wwPDB X-ray Structure Validation Summary Report (i)

Oct 13, 2024 – 06:56 am BST

PDB ID	:	2C11
Title	:	Crystal structure of the 2-hydrazinopyridine of semicarbazide- sensitive amine oxidase
Authors	:	Jakobsson, E.; Kleywegt, G.J.
Deposited on	:	2005-09-09
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

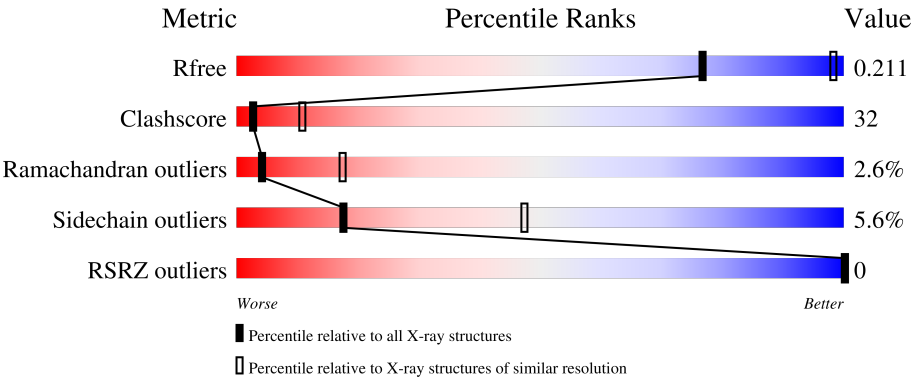
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 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}	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (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 of 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	735	39% 45% 7% 9%
1	B	735	47% 41% . 9%
1	C	735	39% 46% 6% 9%
1	D	735	47% 41% . 9%
2	E	2	100%

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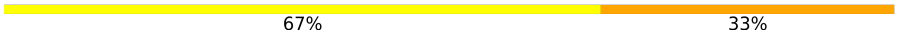
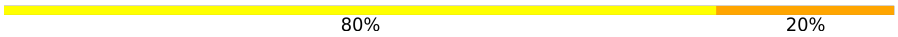
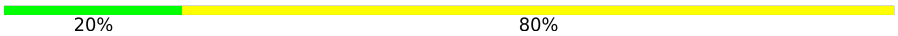
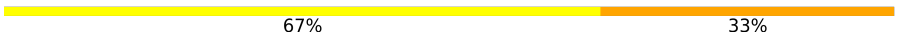
Mol	Chain	Length	Quality of chain
2	I	2	
3	F	2	
4	G	3	
4	K	3	
5	H	5	
5	L	5	
6	J	3	

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
1	PAQ	A	471	X	-	-	-
1	PAQ	B	471	X	-	-	-
1	PAQ	C	471	X	-	-	-
1	PAQ	D	471	X	-	-	-
3	FUC	F	2	X	-	-	-
5	NAG	H	1	X	-	-	-
5	FUC	H	5	X	-	-	-
5	NAG	L	1	X	-	-	-
5	FUC	L	5	X	-	-	-
6	FUC	J	3	X	-	-	-
7	NAG	D	1736	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 21917 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 MEMBRANE COPPER AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	672	Total	C	N	O	S	0	0	1
			5340	3434	924	965	17			
1	B	672	Total	C	N	O	S	0	0	1
			5340	3434	924	965	17			
1	C	672	Total	C	N	O	S	0	0	1
			5340	3434	924	965	17			
1	D	672	Total	C	N	O	S	0	0	1
			5340	3434	924	965	17			

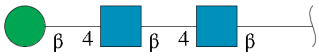
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

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

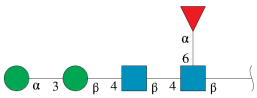
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O	0	0	0
			24	14	1	9			

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



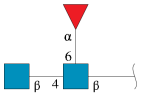
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	K	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



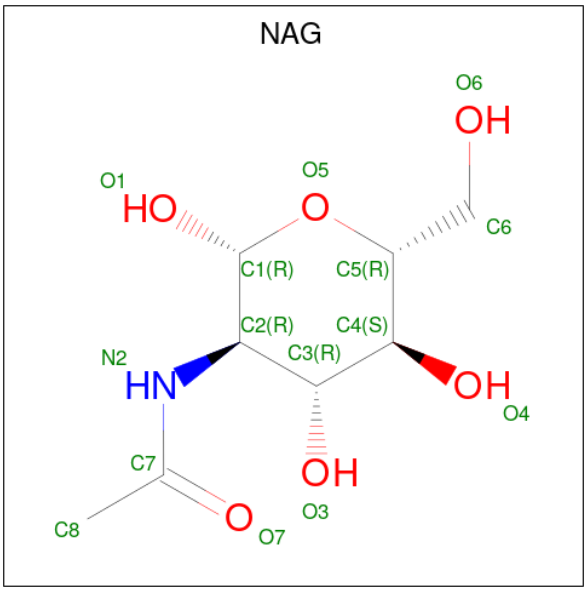
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	5	Total	C	N	O	0	0	0
			60	34	2	24			
5	L	5	Total	C	N	O	0	0	0
			60	34	2	24			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	3	Total	C	N	O	0	0	0
			38	22	2	14			

- 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
7	A	1	Total C N O 14 8 1 5	0	0
7	A	1	Total C N O 14 8 1 5	0	0
7	B	1	Total C N O 14 8 1 5	0	0
7	B	1	Total C N O 14 8 1 5	0	0
7	B	1	Total C N O 14 8 1 5	0	0
7	C	1	Total C N O 14 8 1 5	0	0
7	C	1	Total C N O 14 8 1 5	0	0
7	D	1	Total C N O 14 8 1 5	0	0
7	D	1	Total C N O 14 8 1 5	0	0
7	D	1	Total C N O 14 8 1 5	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	2	Total Ca 2 2	0	0
8	B	2	Total Ca 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	2	Total Ca 2 2	0	0
8	D	2	Total Ca 2 2	0	0

- Molecule 9 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	7	Total Cu 7 7	0	0
9	B	8	Total Cu 8 8	0	0
9	C	8	Total Cu 8 8	0	0
9	D	7	Total Cu 7 7	0	0

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	2	Total Cl 2 2	0	0
10	C	1	Total Cl 1 1	0	0
10	D	1	Total Cl 1 1	0	0

- Molecule 11 is water.

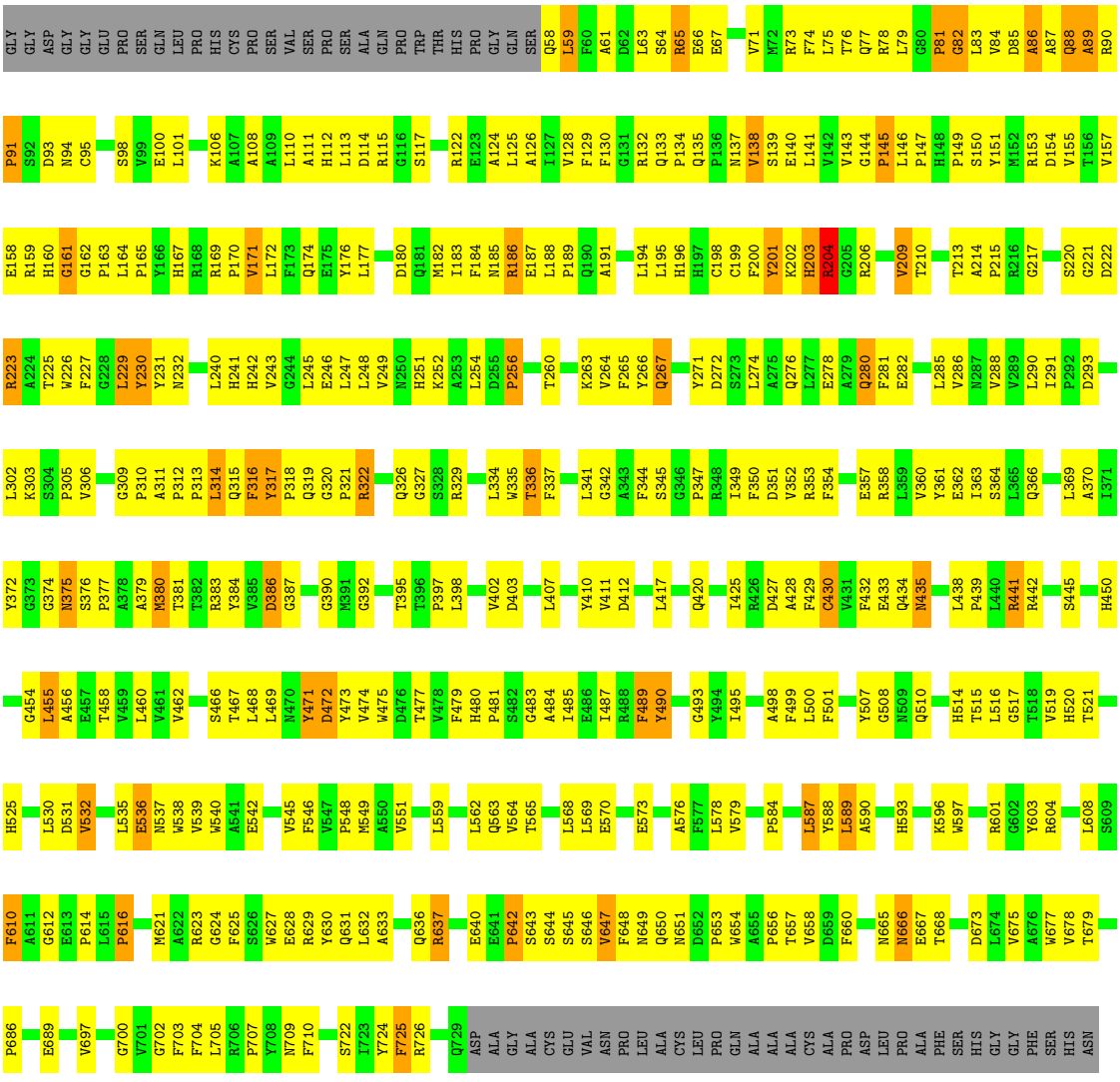
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	19	Total O 19 19	0	0
11	B	20	Total O 20 20	0	0
11	C	11	Total O 11 11	0	0
11	D	9	Total O 9 9	0	0

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.

