Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2023 – 09:50 am GMT

PDB ID	:	8PMS
Title	:	NADase from Aspergillus fumigatus with replaced C-terminus from Neurospora crassa
Authors	:	Kallio, J.P.; Ferrario, E.; Stromland, O.; Ziegler, M.
Deposited on	:	2023-06-29
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ 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 ⓘ) were used in the production of this report:

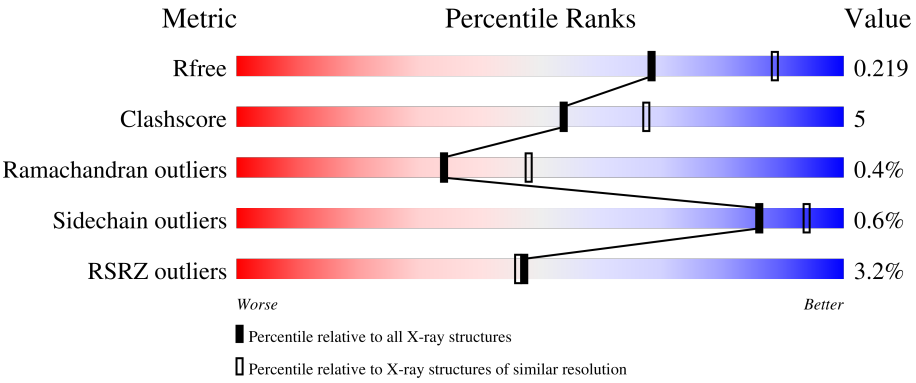
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	239	% 65% 13% 21%
1	B	239	69% 10% 21%
1	C	239	4% 71% 7% 21%
1	D	239	5% 70% 9% 21%
2	E	3	33% 67%

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Mol	Chain	Length	Quality of chain
3	F	5	20% 80%
4	G	2	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	301	-	-	-	X
8	AKR	A	305	-	X	-	-
8	AKR	A	306	-	X	-	-
8	AKR	C	303	-	X	-	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6528 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 Conidial surface nicotinamide adenine dinucleotide glycohydrolase nadA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	7	0
			1545	1003	250	285	7			
1	B	189	Total	C	N	O	S	0	9	0
			1563	1017	252	287	7			
1	C	188	Total	C	N	O	S	0	0	0
			1479	962	237	273	7			
1	D	189	Total	C	N	O	S	0	0	0
			1486	967	238	274	7			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	213	GLU	LEU	engineered mutation	UNP Q4WL81
A	215	PRO	GLU	engineered mutation	UNP Q4WL81
A	216	GLN	SER	engineered mutation	UNP Q4WL81
A	217	ARG	GLU	engineered mutation	UNP Q4WL81
A	218	LEU	TYR	engineered mutation	UNP Q4WL81
A	219	VAL	ASP	engineered mutation	UNP Q4WL81
A	220	PRO	GLU	engineered mutation	UNP Q4WL81
A	221	ARG	LYS	engineered mutation	UNP Q4WL81
A	222	ASN	VAL	engineered mutation	UNP Q4WL81
A	223	TYR	GLU	engineered mutation	UNP Q4WL81
A	224	GLY	-	expression tag	UNP Q4WL81
A	225	THR	-	expression tag	UNP Q4WL81
A	226	ASP	-	expression tag	UNP Q4WL81
A	227	VAL	-	expression tag	UNP Q4WL81
A	228	LEU	-	expression tag	UNP Q4WL81
A	229	PHE	-	expression tag	UNP Q4WL81
A	230	GLN	-	expression tag	UNP Q4WL81
A	231	GLY	-	expression tag	UNP Q4WL81
A	232	PRO	-	expression tag	UNP Q4WL81
A	233	GLY	-	expression tag	UNP Q4WL81

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Chain	Residue	Modelled	Actual	Comment	Reference
A	234	HIS	-	expression tag	UNP Q4WL81
A	235	HIS	-	expression tag	UNP Q4WL81
A	236	HIS	-	expression tag	UNP Q4WL81
A	237	HIS	-	expression tag	UNP Q4WL81
A	238	HIS	-	expression tag	UNP Q4WL81
A	239	HIS	-	expression tag	UNP Q4WL81
B	213	GLU	LEU	engineered mutation	UNP Q4WL81
B	215	PRO	GLU	engineered mutation	UNP Q4WL81
B	216	GLN	SER	engineered mutation	UNP Q4WL81
B	217	ARG	GLU	engineered mutation	UNP Q4WL81
B	218	LEU	TYR	engineered mutation	UNP Q4WL81
B	219	VAL	ASP	engineered mutation	UNP Q4WL81
B	220	PRO	GLU	engineered mutation	UNP Q4WL81
B	221	ARG	LYS	engineered mutation	UNP Q4WL81
B	222	ASN	VAL	engineered mutation	UNP Q4WL81
B	223	TYR	GLU	engineered mutation	UNP Q4WL81
B	224	GLY	-	expression tag	UNP Q4WL81
B	225	THR	-	expression tag	UNP Q4WL81
B	226	ASP	-	expression tag	UNP Q4WL81
B	227	VAL	-	expression tag	UNP Q4WL81
B	228	LEU	-	expression tag	UNP Q4WL81
B	229	PHE	-	expression tag	UNP Q4WL81
B	230	GLN	-	expression tag	UNP Q4WL81
B	231	GLY	-	expression tag	UNP Q4WL81
B	232	PRO	-	expression tag	UNP Q4WL81
B	233	GLY	-	expression tag	UNP Q4WL81
B	234	HIS	-	expression tag	UNP Q4WL81
B	235	HIS	-	expression tag	UNP Q4WL81
B	236	HIS	-	expression tag	UNP Q4WL81
B	237	HIS	-	expression tag	UNP Q4WL81
B	238	HIS	-	expression tag	UNP Q4WL81
B	239	HIS	-	expression tag	UNP Q4WL81
C	213	GLU	LEU	engineered mutation	UNP Q4WL81
C	215	PRO	GLU	engineered mutation	UNP Q4WL81
C	216	GLN	SER	engineered mutation	UNP Q4WL81
C	217	ARG	GLU	engineered mutation	UNP Q4WL81
C	218	LEU	TYR	engineered mutation	UNP Q4WL81
C	219	VAL	ASP	engineered mutation	UNP Q4WL81
C	220	PRO	GLU	engineered mutation	UNP Q4WL81
C	221	ARG	LYS	engineered mutation	UNP Q4WL81
C	222	ASN	VAL	engineered mutation	UNP Q4WL81
C	223	TYR	GLU	engineered mutation	UNP Q4WL81

