



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:35 PM UTC

PDB ID : 3KL5 / pdb\_00003kl5  
Title : Structure Analysis of a Xylanase From Glycosyl Hydrolase Family Thirty: Carbohydrate Ligand Complexes Reveal this Family of Enzymes Unique Mechanism of Substrate Specificity and Recognition  
Authors : St John, F.J.; Hurlbert, J.C.; Pozharski, E.  
Deposited on : 2009-11-06  
Resolution : 2.59 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](mailto: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>.

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

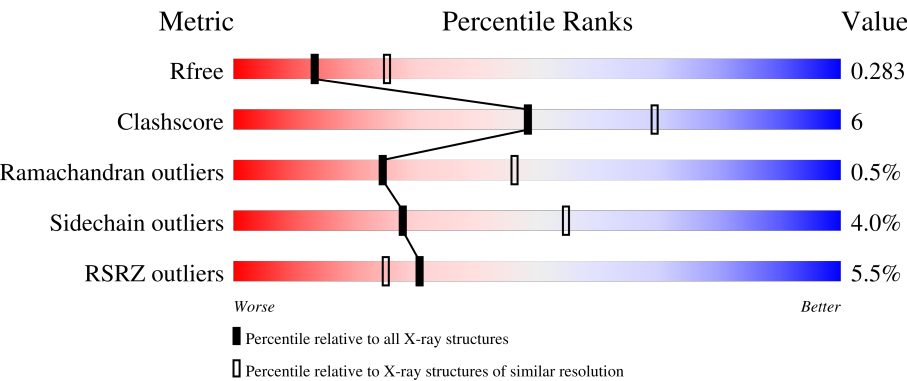
MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.59 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.



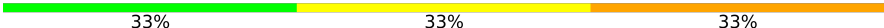
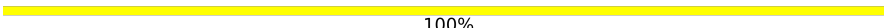
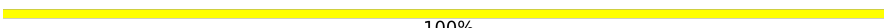
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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  $\geq 3$ , 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	401	<div><div>%</div><div>85%12%.</div></div>
1	B	401	<div><div>2%</div><div>85%12%..</div></div>
1	C	401	<div><div>2%</div><div>83%13%.</div></div>
1	D	401	<div><div>15%</div><div>68%22%.8%</div></div>
2	E	3	<div><div></div><div>100%</div></div>

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Mol	Chain	Length	Quality of chain
2	F	3	 33% 33% 33%
2	G	3	 100%
2	H	3	 100%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12477 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 Glucuronoxylanase xynC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	1	0
			3109	1966	552	582	9			
1	B	390	Total	C	N	O	S	0	3	0
			3136	1984	557	586	9			
1	C	389	Total	C	N	O	S	0	1	0
			3110	1967	552	582	9			
1	D	367	Total	C	N	O	S	0	0	0
			2948	1878	516	545	9			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q45070
A	392	LEU	-	expression tag	UNP Q45070
A	393	GLU	-	expression tag	UNP Q45070
A	394	HIS	-	expression tag	UNP Q45070
A	395	HIS	-	expression tag	UNP Q45070
A	396	HIS	-	expression tag	UNP Q45070
A	397	HIS	-	expression tag	UNP Q45070
A	398	HIS	-	expression tag	UNP Q45070
A	399	HIS	-	expression tag	UNP Q45070
A	400	HIS	-	expression tag	UNP Q45070
A	401	HIS	-	expression tag	UNP Q45070
B	1	MET	-	expression tag	UNP Q45070
B	392	LEU	-	expression tag	UNP Q45070
B	393	GLU	-	expression tag	UNP Q45070
B	394	HIS	-	expression tag	UNP Q45070
B	395	HIS	-	expression tag	UNP Q45070
B	396	HIS	-	expression tag	UNP Q45070
B	397	HIS	-	expression tag	UNP Q45070
B	398	HIS	-	expression tag	UNP Q45070
B	399	HIS	-	expression tag	UNP Q45070
B	400	HIS	-	expression tag	UNP Q45070

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Chain	Residue	Modelled	Actual	Comment	Reference
B	401	HIS	-	expression tag	UNP Q45070
C	1	MET	-	expression tag	UNP Q45070
C	392	LEU	-	expression tag	UNP Q45070
C	393	GLU	-	expression tag	UNP Q45070
C	394	HIS	-	expression tag	UNP Q45070
C	395	HIS	-	expression tag	UNP Q45070
C	396	HIS	-	expression tag	UNP Q45070
C	397	HIS	-	expression tag	UNP Q45070
C	398	HIS	-	expression tag	UNP Q45070
C	399	HIS	-	expression tag	UNP Q45070
C	400	HIS	-	expression tag	UNP Q45070
C	401	HIS	-	expression tag	UNP Q45070
D	1	MET	-	expression tag	UNP Q45070
D	392	LEU	-	expression tag	UNP Q45070
D	393	GLU	-	expression tag	UNP Q45070
D	394	HIS	-	expression tag	UNP Q45070
D	395	HIS	-	expression tag	UNP Q45070
D	396	HIS	-	expression tag	UNP Q45070
D	397	HIS	-	expression tag	UNP Q45070
D	398	HIS	-	expression tag	UNP Q45070
D	399	HIS	-	expression tag	UNP Q45070
D	400	HIS	-	expression tag	UNP Q45070
D	401	HIS	-	expression tag	UNP Q45070

- Molecule 2 is an oligosaccharide called 4-O-methyl-alpha-D-glucopyranuronic acid-(1-2)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	3	Total	C	O	0	0	0
			32	17	15			
2	F	3	Total	C	O	0	0	0
			32	17	15			
2	G	3	Total	C	O	0	0	0
			31	17	14			
2	H	3	Total	C	O	0	0	0
			32	17	15			

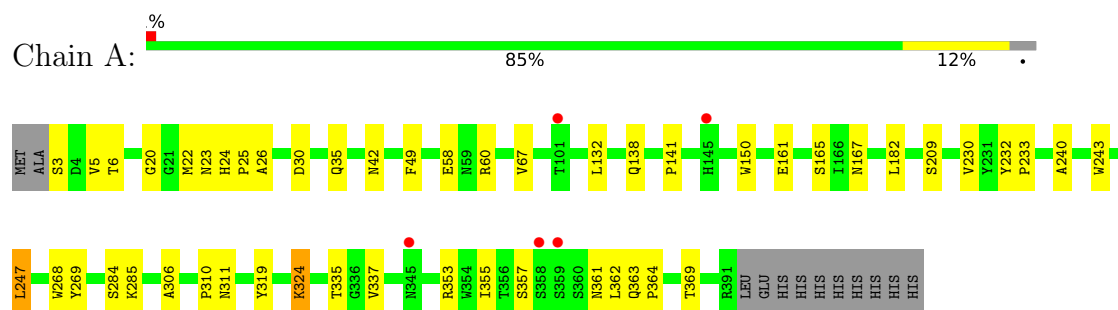
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total 10	O 10	0	0
3	B	17	Total 17	O 17	0	0
3	C	19	Total 19	O 19	0	0
3	D	1	Total 1	O 1	0	0

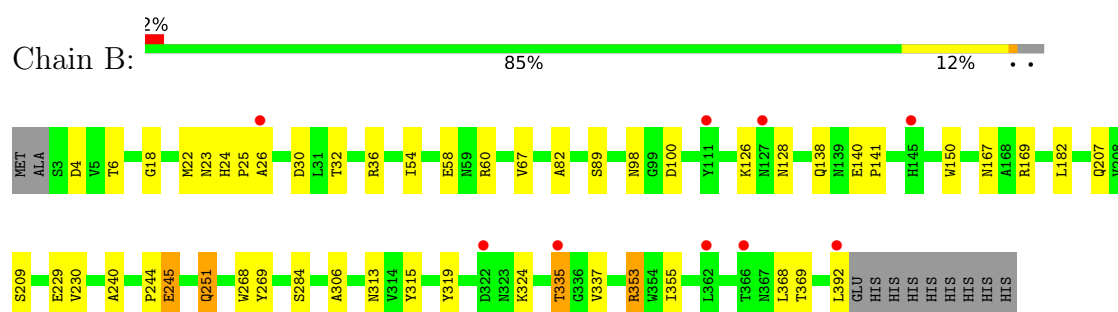
### 3 Residue-property plots [i](#)

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.