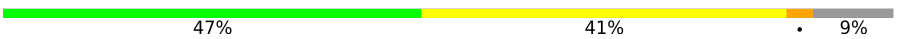
• Molecule 1: MEMBRANE COPPER AMINE OXIDASE

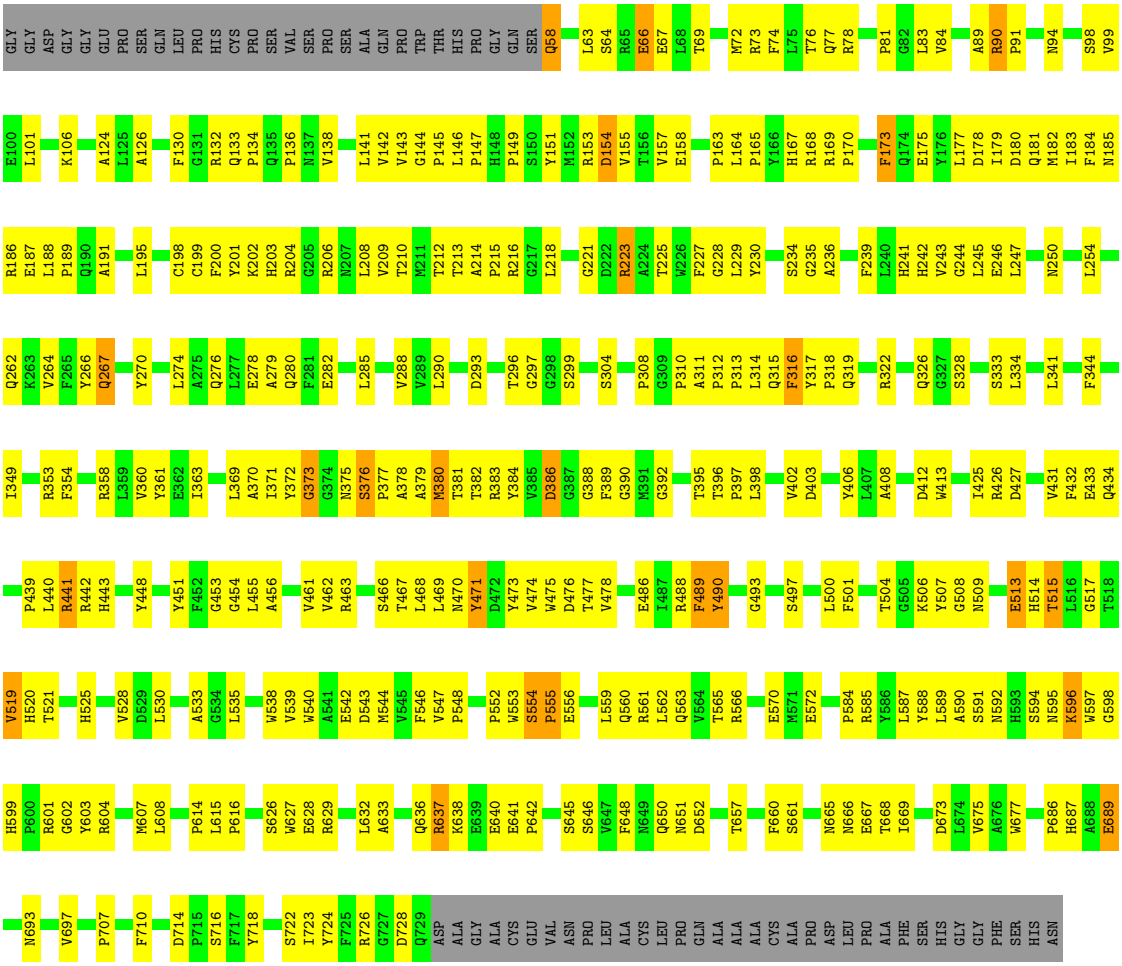
Chain A:



• Molecule 1: MEMBRANE COPPER AMINE OXIDASE

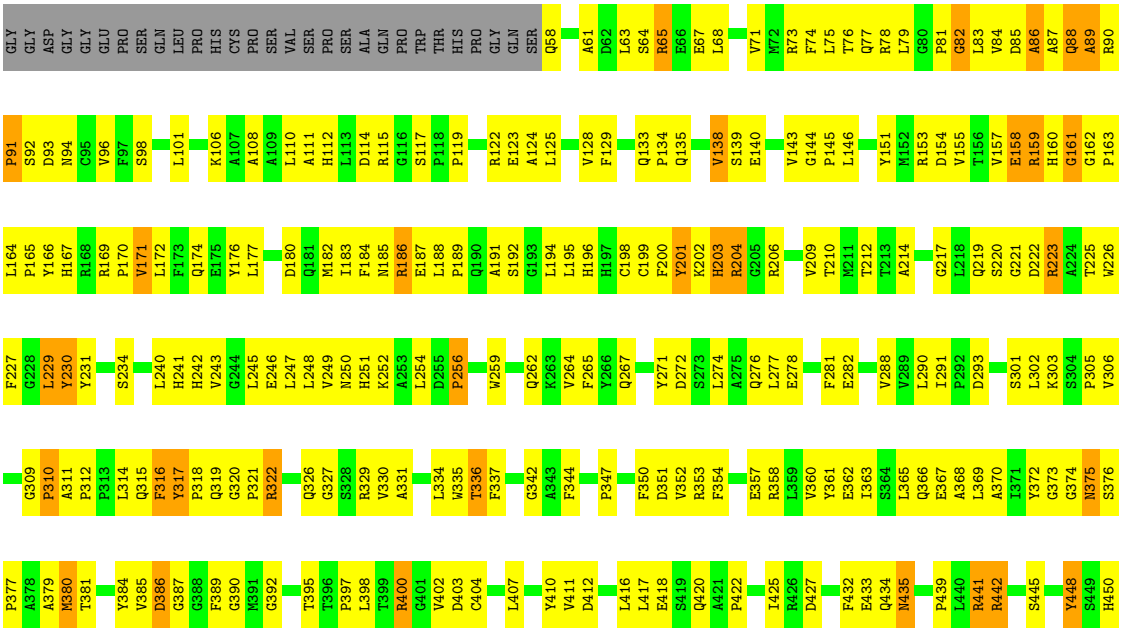
Chain B:

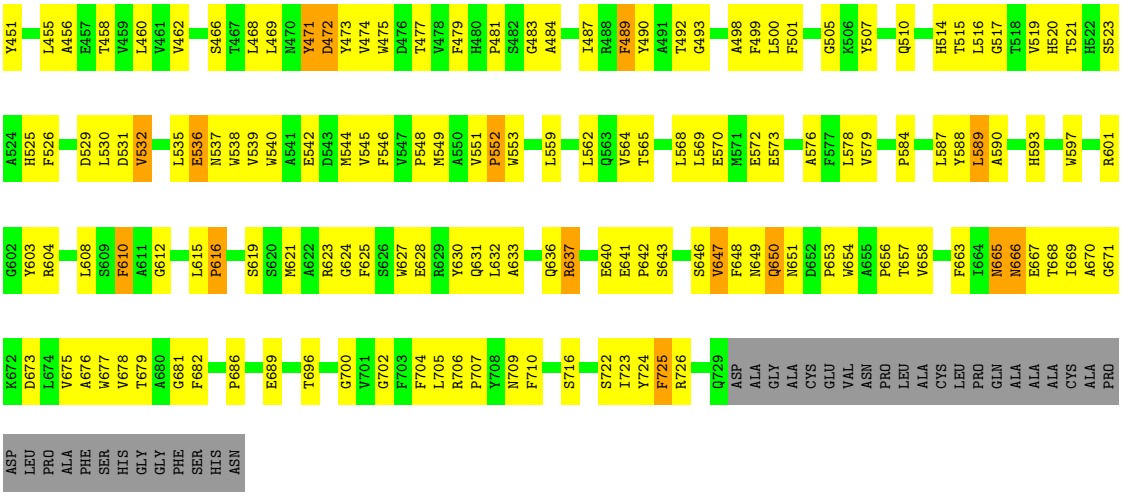




• Molecule 1: MEMBRANE COPPER AMINE OXIDASE

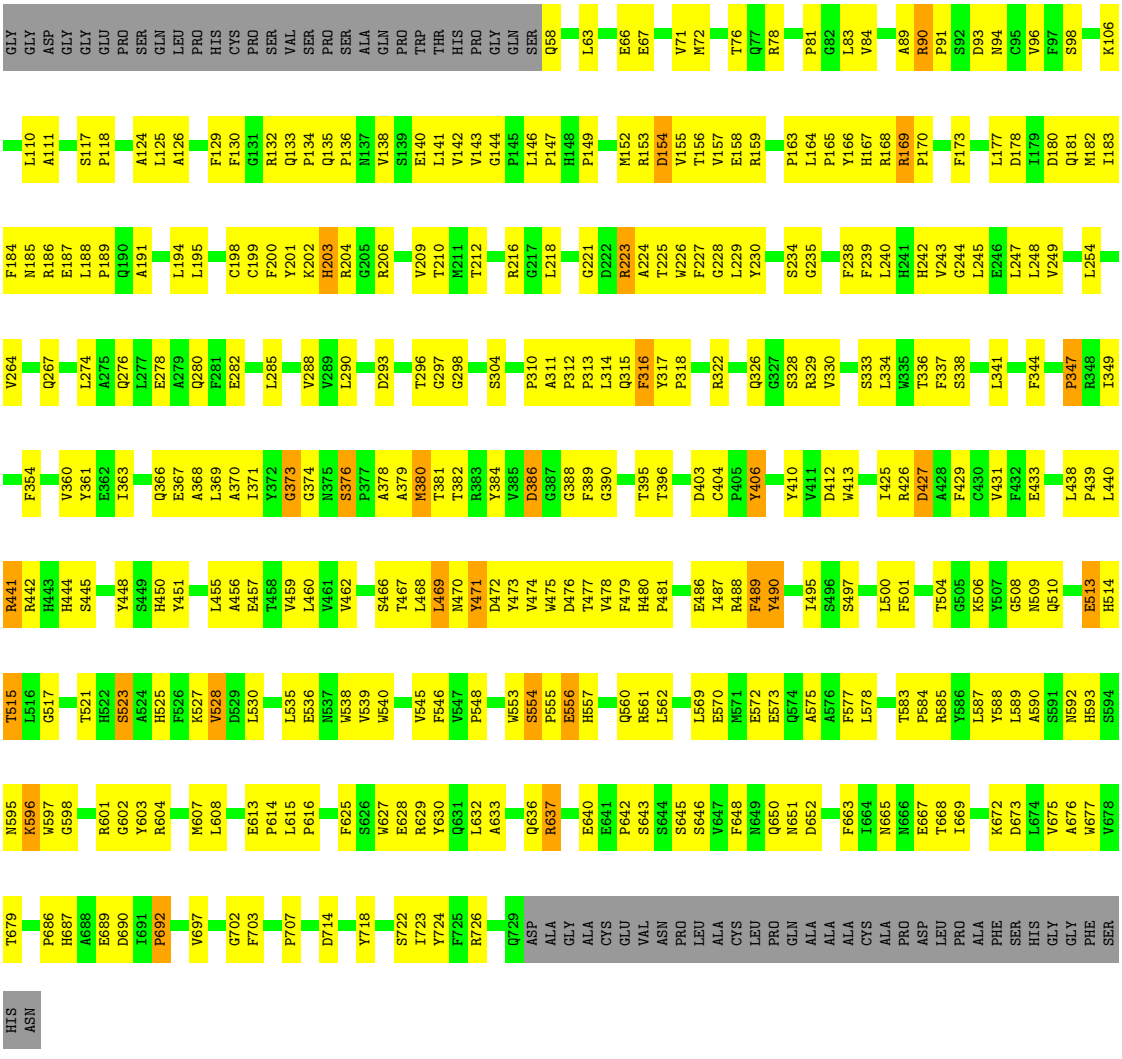
Chain C:





• Molecule 1: MEMBRANE COPPER AMINE OXIDASE

Chain D:



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

Chain E:

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

Chain I:

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

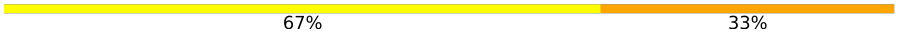
Chain F:

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

Chain G:

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

Chain K:

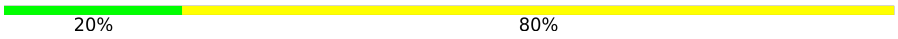


• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

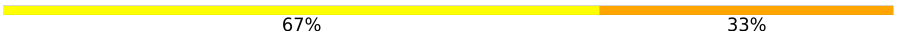
• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



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

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	127.40Å 127.40Å 219.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	90.7 (20.00-2.90) 94.7 (20.00-2.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.276 0.215 , 0.211	Depositor DCC
R_{free} test set	3370 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å^2)	55.3	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 27.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.458 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	21917	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: FUC, BMA, CL, CU, PAQ, NAG, CA, 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	0.50	0/5488	0.72	2/7481 (0.0%)
1	B	0.48	0/5488	0.72	1/7481 (0.0%)
1	C	0.49	0/5488	0.71	2/7481 (0.0%)
1	D	0.48	0/5488	0.72	1/7481 (0.0%)
All	All	0.49	0/21952	0.72	6/29924 (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	1	0
1	B	1	0
1	C	1	0
1	D	1	0
All	All	4	0

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	59	LEU	CA-CB-CG	7.19	131.83	115.30
1	D	373	GLY	N-CA-C	-6.13	97.78	113.10
1	B	373	GLY	N-CA-C	-5.95	98.23	113.10
1	C	204	ARG	N-CA-C	5.47	125.78	111.00
1	A	204	ARG	N-CA-C	5.24	125.15	111.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	471	PAQ	CG
1	B	471	PAQ	CG
1	C	471	PAQ	CG
1	D	471	PAQ	CG

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	5340	0	5112	410	0
1	B	5340	0	5110	323	0
1	C	5340	0	5112	399	0
1	D	5340	0	5111	338	0
2	E	28	0	25	2	0
2	I	28	0	25	3	0
3	F	24	0	22	4	0
4	G	39	0	34	1	0
4	K	39	0	34	5	0
5	H	60	0	52	3	0
5	L	60	0	52	0	0
6	J	38	0	34	5	0
7	A	28	0	26	4	0
7	B	42	0	39	3	0
7	C	28	0	26	2	0
7	D	42	0	39	2	0
8	A	2	0	0	0	0
8	B	2	0	0	0	0
8	C	2	0	0	0	0
8	D	2	0	0	0	0
9	A	7	0	0	0	0
9	B	8	0	0	0	0
9	C	8	0	0	0	0
9	D	7	0	0	0	0
10	A	2	0	0	0	0
10	C	1	0	0	0	0
10	D	1	0	0	0	0
11	A	19	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	B	20	0	0	5	0
11	C	11	0	0	5	0
11	D	9	0	0	4	0
All	All	21917	0	20853	1388	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 32.

The worst 5 of 1388 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)
1:B:360:VAL:HG11	1:B:363:ILE:HG13	1.37	1.04
1:C:90:ARG:HG2	1:C:91:PRO:HD2	1.42	1.02
1:B:106:LYS:HB2	1:B:637:ARG:HH21	1.27	0.99
1:A:90:ARG:HG2	1:A:91:PRO:HD2	1.43	0.96
1:A:344:PHE:HA	1:A:390:GLY:HA2	1.45	0.95

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	669/735 (91%)	571 (85%)	72 (11%)	26 (4%)	2 10
1	B	669/735 (91%)	585 (87%)	76 (11%)	8 (1%)	11 35
1	C	669/735 (91%)	575 (86%)	69 (10%)	25 (4%)	2 11
1	D	669/735 (91%)	587 (88%)	71 (11%)	11 (2%)	8 28
All	All	2676/2940 (91%)	2318 (87%)	288 (11%)	70 (3%)	4 17

5 of 70 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	380	MET
1	A	637	ARG
1	B	267	GLN
1	B	386	ASP
1	B	596	LYS

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	562/609 (92%)	523 (93%)	39 (7%)	13	37
1	B	562/609 (92%)	538 (96%)	24 (4%)	25	57
1	C	562/609 (92%)	527 (94%)	35 (6%)	15	43
1	D	562/609 (92%)	535 (95%)	27 (5%)	21	54
All	All	2248/2436 (92%)	2123 (94%)	125 (6%)	17	47

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	519	VAL
1	D	429	PHE
1	C	209	VAL
1	D	427	ASP
1	D	528	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	185	ASN
1	C	326	GLN
1	D	650	GLN
1	D	319	GLN
1	C	203	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)

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	PAQ	D	471	1	17,22,23	2.12	5 (29%)	16,29,31	2.39	3 (18%)
1	PAQ	B	471	1	17,22,23	2.12	5 (29%)	16,29,31	2.45	4 (25%)
1	PAQ	A	471	1	17,22,23	2.12	5 (29%)	16,29,31	2.42	3 (18%)
1	PAQ	C	471	1	17,22,23	2.16	7 (41%)	16,29,31	2.47	4 (25%)

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
1	PAQ	D	471	1	1/1/5/10	6/8/27/29	0/2/2/2
1	PAQ	B	471	1	1/1/5/10	5/8/27/29	0/2/2/2
1	PAQ	A	471	1	1/1/5/10	6/8/27/29	0/2/2/2
1	PAQ	C	471	1	1/1/5/10	6/8/27/29	0/2/2/2

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	471	PAQ	CG-CD2	-5.60	1.39	1.50
1	D	471	PAQ	CG-CD2	-5.58	1.39	1.50
1	C	471	PAQ	CG-CD2	-5.56	1.39	1.50
1	B	471	PAQ	CG-CD2	-5.55	1.39	1.50
1	C	471	PAQ	N2-N1	-3.50	1.32	1.39

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	471	PAQ	CD2-CG-CD1	6.03	119.02	104.65
1	B	471	PAQ	CD2-CG-CD1	6.03	119.01	104.65
1	A	471	PAQ	CD2-CG-CD1	5.99	118.92	104.65
1	C	471	PAQ	CD2-CG-CD1	5.96	118.86	104.65
1	C	471	PAQ	CD2-CE2-N1	-5.82	117.45	125.57

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	471	PAQ	CG
1	B	471	PAQ	CG
1	C	471	PAQ	CG
1	D	471	PAQ	CG

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	471	PAQ	N-CA-CB-CG
1	A	471	PAQ	C-CA-CB-CG
1	A	471	PAQ	CA-CB-CG-CD1
1	A	471	PAQ	C2-C1-N2-N1
1	A	471	PAQ	N3-C1-N2-N1

There are no ring outliers.

4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	471	PAQ	4	0
1	B	471	PAQ	5	0
1	A	471	PAQ	5	0
1	C	471	PAQ	4	0

5.5 Carbohydrates (i)

25 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	$\#\|Z\| > 2$
2	NAG	E	1	2,1	14,14,15	0.54	0	17,19,21	1.01	1 (5%)
2	NAG	E	2	2	14,14,15	0.55	0	17,19,21	0.82	1 (5%)
3	NAG	F	1	1,3	14,14,15	0.79	1 (7%)	17,19,21	0.96	1 (5%)
3	FUC	F	2	3	10,10,11	0.60	0	14,14,16	0.88	0
4	NAG	G	1	4,1	14,14,15	0.75	0	17,19,21	0.84	0
4	NAG	G	2	4	14,14,15	0.97	0	17,19,21	0.95	2 (11%)
4	BMA	G	3	4	11,11,12	0.94	0	15,15,17	0.58	0
5	NAG	H	1	1,5	14,14,15	0.80	0	17,19,21	1.63	3 (17%)
5	NAG	H	2	5	14,14,15	0.69	0	17,19,21	0.88	0
5	BMA	H	3	5	11,11,12	0.94	0	15,15,17	1.21	1 (6%)
5	MAN	H	4	5	11,11,12	0.72	0	15,15,17	0.85	1 (6%)
5	FUC	H	5	5	10,10,11	0.73	0	14,14,16	0.57	0
2	NAG	I	1	2,1	14,14,15	0.60	0	17,19,21	0.72	0
2	NAG	I	2	2	14,14,15	0.57	0	17,19,21	0.96	1 (5%)
6	NAG	J	1	1,6	14,14,15	0.64	0	17,19,21	1.20	2 (11%)
6	NAG	J	2	6	14,14,15	0.46	0	17,19,21	0.68	0
6	FUC	J	3	6	10,10,11	0.51	0	14,14,16	0.62	0
4	NAG	K	1	4,1	14,14,15	0.55	0	17,19,21	0.70	0
4	NAG	K	2	4	14,14,15	0.75	0	17,19,21	0.74	0
4	BMA	K	3	4	11,11,12	0.64	0	15,15,17	0.83	1 (6%)
5	NAG	L	1	1,5	14,14,15	0.77	0	17,19,21	1.11	1 (5%)
5	NAG	L	2	5	14,14,15	0.84	0	17,19,21	0.88	1 (5%)
5	BMA	L	3	5	11,11,12	1.05	1 (9%)	15,15,17	0.62	0
5	MAN	L	4	5	11,11,12	0.97	1 (9%)	15,15,17	0.66	1 (6%)
5	FUC	L	5	5	10,10,11	0.82	0	14,14,16	0.59	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
2	NAG	E	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	5/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	4/6/23/26	0/1/1/1
3	FUC	F	2	3	1/1/4/5	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	2/2/19/22	0/1/1/1
5	NAG	H	1	1,5	1/1/5/7	4/6/23/26	0/1/1/1
5	NAG	H	2	5	-	4/6/23/26	0/1/1/1
5	BMA	H	3	5	-	2/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	FUC	H	5	5	1/1/4/5	-	0/1/1/1
2	NAG	I	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	I	2	2	-	5/6/23/26	0/1/1/1
6	NAG	J	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	J	2	6	-	6/6/23/26	0/1/1/1
6	FUC	J	3	6	1/1/4/5	-	0/1/1/1
4	NAG	K	1	4,1	-	6/6/23/26	0/1/1/1
4	NAG	K	2	4	-	5/6/23/26	0/1/1/1
4	BMA	K	3	4	-	2/2/19/22	0/1/1/1
5	NAG	L	1	1,5	1/1/5/7	1/6/23/26	0/1/1/1
5	NAG	L	2	5	-	4/6/23/26	0/1/1/1
5	BMA	L	3	5	-	2/2/19/22	0/1/1/1
5	MAN	L	4	5	-	1/2/19/22	1/1/1/1
5	FUC	L	5	5	1/1/4/5	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	3	BMA	C2-C3	2.54	1.56	1.52
5	L	4	MAN	C2-C3	2.29	1.55	1.52
3	F	1	NAG	C1-C2	2.13	1.55	1.52

