Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2024 – 04:56 PM EST

PDB ID	:	4OJP
Title	:	Crystal Structure of Putative Tailspike Protein (TSP1, orf210) from Escherichia coli O157:H7 Bacteriohage CBA120 in Complex with Maltose
Authors	:	Chen, C.; Herzberg, O.
Deposited on	:	2014-01-21
Resolution	:	1.95 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:

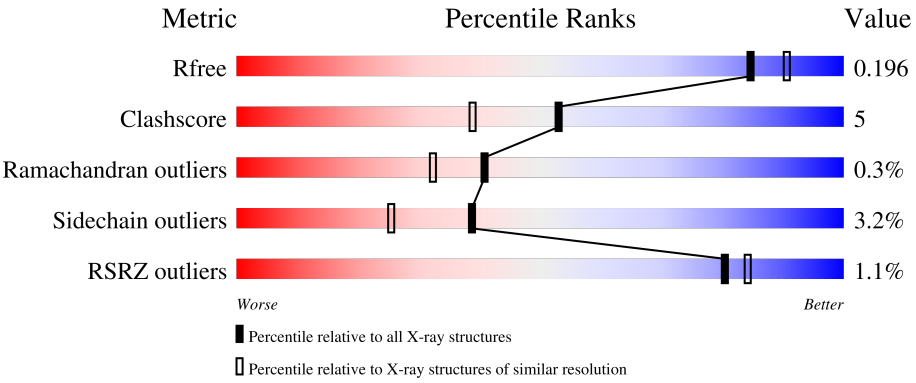
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.95 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	776	88% 9%
1	B	776	2% 84% 12%
1	C	776	87% 9%
2	D	2	100%
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	F	2	100%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 19572 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 Tailspike protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	758	Total	C	N	O	S	1	0	0
			5670	3576	954	1121	19			
1	B	756	Total	C	N	O	S	0	0	0
			5653	3568	947	1119	19			
1	C	758	Total	C	N	O	S	1	0	0
			5667	3573	955	1120	19			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	771	HIS	-	expression tag	UNP G3M189
A	772	HIS	-	expression tag	UNP G3M189
A	773	HIS	-	expression tag	UNP G3M189
A	774	HIS	-	expression tag	UNP G3M189
A	775	HIS	-	expression tag	UNP G3M189
A	776	HIS	-	expression tag	UNP G3M189
B	771	HIS	-	expression tag	UNP G3M189
B	772	HIS	-	expression tag	UNP G3M189
B	773	HIS	-	expression tag	UNP G3M189
B	774	HIS	-	expression tag	UNP G3M189
B	775	HIS	-	expression tag	UNP G3M189
B	776	HIS	-	expression tag	UNP G3M189
C	771	HIS	-	expression tag	UNP G3M189
C	772	HIS	-	expression tag	UNP G3M189
C	773	HIS	-	expression tag	UNP G3M189
C	774	HIS	-	expression tag	UNP G3M189
C	775	HIS	-	expression tag	UNP G3M189
C	776	HIS	-	expression tag	UNP G3M189

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	D	2	Total C O 23 12 11	0	0	0
2	E	2	Total C O 23 12 11	0	0	0
2	F	2	Total C O 23 12 11	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	1

- Molecule 4 is water.

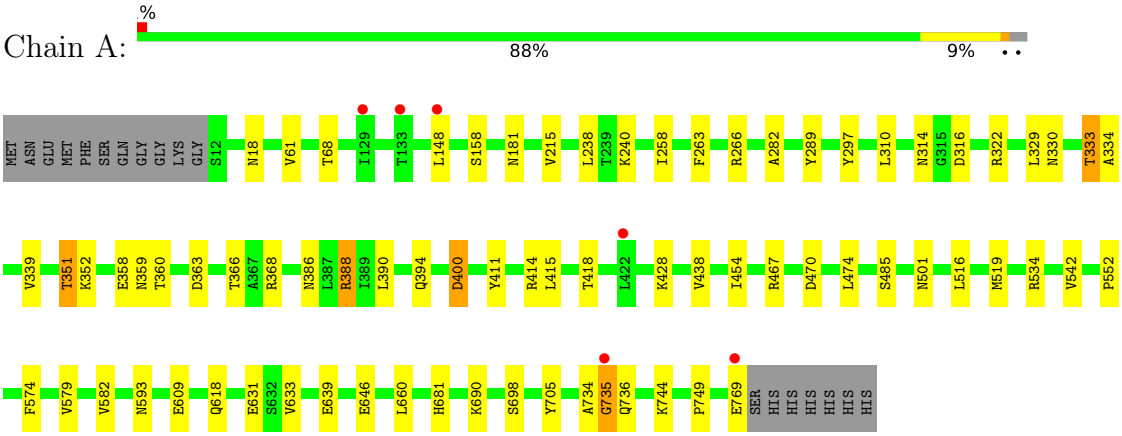
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	774	Total O 774 774	0	0
4	B	819	Total O 819 819	0	0
4	C	919	Total O 919 919	0	0

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.

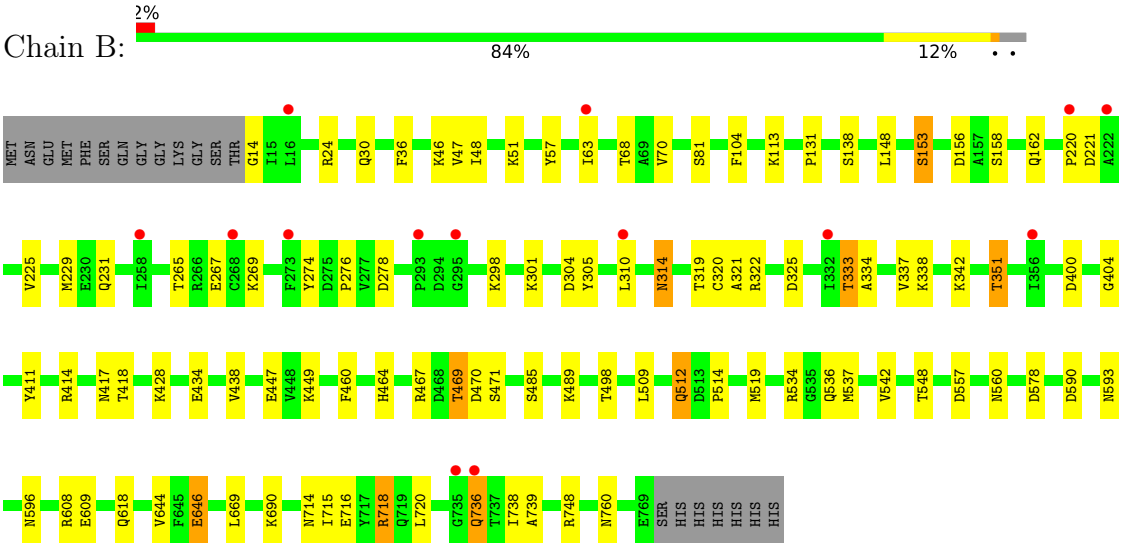
• Molecule 1: Tailspike protein

Chain A:



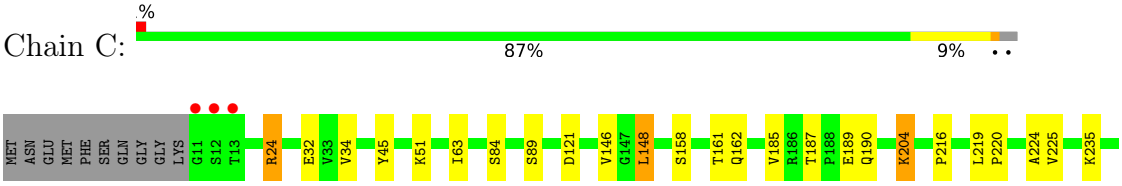
• Molecule 1: Tailspike protein

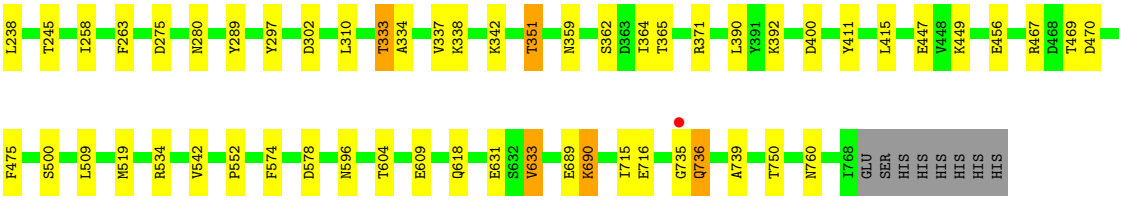
Chain B:



• Molecule 1: Tailspike protein

Chain C:





• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

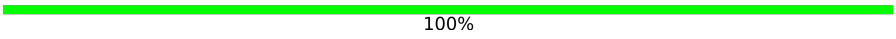
Chain D:

• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain E:

• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	123.44Å 147.98Å 171.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.70 – 1.95 67.91 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.5 (61.70-1.95) 98.5 (67.91-1.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.192 , 0.220 0.194 , 0.196	Depositor DCC
R_{free} test set	11323 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	22.6	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19572	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: ZN, GLC

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	0/5774	0.65	0/7850
1	B	0.39	0/5757	0.68	2/7828 (0.0%)
1	C	0.41	0/5771	0.68	0/7846
All	All	0.39	0/17302	0.67	2/23524 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	718	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	B	718	ARG	NE-CZ-NH1	6.81	123.70	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5670	0	5629	50	0
1	B	5653	0	5600	90	0
1	C	5667	0	5624	49	0
2	D	23	0	21	0	0
2	E	23	0	21	0	0
2	F	23	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
4	A	774	0	0	17	0
4	B	819	0	0	53	1
4	C	919	0	0	24	0
All	All	19572	0	16916	183	1

