

wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2023 – 06:04 PM EDT

PDB ID : 7K4O

Title : Tannin acyl hydrolase from Aspergillus niger

Authors : Ren, B. Deposited on : 2020-09-15

Resolution : 1.65 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 (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.35.1

 $buster\text{-report}\quad :\quad 1.1.7\ (2018)$

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

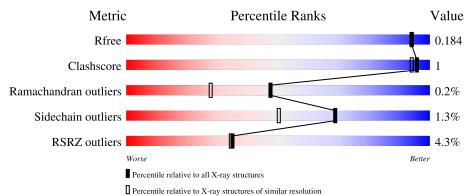
Validation Pipeline (wwPDB-VP) : 2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.65 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	554	96%	
2	В	8	88%	12%
3	С	6	100%	
4	D	2	100%	
4	Е	2	100%	

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Mol	Chain	Length	Quality of chain
4	F	2	100%
4	G	2	100%



2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 9900 atoms, of which 4423 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 Carboxylic ester hydrolase.

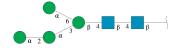
Mol	Chain	Residues		Atoms						AltConf	Trace
1	A	554	Total 8477	C 2757	H 4112	N 704	O 881	S 23	249	18	0

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



Mol	Chain	Residues		\mathbf{At}	oms			ZeroOcc	AltConf	Trace
2	В	8	Total 179	C 52	H 86	N 2	O 39	23	0	0

• Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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		
9	C	6	Total	С	Н	N	О	17	0	0
3		0	139	40	67	2	30	17	0	0

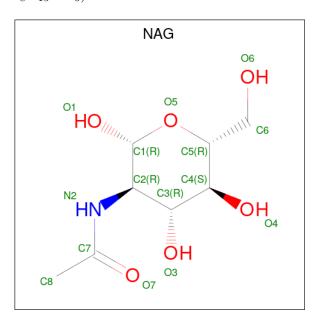
• Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.





Mol	Chain	Residues		\mathbf{At}	oms			ZeroOcc	AltConf	Trace	
1	D	2	Total	С	Н	N	О	5	0	0	
4	D	2	55	16	27	2	10	5	0	0	
1	Е	2	Total	С	Н	N	О	5	0	0	
4	<u> 1</u> 2	2	55	16	27	2	10	5		0	
1	F	2	Total	С	Н	N	О	5	0	0	
4	I'	2	55	16	27	2	10		0		
1	C	2	Total	С	Н	N	О	5	0	0	
4	G	2	55	16	27	2	10	0	U		

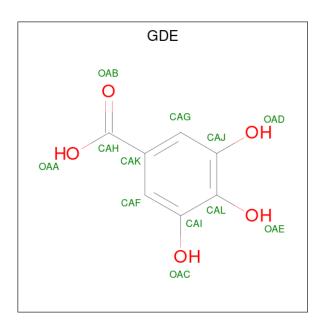
 \bullet Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $\rm C_8H_{15}NO_6).$



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	
5	Λ	1	Total	С	Н	N	О	2	0	
9	A	1	28	8	14	1	5	3	U	
5	Λ	1	Total	С	Н	N	О	2	0	
3	A	1	28	8	14	1	5	3	0	

• Molecule 6 is 3,4,5-trihydroxybenzoic acid (three-letter code: GDE) (formula: $C_7H_6O_5$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	A	tor	ns		ZeroOcc	AltConf
6	A	1	Total 17	C 7	H 5	O 5	3	0

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

Mol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0

• Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	4	Total Zn 4 4	0	0

• Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

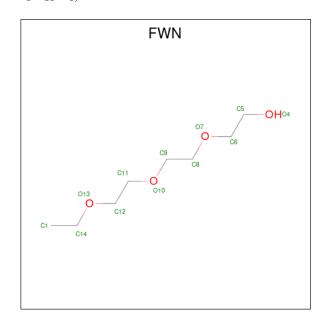
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	2	Total Cl 2 2	0	0

• Molecule 10 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total Na 1 1	0	0



 \bullet Molecule 11 is 2-[2-(2-ethoxyethoxy)ethoxy]ethanol (three-letter code: FWN) (formula: $C_8H_{18}O_4).$



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	٨	1	Total	С	Н	О	9	0
11	A	1	29	8	17	4	2	0

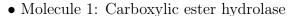
• Molecule 12 is water.

