Full wwPDB X-ray Structure Validation Report ⓘ

Jun 1, 2023 – 01:48 pm BST

PDB ID	:	8B48
Title	:	Structure of Lentithecium fluviatile carbohydrate esterase from the CE15 family (LfCE15C)
Authors	:	Scholzen, K.; Mazurkewich, S.; Poulsen, J.C.N.; Larsbrink, J.; Lo Leggio, L.
Deposited on	:	2022-09-20
Resolution	:	2.65 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:

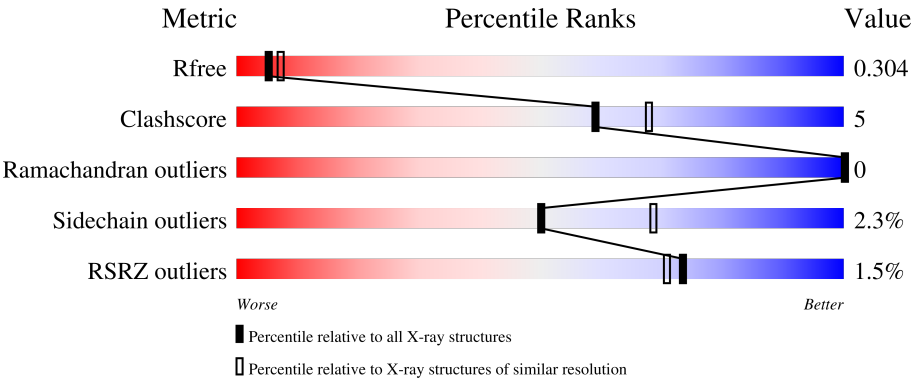
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.33
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 2.65 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	394	82% 12% 6%
1	B	394	79% 14% 6%
1	C	394	83% 11% 6%
1	D	394	3% 84% 10% 6%
2	E	4	75% 25%

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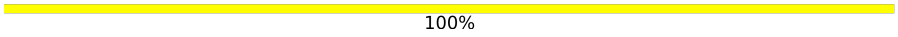
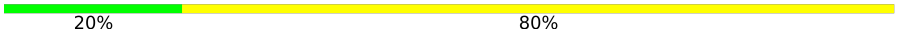
Mol	Chain	Length	Quality of chain
3	F	5	
3	H	5	
4	G	6	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11960 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 Carbohydrate esterase family 15 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	2	0
			2853	1813	492	533	15			
1	B	370	Total	C	N	O	S	0	3	0
			2866	1823	496	534	13			
1	C	370	Total	C	N	O	S	0	0	0
			2847	1809	492	533	13			
1	D	369	Total	C	N	O	S	0	0	0
			2841	1806	491	531	13			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	388	GLY	-	expression tag	UNP A0A6G1IIU9
A	389	LEU	-	expression tag	UNP A0A6G1IIU9
A	390	GLU	-	expression tag	UNP A0A6G1IIU9
A	391	GLN	-	expression tag	UNP A0A6G1IIU9
A	392	LYS	-	expression tag	UNP A0A6G1IIU9
A	393	LEU	-	expression tag	UNP A0A6G1IIU9
A	394	ILE	-	expression tag	UNP A0A6G1IIU9
A	395	SER	-	expression tag	UNP A0A6G1IIU9
A	396	GLU	-	expression tag	UNP A0A6G1IIU9
A	397	GLU	-	expression tag	UNP A0A6G1IIU9
A	398	ASP	-	expression tag	UNP A0A6G1IIU9
A	399	LEU	-	expression tag	UNP A0A6G1IIU9
A	400	ASN	-	expression tag	UNP A0A6G1IIU9
A	401	SER	-	expression tag	UNP A0A6G1IIU9
A	402	ALA	-	expression tag	UNP A0A6G1IIU9
A	403	VAL	-	expression tag	UNP A0A6G1IIU9
A	404	ASP	-	expression tag	UNP A0A6G1IIU9
A	405	HIS	-	expression tag	UNP A0A6G1IIU9
A	406	HIS	-	expression tag	UNP A0A6G1IIU9
A	407	HIS	-	expression tag	UNP A0A6G1IIU9
A	408	HIS	-	expression tag	UNP A0A6G1IIU9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	409	HIS	-	expression tag	UNP A0A6G1IIU9
A	410	HIS	-	expression tag	UNP A0A6G1IIU9
B	388	GLY	-	expression tag	UNP A0A6G1IIU9
B	389	LEU	-	expression tag	UNP A0A6G1IIU9
B	390	GLU	-	expression tag	UNP A0A6G1IIU9
B	391	GLN	-	expression tag	UNP A0A6G1IIU9
B	392	LYS	-	expression tag	UNP A0A6G1IIU9
B	393	LEU	-	expression tag	UNP A0A6G1IIU9
B	394	ILE	-	expression tag	UNP A0A6G1IIU9
B	395	SER	-	expression tag	UNP A0A6G1IIU9
B	396	GLU	-	expression tag	UNP A0A6G1IIU9
B	397	GLU	-	expression tag	UNP A0A6G1IIU9
B	398	ASP	-	expression tag	UNP A0A6G1IIU9
B	399	LEU	-	expression tag	UNP A0A6G1IIU9
B	400	ASN	-	expression tag	UNP A0A6G1IIU9
B	401	SER	-	expression tag	UNP A0A6G1IIU9
B	402	ALA	-	expression tag	UNP A0A6G1IIU9
B	403	VAL	-	expression tag	UNP A0A6G1IIU9
B	404	ASP	-	expression tag	UNP A0A6G1IIU9
B	405	HIS	-	expression tag	UNP A0A6G1IIU9
B	406	HIS	-	expression tag	UNP A0A6G1IIU9
B	407	HIS	-	expression tag	UNP A0A6G1IIU9
B	408	HIS	-	expression tag	UNP A0A6G1IIU9
B	409	HIS	-	expression tag	UNP A0A6G1IIU9
B	410	HIS	-	expression tag	UNP A0A6G1IIU9
C	388	GLY	-	expression tag	UNP A0A6G1IIU9
C	389	LEU	-	expression tag	UNP A0A6G1IIU9
C	390	GLU	-	expression tag	UNP A0A6G1IIU9
C	391	GLN	-	expression tag	UNP A0A6G1IIU9
C	392	LYS	-	expression tag	UNP A0A6G1IIU9
C	393	LEU	-	expression tag	UNP A0A6G1IIU9
C	394	ILE	-	expression tag	UNP A0A6G1IIU9
C	395	SER	-	expression tag	UNP A0A6G1IIU9
C	396	GLU	-	expression tag	UNP A0A6G1IIU9
C	397	GLU	-	expression tag	UNP A0A6G1IIU9
C	398	ASP	-	expression tag	UNP A0A6G1IIU9
C	399	LEU	-	expression tag	UNP A0A6G1IIU9
C	400	ASN	-	expression tag	UNP A0A6G1IIU9
C	401	SER	-	expression tag	UNP A0A6G1IIU9
C	402	ALA	-	expression tag	UNP A0A6G1IIU9
C	403	VAL	-	expression tag	UNP A0A6G1IIU9
C	404	ASP	-	expression tag	UNP A0A6G1IIU9

