Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 09:40 PM BST

PDB ID	:	3W5F
Title	:	Crystal structure of tomato beta-galactosidase 4
Authors	:	Eda, M.; Tada, T.
Deposited on	:	2013-01-29
Resolution	:	1.65 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:

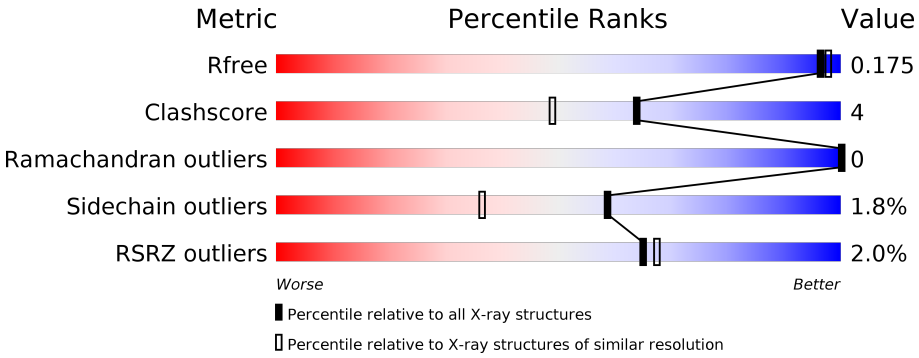
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	718	2% 89% 8%
1	B	718	2% 88% 9%
2	C	2	100%
2	D	2	50% 50%
2	E	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EPE	A	804	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13091 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 Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	701	Total	C	N	O	S	0	0	0
			5503	3521	940	1015	27			
1	B	701	Total	C	N	O	S	0	0	0
			5503	3521	940	1015	27			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLU	-	expression tag	UNP O81100
A	19	ALA	-	expression tag	UNP O81100
A	20	GLU	-	expression tag	UNP O81100
A	21	ALA	-	expression tag	UNP O81100
A	22	GLU	-	expression tag	UNP O81100
A	23	PHE	-	expression tag	UNP O81100
A	725	SER	-	expression tag	UNP O81100
A	726	ALA	-	expression tag	UNP O81100
A	727	ALA	-	expression tag	UNP O81100
A	728	ALA	-	expression tag	UNP O81100
A	729	ALA	-	expression tag	UNP O81100
A	730	SER	-	expression tag	UNP O81100
A	731	PHE	-	expression tag	UNP O81100
A	732	LEU	-	expression tag	UNP O81100
A	733	GLU	-	expression tag	UNP O81100
A	734	GLN	-	expression tag	UNP O81100
A	735	LYS	-	expression tag	UNP O81100
B	18	GLU	-	expression tag	UNP O81100
B	19	ALA	-	expression tag	UNP O81100
B	20	GLU	-	expression tag	UNP O81100
B	21	ALA	-	expression tag	UNP O81100
B	22	GLU	-	expression tag	UNP O81100
B	23	PHE	-	expression tag	UNP O81100
B	725	SER	-	expression tag	UNP O81100
B	726	ALA	-	expression tag	UNP O81100

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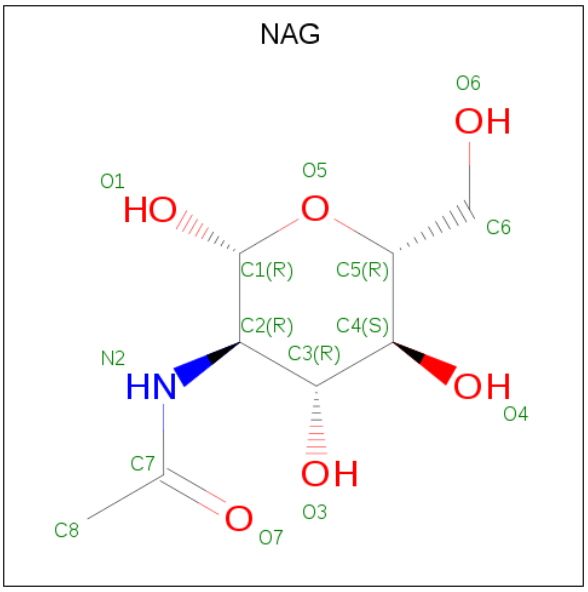
Chain	Residue	Modelled	Actual	Comment	Reference
B	727	ALA	-	expression tag	UNP O81100
B	728	ALA	-	expression tag	UNP O81100
B	729	ALA	-	expression tag	UNP O81100
B	730	SER	-	expression tag	UNP O81100
B	731	PHE	-	expression tag	UNP O81100
B	732	LEU	-	expression tag	UNP O81100
B	733	GLU	-	expression tag	UNP O81100
B	734	GLN	-	expression tag	UNP O81100
B	735	LYS	-	expression tag	UNP O81100

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

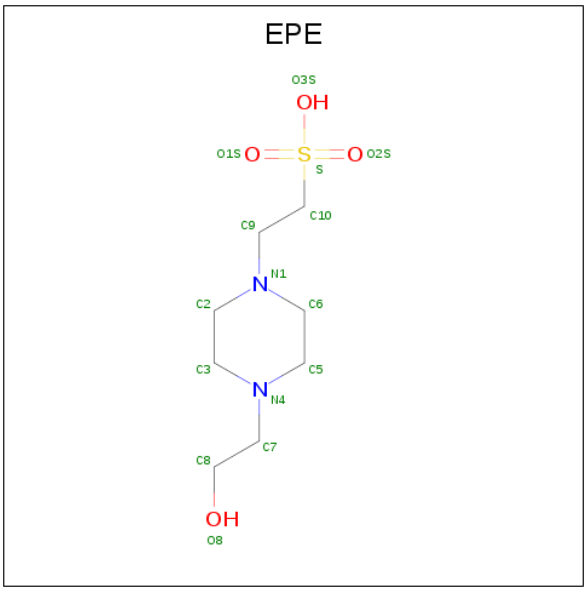
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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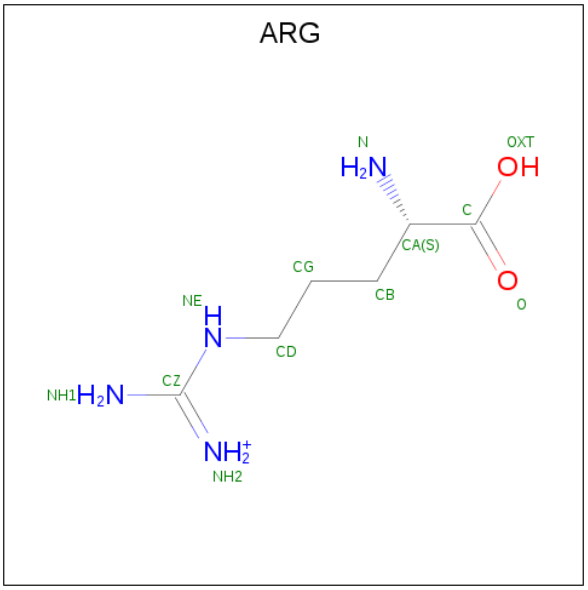
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O S 15 8 2 4 1	0	0
4	B	1	Total C N O S 15 8 2 4 1	0	0

- Molecule 5 is ARGININE (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 12 6 4 2	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	5	Total Cl 5 5	0	0
6	A	4	Total Cl 4 4	0	0

- Molecule 7 is water.

