



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 04:38 AM BST

PDB ID : 3NDZ
Title : The structure of the catalytic and carbohydrate binding domain of endoglucanase D from *Clostridium cellulovorans* bound to cellotriose
Authors : Bianchetti, C.M.; Smith, R.W.; Bingman, C.A.; Phillips Jr., G.N.
Deposited on : 2010-06-08
Resolution : 2.08 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

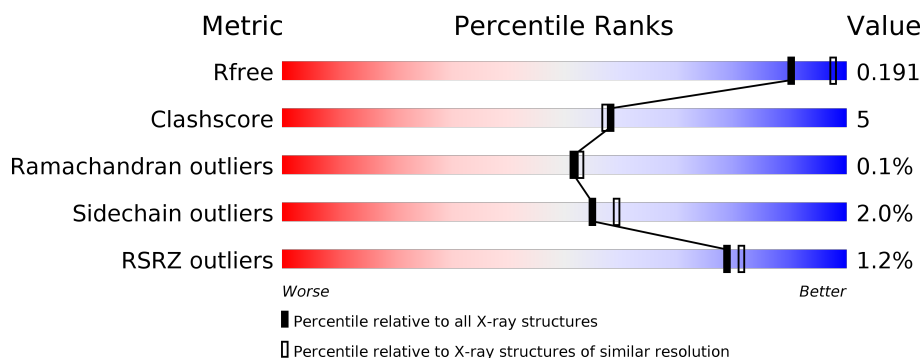
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	345	<div> <div>92%</div> <div>8%</div> </div>
1	B	345	<div> <div>86%</div> <div>14%</div> </div>
1	C	345	<div> <div>90%</div> <div>9%</div> </div>
1	D	345	<div> <div>88%</div> <div>11%</div> </div>
2	E	107	<div> <div>4%</div> <div>88%</div> <div>12%</div> </div>
2	F	107	<div> <div>2%</div> <div>87%</div> <div>13%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	107	<div><div></div><div>6%</div><div>89%</div><div>11%</div></div>
2	H	107	<div><div></div><div>%</div><div>93%</div><div>6%</div></div>
3	I	3	<div><div></div><div>33%</div><div>67%</div></div>
3	J	3	<div><div></div><div>100%</div></div>
3	K	3	<div><div></div><div>67%</div><div>33%</div></div>
3	L	3	<div><div></div><div>100%</div></div>
3	M	3	<div><div></div><div>67%</div><div>33%</div></div>
3	N	3	<div><div></div><div>67%</div><div>33%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16122 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

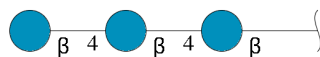
- Molecule 1 is a protein called Endoglucanase D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	2	0
			2715	1721	465	515	14			
1	B	345	Total	C	N	O	S	0	0	0
			2707	1714	465	514	14			
1	C	345	Total	C	N	O	S	0	3	0
			2723	1724	466	519	14			
1	D	345	Total	C	N	O	S	0	1	0
			2712	1717	466	515	14			

- Molecule 2 is a protein called Endoglucanase D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	107	Total	C	N	O	S	0	0	0
			782	491	130	158	3			
2	F	107	Total	C	N	O	S	0	0	0
			782	491	130	158	3			
2	G	107	Total	C	N	O	S	0	1	0
			786	494	130	159	3			
2	H	107	Total	C	N	O	S	0	1	0
			784	492	130	159	3			

- Molecule 3 is an oligosaccharide called beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	I	3	Total	C	O	0	0	0
			34	18	16			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	J	3	Total	C	O	0	0	0
			34	18	16			
3	K	3	Total	C	O	0	0	0
			34	18	16			
3	L	3	Total	C	O	0	0	0
			34	18	16			
3	M	3	Total	C	O	0	0	0
			34	18	16			
3	N	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	417	Total	O	0	0
			417	417		
4	E	91	Total	O	0	0
			91	91		
4	B	362	Total	O	0	0
			362	362		
4	F	110	Total	O	0	0
			110	110		
4	C	400	Total	O	0	0
			400	400		
4	G	88	Total	O	0	0
			88	88		
4	D	355	Total	O	0	0
			355	355		
4	H	104	Total	O	0	0
			104	104		

3 Residue-property plots


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.

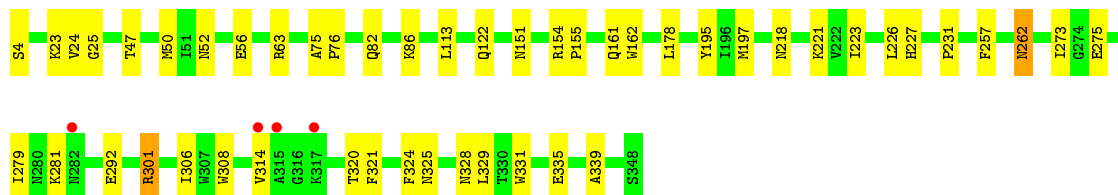
• Molecule 1: Endoglucanase D

Chain A: 



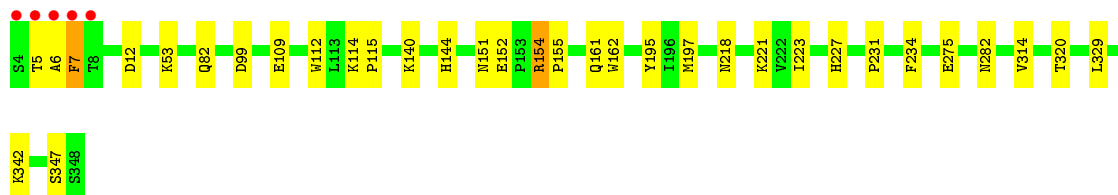
• Molecule 1: Endoglucanase D

Chain B: 




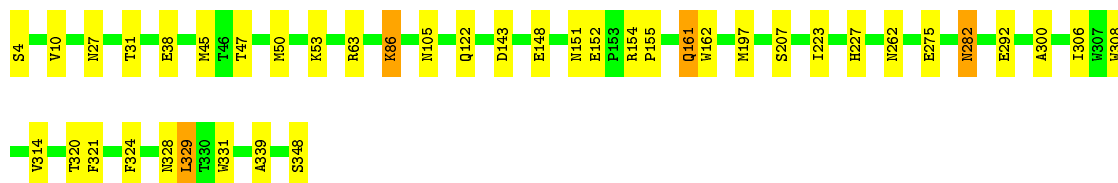
• Molecule 1: Endoglucanase D

Chain C: 

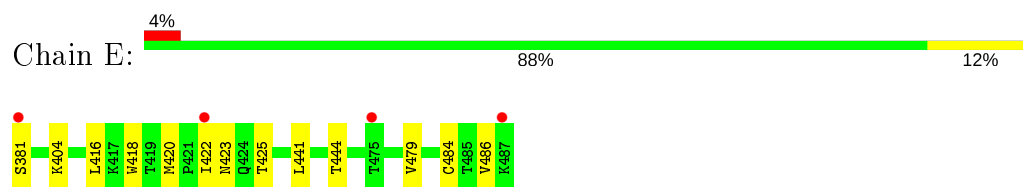


• Molecule 1: Endoglucanase D

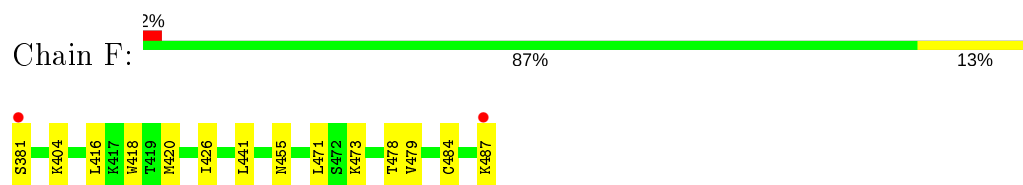
Chain D: 



