



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 05:57 PM BST

PDB ID : 3VI4  
Title : Crystal structure of alpha5beta1 integrin headpiece in complex with RGD peptide  
Authors : Nagae, M.; Nogi, T.; Takagi, J.  
Deposited on : 2011-09-21  
Resolution : 2.90 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.

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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

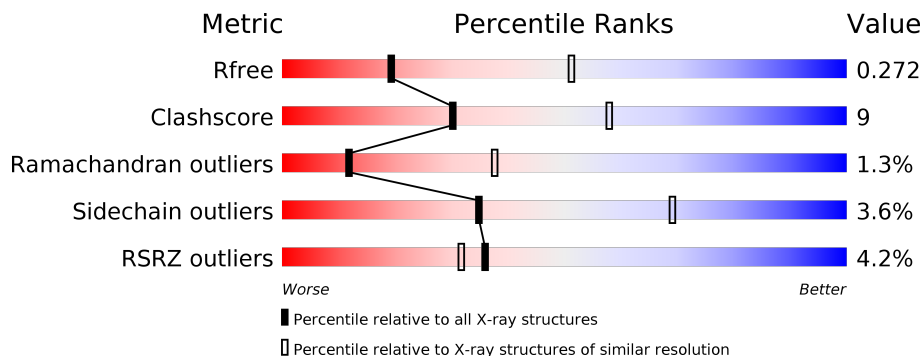
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 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	
1	C	632	
2	B	454	
2	D	454	
3	E	219	
3	L	219	

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Mol	Chain	Length	Quality of chain
4	F	218	<p>% 74% 24%</p>
4	H	218	<p>% 82% 18%</p>
5	G	5	<p>60% 20% 20%</p>
5	I	5	<p>60% 40%</p>
6	J	2	<p>50% 50%</p>
6	M	2	<p>100%</p>
7	K	6	<p>17% 83%</p>
7	N	6	<p>83% 17%</p>

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 22882 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 Integrin alpha-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	601	Total	C	N	O	S	0	0	0
			4567	2892	768	893	14			
1	C	589	Total	C	N	O	S	0	0	0
			4466	2828	747	877	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	624	GLY	-	expression tag	UNP P08648
A	625	GLY	-	expression tag	UNP P08648
A	626	LEU	-	expression tag	UNP P08648
A	627	GLU	-	expression tag	UNP P08648
A	628	ASN	-	expression tag	UNP P08648
A	629	LEU	-	expression tag	UNP P08648
A	630	TYR	-	expression tag	UNP P08648
A	631	PHE	-	expression tag	UNP P08648
A	632	GLN	-	expression tag	UNP P08648
C	624	GLY	-	expression tag	UNP P08648
C	625	GLY	-	expression tag	UNP P08648
C	626	LEU	-	expression tag	UNP P08648
C	627	GLU	-	expression tag	UNP P08648
C	628	ASN	-	expression tag	UNP P08648
C	629	LEU	-	expression tag	UNP P08648
C	630	TYR	-	expression tag	UNP P08648
C	631	PHE	-	expression tag	UNP P08648
C	632	GLN	-	expression tag	UNP P08648

- Molecule 2 is a protein called Integrin beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	431	Total	C	N	O	S	0	0	0
			3353	2096	572	661	24			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	433	3372	2109	575	664	24	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	92	HIS	THR	SEE REMARK 999	UNP P05556
B	195	THR	SER	SEE REMARK 999	UNP P05556
B	446	GLY	-	expression tag	UNP P05556
B	447	GLY	-	expression tag	UNP P05556
B	448	LEU	-	expression tag	UNP P05556
B	449	GLU	-	expression tag	UNP P05556
B	450	ASN	-	expression tag	UNP P05556
B	451	LEU	-	expression tag	UNP P05556
B	452	TYR	-	expression tag	UNP P05556
B	453	PHE	-	expression tag	UNP P05556
B	454	GLN	-	expression tag	UNP P05556
D	92	HIS	THR	SEE REMARK 999	UNP P05556
D	195	THR	SER	SEE REMARK 999	UNP P05556
D	446	GLY	-	expression tag	UNP P05556
D	447	GLY	-	expression tag	UNP P05556
D	448	LEU	-	expression tag	UNP P05556
D	449	GLU	-	expression tag	UNP P05556
D	450	ASN	-	expression tag	UNP P05556
D	451	LEU	-	expression tag	UNP P05556
D	452	TYR	-	expression tag	UNP P05556
D	453	PHE	-	expression tag	UNP P05556
D	454	GLN	-	expression tag	UNP P05556

- Molecule 3 is a protein called SG/19 Fab fragment (Light chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	219	1701	1066	292	335	8	0	0	0
3	E	219	1701	1066	292	335	8	0	0	0

- Molecule 4 is a protein called SG/19 Fab fragment (Heavy chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	218	1651	1051	268	324	8	0	0	0

*Continued on next page...*

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	218	1651	1051	268	324	8	0	0	0

- Molecule 5 is a protein called RGD peptide.

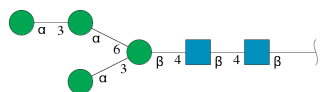
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	G	4	31	16	8	7	0	0	0
5	I	3	23	12	6	5	0	0	0

- 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
			Total	C	N	O			
6	J	2	28	16	2	10	0	0	0
6	M	2	28	16	2	10	0	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

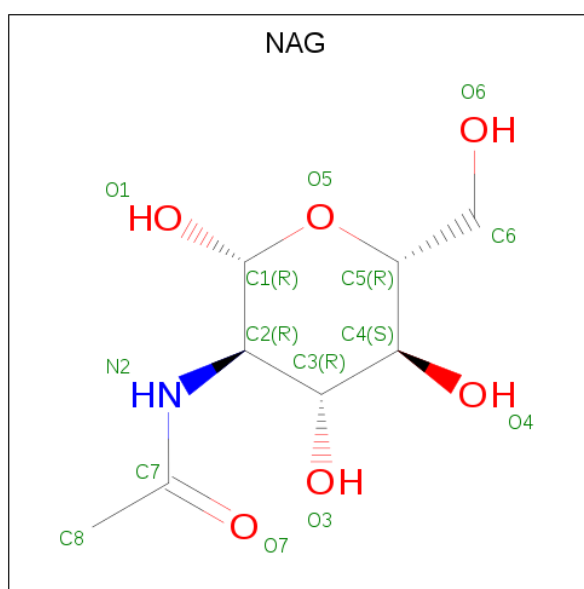


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	K	6	72	40	2	30	0	0	0
7	N	6	72	40	2	30	0	0	0

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Ca 1 1	0	0
8	A	4	Total Ca 4 4	0	0
8	D	1	Total Ca 1 1	0	0
8	C	4	Total Ca 4 4	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

