



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:57 PM UTC

PDB ID : 2D23 / pdb_00002d23
Title : Crystal structure of EP complex of catalytic-site mutant xylanase from *Streptomyces olivaceoviridis* E-86
Authors : Suzuki, R.; Kuno, A.; Fujimoto, Z.; Ito, S.; Kawahara, S.I.; Kaneko, S.; Hasegawa, T.; Taira, K.
Deposited on : 2005-09-02
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

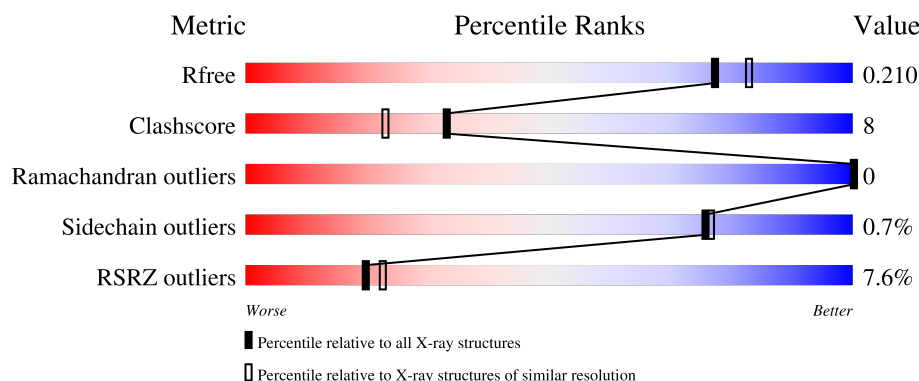
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	436	7% 81% 16% .
1	B	436	8% 83% 15% .
2	C	2	100%
2	D	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
2	XYS	C	1	X	-	-	-
2	XYS	C	2	X	-	-	-
2	XYS	D	1	X	-	-	-
2	XYS	D	2	X	-	-	-
4	GOL	B	963	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7304 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 ENDO-1,4-BETA-D-XYLANASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3233	1988	588	641	16			
1	B	427	Total	C	N	O	S	0	0	0
			3233	1988	588	641	16			

There are 4 discrepancies between the modelled and reference sequences:

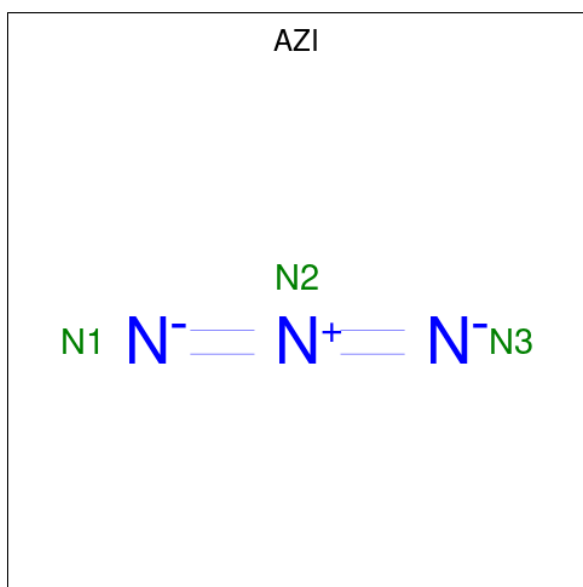
Chain	Residue	Modelled	Actual	Comment	Reference
A	127	SER	ASN	engineered mutation	UNP Q7SI98
A	128	HIS	GLU	engineered mutation	UNP Q7SI98
B	627	SER	ASN	engineered mutation	UNP Q7SI98
B	628	HIS	GLU	engineered mutation	UNP Q7SI98

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



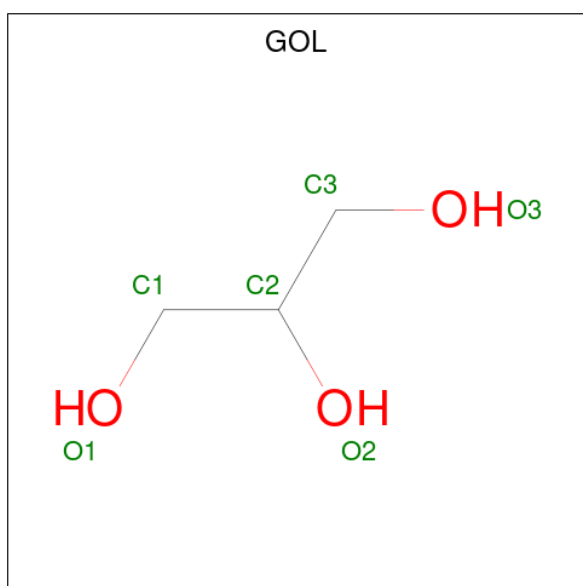
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			18	10	8			
2	D	2	Total	C	O	0	0	0
			18	10	8			

- Molecule 3 is AZIDE ION (CCD ID: AZI) (formula: N₃).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	N	0	0
			3	3		
3	B	1	Total	N	0	0
			3	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

Continued on next page...

