Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 11:12 AM EDT

PDB ID	:	5N2J
Title	:	UDP-Glucose Glycoprotein Glucosyltransferase from Chaetomium thermophilum (closed form)
Authors	:	Roversi, P.; Caputo, A.T.; Hill, J.; Alonzi, D.S.; Zitzmann, N.
Deposited on	:	2017-02-07
Resolution	:	4.40 Å(reported)

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

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

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

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

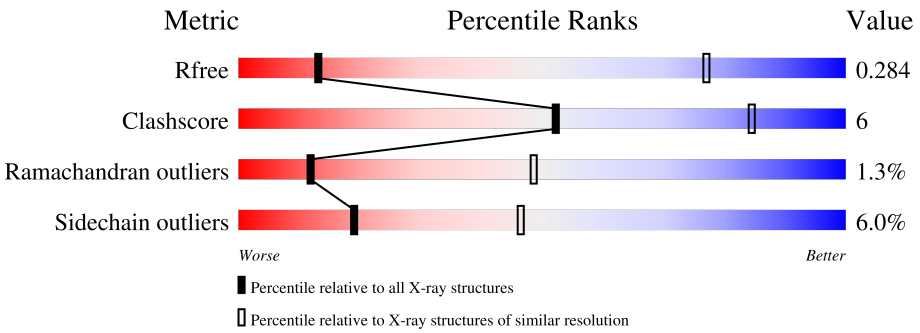
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.40 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	1043 (5.00-3.80)
Clashscore	141614	1111 (5.00-3.80)
Ramachandran outliers	138981	1059 (5.00-3.80)
Sidechain outliers	138945	1041 (5.00-3.80)

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%

Mol	Chain	Length	Quality of chain
1	A	1494	75% 16% • 8%
1	B	1494	74% 17% • 8%
2	C	3	100%
2	F	3	100%
3	D	5	20% 80%
3	G	5	20% 80%
4	E	2	100%

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Mol	Chain	Length	Quality of chain
4	H	2	100%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 44580 atoms, of which 22133 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.

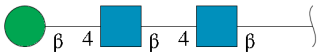
- Molecule 1 is a protein called UDP-glucose-glycoprotein glucosyltransferase-like protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	1373	21929	7057	10895	1880	2065	32	0	0	0
1	B	1381	22060	7098	10964	1889	2077	32	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

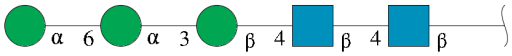
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLU	-	expression tag	UNP G0SB58
A	22	THR	-	expression tag	UNP G0SB58
A	23	GLY	-	expression tag	UNP G0SB58
A	1506	GLY	-	expression tag	UNP G0SB58
A	1507	THR	-	expression tag	UNP G0SB58
A	1508	LYS	-	expression tag	UNP G0SB58
A	1509	HIS	-	expression tag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

- Molecule 2 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
			Total	C	H	N	O			
2	C	3	73	22	34	2	15	0	0	0
2	F	3	73	22	34	2	15	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.

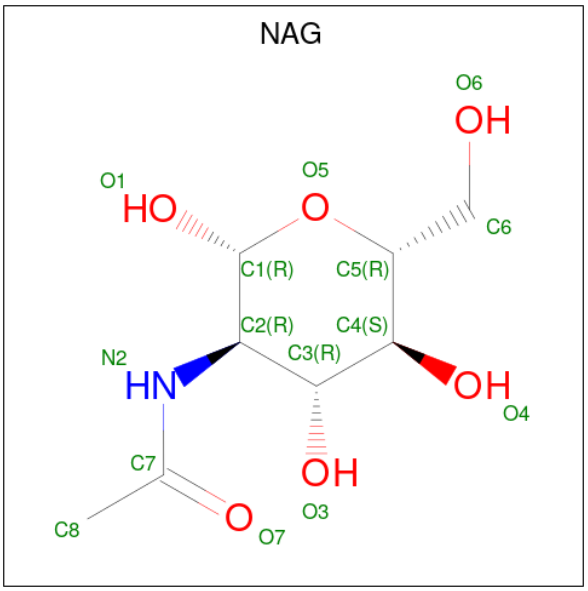


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
3	D	5	113	34	52	2	25	0	0	0
3	G	5	113	34	52	2	25	0	0	0

- Molecule 4 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
			Total	C	H	N	O			
4	E	2	53	16	25	2	10	0	0	0
4	H	2	53	16	25	2	10	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

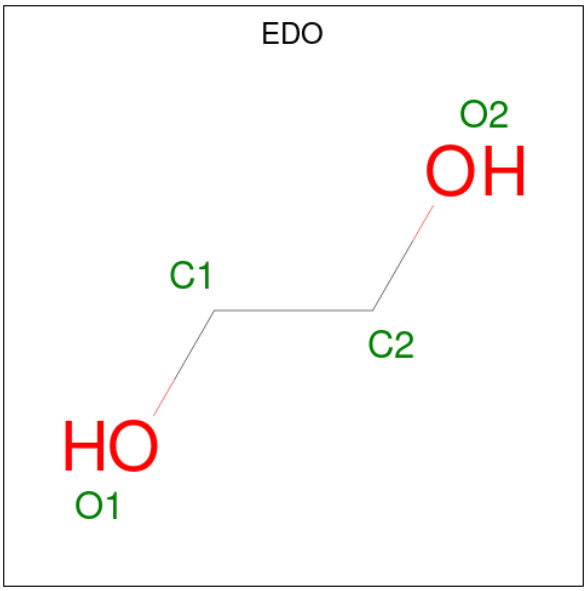


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
5	A	1	27	8	13	1	5	0	0
			Total	C	H	N	O		
5	A	1	27	8	13	1	5	0	0
			Total	C	H	N	O		
5	B	1	27	8	13	1	5	0	0
			Total	C	H	N	O		
5	B	1	27	8	13	1	5	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
6	A	1	1	1	0	0
			Total	Ca		
6	B	1	1	1	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O 1 1	0	0

- Molecule 8 is water.

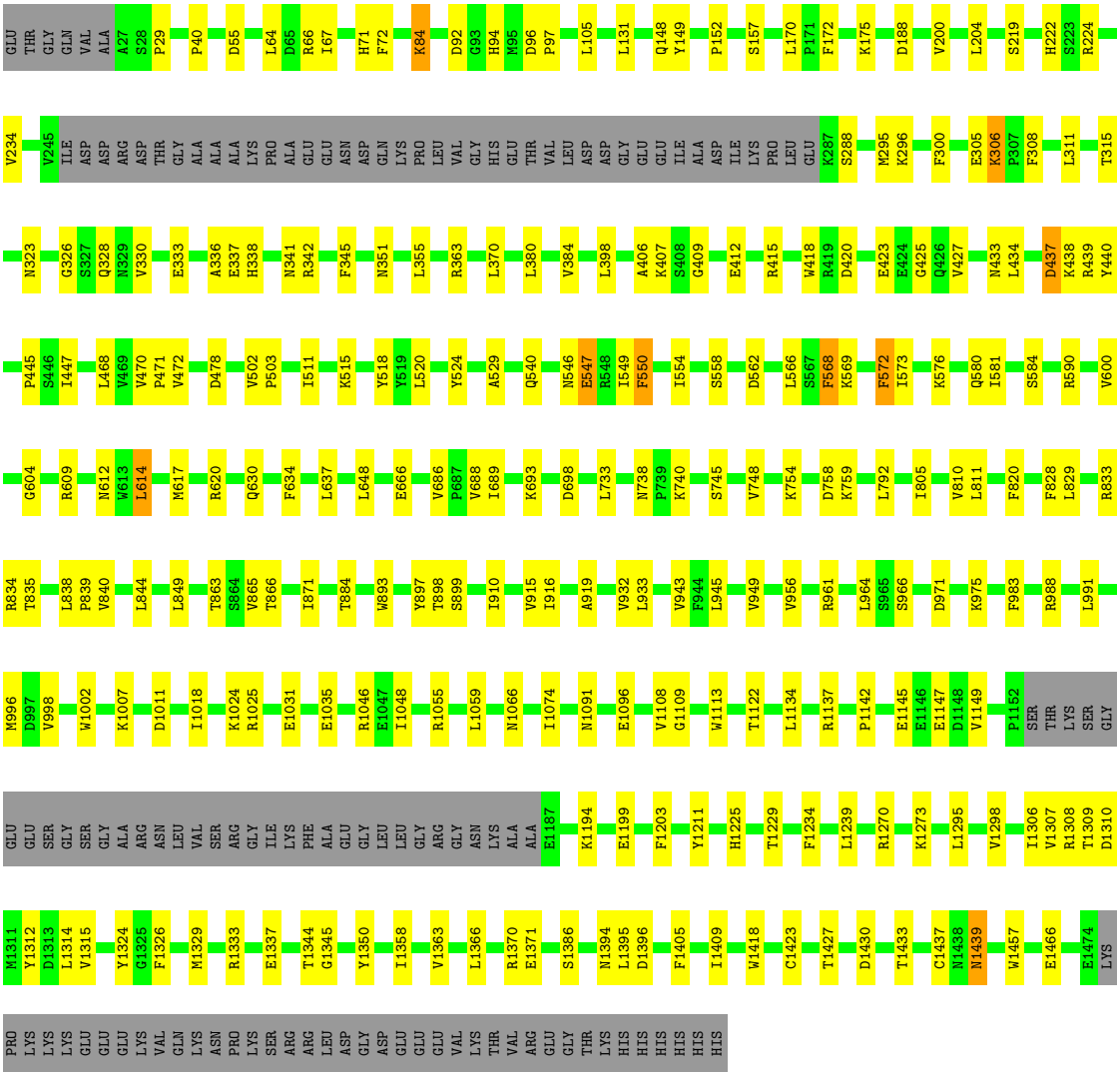
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O 1 1	0	0
8	B	1	Total O 1 1	0	0

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. 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. 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.

