



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 07:53 pm BST

PDB ID : 8PEJ  
Title : CjGH35 with a Galactosidase Activity-Based Probe  
Authors : Offen, W.A.; Davies, G.J.  
Deposited on : 2023-06-14  
Resolution : 1.50 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 : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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

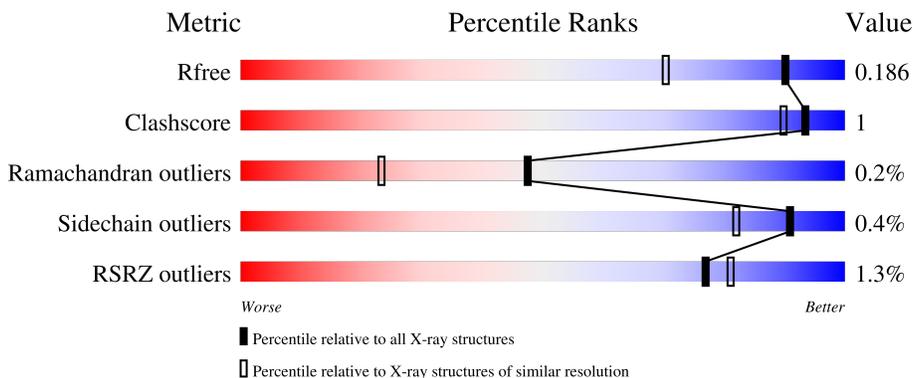
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

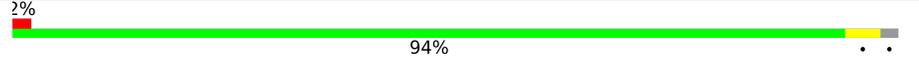
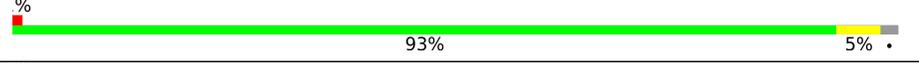
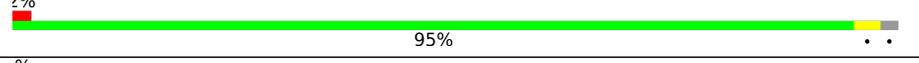
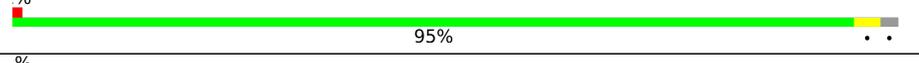
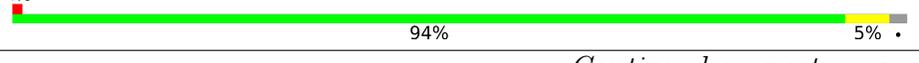
The reported resolution of this entry is 1.50 Å.

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.



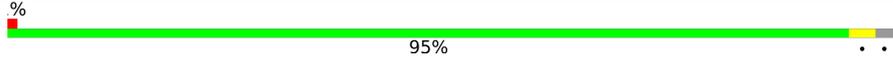
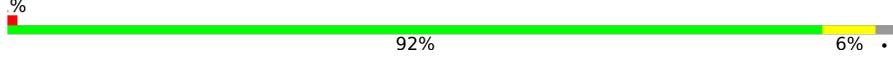
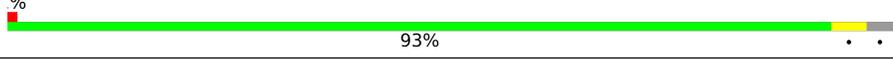
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	550	 2% 94% 5%
1	B	550	 1% 93% 5%
1	C	550	 2% 95% 5%
1	D	550	 1% 95% 5%
1	E	550	 1% 94% 5%

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Mol	Chain	Length	Quality of chain
1	F	550	 <p>% 95% 6% . .</p>
1	G	550	 <p>% 92% 6% . .</p>
1	H	550	 <p>% 93% 6% . .</p>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 72581 atoms, of which 33577 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 Beta-galactosidase, putative, bgl35A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	537	8365	2721	4118	722	788	16	110	7	0
1	B	540	8419	2735	4143	731	794	16	113	6	0
1	C	540	8451	2747	4159	734	795	16	118	8	0
1	D	539	8471	2752	4174	727	802	16	108	10	0
1	E	540	8509	2762	4199	730	802	16	109	11	0
1	F	539	8558	2772	4225	738	807	16	108	12	0
1	G	540	8574	2779	4226	741	812	16	110	14	0
1	H	535	8488	2755	4187	730	801	15	113	12	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	initiating methionine	UNP B3PBE0
A	27	GLY	-	expression tag	UNP B3PBE0
A	28	SER	-	expression tag	UNP B3PBE0
A	29	SER	-	expression tag	UNP B3PBE0
A	30	HIS	-	expression tag	UNP B3PBE0
A	31	HIS	-	expression tag	UNP B3PBE0
A	32	HIS	-	expression tag	UNP B3PBE0
A	33	HIS	-	expression tag	UNP B3PBE0
A	34	HIS	-	expression tag	UNP B3PBE0
A	35	HIS	-	expression tag	UNP B3PBE0
B	26	MET	-	initiating methionine	UNP B3PBE0
B	27	GLY	-	expression tag	UNP B3PBE0
B	28	SER	-	expression tag	UNP B3PBE0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	29	SER	-	expression tag	UNP B3PBE0
B	30	HIS	-	expression tag	UNP B3PBE0
B	31	HIS	-	expression tag	UNP B3PBE0
B	32	HIS	-	expression tag	UNP B3PBE0
B	33	HIS	-	expression tag	UNP B3PBE0
B	34	HIS	-	expression tag	UNP B3PBE0
B	35	HIS	-	expression tag	UNP B3PBE0
C	26	MET	-	initiating methionine	UNP B3PBE0
C	27	GLY	-	expression tag	UNP B3PBE0
C	28	SER	-	expression tag	UNP B3PBE0
C	29	SER	-	expression tag	UNP B3PBE0
C	30	HIS	-	expression tag	UNP B3PBE0
C	31	HIS	-	expression tag	UNP B3PBE0
C	32	HIS	-	expression tag	UNP B3PBE0
C	33	HIS	-	expression tag	UNP B3PBE0
C	34	HIS	-	expression tag	UNP B3PBE0
C	35	HIS	-	expression tag	UNP B3PBE0
D	26	MET	-	initiating methionine	UNP B3PBE0
D	27	GLY	-	expression tag	UNP B3PBE0
D	28	SER	-	expression tag	UNP B3PBE0
D	29	SER	-	expression tag	UNP B3PBE0
D	30	HIS	-	expression tag	UNP B3PBE0
D	31	HIS	-	expression tag	UNP B3PBE0
D	32	HIS	-	expression tag	UNP B3PBE0
D	33	HIS	-	expression tag	UNP B3PBE0
D	34	HIS	-	expression tag	UNP B3PBE0
D	35	HIS	-	expression tag	UNP B3PBE0
E	26	MET	-	initiating methionine	UNP B3PBE0
E	27	GLY	-	expression tag	UNP B3PBE0
E	28	SER	-	expression tag	UNP B3PBE0
E	29	SER	-	expression tag	UNP B3PBE0
E	30	HIS	-	expression tag	UNP B3PBE0
E	31	HIS	-	expression tag	UNP B3PBE0
E	32	HIS	-	expression tag	UNP B3PBE0
E	33	HIS	-	expression tag	UNP B3PBE0
E	34	HIS	-	expression tag	UNP B3PBE0
E	35	HIS	-	expression tag	UNP B3PBE0
F	26	MET	-	initiating methionine	UNP B3PBE0
F	27	GLY	-	expression tag	UNP B3PBE0
F	28	SER	-	expression tag	UNP B3PBE0
F	29	SER	-	expression tag	UNP B3PBE0
F	30	HIS	-	expression tag	UNP B3PBE0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	31	HIS	-	expression tag	UNP B3PBE0
F	32	HIS	-	expression tag	UNP B3PBE0
F	33	HIS	-	expression tag	UNP B3PBE0
F	34	HIS	-	expression tag	UNP B3PBE0
F	35	HIS	-	expression tag	UNP B3PBE0
G	26	MET	-	initiating methionine	UNP B3PBE0
G	27	GLY	-	expression tag	UNP B3PBE0
G	28	SER	-	expression tag	UNP B3PBE0
G	29	SER	-	expression tag	UNP B3PBE0
G	30	HIS	-	expression tag	UNP B3PBE0
G	31	HIS	-	expression tag	UNP B3PBE0
G	32	HIS	-	expression tag	UNP B3PBE0
G	33	HIS	-	expression tag	UNP B3PBE0
G	34	HIS	-	expression tag	UNP B3PBE0
G	35	HIS	-	expression tag	UNP B3PBE0
H	26	MET	-	initiating methionine	UNP B3PBE0
H	27	GLY	-	expression tag	UNP B3PBE0
H	28	SER	-	expression tag	UNP B3PBE0
H	29	SER	-	expression tag	UNP B3PBE0
H	30	HIS	-	expression tag	UNP B3PBE0
H	31	HIS	-	expression tag	UNP B3PBE0
H	32	HIS	-	expression tag	UNP B3PBE0
H	33	HIS	-	expression tag	UNP B3PBE0
H	34	HIS	-	expression tag	UNP B3PBE0
H	35	HIS	-	expression tag	UNP B3PBE0

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

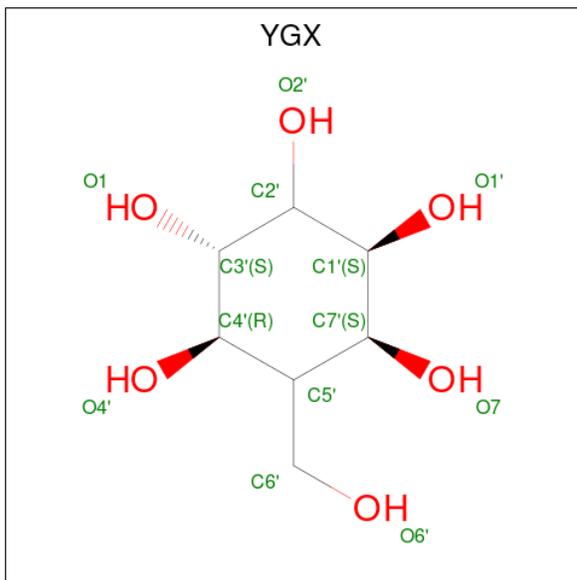
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Na 4 4	0	0
2	B	2	Total Na 2 2	0	0
2	C	4	Total Na 4 4	0	0
2	D	5	Total Na 5 5	0	0
2	E	6	Total Na 6 6	0	0
2	F	4	Total Na 4 4	0	0
2	G	5	Total Na 5 5	0	0

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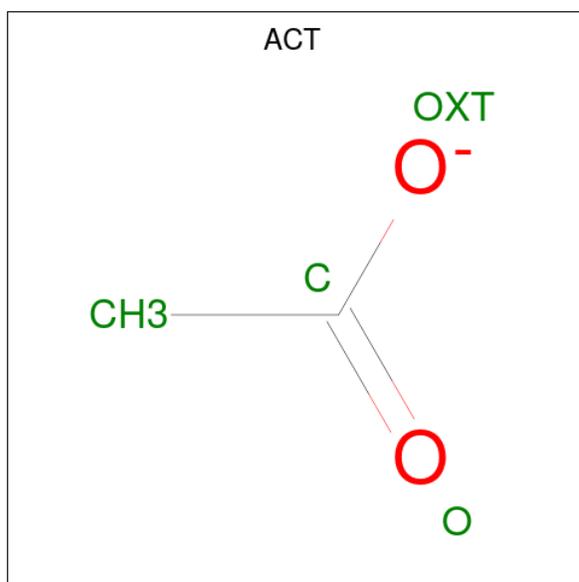
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	5	Total	Na	0	0
			5	5		

