Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 06:02 AM EDT

PDB ID	:	3CCB
Title	:	Crystal Structure of Human DPP4 in complex with a benzimidazole derivative
Authors	:	Wallace, M.B.; Skene, R.J.
Deposited on	:	2008-02-25
Resolution	:	2.49 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:

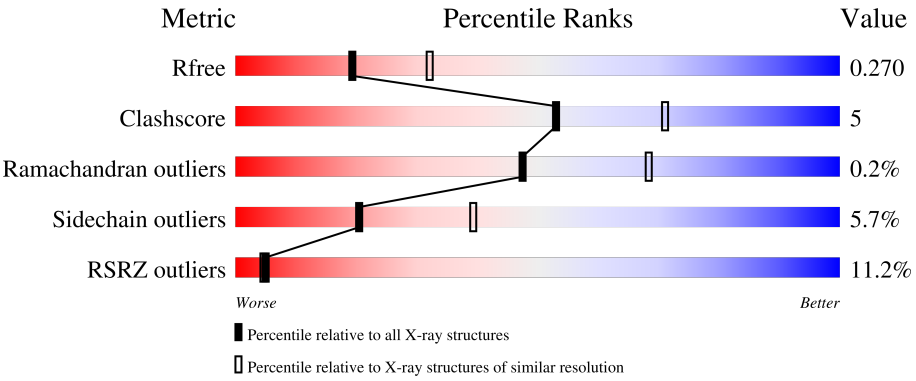
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.49 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	740	11% 81% 15%
1	B	740	5% 83% 13%
1	C	740	12% 83% 14%
1	D	740	16% 81% 15%
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	F	2	50% 50%
2	G	2	100%
2	H	2	50% 50%
2	I	2	50% 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	D	804	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 24805 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	724	Total	C	N	O	S	0	1	0
			5935	3812	977	1120	26			
1	B	729	Total	C	N	O	S	0	0	0
			5965	3830	983	1126	26			
1	C	724	Total	C	N	O	S	0	1	0
			5936	3813	977	1120	26			
1	D	724	Total	C	N	O	S	0	0	0
			5929	3809	974	1120	26			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	-	expression tag	UNP P27487
A	28	ASP	-	expression tag	UNP P27487
A	29	PRO	-	expression tag	UNP P27487
A	30	GLY	-	expression tag	UNP P27487
A	31	GLY	-	expression tag	UNP P27487
A	32	SER	-	expression tag	UNP P27487
A	33	HIS	-	expression tag	UNP P27487
A	34	HIS	-	expression tag	UNP P27487
A	35	HIS	-	expression tag	UNP P27487
A	36	HIS	-	expression tag	UNP P27487
A	37	HIS	-	expression tag	UNP P27487
A	38	HIS	-	expression tag	UNP P27487
B	27	ALA	-	expression tag	UNP P27487
B	28	ASP	-	expression tag	UNP P27487
B	29	PRO	-	expression tag	UNP P27487
B	30	GLY	-	expression tag	UNP P27487
B	31	GLY	-	expression tag	UNP P27487
B	32	SER	-	expression tag	UNP P27487
B	33	HIS	-	expression tag	UNP P27487
B	34	HIS	-	expression tag	UNP P27487
B	35	HIS	-	expression tag	UNP P27487

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Chain	Residue	Modelled	Actual	Comment	Reference
B	36	HIS	-	expression tag	UNP P27487
B	37	HIS	-	expression tag	UNP P27487
B	38	HIS	-	expression tag	UNP P27487
C	27	ALA	-	expression tag	UNP P27487
C	28	ASP	-	expression tag	UNP P27487
C	29	PRO	-	expression tag	UNP P27487
C	30	GLY	-	expression tag	UNP P27487
C	31	GLY	-	expression tag	UNP P27487
C	32	SER	-	expression tag	UNP P27487
C	33	HIS	-	expression tag	UNP P27487
C	34	HIS	-	expression tag	UNP P27487
C	35	HIS	-	expression tag	UNP P27487
C	36	HIS	-	expression tag	UNP P27487
C	37	HIS	-	expression tag	UNP P27487
C	38	HIS	-	expression tag	UNP P27487
D	27	ALA	-	expression tag	UNP P27487
D	28	ASP	-	expression tag	UNP P27487
D	29	PRO	-	expression tag	UNP P27487
D	30	GLY	-	expression tag	UNP P27487
D	31	GLY	-	expression tag	UNP P27487
D	32	SER	-	expression tag	UNP P27487
D	33	HIS	-	expression tag	UNP P27487
D	34	HIS	-	expression tag	UNP P27487
D	35	HIS	-	expression tag	UNP P27487
D	36	HIS	-	expression tag	UNP P27487
D	37	HIS	-	expression tag	UNP P27487
D	38	HIS	-	expression tag	UNP P27487

- Molecule 2 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
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

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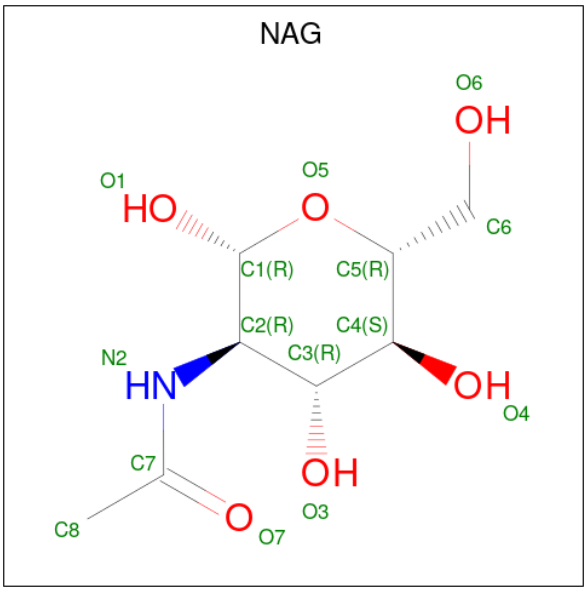
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	H	2	Total C N O 28 16 2 10	0	0	0
2	I	2	Total C N O 28 16 2 10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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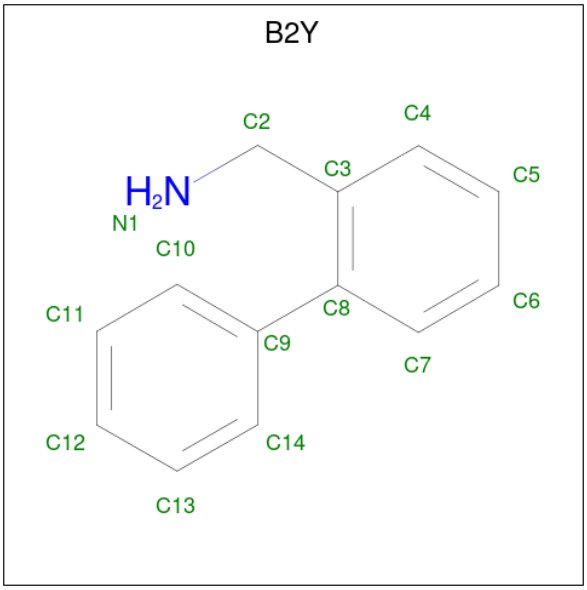
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is 1-biphenyl-2-ylmethanamine (three-letter code: B2Y) (formula: $C_{13}H_{13}N$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 14 13 1	0	0
4	B	1	Total C N 14 13 1	0	0
4	C	1	Total C N 14 13 1	0	0
4	D	1	Total C N 14 13 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	206	Total O 206 206	0	0
5	B	191	Total O 191 191	0	0

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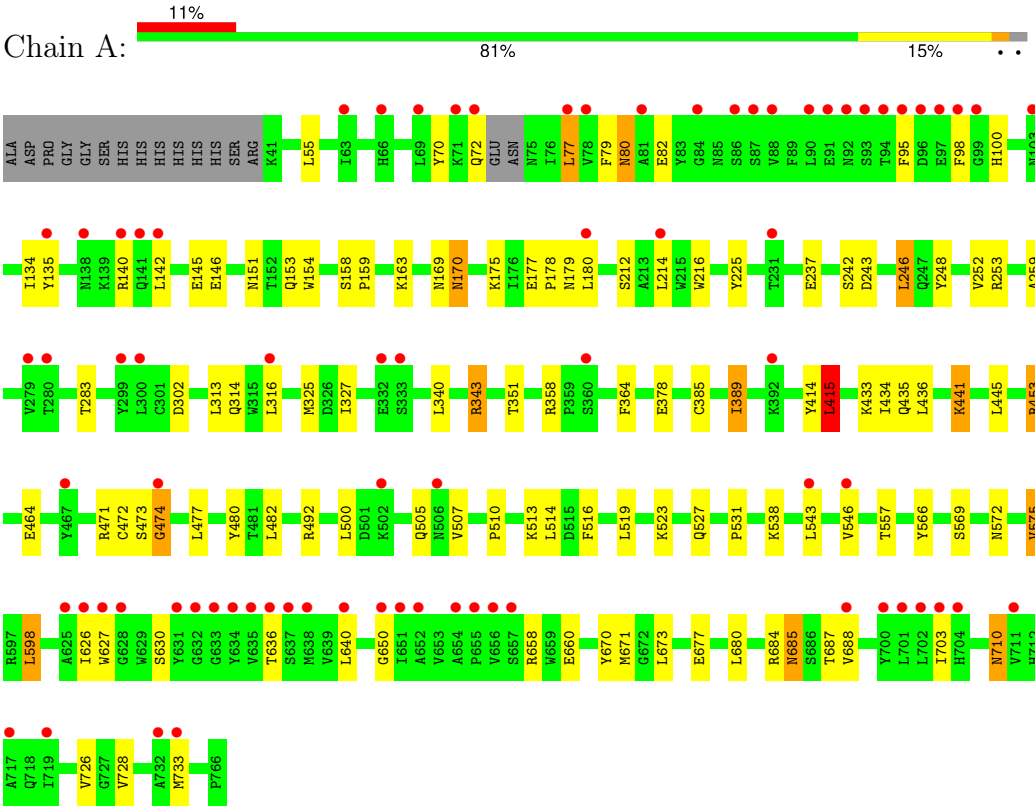
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	189	Total O 189 189	0	0
5	D	90	Total O 90 90	0	0

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.

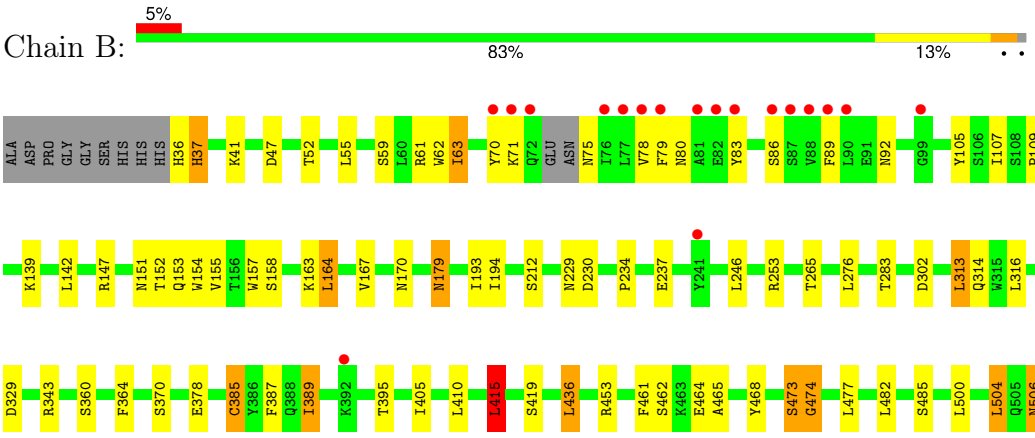
• Molecule 1: Dipeptidyl peptidase 4

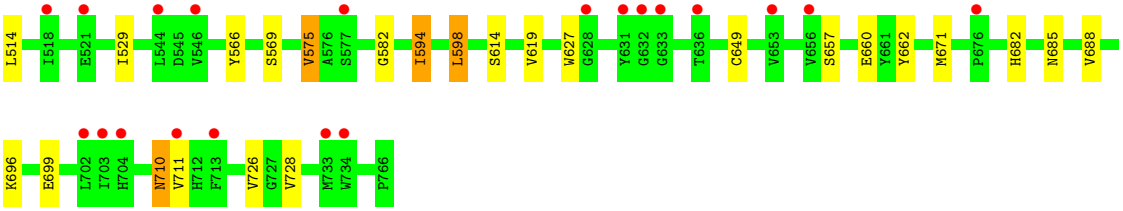
Chain A:



