wwPDB X-ray Structure Validation Summary Report (i)

Aug 7, 2020 – 11:40 PM BST

PDB ID	:	4X4M
Title	:	Structure of FcgammaRI in complex with Fc reveals the importance of glycan recognition for high affinity IgG binding
Authors	:	Lu, J.; Sun, P.D.
Deposited on	:	2014-12-03
Resolution	:	3.48 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

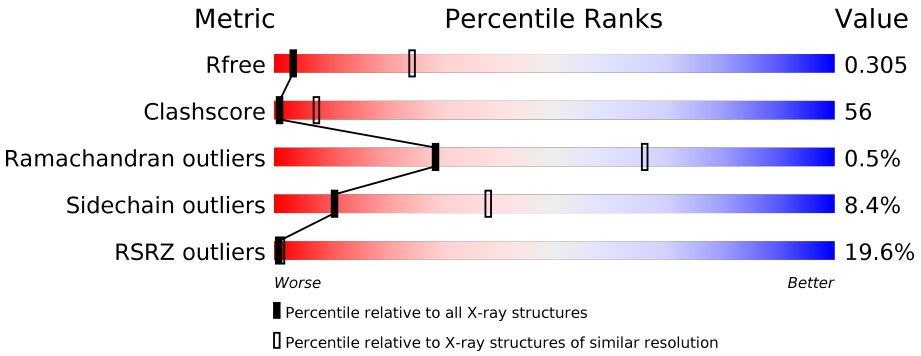
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.48 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	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

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 <=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	219	9% 42% 54% •
1	B	219	11% 38% 53% 7% •
1	C	219	7% 45% 47% 5% •
1	D	219	13% 38% 53% 6% •
2	E	275	34% 30% 55% 9% 6%
2	F	275	32% 26% 59% 8% • 6%

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Mol	Chain	Length	Quality of chain
3	G	8	100%
3	H	8	100%
4	I	9	11% 89%
5	J	6	17% 83%
6	K	2	50% 50%

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
3	BMA	G	3	-	-	X	-
3	MAN	G	6	-	-	X	-
3	MAN	H	4	-	-	X	-
4	NAG	I	2	-	-	X	-
4	BMA	I	3	-	-	X	-
4	MAN	I	4	-	-	X	-
4	MAN	I	7	-	-	X	-
5	NAG	J	4	-	-	X	-
7	NAG	D	1001	-	-	X	-
8	FUL	D	1008	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11374 atoms, of which 8 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 Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	218	Total	C	H	N	O	S	0	0	0
			1737	1101	8	290	331	7			
1	B	216	Total	C		N	O	S	0	0	0
			1716	1093		288	329	6			
1	C	212	Total	C		N	O	S	0	0	0
			1694	1080		284	324	6			
1	D	214	Total	C		N	O	S	0	0	0
			1705	1086		286	327	6			

- Molecule 2 is a protein called High affinity immunoglobulin gamma Fc receptor I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	259	Total	C	N	O	S	0	0	0
			2046	1299	352	386	9			
2	F	258	Total	C	N	O	S	0	0	0
			2038	1293	351	385	9			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	25	LYS	THR	engineered mutation	UNP P12314
E	38	SER	THR	engineered mutation	UNP P12314
E	46	PRO	LEU	engineered mutation	UNP P12314
E	63	ILE	THR	engineered mutation	UNP P12314
E	69	THR	SER	engineered mutation	UNP P12314
E	71	HIS	ARG	engineered mutation	UNP P12314
E	77	GLU	VAL	engineered mutation	UNP P12314
E	78	ASP	ASN	engineered mutation	UNP P12314
E	100	VAL	ILE	engineered mutation	UNP P12314
E	114	LEU	PHE	engineered mutation	UNP P12314
E	160	MET	ILE	engineered mutation	UNP P12314
E	163	SER	ASN	engineered mutation	UNP P12314

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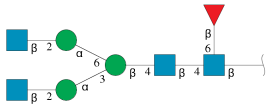
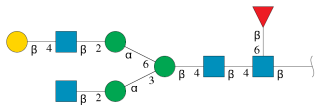
Chain	Residue	Modelled	Actual	Comment	Reference
E	195	THR	ASN	engineered mutation	UNP P12314
E	206	THR	ASN	engineered mutation	UNP P12314
E	207	PRO	LEU	engineered mutation	UNP P12314
E	240	ASP	ASN	engineered mutation	UNP P12314
E	283	HIS	LEU	engineered mutation	UNP P12314
E	285	GLN	LEU	engineered mutation	UNP P12314
E	290	HIS	-	expression tag	UNP P12314
E	291	HIS	-	expression tag	UNP P12314
E	292	HIS	-	expression tag	UNP P12314
E	293	HIS	-	expression tag	UNP P12314
E	294	HIS	-	expression tag	UNP P12314
E	295	HIS	-	expression tag	UNP P12314
F	25	LYS	THR	engineered mutation	UNP P12314
F	38	SER	THR	engineered mutation	UNP P12314
F	46	PRO	LEU	engineered mutation	UNP P12314
F	63	ILE	THR	engineered mutation	UNP P12314
F	69	THR	SER	engineered mutation	UNP P12314
F	71	HIS	ARG	engineered mutation	UNP P12314
F	77	GLU	VAL	engineered mutation	UNP P12314
F	78	ASP	ASN	engineered mutation	UNP P12314
F	100	VAL	ILE	engineered mutation	UNP P12314
F	114	LEU	PHE	engineered mutation	UNP P12314
F	160	MET	ILE	engineered mutation	UNP P12314
F	163	SER	ASN	engineered mutation	UNP P12314
F	195	THR	ASN	engineered mutation	UNP P12314
F	206	THR	ASN	engineered mutation	UNP P12314
F	207	PRO	LEU	engineered mutation	UNP P12314
F	240	ASP	ASN	engineered mutation	UNP P12314
F	283	HIS	LEU	engineered mutation	UNP P12314
F	285	GLN	LEU	engineered mutation	UNP P12314
F	290	HIS	-	expression tag	UNP P12314
F	291	HIS	-	expression tag	UNP P12314
F	292	HIS	-	expression tag	UNP P12314
F	293	HIS	-	expression tag	UNP P12314
F	294	HIS	-	expression tag	UNP P12314
F	295	HIS	-	expression tag	UNP P12314

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



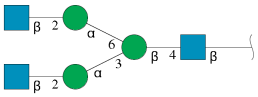
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	8	Total	C	N	O	0	0	0
			99	56	4	39			
3	H	8	Total	C	N	O	0	0	0
			99	56	4	39			

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



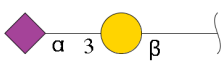
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	9	Total	C	N	O	0	0	0
			110	62	4	44			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



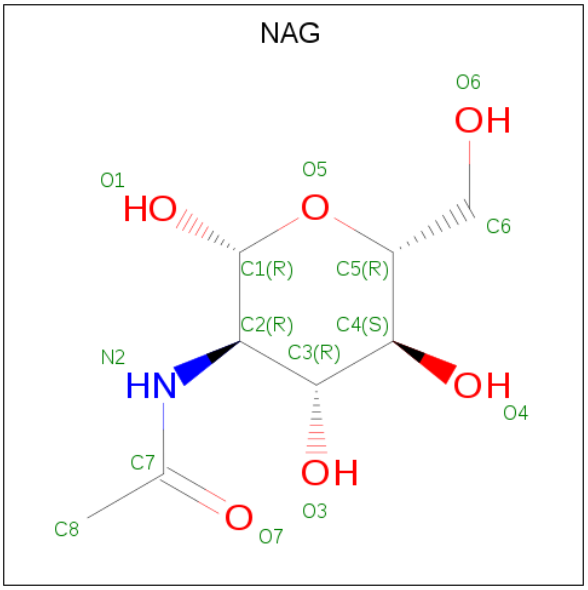
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	J	6	Total	C	N	O	0	0	0
			75	42	3	30			

- Molecule 6 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose.



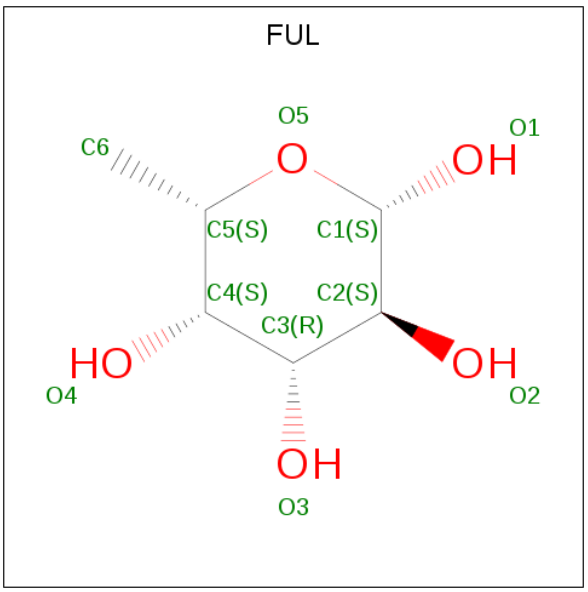
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	K	2	31	17	1	13	0	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is beta-L-fucopyranose (three-letter code: FUL) (formula: $C_6H_{12}O_5$).



