



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 29, 2023 – 12:13 PM JST

PDB ID : 8JQO
Title : Protocatechuate hydroxylase from *Xylophilus ampelinus* complexed with imidazole
Authors : Fukushima, R.; Katsuki, N.; Fushinobu, S.; Takaya, N.
Deposited on : 2023-06-14
Resolution : 1.60 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

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 : 2.36
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) : 2.36

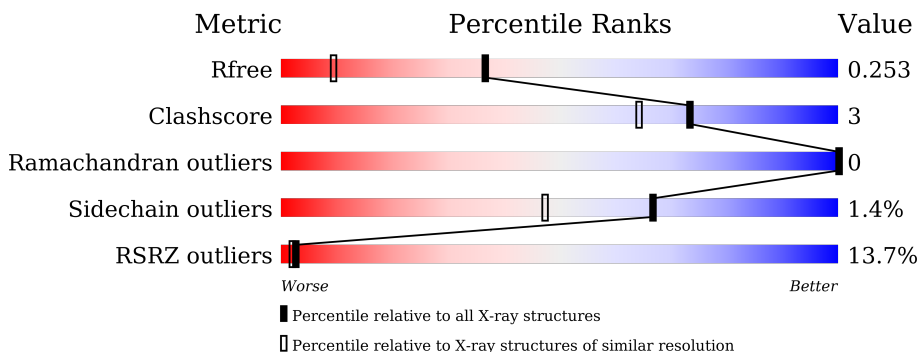
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

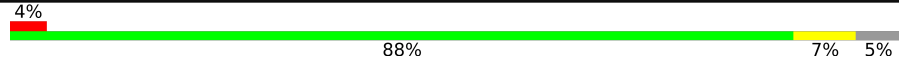
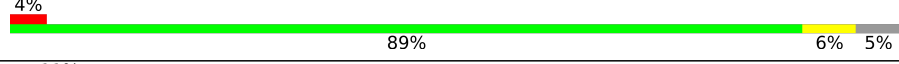


The reported resolution of this entry is 1.60 Å.

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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 ≥ 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	411	 4% 88% 7% 5%
1	B	411	 4% 89% 6% 5%
1	C	411	 11% 84% 9% 6%
1	D	411	 31% 64% 11% 25%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12403 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 4-hydroxybenzoate 3-monooxygenase (NAD(P)H).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	391	Total 3029	C 1884	N 569	O 552	S 24	0	0	0
1	B	391	Total 3029	C 1884	N 569	O 552	S 24	0	0	0
1	C	387	Total 2999	C 1868	N 562	O 545	S 24	0	0	0
1	D	309	Total 2410	C 1503	N 451	O 436	S 20	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A978C2P2
A	-18	GLN	-	expression tag	UNP A0A978C2P2
A	-17	LEU	-	expression tag	UNP A0A978C2P2
A	-16	SER	-	expression tag	UNP A0A978C2P2
A	-15	HIS	-	expression tag	UNP A0A978C2P2
A	-14	HIS	-	expression tag	UNP A0A978C2P2
A	-13	HIS	-	expression tag	UNP A0A978C2P2
A	-12	HIS	-	expression tag	UNP A0A978C2P2
A	-11	HIS	-	expression tag	UNP A0A978C2P2
A	-10	HIS	-	expression tag	UNP A0A978C2P2
A	-9	SER	-	expression tag	UNP A0A978C2P2
A	-8	SER	-	expression tag	UNP A0A978C2P2
A	-7	GLY	-	expression tag	UNP A0A978C2P2
A	-6	LEU	-	expression tag	UNP A0A978C2P2
A	-5	VAL	-	expression tag	UNP A0A978C2P2
A	-4	PRO	-	expression tag	UNP A0A978C2P2
A	-3	ARG	-	expression tag	UNP A0A978C2P2
A	-2	GLY	-	expression tag	UNP A0A978C2P2
A	-1	SER	-	expression tag	UNP A0A978C2P2
A	0	HIS	-	expression tag	UNP A0A978C2P2
A	1	MET	-	expression tag	UNP A0A978C2P2

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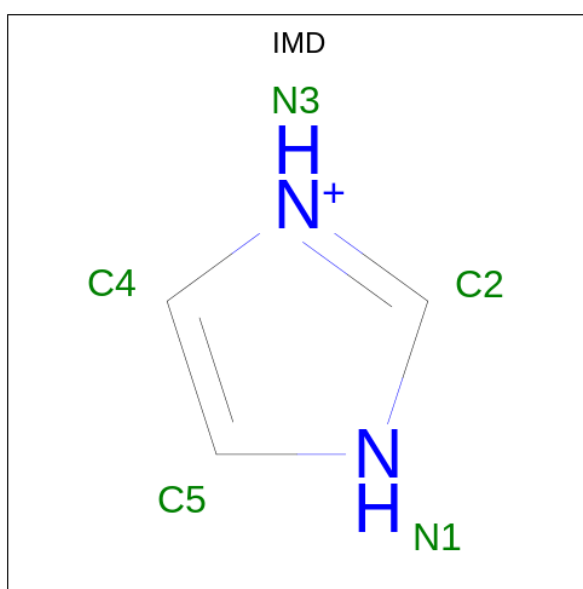
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP A0A978C2P2
B	-18	GLN	-	expression tag	UNP A0A978C2P2
B	-17	LEU	-	expression tag	UNP A0A978C2P2
B	-16	SER	-	expression tag	UNP A0A978C2P2
B	-15	HIS	-	expression tag	UNP A0A978C2P2
B	-14	HIS	-	expression tag	UNP A0A978C2P2
B	-13	HIS	-	expression tag	UNP A0A978C2P2
B	-12	HIS	-	expression tag	UNP A0A978C2P2
B	-11	HIS	-	expression tag	UNP A0A978C2P2
B	-10	HIS	-	expression tag	UNP A0A978C2P2
B	-9	SER	-	expression tag	UNP A0A978C2P2
B	-8	SER	-	expression tag	UNP A0A978C2P2
B	-7	GLY	-	expression tag	UNP A0A978C2P2
B	-6	LEU	-	expression tag	UNP A0A978C2P2
B	-5	VAL	-	expression tag	UNP A0A978C2P2
B	-4	PRO	-	expression tag	UNP A0A978C2P2
B	-3	ARG	-	expression tag	UNP A0A978C2P2
B	-2	GLY	-	expression tag	UNP A0A978C2P2
B	-1	SER	-	expression tag	UNP A0A978C2P2
B	0	HIS	-	expression tag	UNP A0A978C2P2
B	1	MET	-	expression tag	UNP A0A978C2P2
C	-19	MET	-	initiating methionine	UNP A0A978C2P2
C	-18	GLN	-	expression tag	UNP A0A978C2P2
C	-17	LEU	-	expression tag	UNP A0A978C2P2
C	-16	SER	-	expression tag	UNP A0A978C2P2
C	-15	HIS	-	expression tag	UNP A0A978C2P2
C	-14	HIS	-	expression tag	UNP A0A978C2P2
C	-13	HIS	-	expression tag	UNP A0A978C2P2
C	-12	HIS	-	expression tag	UNP A0A978C2P2
C	-11	HIS	-	expression tag	UNP A0A978C2P2
C	-10	HIS	-	expression tag	UNP A0A978C2P2
C	-9	SER	-	expression tag	UNP A0A978C2P2
C	-8	SER	-	expression tag	UNP A0A978C2P2
C	-7	GLY	-	expression tag	UNP A0A978C2P2
C	-6	LEU	-	expression tag	UNP A0A978C2P2
C	-5	VAL	-	expression tag	UNP A0A978C2P2
C	-4	PRO	-	expression tag	UNP A0A978C2P2
C	-3	ARG	-	expression tag	UNP A0A978C2P2
C	-2	GLY	-	expression tag	UNP A0A978C2P2
C	-1	SER	-	expression tag	UNP A0A978C2P2
C	0	HIS	-	expression tag	UNP A0A978C2P2
C	1	MET	-	expression tag	UNP A0A978C2P2

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	D	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 3 is IMIDAZOLE (three-letter code: IMD) (formula: C₃H₅N₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
3	A	1	Total 5	C 3	N 2	0	0
3	A	1	Total 5	C 3	N 2	0	0
3	B	1	Total 5	C 3	N 2	0	0
3	B	1	Total 5	C 3	N 2	0	0
3	C	1	Total 5	C 3	N 2	0	0
3	C	1	Total 5	C 3	N 2	0	0
3	D	1	Total 5	C 3	N 2	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

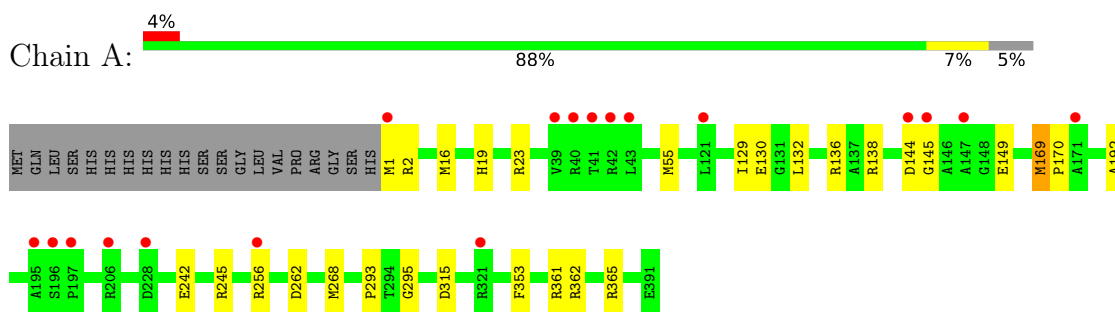
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	229	Total O 229 229	0	0
5	B	224	Total O 224 224	0	0
5	C	152	Total O 152 152	0	0
5	D	80	Total O 80 80	0	0

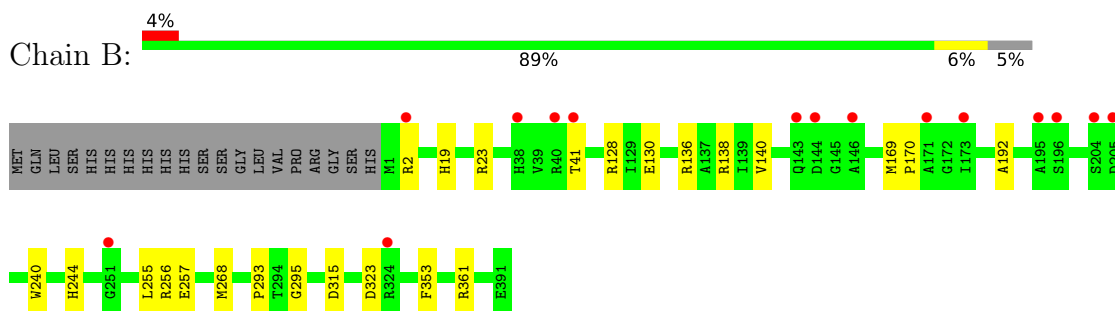
3 Residue-property plots [i](#)

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.

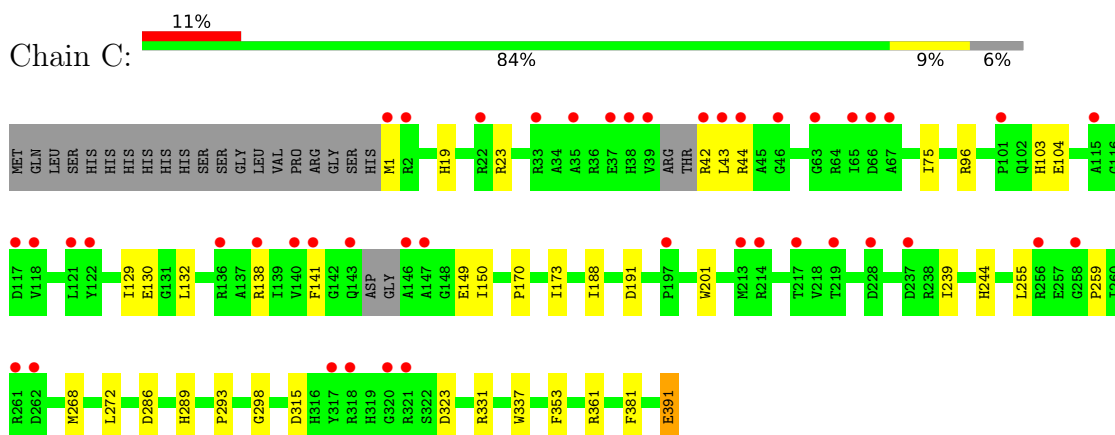
- Molecule 1: 4-hydroxybenzoate 3-monooxygenase (NAD(P)H)



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- Molecule 1: 4-hydroxybenzoate 3-monooxygenase (NAD(P)H)

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.26Å 67.39Å 128.23Å 90.00° 90.67° 90.00°	Depositor
Resolution (Å)	46.45 – 1.60 46.45 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (46.45-1.60) 95.3 (46.45-1.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 1.60Å)	Xtrriage
Refinement program	REFMAC 5.0.32, PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.223 , 0.246 0.231 , 0.253	Depositor DCC
R_{free} test set	9831 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtrriage
Anisotropy	0.037	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.197 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12403	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IMD, CA, FAD

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	0.36	0/3095	0.64	0/4182
1	B	0.34	0/3095	0.63	0/4182
1	C	0.30	0/3063	0.58	0/4136
1	D	0.29	0/2463	0.55	0/3319
All	All	0.33	0/11716	0.60	0/15819

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3029	0	2958	15	0
1	B	3029	0	2958	13	0
1	C	2999	0	2929	22	0
1	D	2410	0	2329	26	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	2	0
2	D	53	0	31	1	0
3	A	10	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	10	1	0
3	C	10	0	10	1	0
3	D	5	0	5	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	229	0	0	0	0
5	B	224	0	0	0	0
5	C	152	0	0	0	0
5	D	80	0	0	0	0
All	All	12403	0	11333	76	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 3.

