Full wwPDB X-ray Structure Validation Report (i)

Sep 6, 2023 – 02:47 PM EDT

PDB ID	:	4FQK
Title	:	Influenza B/Brisbane/60/2008 hemagglutinin Fab CR8059 complex
Authors	:	Dreyfus, C.; Laursen, N.S.; Wilson, I.A.
Deposited on	:	2012-06-25
Resolution	:	5.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

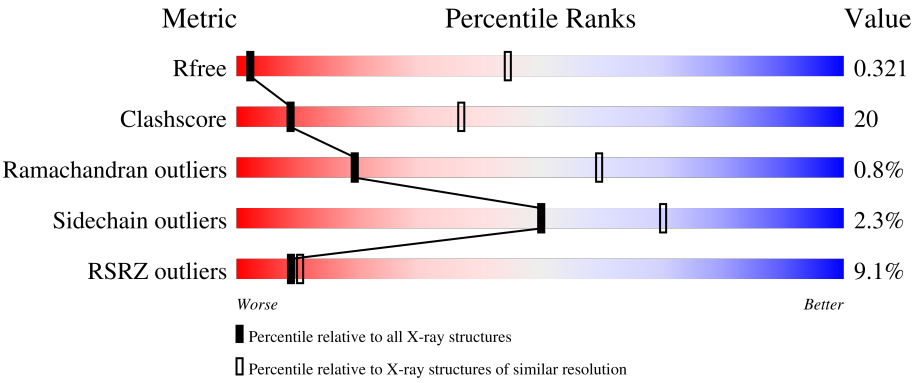
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 5.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1006 (7.40-3.84)
Clashscore	141614	1018 (7.40-3.90)
Ramachandran outliers	138981	1001 (7.40-3.84)
Sidechain outliers	138945	1203 (7.50-3.80)
RSRZ outliers	127900	1000 (7.54-3.78)

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	347	11% 56% 39%
1	C	347	8% 57% 38%
2	B	179	6% 56% 21% 22%
2	D	179	8% 56% 21% 22%
3	E	234	11% 71% 21% 6%

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Mol	Chain	Length	Quality of chain
3	H	234	9% 71% 22% 6%
4	F	216	8% 79% 20%
4	L	216	6% 81% 17%
5	G	2	50% 50%
5	I	2	100%
5	J	2	100%
5	N	2	100%
5	O	2	100%
5	P	2	50% 50%
6	K	3	67% 33%
6	M	3	67% 33%

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
5	NAG	G	2	-	-	-	X
5	NAG	J	2	-	-	-	X
5	NAG	O	2	-	-	-	X
6	NAG	K	1	-	-	-	X
7	NAG	A	410	-	-	-	X
7	NAG	C	410	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 14080 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 Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2560	1607	458	480	15			
1	C	337	Total	C	N	O	S	0	0	0
			2560	1607	458	480	15			

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	139	Total	C	N	O	S	0	0	0
			1054	652	182	215	5			
2	D	140	Total	C	N	O	S	0	0	0
			1062	658	183	216	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	524	SER	-	linker	UNP C0LT38
B	525	GLY	-	linker	UNP C0LT38
B	526	ARG	-	linker	UNP C0LT38
D	524	SER	-	linker	UNP C0LT38
D	525	GLY	-	linker	UNP C0LT38
D	526	ARG	-	linker	UNP C0LT38

- Molecule 3 is a protein called Antibody CR8059 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	220	Total	C	N	O	S	0	0	0
			1673	1061	278	327	7			
3	H	221	Total	C	N	O	S	0	0	0
			1679	1064	279	328	8			

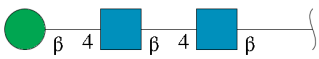
- Molecule 4 is a protein called Antibody CR8059 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	213	Total	C	N	O	S	0	0	0
			1606	1006	269	327	4			
4	L	214	Total	C	N	O	S	0	0	0
			1612	1009	270	328	5			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

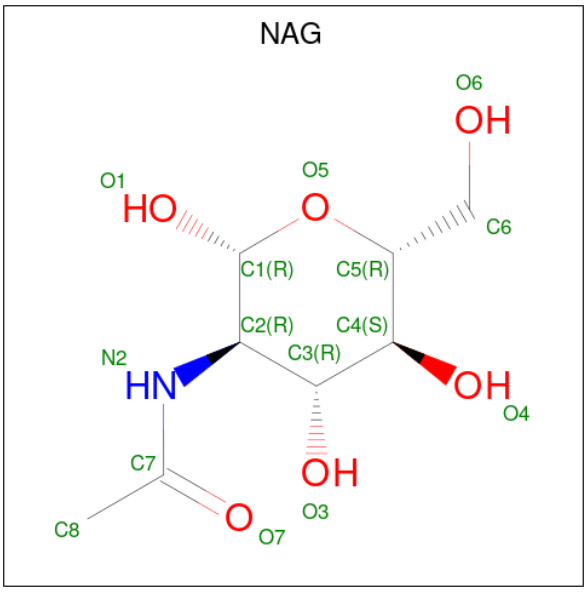
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 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
6	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	M	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

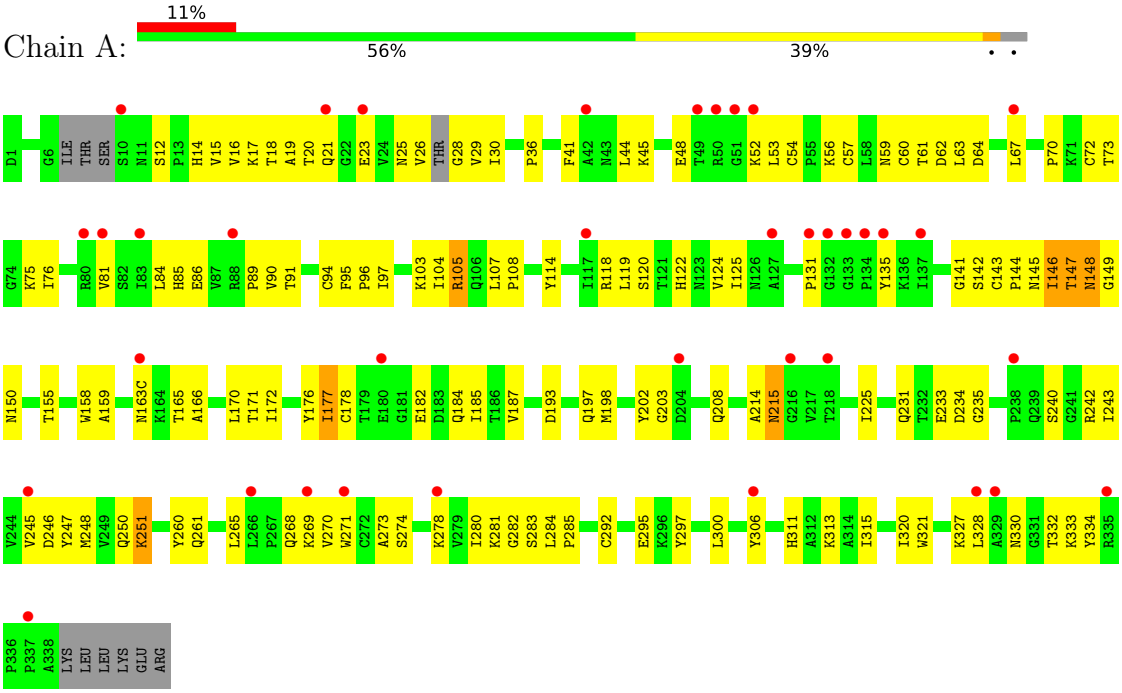


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 14 8 1 5	0	0
7	C	1	Total C N O 14 8 1 5	0	0

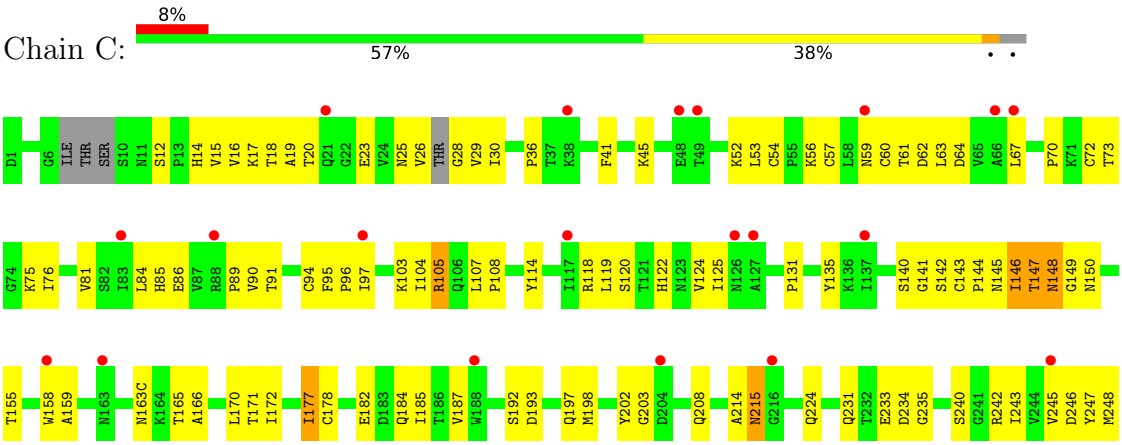
3 Residue-property plots (i)

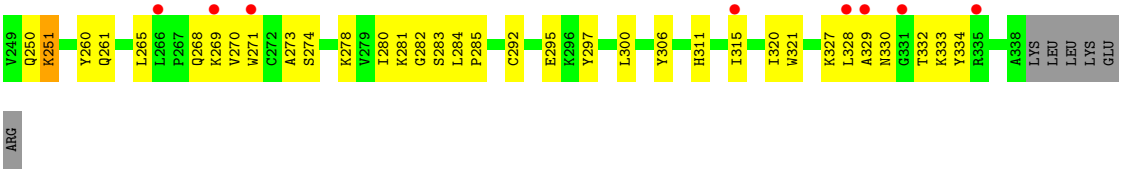
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Hemagglutinin HA1

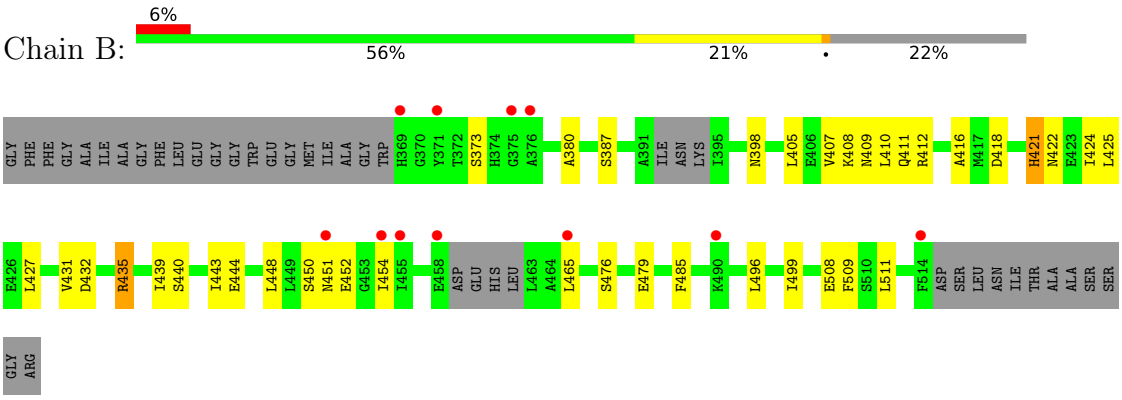


• Molecule 1: Hemagglutinin HA1

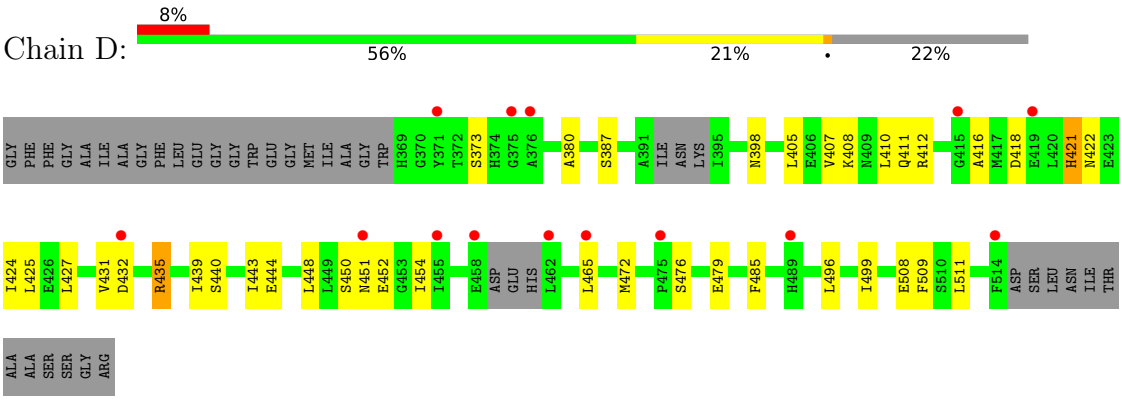




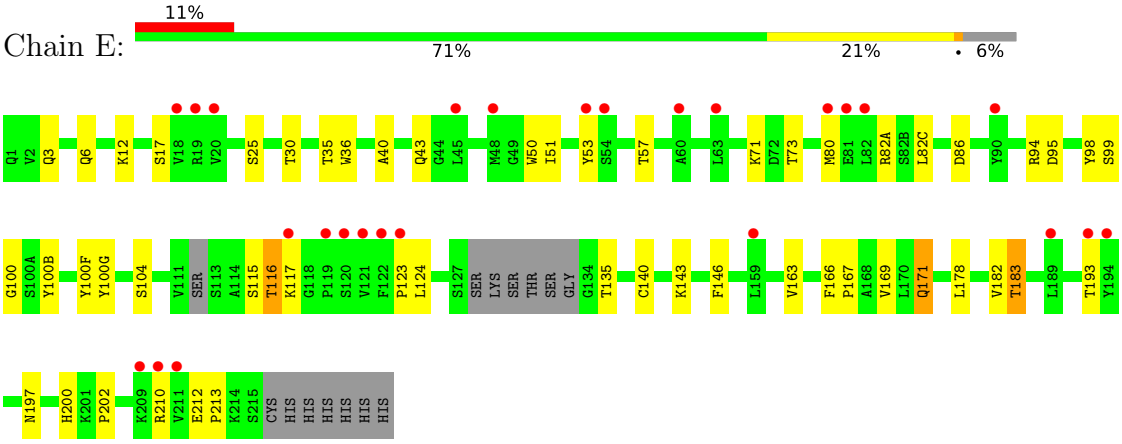
• Molecule 2: Hemagglutinin HA2



• Molecule 2: Hemagglutinin HA2

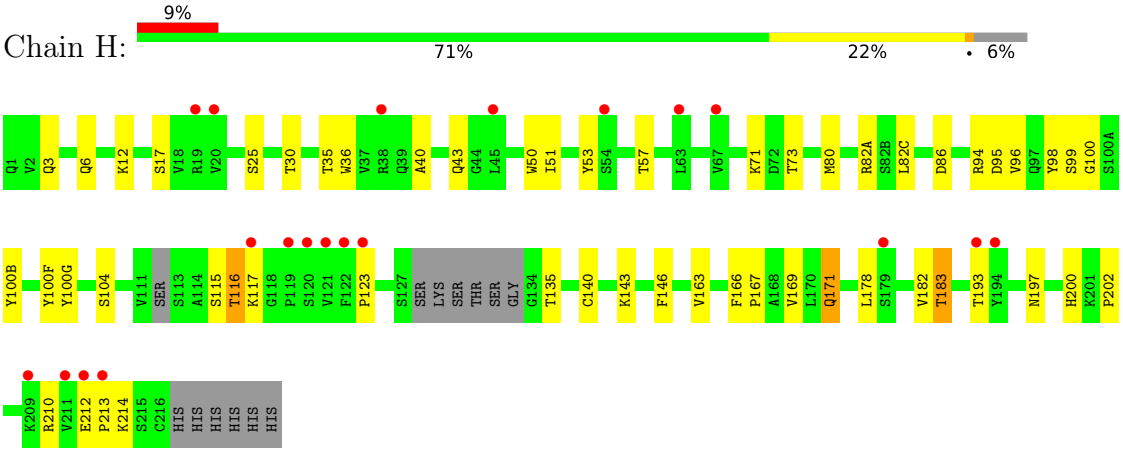


• Molecule 3: Antibody CR8059 Heavy Chain



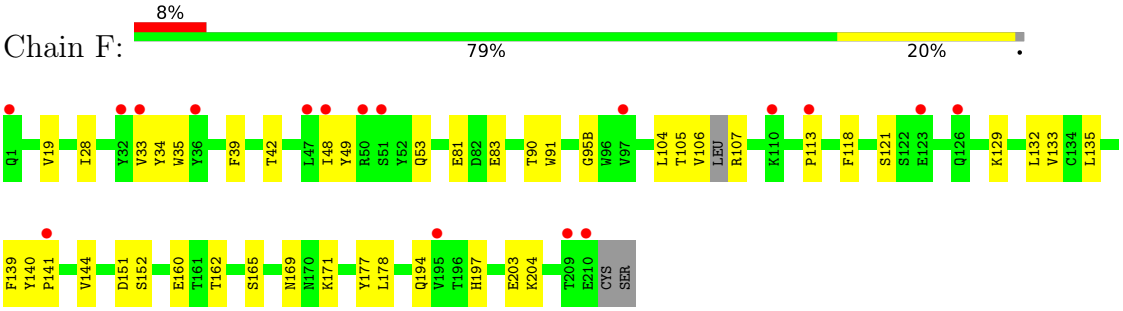
• Molecule 3: Antibody CR8059 Heavy Chain