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 (183) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:371:ARG:HB2	4:C:1746:HOH:O	1.28	1.27
1:C:235:LYS:HE3	4:C:1540:HOH:O	1.38	1.20
1:B:47:VAL:HG13	4:B:1701:HOH:O	1.38	1.19
1:C:338:LYS:HA	4:C:1746:HOH:O	1.46	1.16
1:A:593:ASN:ND2	4:A:1358:HOH:O	1.81	1.12
1:B:24:ARG:NE	4:B:1479:HOH:O	1.80	1.12
1:B:229:MET:SD	4:B:1465:HOH:O	2.08	1.10
1:B:57:TYR:C	4:B:1701:HOH:O	1.92	1.05
1:B:618:GLN:HG3	4:B:1390:HOH:O	1.56	1.03
1:B:24:ARG:CZ	4:B:1479:HOH:O	2.04	1.02
1:B:63:ILE:O	4:B:1424:HOH:O	1.82	0.97
1:B:512:GLN:O	4:B:1561:HOH:O	1.82	0.96
1:B:57:TYR:O	4:B:1701:HOH:O	1.81	0.96
1:C:338:LYS:O	4:C:1746:HOH:O	1.83	0.95
1:C:534:ARG:CZ	4:C:1547:HOH:O	2.15	0.94
1:B:24:ARG:NH2	4:B:1479:HOH:O	1.99	0.93
1:C:162:GLN:CG	4:C:1806:HOH:O	2.15	0.93
1:A:68:THR:OG1	4:A:1587:HOH:O	1.86	0.92
1:B:68:THR:O	4:B:1583:HOH:O	1.88	0.90
1:A:681:HIS:HD2	1:A:705:TYR:H	1.21	0.89
1:A:400:ASP:OD2	4:A:1606:HOH:O	1.92	0.88
1:B:351:THR:CG2	4:B:1482:HOH:O	2.21	0.87
1:B:70:VAL:HG23	4:B:1583:HOH:O	1.74	0.86
1:B:609:GLU:OE2	4:B:1395:HOH:O	1.94	0.85
1:A:769:GLU:N	4:A:1333:HOH:O	2.07	0.85
1:B:548:THR:HG22	4:B:1408:HOH:O	1.76	0.85
1:A:18:ASN:OD1	4:B:1479:HOH:O	1.93	0.84
1:B:449:LYS:NZ	4:B:991:HOH:O	2.11	0.83
1:B:278:ASP:OD2	4:B:1515:HOH:O	1.96	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:GLU:HB3	4:A:1569:HOH:O	1.80	0.82
1:A:388:ARG:NH2	4:A:954:HOH:O	2.14	0.80
1:B:81:SER:N	4:B:1583:HOH:O	2.14	0.80
1:C:302:ASP:HB2	4:C:1760:HOH:O	1.81	0.79
1:B:57:TYR:N	4:B:1701:HOH:O	2.15	0.79
1:A:351:THR:CG2	4:A:1406:HOH:O	2.32	0.78
1:C:338:LYS:CA	4:C:1746:HOH:O	2.13	0.77
1:A:646:GLU:CG	4:A:1411:HOH:O	2.34	0.75
1:C:63:ILE:O	4:C:1203:HOH:O	2.03	0.75
1:B:469:THR:HG21	4:B:1474:HOH:O	1.87	0.75
1:B:156:ASP:OD2	4:B:1001:HOH:O	2.05	0.73
1:A:534:ARG:CZ	4:C:1547:HOH:O	2.36	0.72
1:B:322:ARG:NH1	4:B:958:HOH:O	2.22	0.71
1:C:162:GLN:CG	4:C:1805:HOH:O	2.39	0.70
1:C:216:PRO:HG2	1:C:219:LEU:HD21	1.74	0.69
1:A:735:GLY:O	4:A:923:HOH:O	2.11	0.67
1:A:181:ASN:O	1:C:187:THR:HG21	1.94	0.67
1:B:325:ASP:OD2	4:B:1399:HOH:O	2.11	0.67
1:B:578:ASP:CB	4:B:1481:HOH:O	2.42	0.67
1:C:689:GLU:OE1	4:C:1475:HOH:O	2.12	0.67
1:B:434:GLU:OE2	4:B:1440:HOH:O	2.13	0.65
1:B:736:GLN:HA	1:B:760:ASN:O	1.96	0.65
1:B:414:ARG:NH2	1:B:418:THR:O	2.30	0.65
1:B:618:GLN:NE2	4:B:1390:HOH:O	2.30	0.65
1:C:604:THR:O	4:C:1464:HOH:O	2.14	0.65
1:B:51:LYS:O	4:B:1603:HOH:O	2.15	0.64
1:B:14:GLY:N	4:B:1458:HOH:O	2.30	0.63
1:A:681:HIS:CD2	1:A:705:TYR:H	2.11	0.62
1:A:314:ASN:ND2	1:A:316:ASP:OD2	2.34	0.61
1:B:321:ALA:N	4:B:1465:HOH:O	2.34	0.60
1:A:351:THR:HG23	4:A:1406:HOH:O	1.99	0.58
1:B:578:ASP:HB2	4:B:1481:HOH:O	2.02	0.58
1:B:304:ASP:OD1	1:B:338:LYS:NZ	2.29	0.57
1:C:338:LYS:C	4:C:1746:HOH:O	2.20	0.57
1:A:414:ARG:NH2	1:A:418:THR:O	2.37	0.57
1:A:358:GLU:OE1	1:A:368:ARG:HD3	2.04	0.57
1:C:690:LYS:NZ	1:C:716:GLU:OE2	2.35	0.57
1:C:32:GLU:OE1	4:C:1368:HOH:O	2.18	0.57
1:B:590:ASP:OD2	4:B:1270:HOH:O	2.18	0.56
1:B:578:ASP:HB3	4:B:1481:HOH:O	2.06	0.56
1:C:24:ARG:NH2	4:C:1124:HOH:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:THR:HG22	1:C:190:GLN:HG3	1.87	0.56
1:A:359:ASN:ND2	4:A:1156:HOH:O	2.34	0.55
1:A:314:ASN:HB3	1:A:316:ASP:H	1.71	0.55
1:A:552:PRO:HB3	1:A:574:PHE:O	2.07	0.54
1:B:428:LYS:HE3	4:B:1428:HOH:O	2.07	0.54
1:B:320:CYS:HA	4:B:1465:HOH:O	2.07	0.53
1:A:534:ARG:HD3	4:A:1408:HOH:O	2.09	0.53
1:B:514:PRO:HA	4:B:1464:HOH:O	2.09	0.52
1:B:351:THR:HG23	4:B:1482:HOH:O	1.94	0.52
1:A:474:LEU:HD21	1:A:501:ASN:HD22	1.74	0.52
1:B:718:ARG:HD3	4:C:923:HOH:O	2.10	0.52
1:A:240:LYS:HE2	4:A:1118:HOH:O	2.10	0.51
1:C:631:GLU:HG2	1:C:633:VAL:HG12	1.92	0.51
1:B:351:THR:HG22	4:B:1482:HOH:O	1.97	0.51
1:C:310:LEU:HB3	4:C:1748:HOH:O	2.11	0.51
1:A:744:LYS:HD2	1:B:736:GLN:HG2	1.92	0.51
1:B:274:TYR:CE2	1:B:276:PRO:HG3	2.46	0.51
1:B:322:ARG:HG3	1:B:322:ARG:HH11	1.75	0.51
1:B:593:ASN:ND2	4:B:1270:HOH:O	2.06	0.51
1:C:618:GLN:NE2	4:C:1604:HOH:O	1.93	0.50
1:A:238:LEU:HB2	1:A:258:ILE:HG12	1.94	0.50
1:B:320:CYS:CA	4:B:1465:HOH:O	2.59	0.50