Continued from previous page...

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

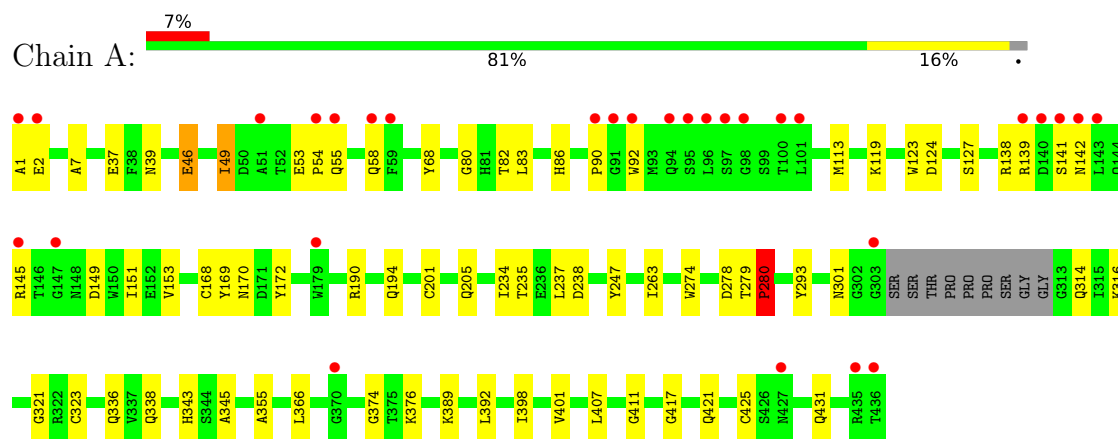
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	314	Total 314	O 314	0	0
5	B	434	Total 434	O 434	0	0

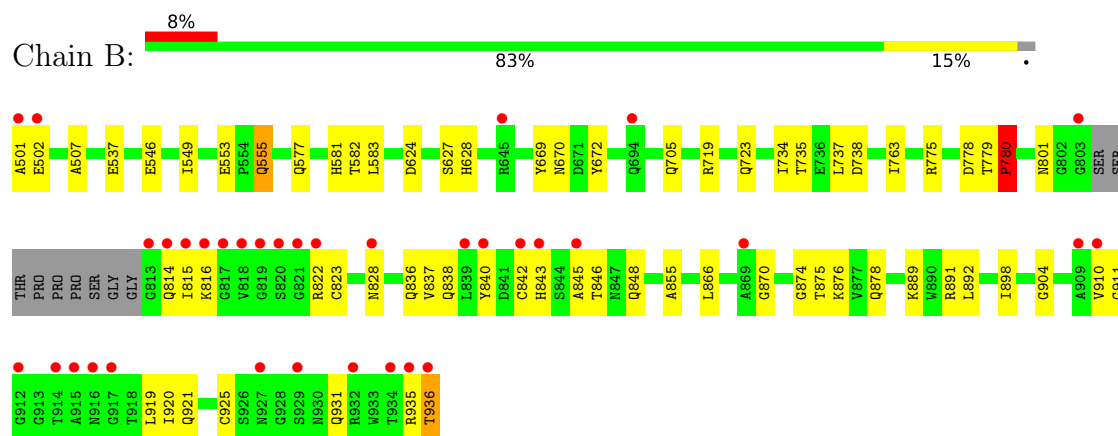
3 Residue-property plots [i](#)

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.

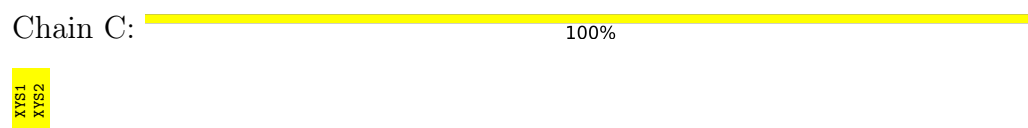
• Molecule 1: ENDO-1,4-BETA-D-XYLANASE



• Molecule 1: ENDO-1,4-BETA-D-XYLANASE



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



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.93Å 94.09Å 139.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.05 – 1.95 47.05 – 1.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (47.05-1.95) 98.3 (47.05-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.03 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.183 , 0.211 0.183 , 0.210	Depositor DCC
R_{free} test set	3807 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7304	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, XYS, AZI