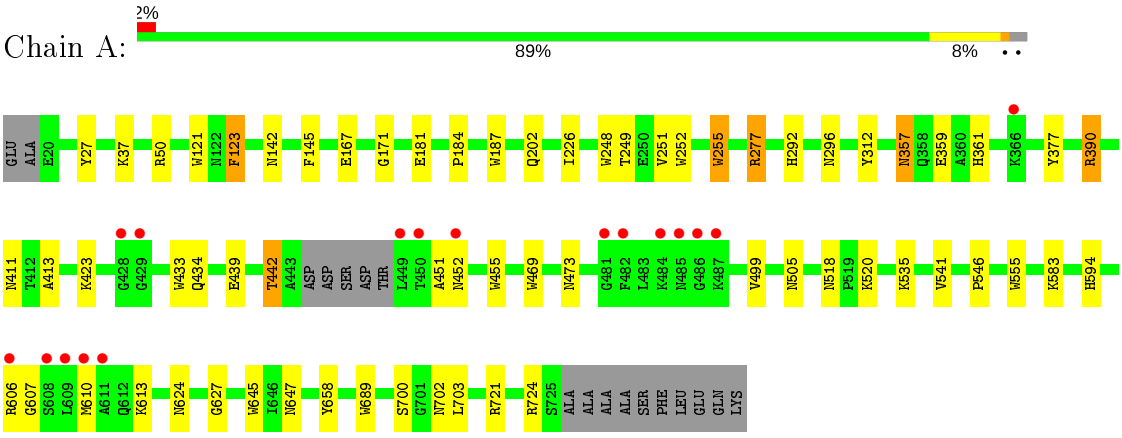
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	908	Total O 908 908	0	0
7	B	998	Total O 998 998	0	0

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.

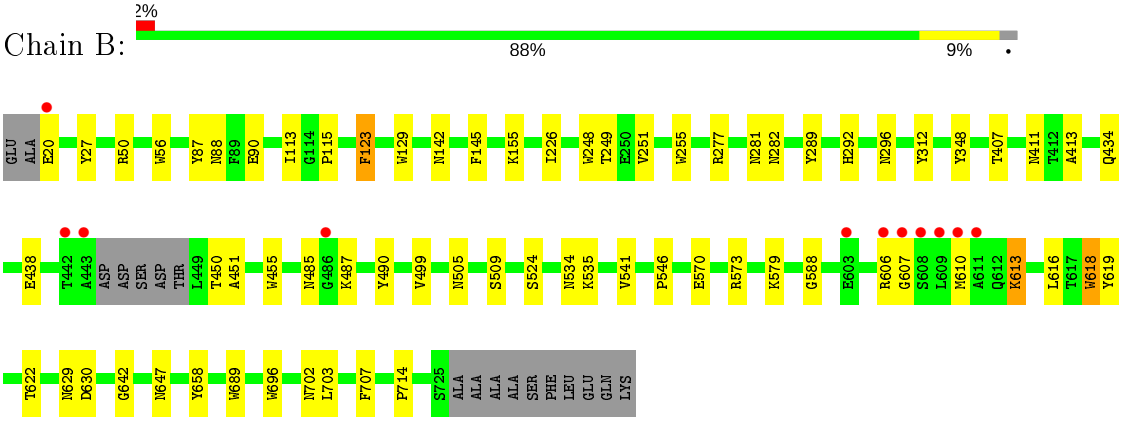
• Molecule 1: Beta-galactosidase

Chain A:



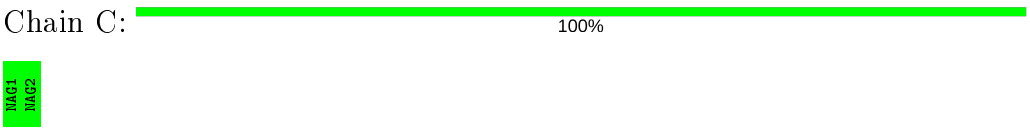
• Molecule 1: Beta-galactosidase

Chain B:



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

Chain C:

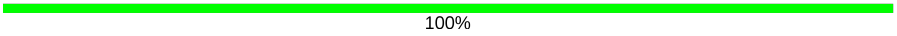


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

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

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.82Å 96.30Å 159.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.09 – 1.65 46.09 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.09-1.65) 99.6 (46.09-1.65)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.72 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.129 , 0.176 0.127 , 0.175	Depositor DCC
R_{free} test set	8537 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	13.4	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 40.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	13091	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 3.73% 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: EPE, NAG, CL

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	0.56	4/5665 (0.1%)	0.59	0/7697
1	B	0.57	6/5665 (0.1%)	0.60	0/7697
All	All	0.56	10/11330 (0.1%)	0.59	0/15394

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	255	TRP	CD2-CE2	5.40	1.47	1.41
1	A	255	TRP	CD2-CE2	5.28	1.47	1.41
1	A	689	TRP	CD2-CE2	5.22	1.47	1.41
1	A	121	TRP	CD2-CE2	5.19	1.47	1.41
1	B	618	TRP	CD2-CE2	5.16	1.47	1.41
1	B	689	TRP	CD2-CE2	5.10	1.47	1.41
1	B	56	TRP	CD2-CE2	5.08	1.47	1.41
1	A	555	TRP	CD2-CE2	5.04	1.47	1.41
1	B	696	TRP	CD2-CE2	5.04	1.47	1.41
1	B	129	TRP	CD2-CE2	5.00	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5503	0	5331	46	0
1	B	5503	0	5330	42	0
2	C	28	0	25	0	0
2	D	28	0	25	2	0
2	E	28	0	25	0	0
3	A	14	0	13	0	0
4	A	30	0	36	7	0
4	B	30	0	36	2	0
5	A	12	0	12	0	0
6	A	4	0	0	0	0
6	B	5	0	0	0	0
7	A	908	0	0	10	0
7	B	998	0	0	6	0
All	All	13091	0	10833	93	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 4.

