



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 07:24 PM BST

PDB ID : 5JW4
Title : Structure of MEDI8852 Fab Fragment in Complex with H5 HA
Authors : Neu, U.; Collins, P.J.; Walker, P.A.; Vorlaender, M.K.; Ogradowicz, R.W.;
Martin, S.R.; Gamblin, S.J.; Skehel, J.J.
Deposited on : 2016-05-11
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

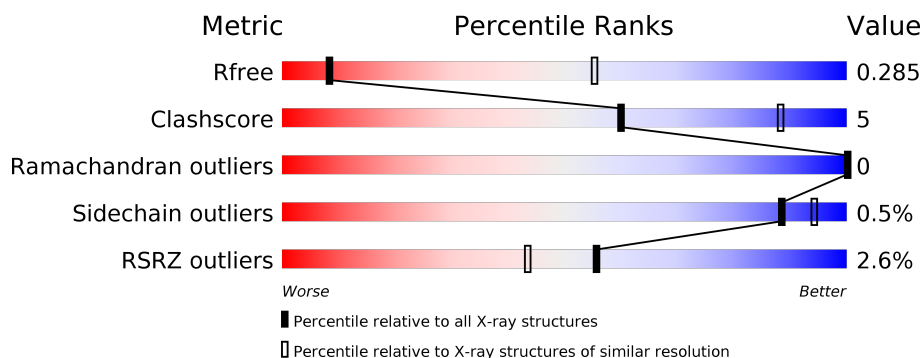
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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.



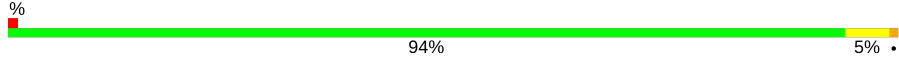
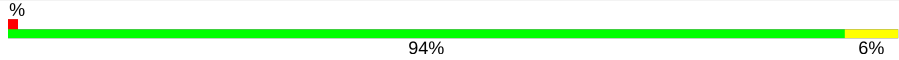
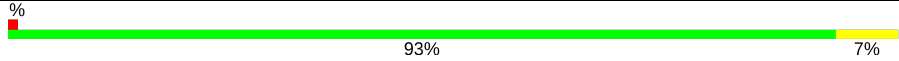
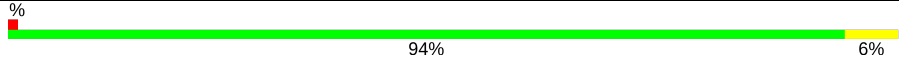
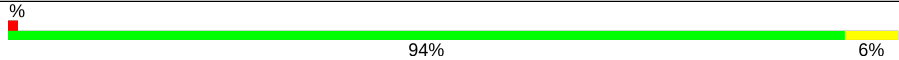
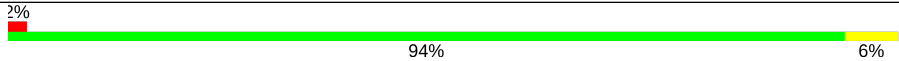
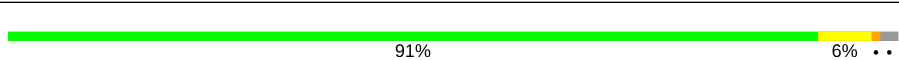
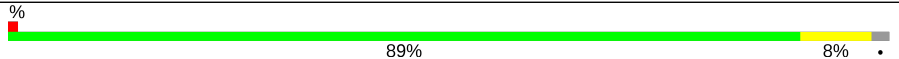
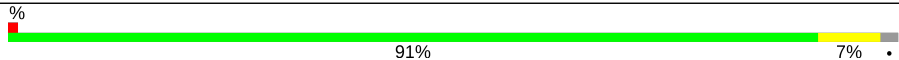
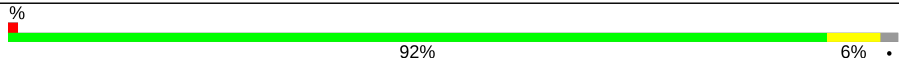
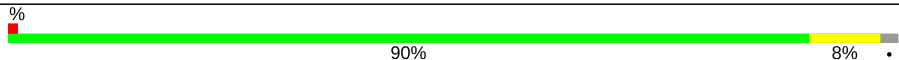
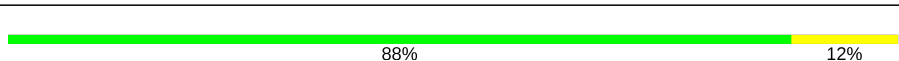
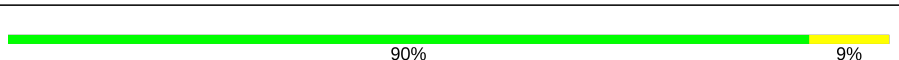

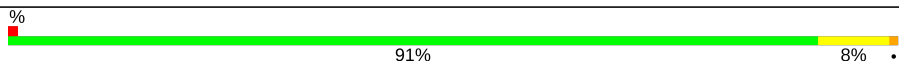
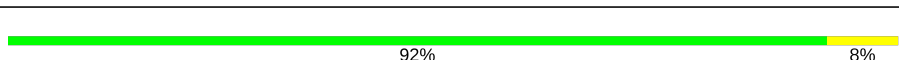
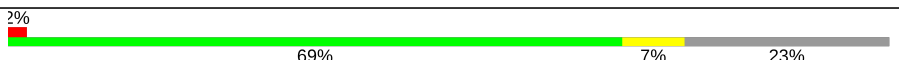
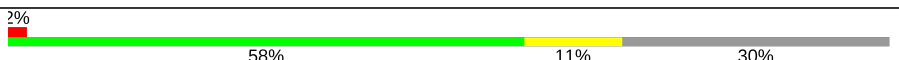

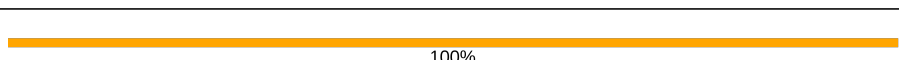
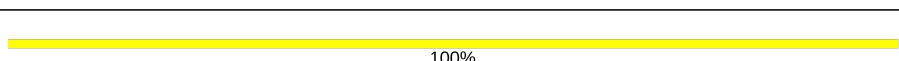
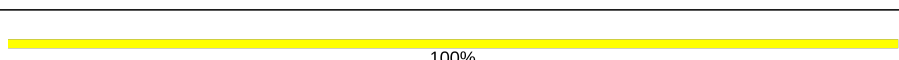
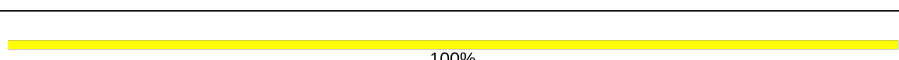
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	321	<div> <div>5%</div> <div> <div></div> <div>96%</div> <div>.</div> </div> </div>
1	C	321	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>
1	E	321	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>
1	G	321	<div> <div>7%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>
1	I	321	<div> <div>11%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
1	K	321	<div> <div>6%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	B	162	
2	D	162	
2	F	162	
2	H	162	
2	J	162	
2	L	162	
3	M	227	
3	O	227	
3	S	227	
3	U	227	
3	W	227	
4	N	206	
4	P	206	
4	T	206	
4	V	206	
4	X	206	
5	Q	231	
6	R	210	
7	Y	2	
7	Z	2	
7	a	2	
7	b	2	
7	c	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
7	NAG	Y	1	X	-	-	-
7	NAG	Z	2	-	-	X	-
7	NAG	a	1	X	-	-	-
7	NAG	b	1	X	-	-	-
7	NAG	c	1	X	-	-	-
8	NAG	D	201	X	-	-	-
8	NAG	L	201	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 42466 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	1	0
			2551	1613	439	484	15			
1	C	321	Total	C	N	O	S	0	1	0
			2551	1613	439	484	15			
1	E	321	Total	C	N	O	S	0	1	0
			2551	1613	439	484	15			
1	G	321	Total	C	N	O	S	0	1	0
			2551	1613	439	484	15			
1	I	321	Total	C	N	O	S	0	1	0
			2551	1613	439	484	15			
1	K	321	Total	C	N	O	S	0	1	0
			2551	1613	439	484	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	LYS	ASN	engineered mutation	UNP Q6DQ34
C	182	LYS	ASN	engineered mutation	UNP Q6DQ34
E	182	LYS	ASN	engineered mutation	UNP Q6DQ34
G	182	LYS	ASN	engineered mutation	UNP Q6DQ34
I	182	LYS	ASN	engineered mutation	UNP Q6DQ34
K	182	LYS	ASN	engineered mutation	UNP Q6DQ34