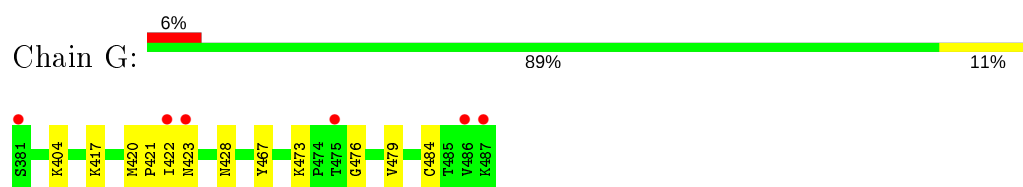
- Molecule 2: Endoglucanase D



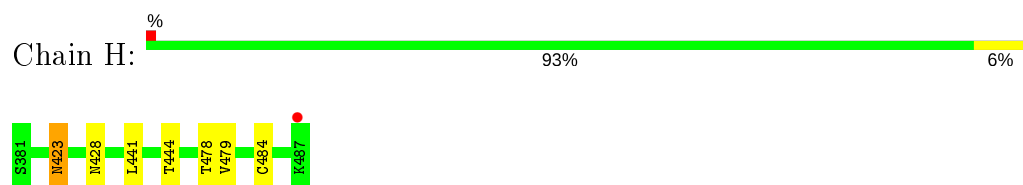
- Molecule 2: Endoglucanase D



- Molecule 2: Endoglucanase D



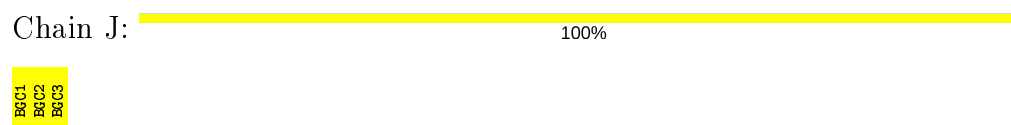
- Molecule 2: Endoglucanase D



- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose




- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose





- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain L:  100%

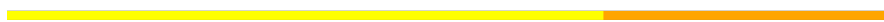


- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain M:  67% 33%



- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain N:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.30Å 119.05Å 198.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.70 – 2.08 41.70 – 2.08	Depositor EDS
% Data completeness (in resolution range)	93.0 (41.70-2.08) 93.0 (41.70-2.08)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.144 , 0.193 0.141 , 0.191	Depositor DCC
R_{free} test set	5697 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16122	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: BGC

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	0.38	0/2789	0.54	0/3792
1	B	0.35	0/2775	0.50	0/3773
1	C	0.38	0/2800	0.52	0/3807
1	D	0.36	0/2783	0.51	0/3784
2	E	0.35	0/799	0.53	0/1095
2	F	0.36	0/799	0.53	0/1095
2	G	0.35	0/806	0.53	0/1105
2	H	0.36	0/804	0.54	0/1102
All	All	0.36	0/14355	0.52	0/19553