- Molecule 3 is (1 {S},2 {S},4 {S},5 {R})-6-(hydroxymethyl)cyclohexane-1,2,3,4,5-pentol (three-letter code: YGX) (formula: C<sub>7</sub>H<sub>14</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	4	0
			25	7	13	5		
3	B	1	Total	C	H	O	4	0
			25	7	13	5		
3	C	1	Total	C	H	O	4	0
			25	7	13	5		
3	D	1	Total	C	H	O	4	0
			25	7	13	5		
3	E	1	Total	C	H	O	4	0
			25	7	13	5		
3	F	1	Total	C	H	O	4	0
			25	7	13	5		
3	G	1	Total	C	H	O	4	0
			25	7	13	5		
3	H	1	Total	C	H	O	4	0
			25	7	13	5		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	7	2	3	2	0	0
4	D	1	7	2	3	2	0	0
4	D	1	7	2	3	2	0	0
4	D	1	7	2	3	2	0	0
4	E	1	7	2	3	2	0	0
4	E	1	7	2	3	2	0	0
4	F	1	7	2	3	2	0	0
4	F	1	7	2	3	2	0	0
4	G	1	7	2	3	2	0	0
4	G	1	7	2	3	2	0	0
4	G	1	7	2	3	2	0	0
4	G	1	7	2	3	2	0	0
4	H	1	7	2	3	2	0	0
4	H	1	7	2	3	2	0	0

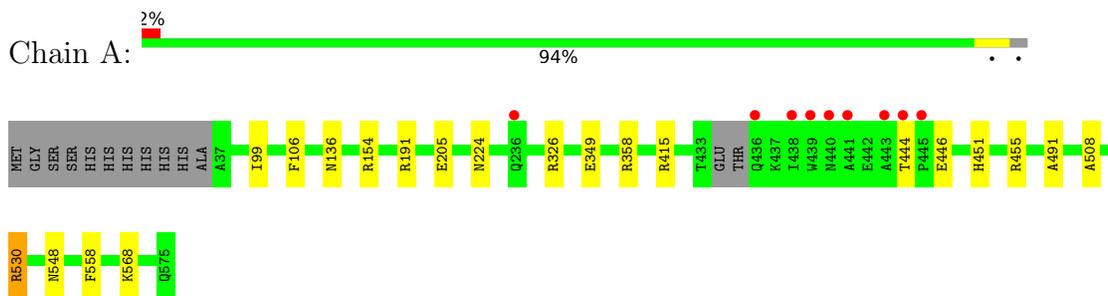
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	468	Total O 468 468	0	0
5	B	552	Total O 552 552	0	0
5	C	467	Total O 467 467	0	0
5	D	590	Total O 590 590	0	0
5	E	635	Total O 635 635	0	0
5	F	569	Total O 569 569	0	0
5	G	635	Total O 635 635	0	0
5	H	497	Total O 497 497	0	0

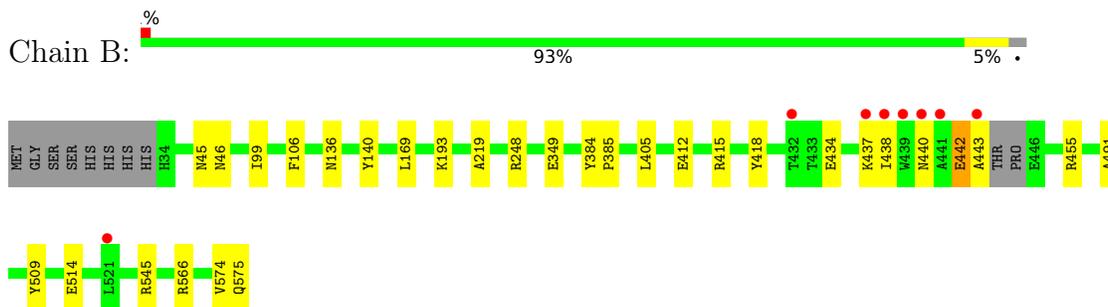
### 3 Residue-property plots [i](#)

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.

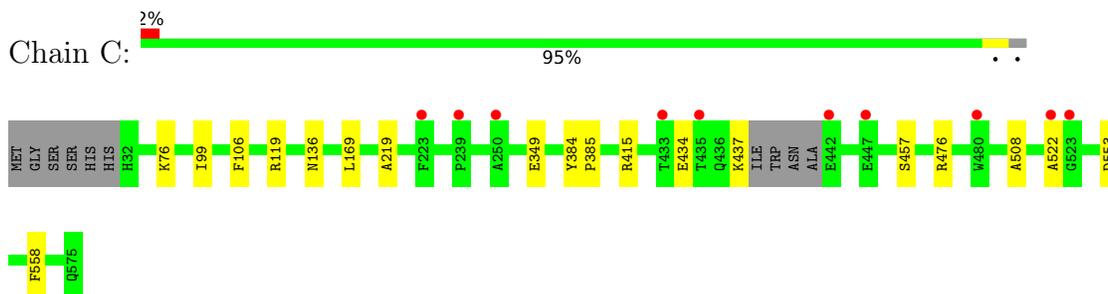
- Molecule 1: Beta-galactosidase, putative, bgl35A



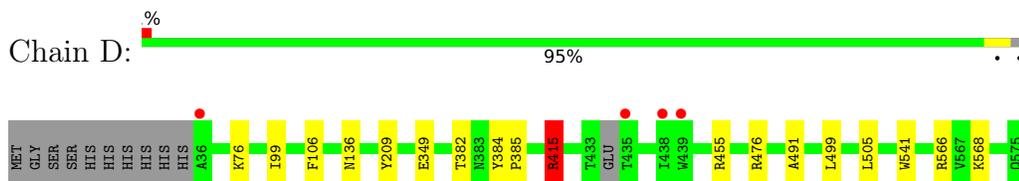
- Molecule 1: Beta-galactosidase, putative, bgl35A



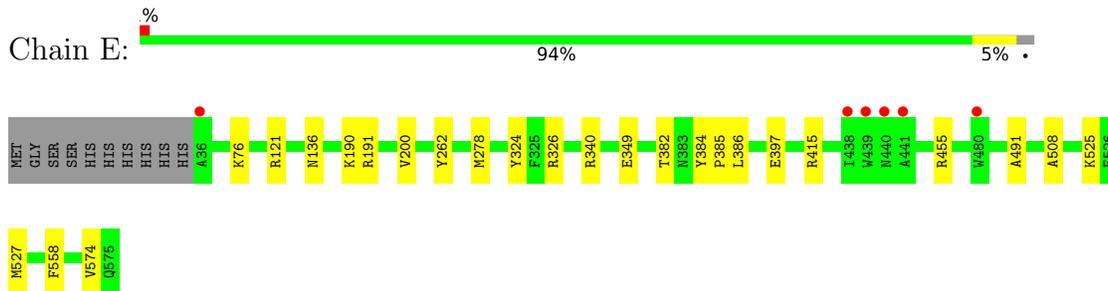
- Molecule 1: Beta-galactosidase, putative, bgl35A



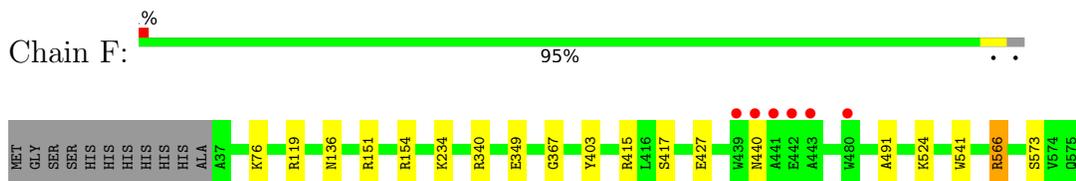
- Molecule 1: Beta-galactosidase, putative, bgl35A



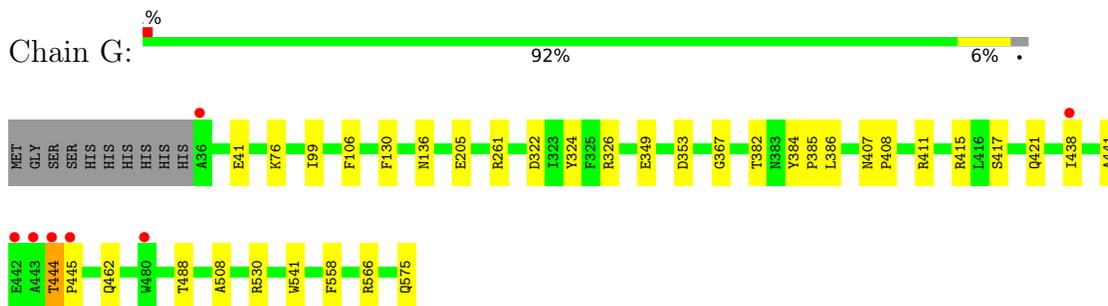
- Molecule 1: Beta-galactosidase, putative, bgl35A



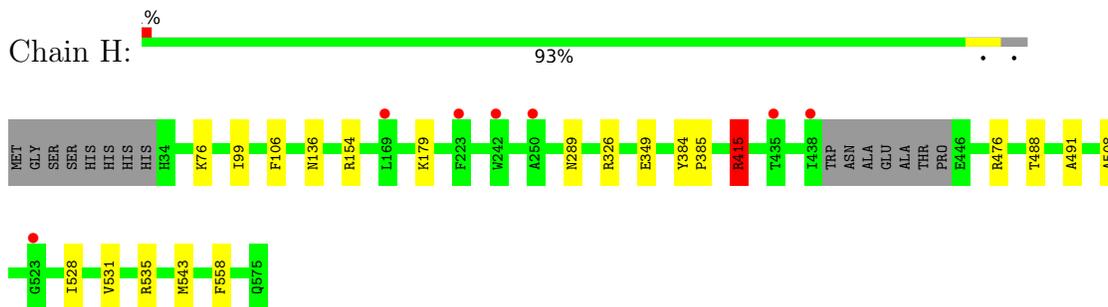
- Molecule 1: Beta-galactosidase, putative, bgl35A



- Molecule 1: Beta-galactosidase, putative, bgl35A



- Molecule 1: Beta-galactosidase, putative, bgl35A



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.32Å 116.21Å 116.40Å 90.24° 89.89° 90.09°	Depositor
Resolution (Å)	82.54 – 1.50 82.41 – 1.50	Depositor EDS
% Data completeness (in resolution range)	96.3 (82.54-1.50) 94.4 (82.41-1.50)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 1.50Å)	Xtrriage
Refinement program	REFMAC 5.8.0411, REFMAC 5.8.0411	Depositor
R, $R_{free}$	0.157 , 0.181 0.165 , 0.186	Depositor DCC
$R_{free}$ test set	39512 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.8	Xtrriage
Anisotropy	0.340	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 49.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.008 for h,-l,k 0.008 for h,l,-k 0.009 for h,-k,-l 0.000 for -h,k,-l 0.000 for -h,-k,l 0.000 for -h,-l,-k 0.000 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	72581	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.75% 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: NA, YGX, ACT

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	0.57	3/4363 (0.1%)	0.84	2/5945 (0.0%)
1	B	0.56	3/4393 (0.1%)	0.86	1/5986 (0.0%)
1	C	0.54	2/4408 (0.0%)	0.85	4/6007 (0.1%)
1	D	0.61	2/4413 (0.0%)	0.92	4/6013 (0.1%)
1	E	0.65	2/4433 (0.0%)	0.92	3/6039 (0.0%)
1	F	0.62	2/4447 (0.0%)	0.94	5/6052 (0.1%)
1	G	0.65	1/4462 (0.0%)	0.95	5/6076 (0.1%)
1	H	0.56	1/4418 (0.0%)	0.87	5/6017 (0.1%)
All	All	0.60	16/35337 (0.0%)	0.90	29/48135 (0.1%)

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	4
1	D	0	1
1	E	0	3
1	F	0	2
1	G	0	1
1	H	0	3
All	All	0	14

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	349	GLU	CD-OE1	12.56	1.39	1.25
1	H	349	GLU	CD-OE1	10.34	1.37	1.25
1	F	349	GLU	CD-OE1	8.94	1.35	1.25
1	A	349	GLU	CD-OE1	8.90	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	349	GLU	CD-OE1	8.86	1.35	1.25
1	G	349	GLU	CD-OE1	8.33	1.34	1.25
1	C	349	GLU	CD-OE1	7.59	1.34	1.25
1	C	349	GLU	CD-OE2	7.30	1.33	1.25
1	A	349	GLU	CD-OE2	7.19	1.33	1.25
1	D	349	GLU	CD-OE1	6.37	1.32	1.25
1	B	514	GLU	CD-OE1	5.99	1.32	1.25
1	D	349	GLU	CD-OE2	5.98	1.32	1.25
1	E	397	GLU	CD-OE1	5.71	1.31	1.25
1	F	427	GLU	CD-OE2	5.56	1.31	1.25
1	B	412	GLU	CD-OE1	5.53	1.31	1.25
1	A	205	GLU	CD-OE2	5.14	1.31	1.25

