



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 07:57 PM BST

PDB ID : 6VBN
Title : Crystal Structure of hTDO2 bound to inhibitor GNE1
Authors : Harris, S.F.; Oh, A.
Deposited on : 2019-12-19
Resolution : 3.18 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 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 : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

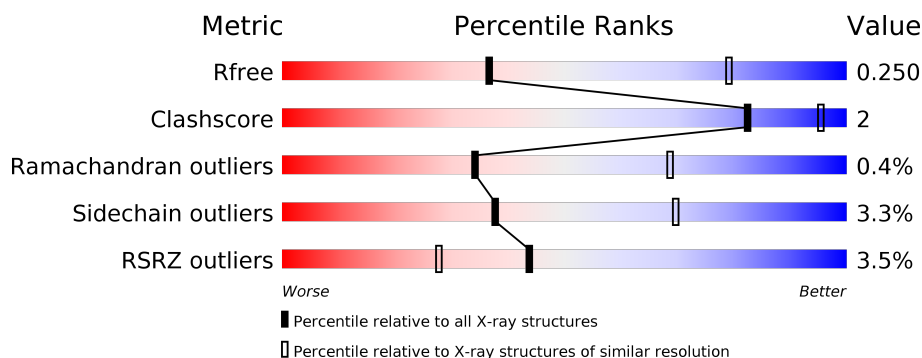
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.18 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	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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 on 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	385	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 82%, yellow 82%, yellow 89%, grey 89%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 82% 7% 11% </div> </div>
1	B	385	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 5%, green 5%, green 80%, yellow 80%, yellow 89%, grey 89%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 5% 80% 9% 11% </div> </div>
1	C	385	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, green 3%, green 79%, yellow 79%, yellow 89%, grey 89%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 79% 10% 10% </div> </div>
1	D	385	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 4%, green 4%, green 81%, yellow 81%, yellow 89%, grey 89%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 4% 81% 8% 11% </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11885 atoms, of which 12 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 Tryptophan 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2899	1858	509	521	11			
1	B	343	Total	C	N	O	S	0	0	0
			2892	1853	508	520	11			
1	C	345	Total	C	N	O	S	0	0	0
			2906	1862	510	523	11			
1	D	343	Total	C	N	O	S	0	0	0
			2892	1853	508	520	11			

There are 56 discrepancies between the modelled and reference sequences:

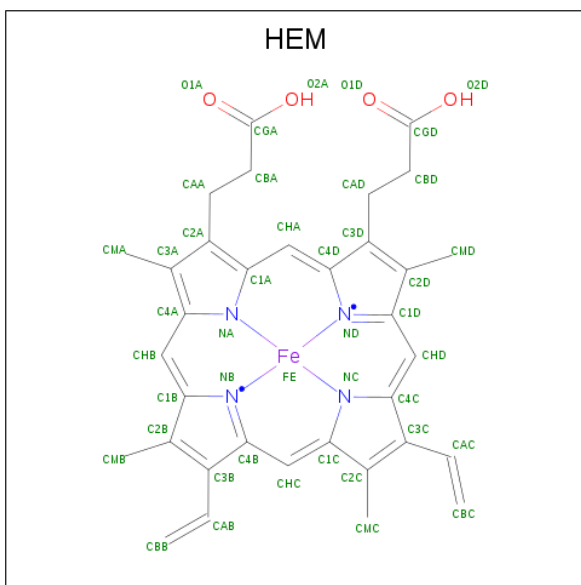
Chain	Residue	Modelled	Actual	Comment	Reference
A	15	MET	-	expression tag	UNP P48775
A	16	GLY	-	expression tag	UNP P48775
A	17	SER	-	expression tag	UNP P48775
A	389	GLY	-	expression tag	UNP P48775
A	390	ASN	-	expression tag	UNP P48775
A	391	SER	-	expression tag	UNP P48775
A	392	ASP	-	expression tag	UNP P48775
A	393	TYR	-	expression tag	UNP P48775
A	394	LYS	-	expression tag	UNP P48775
A	395	ASP	-	expression tag	UNP P48775
A	396	ASP	-	expression tag	UNP P48775
A	397	ASP	-	expression tag	UNP P48775
A	398	ASP	-	expression tag	UNP P48775
A	399	LYS	-	expression tag	UNP P48775
B	15	MET	-	expression tag	UNP P48775
B	16	GLY	-	expression tag	UNP P48775
B	17	SER	-	expression tag	UNP P48775
B	389	GLY	-	expression tag	UNP P48775
B	390	ASN	-	expression tag	UNP P48775
B	391	SER	-	expression tag	UNP P48775
B	392	ASP	-	expression tag	UNP P48775

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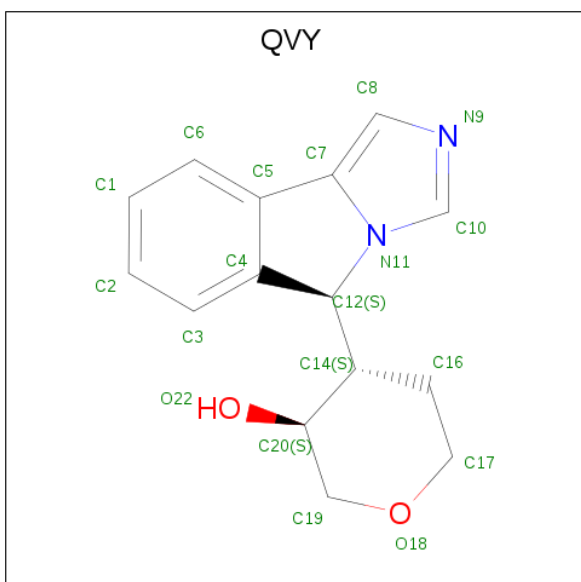
Chain	Residue	Modelled	Actual	Comment	Reference
B	393	TYR	-	expression tag	UNP P48775
B	394	LYS	-	expression tag	UNP P48775
B	395	ASP	-	expression tag	UNP P48775
B	396	ASP	-	expression tag	UNP P48775
B	397	ASP	-	expression tag	UNP P48775
B	398	ASP	-	expression tag	UNP P48775
B	399	LYS	-	expression tag	UNP P48775
C	15	MET	-	expression tag	UNP P48775
C	16	GLY	-	expression tag	UNP P48775
C	17	SER	-	expression tag	UNP P48775
C	389	GLY	-	expression tag	UNP P48775
C	390	ASN	-	expression tag	UNP P48775
C	391	SER	-	expression tag	UNP P48775
C	392	ASP	-	expression tag	UNP P48775
C	393	TYR	-	expression tag	UNP P48775
C	394	LYS	-	expression tag	UNP P48775
C	395	ASP	-	expression tag	UNP P48775
C	396	ASP	-	expression tag	UNP P48775
C	397	ASP	-	expression tag	UNP P48775
C	398	ASP	-	expression tag	UNP P48775
C	399	LYS	-	expression tag	UNP P48775
D	15	MET	-	expression tag	UNP P48775
D	16	GLY	-	expression tag	UNP P48775
D	17	SER	-	expression tag	UNP P48775
D	389	GLY	-	expression tag	UNP P48775
D	390	ASN	-	expression tag	UNP P48775
D	391	SER	-	expression tag	UNP P48775
D	392	ASP	-	expression tag	UNP P48775
D	393	TYR	-	expression tag	UNP P48775
D	394	LYS	-	expression tag	UNP P48775
D	395	ASP	-	expression tag	UNP P48775
D	396	ASP	-	expression tag	UNP P48775
D	397	ASP	-	expression tag	UNP P48775
D	398	ASP	-	expression tag	UNP P48775
D	399	LYS	-	expression tag	UNP P48775

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 1,5-anhydro-2,3-dideoxy-3-[(5S)-5H-imidazo[5,1-a]isoindol-5-yl]-D-threo-pentitol (three-letter code: QVY) (formula: C₁₅H₁₆N₂O₂) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			22	15	3	2	2		
3	B	1	Total	C	H	N	O	0	0
			22	15	3	2	2		
3	C	1	Total	C	H	N	O	0	0
			22	15	3	2	2		
3	C	1	Total	C	H	N	O	0	0
			22	15	3	2	2		

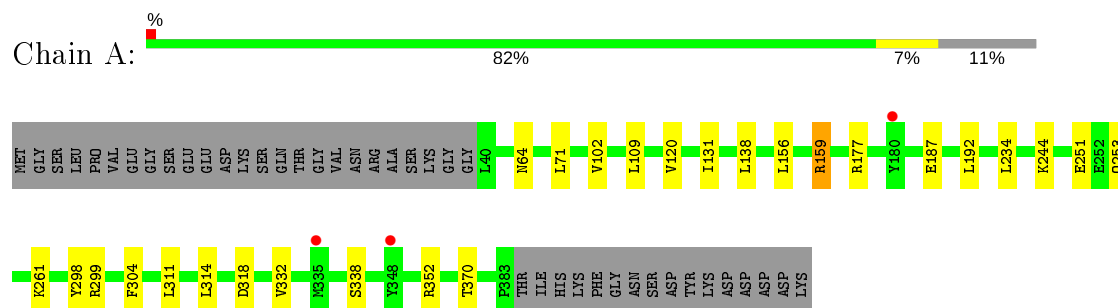
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	O	0	0
			13	13		
4	B	12	Total	O	0	0
			12	12		
4	C	4	Total	O	0	0
			4	4		
4	D	7	Total	O	0	0
			7	7		

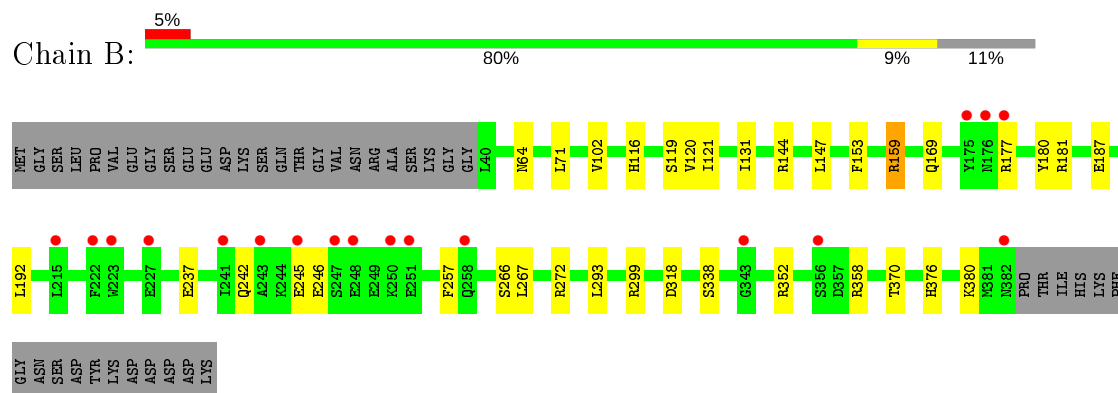
3 Residue-property plots [i](#)

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.

