wwPDB X-ray Structure Validation Summary Report (i)

Aug 7, 2020 – 06:23 AM BST

PDB ID	:	3K72
Title	:	Structure of integrin alphaX beta2
Authors	:	Xie, C.; Zhu, J.; Chen, X.; Mi, L.; Nishida, N.; Springer, T.A.
Deposited on	:	2009-10-11
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 (i) symbol.

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

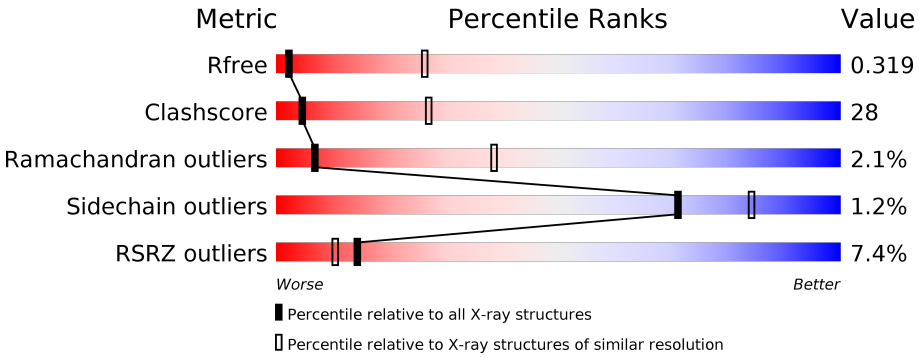
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.70 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 <=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	1095	3% 43% 35% . 19%
1	C	1095	3% 44% 34% . 19%
2	B	687	10% 62% 34% ..
2	D	687	13% 62% 34% ..
3	E	2	50% 50%
3	I	2	50% 50%

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Mol	Chain	Length	Quality of chain
4	F	5	20% 80%
4	J	5	40% 60%
5	G	3	33% 67%
5	H	3	100%
5	K	3	100%

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	NAG	I	2	-	-	-	X
4	NAG	F	1	X	-	-	-
4	MAN	F	3	X	-	-	-
4	MAN	F	4	-	-	-	X
4	NAG	J	1	X	-	-	-
4	MAN	J	3	X	-	-	-
5	MAN	G	3	X	-	-	-
5	MAN	H	3	X	-	-	X
5	NAG	K	1	-	-	X	-
5	MAN	K	3	X	-	-	-
6	NAG	B	3479	-	X	-	-
6	NAG	D	3094	-	-	-	X
8	MAN	C	3378	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 24382 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-X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	884	Total	C	N	O	S	0	0	0
			6814	4305	1178	1297	34			
1	C	882	Total	C	N	O	S	0	0	0
			6802	4299	1176	1293	34			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1085	GLY	-	expression tag	UNP P20702
A	1086	CYS	-	expression tag	UNP P20702
A	1087	GLY	-	expression tag	UNP P20702
A	1088	GLY	-	expression tag	UNP P20702
A	1089	LEU	-	expression tag	UNP P20702
A	1090	GLU	-	expression tag	UNP P20702
A	1091	ASN	-	expression tag	UNP P20702
A	1092	LEU	-	expression tag	UNP P20702
A	1093	TYR	-	expression tag	UNP P20702
A	1094	PHE	-	expression tag	UNP P20702
A	1095	GLN	-	expression tag	UNP P20702
C	1085	GLY	-	expression tag	UNP P20702
C	1086	CYS	-	expression tag	UNP P20702
C	1087	GLY	-	expression tag	UNP P20702
C	1088	GLY	-	expression tag	UNP P20702
C	1089	LEU	-	expression tag	UNP P20702
C	1090	GLU	-	expression tag	UNP P20702
C	1091	ASN	-	expression tag	UNP P20702
C	1092	LEU	-	expression tag	UNP P20702
C	1093	TYR	-	expression tag	UNP P20702
C	1094	PHE	-	expression tag	UNP P20702
C	1095	GLN	-	expression tag	UNP P20702

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	673	Total	C	N	O	S	0	0	0
			5177	3181	929	1003	64			
2	D	673	Total	C	N	O	S	0	0	0
			5177	3181	929	1003	64			

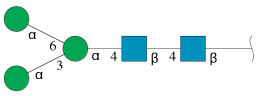
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	678	ASP	-	expression tag	UNP P05107
B	679	GLY	-	expression tag	UNP P05107
B	680	CYS	-	expression tag	UNP P05107
B	681	GLY	-	expression tag	UNP P05107
B	682	GLU	-	expression tag	UNP P05107
B	684	LEU	-	expression tag	UNP P05107
B	685	TYR	-	expression tag	UNP P05107
B	686	PHE	-	expression tag	UNP P05107
B	687	GLN	-	expression tag	UNP P05107
D	678	ASP	-	expression tag	UNP P05107
D	679	GLY	-	expression tag	UNP P05107
D	680	CYS	-	expression tag	UNP P05107
D	681	GLY	-	expression tag	UNP P05107
D	682	GLU	-	expression tag	UNP P05107
D	684	LEU	-	expression tag	UNP P05107
D	685	TYR	-	expression tag	UNP P05107
D	686	PHE	-	expression tag	UNP P05107
D	687	GLN	-	expression tag	UNP P05107

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

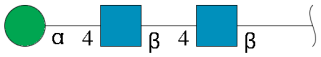
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



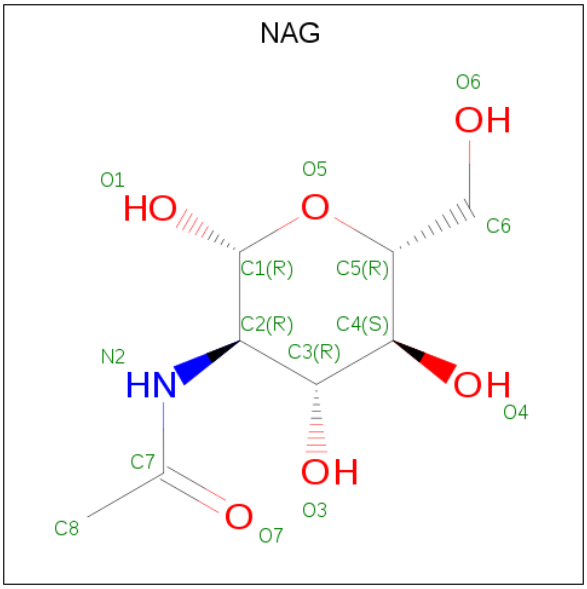
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	F	5	Total C N O 61 34 2 25	0	0	0
4	J	5	Total C N O 61 34 2 25	0	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	G	3	Total C N O 39 22 2 15	0	0	0
5	H	3	Total C N O 39 22 2 15	0	0	0
5	K	3	Total C N O 39 22 2 15	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

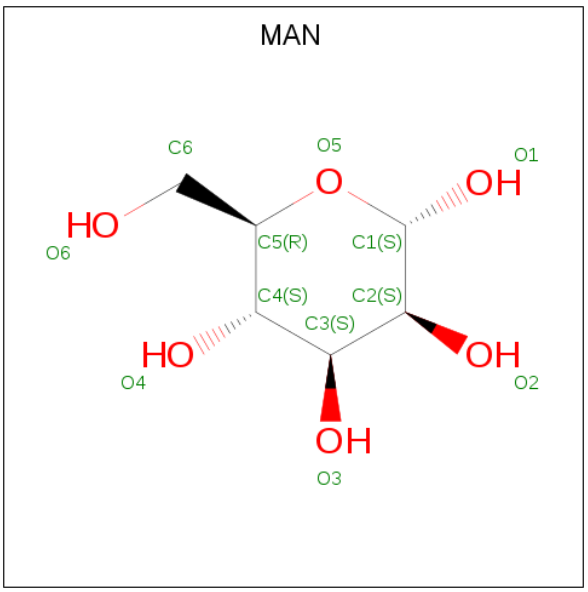


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0
6	C	1	Total C N O 14 8 1 5	0	0
6	C	1	Total C N O 14 8 1 5	0	0
6	D	1	Total C N O 14 8 1 5	0	0
6	D	1	Total C N O 14 8 1 5	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Ca 1 1	0	0
7	A	3	Total Ca 3 3	0	0
7	D	1	Total Ca 1 1	0	0
7	C	3	Total Ca 3 3	0	0

- Molecule 8 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



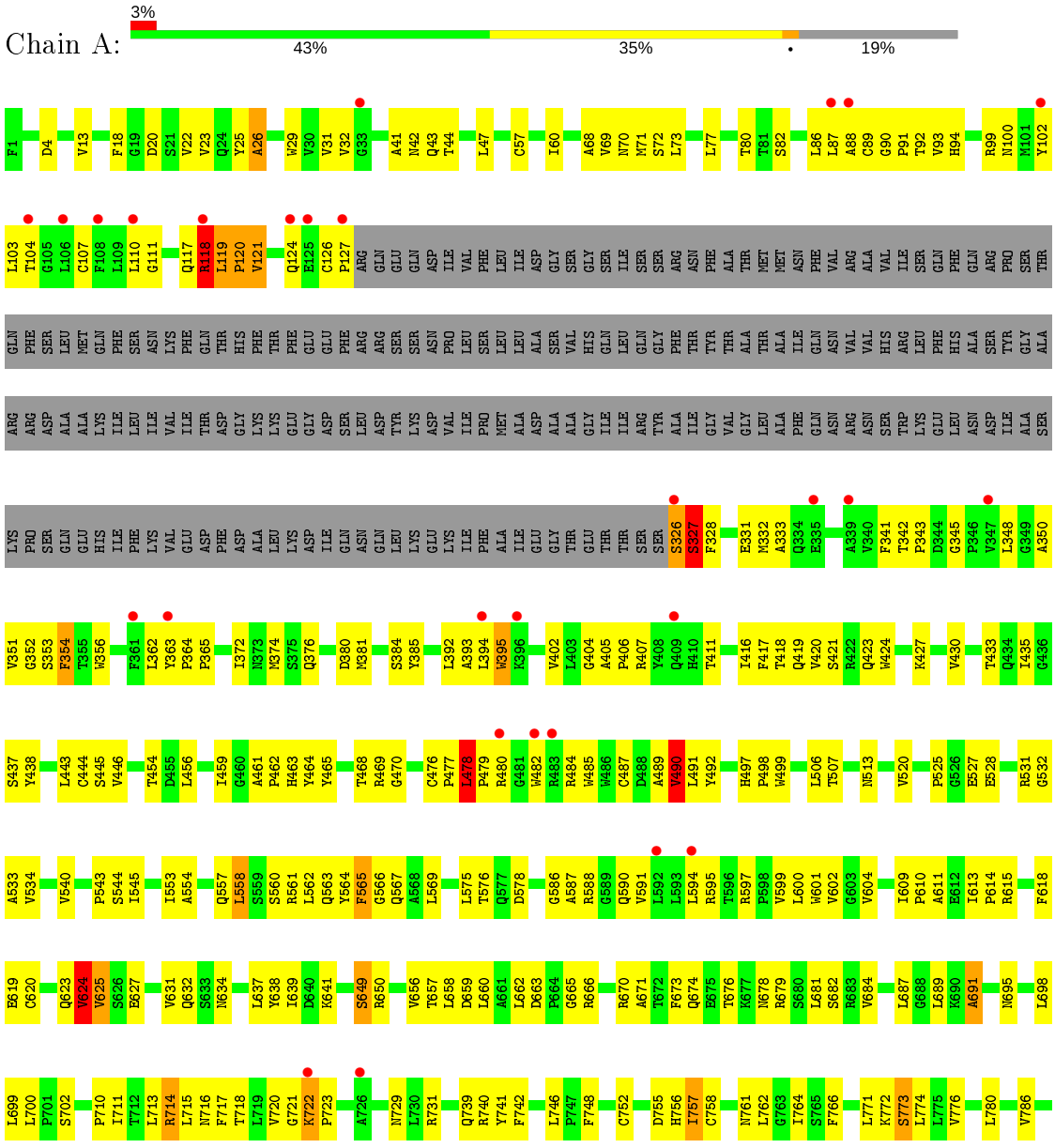
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			11	6	5		