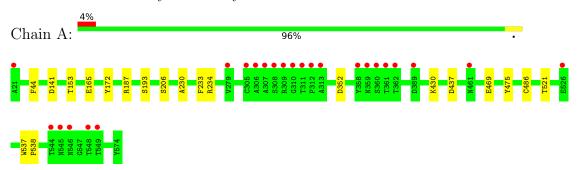
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	775	Total O 775 775	0	0



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

Chain B: 88% 12%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6 MAN7 MAN8

• Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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 C:

NAG1 NAG2 BMA3 MAN4 MAN5

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

Chain D: 100%





• Molecule 4: opyranose	2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc
Chain E:	100%
NAG2	
• Molecule 4: opyranose	$2\hbox{-}acetamido-2\hbox{-}deoxy-beta-D-glucopyranose-(1-4)-2\hbox{-}acetamido-2\hbox{-}deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido$
Chain F:	100%
NAG1 NAG2	
• Molecule 4: opyranose	$2\hbox{-}acetamido-2\hbox{-}deoxy-beta-D-glucopyranose-(1-4)-2\hbox{-}acetamido-2\hbox{-}deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido$
Chain G:	100%
NAG2	



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants	170.92Å 170.92Å 111.06Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.76 - 1.65	Depositor
resolution (A)	19.76 - 1.65	EDS
% Data completeness	99.9 (19.76-1.65)	Depositor
(in resolution range)	100.0 (19.76-1.65)	EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.10 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
P.P.	0.152 , 0.174	Depositor
R, R_{free}	0.164 , 0.184	DCC
R_{free} test set	5698 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.37,65.6	EDS
L-test for twinning ²	$ < L > = 0.50, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	9900	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.86% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GDE, FWN, BMA, NAG, NA, MAN, CL, ZN, CA

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	Boı	nd lengths	Bo	nd angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.79	$2/4541 \ (0.0\%)$	0.84	1/6201 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(A)
1	A	469	GLU	CD-OE2	5.33	1.31	1.25
1	A	165	GLU	CD-OE1	5.13	1.31	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	${f Z}$	$\operatorname{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
1	A	234	ARG	NE-CZ-NH2	-5.18	117.71	120.30

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	4365	4112	4120	9	0
2	В	93	86	76	1	0
3	С	72	67	61	0	0
4	D	28	27	25	0	0
4	Ε	28	27	25	0	0

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Continued	trom	mmoninonic	maaa
COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Mol	Chain	Non-H	H(model)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
4	F	28	27	25	0	0
4	G	28	27	25	0	0
5	A	28	28	26	0	0
6	A	12	5	4	2	0
7	A	1	0	0	0	0
8	A	4	0	0	0	0
9	A	2	0	0	0	0
10	A	1	0	0	0	0
11	A	12	17	0	0	0
12	A	775	0	0	2	2
All	All	5477	4423	4387	9	2

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 1.

The worst 5 of 9 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:206[A]:SER:OG	6:A:603:GDE:CAH	2.48	0.61
1:A:206[B]:SER:OG	1:A:486:CYS:SG	2.65	0.52
1:A:153:THR:HG21	12:A:1068:HOH:O	2.14	0.47
1:A:537:TRP:CD2	1:A:538:PRO:HA	2.52	0.45
1:A:430[A]:LYS:NZ	12:A:721:HOH:O	2.50	0.45

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
12:A:1075:HOH:O	12:A:1075:HOH:O[10_555]	2.13	0.07
12:A:1208:HOH:O	12:A:1433:HOH:O[9_555]	2.19	0.01

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	573/554 (103%)	560 (98%)	12 (2%)	1 (0%)	47 28	

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	TYR

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	479/458 (105%)	473 (99%)	6 (1%)	69 50		

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	352	ASP
1	A	437	ASP
1	A	475	TYR
1	A	141	ASP
1	A	44	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

