



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 07:30 PM JST

PDB ID : 7E0U / pdb_00007e0u
Title : Crystal Structure of Human Indoleamine 2,3-dioxygenase 1 (hIDO1) Complexed with 6-Bromo-N-(((1S,2S)-2-chlorocyclohexyl)methyl)-1H-indazol-4-amine (39)
Authors : Li, G.-B.; Ning, X.-L.
Deposited on : 2021-01-28
Resolution : 2.28 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	:	1.8.5 (274361), CSD as541be (2020)
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

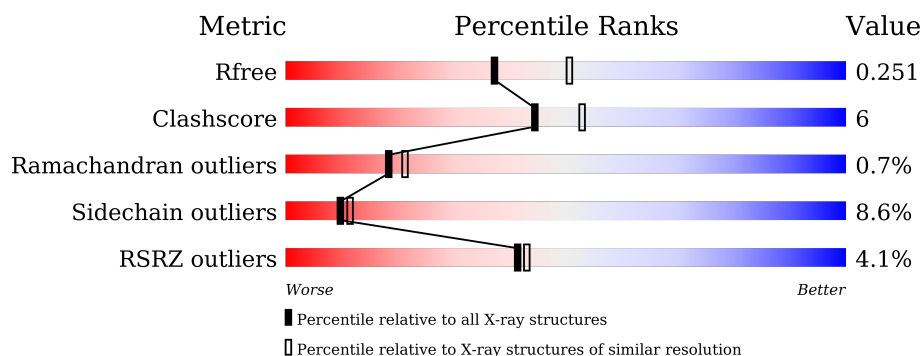
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	392	3% 83% 11% • •
1	B	392	5% 76% 18% • •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6258 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.

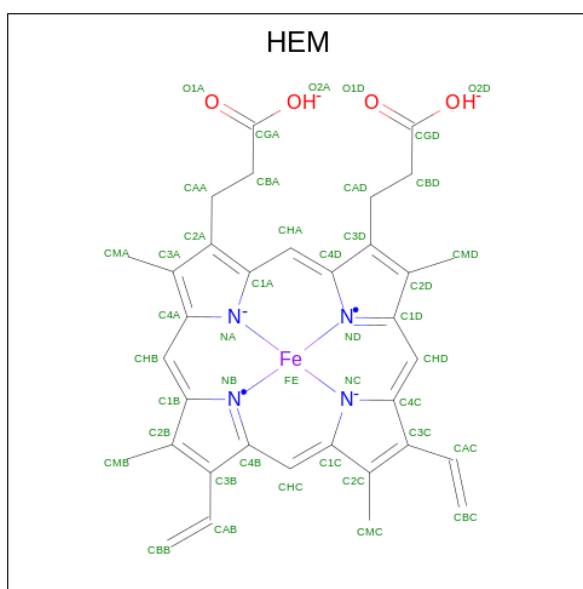
- Molecule 1 is a protein called Indoleamine 2,3-dioxygenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	1	0
			3013	1933	516	547	17			
1	B	380	Total	C	N	O	S	0	1	0
			3013	1933	516	547	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	374	GLU	LEU	conflict	UNP P14902
B	374	GLU	LEU	conflict	UNP P14902

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



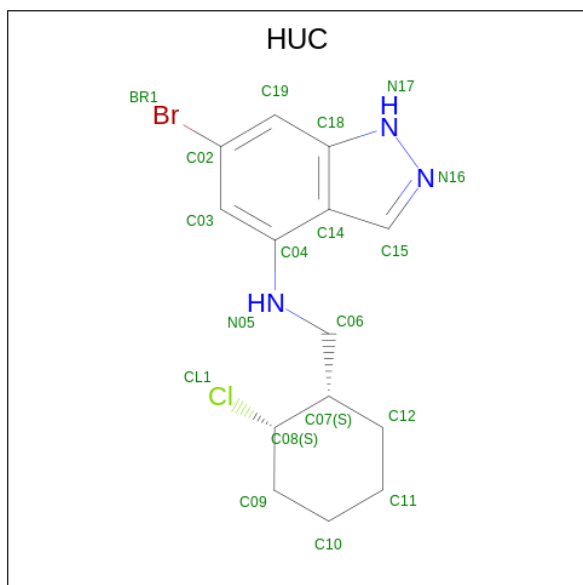
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is 6-bromanyl- {N}-[[[(1 {S},2 {S})-2-chloranylcyclohexyl)methyl]-1 {H}-indazol-4-amine (CCD ID: HUC) (formula: C₁₄H₁₇BrClN₃) (labeled as "Ligand of Interest" by depositor).

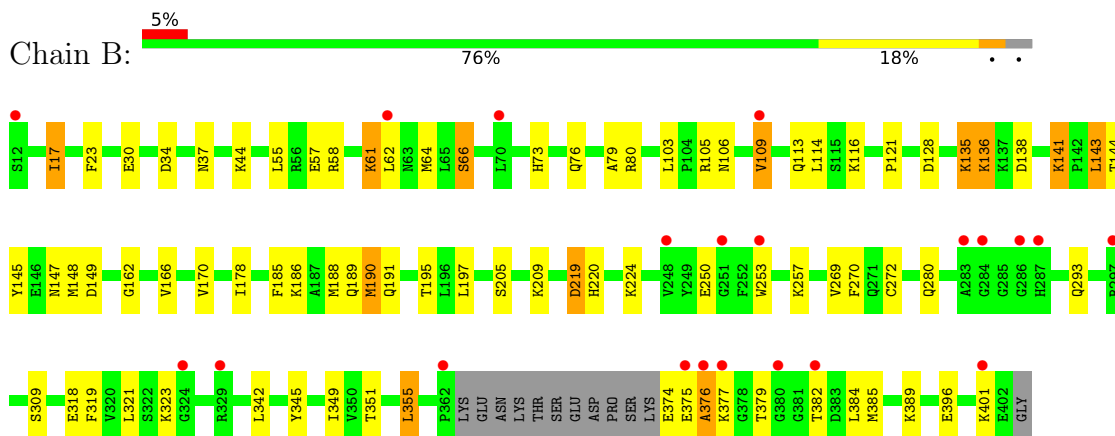


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 19	Br 1	C 14	Cl 1	N 3	0	0
3	B	1	Total 19	Br 1	C 14	Cl 1	N 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	71	Total	O	0	0
			71	71		
4	B	37	Total	O	0	0
			37	37		

