



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 12, 2024 – 09:46 PM EDT

PDB ID : 8VUG
Title : Crystal Structure of human Tryptophan 2,3-dioxygenase in complex with PPN1 inhibitor
Authors : Geeraerts, Z.; Yeh, S.
Deposited on : 2024-01-29
Resolution : 2.05 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)
Xtrriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

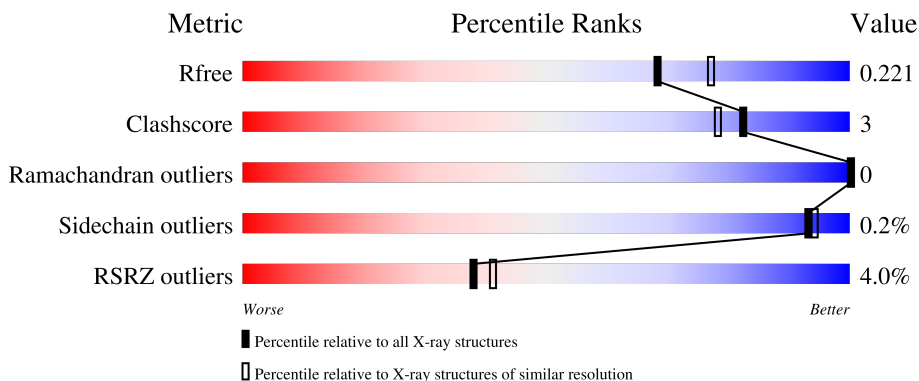
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	380	 2% 88% 5% 7%
1	B	380	 4% 86% 7% 7%
1	C	380	 7% 82% 8% 9%
1	D	380	 2% 82% 7% 10%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12216 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 Tryptophan 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	352	2971	1906	522	532	11	0	0	0
1	B	353	2975	1908	523	533	11	0	0	0
1	C	345	2919	1877	513	518	11	0	0	0
1	D	341	2890	1859	507	513	11	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

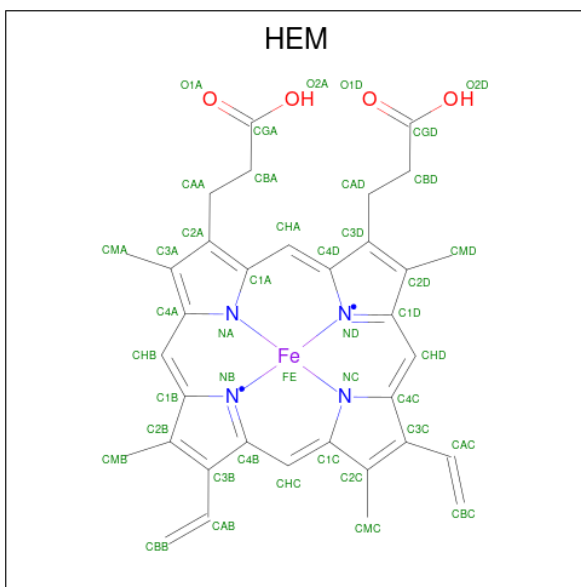
Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MET	-	initiating methionine	UNP P48775
A	390	GLU	-	expression tag	UNP P48775
A	391	HIS	-	expression tag	UNP P48775
A	392	HIS	-	expression tag	UNP P48775
A	393	HIS	-	expression tag	UNP P48775
A	394	HIS	-	expression tag	UNP P48775
A	395	HIS	-	expression tag	UNP P48775
A	396	HIS	-	expression tag	UNP P48775
B	17	MET	-	initiating methionine	UNP P48775
B	390	GLU	-	expression tag	UNP P48775
B	391	HIS	-	expression tag	UNP P48775
B	392	HIS	-	expression tag	UNP P48775
B	393	HIS	-	expression tag	UNP P48775
B	394	HIS	-	expression tag	UNP P48775
B	395	HIS	-	expression tag	UNP P48775
B	396	HIS	-	expression tag	UNP P48775
C	17	MET	-	initiating methionine	UNP P48775
C	390	GLU	-	expression tag	UNP P48775
C	391	HIS	-	expression tag	UNP P48775
C	392	HIS	-	expression tag	UNP P48775
C	393	HIS	-	expression tag	UNP P48775

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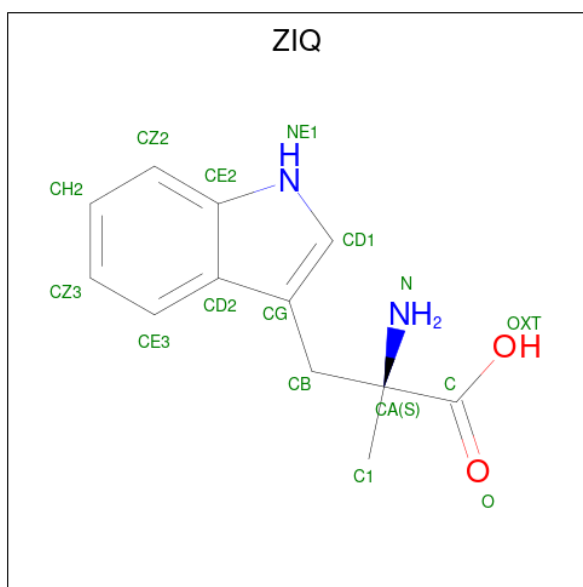
Chain	Residue	Modelled	Actual	Comment	Reference
C	394	HIS	-	expression tag	UNP P48775
C	395	HIS	-	expression tag	UNP P48775
C	396	HIS	-	expression tag	UNP P48775
D	17	MET	-	initiating methionine	UNP P48775
D	390	GLU	-	expression tag	UNP P48775
D	391	HIS	-	expression tag	UNP P48775
D	392	HIS	-	expression tag	UNP P48775
D	393	HIS	-	expression tag	UNP P48775
D	394	HIS	-	expression tag	UNP P48775
D	395	HIS	-	expression tag	UNP P48775
D	396	HIS	-	expression tag	UNP P48775

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



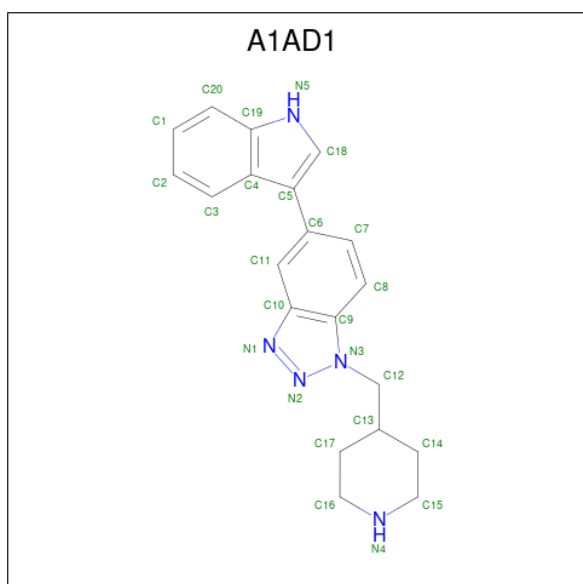
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is alpha-methyl-L-tryptophan (three-letter code: ZIQ) (formula: $C_{12}H_{14}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			
3	A	1	Total	16	12	2	2	0	0
3	B	1	Total	16	12	2	2	0	0
3	C	1	Total	16	12	2	2	0	0
3	D	1	Total	16	12	2	2	0	0

- Molecule 4 is (5P)-5-(1H-indol-3-yl)-1-[(piperidin-4-yl)methyl]-1H-benzotriazole (three-letter code: A1AD1) (formula: C₂₀H₂₁N₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			25	20	5		
4	B	1	Total	C	N	0	0
			25	20	5		
4	C	1	Total	C	N	0	0
			25	20	5		
4	D	1	Total	C	N	0	0
			25	20	5		

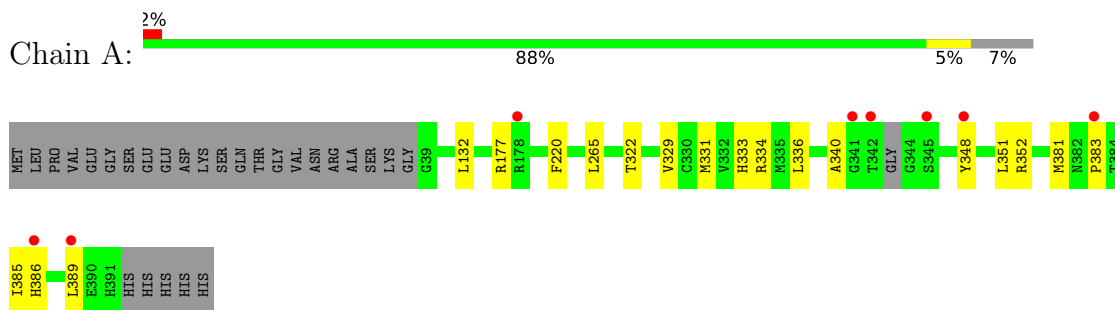
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	44	Total	O	0	0
			44	44		
5	B	33	Total	O	0	0
			33	33		
5	C	20	Total	O	0	0
			20	20		
5	D	28	Total	O	0	0
			28	28		

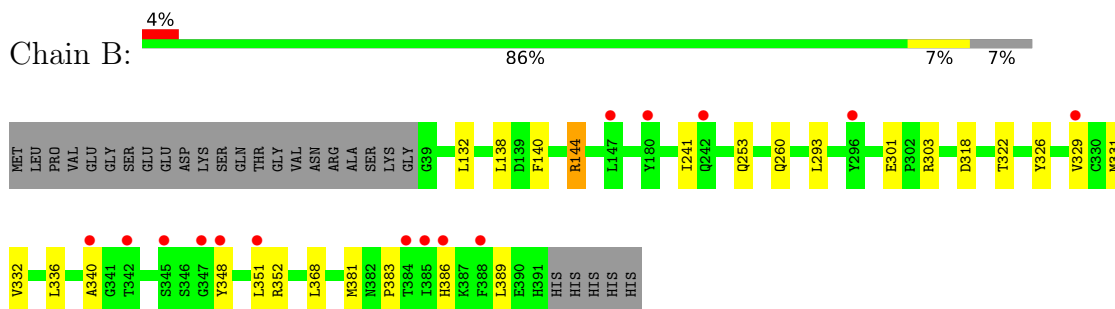
3 Residue-property plots [i](#)

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.