22 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	Trino	Chain	Dag	Link	Вс	ond leng	ths	В	ond ang	gles
MIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	NAG	В	1	2,1	14,14,15	1.24	3 (21%)	17,19,21	1.83	2 (11%)
2	NAG	В	2	2	14,14,15	1.08	0	17,19,21	1.74	3 (17%)
2	BMA	В	3	2	11,11,12	0.52	0	15,15,17	1.41	3 (20%)
2	MAN	В	4	2	11,11,12	0.78	0	15,15,17	1.79	4 (26%)
2	MAN	В	5	2	11,11,12	0.70	0	15,15,17	1.31	3 (20%)
2	MAN	В	6	2	11,11,12	0.98	1 (9%)	15,15,17	1.77	6 (40%)
2	MAN	В	7	2	10,10,12	0.57	0	14,14,17	1.71	4 (28%)
2	MAN	В	8	2	11,11,12	0.54	0	15,15,17	1.57	4 (26%)
3	NAG	С	1	3,1	14,14,15	1.44	3 (21%)	17,19,21	0.93	0
3	NAG	С	2	3	14,14,15	0.89	0	17,19,21	1.31	2 (11%)
3	BMA	С	3	3	11,11,12	1.10	1 (9%)	15,15,17	1.38	2 (13%)
3	MAN	С	4	3	11,11,12	0.77	0	15,15,17	2.08	5 (33%)
3	MAN	С	5	3	11,11,12	0.66	0	15,15,17	1.54	3 (20%)
3	MAN	С	6	3	11,11,12	0.49	0	15,15,17	1.97	3 (20%)
4	NAG	D	1	4,1	14,14,15	0.84	0	17,19,21	1.40	3 (17%)
4	NAG	D	2	4	14,14,15	0.36	0	17,19,21	0.96	1 (5%)
4	NAG	Е	1	4,1	14,14,15	1.40	3 (21%)	17,19,21	1.96	5 (29%)
4	NAG	E	2	4	14,14,15	0.39	0	17,19,21	1.27	2 (11%)
4	NAG	F	1	4,1	14,14,15	1.01	1 (7%)	17,19,21	1.38	3 (17%)
4	NAG	F	2	4	14,14,15	0.61	0	17,19,21	1.20	3 (17%)
4	NAG	G	1	4,1	14,14,15	0.66	0	17,19,21	1.60	3 (17%)
4	NAG	G	2	4	14,14,15	0.44	0	17,19,21	1.42	3 (17%)

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	В	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	В	2	2	-	0/6/23/26	0/1/1/1
2	BMA	В	3	2	-	0/2/19/22	0/1/1/1
2	MAN	В	4	2	-	1/2/19/22	0/1/1/1
2	MAN	В	5	2	-	0/2/19/22	0/1/1/1
2	MAN	В	6	2	-	0/2/19/22	0/1/1/1
2	MAN	В	7	2	-	-	0/1/1/1
2	MAN	В	8	2	-	2/2/19/22	0/1/1/1
3	NAG	С	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	С	2	3	-	0/6/23/26	0/1/1/1
3	BMA	С	3	3	-	0/2/19/22	0/1/1/1
3	MAN	С	4	3	-	2/2/19/22	0/1/1/1
3	MAN	С	5	3	-	2/2/19/22	0/1/1/1
3	MAN	С	6	3	-	0/2/19/22	0/1/1/1
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	Ε	2	4	-	1/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$Ideal(\AA)$
4	Е	1	NAG	C1-C2	3.18	1.57	1.52
3	С	1	NAG	O5-C1	-3.06	1.38	1.43
3	С	1	NAG	C8-C7	-2.87	1.44	1.50
4	Е	1	NAG	O5-C1	-2.78	1.39	1.43
3	С	3	BMA	O5-C1	-2.63	1.39	1.43

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$\operatorname{Ideal}(^{o})$
2	В	2	NAG	O3-C3-C2	-4.82	99.49	109.47
2	В	1	NAG	C8-C7-N2	4.65	123.97	116.10
2	В	1	NAG	O7-C7-C8	-4.58	113.55	122.06
3	С	6	MAN	O5-C1-C2	-4.26	104.20	110.77
3	С	4	MAN	C1-O5-C5	4.19	117.86	112.19

There are no chirality outliers.



5 of 10 torsion outliers are listed below:

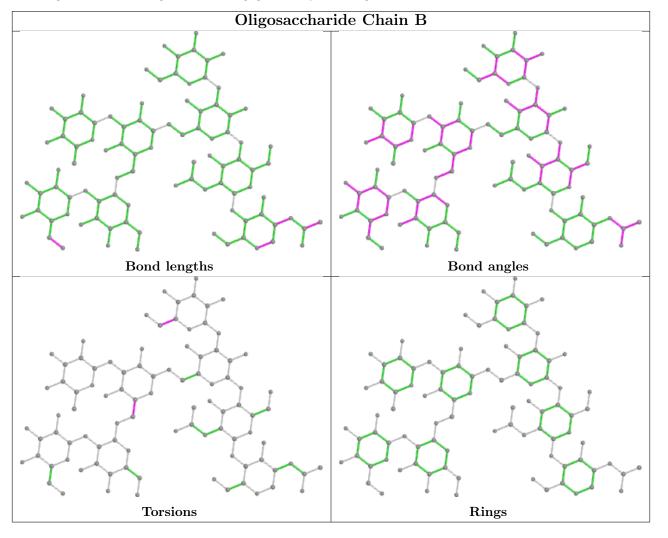
Mol	Chain	Res	Type	Atoms
3	С	4	MAN	O5-C5-C6-O6
3	С	4	MAN	C4-C5-C6-O6
3	С	5	MAN	O5-C5-C6-O6
3	С	5	MAN	C4-C5-C6-O6
2	В	8	MAN	O5-C5-C6-O6

There are no ring outliers.

