Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2024 – 05:25 pm GMT

PDB ID	:	5MZO
Title	:	UDP-Glucose Glycoprotein Glucosyltransferase from Chaetomium thermophilum (open conformation)
Authors	:	Roversi, P.; Caputo, A.T.; Hill, J.; Alonzi, D.S.; Zitzmann, N.
Deposited on	:	2017-02-01
Resolution	:	3.48 Å(reported)

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

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

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

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

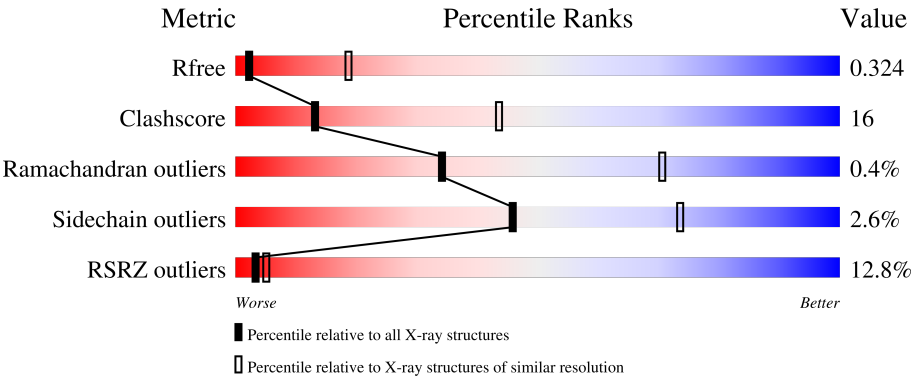
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.48 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	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

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	1494	12% 65% 25% • 8%
2	B	2	50% 50%
2	D	2	100%
2	E	2	100%
3	C	5	60% 40%

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
2	NAG	D	2	-	-	-	X
5	CA	A	1613	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11227 atoms, of which 12 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 UDP-glucose-glycoprotein glucosyltransferase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1373	Total	C	N	O	S	0	0	0
			11035	7063	1879	2062	31			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLU	-	expression tag	UNP G0SB58
A	22	THR	-	expression tag	UNP G0SB58
A	23	GLY	-	expression tag	UNP G0SB58
A	1506	GLY	-	expression tag	UNP G0SB58
A	1507	THR	-	expression tag	UNP G0SB58
A	1508	LYS	-	expression tag	UNP G0SB58
A	1509	HIS	-	expression tag	UNP G0SB58
A	1510	HIS	-	expression tag	UNP G0SB58
A	1511	HIS	-	expression tag	UNP G0SB58
A	1512	HIS	-	expression tag	UNP G0SB58
A	1513	HIS	-	expression tag	UNP G0SB58
A	1514	HIS	-	expression tag	UNP G0SB58

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

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

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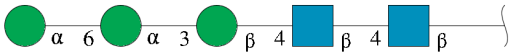
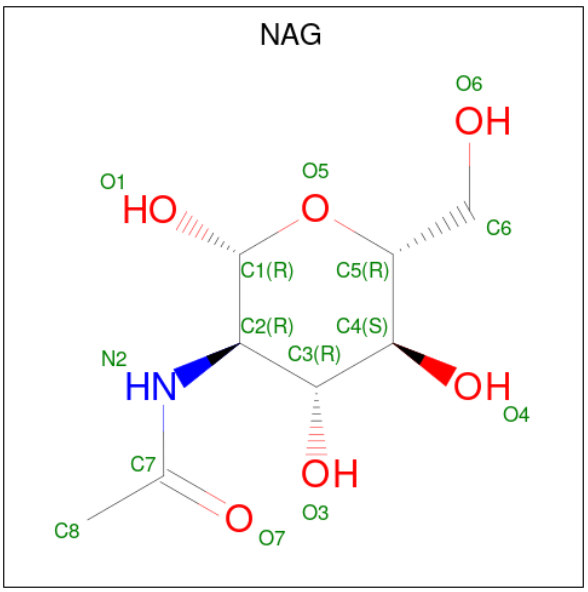
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	E	2	Total C N O 28 16 2 10	0	0	0

- Molecule 3 is an oligosaccharide called alpha-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
3	C	5	Total C N O 61 34 2 25	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

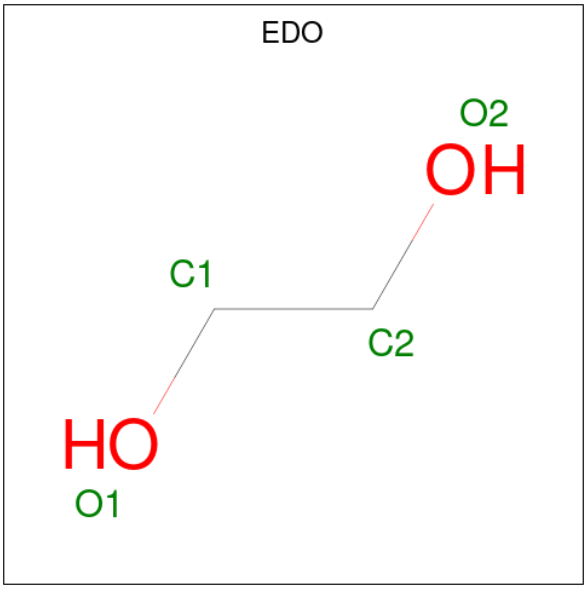


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H O 10 2 6 2	0	0
6	A	1	Total C H O 10 2 6 2	0	0

- Molecule 7 is water.

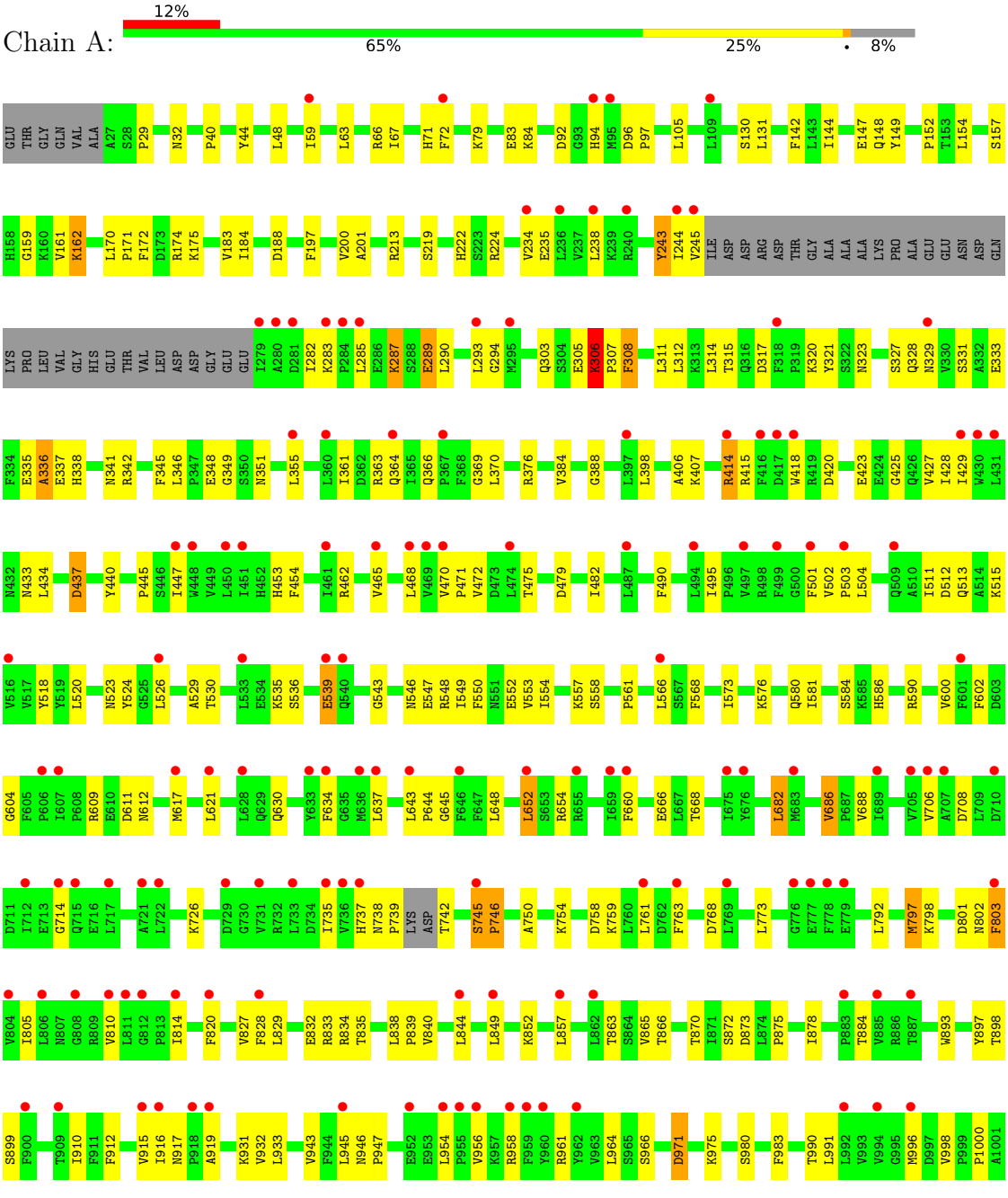
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	12	Total O 12 12	0	0