All (76) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ARG:NH1	1:C:43:LEU:O	2.19	0.74
1:A:192:ALA:HB1	1:A:256:ARG:HG3	1.75	0.68
1:D:71:GLU:OE2	1:D:96:ARG:NH1	2.27	0.68
1:B:19:HIS:CE1	1:B:23:ARG:HD2	2.31	0.65
1:D:295:GLY:H	3:D:402:IMD:HN1	1.45	0.65
1:B:295:GLY:H	3:B:402:IMD:HN1	1.46	0.62
1:C:331:ARG:HB3	1:C:391:GLU:HG3	1.80	0.62
1:A:295:GLY:H	3:A:402:IMD:HN3	1.49	0.60
1:B:2:ARG:HH21	1:B:136:ARG:HE	1.50	0.58
1:C:103:HIS:CD2	1:C:104:GLU:HG3	2.40	0.57
1:B:130:GLU:HG3	1:B:138:ARG:HB2	1.87	0.56
1:A:144:ASP:OD1	1:A:145:GLY:N	2.39	0.56
1:A:19:HIS:CE1	1:A:23:ARG:HD2	2.42	0.55
1:C:19:HIS:NE2	1:C:23:ARG:HD2	2.21	0.55
1:C:170:PRO:HG2	1:C:173:ILE:HG13	1.89	0.54
1:A:268:MET:SD	1:A:293:PRO:HD2	2.49	0.53
1:D:75:ILE:HD12	1:D:381:PHE:HZ	1.74	0.53
1:C:42:ARG:HH21	1:C:44:ARG:HH21	1.57	0.52
1:D:193:PRO:HD2	1:D:256:ARG:HG2	1.92	0.51
1:B:128:ARG:HH21	1:B:140:VAL:HG21	1.76	0.51
1:A:130:GLU:HG3	1:A:138:ARG:HB2	1.93	0.51
1:D:353:PHE:O	1:D:361:ARG:NH2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HG3	1:A:149:GLU:O	2.11	0.51
1:C:268:MET:SD	1:C:293:PRO:HD2	2.53	0.49
1:D:92:SER:HB2	1:D:382:ALA:HB1	1.95	0.48
1:C:19:HIS:CE1	1:C:23:ARG:HD2	2.48	0.48
1:B:192:ALA:HB1	1:B:256:ARG:HG2	1.96	0.48
1:C:1:MET:HG3	1:C:149:GLU:O	2.13	0.48
1:C:353:PHE:O	1:C:361:ARG:NH2	2.46	0.48
1:D:268:MET:SD	1:D:293:PRO:HD2	2.54	0.48
1:C:298:GLY:HA3	2:C:401:FAD:H1'2	1.96	0.48
1:A:353:PHE:O	1:A:361:ARG:NH2	2.47	0.48
1:A:2:ARG:HH21	1:A:136:ARG:NE	2.11	0.47
1:D:180:ILE:HG12	1:D:269:ARG:HG3	1.97	0.47
1:C:201:TRP:HZ2	3:C:402:IMD:H2	1.79	0.46
1:B:2:ARG:HH21	1:B:136:ARG:NE	2.12	0.46
1:B:268:MET:SD	1:B:293:PRO:HD2	2.56	0.46
1:D:3:THR:OG1	1:D:4:GLN:N	2.49	0.46
1:D:298:GLY:HA3	2:D:401:FAD:H1'2	1.97	0.46
1:A:169:MET:HG3	1:A:170:PRO:HD2	1.97	0.45
1:D:289:HIS:O	1:D:289:HIS:ND1	2.48	0.45
1:B:244:HIS:CE1	1:B:255:LEU:HB2	2.53	0.44
1:A:129:ILE:HG22	1:A:132:LEU:HD21	1.98	0.44
1:D:177:TYR:O	1:D:271:PHE:HA	2.18	0.44
1:A:192:ALA:HB1	1:A:256:ARG:CG	2.45	0.44
1:A:16:MET:HE2	1:A:55:MET:HG2	2.01	0.43
1:A:242:GLU:OE2	1:A:245:ARG:NH2	2.51	0.43
1:C:75:ILE:HD12	1:C:381:PHE:HZ	1.83	0.43
1:C:141:PHE:HE1	1:C:150:ILE:HG13	1.83	0.43
1:D:190:ALA:HB3	1:D:219:THR:HG23	2.01	0.43
1:C:129:ILE:HG22	1:C:132:LEU:HD21	2.01	0.43
1:D:75:ILE:HD12	1:D:381:PHE:CZ	2.53	0.43
1:C:391:GLU:H	1:C:391:GLU:HG2	1.62	0.42
1:D:314:VAL:O	1:D:318:ARG:HB3	2.18	0.42
1:C:191:ASP:HB2	1:C:259:PRO:HD2	2.00	0.42
1:D:282:PHE:CZ	1:D:325:LEU:HD22	2.55	0.42
1:C:244:HIS:CE1	1:C:255:LEU:HB2	2.55	0.42
1:D:271:PHE:HB3	1:D:290:ILE:HG12	2.02	0.42
1:B:240:TRP:CD2	1:B:257:GLU:HG2	2.56	0.41
1:C:188:ILE:HD13	1:C:239:ILE:HG21	2.02	0.41
1:D:132:LEU:HD22	1:D:281:LEU:HB2	2.03	0.41
1:D:137:ALA:O	1:D:152:CYS:N	2.53	0.41
1:D:321:ARG:HG2	1:D:323:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:401:FAD:H9	2:C:401:FAD:H1'1	1.89	0.41
1:D:75:ILE:HD11	1:D:385:PHE:CZ	2.55	0.41
1:C:286:ASP:HA	1:C:289:HIS:O	2.21	0.41
1:B:323:ASP:OD1	1:B:323:ASP:N	2.54	0.41
1:D:166:ARG:HD3	1:D:287:ALA:O	2.21	0.41
1:D:213:MET:SD	1:D:213:MET:N	2.94	0.41
1:D:231:PRO:HB2	1:D:263:LYS:HE3	2.02	0.41
1:B:169:MET:HG3	1:B:170:PRO:HD2	2.02	0.41
1:A:362:ARG:HG2	1:D:337:TRP:CZ2	2.56	0.40
1:C:130:GLU:HG3	1:C:138:ARG:HB2	2.04	0.40
1:B:353:PHE:O	1:B:361:ARG:NH2	2.54	0.40
1:C:272:LEU:HD22	1:C:337:TRP:CZ2	2.56	0.40
1:D:255:LEU:HD12	1:D:255:LEU:HA	1.97	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	389/411 (95%)	380 (98%)	9 (2%)	0	100	100
1	B	389/411 (95%)	381 (98%)	8 (2%)	0	100	100
1	C	381/411 (93%)	374 (98%)	7 (2%)	0	100	100
1	D	297/411 (72%)	290 (98%)	7 (2%)	0	100	100
All	All	1456/1644 (89%)	1425 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	307/325 (94%)	303 (99%)	4 (1%)	69	50
1	B	307/325 (94%)	305 (99%)	2 (1%)	84	73
1	C	304/325 (94%)	300 (99%)	4 (1%)	69	50
1	D	246/325 (76%)	240 (98%)	6 (2%)	49	24
All	All	1164/1300 (90%)	1148 (99%)	16 (1%)	67	47

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	MET
1	A	262	ASP
1	A	315	ASP
1	A	365	ARG
1	B	41	THR
1	B	315	ASP
1	C	96	ARG
1	C	315	ASP
1	C	323	ASP
1	C	391	GLU
1	D	73	HIS
1	D	96	ARG
1	D	136	ARG
1	D	179	ARG
1	D	212	SER
1	D	213	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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
3	IMD	C	403	-	3,5,5	0.42	0	4,5,5	0.60	0
3	IMD	D	402	-	3,5,5	0.40	0	4,5,5	0.58	0
2	FAD	D	401	-	53,58,58	0.43	0	68,89,89	0.53	2 (2%)
2	FAD	A	401	-	53,58,58	0.57	0	68,89,89	0.60	1 (1%)
3	IMD	B	403	-	3,5,5	0.40	0	4,5,5	0.57	0
3	IMD	A	403	-	3,5,5	0.39	0	4,5,5	0.62	0
2	FAD	C	401	-	53,58,58	0.49	0	68,89,89	0.54	1 (1%)
3	IMD	A	402	-	3,5,5	0.39	0	4,5,5	0.64	0
3	IMD	C	402	-	3,5,5	0.37	0	4,5,5	0.53	0
3	IMD	B	402	-	3,5,5	0.41	0	4,5,5	0.57	0
2	FAD	B	401	-	53,58,58	0.53	0	68,89,89	0.57	1 (1%)

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	IMD	C	403	-	-	-	0/1/1/1
3	IMD	D	402	-	-	-	0/1/1/1
2	FAD	D	401	-	-	9/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	401	-	-	3/30/50/50	0/6/6/6
3	IMD	B	403	-	-	-	0/1/1/1
3	IMD	A	403	-	-	-	0/1/1/1
2	FAD	C	401	-	-	1/30/50/50	0/6/6/6
3	IMD	A	402	-	-	-	0/1/1/1
3	IMD	C	402	-	-	-	0/1/1/1
3	IMD	B	402	-	-	-	0/1/1/1
2	FAD	B	401	-	-	4/30/50/50	0/6/6/6

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	FAD	C5A-C6A-N6A	2.36	123.94	120.35
2	C	401	FAD	C5A-C6A-N6A	2.35	123.92	120.35
2	A	401	FAD	C5A-C6A-N6A	2.34	123.92	120.35
2	D	401	FAD	P-O3P-PA	-2.32	124.86	132.83
2	D	401	FAD	C5A-C6A-N6A	2.31	123.86	120.35

There are no chirality outliers.

All (17) torsion outliers are listed below:

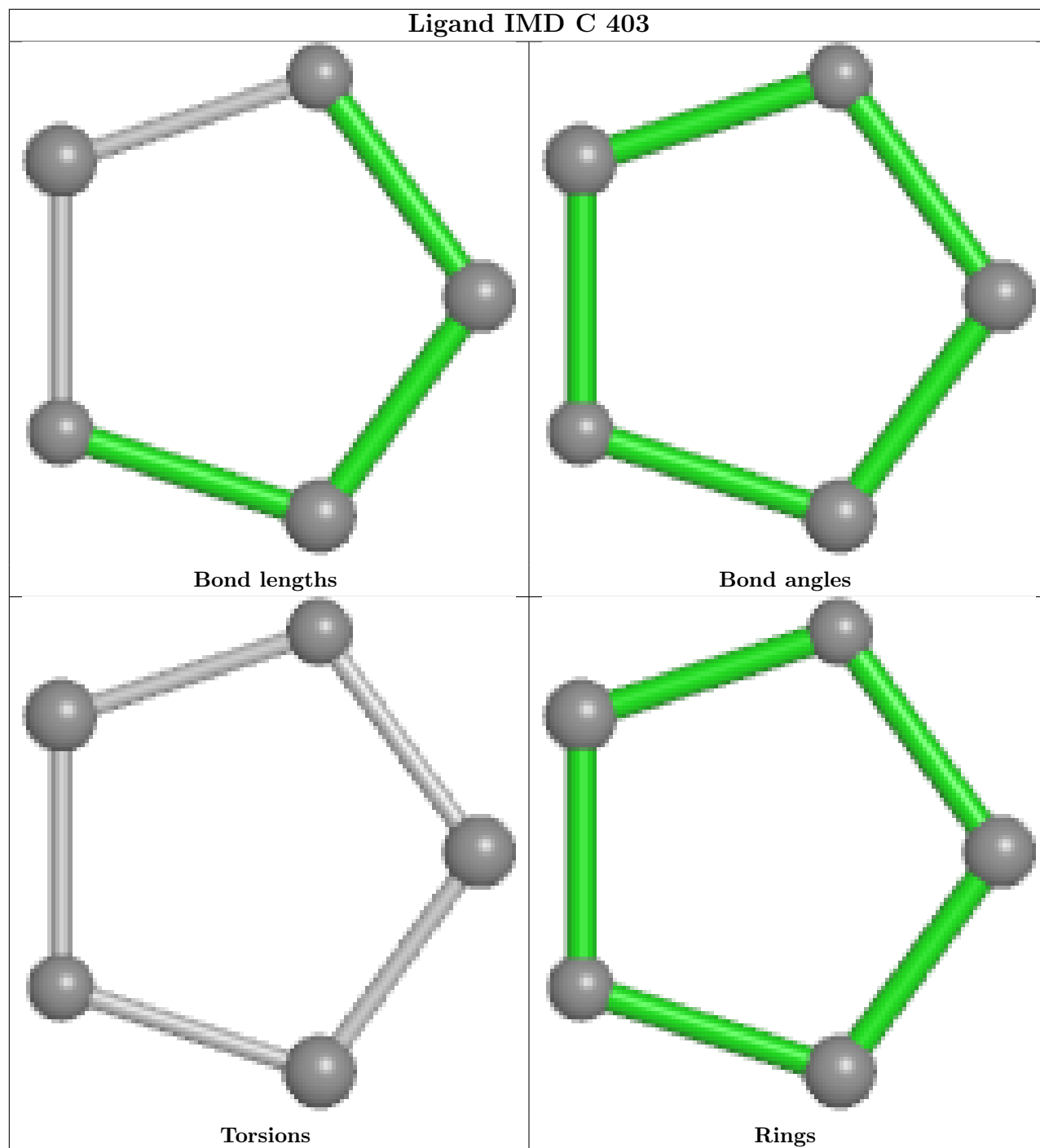
Mol	Chain	Res	Type	Atoms
2	D	401	FAD	O4B-C4B-C5B-O5B
2	D	401	FAD	C2'-C3'-C4'-C5'
2	D	401	FAD	O3'-C3'-C4'-C5'
2	D	401	FAD	O3'-C3'-C4'-O4'
2	D	401	FAD	C2'-C3'-C4'-O4'
2	D	401	FAD	C3B-C4B-C5B-O5B
2	D	401	FAD	C5B-O5B-PA-O2A
2	B	401	FAD	O4B-C4B-C5B-O5B
2	B	401	FAD	C2'-C3'-C4'-C5'
2	B	401	FAD	O3'-C3'-C4'-C5'
2	D	401	FAD	C5B-O5B-PA-O3P
2	A	401	FAD	O3'-C3'-C4'-C5'
2	A	401	FAD	O4B-C4B-C5B-O5B
2	C	401	FAD	O4B-C4B-C5B-O5B
2	A	401	FAD	C2'-C3'-C4'-C5'
2	B	401	FAD	C2'-C3'-C4'-O4'
2	D	401	FAD	C5B-O5B-PA-O1A

