



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:05 PM UTC

PDB ID : 6XN2 / pdb_00006xn2
Title : Crystal structure of the GH43_1 enzyme from Xanthomonas citri complexed with xylotriose
Authors : Morais, M.A.B.; Tonoli, C.C.C.; Santos, C.R.; Murakami, M.T.
Deposited on : 2020-07-02
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 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

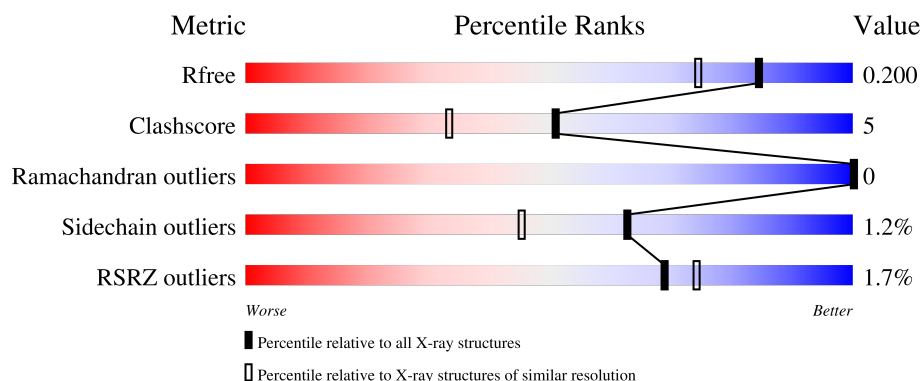
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

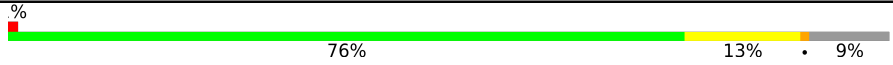
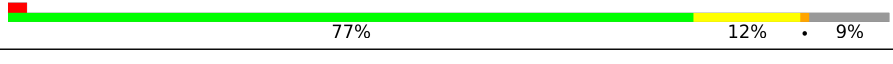
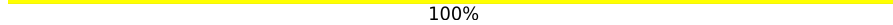
The reported resolution of this entry is 1.65 Å.

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}	180053	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (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 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	364	
1	B	364	
2	C	3	

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
6	GOL	B	409	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5829 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 Xylosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2589	1653	455	473	8			
1	B	331	Total	C	N	O	S	0	1	0
			2614	1668	461	477	8			

There are 40 discrepancies between the modelled and reference sequences:

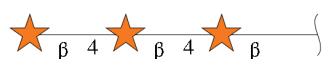
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q8PET2
A	-18	GLY	-	expression tag	UNP Q8PET2
A	-17	SER	-	expression tag	UNP Q8PET2
A	-16	SER	-	expression tag	UNP Q8PET2
A	-15	HIS	-	expression tag	UNP Q8PET2
A	-14	HIS	-	expression tag	UNP Q8PET2
A	-13	HIS	-	expression tag	UNP Q8PET2
A	-12	HIS	-	expression tag	UNP Q8PET2
A	-11	HIS	-	expression tag	UNP Q8PET2
A	-10	HIS	-	expression tag	UNP Q8PET2
A	-9	SER	-	expression tag	UNP Q8PET2
A	-8	SER	-	expression tag	UNP Q8PET2
A	-7	GLY	-	expression tag	UNP Q8PET2
A	-6	LEU	-	expression tag	UNP Q8PET2
A	-5	VAL	-	expression tag	UNP Q8PET2
A	-4	PRO	-	expression tag	UNP Q8PET2
A	-3	ARG	-	expression tag	UNP Q8PET2
A	-2	GLY	-	expression tag	UNP Q8PET2
A	-1	SER	-	expression tag	UNP Q8PET2
A	0	HIS	-	expression tag	UNP Q8PET2
B	-19	MET	-	initiating methionine	UNP Q8PET2
B	-18	GLY	-	expression tag	UNP Q8PET2
B	-17	SER	-	expression tag	UNP Q8PET2
B	-16	SER	-	expression tag	UNP Q8PET2
B	-15	HIS	-	expression tag	UNP Q8PET2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q8PET2
B	-13	HIS	-	expression tag	UNP Q8PET2
B	-12	HIS	-	expression tag	UNP Q8PET2
B	-11	HIS	-	expression tag	UNP Q8PET2
B	-10	HIS	-	expression tag	UNP Q8PET2
B	-9	SER	-	expression tag	UNP Q8PET2
B	-8	SER	-	expression tag	UNP Q8PET2
B	-7	GLY	-	expression tag	UNP Q8PET2
B	-6	LEU	-	expression tag	UNP Q8PET2
B	-5	VAL	-	expression tag	UNP Q8PET2
B	-4	PRO	-	expression tag	UNP Q8PET2
B	-3	ARG	-	expression tag	UNP Q8PET2
B	-2	GLY	-	expression tag	UNP Q8PET2
B	-1	SER	-	expression tag	UNP Q8PET2
B	0	HIS	-	expression tag	UNP Q8PET2