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	0.34	0/3298	0.90	12/4473 (0.3%)
1	B	0.34	0/3298	0.92	13/4473 (0.3%)
All	All	0.34	0/6596	0.91	25/8946 (0.3%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	THR	N-CA-C	9.05	124.76	112.90
1	B	735	THR	N-CA-C	8.09	123.50	112.90
1	B	583	LEU	N-CA-C	7.42	120.81	111.69
1	B	537	GLU	N-CA-C	6.82	121.68	113.23
1	A	37	GLU	N-CA-C	6.78	121.64	113.23
1	B	669	TYR	N-CA-C	-6.76	98.22	109.24
1	A	366	LEU	N-CA-C	-6.73	100.07	110.10
1	B	546	GLU	N-CA-C	6.60	120.79	112.87
1	B	549	ILE	N-CA-C	6.42	116.58	110.42
1	A	83	LEU	N-CA-C	6.24	119.36	111.69
1	B	737	LEU	N-CA-C	6.17	119.29	110.10
1	A	169	TYR	N-CA-C	-6.03	99.36	109.07
1	A	407	LEU	N-CA-C	-6.00	100.95	109.96
1	B	866	LEU	N-CA-C	-5.98	101.05	109.96
1	B	553	GLU	CA-C-N	5.95	126.10	119.32
1	B	553	GLU	C-N-CA	5.95	126.10	119.32
1	A	46	GLU	N-CA-C	5.74	119.80	112.34
1	A	49	ILE	N-CA-C	5.72	116.37	110.36
1	A	323	CYS	N-CA-C	5.48	118.99	110.17
1	A	237	LEU	N-CA-C	5.46	118.24	110.10
1	B	780	PRO	N-CA-C	5.16	122.13	114.80
1	B	577	GLN	N-CA-C	-5.14	103.14	110.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	PRO	N-CA-C	5.13	122.08	114.80
1	A	274	TRP	N-CA-C	-5.07	106.93	113.01
1	B	904	GLY	N-CA-C	-5.04	108.29	115.30

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	3233	0	3043	52	0
1	B	3233	0	3040	46	0
2	C	18	0	15	0	0
2	D	18	0	15	0	0
3	A	3	0	0	0	0
3	B	3	0	0	1	0
4	A	18	0	24	9	0
4	B	30	0	40	9	0
5	A	314	0	0	2	0
5	B	434	0	0	4	0
All	All	7304	0	6177	99	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 8.

