wwPDB X-ray Structure Validation Summary Report (i)

Nov 9, 2023 – 09:55 am GMT

PDB ID	:	8PMR
Title	:	NADase from Aspergillus fumigatus with mutated calcium binding motif (D219A/E220A)
Authors	:	Kallio, J.P.; Ferrario, E.; Stromland, O.; Ziegler, M.
Deposited on	:	2023-06-29
Resolution	:	1.94 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:

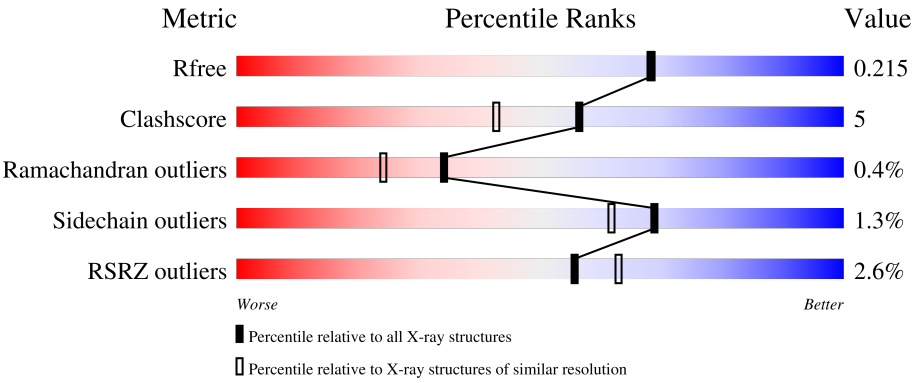
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.94 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	248	78% 7% 15%
1	B	248	77% 8% 15%
1	C	248	73% 10% 16%
1	D	248	69% 13% 17%
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	F	4	25% 75%
4	G	2	100%
4	I	2	100%
5	H	5	60% 40%
6	J	3	33% 33% 33%
6	K	3	67% 33%
6	L	3	33% 67%

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
4	FUC	G	2	-	-	-	X
4	FUC	I	2	-	-	-	X

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 7691 atoms, of which 74 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 Conidial surface nicotinamide adenine dinucleotide glycohydrolase nadA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1661	1076	265	313	7			
1	B	210	Total	C	N	O	S	0	1	0
			1662	1077	265	313	7			
1	C	208	Total	C	N	O	S	0	0	0
			1642	1065	261	309	7			
1	D	207	Total	C	N	O	S	0	0	0
			1632	1059	258	308	7			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	ALA	ASP	engineered mutation	UNP Q4WL81
A	220	ALA	GLU	engineered mutation	UNP Q4WL81
A	235	ASP	-	expression tag	UNP Q4WL81
A	236	VAL	-	expression tag	UNP Q4WL81
A	237	LEU	-	expression tag	UNP Q4WL81
A	238	PHE	-	expression tag	UNP Q4WL81
A	239	GLN	-	expression tag	UNP Q4WL81
A	240	GLY	-	expression tag	UNP Q4WL81
A	241	PRO	-	expression tag	UNP Q4WL81
A	242	GLY	-	expression tag	UNP Q4WL81
A	243	HIS	-	expression tag	UNP Q4WL81
A	244	HIS	-	expression tag	UNP Q4WL81
A	245	HIS	-	expression tag	UNP Q4WL81
A	246	HIS	-	expression tag	UNP Q4WL81
A	247	HIS	-	expression tag	UNP Q4WL81
A	248	HIS	-	expression tag	UNP Q4WL81
B	219	ALA	ASP	engineered mutation	UNP Q4WL81
B	220	ALA	GLU	engineered mutation	UNP Q4WL81
B	235	ASP	-	expression tag	UNP Q4WL81
B	236	VAL	-	expression tag	UNP Q4WL81

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Chain	Residue	Modelled	Actual	Comment	Reference
B	237	LEU	-	expression tag	UNP Q4WL81
B	238	PHE	-	expression tag	UNP Q4WL81
B	239	GLN	-	expression tag	UNP Q4WL81
B	240	GLY	-	expression tag	UNP Q4WL81
B	241	PRO	-	expression tag	UNP Q4WL81
B	242	GLY	-	expression tag	UNP Q4WL81
B	243	HIS	-	expression tag	UNP Q4WL81
B	244	HIS	-	expression tag	UNP Q4WL81
B	245	HIS	-	expression tag	UNP Q4WL81
B	246	HIS	-	expression tag	UNP Q4WL81
B	247	HIS	-	expression tag	UNP Q4WL81
B	248	HIS	-	expression tag	UNP Q4WL81
C	219	ALA	ASP	engineered mutation	UNP Q4WL81
C	220	ALA	GLU	engineered mutation	UNP Q4WL81
C	235	ASP	-	expression tag	UNP Q4WL81
C	236	VAL	-	expression tag	UNP Q4WL81
C	237	LEU	-	expression tag	UNP Q4WL81
C	238	PHE	-	expression tag	UNP Q4WL81
C	239	GLN	-	expression tag	UNP Q4WL81
C	240	GLY	-	expression tag	UNP Q4WL81
C	241	PRO	-	expression tag	UNP Q4WL81
C	242	GLY	-	expression tag	UNP Q4WL81
C	243	HIS	-	expression tag	UNP Q4WL81
C	244	HIS	-	expression tag	UNP Q4WL81
C	245	HIS	-	expression tag	UNP Q4WL81
C	246	HIS	-	expression tag	UNP Q4WL81
C	247	HIS	-	expression tag	UNP Q4WL81
C	248	HIS	-	expression tag	UNP Q4WL81
D	219	ALA	ASP	engineered mutation	UNP Q4WL81
D	220	ALA	GLU	engineered mutation	UNP Q4WL81
D	235	ASP	-	expression tag	UNP Q4WL81
D	236	VAL	-	expression tag	UNP Q4WL81
D	237	LEU	-	expression tag	UNP Q4WL81
D	238	PHE	-	expression tag	UNP Q4WL81
D	239	GLN	-	expression tag	UNP Q4WL81
D	240	GLY	-	expression tag	UNP Q4WL81
D	241	PRO	-	expression tag	UNP Q4WL81
D	242	GLY	-	expression tag	UNP Q4WL81
D	243	HIS	-	expression tag	UNP Q4WL81
D	244	HIS	-	expression tag	UNP Q4WL81
D	245	HIS	-	expression tag	UNP Q4WL81
D	246	HIS	-	expression tag	UNP Q4WL81

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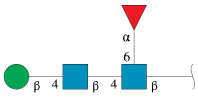
Chain	Residue	Modelled	Actual	Comment	Reference
D	247	HIS	-	expression tag	UNP Q4WL81
D	248	HIS	-	expression tag	UNP Q4WL81

- 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			

- Molecule 3 is an oligosaccharide called 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.



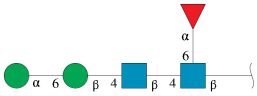
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	4	Total	C	N	O	0	0	0
			49	28	2	19			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O	0	0	0
			24	14	1	9			
4	I	2	Total	C	N	O	0	0	0
			24	14	1	9			

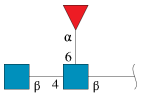
- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acet

amido-2-deoxy-beta-D-glucopyranose.



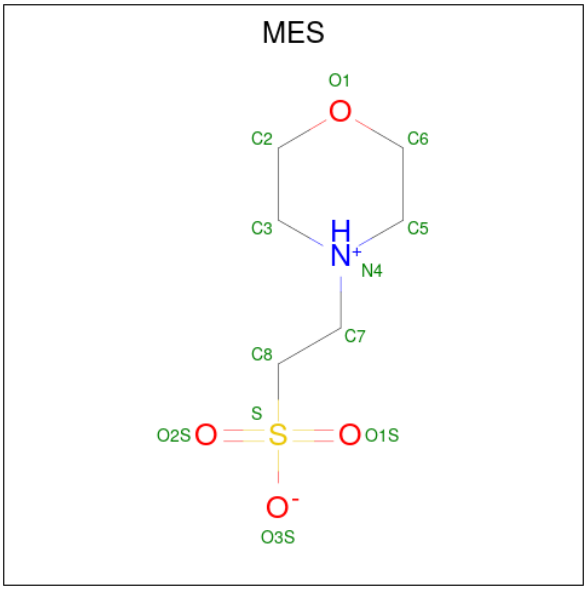
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	5	Total	C	N	O	0	0	0
			60	34	2	24			

- 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.



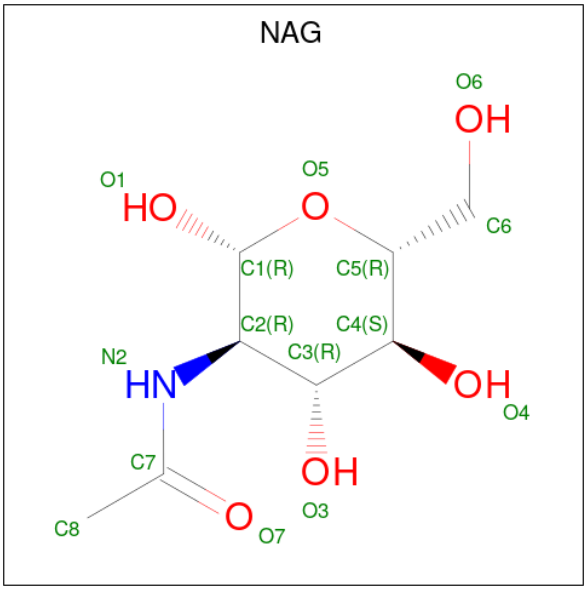
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	3	Total	C	N	O	0	0	0
			38	22	2	14			
6	K	3	Total	C	N	O	0	0	0
			38	22	2	14			
6	L	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



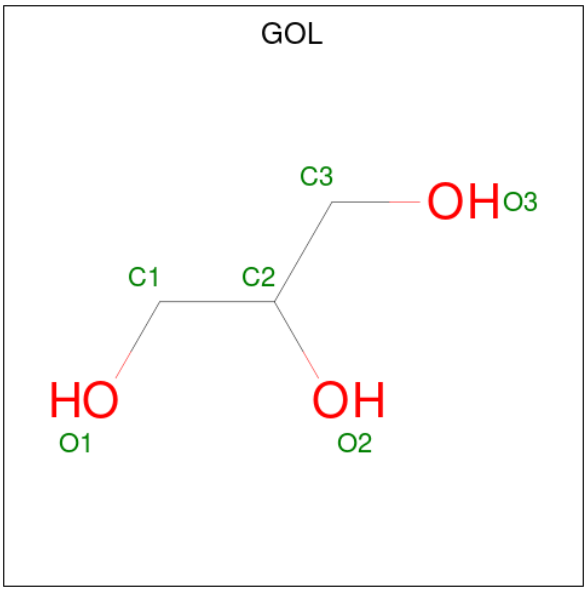
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
7	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