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	2715	0	2621	17	0
1	B	2707	0	2605	32	0
1	C	2723	0	2621	23	0
1	D	2712	0	2611	24	0
2	E	782	0	755	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	782	0	755	13	0
2	G	786	0	762	11	0
2	H	784	0	755	6	0
3	I	34	0	30	2	0
3	J	34	0	30	0	0
3	K	34	0	30	3	0
3	L	34	0	30	0	0
3	M	34	0	30	1	0
3	N	34	0	30	2	0
4	A	417	0	0	3	0
4	B	362	0	0	8	0
4	C	400	0	0	4	0
4	D	355	0	0	3	0
4	E	91	0	0	4	0
4	F	110	0	0	4	0
4	G	88	0	0	6	0
4	H	104	0	0	1	0
All	All	16122	0	13665	133	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (133) 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)
2:H:423:ASN:HD22	2:H:423:ASN:H	1.29	0.80
2:F:479:VAL:HG23	2:F:484:CYS:SG	2.25	0.76
1:B:262:ASN:HB3	4:B:816:HOH:O	1.84	0.75
1:C:82[A]:GLN:HG3	4:C:899:HOH:O	1.86	0.75
1:A:262:ASN:HB2	4:A:627:HOH:O	1.87	0.74
1:C:275:GLU:OE1	3:M:1:BGC:H1	1.89	0.73
1:C:53:LYS:HE2	4:C:898:HOH:O	1.88	0.72
2:F:418:TRP:CZ2	2:F:441:LEU:HD23	2.24	0.71
1:B:314:VAL:O	1:B:320:THR:HG21	1.92	0.69
2:G:476:GLY:HA2	4:G:587:HOH:O	1.91	0.69
2:H:423:ASN:ND2	2:H:423:ASN:H	1.94	0.66
2:F:404:LYS:HE3	4:F:555:HOH:O	1.96	0.66
1:D:275:GLU:OE1	3:N:1:BGC:H1	1.98	0.64
2:F:416:LEU:HD13	2:F:479:VAL:HG22	1.80	0.64
2:E:479:VAL:HG23	2:E:484:CYS:SG	2.37	0.63
1:C:5:THR:HG23	1:C:99[B]:ASP:OD2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:GLN:OE1	4:D:509:HOH:O	2.16	0.61
1:C:5:THR:HG21	1:C:144:HIS:CD2	2.36	0.61
2:H:428:ASN:HB2	4:H:564:HOH:O	2.01	0.60
1:D:314:VAL:O	1:D:320:THR:HG21	2.02	0.59
1:B:151:ASN:ND2	1:B:227:HIS:HE1	2.00	0.59
2:E:420:MET:HG2	2:E:441:LEU:HB2	1.85	0.58
2:G:428:ASN:HB2	4:G:526:HOH:O	2.03	0.58
1:B:82:GLN:O	1:B:86:LYS:HG2	2.03	0.58
1:C:82[A]:GLN:NE2	4:C:890:HOH:O	2.38	0.56
1:B:122:GLN:HG3	4:B:847:HOH:O	2.06	0.56
1:C:7:PHE:HE2	1:C:140:LYS:HD2	1.70	0.56
1:B:231:PRO:HG3	4:B:518:HOH:O	2.05	0.56
1:B:151:ASN:HD21	1:B:227:HIS:HE1	1.52	0.56
1:D:161:GLN:HG2	1:D:162:TRP:CD1	2.41	0.56
2:G:423:ASN:O	2:G:467:TYR:HA	2.05	0.56
1:D:4:SER:N	4:D:709:HOH:O	2.38	0.55
1:C:314:VAL:O	1:C:320:THR:HG21	2.07	0.55
2:E:381:SER:HA	4:E:535:HOH:O	2.06	0.54
1:A:151:ASN:ND2	1:A:227:HIS:HE1	2.06	0.53
1:A:275:GLU:OE1	3:I:1:BGC:H1	2.08	0.53
1:A:250:LYS:HE2	4:A:908:HOH:O	2.09	0.53
2:H:479:VAL:HG23	2:H:484:CYS:SG	2.48	0.52
2:F:478:THR:HG22	4:F:558:HOH:O	2.10	0.52
2:G:422:ILE:O	2:G:423:ASN:HB2	2.10	0.51
1:C:347:SER:O	2:G:428:ASN:HA	2.11	0.51
1:B:324:PHE:HB2	1:B:331:TRP:CZ3	2.45	0.51
1:A:151:ASN:HD21	1:A:227:HIS:HE1	1.59	0.50
1:B:25:GLY:C	1:B:306:ILE:HG23	2.32	0.50
1:C:342:LYS:HE2	4:G:542:HOH:O	2.11	0.50
1:A:219:ASP:HB3	1:A:222:VAL:HG23	1.92	0.50
1:A:10:VAL:HG13	1:A:143:ASP:HB3	1.94	0.49
1:C:5:THR:CG2	1:C:99[B]:ASP:OD2	2.60	0.49
2:F:416:LEU:CD1	2:F:479:VAL:HG22	2.41	0.49
2:E:422:ILE:O	2:E:423:ASN:HB2	2.12	0.49
2:F:381:SER:N	4:F:590:HOH:O	2.45	0.49
1:C:154:ARG:HB2	1:C:155:PRO:HD2	1.94	0.49
1:C:151:ASN:ND2	1:C:227:HIS:HE1	2.10	0.48
1:B:275:GLU:OE1	3:K:1:BGC:H1	2.12	0.48
1:B:308:TRP:O	1:B:321:PHE:HB3	2.13	0.48
1:C:12:ASP:HB2	4:C:893:HOH:O	2.12	0.48
2:F:420:MET:HG2	4:F:536:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ASN:OD1	1:B:328:ASN:HB2	2.13	0.48
2:G:473:LYS:HD2	4:G:585:HOH:O	2.13	0.48
1:B:178:LEU:HD21	1:C:12:ASP:OD2	2.14	0.48
1:B:257:PHE:HB3	1:B:301:ARG:HD3	1.95	0.48
1:B:257:PHE:CB	1:B:301:ARG:HD3	2.43	0.48
1:D:86:LYS:HD2	1:D:86:LYS:HA	1.63	0.48
1:B:279:ILE:HD11	1:B:281:LYS:HE3	1.95	0.48
1:C:195:TYR:CE2	1:C:221:LYS:HD2	2.48	0.48
1:A:314:VAL:O	1:A:320:THR:HG21	2.13	0.48
2:G:479:VAL:HG23	2:G:484:CYS:SG	2.54	0.48
1:D:154:ARG:HB2	1:D:155:PRO:HD2	1.97	0.47
2:E:422:ILE:HA	4:E:526:HOH:O	2.14	0.47
2:F:426:ILE:HD11	2:F:441:LEU:HD21	1.96	0.47
1:D:63:ARG:HH22	1:D:151:ASN:ND2	2.13	0.46
1:B:218:ASN:CB	4:B:827:HOH:O	2.63	0.46
1:B:75:ALA:HB1	1:B:76:PRO:HA	1.97	0.46
1:A:63:ARG:HH22	1:A:151:ASN:ND2	2.13	0.46
2:E:404:LYS:NZ	4:E:590:HOH:O	2.49	0.46
1:C:197:MET:HA	1:C:223:ILE:O	2.16	0.45
1:B:226:LEU:O	1:B:273:ILE:HA	2.17	0.45
2:F:426:ILE:CD1	2:F:441:LEU:HD21	2.46	0.45
1:B:52:ASN:O	1:B:56:GLU:HG3	2.16	0.45
1:B:218:ASN:HB2	4:B:827:HOH:O	2.17	0.45
1:C:161:GLN:HG2	1:C:162:TRP:CD1	2.52	0.45
1:D:151:ASN:ND2	1:D:227:HIS:HE1	2.15	0.45
1:D:53:LYS:HE2	4:D:776:HOH:O	2.17	0.44
1:B:161:GLN:HG2	1:B:162:TRP:CD1	2.52	0.44
1:C:151:ASN:HD21	1:C:227:HIS:HE1	1.64	0.44
1:B:195:TYR:CE2	1:B:221:LYS:HD3	2.53	0.44
1:C:114:LYS:HA	1:C:115:PRO:HD3	1.76	0.44
3:K:1:BGC:H6C2	3:K:2:BGC:C1	2.47	0.44
1:C:109:GLU:HB3	1:C:112:TRP:NE1	2.32	0.43
2:E:416:LEU:HD13	2:E:479:VAL:HG22	2.01	0.43
2:E:404:LYS:HE3	4:E:562:HOH:O	2.17	0.43
1:B:292:GLU:HB2	1:B:339:ALA:HB1	2.01	0.43
1:D:324:PHE:HB2	1:D:331:TRP:CZ3	2.54	0.43
1:D:47:THR:OG1	1:D:50:MET:HG3	2.19	0.43
1:A:113[B]:LEU:HD21	1:A:150:MET:SD	2.59	0.43
1:C:231:PRO:HG2	1:C:234:PHE:HB3	2.01	0.43
2:E:418:TRP:CZ2	2:E:441:LEU:CD2	3.02	0.42
2:G:420:MET:SD	2:G:421:PRO:HD2	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:ASN:CG	4:B:827:HOH:O	2.57	0.42
1:A:197:MET:HA	1:A:223:ILE:O	2.18	0.42
1:D:31:THR:HG22	1:D:38:GLU:HG3	2.01	0.42
1:D:152:GLU:OE2	3:N:1:BGC:O1	2.34	0.42
1:D:27:ASN:ND2	1:D:306:ILE:HG22	2.35	0.42
3:K:1:BGC:C6	3:K:2:BGC:C1	2.98	0.42
1:A:76:PRO:HD2	4:A:736:HOH:O	2.18	0.42
1:D:282:ASN:HA	1:D:282:ASN:HD22	1.64	0.42
1:D:328:ASN:O	1:D:329:LEU:HB2	2.20	0.42
1:B:23:LYS:HG2	1:B:24:VAL:HG12	2.02	0.41
1:A:120:GLU:OE1	1:A:175:ARG:NH1	2.48	0.41
1:B:63:ARG:HH22	1:B:151:ASN:ND2	2.18	0.41
1:A:14:PRO:HG2	2:F:455:ASN:HB3	2.02	0.41
1:D:300:ALA:HA	2:H:444:THR:CG2	2.50	0.41
1:D:292:GLU:HB2	1:D:339:ALA:HB1	2.02	0.41
2:G:422:ILE:HA	4:G:574:HOH:O	2.21	0.41
1:D:151:ASN:HD21	1:D:227:HIS:HE1	1.68	0.41
1:A:300:ALA:HA	2:E:444:THR:CG2	2.51	0.41
2:G:404:LYS:HE3	4:G:509:HOH:O	2.20	0.41
1:A:282:ASN:HD22	1:A:282:ASN:HA	1.70	0.41
1:B:197:MET:HA	1:B:223:ILE:O	2.20	0.41
2:F:487:LYS:HE2	2:F:487:LYS:HB3	1.82	0.41
1:D:105:ASN:HB3	1:D:148:GLU:HB3	2.02	0.41
1:B:4:SER:N	4:B:670:HOH:O	2.53	0.41
1:C:152:GLU:OE1	1:C:154:ARG:NH2	2.54	0.41
1:B:154:ARG:HB2	1:B:155:PRO:HD2	2.02	0.41
2:G:417:LYS:HB2	2:G:417:LYS:HE3	1.69	0.41
1:D:197:MET:HA	1:D:223:ILE:O	2.21	0.41
2:F:479:VAL:HG23	2:F:484:CYS:HG	1.86	0.40
1:A:41:TRP:CD2	3:I:3:BGC:H5	2.55	0.40
1:B:335:GLU:HG2	4:B:850:HOH:O	2.21	0.40
1:B:47:THR:OG1	1:B:50:MET:HG3	2.20	0.40
1:D:10:VAL:HG13	1:D:143:ASP:HB3	2.03	0.40
1:D:308:TRP:O	1:D:321:PHE:HB3	2.22	0.40
2:H:423:ASN:HD22	2:H:423:ASN:N	2.08	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	345/345 (100%)	331 (96%)	14 (4%)	0	100	100
1	B	343/345 (99%)	329 (96%)	14 (4%)	0	100	100
1	C	346/345 (100%)	332 (96%)	13 (4%)	1 (0%)	41	39
1	D	344/345 (100%)	329 (96%)	15 (4%)	0	100	100
2	E	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
2	F	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
2	G	106/107 (99%)	101 (95%)	5 (5%)	0	100	100
2	H	106/107 (99%)	103 (97%)	3 (3%)	0	100	100
All	All	1800/1808 (100%)	1727 (96%)	72 (4%)	1 (0%)	51	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	6	ALA