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	162	Total	C	N	O	S	0	0	0
			1312	819	226	259	8			
2	D	162	Total	C	N	O	S	0	0	0
			1312	819	226	259	8			
2	F	162	Total	C	N	O	S	0	0	0
			1312	819	226	259	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	162	Total	C	N	O	S	0	0	0
			1312	819	226	259	8			
2	J	162	Total	C	N	O	S	0	0	0
			1312	819	226	259	8			
2	L	162	Total	C	N	O	S	0	0	0
			1312	819	226	259	8			

- Molecule 3 is a protein called MEDI8852 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	223	Total	C	N	O	S	0	1	0
			1697	1071	285	335	6			
3	O	223	Total	C	N	O	S	0	1	0
			1697	1071	285	335	6			
3	S	223	Total	C	N	O	S	0	1	0
			1697	1071	285	335	6			
3	U	223	Total	C	N	O	S	0	1	0
			1697	1071	285	335	6			
3	W	223	Total	C	N	O	S	0	1	0
			1697	1071	285	335	6			

- Molecule 4 is a protein called MEDI8852 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	206	Total	C	N	O	S	0	0	0
			1577	980	270	322	5			
4	P	206	Total	C	N	O	S	0	0	0
			1577	980	270	322	5			
4	T	206	Total	C	N	O	S	0	0	0
			1577	980	270	322	5			
4	V	206	Total	C	N	O	S	0	0	0
			1577	980	270	322	5			
4	X	206	Total	C	N	O	S	0	0	0
			1577	980	270	322	5			

- Molecule 5 is a protein called MEDI8852 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	Q	177	Total	C	N	O	S	0	0	0
			1369	867	230	267	5			

- Molecule 6 is a protein called MEDI8852 light chain.

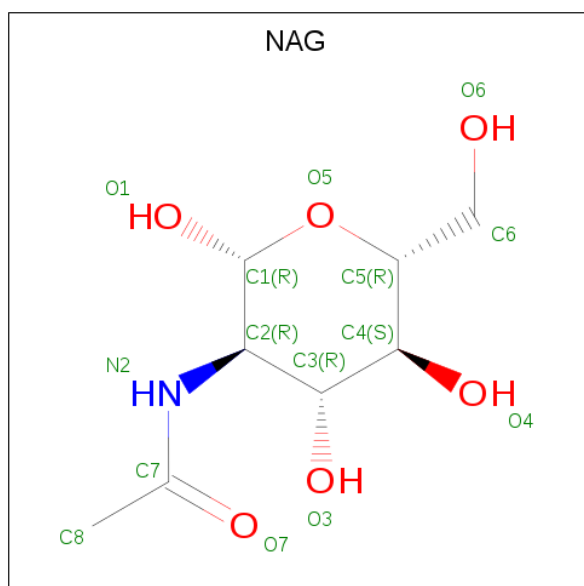
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	R	148	Total	C	N	O	S	0	0	0
			1129	701	193	230	5			

- 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	Y	2	Total	C	N	O		0	0	0
			28	16	2	10				
7	Z	2	Total	C	N	O		0	0	0
			28	16	2	10				
7	a	2	Total	C	N	O		0	0	0
			28	16	2	10				
7	b	2	Total	C	N	O		0	0	0
			28	16	2	10				
7	c	2	Total	C	N	O		0	0	0
			28	16	2	10				

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

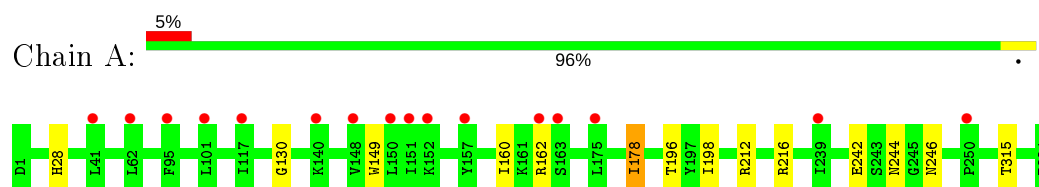


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	D	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1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

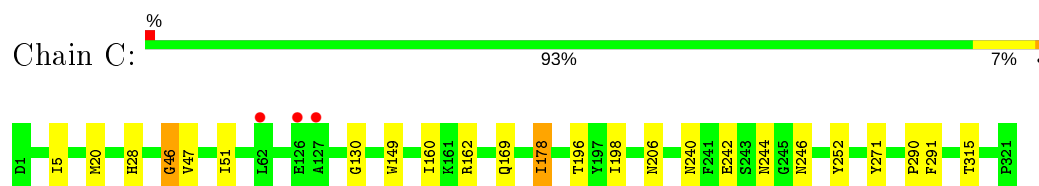
3 Residue-property plots [i](#)

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.

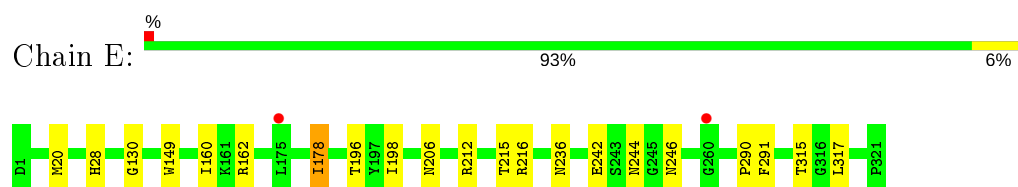
- Molecule 1: Hemagglutinin



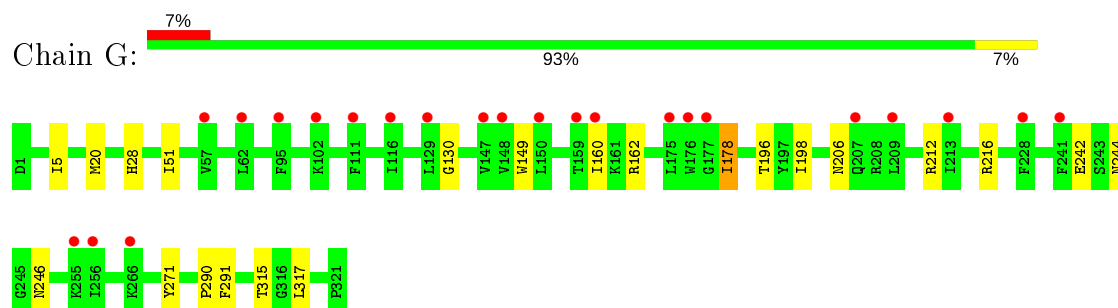
- Molecule 1: Hemagglutinin



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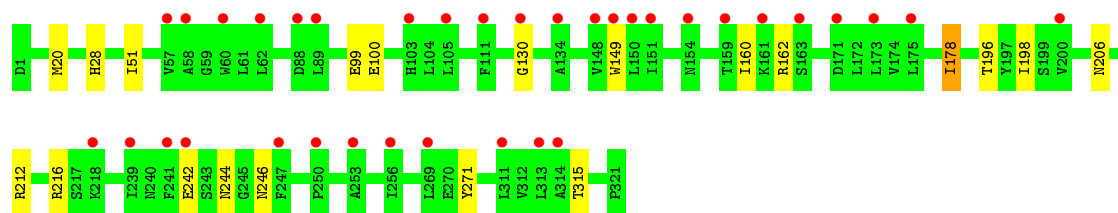