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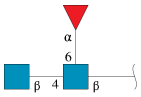
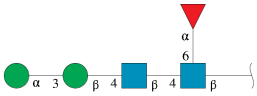
Chain	Residue	Modelled	Actual	Comment	Reference
C	224	GLY	-	expression tag	UNP Q4WL81
C	225	THR	-	expression tag	UNP Q4WL81
C	226	ASP	-	expression tag	UNP Q4WL81
C	227	VAL	-	expression tag	UNP Q4WL81
C	228	LEU	-	expression tag	UNP Q4WL81
C	229	PHE	-	expression tag	UNP Q4WL81
C	230	GLN	-	expression tag	UNP Q4WL81
C	231	GLY	-	expression tag	UNP Q4WL81
C	232	PRO	-	expression tag	UNP Q4WL81
C	233	GLY	-	expression tag	UNP Q4WL81
C	234	HIS	-	expression tag	UNP Q4WL81
C	235	HIS	-	expression tag	UNP Q4WL81
C	236	HIS	-	expression tag	UNP Q4WL81
C	237	HIS	-	expression tag	UNP Q4WL81
C	238	HIS	-	expression tag	UNP Q4WL81
C	239	HIS	-	expression tag	UNP Q4WL81
D	213	GLU	LEU	engineered mutation	UNP Q4WL81
D	215	PRO	GLU	engineered mutation	UNP Q4WL81
D	216	GLN	SER	engineered mutation	UNP Q4WL81
D	217	ARG	GLU	engineered mutation	UNP Q4WL81
D	218	LEU	TYR	engineered mutation	UNP Q4WL81
D	219	VAL	ASP	engineered mutation	UNP Q4WL81
D	220	PRO	GLU	engineered mutation	UNP Q4WL81
D	221	ARG	LYS	engineered mutation	UNP Q4WL81
D	222	ASN	VAL	engineered mutation	UNP Q4WL81
D	223	TYR	GLU	engineered mutation	UNP Q4WL81
D	224	GLY	-	expression tag	UNP Q4WL81
D	225	THR	-	expression tag	UNP Q4WL81
D	226	ASP	-	expression tag	UNP Q4WL81
D	227	VAL	-	expression tag	UNP Q4WL81
D	228	LEU	-	expression tag	UNP Q4WL81
D	229	PHE	-	expression tag	UNP Q4WL81
D	230	GLN	-	expression tag	UNP Q4WL81
D	231	GLY	-	expression tag	UNP Q4WL81
D	232	PRO	-	expression tag	UNP Q4WL81
D	233	GLY	-	expression tag	UNP Q4WL81
D	234	HIS	-	expression tag	UNP Q4WL81
D	235	HIS	-	expression tag	UNP Q4WL81
D	236	HIS	-	expression tag	UNP Q4WL81
D	237	HIS	-	expression tag	UNP Q4WL81
D	238	HIS	-	expression tag	UNP Q4WL81
D	239	HIS	-	expression tag	UNP Q4WL81

- Molecule 2 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
2	E	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 3 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.

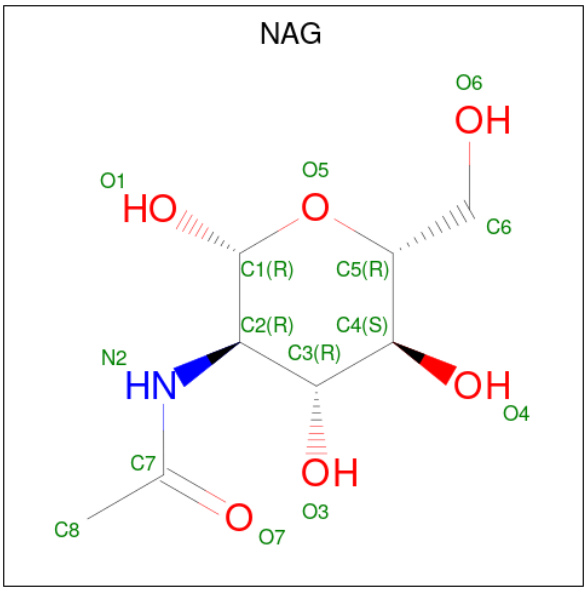


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	5	Total	C	N	O	0	0	0
			60	34	2	24			

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

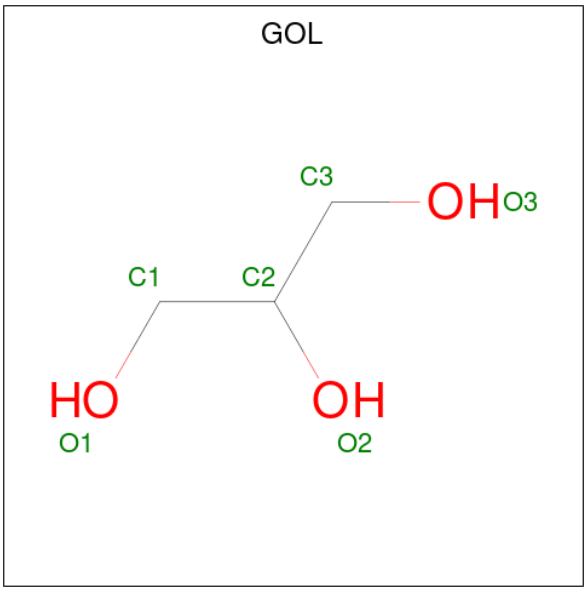
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



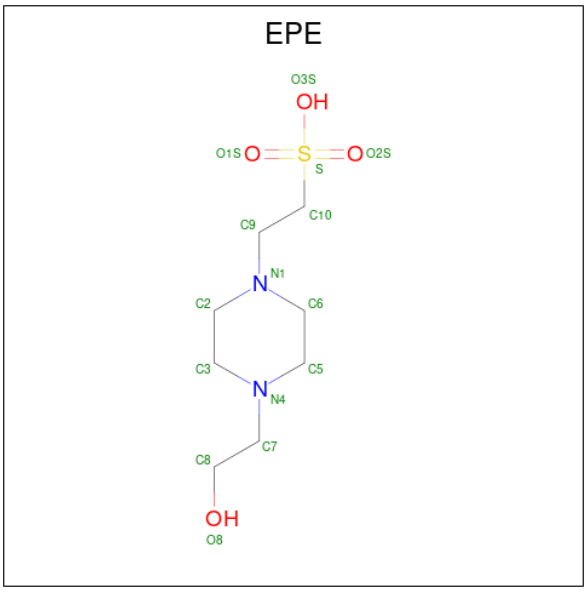
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	C	1	Total C N O 14 8 1 5	0	0
5	D	1	Total C N O 14 8 1 5	0	0
5	D	1	Total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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



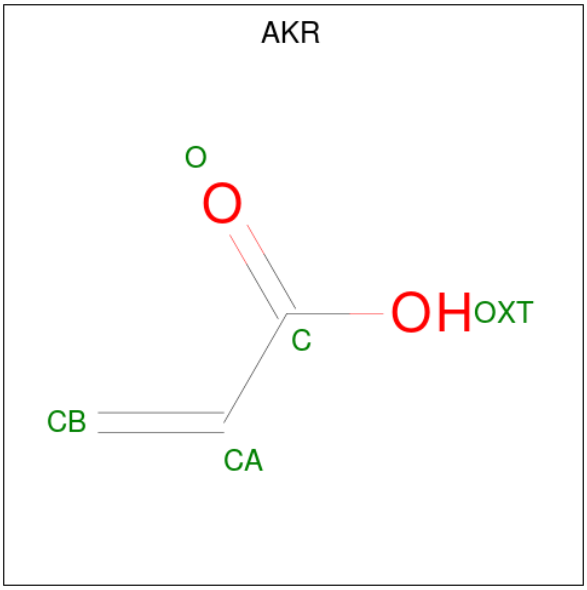
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O S 15 8 2 4 1	0	0
7	B	1	Total C N O S 15 8 2 4 1	0	0

- Molecule 8 is ACRYLIC ACID (three-letter code: AKR) (formula: $C_3H_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 5 3 2	0	0
8	A	1	Total C O 5 3 2	0	0
8	B	1	Total C O 5 3 2	0	0
8	C	1	Total C O 5 3 2	0	0

- Molecule 9 is water.

