Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 04:24 PM BST

PDB ID	:	4MMY
Title	:	Integrin AlphaVBeta3 ectodomain bound to the tenth domain of Fibronectin with the IAKGDWND motif
Authors	:	van Agthoven, J.; Xiong, J.; Arnaout, M.A.
Deposited on	:	2013-09-09
Resolution	:	3.18 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 following versions of software and data (see references ①) were used in the production of this report:

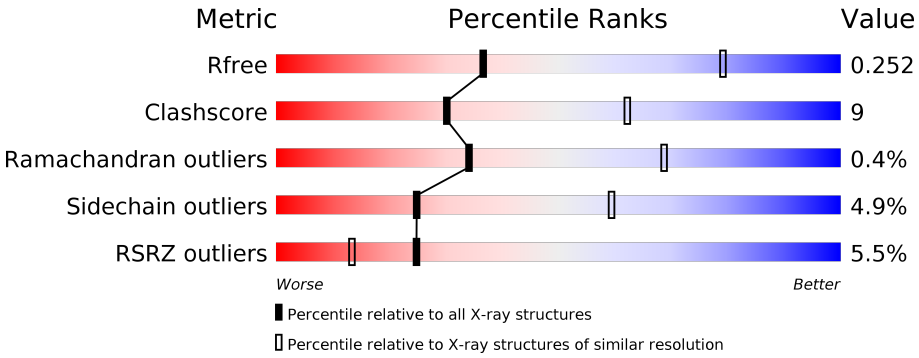
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 3.18 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	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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 on 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	959	3%, 74%, 21%, • •
2	B	692	9%, 74%, 23%, •
3	C	98	3%, 6%, •, 92%
4	D	4	75%, 25%
4	G	4	50%, 50%
5	E	2	100%

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Mol	Chain	Length	Quality of chain
5	H	2	100%
5	I	2	50% 50%
5	K	2	50% 50%
6	F	6	50% 50%
7	J	3	33% 67%
7	L	3	33% 67%

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
8	NAG	A	1017	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13000 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 Integrin alpha-V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	924	Total	C	N	O	S	0	0	0
			7196	4556	1221	1384	35			

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	690	Total	C	N	O	S	0	0	0
			5294	3250	904	1070	70			

- Molecule 3 is a protein called Fibronectin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	0	0	0
			65	41	13	11			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1491	ILE	THR	engineered mutation	UNP P02751
C	1492	ALA	GLY	engineered mutation	UNP P02751
C	1496	TRP	SER	engineered mutation	UNP P02751
C	1497	ASN	PRO	engineered mutation	UNP P02751
C	1498	ASP	ALA	engineered mutation	UNP P02751
C	1499	GLY	SER	engineered mutation	UNP P02751
C	1510	GLY	-	expression tag	UNP P02751
C	1511	LYS	-	expression tag	UNP P02751
C	1512	LYS	-	expression tag	UNP P02751
C	1513	GLY	-	expression tag	UNP P02751
C	1514	LYS	-	expression tag	UNP P02751

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

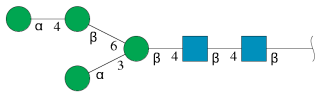
pyranose.

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

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

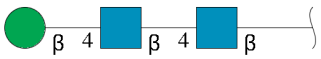
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



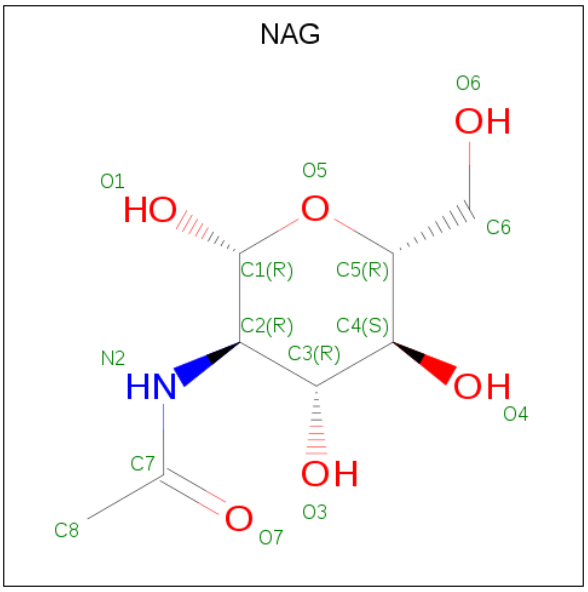
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 7 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
7	J	3	Total C N O 39 22 2 15	0	0	0
7	L	3	Total C N O 39 22 2 15	0	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 9 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	3	Total Mn 3 3	0	0
9	A	5	Total Mn 5 5	0	0

- Molecule 10 is water.

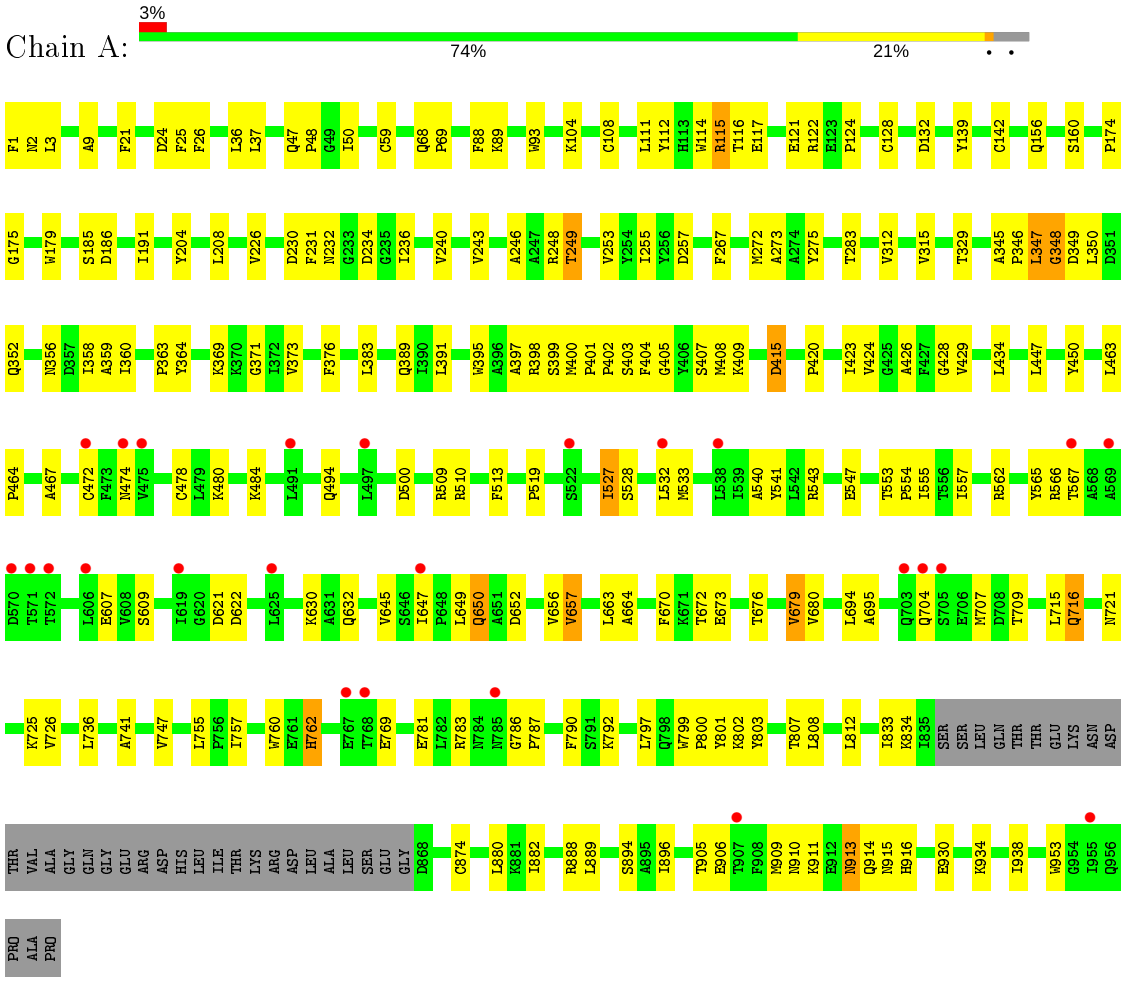
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	3	Total O 3 3	0	0
10	B	2	Total O 2 2	0	0

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.

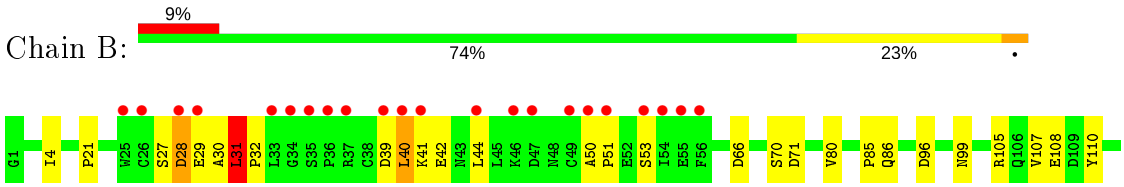
- Molecule 1: Integrin alpha-V

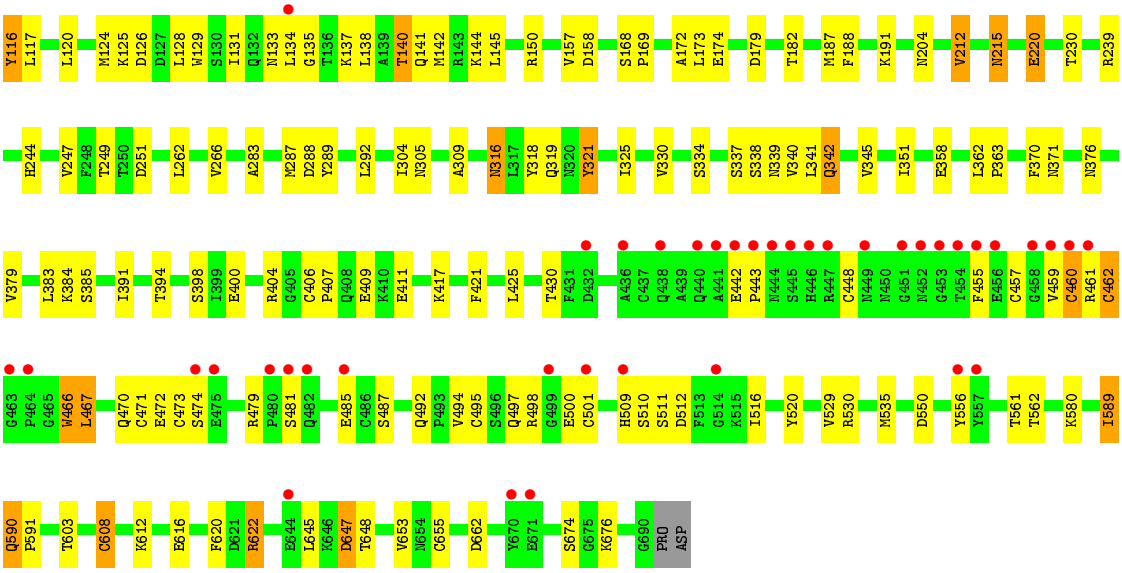
Chain A:



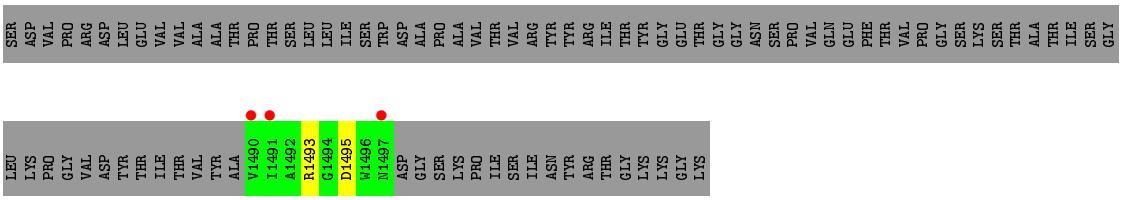
- Molecule 2: Integrin beta-3

Chain B:





• Molecule 3: Fibronectin



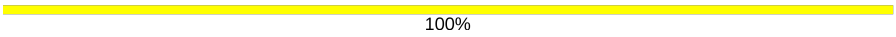
• Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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

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

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

Chain H:



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

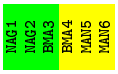
Chain I:

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

Chain K:

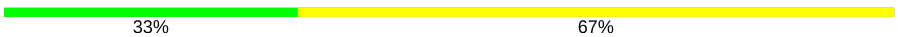
• Molecule 6: alpha-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



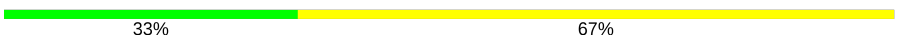
• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



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

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	130.02Å 130.02Å 308.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.02 – 3.18 49.69 – 3.18	Depositor EDS
% Data completeness (in resolution range)	99.4 (41.02-3.18) 99.4 (49.69-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.211 , 0.252 0.214 , 0.252	Depositor DCC
R_{free} test set	2536 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	95.8	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 64.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	13000	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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, MN, MAN

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	0.23	0/7352	0.44	0/9967
2	B	0.22	0/5390	0.47	0/7289
3	C	0.17	0/66	0.49	0/89
All	All	0.23	0/12808	0.45	0/17345

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7196	0	7013	129	0
2	B	5294	0	5024	109	0
3	C	65	0	60	1	0
4	D	50	0	43	0	0
4	G	50	0	43	0	0
5	E	28	0	25	0	0
5	H	28	0	25	1	0
5	I	28	0	25	0	0
5	K	28	0	25	2	0
6	F	72	0	61	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	J	39	0	34	0	0
7	L	39	0	34	0	0
8	A	42	0	39	0	0
8	B	28	0	26	2	0
9	A	5	0	0	0	0
9	B	3	0	0	0	0
10	A	3	0	0	0	0
10	B	2	0	0	0	0
All	All	13000	0	12477	237	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 9.

