



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2025 – 01:18 pm BST

PDB ID : 9I1Q / pdb\_00009i1q  
Title : HER3 receptor in complex with the Fab fragment of TK-hu A3 monoclonal antibody  
Authors : Bulfaro, G.; Savino, C.; Costanzo, A.; Fata, F.; Vallone, B.; Montemiglio, L.C.  
Deposited on : 2025-01-16  
Resolution : 2.80 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](mailto: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>.

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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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

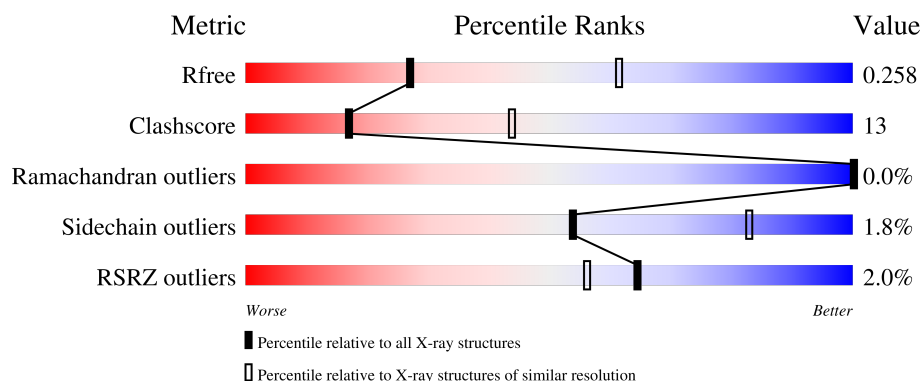
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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  $\geq 3$ , 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	632	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>7%</div> </div> </div>
1	B	632	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>24%</div> <div>7%</div> </div> </div>
1	C	632	<div> <div>3%</div> <div> <div></div> <div>61%</div> <div>22%</div> <div>16%</div> </div> </div>
1	D	632	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>21%</div> <div>6%</div> </div> </div>
2	E	220	<div> <div></div> <div> <div></div> <div>71%</div> <div>27%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	220	
2	G	220	
2	H	220	
3	I	223	
3	J	223	
3	K	223	
3	L	223	
4	M	3	
4	O	3	
5	N	4	
6	P	2	
6	Q	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	SCN	D	709	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 31872 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 Receptor tyrosine-protein kinase erbB-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	216	1	0
			4511	2791	815	846	59			
1	B	588	Total	C	N	O	S	202	0	0
			4522	2799	816	848	59			
1	C	531	Total	C	N	O	S	178	0	0
			4093	2540	735	767	51			
1	D	592	Total	C	N	O	S	198	0	0
			4554	2819	823	853	59			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	625	VAL	-	expression tag	UNP P21860
A	626	ASP	-	expression tag	UNP P21860
A	627	HIS	-	expression tag	UNP P21860
A	628	HIS	-	expression tag	UNP P21860
A	629	HIS	-	expression tag	UNP P21860
A	630	HIS	-	expression tag	UNP P21860
A	631	HIS	-	expression tag	UNP P21860
A	632	HIS	-	expression tag	UNP P21860
B	625	VAL	-	expression tag	UNP P21860
B	626	ASP	-	expression tag	UNP P21860
B	627	HIS	-	expression tag	UNP P21860
B	628	HIS	-	expression tag	UNP P21860
B	629	HIS	-	expression tag	UNP P21860
B	630	HIS	-	expression tag	UNP P21860
B	631	HIS	-	expression tag	UNP P21860
B	632	HIS	-	expression tag	UNP P21860
C	625	VAL	-	expression tag	UNP P21860
C	626	ASP	-	expression tag	UNP P21860
C	627	HIS	-	expression tag	UNP P21860
C	628	HIS	-	expression tag	UNP P21860
C	629	HIS	-	expression tag	UNP P21860

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Chain	Residue	Modelled	Actual	Comment	Reference
C	630	HIS	-	expression tag	UNP P21860
C	631	HIS	-	expression tag	UNP P21860
C	632	HIS	-	expression tag	UNP P21860
D	625	VAL	-	expression tag	UNP P21860
D	626	ASP	-	expression tag	UNP P21860
D	627	HIS	-	expression tag	UNP P21860
D	628	HIS	-	expression tag	UNP P21860
D	629	HIS	-	expression tag	UNP P21860
D	630	HIS	-	expression tag	UNP P21860
D	631	HIS	-	expression tag	UNP P21860
D	632	HIS	-	expression tag	UNP P21860

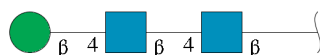
- Molecule 2 is a protein called light chain hA3-Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	220	Total	C	N	O	S	0	0	0
			1705	1072	288	339	6			
2	F	220	Total	C	N	O	S	0	0	0
			1705	1072	288	339	6			
2	G	220	Total	C	N	O	S	0	0	0
			1705	1072	288	339	6			
2	H	218	Total	C	N	O	S	0	0	0
			1690	1064	286	335	5			

- Molecule 3 is a protein called heavy chain hA3-Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	221	Total	C	N	O	S	0	0	0
			1679	1072	272	327	8			
3	J	223	Total	C	N	O	S	0	1	0
			1700	1084	277	331	8			
3	K	223	Total	C	N	O	S	0	0	0
			1692	1079	274	331	8			
3	L	219	Total	C	N	O	S	0	0	0
			1664	1062	269	326	7			

- Molecule 4 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.



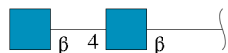
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	O	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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	N	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 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
6	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



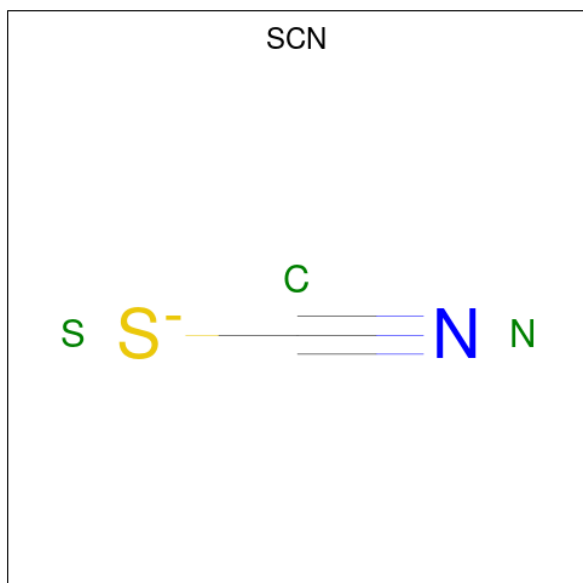
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 8 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	S	0	0
			3	1	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total 3	C 1	N 1	S 1	0	0
8	D	1	Total 3	C 1	N 1	S 1	0	0
8	D	1	Total 3	C 1	N 1	S 1	0	0
8	H	1	Total 3	C 1	N 1	S 1	0	0
8	H	1	Total 3	C 1	N 1	S 1	0	0
8	I	1	Total 3	C 1	N 1	S 1	0	0
8	I	1	Total 3	C 1	N 1	S 1	0	0
8	L	1	Total 3	C 1	N 1	S 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	12	Total 12	O 12	0	0
9	B	10	Total 10	O 10	0	0
9	C	6	Total 6	O 6	0	0
9	D	24	Total 24	O 24	0	0
9	E	4	Total 4	O 4	0	0
9	F	15	Total 15	O 15	0	0
9	G	2	Total 2	O 2	0	0
9	H	6	Total 6	O 6	0	0
9	I	9	Total 9	O 9	0	0
9	J	7	Total 7	O 7	0	0
9	K	4	Total 4	O 4	0	0

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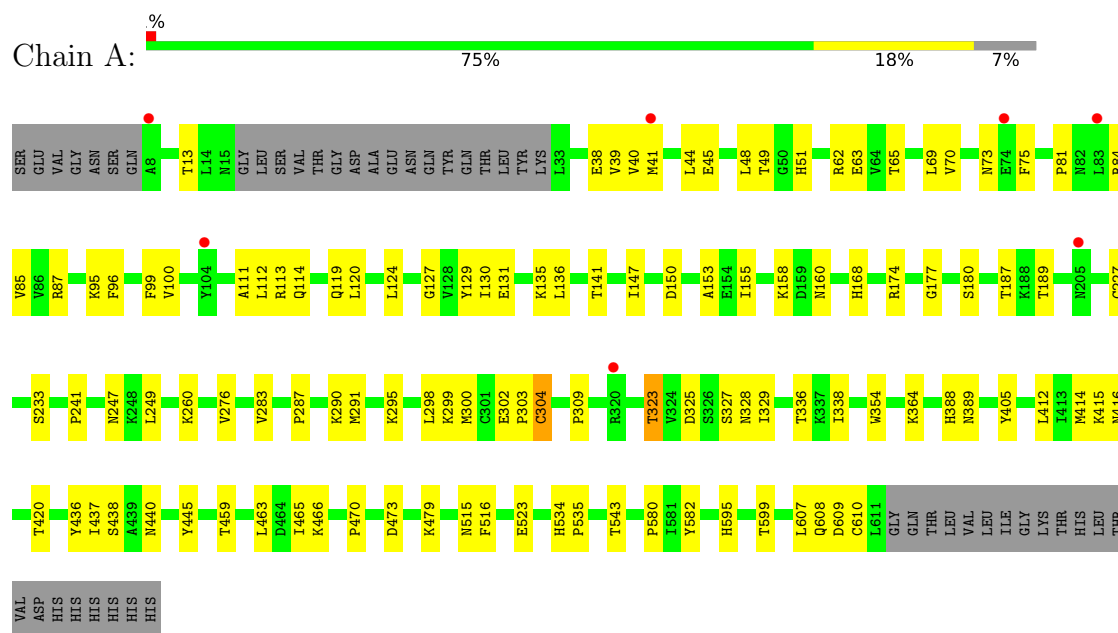
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	6	Total	O	0	0
			6	6		

