



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:12 PM UTC

PDB ID : 8JC4 / pdb_00008jc4
Title : Crystal structure of the P450 BM3 heme domain mutant F87A-T268V in complex with Pyd-Pid-Phe and hydroxylamine
Authors : Jiang, Y.; Dong, S.; Feng, Y.; Cong, Z.
Deposited on : 2023-05-10
Resolution : 2.64 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

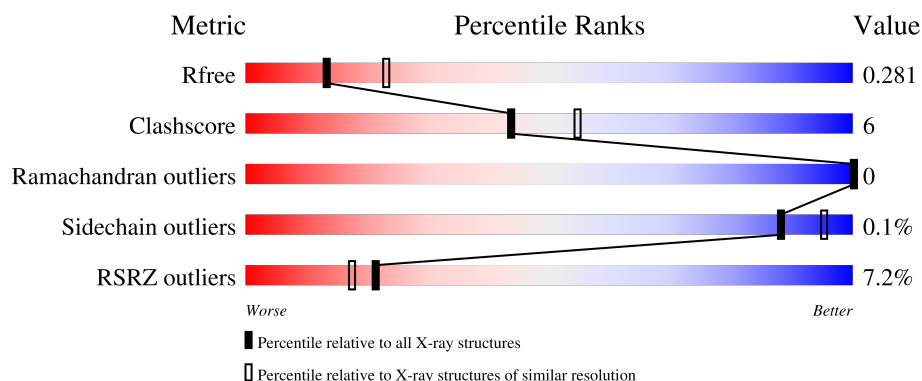
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	465	6% 81% 15% .
1	B	465	8% 85% 12% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7503 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.

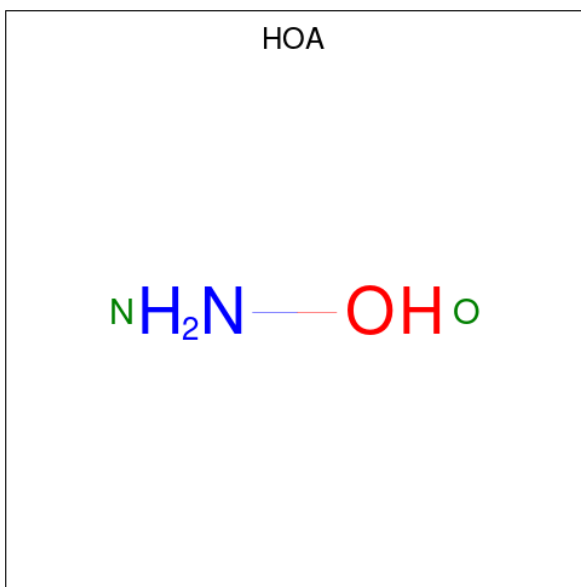
- Molecule 1 is a protein called Bifunctional cytochrome P450/NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	0
			3513	2249	597	650	17			
1	B	448	Total	C	N	O	S	0	0	0
			3543	2264	603	659	17			

There are 22 discrepancies between the modelled and reference sequences:

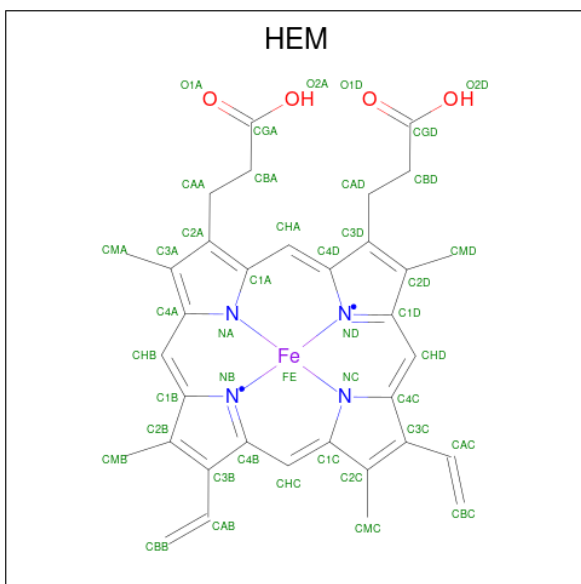
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P14779
A	87	ALA	PHE	engineered mutation	UNP P14779
A	268	VAL	THR	engineered mutation	UNP P14779
A	456	LEU	-	expression tag	UNP P14779
A	457	GLU	-	expression tag	UNP P14779
A	458	HIS	-	expression tag	UNP P14779
A	459	HIS	-	expression tag	UNP P14779
A	460	HIS	-	expression tag	UNP P14779
A	461	HIS	-	expression tag	UNP P14779
A	462	HIS	-	expression tag	UNP P14779
A	463	HIS	-	expression tag	UNP P14779
B	-1	GLY	-	expression tag	UNP P14779
B	87	ALA	PHE	engineered mutation	UNP P14779
B	268	VAL	THR	engineered mutation	UNP P14779
B	456	LEU	-	expression tag	UNP P14779
B	457	GLU	-	expression tag	UNP P14779
B	458	HIS	-	expression tag	UNP P14779
B	459	HIS	-	expression tag	UNP P14779
B	460	HIS	-	expression tag	UNP P14779
B	461	HIS	-	expression tag	UNP P14779
B	462	HIS	-	expression tag	UNP P14779
B	463	HIS	-	expression tag	UNP P14779

