Full wwPDB X-ray Structure Validation Report (i)

Jan 8, 2024 – 05:27 am GMT

PDB ID	:	6FG8
Title	:	Crystal structure of the BIR3 - SERK1 complex from Arabidopsis thaliana.
Authors	:	Hothorn, M.; Hohmann, U.
Deposited on	:	2018-01-10
Resolution	:	1.25 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 (1)) were used in the production of this report:

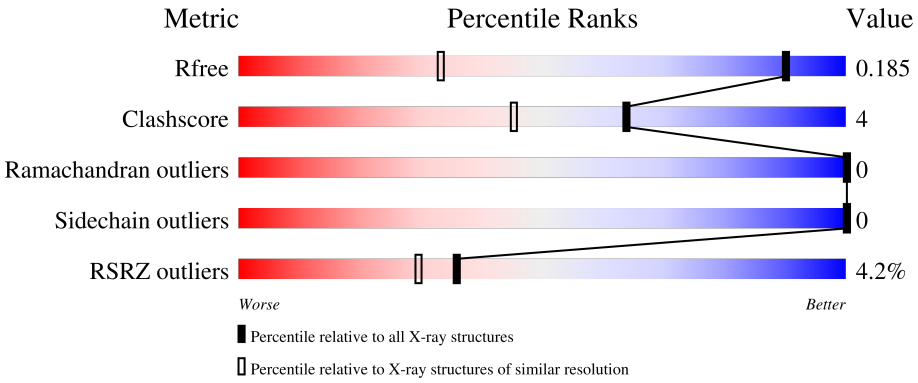
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.25 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	1023 (1.28-1.24)
Clashscore	141614	1060 (1.28-1.24)
Ramachandran outliers	138981	1029 (1.28-1.24)
Sidechain outliers	138945	1028 (1.28-1.24)
RSRZ outliers	127900	1004 (1.28-1.24)

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	265	3% 68% . 29%
2	B	241	3% 71% 7% 22%
3	C	2	100%
3	D	2	50% 50%
3	F	2	50% 50%

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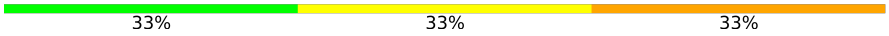
Mol	Chain	Length	Quality of chain
3	G	2	
4	E	3	
5	H	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BMA	E	3	-	-	-	X
5	FUC	H	2	-	-	-	X
5	NAG	H	3	-	-	-	X
6	PEG	B	304	-	X	X	-
6	PEG	B	305	-	-	X	-
6	PEG	B	306	-	X	-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 3628 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 Somatic embryogenesis receptor kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	6	0
			1453	917	246	284	6			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q94AG2
A	2	THR	-	expression tag	UNP Q94AG2
A	3	ARG	-	expression tag	UNP Q94AG2
A	4	LEU	-	expression tag	UNP Q94AG2
A	5	THR	-	expression tag	UNP Q94AG2
A	6	VAL	-	expression tag	UNP Q94AG2
A	7	LEU	-	expression tag	UNP Q94AG2
A	8	ALA	-	expression tag	UNP Q94AG2
A	9	LEU	-	expression tag	UNP Q94AG2
A	10	LEU	-	expression tag	UNP Q94AG2
A	11	ALA	-	expression tag	UNP Q94AG2
A	12	GLY	-	expression tag	UNP Q94AG2
A	13	LEU	-	expression tag	UNP Q94AG2
A	14	LEU	-	expression tag	UNP Q94AG2
A	15	ALA	-	expression tag	UNP Q94AG2
A	16	SER	-	expression tag	UNP Q94AG2
A	17	SER	-	expression tag	UNP Q94AG2
A	18	ARG	-	expression tag	UNP Q94AG2
A	19	ALA	-	expression tag	UNP Q94AG2
A	20	GLY	-	expression tag	UNP Q94AG2
A	21	SER	-	expression tag	UNP Q94AG2
A	22	SER	-	expression tag	UNP Q94AG2
A	23	MET	-	expression tag	UNP Q94AG2
A	209	PRO	-	expression tag	UNP Q94AG2
A	210	CYS	-	expression tag	UNP Q94AG2
A	211	PRO	-	expression tag	UNP Q94AG2
A	212	GLY	-	expression tag	UNP Q94AG2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	213	SER	-	expression tag	UNP Q94AG2
A	214	LEU	-	expression tag	UNP Q94AG2
A	215	GLU	-	expression tag	UNP Q94AG2
A	216	GLY	-	expression tag	UNP Q94AG2
A	217	SER	-	expression tag	UNP Q94AG2
A	218	GLU	-	expression tag	UNP Q94AG2
A	219	ASN	-	expression tag	UNP Q94AG2
A	220	LEU	-	expression tag	UNP Q94AG2
A	221	TYR	-	expression tag	UNP Q94AG2
A	222	PHE	-	expression tag	UNP Q94AG2
A	223	GLN	-	expression tag	UNP Q94AG2
A	224	GLY	-	expression tag	UNP Q94AG2
A	225	SER	-	expression tag	UNP Q94AG2
A	226	ALA	-	expression tag	UNP Q94AG2
A	227	TRP	-	expression tag	UNP Q94AG2
A	228	SER	-	expression tag	UNP Q94AG2
A	229	HIS	-	expression tag	UNP Q94AG2
A	230	PRO	-	expression tag	UNP Q94AG2
A	231	GLN	-	expression tag	UNP Q94AG2
A	232	PHE	-	expression tag	UNP Q94AG2
A	233	GLU	-	expression tag	UNP Q94AG2
A	234	LYS	-	expression tag	UNP Q94AG2
A	235	GLY	-	expression tag	UNP Q94AG2
A	236	GLY	-	expression tag	UNP Q94AG2
A	237	GLY	-	expression tag	UNP Q94AG2
A	238	SER	-	expression tag	UNP Q94AG2
A	239	GLY	-	expression tag	UNP Q94AG2
A	240	GLY	-	expression tag	UNP Q94AG2
A	241	GLY	-	expression tag	UNP Q94AG2
A	242	SER	-	expression tag	UNP Q94AG2
A	243	GLY	-	expression tag	UNP Q94AG2
A	244	GLY	-	expression tag	UNP Q94AG2
A	245	SER	-	expression tag	UNP Q94AG2
A	246	ALA	-	expression tag	UNP Q94AG2
A	247	TRP	-	expression tag	UNP Q94AG2
A	248	SER	-	expression tag	UNP Q94AG2
A	249	HIS	-	expression tag	UNP Q94AG2
A	250	PRO	-	expression tag	UNP Q94AG2
A	251	GLN	-	expression tag	UNP Q94AG2
A	252	PHE	-	expression tag	UNP Q94AG2
A	253	GLU	-	expression tag	UNP Q94AG2
A	254	LYS	-	expression tag	UNP Q94AG2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	255	GLY	-	expression tag	UNP Q94AG2
A	256	ALA	-	expression tag	UNP Q94AG2
A	257	HIS	-	expression tag	UNP Q94AG2
A	258	HIS	-	expression tag	UNP Q94AG2
A	259	HIS	-	expression tag	UNP Q94AG2
A	260	HIS	-	expression tag	UNP Q94AG2
A	261	HIS	-	expression tag	UNP Q94AG2
A	262	HIS	-	expression tag	UNP Q94AG2
A	263	HIS	-	expression tag	UNP Q94AG2
A	264	HIS	-	expression tag	UNP Q94AG2
A	265	HIS	-	expression tag	UNP Q94AG2