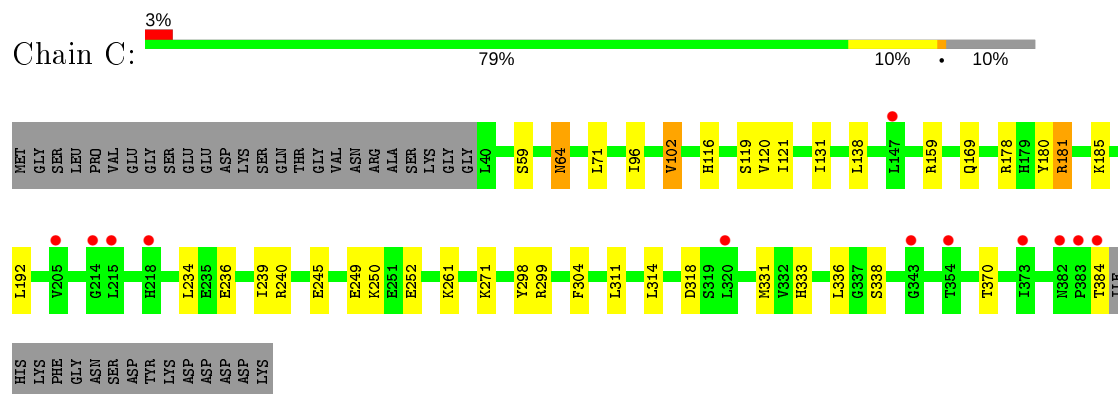
- Molecule 1: Tryptophan 2,3-dioxygenase



- Molecule 1: Tryptophan 2,3-dioxygenase



- Molecule 1: Tryptophan 2,3-dioxygenase



- Molecule 1: Tryptophan 2,3-dioxygenase

[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.47Å 143.04Å 147.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.37 – 3.18 102.60 – 3.18	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.37-3.18) 99.8 (102.60-3.18)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 3.19Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.196 , 0.245 0.210 , 0.250	Depositor DCC
R_{free} test set	1383 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	94.6	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 69.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11885	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: HEM, QVY

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	0.44	0/2966	0.60	0/3992
1	B	0.43	0/2958	0.60	0/3980
1	C	0.42	0/2973	0.59	0/4002
1	D	0.43	0/2958	0.62	0/3980
All	All	0.43	0/11855	0.60	0/15954

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	2899	0	2883	18	0
1	B	2892	0	2876	15	0
1	C	2906	0	2890	19	0
1	D	2892	0	2876	21	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0
2	C	43	0	30	0	0
2	D	43	0	30	1	0
3	A	19	3	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	19	3	0	0	0
3	C	38	6	0	0	0
4	A	13	0	0	0	0
4	B	12	0	0	0	0
4	C	4	0	0	1	0
4	D	7	0	0	0	0
All	All	11873	12	11645	58	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 2.

All (58) 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:D:346:SER:HB3	1:D:349:HIS:HB3	1.58	0.83
1:A:338:SER:H	1:C:370:THR:HG22	1.58	0.68
1:D:169:GLN:HA	1:D:172:ARG:HD2	1.77	0.67
1:B:153:PHE:CE2	2:B:401:HEM:HBA1	2.32	0.65
1:B:144:ARG:HA	1:B:147:LEU:HD12	1.83	0.60
1:A:299:ARG:HD3	1:C:138:LEU:HD12	1.85	0.58
1:D:159:ARG:HB3	1:D:192:LEU:HD11	1.84	0.58
1:C:245:GLU:HB3	4:C:502:HOH:O	2.03	0.57
1:D:133:GLU:HA	1:D:334:ARG:HH21	1.68	0.57
1:C:311:LEU:HA	1:C:314:LEU:HD12	1.87	0.56
1:B:338:SER:H	1:D:370:THR:HG22	1.71	0.56
1:B:181:ARG:HG3	1:B:192:LEU:HD23	1.88	0.55
1:A:131:ILE:HD13	1:B:120:VAL:HG12	1.88	0.55
1:B:266:SER:HB2	1:B:272:ARG:HD3	1.92	0.52
1:A:159:ARG:HB3	1:A:192:LEU:HD11	1.92	0.50
1:C:131:ILE:HD12	1:D:121:ILE:HA	1.94	0.49
1:A:120:VAL:HG12	1:B:131:ILE:HD13	1.95	0.48
1:B:370:THR:HG22	1:D:338:SER:H	1.80	0.47
1:B:237:GLU:HB3	1:B:257:PHE:HE1	1.80	0.47
1:C:298:TYR:O	1:C:304:PHE:HB2	2.14	0.47
1:D:298:TYR:O	1:D:304:PHE:HB2	2.14	0.47
1:A:109:LEU:HD21	1:D:305:GLN:HG2	1.96	0.47
1:A:311:LEU:HA	1:A:314:LEU:HD12	1.96	0.47
1:A:156:LEU:HD12	1:A:192:LEU:HD13	1.96	0.47
1:C:131:ILE:HD13	1:D:120:VAL:HG12	1.96	0.46
1:A:298:TYR:O	1:A:304:PHE:HB2	2.15	0.46
1:B:299:ARG:HD3	1:D:138:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ILE:HG22	1:C:102:VAL:HG13	1.97	0.46
1:A:109:LEU:HD11	1:D:305:GLN:CD	2.36	0.46
1:A:138:LEU:HD12	1:C:299:ARG:HD3	1.97	0.46
1:C:120:VAL:HG12	1:D:131:ILE:HD13	1.96	0.46
1:C:236:GLU:O	1:C:240:ARG:HG2	2.16	0.46
1:B:159:ARG:HB3	1:B:192:LEU:HD11	1.98	0.45
1:A:332:VAL:HG12	2:A:401:HEM:CHB	2.46	0.45
1:D:234:LEU:HD13	1:D:261:LYS:HG3	1.98	0.45
1:A:234:LEU:HD13	1:A:261:LYS:HG3	1.99	0.44
1:D:326:TYR:O	1:D:329:VAL:HG12	2.17	0.44
1:D:169:GLN:CD	1:D:169:GLN:H	2.20	0.44
1:B:267:LEU:HD11	1:B:293:LEU:HD11	2.00	0.44
1:A:244:LYS:HE2	1:A:253:GLN:HE22	1.82	0.43
1:A:177:ARG:HE	1:A:177:ARG:HB3	1.51	0.43
1:C:159:ARG:HD3	1:C:180:TYR:HD1	1.83	0.43
1:C:333:HIS:CE1	1:C:338:SER:HB3	2.53	0.43
1:D:329:VAL:HA	1:D:332:VAL:HG22	2.02	0.42
1:A:332:VAL:HG12	2:A:401:HEM:C1B	2.54	0.42
1:A:71:LEU:HD11	1:A:131:ILE:HG22	2.00	0.41
1:C:181:ARG:HG2	1:C:192:LEU:HD23	2.02	0.41
1:D:151:SER:O	1:D:154:GLN:HB2	2.20	0.41
1:C:121:ILE:HA	1:D:131:ILE:HD12	2.02	0.41
1:B:71:LEU:HD11	1:B:131:ILE:HG22	2.02	0.41
1:C:71:LEU:HD11	1:C:131:ILE:HG22	2.02	0.41
1:B:116:HIS:O	1:B:119:SER:HB3	2.20	0.41
1:C:234:LEU:HD13	1:C:261:LYS:HG3	2.03	0.41
1:D:332:VAL:HG12	2:D:401:HEM:C1B	2.56	0.41
1:C:59:SER:HB2	1:C:64:ASN:O	2.21	0.40
1:D:116:HIS:O	1:D:119:SER:HB3	2.20	0.40
1:A:131:ILE:HD12	1:B:121:ILE:HA	2.03	0.40
1:C:116:HIS:O	1:C:119:SER:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	342/385 (89%)	330 (96%)	11 (3%)	1 (0%)	41	73
1	B	341/385 (89%)	327 (96%)	13 (4%)	1 (0%)	41	73
1	C	343/385 (89%)	328 (96%)	13 (4%)	2 (1%)	25	63
1	D	341/385 (89%)	327 (96%)	13 (4%)	1 (0%)	41	73
All	All	1367/1540 (89%)	1312 (96%)	50 (4%)	5 (0%)	34	69

