



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 16, 2023 – 08:55 PM EDT

PDB ID : 2F2H  
Title : Structure of the YicI thiosugar Michaelis complex  
Authors : Kim, Y.-W.; Lovering, A.L.; Strynadka, N.C.J.; Withers, S.G.  
Deposited on : 2005-11-16  
Resolution : 1.95 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](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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

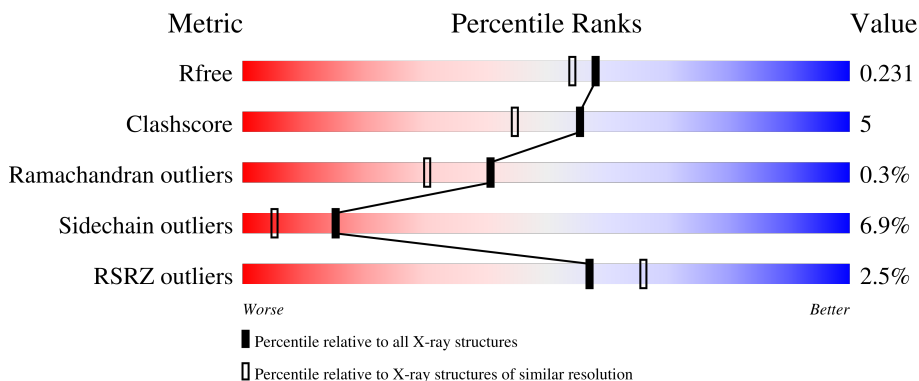
# 1 Overall quality at a glance

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))
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (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  $\geq 3$ , 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	773	 2% 85% 12% .
1	B	773	 3% 86% 12% .
1	C	773	 2% 84% 13% .
1	D	773	 3% 85% 12% .
1	E	773	 3% 83% 14% . .

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Mol	Chain	Length	Quality of chain
1	F	773	 2% 84% 13%

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	SO4	F	3001	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 39799 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 Putative family 31 glucosidase yicI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	773	6232	3981	1071	1148	32	0	0	0
1	B	773	6232	3981	1071	1148	32	0	0	0
1	C	773	6232	3981	1071	1148	32	0	0	0
1	D	773	6232	3981	1071	1148	32	0	0	0
1	E	773	6232	3981	1071	1148	32	0	0	0
1	F	773	6232	3981	1071	1148	32	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

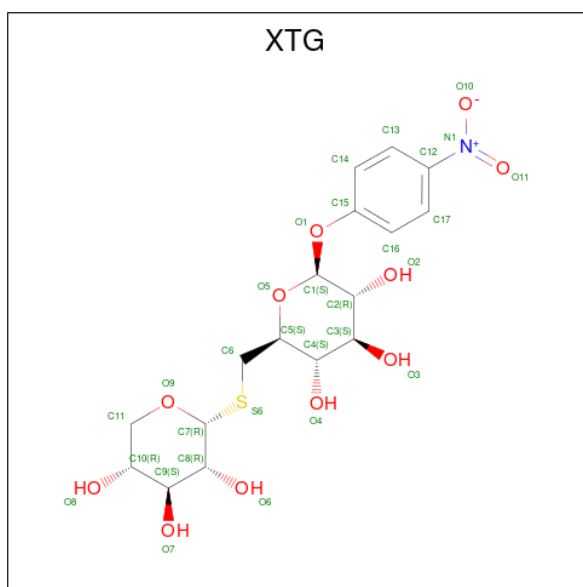
Chain	Residue	Modelled	Actual	Comment	Reference
A	773	HIS	-	expression tag	UNP P31434
B	773	HIS	-	expression tag	UNP P31434
C	773	HIS	-	expression tag	UNP P31434
D	773	HIS	-	expression tag	UNP P31434
E	773	HIS	-	expression tag	UNP P31434
F	773	HIS	-	expression tag	UNP P31434

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0

- Molecule 3 is 4-NITROPHENYL 6-THIO-6-S-ALPHA-D-XYLOPYRANOSYL-BETA-D-G LUCOPYRANOSIDE (three-letter code: XTG) (formula: C<sub>17</sub>H<sub>23</sub>NO<sub>11</sub>S).



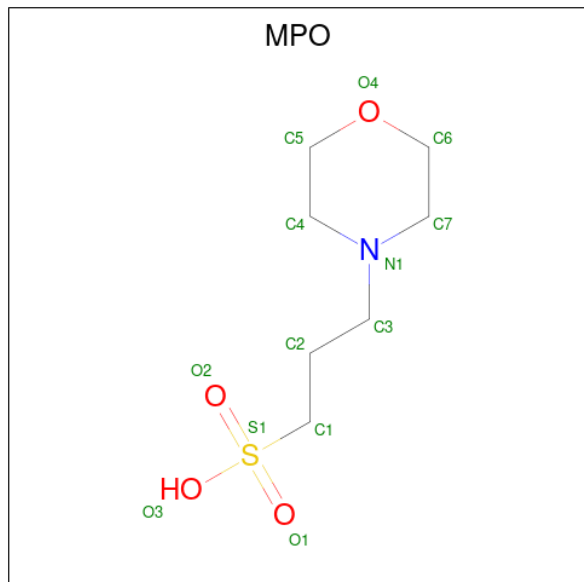
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	Total	C	N	O	S	0	0
			30	17	1	11	1		
3	B	1	Total	C	N	O	S	0	0
			30	17	1	11	1		
3	C	1	Total	C	N	O	S	0	0
			30	17	1	11	1		
3	D	1	Total	C	N	O	S	0	0
			30	17	1	11	1		
3	E	1	Total	C	N	O	S	0	0
			30	17	1	11	1		
3	F	1	Total	C	N	O	S	0	0
			30	17	1	11	1		
3	F	1	Total	C	N	O	S	0	0
			30	17	1	11	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 5 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: C<sub>7</sub>H<sub>15</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	B	1	Total 13	C 7	N 1	O 4	S 1	0	0
5	C	1	Total 13	C 7	N 1	O 4	S 1	0	0
5	D	1	Total 13	C 7	N 1	O 4	S 1	0	0
5	E	1	Total 13	C 7	N 1	O 4	S 1	0	0
5	F	1	Total 13	C 7	N 1	O 4	S 1	5	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	373	Total 373	O 373	0	0
6	B	290	Total 290	O 290	0	0
6	C	344	Total 344	O 344	0	0
6	D	370	Total 370	O 370	0	0
6	E	300	Total 300	O 300	0	0

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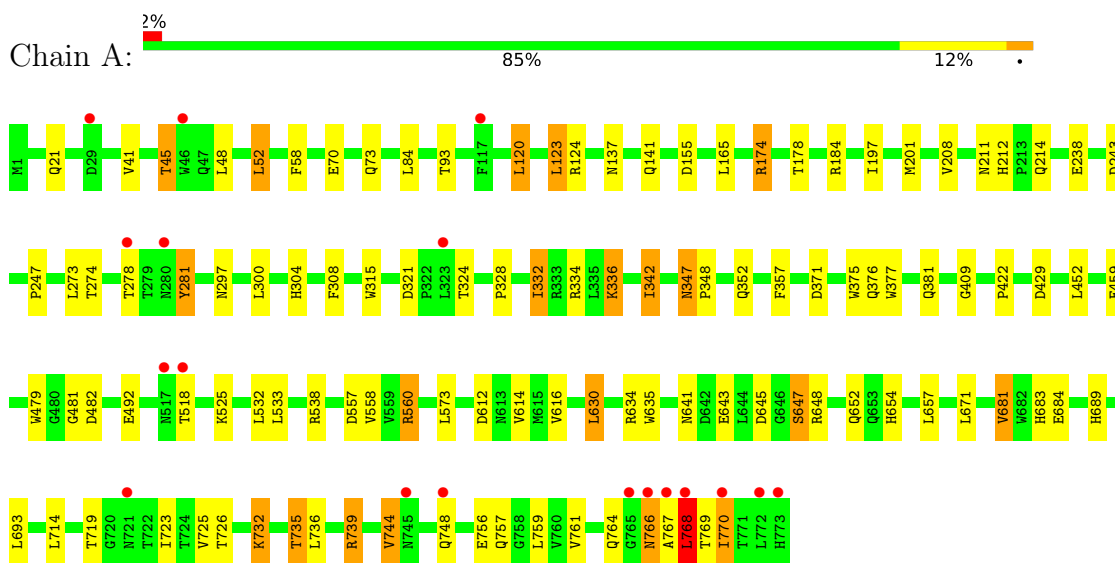
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	F	326	Total 326	O 326	0	0