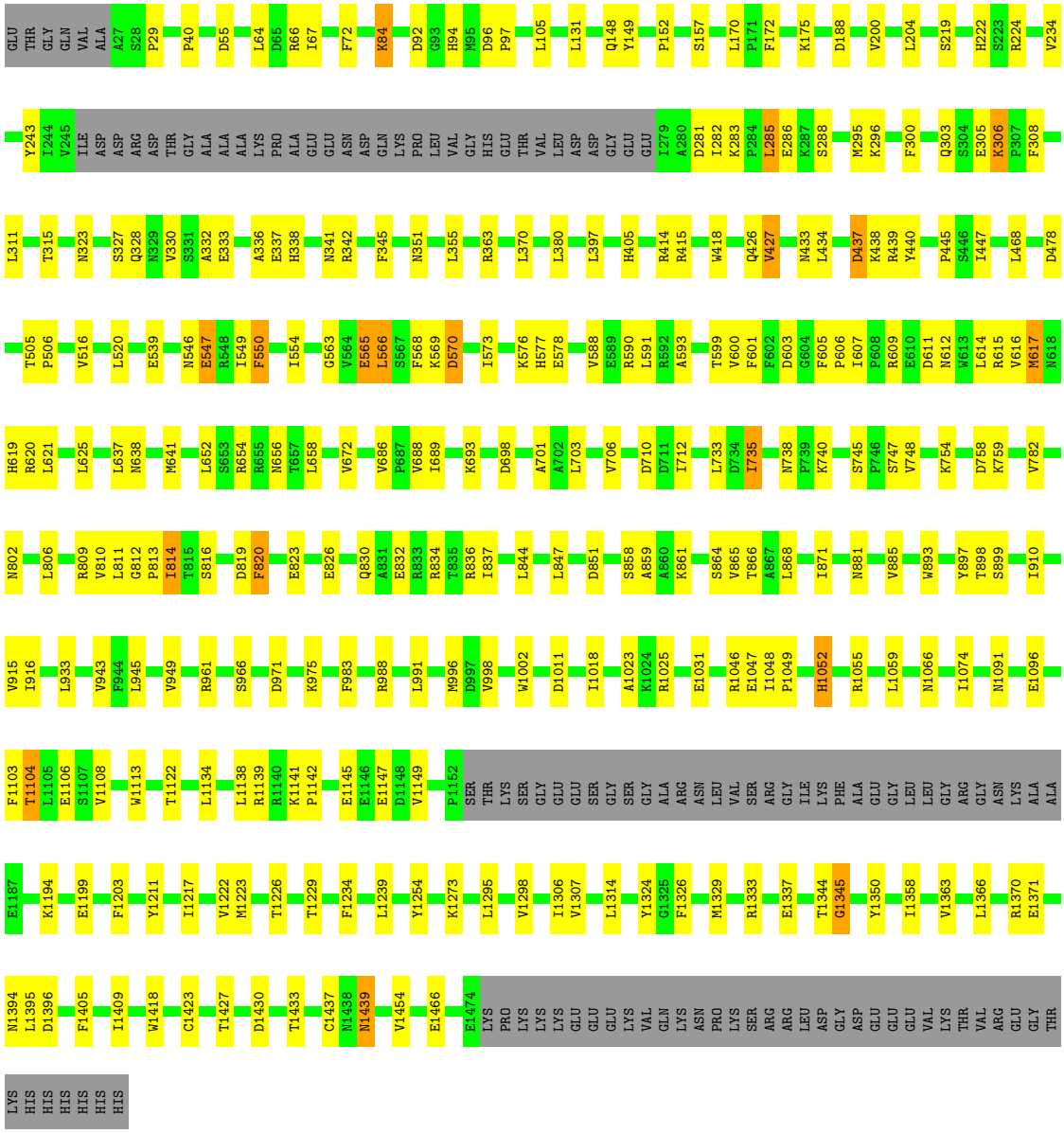
- Molecule 1: UDP-glucose-glycoprotein glucosyltransferase-like protein

Chain A:



- Molecule 1: UDP-glucose-glycoprotein glucosyltransferase-like protein

Chain B:



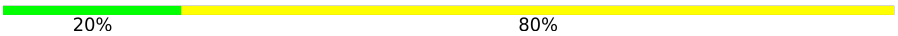
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 100%

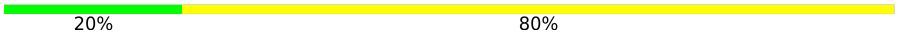
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%

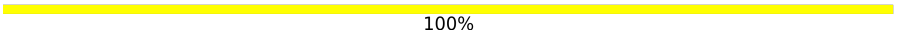
• Molecule 3: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 

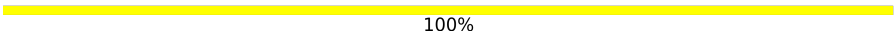
• Molecule 3: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 

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

Chain E: 

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

Chain H: 

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	148.60Å 148.60Å 179.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	114.59 – 4.40 114.59 – 4.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (114.59-4.40) 100.0 (114.59-4.30)	Depositor EDS
R_{merge}	0.78	Depositor
R_{sym}	0.81	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 4.30Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.201 , 0.259 0.227 , 0.284	Depositor DCC
R_{free} test set	1363 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	126.7	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 245.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.34$, $< L^2 > = 0.17$	Xtriage
Estimated twinning fraction	0.167 for h,-k,-l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	44580	wwPDB-VP
Average B, all atoms (Å^2)	243.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MAN, EDO, NAG, BMA

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	0.49	0/11298	0.74	2/15323 (0.0%)
1	B	0.55	0/11361	0.77	3/15409 (0.0%)
All	All	0.52	0/22659	0.75	5/30732 (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	5.80	136.21	121.70
1	B	305	GLU	C-N-CA	5.80	136.21	121.70
1	B	565	GLU	C-N-CA	5.52	135.50	121.70
1	B	306	LYS	N-CA-C	-5.42	96.38	111.00
1	A	306	LYS	N-CA-C	-5.29	96.70	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	11034	10895	10898	144	0
1	B	11096	10964	10966	105	0
2	C	39	34	34	0	0
2	F	39	34	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	61	52	52	0	0
3	G	61	52	52	0	0
4	E	28	25	25	0	0
4	H	28	25	25	0	0
5	A	28	26	26	0	0
5	B	28	26	26	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	1	0	0	0	0
8	A	1	0	0	1	0
8	B	1	0	0	0	0
All	All	22447	22133	22138	247	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 6.