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	C	336	LEU
1	B	64	ASN
1	C	64	ASN
1	D	64	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	317/351 (90%)	310 (98%)	7 (2%)	52	78
1	B	316/351 (90%)	302 (96%)	14 (4%)	28	62
1	C	318/351 (91%)	305 (96%)	13 (4%)	30	64
1	D	316/351 (90%)	308 (98%)	8 (2%)	47	76
All	All	1267/1404 (90%)	1225 (97%)	42 (3%)	38	70

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	VAL
1	A	159	ARG
1	A	187	GLU

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Mol	Chain	Res	Type
1	A	251	GLU
1	A	318	ASP
1	A	352	ARG
1	A	370	THR
1	B	102	VAL
1	B	159	ARG
1	B	169	GLN
1	B	177	ARG
1	B	180	TYR
1	B	187	GLU
1	B	242	GLN
1	B	245	GLU
1	B	246	GLU
1	B	318	ASP
1	B	352	ARG
1	B	358	ARG
1	B	376	HIS
1	B	380	LYS
1	C	102	VAL
1	C	169	GLN
1	C	178	ARG
1	C	181	ARG
1	C	185	LYS
1	C	239	ILE
1	C	249	GLU
1	C	250	LYS
1	C	252	GLU
1	C	271	LYS
1	C	318	ASP
1	C	331	MET
1	C	384	THR
1	D	153	PHE
1	D	154	GLN
1	D	159	ARG
1	D	177	ARG
1	D	185	LYS
1	D	193	LEU
1	D	370	THR
1	D	381	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	176	ASN
1	A	253	GLN
1	B	44	ASN
1	B	176	ASN
1	B	253	GLN
1	C	44	ASN
1	C	229	ASN
1	D	44	ASN
1	D	170	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](#)

8 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	QVY	B	402	2	20,22,22	0.51	0	21,32,32	1.11	2 (9%)
3	QVY	A	402	2	20,22,22	0.54	0	21,32,32	1.12	2 (9%)
2	HEM	D	401	1,3	27,50,50	1.29	3 (11%)	17,82,82	1.94	3 (17%)
2	HEM	B	401	1,3	27,50,50	1.27	3 (11%)	17,82,82	2.12	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	A	401	1,3	27,50,50	1.35	3 (11%)	17,82,82	2.00	4 (23%)
3	QVY	C	402	2	20,22,22	0.53	0	21,32,32	1.16	2 (9%)
3	QVY	C	403	2	20,22,22	0.57	0	21,32,32	1.18	2 (9%)
2	HEM	C	401	1,3	27,50,50	1.35	4 (14%)	17,82,82	1.91	4 (23%)

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	QVY	B	402	2	-	0/3/27/27	0/4/4/4
3	QVY	A	402	2	-	0/3/27/27	0/4/4/4
2	HEM	D	401	1,3	-	0/6/54/54	-
2	HEM	B	401	1,3	-	0/6/54/54	-
2	HEM	A	401	1,3	-	0/6/54/54	-
3	QVY	C	402	2	-	0/3/27/27	0/4/4/4
3	QVY	C	403	2	-	0/3/27/27	0/4/4/4
2	HEM	C	401	1,3	-	0/6/54/54	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	HEM	C3B-C2B	-3.91	1.34	1.40
2	D	401	HEM	C3B-C2B	-3.86	1.35	1.40
2	C	401	HEM	C3B-C2B	-3.62	1.35	1.40
2	A	401	HEM	C3B-C2B	-3.52	1.35	1.40
2	C	401	HEM	C4D-C3D	3.21	1.49	1.42
2	A	401	HEM	C4D-C3D	2.99	1.49	1.42
2	B	401	HEM	C4D-C3D	2.99	1.49	1.42
2	D	401	HEM	C4D-C3D	2.95	1.49	1.42
2	D	401	HEM	C3C-C2C	-2.37	1.37	1.40
2	C	401	HEM	C3C-C2C	-2.35	1.37	1.40
2	A	401	HEM	C3C-C2C	-2.21	1.37	1.40
2	C	401	HEM	CAA-C2A	-2.12	1.48	1.52
2	B	401	HEM	C3C-C2C	-2.06	1.37	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	HEM	CBD-CAD-C3D	-5.44	102.45	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	HEM	CBD-CAD-C3D	-5.16	102.98	112.48
2	C	401	HEM	CBD-CAD-C3D	-5.11	103.06	112.48
2	D	401	HEM	CBD-CAD-C3D	-5.04	103.19	112.48
3	C	403	QVY	C6-C5-C7	3.78	130.75	123.45
3	C	402	QVY	C6-C5-C7	3.74	130.68	123.45
3	A	402	QVY	C6-C5-C7	3.49	130.20	123.45
3	B	402	QVY	C6-C5-C7	3.39	130.00	123.45
2	B	401	HEM	CAD-CBD-CGD	3.16	117.97	112.67
2	D	401	HEM	CAD-CBD-CGD	3.13	117.92	112.67
2	B	401	HEM	CBA-CAA-C2A	-2.96	107.03	112.49
2	A	401	HEM	CAD-CBD-CGD	2.95	117.62	112.67
2	A	401	HEM	CBA-CAA-C2A	-2.89	107.15	112.49
2	C	401	HEM	CAD-CBD-CGD	2.72	117.23	112.67
2	C	401	HEM	CBA-CAA-C2A	-2.53	107.82	112.49
2	D	401	HEM	CBA-CAA-C2A	-2.49	107.89	112.49
3	B	402	QVY	C5-C7-N11	-2.35	105.28	112.38
2	B	401	HEM	C4A-C3A-C2A	-2.32	105.38	107.00
3	C	403	QVY	C5-C7-N11	-2.32	105.38	112.38
3	C	402	QVY	C5-C7-N11	-2.31	105.40	112.38
3	A	402	QVY	C5-C7-N11	-2.29	105.46	112.38
2	A	401	HEM	CMB-C2B-C3B	2.29	128.96	124.68
2	C	401	HEM	CMB-C2B-C3B	2.25	128.90	124.68
2	B	401	HEM	CMB-C2B-C3B	2.22	128.84	124.68

There are no chirality outliers.

There are no torsion outliers.

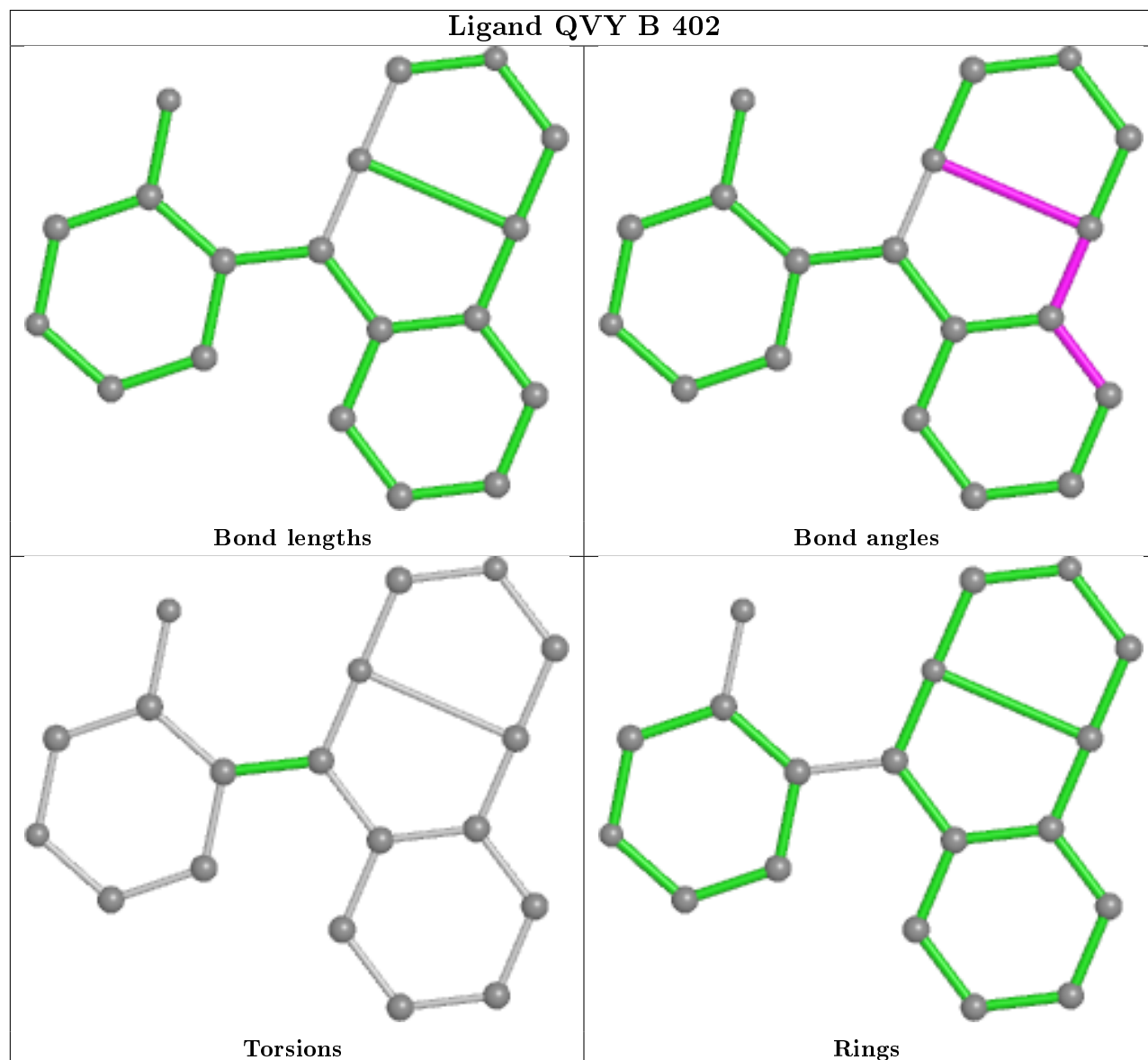
There are no ring outliers.