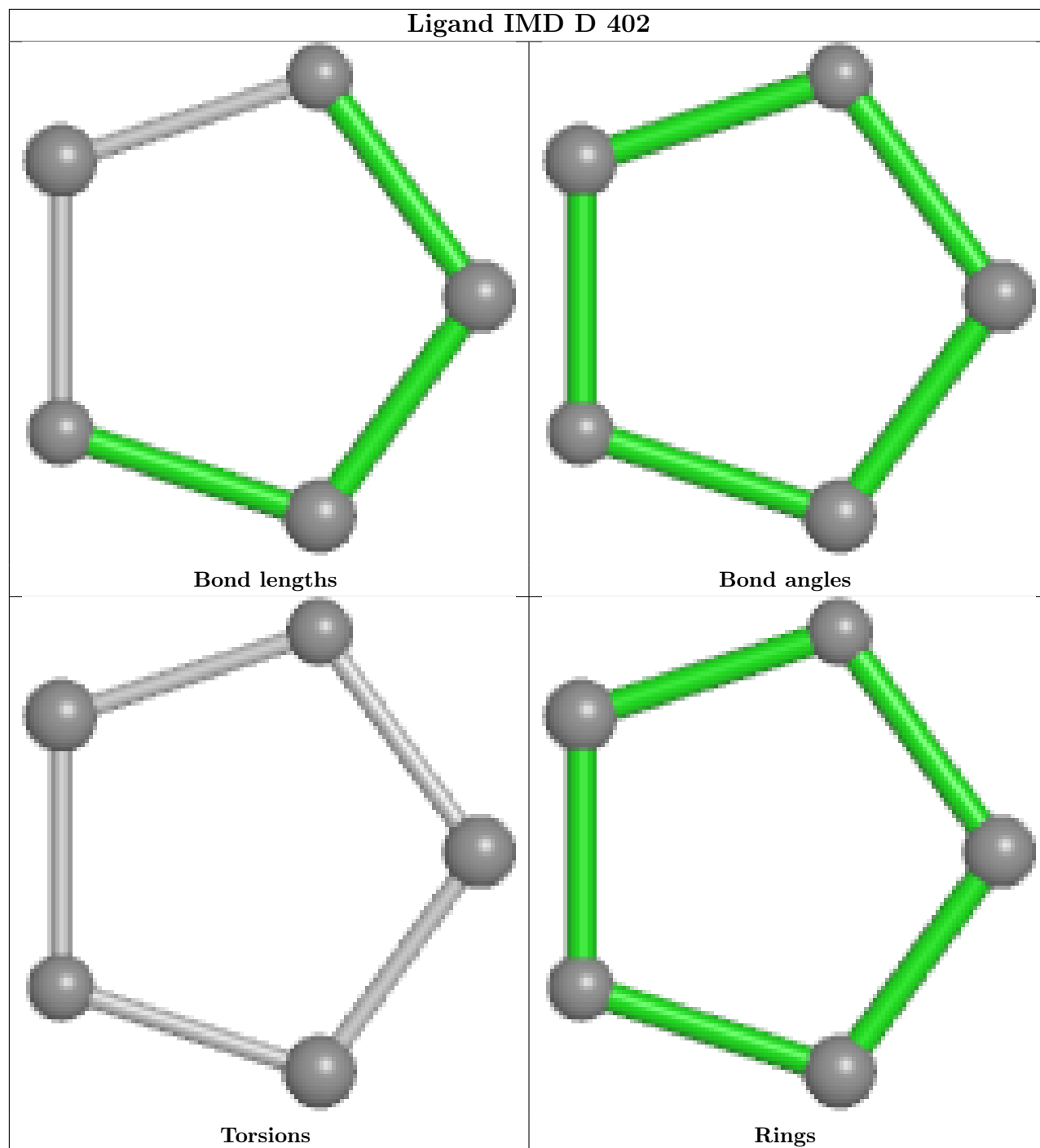
There are no ring outliers.

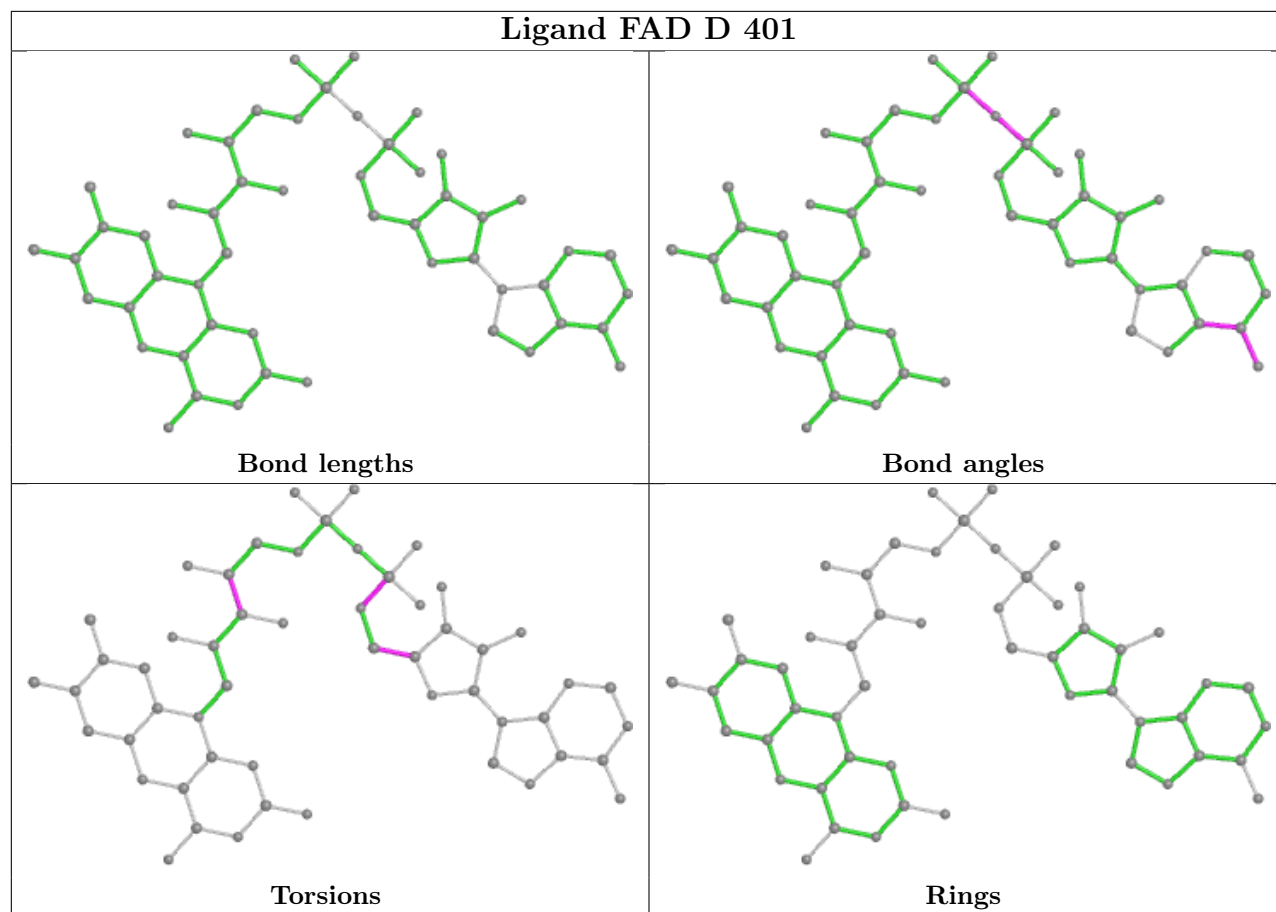
6 monomers are involved in 7 short contacts:

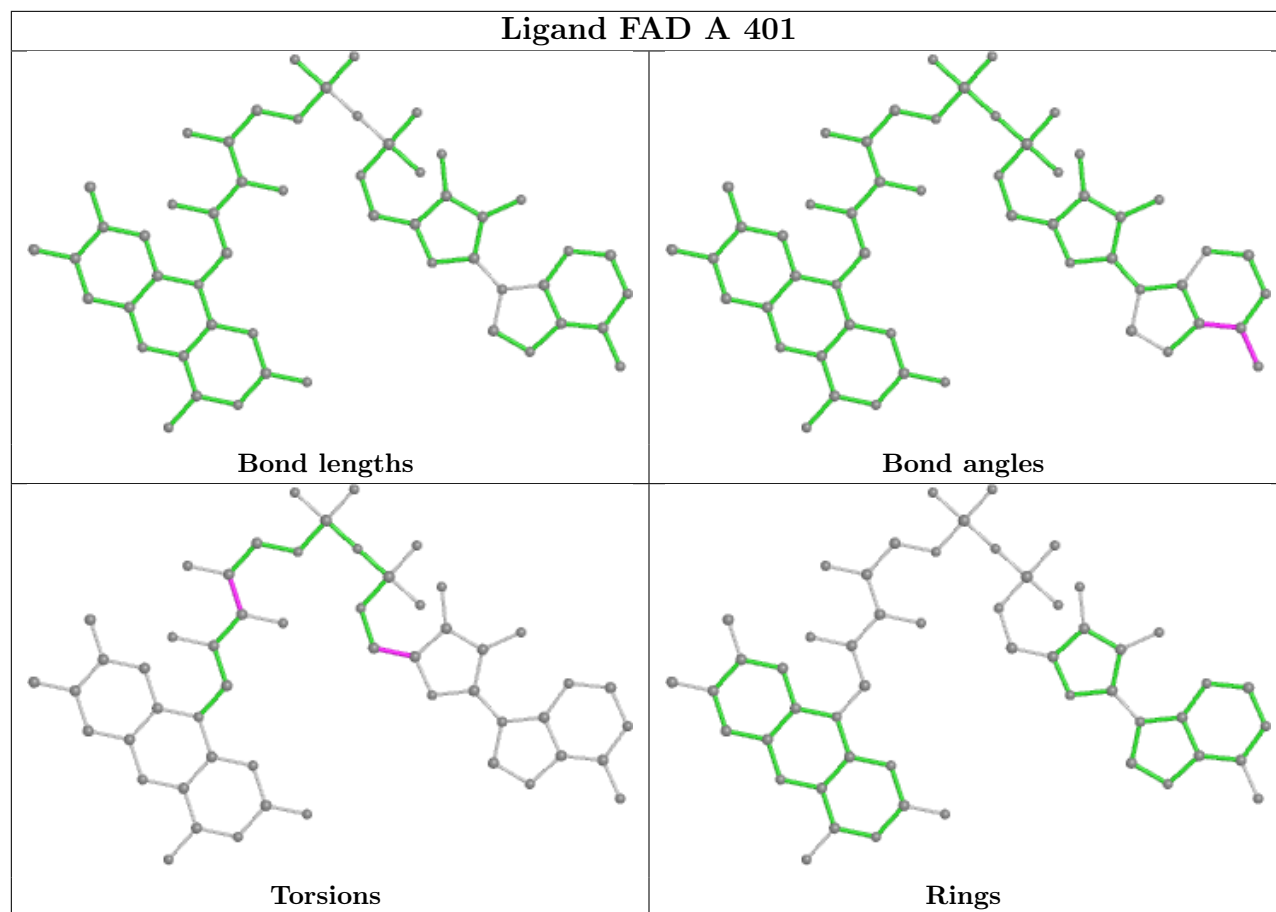
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	IMD	1	0
2	D	401	FAD	1	0
2	C	401	FAD	2	0
3	A	402	IMD	1	0
3	C	402	IMD	1	0
3	B	402	IMD	1	0

