Full wwPDB X-ray Structure Validation Report (i)

Jun 4, 2025 – 04:07 pm BST

PDB ID	:	9QQN / pdb_00009qqn
Title	:	Junin virus GP1-GP2 heterodimer in complex with Fab of JUN1
Authors	:	Bowden, T.A.; Paesen, G.C.
Deposited on	:	2025-04-01
Resolution	:	2.55 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

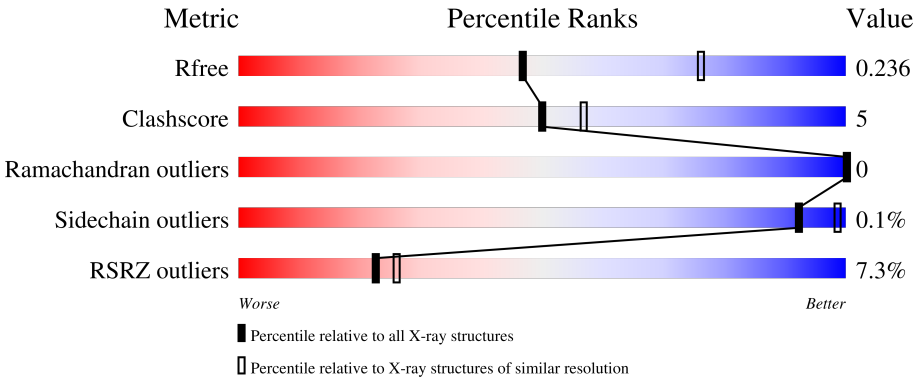
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.55 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}	164625	1004 (2.54-2.54)
Clashscore	180529	1055 (2.54-2.54)
Ramachandran outliers	177936	1048 (2.54-2.54)
Sidechain outliers	177891	1048 (2.54-2.54)
RSRZ outliers	164620	1004 (2.54-2.54)

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	454	3% 35% 6% 60%
1	B	454	4% 27% 5% 69%
2	C	217	7% 85% 12% .
3	D	242	5% 81% 12% 7%
4	E	4	50% 50%

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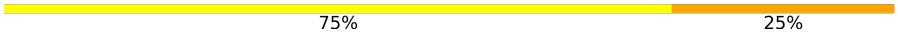
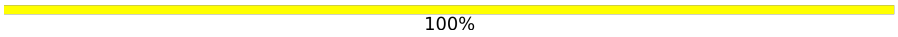
Mol	Chain	Length	Quality of chain
5	F	3	
6	G	4	
7	H	5	
8	I	2	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6406 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 Pre-glycoprotein polyprotein GP complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	0	0
			1478	948	253	265	12			
1	B	142	Total	C	N	O	S	0	0	0
			1166	750	191	212	13			

There are 86 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	CYS	LEU	conflict	UNP C1K9J9
A	249	ARG	SER	conflict	UNP C1K9J9
A	250	ARG	LEU	conflict	UNP C1K9J9
A	251	ARG	LYS	conflict	UNP C1K9J9
A	329	CYS	MET	conflict	UNP C1K9J9
A	417	SER	-	expression tag	UNP C1K9J9
A	418	GLY	-	expression tag	UNP C1K9J9
A	419	ASP	-	expression tag	UNP C1K9J9
A	420	ASP	-	expression tag	UNP C1K9J9
A	421	ASP	-	expression tag	UNP C1K9J9
A	422	ASP	-	expression tag	UNP C1K9J9
A	423	LYS	-	expression tag	UNP C1K9J9
A	424	GLY	-	expression tag	UNP C1K9J9
A	425	SER	-	expression tag	UNP C1K9J9
A	426	GLY	-	expression tag	UNP C1K9J9
A	427	TRP	-	expression tag	UNP C1K9J9
A	428	SER	-	expression tag	UNP C1K9J9
A	429	HIS	-	expression tag	UNP C1K9J9
A	430	PRO	-	expression tag	UNP C1K9J9
A	431	GLN	-	expression tag	UNP C1K9J9
A	432	PHE	-	expression tag	UNP C1K9J9
A	433	GLU	-	expression tag	UNP C1K9J9
A	434	LYS	-	expression tag	UNP C1K9J9
A	435	GLY	-	expression tag	UNP C1K9J9
A	436	GLY	-	expression tag	UNP C1K9J9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	437	GLY	-	expression tag	UNP C1K9J9
A	438	SER	-	expression tag	UNP C1K9J9
A	439	GLY	-	expression tag	UNP C1K9J9
A	440	GLY	-	expression tag	UNP C1K9J9
A	441	GLY	-	expression tag	UNP C1K9J9
A	442	SER	-	expression tag	UNP C1K9J9
A	443	GLY	-	expression tag	UNP C1K9J9
A	444	GLY	-	expression tag	UNP C1K9J9
A	445	SER	-	expression tag	UNP C1K9J9
A	446	ALA	-	expression tag	UNP C1K9J9
A	447	TRP	-	expression tag	UNP C1K9J9
A	448	SER	-	expression tag	UNP C1K9J9
A	449	HIS	-	expression tag	UNP C1K9J9
A	450	PRO	-	expression tag	UNP C1K9J9
A	451	GLN	-	expression tag	UNP C1K9J9
A	452	PHE	-	expression tag	UNP C1K9J9
A	453	GLU	-	expression tag	UNP C1K9J9
A	454	LYS	-	expression tag	UNP C1K9J9
B	88	CYS	LEU	conflict	UNP C1K9J9
B	249	ARG	SER	conflict	UNP C1K9J9
B	250	ARG	LEU	conflict	UNP C1K9J9
B	251	ARG	LYS	conflict	UNP C1K9J9
B	329	CYS	MET	conflict	UNP C1K9J9
B	417	SER	-	expression tag	UNP C1K9J9
B	418	GLY	-	expression tag	UNP C1K9J9
B	419	ASP	-	expression tag	UNP C1K9J9
B	420	ASP	-	expression tag	UNP C1K9J9
B	421	ASP	-	expression tag	UNP C1K9J9
B	422	ASP	-	expression tag	UNP C1K9J9
B	423	LYS	-	expression tag	UNP C1K9J9
B	424	GLY	-	expression tag	UNP C1K9J9
B	425	SER	-	expression tag	UNP C1K9J9
B	426	GLY	-	expression tag	UNP C1K9J9
B	427	TRP	-	expression tag	UNP C1K9J9
B	428	SER	-	expression tag	UNP C1K9J9
B	429	HIS	-	expression tag	UNP C1K9J9
B	430	PRO	-	expression tag	UNP C1K9J9
B	431	GLN	-	expression tag	UNP C1K9J9
B	432	PHE	-	expression tag	UNP C1K9J9
B	433	GLU	-	expression tag	UNP C1K9J9
B	434	LYS	-	expression tag	UNP C1K9J9
B	435	GLY	-	expression tag	UNP C1K9J9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	436	GLY	-	expression tag	UNP C1K9J9
B	437	GLY	-	expression tag	UNP C1K9J9
B	438	SER	-	expression tag	UNP C1K9J9
B	439	GLY	-	expression tag	UNP C1K9J9
B	440	GLY	-	expression tag	UNP C1K9J9
B	441	GLY	-	expression tag	UNP C1K9J9
B	442	SER	-	expression tag	UNP C1K9J9
B	443	GLY	-	expression tag	UNP C1K9J9
B	444	GLY	-	expression tag	UNP C1K9J9
B	445	SER	-	expression tag	UNP C1K9J9
B	446	ALA	-	expression tag	UNP C1K9J9
B	447	TRP	-	expression tag	UNP C1K9J9
B	448	SER	-	expression tag	UNP C1K9J9
B	449	HIS	-	expression tag	UNP C1K9J9
B	450	PRO	-	expression tag	UNP C1K9J9
B	451	GLN	-	expression tag	UNP C1K9J9
B	452	PHE	-	expression tag	UNP C1K9J9
B	453	GLU	-	expression tag	UNP C1K9J9
B	454	LYS	-	expression tag	UNP C1K9J9

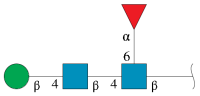
- Molecule 2 is a protein called Chains: C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	211	Total	C	N	O	S	0	0	0
			1637	1023	275	332	7			

- Molecule 3 is a protein called Chains: D.

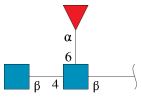
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	226	Total	C	N	O	S	0	0	0
			1724	1090	289	337	8			

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



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

- Molecule 5 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.