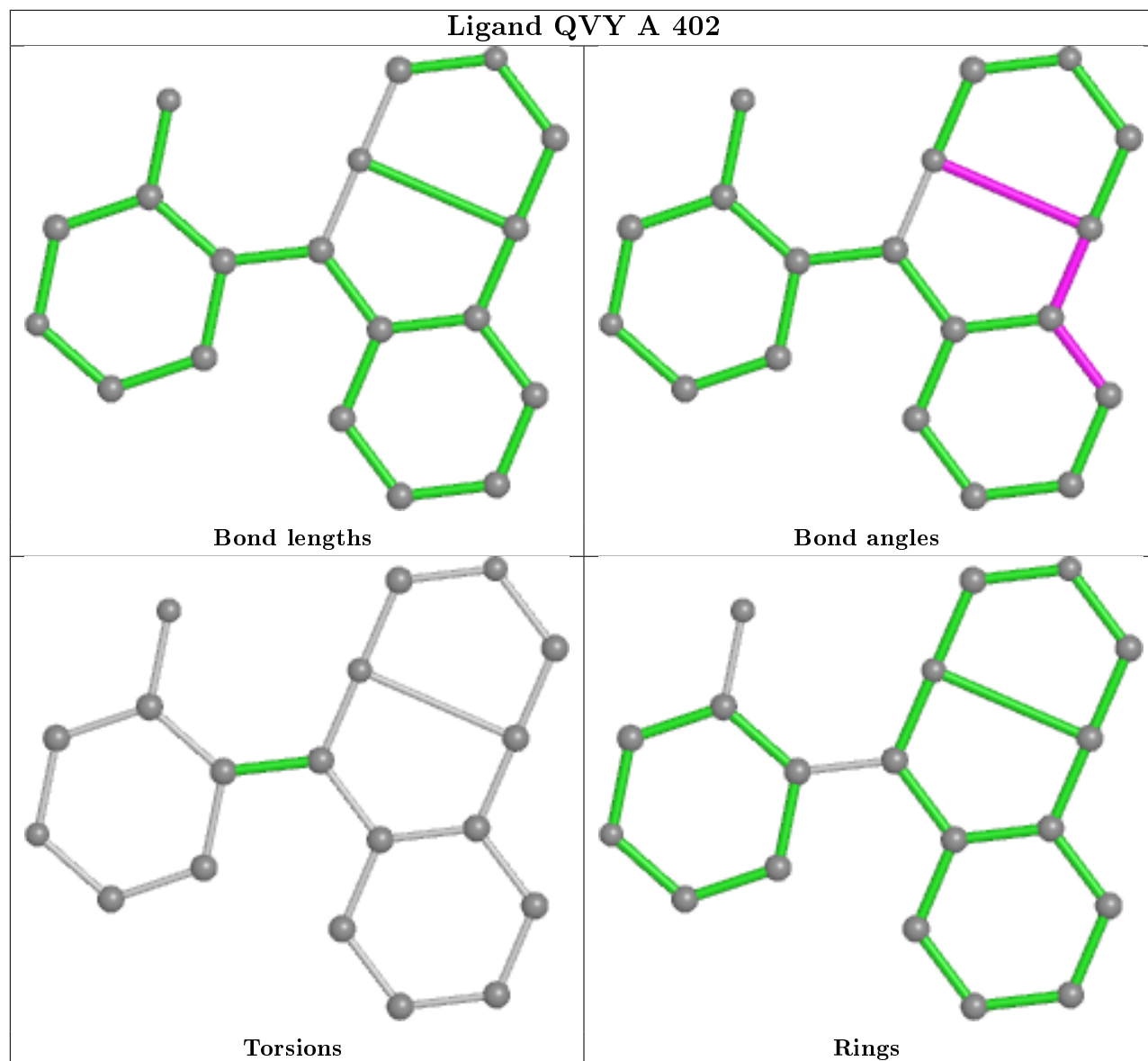
3 monomers are involved in 4 short contacts:

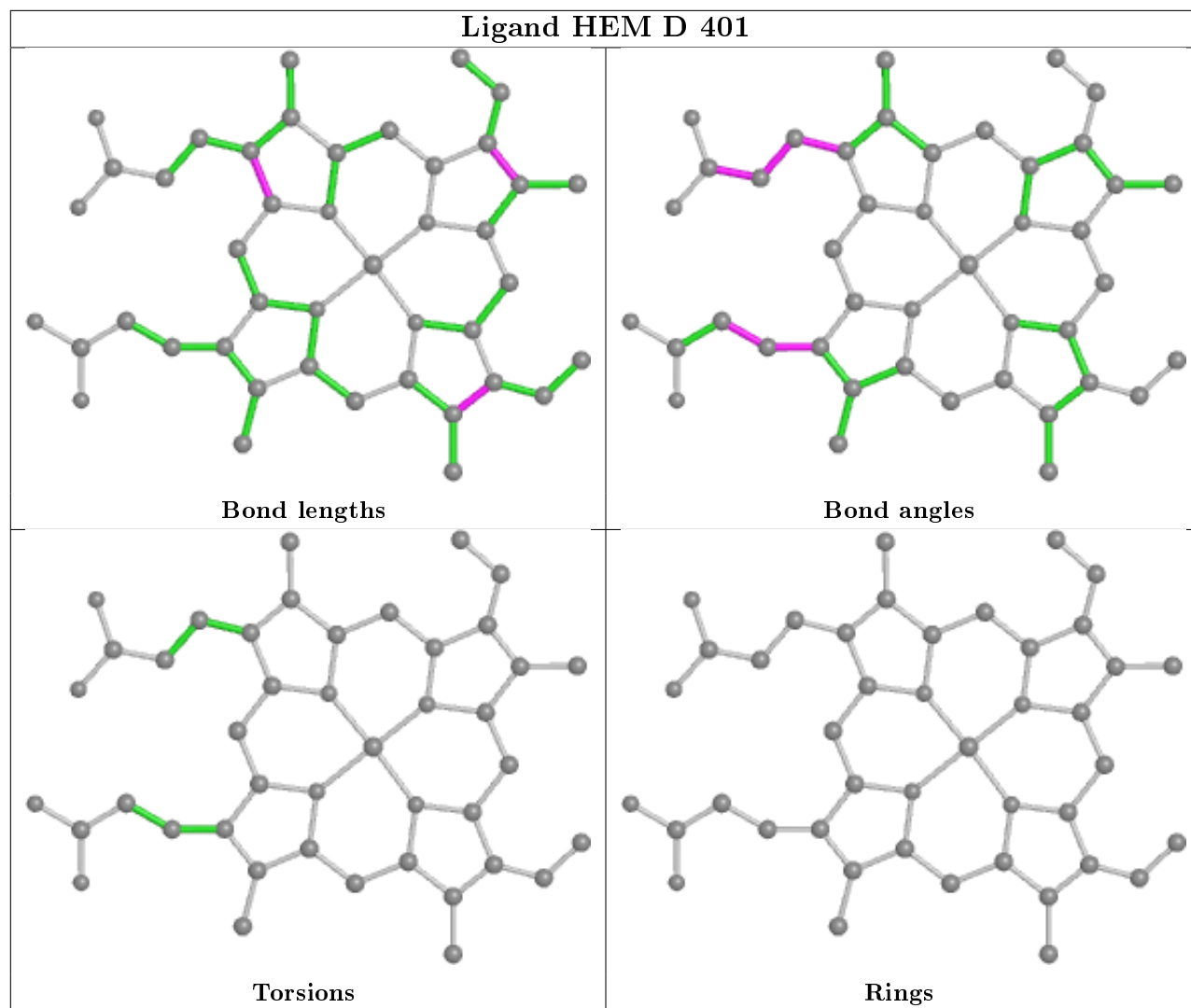
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	HEM	1	0
2	B	401	HEM	1	0
2	A	401	HEM	2	0