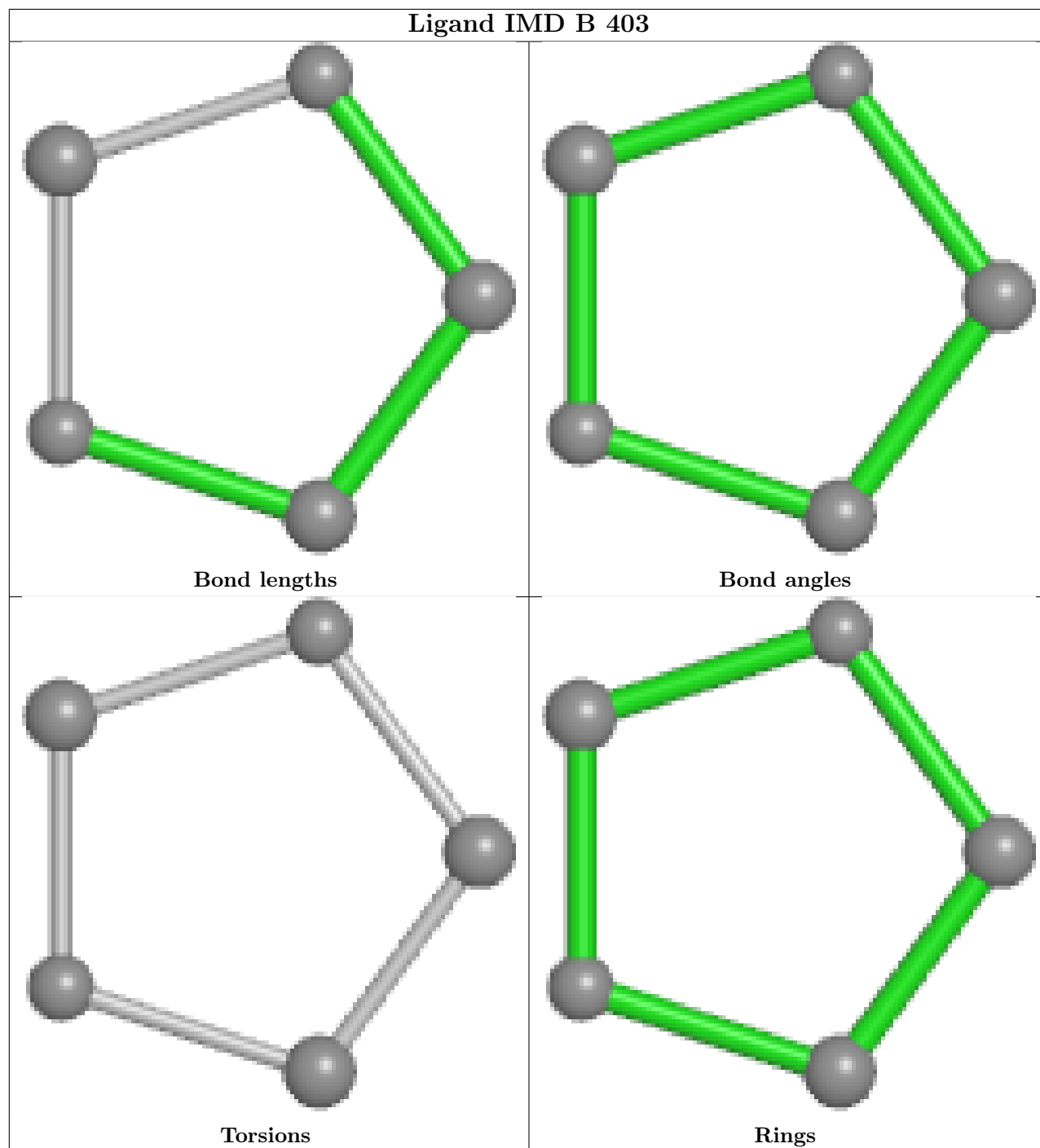
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