All (93) 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:390:ARG:HG3	1:A:390:ARG:HH11	1.13	1.04
1:A:390:ARG:HG3	1:A:390:ARG:NH1	1.89	0.85
1:B:348:TYR:CE2	2:D:1:NAG:O6	2.33	0.81
1:A:434:GLN:HA	1:A:610:MET:HE1	1.72	0.71
1:B:348:TYR:CD2	2:D:1:NAG:O6	2.38	0.69
1:A:50:ARG:HH21	1:A:296:ASN:HD21	1.42	0.67
1:A:37:LYS:HE2	7:A:1356:HOH:O	1.95	0.66
1:A:505:ASN:ND2	1:A:535:LYS:H	1.93	0.66
1:B:50:ARG:HH21	1:B:296:ASN:HD21	1.44	0.64
1:A:442:THR:HG23	1:A:535:LYS:HD2	1.80	0.63
1:B:451:ALA:HB2	1:B:455:TRP:CZ2	2.34	0.62
1:B:570:GLU:HG3	7:B:1360:HOH:O	1.97	0.62
1:B:613:LYS:HG2	7:B:1471:HOH:O	2.00	0.61
1:A:142:ASN:HD22	1:A:145:PHE:H	1.49	0.61
1:A:411:ASN:ND2	1:A:413:ALA:H	1.99	0.60
1:B:607:GLY:O	1:B:610:MET:HG2	2.01	0.60
1:B:647:ASN:HD21	1:B:702:ASN:HA	1.67	0.59
1:B:573:ARG:HG3	7:B:1360:HOH:O	2.03	0.57
1:A:647:ASN:HD21	1:A:702:ASN:HA	1.70	0.56
1:B:411:ASN:ND2	1:B:413:ALA:H	2.02	0.56
1:B:142:ASN:HD22	1:B:145:PHE:H	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ARG:CG	1:A:390:ARG:NH1	2.66	0.56
1:A:473:ASN:HD21	1:A:535:LYS:NZ	2.04	0.55
1:B:289:TYR:CE1	4:B:805:EPE:H81	2.41	0.55
1:B:647:ASN:ND2	1:B:703:LEU:H	2.05	0.55
1:B:50:ARG:HE	1:B:296:ASN:ND2	2.04	0.55
4:A:804:EPE:H61	7:A:1129:HOH:O	2.08	0.53
1:B:292:HIS:HD2	7:B:905:HOH:O	1.91	0.52
1:B:505:ASN:ND2	1:B:535:LYS:H	2.08	0.52
1:A:357:ASN:HD22	1:A:377:TYR:HB2	1.74	0.52
1:B:407:THR:HG22	7:B:1436:HOH:O	2.10	0.51
1:A:277:ARG:HG2	7:A:1121:HOH:O	2.10	0.51
1:A:647:ASN:ND2	1:A:703:LEU:H	2.09	0.50
1:A:423:LYS:HD2	7:A:1582:HOH:O	2.11	0.50
1:A:520:LYS:HG2	7:A:1797:HOH:O	2.11	0.49
1:B:450:THR:HG21	1:B:579:LYS:HE3	1.94	0.49
1:B:490:TYR:CE2	1:B:524:SER:OG	2.65	0.49
1:A:142:ASN:ND2	1:A:145:PHE:H	2.09	0.49
1:B:505:ASN:HD21	1:B:534:ASN:HA	1.77	0.48
1:A:248:TRP:CD2	1:A:251:VAL:HG22	2.48	0.48
1:A:451:ALA:HB2	1:A:455:TRP:CZ2	2.50	0.47
4:A:804:EPE:H81	7:A:944:HOH:O	2.15	0.47
1:A:181:GLU:OE1	4:A:804:EPE:H101	2.15	0.46
1:B:642:GLY:HA3	1:B:707:PHE:O	2.16	0.46
1:A:499:VAL:HB	1:A:541:VAL:HB	1.98	0.46
1:A:50:ARG:HE	1:A:296:ASN:ND2	2.13	0.46
1:B:113:ILE:O	1:B:115:PRO:HA	2.16	0.46
1:B:123:PHE:HA	1:B:546:PRO:O	2.16	0.45
1:A:469:TRP:HB2	1:A:583:LYS:HB3	1.99	0.45
1:A:248:TRP:CE2	1:A:251:VAL:HG22	2.51	0.45
1:A:433:TRP:O	1:A:606:ARG:NH1	2.50	0.45
1:B:485:ASN:OD1	1:B:487:LYS:HB2	2.17	0.44
4:A:804:EPE:H81	4:A:804:EPE:H51	1.56	0.44
1:B:588:GLY:HA3	1:B:618:TRP:CE2	2.52	0.44
1:B:88:ASN:OD1	1:B:90:GLU:HG2	2.17	0.44
1:B:610:MET:CE	1:B:714:PRO:HG2	2.47	0.44
1:B:438:GLU:HB3	1:B:616:LEU:O	2.17	0.44
1:B:50:ARG:HE	1:B:296:ASN:HD21	1.66	0.44
1:B:588:GLY:HA3	1:B:618:TRP:CZ2	2.53	0.44
1:B:619:TYR:CE1	1:B:714:PRO:HG3	2.52	0.44
1:A:292:HIS:HD2	7:A:910:HOH:O	2.00	0.43
1:A:252:TRP:CZ2	4:A:804:EPE:H31	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:GLN:HG2	1:A:606:ARG:HD2	2.01	0.43
1:A:518:ASN:HB3	7:A:1797:HOH:O	2.19	0.43
1:A:594:HIS:HB2	1:A:645:TRP:CG	2.52	0.43
4:A:804:EPE:H51	7:A:944:HOH:O	2.19	0.43
1:A:624:ASN:HD22	1:A:700:SER:HA	1.83	0.43
1:B:87:TYR:CD1	1:B:155:LYS:HE2	2.54	0.43
1:A:184:PRO:HA	1:A:187:TRP:CE3	2.54	0.43
1:A:724:ARG:HB2	7:A:1349:HOH:O	2.19	0.43
1:B:281:ASN:O	1:B:282:ASN:HB2	2.19	0.42
1:A:184:PRO:HA	1:A:187:TRP:CD2	2.53	0.42
1:B:629:ASN:ND2	7:B:1452:HOH:O	2.52	0.42
1:A:606:ARG:NH1	1:A:607:GLY:H	2.17	0.42
1:A:610:MET:HE2	1:A:610:MET:HA	2.02	0.42
1:A:255:TRP:CH2	4:A:804:EPE:H32	2.55	0.42
1:A:123:PHE:HA	1:A:546:PRO:O	2.20	0.42
1:B:610:MET:HE1	1:B:714:PRO:HG2	2.02	0.42
1:A:606:ARG:HG3	1:A:607:GLY:N	2.34	0.42
1:B:142:ASN:ND2	1:B:145:PHE:H	2.18	0.42
1:B:499:VAL:HB	1:B:541:VAL:HB	2.01	0.42
4:B:806:EPE:H81	4:B:806:EPE:H52	1.75	0.42
1:B:438:GLU:HB3	1:B:616:LEU:HB3	2.01	0.42
1:A:359:GLU:OE1	1:A:361:HIS:HE1	2.03	0.41
1:B:622:THR:HA	1:B:702:ASN:O	2.21	0.41
1:A:27:TYR:CD2	1:A:226:ILE:HD11	2.55	0.41
1:B:27:TYR:CD2	1:B:226:ILE:HD11	2.56	0.41
1:A:627:GLY:O	1:A:721:ARG:NH1	2.39	0.41
1:A:610:MET:HE3	1:A:610:MET:HB2	1.61	0.41
1:A:167:GLU:HA	1:A:171:GLY:O	2.20	0.41
1:B:248:TRP:CD2	1:B:251:VAL:HG22	2.56	0.41
1:B:434:GLN:HG2	1:B:606:ARG:HD3	2.02	0.41
1:A:610:MET:CE	1:A:610:MET:HA	2.52	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	697/718 (97%)	678 (97%)	19 (3%)	0	100	100
1	B	697/718 (97%)	680 (98%)	17 (2%)	0	100	100
All	All	1394/1436 (97%)	1358 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	587/599 (98%)	575 (98%)	12 (2%)	55	32
1	B	587/599 (98%)	578 (98%)	9 (2%)	65	44
All	All	1174/1198 (98%)	1153 (98%)	21 (2%)	59	36

