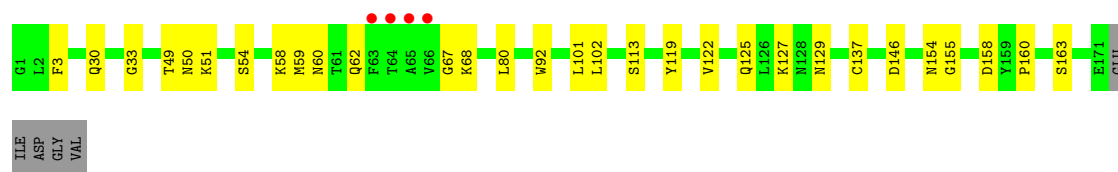
- Molecule 2: Hemagglutinin HA2 chain

Chain D:  81% 14%

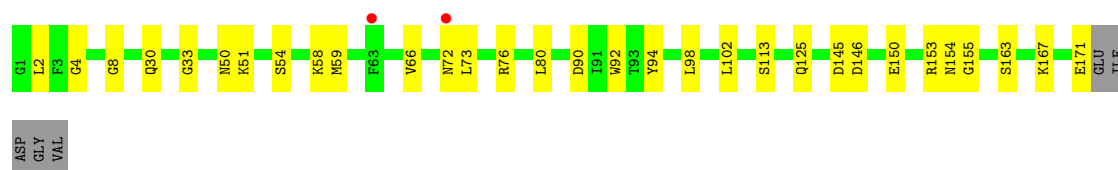
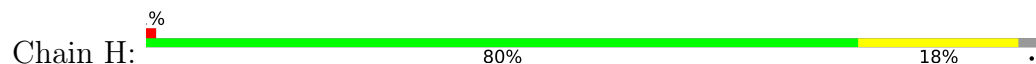


- Molecule 2: Hemagglutinin HA2 chain

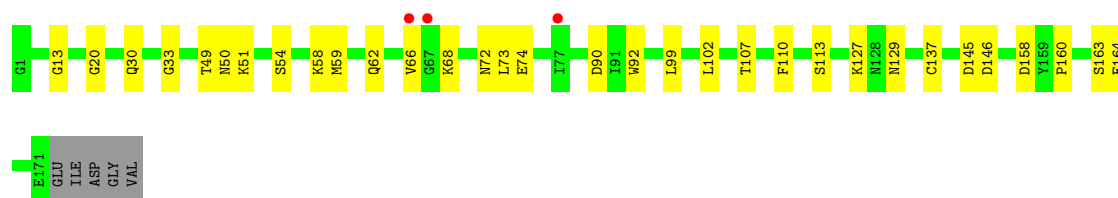
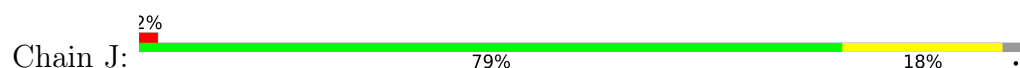
Chain F:  80% 17%



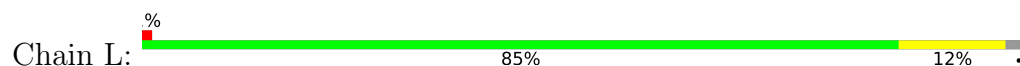
- Molecule 2: Hemagglutinin HA2 chain



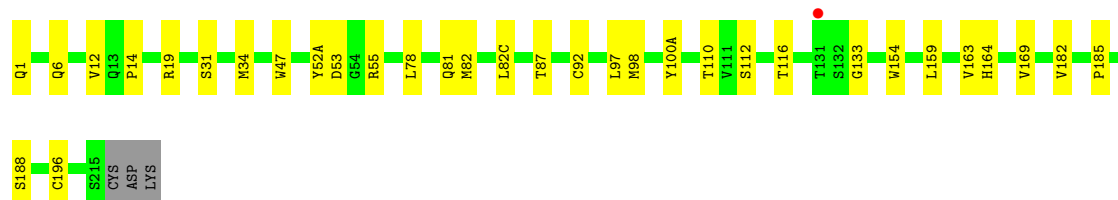
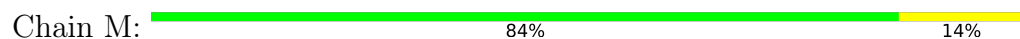
- Molecule 2: Hemagglutinin HA2 chain



- Molecule 2: Hemagglutinin HA2 chain



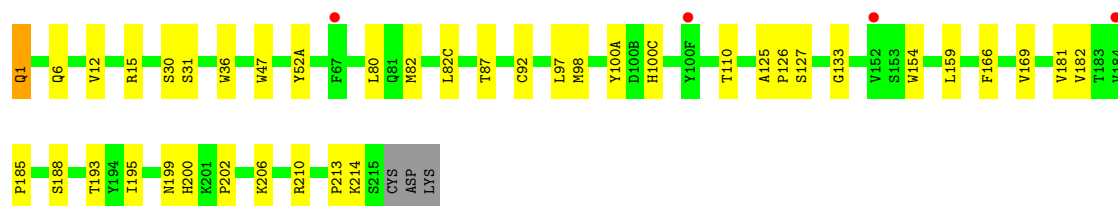
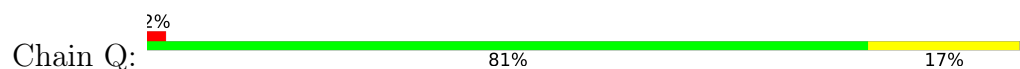
- Molecule 3: Antibody 1F1, heavy chain



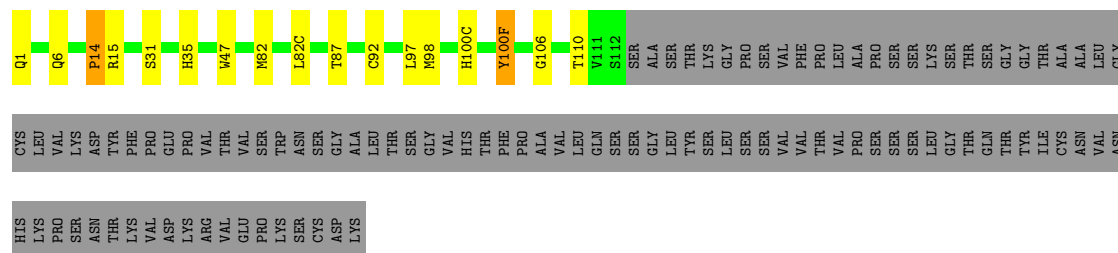
- Molecule 3: Antibody 1F1, heavy chain



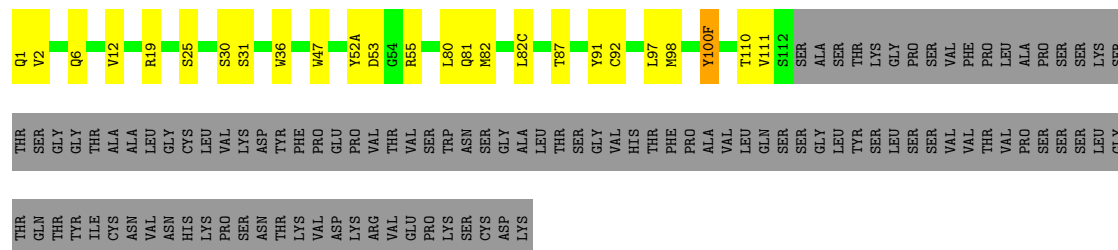
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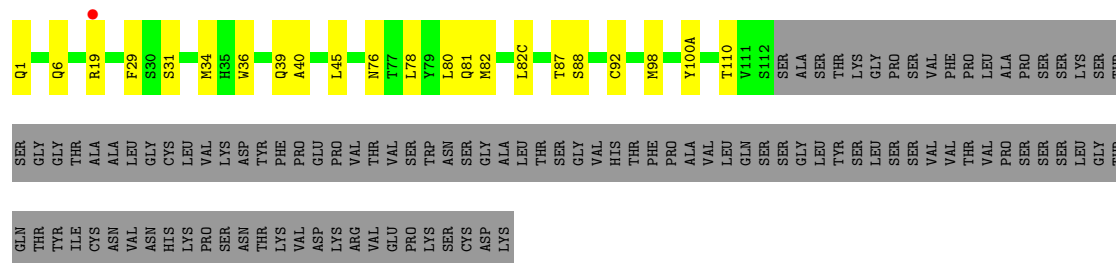


