wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 4, 2023 – 01:16 am GMT

PDB ID	:	2C10
Title	:	The structure of a truncated, soluble version of semicarbazide- sensitive amine oxidase
Authors	:	Jakobsson, E.; Kleywegt, G.J.
Deposited on	:	2005-09-09
Resolution	:	2.50 Å(reported)

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

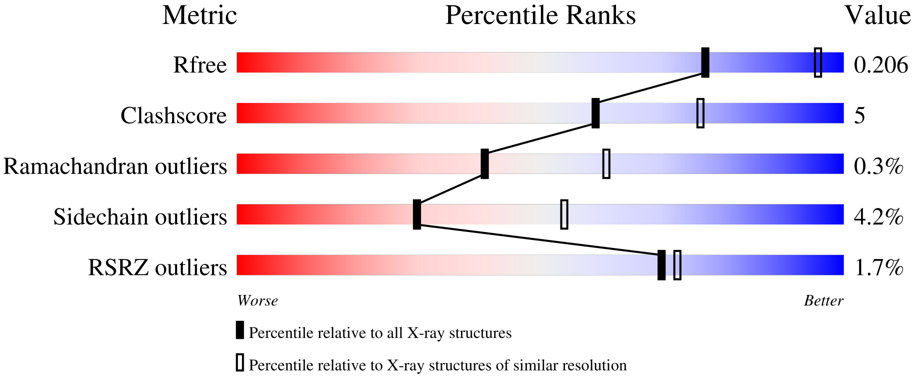
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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

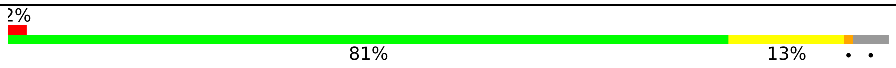
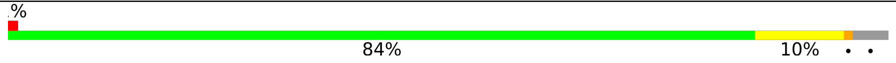
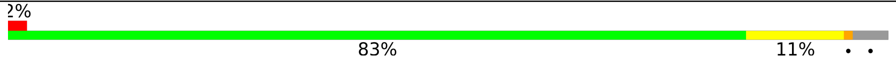
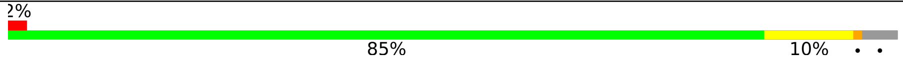
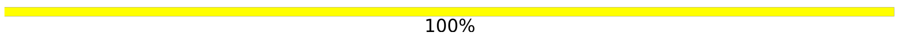
The reported resolution of this entry is 2.50 Å.

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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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	
1	B	735	
1	C	735	
1	D	735	
2	E	3	

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Mol	Chain	Length	Quality of chain
2	H	3	33% 67%
2	K	3	100%
3	F	3	100%
3	L	3	33% 67%
4	G	2	100%
4	J	2	100%
4	M	2	100%
4	P	2	100%
5	I	5	80% 20%
5	O	5	100%
6	N	4	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	F	1	X	-	-	-
3	FUC	F	3	X	-	-	-
3	NAG	L	1	X	-	-	-
3	FUC	L	3	X	-	-	-
4	NAG	G	2	-	-	-	X
5	NAG	I	1	X	-	-	-
5	FUC	I	5	X	-	-	-
5	NAG	O	1	X	-	-	-
5	FUC	O	5	X	-	-	-

2 Entry composition ⓘ

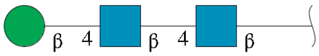
There are 11 unique types of molecules in this entry. The entry contains 23470 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

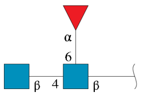
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	706	Total 5563	C 3571	N 960	O 1011	S 21	0	0	1
1	B	709	Total 5587	C 3587	N 965	O 1014	S 21	0	0	1
1	C	706	Total 5563	C 3571	N 960	O 1011	S 21	0	0	1
1	D	709	Total 5587	C 3587	N 965	O 1014	S 21	0	0	1

- Molecule 2 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.



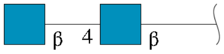
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total 39	C 22	N 2	O 15	0	0	0
2	H	3	Total 39	C 22	N 2	O 15	0	0	0
2	K	3	Total 39	C 22	N 2	O 15	0	0	0

- Molecule 3 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.



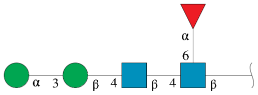
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	F	3	Total C N O 38 22 2 14	0	0	0
3	L	3	Total C N O 38 22 2 14	0	0	0

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



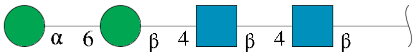
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	G	2	Total C N O 28 16 2 10	0	0	0
4	J	2	Total C N O 28 16 2 10	0	0	0
4	M	2	Total C N O 28 16 2 10	0	0	0
4	P	2	Total C N O 28 16 2 10	0	0	0

- 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.



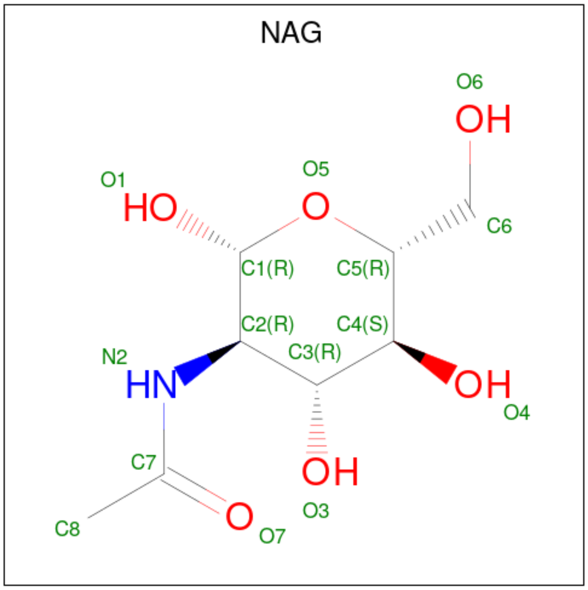
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	I	5	Total C N O 60 34 2 24	0	0	0
5	O	5	Total C N O 60 34 2 24	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	N	4	50	28	2	20	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	14	8	1	5	0	0
7	B	1	14	8	1	5	0	0
7	B	1	14	8	1	5	0	0
7	B	1	14	8	1	5	0	0
7	C	1	14	8	1	5	0	0
7	D	1	14	8	1	5	0	0
7	D	1	14	8	1	5	0	0
7	D	1	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
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	1	Total Cu 1 1	0	0
9	B	1	Total Cu 1 1	0	0
9	C	1	Total Cu 1 1	0	0
9	D	1	Total Cu 1 1	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	B	2	Total Cl 2 2	0	0
10	C	2	Total Cl 2 2	0	0
10	D	2	Total Cl 2 2	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	141	Total O 141 141	0	0
11	B	139	Total O 139 139	0	0
11	C	141	Total O 141 141	0	0

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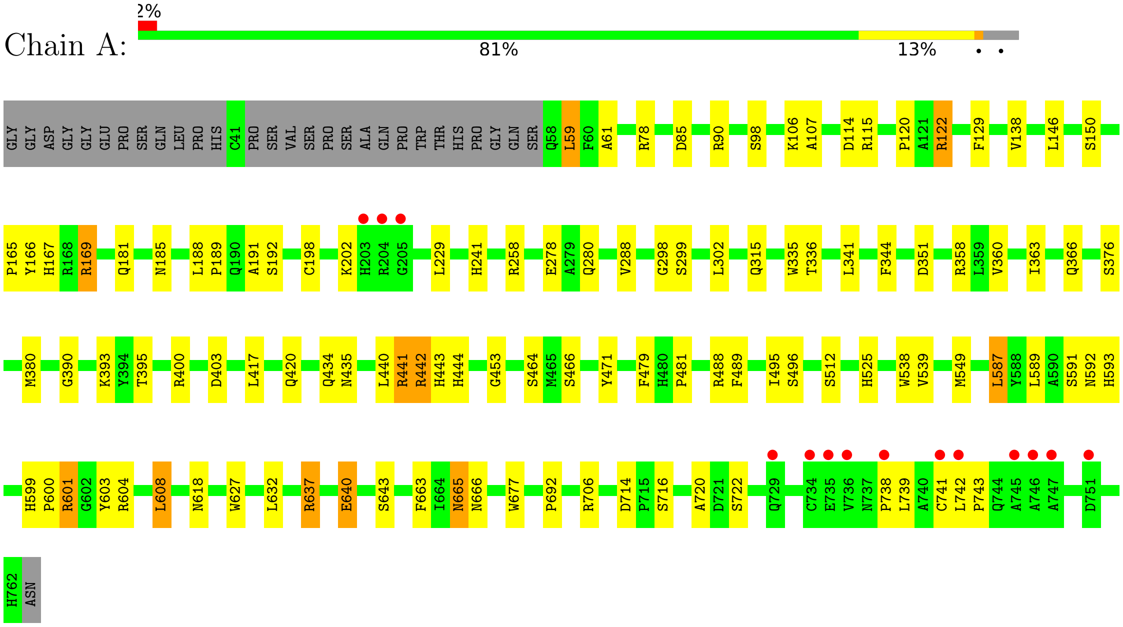
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	D	142	Total O 142 142	0	0