All (99) 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:B:889:LYS:HE3	5:B:1211:HOH:O	1.73	0.89
1:A:336:GLN:HB2	1:A:376:LYS:HE3	1.55	0.89
1:B:935:ARG:HA	1:B:936:THR:OG1	1.77	0.83
1:B:911:GLY:H	4:B:964:GOL:H31	1.52	0.74
1:A:39:ASN:HB3	4:A:1462:GOL:H11	1.70	0.74
1:B:836:GLN:HB2	1:B:876:LYS:HE3	1.71	0.72
1:A:421:GLN:HE22	4:A:1461:GOL:H32	1.58	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:501:ALA:N	1:B:507:ALA:HB1	2.07	0.69
1:B:502:GLU:HG3	1:B:801:ASN:OD1	1.94	0.67
1:A:411:GLY:H	4:A:1461:GOL:H31	1.60	0.67
1:A:238:ASP:HB2	1:A:280:PRO:HB2	1.78	0.66
1:B:672:TYR:HB3	1:B:705:GLN:NE2	2.11	0.65
1:A:374:GLY:HA2	1:A:421:GLN:OE1	1.96	0.65
1:A:421:GLN:NE2	4:A:1461:GOL:H32	2.12	0.63
1:B:874:GLY:HA2	1:B:921:GLN:OE1	1.99	0.62
1:A:392:LEU:HD22	1:A:398:ILE:HG12	1.82	0.61
1:B:501:ALA:HB3	5:B:1212:HOH:O	2.01	0.61
1:A:2:GLU:HB2	1:A:301:ASN:OD1	2.01	0.60
1:B:855:ALA:O	1:B:889:LYS:HD2	2.01	0.60
1:B:775:ARG:HH12	4:B:962:GOL:H32	1.66	0.60
1:B:921:GLN:NE2	4:B:964:GOL:H32	2.16	0.59
1:B:778:ASP:O	1:B:779:THR:C	2.44	0.59
1:A:54:PRO:HB2	1:A:55:GLN:NE2	2.18	0.59
1:B:838:GLN:NE2	4:B:963:GOL:H32	2.19	0.58
1:A:127:SER:HA	1:A:170:ASN:O	2.06	0.56
1:A:54:PRO:HB2	1:A:55:GLN:HE22	1.70	0.56
1:B:921:GLN:HE22	4:B:964:GOL:H32	1.70	0.55
1:A:234:ILE:HD12	1:A:263:ILE:HG12	1.90	0.53
1:A:278:ASP:O	1:A:279:THR:C	2.50	0.53
1:B:815:ILE:HG12	1:B:935:ARG:HE	1.74	0.53
1:A:389:LYS:HE3	5:A:1482:HOH:O	2.09	0.53
1:A:141:SER:O	1:A:145:ARG:HG3	2.09	0.52
1:B:738:ASP:HB2	1:B:780:PRO:HB2	1.89	0.52
1:A:172:TYR:HB3	1:A:205:GLN:NE2	2.24	0.52
1:A:68:TYR:OH	1:A:119:LYS:HD3	2.10	0.52
1:A:55:GLN:HB2	1:A:58:GLN:HB2	1.91	0.52
4:B:960:GOL:H31	5:B:1261:HOH:O	2.10	0.52
1:A:279:THR:N	1:A:280:PRO:HD3	2.24	0.51
1:A:82:THR:HG23	1:A:124:ASP:O	2.10	0.51
1:A:389:LYS:HB3	1:A:401:VAL:HG21	1.93	0.51
1:A:7:ALA:N	4:A:1462:GOL:H32	2.25	0.51
1:B:627:SER:HA	1:B:670:ASN:O	2.11	0.50
1:A:142:ASN:HA	1:A:145:ARG:HH11	1.76	0.50
1:B:891:ARG:CB	1:B:891:ARG:HH11	2.25	0.50
1:B:581:HIS:ND1	1:B:582:THR:OG1	2.45	0.49
1:A:168:CYS:HA	1:A:201:CYS:O	2.12	0.49
1:B:779:THR:N	1:B:780:PRO:HD3	2.27	0.49
1:B:843:HIS:NE2	1:B:845:ALA:HB3	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:ALA:HB3	1:A:7:ALA:HB1	1.95	0.49
1:A:49:ILE:HG22	1:A:90:PRO:HD3	1.96	0.48
1:A:53:GLU:HG2	1:A:92:TRP:CZ2	2.48	0.48
1:B:842:CYS:HA	1:B:848:GLN:OE1	2.13	0.48
1:B:843:HIS:HE1	4:B:963:GOL:O1	1.97	0.48
1:B:935:ARG:HA	1:B:936:THR:CB	2.44	0.47
1:A:338:GLN:NE2	4:A:1460:GOL:H32	2.30	0.47
1:B:502:GLU:HG2	1:B:801:ASN:ND2	2.30	0.47
1:B:719:ARG:O	1:B:723:GLN:HG3	2.15	0.47
1:A:53:GLU:HG2	1:A:92:TRP:HZ2	1.79	0.47
1:B:837:VAL:HG23	1:B:920:ILE:HB	1.97	0.46
1:A:142:ASN:HA	1:A:145:ARG:NH1	2.31	0.46
1:A:190:ARG:O	1:A:194:GLN:HG3	2.16	0.46
1:A:338:GLN:HE22	4:A:1460:GOL:H32	1.78	0.46
1:B:816:LYS:HB3	1:B:823:CYS:SG	2.55	0.46
1:A:343:HIS:HE1	4:A:1460:GOL:O1	1.98	0.46
1:B:822:ARG:HD2	1:B:840:TYR:C	2.40	0.46
1:B:501:ALA:N	5:B:1209:HOH:O	2.49	0.46
1:B:582:THR:HG23	1:B:624:ASP:O	2.17	0.45
1:A:425:CYS:HA	1:A:431:GLN:OE1	2.17	0.45
1:A:7:ALA:H	4:A:1462:GOL:C3	2.29	0.44
1:A:389:LYS:HB3	1:A:401:VAL:CG2	2.47	0.44
1:B:876:LYS:HE2	1:B:878:GLN:OE1	2.18	0.44
1:B:910:VAL:HG23	1:B:919:LEU:O	2.18	0.44
1:A:80:GLY:HA3	1:A:123:TRP:CE3	2.53	0.44
1:A:314:GLN:NE2	1:A:343:HIS:O	2.49	0.44
1:A:2:GLU:CB	1:A:301:ASN:OD1	2.65	0.44
1:B:828:ASN:H	4:B:963:GOL:H31	1.82	0.43
1:B:628:HIS:NE2	3:B:953:AZI:N1	2.66	0.43
1:B:892:LEU:HD22	1:B:898:ILE:HG12	2.01	0.43
1:A:316:LYS:HE3	1:A:321:GLY:O	2.19	0.43
1:A:338:GLN:OE1	1:A:417:GLY:HA2	2.18	0.43
1:B:925:CYS:HA	1:B:931:GLN:OE1	2.19	0.43
1:A:355:ALA:O	1:A:389:LYS:HE2	2.19	0.43
1:B:814:GLN:H	1:B:814:GLN:CD	2.26	0.42
1:B:734:ILE:HD12	1:B:763:ILE:HG12	2.01	0.42
1:A:68:TYR:OH	1:A:119:LYS:HB3	2.20	0.42
1:A:138:ARG:CZ	1:A:151:ILE:HD12	2.50	0.42
1:A:293:TYR:CD1	1:A:293:TYR:C	2.98	0.42
1:A:149:ASP:O	1:A:153:VAL:HG23	2.20	0.41
1:B:891:ARG:HB2	1:B:891:ARG:NH1	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:LYS:CD	5:A:1482:HOH:O	2.67	0.41
1:B:870:GLY:H	1:B:875:THR:CG2	2.33	0.41
1:B:555:GLN:HE21	1:B:555:GLN:HB2	1.71	0.41
1:B:582:THR:HG21	1:B:627:SER:OG	2.20	0.41
1:B:838:GLN:HE22	4:B:963:GOL:H32	1.85	0.41
1:A:113:MET:HE3	1:A:123:TRP:CD1	2.56	0.41
1:A:46:GLU:H	1:A:46:GLU:CD	2.26	0.41
1:A:86:HIS:NE2	1:A:139:ARG:NH1	2.69	0.41
1:B:846:THR:C	1:B:848:GLN:H	2.29	0.41
1:A:343:HIS:NE2	1:A:345:ALA:HB3	2.36	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	423/436 (97%)	412 (97%)	11 (3%)	0	100	100
1	B	423/436 (97%)	401 (95%)	22 (5%)	0	100	100
All	All	846/872 (97%)	813 (96%)	33 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	334/341 (98%)	332 (99%)	2 (1%)	78	79
1	B	334/341 (98%)	331 (99%)	3 (1%)	70	70
All	All	668/682 (98%)	663 (99%)	5 (1%)	76	76