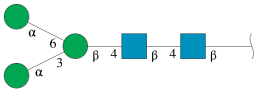


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	F	3	Total C N O 38 22 2 14	0	0	0

- Molecule 6 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
6	G	4	Total C N O 50 28 2 20	0	0	0

- Molecule 7 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
7	H	5	Total C N O 61 34 2 25	0	0	0

- Molecule 8 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
8	I	2	Total C N O 28 16 2 10	0	0	0

- Molecule 9 is water.

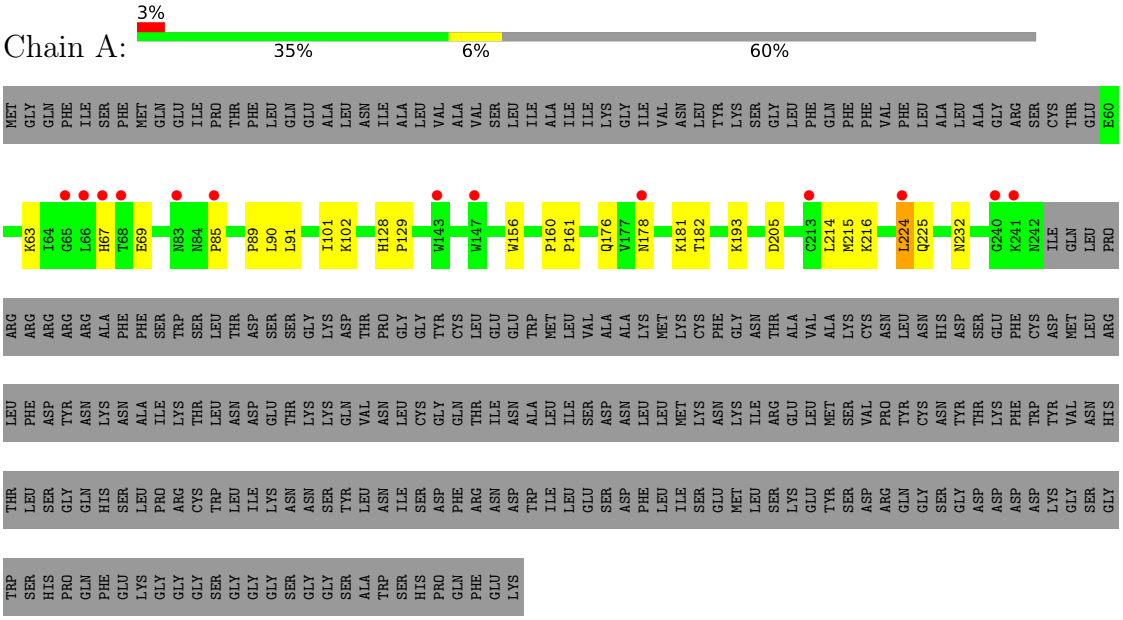
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	59	Total O 59 59	0	0
9	B	28	Total O 28 28	0	0
9	C	45	Total O 45 45	0	0
9	D	43	Total O 43 43	0	0

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.

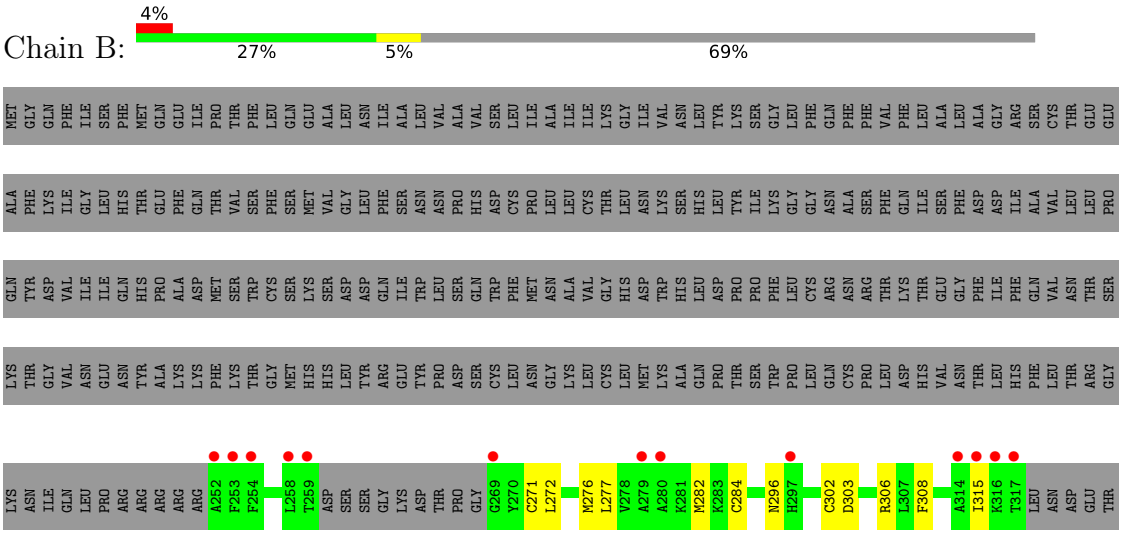
• Molecule 1: Pre-glycoprotein polyprotein GP complex

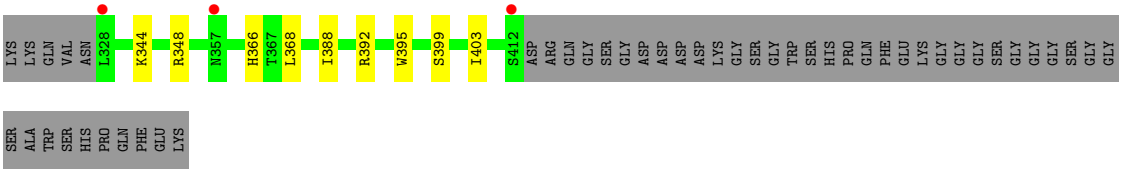
Chain A:



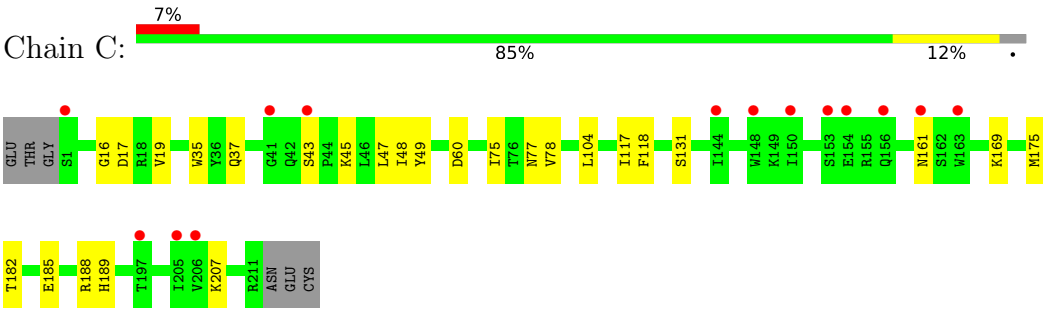
• Molecule 1: Pre-glycoprotein polyprotein GP complex

Chain B:

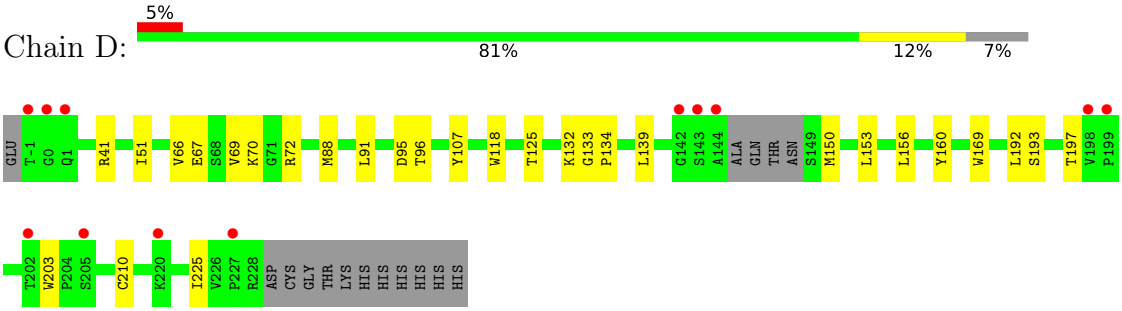




• Molecule 2: Chains: C



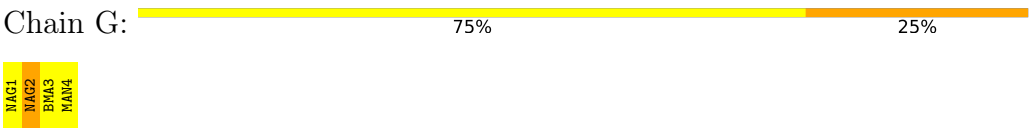
• Molecule 3: Chains: D



• Molecule 4: 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

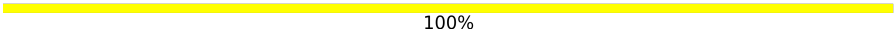
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