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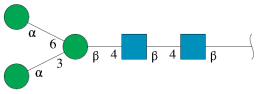
Chain	Residue	Modelled	Actual	Comment	Reference
C	405	HIS	-	expression tag	UNP A0A6G1IIU9
C	406	HIS	-	expression tag	UNP A0A6G1IIU9
C	407	HIS	-	expression tag	UNP A0A6G1IIU9
C	408	HIS	-	expression tag	UNP A0A6G1IIU9
C	409	HIS	-	expression tag	UNP A0A6G1IIU9
C	410	HIS	-	expression tag	UNP A0A6G1IIU9
D	388	GLY	-	expression tag	UNP A0A6G1IIU9
D	389	LEU	-	expression tag	UNP A0A6G1IIU9
D	390	GLU	-	expression tag	UNP A0A6G1IIU9
D	391	GLN	-	expression tag	UNP A0A6G1IIU9
D	392	LYS	-	expression tag	UNP A0A6G1IIU9
D	393	LEU	-	expression tag	UNP A0A6G1IIU9
D	394	ILE	-	expression tag	UNP A0A6G1IIU9
D	395	SER	-	expression tag	UNP A0A6G1IIU9
D	396	GLU	-	expression tag	UNP A0A6G1IIU9
D	397	GLU	-	expression tag	UNP A0A6G1IIU9
D	398	ASP	-	expression tag	UNP A0A6G1IIU9
D	399	LEU	-	expression tag	UNP A0A6G1IIU9
D	400	ASN	-	expression tag	UNP A0A6G1IIU9
D	401	SER	-	expression tag	UNP A0A6G1IIU9
D	402	ALA	-	expression tag	UNP A0A6G1IIU9
D	403	VAL	-	expression tag	UNP A0A6G1IIU9
D	404	ASP	-	expression tag	UNP A0A6G1IIU9
D	405	HIS	-	expression tag	UNP A0A6G1IIU9
D	406	HIS	-	expression tag	UNP A0A6G1IIU9
D	407	HIS	-	expression tag	UNP A0A6G1IIU9
D	408	HIS	-	expression tag	UNP A0A6G1IIU9
D	409	HIS	-	expression tag	UNP A0A6G1IIU9
D	410	HIS	-	expression tag	UNP A0A6G1IIU9

- Molecule 2 is an oligosaccharide called 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-glucopyranose.

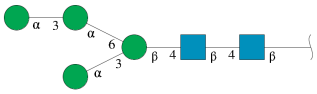
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	4	50	28	2	20	0	0	0

- Molecule 3 is an oligosaccharide called 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.



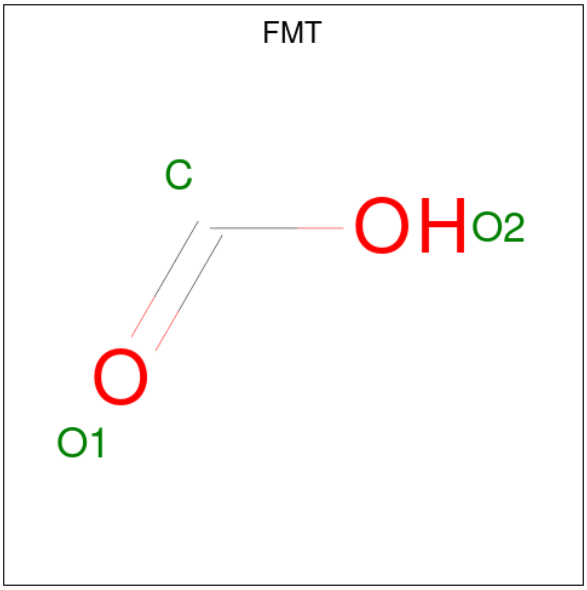
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	H	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is an oligosaccharide called 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-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



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

- Molecule 6 is water.

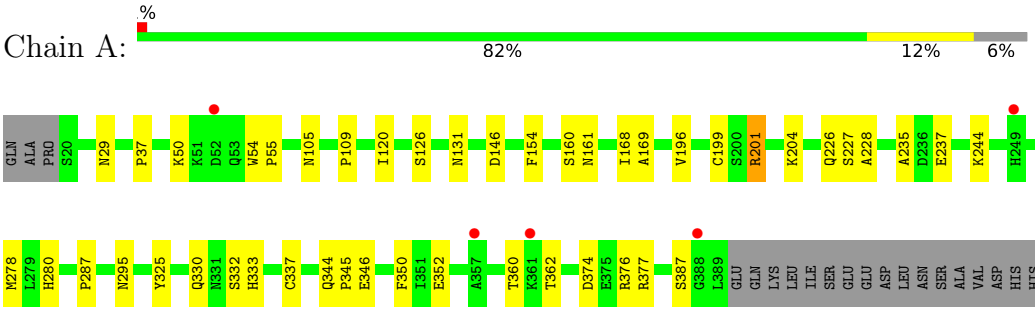
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	78	Total O 78 78	0	0
6	B	80	Total O 80 80	0	0
6	C	76	Total O 76 76	0	0
6	D	69	Total O 69 69	0	0

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.

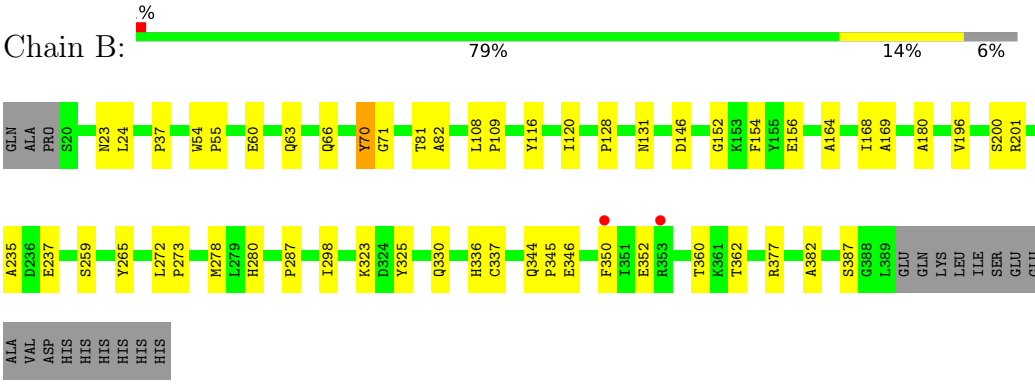
• Molecule 1: Carbohydrate esterase family 15 protein

Chain A:



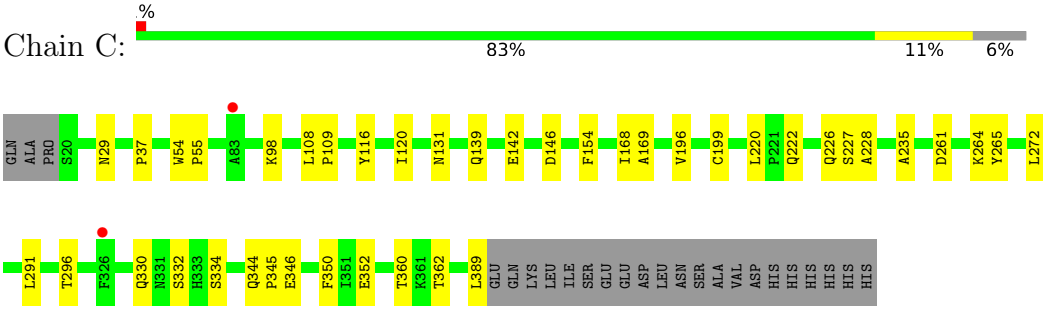
• Molecule 1: Carbohydrate esterase family 15 protein

Chain B:



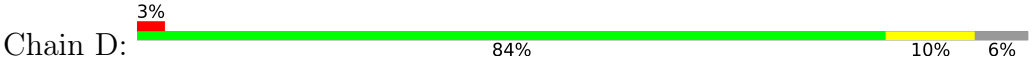
• Molecule 1: Carbohydrate esterase family 15 protein

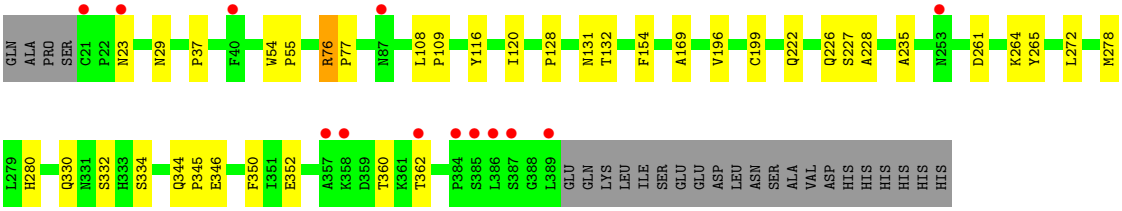
Chain C:



• Molecule 1: Carbohydrate esterase family 15 protein

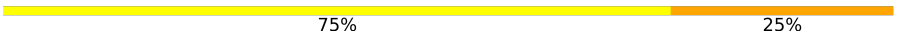
Chain D:





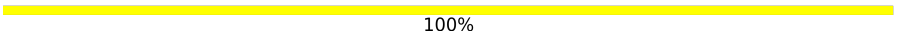
• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



• Molecule 3: 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 F:

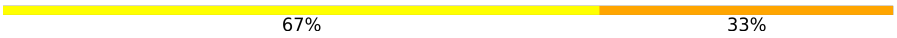


• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

• Molecule 4: 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-glucopyranose

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	70.74Å 79.57Å 86.01Å 113.32° 98.53° 94.44°	Depositor
Resolution (Å)	47.25 – 2.65 47.21 – 2.65	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.25-2.65) 97.6 (47.21-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.238 , 0.298 0.241 , 0.304	Depositor DCC
R_{free} test set	2294 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	50.5	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 35.2	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	0.93	EDS
Total number of atoms	11960	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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: FMT, MAN, NAG, BMA

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	0.66	0/2937	0.78	0/3992
1	B	0.66	0/2954	0.79	0/4014
1	C	0.66	0/2925	0.78	0/3976
1	D	0.65	0/2919	0.77	0/3968
All	All	0.66	0/11735	0.78	0/15950

There are no bond length outliers.

There are no bond angle outliers.

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	2853	0	2783	28	0
1	B	2866	0	2801	37	0
1	C	2847	0	2773	22	0
1	D	2841	0	2768	20	0
2	E	50	0	43	1	0
3	F	61	0	52	0	0
3	H	61	0	52	0	0
4	G	72	0	61	1	0
5	A	3	0	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	3	0	1	0	0
6	A	78	0	0	3	0
6	B	80	0	0	6	0
6	C	76	0	0	2	0
6	D	69	0	0	3	0
All	All	11960	0	11335	108	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 (108) 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:298:ILE:HD12	1:B:336[A]:HIS:CE1	2.18	0.77
1:B:273:PRO:O	6:B:501:HOH:O	2.11	0.68
1:B:200:SER:HB2	1:B:336[B]:HIS:NE2	2.09	0.66
1:C:139:GLN:HB3	1:C:142:GLU:OE1	1.94	0.66
1:A:201:ARG:HG2	1:A:201:ARG:HH11	1.60	0.66
4:G:3:BMA:H2	4:G:6:MAN:H5	1.80	0.64
1:B:71:GLY:HA3	1:B:164:ALA:HA	1.79	0.63
1:A:201:ARG:HG2	1:A:201:ARG:NH1	2.11	0.62
1:D:261:ASP:O	1:D:264:LYS:HG2	2.02	0.60
1:C:261:ASP:O	1:C:264:LYS:HG2	2.02	0.59
1:D:132:THR:HG21	6:D:603:HOH:O	2.05	0.56
1:B:152:GLY:O	1:B:156:GLU:HG3	2.07	0.55
1:B:63:GLN:HA	1:B:66[B]:GLN:HG2	1.88	0.54
1:A:295:ASN:ND2	1:A:333:HIS:CD2	2.76	0.53
1:A:161:ASN:HB2	6:A:660:HOH:O	2.08	0.53
1:B:71:GLY:O	1:B:168:ILE:HG21	2.09	0.53
1:B:382:ALA:HA	6:B:510:HOH:O	2.08	0.53
1:A:265:TYR:HB3	1:A:272:LEU:HD21	1.90	0.52
1:D:23:ASN:ND2	6:D:604:HOH:O	2.44	0.51
1:B:352:GLU:OE1	1:B:360:THR:HG21	2.11	0.51
1:C:352:GLU:OE1	1:C:360:THR:HG21	2.10	0.51
1:B:109:PRO:HB2	1:B:131:ASN:O	2.11	0.50
1:B:108:LEU:HD12	1:B:116:TYR:CD2	2.46	0.50
1:A:109:PRO:HB2	1:A:131:ASN:O	2.11	0.50
1:D:352:GLU:OE1	1:D:360:THR:HG21	2.12	0.50
1:B:237:GLU:OE2	1:B:377:ARG:NH2	2.43	0.49
1:C:139:GLN:HB3	1:C:142:GLU:HB3	1.94	0.49
1:D:109:PRO:HB2	1:D:131:ASN:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:TYR:HB3	1:D:272:LEU:HD21	1.94	0.49
1:B:265:TYR:HB3	1:B:272:LEU:HD21	1.94	0.49
1:A:352:GLU:OE1	1:A:360:THR:HG21	2.13	0.49
1:C:109:PRO:HB2	1:C:131:ASN:O	2.13	0.49
1:B:226:GLN:HE21	1:B:235:ALA:HB2	1.79	0.48
1:C:226:GLN:HE21	1:C:235:ALA:HB2	1.78	0.48
1:A:344:GLN:N	1:A:345:PRO:HD2	2.29	0.48
1:A:237:GLU:OE2	1:A:377:ARG:NH2	2.42	0.48
1:C:265:TYR:HB3	1:C:272:LEU:HD21	1.96	0.48
1:D:344:GLN:N	1:D:345:PRO:HD2	2.29	0.47
1:A:120:ILE:O	1:A:196:VAL:HA	2.15	0.47
1:C:98:LYS:HA	6:C:548:HOH:O	2.15	0.47
1:D:120:ILE:O	1:D:196:VAL:HA	2.16	0.46
1:A:226:GLN:HE21	1:A:235:ALA:HB2	1.80	0.46
1:B:336[B]:HIS:CD2	1:B:337:CYS:SG	3.09	0.46
1:C:296:THR:HG23	1:C:330:GLN:HB3	1.95	0.46
1:D:226:GLN:HE21	1:D:235:ALA:HB2	1.78	0.46
1:B:120:ILE:O	1:B:196:VAL:HA	2.16	0.46
1:C:344:GLN:N	1:C:345:PRO:HD2	2.31	0.46
1:A:374:ASP:OD1	1:A:376:ARG:HG3	2.16	0.46
1:A:201:ARG:HH11	1:A:201:ARG:CG	2.25	0.46
1:B:344:GLN:N	1:B:345:PRO:HD2	2.30	0.45
1:D:228:ALA:O	1:D:280:HIS:HE1	1.99	0.45
1:C:120:ILE:O	1:C:196:VAL:HA	2.16	0.45
1:C:228:ALA:O	1:C:280:HIS:HE1	2.00	0.45
1:A:228:ALA:O	1:A:280:HIS:HE1	2.00	0.45
1:A:37:PRO:HB2	1:A:278:MET:CE	2.47	0.44
1:B:298:ILE:CG2	1:B:336[A]:HIS:HE1	2.30	0.44
1:B:82:ALA:HB2	1:B:180:ALA:HB1	1.99	0.44
1:D:37:PRO:HB2	1:D:278:MET:CE	2.48	0.44
1:D:199:CYS:HA	1:D:222:GLN:O	2.18	0.44
1:D:132:THR:CG2	6:D:603:HOH:O	2.63	0.44
1:B:37:PRO:HB2	1:B:278:MET:CE	2.47	0.44
1:B:228:ALA:O	1:B:280:HIS:HE1	2.01	0.43
1:D:108:LEU:HD12	1:D:116:TYR:CD2	2.53	0.43
1:C:146:ASP:HB3	6:C:511:HOH:O	2.16	0.43
1:C:54:TRP:N	1:C:55:PRO:CD	2.82	0.43
1:A:237:GLU:HG2	2:E:1:NAG:H82	2.00	0.43
1:B:128:PRO:HG2	1:B:344:GLN:HE22	1.84	0.43
1:A:146:ASP:OD2	1:A:201:ARG:NH1	2.52	0.43
1:C:226:GLN:NE2	1:C:235:ALA:HB2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LYS:HE2	6:A:639:HOH:O	2.18	0.43
1:B:54:TRP:N	1:B:55:PRO:CD	2.82	0.43
1:C:108:LEU:HD12	1:C:116:TYR:CD2	2.54	0.42
1:D:154:PHE:CG	1:D:169:ALA:HB1	2.54	0.42
1:B:259:SER:HB2	6:B:521:HOH:O	2.19	0.42
1:A:126:SER:OG	1:A:199[B]:CYS:SG	2.72	0.42
1:A:54:TRP:N	1:A:55:PRO:CD	2.82	0.42
1:C:168:ILE:HD12	1:C:168:ILE:HA	1.95	0.42
1:B:226:GLN:NE2	1:B:235:ALA:HB2	2.34	0.42
1:B:287:PRO:HB2	1:B:325:TYR:CE2	2.55	0.42
1:D:54:TRP:N	1:D:55:PRO:CD	2.82	0.42
1:A:168:ILE:HD12	1:A:168:ILE:HA	1.95	0.42
1:B:154:PHE:CG	1:B:169:ALA:HB1	2.55	0.42
1:D:226:GLN:NE2	1:D:235:ALA:HB2	2.35	0.42
1:A:154:PHE:CG	1:A:169:ALA:HB1	2.54	0.41
1:B:70:TYR:CD1	1:B:70:TYR:N	2.85	0.41
1:C:350:PHE:CE1	1:C:362:THR:HB	2.55	0.41
1:C:37:PRO:HB2	1:C:278:MET:CE	2.49	0.41
1:B:168:ILE:HD12	1:B:168:ILE:HA	1.93	0.41
1:B:81:THR:N	6:B:509:HOH:O	2.53	0.41
1:A:226:GLN:NE2	1:A:235:ALA:HB2	2.35	0.41
1:A:50:LYS:HD2	1:A:387:SER:OG	2.20	0.41
1:A:105:ASN:OD1	6:A:601:HOH:O	2.22	0.41
1:A:287:PRO:HB2	1:A:325:TYR:CE2	2.55	0.41
1:A:350:PHE:CE1	1:A:362:THR:HB	2.55	0.41
1:B:60:GLU:HA	6:B:511:HOH:O	2.19	0.41
1:B:323[B]:LYS:HD3	1:B:323[B]:LYS:H	1.85	0.41
1:D:350:PHE:CE1	1:D:362:THR:HB	2.55	0.41
1:B:66[B]:GLN:HA	1:B:70:TYR:O	2.21	0.40
1:B:146:ASP:OD2	1:B:201:ARG:NH2	2.54	0.40
1:C:154:PHE:CG	1:C:169:ALA:HB1	2.56	0.40
1:B:387:SER:HB2	6:B:571:HOH:O	2.21	0.40
1:C:199:CYS:HA	1:C:222:GLN:O	2.22	0.40
1:C:220:LEU:HD23	1:C:291:LEU:HB3	2.03	0.40
1:D:128:PRO:CG	1:D:344:GLN:HE22	2.34	0.40
1:D:76:ARG:HA	1:D:77:PRO:HD3	1.96	0.40
1:B:350:PHE:CE1	1:B:362:THR:HB	2.56	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	370/394 (94%)	347 (94%)	23 (6%)	0	100	100
1	B	371/394 (94%)	348 (94%)	23 (6%)	0	100	100
1	C	368/394 (93%)	348 (95%)	20 (5%)	0	100	100
1	D	367/394 (93%)	345 (94%)	22 (6%)	0	100	100
All	All	1476/1576 (94%)	1388 (94%)	88 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	301/321 (94%)	293 (97%)	8 (3%)	44	63
1	B	302/321 (94%)	296 (98%)	6 (2%)	55	73
1	C	299/321 (93%)	293 (98%)	6 (2%)	55	73
1	D	298/321 (93%)	291 (98%)	7 (2%)	50	68
All	All	1200/1284 (94%)	1173 (98%)	27 (2%)	50	68