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

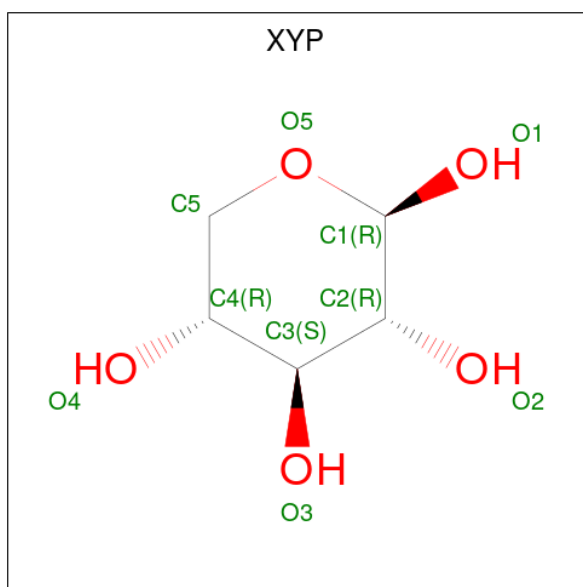


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	3	Total	C	O	0	1	0
			37	20	17			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

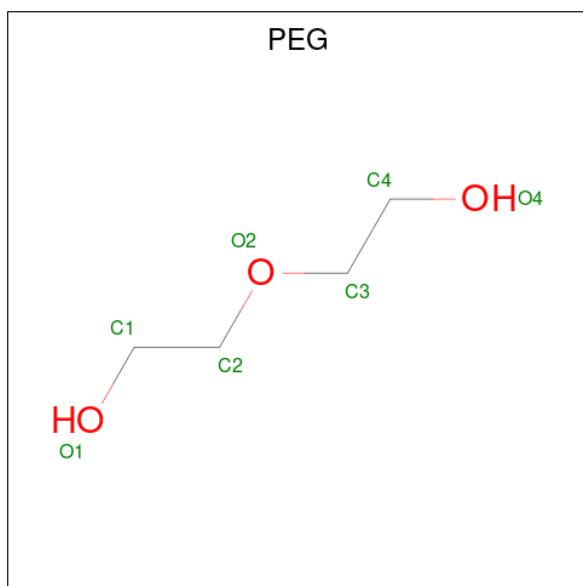
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is beta-D-xylopyranose (CCD ID: XYP) (formula: C₅H₁₀O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	5	5		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



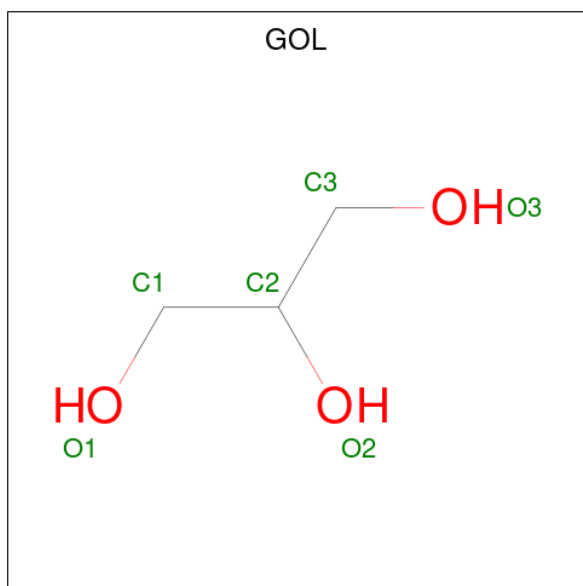
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		

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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	256	Total	O	0	0
			256	256		

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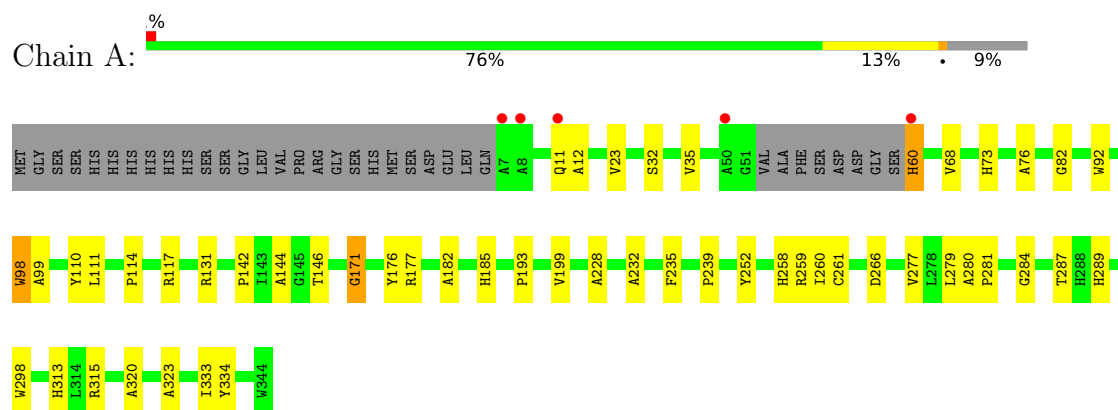
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	246	Total 246	O 246	0	0

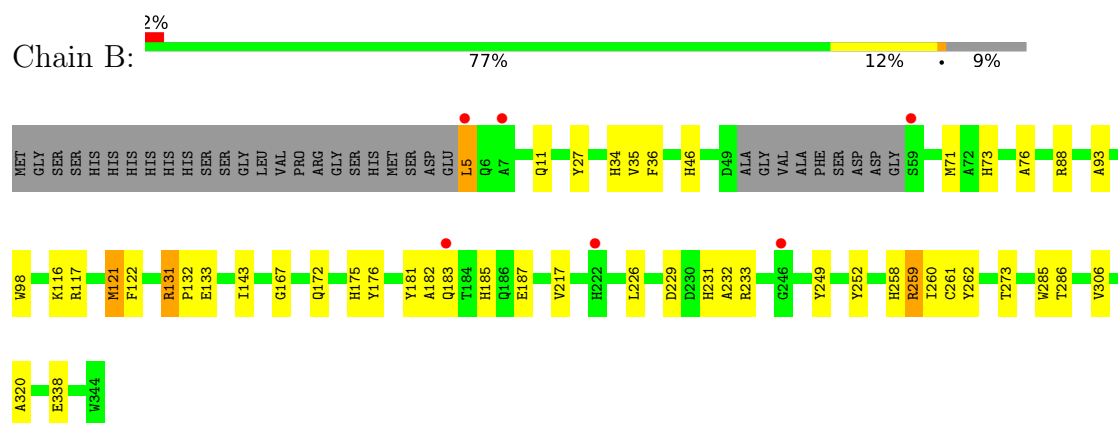
3 Residue-property plots [i](#)