All (247) 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:1225:HIS:ND1	1:A:1308:ARG:HA	1.68	1.07
1:B:243:TYR:O	1:B:285:LEU:HG	1.65	0.96
1:A:1225:HIS:CE1	1:A:1308:ARG:HA	2.04	0.93
1:A:1149:VAL:HG13	1:A:1371:GLU:O	1.71	0.90
1:B:1149:VAL:HG13	1:B:1371:GLU:O	1.73	0.87
1:A:326:GLY:HA2	1:A:330:VAL:HG11	1.59	0.84
1:A:67:ILE:HG22	1:A:72:PHE:CD2	2.16	0.81
1:B:67:ILE:HG22	1:B:72:PHE:CD2	2.18	0.79
1:A:554:ILE:HG23	1:A:558:SER:HB2	1.65	0.77
1:A:1295:LEU:HD21	1:A:1298:VAL:CG2	2.15	0.76
1:B:1295:LEU:HD21	1:B:1298:VAL:CG2	2.17	0.74
1:A:566:LEU:HD13	1:A:568:PHE:CD2	2.24	0.71
1:A:524:TYR:HE2	1:A:558:SER:HG	1.38	0.70
1:A:1225:HIS:ND1	1:A:1308:ARG:CA	2.53	0.70
1:A:1059:LEU:HD11	1:A:1074:ILE:HD11	1.74	0.69
1:A:515:LYS:HG3	1:A:581:ILE:HD11	1.75	0.69
1:B:1059:LEU:HD11	1:B:1074:ILE:HD11	1.76	0.68
1:B:414:ARG:HD2	1:B:652:LEU:HD11	1.76	0.67
1:A:384:VAL:HG23	1:A:865:VAL:HG11	1.77	0.66
1:A:834:ARG:O	1:A:839:PRO:HD3	1.97	0.65
1:A:686:VAL:O	1:A:754:LYS:HE2	1.98	0.64
1:A:1048:ILE:HD11	1:A:1137:ARG:HB3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1329:MET:HG2	1:A:1358:ILE:HD11	1.80	0.64
1:B:447:ILE:HD11	1:B:637:LEU:HB3	1.79	0.63
1:A:420:ASP:OD1	1:A:427:VAL:CG1	2.46	0.63
1:A:418:TRP:HE1	1:A:648:LEU:HD11	1.64	0.62
1:B:1329:MET:HG2	1:B:1358:ILE:HD11	1.81	0.62
1:A:515:LYS:CG	1:A:581:ILE:HD11	2.30	0.62
1:B:686:VAL:O	1:B:754:LYS:HE2	1.99	0.62
1:A:447:ILE:HD11	1:A:637:LEU:HB3	1.80	0.62
1:A:398:LEU:CD2	1:A:866:THR:HG22	2.29	0.61
1:B:1306:ILE:HD13	1:B:1454:VAL:HG21	1.83	0.60
1:A:338:HIS:HD2	1:A:898:THR:HG23	1.65	0.60
1:A:338:HIS:O	1:A:341:ASN:HB2	2.02	0.60
1:B:338:HIS:HD2	1:B:898:THR:HG23	1.67	0.59
1:A:295:MET:CE	1:A:949:VAL:HG12	2.32	0.59
1:A:152:PRO:HB3	1:A:200:VAL:HG21	1.85	0.58
1:A:470:VAL:HG23	1:A:600:VAL:HG22	1.85	0.58
1:A:384:VAL:CG2	1:A:865:VAL:HG11	2.33	0.58
1:A:420:ASP:OD1	1:A:427:VAL:HG13	2.04	0.58
1:A:1199:GLU:HG3	1:A:1229:THR:OG1	2.03	0.58
1:B:295:MET:CE	1:B:949:VAL:HG12	2.33	0.58
1:B:152:PRO:HB3	1:B:200:VAL:HG21	1.85	0.58
1:A:311:LEU:O	1:A:315:THR:HG22	2.04	0.58
1:A:420:ASP:HB3	1:A:425:GLY:HA2	1.87	0.57
1:A:829:LEU:O	1:A:833:ARG:HB2	2.04	0.57
1:B:1199:GLU:HG3	1:B:1229:THR:OG1	2.03	0.57
1:A:1307:VAL:HG13	1:A:1433:THR:HG22	1.87	0.57
1:B:338:HIS:O	1:B:341:ASN:HB2	2.04	0.57
1:A:554:ILE:O	1:A:558:SER:HB3	2.05	0.56
1:B:802:ASN:O	1:B:813:PRO:HA	2.05	0.56
1:A:67:ILE:HG22	1:A:72:PHE:HD2	1.71	0.56
1:A:573:ILE:HB	1:A:576:LYS:HB3	1.87	0.56
1:B:1108:VAL:HG12	1:B:1134:LEU:HD22	1.88	0.56
1:A:600:VAL:CG2	1:A:609:ARG:HG2	2.35	0.56
1:A:1108:VAL:HG12	1:A:1134:LEU:HD22	1.87	0.56
1:A:554:ILE:HG23	1:A:558:SER:CB	2.33	0.55
1:B:745:SER:O	1:B:748:VAL:HG22	2.07	0.55
1:A:554:ILE:O	1:A:558:SER:CB	2.54	0.55
1:A:66:ARG:O	1:A:71:HIS:HB3	2.07	0.55
1:B:311:LEU:O	1:B:315:THR:HG22	2.07	0.54
1:A:398:LEU:HD23	1:A:866:THR:HG22	1.89	0.54
1:A:524:TYR:HE2	1:A:558:SER:OG	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:LEU:HD23	1:B:440:TYR:CE2	2.43	0.54
1:A:745:SER:O	1:A:748:VAL:HG22	2.07	0.54
1:A:96:ASP:HB2	1:A:97:PRO:HD2	1.90	0.54
1:B:899:SER:HA	1:B:943:VAL:O	2.08	0.54
1:A:337:GLU:OE1	1:A:897:TYR:CD2	2.61	0.54
1:A:1418:TRP:HE1	1:A:1427:THR:HB	1.73	0.54
1:A:434:LEU:HD23	1:A:440:TYR:CE2	2.43	0.53
1:A:899:SER:HA	1:A:943:VAL:O	2.08	0.53
1:A:1091:ASN:OD1	1:A:1122:THR:HG23	2.09	0.53
1:A:170:LEU:HD11	1:A:172:PHE:CE1	2.43	0.53
1:B:234:VAL:HG22	1:B:996:MET:CE	2.38	0.53
1:A:566:LEU:HD13	1:A:568:PHE:CE2	2.44	0.53
1:B:170:LEU:HD11	1:B:172:PHE:CE1	2.44	0.53
1:A:72:PHE:CE1	1:A:84:LYS:HG3	2.44	0.53
1:A:420:ASP:OD1	1:A:427:VAL:HG12	2.10	0.52
1:B:735:ILE:N	1:B:735:ILE:HD12	2.24	0.52
1:A:29:PRO:HB2	1:A:1018:ILE:HD13	1.91	0.52
1:A:234:VAL:HG22	1:A:996:MET:CE	2.38	0.52
1:A:600:VAL:HG23	1:A:609:ARG:CG	2.40	0.52
1:A:630:GLN:O	1:A:634:PHE:HD1	1.93	0.52
1:B:1418:TRP:HE1	1:B:1427:THR:HB	1.74	0.52
1:B:96:ASP:HB2	1:B:97:PRO:HD2	1.92	0.52
1:B:333:GLU:CD	1:B:336:ALA:HB2	2.30	0.52
1:B:1091:ASN:OD1	1:B:1122:THR:HG23	2.10	0.52
1:B:1103:PHE:HB3	1:B:1138:LEU:HD22	1.92	0.52
1:A:296:LYS:HE2	1:A:330:VAL:HG13	1.92	0.51
1:A:547:GLU:HA	1:A:550:PHE:HB3	1.92	0.51
1:A:1048:ILE:CD1	1:A:1137:ARG:HB3	2.40	0.51
1:A:64:LEU:HD12	1:A:67:ILE:HD11	1.92	0.51
1:B:1222:VAL:O	1:B:1226:THR:HG22	2.10	0.51
1:A:1199:GLU:HB2	1:A:1229:THR:O	2.10	0.51
1:B:64:LEU:HD12	1:B:67:ILE:HD11	1.92	0.51
1:B:355:LEU:HD11	1:B:910:ILE:HG23	1.93	0.51
1:A:333:GLU:CD	1:A:336:ALA:HB2	2.32	0.51
1:A:524:TYR:HE2	1:A:558:SER:CB	2.24	0.50
1:B:337:GLU:OE1	1:B:897:TYR:CD2	2.64	0.50
1:A:1059:LEU:CD1	1:A:1074:ILE:HD11	2.40	0.50
1:B:547:GLU:HA	1:B:550:PHE:HB3	1.93	0.50
1:B:1059:LEU:CD1	1:B:1074:ILE:HD11	2.41	0.50
1:A:1306:ILE:HD11	1:A:1457:TRP:HD1	1.75	0.50
1:B:1104:THR:HG23	1:B:1139:ARG:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1307:VAL:HG13	1:B:1433:THR:HG22	1.93	0.50
1:B:72:PHE:CE1	1:B:84:LYS:HG3	2.46	0.50
1:B:29:PRO:HB2	1:B:1018:ILE:HD13	1.93	0.50
1:A:518:TYR:HB3	1:A:580:GLN:OE1	2.12	0.49
1:B:1046:ARG:HA	1:B:1052:HIS:O	2.12	0.49
1:A:468:LEU:HD22	1:A:617:MET:SD	2.53	0.49
1:B:380:LEU:HG	1:B:865:VAL:HG13	1.95	0.49
1:A:472:VAL:O	1:A:503:PRO:HA	2.11	0.49
1:A:355:LEU:HD11	1:A:910:ILE:HG23	1.93	0.49
1:A:511:ILE:HG23	1:A:581:ILE:HD13	1.94	0.49
1:B:590:ARG:O	1:B:654:ARG:HA	2.13	0.48
1:A:1324:TYR:CD1	1:A:1326:PHE:HE1	2.31	0.48
1:B:1199:GLU:HB2	1:B:1229:THR:O	2.11	0.48
1:A:1295:LEU:HD21	1:A:1298:VAL:HG22	1.94	0.48
1:A:546:ASN:HB3	1:A:549:ILE:HG22	1.96	0.48
1:A:1048:ILE:HD11	1:A:1137:ARG:HD2	1.95	0.48
1:A:1324:TYR:CE1	1:A:1409:ILE:HG12	2.48	0.48
1:A:1109:GLY:HA2	8:A:1701:HOH:O	2.14	0.48
1:B:1104:THR:HG22	1:B:1141:LYS:HG3	1.96	0.48
1:B:1048:ILE:HG22	1:B:1049:PRO:HA	1.95	0.48
1:B:1329:MET:SD	1:B:1358:ILE:HD11	2.54	0.48
1:B:1324:TYR:CE1	1:B:1409:ILE:HG12	2.49	0.48
1:A:524:TYR:CD2	1:A:558:SER:HA	2.49	0.47
1:A:835:THR:O	1:A:839:PRO:HD2	2.14	0.47
1:A:840:VAL:HG21	1:A:863:THR:HA	1.96	0.47
1:B:554:ILE:HG21	1:B:568:PHE:CE2	2.49	0.47
1:A:345:PHE:HB3	1:A:893:TRP:CZ2	2.50	0.47
1:A:370:LEU:HD13	1:A:933:LEU:HD11	1.96	0.47
1:A:468:LEU:HD11	1:A:600:VAL:CG1	2.45	0.47
1:A:1350:TYR:O	1:A:1405:PHE:HZ	1.97	0.47
1:B:1047:GLU:HG2	1:B:1052:HIS:HB2	1.96	0.47
1:A:614:LEU:HD12	1:A:617:MET:CE	2.45	0.47
1:A:433:ASN:O	1:A:437:ASP:HB2	2.15	0.47
1:A:471:PRO:HA	1:A:502:VAL:O	2.14	0.47
1:B:296:LYS:HG2	1:B:330:VAL:HG13	1.95	0.47
1:A:200:VAL:O	1:A:204:LEU:HG	2.14	0.47
1:A:338:HIS:CD2	1:A:898:THR:HG23	2.48	0.47
1:A:600:VAL:HG23	1:A:609:ARG:HG2	1.95	0.47
1:A:1329:MET:CG	1:A:1358:ILE:HD11	2.44	0.47
1:B:370:LEU:HD13	1:B:933:LEU:HD11	1.97	0.47
1:B:546:ASN:HB3	1:B:549:ILE:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:LEU:HG	1:A:865:VAL:HG13	1.98	0.46
1:B:810:VAL:HG12	1:B:811:LEU:N	2.30	0.46
1:A:407:LYS:NZ	1:A:884:THR:HB	2.30	0.46
1:A:961:ARG:HG2	1:A:983:PHE:CE2	2.50	0.46
1:A:1329:MET:SD	1:A:1358:ILE:HD11	2.56	0.46
1:A:1333:ARG:HG2	1:A:1423:CYS:C	2.35	0.46
1:B:345:PHE:HB3	1:B:893:TRP:CZ2	2.51	0.46
1:A:92:ASP:HB2	1:A:94:HIS:CD2	2.51	0.46
1:B:961:ARG:HG2	1:B:983:PHE:CE2	2.51	0.46
1:B:1046:ARG:NH2	1:B:1113:TRP:O	2.49	0.46
1:B:1329:MET:CG	1:B:1358:ILE:HD11	2.45	0.46
1:B:686:VAL:O	1:B:688:VAL:HG23	2.16	0.46
1:A:998:VAL:HG22	1:A:1002:TRP:HB2	1.98	0.46
1:B:1223:MET:HG3	1:B:1254:TYR:HB3	1.98	0.46
1:B:1324:TYR:CD1	1:B:1326:PHE:HE1	2.34	0.46
1:A:188:ASP:OD1	1:A:219:SER:HB3	2.16	0.45
1:A:1046:ARG:NH2	1:A:1113:TRP:O	2.50	0.45
1:A:1314:LEU:HG	1:A:1363:VAL:CG2	2.47	0.45
1:B:1295:LEU:HD21	1:B:1298:VAL:HG22	1.95	0.45
1:B:92:ASP:HB2	1:B:94:HIS:CD2	2.52	0.45
1:B:1333:ARG:HG2	1:B:1423:CYS:C	2.37	0.45
1:A:415:ARG:HA	1:A:604:GLY:O	2.17	0.45
1:A:520:LEU:HD23	1:A:529:ALA:HA	1.99	0.45
1:A:573:ILE:CG2	1:B:1023:ALA:O	2.65	0.45
1:A:738:ASN:HD22	1:A:792:LEU:HD11	1.82	0.45
1:B:67:ILE:HG22	1:B:72:PHE:HD2	1.74	0.45
1:A:326:GLY:CA	1:A:330:VAL:HG11	2.38	0.45
1:A:1309:THR:HG22	1:A:1310:ASP:O	2.17	0.45
1:A:418:TRP:NE1	1:A:648:LEU:HD11	2.30	0.45
1:A:600:VAL:CG2	1:A:609:ARG:CG	2.94	0.44
1:B:1366:LEU:O	1:B:1370:ARG:HG3	2.17	0.44
1:B:433:ASN:O	1:B:437:ASP:HB2	2.17	0.44
1:B:812:GLY:CA	1:B:814:ILE:HD13	2.47	0.44
1:A:686:VAL:O	1:A:688:VAL:HG23	2.17	0.44
1:A:573:ILE:HG22	1:B:1023:ALA:O	2.17	0.44
1:A:1366:LEU:O	1:A:1370:ARG:HG3	2.16	0.44
1:B:658:LEU:HD22	1:B:814:ILE:HD12	1.99	0.44
1:A:370:LEU:HD13	1:A:933:LEU:CD1	2.48	0.44
1:A:406:ALA:HB2	1:A:839:PRO:HG2	1.99	0.44
1:B:397:LEU:HD21	1:B:866:THR:CG2	2.48	0.44
1:B:998:VAL:HG22	1:B:1002:TRP:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1314:LEU:HG	1:B:1363:VAL:CG2	2.48	0.44
1:B:131:LEU:HD11	1:B:148:GLN:OE1	2.17	0.44
1:A:572:PHE:CD2	1:A:572:PHE:N	2.85	0.44
1:B:812:GLY:HA2	1:B:814:ILE:HD13	1.99	0.44
1:A:149:TYR:CE1	1:A:157:SER:HB3	2.52	0.44
1:A:351:ASN:HA	1:A:915:VAL:O	2.18	0.44
1:B:370:LEU:HD13	1:B:933:LEU:CD1	2.48	0.43
1:B:188:ASP:OD1	1:B:219:SER:HB3	2.18	0.43
1:A:105:LEU:HD13	1:A:966:SER:HA	2.00	0.43
1:A:844:LEU:HD12	1:A:849:LEU:HB2	1.99	0.43
1:B:105:LEU:HD13	1:B:966:SER:HA	2.00	0.43
1:B:295:MET:HE3	1:B:949:VAL:HG12	2.01	0.43
1:B:588:VAL:HG13	1:B:593:ALA:O	2.18	0.43
1:A:1234:PHE:HB3	1:A:1239:LEU:HD11	2.01	0.43
1:B:1048:ILE:HD12	1:B:1106:GLU:OE1	2.19	0.43
1:B:338:HIS:CD2	1:B:898:THR:HG23	2.49	0.43
1:B:351:ASN:HA	1:B:915:VAL:O	2.19	0.43
1:B:505:THR:N	1:B:506:PRO:HD3	2.34	0.43
1:A:689:ILE:HD12	1:A:733:LEU:HD23	2.01	0.42
1:B:149:TYR:CE1	1:B:157:SER:HB3	2.54	0.42
1:B:1395:LEU:HD12	1:B:1396:ASP:N	2.34	0.42
1:A:811:LEU:HD11	1:A:828:PHE:CE1	2.54	0.42
1:A:40:PRO:HB3	1:A:224:ARG:HD2	2.01	0.42
1:A:131:LEU:HD11	1:A:148:GLN:OE1	2.18	0.42
1:B:591:LEU:HD22	1:B:601:PHE:CZ	2.55	0.42
1:A:427:VAL:CG2	1:A:584:SER:HA	2.50	0.42
1:A:1011:ASP:CG	1:A:1025:ARG:HH22	2.22	0.42
1:B:689:ILE:HD12	1:B:733:LEU:HD23	2.01	0.42
1:A:916:ILE:O	1:A:945:LEU:HA	2.19	0.42
1:A:919:ALA:O	1:A:956:VAL:HG23	2.20	0.42
1:A:1314:LEU:HG	1:A:1363:VAL:HG22	2.02	0.42
1:A:1395:LEU:HD12	1:A:1396:ASP:N	2.34	0.42
1:B:617:MET:SD	1:B:617:MET:N	2.93	0.42
1:B:916:ILE:O	1:B:945:LEU:HA	2.20	0.42
1:B:1234:PHE:HB3	1:B:1239:LEU:HD11	2.01	0.42
1:A:600:VAL:HG23	1:A:609:ARG:HG3	2.02	0.42
1:B:599:THR:CG2	1:B:606:PRO:HB2	2.50	0.42
1:A:805:ILE:HG12	1:A:810:VAL:HG22	2.01	0.42
1:B:600:VAL:N	1:B:607:ILE:O	2.53	0.42
1:A:838:LEU:HD23	1:A:838:LEU:HA	1.80	0.41
1:B:40:PRO:HB3	1:B:224:ARG:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:988:ARG:HA	1:B:1018:ILE:HB	2.00	0.41
1:A:1312:TYR:O	1:A:1315:VAL:N	2.52	0.41
1:A:1007:LYS:HG3	1:A:1035:GLU:HB2	2.02	0.41
1:B:327:SER:O	1:B:330:VAL:HB	2.20	0.41
1:A:1108:VAL:CG1	1:A:1134:LEU:HD22	2.51	0.41
1:A:1344:THR:HG22	1:A:1345:GLY:N	2.35	0.41
1:B:814:ILE:HG21	1:B:820:PHE:HB2	2.02	0.41
1:B:380:LEU:HD11	1:B:868:LEU:HB2	2.03	0.41
1:B:1011:ASP:CG	1:B:1025:ARG:HH22	2.23	0.41
1:B:1344:THR:HG22	1:B:1345:GLY:N	2.36	0.41
1:A:932:VAL:HG11	1:A:964:LEU:HG	2.03	0.41
1:A:524:TYR:CE2	1:A:558:SER:HA	2.56	0.41
1:A:1270:ARG:HD2	1:A:1386:SER:OG	2.20	0.41
1:B:568:PHE:O	1:B:570:ASP:N	2.52	0.41
1:B:672:VAL:HG23	1:B:864:SER:OG	2.20	0.41
1:B:836:ARG:C	1:B:837:ILE:HD12	2.41	0.41
1:A:423:GLU:OE1	1:A:590:ARG:NH1	2.54	0.41
1:B:303:GLN:HE22	1:B:330:VAL:HA	1.86	0.41
1:B:1350:TYR:O	1:B:1405:PHE:HZ	2.04	0.40
1:A:149:TYR:HE1	1:A:157:SER:HB3	1.87	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	1367/1494 (92%)	1297 (95%)	59 (4%)	11 (1%)	19 60
1	B	1375/1494 (92%)	1265 (92%)	84 (6%)	26 (2%)	8 41
All	All	2742/2988 (92%)	2562 (93%)	143 (5%)	37 (1%)	12 48