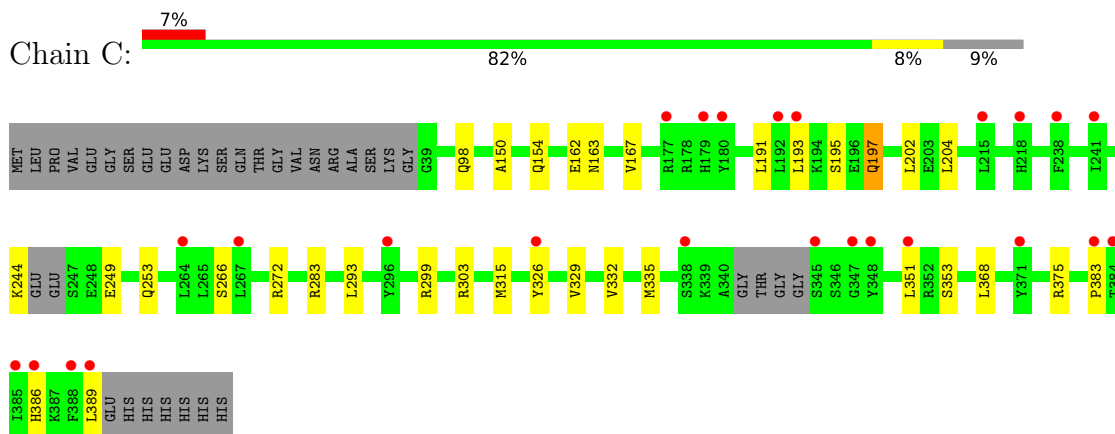
- Molecule 1: Tryptophan 2,3-dioxygenase



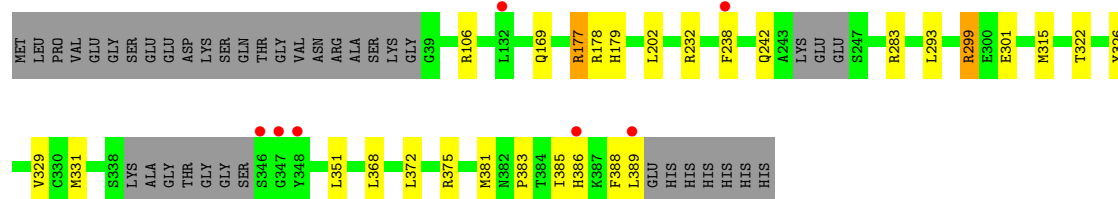
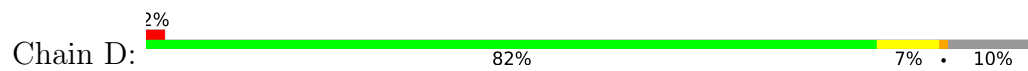
- Molecule 1: Tryptophan 2,3-dioxygenase



- Molecule 1: Tryptophan 2,3-dioxygenase



- Molecule 1: Tryptophan 2,3-dioxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	143.81Å 154.93Å 88.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	105.62 – 2.05 105.40 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.4 (105.62-2.05) 99.3 (105.40-2.05)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.05Å)	Xtrriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.194 , 0.215 0.202 , 0.221	Depositor DCC
R_{free} test set	6083 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	53.0	Xtrriage
Anisotropy	0.406	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12216	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: ZIQ, A1AD1, 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	0.44	0/3040	0.75	0/4090
1	B	0.42	0/3045	0.74	0/4098
1	C	0.39	0/2986	0.73	2/4016 (0.0%)
1	D	0.43	0/2957	0.76	4/3979 (0.1%)
All	All	0.42	0/12028	0.75	6/16183 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	D	0	4
All	All	0	8

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	331	MET	CG-SD-CE	-7.81	87.70	100.20
1	D	178	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	D	177	ARG	NE-CZ-NH2	7.14	123.87	120.30
1	D	315	MET	CG-SD-CE	6.77	111.04	100.20
1	C	315	MET	CG-SD-CE	6.53	110.65	100.20
1	C	335	MET	CG-SD-CE	5.21	108.53	100.20

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	ARG	Sidechain
1	A	334	ARG	Sidechain
1	A	352	ARG	Sidechain
1	B	144	ARG	Sidechain
1	D	106	ARG	Sidechain
1	D	177	ARG	Sidechain
1	D	232	ARG	Sidechain
1	D	299	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2971	0	2953	10	0
1	B	2975	0	2957	16	0
1	C	2919	0	2914	21	0
1	D	2890	0	2878	14	0
2	A	43	0	30	1	0
2	B	43	0	30	2	0
2	C	43	0	30	1	0
2	D	43	0	30	2	0
3	A	16	0	0	0	0
3	B	16	0	0	0	0
3	C	16	0	0	0	0
3	D	16	0	0	0	0
4	A	25	0	0	0	0
4	B	25	0	0	0	0
4	C	25	0	0	0	0
4	D	25	0	0	0	0
5	A	44	0	0	0	0
5	B	33	0	0	0	0
5	C	20	0	0	0	0
5	D	28	0	0	0	0
All	All	12216	0	11822	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:C:383:PRO:HA	1:C:386:HIS:HB3	1.65	0.77
1:C:193:LEU:O	1:C:197:GLN:HG2	1.86	0.75
1:B:383:PRO:HA	1:B:386:HIS:HB3	1.70	0.72
1:A:322:THR:HG22	1:C:326:TYR:OH	1.91	0.71
1:C:386:HIS:HD2	1:C:389:LEU:HB2	1.61	0.65
1:B:326:TYR:OH	1:D:322:THR:HG22	1.98	0.64
1:B:241:ILE:HG12	1:B:253:GLN:HE21	1.64	0.62
1:A:381:MET:SD	1:A:389:LEU:HD12	2.42	0.60
1:B:381:MET:SD	1:B:389:LEU:HD12	2.42	0.59
1:C:163:ASN:HB2	1:C:195:SER:OG	2.02	0.59
1:C:249:GLU:HG2	1:C:253:GLN:HE21	1.66	0.59
1:A:383:PRO:HA	1:A:386:HIS:HB3	1.84	0.58
1:B:322:THR:HG22	1:D:326:TYR:OH	2.04	0.57
1:D:381:MET:SD	1:D:389:LEU:HD12	2.45	0.56
1:D:383:PRO:HA	1:D:386:HIS:HB3	1.91	0.52
1:C:162:GLU:HB3	1:C:167:VAL:HG11	1.92	0.51
1:C:329:VAL:HG22	1:C:351:LEU:HB3	1.92	0.51
1:B:329:VAL:HG22	1:B:351:LEU:HB3	1.93	0.50
1:A:322:THR:CG2	1:C:326:TYR:OH	2.60	0.50
1:C:299:ARG:HH12	1:C:375:ARG:HH22	1.60	0.49
1:A:220:PHE:HD1	1:A:385:ILE:HG12	1.79	0.47
1:B:336:LEU:HB3	1:B:340:ALA:HB3	1.96	0.47
1:C:303:ARG:HD3	1:C:389:LEU:HA	1.97	0.47
1:D:329:VAL:HG22	1:D:351:LEU:HB3	1.97	0.47
1:D:238:PHE:O	1:D:242:GLN:HG2	2.15	0.47
2:D:401:HEM:HBC2	2:D:401:HEM:HHD	1.95	0.46
1:A:336:LEU:HB3	1:A:340:ALA:HB3	1.97	0.46
1:A:329:VAL:HG22	1:A:351:LEU:HB3	1.97	0.46
2:B:401:HEM:HBC2	2:B:401:HEM:HHD	1.98	0.46
1:C:202:LEU:HD22	1:C:283:ARG:NH1	2.31	0.46
1:B:138:LEU:HD23	1:D:372:LEU:HD22	1.99	0.45
1:C:98:GLN:HG3	1:C:204:LEU:HD21	1.98	0.45
1:D:202:LEU:HD22	1:D:283:ARG:NH1	2.32	0.44
1:B:132:LEU:HD23	1:B:331:MET:HE1	1.99	0.44
1:A:132:LEU:HD23	1:A:331:MET:HE1	2.00	0.44
1:D:385:ILE:HG13	1:D:388:PHE:CD1	2.53	0.43
1:C:386:HIS:O	1:C:389:LEU:N	2.48	0.43
1:B:348:TYR:CZ	1:B:352:ARG:HD2	2.52	0.43
2:A:401:HEM:HBC2	2:A:401:HEM:HHD	2.00	0.43
1:C:150:ALA:HA	1:C:154:GLN:OE1	2.18	0.43
1:C:332:VAL:HG22	2:C:401:HEM:C1B	2.54	0.43
1:D:299:ARG:HH12	1:D:375:ARG:HH12	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:SER:HB2	1:C:272:ARG:NH2	2.34	0.42
1:C:191:LEU:HD23	1:C:191:LEU:HA	1.89	0.42
1:B:293:LEU:HD13	1:B:368:LEU:HD22	2.00	0.42
1:B:303:ARG:HD3	1:B:389:LEU:HA	2.01	0.42
1:C:244:LYS:HE2	1:C:253:GLN:NE2	2.34	0.42
1:D:293:LEU:HD13	1:D:368:LEU:HD22	2.00	0.42
1:B:332:VAL:HG22	2:B:401:HEM:C1B	2.54	0.42
1:D:202:LEU:CD2	1:D:283:ARG:NH1	2.83	0.42
1:D:301:GLU:OE1	1:D:386:HIS:NE2	2.53	0.42
1:A:333:HIS:HB2	1:A:348:TYR:CE1	2.54	0.42
1:D:169:GLN:HB2	1:D:179:HIS:HE2	1.85	0.41
1:B:260:GLN:HA	1:B:260:GLN:OE1	2.20	0.41
1:B:140:PHE:CE2	1:B:144:ARG:HD3	2.55	0.41
1:C:293:LEU:HD13	1:C:368:LEU:HD22	2.03	0.41
1:B:301:GLU:OE1	1:B:386:HIS:NE2	2.54	0.41
1:A:265:LEU:HD23	1:A:265:LEU:HA	1.94	0.41
1:C:202:LEU:CD2	1:C:283:ARG:NH1	2.85	0.40
2:D:401:HEM:HBB2	2:D:401:HEM:CMB	2.51	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	348/380 (92%)	342 (98%)	6 (2%)	0	100	100
1	B	351/380 (92%)	345 (98%)	6 (2%)	0	100	100
1	C	339/380 (89%)	335 (99%)	4 (1%)	0	100	100
1	D	335/380 (88%)	329 (98%)	6 (2%)	0	100	100
All	All	1373/1520 (90%)	1351 (98%)	22 (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	325/348 (93%)	325 (100%)	0	100	100
1	B	325/348 (93%)	324 (100%)	1 (0%)	92	93
1	C	320/348 (92%)	318 (99%)	2 (1%)	86	87
1	D	317/348 (91%)	317 (100%)	0	100	100
All	All	1287/1392 (92%)	1284 (100%)	3 (0%)	93	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	318	ASP
1	C	197	GLN
1	C	353	SER

