Full wwPDB X-ray Structure Validation Report ⓘ

Dec 9, 2023 – 12:51 pm GMT

PDB ID	:	2UVF
Title	:	Structure of Yersinia enterocolitica Family 28 Exopolygalacturonase in Complex with Digalaturonic Acid
Authors	:	Abbott, D.W.; Boraston, A.B.
Deposited on	:	2007-03-09
Resolution	:	2.10 Å(reported)

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

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

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

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

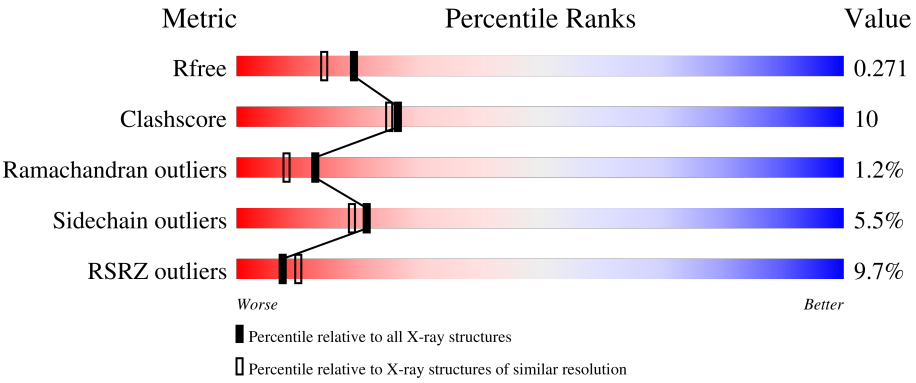
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	608	13% 68% 22% • 6%
1	B	608	5% 75% 16% • 7%
2	C	2	50% 50%

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
3	SO4	A	1612	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9493 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.

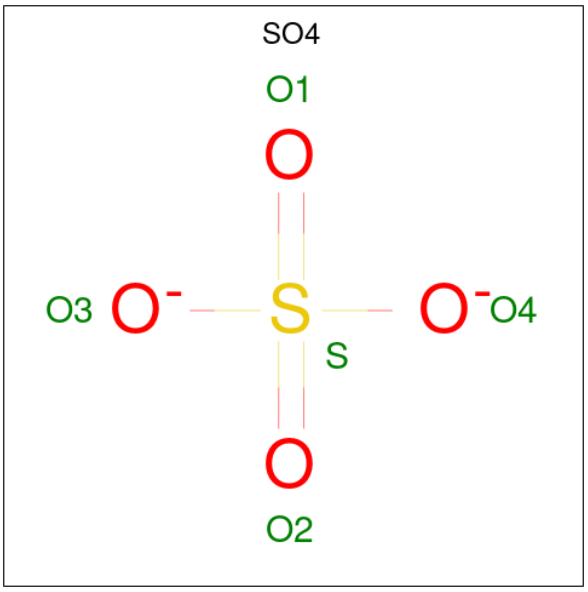
- Molecule 1 is a protein called EXOPOLYGALACTURONASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	571	Total	C	N	O	S	0	4	0
			4459	2795	781	868	15			
1	B	567	Total	C	N	O	S	0	0	0
			4392	2760	766	851	15			

- Molecule 2 is an oligosaccharide called alpha-D-galactopyranuronic acid-(1-4)-alpha-D-galac topyranuronic acid.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			25	12	13			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

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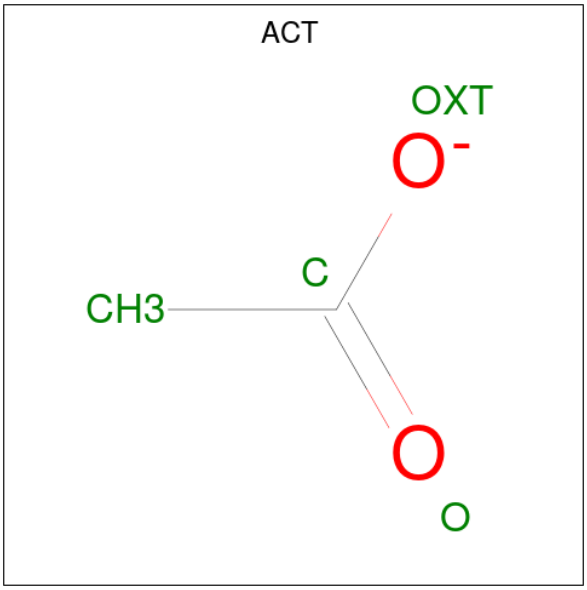
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

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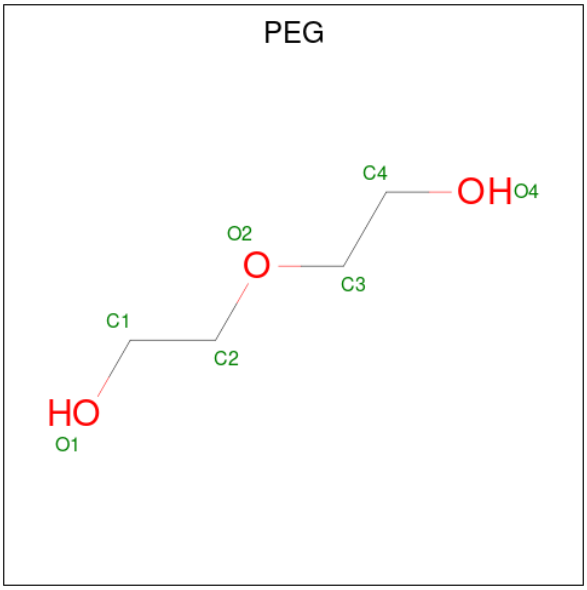
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0

- Molecule 7 is water.