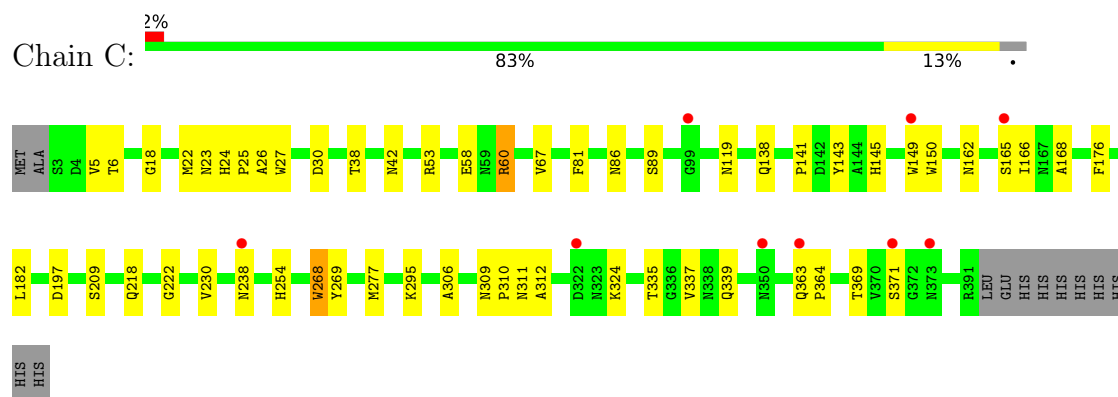
#### • Molecule 1: Glucuronoxylanase xynC



#### • Molecule 1: Glucuronoxylanase xynC

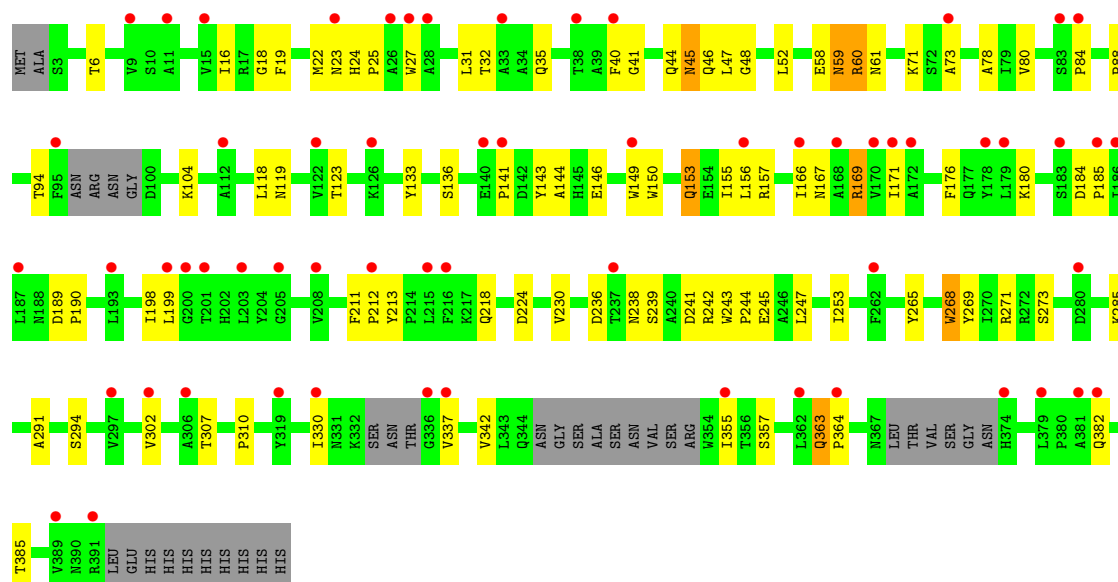


#### • Molecule 1: Glucuronoxylanase xynC



#### • Molecule 1: Glucuronoxylanase xynC





- Molecule 2: 4-O-methyl-alpha-D-glucopyranuronic acid-(1-2)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain E: 100%

XYP1  
XYP2  
GCV3

- Molecule 2: 4-O-methyl-alpha-D-glucopyranuronic acid-(1-2)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain F: 33% 33% 33%

XYP1  
XYP2  
GCV3

- Molecule 2: 4-O-methyl-alpha-D-glucopyranuronic acid-(1-2)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain G: 100%

XYP1  
XYP2  
GCV3

- Molecule 2: 4-O-methyl-alpha-D-glucopyranuronic acid-(1-2)-beta-D-xylopyranose-(1-4)-beta-D-xylopyranose

Chain H: 100%

XYP1  
XYP2  
GCV3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.72Å 194.01Å 65.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.59 50.00 – 2.59	Depositor EDS
% Data completeness (in resolution range)	97.5 (50.00-2.59) 97.9 (50.00-2.59)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.241 , 0.290 0.237 , 0.283	Depositor DCC
$R_{free}$ test set	2778 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.9	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 37.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12477	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GCV, XYP

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	0.68	0/3196	0.83	1/4353 (0.0%)
1	B	0.71	0/3224	0.89	6/4390 (0.1%)
1	C	0.74	5/3197 (0.2%)	0.87	5/4354 (0.1%)
1	D	0.57	0/3031	0.80	1/4123 (0.0%)
All	All	0.68	5/12648 (0.0%)	0.85	13/17220 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	162	ASN	CG-ND2	-6.40	1.19	1.33
1	C	339	GLN	CD-NE2	-6.05	1.20	1.33
1	C	86	ASN	CG-ND2	-5.99	1.20	1.33
1	C	162	ASN	CG-OD1	-5.96	1.12	1.23
1	C	339	GLN	CD-OE1	-5.26	1.13	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	60	ARG	NE-CZ-NH2	8.38	126.75	119.20
1	B	169	ARG	NE-CZ-NH1	-8.29	113.21	121.50
1	B	169	ARG	NE-CZ-NH2	7.93	126.34	119.20
1	C	60	ARG	NE-CZ-NH1	-7.57	113.93	121.50
1	B	169	ARG	CD-NE-CZ	5.99	132.79	124.40
1	A	67	VAL	N-CA-C	5.90	116.07	110.53
1	C	67	VAL	N-CA-C	5.80	115.98	110.53
1	D	18	GLY	N-CA-C	5.79	118.74	110.46
1	B	18	GLY	N-CA-C	5.77	118.22	110.43
1	B	67	VAL	N-CA-C	5.75	115.94	110.53
1	C	18	GLY	N-CA-C	5.54	118.38	110.46
1	C	60	ARG	CD-NE-CZ	5.39	131.94	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	ASN	CB-CA-C	-5.34	104.60	111.22

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	3109	0	2963	26	0
1	B	3136	0	2993	29	0
1	C	3110	0	2965	35	0
1	D	2948	0	2810	58	0
2	E	32	0	9	0	0
2	F	32	0	9	2	0
2	G	31	0	9	0	0
2	H	32	0	9	0	0
3	A	10	0	0	2	0
3	B	17	0	0	0	0
3	C	19	0	0	4	0
3	D	1	0	0	0	0
All	All	12477	0	11767	133	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 6.