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

Mol	Chain	Res	Type
1	C	253	GLN
1	C	386	HIS
1	D	229	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](#)

12 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	ZIQ	D	402	-	13,17,17	0.84	0	14,25,25	0.92	0
4	A1AD1	A	403	-	26,29,29	0.85	1 (3%)	27,41,41	1.13	2 (7%)
2	HEM	D	401	1	41,50,50	1.47	6 (14%)	45,82,82	1.87	11 (24%)
3	ZIQ	A	402	-	13,17,17	0.83	0	14,25,25	1.00	1 (7%)
3	ZIQ	C	402	-	13,17,17	0.75	0	14,25,25	1.05	1 (7%)
4	A1AD1	D	403	-	26,29,29	0.82	1 (3%)	27,41,41	1.08	2 (7%)
4	A1AD1	C	403	-	26,29,29	0.80	1 (3%)	27,41,41	0.99	2 (7%)
2	HEM	C	401	1	41,50,50	1.33	5 (12%)	45,82,82	1.88	10 (22%)
2	HEM	B	401	1	41,50,50	1.38	6 (14%)	45,82,82	1.92	10 (22%)
2	HEM	A	401	1	41,50,50	1.48	6 (14%)	45,82,82	1.90	12 (26%)
4	A1AD1	B	403	-	26,29,29	0.77	0	27,41,41	0.97	2 (7%)
3	ZIQ	B	402	-	13,17,17	0.74	0	14,25,25	0.87	1 (7%)

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	ZIQ	D	402	-	-	2/9/11/11	0/2/2/2
4	A1AD1	A	403	-	-	0/7/16/16	0/5/5/5
2	HEM	D	401	1	-	2/12/54/54	-
3	ZIQ	A	402	-	-	1/9/11/11	0/2/2/2
3	ZIQ	C	402	-	-	4/9/11/11	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A1AD1	D	403	-	-	2/7/16/16	0/5/5/5
4	A1AD1	C	403	-	-	2/7/16/16	0/5/5/5
2	HEM	C	401	1	-	2/12/54/54	-
2	HEM	B	401	1	-	2/12/54/54	-
2	HEM	A	401	1	-	2/12/54/54	-
4	A1AD1	B	403	-	-	2/7/16/16	0/5/5/5
3	ZIQ	B	402	-	-	4/9/11/11	0/2/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	HEM	C1B-NB	-4.12	1.33	1.40
2	D	401	HEM	C1B-NB	-3.99	1.33	1.40
2	A	401	HEM	C1B-NB	-3.64	1.34	1.40
2	C	401	HEM	C1B-NB	-3.57	1.34	1.40
2	C	401	HEM	C4D-ND	-3.52	1.34	1.40
2	A	401	HEM	C1D-ND	-3.38	1.31	1.38
2	D	401	HEM	C4D-ND	-3.30	1.34	1.40
2	D	401	HEM	C4B-NB	-3.26	1.32	1.38
2	A	401	HEM	C4B-NB	-3.14	1.32	1.38
2	B	401	HEM	FE-NB	2.84	2.10	1.96
2	B	401	HEM	C4D-ND	-2.84	1.35	1.40
2	C	401	HEM	FE-NB	2.76	2.10	1.96
2	A	401	HEM	CHB-C1B	2.59	1.41	1.35
2	B	401	HEM	C4B-NB	-2.50	1.33	1.38
2	D	401	HEM	CHB-C1B	2.50	1.41	1.35
2	A	401	HEM	FE-NB	2.45	2.09	1.96
2	D	401	HEM	FE-NB	2.43	2.08	1.96
2	C	401	HEM	C4B-NB	-2.39	1.33	1.38
2	D	401	HEM	O1D-CGD	2.21	1.29	1.22
4	A	403	A1AD1	N1-N2	-2.14	1.30	1.34
2	A	401	HEM	C3C-C2C	-2.14	1.37	1.40
2	C	401	HEM	C1D-ND	-2.14	1.34	1.38
4	D	403	A1AD1	N1-N2	-2.11	1.30	1.34
4	C	403	A1AD1	N1-N2	-2.10	1.30	1.34
2	B	401	HEM	C1D-ND	-2.08	1.34	1.38
2	B	401	HEM	CHB-C1B	2.06	1.40	1.35

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	HEM	C1B-NB-C4B	4.86	110.09	105.07
2	C	401	HEM	CHC-C4B-NB	4.86	129.71	124.43
2	D	401	HEM	CHD-C1D-ND	4.71	129.54	124.43
2	C	401	HEM	C1B-NB-C4B	4.65	109.88	105.07
2	B	401	HEM	CHD-C1D-ND	4.61	129.44	124.43
2	B	401	HEM	CHC-C4B-NB	4.58	129.41	124.43
2	A	401	HEM	C1B-NB-C4B	4.58	109.80	105.07
2	D	401	HEM	C1B-NB-C4B	4.52	109.74	105.07
2	A	401	HEM	CHC-C4B-NB	4.44	129.25	124.43
2	A	401	HEM	CHD-C1D-ND	4.36	129.17	124.43
2	A	401	HEM	CHA-C4D-ND	4.05	129.38	124.38
2	C	401	HEM	CHD-C1D-ND	3.82	128.58	124.43
2	D	401	HEM	CHB-C1B-NB	3.81	129.09	124.38
2	D	401	HEM	CHC-C4B-NB	3.80	128.56	124.43
2	C	401	HEM	CHB-C1B-NB	3.76	129.02	124.38
2	B	401	HEM	CHA-C4D-ND	3.44	128.63	124.38
2	A	401	HEM	CHB-C1B-NB	3.36	128.53	124.38
2	B	401	HEM	CBD-CAD-C3D	-3.28	103.51	112.63
2	D	401	HEM	CHA-C4D-ND	3.24	128.39	124.38
2	C	401	HEM	CBD-CAD-C3D	-3.23	103.65	112.63
2	D	401	HEM	CBD-CAD-C3D	-3.22	103.68	112.63
2	B	401	HEM	CHB-C1B-NB	3.17	128.29	124.38
4	A	403	A1AD1	C6-C11-C10	-3.12	118.71	121.44
2	C	401	HEM	CHA-C4D-ND	3.09	128.19	124.38
4	A	403	A1AD1	C12-N3-N2	3.06	121.16	116.67
2	A	401	HEM	CBD-CAD-C3D	-3.05	104.16	112.63
2	A	401	HEM	CHD-C1D-C2D	-2.90	120.45	124.98
2	B	401	HEM	CHD-C1D-C2D	-2.90	120.45	124.98
2	C	401	HEM	CBA-CAA-C2A	-2.86	107.74	112.62
4	D	403	A1AD1	C12-N3-N2	2.72	120.66	116.67
2	D	401	HEM	CHD-C1D-C2D	-2.68	120.79	124.98
4	B	403	A1AD1	C12-N3-N2	2.62	120.52	116.67
4	D	403	A1AD1	C6-C11-C10	-2.59	119.17	121.44
4	C	403	A1AD1	C6-C11-C10	-2.55	119.21	121.44
2	D	401	HEM	CBA-CAA-C2A	-2.52	108.33	112.62
2	C	401	HEM	C4D-ND-C1D	2.46	107.61	105.07
2	B	401	HEM	O2A-CGA-CBA	2.45	121.91	114.03
2	D	401	HEM	CMD-C2D-C1D	2.44	128.75	125.04
2	B	401	HEM	CBA-CAA-C2A	-2.40	108.53	112.62
2	C	401	HEM	CHD-C1D-C2D	-2.38	121.27	124.98
4	C	403	A1AD1	C12-N3-N2	2.31	120.06	116.67
2	B	401	HEM	C4D-ND-C1D	2.26	107.41	105.07
2	A	401	HEM	CHA-C4D-C3D	-2.25	121.11	125.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	HEM	O2D-CGD-O1D	-2.17	117.90	123.30
2	A	401	HEM	O2A-CGA-CBA	2.16	120.98	114.03
2	C	401	HEM	C4B-C3B-C2B	-2.15	105.40	107.11
3	C	402	ZIQ	CH2-CZ2-CE2	-2.15	116.98	120.08
2	A	401	HEM	C4D-ND-C1D	2.14	107.28	105.07
4	B	403	A1AD1	C6-C11-C10	-2.12	119.58	121.44
2	D	401	HEM	CHA-C4D-C3D	-2.10	121.38	125.33
3	A	402	ZIQ	CH2-CZ2-CE2	-2.07	117.10	120.08
2	D	401	HEM	CHB-C1B-C2B	-2.05	121.05	126.72
2	A	401	HEM	O2A-CGA-O1A	-2.04	118.21	123.30
3	B	402	ZIQ	CH2-CZ2-CE2	-2.01	117.18	120.08

There are no chirality outliers.