- Molecule 2 is HYDROXYAMINE (CCD ID: HOA) (formula: H_3NO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	N	O		0	0
			2	1	1			
2	B	1	Total	N	O		0	0
			2	1	1			

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



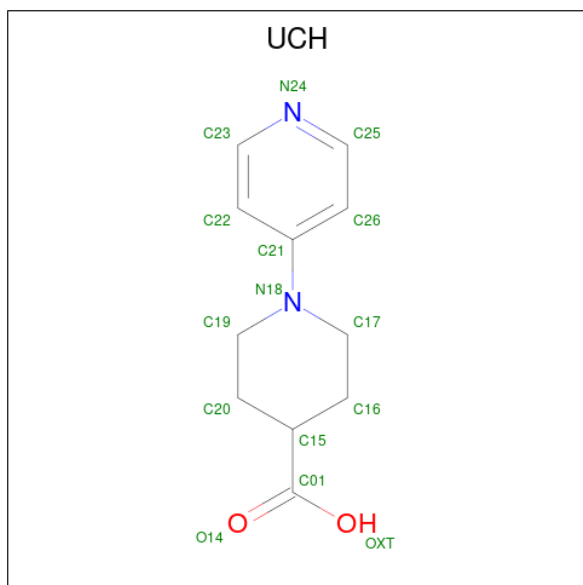
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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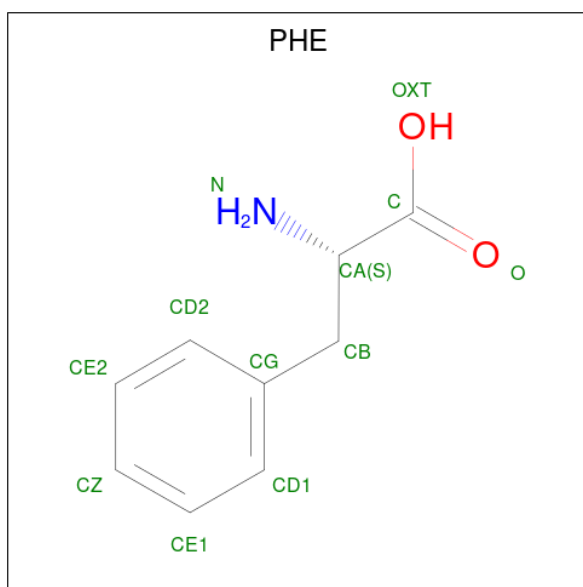
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is 1-pyridin-4-ylpiperidine-4-carboxylic acid (CCD ID: UCH) (formula: $C_{11}H_{14}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	1
			14	11	2	1		
4	A	1	Total	C	N	O	0	1
			14	11	2	1		
4	B	1	Total	C	N	O	0	1
			14	11	2	1		
4	B	1	Total	C	N	O	0	1
			14	11	2	1		

- Molecule 5 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	1
			12	9	1	2		
5	A	1	Total	C	N	O	0	1
			12	9	1	2		
5	B	1	Total	C	N	O	0	1
			12	9	1	2		
5	B	1	Total	C	N	O	0	1
			12	9	1	2		

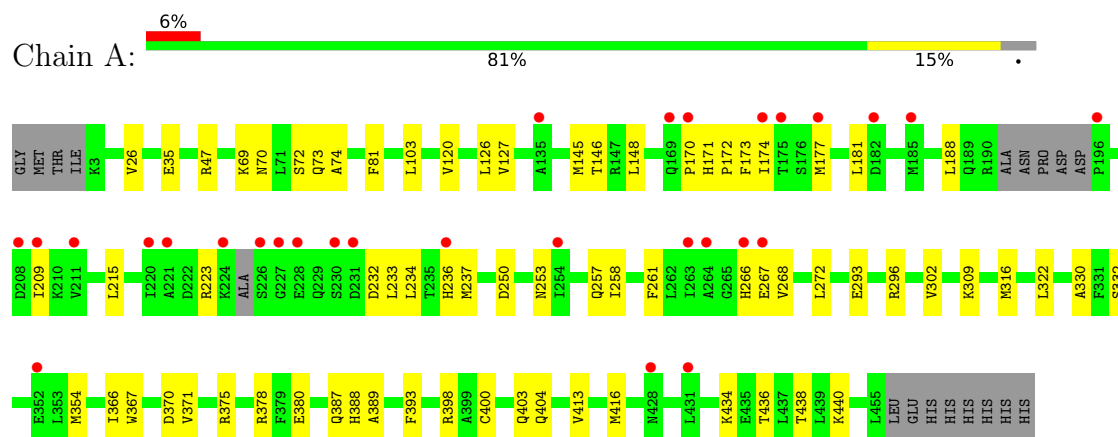
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	119	Total	O	0	0
			119	119		
6	B	134	Total	O	0	0
			134	134		