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	160	SER

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Mol	Chain	Res	Type
1	A	201	ARG
1	A	227	SER
1	A	244	LYS
1	A	330	GLN
1	A	332	SER
1	A	346	GLU
1	B	23	ASN
1	B	24	LEU
1	B	70	TYR
1	B	227	SER
1	B	330	GLN
1	B	346	GLU
1	C	29	ASN
1	C	227	SER
1	C	332	SER
1	C	334	SER
1	C	346	GLU
1	C	389	LEU
1	D	29	ASN
1	D	76	ARG
1	D	227	SER
1	D	330	GLN
1	D	332	SER
1	D	334	SER
1	D	346	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	HIS
1	A	226	GLN
1	A	280	HIS
1	A	308	HIS
1	A	330	GLN
1	A	333	HIS
1	A	344	GLN
1	B	226	GLN
1	B	250	GLN
1	B	280	HIS
1	B	308	HIS
1	B	330	GLN
1	B	344	GLN

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Mol	Chain	Res	Type
1	C	29	ASN
1	C	226	GLN
1	C	280	HIS
1	C	308	HIS
1	C	344	GLN
1	D	23	ASN
1	D	226	GLN
1	D	280	HIS
1	D	308	HIS
1	D	317	HIS
1	D	330	GLN
1	D	344	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)

20 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	1.19	2 (14%)	17,19,21	2.18	5 (29%)
2	NAG	E	2	2	14,14,15	0.54	0	17,19,21	1.13	1 (5%)
2	BMA	E	3	2	11,11,12	0.43	0	15,15,17	2.11	4 (26%)
2	MAN	E	4	2	11,11,12	0.51	0	15,15,17	1.61	3 (20%)
3	NAG	F	1	3,1	14,14,15	0.47	0	17,19,21	2.87	10 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	F	2	3	14,14,15	0.58	0	17,19,21	2.48	6 (35%)
3	BMA	F	3	3	11,11,12	0.39	0	15,15,17	1.08	2 (13%)
3	MAN	F	4	3	11,11,12	0.31	0	15,15,17	1.32	3 (20%)
3	MAN	F	5	3	11,11,12	0.33	0	15,15,17	0.87	1 (6%)
4	NAG	G	1	4,1	14,14,15	0.45	0	17,19,21	2.05	2 (11%)
4	NAG	G	2	4	14,14,15	0.41	0	17,19,21	1.62	4 (23%)
4	BMA	G	3	4	11,11,12	0.38	0	15,15,17	1.48	3 (20%)
4	MAN	G	4	4	11,11,12	0.59	0	15,15,17	1.64	3 (20%)
4	MAN	G	5	4	11,11,12	0.33	0	15,15,17	1.56	3 (20%)
4	MAN	G	6	4	11,11,12	0.48	0	15,15,17	1.57	2 (13%)
3	NAG	H	1	3,1	14,14,15	0.54	0	17,19,21	2.24	4 (23%)
3	NAG	H	2	3	14,14,15	0.55	0	17,19,21	0.96	0
3	BMA	H	3	3	11,11,12	0.24	0	15,15,17	1.86	6 (40%)
3	MAN	H	4	3	11,11,12	0.40	0	15,15,17	1.04	1 (6%)
3	MAN	H	5	3	11,11,12	0.53	0	15,15,17	1.20	1 (6%)

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	-	1/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
2	MAN	E	4	2	-	2/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	5/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	F	5	3	-	0/2/19/22	0/1/1/1
4	NAG	G	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	2/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
4	MAN	G	5	4	-	1/2/19/22	0/1/1/1
4	MAN	G	6	4	-	0/2/19/22	0/1/1/1

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAG	O5-C5	-2.48	1.38	1.43
2	E	1	NAG	C2-N2	-2.25	1.42	1.46