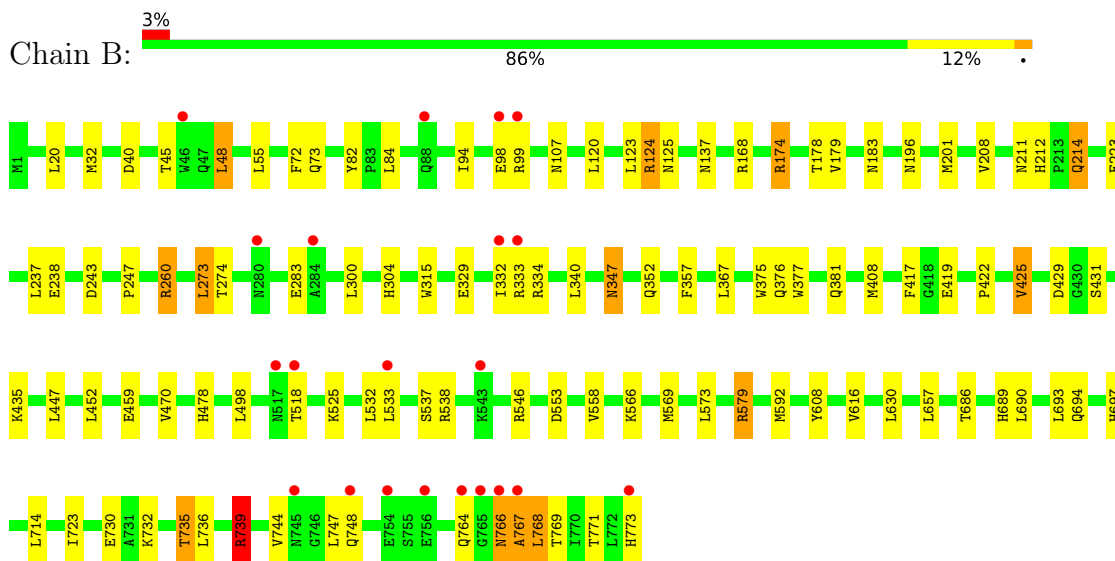
### 3 Residue-property plots [i](#)

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.

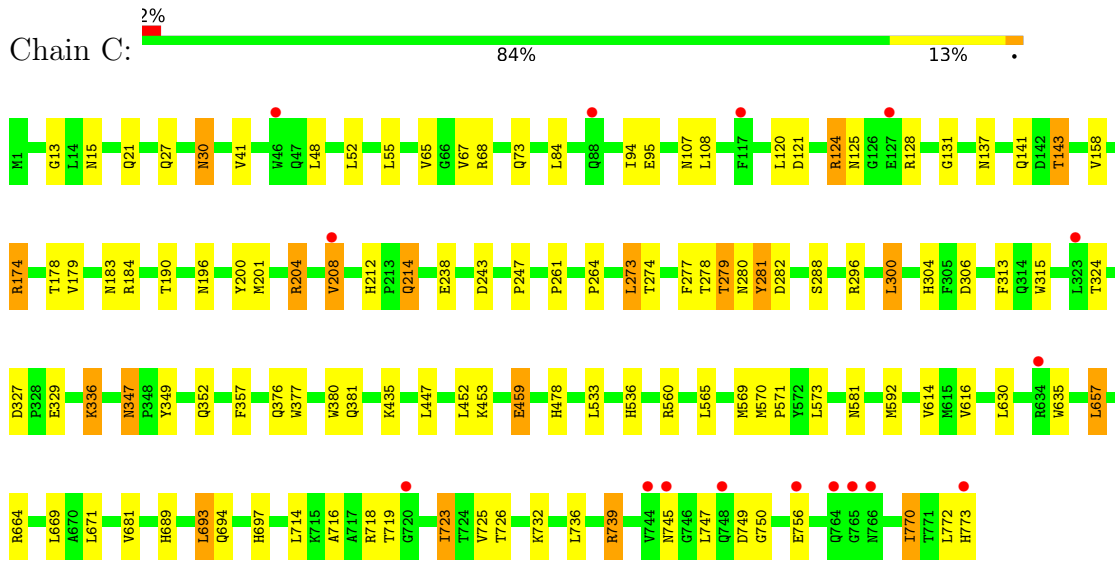
- Molecule 1: Putative family 31 glucosidase yicI



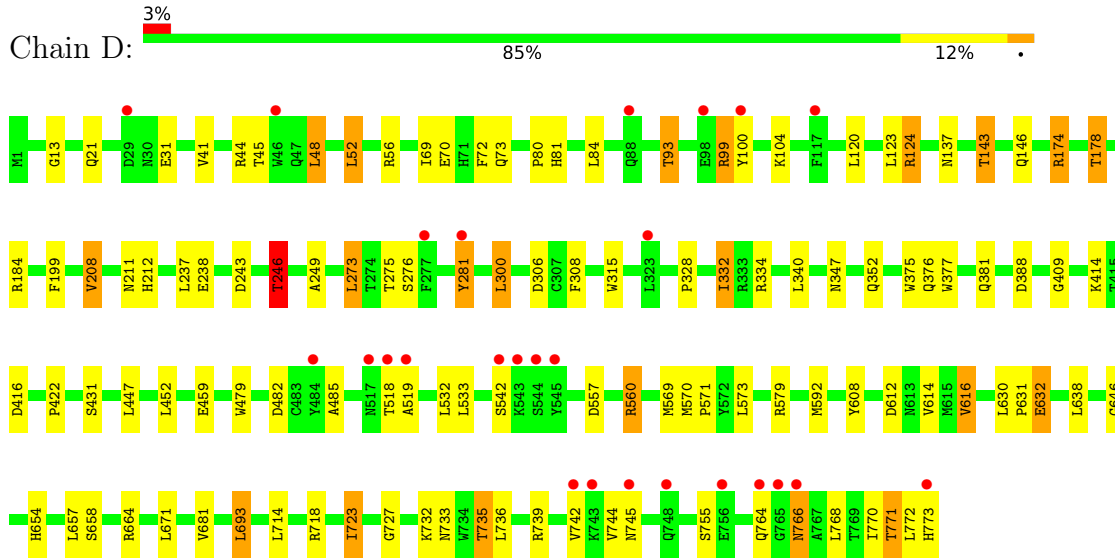
- Molecule 1: Putative family 31 glucosidase yicI



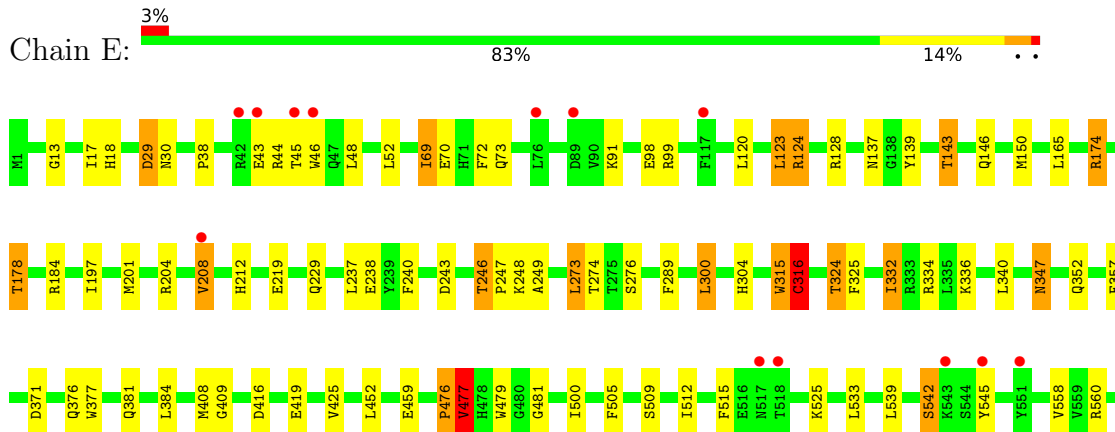
- Molecule 1: Putative family 31 glucosidase yicI