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	543	MET	CG-SD-CE	-9.32	85.29	100.20
1	D	455	ARG	NE-CZ-NH1	-6.61	117.00	120.30
1	E	262	TYR	CB-CG-CD1	6.41	124.85	121.00
1	E	262	TYR	CB-CG-CD2	-6.29	117.23	121.00
1	A	530	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	F	340	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	H	476	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	D	415	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	A	358	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	G	353	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	G	261	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	545	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	G	130	PHE	CB-CG-CD1	5.74	124.82	120.80
1	D	209	TYR	CB-CG-CD2	-5.70	117.58	121.00
1	C	476	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	E	340	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	F	340	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	C	476	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	G	411	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	G	130	PHE	CB-CG-CD2	-5.42	117.01	120.80
1	D	476	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	C	553	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	C	119	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	H	326	ARG	NE-CZ-NH1	-5.15	117.73	120.30
1	H	415[A]	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	H	415[B]	ARG	NE-CZ-NH2	-5.12	117.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	151	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	F	119	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	F	403	TYR	CB-CG-CD2	-5.06	117.96	121.00

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	ARG	Sidechain
1	A	191[A]	ARG	Sidechain
1	A	415[A]	ARG	Sidechain
1	A	530	ARG	Sidechain
1	D	415	ARG	Sidechain
1	E	121[A]	ARG	Sidechain
1	E	121[B]	ARG	Sidechain
1	E	415	ARG	Sidechain
1	F	154	ARG	Sidechain
1	F	566	ARG	Sidechain
1	G	530[A]	ARG	Sidechain
1	H	154	ARG	Sidechain
1	H	415[A]	ARG	Sidechain
1	H	535	ARG	Sidechain

## 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	4247	4118	4058	11	0
1	B	4276	4143	4087	20	0
1	C	4292	4159	4091	10	0
1	D	4297	4174	4122	8	0
1	E	4310	4199	4146	11	0
1	F	4333	4225	4169	7	0
1	G	4348	4226	4166	19	0
1	H	4301	4187	4133	8	0
2	A	4	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	4	0	0	0	0
2	D	5	0	0	0	0
2	E	6	0	0	0	0
2	F	4	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
3	A	12	13	0	0	0
3	B	12	13	0	0	0
3	C	12	13	0	0	0
3	D	12	13	0	0	0
3	E	12	13	0	0	0
3	F	12	13	0	0	0
3	G	12	13	0	0	0
3	H	12	13	0	0	0
4	A	4	3	3	0	0
4	D	12	9	9	0	0
4	E	8	6	6	0	0
4	F	8	6	6	0	0
4	G	16	12	12	0	0
4	H	8	6	6	0	0
5	A	468	0	0	4	0
5	B	552	0	0	8	0
5	C	467	0	0	5	0
5	D	590	0	0	5	2
5	E	635	0	0	4	1
5	F	569	0	0	4	4
5	G	635	0	0	7	3
5	H	497	0	0	4	0
All	All	39004	33577	33014	93	5

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 1.

All (93) 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:248:ARG:HD2	5:B:711:HOH:O	1.28	1.31
1:G:326[B]:ARG:NH1	5:G:701:HOH:O	1.82	1.13
1:A:326[A]:ARG:NH1	5:A:701:HOH:O	1.92	0.99
1:H:415[A]:ARG:HD2	5:H:801:HOH:O	1.73	0.89
1:E:326[B]:ARG:NH1	5:E:701:HOH:O	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:457:SER:O	5:C:701:HOH:O	2.02	0.76
1:E:76:LYS:HE2	5:E:947:HOH:O	1.92	0.69
1:G:41:GLU:OE2	5:G:702:HOH:O	2.10	0.68
1:D:76:LYS:HE2	5:D:740:HOH:O	1.93	0.67
1:H:179:LYS:CD	5:H:880:HOH:O	2.42	0.66
1:E:382[A]:THR:HG23	5:E:1194:HOH:O	1.96	0.65
1:G:444:THR:HG22	1:G:445:PRO:HD2	1.79	0.65
1:B:415:ARG:NH2	5:B:703:HOH:O	2.37	0.57
1:G:541:TRP:CE2	1:G:566:ARG:HD3	2.40	0.56
1:E:455:ARG:NH1	5:E:704:HOH:O	2.32	0.56
1:A:326[A]:ARG:HG3	1:A:326[A]:ARG:HH11	1.71	0.56
1:C:415[A]:ARG:CZ	5:C:707:HOH:O	2.54	0.56
1:C:434:GLU:O	1:C:437:LYS:N	2.40	0.55
1:D:415:ARG:NE	5:D:703:HOH:O	2.40	0.55
1:B:574:VAL:O	1:B:575:GLN:CB	2.55	0.54
1:A:568:LYS:HE2	5:A:803:HOH:O	2.08	0.53
1:F:415[A]:ARG:CZ	5:F:712:HOH:O	2.56	0.53
1:G:575:GLN:O	5:G:703:HOH:O	2.18	0.53
1:B:415:ARG:CZ	5:B:703:HOH:O	2.56	0.53
1:E:190:LYS:HG3	1:E:191:ARG:HG2	1.91	0.52
1:B:384:TYR:CD1	1:B:385:PRO:HA	2.44	0.52
1:H:384:TYR:CD1	1:H:385:PRO:HA	2.45	0.52
1:C:384:TYR:CD1	1:C:385:PRO:HA	2.45	0.51
1:G:462:GLN:HG2	5:G:741:HOH:O	2.11	0.51
1:A:444:THR:C	1:A:446:GLU:H	2.14	0.50
1:B:455:ARG:NH1	5:B:708:HOH:O	2.42	0.50
1:G:488[A]:THR:HG23	5:G:1244:HOH:O	2.10	0.49
1:D:499:LEU:HD11	1:D:505[B]:LEU:HG	1.95	0.49
1:B:434:GLU:HA	1:B:437:LYS:CB	2.43	0.49
1:D:541:TRP:CE2	1:D:566:ARG:HD3	2.48	0.48
1:G:438:ILE:O	1:G:441:ALA:HB3	2.13	0.48
1:C:415[A]:ARG:NH2	5:C:707:HOH:O	2.46	0.48
1:C:169:LEU:HD13	1:C:219:ALA:HA	1.96	0.48
1:F:415[A]:ARG:NE	5:F:712:HOH:O	2.45	0.48
1:C:76:LYS:CE	5:C:821:HOH:O	2.61	0.47
1:C:415[A]:ARG:NE	5:C:707:HOH:O	2.47	0.47
1:F:234:LYS:NZ	5:F:715:HOH:O	2.47	0.47
1:F:541:TRP:CE2	1:F:566:ARG:HD3	2.48	0.47
1:B:438:ILE:C	1:B:440:ASN:H	2.17	0.47
1:D:384:TYR:CD1	1:D:385:PRO:HA	2.49	0.47
1:F:76[A]:LYS:HE2	5:F:755:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:76:LYS:HE2	5:H:888:HOH:O	2.15	0.47
1:A:326[A]:ARG:HD3	5:A:943:HOH:O	2.14	0.47
1:G:99:ILE:O	1:G:106:PHE:HA	2.16	0.46
1:B:442:GLU:O	1:B:443:ALA:C	2.54	0.46
1:F:524[A]:LYS:HE2	1:F:573[A]:SER:OG	2.15	0.45
1:A:508:ALA:HB3	1:A:558:PHE:CD1	2.52	0.45
1:A:99:ILE:O	1:A:106:PHE:HA	2.17	0.45
1:B:45:ASN:ND2	1:B:418:TYR:OH	2.38	0.45
1:G:508:ALA:HB3	1:G:558:PHE:CD1	2.52	0.45
1:A:326[A]:ARG:NH1	1:A:326[A]:ARG:HG3	2.31	0.45
1:B:193:LYS:HG3	5:B:1021:HOH:O	2.16	0.45
1:A:224:ASN:ND2	5:A:708:HOH:O	2.46	0.45
1:C:99:ILE:O	1:C:106:PHE:HA	2.17	0.45
1:E:525[B]:LYS:HD3	1:E:574:VAL:HG11	1.97	0.45
1:G:76:LYS:HD3	5:G:1220:HOH:O	2.17	0.45
1:D:76:LYS:CE	5:D:740:HOH:O	2.60	0.44
1:G:541:TRP:CH2	1:G:566:ARG:HG3	2.52	0.44
1:E:384:TYR:CD1	1:E:385:PRO:HA	2.52	0.44
1:B:566:ARG:NE	5:B:710:HOH:O	2.49	0.44
1:B:99:ILE:O	1:B:106:PHE:HA	2.17	0.44
1:B:46:ASN:OD1	5:B:701:HOH:O	2.21	0.43
1:F:367:GLY:HA2	1:F:417[A]:SER:OG	2.17	0.43
1:B:405:LEU:HD11	1:B:509:TYR:HB2	1.99	0.43
5:D:732:HOH:O	1:E:527:MET:CE	2.67	0.43
1:D:568:LYS:HE3	5:D:1118:HOH:O	2.18	0.42
1:E:508:ALA:HB3	1:E:558:PHE:CD1	2.54	0.42
1:H:508:ALA:HB3	1:H:558:PHE:CD1	2.55	0.42
1:G:205:GLU:OE2	1:G:322:ASP:OD2	2.37	0.42
1:H:99:ILE:O	1:H:106:PHE:HA	2.20	0.42
1:E:324:TYR:CE1	1:E:386:LEU:HB3	2.55	0.42
1:H:528:ILE:HG21	1:H:531:VAL:HG23	2.02	0.42
1:H:488[B]:THR:HG22	5:H:1033:HOH:O	2.19	0.41
1:G:367:GLY:HA2	1:G:417[A]:SER:OG	2.20	0.41
1:B:169:LEU:CD1	1:B:219:ALA:HA	2.50	0.41
1:G:384:TYR:CD1	1:G:385:PRO:HA	2.56	0.41
1:B:248:ARG:CD	5:B:711:HOH:O	2.12	0.41
1:C:508:ALA:HB3	1:C:558:PHE:CD1	2.56	0.41
1:G:324:TYR:CE1	1:G:386:LEU:HB3	2.55	0.41
1:G:407:ASN:N	1:G:408:PRO:CD	2.83	0.41
1:G:541:TRP:CE2	1:G:566:ARG:CD	3.04	0.41
1:D:99:ILE:O	1:D:106:PHE:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:TYR:CG	1:B:385:PRO:HA	2.55	0.40
1:G:415[B]:ARG:NE	5:G:724:HOH:O	2.54	0.40
1:A:451:HIS:NE2	1:A:455:ARG:HD2	2.37	0.40
1:A:548:ASN:HB3	1:B:140:TYR:CZ	2.56	0.40
1:B:455:ARG:HH11	1:B:455:ARG:HD3	1.68	0.40
1:E:200:VAL:O	1:E:278:MET:HA	2.22	0.40

All (5) 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)
5:F:943:HOH:O	5:G:704:HOH:O[1_565]	2.07	0.13
5:F:997:HOH:O	5:G:1163:HOH:O[1_565]	2.07	0.13
5:D:1210:HOH:O	5:G:1305:HOH:O[1_565]	2.10	0.10
5:D:906:HOH:O	5:F:704:HOH:O[1_554]	2.16	0.04
5:E:1235:HOH:O	5:F:1249:HOH:O[1_554]	2.16	0.04

## 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	540/550 (98%)	519 (96%)	20 (4%)	1 (0%)	47 23
1	B	542/550 (98%)	520 (96%)	20 (4%)	2 (0%)	34 13
1	C	544/550 (99%)	524 (96%)	19 (4%)	1 (0%)	47 23
1	D	545/550 (99%)	526 (96%)	18 (3%)	1 (0%)	47 23
1	E	549/550 (100%)	529 (96%)	19 (4%)	1 (0%)	47 23
1	F	549/550 (100%)	527 (96%)	20 (4%)	2 (0%)	34 13
1	G	552/550 (100%)	534 (97%)	18 (3%)	0	100 100
1	H	543/550 (99%)	524 (96%)	18 (3%)	1 (0%)	47 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4364/4400 (99%)	4203 (96%)	152 (4%)	9 (0%)	47 23

