



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:40 PM UTC

PDB ID : 6VBN / pdb_00006vbn
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 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

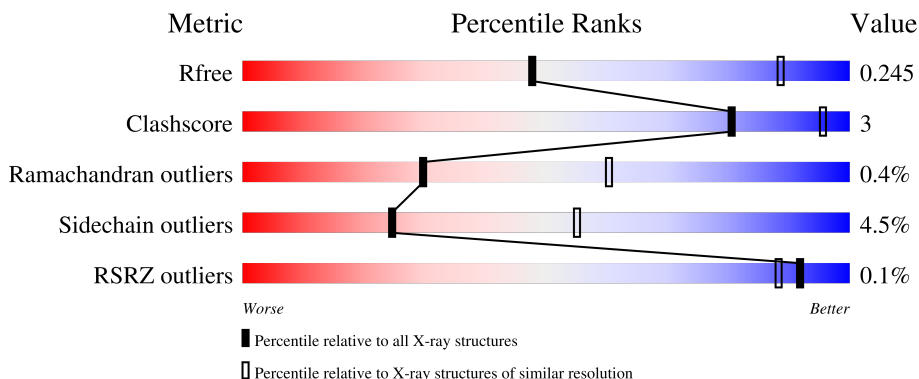
1 Overall quality at a glance

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}	180053	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (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 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	385	 80% 8% • 11%
1	B	385	 79% 9% • 11%
1	C	385	 77% 12% • 10%
1	D	385	 80% 8% • 11%

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:

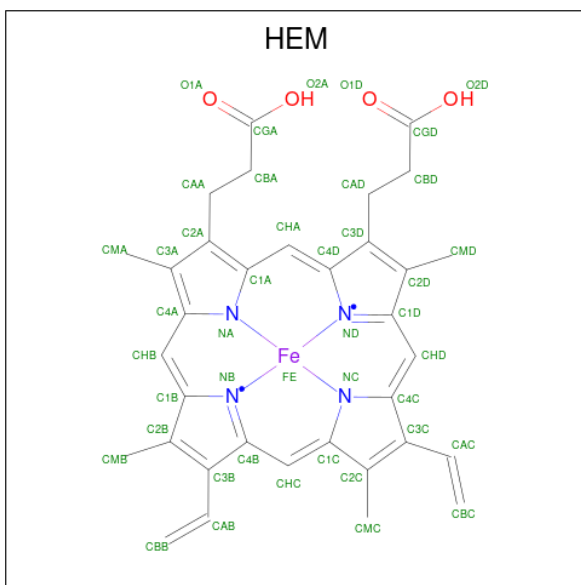
Chain	Residue	Modelled	Actual	Comment	Reference
A	15	MET	-	expression tag	UNP P48775
A	16	GLY	-	expression tag	UNP P48775
A	17	SER	-	expression tag	UNP P48775
A	389	GLY	-	expression tag	UNP P48775
A	390	ASN	-	expression tag	UNP P48775
A	391	SER	-	expression tag	UNP P48775
A	392	ASP	-	expression tag	UNP 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

Continued on next page...

Continued from previous page...

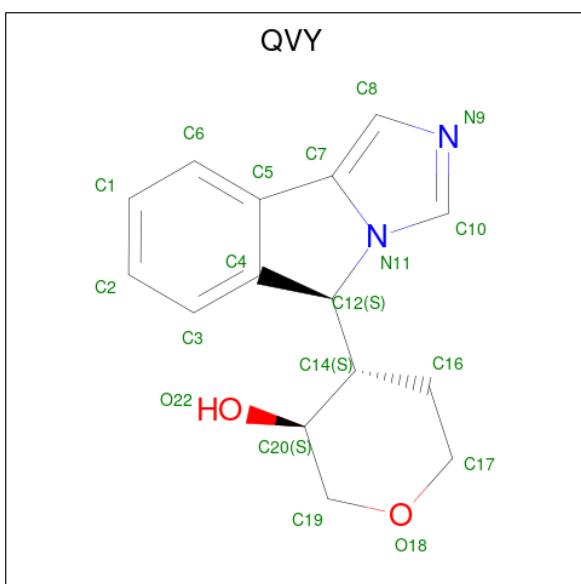
Chain	Residue	Modelled	Actual	Comment	Reference
B	393	TYR	-	expression tag	UNP P48775
B	394	LYS	-	expression tag	UNP P48775
B	395	ASP	-	expression tag	UNP P48775
B	396	ASP	-	expression tag	UNP P48775
B	397	ASP	-	expression tag	UNP P48775
B	398	ASP	-	expression tag	UNP P48775
B	399	LYS	-	expression tag	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 (CCD ID: 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 (CCD ID: QVY) (formula: $C_{15}H_{16}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



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.

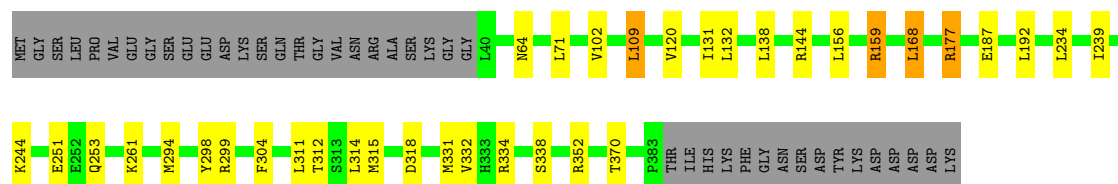
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	O	0	0
			13	13		
4	B	12	Total	O	0	0
			12	12		
4	C	4	Total	O	0	0
			4	4		
4	D	7	Total	O	0	0
			7	7		

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.

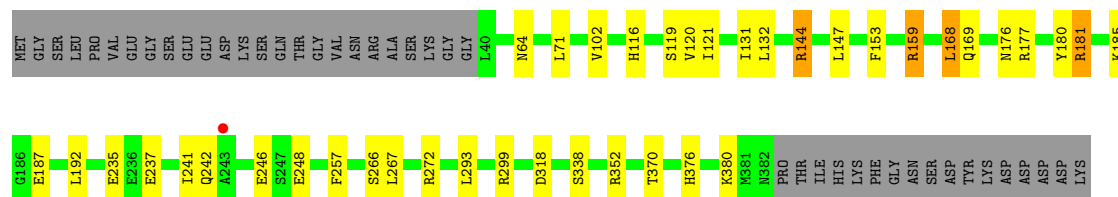
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain A: 



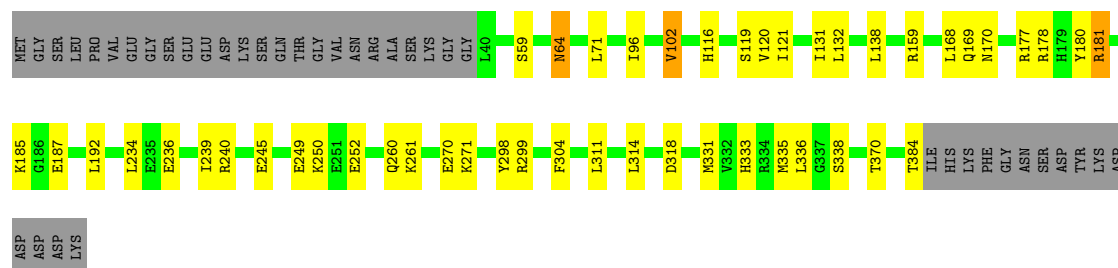
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain B: 



• Molecule 1: Tryptophan 2,3-dioxygenase

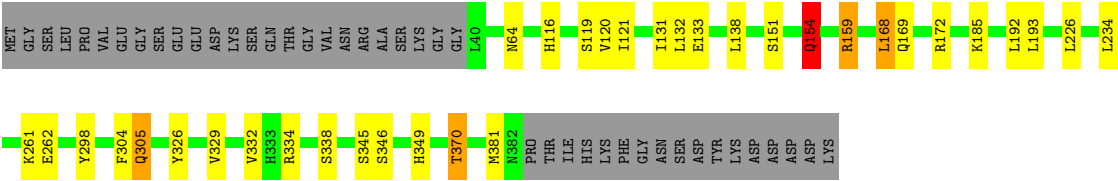
Chain C: 



• Molecule 1: Tryptophan 2,3-dioxygenase

Chain D: 





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 39.37 – 3.18	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.37-3.18) 99.7 (39.37-3.18)	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 0.207 , 0.245	Depositor DCC
R_{free} test set	1383 reflections (4.84%)	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 , 67.9	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	0.95	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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: QVY, HEM