• Molecule 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



• Molecule 7: 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 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	226.47Å 73.03Å 80.73Å 90.00° 95.78° 90.00°	Depositor
Resolution (Å)	80.32 – 2.55 80.32 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.3 (80.32-2.55) 99.3 (80.32-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.201 , 0.237 0.202 , 0.236	Depositor DCC
R_{free} test set	2100 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	64.0	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 73.9	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	0.95	EDS
Total number of atoms	6406	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.12	0/1524	0.36	0/2069
1	B	0.13	0/1193	0.32	0/1609
2	C	0.12	0/1673	0.30	0/2273
3	D	0.12	0/1767	0.34	0/2409
All	All	0.12	0/6157	0.33	0/8360

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	1478	0	1414	18	0
1	B	1166	0	1125	14	0
2	C	1637	0	1580	18	0
3	D	1724	0	1684	18	0
4	E	49	0	43	0	0
5	F	38	0	34	0	0
6	G	50	0	43	1	0
7	H	61	0	52	0	0
8	I	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	59	0	0	0	0
9	B	28	0	0	0	0
9	C	45	0	0	0	0
9	D	43	0	0	0	0
All	All	6406	0	6000	64	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 (64) 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:272:LEU:HD23	1:B:277:LEU:HD21	1.70	0.74
1:A:178:ASN:HA	1:A:214:LEU:HD23	1.70	0.73
3:D:139:LEU:HD21	3:D:156:LEU:HB2	1.71	0.72
1:A:225:GLN:N	1:A:225:GLN:OE1	2.25	0.69
3:D:96:THR:HG23	3:D:125:THR:HA	1.75	0.68
2:C:37:GLN:HB2	2:C:47:LEU:HD11	1.75	0.68
1:B:303:ASP:OD1	1:B:306:ARG:NH1	2.31	0.64
1:A:182:THR:HG21	6:G:2:NAG:H82	1.80	0.62
1:B:276:MET:HE2	1:B:308:PHE:HB3	1.82	0.62
3:D:132:LYS:HD3	3:D:133:GLY:N	2.19	0.57
3:D:88:MET:HE2	3:D:91:LEU:HD21	1.87	0.57
2:C:188:ARG:HD2	2:C:189:HIS:HE1	1.71	0.56
1:B:392:ARG:HA	1:B:395:TRP:NE1	2.20	0.56
1:A:63:LYS:HG2	1:A:69:GLU:HG3	1.87	0.56
1:A:85:PRO:HD3	1:B:315:ILE:HG22	1.87	0.55
1:A:128:HIS:ND1	1:A:129:PRO:HD2	2.22	0.54
2:C:131:SER:HA	2:C:179:LEU:O	2.08	0.54
2:C:16:GLY:HA2	2:C:77:ASN:HD22	1.74	0.53
2:C:188:ARG:HD2	2:C:189:HIS:CE1	2.45	0.52
3:D:150:MET:HE2	3:D:197:THR:HG22	1.93	0.50
1:B:388:ILE:H	1:B:388:ILE:HD12	1.76	0.50
2:C:35:TRP:HB2	2:C:48:ILE:HB	1.93	0.49
3:D:153:LEU:HD13	3:D:225:ILE:HG21	1.95	0.49
2:C:19:VAL:HG12	2:C:75:ILE:HB	1.95	0.49
1:B:392:ARG:HA	1:B:395:TRP:CE2	2.48	0.48
1:B:296:ASN:O	1:B:306:ARG:NH2	2.47	0.48
1:B:366:HIS:CD2	1:B:368:LEU:HB3	2.49	0.48
1:A:176:GLN:HA	1:A:215:MET:O	2.15	0.47
3:D:41:ARG:HD3	3:D:51:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:134:PRO:HB3	3:D:160:TYR:HB3	1.96	0.47
1:A:224:LEU:HD22	1:A:224:LEU:H	1.80	0.46
1:A:129:PRO:HD3	1:A:156:TRP:CD2	2.51	0.45
3:D:192:LEU:HD23	3:D:193:SER:H	1.81	0.45
3:D:169:TRP:CZ3	3:D:210:CYS:HB3	2.52	0.45
1:A:193:LYS:NZ	1:A:205:ASP:OD2	2.45	0.45
2:C:182:THR:HG23	2:C:185:GLU:H	1.82	0.45
3:D:192:LEU:HD23	3:D:193:SER:N	2.32	0.44
1:A:90:LEU:O	1:A:101:ILE:HA	2.17	0.44
1:B:272:LEU:O	1:B:282:MET:HA	2.18	0.44
3:D:153:LEU:HD11	3:D:203:TRP:CD2	2.53	0.44
2:C:118:PHE:CD1	3:D:139:LEU:HB3	2.52	0.44
3:D:72:ARG:NH2	3:D:95:ASP:OD2	2.48	0.44
1:B:399:SER:O	1:B:403:ILE:HG12	2.17	0.44
3:D:67:GLU:HA	3:D:70:LYS:HE3	2.01	0.43
1:A:67:HIS:ND1	1:A:67:HIS:N	2.67	0.43
2:C:60:ASP:N	2:C:60:ASP:OD1	2.45	0.43
2:C:169:LYS:HA	2:C:169:LYS:HD3	1.76	0.43
1:A:181:LYS:NZ	1:A:205:ASP:OD2	2.46	0.42
1:A:129:PRO:HD3	1:A:156:TRP:CE3	2.53	0.42
3:D:66:VAL:HG12	3:D:69:VAL:HG22	2.00	0.42
2:C:43:SER:OG	3:D:118:TRP:HB2	2.20	0.42
2:C:161:ASN:HB3	2:C:175:MET:HE3	2.01	0.42
2:C:17:ASP:O	2:C:78:VAL:HG23	2.20	0.42
2:C:19:VAL:HG21	2:C:104:LEU:HD11	2.03	0.41
2:C:49:TYR:CD1	3:D:107:TYR:HB3	2.55	0.41
1:A:91:LEU:HB2	1:A:232:ASN:HB3	2.02	0.41
2:C:117:ILE:HG22	2:C:207:LYS:HB3	2.03	0.41
1:A:89:PRO:HA	1:A:102:LYS:O	2.21	0.41
1:A:160:PRO:HA	1:A:161:PRO:HD3	1.92	0.41
1:B:344:LYS:O	1:B:348:ARG:HG3	2.21	0.41
1:B:271:CYS:HA	1:B:284:CYS:HA	2.04	0.40
1:A:216:LYS:HB2	1:A:216:LYS:HE2	1.87	0.40
1:B:302:CYS:O	1:B:306:ARG:HG3	2.21	0.40
2:C:45:LYS:HB3	2:C:45:LYS:HE3	1.83	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	181/454 (40%)	172 (95%)	9 (5%)	0	100	100
1	B	136/454 (30%)	129 (95%)	7 (5%)	0	100	100
2	C	209/217 (96%)	202 (97%)	7 (3%)	0	100	100
3	D	222/242 (92%)	216 (97%)	6 (3%)	0	100	100
All	All	748/1367 (55%)	719 (96%)	29 (4%)	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	166/401 (41%)	165 (99%)	1 (1%)	84	92
1	B	131/401 (33%)	131 (100%)	0	100	100
2	C	187/192 (97%)	187 (100%)	0	100	100
3	D	195/209 (93%)	195 (100%)	0	100	100
All	All	679/1203 (56%)	678 (100%)	1 (0%)	92	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	224	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	127	GLN
2	C	77	ASN
2	C	189	HIS
3	D	1	GLN
3	D	64	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