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	522	ALA
1	D	491	ALA
1	A	491	ALA
1	B	491	ALA
1	E	491	ALA
1	B	442	GLU
1	F	440	ASN
1	F	491	ALA
1	H	491	ALA

### 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	431/461 (94%)	430 (100%)	1 (0%)	93 86
1	B	436/461 (95%)	435 (100%)	1 (0%)	93 86
1	C	436/461 (95%)	435 (100%)	1 (0%)	93 86
1	D	441/461 (96%)	439 (100%)	2 (0%)	88 78
1	E	442/461 (96%)	441 (100%)	1 (0%)	93 86
1	F	445/461 (96%)	444 (100%)	1 (0%)	93 86
1	G	445/461 (96%)	440 (99%)	5 (1%)	73 53
1	H	443/461 (96%)	441 (100%)	2 (0%)	88 78
All	All	3519/3688 (95%)	3505 (100%)	14 (0%)	91 82

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	ASN

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Mol	Chain	Res	Type
1	B	136	ASN
1	C	136	ASN
1	D	136	ASN
1	D	382	THR
1	E	136	ASN
1	F	136	ASN
1	G	136	ASN
1	G	382	THR
1	G	421[A]	GLN
1	G	421[B]	GLN
1	G	444	THR
1	H	136	ASN
1	H	289	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	ASN
1	D	45	ASN
1	H	46	ASN

### 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](#)

Of 57 ligands modelled in this entry, 35 are monoatomic - leaving 22 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ACT	G	605	-	3,3,3	0.73	0	3,3,3	0.99	0
4	ACT	H	604	-	3,3,3	1.21	0	3,3,3	1.03	0
3	YGX	E	604	1	12,12,13	0.72	0	14,17,19	0.90	0
4	ACT	A	603	-	3,3,3	0.92	0	3,3,3	0.78	0
3	YGX	D	605	1	12,12,13	0.72	0	14,17,19	0.81	0
4	ACT	G	604	-	3,3,3	1.09	0	3,3,3	0.59	0
4	ACT	D	604	-	3,3,3	0.92	0	3,3,3	1.22	0
4	ACT	E	605	-	3,3,3	1.16	0	3,3,3	0.60	0
3	YGX	F	604	1	12,12,13	1.04	1 (8%)	14,17,19	0.78	0
3	YGX	H	602	1	12,12,13	0.64	0	14,17,19	0.96	1 (7%)
4	ACT	D	606	-	3,3,3	0.80	0	3,3,3	0.99	0
4	ACT	G	607	-	3,3,3	0.94	0	3,3,3	1.02	0
4	ACT	H	603	-	3,3,3	0.94	0	3,3,3	1.03	0
4	ACT	G	606	-	3,3,3	1.37	0	3,3,3	0.38	0
4	ACT	F	606	-	3,3,3	0.92	0	3,3,3	0.74	0
3	YGX	G	603	1	12,12,13	0.56	0	14,17,19	0.83	0
4	ACT	F	605	-	3,3,3	1.06	0	3,3,3	0.80	0
3	YGX	B	602	1	12,12,13	0.60	0	14,17,19	0.79	1 (7%)
3	YGX	A	602	1	12,12,13	0.55	0	14,17,19	0.88	0
4	ACT	D	607	-	3,3,3	1.08	0	3,3,3	0.88	0
3	YGX	C	603	1	12,12,13	0.47	0	14,17,19	1.13	1 (7%)
4	ACT	E	606	-	3,3,3	0.76	0	3,3,3	1.05	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	YGX	D	605	1	-	0/2/22/26	0/1/1/1
3	YGX	H	602	1	-	0/2/22/26	0/1/1/1
3	YGX	B	602	1	-	0/2/22/26	0/1/1/1
3	YGX	A	602	1	-	0/2/22/26	0/1/1/1
3	YGX	F	604	1	-	0/2/22/26	0/1/1/1
3	YGX	C	603	1	-	0/2/22/26	0/1/1/1
3	YGX	E	604	1	-	0/2/22/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	YGX	G	603	1	-	0/2/22/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	604	YGX	C3'-C2'	-2.32	1.48	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	602	YGX	C3'-C2'-C1'	-2.57	106.95	110.69
3	C	603	YGX	C3'-C2'-C1'	-2.24	107.42	110.69
3	B	602	YGX	O1'-C1'-C2'	2.11	114.04	109.99

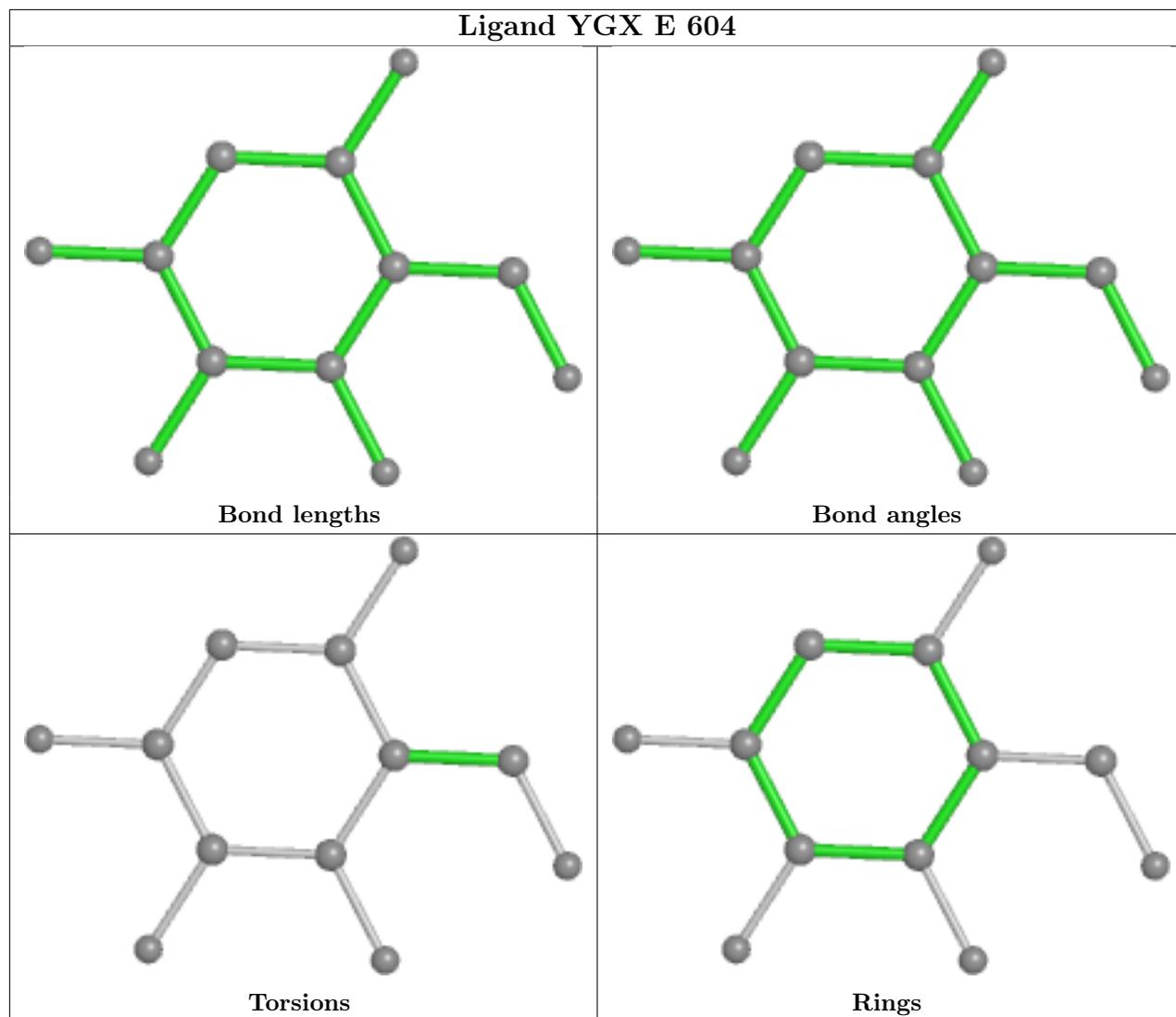
There are no chirality outliers.

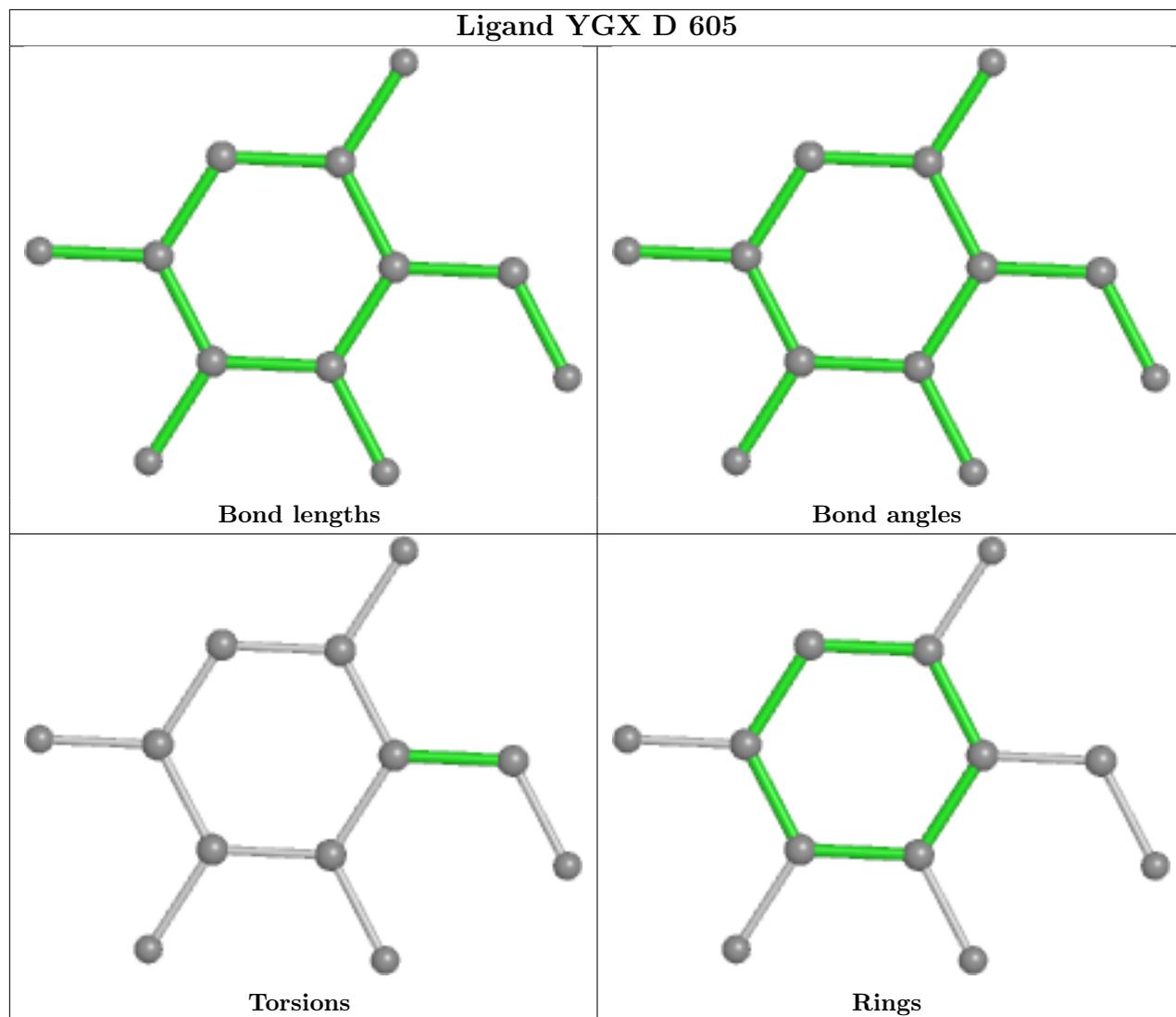
There are no torsion outliers.