- Molecule 1: Indoleamine 2,3-dioxygenase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.49Å 91.50Å 128.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.45 – 2.28 74.45 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.6 (74.45-2.28) 99.6 (74.45-2.28)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.190 , 0.248 0.201 , 0.251	Depositor DCC
R_{free} test set	1999 reflections (4.29%)	wwPDB-VP
Wilson B-factor (Å ²)	53.6	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6258	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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, HUC

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	0.67	0/3082	0.78	2/4168 (0.0%)
1	B	0.55	1/3082 (0.0%)	0.71	0/4168
All	All	0.61	1/6164 (0.0%)	0.75	2/8336 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	121	PRO	C-N	5.44	1.46	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	GLU	CA-C-N	5.47	131.54	121.70
1	A	375	GLU	C-N-CA	5.47	131.54	121.70

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	3013	0	3016	28	0
1	B	3013	0	3016	42	0
2	A	43	0	30	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	43	0	30	4	0
3	A	19	0	0	0	0
3	B	19	0	0	0	0
4	A	71	0	0	5	1
4	B	37	0	0	1	1
All	All	6258	0	6092	73	1

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 6.

All (73) 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:B:62:LEU:O	1:B:106:ASN:ND2	2.10	0.81
1:A:402:GLU:O	4:A:601:HOH:O	2.08	0.71
1:A:297:ARG:NH2	1:B:293:GLN:OE1	2.25	0.69
1:A:393:SER:OG	1:A:397:LYS:HE2	1.96	0.65
1:B:345:TYR:CE2	1:B:349:ILE:HD11	2.32	0.65
1:A:345:TYR:CE2	1:A:349:ILE:HD11	2.38	0.58
1:B:105:ARG:HB3	1:B:250:GLU:HG2	1.86	0.57
1:A:136:LYS:HE2	1:A:141:LYS:O	2.06	0.55
1:B:34:ASP:O	1:B:37:ASN:OD1	2.24	0.54
1:B:66:SER:HA	4:B:607:HOH:O	2.07	0.54
1:B:145:TYR:CE2	1:B:220:HIS:CD2	2.95	0.54
1:B:23:PHE:HD2	1:B:269:VAL:HG13	1.72	0.53
1:A:214:PHE:CE1	1:A:349:ILE:HD13	2.43	0.53
1:B:170:VAL:CG1	2:B:501:HEM:HBC1	2.41	0.51
1:A:106:ASN:HB3	4:A:667:HOH:O	2.09	0.51
1:A:255:ASP:HB3	1:A:256:PRO:HD2	1.93	0.50
1:B:144:THR:O	1:B:148:MET:HG3	2.12	0.50
1:A:208:GLU:OE2	4:A:602:HOH:O	2.18	0.50
1:A:254:GLU:HB2	4:A:604:HOH:O	2.11	0.50
1:A:190:MET:HA	1:A:190:MET:HE2	1.93	0.50
1:B:30:GLU:OE1	1:B:135:LYS:HE2	2.11	0.50
1:B:170:VAL:HB	2:B:501:HEM:CBC	2.43	0.49
1:A:109:VAL:O	1:A:113:GLN:HG3	2.12	0.49
2:A:501:HEM:HHA	2:A:501:HEM:HBA2	1.95	0.48
1:B:185:PHE:CD1	1:B:188:MET:HE2	2.48	0.48
1:B:253:TRP:CE3	1:B:257:LYS:HD2	2.48	0.48
1:A:161:LYS:NZ	4:A:616:HOH:O	2.47	0.48
1:B:219:ASP:HB2	1:B:220:HIS:CE1	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:LYS:HD2	1:B:143:LEU:HD23	1.95	0.47
1:A:55:LEU:O	1:A:55:LEU:HG	2.11	0.47
1:B:109:VAL:O	1:B:113:GLN:HG3	2.14	0.47
1:B:318:GLU:O	1:B:319:PHE:C	2.56	0.47
1:A:46:LEU:O	1:A:50:ILE:HG13	2.15	0.47
1:A:189:GLN:OE1	1:A:190:MET:HE3	2.15	0.46
1:B:105:ARG:HA	1:B:250:GLU:O	2.16	0.46
1:B:185:PHE:HD1	1:B:188:MET:HE2	1.81	0.46
1:B:269:VAL:O	1:B:272:CYS:HB2	2.16	0.46
1:A:28:PRO:HD3	1:A:134:TRP:CZ2	2.50	0.45
1:B:17:ILE:CD1	1:B:23:PHE:CE1	3.00	0.45
1:A:253:TRP:CE3	1:A:257:LYS:CD	3.00	0.45
1:A:282:THR:HA	1:A:289:ALA:HB1	1.99	0.45
1:A:253:TRP:CG	1:A:257:LYS:HE2	2.51	0.44
1:B:190:MET:HA	1:B:190:MET:HE2	1.99	0.44
1:B:375:GLU:HA	1:B:376:ALA:O	2.18	0.44
1:A:197:LEU:HD23	1:A:197:LEU:C	2.42	0.44
1:B:178:ILE:HD11	1:B:269:VAL:HG12	1.99	0.44
1:A:253:TRP:CE3	1:A:257:LYS:HD2	2.52	0.44
1:A:345:TYR:CE2	1:A:349:ILE:CD1	3.00	0.44
1:B:269:VAL:HG23	1:B:270:PHE:CD2	2.53	0.44
1:B:80:ARG:NH2	1:B:128:ASP:OD2	2.49	0.44
1:B:170:VAL:HB	2:B:501:HEM:HBC1	1.99	0.44
1:B:384:LEU:HD12	1:B:385:MET:N	2.33	0.43
1:A:268:SER:O	1:A:272:CYS:HB3	2.19	0.43
1:B:64:MET:HG3	1:B:106:ASN:HA	2.01	0.43
1:B:105:ARG:CB	1:B:250:GLU:HG2	2.47	0.43
1:B:147:ASN:O	1:B:147:ASN:CG	2.62	0.43
1:B:138:ASP:HB3	1:B:141:LYS:HD2	2.00	0.42
1:B:55:LEU:O	1:B:55:LEU:HG	2.20	0.42
2:A:501:HEM:HHD	2:A:501:HEM:CBC	2.49	0.42
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	2.02	0.42
1:A:136:LYS:CE	1:A:141:LYS:O	2.67	0.42
1:B:103:LEU:O	1:B:250:GLU:HB3	2.19	0.42
1:B:162:GLY:O	1:B:166:VAL:HG23	2.20	0.41
2:A:501:HEM:HHD	2:A:501:HEM:HBC2	2.02	0.41
1:B:61:LYS:O	1:B:61:LYS:HG3	2.21	0.41
1:B:79:ALA:HB3	1:B:114:LEU:HD21	2.03	0.41
1:B:379:THR:O	1:B:382:THR:HG23	2.21	0.41
1:A:59:VAL:HG11	1:A:90:TYR:CD2	2.55	0.41
1:A:280:GLN:OE1	1:A:280:GLN:HA	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:LEU:C	1:B:197:LEU:HD23	2.46	0.41
1:B:351:THR:HA	1:B:355:LEU:HB2	2.02	0.41
1:A:383:ASP:OD1	1:A:383:ASP:C	2.64	0.40
1:B:73:HIS:HA	1:B:76:GLN:OE1	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:660:HOH:O	4:B:637:HOH:O[3_445]	2.05	0.15