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: Xylosidase



- Molecule 1: Xylosidase



- Molecule 2: beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	63.59Å 165.87Å 158.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.41 – 1.65 29.41 – 1.65	Depositor EDS
% Data completeness (in resolution range)	63.6 (29.41-1.65) 63.6 (29.41-1.65)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 1.65Å)	Xtriage
Refinement program	PHENIX 1.8	Depositor
R, R_{free}	0.177 , 0.201 0.179 , 0.200	Depositor DCC
R_{free} test set	3168 reflections (3.15%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5829	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 4.51% 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: PEG, XYP, GOL, CA

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	1.45	28/2678 (1.0%)	0.96	7/3665 (0.2%)
1	B	1.44	23/2703 (0.9%)	0.97	9/3698 (0.2%)
All	All	1.44	51/5381 (0.9%)	0.96	16/7363 (0.2%)

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	1
1	B	0	1
All	All	0	2

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	187	GLU	C-N	10.75	1.48	1.33
1	A	68	VAL	C-O	-6.91	1.16	1.24
1	A	261	CYS	C-O	-6.91	1.15	1.23
1	B	285	TRP	C-O	-6.83	1.16	1.24
1	B	306	VAL	C-O	-6.76	1.16	1.24
1	A	110	TYR	C-O	-6.63	1.16	1.24
1	B	27	TYR	C-O	-6.61	1.16	1.24
1	A	177	ARG	C-O	-6.34	1.16	1.23
1	A	239	PRO	C-O	-6.16	1.16	1.23
1	A	199	VAL	C-O	-6.12	1.17	1.24
1	A	111	LEU	C-O	-6.07	1.17	1.24
1	A	99	ALA	C-O	-6.06	1.16	1.24
1	B	143	ILE	C-O	-5.79	1.18	1.24
1	B	252	TYR	C-O	-5.75	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	333	ILE	C-O	-5.74	1.17	1.24
1	B	320	ALA	C-O	-5.73	1.18	1.24
1	A	176	TYR	C-O	-5.65	1.16	1.24
1	A	284	GLY	C-O	-5.64	1.17	1.24
1	A	320	ALA	C-O	-5.60	1.18	1.24
1	B	232	ALA	C-O	-5.58	1.17	1.24
1	A	334	TYR	C-O	-5.56	1.18	1.24
1	B	273	THR	C-O	-5.53	1.17	1.24
1	B	93	ALA	C-O	-5.52	1.17	1.23
1	B	121	MET	C-O	-5.51	1.17	1.24
1	A	146	THR	C-O	-5.47	1.17	1.23
1	A	252	TYR	C-O	-5.46	1.17	1.23
1	A	228	ALA	C-O	-5.43	1.17	1.24
1	A	279	LEU	C-O	-5.39	1.17	1.24
1	A	82	GLY	C-O	-5.37	1.17	1.23
1	A	235	PHE	C-O	-5.33	1.17	1.23
1	B	217	VAL	C-O	-5.29	1.18	1.24
1	B	226	LEU	C-O	-5.28	1.17	1.23
1	A	287	THR	C-O	-5.27	1.17	1.23
1	A	12	ALA	C-O	-5.26	1.18	1.24
1	B	167	GLY	C-O	-5.24	1.16	1.23
1	A	131	ARG	C-O	-5.21	1.18	1.24
1	B	98	TRP	C-O	-5.21	1.17	1.23
1	A	32	SER	C-O	-5.17	1.18	1.24
1	A	193	PRO	C-O	-5.15	1.17	1.23
1	B	233	ARG	C-O	-5.15	1.17	1.24
1	A	260	ILE	C-O	-5.12	1.18	1.24
1	B	231	HIS	C-O	-5.11	1.17	1.24
1	B	261	CYS	C-O	-5.10	1.17	1.23
1	A	23	VAL	C-O	-5.09	1.18	1.23
1	B	249	TYR	C-O	-5.09	1.18	1.24
1	A	98	TRP	C-O	-5.06	1.18	1.23
1	B	229	ASP	C-O	-5.05	1.17	1.24
1	A	144	ALA	C-O	-5.04	1.17	1.23
1	B	46	HIS	C-O	-5.04	1.18	1.23
1	B	286	THR	C-O	-5.03	1.17	1.23
1	B	262	TYR	C-O	-5.02	1.17	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	187	GLU	CA-C-N	10.84	130.94	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	187	GLU	C-N-CA	10.84	130.94	119.78
1	A	258	HIS	N-CA-C	9.24	124.07	112.24
1	B	258	HIS	N-CA-C	7.93	122.33	111.54
1	B	187	GLU	O-C-N	-6.90	115.16	121.30
1	A	289	HIS	N-CA-C	6.32	117.82	108.60
1	B	5	LEU	CA-C-N	-6.25	111.01	121.39
1	B	5	LEU	C-N-CA	-6.25	111.01	121.39
1	B	338	GLU	CA-C-N	-6.09	112.91	122.65
1	B	338	GLU	C-N-CA	-6.09	112.91	122.65
1	A	266	ASP	N-CA-C	-5.50	106.25	113.17
1	A	323	ALA	N-CA-C	5.31	117.56	108.90
1	A	171	GLY	CA-C-O	-5.22	113.29	119.45
1	B	260	ILE	N-CA-C	-5.03	100.65	107.99
1	A	131	ARG	CA-C-N	5.02	124.80	119.28
1	A	131	ARG	C-N-CA	5.02	124.80	119.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	171	GLY	Mainchain
1	B	259[A]	ARG	Mainchain