All (237) 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:A:346:PRO:C	1:A:347:LEU:HD23	1.66	1.15
1:A:347:LEU:N	1:A:347:LEU:HD23	1.50	1.08
2:B:27:SER:O	2:B:28:ASP:HB2	1.30	1.07
2:B:30:ALA:O	2:B:31:LEU:HD23	1.61	1.00
1:A:347:LEU:N	1:A:347:LEU:CD2	2.30	0.94
2:B:27:SER:O	2:B:28:ASP:CB	2.16	0.91
2:B:27:SER:HB2	2:B:53:SER:HB2	1.50	0.91
2:B:30:ALA:O	2:B:31:LEU:HB3	1.79	0.83
2:B:28:ASP:O	2:B:29:GLU:HB2	1.77	0.83
2:B:30:ALA:O	2:B:31:LEU:CB	2.30	0.80
2:B:510:SER:HB3	2:B:511:SER:HA	1.65	0.78
2:B:31:LEU:HD12	2:B:31:LEU:O	1.84	0.77
2:B:30:ALA:O	2:B:31:LEU:CD2	2.32	0.76
2:B:455:PHE:HA	2:B:460:CYS:HA	1.69	0.74
1:A:415:ASP:OD1	1:A:415:ASP:N	2.16	0.73
1:A:707:MET:HG2	1:A:934:LYS:H	1.53	0.73
1:A:609:SER:HB2	1:A:630:LYS:HB3	1.70	0.73
1:A:348:GLY:O	1:A:356:ASN:CB	2.36	0.73
2:B:141:GLN:HE21	2:B:345:VAL:HG23	1.53	0.73
1:A:664:ALA:HB3	1:A:695:ALA:HB2	1.73	0.71
1:A:348:GLY:O	1:A:356:ASN:HB3	1.90	0.70
2:B:616:GLU:HG3	2:B:622:ARG:HB3	1.75	0.68
2:B:169:PRO:HD2	2:B:172:ALA:HB2	1.76	0.68
1:A:645:VAL:HB	1:A:679:VAL:HG13	1.78	0.66
1:A:402:PRO:HA	1:A:428:GLY:HA3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:498:ARG:HD3	2:B:516:ILE:HD13	1.77	0.66
1:A:371:GLY:HA3	1:A:404:PHE:HB3	1.78	0.64
1:A:565:TYR:O	1:A:566:ARG:NH1	2.28	0.64
1:A:741:ALA:H	1:A:786:GLY:HA3	1.61	0.64
2:B:417:LYS:NZ	2:B:421:PHE:O	2.29	0.64
2:B:404:ARG:NH1	2:B:550:ASP:OD1	2.28	0.64
1:A:650:GLN:HE21	1:A:704:GLN:HB2	1.62	0.64
2:B:487:SER:HB2	2:B:492:GLN:HB3	1.80	0.63
2:B:292:LEU:HD22	2:B:325:ILE:HD11	1.81	0.63
1:A:348:GLY:O	1:A:356:ASN:HA	2.00	0.61
2:B:28:ASP:O	2:B:29:GLU:CB	2.48	0.61
1:A:348:GLY:O	1:A:356:ASN:CA	2.49	0.61
1:A:725:LYS:HG3	1:A:726:VAL:HG13	1.81	0.61
2:B:473:CYS:SG	2:B:474:SER:N	2.71	0.60
2:B:383:LEU:HG	2:B:385:SER:H	1.66	0.60
1:A:248:ARG:NH1	1:A:272:MET:SD	2.74	0.60
1:A:346:PRO:C	1:A:347:LEU:CD2	2.58	0.60
1:A:345:ALA:O	1:A:347:LEU:HD21	2.02	0.59
1:A:402:PRO:HB3	1:A:429:VAL:HG13	1.85	0.59
2:B:30:ALA:O	2:B:31:LEU:CG	2.51	0.59
2:B:137:LYS:HB3	2:B:341:LEU:HD21	1.85	0.59
2:B:318:TYR:HA	2:B:321:TYR:HB2	1.85	0.58
1:A:3:LEU:HG	1:A:350:LEU:HD21	1.85	0.58
1:A:802:LYS:HG2	1:A:807:THR:HA	1.84	0.58
2:B:134:LEU:O	2:B:137:LYS:N	2.37	0.58
2:B:129:TRP:HZ3	2:B:339:ASN:HD21	1.52	0.58
1:A:395:TRP:HB3	1:A:429:VAL:HG11	1.86	0.57
1:A:543:ARG:NH1	1:A:547:GLU:OE1	2.34	0.57
2:B:411:GLU:HG2	2:B:430:THR:HG22	1.86	0.57
2:B:99:ASN:HD22	8:B:701:NAG:H62	1.69	0.57
1:A:909:MET:HA	1:A:914:GLN:HA	1.87	0.56
1:A:645:VAL:HG22	1:A:715:LEU:HD22	1.88	0.56
2:B:31:LEU:CD1	2:B:31:LEU:O	2.52	0.55
1:A:114:TRP:CD2	1:A:116:THR:HA	2.42	0.55
1:A:114:TRP:CE2	1:A:116:THR:HA	2.41	0.55
2:B:674:SER:HB3	2:B:676:LYS:HG3	1.89	0.55
1:A:397:ALA:HB2	1:A:402:PRO:HD3	1.90	0.54
1:A:913:ASN:ND2	1:A:913:ASN:O	2.40	0.54
2:B:31:LEU:CG	2:B:31:LEU:O	2.55	0.54
2:B:230:THR:HG23	2:B:304:ILE:HD12	1.89	0.54
2:B:288:ASP:OD1	2:B:289:TYR:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:510:SER:H	2:B:511:SER:HB3	1.73	0.54
1:A:450:TYR:HB2	1:A:474:ASN:HB2	1.89	0.54
1:A:253:VAL:HB	1:A:267:PHE:HB2	1.90	0.54
2:B:29:GLU:O	2:B:30:ALA:C	2.47	0.53
1:A:621:ASP:OD1	1:A:622:ASP:N	2.40	0.53
2:B:608:CYS:O	2:B:612:LYS:N	2.41	0.53
2:B:31:LEU:H	2:B:32:PRO:HD3	1.73	0.53
2:B:459:VAL:HG12	2:B:461:ARG:H	1.74	0.53
1:A:315:VAL:HG21	1:A:360:ILE:HD13	1.91	0.52
2:B:620:PHE:HB3	2:B:622:ARG:HE	1.75	0.52
1:A:124:PRO:HB2	1:A:156:GLN:HG2	1.91	0.52
1:A:915:ASN:HA	1:A:953:TRP:CD1	2.44	0.52
1:A:607:GLU:OE1	1:A:632:GLN:NE2	2.42	0.52
2:B:120:LEU:HD12	2:B:188:PHE:HZ	1.75	0.52
2:B:530:ARG:HG2	2:B:535:MET:HA	1.90	0.52
2:B:144:LYS:HG3	2:B:145:LEU:HD13	1.91	0.52
1:A:349:ASP:O	1:A:420:PRO:HG3	2.09	0.52
2:B:580:LYS:HG2	2:B:589:ILE:HD11	1.92	0.52
1:A:906:GLU:O	1:A:910:ASN:ND2	2.42	0.51
2:B:529:VAL:HG11	2:B:556:TYR:HE1	1.76	0.51
1:A:231:PHE:CD2	1:A:231:PHE:N	2.77	0.51
2:B:133:ASN:O	2:B:204:ASN:ND2	2.43	0.51
1:A:801:TYR:HB2	1:A:880:LEU:HB2	1.93	0.51
2:B:494:VAL:HG22	2:B:495:CYS:H	1.75	0.51
1:A:50:ILE:HD12	1:A:89:LYS:HB2	1.93	0.51
1:A:21:PHE:HE1	2:B:266:VAL:HG11	1.75	0.51
2:B:316:ASN:HB3	8:B:702:NAG:H82	1.93	0.51
1:A:345:ALA:O	1:A:347:LEU:CD2	2.59	0.51
1:A:510:ARG:NH2	1:A:553:THR:O	2.25	0.50
2:B:215:ASN:O	3:C:1495:ASP:HB3	2.12	0.50
2:B:50:ALA:N	2:B:51:PRO:HD2	2.27	0.49
1:A:36:LEU:HB2	1:A:59:CYS:HB2	1.94	0.49
1:A:185:SER:HB3	1:A:208:LEU:HB2	1.95	0.49
1:A:104:LYS:HD3	1:A:132:ASP:HB2	1.93	0.49
1:A:649:LEU:HD13	1:A:704:GLN:HG3	1.94	0.49
1:A:232:ASN:ND2	1:A:257:ASP:OD1	2.45	0.49
1:A:24:ASP:OD1	1:A:25:PHE:N	2.45	0.49
1:A:26:PHE:HB2	1:A:37:LEU:HG	1.93	0.49
1:A:513:PHE:HA	1:A:540:ALA:HA	1.95	0.49
1:A:909:MET:HA	1:A:914:GLN:HG3	1.94	0.49
1:A:408:MET:HG2	1:A:424:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:PHE:HA	1:A:389:GLN:HB2	1.95	0.49
2:B:362:LEU:HD12	2:B:363:PRO:HD2	1.94	0.48
2:B:442:GLU:HG3	2:B:443:PRO:HD2	1.95	0.48
1:A:423:ILE:HG12	1:A:434:LEU:HD23	1.94	0.48
2:B:400:GLU:HB2	5:K:1:NAG:H83	1.94	0.48
2:B:358:GLU:N	2:B:417:LYS:O	2.42	0.48
2:B:124:MET:HG2	2:B:251:ASP:HB2	1.95	0.48
1:A:249:THR:HG23	1:A:273:ALA:H	1.79	0.48
1:A:349:ASP:O	1:A:420:PRO:CG	2.61	0.48
1:A:2:ASN:OD1	1:A:2:ASN:N	2.47	0.47
2:B:338:SER:HB3	2:B:342:GLN:HB2	1.96	0.47
2:B:479:ARG:O	2:B:481:SER:N	2.45	0.47
2:B:608:CYS:HB3	2:B:655:CYS:HB3	1.58	0.47
5:K:1:NAG:H62	5:K:2:NAG:H83	1.96	0.47
2:B:116:TYR:HA	2:B:247:VAL:HG13	1.97	0.47
1:A:480:LYS:HB3	1:A:533:MET:HG2	1.96	0.47
2:B:133:ASN:ND2	2:B:137:LYS:HE3	2.29	0.47
2:B:319:GLN:HA	2:B:330:VAL:HG21	1.96	0.47
2:B:66:ASP:HB3	2:B:85:PRO:HB3	1.97	0.47
2:B:134:LEU:O	2:B:138:LEU:N	2.39	0.46
1:A:792:LYS:HB2	1:A:930:GLU:HG2	1.97	0.46
1:A:405:GLY:C	1:A:407:SER:H	2.19	0.46
1:A:243:VAL:HG22	1:A:246:ALA:HB2	1.97	0.46
2:B:158:ASP:HB3	2:B:187:MET:HE1	1.98	0.46
1:A:447:LEU:HD21	1:A:557:ILE:HG22	1.98	0.46
2:B:157:VAL:O	2:B:220:GLU:HG3	2.16	0.46
1:A:108:CYS:HA	1:A:128:CYS:HA	1.98	0.46
2:B:135:GLY:HA2	2:B:138:LEU:HB2	1.97	0.46
1:A:400:MET:HB2	1:A:401:PRO:HD2	1.96	0.45
1:A:24:ASP:HA	1:A:409:LYS:HG2	1.98	0.45
2:B:137:LYS:O	2:B:140:THR:HG22	2.16	0.45
1:A:527:ILE:HG22	1:A:528:SER:H	1.82	0.45
1:A:803:TYR:HB2	1:A:808:LEU:HD11	1.98	0.45
1:A:139:TYR:OH	1:A:186:ASP:OD2	2.31	0.45
1:A:797:LEU:HD23	1:A:882:ILE:HD12	1.98	0.45
1:A:240:VAL:HG22	1:A:255:ILE:HG12	1.98	0.45
2:B:41:LYS:HD2	2:B:41:LYS:HA	1.69	0.45
2:B:590:GLN:CD	2:B:591:PRO:HD2	2.36	0.45
1:A:9:ALA:HB3	1:A:434:LEU:HB3	1.98	0.45
1:A:652:ASP:N	1:A:652:ASP:OD1	2.50	0.45
1:A:472:CYS:HA	1:A:541:TYR:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:SER:HB2	1:A:226:VAL:HG22	1.98	0.45
2:B:305:ASN:HB3	2:B:351:ILE:HD13	1.98	0.45
2:B:371:ASN:HB2	2:B:398:SER:OG	2.17	0.45
1:A:93:TRP:CD1	1:A:111:LEU:HD22	2.52	0.45
2:B:249:THR:HA	2:B:309:ALA:O	2.17	0.45
1:A:494:GLN:HB2	1:A:562:ARG:HB3	1.99	0.45
1:A:769:GLU:HG2	1:A:812:LEU:HD21	1.99	0.44
2:B:133:ASN:HD22	2:B:137:LYS:HE3	1.82	0.44
1:A:352:GLN:O	1:A:484:LYS:NZ	2.49	0.44
2:B:244:HIS:HB2	2:B:304:ILE:HA	1.99	0.44
1:A:350:LEU:HA	1:A:350:LEU:HD12	1.74	0.44
1:A:500:ASP:HB2	1:A:555:ILE:HG23	1.98	0.44
1:A:888:ARG:HD2	1:A:888:ARG:HA	1.73	0.44
1:A:364:TYR:HB3	1:A:369:LYS:HE3	2.00	0.44
2:B:105:ARG:HB2	2:B:394:THR:HG23	1.98	0.44
1:A:398:ARG:HG3	1:A:399:SER:H	1.82	0.44
2:B:125:LYS:HG3	2:B:212:VAL:HG21	1.99	0.44
1:A:175:GLY:HA2	1:A:179:TRP:CD1	2.53	0.44
2:B:21:PRO:HB3	2:B:96:ASP:HB2	2.00	0.44
1:A:799:TRP:HA	1:A:800:PRO:HD3	1.79	0.43
2:B:497:GLN:HB3	2:B:498:ARG:H	1.54	0.43
1:A:783:ARG:HG3	1:A:894:SER:HB2	1.99	0.43
1:A:762:HIS:ND1	1:A:906:GLU:OE1	2.46	0.43
2:B:466:TRP:CD2	2:B:471:CYS:HB3	2.53	0.43
2:B:494:VAL:HG21	2:B:500:GLU:HB2	1.99	0.43
1:A:88:PHE:CE2	1:A:122:ARG:HG2	2.54	0.43
1:A:347:LEU:HD11	1:A:359:ALA:HB2	1.99	0.43
2:B:173:LEU:O	2:B:174:GLU:HB3	2.18	0.43
5:H:1:NAG:H4	5:H:2:NAG:H2	1.83	0.43
1:A:47:GLN:HA	1:A:48:PRO:HD3	1.88	0.43
2:B:462:CYS:HB3	2:B:467:LEU:H	1.83	0.43
2:B:141:GLN:O	2:B:144:LYS:HG2	2.17	0.43
2:B:407:PRO:HB2	2:B:409:GLU:HG2	2.00	0.43
1:A:509:ARG:HH11	1:A:519:PRO:HB2	1.83	0.43
2:B:131:ILE:HA	2:B:131:ILE:HD12	1.87	0.43
2:B:86:GLN:O	2:B:425:LEU:HD12	2.19	0.43
1:A:234:ASP:HB2	1:A:236:ILE:HD12	2.00	0.43
2:B:39:ASP:HB3	2:B:40:LEU:H	1.59	0.43
1:A:747:VAL:HG13	2:B:603:THR:HB	2.01	0.43
1:A:347:LEU:O	1:A:349:ASP:N	2.51	0.43
2:B:70:SER:HB2	2:B:107:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:647:ASP:OD1	2:B:647:ASP:N	2.52	0.43
2:B:188:PHE:CZ	2:B:191:LYS:HE3	2.53	0.42
1:A:364:TYR:O	1:A:369:LYS:HG3	2.19	0.42
1:A:115:ARG:HD3	1:A:115:ARG:O	2.19	0.42
2:B:150:ARG:HG3	2:B:239:ARG:CZ	2.49	0.42
2:B:108:GLU:HG2	2:B:391:ILE:HG22	2.01	0.42
2:B:4:ILE:HD12	2:B:4:ILE:H	1.84	0.42
1:A:346:PRO:HA	1:A:358:ILE:HG13	2.02	0.42
2:B:137:LYS:O	2:B:141:GLN:HG2	2.18	0.42
1:A:68:GLN:HA	1:A:69:PRO:HD3	1.92	0.42
1:A:716:GLN:HB2	1:A:716:GLN:HE21	1.62	0.42
2:B:134:LEU:HA	2:B:134:LEU:HD12	1.92	0.42
1:A:709:THR:O	1:A:736:LEU:HB2	2.20	0.42
1:A:174:PRO:HB2	2:B:262:LEU:HD21	2.02	0.42
2:B:71:ASP:OD1	2:B:71:ASP:N	2.45	0.42
1:A:403:SER:O	1:A:426:ALA:HA	2.20	0.41
1:A:621:ASP:HB2	1:A:787:PRO:HB3	2.02	0.41
2:B:80:VAL:HG11	2:B:110:TYR:HE1	1.85	0.41
1:A:230:ASP:OD1	1:A:234:ASP:O	2.38	0.41
2:B:334:SER:OG	2:B:337:SER:OG	2.37	0.41
1:A:911:LYS:C	1:A:913:ASN:H	2.22	0.41
2:B:406:CYS:HA	2:B:407:PRO:HD3	1.81	0.41
1:A:191:ILE:HA	1:A:204:TYR:CE2	2.54	0.41
1:A:464:PRO:HG2	1:A:467:ALA:HB3	2.01	0.41
2:B:141:GLN:HG3	2:B:142:MET:H	1.85	0.41
1:A:760:TRP:CZ2	1:A:905:THR:HB	2.56	0.41
1:A:112:TYR:O	1:A:124:PRO:HA	2.21	0.41
1:A:373:VAL:HB	1:A:391:LEU:HB2	2.02	0.41
1:A:553:THR:HA	1:A:554:PRO:HD3	1.93	0.41
2:B:283:ALA:HB1	2:B:287:MET:HG2	2.02	0.41
1:A:376:PHE:HB3	1:A:383:LEU:HD11	2.02	0.41
1:A:647:ILE:HD11	1:A:670:PHE:HE1	1.86	0.41
1:A:790:PHE:CZ	1:A:889:LEU:HB2	2.55	0.41
1:A:721:ASN:O	1:A:725:LYS:HE2	2.20	0.41
1:A:755:LEU:HD23	1:A:757:ILE:HD13	2.03	0.41
1:A:781:GLU:HG3	1:A:896:ILE:HG13	2.03	0.41
2:B:495:CYS:HB3	2:B:520:TYR:O	2.21	0.41
2:B:126:ASP:OD1	2:B:126:ASP:N	2.52	0.41
1:A:115:ARG:HA	1:A:121:GLU:HB2	2.03	0.41
1:A:657:VAL:HG21	1:A:663:LEU:HD13	2.03	0.41
1:A:232:ASN:OD1	1:A:232:ASN:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:CYS:HB3	1:A:533:MET:HB2	2.03	0.40
1:A:363:PRO:HA	1:A:404:PHE:O	2.21	0.40
2:B:117:LEU:HA	2:B:117:LEU:HD23	1.95	0.40
2:B:150:ARG:CZ	2:B:239:ARG:HD3	2.51	0.40
2:B:370:PHE:CG	2:B:384:LYS:HG2	2.56	0.40
1:A:673:GLU:O	1:A:676:THR:OG1	2.31	0.40
1:A:797:LEU:HB3	1:A:882:ILE:HB	2.02	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	920/959 (96%)	853 (93%)	65 (7%)	2 (0%)	47 78
2	B	688/692 (99%)	595 (86%)	89 (13%)	4 (1%)	25 63
3	C	6/98 (6%)	5 (83%)	1 (17%)	0	100 100
All	All	1614/1749 (92%)	1453 (90%)	155 (10%)	6 (0%)	34 69

