



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 27, 2025 – 09:12 am GMT

PDB ID : 9H6G / pdb_00009h6g
Title : Inactive Bacteroides ovatus GH98 endoxylanase E361A in complex with arabino-xylooligosaccharide
Authors : Tomlinson, C.W.E.; Cartmell, A.; Bolam, D.N.
Deposited on : 2024-10-24
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

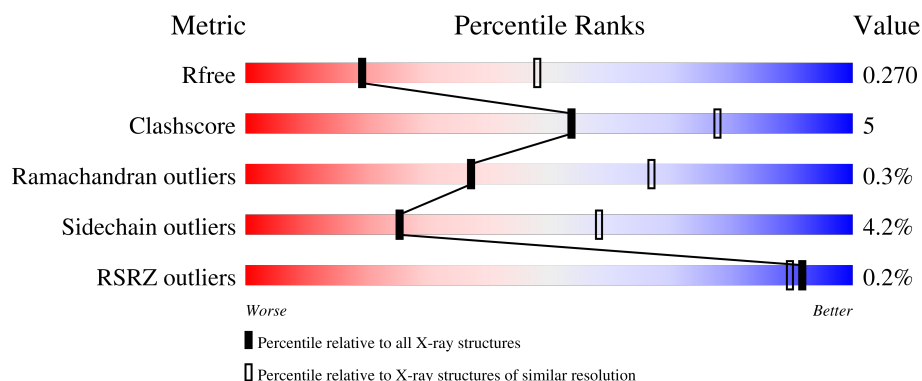
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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	895	
1	B	895	
2	E	9	
3	F	8	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 28503 atoms, of which 13801 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.

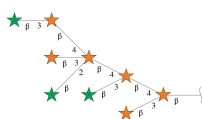
- Molecule 1 is a protein called Glycoside hydrolase family 98 domain-containing protein.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	894	Total	C	H	N	O	P	S	214	0	0
			13938	4518	6827	1183	1386	1	23			
1	B	895	Total	C	H	N	O	P	S	214	0	0
			13952	4522	6835	1184	1387	1	23			

There are 2 discrepancies between the modelled and reference sequences:

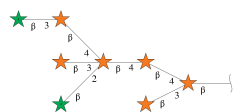
Chain	Residue	Modelled	Actual	Comment	Reference
A	353	ALA	GLU	engineered mutation	UNP A0A6N3VET1
B	353	ALA	GLU	engineered mutation	UNP A0A6N3VET1

- Molecule 2 is an oligosaccharide called beta-L-arabinofuranose-(1-3)-beta-D-xylopyranose-(1-4)-[beta-L-arabinofuranose-(1-2)][beta-D-xylopyranose-(1-3)]beta-D-xylopyranose-(1-4)-[beta-L-arabinofuranose-(1-3)]beta-D-xylopyranose-(1-4)-[beta-D-xylopyranose-(1-3)]beta-D-xylopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	9	Total	C	H	O	20	0	0
			156	45	74	37			

- Molecule 3 is an oligosaccharide called beta-L-arabinofuranose-(1-3)-beta-D-xylopyranose-(1-4)-[beta-L-arabinofuranose-(1-2)][beta-D-xylopyranose-(1-3)]beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-[beta-D-xylopyranose-(1-3)]beta-D-xylopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	8	Total	C	H	O	17	0	0
			138	40	65	33			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