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	377/392 (96%)	355 (94%)	19 (5%)	3 (1%)	16	18
1	B	377/392 (96%)	361 (96%)	14 (4%)	2 (0%)	24	29
All	All	754/784 (96%)	716 (95%)	33 (4%)	5 (1%)	18	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	375	GLU
1	B	143	LEU
1	B	376	ALA
1	A	179	LYS
1	A	376	ALA

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	327/339 (96%)	303 (93%)	24 (7%)	13	16
1	B	327/339 (96%)	295 (90%)	32 (10%)	7	8
All	All	654/678 (96%)	598 (91%)	56 (9%)	10	11

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLU
1	A	44	LYS
1	A	54	GLN
1	A	55	LEU
1	A	57	GLU
1	A	59	VAL
1	A	66	SER
1	A	106	ASN
1	A	109	VAL
1	A	116	LYS
1	A	135	LYS
1	A	141	LYS
1	A	179	LYS
1	A	189	GLN
1	A	191	GLN
1	A	209	LYS
1	A	237	TRP
1	A	269	VAL
1	A	272	CYS
1	A	309	SER
1	A	323	LYS
1	A	349	ILE
1	A	374	GLU
1	A	377	LYS
1	B	17	ILE
1	B	44	LYS
1	B	57	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	58	ARG
1	B	61	LYS
1	B	66	SER
1	B	109	VAL
1	B	116	LYS
1	B	135	LYS
1	B	136	LYS
1	B	141	LYS
1	B	149	ASP
1	B	186	LYS
1	B	189	GLN
1	B	190	MET
1	B	191	GLN
1	B	195	THR
1	B	205	SER
1	B	209	LYS
1	B	219	ASP
1	B	224	LYS
1	B	280	GLN
1	B	309	SER
1	B	321	LEU
1	B	323	LYS
1	B	342	LEU
1	B	355	LEU
1	B	374	GLU
1	B	377	LYS
1	B	389	LYS
1	B	396	GLU
1	B	401	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	HIS
1	A	113	GLN
1	A	191	GLN
1	A	212	GLN
1	A	348	GLN
1	B	54	GLN
1	B	73	HIS
1	B	113	GLN
1	B	303	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	HUC	A	502	2	19,21,21	1.42	1 (5%)	20,29,29	3.48	7 (35%)
2	HEM	A	501	3,1	50,50,50	1.21	6 (12%)	66,82,82	1.25	8 (12%)
2	HEM	B	501	3,1	50,50,50	1.32	4 (8%)	66,82,82	1.47	11 (16%)
3	HUC	B	502	2	19,21,21	1.37	2 (10%)	20,29,29	3.40	6 (30%)

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	HUC	A	502	2	-	2/5/16/16	0/3/3/3
2	HEM	A	501	3,1	-	4/14/54/54	-
2	HEM	B	501	3,1	-	5/14/54/54	-
3	HUC	B	502	2	-	2/5/16/16	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	HUC	C14-C18	-4.65	1.36	1.41
3	B	502	HUC	C14-C18	-3.65	1.37	1.41
2	B	501	HEM	CAB-C3B	3.21	1.56	1.47
2	B	501	HEM	FE-ND	2.99	2.04	1.94
2	B	501	HEM	C3B-C2B	-2.60	1.32	1.37
3	B	502	HUC	C04-N05	2.55	1.44	1.37
2	A	501	HEM	FE-NB	2.44	2.02	1.94
2	A	501	HEM	C3C-C2C	-2.36	1.32	1.37
2	A	501	HEM	C3D-C2D	-2.18	1.32	1.36
2	A	501	HEM	CAB-C3B	2.18	1.53	1.47
2	B	501	HEM	CAC-C3C	2.17	1.53	1.47
2	A	501	HEM	CAC-C3C	2.14	1.53	1.47
2	A	501	HEM	CMD-C2D	2.11	1.55	1.50