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	0.76	0/2966	1.37	6/3992 (0.2%)
1	B	0.76	0/2958	1.38	9/3980 (0.2%)
1	C	0.74	0/2973	1.37	2/4002 (0.0%)
1	D	0.75	0/2958	1.40	10/3980 (0.3%)
All	All	0.75	0/11855	1.38	27/15954 (0.2%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	305	GLN	CB-CG-CD	-7.65	99.59	112.60
1	D	168	LEU	CA-C-N	7.36	130.46	120.38
1	D	168	LEU	C-N-CA	7.36	130.46	120.38
1	B	248	GLU	CA-C-N	6.54	129.69	120.28
1	B	248	GLU	C-N-CA	6.54	129.69	120.28
1	D	345	SER	CA-C-N	6.52	130.60	120.82
1	D	345	SER	C-N-CA	6.52	130.60	120.82
1	D	154	GLN	N-CA-C	-6.36	104.78	113.30
1	B	235	GLU	CA-C-N	6.23	128.63	120.28
1	B	235	GLU	C-N-CA	6.23	128.63	120.28
1	B	168	LEU	CA-C-N	5.82	128.08	120.28
1	B	168	LEU	C-N-CA	5.82	128.08	120.28
1	A	168	LEU	CA-C-N	5.81	128.07	120.28
1	A	168	LEU	C-N-CA	5.81	128.07	120.28
1	A	239	ILE	CA-C-N	5.42	127.49	120.44
1	A	239	ILE	C-N-CA	5.42	127.49	120.44
1	D	262	GLU	CA-C-N	5.37	127.33	120.56
1	D	262	GLU	C-N-CA	5.37	127.33	120.56
1	B	176	ASN	CA-CB-CG	5.17	117.78	112.60
1	A	144	ARG	CA-C-N	5.10	127.37	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	ARG	C-N-CA	5.10	127.37	120.38
1	D	226	LEU	CA-C-N	5.10	127.37	120.38
1	D	226	LEU	C-N-CA	5.10	127.37	120.38
1	C	270	GLU	CA-C-N	5.07	127.08	120.28
1	C	270	GLU	C-N-CA	5.07	127.08	120.28
1	B	144	ARG	CA-C-N	5.05	127.05	120.28
1	B	144	ARG	C-N-CA	5.05	127.05	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	20	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
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	60	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 (60) 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:331:MET:HE1	1:A:334:ARG:HH21	1.56	0.70
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:109:LEU:HD11	1:D:305:GLN:CD	2.36	0.51
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:D:169:GLN:H	1:D:169:GLN:CD	2.20	0.48
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:A:109:LEU:HD21	1:D:305:GLN:HG2	1.96	0.47
1:D:298:TYR:O	1:D:304:PHE:HB2	2.14	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
1:C:96:ILE:HG22	1:C:102:VAL:HG13	1.97	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:312:THR:HA	1:A:315:MET:HE3	2.00	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 [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	342/385 (89%)	330 (96%)	11 (3%)	1 (0%)	36	66
1	B	341/385 (89%)	327 (96%)	13 (4%)	1 (0%)	36	66
1	C	343/385 (89%)	328 (96%)	13 (4%)	2 (1%)	21	53
1	D	341/385 (89%)	327 (96%)	13 (4%)	1 (0%)	36	66
All	All	1367/1540 (89%)	1312 (96%)	50 (4%)	5 (0%)	30	60

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%)	305 (96%)	12 (4%)	29	59
1	B	316/351 (90%)	299 (95%)	17 (5%)	20	50
1	C	318/351 (91%)	298 (94%)	20 (6%)	16	45
1	D	316/351 (90%)	308 (98%)	8 (2%)	42	66
All	All	1267/1404 (90%)	1210 (96%)	57 (4%)	24	55

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	VAL
1	A	109	LEU
1	A	132	LEU
1	A	159	ARG
1	A	168	LEU
1	A	177	ARG
1	A	187	GLU
1	A	251	GLU
1	A	294	MET
1	A	318	ASP
1	A	352	ARG
1	A	370	THR
1	B	102	VAL
1	B	132	LEU
1	B	159	ARG
1	B	168	LEU
1	B	169	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	177	ARG
1	B	180	TYR
1	B	181	ARG
1	B	185	LYS
1	B	187	GLU
1	B	241	ILE
1	B	242	GLN
1	B	246	GLU
1	B	318	ASP
1	B	352	ARG
1	B	376	HIS
1	B	380	LYS
1	C	102	VAL
1	C	132	LEU
1	C	168	LEU
1	C	169	GLN
1	C	170	ASN
1	C	177	ARG
1	C	178	ARG
1	C	181	ARG
1	C	185	LYS
1	C	187	GLU
1	C	239	ILE
1	C	249	GLU
1	C	250	LYS
1	C	252	GLU
1	C	260	GLN
1	C	271	LYS
1	C	318	ASP
1	C	331	MET
1	C	335	MET
1	C	384	THR
1	D	132	LEU
1	D	154	GLN
1	D	159	ARG
1	D	168	LEU
1	D	185	LYS
1	D	193	LEU
1	D	370	THR
1	D	381	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	55	GLN
1	A	116	HIS
1	A	128	GLN
1	A	229	ASN
1	A	242	GLN
1	A	253	GLN
1	A	260	GLN
1	A	382	ASN
1	B	44	ASN
1	B	116	HIS
1	B	128	GLN
1	B	163	ASN
1	B	176	ASN
1	B	253	GLN
1	C	44	ASN
1	C	116	HIS
1	C	163	ASN
1	C	169	GLN
1	C	179	HIS
1	C	229	ASN
1	C	309	GLN
1	C	333	HIS
1	C	349	HIS
1	D	44	ASN
1	D	116	HIS
1	D	128	GLN
1	D	170	ASN
1	D	176	ASN
1	D	183	ASN
1	D	229	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	C	402	2	21,22,22	0.29	0	22,32,32	1.76	4 (18%)
2	HEM	C	401	3,1	50,50,50	1.22	7 (14%)	67,82,82	1.28	7 (10%)
2	HEM	D	401	3,1	50,50,50	1.16	7 (14%)	67,82,82	1.24	6 (8%)
2	HEM	A	401	3,1	50,50,50	1.14	6 (12%)	67,82,82	1.33	6 (8%)
3	QVY	C	403	2	21,22,22	0.37	0	22,32,32	1.76	4 (18%)
3	QVY	B	402	2	21,22,22	0.32	0	22,32,32	1.86	3 (13%)
2	HEM	B	401	3,1	50,50,50	1.12	6 (12%)	67,82,82	1.29	5 (7%)
3	QVY	A	402	2	21,22,22	0.30	0	22,32,32	1.81	3 (13%)

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	C	402	2	-	0/4/27/27	0/4/4/4
2	HEM	C	401	3,1	-	7/14/54/54	-
2	HEM	D	401	3,1	-	7/14/54/54	-
2	HEM	A	401	3,1	-	8/14/54/54	-
3	QVY	C	403	2	-	0/4/27/27	0/4/4/4
3	QVY	B	402	2	-	0/4/27/27	0/4/4/4
2	HEM	B	401	3,1	-	8/14/54/54	-
3	QVY	A	402	2	-	0/4/27/27	0/4/4/4

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	HEM	C4D-ND	-2.92	1.35	1.40
2	C	401	HEM	C4D-C3D	2.83	1.49	1.45
2	B	401	HEM	C1B-NB	-2.78	1.35	1.40
2	A	401	HEM	C4D-ND	-2.75	1.35	1.40
2	D	401	HEM	C4D-ND	-2.65	1.35	1.40
2	A	401	HEM	C3B-C4B	2.55	1.49	1.44
2	A	401	HEM	C4D-C3D	2.54	1.49	1.45
2	B	401	HEM	C4D-C3D	2.53	1.49	1.45
2	D	401	HEM	C1B-NB	-2.52	1.35	1.40
2	B	401	HEM	C3B-C4B	2.52	1.49	1.44
2	D	401	HEM	C4D-C3D	2.48	1.49	1.45
2	B	401	HEM	C1D-ND	-2.45	1.34	1.38
2	A	401	HEM	C1D-ND	-2.44	1.34	1.38
2	B	401	HEM	C4D-ND	-2.42	1.36	1.40
2	D	401	HEM	C1D-ND	-2.33	1.34	1.38
2	D	401	HEM	C3B-C4B	2.32	1.49	1.44
2	D	401	HEM	C1A-C2A	-2.31	1.40	1.44
2	C	401	HEM	C3B-C4B	2.27	1.49	1.44
2	D	401	HEM	C1C-C2C	-2.20	1.41	1.45
2	C	401	HEM	C1D-ND	-2.19	1.34	1.38
2	C	401	HEM	C1D-C2D	2.16	1.48	1.44
2	C	401	HEM	C1B-NB	-2.12	1.36	1.40
2	A	401	HEM	C1B-NB	-2.11	1.36	1.40
2	C	401	HEM	C1A-C2A	-2.06	1.40	1.44
2	B	401	HEM	C1D-C2D	2.06	1.48	1.44
2	A	401	HEM	C1D-C2D	2.02	1.48	1.44