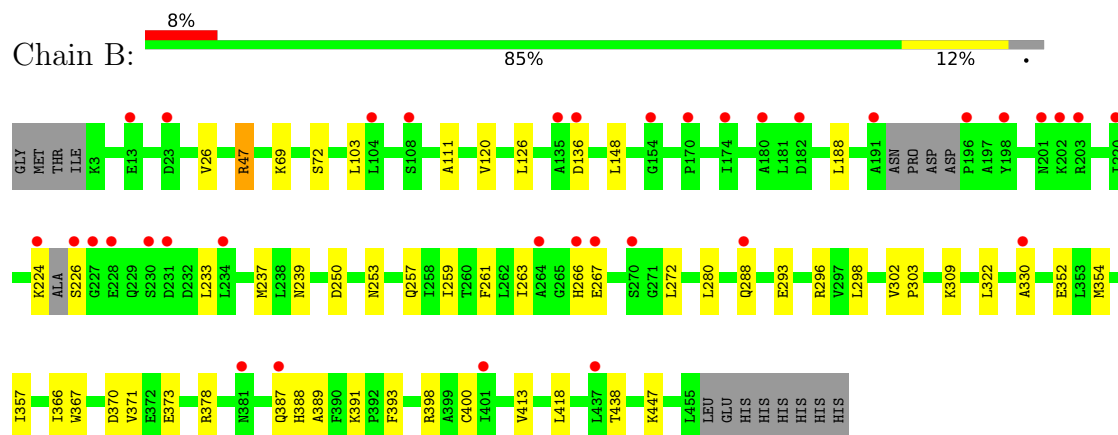
3 Residue-property plots [i](#)

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: Bifunctional cytochrome P450/NADPH-P450 reductase



- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.84Å 148.29Å 64.92Å 90.00° 100.38° 90.00°	Depositor
Resolution (Å)	19.89 – 2.64 19.89 – 2.64	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.89-2.64) 98.4 (19.89-2.64)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.77 (at 2.63Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.245 , 0.280 0.245 , 0.281	Depositor DCC
R_{free} test set	2000 reflections (3.67%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	7503	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.6303e-03.*

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: UCH, HEM, HOA

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	0.15	1/3592 (0.0%)	0.35	2/4866 (0.0%)
1	B	0.15	0/3622	0.32	0/4904
All	All	0.15	1/7214 (0.0%)	0.34	2/9770 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	404	GLN	C-N	-6.05	1.26	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	436	THR	N-CA-C	-8.17	100.91	108.75
1	A	403	GLN	O-C-N	5.88	128.13	122.07

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	3513	0	3426	44	0
1	B	3543	0	3464	37	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
3	A	43	0	30	2	0
3	B	43	0	30	2	0
4	A	28	0	0	1	0
4	B	28	0	0	2	0
5	A	24	0	16	1	0
5	B	24	0	16	4	0
6	A	119	0	0	4	0
6	B	134	0	0	7	0
All	All	7503	0	6982	87	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 6.