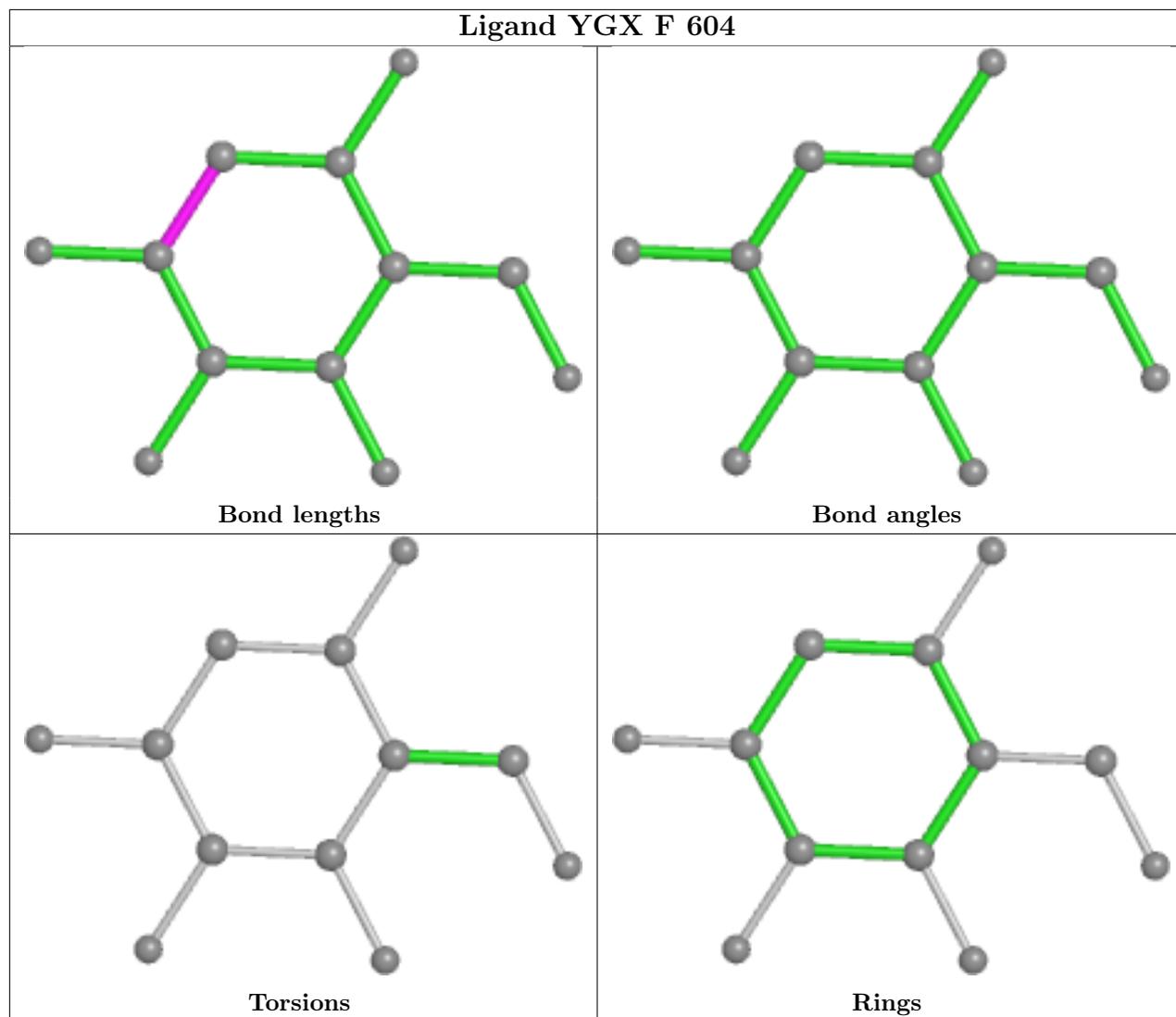
There are no ring outliers.

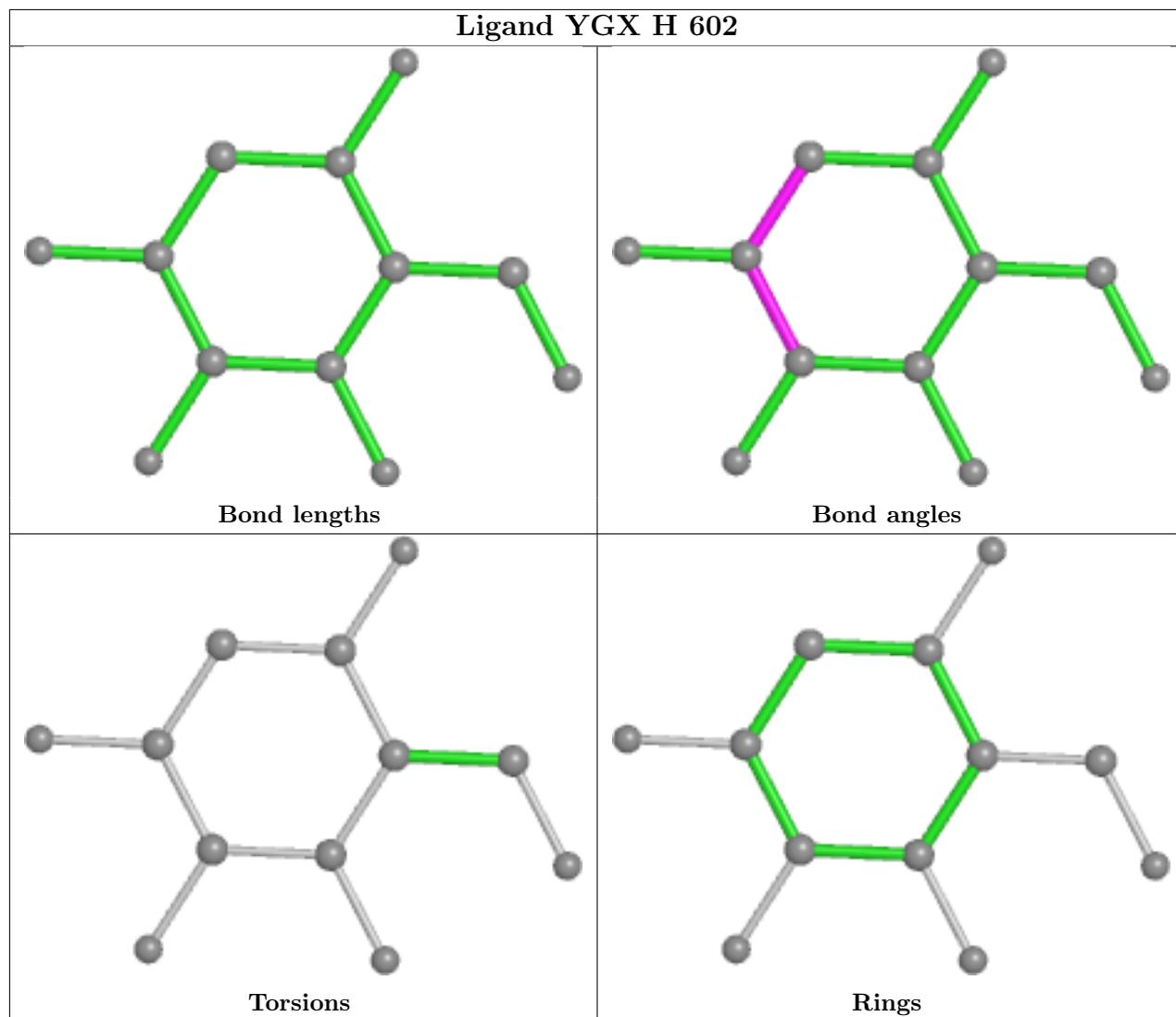
No monomer is involved in short contacts.

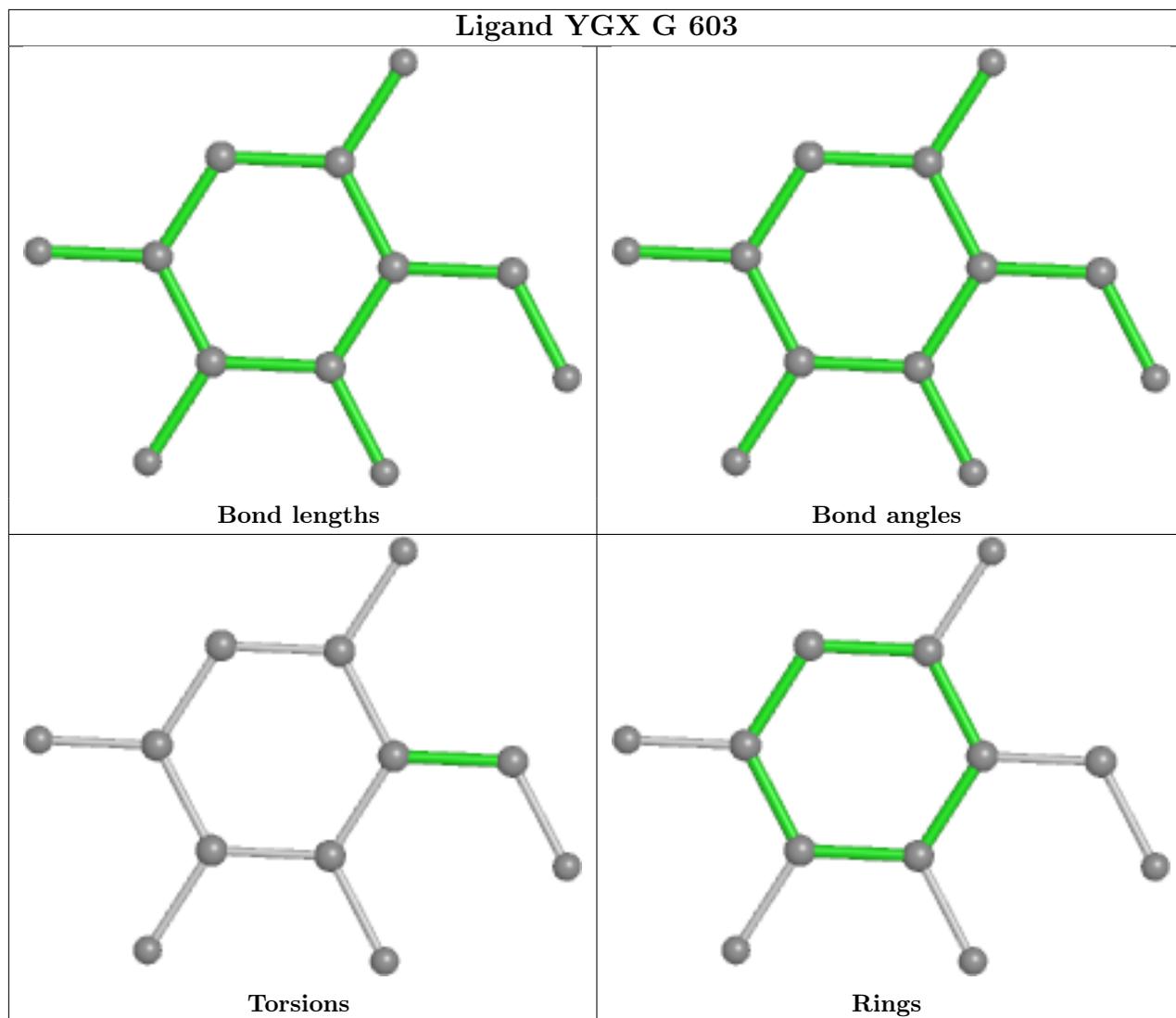
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