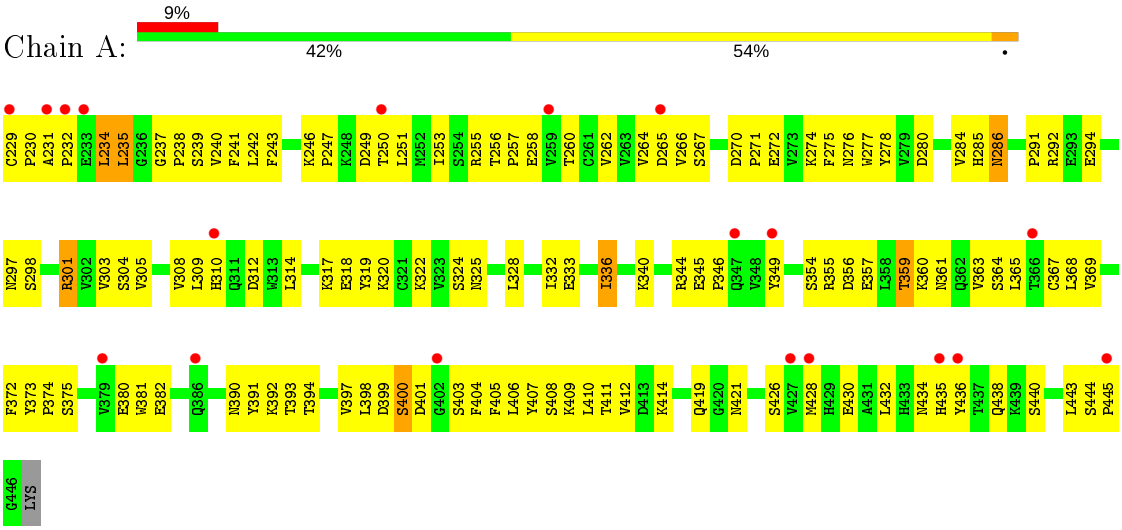
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	D	1	10	6	4	0	0

3 Residue-property plots (i)

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

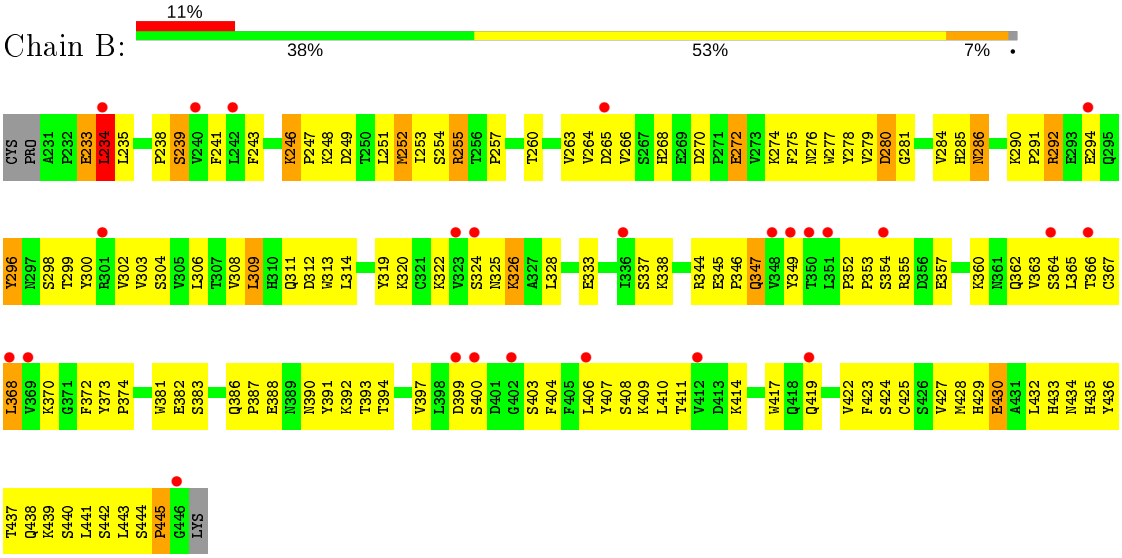
- Molecule 1: Ig gamma-1 chain C region

Chain A:



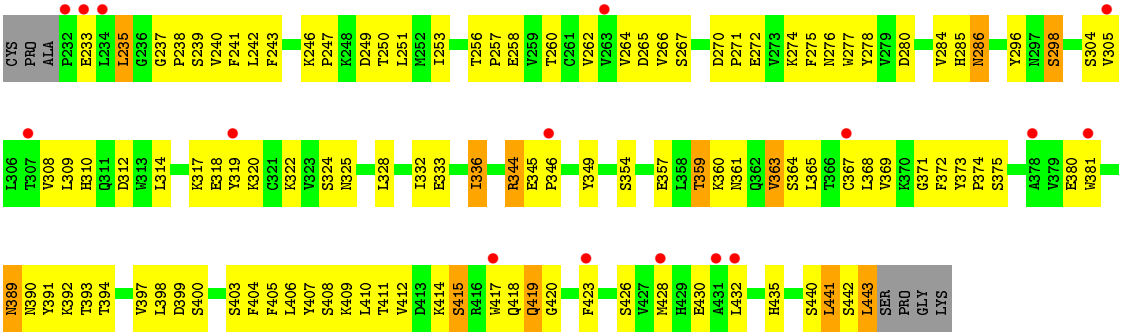
- Molecule 1: Ig gamma-1 chain C region

Chain B:



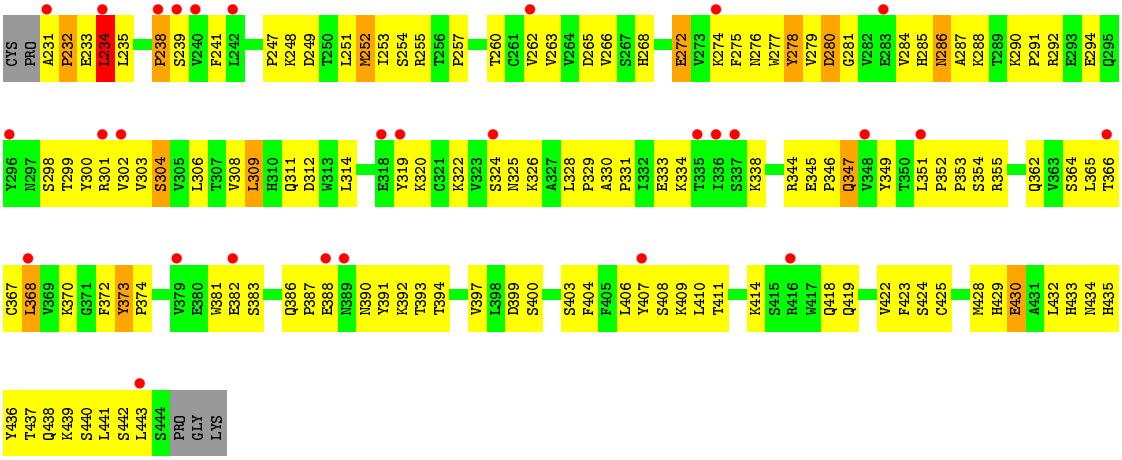
- Molecule 1: Ig gamma-1 chain C region

Chain C:



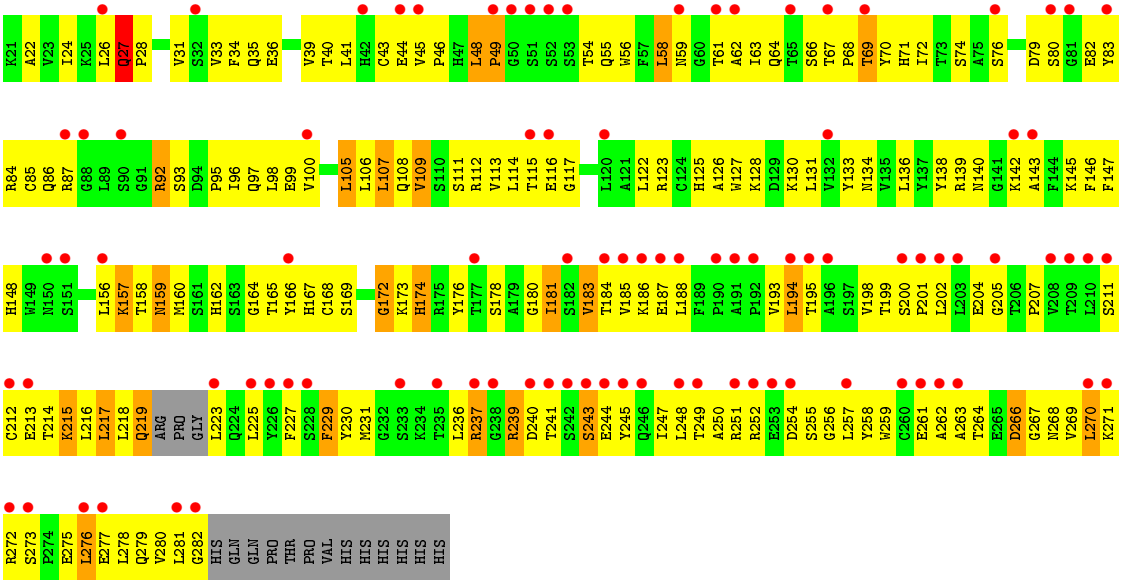
• Molecule 1: Ig gamma-1 chain C region

Chain D:



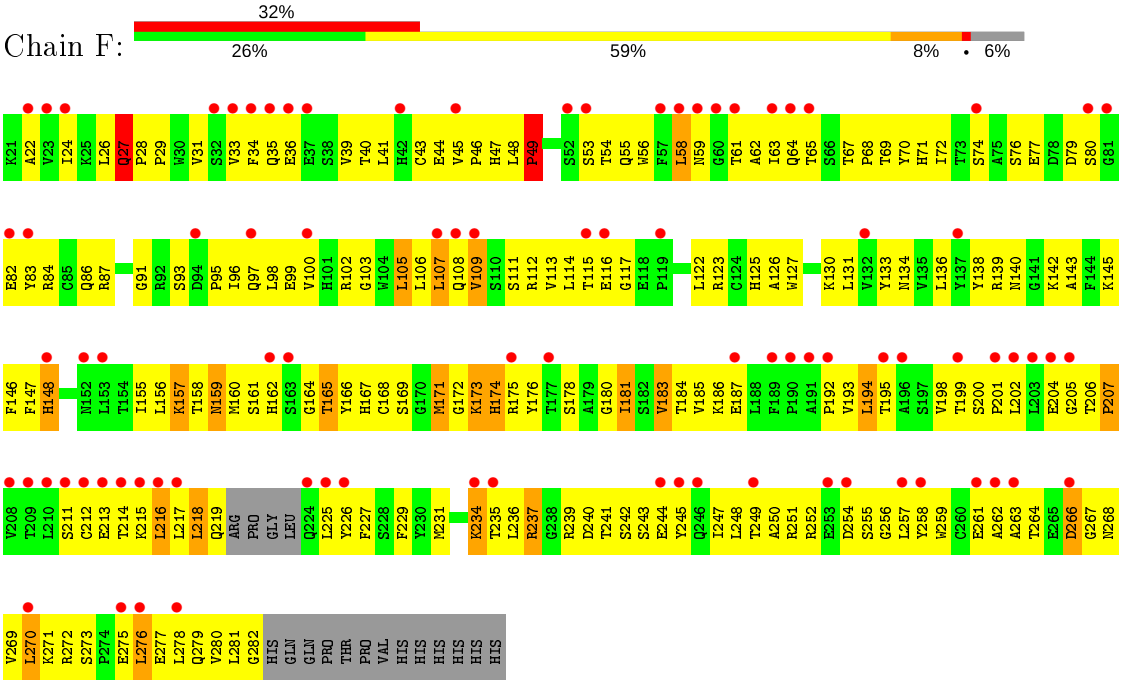
• Molecule 2: High affinity immunoglobulin gamma Fc receptor I

Chain E:



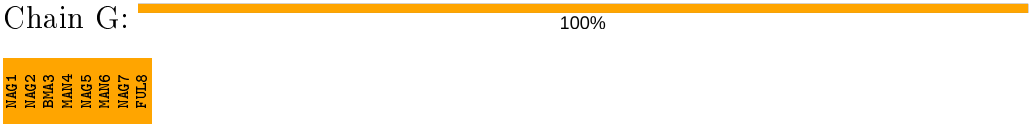
• Molecule 2: High affinity immunoglobulin gamma Fc receptor I

Chain F:



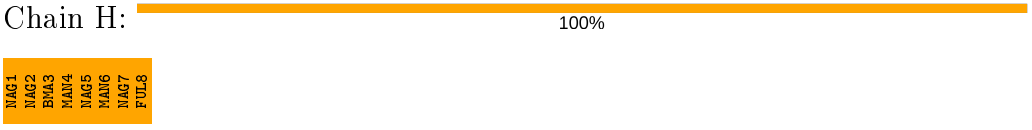
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain H:



• Molecule 4: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

• Molecule 6: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain K:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	59.92Å 67.99Å 125.03Å 89.86° 112.25° 89.96°	Depositor
Resolution (Å)	40.66 – 3.48 40.67 – 3.49	Depositor EDS
% Data completeness (in resolution range)	89.9 (40.66-3.48) 85.6 (40.67-3.49)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.245 , 0.296 0.261 , 0.305	Depositor DCC
R_{free} test set	1037 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	129.1	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 127.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.250 for -h,k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11374	wwPDB-VP
Average B, all atoms (Å^2)	182.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, SIA, GAL, FUL, MAN

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	0.38	0/1778	0.72	4/2425 (0.2%)
1	B	0.35	0/1764	0.74	1/2405 (0.0%)
1	C	0.37	0/1741	0.66	2/2372 (0.1%)
1	D	0.47	2/1752 (0.1%)	0.76	3/2388 (0.1%)
2	E	0.37	0/2096	0.90	9/2847 (0.3%)
2	F	0.38	1/2088 (0.0%)	0.76	2/2836 (0.1%)
All	All	0.39	3/11219 (0.0%)	0.76	21/15273 (0.1%)

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	A	0	1
1	B	0	2
1	D	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	234	LEU	C-N	10.83	1.58	1.34
1	D	238	PRO	N-CD	8.36	1.59	1.47
2	F	49	PRO	N-CD	5.10	1.54	1.47

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	237	ARG	NE-CZ-NH1	16.95	128.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	237	ARG	NE-CZ-NH2	-12.05	114.27	120.30
1	B	234	LEU	CB-CA-C	-11.04	89.23	110.20
1	D	231	ALA	CB-CA-C	-10.99	93.62	110.10
2	E	243	SER	N-CA-CB	-9.22	96.66	110.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	301	ARG	Sidechain
1	B	233	GLU	Mainchain
1	B	234	LEU	Peptide
1	D	234	LEU	Peptide

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	1729	8	1695	132	0
1	B	1716	0	1683	198	1
1	C	1694	0	1664	130	0
1	D	1705	0	1673	205	1
2	E	2046	0	2013	287	1
2	F	2038	0	2002	300	1
3	G	99	0	85	24	0
3	H	99	0	85	19	0
4	I	110	0	93	26	0
5	J	75	0	64	23	0
6	K	31	0	26	9	0
7	D	14	0	12	13	0
8	D	10	0	10	5	0
All	All	11366	8	11105	1255	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 56.

The worst 5 of 1255 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)
5:J:4:NAG:H4	6:K:1:GAL:C1	1.37	1.50
2:F:45:VAL:HG22	2:F:87:ARG:NH2	1.34	1.36
1:C:417:TRP:HZ3	1:C:423:PHE:CD2	1.43	1.35
2:F:99:GLU:OE2	2:F:112:ARG:NH2	1.64	1.28
2:E:227:PHE:O	2:E:241:THR:CG2	1.80	1.28

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:B:296:TYR:OH	1:D:309:LEU:CD2[1_565]	1.84	0.36
2:E:237:ARG:NH1	2:F:244:GLU:OE1[1_646]	2.19	0.01

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	216/219 (99%)	197 (91%)	18 (8%)	1 (0%)	29	66
1	B	214/219 (98%)	200 (94%)	13 (6%)	1 (0%)	29	66
1	C	210/219 (96%)	197 (94%)	13 (6%)	0	100	100
1	D	212/219 (97%)	200 (94%)	11 (5%)	1 (0%)	29	66
2	E	255/275 (93%)	241 (94%)	12 (5%)	2 (1%)	19	57
2	F	254/275 (92%)	245 (96%)	7 (3%)	2 (1%)	19	57
All	All	1361/1426 (95%)	1280 (94%)	74 (5%)	7 (0%)	29	66

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	445	PRO
1	A	445	PRO
1	D	232	PRO

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Mol	Chain	Res	Type
2	E	49	PRO
2	F	49	PRO

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	201/202 (100%)	193 (96%)	8 (4%)	31 62
1	B	199/202 (98%)	183 (92%)	16 (8%)	12 40
1	C	197/202 (98%)	184 (93%)	13 (7%)	16 48
1	D	198/202 (98%)	184 (93%)	14 (7%)	14 45
2	E	229/244 (94%)	205 (90%)	24 (10%)	7 29
2	F	228/244 (93%)	198 (87%)	30 (13%)	4 19
All	All	1252/1296 (97%)	1147 (92%)	105 (8%)	11 38

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	368	LEU
2	E	128	LYS
2	F	218	LEU
1	D	373	TYR
2	E	69	THR

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

Mol	Chain	Res	Type
1	D	268	HIS
1	D	342	GLN
2	F	134	ASN
1	D	295	GLN
1	D	384	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