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	28	ASP
2	B	31	LEU
1	A	833	ILE
2	B	457	CYS
1	A	348	GLY
2	B	379	VAL

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	784/813 (96%)	756 (96%)	28 (4%)	35 68
2	B	612/614 (100%)	572 (94%)	40 (6%)	17 48
3	C	6/81 (7%)	5 (83%)	1 (17%)	2 9
All	All	1402/1508 (93%)	1333 (95%)	69 (5%)	25 59

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	ARG
1	A	117	GLU
1	A	142	CYS
1	A	249	THR
1	A	275	TYR
1	A	283	THR
1	A	312	VAL
1	A	329	THR
1	A	347	LEU
1	A	415	ASP
1	A	463	LEU
1	A	527	ILE
1	A	532	LEU
1	A	567	THR
1	A	650	GLN
1	A	656	VAL
1	A	657	VAL
1	A	672	THR
1	A	679	VAL
1	A	680	VAL
1	A	694	LEU
1	A	716	GLN
1	A	762	HIS
1	A	834	LYS
1	A	874	CYS
1	A	913	ASN

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Mol	Chain	Res	Type
1	A	916	HIS
1	A	938	ILE
2	B	31	LEU
2	B	40	LEU
2	B	42	GLU
2	B	44	LEU
2	B	116	TYR
2	B	128	LEU
2	B	140	THR
2	B	168	SER
2	B	179	ASP
2	B	182	THR
2	B	212	VAL
2	B	215	ASN
2	B	220	GLU
2	B	316	ASN
2	B	321	TYR
2	B	340	VAL
2	B	342	GLN
2	B	376	ASN
2	B	448	CYS
2	B	460	CYS
2	B	462	CYS
2	B	466	TRP
2	B	467	LEU
2	B	470	GLN
2	B	472	GLU
2	B	485	GLU
2	B	501	CYS
2	B	509	HIS
2	B	512	ASP
2	B	561	THR
2	B	562	THR
2	B	589	ILE
2	B	590	GLN
2	B	608	CYS
2	B	622	ARG
2	B	645	LEU
2	B	647	ASP
2	B	648	THR
2	B	653	VAL
2	B	662	ASP

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Mol	Chain	Res	Type
3	C	1493	ARG