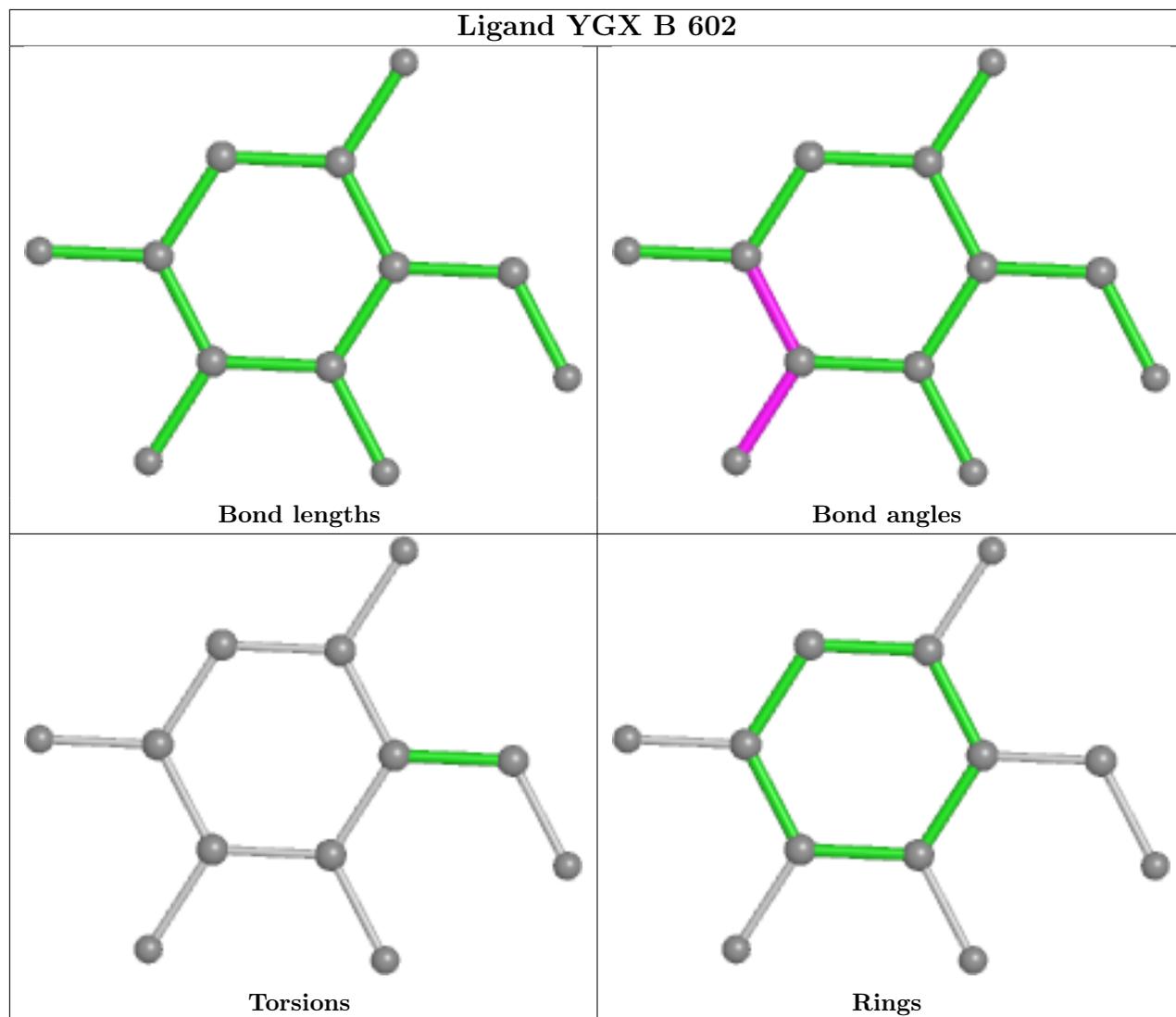


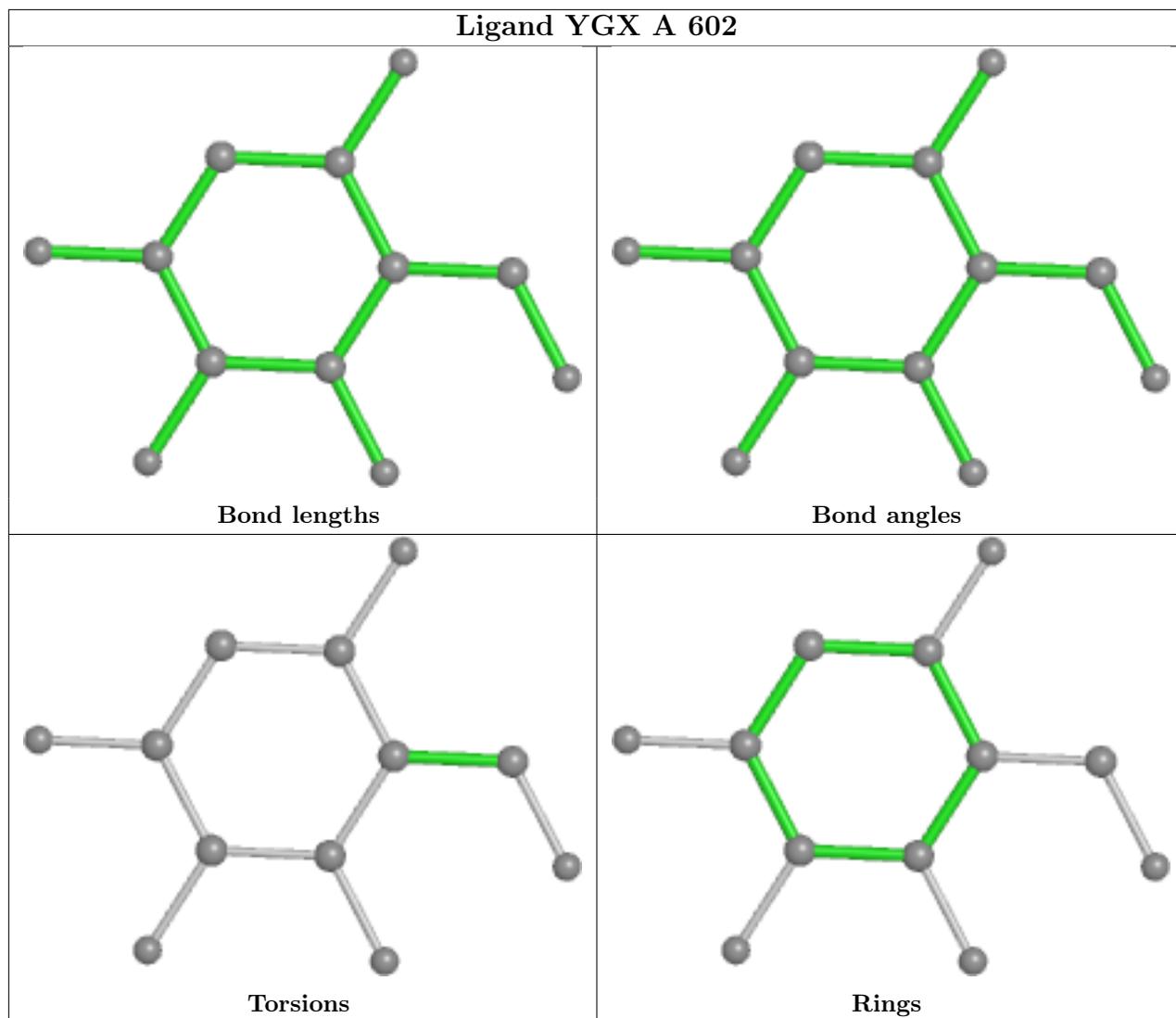


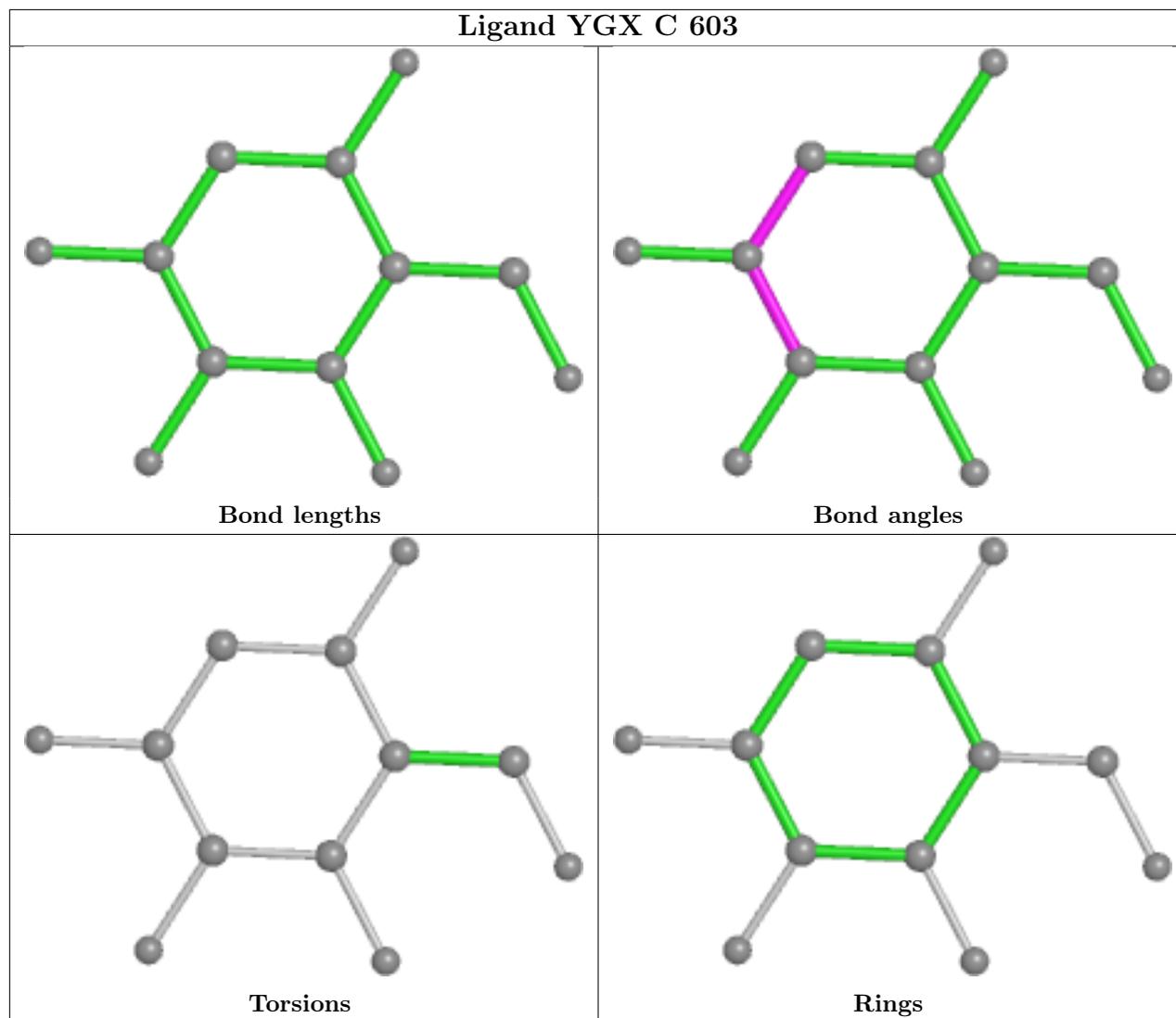












## 5.7 Other polymers [i](#)

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

### 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	537/550 (97%)	-0.24	9 (1%) 70 75	17, 25, 43, 68	41 (7%)
1	B	540/550 (98%)	-0.35	8 (1%) 73 78	16, 23, 39, 66	34 (6%)
1	C	540/550 (98%)	-0.21	10 (1%) 66 71	18, 25, 41, 63	34 (6%)
1	D	539/550 (98%)	-0.33	4 (0%) 87 90	15, 21, 38, 61	32 (5%)
1	E	540/550 (98%)	-0.31	6 (1%) 80 84	14, 20, 37, 59	33 (6%)
1	F	539/550 (98%)	-0.28	6 (1%) 80 84	14, 21, 41, 61	35 (6%)
1	G	540/550 (98%)	-0.26	7 (1%) 77 81	14, 20, 39, 59	31 (5%)
1	H	535/550 (97%)	-0.28	7 (1%) 77 81	17, 24, 39, 70	44 (8%)
All	All	4310/4400 (97%)	-0.28	57 (1%) 77 81	14, 23, 41, 70	284 (6%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	439	TRP	8.5
1	A	439	TRP	7.6
1	B	439	TRP	6.9
1	D	439	TRP	6.8
1	A	438	ILE	6.4
1	A	441	ALA	6.2
1	B	441	ALA	5.5
1	H	438	ILE	5.5
1	B	443	ALA	5.5
1	A	440	ASN	4.9
1	G	445	PRO	4.7
1	E	36	ALA	4.7
1	G	444	THR	4.7
1	D	435	THR	4.1
1	B	440	ASN	4.0
1	A	443	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	G	443	ALA	3.9
1	G	438	ILE	3.9
1	C	435	THR	3.9
1	D	438	ILE	3.7
1	F	440	ASN	3.7
1	B	521	LEU	3.6
1	F	439	TRP	3.4
1	A	444	THR	3.4
1	H	523	GLY	3.3
1	E	441	ALA	3.2
1	C	433	THR	3.0
1	H	435	THR	2.9
1	E	438	ILE	2.9
1	H	242	TRP	2.7
1	E	440	ASN	2.7
1	E	480	TRP	2.6
1	C	250	ALA	2.6
1	A	436	GLN	2.6
1	H	169[A]	LEU	2.6
1	B	432	THR	2.6
1	G	36	ALA	2.5
1	C	522	ALA	2.5
1	F	441	ALA	2.5
1	B	438	ILE	2.5
1	F	443	ALA	2.5
1	C	480	TRP	2.4
1	C	442	GLU	2.4
1	G	442	GLU	2.3
1	F	480	TRP	2.3
1	C	447	GLU	2.3
1	D	36	ALA	2.2
1	H	223	PHE	2.2
1	C	523	GLY	2.2
1	A	236	GLN	2.2
1	C	239	PRO	2.2
1	G	480	TRP	2.2
1	B	437	LYS	2.2
1	F	442	GLU	2.1
1	C	223	PHE	2.1
1	A	445	PRO	2.1
1	H	250	ALA	2.1