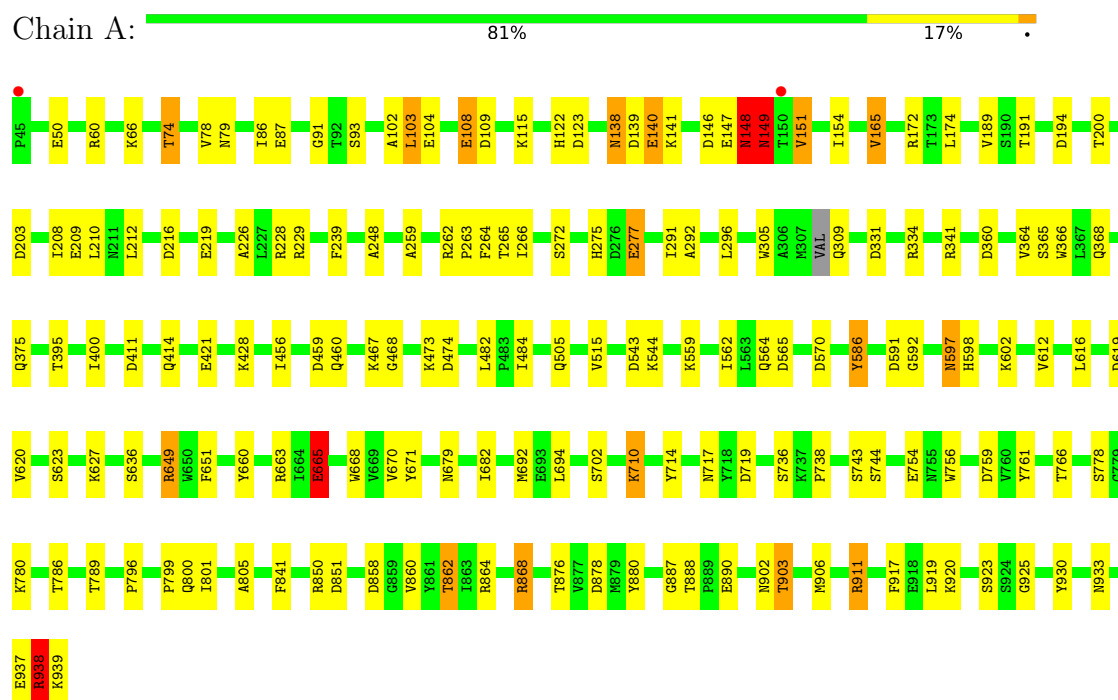
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	179	Total	O	0	0
			179	179		
5	B	138	Total	O	0	0
			138	138		

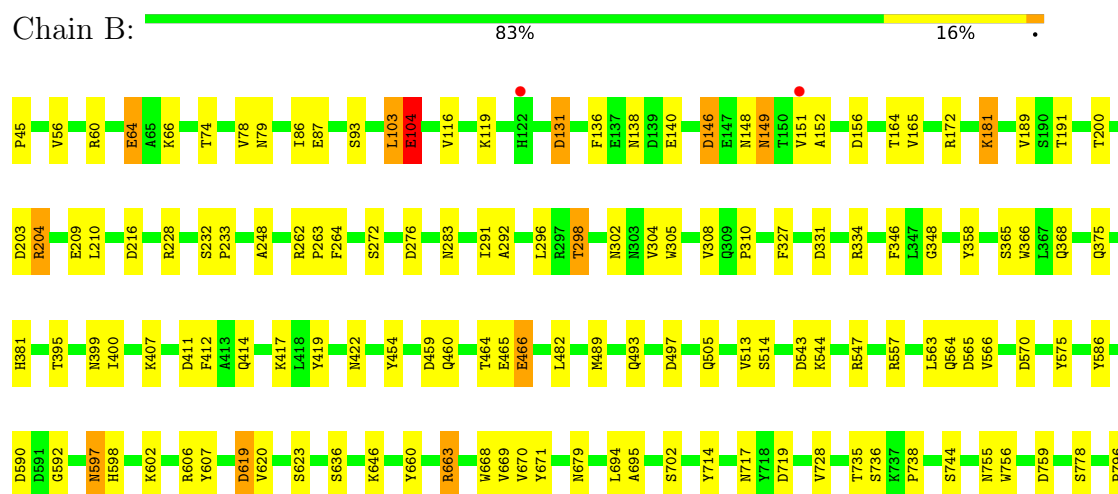
3 Residue-property plots

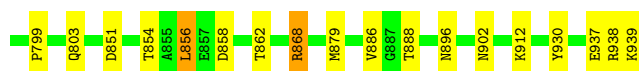
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glycoside hydrolase family 98 domain-containing protein