Chain H:



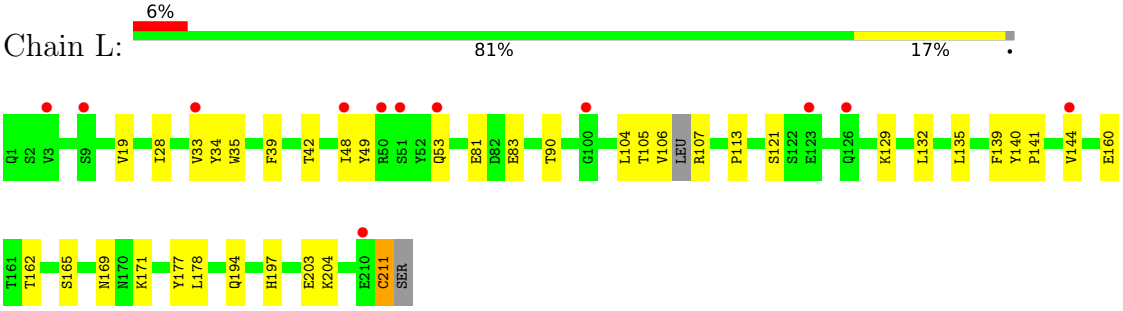
• Molecule 4: Antibody CR8059 Light Chain

Chain F:



• Molecule 4: Antibody CR8059 Light Chain

Chain L:

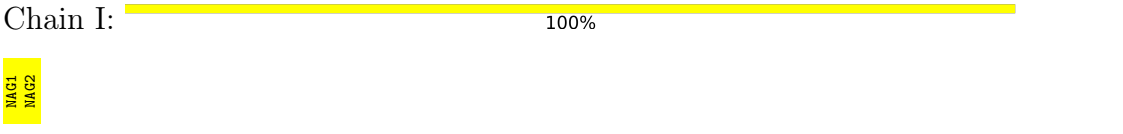


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

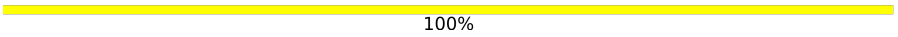
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



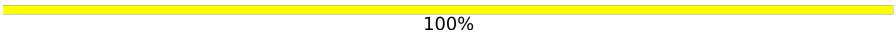
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



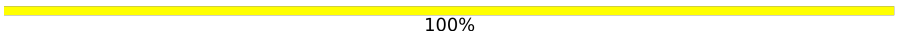
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

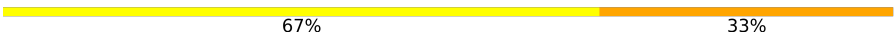
Chain P:

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

Chain K:

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

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	189.20Å 189.20Å 319.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.93 – 5.65 48.93 – 5.65	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.93-5.65) 99.9 (48.93-5.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.66 (at 5.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.306 , 0.324 0.298 , 0.321	Depositor DCC
R_{free} test set	1275 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	243.5	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 139.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.429 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	14080	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	0.64	0/2618	0.94	3/3553 (0.1%)
1	C	0.64	0/2618	0.94	2/3553 (0.1%)
2	B	0.45	0/1063	0.70	0/1429
2	D	0.45	0/1071	0.71	0/1440
3	E	0.44	0/1714	0.61	0/2335
3	H	0.44	0/1720	0.61	0/2343
4	F	0.43	0/1648	0.57	0/2250
4	L	0.43	0/1654	0.57	0/2258
All	All	0.52	0/14106	0.75	5/19161 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	84	LEU	CB-CG-CD2	-5.77	101.19	111.00
1	A	84	LEU	CB-CG-CD2	-5.73	101.26	111.00
1	C	67	LEU	CB-CG-CD2	-5.72	101.28	111.00
1	A	67	LEU	CB-CG-CD2	-5.71	101.30	111.00
1	A	44	LEU	CA-CB-CG	-5.01	103.78	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	2560	0	2559	201	0
1	C	2560	0	2559	195	0
2	B	1054	0	1043	65	0
2	D	1062	0	1054	59	0
3	E	1673	0	1633	50	0
3	H	1679	0	1638	49	0
4	F	1606	0	1541	34	0
4	L	1612	0	1546	29	0
5	G	28	0	25	1	0
5	I	28	0	25	0	0
5	J	28	0	25	0	0
5	N	28	0	25	0	0
5	O	28	0	25	0	0
5	P	28	0	25	5	0
6	K	39	0	34	3	0
6	M	39	0	34	1	0
7	A	14	0	13	0	0
7	C	14	0	13	0	0
All	All	14080	0	13817	567	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 20.

