



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2023 – 09:22 PM EDT

PDB ID : 3GH8  
Title : Crystal structure of Mus musculus iodotyrosine deiodinase (IYD) bound to FMN and di-iodotyrosine (DIT)  
Authors : Thomas, S.R.; McTamney, P.M.; Adler, J.M.; LaRonde-LeBlanc, N.; Rokita, S.E.  
Deposited on : 2009-03-03  
Resolution : 2.61 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>.

---

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

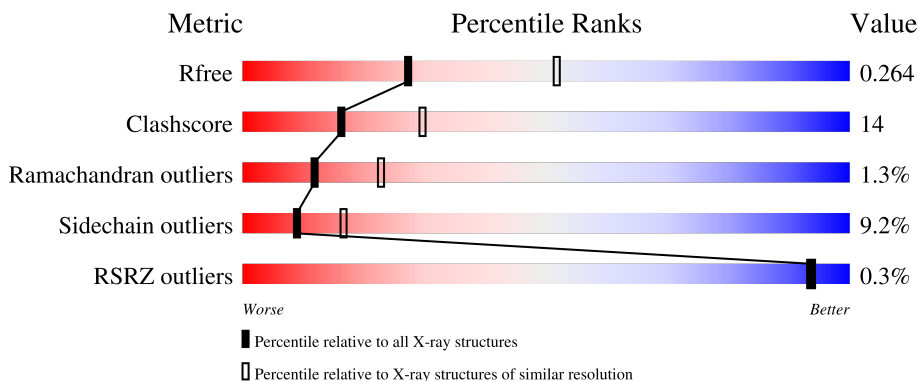
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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	259	
1	B	259	
1	C	259	
1	D	259	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	E	259	 60% 23% • 15%
1	F	259	 58% 22% • 15%
1	G	259	 58% 23% •• 15%
1	H	259	 57% 25% • 15%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14910 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 Iodotyrosine dehalogenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	221	Total 1783	C 1142	N 317	O 315	S 9	0	0	0
1	B	220	Total 1773	C 1136	N 314	O 314	S 9	0	0	0
1	C	221	Total 1783	C 1142	N 317	O 315	S 9	0	0	0
1	D	220	Total 1777	C 1139	N 316	O 313	S 9	0	0	0
1	E	221	Total 1783	C 1142	N 317	O 315	S 9	0	0	0
1	F	220	Total 1773	C 1136	N 314	O 314	S 9	0	0	0
1	G	221	Total 1783	C 1142	N 317	O 315	S 9	0	0	0
1	H	220	Total 1777	C 1139	N 316	O 313	S 9	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	MET	-	expression tag	UNP Q9DCX8
A	286	HIS	-	expression tag	UNP Q9DCX8
A	287	HIS	-	expression tag	UNP Q9DCX8
A	288	HIS	-	expression tag	UNP Q9DCX8
A	289	HIS	-	expression tag	UNP Q9DCX8
A	290	HIS	-	expression tag	UNP Q9DCX8
A	291	HIS	-	expression tag	UNP Q9DCX8
B	33	MET	-	expression tag	UNP Q9DCX8
B	286	HIS	-	expression tag	UNP Q9DCX8
B	287	HIS	-	expression tag	UNP Q9DCX8
B	288	HIS	-	expression tag	UNP Q9DCX8
B	289	HIS	-	expression tag	UNP Q9DCX8
B	290	HIS	-	expression tag	UNP Q9DCX8

*Continued on next page...*

*Continued from previous page...*

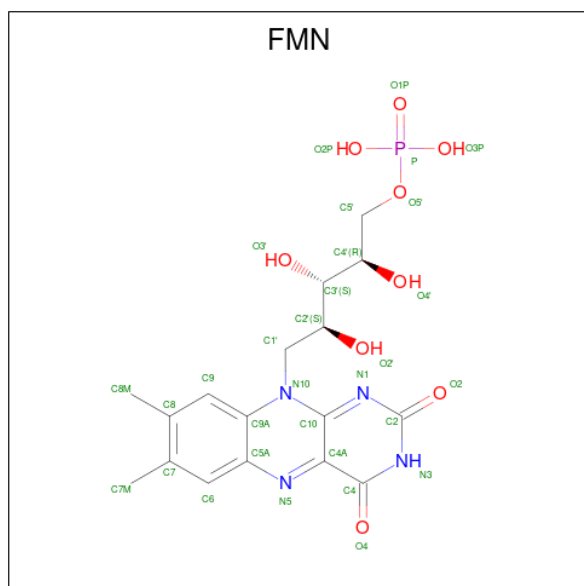
Chain	Residue	Modelled	Actual	Comment	Reference
B	291	HIS	-	expression tag	UNP Q9DCX8
C	33	MET	-	expression tag	UNP Q9DCX8
C	286	HIS	-	expression tag	UNP Q9DCX8
C	287	HIS	-	expression tag	UNP Q9DCX8
C	288	HIS	-	expression tag	UNP Q9DCX8
C	289	HIS	-	expression tag	UNP Q9DCX8
C	290	HIS	-	expression tag	UNP Q9DCX8
C	291	HIS	-	expression tag	UNP Q9DCX8
D	33	MET	-	expression tag	UNP Q9DCX8
D	286	HIS	-	expression tag	UNP Q9DCX8
D	287	HIS	-	expression tag	UNP Q9DCX8
D	288	HIS	-	expression tag	UNP Q9DCX8
D	289	HIS	-	expression tag	UNP Q9DCX8
D	290	HIS	-	expression tag	UNP Q9DCX8
D	291	HIS	-	expression tag	UNP Q9DCX8
E	33	MET	-	expression tag	UNP Q9DCX8
E	286	HIS	-	expression tag	UNP Q9DCX8
E	287	HIS	-	expression tag	UNP Q9DCX8
E	288	HIS	-	expression tag	UNP Q9DCX8
E	289	HIS	-	expression tag	UNP Q9DCX8
E	290	HIS	-	expression tag	UNP Q9DCX8
E	291	HIS	-	expression tag	UNP Q9DCX8
F	33	MET	-	expression tag	UNP Q9DCX8
F	286	HIS	-	expression tag	UNP Q9DCX8
F	287	HIS	-	expression tag	UNP Q9DCX8
F	288	HIS	-	expression tag	UNP Q9DCX8
F	289	HIS	-	expression tag	UNP Q9DCX8
F	290	HIS	-	expression tag	UNP Q9DCX8
F	291	HIS	-	expression tag	UNP Q9DCX8
G	33	MET	-	expression tag	UNP Q9DCX8
G	286	HIS	-	expression tag	UNP Q9DCX8
G	287	HIS	-	expression tag	UNP Q9DCX8
G	288	HIS	-	expression tag	UNP Q9DCX8
G	289	HIS	-	expression tag	UNP Q9DCX8
G	290	HIS	-	expression tag	UNP Q9DCX8
G	291	HIS	-	expression tag	UNP Q9DCX8
H	33	MET	-	expression tag	UNP Q9DCX8
H	286	HIS	-	expression tag	UNP Q9DCX8
H	287	HIS	-	expression tag	UNP Q9DCX8
H	288	HIS	-	expression tag	UNP Q9DCX8
H	289	HIS	-	expression tag	UNP Q9DCX8
H	290	HIS	-	expression tag	UNP Q9DCX8

*Continued on next page...*

Continued from previous page...

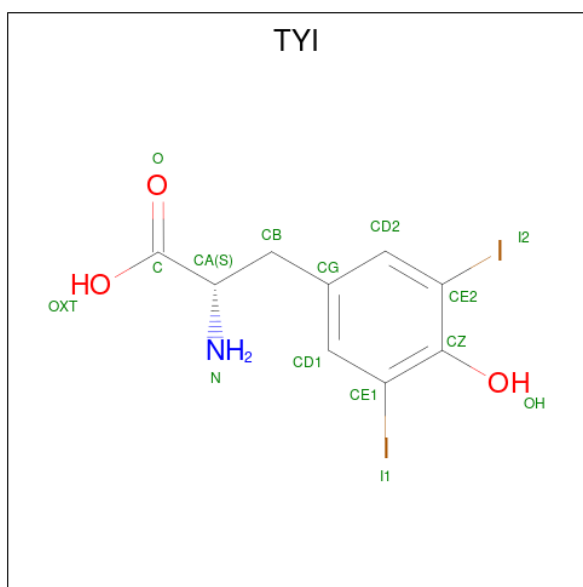
Chain	Residue	Modelled	Actual	Comment	Reference
H	291	HIS	-	expression tag	UNP Q9DCX8

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	E	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	F	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is 3,5-DIODOTYROSINE (three-letter code: TYI) (formula:  $C_9H_9I_2NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	I	N			O
3	A	1	Total	C	I	N	O	0	0
			15	9	2	1	3		
3	B	1	Total	C	I	N	O	0	0
			15	9	2	1	3		
3	C	1	Total	C	I	N	O	0	0
			15	9	2	1	3		
3	D	1	Total	C	I	N	O	0	0
			15	9	2	1	3		
3	E	1	Total	C	I	N	O	0	0
			15	9	2	1	3		
3	F	1	Total	C	I	N	O	0	0
			15	9	2	1	3		
3	G	1	Total	C	I	N	O	0	0
			15	9	2	1	3		
3	H	1	Total	C	I	N	O	0	0
			15	9	2	1	3		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	P	0	0
			5	4	1		
4	G	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

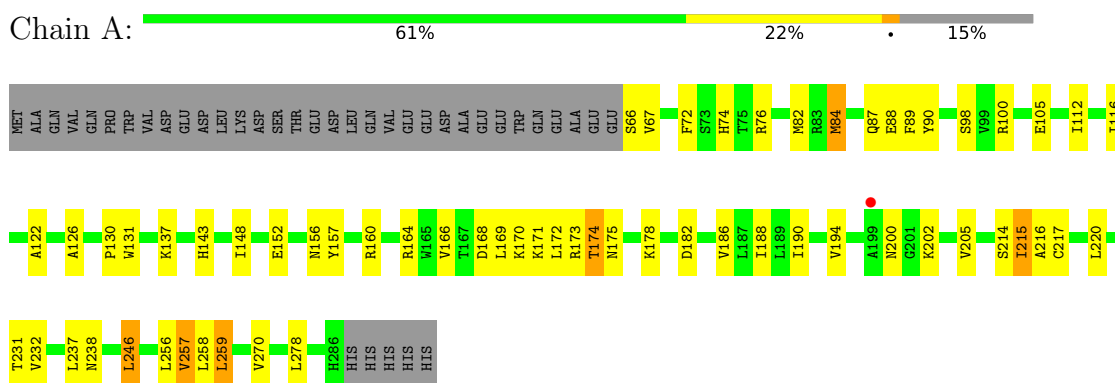
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	36	Total	O	0	0
			36	36		
5	B	38	Total	O	0	0
			38	38		
5	C	39	Total	O	0	0
			39	39		
5	D	23	Total	O	0	0
			23	23		
5	E	48	Total	O	0	0
			48	48		
5	F	40	Total	O	0	0
			40	40		
5	G	38	Total	O	0	0
			38	38		
5	H	38	Total	O	0	0
			38	38		



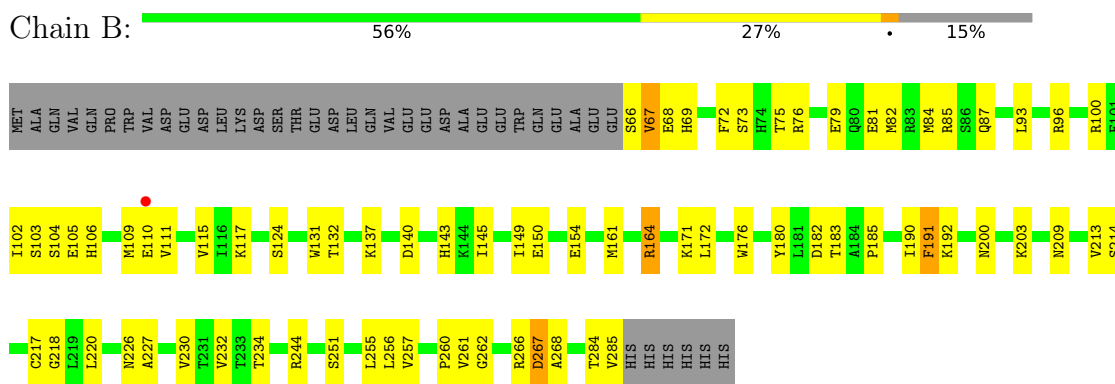
### 3 Residue-property plots i

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.

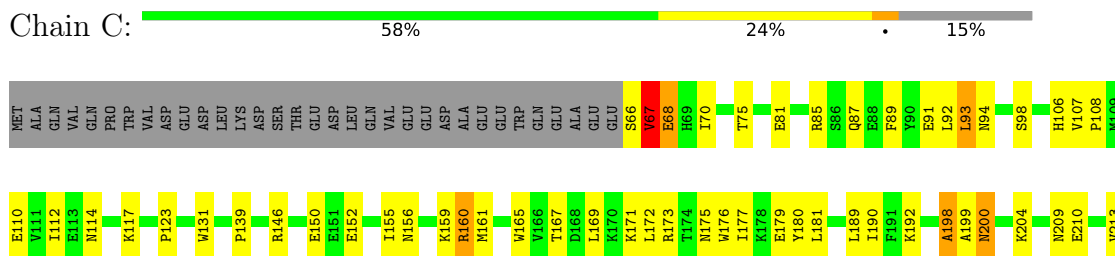
- Molecule 1: Iodotyrosine dehalogenase 1

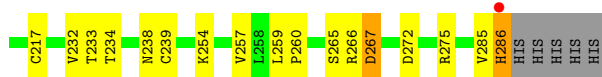


- Molecule 1: Iodotyrosine dehalogenase 1

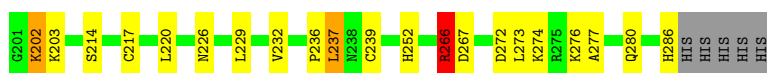
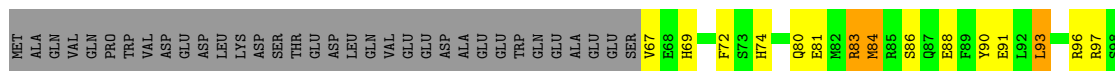


- Molecule 1: Iodotyrosine dehalogenase 1

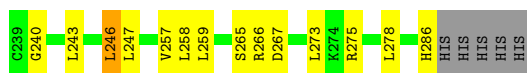
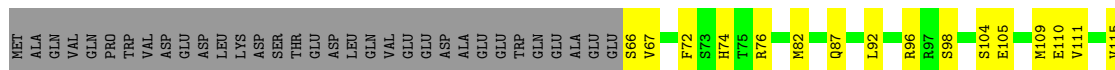




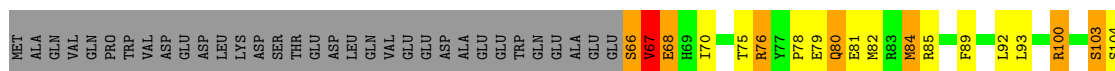
- Molecule 1: Iodotyrosine dehalogenase 1



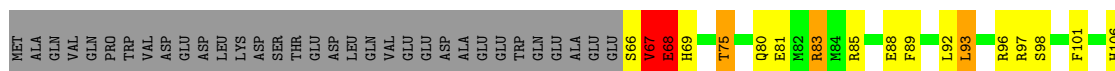
- Molecule 1: Iodotyrosine dehalogenase 1

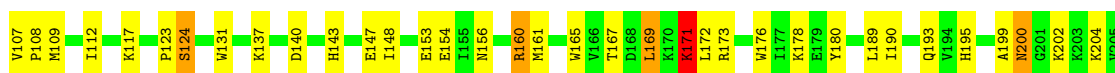


- Molecule 1: Iodotyrosine dehalogenase 1

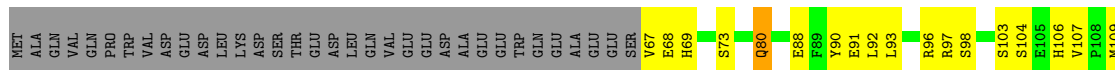


- Molecule 1: Iodotyrosine dehalogenase 1





● Molecule 1: Iodotyrosine dehalogenase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.61Å 112.57Å 189.25Å 90.00° 89.92° 90.00°	Depositor
Resolution (Å)	30.00 – 2.61 48.37 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.8 (30.00-2.61) 96.7 (48.37-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.26 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.181 , 0.264 0.182 , 0.264	Depositor DCC
$R_{free}$ test set	3203 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.1	Xtrriage
Anisotropy	0.986	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 14.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.457 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14910	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.42% 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: PO4, TYI, FMN

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	0.92	0/1823	0.92	2/2468 (0.1%)
1	B	0.89	1/1812 (0.1%)	0.93	1/2453 (0.0%)
1	C	0.86	0/1823	0.91	1/2468 (0.0%)
1	D	0.88	0/1817	0.90	4/2460 (0.2%)
1	E	0.93	2/1823 (0.1%)	0.90	1/2468 (0.0%)
1	F	0.91	1/1812 (0.1%)	0.96	4/2453 (0.2%)
1	G	0.88	0/1823	0.92	0/2468
1	H	0.92	1/1817 (0.1%)	0.90	2/2460 (0.1%)
All	All	0.90	5/14550 (0.0%)	0.92	15/19698 (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	C	0	1
1	F	1	1
1	G	0	1
All	All	1	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	191	PHE	CE2-CZ	6.18	1.49	1.37
1	E	207	TYR	CE2-CZ	5.95	1.46	1.38
1	E	217	CYS	CB-SG	-5.74	1.72	1.81
1	H	239	CYS	CB-SG	-5.20	1.73	1.81
1	F	217	CYS	CB-SG	-5.05	1.73	1.81

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	100	ARG	NE-CZ-NH1	-11.56	114.52	120.30
1	F	100	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	A	246	LEU	CA-CB-CG	6.47	130.18	115.30
1	E	246	LEU	CA-CB-CG	6.33	129.85	115.30
1	H	237	LEU	CA-CB-CG	5.95	128.98	115.30
1	D	160	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	B	102	ILE	CG1-CB-CG2	-5.89	98.44	111.40
1	D	83	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	A	168	ASP	CB-CG-OD1	5.58	123.33	118.30
1	F	259	LEU	CA-CB-CG	5.56	128.09	115.30
1	H	266	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	F	67	VAL	N-CA-C	5.43	125.67	111.00
1	D	266	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	D	237	LEU	CA-CB-CG	5.18	127.22	115.30
1	C	204	LYS	CD-CE-NZ	5.03	123.27	111.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	67	VAL	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	285	VAL	Peptide
1	F	66	SER	Peptide
1	G	285	VAL	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	1783	0	1839	42	0
1	B	1773	0	1832	58	0
1	C	1783	0	1839	69	0
1	D	1777	0	1834	70	0
1	E	1783	0	1839	34	0
1	F	1773	0	1832	58	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1783	0	1839	55	0
1	H	1777	0	1834	68	0
2	A	31	0	19	3	0
2	B	31	0	19	4	0
2	C	31	0	19	2	0
2	D	31	0	19	0	0
2	E	31	0	19	1	0
2	F	31	0	19	1	0
2	G	31	0	19	1	0
2	H	31	0	19	1	0
3	A	15	0	8	3	0
3	B	15	0	8	4	0
3	C	15	0	8	2	0
3	D	15	0	7	2	0
3	E	15	0	8	0	0
3	F	15	0	8	3	0
3	G	15	0	8	1	0
3	H	15	0	7	3	0
4	C	5	0	0	0	0
4	G	5	0	0	0	0
5	A	36	0	0	8	0
5	B	38	0	0	12	0
5	C	39	0	0	10	0
5	D	23	0	0	7	0
5	E	48	0	0	8	0
5	F	40	0	0	13	0
5	G	38	0	0	12	0
5	H	38	0	0	19	0
All	All	14910	0	14902	424	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 14.