- Molecule 3: Antibody 1F1, heavy chain



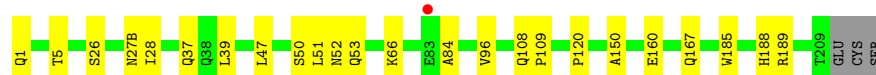
- Molecule 3: Antibody 1F1, heavy chain





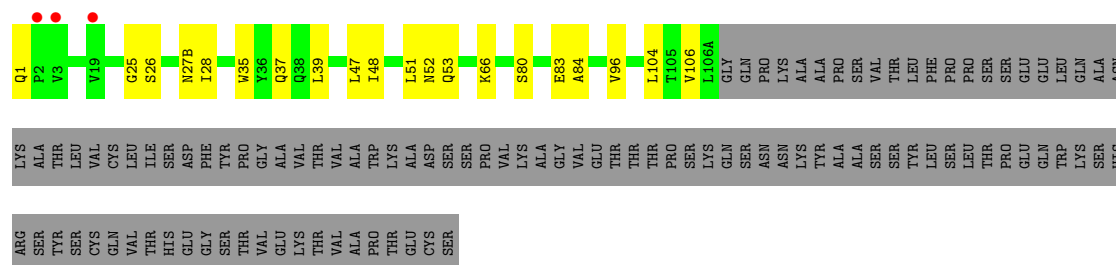
• Molecule 4: Antibody 1F1, light chain

Chain N: 88% 11%



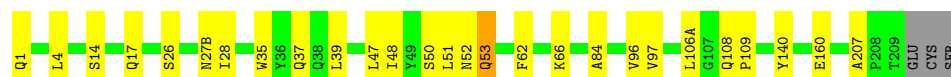
• Molecule 4: Antibody 1F1, light chain

Chain P: 42% 9% 49%



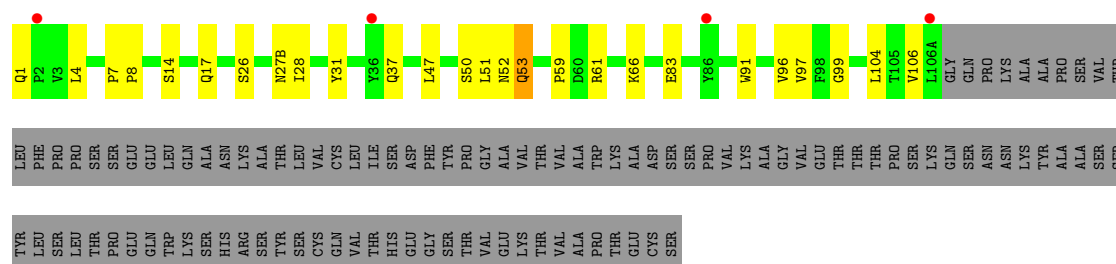
• Molecule 4: Antibody 1F1, light chain

Chain R: 86% 12%



• Molecule 4: Antibody 1F1, light chain

Chain T: 39% 12% 49%



• Molecule 4: Antibody 1F1, light chain

Chain b:  67% 33%



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

Chain c:  100%



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

Chain d:  33% 33% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	153.71Å 176.27Å 168.12Å 90.00° 92.14° 90.00°	Depositor
Resolution (Å)	35.04 – 3.29 35.04 – 3.29	Depositor EDS
% Data completeness (in resolution range)	80.1 (35.04-3.29) 80.3 (35.04-3.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.219 , 0.255 0.220 , 0.258	Depositor DCC
R_{free} test set	5441 reflections (4.02%)	wwPDB-VP
Wilson B-factor (Å ²)	104.3	Xtriage
Anisotropy	0.548	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 78.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	38412	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, PCA, 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	0.37	0/2633	0.94	5/3588 (0.1%)
1	C	0.43	0/2641	1.08	13/3599 (0.4%)
1	E	0.40	0/2641	0.95	9/3599 (0.3%)
1	G	0.36	0/2641	0.89	6/3599 (0.2%)
1	I	0.34	0/2641	0.86	3/3599 (0.1%)
1	K	0.36	0/2641	0.92	6/3599 (0.2%)
2	B	0.39	0/1426	0.91	4/1920 (0.2%)
2	D	0.44	0/1426	0.99	8/1920 (0.4%)
2	F	0.43	0/1426	0.94	6/1920 (0.3%)
2	H	0.36	0/1426	0.80	2/1920 (0.1%)
2	J	0.39	0/1426	0.86	4/1920 (0.2%)
2	L	0.42	0/1426	0.88	3/1920 (0.2%)
3	M	0.35	0/1794	0.85	0/2444
3	O	0.29	0/1020	0.78	0/1383
3	Q	0.33	0/1802	0.85	0/2454
3	S	0.31	0/1020	0.84	2/1383 (0.1%)
3	U	0.33	0/1020	0.83	1/1383 (0.1%)
3	W	0.32	0/1020	0.80	0/1383
4	N	0.36	0/1662	0.86	1/2276 (0.0%)
4	P	0.35	0/869	0.86	1/1189 (0.1%)
4	R	0.34	0/1662	0.97	3/2276 (0.1%)
4	T	0.33	0/869	0.83	1/1189 (0.1%)
4	V	0.36	0/869	0.89	0/1189
4	X	0.33	0/869	0.76	2/1189 (0.2%)
All	All	0.37	0/38870	0.90	80/52841 (0.2%)

There are no bond length outliers.

The worst 5 of 80 bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	207	ALA	CA-C-N	-14.94	104.82	119.76
4	R	207	ALA	C-N-CA	-14.94	104.82	119.76
1	C	264	SER	N-CA-C	12.25	127.09	110.55
1	C	220	ARG	CA-C-N	-10.05	110.08	120.03
1	C	220	ARG	C-N-CA	-10.05	110.08	120.03

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	2568	0	2488	40	0
1	C	2576	0	2493	54	1
1	E	2576	0	2493	52	0
1	G	2576	0	2493	32	0
1	I	2576	0	2493	33	0
1	K	2576	0	2493	24	0
2	B	1399	0	1312	23	0
2	D	1399	0	1312	24	0
2	F	1399	0	1312	20	0
2	H	1399	0	1312	24	0
2	J	1399	0	1312	25	0
2	L	1399	0	1312	14	0
3	M	1758	0	1718	23	0
3	O	1003	0	968	15	0
3	Q	1766	0	1726	29	0
3	S	1003	0	968	15	0
3	U	1003	0	968	21	0
3	W	1003	0	968	12	0
4	N	1620	0	1589	20	1
4	P	848	0	834	15	0
4	R	1620	0	1589	21	0
4	T	848	0	834	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	V	848	0	834	21	0
4	X	848	0	834	16	0
5	Y	39	0	34	1	0
5	Z	39	0	34	0	0
5	a	39	0	34	0	0
5	b	39	0	34	1	0
5	c	39	0	34	0	0
5	d	39	0	34	1	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
6	C	14	0	13	0	0
6	D	14	0	13	0	0
6	E	14	0	13	0	0
6	F	14	0	13	1	0
6	G	14	0	13	0	0
6	H	14	0	13	1	0
6	I	14	0	13	0	0
6	J	14	0	13	0	0
6	K	14	0	13	0	0
6	L	14	0	13	1	0
All	All	38412	0	37015	477	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 6.

The worst 5 of 477 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)
4:X:27(B):ASN:HD22	4:X:28:ILE:H	1.15	0.95
4:R:27(B):ASN:HD22	4:R:28:ILE:H	1.14	0.95
4:T:27(B):ASN:HD22	4:T:28:ILE:H	1.15	0.94
4:V:27(B):ASN:HD22	4:V:28:ILE:H	1.15	0.94
4:P:27(B):ASN:HD22	4:P:28:ILE:H	1.13	0.91

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)
1:C:264:SER:OG	4:N:189:ARG:N[2_444]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone