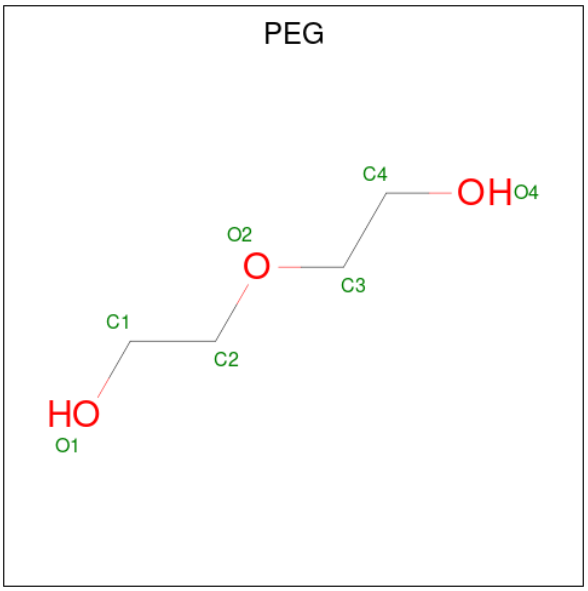
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



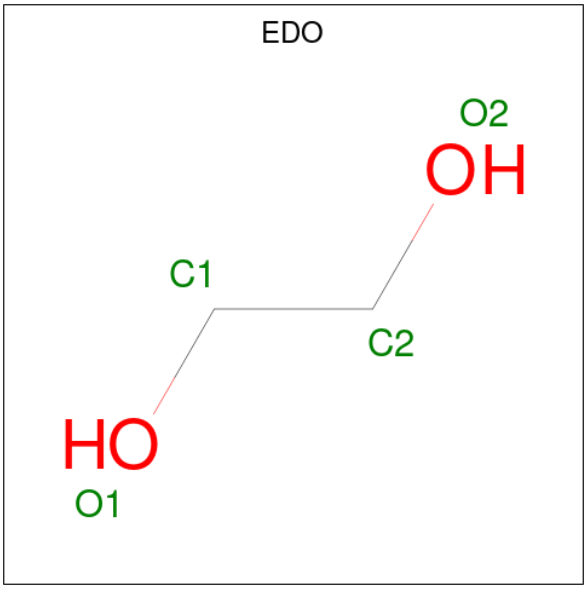
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C H O 14 3 8 3	0	0
9	C	1	Total C H O 14 3 8 3	0	0
9	D	1	Total C H O 14 3 8 3	0	0
9	D	1	Total C H O 14 3 8 3	0	0

- Molecule 10 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 11 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	D	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 12 is water.

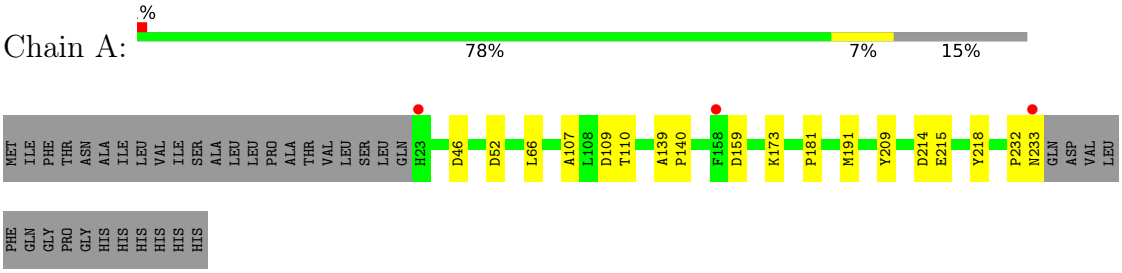
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	183	Total	O	0	5
			188	188		
12	B	168	Total	O	0	3
			171	171		
12	C	154	Total	O	0	4
			158	158		
12	D	102	Total	O	0	1
			103	103		

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.

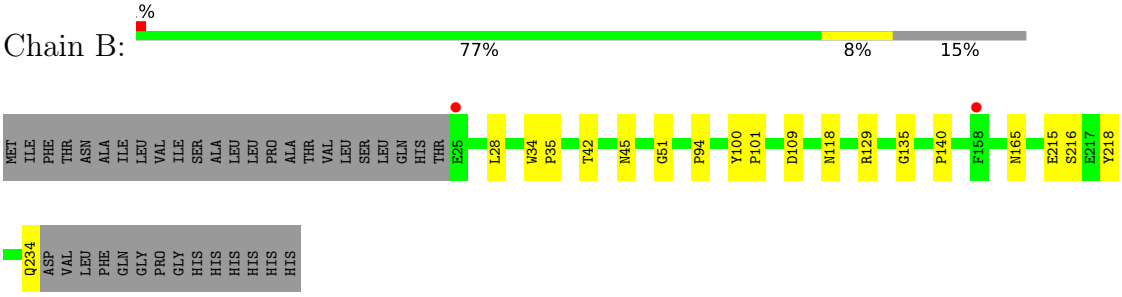
• Molecule 1: Conidial surface nicotinamide adenine dinucleotide glycohydrolase nadA

Chain A:



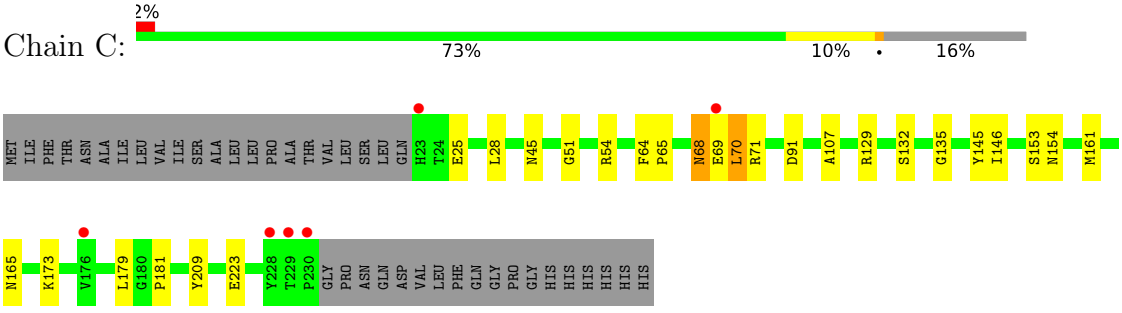
• Molecule 1: Conidial surface nicotinamide adenine dinucleotide glycohydrolase nadA

Chain B:



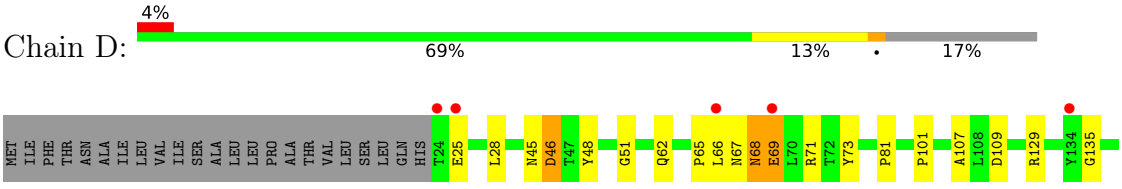
• Molecule 1: Conidial surface nicotinamide adenine dinucleotide glycohydrolase nadA

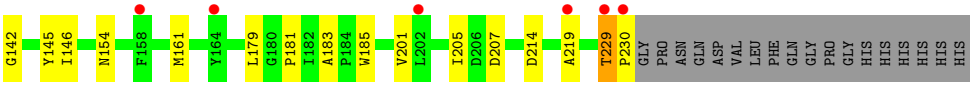
Chain C:



• Molecule 1: Conidial surface nicotinamide adenine dinucleotide glycohydrolase nadA

Chain D:



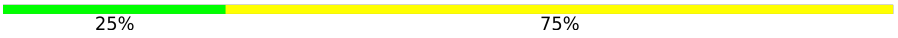


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

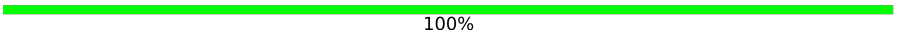
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



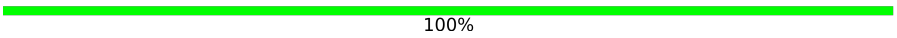
• Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain I:

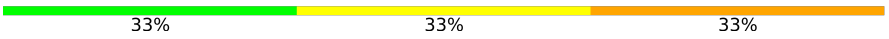


• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

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

Chain J:



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

Chain K:

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

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	65.90Å 65.90Å 488.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.32 – 1.94 49.27 – 1.94	Depositor EDS
% Data completeness (in resolution range)	96.4 (39.32-1.94) 96.6 (49.27-1.94)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.182 , 0.216 0.182 , 0.215	Depositor DCC
R_{free} test set	4243 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	39.0	Xtriage
Anisotropy	0.541	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.084 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7691	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MES, GOL, NAG, FUC, PEG, EDO, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.43	0/1719	0.67	4/2359 (0.2%)
1	B	0.44	0/1719	0.63	1/2357 (0.0%)
1	C	0.47	0/1699	0.69	0/2331
1	D	0.52	0/1688	0.70	1/2316 (0.0%)
All	All	0.46	0/6825	0.67	6/9363 (0.1%)

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	109	ASP	CB-CG-OD1	6.15	123.83	118.30
1	A	159	ASP	CB-CG-OD1	6.04	123.73	118.30
1	D	109	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	109	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	46	ASP	CB-CG-OD1	5.26	123.03	118.30

There are no chirality outliers.

There are no planarity outliers.