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	PHE
1	A	202	GLN
1	A	249	THR
1	A	277	ARG
1	A	312	TYR
1	A	357	ASN
1	A	390	ARG
1	A	439	GLU
1	A	442	THR
1	A	452	ASN
1	A	613	LYS
1	A	658	TYR
1	B	20	GLU
1	B	123	PHE
1	B	249	THR

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Mol	Chain	Res	Type
1	B	277	ARG
1	B	312	TYR
1	B	509	SER
1	B	613	LYS
1	B	630	ASP
1	B	658	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	143	GLN
1	A	154	GLN
1	A	202	GLN
1	A	292	HIS
1	A	296	ASN
1	A	357	ASN
1	A	411	ASN
1	A	416	ASN
1	A	473	ASN
1	A	505	ASN
1	A	594	HIS
1	A	624	ASN
1	A	647	ASN
1	B	142	ASN
1	B	292	HIS
1	B	296	ASN
1	B	411	ASN
1	B	437	ASN
1	B	505	ASN
1	B	526	ASN
1	B	629	ASN
1	B	647	ASN

5.3.3 RNA

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	NAG	C	1	1,2	14,14,15	0.34	0	17,19,21	0.82	0
2	NAG	C	2	2	14,14,15	0.30	0	17,19,21	0.61	0
2	NAG	D	1	1,2	14,14,15	0.33	0	17,19,21	0.72	0
2	NAG	D	2	2	14,14,15	0.29	0	17,19,21	0.61	0
2	NAG	E	1	1,2	14,14,15	0.30	0	17,19,21	0.62	0
2	NAG	E	2	2	14,14,15	0.29	0	17,19,21	0.62	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	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

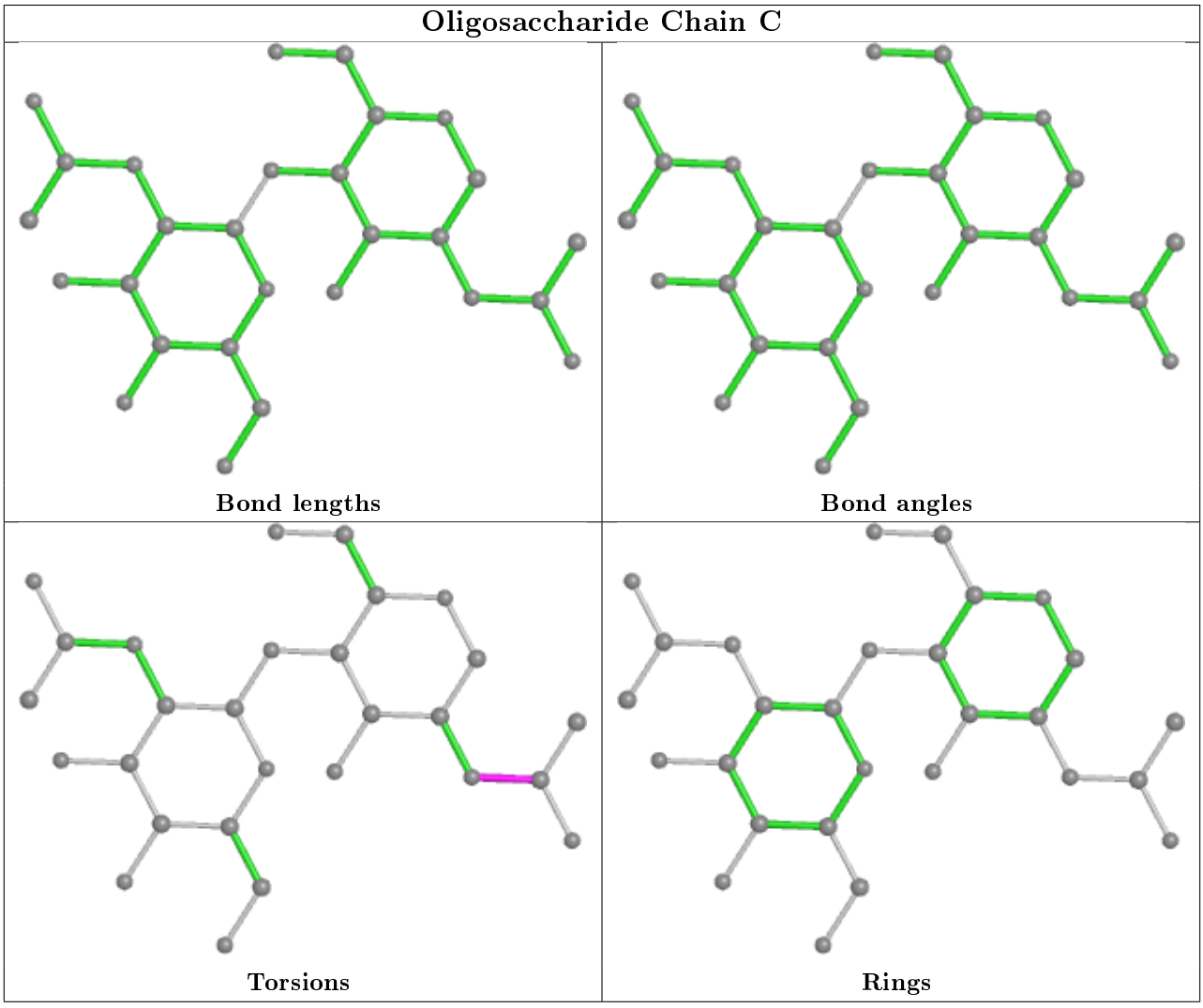
Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2