- Molecule 2 is a protein called Probable inactive receptor kinase At1g27190.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	189	Total	C	N	O	S	0	20	0
			1509	947	255	297	10			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	215	GLU	-	expression tag	UNP O04567
B	216	ASN	-	expression tag	UNP O04567
B	217	LEU	-	expression tag	UNP O04567
B	218	TYR	-	expression tag	UNP O04567
B	219	PHE	-	expression tag	UNP O04567
B	220	GLN	-	expression tag	UNP O04567
B	221	GLY	-	expression tag	UNP O04567
B	222	ALA	-	expression tag	UNP O04567
B	223	TRP	-	expression tag	UNP O04567
B	224	SER	-	expression tag	UNP O04567
B	225	HIS	-	expression tag	UNP O04567
B	226	PRO	-	expression tag	UNP O04567
B	227	GLN	-	expression tag	UNP O04567
B	228	PHE	-	expression tag	UNP O04567
B	229	GLU	-	expression tag	UNP O04567
B	230	LYS	-	expression tag	UNP O04567
B	231	GLY	-	expression tag	UNP O04567
B	232	SER	-	expression tag	UNP O04567
B	233	HIS	-	expression tag	UNP O04567
B	234	HIS	-	expression tag	UNP O04567
B	235	HIS	-	expression tag	UNP O04567

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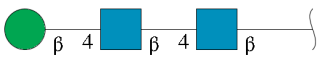
Chain	Residue	Modelled	Actual	Comment	Reference
B	236	HIS	-	expression tag	UNP O04567
B	237	HIS	-	expression tag	UNP O04567
B	238	HIS	-	expression tag	UNP O04567
B	239	HIS	-	expression tag	UNP O04567
B	240	HIS	-	expression tag	UNP O04567
B	241	HIS	-	expression tag	UNP O04567

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

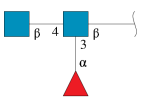
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



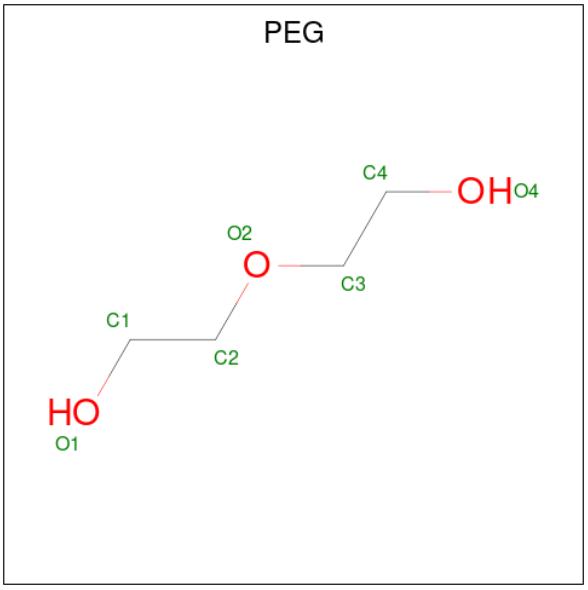
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



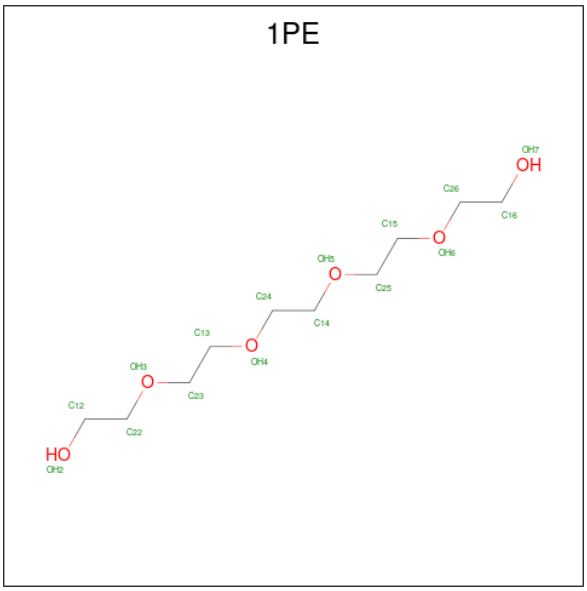
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	H	3	Total C N O 38 22 2 14	0	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 16 10 6	0	0

- Molecule 8 is water.

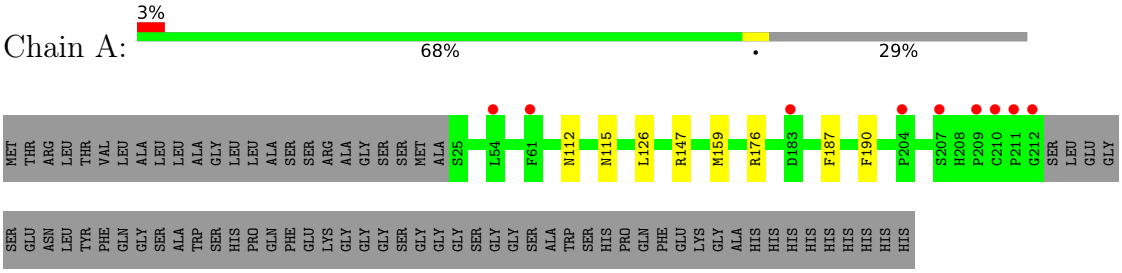
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	219	Total O 219 219	0	0
8	B	214	Total O 214 214	0	0

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.

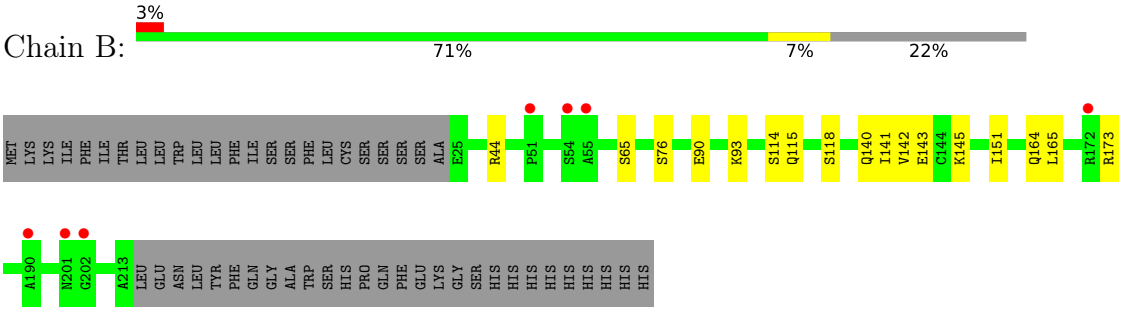
• Molecule 1: Somatic embryogenesis receptor kinase 1

Chain A:



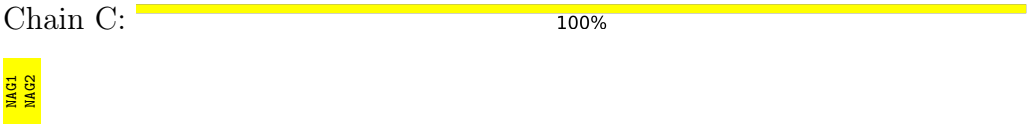
• Molecule 2: Probable inactive receptor kinase At1g27190

Chain B:



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

Chain C:



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

Chain D:

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

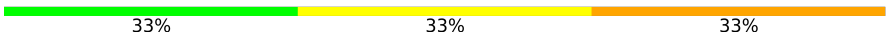
Chain F:

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

Chain G:

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

Chain E:



• Molecule 5: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	52.17Å 50.76Å 77.42Å 90.00° 96.72° 90.00°	Depositor
Resolution (Å)	40.81 – 1.25 40.81 – 1.25	Depositor EDS
% Data completeness (in resolution range)	98.7 (40.81-1.25) 98.7 (40.81-1.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 1.25Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.151 , 0.184 0.153 , 0.185	Depositor DCC
R_{free} test set	5491 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	12.8	Xtriage
Anisotropy	0.850	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.2	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	0.98	EDS
Total number of atoms	3628	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.12% 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: FUC, PEG, BMA, 1PE, NAG

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	0.61	0/1502	0.79	2/2058 (0.1%)
2	B	0.58	0/1585	0.78	1/2139 (0.0%)
All	All	0.60	0/3087	0.78	3/4197 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	176	ARG	NE-CZ-NH2	6.37	123.49	120.30
2	B	44	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	147	ARG	NE-CZ-NH1	5.21	122.91	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1453	0	1446	7	0
2	B	1509	0	1576	19	0
3	C	28	0	25	0	0
3	D	28	0	25	1	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	39	0	34	1	0
5	H	38	0	34	0	0
6	A	7	0	10	1	0
6	B	21	0	30	14	0
7	A	16	0	22	1	0
8	A	219	0	0	1	0
8	B	214	0	0	0	0
All	All	3628	0	3252	27	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 4.