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	330/331 (100%)	322 (98%)	8 (2%)	0	100	100
1	C	331/331 (100%)	324 (98%)	7 (2%)	0	100	100
1	E	331/331 (100%)	322 (97%)	9 (3%)	0	100	100
1	G	331/331 (100%)	324 (98%)	7 (2%)	0	100	100
1	I	331/331 (100%)	324 (98%)	7 (2%)	0	100	100
1	K	331/331 (100%)	322 (97%)	9 (3%)	0	100	100
2	B	172/176 (98%)	169 (98%)	3 (2%)	0	100	100
2	D	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
2	F	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
2	H	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
2	J	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
2	L	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
3	M	230/231 (100%)	224 (97%)	5 (2%)	1 (0%)	30	60
3	O	125/231 (54%)	123 (98%)	2 (2%)	0	100	100
3	Q	231/231 (100%)	225 (97%)	5 (2%)	1 (0%)	30	60
3	S	125/231 (54%)	123 (98%)	2 (2%)	0	100	100
3	U	125/231 (54%)	123 (98%)	2 (2%)	0	100	100
3	W	125/231 (54%)	123 (98%)	2 (2%)	0	100	100
4	N	219/217 (101%)	214 (98%)	5 (2%)	0	100	100
4	P	116/217 (54%)	113 (97%)	3 (3%)	0	100	100
4	R	219/217 (101%)	215 (98%)	4 (2%)	0	100	100
4	T	116/217 (54%)	113 (97%)	3 (3%)	0	100	100
4	V	116/217 (54%)	113 (97%)	3 (3%)	0	100	100
4	X	116/217 (54%)	113 (97%)	3 (3%)	0	100	100
All	All	4880/5730 (85%)	4779 (98%)	99 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	133	GLY
3	Q	133	GLY

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
4	PCA	X	1	4	7,8,9	1.89	1 (14%)	9,10,12	2.24	6 (66%)
3	PCA	M	1	3	7,8,9	1.97	1 (14%)	9,10,12	2.18	4 (44%)
3	PCA	Q	1	3	7,8,9	1.82	1 (14%)	9,10,12	2.12	4 (44%)
4	PCA	V	1	4	7,8,9	1.98	1 (14%)	9,10,12	2.54	5 (55%)
4	PCA	R	1	4	7,8,9	1.96	1 (14%)	9,10,12	2.39	5 (55%)
4	PCA	P	1	4	7,8,9	2.03	1 (14%)	9,10,12	2.61	5 (55%)
4	PCA	N	1	4	7,8,9	1.99	1 (14%)	9,10,12	2.55	6 (66%)
3	PCA	O	1	3	7,8,9	1.85	1 (14%)	9,10,12	2.10	4 (44%)
4	PCA	T	1	4	7,8,9	1.95	1 (14%)	9,10,12	2.29	6 (66%)
3	PCA	W	1	3	7,8,9	1.95	1 (14%)	9,10,12	2.12	4 (44%)
3	PCA	U	1	3	7,8,9	1.93	1 (14%)	9,10,12	1.99	4 (44%)
3	PCA	S	1	3	7,8,9	1.95	1 (14%)	9,10,12	2.09	4 (44%)

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
4	PCA	X	1	4	-	0/0/11/13	0/1/1/1
3	PCA	M	1	3	-	0/0/11/13	0/1/1/1
3	PCA	Q	1	3	-	0/0/11/13	0/1/1/1
4	PCA	V	1	4	-	0/0/11/13	0/1/1/1
4	PCA	R	1	4	-	0/0/11/13	0/1/1/1
4	PCA	P	1	4	-	0/0/11/13	0/1/1/1
4	PCA	N	1	4	-	0/0/11/13	0/1/1/1
3	PCA	O	1	3	-	0/0/11/13	0/1/1/1
4	PCA	T	1	4	-	0/0/11/13	0/1/1/1
3	PCA	W	1	3	-	0/0/11/13	0/1/1/1
3	PCA	U	1	3	-	0/0/11/13	0/1/1/1
3	PCA	S	1	3	-	0/0/11/13	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	1	PCA	CD-N	5.23	1.47	1.34
4	V	1	PCA	CD-N	5.08	1.47	1.34
3	M	1	PCA	CD-N	5.07	1.47	1.34
4	N	1	PCA	CD-N	5.05	1.47	1.34
3	S	1	PCA	CD-N	5.04	1.47	1.34

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	1	PCA	CB-CA-C	-4.26	106.81	112.66
4	V	1	PCA	OE-CD-CG	-3.82	119.90	126.72
4	P	1	PCA	OE-CD-CG	-3.73	120.07	126.72
4	N	1	PCA	OE-CD-CG	-3.72	120.08	126.72
4	N	1	PCA	CA-N-CD	-3.52	101.53	113.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	1	PCA	1	0
3	O	1	PCA	1	0

5.5 Carbohydrates [i](#)

18 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	Y	1	1,5	14,14,15	0.50	0	17,19,21	1.20	4 (23%)
5	NAG	Y	2	5	14,14,15	0.59	0	17,19,21	1.09	1 (5%)
5	BMA	Y	3	5	11,11,12	0.68	0	15,15,17	0.69	0
5	NAG	Z	1	1,5	14,14,15	0.54	0	17,19,21	0.92	1 (5%)
5	NAG	Z	2	5	14,14,15	0.49	0	17,19,21	0.85	0
5	BMA	Z	3	5	11,11,12	0.76	0	15,15,17	0.65	0
5	NAG	a	1	1,5	14,14,15	0.54	0	17,19,21	0.95	1 (5%)
5	NAG	a	2	5	14,14,15	0.55	0	17,19,21	1.14	1 (5%)
5	BMA	a	3	5	11,11,12	0.73	0	15,15,17	0.70	0
5	NAG	b	1	1,5	14,14,15	0.55	0	17,19,21	0.77	0
5	NAG	b	2	5	14,14,15	0.61	0	17,19,21	1.14	3 (17%)
5	BMA	b	3	5	11,11,12	0.71	0	15,15,17	0.65	0
5	NAG	c	1	1,5	14,14,15	0.53	0	17,19,21	1.05	2 (11%)
5	NAG	c	2	5	14,14,15	0.60	0	17,19,21	1.15	1 (5%)
5	BMA	c	3	5	11,11,12	1.00	2 (18%)	15,15,17	1.34	1 (6%)
5	NAG	d	1	1,5	14,14,15	0.55	0	17,19,21	0.59	0
5	NAG	d	2	5	14,14,15	0.62	0	17,19,21	1.26	1 (5%)
5	BMA	d	3	5	11,11,12	0.78	0	15,15,17	0.70	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
5	NAG	Y	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	1/6/23/26	0/1/1/1
5	BMA	Y	3	5	-	2/2/19/22	0/1/1/1
5	NAG	Z	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	3/6/23/26	0/1/1/1
5	BMA	Z	3	5	-	2/2/19/22	0/1/1/1
5	NAG	a	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	a	2	5	-	4/6/23/26	0/1/1/1
5	BMA	a	3	5	-	2/2/19/22	0/1/1/1
5	NAG	b	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	b	2	5	-	3/6/23/26	0/1/1/1
5	BMA	b	3	5	-	0/2/19/22	0/1/1/1
5	NAG	c	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	c	2	5	-	3/6/23/26	0/1/1/1
5	BMA	c	3	5	-	0/2/19/22	0/1/1/1
5	NAG	d	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	d	2	5	-	2/6/23/26	0/1/1/1
5	BMA	d	3	5	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	c	3	BMA	C1-C2	2.32	1.57	1.52
5	c	3	BMA	C2-C3	2.20	1.55	1.52

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	d	2	NAG	C4-C3-C2	3.66	116.39	111.02
5	c	2	NAG	C4-C3-C2	3.63	116.33	111.02
5	c	3	BMA	C1-C2-C3	3.19	114.28	109.64
5	a	2	NAG	C4-C3-C2	3.15	115.64	111.02
5	Y	2	NAG	C4-C3-C2	3.13	115.61	111.02