All (567) 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:214:ALA:HB2	1:C:248:MET:CE	1.62	1.29
1:A:214:ALA:HB2	1:A:248:MET:CE	1.62	1.27
1:A:20:THR:CG2	2:B:452:GLU:HG3	1.78	1.13
1:A:320:ILE:CD1	2:B:405:LEU:HD22	1.78	1.12
1:C:320:ILE:CD1	2:D:405:LEU:HD22	1.80	1.11
1:C:131:PRO:HG2	1:C:172:ILE:HD11	1.33	1.11
1:A:280:ILE:HD11	1:A:315:ILE:HG23	1.25	1.10
1:C:280:ILE:HD11	1:C:315:ILE:HG23	1.25	1.10
1:C:214:ALA:HB2	1:C:248:MET:HE3	1.32	1.10
1:A:20:THR:CG2	2:B:452:GLU:CG	2.31	1.08
1:A:214:ALA:HB2	1:A:248:MET:HE3	1.32	1.06
1:A:124:VAL:HG12	1:A:177:ILE:HG13	1.38	1.06
1:A:56:LYS:NZ	1:A:75:LYS:HE3	1.72	1.05
1:C:124:VAL:HG12	1:C:177:ILE:HG13	1.38	1.04
1:A:280:ILE:CD1	1:A:315:ILE:HG12	1.87	1.04
1:C:56:LYS:NZ	1:C:75:LYS:HE3	1.72	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:PRO:HG2	1:A:172:ILE:HD11	1.33	1.03
1:C:280:ILE:CD1	1:C:315:ILE:HG12	1.87	1.03
1:C:96:PRO:O	1:C:243:ILE:HG22	1.59	1.02
1:C:283:SER:HB2	3:E:99:SER:O	1.57	1.02
1:A:96:PRO:O	1:A:243:ILE:HG22	1.59	1.01
1:A:20:THR:HG22	2:B:452:GLU:CG	1.91	1.01
1:A:119:LEU:HD21	1:A:269:LYS:HB3	1.43	1.01
4:F:105:THR:HG21	4:F:141:PRO:HB3	1.43	1.01
1:C:131:PRO:HG2	1:C:172:ILE:CD1	1.91	1.00
2:D:416:ALA:HB1	2:D:425:LEU:HD21	1.42	1.00
1:A:328:LEU:HD12	2:B:451:ASN:OD1	1.62	1.00
1:C:328:LEU:HD12	2:D:451:ASN:OD1	1.62	0.99
1:A:131:PRO:HG2	1:A:172:ILE:CD1	1.91	0.99
2:B:416:ALA:HB1	2:B:425:LEU:HD21	1.42	0.99
1:C:119:LEU:HD21	1:C:269:LYS:HB3	1.43	0.98
1:A:283:SER:HB2	3:H:99:SER:O	1.63	0.97
1:A:20:THR:HG21	2:B:452:GLU:CG	1.93	0.97
1:A:215:ASN:OD1	1:A:251:LYS:HG2	1.65	0.97
1:C:215:ASN:OD1	1:C:251:LYS:HG2	1.65	0.96
1:C:283:SER:HB3	3:E:100:GLY:HA3	1.48	0.96
1:C:214:ALA:HB2	1:C:248:MET:HE2	1.47	0.96
1:A:280:ILE:HD12	1:A:315:ILE:HG12	1.48	0.94
1:A:281:LYS:HD2	2:B:412:ARG:CZ	1.98	0.94
1:C:280:ILE:HD12	1:C:315:ILE:HG12	1.48	0.94
4:L:105:THR:HG21	4:L:141:PRO:HB3	1.50	0.94
1:A:214:ALA:HB2	1:A:248:MET:HE2	1.48	0.94
2:D:421:HIS:O	2:D:425:LEU:HG	1.68	0.93
2:B:421:HIS:O	2:B:425:LEU:HG	1.68	0.93
1:A:240:SER:OG	6:K:1:NAG:H82	1.69	0.93
1:A:280:ILE:HD11	1:A:315:ILE:CG2	1.99	0.92
1:A:285:PRO:HD2	3:H:100(F):TYR:CE2	2.04	0.92
1:C:280:ILE:HD11	1:C:315:ILE:CG2	1.99	0.92
1:C:240:SER:OG	5:P:1:NAG:H82	1.69	0.92
1:A:171:THR:O	1:A:172:ILE:HD13	1.71	0.91
1:A:119:LEU:HD23	1:A:120:SER:N	1.86	0.91
1:C:171:THR:O	1:C:172:ILE:HD13	1.71	0.90
1:A:20:THR:HG21	2:B:452:GLU:HG3	1.50	0.90
1:C:278:LYS:HD2	2:D:411:GLN:NE2	1.87	0.89
1:C:285:PRO:HD2	3:E:100(F):TYR:CE2	2.07	0.89
1:A:131:PRO:CG	1:A:172:ILE:HD11	2.01	0.89
1:C:119:LEU:HD23	1:C:120:SER:N	1.87	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:PRO:CG	1:C:172:ILE:HD11	2.01	0.89
3:E:167:PRO:HG2	4:F:165:SER:OG	1.70	0.89
1:A:20:THR:CG2	2:B:452:GLU:HG2	2.03	0.89
1:C:281:LYS:HD2	2:D:412:ARG:NH2	1.87	0.89
1:C:320:ILE:HD11	2:D:405:LEU:HD22	1.54	0.88
3:H:167:PRO:HG2	4:L:165:SER:OG	1.73	0.88
1:A:320:ILE:HD11	2:B:405:LEU:HD22	1.54	0.86
1:C:155:THR:CG2	1:C:187:VAL:HB	2.05	0.86
1:C:215:ASN:O	1:C:215:ASN:ND2	2.09	0.86
1:A:155:THR:CG2	1:A:187:VAL:HB	2.05	0.86
1:A:18:THR:HG22	2:B:451:ASN:HB2	1.58	0.85
1:A:215:ASN:ND2	1:A:215:ASN:O	2.09	0.85
1:C:281:LYS:HD2	2:D:412:ARG:CZ	2.07	0.84
1:A:56:LYS:NZ	1:A:75:LYS:CE	2.40	0.84
1:A:283:SER:HB3	3:H:100:GLY:HA3	1.58	0.84
1:C:56:LYS:NZ	1:C:75:LYS:CE	2.40	0.84
1:C:26:VAL:HG12	1:C:28:GLY:O	1.78	0.83
1:A:214:ALA:CB	1:A:248:MET:HE3	2.08	0.83
1:C:214:ALA:CB	1:C:248:MET:HE3	2.09	0.83
1:C:56:LYS:HZ3	1:C:75:LYS:HE3	1.42	0.82
1:A:281:LYS:HD2	2:B:412:ARG:NH2	1.92	0.82
1:A:320:ILE:CD1	2:B:405:LEU:CD2	2.58	0.82
2:B:416:ALA:HB1	2:B:425:LEU:CD2	2.09	0.82
1:C:18:THR:HG22	2:D:451:ASN:HB2	1.61	0.81
2:D:416:ALA:HB1	2:D:425:LEU:CD2	2.09	0.81
1:A:18:THR:HG22	2:B:451:ASN:CB	2.11	0.80
1:C:52:LYS:HE3	3:E:53:TYR:CE1	2.17	0.79
1:A:20:THR:HG22	2:B:452:GLU:HG3	1.50	0.79
1:C:18:THR:HG22	2:D:451:ASN:CB	2.13	0.78
1:A:26:VAL:HG12	1:A:28:GLY:O	1.84	0.77
1:A:320:ILE:HD11	2:B:405:LEU:CD2	2.15	0.77
1:A:52:LYS:HE3	3:H:53:TYR:CE1	2.21	0.76
1:A:284:LEU:HB3	1:A:285:PRO:HA	1.67	0.76
1:A:59:ASN:OD1	3:H:30:THR:HG21	1.85	0.75
1:C:320:ILE:CD1	2:D:405:LEU:CD2	2.64	0.75
1:C:52:LYS:CE	3:E:53:TYR:CE1	2.70	0.75
1:A:278:LYS:HD2	2:B:411:GLN:NE2	2.01	0.74
1:C:284:LEU:HB3	1:C:285:PRO:HA	1.67	0.74
1:A:56:LYS:HZ3	1:A:75:LYS:HE3	1.48	0.74
1:A:215:ASN:C	1:A:215:ASN:HD22	1.91	0.74
1:C:20:THR:HB	2:D:452:GLU:HG3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:ASN:OD1	3:E:30:THR:HG21	1.88	0.74
1:C:215:ASN:C	1:C:215:ASN:HD22	1.91	0.73
1:A:119:LEU:HD21	1:A:269:LYS:CB	2.18	0.73
1:C:36:PRO:HB2	1:C:297:TYR:CD1	2.24	0.73
1:C:283:SER:CB	3:E:99:SER:O	2.35	0.73
1:A:52:LYS:CE	3:H:53:TYR:CE1	2.72	0.73
1:C:283:SER:CB	3:E:100:GLY:HA3	2.18	0.73
1:A:56:LYS:HZ3	1:A:75:LYS:CE	2.01	0.73
1:A:36:PRO:HB2	1:A:297:TYR:CD1	2.24	0.73
1:C:193:ASP:OD1	1:C:198:MET:SD	2.46	0.73
1:A:193:ASP:OD1	1:A:198:MET:SD	2.46	0.72
1:A:158:TRP:HA	1:A:265:LEU:HD23	1.70	0.72
1:A:280:ILE:HG23	1:A:295:GLU:HG3	1.71	0.72
4:F:106:VAL:O	4:F:106:VAL:HG22	1.89	0.72
1:C:119:LEU:HD23	1:C:120:SER:H	1.54	0.72
1:C:119:LEU:HD21	1:C:269:LYS:CB	2.18	0.72
1:A:292:CYS:HB3	1:A:300:LEU:HB3	1.72	0.72
1:C:158:TRP:HA	1:C:265:LEU:HD23	1.70	0.71
1:C:280:ILE:HD11	1:C:315:ILE:HG12	1.73	0.71
1:C:292:CYS:HB3	1:C:300:LEU:HB3	1.72	0.71
4:L:106:VAL:HG22	4:L:106:VAL:O	1.89	0.71
1:A:56:LYS:HZ1	1:A:75:LYS:HE3	1.54	0.71
2:B:479:GLU:OE1	2:B:485:PHE:CE2	2.44	0.71
1:A:16:VAL:CG2	1:A:29:VAL:CG1	2.69	0.70
1:C:320:ILE:HD11	2:D:405:LEU:CD2	2.20	0.70
1:A:19:ALA:H	2:B:448:LEU:HB3	1.57	0.70
1:C:280:ILE:HG23	1:C:295:GLU:HG3	1.72	0.70
1:A:119:LEU:HD23	1:A:120:SER:H	1.54	0.70
2:B:479:GLU:OE1	2:B:485:PHE:CZ	2.45	0.70
1:C:172:ILE:HG13	1:C:260:TYR:HE2	1.56	0.70
2:D:479:GLU:OE1	2:D:485:PHE:CE2	2.44	0.70
1:A:85:HIS:HB2	3:H:99:SER:HB3	1.74	0.70
2:D:479:GLU:OE1	2:D:485:PHE:CZ	2.45	0.69
1:A:243:ILE:HD11	1:A:265:LEU:HD11	1.73	0.69
1:C:56:LYS:HZ3	1:C:75:LYS:CE	2.02	0.69
1:A:16:VAL:HG13	1:A:327:LYS:O	1.93	0.69
1:A:280:ILE:HD11	1:A:315:ILE:HG12	1.73	0.69
1:A:85:HIS:HB2	3:H:99:SER:CB	2.23	0.69
1:A:172:ILE:HG13	1:A:260:TYR:HE2	1.56	0.69
1:A:283:SER:CB	3:H:99:SER:O	2.40	0.68
1:C:14:HIS:CD2	1:C:28:GLY:HA2	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:HIS:HB2	3:E:99:SER:CB	2.24	0.68
1:C:243:ILE:HD11	1:C:265:LEU:HD11	1.73	0.68
1:A:284:LEU:HD13	3:H:98:TYR:OH	1.93	0.68
1:A:16:VAL:CG2	1:A:29:VAL:HG12	2.24	0.68
1:A:56:LYS:HZ3	1:A:75:LYS:NZ	1.92	0.67
1:A:19:ALA:N	2:B:448:LEU:HB3	2.09	0.67
1:A:26:VAL:HA	1:A:332:THR:O	1.93	0.67
1:C:36:PRO:HB2	1:C:297:TYR:HD1	1.58	0.67
1:C:53:LEU:CD1	1:C:62:ASP:HB3	2.25	0.67
1:A:52:LYS:HE2	3:H:53:TYR:HE1	1.60	0.67
1:C:284:LEU:HD13	3:E:98:TYR:OH	1.95	0.67
1:C:56:LYS:HZ1	1:C:75:LYS:HE3	1.60	0.67
1:A:16:VAL:HG23	1:A:29:VAL:CG1	2.25	0.66
1:C:85:HIS:HB2	3:E:99:SER:HB3	1.77	0.66
1:A:53:LEU:CD1	1:A:62:ASP:HB3	2.25	0.66
1:C:52:LYS:HE2	3:E:53:TYR:HE1	1.59	0.66
1:C:56:LYS:NZ	1:C:75:LYS:NZ	2.44	0.66
4:F:83:GLU:HG2	4:F:106:VAL:HG13	1.77	0.66
1:A:56:LYS:NZ	1:A:75:LYS:NZ	2.44	0.66
1:A:36:PRO:HB2	1:A:297:TYR:HD1	1.58	0.66
1:A:85:HIS:HD2	1:A:86:GLU:HG3	1.61	0.66
3:H:166:PHE:CZ	4:L:135:LEU:HB3	2.29	0.66
2:D:373:SER:HB2	2:D:380:ALA:HB3	1.77	0.66
3:E:3:GLN:HB2	3:E:25:SER:HB2	1.78	0.66
2:B:373:SER:HB2	2:B:380:ALA:HB3	1.78	0.65
1:C:89:PRO:HG2	1:C:105:ARG:O	1.96	0.65
3:H:3:GLN:HB2	3:H:25:SER:HB2	1.78	0.65
1:A:14:HIS:CD2	1:A:28:GLY:HA2	2.31	0.65
4:F:33:VAL:HA	4:F:90:THR:HG22	1.78	0.65
1:A:214:ALA:O	1:A:215:ASN:ND2	2.30	0.65
1:C:16:VAL:HG13	1:C:327:LYS:O	1.97	0.65
1:C:85:HIS:HD2	1:C:86:GLU:HG3	1.61	0.65
4:L:33:VAL:HA	4:L:90:THR:HG22	1.78	0.65
1:A:306:TYR:CE2	2:B:443:ILE:HD13	2.32	0.65
4:L:83:GLU:HG2	4:L:106:VAL:HG13	1.77	0.65
1:A:89:PRO:HG2	1:A:105:ARG:O	1.96	0.65
1:A:20:THR:HG23	1:A:21:GLN:HG2	1.78	0.64
1:C:214:ALA:O	1:C:215:ASN:ND2	2.30	0.64
2:D:508:GLU:HG3	2:D:509:PHE:H	1.63	0.64
3:E:169:VAL:HA	4:F:162:THR:HG22	1.79	0.64
2:B:427:LEU:O	2:B:431:VAL:HG23	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:ILE:CG1	1:C:260:TYR:HE2	2.11	0.64
2:D:427:LEU:O	2:D:431:VAL:HG23	1.97	0.64
3:H:212:GLU:CG	3:H:213:PRO:HD2	2.28	0.64
1:A:147:THR:O	1:A:148:ASN:CG	2.37	0.63
3:E:212:GLU:CG	3:E:213:PRO:HD2	2.28	0.63
1:C:147:THR:O	1:C:148:ASN:CG	2.37	0.63
2:B:508:GLU:HG3	2:B:509:PHE:H	1.63	0.63
1:C:26:VAL:CG1	1:C:28:GLY:O	2.46	0.63
1:C:26:VAL:HA	1:C:332:THR:O	1.98	0.63
1:C:214:ALA:CB	1:C:248:MET:CE	2.57	0.63
1:A:16:VAL:HG23	1:A:29:VAL:HG11	1.80	0.63
1:C:94:CYS:HA	1:C:142:SER:O	1.99	0.63
1:A:172:ILE:CG1	1:A:260:TYR:HE2	2.10	0.62
1:C:171:THR:O	1:C:172:ILE:CD1	2.46	0.62
1:A:94:CYS:HA	1:A:142:SER:O	1.99	0.62
1:A:214:ALA:CB	1:A:248:MET:CE	2.57	0.62
4:F:106:VAL:O	4:F:106:VAL:CG2	2.48	0.61
1:A:16:VAL:CG2	1:A:29:VAL:HG11	2.30	0.61
1:A:171:THR:O	1:A:172:ILE:CD1	2.46	0.61
1:C:85:HIS:HB2	3:E:99:SER:OG	2.01	0.61
1:C:311:HIS:HB2	1:C:321:TRP:CD1	2.36	0.61
2:D:435:ARG:HD3	2:D:439:ILE:CG1	2.31	0.61
1:A:311:HIS:HB2	1:A:321:TRP:CD1	2.36	0.61
1:C:320:ILE:HD13	2:D:405:LEU:HD22	1.78	0.61
1:A:283:SER:CB	3:H:100:GLY:HA3	2.28	0.60
2:D:398:ASN:HD21	2:D:450:SER:HB3	1.66	0.60
2:B:398:ASN:HD21	2:B:450:SER:HB3	1.66	0.60
3:H:169:VAL:HA	4:L:162:THR:HG22	1.82	0.60
4:L:106:VAL:O	4:L:106:VAL:CG2	2.48	0.60
3:E:163:VAL:HG22	3:E:182:VAL:HG22	1.83	0.60
1:A:41:PHE:CZ	1:A:282:GLY:HA2	2.37	0.60
2:B:435:ARG:HD3	2:B:439:ILE:CG1	2.31	0.60
1:C:280:ILE:CD1	1:C:315:ILE:CG1	2.73	0.60
1:A:119:LEU:CD2	1:A:269:LYS:HB3	2.27	0.59
1:C:70:PRO:HB2	1:C:144:PRO:O	2.01	0.59
4:L:83:GLU:CG	4:L:106:VAL:HG13	2.32	0.59
1:A:16:VAL:HG21	1:A:29:VAL:HG12	1.82	0.59
1:A:26:VAL:CG1	1:A:28:GLY:O	2.48	0.59
1:A:280:ILE:CD1	1:A:315:ILE:CG1	2.73	0.59
2:B:418:ASP:O	2:B:422:ASN:ND2	2.36	0.59
2:D:418:ASP:O	2:D:422:ASN:ND2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:163:VAL:HG22	3:H:182:VAL:HG22	1.83	0.59
1:A:70:PRO:HB2	1:A:144:PRO:O	2.01	0.59
1:C:41:PHE:CZ	1:C:282:GLY:HA2	2.37	0.59
4:F:83:GLU:CG	4:F:106:VAL:HG13	2.32	0.59
2:B:421:HIS:HB3	2:B:424:ILE:HD12	1.84	0.59
2:D:421:HIS:HB3	2:D:424:ILE:HD12	1.84	0.59
1:A:283:SER:O	3:H:100(F):TYR:OH	2.20	0.58
1:C:25:ASN:O	1:C:333:LYS:HA	2.02	0.58
3:H:212:GLU:HG3	3:H:213:PRO:HD2	1.85	0.58
1:C:281:LYS:CD	2:D:412:ARG:NH2	2.65	0.58
2:B:421:HIS:O	2:B:425:LEU:CG	2.48	0.58
3:E:193:THR:HG22	3:E:210:ARG:HH22	1.69	0.58
1:C:16:VAL:CG2	1:C:29:VAL:CG1	2.81	0.58
1:A:155:THR:HG23	1:A:187:VAL:HB	1.84	0.58
1:C:119:LEU:CD2	1:C:269:LYS:HB3	2.26	0.58
1:A:281:LYS:CD	2:B:412:ARG:NH2	2.65	0.58
1:C:292:CYS:SG	1:C:300:LEU:HD23	2.44	0.58
1:A:131:PRO:CD	1:A:172:ILE:HD11	2.34	0.57
1:C:131:PRO:CD	1:C:172:ILE:HD11	2.34	0.57
1:C:328:LEU:HD11	2:D:454:ILE:HD12	1.87	0.57
1:A:85:HIS:HB2	3:H:99:SER:OG	2.05	0.57
3:E:212:GLU:HG3	3:E:213:PRO:HD2	1.85	0.57
3:H:193:THR:HG22	3:H:210:ARG:HH22	1.69	0.57
1:A:18:THR:HG22	2:B:451:ASN:HB3	1.86	0.56
1:A:104:ILE:HD13	1:A:245:VAL:HG12	1.87	0.56
1:A:320:ILE:HD12	2:B:405:LEU:HD22	1.81	0.56
1:C:155:THR:HG23	1:C:187:VAL:HB	1.84	0.56
1:C:131:PRO:CG	1:C:172:ILE:CD1	2.71	0.56
1:A:292:CYS:SG	1:A:300:LEU:HD23	2.44	0.56
1:C:19:ALA:N	2:D:448:LEU:HB3	2.20	0.56
1:A:197:GLN:HA	1:A:197:GLN:OE1	2.06	0.56
1:C:197:GLN:OE1	1:C:197:GLN:HA	2.06	0.56
1:C:280:ILE:HD12	1:C:315:ILE:CG1	2.30	0.56
1:C:16:VAL:HG23	1:C:29:VAL:CG1	2.35	0.56
1:C:104:ILE:HD13	1:C:245:VAL:HG12	1.87	0.56
1:C:59:ASN:OD1	3:E:73:THR:CG2	2.53	0.56
3:H:36:TRP:CE2	3:H:80:MET:HB2	2.41	0.56
1:A:25:ASN:O	1:A:333:LYS:HA	2.05	0.56
3:E:166:PHE:CZ	4:F:135:LEU:HB3	2.41	0.56
1:C:16:VAL:CG2	1:C:29:VAL:HG12	2.36	0.55
2:D:508:GLU:HG3	2:D:509:PHE:CD1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:36:TRP:CE2	3:E:80:MET:HB2	2.41	0.55
1:C:19:ALA:H	2:D:448:LEU:HB3	1.71	0.55
2:D:421:HIS:O	2:D:425:LEU:CG	2.48	0.55
2:D:476:SER:HB3	2:D:511:LEU:HD13	1.89	0.55
4:L:83:GLU:HG2	4:L:106:VAL:CG1	2.37	0.55
2:B:435:ARG:HD3	2:B:439:ILE:HG13	1.89	0.55
3:E:200:HIS:NE2	3:E:202:PRO:HG2	2.22	0.55
1:C:26:VAL:O	1:C:28:GLY:N	2.41	0.54
3:H:200:HIS:NE2	3:H:202:PRO:HG2	2.22	0.54
2:B:476:SER:HB3	2:B:511:LEU:HD13	1.89	0.54
1:C:280:ILE:HD11	1:C:315:ILE:CG1	2.37	0.54
1:C:56:LYS:HZ3	1:C:75:LYS:NZ	2.05	0.54
1:C:278:LYS:HD2	2:D:411:GLN:HE21	1.67	0.54
1:C:16:VAL:HG23	1:C:29:VAL:HG11	1.89	0.54
1:A:59:ASN:OD1	3:H:73:THR:CG2	2.56	0.54
2:D:410:LEU:HG	2:D:432:ASP:OD2	2.08	0.54
2:D:435:ARG:HD3	2:D:439:ILE:HG13	1.89	0.54
4:F:83:GLU:HG2	4:F:106:VAL:CG1	2.37	0.54
3:H:35:THR:HG22	3:H:50:TRP:HB2	1.88	0.54
2:B:508:GLU:HG3	2:B:509:PHE:CD1	2.42	0.54
1:A:20:THR:HG21	2:B:452:GLU:HG2	1.76	0.53
1:C:283:SER:O	3:E:100(F):TYR:OH	2.26	0.53
3:E:35:THR:HG22	3:E:50:TRP:HB2	1.89	0.53
1:A:284:LEU:CB	1:A:285:PRO:HA	2.36	0.53
2:B:410:LEU:HG	2:B:432:ASP:OD2	2.08	0.53
2:D:422:ASN:HA	2:D:425:LEU:HD12	1.90	0.53