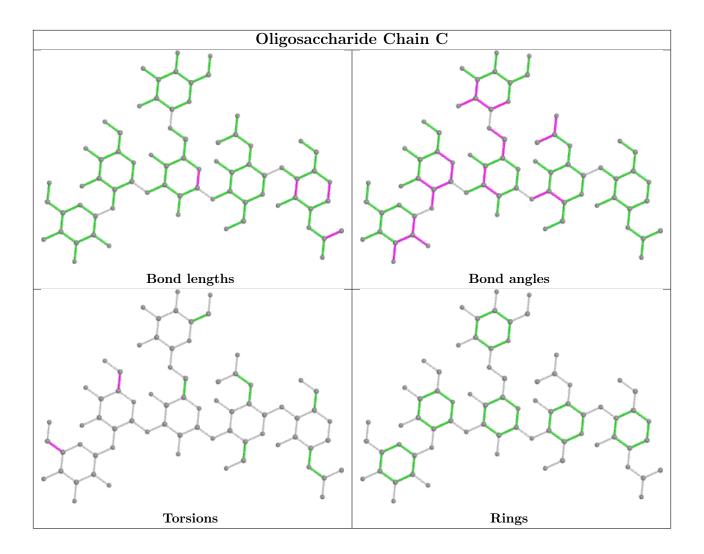
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	6	MAN	1	0

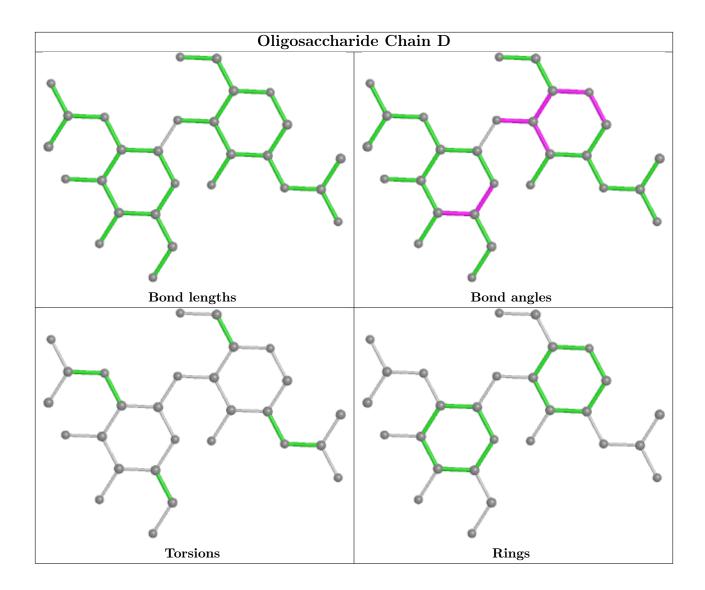
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