18 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	$\#\|Z\| > 2$
4	NAG	E	1	1,4	14,14,15	0.66	0	17,19,21	0.95	1 (5%)
4	NAG	E	2	4	14,14,15	0.72	0	17,19,21	0.94	0
4	BMA	E	3	4	11,11,12	0.90	0	15,15,17	2.55	7 (46%)
4	FUC	E	4	4	10,10,11	0.81	0	14,14,16	1.01	0
5	NAG	F	1	1,5	14,14,15	0.74	0	17,19,21	1.30	1 (5%)
5	NAG	F	2	5	14,14,15	0.73	0	17,19,21	0.78	0
5	FUC	F	3	5	10,10,11	0.82	0	14,14,16	0.99	0
6	NAG	G	1	1,6	14,14,15	0.77	0	17,19,21	1.10	1 (5%)
6	NAG	G	2	6	14,14,15	0.70	0	17,19,21	1.04	1 (5%)
6	BMA	G	3	6	11,11,12	0.86	0	15,15,17	2.88	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	MAN	G	4	6	11,11,12	0.62	0	15,15,17	1.68	1 (6%)
7	NAG	H	1	1,7	14,14,15	0.69	0	17,19,21	1.34	2 (11%)
7	NAG	H	2	7	14,14,15	0.71	0	17,19,21	0.99	1 (5%)
7	BMA	H	3	7	11,11,12	0.89	0	15,15,17	2.64	7 (46%)
7	MAN	H	4	7	11,11,12	0.67	0	15,15,17	1.71	1 (6%)
7	MAN	H	5	7	11,11,12	0.75	0	15,15,17	1.06	1 (6%)
8	NAG	I	1	1,8	14,14,15	0.74	0	17,19,21	1.21	2 (11%)
8	NAG	I	2	8	14,14,15	0.70	0	17,19,21	0.86	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
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	FUC	E	4	4	-	-	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	FUC	F	3	5	-	-	0/1/1/1
6	NAG	G	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	G	2	6	-	0/6/23/26	0/1/1/1
6	BMA	G	3	6	-	0/2/19/22	0/1/1/1
6	MAN	G	4	6	-	1/2/19/22	0/1/1/1
7	NAG	H	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	H	2	7	-	2/6/23/26	0/1/1/1
7	BMA	H	3	7	-	0/2/19/22	0/1/1/1
7	MAN	H	4	7	-	1/2/19/22	1/1/1/1
7	MAN	H	5	7	-	0/2/19/22	0/1/1/1
8	NAG	I	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	I	2	8	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	3	BMA	C1-O5-C5	9.09	124.51	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	H	3	BMA	C1-O5-C5	8.00	123.03	112.19
4	E	3	BMA	C1-O5-C5	7.09	121.80	112.19
6	G	4	MAN	C1-O5-C5	5.63	119.82	112.19
7	H	4	MAN	C1-O5-C5	5.41	119.53	112.19
7	H	1	NAG	C1-O5-C5	4.00	117.62	112.19
5	F	1	NAG	C1-O5-C5	3.63	117.11	112.19
4	E	3	BMA	C3-C4-C5	3.36	116.24	110.24
6	G	3	BMA	C3-C4-C5	3.27	116.07	110.24
4	E	3	BMA	C2-C3-C4	3.25	116.52	110.89
8	I	1	NAG	O4-C4-C3	-2.97	103.48	110.35
7	H	3	BMA	C3-C4-C5	2.88	115.37	110.24
7	H	5	MAN	C1-O5-C5	2.85	116.05	112.19
6	G	3	BMA	O5-C5-C4	2.58	117.09	110.83
7	H	3	BMA	C2-C3-C4	2.55	115.31	110.89
6	G	2	NAG	O5-C1-C2	-2.47	107.39	111.29
6	G	3	BMA	C2-C3-C4	2.46	115.16	110.89
4	E	3	BMA	O4-C4-C3	-2.46	104.66	110.35
7	H	2	NAG	O5-C1-C2	-2.45	107.42	111.29
7	H	3	BMA	C1-C2-C3	2.42	112.64	109.67
7	H	3	BMA	O4-C4-C3	-2.34	104.93	110.35
6	G	1	NAG	O4-C4-C3	-2.29	105.05	110.35
4	E	3	BMA	O3-C3-C2	-2.29	105.61	109.99
6	G	3	BMA	O3-C3-C2	-2.27	105.64	109.99
4	E	3	BMA	C1-C2-C3	2.17	112.34	109.67
7	H	3	BMA	O5-C5-C4	2.11	115.95	110.83
8	I	1	NAG	O5-C1-C2	-2.05	108.05	111.29
4	E	1	NAG	O5-C1-C2	-2.04	108.07	111.29
6	G	3	BMA	O4-C4-C3	-2.04	105.63	110.35
4	E	3	BMA	O5-C5-C4	2.04	115.78	110.83
7	H	3	BMA	O3-C3-C2	-2.00	106.16	109.99
7	H	1	NAG	O5-C1-C2	-2.00	108.13	111.29

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	1	NAG	C8-C7-N2-C2
6	G	1	NAG	O7-C7-N2-C2
7	H	1	NAG	C8-C7-N2-C2
7	H	1	NAG	O7-C7-N2-C2
7	H	2	NAG	C8-C7-N2-C2
7	H	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
8	I	2	NAG	C8-C7-N2-C2
8	I	2	NAG	O7-C7-N2-C2
6	G	4	MAN	O5-C5-C6-O6
7	H	4	MAN	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

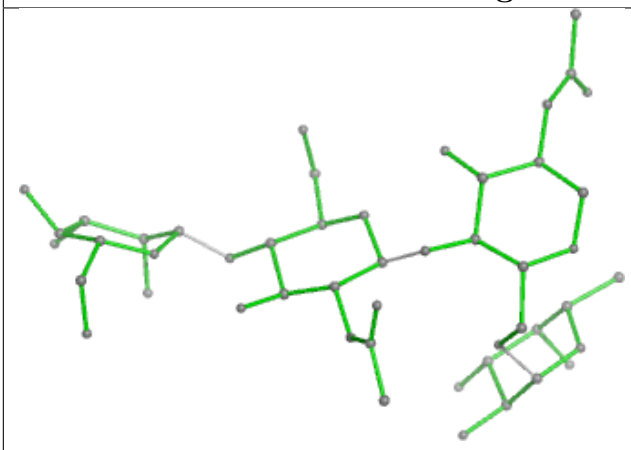
Mol	Chain	Res	Type	Atoms
7	H	4	MAN	C1-C2-C3-C4-C5-O5

1 monomer is involved in 1 short contact:

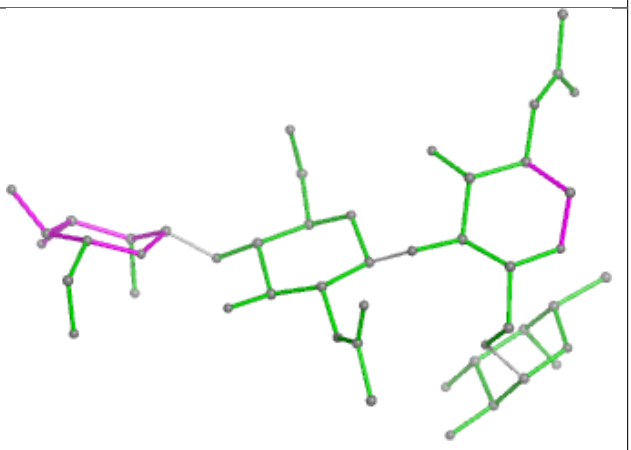
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	2	NAG	1	0