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Z	2	NAG	C1-C2-N2-C7

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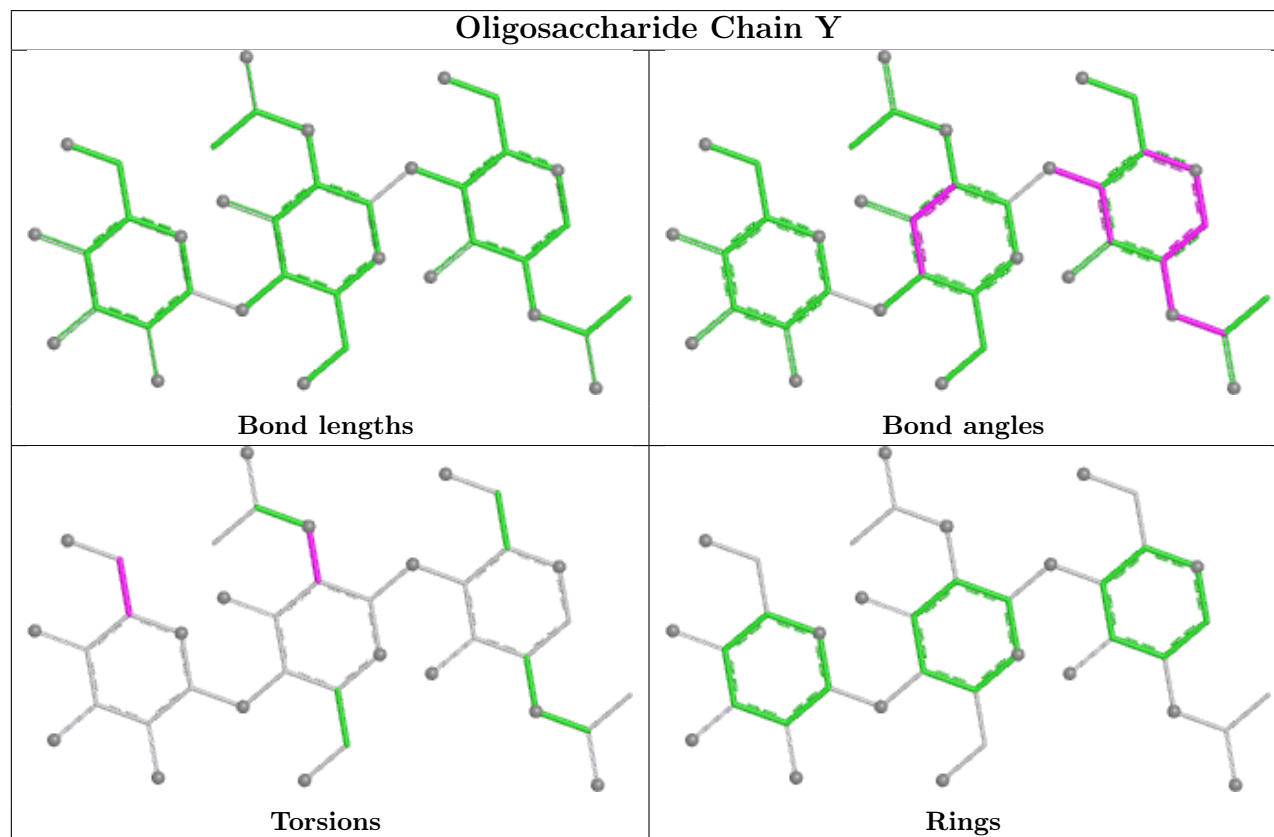
Mol	Chain	Res	Type	Atoms
5	Z	2	NAG	C8-C7-N2-C2
5	Z	2	NAG	O7-C7-N2-C2
5	a	1	NAG	C8-C7-N2-C2
5	a	1	NAG	O7-C7-N2-C2

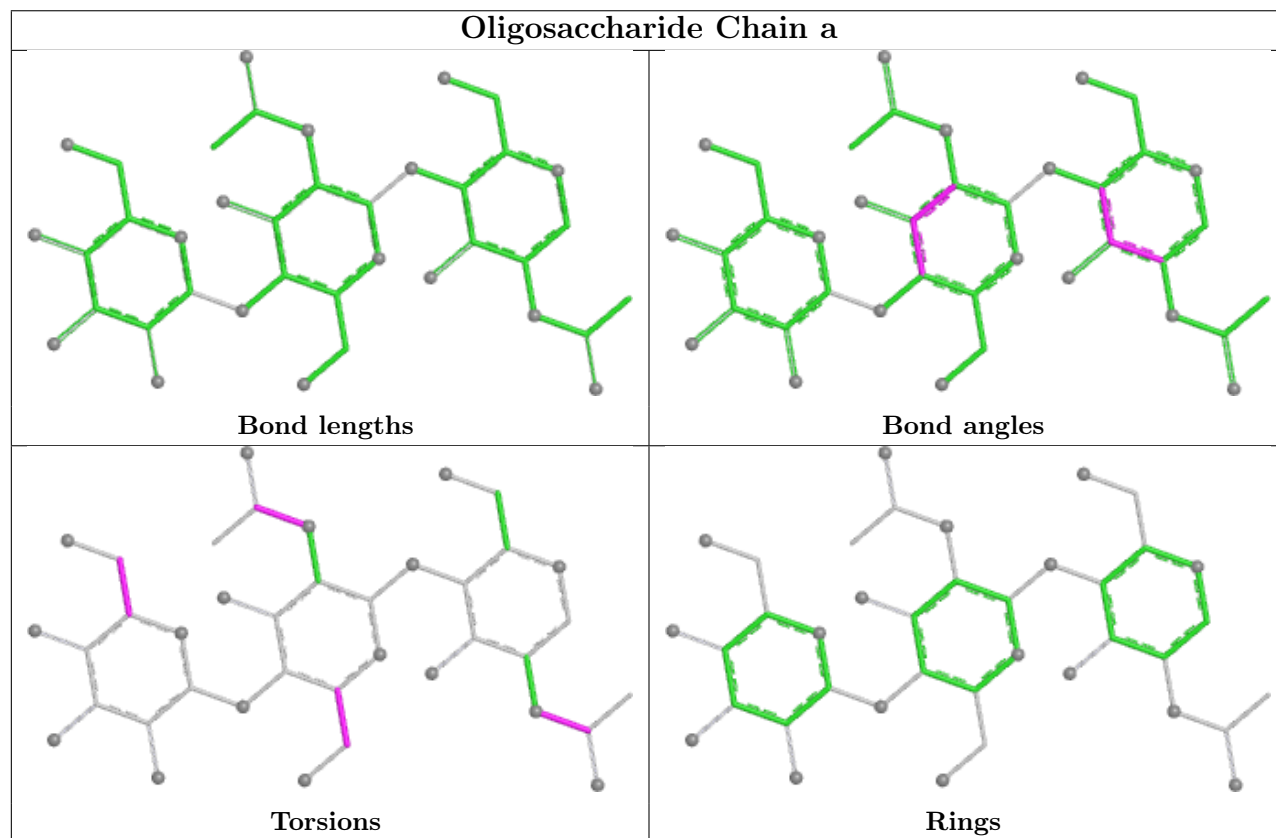
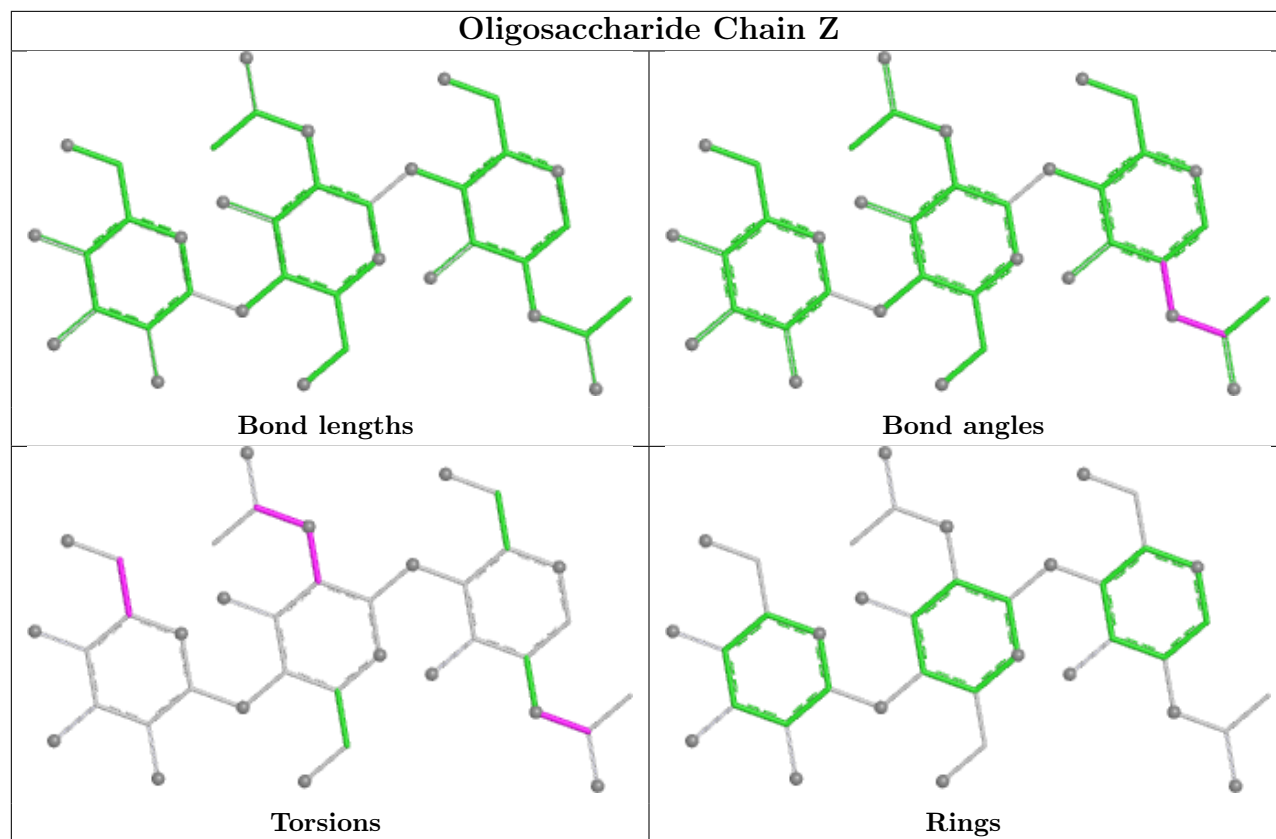
There are no ring outliers.