1:C:124:VAL:HG12	1:C:177:ILE:CG1	2.26	0.53
2:D:508:GLU:HG3	2:D:509:PHE:N	2.24	0.53
1:C:85:HIS:CD2	1:C:86:GLU:HG3	2.42	0.53
1:A:18:THR:CG2	2:B:451:ASN:HB3	2.39	0.53
1:A:240:SER:OG	6:K:1:NAG:C8	2.51	0.53
1:A:280:ILE:HD12	1:A:315:ILE:CG1	2.30	0.53
1:C:18:THR:HG22	2:D:451:ASN:HB3	1.89	0.53
1:C:306:TYR:CE2	2:D:443:ILE:HD13	2.44	0.53
2:B:408:LYS:O	2:B:435:ARG:NH2	2.42	0.52
2:B:422:ASN:HA	2:B:425:LEU:HD12	1.90	0.52
1:C:16:VAL:CG1	1:C:327:LYS:O	2.58	0.52
3:H:123:PRO:O	4:L:121:SER:HB3	2.10	0.52
1:A:56:LYS:HZ3	1:A:75:LYS:HZ2	1.58	0.52
1:A:280:ILE:CG2	1:A:295:GLU:HG3	2.39	0.52
2:B:508:GLU:CG	2:B:509:PHE:H	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:VAL:CG1	1:A:327:LYS:O	2.57	0.52
1:A:208:GLN:HB3	1:A:261:GLN:HB2	1.92	0.52
1:C:53:LEU:HD11	1:C:62:ASP:HB3	1.91	0.52
1:A:20:THR:HG22	2:B:452:GLU:HG2	1.71	0.52
2:D:508:GLU:CG	2:D:509:PHE:H	2.22	0.52
1:A:85:HIS:CD2	1:A:86:GLU:HG3	2.42	0.52
1:A:53:LEU:HD11	1:A:62:ASP:HB3	1.91	0.52
1:C:56:LYS:HZ2	1:C:75:LYS:NZ	2.07	0.52
1:A:103:LYS:NZ	1:A:246:ASP:OD1	2.38	0.52
1:C:208:GLN:HB3	1:C:261:GLN:HB2	1.92	0.52
3:H:115:SER:O	3:H:115:SER:OG	2.23	0.52
1:A:52:LYS:HE2	3:H:53:TYR:CE1	2.38	0.51
2:B:439:ILE:O	2:B:443:ILE:HG13	2.10	0.51
1:C:103:LYS:NZ	1:C:246:ASP:OD1	2.38	0.51
4:L:28:ILE:HG12	4:L:90:THR:HG21	1.92	0.51
1:A:280:ILE:HD11	1:A:315:ILE:CG1	2.37	0.51
2:B:508:GLU:HG3	2:B:509:PHE:N	2.24	0.51
3:E:115:SER:O	3:E:115:SER:OG	2.23	0.51
1:C:16:VAL:HG22	1:C:327:LYS:HB2	1.92	0.51
1:A:94:CYS:O	1:A:235:GLY:N	2.43	0.51
1:A:320:ILE:HD13	2:B:405:LEU:HD22	1.81	0.51
1:A:26:VAL:O	1:A:28:GLY:N	2.44	0.51
2:D:408:LYS:O	2:D:435:ARG:NH2	2.42	0.51
1:C:131:PRO:O	1:C:170:LEU:HD13	2.11	0.51
1:C:97:ILE:HA	1:C:243:ILE:HG23	1.93	0.51
2:D:416:ALA:O	2:D:421:HIS:ND1	2.43	0.51
2:D:439:ILE:O	2:D:443:ILE:HG13	2.10	0.51
4:F:28:ILE:HG12	4:F:90:THR:HG21	1.92	0.51
3:H:167:PRO:CG	4:L:165:SER:OG	2.55	0.51
2:B:416:ALA:O	2:B:421:HIS:ND1	2.43	0.50
1:A:105:ARG:NH2	1:A:233:GLU:OE1	2.45	0.50
1:C:59:ASN:OD1	3:E:73:THR:HG23	2.11	0.50
1:A:59:ASN:OD1	3:H:73:THR:HG23	2.12	0.50
1:A:131:PRO:O	1:A:170:LEU:HD13	2.11	0.50
1:C:94:CYS:O	1:C:235:GLY:N	2.43	0.50
1:C:145:ASN:O	1:C:146:ILE:C	2.50	0.50
1:A:149:GLY:HA3	5:G:1:NAG:O6	2.11	0.50
1:C:16:VAL:CG2	1:C:29:VAL:HG11	2.41	0.50
1:C:105:ARG:NH2	1:C:233:GLU:OE1	2.44	0.50
1:A:145:ASN:O	1:A:146:ILE:C	2.50	0.50
1:C:18:THR:CG2	2:D:451:ASN:HB3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:GLY:HA3	6:M:1:NAG:O6	2.11	0.50
1:C:240:SER:OG	5:P:1:NAG:C8	2.51	0.50
4:F:144:VAL:HG12	4:F:197:HIS:HB2	1.94	0.50
3:E:95:ASP:OD2	3:E:100(B):TYR:OH	2.30	0.50
3:H:212:GLU:HG2	3:H:213:PRO:HD2	1.93	0.50
1:A:124:VAL:HG12	1:A:177:ILE:CG1	2.26	0.49
3:E:167:PRO:CG	4:F:165:SER:OG	2.53	0.49
3:H:6:GLN:OE1	3:H:104:SER:OG	2.29	0.49
3:H:171:GLN:HG3	4:L:160:GLU:HG3	1.93	0.49
3:E:171:GLN:HG3	4:F:160:GLU:HG3	1.93	0.49
1:A:131:PRO:HD2	1:A:172:ILE:HD11	1.94	0.49
3:H:169:VAL:HG11	4:L:177:TYR:CD1	2.47	0.49
1:C:131:PRO:HD2	1:C:172:ILE:HD11	1.94	0.49
4:F:105:THR:CG2	4:F:141:PRO:HB3	2.28	0.49
1:A:97:ILE:HA	1:A:243:ILE:HG23	1.93	0.49
1:A:172:ILE:HG13	1:A:260:TYR:CE2	2.44	0.49
3:E:12:LYS:HE2	3:E:17:SER:O	2.12	0.49
4:L:144:VAL:HG12	4:L:197:HIS:HB2	1.94	0.49
1:C:16:VAL:HG22	1:C:327:LYS:CB	2.42	0.49
3:E:6:GLN:OE1	3:E:104:SER:OG	2.29	0.49
1:C:97:ILE:HA	1:C:243:ILE:CG2	2.43	0.49
1:C:280:ILE:CG2	1:C:295:GLU:HG3	2.39	0.48
3:H:12:LYS:HE2	3:H:17:SER:O	2.12	0.48
1:C:36:PRO:HB2	1:C:297:TYR:CE1	2.48	0.48
3:E:212:GLU:HG2	3:E:213:PRO:HD2	1.94	0.48
3:H:214:LYS:HG3	4:L:211:CYS:SG	2.52	0.48
4:F:107:ARG:N	4:F:140:TYR:HH	2.11	0.48
1:A:131:PRO:CG	1:A:172:ILE:CD1	2.72	0.48
1:A:163(C):ASN:O	1:A:165:THR:HG22	2.14	0.48
1:C:172:ILE:HG13	1:C:260:TYR:CE2	2.44	0.48
4:L:107:ARG:N	4:L:140:TYR:HH	2.11	0.48
1:A:36:PRO:HB2	1:A:297:TYR:CE1	2.48	0.48
3:H:100(G):TYR:HB3	4:L:34:TYR:CZ	2.49	0.47
1:C:26:VAL:C	1:C:28:GLY:N	2.67	0.47
1:C:52:LYS:HD3	1:C:62:ASP:OD1	2.14	0.47
1:A:16:VAL:HG22	1:A:327:LYS:CB	2.44	0.47
1:C:163(C):ASN:O	1:C:165:THR:HG22	2.14	0.47
1:C:16:VAL:HG21	1:C:29:VAL:HG12	1.95	0.47
1:C:63:LEU:HA	1:C:108:PRO:HG3	1.96	0.47
1:C:182:GLU:HG2	1:C:274:SER:HB3	1.96	0.47
1:A:63:LEU:HA	1:A:108:PRO:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:ILE:HG13	1:C:330:ASN:HB2	1.97	0.47
1:A:52:LYS:HD3	1:A:62:ASP:OD1	2.14	0.47
1:A:122:HIS:O	1:A:269:LYS:HD3	2.15	0.47
2:B:435:ARG:HD3	2:B:439:ILE:HG12	1.96	0.47
1:C:193:ASP:OD1	1:C:198:MET:HB2	2.14	0.47
1:A:81:VAL:CG1	1:A:315:ILE:HD11	2.45	0.47
1:A:193:ASP:OD1	1:A:198:MET:HB2	2.14	0.47
2:D:435:ARG:HD3	2:D:439:ILE:HG12	1.96	0.47
1:A:197:GLN:CD	6:K:1:NAG:O7	2.54	0.47
1:A:97:ILE:HA	1:A:243:ILE:CG2	2.44	0.47
1:C:122:HIS:O	1:C:269:LYS:HD3	2.15	0.47
1:C:178:CYS:SG	1:C:184:GLN:HG3	2.55	0.47
3:E:100(G):TYR:HB3	4:F:34:TYR:CZ	2.50	0.47
1:A:313:LYS:HB3	2:B:411:GLN:HA	1.98	0.46
1:C:81:VAL:CG1	1:C:315:ILE:HD11	2.45	0.46
1:C:197:GLN:CD	5:P:1:NAG:O7	2.54	0.46
3:H:95:ASP:OD2	3:H:100(B):TYR:OH	2.30	0.46
1:C:114:TYR:CG	1:C:273:ALA:HB1	2.51	0.46
1:A:12:SER:HB2	1:A:334:TYR:HB2	1.96	0.46
1:A:292:CYS:HB3	1:A:300:LEU:HD23	1.98	0.46
1:C:103:LYS:HG3	1:C:247:TYR:CE1	2.50	0.46
1:C:197:GLN:HE21	5:P:1:NAG:H81	1.81	0.46
1:A:26:VAL:C	1:A:28:GLY:N	2.69	0.46
1:A:30:ILE:HG13	1:A:330:ASN:HB2	1.97	0.46
1:A:103:LYS:HG3	1:A:247:TYR:CE1	2.50	0.46
1:A:182:GLU:HG2	1:A:274:SER:HB3	1.96	0.46
1:C:135:TYR:CD1	1:C:159:ALA:HB1	2.50	0.46
4:L:204:LYS:HD3	4:L:204:LYS:HA	1.76	0.46
1:A:250:GLN:O	1:A:251:LYS:O	2.33	0.46
1:C:184:GLN:NE2	1:C:270:VAL:HG11	2.31	0.46
3:E:169:VAL:HG11	4:F:177:TYR:CD1	2.50	0.46
1:A:114:TYR:CG	1:A:273:ALA:HB1	2.51	0.46
1:A:184:GLN:NE2	1:A:270:VAL:HG11	2.31	0.46
1:A:231:GLN:HG2	1:A:242:ARG:NH2	2.31	0.46
1:C:231:GLN:HG2	1:C:242:ARG:NH2	2.31	0.46
1:C:250:GLN:O	1:C:251:LYS:O	2.33	0.46
1:A:178:CYS:SG	1:A:184:GLN:HG3	2.55	0.46
1:A:16:VAL:HG22	1:A:327:LYS:HB2	1.98	0.45
1:C:215:ASN:ND2	1:C:215:ASN:C	2.63	0.45
1:A:135:TYR:CD1	1:A:159:ALA:HB1	2.50	0.45
2:B:407:VAL:HG12	2:B:435:ARG:HH21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:THR:O	1:C:64:ASP:HB2	2.16	0.45
3:E:116:THR:HA	3:E:146:PHE:O	2.17	0.45
1:C:292:CYS:HB3	1:C:300:LEU:HD23	1.98	0.45
2:D:407:VAL:HG12	2:D:435:ARG:HH21	1.82	0.45
1:A:59:ASN:OD1	3:H:30:THR:CG2	2.62	0.45
1:C:131:PRO:CD	1:C:172:ILE:CD1	2.95	0.45
1:A:61:THR:O	1:A:64:ASP:HB2	2.16	0.45
1:A:313:LYS:HD3	2:B:412:ARG:N	2.32	0.45
1:A:131:PRO:CD	1:A:172:ILE:CD1	2.95	0.45
1:C:26:VAL:HG21	1:C:329:ALA:HB1	1.99	0.45
1:C:131:PRO:HD2	1:C:172:ILE:CD1	2.47	0.45
1:C:72:CYS:O	1:C:73:THR:HG23	2.17	0.44
1:C:165:THR:HA	1:C:203:GLY:HA3	1.99	0.44
1:C:231:GLN:HB3	1:C:234:ASP:OD2	2.18	0.44
3:E:51:ILE:HB	3:E:57:THR:HG22	1.99	0.44
1:A:147:THR:O	1:A:148:ASN:OD1	2.36	0.44
1:A:165:THR:HA	1:A:203:GLY:HA3	1.98	0.44
1:A:72:CYS:O	1:A:73:THR:HG23	2.17	0.44
1:C:20:THR:HB	2:D:452:GLU:CG	2.45	0.44
4:F:49:TYR:CE1	4:F:53:GLN:HB3	2.52	0.44
4:L:39:PHE:O	4:L:42:THR:OG1	2.33	0.44
3:H:17:SER:HB3	3:H:82(A):ARG:HA	2.00	0.44
1:C:53:LEU:HG	1:C:62:ASP:CG	2.38	0.44
1:C:165:THR:OG1	1:C:166:ALA:N	2.51	0.44
4:F:194:GLN:HB3	4:F:203:GLU:HG3	2.00	0.44
3:H:51:ILE:HB	3:H:57:THR:HG22	1.99	0.44
1:A:131:PRO:HD2	1:A:172:ILE:CD1	2.47	0.44
1:C:185:ILE:HB	1:C:271:TRP:HB2	2.00	0.44
3:H:117:LYS:HB3	3:H:117:LYS:HE2	1.86	0.44
1:A:53:LEU:HG	1:A:62:ASP:CG	2.38	0.43
2:B:444:GLU:O	2:B:448:LEU:HG	2.17	0.43
3:E:123:PRO:O	4:F:121:SER:HB3	2.18	0.43
4:L:169:ASN:OD1	4:L:171:LYS:HB2	2.18	0.43
1:A:185:ILE:HB	1:A:271:TRP:HB2	2.00	0.43
4:L:49:TYR:CE1	4:L:53:GLN:HB3	2.52	0.43
1:A:165:THR:OG1	1:A:166:ALA:N	2.51	0.43
1:C:17:LYS:O	2:D:448:LEU:HD23	2.18	0.43
1:C:95:PHE:CD1	1:C:96:PRO:HD2	2.53	0.43
4:L:105:THR:CG2	4:L:141:PRO:HB3	2.36	0.43
1:C:320:ILE:HD13	2:D:405:LEU:CD2	2.44	0.43
1:A:95:PHE:CD1	1:A:96:PRO:HD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:ILE:O	1:C:268:GLN:NE2	2.47	0.43
1:C:320:ILE:HG21	2:D:443:ILE:HD11	2.01	0.43
3:E:117:LYS:HB3	3:E:117:LYS:HE2	1.86	0.43
2:D:444:GLU:O	2:D:448:LEU:HG	2.17	0.43
2:D:508:GLU:CG	2:D:509:PHE:N	2.81	0.43
4:F:169:ASN:OD1	4:F:171:LYS:HB2	2.18	0.43
3:H:116:THR:HA	3:H:146:PHE:O	2.17	0.43
3:H:135:THR:OG1	3:H:183:THR:HG23	2.19	0.43
2:D:496:LEU:HD12	2:D:499:ILE:HD12	2.01	0.43
4:L:35:TRP:HB2	4:L:48:ILE:HB	2.00	0.43
1:A:48:GLU:H	1:A:48:GLU:HG2	1.69	0.43
1:A:328:LEU:HD11	2:B:454:ILE:HD12	2.00	0.43
2:B:496:LEU:HD12	2:B:499:ILE:HD12	2.01	0.43
1:C:81:VAL:HG13	1:C:315:ILE:CD1	2.49	0.43
3:E:17:SER:HB3	3:E:82(A):ARG:HA	2.00	0.43
1:A:231:GLN:HB3	1:A:234:ASP:OD2	2.18	0.43
3:E:135:THR:OG1	3:E:183:THR:HG23	2.19	0.43
4:F:204:LYS:HD3	4:F:204:LYS:HA	1.77	0.43
1:C:56:LYS:HZ3	1:C:75:LYS:HZ2	1.66	0.43
1:C:147:THR:O	1:C:148:ASN:OD1	2.36	0.43
1:A:90:VAL:HG12	1:A:91:THR:O	2.19	0.42
2:B:508:GLU:CG	2:B:509:PHE:N	2.82	0.42
1:C:292:CYS:CB	1:C:300:LEU:HD23	2.49	0.42
2:D:387:SER:HB2	2:D:465:LEU:HD11	2.01	0.42
1:A:150:ASN:OD1	1:A:150:ASN:N	2.50	0.42
1:A:155:THR:HG21	1:A:187:VAL:HB	1.97	0.42
2:B:387:SER:HB2	2:B:465:LEU:HD11	2.01	0.42
1:C:12:SER:HB2	1:C:334:TYR:HB2	2.01	0.42
1:C:329:ALA:N	2:D:451:ASN:OD1	2.43	0.42
1:A:17:LYS:O	2:B:448:LEU:HD23	2.18	0.42
4:L:113:PRO:HB3	4:L:139:PHE:HB3	2.01	0.42
4:L:194:GLN:HB3	4:L:203:GLU:HG3	2.00	0.42
1:C:57:CYS:O	1:C:60:CYS:HB2	2.20	0.42
1:C:107:LEU:HB3	1:C:108:PRO:HD3	2.01	0.42
1:C:150:ASN:OD1	1:C:150:ASN:N	2.50	0.42
4:F:39:PHE:O	4:F:42:THR:OG1	2.33	0.42
3:H:212:GLU:CG	3:H:213:PRO:CD	2.97	0.42
1:A:320:ILE:HD13	2:B:405:LEU:CD2	2.42	0.42
1:C:141:GLY:C	1:C:143:CYS:H	2.23	0.42
1:C:284:LEU:CB	1:C:285:PRO:HA	2.36	0.42
4:L:132:LEU:HD12	4:L:178:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:CYS:CB	1:A:300:LEU:HD23	2.49	0.42
4:F:35:TRP:HB2	4:F:48:ILE:HB	2.00	0.42
1:A:81:VAL:HG13	1:A:315:ILE:CD1	2.49	0.42
1:C:90:VAL:HG12	1:C:91:THR:O	2.19	0.42
1:C:192:SER:OG	1:C:224:GLN:O	2.28	0.42
2:D:435:ARG:CD	2:D:439:ILE:HG13	2.50	0.42
1:A:145:ASN:O	1:A:147:THR:N	2.52	0.42
1:C:15:VAL:HG22	1:C:23:GLU:HG2	2.02	0.42
1:C:59:ASN:OD1	3:E:30:THR:CG2	2.65	0.42
1:C:81:VAL:HG11	1:C:315:ILE:HD11	2.02	0.42
3:H:82(C):LEU:HA	3:H:86:ASP:OD2	2.20	0.42
2:D:440:SER:O	2:D:444:GLU:HG3	2.20	0.41
3:E:169:VAL:CA	4:F:162:THR:HG22	2.47	0.41
1:C:158:TRP:CD1	1:C:158:TRP:C	2.92	0.41
1:C:281:LYS:HB2	1:C:295:GLU:HG2	2.02	0.41
4:F:132:LEU:HD12	4:F:178:LEU:HD23	2.02	0.41
1:A:176:TYR:OH	1:A:182:GLU:O	2.35	0.41
1:A:20:THR:CG2	1:A:21:GLN:HG2	2.47	0.41
1:A:81:VAL:HG11	1:A:315:ILE:HD11	2.02	0.41
1:A:107:LEU:HB3	1:A:108:PRO:HD3	2.01	0.41
2:B:440:SER:O	2:B:444:GLU:HG3	2.20	0.41
1:C:145:ASN:O	1:C:147:THR:N	2.53	0.41
1:A:141:GLY:C	1:A:143:CYS:H	2.23	0.41
1:C:278:LYS:HD2	2:D:411:GLN:CD	2.39	0.41
3:E:82(C):LEU:HA	3:E:86:ASP:OD2	2.19	0.41
4:F:113:PRO:HB3	4:F:139:PHE:HB3	2.02	0.41
1:A:57:CYS:O	1:A:60:CYS:HB2	2.20	0.41
1:A:243:ILE:HD11	1:A:265:LEU:CD1	2.47	0.41
1:A:285:PRO:HD3	3:H:96:VAL:O	2.21	0.41
1:C:214:ALA:CB	1:C:248:MET:HE2	2.33	0.41
2:D:472:MET:H	2:D:472:MET:HG2	1.70	0.41
3:E:169:VAL:HG11	4:F:177:TYR:CE1	2.56	0.41
1:A:53:LEU:O	1:A:76:ILE:HG23	2.21	0.41
1:A:225:ILE:HA	1:A:225:ILE:HD13	1.71	0.41
3:E:212:GLU:CG	3:E:213:PRO:CD	2.97	0.41
1:A:172:ILE:CG1	1:A:260:TYR:CE2	2.97	0.41
1:C:41:PHE:CE1	1:C:282:GLY:HA2	2.56	0.41
1:C:53:LEU:O	1:C:76:ILE:HG23	2.21	0.41
4:F:118:PHE:HB2	4:F:133:VAL:HB	2.03	0.41
1:A:15:VAL:HG22	1:A:23:GLU:HG2	2.02	0.41
1:A:125:ILE:O	1:A:268:GLN:NE2	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:TRP:C	1:A:158:TRP:CD1	2.92	0.41
2:B:409:ASN:O	2:B:410:LEU:HB2	2.21	0.41
2:B:435:ARG:CD	2:B:439:ILE:HG13	2.50	0.41
1:C:197:GLN:NE2	5:P:1:NAG:H81	2.35	0.41
4:F:91:TRP:CZ3	4:F:95(B):GLY:HA2	2.56	0.41
1:C:16:VAL:HG12	1:C:17:LYS:N	2.36	0.41
1:C:52:LYS:HE2	3:E:53:TYR:CE1	2.39	0.41
3:E:124:LEU:HB3	4:F:118:PHE:CD1	2.56	0.41
3:E:40:ALA:HB3	3:E:43:GLN:HG3	2.03	0.40
3:H:40:ALA:HB3	3:H:43:GLN:HG3	2.03	0.40
4:F:19:VAL:HG21	4:F:104:LEU:CD1	2.52	0.40
4:L:19:VAL:HG21	4:L:104:LEU:CD1	2.52	0.40
1:A:16:VAL:HG12	1:A:17:LYS:N	2.36	0.40
2:B:418:ASP:HA	2:B:425:LEU:HD11	2.03	0.40
2:D:418:ASP:HA	2:D:425:LEU:HD11	2.03	0.40
1:C:140:SER:C	1:C:141:GLY:O	2.60	0.40
1:A:281:LYS:HB2	1:A:295:GLU:HG2	2.02	0.40
4:F:151:ASP:HB2	4:F:152:SER:H	1.71	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	331/347 (95%)	303 (92%)	22 (7%)	6 (2%)	8 40
1	C	331/347 (95%)	303 (92%)	22 (7%)	6 (2%)	8 40
2	B	133/179 (74%)	128 (96%)	5 (4%)	0	100 100
2	D	134/179 (75%)	129 (96%)	5 (4%)	0	100 100
3	E	214/234 (92%)	202 (94%)	11 (5%)	1 (0%)	29 69
3	H	215/234 (92%)	203 (94%)	11 (5%)	1 (0%)	29 69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	F	209/216 (97%)	202 (97%)	7 (3%)	0	100	100
4	L	210/216 (97%)	203 (97%)	7 (3%)	0	100	100
All	All	1777/1952 (91%)	1673 (94%)	90 (5%)	14 (1%)	19	60