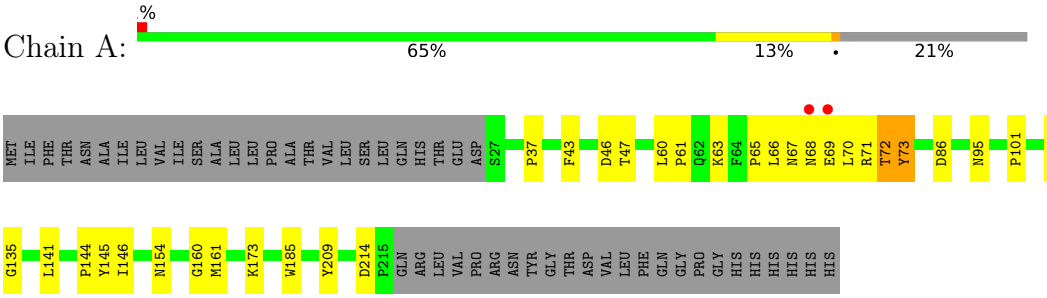
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	51	Total O 52 52	0	1
9	B	63	Total O 63 63	0	0
9	C	7	Total O 7 7	0	0
9	D	13	Total O 13 13	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

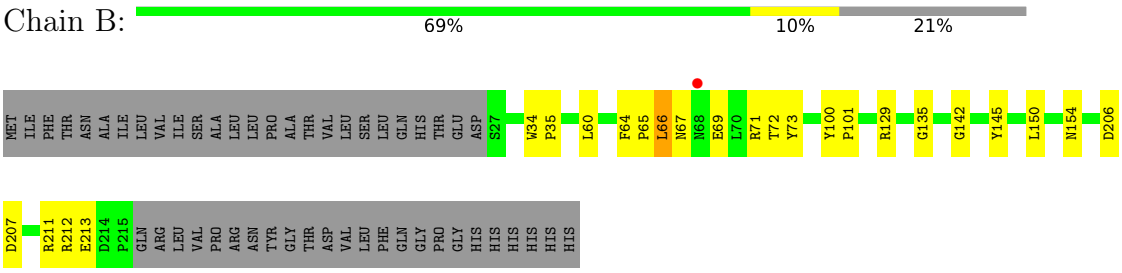
• Molecule 1: Conidial surface nicotinamide adenine dinucleotide glycohydrolase nadA

Chain A:



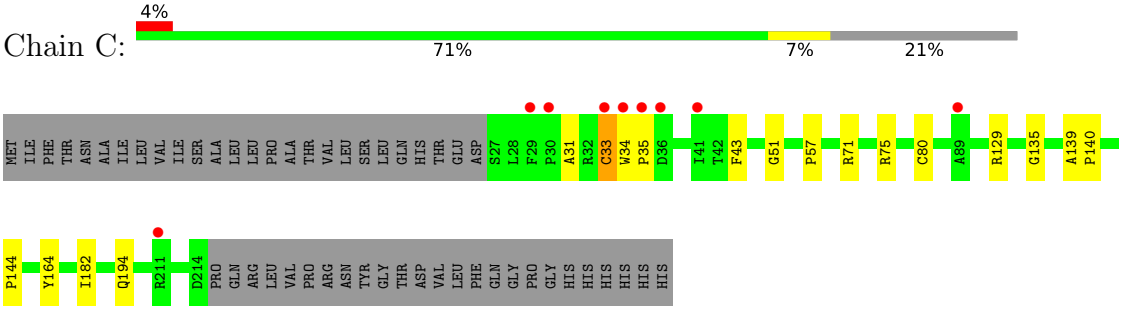
• Molecule 1: Conidial surface nicotinamide adenine dinucleotide glycohydrolase nadA

Chain B:



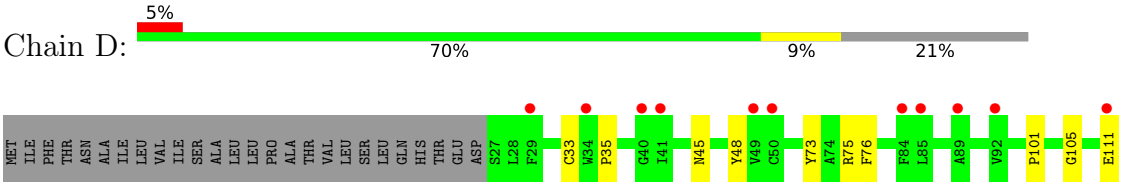
• Molecule 1: Conidial surface nicotinamide adenine dinucleotide glycohydrolase nadA

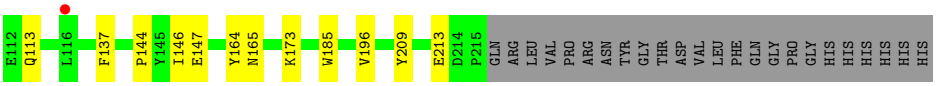
Chain C:



• Molecule 1: Conidial surface nicotinamide adenine dinucleotide glycohydrolase nadA

Chain D:



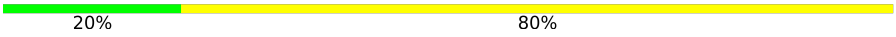


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

• Molecule 3: 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 F:



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

Chain G:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	101.02Å 101.02Å 366.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.67 – 2.40 48.69 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.67-2.40) 99.8 (48.69-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.204 , 0.224 0.197 , 0.219	Depositor DCC
R_{free} test set	3633 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	72.5	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 59.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6528	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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: EPE, AKR, NAG, BMA, FUC, GOL, 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	0.49	0/1598	0.86	4/2191 (0.2%)
1	B	0.50	0/1618	0.86	1/2219 (0.0%)
1	C	0.44	1/1530 (0.1%)	0.78	3/2098 (0.1%)
1	D	0.44	0/1538	0.79	0/2110
All	All	0.47	1/6284 (0.0%)	0.83	8/8618 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	33	CYS	CB-SG	-5.55	1.72	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	86	ASP	CB-CG-OD2	-8.01	111.09	118.30
1	A	86	ASP	CB-CG-OD1	6.50	124.15	118.30
1	C	33	CYS	CA-CB-SG	-6.34	102.59	114.00
1	B	73	TYR	CB-CG-CD2	-6.24	117.26	121.00
1	A	73	TYR	CB-CG-CD2	-5.24	117.85	121.00
1	C	80	CYS	CA-CB-SG	-5.24	104.56	114.00
1	A	73	TYR	CB-CG-CD1	5.17	124.10	121.00
1	C	164	TYR	CA-CB-CG	5.06	123.01	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1545	0	1470	26	0
1	B	1563	0	1486	16	0
1	C	1479	0	1405	12	0
1	D	1486	0	1412	12	0
2	E	38	0	34	1	0
3	F	60	0	52	0	0
4	G	28	0	25	0	0
5	A	28	0	26	2	0
5	B	28	0	26	0	0
5	C	42	0	39	1	0
5	D	28	0	26	1	0
6	A	6	0	8	0	0
6	B	12	0	16	0	0
7	A	15	0	17	2	0
7	B	15	0	17	2	0
8	A	10	0	6	0	0
8	B	5	0	3	0	0
8	C	5	0	3	0	0
9	A	52	0	0	1	0
9	B	63	0	0	1	0
9	C	7	0	0	0	0
9	D	13	0	0	1	0
All	All	6528	0	6071	66	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.