There are no ring outliers.

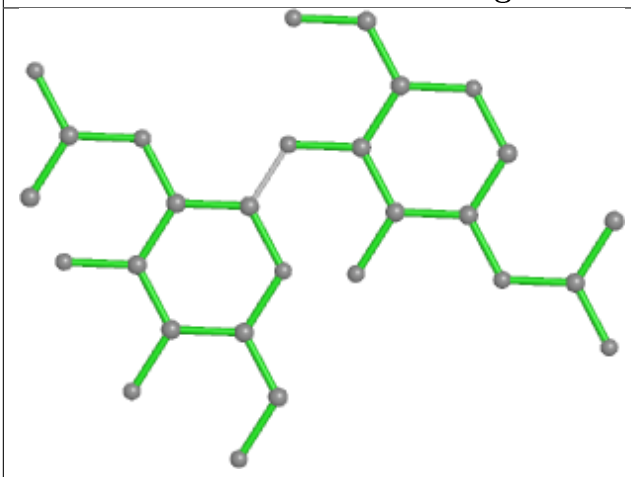
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	2	0

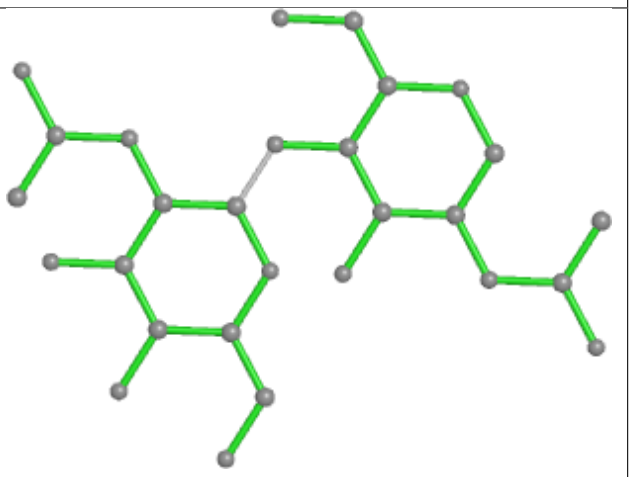
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