All (133) 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:C:254:HIS:HD2	3:C:411:HOH:O	1.57	0.87
1:B:244[B]:PRO:O	1:B:245[B]:GLU:HB2	1.76	0.82
1:B:244[B]:PRO:O	1:B:245[B]:GLU:CB	2.30	0.76
1:D:144:ALA:HB3	1:D:149:TRP:HD1	1.53	0.74
1:B:315:TYR:OH	1:C:222:GLY:HA2	1.86	0.74
1:C:238:ASN:OD1	1:D:27:TRP:HA	1.92	0.69
1:B:353[A]:ARG:HD2	1:B:355:ILE:HD11	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:PRO:HB3	1:D:150:TRP:HB2	1.76	0.68
1:C:145:HIS:ND1	1:C:149:TRP:HZ2	1.93	0.67
1:D:144:ALA:HB3	1:D:149:TRP:CD1	2.30	0.67
1:B:353[A]:ARG:HH21	1:B:368:LEU:HD21	1.60	0.66
1:D:24:HIS:CG	1:D:27:TRP:HB2	2.31	0.65
1:D:24:HIS:CE1	1:D:27:TRP:CD1	2.85	0.65
1:D:156:LEU:HD13	1:D:185:PRO:O	1.97	0.65
1:D:59:ASN:HB2	1:D:88:PRO:HB3	1.79	0.65
1:A:141:PRO:HG2	1:A:182:LEU:HD21	1.80	0.61
1:D:23:ASN:HB3	1:D:52:LEU:HD11	1.83	0.60
1:A:42:ASN:ND2	1:B:98:ASN:OD1	2.34	0.60
1:D:144:ALA:C	1:D:146:GLU:H	2.09	0.60
1:D:243:TRP:CE2	1:D:247:LEU:HD11	2.38	0.59
1:A:324:LYS:HE3	1:B:100:ASP:HB2	1.84	0.58
1:D:239:SER:HB3	1:D:242:ARG:HH11	1.69	0.58
1:C:145:HIS:ND1	1:C:149:TRP:CZ2	2.72	0.58
1:C:25:PRO:HB3	1:C:30:ASP:HB2	1.87	0.57
1:B:25:PRO:HB3	1:B:30:ASP:HB2	1.87	0.57
1:A:25:PRO:HB3	1:A:30:ASP:HB2	1.87	0.56
1:A:353:ARG:HD2	1:A:355:ILE:HD11	1.86	0.56
1:B:141:PRO:HG2	1:B:182:LEU:HD21	1.87	0.56
1:D:198:ILE:HG12	1:D:224:ASP:HB2	1.86	0.56
1:C:141:PRO:HG2	1:C:182:LEU:HD21	1.86	0.56
1:D:241:ASP:HA	1:D:285:LYS:HB2	1.86	0.56
1:D:143:TYR:HB2	1:D:176:PHE:CD2	2.41	0.56
1:D:268:TRP:CG	1:D:269:TYR:H	2.25	0.55
1:C:218:GLN:HG3	3:C:417:HOH:O	2.07	0.54
1:A:167[B]:ASN:O	1:A:167[B]:ASN:CG	2.51	0.54
1:D:355:ILE:HG12	1:D:385:THR:HG23	1.90	0.53
1:C:6:THR:O	1:C:306:ALA:HA	2.10	0.52
1:C:254:HIS:CD2	3:C:411:HOH:O	2.43	0.52
1:C:268:TRP:CG	1:C:269:TYR:H	2.27	0.52
1:D:44:GLN:O	1:D:45:ASN:CB	2.58	0.52
1:A:285:LYS:NZ	1:A:357:SER:O	2.42	0.52
1:C:238:ASN:OD1	1:D:27:TRP:CG	2.64	0.51
1:D:244:PRO:HB3	1:D:382:GLN:CG	2.41	0.51
1:B:353[A]:ARG:O	1:B:353[A]:ARG:HG3	2.09	0.51
1:C:238:ASN:CG	1:D:27:TRP:CD1	2.88	0.51
1:C:310:PRO:O	1:C:311:ASN:ND2	2.41	0.51
1:D:236:ASP:HB2	1:D:239:SER:HB3	1.92	0.50
1:D:180:LYS:HD2	1:D:213:TYR:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:TYR:CZ	1:C:222:GLY:HA2	2.46	0.50
1:A:138:GLN:HG2	1:A:150:TRP:CD1	2.47	0.50
1:D:40:PHE:HZ	1:D:52:LEU:HD13	1.77	0.50
1:C:5:VAL:HG22	1:C:310:PRO:HG3	1.94	0.49
1:D:31:LEU:HA	1:D:271:ARG:HH22	1.77	0.49
1:D:94:THR:HG22	1:D:104:LYS:HG2	1.94	0.49
1:A:268:TRP:CG	1:A:269:TYR:H	2.30	0.49
1:B:335:THR:HB	1:C:168:ALA:HA	1.94	0.49
1:D:144:ALA:C	1:D:146:GLU:N	2.70	0.49
1:D:244:PRO:HB3	1:D:382:GLN:HG3	1.93	0.49
1:B:138:GLN:HG2	1:B:150:TRP:CD1	2.47	0.49
1:B:140:GLU:OE2	2:F:1:XYP:O1	2.31	0.49
1:D:291:ALA:HA	1:D:294:SER:HB3	1.94	0.49
1:D:238:ASN:H	1:D:273:SER:HB2	1.78	0.49
1:D:153:GLN:HE21	1:D:153:GLN:H	1.60	0.48
1:A:165:SER:HA	1:C:309:ASN:O	2.12	0.48
1:D:32:THR:OG1	1:D:35:GLN:HB2	2.14	0.48
1:D:84:PRO:HG3	1:D:118:LEU:HD21	1.96	0.48
1:A:243:TRP:CH2	1:A:247:LEU:HD13	2.49	0.47
1:A:161:GLU:O	1:C:312:ALA:HA	2.14	0.47
1:D:184:ASP:N	1:D:185:PRO:CD	2.77	0.47
1:B:22:MET:HG3	1:B:23:ASN:N	2.28	0.47
1:A:3:SER:N	1:A:311:ASN:HD21	2.13	0.47
1:C:119:ASN:ND2	1:C:166:ILE:HA	2.30	0.47
1:A:268:TRP:O	1:A:269:TYR:C	2.57	0.47
1:D:60:ARG:N	1:D:60:ARG:HD2	2.30	0.47
1:B:207:GLN:HG2	1:C:218:GLN:HA	1.96	0.46
1:C:138:GLN:HG2	1:C:150:TRP:CD1	2.51	0.46
1:C:119:ASN:ND2	1:C:165:SER:O	2.43	0.46
1:B:24:HIS:CE1	1:B:26:ALA:HB3	2.50	0.46
1:A:35:GLN:HA	3:A:405:HOH:O	2.15	0.46
1:B:54:ILE:O	1:B:82:ALA:HA	2.16	0.46
1:B:268:TRP:CG	1:B:269:TYR:H	2.34	0.46
1:D:22:MET:HE3	1:D:24:HIS:CD2	2.51	0.46
1:D:119:ASN:HD21	1:D:166:ILE:HA	1.81	0.46
1:B:6:THR:O	1:B:306:ALA:HA	2.15	0.46
1:B:32:THR:O	1:B:36:ARG:HG3	2.16	0.46
1:C:42:ASN:OD1	1:C:295:LYS:HG2	2.16	0.46
1:D:239:SER:CB	1:D:242:ARG:HH11	2.29	0.46
1:C:5:VAL:CG2	1:C:310:PRO:HG3	2.46	0.45
1:D:19:PHE:CD1	1:D:265:TYR:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:TRP:CZ2	1:D:357:SER:HA	2.52	0.45
1:C:238:ASN:OD1	1:D:27:TRP:CD1	2.70	0.45
1:B:251:GLN:OE1	1:C:222:GLY:HA3	2.17	0.44
1:D:253:ILE:HG12	1:D:265:TYR:CE2	2.53	0.44
1:A:165:SER:HB3	3:A:409:HOH:O	2.17	0.44
1:B:268:TRP:O	1:B:269:TYR:C	2.60	0.44
1:D:363:GLN:HA	1:D:364:PRO:HD3	1.88	0.44
1:C:24:HIS:CE1	1:C:26:ALA:HB3	2.52	0.44
1:D:133:TYR:O	1:D:169:ARG:HD3	2.17	0.44
1:C:38:THR:HB	1:C:277:MET:HE2	1.99	0.44
1:D:41:GLY:O	1:D:48:GLY:N	2.51	0.44
1:C:27:TRP:CD1	1:D:238:ASN:HB2	2.53	0.44
1:D:31:LEU:HA	1:D:271:ARG:NH2	2.33	0.43
1:A:24:HIS:CE1	1:A:26:ALA:HB3	2.53	0.43
1:A:6:THR:O	1:A:306:ALA:HA	2.18	0.43
1:A:22:MET:HG3	1:A:23:ASN:N	2.33	0.43
1:C:53:ARG:HD2	1:C:81:PHE:CZ	2.53	0.43
1:D:141:PRO:CB	1:D:150:TRP:HB2	2.47	0.43
1:A:5:VAL:HG22	1:A:310:PRO:HG3	2.01	0.43
1:A:20:GLY:HA2	1:A:49:PHE:CG	2.54	0.43
1:D:24:HIS:HA	1:D:25:PRO:HD3	1.86	0.43
1:D:47:LEU:HD23	1:D:291:ALA:HB2	1.99	0.43
1:A:232:TYR:CG	1:A:233:PRO:HA	2.54	0.42
1:A:361:ASN:O	1:A:362:LEU:C	2.63	0.42
1:C:22:MET:HG3	1:C:23:ASN:N	2.33	0.42
1:D:61:ASN:H	1:D:61:ASN:HD22	1.67	0.42
1:C:143:TYR:HB2	1:C:176:PHE:CD2	2.55	0.42
1:B:313:ASN:OD1	1:C:197:ASP:HB3	2.19	0.41
1:D:189:ASP:HA	1:D:190:PRO:HD3	1.81	0.41
1:D:243:TRP:CZ2	1:D:247:LEU:HD11	2.54	0.41
1:B:335:THR:HG21	3:C:422:HOH:O	2.20	0.41
1:A:363:GLN:HA	1:A:364:PRO:HD3	1.97	0.41
1:B:229:GLU:OE2	2:F:1:XYP:C1	2.68	0.41
1:B:240:ALA:HB1	1:B:284:SER:HB2	2.02	0.41
1:B:319:TYR:CD2	1:B:319:TYR:N	2.89	0.41
1:D:211:PHE:N	1:D:212:PRO:HD2	2.34	0.41
1:A:319:TYR:CD2	1:A:319:TYR:N	2.88	0.41
1:D:73:ALA:O	1:D:78:ALA:HB3	2.21	0.41
1:D:136:SER:HA	1:D:171:ILE:HB	2.03	0.41
1:A:240:ALA:HB1	1:A:284:SER:HB2	2.04	0.40
1:C:363:GLN:HA	1:C:364:PRO:HD3	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:THR:HA	1:D:342:VAL:HG22	2.03	0.40
1:B:126:LYS:C	1:B:128:ASN:H	2.30	0.40
1:D:84:PRO:HD2	1:D:136:SER:HB3	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	388/401 (97%)	373 (96%)	15 (4%)	0	100	100
1	B	391/401 (98%)	373 (95%)	15 (4%)	3 (1%)	16	34
1	C	388/401 (97%)	373 (96%)	14 (4%)	1 (0%)	36	58
1	D	357/401 (89%)	316 (88%)	36 (10%)	5 (1%)	9	19
All	All	1524/1604 (95%)	1435 (94%)	80 (5%)	9 (1%)	24	42