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	QVY	C5-C7-N11	-6.25	105.28	107.44
3	C	403	QVY	C5-C7-N11	-5.97	105.38	107.44
3	C	402	QVY	C5-C7-N11	-5.93	105.40	107.44
3	A	402	QVY	C5-C7-N11	-5.73	105.46	107.44
3	A	402	QVY	C5-C7-C8	4.48	149.03	146.18
3	C	403	QVY	C5-C7-C8	4.46	149.01	146.18
3	B	402	QVY	C5-C7-C8	4.37	148.96	146.18
3	C	402	QVY	C5-C7-C8	4.37	148.95	146.18
2	B	401	HEM	C2B-C1B-NB	3.90	114.33	109.84
2	A	401	HEM	C2B-C1B-NB	3.85	114.27	109.84
2	C	401	HEM	C2B-C1B-NB	3.80	114.21	109.84
2	B	401	HEM	CBD-CAD-C3D	-3.65	102.45	112.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	HEM	C2B-C1B-NB	3.55	113.92	109.84
2	A	401	HEM	CBD-CAD-C3D	-3.46	102.98	112.53
2	C	401	HEM	CBD-CAD-C3D	-3.43	103.06	112.53
3	A	402	QVY	C4-C5-C7	3.39	109.76	107.78
2	D	401	HEM	CBD-CAD-C3D	-3.38	103.19	112.53
3	B	402	QVY	C4-C5-C7	3.11	109.59	107.78
2	A	401	HEM	O2A-CGA-CBA	3.10	123.81	114.00
2	C	401	HEM	O2A-CGA-CBA	3.09	123.75	114.00
2	B	401	HEM	O2A-CGA-CBA	2.66	122.39	114.00
2	D	401	HEM	O2A-CGA-CBA	2.44	121.71	114.00
2	C	401	HEM	C3B-C4B-NB	2.44	111.22	109.47
3	C	402	QVY	C4-C5-C7	2.38	109.17	107.78
2	D	401	HEM	C4B-C3B-C2B	-2.37	105.11	107.28
2	D	401	HEM	C3B-C4B-NB	2.31	111.13	109.47
2	A	401	HEM	CHB-C1B-C2B	-2.28	120.48	126.95
2	A	401	HEM	C3B-C4B-NB	2.20	111.05	109.47
2	A	401	HEM	CHD-C1D-C2D	-2.16	121.62	125.03
2	C	401	HEM	CHB-C1B-C2B	-2.14	120.86	126.95
3	C	403	QVY	C4-C5-C7	2.11	109.01	107.78
2	B	401	HEM	CHB-C1B-C2B	-2.10	120.98	126.95
2	D	401	HEM	CHB-C1B-C2B	-2.08	121.03	126.95
2	B	401	HEM	CHD-C1D-C2D	-2.07	121.76	125.03
3	C	402	QVY	N11-C10-N9	2.05	113.62	111.68
2	C	401	HEM	C4B-C3B-C2B	-2.04	105.41	107.28
3	C	403	QVY	N11-C10-N9	2.02	113.60	111.68
2	C	401	HEM	CHD-C1D-C2D	-2.02	121.84	125.03

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	HEM	C2C-C3C-CAC-CBC
2	B	401	HEM	C2C-C3C-CAC-CBC
2	C	401	HEM	C2C-C3C-CAC-CBC
2	D	401	HEM	C2C-C3C-CAC-CBC
2	A	401	HEM	C2B-C3B-CAB-CBB
2	D	401	HEM	C2B-C3B-CAB-CBB
2	A	401	HEM	C4C-C3C-CAC-CBC
2	B	401	HEM	C4C-C3C-CAC-CBC
2	C	401	HEM	C4C-C3C-CAC-CBC
2	D	401	HEM	C4C-C3C-CAC-CBC
2	B	401	HEM	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

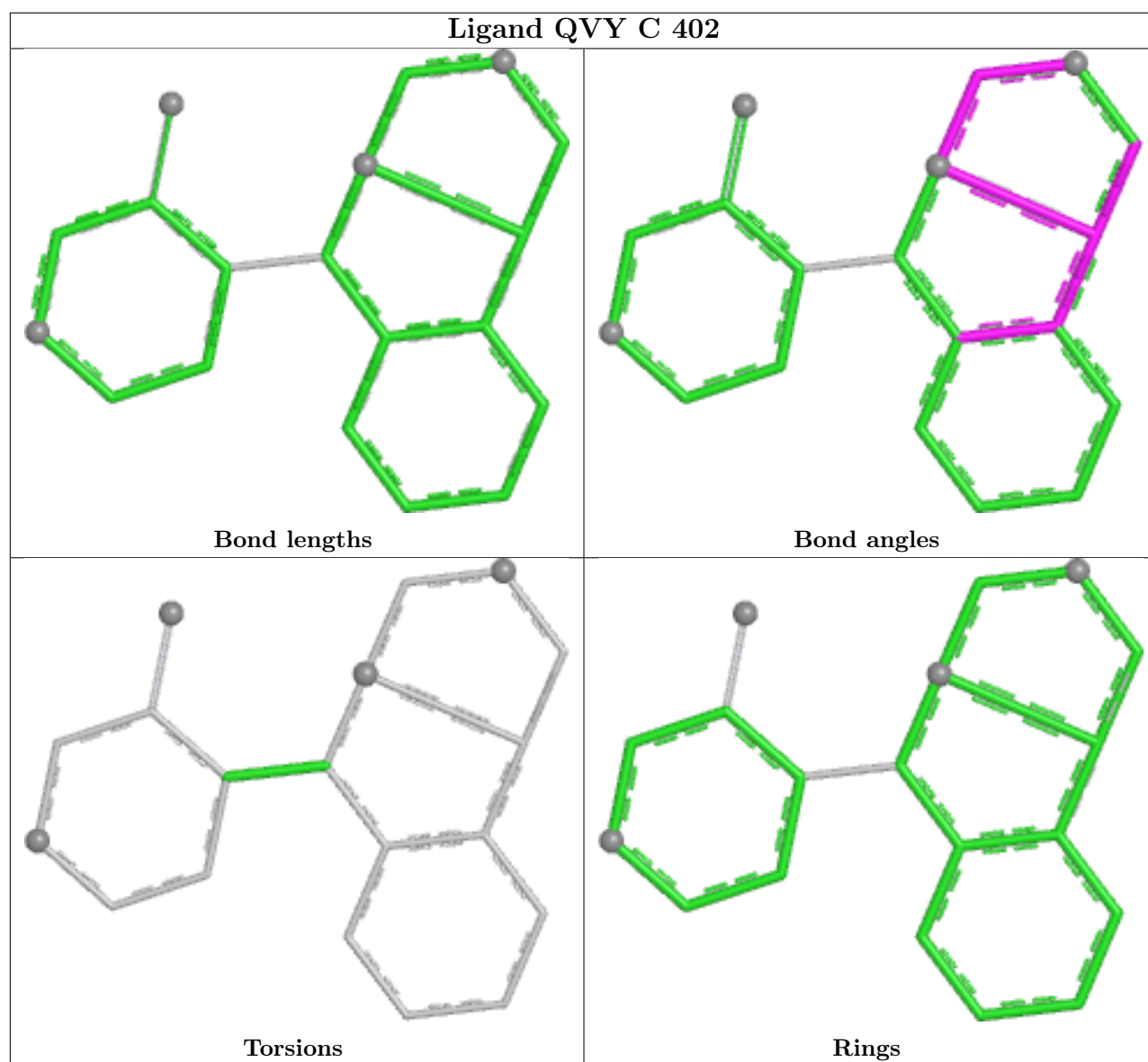
Mol	Chain	Res	Type	Atoms
2	C	401	HEM	C4B-C3B-CAB-CBB
2	D	401	HEM	CAA-CBA-CGA-O2A
2	B	401	HEM	CAA-CBA-CGA-O1A
2	A	401	HEM	CAA-CBA-CGA-O1A
2	C	401	HEM	CAA-CBA-CGA-O1A
2	B	401	HEM	CAA-CBA-CGA-O2A
2	A	401	HEM	CAA-CBA-CGA-O2A
2	C	401	HEM	CAA-CBA-CGA-O2A
2	D	401	HEM	CAA-CBA-CGA-O1A
2	B	401	HEM	C2B-C3B-CAB-CBB
2	C	401	HEM	C2B-C3B-CAB-CBB
2	A	401	HEM	C4B-C3B-CAB-CBB
2	D	401	HEM	C4B-C3B-CAB-CBB
2	C	401	HEM	CAD-CBD-CGD-O2D
2	D	401	HEM	CAD-CBD-CGD-O2D
2	B	401	HEM	CAD-CBD-CGD-O2D
2	A	401	HEM	CAD-CBD-CGD-O2D
2	A	401	HEM	CAD-CBD-CGD-O1D
2	B	401	HEM	CAD-CBD-CGD-O1D

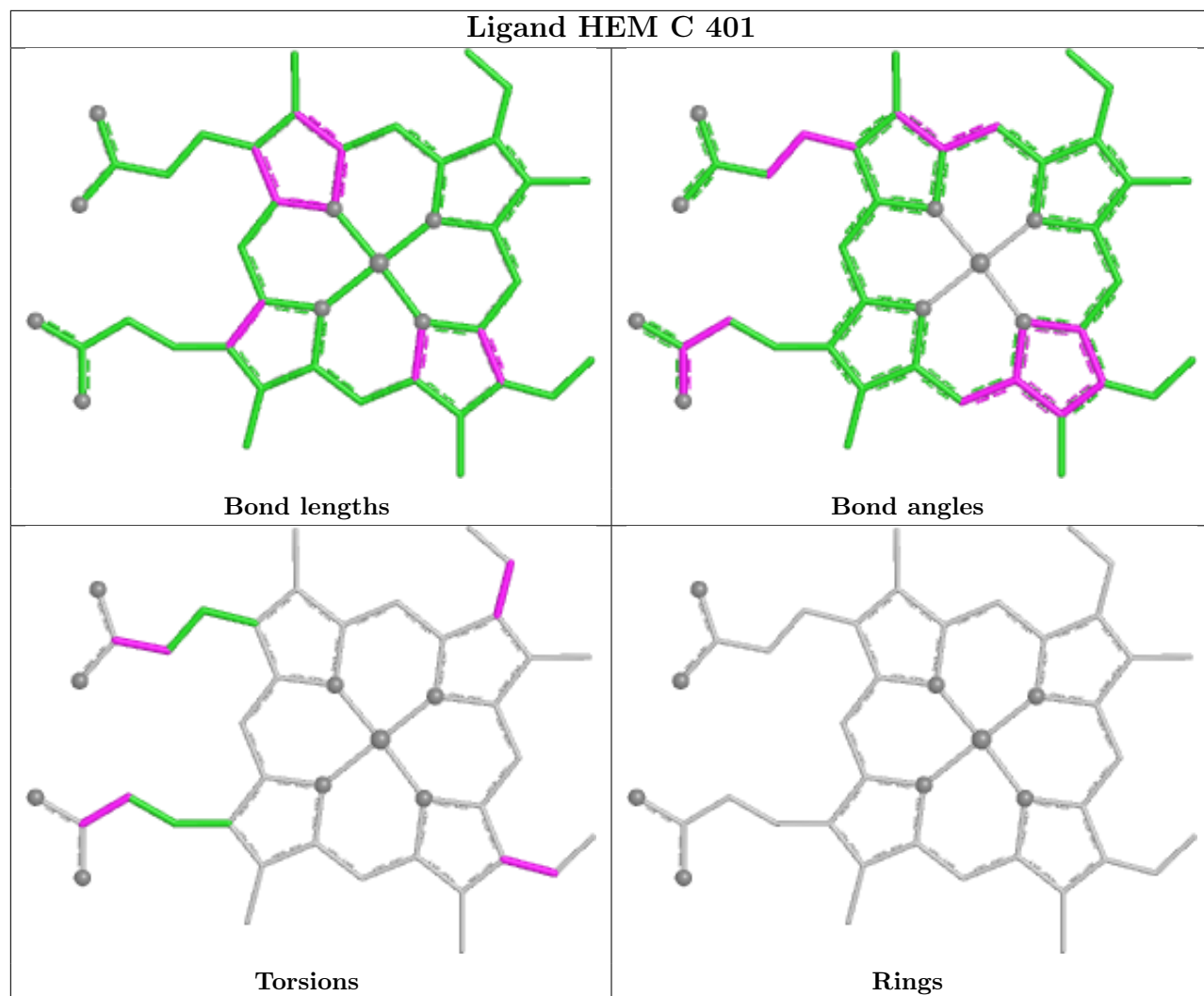
There are no ring outliers.