All (87) 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:330:ALA:HB3	4:B:505[B]:UCH:C16	2.02	0.89
1:B:391:LYS:HA	6:B:623:HOH:O	1.79	0.81
3:A:502:HEM:HBC2	3:A:502:HEM:HHD	1.74	0.69
1:B:370:ASP:O	1:B:378:ARG:NH2	2.25	0.66
1:A:74:ALA:HB2	1:A:188:LEU:HD11	1.79	0.65
3:B:502:HEM:HBC2	3:B:502:HEM:HHD	1.76	0.65
1:A:232:ASP:O	1:A:236:HIS:ND1	2.30	0.63
1:B:288:GLN:NE2	6:B:615:HOH:O	2.34	0.61
1:B:148:LEU:HD21	1:B:413:VAL:HG21	1.84	0.60
1:A:146:THR:HG23	1:A:266:HIS:HD2	1.67	0.59
1:A:170:PRO:HB3	1:A:174:ILE:HD11	1.84	0.59
1:A:316:MET:HE2	1:A:380:GLU:HA	1.84	0.59
1:A:367:TRP:HB2	1:A:371:VAL:HG12	1.84	0.59
1:A:81:PHE:HB3	1:A:209:ILE:HG12	1.85	0.58
1:A:268:VAL:HG22	1:A:438:THR:HG21	1.85	0.58
1:B:224:LYS:O	1:B:226:SER:N	2.36	0.58
1:A:120:VAL:HG11	1:A:302:VAL:HG13	1.86	0.56
3:B:502:HEM:HBB2	3:B:502:HEM:HMB1	1.86	0.56
1:A:148:LEU:HD21	1:A:413:VAL:HG21	1.85	0.56
3:A:502:HEM:HBB2	3:A:502:HEM:HMB2	1.87	0.56
1:B:367:TRP:HB2	1:B:371:VAL:HG12	1.89	0.54
1:A:47:ARG:NH1	6:A:620:HOH:O	2.40	0.53
1:A:296:ARG:NH2	6:A:621:HOH:O	2.40	0.53
1:A:375:ARG:NH2	6:A:619:HOH:O	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:LEU:HD13	1:B:261:PHE:HZ	1.73	0.53
1:A:223:ARG:NH2	1:A:232:ASP:OD2	2.36	0.52
1:B:120:VAL:HG11	1:B:302:VAL:HG13	1.91	0.52
1:A:103:LEU:HD13	1:A:261:PHE:HZ	1.74	0.51
1:A:234:LEU:HD13	1:A:258:ILE:HD11	1.93	0.51
1:A:293:GLU:HG3	1:A:296:ARG:HH11	1.76	0.51
1:A:370:ASP:O	1:A:378:ARG:NH2	2.38	0.51
1:A:47:ARG:NH1	1:A:73:GLN:HB2	2.26	0.50
1:B:293:GLU:HA	1:B:296:ARG:HG2	1.93	0.49
1:B:266:HIS:CG	1:B:267:GLU:N	2.80	0.49
1:B:272:LEU:HD13	1:B:322:LEU:HG	1.94	0.48
1:B:47:ARG:HH22	1:B:354:MET:HE3	1.78	0.48
1:B:111:ALA:HA	6:B:608:HOH:O	2.12	0.48
1:A:272:LEU:HD13	1:A:322:LEU:HG	1.96	0.47
1:A:366:ILE:HG21	1:A:389:ALA:HB1	1.97	0.47
1:A:177:MET:O	1:A:181:LEU:HD13	2.15	0.47
1:B:253:ASN:O	1:B:257:GLN:HG2	2.14	0.47
1:B:26:VAL:HG22	5:B:504[A]:PHE:HB3	1.98	0.46
1:A:26:VAL:HG22	5:A:504[A]:PHE:HB3	1.96	0.46
1:B:366:ILE:HG21	1:B:389:ALA:HB1	1.97	0.46
1:A:126:LEU:HD22	1:A:148:LEU:HD13	1.97	0.46
1:B:72:SER:HB2	5:B:506[B]:PHE:OXT	2.16	0.45
1:A:174:ILE:HA	1:A:177:MET:HB3	1.97	0.45
1:A:127:VAL:HG21	1:A:416:MET:HE2	1.97	0.45
1:A:266:HIS:CG	1:A:267:GLU:N	2.83	0.45
1:A:126:LEU:HD21	1:A:145:MET:HE1	1.98	0.45
1:B:373:GLU:HA	6:B:642:HOH:O	2.16	0.45
1:B:267:GLU:HG3	1:B:438:THR:HG21	1.99	0.45
5:B:506[B]:PHE:O	5:B:506[B]:PHE:CG	2.70	0.45
1:A:233:LEU:O	1:A:237:MET:HG3	2.18	0.44
1:A:253:ASN:O	1:A:257:GLN:HG2	2.17	0.44
1:B:126:LEU:HD22	1:B:148:LEU:HD13	2.00	0.44
1:A:250:ASP:N	1:A:250:ASP:OD1	2.50	0.44
1:B:136:ASP:O	1:B:447:LYS:NZ	2.50	0.44
1:A:387:GLN:HG2	1:A:388:HIS:CD2	2.53	0.43
1:A:35:GLU:O	6:A:602:HOH:O	2.21	0.43
1:B:387:GLN:HG2	1:B:388:HIS:CD2	2.53	0.43
1:B:188:LEU:HD23	1:B:188:LEU:HA	1.87	0.43
1:B:280:LEU:HD13	1:B:418:LEU:HD21	2.01	0.43
1:A:393:PHE:HB3	1:A:400:CYS:HB3	2.01	0.43
1:B:47:ARG:NH1	1:B:352:GLU:OE1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:LYS:HD3	1:A:440:LYS:NZ	2.33	0.42
1:B:233:LEU:O	1:B:237:MET:HG3	2.20	0.42
1:B:239:ASN:HB2	6:B:710:HOH:O	2.18	0.42
1:B:393:PHE:HB3	1:B:400:CYS:HB3	2.01	0.42
1:A:70:ASN:O	1:A:332:SER:HB3	2.20	0.42
1:A:173:PHE:HB2	1:A:215:LEU:HD13	2.00	0.42
4:B:503[A]:UCH:C22	6:B:695:HOH:O	2.67	0.42
1:B:309:LYS:HA	1:B:309:LYS:HD3	1.80	0.42
1:A:103:LEU:HD21	1:A:237:MET:HG2	2.02	0.42
1:B:250:ASP:OD1	1:B:250:ASP:N	2.53	0.41
1:A:171:HIS:CG	1:A:172:PRO:HD2	2.55	0.41
1:A:330:ALA:HB3	4:A:505[B]:UCH:C16	2.51	0.41
1:B:188:LEU:HD22	5:B:506[B]:PHE:HD1	1.86	0.41
1:B:69:LYS:HD3	1:B:398:ARG:CZ	2.51	0.41
1:B:259:ILE:O	1:B:263:ILE:HG13	2.21	0.41
1:B:298:LEU:HD22	1:B:303:PRO:HB3	2.03	0.41
1:A:69:LYS:HB3	1:A:398:ARG:HG3	2.03	0.40
1:A:173:PHE:CD1	1:A:215:LEU:HD22	2.56	0.40
1:B:330:ALA:HA	1:B:357:ILE:HG13	2.03	0.40
1:A:72:SER:HB3	1:A:354:MET:HE1	2.04	0.40
1:A:309:LYS:HA	1:A:309:LYS:HD3	1.81	0.40
1:B:352:GLU:HB3	6:B:601:HOH:O	2.22	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	441/465 (95%)	423 (96%)	18 (4%)	0	100	100
1	B	442/465 (95%)	424 (96%)	18 (4%)	0	100	100
All	All	883/930 (95%)	847 (96%)	36 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	369/407 (91%)	369 (100%)	0	100	100
1	B	375/407 (92%)	374 (100%)	1 (0%)	86	93
All	All	744/814 (91%)	743 (100%)	1 (0%)	88	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	47	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	73	GLN
1	A	134	ASN
1	A	204	GLN
1	A	229	GLN
1	A	266	HIS
1	A	403	GLN
1	B	206	GLN
1	B	229	GLN
1	B	239	ASN
1	B	403	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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	HEM	A	502	2	50,50,50	1.46	8 (16%)	67,82,82	1.20	5 (7%)
4	UCH	B	503[A]	5	15,15,16	1.23	4 (26%)	19,19,21	1.59	4 (21%)
2	HOA	B	501	3	0,1,1	-	-	-		
4	UCH	A	505[B]	5	15,15,16	1.21	2 (13%)	19,19,21	1.78	6 (31%)
3	HEM	B	502	2	50,50,50	1.44	7 (14%)	67,82,82	1.18	5 (7%)
5	PHE	B	506[B]	4	11,12,12	0.77	1 (9%)	11,15,15	1.09	1 (9%)
2	HOA	A	501	3	0,1,1	-	-	-		
4	UCH	B	505[B]	5	15,15,16	1.28	3 (20%)	19,19,21	1.60	4 (21%)
5	PHE	A	506[B]	4	11,12,12	0.67	0	11,15,15	0.83	0
5	PHE	B	504[A]	4	11,12,12	0.69	0	11,15,15	0.71	0
4	UCH	A	503[A]	5	15,15,16	1.24	3 (20%)	19,19,21	1.65	8 (42%)
5	PHE	A	504[A]	4	11,12,12	0.69	0	11,15,15	0.71	0