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	1661	0	1564	8	0
1	B	1662	0	1570	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1642	0	1548	26	0
1	D	1632	0	1542	29	0
2	E	28	0	25	1	0
3	F	49	0	43	0	0
4	G	24	0	22	0	0
4	I	24	0	22	0	0
5	H	60	0	52	0	0
6	J	38	0	34	1	0
6	K	38	0	34	0	0
6	L	38	0	34	0	0
7	A	12	13	12	0	0
7	B	12	13	12	0	0
8	B	14	0	13	0	0
8	C	14	0	13	1	0
8	D	14	0	13	0	0
9	C	12	16	15	1	0
9	D	12	16	16	0	0
10	C	7	10	10	2	0
11	D	4	6	6	2	0
12	A	188	0	0	0	0
12	B	171	0	0	3	0
12	C	158	0	0	1	0
12	D	103	0	0	1	0
All	All	7617	74	6600	68	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 68 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:C:65:PRO:HB3	1:D:69:GLU:HB2	1.46	0.95
1:C:69:GLU:HB3	1:D:65:PRO:HB3	1.63	0.78
1:D:154:ASN:OD1	12:D:401:HOH:O	2.13	0.67
1:C:68:ASN:ND2	1:C:146:ILE:HG21	2.13	0.63
1:D:229:THR:HB	1:D:230:PRO:HD3	1.81	0.62

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	209/248 (84%)	208 (100%)	1 (0%)	0	100 100
1	B	209/248 (84%)	208 (100%)	1 (0%)	0	100 100
1	C	206/248 (83%)	202 (98%)	3 (2%)	1 (0%)	29 17
1	D	205/248 (83%)	196 (96%)	7 (3%)	2 (1%)	15 6
All	All	829/992 (84%)	814 (98%)	12 (1%)	3 (0%)	34 24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	70	LEU
1	D	69	GLU
1	D	229	THR

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	177/209 (85%)	176 (99%)	1 (1%)	86 85
1	B	177/209 (85%)	177 (100%)	0	100 100
1	C	175/209 (84%)	172 (98%)	3 (2%)	60 49
1	D	174/209 (83%)	169 (97%)	5 (3%)	42 28
All	All	703/836 (84%)	694 (99%)	9 (1%)	69 62

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	207	ASP
1	D	214	ASP
1	C	223	GLU
1	D	46	ASP
1	D	68	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	68	ASN
1	D	68	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

24 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	0.41	0	17,19,21	0.52	0
2	NAG	E	2	2	14,14,15	0.28	0	17,19,21	0.80	1 (5%)
3	NAG	F	1	3,1	14,14,15	0.20	0	17,19,21	0.61	0
3	NAG	F	2	3	14,14,15	0.78	1 (7%)	17,19,21	1.39	2 (11%)
3	BMA	F	3	3	11,11,12	3.24	5 (45%)	15,15,17	2.99	6 (40%)
3	FUC	F	4	3	10,10,11	1.27	2 (20%)	14,14,16	1.10	0
4	NAG	G	1	1,4	14,14,15	0.59	0	17,19,21	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	FUC	G	2	4	10,10,11	0.86	0	14,14,16	0.70	0
5	NAG	H	1	5,1	14,14,15	0.25	0	17,19,21	0.56	0
5	NAG	H	2	5	14,14,15	0.51	0	17,19,21	0.51	0
5	BMA	H	3	5	11,11,12	0.98	1 (9%)	15,15,17	1.07	2 (13%)
5	MAN	H	4	5	11,11,12	0.93	0	15,15,17	1.27	3 (20%)
5	FUC	H	5	5	10,10,11	0.79	0	14,14,16	0.71	0
4	NAG	I	1	1,4	14,14,15	0.33	0	17,19,21	0.57	0
4	FUC	I	2	4	10,10,11	0.89	0	14,14,16	0.78	0
6	NAG	J	1	1,6	14,14,15	2.14	1 (7%)	17,19,21	1.98	4 (23%)
6	NAG	J	2	6	14,14,15	0.17	0	17,19,21	0.79	1 (5%)
6	FUC	J	3	6	10,10,11	0.94	0	14,14,16	0.71	0
6	NAG	K	1	1,6	14,14,15	0.34	0	17,19,21	0.45	0
6	NAG	K	2	6	14,14,15	0.21	0	17,19,21	0.69	1 (5%)
6	FUC	K	3	6	10,10,11	0.75	0	14,14,16	0.64	0
6	NAG	L	1	1,6	14,14,15	0.35	0	17,19,21	0.53	0
6	NAG	L	2	6	14,14,15	0.57	0	17,19,21	0.75	1 (5%)
6	FUC	L	3	6	10,10,11	0.82	1 (10%)	14,14,16	0.61	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	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	FUC	F	4	3	-	-	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	FUC	G	2	4	-	-	0/1/1/1
5	NAG	H	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	FUC	H	5	5	-	-	0/1/1/1
4	NAG	I	1	1,4	-	3/6/23/26	0/1/1/1
4	FUC	I	2	4	-	-	0/1/1/1
6	NAG	J	1	1,6	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	J	2	6	-	2/6/23/26	0/1/1/1
6	FUC	J	3	6	-	-	0/1/1/1
6	NAG	K	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1
6	FUC	K	3	6	-	-	0/1/1/1
6	NAG	L	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	L	2	6	-	2/6/23/26	0/1/1/1
6	FUC	L	3	6	-	-	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	1	NAG	O5-C1	-7.72	1.31	1.43
3	F	3	BMA	O5-C1	6.09	1.53	1.43
3	F	3	BMA	C1-C2	6.00	1.65	1.52
3	F	3	BMA	C4-C3	4.21	1.63	1.52
3	F	3	BMA	C2-C3	-3.40	1.47	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	3	BMA	C1-C2-C3	-7.43	100.53	109.67
3	F	3	BMA	C1-O5-C5	-6.21	103.77	112.19
6	J	1	NAG	C2-N2-C7	4.76	129.68	122.90
3	F	3	BMA	O5-C5-C6	4.10	113.63	107.20
3	F	2	NAG	O3-C3-C2	-3.55	102.12	109.47

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	J	1	NAG	C8-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
4	I	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2

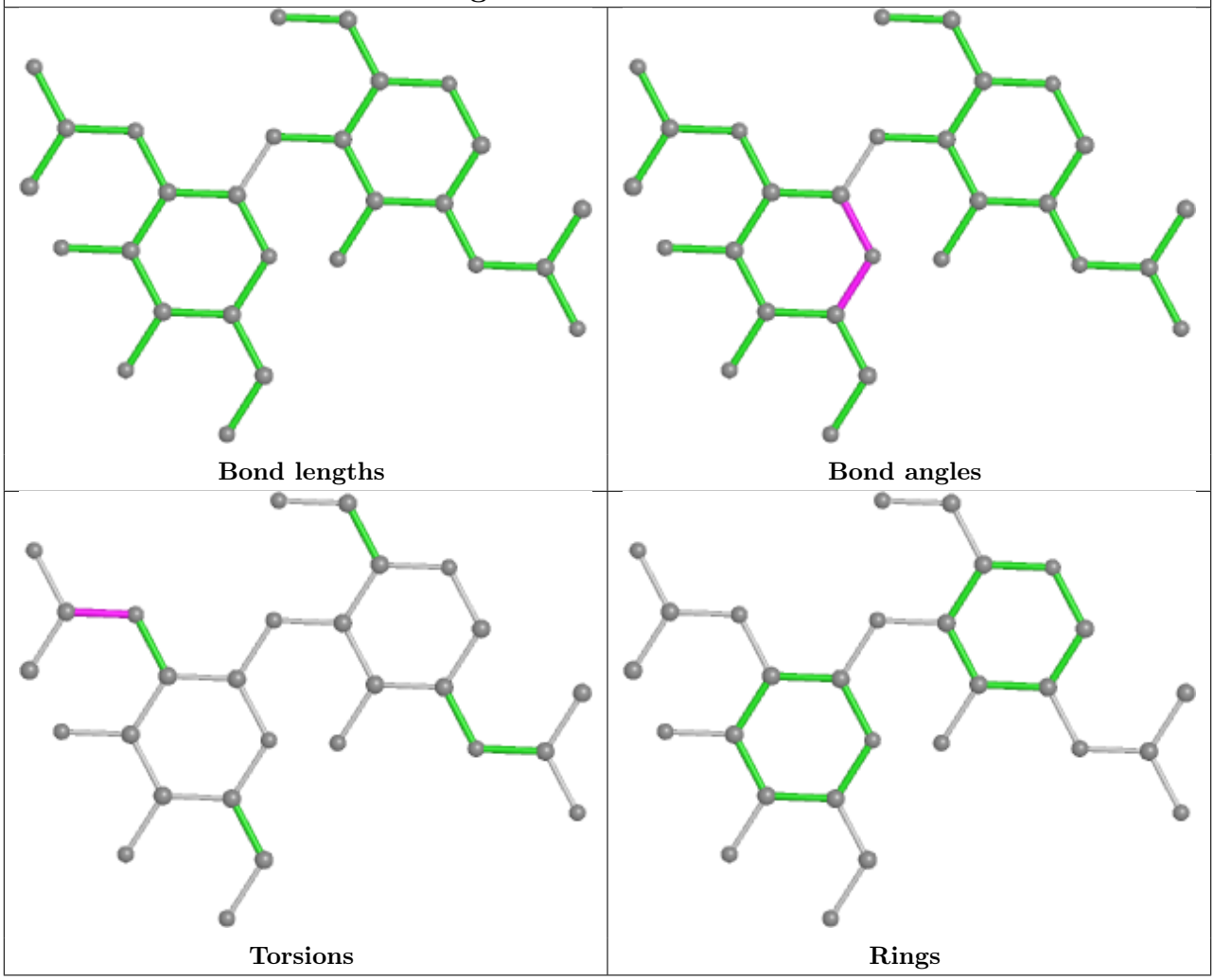
There are no ring outliers.

3 monomers are involved in 2 short contacts:

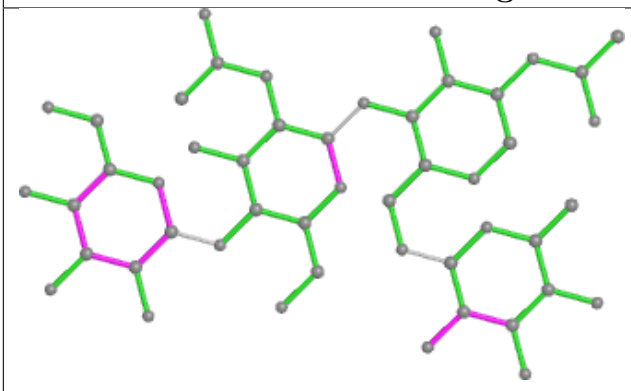
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	1	NAG	1	0
2	E	1	NAG	1	0
2	E	2	NAG	1	0