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	247	TYR
1	A	280	PRO
1	B	555	GLN
1	B	780	PRO
1	B	936	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	173	ASN
1	A	343	HIS
1	A	349	GLN
1	B	511	GLN
1	B	555	GLN
1	B	673	ASN
1	B	843	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

4 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	XYS	C	1	3,2	9,9,10	0.54	0	10,12,14	0.96	1 (10%)
2	XYS	C	2	2	9,9,10	0.63	0	10,12,14	0.78	1 (10%)
2	XYS	D	1	3,2	9,9,10	0.50	0	10,12,14	1.05	1 (10%)
2	XYS	D	2	2	9,9,10	0.61	0	10,12,14	0.75	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	XYS	C	1	3,2	1/1/3/4	-	0/1/1/1
2	XYS	C	2	2	1/1/3/4	-	0/1/1/1
2	XYS	D	1	3,2	1/1/3/4	-	0/1/1/1
2	XYS	D	2	2	1/1/3/4	-	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	XYS	C4-C3-C2	-3.07	107.28	110.92
2	C	1	XYS	C4-C3-C2	-2.76	107.64	110.92
2	C	2	XYS	C4-C3-C2	-2.21	108.30	110.92

All (4) chirality outliers are listed below:

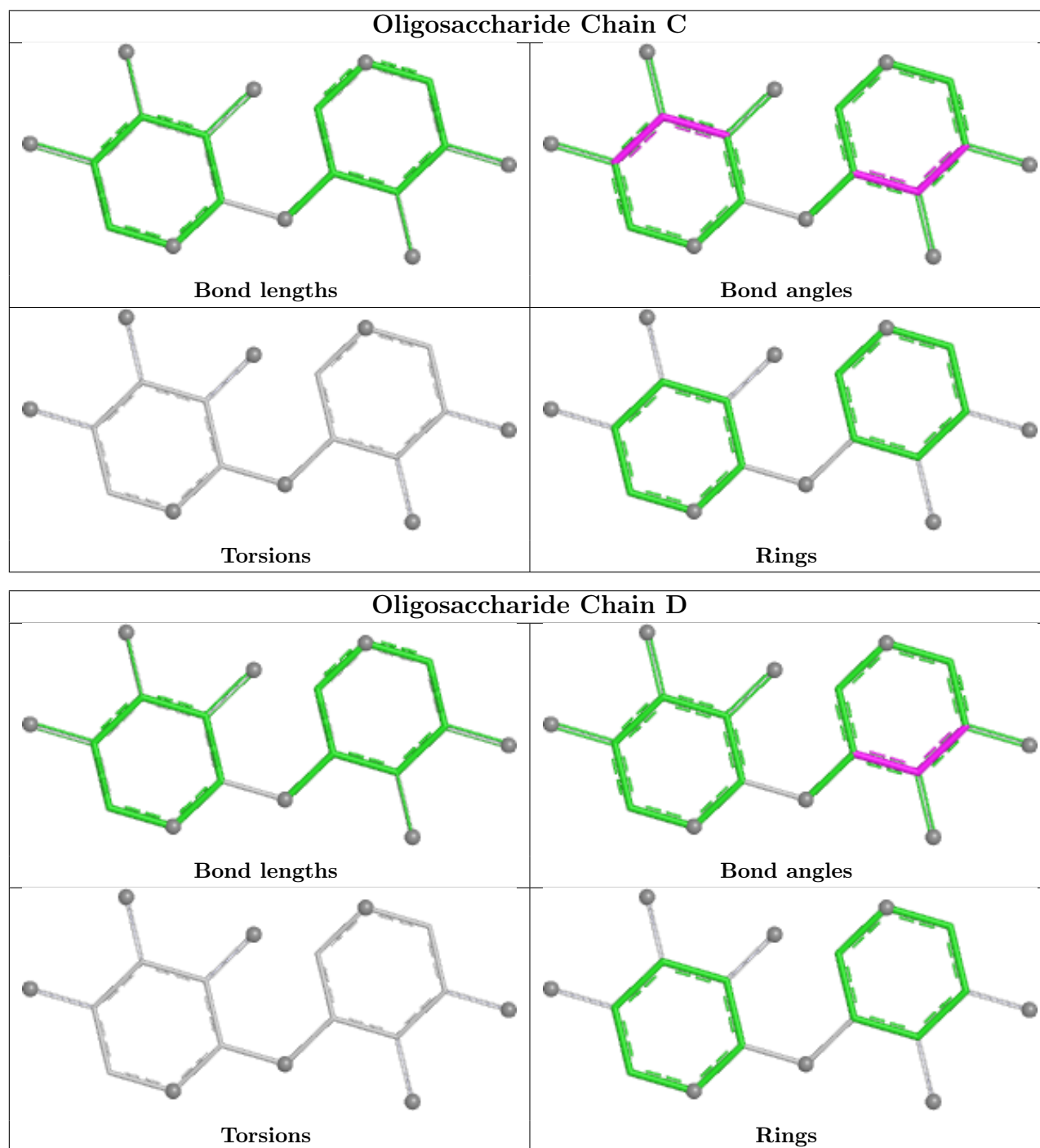
Mol	Chain	Res	Type	Atom
2	C	1	XYS	C1
2	C	2	XYS	C1
2	D	1	XYS	C1
2	D	2	XYS	C1