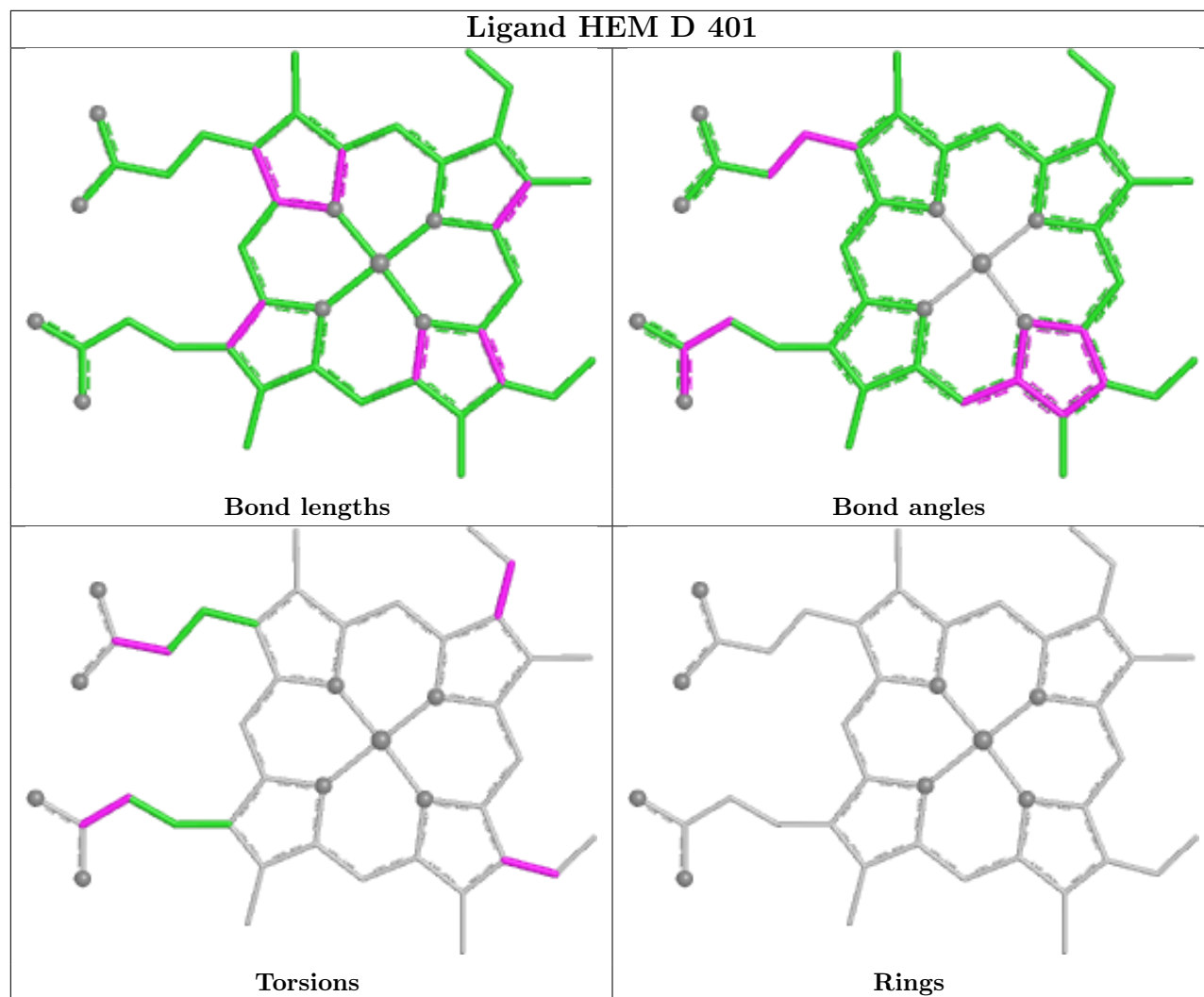
3 monomers are involved in 4 short contacts:

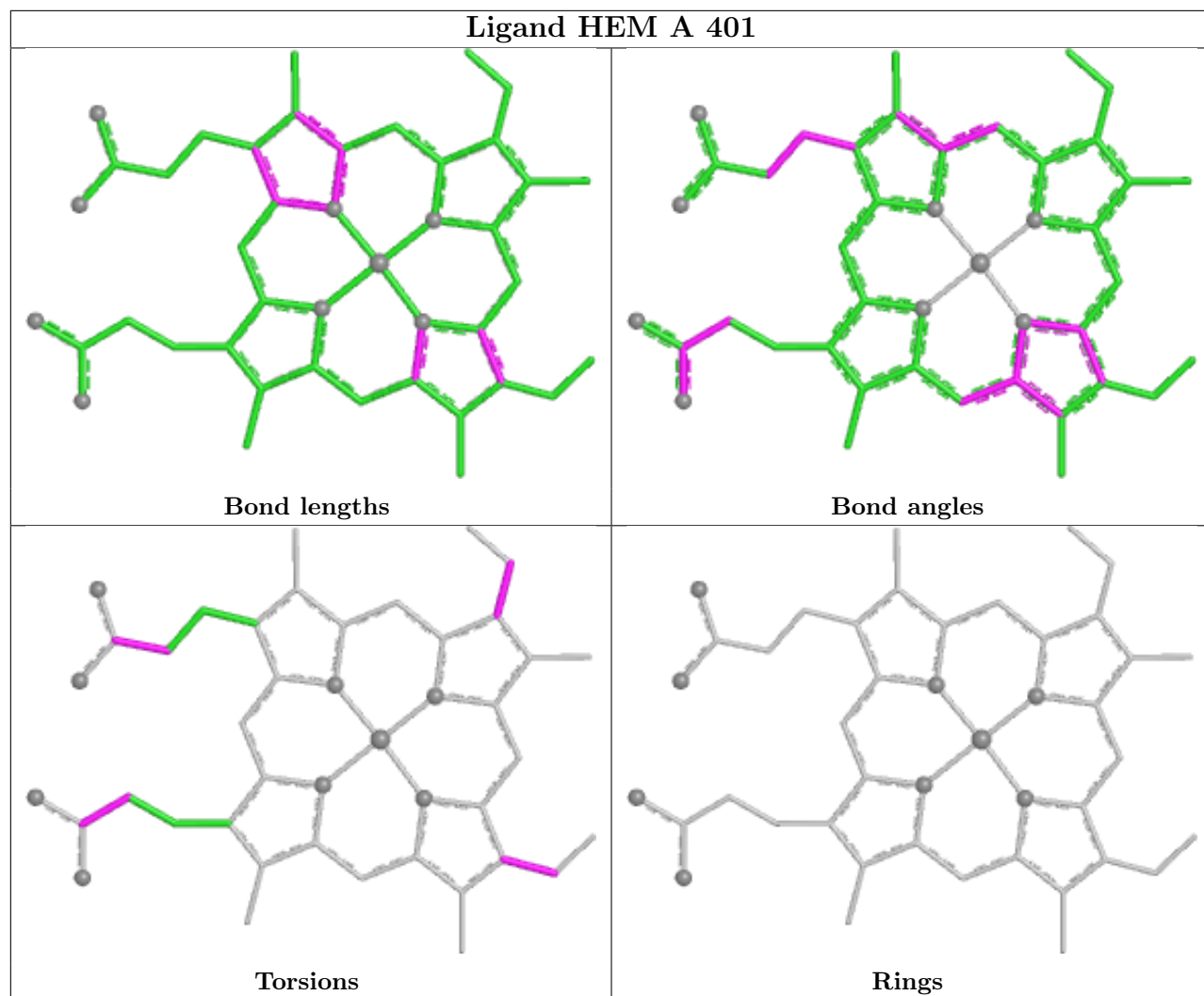
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	HEM	1	0
2	A	401	HEM	2	0
2	B	401	HEM	1	0