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	HUC	C14-C15-N16	-10.87	107.96	111.41
3	B	502	HUC	C14-C15-N16	-10.34	108.13	111.41
3	B	502	HUC	C15-N16-N17	5.95	109.17	106.02
3	A	502	HUC	C15-N16-N17	5.89	109.14	106.02
3	A	502	HUC	C03-C04-N05	-5.69	112.60	121.58
3	B	502	HUC	C03-C04-N05	-5.51	112.89	121.58
3	B	502	HUC	C07-C06-N05	-4.87	104.20	112.09
3	A	502	HUC	C07-C06-N05	-4.73	104.43	112.09
2	B	501	HEM	C3B-C2B-C1B	4.38	109.73	106.49
3	A	502	HUC	C14-C18-N17	3.73	109.49	106.47
3	B	502	HUC	C14-C18-N17	3.69	109.46	106.47
2	B	501	HEM	CAA-CBA-CGA	-3.55	105.97	113.60
2	B	501	HEM	CHB-C1B-NB	3.29	128.43	124.37
2	A	501	HEM	CBD-CAD-C3D	-2.90	104.58	112.63
3	A	502	HUC	BR1-C02-C03	-2.87	115.28	119.27
2	A	501	HEM	CMB-C2B-C1B	-2.85	120.70	125.04
2	B	501	HEM	CHD-C4C-NC	2.81	127.48	124.44
2	B	501	HEM	CAB-C3B-C2B	-2.81	119.36	128.60
2	B	501	HEM	CHC-C4B-NB	-2.75	121.43	124.42
2	A	501	HEM	O1D-CGD-CBD	-2.65	114.56	123.08
2	A	501	HEM	C1C-CHC-C4B	-2.53	120.59	126.06
2	B	501	HEM	CAD-CBD-CGD	-2.45	108.32	113.60
2	A	501	HEM	O2D-CGD-CBD	2.39	121.71	114.03
2	A	501	HEM	C4A-C3A-C2A	2.33	109.56	106.83
2	B	501	HEM	CHC-C4B-C3B	2.31	130.10	125.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	CAC-C3C-C4C	-2.29	119.36	124.90
2	A	501	HEM	CHC-C1C-NC	2.25	126.87	124.44
2	B	501	HEM	C4D-ND-C1D	2.24	107.38	105.07
3	B	502	HUC	C12-C07-C06	-2.15	105.71	110.30
2	A	501	HEM	CBC-CAC-C3C	-2.13	117.02	127.62
2	B	501	HEM	CAB-C3B-C4B	2.11	134.28	124.47
3	A	502	HUC	C19-C18-C14	-2.00	120.16	122.22

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	HUC	C03-C04-N05-C06
3	A	502	HUC	C14-C04-N05-C06
3	B	502	HUC	C03-C04-N05-C06
3	B	502	HUC	C14-C04-N05-C06
2	A	501	HEM	C1A-C2A-CAA-CBA
2	B	501	HEM	C1A-C2A-CAA-CBA
2	A	501	HEM	C3D-CAD-CBD-CGD
2	B	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	CAA-CBA-CGA-O1A
2	B	501	HEM	C3A-C2A-CAA-CBA
2	B	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	C3A-C2A-CAA-CBA
2	A	501	HEM	CAD-CBD-CGD-O2D

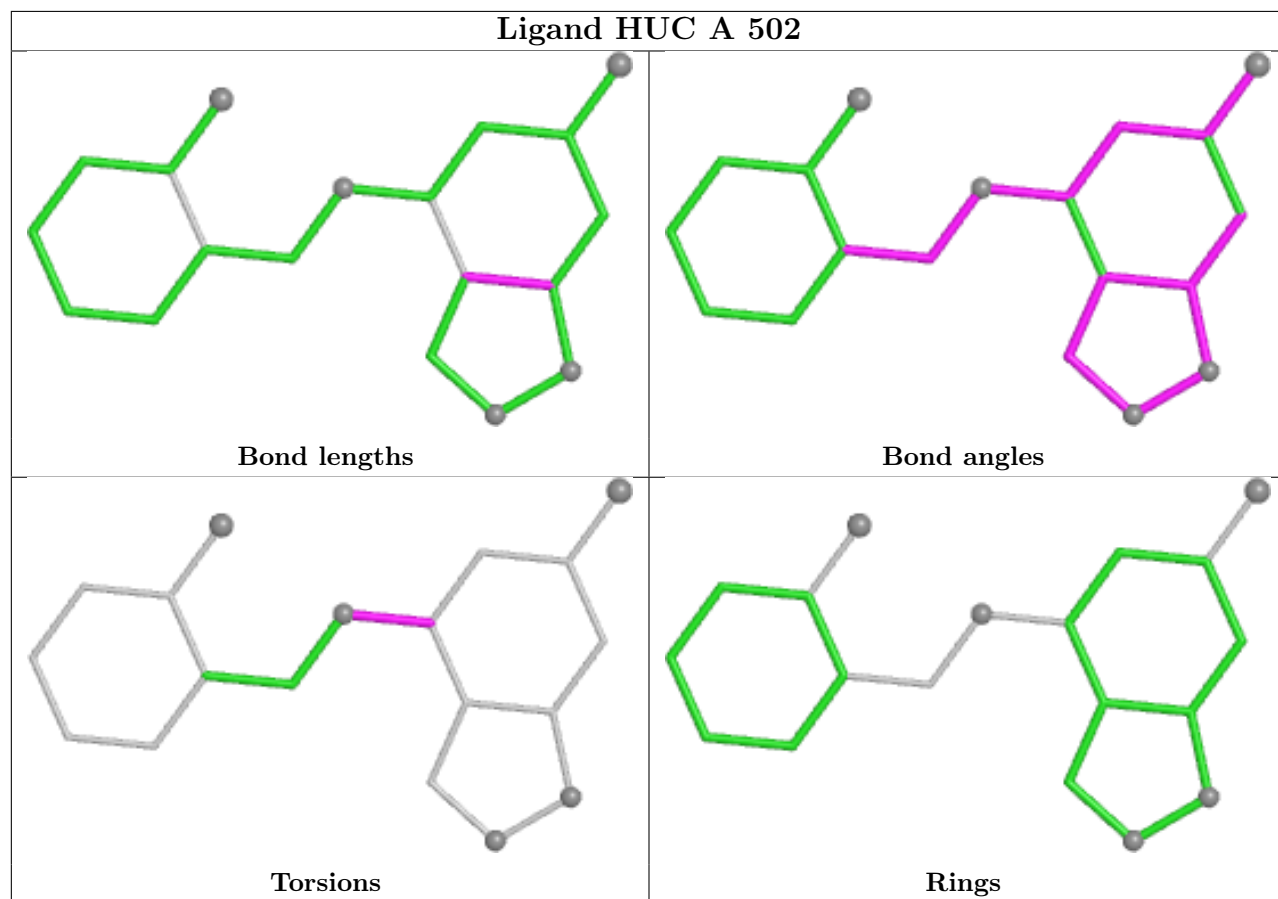
There are no ring outliers.