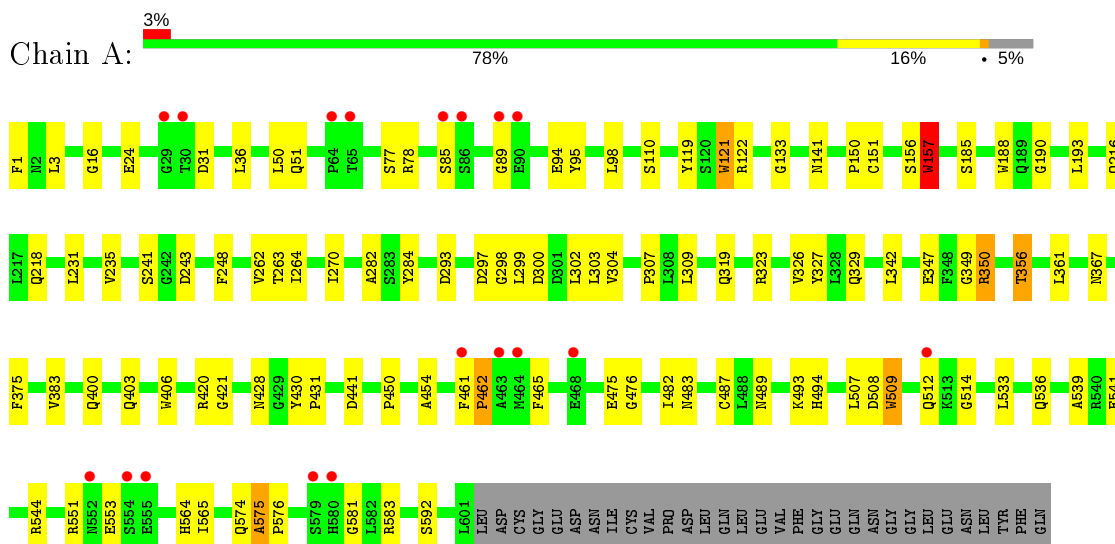
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	Mg	0	0
			1	1		
10	D	1	Total	Mg	0	0
			1	1		



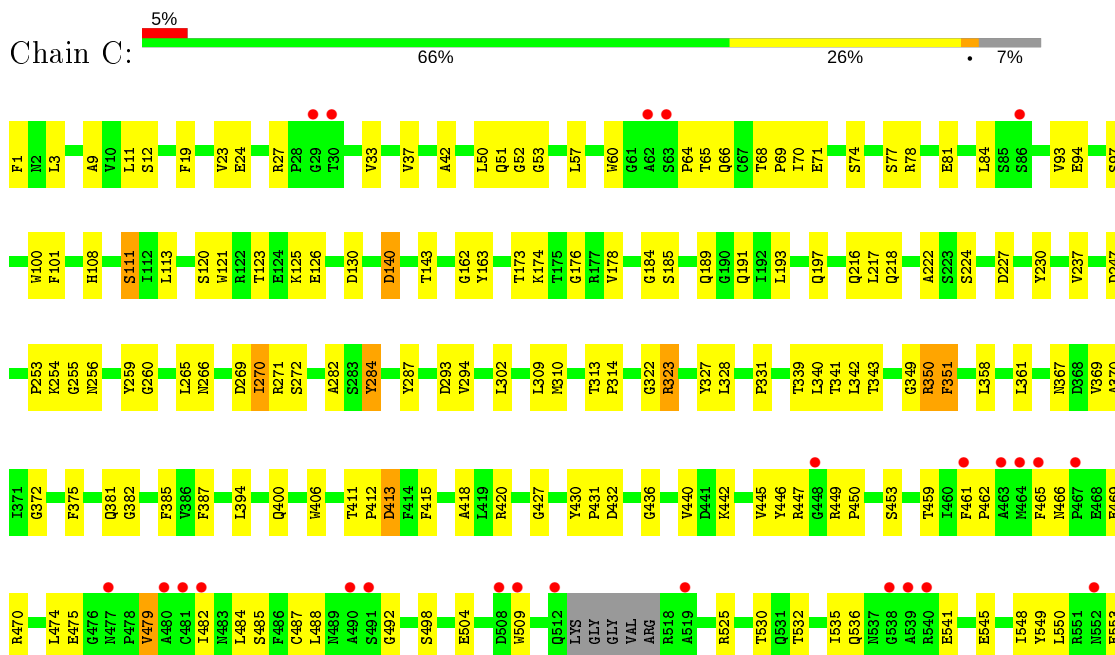
### 3 Residue-property plots [i](#)

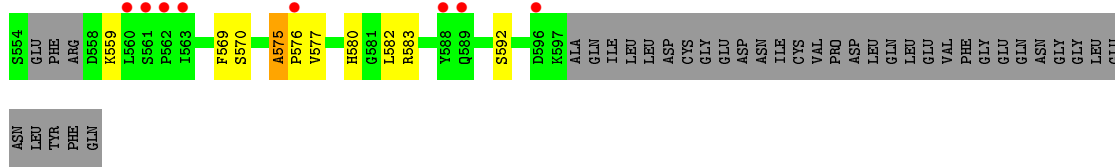
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Integrin alpha-5