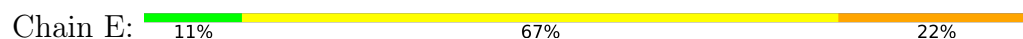


- Molecule 1: Glycoside hydrolase family 98 domain-containing protein

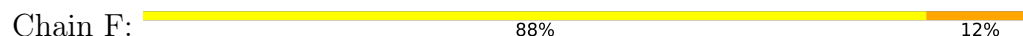




- Molecule 2: beta-L-arabinofuranose-(1-3)-beta-D-xylopyranose-(1-4)-[beta-L-arabinofuranose-(1-2)][beta-D-xylopyranose-(1-3)]beta-D-xylopyranose-(1-4)-[beta-L-arabinofuranose-(1-3)]beta-D-xylopyranose-(1-4)-[beta-D-xylopyranose-(1-3)]beta-D-xylopyranose



- Molecule 3: beta-L-arabinofuranose-(1-3)-beta-D-xylopyranose-(1-4)-[beta-L-arabinofuranose-(1-2)][beta-D-xylopyranose-(1-3)]beta-D-xylopyranose-(1-4)-beta-D-xylopyranose-(1-4)-[beta-D-xylopyranose-(1-3)]beta-D-xylopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	186.05Å 63.48Å 180.90Å 90.00° 118.44° 90.00°	Depositor
Resolution (Å)	53.02 – 2.80 53.02 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (53.02-2.80) 99.7 (53.02-2.80)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.88)	Depositor
R, R_{free}	0.186 , 0.268 0.185 , 0.270	Depositor DCC
R_{free} test set	2397 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	28503	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.49% 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: CA, FUB, XYP, PHD

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	0.66	0/7277	1.23	41/9896 (0.4%)
1	B	0.63	0/7283	1.20	31/9905 (0.3%)
All	All	0.64	0/14560	1.22	72/19801 (0.4%)

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	10
1	B	0	7
All	All	0	17

There are no bond length outliers.

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	THR	CA-CB-OG1	-9.17	95.85	109.60
1	B	74	THR	CA-CB-OG1	-8.81	96.39	109.60
1	A	203	ASP	CA-CB-CG	8.11	120.71	112.60
1	A	194	ASP	CA-CB-CG	7.98	120.58	112.60
1	A	421	GLU	CB-CG-CD	7.54	125.42	112.60

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	172	ARG	Sidechain
1	A	228	ARG	Sidechain
1	A	229	ARG	Sidechain
1	A	60	ARG	Sidechain

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	7111	6827	6813	70	1
1	B	7117	6835	6821	65	0
2	E	82	74	0	2	0
3	F	73	65	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	179	0	0	10	0
5	B	138	0	0	9	0
All	All	14702	13801	13634	135	1

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

The worst 5 of 135 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:358:TYR:CE2	1:B:358:TYR:CG	2.37	1.05
1:A:665:GLU:HG2	5:A:1165:HOH:O	1.63	0.95
1:A:138:ASN:OD1	1:A:139:ASP:N	2.21	0.74
1:A:66:LYS:HD2	5:A:1115:HOH:O	1.87	0.74
1:B:131:ASP:OD1	1:B:203:ASP:O	2.08	0.71

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ASP:OD2	1:A:649:ARG:NH2[3_545]	2.02	0.18

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	889/895 (99%)	842 (95%)	44 (5%)	3 (0%)	37	67
1	B	892/895 (100%)	843 (94%)	46 (5%)	3 (0%)	37	67
All	All	1781/1790 (100%)	1685 (95%)	90 (5%)	6 (0%)	37	67

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	717	ASN
1	B	104	GLU
1	A	102	ALA
1	B	204	ARG

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	771/772 (100%)	738 (96%)	33 (4%)	25	57
1	B	772/772 (100%)	740 (96%)	32 (4%)	26	59
All	All	1543/1544 (100%)	1478 (96%)	65 (4%)	25	58

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	744	SER
1	B	778	SER
1	A	754	GLU
1	A	744	SER
1	B	856	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	302	ASN
1	B	453	GLN
1	B	422	ASN
1	B	511	ASN
1	A	751	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	PHD	A	851	1	9,11,12	1.99	2 (22%)	10,15,17	1.97	4 (40%)
1	PHD	B	851	1	9,11,12	2.25	1 (11%)	10,15,17	2.01	4 (40%)