33 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	$\#\|Z\| > 2$
3	NAG	G	1	1,3	14,14,15	1.62	3 (21%)	17,19,21	1.80	3 (17%)
3	NAG	G	2	3	14,14,15	1.58	3 (21%)	17,19,21	1.62	4 (23%)
3	BMA	G	3	3	11,11,12	1.75	2 (18%)	15,15,17	2.68	7 (46%)
3	MAN	G	4	3	11,11,12	1.98	2 (18%)	15,15,17	1.79	3 (20%)
3	NAG	G	5	3	14,14,15	1.59	3 (21%)	17,19,21	1.55	4 (23%)
3	MAN	G	6	3	11,11,12	1.73	3 (27%)	15,15,17	1.18	1 (6%)
3	NAG	G	7	3	14,14,15	1.53	3 (21%)	17,19,21	1.43	3 (17%)
3	FUL	G	8	3	10,10,11	1.75	2 (20%)	14,14,16	1.05	1 (7%)
3	NAG	H	1	1,3	14,14,15	1.73	4 (28%)	17,19,21	1.87	6 (35%)
3	NAG	H	2	3	14,14,15	1.61	3 (21%)	17,19,21	1.24	2 (11%)
3	BMA	H	3	3	11,11,12	1.66	2 (18%)	15,15,17	2.58	4 (26%)
3	MAN	H	4	3	11,11,12	1.34	1 (9%)	15,15,17	2.55	5 (33%)
3	NAG	H	5	3	14,14,15	1.75	3 (21%)	17,19,21	1.82	4 (23%)
3	MAN	H	6	3	11,11,12	1.74	3 (27%)	15,15,17	1.28	2 (13%)
3	NAG	H	7	3	14,14,15	1.72	3 (21%)	17,19,21	2.08	5 (29%)
3	FUL	H	8	3	10,10,11	1.76	2 (20%)	14,14,16	1.16	2 (14%)
4	NAG	I	1	1,4	14,14,15	1.69	3 (21%)	17,19,21	2.23	8 (47%)
4	NAG	I	2	4	14,14,15	1.64	3 (21%)	17,19,21	1.44	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	BMA	I	3	4	11,11,12	1.84	2 (18%)	15,15,17	2.05	6 (40%)
4	MAN	I	4	4	11,11,12	1.71	2 (18%)	15,15,17	1.14	1 (6%)
4	NAG	I	5	4	14,14,15	1.56	3 (21%)	17,19,21	1.03	1 (5%)
4	GAL	I	6	4	11,11,12	1.50	2 (18%)	15,15,17	2.02	6 (40%)
4	MAN	I	7	4	11,11,12	1.68	3 (27%)	15,15,17	1.29	1 (6%)
4	NAG	I	8	4	14,14,15	1.57	2 (14%)	17,19,21	1.33	1 (5%)
4	FUL	I	9	4	10,10,11	1.92	2 (20%)	14,14,16	0.96	1 (7%)
5	NAG	J	1	5	14,14,15	1.33	2 (14%)	17,19,21	2.01	4 (23%)
5	BMA	J	2	5	11,11,12	0.50	0	15,15,17	2.20	4 (26%)
5	MAN	J	3	5	11,11,12	0.24	0	15,15,17	0.93	1 (6%)
5	NAG	J	4	5	14,14,15	0.50	0	17,19,21	1.75	2 (11%)
5	MAN	J	5	5	11,11,12	0.44	0	15,15,17	1.93	4 (26%)
5	NAG	J	6	5	14,14,15	0.27	0	17,19,21	0.72	0
6	GAL	K	1	6	11,11,12	1.71	3 (27%)	15,15,17	2.04	6 (40%)
6	SIA	K	2	6	17,20,21	0.27	0	21,28,31	0.87	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
3	NAG	G	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1
3	BMA	G	3	3	-	1/2/19/22	0/1/1/1
3	MAN	G	4	3	-	2/2/19/22	0/1/1/1
3	NAG	G	5	3	-	6/6/23/26	0/1/1/1
3	MAN	G	6	3	-	2/2/19/22	1/1/1/1
3	NAG	G	7	3	-	3/6/23/26	0/1/1/1
3	FUL	G	8	3	-	-	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	4/6/23/26	0/1/1/1
3	BMA	H	3	3	-	2/2/19/22	0/1/1/1
3	MAN	H	4	3	-	1/2/19/22	0/1/1/1
3	NAG	H	5	3	-	2/6/23/26	0/1/1/1
3	MAN	H	6	3	-	2/2/19/22	0/1/1/1
3	NAG	H	7	3	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUL	H	8	3	-	-	0/1/1/1
4	NAG	I	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	BMA	I	3	4	-	2/2/19/22	0/1/1/1
4	MAN	I	4	4	-	1/2/19/22	1/1/1/1
4	NAG	I	5	4	-	3/6/23/26	0/1/1/1
4	GAL	I	6	4	-	2/2/19/22	0/1/1/1
4	MAN	I	7	4	-	2/2/19/22	0/1/1/1
4	NAG	I	8	4	-	5/6/23/26	0/1/1/1
4	FUL	I	9	4	-	-	0/1/1/1
5	NAG	J	1	5	-	4/6/23/26	0/1/1/1
5	BMA	J	2	5	-	0/2/19/22	0/1/1/1
5	MAN	J	3	5	-	0/2/19/22	0/1/1/1
5	NAG	J	4	5	-	2/6/23/26	0/1/1/1
5	MAN	J	5	5	-	1/2/19/22	0/1/1/1
5	NAG	J	6	5	-	3/6/23/26	0/1/1/1
6	GAL	K	1	6	-	1/2/19/22	0/1/1/1
6	SIA	K	2	6	-	13/14/34/38	0/1/1/1

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	5	NAG	O5-C1	4.61	1.51	1.43
3	G	4	MAN	O5-C1	4.51	1.50	1.43
3	H	7	NAG	O5-C1	4.34	1.50	1.43
3	H	1	NAG	O5-C1	4.11	1.50	1.43
3	H	6	MAN	O5-C1	4.00	1.50	1.43

The worst 5 of 106 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	3	BMA	C1-C2-C3	7.22	118.54	109.67
3	H	3	BMA	C1-C2-C3	6.99	118.26	109.67
3	H	4	MAN	C1-C2-C3	6.56	117.72	109.67
5	J	4	NAG	C1-O5-C5	5.62	119.80	112.19
5	J	2	BMA	C1-O5-C5	5.18	119.22	112.19

There are no chirality outliers.

5 of 80 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	1	NAG	C3-C2-N2-C7
6	K	2	SIA	C5-C6-C7-C8
6	K	2	SIA	C5-C6-C7-O7
6	K	2	SIA	O6-C6-C7-C8
6	K	2	SIA	O6-C6-C7-O7

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	6	MAN	C1-C2-C3-C4-C5-O5
4	I	4	MAN	C1-C2-C3-C4-C5-O5

32 monomers are involved in 96 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	5	NAG	3	0
5	J	5	MAN	2	0
3	H	7	NAG	2	0
3	G	4	MAN	1	0
4	I	1	NAG	2	0
3	H	1	NAG	2	0
3	G	8	FUL	2	0
6	K	1	GAL	5	0
4	I	4	MAN	7	0
3	H	5	NAG	5	0
3	G	6	MAN	10	0
4	I	7	MAN	7	0
4	I	2	NAG	7	0
3	H	8	FUL	2	0
4	I	6	GAL	3	0
3	H	2	NAG	5	0
3	H	3	BMA	1	0
5	J	1	NAG	2	0
3	G	1	NAG	4	0
6	K	2	SIA	4	0
5	J	3	MAN	1	0
5	J	4	NAG	13	0
4	I	8	NAG	5	0
3	G	2	NAG	5	0
4	I	5	NAG	4	0
3	G	3	BMA	7	0
5	J	6	NAG	6	0
3	H	6	MAN	5	0