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

Mol	Chain	Res	Type
1	A	650	GLN
2	B	141	GLN

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

28 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	D	1	1,4	14,14,15	0.56	0	17,19,21	0.46	0
4	NAG	D	2	4	14,14,15	0.18	0	17,19,21	0.39	0
4	BMA	D	3	4	11,11,12	0.62	0	15,15,17	0.74	0
4	MAN	D	4	4	11,11,12	0.72	0	15,15,17	1.05	2 (13%)
5	NAG	E	1	1,5	14,14,15	0.24	0	17,19,21	0.41	0
5	NAG	E	2	5	14,14,15	0.23	0	17,19,21	0.41	0
6	NAG	F	1	1,6	14,14,15	0.31	0	17,19,21	0.39	0
6	NAG	F	2	6	14,14,15	0.20	0	17,19,21	0.45	0
6	BMA	F	3	6	11,11,12	0.69	0	15,15,17	0.73	0
6	BMA	F	4	6	11,11,12	1.34	3 (27%)	15,15,17	1.15	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	MAN	F	5	6	11,11,12	0.72	0	15,15,17	1.01	2 (13%)
6	MAN	F	6	6	11,11,12	0.69	0	15,15,17	1.07	2 (13%)
4	NAG	G	1	1,4	14,14,15	0.37	0	17,19,21	0.40	0
4	NAG	G	2	4	14,14,15	0.33	0	17,19,21	0.40	0
4	BMA	G	3	4	11,11,12	0.80	0	15,15,17	0.99	2 (13%)
4	MAN	G	4	4	11,11,12	0.82	0	15,15,17	1.02	1 (6%)
5	NAG	H	1	1,5	14,14,15	0.19	0	17,19,21	0.45	0
5	NAG	H	2	5	14,14,15	0.25	0	17,19,21	0.38	0
5	NAG	I	1	1,5	14,14,15	0.28	0	17,19,21	0.49	0
5	NAG	I	2	5	14,14,15	0.52	0	17,19,21	0.68	1 (5%)
7	NAG	J	1	1,7	14,14,15	0.25	0	17,19,21	0.45	0
7	NAG	J	2	7	14,14,15	0.76	1 (7%)	17,19,21	0.91	1 (5%)
7	BMA	J	3	7	11,11,12	1.23	2 (18%)	15,15,17	1.81	4 (26%)
5	NAG	K	1	2,5	14,14,15	0.25	0	17,19,21	0.39	0
5	NAG	K	2	5	14,14,15	0.74	1 (7%)	17,19,21	0.91	1 (5%)
7	NAG	L	1	2,7	14,14,15	0.29	0	17,19,21	0.46	0
7	NAG	L	2	7	14,14,15	0.71	1 (7%)	17,19,21	0.89	1 (5%)
7	BMA	L	3	7	11,11,12	0.78	0	15,15,17	1.23	2 (13%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	G	3	4	-	1/2/19/22	0/1/1/1
4	MAN	G	4	4	-	2/2/19/22	0/1/1/1
5	NAG	H	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	1/6/23/26	0/1/1/1
5	NAG	I	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
7	NAG	J	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	2/6/23/26	0/1/1/1
7	BMA	J	3	7	-	1/2/19/22	0/1/1/1
5	NAG	K	1	2,5	-	1/6/23/26	0/1/1/1
5	NAG	K	2	5	-	4/6/23/26	0/1/1/1
7	NAG	L	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	L	2	7	-	2/6/23/26	0/1/1/1
7	BMA	L	3	7	-	1/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	3	BMA	C2-C3	2.87	1.56	1.52
6	F	4	BMA	C4-C5	2.69	1.58	1.53
5	K	2	NAG	O5-C1	2.54	1.47	1.43
6	F	4	BMA	O5-C1	-2.41	1.39	1.43
7	J	3	BMA	C1-C2	2.40	1.57	1.52
7	L	2	NAG	O5-C1	2.37	1.47	1.43
7	J	2	NAG	O5-C1	2.31	1.47	1.43
6	F	4	BMA	C4-C3	2.06	1.57	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	J	3	BMA	C1-C2-C3	4.34	115.00	109.67
5	K	2	NAG	C1-O5-C5	3.47	116.90	112.19
7	J	2	NAG	C1-O5-C5	3.42	116.83	112.19
7	L	2	NAG	C1-O5-C5	3.38	116.77	112.19
7	J	3	BMA	O5-C1-C2	3.26	115.81	110.77
7	L	3	BMA	C1-O5-C5	2.73	115.89	112.19
5	I	2	NAG	C1-O5-C5	2.51	115.59	112.19
7	J	3	BMA	C2-C3-C4	2.36	114.97	110.89
4	G	4	MAN	O2-C2-C3	-2.33	105.47	110.14
4	D	4	MAN	O2-C2-C3	-2.31	105.51	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	4	BMA	C3-C4-C5	2.30	114.34	110.24
4	G	3	BMA	C1-C2-C3	-2.27	106.88	109.67
4	G	3	BMA	O3-C3-C2	2.26	114.32	109.99
6	F	5	MAN	O2-C2-C3	-2.25	105.63	110.14
7	J	3	BMA	O5-C5-C4	-2.23	105.41	110.83
6	F	6	MAN	O2-C2-C3	-2.21	105.71	110.14
7	L	3	BMA	O5-C1-C2	2.19	114.16	110.77
6	F	6	MAN	C1-O5-C5	2.18	115.14	112.19
4	D	4	MAN	C1-O5-C5	2.03	114.94	112.19
6	F	5	MAN	C1-O5-C5	2.02	114.94	112.19
6	F	4	BMA	C2-C3-C4	2.02	114.39	110.89

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	2	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
7	L	1	NAG	O5-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
7	L	2	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
6	F	3	BMA	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	G	4	MAN	O5-C5-C6-O6
7	J	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
7	L	2	NAG	O5-C5-C6-O6
7	L	1	NAG	C4-C5-C6-O6
5	I	2	NAG	C8-C7-N2-C2
5	I	2	NAG	O7-C7-N2-C2
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
5	K	2	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
7	J	2	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
4	G	4	MAN	C4-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	L	3	BMA	O5-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6
7	J	3	BMA	O5-C5-C6-O6
6	F	6	MAN	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
6	F	3	BMA	C4-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6

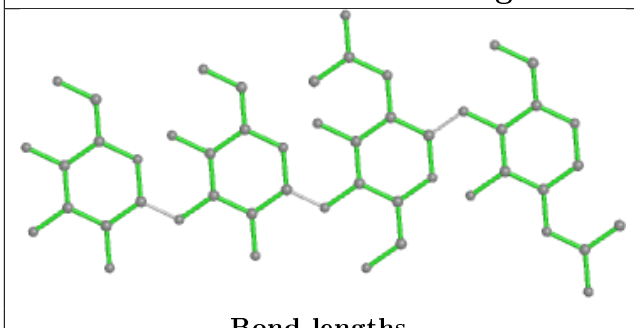
There are no ring outliers.

4 monomers are involved in 3 short contacts:

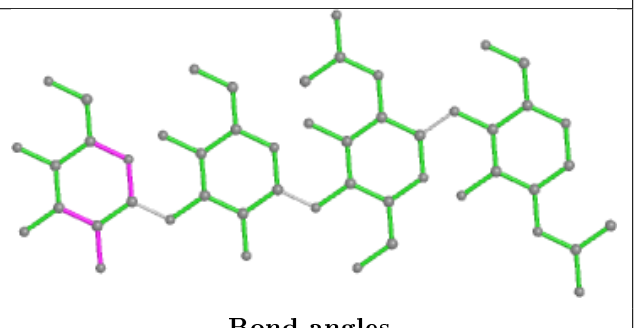
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1	NAG	1	0
5	H	2	NAG	1	0
5	K	1	NAG	2	0
5	K	2	NAG	1	0