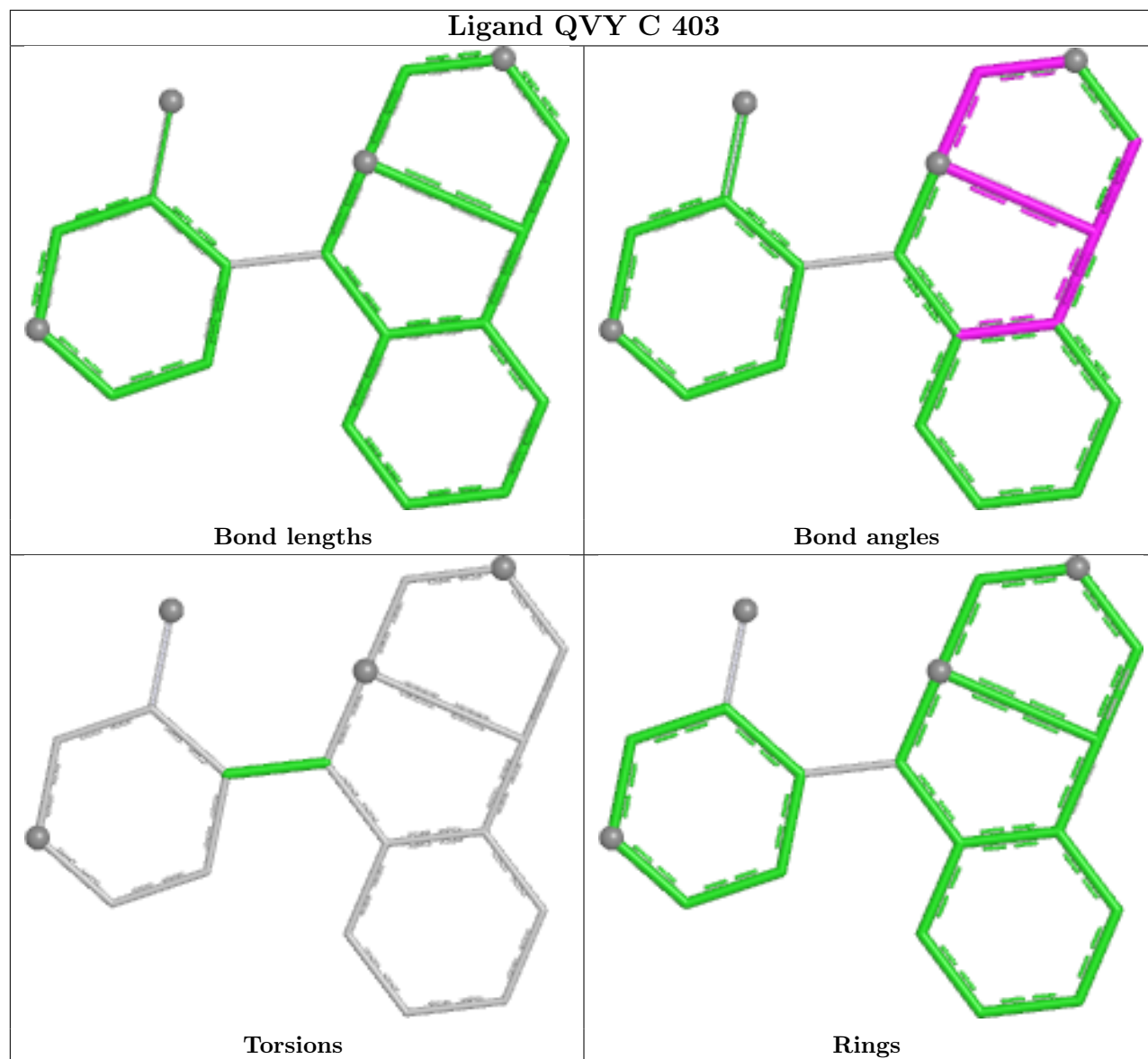
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