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

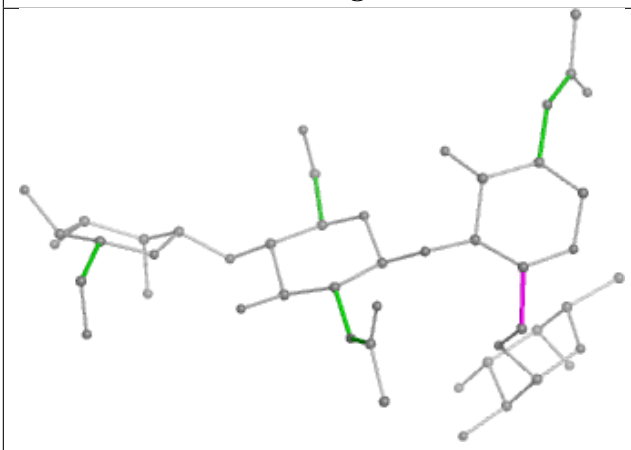
Oligosaccharide Chain E



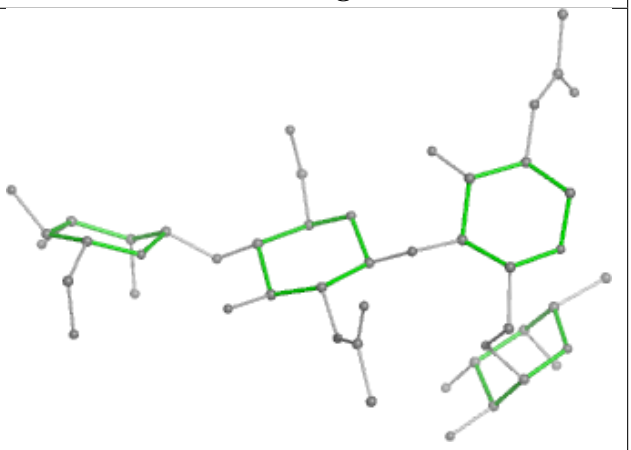
Bond lengths



Bond angles

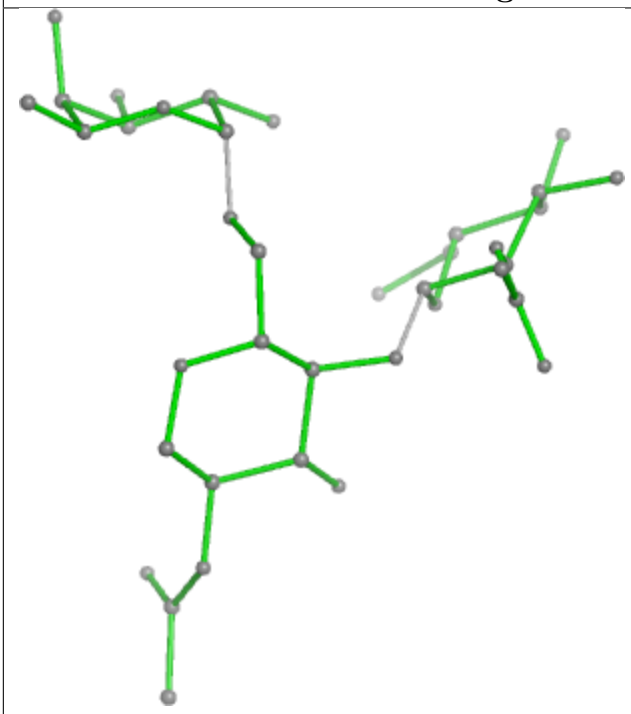


Torsions

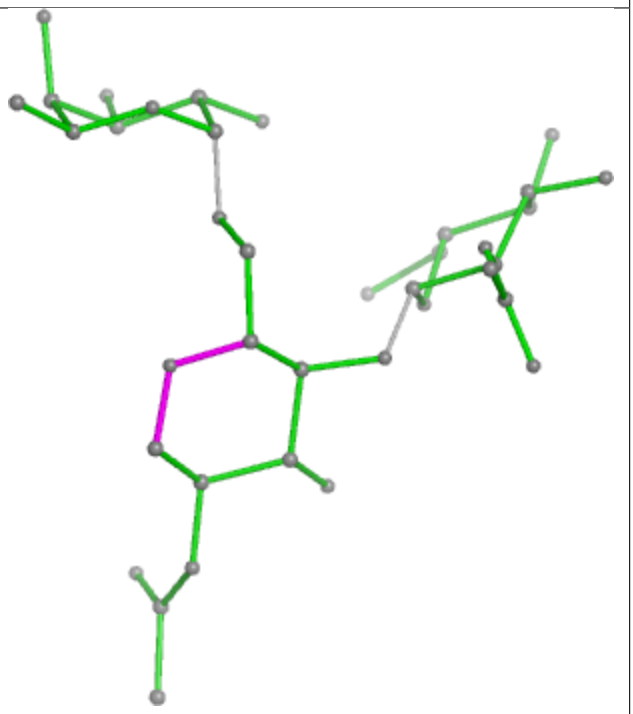


Rings

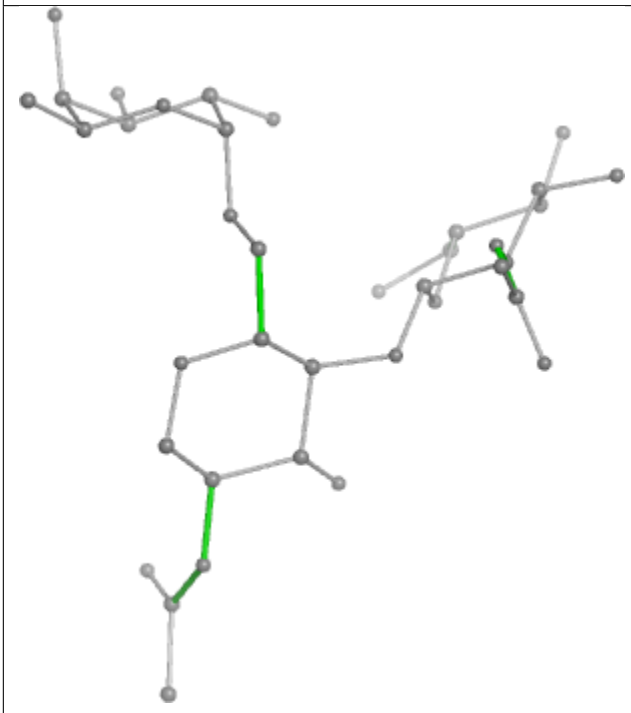
Oligosaccharide Chain F



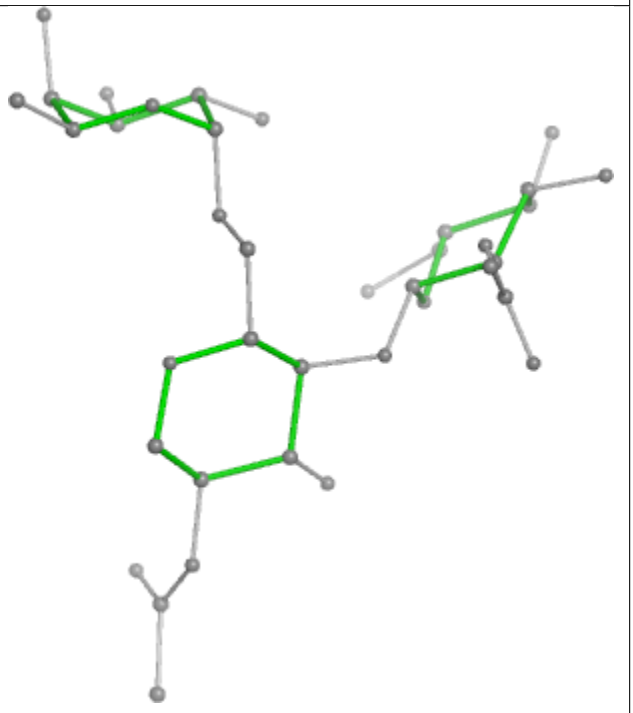
Bond lengths



Bond angles

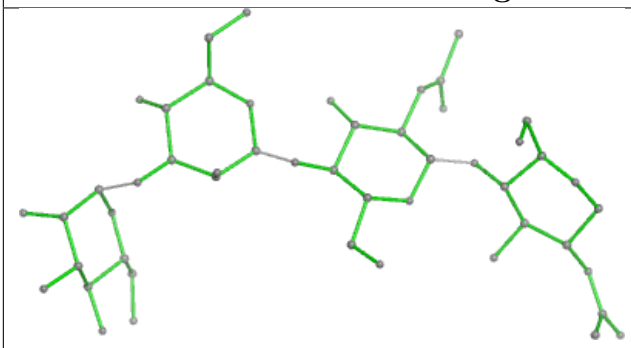


Torsions

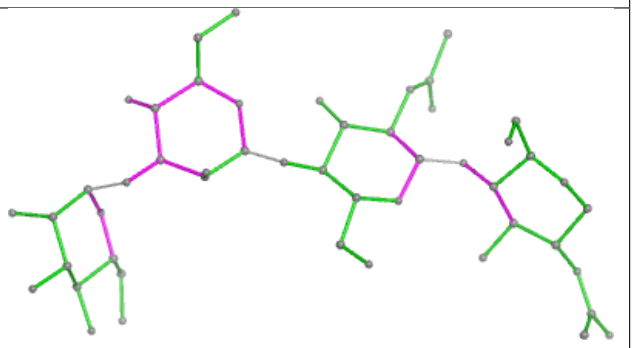


Rings

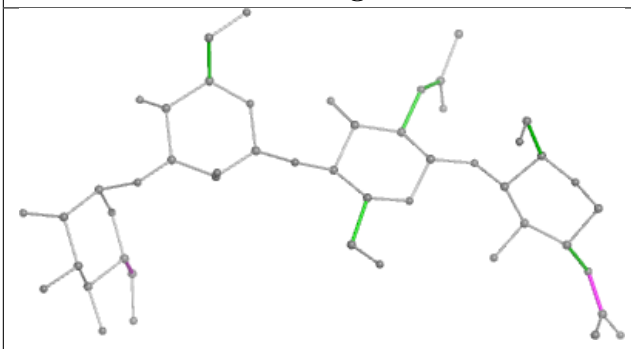
Oligosaccharide Chain G



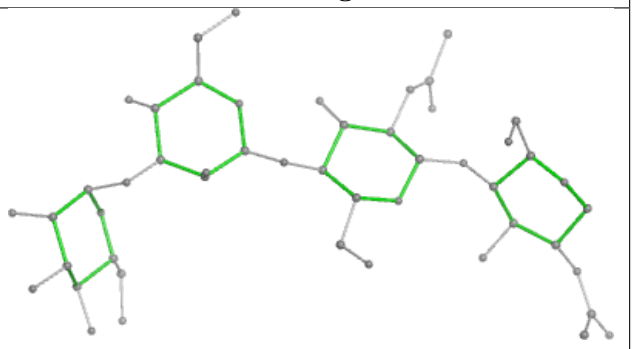
Bond lengths



Bond angles

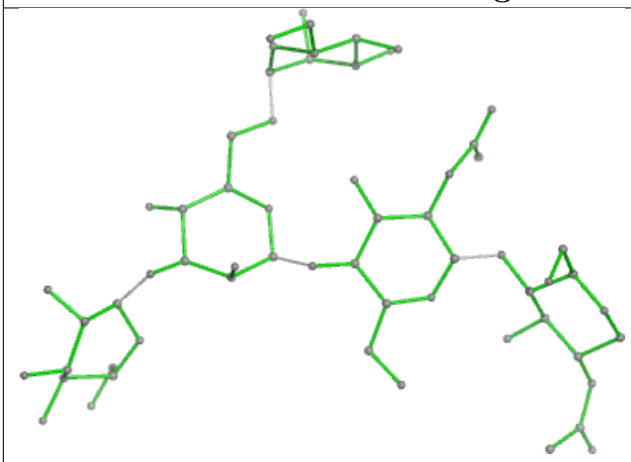


Torsions

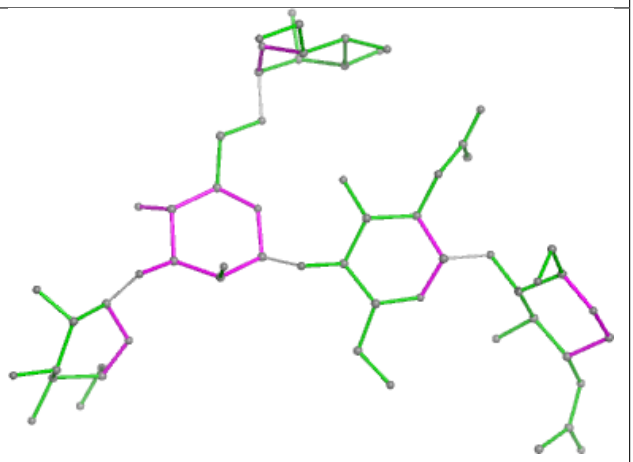


Rings

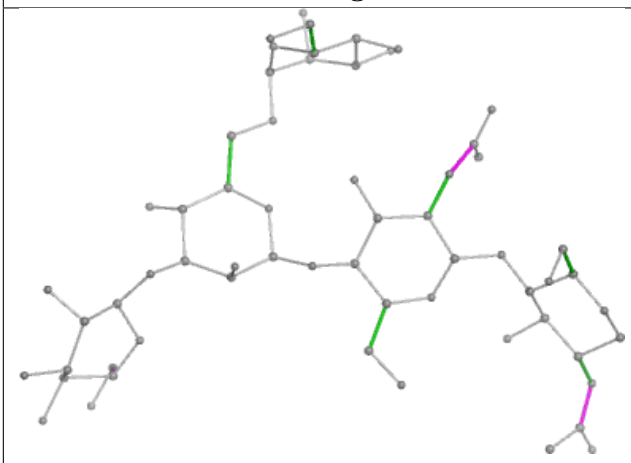
Oligosaccharide Chain H



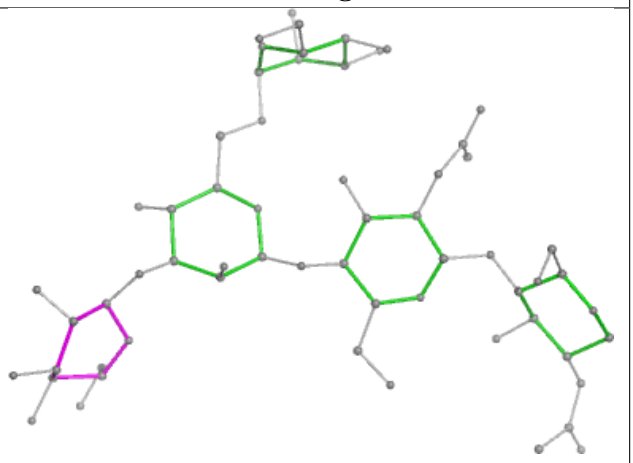
Bond lengths



Bond angles

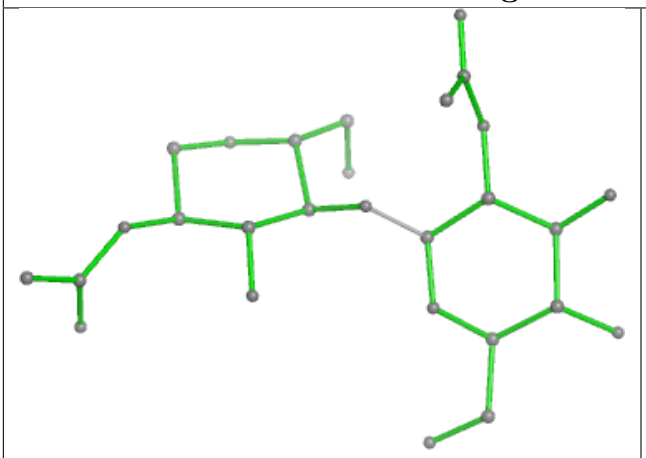


Torsions

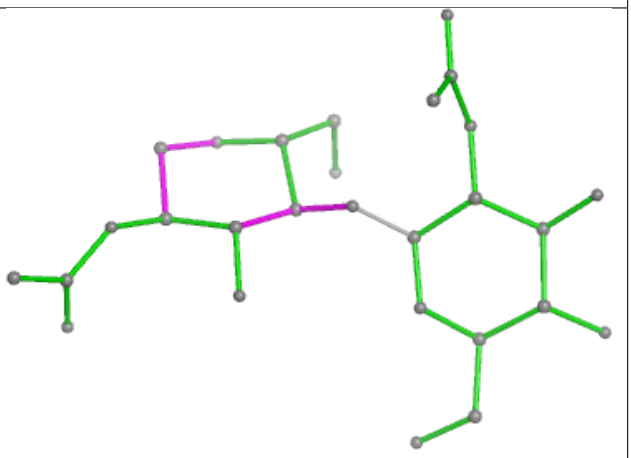


Rings

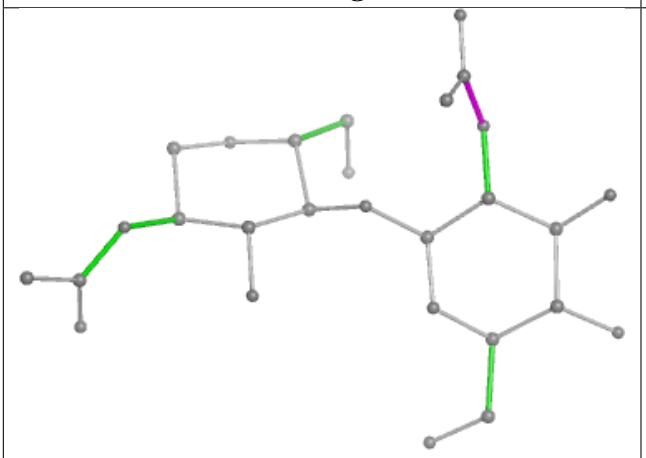
Oligosaccharide Chain I



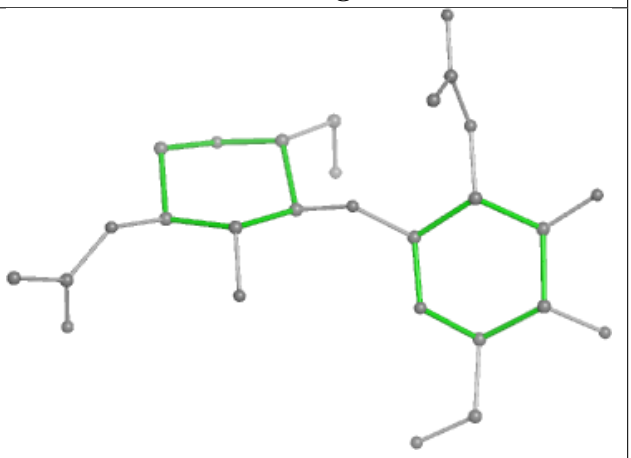
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	183/454 (40%)	0.18	13 (7%)	23	27	44, 64, 105, 141	0