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	1	NAG	C1-O5-C5	7.45	122.29	112.19
3	F	1	NAG	C1-O5-C5	7.29	122.08	112.19
4	G	1	NAG	C1-O5-C5	6.50	121.00	112.19
3	F	2	NAG	C1-O5-C5	-5.15	105.22	112.19
2	E	3	BMA	C1-O5-C5	5.00	118.96	112.19
3	F	1	NAG	C3-C4-C5	4.76	118.73	110.24
2	E	1	NAG	O5-C1-C2	-4.34	104.43	111.29
3	F	2	NAG	C8-C7-N2	4.29	123.37	116.10
4	G	3	BMA	C1-O5-C5	4.28	117.99	112.19
3	F	2	NAG	C4-C3-C2	-4.23	104.83	111.02
2	E	3	BMA	C1-C2-C3	4.21	114.84	109.67
2	E	1	NAG	O3-C3-C4	-3.95	101.22	110.35
4	G	1	NAG	C3-C4-C5	3.93	117.26	110.24
4	G	2	NAG	C3-C4-C5	3.86	117.13	110.24
4	G	6	MAN	O5-C5-C6	3.83	113.21	107.20
3	H	3	BMA	C1-O5-C5	3.82	117.36	112.19
2	E	4	MAN	O5-C5-C6	3.66	112.94	107.20
2	E	1	NAG	O4-C4-C3	-3.58	102.08	110.35
3	H	3	BMA	C2-C3-C4	-3.55	104.75	110.89
4	G	4	MAN	C1-O5-C5	3.50	116.94	112.19
3	F	1	NAG	C1-C2-N2	-3.45	104.59	110.49
3	F	2	NAG	O7-C7-N2	-3.41	115.69	121.95
3	F	2	NAG	C2-N2-C7	3.39	127.73	122.90
4	G	4	MAN	C3-C4-C5	3.28	116.10	110.24
4	G	5	MAN	C1-O5-C5	3.23	116.56	112.19
2	E	4	MAN	C1-O5-C5	3.21	116.53	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	3	BMA	C2-C3-C4	-3.06	105.60	110.89
2	E	1	NAG	C2-N2-C7	-3.04	118.58	122.90
3	H	5	MAN	C1-O5-C5	3.03	116.29	112.19
3	F	1	NAG	C6-C5-C4	-3.02	105.92	113.00
3	F	1	NAG	C2-N2-C7	2.94	127.09	122.90
2	E	1	NAG	C3-C4-C5	2.86	115.35	110.24
3	H	1	NAG	O5-C5-C6	2.80	111.59	107.20
4	G	5	MAN	O5-C1-C2	-2.78	106.48	110.77
2	E	2	NAG	C3-C4-C5	2.78	115.19	110.24
3	F	1	NAG	O3-C3-C4	-2.77	103.94	110.35
3	H	3	BMA	O2-C2-C1	-2.69	103.64	109.15
3	F	3	BMA	C2-C3-C4	-2.62	106.36	110.89
4	G	6	MAN	O5-C1-C2	-2.60	106.75	110.77
3	F	1	NAG	C4-C3-C2	2.59	114.81	111.02
4	G	2	NAG	C4-C3-C2	2.56	114.77	111.02
4	G	4	MAN	O4-C4-C3	-2.55	104.46	110.35
3	H	4	MAN	C2-C3-C4	-2.49	106.59	110.89
2	E	4	MAN	C1-C2-C3	2.43	112.66	109.67
3	F	4	MAN	C2-C3-C4	-2.41	106.72	110.89
3	H	3	BMA	C1-C2-C3	2.40	112.62	109.67
3	F	4	MAN	C1-O5-C5	2.35	115.37	112.19
4	G	2	NAG	C1-C2-N2	-2.33	106.50	110.49
2	E	3	BMA	O2-C2-C1	-2.30	104.45	109.15
4	G	5	MAN	C1-C2-C3	-2.26	106.89	109.67
3	F	4	MAN	O5-C1-C2	-2.26	107.29	110.77
3	F	3	BMA	O3-C3-C4	2.24	115.54	110.35
4	G	2	NAG	O3-C3-C2	-2.24	104.83	109.47
3	F	1	NAG	C8-C7-N2	2.22	119.87	116.10
3	H	3	BMA	C3-C4-C5	-2.18	106.34	110.24
4	G	3	BMA	C1-C2-C3	-2.17	107.00	109.67
3	F	1	NAG	O7-C7-N2	-2.15	118.00	121.95
3	F	2	NAG	O5-C5-C4	-2.12	105.68	110.83
3	F	1	NAG	O3-C3-C2	2.11	113.83	109.47
3	H	1	NAG	C6-C5-C4	-2.10	108.09	113.00
4	G	3	BMA	C2-C3-C4	-2.08	107.29	110.89
3	H	3	BMA	O4-C4-C5	2.06	114.41	109.30
3	H	1	NAG	C2-N2-C7	2.05	125.82	122.90
3	F	5	MAN	C1-C2-C3	2.02	112.15	109.67

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	2	NAG	O5-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
4	G	3	BMA	C4-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
2	E	4	MAN	C4-C5-C6-O6
3	F	3	BMA	C4-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6
2	E	4	MAN	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	H	3	BMA	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
3	H	3	BMA	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
3	H	5	MAN	C4-C5-C6-O6
3	H	4	MAN	C4-C5-C6-O6
4	G	5	MAN	O5-C5-C6-O6
3	F	2	NAG	C3-C2-N2-C7
3	H	4	MAN	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6
3	H	5	MAN	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6

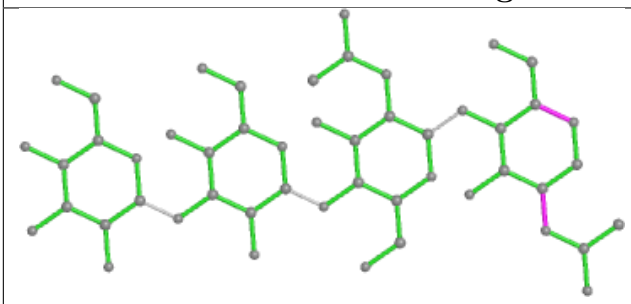
There are no ring outliers.

3 monomers are involved in 2 short contacts:

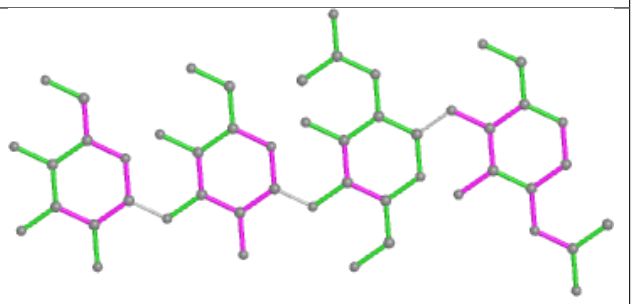
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	1	0
4	G	3	BMA	1	0
4	G	6	MAN	1	0