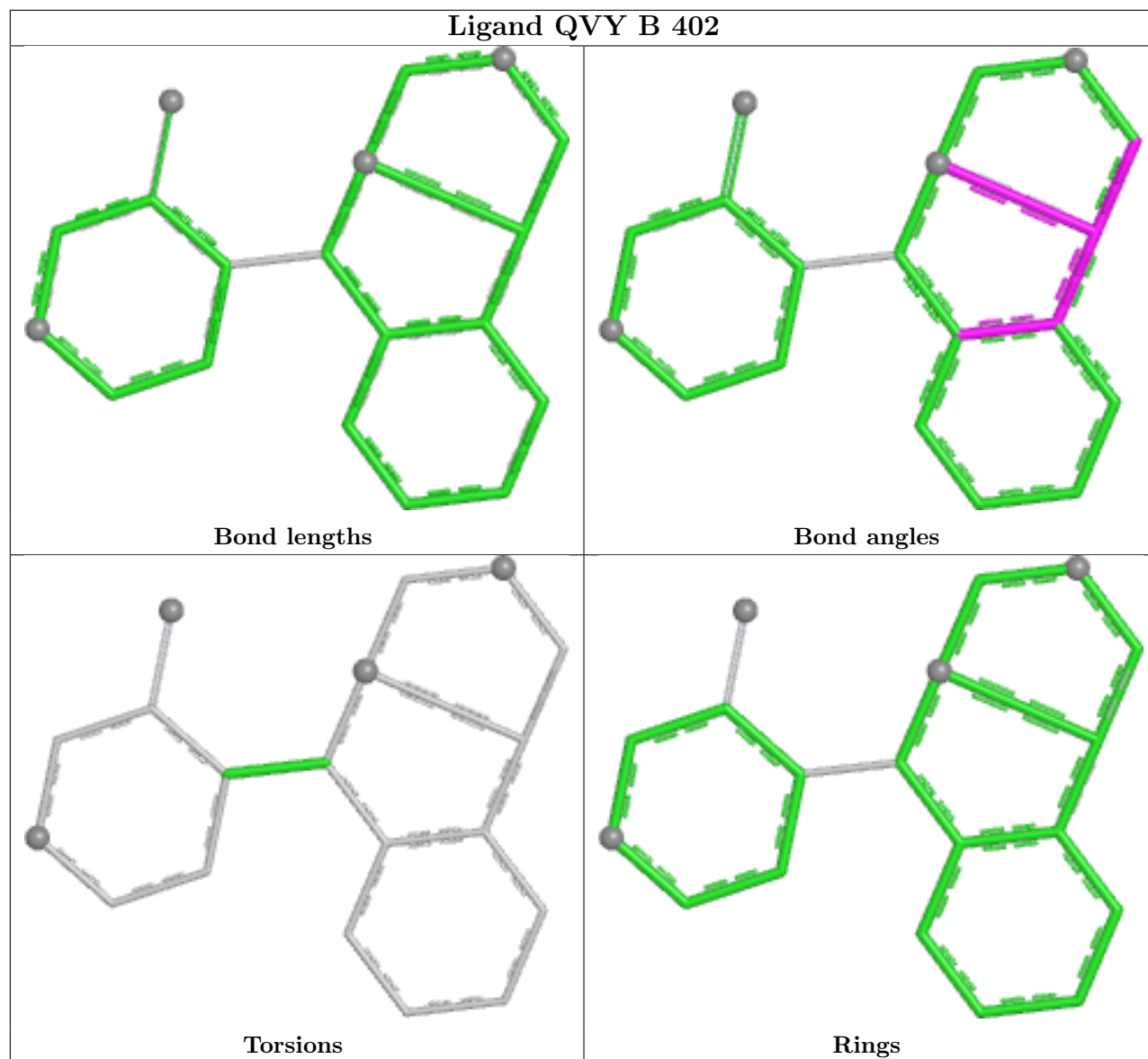


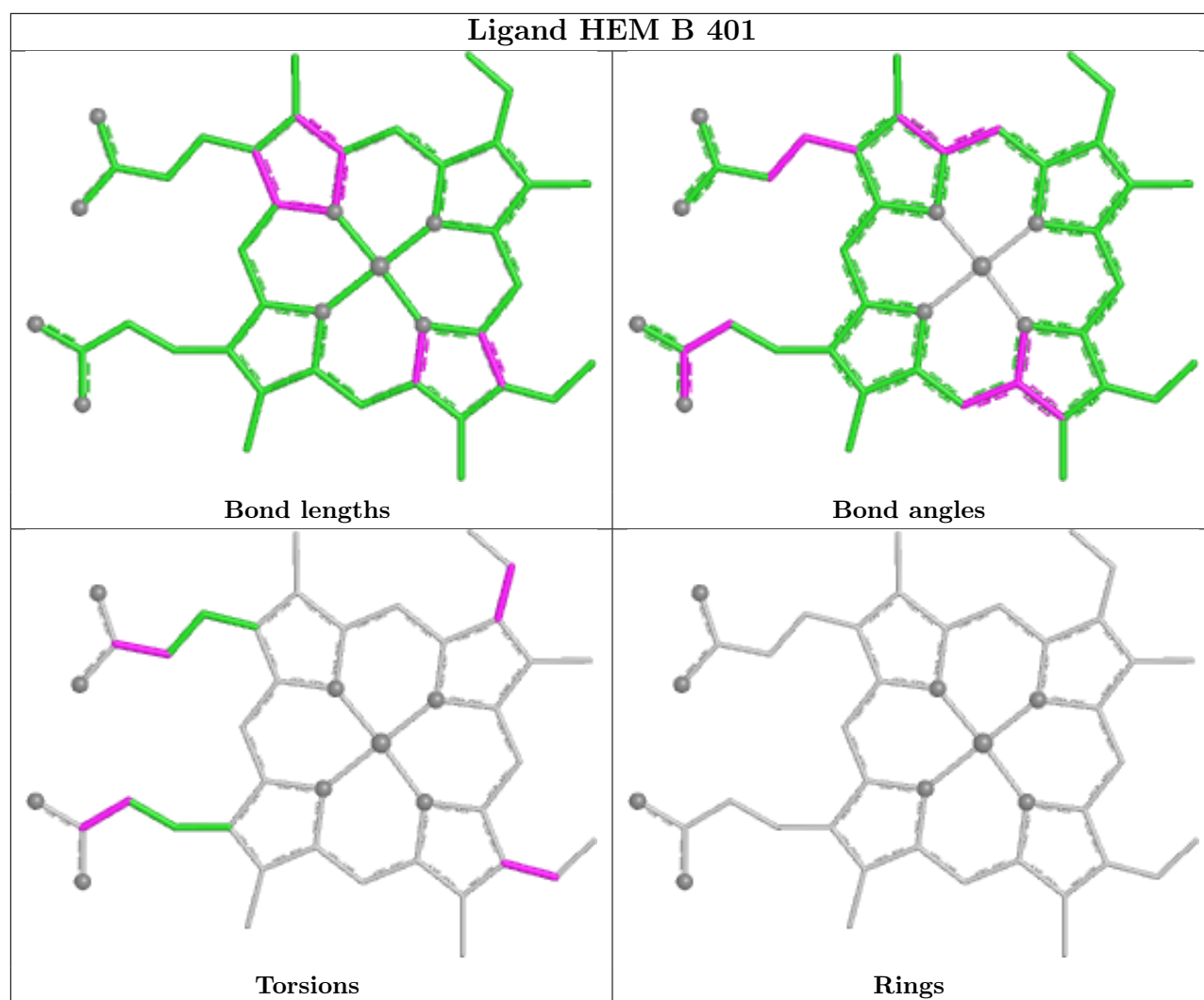


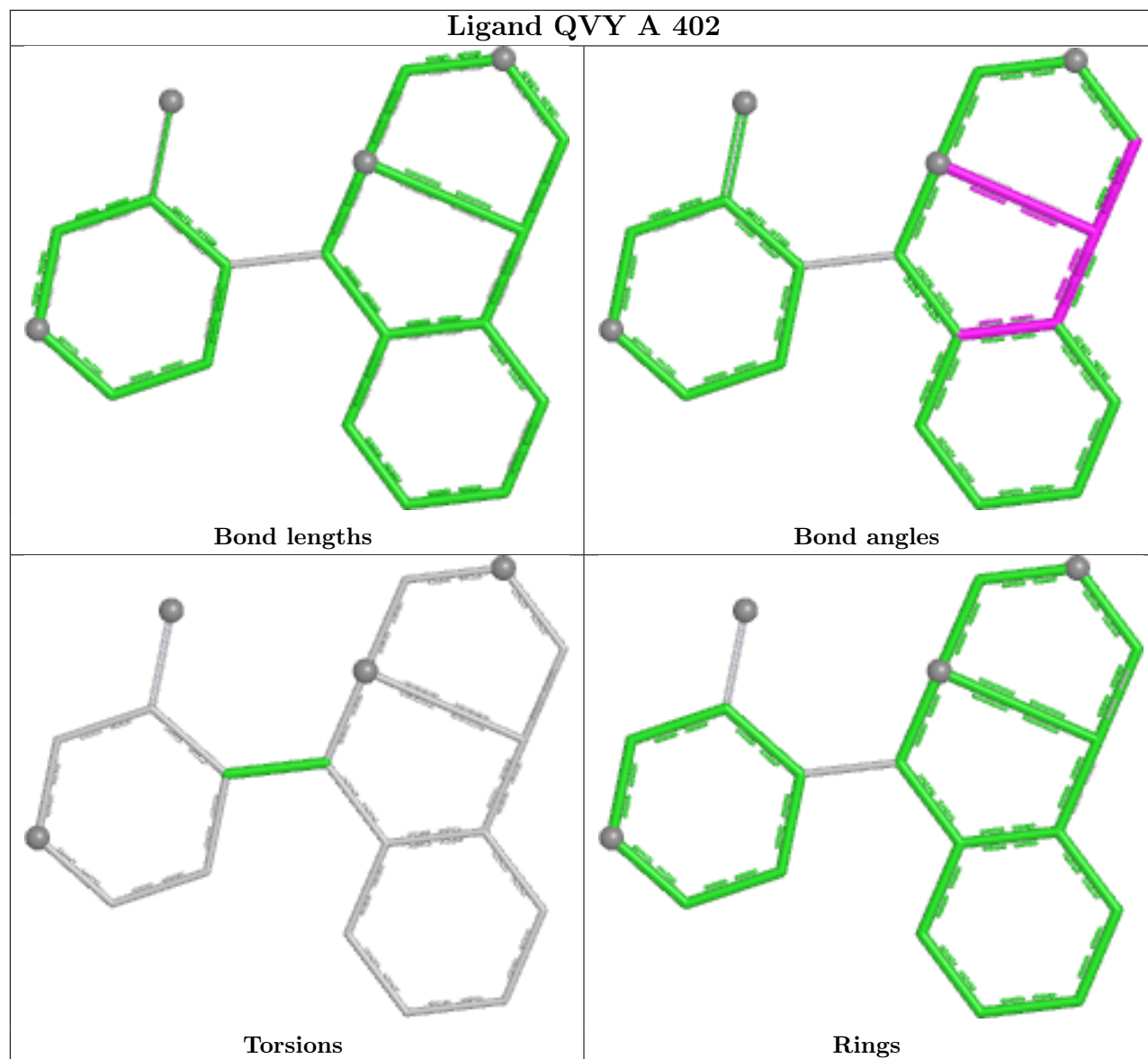












5.7 Other polymers [i](#)

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	344/385 (89%)	-0.50	0 100 100	58, 94, 146, 167	0
1	B	343/385 (89%)	-0.40	1 (0%) 90 81	61, 113, 167, 200	0
1	C	345/385 (89%)	-0.33	0 100 100	68, 125, 173, 193	0
1	D	343/385 (89%)	-0.45	0 100 100	58, 98, 159, 178	0
All	All	1375/1540 (89%)	-0.42	1 (0%) 92 88	58, 107, 163, 200	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	243	ALA	2.5

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 oligosaccharides 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.

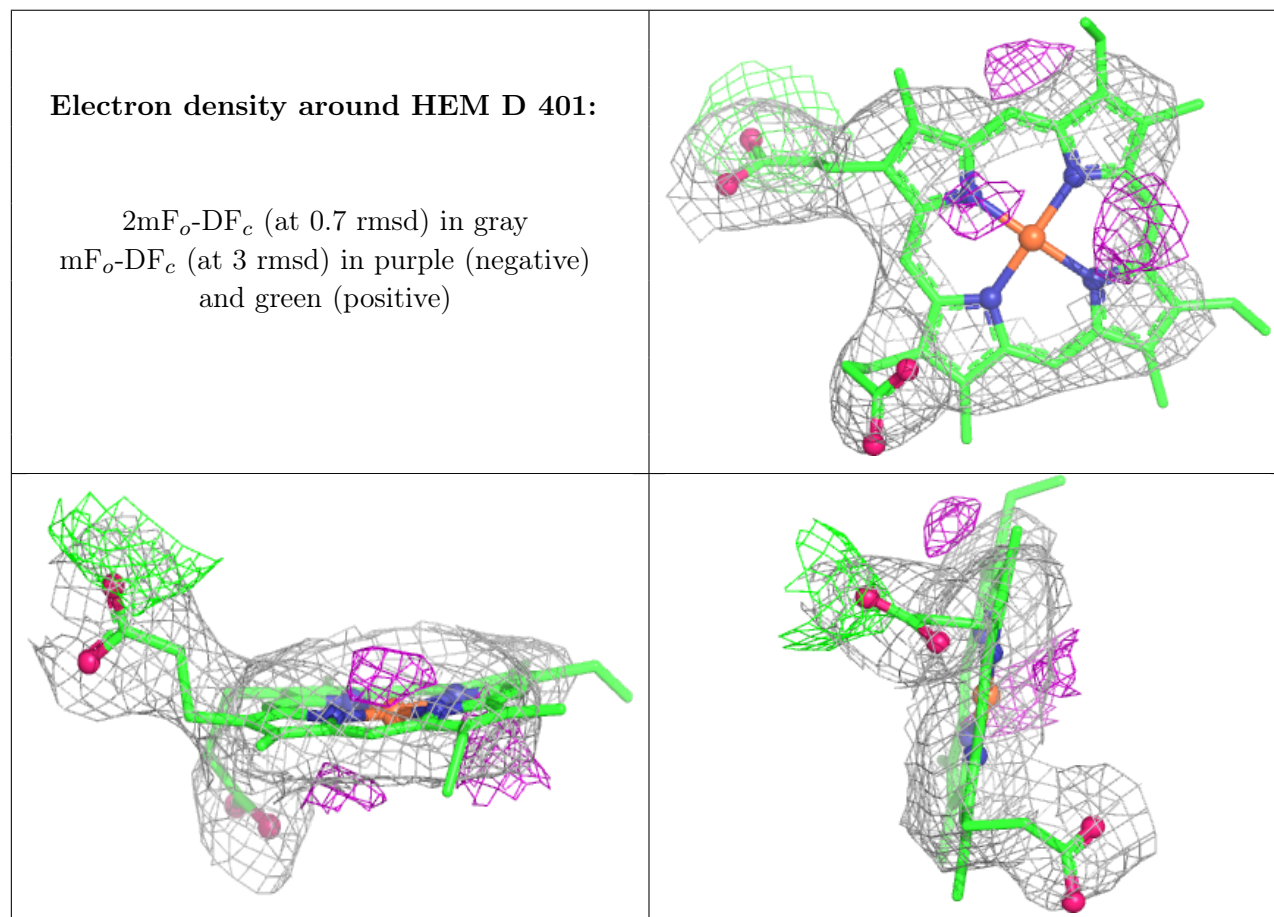
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HEM	D	401	43/43	0.91	0.12	123,124,128,129	0

Continued on next page...