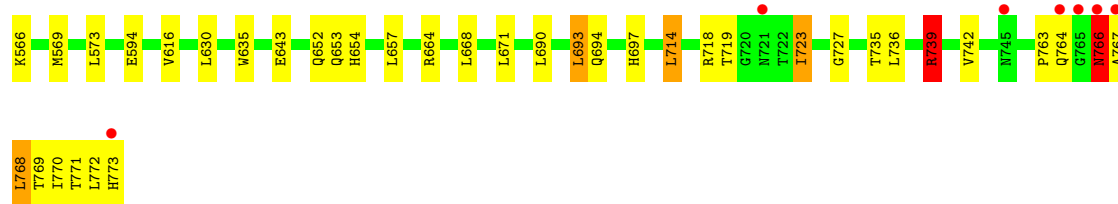


- Molecule 1: Putative family 31 glucosidase yicI

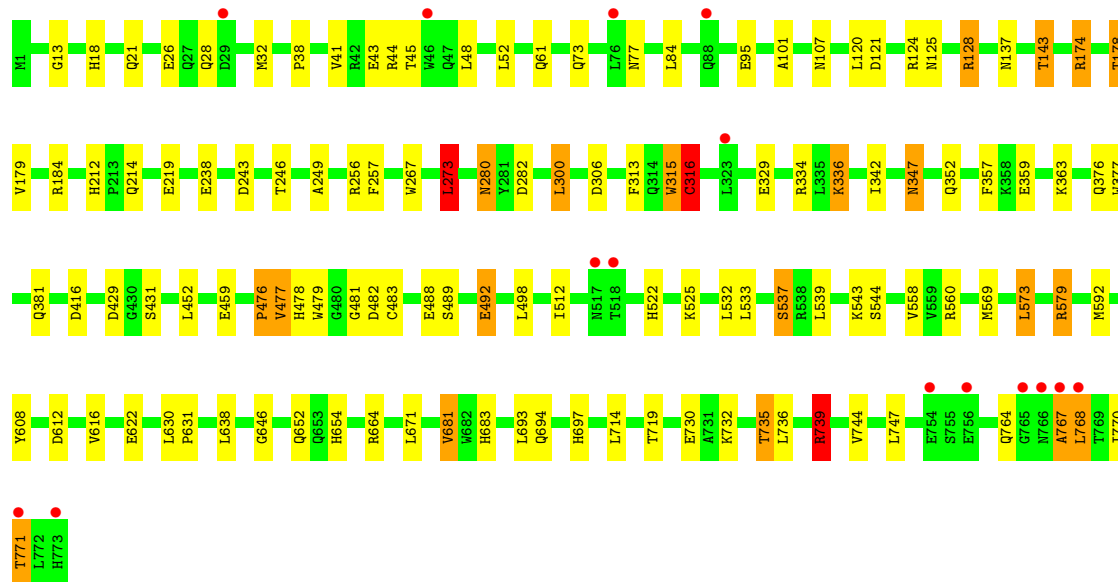
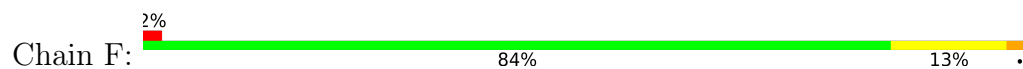


- Molecule 1: Putative family 31 glucosidase yicI





● Molecule 1: Putative family 31 glucosidase yicI



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.32Å 175.84Å 210.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.64 – 1.95 28.64 – 1.95	Depositor EDS
% Data completeness (in resolution range)	86.4 (28.64-1.95) 86.4 (28.64-1.95)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.58 (at 1.95Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.180 , 0.225 0.188 , 0.231	Depositor DCC
$R_{free}$ test set	18828 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.2	Xtrriage
Anisotropy	0.526	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	39799	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MPO, XTG, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.90	2/6416 (0.0%)	0.97	28/8719 (0.3%)
1	B	0.83	2/6416 (0.0%)	0.89	15/8719 (0.2%)
1	C	0.85	1/6416 (0.0%)	0.91	13/8719 (0.1%)
1	D	0.88	2/6416 (0.0%)	0.93	16/8719 (0.2%)
1	E	0.85	1/6416 (0.0%)	0.93	17/8719 (0.2%)
1	F	0.90	5/6416 (0.1%)	0.94	21/8719 (0.2%)
All	All	0.87	13/38496 (0.0%)	0.93	110/52314 (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	D	0	1
1	E	0	6
1	F	0	4
All	All	0	12

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	483	CYS	CB-SG	-8.95	1.67	1.82
1	F	537	SER	CB-OG	8.53	1.53	1.42
1	F	43	GLU	CG-CD	7.21	1.62	1.51
1	A	214	GLN	CB-CG	-6.47	1.35	1.52
1	C	336	LYS	CD-CE	6.32	1.67	1.51

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	174	ARG	NE-CZ-NH2	-16.54	112.03	120.30
1	E	174	ARG	NE-CZ-NH1	15.85	128.23	120.30
1	A	174	ARG	NE-CZ-NH2	-14.53	113.04	120.30
1	A	174	ARG	NE-CZ-NH1	14.36	127.48	120.30
1	F	174	ARG	NE-CZ-NH2	-13.02	113.79	120.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	766	ASN	Peptide
1	D	766	ASN	Peptide
1	E	315	TRP	Peptide,Mainchain
1	E	476	PRO	Peptide,Mainchain
1	E	763	PRO	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6232	0	5939	63	0
1	B	6232	0	5939	59	0
1	C	6232	0	5939	65	0
1	D	6232	0	5939	74	0
1	E	6232	0	5939	71	0
1	F	6232	0	5939	67	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	1	0
2	E	10	0	0	1	0
2	F	15	0	0	3	0
3	A	30	0	23	2	0
3	B	30	0	23	1	0
3	C	30	0	23	0	0
3	D	30	0	23	7	0
3	E	30	0	23	1	0
3	F	60	0	46	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	18	0	24	5	0
4	B	12	0	16	2	0
4	C	18	0	24	1	0
4	D	12	0	16	2	0
4	E	12	0	16	0	0
4	F	12	0	16	1	0
5	B	13	0	15	0	0
5	C	13	0	15	0	0
5	D	13	0	15	0	0
5	E	13	0	15	0	0
5	F	13	0	15	0	0
6	A	373	0	0	4	0
6	B	290	0	0	4	0
6	C	344	0	0	6	0
6	D	370	0	0	10	0
6	E	300	0	0	9	0
6	F	326	0	0	6	0
All	All	39799	0	35982	379	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.

The worst 5 of 379 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:124:ARG:NH2	1:A:243:ASP:OD1	1.88	1.04
1:D:569:MET:HE2	1:D:638:LEU:HD21	1.51	0.91
1:B:32:MET:CE	1:B:94:ILE:HG23	2.03	0.89
1:C:30:ASN:HD22	1:C:30:ASN:H	1.19	0.88
1:C:352:GLN:NE2	1:D:73:GLN:H	1.72	0.86

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	771/773 (100%)	744 (96%)	25 (3%)	2 (0%)	41	30
1	B	771/773 (100%)	736 (96%)	33 (4%)	2 (0%)	41	30
1	C	771/773 (100%)	740 (96%)	30 (4%)	1 (0%)	51	43
1	D	771/773 (100%)	743 (96%)	28 (4%)	0	100	100
1	E	771/773 (100%)	740 (96%)	27 (4%)	4 (0%)	29	17
1	F	771/773 (100%)	737 (96%)	28 (4%)	6 (1%)	19	9
All	All	4626/4638 (100%)	4440 (96%)	171 (4%)	15 (0%)	41	30

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	768	LEU
1	B	768	LEU
1	E	316	CYS
1	E	477	VAL
1	F	316	CYS

### 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	660/660 (100%)	617 (94%)	43 (6%)	17	6
1	B	660/660 (100%)	618 (94%)	42 (6%)	17	6
1	C	660/660 (100%)	614 (93%)	46 (7%)	15	5
1	D	660/660 (100%)	610 (92%)	50 (8%)	13	4
1	E	660/660 (100%)	609 (92%)	51 (8%)	13	4
1	F	660/660 (100%)	617 (94%)	43 (6%)	17	6
All	All	3960/3960 (100%)	3685 (93%)	275 (7%)	15	5

5 of 275 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	773	HIS
1	F	137	ASN
1	F	592	MET
1	C	214	GLN
1	C	178	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 105 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	133	GLN
1	E	73	GLN
1	F	478	HIS
1	D	141	GLN
1	D	381	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