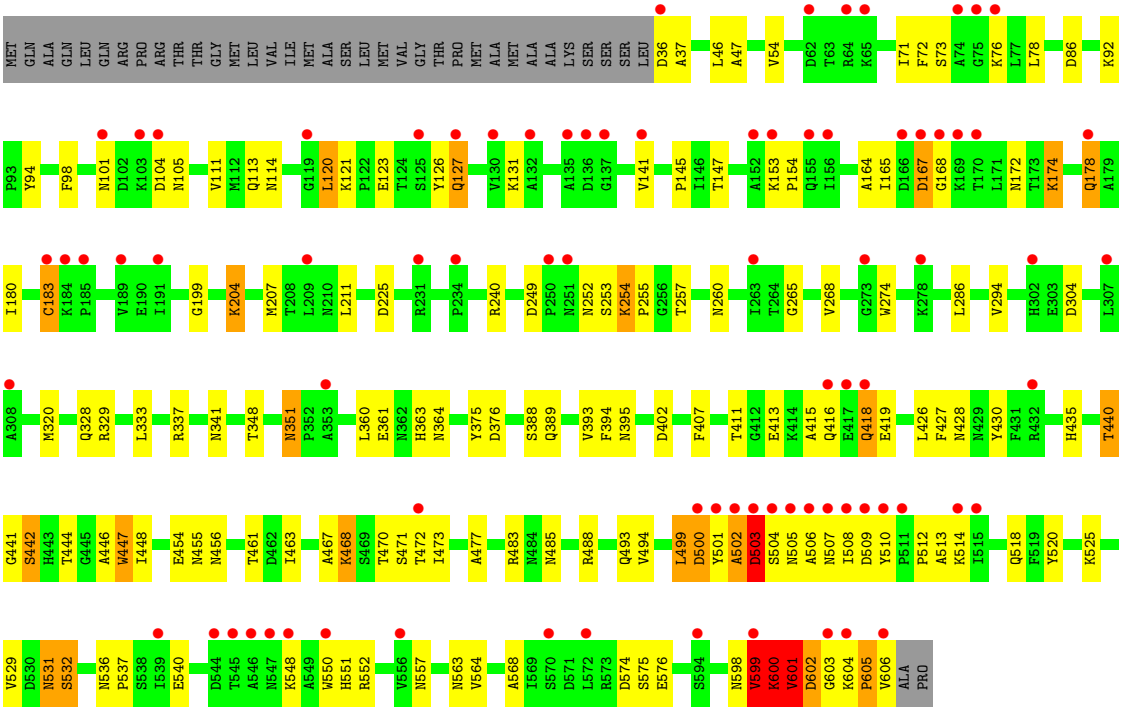
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	184	Total O 184 184	0	0
7	B	303	Total O 303 303	0	0

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.

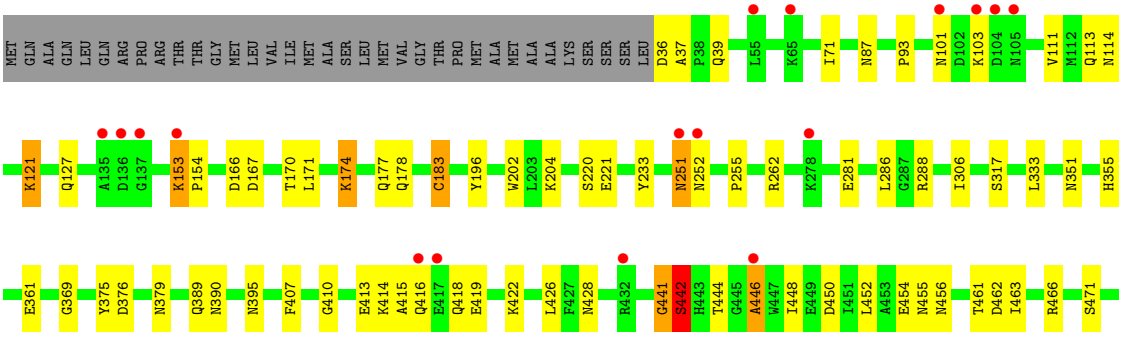
• Molecule 1: EXOPOLYGALACTURONASE

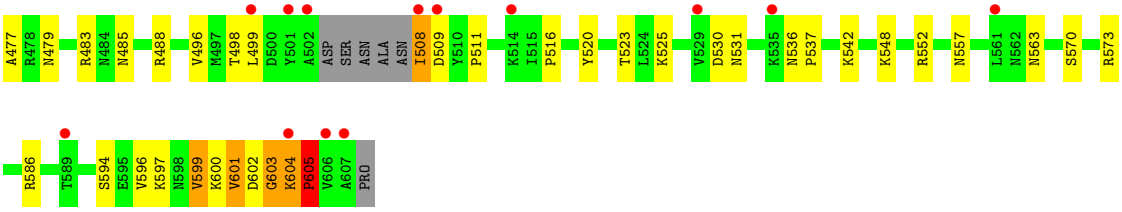
Chain A:



• Molecule 1: EXOPOLYGALACTURONASE

Chain B:





• Molecule 2: alpha-D-galactopyranuronic acid-(1-4)-alpha-D-galactopyranuronic acid

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	91.02Å 79.66Å 98.49Å 90.00° 103.90° 90.00°	Depositor
Resolution (Å)	19.72 – 2.10 19.72 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.72-2.10) 99.0 (19.72-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.232 , 0.284 0.225 , 0.271	Depositor DCC
R_{free} test set	3976 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	33.3	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 61.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9493	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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: PEG, ACT, NI, ADA, SO4

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	0.59	0/4552	0.71	2/6179 (0.0%)
1	B	0.71	1/4482 (0.0%)	0.79	4/6083 (0.1%)
All	All	0.65	1/9034 (0.0%)	0.75	6/12262 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	1	5
All	All	1	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	183	CYS	CB-SG	-6.50	1.71	1.82

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	262	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	B	262	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	A	601	VAL	N-CA-C	7.93	132.42	111.00
1	B	442	SER	N-CA-CB	6.48	120.22	110.50
1	B	446	ALA	N-CA-C	-5.82	95.29	111.00
1	A	599	VAL	C-N-CA	5.11	134.47	121.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	442	SER	CA

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	440	THR	Peptide
1	A	502	ALA	Peptide
1	A	600	LYS	Peptide
1	A	602	ASP	Peptide
1	A	604	LYS	Peptide
1	B	251	ASN	Peptide
1	B	441	GLY	Peptide
1	B	602	ASP	Peptide
1	B	603	GLY	Peptide
1	B	604	LYS	Peptide

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	4459	0	4340	109	0
1	B	4392	0	4289	73	0
2	C	25	0	15	1	0
3	A	30	0	0	0	0
3	B	60	0	0	0	0
4	A	4	0	0	0	0
4	B	6	0	0	0	0
5	B	16	0	12	1	0
6	B	14	0	20	2	0
7	A	184	0	0	3	0
7	B	303	0	0	9	0
All	All	9493	0	8676	182	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 10.