Continued from previous page...

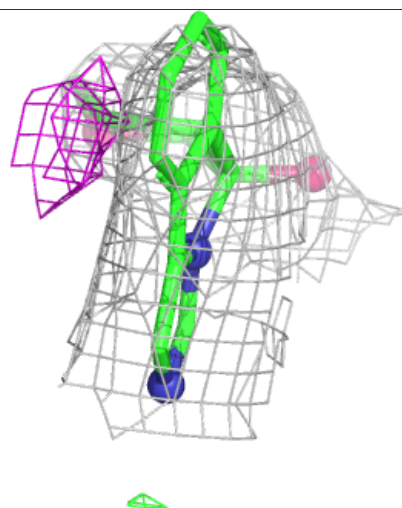
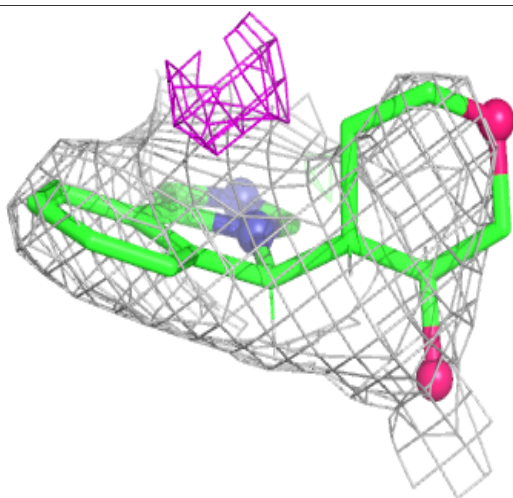
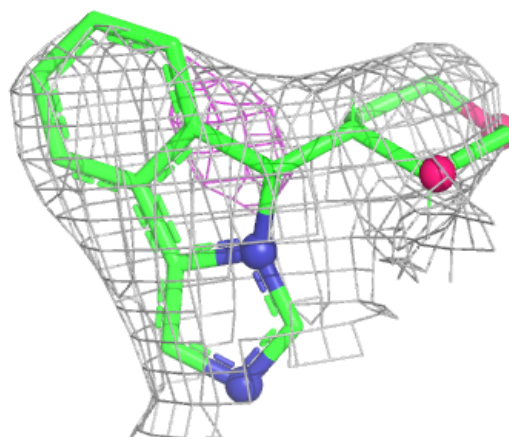
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	QVY	C	403	19/19	0.95	0.07	85,92,107,108	0
3	QVY	A	402	19/19	0.96	0.07	90,95,98,98	0
3	QVY	B	402	19/19	0.96	0.06	83,87,92,94	0
3	QVY	C	402	19/19	0.96	0.06	112,116,118,119	0
2	HEM	C	401	43/43	0.96	0.09	115,116,120,121	0
2	HEM	B	401	43/43	0.97	0.07	109,110,114,115	0
2	HEM	A	401	43/43	0.98	0.07	97,99,103,104	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.



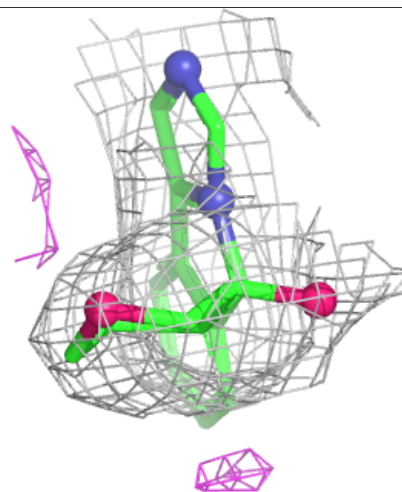
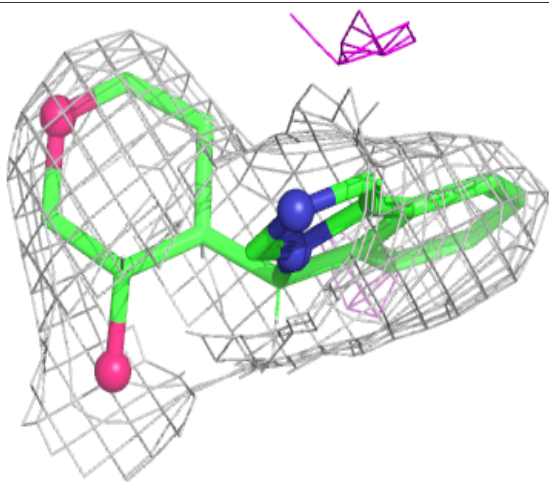
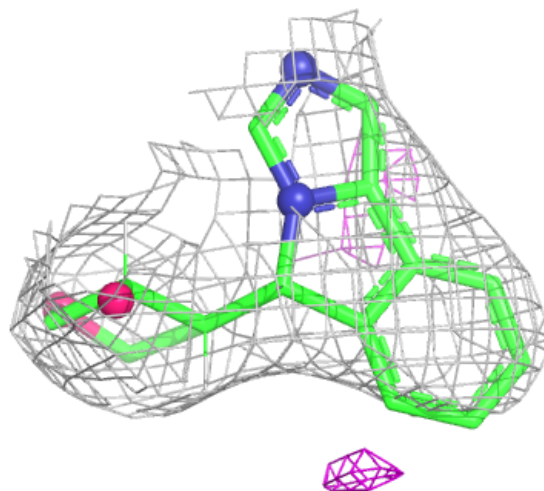
Electron density around QVY C 403:

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



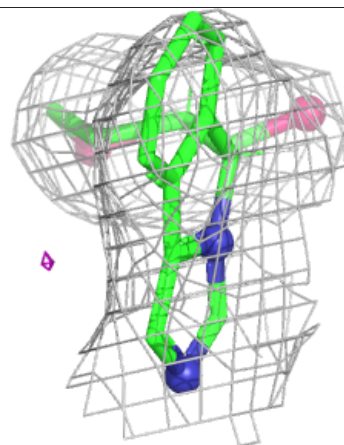
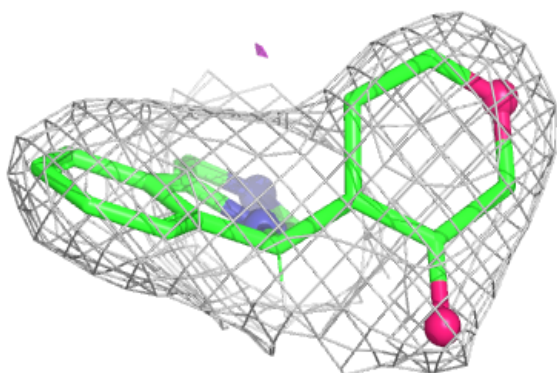
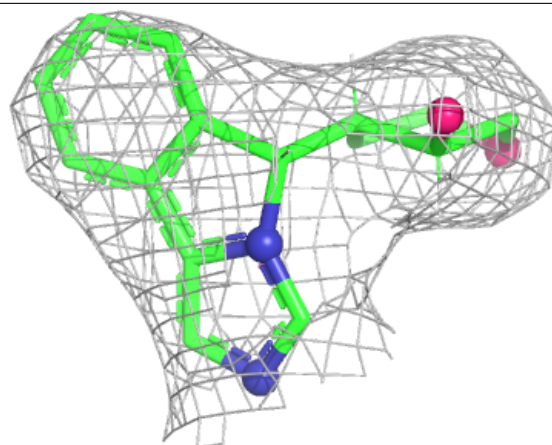
Electron density around QVY A 402:

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



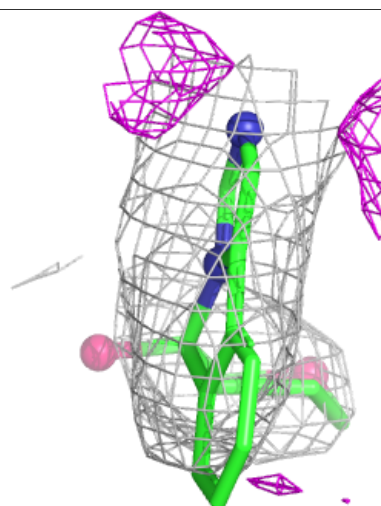
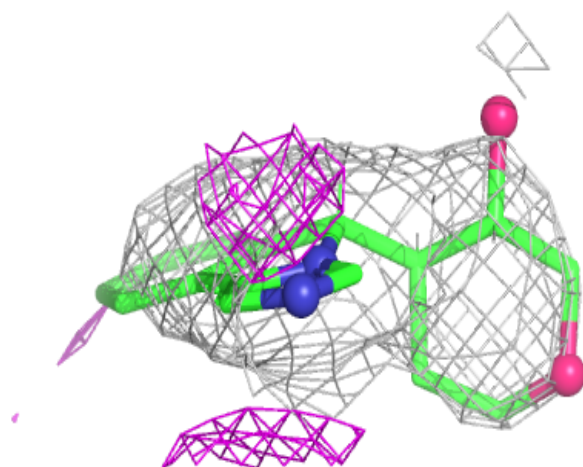
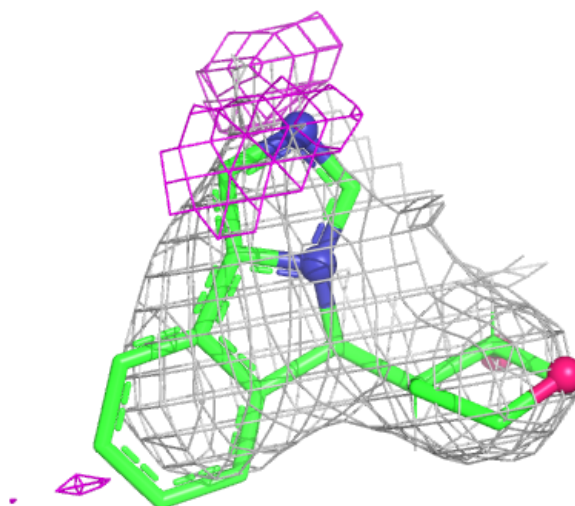
Electron density around QVY B 402:

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



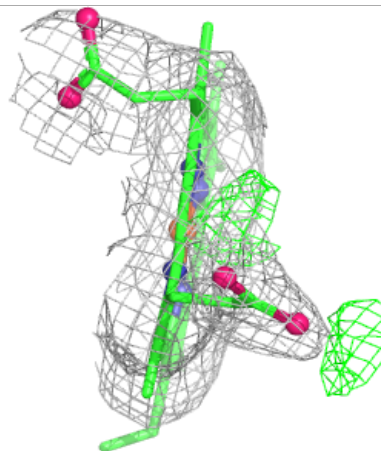
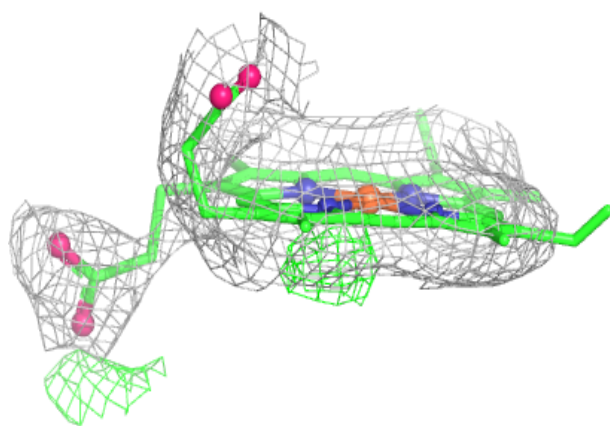
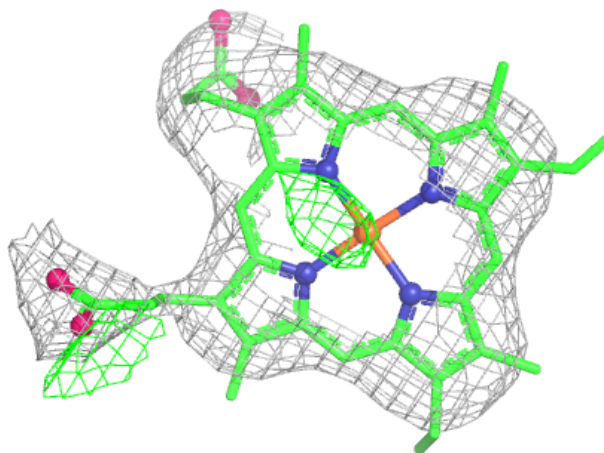
Electron density around QVY C 402:

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



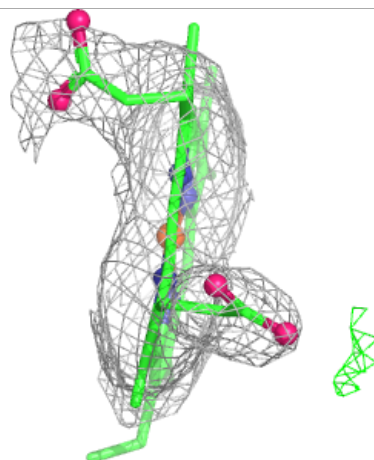
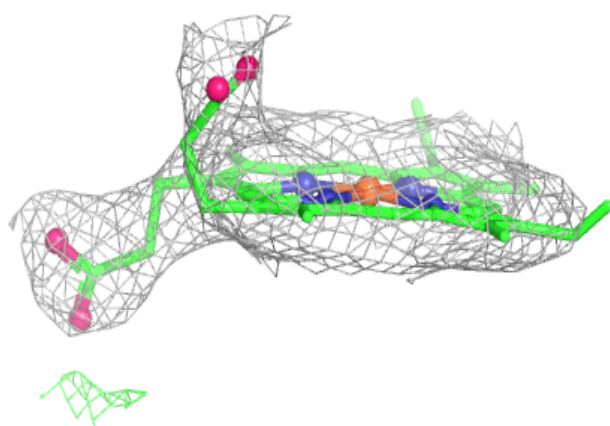
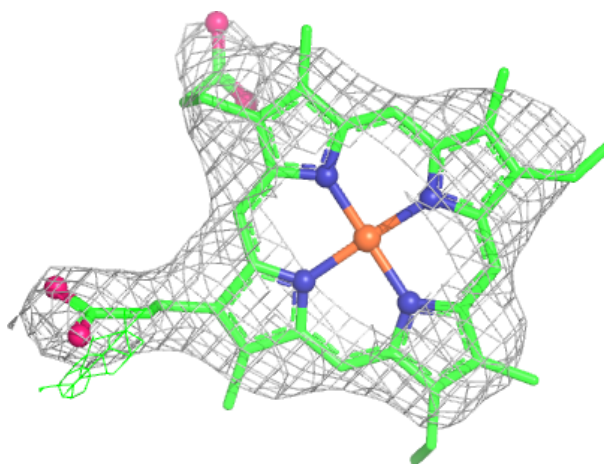
Electron density around HEM C 401:

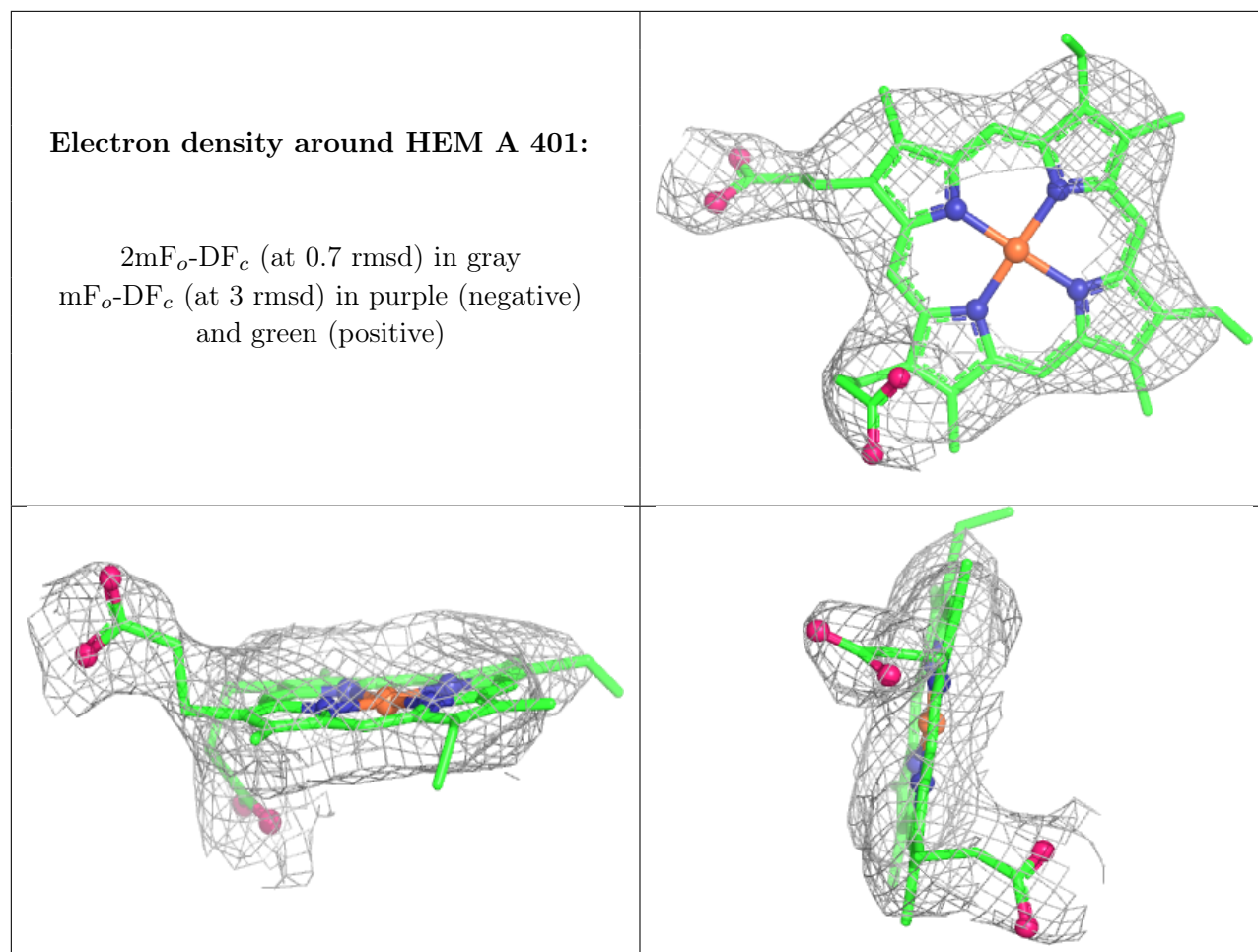
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.