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	268	TRP
1	B	245[A]	GLU
1	B	245[B]	GLU
1	B	4	ASP
1	D	58	GLU
1	D	59	ASN
1	D	310	PRO
1	C	268	TRP
1	D	45	ASN

### 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	331/341 (97%)	321 (97%)	10 (3%)	36	64
1	B	334/341 (98%)	321 (96%)	13 (4%)	28	55
1	C	331/341 (97%)	321 (97%)	10 (3%)	36	64
1	D	312/341 (92%)	292 (94%)	20 (6%)	16	35
All	All	1308/1364 (96%)	1255 (96%)	53 (4%)	28	54

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
1	A	60	ARG
1	A	132	LEU
1	A	209	SER
1	A	230	VAL
1	A	247	LEU
1	A	324	LYS
1	A	335	THR
1	A	337	VAL
1	A	369	THR
1	B	58	GLU
1	B	60	ARG
1	B	89	SER
1	B	209	SER
1	B	230	VAL
1	B	251	GLN
1	B	324	LYS
1	B	335	THR
1	B	337	VAL
1	B	353[A]	ARG
1	B	353[B]	ARG
1	B	369	THR
1	B	392	LEU
1	C	58	GLU

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Mol	Chain	Res	Type
1	C	60	ARG
1	C	89	SER
1	C	209	SER
1	C	230	VAL
1	C	324	LYS
1	C	335	THR
1	C	337	VAL
1	C	369	THR
1	C	371	SER
1	D	16	ILE
1	D	46	GLN
1	D	60	ARG
1	D	71	LYS
1	D	80	VAL
1	D	123	THR
1	D	153	GLN
1	D	155	ILE
1	D	157	ARG
1	D	167	ASN
1	D	169	ARG
1	D	199	LEU
1	D	218	GLN
1	D	230	VAL
1	D	245	GLU
1	D	302	VAL
1	D	307	THR
1	D	330	ILE
1	D	337	VAL
1	D	363	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	131	ASN
1	A	210	GLN
1	A	311	ASN
1	A	313	ASN
1	A	338	ASN
1	A	339	GLN
1	A	373	ASN
1	A	378	HIS

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Mol	Chain	Res	Type
1	B	131	ASN
1	C	59	ASN
1	C	131	ASN
1	C	153	GLN
1	C	162	ASN
1	C	210	GLN
1	C	313	ASN
1	C	340	ASN
1	C	363	GLN
1	D	8	ASN
1	D	23	ASN
1	D	24	HIS
1	D	61	ASN
1	D	76	HIS
1	D	86	ASN
1	D	116	GLN
1	D	119	ASN
1	D	128	ASN
1	D	145	HIS
1	D	153	GLN
1	D	340	ASN
1	D	363	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 ⓘ

12 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	0.96	1 (10%)	14,14,14	0.86	0
2	XYP	E	2	2	9,9,10	1.79	3 (33%)	10,12,14	1.89	3 (30%)
2	GCV	E	3	2	13,13,14	1.51	2 (15%)	14,18,20	1.01	0
2	XYP	F	1	2	10,10,10	1.09	1 (10%)	14,14,14	1.52	2 (14%)
2	XYP	F	2	2	9,9,10	0.87	0	10,12,14	1.45	1 (10%)
2	GCV	F	3	2	13,13,14	0.85	0	14,18,20	0.77	0
2	XYP	G	1	2	9,9,10	1.45	1 (11%)	10,12,14	1.67	2 (20%)
2	XYP	G	2	2	9,9,10	1.94	3 (33%)	10,12,14	1.91	2 (20%)
2	GCV	G	3	2	13,13,14	1.73	3 (23%)	14,18,20	1.36	2 (14%)
2	XYP	H	1	2	10,10,10	2.07	5 (50%)	14,14,14	1.51	2 (14%)
2	XYP	H	2	2	9,9,10	1.91	4 (44%)	10,12,14	2.64	2 (20%)
2	GCV	H	3	2	13,13,14	1.58	2 (15%)	14,18,20	1.70	3 (21%)

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	GCV	E	3	2	-	1/6/23/26	0/1/1/1
2	XYP	F	1	2	-	-	0/1/1/1
2	XYP	F	2	2	-	-	0/1/1/1
2	GCV	F	3	2	-	0/6/23/26	0/1/1/1
2	XYP	G	1	2	-	-	0/1/1/1
2	XYP	G	2	2	-	-	0/1/1/1
2	GCV	G	3	2	-	0/6/23/26	0/1/1/1
2	XYP	H	1	2	-	-	0/1/1/1
2	XYP	H	2	2	-	-	0/1/1/1
2	GCV	H	3	2	-	0/6/23/26	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	2	XYP	O5-C1	3.91	1.50	1.43
2	G	3	GCV	C4-C5	3.82	1.59	1.52
2	H	3	GCV	O5-C1	3.37	1.49	1.43
2	H	1	XYP	O4-C4	3.24	1.50	1.43
2	H	2	XYP	O5-C1	3.13	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	XYP	C4-C3	3.11	1.57	1.52
2	E	2	XYP	C2-C3	2.95	1.57	1.52
2	E	3	GCV	O5-C5	2.72	1.48	1.43
2	E	2	XYP	O5-C1	2.59	1.47	1.43
2	H	1	XYP	O5-C5	2.54	1.48	1.43
2	H	3	GCV	O5-C5	2.53	1.48	1.43
2	G	2	XYP	O5-C5	2.50	1.47	1.43
2	F	1	XYP	C4-C3	2.49	1.56	1.52
2	H	2	XYP	C1-C2	2.46	1.58	1.52
2	G	1	XYP	O5-C5	2.44	1.47	1.43
2	G	2	XYP	C1-C2	2.42	1.58	1.52
2	G	3	GCV	O5-C5	2.42	1.48	1.43
2	G	3	GCV	C2-C3	2.42	1.56	1.52
2	H	1	XYP	C5-C4	2.41	1.58	1.52
2	H	1	XYP	O5-C1	2.41	1.47	1.43
2	E	2	XYP	O5-C5	2.23	1.47	1.43
2	H	2	XYP	O2-C2	2.22	1.48	1.43
2	E	3	GCV	C2-C3	2.20	1.55	1.52
2	E	1	XYP	C4-C3	2.05	1.55	1.52
2	H	2	XYP	O5-C5	2.00	1.46	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2	XYP	C1-C2-C3	-5.92	101.02	109.64
2	H	2	XYP	O2-C2-C1	4.91	120.45	109.22
2	G	1	XYP	C5-C4-C3	-4.22	103.50	109.64
2	F	2	XYP	C1-C2-C3	4.01	115.48	109.64
2	G	2	XYP	C5-O5-C1	3.98	117.85	111.42
2	E	2	XYP	C1-C2-C3	3.87	115.28	109.64
2	H	3	GCV	O5-C1-C2	3.77	119.77	110.79
2	G	2	XYP	C1-C2-C3	3.66	114.98	109.64
2	H	1	XYP	O4-C4-C3	3.43	117.25	110.15
2	F	1	XYP	O4-C4-C5	-3.39	101.46	109.22
2	G	3	GCV	O4-C4-C3	-3.29	102.87	110.39
2	H	3	GCV	C1-C2-C3	3.27	114.41	109.64
2	H	1	XYP	O5-C5-C4	3.25	118.54	110.79
2	E	2	XYP	O2-C2-C3	3.12	116.62	110.15
2	H	3	GCV	C4-C5-C6	-2.93	108.11	112.15
2	F	1	XYP	O1-C1-O5	2.28	115.77	109.91
2	G	1	XYP	C5-O5-C1	2.28	115.09	111.42
2	G	3	GCV	C4-C5-C6	2.22	115.22	112.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	XYP	C5-O5-C1	2.16	114.91	111.42