1:C:596:ASN:OD1	1:C:609:GLU:HG2	2.12	0.49
1:A:467:ARG:HD2	1:A:470:ASP:OD1	2.13	0.49
1:B:24:ARG:NH2	4:B:1127:HOH:O	2.45	0.49
1:C:364:ILE:HD11	1:C:392:LYS:HA	1.94	0.49
1:A:352:LYS:HE2	4:B:1399:HOH:O	2.11	0.49
1:A:333:THR:HG23	1:A:334:ALA:O	2.14	0.48
1:B:534:ARG:HG2	1:B:557:ASP:HB3	1.95	0.48
1:B:467:ARG:HD2	1:B:470:ASP:OD1	2.13	0.48
1:B:748:ARG:NH2	4:B:1497:HOH:O	2.47	0.48
1:B:417:ASN:ND2	1:B:485:SER:O	2.47	0.47
1:A:749:PRO:HA	4:A:1477:HOH:O	2.14	0.47
1:C:578:ASP:HB2	4:C:1815:HOH:O	2.13	0.47
1:C:736:GLN:HA	1:C:760:ASN:O	2.14	0.47
1:B:153:SER:OG	4:B:1393:HOH:O	2.19	0.47
1:C:289:TYR:HB3	1:C:297:TYR:HB3	1.96	0.47
1:A:639:GLU:HA	1:A:660:LEU:HB2	1.96	0.47
1:B:298:LYS:NZ	4:B:1586:HOH:O	2.47	0.47
1:B:231:GLN:HB3	4:B:1536:HOH:O	2.15	0.46
1:A:618:GLN:HG3	4:A:1433:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:519:MET:HE3	1:B:542:VAL:HG21	1.97	0.46
1:C:245:THR:HG22	1:C:275:ASP:O	2.16	0.46
1:A:360:THR:O	4:A:1307:HOH:O	2.21	0.46
1:C:359:ASN:OD1	1:C:415:LEU:HD11	2.16	0.46
1:B:320:CYS:C	4:B:1465:HOH:O	2.54	0.46
1:B:690:LYS:NZ	1:B:716:GLU:OE2	2.43	0.46
1:A:363:ASP:O	1:A:366:THR:HG22	2.16	0.45
1:C:467:ARG:HD2	1:C:470:ASP:OD1	2.16	0.45
1:B:489:LYS:HE3	1:B:509:LEU:HD21	1.98	0.45
1:B:596:ASN:OD1	1:B:609:GLU:HG2	2.17	0.45
1:A:474:LEU:HD21	1:A:501:ASN:ND2	2.31	0.45
1:C:204:LYS:HD3	4:C:1050:HOH:O	2.16	0.45
1:C:519:MET:HE3	1:C:542:VAL:HG21	1.99	0.45
1:B:131:PRO:HG3	4:B:1654:HOH:O	2.17	0.45
1:B:158:SER:O	1:B:162:GLN:HG3	2.17	0.45
1:C:552:PRO:HB3	1:C:574:PHE:O	2.17	0.45
1:A:744:LYS:HE2	1:B:736:GLN:OE1	2.17	0.44
1:B:618:GLN:CG	4:B:1390:HOH:O	2.35	0.44
1:A:258:ILE:HD12	1:A:330:ASN:H	1.83	0.44
1:A:289:TYR:HB3	1:A:297:TYR:HB3	2.00	0.44
1:B:229:MET:CG	4:B:1465:HOH:O	2.54	0.44
1:A:263:PHE:O	1:B:322:ARG:HD3	2.18	0.44
1:B:715:ILE:O	1:B:739:ALA:HA	2.18	0.44
1:B:57:TYR:CA	4:B:1701:HOH:O	2.42	0.44
1:A:282:ALA:HA	1:A:339:VAL:O	2.18	0.44
1:A:386:ASN:OD1	1:A:388:ARG:NH1	2.51	0.44
1:C:220:PRO:HD2	1:C:224:ALA:CB	2.47	0.44
1:C:715:ILE:O	1:C:739:ALA:HA	2.18	0.43
1:B:536:GLN:HG2	1:B:537:MET:O	2.18	0.43
1:C:351:THR:CG2	4:C:1572:HOH:O	2.65	0.43
1:B:24:ARG:HA	1:B:24:ARG:HD3	1.81	0.43
1:B:342:LYS:HE2	1:B:342:LYS:HB3	1.68	0.43
1:B:333:THR:HG23	1:B:334:ALA:O	2.19	0.43
1:B:104:PHE:HB3	1:B:138:SER:O	2.18	0.43
1:C:333:THR:HG23	1:C:334:ALA:O	2.19	0.43
1:B:438:VAL:HG22	1:B:460:PHE:HB2	2.01	0.43
1:B:464:HIS:HD2	1:B:498:THR:HG21	1.83	0.43
1:B:467:ARG:HD3	1:B:469:THR:HG22	2.00	0.43
1:B:319:THR:CG2	1:B:321:ALA:H	2.31	0.42
1:C:449:LYS:NZ	4:C:1439:HOH:O	2.52	0.42
1:B:305:TYR:O	1:B:342:LYS:NZ	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:LEU:O	1:B:314:ASN:N	2.46	0.42
1:C:24:ARG:HD3	1:C:24:ARG:HA	1.54	0.42
1:B:644:VAL:HG12	1:B:646:GLU:HG2	2.02	0.42
1:C:475:PHE:HB3	1:C:500:SER:HB3	2.02	0.42
1:A:258:ILE:HD12	1:A:329:LEU:HA	2.01	0.42
1:A:394:GLN:HA	1:A:438:VAL:O	2.19	0.42
1:A:519:MET:HE3	1:A:542:VAL:HG21	2.02	0.42
1:A:631:GLU:HG2	1:A:633:VAL:HG12	2.02	0.41
1:C:280:ASN:ND2	4:C:995:HOH:O	2.47	0.41
1:B:269:LYS:HA	1:B:269:LYS:HD2	1.92	0.41
1:C:333:THR:HG23	1:C:337:VAL:HB	2.01	0.41
1:C:148:LEU:HD12	1:C:148:LEU:HA	1.87	0.41
1:B:334:ALA:O	1:B:337:VAL:HG23	2.21	0.41
1:B:714:ASN:HA	1:B:738:ILE:HG13	2.01	0.41
1:C:121:ASP:HB2	1:C:161:THR:HG21	2.02	0.41
1:A:454:ILE:HD11	1:B:404:GLY:HA3	2.01	0.41
4:A:1034:HOH:O	1:B:534:ARG:HD3	2.20	0.41
1:B:36:PHE:HB2	1:B:48:ILE:HD11	2.02	0.41
1:C:34:VAL:HB	1:C:45:TYR:CG	2.55	0.41
1:C:187:THR:OG1	1:C:189:GLU:OE1	2.36	0.41
1:C:238:LEU:HB2	1:C:258:ILE:HG12	2.03	0.41
1:C:342:LYS:HB3	1:C:342:LYS:HE2	1.84	0.41
1:B:221:ASP:O	1:B:225:VAL:HG23	2.21	0.41
1:A:322:ARG:HD3	1:C:263:PHE:O	2.21	0.41
1:A:579:VAL:CG1	1:A:582:VAL:HB	2.51	0.41
1:B:536:GLN:HA	1:B:560:ASN:HB3	2.02	0.41
1:A:266:ARG:HA	1:A:359:ASN:O	2.21	0.40
1:A:359:ASN:OD1	1:A:415:LEU:HD11	2.22	0.40
1:B:46:LYS:NZ	4:B:1407:HOH:O	2.11	0.40
1:B:310:LEU:O	1:B:314:ASN:HB2	2.22	0.40
1:B:113:LYS:HE3	4:B:1406:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1282:HOH:O	4:B:1674:HOH:O[2_585]	1.57	0.63