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
1	PHD	A	851	1	-	4/8/11/13	-
1	PHD	B	851	1	-	4/8/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	851	PHD	P-OD1	6.31	1.68	1.59
1	A	851	PHD	P-OD1	5.40	1.67	1.59
1	A	851	PHD	OD2-CG	-2.04	1.16	1.22

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	851	PHD	OD2-CG-CB	-3.18	117.70	124.73
1	A	851	PHD	OD1-CG-CB	3.13	119.71	111.11
1	B	851	PHD	CA-CB-CG	3.06	119.27	112.86
1	A	851	PHD	OP3-P-OD1	2.89	114.06	105.25
1	A	851	PHD	OD2-CG-CB	-2.63	118.93	124.73

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	851	PHD	C-CA-CB-CG
1	B	851	PHD	C-CA-CB-CG
1	A	851	PHD	N-CA-CB-CG
1	B	851	PHD	CA-CB-CG-OD2
1	B	851	PHD	CA-CB-CG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

17 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	E	1	2	10,10,10	0.39	0	14,14,14	1.70	4 (28%)
2	XYP	E	2	2	9,9,10	0.65	0	10,12,14	1.23	1 (10%)
2	XYP	E	3	2	9,9,10	0.56	0	10,12,14	2.91	6 (60%)
2	XYP	E	4	2	9,9,10	0.94	1 (11%)	10,12,14	2.35	4 (40%)
2	FUB	E	5	2	9,9,10	0.60	0	10,12,14	1.61	2 (20%)
2	FUB	E	6	2	9,9,10	0.58	0	10,12,14	1.89	3 (30%)
2	XYP	E	7	2	9,9,10	0.32	0	10,12,14	1.12	1 (10%)
2	FUB	E	8	2	9,9,10	0.32	0	10,12,14	1.12	0
2	XYP	E	9	2	9,9,10	0.52	0	10,12,14	1.67	3 (30%)
3	XYP	F	1	3	10,10,10	0.63	0	14,14,14	1.70	3 (21%)
3	XYP	F	2	3	9,9,10	0.61	0	10,12,14	1.39	1 (10%)
3	XYP	F	3	3	9,9,10	0.81	0	10,12,14	2.38	5 (50%)
3	XYP	F	4	3	9,9,10	0.72	0	10,12,14	1.47	2 (20%)
3	FUB	F	5	3	9,9,10	0.57	0	10,12,14	1.44	1 (10%)
3	FUB	F	6	3	9,9,10	0.41	0	10,12,14	1.14	1 (10%)
3	XYP	F	7	3	9,9,10	0.26	0	10,12,14	1.88	4 (40%)
3	XYP	F	8	3	9,9,10	0.40	0	10,12,14	0.80	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	E	1	2	-	-	0/1/1/1
2	XYP	E	2	2	-	-	0/1/1/1
2	XYP	E	3	2	-	-	0/1/1/1
2	XYP	E	4	2	-	-	0/1/1/1
2	FUB	E	5	2	-	2/2/15/18	0/1/1/1
2	FUB	E	6	2	-	0/2/15/18	0/1/1/1
2	XYP	E	7	2	-	-	0/1/1/1
2	FUB	E	8	2	-	0/2/15/18	0/1/1/1
2	XYP	E	9	2	-	-	0/1/1/1
3	XYP	F	1	3	-	-	0/1/1/1
3	XYP	F	2	3	-	-	0/1/1/1
3	XYP	F	3	3	-	-	1/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	XYP	F	4	3	-	-	0/1/1/1
3	FUB	F	5	3	-	2/2/15/18	0/1/1/1
3	FUB	F	6	3	-	2/2/15/18	0/1/1/1
3	XYP	F	7	3	-	-	0/1/1/1
3	XYP	F	8	3	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	4	XYP	O3-C3	2.00	1.47	1.43

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	XYP	C4-C3-C2	-5.35	104.56	110.92
2	E	3	XYP	O4-C4-C3	5.08	120.32	110.14
3	F	1	XYP	O3-C3-C4	-4.43	101.51	109.99
2	E	1	XYP	O3-C3-C4	-4.38	101.61	109.99
2	E	6	FUB	O4-C4-C3	-4.05	101.12	104.70