All (66) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67[B]:ASN:HB2	1:B:72:THR:HA	1.68	0.74
1:D:165:ASN:OD1	9:D:401:HOH:O	2.06	0.72
7:B:305:EPE:H32	9:B:410:HOH:O	1.92	0.69
1:C:33:CYS:C	1:C:35:PRO:HD2	2.15	0.67
1:D:73:TYR:HD1	1:D:146:ILE:HG22	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:ALA:HA	1:C:34:TRP:CD1	2.34	0.62
1:A:71[B]:ARG:O	1:A:72:THR:OG1	2.13	0.62
1:D:75:ARG:HD2	1:D:76:PHE:CZ	2.34	0.62
5:D:301:NAG:H3	5:D:301:NAG:H83	1.84	0.60
1:A:60:LEU:HD13	1:A:66[B]:LEU:CD1	2.33	0.58
1:A:68[B]:ASN:HD22	1:A:144:PRO:HG3	1.68	0.58
1:D:111:GLU:HG2	1:D:113:GLN:HG2	1.86	0.57
1:C:57:PRO:O	1:C:75:ARG:NH1	2.33	0.57
7:A:304:EPE:H52	9:A:414:HOH:O	2.07	0.54
1:D:101:PRO:HB3	1:D:185:TRP:CE3	2.42	0.53
1:A:68[B]:ASN:HB3	1:A:144:PRO:HB3	1.89	0.53
1:A:65[B]:PRO:O	1:A:67[B]:ASN:N	2.42	0.53
1:A:129:ARG:NH2	1:A:135:GLY:HA3	2.24	0.53
1:D:173:LYS:HD3	1:D:209:TYR:CE1	2.45	0.52
1:A:173:LYS:HD2	1:A:209:TYR:CE1	2.45	0.52
1:A:73:TYR:HD1	1:A:146:ILE:HG22	1.75	0.52
1:A:63:LYS:HB2	1:A:161:MET:O	2.10	0.51
1:C:71:ARG:HH22	1:C:144:PRO:HG2	1.75	0.51
5:C:304:NAG:H83	5:C:304:NAG:H3	1.92	0.51
1:C:31:ALA:HA	1:C:34:TRP:NE1	2.26	0.50
1:B:129:ARG:NH2	1:B:135:GLY:HA3	2.25	0.50
1:D:101:PRO:HB3	1:D:185:TRP:CD2	2.47	0.49
1:A:70[B]:LEU:H	1:B:142:GLY:HA3	1.77	0.49
1:A:61:PRO:HA	1:A:160:GLY:O	2.12	0.48
1:A:144:PRO:HA	1:B:69[A]:GLU:HG3	1.94	0.48
1:B:206:ASP:OD2	1:D:164:TYR:HE1	1.96	0.48
1:C:139:ALA:HB1	1:C:140:PRO:HD2	1.94	0.48
1:A:69[B]:GLU:HG3	1:A:146:ILE:HD11	1.96	0.47
1:D:137:PHE:CE2	1:D:196:VAL:HG12	2.49	0.47
1:A:73:TYR:CD1	1:A:146:ILE:HG22	2.49	0.47
1:A:37:PRO:HD2	7:A:304:EPE:H52	1.97	0.47
1:A:47:THR:OG1	5:A:301:NAG:H83	2.15	0.47
1:A:141:LEU:O	1:B:71[A]:ARG:HD2	2.14	0.47
1:C:129:ARG:NH2	1:C:135:GLY:HA3	2.30	0.46
1:A:95:ASN:N	1:A:95:ASN:OD1	2.48	0.45
5:A:301:NAG:O3	5:A:301:NAG:H82	2.17	0.44
1:B:211:ARG:HG2	1:B:212:ARG:N	2.32	0.44
1:C:33:CYS:O	1:C:35:PRO:HD2	2.16	0.44
1:C:182:ILE:HG12	1:C:194:GLN:HB3	1.98	0.44
1:A:43:PHE:HZ	1:A:46:ASP:HB3	1.83	0.44
1:A:144:PRO:HA	1:B:69[A]:GLU:CG	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:PHE:CD1	1:C:51:GLY:HA3	2.54	0.43
1:C:31:ALA:O	1:C:34:TRP:HD1	2.02	0.43
1:B:211:ARG:NH1	1:B:213:GLU:OE2	2.46	0.43
1:C:71:ARG:NH2	1:C:144:PRO:HG2	2.33	0.43
1:B:100:TYR:HB3	1:B:101:PRO:HD2	2.01	0.43
1:B:145:TYR:OH	1:B:154:ASN:HB2	2.19	0.43
1:B:34:TRP:HB3	1:B:35:PRO:HA	2.01	0.42
1:B:60:LEU:HD13	1:B:66[A]:LEU:HD11	2.02	0.42
1:D:101:PRO:HG2	1:D:105:GLY:HA2	2.02	0.42
1:A:68[A]:ASN:CG	1:B:65[A]:PRO:HB3	2.40	0.42
1:A:72:THR:HG22	1:A:73:TYR:N	2.34	0.42
7:B:305:EPE:H101	7:B:305:EPE:H21	1.77	0.42
1:A:67[B]:ASN:HB3	1:A:72:THR:HA	2.00	0.42
1:B:150:LEU:HB3	1:B:154:ASN:HD22	1.85	0.42
1:D:45:ASN:HB3	1:D:48:TYR:CD2	2.55	0.42
1:B:64[A]:PHE:CG	1:B:65[A]:PRO:HD2	2.56	0.41
1:A:101:PRO:HB3	1:A:185:TRP:CD2	2.56	0.41
1:A:145:TYR:OH	1:A:154:ASN:HB2	2.21	0.41
1:A:118:ASN:HD22	2:E:1:NAG:H83	1.85	0.40
1:D:144:PRO:O	1:D:147:GLU:HG2	2.22	0.40

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	194/239 (81%)	185 (95%)	8 (4%)	1 (0%)	29	41
1	B	196/239 (82%)	186 (95%)	8 (4%)	2 (1%)	15	23
1	C	186/239 (78%)	182 (98%)	4 (2%)	0	100	100
1	D	187/239 (78%)	181 (97%)	5 (3%)	1 (0%)	29	41
All	All	763/956 (80%)	734 (96%)	25 (3%)	4 (0%)	34	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	THR
1	B	66[A]	LEU
1	B	66[B]	LEU
1	D	35	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	165/202 (82%)	164 (99%)	1 (1%)	86 94
1	B	167/202 (83%)	166 (99%)	1 (1%)	86 94
1	C	157/202 (78%)	157 (100%)	0	100 100
1	D	158/202 (78%)	156 (99%)	2 (1%)	69 84
All	All	647/808 (80%)	643 (99%)	4 (1%)	86 94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	ASP
1	B	207	ASP
1	D	33	CYS
1	D	213	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	44	GLN

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)

10 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	0.26	0	17,19,21	0.48	0
2	NAG	E	2	2	14,14,15	0.58	0	17,19,21	0.46	0
2	FUC	E	3	2	10,10,11	0.99	0	14,14,16	1.04	1 (7%)
3	NAG	F	1	3,1	14,14,15	0.61	1 (7%)	17,19,21	0.58	0
3	NAG	F	2	3	14,14,15	0.33	0	17,19,21	0.44	0
3	BMA	F	3	3	11,11,12	1.04	2 (18%)	15,15,17	1.44	3 (20%)
3	MAN	F	4	3	11,11,12	1.17	2 (18%)	15,15,17	1.44	2 (13%)
3	FUC	F	5	3	10,10,11	0.56	0	14,14,16	0.96	1 (7%)
4	NAG	G	1	1,4	14,14,15	0.95	1 (7%)	17,19,21	1.06	1 (5%)
4	NAG	G	2	4	14,14,15	0.49	0	17,19,21	0.48	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	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	FUC	E	3	2	-	-	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	FUC	F	5	3	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1	NAG	O5-C1	3.17	1.48	1.43
3	F	4	MAN	O5-C5	2.36	1.48	1.43
3	F	4	MAN	C1-C2	2.28	1.57	1.52
3	F	3	BMA	C4-C3	2.11	1.57	1.52
3	F	1	NAG	C1-C2	2.11	1.55	1.52
3	F	3	BMA	C4-C5	2.01	1.57	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	4	MAN	C1-O5-C5	4.50	118.29	112.19
4	G	1	NAG	C1-O5-C5	3.73	117.25	112.19
3	F	3	BMA	C3-C4-C5	3.02	115.63	110.24
3	F	3	BMA	C2-C3-C4	2.54	115.29	110.89
3	F	3	BMA	C1-C2-C3	2.26	112.44	109.67
3	F	4	MAN	O2-C2-C3	-2.13	105.88	110.14
2	E	3	FUC	C1-C2-C3	-2.10	107.08	109.67
3	F	5	FUC	C1-O5-C5	2.01	117.33	112.78

There are no chirality outliers.