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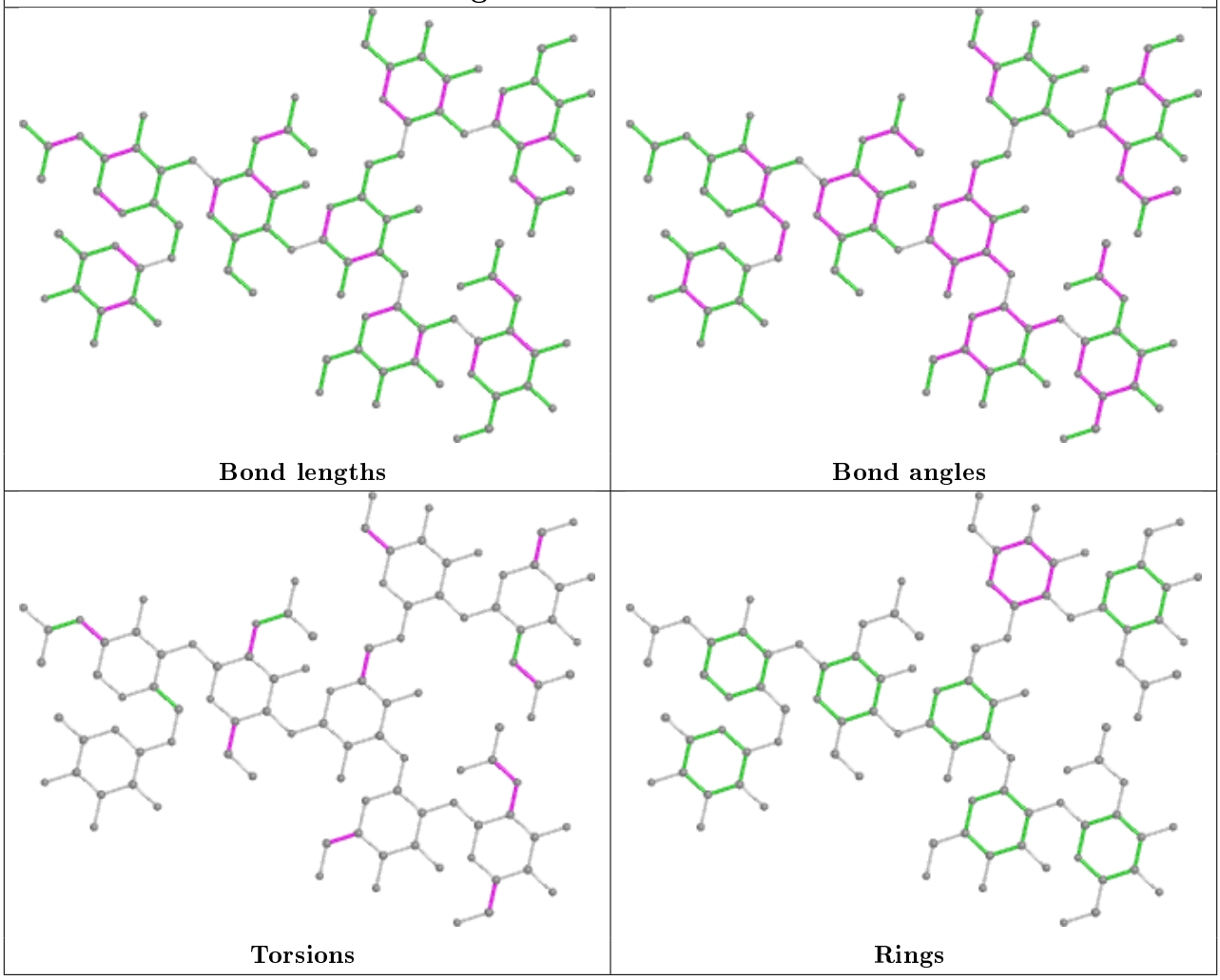
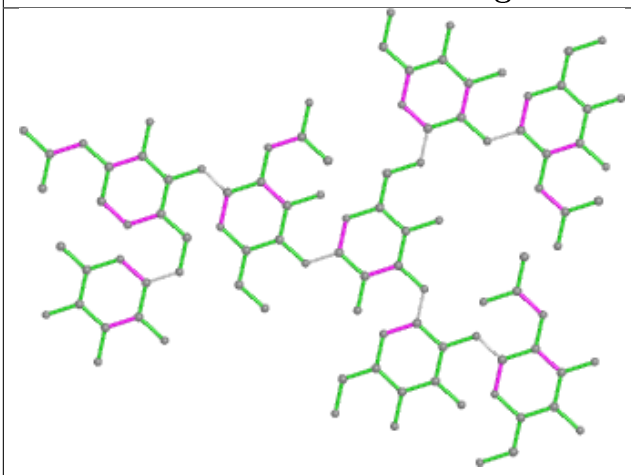
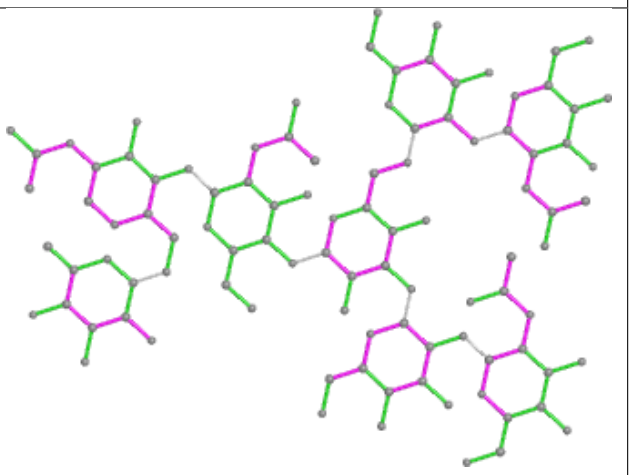
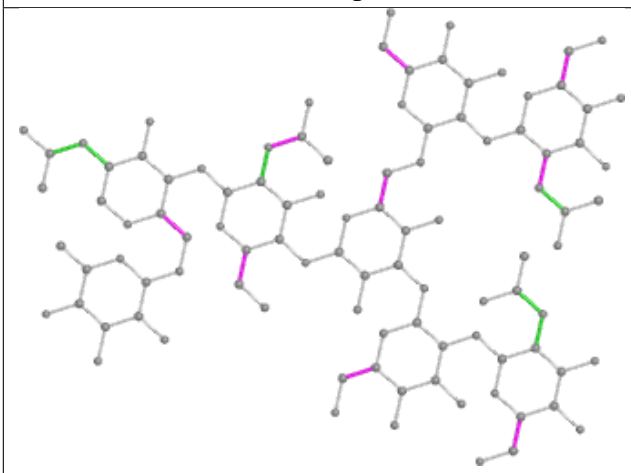
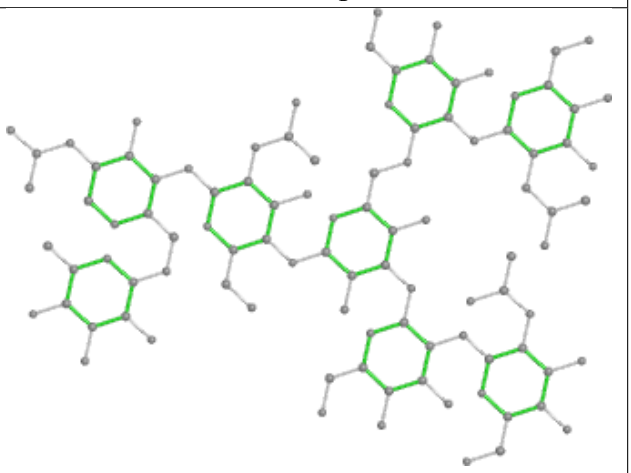
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	7	NAG	5	0
5	J	2	BMA	2	0
4	I	3	BMA	7	0
3	H	4	MAN	7	0

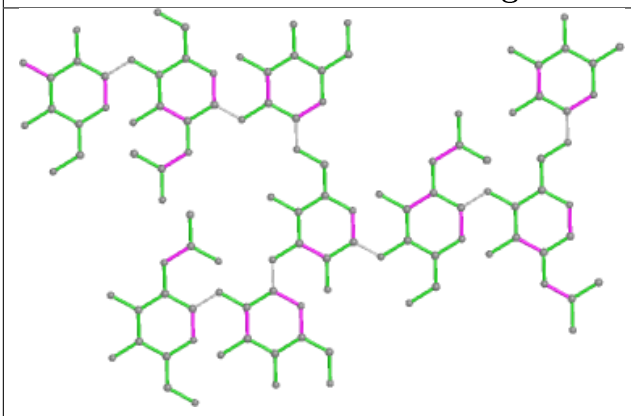
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain G