1	B	142/454 (31%)	0.68	16 (11%)	11	14	51, 75, 115, 143	0
2	C	211/217 (97%)	0.55	15 (7%)	23	27	42, 80, 129, 143	0
3	D	226/242 (93%)	0.40	12 (5%)	33	37	46, 78, 108, 131	0
All	All	762/1367 (55%)	0.44	56 (7%)	22	26	42, 73, 123, 143	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	328	LEU	5.4
1	B	317	THR	3.8
1	B	252	ALA	3.8
3	D	-1	THR	3.8
1	B	269	GLY	3.5
1	A	224	LEU	3.1
2	C	161	ASN	3.1
1	B	297	HIS	3.1
3	D	198	VAL	3.0
3	D	202	THR	2.9
1	A	66	LEU	2.9
1	B	412	SER	2.9
1	B	254	PHE	2.9
1	B	259	THR	2.8
2	C	148	TRP	2.8
2	C	163	TRP	2.8
2	C	154	GLU	2.7
3	D	142	GLY	2.7
3	D	143	SER	2.7
2	C	180	THR	2.7
2	C	1	SER	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	144	ILE	2.6
1	B	279	ALA	2.6
1	A	85	PRO	2.6
1	A	65	GLY	2.6
2	C	156	GLN	2.5
1	B	316	LYS	2.5
1	B	315	ILE	2.5
1	A	178	ASN	2.5
1	B	253	PHE	2.5
3	D	144	ALA	2.4
1	A	83	ASN	2.4
2	C	205	ILE	2.4
1	B	314	ALA	2.4
3	D	1	GLN	2.4
1	A	67	HIS	2.3
1	B	357	ASN	2.3
1	A	213	CYS	2.3
2	C	206	VAL	2.2
2	C	43	SER	2.2
1	B	258	LEU	2.2
3	D	220	LYS	2.2
1	B	280	ALA	2.2
2	C	41	GLY	2.1
1	A	143	TRP	2.1
3	D	227	PRO	2.1
3	D	205	SER	2.1
2	C	150	ILE	2.1
1	A	241	LYS	2.0
2	C	197	THR	2.0
3	D	199	PRO	2.0
1	A	240	GLY	2.0
3	D	0	GLY	2.0
1	A	147	TRP	2.0
1	A	68	THR	2.0
2	C	153	SER	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)