All (11) torsion outliers are listed below:

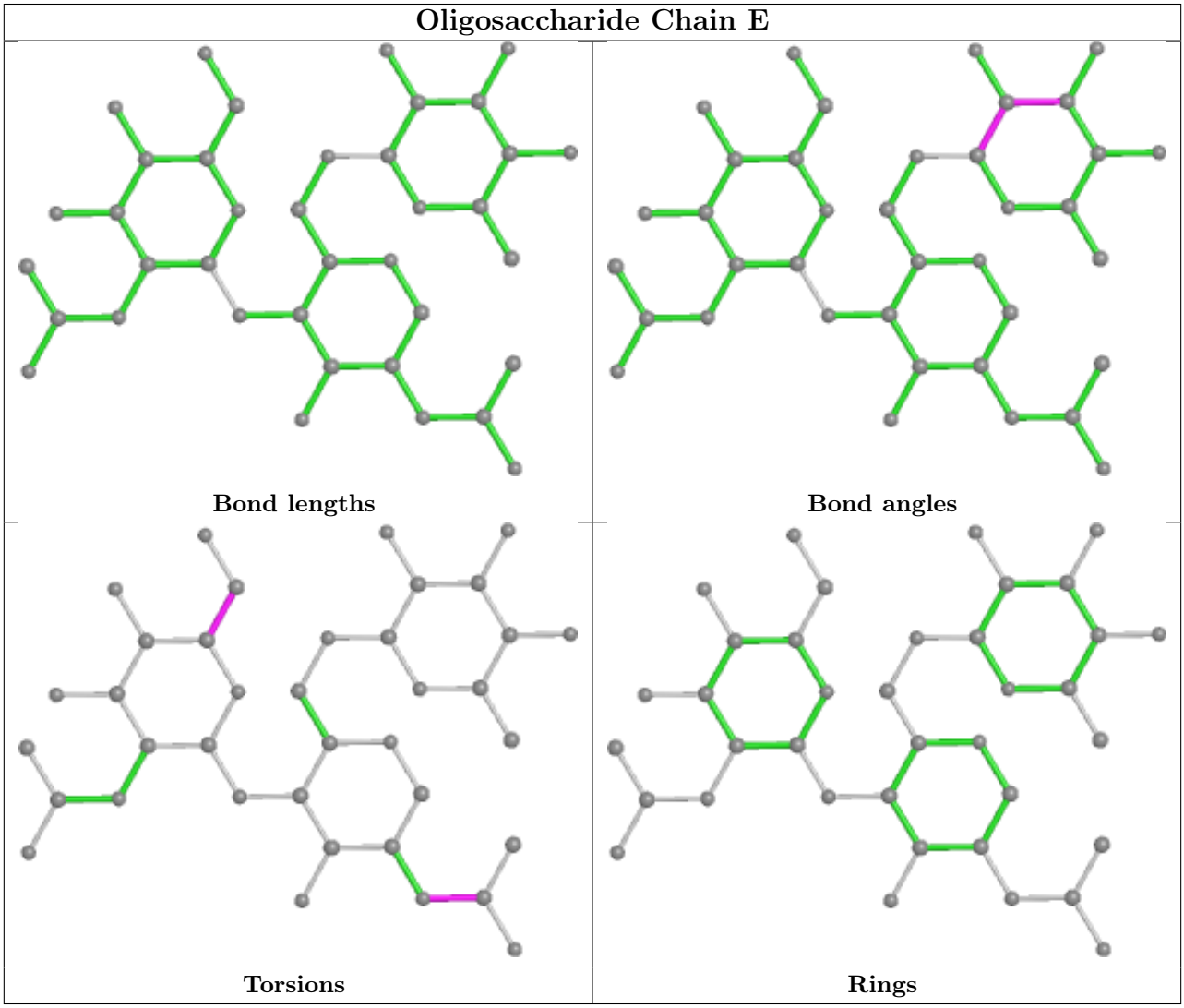
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
3	F	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6

There are no ring outliers.

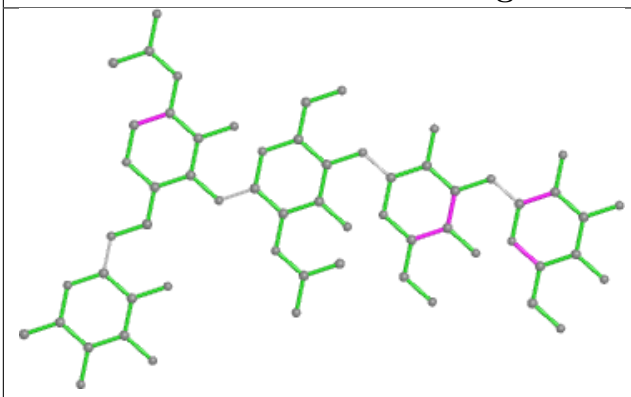
1 monomer is involved in 1 short contact:

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

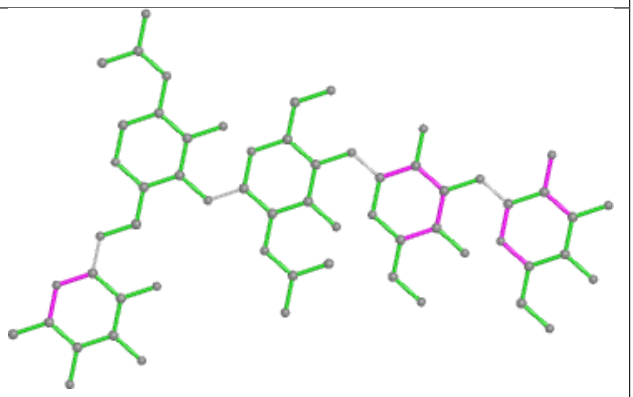
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