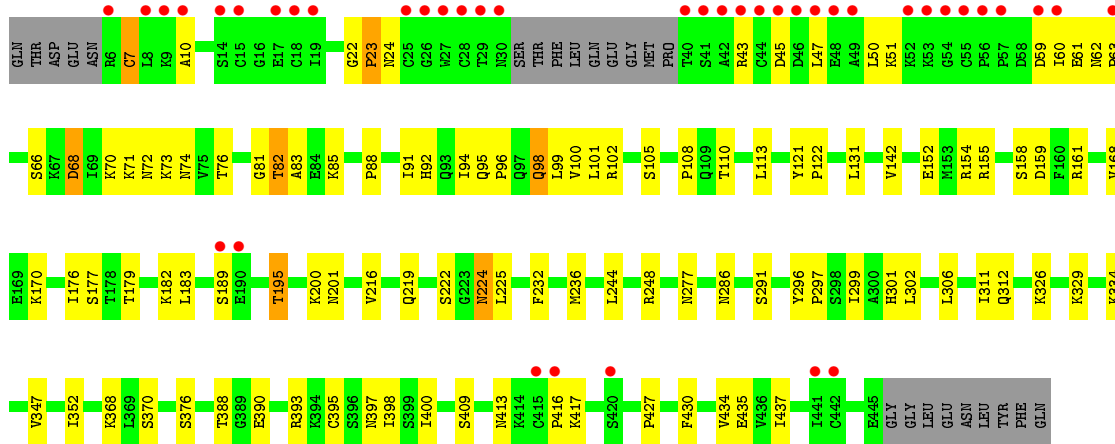


- Molecule 1: Integrin alpha-5

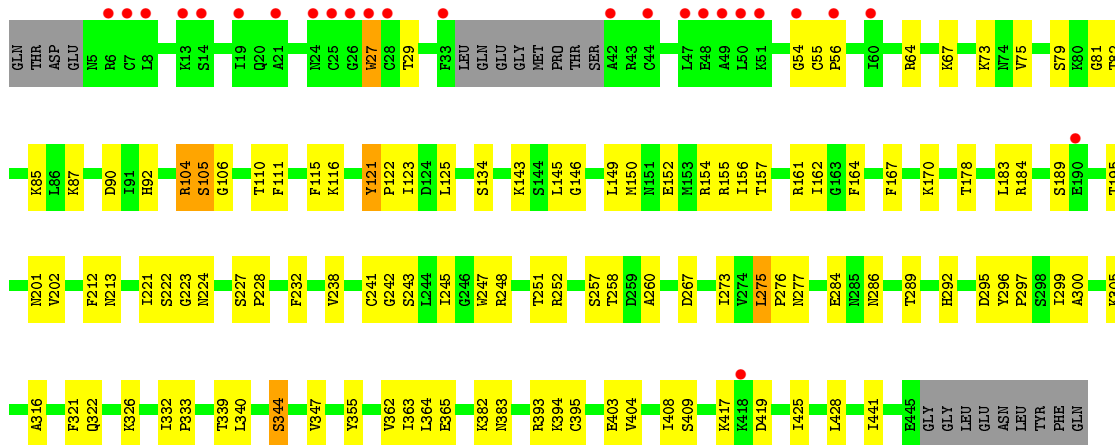




• Molecule 2: Integrin beta-1



• Molecule 2: Integrin beta-1

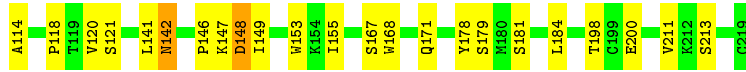
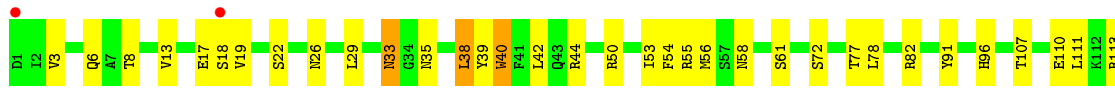
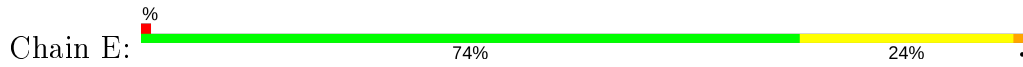


• Molecule 3: SG/19 Fab fragment (Light chain)

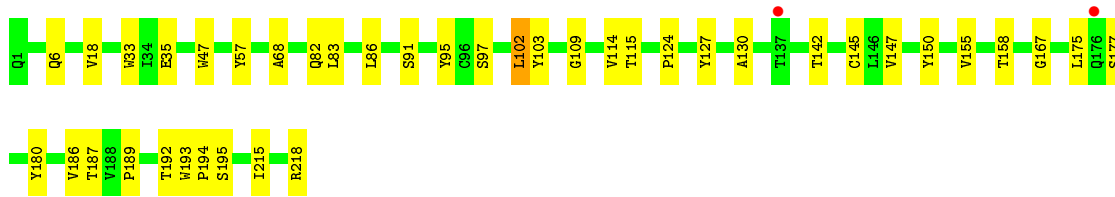
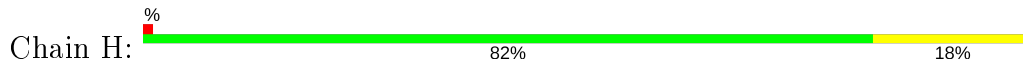




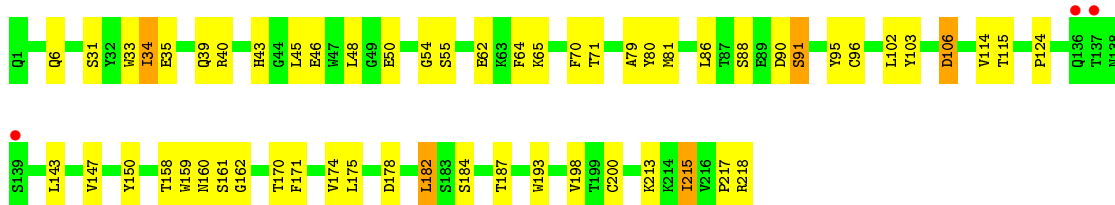
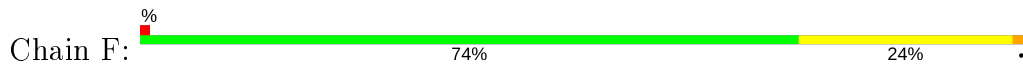
- Molecule 3: SG/19 Fab fragment (Light chain)



- Molecule 4: SG/19 Fab fragment (Heavy chain)



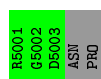
- Molecule 4: SG/19 Fab fragment (Heavy chain)