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	5	FUB	O4-C4-C5-O5
2	E	5	FUB	C3-C4-C5-O5
3	F	5	FUB	O4-C4-C5-O5
3	F	5	FUB	C3-C4-C5-O5
3	F	6	FUB	C3-C4-C5-O5

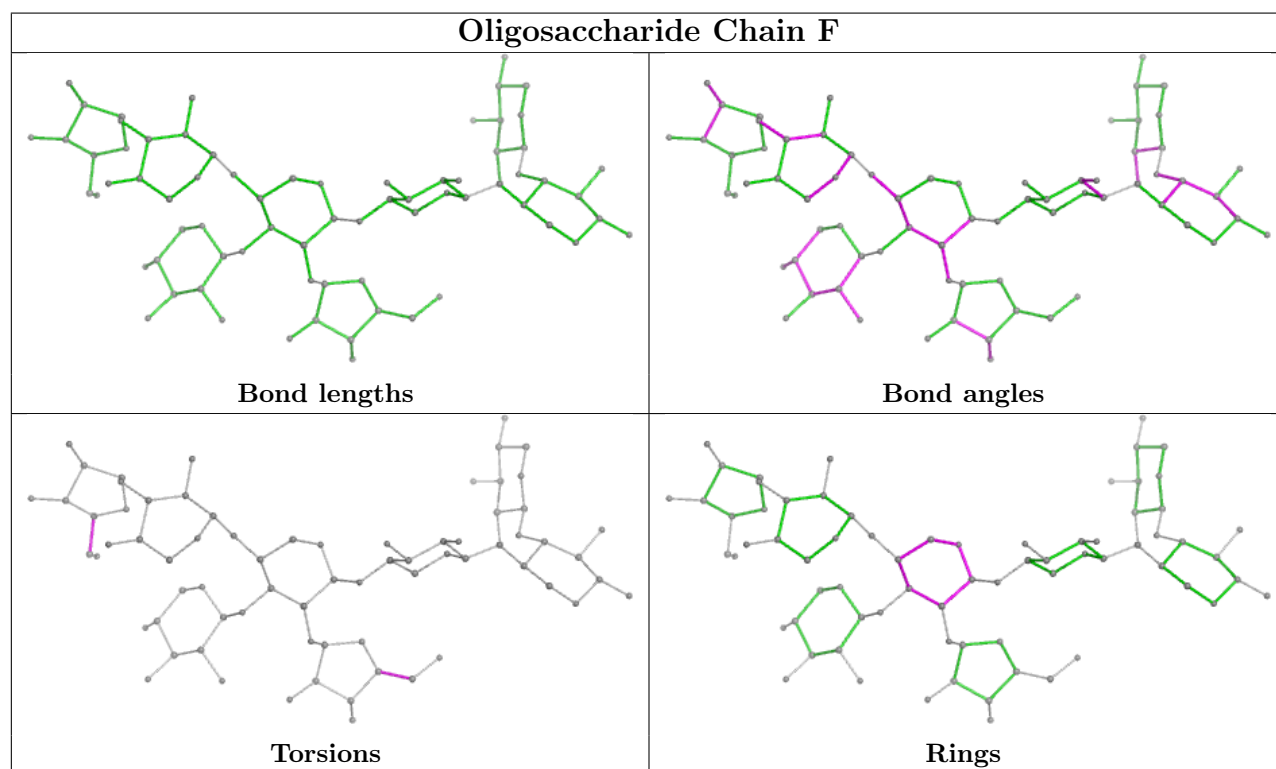
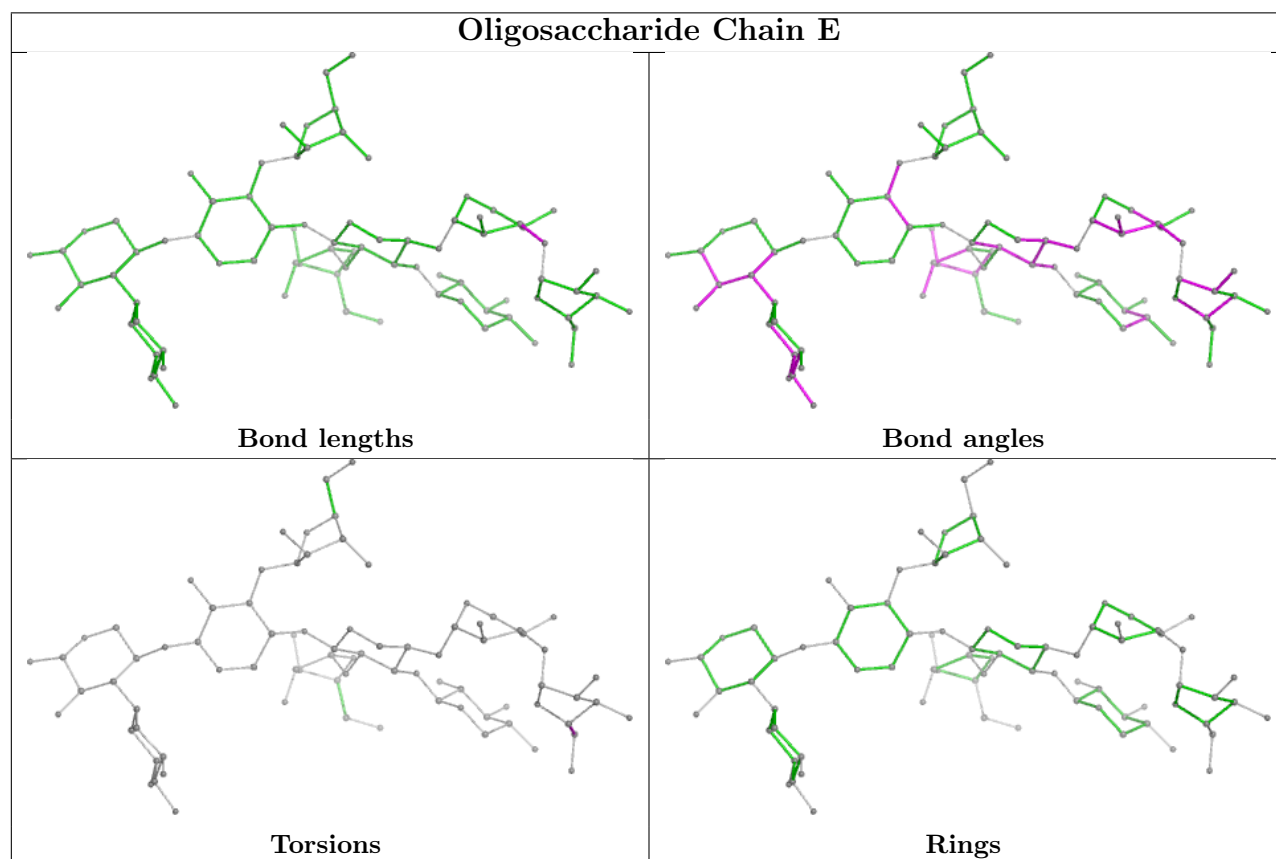
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	3	XYP	C1-C2-C3-C4-C5-O5