• Molecule 1: Dipeptidyl peptidase 4

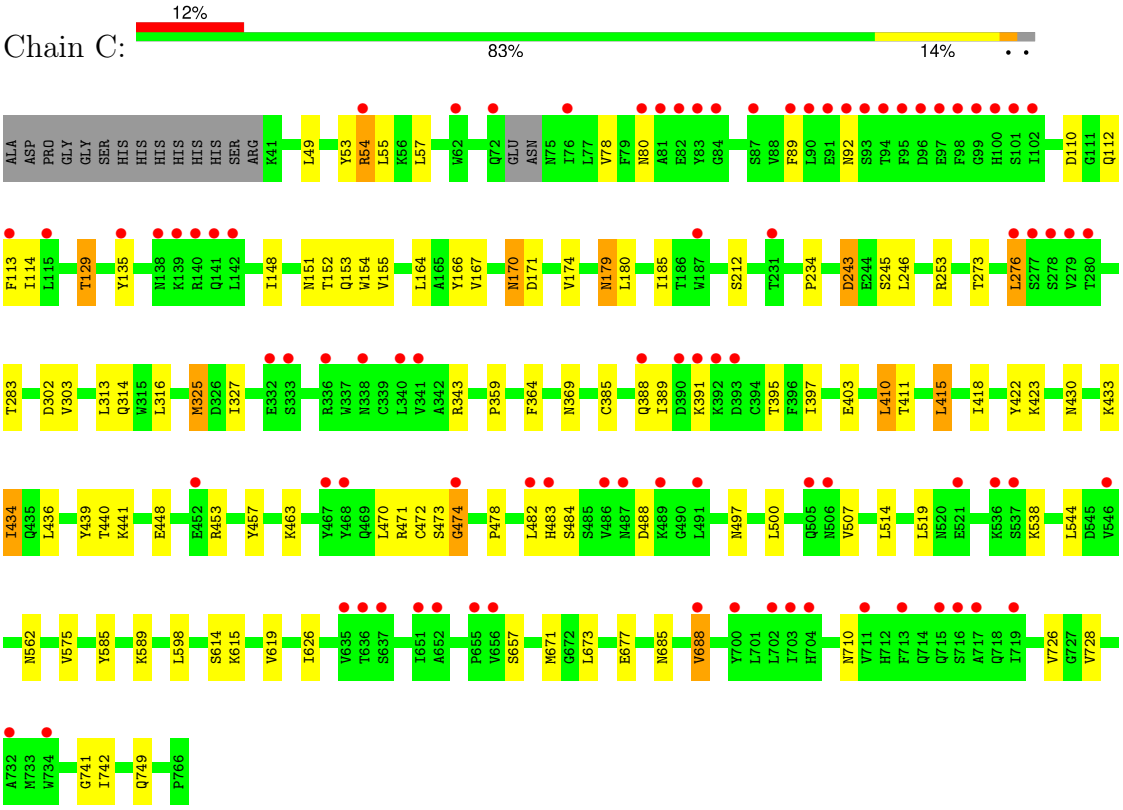
Chain B:





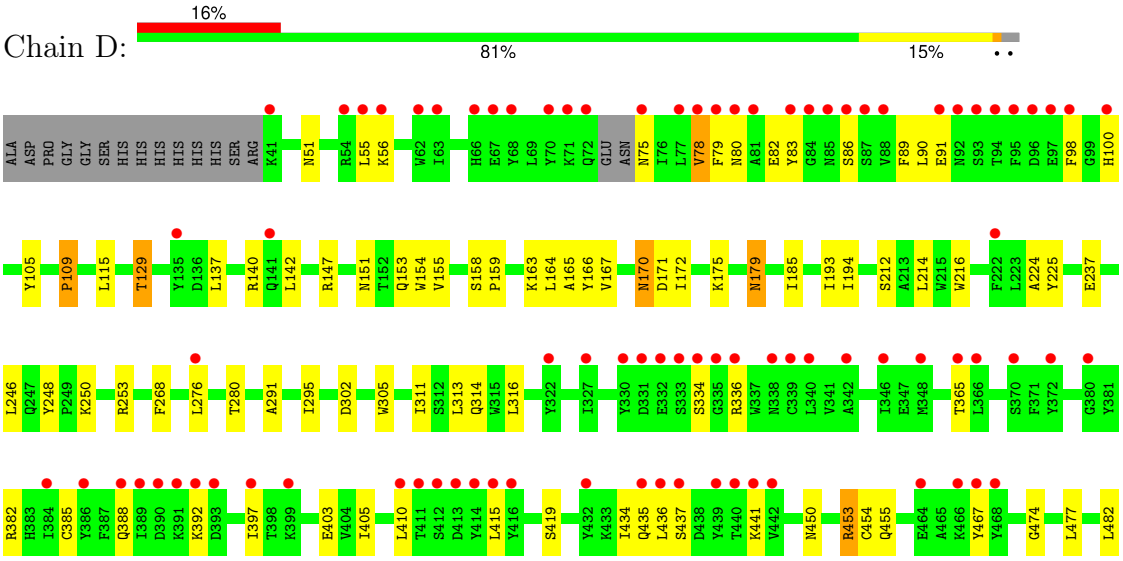
• Molecule 1: Dipeptidyl peptidase 4

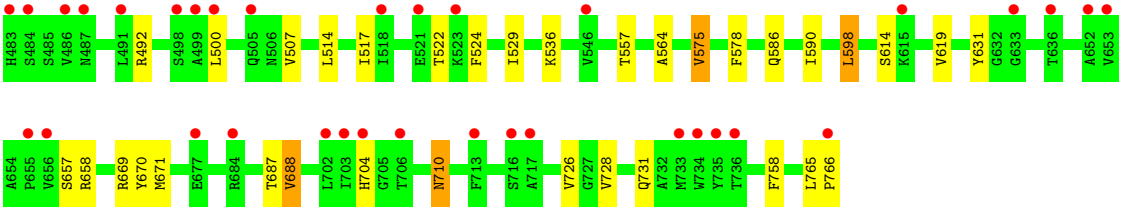
Chain C:



• Molecule 1: Dipeptidyl peptidase 4

Chain D:





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

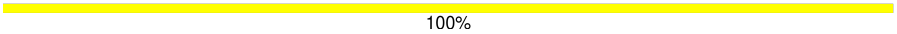
Chain E:

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

Chain F:

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

Chain G:



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

Chain H:

• Molecule 2: 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	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	122.09Å 123.01Å 144.65Å 90.00° 114.84° 90.00°	Depositor
Resolution (Å)	32.80 – 2.49 32.82 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.3 (32.80-2.49) 98.3 (32.82-2.49)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.37 (at 2.48Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.244 0.234 , 0.270	Depositor DCC
R_{free} test set	6730 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	44.1	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	24805	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: B2Y, 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	0.45	0/6111	0.62	1/8311 (0.0%)
1	B	0.44	0/6138	0.62	1/8348 (0.0%)
1	C	0.44	0/6111	0.61	1/8311 (0.0%)
1	D	0.42	0/6100	0.58	0/8296
All	All	0.44	0/24460	0.61	3/33266 (0.0%)

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	C	415	LEU	CA-CB-CG	5.83	128.71	115.30
1	A	415	LEU	CA-CB-CG	5.37	127.66	115.30
1	B	415	LEU	CA-CB-CG	5.13	127.11	115.30