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	HEM	A	502	2	-	3/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	UCH	B	503[A]	5	-	0/6/16/18	0/2/2/2
4	UCH	A	505[B]	5	-	6/6/16/18	0/2/2/2
5	PHE	B	506[B]	4	-	2/8/8/8	0/1/1/1
3	HEM	B	502	2	-	3/14/54/54	-
4	UCH	B	505[B]	5	-	6/6/16/18	0/2/2/2
5	PHE	A	506[B]	4	-	0/8/8/8	0/1/1/1
5	PHE	B	504[A]	4	-	0/8/8/8	0/1/1/1
4	UCH	A	503[A]	5	-	0/6/16/18	0/2/2/2
5	PHE	A	504[A]	4	-	0/8/8/8	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	HEM	FE-NC	3.55	2.06	1.95
3	A	502	HEM	FE-NB	3.53	2.05	1.94
3	B	502	HEM	FE-NB	3.49	2.05	1.94
3	A	502	HEM	FE-NC	3.46	2.06	1.95
3	A	502	HEM	FE-NA	3.38	2.06	1.95
3	A	502	HEM	FE-ND	3.14	2.04	1.94
3	B	502	HEM	CAB-C3B	3.10	1.55	1.47
3	A	502	HEM	CAB-C3B	3.10	1.55	1.47
3	B	502	HEM	FE-ND	3.01	2.04	1.94
3	B	502	HEM	FE-NA	2.98	2.05	1.95
3	A	502	HEM	CAC-C3C	2.96	1.55	1.47
3	B	502	HEM	CAC-C3C	2.88	1.55	1.47
4	A	505[B]	UCH	C21-N18	2.65	1.46	1.38
4	B	505[B]	UCH	C20-C15	-2.62	1.47	1.53
4	A	503[A]	UCH	C21-N18	2.54	1.45	1.38
4	B	503[A]	UCH	C21-N18	2.48	1.45	1.38
4	B	505[B]	UCH	C21-N18	2.44	1.45	1.38
4	B	505[B]	UCH	C16-C15	-2.12	1.48	1.53
3	A	502	HEM	CMB-C2B	2.10	1.55	1.50
3	B	502	HEM	CMB-C2B	2.10	1.55	1.50
4	A	505[B]	UCH	C16-C15	-2.06	1.48	1.53
4	B	503[A]	UCH	C20-C15	-2.04	1.48	1.53
4	A	503[A]	UCH	C16-C15	-2.04	1.48	1.53
3	A	502	HEM	CMA-C3A	2.04	1.54	1.50
4	A	503[A]	UCH	C20-C15	-2.03	1.48	1.53
5	B	506[B]	PHE	OXT-C	-2.02	1.24	1.30
4	B	503[A]	UCH	C16-C15	-2.02	1.48	1.53
4	B	503[A]	UCH	C17-N18	2.02	1.50	1.46