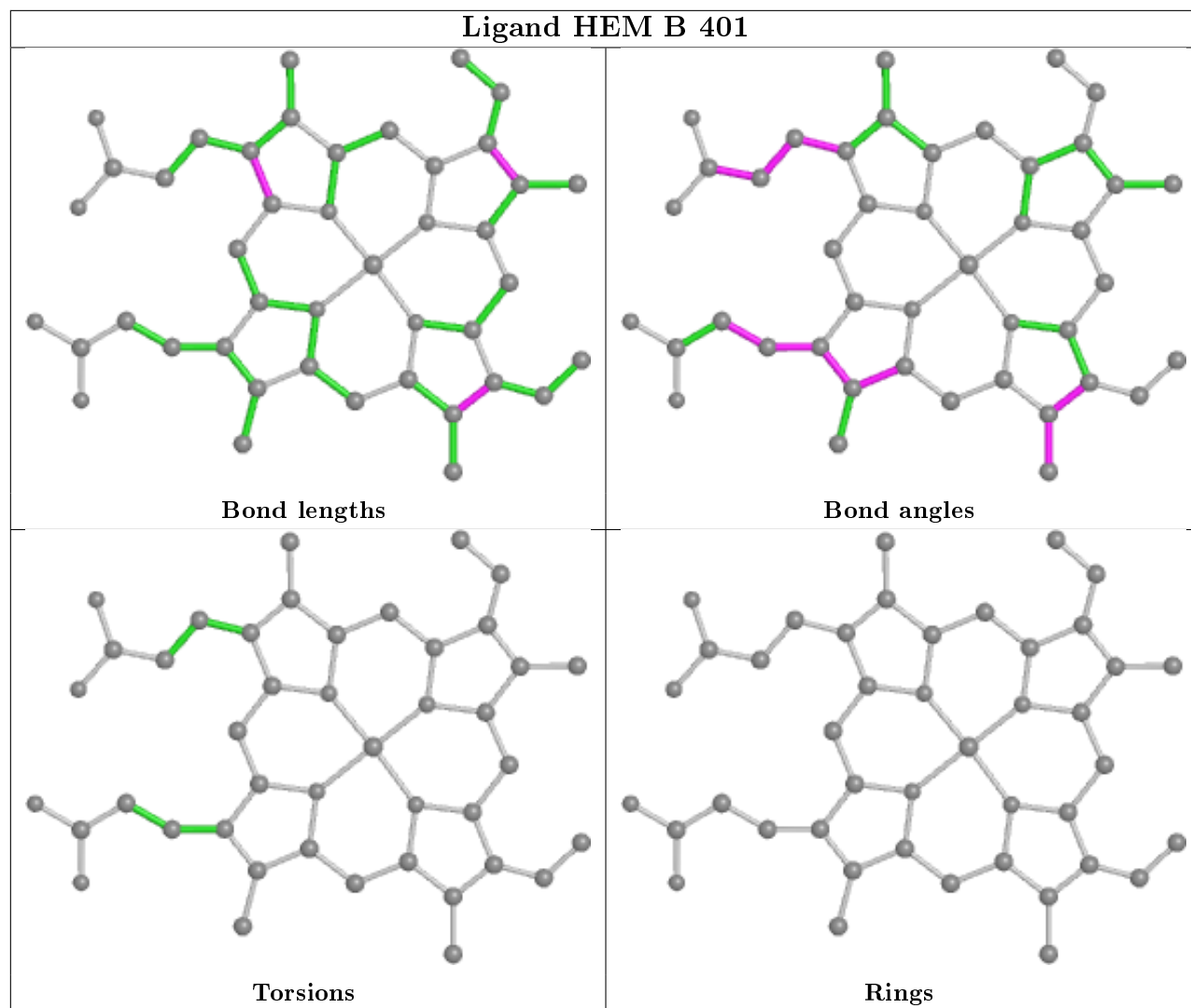
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

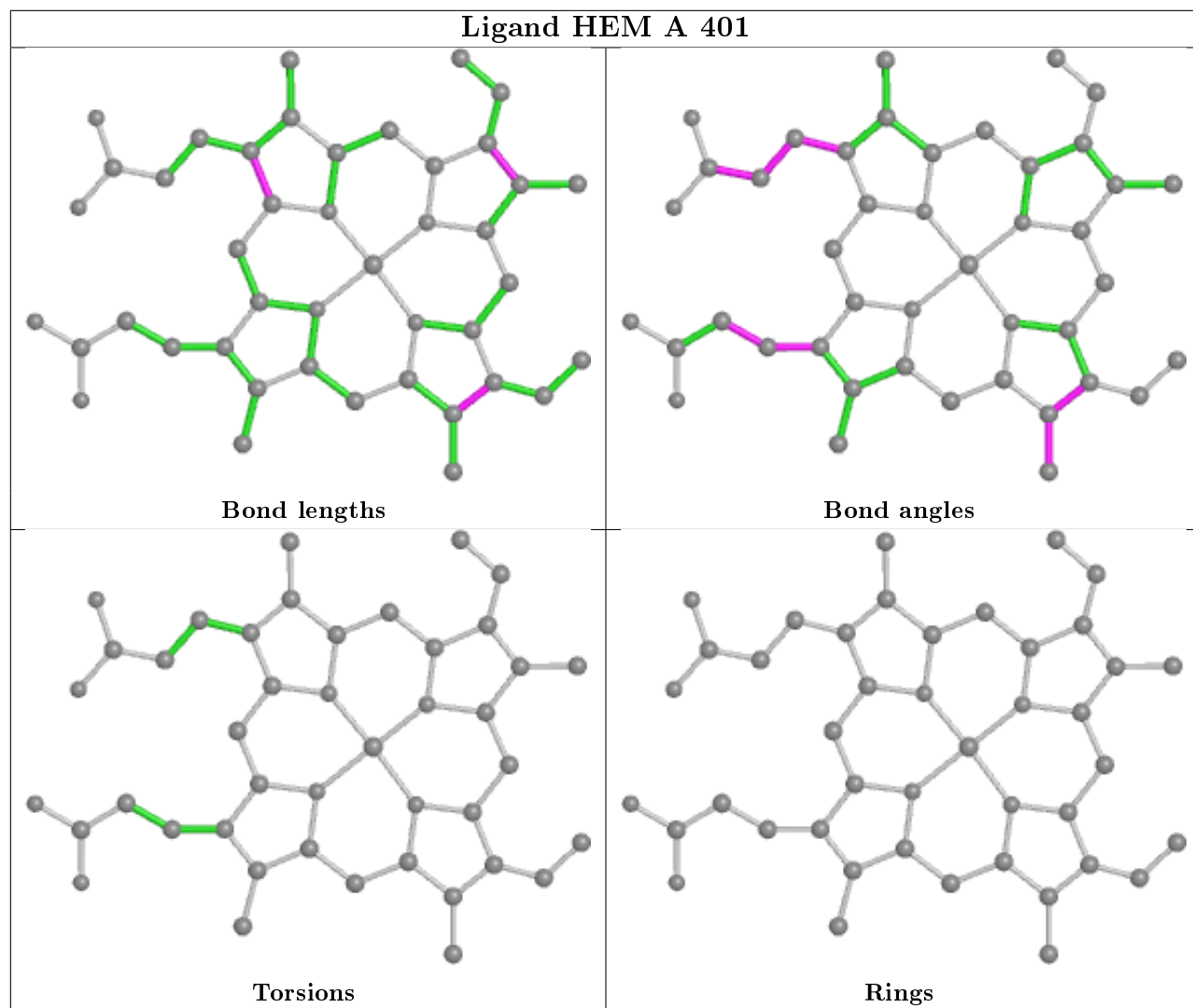
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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