All (424) 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:E:164:ARG:HD3	5:E:305:HOH:O	1.38	1.21
1:B:191:PHE:HB2	5:B:294:HOH:O	1.43	1.14
1:D:266:ARG:CB	1:D:266:ARG:HH11	1.61	1.13
1:B:132:THR:HB	5:B:294:HOH:O	1.51	1.08
1:E:110:GLU:HA	5:E:403:HOH:O	1.53	1.07

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:ARG:HH11	1:D:266:ARG:HB3	1.16	1.06
1:G:156:ASN:HD22	1:G:160:ARG:HD3	1.08	1.06
1:G:156:ASN:ND2	1:G:160:ARG:HD3	1.69	1.06
1:F:84:MET:HG3	5:F:297:HOH:O	1.57	1.03
1:B:67:VAL:HG12	1:B:68:GLU:N	1.77	1.00
1:A:164:ARG:HG3	5:A:461:HOH:O	1.63	0.98
1:B:106:HIS:HB2	5:B:311:HOH:O	1.64	0.96
1:G:67:VAL:HG13	1:H:171:LYS:HA	1.44	0.96
1:D:164:ARG:HG3	1:D:164:ARG:HH11	1.30	0.95
1:F:67:VAL:O	1:F:68:GLU:CB	2.16	0.94
1:C:200:ASN:HD22	1:C:200:ASN:H	1.14	0.93
1:G:67:VAL:O	1:G:68:GLU:HB3	1.65	0.93
1:G:200:ASN:HD22	1:G:200:ASN:H	1.12	0.92
1:F:76:ARG:HG2	1:F:76:ARG:HH11	1.37	0.89
1:B:67:VAL:HG12	1:B:68:GLU:H	1.35	0.88
1:C:173:ARG:HG3	1:D:69:HIS:CE1	2.09	0.87
1:F:67:VAL:O	1:F:68:GLU:HB3	1.73	0.86
1:B:172:LEU:HD13	3:B:302:TYI:I1	2.47	0.85
1:D:156:ASN:HA	1:D:160:ARG:HB2	1.58	0.85
1:G:200:ASN:H	1:G:200:ASN:ND2	1.73	0.85
1:D:266:ARG:HB3	1:D:266:ARG:NH1	1.92	0.84
1:E:171:LYS:HD2	5:E:432:HOH:O	1.77	0.83
1:D:156:ASN:ND2	1:D:160:ARG:NH1	2.25	0.82
1:G:106:HIS:HD2	5:H:414:HOH:O	1.63	0.82
1:C:286:HIS:HB3	5:C:296:HOH:O	1.78	0.81
1:B:284:THR:HG22	5:B:493:HOH:O	1.80	0.81
1:A:171:LYS:HA	1:B:67:VAL:HG22	1.63	0.80
1:F:202:LYS:HE2	1:F:202:LYS:HA	1.63	0.80
1:A:157:TYR:OH	1:A:174:THR:HG23	1.82	0.80
1:E:164:ARG:HG2	5:E:294:HOH:O	1.83	0.78
1:C:156:ASN:HD22	1:C:160:ARG:HD2	1.48	0.77
1:C:198:ALA:CB	1:C:200:ASN:HD21	1.95	0.77
1:C:67:VAL:O	1:C:68:GLU:CB	2.32	0.77
5:A:409:HOH:O	1:B:82:MET:CE	2.33	0.75
1:E:157:TYR:OH	1:E:174:THR:HG23	1.86	0.75
1:D:164:ARG:HG3	1:D:164:ARG:NH1	1.97	0.74
1:C:156:ASN:ND2	1:C:160:ARG:HD2	2.03	0.74
1:D:266:ARG:CB	1:D:266:ARG:NH1	2.45	0.74
1:E:98:SER:HB3	1:E:232:VAL:HG23	1.70	0.74
1:F:172:LEU:HD13	3:F:302:TYI:I1	2.57	0.74
1:D:266:ARG:HH11	1:D:266:ARG:HB2	1.54	0.73

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:156:ASN:HD22	1:G:160:ARG:CD	1.95	0.73
1:A:72:PHE:CE2	1:A:74:HIS:HB2	2.23	0.73
1:H:181:LEU:HB3	5:H:297:HOH:O	1.87	0.72
1:C:198:ALA:CB	1:C:200:ASN:ND2	2.53	0.72
2:F:301:FMN:O1P	5:F:423:HOH:O	2.06	0.72
1:H:146:ARG:CA	5:H:297:HOH:O	2.38	0.71
1:C:114:ASN:HB2	1:D:86:SER:HB2	1.72	0.71
1:C:198:ALA:HB3	1:C:200:ASN:ND2	2.06	0.71
1:D:172:LEU:HD13	3:D:302:TYI:I1	2.60	0.71
1:C:67:VAL:O	1:C:68:GLU:HB3	1.89	0.71
1:H:146:ARG:N	5:H:297:HOH:O	2.22	0.71
1:H:111:VAL:O	1:H:115:VAL:HG13	1.90	0.70
1:H:200:ASN:HD22	1:H:202:LYS:H	1.38	0.70
1:F:81:GLU:O	1:F:85:ARG:HG3	1.91	0.70
1:C:233:THR:HA	1:C:259:LEU:HD23	1.71	0.70
1:C:200:ASN:HD22	1:C:200:ASN:N	1.88	0.70
1:D:286:HIS:CE1	5:D:358:HOH:O	2.44	0.69
1:C:190:ILE:HD12	1:C:257:VAL:HG23	1.73	0.69
1:C:200:ASN:H	1:C:200:ASN:ND2	1.90	0.69
1:F:200:ASN:ND2	5:F:415:HOH:O	2.26	0.69
1:H:286:HIS:O	5:H:481:HOH:O	2.10	0.69
1:E:111:VAL:O	1:E:115:VAL:HG13	1.93	0.69
1:B:143:HIS:HD2	1:B:182:ASP:OD2	1.76	0.68
1:E:162:GLY:O	1:E:166:VAL:HG12	1.93	0.68
1:B:140:ASP:HB3	5:B:364:HOH:O	1.92	0.68
1:D:200:ASN:C	1:D:200:ASN:HD22	1.97	0.68
1:B:81:GLU:O	1:B:85:ARG:HG3	1.94	0.67
1:C:173:ARG:HD2	5:C:305:HOH:O	1.93	0.67
1:A:76:ARG:NH2	1:B:105:GLU:OE2	2.28	0.67
1:D:277:ALA:N	1:D:280:GLN:OE1	2.22	0.66
1:G:173:ARG:HD2	1:H:69:HIS:CE1	2.31	0.66
1:A:257:VAL:HG23	1:A:259:LEU:HD23	1.77	0.66
1:F:103:SER:OG	1:F:105:GLU:HG3	1.96	0.66
1:G:83:ARG:HG2	1:H:110:GLU:HG2	1.77	0.66
1:H:156:ASN:ND2	1:H:160:ARG:HH11	1.93	0.66
1:B:244:ARG:HG2	1:B:244:ARG:HH11	1.61	0.66
1:A:112:ILE:O	1:A:116:ILE:HG13	1.96	0.66
5:C:340:HOH:O	1:D:69:HIS:HD2	1.78	0.66
1:F:76:ARG:HH11	1:F:76:ARG:CG	2.07	0.65
1:F:142:LYS:HE3	1:F:184:ALA:O	1.96	0.65
1:F:266:ARG:HG3	5:F:300:HOH:O	1.97	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:161:MET:HE3	3:H:302:TYI:HB2	1.77	0.65
1:F:104:SER:HB2	5:F:449:HOH:O	1.96	0.65
1:H:106:HIS:CE1	5:H:296:HOH:O	2.49	0.65
1:E:192:LYS:NZ	1:E:210:GLU:OE1	2.31	0.64
1:A:257:VAL:HG23	1:A:259:LEU:CD2	2.26	0.64
1:D:67:VAL:N	5:D:322:HOH:O	2.30	0.64
1:B:150:GLU:HG2	1:B:176:TRP:O	1.96	0.64
1:F:198:ALA:HB3	5:F:415:HOH:O	1.97	0.64
1:C:81:GLU:O	1:C:85:ARG:HG3	1.97	0.64
1:G:117:LYS:HB3	1:H:90:TYR:CD1	2.33	0.64
1:D:109:MET:O	1:D:113:GLU:HG3	1.97	0.63
1:E:66:SER:N	5:E:452:HOH:O	2.30	0.63
1:A:202:LYS:HG2	5:A:384:HOH:O	1.98	0.63
1:C:156:ASN:ND2	1:C:160:ARG:HH11	1.96	0.63
1:A:172:LEU:HD13	3:A:302:TYI:I1	2.69	0.62
1:A:137:LYS:HE2	5:A:294:HOH:O	1.99	0.62
1:C:198:ALA:HB1	1:C:200:ASN:HD21	1.62	0.62
1:G:81:GLU:O	1:G:85:ARG:HG3	1.98	0.62
5:E:432:HOH:O	1:F:67:VAL:HG21	1.98	0.62
1:B:87:GLN:HA	5:B:297:HOH:O	1.99	0.62
1:G:178:LYS:HD2	1:G:180:TYR:OH	1.98	0.62
1:F:266:ARG:HH11	1:F:266:ARG:CG	2.13	0.62
1:F:274:LYS:HE2	5:F:451:HOH:O	1.99	0.62
1:H:156:ASN:HD22	1:H:160:ARG:HD2	1.63	0.62
1:C:173:ARG:CD	5:C:305:HOH:O	2.47	0.61
1:C:233:THR:HA	1:C:259:LEU:CD2	2.29	0.61
1:D:136:VAL:HG13	1:D:187:LEU:HB2	1.81	0.61
1:F:67:VAL:O	1:F:68:GLU:HB2	2.00	0.61
1:C:232:VAL:O	1:C:234:THR:HG23	2.01	0.61
1:H:200:ASN:ND2	1:H:202:LYS:H	1.98	0.61
1:C:67:VAL:HG13	5:C:433:HOH:O	1.99	0.60
1:D:156:ASN:ND2	1:D:160:ARG:HH11	1.97	0.60
1:H:172:LEU:HD13	3:H:302:TYI:I1	2.71	0.60
1:D:155:ILE:HG22	1:D:160:ARG:HD3	1.83	0.60
1:B:67:VAL:CG1	1:B:68:GLU:N	2.51	0.60
1:B:232:VAL:O	1:B:234:THR:HG23	2.01	0.60
1:D:214:SER:O	1:D:217:CYS:HB3	2.02	0.60
5:G:470:HOH:O	1:H:109:MET:HE2	2.02	0.60
1:F:104:SER:CB	5:F:370:HOH:O	2.49	0.60
1:H:278:LEU:HD11	1:H:282:MET:SD	2.42	0.60
1:E:127:HIS:CG	1:E:127:HIS:O	2.55	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:266:ARG:HG3	1:F:266:ARG:HH11	1.67	0.59
1:C:172:LEU:HD13	3:C:302:TYI:I1	2.72	0.59
1:C:139:PRO:HG2	1:H:73:SER:HB3	1.85	0.59
1:H:80:GLN:HA	1:H:80:GLN:NE2	2.17	0.59
1:C:110:GLU:HG3	5:C:294:HOH:O	2.02	0.59
1:G:232:VAL:O	1:G:234:THR:HG23	2.03	0.59
1:H:137:LYS:NZ	5:H:400:HOH:O	2.34	0.59
1:G:83:ARG:HD2	5:G:327:HOH:O	2.04	0.58
1:A:148:ILE:O	1:A:152:GLU:HG2	2.02	0.58
1:E:267:ASP:OD1	1:E:267:ASP:N	2.34	0.58
1:A:82:MET:HG2	1:B:227:ALA:O	2.02	0.58
1:G:83:ARG:CG	1:H:110:GLU:HG2	2.34	0.58
1:G:171:LYS:HB2	5:G:482:HOH:O	2.04	0.58
1:D:136:VAL:CG1	1:D:187:LEU:HB2	2.34	0.58
1:A:205:VAL:H	1:B:164:ARG:NH2	2.02	0.57
5:A:409:HOH:O	1:B:82:MET:HE2	1.99	0.57
2:B:301:FMN:O1P	5:B:300:HOH:O	2.17	0.57
1:H:266:ARG:NH1	1:H:266:ARG:HB3	2.20	0.57
1:E:258:LEU:HD23	1:E:259:LEU:N	2.20	0.57
1:B:180:TYR:CD2	1:B:260:PRO:HG3	2.40	0.57
1:D:104:SER:HA	1:D:183:THR:O	2.04	0.57
1:F:66:SER:HB2	1:F:67:VAL:HG23	1.87	0.57
1:A:100:ARG:NH2	3:A:302:TYI:I1	3.08	0.56
5:G:498:HOH:O	1:H:69:HIS:HD2	1.88	0.56
1:G:200:ASN:ND2	1:G:200:ASN:N	2.49	0.56
1:H:146:ARG:HG3	1:H:181:LEU:HB2	1.87	0.56
1:B:180:TYR:CE2	1:B:260:PRO:HG3	2.40	0.56
1:D:146:ARG:HG3	1:D:181:LEU:HB2	1.88	0.56
1:D:198:ALA:HB3	1:D:200:ASN:ND2	2.21	0.56
1:C:156:ASN:HD21	1:C:238:ASN:HD22	1.53	0.55
1:G:109:MET:SD	1:G:137:LYS:HD3	2.47	0.55
1:A:175:ASN:HB2	5:A:408:HOH:O	2.05	0.55
1:C:198:ALA:HB1	1:C:200:ASN:ND2	2.19	0.55
1:H:80:GLN:HB2	5:H:359:HOH:O	2.06	0.55
1:H:98:SER:HB3	1:H:232:VAL:HG23	1.88	0.55
1:F:140:ASP:O	1:F:144:LYS:HG3	2.07	0.55
1:F:180:TYR:CD2	1:F:260:PRO:HG3	2.41	0.55
1:E:190:ILE:HD12	1:E:257:VAL:HG23	1.87	0.55
1:D:106:HIS:HD2	5:D:313:HOH:O	1.89	0.55
1:C:159:LYS:HG3	1:C:160:ARG:N	2.22	0.55
1:F:106:HIS:HB2	5:F:21:HOH:O	2.06	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:MET:HE1	3:F:302:TYI:HB2	1.89	0.54
1:C:107:VAL:HG23	1:C:112:ILE:HD13	1.88	0.54
1:C:198:ALA:HB3	1:C:200:ASN:HD21	1.68	0.54
1:G:204:LYS:NZ	5:G:361:HOH:O	2.40	0.54
1:C:107:VAL:HG21	1:C:112:ILE:HD11	1.90	0.54
1:G:284:THR:HG21	5:G:470:HOH:O	2.07	0.54
1:G:101:PHE:HB3	5:G:490:HOH:O	2.08	0.54
1:D:72:PHE:CE2	1:D:74:HIS:HB2	2.43	0.54
1:E:76:ARG:HH22	1:F:105:GLU:CD	2.11	0.53
1:G:68:GLU:OE1	1:G:69:HIS:N	2.41	0.53
1:A:98:SER:OG	2:A:301:FMN:O2P	2.25	0.53
1:G:143:HIS:HB3	5:G:456:HOH:O	2.08	0.53
1:E:171:LYS:CD	5:E:432:HOH:O	2.44	0.53
1:D:107:VAL:HG21	1:D:112:ILE:HD11	1.90	0.53
5:G:470:HOH:O	1:H:109:MET:CE	2.55	0.53
1:D:156:ASN:HD21	1:D:160:ARG:NH1	2.05	0.53
1:D:194:VAL:HG22	1:D:252:HIS:O	2.08	0.53
1:A:190:ILE:HD13	1:A:257:VAL:HG22	1.89	0.53
1:D:198:ALA:HB3	1:D:200:ASN:HD21	1.73	0.53
1:D:286:HIS:HE1	5:D:358:HOH:O	1.87	0.53
1:G:66:SER:O	1:H:171:LYS:HB3	2.09	0.53
1:B:145:ILE:O	1:B:149:ILE:HG13	2.09	0.52
1:F:185:PRO:HD2	1:F:261:VAL:O	2.09	0.52
1:H:209:ASN:O	1:H:213:VAL:HG23	2.09	0.52
1:A:257:VAL:CG2	1:A:259:LEU:HD21	2.39	0.52
5:A:409:HOH:O	1:B:82:MET:HE3	2.04	0.52
1:D:202:LYS:HD2	1:D:203:LYS:H	1.74	0.52
1:E:189:LEU:HG	1:E:258:LEU:HG	1.91	0.52
1:B:109:MET:CE	5:B:438:HOH:O	2.57	0.52
1:C:171:LYS:HG2	1:D:67:VAL:HG12	1.90	0.52
2:A:301:FMN:H4'	1:B:124:SER:O	2.09	0.52
1:B:105:GLU:O	1:B:185:PRO:HG3	2.10	0.52
1:F:100:ARG:NH2	3:F:302:TYI:I1	3.13	0.52
1:B:244:ARG:HG2	1:B:244:ARG:NH1	2.24	0.52
1:C:67:VAL:HG13	1:D:171:LYS:HA	1.91	0.51
1:C:150:GLU:HG2	1:C:176:TRP:O	2.10	0.51
1:C:98:SER:HB3	1:C:232:VAL:HG23	1.92	0.51
1:H:96:ARG:O	1:H:97:ARG:HD2	2.09	0.51
1:H:202:LYS:HD2	1:H:203:LYS:H	1.74	0.51
1:A:122:ALA:HB2	1:A:216:ALA:HA	1.92	0.51
1:D:110:GLU:HB3	5:D:295:HOH:O	2.11	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:FMN:O4	3:B:302:TYI:N	2.43	0.51
1:H:156:ASN:HA	1:H:160:ARG:HB2	1.91	0.51
1:D:276:LYS:HB3	1:D:280:GLN:HB2	1.92	0.51
1:C:175:ASN:HD21	1:C:177:ILE:HD12	1.76	0.51
1:G:258:LEU:C	1:G:258:LEU:HD23	2.32	0.51
1:H:171:LYS:HD3	5:H:314:HOH:O	2.11	0.51
1:H:185:PRO:HB2	5:H:400:HOH:O	2.10	0.50
1:C:161:MET:HG2	1:C:165:TRP:CD2	2.46	0.50
1:C:152:GLU:HB2	1:C:239:CYS:SG	2.52	0.50
1:D:200:ASN:ND2	1:D:202:LYS:H	2.10	0.50
1:G:190:ILE:HD12	1:G:257:VAL:HG23	1.92	0.50
1:D:96:ARG:O	1:D:97:ARG:HD2	2.11	0.50
1:F:156:ASN:HA	1:F:160:ARG:HB2	1.93	0.50
1:B:96:ARG:NH1	5:B:303:HOH:O	2.39	0.50
1:G:225:GLN:HA	5:G:506:HOH:O	2.11	0.50
1:H:162:GLY:O	1:H:166:VAL:HG23	2.12	0.50
1:H:266:ARG:HB3	1:H:266:ARG:HH11	1.75	0.50
1:F:89:PHE:HA	5:F:410:HOH:O	2.12	0.49
1:F:154:GLU:O	1:F:158:MET:HG3	2.12	0.49
1:E:214:SER:O	1:E:217:CYS:HB3	2.12	0.49
1:F:154:GLU:HG3	1:F:176:TRP:CE2	2.48	0.49
1:C:117:LYS:HB3	1:D:90:TYR:CD1	2.47	0.49
1:A:173:ARG:NE	1:B:67:VAL:HG11	2.28	0.49
1:D:165:TRP:HD1	1:D:165:TRP:O	1.95	0.49
5:G:406:HOH:O	1:H:235:THR:HB	2.13	0.49
1:A:156:ASN:HA	1:A:160:ARG:HB3	1.94	0.49
1:G:153:GLU:HA	1:G:156:ASN:HB2	1.95	0.49
1:F:111:VAL:O	1:F:115:VAL:HG13	2.13	0.48
1:H:146:ARG:CB	5:H:297:HOH:O	2.58	0.48
1:B:161:MET:HE2	3:B:302:TYI:HB2	1.94	0.48
1:B:214:SER:O	1:B:217:CYS:HB3	2.13	0.48
1:H:156:ASN:ND2	1:H:160:ARG:HD2	2.28	0.48
1:B:209:ASN:O	1:B:213:VAL:HG23	2.13	0.48
1:H:180:TYR:CD2	1:H:260:PRO:HG3	2.47	0.48
1:C:180:TYR:CD2	1:C:260:PRO:HG3	2.48	0.48
1:D:130:PRO:HG3	5:D:17:HOH:O	2.12	0.48
1:E:273:LEU:HD13	1:F:127:HIS:CG	2.49	0.48
1:B:190:ILE:O	1:B:255:LEU:HD12	2.14	0.48
1:D:81:GLU:HA	1:D:84:MET:SD	2.53	0.47
1:H:112:ILE:O	1:H:116:ILE:HG12	2.14	0.47
1:A:278:LEU:HD13	1:B:117:LYS:HG2	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:ASN:C	1:D:200:ASN:ND2	2.67	0.47
1:E:98:SER:OG	2:E:301:FMN:O2P	2.33	0.47
1:C:89:PHE:HB2	1:D:226:ASN:ND2	2.29	0.47
1:G:172:LEU:HD13	3:G:302:TYI:I1	2.84	0.47
1:A:178:LYS:NZ	3:A:302:TYI:OXT	2.38	0.47
1:C:67:VAL:O	1:C:68:GLU:HB2	2.12	0.47
1:H:144:LYS:O	1:H:148:ILE:HG13	2.15	0.47
1:D:163:LYS:HD3	1:D:163:LYS:N	2.30	0.47
1:F:180:TYR:HA	1:F:183:THR:OG1	2.15	0.47
1:C:106:HIS:CE1	5:C:405:HOH:O	2.68	0.47
1:C:171:LYS:O	1:D:69:HIS:HE1	1.98	0.47
1:A:215:ILE:HG23	1:B:218:GLY:HA2	1.95	0.47
2:C:301:FMN:O4	3:C:302:TYI:N	2.48	0.47
1:A:143:HIS:HD2	1:A:182:ASP:OD2	1.97	0.46
1:D:99:VAL:HG12	1:D:101:PHE:H	1.80	0.46
1:D:146:ARG:O	1:D:150:GLU:HG3	2.15	0.46
1:F:127:HIS:CG	1:F:127:HIS:O	2.67	0.46
1:B:285:VAL:C	5:B:493:HOH:O	2.53	0.46
1:A:90:TYR:CE1	1:B:117:LYS:HB3	2.51	0.46
1:B:192:LYS:CB	1:B:213:VAL:HG21	2.46	0.46
1:C:66:SER:HB3	5:C:297:HOH:O	2.16	0.46
1:E:72:PHE:CE2	1:E:74:HIS:HB2	2.50	0.46
1:E:96:ARG:O	1:E:275:ARG:NH2	2.47	0.46
1:H:96:ARG:HD2	5:H:321:HOH:O	2.15	0.46
1:G:106:HIS:CD2	5:H:414:HOH:O	2.51	0.46
1:H:266:ARG:NH1	1:H:266:ARG:CB	2.79	0.46
1:D:164:ARG:HH11	1:D:164:ARG:CG	2.14	0.46
1:F:232:VAL:O	1:F:234:THR:HG23	2.16	0.46
1:H:165:TRP:HB2	5:H:356:HOH:O	2.16	0.46
1:A:171:LYS:HA	1:B:67:VAL:CG2	2.42	0.45
1:B:96:ARG:HG2	1:B:96:ARG:HH11	1.80	0.45
1:G:123:PRO:HB2	2:H:301:FMN:HM81	1.98	0.45
1:H:146:ARG:HB2	5:H:297:HOH:O	2.14	0.45
1:H:180:TYR:CE2	1:H:260:PRO:HG3	2.51	0.45
1:A:171:LYS:HG2	5:A:296:HOH:O	2.16	0.45
1:G:68:GLU:OE1	1:G:68:GLU:C	2.54	0.45
1:H:169:LEU:HD22	3:H:302:TYI:CE1	2.46	0.45
5:E:419:HOH:O	1:F:82:MET:CE	2.64	0.45
1:F:246:LEU:O	1:F:246:LEU:HG	2.16	0.45
1:A:84:MET:O	1:A:88:GLU:HG3	2.16	0.45
1:B:96:ARG:NH1	1:B:96:ARG:HG2	2.31	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:VAL:O	1:D:115:VAL:HG13	2.16	0.45
2:G:301:FMN:HM83	2:G:301:FMN:HM71	1.78	0.45
1:B:104:SER:HB3	5:B:295:HOH:O	2.17	0.45
1:D:156:ASN:O	1:D:161:MET:HG3	2.16	0.45
1:E:171:LYS:O	1:F:67:VAL:HG12	2.17	0.45
1:E:209:ASN:O	1:E:213:VAL:HG23	2.16	0.45
1:G:161:MET:HG2	1:G:165:TRP:CE3	2.51	0.45
1:A:256:LEU:O	1:A:257:VAL:HG12	2.17	0.45
1:F:150:GLU:HG2	1:F:176:TRP:O	2.17	0.45
1:G:96:ARG:HG2	1:G:97:ARG:N	2.32	0.45
1:G:195:HIS:CE1	1:G:252:HIS:HB3	2.52	0.45
1:E:82:MET:HG2	1:F:227:ALA:O	2.18	0.44
1:F:112:ILE:O	1:F:115:VAL:HG22	2.16	0.44
1:H:165:TRP:O	1:H:165:TRP:HD1	2.00	0.44
1:C:189:LEU:N	1:C:189:LEU:HD12	2.32	0.44
1:D:93:LEU:HD12	1:D:93:LEU:HA	1.78	0.44
1:D:236:PRO:HB2	1:D:239:CYS:HB2	2.00	0.44
1:C:87:GLN:HG3	1:C:91:GLU:OE2	2.17	0.44
1:C:146:ARG:HA	1:C:181:LEU:HD13	2.00	0.44
1:H:164:ARG:HD2	5:H:295:HOH:O	2.17	0.44
1:A:231:THR:OG1	1:A:232:VAL:N	2.51	0.44
1:B:100:ARG:NH2	3:B:302:TYI:I1	3.21	0.44
1:B:267:ASP:HA	5:B:436:HOH:O	2.17	0.44
5:C:405:HOH:O	1:G:267:ASP:HB2	2.18	0.44
1:F:171:LYS:H	1:F:171:LYS:HG2	1.55	0.44
2:B:301:FMN:C9	2:B:301:FMN:H2'	2.48	0.43
1:C:267:ASP:OD1	1:C:267:ASP:N	2.51	0.43
1:E:162:GLY:O	1:E:166:VAL:CG1	2.64	0.43
1:F:258:LEU:C	1:F:258:LEU:HD23	2.38	0.43
1:G:140:ASP:HA	5:G:456:HOH:O	2.18	0.43
1:G:156:ASN:OD1	1:G:237:LEU:HB3	2.18	0.43
1:F:146:ARG:NH2	1:F:179:GLU:HA	2.33	0.43
1:G:171:LYS:HG2	1:H:67:VAL:HG12	2.00	0.43
1:C:161:MET:HG2	1:C:165:TRP:CE3	2.53	0.43
1:D:80:GLN:NE2	1:D:83:ARG:HH21	2.17	0.43
1:E:197:PHE:HA	1:E:202:LYS:O	2.19	0.43
1:F:266:ARG:HD3	5:F:298:HOH:O	2.17	0.43
1:G:180:TYR:CD2	1:G:260:PRO:HG3	2.53	0.43
1:B:180:TYR:HA	1:B:183:THR:OG1	2.19	0.43
1:C:94:ASN:ND2	1:C:275:ARG:HH11	2.17	0.43
1:C:98:SER:OG	2:C:301:FMN:O2P	2.27	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:ASN:CB	1:D:86:SER:HB2	2.45	0.43
1:C:200:ASN:ND2	1:C:200:ASN:N	2.58	0.43
1:D:161:MET:HE3	3:D:302:TYI:HB2	2.01	0.43
1:F:76:ARG:CG	1:F:76:ARG:NH1	2.77	0.43
1:G:112:ILE:HD13	1:G:112:ILE:HA	1.78	0.43
1:D:274:LYS:HD3	1:D:274:LYS:HA	1.67	0.43
1:F:230:VAL:HG22	1:F:262:GLY:O	2.18	0.43
1:H:104:SER:HA	1:H:183:THR:O	2.19	0.43
1:H:266:ARG:HH11	1:H:266:ARG:CG	2.31	0.43
1:E:122:ALA:HB1	1:E:123:PRO:HD2	2.01	0.43
1:C:272:ASP:O	1:D:67:VAL:HG21	2.18	0.43
1:D:148:ILE:O	1:D:152:GLU:HG2	2.19	0.43
1:G:98:SER:HB3	1:G:232:VAL:HG23	2.00	0.43
1:C:123:PRO:HD3	1:D:96:ARG:CZ	2.49	0.43
1:G:80:GLN:OE1	1:G:80:GLN:HA	2.19	0.43
1:C:107:VAL:CG2	1:C:112:ILE:CD1	2.97	0.42
1:D:156:ASN:HD22	1:D:160:ARG:HH11	1.65	0.42
1:H:156:ASN:HD22	1:H:160:ARG:CD	2.30	0.42
1:A:270:VAL:HG13	1:B:72:PHE:HB2	2.00	0.42
1:C:209:ASN:O	1:C:213:VAL:HG23	2.19	0.42
1:D:286:HIS:C	5:D:10:HOH:O	2.58	0.42
1:A:98:SER:HG	2:A:301:FMN:P	2.42	0.42
1:A:156:ASN:ND2	1:A:237:LEU:HB3	2.35	0.42
1:C:146:ARG:NE	1:C:150:GLU:OE2	2.50	0.42
1:G:156:ASN:HD21	1:G:238:ASN:HD22	1.67	0.42
1:H:231:THR:OG1	1:H:232:VAL:N	2.53	0.42
1:H:266:ARG:HH11	1:H:266:ARG:CB	2.32	0.42
1:A:89:PHE:HB2	1:B:226:ASN:ND2	2.35	0.42
1:B:143:HIS:CD2	1:B:182:ASP:OD2	2.65	0.42
1:D:273:LEU:O	1:D:274:LYS:HD3	2.20	0.42
1:E:235:THR:HG22	1:E:257:VAL:HG12	2.02	0.42
1:G:244:ARG:HG2	1:G:244:ARG:HH11	1.85	0.42
1:H:239:CYS:HB3	1:H:243:LEU:CD1	2.49	0.42
1:B:66:SER:O	1:B:67:VAL:HB	2.20	0.42
1:C:266:ARG:HD3	1:C:266:ARG:HA	1.88	0.42
1:D:229:LEU:HD23	1:D:229:LEU:HA	1.83	0.42
1:A:257:VAL:HG21	1:A:259:LEU:HD21	2.01	0.42
1:B:256:LEU:HD12	1:B:256:LEU:HA	1.89	0.42
1:C:171:LYS:HB2	5:C:348:HOH:O	2.20	0.42
1:B:67:VAL:CG1	1:B:69:HIS:HD2	2.32	0.42
1:C:68:GLU:HA	1:C:68:GLU:OE1	2.20	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:ASN:HD22	1:D:202:LYS:H	1.67	0.42
1:H:107:VAL:HG21	1:H:112:ILE:HD11	2.01	0.42
1:H:256:LEU:HG	1:H:257:VAL:HG23	2.02	0.42
1:A:258:LEU:C	1:A:259:LEU:HD23	2.41	0.41
1:G:154:GLU:HG3	1:G:176:TRP:CE2	2.54	0.41
1:E:146:ARG:HE	1:E:150:GLU:CD	2.23	0.41
1:E:278:LEU:HD13	1:F:117:LYS:HG2	2.02	0.41
1:G:193:GLN:HE21	1:G:206:HIS:HE1	1.67	0.41
1:C:192:LYS:NZ	1:C:210:GLU:OE1	2.52	0.41
1:G:124:SER:HA	1:G:212:SER:HB3	2.02	0.41
1:A:156:ASN:OD1	1:A:160:ARG:NE	2.48	0.41
1:A:214:SER:O	1:A:217:CYS:HB3	2.19	0.41
1:B:185:PRO:HD2	1:B:261:VAL:O	2.20	0.41
1:D:138:ASP:HA	1:D:139:PRO:HD3	1.81	0.41
1:H:250:PRO:HB2	1:H:252:HIS:CE1	2.56	0.41
1:B:66:SER:C	1:B:67:VAL:HG23	2.41	0.41
1:G:189:LEU:HD12	1:G:189:LEU:N	2.36	0.41
1:G:89:PHE:HB2	1:H:226:ASN:ND2	2.36	0.41
1:H:207:TYR:HA	5:H:7:HOH:O	2.20	0.41
1:D:146:ARG:HA	1:D:181:LEU:HD13	2.02	0.41
1:F:189:LEU:N	1:F:189:LEU:HD12	2.36	0.41
1:F:266:ARG:HH11	1:F:266:ARG:CB	2.34	0.41
1:C:107:VAL:HG23	1:C:112:ILE:CD1	2.51	0.41
1:E:184:ALA:HA	1:E:185:PRO:HD2	1.90	0.41
1:F:104:SER:HB2	5:F:370:HOH:O	2.19	0.41
1:G:107:VAL:HA	1:G:108:PRO:HD3	1.89	0.41
1:G:165:TRP:CD1	1:G:169:LEU:HD22	2.56	0.41
1:H:265:SER:HB3	1:H:267:ASP:OD1	2.21	0.41
1:B:111:VAL:O	1:B:115:VAL:HG13	2.21	0.41
1:B:230:VAL:HG22	1:B:262:GLY:O	2.20	0.41
1:C:93:LEU:HD12	1:C:93:LEU:HA	1.74	0.41
1:C:217:CYS:SG	1:C:257:VAL:HG21	2.61	0.41
1:F:104:SER:HB3	5:F:370:HOH:O	2.18	0.41
1:F:266:ARG:CB	1:F:266:ARG:NH1	2.84	0.41
1:A:173:ARG:HE	1:B:67:VAL:HG11	1.85	0.40
1:E:243:LEU:O	1:E:247:LEU:HD12	2.21	0.40
1:H:134:VAL:HG21	1:H:249:ARG:HD3	2.02	0.40
1:E:127:HIS:CG	1:F:273:LEU:HD13	2.57	0.40
1:H:106:HIS:HE1	5:H:296:HOH:O	1.98	0.40
1:A:130:PRO:HD2	1:A:131:TRP:CE3	2.57	0.40
2:B:301:FMN:H2'	2:B:301:FMN:H9	2.03	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:ILE:O	1:C:70:ILE:HG13	2.21	0.40
1:H:152:GLU:HB2	1:H:239:CYS:SG	2.61	0.40
1:C:107:VAL:HA	1:C:108:PRO:HD3	1.82	0.40
1:D:163:LYS:N	1:D:163:LYS:CD	2.85	0.40
1:F:78:PRO:O	1:F:80:GLN:N	2.55	0.40
1:F:271:PRO:HB2	1:F:273:LEU:HG	2.04	0.40
1:G:93:LEU:HD12	1:G:93:LEU:HA	1.69	0.40
1:G:266:ARG:HA	1:G:266:ARG:HD3	1.72	0.40
1:H:106:HIS:HA	5:H:400:HOH:O	2.21	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	219/259 (85%)	201 (92%)	16 (7%)	2 (1%)	17	33
1	B	218/259 (84%)	199 (91%)	16 (7%)	3 (1%)	11	21
1	C	219/259 (85%)	202 (92%)	13 (6%)	4 (2%)	8	15
1	D	218/259 (84%)	204 (94%)	13 (6%)	1 (0%)	29	50
1	E	219/259 (85%)	206 (94%)	10 (5%)	3 (1%)	11	21
1	F	218/259 (84%)	201 (92%)	13 (6%)	4 (2%)	8	15
1	G	219/259 (85%)	200 (91%)	14 (6%)	5 (2%)	6	10
1	H	218/259 (84%)	203 (93%)	14 (6%)	1 (0%)	29	50
All	All	1748/2072 (84%)	1616 (92%)	109 (6%)	23 (1%)	12	23