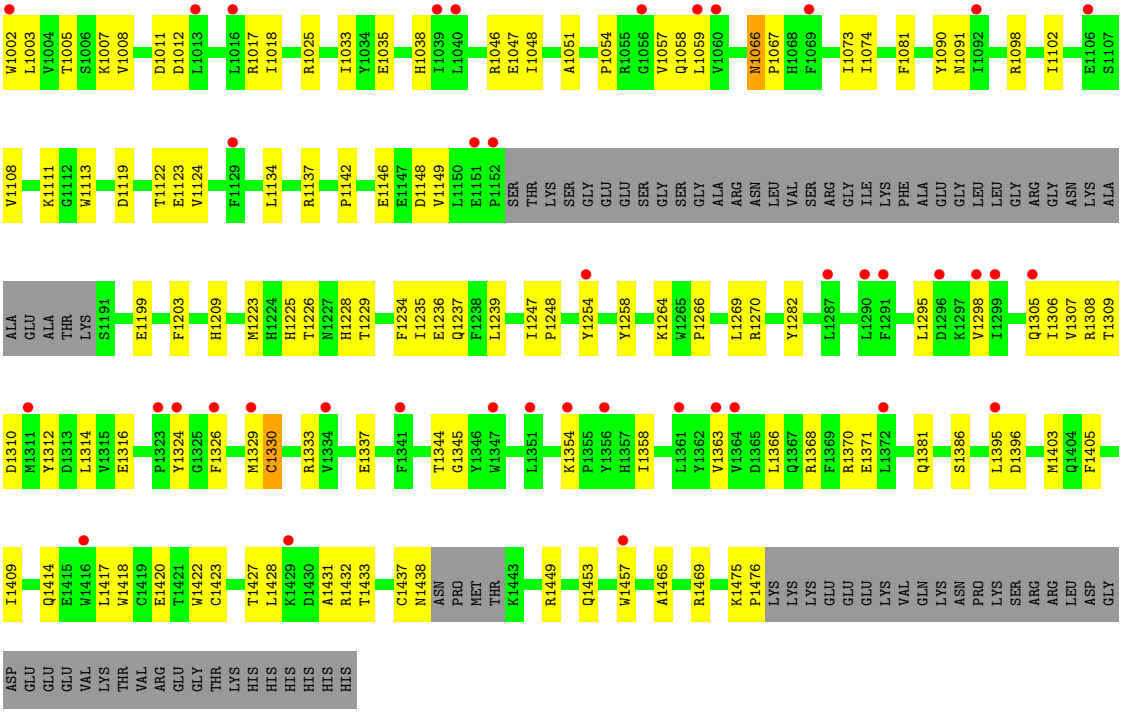
3 Residue-property plots (i)

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: UDP-glucose-glycoprotein glucosyltransferase-like protein

Chain A:



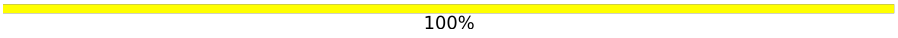


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

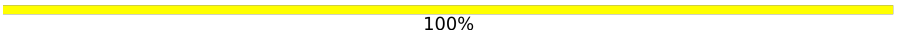
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



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

Chain E:



• Molecule 3: alpha-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 C:


NAG1
NAG2
BMA3
MAN4
MAN5

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	163.57Å 163.57Å 248.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	102.00 – 3.48 123.08 – 3.48	Depositor EDS
% Data completeness (in resolution range)	98.0 (102.00-3.48) 99.7 (123.08-3.48)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	0.26	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 3.49Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.251 , 0.278 0.283 , 0.324	Depositor DCC
R_{free} test set	1602 reflections (6.23%)	wwPDB-VP
Wilson B-factor (Å^2)	129.9	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 118.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11227	wwPDB-VP
Average B, all atoms (Å^2)	171.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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, EDO, NAG, MAN, CA

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	0.44	0/11298	0.74	5/15321 (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	A	305	GLU	C-N-CA	7.51	140.47	121.70
1	A	287	LYS	C-N-CA	6.70	138.44	121.70
1	A	243	TYR	C-N-CA	5.95	136.57	121.70
1	A	336	ALA	N-CA-C	-5.32	96.63	111.00
1	A	306	LYS	N-CA-C	-5.08	97.27	111.00

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	11035	0	10907	360	0
2	B	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
3	C	61	0	52	2	0
4	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
6	A	8	12	12	0	0
7	A	12	0	0	1	0
All	All	11215	12	11059	362	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 16.