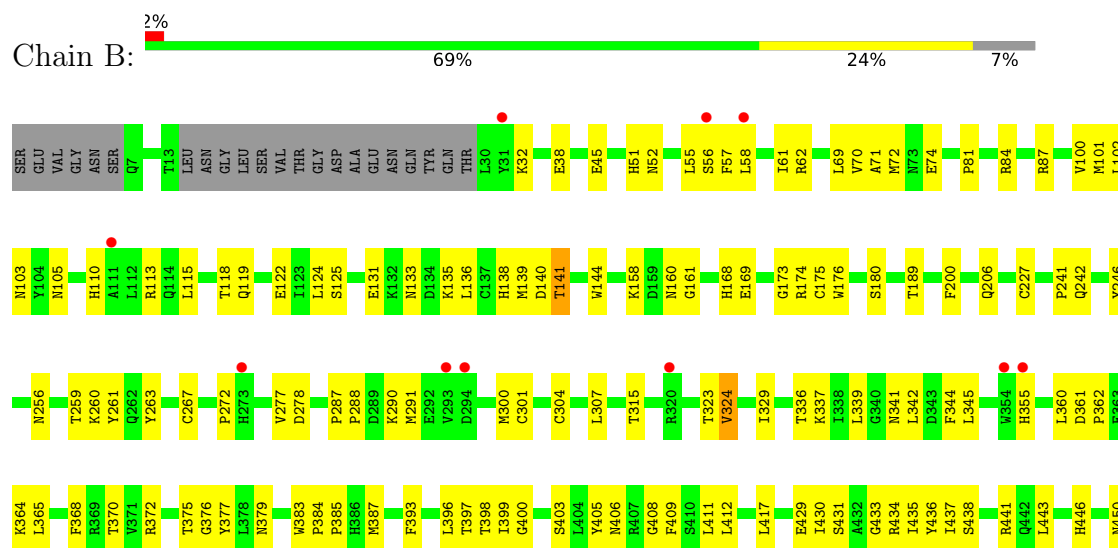
### 3 Residue-property plots [i](#)

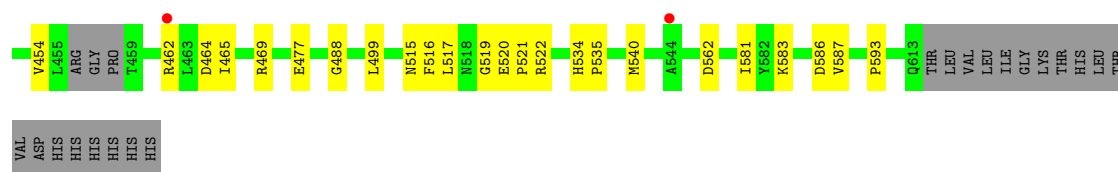
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Receptor tyrosine-protein kinase erbB-3

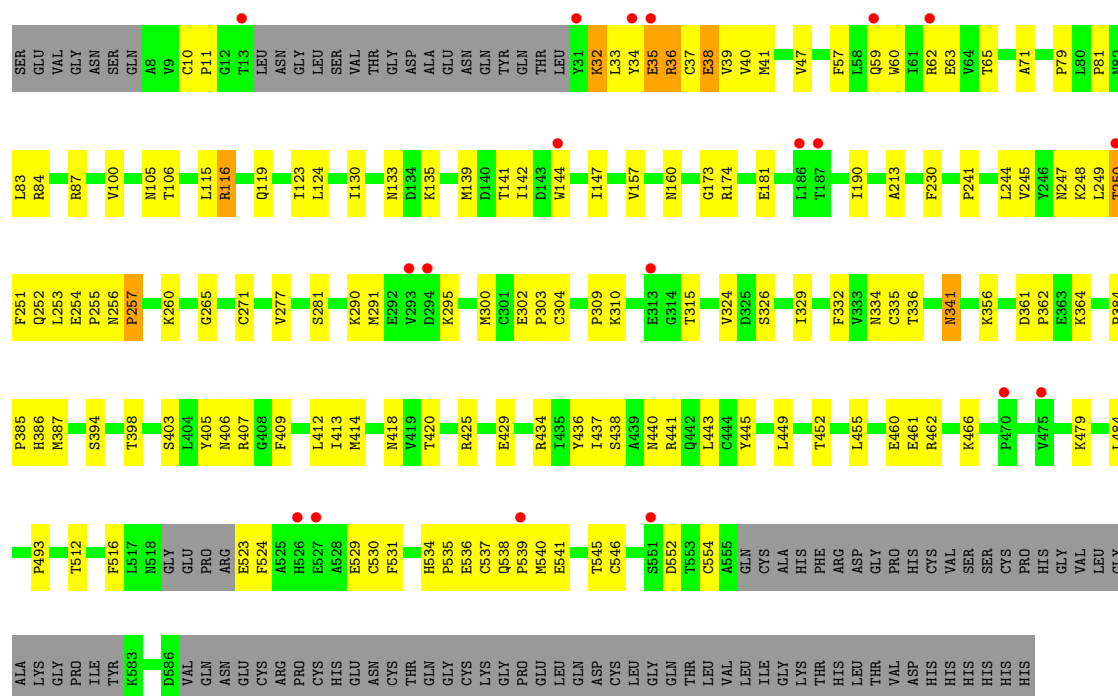


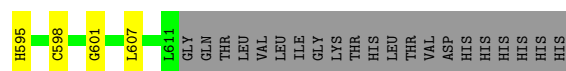
#### • Molecule 1: Receptor tyrosine-protein kinase erbB-3



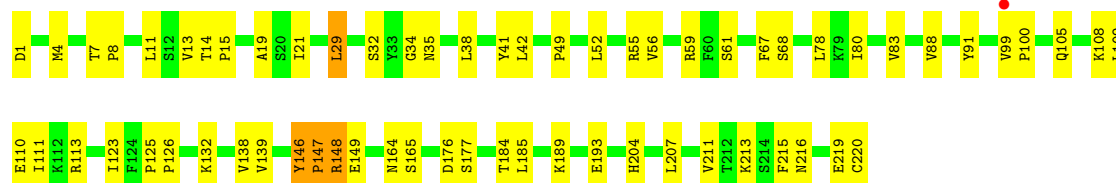


• Molecule 1: Receptor tyrosine-protein kinase erbB-3

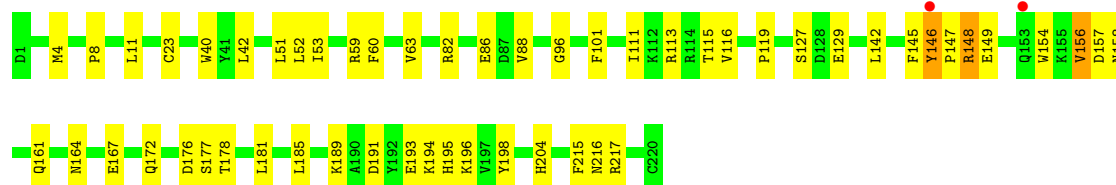
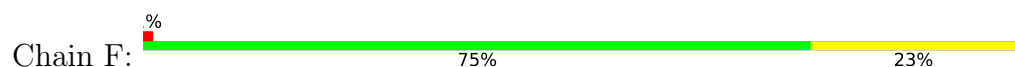