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	5935	0	5657	72	0
1	B	5965	0	5672	63	0
1	C	5936	0	5660	65	0
1	D	5929	0	5651	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	1	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
3	A	56	0	52	0	0
3	B	56	0	52	1	0
3	C	28	0	26	0	0
3	D	28	0	26	1	0
4	A	14	0	13	0	0
4	B	14	0	13	1	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
5	A	206	0	0	2	0
5	B	191	0	0	0	0
5	C	189	0	0	1	0
5	D	90	0	0	0	0
All	All	24805	0	22973	253	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 (253) 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:C:343:ARG:HD2	1:C:389:ILE:HG22	1.42	0.98
1:C:153:GLN:HE22	1:C:170:ASN:H	1.14	0.93
1:A:153:GLN:HE22	1:A:170:ASN:H	1.18	0.90
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.14	0.90
1:C:54:ARG:HG2	1:C:54:ARG:HH21	1.39	0.88
1:A:325:MET:HE3	1:A:327:ILE:HD11	1.56	0.88
1:C:253:ARG:HH21	1:D:253:ARG:NH2	1.71	0.88
1:C:253:ARG:NH2	1:D:253:ARG:HH21	1.71	0.87
1:D:658:ARG:HB2	1:D:687:THR:HG22	1.58	0.85
1:D:153:GLN:HE22	1:D:170:ASN:H	1.22	0.84
1:C:253:ARG:HH21	1:D:253:ARG:HH21	0.88	0.83
1:B:343:ARG:HD3	1:B:389:ILE:HG23	1.59	0.82
1:B:153:GLN:HE22	1:B:170:ASN:H	1.27	0.82
1:A:325:MET:CE	1:A:327:ILE:HD11	2.11	0.81
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.64	0.79
1:C:434:ILE:HD11	1:C:439:TYR:HB2	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:THR:HG23	1:A:151:ASN:HA	1.70	0.73
1:A:598:LEU:HD22	1:A:671:MET:HG2	1.73	0.70
1:D:179:ASN:H	1:D:179:ASN:HD22	1.42	0.67
1:A:129:THR:CG2	1:A:151:ASN:HA	2.25	0.67
1:C:726:VAL:HG23	1:C:728:VAL:HG23	1.79	0.64
1:A:253:ARG:HH21	1:B:253:ARG:NH2	1.92	0.64
1:B:36:HIS:O	1:B:37:HIS:HB2	1.98	0.63
1:B:614:SER:HA	1:B:619:VAL:HB	1.79	0.63
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.28	0.63
1:B:696:LYS:HG3	1:B:728:VAL:HG22	1.80	0.62
1:C:343:ARG:HD2	1:C:389:ILE:CG2	2.23	0.62
1:A:134:ILE:HG21	1:A:178:PRO:HB3	1.82	0.62
1:C:153:GLN:NE2	1:C:170:ASN:H	1.94	0.62
1:D:147:ARG:HE	3:D:801:NAG:H83	1.66	0.61
1:A:135:TYR:HD1	1:A:142:LEU:HD13	1.65	0.61
1:B:327:ILE:HD13	1:B:389:ILE:HG13	1.83	0.61
1:A:516:PHE:CD1	1:A:523:LYS:HG2	2.36	0.60
1:C:174:VAL:HG23	1:C:185:ILE:HD11	1.83	0.60
1:A:253:ARG:NH2	1:B:253:ARG:HH21	1.92	0.60
1:D:564:ALA:HB1	1:D:575:VAL:HG11	1.84	0.60
1:C:327:ILE:HD13	1:C:389:ILE:HD12	1.84	0.60
1:D:155:VAL:HG12	1:D:166:TYR:HB3	1.85	0.59
1:C:314:GLN:HG2	1:C:325:MET:HB2	1.85	0.59
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.85	0.59
1:B:711:VAL:CG2	4:B:800:B2Y:H11	2.32	0.58
1:C:388:GLN:HB2	1:C:391:LYS:HG2	1.84	0.58
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.86	0.58
1:B:529:ILE:HB	1:B:575:VAL:HG13	1.84	0.58
1:C:472:CYS:O	1:C:478:PRO:HA	2.04	0.57
1:A:364:PHE:HE2	1:A:389:ILE:HD11	1.67	0.57
1:D:522:THR:HB	1:D:524:PHE:CE2	2.40	0.57
1:D:382:ARG:H	1:D:403:GLU:HG2	1.69	0.57
1:D:415:LEU:HB2	1:D:436:LEU:HD11	1.86	0.57
1:A:415:LEU:HB3	1:A:434:ILE:HG23	1.86	0.56
1:D:529:ILE:HB	1:D:575:VAL:HG13	1.87	0.56
1:A:471:ARG:HG3	1:A:480:TYR:CE1	2.40	0.56
1:C:152:THR:HG21	1:C:155:VAL:HG13	1.88	0.55
1:B:582:GLY:HA2	1:B:594:ILE:HD12	1.88	0.55
1:B:364:PHE:HE2	1:B:389:ILE:HD11	1.71	0.55
1:D:78:VAL:HG22	1:D:89:PHE:HB2	1.88	0.55
1:D:726:VAL:HG23	1:D:728:VAL:HG23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:TRP:CE2	1:C:212:SER:HB3	2.42	0.54
1:C:153:GLN:HE22	1:C:170:ASN:N	1.95	0.54
1:B:343:ARG:HD3	1:B:389:ILE:CG2	2.32	0.54
1:D:172:ILE:HG22	1:D:185:ILE:HD13	1.89	0.54
1:B:89:PHE:HE1	1:B:107:ILE:HD12	1.73	0.54
1:A:351:THR:OG1	1:A:592:HIS:HD2	1.91	0.54
1:D:614:SER:HA	1:D:619:VAL:HB	1.89	0.53
1:A:340:LEU:HD22	1:A:343:ARG:HH11	1.74	0.53
1:B:78:VAL:HG23	1:B:89:PHE:HB2	1.89	0.53
1:C:174:VAL:HG23	1:C:185:ILE:CD1	2.39	0.53
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.90	0.52
1:A:135:TYR:HE2	1:A:140:ARG:HG2	1.74	0.52
1:C:170:ASN:N	1:C:170:ASN:HD22	2.08	0.52
1:A:170:ASN:N	1:A:170:ASN:HD22	2.08	0.51
1:C:53:TYR:HB3	1:C:500:LEU:HD11	1.92	0.51
1:C:174:VAL:CG2	1:C:185:ILE:HD11	2.40	0.51
1:D:657:SER:HA	1:D:688:VAL:HG13	1.91	0.51
1:B:179:ASN:H	1:B:179:ASN:HD22	1.57	0.51
1:C:114:ILE:HG23	1:C:135:TYR:HB3	1.93	0.51
1:B:147:ARG:HE	3:B:802:NAG:H83	1.75	0.51
1:B:154:TRP:CE2	1:B:212:SER:HB3	2.46	0.51
1:D:453:ARG:NH2	1:D:477:LEU:O	2.43	0.51
1:C:369:ASN:C	1:C:389:ILE:HG12	2.32	0.51
1:C:369:ASN:O	1:C:389:ILE:HG12	2.11	0.50
1:C:273:THR:HA	1:C:276:LEU:HD22	1.93	0.50
1:C:153:GLN:NE2	1:C:167:VAL:HG12	2.27	0.50
1:D:598:LEU:HG	1:D:631:TYR:OH	2.12	0.49
1:A:55:LEU:HD23	1:A:500:LEU:HD22	1.93	0.49
1:D:334:SER:HB2	1:D:336:ARG:H	1.77	0.49
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.94	0.49
1:B:158:SER:HB3	1:B:163:LYS:HB2	1.93	0.49
1:C:54:ARG:HG2	1:C:54:ARG:NH2	2.16	0.49
1:B:79:PHE:HA	1:B:86:SER:HB3	1.94	0.49
1:B:504:LEU:HA	1:B:507:VAL:CG1	2.43	0.49
1:A:153:GLN:NE2	1:A:170:ASN:H	1.99	0.49
1:B:47:ASP:HA	1:B:52:THR:OG1	2.12	0.49
1:B:80:ASN:HD22	1:B:83:TYR:H	1.59	0.49
1:B:229:ASN:HB3	1:B:265:THR:OG1	2.13	0.49
1:D:82:GLU:HG2	1:D:467:TYR:OH	2.13	0.49
1:C:110:ASP:OD2	1:C:112:GLN:HG2	2.13	0.48
1:C:129:THR:HG23	1:C:151:ASN:HA	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:ILE:HD13	1:C:389:ILE:HG23	1.95	0.48
1:D:75:ASN:OD1	1:D:91:GLU:HG3	2.12	0.48
1:C:473:SER:O	1:C:474:GLY:O	2.32	0.48
1:B:598:LEU:HB2	1:B:671:MET:SD	2.54	0.48
1:A:154:TRP:CE2	1:A:212:SER:HB3	2.48	0.48
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.95	0.48
1:B:329:ASP:OD2	1:B:343:ARG:NH1	2.46	0.48
1:A:435:GLN:OE1	1:A:441:LYS:HE2	2.14	0.48
1:A:159:PRO:HD3	1:A:216:TRP:HB3	1.96	0.47
1:B:473:SER:O	1:B:474:GLY:O	2.32	0.47
1:C:403:GLU:OE2	1:C:585:TYR:HA	2.13	0.47
1:B:157:TRP:CE3	1:B:164:LEU:HD13	2.48	0.47
1:B:71:LYS:HA	1:B:75:ASN:O	2.14	0.47
1:C:179:ASN:C	1:C:179:ASN:HD22	2.18	0.47
1:A:153:GLN:HE22	1:A:170:ASN:N	2.00	0.47
1:B:109:PRO:HG2	1:B:158:SER:O	2.14	0.47
1:A:626:ILE:HG23	1:A:636:THR:HG23	1.96	0.47
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.96	0.47
1:D:305:TRP:CE2	1:D:311:ILE:HD12	2.49	0.47
2:G:1:NAG:H62	2:G:2:NAG:N2	2.30	0.47
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.96	0.47
1:C:364:PHE:HE2	1:C:389:ILE:HD11	1.80	0.47
1:D:80:ASN:HD22	1:D:83:TYR:HB2	1.80	0.47
1:D:435:GLN:HE21	1:D:437:SER:HG	1.63	0.47
1:B:465:ALA:O	1:B:485:SER:OG	2.25	0.47
1:C:303:VAL:HG22	1:C:313:LEU:HD12	1.97	0.47
1:D:154:TRP:CE2	1:D:212:SER:HB3	2.49	0.46
1:D:586:GLN:HB3	1:D:590:ILE:HD12	1.97	0.46
1:D:158:SER:OG	1:D:163:LYS:HB2	2.15	0.46
1:D:170:ASN:N	1:D:170:ASN:HD22	2.14	0.46
1:A:685:ASN:ND2	5:A:866:HOH:O	2.48	0.46
1:D:710:ASN:C	1:D:710:ASN:HD22	2.19	0.46
1:B:314:GLN:HG2	1:B:325:MET:HB2	1.97	0.46
1:A:214:LEU:HD23	1:A:225:TYR:HB3	1.98	0.46
1:A:710:ASN:HD22	1:A:710:ASN:C	2.20	0.46
1:C:55:LEU:HD23	1:C:500:LEU:HD22	1.98	0.46
1:C:657:SER:HA	1:C:688:VAL:HG13	1.98	0.46
1:D:302:ASP:HB3	1:D:314:GLN:HB2	1.98	0.46
1:D:193:ILE:HG22	1:D:194:ILE:HG12	1.98	0.46
1:B:153:GLN:NE2	1:B:167:VAL:HG12	2.31	0.45
1:A:531:PRO:HB3	1:A:572:ASN:HD22	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:405:ILE:HG12	1:D:419:SER:HA	1.98	0.45
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.98	0.45
1:C:598:LEU:HD22	1:C:671:MET:HG2	1.98	0.45
1:C:741:GLY:O	1:C:742:ILE:C	2.55	0.45
1:D:214:LEU:HD23	1:D:225:TYR:HB3	1.98	0.45
1:D:669:ARG:HD2	1:D:670:TYR:CZ	2.52	0.45
1:B:598:LEU:HD22	1:B:671:MET:HG2	1.97	0.45
1:D:159:PRO:HD3	1:D:216:TRP:CB	2.47	0.45
1:A:455:GLN:HE21	1:A:557:THR:HG21	1.82	0.45
1:B:129:THR:HG23	1:B:151:ASN:HA	1.97	0.45
1:C:410:LEU:HD22	1:C:411:THR:O	2.16	0.45
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.52	0.45
1:B:153:GLN:NE2	1:B:170:ASN:H	2.06	0.45
1:A:325:MET:HE2	1:A:327:ILE:HD11	1.94	0.45
1:D:129:THR:HG23	1:D:151:ASN:HA	1.98	0.45
1:D:731:GLN:HG3	1:D:758:PHE:HE1	1.82	0.44
1:A:135:TYR:CE2	1:A:140:ARG:HA	2.52	0.44
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.99	0.44
1:B:62:TRP:CG	1:B:462:SER:HA	2.53	0.44
1:B:75:ASN:ND2	1:B:92:ASN:HD22	2.15	0.44
1:C:470:LEU:HD12	1:C:483:HIS:NE2	2.33	0.44
1:C:614:SER:HA	1:C:619:VAL:HB	2.00	0.44
1:A:98:PHE:CD1	1:A:100:HIS:HB2	2.52	0.44
1:B:152:THR:HG21	1:B:155:VAL:HG22	1.98	0.44
1:B:193:ILE:HG22	1:B:194:ILE:HG12	2.00	0.44
1:B:378:GLU:CD	1:B:378:GLU:H	2.21	0.44
1:D:455:GLN:HE21	1:D:557:THR:HG21	1.82	0.44
1:B:75:ASN:HD21	1:B:92:ASN:HD22	1.66	0.43
1:D:517:ILE:HD11	1:D:578:PHE:CE1	2.53	0.43
1:C:78:VAL:HG23	1:C:89:PHE:HB2	2.00	0.43
1:C:422:TYR:CE1	1:C:423:LYS:HE3	2.54	0.43
1:B:405:ILE:HG12	1:B:419:SER:HA	2.00	0.43
1:D:397:ILE:HD12	1:D:434:ILE:HD13	2.01	0.43
1:B:302:ASP:HB3	1:B:314:GLN:HB2	2.00	0.43
1:C:544:LEU:HD23	1:C:626:ILE:HD12	2.00	0.43
1:D:224:ALA:HB1	1:D:268:PHE:CZ	2.53	0.43
1:B:385:CYS:HB3	1:B:387:PHE:CE2	2.54	0.43
1:A:473:SER:O	1:A:474:GLY:O	2.36	0.43
1:D:291:ALA:O	1:D:295:ILE:HG23	2.18	0.43
1:A:596:ARG:HA	1:A:670:TYR:O	2.19	0.43
1:C:234:PRO:HB2	1:D:248:TYR:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:ALA:HB2	1:D:216:TRP:CZ2	2.54	0.43
1:D:268:PHE:CD2	1:D:313:LEU:HD21	2.54	0.43
1:A:453:ARG:HG3	1:A:454:CYS:SG	2.58	0.43
1:C:112:GLN:HG3	1:C:113:PHE:CD2	2.53	0.43
1:C:148:ILE:HD11	1:C:164:LEU:HD21	2.01	0.43
1:A:680:LEU:HD11	1:A:684:ARG:CZ	2.49	0.42
1:D:268:PHE:CE2	1:D:313:LEU:HD11	2.54	0.42
1:A:72:GLN:HB2	1:A:77:LEU:HD21	2.01	0.42
1:A:80:ASN:HD22	1:A:82:GLU:H	1.66	0.42
1:B:415:LEU:HB2	1:B:436:LEU:HD11	2.02	0.42
1:A:268:PHE:CD2	1:A:313:LEU:HD21	2.54	0.42
1:A:433:LYS:HE2	1:A:445:LEU:HD21	2.01	0.42
1:C:54:ARG:HH21	1:C:54:ARG:CG	2.19	0.42
1:C:55:LEU:HD23	1:C:500:LEU:CD2	2.50	0.42
1:C:418:ILE:HA	1:C:430:ASN:O	2.19	0.42
1:A:129:THR:HG22	5:A:1002:HOH:O	2.18	0.42
1:C:155:VAL:HG12	1:C:166:TYR:HB3	2.01	0.42
1:D:450:ASN:O	1:D:454:CYS:HB2	2.20	0.42
1:A:596:ARG:N	1:A:670:TYR:O	2.47	0.42
1:C:179:ASN:HD22	1:C:180:LEU:N	2.17	0.42
1:D:435:GLN:OE1	1:D:441:LYS:HD3	2.19	0.42
1:D:765:LEU:HA	1:D:766:PRO:HD3	1.91	0.42
1:A:259:ALA:HB3	1:A:660:GLU:HA	2.02	0.41
1:A:658:ARG:HB2	1:A:687:THR:HG22	2.01	0.41
1:B:70:TYR:CG	1:B:71:LYS:N	2.88	0.41
1:B:313:LEU:O	1:B:325:MET:HA	2.19	0.41
1:C:167:VAL:HA	1:C:171:ASP:O	2.20	0.41
1:C:302:ASP:HB3	1:C:314:GLN:HB2	2.01	0.41
1:A:378:GLU:CD	1:A:378:GLU:H	2.23	0.41
1:A:513:LYS:O	1:A:527:GLN:HA	2.20	0.41
1:B:506:ASN:HB2	1:C:440:THR:CG2	2.49	0.41
1:C:397:ILE:HD12	1:C:434:ILE:HD13	2.03	0.41
1:D:79:PHE:CD2	1:D:86:SER:HB3	2.54	0.41
1:D:98:PHE:CD1	1:D:100:HIS:HB2	2.55	0.41
1:A:70:TYR:HB3	1:A:79:PHE:CE1	2.55	0.41
1:A:458:SER:OG	1:A:471:ARG:HB3	2.21	0.41
1:A:703:ILE:HA	1:A:733:MET:O	2.21	0.41
1:B:662:TYR:HE1	1:B:710:ASN:HD22	1.69	0.41
1:C:457:TYR:HA	1:C:471:ARG:O	2.20	0.41
1:D:237:GLU:HG2	1:D:253:ARG:HG2	2.02	0.41
1:D:598:LEU:HB2	1:D:671:MET:SD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:PHE:CD2	1:B:468:TYR:HB3	2.56	0.41
1:D:105:TYR:HA	1:D:115:LEU:O	2.20	0.41
1:A:98:PHE:CE1	1:A:100:HIS:HB2	2.56	0.41
1:A:135:TYR:CE2	1:A:140:ARG:HG2	2.55	0.41
1:C:478:PRO:HB2	1:C:497:ASN:ND2	2.36	0.41
1:D:55:LEU:HD23	1:D:500:LEU:HD22	2.02	0.41
1:D:598:LEU:HD22	1:D:671:MET:HG2	2.02	0.41
1:B:657:SER:HA	1:B:688:VAL:HG13	2.02	0.41
1:C:49:LEU:HD22	1:C:749:GLN:HA	2.03	0.41
1:A:242:SER:OG	1:A:243:ASP:N	2.53	0.41
1:D:167:VAL:HA	1:D:171:ASP:O	2.21	0.41
1:A:146:GLU:O	1:A:175:LYS:NZ	2.52	0.41
1:A:154:TRP:CD2	1:A:212:SER:HB3	2.56	0.41
1:A:177:GLU:HB2	1:A:180:LEU:HG	2.02	0.41
1:A:389:ILE:HD13	1:A:389:ILE:HA	1.77	0.41
1:A:598:LEU:HB2	1:A:671:MET:SD	2.60	0.41
1:B:55:LEU:HD23	1:B:500:LEU:CD2	2.51	0.41
1:B:598:LEU:O	1:B:682:HIS:NE2	2.52	0.41
1:C:562:ASN:HB2	5:C:841:HOH:O	2.20	0.41
1:A:543:LEU:O	1:A:575:VAL:HA	2.22	0.41
1:B:582:GLY:CA	1:B:594:ILE:HD12	2.50	0.40
1:C:484:SER:O	1:C:488:ASP:HA	2.20	0.40
1:D:55:LEU:HD23	1:D:500:LEU:CD2	2.51	0.40
1:A:158:SER:OG	1:A:163:LYS:HB2	2.22	0.40
1:A:237:GLU:HA	1:A:252:VAL:O	2.21	0.40
1:A:546:VAL:HG12	1:A:627:TRP:O	2.21	0.40
1:B:649:CYS:HB3	1:B:699:GLU:HB2	2.02	0.40
1:D:164:LEU:HB3	1:D:175:LYS:HB2	2.03	0.40
1:A:414:TYR:CE2	1:A:433:LYS:HD3	2.57	0.40
1:B:63:ILE:HD12	1:B:63:ILE:HA	1.81	0.40
1:C:243:ASP:C	1:C:245:SER:N	2.75	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	721/740 (97%)	684 (95%)	36 (5%)	1 (0%)	51	73
1	B	725/740 (98%)	698 (96%)	25 (3%)	2 (0%)	41	61
1	C	721/740 (97%)	688 (95%)	31 (4%)	2 (0%)	41	61
1	D	720/740 (97%)	684 (95%)	34 (5%)	2 (0%)	41	61
All	All	2887/2960 (98%)	2754 (95%)	126 (4%)	7 (0%)	47	68