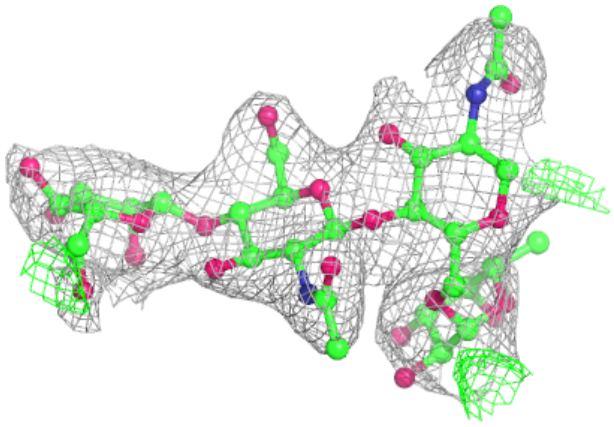
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

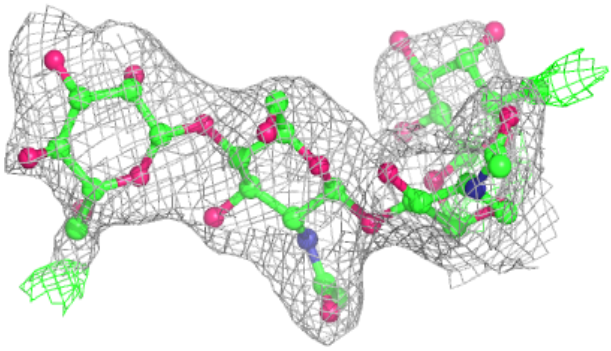
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	MAN	H	4	11/12	0.42	0.12	121,151,155,162	0
7	MAN	H	5	11/12	0.48	0.15	111,129,144,147	0
4	FUC	E	4	10/11	0.52	0.18	102,131,137,150	0
4	BMA	E	3	11/12	0.54	0.14	118,125,131,136	0
8	NAG	I	2	14/15	0.58	0.15	103,127,136,143	0
7	BMA	H	3	11/12	0.66	0.11	118,134,144,149	0
6	MAN	G	4	11/12	0.76	0.17	88,103,112,118	0
7	NAG	H	2	14/15	0.77	0.17	85,103,124,142	0
5	NAG	F	2	14/15	0.78	0.12	89,105,117,120	0
6	BMA	G	3	11/12	0.81	0.12	76,84,113,119	0
4	NAG	E	2	14/15	0.86	0.10	87,106,118,130	0
6	NAG	G	1	14/15	0.90	0.14	51,65,74,87	0
5	FUC	F	3	10/11	0.90	0.13	68,92,100,101	0
4	NAG	E	1	14/15	0.91	0.10	84,93,107,110	0
7	NAG	H	1	14/15	0.93	0.10	50,60,74,78	0
8	NAG	I	1	14/15	0.94	0.10	78,90,108,122	0
6	NAG	G	2	14/15	0.95	0.08	60,67,78,88	0
5	NAG	F	1	14/15	0.95	0.09	62,75,90,103	0

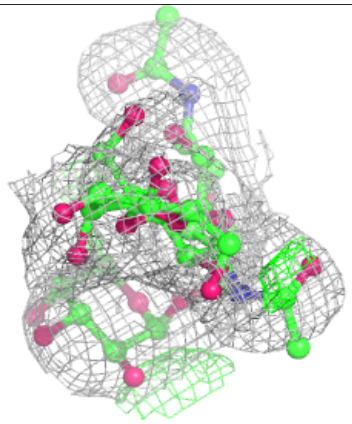
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

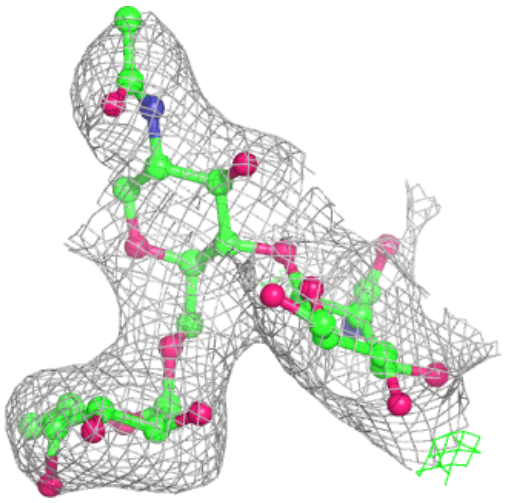


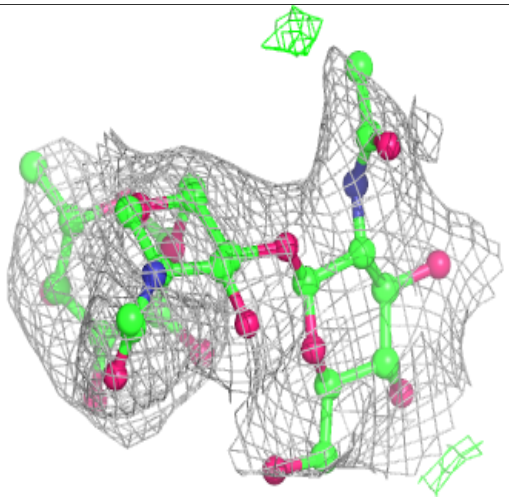


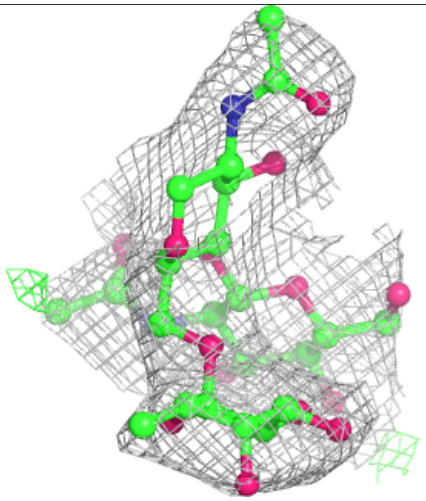


Electron density around Chain F:

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

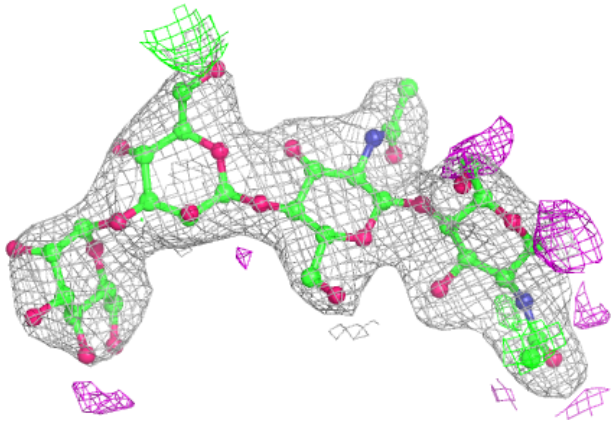


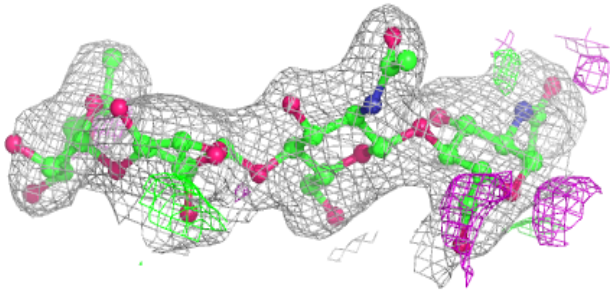


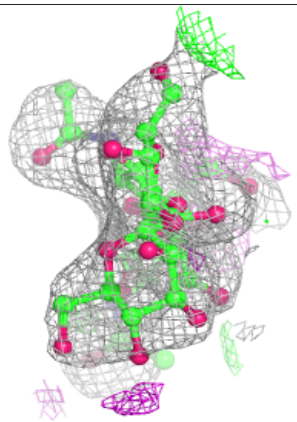


Electron density around Chain G:

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

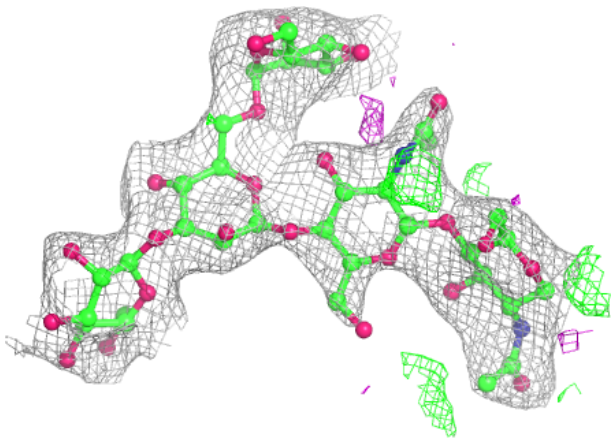


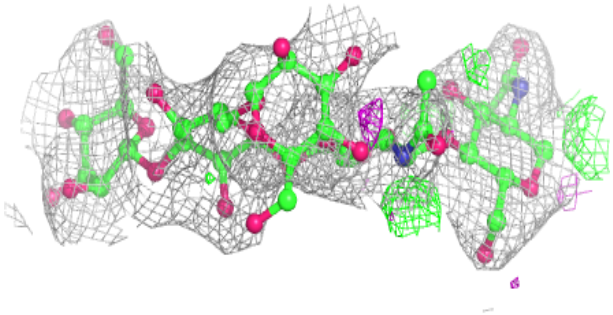


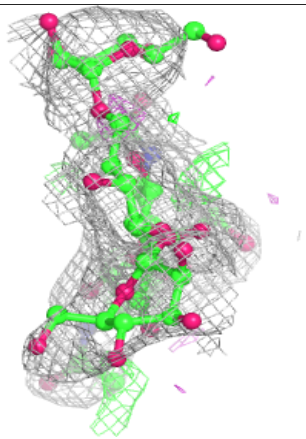


Electron density around Chain H:

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

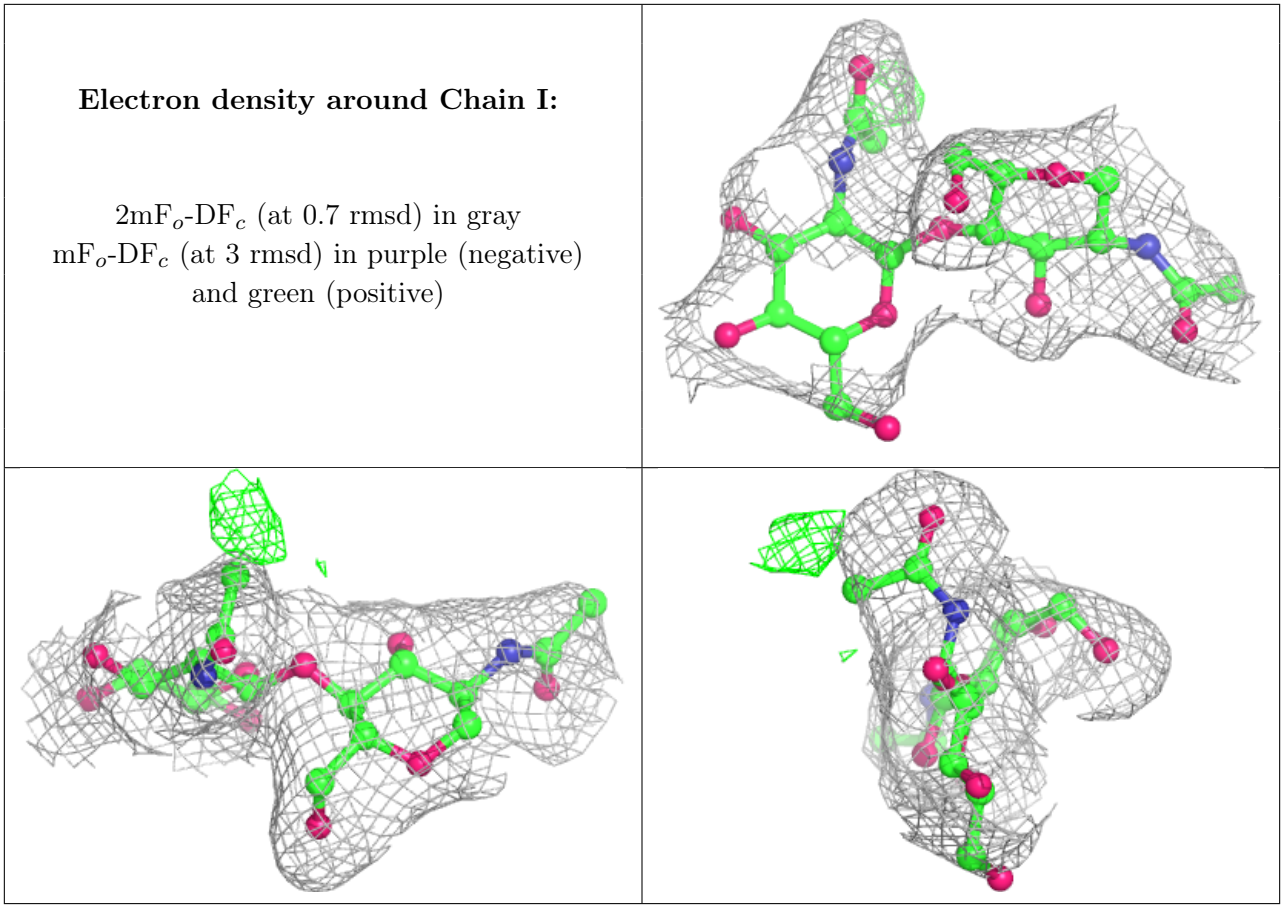






Electron density around Chain I:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.