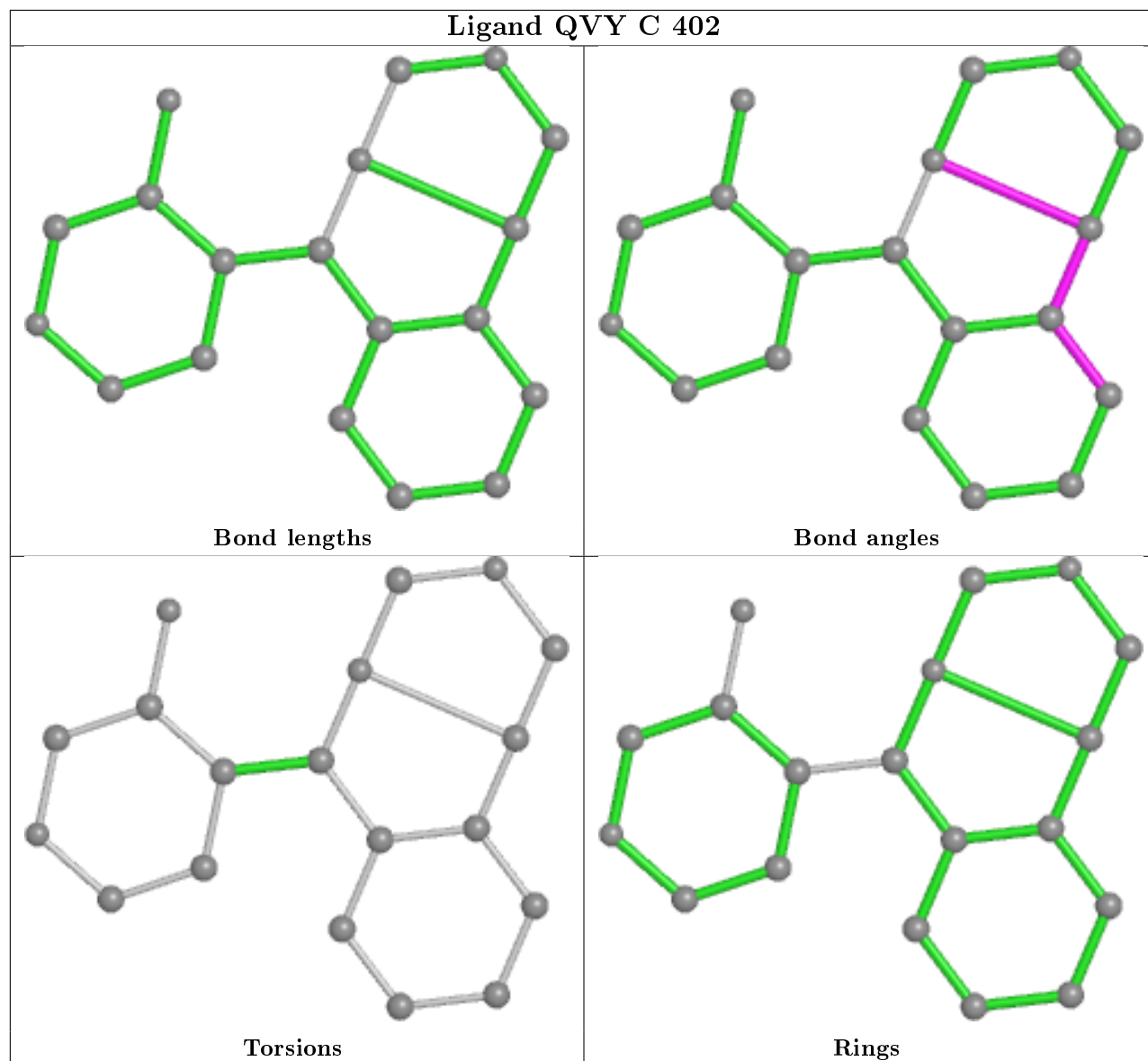


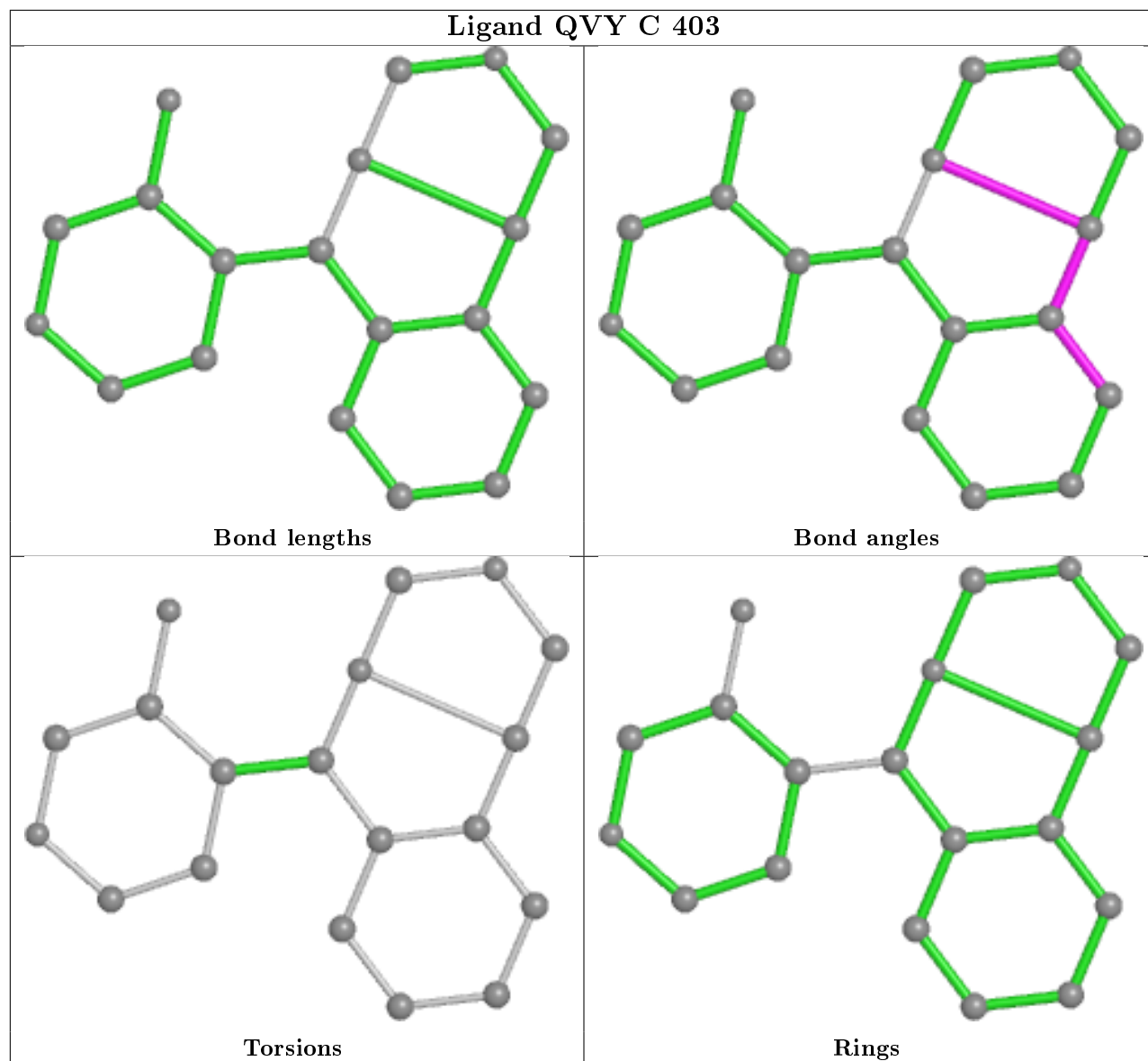


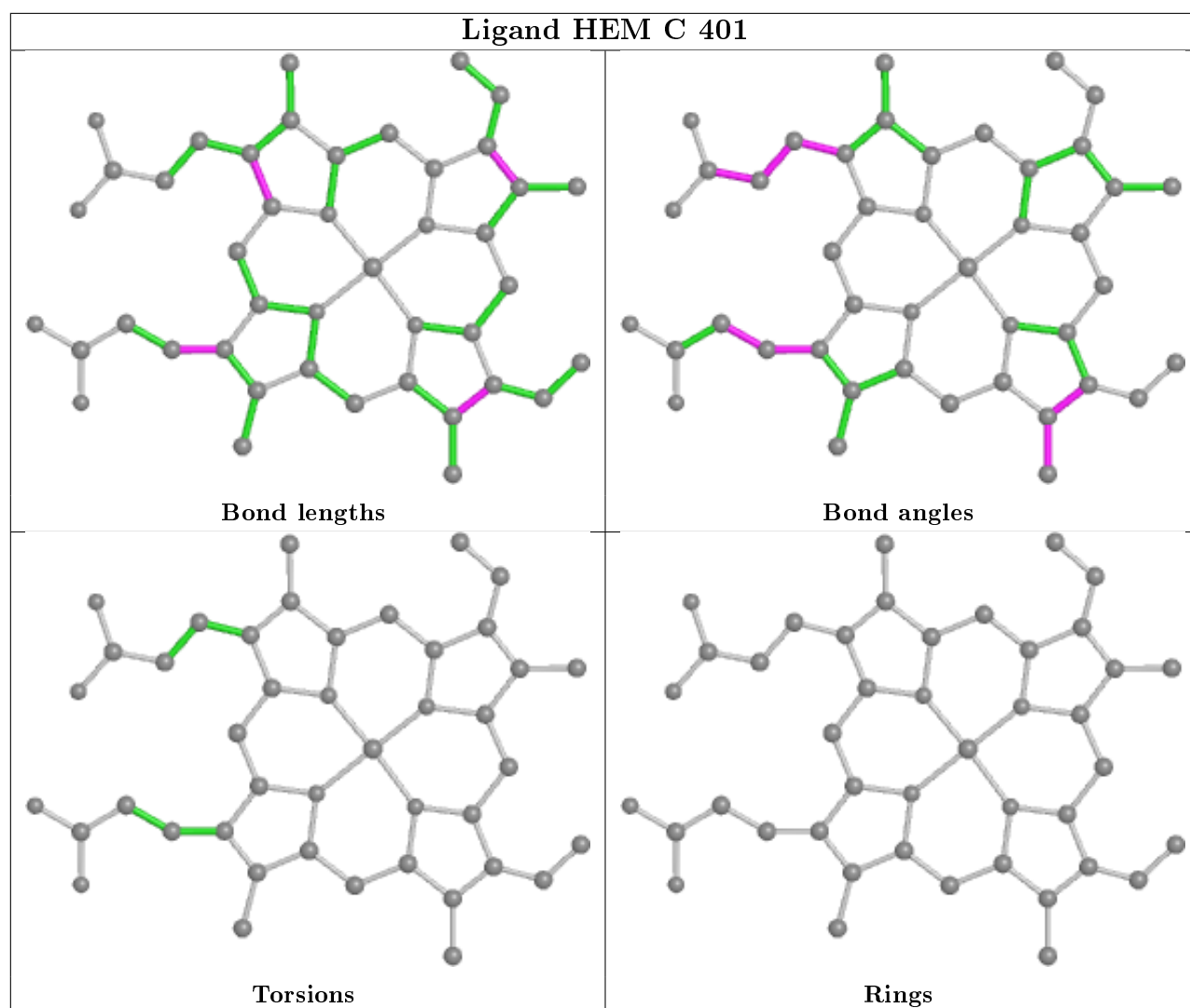












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	344/385 (89%)	0.09	3 (0%) 84 75	58, 94, 146, 167	0
1	B	343/385 (89%)	0.39	18 (5%) 27 15	61, 113, 167, 200	0
1	C	345/385 (89%)	0.26	12 (3%) 44 28	68, 125, 173, 193	0
1	D	343/385 (89%)	0.31	15 (4%) 34 20	58, 98, 159, 178	0
All	All	1375/1540 (89%)	0.26	48 (3%) 44 28	58, 107, 163, 200	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	258	GLN	6.1
1	D	344	GLY	5.8
1	B	243	ALA	5.4
1	D	171	MET	5.4
1	B	247	SER	5.2
1	D	342	THR	5.1
1	C	384	THR	4.7
1	D	343	GLY	4.4
1	D	345	SER	4.3
1	D	338	SER	4.1
1	D	175	TYR	3.9
1	B	248	GLU	3.8
1	B	382	ASN	3.8
1	B	343	GLY	3.7
1	B	176	ASN	3.6
1	B	177	ARG	3.3
1	D	180	TYR	3.2
1	B	245	GLU	3.2
1	D	176	ASN	3.1
1	B	175	TYR	2.9
1	B	250	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	177	ARG	2.8
1	D	382	ASN	2.8
1	B	227	GLU	2.7
1	A	348	TYR	2.7
1	B	215	LEU	2.4
1	A	335	MET	2.4
1	D	153	PHE	2.4
1	C	215	LEU	2.4
1	C	354	THR	2.4
1	B	223	TRP	2.4
1	D	183	ASN	2.4
1	C	214	GLY	2.4
1	B	251	GLU	2.3
1	C	383	PRO	2.2
1	C	218	HIS	2.2
1	C	373	ILE	2.2
1	C	147	LEU	2.2
1	A	180	TYR	2.2
1	B	222	PHE	2.1
1	C	320	LEU	2.1
1	C	205	VAL	2.1
1	C	343	GLY	2.1
1	C	382	ASN	2.1
1	D	170	ASN	2.1
1	D	42	TYR	2.1
1	B	241	ILE	2.1
1	B	356	SER	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,