5.3.2 Protein sidechains ⓘ

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	286/284 (101%)	281 (98%)	5 (2%)	60	65
1	B	284/284 (100%)	280 (99%)	4 (1%)	67	72
1	C	287/284 (101%)	282 (98%)	5 (2%)	60	65
1	D	285/284 (100%)	277 (97%)	8 (3%)	43	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	86/86 (100%)	84 (98%)	2 (2%)	50	53
2	F	86/86 (100%)	84 (98%)	2 (2%)	50	53
2	G	87/86 (101%)	87 (100%)	0	100	100
2	H	86/86 (100%)	82 (95%)	4 (5%)	26	24
All	All	1487/1480 (100%)	1457 (98%)	30 (2%)	55	59

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	MET
1	A	161	GLN
1	A	218	ASN
1	A	282	ASN
1	A	329	LEU
2	E	425	THR
2	E	486	VAL
1	B	113	LEU
1	B	262	ASN
1	B	301	ARG
1	B	329	LEU
2	F	471	LEU
2	F	473	LYS
1	C	7	PHE
1	C	154	ARG
1	C	218	ASN
1	C	282	ASN
1	C	329	LEU
1	D	45	MET
1	D	86	LYS
1	D	161	GLN
1	D	207	SER
1	D	262	ASN
1	D	282	ASN
1	D	329	LEU
1	D	348	SER
2	H	423	ASN
2	H	441	LEU
2	H	478[A]	THR
2	H	478[B]	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	A	151	ASN
1	A	218	ASN
1	A	262	ASN
1	A	282	ASN
1	B	151	ASN
1	B	282	ASN
1	C	151	ASN
1	D	110	ASN
1	D	151	ASN
1	D	282	ASN
2	H	423	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

18 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BGC	I	1	3	12,12,12	1.25	1 (8%)	17,17,17	1.37	3 (17%)
3	BGC	I	2	3	11,11,12	1.01	1 (9%)	15,15,17	1.36	2 (13%)
3	BGC	I	3	3	11,11,12	0.51	0	15,15,17	1.00	1 (6%)
3	BGC	J	1	3	12,12,12	1.20	2 (16%)	17,17,17	1.28	3 (17%)
3	BGC	J	2	3	11,11,12	0.92	1 (9%)	15,15,17	1.81	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BGC	J	3	3	11,11,12	0.56	0	15,15,17	1.23	1 (6%)
3	BGC	K	1	3	12,12,12	0.80	0	17,17,17	1.00	0
3	BGC	K	2	3	11,11,12	0.57	0	15,15,17	2.69	5 (33%)
3	BGC	K	3	3	11,11,12	0.57	0	15,15,17	2.17	4 (26%)
3	BGC	L	1	3	12,12,12	1.07	1 (8%)	17,17,17	1.17	2 (11%)
3	BGC	L	2	3	11,11,12	0.98	1 (9%)	15,15,17	1.79	4 (26%)
3	BGC	L	3	3	11,11,12	0.55	0	15,15,17	1.41	2 (13%)
3	BGC	M	1	3	12,12,12	1.16	1 (8%)	17,17,17	1.50	2 (11%)
3	BGC	M	2	3	11,11,12	0.86	0	15,15,17	2.52	4 (26%)
3	BGC	M	3	3	11,11,12	0.61	0	15,15,17	1.22	2 (13%)
3	BGC	N	1	3	12,12,12	1.17	1 (8%)	17,17,17	1.13	1 (5%)
3	BGC	N	2	3	11,11,12	0.81	0	15,15,17	2.50	5 (33%)
3	BGC	N	3	3	11,11,12	0.64	0	15,15,17	2.19	6 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	I	1	3	-	0/2/22/22	0/1/1/1
3	BGC	I	2	3	-	0/2/19/22	0/1/1/1
3	BGC	I	3	3	-	0/2/19/22	0/1/1/1
3	BGC	J	1	3	-	0/2/22/22	0/1/1/1
3	BGC	J	2	3	-	0/2/19/22	0/1/1/1
3	BGC	J	3	3	-	0/2/19/22	0/1/1/1
3	BGC	K	1	3	-	0/2/22/22	0/1/1/1
3	BGC	K	2	3	-	0/2/19/22	0/1/1/1
3	BGC	K	3	3	-	0/2/19/22	0/1/1/1
3	BGC	L	1	3	-	0/2/22/22	0/1/1/1
3	BGC	L	2	3	-	0/2/19/22	0/1/1/1
3	BGC	L	3	3	-	0/2/19/22	0/1/1/1
3	BGC	M	1	3	-	0/2/22/22	0/1/1/1
3	BGC	M	2	3	-	0/2/19/22	0/1/1/1
3	BGC	M	3	3	-	0/2/19/22	0/1/1/1
3	BGC	N	1	3	-	0/2/22/22	0/1/1/1
3	BGC	N	2	3	-	0/2/19/22	0/1/1/1
3	BGC	N	3	3	-	0/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1	BGC	C4-C5	3.69	1.60	1.53
3	M	1	BGC	C4-C5	3.57	1.60	1.53
3	N	1	BGC	C4-C5	3.50	1.60	1.53
3	L	2	BGC	C4-C5	2.75	1.58	1.53
3	J	2	BGC	C4-C5	2.55	1.58	1.53
3	I	2	BGC	O5-C1	2.52	1.47	1.43
3	J	1	BGC	C4-C5	-2.49	1.47	1.53
3	L	1	BGC	C4-C5	-2.32	1.48	1.53
3	J	1	BGC	C6-C5	2.24	1.59	1.51

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	2	BGC	C6-C5-C4	-6.89	96.86	113.00
3	K	2	BGC	C6-C5-C4	-6.17	98.55	113.00
3	N	2	BGC	C6-C5-C4	-6.00	98.95	113.00
3	N	3	BGC	C6-C5-C4	-5.96	99.04	113.00
3	K	2	BGC	O4-C4-C3	5.95	124.11	110.35
3	N	2	BGC	O4-C4-C3	5.53	123.12	110.35
3	K	3	BGC	C6-C5-C4	-5.40	100.35	113.00
3	M	2	BGC	O4-C4-C3	5.00	121.90	110.35
3	L	2	BGC	C3-C4-C5	-4.27	102.63	110.24
3	L	3	BGC	C6-C5-C4	-4.08	103.44	113.00
3	M	1	BGC	O1-C1-O5	-3.88	98.73	110.38
3	K	3	BGC	O5-C5-C6	3.78	113.13	107.20
3	K	2	BGC	C2-C3-C4	-3.61	104.65	110.89
3	J	2	BGC	C3-C4-C5	-3.55	103.90	110.24
3	J	2	BGC	O3-C3-C2	-3.45	103.38	109.99
3	N	2	BGC	C2-C3-C4	-3.40	105.01	110.89
3	L	2	BGC	O3-C3-C2	-3.37	103.53	109.99
3	M	2	BGC	C2-C3-C4	-3.29	105.21	110.89
3	N	3	BGC	O5-C5-C6	3.29	112.36	107.20
3	J	3	BGC	C2-C3-C4	-3.27	105.23	110.89
3	K	3	BGC	O2-C2-C3	-3.22	103.70	110.14
3	I	2	BGC	C6-C5-C4	-3.14	105.64	113.00
3	J	2	BGC	C1-C2-C3	-3.03	105.94	109.67
3	N	3	BGC	O2-C2-C3	-3.00	104.14	110.14
3	J	2	BGC	O5-C1-C2	2.90	115.24	110.77
3	L	2	BGC	O5-C1-C2	2.83	115.15	110.77
3	L	3	BGC	C2-C3-C4	-2.80	106.05	110.89
3	I	1	BGC	O5-C1-C2	2.78	115.24	110.28
3	I	2	BGC	C1-C2-C3	-2.77	106.26	109.67
3	M	3	BGC	O2-C2-C3	-2.74	104.65	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	2	BGC	O5-C5-C6	-2.70	102.98	107.20
3	K	2	BGC	O4-C4-C5	-2.68	102.65	109.30
3	I	3	BGC	C2-C3-C4	-2.55	106.48	110.89
3	M	2	BGC	O5-C1-C2	-2.54	106.86	110.77
3	N	1	BGC	O1-C1-O5	-2.50	102.89	110.38
3	J	1	BGC	C1-C2-C3	-2.45	105.24	110.31
3	M	1	BGC	C4-C3-C2	-2.42	106.60	110.82
3	K	3	BGC	C1-C2-C3	-2.37	106.75	109.67
3	I	1	BGC	C4-C3-C2	-2.33	106.75	110.82
3	L	1	BGC	C6-C5-C4	-2.29	107.64	113.00
3	L	1	BGC	C1-C2-C3	-2.29	105.57	110.31
3	N	2	BGC	O5-C1-C2	-2.19	107.39	110.77
3	J	1	BGC	C6-C5-C4	-2.18	107.90	113.00
3	L	2	BGC	C1-C2-C3	-2.17	107.00	109.67
3	N	3	BGC	C1-O5-C5	-2.15	109.28	112.19
3	M	3	BGC	O5-C5-C6	2.14	110.56	107.20
3	N	3	BGC	C1-C2-C3	-2.13	107.05	109.67
3	N	2	BGC	O4-C4-C5	-2.07	104.16	109.30
3	N	3	BGC	C2-C3-C4	-2.06	107.32	110.89
3	J	1	BGC	O5-C5-C6	2.06	111.57	106.44
3	I	1	BGC	O1-C1-O5	-2.05	104.22	110.38