All (27) 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)
2:B:143:GLU:HG3	6:B:304:PEG:H21	1.33	1.05
2:B:115:GLN:HG2	6:B:305:PEG:H41	1.59	0.83
1:A:112[B]:ASN:OD1	3:D:1:NAG:C1	2.28	0.80
1:A:112[B]:ASN:OD1	1:A:115:ASN:ND2	2.25	0.70
2:B:143:GLU:HG3	6:B:304:PEG:C2	2.16	0.69
2:B:140:GLN:HG2	6:B:304:PEG:H42	1.77	0.67
2:B:114:SER:O	6:B:304:PEG:H41	1.97	0.63
1:A:159[B]:MET:HE3	1:A:159[B]:MET:HA	1.87	0.57
2:B:115:GLN:NE2	6:B:305:PEG:O2	2.40	0.53
2:B:115:GLN:HE21	6:B:305:PEG:C4	2.23	0.52
2:B:143:GLU:CG	6:B:304:PEG:H21	2.24	0.52
1:A:126:LEU:HD11	4:E:1:NAG:H82	1.93	0.51
2:B:115:GLN:HE21	6:B:305:PEG:C3	2.26	0.49
2:B:151[B]:ILE:HD11	2:B:173[B]:ARG:NH2	2.27	0.49
2:B:93:LYS:CD	6:B:306:PEG:H41	2.45	0.47
7:A:313:1PE:H131	2:B:145:LYS:HE2	1.97	0.46
1:A:187:PHE:HA	1:A:190:PHE:CD2	2.52	0.45
2:B:93:LYS:HD2	6:B:306:PEG:H41	1.99	0.44
1:A:159[B]:MET:HE2	1:A:159[B]:MET:HB3	1.84	0.43
2:B:115:GLN:NE2	6:B:305:PEG:C2	2.81	0.42
6:A:312:PEG:H22	8:A:492:HOH:O	2.19	0.42
2:B:90:GLU:CD	6:B:305:PEG:O4	2.57	0.42
2:B:118[B]:SER:HB2	6:B:304:PEG:H31	2.01	0.41
1:A:159[B]:MET:HE3	1:A:159[B]:MET:CA	2.49	0.41
2:B:141:ILE:HG21	2:B:165:LEU:HD21	2.03	0.40
2:B:142:VAL:HB	2:B:164:GLN:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:SER:HB2	2:B:76[B]:SER:OG	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	192/265 (72%)	182 (95%)	10 (5%)	0	100	100
2	B	207/241 (86%)	199 (96%)	8 (4%)	0	100	100
All	All	399/506 (79%)	381 (96%)	18 (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	177/227 (78%)	177 (100%)	0	100	100
2	B	186/214 (87%)	186 (100%)	0	100	100
All	All	363/441 (82%)	363 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	174	ASN
1	A	197	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)

14 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	$\#\|Z\| > 2$
3	NAG	C	1	1,3	14,14,15	0.41	0	17,19,21	1.06	2 (11%)
3	NAG	C	2	3	14,14,15	0.37	0	17,19,21	1.11	2 (11%)
3	NAG	D	1	1,3	14,14,15	0.58	0	17,19,21	1.42	4 (23%)
3	NAG	D	2	3	14,14,15	0.27	0	17,19,21	0.72	0
4	NAG	E	1	4,1	14,14,15	0.47	0	17,19,21	0.98	1 (5%)
4	NAG	E	2	4	14,14,15	0.39	0	17,19,21	1.13	1 (5%)
4	BMA	E	3	4	11,11,12	0.41	0	15,15,17	0.55	0
3	NAG	F	1	1,3	14,14,15	0.38	0	17,19,21	1.31	3 (17%)
3	NAG	F	2	3	14,14,15	0.33	0	17,19,21	0.86	0
3	NAG	G	1	1,3	14,14,15	0.35	0	17,19,21	1.28	2 (11%)
3	NAG	G	2	3	14,14,15	0.37	0	17,19,21	0.99	0
5	NAG	H	1	2,5	14,14,15	0.29	0	17,19,21	1.15	1 (5%)
5	FUC	H	2	5	10,10,11	0.53	0	14,14,16	0.95	0
5	NAG	H	3	5	14,14,15	0.38	0	17,19,21	0.83	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
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
5	NAG	H	1	2,5	-	0/6/23/26	0/1/1/1
5	FUC	H	2	5	-	-	0/1/1/1
5	NAG	H	3	5	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	1	NAG	C1-O5-C5	3.69	117.19	112.19
3	D	1	NAG	C1-C2-N2	-2.84	105.64	110.49
3	F	1	NAG	C1-O5-C5	2.78	115.96	112.19
3	F	1	NAG	O5-C1-C2	-2.77	106.91	111.29
3	C	1	NAG	C1-O5-C5	2.75	115.92	112.19
4	E	1	NAG	O5-C1-C2	-2.59	107.20	111.29
3	C	2	NAG	C4-C3-C2	2.52	114.71	111.02
3	D	1	NAG	O5-C5-C4	-2.46	104.84	110.83
4	E	2	NAG	C3-C4-C5	2.40	114.52	110.24
5	H	1	NAG	C1-O5-C5	2.36	115.39	112.19
3	C	1	NAG	C1-C2-N2	-2.35	106.47	110.49
3	F	1	NAG	O5-C5-C6	2.27	110.77	107.20
3	D	1	NAG	C6-C5-C4	2.27	118.33	113.00
3	C	2	NAG	O5-C5-C6	2.23	110.70	107.20
3	D	1	NAG	C4-C3-C2	2.14	114.16	111.02
3	G	1	NAG	C4-C3-C2	2.11	114.11	111.02

There are no chirality outliers.

All (5) torsion outliers are listed below:

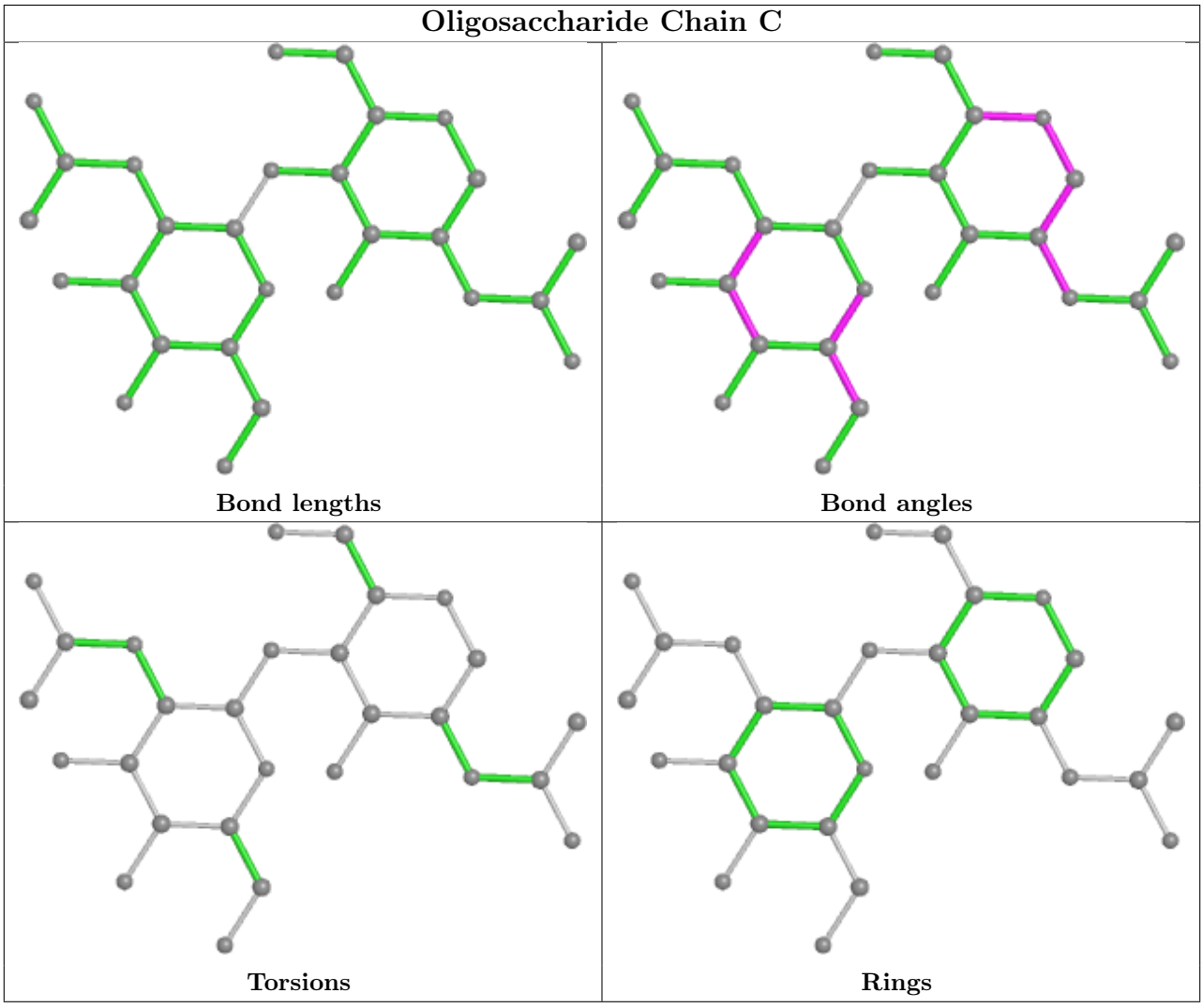
Mol	Chain	Res	Type	Atoms
5	H	3	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
5	H	3	NAG	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6