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	505[B]	UCH	C20-C19-N18	4.10	120.23	110.92
4	A	505[B]	UCH	C19-C20-C15	3.32	116.03	110.99
4	A	503[A]	UCH	C19-N18-C17	3.24	118.85	111.57
5	B	506[B]	PHE	OXT-C-O	-3.23	116.75	124.08
4	A	505[B]	UCH	C19-N18-C17	3.13	118.61	111.57
4	A	505[B]	UCH	C20-C19-N18	3.10	117.95	110.92
4	B	503[A]	UCH	C19-N18-C21	-2.99	109.96	118.11
4	B	503[A]	UCH	C19-N18-C17	2.86	117.99	111.57
4	A	503[A]	UCH	C19-N18-C21	-2.76	110.59	118.11
4	B	505[B]	UCH	C19-C20-C15	2.64	114.99	110.99
3	A	502	HEM	C4D-ND-C1D	2.64	108.33	105.21
3	B	502	HEM	C4D-ND-C1D	2.62	108.31	105.21
4	A	505[B]	UCH	O14-C01-C15	-2.48	119.56	125.24
4	B	505[B]	UCH	C19-N18-C17	2.46	117.10	111.57
4	A	503[A]	UCH	C25-N24-C23	2.39	122.33	116.86
3	A	502	HEM	C1B-NB-C4B	2.32	107.95	105.21
3	A	502	HEM	C3D-C4D-ND	-2.26	107.70	110.17
4	A	503[A]	UCH	C20-C19-N18	2.25	116.03	110.92
3	B	502	HEM	C3D-C4D-ND	-2.23	107.72	110.17
3	B	502	HEM	C2A-C1A-NA	-2.23	107.68	110.15
3	A	502	HEM	C2A-C1A-NA	-2.22	107.69	110.15
4	B	505[B]	UCH	O14-C01-C15	-2.20	120.21	125.24
4	B	503[A]	UCH	C25-N24-C23	2.20	121.89	116.86
4	A	505[B]	UCH	C25-N24-C23	2.19	121.87	116.86
3	B	502	HEM	C1B-NB-C4B	2.15	107.75	105.21
3	A	502	HEM	C3B-C2B-C1B	2.14	108.02	106.41
3	B	502	HEM	C3B-C2B-C1B	2.12	108.00	106.41
4	A	503[A]	UCH	C17-N18-C21	-2.11	112.36	118.11
4	A	505[B]	UCH	C19-N18-C21	-2.07	112.45	118.11
4	A	503[A]	UCH	O14-C01-C15	-2.06	120.54	125.24
4	A	503[A]	UCH	C26-C25-N24	-2.05	120.10	123.60
4	B	503[A]	UCH	C16-C17-N18	2.02	115.51	110.92
4	A	503[A]	UCH	C16-C17-N18	2.01	115.48	110.92

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	505[B]	UCH	O14-C01-C15-C16
4	B	505[B]	UCH	O14-C01-C15-C16
4	B	505[B]	UCH	C22-C21-N18-C17

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Mol	Chain	Res	Type	Atoms
4	B	505[B]	UCH	C26-C21-N18-C17
4	A	505[B]	UCH	C22-C21-N18-C19
4	B	505[B]	UCH	C22-C21-N18-C19
4	A	505[B]	UCH	C22-C21-N18-C17
4	A	505[B]	UCH	C26-C21-N18-C19
4	A	505[B]	UCH	C26-C21-N18-C17
4	B	505[B]	UCH	C26-C21-N18-C19
4	B	505[B]	UCH	O14-C01-C15-C20
3	A	502	HEM	C4C-C3C-CAC-CBC
3	B	502	HEM	C4C-C3C-CAC-CBC
5	B	506[B]	PHE	O-C-CA-CB
5	B	506[B]	PHE	OXT-C-CA-CB
3	A	502	HEM	CAD-CBD-CGD-O1D
3	B	502	HEM	CAD-CBD-CGD-O1D
3	A	502	HEM	CAD-CBD-CGD-O2D
3	B	502	HEM	CAD-CBD-CGD-O2D
4	A	505[B]	UCH	O14-C01-C15-C20