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	3	GCV	O5-C5-C6-O6B

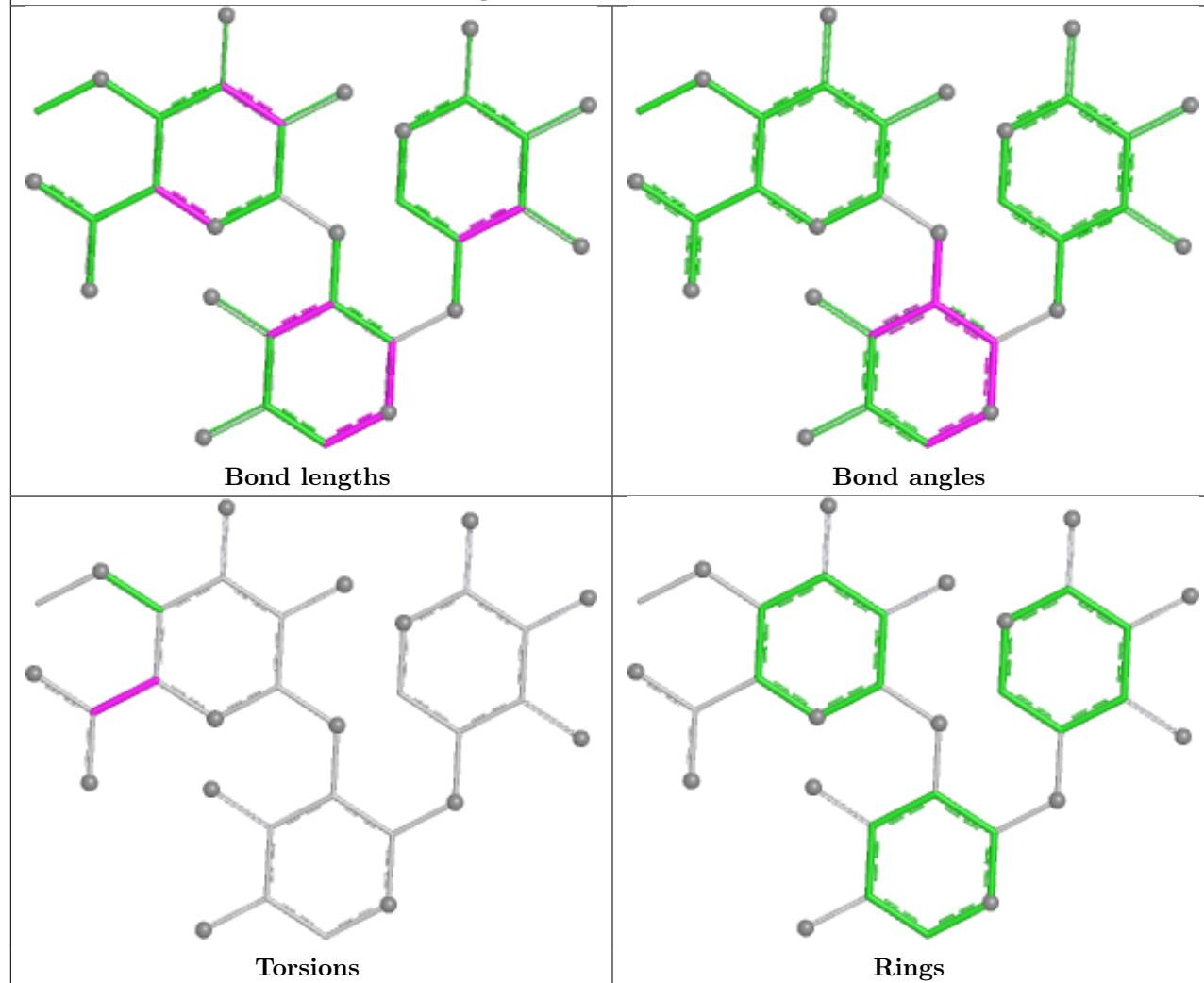
There are no ring outliers.

1 monomer is involved in 2 short contacts:

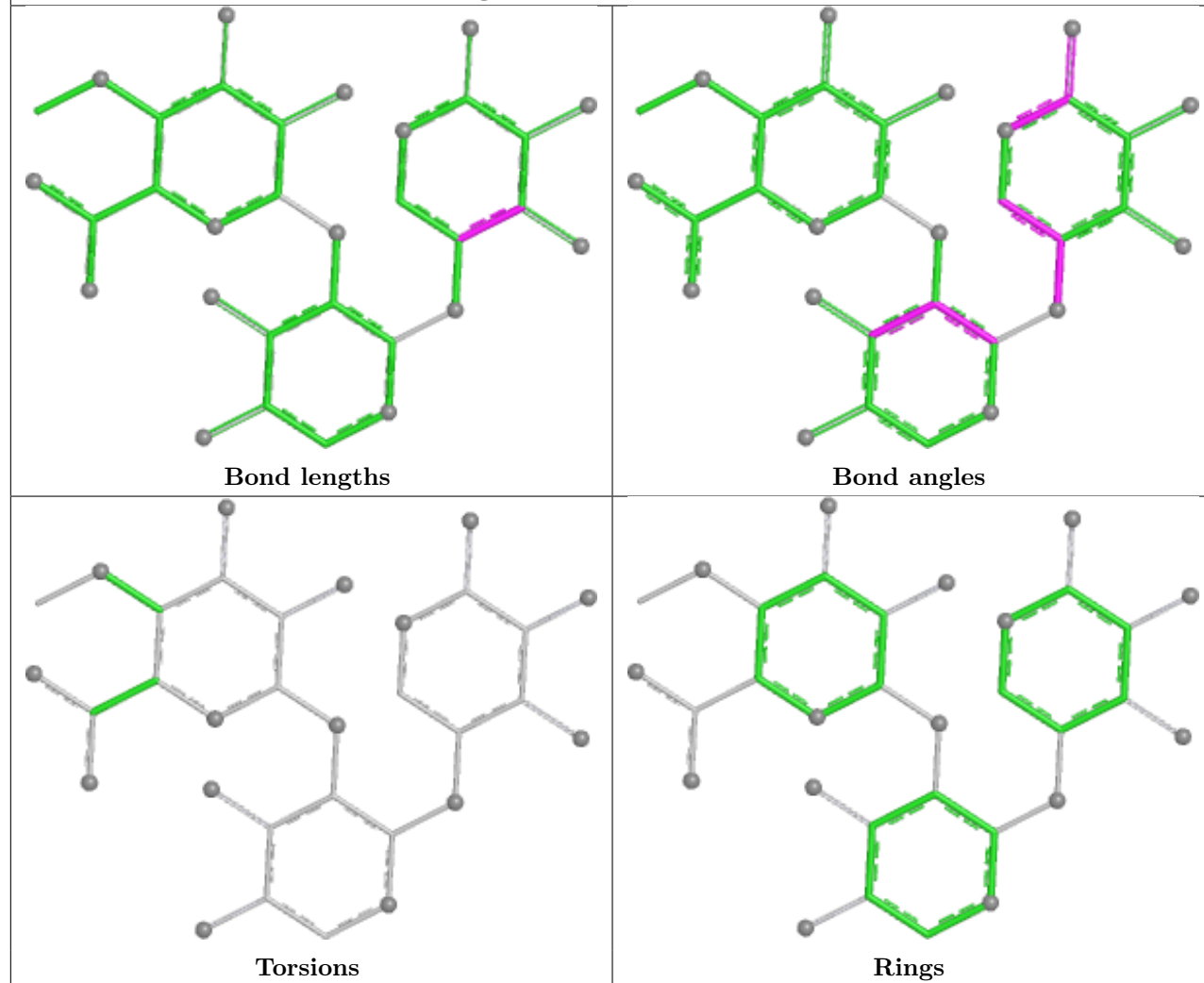
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	XYP	2	0