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	VAL

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	126	ALA
1	B	67	VAL
1	B	79	GLU
1	C	68	GLU
1	C	198	ALA
1	E	67	VAL
1	F	67	VAL
1	F	68	GLU
1	F	79	GLU
1	G	68	GLU
1	C	199	ALA
1	F	199	ALA
1	G	171	LYS
1	G	199	ALA
1	D	272	ASP
1	G	75	THR
1	C	67	VAL
1	B	268	ALA
1	E	236	PRO
1	H	199	ALA
1	G	67	VAL
1	E	240	GLY

### 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	198/233 (85%)	180 (91%)	18 (9%)	9 17
1	B	197/233 (84%)	178 (90%)	19 (10%)	8 15
1	C	198/233 (85%)	183 (92%)	15 (8%)	13 25
1	D	197/233 (84%)	178 (90%)	19 (10%)	8 15
1	E	198/233 (85%)	176 (89%)	22 (11%)	6 10
1	F	197/233 (84%)	178 (90%)	19 (10%)	8 15
1	G	198/233 (85%)	180 (91%)	18 (9%)	9 17

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	197/233 (84%)	181 (92%)	16 (8%)	11	22
All	All	1580/1864 (85%)	1434 (91%)	146 (9%)	9	16

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	SER
1	A	84	MET
1	A	87	GLN
1	A	105	GLU
1	A	166	VAL
1	A	169	LEU
1	A	170	LYS
1	A	174	THR
1	A	186	VAL
1	A	188	ILE
1	A	194	VAL
1	A	200	ASN
1	A	215	ILE
1	A	220	LEU
1	A	238	ASN
1	A	246	LEU
1	A	257	VAL
1	A	259	LEU
1	B	73	SER
1	B	75	THR
1	B	76	ARG
1	B	84	MET
1	B	93	LEU
1	B	103	SER
1	B	110	GLU
1	B	131	TRP
1	B	137	LYS
1	B	154	GLU
1	B	164	ARG
1	B	171	LYS
1	B	200	ASN
1	B	203	LYS
1	B	220	LEU
1	B	251	SER
1	B	257	VAL
1	B	266	ARG

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	267	ASP
1	C	67	VAL
1	C	75	THR
1	C	92	LEU
1	C	93	LEU
1	C	131	TRP
1	C	155	ILE
1	C	160	ARG
1	C	167	THR
1	C	169	LEU
1	C	179	GLU
1	C	200	ASN
1	C	254	LYS
1	C	265	SER
1	C	267	ASP
1	C	286	HIS
1	D	84	MET
1	D	88	GLU
1	D	91	GLU
1	D	93	LEU
1	D	103	SER
1	D	131	TRP
1	D	137	LYS
1	D	158	MET
1	D	160	ARG
1	D	163	LYS
1	D	164	ARG
1	D	171	LYS
1	D	200	ASN
1	D	202	LYS
1	D	220	LEU
1	D	232	VAL
1	D	237	LEU
1	D	266	ARG
1	D	267	ASP
1	E	87	GLN
1	E	92	LEU
1	E	104	SER
1	E	105	GLU
1	E	109	MET
1	E	137	LYS
1	E	158	MET

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	164	ARG
1	E	166	VAL
1	E	169	LEU
1	E	170	LYS
1	E	171	LYS
1	E	172	LEU
1	E	186	VAL
1	E	203	LYS
1	E	209	ASN
1	E	220	LEU
1	E	238	ASN
1	E	246	LEU
1	E	265	SER
1	E	266	ARG
1	E	286	HIS
1	F	67	VAL
1	F	70	ILE
1	F	75	THR
1	F	76	ARG
1	F	80	GLN
1	F	84	MET
1	F	92	LEU
1	F	93	LEU
1	F	103	SER
1	F	106	HIS
1	F	163	LYS
1	F	164	ARG
1	F	171	LYS
1	F	202	LYS
1	F	220	LEU
1	F	235	THR
1	F	257	VAL
1	F	266	ARG
1	F	267	ASP
1	G	67	VAL
1	G	68	GLU
1	G	75	THR
1	G	83	ARG
1	G	88	GLU
1	G	92	LEU
1	G	93	LEU
1	G	124	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	131	TRP
1	G	147	GLU
1	G	148	ILE
1	G	160	ARG
1	G	167	THR
1	G	169	LEU
1	G	171	LYS
1	G	200	ASN
1	G	202	LYS
1	G	286	HIS
1	H	68	GLU
1	H	80	GLN
1	H	88	GLU
1	H	91	GLU
1	H	92	LEU
1	H	93	LEU
1	H	103	SER
1	H	110	GLU
1	H	112	ILE
1	H	131	TRP
1	H	136	VAL
1	H	158	MET
1	H	200	ASN
1	H	202	LYS
1	H	237	LEU
1	H	266	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	143	HIS
1	B	69	HIS
1	B	143	HIS
1	B	200	ASN
1	B	226	ASN
1	C	87	GLN
1	C	94	ASN
1	C	106	HIS
1	C	143	HIS
1	C	156	ASN
1	C	175	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	193	GLN
1	C	200	ASN
1	C	238	ASN
1	D	69	HIS
1	D	80	GLN
1	D	143	HIS
1	D	156	ASN
1	D	200	ASN
1	D	238	ASN
1	E	74	HIS
1	E	143	HIS
1	F	106	HIS
1	F	114	ASN
1	F	143	HIS
1	F	200	ASN
1	G	74	HIS
1	G	94	ASN
1	G	156	ASN
1	G	193	GLN
1	G	200	ASN
1	G	238	ASN
1	H	69	HIS
1	H	80	GLN
1	H	143	HIS
1	H	156	ASN
1	H	200	ASN
1	H	238	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

18 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
3	TYI	B	302	-	14,15,15	1.82	3 (21%)	20,21,21	2.09	6 (30%)
3	TYI	G	302	-	14,15,15	1.47	3 (21%)	20,21,21	2.18	6 (30%)
2	FMN	E	301	-	33,33,33	1.00	1 (3%)	48,50,50	1.67	13 (27%)
2	FMN	H	301	-	33,33,33	1.04	1 (3%)	48,50,50	1.52	9 (18%)
2	FMN	A	301	-	33,33,33	1.12	2 (6%)	48,50,50	1.65	14 (29%)
4	PO4	C	1	-	4,4,4	0.82	0	6,6,6	0.87	0
3	TYI	F	302	-	14,15,15	1.65	2 (14%)	20,21,21	1.89	7 (35%)
2	FMN	B	301	-	33,33,33	1.25	3 (9%)	48,50,50	2.02	19 (39%)
2	FMN	C	301	-	33,33,33	1.22	2 (6%)	48,50,50	1.48	9 (18%)
3	TYI	D	302	-	14,15,15	1.26	3 (21%)	20,21,21	2.27	7 (35%)
4	PO4	G	2	-	4,4,4	0.85	0	6,6,6	0.70	0
3	TYI	E	302	-	14,15,15	1.54	3 (21%)	20,21,21	1.87	7 (35%)
3	TYI	C	302	-	14,15,15	1.65	3 (21%)	20,21,21	2.13	6 (30%)
3	TYI	H	302	-	14,15,15	0.99	0	20,21,21	1.78	6 (30%)
2	FMN	G	301	-	33,33,33	1.44	5 (15%)	48,50,50	1.72	14 (29%)
3	TYI	A	302	-	14,15,15	1.33	2 (14%)	20,21,21	1.88	5 (25%)
2	FMN	F	301	-	33,33,33	1.31	4 (12%)	48,50,50	1.39	8 (16%)
2	FMN	D	301	-	33,33,33	1.21	2 (6%)	48,50,50	1.58	11 (22%)

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
3	TYI	B	302	-	-	0/8/8/8	0/1/1/1
3	TYI	G	302	-	-	0/8/8/8	0/1/1/1
2	FMN	E	301	-	-	2/18/18/18	0/3/3/3

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	H	301	-	-	0/18/18/18	0/3/3/3
2	FMN	A	301	-	-	0/18/18/18	0/3/3/3
3	TYI	F	302	-	-	0/8/8/8	0/1/1/1
2	FMN	B	301	-	-	5/18/18/18	0/3/3/3
2	FMN	C	301	-	-	1/18/18/18	0/3/3/3
3	TYI	D	302	-	-	0/8/8/8	0/1/1/1
3	TYI	E	302	-	-	0/8/8/8	0/1/1/1
3	TYI	C	302	-	-	0/8/8/8	0/1/1/1
3	TYI	H	302	-	-	0/8/8/8	0/1/1/1
2	FMN	G	301	-	-	6/18/18/18	0/3/3/3
3	TYI	A	302	-	-	0/8/8/8	0/1/1/1
2	FMN	F	301	-	-	1/18/18/18	0/3/3/3
2	FMN	D	301	-	-	0/18/18/18	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	FMN	C4A-N5	4.70	1.39	1.30
3	B	302	TYI	CZ-CE1	4.27	1.49	1.40
2	H	301	FMN	C4A-N5	3.97	1.38	1.30
3	G	302	TYI	CZ-CE2	3.93	1.49	1.40
3	C	302	TYI	CZ-CE2	3.79	1.48	1.40
3	F	302	TYI	CZ-CE1	3.77	1.48	1.40
2	D	301	FMN	C4A-N5	3.75	1.38	1.30
3	F	302	TYI	CZ-CE2	3.70	1.48	1.40
2	F	301	FMN	C4A-N5	3.67	1.37	1.30
3	A	302	TYI	CZ-CE1	3.64	1.48	1.40
2	C	301	FMN	C4A-N5	3.63	1.37	1.30
3	B	302	TYI	CZ-CE2	3.44	1.47	1.40
3	E	302	TYI	CZ-CE1	3.39	1.47	1.40
3	C	302	TYI	CZ-CE1	3.37	1.47	1.40
2	A	301	FMN	C4A-N5	3.34	1.37	1.30
2	B	301	FMN	C4A-N5	3.29	1.37	1.30
2	C	301	FMN	C10-N1	3.12	1.39	1.33
2	E	301	FMN	C4A-N5	2.91	1.36	1.30
2	G	301	FMN	C10-N1	2.80	1.38	1.33
2	G	301	FMN	C4'-C3'	-2.72	1.48	1.53
3	E	302	TYI	CZ-CE2	2.70	1.46	1.40
3	D	302	TYI	CZ-CE2	2.69	1.46	1.40
2	F	301	FMN	C10-N1	2.59	1.38	1.33
3	D	302	TYI	CZ-CE1	2.58	1.45	1.40
3	C	302	TYI	OXT-C	-2.52	1.22	1.30

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	TYI	CE1-I1	-2.46	2.04	2.10
2	B	301	FMN	C5'-C4'	2.46	1.55	1.51
3	E	302	TYI	OXT-C	-2.39	1.22	1.30
2	G	301	FMN	C2'-C3'	-2.36	1.49	1.53
3	G	302	TYI	CZ-CE1	2.30	1.45	1.40
2	B	301	FMN	C4A-C10	-2.28	1.37	1.44
2	A	301	FMN	C10-N1	2.25	1.37	1.33
2	F	301	FMN	O3'-C3'	-2.21	1.37	1.43
2	D	301	FMN	P-O1P	2.14	1.57	1.50
2	F	301	FMN	C4A-C10	-2.12	1.37	1.44
3	G	302	TYI	OXT-C	-2.08	1.23	1.30
3	A	302	TYI	CZ-CE2	2.05	1.44	1.40
3	D	302	TYI	OXT-C	-2.03	1.23	1.30
2	G	301	FMN	O4'-C4'	-2.01	1.39	1.43