All (25) torsion outliers are listed below:

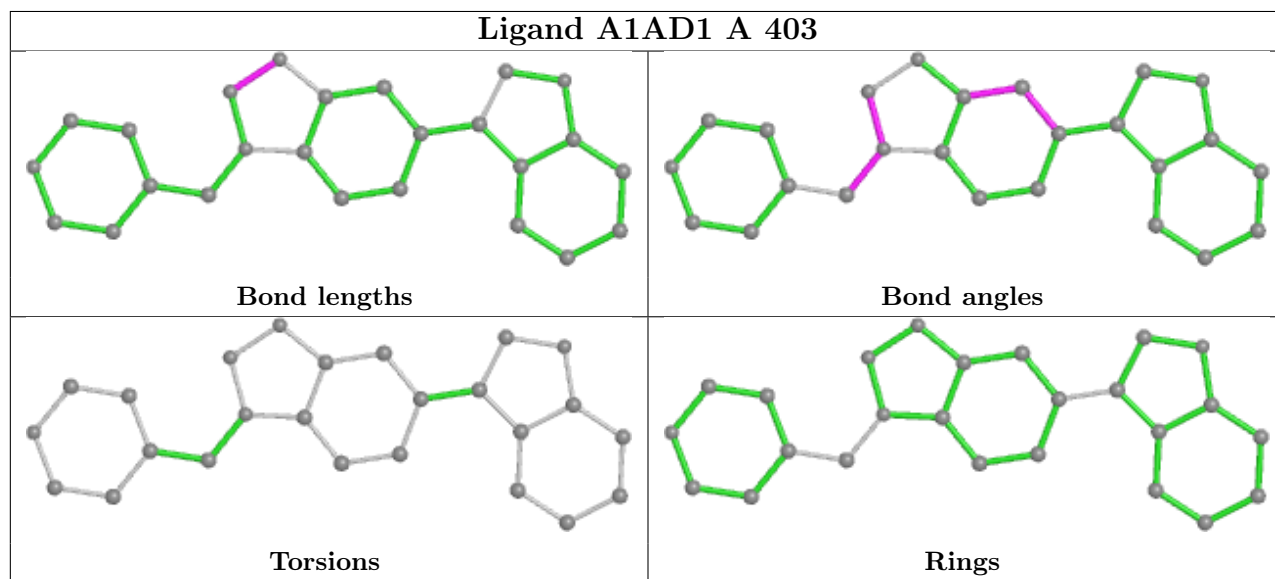
Mol	Chain	Res	Type	Atoms
3	B	402	ZIQ	O-C-CA-C1
3	B	402	ZIQ	OXT-C-CA-C1
3	C	402	ZIQ	OXT-C-CA-C1
4	C	403	A1AD1	N3-C12-C13-C14
4	C	403	A1AD1	N3-C12-C13-C17
4	D	403	A1AD1	N3-C12-C13-C14
4	D	403	A1AD1	N3-C12-C13-C17
3	C	402	ZIQ	O-C-CA-C1
3	B	402	ZIQ	O-C-CA-CB
3	B	402	ZIQ	OXT-C-CA-CB
3	C	402	ZIQ	O-C-CA-CB
3	C	402	ZIQ	OXT-C-CA-CB
2	A	401	HEM	CAA-CBA-CGA-O1A
2	C	401	HEM	CAA-CBA-CGA-O1A
2	D	401	HEM	CAA-CBA-CGA-O1A
3	D	402	ZIQ	O-C-CA-C1
2	C	401	HEM	CAA-CBA-CGA-O2A
2	A	401	HEM	CAA-CBA-CGA-O2A
2	D	401	HEM	CAA-CBA-CGA-O2A
3	A	402	ZIQ	O-C-CA-C1
2	B	401	HEM	CAA-CBA-CGA-O1A
2	B	401	HEM	CAA-CBA-CGA-O2A
4	B	403	A1AD1	C18-C5-C6-C7
3	D	402	ZIQ	OXT-C-CA-C1
4	B	403	A1AD1	C4-C5-C6-C7

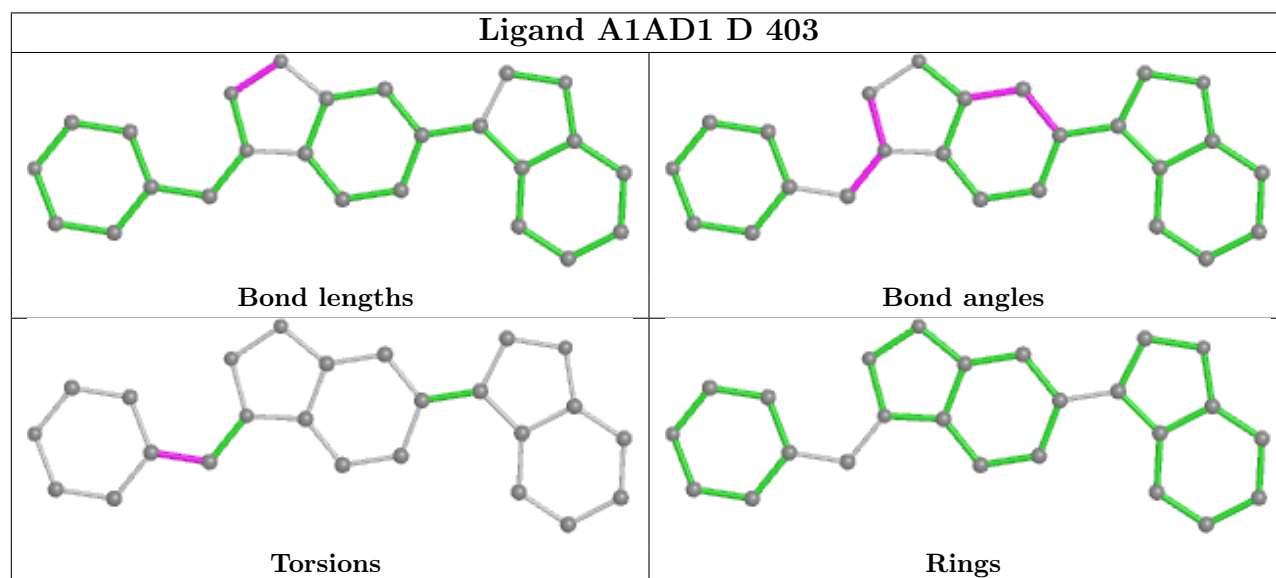
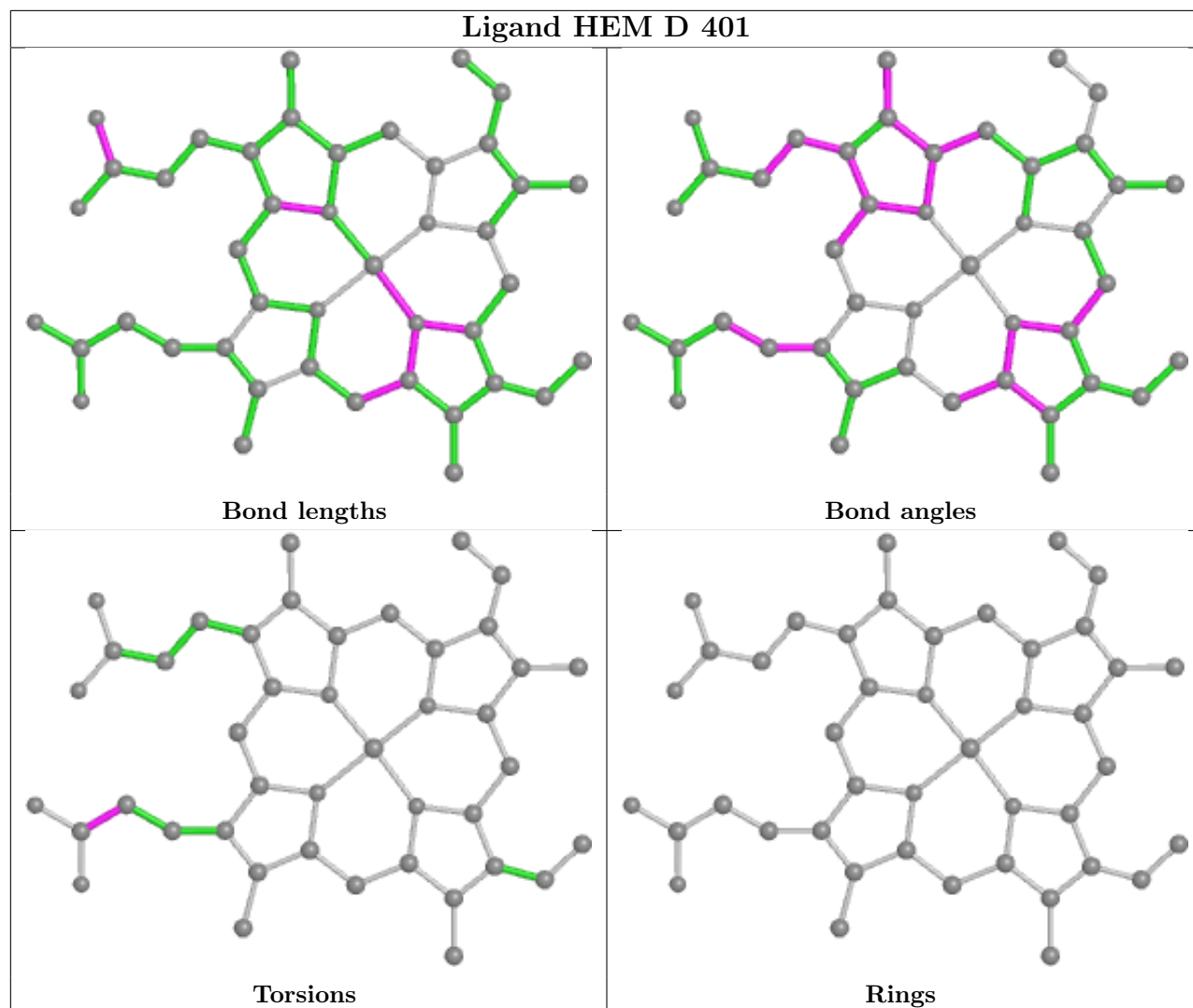
There are no ring outliers.