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	756/776 (97%)	727 (96%)	26 (3%)	3 (0%)	34	24
1	B	754/776 (97%)	724 (96%)	28 (4%)	2 (0%)	41	32
1	C	756/776 (97%)	731 (97%)	23 (3%)	2 (0%)	41	32
All	All	2266/2328 (97%)	2182 (96%)	77 (3%)	7 (0%)	41	32

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	736	GLN
1	B	736	GLN
1	C	735	GLY
1	C	736	GLN
1	A	734	ALA
1	A	735	GLY
1	B	220	PRO

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	619/637 (97%)	603 (97%)	16 (3%)	46	32
1	B	615/637 (96%)	596 (97%)	19 (3%)	40	26
1	C	618/637 (97%)	594 (96%)	24 (4%)	32	17
All	All	1852/1911 (97%)	1793 (97%)	59 (3%)	39	25

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	VAL
1	A	148	LEU
1	A	158	SER
1	A	215	VAL
1	A	310	LEU
1	A	333	THR
1	A	351	THR
1	A	388	ARG
1	A	390	LEU
1	A	400	ASP
1	A	411	TYR
1	A	428	LYS
1	A	485	SER
1	A	516	LEU
1	A	690	LYS
1	A	698	SER
1	B	30	GLN
1	B	148	LEU
1	B	153	SER
1	B	265	THR
1	B	267	GLU
1	B	301	LYS
1	B	314	ASN
1	B	333	THR
1	B	351	THR
1	B	400	ASP
1	B	411	TYR
1	B	447	GLU
1	B	469	THR
1	B	471	SER
1	B	512	GLN
1	B	608	ARG
1	B	646	GLU
1	B	669	LEU
1	B	720	LEU
1	C	24	ARG
1	C	51	LYS
1	C	84	SER
1	C	89	SER
1	C	146	VAL
1	C	148	LEU
1	C	158	SER

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Mol	Chain	Res	Type
1	C	185	VAL
1	C	204	LYS
1	C	225	VAL
1	C	333	THR
1	C	351	THR
1	C	362	SER
1	C	365	THR
1	C	390	LEU
1	C	400	ASP
1	C	411	TYR
1	C	447	GLU
1	C	456	GLU
1	C	469	THR
1	C	509	LEU
1	C	633	VAL
1	C	690	LYS
1	C	750	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	HIS
1	A	262	ASN
1	A	424	GLN
1	A	501	ASN
1	A	681	HIS
1	B	328	ASN
1	C	192	ASN
1	C	262	ASN
1	C	280	ASN
1	C	327	ASN

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)

6 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	GLC	D	1	2	12,12,12	0.54	0	17,17,17	0.70	0
2	GLC	D	2	2	11,11,12	0.50	0	15,15,17	0.93	0
2	GLC	E	1	2	12,12,12	0.57	0	17,17,17	0.94	0
2	GLC	E	2	2	11,11,12	0.56	0	15,15,17	0.92	1 (6%)
2	GLC	F	1	2	12,12,12	0.54	0	17,17,17	0.85	0
2	GLC	F	2	2	11,11,12	0.57	0	15,15,17	0.66	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
2	GLC	D	1	2	-	1/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	GLC	E	1	2	-	0/2/22/22	0/1/1/1
2	GLC	E	2	2	-	0/2/19/22	0/1/1/1
2	GLC	F	1	2	-	2/2/22/22	0/1/1/1
2	GLC	F	2	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2	GLC	O5-C5-C6	2.60	111.28	107.20

There are no chirality outliers.

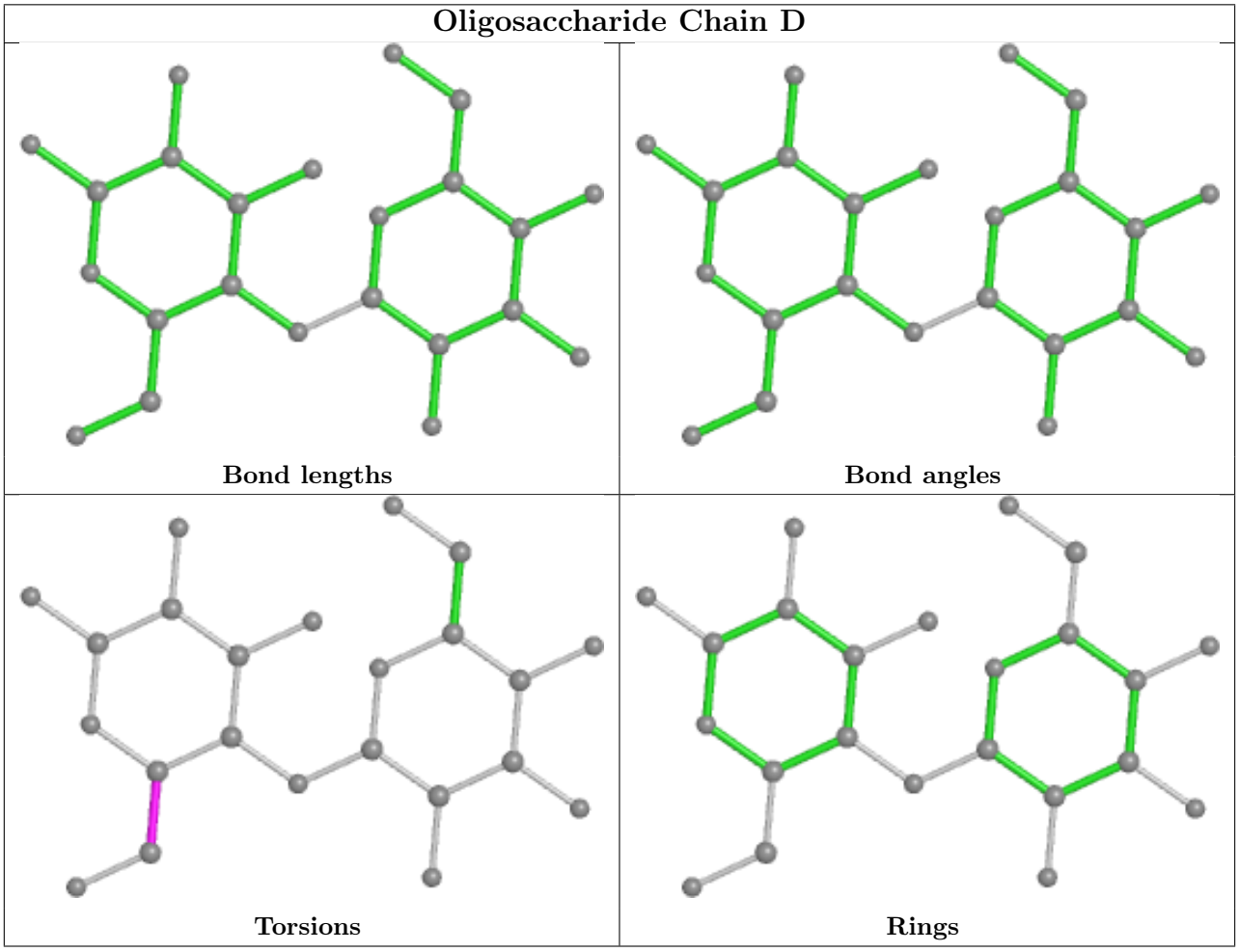
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1	GLC	O5-C5-C6-O6
2	F	1	GLC	C4-C5-C6-O6
2	F	2	GLC	C4-C5-C6-O6
2	F	2	GLC	O5-C5-C6-O6
2	D	1	GLC	C4-C5-C6-O6