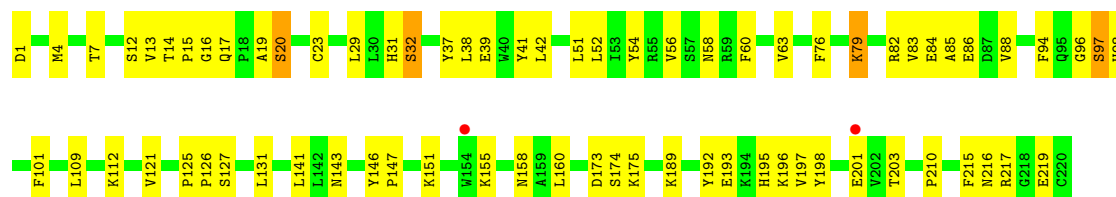
- Molecule 2: light chain hA3-Fab



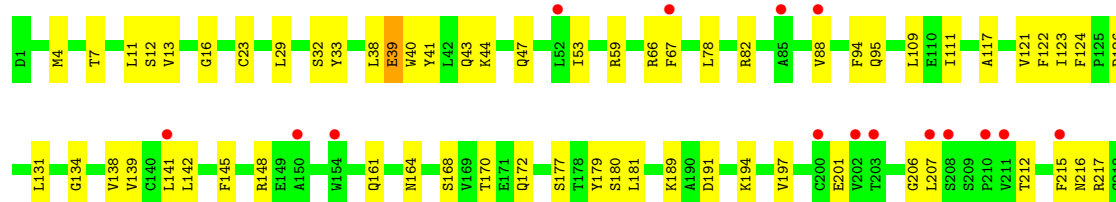
- Molecule 2: light chain hA3-Fab



- Molecule 2: light chain hA3-Fab

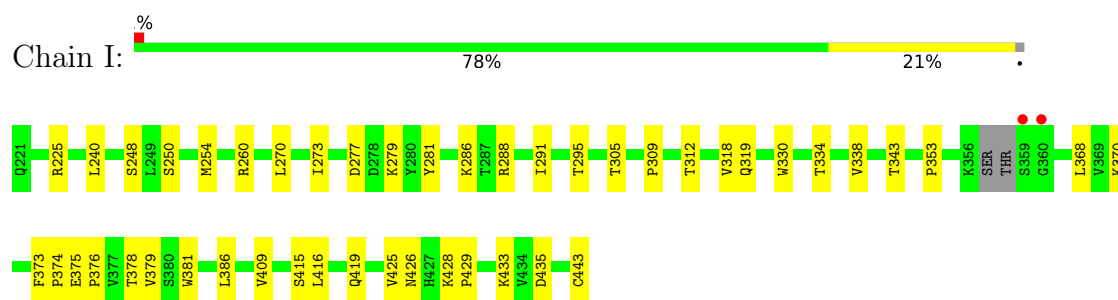


- Molecule 2: light chain hA3-Fab

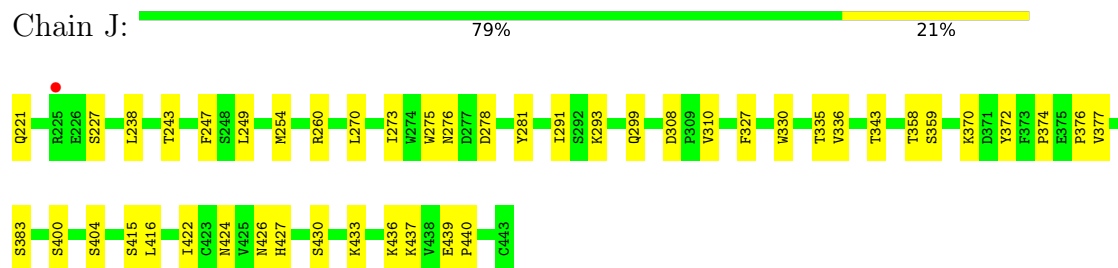


GLU  
CYS

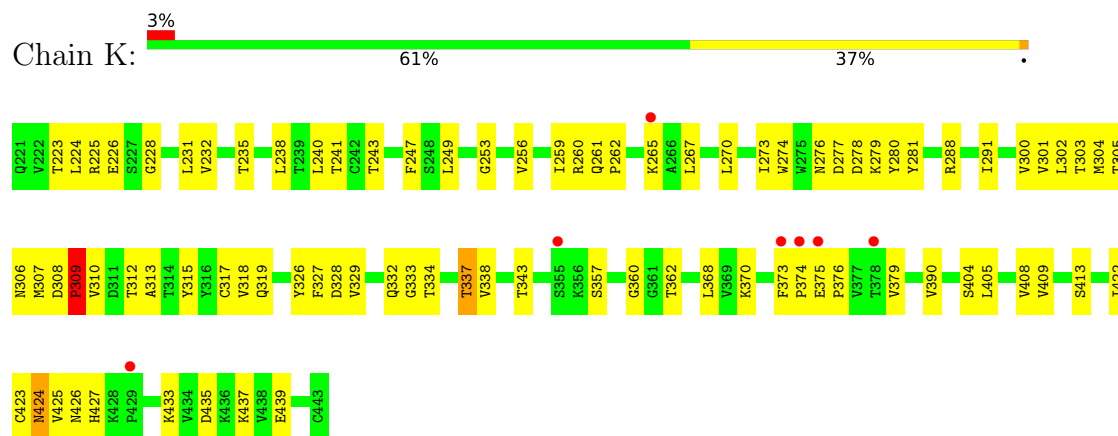
- Molecule 3: heavy chain hA3-Fab



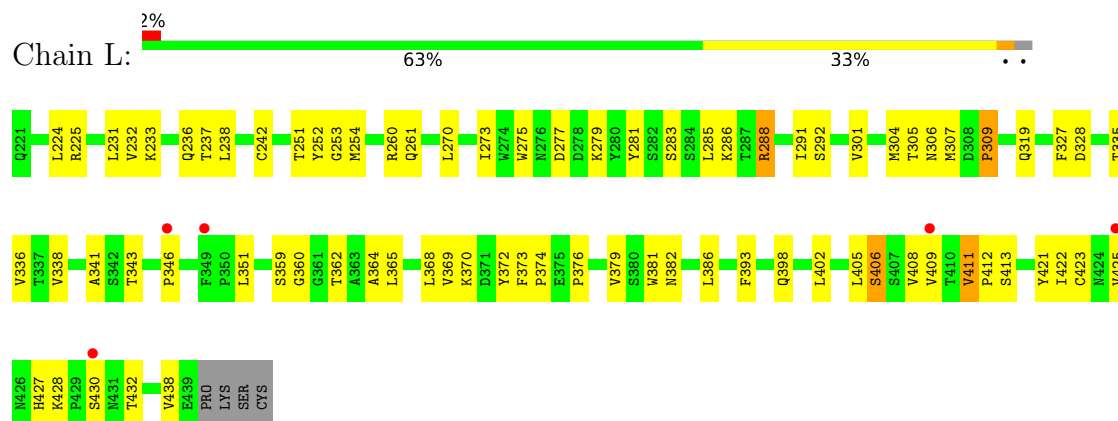
- Molecule 3: heavy chain hA3-Fab



- Molecule 3: heavy chain hA3-Fab



- Molecule 3: heavy chain hA3-Fab



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

Chain M:  100%

MAG1  
MAG2  
BMA3

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

Chain O:  100%

MAG1  
MAG2  
BMA3

- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  50% 50%

MAG1  
MAG2  
BMA3  
MAN4

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

Chain P:  50% 50%

MAG1  
MAG2

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

Chain Q:  100%

MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.03Å 98.81Å 270.38Å 90.00° 99.21° 90.00°	Depositor
Resolution (Å)	49.00 – 2.80 49.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	64.6 (49.00-2.80) 64.6 (49.00-2.80)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 2.55Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.209 , 0.263 0.208 , 0.258	Depositor DCC
$R_{free}$ test set	4143 reflections (2.49%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.0	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 30.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	31872	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MAN, NAG, SCN, 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	0.23	0/4623	0.47	0/6272
1	B	0.22	0/4630	0.46	0/6279
1	C	0.33	0/4189	0.62	6/5680 (0.1%)
1	D	0.22	0/4664	0.46	1/6328 (0.0%)
2	E	0.39	0/1744	0.68	2/2366 (0.1%)
2	F	0.36	0/1744	0.65	1/2366 (0.0%)
2	G	0.35	0/1744	0.67	1/2366 (0.0%)
2	H	0.53	0/1729	0.77	0/2346
3	I	0.24	0/1724	0.58	0/2360
3	J	0.30	0/1749	0.63	2/2395 (0.1%)
3	K	0.43	0/1738	0.74	0/2381
3	L	0.45	0/1709	0.77	3/2342 (0.1%)
All	All	0.32	0/31987	0.59	16/43481 (0.0%)

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
1	C	0	2
1	D	0	1
2	E	0	1
2	F	0	1
2	H	0	2
All	All	0	7

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	416	LEU	N-CA-C	-9.54	101.15	113.17
1	C	36	ARG	N-CA-C	-7.34	97.71	109.39
1	C	34	TYR	N-CA-C	-6.76	103.53	112.72
1	C	257	PRO	N-CA-C	-6.15	104.59	113.75
1	C	250	THR	N-CA-C	-5.92	104.20	113.02

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	116	ARG	Sidechain
1	C	36	ARG	Sidechain
1	D	469	ARG	Sidechain
2	E	148	ARG	Sidechain
2	F	148	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4511	0	4275	80	0
1	B	4522	0	4286	107	0
1	C	4093	0	3890	115	0
1	D	4554	0	4322	88	0
2	E	1705	0	1660	46	0
2	F	1705	0	1660	47	0
2	G	1705	0	1660	56	0
2	H	1690	0	1650	46	0
3	I	1679	0	1654	28	0
3	J	1700	0	1680	32	0
3	K	1692	0	1667	70	0
3	L	1664	0	1638	62	0
4	M	39	0	34	0	0
4	O	39	0	34	0	0
5	N	50	0	43	1	0
6	P	28	0	25	0	0
6	Q	28	0	25	0	0
7	A	84	0	78	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	84	0	78	0	0
7	C	70	0	65	1	0
7	D	98	0	91	2	0
8	B	3	0	0	0	0
8	C	3	0	0	0	0
8	D	6	0	0	0	0
8	H	6	0	0	0	0
8	I	6	0	0	0	0
8	L	3	0	0	0	0
9	A	12	0	0	0	0
9	B	10	0	0	0	0
9	C	6	0	0	0	0
9	D	24	0	0	0	0
9	E	4	0	0	0	0
9	F	15	0	0	0	0
9	G	2	0	0	0	0
9	H	6	0	0	0	0
9	I	9	0	0	1	0
9	J	7	0	0	1	0
9	K	4	0	0	0	0
9	L	6	0	0	0	0
All	All	31872	0	30515	757	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 13.