There are no ring outliers.

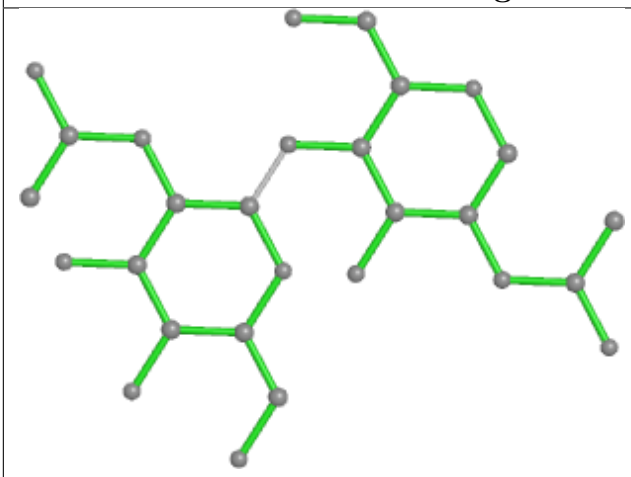
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	NAG	1	0
3	D	1	NAG	1	0

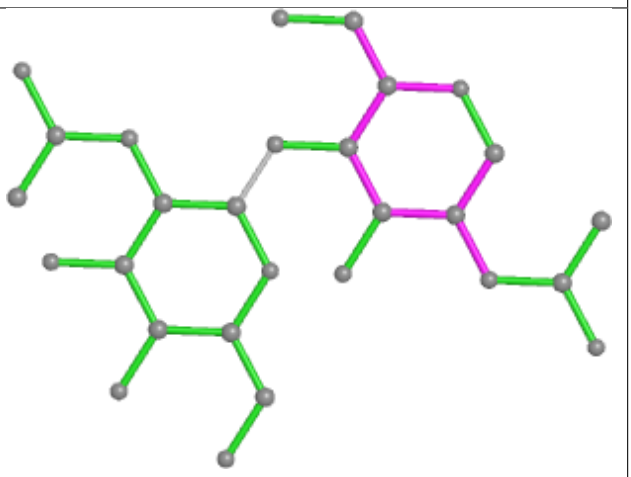
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