- Molecule 5: RGD peptide



- Molecule 5: RGD peptide




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

Chain J:  50% 50%

MAG1  
MAG2

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

Chain M:  100%


MAG1  
MAG2

- Molecule 7: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  17% 83%

MAG3  
MAG2  
EMAG3  
MAN4  
MAN5  
MAN6

- Molecule 7: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  83% 17%

MAG1  
MAG2  
EMAG3  
MAN4  
MAN5  
MAN6

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.81Å 103.87Å 125.26Å 75.72° 70.16° 70.90°	Depositor
Resolution (Å)	100.00 – 2.90 47.92 – 2.89	Depositor EDS
% Data completeness (in resolution range)	98.3 (100.00-2.90) 97.9 (47.92-2.89)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 2.91Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.215 , 0.275 0.213 , 0.272	Depositor DCC
$R_{free}$ test set	4464 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.6	Xtrriage
Anisotropy	0.474	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 33.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	22882	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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, MG, BMA, CA, 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	0.46	4/4684 (0.1%)	0.62	0/6374
1	C	0.48	4/4580 (0.1%)	0.63	0/6234
2	B	0.41	0/3410	0.59	0/4601
2	D	0.43	1/3430 (0.0%)	0.63	0/4628
3	E	0.50	3/1741 (0.2%)	0.65	1/2364 (0.0%)
3	L	0.51	2/1741 (0.1%)	0.63	1/2364 (0.0%)
4	F	0.56	1/1698 (0.1%)	0.63	0/2323
4	H	0.56	1/1698 (0.1%)	0.66	0/2323
5	G	0.49	0/30	0.52	0/38
5	I	0.49	0/22	0.57	0/27
All	All	0.48	16/23034 (0.1%)	0.62	2/31276 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	40	TRP	CD2-CE2	5.51	1.48	1.41
1	C	406	TRP	CD2-CE2	5.48	1.48	1.41
3	E	40	TRP	CD2-CE2	5.46	1.47	1.41
1	A	121	TRP	CD2-CE2	5.43	1.47	1.41
3	L	168	TRP	CD2-CE2	5.34	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	94	LEU	CA-CB-CG	5.70	128.40	115.30
3	E	142	ASN	N-CA-C	5.38	125.53	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4567	0	4363	59	0
1	C	4466	0	4247	102	0
2	B	3353	0	3305	67	0
2	D	3372	0	3321	77	0
3	E	1701	0	1649	43	0
3	L	1701	0	1649	34	0
4	F	1651	0	1610	38	0
4	H	1651	0	1610	21	0
5	G	31	0	25	1	0
5	I	23	0	19	0	0
6	J	28	0	25	1	0
6	M	28	0	25	0	0
7	K	72	0	61	0	0
7	N	72	0	61	1	0
8	A	4	0	0	0	0
8	B	1	0	0	0	0
8	C	4	0	0	0	0
8	D	1	0	0	0	0
9	A	56	0	52	0	0
9	B	28	0	26	0	0
9	C	56	0	52	1	0
9	D	14	0	13	0	0
10	B	1	0	0	0	0
10	D	1	0	0	0	0
All	All	22882	0	22113	417	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 9.

The worst 5 of 417 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)
2:B:110:THR:HG22	2:B:409:SER:HB3	1.15	1.07
2:D:110:THR:HG22	2:D:409:SER:HB3	1.36	1.05
2:B:7:CYS:HB3	2:B:45:ASP:HA	1.39	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:284:GLU:HG2	2:D:289:THR:HG21	1.50	0.94
2:D:110:THR:HG22	2:D:409:SER:CB	1.98	0.93

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	599/632 (95%)	533 (89%)	56 (9%)	10 (2%)	9	31
1	C	583/632 (92%)	504 (86%)	69 (12%)	10 (2%)	9	31
2	B	427/454 (94%)	376 (88%)	46 (11%)	5 (1%)	13	40
2	D	429/454 (94%)	386 (90%)	38 (9%)	5 (1%)	13	40
3	E	217/219 (99%)	193 (89%)	22 (10%)	2 (1%)	17	48
3	L	217/219 (99%)	201 (93%)	13 (6%)	3 (1%)	11	36
4	F	216/218 (99%)	192 (89%)	22 (10%)	2 (1%)	17	48
4	H	216/218 (99%)	199 (92%)	16 (7%)	1 (0%)	29	61
5	G	2/5 (40%)	1 (50%)	1 (50%)	0	100	100
5	I	1/5 (20%)	1 (100%)	0	0	100	100
All	All	2907/3056 (95%)	2586 (89%)	283 (10%)	38 (1%)	12	37

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	575	ALA
2	B	416	PRO
1	C	350	ARG
1	C	575	ALA
1	A	514	GLY



### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	486/513 (95%)	475 (98%)	11 (2%)	50	80
1	C	476/513 (93%)	463 (97%)	13 (3%)	44	77
2	B	382/402 (95%)	361 (94%)	21 (6%)	21	53
2	D	384/402 (96%)	369 (96%)	15 (4%)	32	66
3	E	194/194 (100%)	188 (97%)	6 (3%)	40	74
3	L	194/194 (100%)	188 (97%)	6 (3%)	40	74
4	F	186/186 (100%)	175 (94%)	11 (6%)	19	49
4	H	186/186 (100%)	179 (96%)	7 (4%)	33	67
5	G	3/4 (75%)	3 (100%)	0	100	100
5	I	2/4 (50%)	2 (100%)	0	100	100
All	All	2493/2598 (96%)	2403 (96%)	90 (4%)	35	69

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	369	VAL
2	D	134	SER
4	F	102	LEU
1	C	413	ASP
2	D	27	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	197	GLN
2	D	5	ASN
3	E	194	HIS
1	C	552	ASN
2	D	92	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

16 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	J	1	1,6	14,14,15	0.49	0	17,19,21	2.09	4 (23%)
6	NAG	J	2	6	14,14,15	0.51	0	17,19,21	1.30	2 (11%)
7	NAG	K	1	1,7	14,14,15	0.75	0	17,19,21	0.90	0
7	NAG	K	2	7	14,14,15	0.62	0	17,19,21	2.15	3 (17%)
7	BMA	K	3	7	11,11,12	0.50	0	15,15,17	1.07	1 (6%)
7	MAN	K	4	7	11,11,12	0.58	0	15,15,17	1.43	2 (13%)
7	MAN	K	5	7	11,11,12	0.82	0	15,15,17	1.51	3 (20%)
7	MAN	K	6	7	11,11,12	0.68	0	15,15,17	0.80	1 (6%)
6	NAG	M	1	1,6	14,14,15	0.51	0	17,19,21	2.35	5 (29%)
6	NAG	M	2	6	14,14,15	0.52	0	17,19,21	0.90	1 (5%)
7	NAG	N	1	1,7	14,14,15	0.70	0	17,19,21	1.27	2 (11%)
7	NAG	N	2	7	14,14,15	0.57	0	17,19,21	2.37	3 (17%)
7	BMA	N	3	7	11,11,12	0.41	0	15,15,17	1.03	1 (6%)
7	MAN	N	4	7	11,11,12	0.62	0	15,15,17	1.63	3 (20%)
7	MAN	N	5	7	11,11,12	0.53	0	15,15,17	1.01	2 (13%)
7	MAN	N	6	7	11,11,12	0.66	0	15,15,17	1.26	2 (13%)

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	J	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	2	6	-	2/6/23/26	0/1/1/1
7	NAG	K	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	K	2	7	-	1/6/23/26	0/1/1/1
7	BMA	K	3	7	-	0/2/19/22	0/1/1/1
7	MAN	K	4	7	-	2/2/19/22	0/1/1/1
7	MAN	K	5	7	-	2/2/19/22	0/1/1/1
7	MAN	K	6	7	-	2/2/19/22	0/1/1/1
6	NAG	M	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	M	2	6	-	2/6/23/26	0/1/1/1
7	NAG	N	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	N	2	7	-	1/6/23/26	0/1/1/1
7	BMA	N	3	7	-	0/2/19/22	0/1/1/1
7	MAN	N	4	7	-	0/2/19/22	0/1/1/1
7	MAN	N	5	7	-	2/2/19/22	0/1/1/1
7	MAN	N	6	7	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	2	NAG	C2-N2-C7	7.10	133.02	122.90
6	M	1	NAG	C1-O5-C5	6.07	120.41	112.19
7	K	2	NAG	C2-N2-C7	5.53	130.77	122.90
7	K	2	NAG	C4-C3-C2	-5.33	103.21	111.02
6	J	1	NAG	C1-O5-C5	5.16	119.18	112.19