All (362) 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:1329:MET:SD	1:A:1358:ILE:HD11	1.65	1.36
1:A:337:GLU:OE1	1:A:897:TYR:HD2	1.15	1.26
1:A:1225:HIS:ND1	1:A:1308:ARG:HA	1.62	1.13
1:A:1295:LEU:HD21	1:A:1298:VAL:CG2	1.79	1.12
1:A:337:GLU:OE1	1:A:897:TYR:CD2	2.03	1.11
1:A:67:ILE:HG22	1:A:72:PHE:HD2	1.17	1.08
1:A:67:ILE:HG22	1:A:72:PHE:CD2	1.91	1.06
1:A:1149:VAL:HG13	1:A:1371:GLU:O	1.57	1.03
1:A:1225:HIS:CE1	1:A:1308:ARG:HA	1.97	1.00
1:A:554:ILE:HG21	1:A:568:PHE:HE1	1.28	0.99
1:A:149:TYR:CE1	1:A:157:SER:HB2	1.98	0.98
1:A:1329:MET:SD	1:A:1358:ILE:CD1	2.51	0.98
1:A:1324:TYR:CD1	1:A:1326:PHE:HE1	1.85	0.94
1:A:524:TYR:OH	1:A:566:LEU:HD22	1.67	0.94
1:A:72:PHE:CE1	1:A:84:LYS:HG3	2.04	0.93
1:A:546:ASN:HB3	1:A:549:ILE:HG22	1.50	0.92
1:A:338:HIS:HD2	1:A:898:THR:HG23	1.35	0.91
1:A:338:HIS:O	1:A:341:ASN:HB2	1.72	0.90
1:A:524:TYR:HE2	1:A:558:SER:HG	1.23	0.87
1:A:1048:ILE:HD11	1:A:1137:ARG:HD2	1.57	0.86
1:A:1058:GLN:HG2	1:A:1073:ILE:HG22	1.57	0.86
1:A:566:LEU:HD13	1:A:568:PHE:CD2	2.10	0.86
1:A:243:TYR:O	1:A:285:LEU:HG	1.76	0.85
1:A:554:ILE:HG21	1:A:568:PHE:CE1	2.12	0.85
1:A:482:ILE:HD12	1:A:609:ARG:HH22	1.42	0.85
1:A:739:PRO:C	1:A:746:PRO:HD3	1.98	0.83
1:A:328:GLN:H	1:A:329:ASN:HA	1.44	0.82
1:A:72:PHE:HE1	1:A:84:LYS:HG3	1.44	0.81
1:A:67:ILE:CG2	1:A:72:PHE:HD2	1.91	0.81
1:A:554:ILE:HG23	1:A:558:SER:HB2	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:PRO:HG3	1:A:566:LEU:HD23	1.62	0.80
1:A:1007:LYS:HG3	1:A:1035:GLU:HB2	1.64	0.79
1:A:346:LEU:HD12	1:A:893:TRP:HH2	1.48	0.79
1:A:1059:LEU:HD11	1:A:1074:ILE:HD11	1.65	0.79
1:A:1324:TYR:CD1	1:A:1326:PHE:CE1	2.70	0.79
1:A:686:VAL:O	1:A:754:LYS:HE2	1.82	0.78
1:A:384:VAL:CG2	1:A:865:VAL:HG11	2.13	0.78
1:A:1422:TRP:CZ3	1:A:1437:CYS:SG	2.78	0.77
1:A:1295:LEU:HD21	1:A:1298:VAL:HG23	1.67	0.76
1:A:433:ASN:O	1:A:437:ASP:HB2	1.85	0.76
1:A:338:HIS:CD2	1:A:898:THR:HG23	2.21	0.76
1:A:311:LEU:O	1:A:315:THR:HG22	1.87	0.75
1:A:342:ARG:HD3	1:A:348:GLU:HB3	1.69	0.75
1:A:244:ILE:HA	1:A:285:LEU:HB3	1.67	0.75
1:A:475:THR:HA	1:A:543:GLY:HA3	1.69	0.75
1:A:1225:HIS:ND1	1:A:1308:ARG:CA	2.47	0.74
1:A:797:MET:HB3	1:A:803:PHE:CZ	2.23	0.74
1:A:445:PRO:HG3	1:A:462:ARG:NH2	2.03	0.73
1:A:566:LEU:HD13	1:A:568:PHE:CE2	2.23	0.73
1:A:243:TYR:HD1	1:A:285:LEU:HD23	1.51	0.73
1:A:482:ILE:HD12	1:A:609:ARG:NH2	2.03	0.73
1:A:834:ARG:O	1:A:839:PRO:HD3	1.89	0.73
1:A:282:ILE:HG13	1:A:990:THR:HG22	1.70	0.73
1:A:346:LEU:HD12	1:A:893:TRP:CH2	2.23	0.73
1:A:144:ILE:HG12	1:A:183:VAL:HG12	1.71	0.72
1:A:546:ASN:HB3	1:A:549:ILE:CG2	2.17	0.72
1:A:67:ILE:CG2	1:A:72:PHE:CD2	2.68	0.72
1:A:96:ASP:HB2	1:A:97:PRO:HD2	1.71	0.72
1:A:245:VAL:HB	1:A:287:LYS:HB2	1.72	0.72
1:A:1098:ARG:HH21	1:A:1102:ILE:HD11	1.55	0.72
1:A:1324:TYR:CE1	1:A:1326:PHE:HE1	2.09	0.71
1:A:1295:LEU:HD21	1:A:1298:VAL:HG22	1.72	0.71
1:A:142:PHE:HE1	1:A:197:PHE:HD2	1.38	0.71
1:A:547:GLU:HA	1:A:550:PHE:HB3	1.72	0.71
1:A:1108:VAL:HG12	1:A:1134:LEU:HD22	1.73	0.71
1:A:244:ILE:HD11	1:A:954:LEU:HD13	1.73	0.70
1:A:515:LYS:CG	1:A:581:ILE:HD11	2.21	0.70
1:A:515:LYS:HG3	1:A:581:ILE:HD11	1.73	0.70
1:A:384:VAL:HG23	1:A:865:VAL:HG11	1.72	0.70
1:A:1307:VAL:HG13	1:A:1433:THR:HG22	1.73	0.70
1:A:524:TYR:HE2	1:A:558:SER:OG	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:TYR:HE1	1:A:157:SER:HB2	1.53	0.69
1:A:130:SER:O	1:A:161:VAL:HG13	1.93	0.69
1:A:1314:LEU:HG	1:A:1363:VAL:CG2	2.23	0.69
1:A:346:LEU:CD1	1:A:893:TRP:HH2	2.05	0.69
1:A:573:ILE:HB	1:A:576:LYS:HB3	1.73	0.69
1:A:829:LEU:O	1:A:833:ARG:HB2	1.93	0.69
3:C:2:NAG:H62	3:C:3:BMA:H2	1.75	0.69
1:A:1366:LEU:O	1:A:1370:ARG:HG3	1.92	0.69
1:A:188:ASP:OD1	1:A:219:SER:HB3	1.93	0.68
1:A:376:ARG:HH12	1:A:873:ASP:HB3	1.58	0.68
1:A:420:ASP:HB3	1:A:425:GLY:HA2	1.75	0.68
1:A:1048:ILE:HD11	1:A:1137:ARG:HB3	1.74	0.68
1:A:1247:ILE:HG13	1:A:1248:PRO:HD3	1.75	0.68
1:A:66:ARG:O	1:A:71:HIS:HB3	1.93	0.68
1:A:1418:TRP:HE1	1:A:1427:THR:HB	1.60	0.67
1:A:445:PRO:HG3	1:A:462:ARG:HH21	1.60	0.67
1:A:546:ASN:CB	1:A:549:ILE:HG22	2.22	0.67
1:A:152:PRO:HB3	1:A:200:VAL:HG21	1.77	0.66
1:A:523:ASN:OD1	1:A:566:LEU:HA	1.96	0.66
1:A:1428:LEU:HD12	1:A:1431:ALA:HB3	1.75	0.66
1:A:29:PRO:HB2	1:A:1018:ILE:HD13	1.77	0.66
1:A:1324:TYR:CE1	1:A:1326:PHE:CE1	2.84	0.66
1:A:238:LEU:HD13	1:A:283:LYS:HE2	1.77	0.65
1:A:512:ASP:HA	1:A:515:LYS:HE3	1.78	0.65
1:A:142:PHE:CE1	1:A:197:PHE:HD2	2.14	0.65
1:A:872:SER:HB2	1:A:884:THR:OG1	1.96	0.65
1:A:335:GLU:HA	1:A:337:GLU:HG2	1.79	0.65
1:A:1422:TRP:HZ3	1:A:1437:CYS:SG	2.19	0.64
1:A:243:TYR:CD1	1:A:285:LEU:HD23	2.32	0.64
1:A:600:VAL:CG2	1:A:609:ARG:HG2	2.29	0.63
1:A:1048:ILE:CD1	1:A:1137:ARG:HB3	2.28	0.63
1:A:244:ILE:HG12	1:A:285:LEU:HD12	1.81	0.63
1:A:1329:MET:CG	1:A:1358:ILE:HD11	2.29	0.62
1:A:345:PHE:HB3	1:A:893:TRP:CZ2	2.34	0.62
1:A:706:VAL:HG11	1:A:803:PHE:CE1	2.34	0.62
1:A:170:LEU:HD11	1:A:172:PHE:CE1	2.34	0.62
1:A:1333:ARG:HH21	1:A:1420:GLU:HG2	1.65	0.62
1:A:511:ILE:HG23	1:A:581:ILE:HD13	1.81	0.62
1:A:554:ILE:HG23	1:A:558:SER:CB	2.30	0.62
1:A:283:LYS:HZ1	1:A:285:LEU:HD21	1.63	0.61
1:A:535:LYS:HE2	1:A:552:GLU:OE1	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1438:ASN:HA	1:A:1449:ARG:HH22	1.66	0.61
1:A:234:VAL:HG22	1:A:996:MET:CE	2.30	0.61
1:A:524:TYR:HE2	1:A:558:SER:CB	2.14	0.61
1:A:398:LEU:CD2	1:A:866:THR:HG22	2.30	0.61
1:A:1003:LEU:HD21	1:A:1264:LYS:HB2	1.83	0.60
1:A:398:LEU:HD23	1:A:866:THR:HG22	1.84	0.60
1:A:418:TRP:HE1	1:A:648:LEU:HD11	1.64	0.60
1:A:289:GLU:HA	1:A:289:GLU:OE1	2.01	0.60