- Molecule 1: Hemagglutinin

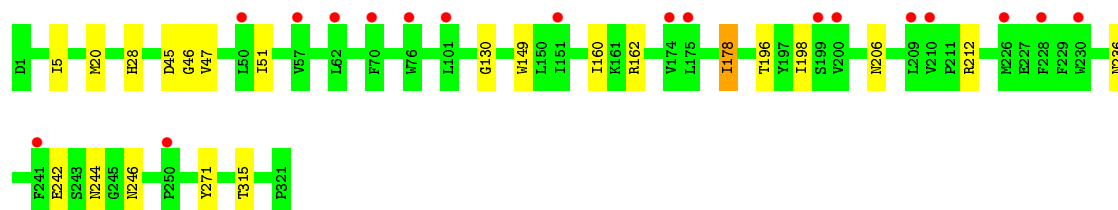
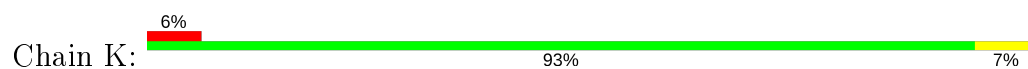


- Molecule 1: Hemagglutinin





• Molecule 1: Hemagglutinin



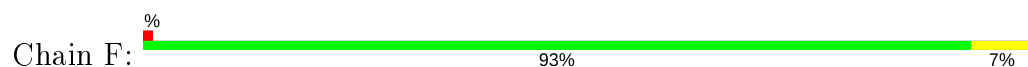
• Molecule 2: Hemagglutinin



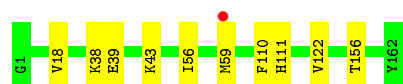
• Molecule 2: Hemagglutinin



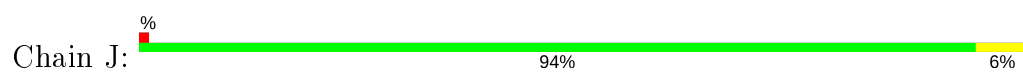
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



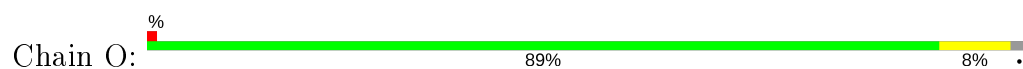
- Molecule 2: Hemagglutinin



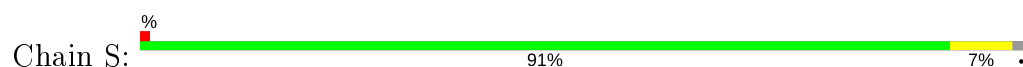
- Molecule 3: MEDI8852 heavy chain



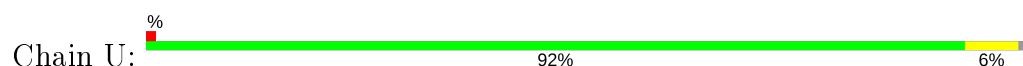
- Molecule 3: MEDI8852 heavy chain



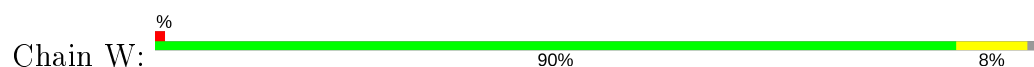
- Molecule 3: MEDI8852 heavy chain




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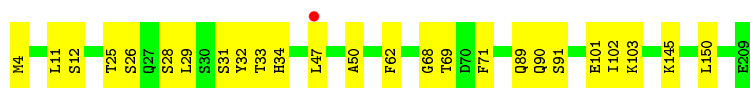


- Molecule 3: MEDI8852 heavy chain




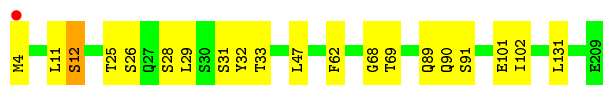
- Molecule 4: MEDI8852 light chain

Chain N:  88% 12%




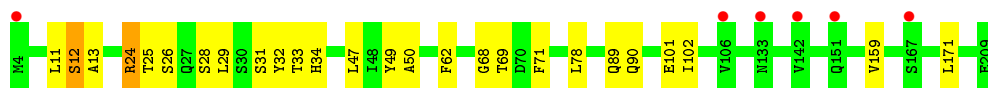
- Molecule 4: MEDI8852 light chain

Chain P:  90% 9%




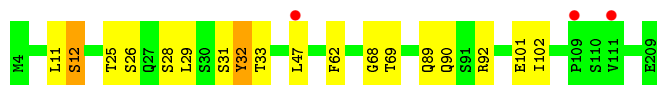
- Molecule 4: MEDI8852 light chain

Chain T:  3% 87% 12%



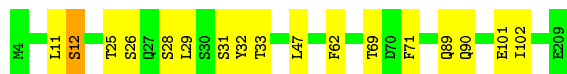
- Molecule 4: MEDI8852 light chain

Chain V:  0% 91% 8%



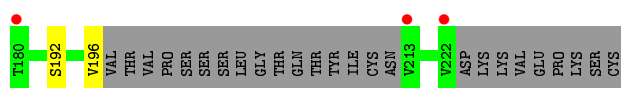
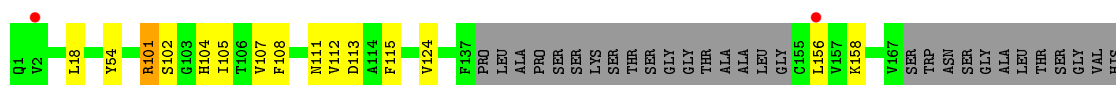
- Molecule 4: MEDI8852 light chain