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	3	BMA	C1-C2-C3	4.33	114.98	109.67
5	H	1	NAG	C4-C3-C2	-4.13	104.97	111.02
5	H	1	NAG	C3-C4-C5	-3.22	104.49	110.24
6	J	1	NAG	C4-C3-C2	-3.14	106.42	111.02
5	H	4	MAN	C1-O5-C5	2.92	116.15	112.19

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	F	2	FUC	C1
5	H	1	NAG	C1
5	H	5	FUC	C1
5	L	1	NAG	C1
5	L	5	FUC	C1

5 of 69 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C1-C2-N2-C7
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2

All (1) ring outliers are listed below:

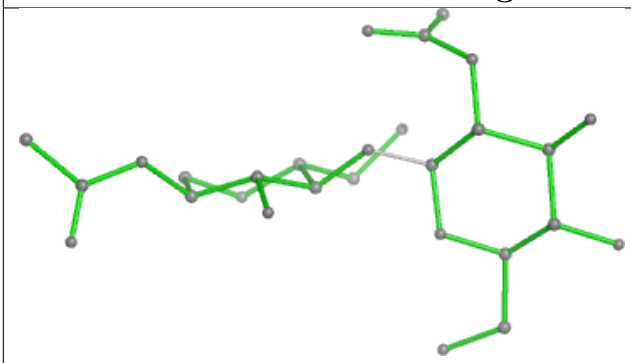
Mol	Chain	Res	Type	Atoms
5	L	4	MAN	C1-C2-C3-C4-C5-O5

16 monomers are involved in 23 short contacts:

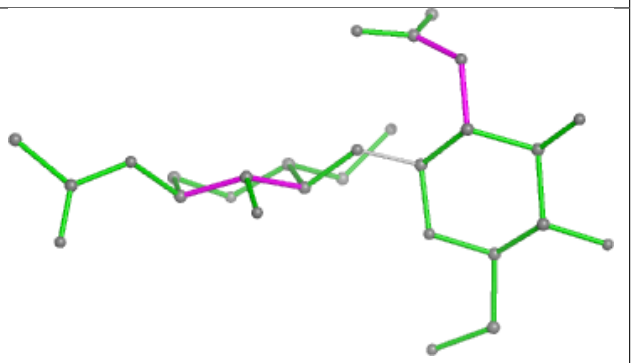
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	2	NAG	3	0
6	J	1	NAG	5	0
2	I	1	NAG	3	0
2	E	2	NAG	2	0
3	F	2	FUC	4	0
5	H	1	NAG	2	0
5	H	2	NAG	2	0
3	F	1	NAG	2	0
4	K	1	NAG	3	0
2	E	1	NAG	2	0
5	H	5	FUC	1	0
6	J	2	NAG	3	0
4	G	1	NAG	1	0
4	K	3	BMA	1	0
6	J	3	FUC	2	0
4	K	2	NAG	3	0