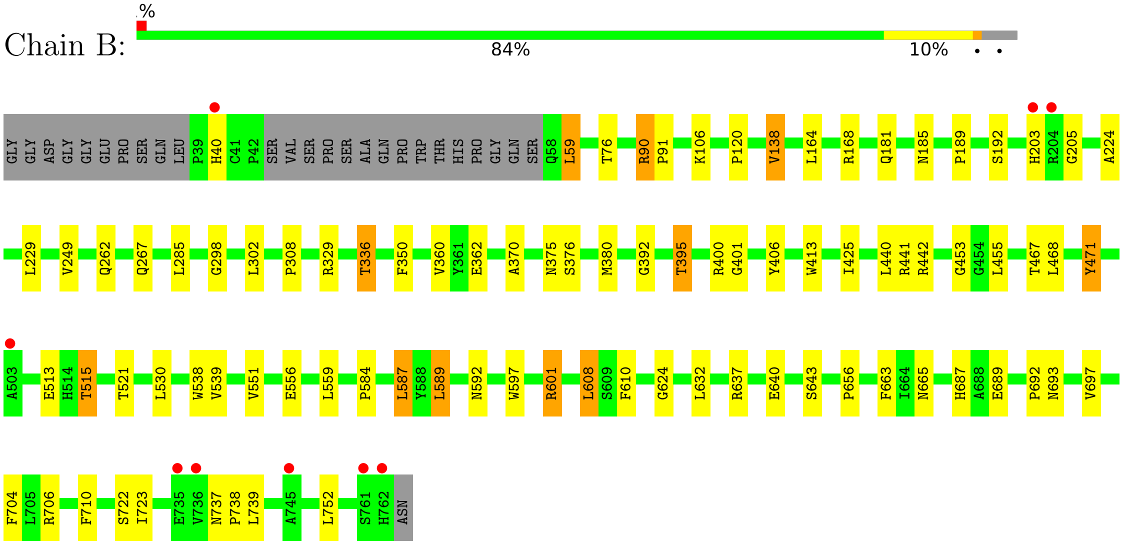
3 Residue-property plots ⓘ

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

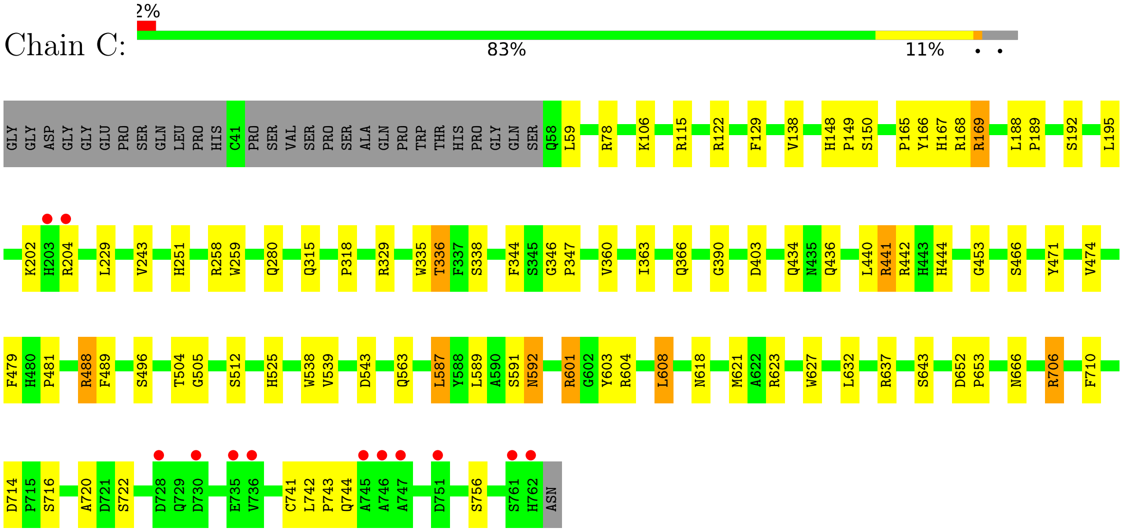


- Molecule 1: MEMBRANE COPPER AMINE OXIDASE



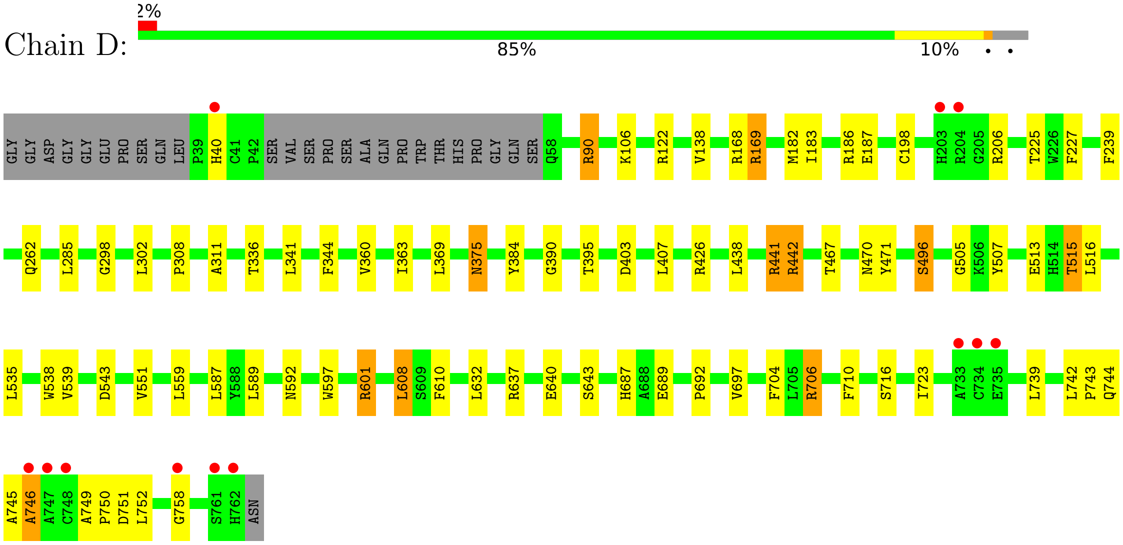
- Molecule 1: MEMBRANE COPPER AMINE OXIDASE

Chain C:



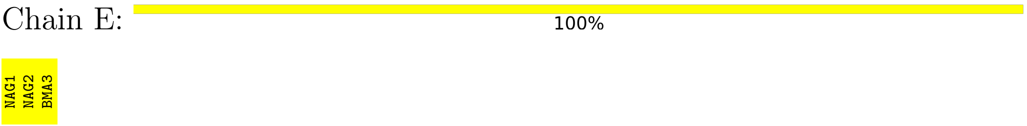
- Molecule 1: MEMBRANE COPPER AMINE OXIDASE

Chain D:



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

Chain E:

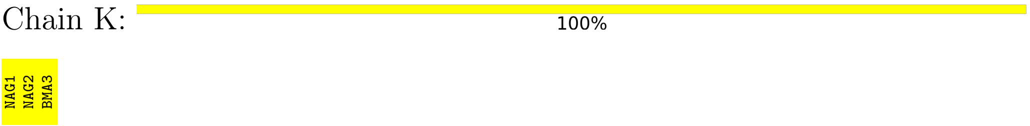


- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

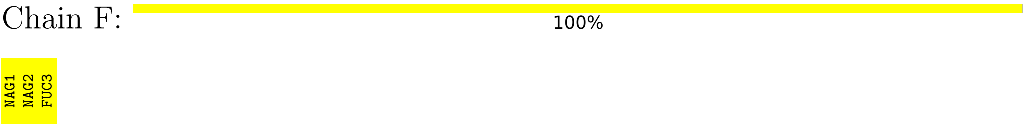
- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



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

Chain F:

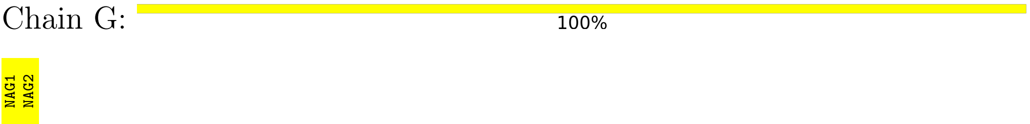


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

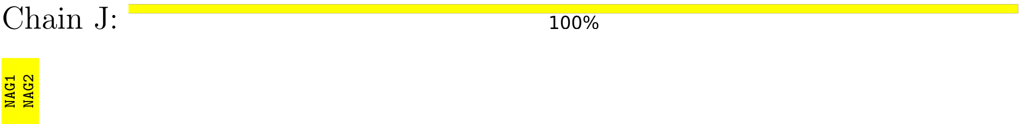
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



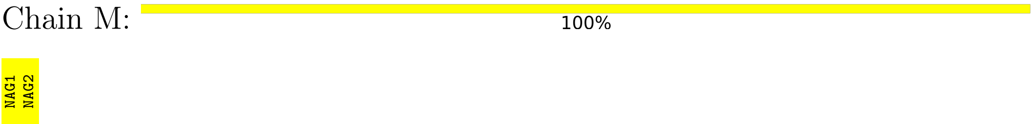
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



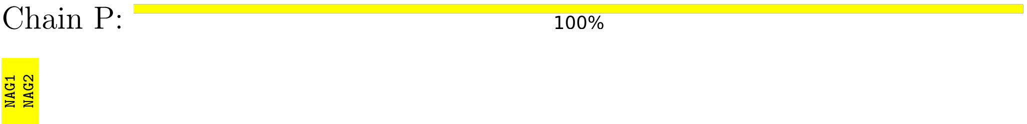
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



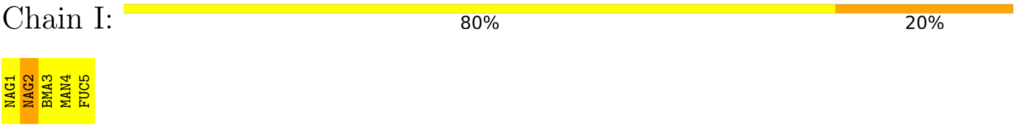
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



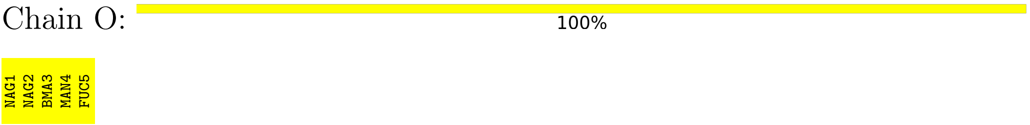
- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



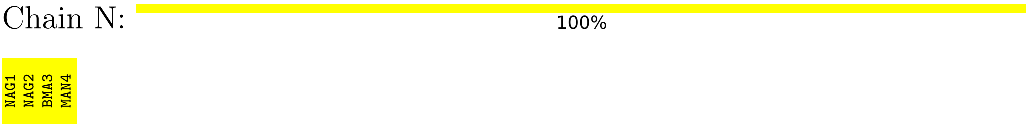
- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