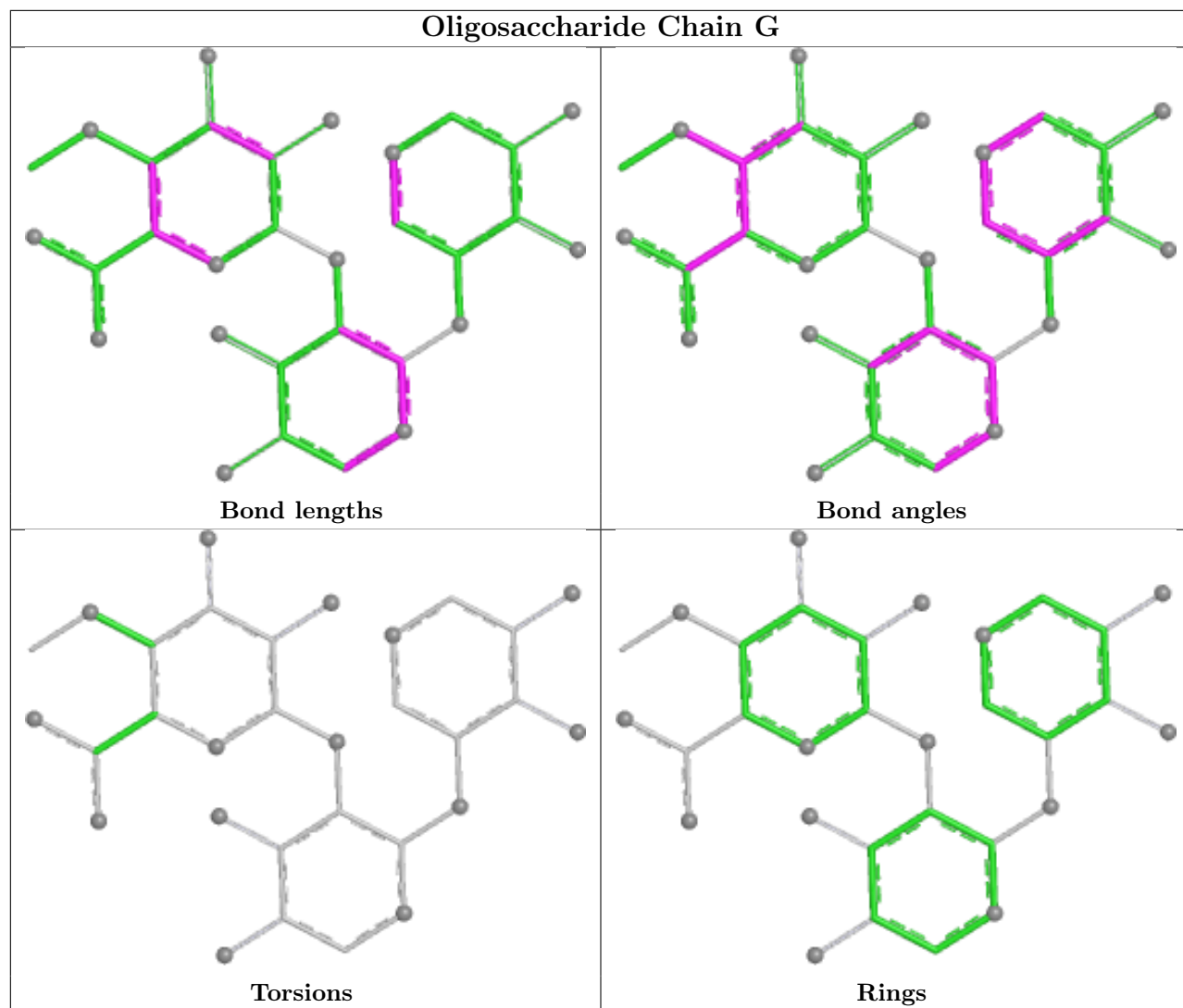
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