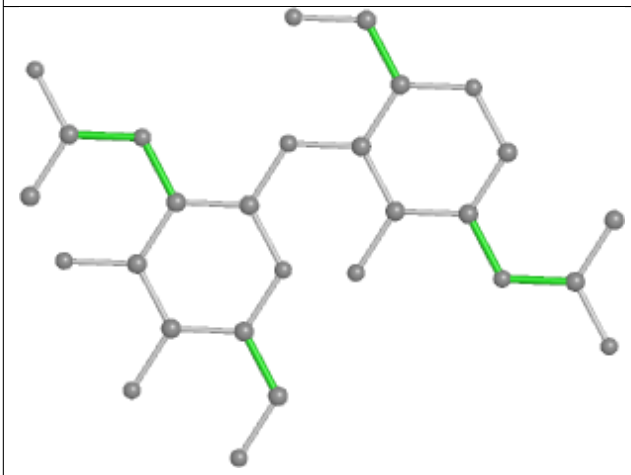
Oligosaccharide Chain D



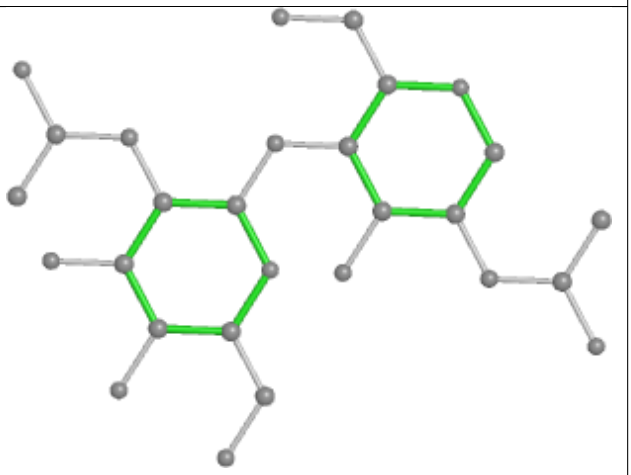
Bond lengths



Bond angles

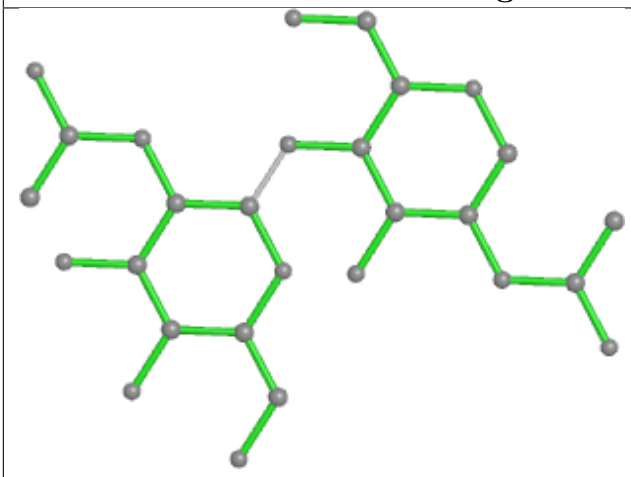


Torsions

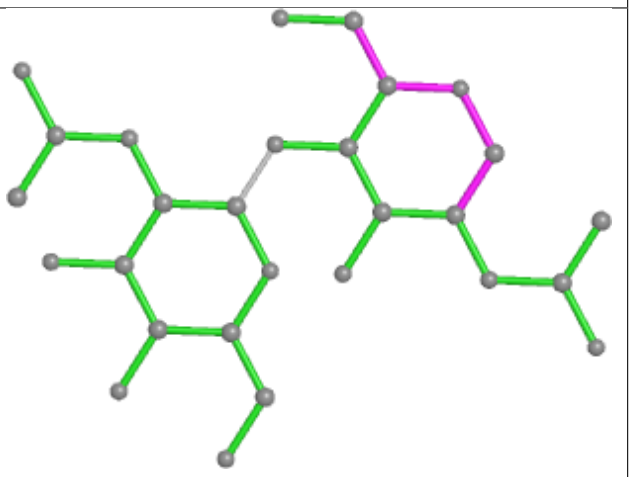


Rings

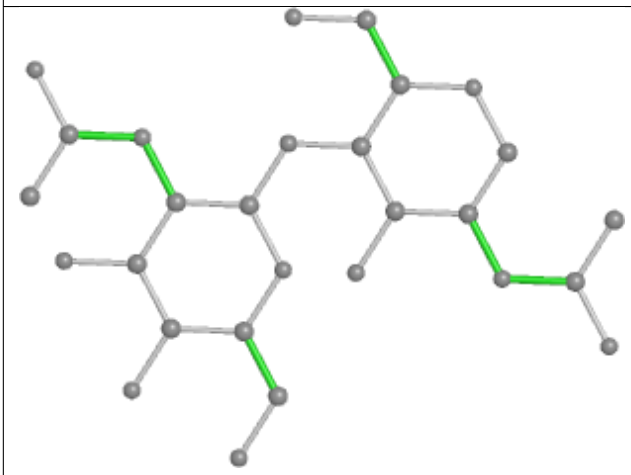
Oligosaccharide Chain F



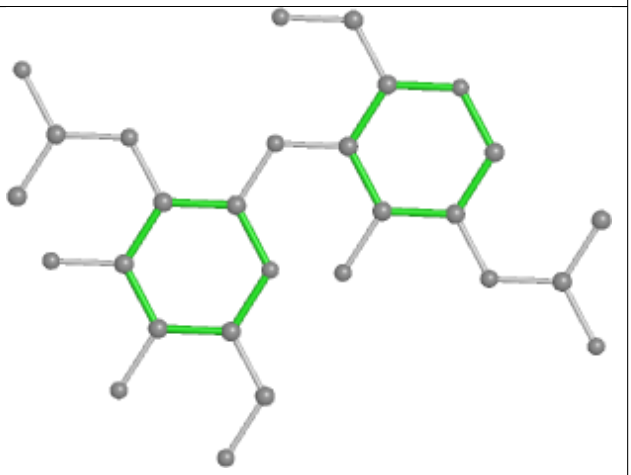
Bond lengths



Bond angles

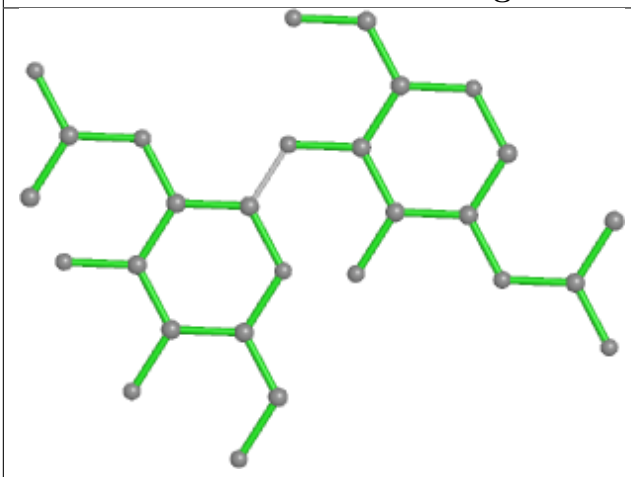


Torsions

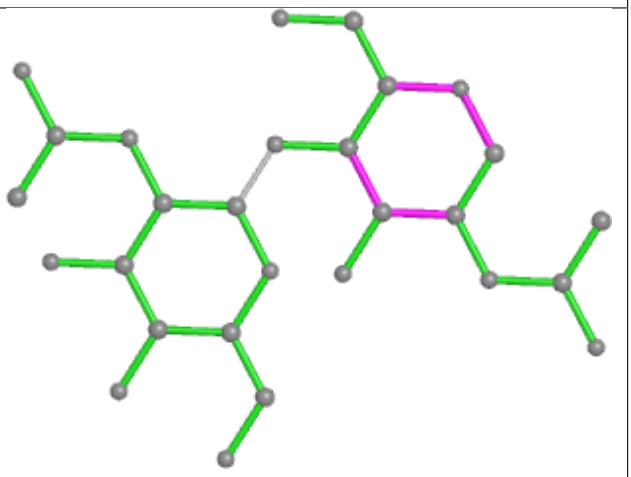


Rings

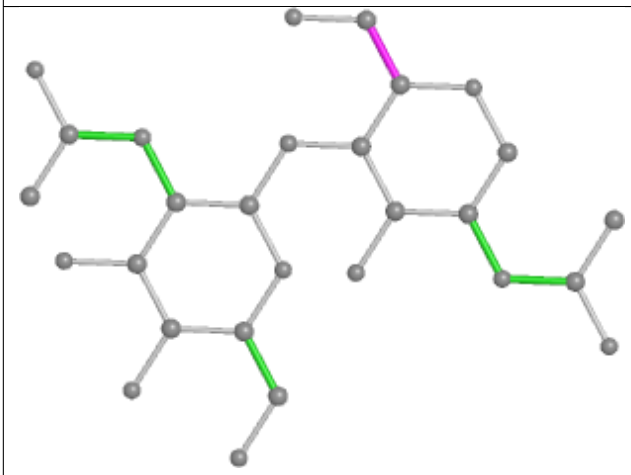
Oligosaccharide Chain G



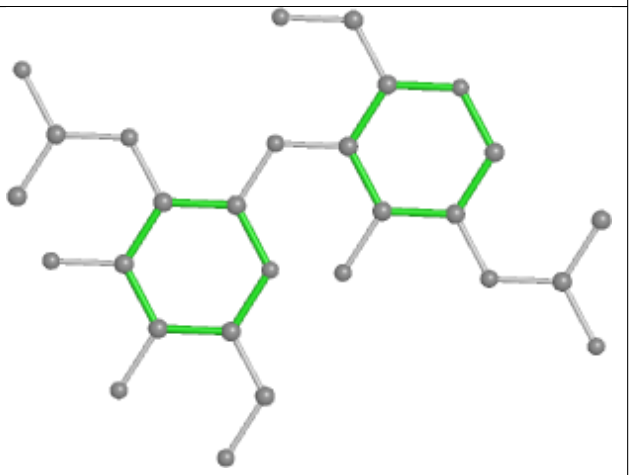
Bond lengths



Bond angles

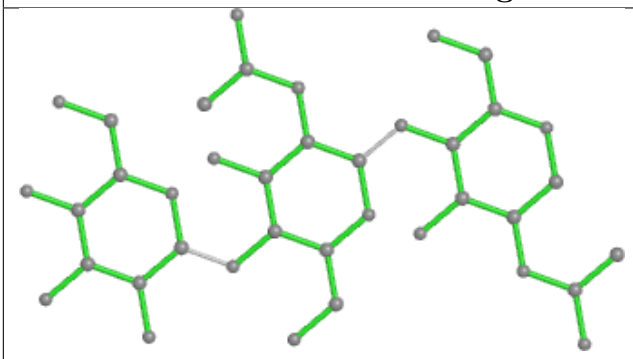


Torsions

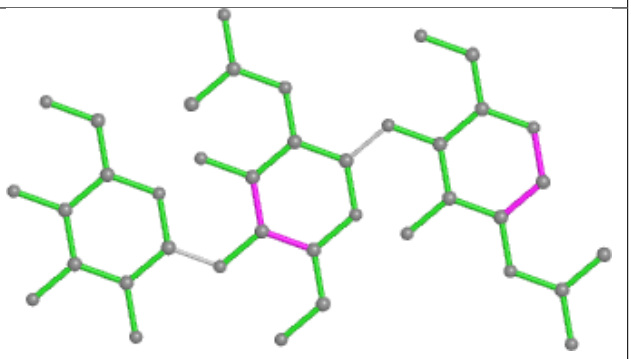


Rings

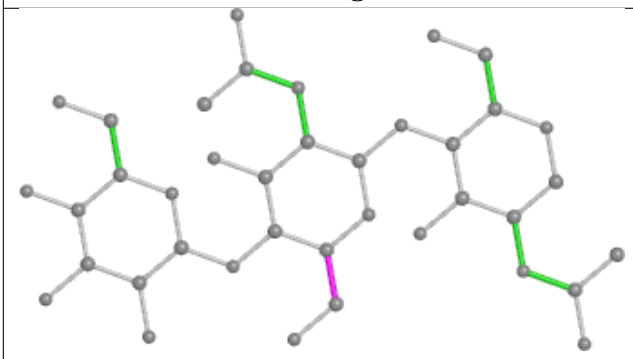
Oligosaccharide Chain E



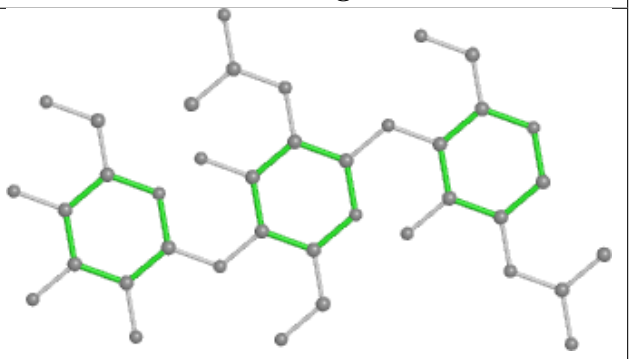
Bond lengths



Bond angles

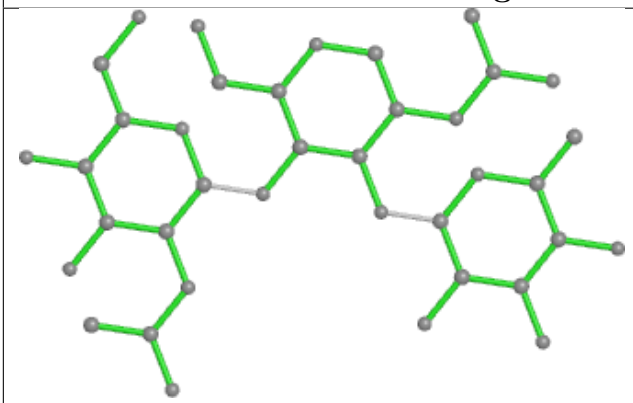


Torsions

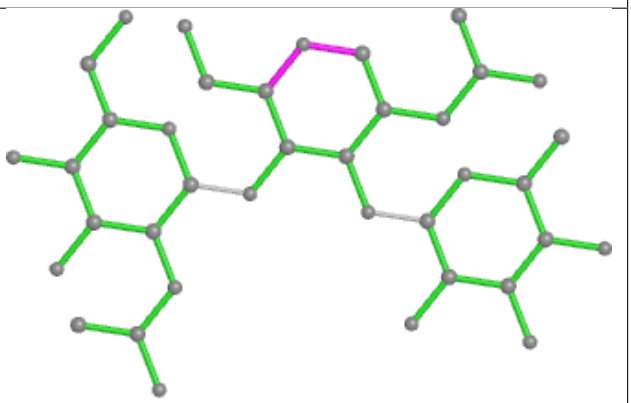


Rings

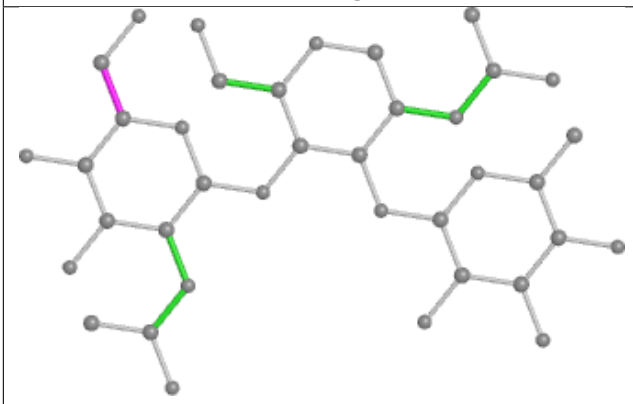
Oligosaccharide Chain H



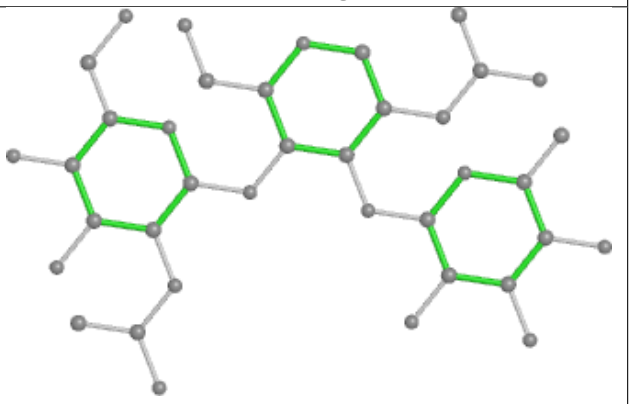
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

5 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	$\#\|Z\| > 2$
6	PEG	A	312	-	6,6,6	0.87	0	5,5,5	1.37	0