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

Chain N:



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	130.24Å 130.24Å 221.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-2.50) 98.2 (19.97-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$[1]	1.67 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.204 , 0.252 0.204 , 0.206	Depositor DCC
R_{free} test set	6351 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	34.6	Xtriage
Anisotropy	0.645	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 12.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.448 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	23470	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, TPQ, CA, FUC, CU, CL, 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	0.52	0/5724	0.64	1/7804 (0.0%)
1	B	0.51	0/5751	0.62	1/7842 (0.0%)
1	C	0.51	0/5724	0.62	1/7804 (0.0%)
1	D	0.51	0/5751	0.63	0/7842
All	All	0.51	0/22950	0.63	3/31292 (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	D	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	LEU	CA-CB-CG	5.25	127.38	115.30
1	B	589	LEU	CA-CB-CG	5.05	126.93	115.30
1	C	592	ASN	N-CA-CB	-5.00	101.60	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	198	CYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5563	0	5311	69	0
1	B	5587	0	5333	49	0
1	C	5563	0	5311	49	0
1	D	5587	0	5332	57	0
2	E	39	0	34	0	0
2	H	39	0	34	1	0
2	K	39	0	34	0	0
3	F	38	0	34	0	0
3	L	38	0	34	1	0
4	G	28	0	25	0	0
4	J	28	0	25	0	0
4	M	28	0	25	0	0
4	P	28	0	25	0	0
5	I	60	0	52	2	0
5	O	60	0	52	0	0
6	N	50	0	43	0	0
7	A	14	0	13	1	0
7	B	42	0	39	1	0
7	C	14	0	13	0	0
7	D	42	0	39	1	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	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	A	2	0	0	0	0
10	B	2	0	0	0	0
10	C	2	0	0	0	0
10	D	2	0	0	0	0
11	A	141	0	0	9	0
11	B	139	0	0	4	0
11	C	141	0	0	5	0
11	D	142	0	0	5	0
All	All	23470	0	21808	209	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 5.

The worst 5 of 209 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:D:360:VAL:HG11	1:D:363:ILE:HG13	1.38	1.04
1:A:360:VAL:HG11	1:A:363:ILE:HG13	1.56	0.85
1:D:426:ARG:HE	1:D:758:GLY:HA3	1.49	0.78
1:A:538:TRP:CZ3	1:A:592:ASN:HB2	2.19	0.77
1:A:488:ARG:HH12	1:A:608:LEU:CD1	1.98	0.77

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	702/735 (96%)	671 (96%)	30 (4%)	1 (0%)	51	73
1	B	704/735 (96%)	675 (96%)	27 (4%)	2 (0%)	41	61
1	C	702/735 (96%)	668 (95%)	32 (5%)	2 (0%)	41	61
1	D	704/735 (96%)	675 (96%)	26 (4%)	3 (0%)	34	54
All	All	2812/2940 (96%)	2689 (96%)	115 (4%)	8 (0%)	41	61

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	746	ALA
1	C	744	GLN
1	B	59	LEU
1	C	204	ARG
1	B	205	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	585/609 (96%)	555 (95%)	30 (5%)	24	45
1	B	588/609 (97%)	568 (97%)	20 (3%)	37	63
1	C	585/609 (96%)	555 (95%)	30 (5%)	24	45
1	D	588/609 (97%)	569 (97%)	19 (3%)	39	65
All	All	2346/2436 (96%)	2247 (96%)	99 (4%)	30	54

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	202	LYS
1	C	603	TYR
1	C	243	VAL
1	C	466	SER
1	C	666	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	181	GLN
1	B	203	HIS
1	D	420	GLN
1	C	185	ASN
1	D	375	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	TPQ	A	471	1	13,14,15	2.18	3 (23%)	15,19,21	1.47	3 (20%)
1	TPQ	B	471	1	13,14,15	2.23	3 (23%)	15,19,21	1.51	3 (20%)
1	TPQ	D	471	1	13,14,15	2.21	3 (23%)	15,19,21	1.60	3 (20%)
1	TPQ	C	471	1	13,14,15	2.21	3 (23%)	15,19,21	1.36	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**
1	TPQ	A	471	1	-	4/5/22/24	0/1/1/1
1	TPQ	B	471	1	-	4/5/22/24	0/1/1/1
1	TPQ	D	471	1	-	4/5/22/24	0/1/1/1
1	TPQ	C	471	1	-	3/5/22/24	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	**Chain**	**Res**	**Type**	**Atoms**	**Z**	**Observed(Å)**	**Ideal(Å)**
1	D	471	TPQ	O5-C5	4.86	1.37	1.24
1	C	471	TPQ	O5-C5	4.86	1.37	1.24
1	B	471	TPQ	O5-C5	4.79	1.37	1.24
1	A	471	TPQ	O5-C5	4.60	1.36	1.24
1	C	471	TPQ	O2-C2	4.52	1.36	1.24

The worst 5 of 12 bond angle outliers are listed below:

Mol	**Chain**	**Res**	**Type**	**Atoms**	**Z**	**Observed(^{o})**	**Ideal(^{o})**
1	B	471	TPQ	C6-C1-C2	2.98	120.92	118.64
1	D	471	TPQ	CA-CB-C1	2.96	119.17	113.51
1	C	471	TPQ	C6-C1-C2	2.86	120.83	118.64
1	D	471	TPQ	C6-C5-C4	2.69	121.59	117.03
1	A	471	TPQ	C6-C5-C4	2.59	121.43	117.03

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	471	TPQ	C-CA-CB-C1
1	A	471	TPQ	C2-C1-CB-CA
1	B	471	TPQ	C-CA-CB-C1
1	B	471	TPQ	C2-C1-CB-CA
1	B	471	TPQ	C6-C1-CB-CA

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	471	TPQ	1	0

5.5 Carbohydrates ⓘ

37 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	1,2	14,14,15	0.62	0	17,19,21	1.33	2 (11%)
2	NAG	E	2	2	14,14,15	0.67	0	17,19,21	1.14	1 (5%)
2	BMA	E	3	2	11,11,12	0.50	0	15,15,17	1.25	1 (6%)
3	NAG	F	1	3,1	14,14,15	0.68	0	17,19,21	1.75	3 (17%)
3	NAG	F	2	3	14,14,15	0.64	0	17,19,21	1.91	4 (23%)
3	FUC	F	3	3	10,10,11	0.69	0	14,14,16	1.66	2 (14%)
4	NAG	G	1	4,1	14,14,15	0.58	0	17,19,21	1.11	3 (17%)
4	NAG	G	2	4	14,14,15	0.61	0	17,19,21	1.42	2 (11%)
2	NAG	H	1	1,2	14,14,15	0.66	0	17,19,21	1.24	2 (11%)
2	NAG	H	2	2	14,14,15	0.51	0	17,19,21	1.16	1 (5%)
2	BMA	H	3	2	11,11,12	0.76	0	15,15,17	1.10	1 (6%)
5	NAG	I	1	1,5	14,14,15	0.59	0	17,19,21	1.80	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	NAG	I	2	5	14,14,15	0.54	0	17,19,21	1.00	1 (5%)
5	BMA	I	3	5	11,11,12	0.71	0	15,15,17	1.96	3 (20%)
5	MAN	I	4	5	11,11,12	0.56	0	15,15,17	1.17	1 (6%)
5	FUC	I	5	5	10,10,11	0.71	0	14,14,16	0.99	0
4	NAG	J	1	4,1	14,14,15	0.64	0	17,19,21	1.00	1 (5%)
4	NAG	J	2	4	14,14,15	0.59	0	17,19,21	1.59	2 (11%)
2	NAG	K	1	1,2	14,14,15	0.57	0	17,19,21	1.02	2 (11%)
2	NAG	K	2	2	14,14,15	0.55	0	17,19,21	1.02	1 (5%)
2	BMA	K	3	2	11,11,12	0.61	0	15,15,17	0.90	1 (6%)
3	NAG	L	1	3,1	14,14,15	0.63	0	17,19,21	2.04	4 (23%)
3	NAG	L	2	3	14,14,15	0.56	0	17,19,21	1.53	3 (17%)
3	FUC	L	3	3	10,10,11	0.80	0	14,14,16	1.52	3 (21%)
4	NAG	M	1	4,1	14,14,15	0.54	0	17,19,21	1.49	3 (17%)
4	NAG	M	2	4	14,14,15	0.61	0	17,19,21	1.67	1 (5%)
6	NAG	N	1	1,6	14,14,15	0.56	0	17,19,21	1.09	1 (5%)
6	NAG	N	2	6	14,14,15	0.56	0	17,19,21	1.99	7 (41%)
6	BMA	N	3	6	11,11,12	0.58	0	15,15,17	1.18	2 (13%)
6	MAN	N	4	6	11,11,12	0.61	0	15,15,17	1.49	3 (20%)
5	NAG	O	1	1,5	14,14,15	0.51	0	17,19,21	2.30	3 (17%)
5	NAG	O	2	5	14,14,15	0.49	0	17,19,21	1.90	4 (23%)
5	BMA	O	3	5	11,11,12	0.91	1 (9%)	15,15,17	2.18	3 (20%)
5	MAN	O	4	5	11,11,12	0.60	0	15,15,17	2.67	4 (26%)
5	FUC	O	5	5	10,10,11	0.77	0	14,14,16	1.41	3 (21%)
4	NAG	P	1	4,1	14,14,15	0.58	0	17,19,21	0.94	1 (5%)
4	NAG	P	2	4	14,14,15	0.61	0	17,19,21	1.14	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
3	NAG	F	1	3,1	1/1/5/7	0/6/23/26	0/1/1/1

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	3	BMA	C2-C3	2.03	1.55	1.52

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	O	4	MAN	C1-O5-C5	8.29	123.42	112.19
5	O	3	BMA	C1-C2-C3	6.78	118.00	109.67
5	O	2	NAG	C1-O5-C5	5.92	120.22	112.19
5	O	1	NAG	C1-O5-C5	5.77	120.02	112.19
5	O	1	NAG	O5-C1-C2	5.72	120.32	111.29

5 of 8 chirality outliers are listed below:

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

5 of 62 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
2	K	2	NAG	C8-C7-N2-C2

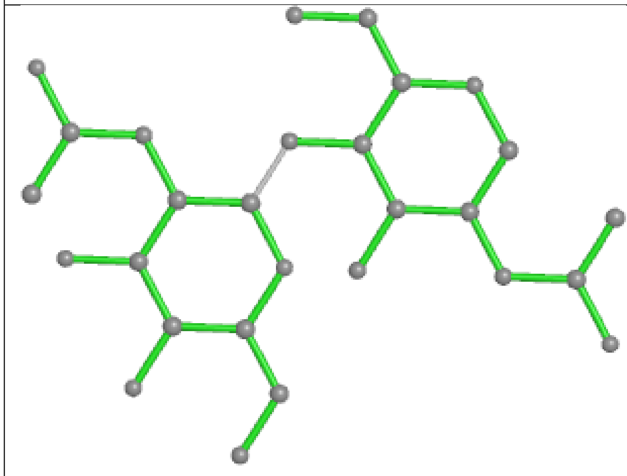
There are no ring outliers.