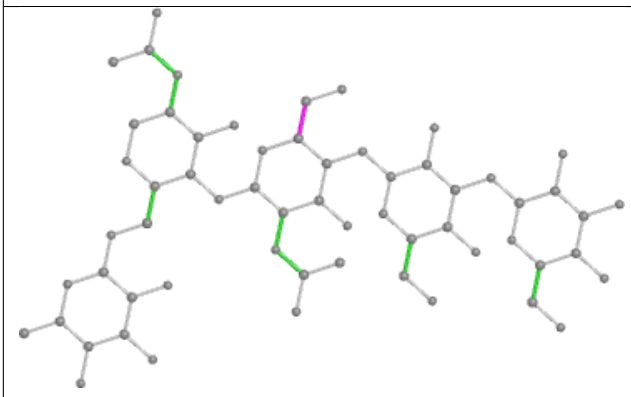
Oligosaccharide Chain F



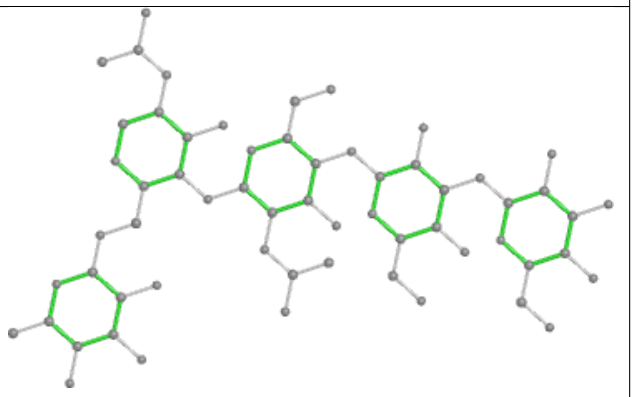
Bond lengths



Bond angles

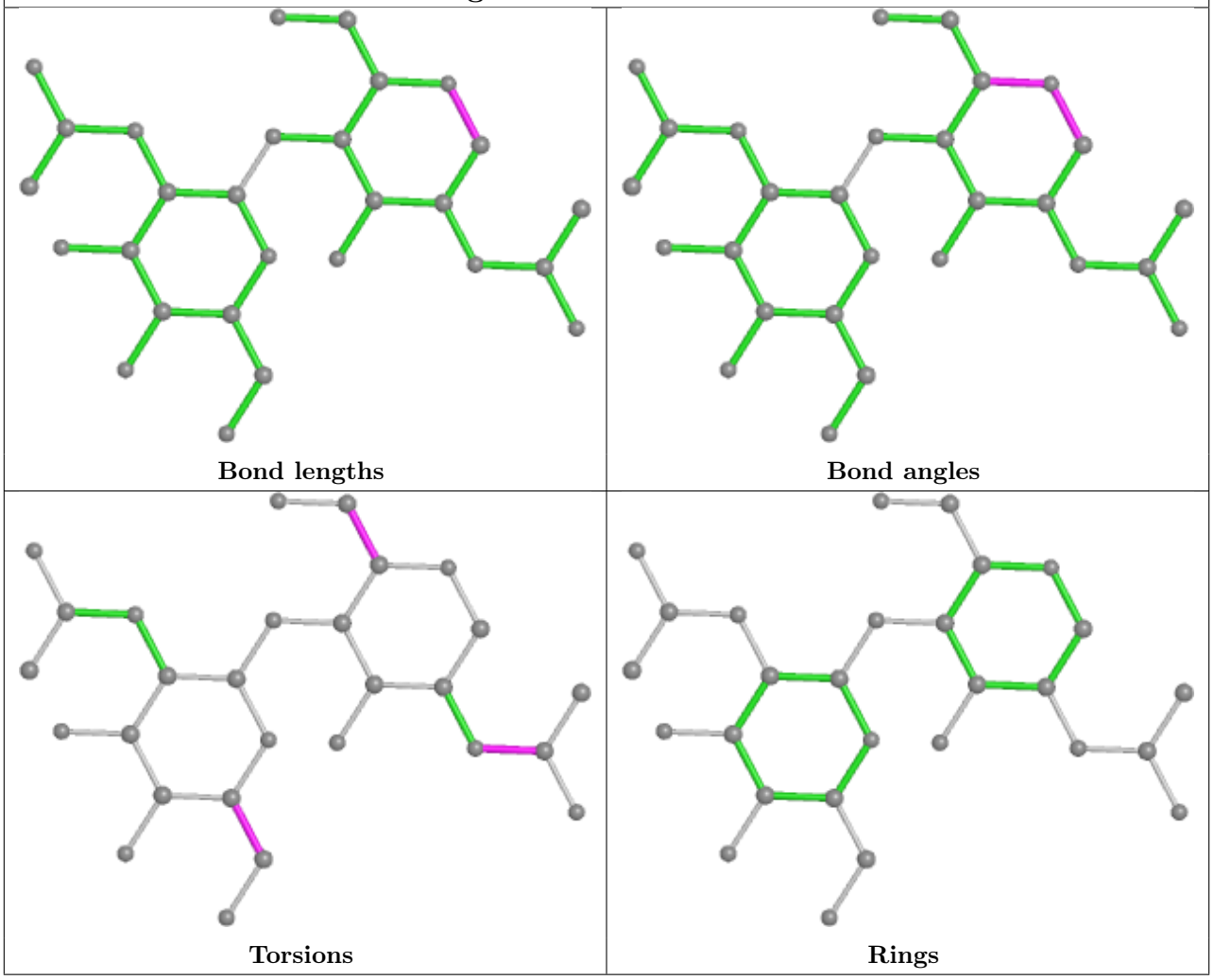


Torsions



Rings

Oligosaccharide Chain G



5.6 Ligand geometry (i)

18 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	$\#\|Z\| > 2$
5	NAG	B	302	1	14,14,15	0.38	0	17,19,21	0.60	0
6	GOL	B	303	-	5,5,5	1.50	1 (20%)	5,5,5	0.87	0
7	EPE	B	305	-	15,15,15	0.87	1 (6%)	18,20,20	1.69	5 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	B	301	1	14,14,15	0.36	0	17,19,21	0.81	1 (5%)
5	NAG	D	302	1	14,14,15	0.44	0	17,19,21	0.52	0
5	NAG	C	302	1	14,14,15	0.25	0	17,19,21	0.40	0
6	GOL	A	303	-	5,5,5	1.40	0	5,5,5	0.70	0
8	AKR	A	305	-	4,4,4	2.24	2 (50%)	4,4,4	2.15	1 (25%)
5	NAG	D	301	1	14,14,15	0.80	1 (7%)	17,19,21	1.21	1 (5%)
5	NAG	C	304	1	14,14,15	0.76	1 (7%)	17,19,21	1.48	3 (17%)
5	NAG	A	302	1	14,14,15	0.81	1 (7%)	17,19,21	0.90	1 (5%)
8	AKR	A	306	-	4,4,4	2.20	1 (25%)	4,4,4	2.24	2 (50%)
6	GOL	B	304	-	5,5,5	0.80	0	5,5,5	1.29	0
7	EPE	A	304	-	15,15,15	1.01	1 (6%)	18,20,20	2.26	7 (38%)
8	AKR	B	306	-	4,4,4	1.74	1 (25%)	4,4,4	4.01	1 (25%)
5	NAG	C	301	1	14,14,15	0.31	0	17,19,21	0.64	1 (5%)
5	NAG	A	301	1	14,14,15	0.56	0	17,19,21	0.78	0
8	AKR	C	303	-	4,4,4	1.95	1 (25%)	4,4,4	2.69	3 (75%)

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
5	NAG	B	302	1	-	4/6/23/26	0/1/1/1
6	GOL	B	303	-	-	4/4/4/4	-
7	EPE	B	305	-	-	1/9/19/19	0/1/1/1
5	NAG	B	301	1	-	3/6/23/26	0/1/1/1
5	NAG	D	302	1	-	4/6/23/26	0/1/1/1
5	NAG	C	302	1	-	2/6/23/26	0/1/1/1
6	GOL	A	303	-	-	2/4/4/4	-
8	AKR	A	305	-	-	2/2/2/2	-
5	NAG	D	301	1	-	3/6/23/26	0/1/1/1
5	NAG	C	304	1	-	5/6/23/26	0/1/1/1
5	NAG	A	302	1	-	2/6/23/26	0/1/1/1
8	AKR	A	306	-	-	1/2/2/2	-
6	GOL	B	304	-	-	2/4/4/4	-
7	EPE	A	304	-	-	5/9/19/19	0/1/1/1
8	AKR	B	306	-	-	0/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	301	1	-	0/6/23/26	0/1/1/1
5	NAG	A	301	1	-	4/6/23/26	0/1/1/1
8	AKR	C	303	-	-	2/2/2/2	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	305	AKR	CA-C	3.73	1.56	1.46
8	A	306	AKR	CA-C	3.68	1.56	1.46
7	A	304	EPE	C10-S	3.65	1.82	1.77
8	C	303	AKR	CA-C	3.33	1.55	1.46
7	B	305	EPE	C10-S	2.84	1.81	1.77
6	B	303	GOL	C1-C2	2.82	1.63	1.51
5	A	302	NAG	O5-C1	2.70	1.48	1.43
8	B	306	AKR	CA-C	2.63	1.53	1.46
5	C	304	NAG	O5-C1	2.61	1.47	1.43
5	D	301	NAG	C1-C2	2.26	1.55	1.52
8	A	305	AKR	O-C	2.24	1.28	1.23

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	306	AKR	CB-CA-C	-7.67	108.44	121.50
7	A	304	EPE	O2S-S-C10	4.77	112.66	106.92
5	C	304	NAG	C2-N2-C7	4.43	129.20	122.90
7	A	304	EPE	C5-N4-C3	4.29	118.47	108.83
8	C	303	AKR	CB-CA-C	-4.09	114.54	121.50
5	D	301	NAG	C2-N2-C7	4.04	128.66	122.90
7	B	305	EPE	O1S-S-C10	3.58	111.22	106.92
8	A	305	AKR	CB-CA-C	-3.42	115.68	121.50
7	A	304	EPE	C7-N4-C3	3.31	119.71	111.23
7	B	305	EPE	C7-N4-C3	3.24	119.52	111.23
8	A	306	AKR	OXT-C-CA	3.18	122.86	114.19
7	B	305	EPE	C7-N4-C5	3.05	119.02	111.23
7	A	304	EPE	O3S-S-C10	3.02	110.65	105.77
5	C	304	NAG	C1-O5-C5	2.89	116.11	112.19
8	C	303	AKR	OXT-C-CA	2.65	121.40	114.19
7	A	304	EPE	C6-C5-N4	2.64	116.06	110.64
7	A	304	EPE	C9-N1-C6	-2.62	104.53	111.23
7	A	304	EPE	C2-C3-N4	2.61	116.00	110.64
7	B	305	EPE	C5-N4-C3	2.52	114.50	108.83
8	A	306	AKR	OXT-C-O	-2.46	117.57	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	302	NAG	C1-O5-C5	2.38	115.42	112.19
5	C	301	NAG	C1-O5-C5	2.25	115.24	112.19
8	C	303	AKR	OXT-C-O	-2.23	118.05	122.67
5	B	301	NAG	C1-O5-C5	2.09	115.02	112.19
5	C	304	NAG	C1-C2-N2	2.07	114.03	110.49
7	B	305	EPE	O3S-S-C10	2.04	109.07	105.77