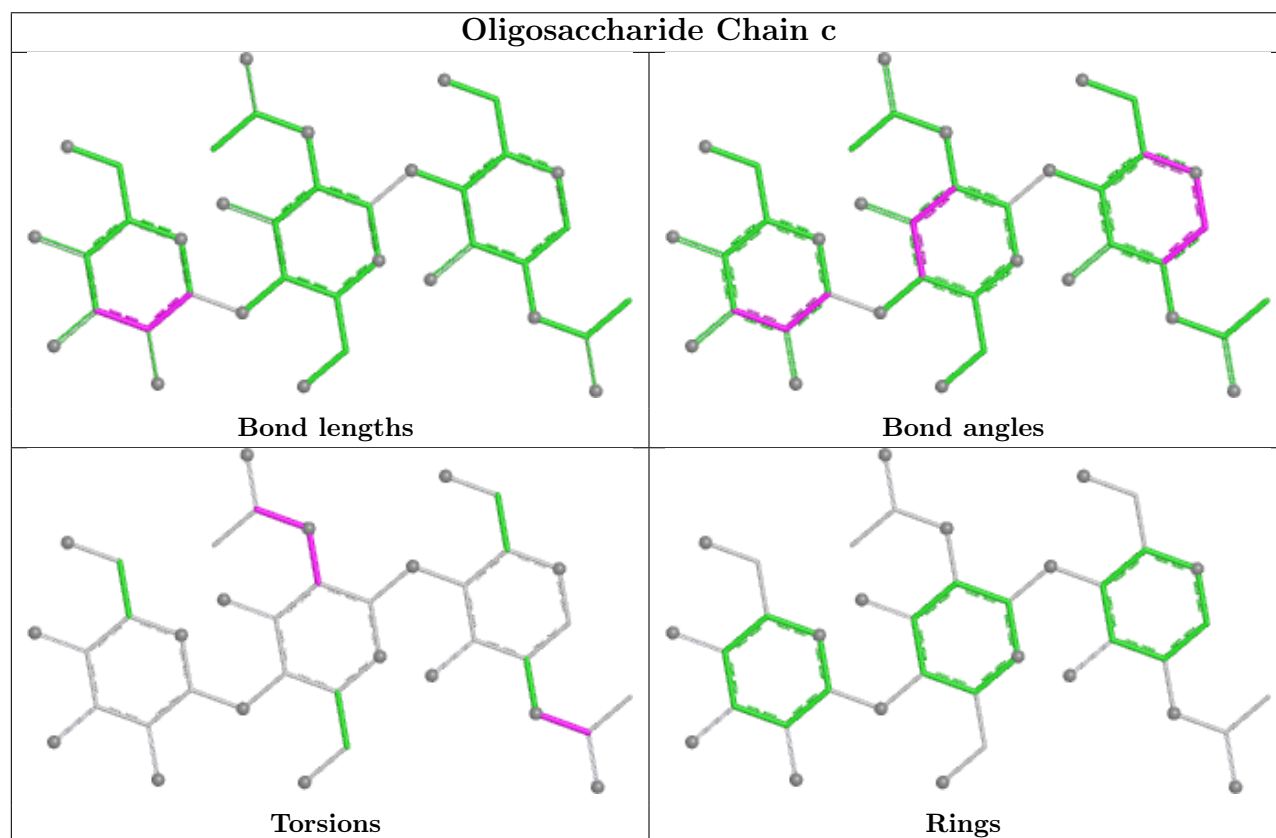
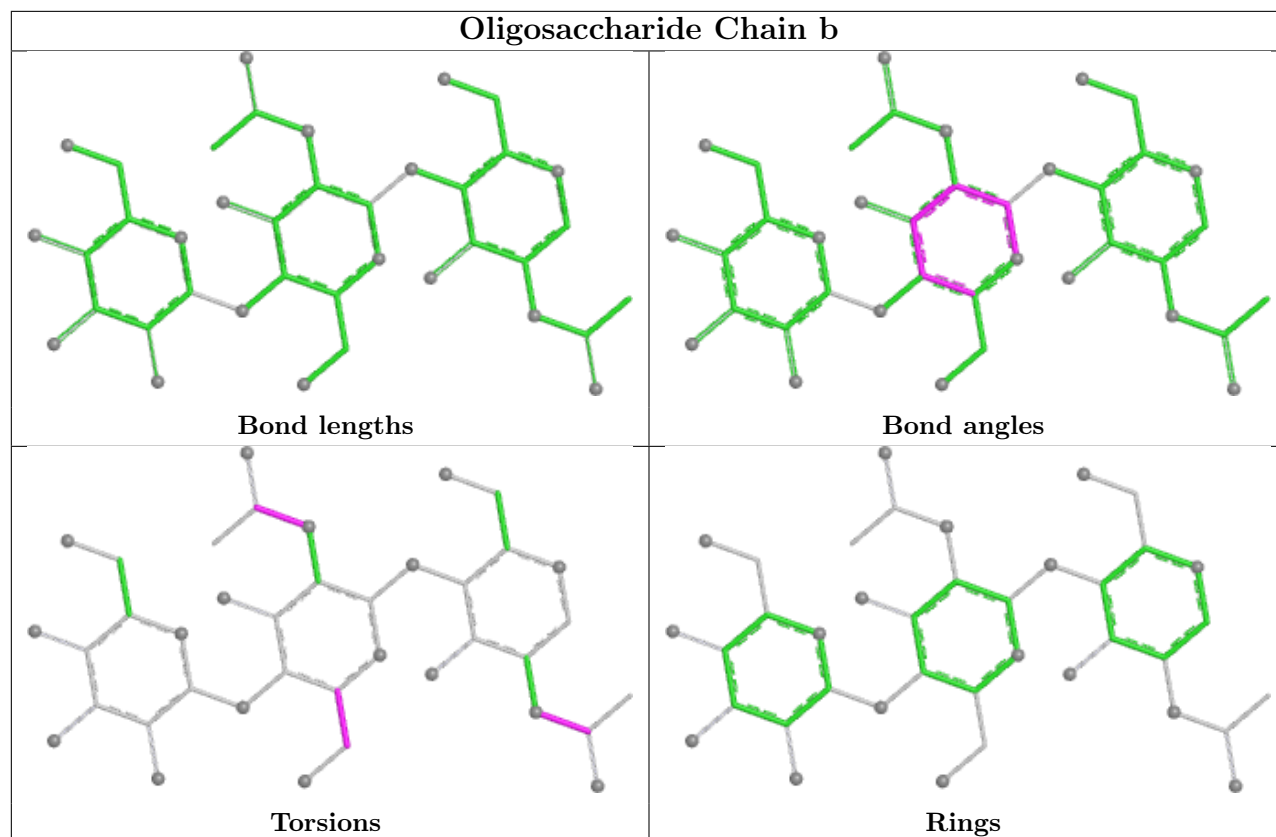
4 monomers are involved in 3 short contacts:

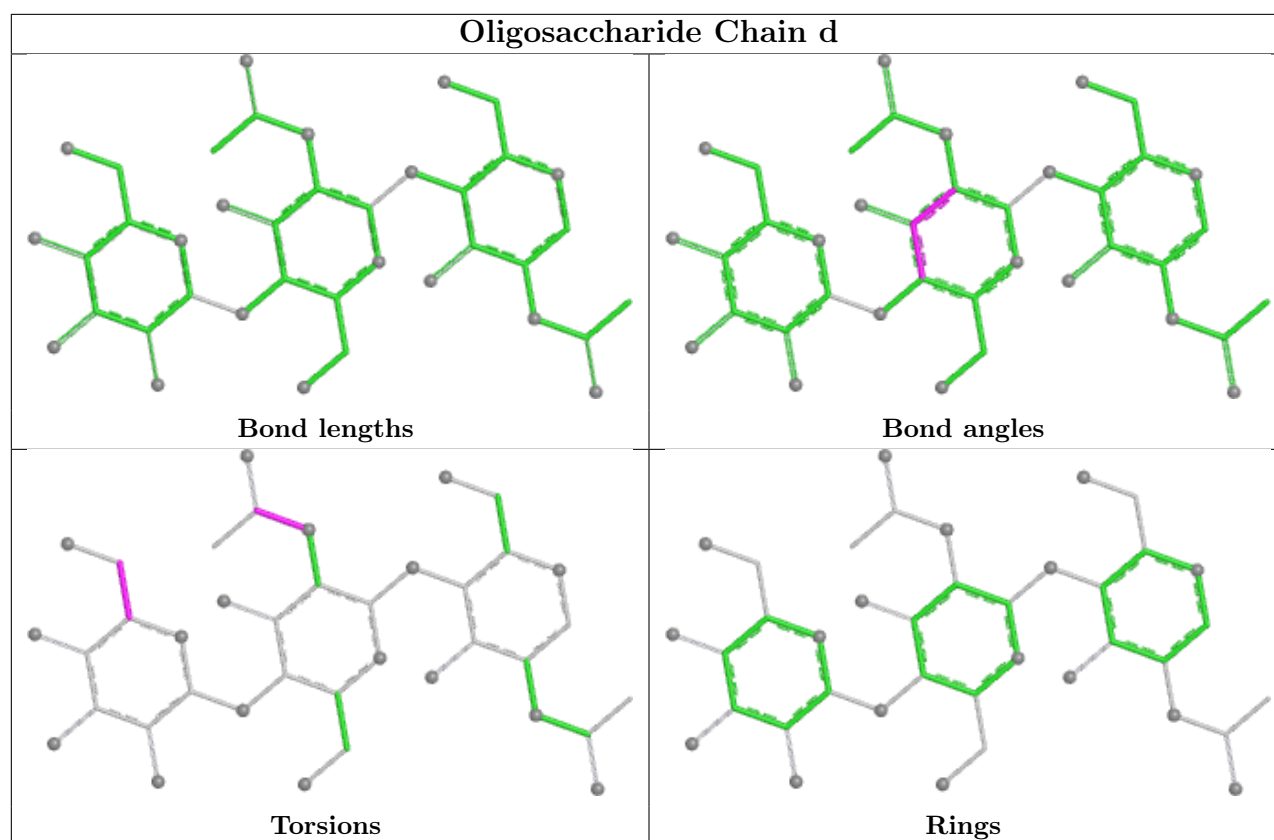
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Y	1	NAG	1	0
5	b	2	NAG	1	0
5	d	1	NAG	1	0
5	d	2	NAG	1	0

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 [i](#)

12 ligands 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	A	401	1	14,14,15	0.42	0	17,19,21	1.12	1 (5%)
6	NAG	D	201	2	14,14,15	0.51	0	17,19,21	0.61	0
6	NAG	F	201	2	14,14,15	0.54	0	17,19,21	1.08	1 (5%)
6	NAG	E	401	1	14,14,15	0.59	0	17,19,21	1.07	2 (11%)
6	NAG	K	401	1	14,14,15	0.56	0	17,19,21	1.55	3 (17%)
6	NAG	I	401	1	14,14,15	0.56	0	17,19,21	1.17	2 (11%)
6	NAG	H	201	2	14,14,15	0.49	0	17,19,21	0.69	0
6	NAG	C	401	1	14,14,15	0.52	0	17,19,21	1.61	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	J	201	2	14,14,15	0.46	0	17,19,21	0.74	0
6	NAG	G	401	1	14,14,15	0.66	0	17,19,21	0.76	0
6	NAG	L	201	2	14,14,15	0.48	0	17,19,21	2.20	2 (11%)
6	NAG	B	201	2	14,14,15	0.55	0	17,19,21	0.92	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	A	401	1	-	2/6/23/26	0/1/1/1
6	NAG	D	201	2	-	2/6/23/26	0/1/1/1
6	NAG	F	201	2	-	4/6/23/26	0/1/1/1
6	NAG	E	401	1	-	6/6/23/26	0/1/1/1
6	NAG	K	401	1	-	4/6/23/26	0/1/1/1
6	NAG	I	401	1	-	3/6/23/26	0/1/1/1
6	NAG	H	201	2	-	2/6/23/26	0/1/1/1
6	NAG	C	401	1	-	3/6/23/26	0/1/1/1
6	NAG	J	201	2	-	0/6/23/26	0/1/1/1
6	NAG	G	401	1	-	5/6/23/26	0/1/1/1
6	NAG	L	201	2	-	2/6/23/26	0/1/1/1
6	NAG	B	201	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	201	NAG	C1-O5-C5	8.11	123.06	112.19
6	K	401	NAG	C1-O5-C5	4.77	118.58	112.19
6	C	401	NAG	C1-O5-C5	4.44	118.13	112.19
6	C	401	NAG	O5-C1-C2	4.38	118.07	111.29
6	A	401	NAG	C1-O5-C5	3.66	117.09	112.19

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	401	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	A	401	NAG	O7-C7-N2-C2
6	C	401	NAG	C8-C7-N2-C2
6	C	401	NAG	O7-C7-N2-C2
6	E	401	NAG	C8-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	201	NAG	1	0
6	H	201	NAG	1	0
6	L	201	NAG	1	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	325/331 (98%)	-0.32	5 (1%) 72 53	26, 85, 149, 213	7 (2%)
1	C	325/331 (98%)	-0.40	7 (2%) 62 43	25, 71, 134, 219	8 (2%)
1	E	325/331 (98%)	-0.42	5 (1%) 72 53	28, 74, 129, 199	8 (2%)
1	G	325/331 (98%)	-0.49	1 (0%) 90 82	36, 104, 146, 175	8 (2%)
1	I	325/331 (98%)	-0.37	2 (0%) 85 73	45, 109, 151, 202	8 (2%)
1	K	325/331 (98%)	-0.40	2 (0%) 85 73	43, 100, 134, 148	8 (2%)
2	B	171/176 (97%)	-0.39	2 (1%) 76 58	33, 107, 161, 207	3 (1%)
2	D	171/176 (97%)	-0.39	3 (1%) 67 49	26, 108, 150, 171	3 (1%)
2	F	171/176 (97%)	-0.47	4 (2%) 61 42	30, 102, 155, 189	3 (1%)
2	H	171/176 (97%)	-0.53	2 (1%) 76 58	46, 100, 152, 206	3 (1%)
2	J	171/176 (97%)	-0.52	3 (1%) 67 49	38, 109, 154, 177	3 (1%)
2	L	171/176 (97%)	-0.54	2 (1%) 76 58	34, 99, 139, 172	3 (1%)
3	M	227/231 (98%)	-0.44	1 (0%) 88 79	33, 89, 151, 210	4 (1%)
3	O	124/231 (53%)	-0.44	1 (0%) 82 68	42, 112, 148, 161	2 (1%)
3	Q	227/231 (98%)	-0.23	4 (1%) 67 49	35, 134, 212, 241	5 (2%)
3	S	124/231 (53%)	-0.40	0 100 100	59, 143, 179, 191	2 (1%)
3	U	124/231 (53%)	-0.23	0 100 100	57, 141, 183, 212	2 (1%)
3	W	124/231 (53%)	-0.26	1 (0%) 82 68	55, 131, 164, 180	2 (1%)
4	N	213/217 (98%)	-0.49	1 (0%) 87 76	33, 76, 116, 156	7 (3%)
4	P	110/217 (50%)	-0.27	3 (2%) 56 37	43, 116, 158, 165	7 (6%)
4	R	213/217 (98%)	-0.36	0 100 100	54, 156, 205, 251	7 (3%)
4	T	110/217 (50%)	-0.27	4 (3%) 46 31	65, 157, 179, 215	7 (6%)
4	V	110/217 (50%)	0.17	6 (5%) 30 21	75, 171, 208, 247	7 (6%)
4	X	110/217 (50%)	-0.25	1 (0%) 81 65	67, 147, 180, 222	7 (6%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4792/5730 (83%)	-0.38	60 (1%) 75 56	25, 105, 175, 251	124 (2%)

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	V	89	ALA	5.2
2	F	66	VAL	4.7
4	P	2	PRO	4.4
4	V	21	ILE	4.0
1	A	264(A)	GLY	4.0

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

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
3	PCA	M	1	8/9	0.10	0.14	120,132,139,146	0
3	PCA	W	1	8/9	0.15	0.13	195,198,202,208	0
3	PCA	S	1	8/9	0.34	0.12	199,209,211,212	0
3	PCA	U	1	8/9	0.34	0.12	170,178,182,187	0
3	PCA	O	1	8/9	0.34	0.12	151,153,157,160	0
4	PCA	X	1	8/9	0.44	0.12	207,212,215,218	0
4	PCA	V	1	8/9	0.61	0.13	206,209,213,215	0
4	PCA	R	1	8/9	0.64	0.16	203,208,217,222	0
4	PCA	T	1	8/9	0.68	0.12	193,201,222,228	0
4	PCA	N	1	8/9	0.70	0.13	172,194,204,208	0
3	PCA	Q	1	8/9	0.71	0.11	155,160,163,164	0
4	PCA	P	1	8/9	0.84	0.17	124,132,163,169	0

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.