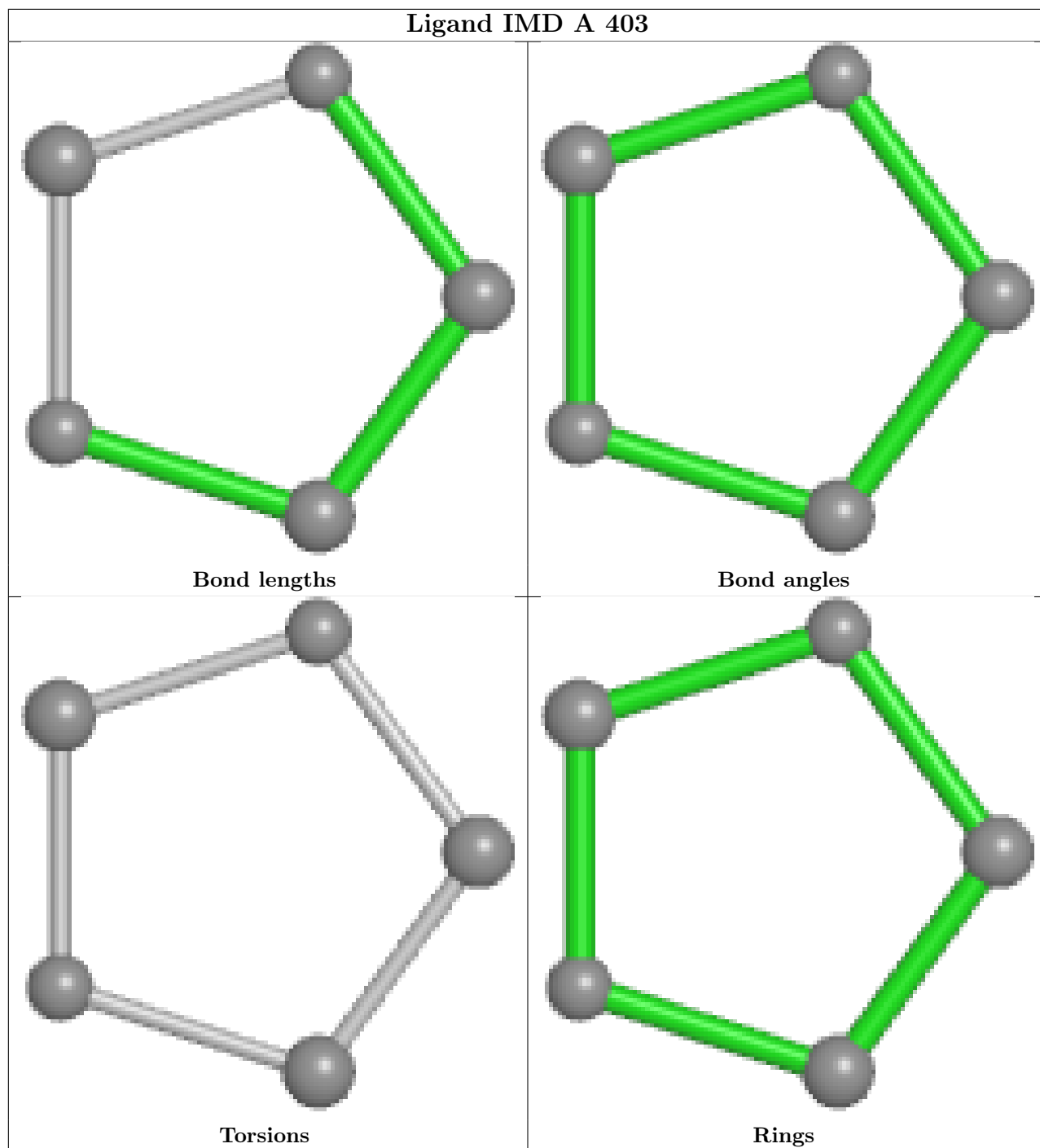


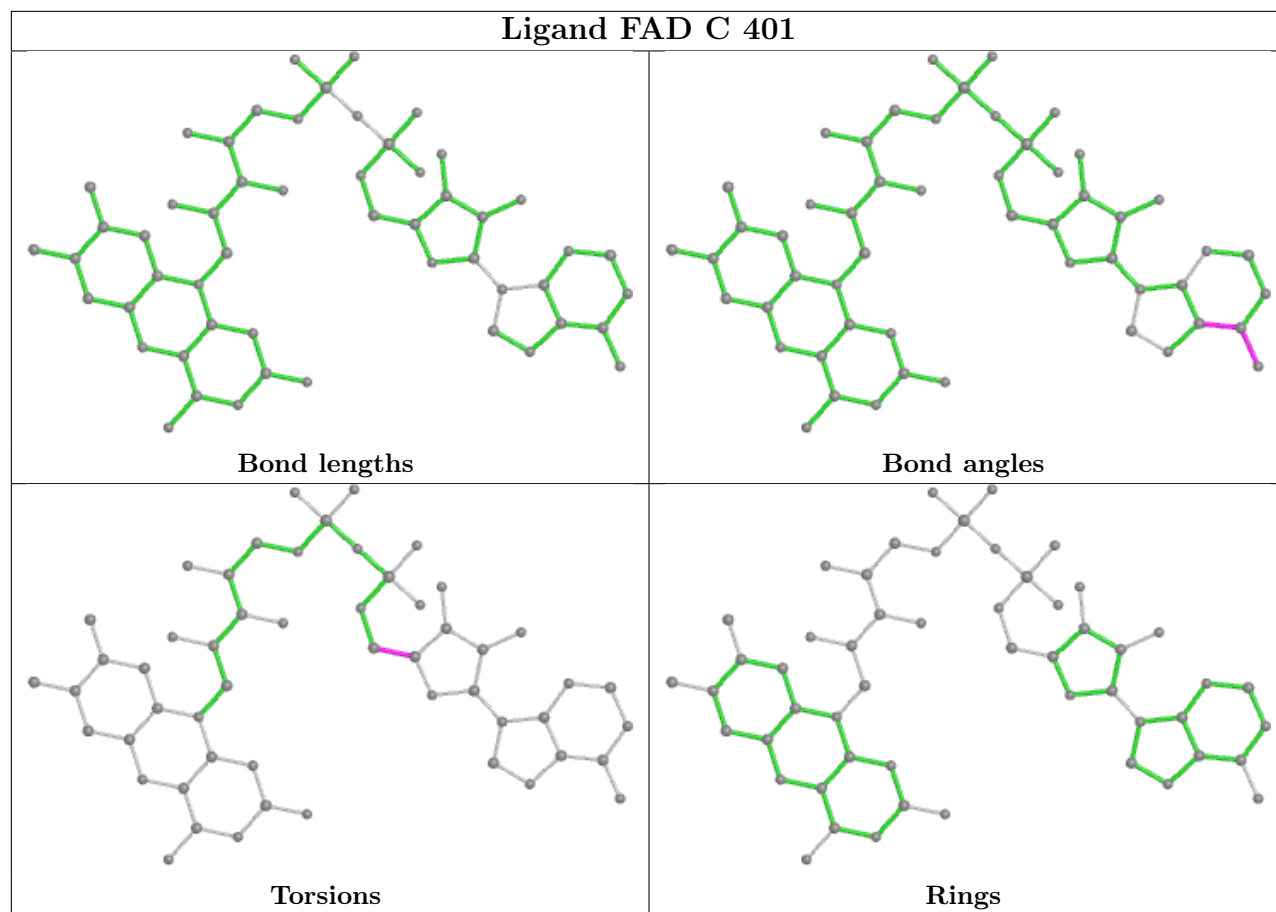


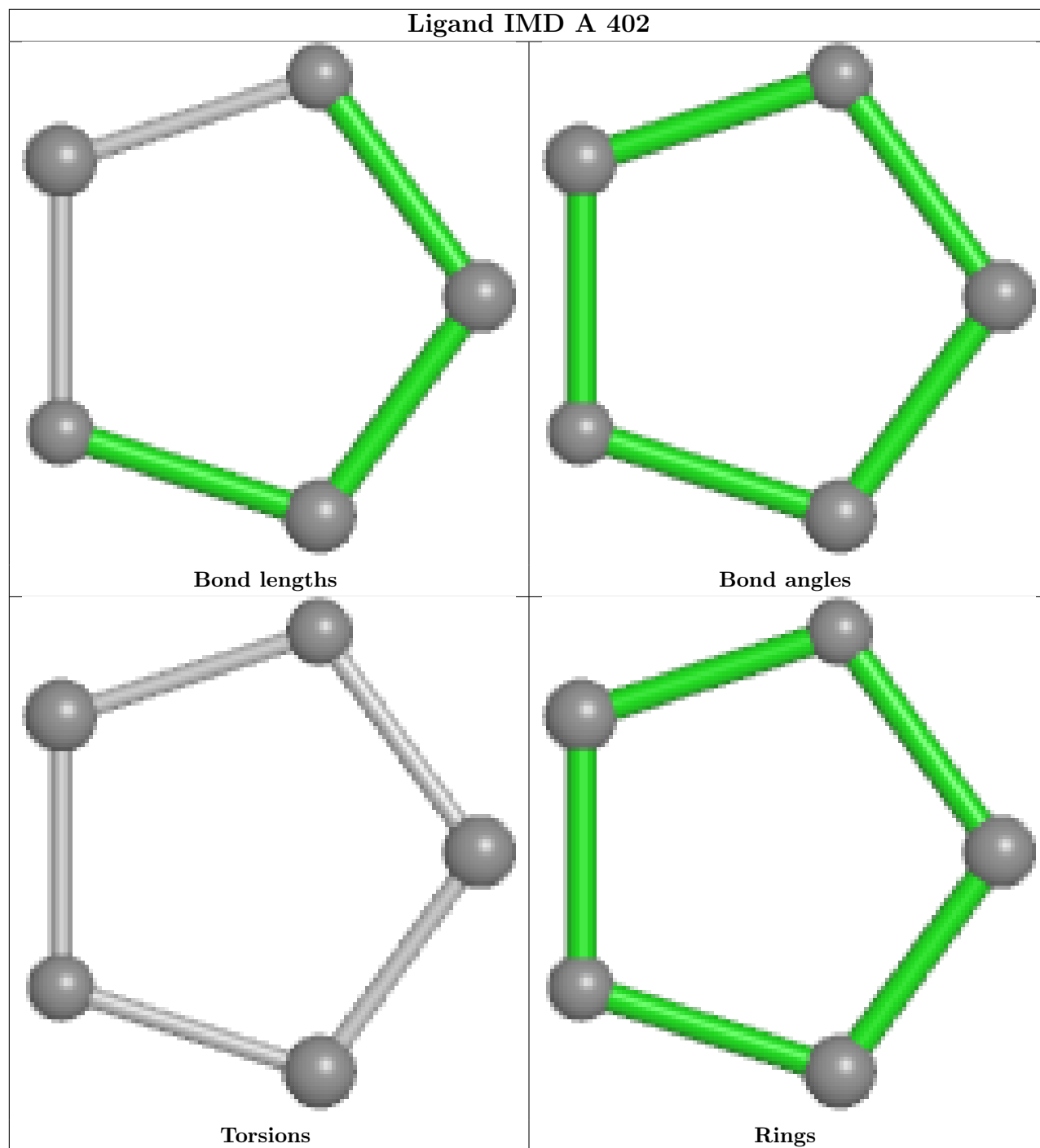


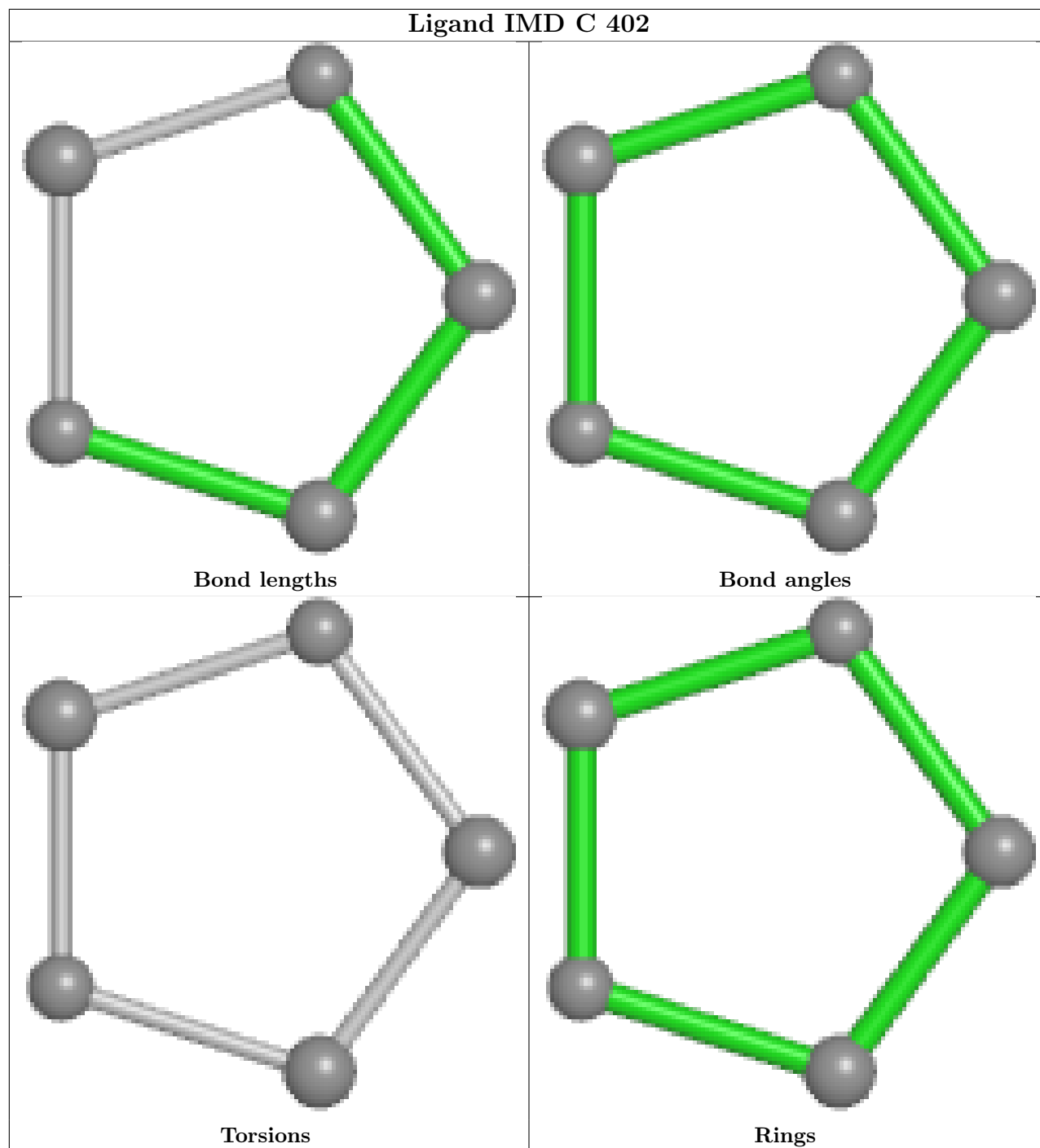


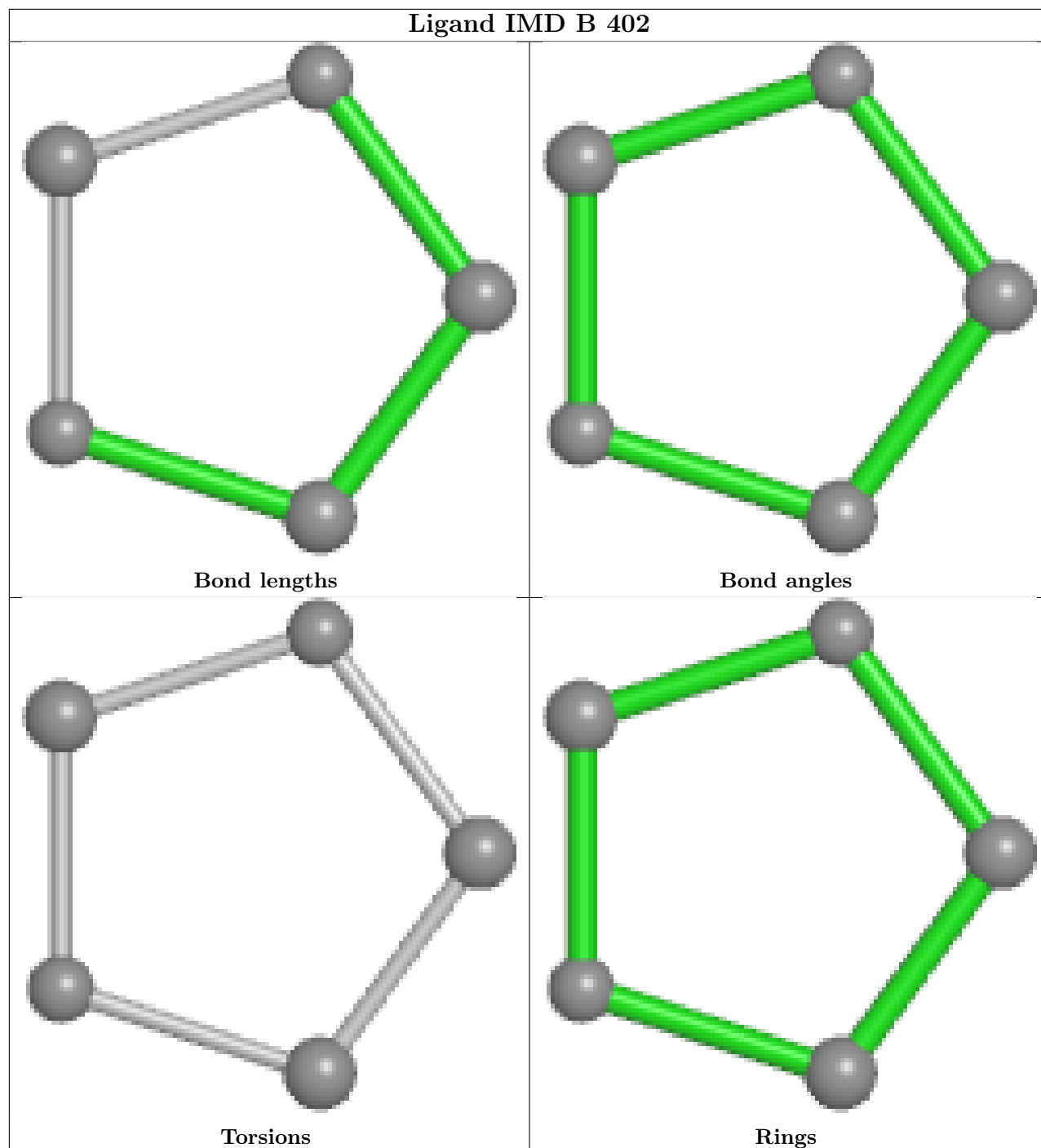


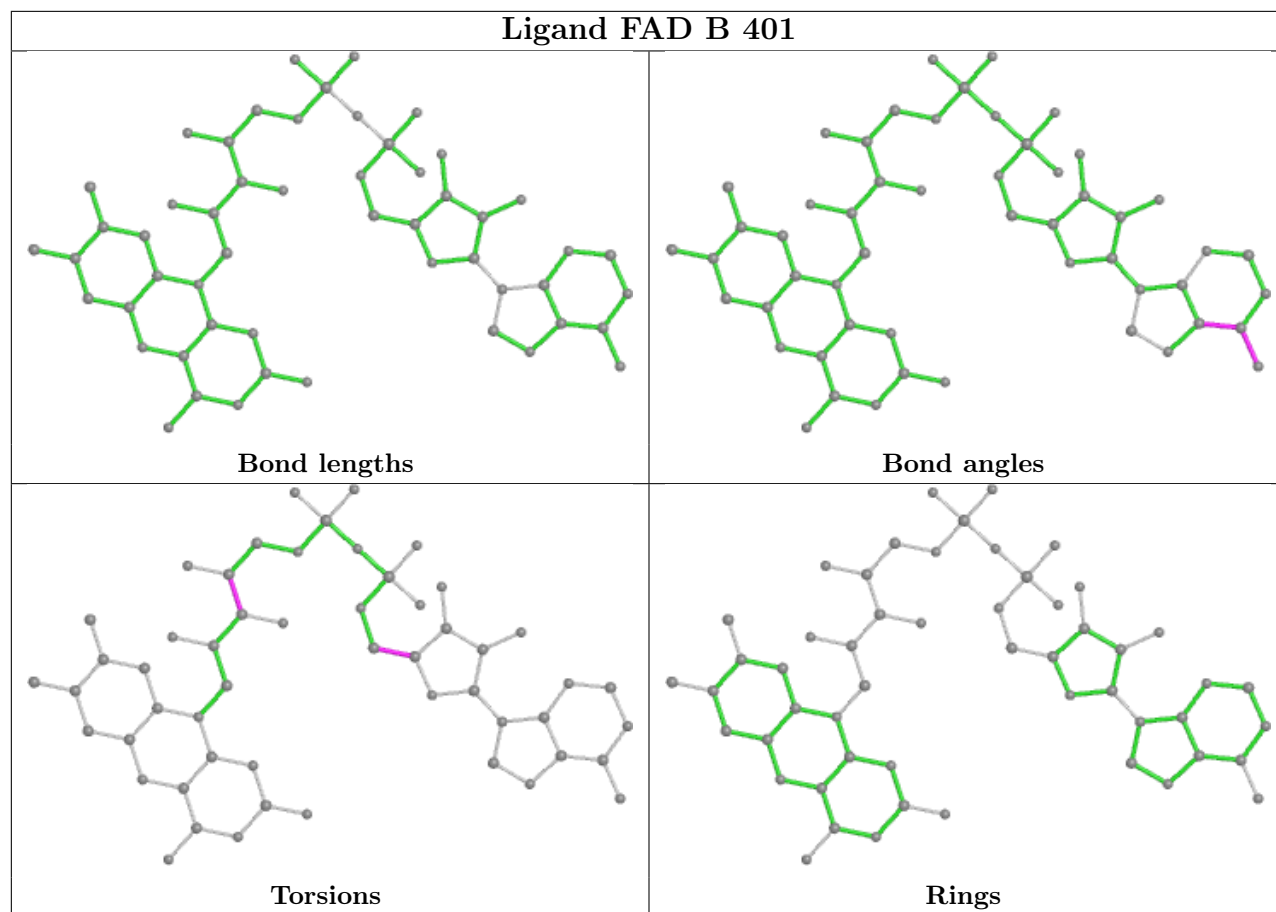












5.7 Other polymers [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	391/411 (95%)	0.01	18 (4%) 32 29	9, 18, 35, 50	0
1	B	391/411 (95%)	-0.00	15 (3%) 40 37	11, 20, 36, 59	0
1	C	387/411 (94%)	0.70	44 (11%) 5 4	12, 29, 52, 79	0
1	D	309/411 (75%)	1.92	126 (40%) 0 0	13, 36, 68, 86	0
All	All	1478/1644 (89%)	0.59	203 (13%) 3 2	9, 23, 58, 86	0

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	17	LEU	11.6
1	D	314	VAL	10.0
1	D	8	VAL	8.6
1	D	139	ILE	8.1
1	D	140	VAL	6.8
1	C	39	VAL	6.7
1	D	173	ILE	6.7
1	C	42	ARG	6.6
1	D	57	ARG	6.5
1	D	18	ALA	6.5
1	D	162	ARG	6.3
1	D	155	VAL	6.3
1	D	152	CYS	6.3
1	D	310	ALA	6.3
1	D	306	ILE	6.3
1	D	7	ILE	6.1
1	A	195	ALA	6.1
1	C	122	TYR	5.9
1	D	279	GLY	5.9
1	D	130	GLU	5.9
1	D	53	VAL	5.9