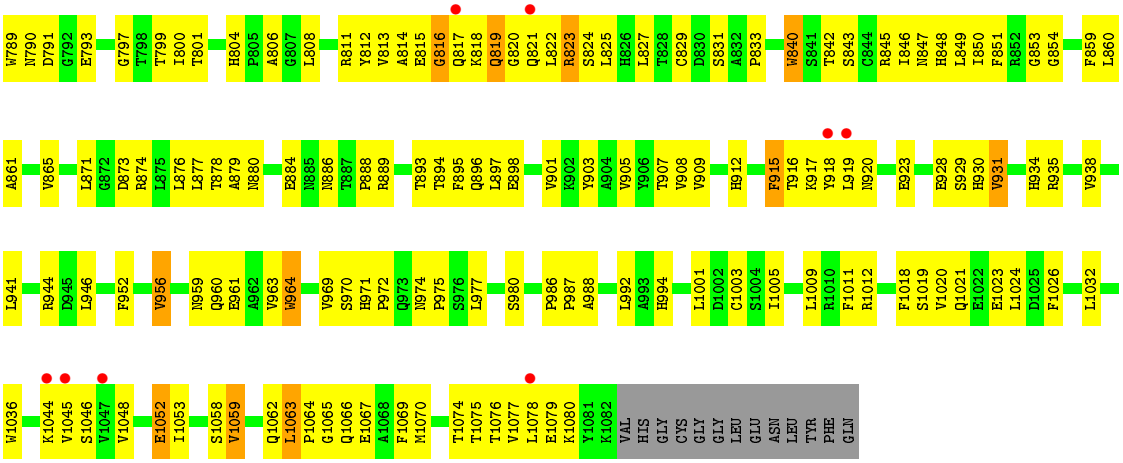
3 Residue-property plots (i)

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: Integrin alpha-X

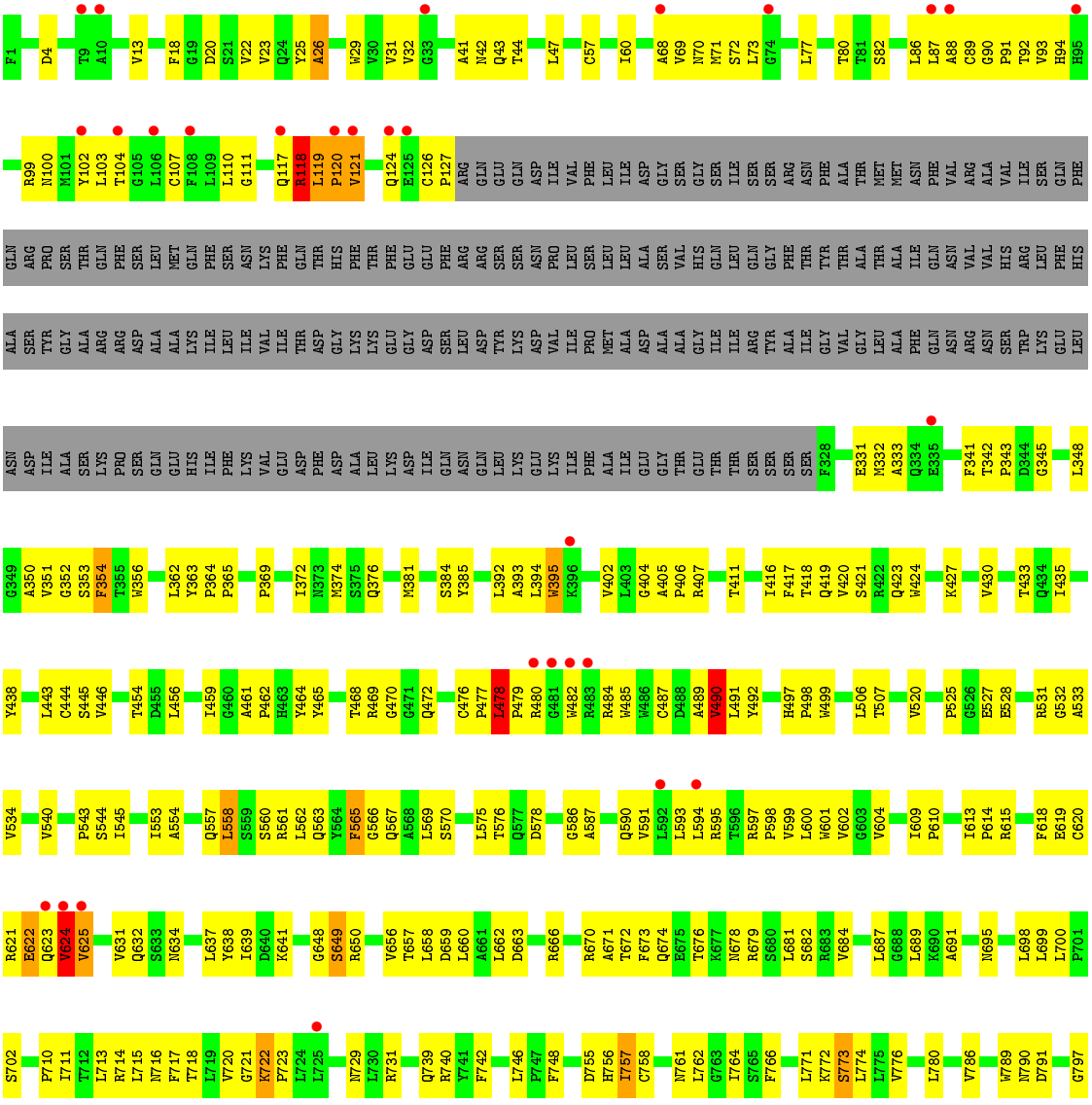
Chain A:

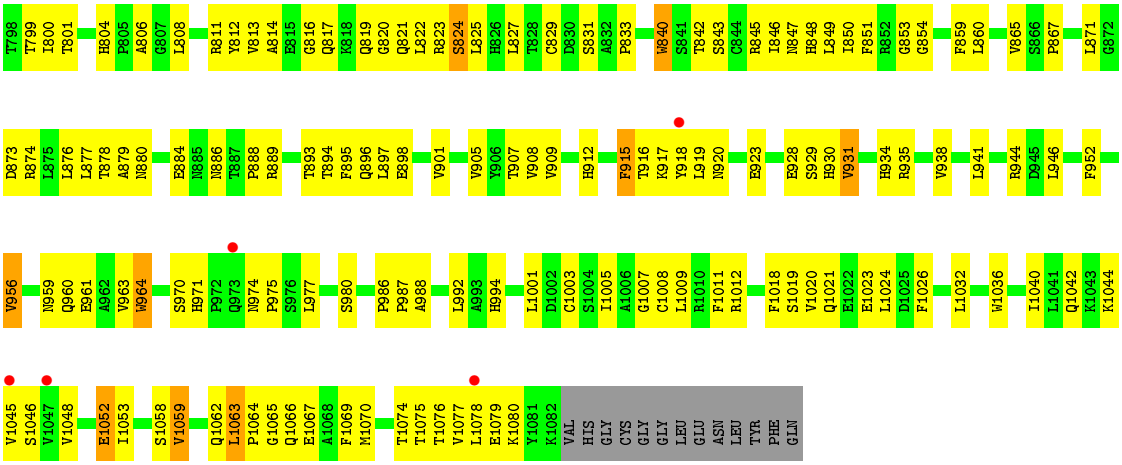




- Molecule 1: Integrin alpha-X

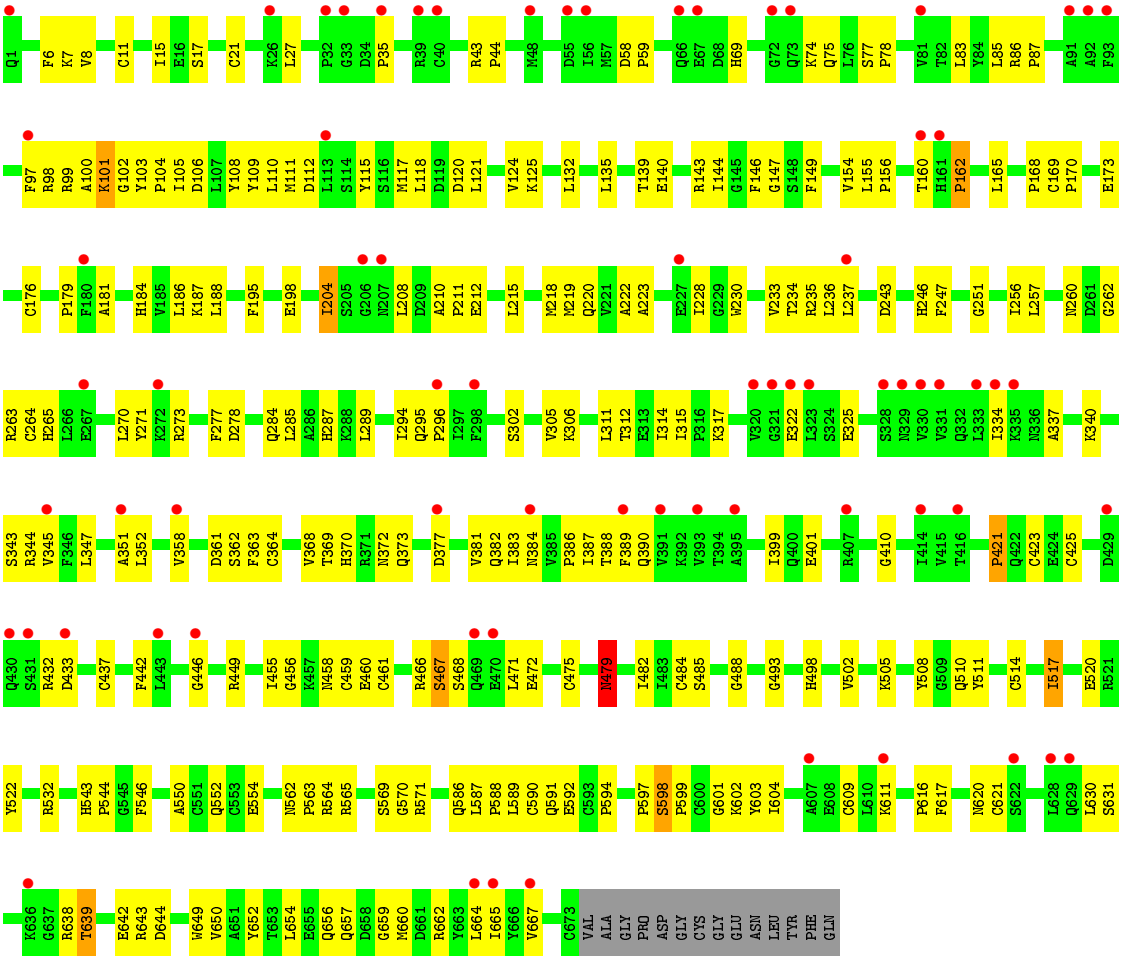
Chain C:





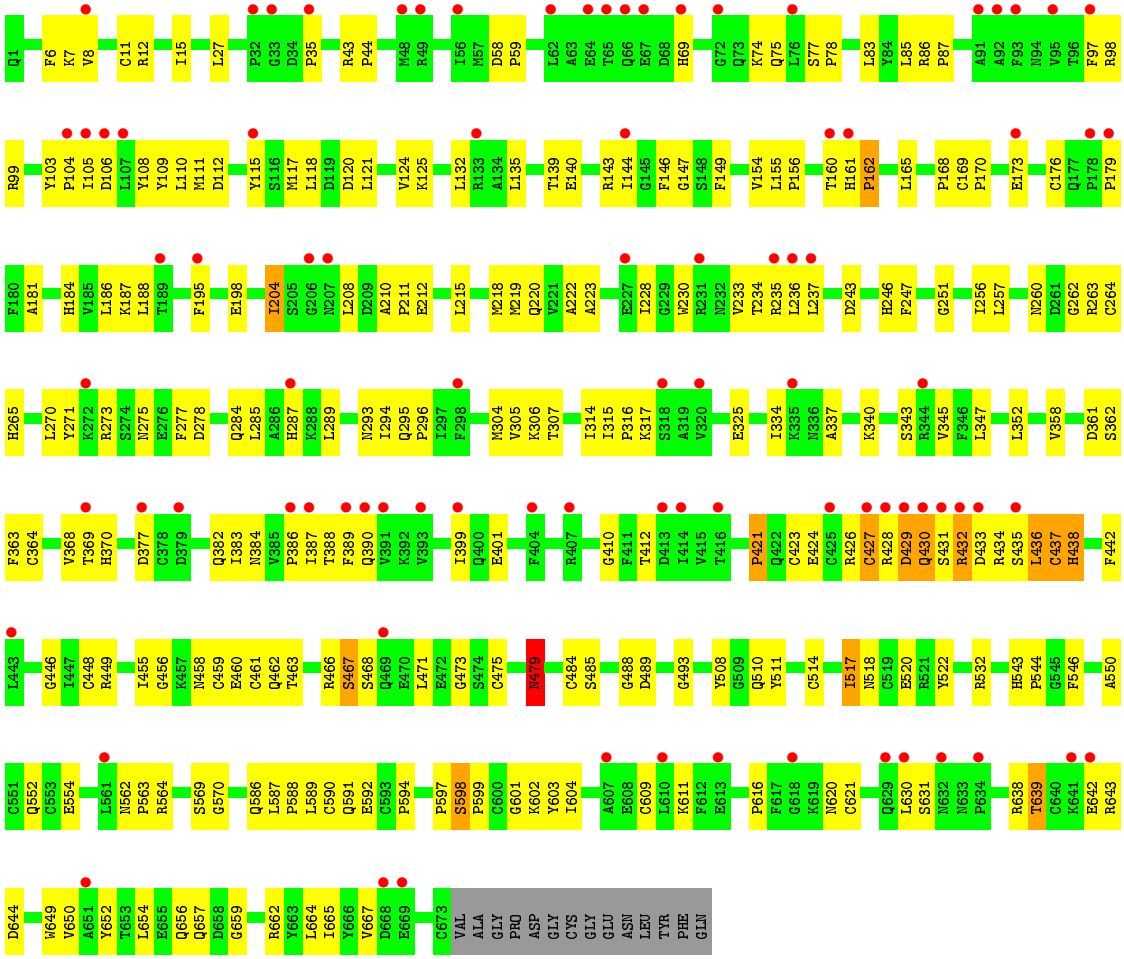
• Molecule 2: Integrin beta-2

Chain B:



• Molecule 2: Integrin beta-2

Chain D:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

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

Chain F:

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

Chain J:

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

Chain G:

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

Chain H:

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

Chain K:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	160.96Å 165.55Å 536.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.48 – 3.70 48.64 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.48-3.70) 99.4 (48.64-3.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.315 , 0.335 0.294 , 0.319	Depositor DCC
R_{free} test set	1136 reflections (1.11%)	wwPDB-VP
Wilson B-factor (Å^2)	92.3	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 151.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.074 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	24382	wwPDB-VP
Average B, all atoms (Å^2)	234.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: CA, NAG, 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	0.43	7/6969 (0.1%)	0.53	3/9480 (0.0%)
1	C	0.38	1/6957 (0.0%)	0.53	2/9464 (0.0%)
2	B	0.29	1/5273 (0.0%)	0.43	0/7119
2	D	0.31	1/5273 (0.0%)	0.43	0/7119
All	All	0.36	10/24472 (0.0%)	0.49	5/33182 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	13
1	C	0	15
2	B	0	2
2	D	0	3
All	All	0	33

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	479	ASN	CB-CG	7.36	1.68	1.51
2	B	479	ASN	CB-CG	6.92	1.67	1.51
1	A	326	SER	CB-OG	6.75	1.51	1.42
1	A	327	SER	CA-CB	6.62	1.62	1.52
1	A	326	SER	CA-CB	6.42	1.62	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	478	LEU	CA-CB-CG	8.42	134.66	115.30
1	A	478	LEU	CA-CB-CG	7.71	133.03	115.30
1	A	478	LEU	CB-CG-CD1	-5.17	102.20	111.00
1	A	118	ARG	NE-CZ-NH1	-5.07	117.76	120.30
1	C	478	LEU	CB-CG-CD1	-5.06	102.39	111.00

There are no chirality outliers.

5 of 33 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ARG	Peptide
1	A	326	SER	Peptide
1	A	327	SER	Peptide
1	A	490	VAL	Peptide
1	A	82	SER	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	6814	0	6671	441	0
1	C	6802	0	6661	442	0
2	B	5177	0	4964	236	0
2	D	5177	0	4964	267	0
3	E	28	0	25	0	0
3	I	28	0	25	0	0
4	F	61	0	52	5	0
4	J	61	0	52	7	0
5	G	39	0	34	4	0
5	H	39	0	34	3	0
5	K	39	0	34	13	0
6	A	14	0	12	0	0
6	B	28	0	26	1	0
6	C	28	0	25	0	0
6	D	28	0	26	1	0
7	A	3	0	0	0	0
7	B	1	0	0	0	0
7	C	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	1	0	0	0	0
8	C	11	0	10	1	0
All	All	24382	0	23615	1353	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 28.

The worst 5 of 1353 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:15:ILE:HG23	2:B:86:ARG:CZ	1.67	1.23
2:D:430:GLN:HB3	2:D:434:ARG:NH2	1.61	1.14
2:D:430:GLN:HG3	2:D:442:PHE:CB	1.78	1.14
2:D:430:GLN:CB	2:D:434:ARG:HH21	1.62	1.10
2:D:430:GLN:HG3	2:D:442:PHE:HB2	1.13	1.09

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	880/1095 (80%)	667 (76%)	192 (22%)	21 (2%)	6 35
1	C	878/1095 (80%)	664 (76%)	195 (22%)	19 (2%)	6 37
2	B	671/687 (98%)	518 (77%)	141 (21%)	12 (2%)	8 41
2	D	671/687 (98%)	512 (76%)	146 (22%)	13 (2%)	8 40
All	All	3100/3564 (87%)	2361 (76%)	674 (22%)	65 (2%)	7 38

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	757	ILE
2	B	162	PRO
2	B	598	SER
1	C	624	VAL
1	C	757	ILE

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	753/934 (81%)	742 (98%)	11 (2%)	65	81
1	C	751/934 (80%)	740 (98%)	11 (2%)	65	81
2	B	582/592 (98%)	579 (100%)	3 (0%)	88	94
2	D	582/592 (98%)	575 (99%)	7 (1%)	71	84
All	All	2668/3052 (87%)	2636 (99%)	32 (1%)	71	84

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	118	ARG
1	C	478	LEU
2	D	479	ASN
1	C	395	TRP
1	C	565	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	295	GLN
1	C	124	GLN
1	C	692	HIS
2	B	159	ASN
2	D	159	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