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	SER
1	A	569	LYS
1	A	1439	ASN
1	B	288	SER
1	B	332	ALA
1	B	426	GLN
1	B	539	GLU
1	B	566	LEU
1	B	603	ASP
1	B	859	ALA
1	B	1439	ASN
1	B	427	VAL
1	B	563	GLY
1	B	569	LYS
1	B	611	ASP
1	B	616	VAL
1	B	710	ASP
1	B	712	ILE
1	B	747	SER
1	B	782	VAL
1	A	568	PHE
1	A	666	GLU
1	A	1337	GLU
1	B	701	ALA
1	B	1337	GLU
1	B	577	HIS
1	B	615	ARG
1	A	306	LYS
1	A	572	PHE
1	A	1142	PRO
1	B	306	LYS
1	B	1142	PRO
1	A	409	GLY
1	B	445	PRO
1	A	445	PRO
1	B	282	ILE
1	B	1345	GLY

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%)	1150 (96%)	49 (4%)	30	56
1	B	1206/1297 (93%)	1110 (92%)	96 (8%)	12	38
All	All	2405/2594 (93%)	2260 (94%)	145 (6%)	19	46

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ASP
1	A	84	LYS
1	A	175	LYS
1	A	222	HIS
1	A	300	PHE
1	A	308	PHE
1	A	323	ASN
1	A	328	GLN
1	A	342	ARG
1	A	363	ARG
1	A	412	GLU
1	A	437	ASP
1	A	438	LYS
1	A	439	ARG
1	A	478	ASP
1	A	540	GLN
1	A	547	GLU
1	A	550	PHE
1	A	562	ASP
1	A	612	ASN
1	A	614	LEU
1	A	620	ARG
1	A	693	LYS
1	A	698	ASP
1	A	740	LYS
1	A	758	ASP
1	A	759	LYS
1	A	820	PHE
1	A	871	ILE
1	A	971	ASP
1	A	975	LYS
1	A	988	ARG
1	A	991	LEU

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Mol	Chain	Res	Type
1	A	1024	LYS
1	A	1031	GLU
1	A	1055	ARG
1	A	1066	ASN
1	A	1096	GLU
1	A	1145	GLU
1	A	1147	GLU
1	A	1194	LYS
1	A	1203	PHE
1	A	1211	TYR
1	A	1273	LYS
1	A	1394	ASN
1	A	1430	ASP
1	A	1437	CYS
1	A	1439	ASN
1	A	1466	GLU
1	B	55	ASP
1	B	66	ARG
1	B	84	LYS
1	B	175	LYS
1	B	204	LEU
1	B	222	HIS
1	B	281	ASP
1	B	283	LYS
1	B	285	LEU
1	B	286	GLU
1	B	300	PHE
1	B	308	PHE
1	B	323	ASN
1	B	328	GLN
1	B	342	ARG
1	B	363	ARG
1	B	405	HIS
1	B	415	ARG
1	B	418	TRP
1	B	427	VAL
1	B	437	ASP
1	B	438	LYS
1	B	439	ARG
1	B	468	LEU
1	B	478	ASP
1	B	516	VAL