6	PEG	B	304	-	6,6,6	0.79	0	5,5,5	2.86	3 (60%)
6	PEG	B	306	-	6,6,6	0.55	0	5,5,5	1.55	2 (40%)
6	PEG	B	305	-	6,6,6	0.78	0	5,5,5	1.09	0
7	1PE	A	313	-	15,15,15	0.50	0	14,14,14	0.66	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
6	PEG	A	312	-	-	2/4/4/4	-
6	PEG	B	304	-	-	4/4/4/4	-
6	PEG	B	306	-	-	4/4/4/4	-
6	PEG	B	305	-	-	1/4/4/4	-
7	1PE	A	313	-	-	9/13/13/13	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	304	PEG	O2-C2-C1	4.20	128.53	110.07
6	B	304	PEG	C3-O2-C2	3.51	128.49	113.29
6	B	304	PEG	O2-C3-C4	2.81	122.41	110.07
6	B	306	PEG	O2-C2-C1	-2.22	100.33	110.07
6	B	306	PEG	O1-C1-C2	-2.07	99.81	111.81

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	304	PEG	C4-C3-O2-C2
7	A	313	1PE	OH6-C15-C25-OH5
7	A	313	1PE	OH5-C14-C24-OH4
6	B	304	PEG	O1-C1-C2-O2
6	B	304	PEG	O2-C3-C4-O4
7	A	313	1PE	OH2-C12-C22-OH3
7	A	313	1PE	OH7-C16-C26-OH6
6	B	305	PEG	O1-C1-C2-O2
6	B	306	PEG	O1-C1-C2-O2
6	B	306	PEG	O2-C3-C4-O4
6	B	306	PEG	C4-C3-O2-C2
7	A	313	1PE	C16-C26-OH6-C15
6	B	304	PEG	C1-C2-O2-C3
6	A	312	PEG	C4-C3-O2-C2
7	A	313	1PE	C23-C13-OH4-C24
6	A	312	PEG	C1-C2-O2-C3
7	A	313	1PE	C25-C15-OH6-C26
7	A	313	1PE	C12-C22-OH3-C23
6	B	306	PEG	C1-C2-O2-C3
7	A	313	1PE	OH4-C13-C23-OH3

There are no ring outliers.