All (182) 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:502:ALA:HB3	1:A:503:ASP:HA	1.30	1.10
1:B:422:LYS:HD3	7:B:2226:HOH:O	1.63	0.98
1:B:601:VAL:O	1:B:603:GLY:HA2	1.67	0.93
1:A:502:ALA:CB	1:A:503:ASP:HA	1.98	0.92
1:B:113:GLN:H	1:B:428:ASN:HD21	1.10	0.89
1:B:177:GLN:HE22	1:B:202:TRP:H	1.26	0.82
1:A:113:GLN:H	1:A:428:ASN:HD21	1.29	0.80
1:A:252:ASN:HB2	7:A:2075:HOH:O	1.85	0.76
1:B:508:ILE:HD12	5:B:1626:ACT:H2	1.69	0.75
1:B:174:LYS:O	1:B:178:GLN:HG3	1.85	0.75
1:B:573:ARG:HH22	6:B:1631:PEG:H12	1.51	0.74
1:A:502:ALA:HB3	1:A:503:ASP:CA	2.15	0.74
1:B:488:ARG:HD2	7:B:2045:HOH:O	1.87	0.74
1:A:167:ASP:CB	1:A:168:GLY:HA2	2.16	0.74
1:A:502:ALA:CB	1:A:503:ASP:CA	2.64	0.73
1:B:452:LEU:HB2	6:B:1630:PEG:H22	1.70	0.73
1:B:415:ALA:HA	1:B:418:GLN:HE21	1.53	0.72
1:A:37:ALA:HB2	1:A:141:VAL:HG23	1.73	0.69
1:A:180:ILE:O	1:A:183:CYS:HB2	1.93	0.69
1:A:531[A]:ASN:HD22	1:A:563[A]:ASN:HB3	1.57	0.68
1:B:355:HIS:HD2	1:B:379:ASN:O	1.76	0.68
1:B:113:GLN:H	1:B:428:ASN:ND2	1.90	0.68
1:A:605:PRO:O	1:A:606:VAL:HG22	1.94	0.67
1:A:504:SER:HA	1:A:505:ASN:C	2.15	0.67
1:A:444:THR:HG22	1:A:448:ILE:HD12	1.79	0.65
1:B:531:ASN:HD22	1:B:563:ASN:HB3	1.62	0.65
1:A:240:ARG:HH21	1:A:328:GLN:HE22	1.45	0.65
1:A:141:VAL:HG22	7:A:2039:HOH:O	1.97	0.64
1:A:240:ARG:HE	1:A:328:GLN:NE2	1.96	0.64
1:B:456:ASN:H	1:B:485:ASN:HD22	1.44	0.63
1:A:167:ASP:CG	1:A:168:GLY:HA2	2.19	0.63
1:A:602:ASP:N	1:A:603:GLY:HA2	2.14	0.63
1:A:599:VAL:HA	1:A:600:LYS:HB2	1.81	0.63
1:A:167:ASP:HB2	1:A:168:GLY:CA	2.30	0.62
1:B:113:GLN:N	1:B:428:ASN:HD21	1.90	0.62
1:B:600:LYS:HG2	1:B:605:PRO:HD3	1.81	0.61
1:B:450:ASP:OD1	7:B:2231:HOH:O	2.16	0.61
1:B:442:SER:HB3	7:B:2229:HOH:O	1.99	0.61
1:A:446:ALA:O	1:A:447:TRP:HB2	1.99	0.61
1:A:456:ASN:H	1:A:485:ASN:HD22	1.48	0.60
1:B:498:THR:HG22	1:B:542:LYS:HD3	1.83	0.59
1:A:294:VAL:HG11	1:A:304:ASP:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:SER:O	1:A:599:VAL:HB	2.03	0.59
1:A:576:GLU:HA	1:A:600:LYS:O	2.03	0.59
1:A:167:ASP:HB2	1:A:168:GLY:HA2	1.83	0.59
1:B:114:ASN:ND2	1:B:395:ASN:HD21	2.01	0.58
1:B:601:VAL:C	1:B:603:GLY:HA2	2.22	0.58
1:B:508:ILE:HA	7:B:2253:HOH:O	2.04	0.57
1:B:255:PRO:HG3	1:B:361:GLU:O	2.05	0.57
1:A:599:VAL:O	1:A:606:VAL:N	2.38	0.57
1:B:600:LYS:HB3	1:B:603:GLY:HA3	1.86	0.56
1:A:341:ASN:ND2	1:A:364:ASN:HD22	2.04	0.55
1:B:111:VAL:H	1:B:455:ASN:ND2	2.03	0.55
1:A:407:PHE:O	1:A:441:GLY:HA3	2.07	0.55
1:A:204:LYS:O	1:A:207:MET:HG2	2.06	0.55
1:A:605:PRO:O	1:A:606:VAL:CG2	2.54	0.55
1:B:498:THR:CG2	1:B:542:LYS:HD3	2.37	0.55
1:B:508:ILE:N	1:B:509:ASP:HB2	2.21	0.55
1:A:167:ASP:CB	1:A:168:GLY:CA	2.84	0.54
1:A:114:ASN:ND2	1:A:395:ASN:HD21	2.04	0.54
1:B:407:PHE:O	1:B:441:GLY:HA3	2.07	0.54
1:A:503:ASP:H	1:A:505:ASN:HB2	1.72	0.54
1:A:72:PHE:HE2	1:A:131:LYS:HG3	1.73	0.53
1:A:111:VAL:H	1:A:455:ASN:ND2	2.07	0.53
1:A:294:VAL:CG1	1:A:304:ASP:HB3	2.38	0.53
1:A:413:GLU:OE1	1:A:513:ALA:HA	2.08	0.53
1:B:114:ASN:HD21	1:B:395:ASN:HD21	1.56	0.53
1:A:499:LEU:HB2	1:A:551:HIS:CE1	2.43	0.53
1:A:531[A]:ASN:ND2	1:A:563[A]:ASN:HB3	2.25	0.52
1:A:199:GLY:HA3	1:A:225:ASP:HB3	1.92	0.52
1:B:450:ASP:OD1	1:B:479:ASN:ND2	2.43	0.51
1:A:114:ASN:HD21	1:A:395:ASN:HD21	1.59	0.51
1:A:471:SER:CB	1:A:501:TYR:HA	2.41	0.51
1:A:548:LYS:HA	1:A:550:TRP:CZ3	2.45	0.50
1:B:444:THR:O	1:B:446:ALA:O	2.28	0.50
1:A:113:GLN:N	1:A:428:ASN:HD21	2.05	0.50
1:A:363:HIS:NE2	1:A:419:GLU:OE1	2.33	0.50
1:A:442:SER:HA	1:A:468:LYS:O	2.11	0.50
1:A:73:SER:HB2	1:A:78:LEU:HD11	1.93	0.50
1:B:557:ASN:ND2	7:B:2268:HOH:O	2.45	0.50
1:B:454:GLU:HA	1:B:483:ARG:O	2.12	0.49
1:A:463:ILE:HA	1:A:493:GLN:O	2.12	0.49
1:B:570:SER:HB2	1:B:594:SER:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:MET:CE	1:A:329:ARG:HD3	2.42	0.49
1:B:536:ASN:HB3	1:B:537:PRO:HD2	1.94	0.49
1:A:413:GLU:HB2	1:A:512:PRO:O	2.13	0.49
1:A:416:GLN:C	1:A:418:GLN:H	2.16	0.49
1:A:501:TYR:CE1	1:A:503:ASP:OD2	2.65	0.49
1:B:171:LEU:HD11	1:B:220:SER:HB2	1.95	0.48
1:B:101:ASN:HB2	7:B:2036:HOH:O	2.11	0.48
1:B:288:ARG:NH1	7:B:2160:HOH:O	2.40	0.48
1:B:520:TYR:HA	1:B:552:ARG:O	2.14	0.47
1:A:164:ALA:HA	1:A:172:ASN:OD1	2.14	0.47