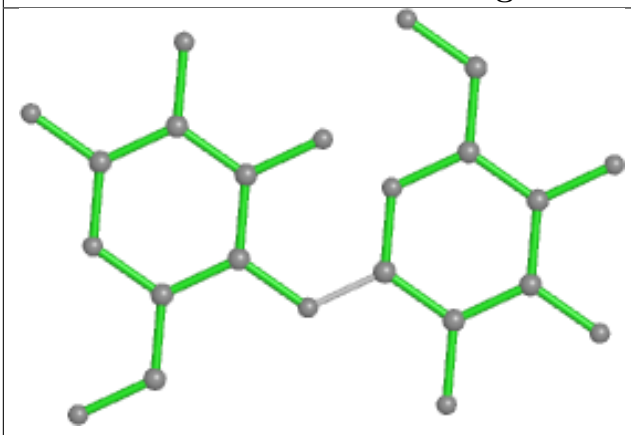
There are no ring outliers.

No monomer is involved in short contacts.

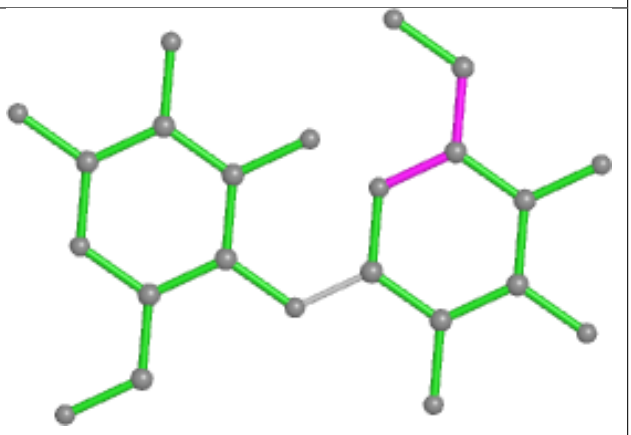
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