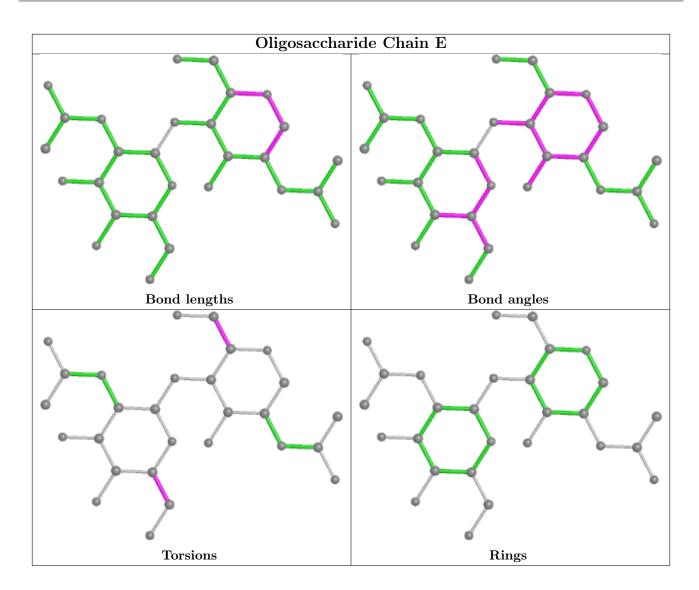




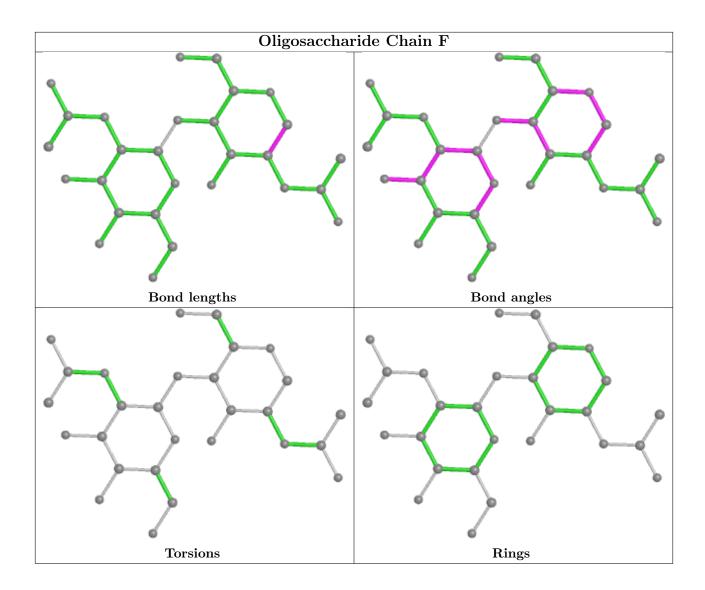




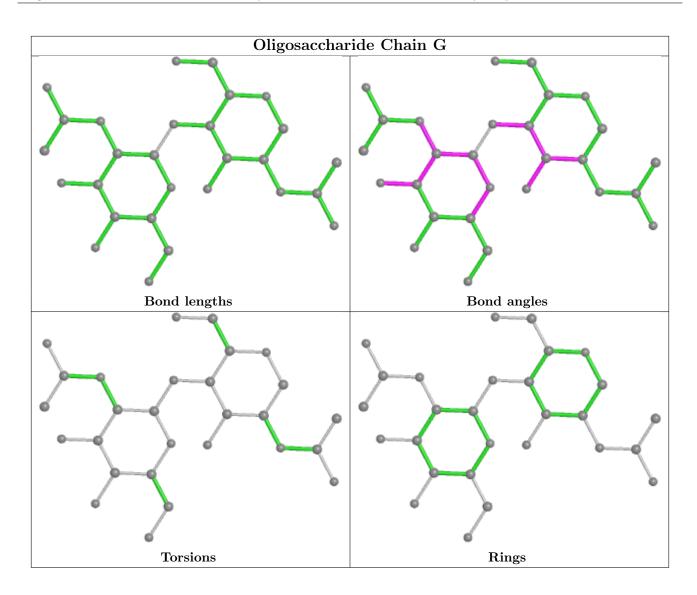












5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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).

Mal	Mol Type Chain Res	Chain	Dec	Res Link	Bond lengths			Bond angles		
MIOI		LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2		
5	NAG	A	601	1	14,14,15	0.66	0	17,19,21	2.47	5 (29%)
11	FWN	A	612	-	11,11,11	0.65	0	10,10,10	1.49	1 (10%)
6	GDE	A	603	-	12,12,12	1.67	5 (41%)	17,17,17	1.88	6 (35%)



Mol	Type	Chain	Res	Ros Lin	Link	Bond lengths			Bond angles		
MIOI	туре			LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
5	NAG	A	602	1	14,14,15	0.66	0	17,19,21	1.52	4 (23%)	

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	A	601	1	-	3/6/23/26	0/1/1/1
11	FWN	A	612	-	-	3/9/9/9	-
6	GDE	A	603	-	-	0/4/4/4	0/1/1/1
5	NAG	A	602	1	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
6	A	603	GDE	OAC-CAI	2.68	1.41	1.36
6	A	603	GDE	CAG-CAJ	2.43	1.42	1.38
6	A	603	GDE	OAE-CAL	2.30	1.42	1.37
6	A	603	GDE	CAI-CAL	2.18	1.42	1.40
6	A	603	GDE	CAJ-CAL	-2.16	1.37	1.40

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	${f Z}$	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
5	A	601	NAG	C1-C2-N2	-6.22	99.86	110.49
5	A	601	NAG	C4-C3-C2	-4.26	104.77	111.02
6	A	603	GDE	CAJ-CAL-CAI	4.17	122.17	119.51
5	A	601	NAG	O4-C4-C5	-3.75	99.97	109.30
6	A	603	GDE	CAG-CAK-CAF	3.20	123.49	119.63