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	ILE
1	A	251	LYS
1	C	177	ILE
1	C	251	LYS
1	A	148	ASN
1	C	148	ASN
3	E	116	THR
3	H	116	THR
1	A	45	LYS
1	A	146	ILE
1	A	147	THR
1	C	45	LYS
1	C	146	ILE
1	C	147	THR

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	284/294 (97%)	279 (98%)	5 (2%)	59	77
1	C	284/294 (97%)	279 (98%)	5 (2%)	59	77
2	B	116/143 (81%)	114 (98%)	2 (2%)	60	78
2	D	117/143 (82%)	115 (98%)	2 (2%)	60	78
3	E	185/198 (93%)	177 (96%)	8 (4%)	29	54
3	H	186/198 (94%)	178 (96%)	8 (4%)	29	54
4	F	180/183 (98%)	178 (99%)	2 (1%)	73	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	L	181/183 (99%)	178 (98%)	3 (2%)	60 78
All	All	1533/1636 (94%)	1498 (98%)	35 (2%)	50 70

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	CYS
1	A	105	ARG
1	A	118	ARG
1	A	202	TYR
1	A	215	ASN
2	B	421	HIS
2	B	435	ARG
1	C	54	CYS
1	C	105	ARG
1	C	118	ARG
1	C	202	TYR
1	C	215	ASN
2	D	421	HIS
2	D	435	ARG
3	E	71	LYS
3	E	94	ARG
3	E	140	CYS
3	E	143	LYS
3	E	171	GLN
3	E	178	LEU
3	E	183	THR
3	E	197	ASN
4	F	81	GLU
4	F	129	LYS
3	H	71	LYS
3	H	94	ARG
3	H	140	CYS
3	H	143	LYS
3	H	171	GLN
3	H	178	LEU
3	H	183	THR
3	H	197	ASN
4	L	81	GLU
4	L	129	LYS
4	L	211	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	85	HIS
1	A	126	ASN
1	A	129	ASN
2	B	398	ASN
2	B	409	ASN
1	C	14	HIS
1	C	85	HIS
1	C	126	ASN
1	C	129	ASN
2	D	398	ASN
2	D	409	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

18 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	G	1	5,1	14,14,15	0.52	0	17,19,21	0.95	1 (5%)
5	NAG	G	2	5	14,14,15	0.49	0	17,19,21	0.86	1 (5%)
5	NAG	I	1	5,1	14,14,15	0.40	0	17,19,21	1.80	3 (17%)
5	NAG	I	2	5	14,14,15	0.45	0	17,19,21	1.27	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	J	1	5,1	14,14,15	0.53	0	17,19,21	0.96	1 (5%)
5	NAG	J	2	5	14,14,15	0.49	0	17,19,21	0.85	1 (5%)
6	NAG	K	1	6,1	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
6	NAG	K	2	6	14,14,15	0.50	0	17,19,21	1.40	3 (17%)
6	BMA	K	3	6	11,11,12	0.66	0	15,15,17	1.46	3 (20%)
6	NAG	M	1	6,1	14,14,15	0.52	0	17,19,21	0.95	1 (5%)
6	NAG	M	2	6	14,14,15	0.49	0	17,19,21	0.86	1 (5%)
6	BMA	M	3	6	11,11,12	0.59	0	15,15,17	0.92	1 (6%)
5	NAG	N	1	5,1	14,14,15	0.40	0	17,19,21	1.80	3 (17%)
5	NAG	N	2	5	14,14,15	0.44	0	17,19,21	1.27	3 (17%)
5	NAG	O	1	5,1	14,14,15	0.51	0	17,19,21	0.96	1 (5%)
5	NAG	O	2	5	14,14,15	0.49	0	17,19,21	0.85	1 (5%)
5	NAG	P	1	5,1	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
5	NAG	P	2	5	14,14,15	0.49	0	17,19,21	1.40	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	3/6/23/26	0/1/1/1
5	NAG	I	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	NAG	J	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	J	2	5	-	3/6/23/26	0/1/1/1
6	NAG	K	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1
6	BMA	K	3	6	-	2/2/19/22	0/1/1/1
6	NAG	M	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	M	2	6	-	3/6/23/26	0/1/1/1
6	BMA	M	3	6	-	0/2/19/22	0/1/1/1
5	NAG	N	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	N	2	5	-	0/6/23/26	0/1/1/1
5	NAG	O	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	P	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	P	2	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	P	1	NAG	O5-C1-C2	-7.39	99.63	111.29
6	K	1	NAG	O5-C1-C2	-7.38	99.64	111.29
5	I	1	NAG	C1-O5-C5	5.94	120.24	112.19
5	N	1	NAG	C1-O5-C5	5.92	120.21	112.19
6	K	2	NAG	O5-C5-C6	-3.58	101.59	107.20
5	P	2	NAG	O5-C5-C6	-3.54	101.66	107.20
5	J	1	NAG	C1-O5-C5	3.20	116.52	112.19
5	O	1	NAG	C1-O5-C5	3.17	116.48	112.19
6	M	1	NAG	C1-O5-C5	3.15	116.46	112.19
5	G	1	NAG	C1-O5-C5	3.14	116.44	112.19
6	K	3	BMA	O2-C2-C3	2.94	116.02	110.14
6	K	1	NAG	O7-C7-C8	-2.79	116.88	122.06
5	P	1	NAG	O7-C7-C8	-2.77	116.91	122.06
6	K	1	NAG	C4-C3-C2	-2.66	107.12	111.02
5	P	1	NAG	C4-C3-C2	-2.64	107.15	111.02
6	K	3	BMA	O4-C4-C5	-2.63	102.77	109.30
5	N	2	NAG	C2-N2-C7	-2.51	119.32	122.90
5	I	2	NAG	C2-N2-C7	-2.47	119.39	122.90
5	N	1	NAG	O5-C5-C4	2.44	116.75	110.83
6	K	3	BMA	C6-C5-C4	-2.42	107.34	113.00
5	I	1	NAG	O5-C5-C4	2.41	116.70	110.83
5	N	2	NAG	O5-C1-C2	-2.35	107.58	111.29
5	P	2	NAG	O5-C1-C2	-2.32	107.63	111.29
6	K	2	NAG	O5-C1-C2	-2.32	107.63	111.29
5	I	2	NAG	O5-C1-C2	-2.28	107.69	111.29
5	I	1	NAG	C3-C4-C5	2.27	114.29	110.24
5	N	1	NAG	C3-C4-C5	2.24	114.24	110.24
5	J	2	NAG	C2-N2-C7	-2.23	119.72	122.90
6	K	2	NAG	C4-C3-C2	-2.23	107.75	111.02
5	P	2	NAG	C4-C3-C2	-2.22	107.76	111.02
5	O	2	NAG	C2-N2-C7	-2.18	119.80	122.90
5	G	2	NAG	C2-N2-C7	-2.13	119.86	122.90
6	M	2	NAG	C2-N2-C7	-2.10	119.91	122.90
6	M	3	BMA	O5-C1-C2	-2.07	107.58	110.77
5	I	2	NAG	C4-C3-C2	-2.06	108.00	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	N	2	NAG	C4-C3-C2	-2.01	108.08	111.02

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	1	NAG	C8-C7-N2-C2
5	N	1	NAG	C8-C7-N2-C2
5	I	1	NAG	O7-C7-N2-C2
5	N	1	NAG	O7-C7-N2-C2
5	N	1	NAG	O5-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
5	G	2	NAG	C8-C7-N2-C2
5	J	2	NAG	C8-C7-N2-C2
5	O	2	NAG	C8-C7-N2-C2
6	M	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
5	J	2	NAG	O7-C7-N2-C2
5	O	2	NAG	O7-C7-N2-C2
6	M	2	NAG	O7-C7-N2-C2
5	G	1	NAG	C8-C7-N2-C2
5	J	1	NAG	C8-C7-N2-C2
5	O	1	NAG	C8-C7-N2-C2
6	M	1	NAG	C8-C7-N2-C2
6	K	3	BMA	C4-C5-C6-O6
6	K	3	BMA	O5-C5-C6-O6
5	G	1	NAG	O7-C7-N2-C2
5	J	1	NAG	O7-C7-N2-C2
5	O	1	NAG	O7-C7-N2-C2
6	M	1	NAG	O7-C7-N2-C2
5	G	2	NAG	O5-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
6	M	2	NAG	O5-C5-C6-O6
5	P	1	NAG	O7-C7-N2-C2
5	J	1	NAG	O5-C5-C6-O6

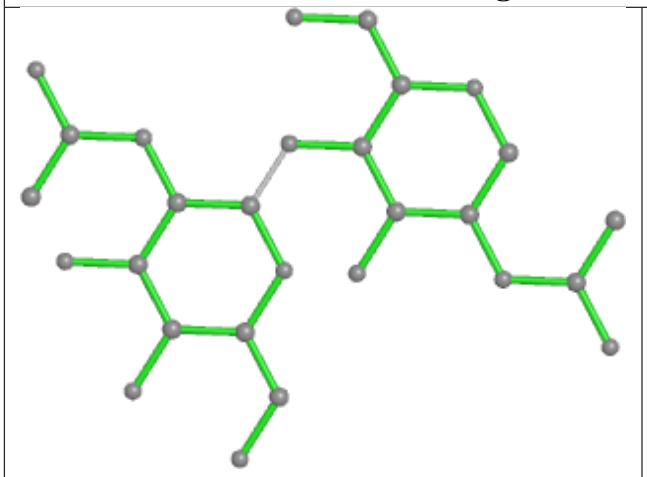
There are no ring outliers.

4 monomers are involved in 10 short contacts:

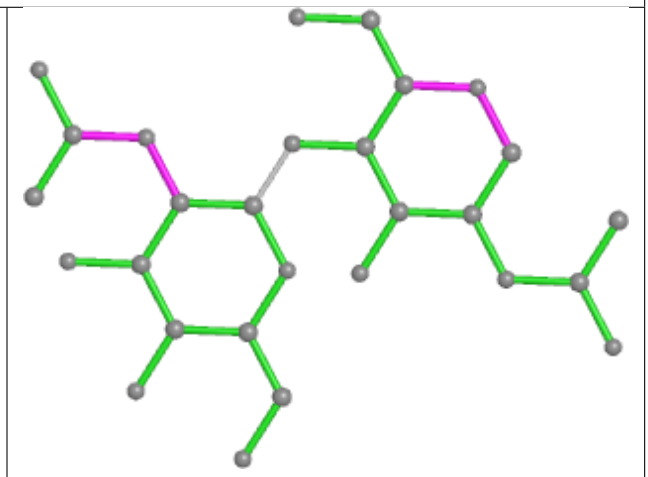
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	1	NAG	1	0
6	K	1	NAG	3	0
5	P	1	NAG	5	0
5	G	1	NAG	1	0