The worst 5 of 757 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:249:LEU:CD2	3:J:293:LYS:HE3	1.86	1.06
3:J:249:LEU:HD22	3:J:293:LYS:HE3	1.40	1.01
2:G:155:LYS:HE3	2:G:158:ASN:HA	1.40	1.00
1:A:412:LEU:HD12	1:A:436:TYR:HB3	1.50	0.93
3:I:312:THR:HG22	3:I:338:VAL:H	1.33	0.93

There are no symmetry-related clashes.

## 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	584/632 (92%)	543 (93%)	41 (7%)	0	100	100
1	B	582/632 (92%)	546 (94%)	36 (6%)	0	100	100
1	C	523/632 (83%)	469 (90%)	54 (10%)	0	100	100
1	D	588/632 (93%)	553 (94%)	34 (6%)	1 (0%)	44	73
2	E	218/220 (99%)	208 (95%)	10 (5%)	0	100	100
2	F	218/220 (99%)	207 (95%)	11 (5%)	0	100	100
2	G	218/220 (99%)	214 (98%)	4 (2%)	0	100	100
2	H	216/220 (98%)	206 (95%)	10 (5%)	0	100	100
3	I	217/223 (97%)	206 (95%)	11 (5%)	0	100	100
3	J	222/223 (100%)	209 (94%)	13 (6%)	0	100	100
3	K	221/223 (99%)	208 (94%)	12 (5%)	1 (0%)	25	56
3	L	217/223 (97%)	208 (96%)	9 (4%)	0	100	100
All	All	4024/4300 (94%)	3777 (94%)	245 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	309	PRO
1	D	353	PRO

### 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	509/548 (93%)	503 (99%)	6 (1%)	67	89
1	B	510/548 (93%)	502 (98%)	8 (2%)	58	85
1	C	461/548 (84%)	453 (98%)	8 (2%)	56	84
1	D	514/548 (94%)	504 (98%)	10 (2%)	52	82
2	E	196/196 (100%)	192 (98%)	4 (2%)	50	81
2	F	196/196 (100%)	195 (100%)	1 (0%)	86	95
2	G	196/196 (100%)	190 (97%)	6 (3%)	35	69
2	H	194/196 (99%)	190 (98%)	4 (2%)	48	80
3	I	194/196 (99%)	191 (98%)	3 (2%)	60	86
3	J	197/196 (100%)	193 (98%)	4 (2%)	50	81
3	K	196/196 (100%)	192 (98%)	4 (2%)	50	81
3	L	192/196 (98%)	186 (97%)	6 (3%)	35	69
All	All	3555/3760 (94%)	3491 (98%)	64 (2%)	54	83

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	K	424	ASN
3	L	319	GLN
1	D	142	ILE
1	D	98	ILE
3	L	362	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
3	J	424	ASN
3	J	426	ASN
1	D	379	ASN
1	D	114	GLN
3	K	261	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 ⓘ

14 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	$\# Z  > 2$
4	NAG	M	1	1,4	14,14,15	0.40	0	17,19,21	0.55	0
4	NAG	M	2	4	14,14,15	0.39	0	17,19,21	0.67	0
4	BMA	M	3	4	11,11,12	0.34	0	15,15,17	0.43	0
5	NAG	N	1	5,1	14,14,15	0.41	0	17,19,21	0.62	0
5	NAG	N	2	5	14,14,15	0.37	0	17,19,21	0.62	0
5	BMA	N	3	5	11,11,12	0.38	0	15,15,17	0.54	0
5	MAN	N	4	5	11,11,12	0.33	0	15,15,17	0.62	0
4	NAG	O	1	1,4	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	O	2	4	14,14,15	0.31	0	17,19,21	0.55	0
4	BMA	O	3	4	11,11,12	0.49	0	15,15,17	0.76	0
6	NAG	P	1	6,1	14,14,15	0.39	0	17,19,21	0.53	0
6	NAG	P	2	6	14,14,15	0.68	0	17,19,21	1.54	2 (11%)
6	NAG	Q	1	6,1	14,14,15	0.37	0	17,19,21	0.54	0
6	NAG	Q	2	6	14,14,15	0.22	0	17,19,21	0.42	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
4	NAG	M	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	1/6/23/26	0/1/1/1
4	BMA	M	3	4	-	0/2/19/22	0/1/1/1
5	NAG	N	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	N	2	5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	N	3	5	-	2/2/19/22	0/1/1/1
5	MAN	N	4	5	-	0/2/19/22	0/1/1/1
4	NAG	O	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	BMA	O	3	4	-	0/2/19/22	0/1/1/1
6	NAG	P	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	P	2	6	-	1/6/23/26	0/1/1/1
6	NAG	Q	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	0/6/23/26	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(°)	Ideal(°)
6	P	2	NAG	C1-O5-C5	4.99	118.95	112.19
6	P	2	NAG	C2-N2-C7	2.83	126.93	122.90

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	P	2	NAG	C3-C2-N2-C7
5	N	3	BMA	C4-C5-C6-O6
4	M	1	NAG	C8-C7-N2-C2
4	M	1	NAG	O7-C7-N2-C2
5	N	3	BMA	O5-C5-C6-O6

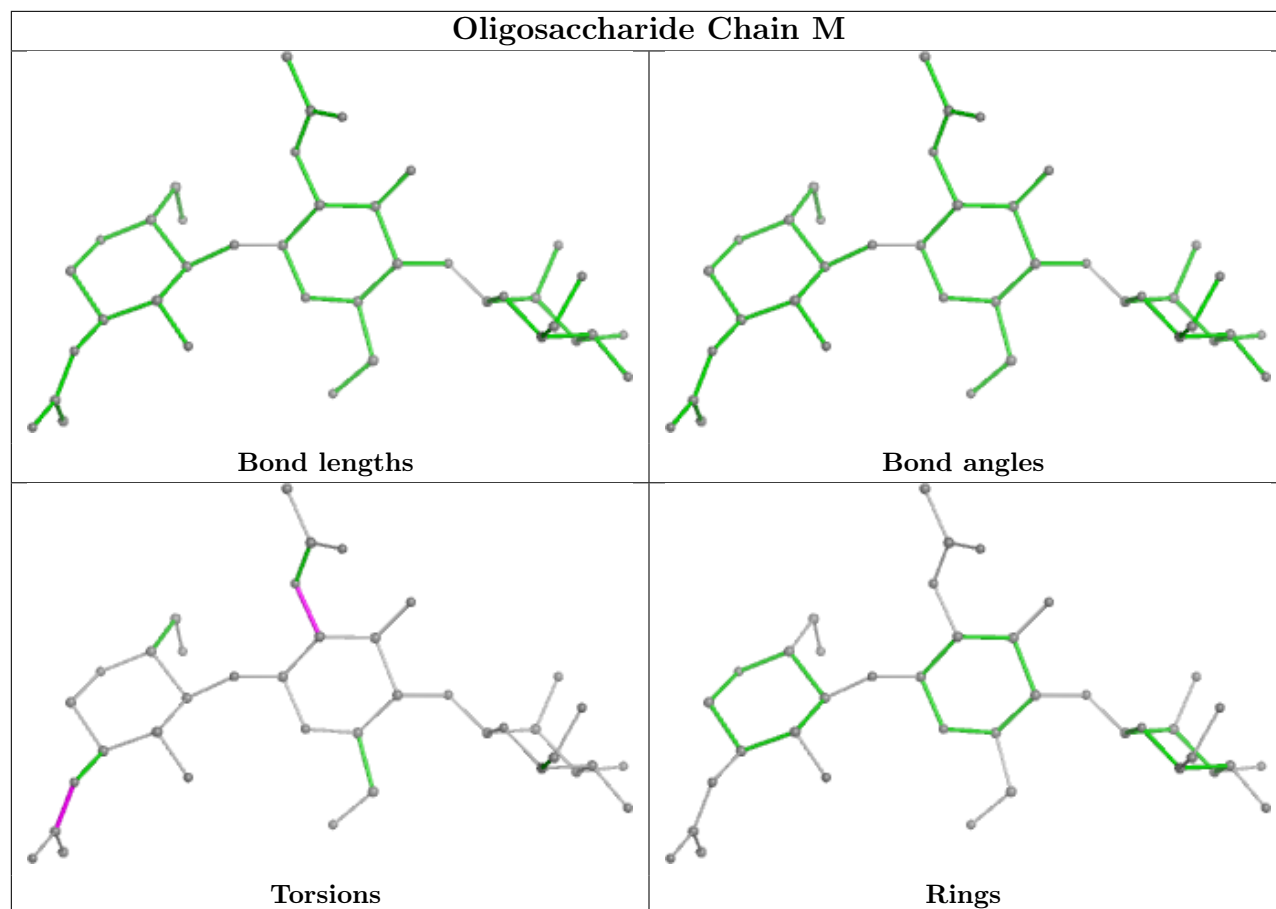
There are no ring outliers.