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	2589	0	2424	28	0
1	B	2614	0	2452	26	0
2	C	37	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	10	0	0	1	0
5	A	35	0	50	7	0
5	B	28	0	40	6	0
6	A	6	0	8	1	0
6	B	6	0	8	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	256	0	0	0	0
7	B	246	0	0	1	0
All	All	5829	0	4982	54	0

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

All (54) 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:60:HIS:HD2	1:A:313:HIS:CD2	1.80	1.00
1:B:181:TYR:HE1	1:B:183:GLN:HE21	1.14	0.95
6:B:409:GOL:H11	7:B:662:HOH:O	1.74	0.87
1:B:181:TYR:HE1	1:B:183:GLN:NE2	1.76	0.84
1:A:60:HIS:CD2	1:A:313:HIS:CG	2.66	0.82
1:A:60:HIS:CD2	1:A:313:HIS:CD2	2.66	0.82
1:B:35:VAL:H	6:B:409:GOL:C3	1.93	0.81
1:A:35:VAL:H	6:A:408:GOL:H11	1.46	0.81
1:B:34:HIS:ND1	6:B:409:GOL:H12	1.95	0.80
1:A:298:TRP:HE1	5:A:403:PEG:H31	1.51	0.76
1:A:259:ARG:HG2	5:A:407:PEG:H22	1.72	0.70
1:B:35:VAL:H	6:B:409:GOL:H32	1.59	0.66
1:B:117:ARG:HH12	5:B:405:PEG:H21	1.59	0.66
5:A:405:PEG:H12	5:A:405:PEG:H42	1.75	0.66
1:A:117:ARG:HH12	5:A:405:PEG:H21	1.62	0.63
1:A:60:HIS:CD2	1:A:313:HIS:CE1	2.88	0.61
1:A:11:GLN:CD	1:B:11:GLN:HG2	2.26	0.60
1:B:36:PHE:HE1	6:B:409:GOL:HO1	1.48	0.59
1:B:172:GLN:HG2	5:B:408:PEG:H41	1.85	0.58
1:A:117:ARG:HH22	5:A:405:PEG:H31	1.70	0.57
1:A:11:GLN:CG	1:B:11:GLN:HG2	2.35	0.56
1:A:60:HIS:NE2	1:A:313:HIS:CE1	2.74	0.56
1:A:281:PRO:HD3	5:A:407:PEG:H31	1.89	0.54
1:A:11:GLN:NE2	1:B:11:GLN:HG2	2.22	0.54
1:B:181:TYR:CE1	1:B:183:GLN:NE2	2.62	0.53
1:A:60:HIS:HD2	1:A:313:HIS:NE2	2.05	0.51
1:A:11:GLN:HG2	1:B:11:GLN:HG2	1.93	0.51
1:B:131:ARG:HB3	1:B:132:PRO:HD2	1.92	0.50
1:B:36:PHE:HE1	6:B:409:GOL:O1	1.95	0.50
1:A:60:HIS:CD2	1:A:313:HIS:NE2	2.79	0.49
1:A:60:HIS:CD2	1:A:313:HIS:ND1	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:HIS:NE2	1:A:313:HIS:ND1	2.60	0.48
1:B:121:MET:HA	1:B:121:MET:HE2	1.97	0.47
1:A:298:TRP:NE1	5:A:403:PEG:H31	2.27	0.46
5:B:407:PEG:H12	5:B:407:PEG:H32	1.67	0.46
1:A:315:ARG:HH12	4:A:402:XYP:C5	2.30	0.44
1:B:34:HIS:ND1	6:B:409:GOL:C1	2.77	0.43
1:A:73:HIS:CD2	1:A:76:ALA:HB2	2.54	0.43
1:A:259:ARG:HD3	1:A:277:VAL:HG22	2.00	0.43
5:B:406:PEG:H31	5:B:406:PEG:H11	1.83	0.43
1:A:92:TRP:CG	1:A:142:PRO:HD3	2.54	0.42
1:B:175:HIS:NE2	5:B:408:PEG:H12	2.35	0.42
1:A:98:TRP:HB2	1:A:114:PRO:HG2	2.00	0.42
1:B:34:HIS:HA	6:B:409:GOL:H31	2.01	0.42
1:B:117:ARG:HH22	5:B:405:PEG:H31	1.84	0.41
1:B:73:HIS:CD2	1:B:76:ALA:HB2	2.55	0.41
1:A:280:ALA:HB1	1:A:281:PRO:HD2	2.02	0.41
1:B:182:ALA:HB3	1:B:185:HIS:CD2	2.55	0.41
1:A:232:ALA:HB1	1:A:259:ARG:NH2	2.36	0.41
1:B:176:TYR:CE2	1:B:181:TYR:HB2	2.56	0.41
1:A:182:ALA:HB3	1:A:185:HIS:CG	2.56	0.41
1:B:71:MET:HE2	1:B:71:MET:HB3	1.94	0.40
1:B:35:VAL:N	6:B:409:GOL:C3	2.75	0.40
1:B:116:LYS:HE3	1:B:122:PHE:CE2	2.57	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	326/364 (90%)	311 (95%)	15 (5%)	0	100	100
1	B	328/364 (90%)	313 (95%)	15 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	654/728 (90%)	624 (95%)	30 (5%)	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	259/288 (90%)	258 (100%)	1 (0%)	84	77
1	B	263/288 (91%)	257 (98%)	6 (2%)	44	21
All	All	522/576 (91%)	515 (99%)	7 (1%)	63	42