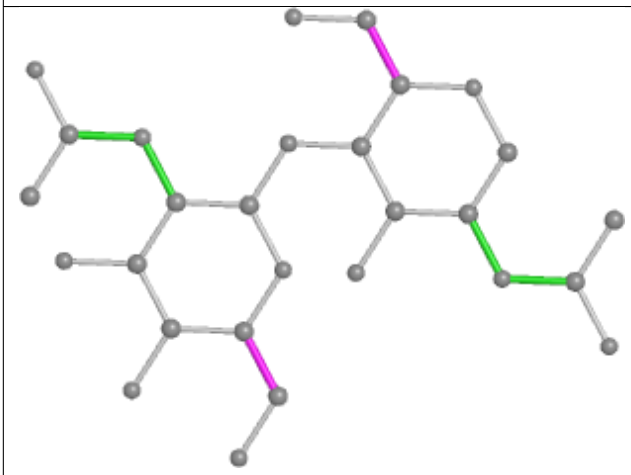
Oligosaccharide Chain D



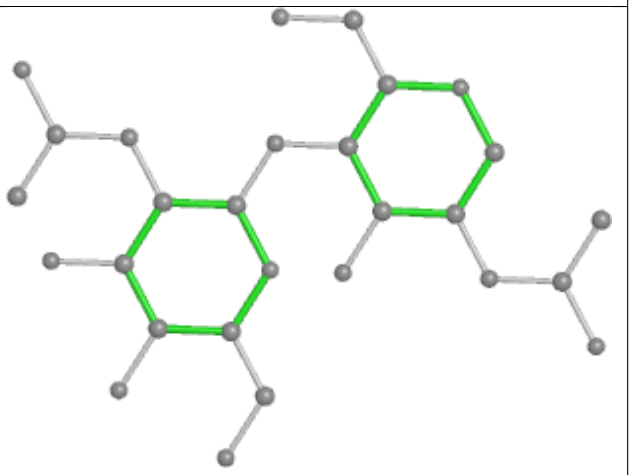
Bond lengths



Bond angles

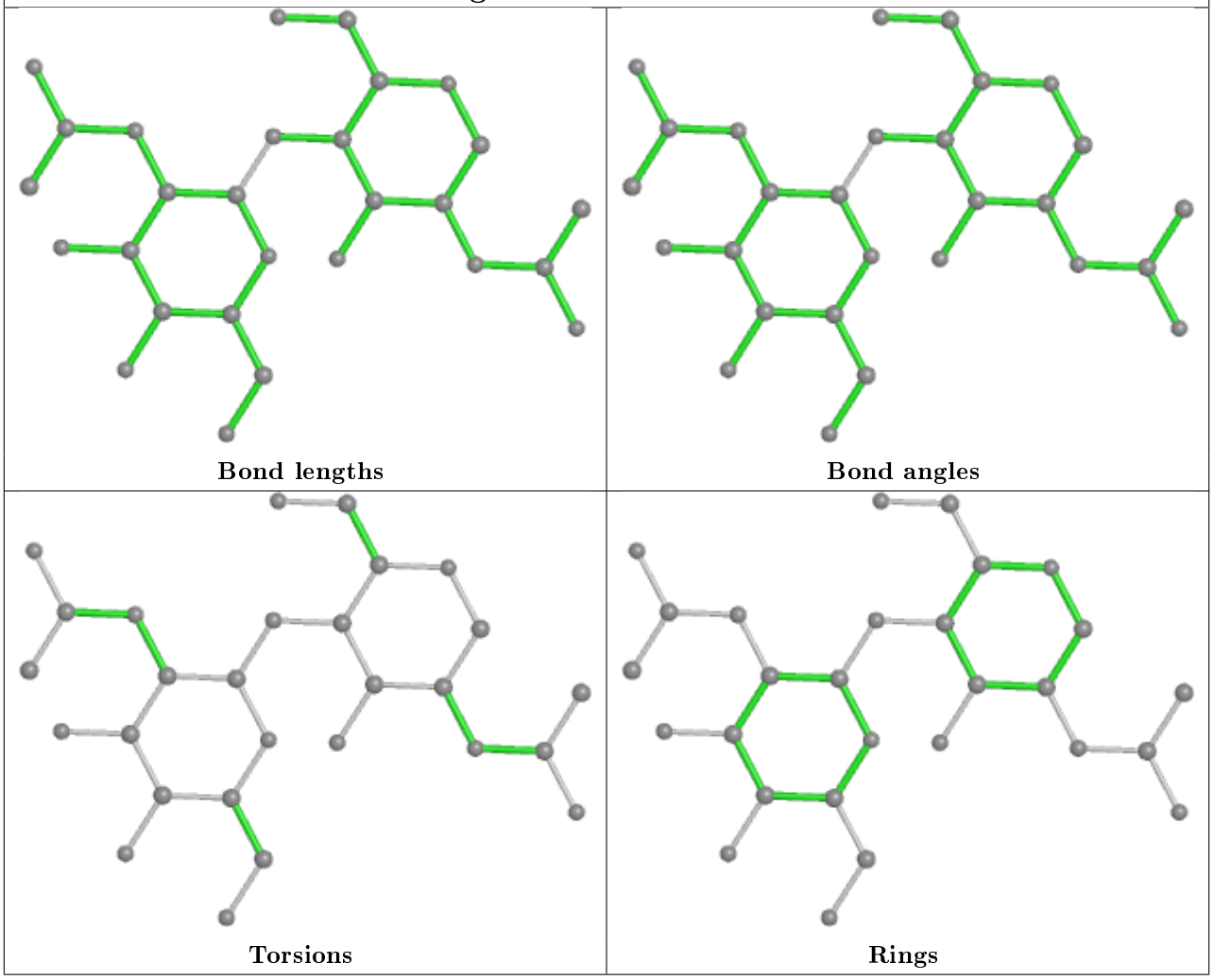


Torsions



Rings

Oligosaccharide Chain E



5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 9 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	EPE	A	805	-	15,15,15	2.31	2 (13%)	18,20,20	1.10	3 (16%)
4	EPE	B	805	-	15,15,15	2.33	2 (13%)	18,20,20	1.11	3 (16%)
4	EPE	B	806	-	15,15,15	2.32	2 (13%)	18,20,20	1.10	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EPE	A	804	-	15,15,15	2.31	2 (13%)	18,20,20	1.10	3 (16%)
3	NAG	A	803	1	14,14,15	1.34	2 (14%)	17,19,21	1.37	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EPE	A	805	-	-	0/9/19/19	0/1/1/1
4	EPE	B	805	-	-	1/9/19/19	0/1/1/1
4	EPE	B	806	-	-	0/9/19/19	0/1/1/1
4	EPE	A	804	-	-	4/9/19/19	0/1/1/1
3	NAG	A	803	1	-	0/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	805	EPE	C10-S	-7.69	1.66	1.77
4	B	806	EPE	C10-S	-7.67	1.66	1.77
4	A	805	EPE	C10-S	-7.61	1.66	1.77
4	A	804	EPE	C10-S	-7.61	1.66	1.77
4	B	805	EPE	O3S-S	4.64	1.64	1.47
4	B	806	EPE	O3S-S	4.62	1.64	1.47
4	A	804	EPE	O3S-S	4.62	1.63	1.47
4	A	805	EPE	O3S-S	4.61	1.63	1.47
3	A	803	NAG	O7-C7	-3.63	1.15	1.23
3	A	803	NAG	O5-C1	-2.47	1.39	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	803	NAG	C1-O5-C5	-2.45	108.88	112.19
4	B	805	EPE	O3S-S-C10	2.30	109.48	105.77
4	B	806	EPE	O3S-S-C10	2.30	109.48	105.77
4	A	805	EPE	O3S-S-C10	2.29	109.47	105.77
4	A	804	EPE	O3S-S-C10	2.29	109.47	105.77
4	B	805	EPE	O1S-S-C10	2.15	109.51	106.92
4	B	806	EPE	O1S-S-C10	2.15	109.50	106.92
4	B	805	EPE	O2S-S-C10	2.14	109.49	106.92
4	A	804	EPE	O2S-S-C10	2.13	109.48	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	805	EPE	O2S-S-C10	2.13	109.48	106.92
4	A	805	EPE	O1S-S-C10	2.13	109.48	106.92
4	B	806	EPE	O2S-S-C10	2.12	109.47	106.92
3	A	803	NAG	C2-N2-C7	2.11	125.91	122.90
4	A	804	EPE	O1S-S-C10	2.11	109.45	106.92
3	A	803	NAG	C1-C2-N2	2.02	113.93	110.49

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	804	EPE	C8-C7-N4-C5
4	A	804	EPE	N4-C7-C8-O8
4	B	805	EPE	N4-C7-C8-O8
4	A	804	EPE	C10-C9-N1-C2
4	A	804	EPE	C10-C9-N1-C6

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	805	EPE	1	0
4	B	806	EPE	1	0
4	A	804	EPE	7	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	701/718 (97%)	-0.42	17 (2%)	59	59	7, 14, 33, 54	0
1	B	701/718 (97%)	-0.52	11 (1%)	72	75	7, 13, 29, 63	0
All	All	1402/1436 (97%)	-0.47	28 (1%)	65	67	7, 13, 31, 63	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	610	MET	6.4
1	B	610	MET	6.0
1	B	609	LEU	5.9
1	B	608	SER	5.3
1	A	429	GLY	4.8
1	A	609	LEU	4.6
1	B	443	ALA	4.1
1	A	485	ASN	3.9
1	B	607	GLY	3.8
1	A	606	ARG	3.5
1	A	611	ALA	3.4
1	A	487	LYS	3.3
1	A	484	LYS	2.9
1	B	606	ARG	2.9
1	A	428	GLY	2.9
1	A	450	THR	2.8
1	B	611	ALA	2.6
1	B	442	THR	2.6
1	A	449	LEU	2.5
1	A	366	LYS	2.5
1	A	486	GLY	2.5
1	B	20	GLU	2.3
1	A	608	SER	2.3
1	A	452	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	603	GLU	2.2
1	A	482	PHE	2.2
1	A	481	GLY	2.2
1	B	486	GLY	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)