35 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	D	3032	-	5,5,5	0.45	0	5,5,5	0.93	0
2	SO4	A	3008	-	4,4,4	0.27	0	6,6,6	0.55	0
2	SO4	F	3003	-	4,4,4	0.30	0	6,6,6	0.40	0
2	SO4	F	3001	-	4,4,4	0.20	0	6,6,6	0.75	0
2	SO4	E	3004	-	4,4,4	0.26	0	6,6,6	0.53	0
3	XTG	F	3020	-	31,32,32	2.72	10 (32%)	42,46,46	2.68	13 (30%)
2	SO4	F	3007	-	4,4,4	0.12	0	6,6,6	0.29	0
3	XTG	E	3019	-	31,32,32	2.54	7 (22%)	42,46,46	2.19	11 (26%)
5	MPO	E	3013	-	13,13,13	1.97	1 (7%)	17,17,17	1.72	3 (17%)
4	GOL	A	3029	-	5,5,5	0.53	0	5,5,5	1.16	1 (20%)
5	MPO	C	3011	-	13,13,13	1.93	1 (7%)	17,17,17	1.50	4 (23%)
2	SO4	E	3009	-	4,4,4	0.16	0	6,6,6	0.52	0
4	GOL	A	3024	-	5,5,5	0.42	0	5,5,5	0.84	0
3	XTG	D	3018	-	31,32,32	3.97	10 (32%)	42,46,46	2.97	15 (35%)
4	GOL	D	3031	-	5,5,5	0.43	0	5,5,5	0.58	0
2	SO4	B	3006	-	4,4,4	0.18	0	6,6,6	0.34	0
4	GOL	C	3030	-	5,5,5	0.47	0	5,5,5	0.52	0
5	MPO	F	3014	-	13,13,13	8.04	2 (15%)	17,17,17	8.56	6 (35%)
4	GOL	B	3026	-	5,5,5	0.31	0	5,5,5	0.79	0
4	GOL	B	3025	-	5,5,5	0.40	0	5,5,5	1.06	0
4	GOL	F	3034	-	5,5,5	0.43	0	5,5,5	0.47	0
5	MPO	B	3010	-	13,13,13	2.04	1 (7%)	17,17,17	1.24	2 (11%)
4	GOL	E	3033	-	5,5,5	0.43	0	5,5,5	0.62	0
3	XTG	C	3017	-	31,32,32	2.99	4 (12%)	42,46,46	1.97	6 (14%)
3	XTG	F	3021	-	31,32,32	2.86	6 (19%)	42,46,46	2.21	8 (19%)
5	MPO	D	3012	-	13,13,13	2.07	1 (7%)	17,17,17	1.47	3 (17%)
3	XTG	A	3015	-	31,32,32	2.98	5 (16%)	42,46,46	2.63	17 (40%)
2	SO4	C	3005	-	4,4,4	0.07	0	6,6,6	0.73	0
2	SO4	D	3002	-	4,4,4	0.22	0	6,6,6	0.47	0
4	GOL	C	3023	-	5,5,5	0.56	0	5,5,5	1.43	1 (20%)
4	GOL	F	3022	-	5,5,5	0.60	0	5,5,5	0.81	0
4	GOL	C	3027	-	5,5,5	0.57	0	5,5,5	0.76	0
4	GOL	A	3028	-	5,5,5	0.36	0	5,5,5	0.66	0
4	GOL	E	3035	-	5,5,5	0.64	0	5,5,5	0.79	0
3	XTG	B	3016	-	31,32,32	3.15	7 (22%)	42,46,46	2.77	13 (30%)

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	D	3032	-	-	0/4/4/4	-
3	XTG	F	3020	-	-	7/11/50/50	0/3/3/3
3	XTG	E	3019	-	-	5/11/50/50	0/3/3/3
5	MPO	E	3013	-	-	5/7/15/15	0/1/1/1
4	GOL	A	3029	-	-	0/4/4/4	-
5	MPO	C	3011	-	-	0/7/15/15	0/1/1/1
4	GOL	A	3024	-	-	4/4/4/4	-
3	XTG	D	3018	-	-	6/11/50/50	0/3/3/3
4	GOL	D	3031	-	-	4/4/4/4	-
4	GOL	C	3030	-	-	2/4/4/4	-
5	MPO	F	3014	-	-	3/7/15/15	0/1/1/1
4	GOL	B	3026	-	-	2/4/4/4	-
4	GOL	B	3025	-	-	4/4/4/4	-
4	GOL	F	3034	-	-	4/4/4/4	-
5	MPO	B	3010	-	-	0/7/15/15	0/1/1/1
4	GOL	E	3033	-	-	3/4/4/4	-
3	XTG	C	3017	-	-	7/11/50/50	0/3/3/3
3	XTG	F	3021	-	-	2/11/50/50	0/3/3/3
5	MPO	D	3012	-	-	2/7/15/15	0/1/1/1
3	XTG	A	3015	-	-	5/11/50/50	0/3/3/3
4	GOL	C	3023	-	-	0/4/4/4	-
4	GOL	F	3022	-	-	4/4/4/4	-
4	GOL	C	3027	-	-	2/4/4/4	-
4	GOL	A	3028	-	-	4/4/4/4	-
4	GOL	E	3035	-	-	1/4/4/4	-
3	XTG	B	3016	-	-	7/11/50/50	0/3/3/3

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	3014	MPO	C4-N1	28.04	2.24	1.46
3	D	3018	XTG	O11-N1	15.42	1.48	1.22
3	C	3017	XTG	O11-N1	14.87	1.48	1.22
3	A	3015	XTG	O11-N1	13.74	1.46	1.22
3	B	3016	XTG	O11-N1	13.20	1.45	1.22

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	3014	MPO	C6-C7-N1	28.67	153.57	110.10
5	F	3014	MPO	C7-N1-C4	-13.89	77.56	108.83
5	F	3014	MPO	C5-C4-N1	11.46	127.48	110.10
3	B	3016	XTG	O5-C5-C6	10.59	124.33	106.48
3	A	3015	XTG	O5-C5-C6	8.96	121.59	106.48

There are no chirality outliers.

5 of 83 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3015	XTG	O5-C5-C6-S6
3	A	3015	XTG	C4-C5-C6-S6
3	A	3015	XTG	O9-C7-S6-C6
3	A	3015	XTG	C8-C7-S6-C6
3	B	3016	XTG	C17-C12-N1-O11

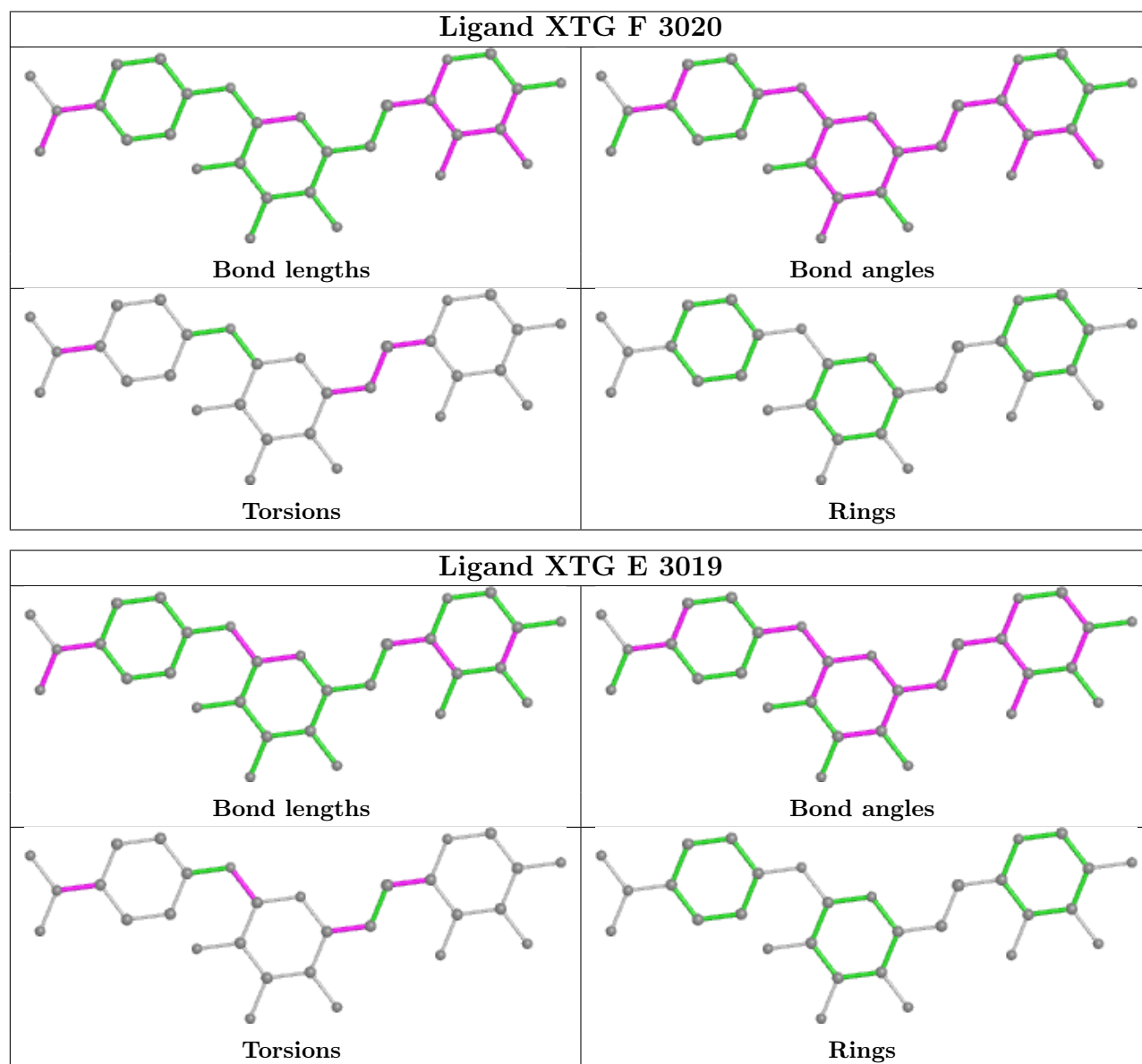
There are no ring outliers.