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	303	GOL	C1-C2-C3-O3
7	A	304	EPE	C9-C10-S-O1S
7	A	304	EPE	C9-C10-S-O2S
7	A	304	EPE	C9-C10-S-O3S
8	A	305	AKR	O-C-CA-CB
8	A	305	AKR	OXT-C-CA-CB
8	A	306	AKR	O-C-CA-CB
8	C	303	AKR	OXT-C-CA-CB
5	B	301	NAG	O5-C5-C6-O6
5	C	304	NAG	O5-C5-C6-O6
5	A	301	NAG	O5-C5-C6-O6
5	A	301	NAG	C4-C5-C6-O6
5	D	302	NAG	O5-C5-C6-O6
5	B	301	NAG	C4-C5-C6-O6
5	C	304	NAG	C4-C5-C6-O6
5	D	302	NAG	C1-C2-N2-C7
5	A	301	NAG	C8-C7-N2-C2
5	A	301	NAG	O7-C7-N2-C2
5	A	302	NAG	C8-C7-N2-C2
5	A	302	NAG	O7-C7-N2-C2
5	C	302	NAG	C8-C7-N2-C2
5	C	302	NAG	O7-C7-N2-C2
5	C	304	NAG	C8-C7-N2-C2
5	C	304	NAG	O7-C7-N2-C2
5	D	301	NAG	C8-C7-N2-C2
5	D	301	NAG	O7-C7-N2-C2
5	D	302	NAG	C4-C5-C6-O6
5	B	302	NAG	C4-C5-C6-O6
5	B	302	NAG	O5-C5-C6-O6
6	A	303	GOL	O1-C1-C2-C3
6	B	303	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	A	303	GOL	O1-C1-C2-O2
5	B	302	NAG	C1-C2-N2-C7
6	B	303	GOL	O2-C2-C3-O3
7	B	305	EPE	N4-C7-C8-O8
7	A	304	EPE	N4-C7-C8-O8
6	B	303	GOL	O1-C1-C2-O2
6	B	304	GOL	O1-C1-C2-O2
8	C	303	AKR	O-C-CA-CB
5	B	301	NAG	C3-C2-N2-C7
7	A	304	EPE	C10-C9-N1-C2
6	B	304	GOL	O1-C1-C2-C3
5	B	302	NAG	C3-C2-N2-C7
5	C	304	NAG	C3-C2-N2-C7
5	D	301	NAG	C3-C2-N2-C7
5	D	302	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	305	EPE	2	0
5	D	301	NAG	1	0
5	C	304	NAG	1	0
7	A	304	EPE	2	0
5	A	301	NAG	2	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	189/239 (79%)	-0.02	2 (1%)	80	79	53, 71, 92, 138	0
1	B	189/239 (79%)	-0.02	1 (0%)	91	89	56, 69, 89, 135	0
1	C	188/239 (78%)	0.20	9 (4%)	30	29	72, 92, 135, 199	0
1	D	189/239 (79%)	0.33	12 (6%)	20	18	67, 94, 138, 208	0
All	All	755/956 (78%)	0.12	24 (3%)	47	46	53, 80, 128, 208	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	34	TRP	5.8
1	D	50	CYS	4.4
1	D	41	ILE	4.2
1	C	29	PHE	3.9
1	A	68[A]	ASN	3.7
1	B	68[A]	ASN	3.5
1	D	85	LEU	3.4
1	A	69[A]	GLU	3.3
1	D	111	GLU	3.2
1	D	84	PHE	3.1
1	D	29	PHE	3.1
1	C	33	CYS	3.1
1	D	34	TRP	3.0
1	C	211	ARG	3.0
1	D	89	ALA	2.9
1	C	30	PRO	2.8
1	D	40	GLY	2.8
1	D	49	VAL	2.7
1	D	116	LEU	2.6
1	C	41	ILE	2.6
1	D	92	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	35	PRO	2.2
1	C	89	ALA	2.0
1	C	36	ASP	2.0

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

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

6.3 Carbohydrates (i)

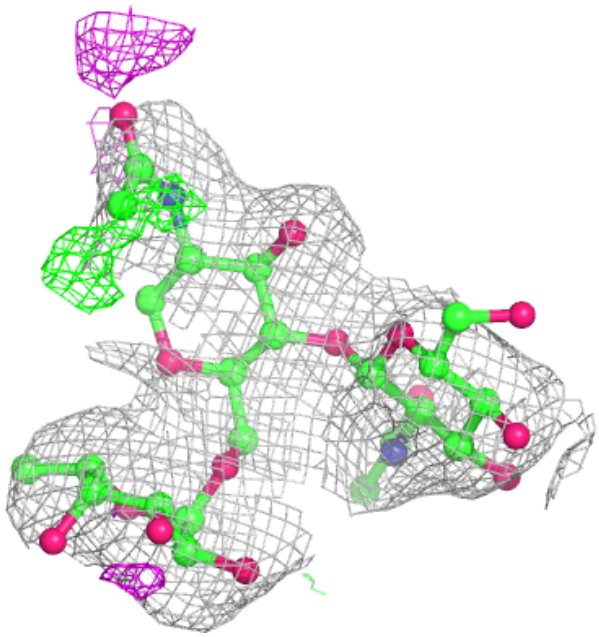
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

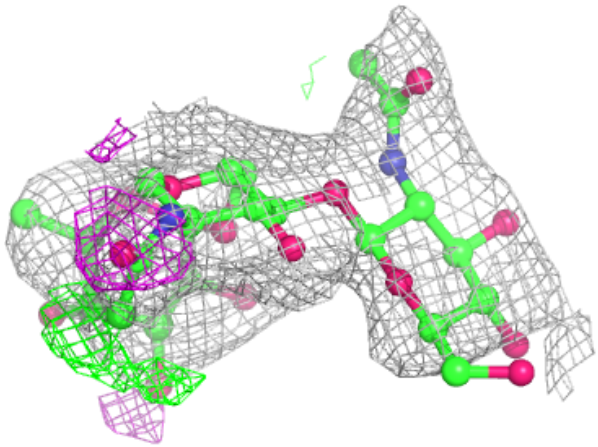
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	G	2	14/15	0.75	0.32	140,156,159,161	0
4	NAG	G	1	14/15	0.76	0.12	110,130,141,151	0
3	BMA	F	3	11/12	0.78	0.20	113,121,129,131	0
2	NAG	E	2	14/15	0.89	0.44	114,149,156,157	0
3	MAN	F	4	11/12	0.89	0.23	114,128,134,135	0
2	NAG	E	1	14/15	0.90	0.26	98,115,126,134	0
2	FUC	E	3	10/11	0.90	0.33	101,126,135,142	0
3	NAG	F	2	14/15	0.96	0.13	86,95,104,104	0
3	NAG	F	1	14/15	0.97	0.12	77,88,92,99	0
3	FUC	F	5	10/11	0.97	0.11	69,88,92,93	0

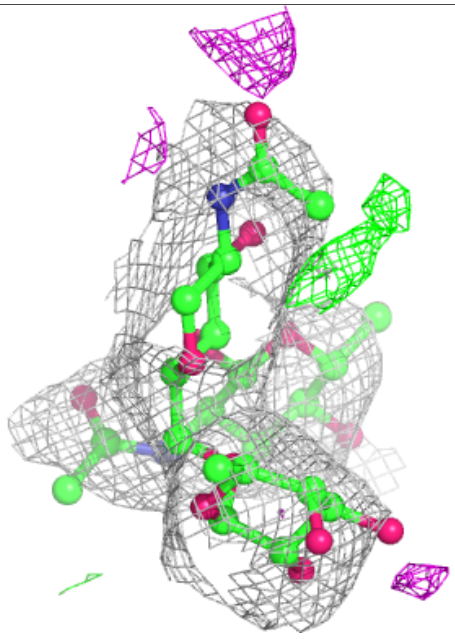
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