23 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	E	1	1,3	14,14,15	0.53	0	17,19,21	0.83	0
3	NAG	E	2	3	14,14,15	0.60	0	17,19,21	1.04	1 (5%)
4	NAG	F	1	1,4	14,14,15	0.59	0	17,19,21	1.10	1 (5%)
4	NAG	F	2	4	14,14,15	0.55	0	17,19,21	1.89	2 (11%)
4	MAN	F	3	4	11,11,12	0.49	0	15,15,17	1.50	3 (20%)
4	MAN	F	4	4	11,11,12	0.73	0	15,15,17	0.95	2 (13%)
4	MAN	F	5	4	11,11,12	0.70	0	15,15,17	0.73	1 (6%)
5	NAG	G	1	1,5	14,14,15	0.51	0	17,19,21	1.72	3 (17%)
5	NAG	G	2	5	14,14,15	0.72	0	17,19,21	1.49	2 (11%)
5	MAN	G	3	5	11,11,12	0.82	0	15,15,17	2.67	2 (13%)
5	NAG	H	1	1,5	14,14,15	0.53	0	17,19,21	2.55	5 (29%)
5	NAG	H	2	5	14,14,15	0.83	1 (7%)	17,19,21	1.23	2 (11%)
5	MAN	H	3	5	11,11,12	0.72	0	15,15,17	2.86	4 (26%)
3	NAG	I	1	1,3	14,14,15	0.50	0	17,19,21	0.76	0
3	NAG	I	2	3	14,14,15	0.56	0	17,19,21	1.19	2 (11%)
4	NAG	J	1	1,4	14,14,15	0.58	0	17,19,21	1.15	2 (11%)
4	NAG	J	2	4	14,14,15	0.53	0	17,19,21	1.97	2 (11%)
4	MAN	J	3	4	11,11,12	0.46	0	15,15,17	1.47	3 (20%)
4	MAN	J	4	4	11,11,12	0.74	0	15,15,17	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	MAN	J	5	4	11,11,12	0.65	0	15,15,17	0.72	0
5	NAG	K	1	1,5	14,14,15	0.59	0	17,19,21	1.46	2 (11%)
5	NAG	K	2	5	14,14,15	0.56	0	17,19,21	1.18	1 (5%)
5	MAN	K	3	5	11,11,12	0.95	1 (9%)	15,15,17	1.35	3 (20%)

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	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
4	NAG	F	1	1,4	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	MAN	F	3	4	1/1/4/5	2/2/19/22	0/1/1/1
4	MAN	F	4	4	-	2/2/19/22	0/1/1/1
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1
5	NAG	G	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	MAN	G	3	5	1/1/4/5	0/2/19/22	0/1/1/1
5	NAG	H	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	MAN	H	3	5	1/1/4/5	0/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
4	NAG	J	1	1,4	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	MAN	J	3	4	1/1/4/5	2/2/19/22	0/1/1/1
4	MAN	J	4	4	-	2/2/19/22	0/1/1/1
4	MAN	J	5	4	-	0/2/19/22	0/1/1/1
5	NAG	K	1	1,5	-	5/6/23/26	0/1/1/1
5	NAG	K	2	5	-	3/6/23/26	0/1/1/1
5	MAN	K	3	5	1/1/4/5	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	2	NAG	C1-C2	2.25	1.55	1.52
5	K	3	MAN	O5-C1	-2.03	1.40	1.43

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	1	NAG	C1-O5-C5	9.04	124.44	112.19
5	G	3	MAN	C1-O5-C5	8.73	124.02	112.19
5	H	3	MAN	C1-C2-C3	-7.71	100.19	109.67
4	J	2	NAG	C1-O5-C5	6.77	121.36	112.19
4	F	2	NAG	C1-O5-C5	6.49	120.99	112.19

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	K	3	MAN	C1
5	G	3	MAN	C1
4	F	1	NAG	C1
5	H	3	MAN	C1
4	J	3	MAN	C1

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	1	NAG	C3-C2-N2-C7
4	J	3	MAN	O5-C5-C6-O6
4	F	3	MAN	O5-C5-C6-O6
4	F	4	MAN	O5-C5-C6-O6
4	J	4	MAN	O5-C5-C6-O6

There are no ring outliers.

17 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	1	NAG	4	0
4	F	4	MAN	1	0
4	F	2	NAG	3	0
5	K	1	NAG	11	0
5	H	2	NAG	2	0
5	K	3	MAN	2	0
5	H	1	NAG	2	0
4	J	4	MAN	1	0

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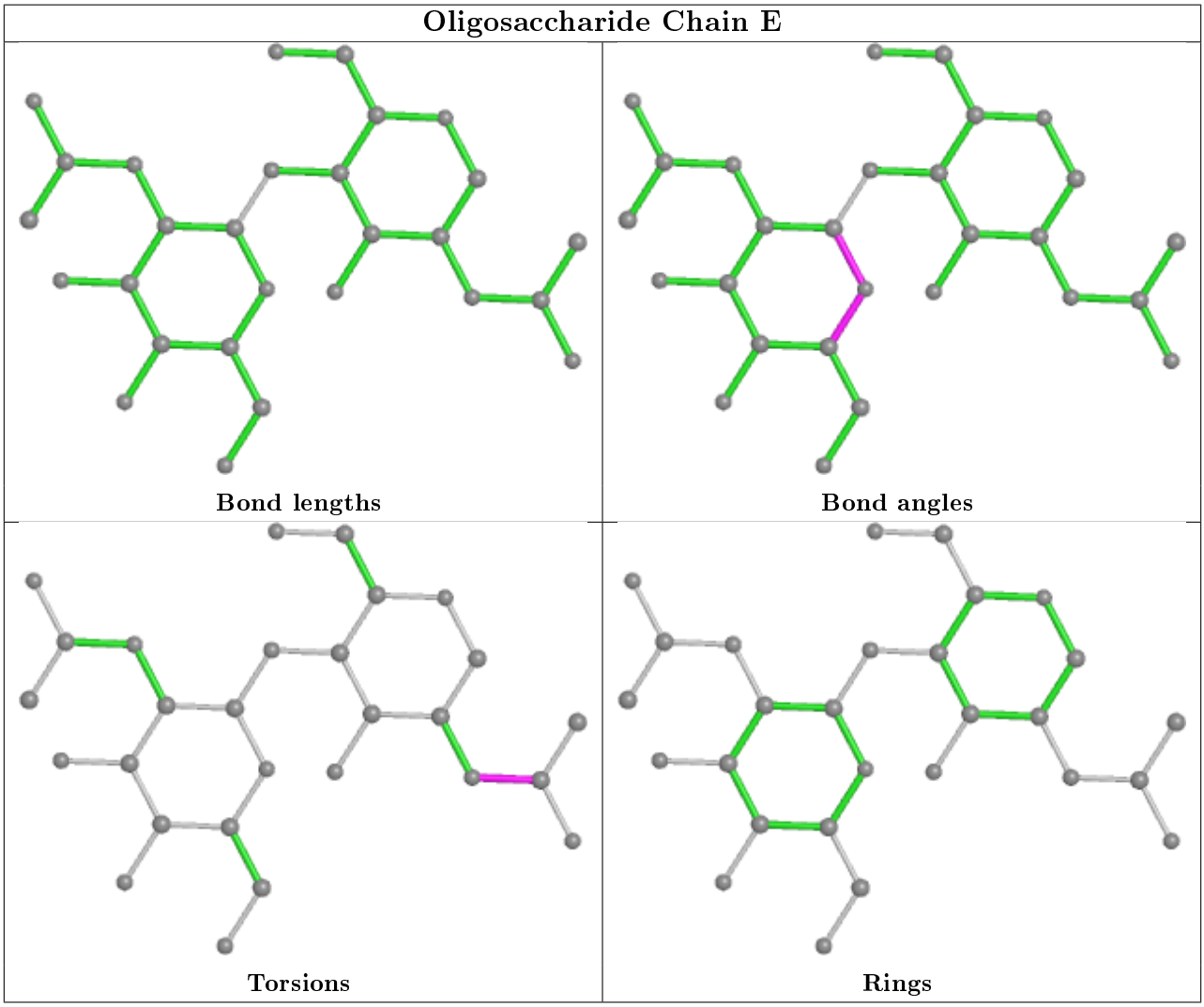
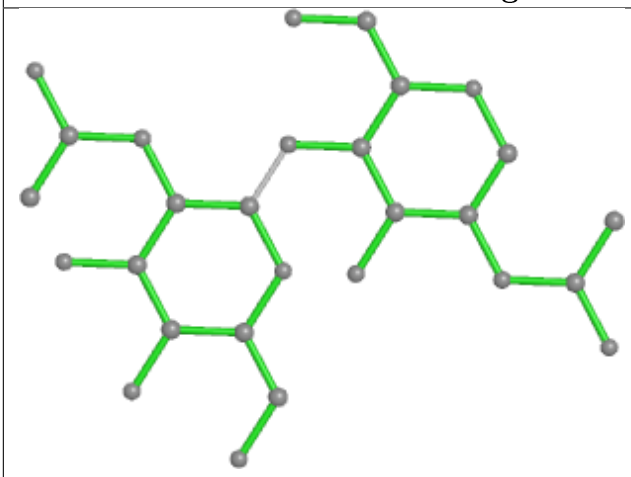
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	2	NAG	1	0
4	J	5	MAN	1	0
4	F	1	NAG	2	0
5	H	3	MAN	1	0
4	J	2	NAG	4	0
4	J	3	MAN	3	0
5	K	2	NAG	4	0
4	J	1	NAG	3	0
4	F	3	MAN	3	0

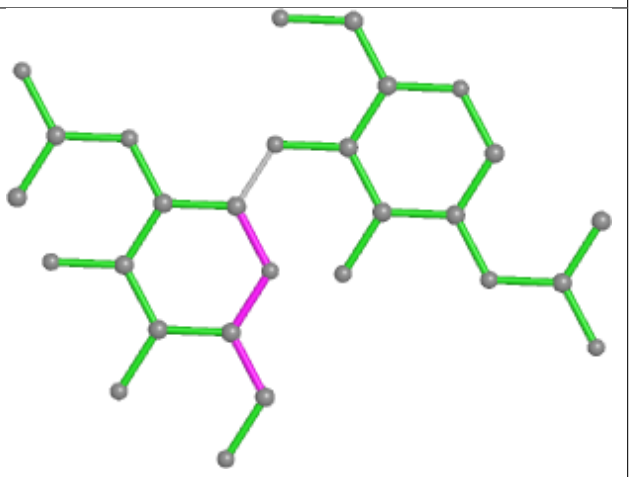
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