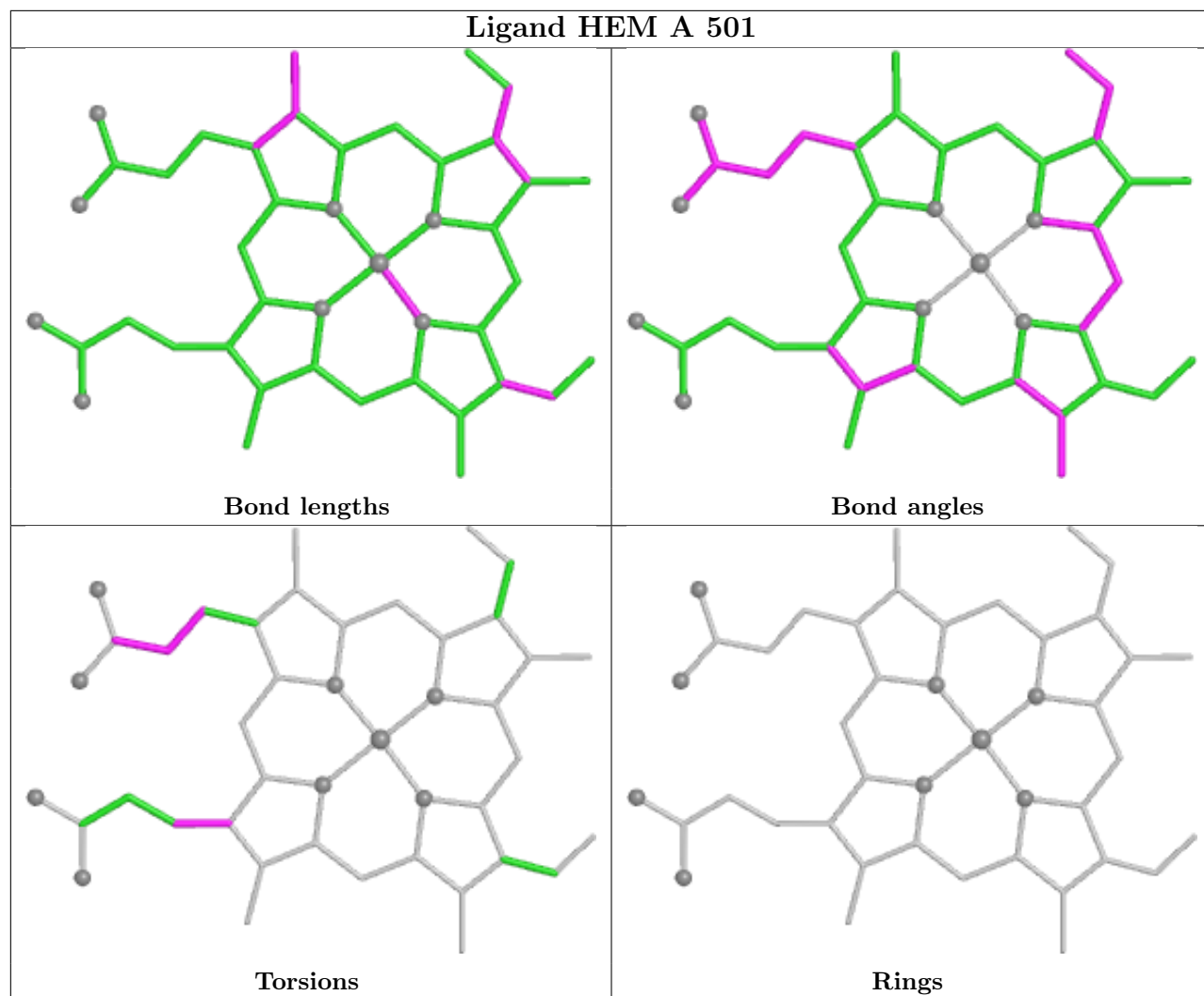
2 monomers are involved in 7 short contacts:

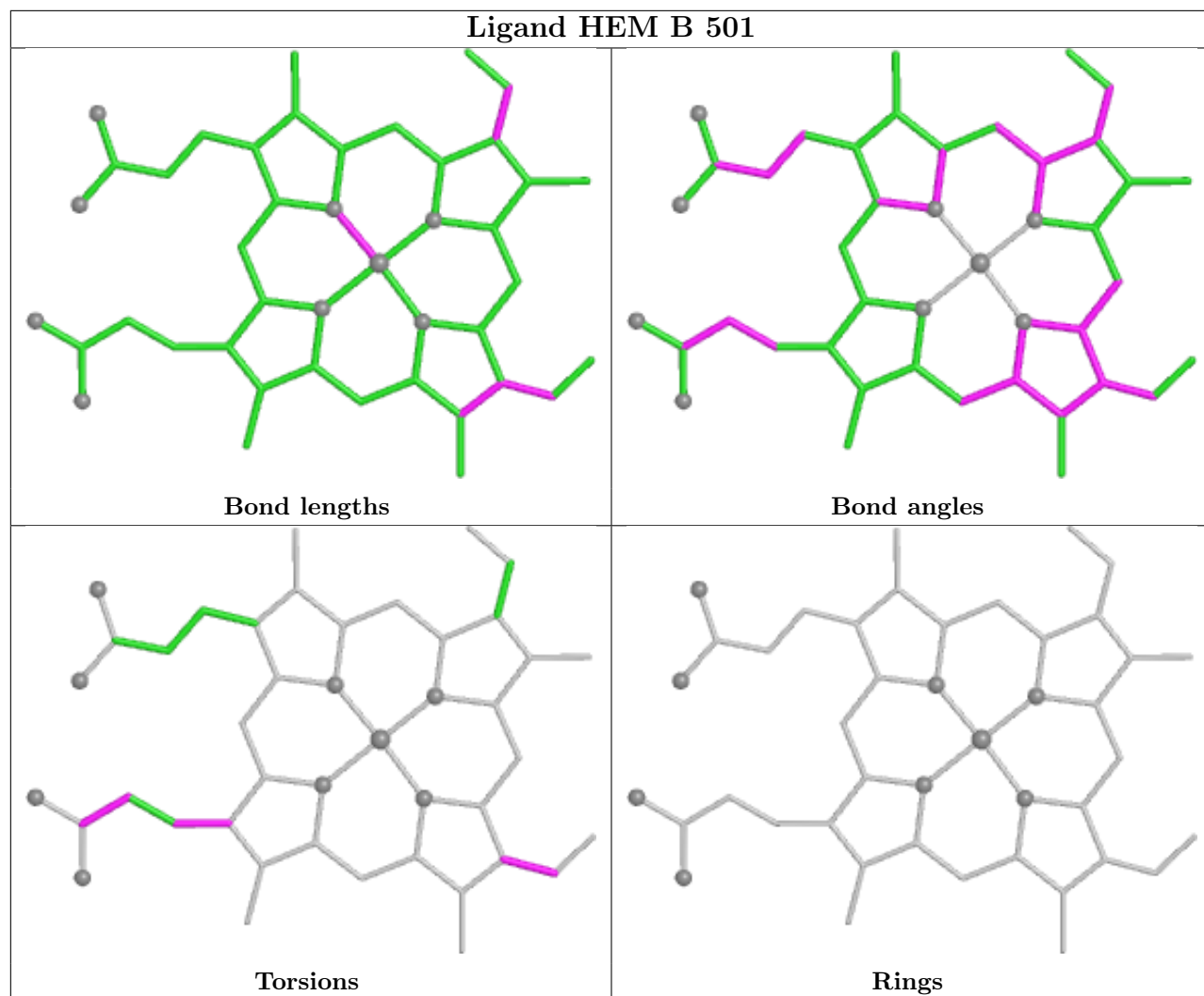
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	3	0
2	B	501	HEM	4	0

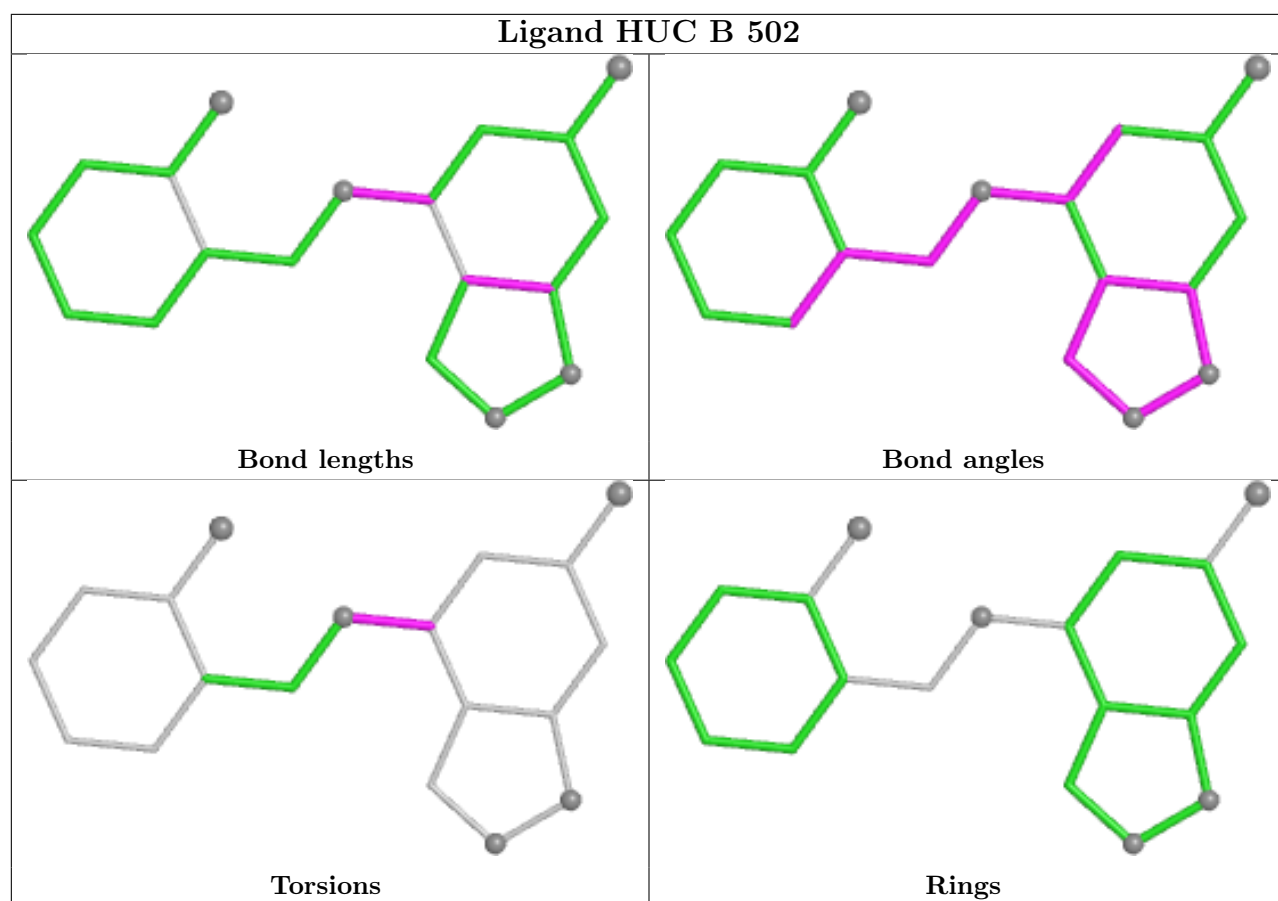
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	380/392 (96%)	0.33	10 (2%) 57 59	28, 57, 79, 120	1 (0%)
1	B	380/392 (96%)	0.70	21 (5%) 30 31	33, 67, 95, 117	1 (0%)
All	All	760/784 (96%)	0.51	31 (4%) 41 43	28, 62, 91, 120	2 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	376	ALA	4.8
1	B	12	SER	4.2
1	B	382	THR	4.0
1	B	362	PRO	3.7
1	A	284	GLY	3.6
1	A	12	SER	3.3
1	A	285	GLY	3.2
1	A	362	PRO	3.2
1	A	376	ALA	2.9
1	B	380	GLY	2.9
1	B	324	GLY	2.7
1	B	284	GLY	2.7
1	B	329[A]	ARG	2.6
1	B	286	GLY	2.6
1	B	287	HIS	2.6
1	B	375	GLU	2.5
1	A	380	GLY	2.5
1	B	251	GLY	2.5
1	B	283	ALA	2.4
1	B	253	TRP	2.4
1	B	248	VAL	2.3
1	B	109	VAL	2.3
1	B	377	LYS	2.3
1	B	70	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	401	LYS	2.2
1	B	297	ARG	2.2
1	B	62	LEU	2.1
1	A	374	GLU	2.1
1	A	253	TRP	2.1
1	A	375	GLU	2.0
1	A	13	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