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	B	5	LEU
1	B	88	ARG
1	B	131	ARG
1	B	133	GLU
1	B	259[A]	ARG
1	B	259[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	104	GLN
1	A	179	ASN
1	B	222	HIS
1	B	311	GLN

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	XYP	C	1	2	10,10,10	0.91	0	14,14,14	1.00	1 (7%)
2	XYP	C	2	2	9,9,10	0.61	0	10,12,14	1.63	2 (20%)
2	XYP	C	3[A]	2	9,9,10	1.14	1 (11%)	10,12,14	3.08	5 (50%)
2	XYP	C	3[B]	2	9,9,10	0.61	0	10,12,14	1.08	1 (10%)

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	XYP	C	1	2	-	-	0/1/1/1
2	XYP	C	2	2	-	-	0/1/1/1
2	XYP	C	3[A]	2	-	-	0/1/1/1
2	XYP	C	3[B]	2	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3[A]	XYP	C2-C3	-2.13	1.49	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3[A]	XYP	C5-O5-C1	6.81	122.42	111.42
2	C	3[A]	XYP	O3-C3-C2	-4.14	101.60	110.05
2	C	3[A]	XYP	C5-C4-C3	3.53	114.79	109.64
2	C	2	XYP	C5-C4-C3	-3.36	104.75	109.64
2	C	3[A]	XYP	C1-C2-C3	3.23	114.34	109.64
2	C	2	XYP	O4-C4-C3	2.30	114.92	110.15
2	C	3[A]	XYP	O4-C4-C3	2.21	114.74	110.15
2	C	3[B]	XYP	O3-C3-C2	-2.21	105.54	110.05
2	C	1	XYP	O4-C4-C3	-2.18	105.64	110.15

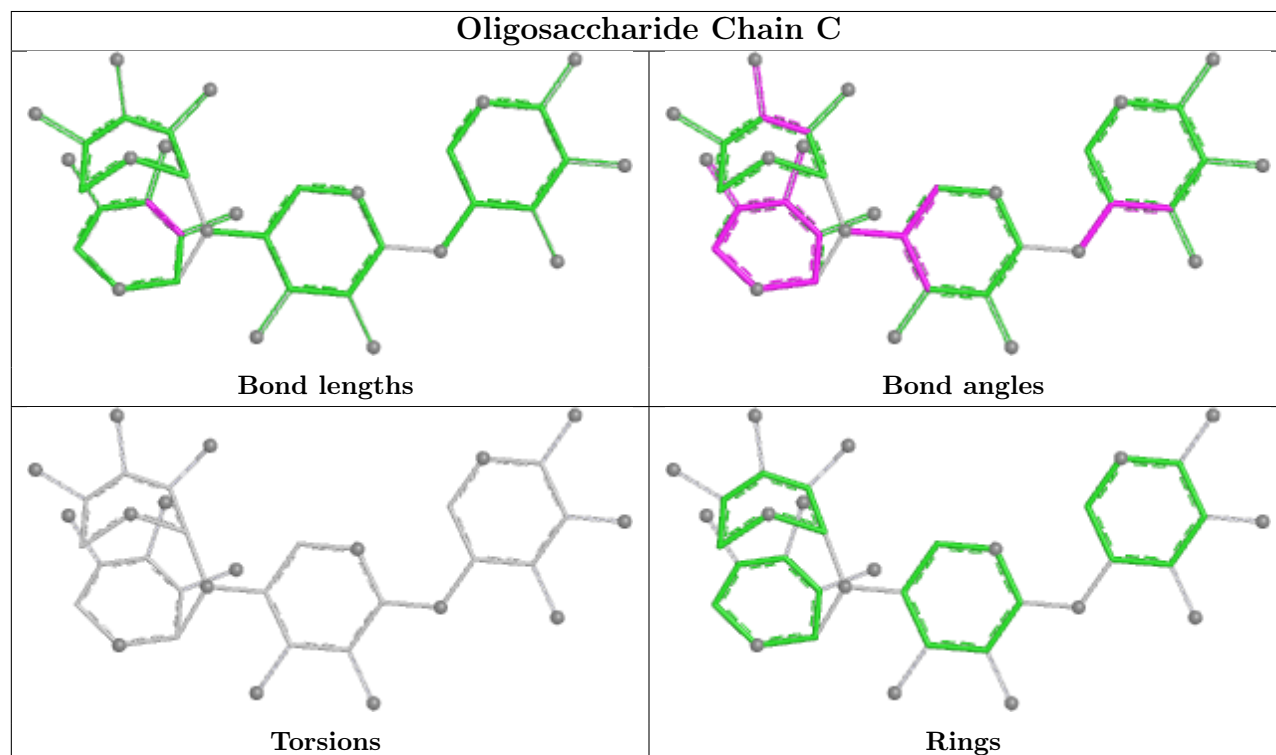
There are no chirality outliers.