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

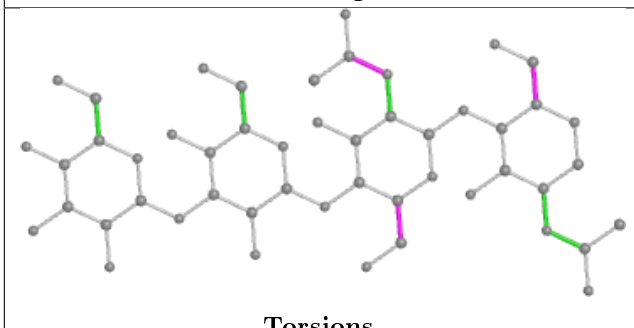
Oligosaccharide Chain D



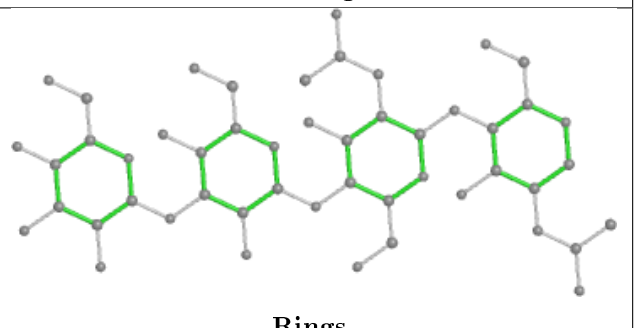
Bond lengths



Bond angles

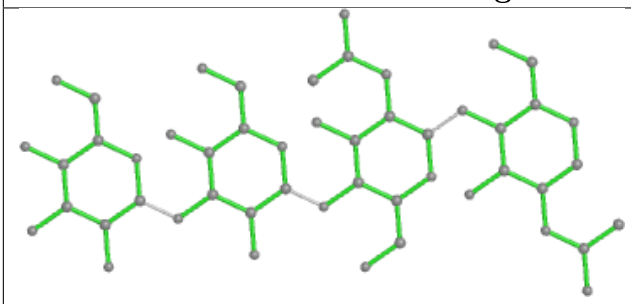


Torsions

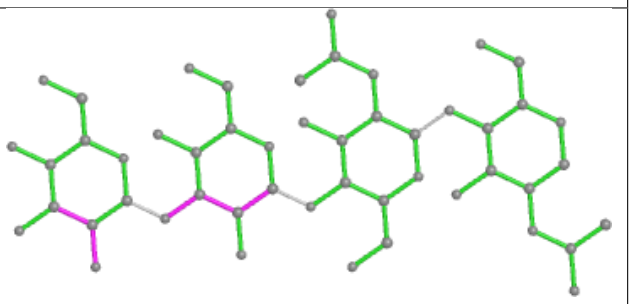


Rings

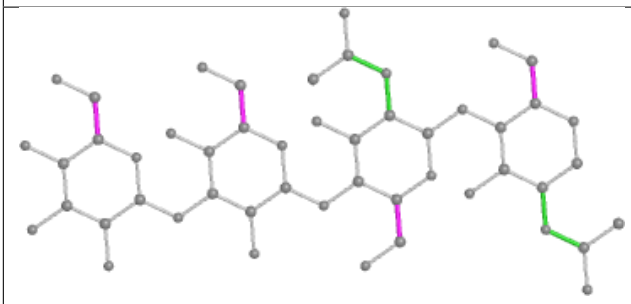
Oligosaccharide Chain G



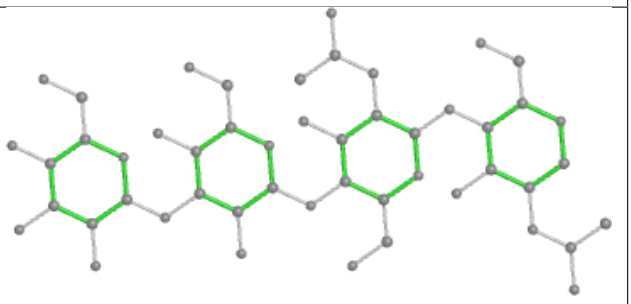
Bond lengths



Bond angles

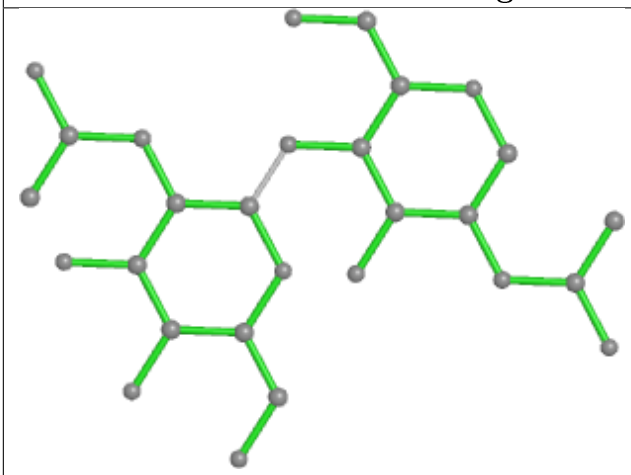


Torsions

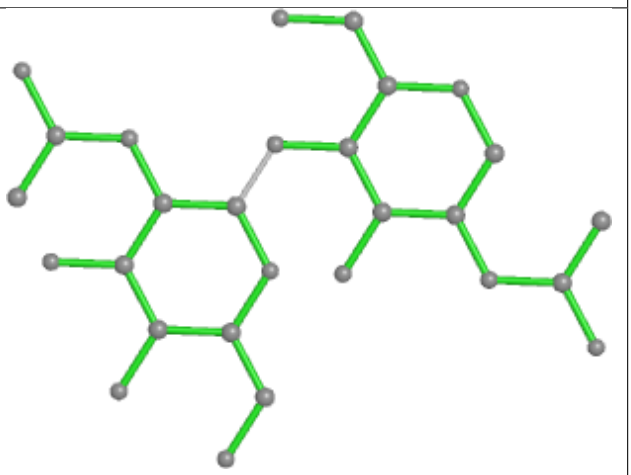


Rings

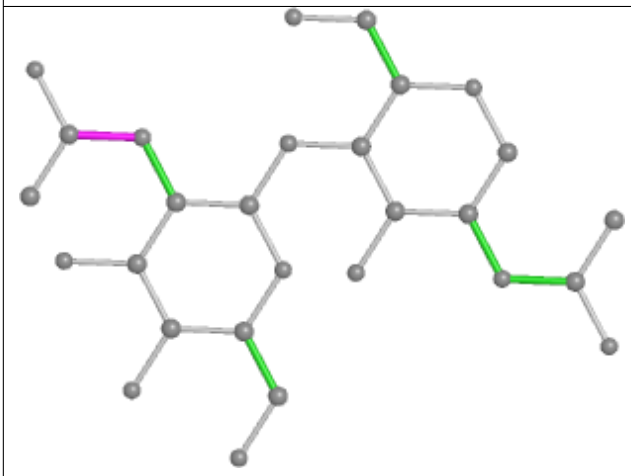
Oligosaccharide Chain E



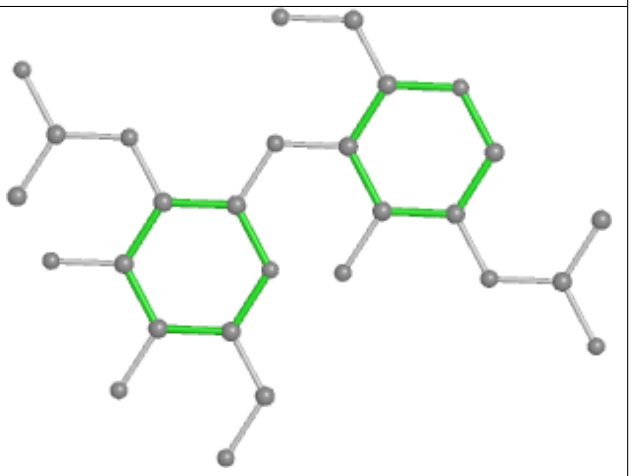
Bond lengths



Bond angles

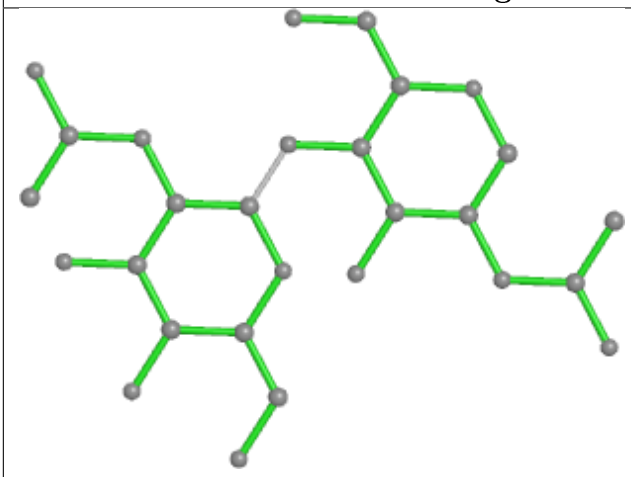


Torsions

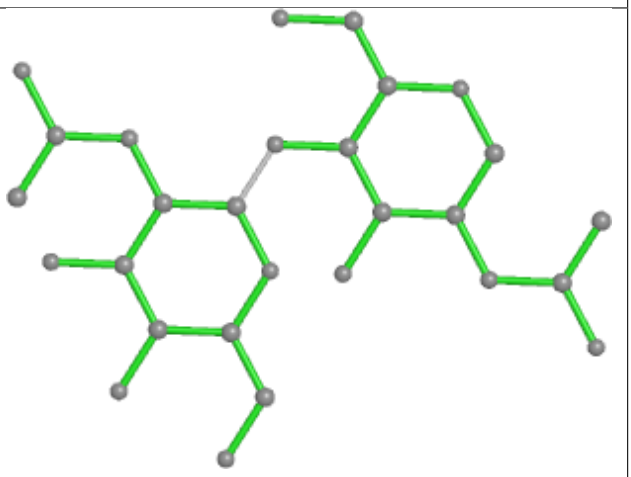


Rings

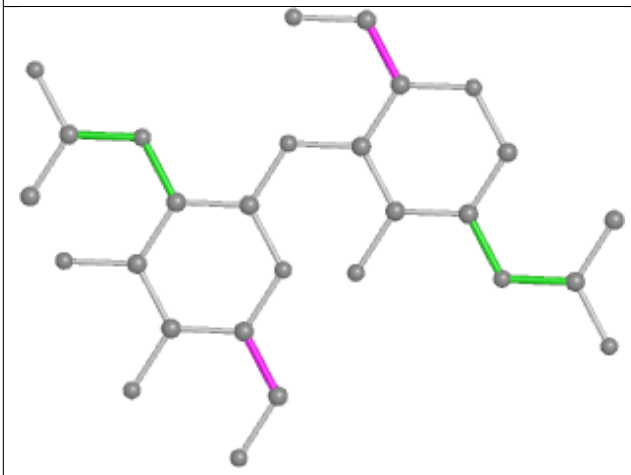
Oligosaccharide Chain H



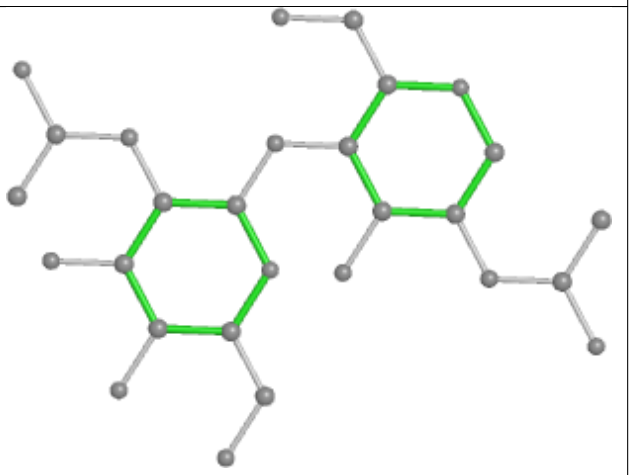
Bond lengths



Bond angles

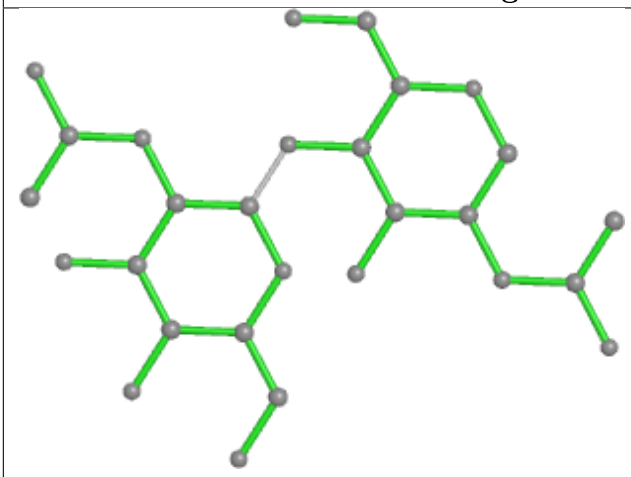


Torsions

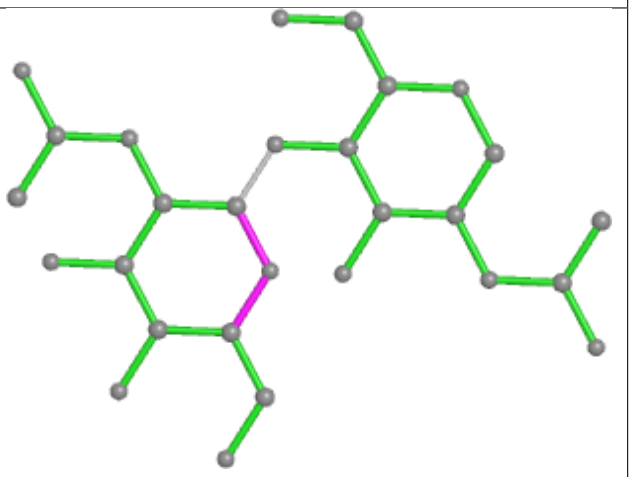


Rings

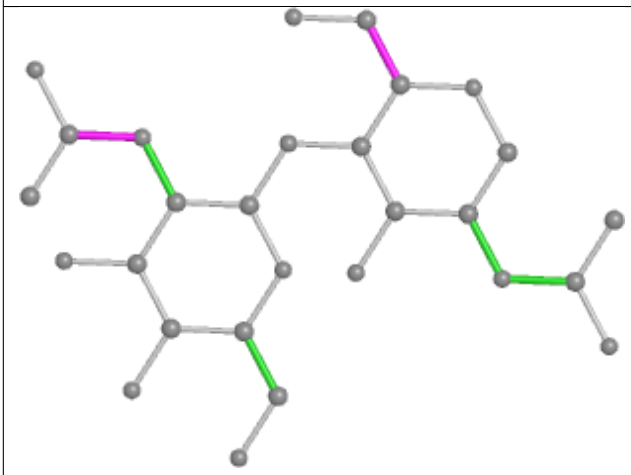
Oligosaccharide Chain I



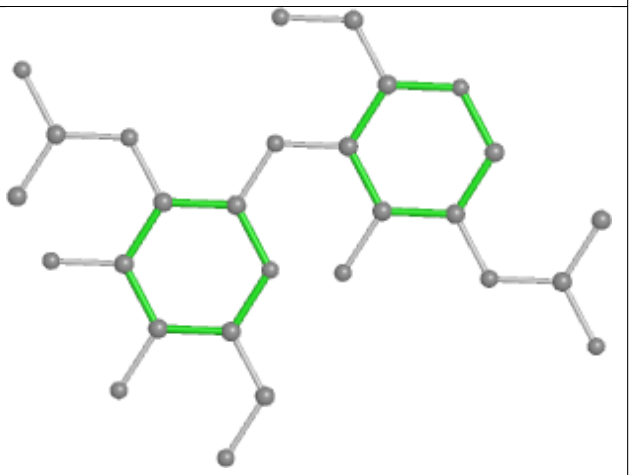
Bond lengths



Bond angles

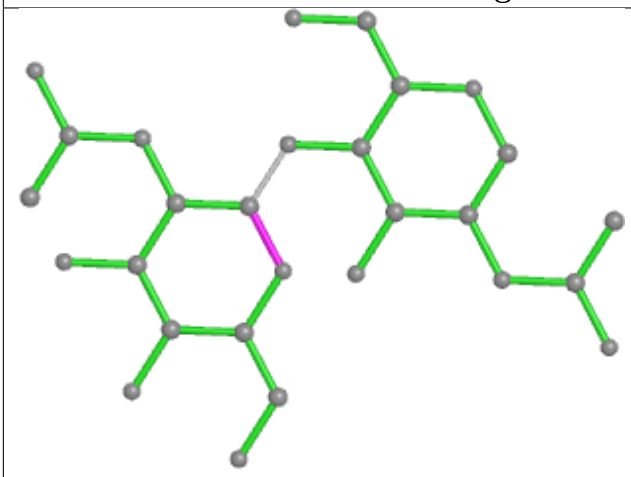


Torsions

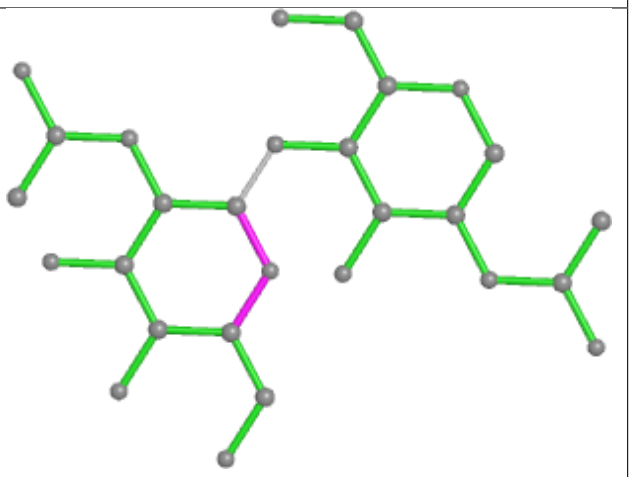


Rings

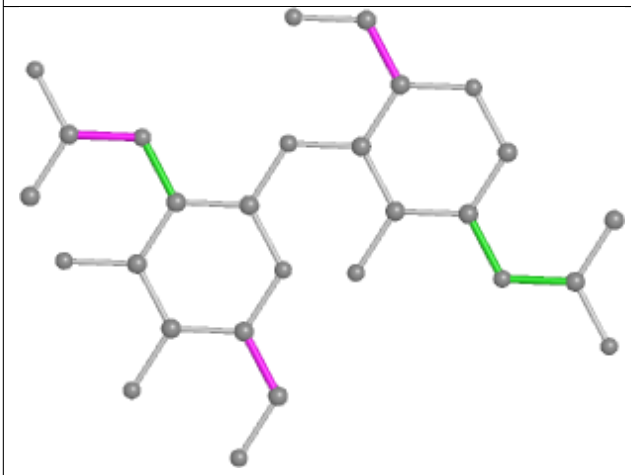
Oligosaccharide Chain K



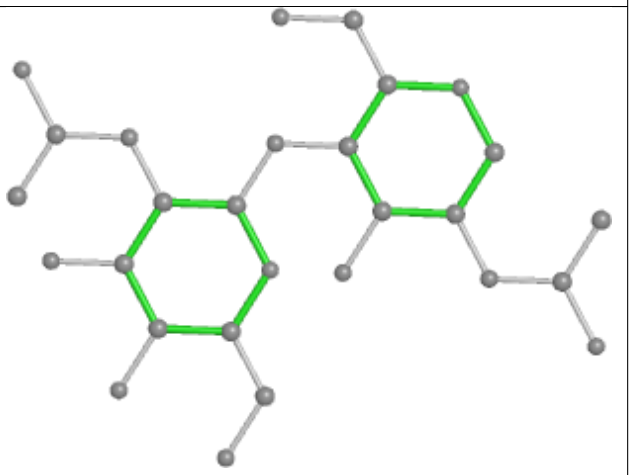
Bond lengths



Bond angles

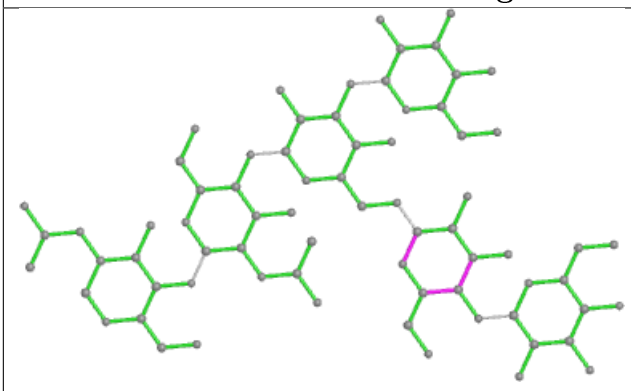


Torsions

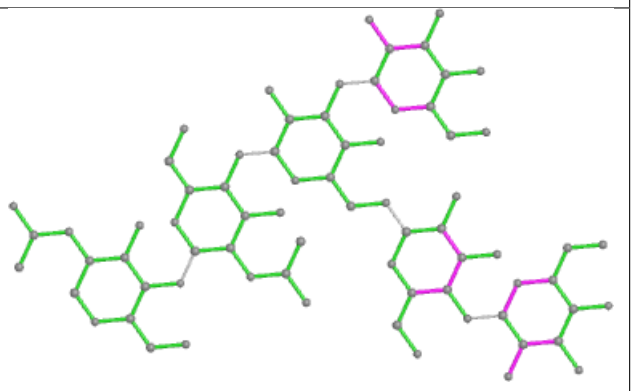


Rings

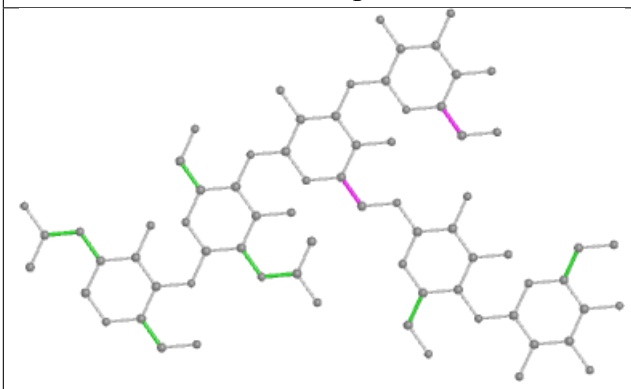
Oligosaccharide Chain F



Bond lengths



Bond angles



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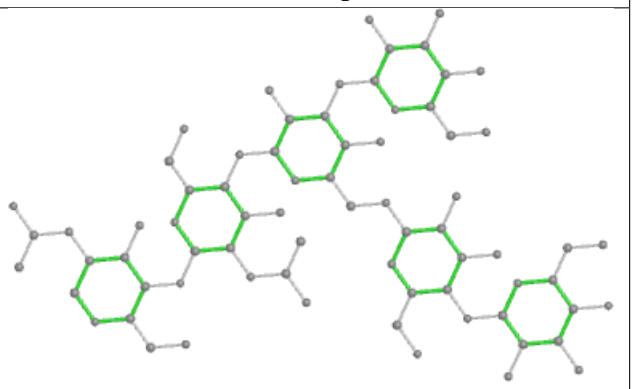
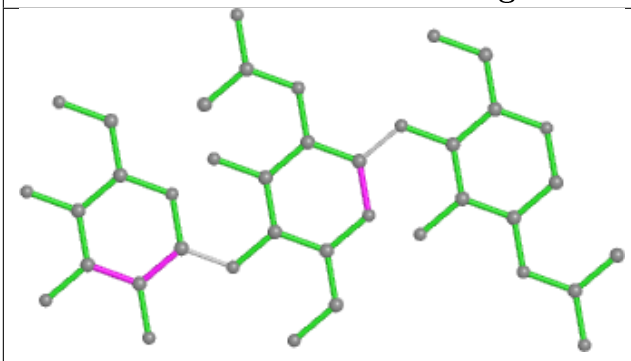
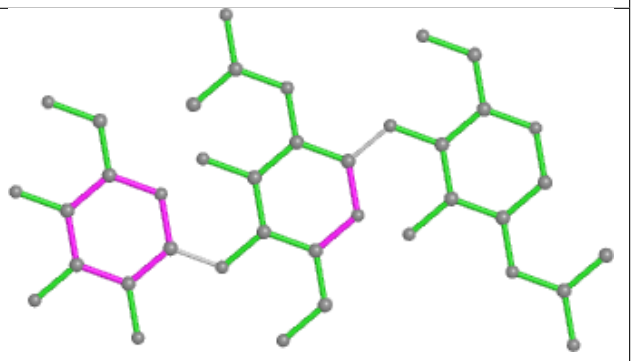


Rings

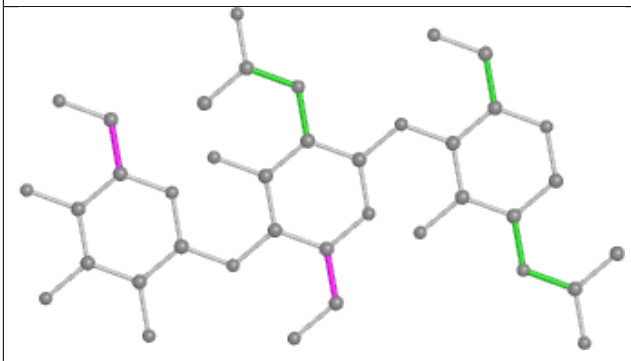
Oligosaccharide Chain J



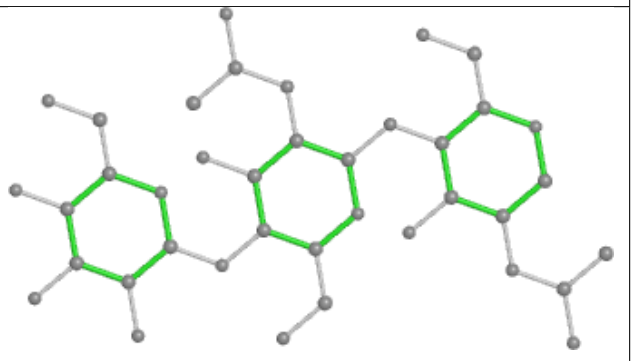
Bond lengths



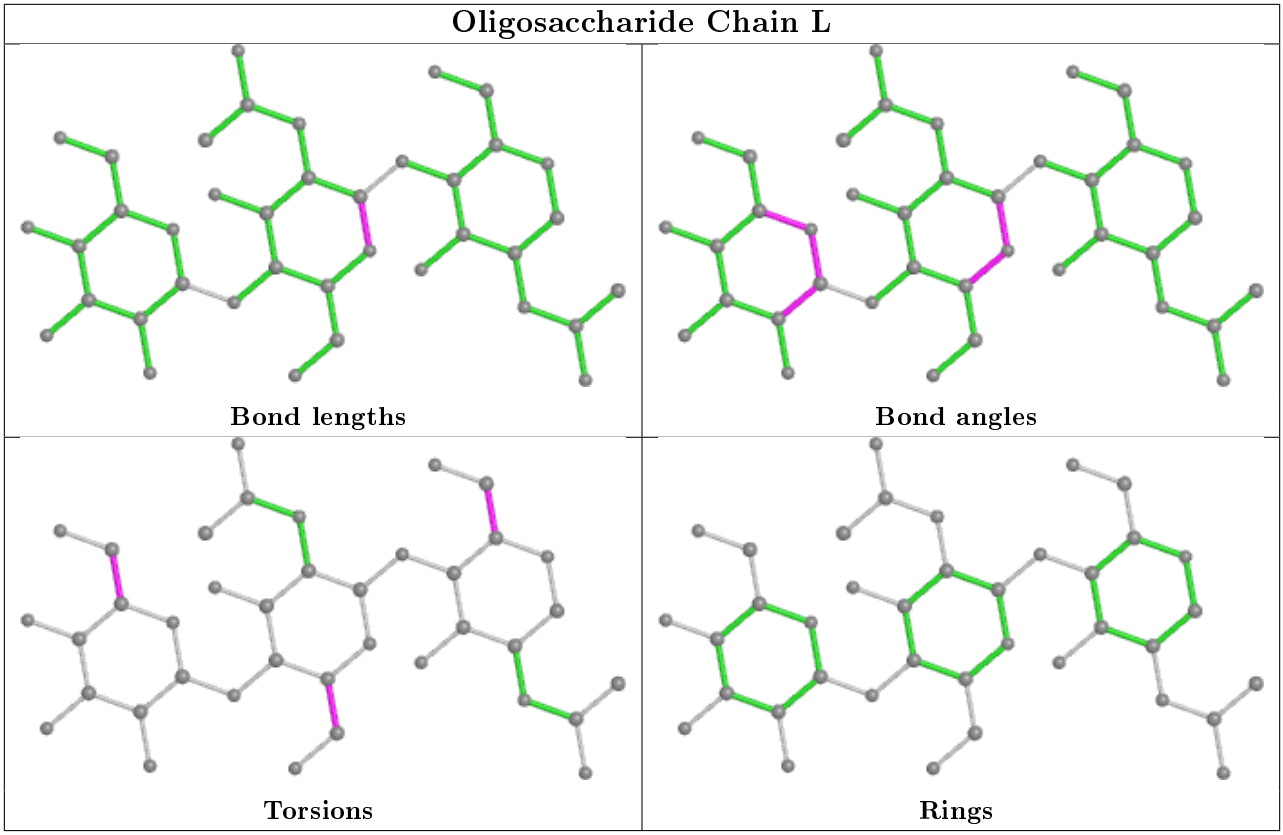
Bond angles



Torsions



Rings



5.6 Ligand geometry

Of 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 for Mogul analysis.

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	$\#\|Z\| > 2$
8	NAG	A	1021	1	14,14,15	0.23	0	17,19,21	0.42	0
8	NAG	B	702	2	14,14,15	0.34	0	17,19,21	0.47	0
8	NAG	A	1020	1	14,14,15	0.25	0	17,19,21	0.46	0
8	NAG	B	701	2	14,14,15	0.71	1 (7%)	17,19,21	0.82	1 (5%)
8	NAG	A	1017	1	14,14,15	0.26	0	17,19,21	0.44	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
8	NAG	A	1021	1	-	0/6/23/26	0/1/1/1
8	NAG	B	702	2	-	2/6/23/26	0/1/1/1