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

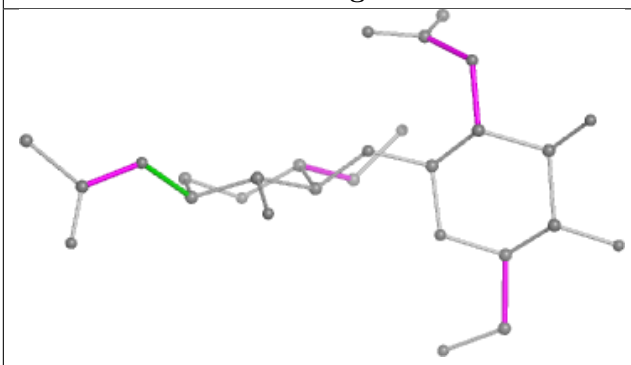
Oligosaccharide Chain E



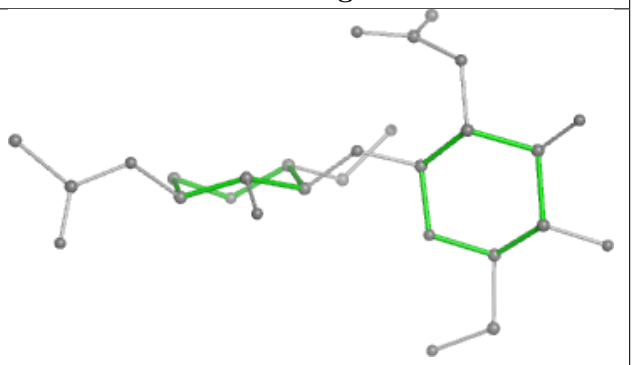
Bond lengths



Bond angles

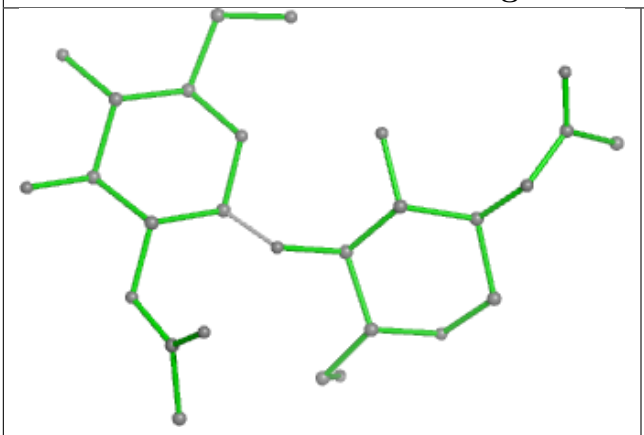


Torsions

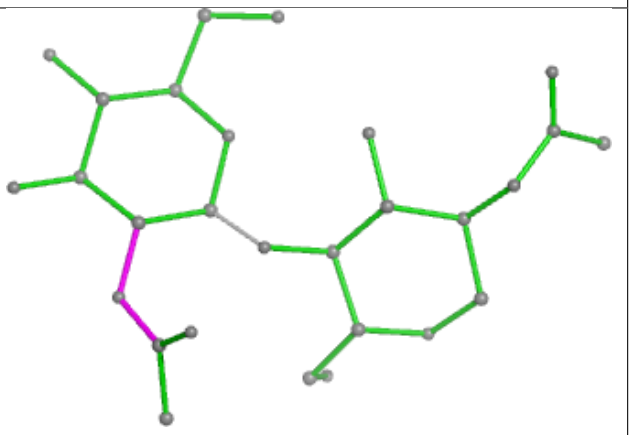


Rings

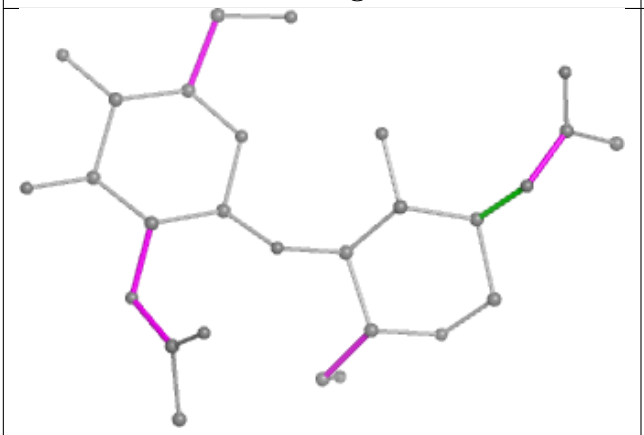
Oligosaccharide Chain I



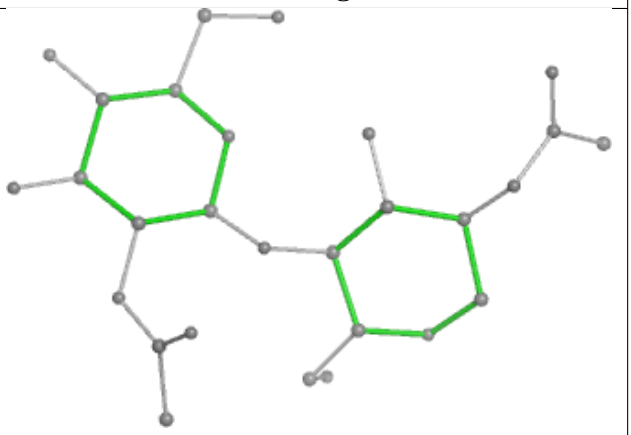
Bond lengths



Bond angles

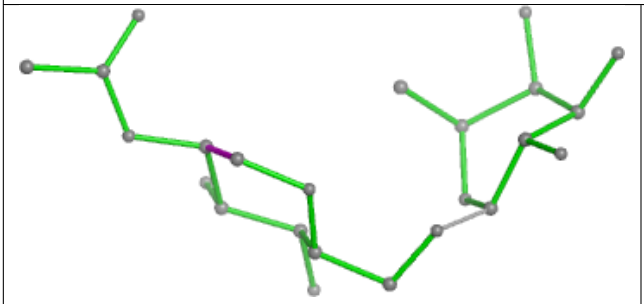


Torsions

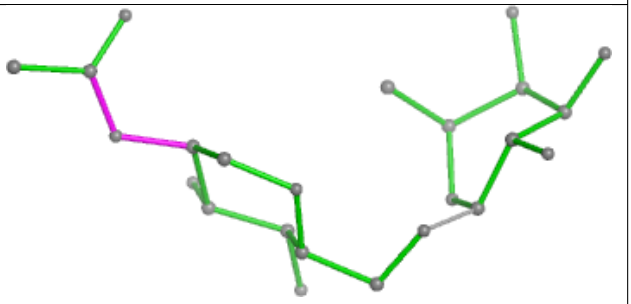


Rings

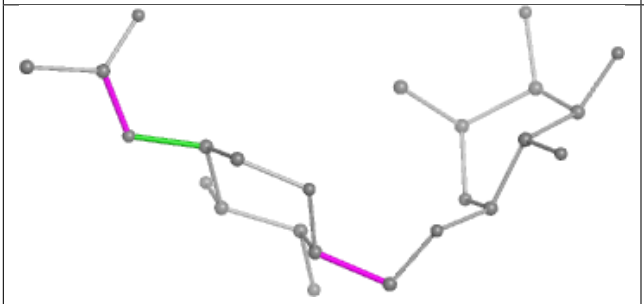
Oligosaccharide Chain F



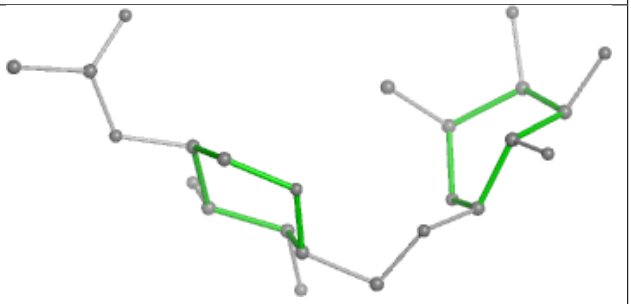
Bond lengths



Bond angles

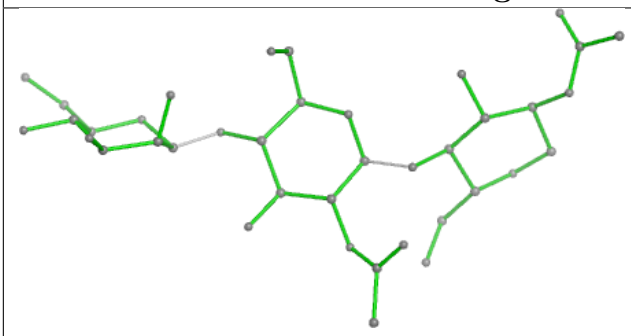


Torsions

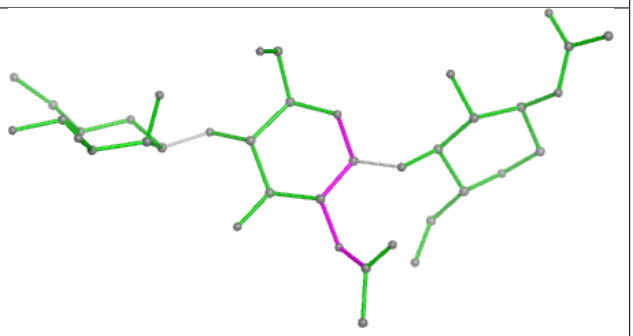


Rings

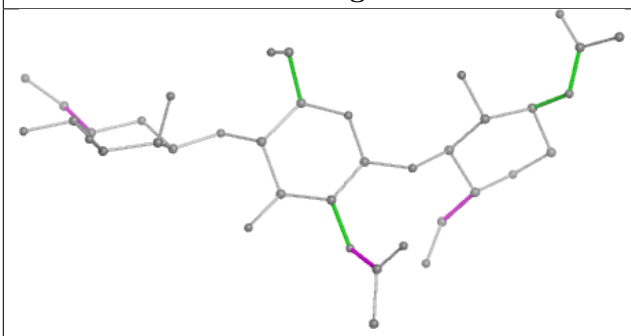
Oligosaccharide Chain G



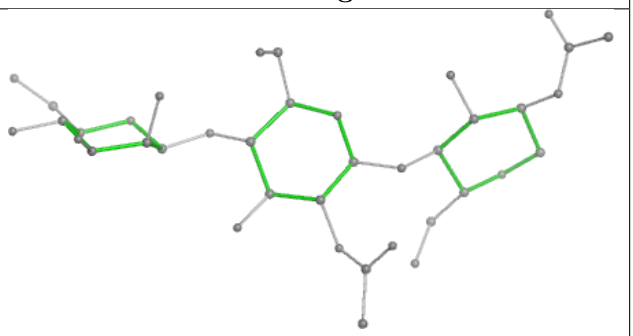
Bond lengths



Bond angles

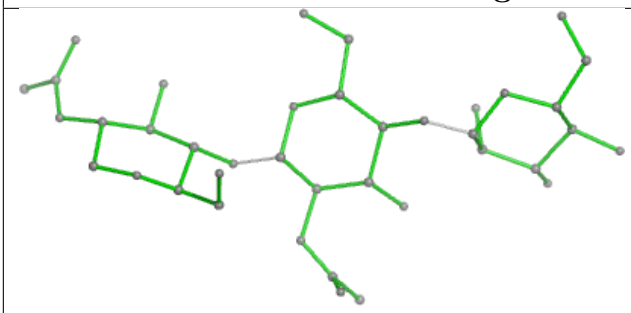


Torsions

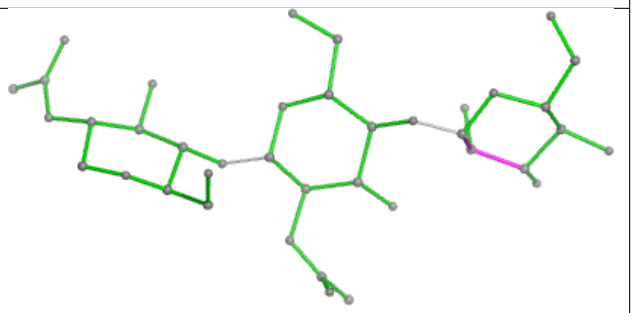


Rings

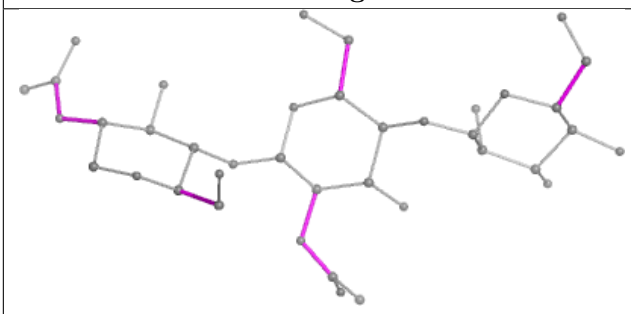
Oligosaccharide Chain K



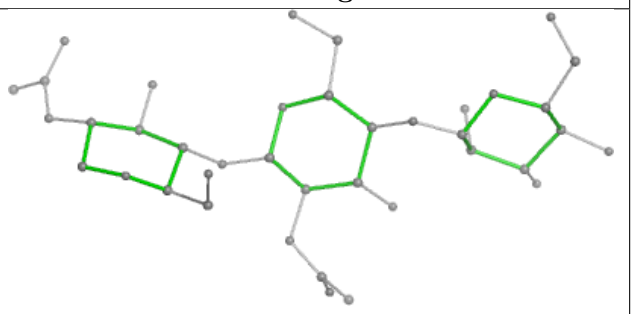
Bond lengths



Bond angles

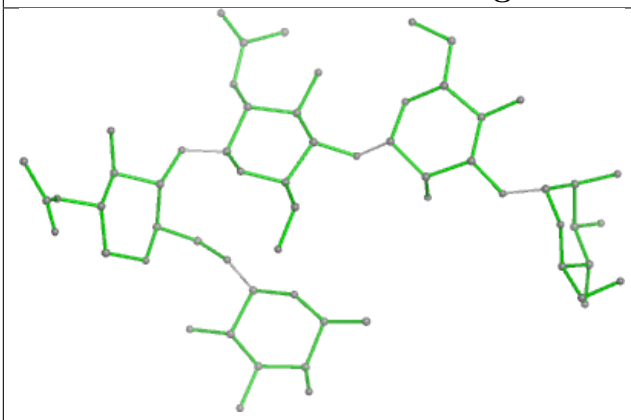


Torsions

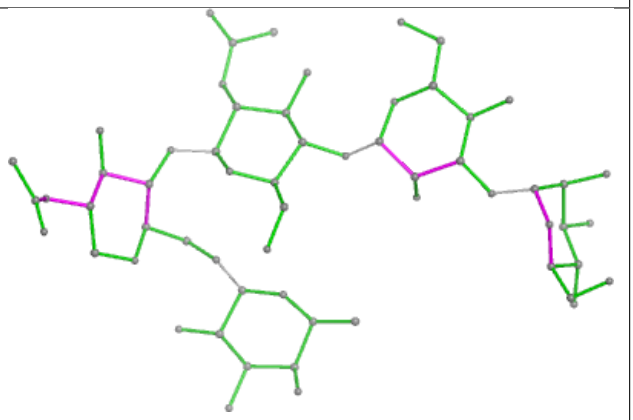


Rings

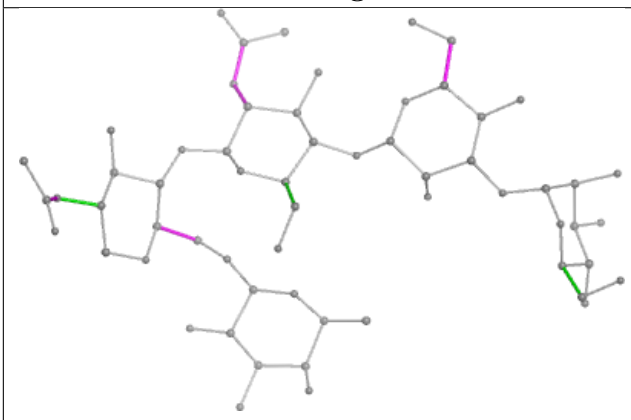
Oligosaccharide Chain H



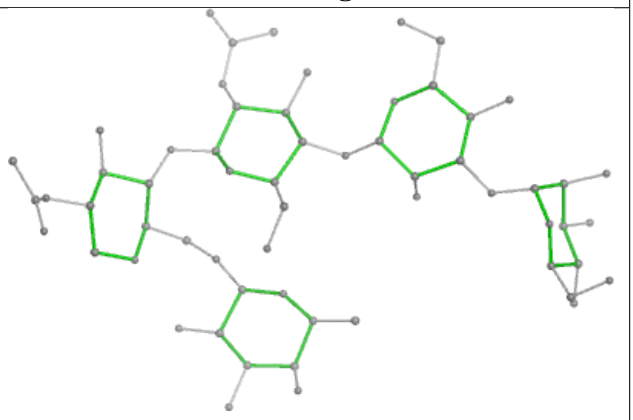
Bond lengths



Bond angles

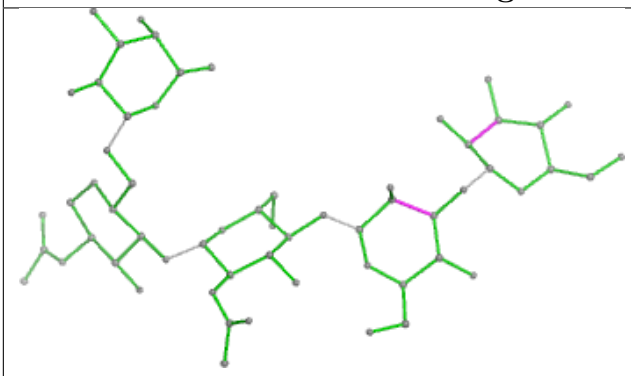


Torsions

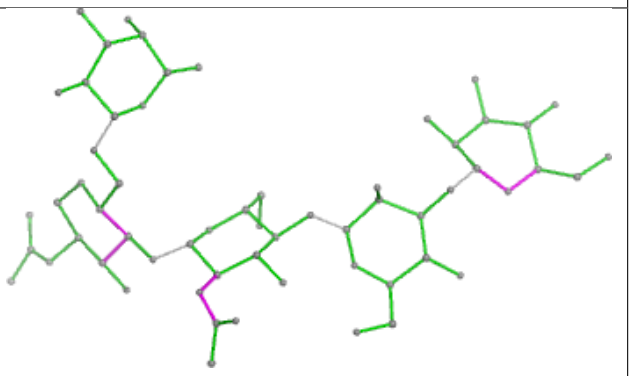


Rings

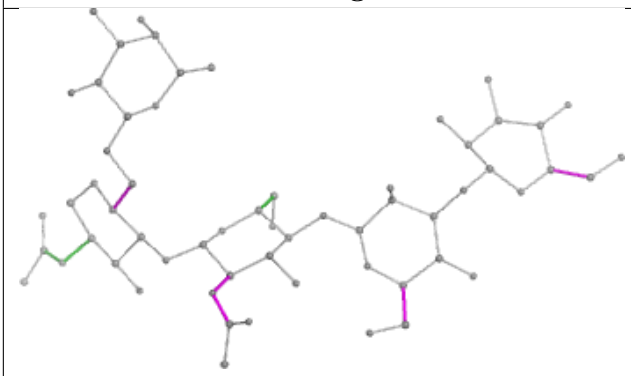
Oligosaccharide Chain L



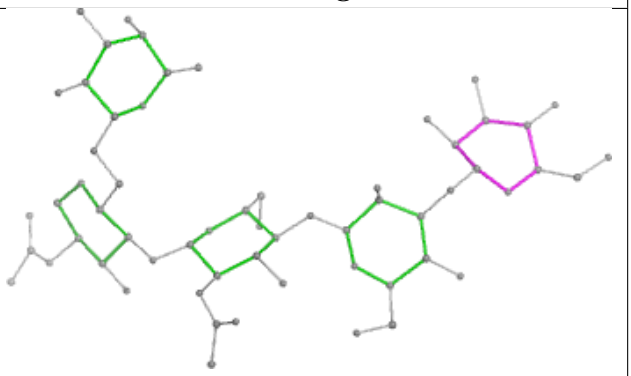
Bond lengths



Bond angles

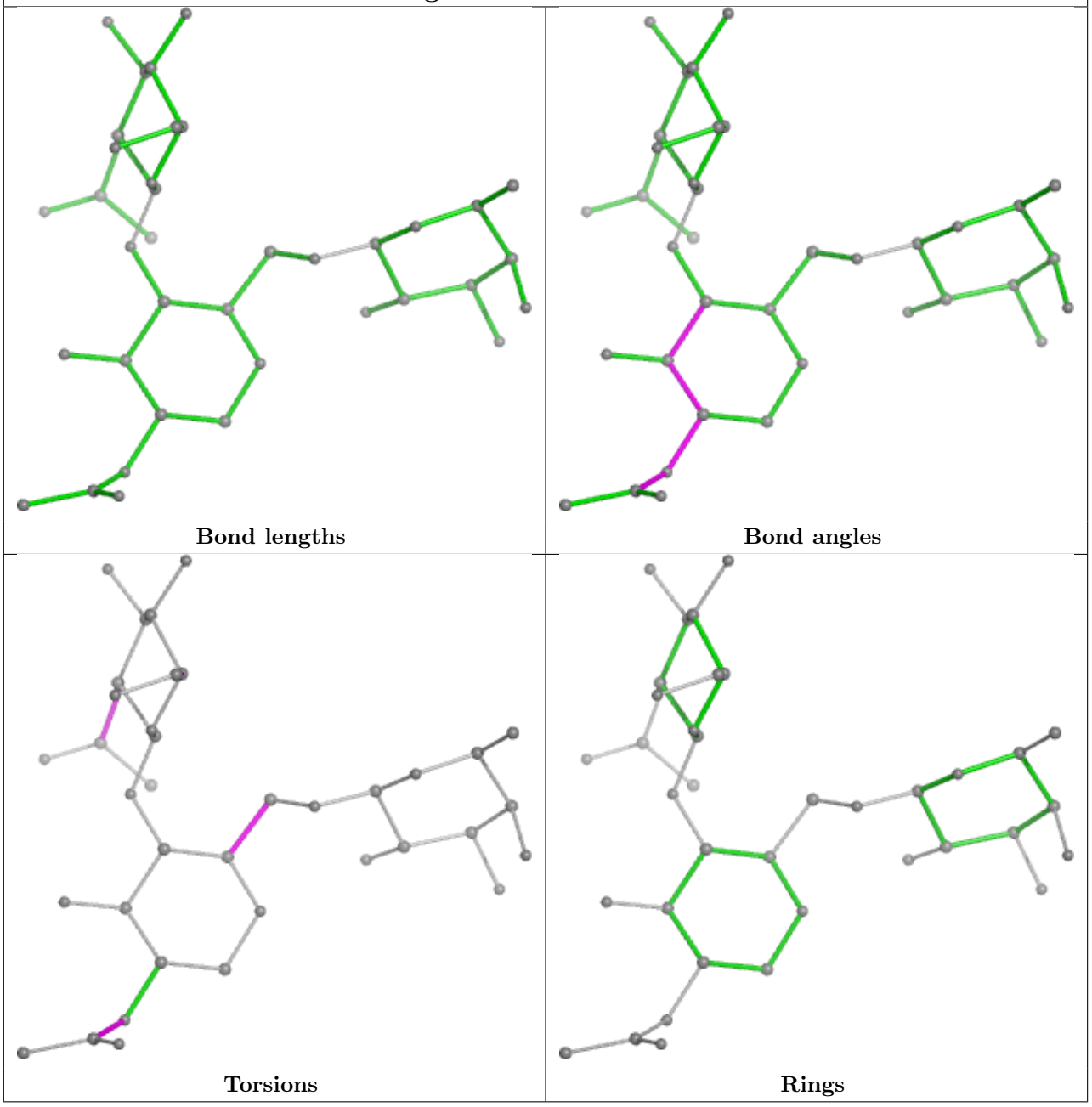


Torsions



Rings

Oligosaccharide Chain J



5.6 Ligand geometry (i)

Of 52 ligands modelled in this entry, 42 are monoatomic - leaving 10 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	$\#\|Z\|>2$