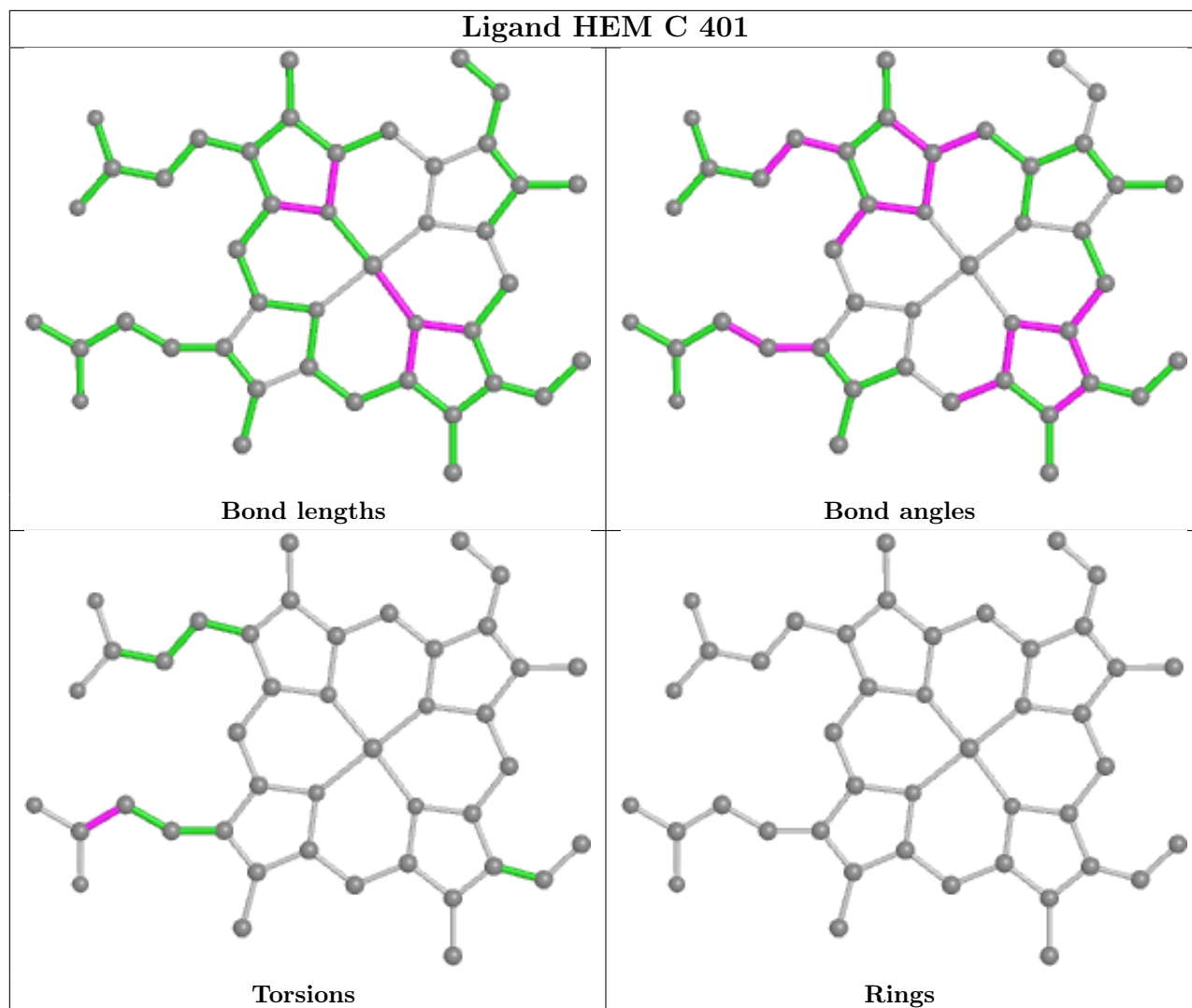
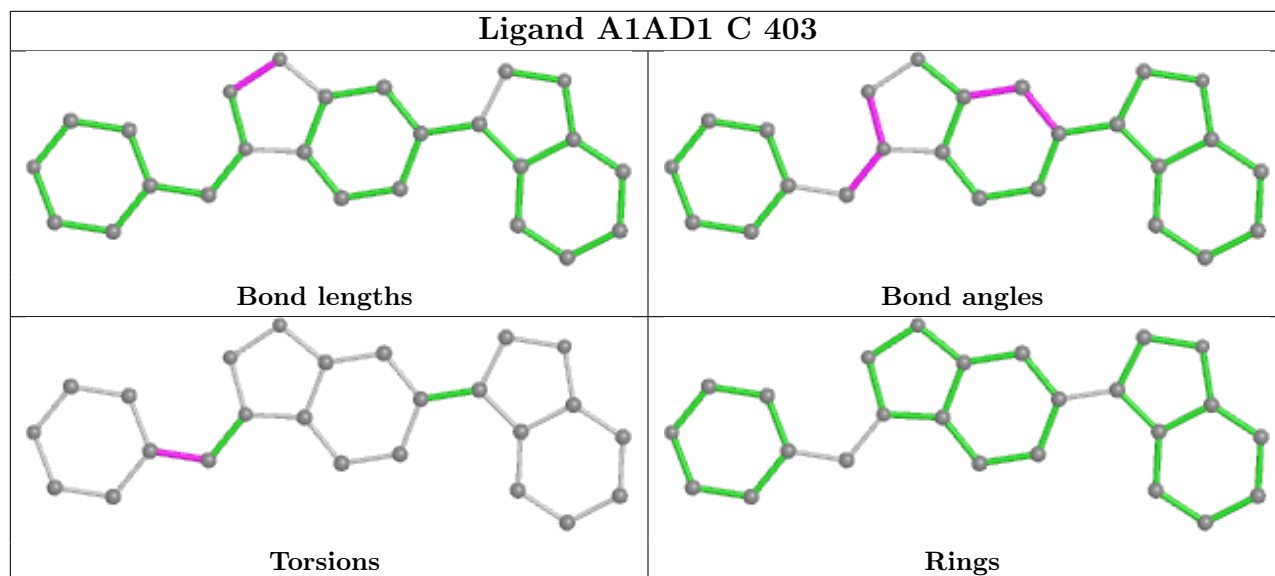
4 monomers are involved in 6 short contacts:

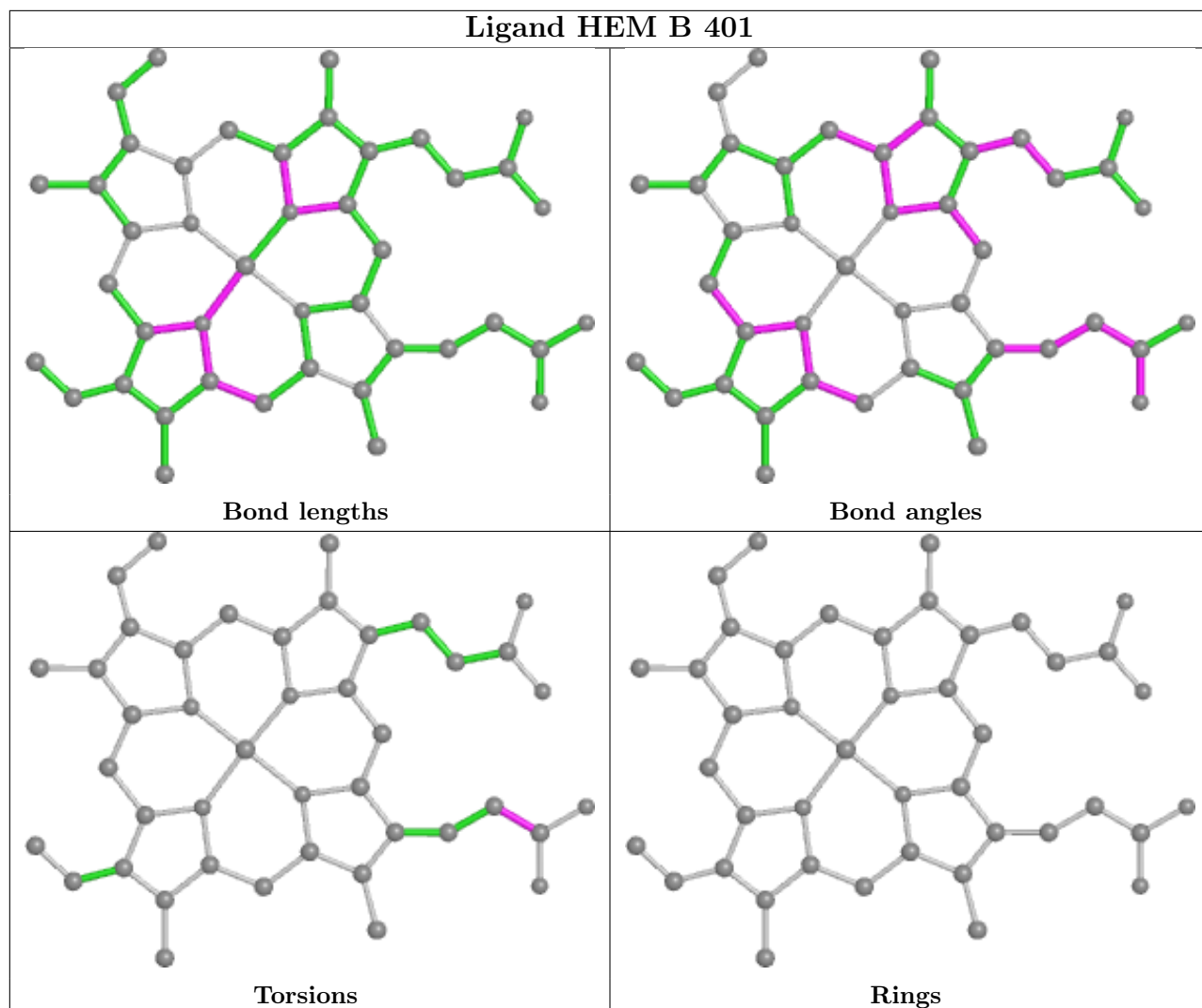
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	HEM	2	0
2	C	401	HEM	1	0
2	B	401	HEM	2	0
2	A	401	HEM	1	0