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	474	GLY
1	A	474	GLY
1	B	37	HIS
1	B	474	GLY
1	D	474	GLY
1	C	92	ASN
1	D	109	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	650/662 (98%)	611 (94%)	39 (6%)	19	37
1	B	652/662 (98%)	611 (94%)	41 (6%)	18	34
1	C	650/662 (98%)	614 (94%)	36 (6%)	21	41
1	D	649/662 (98%)	617 (95%)	32 (5%)	25	47
All	All	2601/2648 (98%)	2453 (94%)	148 (6%)	20	39

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LEU

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Mol	Chain	Res	Type
1	A	80	ASN
1	A	95	PHE
1	A	145	GLU
1	A	169	ASN
1	A	170	ASN
1	A	179	ASN
1	A	246	LEU
1	A	276	LEU
1	A	283	THR
1	A	316	LEU
1	A	343	ARG
1	A	358[A]	ARG
1	A	358[B]	ARG
1	A	385	CYS
1	A	389	ILE
1	A	415	LEU
1	A	436	LEU
1	A	441	LYS
1	A	453	ARG
1	A	464	GLU
1	A	472	CYS
1	A	477	LEU
1	A	482	LEU
1	A	492	ARG
1	A	505	GLN
1	A	507	VAL
1	A	514	LEU
1	A	519	LEU
1	A	538	LYS
1	A	566	TYR
1	A	575	VAL
1	A	598	LEU
1	A	630	SER
1	A	673	LEU
1	A	677	GLU
1	A	685	ASN
1	A	688	VAL
1	A	710	ASN
1	B	41	LYS
1	B	59	SER
1	B	61	ARG
1	B	63	ILE

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Mol	Chain	Res	Type
1	B	129	THR
1	B	139	LYS
1	B	142	LEU
1	B	164	LEU
1	B	179	ASN
1	B	230	ASP
1	B	246	LEU
1	B	276	LEU
1	B	283	THR
1	B	313	LEU
1	B	316	LEU
1	B	325	MET
1	B	360	SER
1	B	370	SER
1	B	385	CYS
1	B	389	ILE
1	B	395	THR
1	B	410	LEU
1	B	415	LEU
1	B	436	LEU
1	B	453	ARG
1	B	464	GLU
1	B	473	SER
1	B	477	LEU
1	B	482	LEU
1	B	504	LEU
1	B	506	ASN
1	B	507	VAL
1	B	514	LEU
1	B	566	TYR
1	B	575	VAL
1	B	594	ILE
1	B	598	LEU
1	B	627	TRP
1	B	660	GLU
1	B	685	ASN
1	B	710	ASN
1	C	54	ARG
1	C	57	LEU
1	C	80	ASN
1	C	129	THR
1	C	170	ASN

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Mol	Chain	Res	Type
1	C	179	ASN
1	C	243	ASP
1	C	246	LEU
1	C	276	LEU
1	C	283	THR
1	C	316	LEU
1	C	325	MET
1	C	385	CYS
1	C	395	THR
1	C	410	LEU
1	C	415	LEU
1	C	433	LYS
1	C	434	ILE
1	C	436	LEU
1	C	441	LYS
1	C	448	GLU
1	C	453	ARG
1	C	463	LYS
1	C	482	LEU
1	C	507	VAL
1	C	514	LEU
1	C	519	LEU
1	C	538	LYS
1	C	575	VAL
1	C	589	LYS
1	C	615	LYS
1	C	673	LEU
1	C	677	GLU
1	C	685	ASN
1	C	688	VAL
1	C	710	ASN
1	D	51	ASN
1	D	56	LYS
1	D	78	VAL
1	D	90	LEU
1	D	109	PRO
1	D	129	THR
1	D	137	LEU
1	D	140	ARG
1	D	142	LEU
1	D	170	ASN
1	D	179	ASN

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Mol	Chain	Res	Type
1	D	246	LEU
1	D	250	LYS
1	D	276	LEU
1	D	280	THR
1	D	316	LEU
1	D	365	THR
1	D	385	CYS
1	D	388	GLN
1	D	392	LYS
1	D	410	LEU
1	D	453	ARG
1	D	482	LEU
1	D	492	ARG
1	D	507	VAL
1	D	514	LEU
1	D	536	LYS
1	D	575	VAL
1	D	598	LEU
1	D	688	VAL
1	D	704	HIS
1	D	710	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	80	ASN
1	A	100	HIS
1	A	153	GLN
1	A	169	ASN
1	A	170	ASN
1	A	179	ASN
1	A	338	ASN
1	A	344	GLN
1	A	455	GLN
1	A	572	ASN
1	A	592	HIS
1	A	710	ASN
1	B	80	ASN
1	B	92	ASN
1	B	123	GLN
1	B	138	ASN

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Mol	Chain	Res	Type
1	B	153	GLN
1	B	169	ASN
1	B	170	ASN
1	B	179	ASN
1	B	430	ASN
1	B	455	GLN
1	B	505	GLN
1	B	506	ASN
1	B	508	GLN
1	B	572	ASN
1	B	592	HIS
1	B	710	ASN
1	C	51	ASN
1	C	80	ASN
1	C	100	HIS
1	C	123	GLN
1	C	138	ASN
1	C	141	GLN
1	C	153	GLN
1	C	170	ASN
1	C	179	ASN
1	C	344	GLN
1	C	430	ASN
1	C	455	GLN
1	C	505	GLN
1	C	697	GLN
1	C	710	ASN
1	C	748	HIS
1	D	80	ASN
1	D	138	ASN
1	D	153	GLN
1	D	169	ASN
1	D	170	ASN
1	D	179	ASN
1	D	344	GLN
1	D	430	ASN
1	D	455	GLN
1	D	508	GLN
1	D	572	ASN
1	D	592	HIS
1	D	621	ASN
1	D	710	ASN

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Mol	Chain	Res	Type
1	D	748	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

10 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	E	1	2,1	14,14,15	0.60	0	17,19,21	0.87	1 (5%)
2	NAG	E	2	2	14,14,15	0.46	0	17,19,21	1.04	0
2	NAG	F	1	2,1	14,14,15	0.55	0	17,19,21	1.45	3 (17%)
2	NAG	F	2	2	14,14,15	0.57	0	17,19,21	0.77	0
2	NAG	G	1	2,1	14,14,15	0.63	0	17,19,21	0.93	0
2	NAG	G	2	2	14,14,15	0.53	0	17,19,21	0.93	0
2	NAG	H	1	2,1	14,14,15	0.64	0	17,19,21	0.98	0
2	NAG	H	2	2	14,14,15	0.62	0	17,19,21	1.26	2 (11%)
2	NAG	I	1	2,1	14,14,15	0.45	0	17,19,21	1.02	1 (5%)
2	NAG	I	2	2	14,14,15	0.61	0	17,19,21	1.00	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	2	NAG	C4-C3-C2	3.87	116.68	111.02
2	F	1	NAG	C1-O5-C5	2.94	116.13	112.19
2	F	1	NAG	O5-C1-C2	-2.66	107.17	111.29
2	I	1	NAG	C1-O5-C5	2.54	115.59	112.19
2	F	1	NAG	C2-N2-C7	-2.35	119.76	122.90
2	E	1	NAG	O5-C1-C2	-2.22	107.85	111.29
2	H	2	NAG	C3-C4-C5	2.15	114.13	110.23

There are no chirality outliers.

All (22) torsion outliers are listed below:

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

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

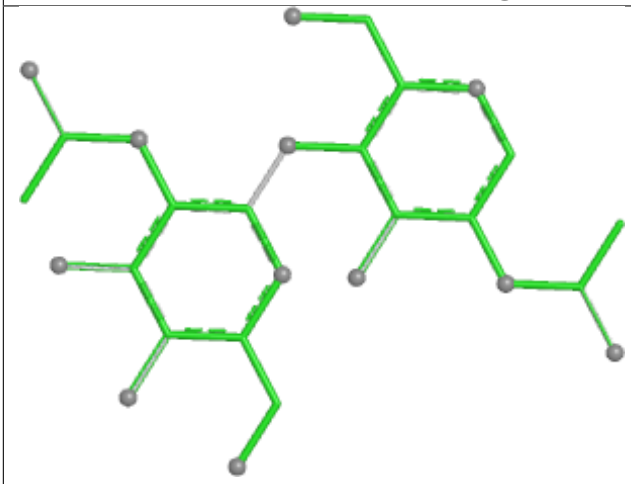
There are no ring outliers.