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

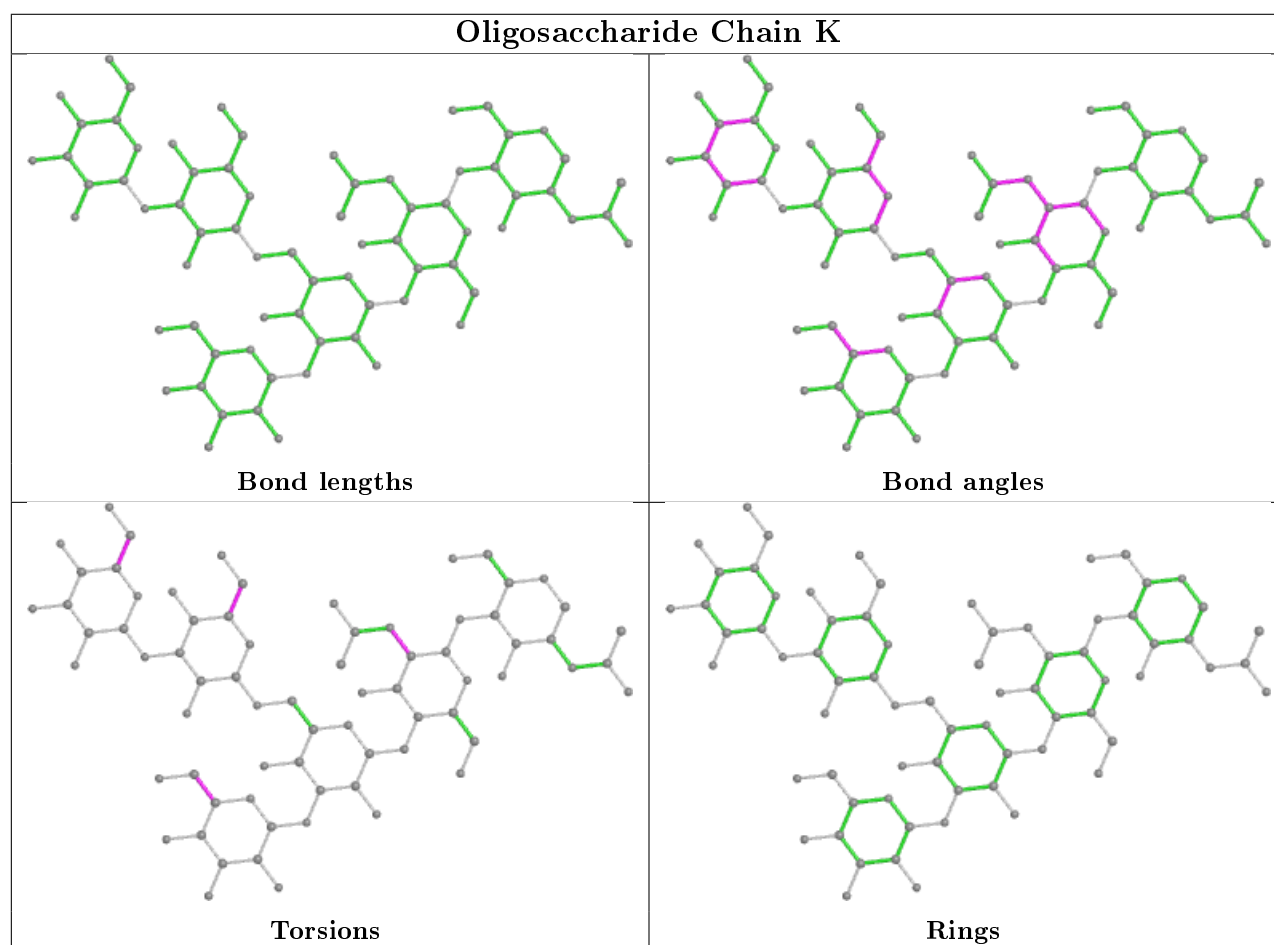
Mol	Chain	Res	Type	Atoms
7	N	2	NAG	C3-C2-N2-C7
6	J	2	NAG	O5-C5-C6-O6
6	M	1	NAG	C4-C5-C6-O6
7	K	6	MAN	O5-C5-C6-O6
6	J	2	NAG	C4-C5-C6-O6

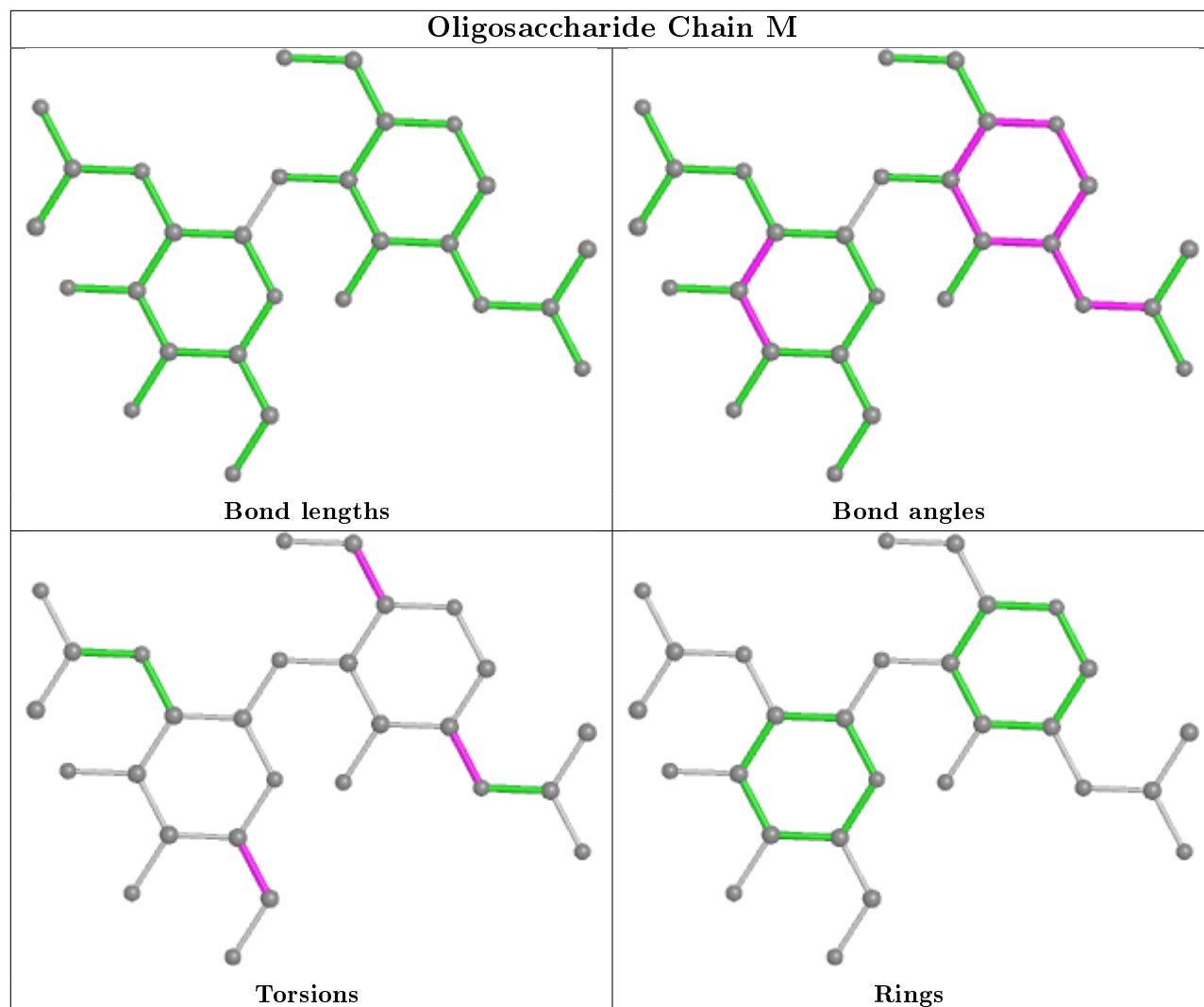
There are no ring outliers.