6 monomers are involved in 4 short contacts:

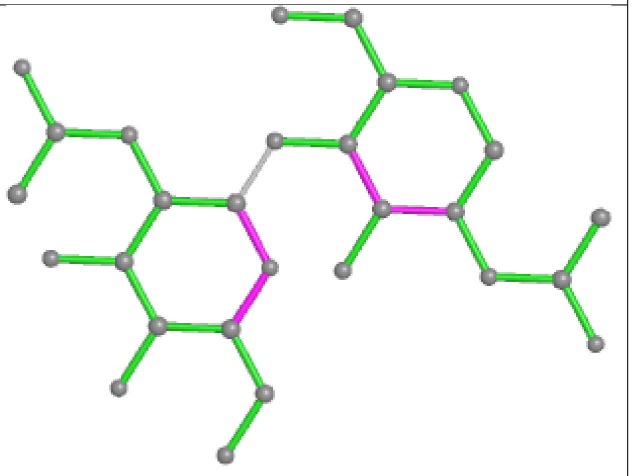
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	3	BMA	1	0
3	L	1	NAG	1	0
3	L	2	NAG	1	0
2	H	2	NAG	1	0
5	I	2	NAG	2	0
5	I	5	FUC	1	0

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

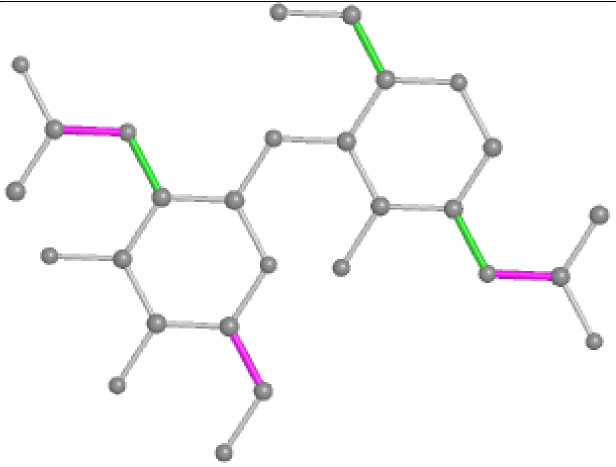
Oligosaccharide Chain P



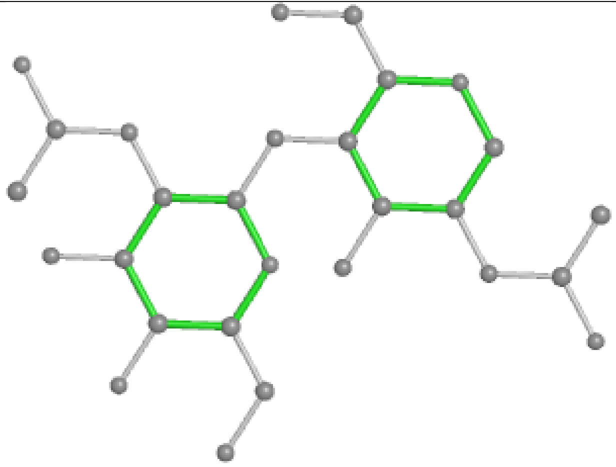
Bond lengths



Bond angles

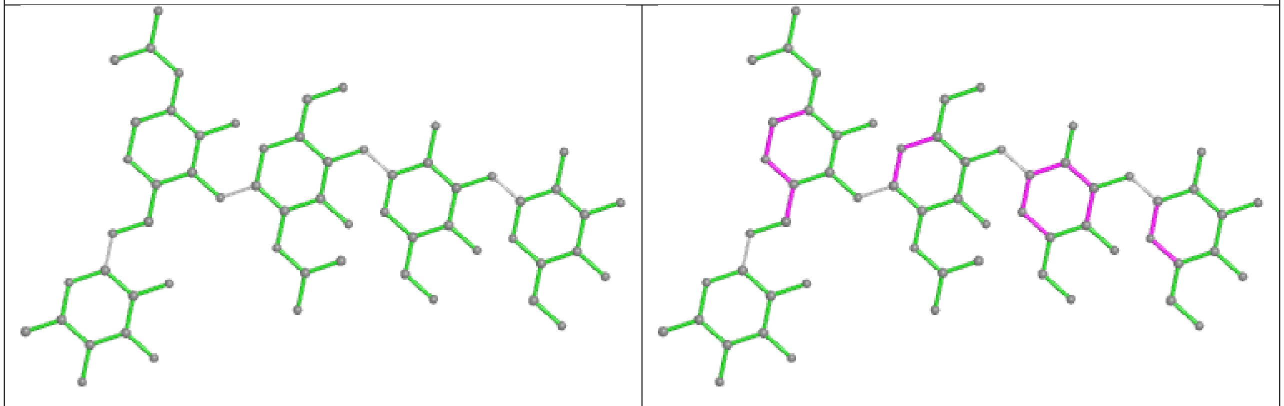


Torsions

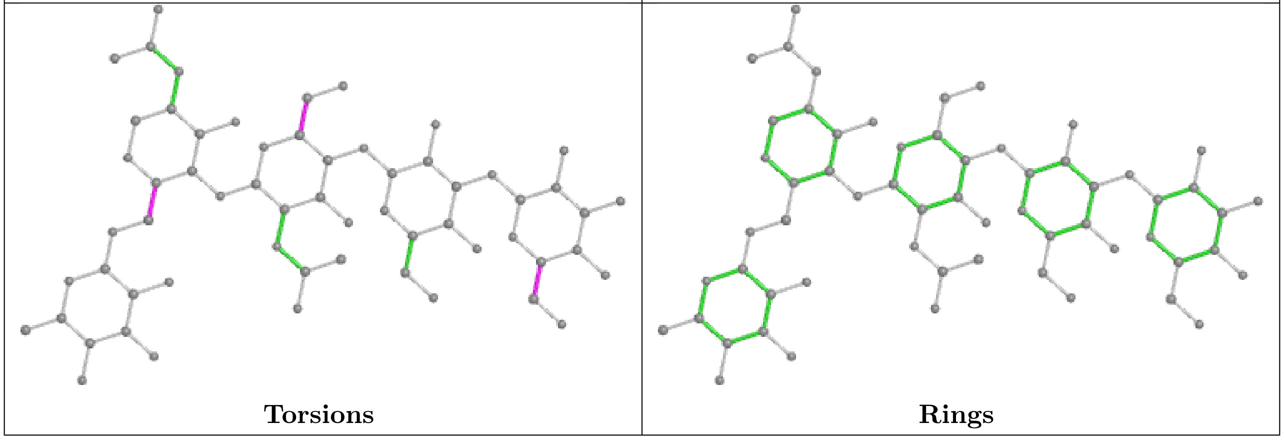


Rings

Oligosaccharide Chain I

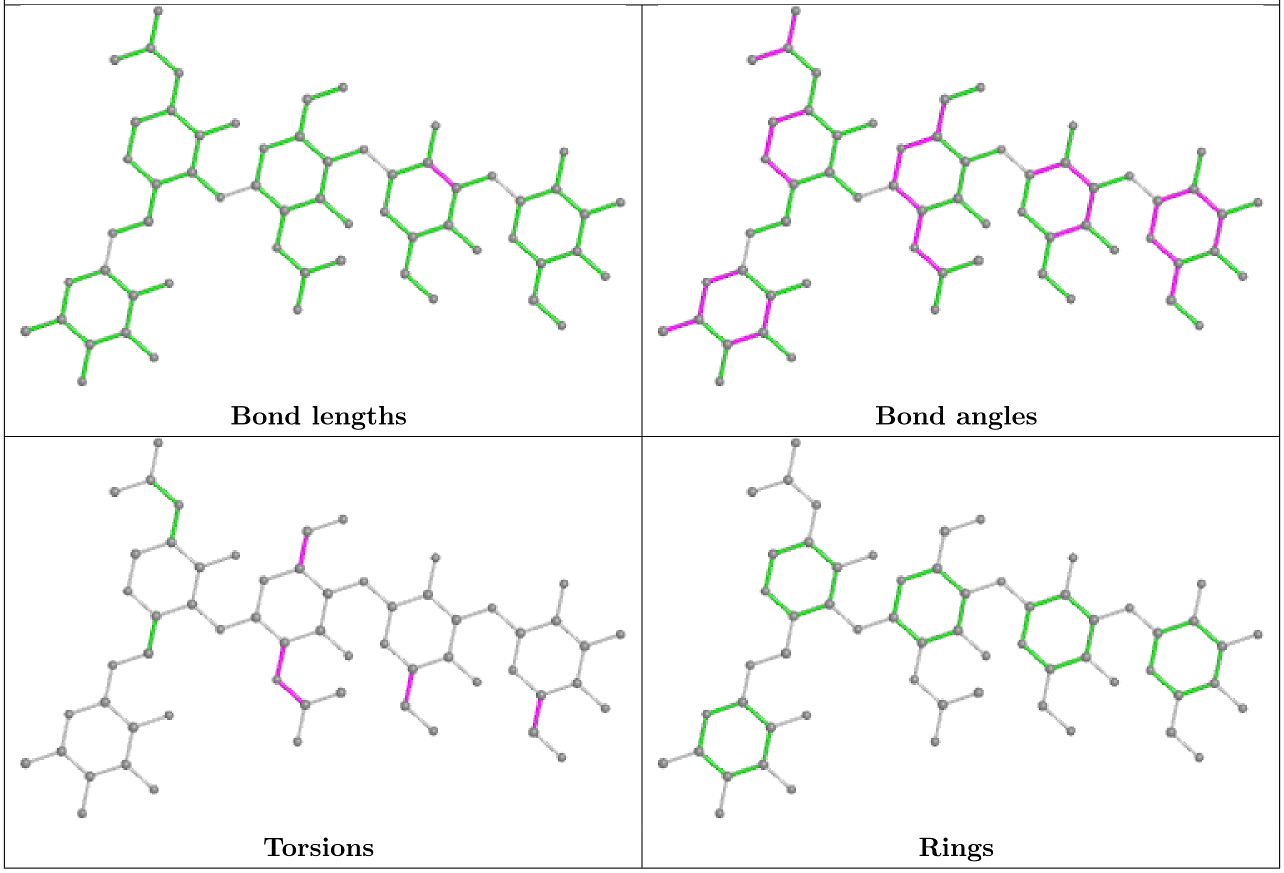


Bond lengths **Bond angles**



Torsions **Rings**

Oligosaccharide Chain O



Bond lengths

Bond angles

Torsions

Rings

5.6 Ligand geometry ⓘ

Of 28 ligands modelled in this entry, 20 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	$\#\|Z\| > 2$
7	NAG	D	1768	1	14,14,15	0.57	0	17,19,21	1.55	3 (17%)
7	NAG	B	1773	-	14,14,15	0.61	0	17,19,21	1.82	4 (23%)
7	NAG	D	1774	-	14,14,15	0.62	0	17,19,21	1.55	2 (11%)
7	NAG	A	1768	1	14,14,15	0.52	0	17,19,21	1.06	2 (11%)
7	NAG	B	1768	1	14,14,15	0.53	0	17,19,21	1.51	1 (5%)
7	NAG	C	1768	1	14,14,15	0.61	0	17,19,21	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	D	1770	1	14,14,15	0.68	0	17,19,21	1.33	2 (11%)
7	NAG	B	1770	1	14,14,15	0.62	0	17,19,21	2.74	6 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	D	1768	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1773	-	-	4/6/23/26	0/1/1/1
7	NAG	D	1774	-	-	3/6/23/26	0/1/1/1
7	NAG	A	1768	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1768	1	-	4/6/23/26	0/1/1/1
7	NAG	C	1768	1	-	2/6/23/26	0/1/1/1
7	NAG	D	1770	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1770	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	1770	NAG	C1-O5-C5	8.24	123.36	112.19
7	B	1768	NAG	C1-O5-C5	5.29	119.35	112.19
7	B	1773	NAG	C2-N2-C7	4.73	129.64	122.90
7	B	1770	NAG	C4-C3-C2	4.03	116.92	111.02
7	D	1774	NAG	C2-N2-C7	3.96	128.54	122.90

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1768	NAG	C8-C7-N2-C2
7	B	1768	NAG	O7-C7-N2-C2
7	D	1774	NAG	C3-C2-N2-C7
7	D	1774	NAG	C8-C7-N2-C2
7	D	1774	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1773	NAG	1	0
7	D	1774	NAG	1	0
7	A	1768	NAG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	705/735 (95%)	-0.39	14 (1%)	65	68	26, 34, 64, 88	0
1	B	708/735 (96%)	-0.40	9 (1%)	77	79	24, 34, 67, 99	0