1:B:167:ASP:OD2	1:B:170:THR:OG1	2.32	0.47
1:A:240:ARG:HE	1:A:328:GLN:HE21	1.61	0.47
1:B:233:TYR:CZ	1:B:410:GLY:HA2	2.50	0.47
1:A:394:PHE:HA	1:A:427:PHE:O	2.15	0.47
1:A:442:SER:HB2	1:A:468:LYS:HD3	1.95	0.47
1:A:174:LYS:O	1:A:178:GLN:HB2	2.14	0.47
1:A:537:PRO:HG2	1:A:568:ALA:HB3	1.97	0.47
1:B:573:ARG:HA	1:B:597:LYS:O	2.15	0.47
1:B:183:CYS:HB2	1:B:204:LYS:HE2	1.96	0.47
1:B:483:ARG:HA	1:B:525:LYS:O	2.14	0.47
1:A:274:TRP:HB2	1:A:351:ASN:HD21	1.80	0.46
1:B:413:GLU:OE2	1:B:416:GLN:NE2	2.48	0.46
1:B:462:ASP:C	1:B:463:ILE:HG13	2.35	0.46
1:B:471:SER:O	1:B:516:PRO:HA	2.14	0.46
1:B:93:PRO:HB2	1:B:286:LEU:HD21	1.97	0.46
1:A:72:PHE:CE2	1:A:131:LYS:HG3	2.51	0.46
1:A:341:ASN:HD22	1:A:364:ASN:HB2	1.81	0.46
1:A:508:ILE:HG22	1:A:510:TYR:O	2.16	0.45
1:B:563:ASN:ND2	1:B:586:ARG:HH11	2.13	0.45
1:A:472:THR:HG23	1:A:502:ALA:HB3	1.99	0.45
1:B:221:GLU:HG3	7:B:2174:HOH:O	2.16	0.45
1:B:448:ILE:O	1:B:477:ALA:HA	2.17	0.45
1:A:471:SER:HB3	1:A:501:TYR:HA	1.99	0.45
1:B:37:ALA:O	1:B:39:GLN:NE2	2.44	0.45
1:B:508:ILE:HG22	1:B:509:ASP:OD2	2.16	0.45
1:B:456:ASN:H	1:B:485:ASN:ND2	2.14	0.45
1:A:253:SER:HB2	1:A:361[A]:GLU:OE2	2.16	0.45
1:B:121:LYS:HB3	1:B:121:LYS:HE2	1.61	0.45
1:A:337:ARG:HA	1:A:360:LEU:O	2.17	0.45
1:A:413:GLU:OE1	1:A:514:LYS:N	2.41	0.45
1:B:71:ILE:HD12	1:B:71:ILE:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:PHE:CE1	1:A:488:ARG:HB3	2.53	0.44
1:A:127:GLN:OE1	1:A:145:PRO:HB3	2.18	0.44
1:A:532:SER:HB2	1:A:564:VAL:HG12	1.99	0.44
1:A:536:ASN:HB2	7:A:2165:HOH:O	2.17	0.44
1:B:171:LEU:HD12	1:B:171:LEU:HA	1.83	0.44
1:B:525:LYS:HE2	1:B:557:ASN:HB2	2.00	0.44
1:A:525:LYS:HA	1:A:557:ASN:O	2.17	0.44
1:A:121:LYS:HE2	1:A:121:LYS:HB2	1.81	0.44
1:A:494:VAL:HG22	1:A:529:VAL:HG21	2.00	0.44
1:B:508:ILE:HG23	1:B:509:ASP:HA	1.99	0.44
1:B:523:THR:HG23	1:B:525:LYS:HE3	2.00	0.44
1:A:415:ALA:O	1:A:418:GLN:HG3	2.17	0.44
1:B:174:LYS:HD2	1:B:174:LYS:HA	1.83	0.44
1:A:167:ASP:OD1	1:A:167:ASP:N	2.51	0.43
1:B:414:LYS:HE3	1:B:511:PRO:HG2	2.00	0.43
1:A:86:ASP:OD1	1:A:92:LYS:NZ	2.52	0.43
1:A:402:ASP:OD1	2:C:1:ADA:H1	2.19	0.43
1:B:375:TYR:HA	1:B:376:ASP:HA	1.84	0.43
1:B:389:GLN:HE22	1:B:419:GLU:HB3	1.83	0.43
1:A:47:ALA:HB1	1:A:54:VAL:HB	2.01	0.42
1:A:113:GLN:H	1:A:428:ASN:ND2	2.07	0.42
1:A:471:SER:HB2	1:A:501:TYR:HA	2.02	0.42
1:B:177:GLN:NE2	1:B:202:TRP:H	2.07	0.42
1:B:525:LYS:HA	1:B:557:ASN:O	2.20	0.42
1:A:254:LYS:HA	1:A:255:PRO:HD3	1.94	0.42
1:B:444:THR:HG22	1:B:448:ILE:HD12	2.02	0.42
1:A:240:ARG:HH21	1:A:328:GLN:NE2	2.15	0.42
1:A:499:LEU:HD11	1:A:518:GLN:HA	2.01	0.42
1:A:388:SER:O	1:A:389:GLN:HG2	2.20	0.42
1:A:448:ILE:O	1:A:477:ALA:HA	2.19	0.42
1:A:120:LEU:HG	1:A:126:TYR:CE2	2.55	0.41
1:A:393:VAL:HB	1:A:426:LEU:HD12	2.02	0.41
1:A:274:TRP:H	1:A:351:ASN:HD21	1.67	0.41
1:A:441:GLY:O	1:A:442:SER:HB3	2.20	0.41
1:A:454:GLU:HA	1:A:483:ARG:O	2.19	0.41
1:A:520:TYR:HA	1:A:552:ARG:O	2.20	0.41
1:B:166:ASP:HB3	1:B:196:TYR:CZ	2.55	0.41
1:A:153:LYS:HD2	1:A:154:PRO:HD2	2.02	0.41
1:A:211:LEU:O	1:A:265:GLY:HA3	2.20	0.41
1:A:341:ASN:HD21	1:A:364:ASN:HD22	1.66	0.41
1:A:500:ASP:N	1:A:500:ASP:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LEU:HD11	1:A:260:ASN:HA	2.02	0.41
1:B:153:LYS:CE	1:B:154:PRO:HD2	2.51	0.41
1:A:470:THR:HB	1:A:500:ASP:O	2.20	0.41
1:A:268:VAL:HG22	1:A:348:THR:HB	2.03	0.41
1:A:411:THR:HA	1:A:473:ILE:HG23	2.03	0.41
1:B:596:VAL:HB	1:B:599:VAL:HG13	2.03	0.41
1:A:94:TYR:HB3	1:A:430:TYR:CE1	2.56	0.40
1:A:540:GLU:HA	1:A:568:ALA:O	2.22	0.40
1:A:440:THR:O	1:A:467:ALA:HA	2.21	0.40
1:A:506:ALA:O	1:A:508:ILE:N	2.54	0.40
1:A:240:ARG:NH2	1:A:328:GLN:HE22	2.17	0.40
1:A:375:TYR:HA	1:A:376:ASP:HA	1.77	0.40
1:B:369:GLY:HA2	1:B:395:ASN:O	2.21	0.40
1:B:530:ASP:O	1:B:531:ASN:HB2	2.21	0.40
1:A:71:ILE:HG22	1:A:78:LEU:HD12	2.04	0.40
1:A:249:ASP:HB2	1:A:257:THR:HG21	2.03	0.40
1:B:466:ARG:HD3	1:B:496:VAL:HB	2.04	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	573/608 (94%)	522 (91%)	41 (7%)	10 (2%)	9 4
1	B	563/608 (93%)	527 (94%)	31 (6%)	5 (1%)	17 12
All	All	1136/1216 (93%)	1049 (92%)	72 (6%)	15 (1%)	13 7