There are no torsion outliers.

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.



5.6 Ligand geometry [i](#)

10 ligands 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
4	GOL	B	961	-	5,5,5	0.14	0	5,5,5	0.32	0
4	GOL	B	962	-	5,5,5	0.17	0	5,5,5	0.34	0
4	GOL	B	963	-	5,5,5	0.16	0	5,5,5	0.34	0
4	GOL	B	964	-	5,5,5	0.17	0	5,5,5	0.34	0
4	GOL	A	1461	-	5,5,5	0.21	0	5,5,5	0.35	0
4	GOL	B	960	-	5,5,5	0.15	0	5,5,5	0.31	0
4	GOL	A	1460	-	5,5,5	0.19	0	5,5,5	0.37	0
4	GOL	A	1462	-	5,5,5	0.17	0	5,5,5	0.37	0
3	AZI	A	453	2	2,2,2	3.00	1 (50%)	0,1,1	-	-
3	AZI	B	953	2	2,2,2	3.16	1 (50%)	0,1,1	-	-

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	GOL	B	961	-	-	0/4/4/4	-
4	GOL	B	962	-	-	0/4/4/4	-
4	GOL	B	963	-	-	0/4/4/4	-
4	GOL	B	964	-	-	0/4/4/4	-
4	GOL	A	1461	-	-	0/4/4/4	-
4	GOL	B	960	-	-	0/4/4/4	-
4	GOL	A	1460	-	-	0/4/4/4	-
4	GOL	A	1462	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	953	AZI	N3-N2	-4.45	1.14	1.23
3	A	453	AZI	N3-N2	-4.23	1.14	1.23