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	302	TYI	CZ-CE1-I1	-5.43	111.06	119.42
3	B	302	TYI	CZ-CE1-I1	-5.40	111.09	119.42
2	B	301	FMN	C4A-C10-N10	5.32	124.26	116.48
3	C	302	TYI	CZ-CE1-I1	-5.20	111.40	119.42
3	G	302	TYI	CD1-CE1-I1	5.20	128.19	118.61
3	D	302	TYI	CD1-CE1-I1	4.87	127.59	118.61
3	D	302	TYI	CG-CB-CA	4.59	123.67	114.13
3	A	302	TYI	CZ-CE2-I2	-4.40	112.63	119.42
2	B	301	FMN	P-O5'-C5'	4.40	130.42	118.30
3	A	302	TYI	CD2-CE2-I2	4.19	126.35	118.61
2	D	301	FMN	O4-C4-C4A	-4.17	115.53	126.60
3	C	302	TYI	CD1-CE1-I1	4.16	126.28	118.61
3	D	302	TYI	CZ-CE1-I1	-4.08	113.13	119.42
2	A	301	FMN	O4-C4-C4A	-3.96	116.10	126.60
3	F	302	TYI	CD1-CE1-I1	3.83	125.67	118.61
2	A	301	FMN	C7M-C7-C6	-3.80	112.47	119.49
2	A	301	FMN	C4A-C10-N10	3.79	122.02	116.48
3	D	302	TYI	CB-CG-CD2	-3.67	114.14	120.44
2	G	301	FMN	C5'-C4'-C3'	-3.59	105.27	112.20
3	C	302	TYI	OXT-C-O	-3.58	115.97	124.09
2	D	301	FMN	O5'-P-O1P	3.54	116.41	106.47
2	B	301	FMN	O3P-P-O5'	3.51	116.07	106.73
2	H	301	FMN	O4-C4-C4A	-3.49	117.34	126.60
3	G	302	TYI	OXT-C-O	-3.49	116.17	124.09

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	FMN	O5'-P-O1P	3.49	116.25	106.47
2	E	301	FMN	C4A-C10-N10	3.46	121.54	116.48
3	B	302	TYI	CB-CG-CD2	-3.46	114.51	120.44
3	F	302	TYI	CZ-CE1-I1	-3.41	114.16	119.42
3	E	302	TYI	CZ-CE2-I2	-3.41	114.17	119.42
2	B	301	FMN	C4-N3-C2	-3.34	119.47	125.64
3	E	302	TYI	OXT-C-CA	3.32	124.70	113.38
3	F	302	TYI	OXT-C-CA	3.32	124.69	113.38
2	G	301	FMN	C4A-C4-N3	3.28	121.51	113.19
2	H	301	FMN	C5A-C9A-N10	3.28	121.34	117.95
2	G	301	FMN	C4-N3-C2	-3.26	119.62	125.64
2	E	301	FMN	O5'-P-O1P	3.23	115.53	106.47
2	G	301	FMN	C4-C4A-N5	3.20	122.79	118.23
2	F	301	FMN	O4-C4-C4A	-3.20	118.12	126.60
2	B	301	FMN	C1'-N10-C9A	3.18	125.82	120.51
3	H	302	TYI	CZ-CE2-I2	-3.17	114.53	119.42
2	E	301	FMN	C4-C4A-C10	3.14	122.08	116.79
2	G	301	FMN	C7M-C7-C8	-3.14	114.30	120.74
3	H	302	TYI	OXT-C-O	-3.13	116.97	124.09
2	B	301	FMN	O2-C2-N1	-3.07	116.75	121.83
2	G	301	FMN	C1'-C2'-C3'	-3.06	101.25	109.79
3	B	302	TYI	CD1-CE1-I1	3.05	124.23	118.61
2	C	301	FMN	C4-N3-C2	-3.03	120.04	125.64
2	G	301	FMN	O4-C4-C4A	-3.03	118.57	126.60
3	E	302	TYI	OH-CZ-CE1	3.02	128.03	120.33
3	H	302	TYI	OXT-C-CA	3.02	123.67	113.38
3	C	302	TYI	CB-CG-CD2	-2.99	115.30	120.44
2	C	301	FMN	C4A-C10-N1	-2.98	117.81	124.73
2	H	301	FMN	C4-N3-C2	-2.94	120.20	125.64
2	B	301	FMN	C9A-N10-C10	-2.91	116.23	120.77
2	F	301	FMN	C4A-C10-N10	2.91	120.74	116.48
3	B	302	TYI	OXT-C-CA	2.90	123.27	113.38
2	E	301	FMN	C9A-N10-C10	-2.89	116.26	120.77
2	G	301	FMN	C4A-C10-N10	2.89	120.71	116.48
3	F	302	TYI	OXT-C-O	-2.88	117.54	124.09
3	F	302	TYI	CD2-CE2-I2	2.88	123.92	118.61
3	H	302	TYI	CG-CB-CA	2.88	120.11	114.13
3	H	302	TYI	CD2-CE2-I2	2.85	123.87	118.61
2	A	301	FMN	O2-C2-N3	2.84	124.17	118.65
3	C	302	TYI	CD2-CE2-I2	2.82	123.81	118.61
2	D	301	FMN	O3'-C3'-C2'	-2.82	102.01	108.81
2	E	301	FMN	C5A-C9A-N10	2.80	120.85	117.95

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	FMN	C4A-C10-N10	2.80	120.58	116.48
2	C	301	FMN	C4A-C10-N10	2.80	120.58	116.48
3	E	302	TYI	CG-CB-CA	2.77	119.89	114.13
2	H	301	FMN	O3P-P-O2P	2.75	118.15	107.64
2	C	301	FMN	C4-C4A-C10	2.74	121.40	116.79
2	E	301	FMN	O2'-C2'-C1'	-2.73	103.20	109.80
2	F	301	FMN	C7M-C7-C6	-2.67	114.55	119.49
3	D	302	TYI	CB-CG-CD1	2.67	125.02	120.44
2	G	301	FMN	C10-C4A-N5	-2.65	119.23	124.86
2	C	301	FMN	C10-C4A-N5	-2.65	119.23	124.86
2	B	301	FMN	O4-C4-C4A	-2.65	119.57	126.60
3	E	302	TYI	OXT-C-O	-2.65	118.07	124.09
3	G	302	TYI	OXT-C-CA	2.64	122.39	113.38
2	B	301	FMN	O2-C2-N3	2.64	123.78	118.65
2	E	301	FMN	O4-C4-C4A	-2.63	119.64	126.60
2	C	301	FMN	C4A-C4-N3	2.62	119.84	113.19
2	E	301	FMN	C4-N3-C2	-2.60	120.84	125.64
2	B	301	FMN	O4'-C4'-C5'	2.60	115.75	109.92
2	A	301	FMN	C9A-N10-C10	-2.59	116.73	120.77
2	F	301	FMN	C4-N3-C2	-2.59	120.86	125.64
2	D	301	FMN	C5A-C9A-N10	2.57	120.61	117.95
2	E	301	FMN	C4A-C10-N1	-2.55	118.81	124.73
2	G	301	FMN	O4-C4-N3	-2.54	115.25	120.12
2	H	301	FMN	C9A-C5A-N5	-2.54	119.67	122.43
2	F	301	FMN	C4A-C4-N3	2.53	119.62	113.19
2	E	301	FMN	C1'-C2'-C3'	2.51	116.80	109.79
2	G	301	FMN	C9A-C5A-N5	-2.45	119.77	122.43
2	A	301	FMN	C5A-C9A-N10	2.45	120.48	117.95
2	G	301	FMN	C8M-C8-C7	-2.44	115.74	120.74
2	D	301	FMN	C8M-C8-C9	-2.43	115.00	119.49
3	A	302	TYI	OXT-C-CA	2.42	121.63	113.38
2	A	301	FMN	C1'-N10-C9A	2.41	124.53	120.51
3	D	302	TYI	OXT-C-CA	2.40	121.56	113.38
3	E	302	TYI	CB-CG-CD2	-2.38	116.35	120.44
3	F	302	TYI	CB-CG-CD2	-2.37	116.37	120.44
2	B	301	FMN	C10-C4A-N5	-2.37	119.84	124.86
2	D	301	FMN	O2P-P-O5'	-2.36	100.46	106.73
2	D	301	FMN	C4-C4A-C10	2.34	120.72	116.79
2	A	301	FMN	O2-C2-N1	-2.31	118.01	121.83
2	F	301	FMN	O2P-P-O5'	2.30	112.86	106.73
2	H	301	FMN	C8M-C8-C9	-2.29	115.25	119.49
2	B	301	FMN	C4A-C4-N3	2.28	118.99	113.19

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	FMN	O4-C4-C4A	-2.28	120.55	126.60
2	G	301	FMN	O3'-C3'-C4'	-2.28	103.31	108.81
3	B	302	TYI	CB-CG-CD1	2.28	124.34	120.44
2	F	301	FMN	C4A-C10-N1	-2.27	119.45	124.73
2	C	301	FMN	O2P-P-O5'	2.27	112.77	106.73
3	A	302	TYI	OH-CZ-CE1	2.25	126.06	120.33
2	C	301	FMN	O3P-P-O5'	2.24	112.70	106.73
2	B	301	FMN	C10-N1-C2	2.22	121.34	116.90
3	C	302	TYI	CD2-CG-CD1	2.22	122.03	118.98
3	A	302	TYI	OXT-C-O	-2.21	119.07	124.09
2	B	301	FMN	C4-C4A-C10	2.20	120.50	116.79
2	H	301	FMN	C4-C4A-C10	2.19	120.47	116.79
2	A	301	FMN	C4A-C4-N3	2.18	118.73	113.19
3	H	302	TYI	CD1-CE1-I1	2.18	122.63	118.61
3	E	302	TYI	CB-CG-CD1	2.17	124.15	120.44
3	B	302	TYI	OXT-C-O	-2.16	119.19	124.09
2	F	301	FMN	C4-C4A-C10	2.16	120.42	116.79
2	A	301	FMN	O5'-P-O1P	2.15	112.51	106.47
2	A	301	FMN	O3'-C3'-C2'	-2.15	103.61	108.81
2	D	301	FMN	O4'-C4'-C5'	-2.15	105.08	109.92
3	D	302	TYI	CD2-CE2-I2	2.15	122.57	118.61
2	B	301	FMN	C6-C5A-C9A	2.14	121.97	118.94
2	E	301	FMN	O3'-C3'-C2'	2.11	113.92	108.81
2	B	301	FMN	C5A-C9A-N10	2.09	120.11	117.95
2	H	301	FMN	C4A-C4-N3	2.08	118.47	113.19
2	B	301	FMN	C7M-C7-C8	-2.07	116.49	120.74
3	G	302	TYI	CD2-CE2-I2	2.06	122.40	118.61
2	B	301	FMN	O5'-C5'-C4'	-2.06	103.87	109.36
2	B	301	FMN	C1'-C2'-C3'	2.05	115.53	109.79
2	A	301	FMN	C4-N3-C2	-2.05	121.86	125.64
2	A	301	FMN	C4-C4A-C10	2.04	120.22	116.79
2	D	301	FMN	C10-C4A-N5	-2.04	120.53	124.86
2	D	301	FMN	O3P-P-O5'	2.04	112.15	106.73
2	G	301	FMN	C6-C5A-N5	2.03	122.07	118.51
3	G	302	TYI	CB-CG-CD2	-2.03	116.95	120.44
3	F	302	TYI	CD2-CG-CD1	2.03	121.77	118.98
2	E	301	FMN	C8M-C8-C9	-2.02	115.75	119.49
2	E	301	FMN	C5'-C4'-C3'	-2.02	108.30	112.20
2	A	301	FMN	C10-N1-C2	2.00	120.91	116.90

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	FMN	C3'-C4'-C5'-O5'
2	B	301	FMN	C5'-O5'-P-O1P
2	B	301	FMN	C5'-O5'-P-O2P
2	B	301	FMN	C5'-O5'-P-O3P
2	G	301	FMN	C2'-C3'-C4'-O4'
2	G	301	FMN	O3'-C3'-C4'-O4'
2	G	301	FMN	C3'-C4'-C5'-O5'
2	G	301	FMN	O4'-C4'-C5'-O5'
2	G	301	FMN	C2'-C3'-C4'-C5'
2	B	301	FMN	O4'-C4'-C5'-O5'
2	G	301	FMN	O3'-C3'-C4'-C5'
2	C	301	FMN	C2'-C3'-C4'-O4'
2	E	301	FMN	C5'-O5'-P-O1P
2	E	301	FMN	C5'-O5'-P-O3P
2	F	301	FMN	C2'-C3'-C4'-O4'

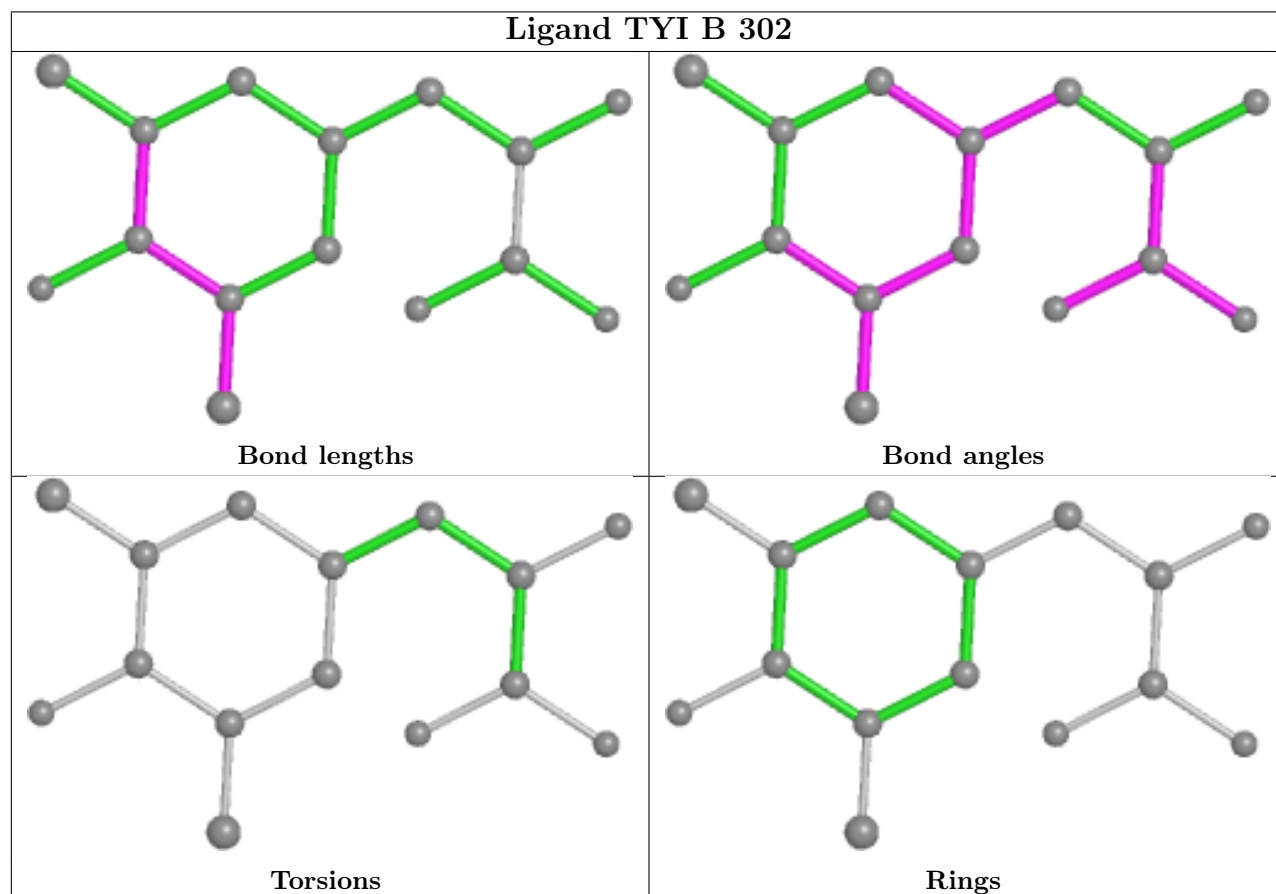
There are no ring outliers.

14 monomers are involved in 29 short contacts:

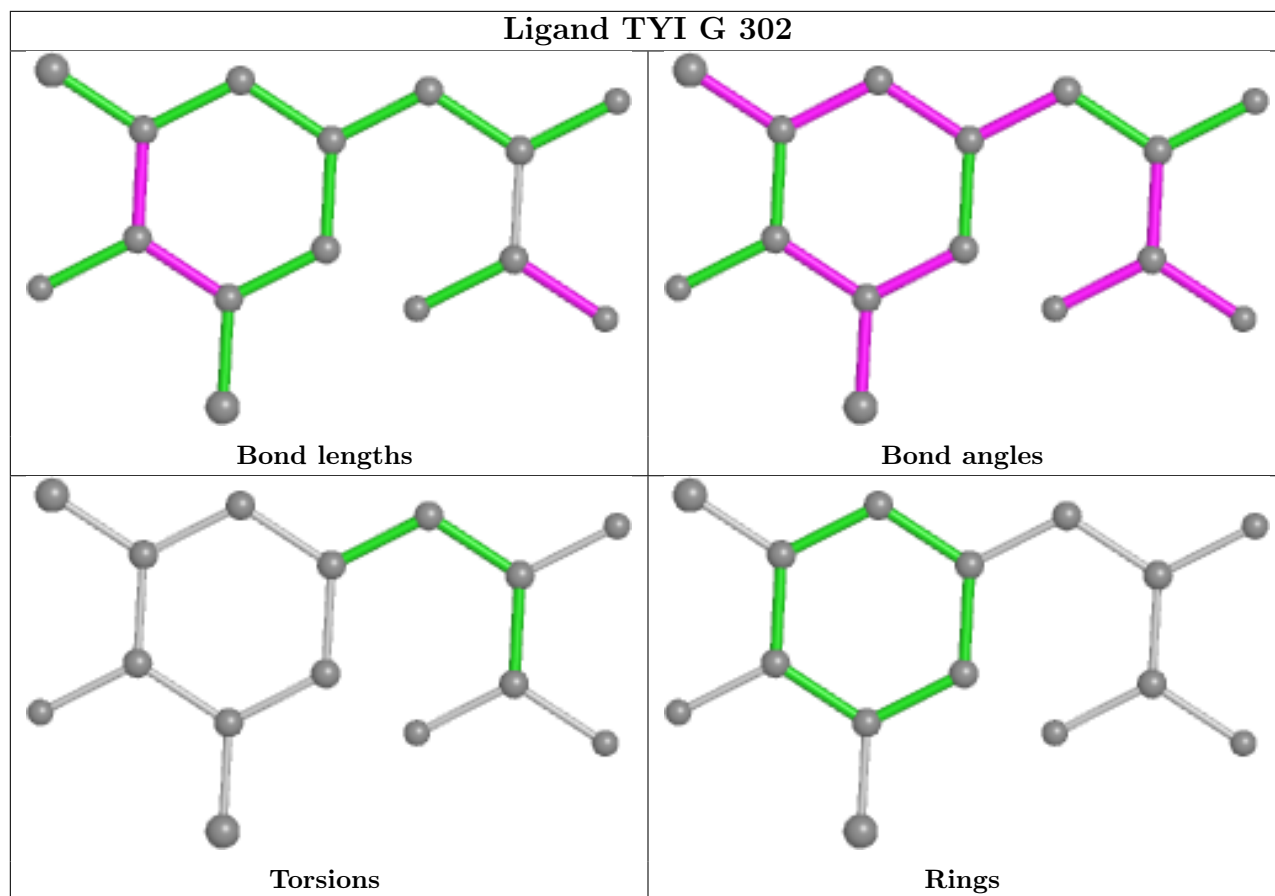
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	TYI	4	0
3	G	302	TYI	1	0
2	E	301	FMN	1	0
2	H	301	FMN	1	0
2	A	301	FMN	3	0
3	F	302	TYI	3	0
2	B	301	FMN	4	0
2	C	301	FMN	2	0
3	D	302	TYI	2	0
3	C	302	TYI	2	0
3	H	302	TYI	3	0
2	G	301	FMN	1	0
3	A	302	TYI	3	0
2	F	301	FMN	1	0

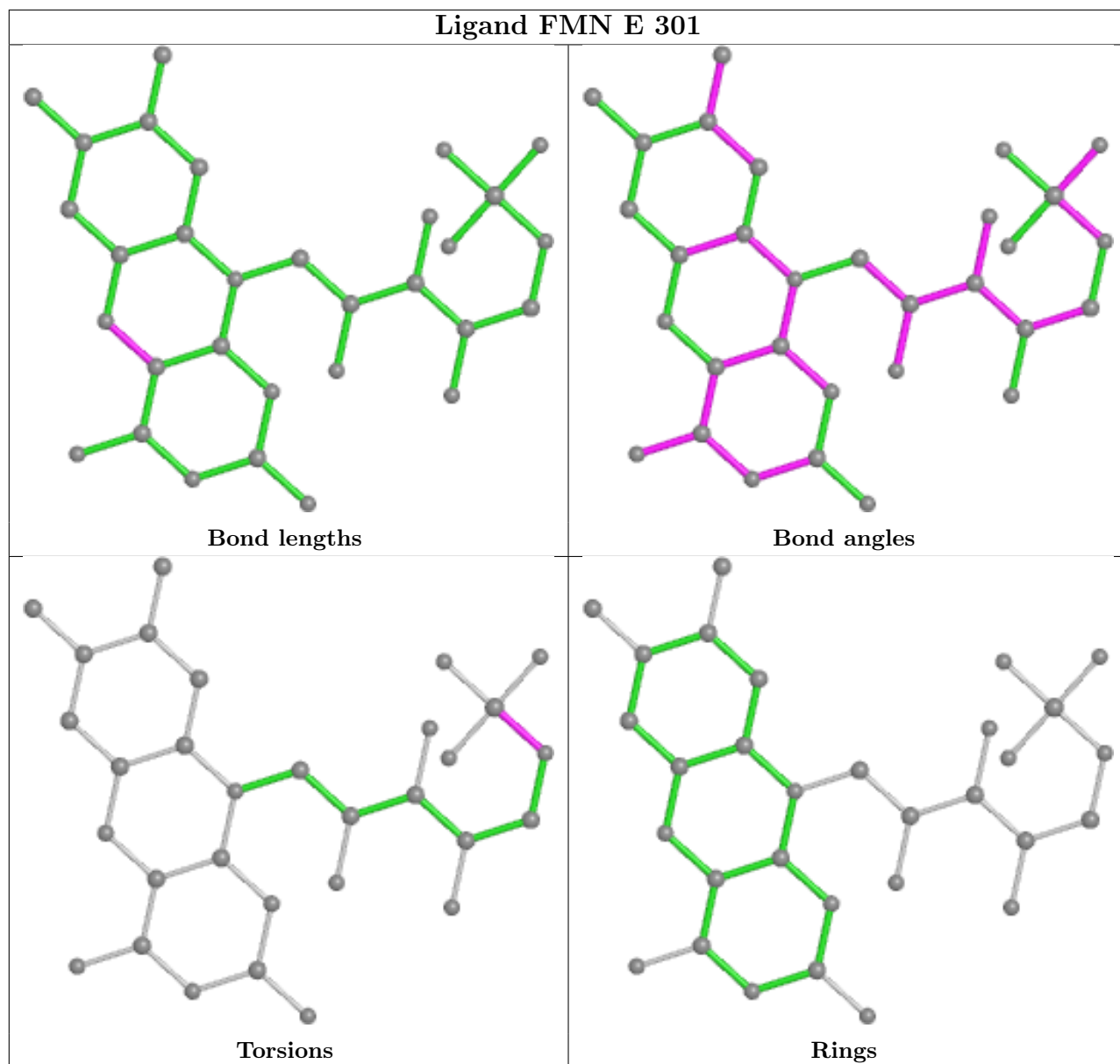
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