There are no chirality outliers.

There are no torsion outliers.

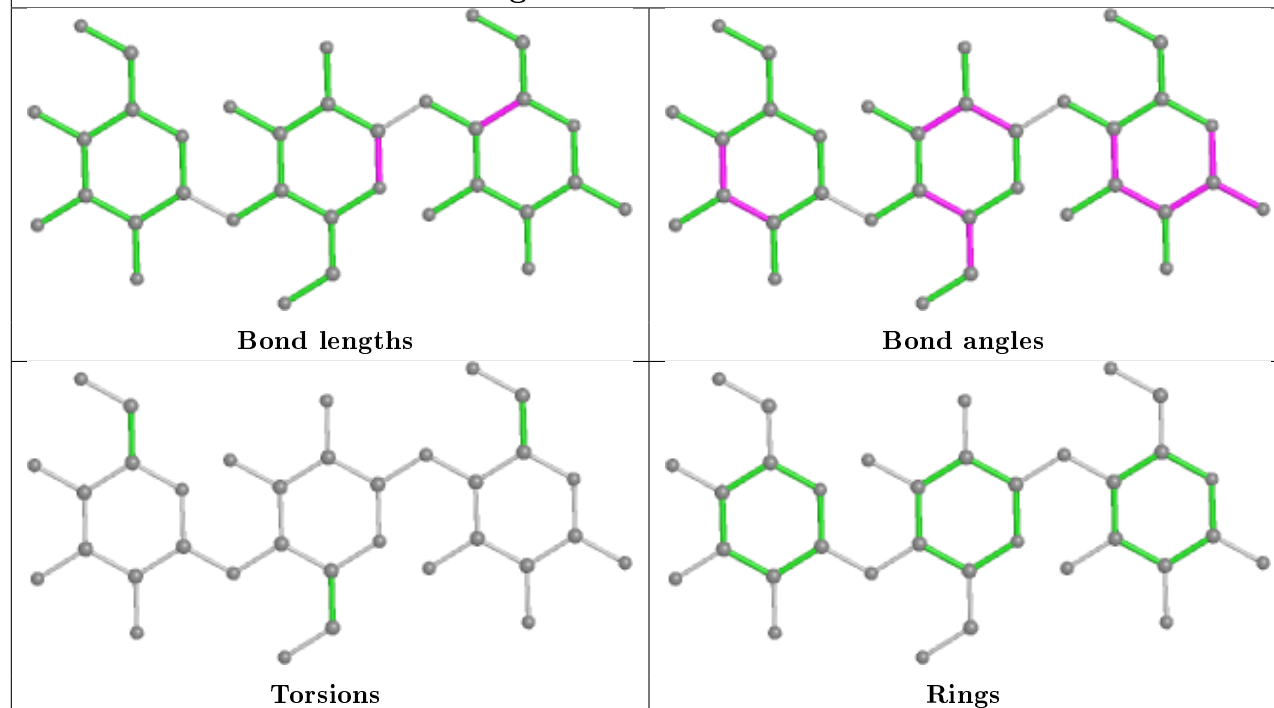
There are no ring outliers.

6 monomers are involved in 8 short contacts:

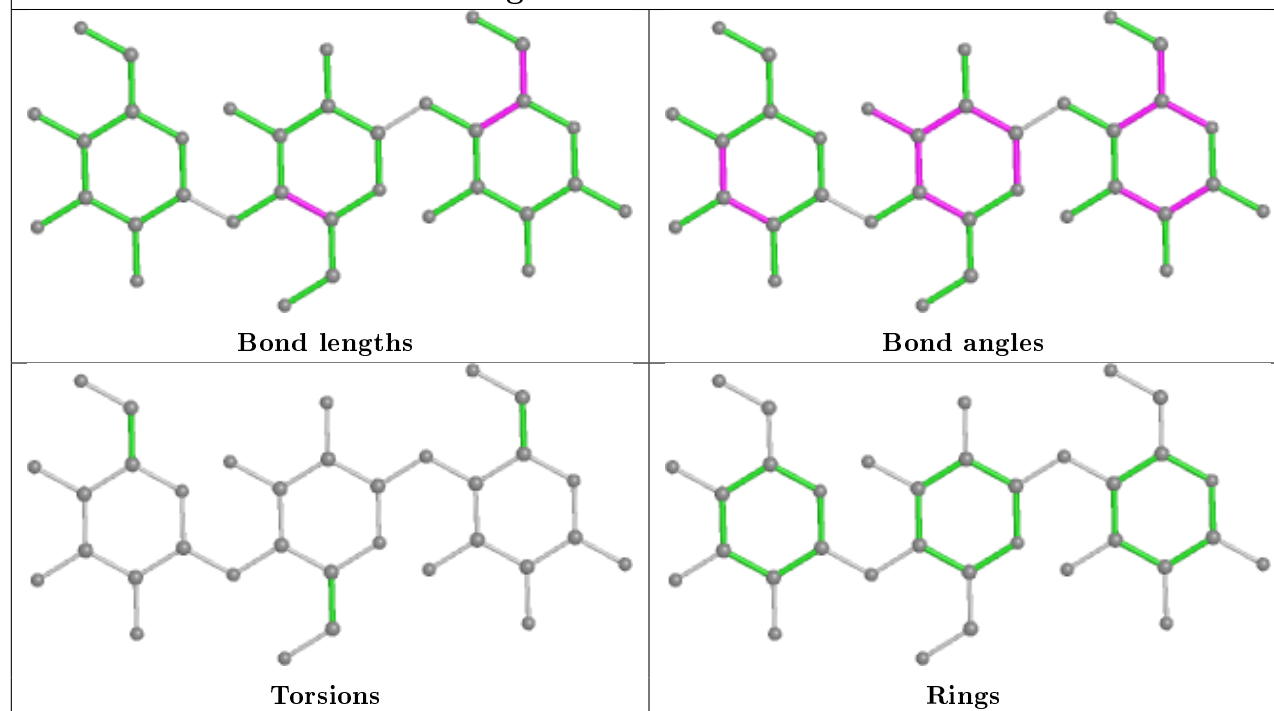
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	1	BGC	3	0
3	I	1	BGC	1	0
3	M	1	BGC	1	0
3	N	1	BGC	2	0
3	I	3	BGC	1	0
3	K	2	BGC	2	0