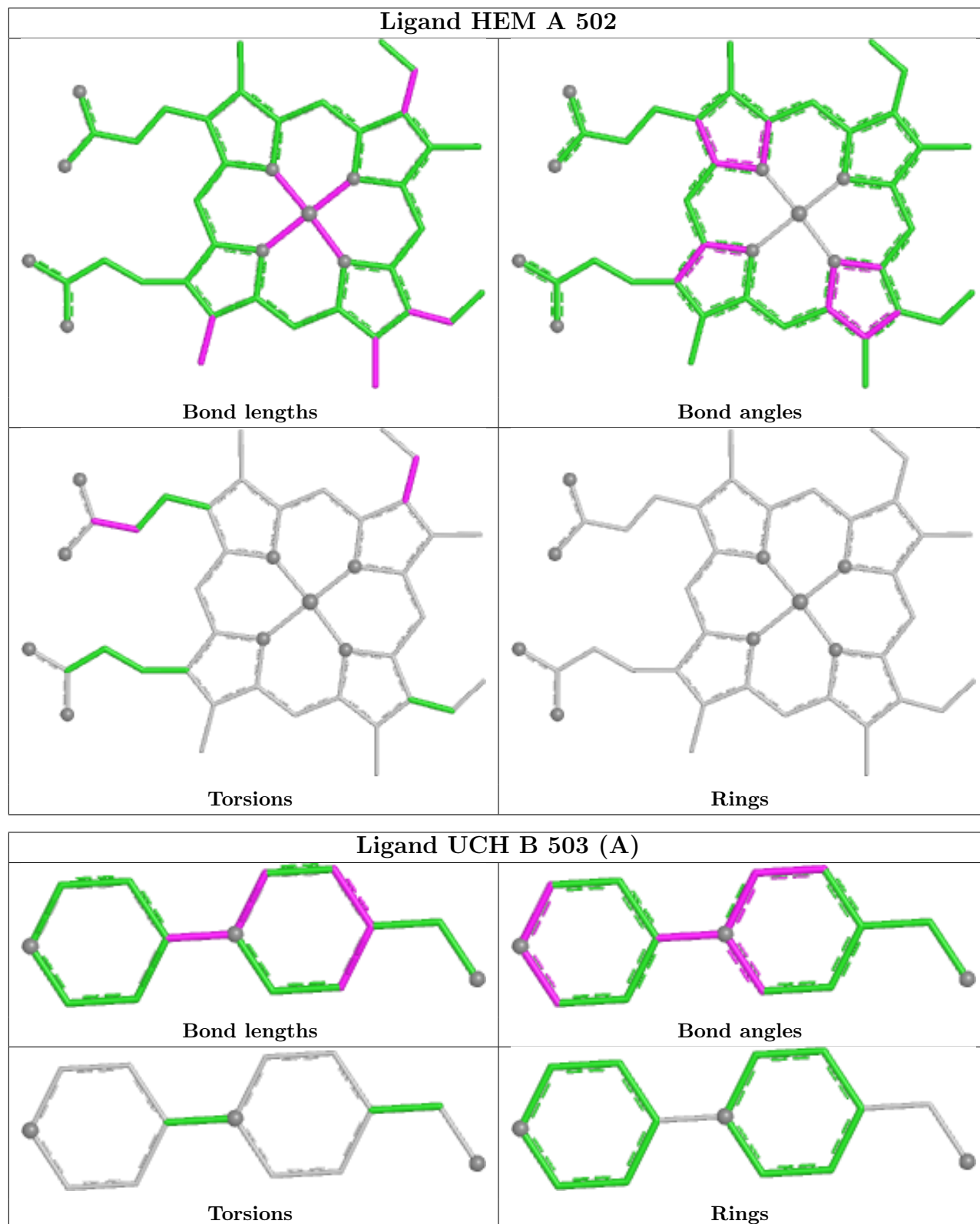
There are no ring outliers.