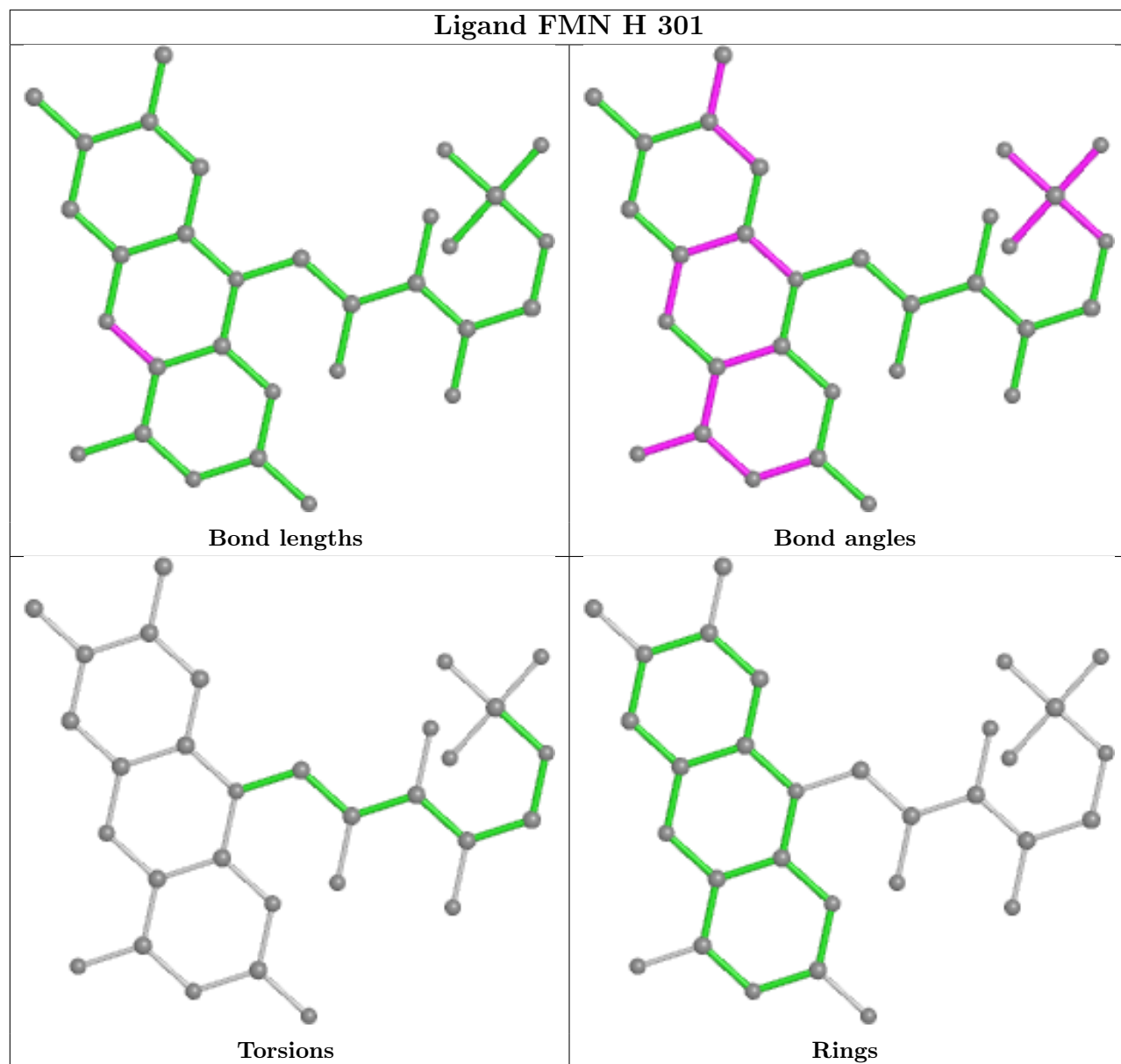
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