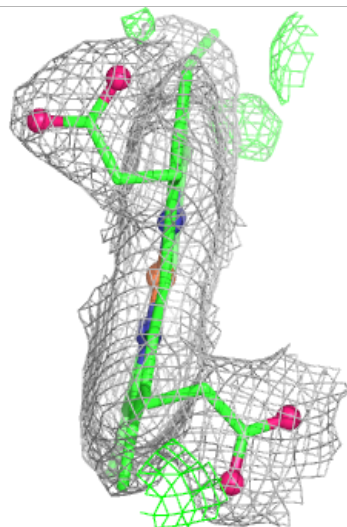
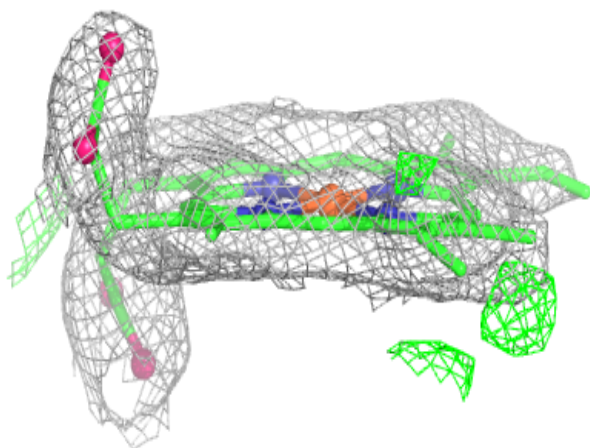
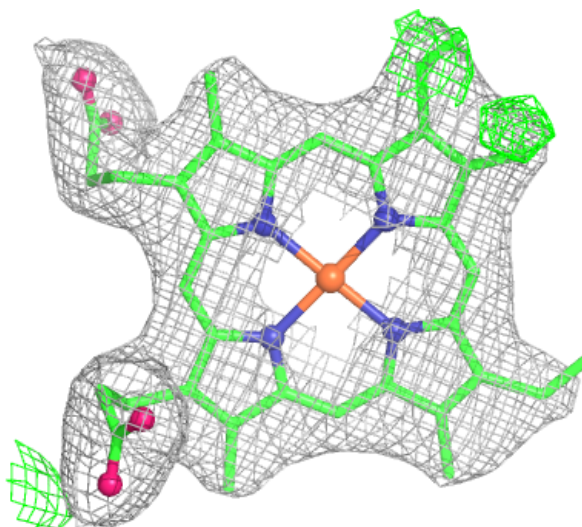
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B	501	43/43	0.98	0.09	42,48,57,73	0
2	HEM	A	501	43/43	0.99	0.06	34,40,48,56	0
3	HUC	A	502	19/19	0.99	0.06	37,45,53,57	0
3	HUC	B	502	19/19	0.99	0.06	45,52,61,77	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.