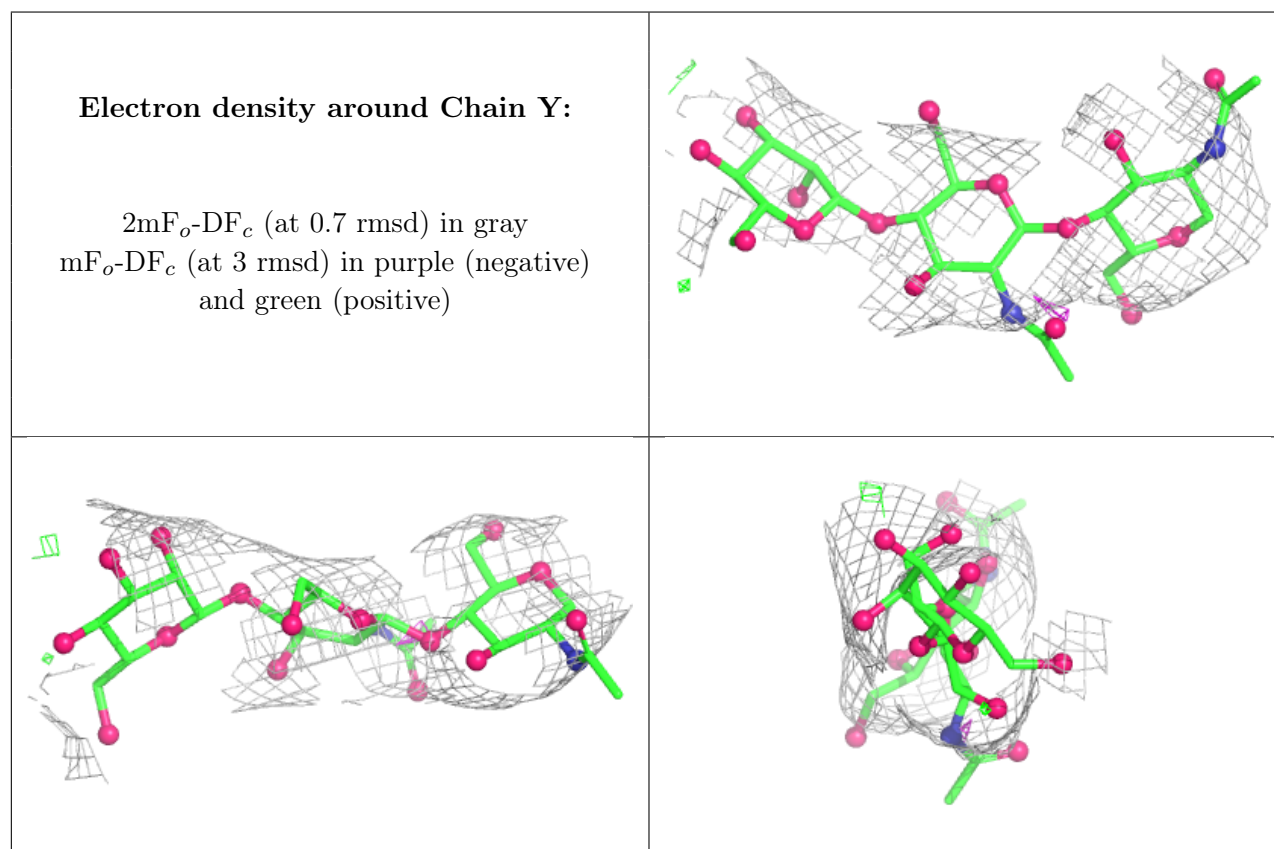
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BMA	Y	3	11/12	0.60	0.10	101,127,129,135	0

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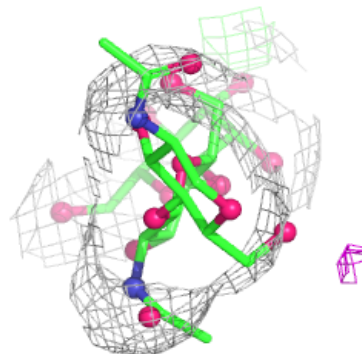
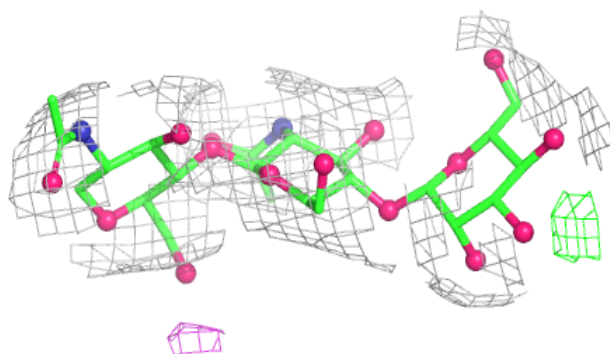
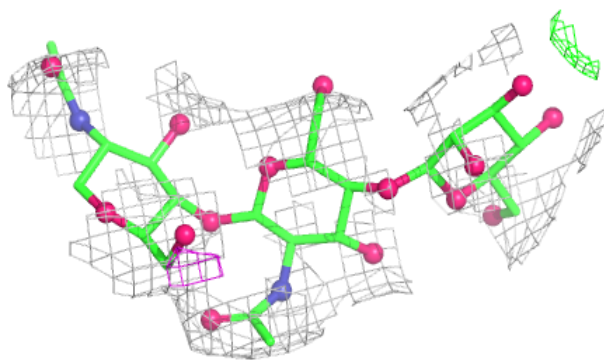
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	BMA	Z	3	11/12	0.80	0.07	83,104,113,124	0
5	NAG	Y	2	14/15	0.93	0.07	107,118,131,133	0
5	NAG	Z	2	14/15	0.94	0.05	96,100,107,110	0
5	NAG	Z	1	14/15	0.94	0.08	62,79,94,98	0
5	NAG	Y	1	14/15	0.95	0.06	99,109,118,126	0
5	NAG	a	1	14/15	-	-	50,70,80,81	0
5	NAG	a	2	14/15	-	-	67,77,90,107	0
5	BMA	a	3	11/12	-	-	122,134,154,160	0
5	NAG	b	1	14/15	-	-	78,90,99,99	0
5	NAG	b	2	14/15	-	-	108,124,132,133	0
5	BMA	b	3	11/12	-	-	114,120,128,131	0
5	NAG	c	1	14/15	-	-	78,102,106,113	0
5	NAG	c	2	14/15	-	-	100,126,130,138	0
5	BMA	c	3	11/12	-	-	99,117,171,172	0
5	NAG	d	1	14/15	-	-	65,106,114,116	0
5	NAG	d	2	14/15	-	-	116,120,133,135	0
5	BMA	d	3	11/12	-	-	122,132,138,140	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.