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	600	LYS

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Mol	Chain	Res	Type
1	A	601	VAL
1	B	605	PRO
1	A	503	ASP
1	A	507	ASN
1	A	442	SER
1	A	605	PRO
1	B	252	ASN
1	B	442	SER
1	A	447	TRP
1	B	604	LYS
1	A	598	ASN
1	A	531[A]	ASN
1	A	531[B]	ASN
1	B	306	ILE

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	481/507 (95%)	450 (94%)	31 (6%)	17	14
1	B	472/507 (93%)	451 (96%)	21 (4%)	28	28
All	All	953/1014 (94%)	901 (94%)	52 (6%)	21	19

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ASP
1	A	76	LYS
1	A	101	ASN
1	A	104	ASP
1	A	105	ASN
1	A	120	LEU
1	A	123	GLU
1	A	127	GLN
1	A	147	THR

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Mol	Chain	Res	Type
1	A	165	ILE
1	A	167	ASP
1	A	174	LYS
1	A	178	GLN
1	A	183	CYS
1	A	204	LYS
1	A	254	LYS
1	A	286	LEU
1	A	333	LEU
1	A	351	ASN
1	A	418	GLN
1	A	435	HIS
1	A	461	THR
1	A	468	LYS
1	A	499	LEU
1	A	500	ASP
1	A	503	ASP
1	A	509	ASP
1	A	532	SER
1	A	574	ASP
1	A	599	VAL
1	A	601	VAL
1	B	36	ASP
1	B	87	ASN
1	B	103	LYS
1	B	121	LYS
1	B	127	GLN
1	B	153	LYS
1	B	174	LYS
1	B	251	ASN
1	B	281	GLU
1	B	317	SER
1	B	333	LEU
1	B	351	ASN
1	B	390	ASN
1	B	426	LEU
1	B	461	THR
1	B	499	LEU
1	B	508	ILE
1	B	548	LYS
1	B	599	VAL
1	B	601	VAL

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Mol	Chain	Res	Type
1	B	605	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	114	ASN
1	A	177	GLN
1	A	328	GLN
1	A	341	ASN
1	A	351	ASN
1	A	390	ASN
1	A	418	GLN
1	A	428	ASN
1	A	455	ASN
1	A	485	ASN
1	A	592	HIS
1	B	105	ASN
1	B	114	ASN
1	B	127	GLN
1	B	177	GLN
1	B	252	ASN
1	B	324	ASN
1	B	351	ASN
1	B	355	HIS
1	B	387	ASN
1	B	416	GLN
1	B	418	GLN
1	B	428	ASN
1	B	455	ASN
1	B	485	ASN
1	B	531	ASN
1	B	557	ASN
1	B	563	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)