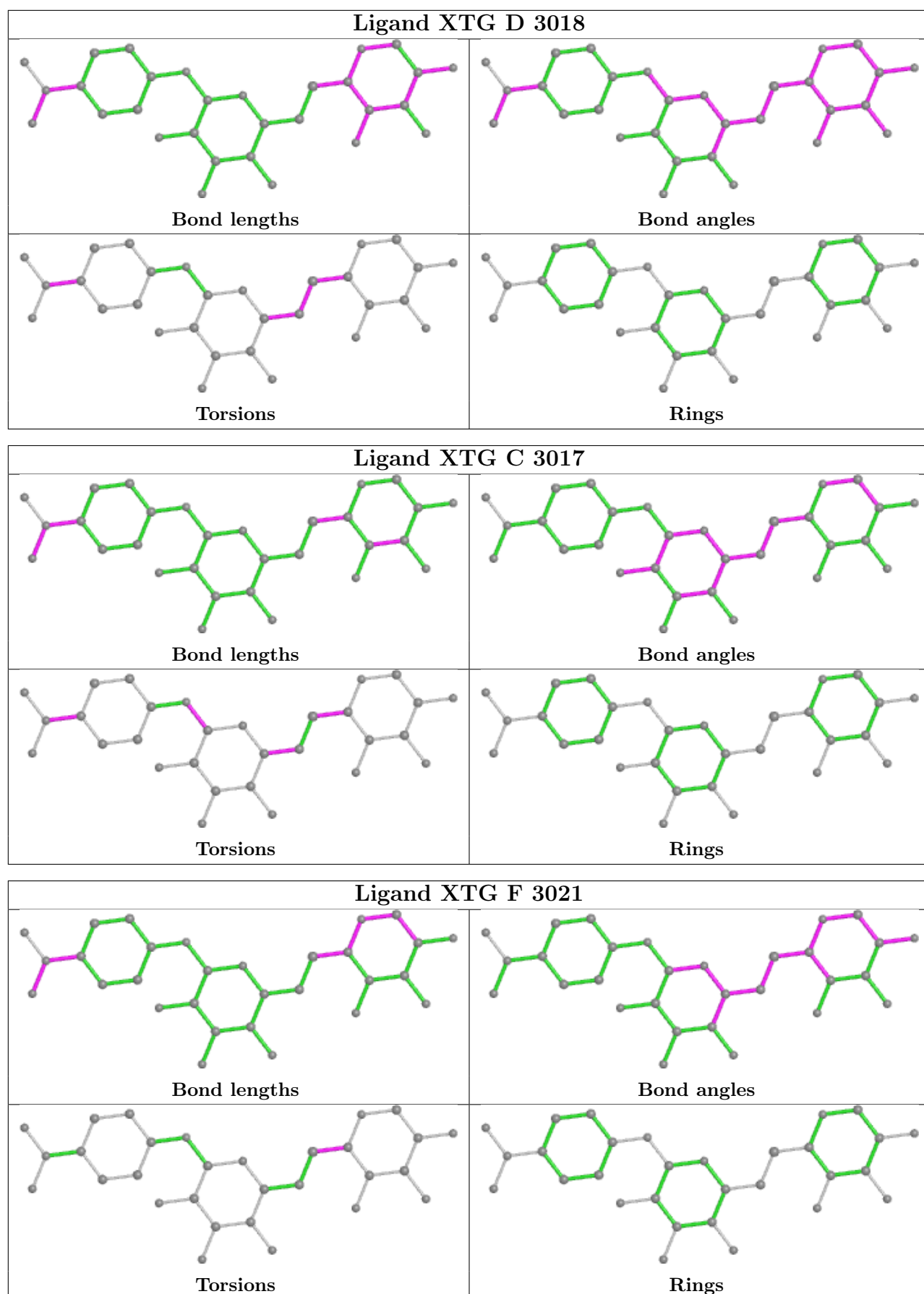
16 monomers are involved in 28 short contacts:

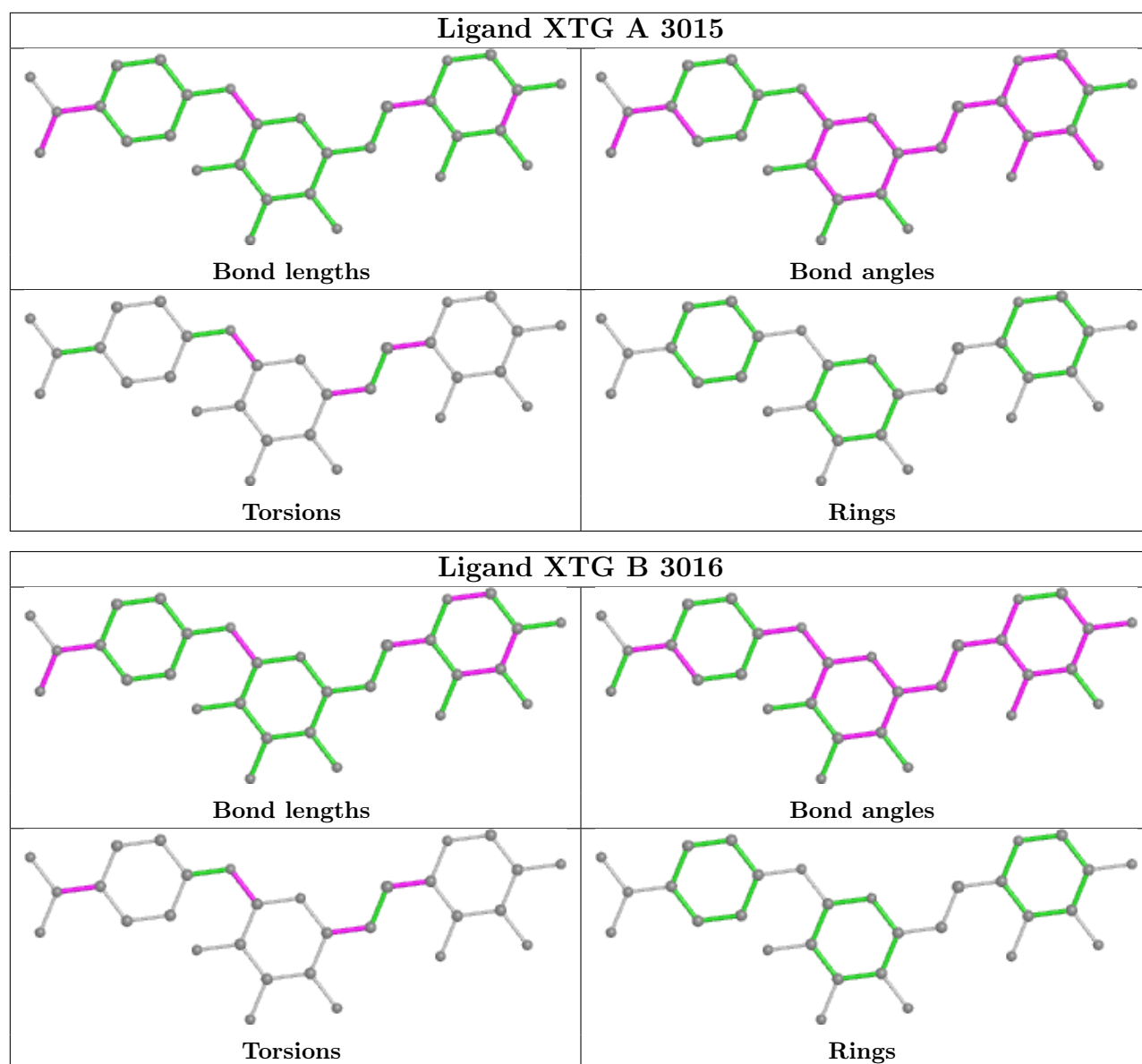
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	3032	GOL	2	0
2	F	3003	SO4	1	0
2	F	3001	SO4	2	0
2	E	3004	SO4	1	0
3	F	3020	XTG	1	0
3	E	3019	XTG	1	0
4	A	3029	GOL	3	0
4	A	3024	GOL	1	0
3	D	3018	XTG	7	0
4	B	3026	GOL	2	0
3	A	3015	XTG	2	0
2	D	3002	SO4	1	0
4	C	3023	GOL	1	0
4	F	3022	GOL	1	0
4	A	3028	GOL	1	0
3	B	3016	XTG	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 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, 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	773/773 (100%)	-0.20	18 (2%) 60 69	8, 14, 35, 53	0
1	B	773/773 (100%)	-0.03	21 (2%) 54 63	11, 20, 38, 58	0
1	C	773/773 (100%)	-0.11	16 (2%) 63 72	9, 18, 35, 50	0
1	D	773/773 (100%)	-0.07	26 (3%) 45 55	8, 17, 41, 55	0
1	E	773/773 (100%)	-0.04	20 (2%) 56 65	10, 20, 39, 55	0
1	F	773/773 (100%)	-0.13	15 (1%) 66 74	9, 17, 37, 54	0
All	All	4638/4638 (100%)	-0.10	116 (2%) 57 66	8, 18, 38, 58	0