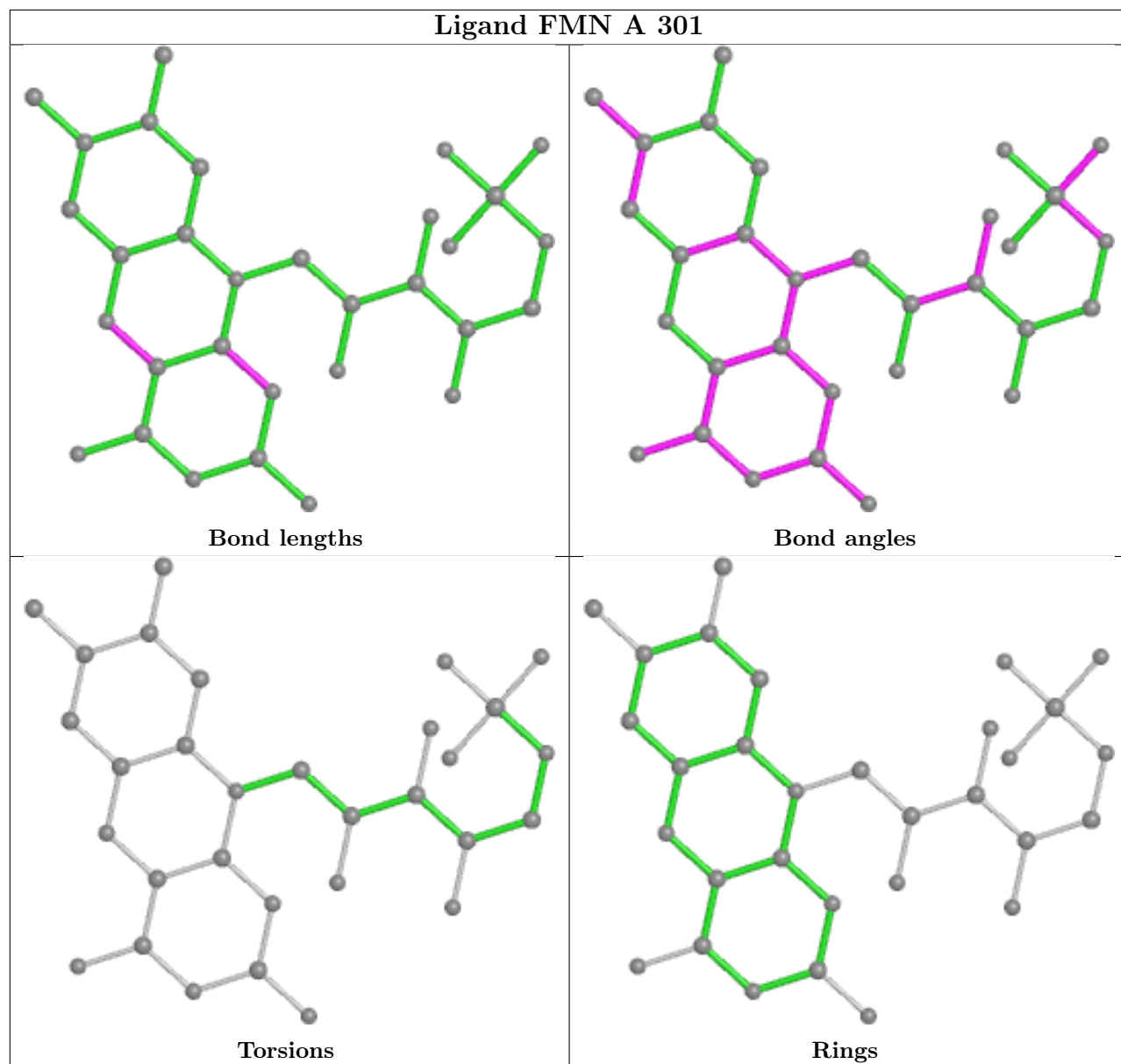


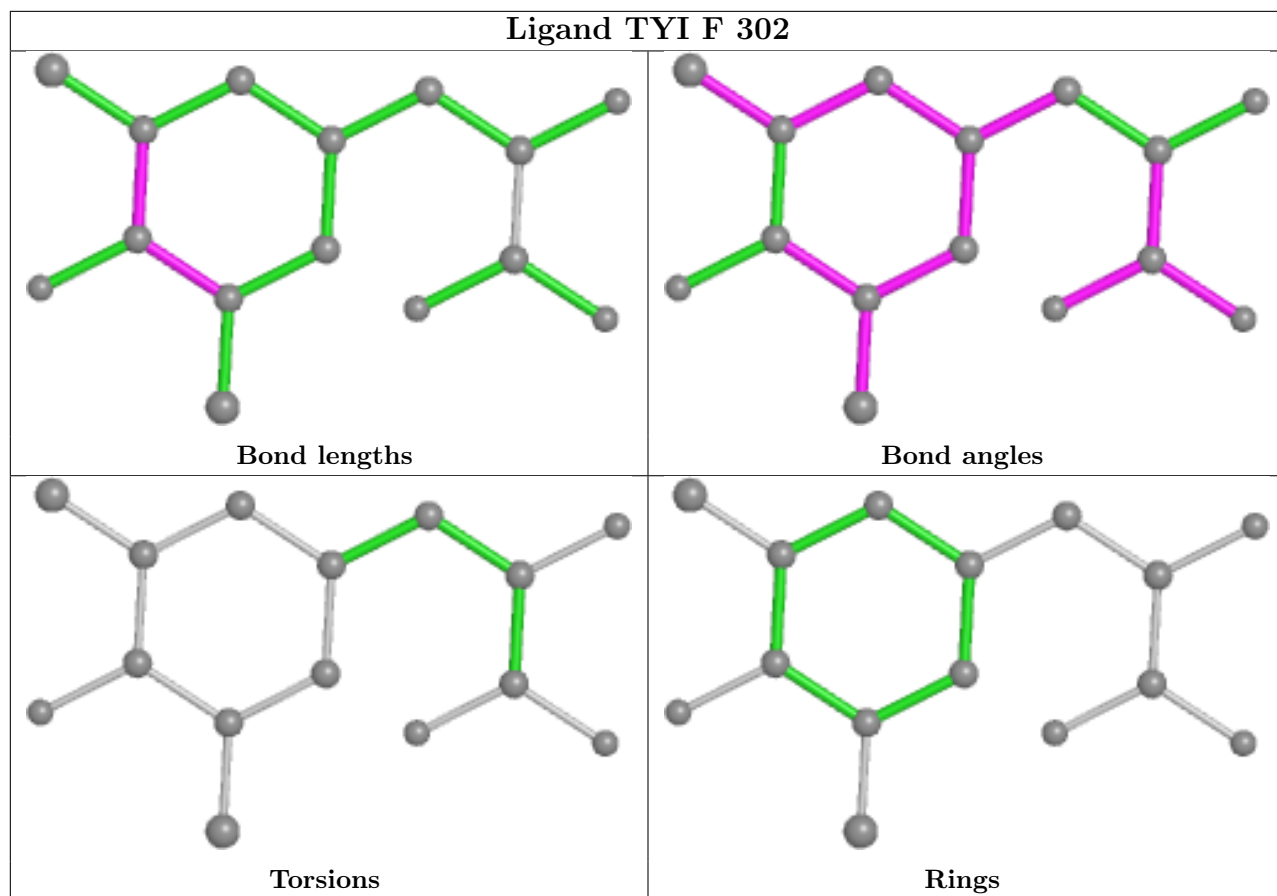


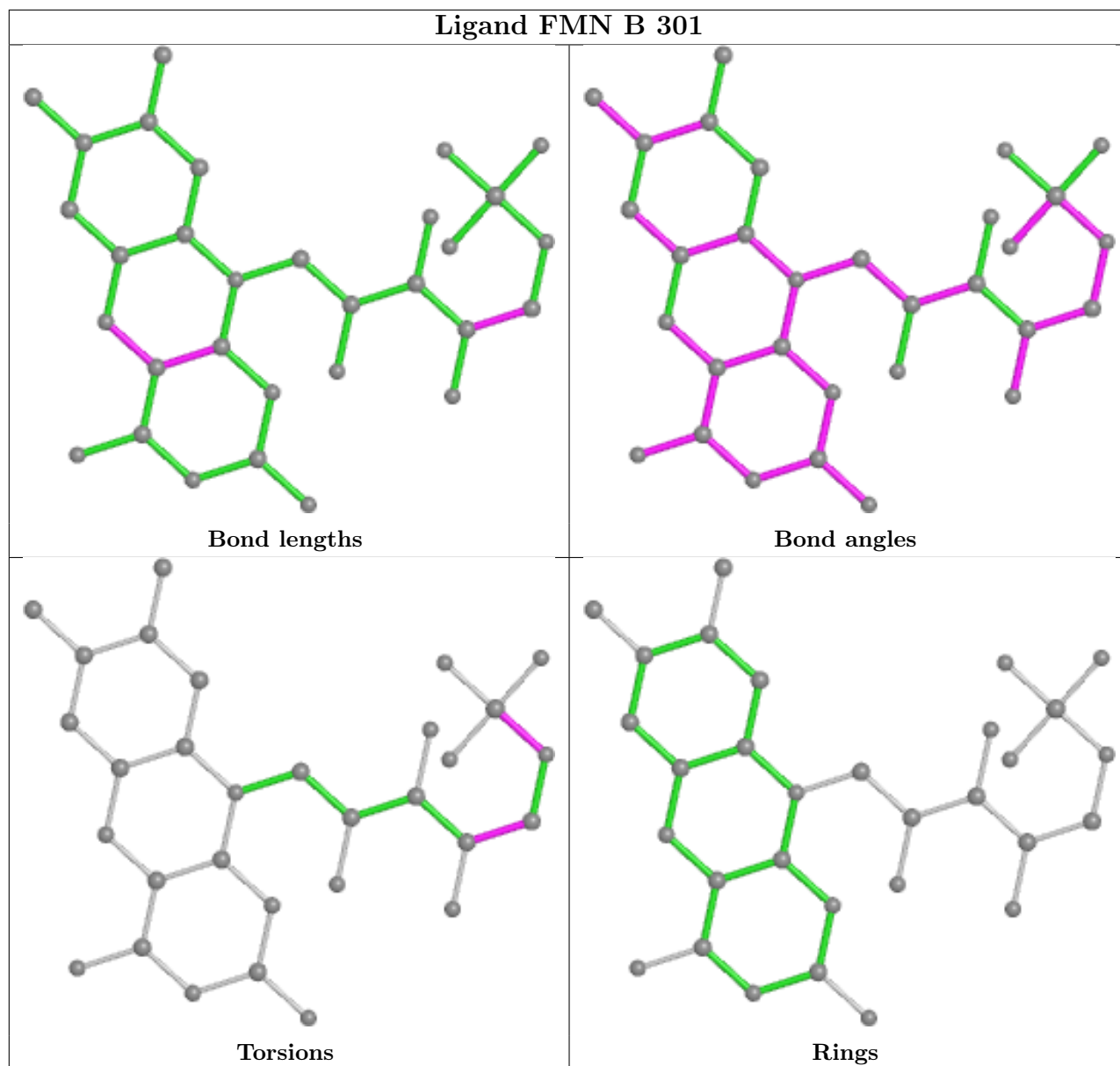


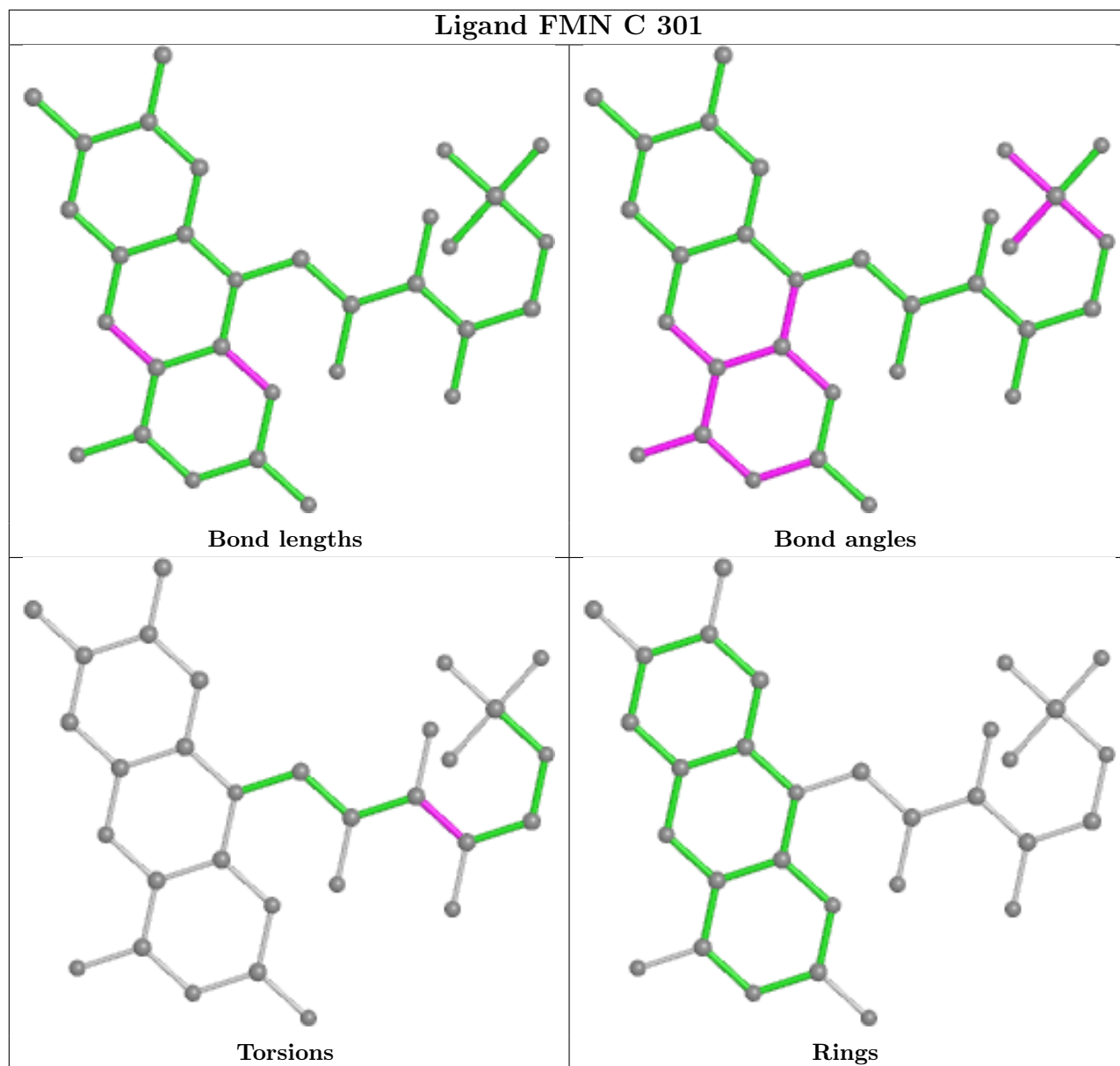


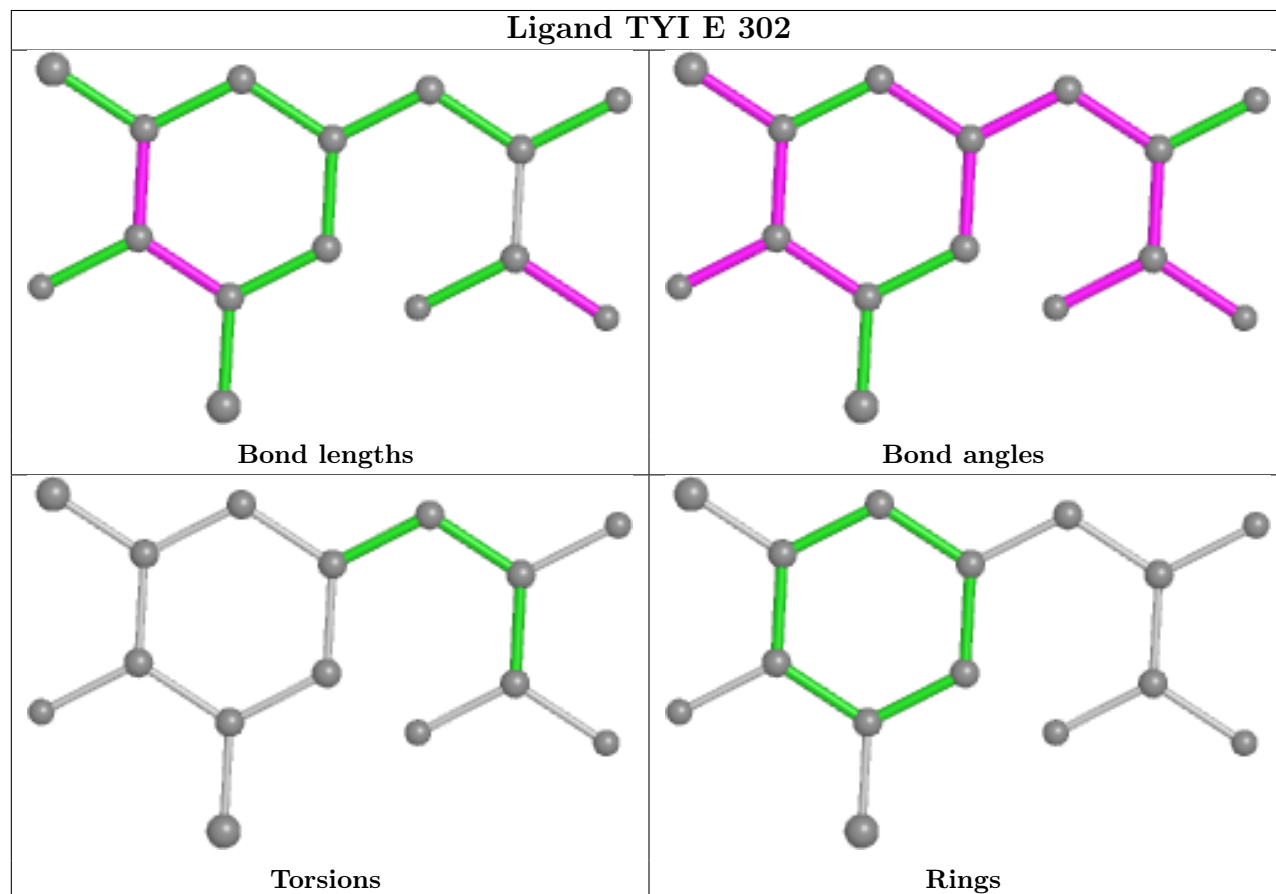
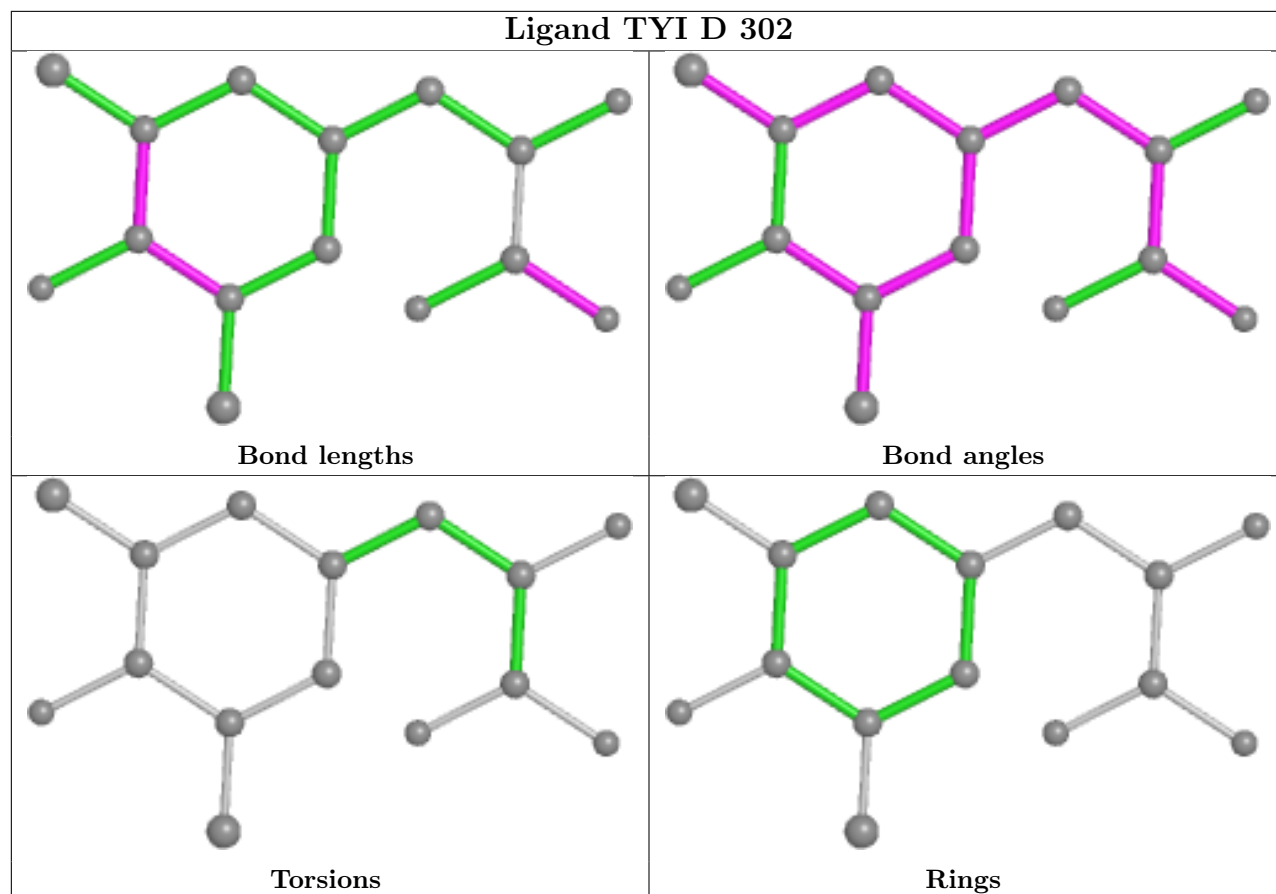




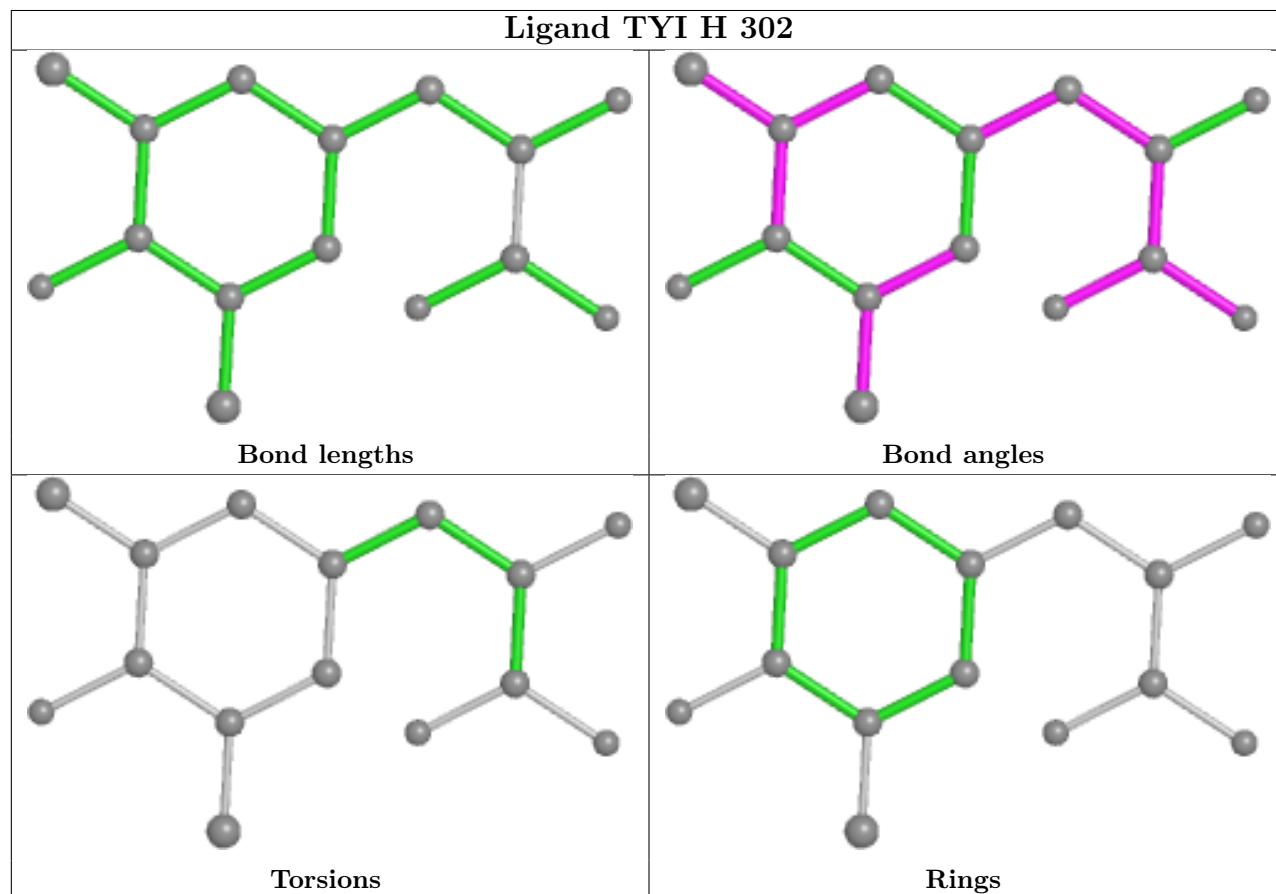
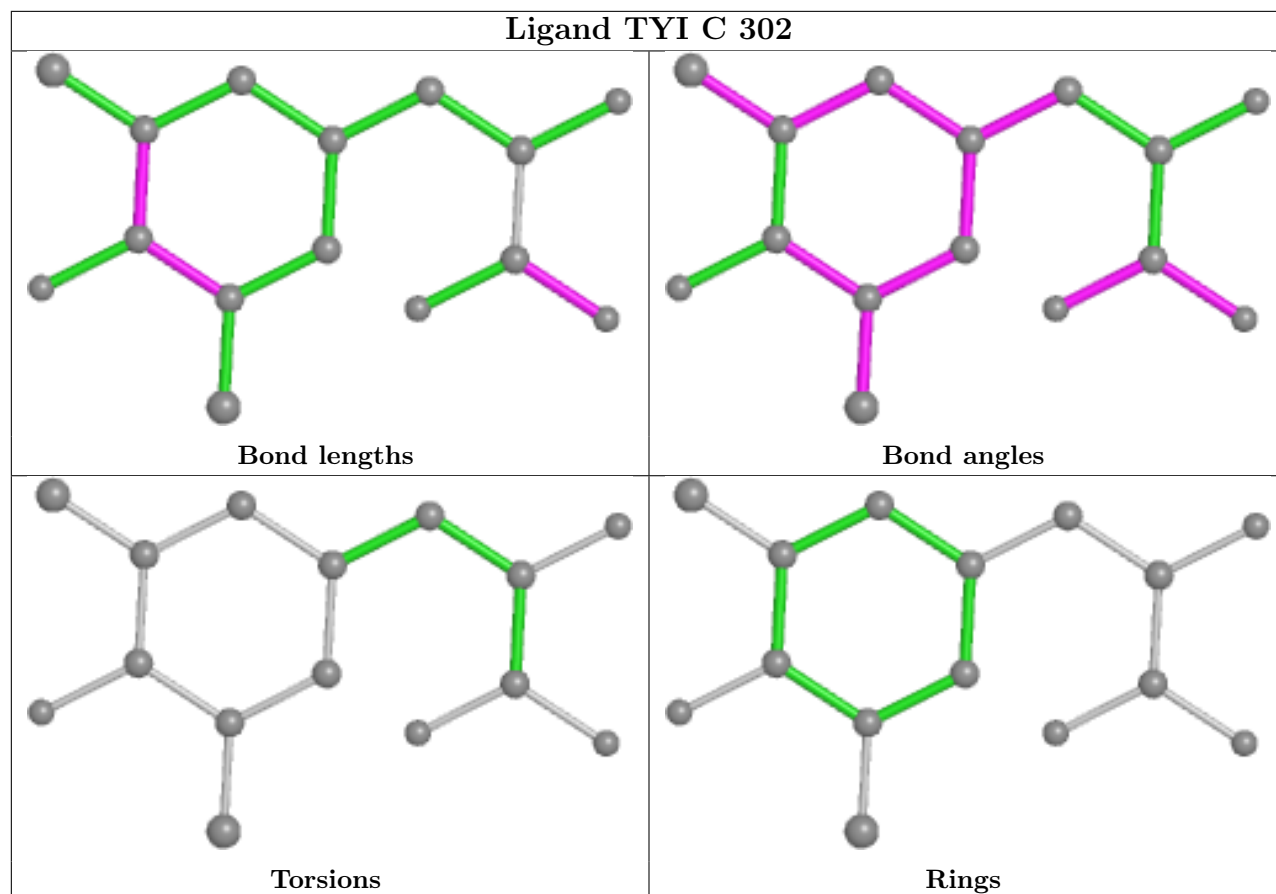