1:A:306:LYS:HG2	1:A:308:PHE:HE1	1.66	0.60
1:A:294:GLY:HA3	1:A:947:PRO:HB3	1.84	0.59
1:A:1199:GLU:HG3	1:A:1229:THR:OG1	2.02	0.59
1:A:630:GLN:O	1:A:634:PHE:HD1	1.86	0.59
1:A:1295:LEU:HD21	1:A:1298:VAL:HG21	1.78	0.59
1:A:1333:ARG:HG2	1:A:1423:CYS:C	2.23	0.59
1:A:1324:TYR:HD1	1:A:1326:PHE:CE1	2.21	0.59
1:A:899:SER:HA	1:A:943:VAL:O	2.02	0.59
1:A:420:ASP:OD1	1:A:427:VAL:CG1	2.51	0.58
1:A:600:VAL:HG23	1:A:609:ARG:CG	2.32	0.58
1:A:470:VAL:HG23	1:A:600:VAL:HG22	1.84	0.58
1:A:328:GLN:HB3	1:A:331:SER:H	1.68	0.58
1:A:590:ARG:HA	1:A:654:ARG:HH21	1.69	0.58
1:A:131:LEU:HD11	1:A:148:GLN:OE1	2.03	0.58
1:A:142:PHE:HE2	1:A:201:ALA:HB2	1.67	0.58
1:A:553:VAL:O	1:A:557:LYS:HB2	2.04	0.58
1:A:561:PRO:CG	1:A:566:LEU:HD23	2.31	0.58
1:A:566:LEU:O	1:A:566:LEU:HD12	2.02	0.58
1:A:738:ASN:HD22	1:A:792:LEU:HD11	1.68	0.58
1:A:1199:GLU:HB2	1:A:1229:THR:O	2.04	0.57
1:A:328:GLN:H	1:A:329:ASN:CA	2.15	0.57
1:A:472:VAL:O	1:A:503:PRO:HA	2.05	0.57
1:A:234:VAL:HG22	1:A:996:MET:HE2	1.86	0.56
1:A:406:ALA:HB2	1:A:839:PRO:HG2	1.85	0.56
1:A:554:ILE:O	1:A:558:SER:CB	2.53	0.56
1:A:600:VAL:HG23	1:A:609:ARG:HG2	1.86	0.56
1:A:174:ARG:O	1:A:213:ARG:HB3	2.05	0.56
1:A:130:SER:HB3	1:A:162:LYS:O	2.06	0.56
1:A:1306:ILE:HD11	1:A:1457:TRP:HD1	1.70	0.56
1:A:482:ILE:CD1	1:A:609:ARG:NH2	2.69	0.56
1:A:147:GLU:HA	1:A:159:GLY:O	2.06	0.56
1:A:961:ARG:HG2	1:A:983:PHE:CE2	2.41	0.56
1:A:465:VAL:HG22	1:A:643:LEU:CD1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:805:ILE:HG12	1:A:810:VAL:HG22	1.88	0.55
1:A:844:LEU:HD12	1:A:849:LEU:HB2	1.88	0.55
1:A:998:VAL:HG22	1:A:1002:TRP:HB2	1.88	0.55
1:A:1295:LEU:CD2	1:A:1298:VAL:CG2	2.70	0.55
1:A:420:ASP:OD1	1:A:427:VAL:HG12	2.05	0.55
1:A:745:SER:HB2	1:A:746:PRO:HA	1.89	0.55
1:A:1054:PRO:HB2	1:A:1057:VAL:HG21	1.87	0.54
1:A:652:LEU:HD13	1:A:660:PHE:CZ	2.43	0.54
1:A:92:ASP:HB2	1:A:94:HIS:CD2	2.43	0.54
1:A:1058:GLN:CG	1:A:1073:ILE:HG22	2.34	0.54
1:A:1422:TRP:CE3	1:A:1437:CYS:SG	3.01	0.54
1:A:915:VAL:HG12	1:A:946:ASN:ND2	2.23	0.54
1:A:235:GLU:HB2	1:A:958:ARG:HD2	1.90	0.54
1:A:546:ASN:O	1:A:549:ILE:HG22	2.07	0.53
1:A:282:ILE:HG13	1:A:990:THR:CG2	2.38	0.53
1:A:290:LEU:HA	1:A:293:LEU:HD13	1.89	0.53
1:A:524:TYR:CD2	1:A:558:SER:HA	2.42	0.53
1:A:1011:ASP:CG	1:A:1025:ARG:HH22	2.11	0.53
1:A:1059:LEU:CD1	1:A:1074:ILE:HD11	2.38	0.53
1:A:554:ILE:HD13	1:A:568:PHE:CE1	2.44	0.53
1:A:524:TYR:CE1	1:A:566:LEU:HB3	2.44	0.52
1:A:932:VAL:HG11	1:A:964:LEU:HG	1.91	0.52
1:A:1005:THR:HG21	1:A:1236:GLU:HG2	1.90	0.52
1:A:708:ASP:OD1	1:A:739:PRO:HD2	2.09	0.52
1:A:1223:MET:HG3	1:A:1254:TYR:HB3	1.91	0.52
1:A:428:ILE:HA	1:A:502:VAL:HG12	1.91	0.52
1:A:536:SER:HA	1:A:549:ILE:HD13	1.90	0.52
1:A:600:VAL:CG2	1:A:609:ARG:CG	2.88	0.52
1:A:602:PHE:HZ	1:A:621:LEU:HD13	1.75	0.52
1:A:763:PHE:HD1	1:A:768:ASP:HB3	1.75	0.52
1:A:376:ARG:NH1	1:A:873:ASP:HB3	2.24	0.52
1:A:1058:GLN:HG2	1:A:1073:ILE:CG2	2.34	0.52
1:A:1048:ILE:HD11	1:A:1137:ARG:CD	2.35	0.52
1:A:434:LEU:HD23	1:A:440:TYR:CE2	2.45	0.52
1:A:554:ILE:O	1:A:558:SER:HB3	2.10	0.51
1:A:1247:ILE:HD12	1:A:1258:TYR:CD2	2.45	0.51
1:A:1324:TYR:CE1	1:A:1409:ILE:HG12	2.46	0.51
1:A:515:LYS:HG2	1:A:581:ILE:HD11	1.91	0.51
1:A:1225:HIS:HE1	1:A:1308:ARG:HG2	1.75	0.51
1:A:355:LEU:HD11	1:A:910:ILE:HG23	1.93	0.51
1:A:142:PHE:HE1	1:A:197:PHE:CD2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:LEU:HD11	1:A:600:VAL:CG1	2.41	0.51
1:A:835:THR:O	1:A:839:PRO:HD2	2.11	0.51
1:A:283:LYS:NZ	1:A:285:LEU:HD21	2.26	0.51
1:A:414:ARG:HE	1:A:652:LEU:HD11	1.76	0.51
1:A:524:TYR:CE2	1:A:558:SER:HA	2.45	0.51
1:A:520:LEU:HD23	1:A:529:ALA:HA	1.92	0.50
1:A:645:GLY:HA2	1:A:648:LEU:HB2	1.94	0.50
1:A:1314:LEU:HG	1:A:1363:VAL:HG22	1.93	0.50
1:A:548:ARG:O	1:A:552:GLU:HG3	2.11	0.50
1:A:1270:ARG:HD2	1:A:1386:SER:OG	2.11	0.50
1:A:427:VAL:CG2	1:A:584:SER:HA	2.41	0.50
1:A:328:GLN:N	1:A:329:ASN:HA	2.21	0.49
1:A:1199:GLU:HG3	1:A:1229:THR:H	1.78	0.49
1:A:535:LYS:C	1:A:549:ILE:HD11	2.32	0.49
1:A:1108:VAL:CG1	1:A:1134:LEU:HD22	2.41	0.49
1:A:447:ILE:HD11	1:A:637:LEU:HB3	1.94	0.49
1:A:1247:ILE:HD12	1:A:1258:TYR:CE2	2.47	0.49
1:A:1309:THR:HG22	1:A:1310:ASP:O	2.12	0.49
1:A:1008:VAL:HB	1:A:1033:ILE:HB	1.95	0.49
1:A:1368:ARG:O	1:A:1368:ARG:HD3	2.13	0.49
1:A:1465:ALA:HB1	1:A:1469:ARG:HH21	1.78	0.49
1:A:652:LEU:HD22	1:A:827:VAL:HG13	1.93	0.49
1:A:415:ARG:HA	1:A:604:GLY:O	2.13	0.49
1:A:1381:GLN:HG3	1:A:1403:MET:SD	2.53	0.48
1:A:144:ILE:HB	1:A:149:TYR:HE2	1.78	0.48
1:A:919:ALA:O	1:A:956:VAL:HG23	2.13	0.48
1:A:745:SER:CB	1:A:746:PRO:HA	2.43	0.48
1:A:1199:GLU:CG	1:A:1229:THR:OG1	2.61	0.48
1:A:1247:ILE:CG1	1:A:1248:PRO:HD3	2.42	0.48
1:A:726:LYS:HE3	1:A:761:LEU:HB2	1.95	0.48
1:A:644:PRO:O	1:A:648:LEU:HD13	2.12	0.48
1:A:1091:ASN:OD1	1:A:1122:THR:HG23	2.13	0.48
1:A:535:LYS:O	1:A:539:GLU:HB2	2.14	0.48
1:A:312:LEU:HD22	1:A:931:LYS:HD3	1.96	0.48
1:A:838:LEU:HD23	1:A:838:LEU:HA	1.76	0.47
1:A:311:LEU:O	1:A:315:THR:CG2	2.60	0.47
1:A:370:LEU:HD13	1:A:933:LEU:HD11	1.95	0.47
1:A:686:VAL:HG22	1:A:735:ILE:O	2.14	0.47
1:A:333:GLU:HG2	1:A:336:ALA:HB2	1.96	0.47
1:A:682:LEU:C	1:A:682:LEU:HD13	2.34	0.47
1:A:366:GLN:OE1	1:A:1000:PRO:HD2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1102:ILE:HD13	1:A:1146:GLU:HB2	1.96	0.47
1:A:142:PHE:HZ	1:A:197:PHE:O	1.96	0.47
1:A:802:ASN:HB2	1:A:814:ILE:HB	1.97	0.47
1:A:1344:THR:HG22	1:A:1345:GLY:N	2.29	0.47
1:A:174:ARG:O	1:A:213:ARG:CB	2.63	0.47
1:A:573:ILE:HB	1:A:576:LYS:CB	2.45	0.47
1:A:366:GLN:HG2	1:A:369:GLY:H	1.80	0.46