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Mol	Chain	Res	Type
1	B	520	LEU
1	B	547	GLU
1	B	550	PHE
1	B	565	GLU
1	B	566	LEU
1	B	570	ASP
1	B	573	ILE
1	B	576	LYS
1	B	578	GLU
1	B	605	PHE
1	B	609	ARG
1	B	612	ASN
1	B	614	LEU
1	B	617	MET
1	B	619	HIS
1	B	620	ARG
1	B	621	LEU
1	B	625	LEU
1	B	638	ASN
1	B	641	MET
1	B	656	ASN
1	B	693	LYS
1	B	698	ASP
1	B	703	LEU
1	B	706	VAL
1	B	735	ILE
1	B	738	ASN
1	B	740	LYS
1	B	758	ASP
1	B	759	LYS
1	B	806	LEU
1	B	809	ARG
1	B	814	ILE
1	B	816	SER
1	B	819	ASP
1	B	820	PHE
1	B	823	GLU
1	B	826	GLU
1	B	830	GLN
1	B	832	GLU
1	B	834	ARG
1	B	844	LEU

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Mol	Chain	Res	Type
1	B	847	LEU
1	B	851	ASP
1	B	858	SER
1	B	861	LYS
1	B	871	ILE
1	B	881	ASN
1	B	885	VAL
1	B	971	ASP
1	B	975	LYS
1	B	991	LEU
1	B	1031	GLU
1	B	1052	HIS
1	B	1055	ARG
1	B	1066	ASN
1	B	1096	GLU
1	B	1104	THR
1	B	1145	GLU
1	B	1147	GLU
1	B	1194	LYS
1	B	1203	PHE
1	B	1211	TYR
1	B	1217	ILE
1	B	1273	LYS
1	B	1394	ASN
1	B	1430	ASP
1	B	1437	CYS
1	B	1439	ASN
1	B	1466	GLU

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

Mol	Chain	Res	Type
1	A	94	HIS
1	A	513	GLN
1	A	751	GLN
1	A	1058	GLN
1	B	94	HIS
1	B	303	GLN
1	B	323	ASN
1	B	400	HIS
1	B	523	ASN
1	B	738	ASN

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Mol	Chain	Res	Type
1	B	751	GLN
1	B	1058	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

20 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	C	1	2,1	14,14,15	0.33	0	17,19,21	0.91	1 (5%)
2	NAG	C	2	2	14,14,15	0.48	0	17,19,21	1.62	2 (11%)
2	BMA	C	3	2	11,11,12	0.50	0	15,15,17	0.83	1 (6%)
3	NAG	D	1	3,1	14,14,15	0.30	0	17,19,21	2.47	2 (11%)
3	NAG	D	2	3	14,14,15	0.36	0	17,19,21	1.70	2 (11%)
3	BMA	D	3	3	11,11,12	0.32	0	15,15,17	0.54	0
3	MAN	D	4	3	11,11,12	0.47	0	15,15,17	0.94	1 (6%)
3	MAN	D	5	3	11,11,12	0.41	0	15,15,17	1.11	1 (6%)
4	NAG	E	1	4,1	14,14,15	0.37	0	17,19,21	0.86	1 (5%)
4	NAG	E	2	4	14,14,15	0.44	0	17,19,21	1.62	2 (11%)
2	NAG	F	1	2,1	14,14,15	0.33	0	17,19,21	0.85	1 (5%)
2	NAG	F	2	2	14,14,15	0.52	0	17,19,21	1.48	2 (11%)
2	BMA	F	3	2	11,11,12	0.54	0	15,15,17	0.91	1 (6%)
3	NAG	G	1	3,1	14,14,15	0.24	0	17,19,21	2.49	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	G	2	3	14,14,15	0.34	0	17,19,21	1.83	2 (11%)
3	BMA	G	3	3	11,11,12	0.36	0	15,15,17	0.56	0
3	MAN	G	4	3	11,11,12	0.41	0	15,15,17	0.94	1 (6%)
3	MAN	G	5	3	11,11,12	0.37	0	15,15,17	1.09	1 (6%)
4	NAG	H	1	4,1	14,14,15	0.36	0	17,19,21	0.92	1 (5%)
4	NAG	H	2	4	14,14,15	0.45	0	17,19,21	1.69	2 (11%)

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	C	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	1/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	0/1/1/1
3	MAN	D	5	3	-	1/2/19/22	1/1/1/1
4	NAG	E	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	1/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	BMA	F	3	2	-	2/2/19/22	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	MAN	G	4	3	-	2/2/19/22	0/1/1/1
3	MAN	G	5	3	-	1/2/19/22	1/1/1/1
4	NAG	H	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	1	NAG	C1-O5-C5	8.40	123.57	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1	NAG	C1-O5-C5	8.39	123.56	112.19
3	G	2	NAG	O5-C1-C2	6.14	120.98	111.29
3	D	2	NAG	O5-C1-C2	5.81	120.46	111.29
4	H	2	NAG	C1-O5-C5	5.19	119.22	112.19
3	G	1	NAG	O5-C1-C2	4.96	119.13	111.29
4	E	2	NAG	C1-O5-C5	4.87	118.78	112.19
3	D	1	NAG	O5-C1-C2	4.85	118.94	111.29
2	C	2	NAG	C1-O5-C5	4.70	118.56	112.19
4	H	2	NAG	O5-C1-C2	4.21	117.94	111.29
2	F	2	NAG	O4-C4-C5	4.15	119.61	109.30
4	E	2	NAG	O5-C1-C2	4.10	117.77	111.29
3	D	5	MAN	C1-O5-C5	3.99	117.60	112.19
3	G	5	MAN	C1-O5-C5	3.92	117.50	112.19
2	F	2	NAG	C1-O5-C5	3.50	116.94	112.19
2	C	2	NAG	O4-C4-C5	3.38	117.70	109.30
3	G	2	NAG	C1-O5-C5	2.90	116.12	112.19
2	C	1	NAG	O5-C1-C2	-2.86	106.77	111.29
3	D	4	MAN	C1-C2-C3	2.64	112.91	109.67
3	D	2	NAG	C1-O5-C5	2.62	115.74	112.19
3	G	4	MAN	C1-C2-C3	2.45	112.68	109.67
4	E	1	NAG	C1-O5-C5	2.41	115.46	112.19
4	H	1	NAG	C1-O5-C5	2.33	115.35	112.19
2	C	3	BMA	C1-O5-C5	2.23	115.21	112.19
2	F	3	BMA	C1-C2-C3	2.18	112.34	109.67
2	F	1	NAG	O5-C1-C2	-2.01	108.12	111.29

There are no chirality outliers.

All (24) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
3	D	5	MAN	O5-C5-C6-O6
3	D	4	MAN	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	F	3	BMA	C4-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
2	F	3	BMA	O5-C5-C6-O6
3	D	2	NAG	C3-C2-N2-C7
3	G	2	NAG	C3-C2-N2-C7

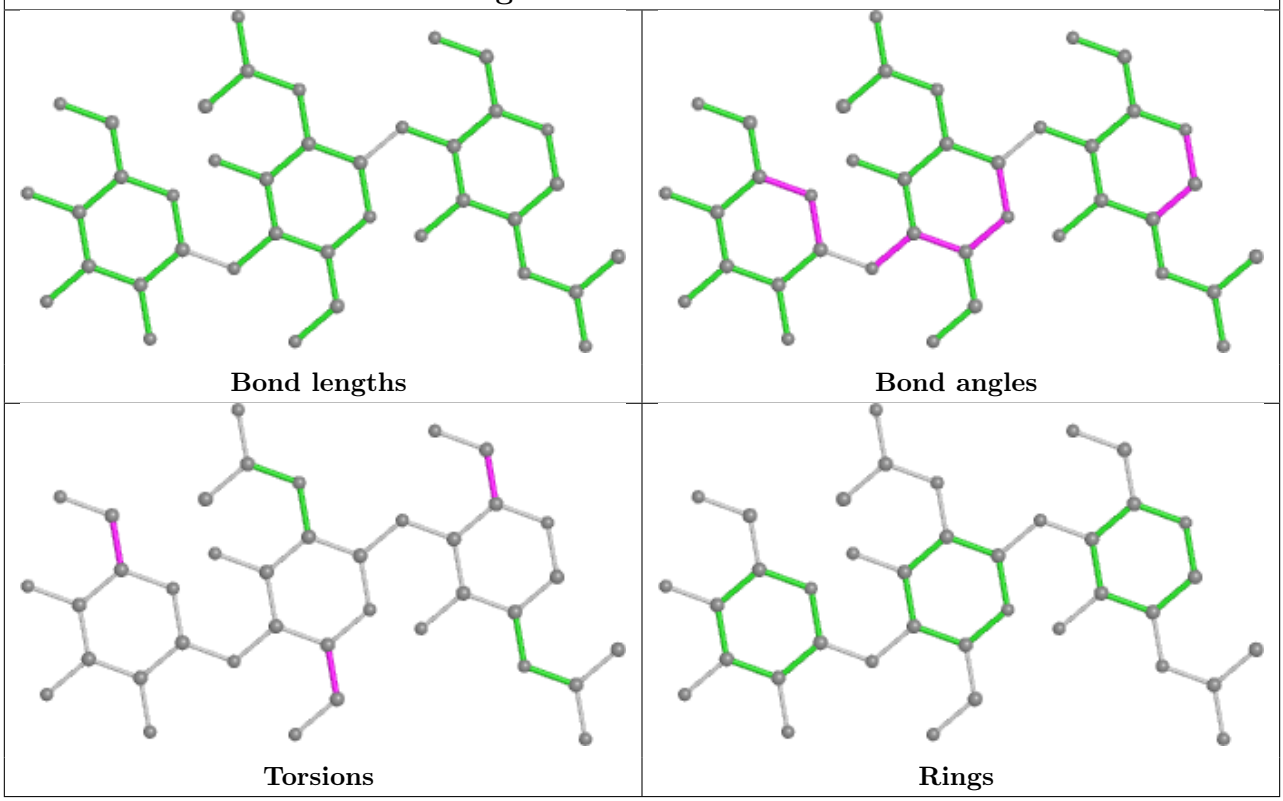
All (2) ring outliers are listed below:

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

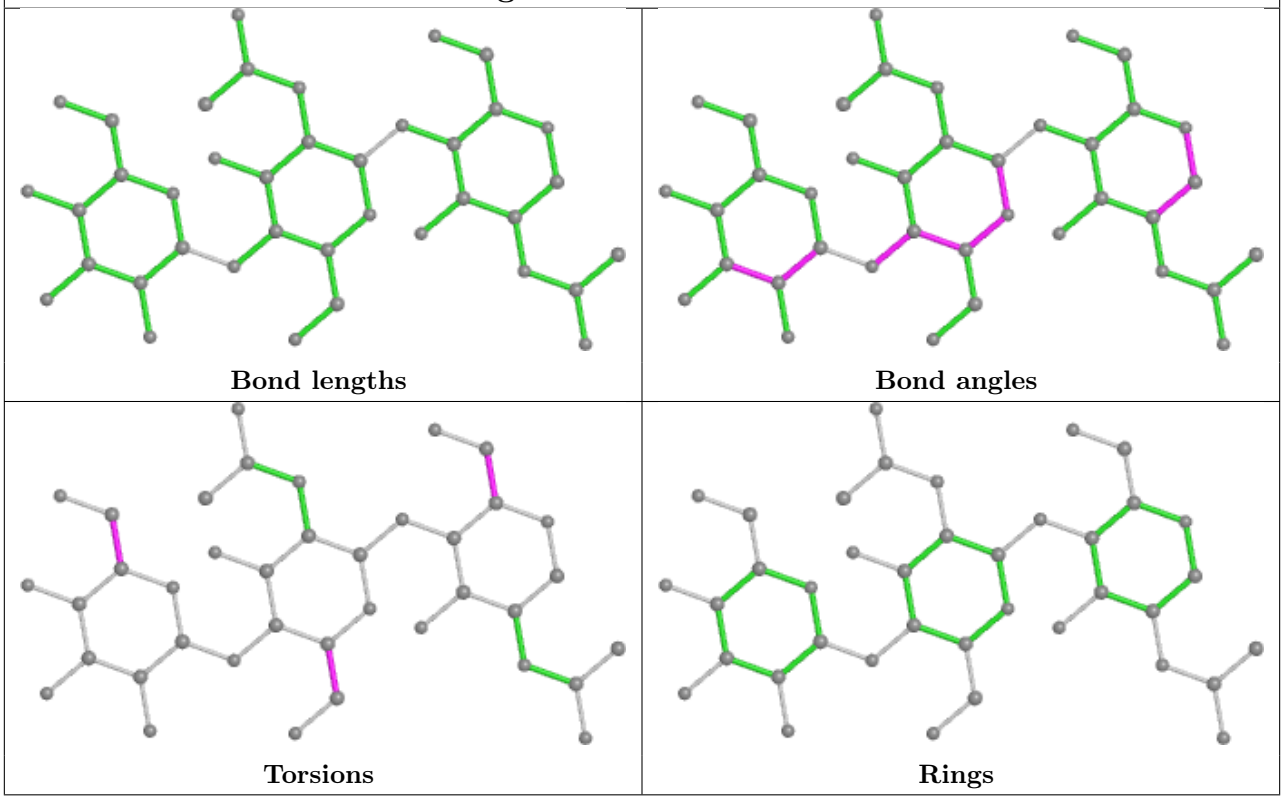
No monomer is involved in short contacts.