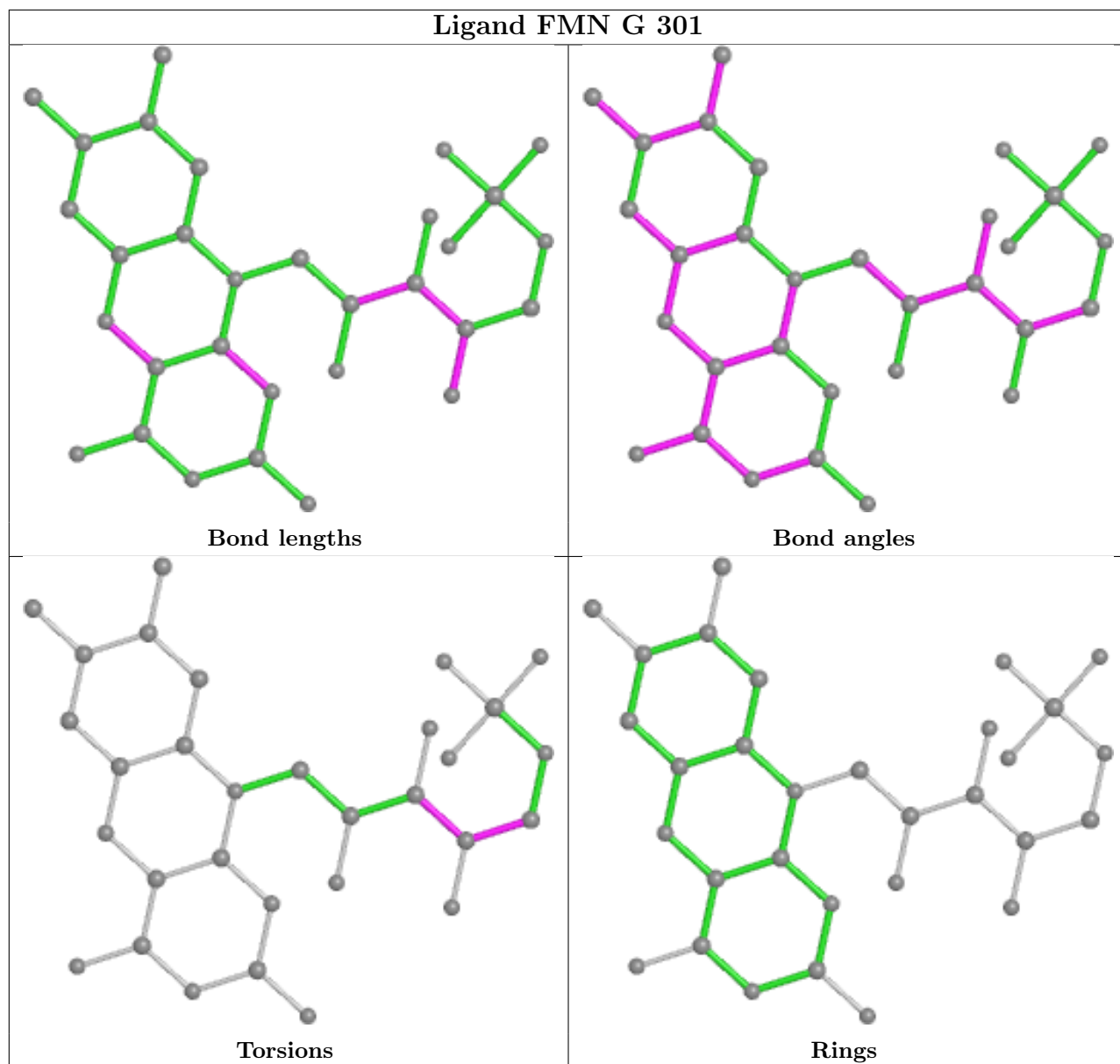


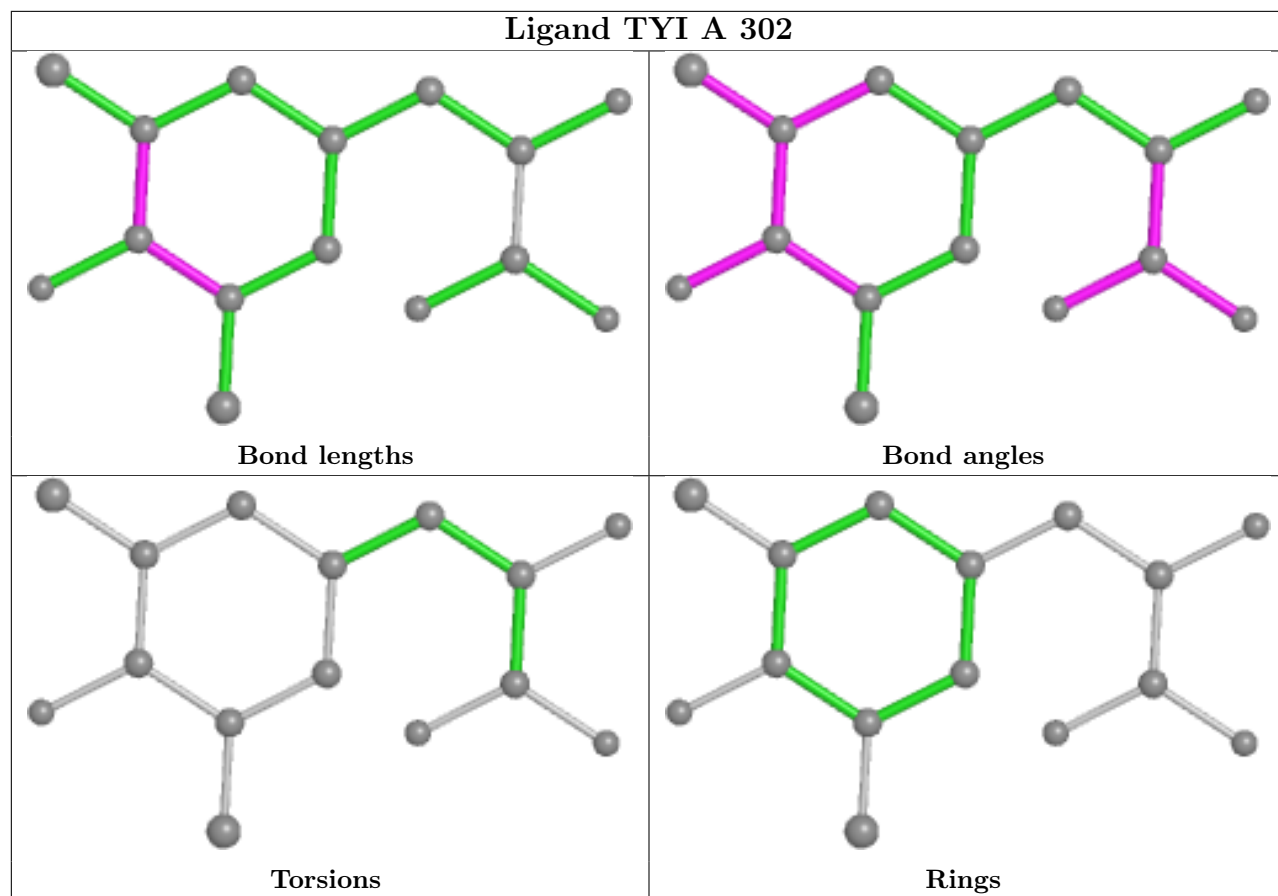


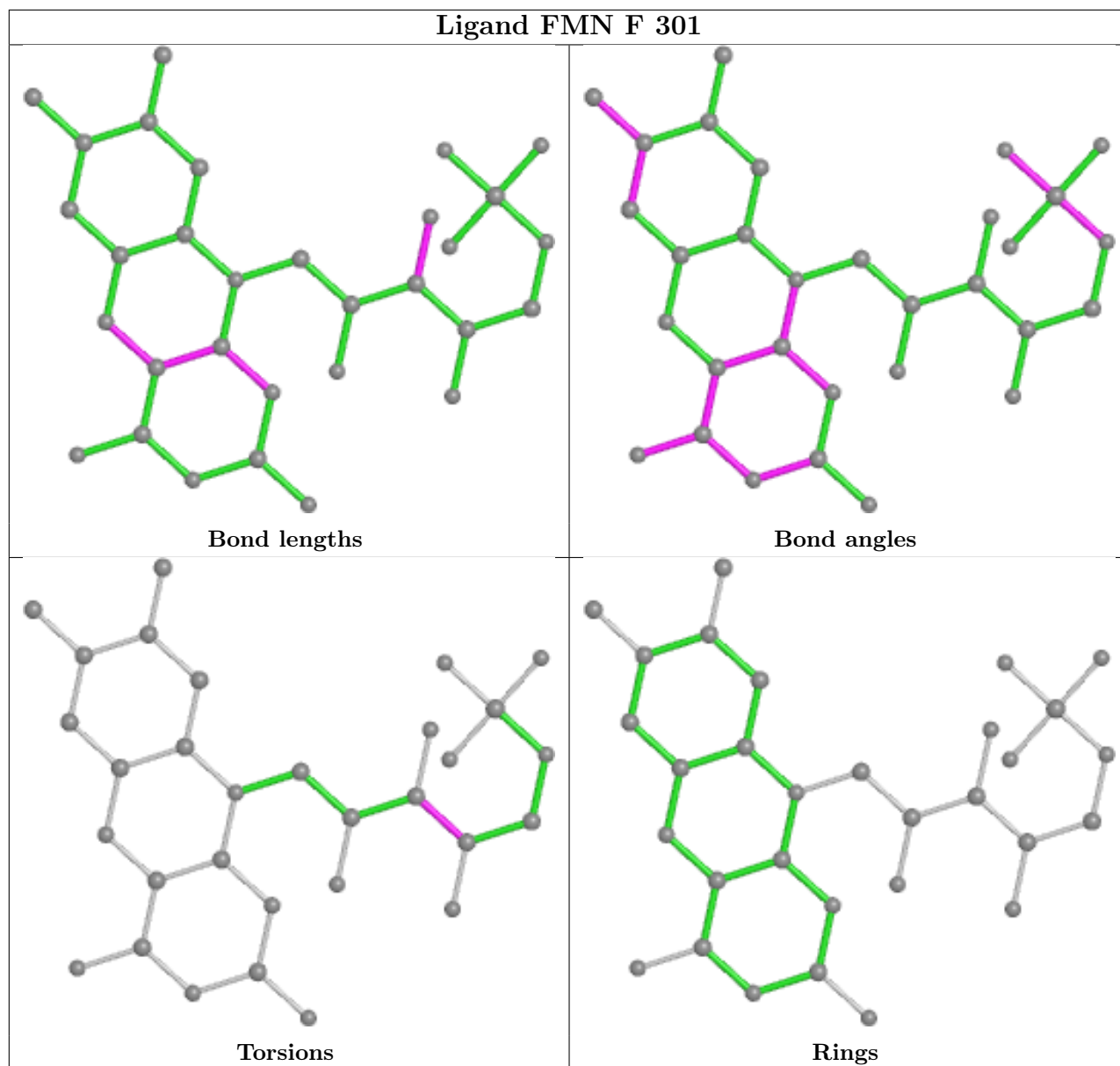


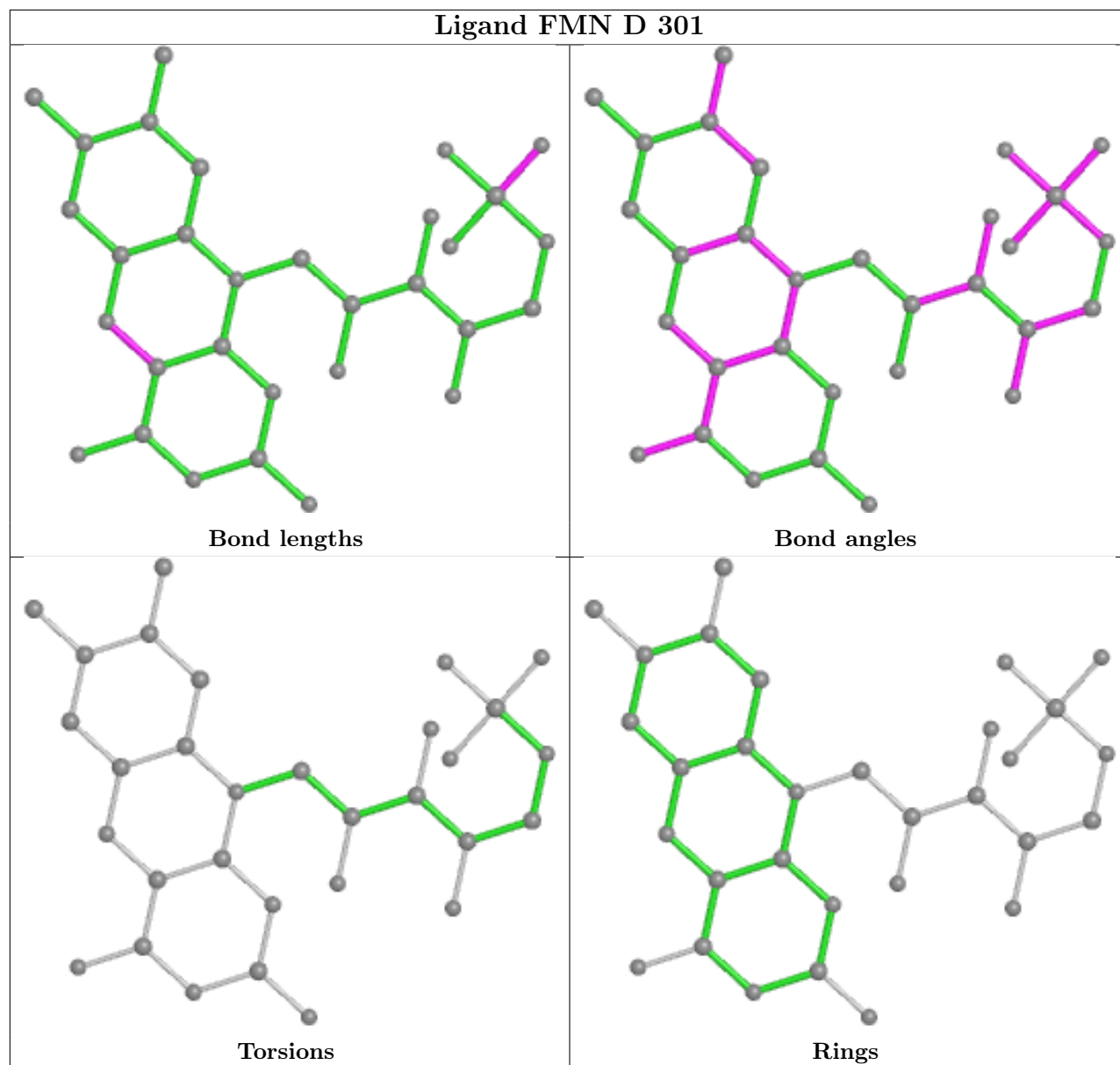












## 5.7 Other polymers [i](#)

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	221/259 (85%)	-0.41	1 (0%) 91   89	24, 33, 45, 56	2 (0%)
1	B	220/259 (84%)	-0.46	1 (0%) 91   89	22, 31, 47, 55	1 (0%)
1	C	221/259 (85%)	-0.38	1 (0%) 91   89	24, 34, 46, 68	0
1	D	220/259 (84%)	-0.46	0 100   100	25, 35, 45, 58	0
1	E	221/259 (85%)	-0.61	0 100   100	18, 35, 51, 63	2 (0%)
1	F	220/259 (84%)	-0.64	0 100   100	18, 33, 52, 61	1 (0%)
1	G	221/259 (85%)	-0.54	2 (0%) 84   82	20, 37, 53, 67	0
1	H	220/259 (84%)	-0.63	0 100   100	22, 36, 51, 56	0
All	All	1764/2072 (85%)	-0.52	5 (0%) 94   93	18, 34, 50, 68	6 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	286	HIS	3.7
1	A	199	ALA	2.8
1	C	286	HIS	2.4
1	B	110	GLU	2.3
1	G	285	VAL	2.2

### 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](#)

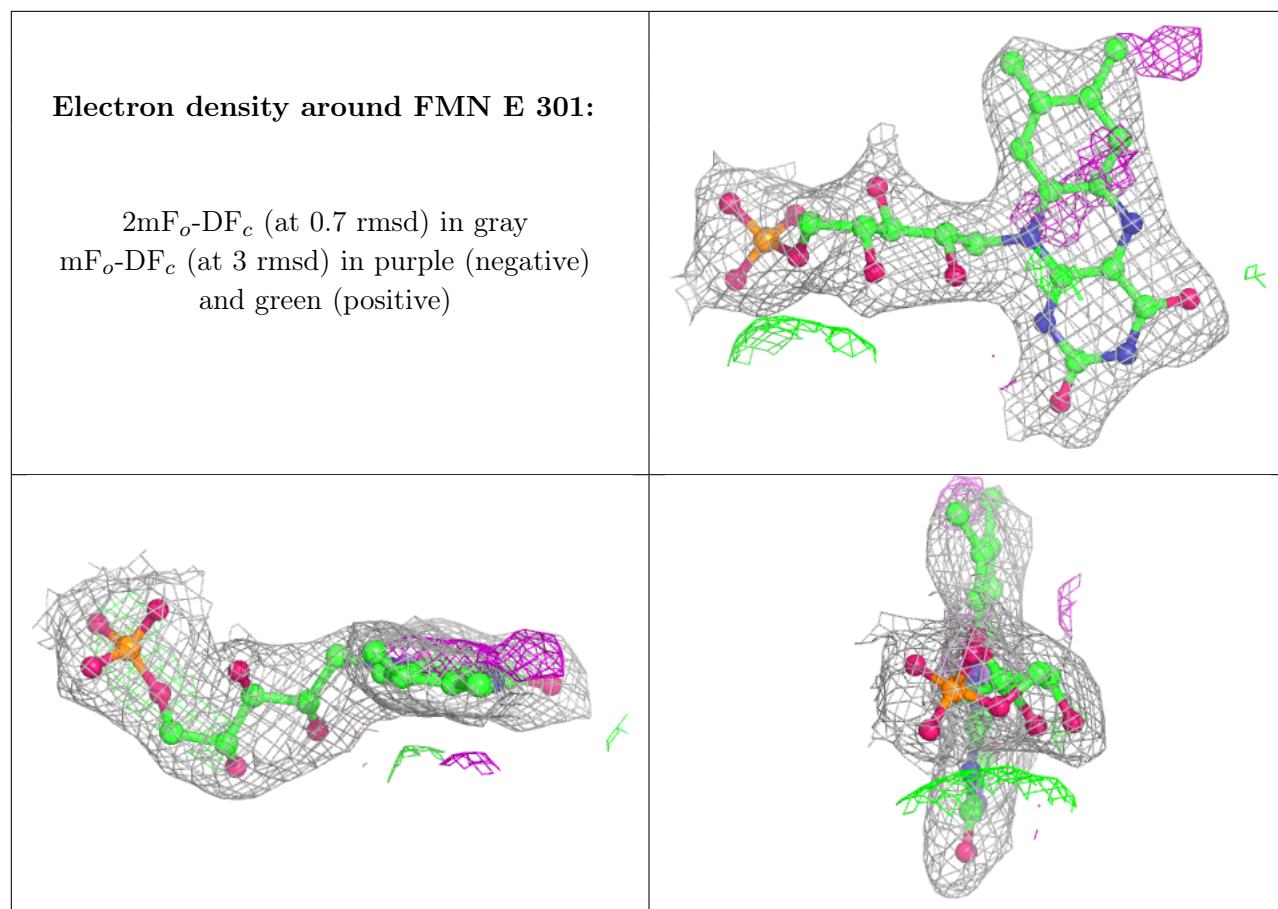
There are no monosaccharides in this entry.

## 6.4 Ligands

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	PO4	C	1	5/5	0.87	0.21	76,79,80,80	0
4	PO4	G	2	5/5	0.92	0.14	78,80,82,82	0
2	FMN	E	301	31/31	0.97	0.14	18,25,28,29	0
2	FMN	H	301	31/31	0.97	0.12	23,27,30,32	0
2	FMN	A	301	31/31	0.97	0.13	16,27,29,30	0
2	FMN	D	301	31/31	0.97	0.12	24,28,29,31	0
2	FMN	B	301	31/31	0.98	0.12	15,24,26,30	0
3	TYI	A	302	15/15	0.98	0.14	37,39,41,42	2
3	TYI	C	302	15/15	0.98	0.10	39,40,45,49	1
3	TYI	D	302	15/15	0.98	0.14	39,41,44,50	1
3	TYI	H	302	15/15	0.98	0.11	33,35,40,47	1
2	FMN	C	301	31/31	0.98	0.11	17,24,26,26	0
2	FMN	G	301	31/31	0.98	0.12	14,24,27,27	0
3	TYI	F	302	15/15	0.99	0.13	38,42,43,50	1
3	TYI	G	302	15/15	0.99	0.14	42,44,48,49	1
2	FMN	F	301	31/31	0.99	0.10	11,21,23,26	0
3	TYI	B	302	15/15	0.99	0.10	35,38,40,46	1
3	TYI	E	302	15/15	0.99	0.12	35,38,41,43	2

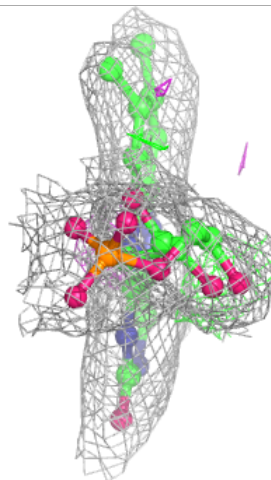
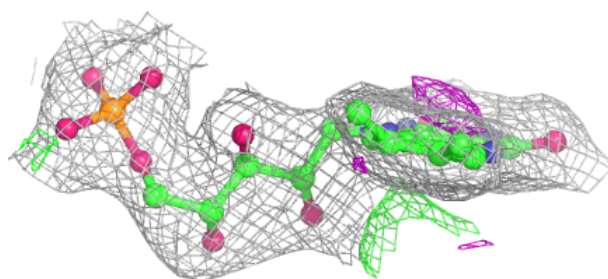
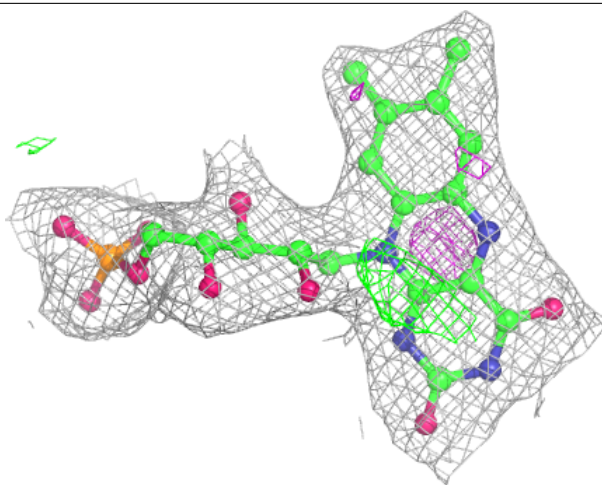
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





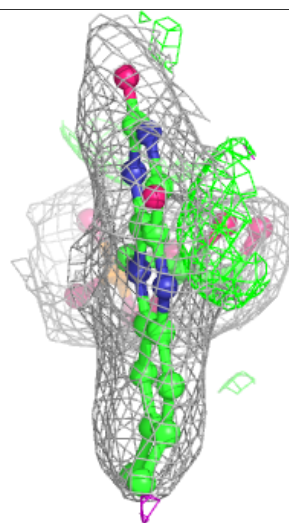
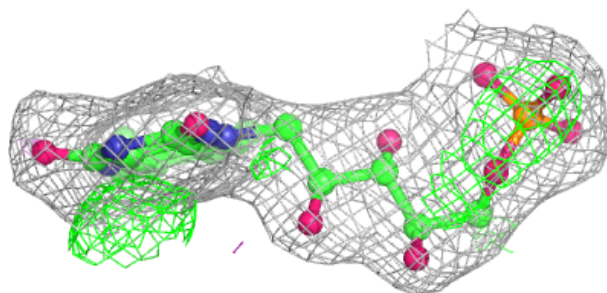
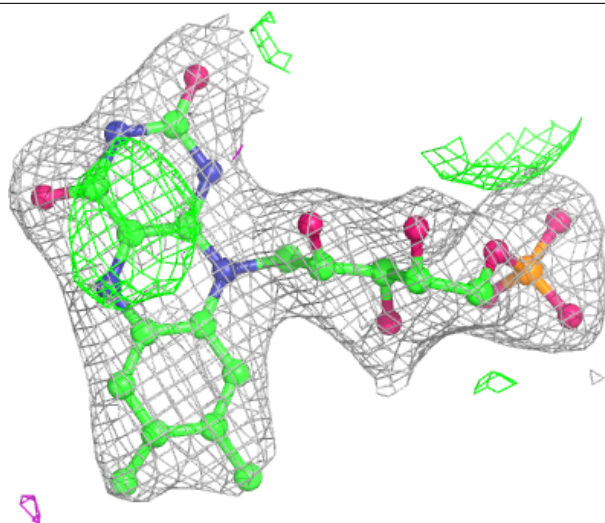
**Electron density around FMN H 301:**

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



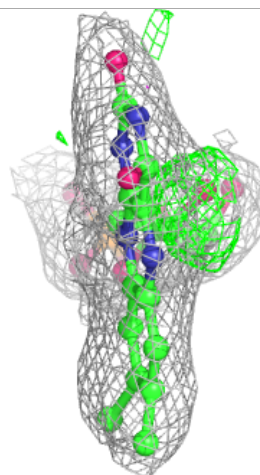
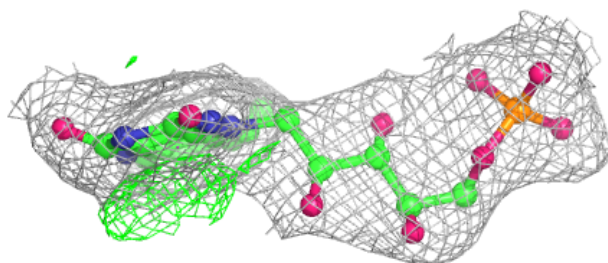
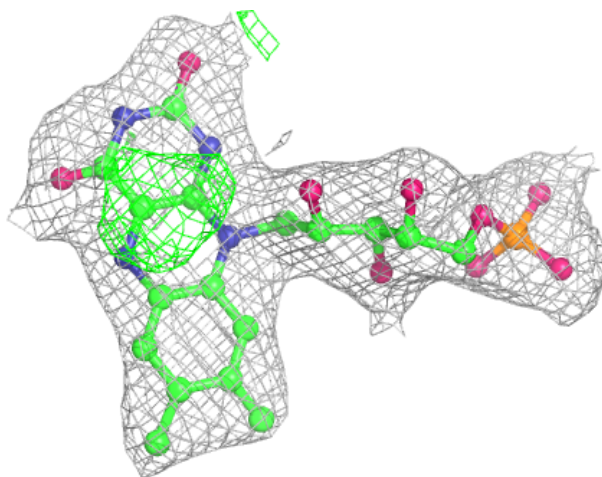
**Electron density around FMN A 301:**

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



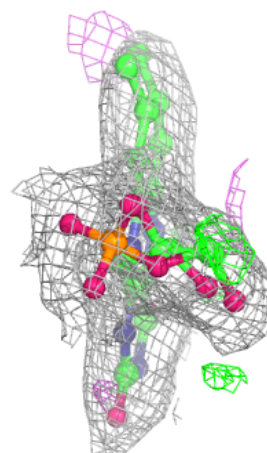
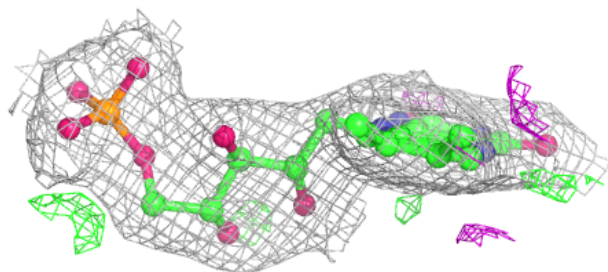
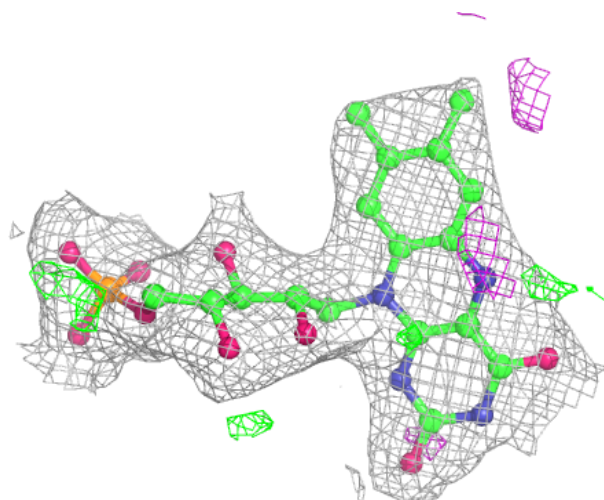
**Electron density around FMN D 301:**

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



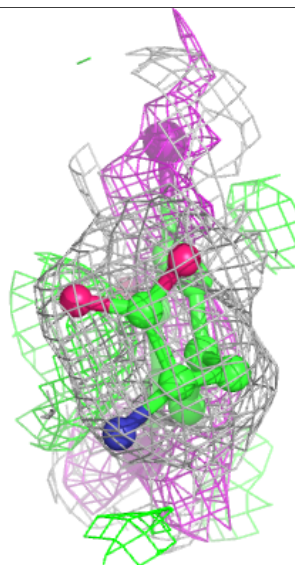
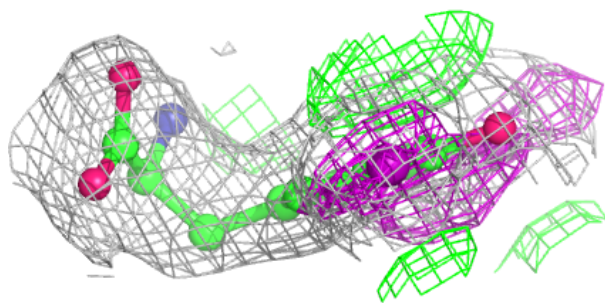
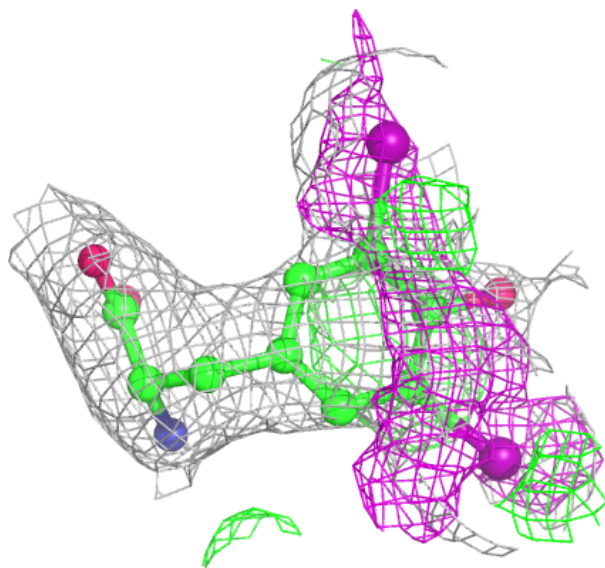
**Electron density around FMN B 301:**

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



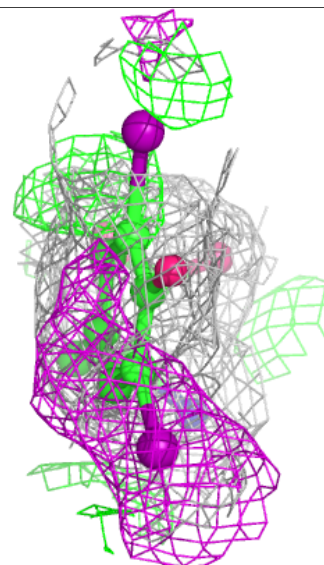
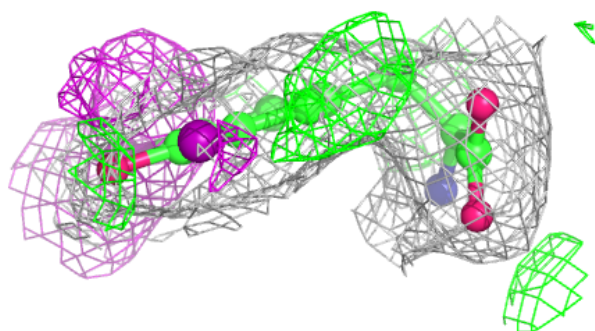
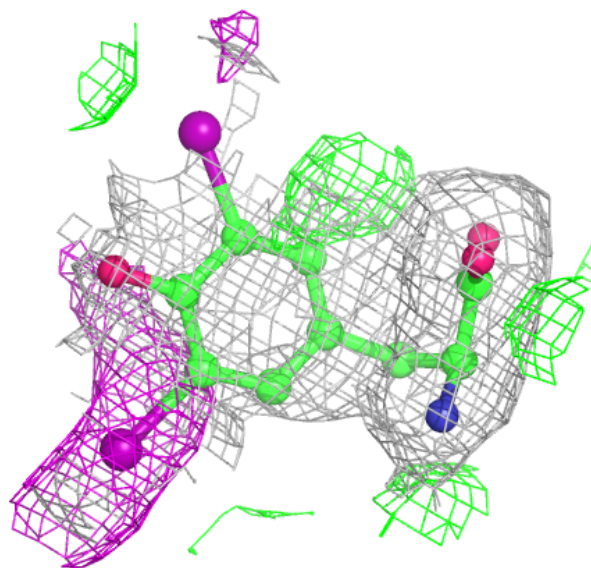
**Electron density around TYI A 302:**