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](#)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	$\# Z > 2$
6	GOL	B	409	-	5,5,5	0.08	0	5,5,5	0.50	0
5	PEG	B	406	-	6,6,6	0.23	0	5,5,5	0.51	0
4	XYP	A	402	-	10,10,10	1.11	0	14,14,14	1.32	1 (7%)
5	PEG	A	405	-	6,6,6	0.30	0	5,5,5	0.58	0
5	PEG	B	405	-	6,6,6	0.33	0	5,5,5	0.50	0
5	PEG	A	407	-	6,6,6	0.23	0	5,5,5	0.90	0
5	PEG	B	407	-	6,6,6	0.24	0	5,5,5	0.39	0
5	PEG	A	404	-	6,6,6	0.34	0	5,5,5	0.63	0
5	PEG	A	403	-	6,6,6	0.31	0	5,5,5	1.04	0
6	GOL	A	408	-	5,5,5	0.27	0	5,5,5	0.73	0
5	PEG	A	406	-	6,6,6	0.30	0	5,5,5	0.50	0
5	PEG	B	408	-	6,6,6	0.42	0	5,5,5	0.63	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	GOL	B	409	-	-	4/4/4/4	-
5	PEG	B	406	-	-	2/4/4/4	-
5	PEG	A	405	-	-	1/4/4/4	-
5	PEG	B	405	-	-	3/4/4/4	-
4	XYP	A	402	-	-	-	0/1/1/1
5	PEG	A	407	-	-	1/4/4/4	-
5	PEG	B	407	-	-	3/4/4/4	-
5	PEG	A	404	-	-	2/4/4/4	-
5	PEG	A	403	-	-	2/4/4/4	-
6	GOL	A	408	-	-	3/4/4/4	-
5	PEG	A	406	-	-	3/4/4/4	-
5	PEG	B	408	-	-	3/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	402	XYP	O3-C3-C2	-3.46	102.22	110.38

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	408	GOL	C1-C2-C3-O3
6	B	409	GOL	C1-C2-C3-O3
5	B	407	PEG	C1-C2-O2-C3
5	B	408	PEG	O2-C3-C4-O4
5	A	403	PEG	O2-C3-C4-O4
6	B	409	GOL	O1-C1-C2-C3
5	A	407	PEG	O2-C3-C4-O4
5	B	406	PEG	O1-C1-C2-O2
5	B	407	PEG	O2-C3-C4-O4
6	A	408	GOL	O2-C2-C3-O3
6	B	409	GOL	O2-C2-C3-O3
5	B	405	PEG	O1-C1-C2-O2
5	B	408	PEG	O1-C1-C2-O2
5	A	406	PEG	O1-C1-C2-O2
5	B	407	PEG	O1-C1-C2-O2
6	B	409	GOL	O1-C1-C2-O2
5	B	406	PEG	C1-C2-O2-C3
5	A	406	PEG	C1-C2-O2-C3
5	B	405	PEG	C4-C3-O2-C2
6	A	408	GOL	O1-C1-C2-C3
5	A	405	PEG	O1-C1-C2-O2
5	A	404	PEG	C4-C3-O2-C2
5	A	406	PEG	O2-C3-C4-O4
5	A	403	PEG	O1-C1-C2-O2
5	B	405	PEG	O2-C3-C4-O4
5	B	408	PEG	C1-C2-O2-C3
5	A	404	PEG	O2-C3-C4-O4

There are no ring outliers.

10 monomers are involved in 24 short contacts:

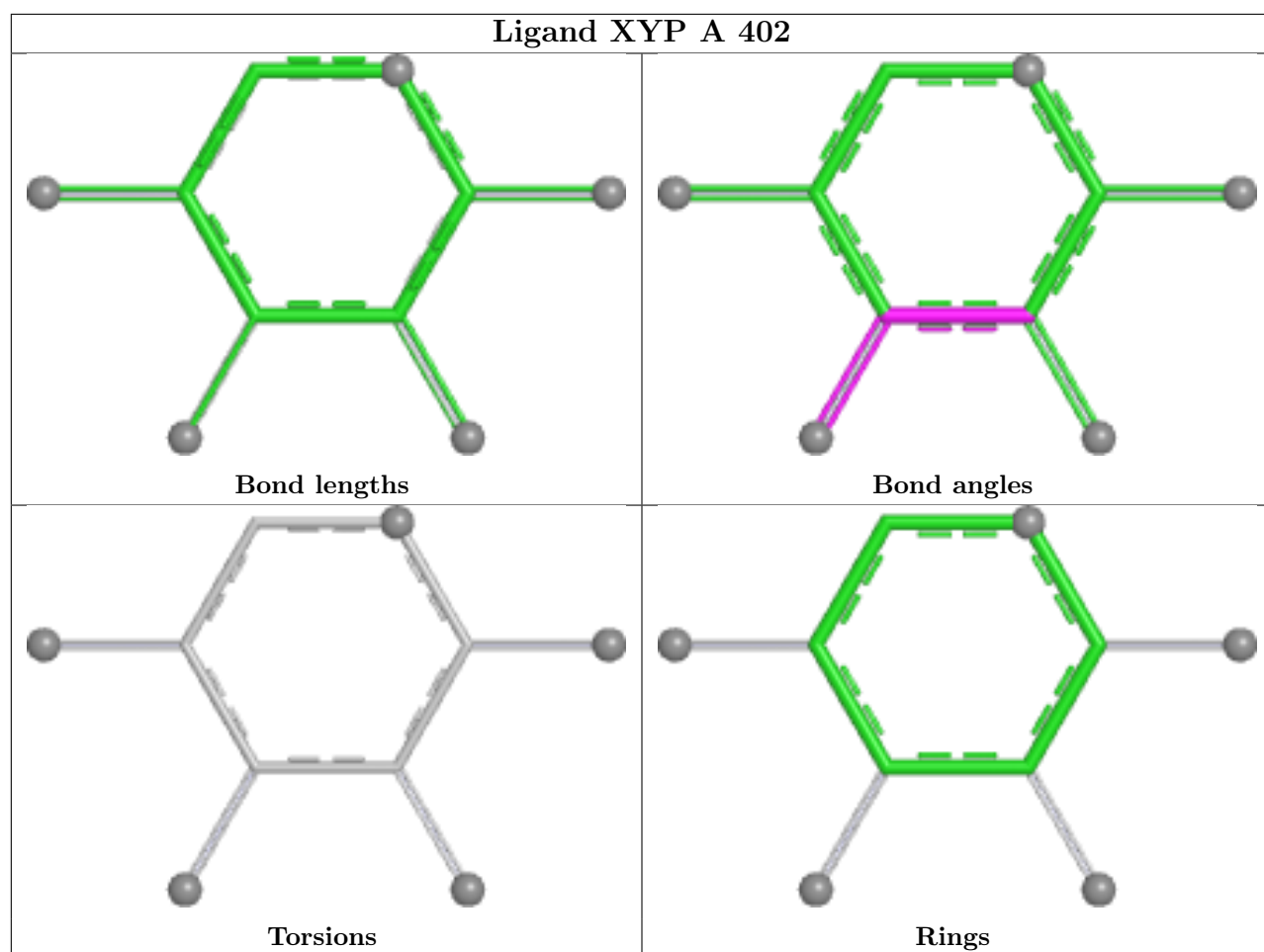
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	409	GOL	9	0
5	B	406	PEG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	402	XYP	1	0
5	A	405	PEG	3	0
5	B	405	PEG	2	0
5	A	407	PEG	2	0
5	B	407	PEG	1	0
5	A	403	PEG	2	0
6	A	408	GOL	1	0
5	B	408	PEG	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	330/364 (90%)	0.05	5 (1%) 72 77	24, 31, 48, 82	0
1	B	331/364 (90%)	0.09	6 (1%) 67 73	15, 32, 51, 76	1 (0%)
All	All	661/728 (90%)	0.07	11 (1%) 69 74	15, 32, 50, 82	1 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	ALA	6.0
1	B	5	LEU	4.9
1	B	183	GLN	4.1
1	A	60	HIS	4.0
1	A	50	ALA	3.0
1	A	11	GLN	2.8
1	A	8	ALA	2.5
1	B	7	ALA	2.5
1	B	246	GLY	2.5
1	B	59	SER	2.2
1	B	222	HIS	2.1