2 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	ADA	C	1	2	13,13,13	1.55	2 (15%)	18,19,19	1.70	3 (16%)
2	ADA	C	2	2	12,12,13	1.29	0	14,17,19	0.73	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	ADA	C	1	2	-	0/4/24/24	0/1/1/1
2	ADA	C	2	2	-	0/4/21/24	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	ADA	O5-C5	3.79	1.49	1.43
2	C	1	ADA	O1-C1	2.07	1.46	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	ADA	C1-O5-C5	3.00	116.64	112.22
2	C	1	ADA	O5-C1-C2	-2.87	105.16	110.28
2	C	1	ADA	C4-C3-C2	-2.87	105.81	110.82

There are no chirality outliers.

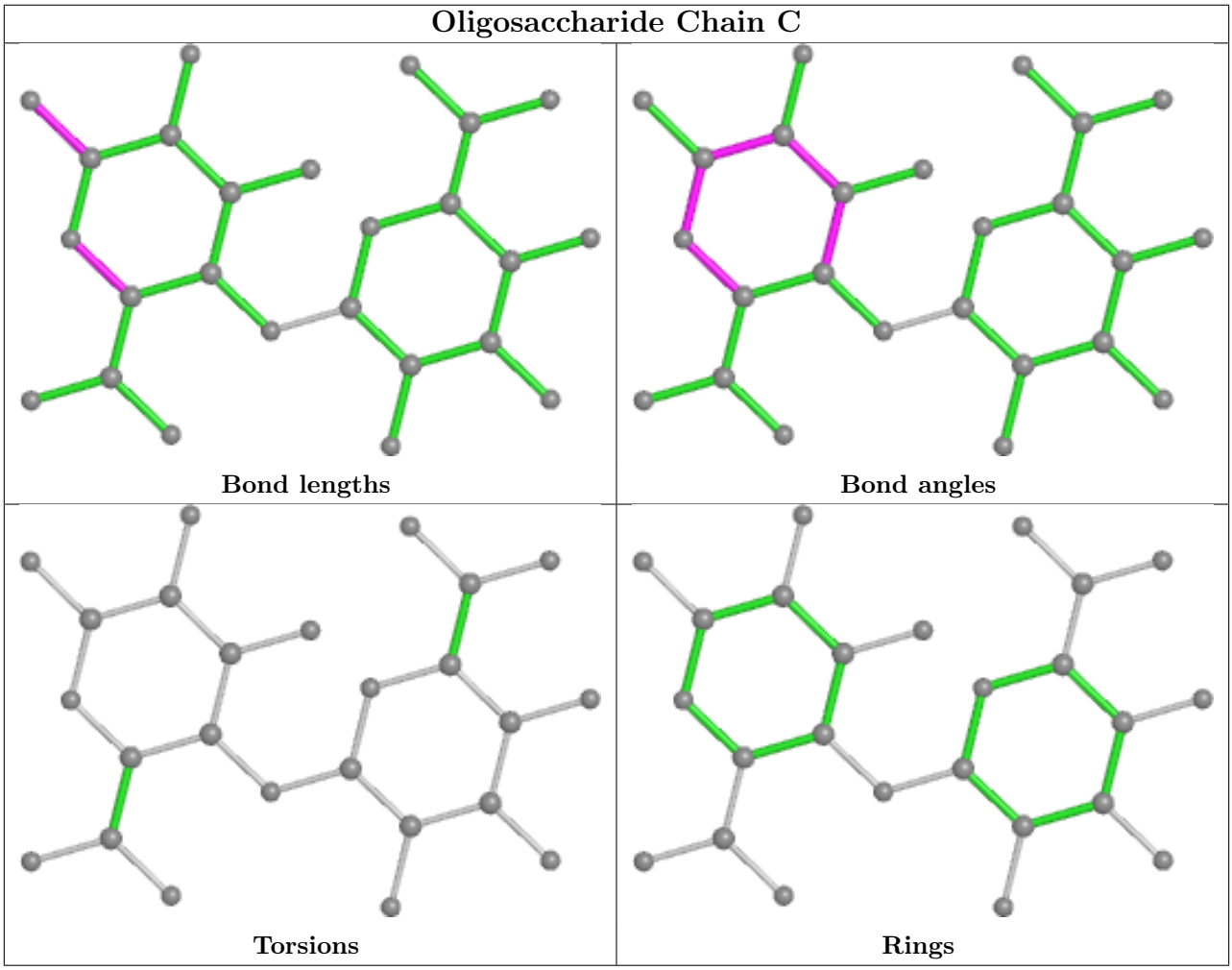
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	ADA	1	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.



5.6 Ligand geometry

Of 34 ligands modelled in this entry, 10 are monoatomic - leaving 24 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	$\#\|Z\| > 2$
3	SO4	B	1611	-	4,4,4	0.15	0	6,6,6	0.08	0
3	SO4	B	1615	-	4,4,4	0.17	0	6,6,6	0.17	0
5	ACT	B	1628	-	3,3,3	0.80	0	3,3,3	0.73	0
3	SO4	B	1618	-	4,4,4	0.16	0	6,6,6	0.27	0
3	SO4	A	1609	-	4,4,4	0.10	0	6,6,6	0.17	0
3	SO4	A	1611	-	4,4,4	0.16	0	6,6,6	0.27	0
3	SO4	B	1614	-	4,4,4	0.15	0	6,6,6	0.33	0
3	SO4	B	1619	-	4,4,4	0.46	0	6,6,6	0.65	0
3	SO4	A	1607	-	4,4,4	0.19	0	6,6,6	0.29	0
3	SO4	B	1617	-	4,4,4	0.14	0	6,6,6	0.23	0
5	ACT	B	1627	-	3,3,3	0.71	0	3,3,3	0.89	0
5	ACT	B	1629	-	3,3,3	0.68	0	3,3,3	1.05	0
6	PEG	B	1631	-	6,6,6	0.57	0	5,5,5	0.16	0
3	SO4	B	1610	-	4,4,4	0.16	0	6,6,6	0.34	0
3	SO4	B	1609	-	4,4,4	0.11	0	6,6,6	0.12	0
3	SO4	A	1612	-	4,4,4	0.12	0	6,6,6	0.16	0
3	SO4	B	1608	-	4,4,4	0.14	0	6,6,6	0.17	0
3	SO4	A	1610	-	4,4,4	0.18	0	6,6,6	0.35	0
3	SO4	B	1612	-	4,4,4	0.12	0	6,6,6	0.14	0
3	SO4	B	1616	-	4,4,4	0.10	0	6,6,6	0.17	0
3	SO4	A	1608	-	4,4,4	0.18	0	6,6,6	0.15	0
3	SO4	B	1613	-	4,4,4	0.15	0	6,6,6	0.18	0
6	PEG	B	1630	-	6,6,6	0.34	0	5,5,5	0.95	0
5	ACT	B	1626	-	3,3,3	0.81	0	3,3,3	1.00	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
6	PEG	B	1631	-	-	3/4/4/4	-
6	PEG	B	1630	-	-	3/4/4/4	-