Chain X:  92% 8%

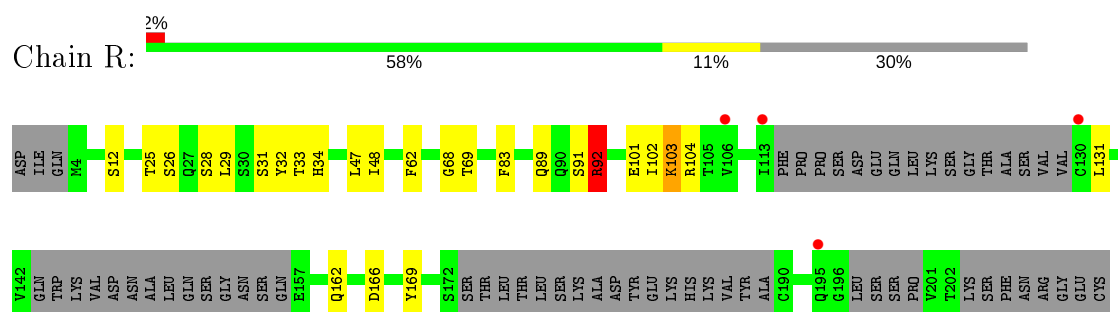


- Molecule 5: MEDI8852 heavy chain

Chain Q:  2% 69% 7% 23%



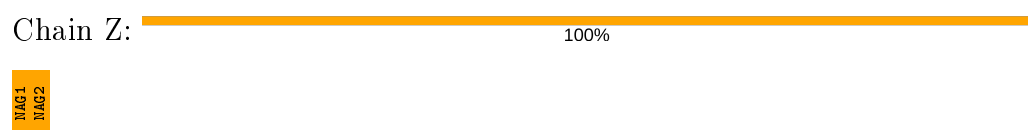
- Molecule 6: MEDI8852 light chain



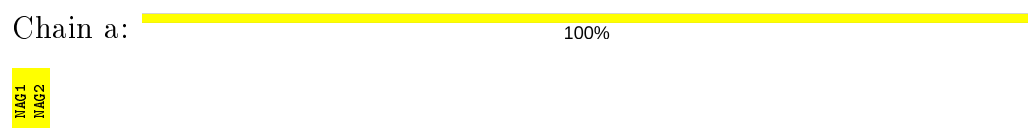
- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



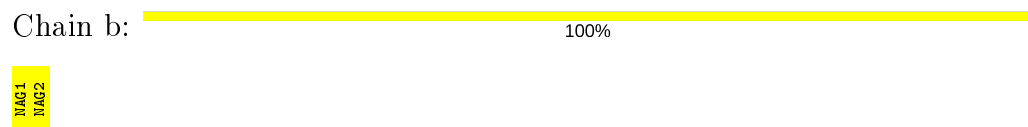
- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



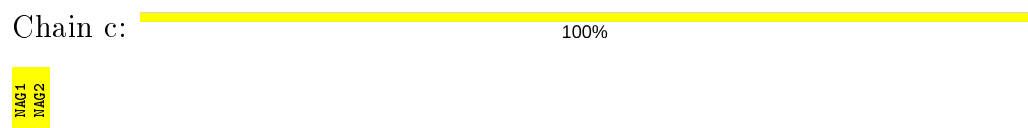
- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.26Å 386.36Å 165.86Å 90.00° 90.44° 90.00°	Depositor
Resolution (Å)	29.80 – 3.70 29.80 – 3.70	Depositor EDS
% Data completeness (in resolution range)	97.6 (29.80-3.70) 97.6 (29.80-3.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 3.75Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.274 , 0.285 0.274 , 0.285	Depositor DCC
R_{free} test set	4769 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	136.3	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 83.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.065 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	42466	wwPDB-VP
Average B, all atoms (Å ²)	152.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.41	0/2616	0.58	0/3553
1	C	0.58	1/2616 (0.0%)	0.62	3/3553 (0.1%)
1	E	0.43	0/2616	0.58	0/3553
1	G	0.40	0/2616	0.58	0/3553
1	I	0.40	0/2616	0.58	0/3553
1	K	0.50	1/2616 (0.0%)	0.62	3/3553 (0.1%)
2	B	0.48	0/1339	0.60	0/1802
2	D	0.50	0/1339	0.61	0/1802
2	F	0.51	0/1339	0.61	0/1802
2	H	0.49	0/1339	0.60	0/1802
2	J	0.49	0/1339	0.62	1/1802 (0.1%)
2	L	0.48	0/1339	0.61	0/1802
3	M	0.75	4/1738 (0.2%)	0.78	4/2374 (0.2%)
3	O	0.59	3/1738 (0.2%)	0.75	4/2374 (0.2%)
3	S	0.61	3/1738 (0.2%)	0.73	1/2374 (0.0%)
3	U	0.62	5/1738 (0.3%)	0.73	3/2374 (0.1%)
3	W	0.79	1/1738 (0.1%)	1.03	4/2374 (0.2%)
4	N	0.56	0/1610	0.72	0/2182
4	P	0.49	0/1610	0.70	0/2182
4	T	0.70	1/1610 (0.1%)	0.77	3/2182 (0.1%)
4	V	0.55	0/1610	0.73	1/2182 (0.0%)
4	X	0.53	0/1610	0.70	0/2182
5	Q	0.57	0/1401	0.79	1/1908 (0.1%)
6	R	0.99	1/1147 (0.1%)	0.95	4/1547 (0.3%)
All	All	0.56	20/43018 (0.0%)	0.69	32/58365 (0.1%)

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	103	LYS	C-N	26.41	1.94	1.34
3	W	195	SER	C-N	25.07	1.91	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	46	GLY	C-N	19.65	1.79	1.34
4	T	24	ARG	C-N	19.10	1.77	1.34
3	M	115	PHE	C-N	17.29	1.73	1.34

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	W	195	SER	O-C-N	-22.98	85.93	122.70
3	W	195	SER	CA-C-N	-22.98	66.65	117.20
3	W	195	SER	C-N-CA	-19.06	74.06	121.70
6	R	103	LYS	O-C-N	-14.20	99.97	122.70
6	R	103	LYS	C-N-CA	11.06	149.34	121.70

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	2551	0	2501	10	0
1	C	2551	0	2500	22	2
1	E	2551	0	2501	27	0
1	G	2551	0	2501	19	0
1	I	2551	0	2500	15	0
1	K	2551	0	2500	19	0
2	B	1312	0	1218	7	0
2	D	1312	0	1218	10	0
2	F	1312	0	1218	14	0
2	H	1312	0	1218	10	0
2	J	1312	0	1218	9	0
2	L	1312	0	1218	8	0
3	M	1697	0	1648	31	0
3	O	1697	0	1649	20	2
3	S	1697	0	1649	14	0
3	U	1697	0	1649	15	0
3	W	1697	0	1647	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	1577	0	1531	28	0
4	P	1577	0	1531	19	0
4	T	1577	0	1530	27	0
4	V	1577	0	1531	23	0
4	X	1577	0	1531	16	0
5	Q	1369	0	1324	18	0
6	R	1129	0	1089	35	0
7	Y	28	0	25	0	0
7	Z	28	0	24	12	0
7	a	28	0	25	0	0
7	b	28	0	25	0	0
7	c	28	0	25	0	0
8	A	42	0	39	1	0
8	C	42	0	39	1	0
8	D	14	0	13	0	0
8	E	28	0	26	0	0
8	G	42	0	39	1	0
8	I	42	0	39	1	0
8	K	56	0	50	6	0
8	L	14	0	13	0	0
All	All	42466	0	41002	387	2

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 5.