1:A:991:LEU:HD23	1:A:1017:ARG:HG3	1.97	0.46
1:A:600:VAL:HG23	1:A:609:ARG:HG3	1.96	0.46
1:A:59:ILE:O	1:A:63:LEU:HG	2.15	0.46
1:A:414:ARG:HE	1:A:652:LEU:CD1	2.28	0.46
1:A:471:PRO:HA	1:A:502:VAL:O	2.16	0.46
1:A:1005:THR:HG22	1:A:1237:GLN:HA	1.97	0.46
1:A:686:VAL:O	1:A:688:VAL:HG23	2.15	0.46
3:C:1:NAG:H61	3:C:2:NAG:C7	2.46	0.46
1:A:414:ARG:NE	1:A:652:LEU:HD11	2.30	0.46
1:A:518:TYR:HB3	1:A:580:GLN:OE1	2.16	0.46
1:A:554:ILE:HD13	1:A:568:PHE:HE1	1.81	0.46
1:A:991:LEU:HG	1:A:1017:ARG:HD2	1.96	0.46
1:A:79:LYS:O	1:A:83:GLU:HG2	2.16	0.46
1:A:586:HIS:O	1:A:590:ARG:HB2	2.16	0.46
1:A:1306:ILE:HD11	1:A:1457:TRP:CD1	2.49	0.46
1:A:916:ILE:O	1:A:945:LEU:HA	2.16	0.45
1:A:1003:LEU:HD12	1:A:1038:HIS:HB2	1.98	0.45
1:A:306:LYS:N	1:A:307:PRO:HD3	2.31	0.45
1:A:418:TRP:NE1	1:A:648:LEU:HD11	2.30	0.45
1:A:566:LEU:CD1	1:A:568:PHE:CE2	2.97	0.45
1:A:708:ASP:O	1:A:714:GLY:HA3	2.16	0.45
1:A:511:ILE:HG22	1:A:515:LYS:HE2	1.96	0.45
1:A:590:ARG:HG2	1:A:654:ARG:HG3	1.99	0.45
1:A:40:PRO:HG2	7:A:1707:HOH:O	2.17	0.45
1:A:170:LEU:HB2	1:A:171:PRO:HD2	1.99	0.45
1:A:303:GLN:HE22	1:A:328:GLN:HE21	1.64	0.45
1:A:407:LYS:HD2	1:A:870:THR:OG1	2.17	0.45
1:A:361:ILE:HG13	1:A:364:GLN:HG3	1.98	0.45
1:A:406:ALA:CB	1:A:839:PRO:HG2	2.47	0.45
1:A:445:PRO:CG	1:A:462:ARG:HH21	2.29	0.45
1:A:1309:THR:OG1	1:A:1432:ARG:HB3	2.17	0.44
1:A:1066:ASN:HA	1:A:1067:PRO:HD3	1.76	0.44
1:A:142:PHE:CE2	1:A:201:ALA:HB2	2.51	0.44
1:A:915:VAL:HG12	1:A:946:ASN:HD22	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1090:TYR:HB2	1:A:1124:VAL:HG23	2.00	0.44
1:A:1047:GLU:O	1:A:1051:ALA:HA	2.18	0.44
1:A:471:PRO:HB2	1:A:504:LEU:HD21	2.00	0.44
1:A:737:HIS:CE1	1:A:750:ALA:HA	2.53	0.44
1:A:1395:LEU:HD12	1:A:1396:ASP:N	2.32	0.44
1:A:351:ASN:HA	1:A:915:VAL:O	2.17	0.44
1:A:971:ASP:HB2	1:A:975:LYS:O	2.18	0.44
1:A:66:ARG:O	1:A:71:HIS:CB	2.63	0.44
1:A:465:VAL:HG22	1:A:643:LEU:HD12	1.99	0.44
1:A:1046:ARG:NH2	1:A:1113:TRP:O	2.51	0.44
1:A:1330:CYS:HA	1:A:1414:GLN:OE1	2.18	0.44
1:A:338:HIS:HD2	1:A:898:THR:CG2	2.19	0.43
1:A:420:ASP:OD1	1:A:427:VAL:HG13	2.17	0.43
1:A:317:ASP:O	1:A:320:LYS:HB3	2.19	0.43
1:A:445:PRO:HD3	1:A:462:ARG:HH21	1.83	0.43
1:A:234:VAL:HG22	1:A:996:MET:HE1	1.98	0.43
1:A:366:GLN:HE21	1:A:369:GLY:HA3	1.84	0.43
1:A:546:ASN:O	1:A:549:ILE:CG2	2.66	0.43
1:A:566:LEU:CD1	1:A:568:PHE:CD2	2.94	0.43
1:A:44:TYR:CE2	1:A:48:LEU:HD11	2.53	0.43
1:A:1098:ARG:HG3	1:A:1148:ASP:OD1	2.18	0.43
1:A:1012:ASP:HB2	1:A:1209:HIS:ND1	2.34	0.43
1:A:366:GLN:CG	1:A:369:GLY:H	2.31	0.43
1:A:1449:ARG:HB3	1:A:1453:GLN:OE1	2.19	0.43
1:A:32:ASN:OD1	1:A:980:SER:HB3	2.19	0.43
1:A:468:LEU:HD22	1:A:617:MET:SD	2.59	0.43
1:A:763:PHE:HD1	1:A:768:ASP:CB	2.32	0.43
1:A:429:ILE:HD11	1:A:501:PHE:CZ	2.54	0.43
1:A:314:LEU:HD12	1:A:321:TYR:HD2	1.84	0.42
1:A:355:LEU:HD13	1:A:912:PHE:CZ	2.54	0.42
1:A:453:HIS:C	1:A:454:PHE:CD2	2.92	0.42
1:A:737:HIS:CD2	1:A:737:HIS:N	2.87	0.42
1:A:840:VAL:HG21	1:A:863:THR:HA	2.01	0.42
1:A:1247:ILE:HG13	1:A:1248:PRO:CD	2.47	0.42
1:A:536:SER:HA	1:A:549:ILE:CD1	2.49	0.42
1:A:1074:ILE:HD13	1:A:1081:PHE:HB3	2.01	0.42
1:A:1305:GLN:HE22	1:A:1417:LEU:HD11	1.83	0.42
1:A:154:LEU:HG	1:A:154:LEU:O	2.20	0.42
1:A:1235:ILE:HD13	1:A:1282:TYR:HB3	2.00	0.42
1:A:511:ILE:HG22	1:A:515:LYS:CE	2.49	0.42
1:A:566:LEU:HD12	1:A:566:LEU:C	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1344:THR:HG22	1:A:1345:GLY:H	1.83	0.42
1:A:998:VAL:CG2	1:A:1002:TRP:HE3	2.33	0.42
1:A:243:TYR:CD1	1:A:285:LEU:CD2	3.03	0.42
1:A:283:LYS:HZ2	1:A:285:LEU:HD11	1.85	0.42
1:A:384:VAL:HG22	1:A:865:VAL:HG11	1.99	0.42
1:A:576:LYS:O	1:A:580:GLN:HB2	2.19	0.42
1:A:1475:LYS:HA	1:A:1476:PRO:HD3	1.95	0.42
1:A:1111:LYS:HG3	1:A:1119:ASP:CB	2.50	0.42
1:A:349:GLY:HA2	1:A:917:ASN:HB2	2.01	0.42
1:A:1354:LYS:HD2	1:A:1405:PHE:CE1	2.55	0.42
1:A:524:TYR:OH	1:A:566:LEU:CD2	2.55	0.42
1:A:526:LEU:O	1:A:530:THR:HG23	2.20	0.41
1:A:828:PHE:O	1:A:832:GLU:HB2	2.20	0.41
1:A:798:LYS:HG2	1:A:801:ASP:OD2	2.20	0.41
1:A:468:LEU:HD11	1:A:600:VAL:HG12	2.03	0.41
1:A:1266:PRO:HD2	1:A:1269:LEU:HD23	2.02	0.41
1:A:142:PHE:HA	1:A:184:ILE:O	2.21	0.41
1:A:490:PHE:HA	1:A:495:ILE:HD12	2.02	0.41
1:A:520:LEU:CD2	1:A:529:ALA:HA	2.51	0.41
1:A:654:ARG:HB2	1:A:827:VAL:HG21	2.03	0.41
1:A:1330:CYS:HB3	1:A:1422:TRP:O	2.21	0.41
1:A:1226:THR:OG1	1:A:1228:HIS:HB2	2.21	0.41
1:A:423:GLU:CD	1:A:590:ARG:HH11	2.24	0.41
1:A:835:THR:O	1:A:839:PRO:CD	2.69	0.41
1:A:1111:LYS:HG3	1:A:1119:ASP:HB3	2.01	0.41
1:A:1234:PHE:HB3	1:A:1239:LEU:HD11	2.03	0.41
1:A:668:THR:HG23	1:A:810:VAL:HB	2.02	0.41
1:A:1098:ARG:HG2	1:A:1148:ASP:HA	2.02	0.41
1:A:1312:TYR:CE1	1:A:1316:GLU:HG3	2.55	0.41
1:A:105:LEU:HD13	1:A:966:SER:HA	2.02	0.41
1:A:549:ILE:HD13	1:A:549:ILE:HG21	1.87	0.41
1:A:998:VAL:CG2	1:A:1002:TRP:CE3	3.04	0.41
1:A:998:VAL:HG23	1:A:1002:TRP:CE3	2.56	0.41
1:A:738:ASN:HD22	1:A:792:LEU:CD1	2.32	0.40
1:A:472:VAL:HG13	1:A:479:ASP:HB3	2.03	0.40
1:A:875:PRO:HB2	1:A:878:ILE:HD12	2.03	0.40
1:A:1333:ARG:NH2	1:A:1420:GLU:HG2	2.32	0.40
1:A:1295:LEU:CD2	1:A:1298:VAL:HG23	2.42	0.40
1:A:303:GLN:NE2	1:A:328:GLN:HE21	2.20	0.40
1:A:370:LEU:HD13	1:A:933:LEU:CD1	2.50	0.40
1:A:388:GLY:O	1:A:852:LYS:HE2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:GLU:OE1	1:A:590:ARG:NH1	2.54	0.40
1:A:244:ILE:CG1	1:A:285:LEU:HD12	2.49	0.40
1:A:285:LEU:HD13	1:A:285:LEU:HA	1.77	0.40
1:A:427:VAL:HG23	1:A:584:SER:HA	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	1363/1494 (91%)	1293 (95%)	64 (5%)	6 (0%)	34 70