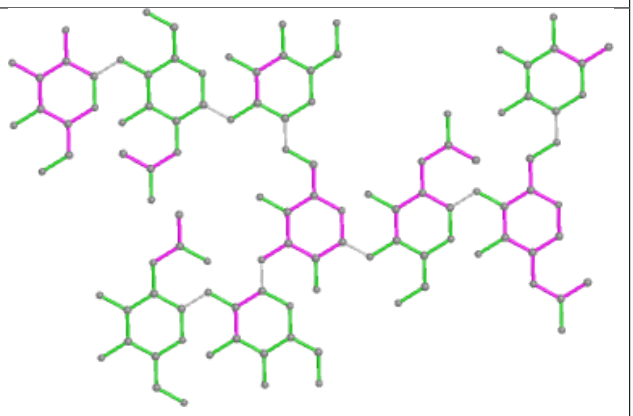


Oligosaccharide Chain H	
 Bond lengths	 Bond angles
 Torsions	 Rings

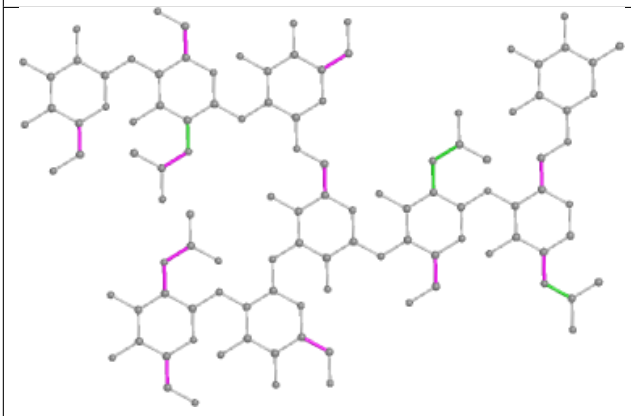
Oligosaccharide Chain I



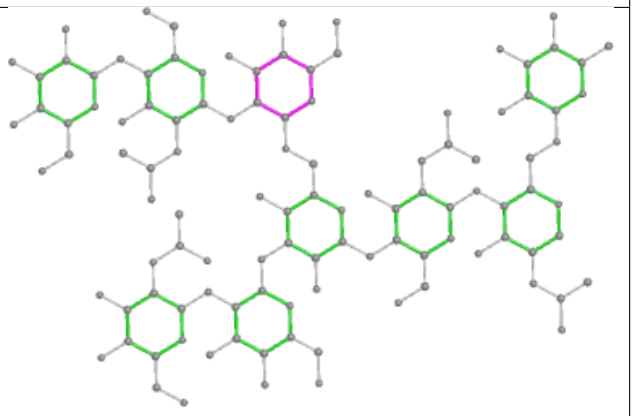
Bond lengths



Bond angles

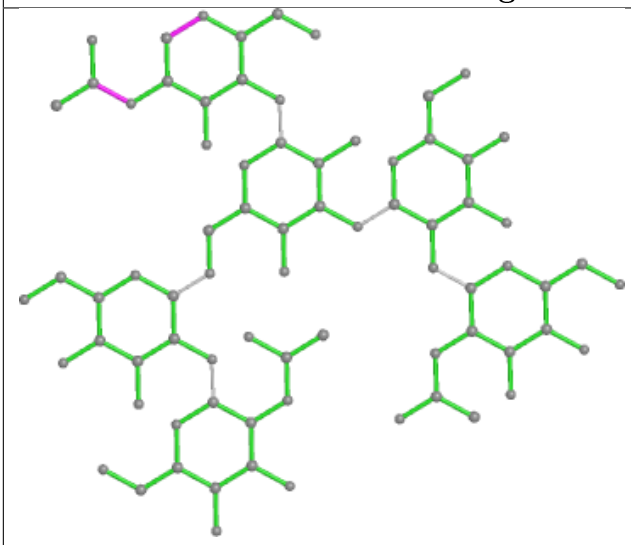


Torsions

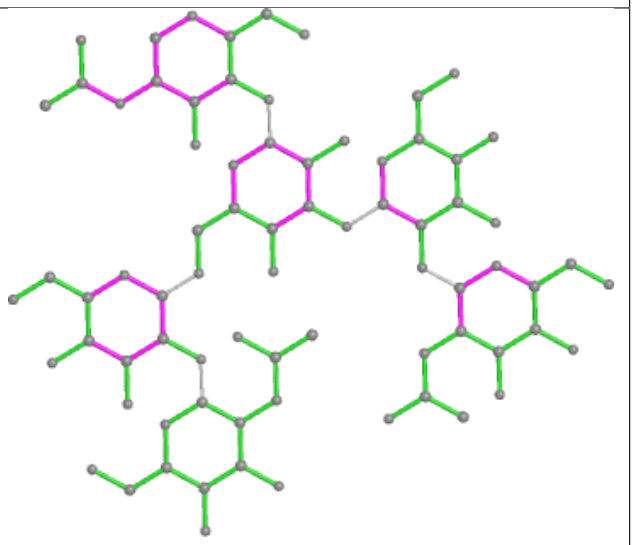


Rings

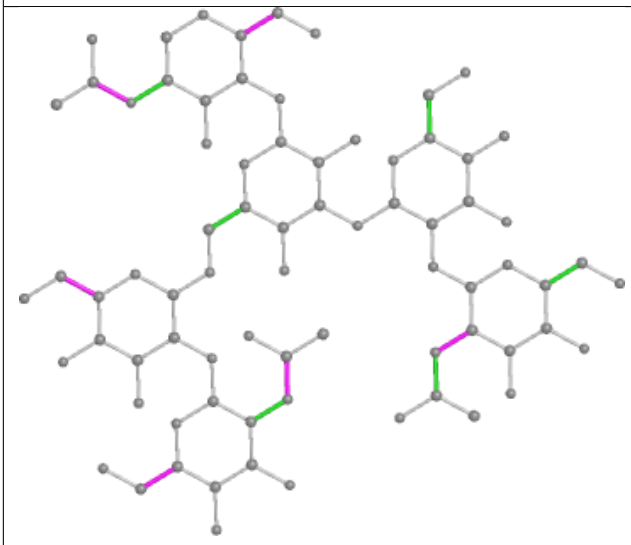
Oligosaccharide Chain J



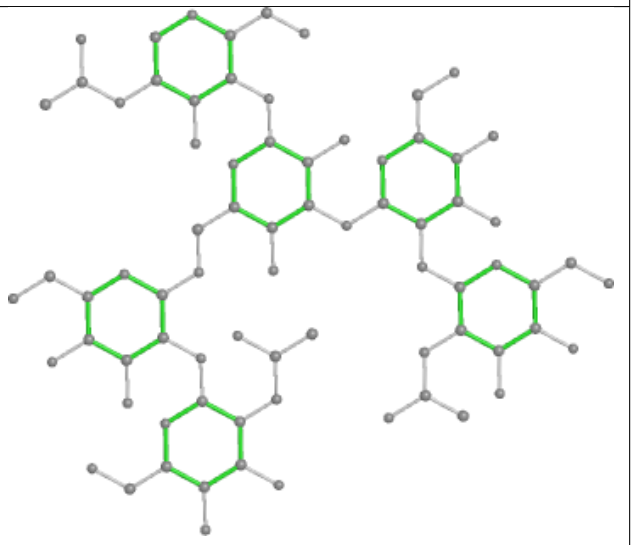
Bond lengths



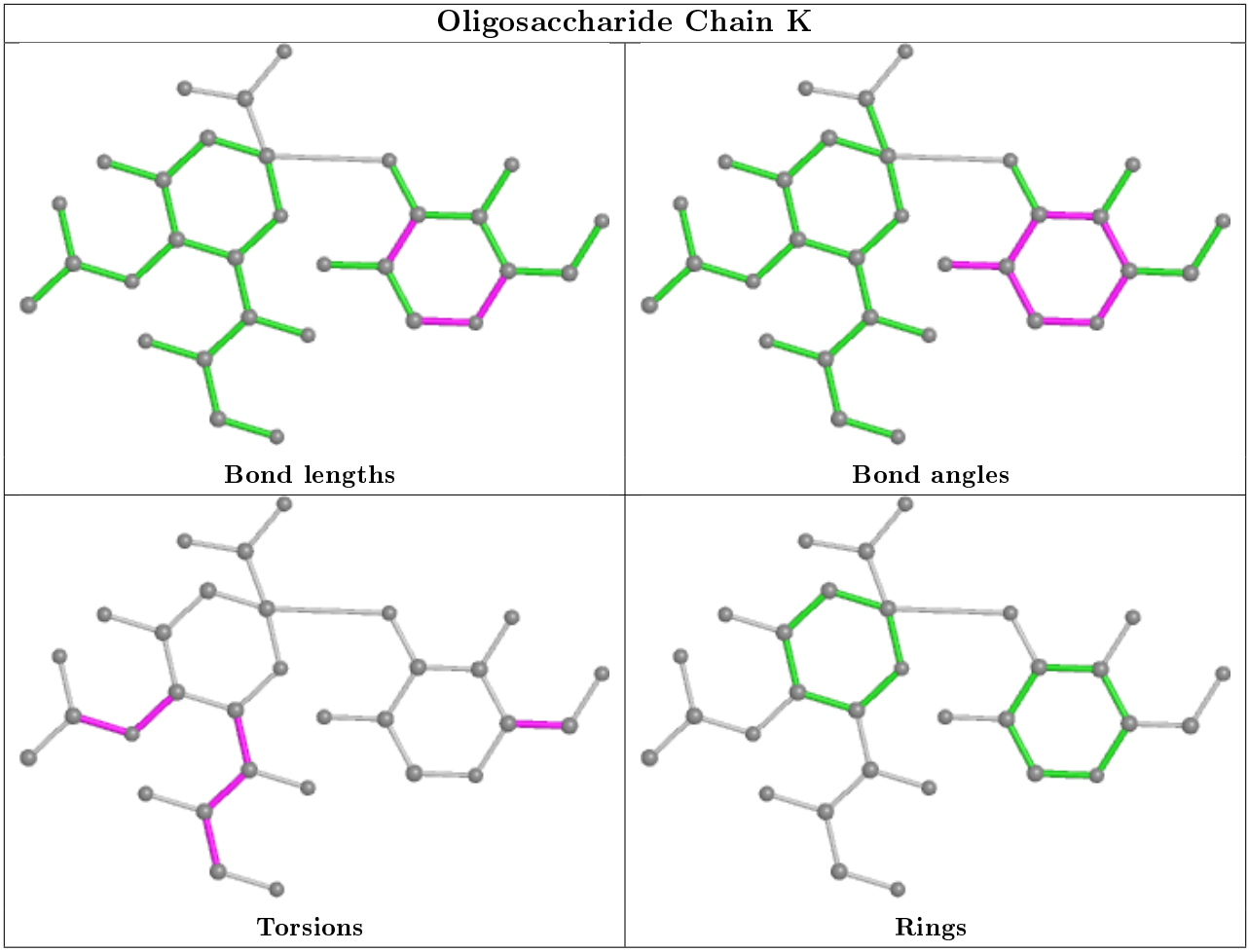
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
7	NAG	D	1001	1	14,14,15	1.60	3 (21%)	17,19,21	1.95	6 (35%)
8	FUL	D	1008	-	10,10,11	1.78	2 (20%)	14,14,16	1.14	2 (14%)