8	NAG	A	1020	1	-	1/6/23/26	0/1/1/1
8	NAG	B	701	2	-	1/6/23/26	0/1/1/1
8	NAG	A	1017	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	701	NAG	O5-C1	2.40	1.47	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	701	NAG	C1-O5-C5	3.14	116.45	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	702	NAG	O5-C5-C6-O6
8	A	1017	NAG	O5-C5-C6-O6
8	B	701	NAG	O5-C5-C6-O6
8	B	702	NAG	C4-C5-C6-O6
8	A	1020	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	702	NAG	1	0
8	B	701	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	924/959 (96%)	0.14	25 (2%) 54 39	56, 105, 149, 190	0
2	B	690/692 (99%)	0.39	62 (8%) 9 5	58, 118, 211, 259	1 (0%)
3	C	8/98 (8%)	1.70	3 (37%) 0 0	99, 135, 152, 157	0
All	All	1622/1749 (92%)	0.25	90 (5%) 25 13	56, 110, 186, 259	1 (0%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	452	ASN	11.6
2	B	443	PRO	8.4
2	B	456	GLU	7.1
2	B	37	ARG	6.9
2	B	36	PRO	6.9
2	B	454	THR	6.4
2	B	35	SER	5.8
2	B	442	GLU	5.6
2	B	453	GLY	5.5
2	B	459	VAL	4.8
2	B	464	PRO	4.3
2	B	440	GLN	4.3
2	B	474	SER	4.1
2	B	455	PHE	4.1
2	B	444	ASN	3.8
1	A	907	THR	3.7
2	B	29	GLU	3.6
1	A	705	SER	3.6
1	A	570	ASP	3.5
2	B	461	ARG	3.5
3	C	1497	ASN	3.4
3	C	1491	ILE	3.4
2	B	481	SER	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	25	TRP	3.3
2	B	671	GLU	3.3
2	B	41	LYS	3.3
2	B	50	ALA	3.2
2	B	451	GLY	3.2
2	B	446	HIS	3.2
2	B	441	ALA	3.1
2	B	644	GLU	3.1
2	B	55	GLU	3.1
2	B	28	ASP	3.1
2	B	449	ASN	3.1
1	A	475	VAL	3.1
1	A	704	GLN	3.0
2	B	482	GLN	3.0
2	B	475	GLU	2.9
1	A	785	ASN	2.9
2	B	46	LYS	2.9
2	B	39	ASP	2.8
1	A	767	GLU	2.8
1	A	567	THR	2.7
2	B	514	GLY	2.7
2	B	49	CYS	2.6
2	B	56	PHE	2.5
1	A	522	SER	2.5
2	B	26	CYS	2.5
2	B	480	PRO	2.5
2	B	53	SER	2.5
1	A	955	ILE	2.5
1	A	647	ILE	2.5
2	B	33	LEU	2.5
3	C	1490	VAL	2.5
1	A	497	LEU	2.4
2	B	509	HIS	2.4
2	B	458	GLY	2.4
2	B	445	SER	2.4
1	A	474	ASN	2.4
1	A	472	CYS	2.4
2	B	501	CYS	2.4
2	B	40	LEU	2.4
2	B	436	ALA	2.4
1	A	569	ALA	2.3
2	B	557	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	670	TYR	2.3
2	B	485	GLU	2.3
2	B	44	LEU	2.3
2	B	432	ASP	2.3
2	B	447	ARG	2.3
2	B	51	PRO	2.2
2	B	438	GLN	2.2
1	A	571	THR	2.2
2	B	134	LEU	2.2
1	A	619	ILE	2.2
2	B	47	ASP	2.1
1	A	625	LEU	2.1
2	B	463	GLY	2.1
1	A	703	GLN	2.1
2	B	34	GLY	2.1
2	B	556	TYR	2.1
1	A	538	LEU	2.1
2	B	54	ILE	2.1
1	A	532	LEU	2.1
2	B	460	CYS	2.1
2	B	499	GLY	2.0
1	A	491	LEU	2.0
1	A	572	THR	2.0
1	A	768	THR	2.0
1	A	606	LEU	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	BMA	J	3	11/12	0.16	0.34	173,182,211,217	0
7	NAG	J	2	14/15	0.71	0.29	170,192,209,217	0
4	BMA	G	3	11/12	0.72	0.34	169,184,221,228	0