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	962	GOL	1	0
4	B	963	GOL	4	0
4	B	964	GOL	3	0
4	A	1461	GOL	3	0
4	B	960	GOL	1	0
4	A	1460	GOL	3	0
4	A	1462	GOL	3	0
3	B	953	AZI	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	427/436 (97%)	0.26	30 (7%) 22 26	11, 21, 41, 51	0
1	B	427/436 (97%)	0.09	35 (8%) 17 20	10, 16, 42, 59	0
All	All	854/872 (97%)	0.17	65 (7%) 20 22	10, 18, 42, 59	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	501	ALA	6.7
1	A	436	THR	6.4
1	A	1	ALA	6.2
1	B	818	VAL	5.9
1	A	303	GLY	5.3
1	B	936	THR	4.5
1	A	95	SER	4.4
1	A	100	THR	4.4
1	A	435	ARG	4.4
1	A	427	ASN	3.9
1	A	97	SER	3.8
1	B	935	ARG	3.8
1	B	927	ASN	3.8
1	A	96	LEU	3.8
1	B	814	GLN	3.6
1	B	820	SER	3.6
1	B	934	THR	3.6
1	A	140	ASP	3.5
1	A	55	GLN	3.4
1	B	819	GLY	3.4
1	B	813	GLY	3.3
1	A	142	ASN	3.3
1	B	803	GLY	3.3
1	B	821	GLY	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	147	GLY	3.0
1	B	845	ALA	3.0
1	B	843	HIS	3.0
1	B	822	ARG	2.9
1	A	101	LEU	2.9
1	B	910	VAL	2.9
1	A	92	TRP	2.9
1	B	914	THR	2.7
1	A	58	GLN	2.7
1	B	817	GLY	2.7
1	B	909	ALA	2.6
1	B	840	TYR	2.5
1	A	145	ARG	2.5
1	A	98	GLY	2.4
1	A	94	GLN	2.4
1	B	912	GLY	2.4
1	A	139	ARG	2.3
1	A	54	PRO	2.3
1	B	917	GLY	2.3
1	B	932	ARG	2.3
1	A	2	GLU	2.3
1	B	839	LEU	2.3
1	B	915	ALA	2.3
1	A	370	GLY	2.3
1	B	645	ARG	2.3
1	A	91	GLY	2.2
1	B	842	CYS	2.2
1	A	141	SER	2.2
1	B	694	GLN	2.2
1	B	869	ALA	2.2
1	B	816	LYS	2.2
1	B	916	ASN	2.2
1	A	51	ALA	2.2
1	B	502	GLU	2.2
1	B	828	ASN	2.1
1	A	179	TRP	2.1
1	A	143	LEU	2.1
1	B	929	SER	2.1
1	A	59	PHE	2.0
1	B	815	ILE	2.0
1	A	90	PRO	2.0

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

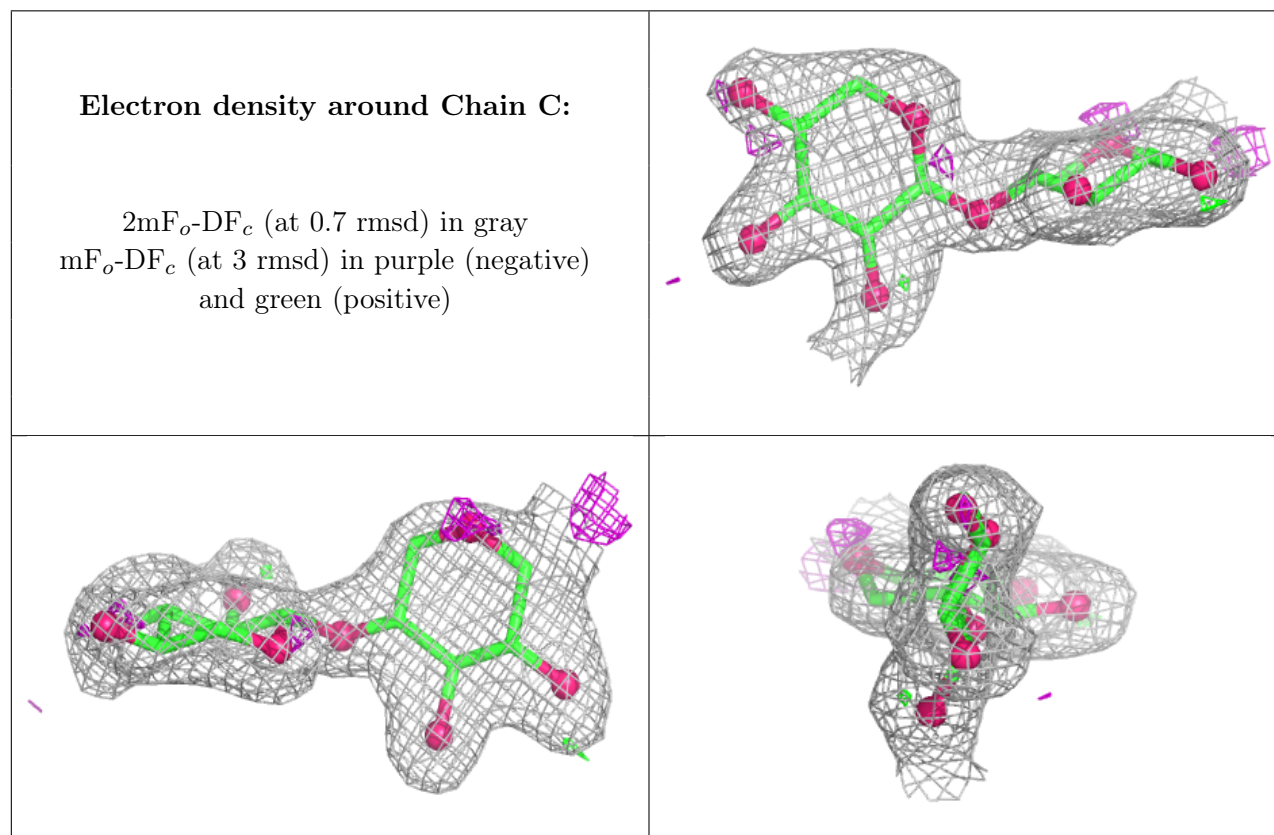
There are no non-standard protein/DNA/RNA residues in this entry.