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

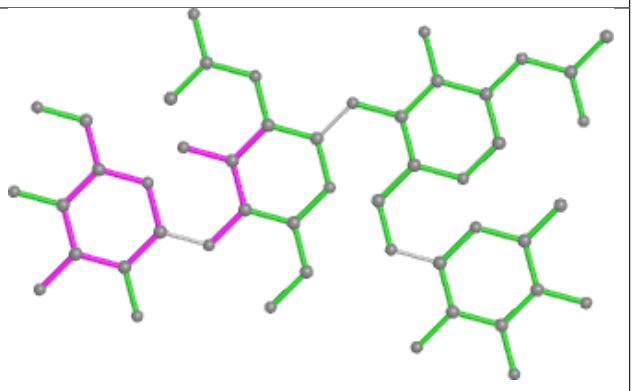
Oligosaccharide Chain E



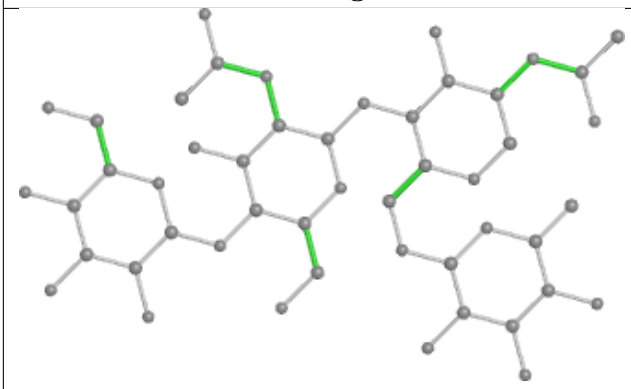
Oligosaccharide Chain F



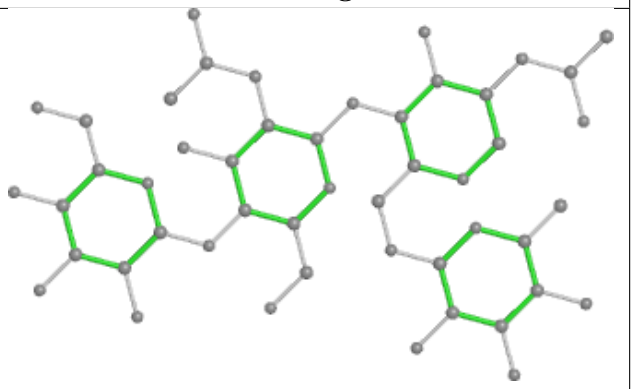
Bond lengths



Bond angles

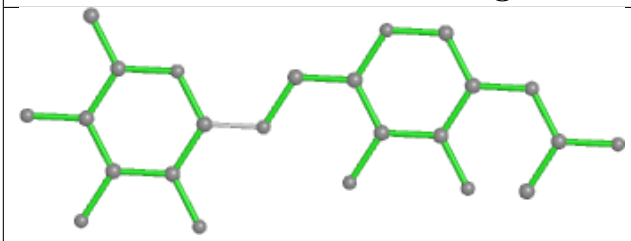


Torsions

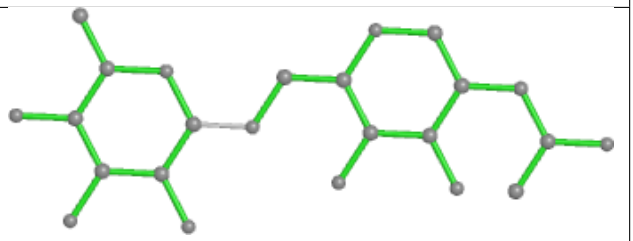


Rings

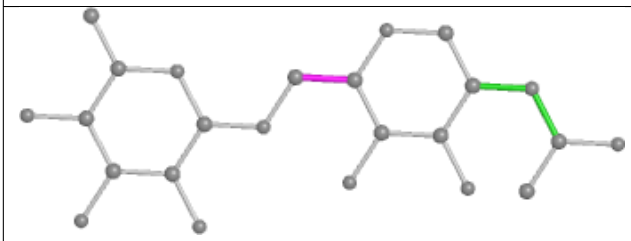
Oligosaccharide Chain G



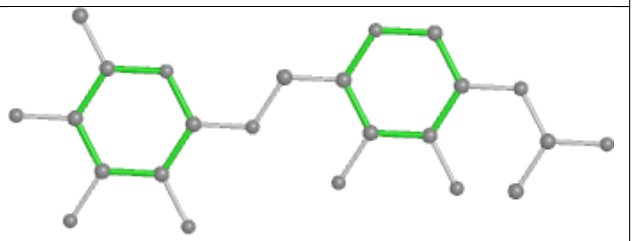
Bond lengths



Bond angles

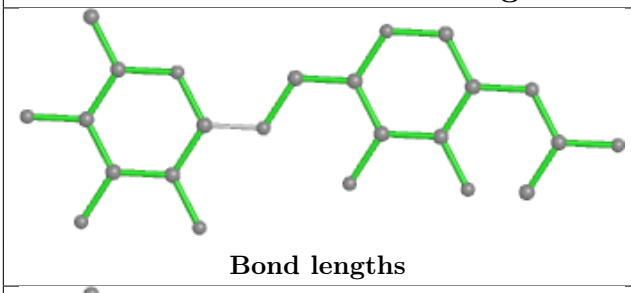


Torsions

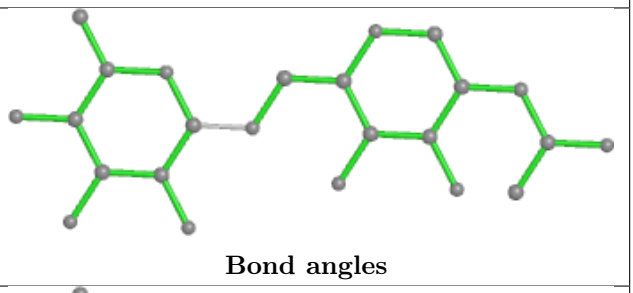


Rings

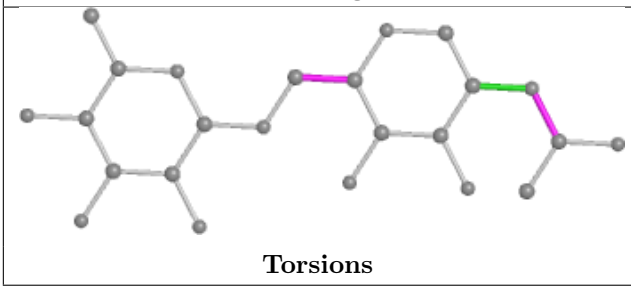
Oligosaccharide Chain I



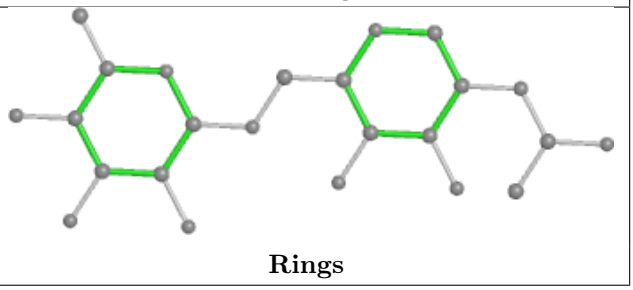
Bond lengths



Bond angles

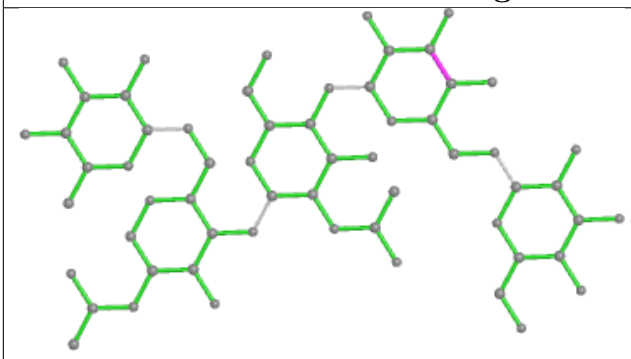


Torsions

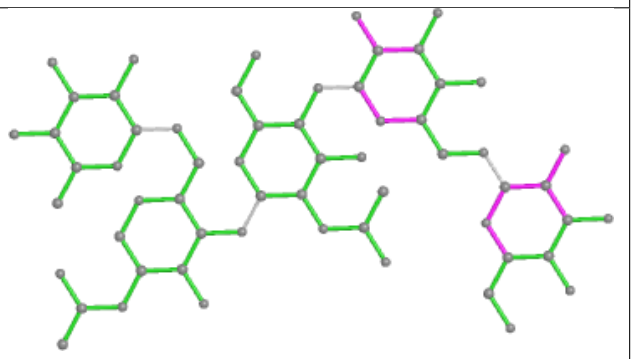


Rings

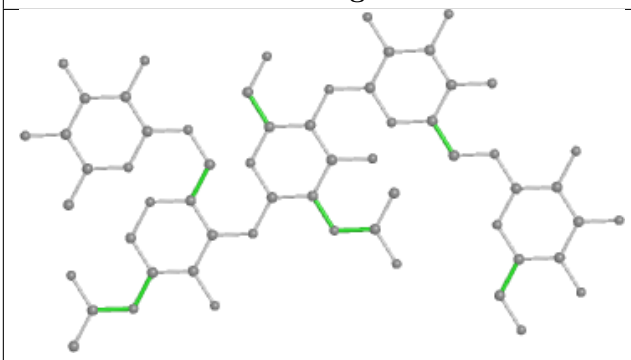
Oligosaccharide Chain H



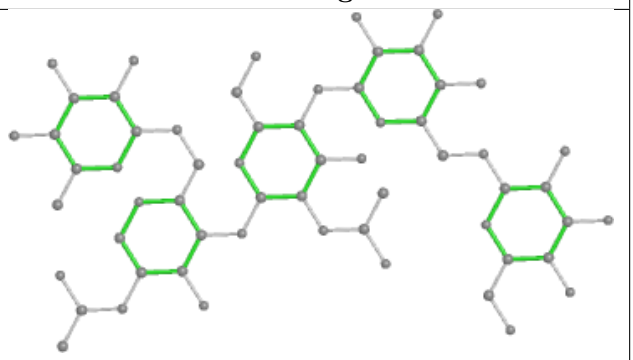
Bond lengths



Bond angles

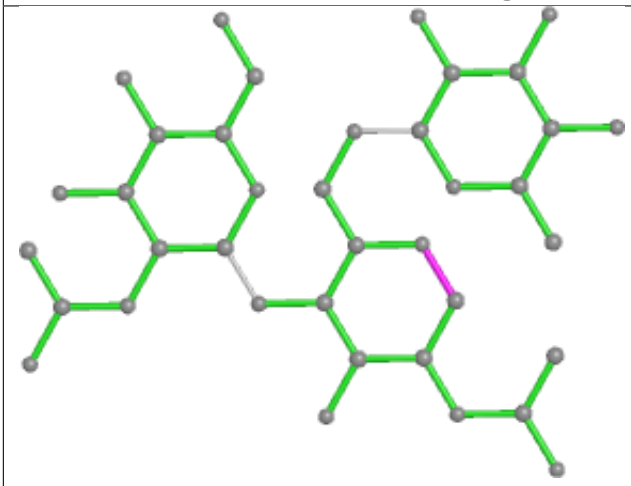


Torsions

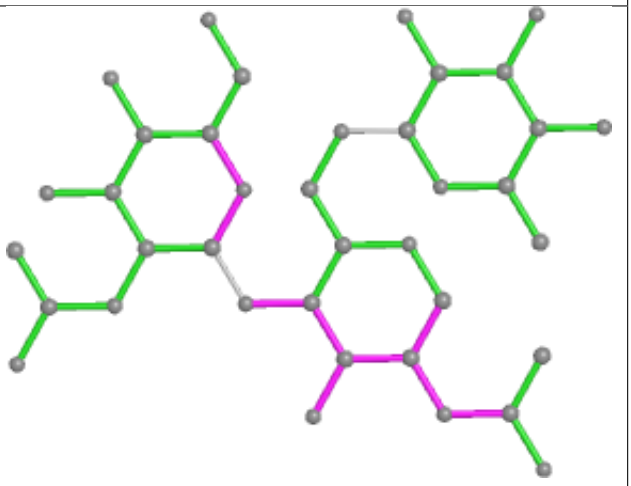


Rings

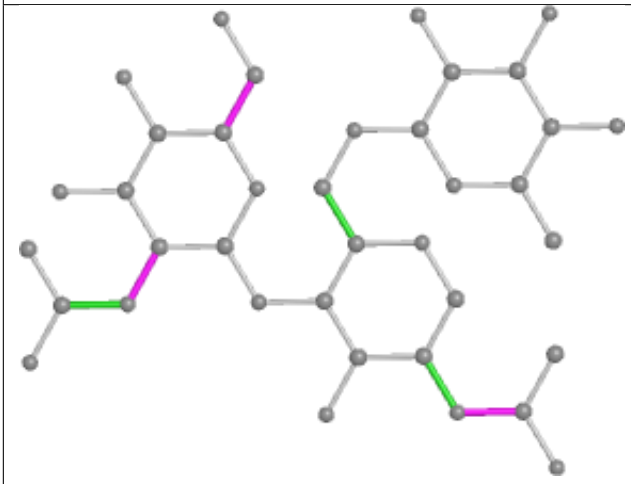
Oligosaccharide Chain J



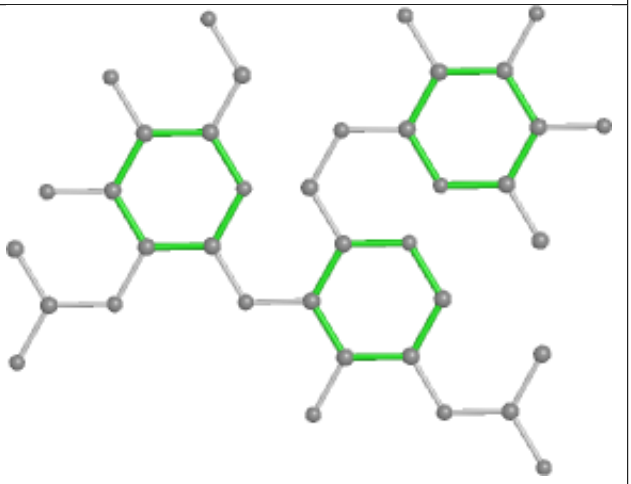
Bond lengths



Bond angles

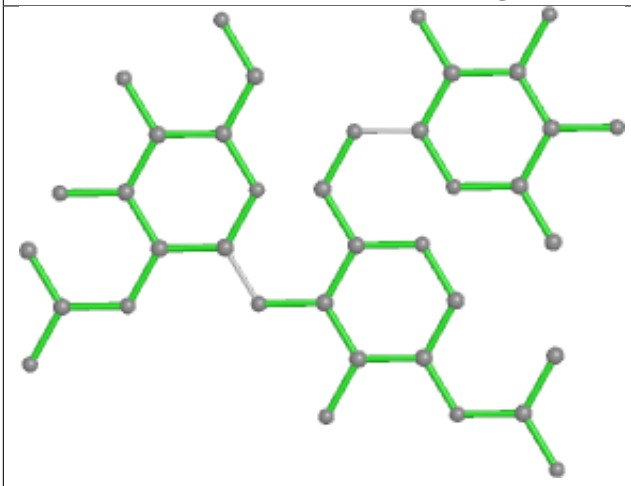


Torsions

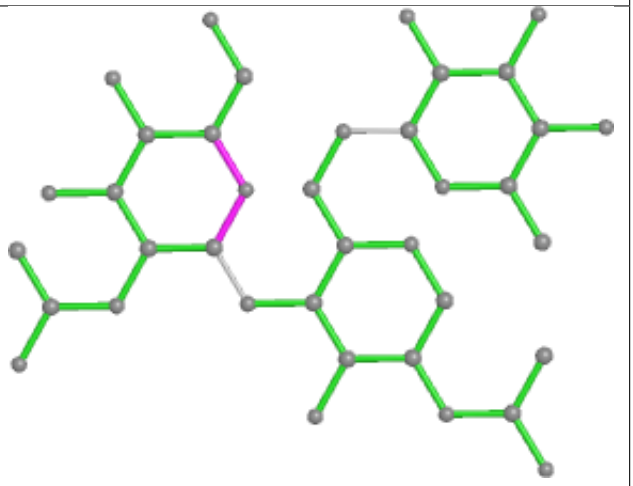


Rings

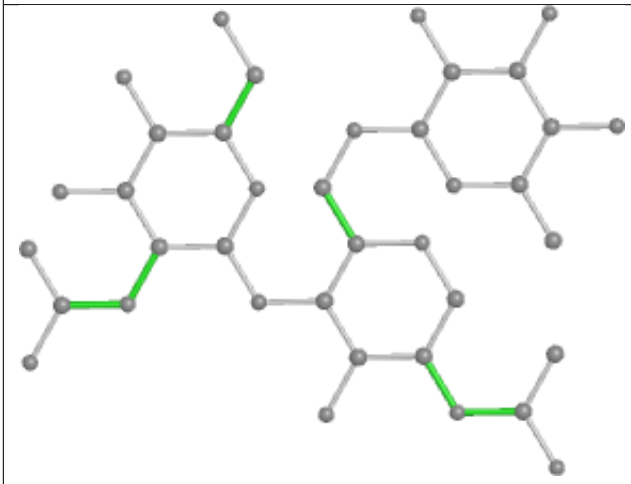
Oligosaccharide Chain K