2 monomers are involved in 1 short contact:

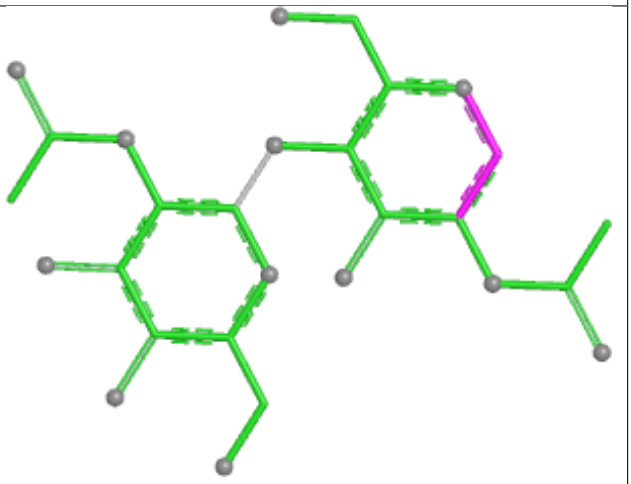
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	NAG	1	0
2	G	1	NAG	1	0

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

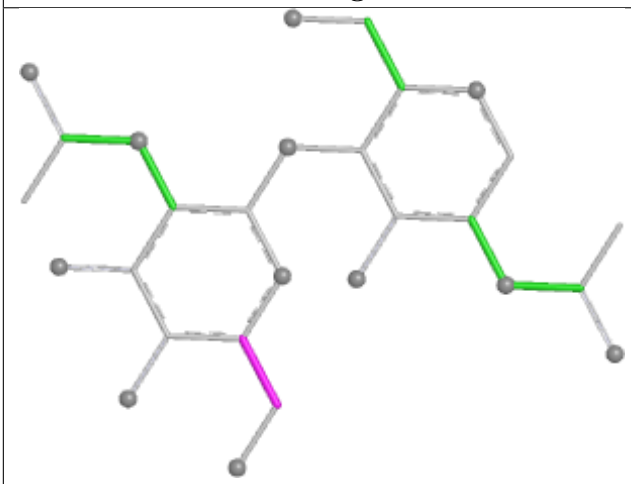
Oligosaccharide Chain E



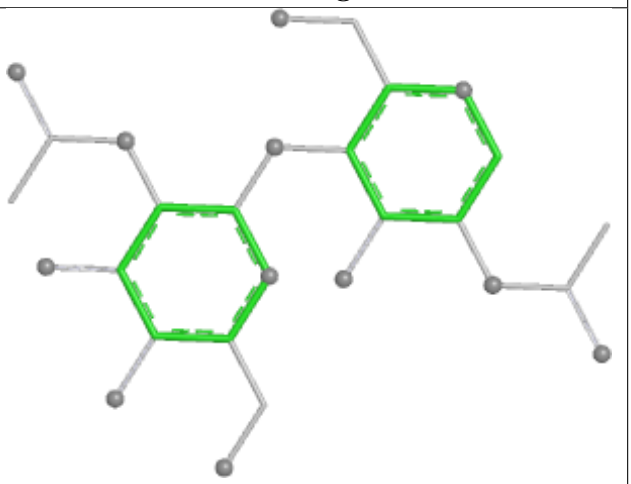
Bond lengths



Bond angles

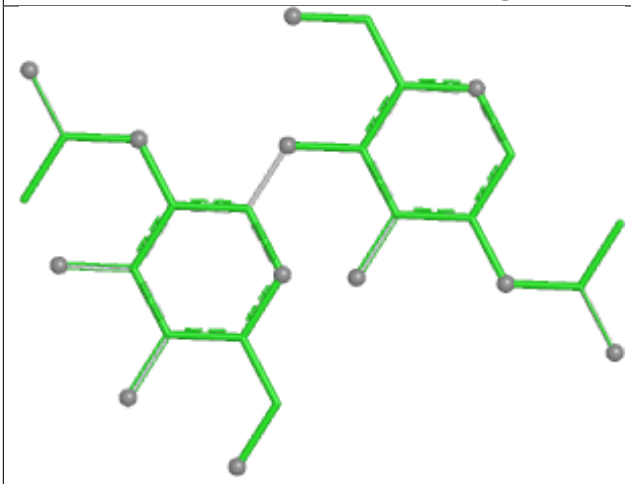


Torsions

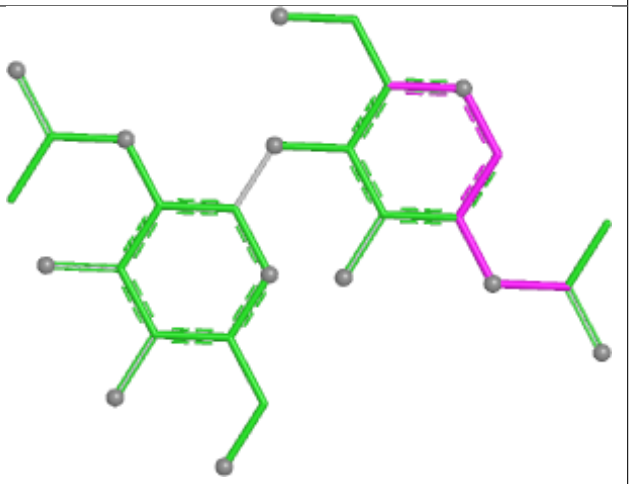


Rings

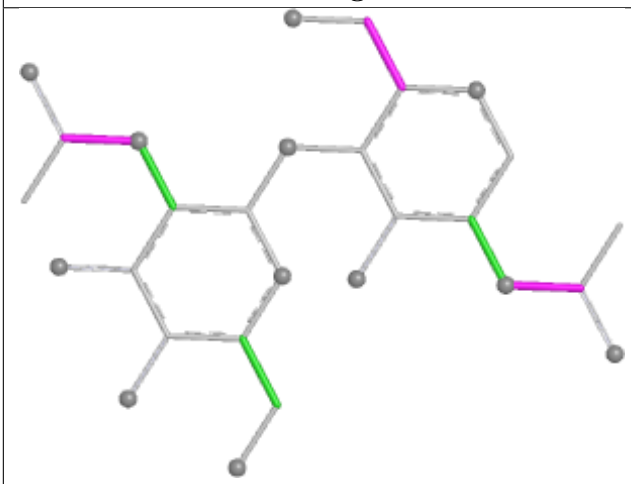
Oligosaccharide Chain F



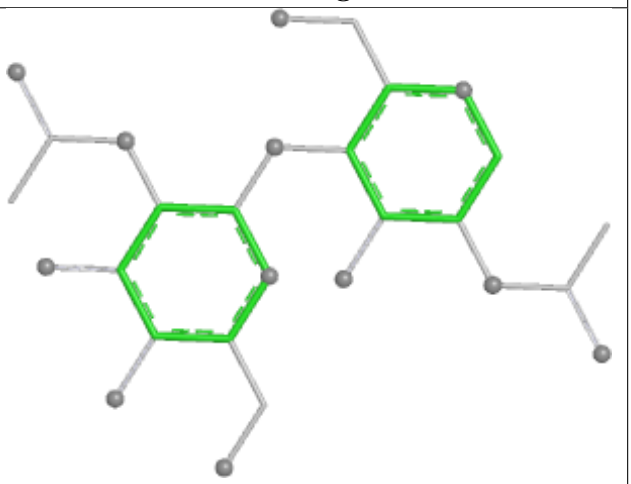
Bond lengths



Bond angles

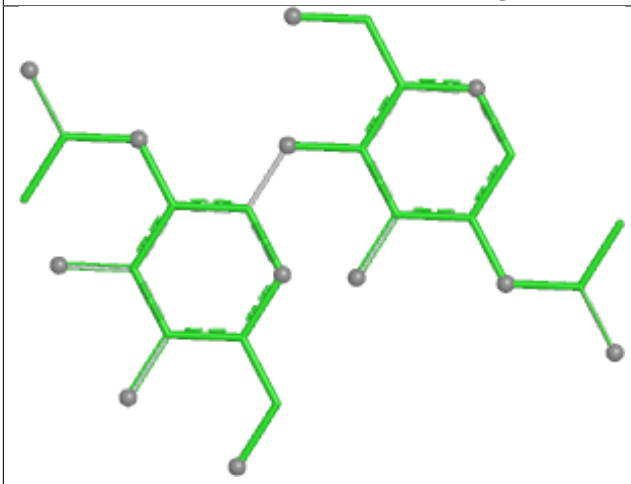


Torsions

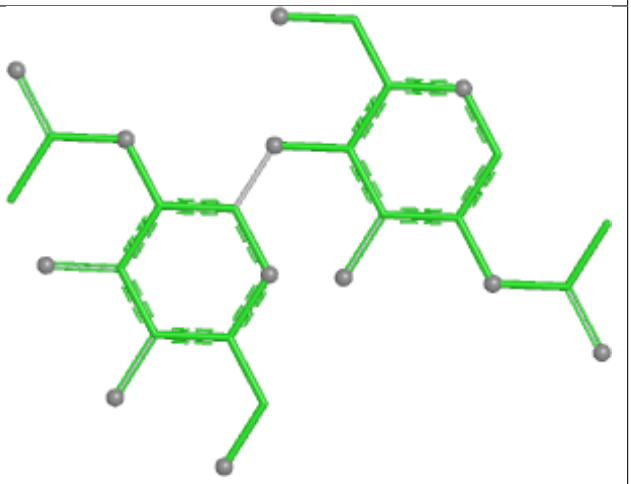


Rings

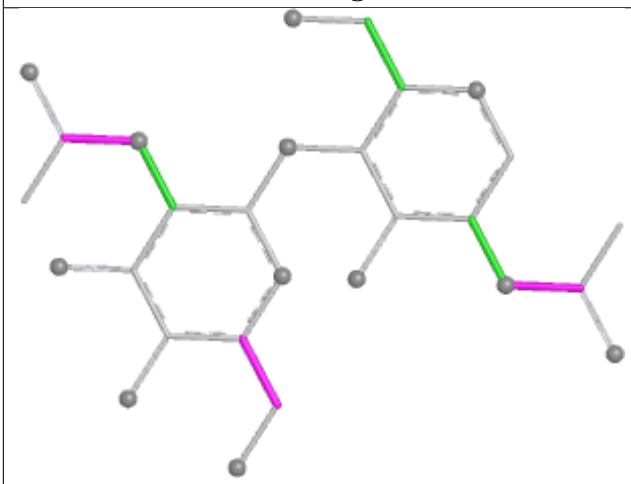
Oligosaccharide Chain G



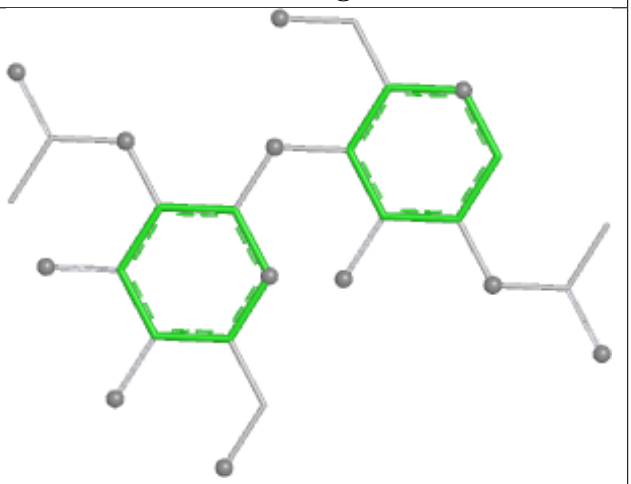
Bond lengths



Bond angles

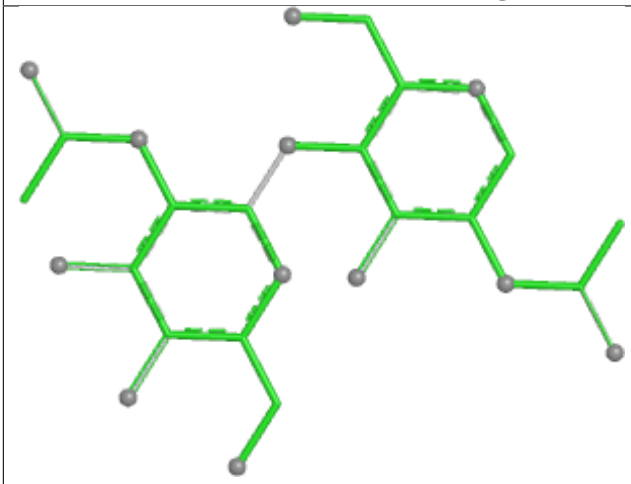


Torsions

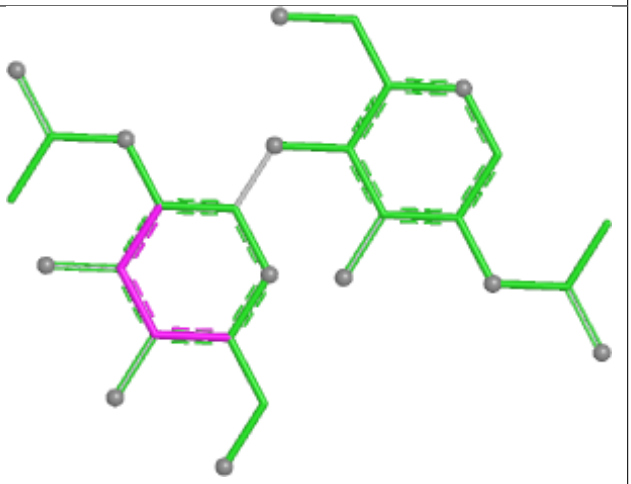


Rings

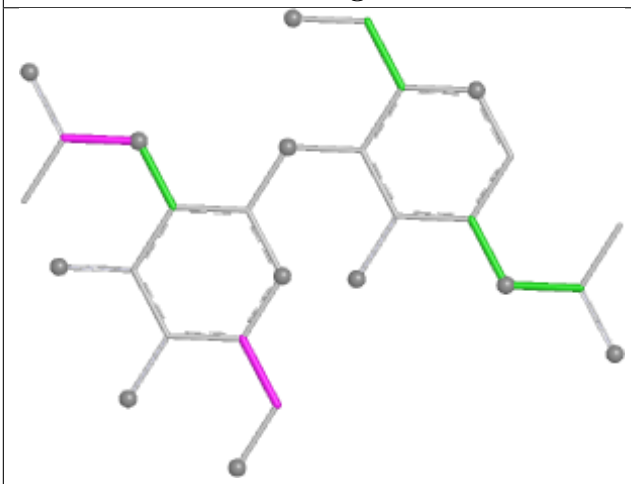
Oligosaccharide Chain H



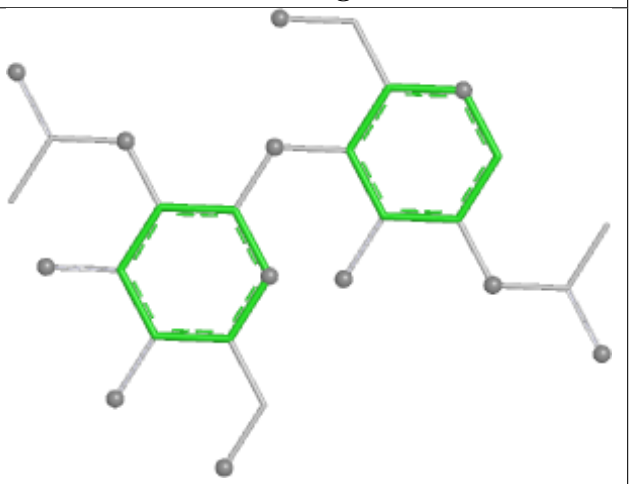
Bond lengths



Bond angles

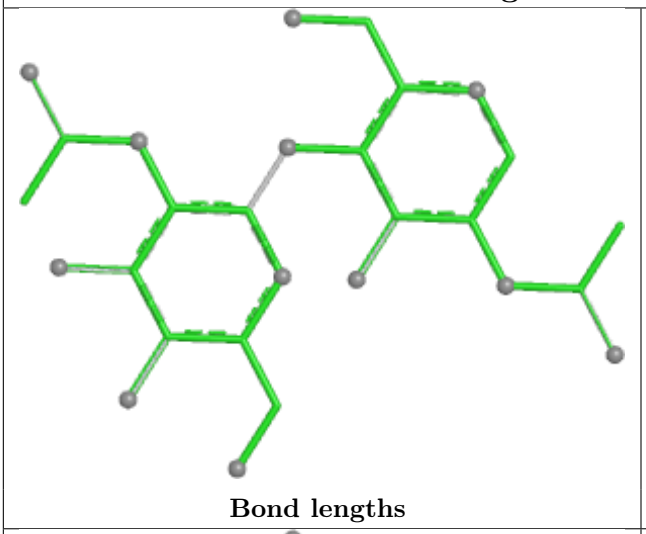


Torsions

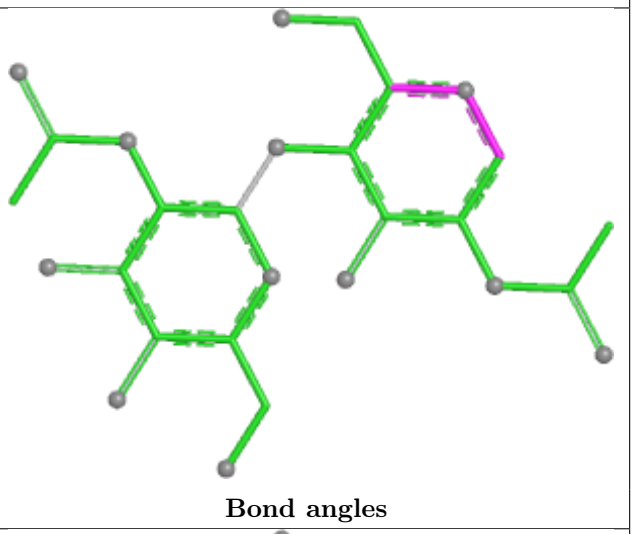


Rings

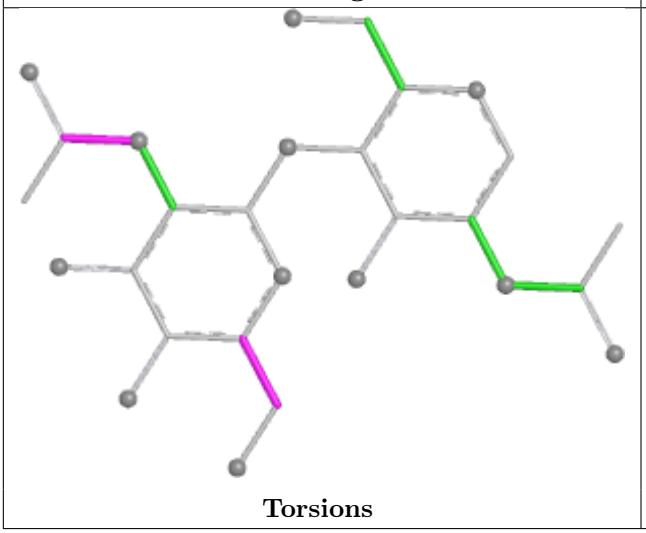
Oligosaccharide Chain I



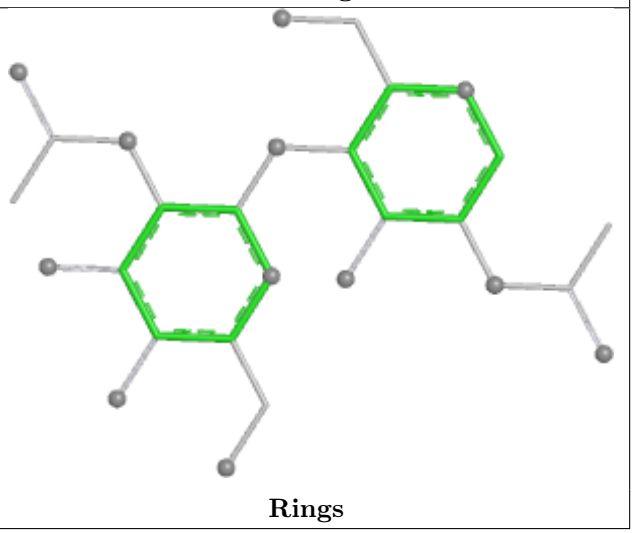
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

16 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	$\#\|Z\| > 2$
3	NAG	A	802	1	14,14,15	0.58	0	17,19,21	1.41	1 (5%)
3	NAG	A	803	1	14,14,15	0.59	0	17,19,21	0.99	1 (5%)
3	NAG	B	806	1	14,14,15	0.56	0	17,19,21	1.64	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	B	803	1	14,14,15	0.63	0	17,19,21	1.21	1 (5%)
3	NAG	D	804	1	14,14,15	0.79	1 (7%)	17,19,21	1.61	3 (17%)
4	B2Y	B	800	-	14,15,15	0.70	0	15,19,19	0.69	0
4	B2Y	C	800	-	14,15,15	0.77	0	15,19,19	0.86	0
3	NAG	C	801	1	14,14,15	0.50	0	17,19,21	1.40	1 (5%)
3	NAG	C	802	1	14,14,15	0.64	0	17,19,21	1.32	1 (5%)
3	NAG	D	801	1	14,14,15	0.60	0	17,19,21	1.06	1 (5%)
4	B2Y	D	800	-	14,15,15	0.72	0	15,19,19	0.77	0
3	NAG	A	801	1	14,14,15	0.59	0	17,19,21	1.44	1 (5%)
4	B2Y	A	800	-	14,15,15	0.81	0	15,19,19	0.87	0
3	NAG	B	801	1	14,14,15	0.78	1 (7%)	17,19,21	1.39	2 (11%)
3	NAG	B	802	1	14,14,15	0.53	0	17,19,21	1.17	1 (5%)
3	NAG	A	808	1	14,14,15	0.57	0	17,19,21	1.41	1 (5%)

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	A	802	1	-	0/6/23/26	0/1/1/1