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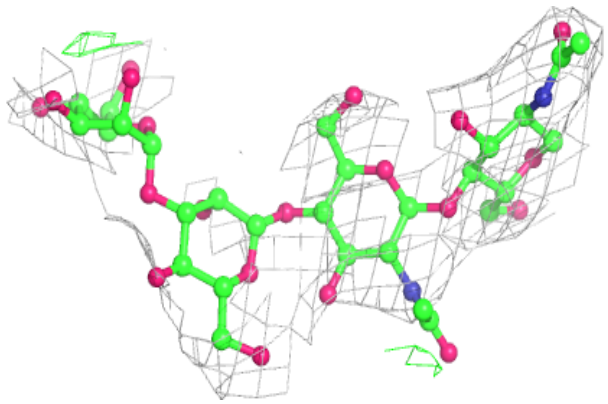
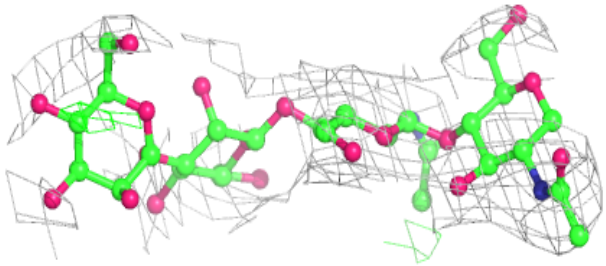
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MAN	D	4	11/12	0.77	0.15	197,201,203,205	0
6	MAN	F	5	11/12	0.77	0.28	147,171,182,182	0
4	MAN	G	4	11/12	0.78	0.38	172,186,195,200	0
4	BMA	D	3	11/12	0.80	0.16	175,189,196,198	0
6	BMA	F	4	11/12	0.82	0.17	136,153,183,190	0
7	BMA	L	3	11/12	0.83	0.15	119,129,139,140	0
4	NAG	G	2	14/15	0.84	0.36	127,164,185,190	0
5	NAG	E	2	14/15	0.84	0.31	153,173,179,180	0
5	NAG	K	2	14/15	0.84	0.18	126,167,175,177	0
5	NAG	H	2	14/15	0.85	0.23	119,145,151,154	0
4	NAG	D	2	14/15	0.87	0.24	139,158,180,182	0
6	MAN	F	6	11/12	0.87	0.14	126,154,167,169	0
6	BMA	F	3	11/12	0.88	0.13	135,145,154,155	0
4	NAG	G	1	14/15	0.89	0.14	86,118,158,166	0
5	NAG	I	2	14/15	0.90	0.17	144,178,183,183	0
5	NAG	H	1	14/15	0.91	0.15	128,152,163,163	0
5	NAG	K	1	14/15	0.92	0.17	94,123,132,149	0
5	NAG	E	1	14/15	0.92	0.19	111,141,164,166	0
7	NAG	L	2	14/15	0.93	0.18	109,115,128,129	0
7	NAG	J	1	14/15	0.93	0.14	86,127,138,145	0
5	NAG	I	1	14/15	0.94	0.11	107,133,152,163	0
4	NAG	D	1	14/15	0.95	0.16	69,87,110,126	0
6	NAG	F	2	14/15	0.96	0.17	66,89,109,133	0
7	NAG	L	1	14/15	0.96	0.21	85,104,125,128	0
6	NAG	F	1	14/15	0.97	0.14	52,69,101,106	0

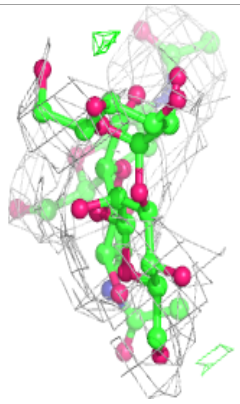
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

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

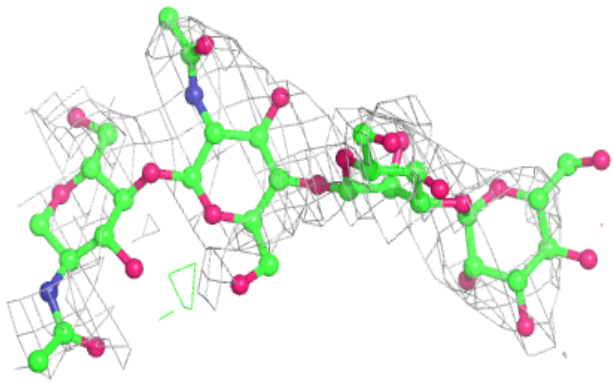


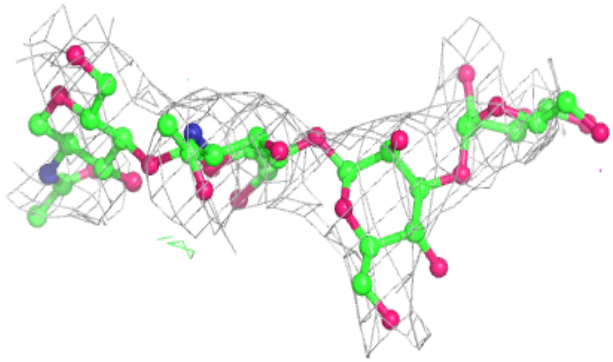


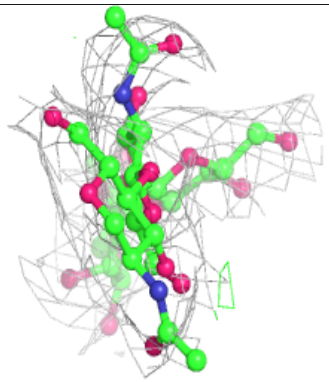


Electron density around Chain G:

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

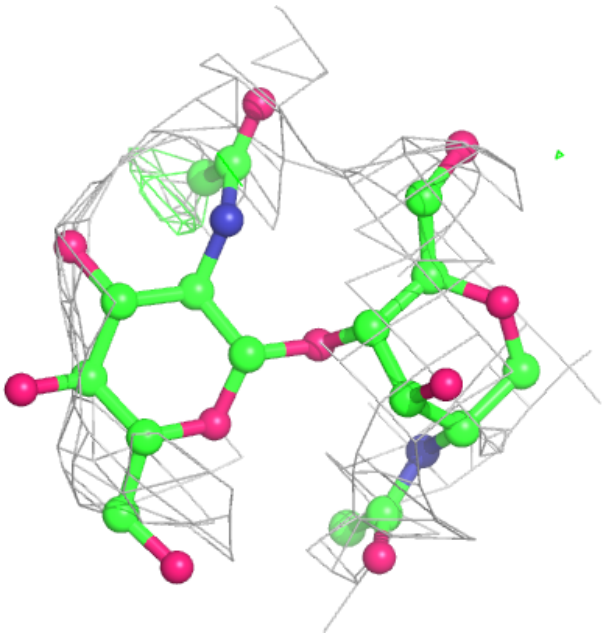


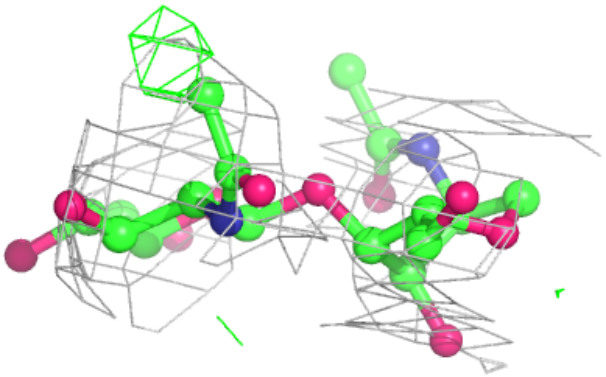


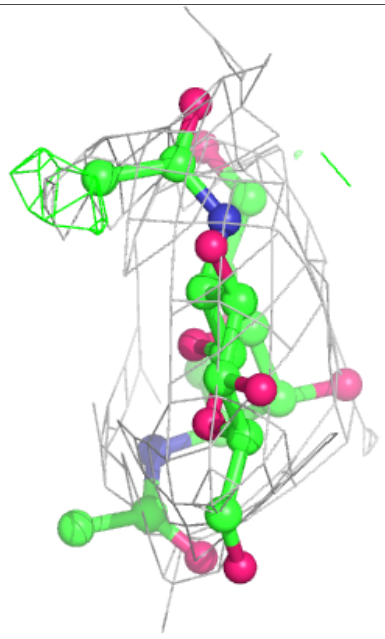


Electron density around Chain E:

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

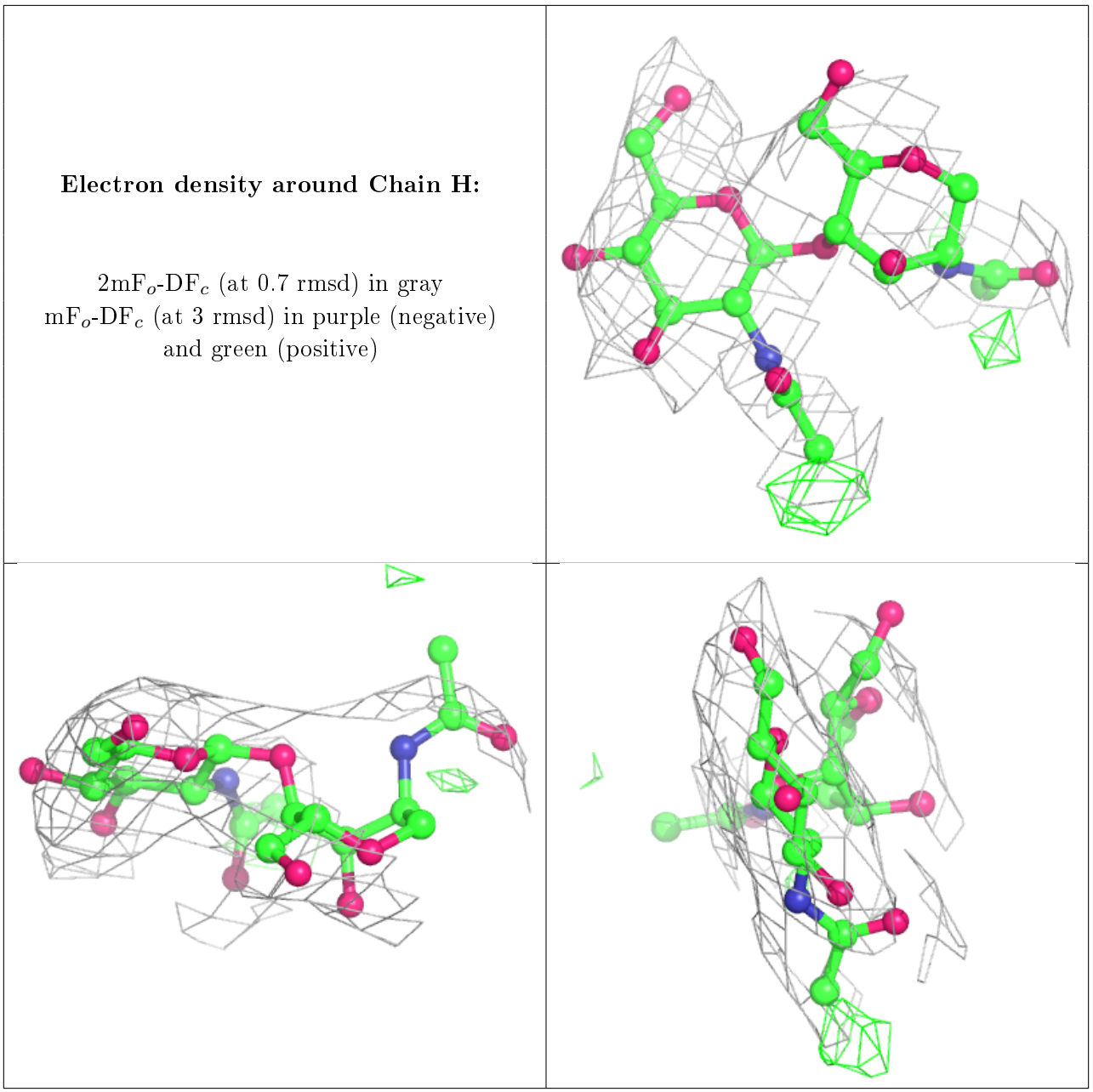






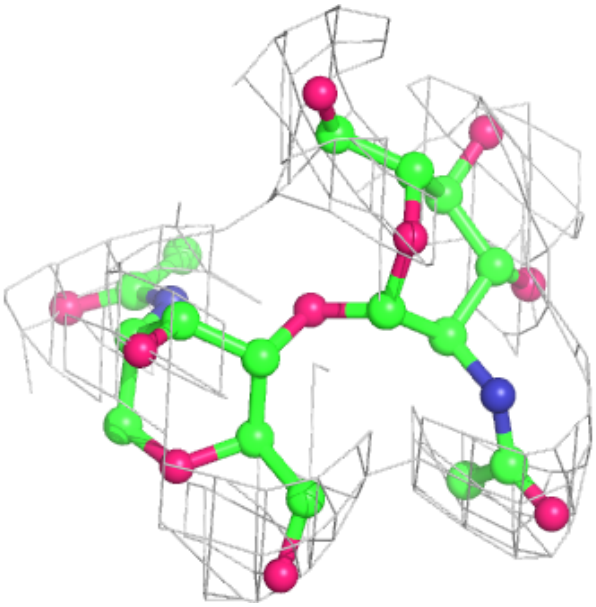
Electron density around Chain H:

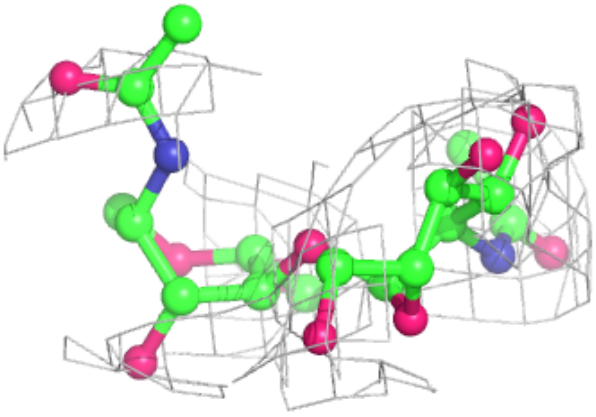
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

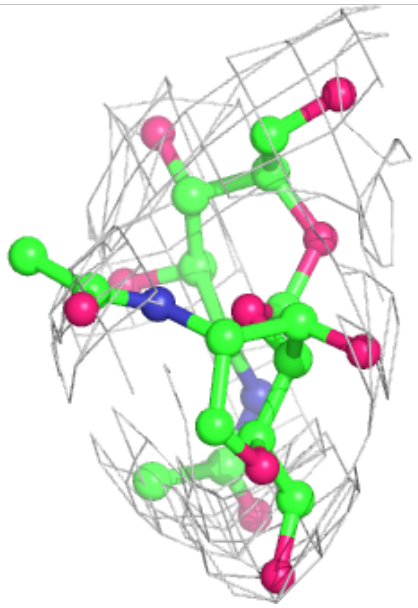


Electron density around Chain I:

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

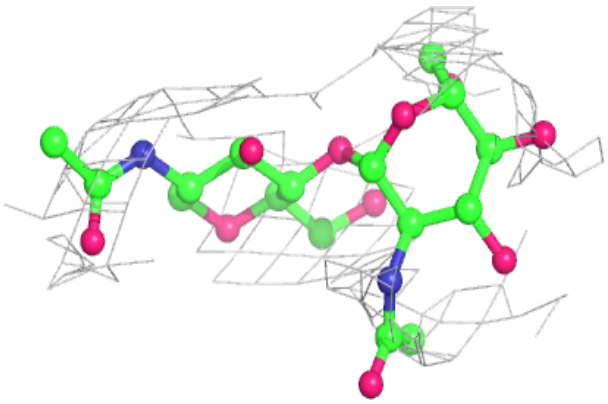


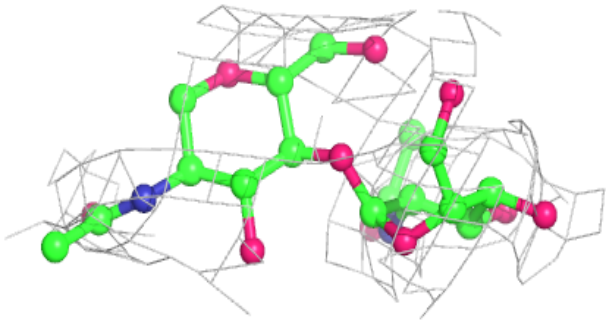


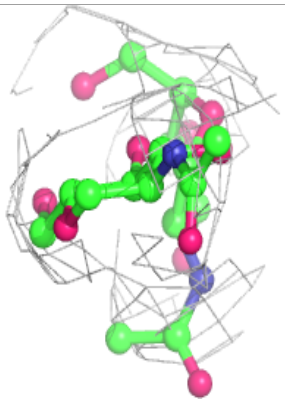


Electron density around Chain K:

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

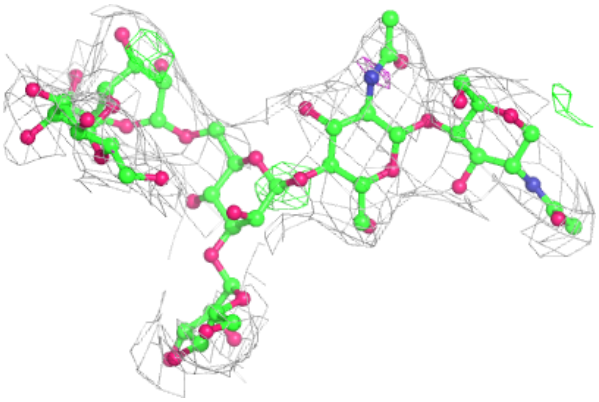


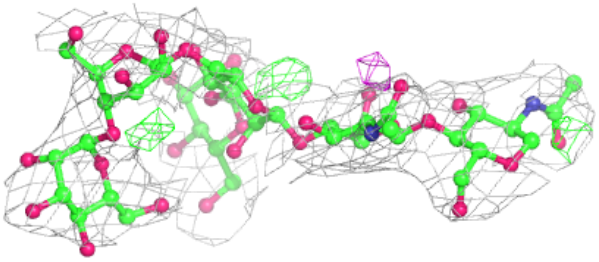


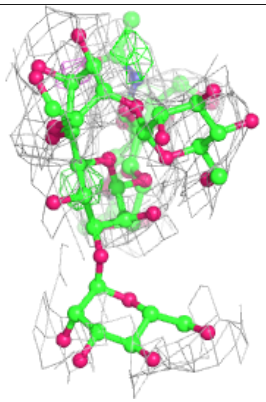


Electron density around Chain F:

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

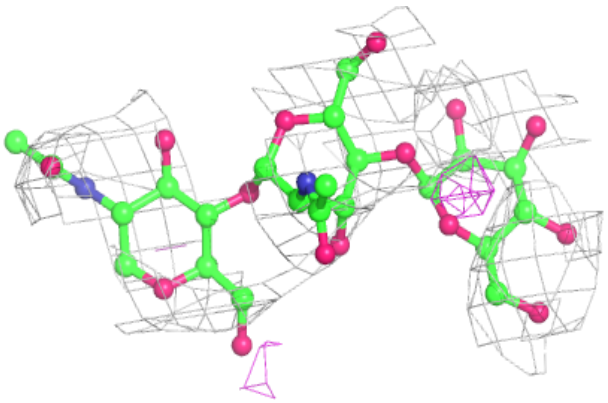


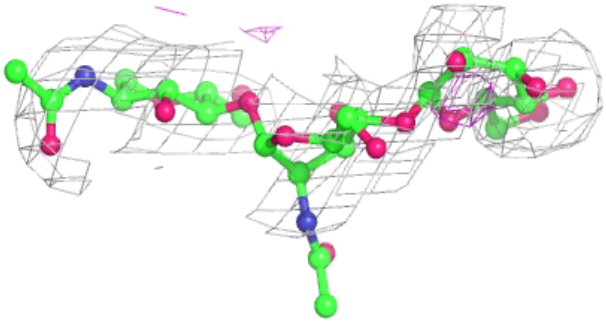


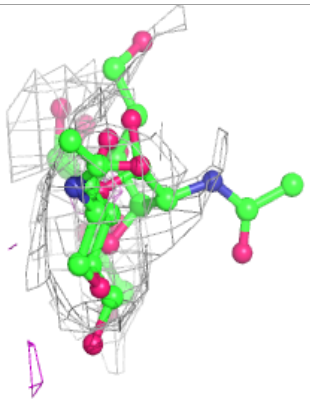


Electron density around Chain J:

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

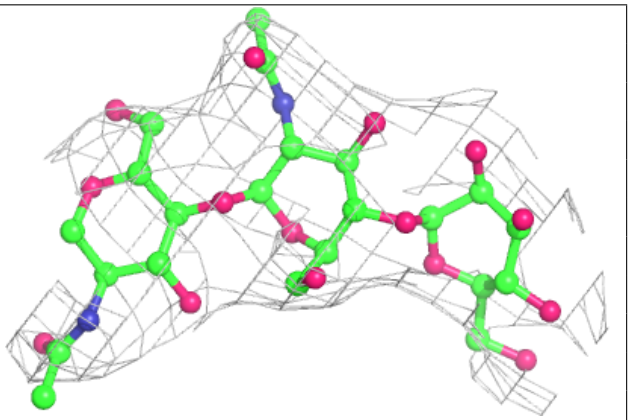


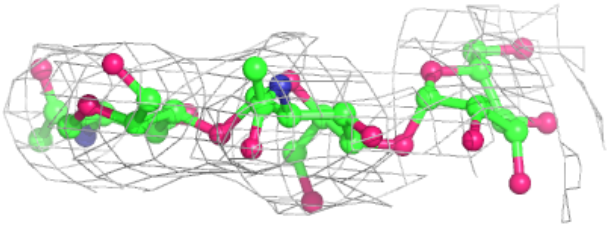


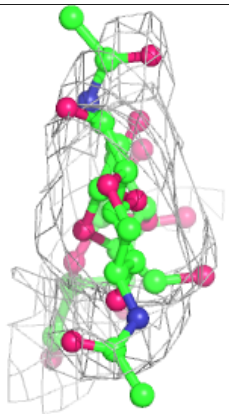


Electron density around Chain L:

$2mF_o$-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
8	NAG	A	1020	14/15	0.67	0.26	156,182,185,188	0
8	NAG	A	1017	14/15	0.68	0.45	143,167,187,187	0
8	NAG	B	701	14/15	0.79	0.39	123,162,179,180	0
8	NAG	A	1021	14/15	0.84	0.26	92,119,132,144	0
9	MN	B	709	1/1	0.91	0.10	115,115,115,115	0
8	NAG	B	702	14/15	0.93	0.16	95,128,144,150	0
9	MN	B	710	1/1	0.93	0.23	99,99,99,99	0
9	MN	A	1028	1/1	0.94	0.06	123,123,123,123	0
9	MN	A	1031	1/1	0.96	0.11	111,111,111,111	0
9	MN	A	1029	1/1	0.96	0.15	131,131,131,131	0
9	MN	A	1030	1/1	0.97	0.11	123,123,123,123	0
9	MN	A	1027	1/1	0.98	0.14	141,141,141,141	0
9	MN	B	708	1/1	1.00	0.15	65,65,65,65	0

6.5 Other polymers

There are no such residues in this entry.