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

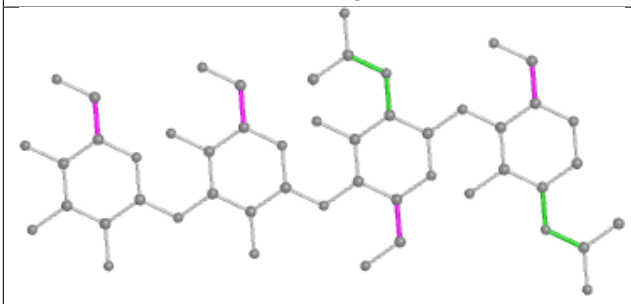
Oligosaccharide Chain E



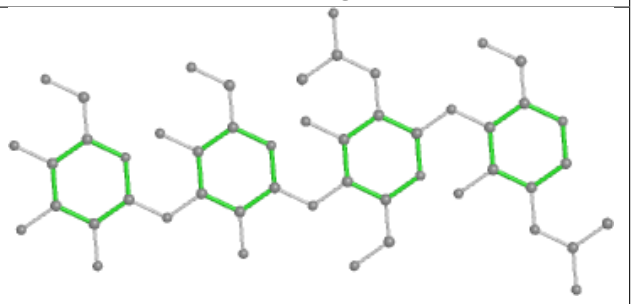
Bond lengths



Bond angles

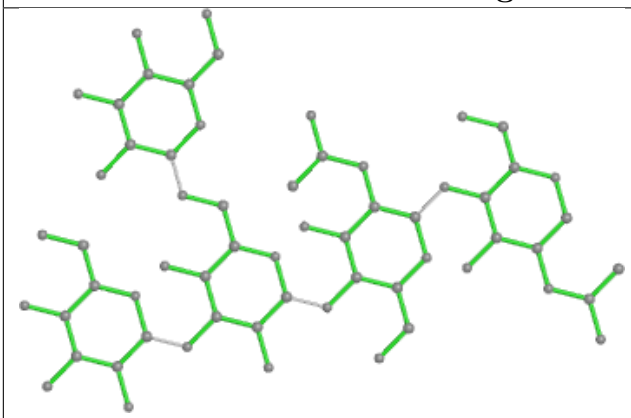


Torsions

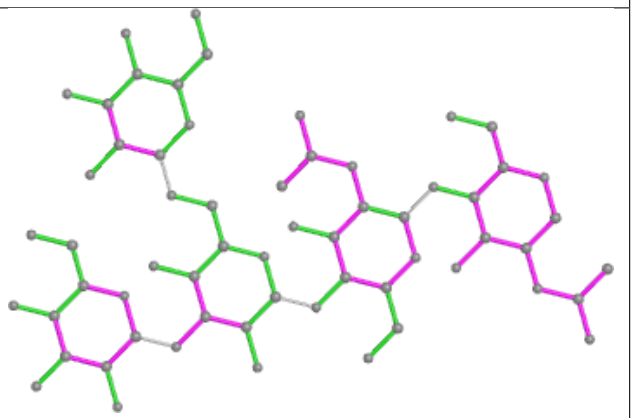


Rings

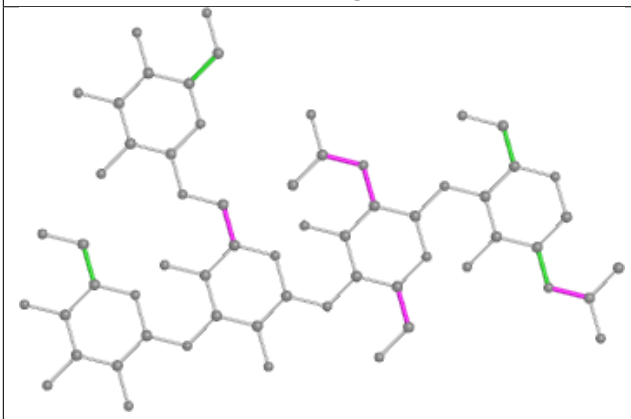
Oligosaccharide Chain F



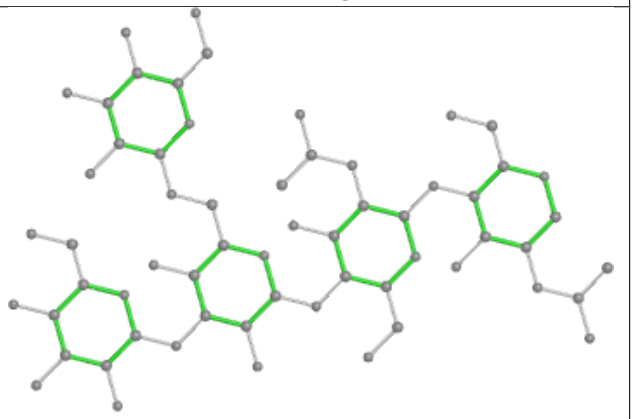
Bond lengths



Bond angles

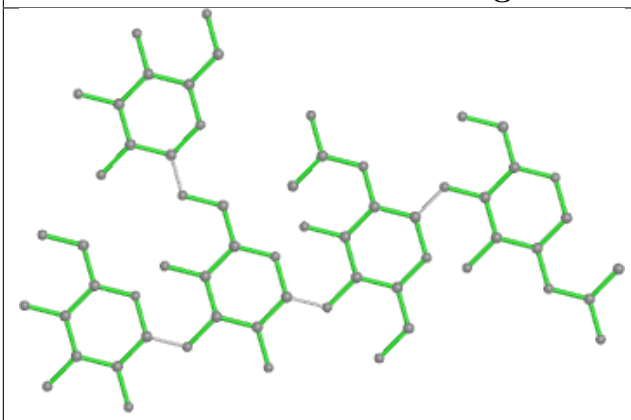


Torsions

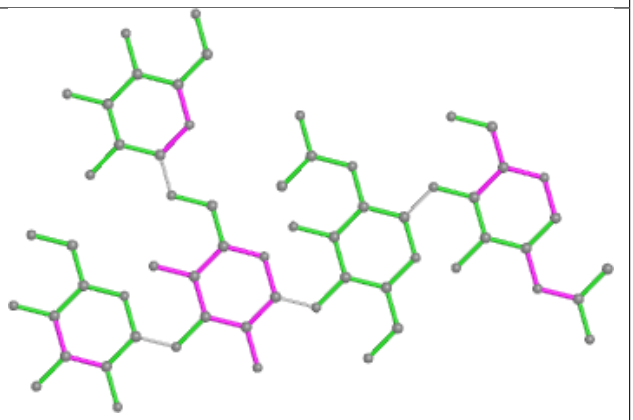


Rings

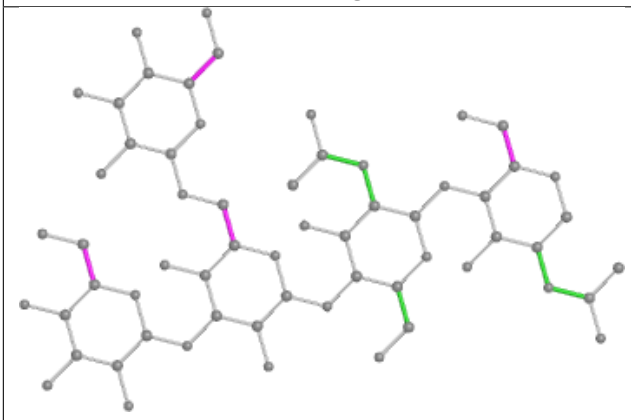
Oligosaccharide Chain H



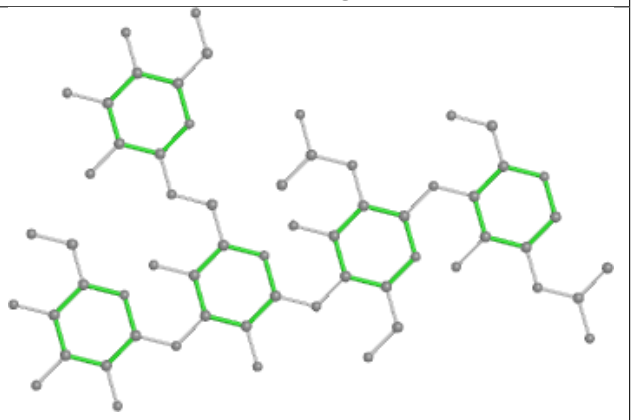
Bond lengths



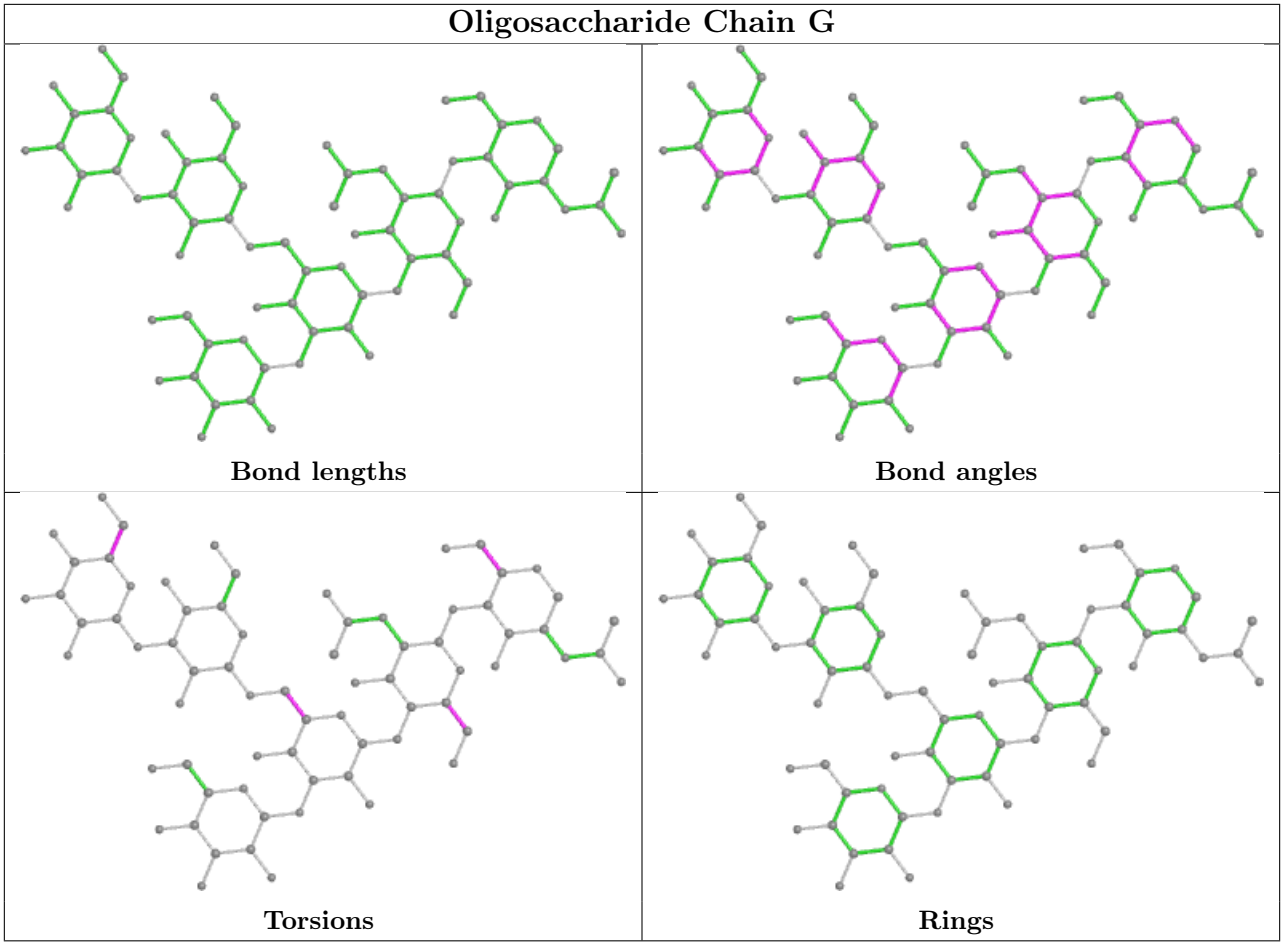
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

2 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	FMT	D	501	-	2,2,2	0.38	0	1,1,1	0.13	0
5	FMT	A	501	-	2,2,2	0.35	0	1,1,1	0.17	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	370/394 (93%)	-0.01	5 (1%)	75	73	40, 61, 84, 107	0
1	B	370/394 (93%)	-0.03	2 (0%)	91	91	35, 56, 77, 129	0
1	C	370/394 (93%)	-0.07	2 (0%)	91	91	39, 59, 87, 144	0
1	D	369/394 (93%)	0.16	13 (3%)	44	40	41, 67, 94, 162	0
All	All	1479/1576 (93%)	0.01	22 (1%)	73	71	35, 60, 88, 162	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	358	LYS	4.2
1	A	388	GLY	3.8
1	D	389	LEU	3.6
1	C	326	PHE	3.4
1	A	52	ASP	3.0
1	A	361	LYS	3.0
1	D	357	ALA	2.8
1	D	87	ASN	2.6