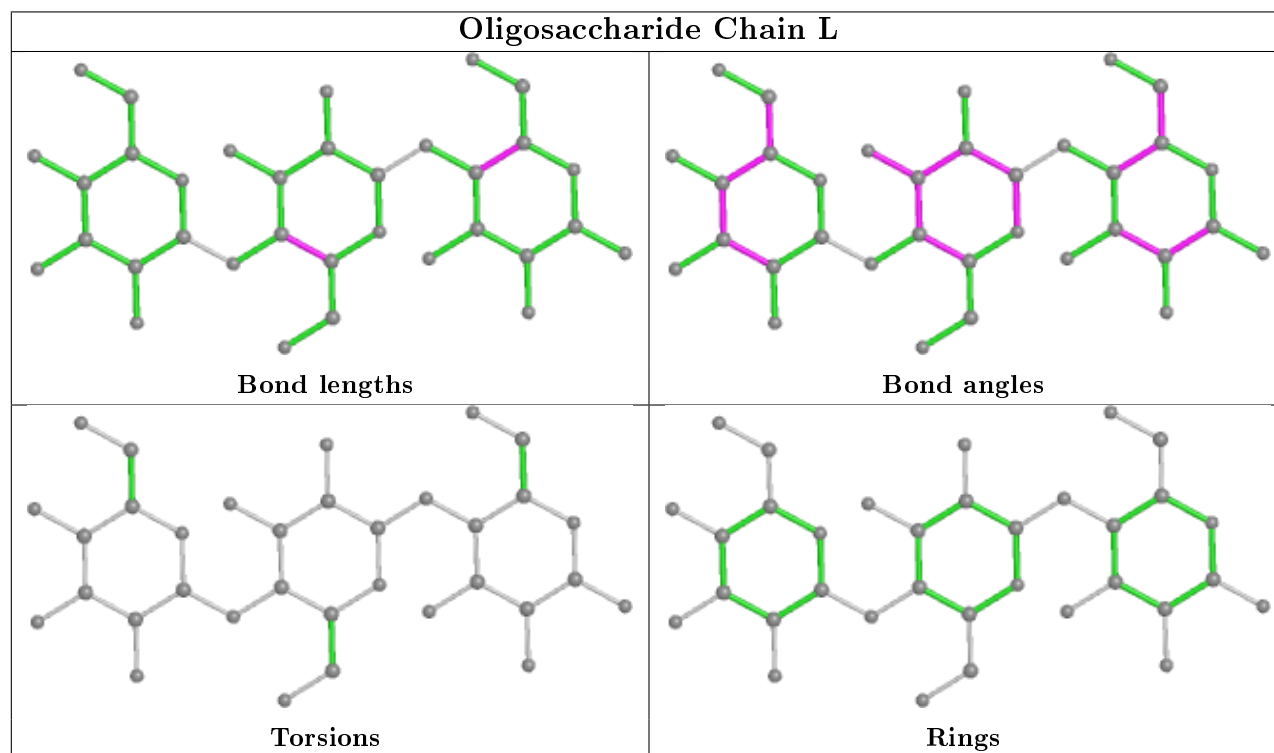
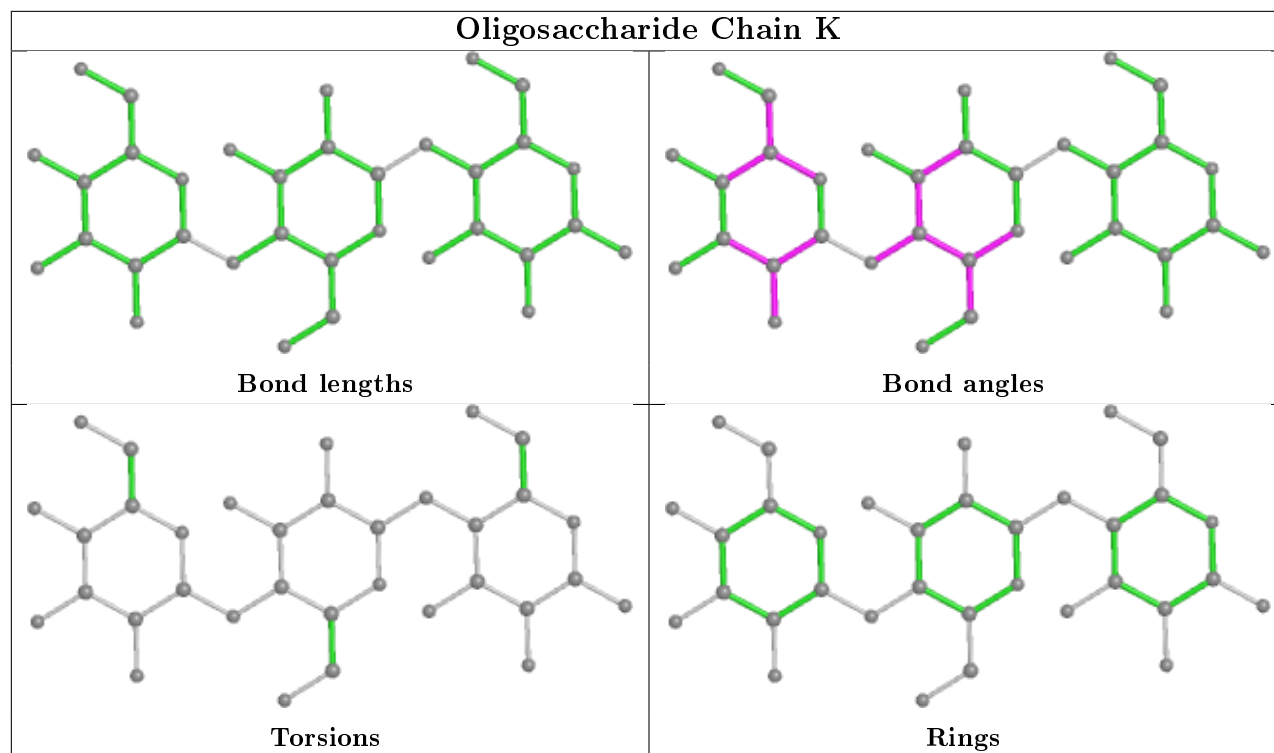
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