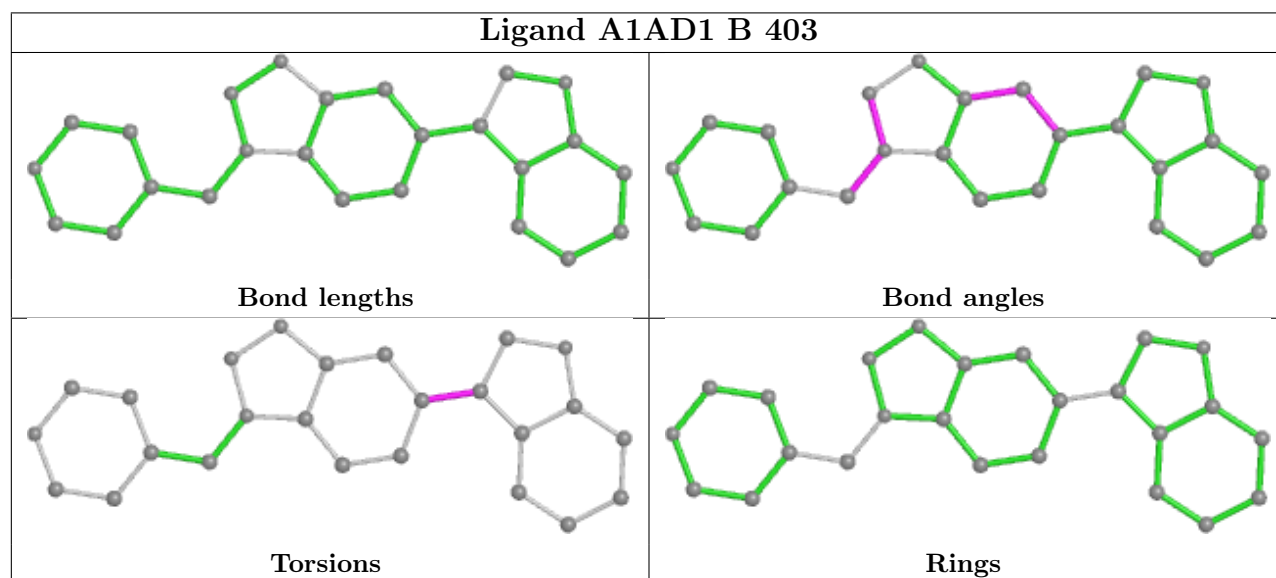
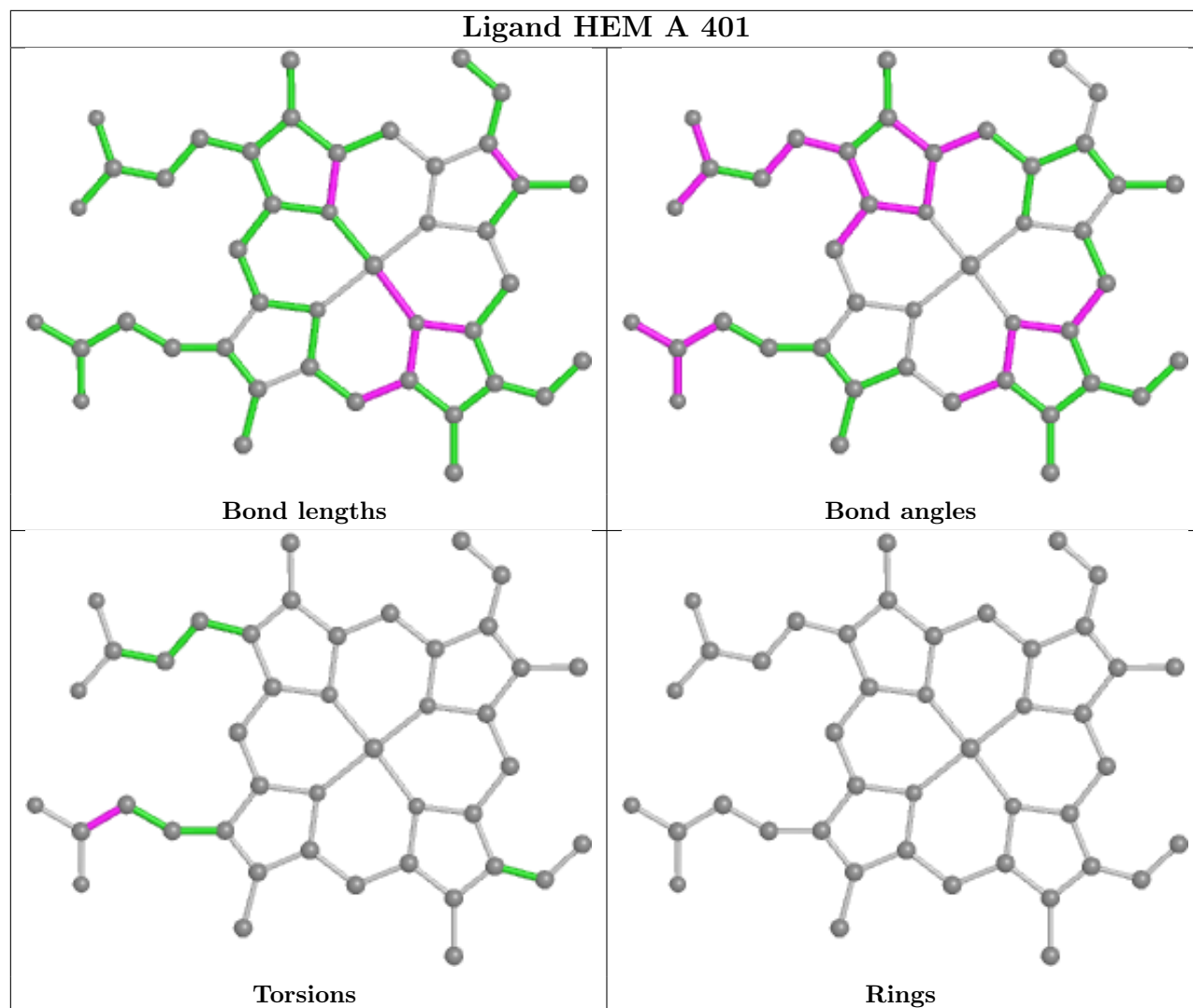
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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	352/380 (92%)	0.46	8 (2%) 60 64	45, 64, 124, 165	0
1	B	353/380 (92%)	0.54	15 (4%) 36 39	47, 70, 125, 174	0
1	C	345/380 (90%)	0.62	25 (7%) 15 17	50, 90, 171, 237	0
1	D	341/380 (89%)	0.43	7 (2%) 63 67	45, 70, 131, 190	0
All	All	1391/1520 (91%)	0.51	55 (3%) 38 41	45, 72, 142, 237	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	386	HIS	6.5
1	B	386	HIS	5.8
1	C	388	PHE	5.6
1	A	386	HIS	5.5
1	B	345	SER	5.2
1	B	342	THR	5.1
1	A	342	THR	4.5
1	C	296	TYR	4.5
1	D	348	TYR	4.4
1	C	179	HIS	4.4
1	D	386	HIS	4.3
1	C	383	PRO	4.3
1	C	371	TYR	4.3
1	D	389	LEU	4.2
1	B	296	TYR	4.1
1	C	389	LEU	3.9
1	C	193	LEU	3.9
1	C	348	TYR	3.9
1	C	345	SER	3.7
1	C	338	SER	3.3
1	A	178	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	385	ILE	3.2
1	B	388	PHE	3.1
1	D	238	PHE	2.9
1	A	345	SER	2.9
1	A	389	LEU	2.9
1	C	326	TYR	2.9
1	C	180	TYR	2.8
1	A	341	GLY	2.8
1	B	351	LEU	2.8
1	D	347	GLY	2.8
1	B	329	VAL	2.7
1	B	384	THR	2.7
1	C	238	PHE	2.6
1	B	348	TYR	2.5
1	D	346	SER	2.5
1	B	340	ALA	2.5
1	A	348	TYR	2.5
1	B	347	GLY	2.4
1	C	177	ARG	2.4
1	B	147	LEU	2.3
1	D	132	LEU	2.3
1	C	351	LEU	2.3
1	C	218	HIS	2.3
1	A	383	PRO	2.3
1	C	241	ILE	2.3
1	C	385	ILE	2.3
1	C	192	LEU	2.2
1	C	347	GLY	2.1
1	C	384	THR	2.1
1	C	264	LEU	2.1
1	B	242	GLN	2.0
1	C	215	LEU	2.0
1	B	180	TYR	2.0
1	C	267	LEU	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](#)