1	C	83	ALA	2.5
1	D	23	ASN	2.5
1	D	385	SER	2.4
1	D	21	CYS	2.3
1	D	253	ASN	2.2
1	D	384	PRO	2.2
1	B	350	PHE	2.2
1	A	249	HIS	2.2
1	D	386	LEU	2.2
1	A	357	ALA	2.1
1	D	40	PHE	2.1
1	D	362	THR	2.1
1	D	387	SER	2.1
1	B	353	ARG	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)

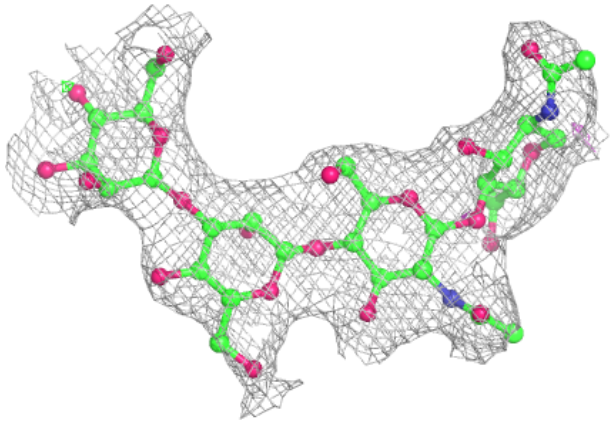
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

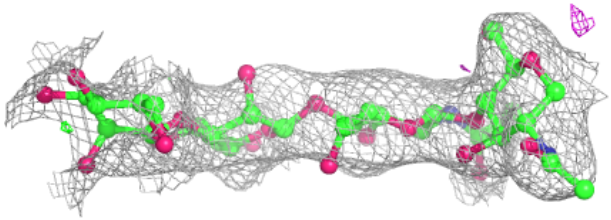
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MAN	F	5	11/12	0.35	0.32	115,157,181,181	0
3	BMA	F	3	11/12	0.42	0.28	138,175,185,200	0
2	MAN	E	4	11/12	0.44	0.22	128,173,182,191	0
3	MAN	F	4	11/12	0.51	0.29	153,172,190,195	0
4	MAN	G	6	11/12	0.57	0.31	107,140,155,164	0
3	MAN	H	5	11/12	0.60	0.36	121,144,152,155	0
3	MAN	H	4	11/12	0.64	0.26	122,145,161,163	0
4	MAN	G	4	11/12	0.67	0.25	71,126,148,181	0
4	MAN	G	5	11/12	0.69	0.21	104,143,165,174	0
3	BMA	H	3	11/12	0.77	0.18	125,135,149,161	0
4	BMA	G	3	11/12	0.82	0.32	121,143,163,168	0
2	BMA	E	3	11/12	0.88	0.21	105,129,138,144	0
3	NAG	F	2	14/15	0.89	0.18	85,95,106,121	0
2	NAG	E	2	14/15	0.90	0.13	62,74,90,90	0
4	NAG	G	2	14/15	0.90	0.20	76,83,94,113	0
3	NAG	H	2	14/15	0.92	0.33	82,99,107,116	0
3	NAG	F	1	14/15	0.94	0.12	58,70,78,81	0
2	NAG	E	1	14/15	0.94	0.18	59,71,86,90	0
4	NAG	G	1	14/15	0.95	0.14	46,65,69,75	0
3	NAG	H	1	14/15	0.96	0.21	49,56,68,69	0

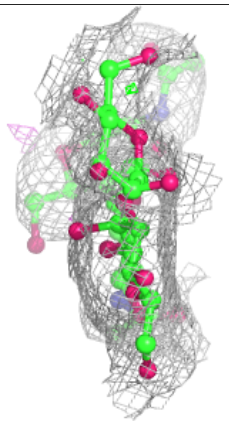
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