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	NAG	C3-C2-N2-C7
5	A	601	NAG	C8-C7-N2-C2
11	A	612	FWN	O4-C5-C6-O7
5	A	601	NAG	O7-C7-N2-C2
11	A	612	FWN	O7-C8-C9-O10



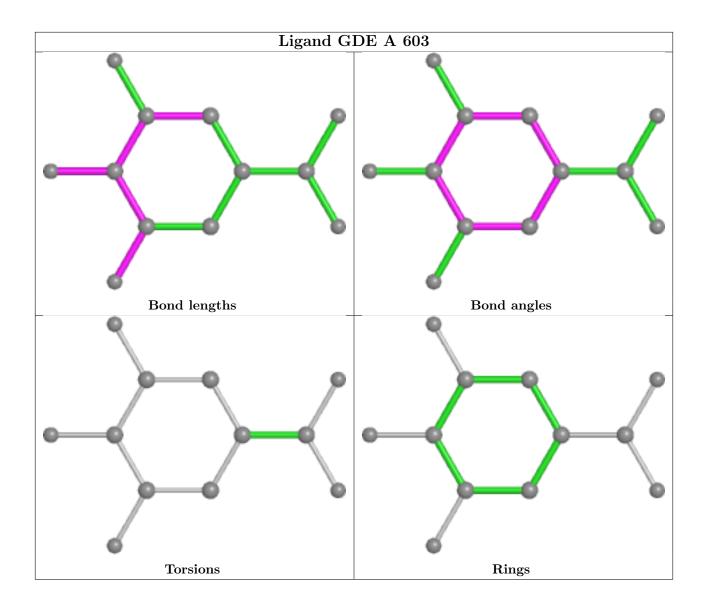
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	603	GDE	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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 (i)

6.1 Protein, DNA and RNA chains (i)

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	$\langle { m RSRZ} \rangle$	#RSF	RZ>2	$OWAB(Å^2)$	Q<0.9
1	A	554/554 (100%)	-0.40	24 (4%)	35 34	19, 27, 53, 136	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	309	ARG	10.0
1	A	361	THR	7.4
1	A	21	ALA	5.8
1	A	310	GLY	4.8
1	A	358	TYR	4.7

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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	MAN	В	7	10/12	0.64	0.34	78,84,89,90	8
3	MAN	С	5	11/12	0.68	0.31	85,94,97,100	11
3	MAN	С	6	11/12	0.69	0.31	76,87,91,92	19
4	NAG	Е	2	14/15	0.73	0.36	71,78,92,102	14
4	NAG	G	2	14/15	0.74	0.40	75,87,95,97	16
2	MAN	В	6	11/12	0.77	0.17	31,37,44,45	11
3	MAN	С	4	11/12	0.78	0.23	42,63,72,75	11

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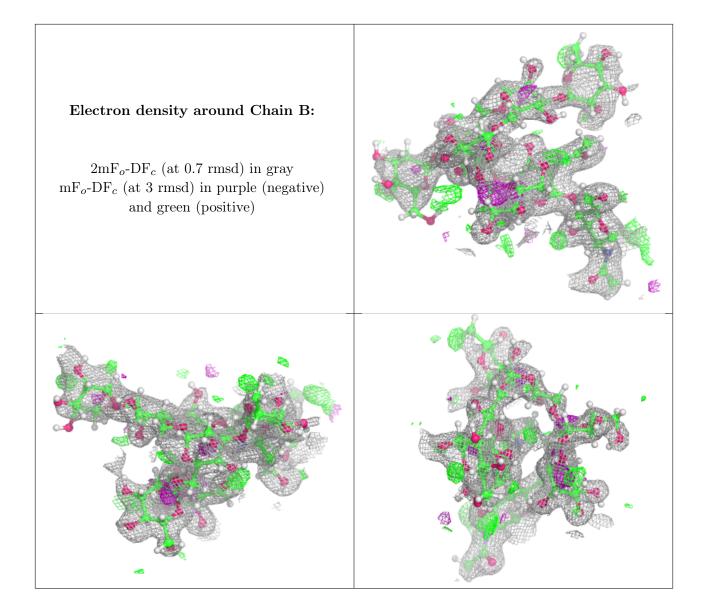