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

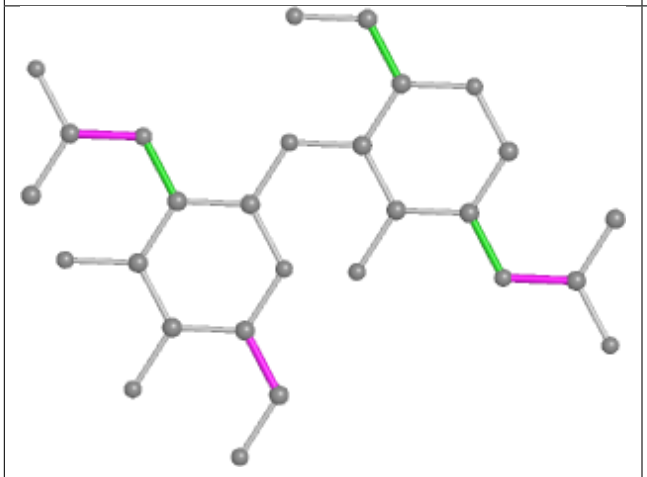
Oligosaccharide Chain G



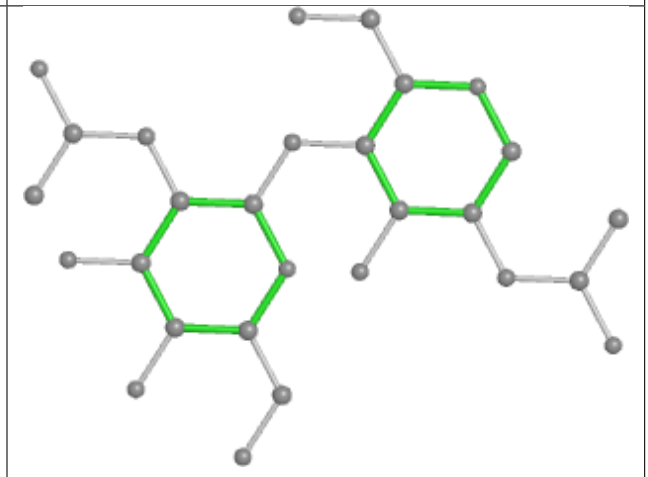
Bond lengths



Bond angles

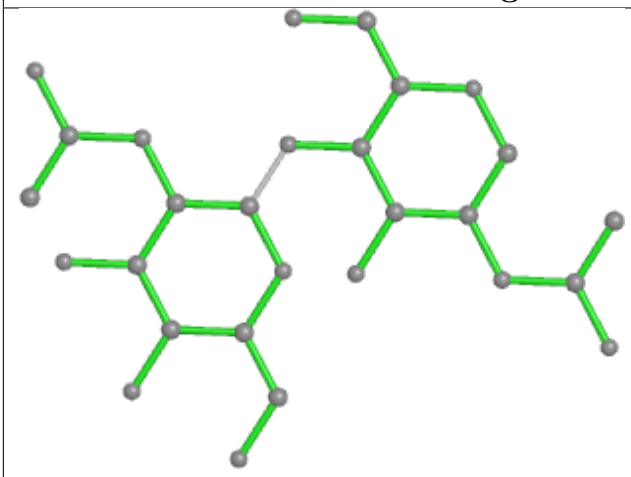


Torsions

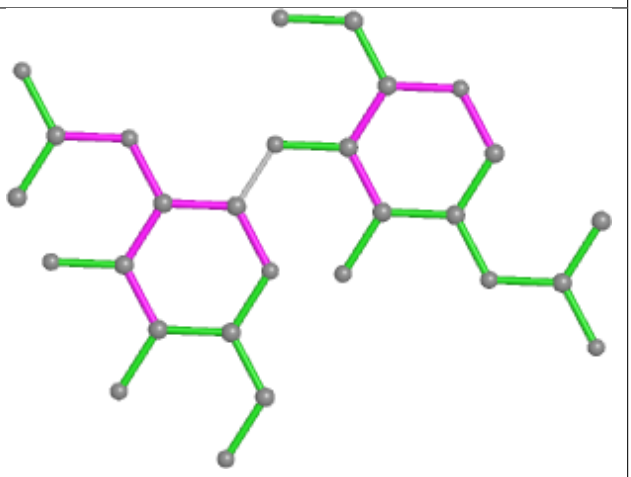


Rings

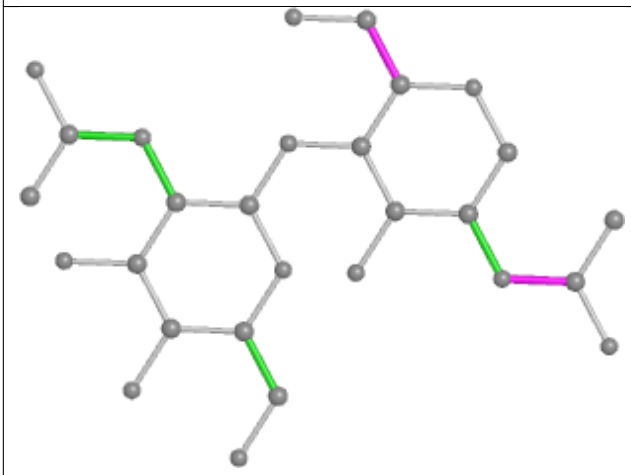
Oligosaccharide Chain I



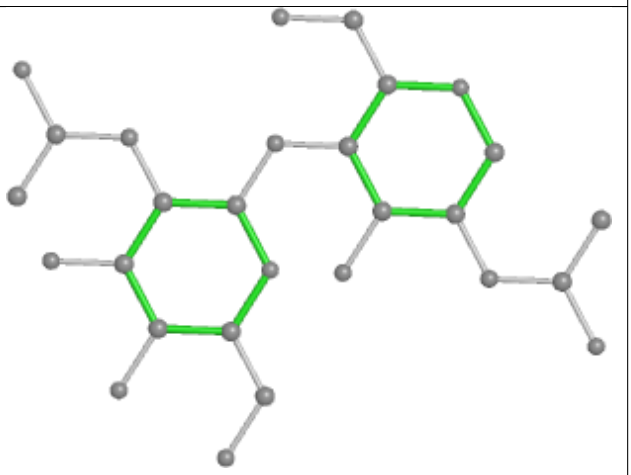
Bond lengths



Bond angles

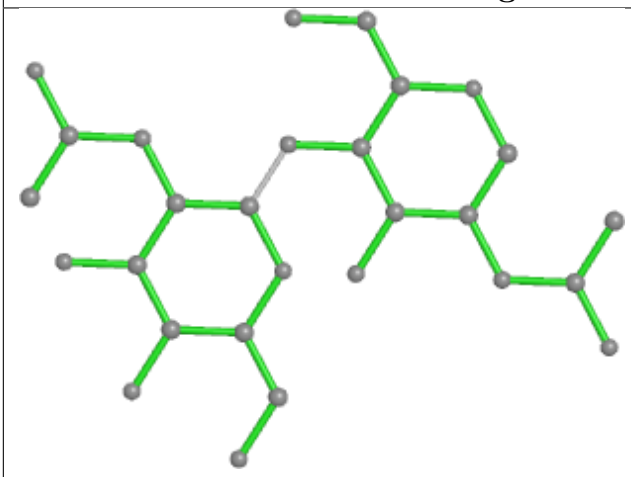


Torsions

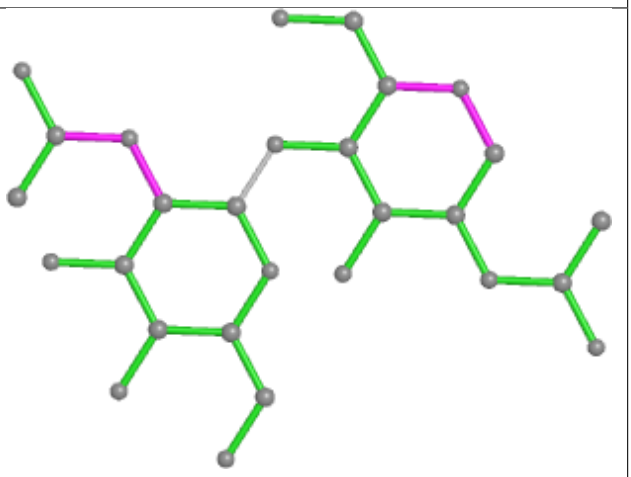


Rings

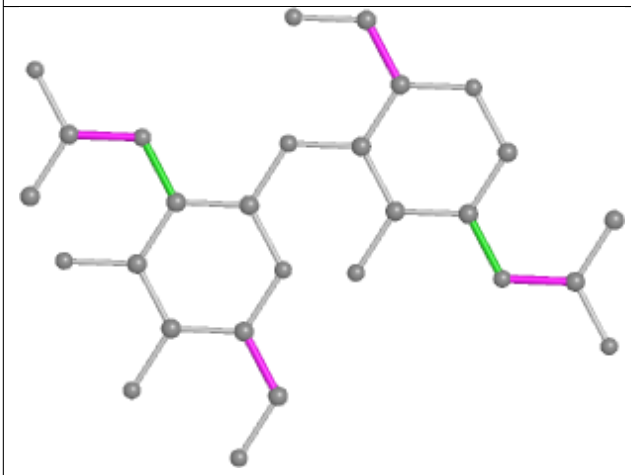
Oligosaccharide Chain J



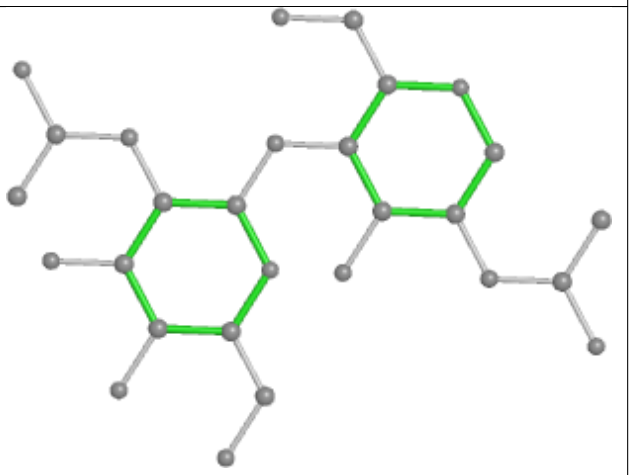
Bond lengths



Bond angles

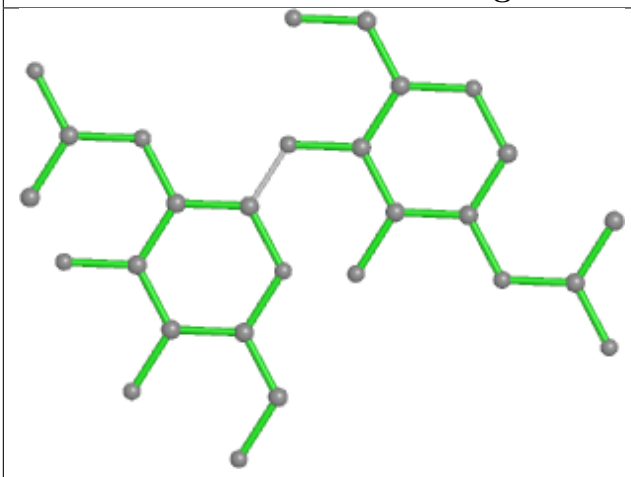


Torsions

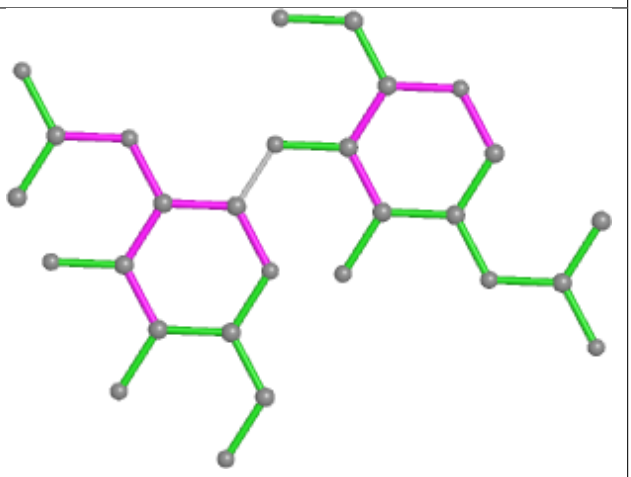


Rings

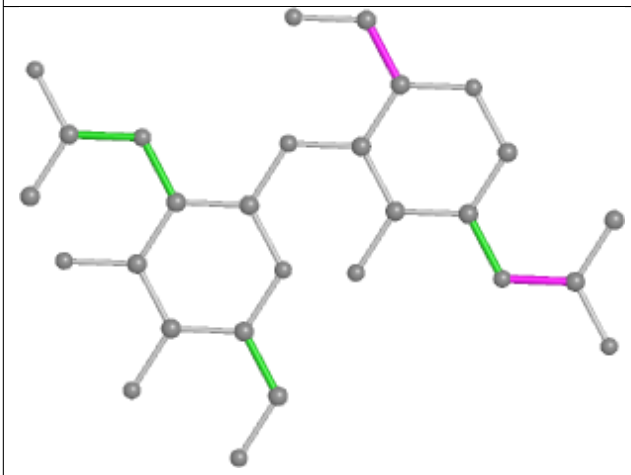
Oligosaccharide Chain N



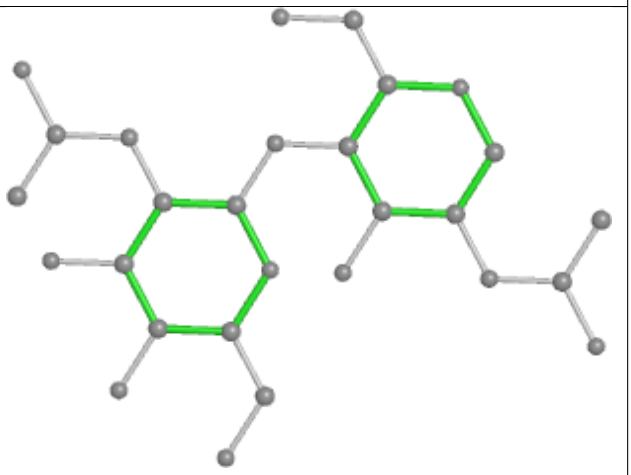
Bond lengths



Bond angles

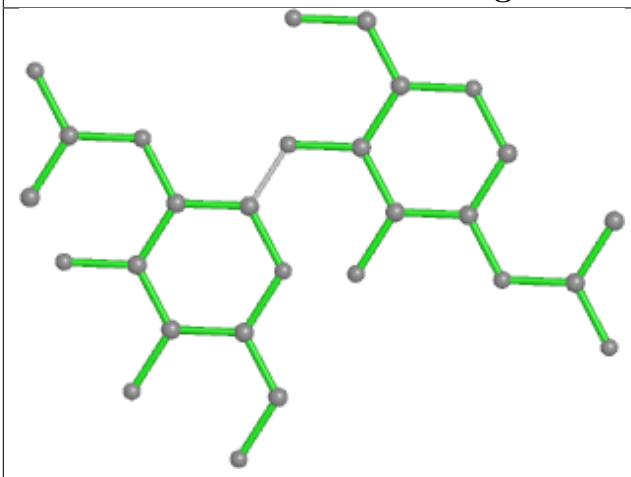


Torsions

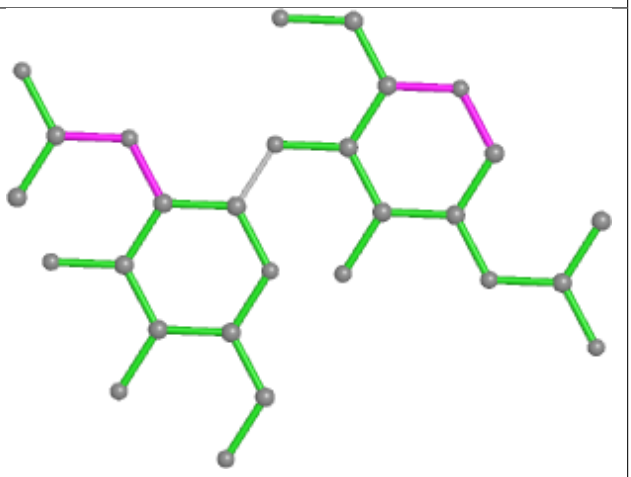


Rings

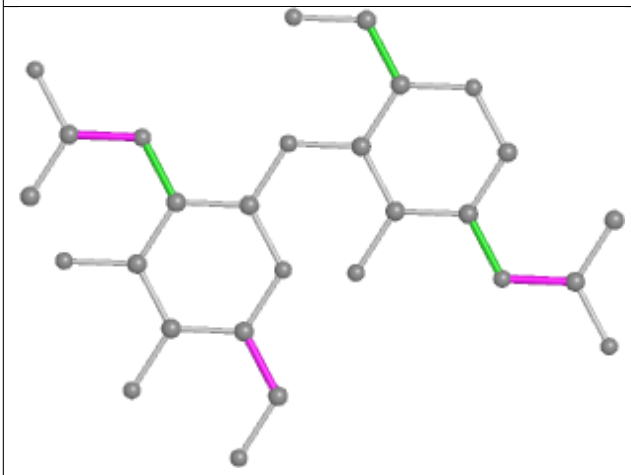
Oligosaccharide Chain O



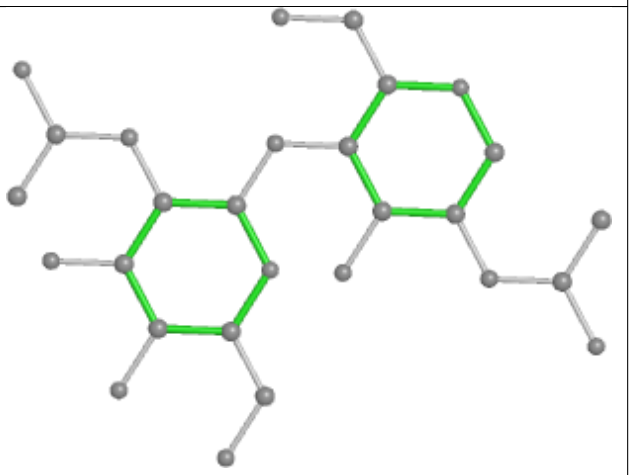
Bond lengths



Bond angles

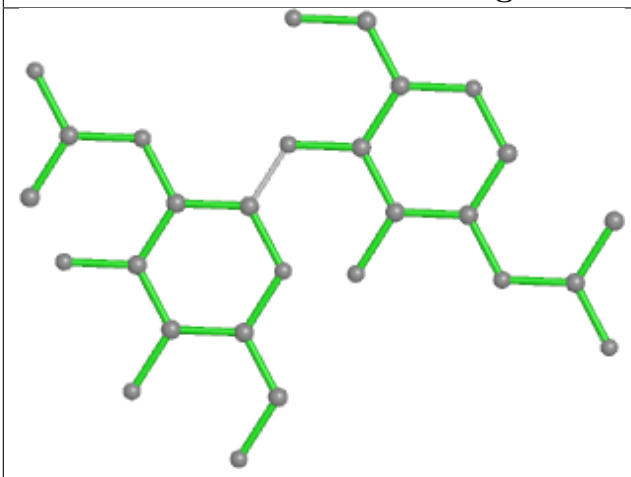


Torsions

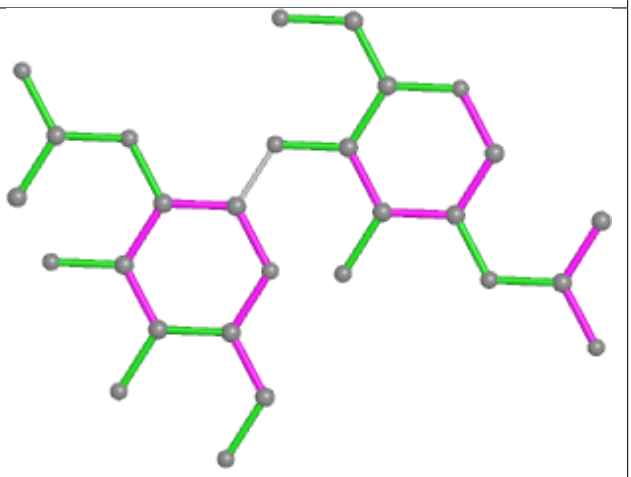


Rings

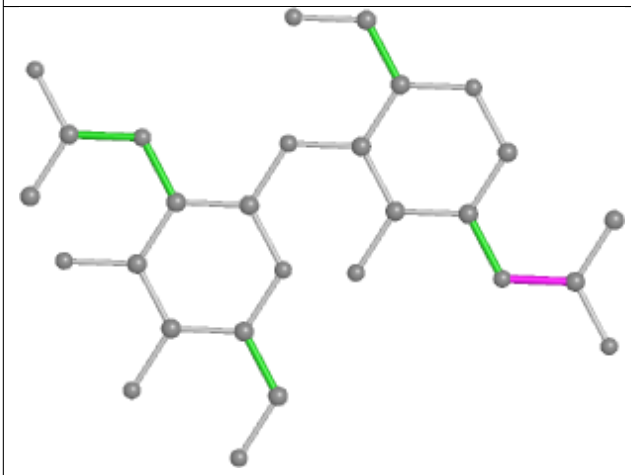
Oligosaccharide Chain P



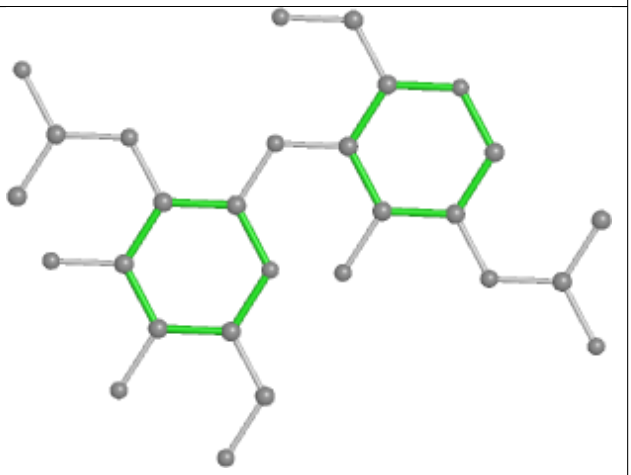
Bond lengths



Bond angles

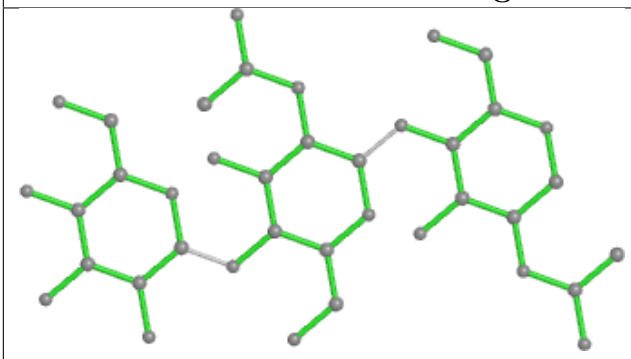


Torsions

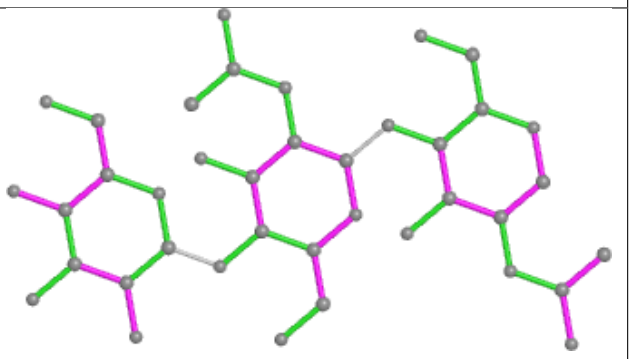


Rings

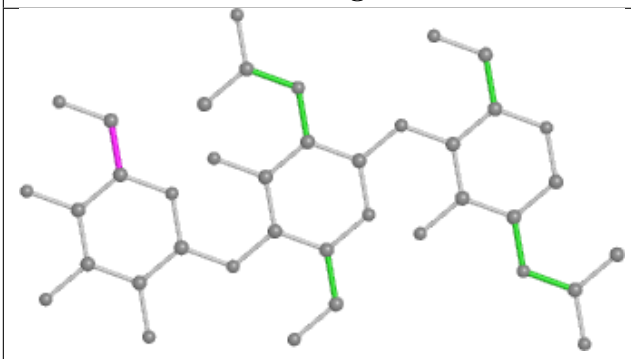
Oligosaccharide Chain K



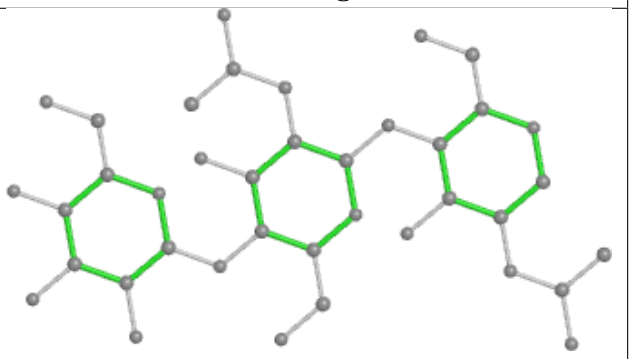
Bond lengths



Bond angles

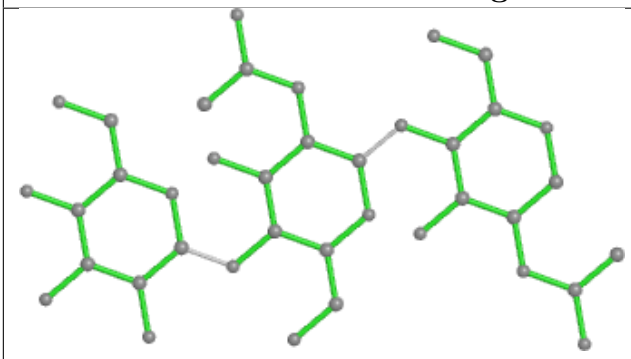


Torsions

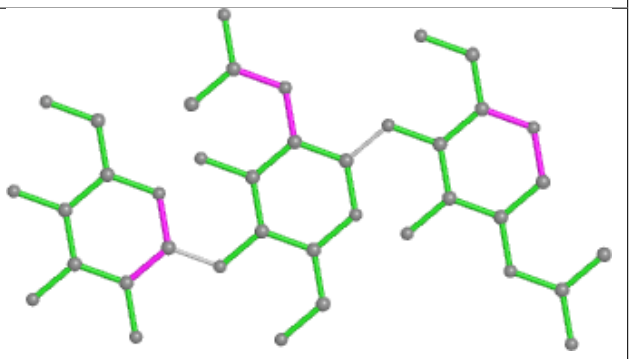


Rings

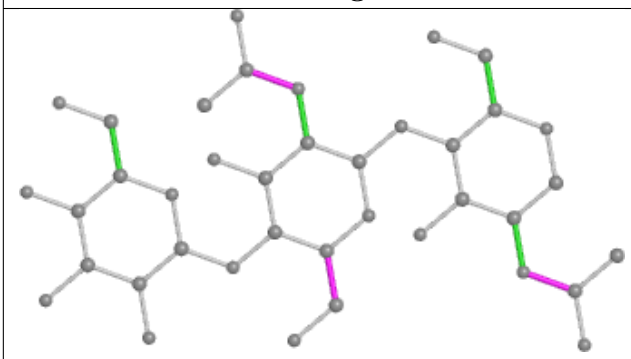
Oligosaccharide Chain M



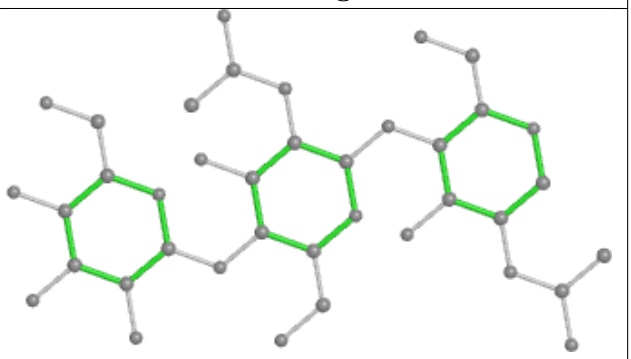
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	C	410	1	14,14,15	0.50	0	17,19,21	0.98	1 (5%)
7	NAG	A	410	1	14,14,15	0.49	0	17,19,21	0.98	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
7	NAG	C	410	1	-	2/6/23/26	0/1/1/1
7	NAG	A	410	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	410	NAG	C1-O5-C5	2.46	115.53	112.19
7	C	410	NAG	C1-O5-C5	2.46	115.52	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	410	NAG	C8-C7-N2-C2
7	C	410	NAG	C8-C7-N2-C2
7	C	410	NAG	O7-C7-N2-C2
7	A	410	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	337/347 (97%)	0.56	37 (10%) 5 8	100, 100, 100, 100	0
1	C	337/347 (97%)	0.52	28 (8%) 11 12	100, 100, 100, 100	0
2	B	139/179 (77%)	0.65	11 (7%) 12 13	100, 100, 100, 100	0
2	D	140/179 (78%)	0.79	14 (10%) 7 9	100, 100, 100, 100	0
3	E	220/234 (94%)	0.66	26 (11%) 4 7	100, 100, 100, 100	0
3	H	221/234 (94%)	0.57	20 (9%) 9 11	100, 100, 100, 100	0
4	F	213/216 (98%)	0.38	17 (7%) 12 13	100, 100, 100, 100	0
4	L	214/216 (99%)	0.30	12 (5%) 24 23	100, 100, 100, 100	0
All	All	1821/1952 (93%)	0.54	165 (9%) 9 10	100, 100, 100, 100	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	194	TYR	6.7
1	C	329	ALA	6.1
4	L	123	GLU	5.4
1	A	329	ALA	4.9
4	F	210	GLU	4.8
1	A	23	GLU	4.7
4	F	1	GLN	4.5
2	D	376	ALA	4.3
1	A	132	GLY	4.3
3	E	193	THR	4.3
3	E	121	VAL	4.2
1	C	127	ALA	4.0
1	C	83	ILE	4.0
3	E	123	PRO	4.0
2	D	465	LEU	3.9
3	H	121	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
3	E	20	VAL	3.8
1	C	21	GLN	3.7
4	F	47	LEU	3.7
3	E	209	LYS	3.6
4	F	32	TYR	3.6
1	A	216	GLY	3.6
3	E	211	VAL	3.6