The worst 5 of 387 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)
8:K:401:NAG:O3	8:K:402:NAG:C1	1.64	1.43
3:W:195:SER:C	3:W:196[A]:VAL:C	1.76	1.42
3:M:115:PHE:C	3:M:116:ASP:N	1.73	1.41
7:Z:1:NAG:O3	7:Z:2:NAG:C1	1.65	1.41
3:W:195:SER:N	3:W:196[B]:VAL:N	1.64	1.40

All (2) 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:169:GLN:CG	3:O:219:ASN:OD1[2_655]	1.93	0.27
1:C:252:TYR:CE1	3:O:79:LYS:CE[2_655]	2.05	0.15

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	320/321 (100%)	311 (97%)	9 (3%)	0	100	100
1	C	320/321 (100%)	311 (97%)	9 (3%)	0	100	100
1	E	320/321 (100%)	311 (97%)	9 (3%)	0	100	100
1	G	320/321 (100%)	311 (97%)	9 (3%)	0	100	100
1	I	320/321 (100%)	311 (97%)	9 (3%)	0	100	100
1	K	320/321 (100%)	311 (97%)	9 (3%)	0	100	100
2	B	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
2	D	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
2	F	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
2	H	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
2	J	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
2	L	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
3	M	217/227 (96%)	210 (97%)	7 (3%)	0	100	100
3	O	217/227 (96%)	211 (97%)	6 (3%)	0	100	100
3	S	217/227 (96%)	212 (98%)	5 (2%)	0	100	100
3	U	217/227 (96%)	211 (97%)	6 (3%)	0	100	100
3	W	217/227 (96%)	210 (97%)	7 (3%)	0	100	100
4	N	204/206 (99%)	200 (98%)	4 (2%)	0	100	100
4	P	204/206 (99%)	200 (98%)	4 (2%)	0	100	100
4	T	204/206 (99%)	200 (98%)	4 (2%)	0	100	100
4	V	204/206 (99%)	200 (98%)	4 (2%)	0	100	100
4	X	204/206 (99%)	199 (98%)	5 (2%)	0	100	100
5	Q	167/231 (72%)	163 (98%)	4 (2%)	0	100	100
6	R	136/210 (65%)	133 (98%)	3 (2%)	0	100	100
All	All	5288/5504 (96%)	5151 (97%)	137 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	290/289 (100%)	288 (99%)	2 (1%)	84	91
1	C	290/289 (100%)	288 (99%)	2 (1%)	84	91
1	E	290/289 (100%)	288 (99%)	2 (1%)	84	91
1	G	290/289 (100%)	288 (99%)	2 (1%)	84	91
1	I	290/289 (100%)	288 (99%)	2 (1%)	84	91
1	K	290/289 (100%)	288 (99%)	2 (1%)	84	91
2	B	138/138 (100%)	137 (99%)	1 (1%)	84	91
2	D	138/138 (100%)	138 (100%)	0	100	100
2	F	138/138 (100%)	138 (100%)	0	100	100
2	H	138/138 (100%)	138 (100%)	0	100	100
2	J	138/138 (100%)	138 (100%)	0	100	100
2	L	138/138 (100%)	138 (100%)	0	100	100
3	M	195/198 (98%)	195 (100%)	0	100	100
3	O	195/198 (98%)	195 (100%)	0	100	100
3	S	195/198 (98%)	194 (100%)	1 (0%)	88	94
3	U	195/198 (98%)	195 (100%)	0	100	100
3	W	195/198 (98%)	195 (100%)	0	100	100
4	N	181/181 (100%)	180 (99%)	1 (1%)	86	93
4	P	181/181 (100%)	179 (99%)	2 (1%)	73	85
4	T	181/181 (100%)	179 (99%)	2 (1%)	73	85
4	V	181/181 (100%)	179 (99%)	2 (1%)	73	85
4	X	181/181 (100%)	179 (99%)	2 (1%)	73	85
5	Q	157/201 (78%)	157 (100%)	0	100	100
6	R	130/185 (70%)	128 (98%)	2 (2%)	65	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4735/4843 (98%)	4710 (100%)	25 (0%)	88 94

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	162	ARG
4	N	26	SER
4	X	12	SER
1	K	178	ILE
4	P	12	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	79	ASN
1	G	246	ASN
1	K	28	HIS
1	E	246	ASN
1	K	236	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

10 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
7	NAG	Y	1	2,7	14,14,15	0.65	0	17,19,21	1.95	5 (29%)
7	NAG	Y	2	7	14,14,15	0.48	0	17,19,21	0.97	0
7	NAG	Z	1	1,7	14,14,15	1.06	2 (14%)	17,19,21	3.19	8 (47%)
7	NAG	Z	2	7	14,14,15	1.40	2 (14%)	17,19,21	3.24	7 (41%)
7	NAG	a	1	2,7	14,14,15	1.11	1 (7%)	17,19,21	1.71	5 (29%)
7	NAG	a	2	7	14,14,15	0.39	0	17,19,21	1.09	1 (5%)
7	NAG	b	1	2,7	14,14,15	0.74	1 (7%)	17,19,21	1.42	4 (23%)
7	NAG	b	2	7	14,14,15	0.41	0	17,19,21	0.99	1 (5%)
7	NAG	c	1	2,7	14,14,15	0.77	0	17,19,21	2.20	5 (29%)
7	NAG	c	2	7	14,14,15	0.49	0	17,19,21	0.99	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
7	NAG	Y	1	2,7	1/1/5/7	3/6/23/26	0/1/1/1
7	NAG	Y	2	7	-	3/6/23/26	0/1/1/1
7	NAG	Z	1	1,7	-	5/6/23/26	0/1/1/1
7	NAG	Z	2	7	-	2/6/23/26	0/1/1/1
7	NAG	a	1	2,7	1/1/5/7	3/6/23/26	0/1/1/1
7	NAG	a	2	7	-	3/6/23/26	0/1/1/1
7	NAG	b	1	2,7	1/1/5/7	2/6/23/26	0/1/1/1
7	NAG	b	2	7	-	3/6/23/26	0/1/1/1
7	NAG	c	1	2,7	1/1/5/7	2/6/23/26	0/1/1/1
7	NAG	c	2	7	-	2/6/23/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Z	2	NAG	C1-C2	4.26	1.58	1.52
7	a	1	NAG	O5-C1	-3.39	1.38	1.43
7	Z	1	NAG	C3-C2	-2.41	1.47	1.52
7	Z	2	NAG	C2-N2	2.30	1.50	1.46
7	Z	1	NAG	O5-C1	-2.24	1.40	1.43

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Z	2	NAG	C1-O5-C5	11.12	127.25	112.19
7	Z	1	NAG	O4-C4-C5	6.79	126.15	109.30
7	Z	1	NAG	O4-C4-C3	-6.25	95.89	110.35
7	Y	1	NAG	C1-O5-C5	5.29	119.35	112.19
7	c	1	NAG	C1-O5-C5	4.92	118.86	112.19

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	Y	1	NAG	C1
7	c	1	NAG	C1
7	b	1	NAG	C1
7	a	1	NAG	C1

5 of 28 torsion outliers are listed below:

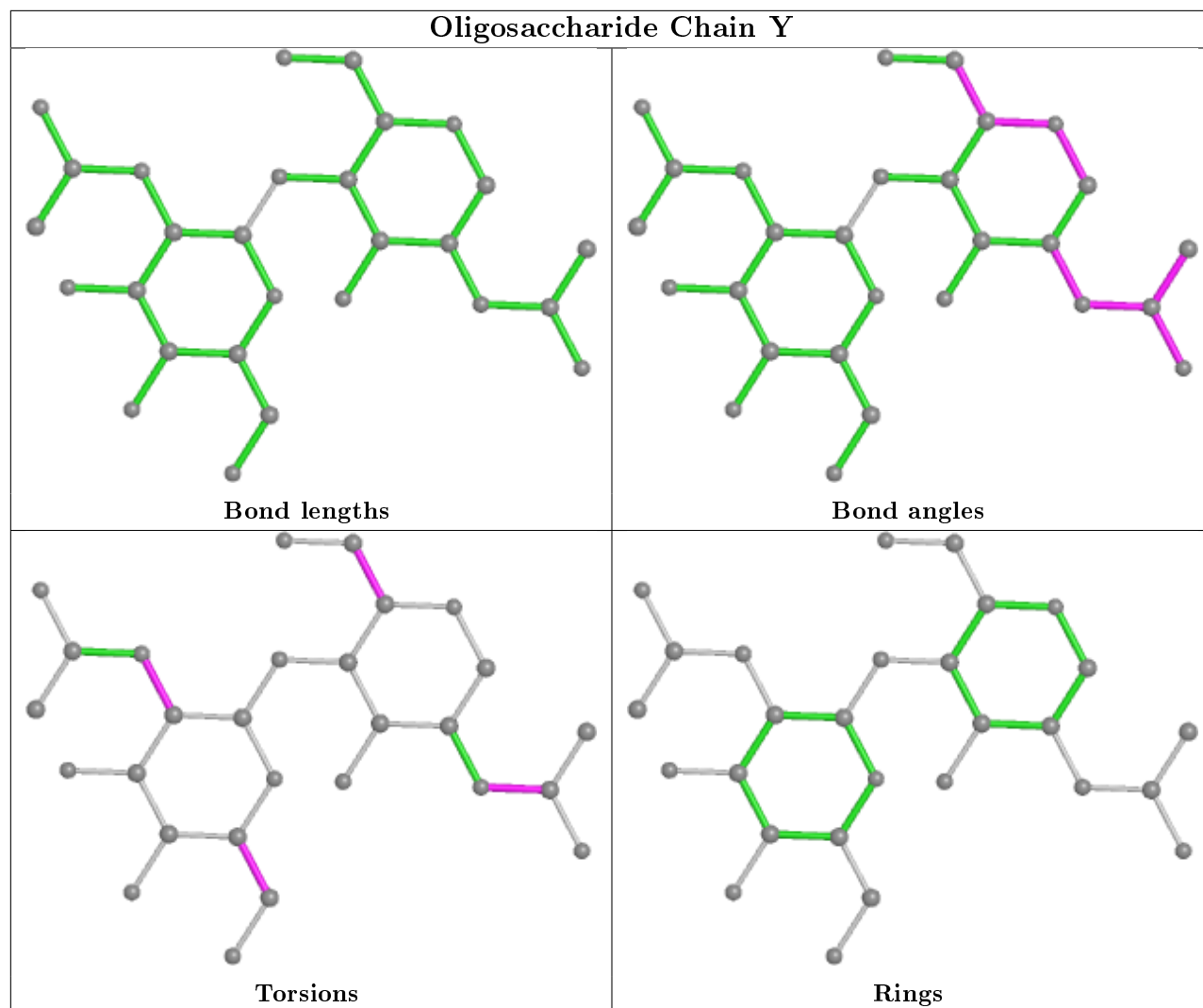
Mol	Chain	Res	Type	Atoms
7	Z	2	NAG	C4-C5-C6-O6
7	Z	1	NAG	C8-C7-N2-C2
7	Z	1	NAG	O7-C7-N2-C2
7	Y	1	NAG	C8-C7-N2-C2
7	Y	1	NAG	O7-C7-N2-C2

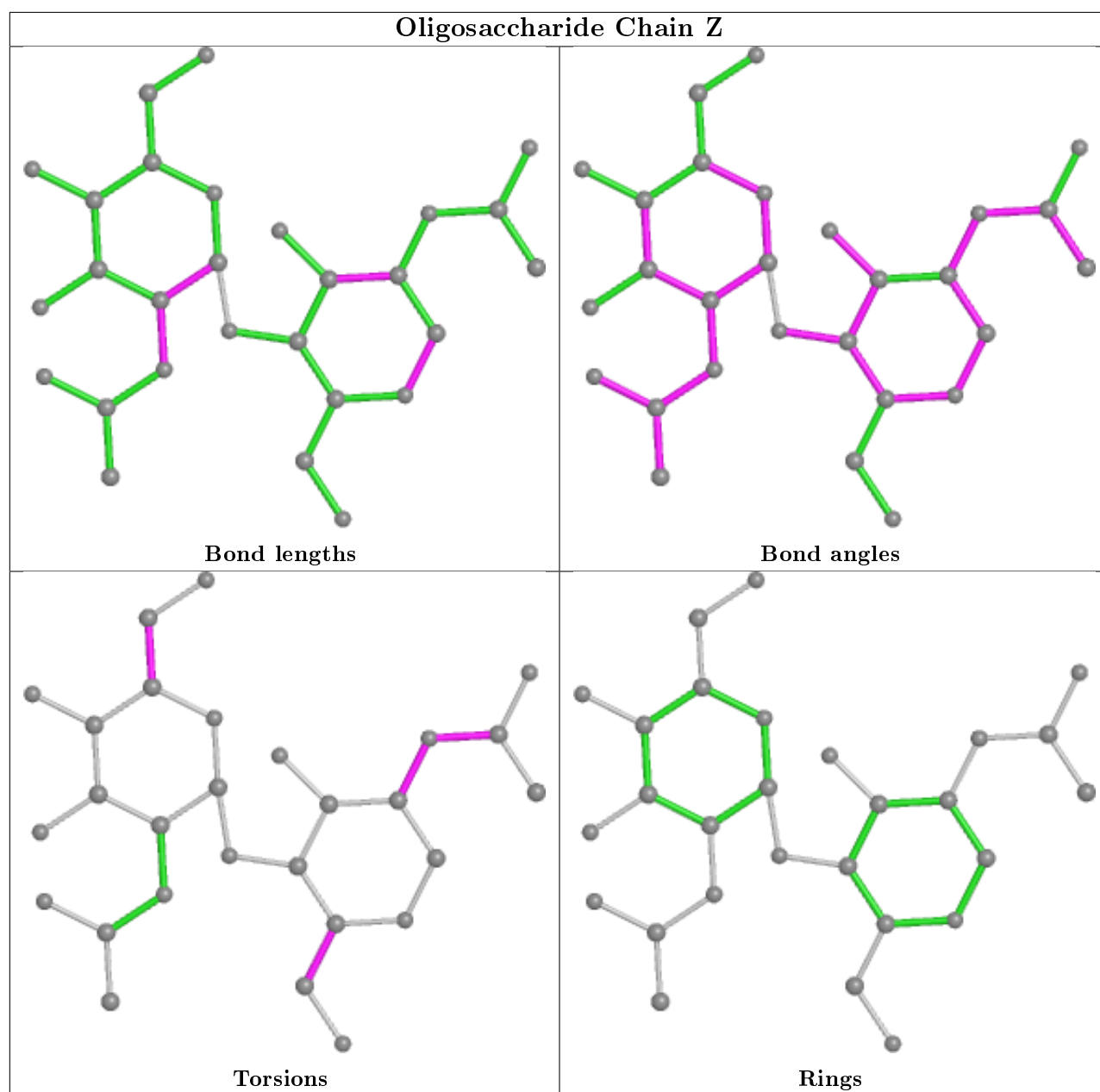
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	Z	1	NAG	3	0
7	Z	2	NAG	11	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](#)