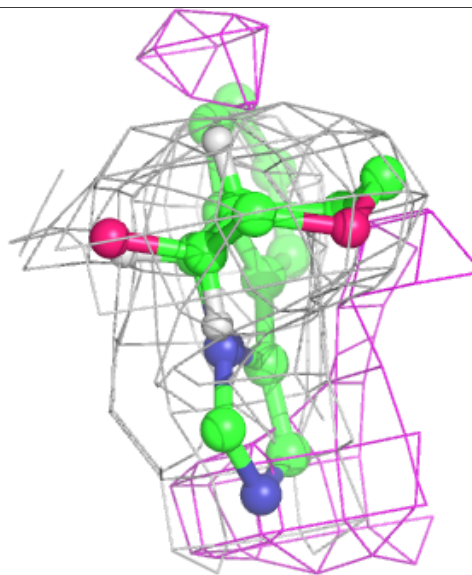
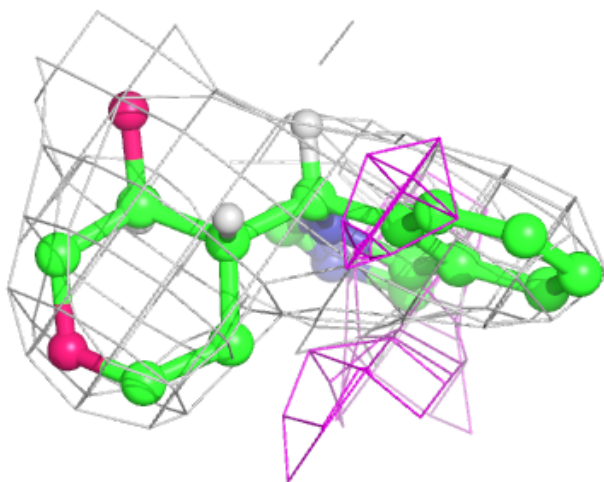
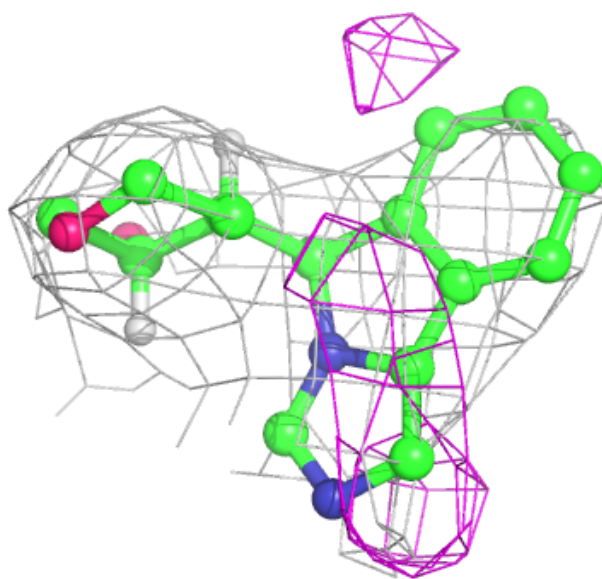
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	QVY	A	402	19/19	0.94	0.34	90,95,98,98	0
2	HEM	D	401	43/43	0.94	0.36	123,124,128,129	0
2	HEM	C	401	43/43	0.96	0.33	115,116,120,121	0
2	HEM	B	401	43/43	0.97	0.32	109,110,114,115	0
2	HEM	A	401	43/43	0.97	0.32	97,99,103,104	0
3	QVY	C	402	19/19	0.97	0.44	112,116,118,119	0
3	QVY	C	403	19/19	0.97	0.36	85,92,107,108	0
3	QVY	B	402	19/19	0.97	0.27	83,87,92,94	0

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

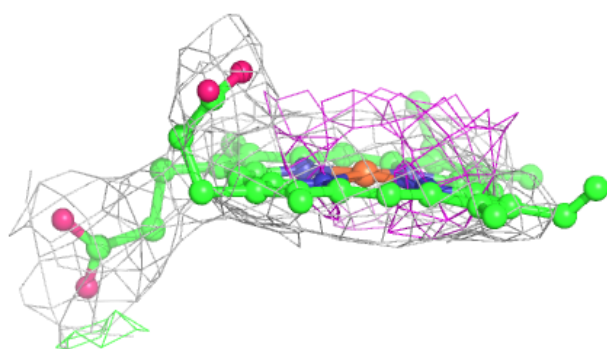
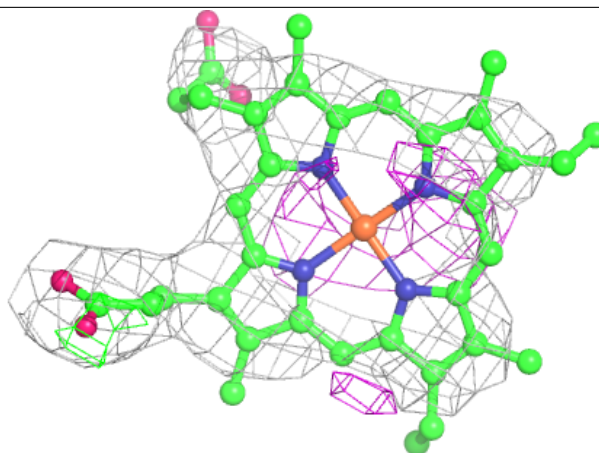
Electron density around QVY A 402:

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



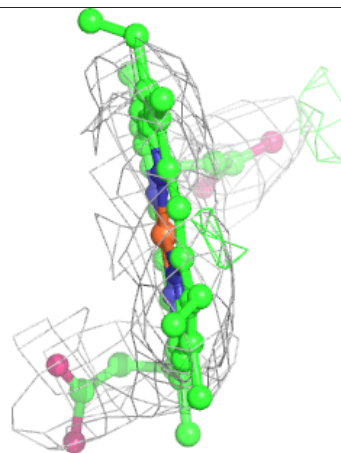
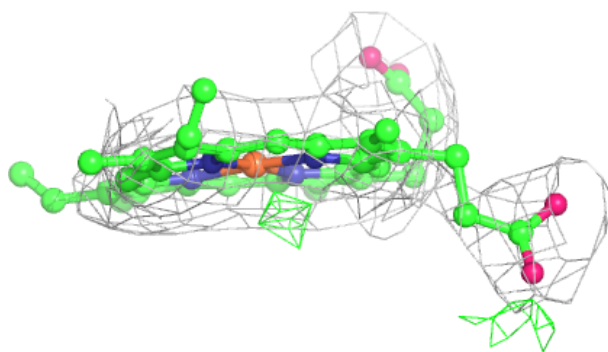
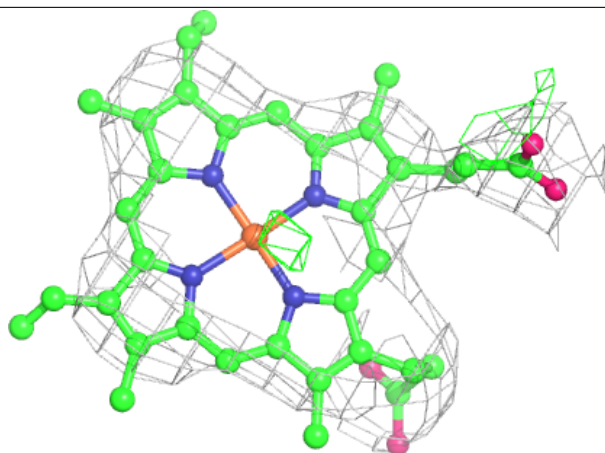
Electron density around HEM D 401:

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



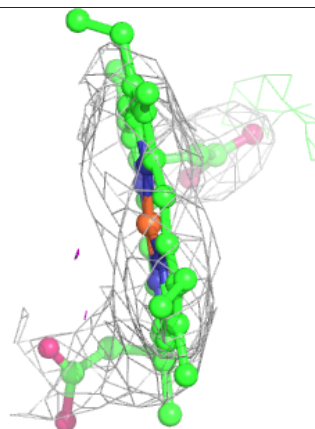
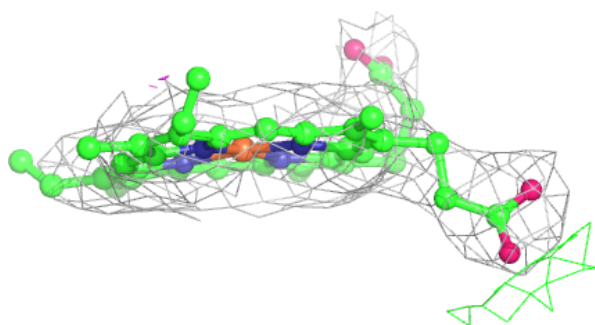
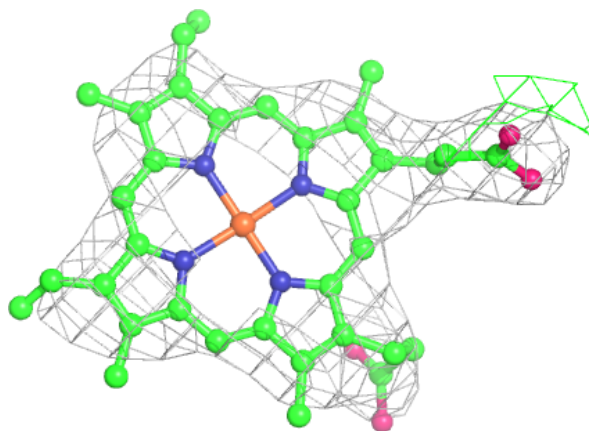
Electron density around HEM C 401:

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



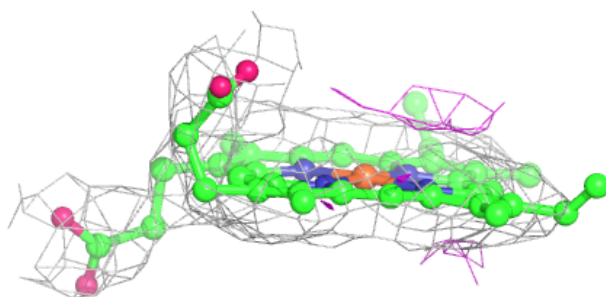
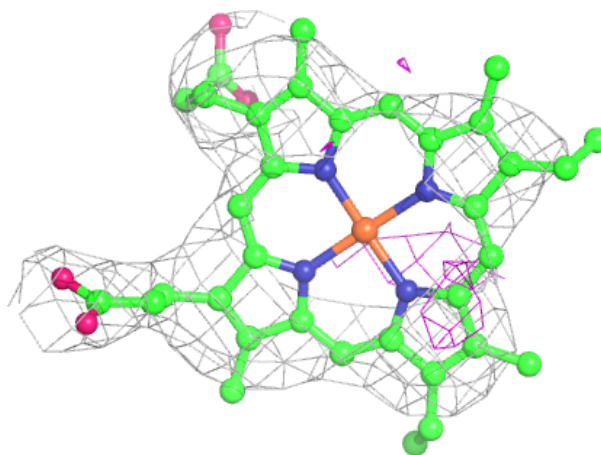
Electron density around HEM B 401:

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



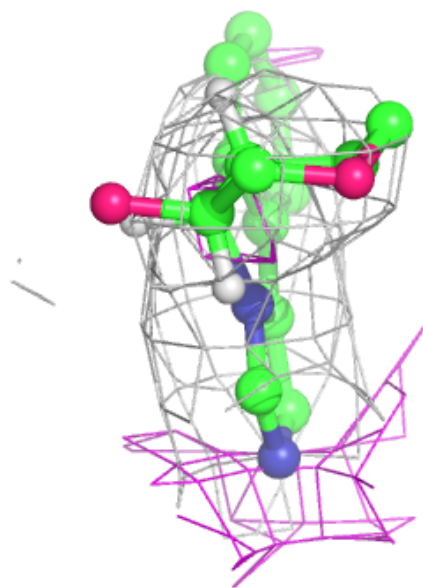
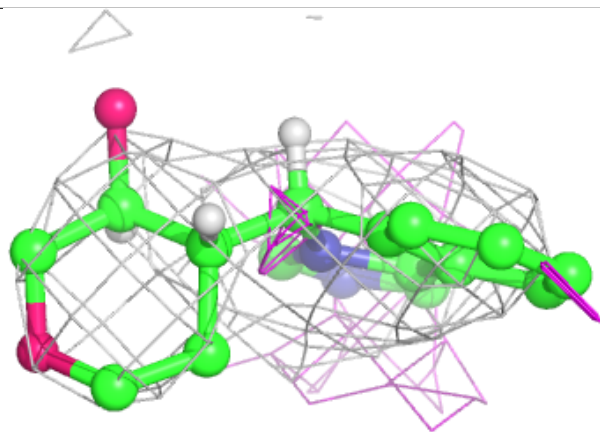
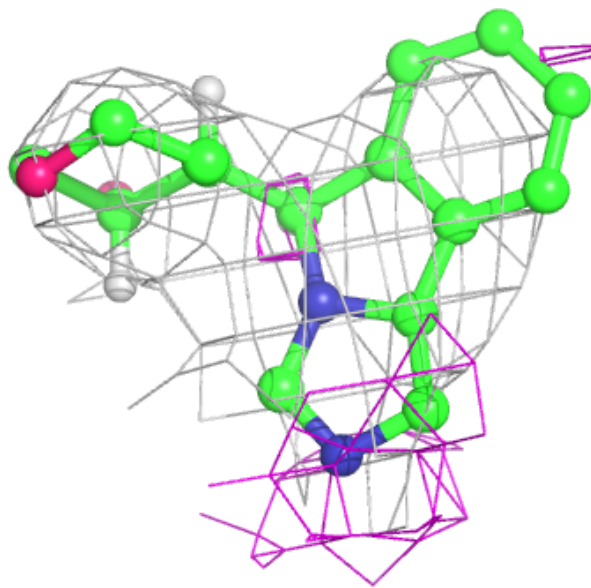
Electron density around HEM A 401:

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



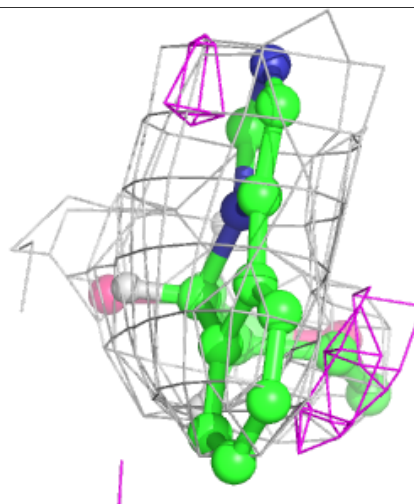
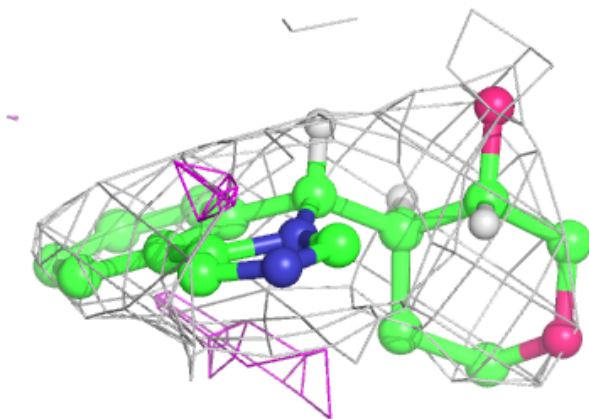
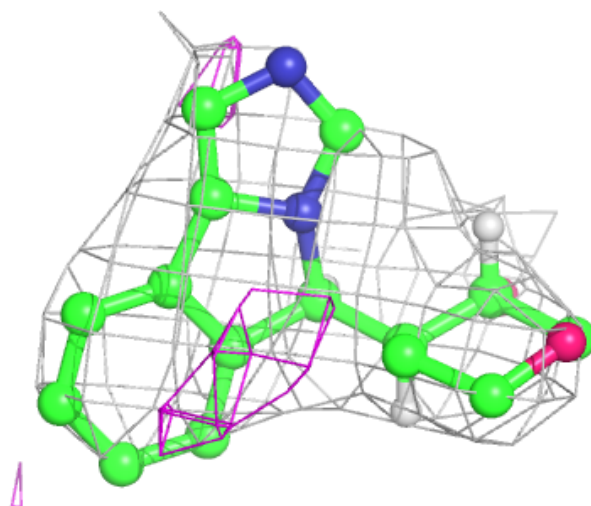
Electron density around QVY C 402:

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



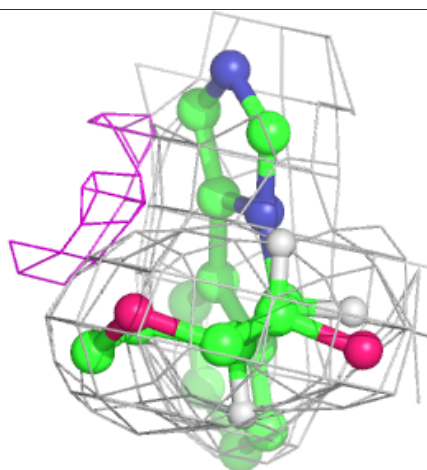
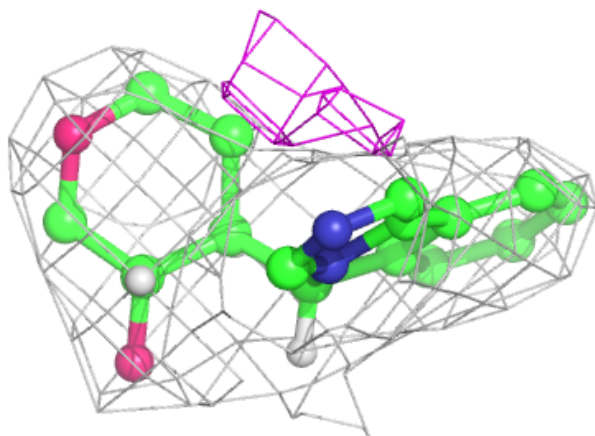
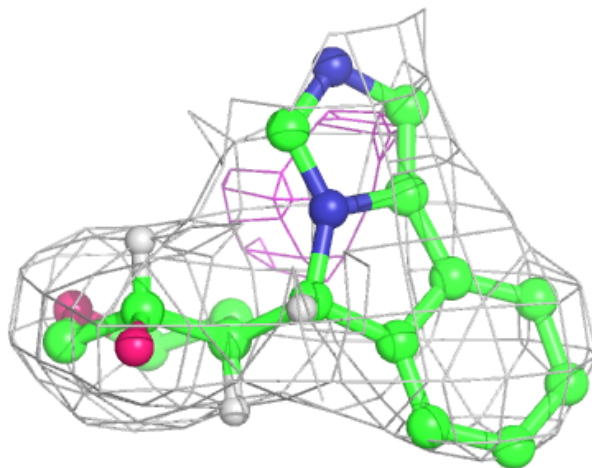
Electron density around QVY C 403:

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



Electron density around QVY 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.