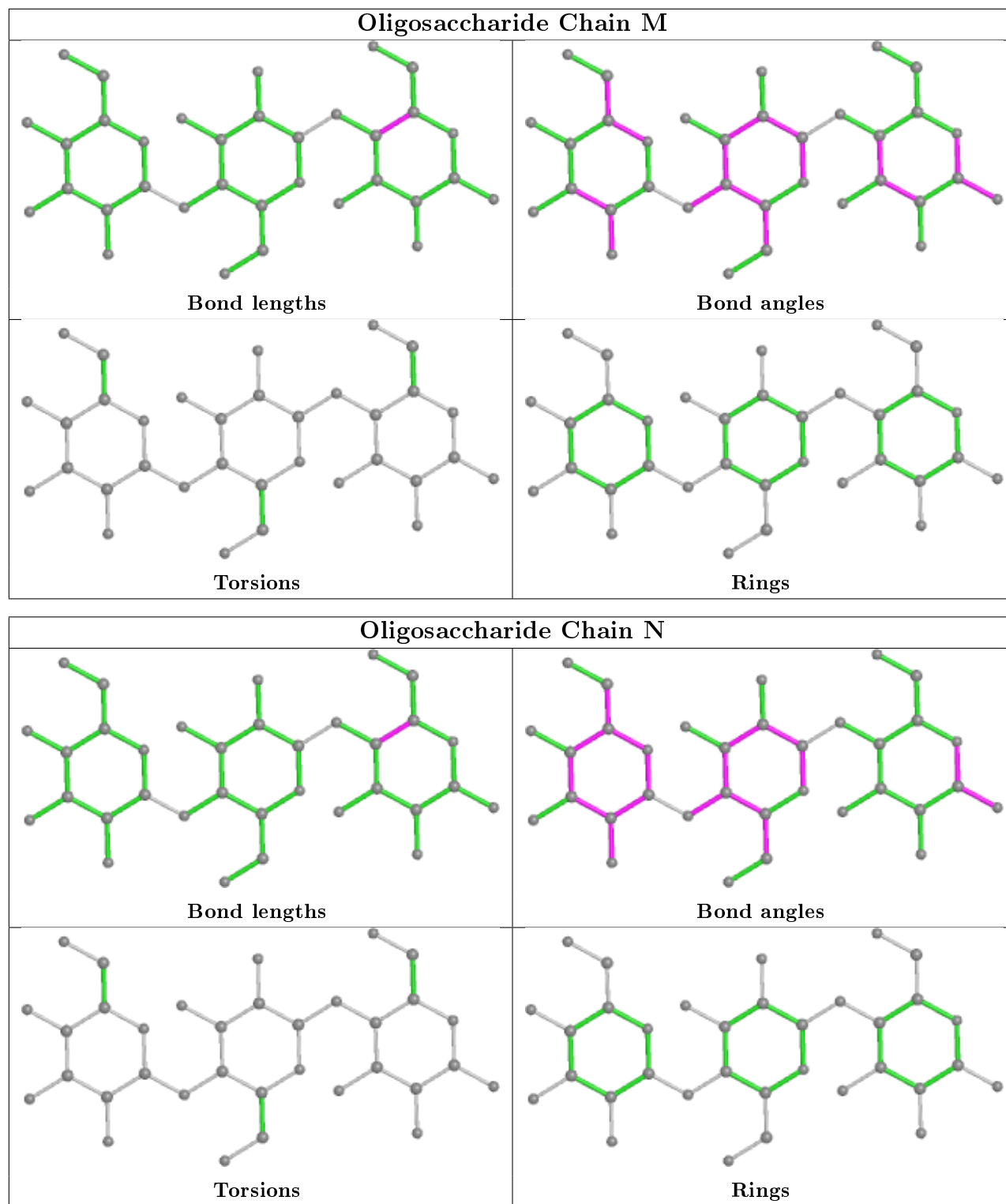
Oligosaccharide Chain I



Oligosaccharide Chain J







5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	345/345 (100%)	-0.82	0 100 100	5, 11, 23, 37	0
1	B	345/345 (100%)	-0.56	4 (1%) 79 81	7, 17, 33, 45	0
1	C	345/345 (100%)	-0.68	5 (1%) 75 78	5, 12, 27, 56	0
1	D	345/345 (100%)	-0.80	0 100 100	7, 14, 30, 41	0
2	E	107/107 (100%)	-0.34	4 (3%) 41 46	9, 18, 46, 59	0
2	F	107/107 (100%)	-0.71	2 (1%) 66 70	10, 15, 28, 48	0
2	G	107/107 (100%)	-0.32	6 (5%) 24 28	8, 17, 41, 52	0
2	H	107/107 (100%)	-0.67	1 (0%) 84 86	8, 16, 33, 56	0
All	All	1808/1808 (100%)	-0.67	22 (1%) 79 81	5, 14, 33, 59	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	7	PHE	6.8
1	C	5	THR	6.1
1	C	6	ALA	5.7
1	C	4	SER	5.7
2	G	422	ILE	3.7
1	C	8	THR	3.4
2	E	475	THR	3.3
2	G	475	THR	3.2
2	G	381	SER	3.0
2	F	381	SER	2.6
1	B	317	LYS	2.5
2	G	487	LYS	2.4
1	B	314	VAL	2.3
2	G	486	VAL	2.3
2	G	423	ASN	2.3
1	B	315	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	381	SER	2.3
1	B	282	ASN	2.2
2	H	487	LYS	2.2
2	E	422	ILE	2.1
2	E	487	LYS	2.1
2	F	487	LYS	2.1

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](#)

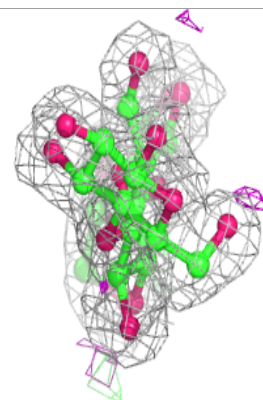
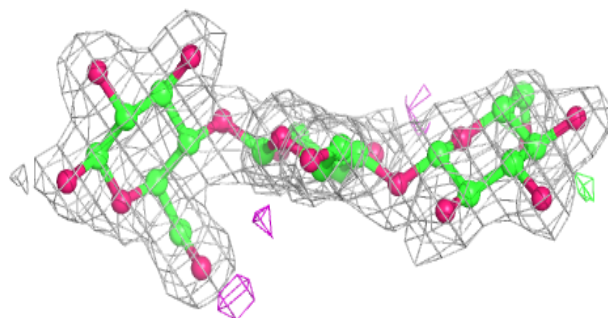
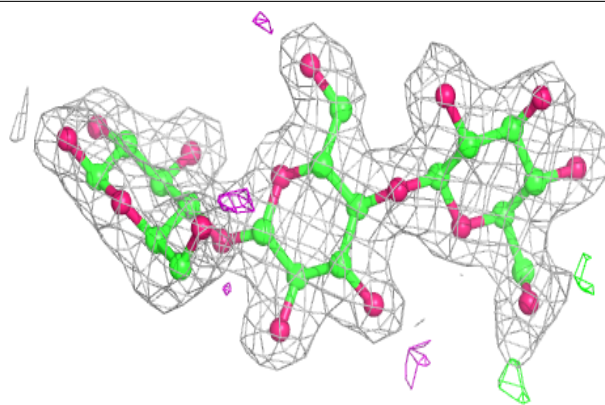
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BGC	L	1	12/12	0.78	0.22	23,34,45,54	0
3	BGC	J	1	12/12	0.78	0.19	18,31,38,44	0
3	BGC	N	1	12/12	0.78	0.16	16,33,43,45	0
3	BGC	L	2	11/12	0.81	0.20	20,31,39,42	0
3	BGC	J	2	11/12	0.83	0.18	18,29,32,33	0
3	BGC	N	3	11/12	0.85	0.19	34,44,52,52	0
3	BGC	N	2	11/12	0.86	0.23	23,33,40,40	0
3	BGC	M	1	12/12	0.86	0.14	14,22,33,35	0
3	BGC	M	2	11/12	0.87	0.14	21,27,33,34	0
3	BGC	K	1	12/12	0.90	0.13	15,28,37,45	0
3	BGC	L	3	11/12	0.90	0.12	25,32,46,47	0
3	BGC	K	2	11/12	0.91	0.18	27,32,37,40	0
3	BGC	J	3	11/12	0.92	0.12	22,29,32,33	0
3	BGC	M	3	11/12	0.93	0.20	24,31,42,44	0
3	BGC	I	3	11/12	0.94	0.11	21,24,31,31	0
3	BGC	K	3	11/12	0.95	0.19	29,38,46,47	0
3	BGC	I	1	12/12	0.96	0.08	12,16,22,28	0
3	BGC	I	2	11/12	0.97	0.10	14,18,22,27	0