1	C	705/735 (95%)	-0.39	12 (1%)	70	72	25, 35, 64, 84	0
1	D	708/735 (96%)	-0.37	12 (1%)	70	72	24, 34, 68, 101	0
All	All	2826/2940 (96%)	-0.39	47 (1%)	70	72	24, 34, 67, 101	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	762	HIS	11.4
1	A	203	HIS	7.0
1	C	762	HIS	6.7
1	C	203	HIS	6.3
1	B	204	ARG	5.7

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	TPQ	A	471	14/15	0.86	0.19	40,48,51,52	0
1	TPQ	D	471	14/15	0.88	0.18	38,46,49,49	0
1	TPQ	B	471	14/15	0.89	0.20	39,47,49,50	0
1	TPQ	C	471	14/15	0.91	0.19	38,46,49,49	0

6.3 Carbohydrates ⓘ

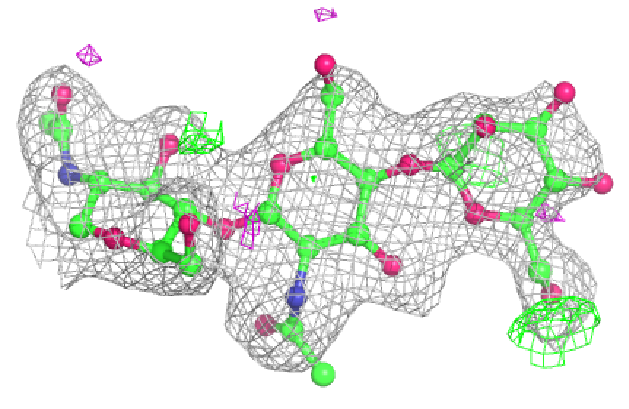
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

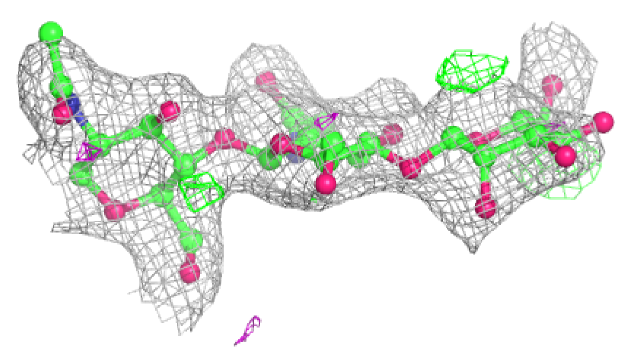
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MAN	N	4	11/12	0.70	0.20	89,90,91,91	0
5	MAN	O	4	11/12	0.73	0.28	79,81,82,82	0
2	BMA	H	3	11/12	0.74	0.18	79,82,82,82	0
4	NAG	G	2	14/15	0.78	0.43	77,81,81,82	0
5	BMA	I	3	11/12	0.82	0.13	69,70,72,75	0
4	NAG	J	2	14/15	0.82	0.29	71,73,73,74	0
4	NAG	P	2	14/15	0.82	0.29	74,75,77,77	0
4	NAG	M	2	14/15	0.83	0.38	76,79,80,81	0
5	BMA	O	3	11/12	0.83	0.14	67,70,72,76	0
5	MAN	I	4	11/12	0.84	0.28	78,79,80,81	0
3	NAG	L	2	14/15	0.84	0.25	62,65,69,69	0
2	BMA	E	3	11/12	0.84	0.24	72,74,75,75	0
3	NAG	F	2	14/15	0.84	0.22	57,61,62,62	0
6	BMA	N	3	11/12	0.85	0.16	79,82,86,88	0
5	FUC	O	5	10/11	0.86	0.18	52,55,57,58	0
2	NAG	H	2	14/15	0.87	0.18	62,66,70,75	0
5	NAG	I	2	14/15	0.88	0.17	54,61,67,68	0
2	BMA	K	3	11/12	0.88	0.23	73,75,75,76	0
2	NAG	E	2	14/15	0.89	0.18	59,63,65,69	0
4	NAG	G	1	14/15	0.89	0.22	58,64,67,73	0
5	FUC	I	5	10/11	0.90	0.22	53,55,56,57	0
6	NAG	N	2	14/15	0.91	0.14	61,64,68,74	0
4	NAG	J	1	14/15	0.91	0.17	58,63,65,68	0
4	NAG	P	1	14/15	0.91	0.17	59,66,68,71	0
3	FUC	F	3	10/11	0.93	0.14	50,51,52,52	0
2	NAG	K	1	14/15	0.93	0.13	43,49,51,55	0
3	FUC	L	3	10/11	0.93	0.15	47,50,52,53	0
2	NAG	K	2	14/15	0.93	0.12	59,61,66,70	0
4	NAG	M	1	14/15	0.94	0.16	58,64,66,72	0
3	NAG	F	1	14/15	0.95	0.12	39,44,48,53	0
3	NAG	L	1	14/15	0.95	0.12	42,48,53,58	0
5	NAG	O	2	14/15	0.95	0.14	55,59,62,66	0
5	NAG	I	1	14/15	0.96	0.12	39,45,51,54	0
2	NAG	H	1	14/15	0.96	0.12	39,43,48,55	0
2	NAG	E	1	14/15	0.96	0.13	43,46,49,55	0
6	NAG	N	1	14/15	0.97	0.12	40,44,49,55	0
5	NAG	O	1	14/15	0.98	0.10	34,43,52,52	0

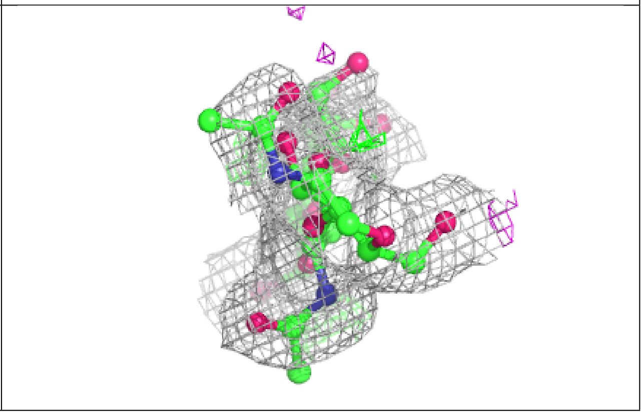
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