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	D	1001	1	-	2/6/23/26	0/1/1/1
8	FUL	D	1008	-	-	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	1008	FUL	O5-C1	3.95	1.50	1.43
7	D	1001	NAG	O5-C1	3.63	1.49	1.43
8	D	1008	FUL	C2-C3	-3.11	1.47	1.52
7	D	1001	NAG	C7-N2	2.74	1.43	1.34
7	D	1001	NAG	C3-C2	-2.52	1.47	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	1001	NAG	C2-N2-C7	-3.48	117.94	122.90
7	D	1001	NAG	C8-C7-N2	3.30	121.68	116.10
7	D	1001	NAG	C1-O5-C5	3.02	116.29	112.19
7	D	1001	NAG	C3-C4-C5	3.00	115.59	110.24
7	D	1001	NAG	O5-C5-C4	2.68	117.34	110.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	1001	NAG	O5-C5-C6-O6
7	D	1001	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	1001	NAG	13	0
8	D	1008	FUL	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	218/219 (99%)	0.51	19 (8%) 10 12	92, 144, 214, 385	0
1	B	216/219 (98%)	0.53	25 (11%) 4 6	86, 150, 207, 283	0
1	C	212/219 (96%)	0.51	16 (7%) 14 16	70, 141, 203, 463	0
1	D	214/219 (97%)	0.77	29 (13%) 3 4	85, 163, 225, 273	0
2	E	259/275 (94%)	1.84	93 (35%) 0 0	100, 218, 411, 457	0
2	F	258/275 (93%)	1.91	88 (34%) 0 0	123, 222, 330, 393	0
All	All	1377/1426 (96%)	1.06	270 (19%) 1 1	70, 167, 316, 463	0

The worst 5 of 270 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	246	GLN	18.2
2	E	212	CYS	17.0
2	E	282	GLY	15.9
2	F	64	GLN	15.6
2	E	243	SER	13.6

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

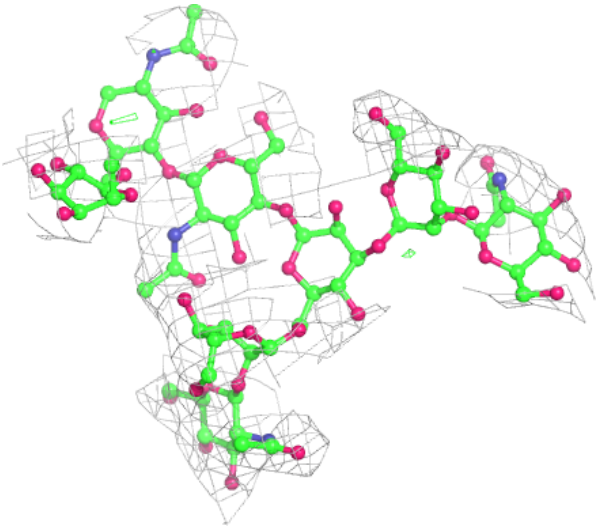
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

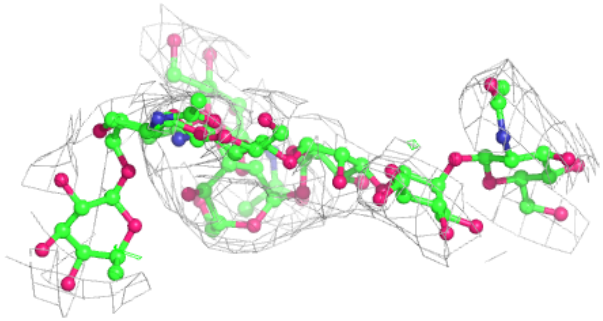
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	J	4	14/15	0.51	0.30	175,258,267,270	0
3	NAG	H	5	14/15	0.58	0.31	170,189,206,207	0
3	FUL	H	8	10/11	0.62	0.28	189,205,221,221	0
6	SIA	K	2	20/21	0.67	0.29	225,279,306,311	0
4	GAL	I	6	11/12	0.69	0.32	178,191,201,214	0
6	GAL	K	1	11/12	0.79	0.17	278,291,310,321	0
3	NAG	H	1	14/15	0.80	0.17	145,188,210,222	0
5	NAG	J	1	14/15	0.82	0.32	185,201,221,225	0
5	NAG	J	6	14/15	0.83	0.20	107,118,130,146	0
5	BMA	J	2	11/12	0.83	0.19	148,167,183,184	0
5	MAN	J	3	11/12	0.84	0.23	205,225,259,266	0
3	MAN	H	4	11/12	0.87	0.15	113,158,179,187	0
5	MAN	J	5	11/12	0.88	0.25	88,100,113,114	0
3	NAG	H	7	14/15	0.89	0.15	107,118,130,146	0
4	NAG	I	8	14/15	0.90	0.17	120,164,176,200	0
4	MAN	I	4	11/12	0.91	0.19	108,118,133,144	0
3	NAG	G	1	14/15	0.91	0.18	116,130,142,155	0
3	MAN	G	4	11/12	0.91	0.18	96,112,146,152	0
4	NAG	I	2	14/15	0.91	0.16	93,112,126,126	0
3	NAG	G	5	14/15	0.92	0.19	135,171,216,235	0
3	FUL	G	8	10/11	0.93	0.21	128,140,150,154	0
4	NAG	I	1	14/15	0.93	0.17	127,140,193,194	0
3	NAG	G	2	14/15	0.94	0.14	78,105,119,125	0
4	NAG	I	5	14/15	0.94	0.18	74,130,156,170	0
3	MAN	H	6	11/12	0.94	0.15	88,100,113,114	0
3	NAG	G	7	14/15	0.94	0.18	70,118,125,126	0
3	NAG	H	2	14/15	0.94	0.16	112,133,150,155	0
4	BMA	I	3	11/12	0.94	0.13	103,120,149,152	0
3	BMA	H	3	11/12	0.94	0.14	110,131,137,146	0
4	FUL	I	9	10/11	0.95	0.18	109,133,138,140	0
3	BMA	G	3	11/12	0.95	0.17	92,95,108,116	0
4	MAN	I	7	11/12	0.97	0.09	156,164,181,186	0
3	MAN	G	6	11/12	0.98	0.14	85,104,131,135	0

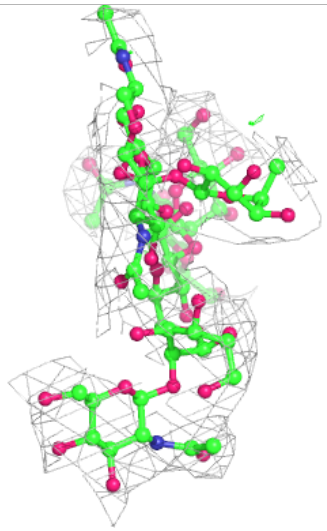
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

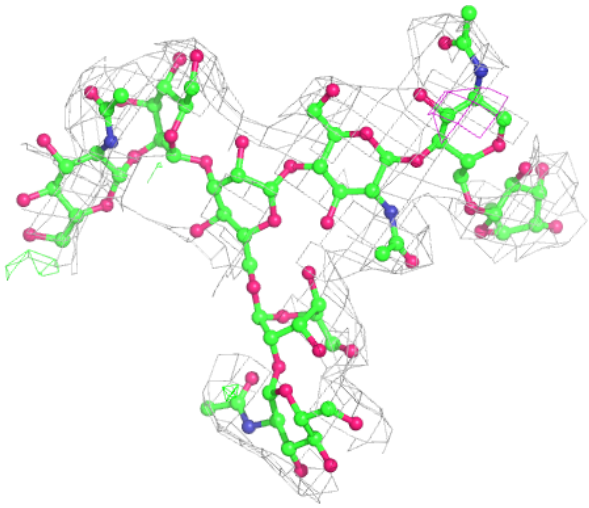


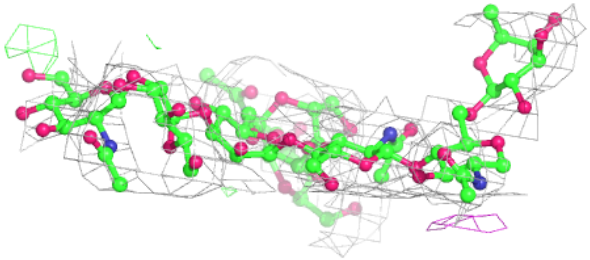


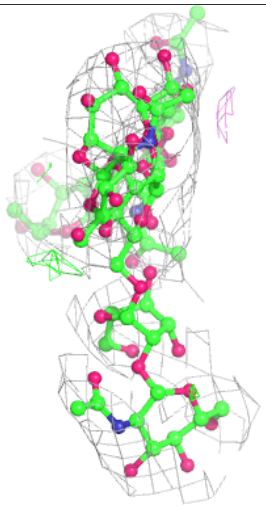


Electron density around Chain H:

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

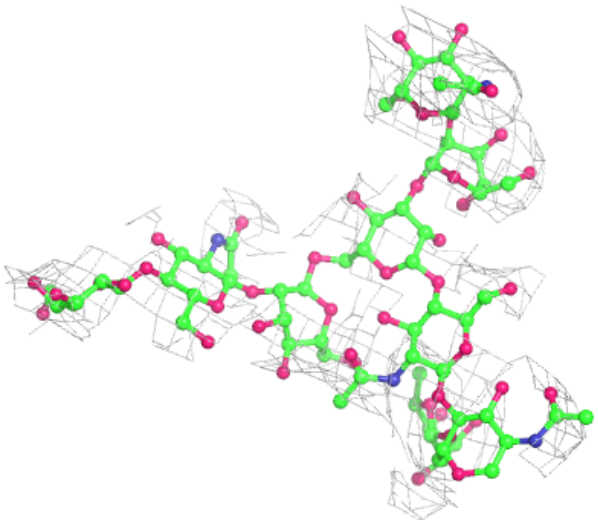


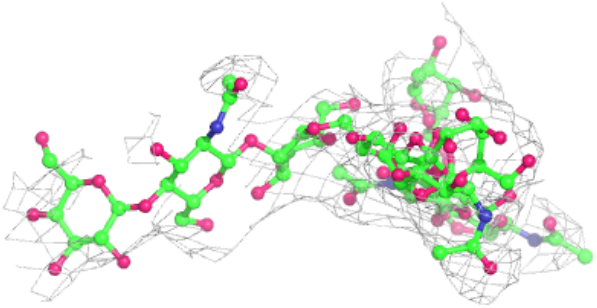


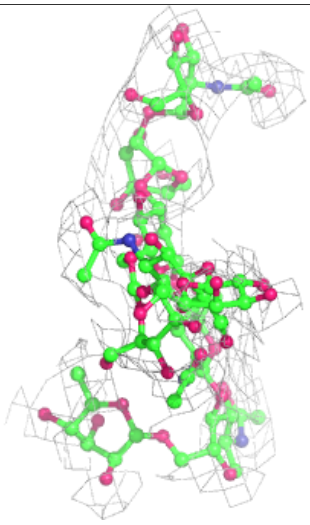


Electron density around Chain I:

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

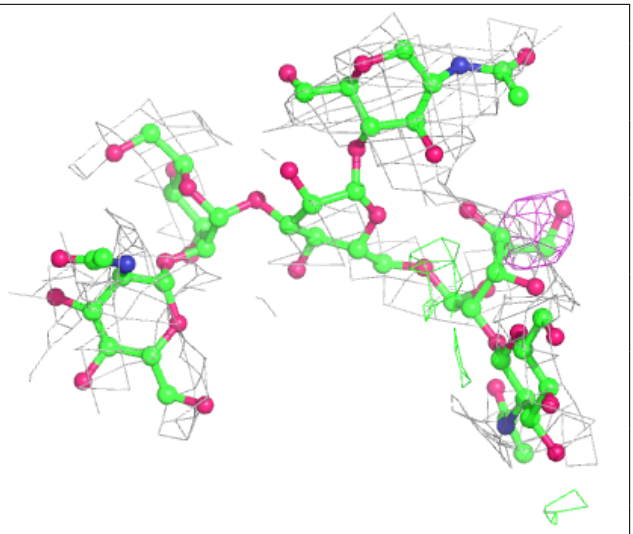


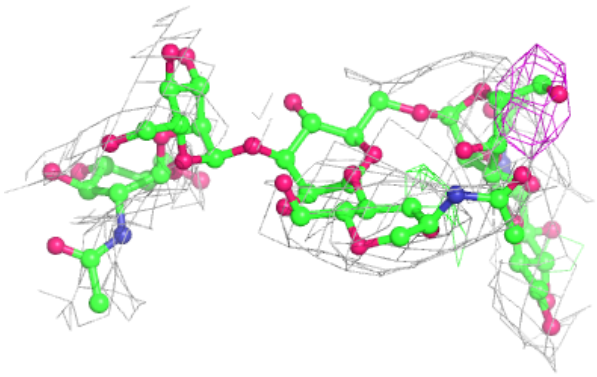


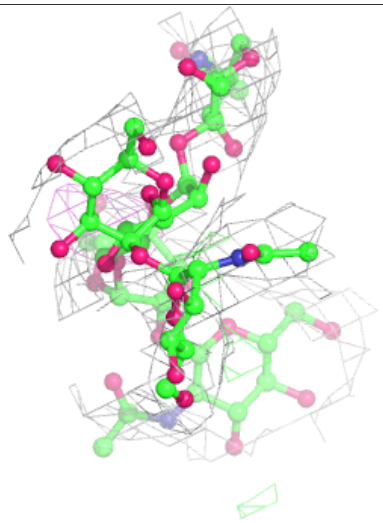


Electron density around Chain J:

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

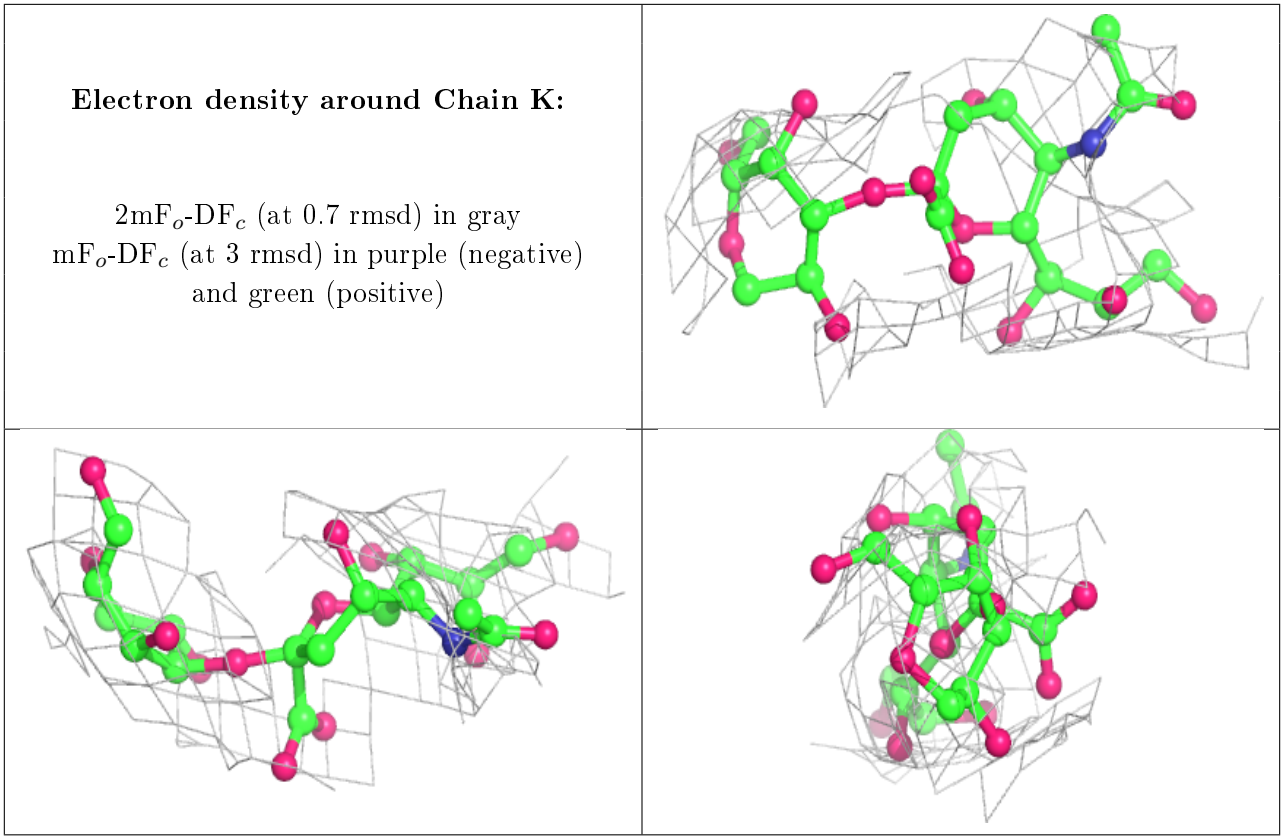






Electron density around Chain K:

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



6.4 Ligands

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^{th} 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	D	1001	14/15	0.74	0.38	184,214,227,227	0
8	FUL	D	1008	10/11	0.75	0.45	189,205,221,221	0

6.5 Other polymers

There are no such residues in this entry.