## Oligosaccharide Chain E

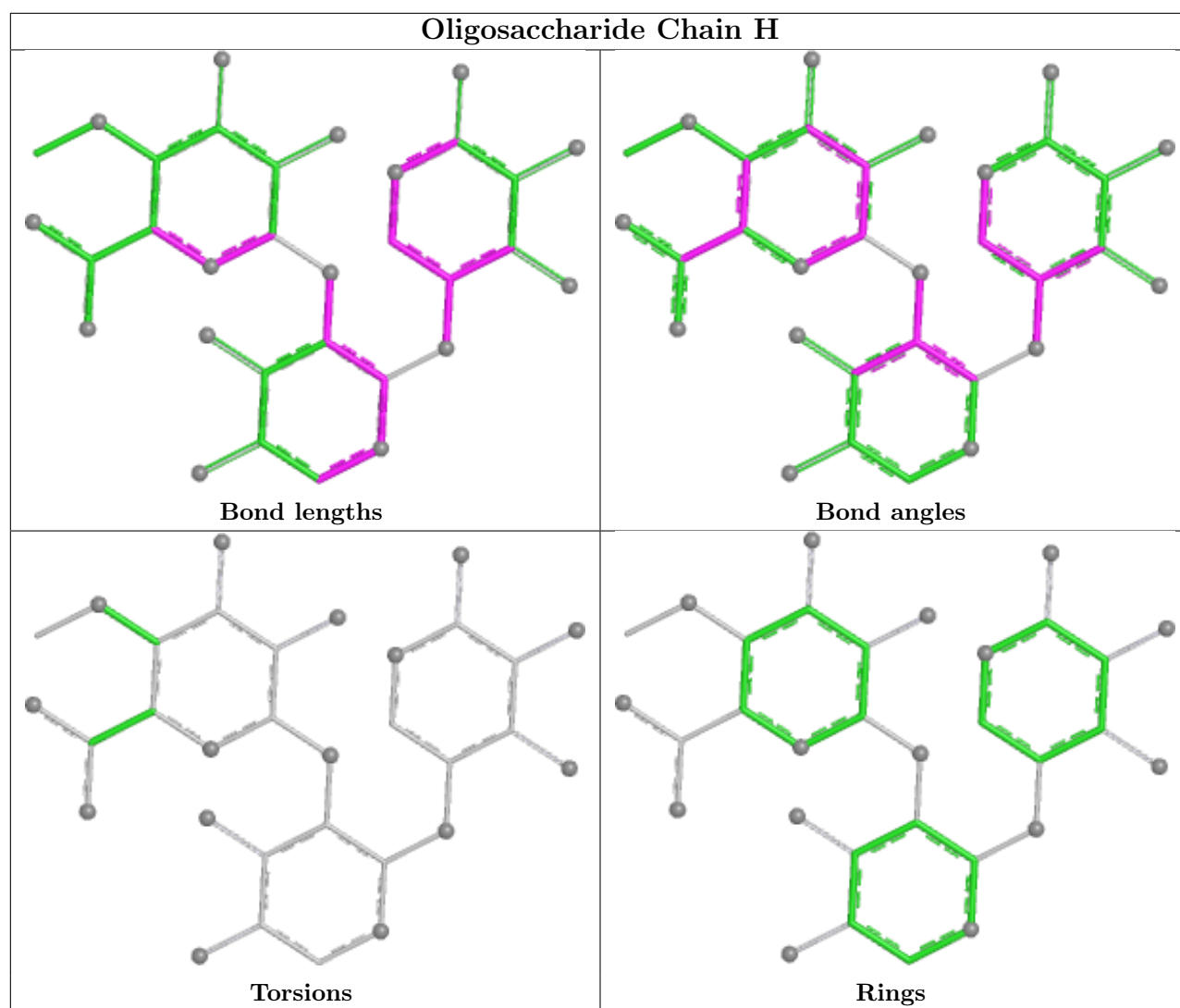


## Oligosaccharide Chain F









## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	389/401 (97%)	0.26	5 (1%) 75 71	28, 58, 72, 80	1 (0%)
1	B	390/401 (97%)	0.42	9 (2%) 61 55	27, 58, 73, 79	4 (1%)
1	C	389/401 (97%)	0.44	9 (2%) 61 55	27, 58, 72, 79	1 (0%)
1	D	367/401 (91%)	1.27	61 (16%) 4 3	60, 96, 124, 164	364 (99%)
All	All	1535/1604 (95%)	0.59	84 (5%) 30 25	27, 62, 112, 164	370 (24%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	337	VAL	3.8
1	D	156	LEU	3.4
1	D	336	GLY	3.2
1	C	322	ASP	3.2
1	D	28	ALA	3.2
1	B	392	LEU	3.0
1	D	200	GLY	3.0
1	D	237	THR	2.9
1	D	171	ILE	2.9
1	A	358	SER	2.8
1	B	335	THR	2.8
1	D	306	ALA	2.8
1	C	371	SER	2.8
1	D	9	VAL	2.8
1	D	149	TRP	2.7
1	D	26	ALA	2.7
1	D	355	ILE	2.6
1	D	203	LEU	2.6
1	D	208	VAL	2.6
1	D	178	TYR	2.6
1	D	319	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	126	LYS	2.6
1	D	95	PHE	2.6
1	C	238	ASN	2.6
1	B	145	HIS	2.6
1	D	389	VAL	2.6
1	D	187	LEU	2.6
1	D	374	HIS	2.6
1	D	179	LEU	2.5
1	D	381	ALA	2.5
1	D	382	GLN	2.5
1	D	27	TRP	2.5
1	D	391	ARG	2.5
1	D	73	ALA	2.5
1	D	141	PRO	2.4
1	D	280	ASP	2.4
1	A	345	ASN	2.4
1	D	302	VAL	2.4
1	D	168	ALA	2.4
1	D	215	LEU	2.4
1	D	262	PHE	2.4
1	B	127	ASN	2.4
1	D	364	PRO	2.4
1	D	185	PRO	2.4
1	D	186	ILE	2.4
1	D	172	ALA	2.4
1	C	99	GLY	2.3
1	D	140	GLU	2.3
1	D	201	THR	2.3
1	D	40	PHE	2.3
1	D	33	ALA	2.3
1	B	366	THR	2.3
1	D	183	SER	2.2
1	D	122	VAL	2.2
1	A	359	SER	2.2
1	D	297	VAL	2.2
1	D	205	GLY	2.2
1	D	83	SER	2.2
1	A	145	HIS	2.2
1	B	362	LEU	2.2
1	D	362	LEU	2.2
1	C	165	SER	2.2
1	A	101	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	166	ILE	2.1
1	D	330	ILE	2.1
1	D	84	PRO	2.1
1	D	112	ALA	2.1
1	D	38	THR	2.1
1	B	322	ASP	2.1
1	D	15	VAL	2.1
1	B	26	ALA	2.1
1	D	23	ASN	2.1
1	D	193	LEU	2.1
1	D	379	LEU	2.1
1	D	216	PHE	2.1
1	D	199	LEU	2.1
1	B	111	TYR	2.1
1	D	212	PRO	2.1
1	D	170	VAL	2.0
1	C	373	ASN	2.0
1	C	149	TRP	2.0
1	C	363	GLN	2.0
1	D	11	ALA	2.0
1	C	350	ASN	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<sup>th</sup> 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.

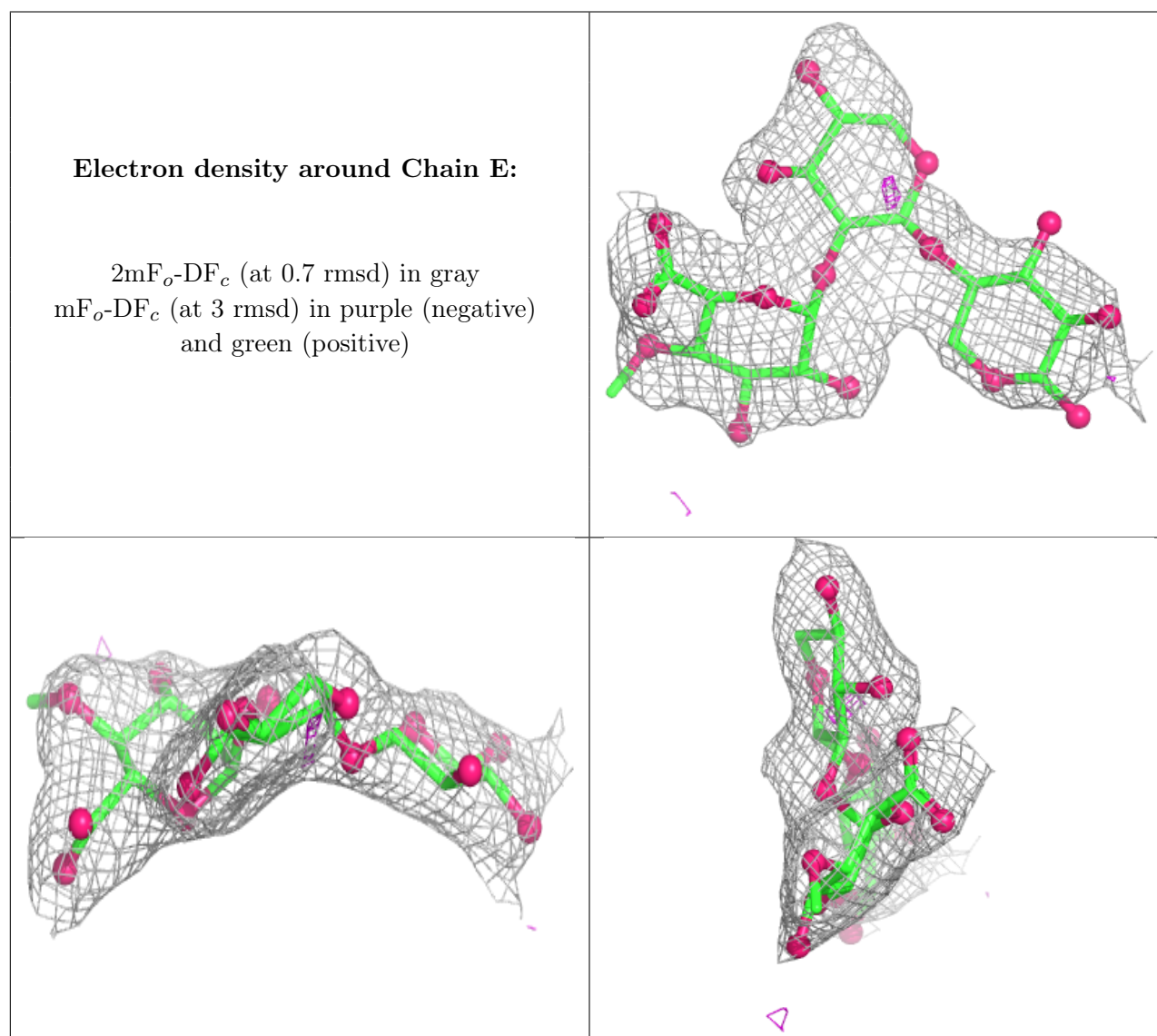
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	XYP	E	2	9/10	0.66	0.15	92,93,94,95	0
2	XYP	G	2	9/10	0.66	0.13	88,90,91,91	0
2	XYP	H	1	10/10	0.74	0.22	118,118,118,119	0
2	XYP	H	2	9/10	0.74	0.26	115,116,117,117	0
2	GCV	G	3	13/14	0.79	0.11	86,88,89,90	0
2	GCV	H	3	13/14	0.82	0.13	112,114,115,115	0
2	XYP	F	1	10/10	0.83	0.13	80,82,83,83	0