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

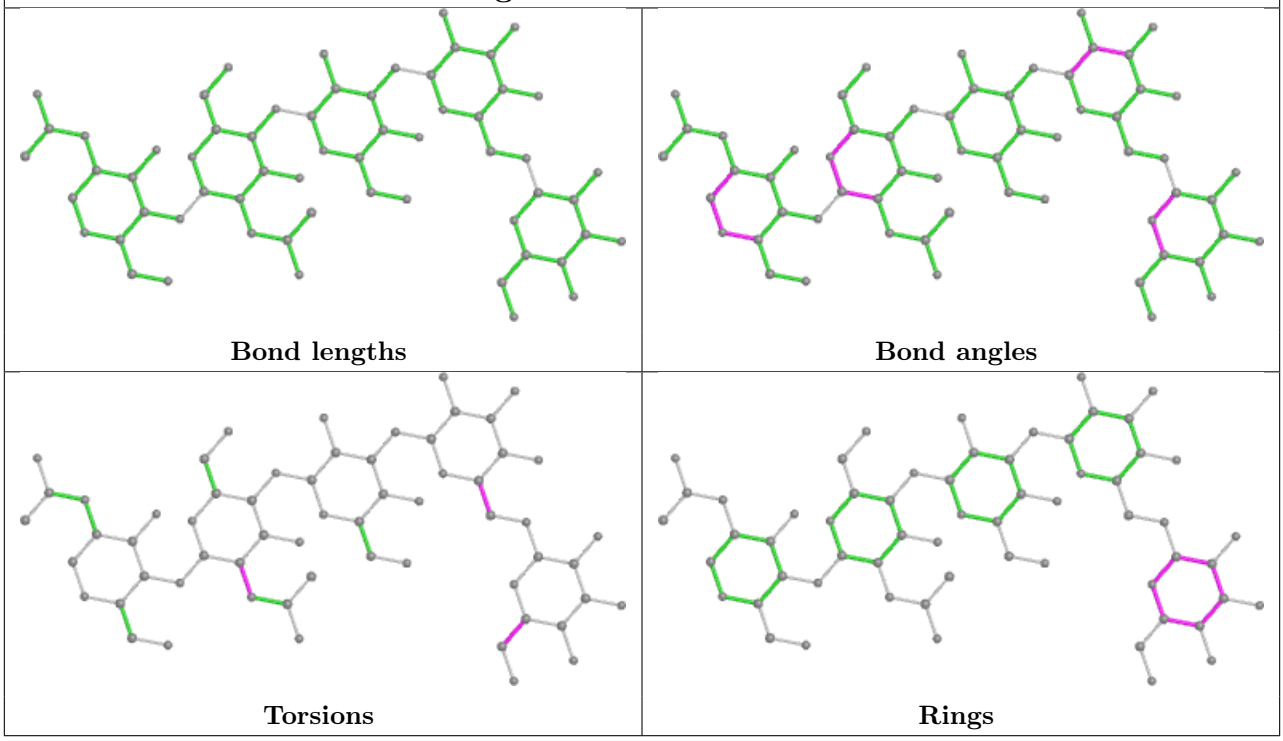
Oligosaccharide Chain C



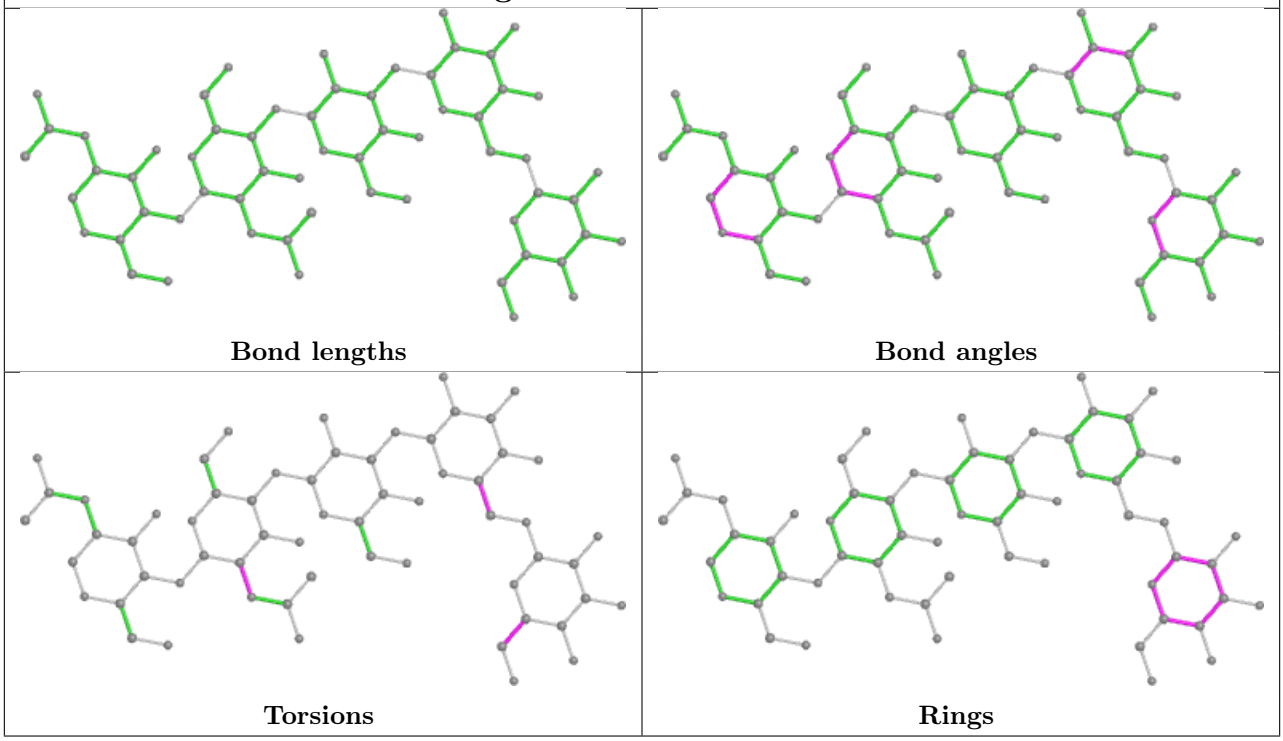
Oligosaccharide Chain F



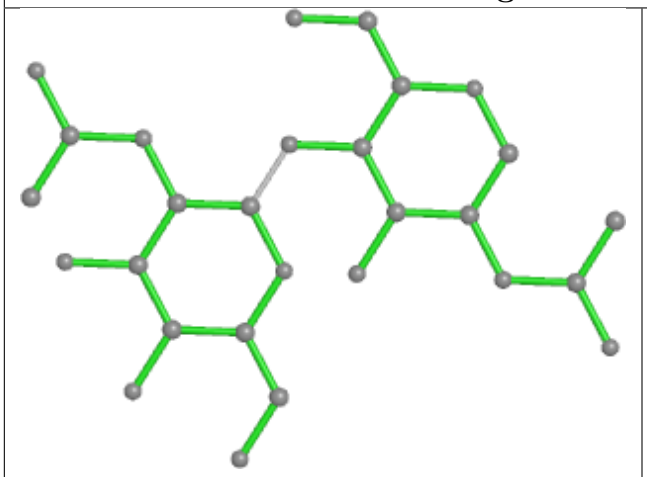
Oligosaccharide Chain D



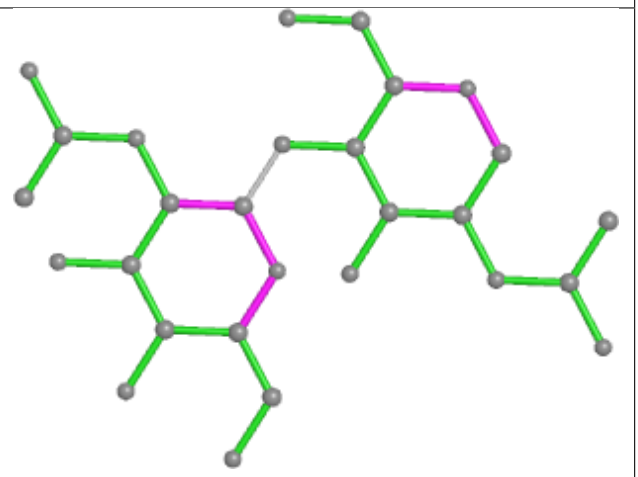
Oligosaccharide Chain G



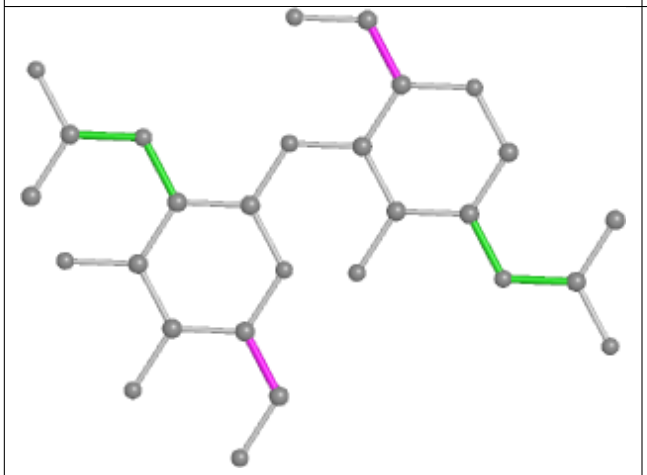
Oligosaccharide Chain E



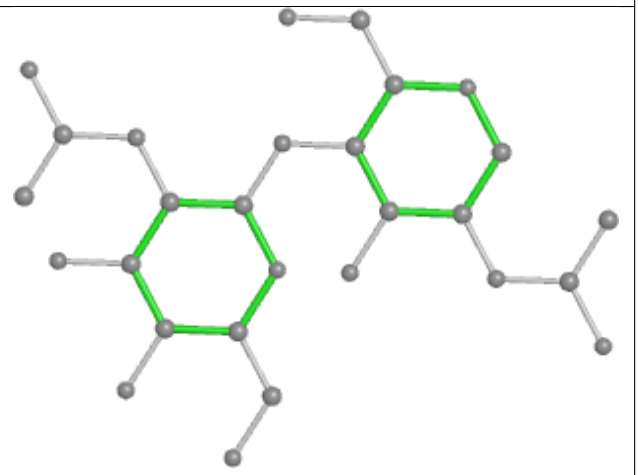
Bond lengths



Bond angles

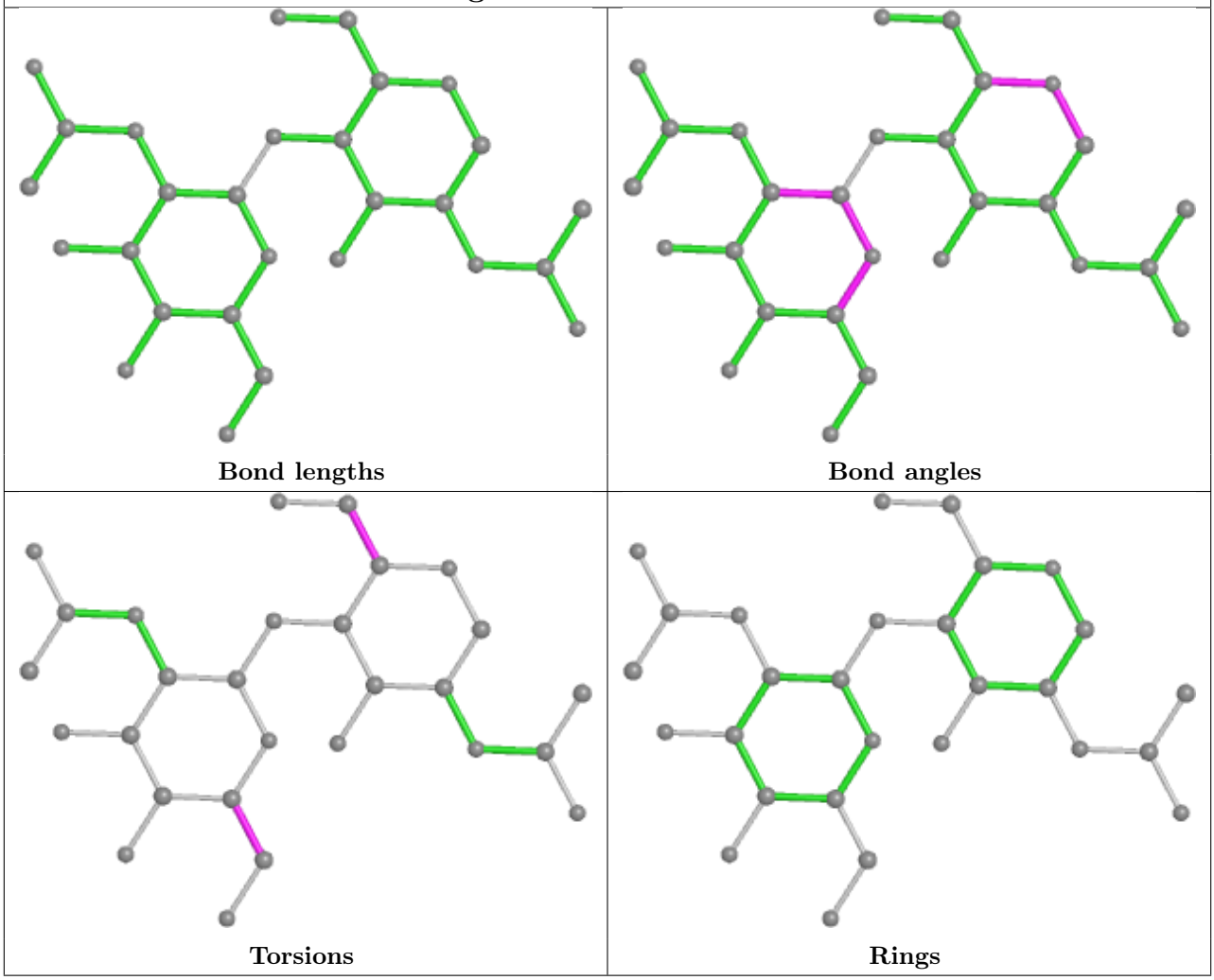


Torsions



Rings

Oligosaccharide Chain H



5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 2 are monoatomic and 1 is modelled with single atom - leaving 4 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	$\#\|Z\| > 2$
5	NAG	A	1601	1	14,14,15	0.40	0	17,19,21	0.71	0
5	NAG	B	1601	1	14,14,15	0.31	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	B	1612	1	14,14,15	0.47	0	17,19,21	2.13	4 (23%)
5	NAG	A	1612	1	14,14,15	0.42	0	17,19,21	2.12	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1601	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1601	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1612	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1612	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1612	NAG	C1-O5-C5	6.89	121.53	112.19
5	B	1612	NAG	C1-O5-C5	6.71	121.29	112.19
5	B	1612	NAG	C1-C2-N2	3.60	116.64	110.49
5	A	1612	NAG	C1-C2-N2	3.34	116.19	110.49
5	B	1612	NAG	C3-C4-C5	2.42	114.56	110.24
5	A	1612	NAG	C3-C4-C5	2.36	114.45	110.24
5	A	1612	NAG	C2-N2-C7	2.28	126.14	122.90
5	B	1612	NAG	C2-N2-C7	2.27	126.14	122.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1612	NAG	C3-C2-N2-C7
5	B	1612	NAG	C3-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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

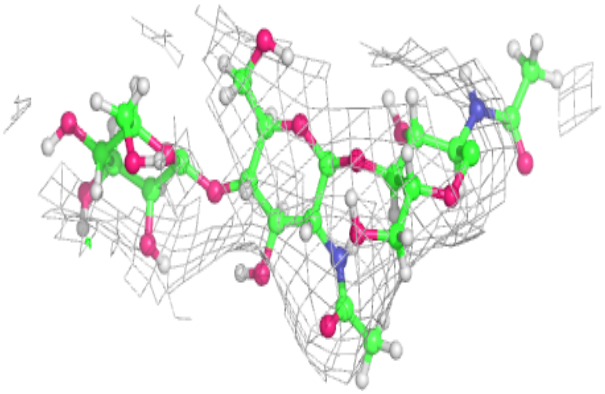
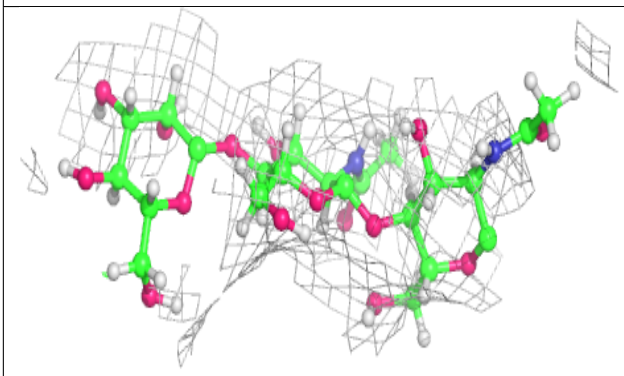
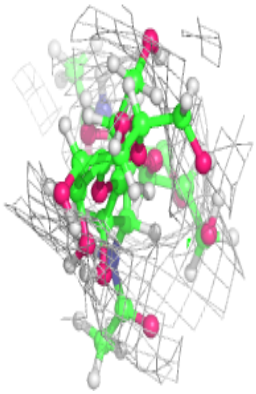
Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