1	C	245	VAL	3.6
2	D	458	GLU	3.5
2	B	376	ALA	3.4
1	A	133	GLY	3.4
2	D	375	GLY	3.3
3	H	179	SER	3.3
3	E	119	PRO	3.2
1	A	271	TRP	3.2
1	A	127	ALA	3.2
1	A	218	THR	3.2
4	L	48	ILE	3.2
2	B	371	TYR	3.1
1	C	269	LYS	3.1
2	B	454	ILE	3.1
1	C	49	THR	3.1
2	B	465	LEU	3.1
3	E	122	PHE	3.1
3	H	193	THR	3.1
3	E	82	LEU	3.0
3	H	211	VAL	3.0
1	A	50	ARG	3.0
2	D	451	ASN	3.0
3	E	117	LYS	3.0
2	D	455	ILE	3.0
1	A	21	GLN	2.9
1	A	245	VAL	2.9
2	B	458	GLU	2.9
1	A	80	ARG	2.9
2	D	432	ASP	2.9
3	E	80	MET	2.9
4	L	210	GLU	2.9
4	F	123	GLU	2.8
3	H	209	LYS	2.8
4	L	100	GLY	2.8
4	L	50	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	67	LEU	2.8
4	F	48	ILE	2.8
1	C	315	ILE	2.7
2	B	455	ILE	2.7
1	A	51	GLY	2.7
1	C	271	TRP	2.7
3	H	19	ARG	2.7
3	H	212	GLU	2.7
1	A	163(C)	ASN	2.7
3	E	120	SER	2.7
1	C	67	LEU	2.7
3	H	194	TYR	2.7
3	H	20	VAL	2.7
3	E	45	LEU	2.7
4	L	126	GLN	2.6
1	C	158	TRP	2.6
3	E	63	LEU	2.6
4	L	51	SER	2.6
1	C	38	LYS	2.6
1	A	131	PRO	2.6
1	C	266	LEU	2.6
2	B	369	HIS	2.6
1	A	269	LYS	2.6
2	D	514	PHE	2.6
1	A	328	LEU	2.6
3	E	54	SER	2.5
4	F	51	SER	2.5
3	H	123	PRO	2.5
1	C	216	GLY	2.5
3	H	67	VAL	2.5
2	D	415	GLY	2.5
4	F	33	VAL	2.5
3	E	210	ARG	2.5
1	A	10	SER	2.4
2	D	419	GLU	2.4
1	A	83	ILE	2.4
1	A	335	ARG	2.4
3	H	54	SER	2.4
3	E	18	VAL	2.4
4	F	50	ARG	2.4
1	A	88	ARG	2.4
1	A	134	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
3	E	53	TYR	2.4
3	H	213	PRO	2.4
4	F	209	THR	2.4
4	L	33	VAL	2.4
1	A	49	THR	2.4
2	D	371	TYR	2.4
1	C	88	ARG	2.3
4	F	113	PRO	2.3
2	D	475	PRO	2.3
3	E	159	LEU	2.3
1	A	81	VAL	2.3
4	F	97	VAL	2.3
3	H	63	LEU	2.3
1	C	328	LEU	2.3
2	B	490	LYS	2.3
1	C	331	GLY	2.3
3	E	48	MET	2.3
3	H	120	SER	2.3
2	B	375	GLY	2.3
1	A	278	LYS	2.3
1	C	59	ASN	2.2
1	A	137	ILE	2.2
3	H	38	ARG	2.2
1	C	48	GLU	2.2
3	E	19	ARG	2.2
1	C	126	ASN	2.2
1	C	97	ILE	2.2
3	H	45	LEU	2.2
4	F	195	VAL	2.2
1	C	163	ASN	2.2
1	A	306	TYR	2.2
1	A	52	LYS	2.2
1	C	204	ASP	2.2
4	F	126	GLN	2.2
1	C	335	ARG	2.2
3	E	81	GLU	2.2
4	L	3	VAL	2.2
4	F	36	TYR	2.2
3	E	90	TYR	2.1
1	A	180	GLU	2.1
1	C	66	ALA	2.1
2	D	489	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	135	TYR	2.1
1	A	266	LEU	2.1
3	E	60	ALA	2.1
4	L	9	SER	2.1
4	F	110	LYS	2.1
1	C	137	ILE	2.1
1	A	204	ASP	2.1
4	L	144	VAL	2.1
1	A	337	PRO	2.1
3	H	119	PRO	2.1
1	A	42	ALA	2.1
4	L	53	GLN	2.1
2	B	514	PHE	2.1
4	F	141	PRO	2.0
2	D	462	LEU	2.0
3	E	189	LEU	2.0
1	A	117	ILE	2.0
1	A	238	PRO	2.0
2	B	451	ASN	2.0
1	C	188	TRP	2.0
3	H	122	PHE	2.0
3	H	117	LYS	2.0
1	C	117	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
5	NAG	G	2	14/15	0.60	0.57	100,100,100,100	0
5	NAG	J	2	14/15	0.67	0.45	100,100,100,100	0
6	BMA	M	3	11/12	0.67	0.38	100,100,100,100	0
5	NAG	P	2	14/15	0.76	0.31	100,100,100,100	0
6	BMA	K	3	11/12	0.76	0.34	100,100,100,100	0

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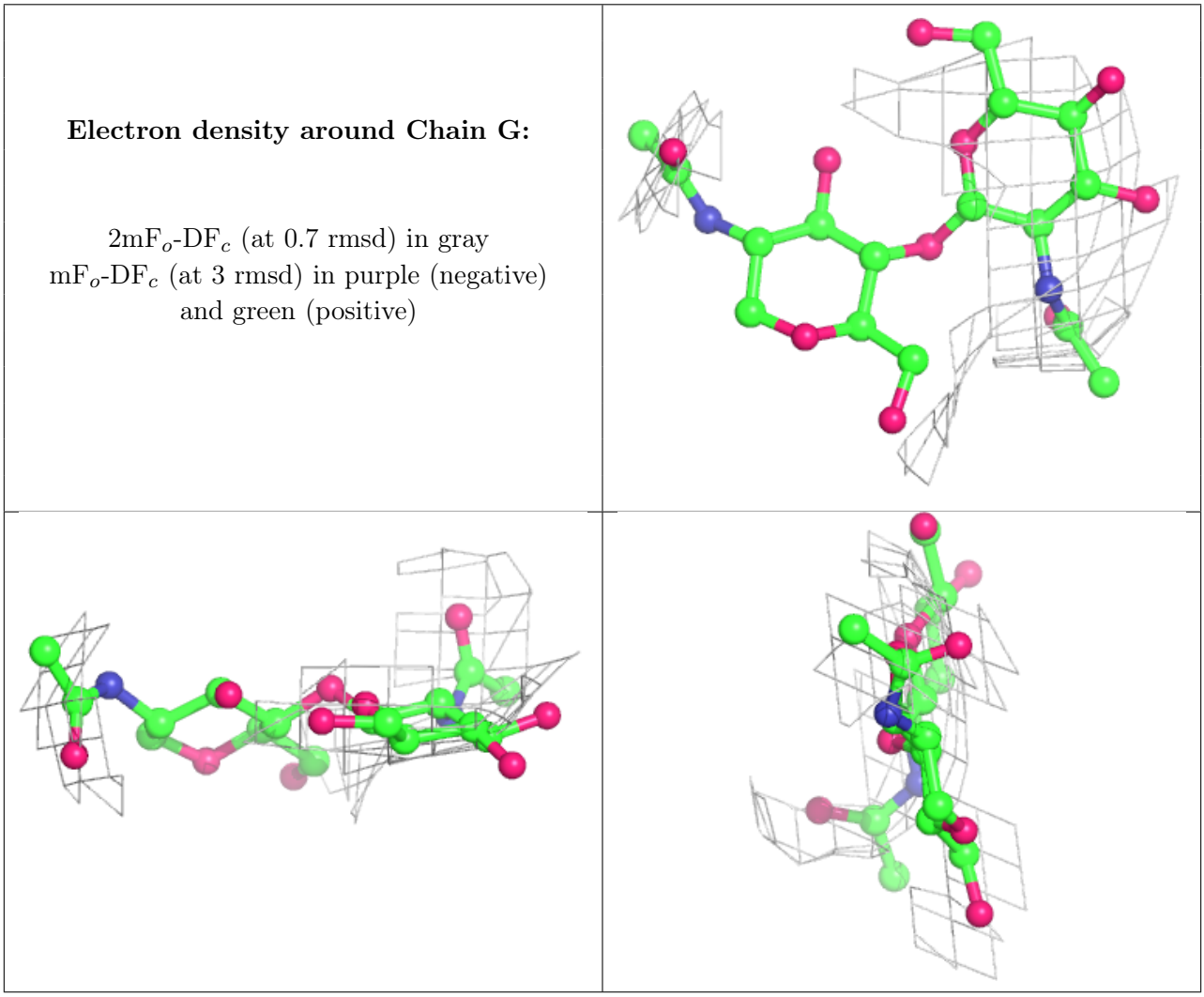
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	O	2	14/15	0.76	0.41	100,100,100,100	0
6	NAG	K	1	14/15	0.77	0.47	100,100,100,100	0
6	NAG	K	2	14/15	0.80	0.25	100,100,100,100	0
6	NAG	M	2	14/15	0.81	0.38	100,100,100,100	0
5	NAG	I	2	14/15	0.81	0.37	100,100,100,100	0
5	NAG	J	1	14/15	0.82	0.45	100,100,100,100	0
5	NAG	O	1	14/15	0.85	0.50	100,100,100,100	0
5	NAG	P	1	14/15	0.85	0.35	100,100,100,100	0
5	NAG	N	2	14/15	0.89	0.32	100,100,100,100	0
6	NAG	M	1	14/15	0.89	0.29	100,100,100,100	0
5	NAG	G	1	14/15	0.91	0.27	100,100,100,100	0
5	NAG	I	1	14/15	0.91	0.36	100,100,100,100	0
5	NAG	N	1	14/15	0.96	0.19	100,100,100,100	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.