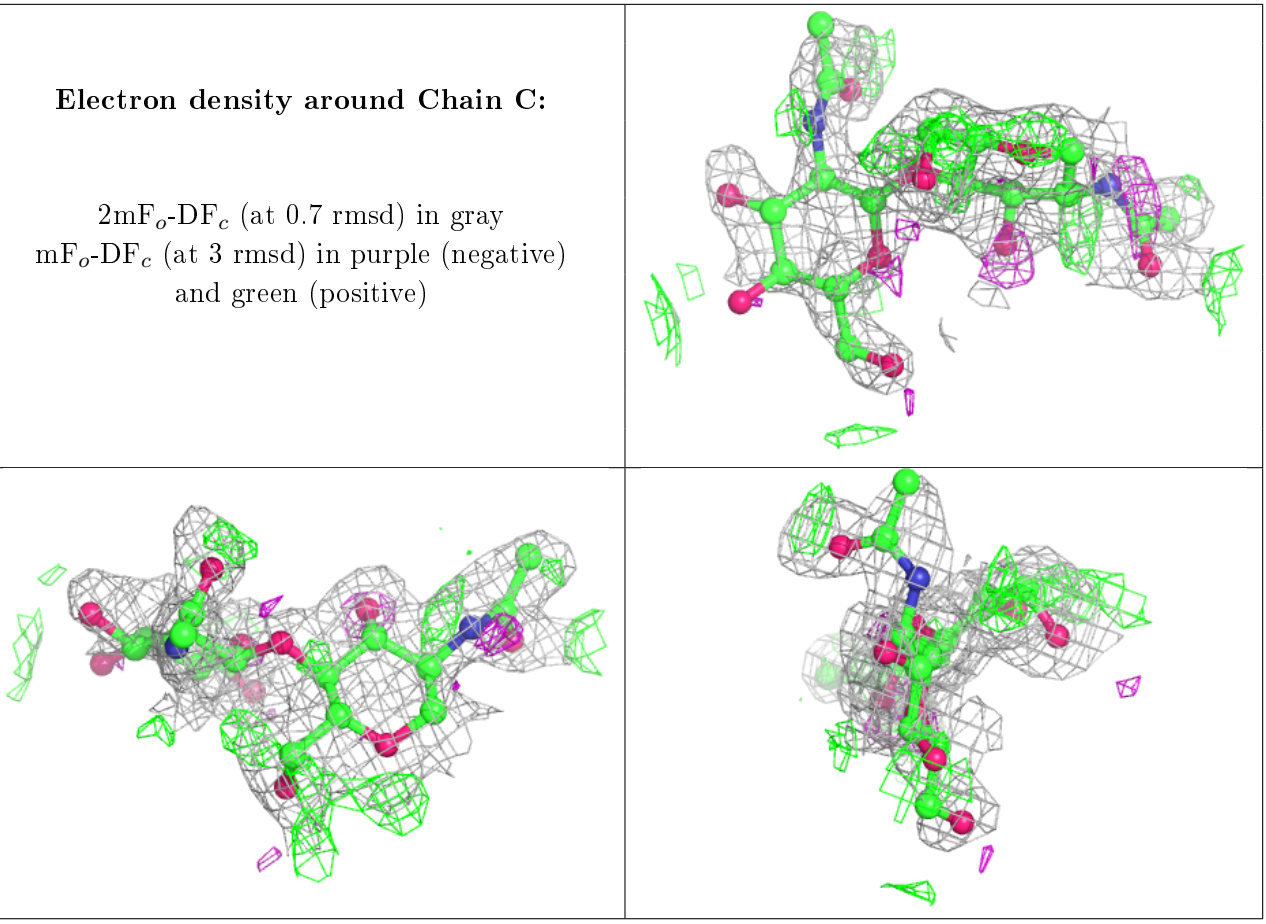
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	NAG	E	2	14/15	0.68	0.33	44,59,66,68	0
2	NAG	C	2	14/15	0.71	0.29	35,50,55,59	0
2	NAG	D	1	14/15	0.80	0.14	18,22,27,34	0
2	NAG	C	1	14/15	0.83	0.14	19,24,31,33	0
2	NAG	D	2	14/15	0.83	0.26	32,38,50,50	0
2	NAG	E	1	14/15	0.93	0.14	21,27,38,47	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.

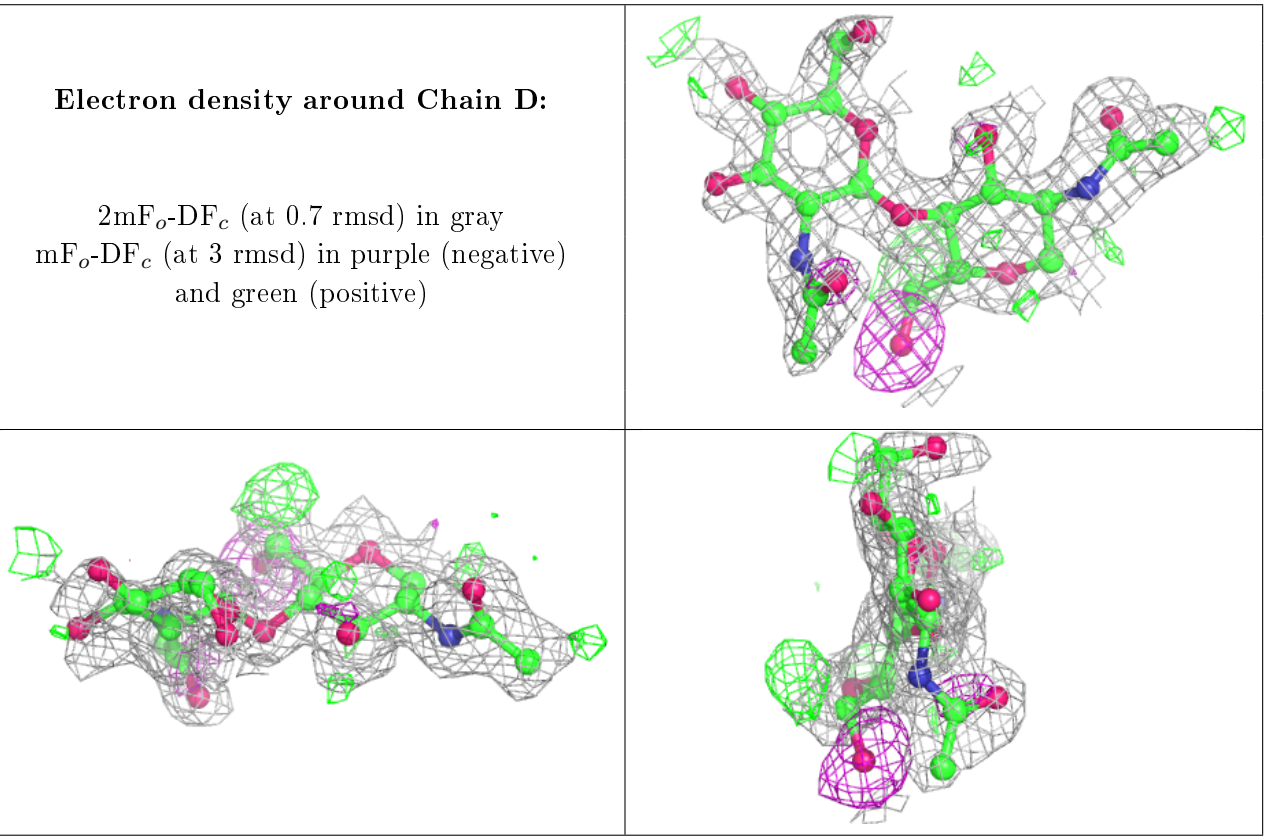
Electron density around Chain C:

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



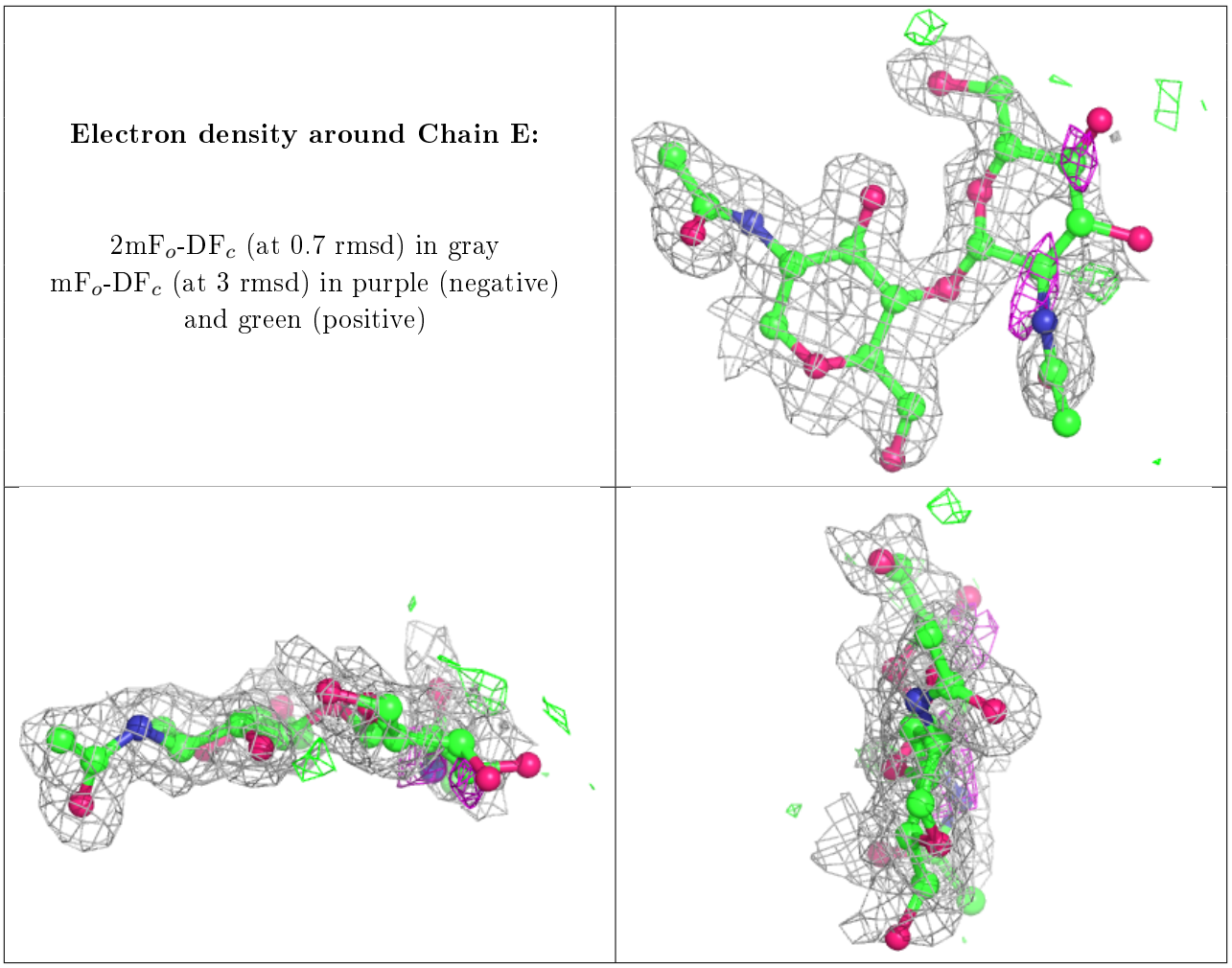
Electron density around Chain D:

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



Electron density around Chain E:

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



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
4	EPE	A	804	15/15	0.65	0.25	22,33,86,89	0
5	ARG	A	806	12/12	0.81	0.19	21,31,37,38	0
4	EPE	A	805	15/15	0.90	0.19	23,28,42,44	0
4	EPE	B	805	15/15	0.92	0.15	18,22,33,39	0
3	NAG	A	803	14/15	0.94	0.13	25,32,40,41	0
4	EPE	B	806	15/15	0.95	0.11	18,22,29,29	0
6	CL	A	810	1/1	0.96	0.22	47,47,47,47	0
6	CL	A	808	1/1	0.99	0.05	27,27,27,27	0
6	CL	A	807	1/1	0.99	0.05	8,8,8,8	0
6	CL	B	808	1/1	0.99	0.14	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CL	B	810	1/1	0.99	0.04	29,29,29,29	0
6	CL	B	811	1/1	0.99	0.05	31,31,31,31	0
6	CL	B	807	1/1	0.99	0.06	8,8,8,8	0
6	CL	A	809	1/1	1.00	0.03	21,21,21,21	0
6	CL	B	809	1/1	1.00	0.05	13,13,13,13	0

6.5 Other polymers

There are no such residues in this entry.