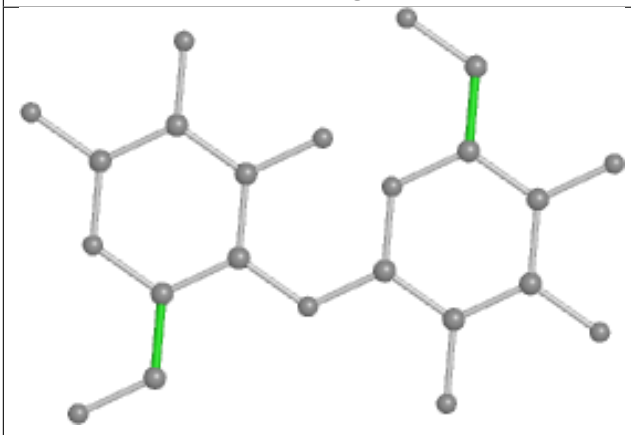
Oligosaccharide Chain E



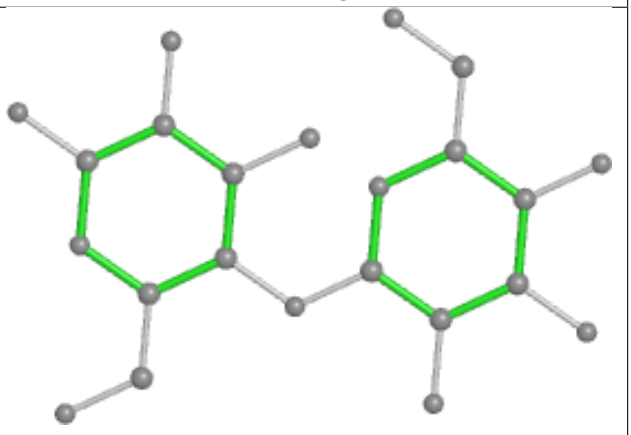
Bond lengths



Bond angles

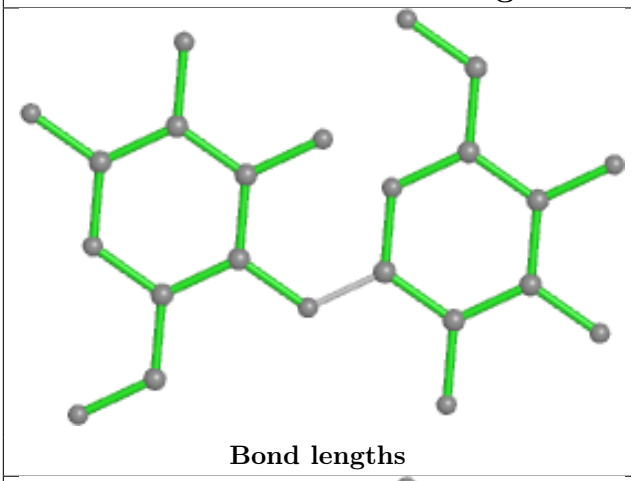


Torsions

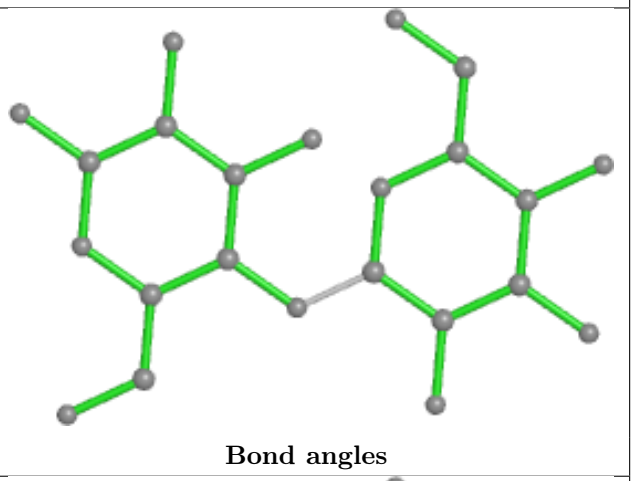


Rings

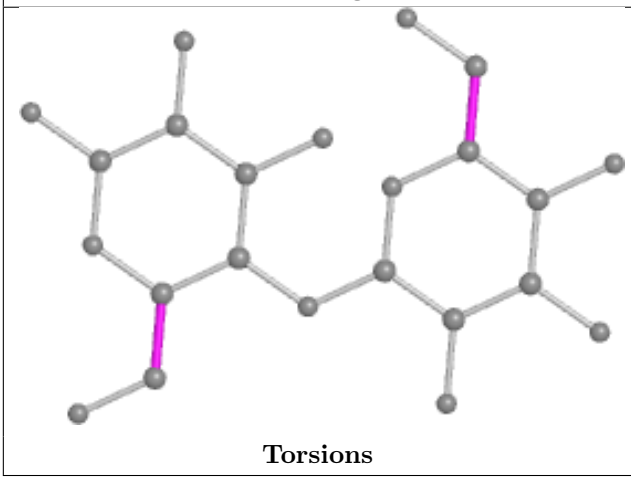
Oligosaccharide Chain F



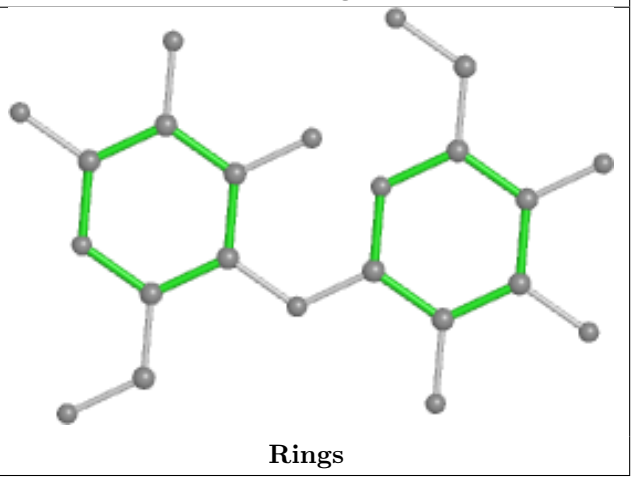
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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	758/776 (97%)	-0.04	6 (0%) 86 89	8, 18, 31, 58	1 (0%)
1	B	756/776 (97%)	0.03	14 (1%) 66 72	5, 15, 32, 49	0
1	C	758/776 (97%)	-0.21	4 (0%) 91 93	3, 12, 29, 67	0
All	All	2272/2328 (97%)	-0.07	24 (1%) 80 84	3, 15, 31, 67	1 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	735	GLY	5.2
1	C	11	GLY	5.2
1	A	129	ILE	3.6
1	B	16	LEU	3.4
1	B	63	ILE	3.4
1	B	222	ALA	3.4
1	C	12	SER	3.1
1	B	310	LEU	3.0
1	C	735	GLY	3.0
1	A	148	LEU	2.9
1	B	220	PRO	2.8
1	B	332	ILE	2.7
1	A	422	LEU	2.7
1	B	258	ILE	2.4
1	B	735	GLY	2.3
1	B	736	GLN	2.3
1	B	295	GLY	2.3
1	A	769	GLU	2.3
1	B	268	CYS	2.3
1	A	133	THR	2.2
1	B	293	PRO	2.2
1	B	273	PHE	2.1
1	C	13	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	356	ILE	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)

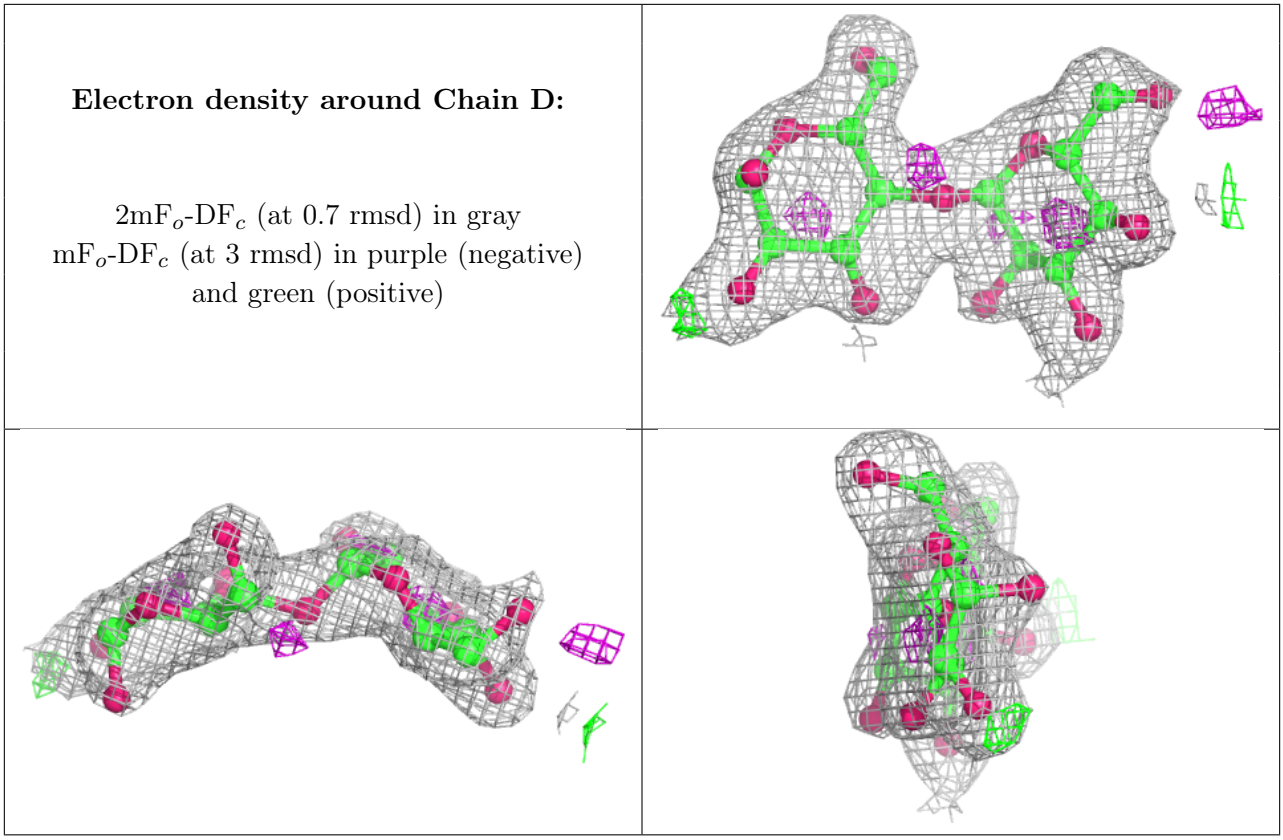
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	GLC	D	1	12/12	0.89	0.28	26,38,42,42	0
2	GLC	E	1	12/12	0.91	0.26	25,38,41,44	0
2	GLC	D	2	11/12	0.92	0.28	25,35,40,41	0
2	GLC	F	1	12/12	0.92	0.27	15,27,36,38	0
2	GLC	F	2	11/12	0.93	0.18	19,25,29,30	0
2	GLC	E	2	11/12	0.94	0.17	24,31,37,40	0