The worst 5 of 116 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	545	TYR	7.5
1	D	773	HIS	5.9
1	B	765	GLY	5.9
1	B	767	ALA	5.7
1	C	773	HIS	5.3

### 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](#)

There are no monosaccharides in this entry.

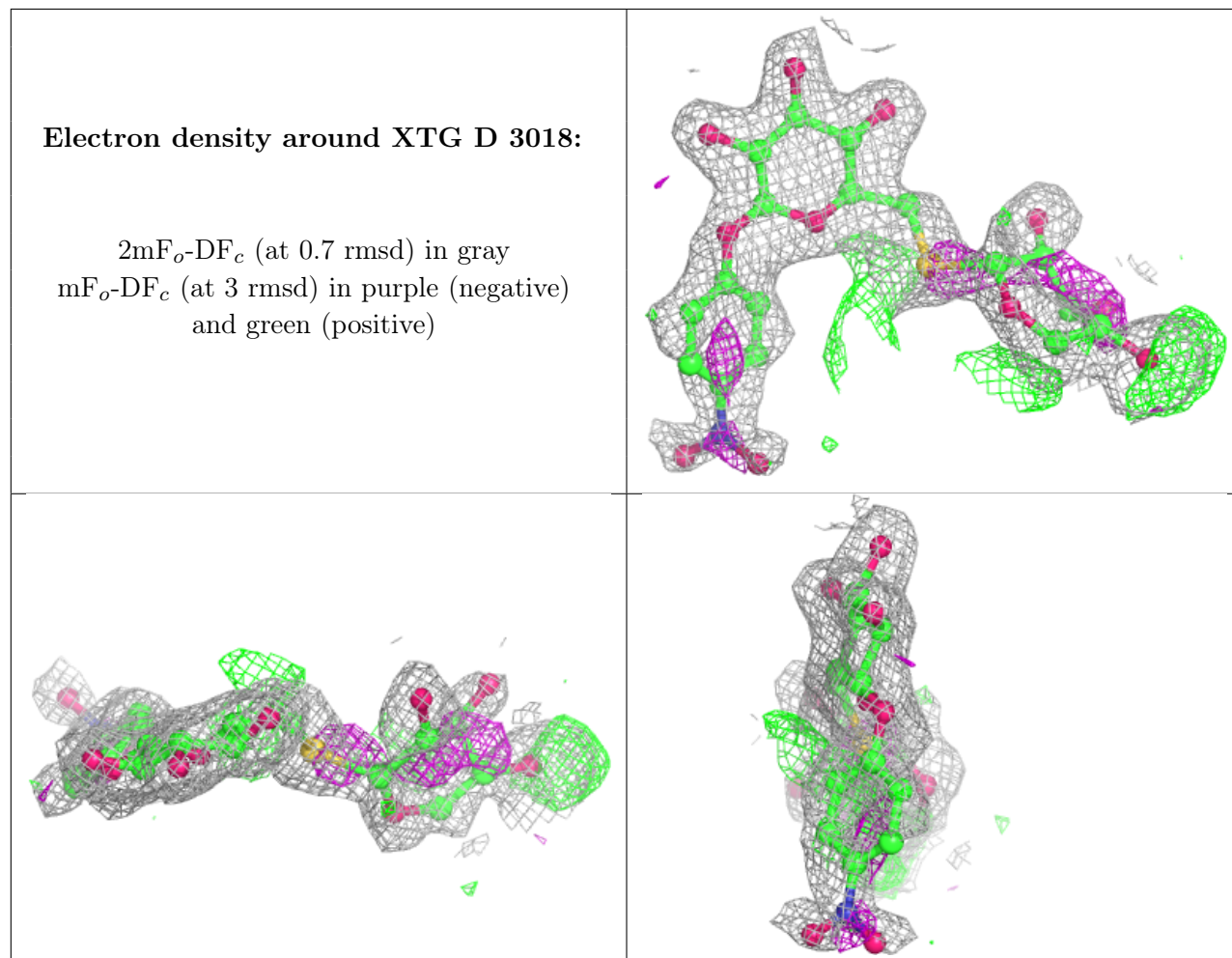
## 6.4 Ligands i

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, 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
5	MPO	F	3014	13/13	0.76	0.27	41,62,71,72	5
4	GOL	E	3035	6/6	0.77	0.19	54,55,56,56	0
3	XTG	D	3018	30/30	0.79	0.20	24,45,53,56	0
4	GOL	A	3029	6/6	0.82	0.24	30,39,39,39	0
4	GOL	A	3028	6/6	0.85	0.20	29,35,37,39	0
4	GOL	E	3033	6/6	0.86	0.14	29,34,35,37	0
4	GOL	A	3024	6/6	0.87	0.25	37,40,40,40	0
4	GOL	C	3027	6/6	0.88	0.16	41,44,45,45	0
4	GOL	D	3031	6/6	0.89	0.13	23,28,30,32	0
2	SO4	E	3009	5/5	0.90	0.26	68,68,69,69	0
4	GOL	B	3026	6/6	0.90	0.21	34,39,40,41	0
4	GOL	F	3034	6/6	0.90	0.16	32,37,38,38	0
4	GOL	D	3032	6/6	0.90	0.16	31,37,40,41	0
4	GOL	C	3030	6/6	0.91	0.14	25,28,30,30	0
3	XTG	E	3019	30/30	0.92	0.13	17,28,42,47	0
4	GOL	C	3023	6/6	0.92	0.12	25,29,29,30	0
3	XTG	F	3020	30/30	0.92	0.14	12,38,41,44	0
3	XTG	F	3021	30/30	0.92	0.16	12,18,54,56	0
4	GOL	B	3025	6/6	0.92	0.15	26,31,31,32	0
3	XTG	B	3016	30/30	0.93	0.11	12,32,41,44	0
2	SO4	E	3004	5/5	0.94	0.26	45,47,48,49	0
3	XTG	C	3017	30/30	0.94	0.13	12,26,39,43	0
2	SO4	A	3008	5/5	0.94	0.24	45,46,48,49	0
3	XTG	A	3015	30/30	0.94	0.12	12,28,37,40	0
2	SO4	F	3001	5/5	0.95	0.20	37,39,41,44	0
5	MPO	C	3011	13/13	0.95	0.16	29,34,37,38	0
5	MPO	E	3013	13/13	0.95	0.16	43,49,55,56	0
2	SO4	B	3006	5/5	0.95	0.24	45,47,49,50	0
5	MPO	D	3012	13/13	0.96	0.15	20,34,40,40	0
2	SO4	C	3005	5/5	0.96	0.21	46,48,49,50	0
2	SO4	D	3002	5/5	0.96	0.23	51,52,53,54	0
2	SO4	F	3007	5/5	0.97	0.19	48,49,50,50	0
5	MPO	B	3010	13/13	0.97	0.14	29,36,43,43	0
4	GOL	F	3022	6/6	0.97	0.08	16,18,20,22	0
2	SO4	F	3003	5/5	0.99	0.08	14,16,20,20	0