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Mol	Chain	Res	Type	RSRZ
1	D	6	GLY	5.9
1	C	146	ALA	5.8
1	D	15	LEU	5.8
1	D	281	LEU	5.7
1	D	12	PRO	5.6
1	D	318	ARG	5.6
1	B	41	THR	5.5
1	A	145	GLY	5.5
1	D	157	GLY	5.5
1	D	138	ARG	5.5
1	B	204	SER	5.4
1	D	164	VAL	5.4
1	D	154	PHE	5.4
1	D	317	TYR	5.3
1	C	321	ARG	5.3
1	C	43	LEU	5.2
1	D	137	ALA	5.1
1	D	391	GLU	5.1
1	C	147	ALA	5.1
1	D	56	LEU	5.0
1	D	132	LEU	5.0
1	D	320	GLY	4.9
1	D	321	ARG	4.9
1	D	3	THR	4.9
1	D	14	GLY	4.9
1	D	313	LEU	4.8
1	D	172	GLY	4.8
1	B	195	ALA	4.7
1	D	19	HIS	4.7
1	D	319	HIS	4.6
1	D	13	ALA	4.6
1	D	98	TRP	4.6
1	D	58	GLU	4.5
1	B	196	SER	4.5
1	D	315	ASP	4.5
1	D	159	ASP	4.4
1	D	5	VAL	4.4
1	B	144	ASP	4.4
1	D	46	GLY	4.4
1	D	290	ILE	4.4
1	C	44	ARG	4.3
1	A	196	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	135	ASP	4.3
1	D	156	ALA	4.2
1	D	99	VAL	4.0
1	D	168	SER	4.0
1	D	288	ALA	4.0
1	D	158	CYS	3.9
1	D	180	ILE	3.9
1	C	1	MET	3.9
1	D	55	MET	3.9
1	D	11	GLY	3.8
1	D	325	LEU	3.7
1	C	214	ARG	3.7
1	D	4	GLN	3.7
1	A	42	ARG	3.7
1	D	136	ARG	3.7
1	D	189	LEU	3.7
1	D	9	GLY	3.6
1	D	16	MET	3.6
1	C	115	ALA	3.6
1	D	322	SER	3.6
1	D	262	ASP	3.5
1	C	2	ARG	3.5
1	D	51	GLY	3.5
1	C	143	GLN	3.4
1	D	133	GLU	3.4
1	D	131	GLY	3.4
1	D	311	ALA	3.4
1	D	134	ASP	3.4
1	D	312	ALA	3.3
1	D	176	GLY	3.3
1	A	147	ALA	3.3
1	D	256	ARG	3.2
1	D	309	LEU	3.2
1	C	37	GLU	3.2
1	C	46	GLY	3.2
1	A	43	LEU	3.2
1	C	256	ARG	3.2
1	B	40	ARG	3.1
1	C	258	GLY	3.1
1	D	328	TYR	3.1
1	D	272	LEU	3.1
1	D	271	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	171	ALA	3.1
1	D	213	MET	3.0
1	B	146	ALA	3.0
1	D	216	PRO	3.0
1	D	287	ALA	3.0
1	C	262	ASP	3.0
1	D	167	GLY	3.0
1	D	197	PRO	2.9
1	D	285	GLY	2.9
1	D	326	ALA	2.9
1	C	228	ASP	2.9
1	D	161	PHE	2.8
1	D	93	GLY	2.8
1	D	291	VAL	2.8
1	D	52	THR	2.8
1	C	38	HIS	2.8
1	D	165	SER	2.8
1	D	301	SER	2.8
1	C	22	ARG	2.8
1	C	136	ARG	2.8
1	D	48	LEU	2.8
1	D	10	ALA	2.8
1	D	214	ARG	2.7
1	D	390	ILE	2.7
1	D	94	GLY	2.7
1	D	286	ASP	2.7
1	C	33	ARG	2.7
1	D	175	ARG	2.7
1	D	304	ALA	2.7
1	D	90	GLU	2.7
1	D	170	PRO	2.7
1	C	63	GLY	2.7
1	C	118	VAL	2.7
1	D	169	MET	2.7
1	A	228	ASP	2.7
1	C	66	ASP	2.7
1	C	217	THR	2.6
1	C	219	THR	2.6
1	A	40	ARG	2.6
1	D	292	PRO	2.6
1	C	261	ARG	2.6
1	C	117	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	276	MET	2.6
1	D	389	PRO	2.6
1	D	174	ALA	2.5
1	B	324	ARG	2.5
1	D	305	ASP	2.5
1	B	2	ARG	2.5
1	D	332	CYS	2.5
1	B	205	ASP	2.5
1	D	71	GLU	2.5
1	D	308	VAL	2.5
1	B	171	ALA	2.5
1	D	273	SER	2.5
1	D	97	ALA	2.4
1	C	197	PRO	2.4
1	D	47	VAL	2.4
1	C	67	ALA	2.4
1	A	206	ARG	2.4
1	C	317	TYR	2.4
1	A	41	THR	2.4
1	D	96	ARG	2.3
1	D	299	LEU	2.3
1	D	282	PHE	2.3
1	B	143	GLN	2.3
1	B	251	GLY	2.3
1	D	190	ALA	2.3
1	A	256	ARG	2.3
1	A	39	VAL	2.3
1	A	197	PRO	2.3
1	C	121	LEU	2.2
1	D	261	ARG	2.2
1	A	121	LEU	2.2
1	D	333	LEU	2.2
1	C	213	MET	2.2
1	A	144	ASP	2.2
1	D	50	GLN	2.2
1	C	101	PRO	2.2
1	D	166	ARG	2.2
1	D	217	THR	2.2
1	A	321	ARG	2.2
1	C	138	ARG	2.2
1	D	278	HIS	2.2
1	D	92	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	160	GLY	2.1
1	D	283	LEU	2.1
1	B	173	ILE	2.1
1	C	320	GLY	2.1
1	C	65	ILE	2.1
1	C	140	VAL	2.1
1	C	237	ASP	2.1
1	C	35	ALA	2.1
1	D	388	LEU	2.1
1	C	318	ARG	2.1
1	D	303	MET	2.1
1	B	38	HIS	2.1
1	A	1	MET	2.1
1	C	141	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

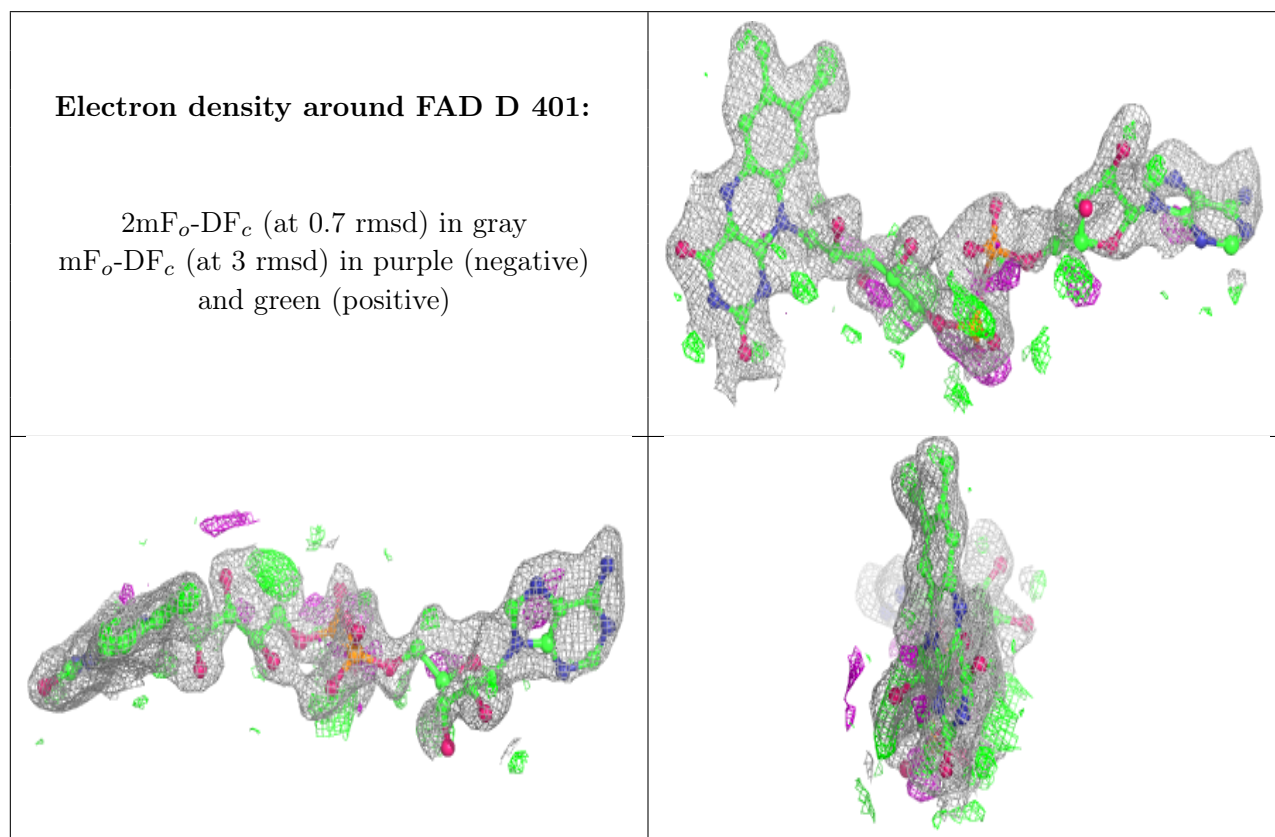
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	D	401	53/53	0.63	0.21	42,53,70,71	3
4	CA	C	404	1/1	0.86	0.13	35,35,35,35	1
3	IMD	B	402	5/5	0.87	0.14	24,25,27,29	0
3	IMD	A	402	5/5	0.89	0.15	22,22,24,26	0
3	IMD	C	403	5/5	0.90	0.20	30,31,34,34	1
3	IMD	D	402	5/5	0.91	0.10	36,38,40,41	0
4	CA	D	403	1/1	0.91	0.18	34,34,34,34	1
2	FAD	C	401	53/53	0.92	0.10	19,27,34,38	0
3	IMD	C	402	5/5	0.93	0.09	26,27,29,30	0

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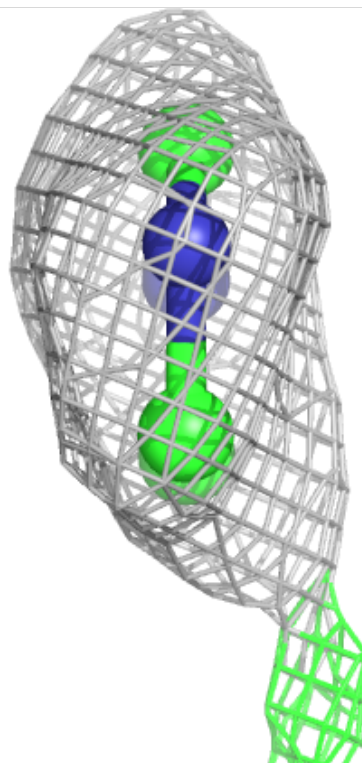
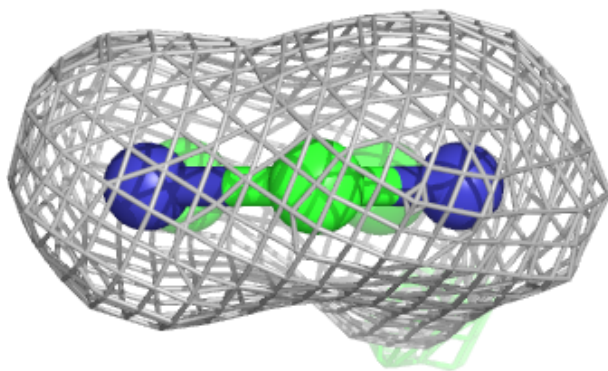
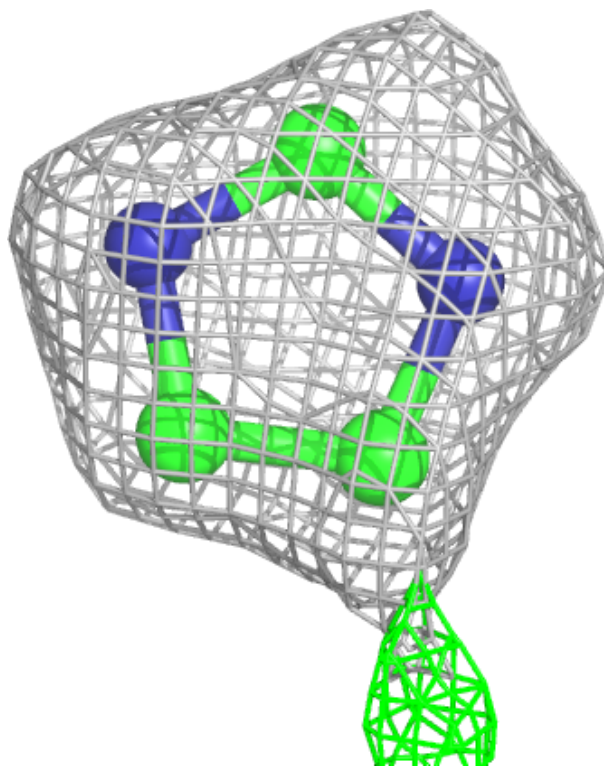
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	IMD	A	403	5/5	0.94	0.10	24,25,27,27	4
2	FAD	B	401	53/53	0.96	0.08	10,14,24,27	0
3	IMD	B	403	5/5	0.97	0.10	24,25,29,29	2
2	FAD	A	401	53/53	0.97	0.08	9,14,25,30	0
4	CA	B	404	1/1	0.98	0.24	22,22,22,22	1
4	CA	A	404	1/1	0.99	0.33	17,17,17,17	1