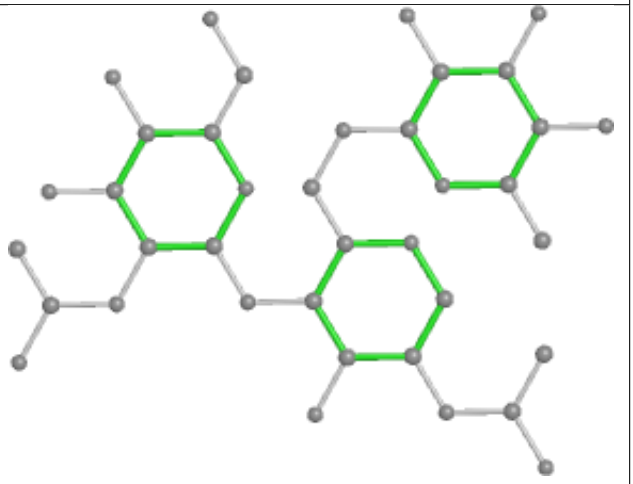
Bond lengths



Bond angles

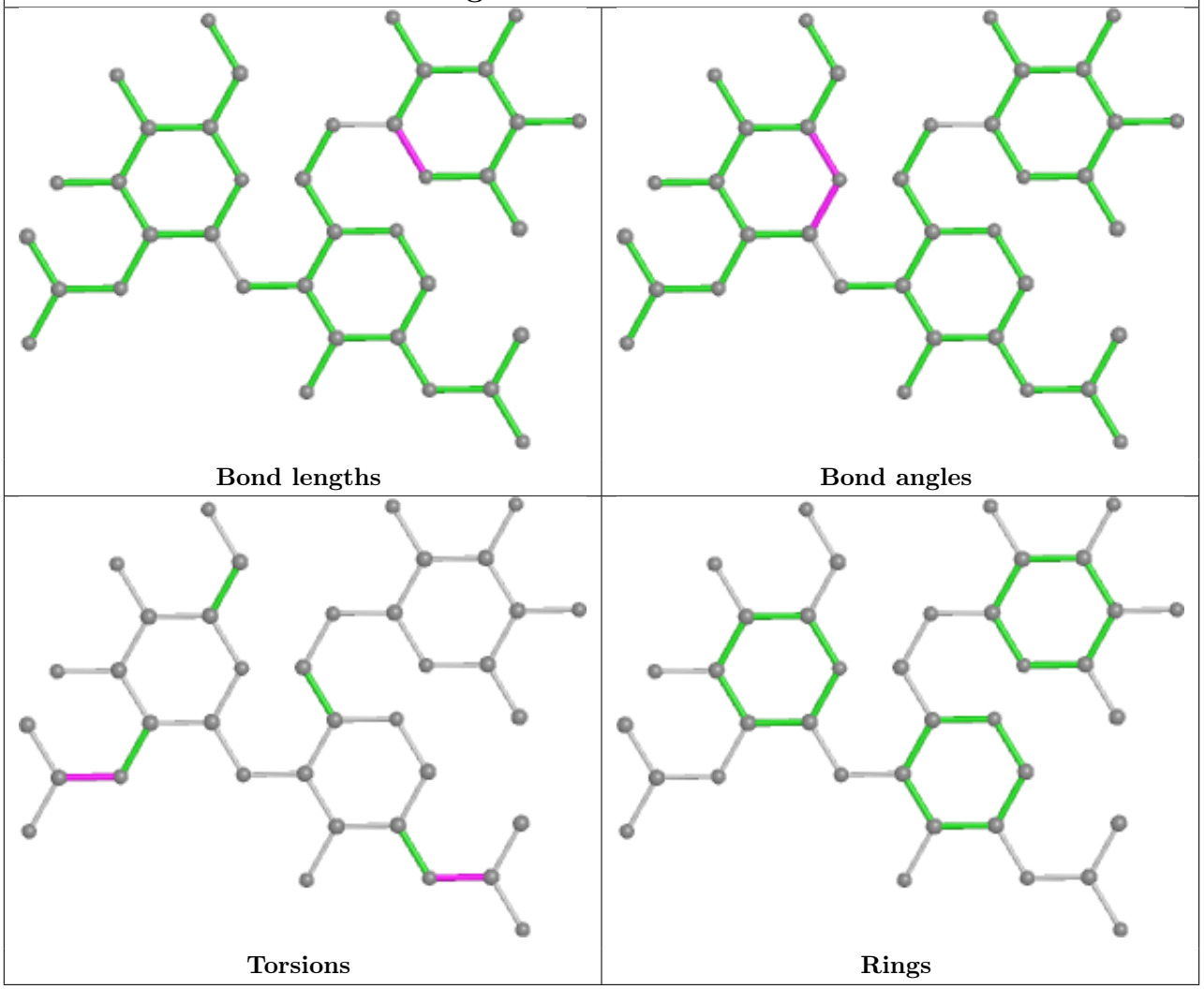


Torsions



Rings

Oligosaccharide Chain L



5.6 Ligand geometry (i)

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	GOL	C	302	-	5,5,5	1.66	1 (20%)	5,5,5	2.00	2 (40%)
10	PEG	C	304	-	6,6,6	0.19	0	5,5,5	0.19	0
7	MES	B	302	-	12,12,12	1.32	1 (8%)	14,16,16	1.93	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	MES	A	600	-	12,12,12	1.66	1 (8%)	14,16,16	1.78	4 (28%)
9	GOL	D	302	-	5,5,5	0.93	0	5,5,5	1.13	1 (20%)
11	EDO	D	303	-	3,3,3	0.54	0	2,2,2	0.71	0
8	NAG	B	301	1	14,14,15	0.67	1 (7%)	17,19,21	0.86	1 (5%)
9	GOL	C	303	-	5,5,5	1.06	0	5,5,5	1.17	0
8	NAG	C	301	1	14,14,15	0.57	0	17,19,21	1.38	2 (11%)
8	NAG	D	301	-	14,14,15	2.06	1 (7%)	17,19,21	1.38	1 (5%)
9	GOL	D	304	-	5,5,5	0.76	0	5,5,5	0.87	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GOL	C	302	-	-	2/4/4/4	-
10	PEG	C	304	-	-	1/4/4/4	-
7	MES	B	302	-	-	1/6/14/14	0/1/1/1
7	MES	A	600	-	-	2/6/14/14	0/1/1/1
9	GOL	D	302	-	-	2/4/4/4	-
11	EDO	D	303	-	-	0/1/1/1	-
8	NAG	B	301	1	-	0/6/23/26	0/1/1/1
9	GOL	C	303	-	-	2/4/4/4	-
8	NAG	C	301	1	-	3/6/23/26	0/1/1/1
8	NAG	D	301	-	-	4/6/23/26	0/1/1/1
9	GOL	D	304	-	-	2/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	301	NAG	O5-C1	7.29	1.55	1.43
7	A	600	MES	C8-S	-5.09	1.70	1.77
7	B	302	MES	C8-S	-4.02	1.71	1.77
8	B	301	NAG	O5-C1	-2.31	1.40	1.43
9	C	302	GOL	C3-C2	2.07	1.60	1.51