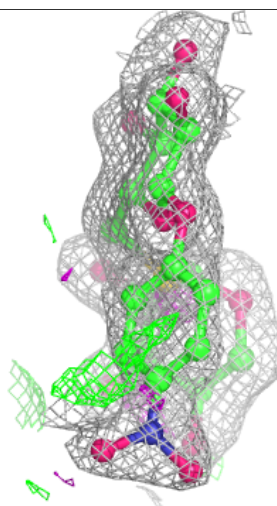
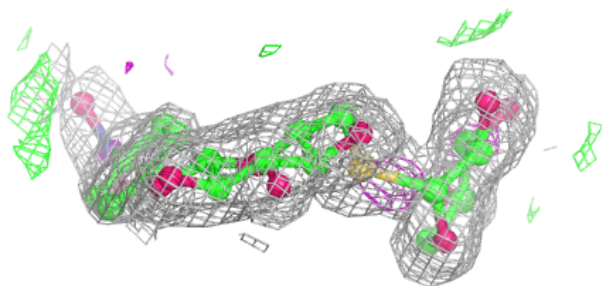
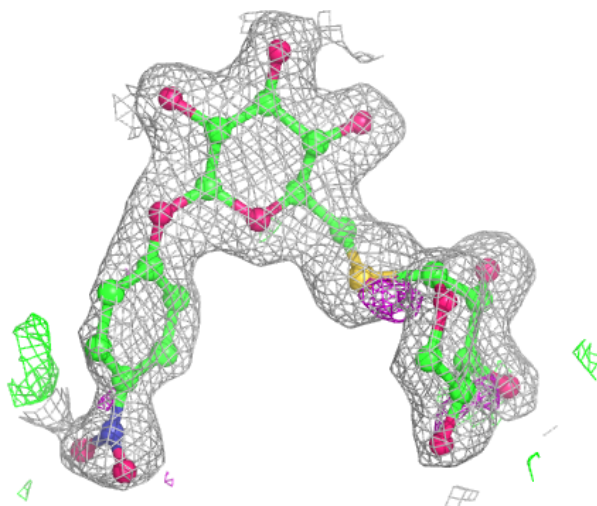
The following is a graphical depiction of the model fit to experimental electron density of all

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.



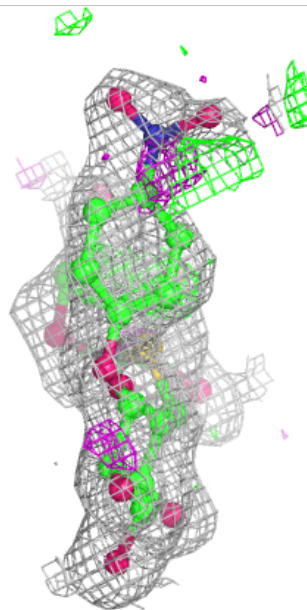
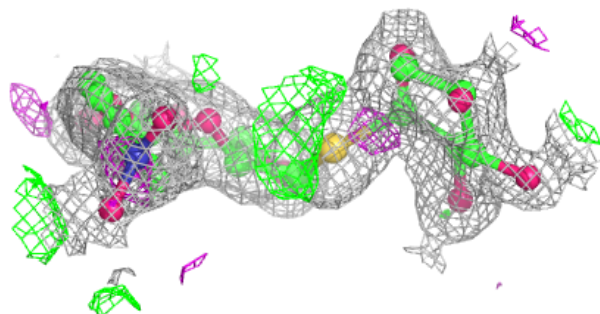
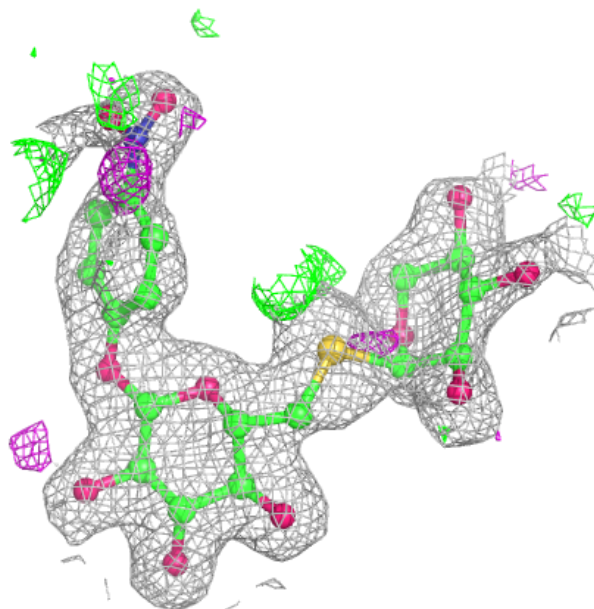
**Electron density around XTG E 3019:**

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



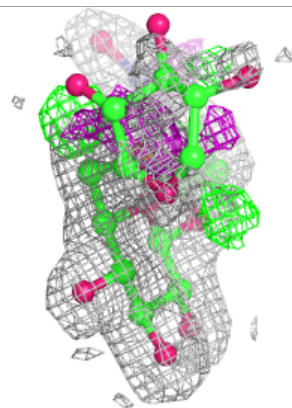
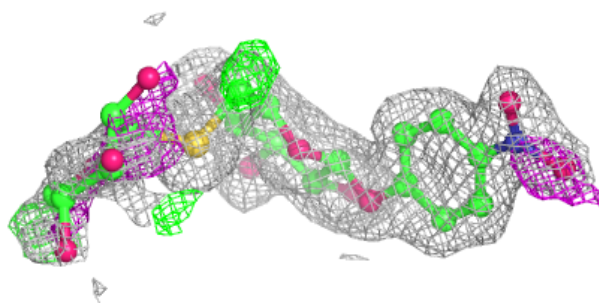
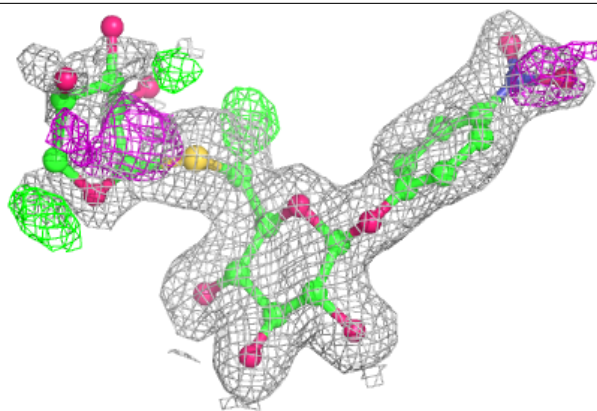
**Electron density around XTG F 3020:**