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

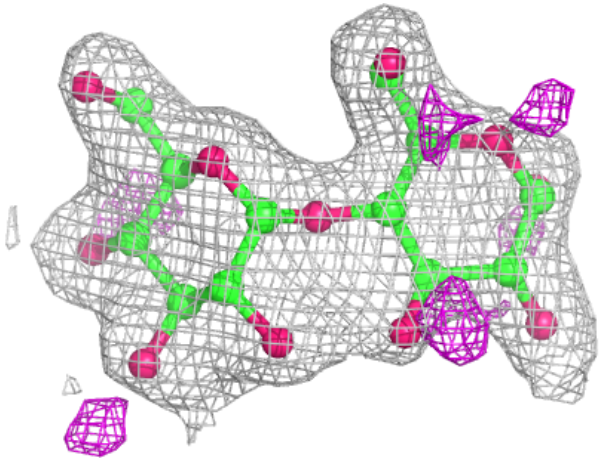
Electron density around Chain D:

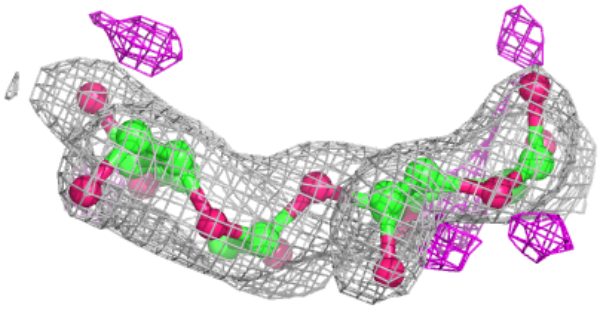
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

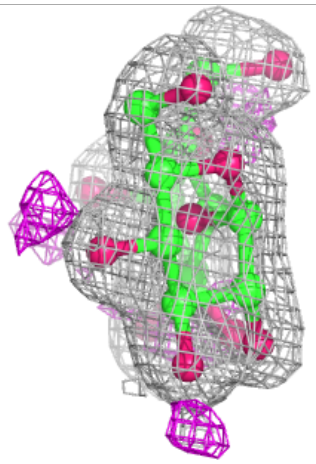


Electron density around Chain E:

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

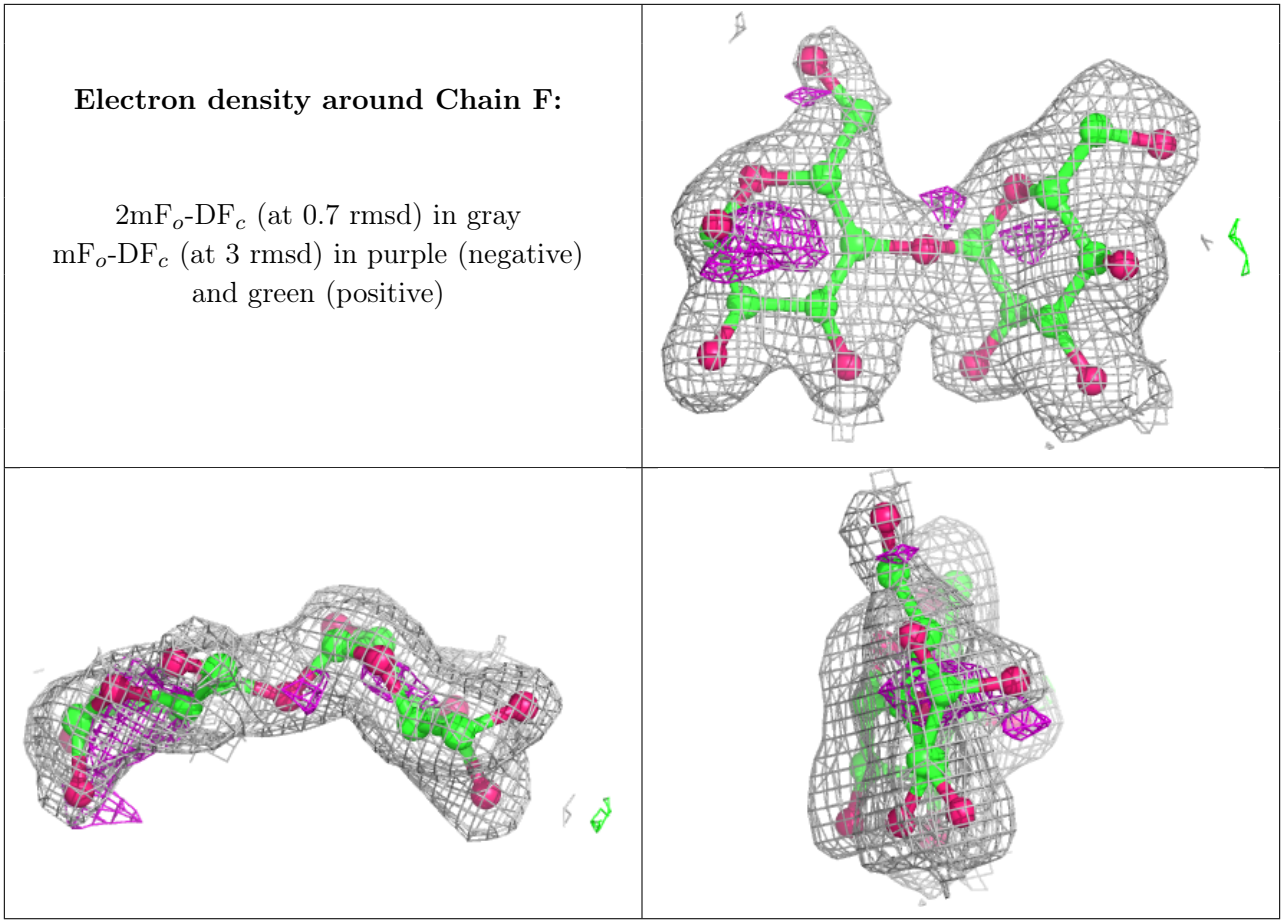






Electron density around Chain F:

$2mF_o$-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
3	ZN	A	802[A]	1/1	0.99	0.06	32,32,32,32	1

6.5 Other polymers

There are no such residues in this entry.