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

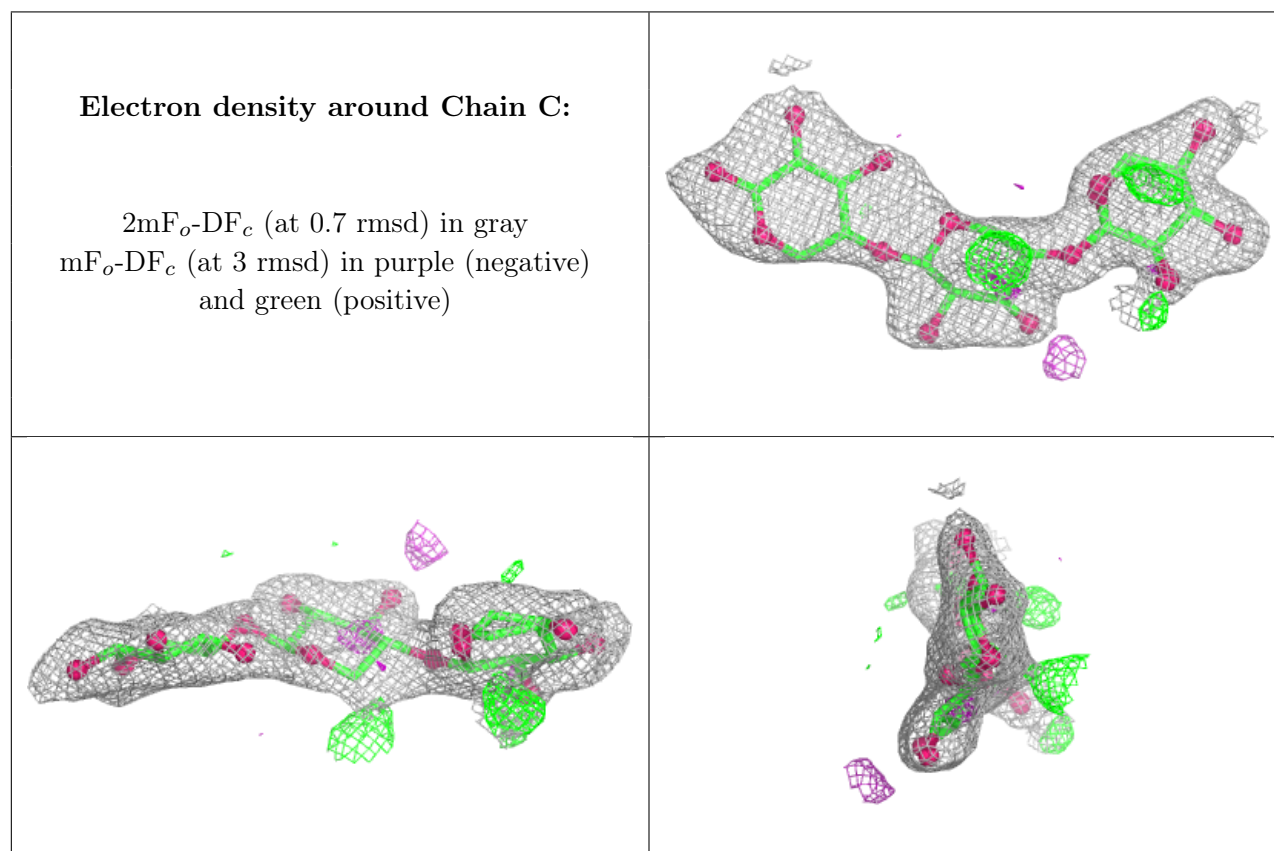
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	XYP	C	3[A]	9/10	0.85	0.13	34,37,43,45	9
2	XYP	C	3[B]	9/10	0.85	0.13	36,39,44,46	9
2	XYP	C	2	9/10	0.86	0.12	50,57,66,69	0
2	XYP	C	1	10/10	0.89	0.10	65,67,69,71	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.