7	NAG	B	1735	1	14,14,15	0.71	0	17,19,21	0.79	0
7	NAG	D	1738	1	14,14,15	1.01	1 (7%)	17,19,21	0.83	0
7	NAG	A	1735	1	14,14,15	0.64	0	17,19,21	0.66	0
7	NAG	C	1736	1	14,14,15	0.78	1 (7%)	17,19,21	0.73	1 (5%)
7	NAG	C	1735	1	14,14,15	0.78	1 (7%)	17,19,21	0.64	0
7	NAG	A	1734	1	14,14,15	0.67	0	17,19,21	0.63	0
7	NAG	D	1735	1	14,14,15	0.84	1 (7%)	17,19,21	0.65	0
7	NAG	B	1736	1	14,14,15	0.83	1 (7%)	17,19,21	0.66	0
7	NAG	D	1736	1	14,14,15	0.72	0	17,19,21	0.71	0
7	NAG	B	1738	1	14,14,15	0.77	0	17,19,21	0.55	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	1735	1	-	1/6/23/26	0/1/1/1
7	NAG	D	1738	1	-	4/6/23/26	0/1/1/1
7	NAG	A	1735	1	-	6/6/23/26	0/1/1/1
7	NAG	C	1736	1	-	4/6/23/26	0/1/1/1
7	NAG	C	1735	1	-	6/6/23/26	0/1/1/1
7	NAG	A	1734	1	-	4/6/23/26	0/1/1/1
7	NAG	D	1735	1	-	4/6/23/26	0/1/1/1
7	NAG	B	1736	1	-	6/6/23/26	0/1/1/1
7	NAG	D	1736	1	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	B	1738	1	-	3/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	1738	NAG	C1-C2	2.99	1.56	1.52
7	B	1736	NAG	C1-C2	2.53	1.56	1.52
7	C	1735	NAG	C1-C2	2.14	1.55	1.52
7	C	1736	NAG	C1-C2	2.09	1.55	1.52
7	D	1735	NAG	C1-C2	2.06	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	1736	NAG	C2-N2-C7	-2.03	120.01	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	D	1736	NAG	C1

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1734	NAG	C8-C7-N2-C2
7	A	1734	NAG	O7-C7-N2-C2
7	A	1735	NAG	C8-C7-N2-C2
7	A	1735	NAG	O7-C7-N2-C2
7	B	1736	NAG	C8-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1735	NAG	2	0
7	C	1735	NAG	2	0
7	A	1734	NAG	4	0
7	D	1735	NAG	2	0
7	B	1738	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	671/735 (91%)	-1.65	0	100	100	43, 64, 79, 87	0
1	B	671/735 (91%)	-1.67	0	100	100	41, 60, 75, 81	0
1	C	671/735 (91%)	-1.70	0	100	100	43, 64, 79, 88	0
1	D	671/735 (91%)	-1.70	0	100	100	41, 60, 75, 81	0
All	All	2684/2940 (91%)	-1.68	0	100	100	41, 62, 77, 88	0

There are no RSRZ outliers to report.