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	LYS
1	A	745	SER
1	A	666	GLU
1	A	746	PRO
1	A	1142	PRO
1	A	1337	GLU

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	1199/1297 (92%)	1168 (97%)	31 (3%)	46 73

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	LYS
1	A	175	LYS
1	A	222	HIS
1	A	224	ARG
1	A	289	GLU
1	A	308	PHE
1	A	323	ASN
1	A	327	SER
1	A	363	ARG
1	A	414	ARG
1	A	437	ASP
1	A	513	GLN
1	A	539	GLU
1	A	611	ASP
1	A	612	ASN
1	A	652	LEU
1	A	682	LEU
1	A	686	VAL
1	A	742	THR
1	A	758	ASP
1	A	759	LYS
1	A	773	LEU
1	A	797	MET
1	A	803	PHE
1	A	820	PHE
1	A	857	LEU
1	A	971	ASP
1	A	1066	ASN
1	A	1123	GLU
1	A	1203	PHE
1	A	1330	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	328	GLN
1	A	513	GLN

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Mol	Chain	Res	Type
1	A	737	HIS

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

11 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	B	1	1,2	14,14,15	0.29	0	17,19,21	0.64	0
2	NAG	B	2	2	14,14,15	0.38	0	17,19,21	1.05	2 (11%)
3	NAG	C	1	1,3	14,14,15	0.35	0	17,19,21	1.34	1 (5%)
3	NAG	C	2	3	14,14,15	0.38	0	17,19,21	1.34	4 (23%)
3	BMA	C	3	3	11,11,12	0.35	0	15,15,17	0.64	0
3	MAN	C	4	3	11,11,12	0.46	0	15,15,17	0.90	1 (6%)
3	MAN	C	5	3	11,11,12	0.45	0	15,15,17	1.12	1 (6%)
2	NAG	D	1	1,2	14,14,15	0.38	0	17,19,21	1.96	2 (11%)
2	NAG	D	2	2	14,14,15	0.39	0	17,19,21	0.86	1 (5%)
2	NAG	E	1	1,2	14,14,15	0.48	0	17,19,21	1.89	3 (17%)
2	NAG	E	2	2	14,14,15	0.34	0	17,19,21	0.83	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
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	1/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	1/2/19/22	0/1/1/1
3	MAN	C	5	3	-	1/2/19/22	1/1/1/1
2	NAG	D	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	NAG	C1-O5-C5	6.54	121.05	112.19
2	D	1	NAG	C1-O5-C5	6.51	121.01	112.19
3	C	1	NAG	O5-C1-C2	-4.22	104.63	111.29
3	C	5	MAN	C1-O5-C5	3.91	117.49	112.19
2	D	1	NAG	O5-C1-C2	3.50	116.82	111.29
2	B	2	NAG	O5-C1-C2	2.90	115.87	111.29
3	C	2	NAG	C1-O5-C5	2.75	115.92	112.19
2	D	2	NAG	C1-O5-C5	2.66	115.80	112.19
3	C	2	NAG	C2-N2-C7	2.56	126.55	122.90
3	C	2	NAG	C1-C2-N2	2.55	114.85	110.49
2	E	1	NAG	C1-C2-N2	2.46	114.69	110.49
3	C	2	NAG	O5-C1-C2	-2.44	107.44	111.29
2	B	2	NAG	C1-O5-C5	2.43	115.48	112.19
2	E	2	NAG	C1-O5-C5	2.41	115.46	112.19
3	C	4	MAN	C1-C2-C3	2.35	112.56	109.67
2	E	1	NAG	C2-N2-C7	2.26	126.13	122.90

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	5	MAN	O5-C5-C6-O6
3	C	4	MAN	O5-C5-C6-O6
2	E	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	C	2	NAG	C3-C2-N2-C7
2	D	1	NAG	C4-C5-C6-O6

All (1) ring outliers are listed below:

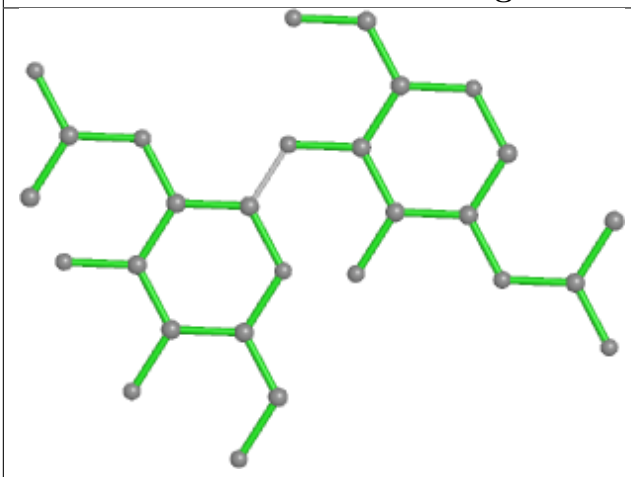
Mol	Chain	Res	Type	Atoms
3	C	5	MAN	C1-C2-C3-C4-C5-O5

3 monomers are involved in 2 short contacts:

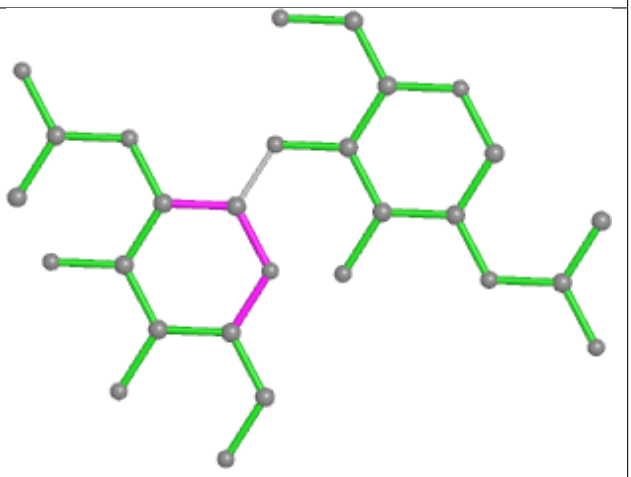
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	1	0
3	C	3	BMA	1	0
3	C	2	NAG	2	0