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	301	NAG	C2-N2-C7	4.20	128.88	122.90
7	B	302	MES	C7-N4-C3	4.06	121.62	111.23
7	A	600	MES	C7-N4-C3	4.05	121.59	111.23
8	D	301	NAG	C1-O5-C5	-3.69	107.19	112.19
7	B	302	MES	O1S-S-C8	3.18	110.75	106.92

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	600	MES	C8-C7-N4-C3
9	D	304	GOL	C1-C2-C3-O3
8	D	301	NAG	C4-C5-C6-O6
8	D	301	NAG	O5-C5-C6-O6
8	C	301	NAG	C8-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	302	GOL	1	0
10	C	304	PEG	2	0
11	D	303	EDO	2	0
8	C	301	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	211/248 (85%)	-0.02	3 (1%)	75	80	34, 44, 62, 78	0
1	B	210/248 (84%)	-0.08	2 (0%)	82	86	36, 44, 64, 83	0
1	C	208/248 (83%)	0.19	6 (2%)	51	59	35, 44, 63, 96	0
1	D	207/248 (83%)	0.20	11 (5%)	26	33	35, 50, 69, 101	0
All	All	836/992 (84%)	0.07	22 (2%)	56	63	34, 45, 65, 101	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	230	PRO	6.5
1	C	228	TYR	5.8
1	A	23	HIS	5.0
1	C	69	GLU	4.9
1	D	229	THR	4.5

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

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

6.3 Carbohydrates

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BMA	F	3	11/12	0.51	0.28	93,95,102,103	0
4	FUC	G	2	10/11	0.71	0.43	88,97,100,100	0

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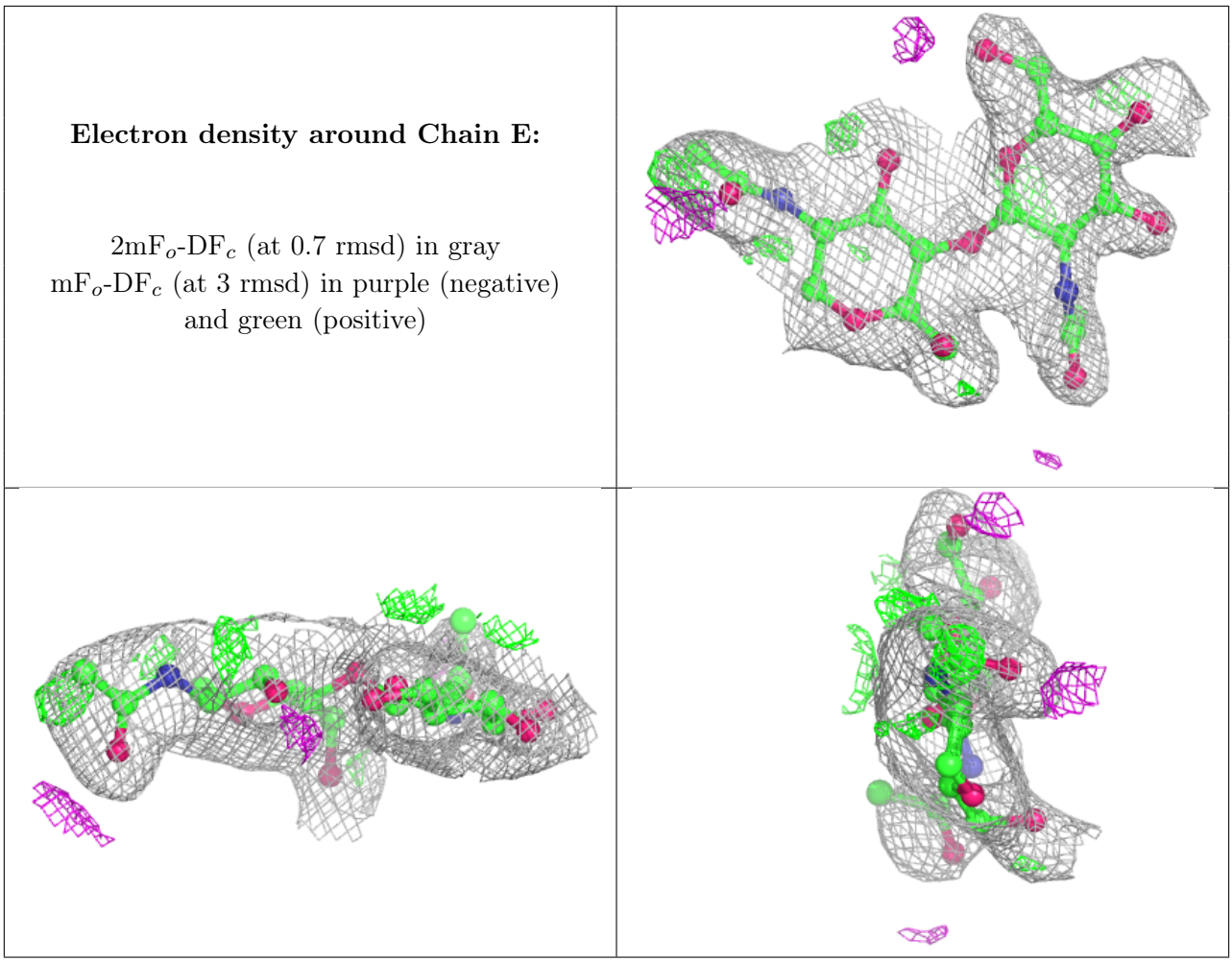
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	E	2	14/15	0.73	0.21	79,82,84,84	0
4	NAG	I	1	14/15	0.73	0.33	74,80,88,88	0
5	BMA	H	3	11/12	0.73	0.16	81,84,87,91	0
3	NAG	F	2	14/15	0.74	0.25	76,84,95,99	0
6	NAG	J	2	14/15	0.76	0.23	85,93,98,106	0
4	FUC	I	2	10/11	0.79	0.46	77,81,88,89	0
5	FUC	H	5	10/11	0.80	0.23	73,81,85,90	0
6	NAG	K	2	14/15	0.81	0.51	72,82,94,97	0
5	MAN	H	4	11/12	0.82	0.26	74,79,85,88	0
2	NAG	E	1	14/15	0.84	0.12	62,70,81,83	0
3	FUC	F	4	10/11	0.85	0.18	65,71,77,79	0
5	NAG	H	1	14/15	0.86	0.10	54,61,69,77	0
5	NAG	H	2	14/15	0.87	0.14	67,72,84,84	0
4	NAG	G	1	14/15	0.88	0.24	64,79,90,91	0
6	FUC	K	3	10/11	0.90	0.42	65,73,75,76	0
6	NAG	J	1	14/15	0.91	0.12	58,68,76,76	0
6	FUC	J	3	10/11	0.92	0.14	68,74,81,87	0
6	NAG	L	1	14/15	0.92	0.07	62,67,71,73	0
6	NAG	L	2	14/15	0.92	0.17	74,78,83,84	0
3	NAG	F	1	14/15	0.93	0.10	53,63,68,74	0
6	NAG	K	1	14/15	0.94	0.24	57,61,71,75	0
6	FUC	L	3	10/11	0.95	0.15	72,78,81,85	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.

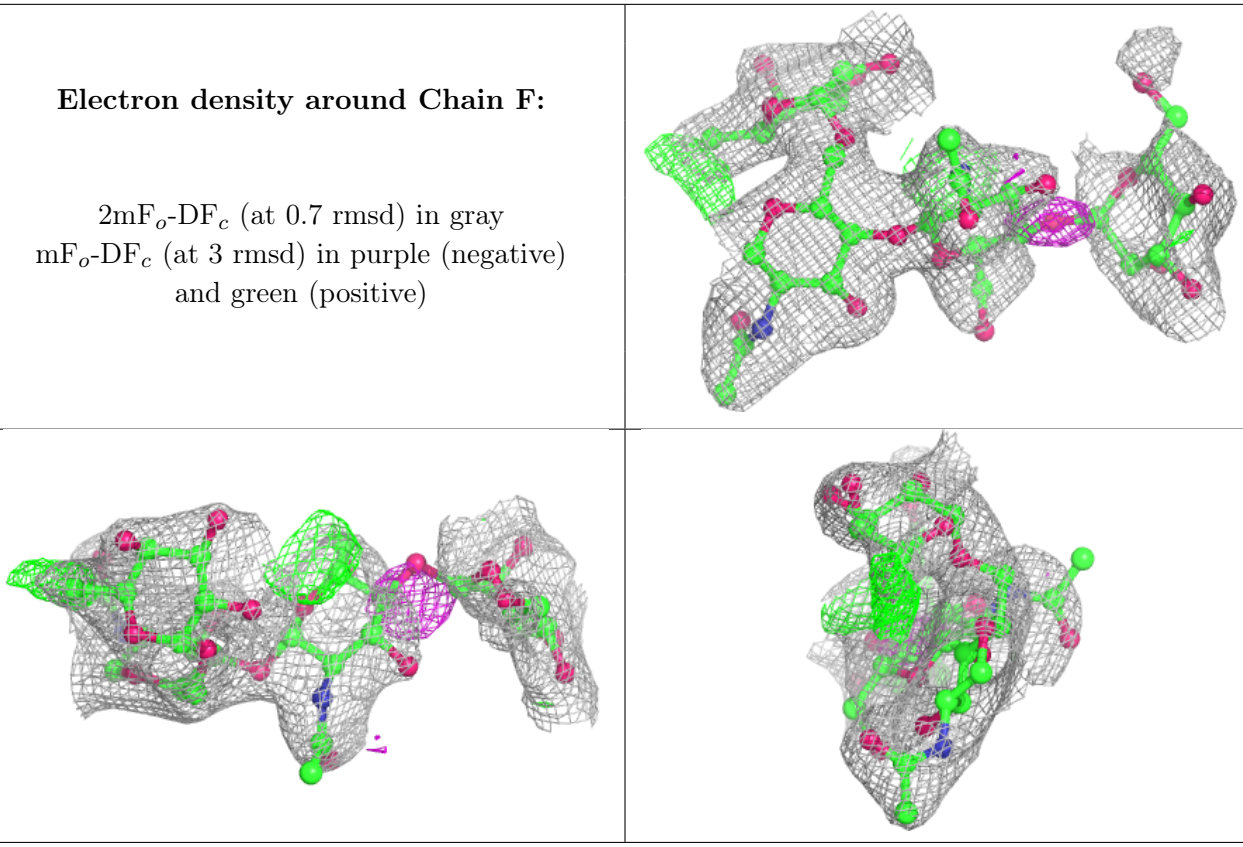
Electron density around Chain E:

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



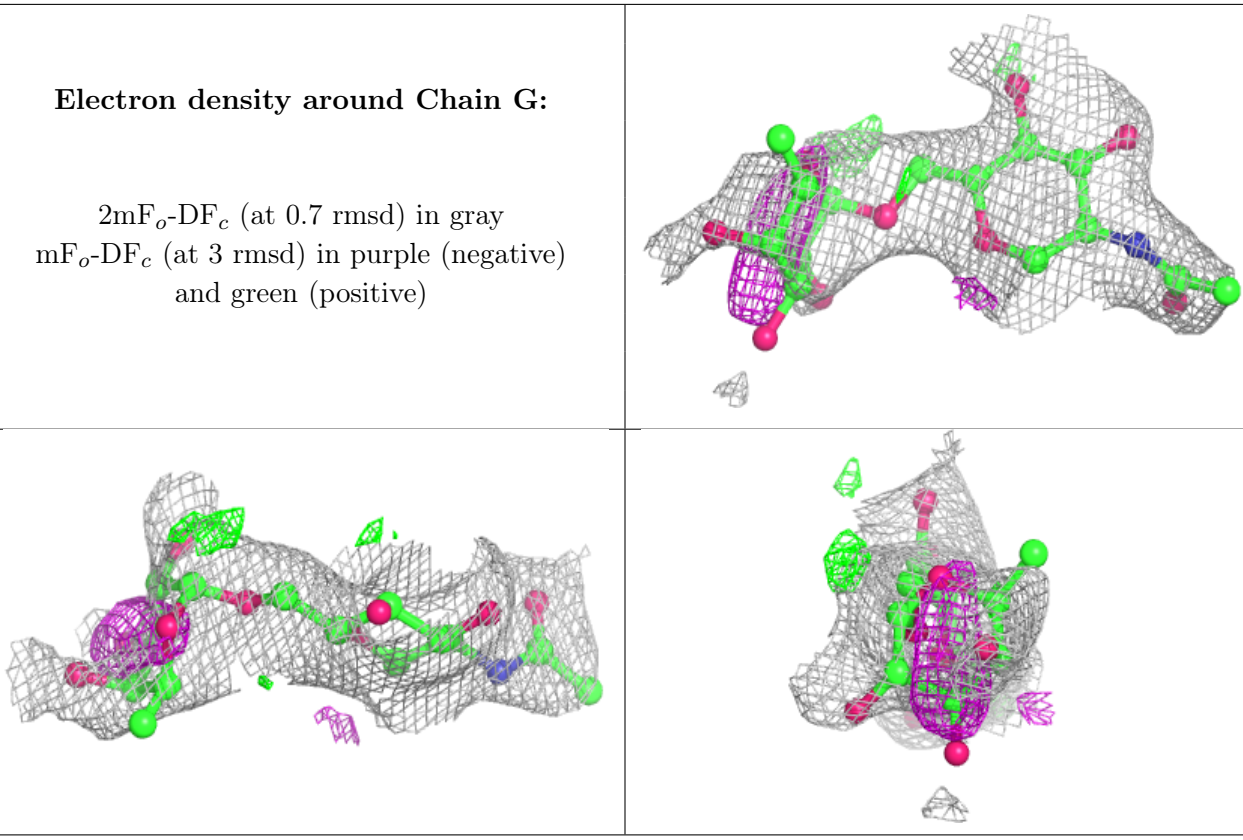
Electron density around Chain F:

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



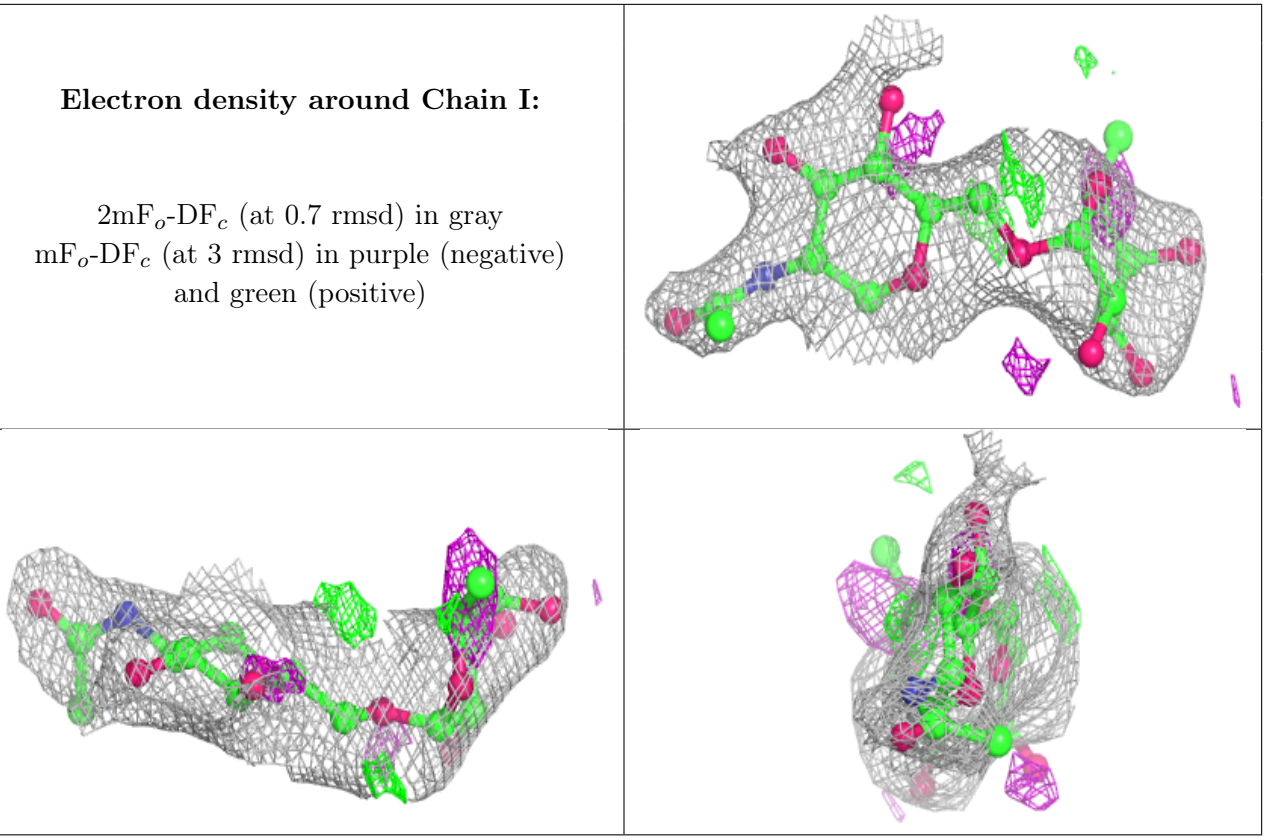
Electron density around Chain G:

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



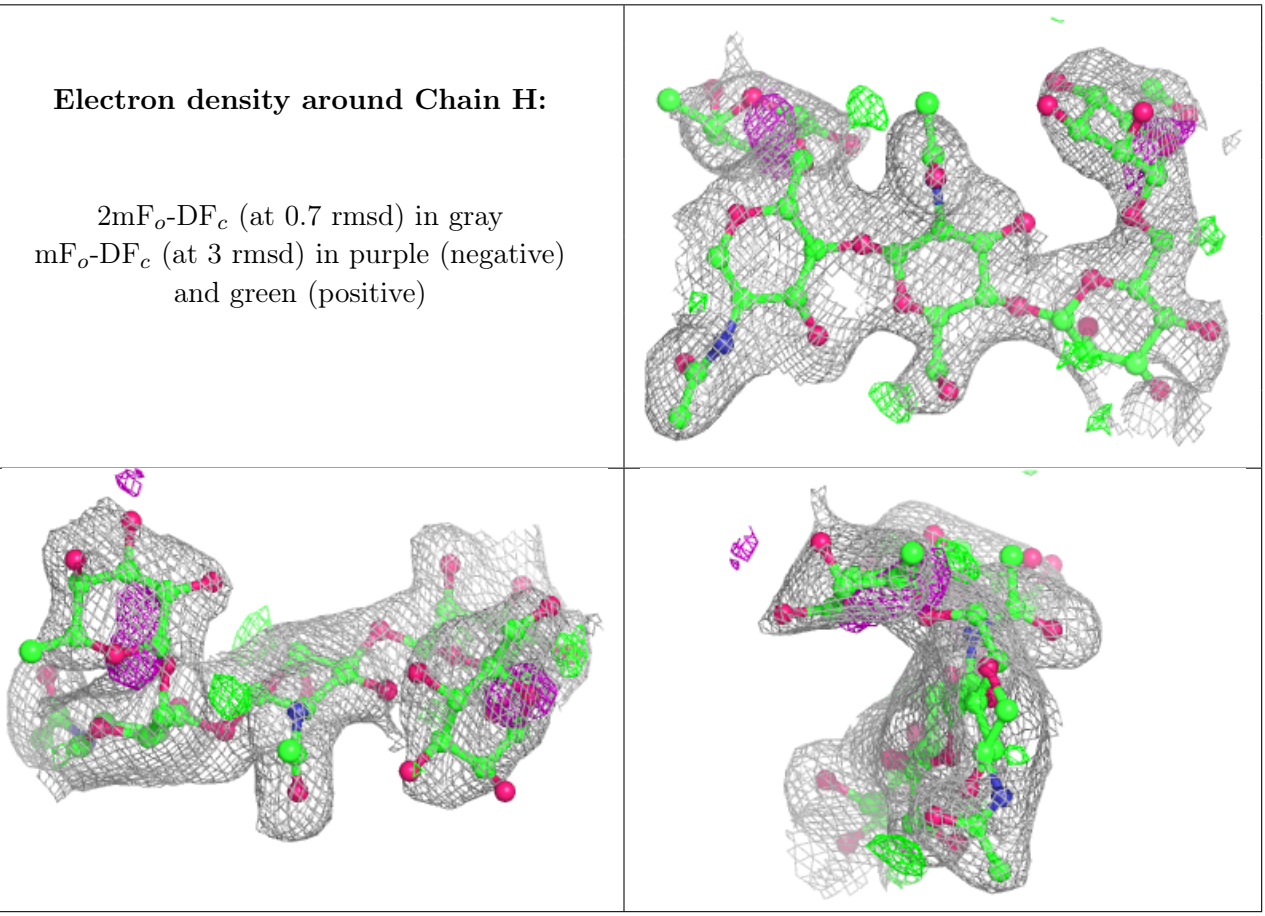
Electron density around Chain I:

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



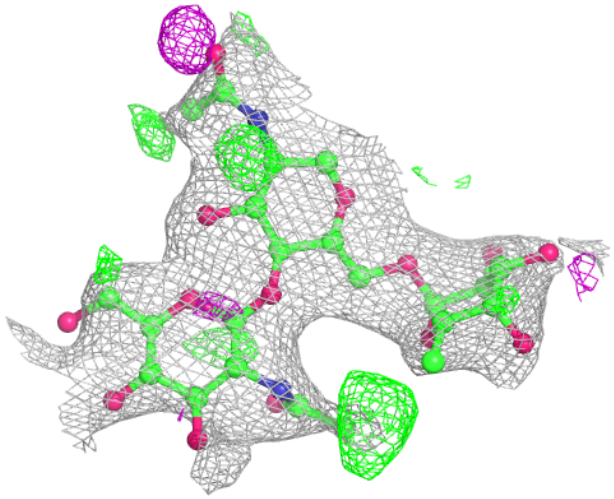
Electron density around Chain H:

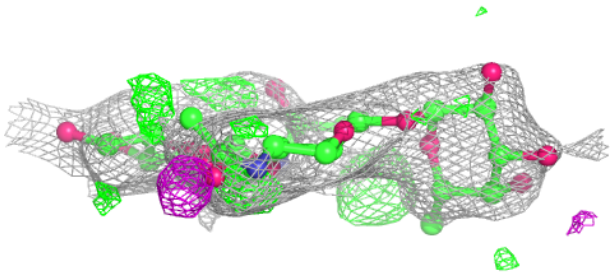
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

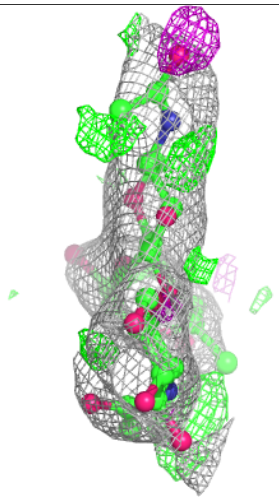


Electron density around Chain J:

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

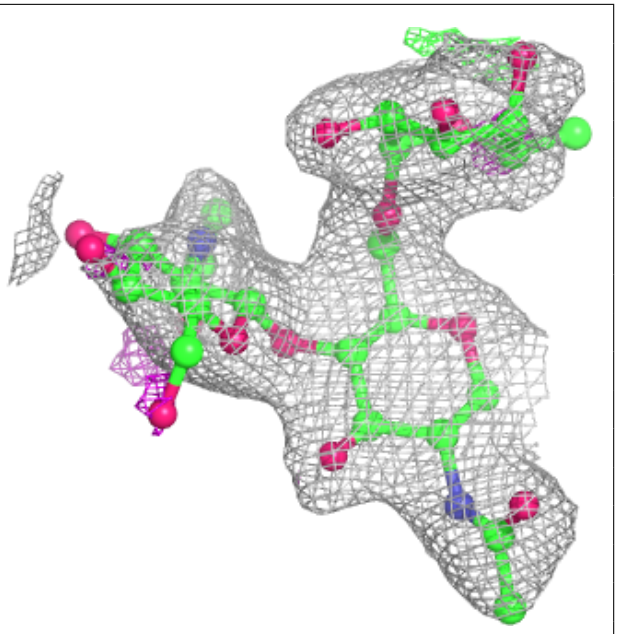


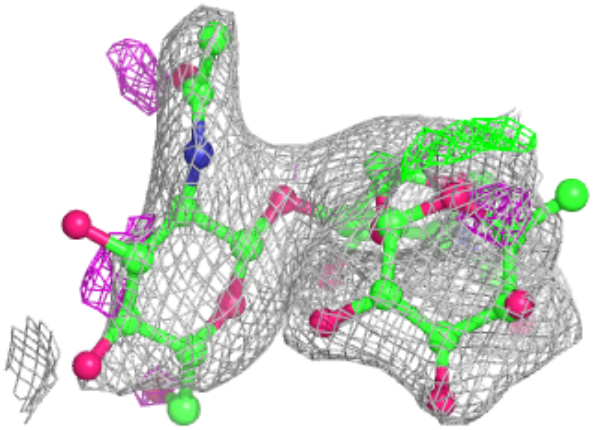


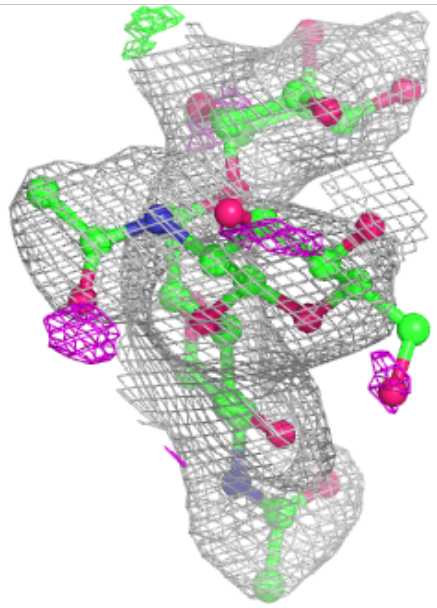


Electron density around Chain K:

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

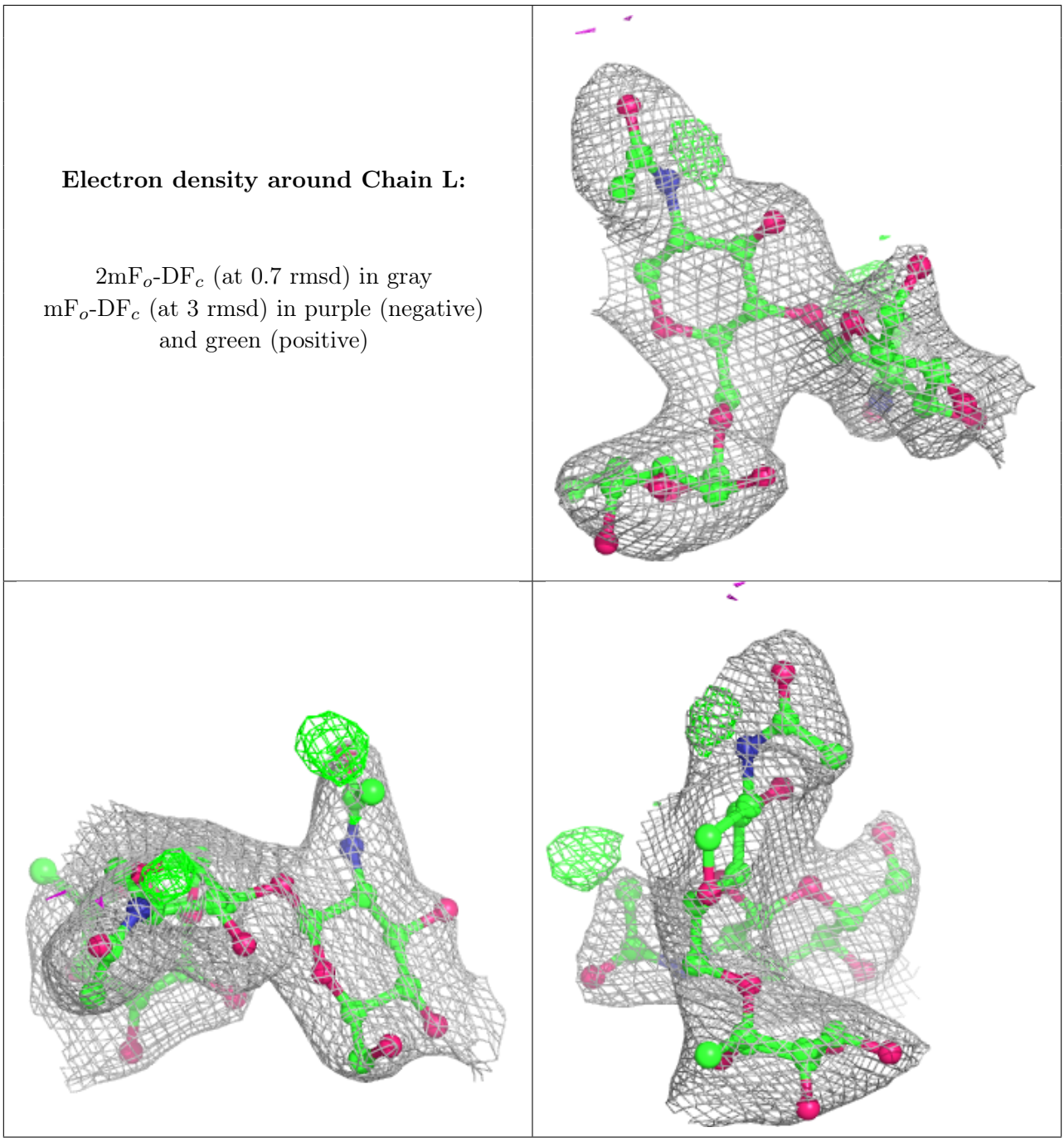






Electron density around Chain L:

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	NAG	D	301	14/15	0.57	0.36	85,91,97,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	EDO	D	303	4/4	0.68	0.13	59,71,85,85	0
8	NAG	C	301	14/15	0.79	0.14	72,78,83,88	0
10	PEG	C	304	7/7	0.81	0.14	42,56,62,69	0
8	NAG	B	301	14/15	0.82	0.16	66,74,83,83	0
9	GOL	C	303	6/6	0.88	0.22	55,66,72,79	0
9	GOL	C	302	6/6	0.89	0.11	39,48,54,60	0
7	MES	A	600	12/12	0.91	0.20	52,68,77,78	25
9	GOL	D	304	6/6	0.91	0.10	54,66,73,79	0
7	MES	B	302	12/12	0.92	0.27	46,67,75,78	25
9	GOL	D	302	6/6	0.94	0.12	45,56,63,69	0

6.5 Other polymers (i)

There are no such residues in this entry.