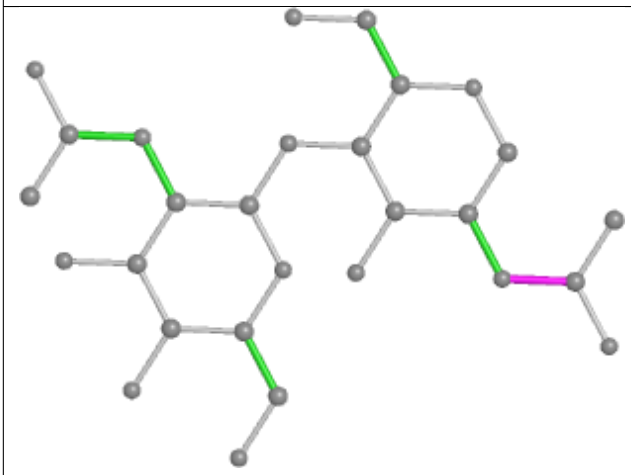
Oligosaccharide Chain I



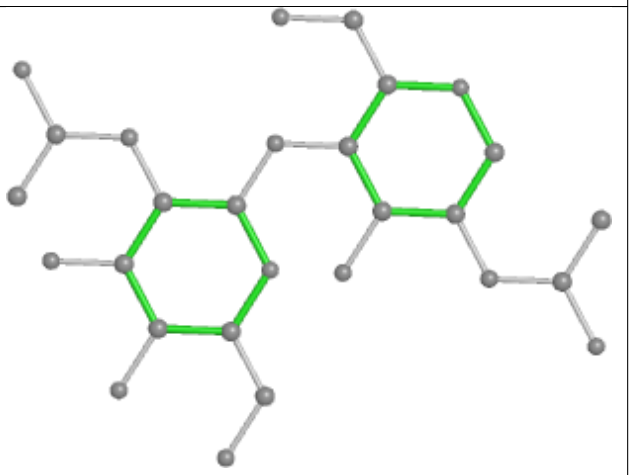
Bond lengths



Bond angles

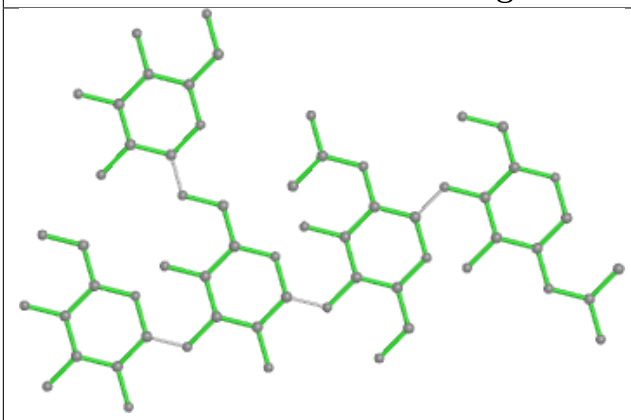


Torsions

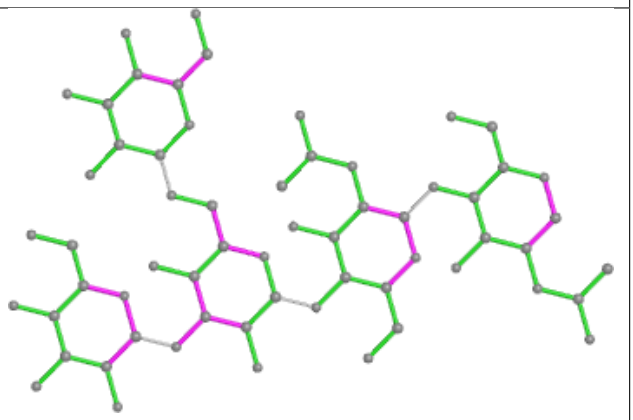


Rings

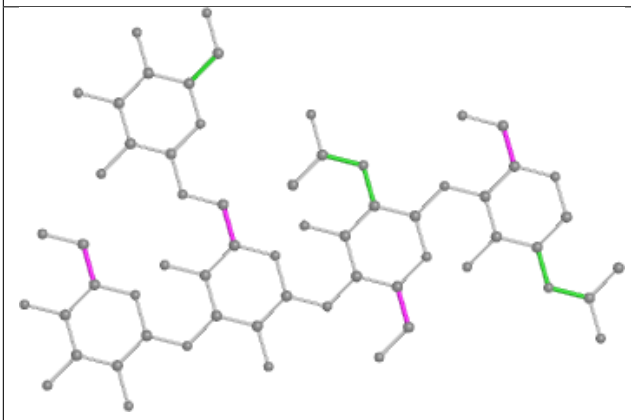
Oligosaccharide Chain F



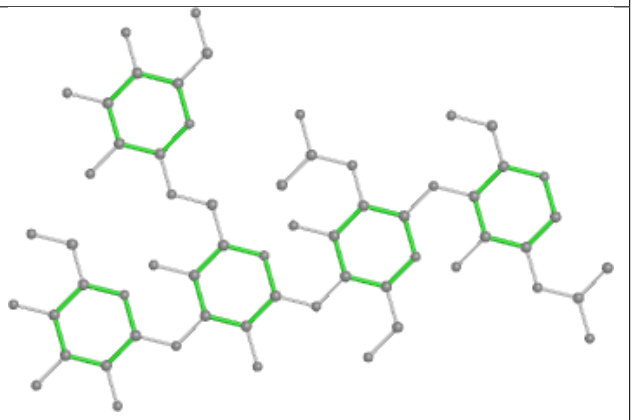
Bond lengths



Bond angles

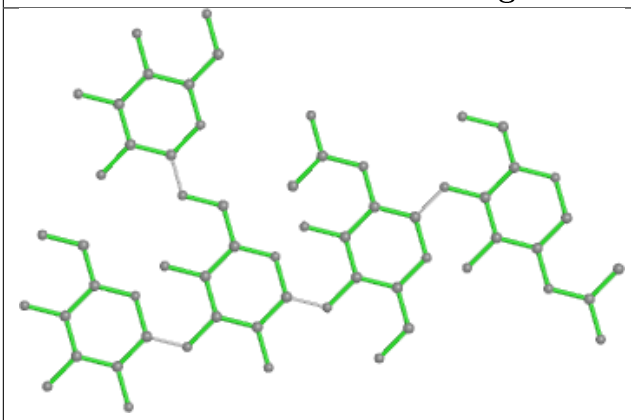


Torsions

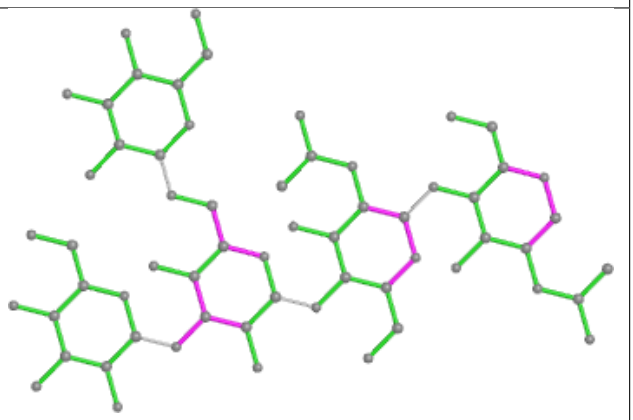


Rings

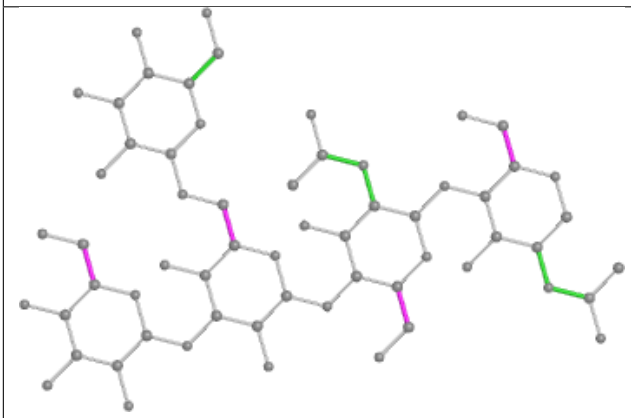
Oligosaccharide Chain J



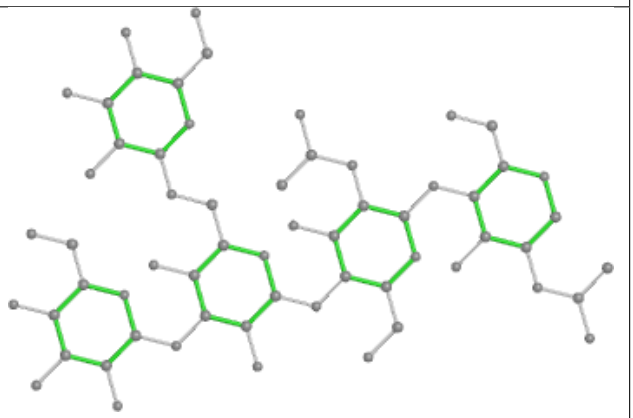
Bond lengths



Bond angles

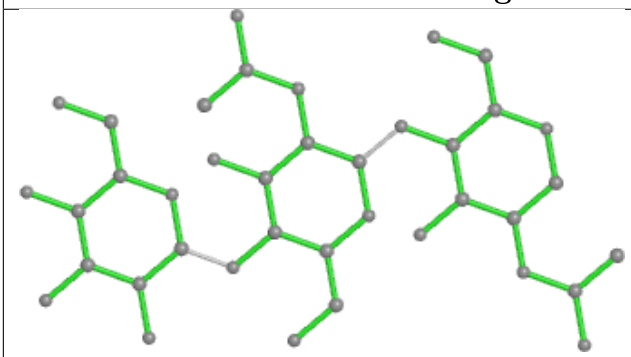


Torsions

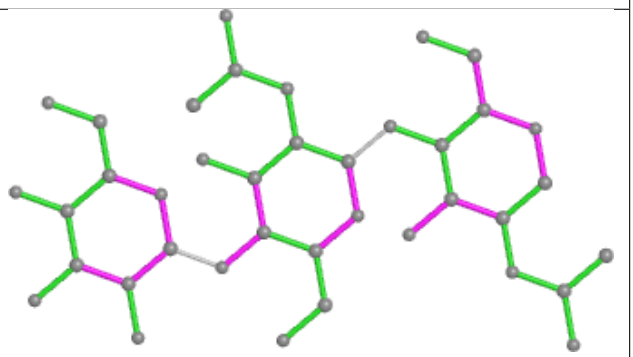


Rings

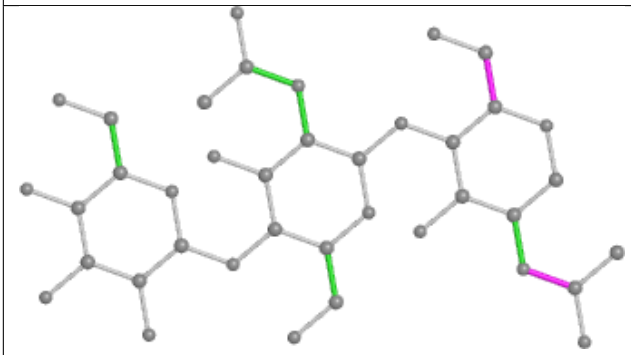
Oligosaccharide Chain G



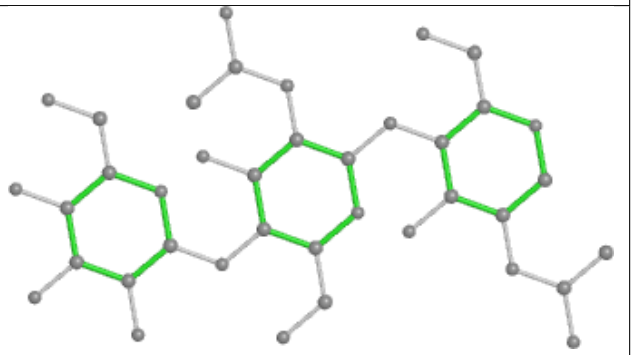
Bond lengths



Bond angles

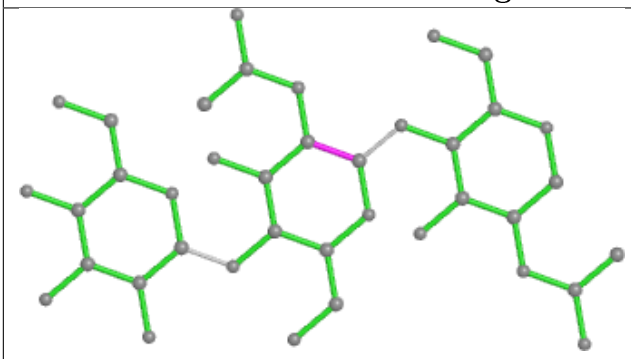


Torsions

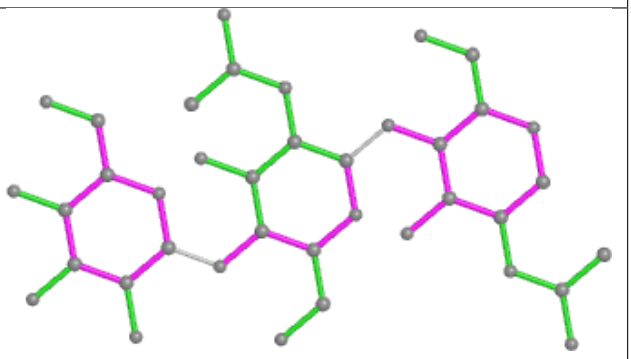


Rings

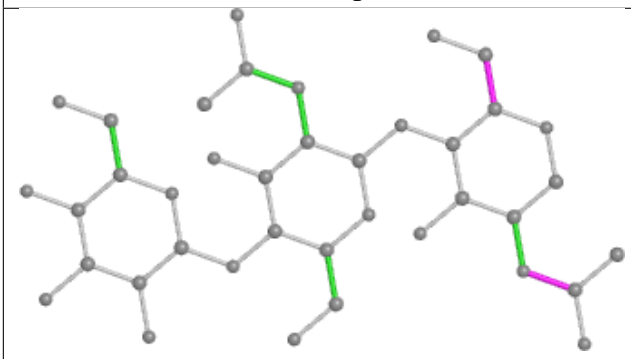
Oligosaccharide Chain H



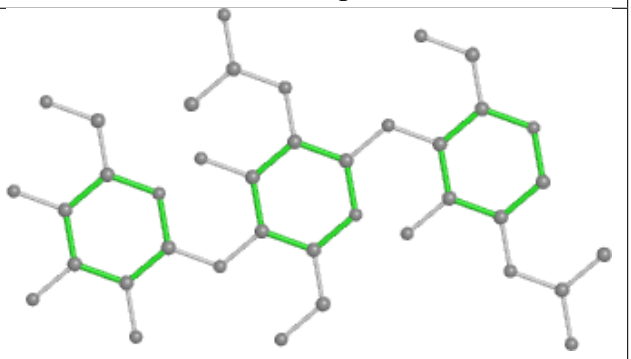
Bond lengths



Bond angles

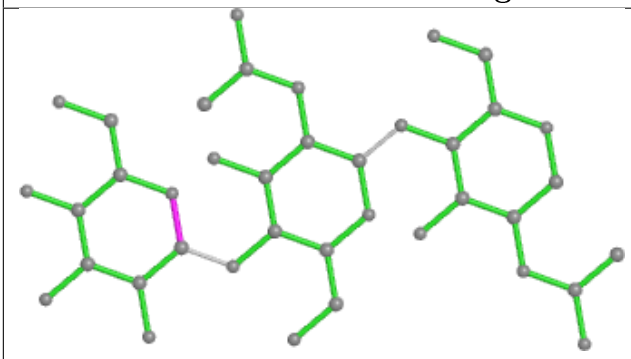


Torsions

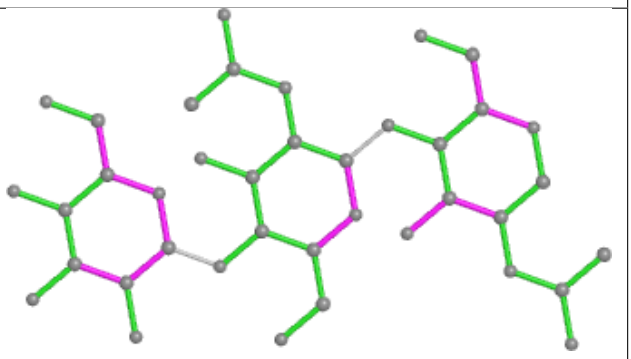


Rings

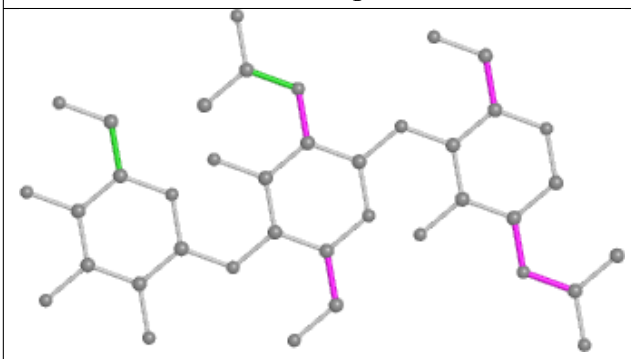
Oligosaccharide Chain K



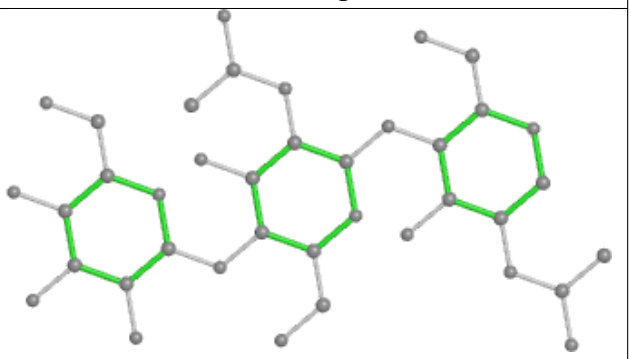