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



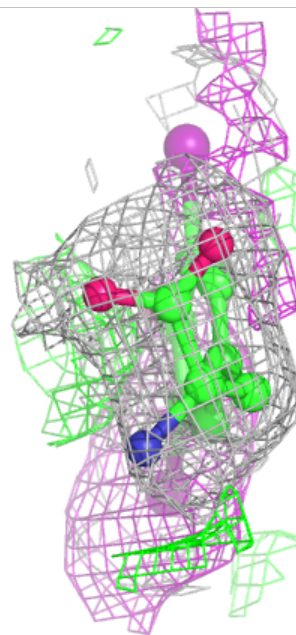
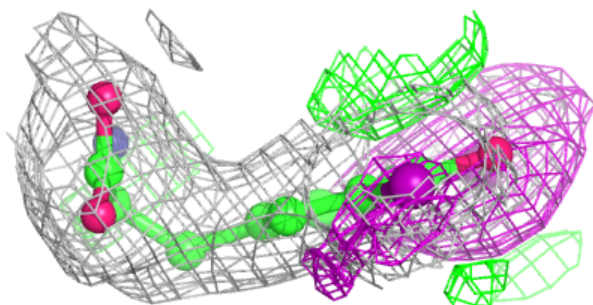
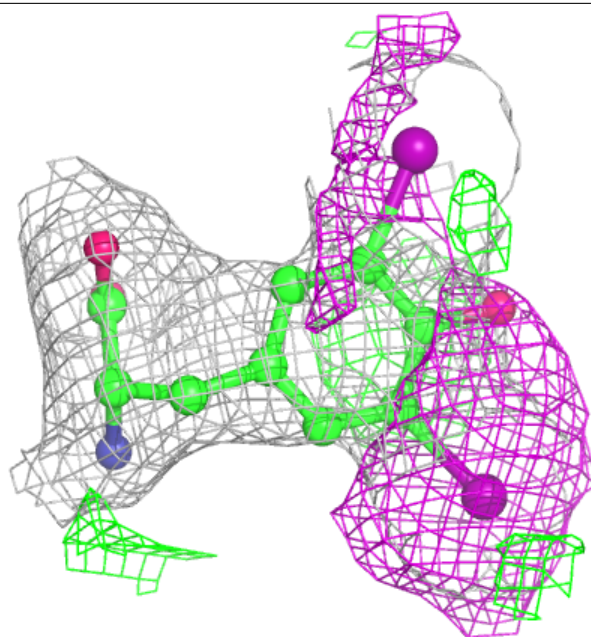
**Electron density around TYI C 302:**

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



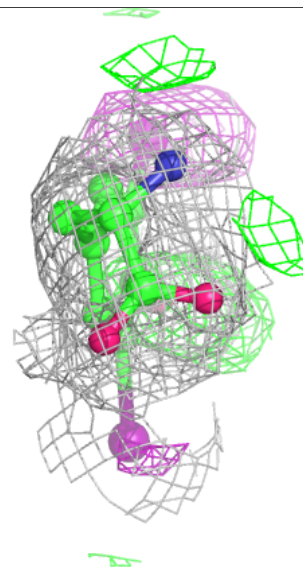
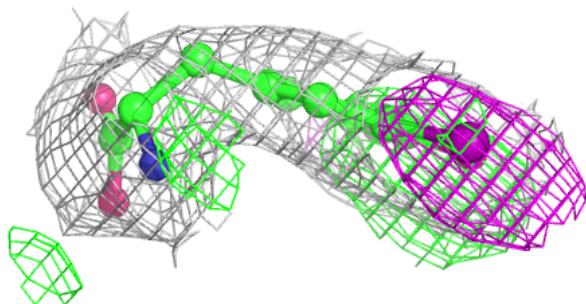
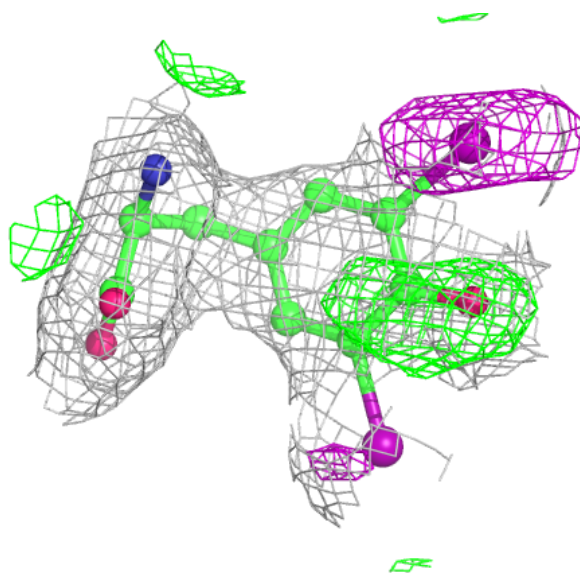
**Electron density around TYI D 302:**

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



**Electron density around TYI H 302:**

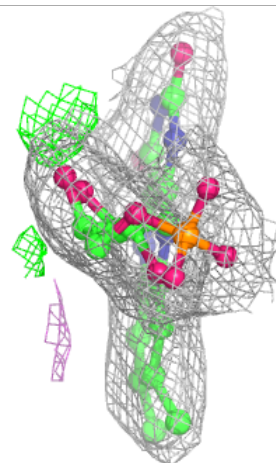
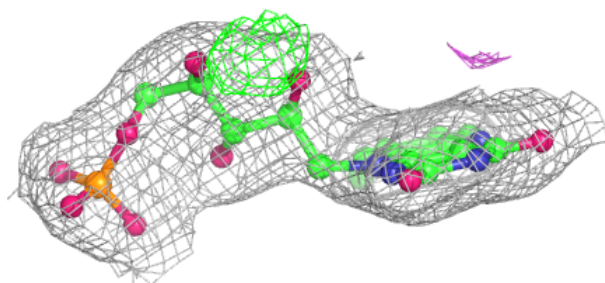
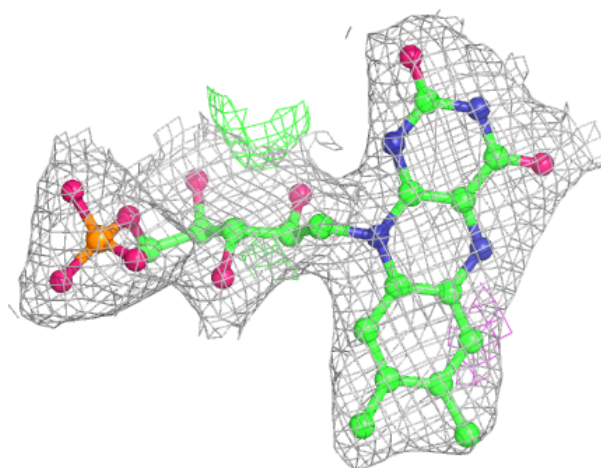
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





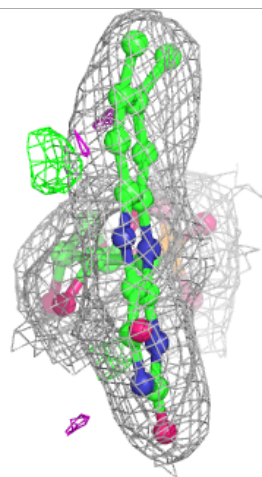
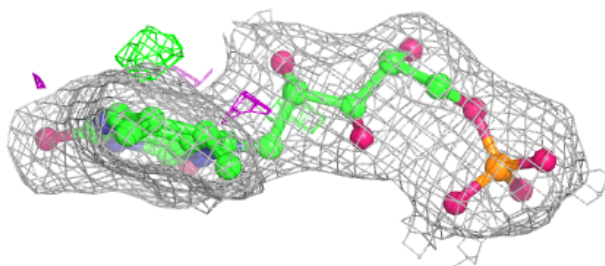
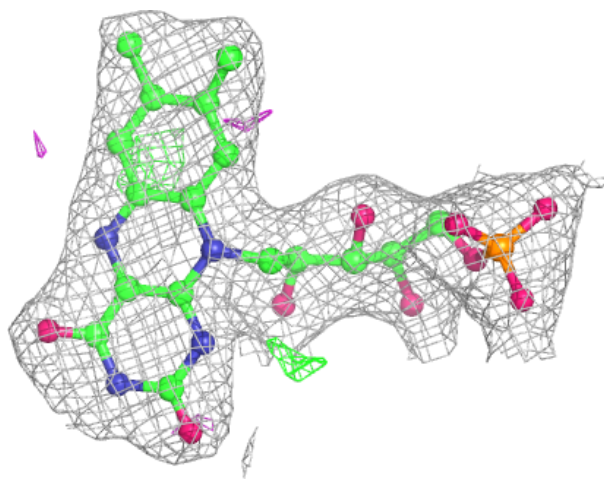
**Electron density around FMN C 301:**

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



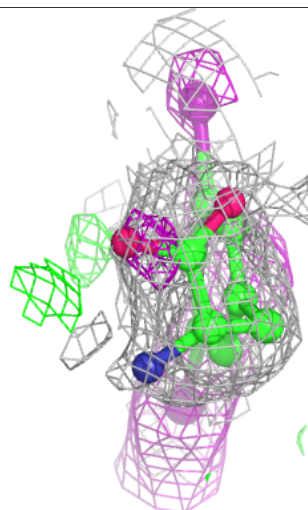
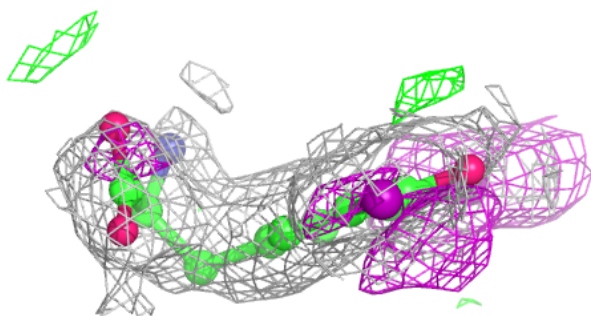
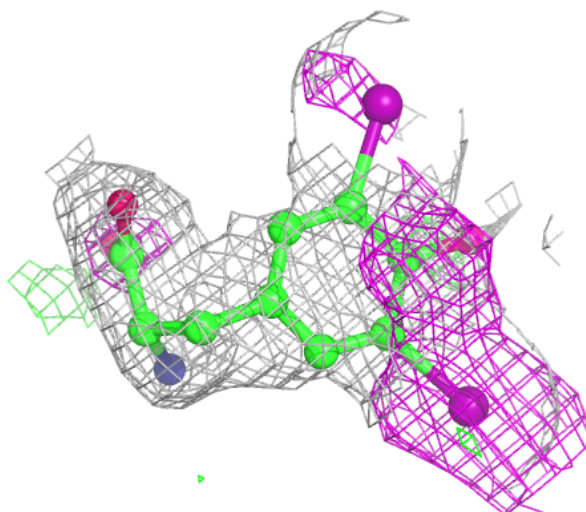
**Electron density around FMN G 301:**

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



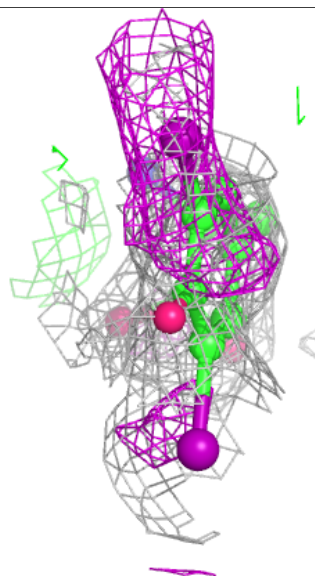
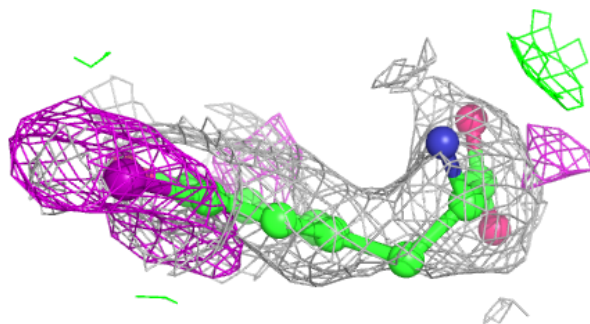
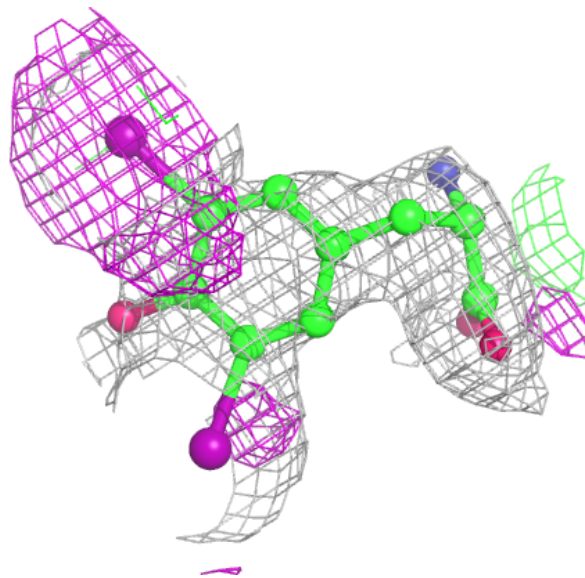
**Electron density around TYI F 302:**

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



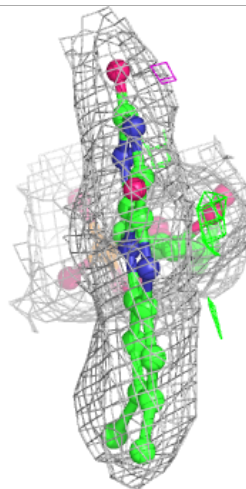
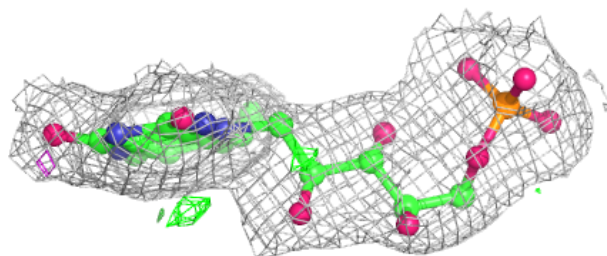
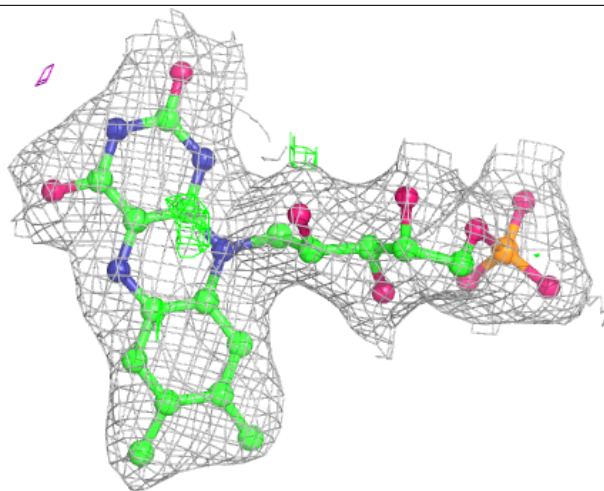
**Electron density around TYI G 302:**

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



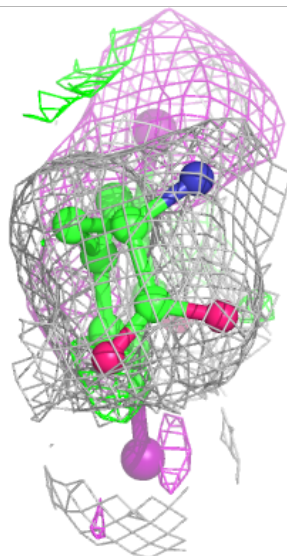
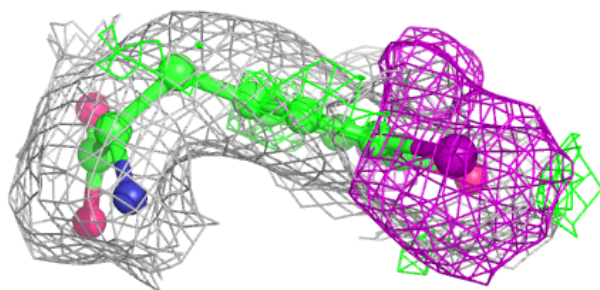
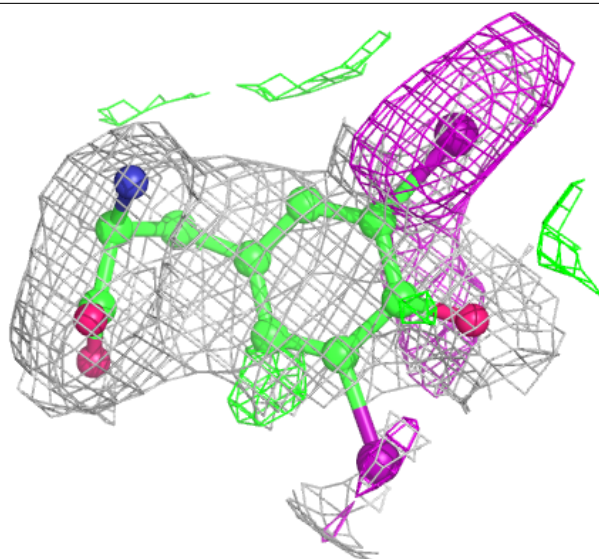
**Electron density around FMN F 301:**

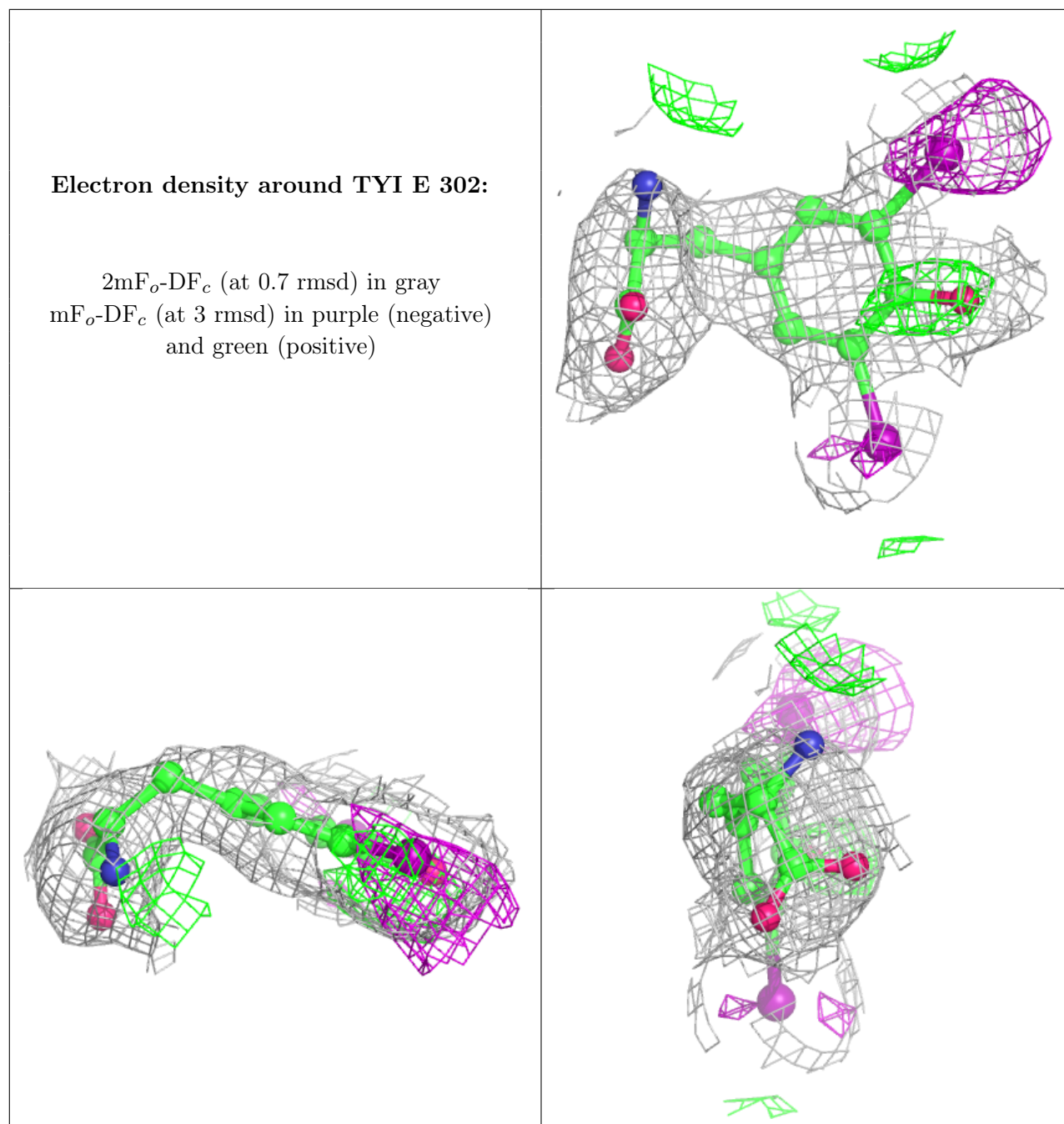
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around TYI B 302:**

$2mF_o-DF_c$  (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.