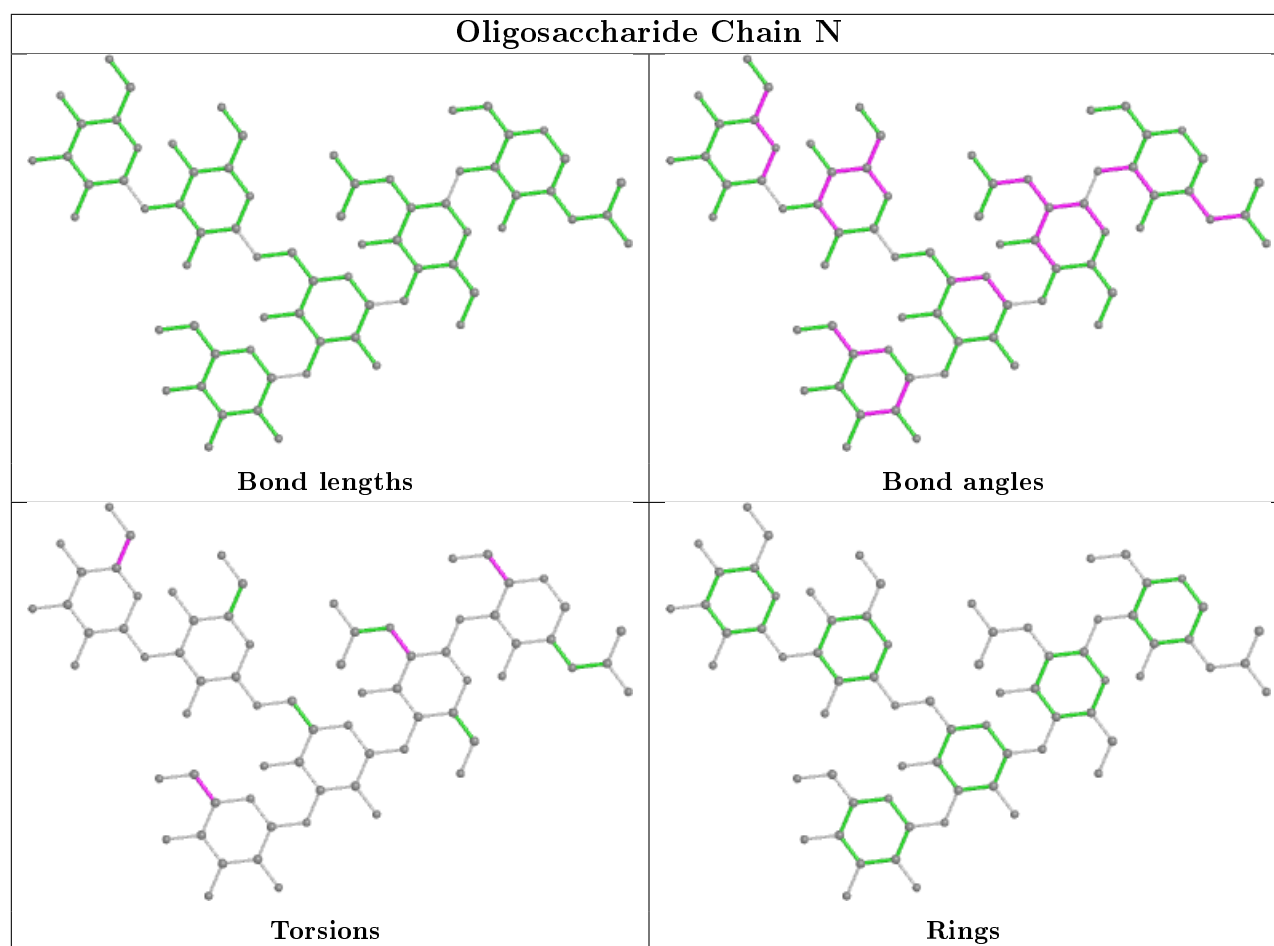
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	1	NAG	1	0
7	N	1	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](#)

Of 23 ligands modelled in this entry, 12 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
9	NAG	C	2008	1	14,14,15	0.53	0	17,19,21	0.96	1 (5%)
9	NAG	A	2007	1	14,14,15	0.50	0	17,19,21	0.84	0
9	NAG	C	2007	1	14,14,15	0.53	0	17,19,21	0.88	1 (5%)
9	NAG	C	2016	1	14,14,15	0.44	0	17,19,21	1.39	1 (5%)
9	NAG	B	503	2	14,14,15	0.57	0	17,19,21	1.00	1 (5%)
9	NAG	D	503	2	14,14,15	0.38	0	17,19,21	1.91	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	A	2006	1	14,14,15	0.57	0	17,19,21	1.06	1 (5%)
9	NAG	B	504	2	14,14,15	0.47	0	17,19,21	1.02	1 (5%)
9	NAG	A	2005	1	14,14,15	0.48	0	17,19,21	1.10	1 (5%)
9	NAG	C	2009	1	14,14,15	0.53	0	17,19,21	1.33	2 (11%)
9	NAG	A	2016	1	14,14,15	0.48	0	17,19,21	2.08	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	C	2008	1	-	0/6/23/26	0/1/1/1
9	NAG	A	2007	1	-	0/6/23/26	0/1/1/1
9	NAG	C	2007	1	-	0/6/23/26	0/1/1/1
9	NAG	C	2016	1	-	1/6/23/26	0/1/1/1
9	NAG	B	503	2	-	0/6/23/26	0/1/1/1
9	NAG	D	503	2	-	2/6/23/26	0/1/1/1
9	NAG	A	2006	1	-	1/6/23/26	0/1/1/1
9	NAG	B	504	2	-	0/6/23/26	0/1/1/1
9	NAG	A	2005	1	-	0/6/23/26	0/1/1/1
9	NAG	C	2009	1	-	2/6/23/26	0/1/1/1
9	NAG	A	2016	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2016	NAG	C1-O5-C5	7.19	121.93	112.19
9	D	503	NAG	C1-O5-C5	6.28	120.69	112.19
9	C	2016	NAG	C1-O5-C5	4.21	117.90	112.19
9	A	2005	NAG	C1-O5-C5	3.53	116.98	112.19
9	C	2009	NAG	C1-O5-C5	3.48	116.90	112.19