2 monomers are involved in 1 short contact:

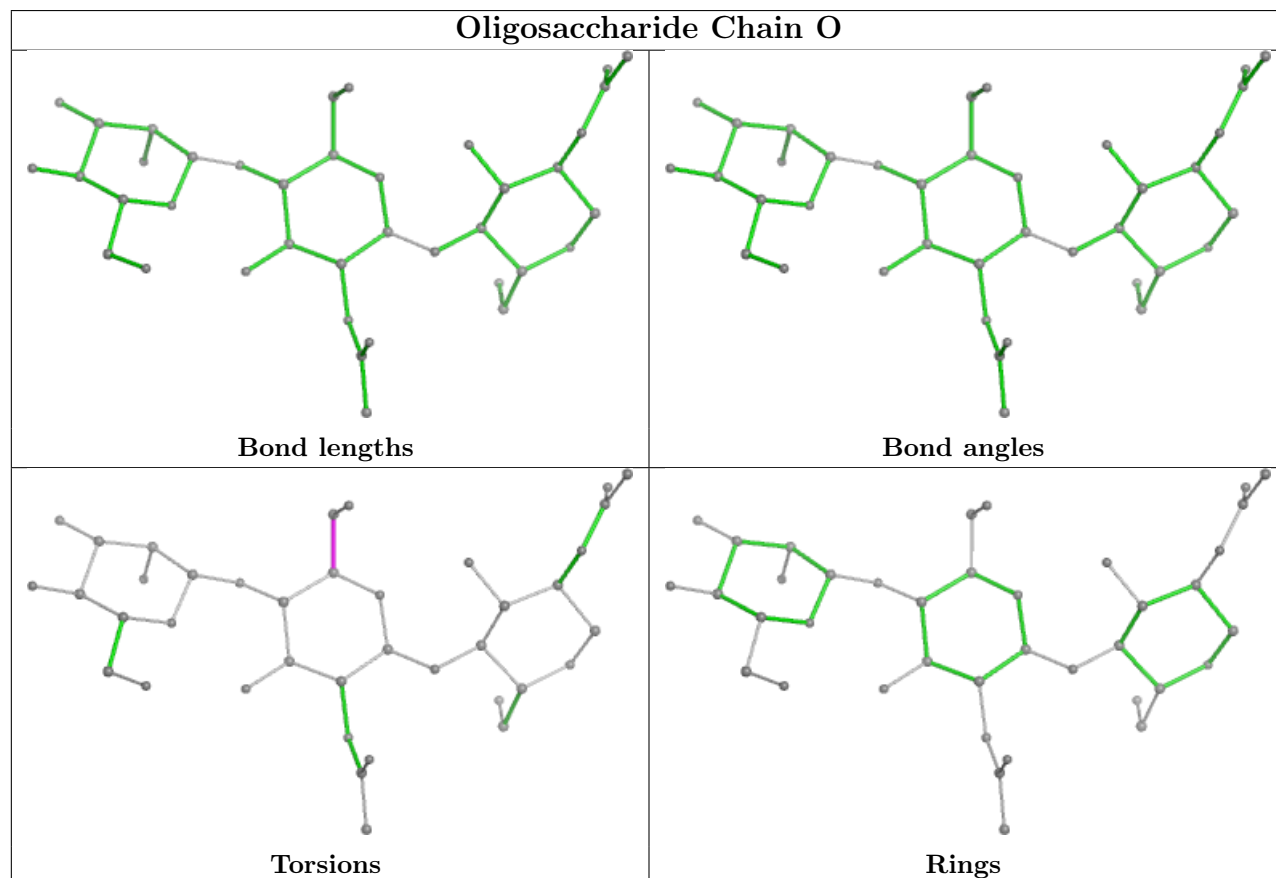
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	N	2	NAG	1	0
5	N	4	MAN	1	0