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
8	MAN	C	3378	-	11,11,12	1.00	1 (9%)	15,15,17	2.37	4 (26%)
6	NAG	C	3880	1	14,14,15	0.32	0	17,19,21	1.58	1 (5%)
6	NAG	D	3094	2	14,14,15	0.53	0	17,19,21	0.65	0
6	NAG	B	3479	2	14,14,15	4.38	14 (100%)	17,19,21	3.51	9 (52%)
6	NAG	B	3094	2	14,14,15	0.62	0	17,19,21	1.01	1 (5%)
6	NAG	C	3678	1	14,14,15	0.53	0	17,19,21	0.67	0
6	NAG	A	3678	1	14,14,15	0.52	0	17,19,21	0.75	0
6	NAG	D	3479	2	14,14,15	4.82	13 (92%)	17,19,21	2.86	9 (52%)

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	MAN	C	3378	-	-	2/2/19/22	0/1/1/1
6	NAG	C	3880	1	-	3/6/23/26	0/1/1/1
6	NAG	D	3094	2	-	0/6/23/26	0/1/1/1
6	NAG	B	3479	2	-	1/6/23/26	0/1/1/1
6	NAG	B	3094	2	-	0/6/23/26	0/1/1/1
6	NAG	C	3678	1	-	0/6/23/26	0/1/1/1
6	NAG	A	3678	1	-	0/6/23/26	0/1/1/1
6	NAG	D	3479	2	-	0/6/23/26	0/1/1/1

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	3479	NAG	C4-C5	6.82	1.67	1.53
6	D	3479	NAG	O5-C5	6.77	1.57	1.43
6	B	3479	NAG	C4-C5	6.53	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	3479	NAG	O7-C7	6.39	1.37	1.23
6	D	3479	NAG	O5-C1	6.38	1.53	1.43

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	3479	NAG	O5-C1-C2	8.23	124.28	111.29
6	D	3479	NAG	C1-O5-C5	7.16	121.90	112.19
8	C	3378	MAN	C1-C2-C3	-6.56	101.60	109.67
6	C	3880	NAG	C1-O5-C5	5.43	119.55	112.19
6	B	3479	NAG	O5-C5-C6	4.64	114.48	107.20