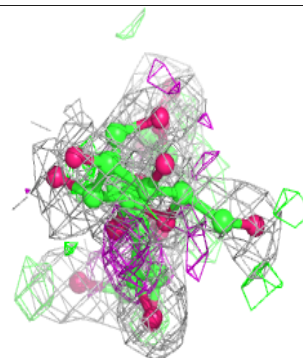
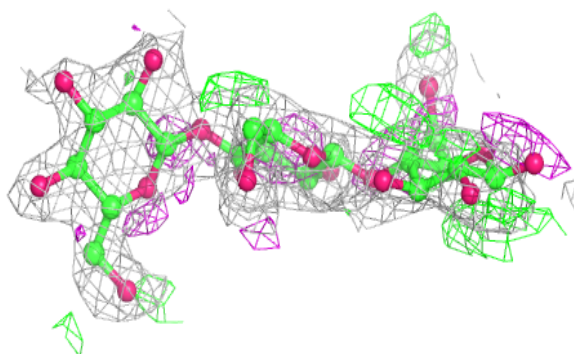
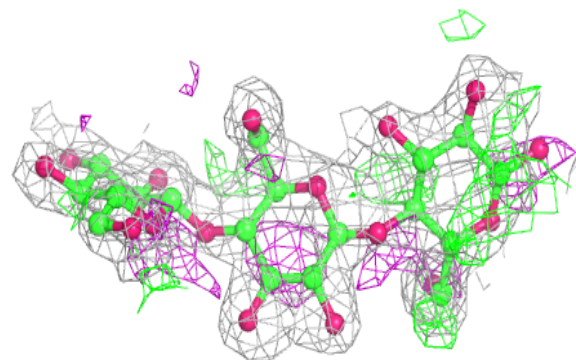
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

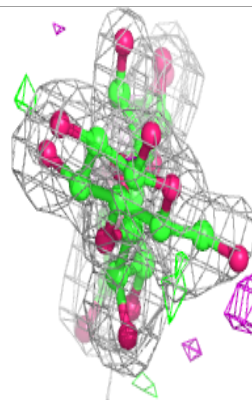
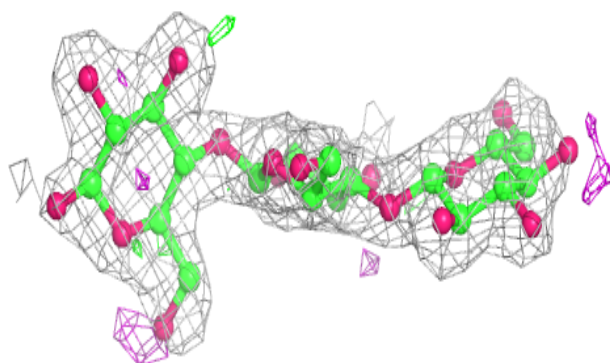
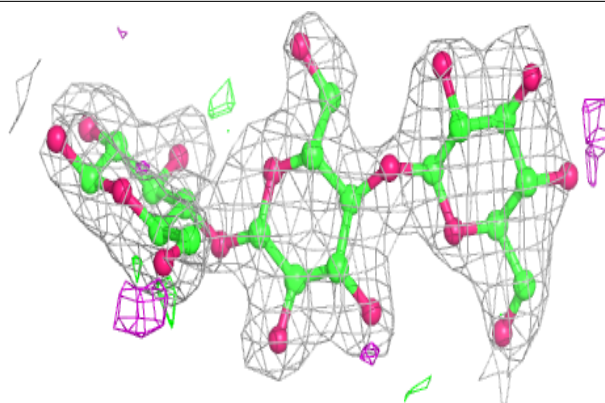
**Electron density around Chain J:**

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

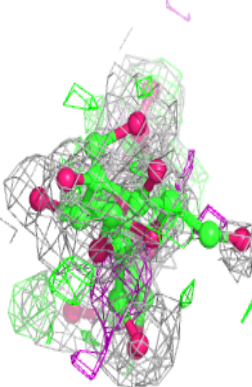
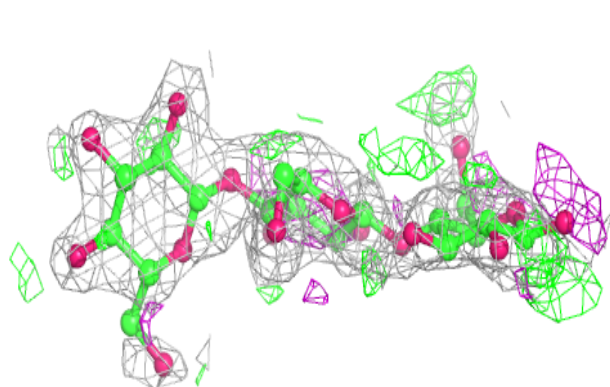
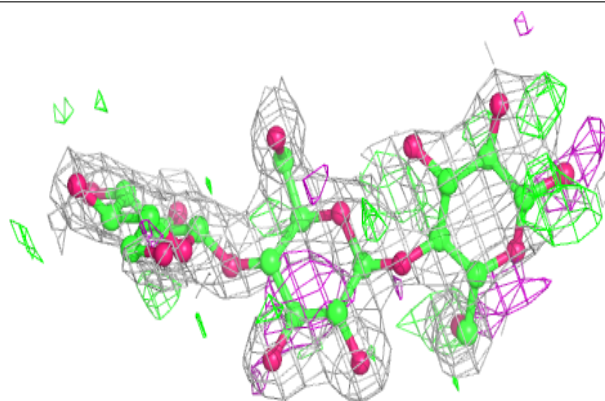


Electron density around Chain K:

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

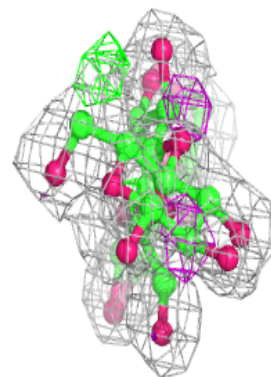
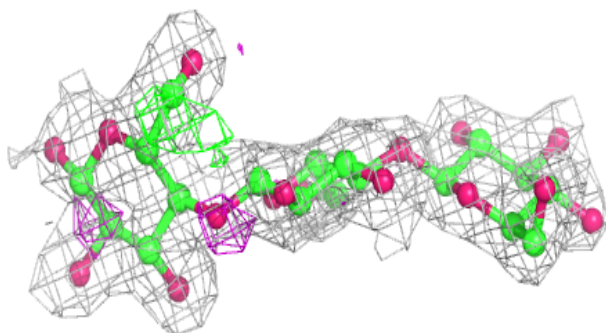
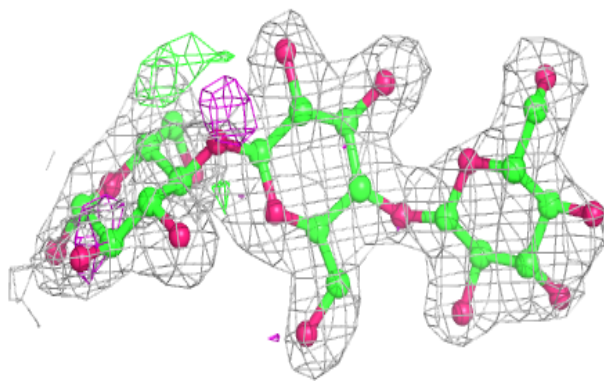
**Electron density around Chain L:**

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

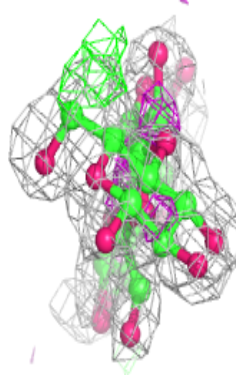
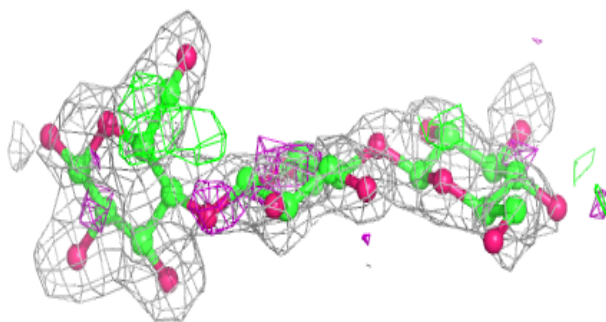


Electron density around Chain M:

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

**Electron density around Chain N:**

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



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.