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

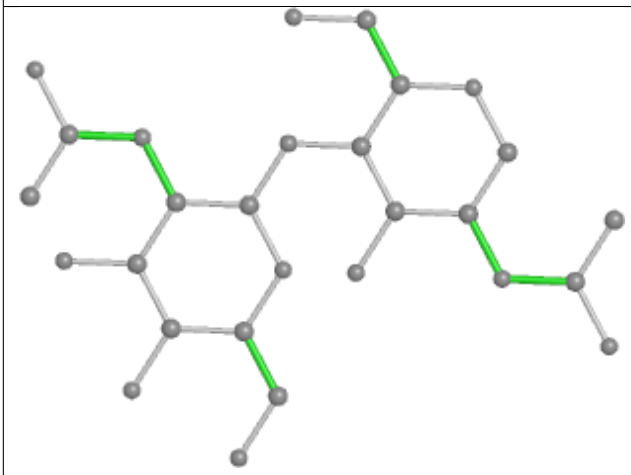
Oligosaccharide Chain B



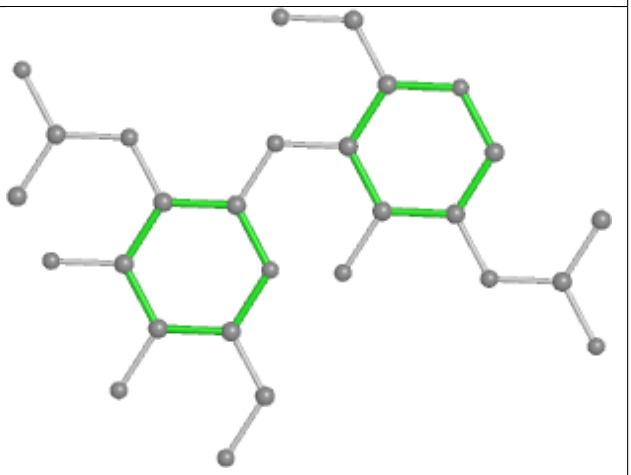
Bond lengths



Bond angles

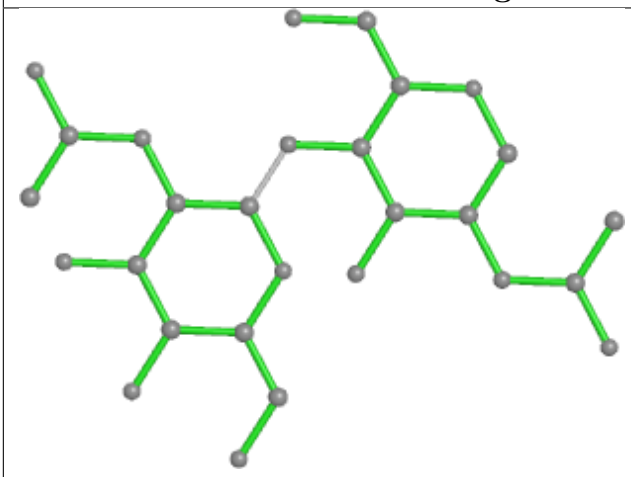


Torsions

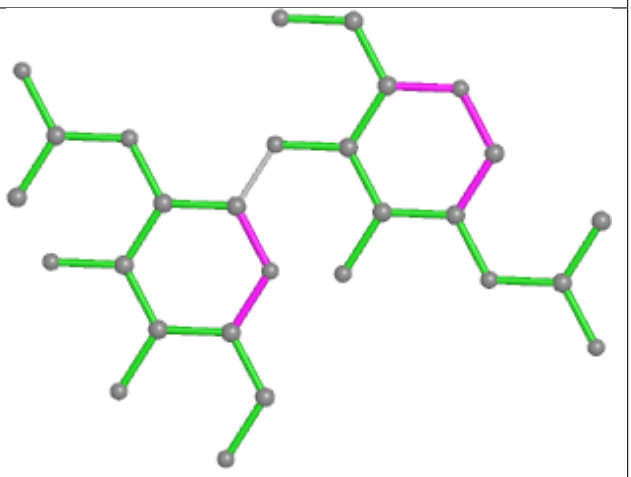


Rings

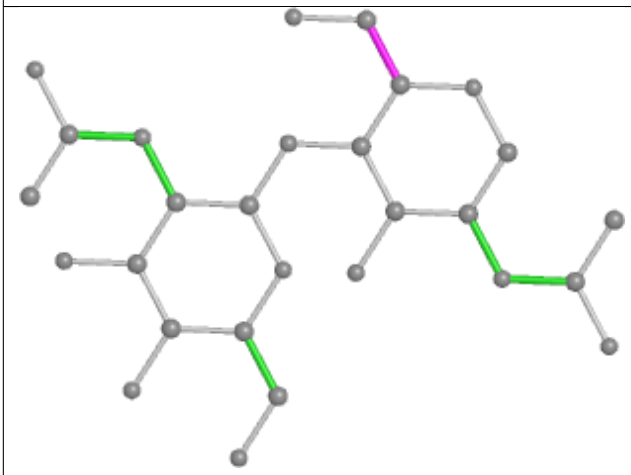
Oligosaccharide Chain D



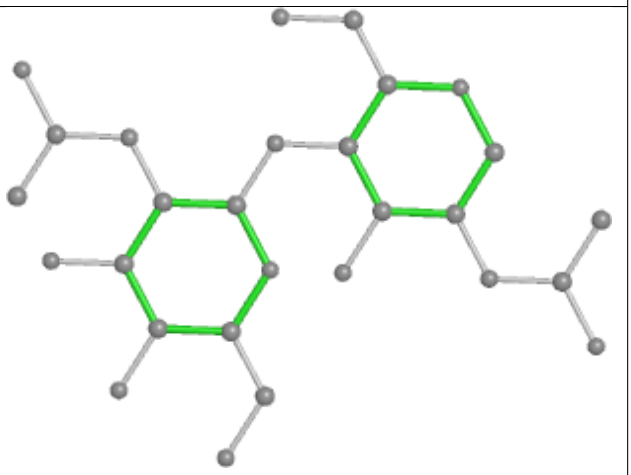
Bond lengths



Bond angles

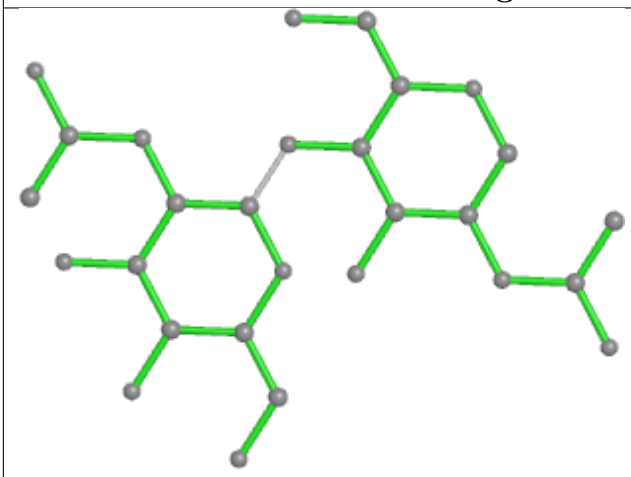


Torsions

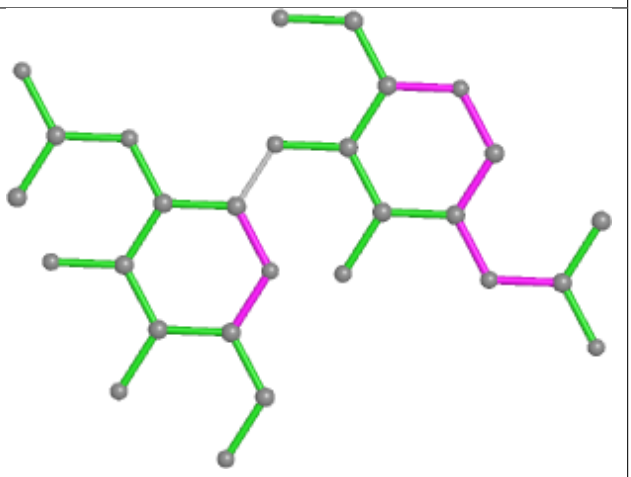


Rings

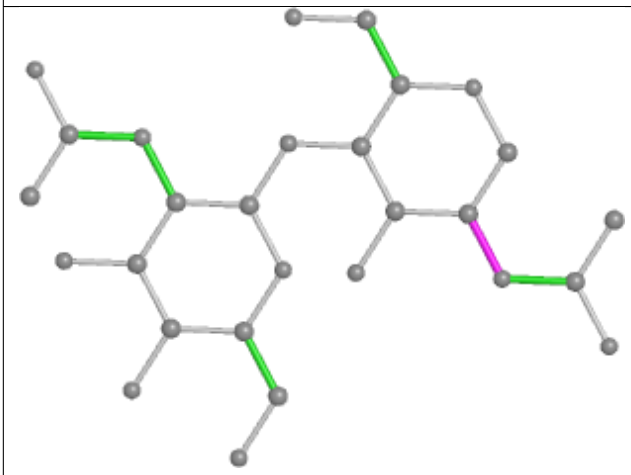
Oligosaccharide Chain E



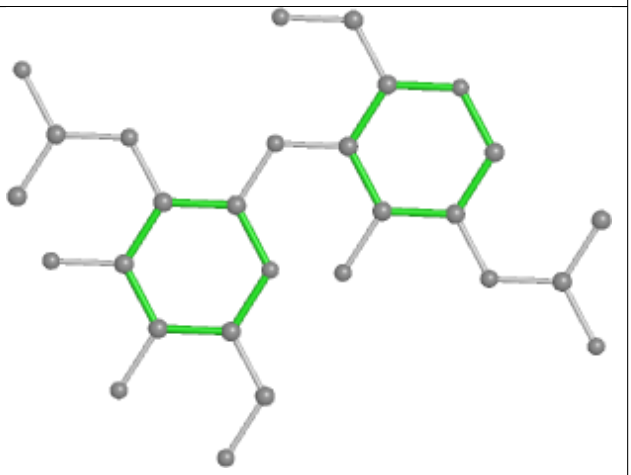
Bond lengths



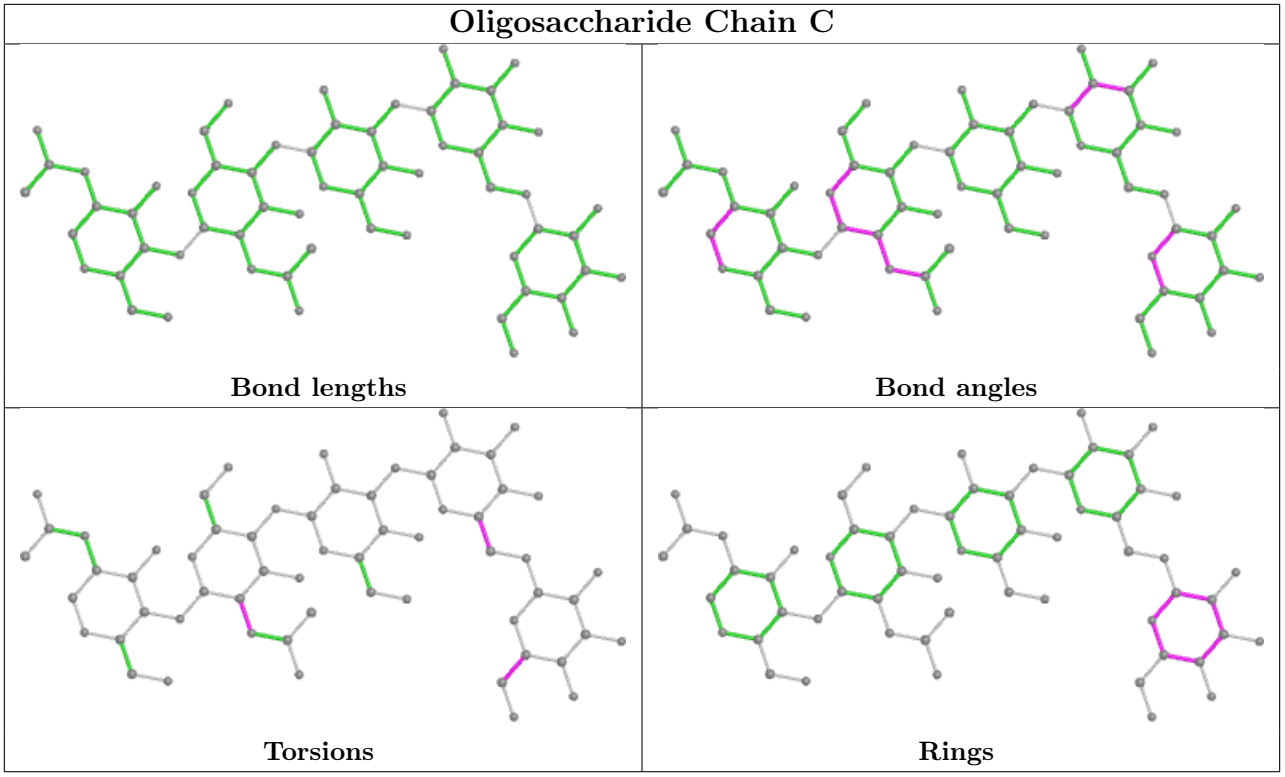
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\#\|Z\| > 2$
4	NAG	A	1601	1	14,14,15	0.38	0	17,19,21	0.74	0
6	EDO	A	1614	-	3,3,3	0.54	0	2,2,2	0.36	0
6	EDO	A	1615	-	3,3,3	0.53	0	2,2,2	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1601	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	1614	-	-	0/1/1/1	-
6	EDO	A	1615	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1601	NAG	C1-C2-N2-C7

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	1373/1494 (91%)	0.75	176 (12%)	3	5	101, 167, 228, 269	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	778	PHE	9.7
1	A	280	ALA	8.4
1	A	279	ILE	7.7
1	A	414	ARG	7.2
1	A	737	HIS	7.2
1	A	447	ILE	5.3
1	A	777	GLU	5.3
1	A	769	LEU	4.6
1	A	804	VAL	4.4
1	A	735	ILE	4.4
1	A	883	PRO	4.4
1	A	776	GLY	4.3
1	A	285	LEU	4.2
1	A	1013	LEU	4.2
1	A	461	ILE	4.1
1	A	236	LEU	4.0
1	A	1324	TYR	4.0
1	A	996	MET	4.0
1	A	540	GLN	4.0
1	A	1341	PHE	4.0
1	A	451	ILE	3.9
1	A	710	ASP	3.9
1	A	1129	PHE	3.9
1	A	814	ILE	3.9
1	A	736	VAL	3.8
1	A	652	LEU	3.8
1	A	706	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	283	LYS	3.8
1	A	474	LEU	3.7
1	A	245	VAL	3.7
1	A	418	TRP	3.7
1	A	1364	VAL	3.6
1	A	992	LEU	3.6
1	A	1354	LYS	3.5
1	A	450	LEU	3.5
1	A	364	GLN	3.5
1	A	539	GLU	3.5
1	A	499	PHE	3.5
1	A	633	TYR	3.4
1	A	646	PHE	3.4
1	A	811	LEU	3.4
1	A	849	LEU	3.4
1	A	676	TYR	3.3
1	A	705	VAL	3.3
1	A	1334	VAL	3.3
1	A	72	PHE	3.3
1	A	516	VAL	3.3
1	A	714	GLY	3.3
1	A	397	LEU	3.2
1	A	1040	LEU	3.2
1	A	1305	GLN	3.2
1	A	683	MET	3.2
1	A	501	PHE	3.2
1	A	1326	PHE	3.2
1	A	1395	LEU	3.2
1	A	954	LEU	3.2
1	A	959	PHE	3.1
1	A	526	LEU	3.1
1	A	470	VAL	3.1
1	A	238	LEU	3.1
1	A	487	LEU	3.1
1	A	95	MET	3.1
1	A	431	LEU	3.1
1	A	707	ALA	3.0
1	A	1059	LEU	3.0
1	A	1092	ILE	3.0
1	A	94	HIS	3.0
1	A	885	VAL	3.0
1	A	318	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	1298	VAL	3.0
1	A	916	ILE	3.0
1	A	900	PHE	3.0
1	A	448	TRP	2.9
1	A	715	GLN	2.9
1	A	731	VAL	2.9
1	A	828	PHE	2.9
1	A	820	PHE	2.9
1	A	1002	TRP	2.9
1	A	1056	GLY	2.9
1	A	655	ARG	2.9
1	A	1287	LEU	2.9
1	A	494	LEU	2.9
1	A	295	MET	2.9
1	A	244	ILE	2.8
1	A	1429	LYS	2.8
1	A	1363	VAL	2.8
1	A	416	PHE	2.8
1	A	722	LEU	2.8
1	A	469	VAL	2.8
1	A	994	VAL	2.8
1	A	1347	TRP	2.8
1	A	465	VAL	2.8
1	A	1039	ILE	2.8
1	A	1329	MET	2.7
1	A	675	ILE	2.7
1	A	918	PRO	2.7
1	A	1457	TRP	2.7
1	A	857	LEU	2.7
1	A	606	PRO	2.7
1	A	763	PHE	2.7
1	A	808	GLY	2.7
1	A	1356	TYR	2.7
1	A	1372	LEU	2.6
1	A	367	PRO	2.6
1	A	844	LEU	2.6
1	A	1069	PHE	2.6
1	A	909	THR	2.6
1	A	712	ILE	2.6
1	A	779	GLU	2.6
1	A	1151	GLU	2.6
1	A	643	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	733	LEU	2.5
1	A	636	MET	2.5
1	A	1351	LEU	2.5
1	A	617	MET	2.5
1	A	1299	ILE	2.5
1	A	721	ALA	2.5
1	A	1361	LEU	2.5
1	A	955	PRO	2.5
1	A	281	ASP	2.4
1	A	812	GLY	2.4
1	A	1296	ASP	2.4
1	A	1152	PRO	2.4
1	A	958	ARG	2.4
1	A	960	TYR	2.3
1	A	887	THR	2.3
1	A	803	PHE	2.3
1	A	956	VAL	2.3
1	A	1311	MET	2.3
1	A	566	LEU	2.3
1	A	919	ALA	2.3
1	A	621	LEU	2.3
1	A	717	LEU	2.3
1	A	729	ASP	2.3
1	A	601	PHE	2.3
1	A	1016	LEU	2.3
1	A	761	LEU	2.3
1	A	607	ILE	2.3
1	A	1254	TYR	2.2
1	A	59	ILE	2.2
1	A	689	ILE	2.2
1	A	810	VAL	2.2
1	A	1323	PRO	2.2
1	A	468	LEU	2.2
1	A	862	LEU	2.2
1	A	1290	LEU	2.2
1	A	360	LEU	2.1
1	A	430	TRP	2.1
1	A	659	ILE	2.1
1	A	284	PRO	2.1
1	A	533	LEU	2.1
1	A	234	VAL	2.1
1	A	429	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	293	LEU	2.1
1	A	240	ARG	2.1
1	A	329	ASN	2.1
1	A	109	LEU	2.1
1	A	1416	TRP	2.1
1	A	806	LEU	2.1
1	A	503	PRO	2.1
1	A	660	PHE	2.1
1	A	745	SER	2.1
1	A	915	VAL	2.1
1	A	634	PHE	2.1
1	A	1060	VAL	2.1
1	A	417	ASP	2.1
1	A	1106	GLU	2.1
1	A	497	VAL	2.1
1	A	962	TYR	2.0
1	A	628	LEU	2.0
1	A	637	LEU	2.0
1	A	945	LEU	2.0
1	A	952	GLU	2.0
1	A	1291	PHE	2.0
1	A	509	GLN	2.0
1	A	355	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
2	NAG	E	1	14/15	0.27	0.34	238,242,245,245	0
2	NAG	B	2	14/15	0.37	0.31	235,238,240,242	0
3	BMA	C	3	11/12	0.41	0.30	238,240,243,246	0
2	NAG	E	2	14/15	0.47	0.35	243,245,246,246	0
3	MAN	C	4	11/12	0.49	0.36	247,249,252,252	0