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	D	503	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	C	2009	NAG	O5-C5-C6-O6
9	D	503	NAG	C4-C5-C6-O6
9	C	2009	NAG	C4-C5-C6-O6
9	A	2016	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	2016	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	601/632 (95%)	-0.06	18 (2%) 50 45	40, 66, 115, 159	0
1	C	589/632 (93%)	0.09	33 (5%) 24 20	37, 65, 131, 164	0
2	B	431/454 (94%)	0.29	41 (9%) 8 6	41, 64, 161, 217	0
2	D	433/454 (95%)	-0.03	25 (5%) 23 19	36, 58, 139, 160	0
3	E	219/219 (100%)	-0.36	2 (0%) 84 84	42, 62, 80, 94	0
3	L	219/219 (100%)	-0.43	0 100 100	38, 55, 73, 85	0
4	F	218/218 (100%)	-0.23	3 (1%) 75 75	44, 66, 106, 127	0
4	H	218/218 (100%)	-0.34	2 (0%) 84 84	35, 58, 97, 111	0
5	G	4/5 (80%)	-0.00	0 100 100	85, 87, 88, 99	0
5	I	3/5 (60%)	-0.27	0 100 100	77, 77, 82, 86	0
All	All	2935/3056 (96%)	-0.06	124 (4%) 36 32	35, 62, 127, 217	0

The worst 5 of 124 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	43	ARG	14.4
2	B	42	ALA	13.4
2	B	41	SER	12.0
2	B	28	CYS	9.3
2	B	19	ILE	7.8

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates

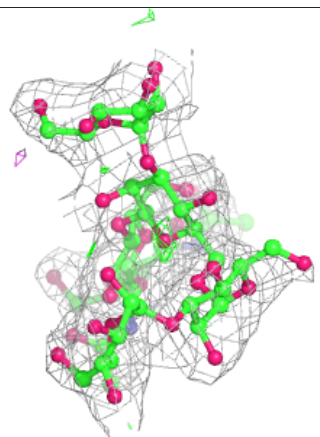
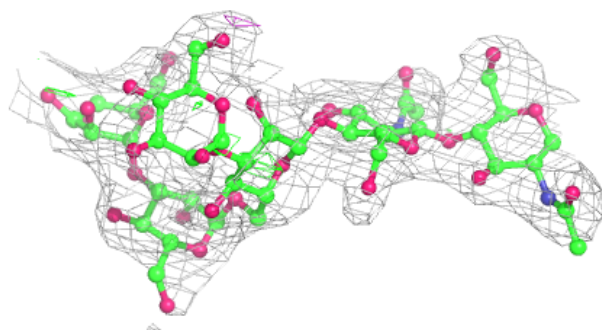
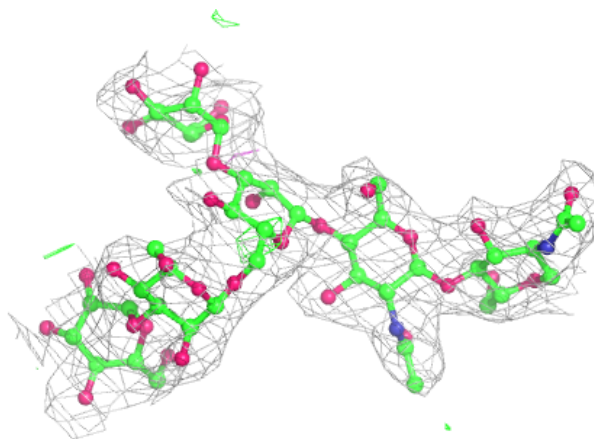
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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
6	NAG	J	2	14/15	0.78	0.31	85,99,103,104	0
7	MAN	N	6	11/12	0.78	0.16	81,91,95,96	0
7	MAN	N	4	11/12	0.83	0.12	83,86,92,97	0
7	BMA	K	3	11/12	0.84	0.13	72,80,84,86	0
7	MAN	K	4	11/12	0.86	0.17	85,95,103,104	0
6	NAG	M	2	14/15	0.87	0.24	88,94,98,100	0
7	MAN	N	5	11/12	0.88	0.15	79,85,97,103	0
7	MAN	K	5	11/12	0.89	0.11	84,89,94,97	0
7	MAN	K	6	11/12	0.90	0.14	78,84,87,95	0
6	NAG	M	1	14/15	0.91	0.19	73,78,87,88	0
7	BMA	N	3	11/12	0.92	0.10	71,76,82,85	0
7	NAG	K	2	14/15	0.93	0.16	61,64,71,75	0
6	NAG	J	1	14/15	0.93	0.22	74,81,86,92	0
7	NAG	N	2	14/15	0.94	0.16	57,61,68,77	0
7	NAG	N	1	14/15	0.96	0.11	50,54,60,64	0
7	NAG	K	1	14/15	0.96	0.11	54,59,62,68	0