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

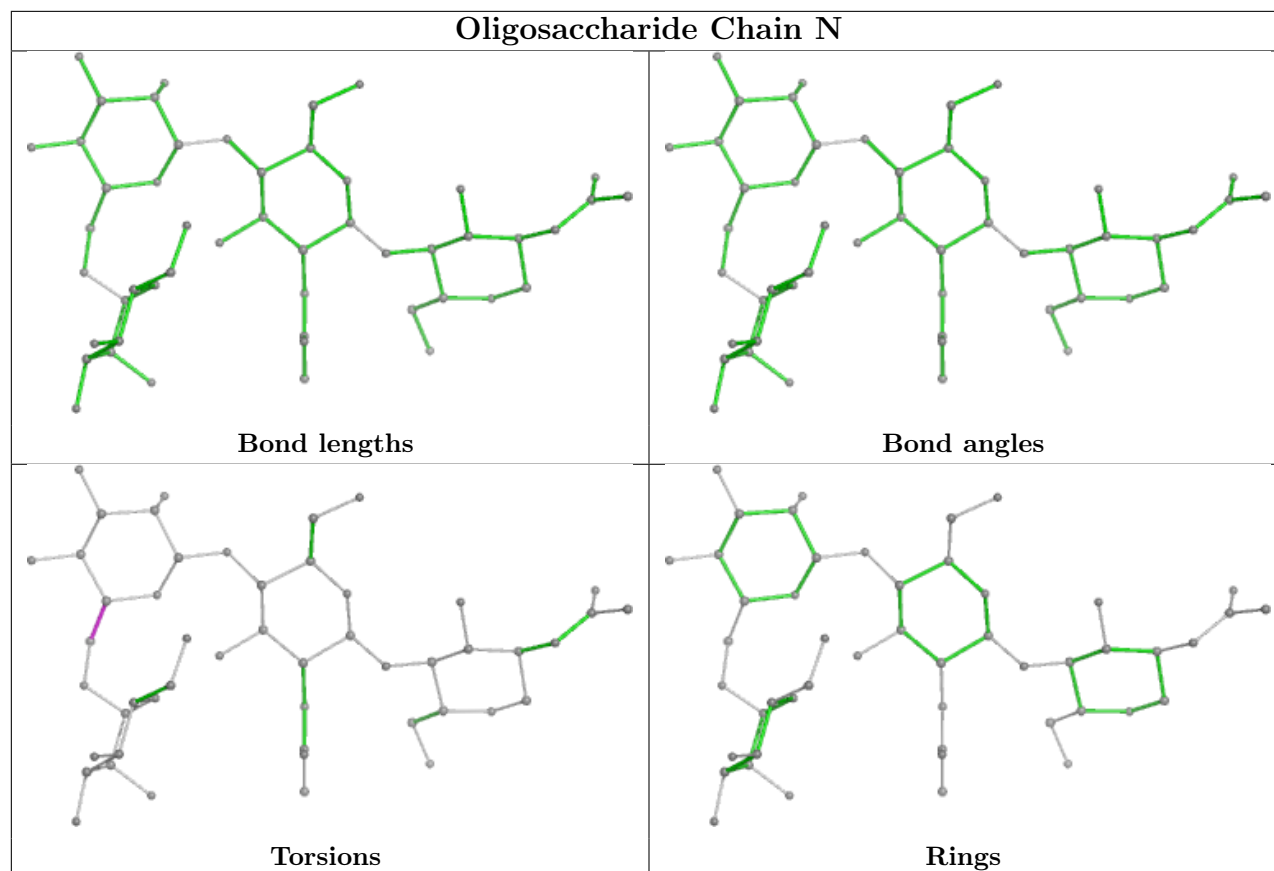
## Oligosaccharide Chain M

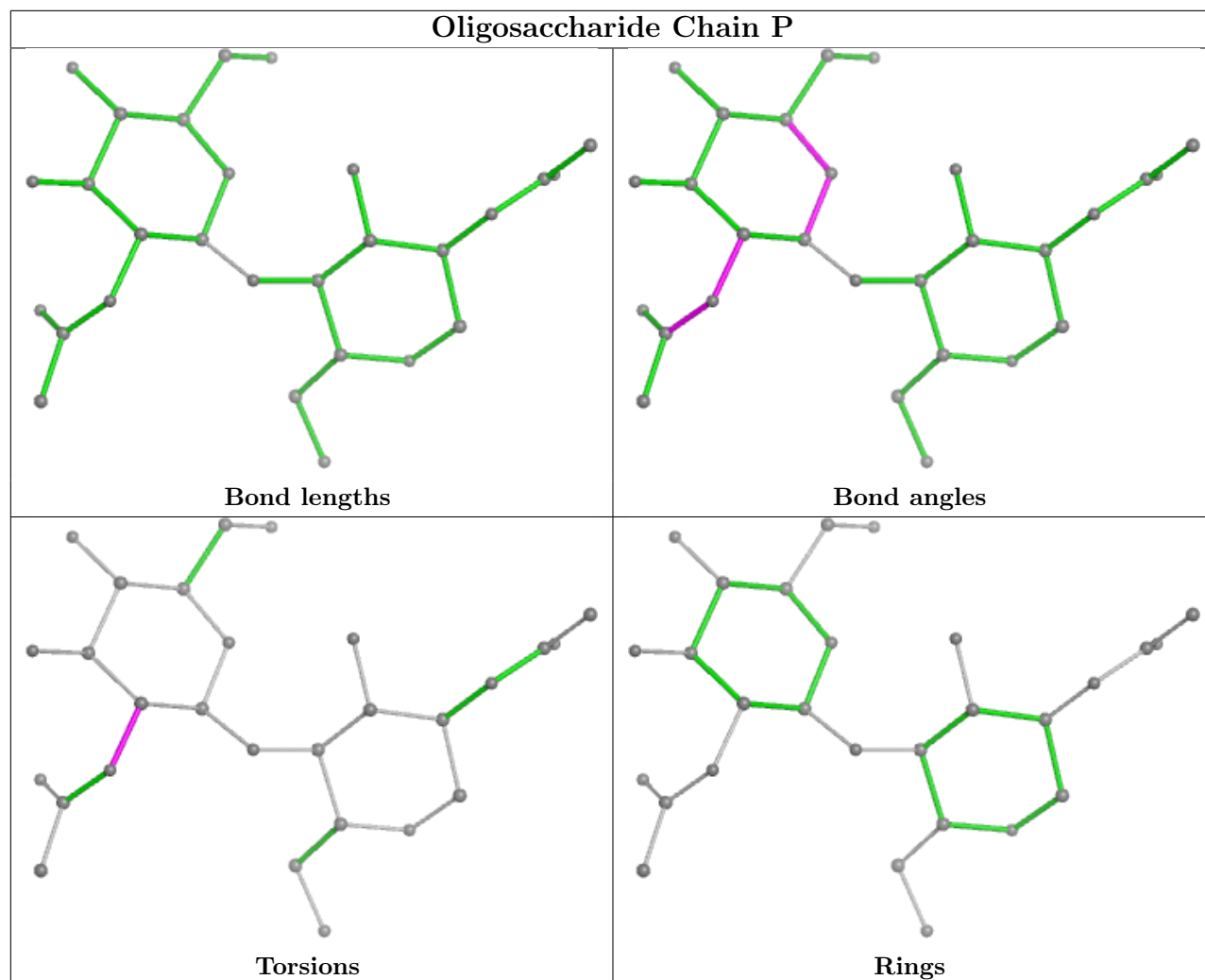


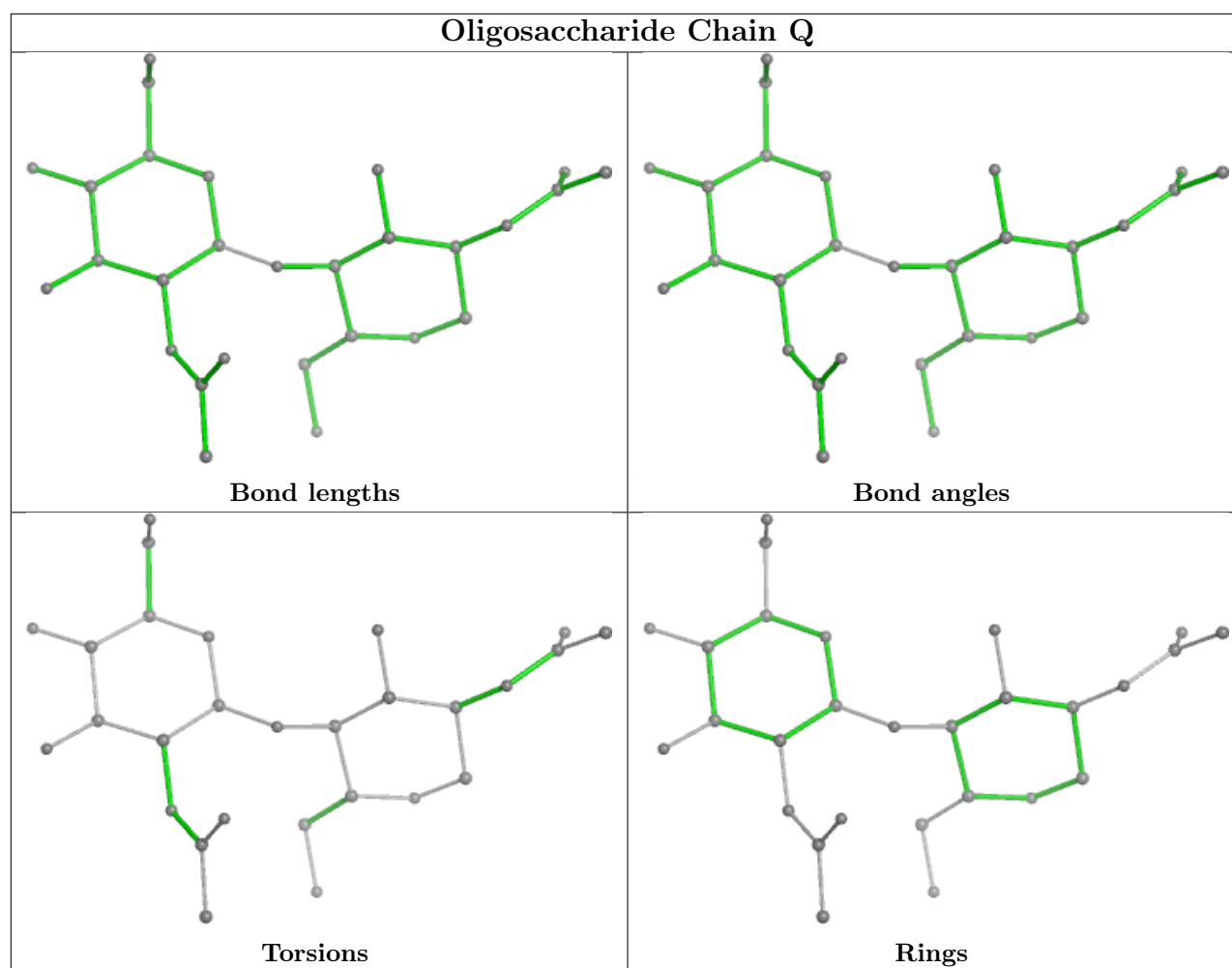
## Oligosaccharide Chain O











## 5.6 Ligand geometry [i](#)

33 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	$\# Z  > 2$
8	SCN	D	708	-	1,2,2	0.28	0	0,1,1	-	-
8	SCN	L	501	-	1,2,2	0.30	0	0,1,1	-	-
7	NAG	A	701	1	14,14,15	0.20	0	17,19,21	0.42	0
7	NAG	A	703	1	14,14,15	0.29	0	17,19,21	0.57	0
7	NAG	B	703	1	14,14,15	0.33	0	17,19,21	0.67	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	SCN	I	502	-	1,2,2	0.35	0	0,1,1	-	-
7	NAG	B	702	1	14,14,15	0.18	0	17,19,21	0.32	0
7	NAG	C	701	1	14,14,15	0.27	0	17,19,21	0.38	0
7	NAG	B	701	1	14,14,15	0.28	0	17,19,21	0.52	0
7	NAG	A	705	1	14,14,15	0.26	0	17,19,21	0.46	0
7	NAG	B	705	1	14,14,15	0.31	0	17,19,21	0.62	1 (5%)
7	NAG	A	702	1	14,14,15	0.27	0	17,19,21	0.51	0
7	NAG	B	706	1	14,14,15	0.19	0	17,19,21	0.43	0
7	NAG	D	707	1	14,14,15	0.47	0	17,19,21	0.64	0
7	NAG	C	703	1	14,14,15	0.19	0	17,19,21	0.43	0
7	NAG	D	701	1	14,14,15	0.48	0	17,19,21	0.55	0
8	SCN	B	707	-	1,2,2	0.14	0	0,1,1	-	-
8	SCN	H	301	-	1,2,2	0.24	0	0,1,1	-	-
8	SCN	I	501	-	1,2,2	0.13	0	0,1,1	-	-
7	NAG	A	704	1	14,14,15	0.24	0	17,19,21	0.54	0
7	NAG	C	705	1	14,14,15	0.23	0	17,19,21	0.42	0
7	NAG	D	703	1	14,14,15	0.24	0	17,19,21	0.61	1 (5%)
7	NAG	D	704	1	14,14,15	0.27	0	17,19,21	0.38	0
8	SCN	D	709	-	1,2,2	0.13	0	0,1,1	-	-
7	NAG	C	702	1	14,14,15	0.21	0	17,19,21	0.40	0
8	SCN	H	302	-	1,2,2	0.41	0	0,1,1	-	-
7	NAG	B	704	1	14,14,15	0.23	0	17,19,21	0.46	0
7	NAG	D	702	1	14,14,15	0.26	0	17,19,21	0.39	0
7	NAG	D	705	1	14,14,15	0.20	0	17,19,21	0.43	0
8	SCN	C	706	-	1,2,2	0.11	0	0,1,1	-	-
7	NAG	D	706	1	14,14,15	0.30	0	17,19,21	0.39	0
7	NAG	A	706	1	14,14,15	0.52	0	17,19,21	0.59	0
7	NAG	C	704	1	14,14,15	0.43	0	17,19,21	0.55	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
7	NAG	A	701	1	-	3/6/23/26	0/1/1/1
7	NAG	A	703	1	-	0/6/23/26	0/1/1/1
7	NAG	B	703	1	-	0/6/23/26	0/1/1/1
7	NAG	B	702	1	-	1/6/23/26	0/1/1/1
7	NAG	C	701	1	-	0/6/23/26	0/1/1/1
7	NAG	B	701	1	-	2/6/23/26	0/1/1/1
7	NAG	A	705	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	705	1	-	3/6/23/26	0/1/1/1
7	NAG	A	702	1	-	0/6/23/26	0/1/1/1
7	NAG	B	706	1	-	0/6/23/26	0/1/1/1
7	NAG	D	707	1	-	1/6/23/26	0/1/1/1
7	NAG	C	703	1	-	3/6/23/26	0/1/1/1
7	NAG	D	701	1	-	0/6/23/26	0/1/1/1
7	NAG	A	704	1	-	1/6/23/26	0/1/1/1
7	NAG	C	705	1	-	1/6/23/26	0/1/1/1
7	NAG	D	703	1	-	0/6/23/26	0/1/1/1
7	NAG	D	704	1	-	1/6/23/26	0/1/1/1
7	NAG	C	702	1	-	0/6/23/26	0/1/1/1
7	NAG	B	704	1	-	2/6/23/26	0/1/1/1
7	NAG	D	702	1	-	0/6/23/26	0/1/1/1
7	NAG	D	705	1	-	2/6/23/26	0/1/1/1
7	NAG	D	706	1	-	2/6/23/26	0/1/1/1
7	NAG	A	706	1	-	2/6/23/26	0/1/1/1
7	NAG	C	704	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	703	NAG	C1-O5-C5	2.37	115.40	112.19
7	D	703	NAG	C1-O5-C5	2.13	115.08	112.19
7	B	705	NAG	C1-O5-C5	2.11	115.05	112.19