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	5	FUB	1	0
2	E	4	XYP	1	0
2	E	5	FUB	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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	893/895 (99%)	-0.60	2 (0%) 92 89	21, 36, 62, 113	0
1	B	894/895 (99%)	-0.26	2 (0%) 92 89	26, 49, 81, 135	0
All	All	1787/1790 (99%)	-0.43	4 (0%) 92 89	21, 42, 76, 135	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	45	PRO	3.9
1	B	151	VAL	2.3
1	A	150	THR	2.2
1	B	122	HIS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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.

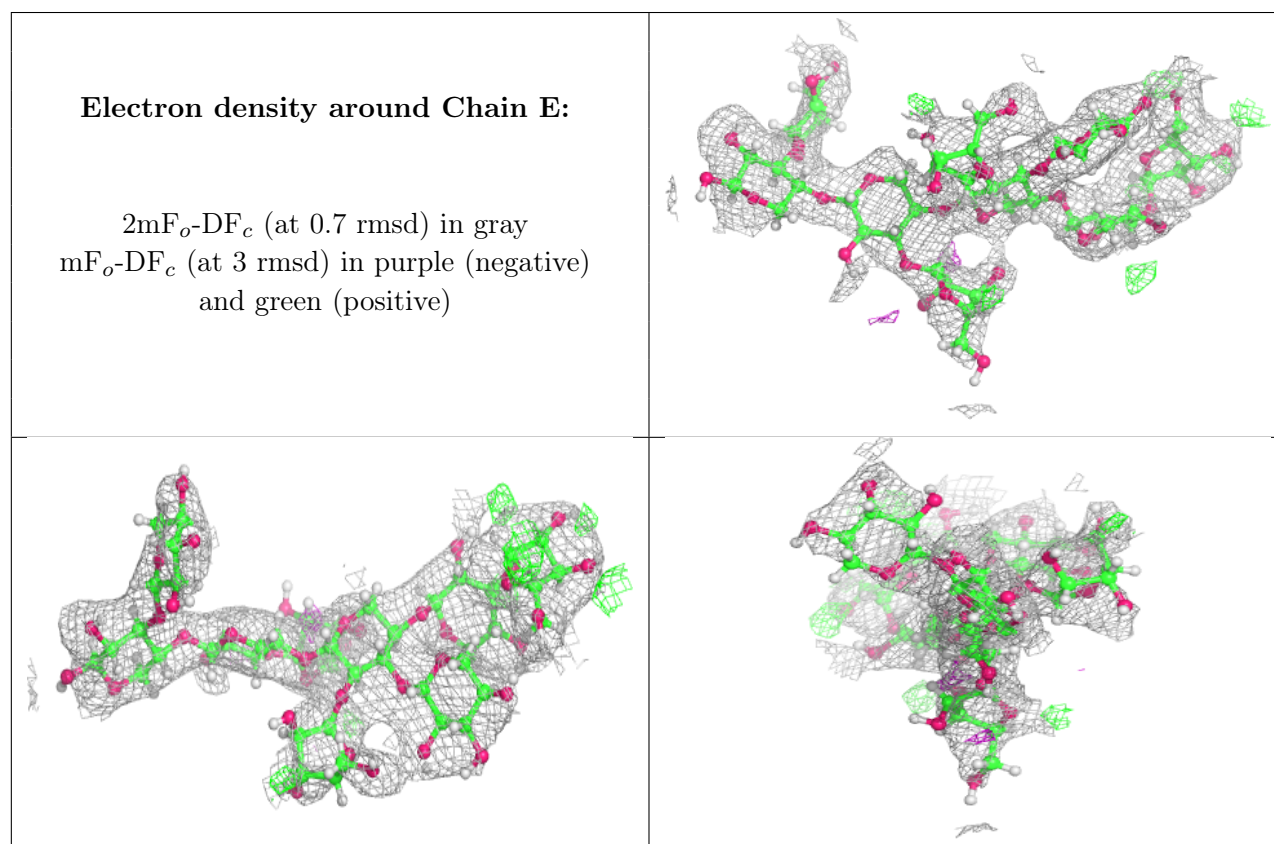
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PHD	B	851	12/13	0.86	0.11	41,47,60,61	0
1	PHD	A	851	12/13	0.92	0.09	28,32,48,49	0