20 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	NAG	C	402	1	14,14,15	0.39	0	17,19,21	1.65	3 (17%)
8	NAG	K	401	1	14,14,15	0.83	1 (7%)	17,19,21	3.17	8 (47%)
8	NAG	A	401	1	14,14,15	0.75	1 (7%)	17,19,21	1.74	4 (23%)
8	NAG	G	402	1	14,14,15	0.39	0	17,19,21	1.41	2 (11%)
8	NAG	I	402	1	14,14,15	0.28	0	17,19,21	1.57	4 (23%)
8	NAG	G	403	1	14,14,15	0.39	0	17,19,21	0.74	0
8	NAG	K	402	-	14,14,15	1.44	2 (14%)	17,19,21	3.02	3 (17%)
8	NAG	A	403	1	14,14,15	0.31	0	17,19,21	1.16	2 (11%)
8	NAG	I	401	1	14,14,15	1.02	1 (7%)	17,19,21	2.16	4 (23%)
8	NAG	E	403	1	14,14,15	0.42	0	17,19,21	1.51	3 (17%)
8	NAG	E	404	1	14,14,15	1.38	1 (7%)	17,19,21	1.54	5 (29%)
8	NAG	I	403	1	14,14,15	0.29	0	17,19,21	1.06	0
8	NAG	C	403	1	14,14,15	0.32	0	17,19,21	0.83	0
8	NAG	L	201	2	14,14,15	0.39	0	17,19,21	1.45	2 (11%)
8	NAG	D	201	2	14,14,15	0.40	0	17,19,21	2.04	4 (23%)
8	NAG	C	401	1	14,14,15	0.41	0	17,19,21	1.93	6 (35%)
8	NAG	K	404	1	14,14,15	0.78	1 (7%)	17,19,21	0.92	0
8	NAG	K	403	1	14,14,15	0.39	0	17,19,21	1.67	4 (23%)
8	NAG	G	401	1	14,14,15	0.70	1 (7%)	17,19,21	2.11	8 (47%)
8	NAG	A	402	1	14,14,15	0.48	0	17,19,21	1.54	3 (17%)

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	C	402	1	-	2/6/23/26	0/1/1/1
8	NAG	K	401	1	-	5/6/23/26	0/1/1/1
8	NAG	A	401	1	-	4/6/23/26	0/1/1/1
8	NAG	G	402	1	-	2/6/23/26	0/1/1/1
8	NAG	I	402	1	-	2/6/23/26	0/1/1/1
8	NAG	G	403	1	-	0/6/23/26	0/1/1/1
8	NAG	K	402	-	-	2/6/23/26	0/1/1/1
8	NAG	A	403	1	-	0/6/23/26	0/1/1/1
8	NAG	I	401	1	-	4/6/23/26	0/1/1/1
8	NAG	E	403	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	E	404	1	-	0/6/23/26	0/1/1/1
8	NAG	I	403	1	-	0/6/23/26	0/1/1/1
8	NAG	C	403	1	-	0/6/23/26	0/1/1/1
8	NAG	A	402	1	-	2/6/23/26	0/1/1/1
8	NAG	D	201	2	1/1/5/7	4/6/23/26	0/1/1/1
8	NAG	C	401	1	-	5/6/23/26	0/1/1/1
8	NAG	K	404	1	-	0/6/23/26	0/1/1/1
8	NAG	K	403	1	-	2/6/23/26	0/1/1/1
8	NAG	G	401	1	-	5/6/23/26	0/1/1/1
8	NAG	L	201	2	1/1/5/7	4/6/23/26	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	K	402	NAG	C1-C2	4.59	1.59	1.52
8	E	404	NAG	C1-C2	4.52	1.59	1.52
8	K	404	NAG	C1-C2	2.83	1.56	1.52
8	I	401	NAG	O5-C1	-2.66	1.39	1.43
8	G	401	NAG	C1-C2	-2.31	1.48	1.52

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	K	402	NAG	C1-O5-C5	11.07	127.18	112.19
8	K	401	NAG	O4-C4-C3	-6.37	95.62	110.35
8	K	401	NAG	O4-C4-C5	6.12	124.50	109.30
8	C	402	NAG	C1-O5-C5	5.22	119.27	112.19
8	I	401	NAG	O5-C1-C2	5.01	119.20	111.29

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	L	201	NAG	C1
8	D	201	NAG	C1

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	G	402	NAG	O5-C5-C6-O6
8	E	403	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	I	401	NAG	O5-C5-C6-O6
8	A	402	NAG	O5-C5-C6-O6
8	I	402	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	K	401	NAG	3	0
8	A	401	NAG	1	0
8	K	402	NAG	5	0
8	I	401	NAG	1	0
8	C	401	NAG	1	0
8	G	401	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	W	4
3	M	3
3	U	2
3	O	2
6	R	2
3	S	2
5	Q	1
1	K	1
1	C	1
4	T	1

The worst 5 of 19 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	196[B]:VAL	C	197:VAL	N	3.54
1	W	196[A]:VAL	C	197:VAL	N	3.43

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Q	128:SER	C	129:ALA	N	3.05
1	O	196[B]:VAL	C	197:VAL	N	2.49
1	R	102:ILE	C	103:LYS	N	2.49

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	321/321 (100%)	0.18	16 (4%) 28 21	107, 166, 215, 249	0
1	C	321/321 (100%)	0.13	3 (0%) 84 76	106, 154, 211, 232	0
1	E	321/321 (100%)	0.17	2 (0%) 89 83	101, 145, 164, 177	0
1	G	321/321 (100%)	0.28	23 (7%) 15 11	118, 199, 244, 262	0
1	I	321/321 (100%)	0.37	35 (10%) 5 4	123, 214, 247, 264	0
1	K	321/321 (100%)	0.21	18 (5%) 24 17	125, 193, 231, 253	0
2	B	162/162 (100%)	0.12	1 (0%) 89 83	104, 122, 149, 161	0
2	D	162/162 (100%)	0.18	1 (0%) 89 83	104, 118, 136, 142	0
2	F	162/162 (100%)	0.12	1 (0%) 89 83	104, 117, 141, 152	0
2	H	162/162 (100%)	0.08	1 (0%) 89 83	112, 132, 173, 191	0
2	J	162/162 (100%)	0.15	2 (1%) 79 69	125, 138, 174, 189	0
2	L	162/162 (100%)	0.09	4 (2%) 57 45	121, 134, 174, 199	0
3	M	223/227 (98%)	0.06	0 100 100	105, 134, 161, 179	0
3	O	223/227 (98%)	0.21	3 (1%) 77 67	109, 139, 186, 205	0
3	S	223/227 (98%)	0.11	3 (1%) 77 67	117, 168, 210, 220	0
3	U	223/227 (98%)	0.04	3 (1%) 77 67	112, 134, 161, 174	0
3	W	223/227 (98%)	0.17	3 (1%) 77 67	120, 145, 182, 196	0
4	N	206/206 (100%)	0.07	1 (0%) 91 85	106, 124, 153, 170	0
4	P	206/206 (100%)	0.04	1 (0%) 91 85	109, 154, 180, 192	0
4	T	206/206 (100%)	0.26	6 (2%) 51 39	134, 188, 231, 238	0
4	V	206/206 (100%)	0.01	3 (1%) 73 63	115, 131, 155, 166	0
4	X	206/206 (100%)	-0.01	0 100 100	124, 151, 182, 189	0
5	Q	177/231 (76%)	0.11	5 (2%) 53 40	101, 124, 161, 161	0
6	R	148/210 (70%)	0.16	4 (2%) 54 42	103, 134, 162, 174	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	5368/5504 (97%)	0.15	139 (2%) 56 43	101, 144, 223, 264	0

The worst 5 of 139 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	150	LEU	8.0
1	G	175	LEU	7.9
1	G	176	TRP	6.2
1	A	150	LEU	5.9
1	I	58	ALA	5.5