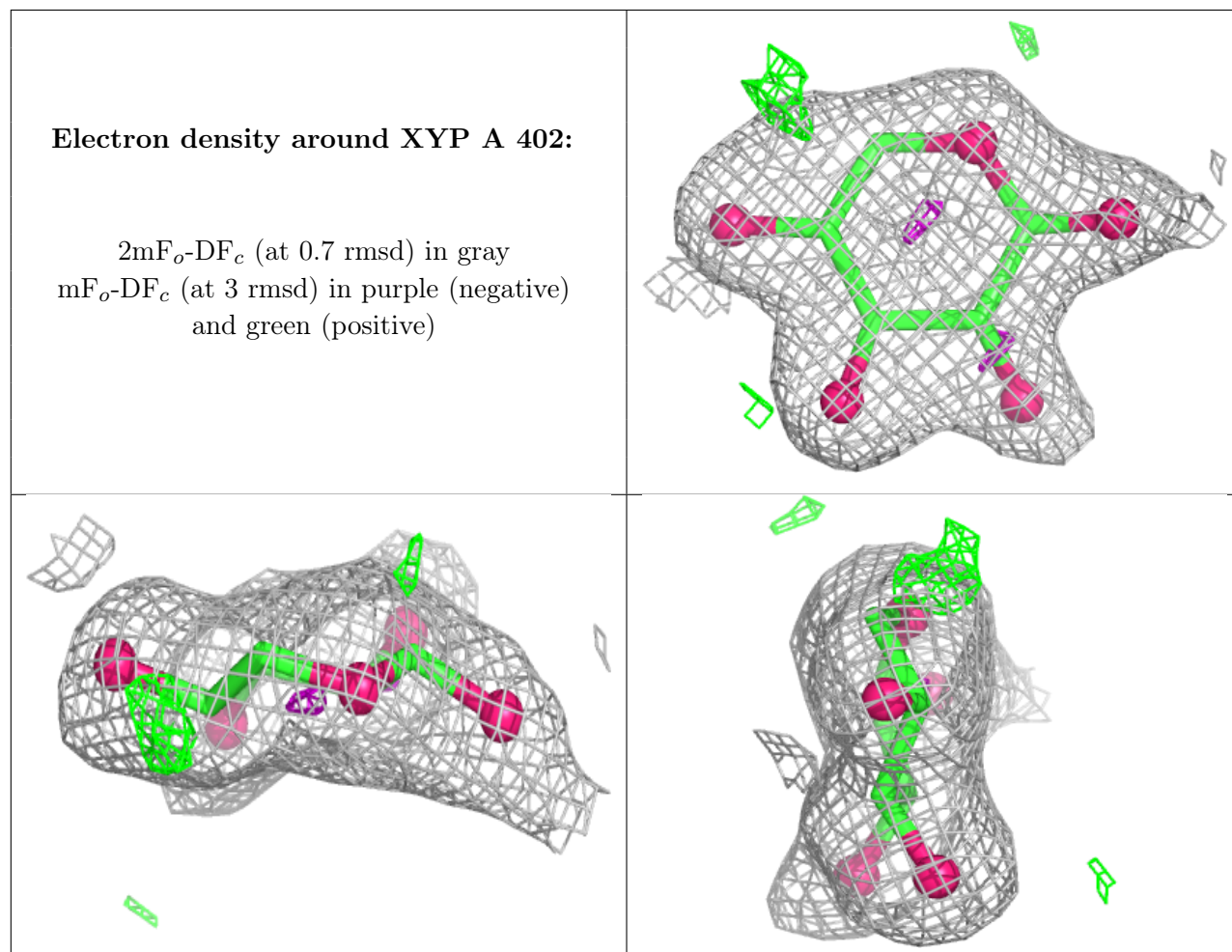
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PEG	B	408	7/7	0.62	0.25	45,54,62,66	0
6	GOL	A	408	6/6	0.78	0.18	27,33,42,45	0
5	PEG	A	406	7/7	0.83	0.15	42,47,54,54	0
5	PEG	B	407	7/7	0.85	0.13	42,44,49,50	0
5	PEG	A	403	7/7	0.85	0.13	43,48,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PEG	A	407	7/7	0.85	0.15	44,50,56,57	0
5	PEG	B	406	7/7	0.86	0.10	37,44,47,49	0
5	PEG	A	405	7/7	0.86	0.14	48,51,57,60	0
5	PEG	B	405	7/7	0.88	0.12	41,45,46,48	0
6	GOL	B	409	6/6	0.90	0.13	24,38,45,53	0
5	PEG	A	404	7/7	0.91	0.10	37,38,43,50	0
4	XYP	A	402	10/10	0.92	0.08	35,38,41,41	0
3	CA	A	401	1/1	0.98	0.04	32,32,32,32	0
3	CA	B	401	1/1	1.00	0.03	31,31,31,31	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.