3	NAG	A	803	1	-	2/6/23/26	0/1/1/1
3	NAG	B	806	1	-	4/6/23/26	0/1/1/1
3	NAG	D	804	1	1/1/5/7	5/6/23/26	0/1/1/1
3	NAG	B	803	1	-	0/6/23/26	0/1/1/1
4	B2Y	B	800	-	-	0/2/6/6	0/2/2/2
4	B2Y	C	800	-	-	1/2/6/6	0/2/2/2
3	NAG	C	801	1	-	0/6/23/26	0/1/1/1
3	NAG	C	802	1	-	2/6/23/26	0/1/1/1
3	NAG	D	801	1	-	0/6/23/26	0/1/1/1
4	B2Y	D	800	-	-	0/2/6/6	0/2/2/2
3	NAG	A	801	1	-	2/6/23/26	0/1/1/1
4	B2Y	A	800	-	-	1/2/6/6	0/2/2/2
3	NAG	B	801	1	-	3/6/23/26	0/1/1/1
3	NAG	B	802	1	-	1/6/23/26	0/1/1/1
3	NAG	A	808	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	804	NAG	C1-C2	2.53	1.55	1.52
3	B	801	NAG	C1-C2	2.18	1.55	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	806	NAG	C1-O5-C5	5.75	119.89	112.19
3	A	802	NAG	C1-O5-C5	5.49	119.54	112.19
3	A	801	NAG	C1-O5-C5	4.90	118.75	112.19
3	A	808	NAG	C1-O5-C5	4.70	118.49	112.19
3	C	801	NAG	C1-O5-C5	4.48	118.19	112.19
3	B	803	NAG	C1-O5-C5	4.04	117.60	112.19
3	B	802	NAG	C1-O5-C5	4.04	117.60	112.19
3	D	804	NAG	C1-O5-C5	3.89	117.40	112.19
3	C	802	NAG	C4-C3-C2	3.80	116.59	111.02
3	B	801	NAG	C4-C3-C2	3.27	115.81	111.02
3	D	801	NAG	C1-O5-C5	2.66	115.75	112.19
3	D	804	NAG	O5-C1-C2	2.66	115.41	111.29
3	A	803	NAG	C4-C3-C2	2.66	114.91	111.02
3	B	801	NAG	O5-C5-C6	2.39	112.32	107.66
3	D	804	NAG	C3-C4-C5	-2.32	106.03	110.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	804	NAG	C1

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	803	NAG	C8-C7-N2-C2
3	A	803	NAG	O7-C7-N2-C2
3	B	801	NAG	C8-C7-N2-C2
3	B	801	NAG	O7-C7-N2-C2
3	B	806	NAG	C8-C7-N2-C2
3	B	806	NAG	O7-C7-N2-C2
3	C	802	NAG	C8-C7-N2-C2
3	C	802	NAG	O7-C7-N2-C2
3	D	804	NAG	C8-C7-N2-C2
3	D	804	NAG	O7-C7-N2-C2
3	B	806	NAG	O5-C5-C6-O6
3	B	806	NAG	C4-C5-C6-O6
3	D	804	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	A	801	NAG	C8-C7-N2-C2
3	A	801	NAG	O7-C7-N2-C2
3	D	804	NAG	C3-C2-N2-C7
3	D	804	NAG	C4-C5-C6-O6
3	B	802	NAG	C4-C5-C6-O6
3	B	801	NAG	C3-C2-N2-C7
4	A	800	B2Y	N1-C2-C3-C8
4	C	800	B2Y	N1-C2-C3-C8

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	800	B2Y	1	0
3	D	801	NAG	1	0
3	B	802	NAG	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	724/740 (97%)	0.60	80 (11%) 5 5	37, 48, 68, 104	0
1	B	729/740 (98%)	0.33	38 (5%) 27 29	36, 47, 67, 83	0
1	C	724/740 (97%)	0.65	86 (11%) 4 4	37, 48, 69, 101	0
1	D	724/740 (97%)	0.74	120 (16%) 1 1	36, 51, 69, 107	0
All	All	2901/2960 (98%)	0.58	324 (11%) 5 4	36, 48, 68, 107	0