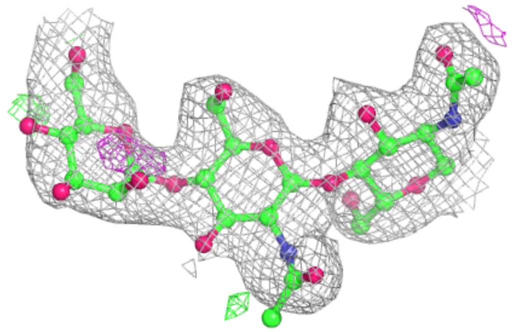


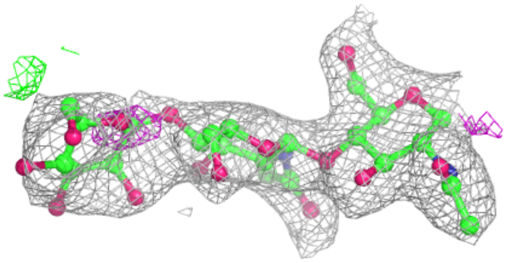


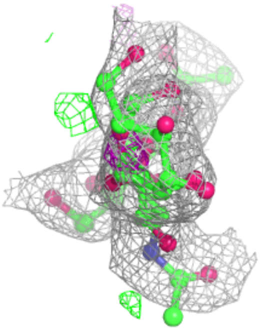


Electron density around Chain H:

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

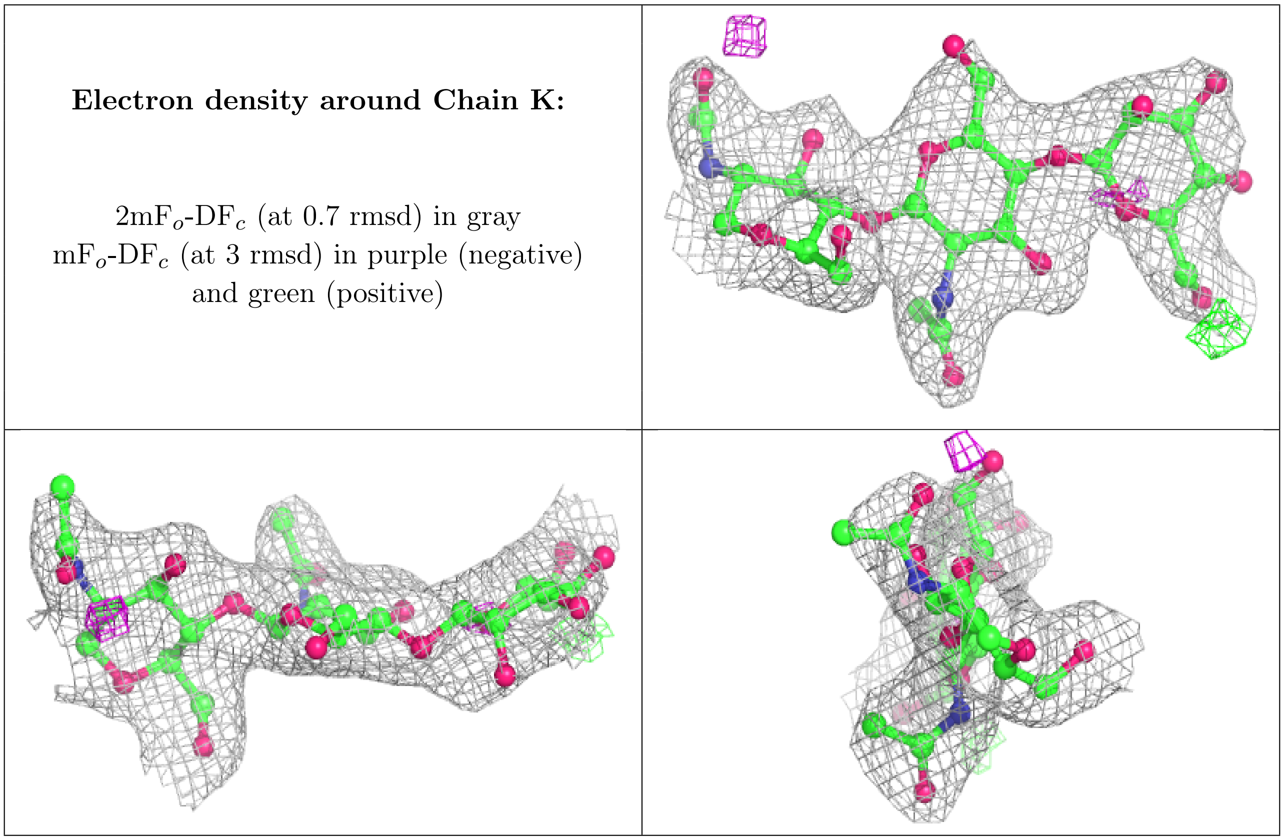






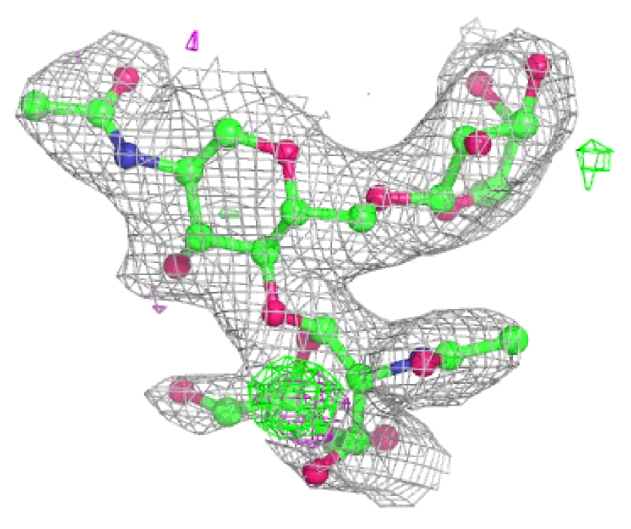
Electron density around Chain K:

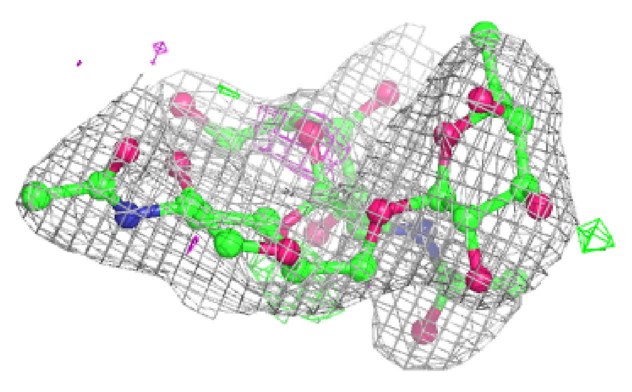
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

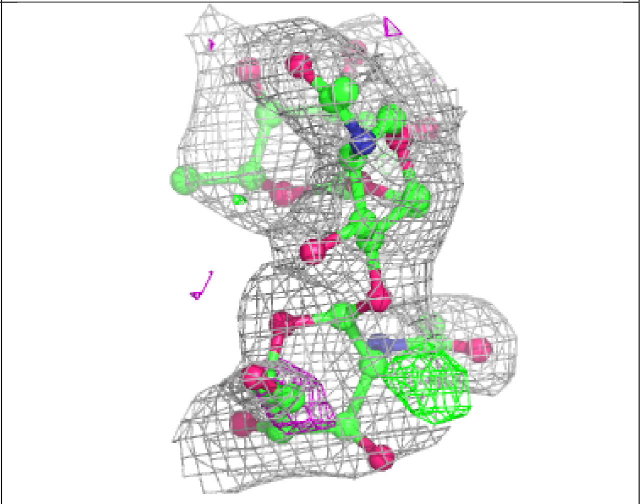


Electron density around Chain F:

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

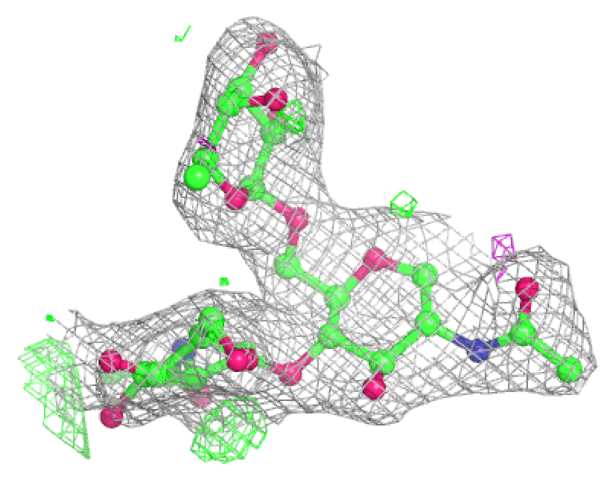


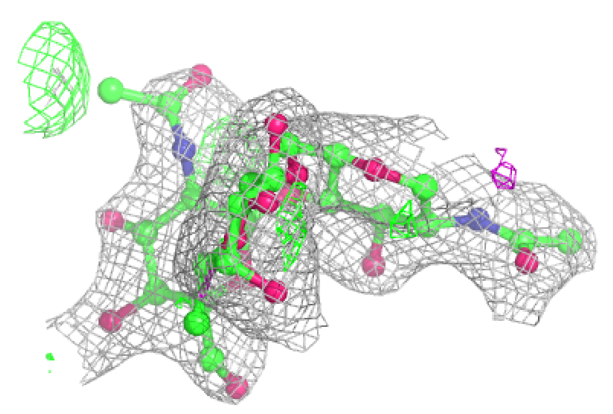


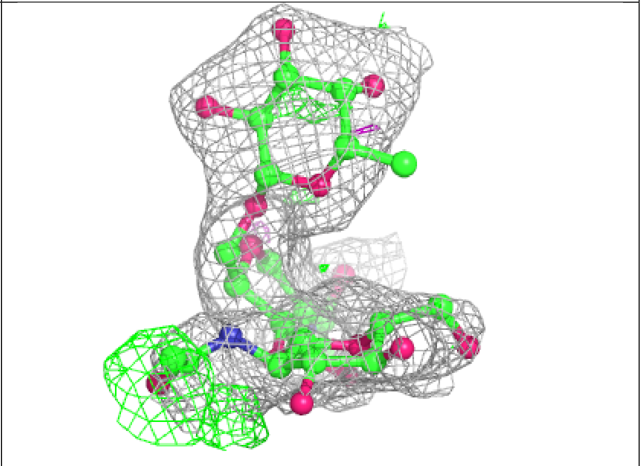


Electron density around Chain L:

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

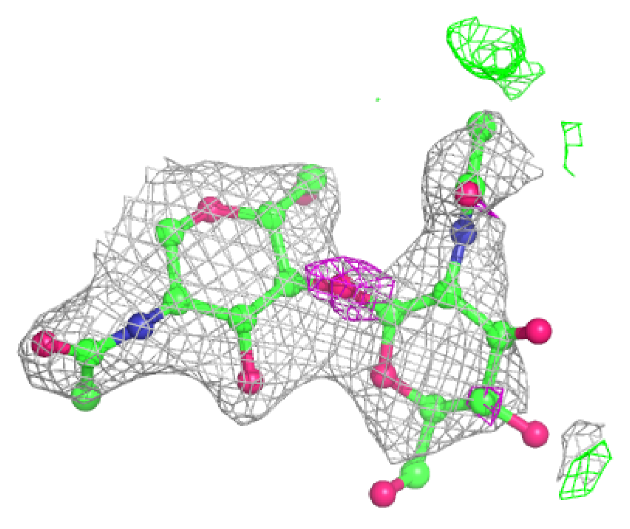


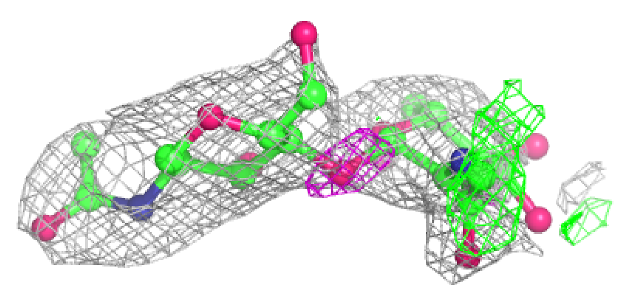


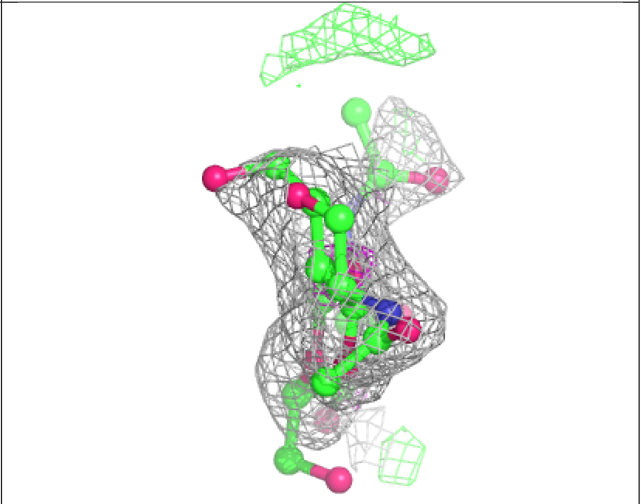


Electron density around Chain G:

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

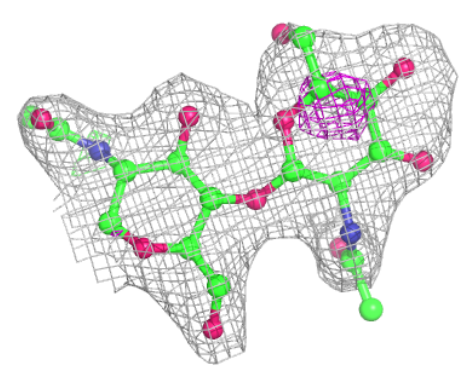


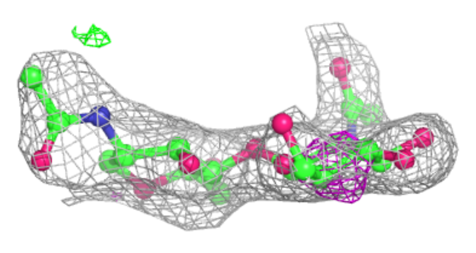


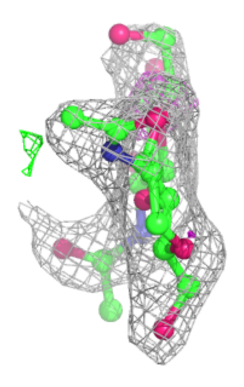


Electron density around Chain J:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

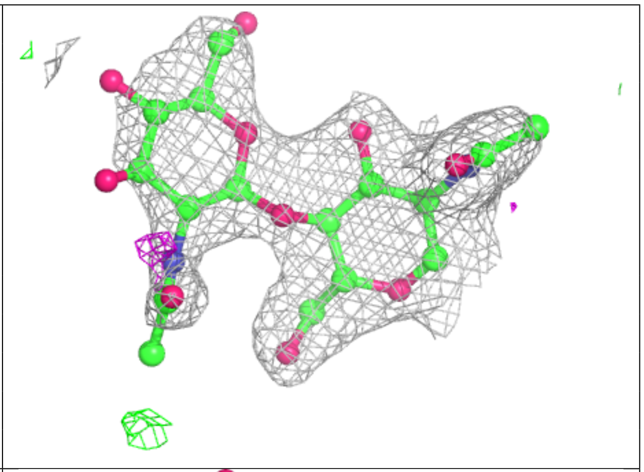


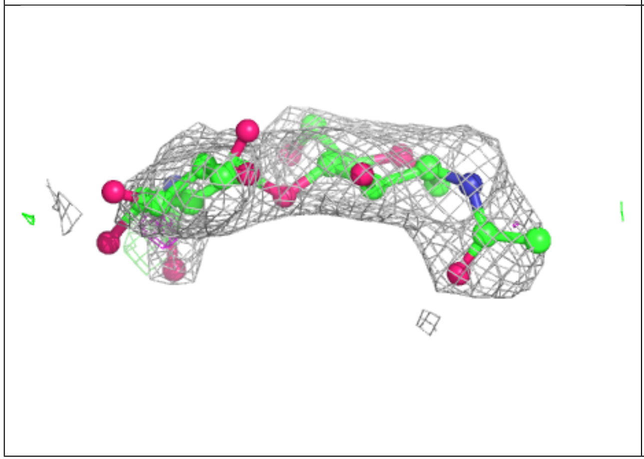


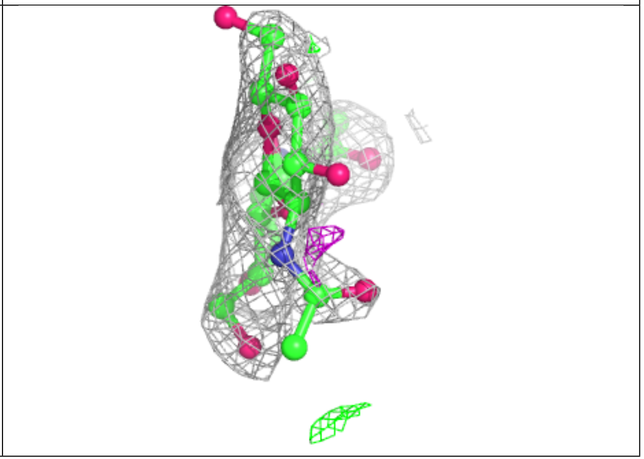


Electron density around Chain M:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

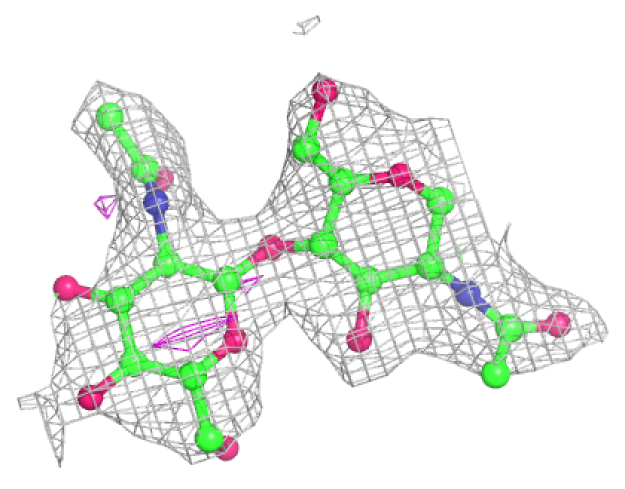


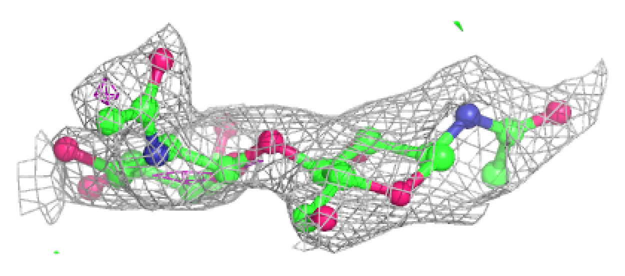


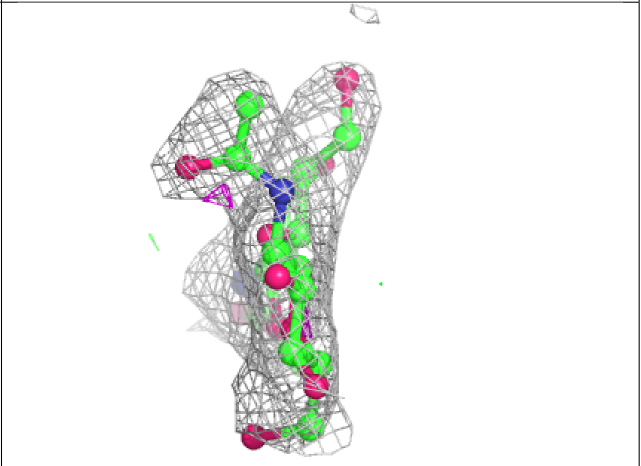


Electron density around Chain P:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