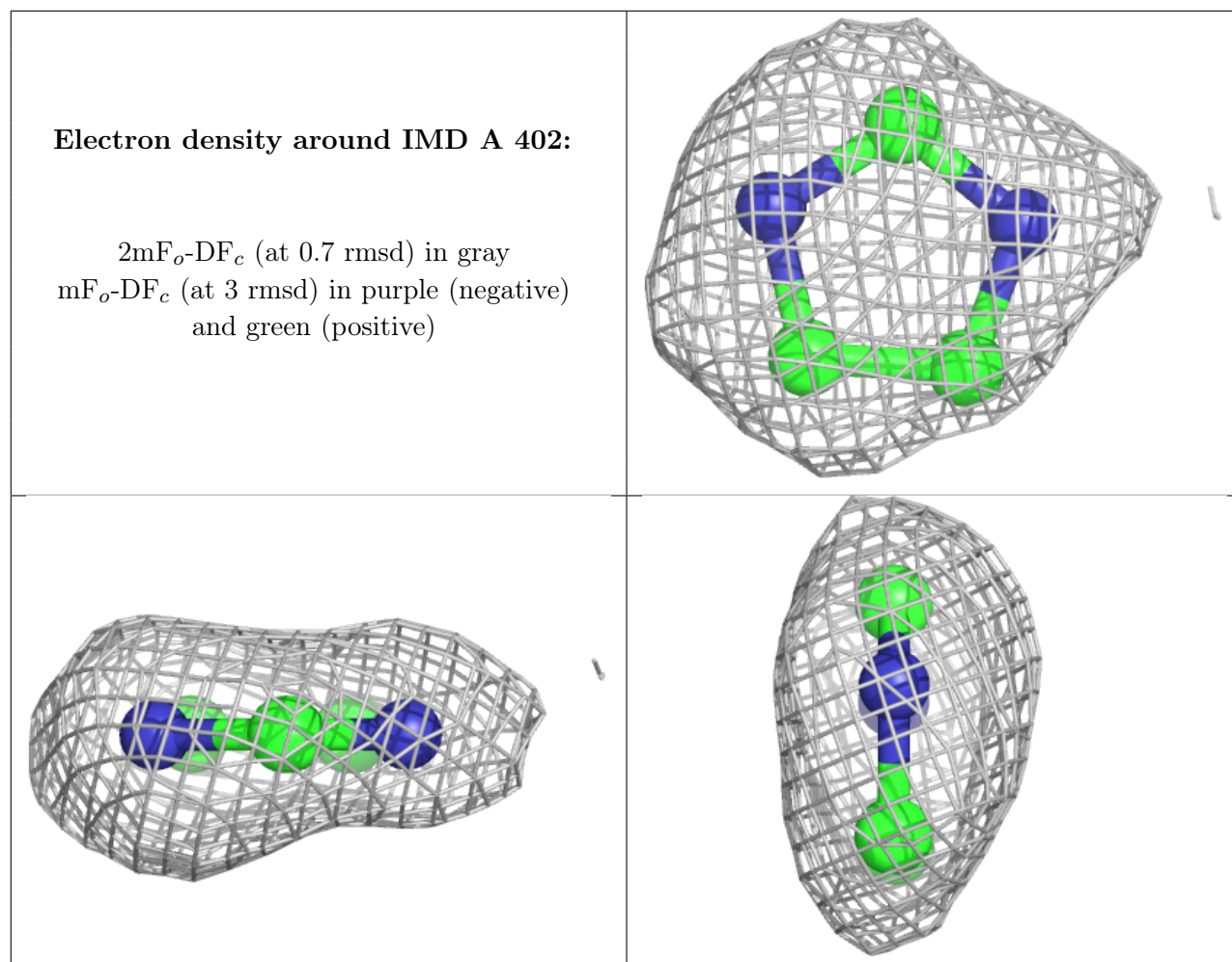
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



Electron density around IMD B 402:

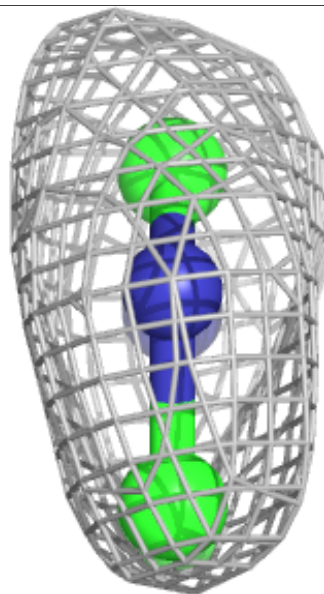
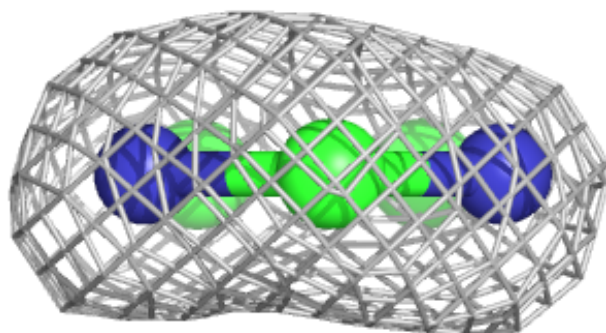
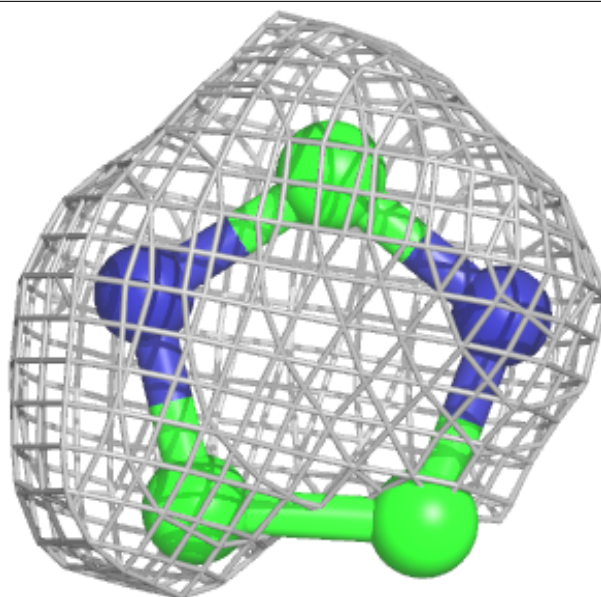
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





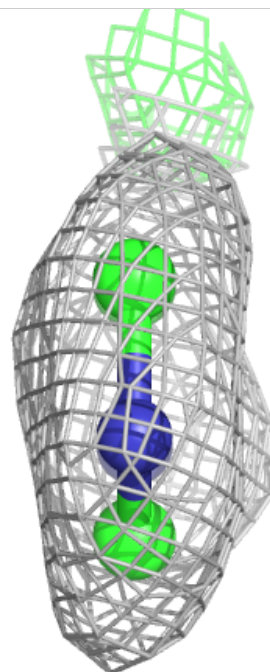
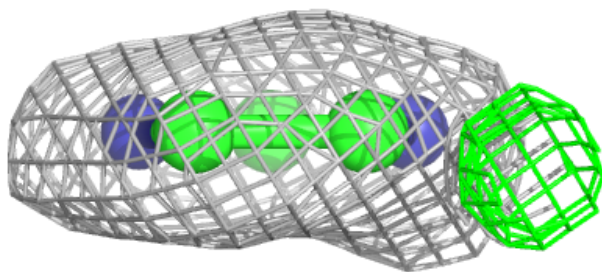
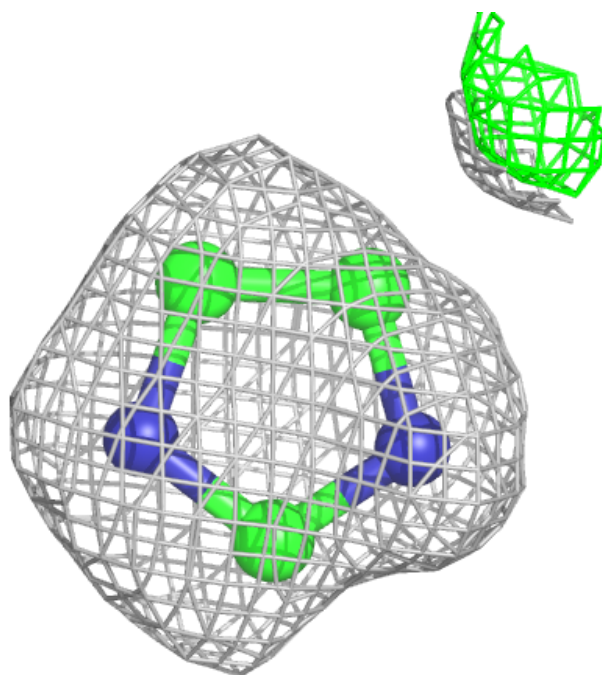
Electron density around IMD C 403:

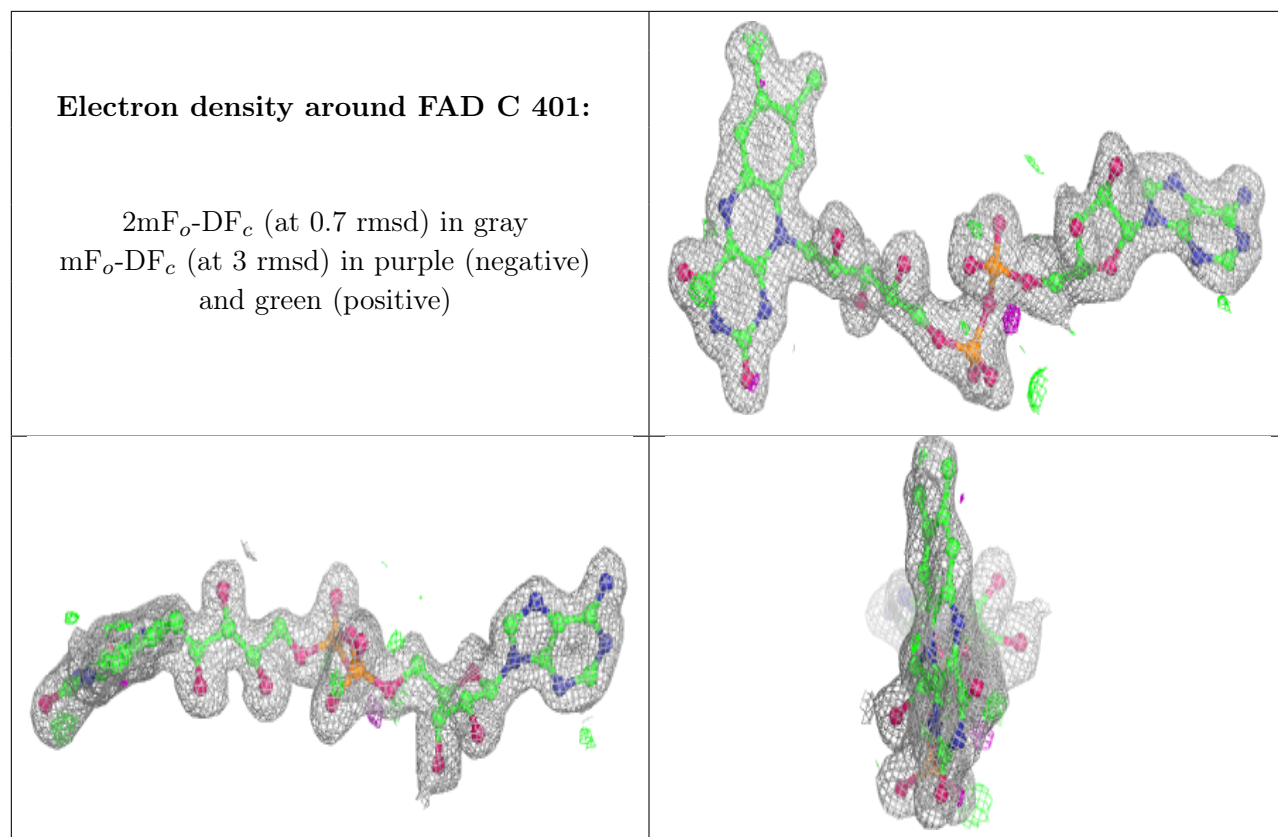
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around IMD D 402:

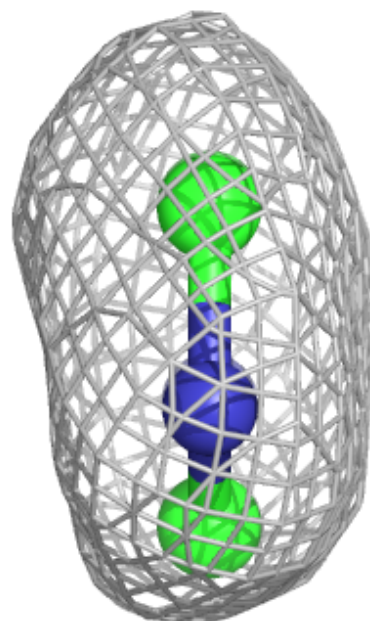
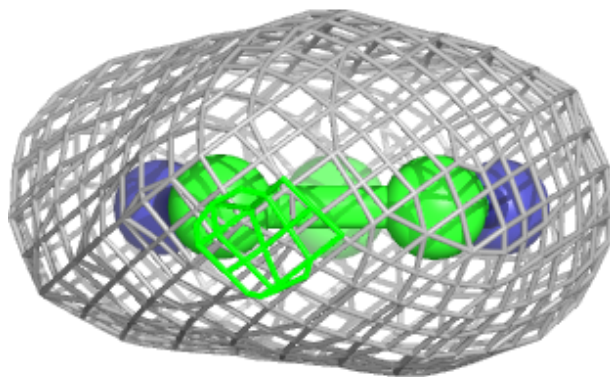
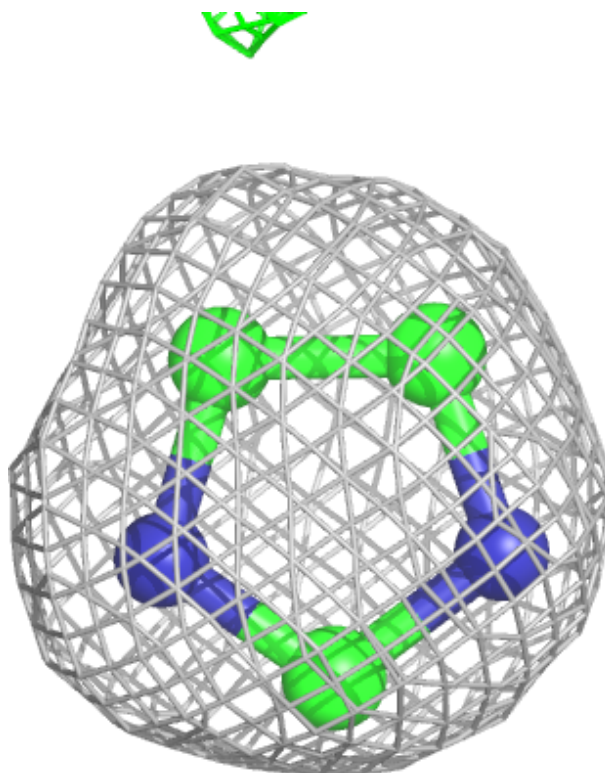
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

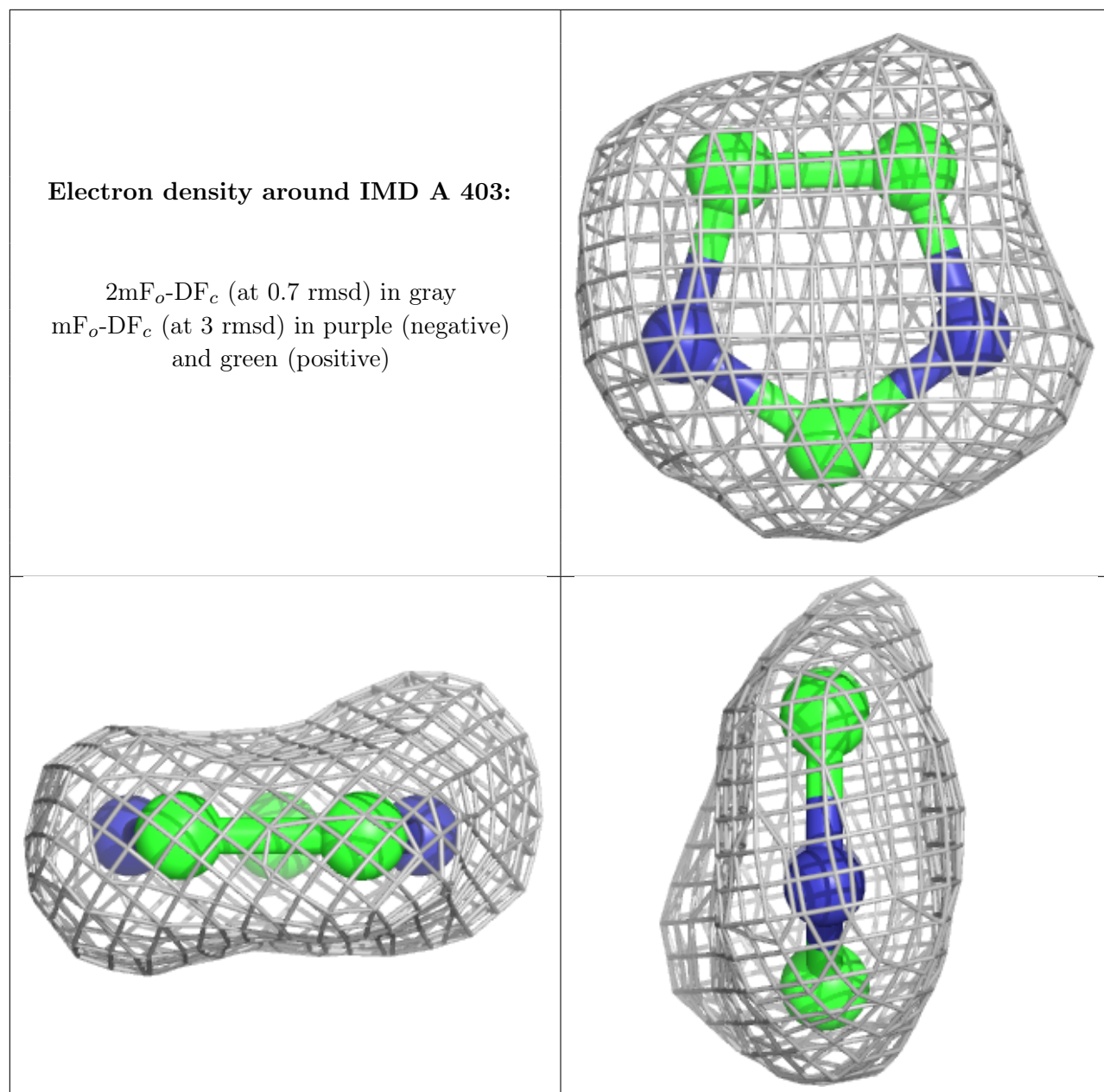




Electron density around IMD C 402:

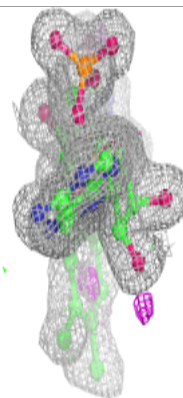
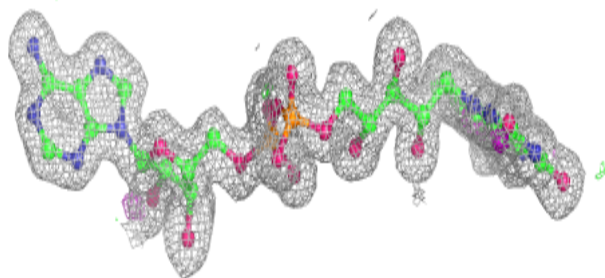
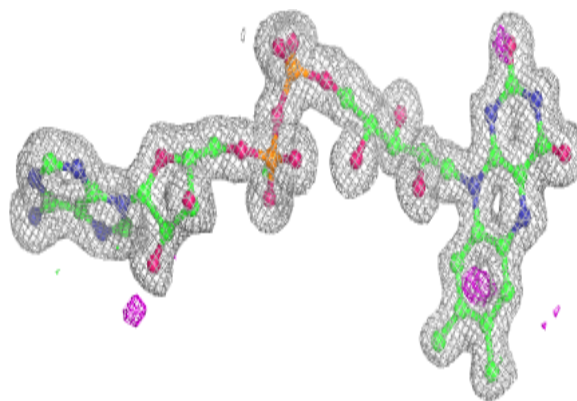
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





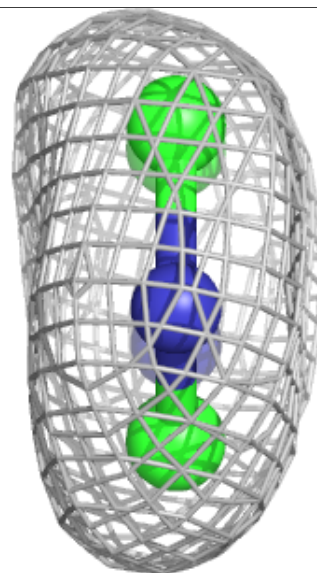
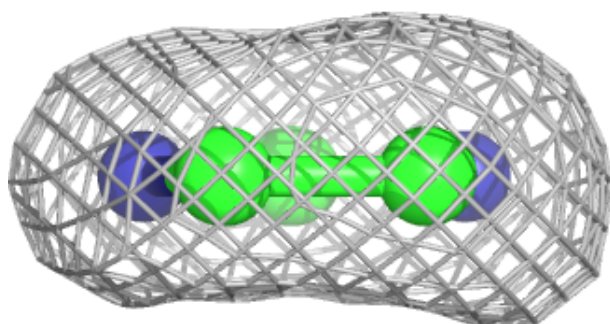
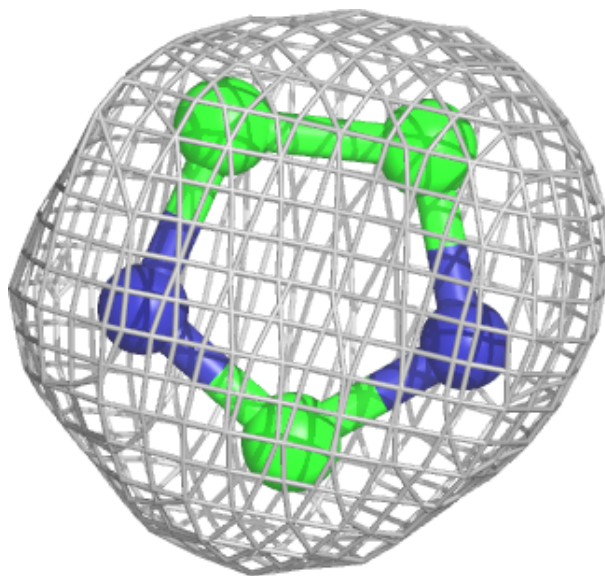
Electron density around FAD B 401:

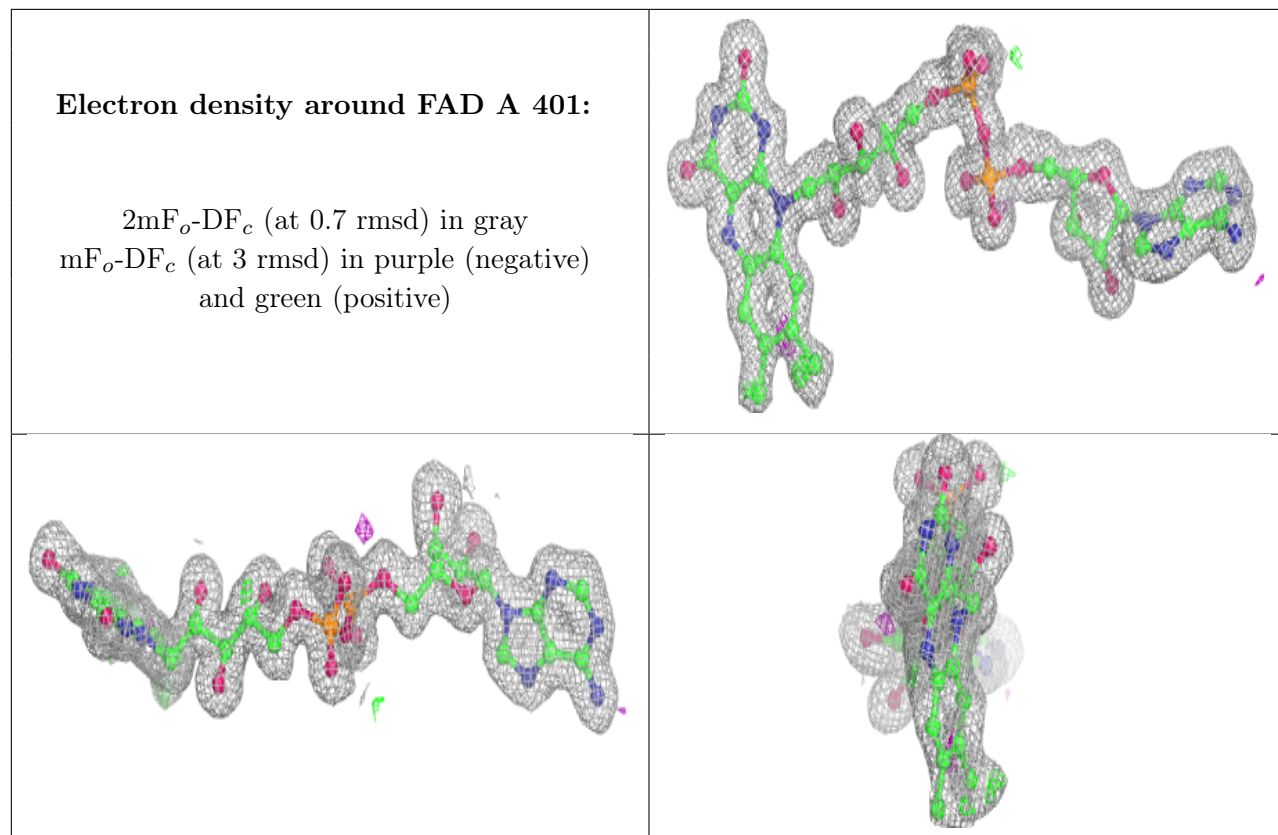
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around IMD B 403:

$2mF_o-DF_c$ (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.