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

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

## 6.3 Carbohydrates [i](#)

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
4	ACT	G	606	4/4	0.76	0.16	30,32,35,36	7
4	ACT	F	606	4/4	0.82	0.15	28,28,29,29	7
4	ACT	D	607	4/4	0.87	0.14	30,39,39,40	7
4	ACT	G	605	4/4	0.87	0.16	34,34,35,36	7
4	ACT	E	606	4/4	0.87	0.15	29,34,34,34	7
4	ACT	D	604	4/4	0.90	0.14	29,33,34,38	0
2	NA	C	601	1/1	0.91	0.08	45,45,45,45	0
4	ACT	D	606	4/4	0.91	0.32	40,40,44,44	7
4	ACT	F	605	4/4	0.91	0.10	28,33,34,35	7
4	ACT	H	603	4/4	0.91	0.12	37,44,44,44	7
4	ACT	H	604	4/4	0.91	0.10	27,31,32,34	7
4	ACT	A	603	4/4	0.92	0.12	27,33,33,34	7
2	NA	E	608	1/1	0.93	0.09	39,39,39,39	0
2	NA	H	608	1/1	0.94	0.06	39,39,39,39	0
4	ACT	G	607	4/4	0.94	0.08	33,34,34,35	7
2	NA	E	607	1/1	0.94	0.07	28,28,28,28	0
2	NA	C	602	1/1	0.94	0.10	38,38,38,38	0
4	ACT	G	604	4/4	0.96	0.14	20,23,24,24	7
4	ACT	E	605	4/4	0.96	0.16	23,24,25,26	7
2	NA	D	601	1/1	0.97	0.09	22,22,22,22	0
3	YGX	C	603	12/13	0.97	0.07	17,19,21,25	4
2	NA	D	609	1/1	0.97	0.07	28,28,28,28	0
2	NA	A	605	1/1	0.97	0.11	34,34,34,34	0
2	NA	A	606	1/1	0.97	0.06	32,32,32,32	0
2	NA	G	608	1/1	0.97	0.06	25,25,25,25	0
2	NA	H	601	1/1	0.97	0.09	34,34,34,34	0
2	NA	H	607	1/1	0.97	0.07	30,30,30,30	1

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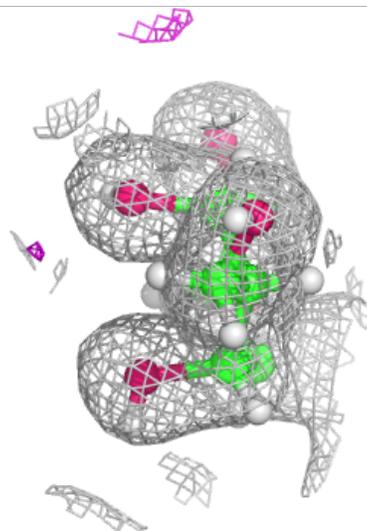
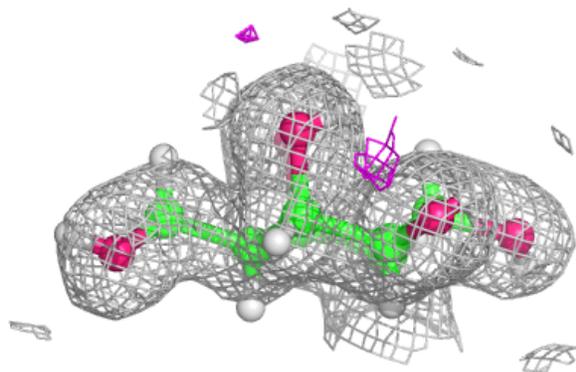
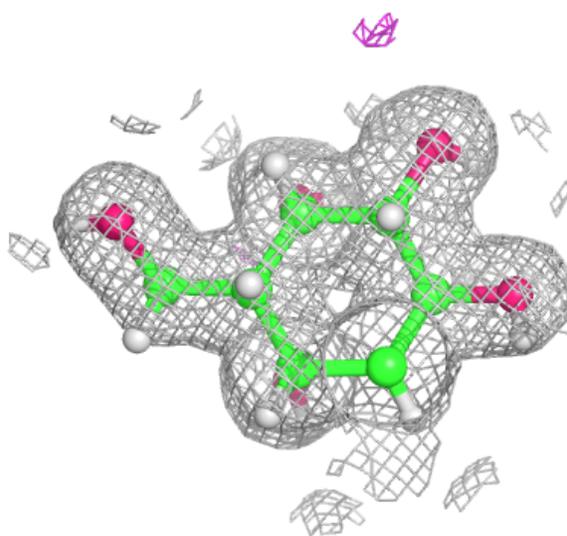
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	YGX	A	602	12/13	0.98	0.06	17,18,21,21	4
3	YGX	B	602	12/13	0.98	0.07	16,17,20,21	4
2	NA	E	601	1/1	0.98	0.06	22,22,22,22	0
3	YGX	D	605	12/13	0.98	0.06	16,16,18,19	4
3	YGX	E	604	12/13	0.98	0.07	14,15,17,18	4
3	YGX	F	604	12/13	0.98	0.08	14,16,17,18	4
3	YGX	G	603	12/13	0.98	0.08	14,15,16,17	4
3	YGX	H	602	12/13	0.98	0.06	17,18,20,20	4
2	NA	D	602	1/1	0.98	0.06	24,24,24,24	0
2	NA	A	604	1/1	0.98	0.05	27,27,27,27	0
2	NA	F	607	1/1	0.98	0.08	26,26,26,26	0
2	NA	A	601	1/1	0.99	0.04	29,29,29,29	0
2	NA	G	602	1/1	0.99	0.05	20,20,20,20	0
2	NA	D	608	1/1	0.99	0.06	24,24,24,24	0
2	NA	G	609	1/1	0.99	0.06	24,24,24,24	0
2	NA	G	610	1/1	0.99	0.05	25,25,25,25	0
2	NA	B	601	1/1	0.99	0.07	31,31,31,31	0
2	NA	H	605	1/1	0.99	0.08	27,27,27,27	0
2	NA	H	606	1/1	0.99	0.05	31,31,31,31	0
2	NA	C	604	1/1	0.99	0.06	28,28,28,28	0
2	NA	E	602	1/1	0.99	0.07	20,20,20,20	0
2	NA	E	603	1/1	0.99	0.07	22,22,22,22	0
2	NA	C	605	1/1	0.99	0.05	30,30,30,30	0
2	NA	B	603	1/1	0.99	0.06	27,27,27,27	0
2	NA	E	609	1/1	0.99	0.08	23,23,23,23	0
2	NA	F	601	1/1	0.99	0.07	23,23,23,23	0
2	NA	F	602	1/1	0.99	0.05	25,25,25,25	0
2	NA	D	603	1/1	1.00	0.07	20,20,20,20	0
2	NA	G	601	1/1	1.00	0.08	24,24,24,24	0
2	NA	F	603	1/1	1.00	0.07	20,20,20,20	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.

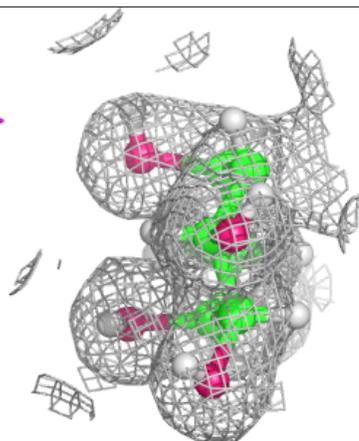
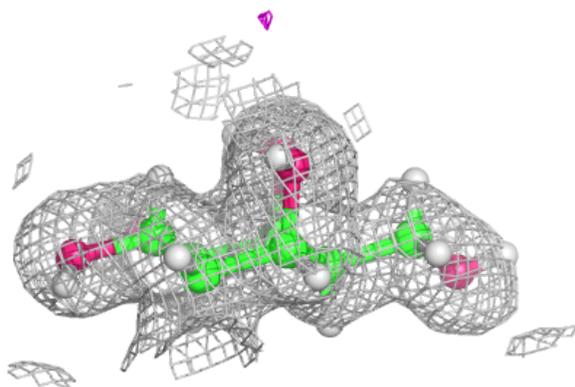
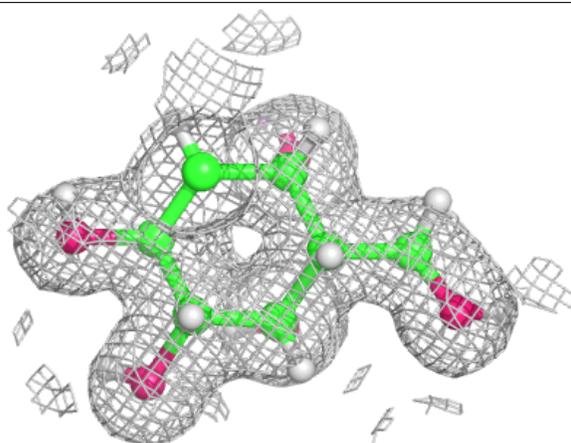
**Electron density around YGX C 603:**

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



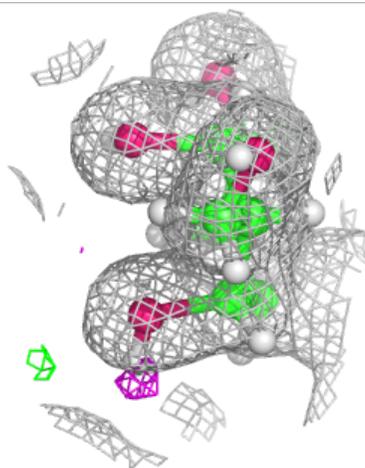
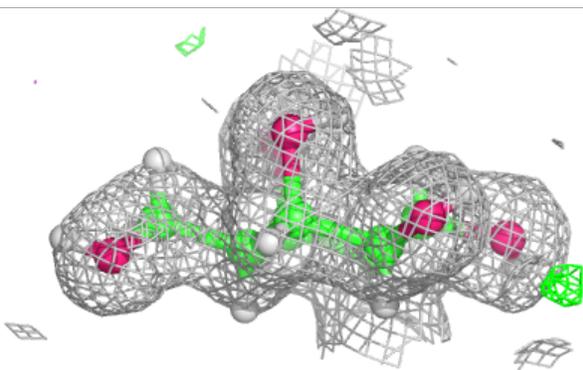
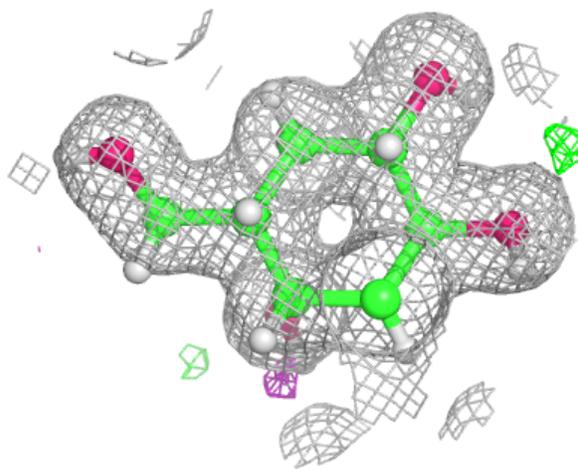
**Electron density around YGX A 602:**