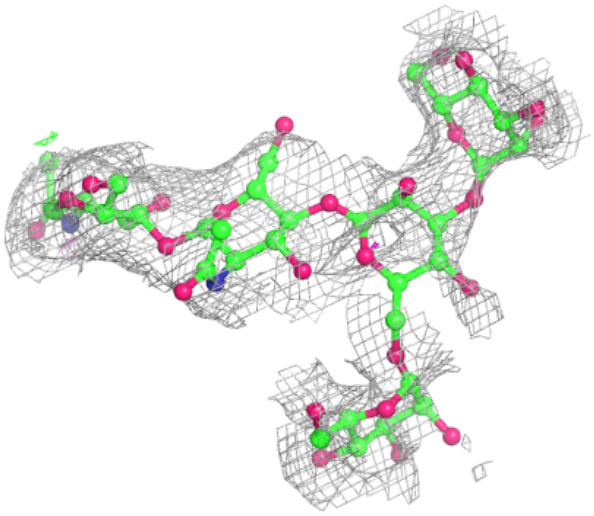


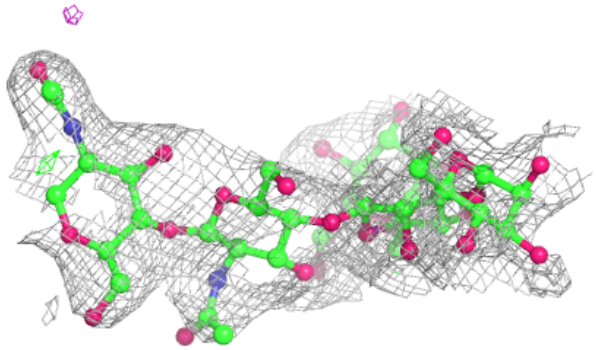


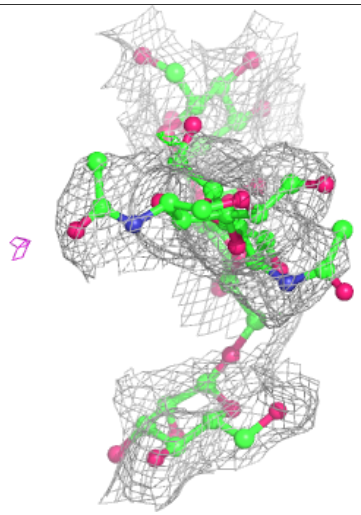


Electron density around Chain F:

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

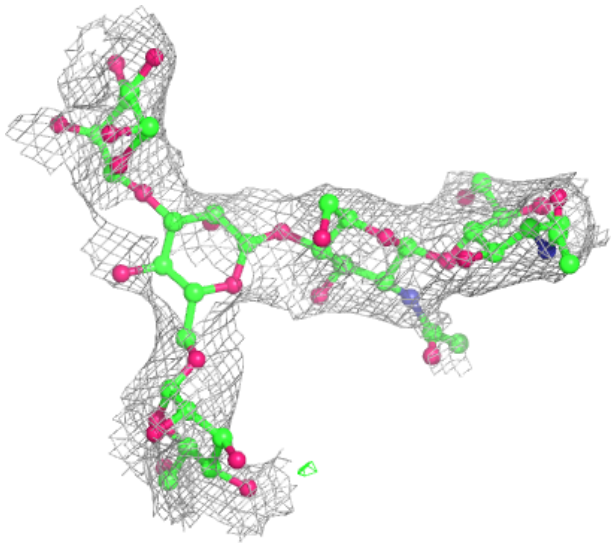


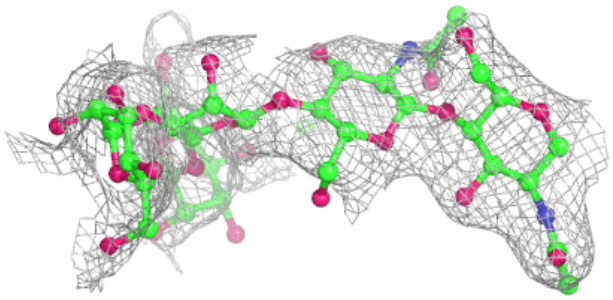


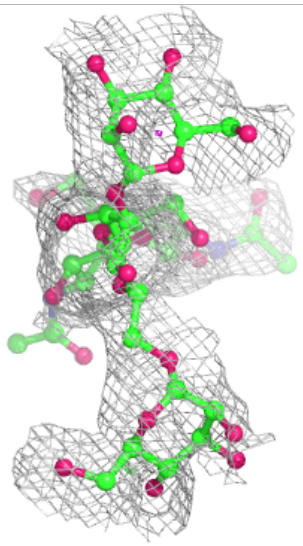


Electron density around Chain H:

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

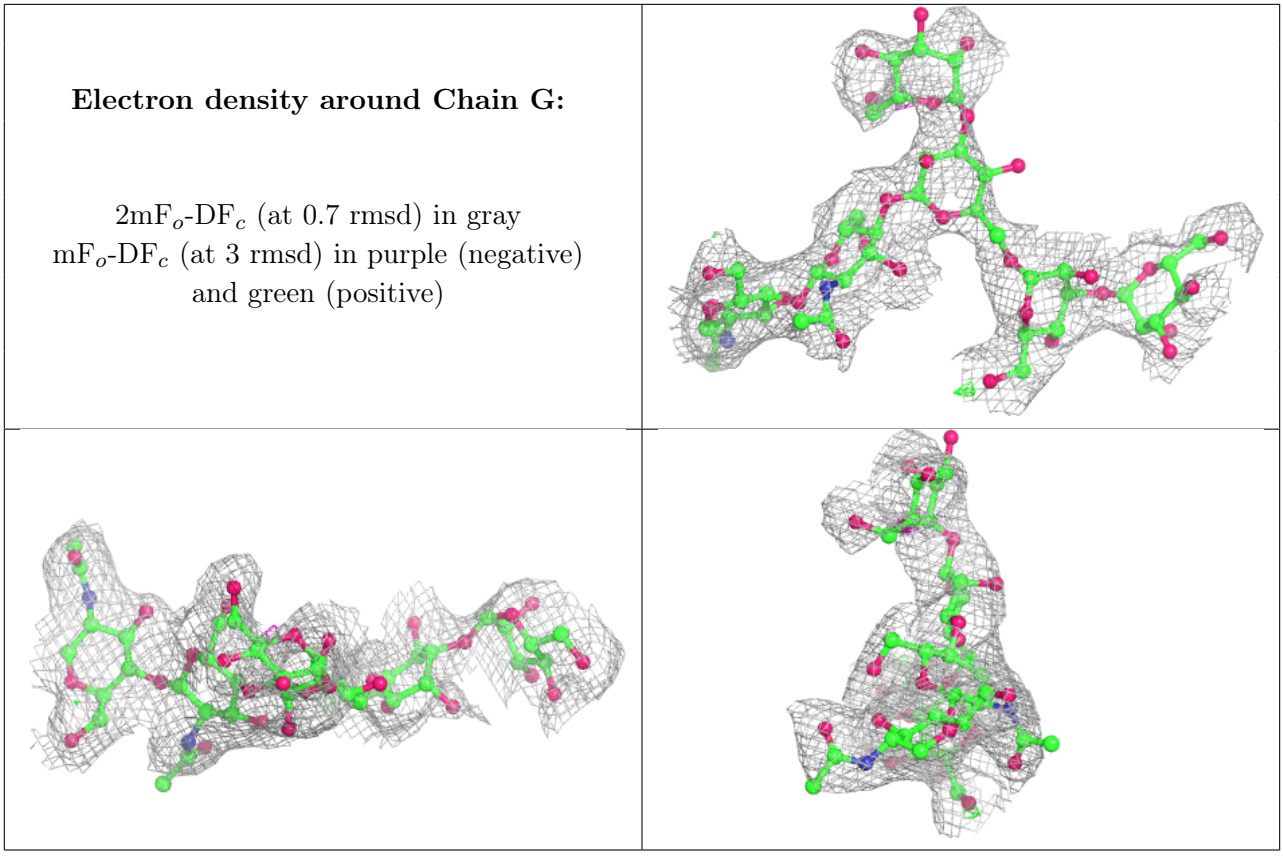






Electron density around Chain G:

$2mF_o$-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
5	FMT	A	501	3/3	0.74	0.17	69,69,73,74	0
5	FMT	D	501	3/3	0.79	0.23	60,60,61,63	0

6.5 Other polymers

There are no such residues in this entry.