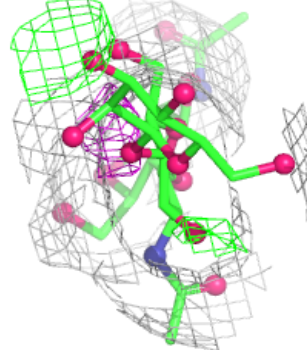
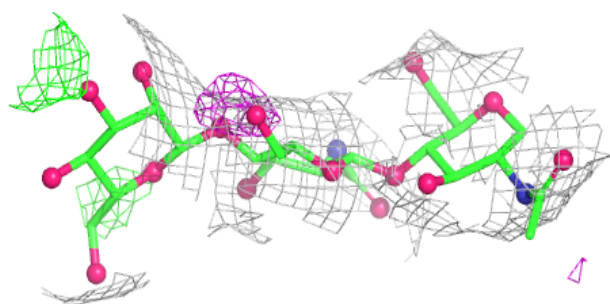
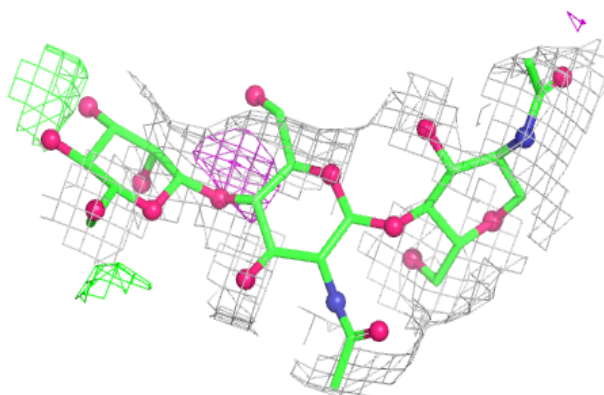


Electron density around Chain Z:

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

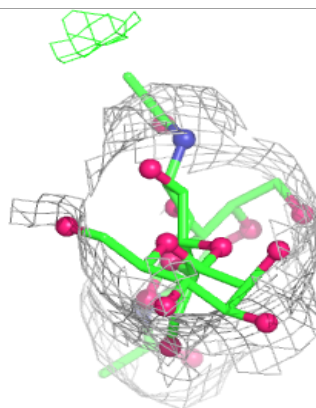
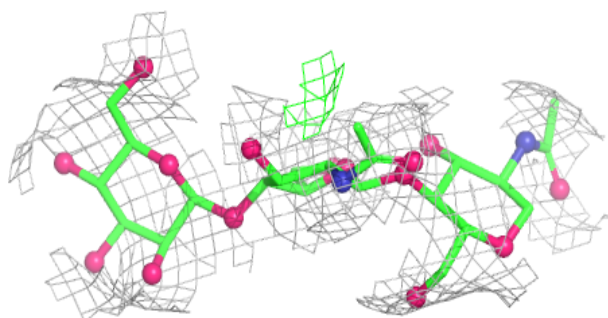
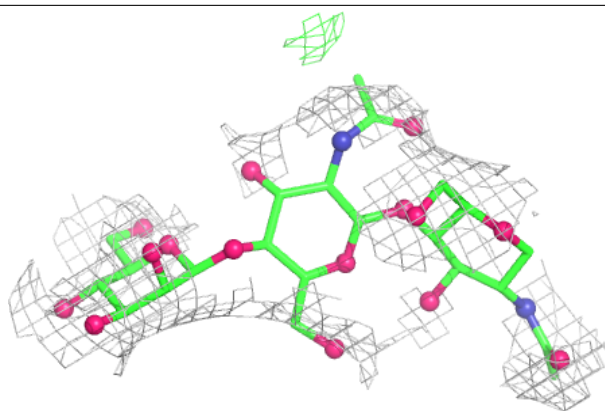
**Electron density around Chain a:**

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

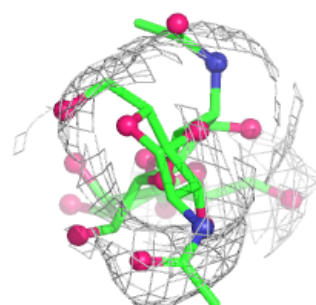
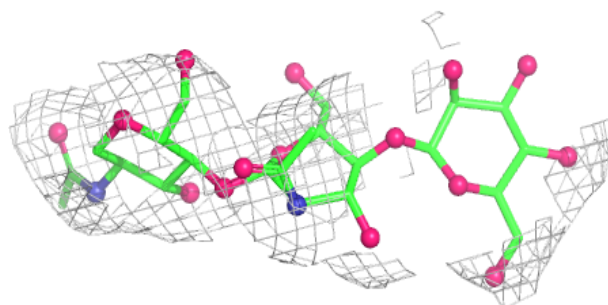
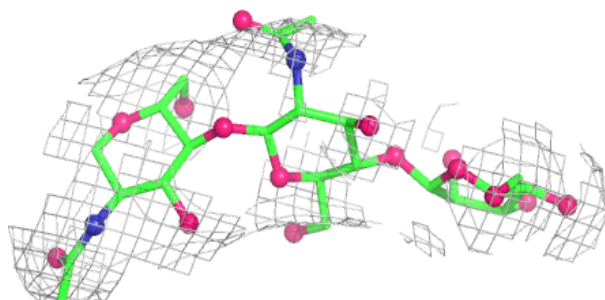


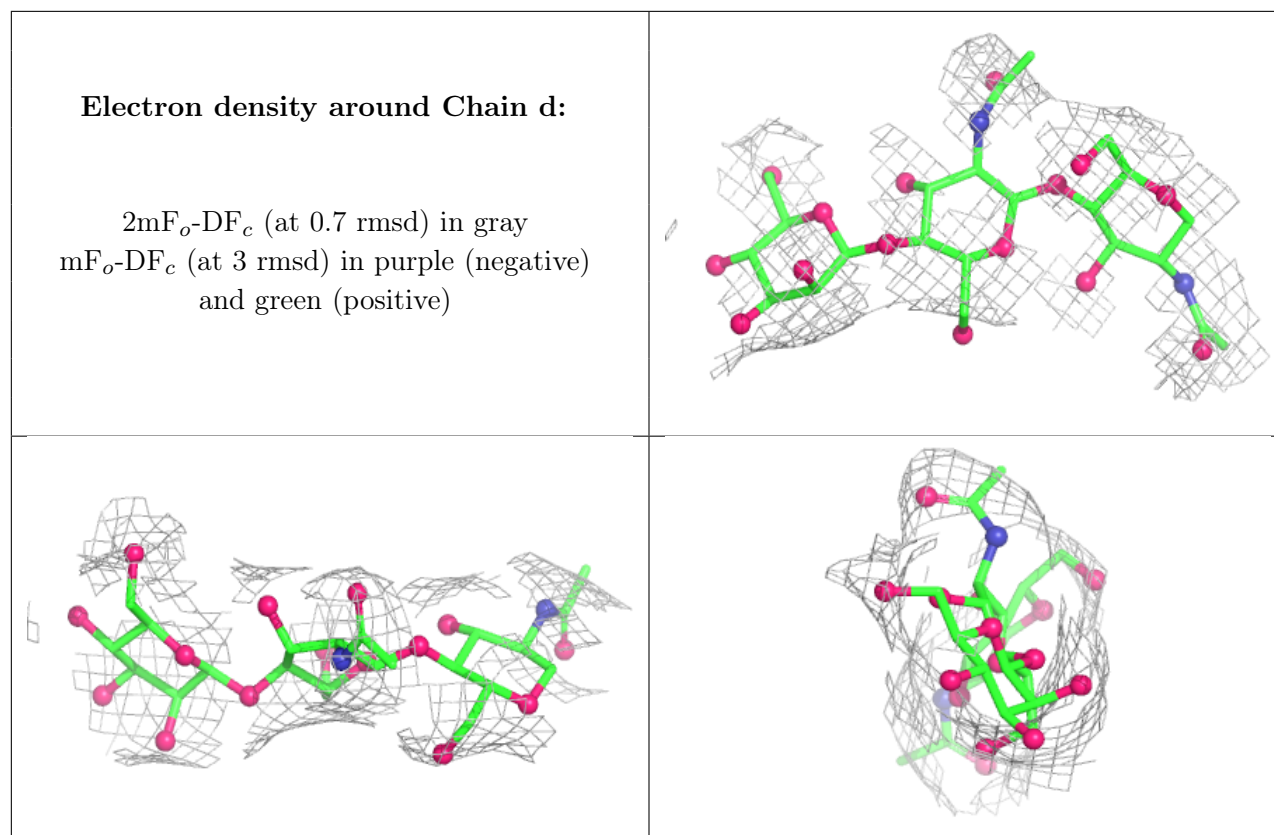
Electron density around Chain b:

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

**Electron density around Chain c:**

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





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	G	401	14/15	0.38	0.11	175,184,195,196	0
6	NAG	A	401	14/15	0.39	0.09	152,185,198,200	0
6	NAG	B	201	14/15	0.51	0.10	153,170,177,180	0
6	NAG	J	201	14/15	0.52	0.10	122,141,152,153	0
6	NAG	K	401	14/15	0.57	0.08	116,156,174,182	0
6	NAG	L	201	14/15	0.59	0.09	140,174,180,183	0
6	NAG	D	201	14/15	0.62	0.10	139,164,173,176	0
6	NAG	C	401	14/15	0.64	0.09	151,163,173,176	0
6	NAG	E	401	14/15	0.64	0.08	186,209,213,218	0
6	NAG	H	201	14/15	0.73	0.10	135,152,165,168	0
6	NAG	F	201	14/15	0.75	0.08	163,181,186,191	0
6	NAG	I	401	14/15	0.77	0.08	179,188,220,226	0

6.5 Other polymers [i](#)

There are no such residues in this entry.