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



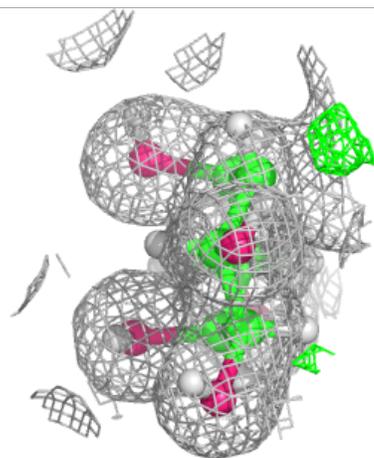
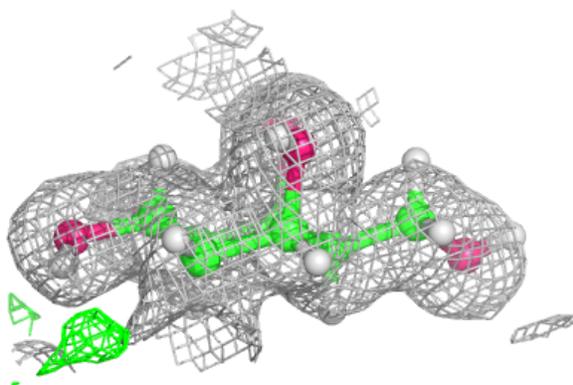
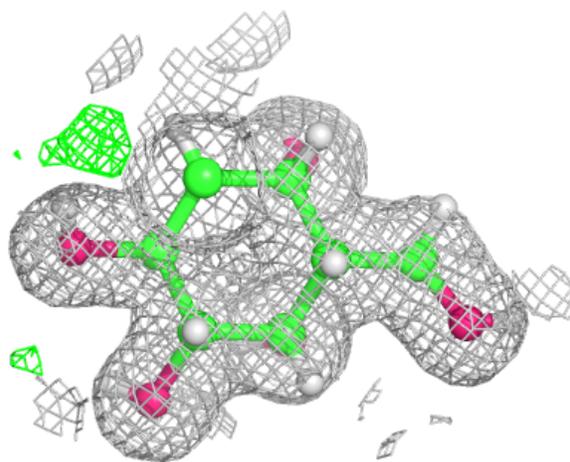
**Electron density around YGX B 602:**

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



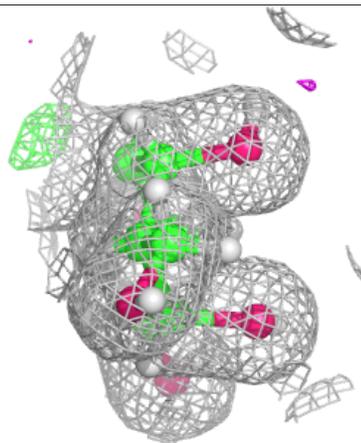
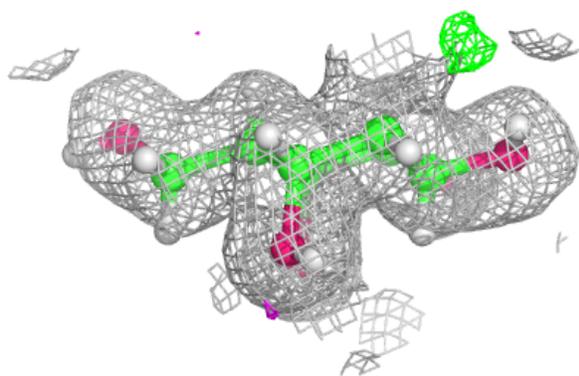
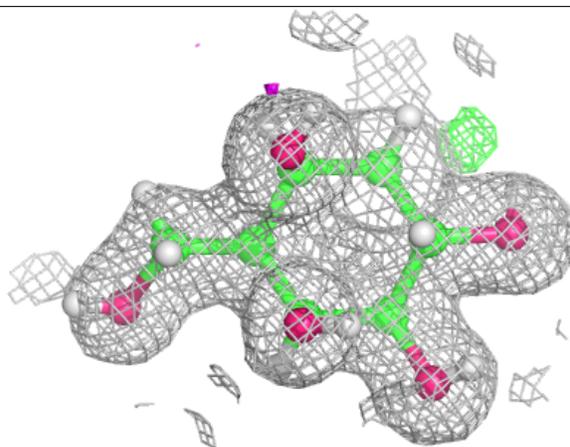
**Electron density around YGX D 605:**

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



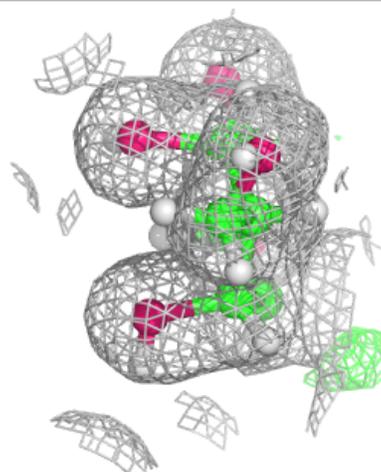
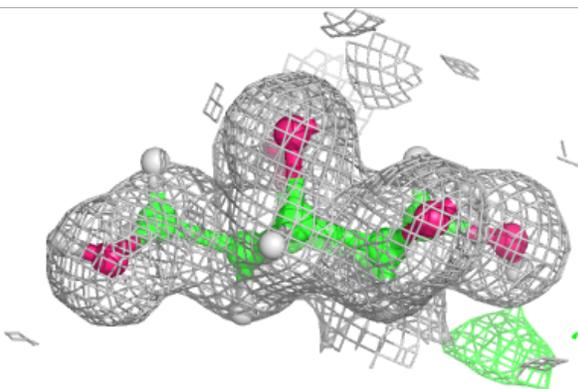
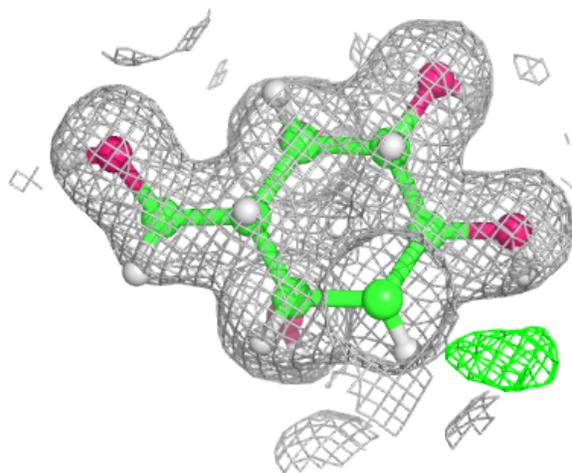
**Electron density around YGX E 604:**

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and green (positive)



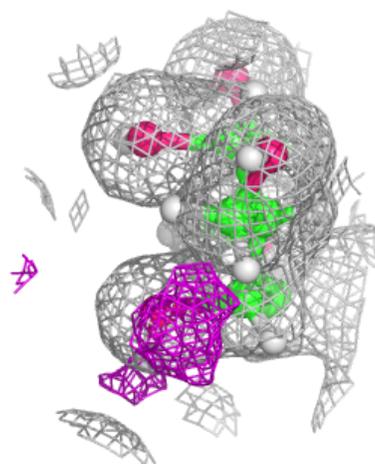
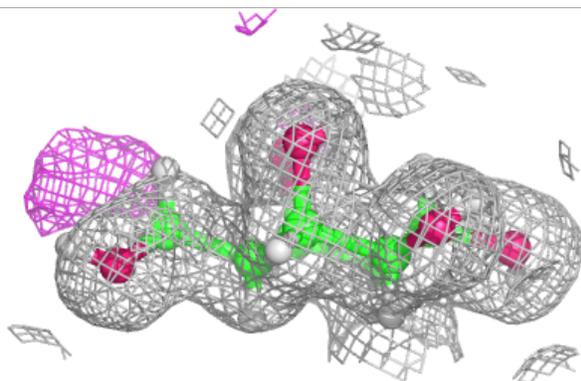
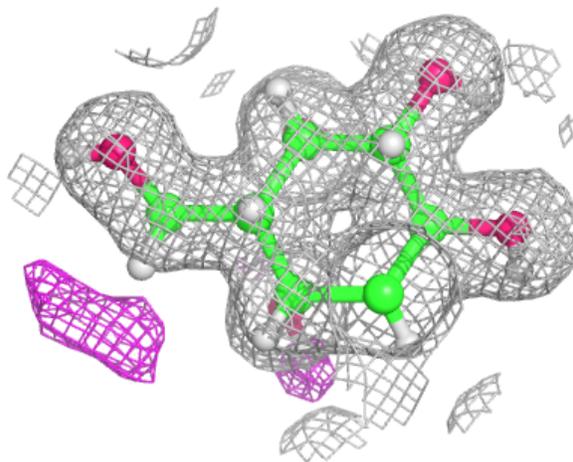
**Electron density around YGX F 604:**

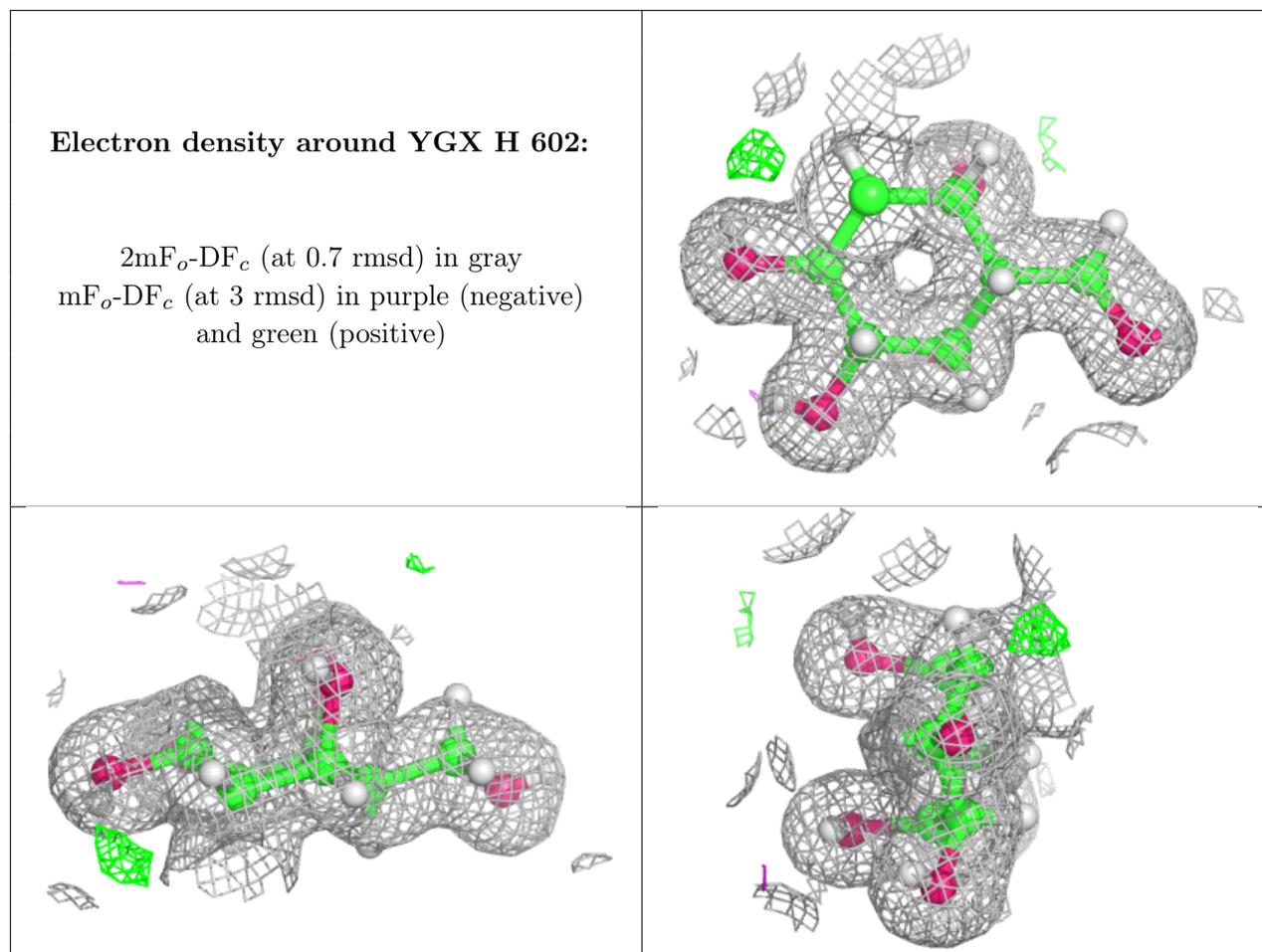
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around YGX G 603:**

$2mF_o-DF_c$  (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.