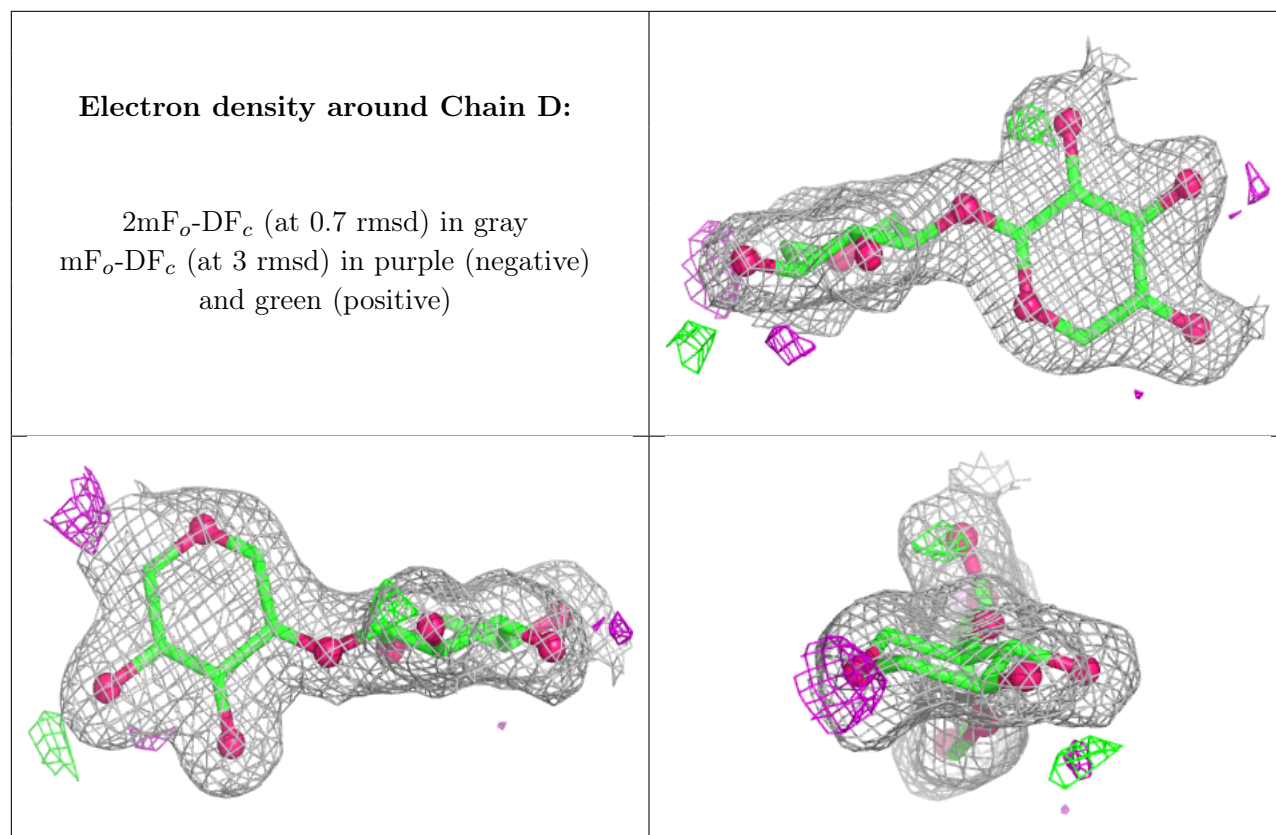
6.3 Carbohydrates [i](#)

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	XYS	C	2	9/10	0.85	0.12	29,31,33,34	0
2	XYS	C	1	9/10	0.90	0.11	26,30,32,33	0
2	XYS	D	2	9/10	0.94	0.07	17,20,22,24	0
2	XYS	D	1	9/10	0.96	0.06	16,22,23,24	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.





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	B	963	6/6	0.70	0.31	65,67,68,69	0
4	GOL	B	960	6/6	0.72	0.24	24,31,32,39	0
4	GOL	A	1460	6/6	0.73	0.26	31,37,41,46	0
4	GOL	B	961	6/6	0.79	0.20	46,48,49,50	0
4	GOL	B	964	6/6	0.79	0.20	46,47,48,50	0
4	GOL	A	1462	6/6	0.80	0.22	26,36,37,39	0
3	AZI	B	953	3/3	0.81	0.24	28,28,28,30	0
4	GOL	A	1461	6/6	0.82	0.18	33,35,36,40	0
4	GOL	B	962	6/6	0.83	0.22	56,57,57,57	0
3	AZI	A	453	3/3	0.88	0.17	32,32,33,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.