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

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

6.3 Carbohydrates ⓘ

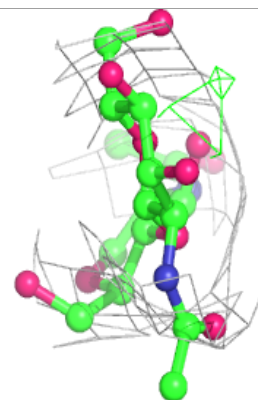
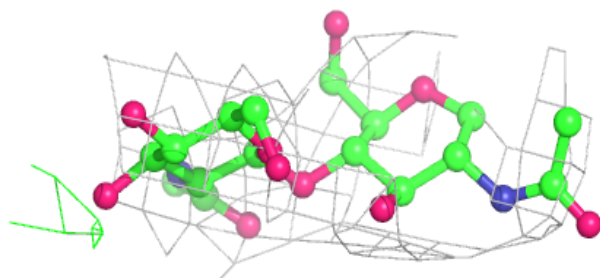
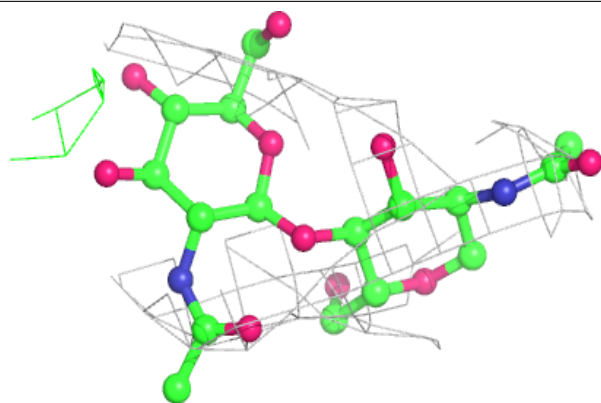
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

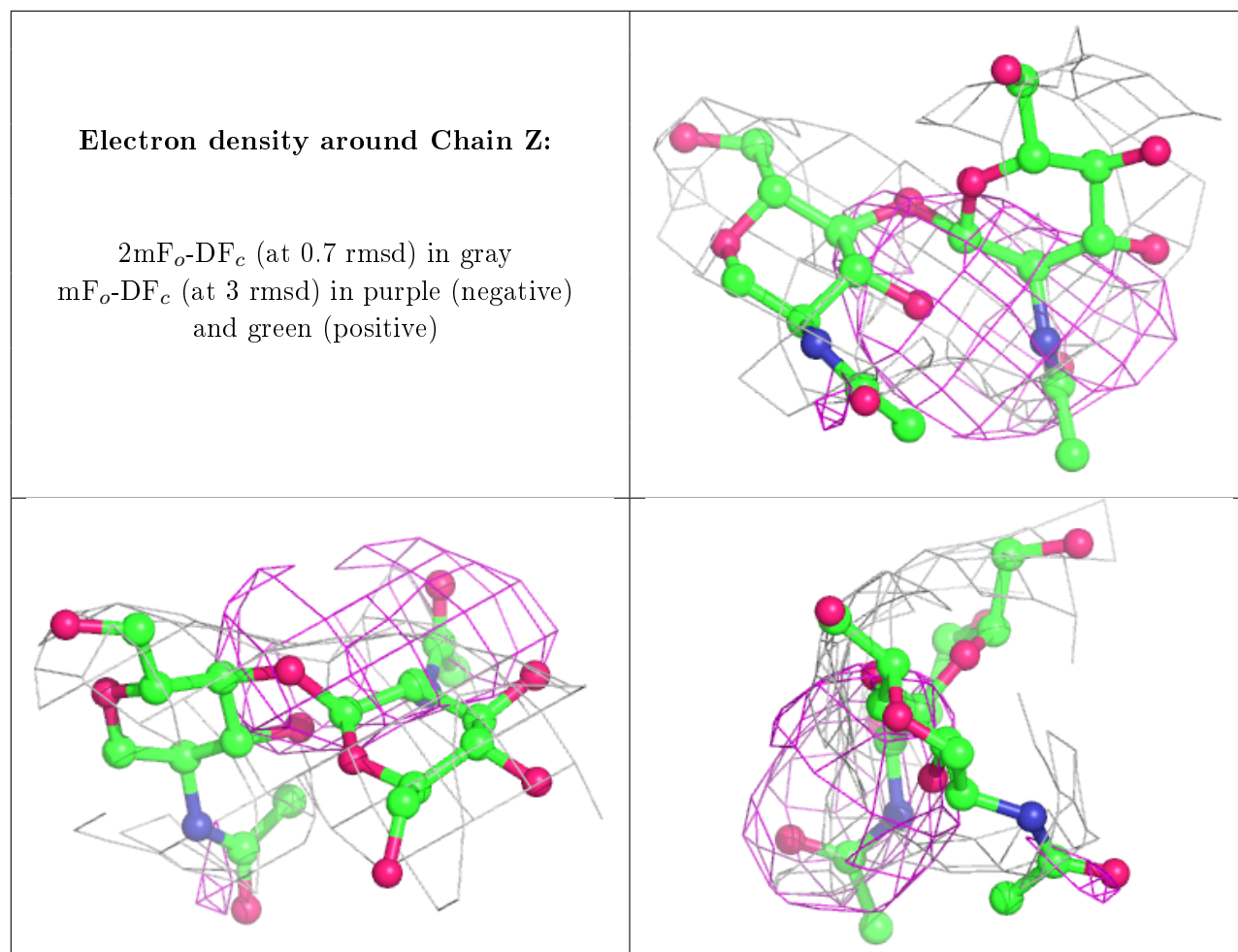
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	Y	2	14/15	0.70	0.32	182,185,188,188	0
7	NAG	c	2	14/15	0.74	0.27	189,190,192,192	0
7	NAG	Z	2	14/15	0.77	0.31	139,139,139,139	0
7	NAG	b	2	14/15	0.81	0.26	193,195,196,197	0
7	NAG	Z	1	14/15	0.86	0.30	139,139,139,139	0
7	NAG	a	2	14/15	0.86	0.27	190,191,194,196	0
7	NAG	c	1	14/15	0.87	0.20	184,186,187,188	0
7	NAG	Y	1	14/15	0.88	0.23	176,178,181,181	0
7	NAG	b	1	14/15	0.89	0.24	188,189,192,192	0
7	NAG	a	1	14/15	0.94	0.21	182,185,189,189	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 Y:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	NAG	D	201	14/15	0.68	0.33	174,176,178,178	0
8	NAG	I	403	14/15	0.69	0.24	139,139,139,139	0
8	NAG	K	403	14/15	0.69	0.28	139,139,139,139	0
8	NAG	C	401	14/15	0.70	0.26	139,139,139,139	0
8	NAG	C	402	14/15	0.75	0.28	139,139,139,139	0
8	NAG	G	403	14/15	0.76	0.23	139,139,139,139	0
8	NAG	A	401	14/15	0.78	0.28	139,139,139,139	0
8	NAG	K	402	14/15	0.78	0.26	139,139,139,139	0
8	NAG	A	402	14/15	0.78	0.26	139,139,139,139	0
8	NAG	L	201	14/15	0.80	0.30	190,192,195,196	0
8	NAG	E	404	14/15	0.81	0.20	139,139,139,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	NAG	E	403	14/15	0.82	0.27	139,139,139,139	0
8	NAG	I	402	14/15	0.83	0.29	139,139,139,139	0
8	NAG	I	401	14/15	0.84	0.16	139,139,139,139	0
8	NAG	G	401	14/15	0.86	0.23	139,139,139,139	0
8	NAG	C	403	14/15	0.86	0.29	139,139,139,139	0
8	NAG	K	404	14/15	0.87	0.31	139,139,139,139	0
8	NAG	G	402	14/15	0.89	0.22	139,139,139,139	0
8	NAG	K	401	14/15	0.91	0.18	139,139,139,139	0
8	NAG	A	403	14/15	0.92	0.15	139,139,139,139	0

6.5 Other polymers [i](#)

There are no such residues in this entry.