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



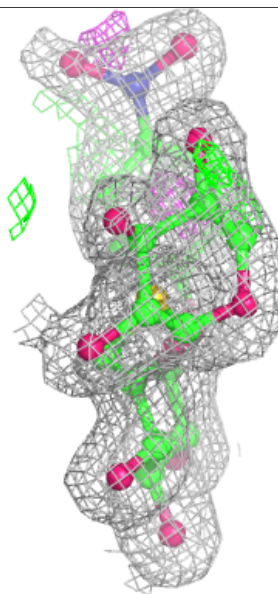
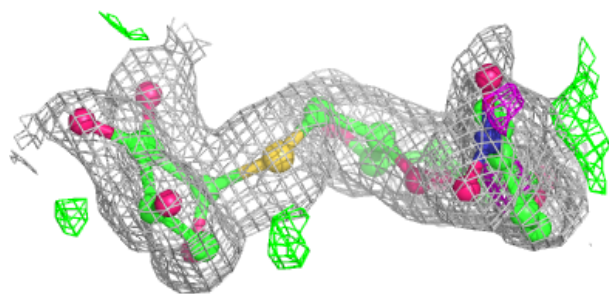
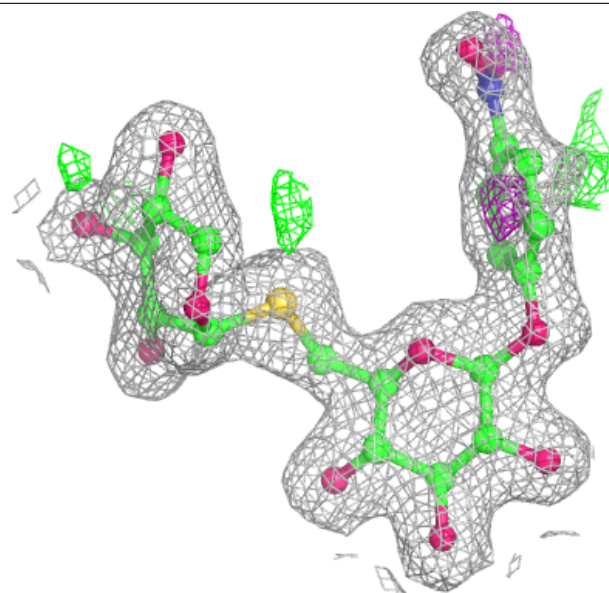
**Electron density around XTG F 3021:**

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



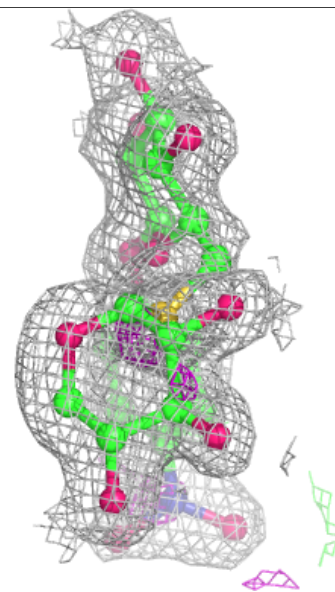
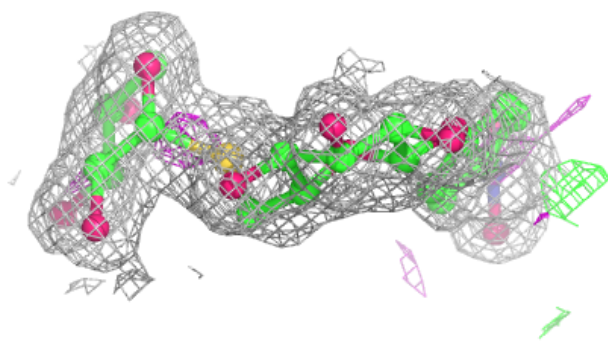
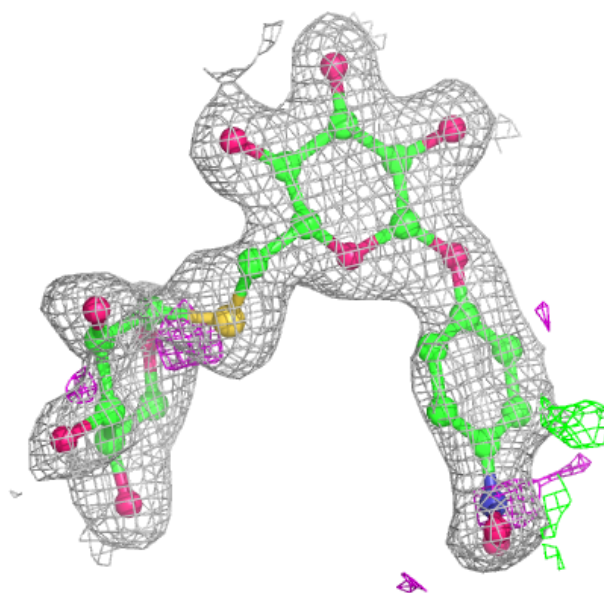
**Electron density around XTG B 3016:**

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

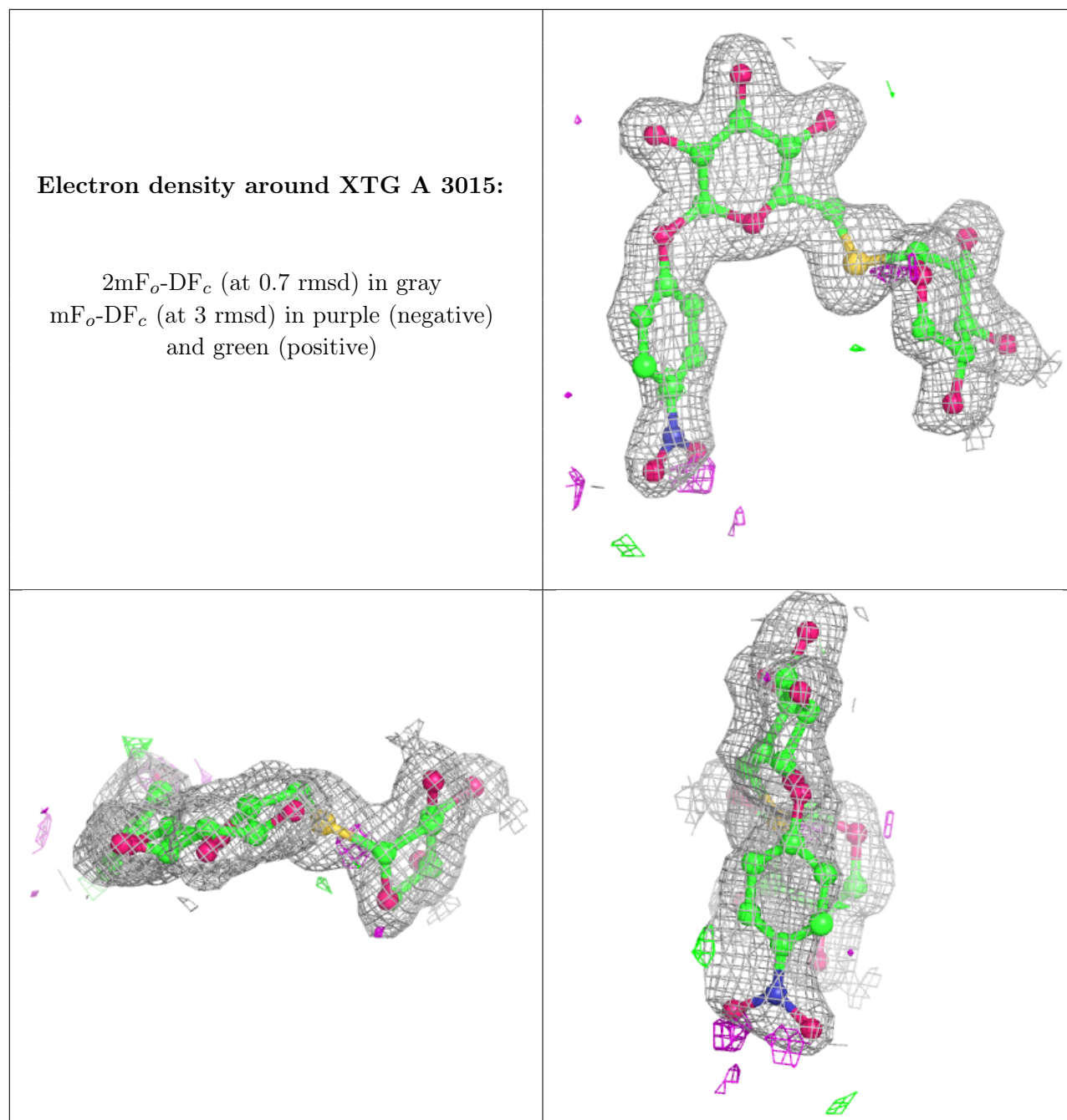


**Electron density around XTG C 3017:**

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







## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.