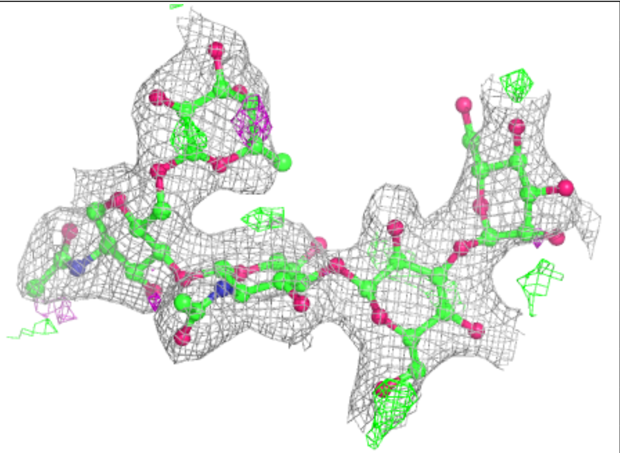


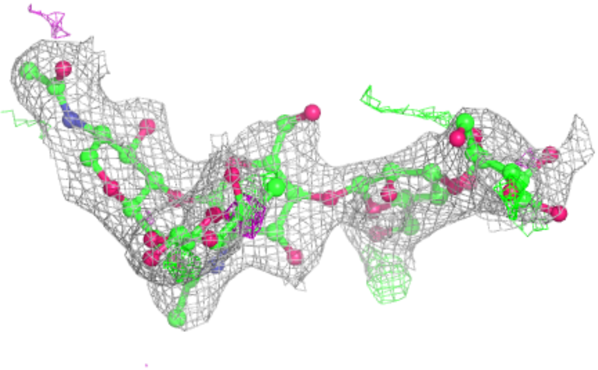


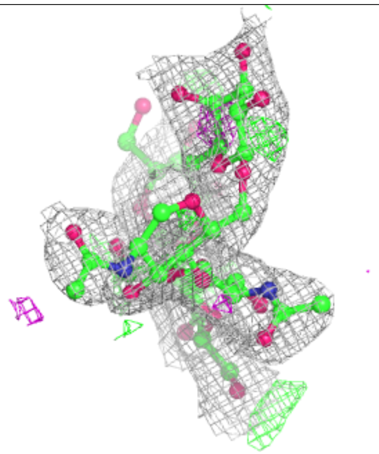


Electron density around Chain I:

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 O:

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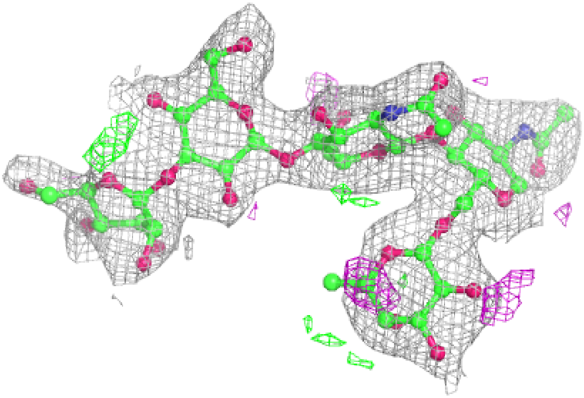
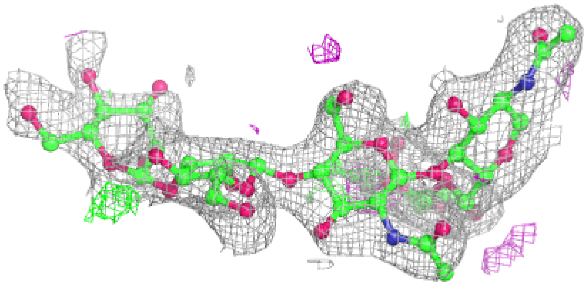
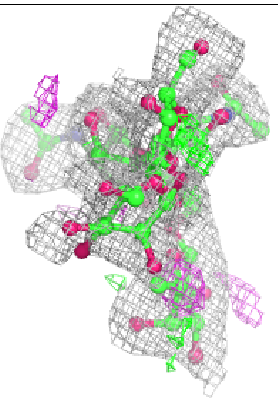
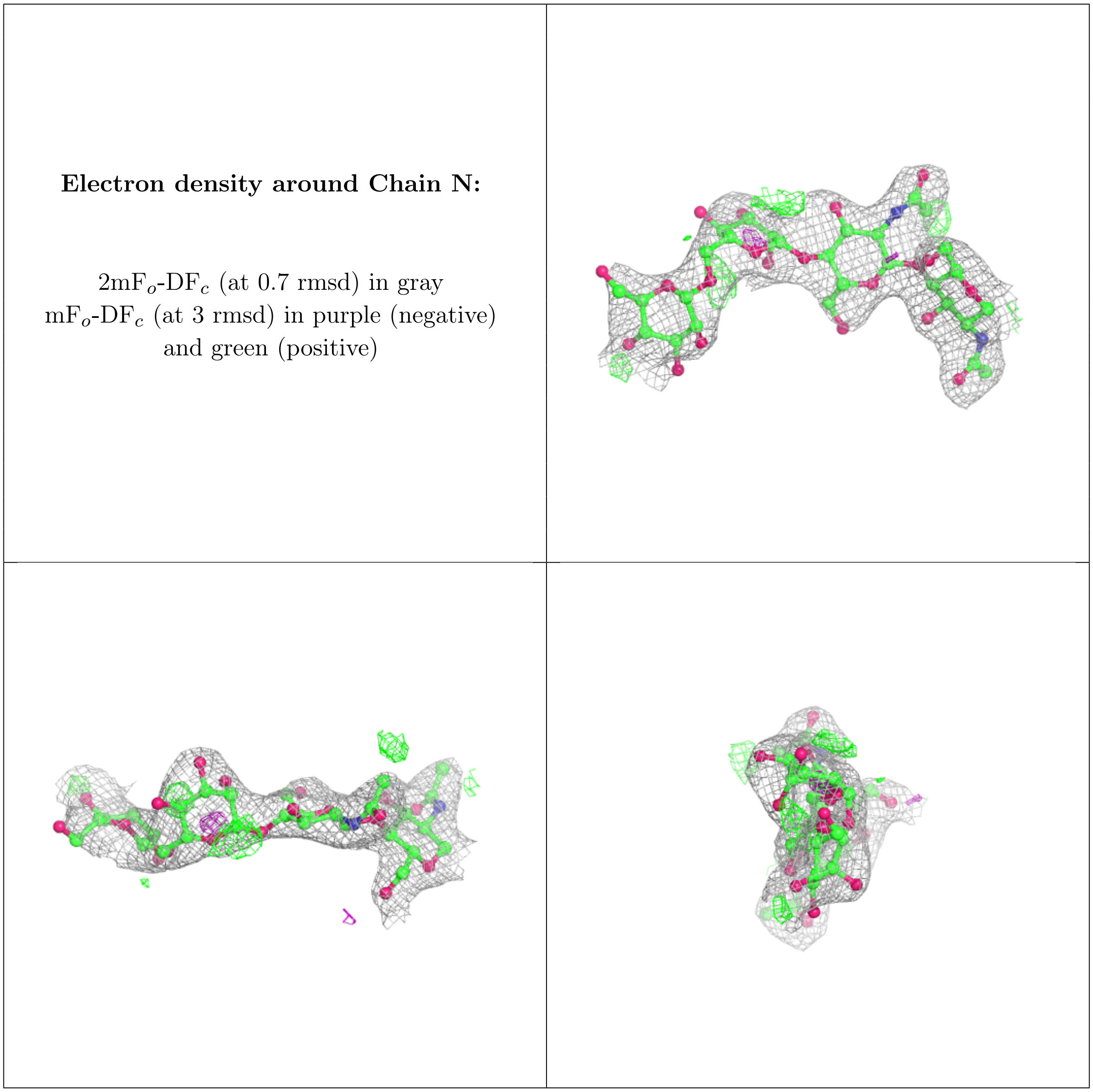
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)









Electron density around Chain N:

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	D	1774	14/15	0.76	0.20	83,86,87,87	0
7	NAG	B	1773	14/15	0.84	0.17	77,78,78,79	0
7	NAG	B	1770	14/15	0.84	0.21	60,65,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
7	NAG	A	1768	14/15	0.85	0.23	64,69,70,70	0
7	NAG	D	1768	14/15	0.87	0.18	62,66,69,70	0
7	NAG	B	1768	14/15	0.87	0.18	62,67,70,71	0
7	NAG	D	1770	14/15	0.88	0.17	60,65,67,67	0
7	NAG	C	1768	14/15	0.88	0.21	61,66,66,68	0
8	CA	C	1773	1/1	0.94	0.07	42,42,42,42	0
10	CL	D	1780	1/1	0.94	0.07	21,21,21,21	1
8	CA	A	1773	1/1	0.97	0.08	40,40,40,40	0
10	CL	C	1775	1/1	0.98	0.09	24,24,24,24	1
8	CA	D	1778	1/1	0.98	0.07	29,29,29,29	0
8	CA	A	1771	1/1	0.99	0.05	29,29,29,29	0
8	CA	D	1776	1/1	0.99	0.07	25,25,25,25	0
8	CA	B	1775	1/1	0.99	0.04	27,27,27,27	0
9	CU	A	1772	1/1	0.99	0.08	33,33,33,33	0
9	CU	C	1772	1/1	0.99	0.06	36,36,36,36	0
9	CU	D	1777	1/1	0.99	0.07	35,35,35,35	0
10	CL	A	1774	1/1	0.99	0.11	19,19,19,19	0
10	CL	A	1775	1/1	0.99	0.06	24,24,24,24	1
10	CL	B	1778	1/1	0.99	0.11	18,18,18,18	0
10	CL	B	1779	1/1	0.99	0.07	18,18,18,18	1
8	CA	B	1777	1/1	0.99	0.07	31,31,31,31	0
10	CL	D	1779	1/1	0.99	0.11	16,16,16,16	0
8	CA	C	1771	1/1	0.99	0.06	28,28,28,28	0
10	CL	C	1774	1/1	1.00	0.10	15,15,15,15	0
9	CU	B	1776	1/1	1.00	0.08	35,35,35,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.