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

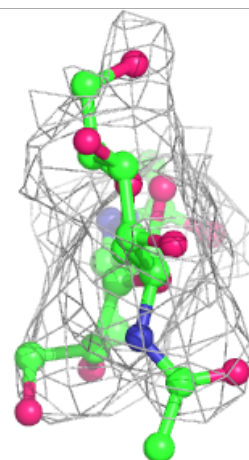
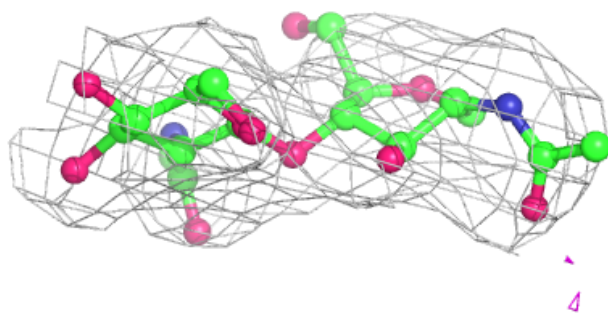
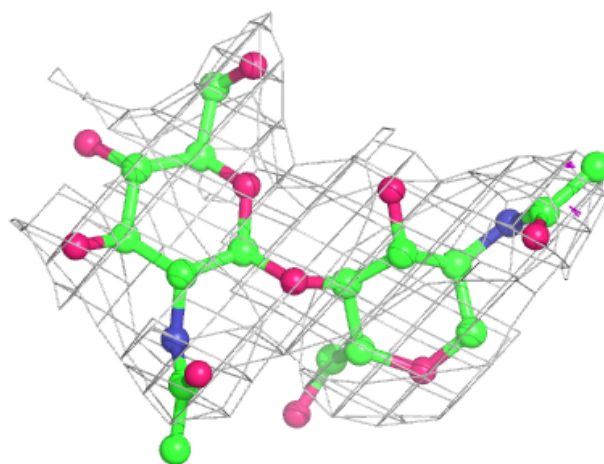
**Electron density around Chain K:**

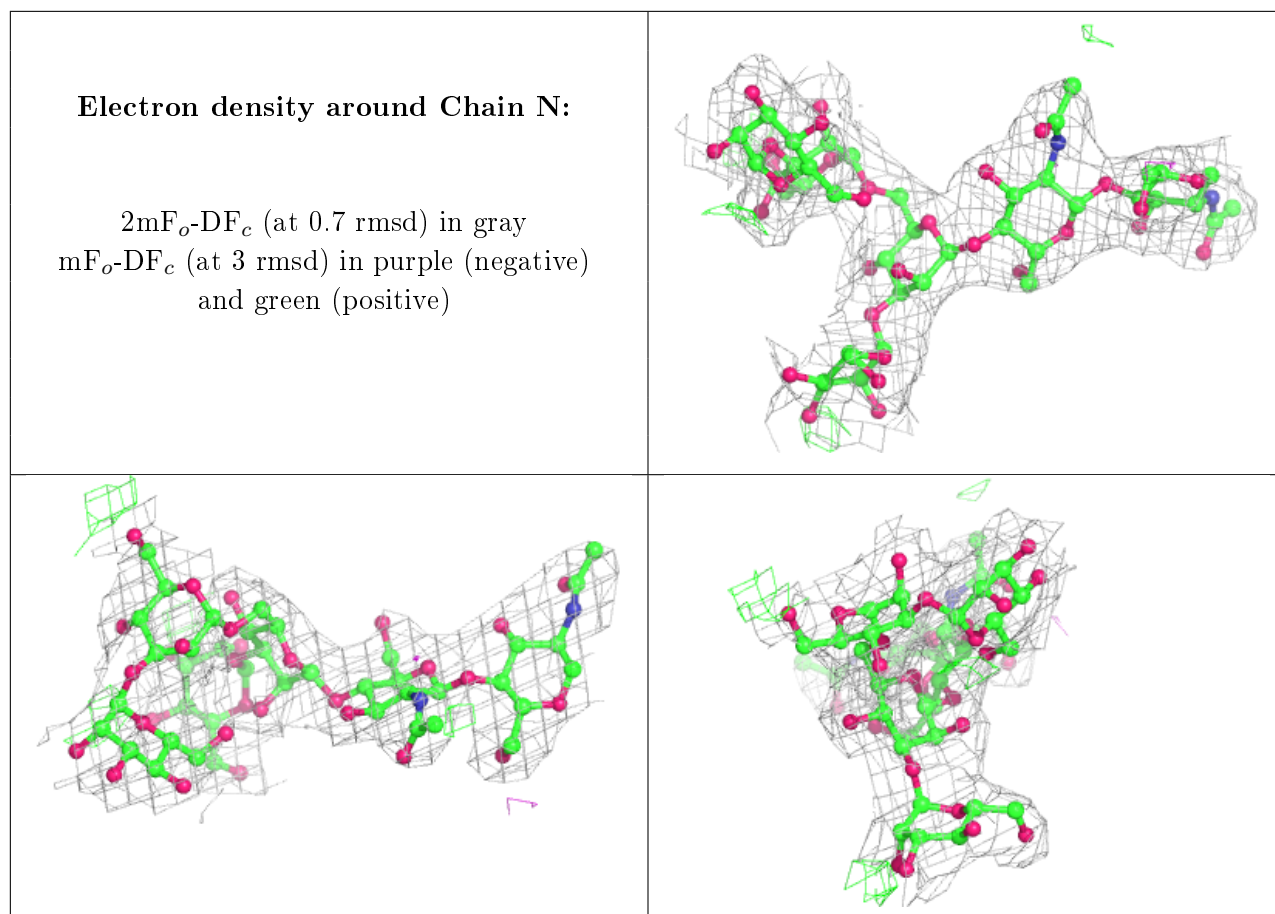
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain M:**

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





## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
9	NAG	C	2007	14/15	0.73	0.18	67,78,85,86	0
9	NAG	C	2008	14/15	0.77	0.18	103,112,114,114	0
9	NAG	A	2006	14/15	0.78	0.16	98,103,109,113	0
9	NAG	C	2016	14/15	0.80	0.19	88,94,106,111	0
10	MG	D	502	1/1	0.80	0.10	66,66,66,66	0
8	CA	A	2004	1/1	0.81	0.13	81,81,81,81	0
9	NAG	D	503	14/15	0.83	0.14	55,62,65,66	0
9	NAG	A	2016	14/15	0.84	0.19	84,89,95,99	0
8	CA	C	2004	1/1	0.86	0.11	76,76,76,76	0
9	NAG	B	503	14/15	0.86	0.15	60,62,67,69	0
9	NAG	A	2007	14/15	0.90	0.14	78,88,93,97	0
9	NAG	B	504	14/15	0.90	0.16	67,70,76,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	NAG	A	2005	14/15	0.90	0.17	64,72,79,79	0
8	CA	A	2002	1/1	0.92	0.06	81,81,81,81	0
9	NAG	C	2009	14/15	0.92	0.14	60,67,71,72	0
8	CA	A	2003	1/1	0.93	0.12	73,73,73,73	0
8	CA	D	501	1/1	0.93	0.12	50,50,50,50	0
8	CA	C	2001	1/1	0.94	0.12	58,58,58,58	0
10	MG	B	502	1/1	0.95	0.21	66,66,66,66	0
8	CA	C	2003	1/1	0.95	0.10	78,78,78,78	0
8	CA	A	2001	1/1	0.96	0.13	69,69,69,69	0
8	CA	C	2002	1/1	0.97	0.07	80,80,80,80	0
8	CA	B	501	1/1	0.99	0.09	59,59,59,59	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.