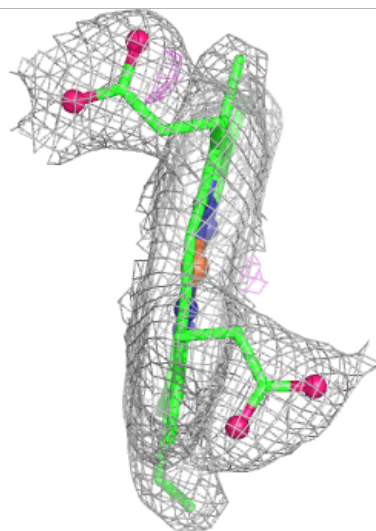
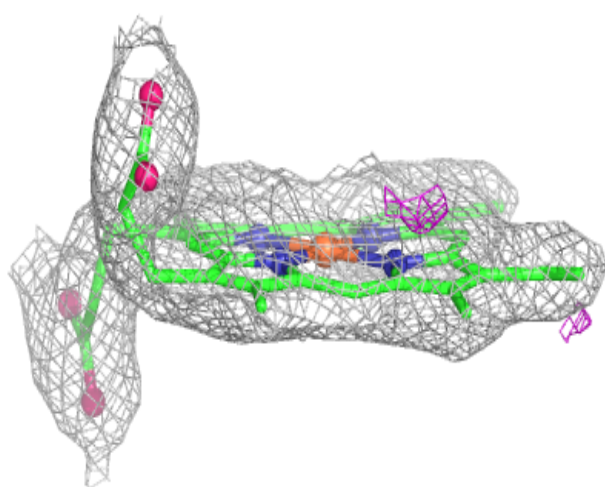
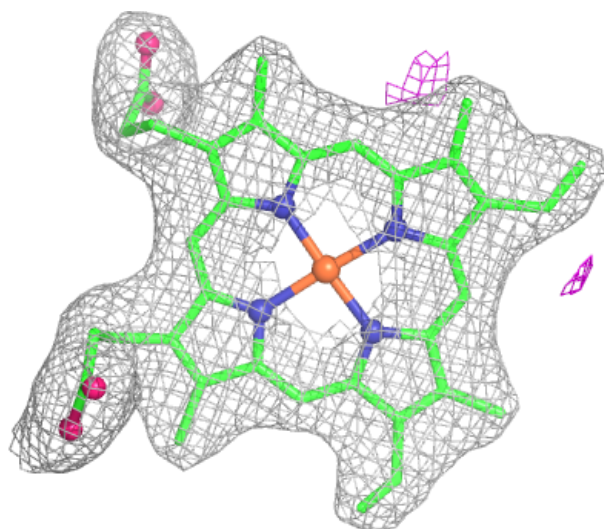
Electron density around HEM B 501:

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



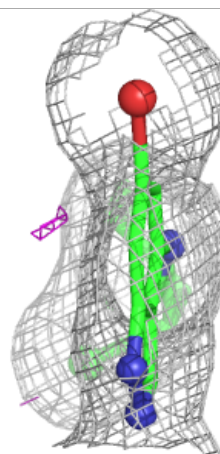
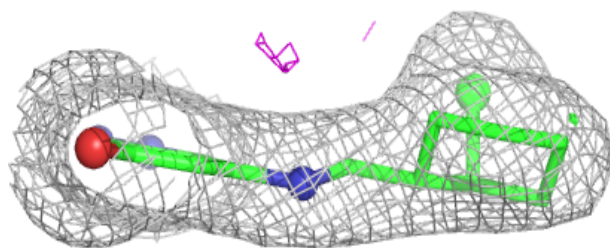
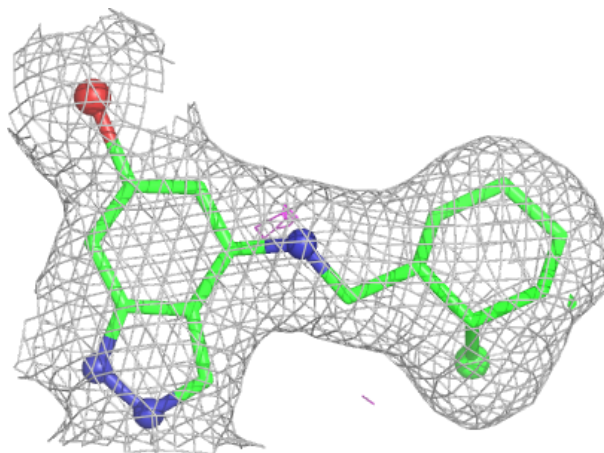
Electron density around HEM A 501:

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



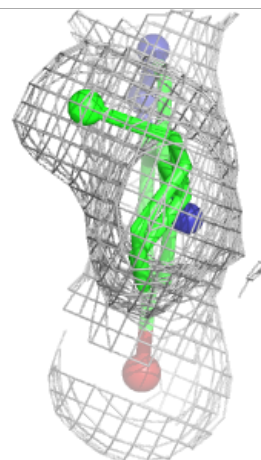
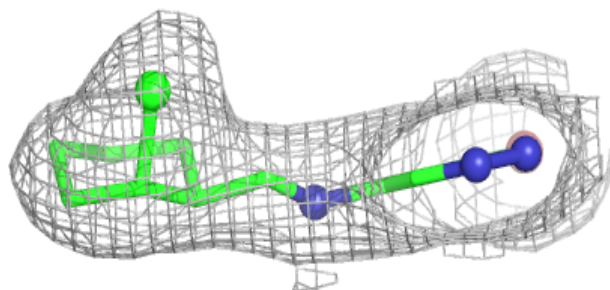
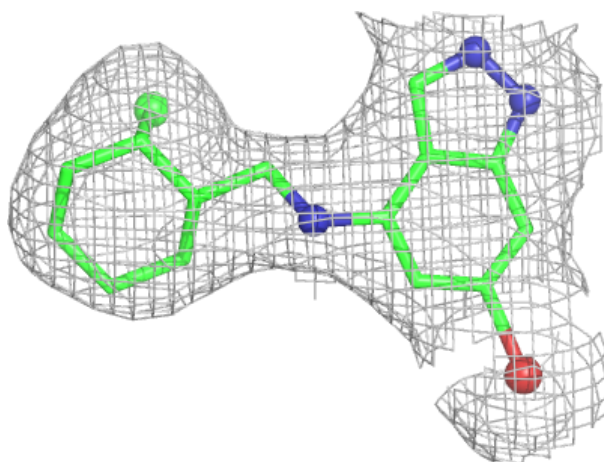
Electron density around HUC A 502:

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



Electron density around HUC B 502:

$2mF_o-DF_c$ (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.