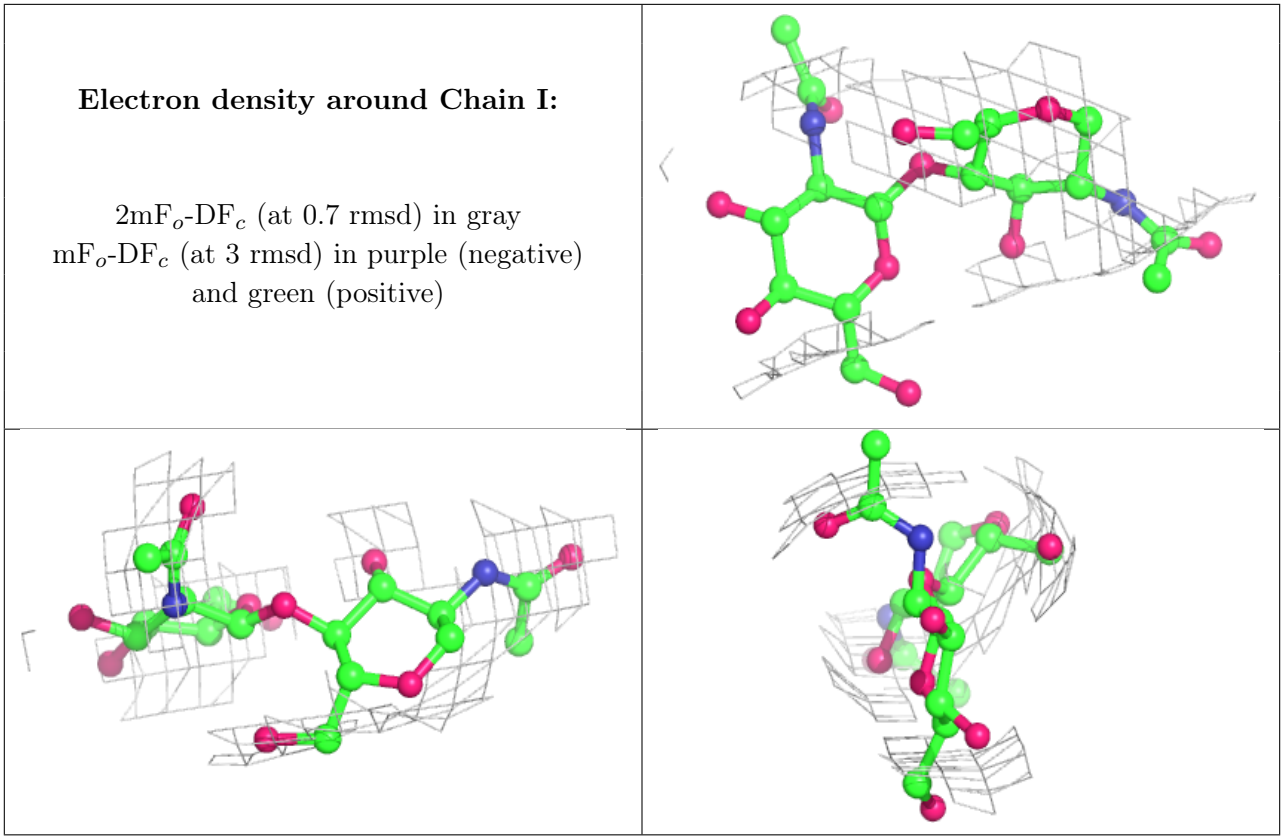
Electron density around Chain G:

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



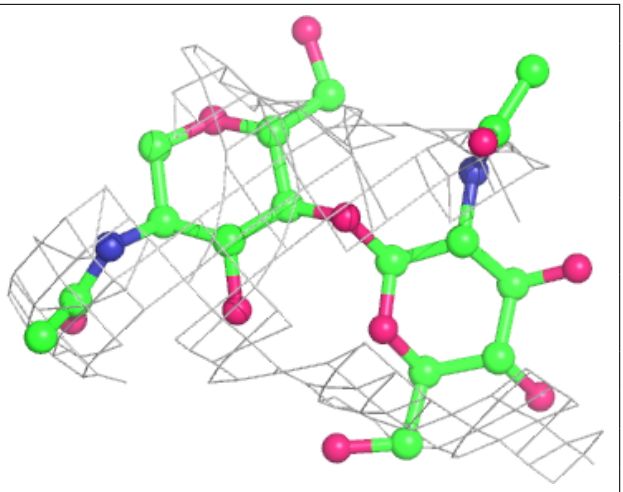
Electron density around Chain I:

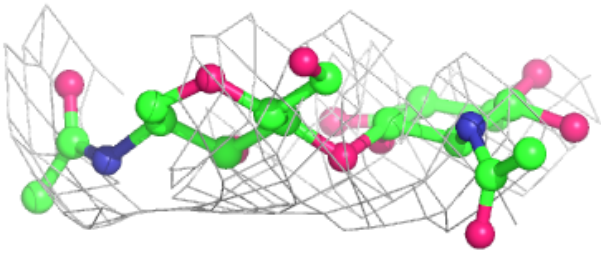
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

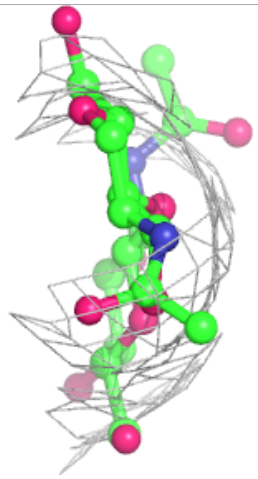


Electron density around Chain J:

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

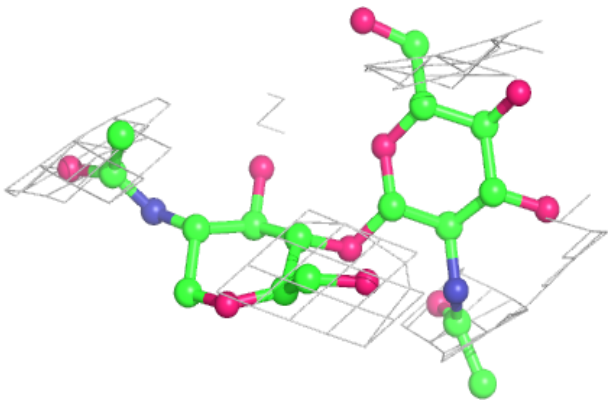


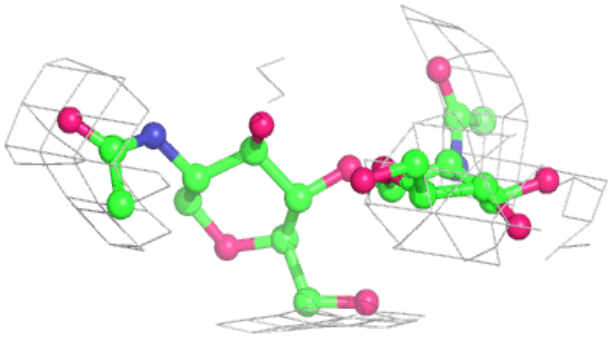


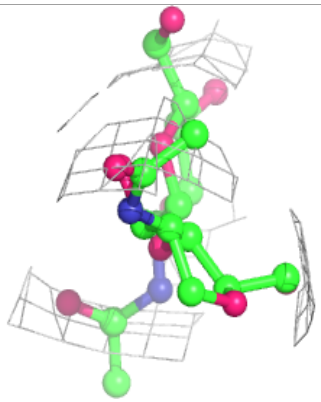


Electron density around Chain N:

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

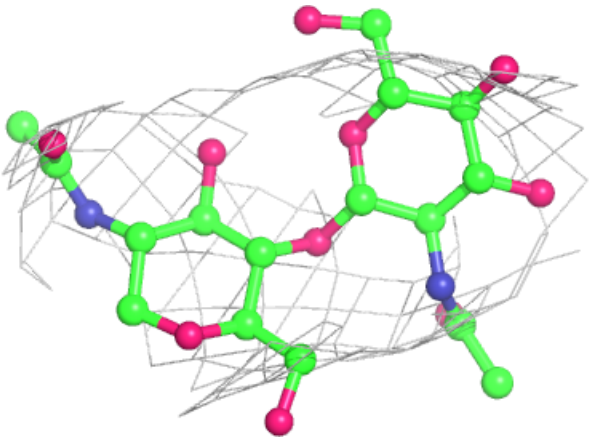


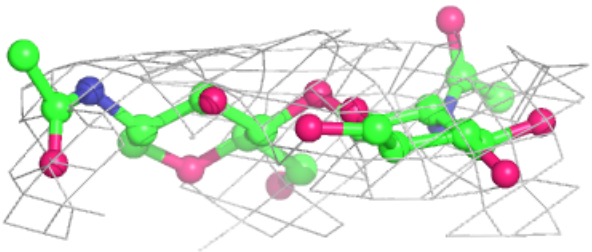


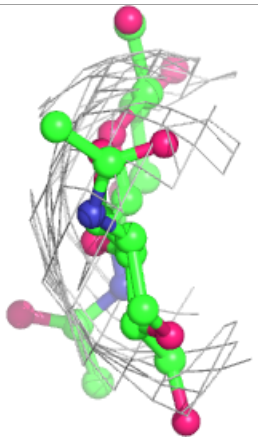


Electron density around Chain O:

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

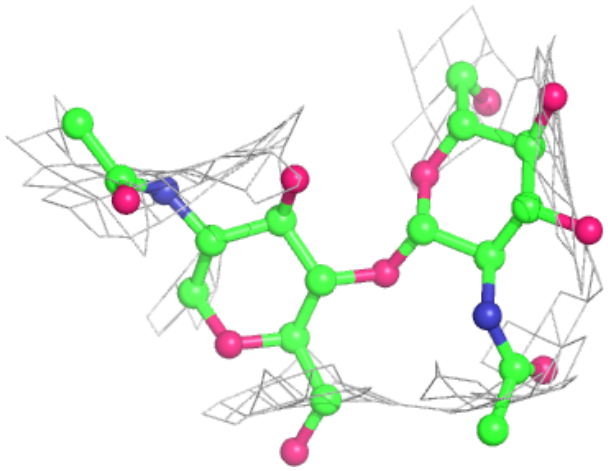


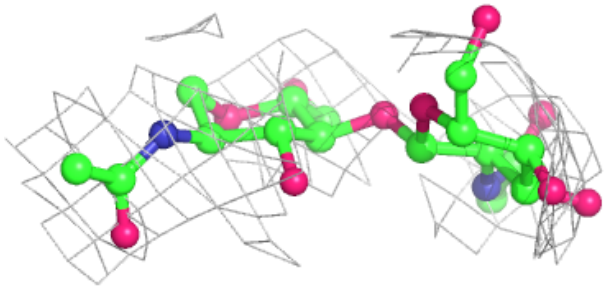


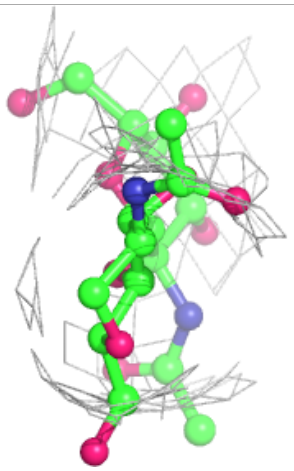


Electron density around Chain P:

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

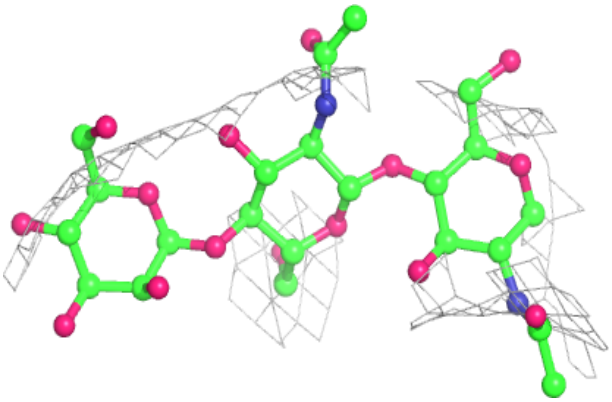


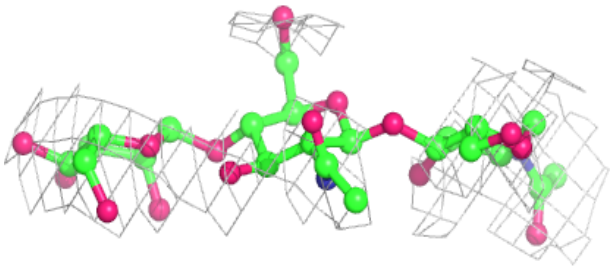


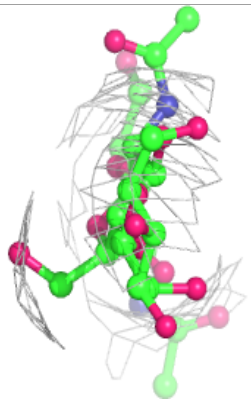


Electron density around Chain K:

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

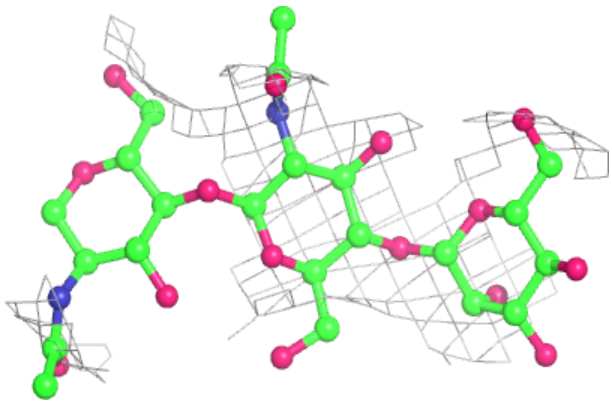


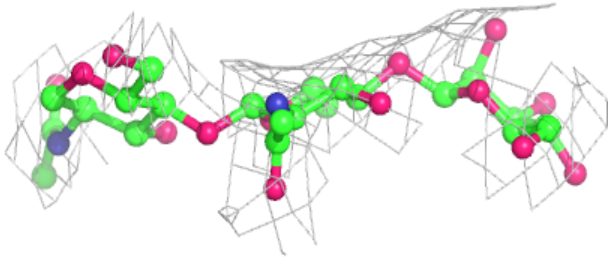


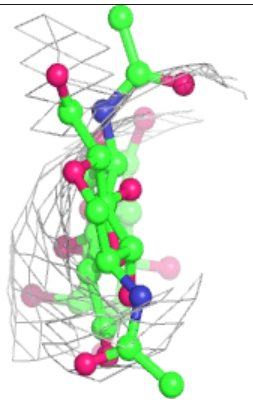


Electron density around Chain M:

$2mF_o$-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	NAG	C	410	14/15	0.62	0.50	100,100,100,100	0
7	NAG	A	410	14/15	0.73	0.47	100,100,100,100	0

6.5 Other polymers

There are no such residues in this entry.