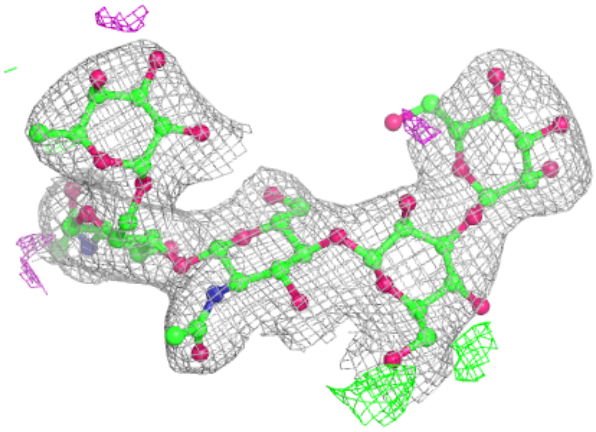


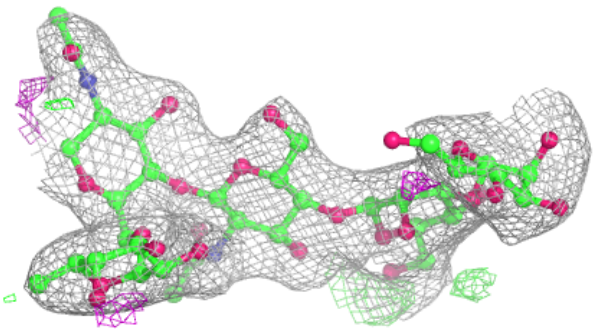


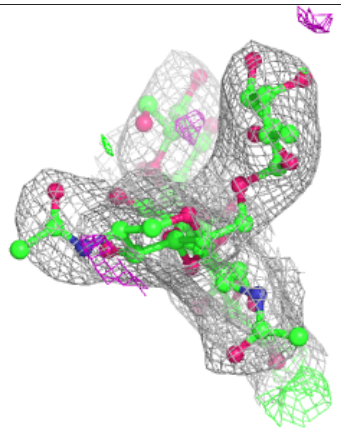


Electron density around Chain F:

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

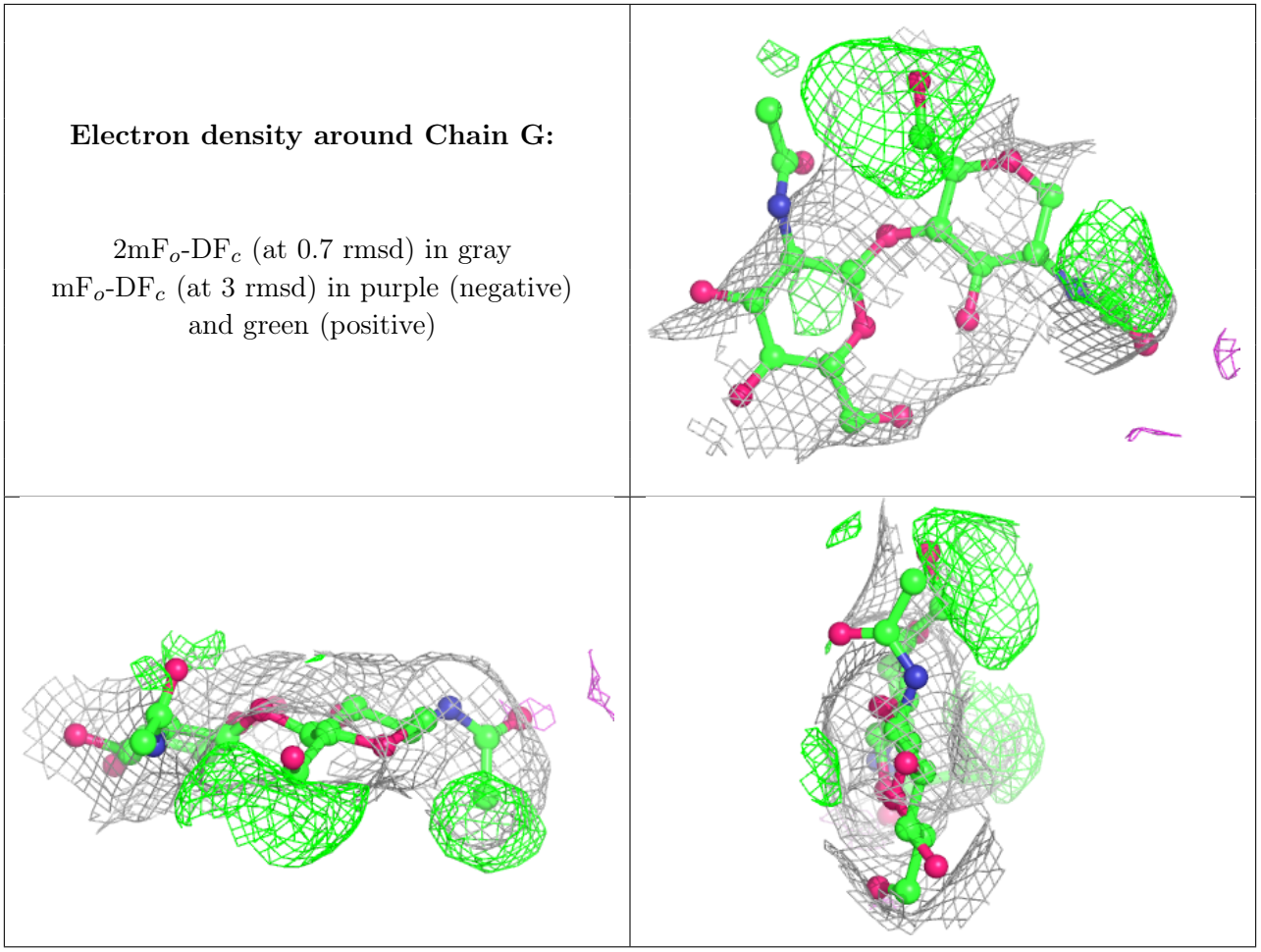






Electron density around Chain G:

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



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	AKR	A	306	5/5	0.43	0.35	69,98,103,115	0
5	NAG	C	304	14/15	0.70	0.24	121,135,142,143	0
5	NAG	D	301	14/15	0.75	0.18	128,145,154,154	0
5	NAG	D	302	14/15	0.76	0.28	120,137,141,141	0
5	NAG	A	301	14/15	0.76	0.44	122,137,141,146	0
8	AKR	C	303	5/5	0.78	0.23	91,97,108,111	0
5	NAG	B	301	14/15	0.80	0.45	136,143,155,156	0
5	NAG	A	302	14/15	0.81	0.19	103,123,129,134	0
6	GOL	B	303	6/6	0.81	0.19	93,98,99,100	0
7	EPE	B	305	15/15	0.82	0.30	74,89,111,129	15
8	AKR	A	305	5/5	0.84	0.20	75,80,83,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	B	302	14/15	0.85	0.26	109,128,133,134	0
5	NAG	C	302	14/15	0.85	0.25	108,126,133,134	0
6	GOL	B	304	6/6	0.88	0.14	86,99,103,104	0
7	EPE	A	304	15/15	0.88	0.16	84,96,110,120	0
5	NAG	C	301	14/15	0.89	0.30	108,122,130,134	0
8	AKR	B	306	5/5	0.92	0.14	74,76,97,100	0
6	GOL	A	303	6/6	0.93	0.14	80,94,106,112	0

6.5 Other polymers (i)

There are no such residues in this entry.