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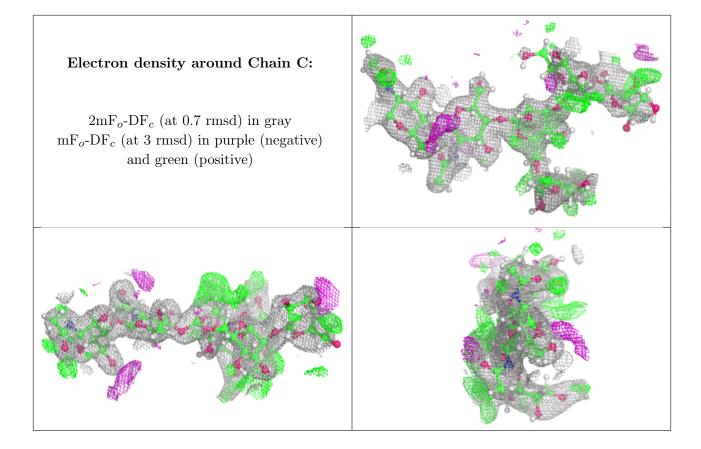
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	MAN	В	4	11/12	0.81	0.33	57,64,69,75	9
4	NAG	F	2	14/15	0.84	0.28	53,60,65,74	21
3	BMA	С	3	11/12	0.85	0.22	42,55,70,83	10
2	MAN	В	5	11/12	0.85	0.25	48,53,59,59	12
4	NAG	D	2	14/15	0.85	0.25	36,50,57,57	17
4	NAG	G	1	14/15	0.87	0.15	51,60,63,69	8
2	MAN	В	8	11/12	0.88	0.35	74,83,90,90	13
4	NAG	F	1	14/15	0.91	0.10	24,32,41,43	17
2	BMA	В	3	11/12	0.91	0.21	49,58,60,63	5
4	NAG	D	1	14/15	0.92	0.07	29,36,42,53	12
4	NAG	E	1	14/15	0.93	0.08	27,41,46,54	15
2	NAG	В	1	14/15	0.94	0.06	26,29,36,38	16
3	NAG	С	2	14/15	0.95	0.07	25,30,38,39	15
2	NAG	В	2	14/15	0.96	0.07	31,37,41,41	12
3	NAG	С	1	14/15	0.97	0.07	19,25,37,37	16

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.