All (324) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	95	PHE	8.2
1	D	83	TYR	7.9
1	C	135	TYR	7.6
1	C	279	VAL	7.1
1	D	93	SER	7.0
1	C	93	SER	6.4
1	D	94	THR	6.2
1	C	94	THR	5.9
1	A	92	ASN	5.7
1	C	99	GLY	5.6
1	A	88	VAL	5.4
1	D	77	LEU	5.4
1	A	135	TYR	5.3
1	D	386	TYR	5.2
1	C	96	ASP	5.1
1	D	414	TYR	5.0
1	A	140	ARG	4.8
1	C	141	GLN	4.7
1	C	83	TYR	4.7
1	C	92	ASN	4.6
1	A	96	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	280	THR	4.6
1	A	86	SER	4.6
1	B	518	ILE	4.5
1	B	81	ALA	4.4
1	D	734	TRP	4.4
1	D	412	SER	4.4
1	D	88	VAL	4.4
1	D	330	TYR	4.4
1	A	95	PHE	4.3
1	D	333	SER	4.3
1	B	88	VAL	4.3
1	D	81	ALA	4.3
1	B	86	SER	4.2
1	D	55	LEU	4.2
1	D	487	ASN	4.2
1	D	518	ILE	4.2
1	D	97	GLU	4.2
1	A	97	GLU	4.2
1	B	87	SER	4.2
1	C	102	ILE	4.2
1	C	187	TRP	4.1
1	A	333	SER	4.1
1	A	635	VAL	4.1
1	C	81	ALA	4.1
1	A	332	GLU	4.0
1	D	78	VAL	4.0
1	A	702	LEU	4.0
1	D	441	LYS	4.0
1	D	505	GLN	3.9
1	B	70	TYR	3.9
1	C	392	LYS	3.9
1	A	138	ASN	3.9
1	C	340	LEU	3.8
1	A	98	PHE	3.8
1	D	436	LEU	3.8
1	D	334	SER	3.8
1	A	93	SER	3.7
1	D	468	TYR	3.7
1	C	489	LYS	3.7
1	C	702	LEU	3.7
1	C	97	GLU	3.7
1	D	62	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	322	TYR	3.7
1	D	85	ASN	3.7
1	D	713	PHE	3.7
1	C	734	TRP	3.7
1	B	72	GLN	3.6
1	D	498	SER	3.6
1	C	467	TYR	3.6
1	D	399	LYS	3.6
1	D	439	TYR	3.5
1	A	700	TYR	3.5
1	D	366	LEU	3.5
1	D	486	VAL	3.5
1	D	766	PRO	3.5
1	D	435	GLN	3.5
1	A	69	LEU	3.5
1	D	86	SER	3.5
1	D	467	TYR	3.5
1	A	81	ALA	3.5
1	D	413	ASP	3.5
1	A	636	THR	3.5
1	D	100	HIS	3.5
1	D	84	GLY	3.4
1	C	332	GLU	3.4
1	D	96	ASP	3.4
1	A	94	THR	3.3
1	D	56	LYS	3.3
1	A	651	ILE	3.3
1	A	713	PHE	3.3
1	D	397	ILE	3.3
1	A	634	TYR	3.3
1	C	487	ASN	3.2
1	A	655	PRO	3.2
1	B	546	VAL	3.2
1	C	390	ASP	3.2
1	C	474	GLY	3.2
1	A	652	ALA	3.2
1	A	656	VAL	3.2
1	D	135	TYR	3.1
1	D	332	GLU	3.1
1	A	626	ILE	3.1
1	C	506	ASN	3.1
1	A	279	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	706	THR	3.1
1	A	701	LEU	3.1
1	D	340	LEU	3.1
1	A	87	SER	3.1
1	D	66	HIS	3.1
1	C	719	ILE	3.1
1	C	732	ALA	3.1
1	D	98	PHE	3.1
1	C	80	ASN	3.0
1	D	92	ASN	3.0
1	C	486	VAL	3.0
1	A	719	ILE	3.0
1	A	84	GLY	3.0
1	D	464	GLU	3.0
1	C	652	ALA	3.0
1	A	637	SER	3.0
1	C	713	PHE	3.0
1	B	734	TRP	3.0
1	C	636	THR	3.0
1	D	491	LEU	3.0
1	A	141	GLN	3.0
1	B	89	PHE	3.0
1	B	83	TYR	3.0
1	C	142	LEU	3.0
1	D	331	ASP	2.9
1	D	483	HIS	2.9
1	B	77	LEU	2.9
1	B	90	LEU	2.9
1	C	717	ALA	2.9
1	C	82	GLU	2.9
1	A	716	SER	2.9
1	A	703	ILE	2.9
1	D	91	GLU	2.9
1	B	78	VAL	2.9
1	D	437	SER	2.9
1	A	627	TRP	2.9
1	D	652	ALA	2.9
1	C	536	LYS	2.9
1	D	466	LYS	2.8
1	C	98	PHE	2.8
1	D	80	ASN	2.8
1	C	505	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	327	ILE	2.8
1	D	521	GLU	2.8
1	D	615	LYS	2.8
1	A	732	ALA	2.8
1	C	91	GLU	2.8
1	D	702	LEU	2.8
1	D	716	SER	2.8
1	D	141	GLN	2.7
1	B	71	LYS	2.7
1	C	391	LYS	2.7
1	C	276	LEU	2.7
1	C	716	SER	2.7
1	C	656	VAL	2.7
1	C	140	ARG	2.7
1	D	372	TYR	2.7
1	D	655	PRO	2.7
1	D	335	GLY	2.7
1	D	338	ASN	2.7
1	C	62	TRP	2.7
1	D	339	CYS	2.7
1	A	72	GLN	2.7
1	C	388	GLN	2.7
1	C	138	ASN	2.7
1	D	703	ILE	2.7
1	C	277	SER	2.7
1	C	700	TYR	2.7
1	B	676	PRO	2.7
1	A	77	LEU	2.6
1	C	482	LEU	2.6
1	A	632	GLY	2.6
1	A	711	VAL	2.6
1	C	231	THR	2.6
1	D	365	THR	2.6
1	B	392	LYS	2.6
1	A	654	ALA	2.6
1	D	68	TYR	2.6
1	B	82	GLU	2.6
1	D	95	PHE	2.6
1	D	546	VAL	2.5
1	A	180	LEU	2.5
1	A	640	LEU	2.5
1	C	100	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	67	GLU	2.5
1	A	717	ALA	2.5
1	D	636	THR	2.5
1	D	389	ILE	2.5
1	D	342	ALA	2.5
1	C	393	ASP	2.5
1	A	392	LYS	2.5
1	C	637	SER	2.5
1	A	715	GLN	2.5
1	D	499	ALA	2.5
1	D	370	SER	2.5
1	D	411	THR	2.5
1	C	139	LYS	2.5
1	B	99	GLY	2.5
1	A	704	HIS	2.5
1	D	442	VAL	2.5
1	C	336	ARG	2.4
1	D	54	ARG	2.4
1	B	703	ILE	2.4
1	B	628	GLY	2.4
1	D	633	GLY	2.4
1	D	432	TYR	2.4
1	D	677	GLU	2.4
1	D	380	GLY	2.4
1	D	523	LYS	2.4
1	D	440	THR	2.4
1	A	546	VAL	2.4
1	B	713	PHE	2.4
1	C	72	GLN	2.4
1	A	688	VAL	2.4
1	B	653	VAL	2.4
1	D	733	MET	2.4
1	D	717	ALA	2.4
1	C	333	SER	2.4
1	C	537	SER	2.4
1	B	733	MET	2.4
1	B	702	LEU	2.4
1	D	656	VAL	2.4
1	B	521	GLU	2.3
1	D	393	ASP	2.3
1	D	70	TYR	2.3
1	A	91	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	63	ILE	2.3
1	A	650	GLY	2.3
1	B	636	THR	2.3
1	C	452	GLU	2.3
1	D	415	LEU	2.3
1	C	711	VAL	2.3
1	A	628	GLY	2.3
1	A	657	SER	2.3
1	A	142	LEU	2.3
1	D	41	LYS	2.3
1	D	704	HIS	2.3
1	C	87	SER	2.3
1	C	715	GLN	2.3
1	D	222	PHE	2.3
1	A	543	LEU	2.3
1	A	631	TYR	2.3
1	B	241	TYR	2.3
1	B	544	LEU	2.3
1	A	103	ASN	2.2
1	C	113	PHE	2.2
1	A	502	LYS	2.2
1	D	71	LYS	2.2
1	C	655	PRO	2.2
1	A	638	MET	2.2
1	B	656	VAL	2.2
1	C	546	VAL	2.2
1	B	577	SER	2.2
1	D	63	ILE	2.2
1	A	280	THR	2.2
1	C	115	LEU	2.2
1	C	703	ILE	2.2
1	A	231	THR	2.2
1	A	474	GLY	2.2
1	B	633	GLY	2.2
1	A	733	MET	2.2
1	C	54	ARG	2.2
1	A	300	LEU	2.2
1	B	632	GLY	2.2
1	D	390	ASP	2.2
1	D	388	GLN	2.2
1	A	71	LYS	2.2
1	C	651	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	75	ASN	2.2
1	A	90	LEU	2.2
1	C	483	HIS	2.2
1	D	72	GLN	2.2
1	B	79	PHE	2.2
1	D	392	LYS	2.1
1	C	704	HIS	2.1
1	B	711	VAL	2.1
1	C	688	VAL	2.1
1	A	506	ASN	2.1
1	A	625	ALA	2.1
1	C	338	ASN	2.1
1	A	99	GLY	2.1
1	C	84	GLY	2.1
1	D	346	ILE	2.1
1	C	521	GLU	2.1
1	D	79	PHE	2.1
1	D	416	TYR	2.1
1	D	735	TYR	2.1
1	C	341	VAL	2.1
1	A	633	GLY	2.1
1	D	384	ILE	2.1
1	C	491	LEU	2.1
1	D	500	LEU	2.1
1	A	299	TYR	2.1
1	B	631	TYR	2.1
1	C	76	ILE	2.1
1	A	66	HIS	2.1
1	D	684	ARG	2.1
1	D	484	SER	2.1
1	D	653	VAL	2.1
1	C	468	TYR	2.1
1	A	214	LEU	2.1
1	A	316	LEU	2.1
1	C	89	PHE	2.1
1	C	101	SER	2.1
1	C	635	VAL	2.1
1	B	704	HIS	2.1
1	A	360	SER	2.1
1	D	87	SER	2.1
1	D	276	LEU	2.1
1	D	336	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	78	VAL	2.0
1	D	736	THR	2.0
1	A	467	TYR	2.0
1	C	90	LEU	2.0
1	D	410	LEU	2.0
1	D	348	MET	2.0
1	D	391	LYS	2.0
1	C	278	SER	2.0
1	B	76	ILE	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)

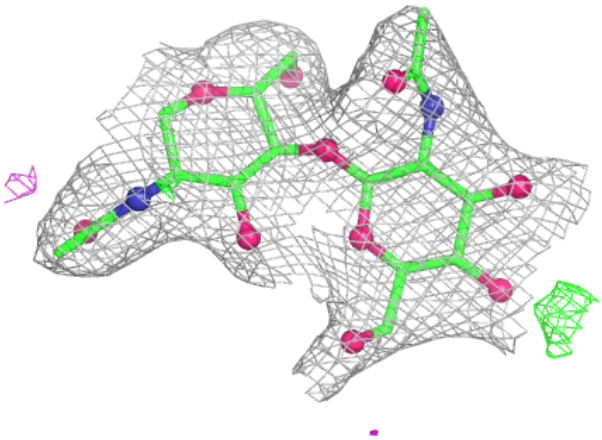
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

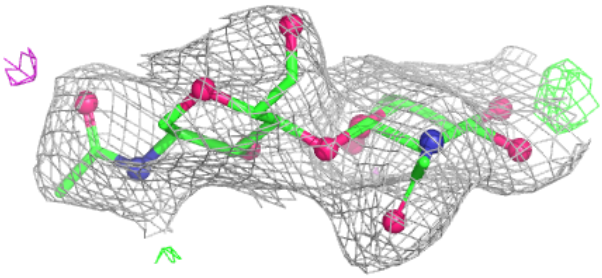
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	F	1	14/15	0.76	0.24	73,76,79,80	0
2	NAG	H	2	14/15	0.81	0.34	73,76,78,78	0
2	NAG	G	2	14/15	0.82	0.43	80,82,83,83	0
2	NAG	F	2	14/15	0.82	0.35	83,84,85,85	0
2	NAG	I	2	14/15	0.83	0.26	67,68,72,72	0
2	NAG	G	1	14/15	0.87	0.22	67,69,73,77	0
2	NAG	E	2	14/15	0.89	0.31	68,70,71,71	0
2	NAG	H	1	14/15	0.89	0.19	63,65,68,72	0
2	NAG	I	1	14/15	0.92	0.16	55,58,61,63	0
2	NAG	E	1	14/15	0.94	0.21	58,60,62,66	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:

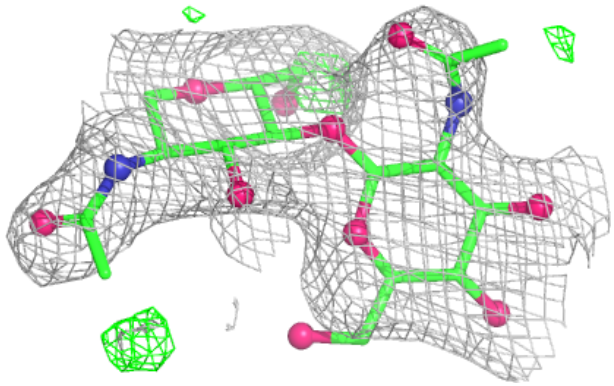
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

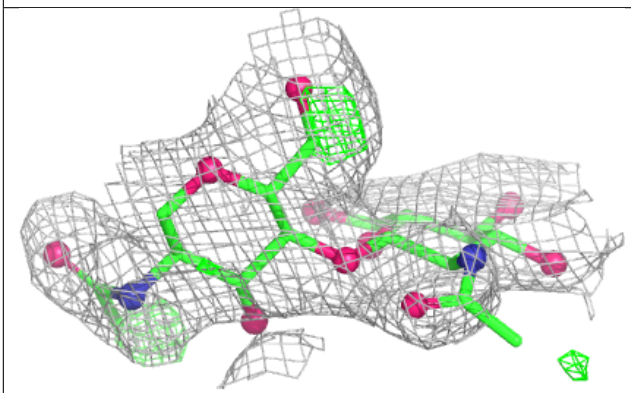


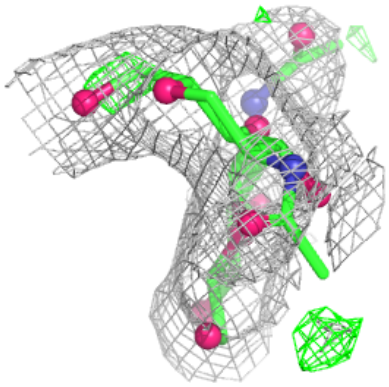


Electron density around Chain F:

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

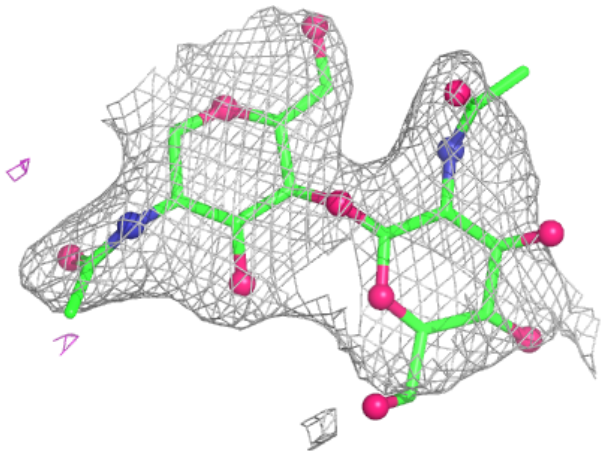


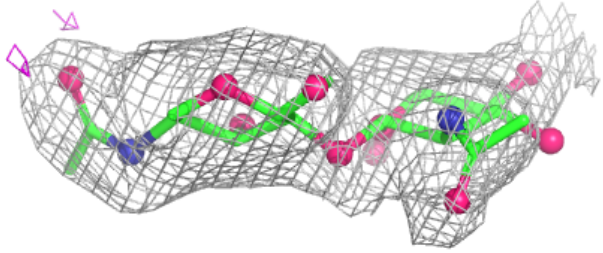


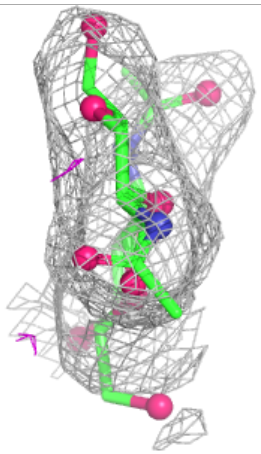


Electron density around Chain G:

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

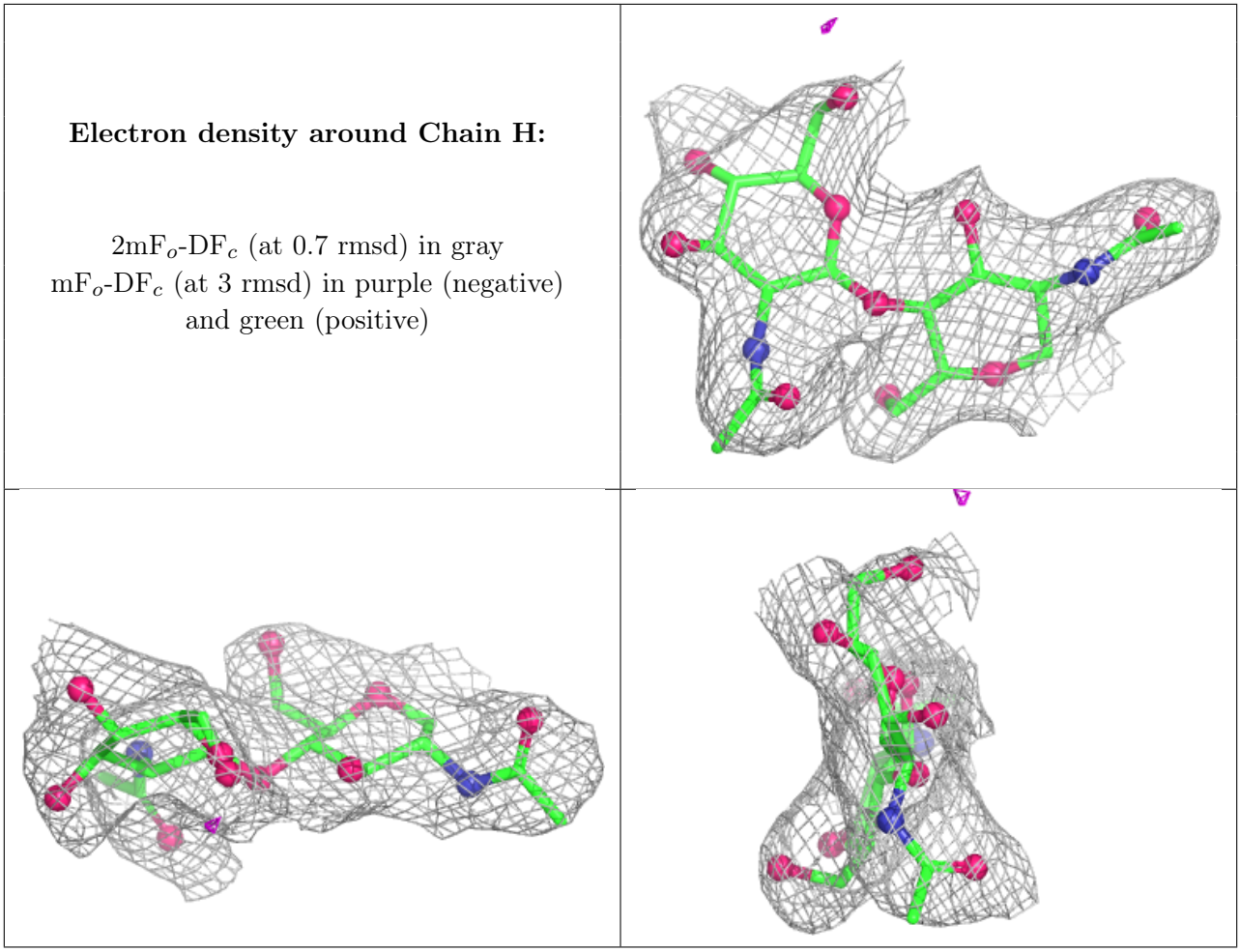






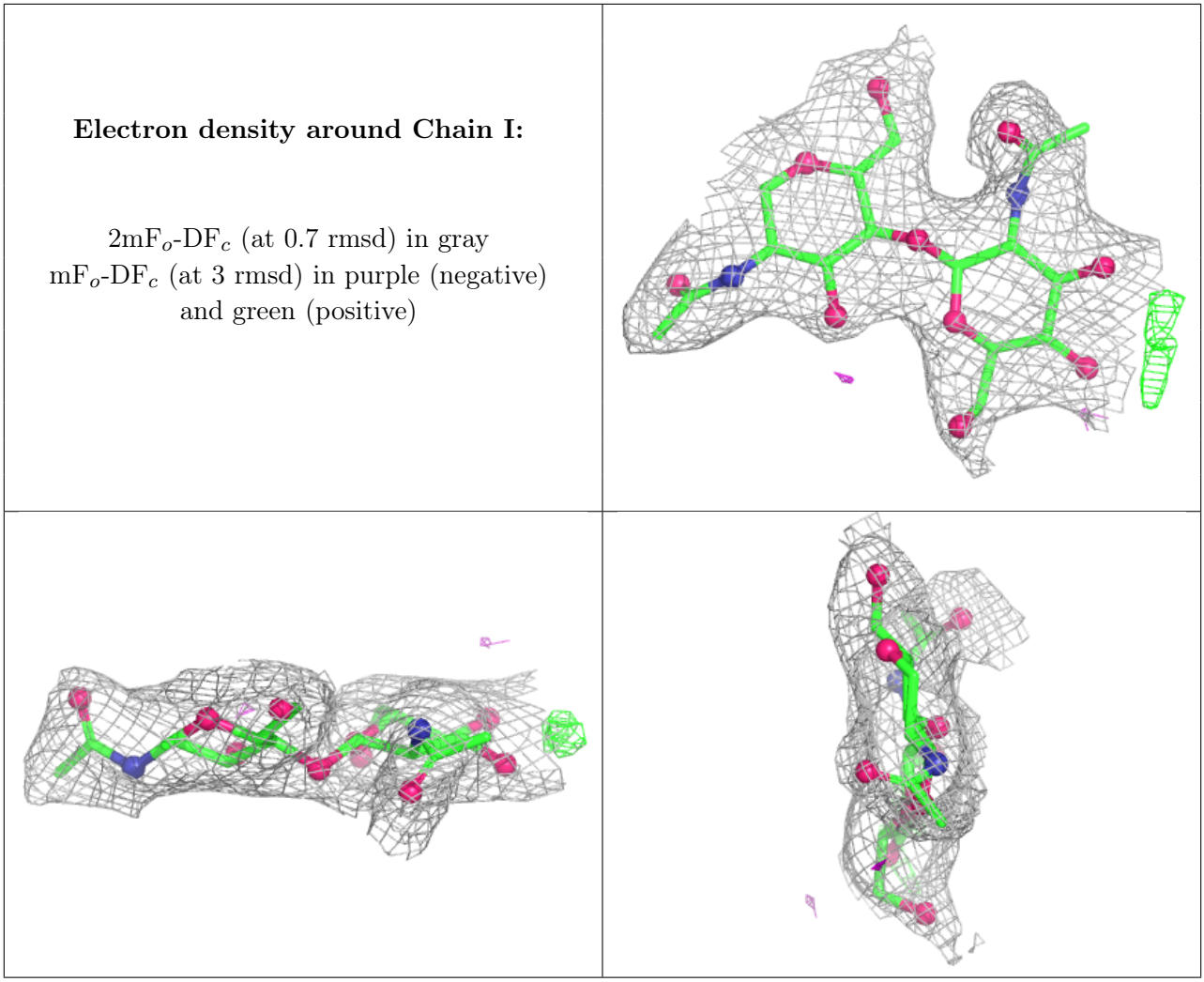
Electron density around Chain H:

$2mF_o$-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

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	NAG	A	801	14/15	0.65	0.32	72,73,74,74	0
3	NAG	A	803	14/15	0.72	0.32	71,73,76,77	0
3	NAG	B	801	14/15	0.73	0.23	78,79,80,80	0
3	NAG	A	802	14/15	0.77	0.30	65,66,68,68	0
3	NAG	C	801	14/15	0.77	0.20	55,55,56,57	0
3	NAG	B	806	14/15	0.80	0.14	67,69,73,74	0
3	NAG	B	803	14/15	0.81	0.33	63,65,68,68	0
3	NAG	D	804	14/15	0.82	0.20	78,80,82,82	0
3	NAG	D	801	14/15	0.86	0.19	58,60,62,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	A	808	14/15	0.86	0.30	61,63,64,64	0
3	NAG	C	802	14/15	0.88	0.32	68,70,74,74	0
4	B2Y	A	800	14/14	0.88	0.24	53,56,58,58	0
4	B2Y	B	800	14/14	0.88	0.28	60,62,63,64	0
3	NAG	B	802	14/15	0.89	0.20	63,64,66,66	0
4	B2Y	C	800	14/14	0.89	0.25	50,54,55,55	0
4	B2Y	D	800	14/14	0.93	0.17	42,44,46,46	0

6.5 Other polymers (i)

There are no such residues in this entry.