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

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
1	PAQ	D	471	21/22	0.98	0.06	54,59,60,61	0
1	PAQ	B	471	21/22	0.99	0.07	55,59,61,61	0
1	PAQ	C	471	21/22	0.99	0.03	56,59,61,61	0
1	PAQ	A	471	21/22	0.99	0.05	56,59,60,63	0

6.3 Carbohydrates

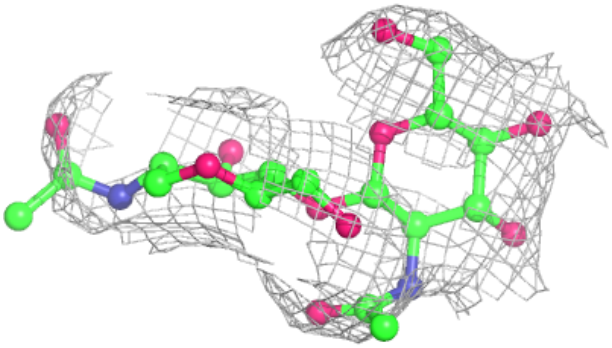
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

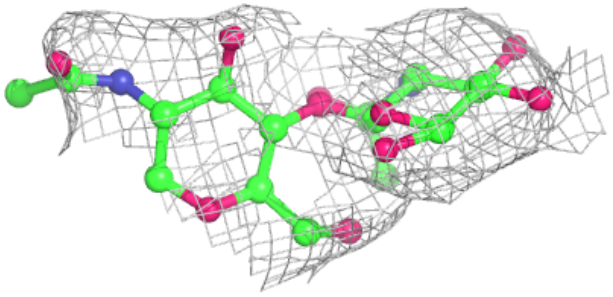
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BMA	G	3	11/12	0.93	0.06	94,94,95,95	0
5	NAG	H	2	14/15	0.97	0.04	95,97,98,98	0
5	BMA	H	3	11/12	0.97	0.04	97,97,98,98	0
5	FUC	H	5	10/11	0.97	0.06	91,93,94,95	0
5	NAG	L	2	14/15	0.97	0.04	92,95,96,97	0
6	NAG	J	2	14/15	0.97	0.05	91,92,93,93	0
4	NAG	K	2	14/15	0.98	0.04	83,85,87,89	0
4	BMA	K	3	11/12	0.98	0.04	89,90,91,91	0
2	NAG	I	1	14/15	0.98	0.05	74,75,77,80	0
2	NAG	I	2	14/15	0.98	0.04	82,84,85,85	0
5	MAN	H	4	11/12	0.98	0.04	96,98,99,99	0
3	NAG	F	1	14/15	0.98	0.05	80,81,83,85	0
5	NAG	L	1	14/15	0.98	0.05	76,79,84,88	0
3	FUC	F	2	10/11	0.98	0.03	78,79,80,80	0
5	BMA	L	3	11/12	0.98	0.04	97,98,98,98	0
5	MAN	L	4	11/12	0.98	0.03	96,98,98,98	0
5	FUC	L	5	10/11	0.98	0.05	84,85,86,86	0
2	NAG	E	2	14/15	0.98	0.04	88,91,92,92	0
2	NAG	E	1	14/15	0.99	0.04	75,77,80,84	0
4	NAG	K	1	14/15	0.99	0.04	75,76,78,81	0
4	NAG	G	1	14/15	0.99	0.04	72,75,77,80	0
4	NAG	G	2	14/15	0.99	0.04	85,86,89,92	0
6	NAG	J	1	14/15	0.99	0.03	80,83,86,89	0
5	NAG	H	1	14/15	0.99	0.03	82,86,91,93	0
6	FUC	J	3	10/11	0.99	0.04	82,83,84,84	0

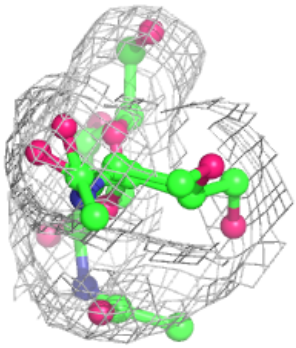
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

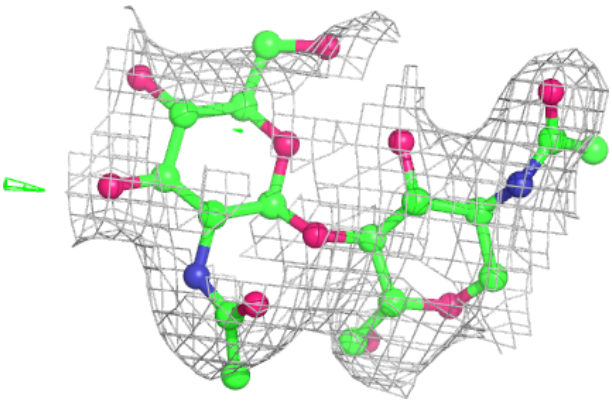


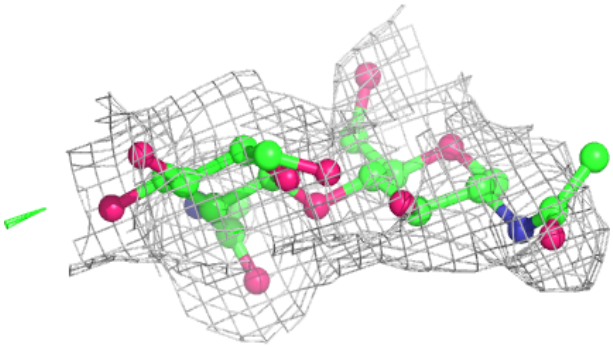


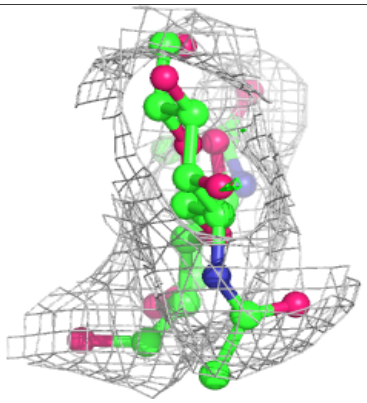


Electron density around Chain I:

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

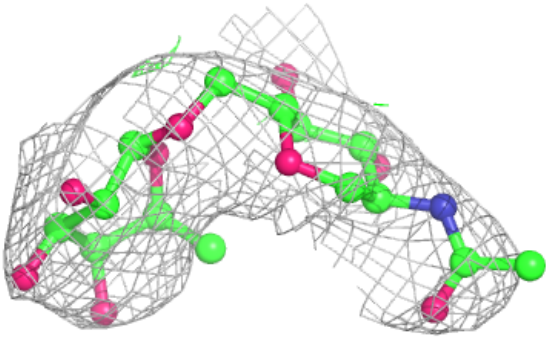


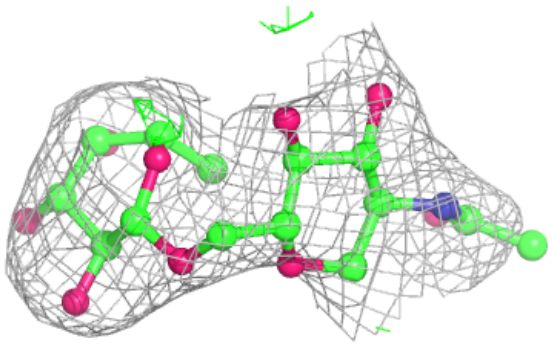


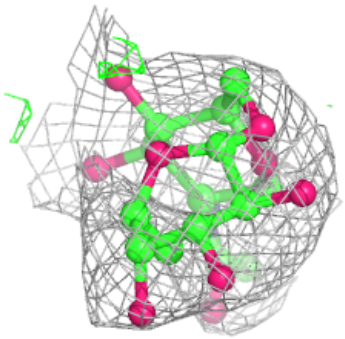


Electron density around Chain F:

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

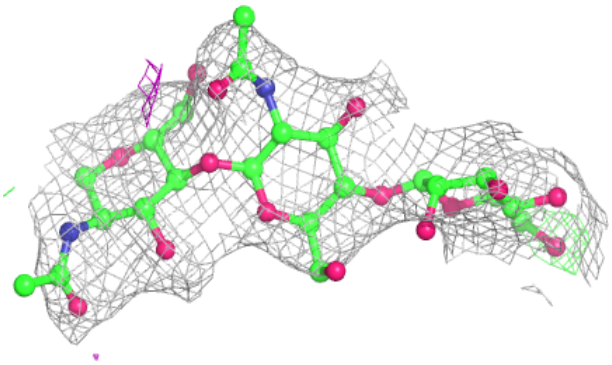


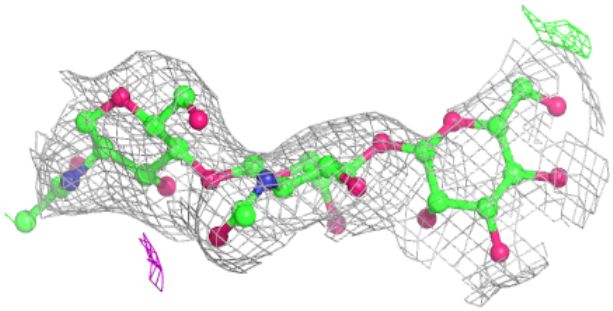


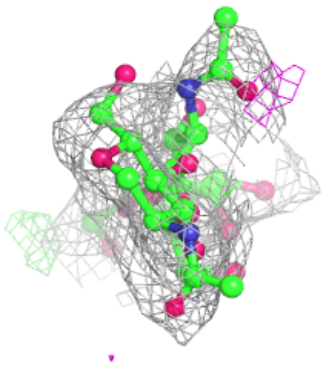


Electron density around Chain G:

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

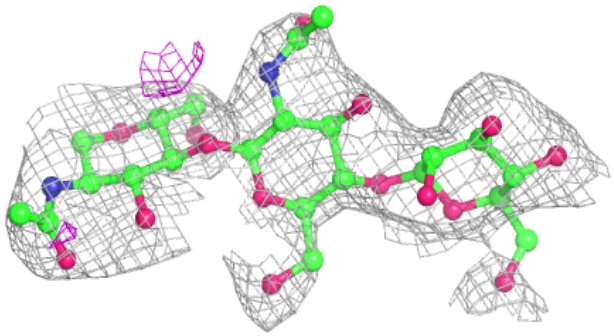


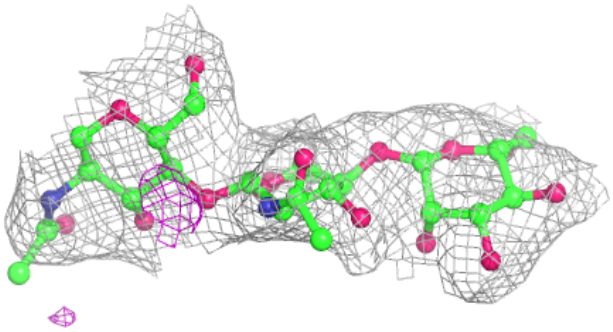


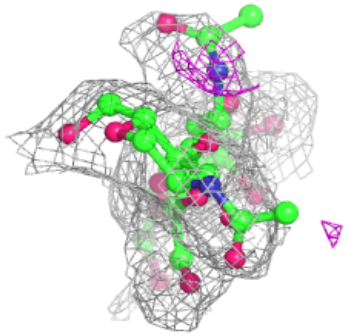


Electron density around Chain K:

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

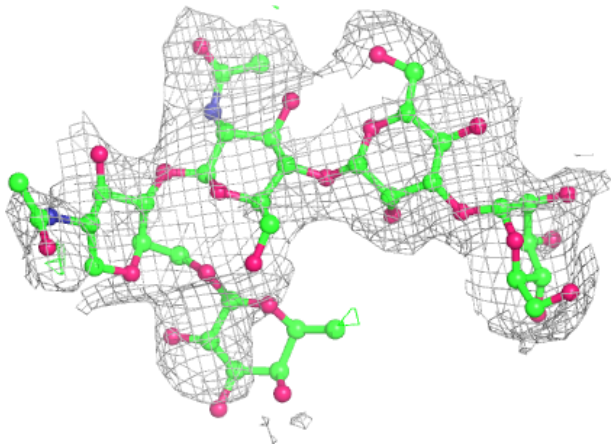


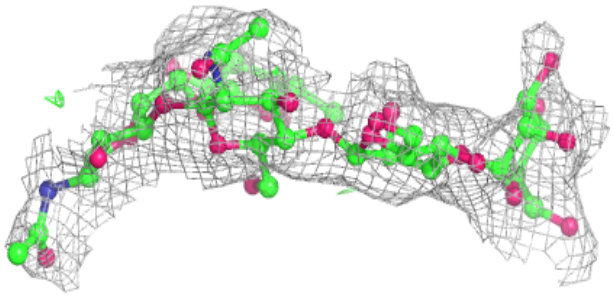


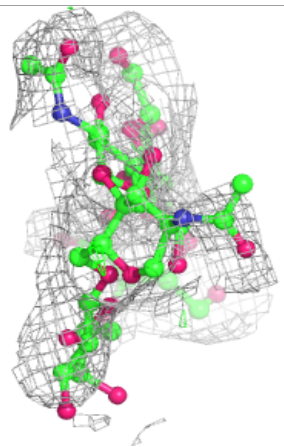


Electron density around Chain H:

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

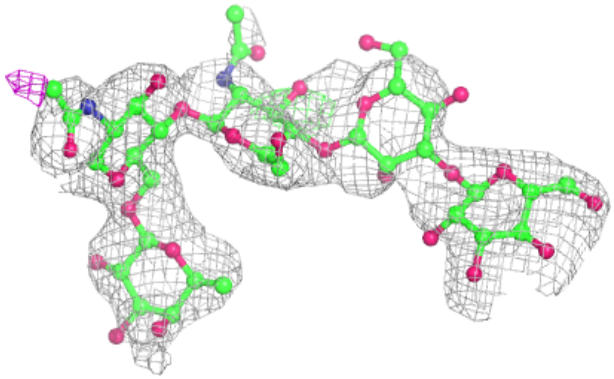


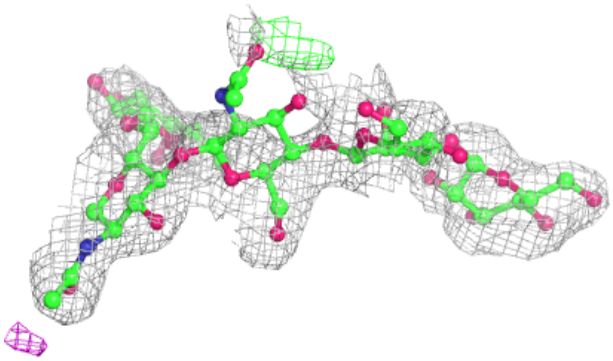


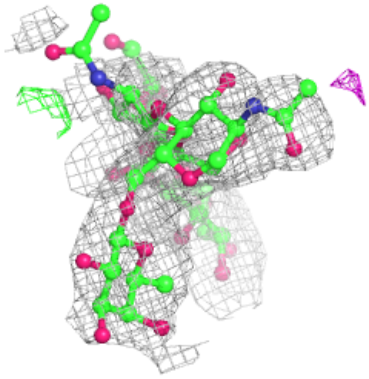


Electron density around Chain L:

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

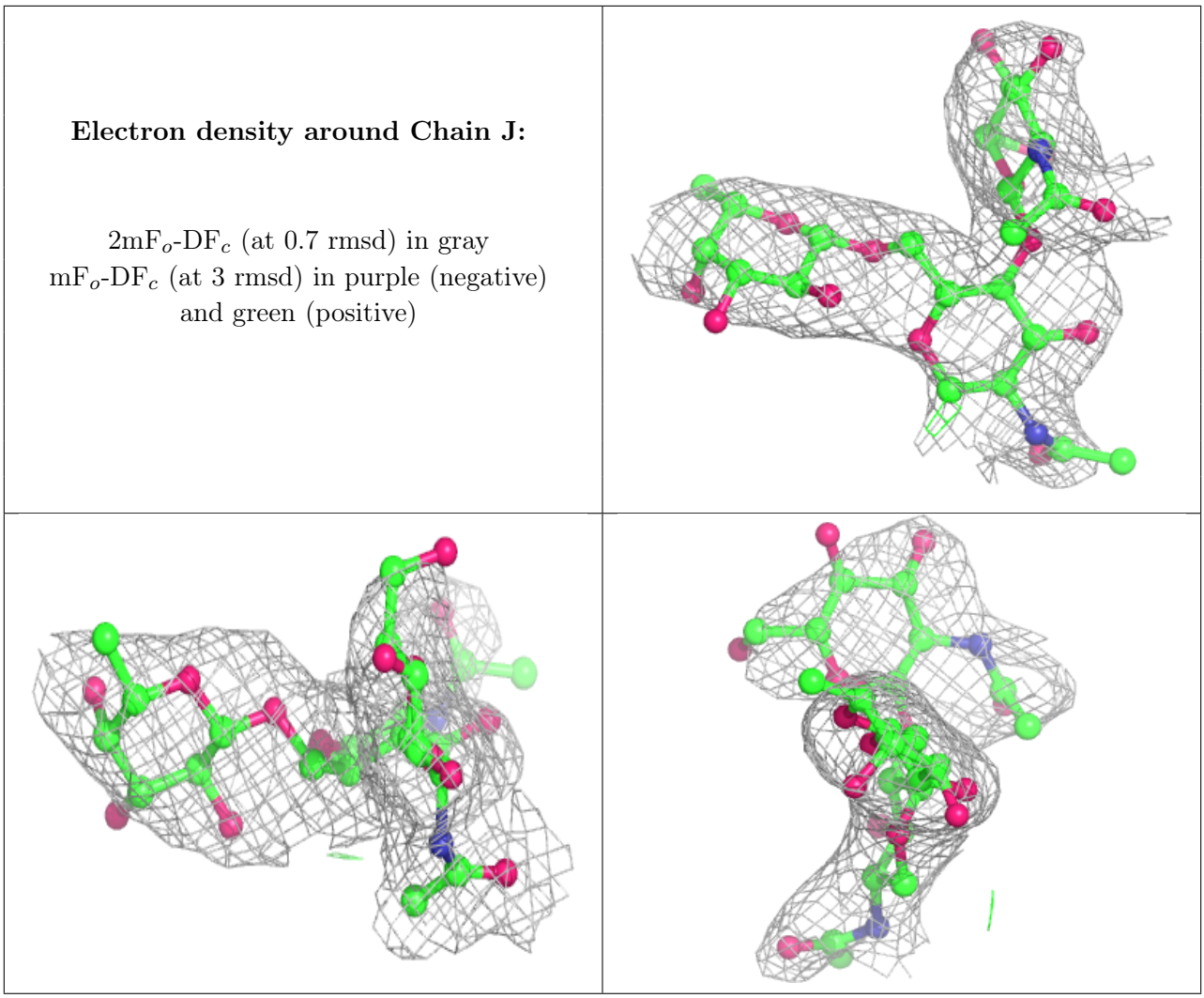






Electron density around Chain J:

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



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	B	1736	14/15	0.94	0.05	84,86,88,88	0
7	NAG	B	1738	14/15	0.94	0.05	81,83,84,85	0
7	NAG	C	1735	14/15	0.96	0.04	70,72,73,74	0
7	NAG	D	1738	14/15	0.96	0.04	81,83,85,85	0
7	NAG	D	1736	14/15	0.97	0.03	83,84,86,86	0
7	NAG	A	1735	14/15	0.98	0.03	84,86,88,89	0
7	NAG	C	1736	14/15	0.98	0.04	82,85,88,88	0
7	NAG	D	1735	14/15	0.99	0.03	71,74,76,77	0
7	NAG	A	1734	14/15	0.99	0.03	71,73,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	B	1735	14/15	0.99	0.04	69,70,73,73	0
8	CA	D	1743	1/1	0.99	0.03	46,46,46,46	0
9	CU	A	1740	1/1	0.99	0.02	81,81,81,81	0
9	CU	A	1743	1/1	0.99	0.02	84,84,84,84	0
9	CU	A	1744	1/1	0.99	0.02	74,74,74,74	0
9	CU	B	1747	1/1	0.99	0.02	81,81,81,81	0
9	CU	B	1748	1/1	0.99	0.02	66,66,66,66	0
9	CU	B	1750	1/1	0.99	0.02	63,63,63,63	0
9	CU	C	1742	1/1	0.99	0.03	84,84,84,84	0
9	CU	C	1744	1/1	0.99	0.03	90,90,90,90	0
9	CU	D	1745	1/1	0.99	0.02	79,79,79,79	0
9	CU	D	1746	1/1	0.99	0.02	78,78,78,78	0
9	CU	D	1747	1/1	0.99	0.07	82,82,82,82	0
8	CA	B	1741	1/1	1.00	0.02	46,46,46,46	0
8	CA	B	1743	1/1	1.00	0.02	47,47,47,47	0
9	CU	A	1745	1/1	1.00	0.02	80,80,80,80	0
9	CU	B	1742	1/1	1.00	0.01	55,55,55,55	0
9	CU	B	1744	1/1	1.00	0.02	76,76,76,76	0
9	CU	B	1745	1/1	1.00	0.01	75,75,75,75	0
9	CU	B	1746	1/1	1.00	0.01	71,71,71,71	0
8	CA	C	1737	1/1	1.00	0.01	50,50,50,50	0
8	CA	C	1739	1/1	1.00	0.01	50,50,50,50	0
9	CU	B	1749	1/1	1.00	0.03	69,69,69,69	0
8	CA	D	1741	1/1	1.00	0.01	47,47,47,47	0
9	CU	C	1738	1/1	1.00	0.01	49,49,49,49	0
9	CU	C	1741	1/1	1.00	0.01	79,79,79,79	0
8	CA	A	1736	1/1	1.00	0.02	52,52,52,52	0
9	CU	C	1743	1/1	1.00	0.02	73,73,73,73	0
9	CU	A	1737	1/1	1.00	0.01	49,49,49,49	0
9	CU	C	1745	1/1	1.00	0.02	77,77,77,77	0
9	CU	C	1746	1/1	1.00	0.03	67,67,67,67	0
9	CU	C	1747	1/1	1.00	0.02	84,84,84,84	0
9	CU	D	1742	1/1	1.00	0.02	52,52,52,52	0
8	CA	A	1738	1/1	1.00	0.02	49,49,49,49	0
9	CU	A	1741	1/1	1.00	0.02	83,83,83,83	0
9	CU	A	1742	1/1	1.00	0.02	77,77,77,77	0
9	CU	D	1748	1/1	1.00	0.01	74,74,74,74	0
9	CU	D	1749	1/1	1.00	0.02	67,67,67,67	0
9	CU	D	1750	1/1	1.00	0.02	67,67,67,67	0
10	CL	A	1739	1/1	1.00	0.03	47,47,47,47	0
10	CL	A	1746	1/1	1.00	0.03	47,47,47,47	0
10	CL	C	1740	1/1	1.00	0.03	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	CL	D	1744	1/1	1.00	0.03	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.