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	701	NAG	C8-C7-N2-C2
7	A	701	NAG	O7-C7-N2-C2
7	A	706	NAG	C8-C7-N2-C2
7	A	706	NAG	O7-C7-N2-C2
7	B	705	NAG	C8-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	701	NAG	1	0
7	D	707	NAG	1	0
7	D	701	NAG	1	0
7	C	704	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	587/632 (92%)	-0.20	7 (1%) 76 69	22, 66, 136, 180	69 (11%)
1	B	588/632 (93%)	-0.25	12 (2%) 64 56	16, 62, 113, 172	65 (11%)
1	C	531/632 (84%)	0.11	19 (3%) 46 38	29, 84, 144, 214	57 (10%)
1	D	592/632 (93%)	-0.18	9 (1%) 71 64	22, 64, 111, 157	68 (11%)
2	E	220/220 (100%)	-0.38	1 (0%) 87 83	22, 53, 95, 115	0
2	F	220/220 (100%)	-0.56	2 (0%) 81 75	14, 48, 93, 124	1 (0%)
2	G	220/220 (100%)	-0.26	2 (0%) 81 75	37, 69, 104, 145	0
2	H	218/220 (99%)	0.49	15 (6%) 24 18	58, 96, 142, 170	0
3	I	221/223 (99%)	-0.59	2 (0%) 81 75	15, 43, 91, 153	0
3	J	223/223 (100%)	-0.58	1 (0%) 89 85	19, 41, 88, 126	1 (0%)
3	K	223/223 (100%)	0.13	7 (3%) 51 43	46, 81, 128, 202	0
3	L	219/223 (98%)	0.06	5 (2%) 61 52	36, 68, 145, 197	0
All	All	4062/4300 (94%)	-0.17	82 (2%) 64 56	14, 66, 128, 214	261 (6%)

The worst 5 of 82 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	31	TYR	6.9
2	H	202	VAL	4.7
1	B	273	HIS	4.6
1	C	13	THR	4.6
1	C	294	ASP	4.0

### 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, 95<sup>th</sup> 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.

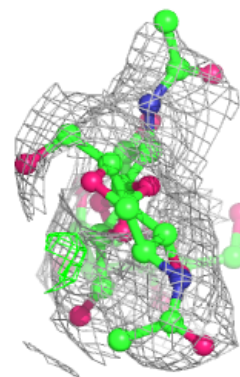
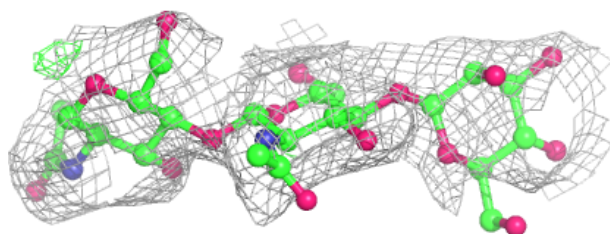
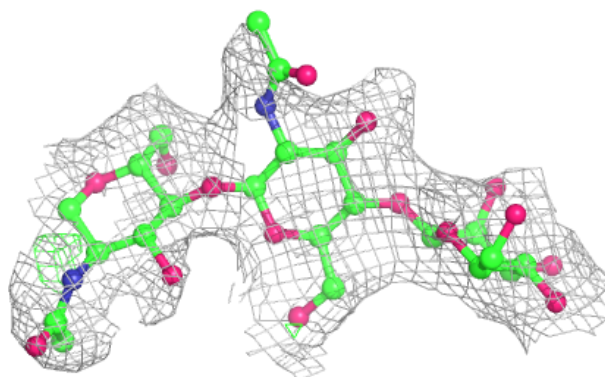
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	BMA	O	3	11/12	0.54	0.10	93,110,124,129	0
4	NAG	M	2	14/15	0.56	0.12	79,107,118,128	0
5	BMA	N	3	11/12	0.57	0.12	91,116,127,129	0
4	BMA	M	3	11/12	0.58	0.11	107,123,130,135	0
5	MAN	N	4	11/12	0.61	0.10	103,123,132,137	0
6	NAG	Q	2	14/15	0.73	0.10	71,92,102,108	0
6	NAG	P	2	14/15	0.74	0.13	93,115,127,132	0
6	NAG	P	1	14/15	0.78	0.09	83,108,117,119	0
5	NAG	N	2	14/15	0.79	0.10	84,95,117,120	0
4	NAG	M	1	14/15	0.83	0.10	57,79,107,116	0
6	NAG	Q	1	14/15	0.85	0.09	53,77,86,89	0
4	NAG	O	1	14/15	0.85	0.10	51,64,81,83	0
4	NAG	O	2	14/15	0.86	0.09	76,90,102,105	0
5	NAG	N	1	14/15	0.95	0.07	43,53,69,78	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.

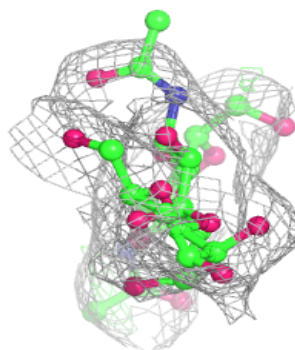
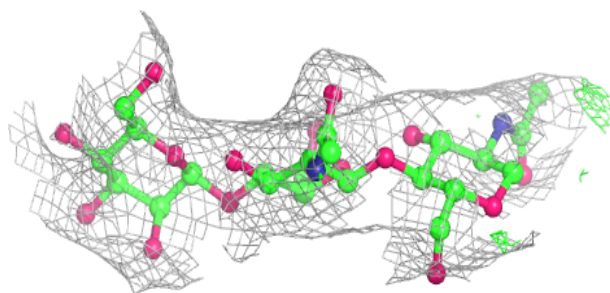
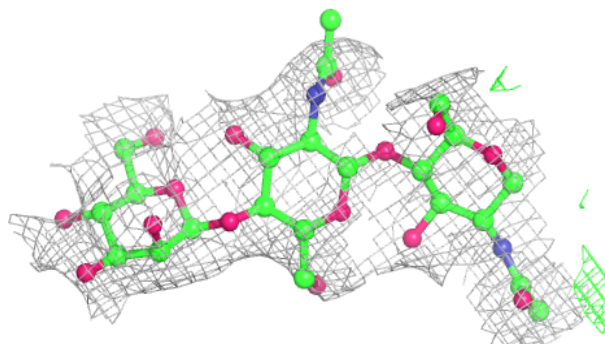