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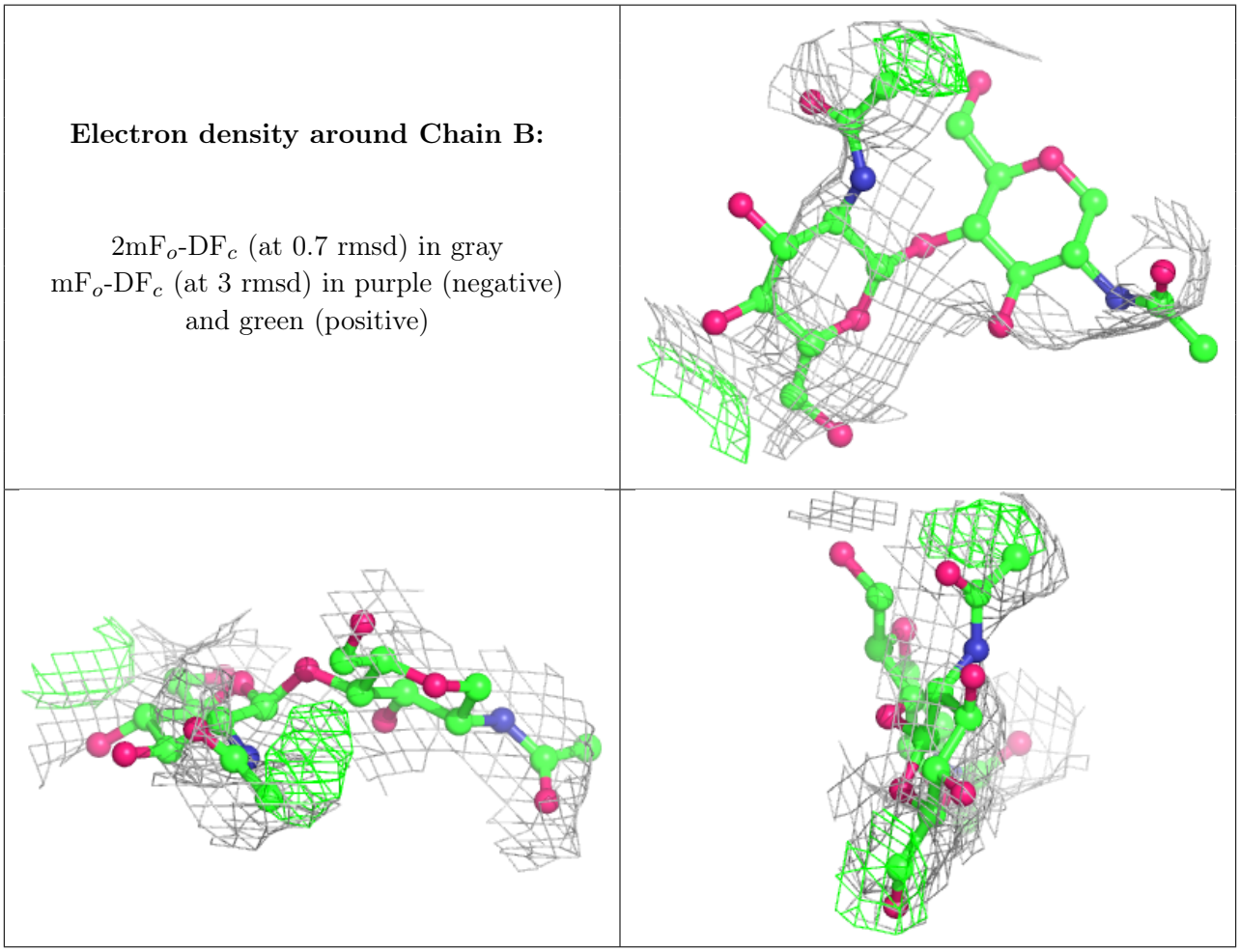
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MAN	C	5	11/12	0.62	0.35	243,247,248,249	0
2	NAG	D	1	14/15	0.68	0.28	207,217,224,228	0
2	NAG	D	2	14/15	0.69	0.42	227,232,234,235	0
3	NAG	C	2	14/15	0.70	0.25	203,214,225,232	0
2	NAG	B	1	14/15	0.77	0.17	213,218,226,231	0
3	NAG	C	1	14/15	0.87	0.23	171,184,192,199	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.

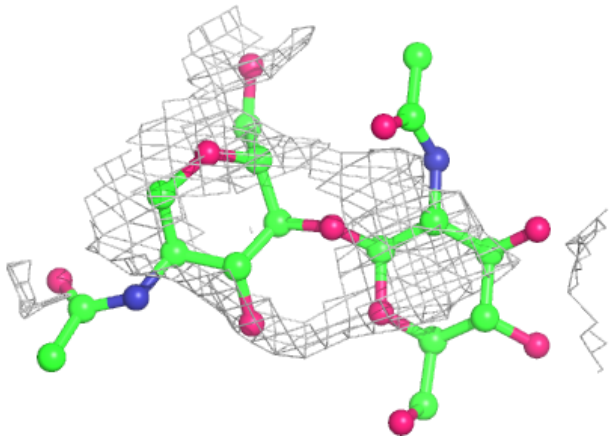
Electron density around Chain B:

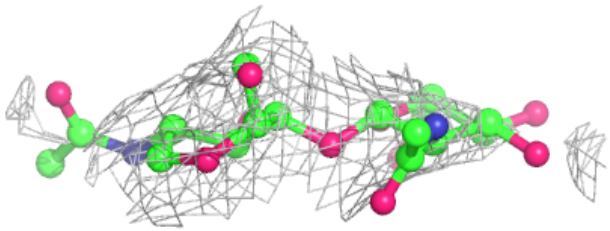
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

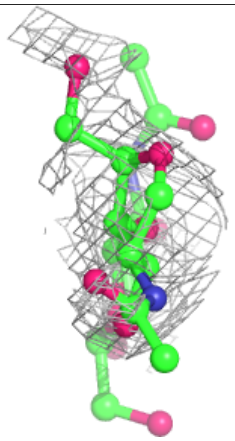


Electron density around Chain D:

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

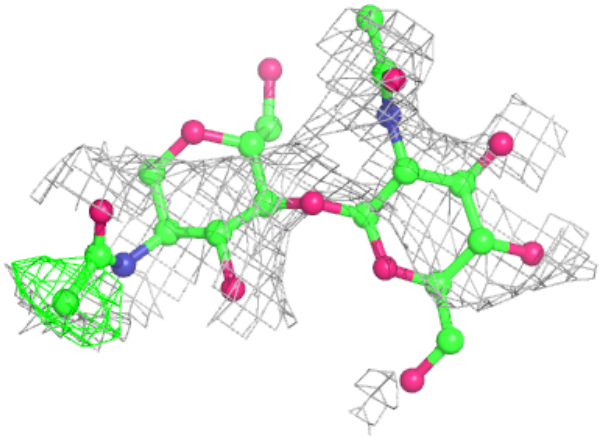


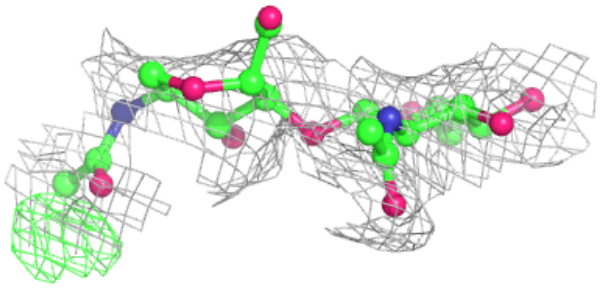


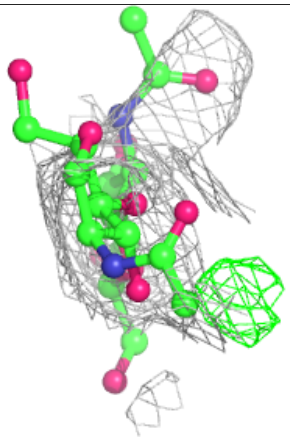


Electron density around Chain E:

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

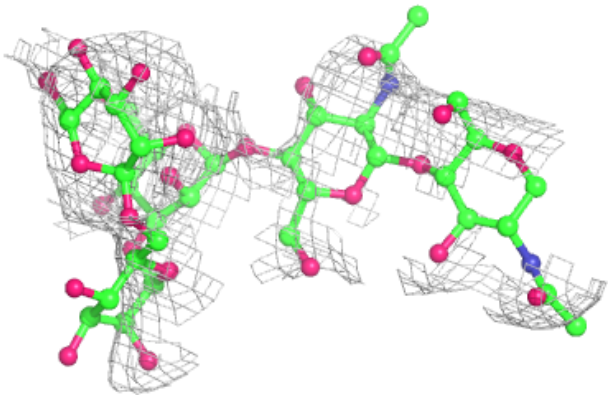


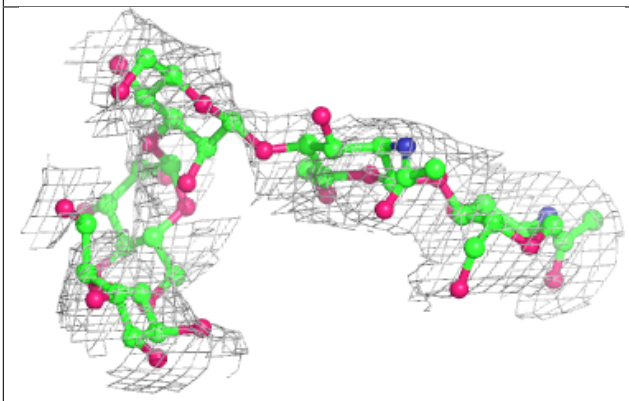


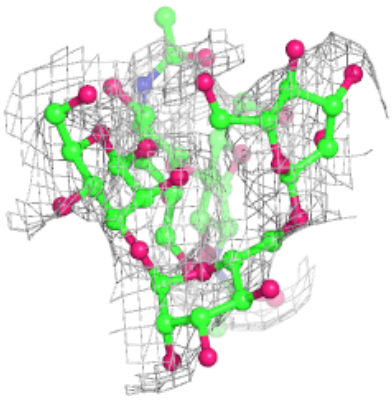


Electron density around Chain C:

$2mF_o$-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
5	CA	A	1613	1/1	0.10	0.46	167,167,167,167	1
4	NAG	A	1601	14/15	0.73	0.20	215,219,223,223	0
6	EDO	A	1614	4/4	0.87	1.14	121,122,122,122	0
6	EDO	A	1615	4/4	0.89	0.24	137,137,137,138	0

6.5 Other polymers

There are no such residues in this entry.