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	3880	NAG	C8-C7-N2-C2
6	C	3880	NAG	O7-C7-N2-C2
8	C	3378	MAN	O5-C5-C6-O6
8	C	3378	MAN	C4-C5-C6-O6
6	C	3880	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	3378	MAN	1	0
6	B	3479	NAG	1	0
6	D	3479	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	884/1095 (80%)	0.13	36 (4%)	37	27	106, 204, 303, 383	0
1	C	882/1095 (80%)	0.09	34 (3%)	39	28	112, 207, 304, 401	0
2	B	673/687 (97%)	0.40	71 (10%)	6	5	133, 256, 325, 426	2 (0%)
2	D	673/687 (97%)	0.52	88 (13%)	3	3	144, 258, 332, 424	2 (0%)
All	All	3112/3564 (87%)	0.26	229 (7%)	14	10	106, 233, 318, 426	4 (0%)

The worst 5 of 229 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	92	ALA	11.5
2	D	433	ASP	10.6
2	B	470	GLU	8.9
2	D	432	ARG	8.6
2	B	323	LEU	7.8

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
4	MAN	F	4	11/12	0.21	0.49	278,313,361,364	0
4	MAN	F	3	11/12	0.27	0.32	221,338,359,359	0

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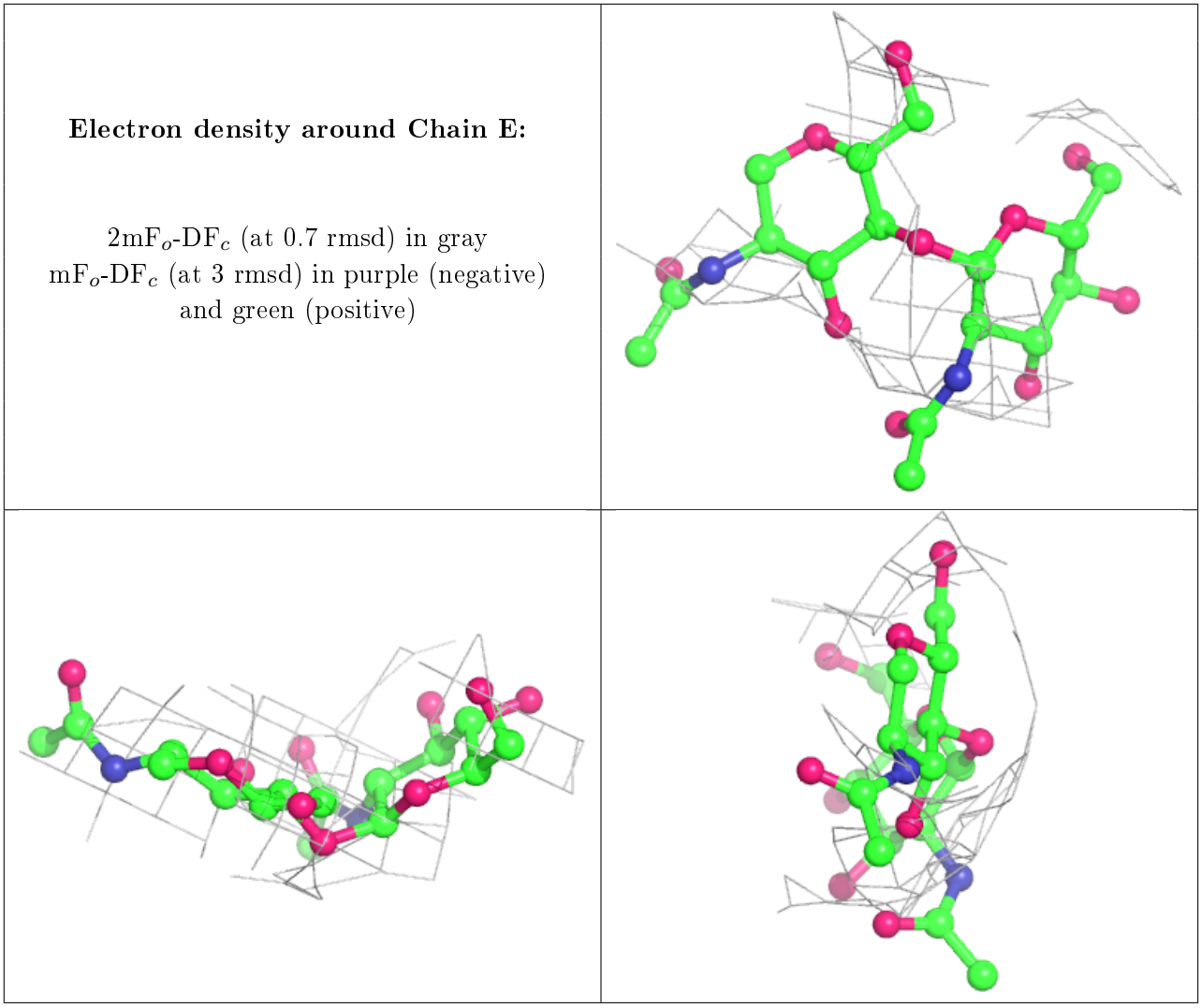
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MAN	J	5	11/12	0.40	0.31	233,301,351,351	0
5	MAN	H	3	11/12	0.43	0.56	310,353,388,410	0
5	MAN	G	3	11/12	0.43	0.20	295,349,390,420	0
4	MAN	J	4	11/12	0.55	0.27	217,294,356,376	0
4	MAN	J	3	11/12	0.56	0.31	271,326,353,354	0
3	NAG	E	2	14/15	0.56	0.28	222,255,345,354	0
3	NAG	I	2	14/15	0.62	0.42	228,295,376,376	0
4	MAN	F	5	11/12	0.69	0.26	241,288,357,366	0
4	NAG	J	2	14/15	0.71	0.29	205,297,391,446	0
4	NAG	F	2	14/15	0.72	0.31	273,293,381,415	0
5	MAN	K	3	11/12	0.73	0.14	313,359,401,410	0
3	NAG	E	1	14/15	0.75	0.32	209,289,325,337	0
5	NAG	H	2	14/15	0.78	0.37	252,291,337,341	0
4	NAG	F	1	14/15	0.80	0.27	181,314,385,389	0
5	NAG	G	2	14/15	0.81	0.22	225,292,336,341	0
4	NAG	J	1	14/15	0.81	0.30	230,326,381,388	0
3	NAG	I	1	14/15	0.82	0.22	219,245,283,285	0
5	NAG	K	2	14/15	0.85	0.22	237,294,351,395	0
5	NAG	H	1	14/15	0.91	0.19	197,234,285,285	0
5	NAG	G	1	14/15	0.93	0.19	84,247,290,297	0
5	NAG	K	1	14/15	0.93	0.18	90,220,322,330	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.

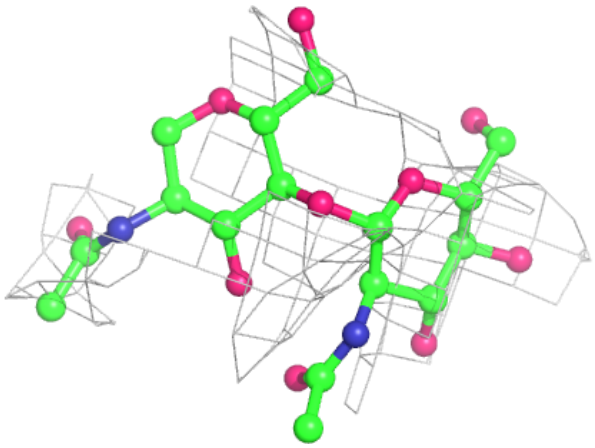
Electron density around Chain E:

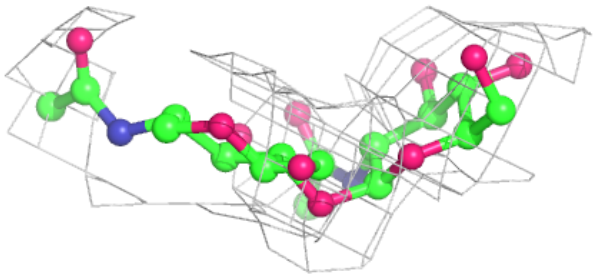
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

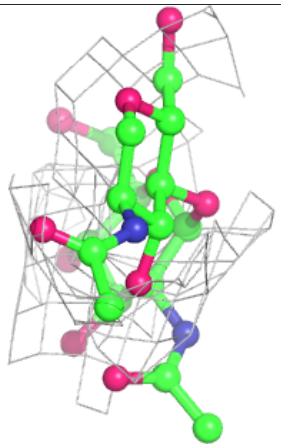


Electron density around Chain I:

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

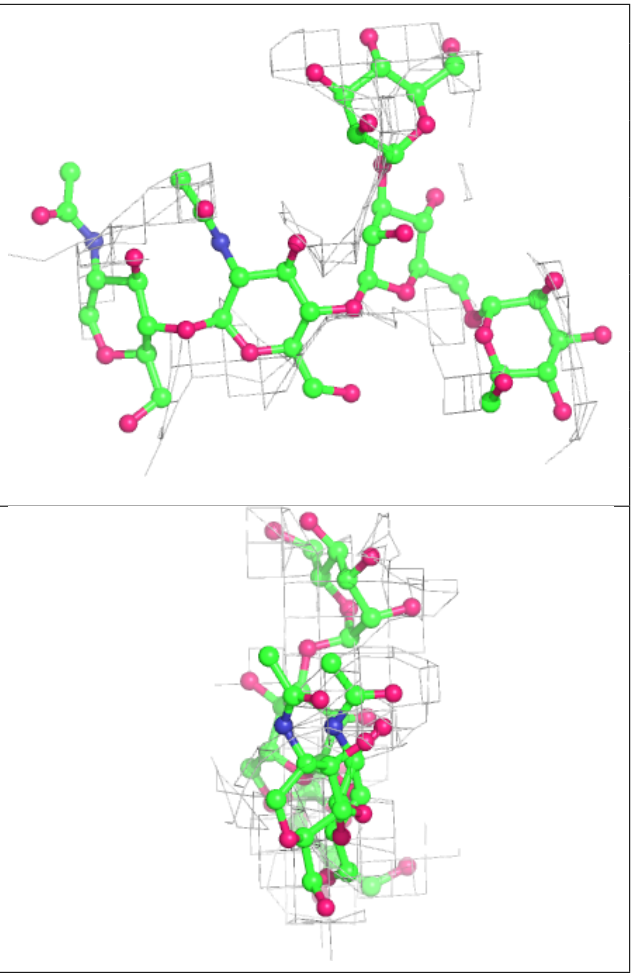






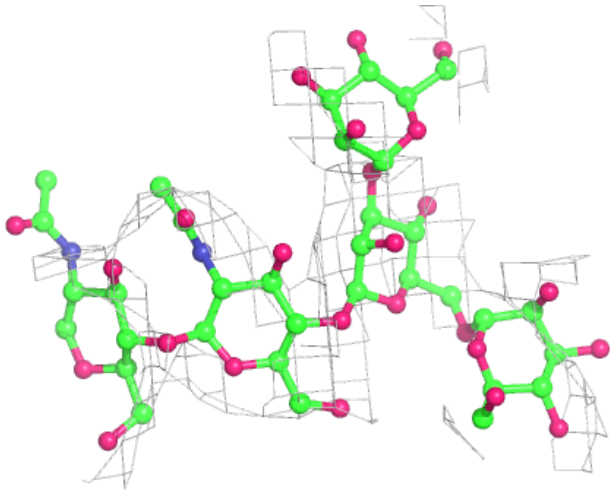
Electron density around Chain F:

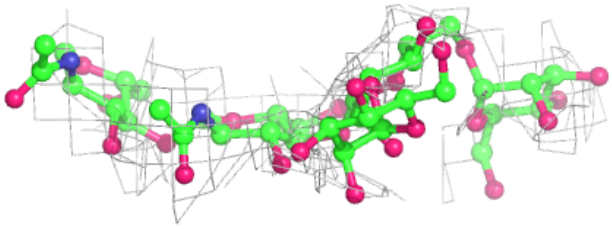
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

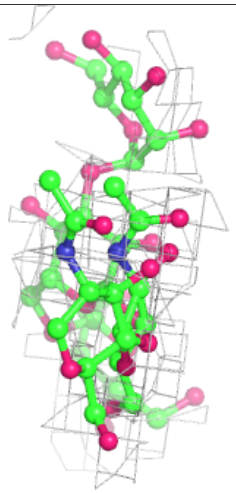


Electron density around Chain J:

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

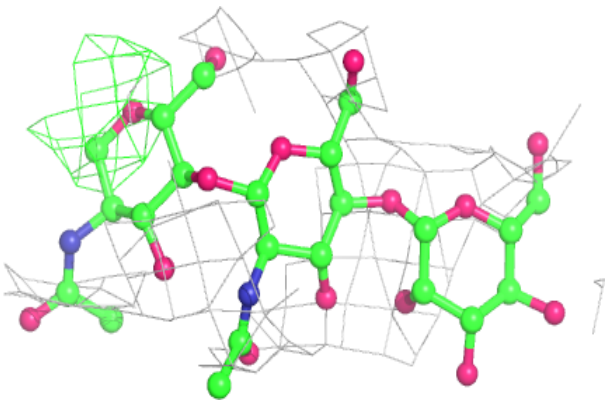


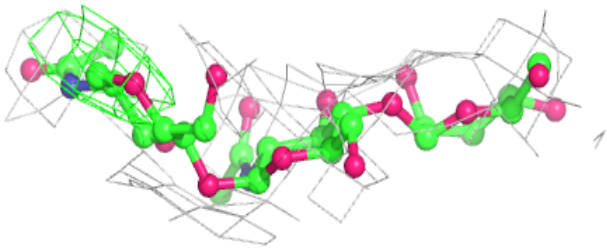


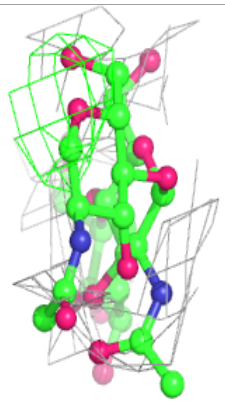


Electron density around Chain G:

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

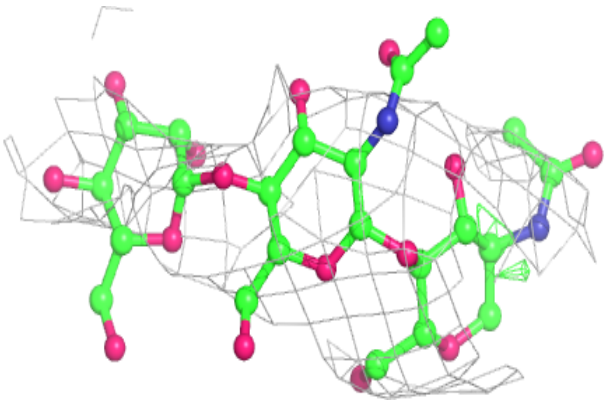


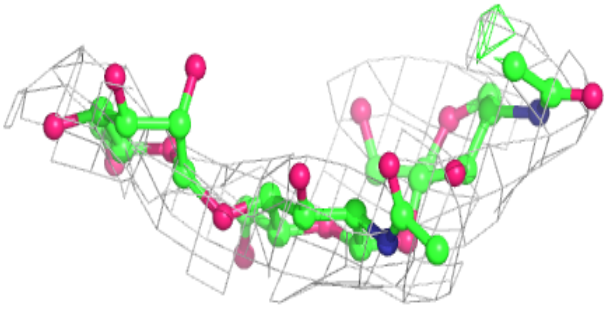


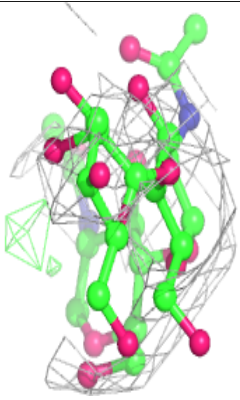


Electron density around Chain H:

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

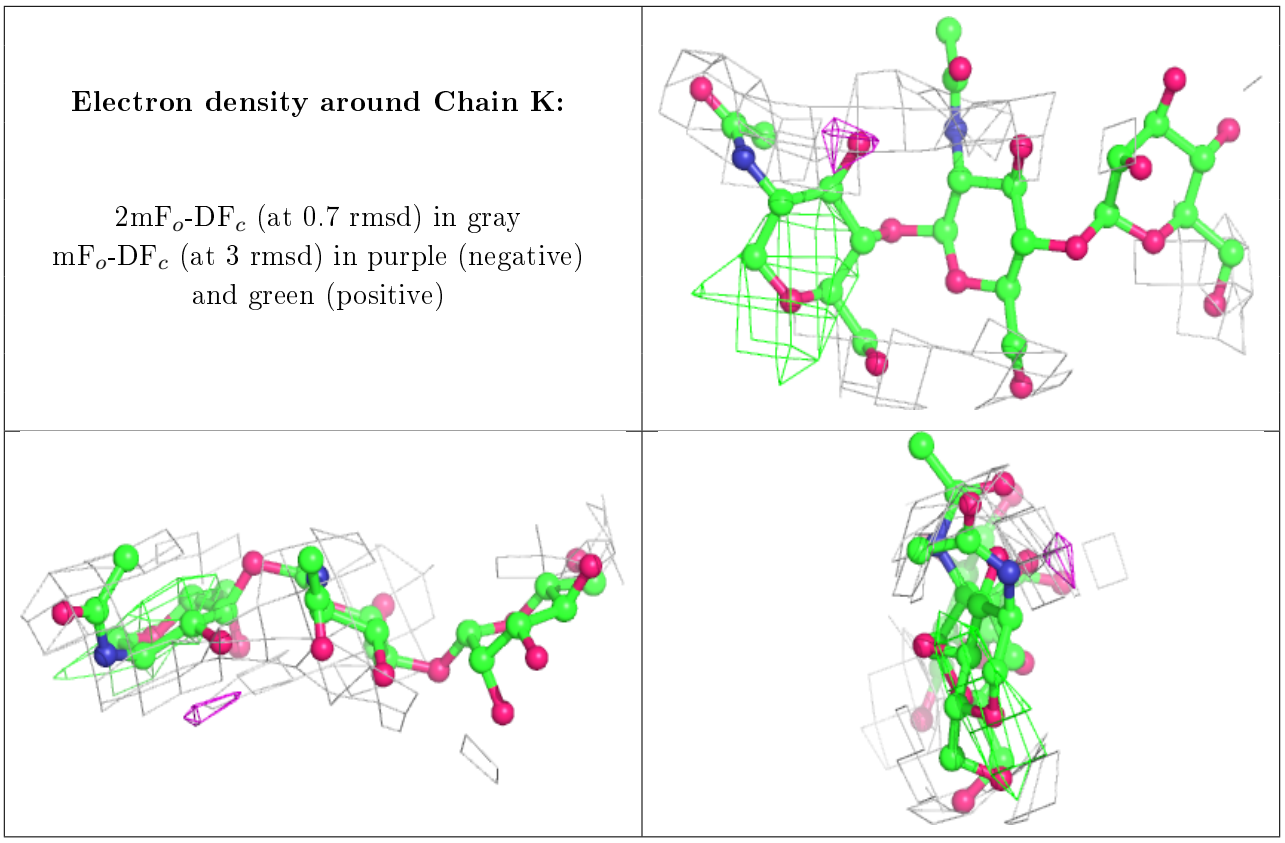






Electron density around Chain K:

$2mF_o$-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
8	MAN	C	3378	11/12	0.36	0.51	241,288,352,362	0
7	CA	B	2002	1/1	0.52	0.23	608,608,608,608	0
7	CA	A	2007	1/1	0.62	0.14	240,240,240,240	0
7	CA	C	2005	1/1	0.63	0.16	215,215,215,215	0
7	CA	C	2007	1/1	0.69	0.14	237,237,237,237	0
7	CA	A	2005	1/1	0.74	0.11	193,193,193,193	0
6	NAG	D	3094	14/15	0.74	0.42	254,283,315,325	0
7	CA	D	2002	1/1	0.76	0.08	594,594,594,594	0
6	NAG	B	3094	14/15	0.79	0.36	232,281,317,341	0
6	NAG	D	3479	14/15	0.79	0.28	191,259,284,291	0
6	NAG	B	3479	14/15	0.82	0.22	213,256,300,333	0
6	NAG	A	3678	14/15	0.86	0.25	167,304,342,378	0
6	NAG	C	3880	14/15	0.87	0.27	136,198,243,253	0
6	NAG	C	3678	14/15	0.90	0.22	177,279,379,392	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	CA	C	2006	1/1	0.90	0.18	147,147,147,147	0
7	CA	A	2006	1/1	0.95	0.17	143,143,143,143	0

6.5 Other polymers (i)

There are no such residues in this entry.