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
6	B	1630	PEG	O1-C1-C2-O2
6	B	1631	PEG	O2-C3-C4-O4
6	B	1630	PEG	O2-C3-C4-O4
6	B	1631	PEG	C1-C2-O2-C3
6	B	1631	PEG	C4-C3-O2-C2
6	B	1630	PEG	C1-C2-O2-C3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1631	PEG	1	0
6	B	1630	PEG	1	0
5	B	1626	ACT	1	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	571/608 (93%)	0.90	80 (14%) 2 3	15, 39, 64, 86	2 (0%)
1	B	567/608 (93%)	0.26	30 (5%) 26 32	14, 27, 42, 58	1 (0%)
All	All	1138/1216 (93%)	0.58	110 (9%) 7 10	14, 32, 56, 86	3 (0%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	546	ALA	13.2
1	A	545	THR	9.5
1	A	502	ALA	8.9
1	A	506	ALA	8.5
1	A	508	ILE	8.4
1	B	508	ILE	8.3
1	A	507	ASN	7.8
1	A	504	SER	7.2
1	A	505	ASN	7.0
1	A	501	TYR	6.8
1	B	432	ARG	6.7
1	A	515	ILE	6.7
1	A	432	ARG	6.7
1	A	548	LYS	6.6
1	B	607	ALA	6.0
1	A	544	ASP	5.7
1	A	168	GLY	5.7
1	B	135	ALA	5.5
1	A	503	ASP	5.3
1	B	501	TYR	5.3
1	A	550	TRP	5.1
1	B	502	ALA	5.0
1	A	603	GLY	5.0
1	A	169	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	417	GLU	4.7
1	A	74	ALA	4.7
1	A	104	ASP	4.5
1	B	251	ASN	4.5
1	A	604	LYS	4.4
1	A	231	ARG	4.1
1	A	137	GLY	4.0
1	A	606	VAL	3.9
1	A	101	ASN	3.9
1	A	103	LYS	3.9
1	A	599	VAL	3.8
1	A	76	LYS	3.7
1	A	572	LEU	3.7
1	A	36	ASP	3.7
1	A	416	GLN	3.6
1	A	472	THR	3.6
1	A	135	ALA	3.5
1	A	500	ASP	3.5
1	B	604	LYS	3.4
1	A	278	LYS	3.4
1	A	307	LEU	3.4
1	A	132	ALA	3.3
1	A	514	LYS	3.3
1	B	514	LYS	3.3
1	A	250	PRO	3.3
1	B	101	ASN	3.2
1	B	104	ASP	3.2
1	B	136	ASP	3.2
1	A	209	LEU	3.1
1	A	75	GLY	3.0
1	A	511	PRO	3.0
1	A	189	VAL	2.9
1	B	65	LYS	2.9
1	A	191	ILE	2.9
1	A	539	ILE	2.8
1	B	153	LYS	2.8
1	A	418	GLN	2.8
1	B	446	ALA	2.8
1	B	509	ASP	2.8
1	A	119	GLY	2.8
1	A	547	ASN	2.8
1	A	509	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	251	ASN	2.7
1	B	417	GLU	2.7
1	A	353	ALA	2.7
1	A	156	ILE	2.7
1	A	302	HIS	2.6
1	A	152	ALA	2.6
1	A	130	VAL	2.6
1	A	141	VAL	2.6
1	A	234	PRO	2.6
1	A	184	LYS	2.5
1	A	185	PRO	2.5
1	A	62	ASP	2.5
1	A	125	SER	2.4
1	B	416	GLN	2.4
1	B	535	LYS	2.4
1	A	570	SER	2.4
1	A	136	ASP	2.4
1	A	155	GLN	2.4
1	A	166	ASP	2.4
1	A	308	ALA	2.3
1	A	167	ASP	2.3
1	A	153	LYS	2.3
1	B	103	LYS	2.3
1	A	170	THR	2.3
1	A	263	ILE	2.3
1	B	55	LEU	2.3
1	B	105	ASN	2.3
1	A	556	VAL	2.2
1	A	183	CYS	2.2
1	A	594	SER	2.2
1	A	127	GLN	2.2
1	B	589	THR	2.2
1	A	64	ARG	2.2
1	A	273	GLY	2.2
1	B	606	VAL	2.1
1	B	561	LEU	2.1
1	B	137	GLY	2.1
1	B	499	LEU	2.1
1	B	529	VAL	2.1
1	A	178	GLN	2.0
1	B	252	ASN	2.0
1	A	65	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	278	LYS	2.0
1	A	510	TYR	2.0