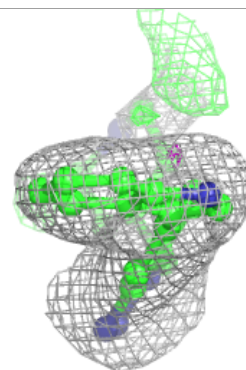
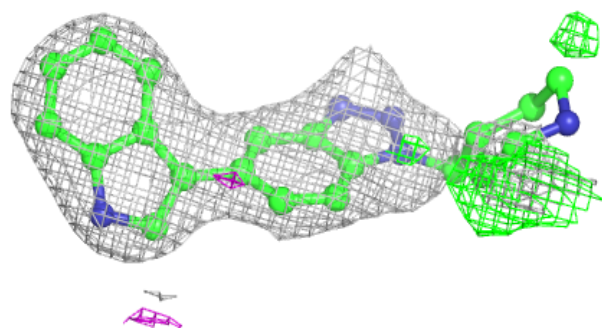
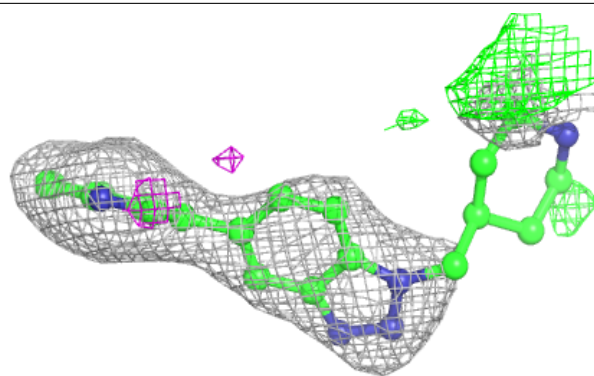
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	A1AD1	C	403	25/25	0.91	0.21	73,93,124,128	0
4	A1AD1	B	403	25/25	0.94	0.19	58,70,105,108	0
3	ZIQ	C	402	16/16	0.95	0.14	75,86,93,96	0
2	HEM	B	401	43/43	0.95	0.19	60,69,81,83	0
2	HEM	C	401	43/43	0.95	0.20	68,82,105,116	0
4	A1AD1	D	403	25/25	0.95	0.17	61,73,103,104	0
4	A1AD1	A	403	25/25	0.96	0.22	61,75,118,120	0
2	HEM	A	401	43/43	0.97	0.14	54,62,74,89	0
3	ZIQ	D	402	16/16	0.97	0.16	53,62,69,74	0
3	ZIQ	B	402	16/16	0.97	0.16	59,68,72,77	0
3	ZIQ	A	402	16/16	0.98	0.15	48,54,61,63	0
2	HEM	D	401	43/43	0.98	0.14	52,58,72,86	0

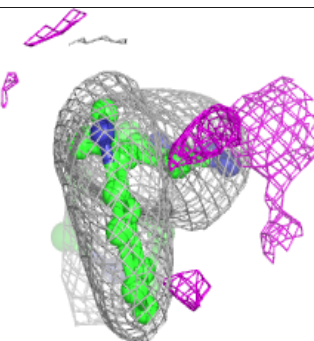
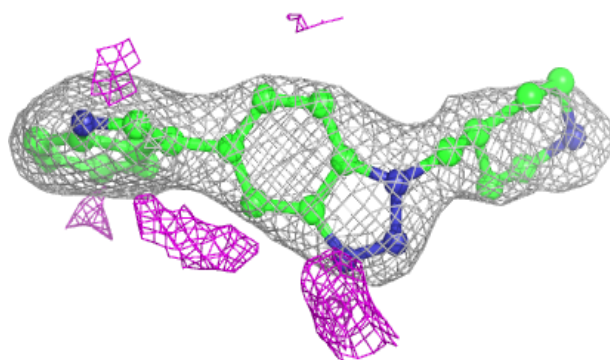
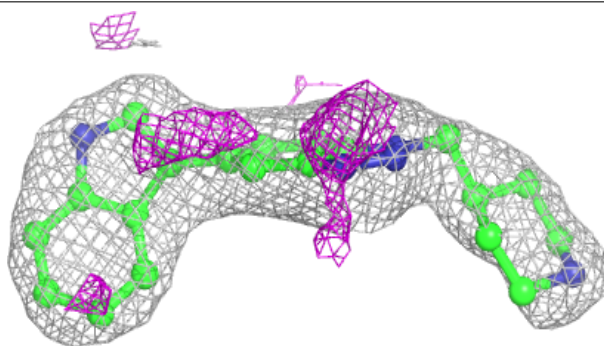
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1AD1 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)

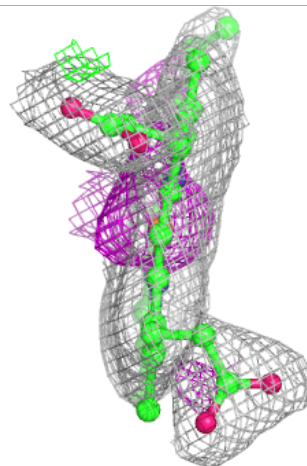
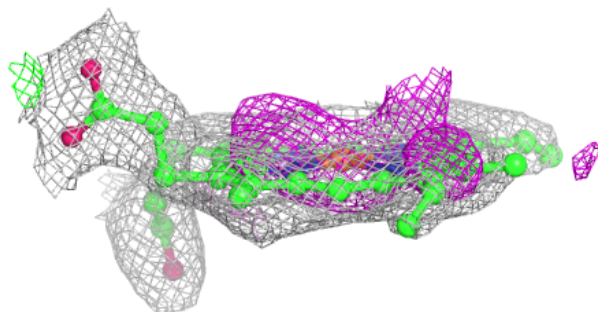
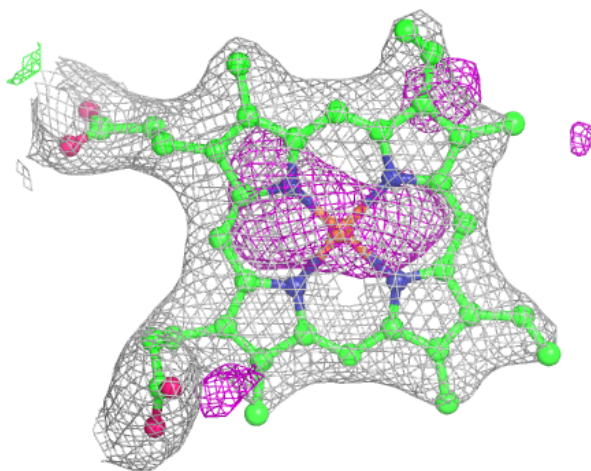
**Electron density around A1AD1 B 403:**

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



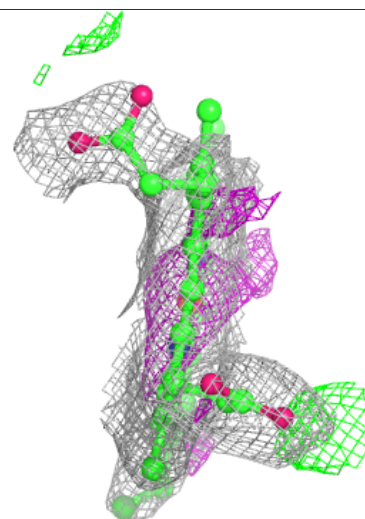
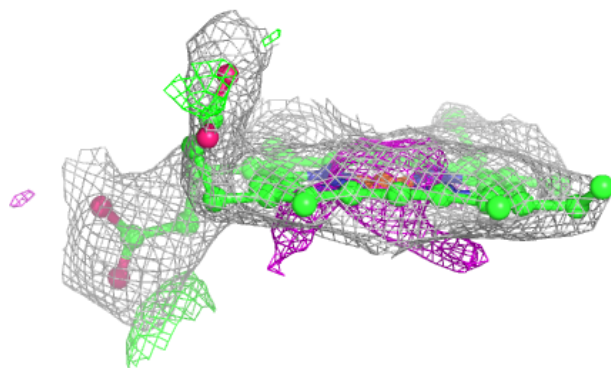
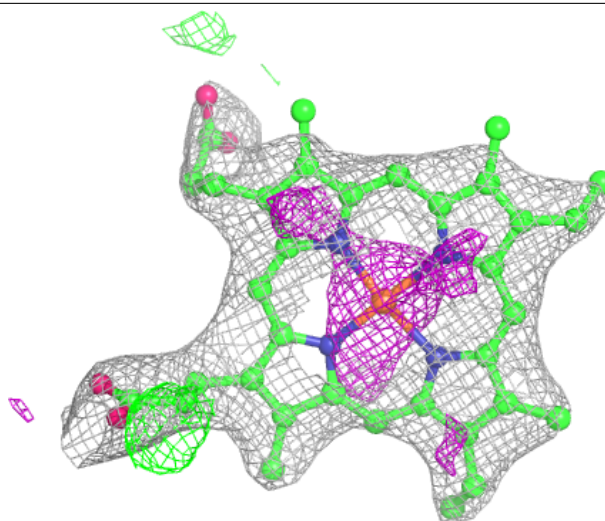
Electron density around HEM B 401:

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



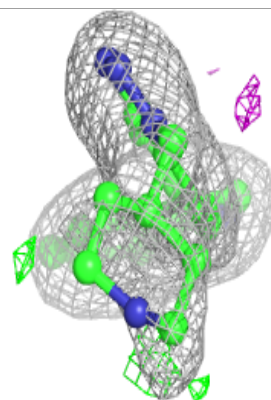
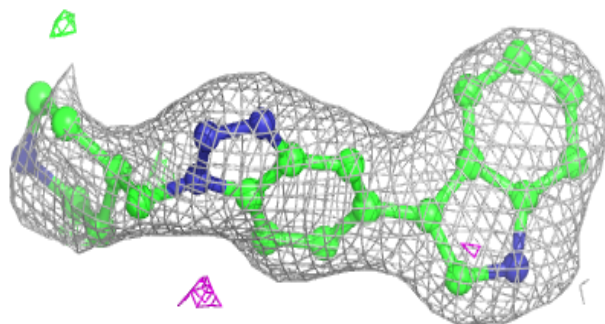
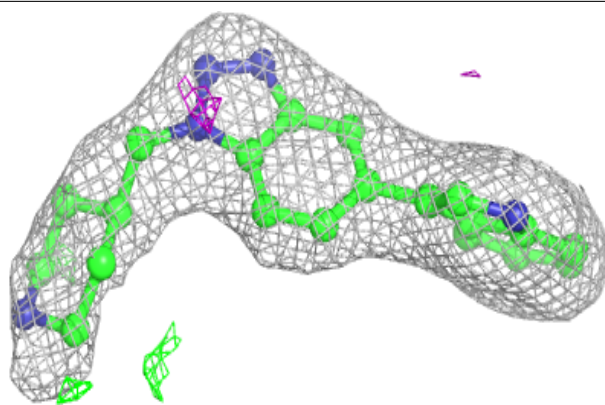
Electron density around HEM C 401:

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

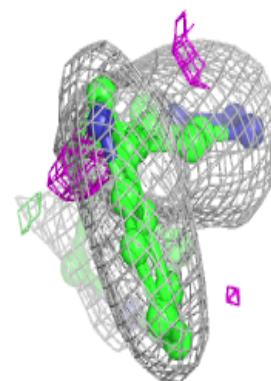
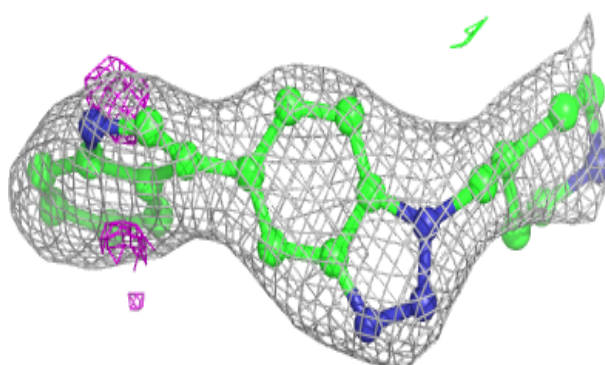
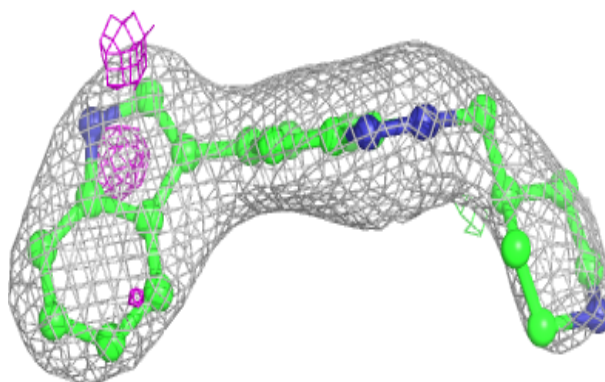


Electron density around A1AD1 D 403:

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

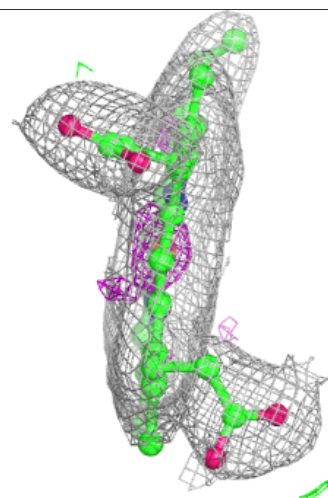
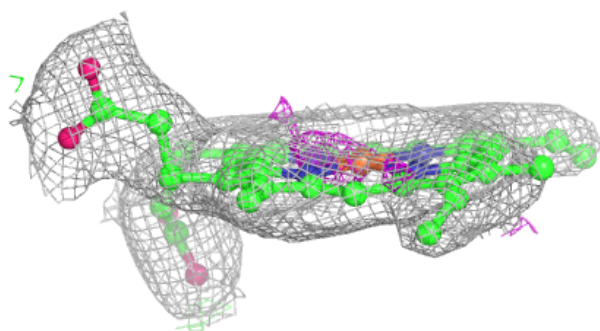
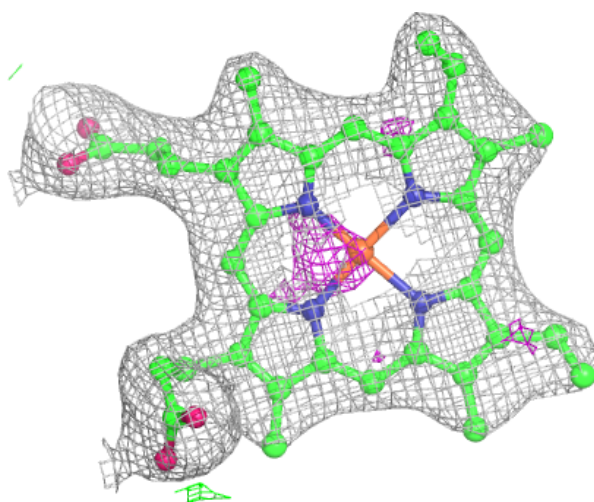
**Electron density around A1AD1 A 403:**

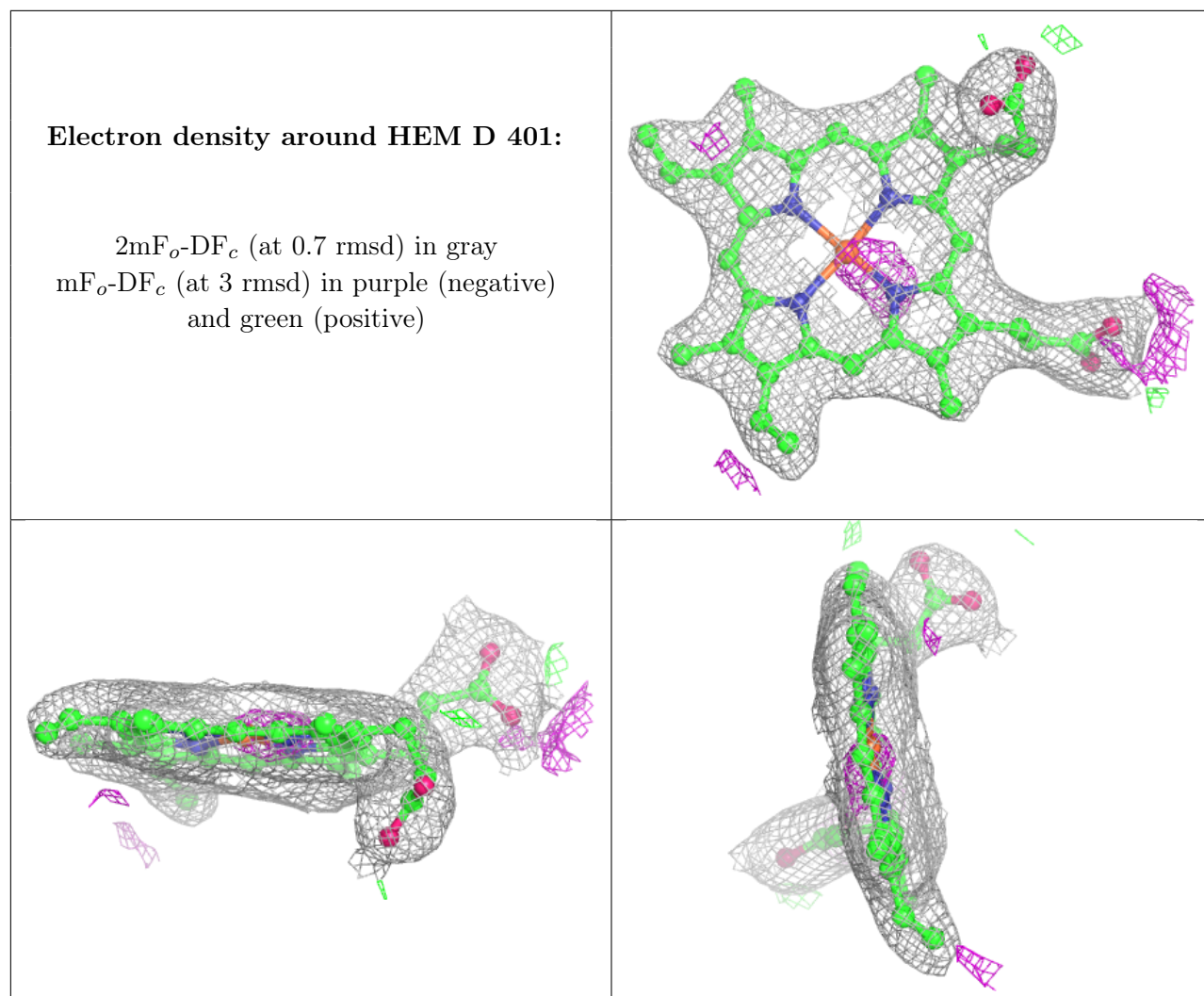
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.