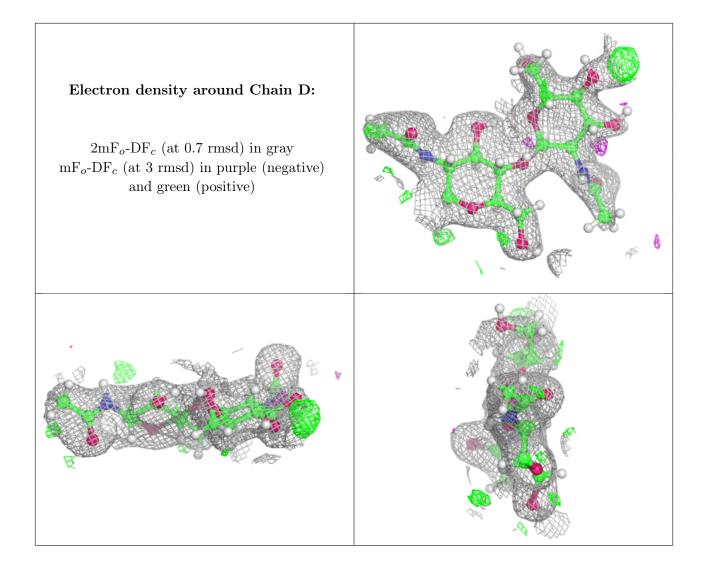




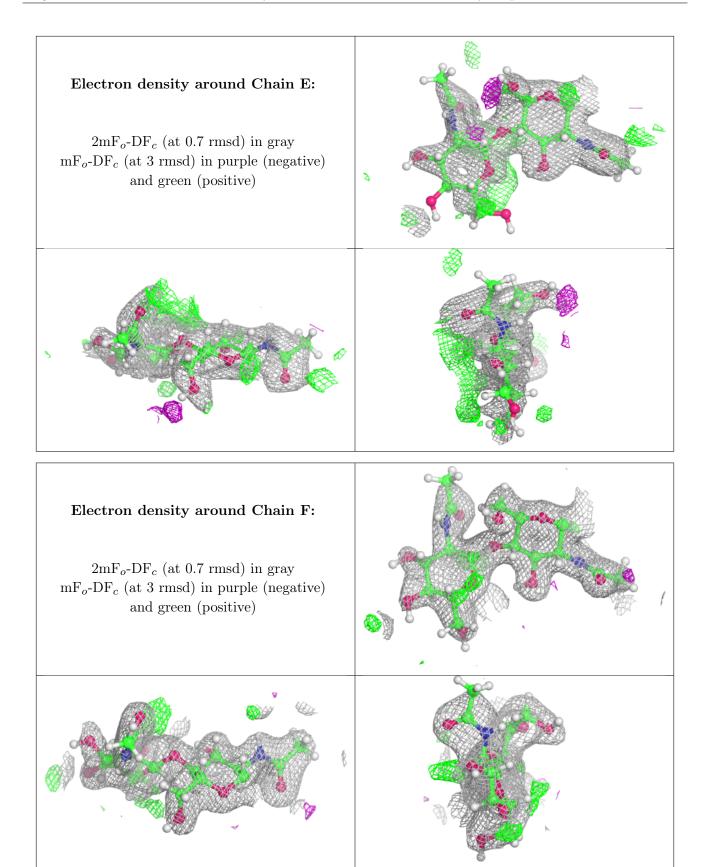




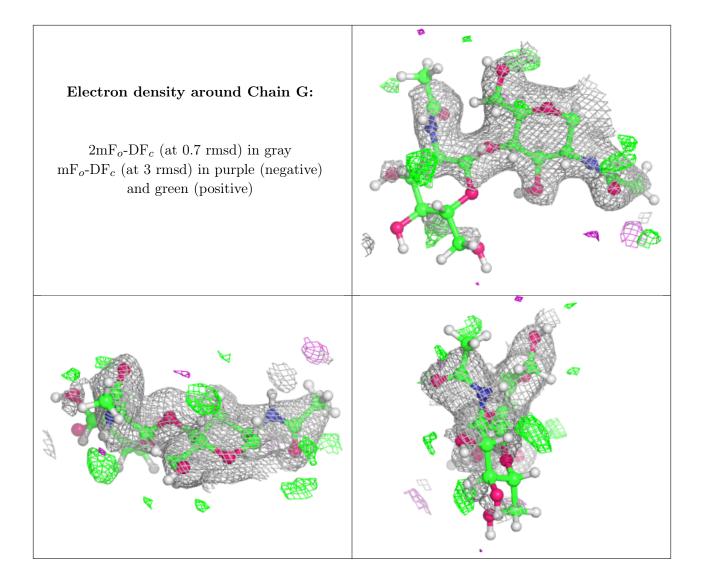












6.4 Ligands (i)

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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
11	FWN	A	612	12/12	0.77	0.21	0,68,77,81	5
5	NAG	A	602	14/15	0.84	0.47	103,112,121,124	9
5	NAG	A	601	14/15	0.85	0.19	40,57,61,75	19
9	CL	A	610	1/1	0.96	0.05	39,39,39,39	1
10	NA	A	611	1/1	0.97	0.10	56,56,56,56	0
8	ZN	A	607	1/1	0.97	0.07	37,37,37,37	1
6	GDE	A	603	12/12	0.98	0.04	22,24,30,31	3
7	CA	A	604	1/1	0.98	0.05	33,33,33,33	0

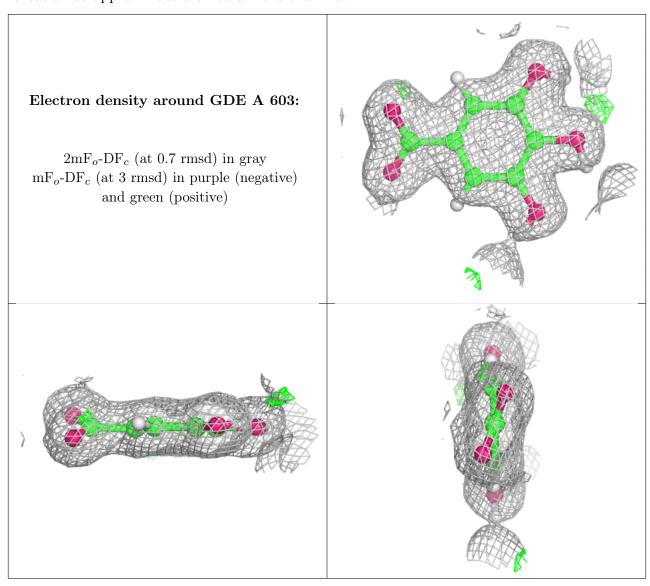
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
9	CL	A	609	1/1	0.99	0.06	40,40,40,40	0
8	ZN	A	608	1/1	0.99	0.07	39,39,39,39	1
8	ZN	A	605	1/1	1.00	0.05	24,24,24,24	1
8	ZN	A	606	1/1	1.00	0.04	22,22,22,22	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers (i)

There are no such residues in this entry.