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

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

6.3 Carbohydrates (i)

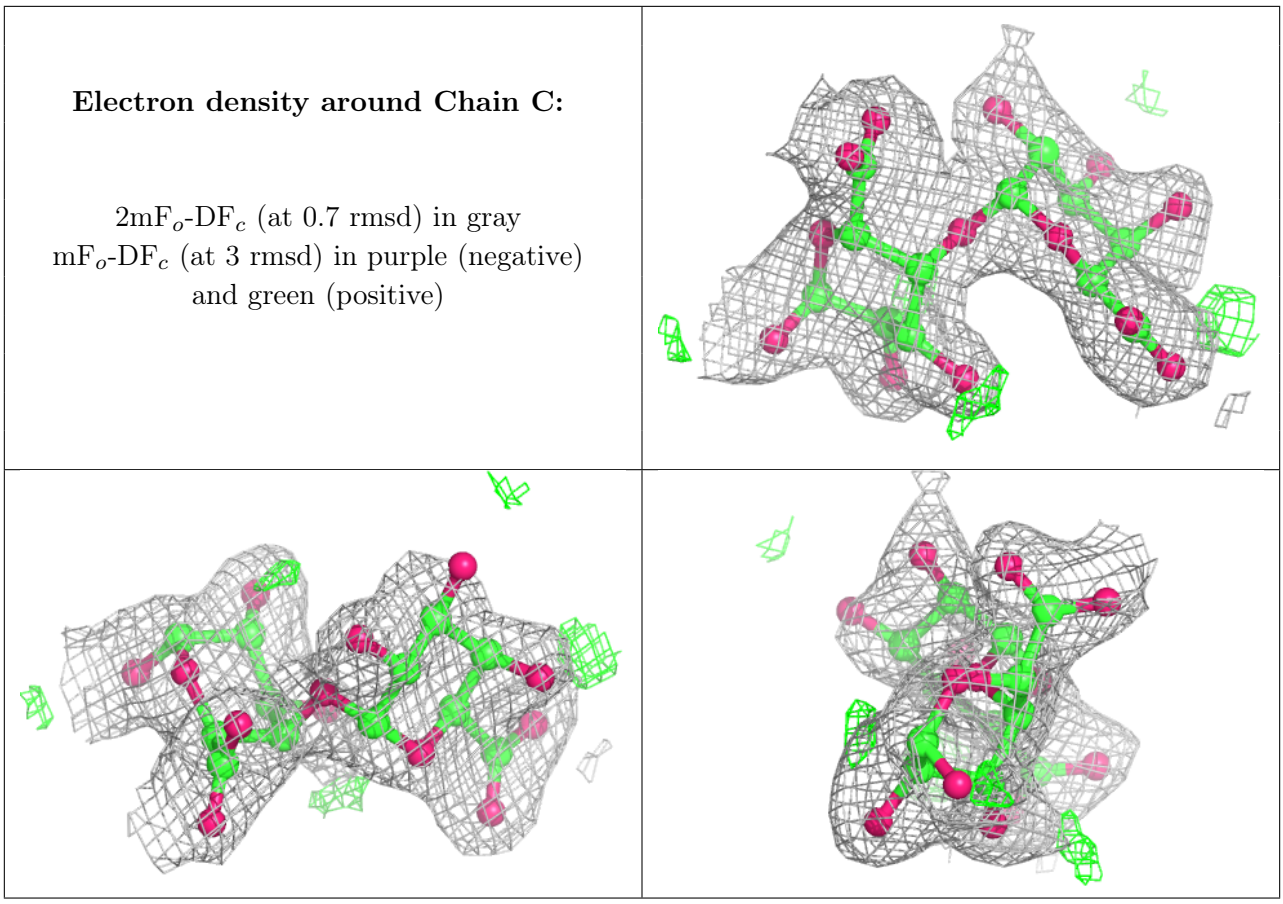
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ADA	C	1	13/13	0.82	0.19	40,47,51,52	0
2	ADA	C	2	12/13	0.87	0.21	43,46,49,50	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)



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	NI	B	1622	1/1	0.49	0.17	93,93,93,93	0
5	ACT	B	1626	4/4	0.60	0.26	44,44,44,44	0
3	SO4	A	1612	5/5	0.75	0.51	104,104,105,105	0
5	ACT	B	1627	4/4	0.82	0.19	48,48,48,49	0
3	SO4	B	1615	5/5	0.86	0.38	97,97,97,98	0
3	SO4	B	1611	5/5	0.86	0.33	112,112,112,112	0
3	SO4	B	1612	5/5	0.86	0.33	97,97,97,98	0
3	SO4	B	1613	5/5	0.86	0.33	87,87,87,87	0
3	SO4	B	1618	5/5	0.87	0.20	73,73,74,74	0
3	SO4	A	1610	5/5	0.87	0.30	82,82,83,83	0
5	ACT	B	1628	4/4	0.87	0.15	42,42,42,43	0
6	PEG	B	1631	7/7	0.87	0.27	46,48,50,50	0
3	SO4	B	1614	5/5	0.88	0.40	77,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NI	A	1616	1/1	0.89	0.06	75,75,75,75	0
6	PEG	B	1630	7/7	0.89	0.27	33,37,43,43	0
4	NI	B	1624	1/1	0.89	0.08	85,85,85,85	0
5	ACT	B	1629	4/4	0.91	0.19	36,36,36,36	0
3	SO4	A	1611	5/5	0.92	0.32	73,73,74,74	0
3	SO4	B	1616	5/5	0.92	0.33	71,71,72,73	0
3	SO4	B	1619	5/5	0.93	0.32	40,41,42,42	0
3	SO4	B	1608	5/5	0.94	0.21	75,75,76,76	0
4	NI	B	1621	1/1	0.94	0.05	50,50,50,50	0
3	SO4	A	1607	5/5	0.95	0.18	52,54,56,56	0
3	SO4	A	1608	5/5	0.95	0.20	61,62,63,63	0
4	NI	B	1625	1/1	0.95	0.03	75,75,75,75	0
3	SO4	A	1609	5/5	0.96	0.12	53,53,55,55	0
3	SO4	B	1617	5/5	0.97	0.20	60,60,60,61	0
3	SO4	B	1609	5/5	0.97	0.15	47,48,49,49	0
4	NI	A	1615	1/1	0.98	0.14	49,49,49,49	0
3	SO4	B	1610	5/5	0.98	0.17	41,42,42,46	0
4	NI	A	1613	1/1	0.98	0.11	32,32,32,32	0
4	NI	B	1623	1/1	0.99	0.13	40,40,40,40	0
4	NI	A	1614	1/1	0.99	0.05	34,34,34,34	0
4	NI	B	1620	1/1	0.99	0.06	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.