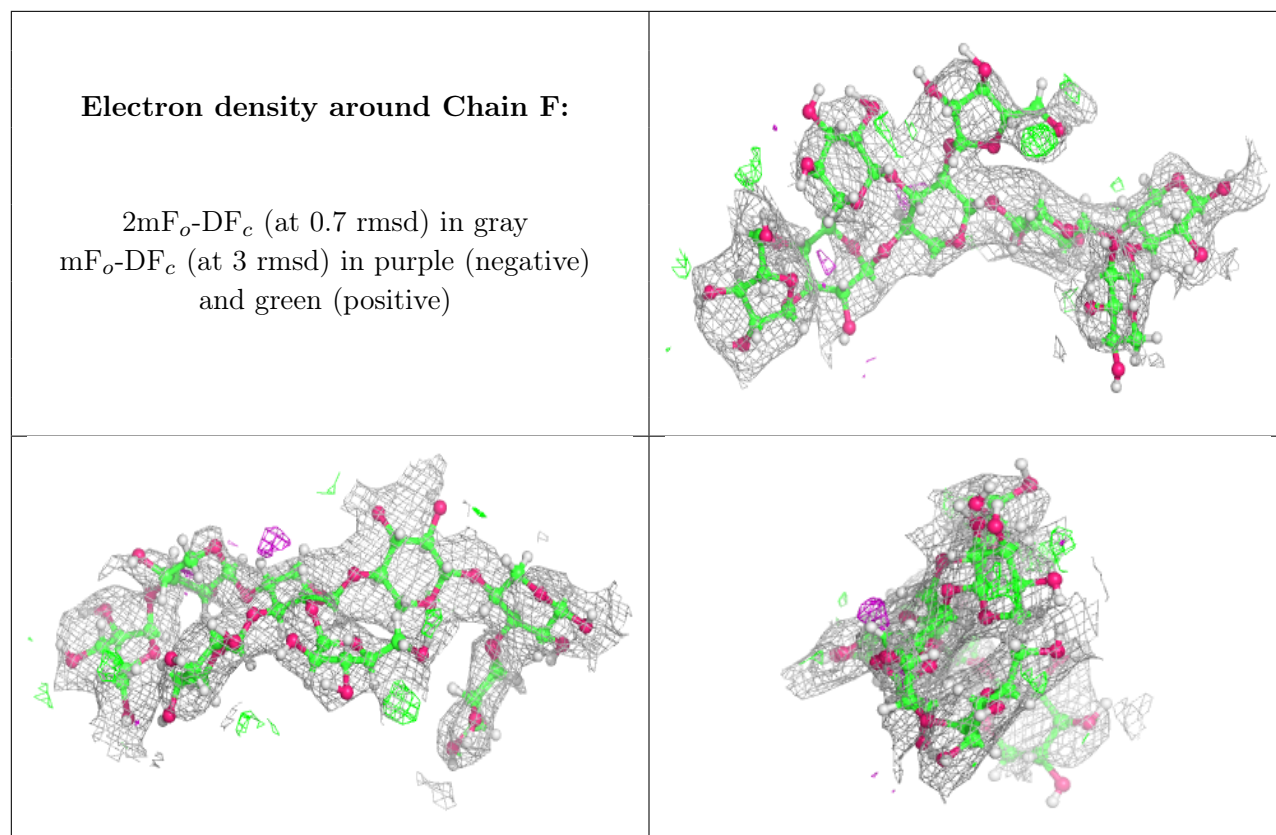
6.3 Carbohydrates [i](#)

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(\AA^2)	Q<0.9
2	XYP	E	1	10/10	-	-	30,73,76,89	2
2	XYP	E	2	9/10	-	-	30,67,80,81	1
2	XYP	E	3	9/10	-	-	60,67,71,92	0
2	XYP	E	4	9/10	-	-	30,66,72,73	2
2	FUB	E	5	9/10	-	-	30,39,44,46	3
2	FUB	E	6	9/10	-	-	30,90,97,98	3
2	XYP	E	7	9/10	-	-	30,70,76,79	3
2	FUB	E	8	9/10	-	-	30,75,87,88	3
2	XYP	E	9	9/10	-	-	30,83,97,103	3
3	XYP	F	1	10/10	-	-	30,92,98,101	2
3	XYP	F	2	9/10	-	-	30,72,80,81	1
3	XYP	F	3	9/10	-	-	75,79,85,94	0
3	XYP	F	4	9/10	-	-	30,89,91,92	2
3	FUB	F	5	9/10	-	-	30,47,62,62	3
3	FUB	F	6	9/10	-	-	30,103,108,119	3
3	XYP	F	7	9/10	-	-	30,67,74,75	3
3	XYP	F	8	9/10	-	-	30,96,101,109	3

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(\AA^2)	Q<0.9
4	CA	B	1001	1/1	0.98	0.03	51,51,51,51	0
4	CA	A	1001	1/1	0.99	0.02	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.