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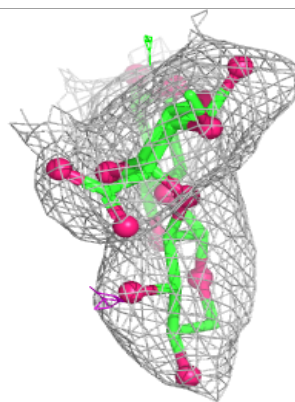
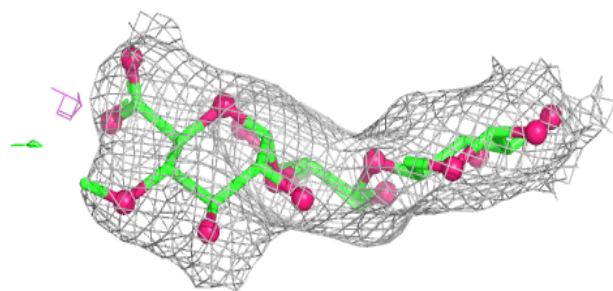
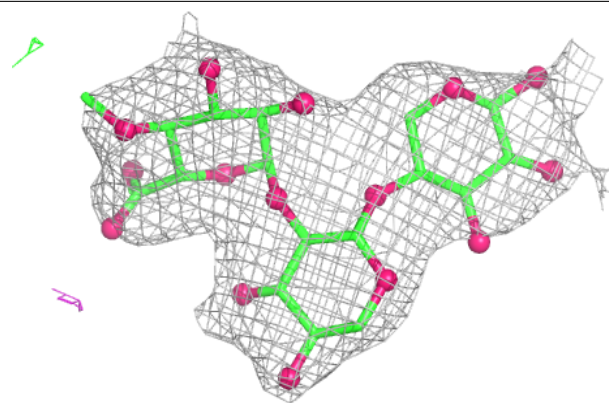
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	XYP	G	1	9/10	0.84	0.08	91,92,92,93	0
2	GCV	E	3	13/14	0.86	0.10	91,94,95,95	0
2	XYP	E	1	10/10	0.89	0.12	92,94,94,95	0
2	GCV	F	3	13/14	0.89	0.09	73,76,78,79	0
2	XYP	F	2	9/10	0.92	0.07	76,77,78,78	0

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.



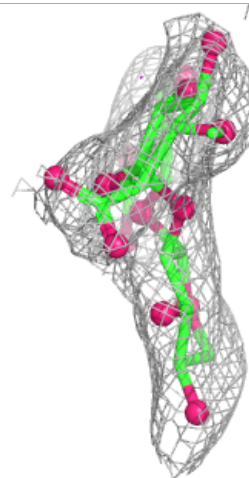
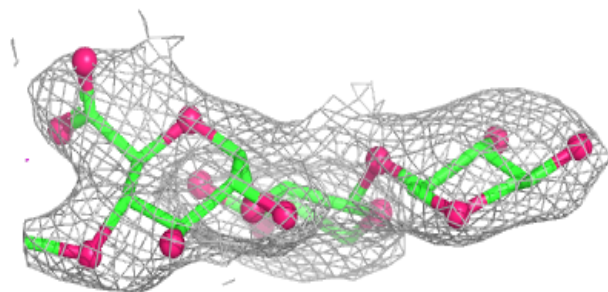
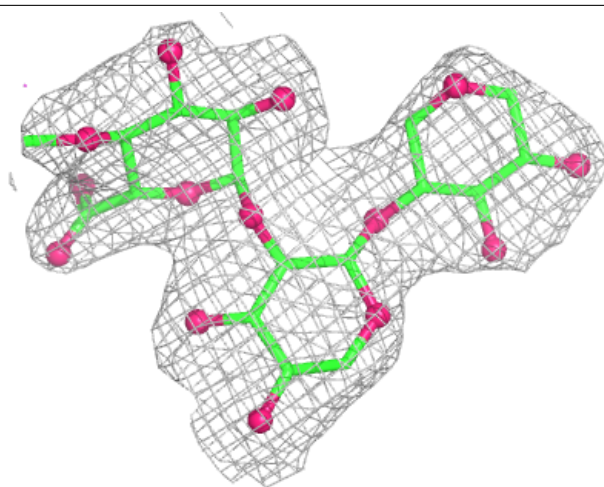
**Electron density around Chain F:**

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

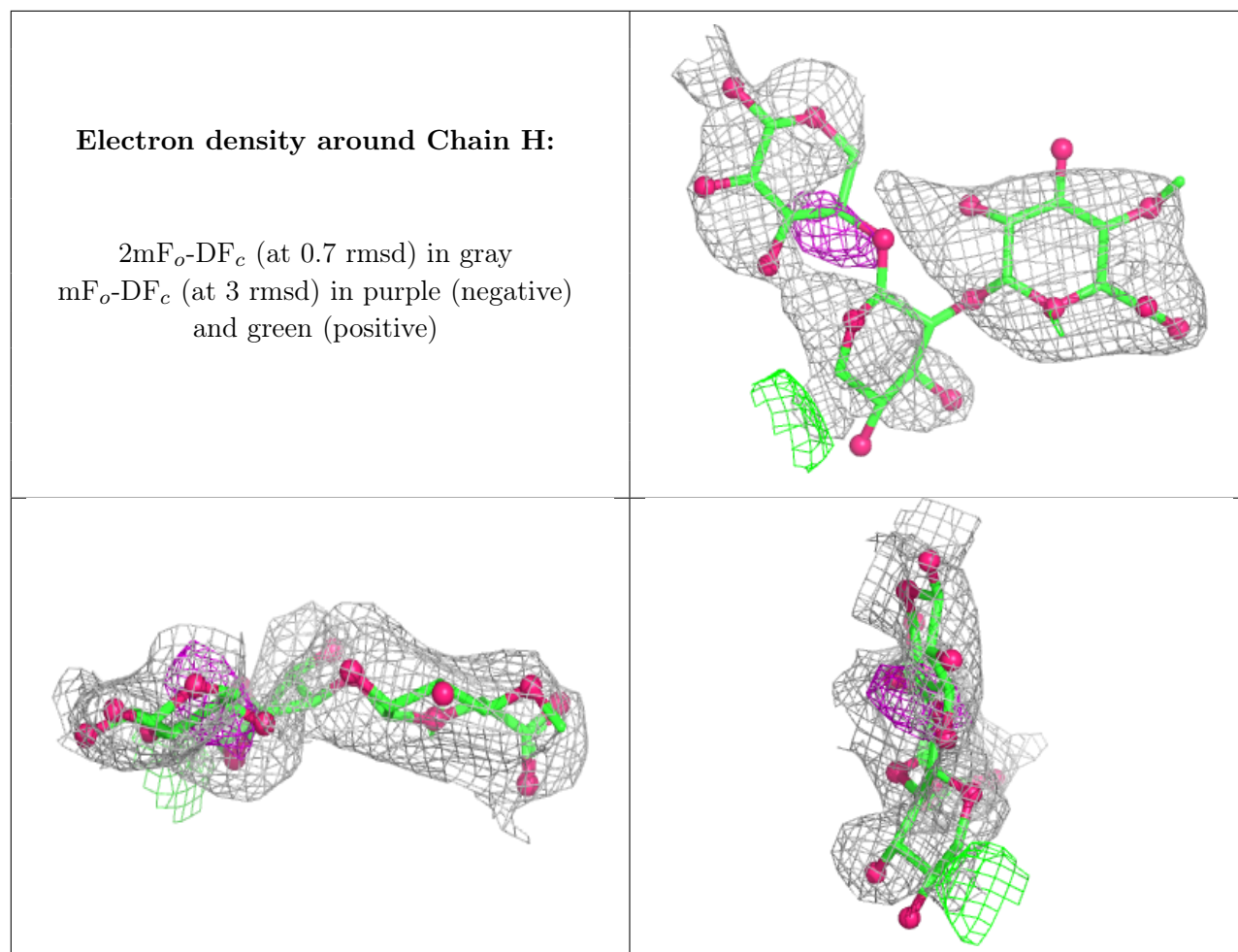


**Electron density around Chain G:**

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







## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.