**Electron density around Chain M:**

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

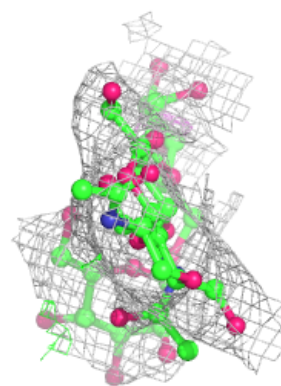
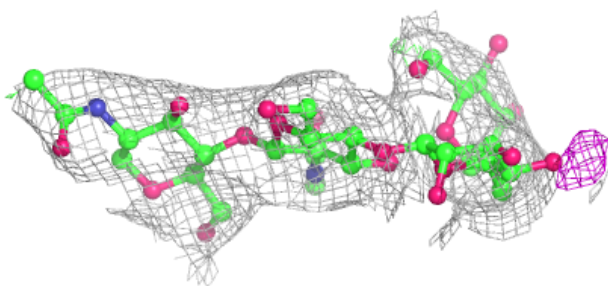
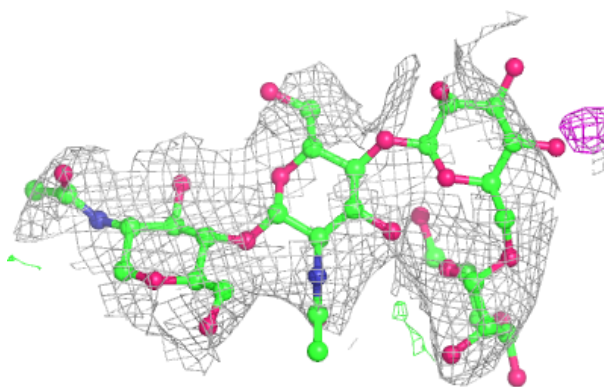
**Electron density around Chain O:**

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

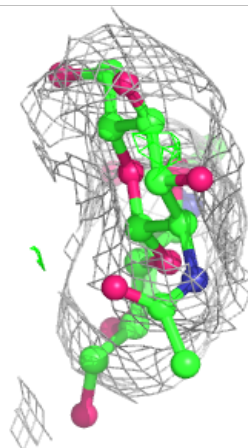
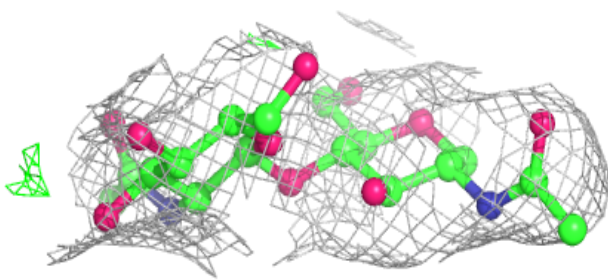
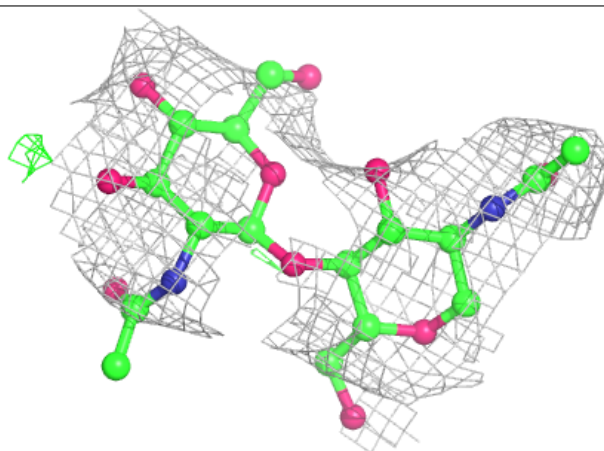


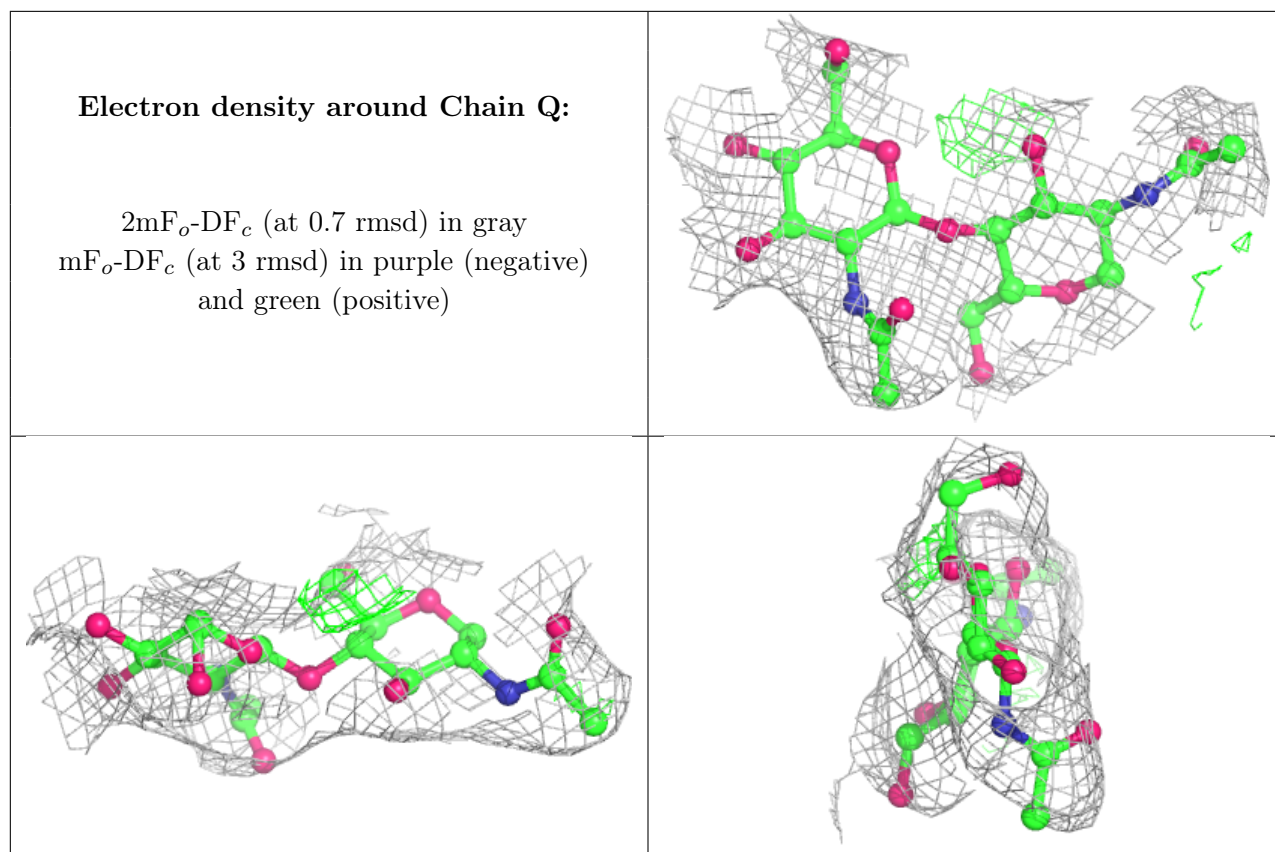
**Electron density around Chain N:**

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

**Electron density around Chain P:**

$2mF_o-DF_c$  (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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
7	NAG	B	705	14/15	0.43	0.12	92,119,131,140	0
7	NAG	A	706	14/15	0.49	0.18	74,101,131,135	0
7	NAG	A	705	14/15	0.54	0.13	116,127,137,141	0
7	NAG	C	703	14/15	0.55	0.10	67,109,128,133	0
8	SCN	B	707	3/3	0.58	0.12	65,65,74,130	0
8	SCN	C	706	3/3	0.59	0.17	77,77,96,109	0
8	SCN	L	501	3/3	0.61	0.15	93,93,99,107	0
8	SCN	D	709	3/3	0.62	0.42	58,58,70,87	0
7	NAG	B	702	14/15	0.65	0.14	89,104,114,123	0
7	NAG	D	706	14/15	0.65	0.17	52,101,117,127	0
8	SCN	I	501	3/3	0.67	0.11	48,48,72,100	0
7	NAG	D	705	14/15	0.67	0.10	106,123,138,140	0
8	SCN	I	502	3/3	0.68	0.16	46,46,74,79	0
7	NAG	B	706	14/15	0.69	0.10	74,121,134,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	NAG	D	701	14/15	0.71	0.12	64,88,103,105	0
7	NAG	D	707	14/15	0.72	0.14	83,101,117,129	0
7	NAG	D	704	14/15	0.73	0.10	76,96,107,114	0
7	NAG	D	703	14/15	0.73	0.10	58,90,103,114	0
7	NAG	C	704	14/15	0.74	0.10	84,98,109,115	0
7	NAG	B	703	14/15	0.76	0.11	66,87,97,97	0
8	SCN	H	301	3/3	0.77	0.07	63,63,83,108	0
7	NAG	B	704	14/15	0.77	0.09	93,101,120,122	0
7	NAG	C	705	14/15	0.79	0.09	63,98,113,122	0
7	NAG	C	702	14/15	0.79	0.09	82,100,110,114	0
7	NAG	D	702	14/15	0.79	0.09	90,107,125,126	0
7	NAG	C	701	14/15	0.82	0.10	60,88,106,108	0
7	NAG	A	701	14/15	0.82	0.12	67,81,98,104	0
8	SCN	H	302	3/3	0.82	0.12	54,54,62,113	0
7	NAG	A	704	14/15	0.83	0.08	71,87,101,109	0
7	NAG	A	703	14/15	0.83	0.14	30,65,85,88	0
8	SCN	D	708	3/3	0.85	0.16	32,32,53,72	0
7	NAG	A	702	14/15	0.88	0.09	54,68,94,106	0
7	NAG	B	701	14/15	0.94	0.08	29,47,73,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.