5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	312	PEG	1	0
6	B	304	PEG	6	0
6	B	306	PEG	2	0
6	B	305	PEG	6	0
7	A	313	1PE	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	188/265 (70%)	0.07	9 (4%)	30	25	12, 17, 34, 87	0
2	B	189/241 (78%)	0.04	7 (3%)	41	34	12, 19, 45, 59	0
All	All	377/506 (74%)	0.06	16 (4%)	36	29	12, 18, 42, 87	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	212	GLY	10.7
1	A	211	PRO	6.9
1	A	210	CYS	4.5
2	B	190	ALA	4.3
1	A	207	SER	3.8
2	B	201	ASN	3.6
2	B	55	ALA	2.9
1	A	183	ASP	2.9
1	A	204	PRO	2.8
2	B	202	GLY	2.8
2	B	54	SER	2.5
1	A	209	PRO	2.5
1	A	61	PHE	2.3
1	A	54	LEU	2.3
2	B	51	PRO	2.3
2	B	172	ARG	2.1

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

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

6.3 Carbohydrates (i)

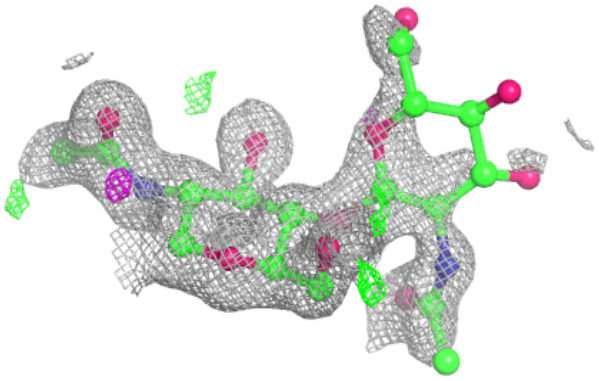
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

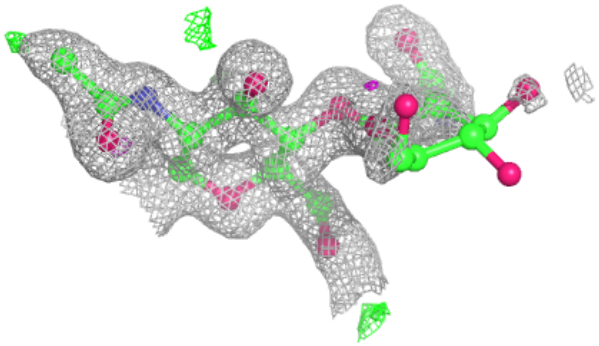
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	H	3	14/15	0.36	0.52	104,127,132,132	0
3	NAG	D	2	14/15	0.52	0.39	82,92,102,102	0
3	NAG	G	2	14/15	0.66	0.36	78,83,89,97	0
4	BMA	E	3	11/12	0.67	0.41	55,58,68,71	0
3	NAG	F	2	14/15	0.70	0.32	70,87,92,94	0
4	NAG	E	2	14/15	0.75	0.25	60,69,76,82	0
5	FUC	H	2	10/11	0.77	0.48	109,114,118,121	0
3	NAG	D	1	14/15	0.77	0.20	37,44,56,65	0
3	NAG	F	1	14/15	0.78	0.14	39,48,63,63	0
5	NAG	H	1	14/15	0.81	0.22	59,87,104,117	0
3	NAG	C	2	14/15	0.83	0.41	61,71,93,107	0
3	NAG	G	1	14/15	0.89	0.16	35,43,57,63	0
4	NAG	E	1	14/15	0.92	0.09	25,39,46,48	0
3	NAG	C	1	14/15	0.94	0.17	27,33,45,55	0

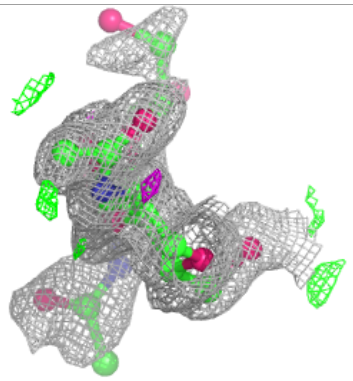
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

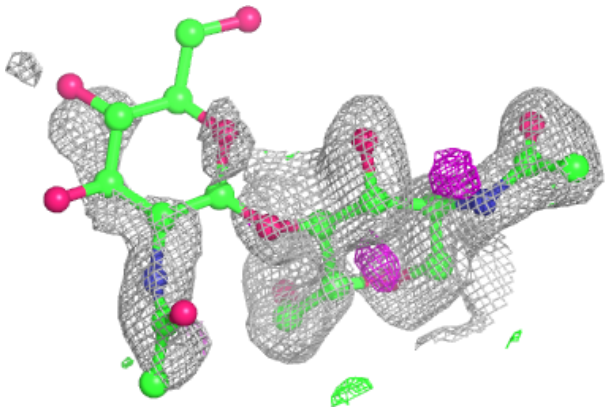


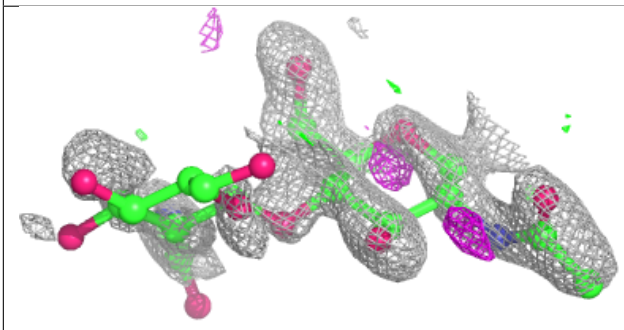


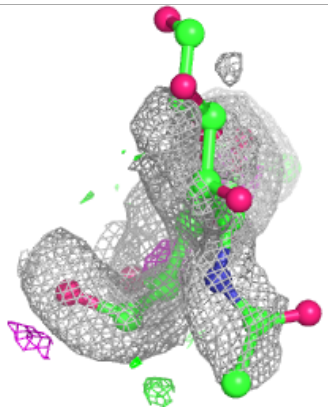


Electron density around Chain D:

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

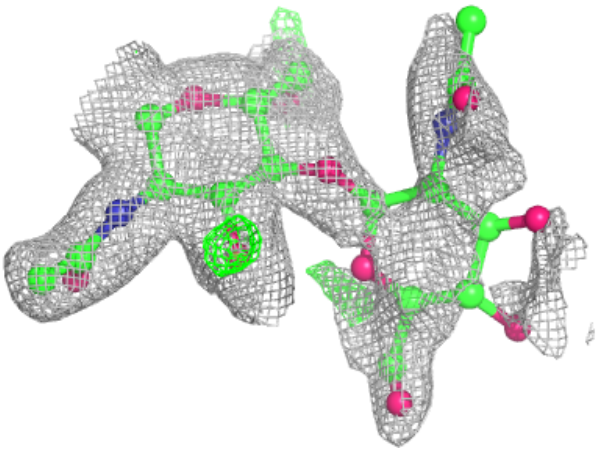


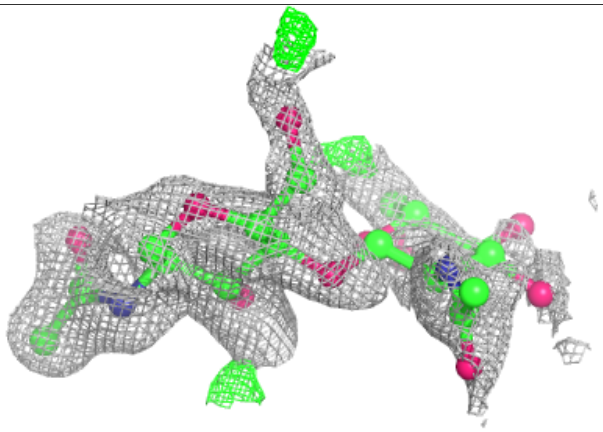


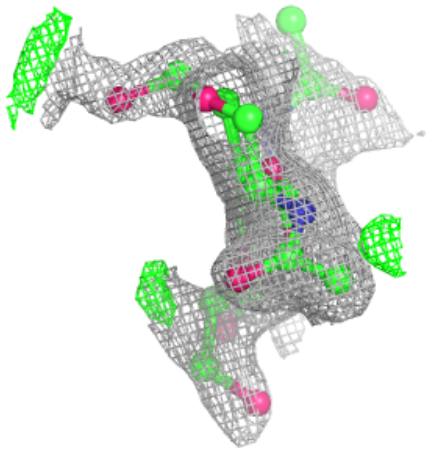


Electron density around Chain F:

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

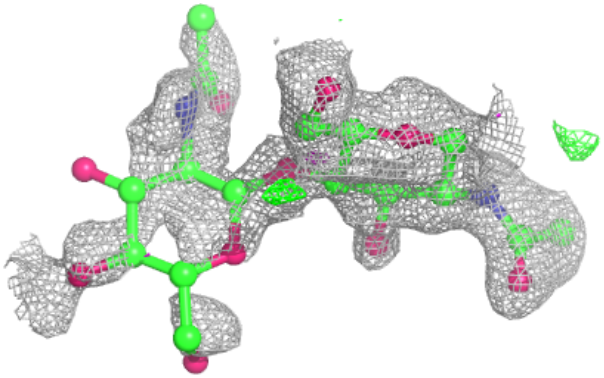


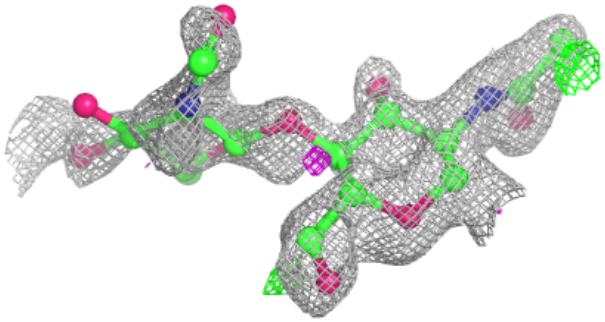


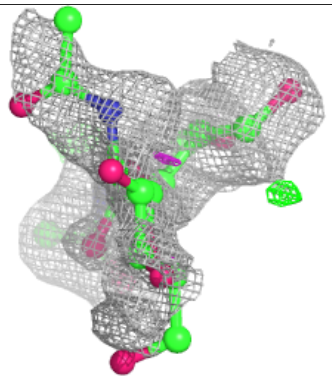


Electron density around Chain G:

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

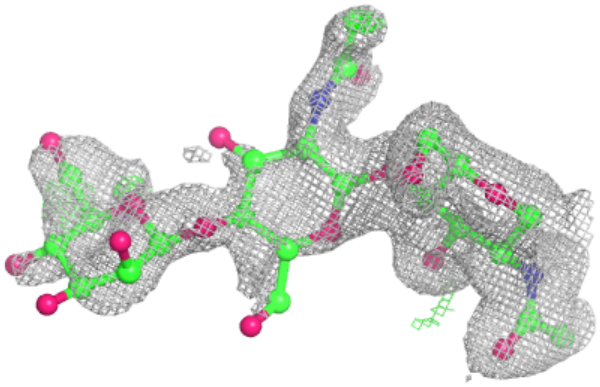


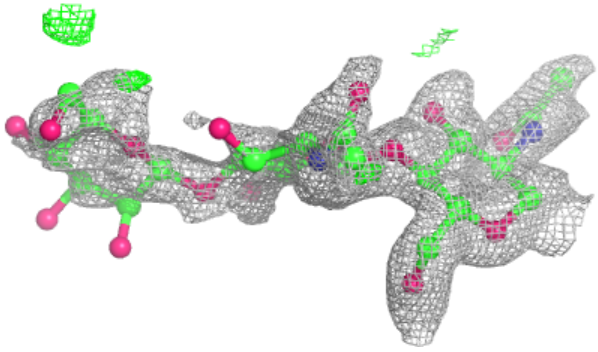


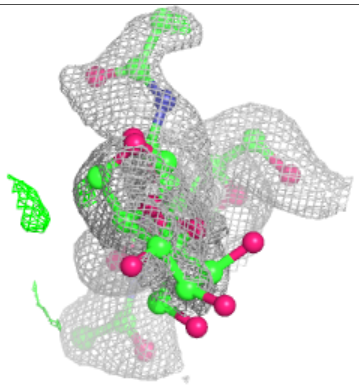


Electron density around Chain E:

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

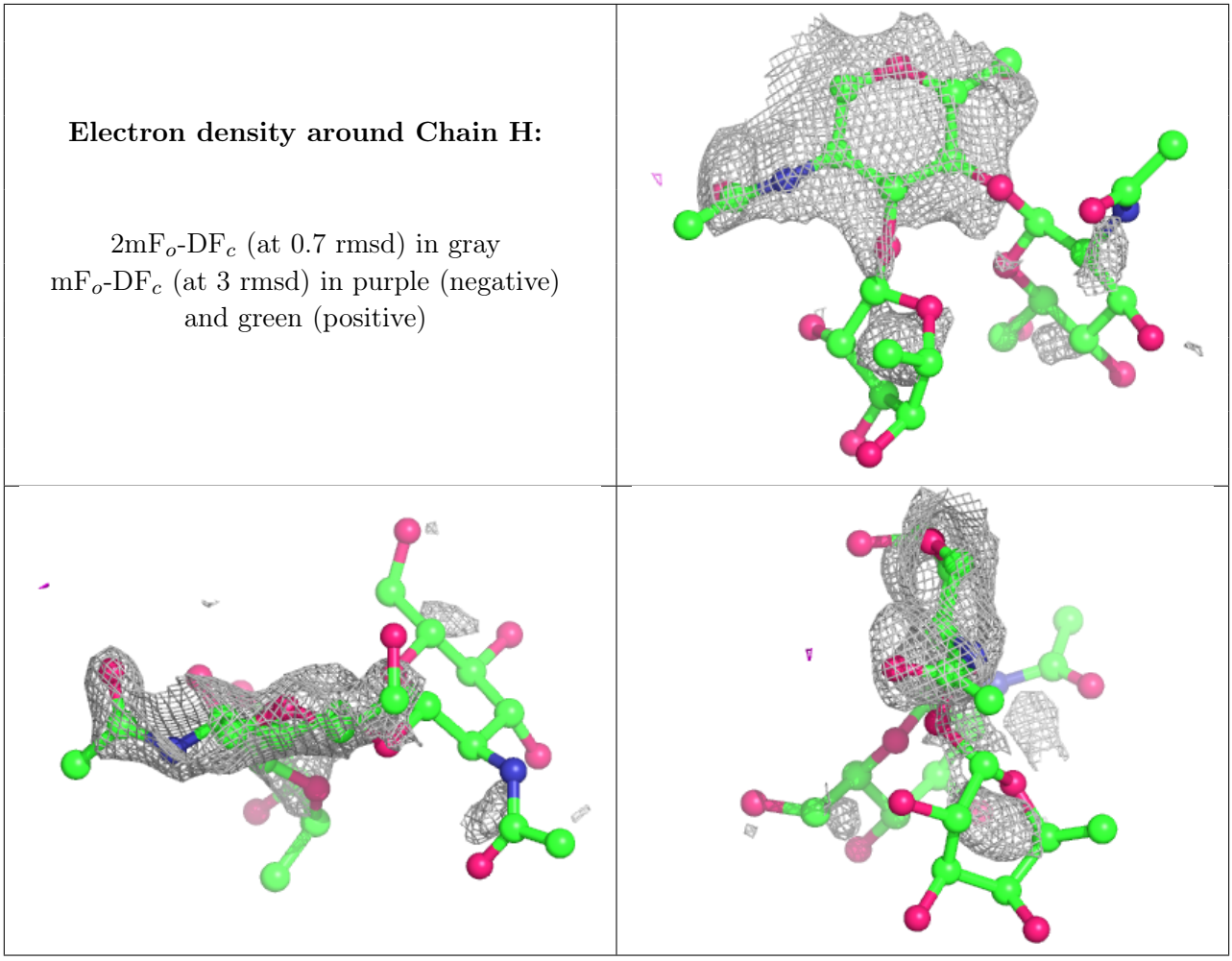






Electron density around Chain H:

$2mF_o$-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
7	1PE	A	313	16/16	0.75	0.26	36,51,68,74	0
6	PEG	B	305	7/7	0.84	0.23	31,37,50,56	0
6	PEG	B	304	7/7	0.85	0.16	25,36,41,48	0
6	PEG	A	312	7/7	0.87	0.23	30,36,44,49	0
6	PEG	B	306	7/7	0.93	0.23	19,37,43,43	0

6.5 Other polymers

There are no such residues in this entry.