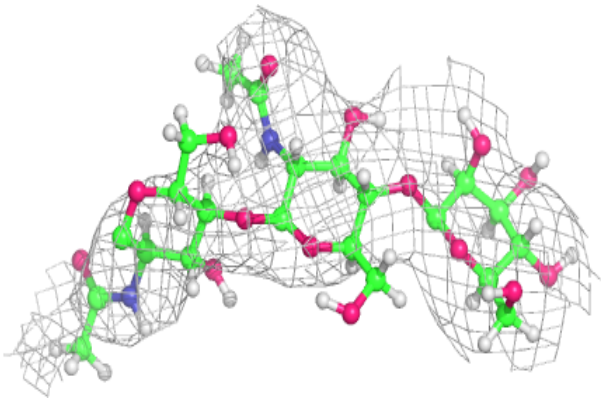
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

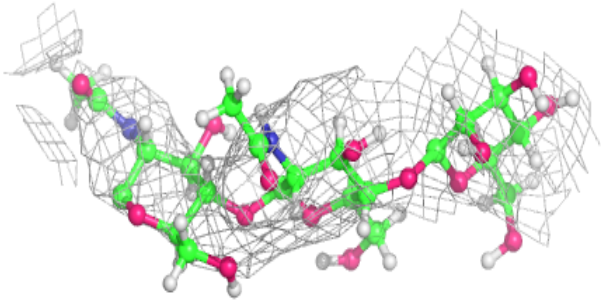
<table>
<tr><td>Electron density around Chain C:

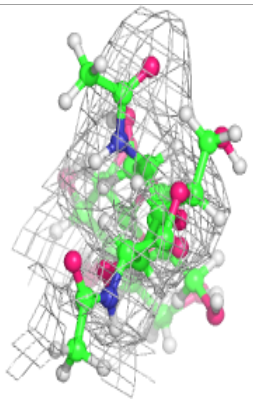
2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)</td><td>  </td></tr>
<tr><td>  </td><td>  </td></tr>
</table>

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)

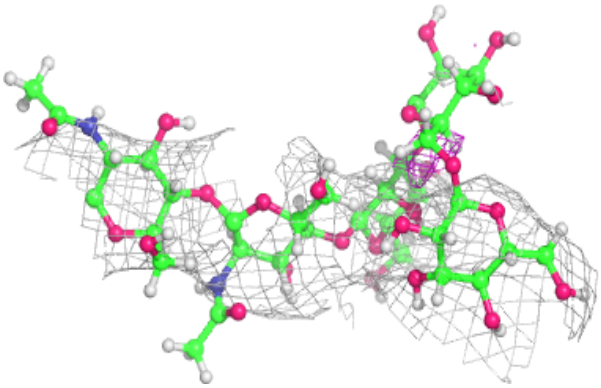


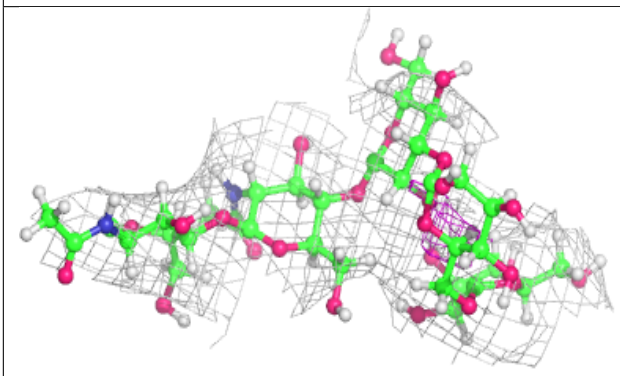


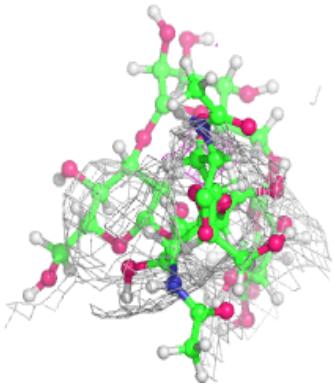


Electron density around Chain D:

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

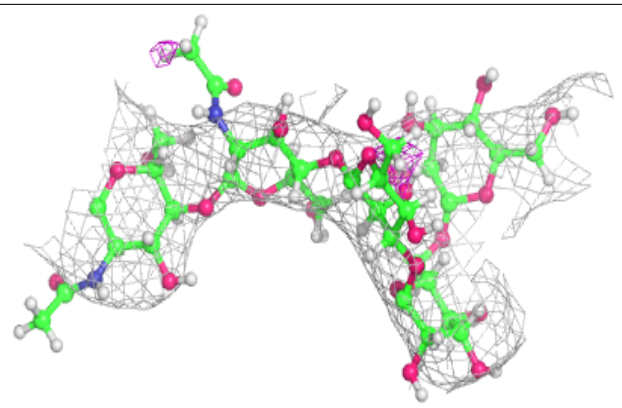


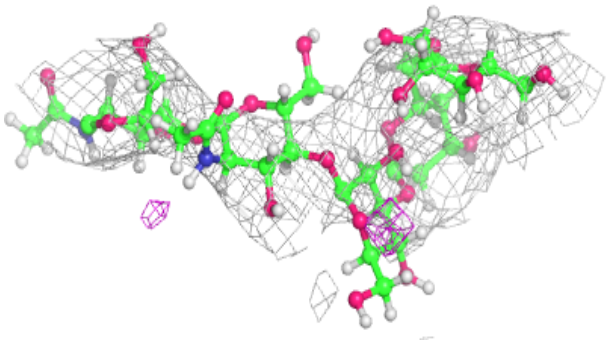


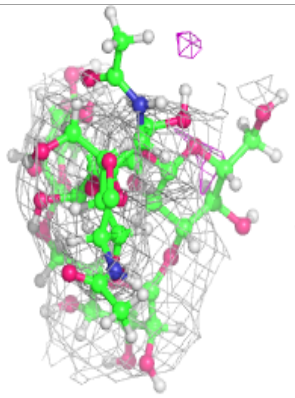


Electron density around Chain G:

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

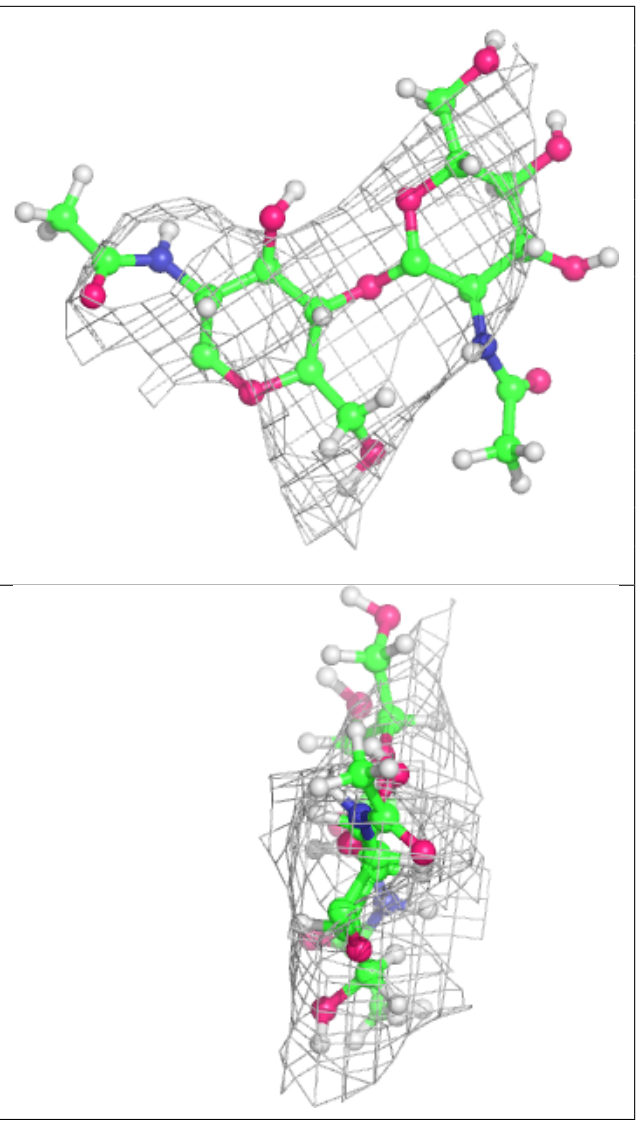


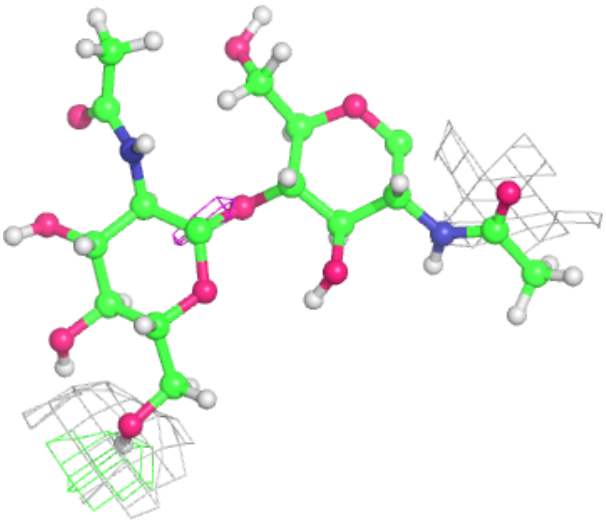
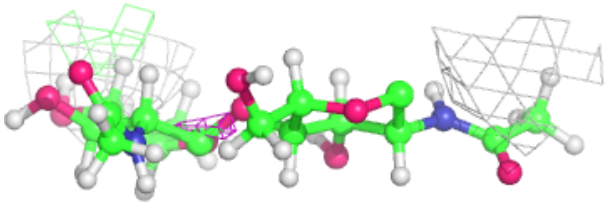
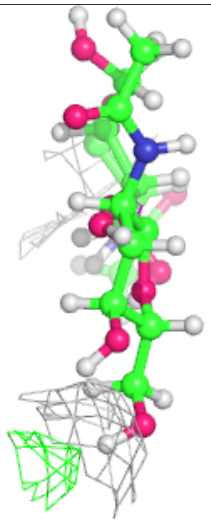




Electron density around Chain E:

$2mF_o$-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)	
	

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.