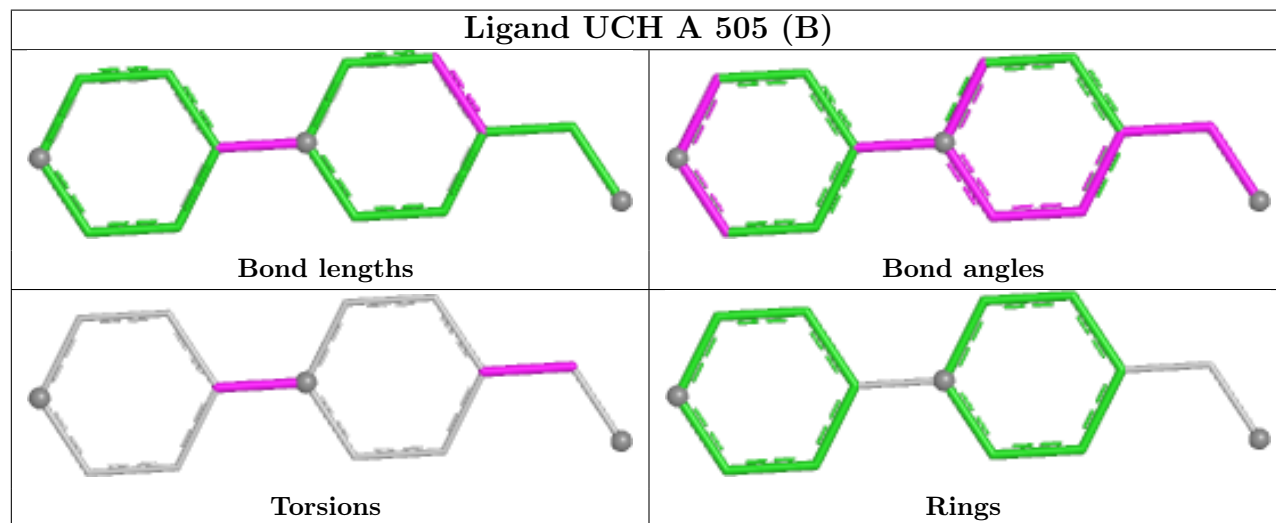
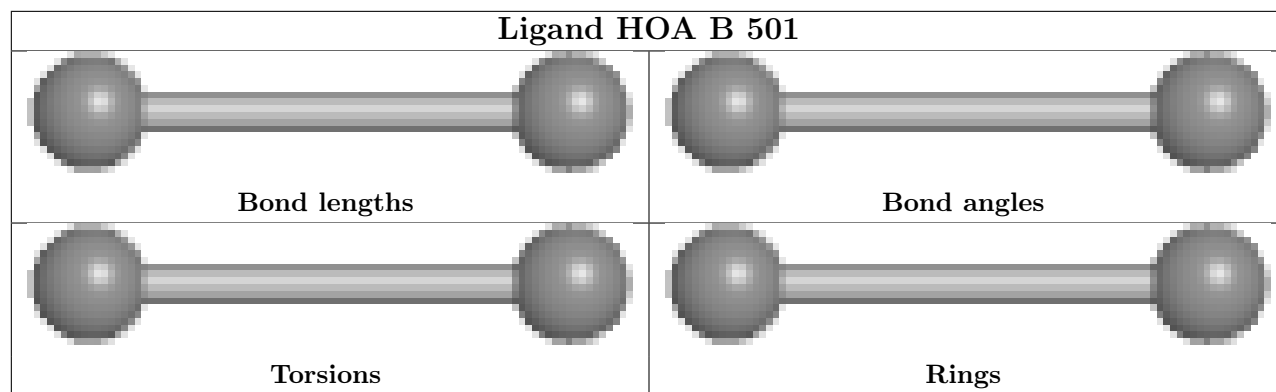
8 monomers are involved in 12 short contacts:

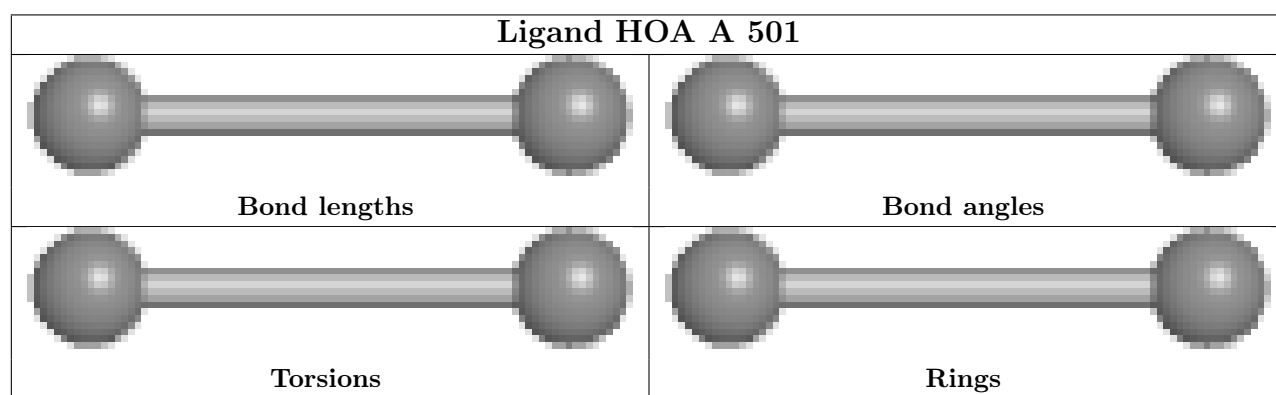
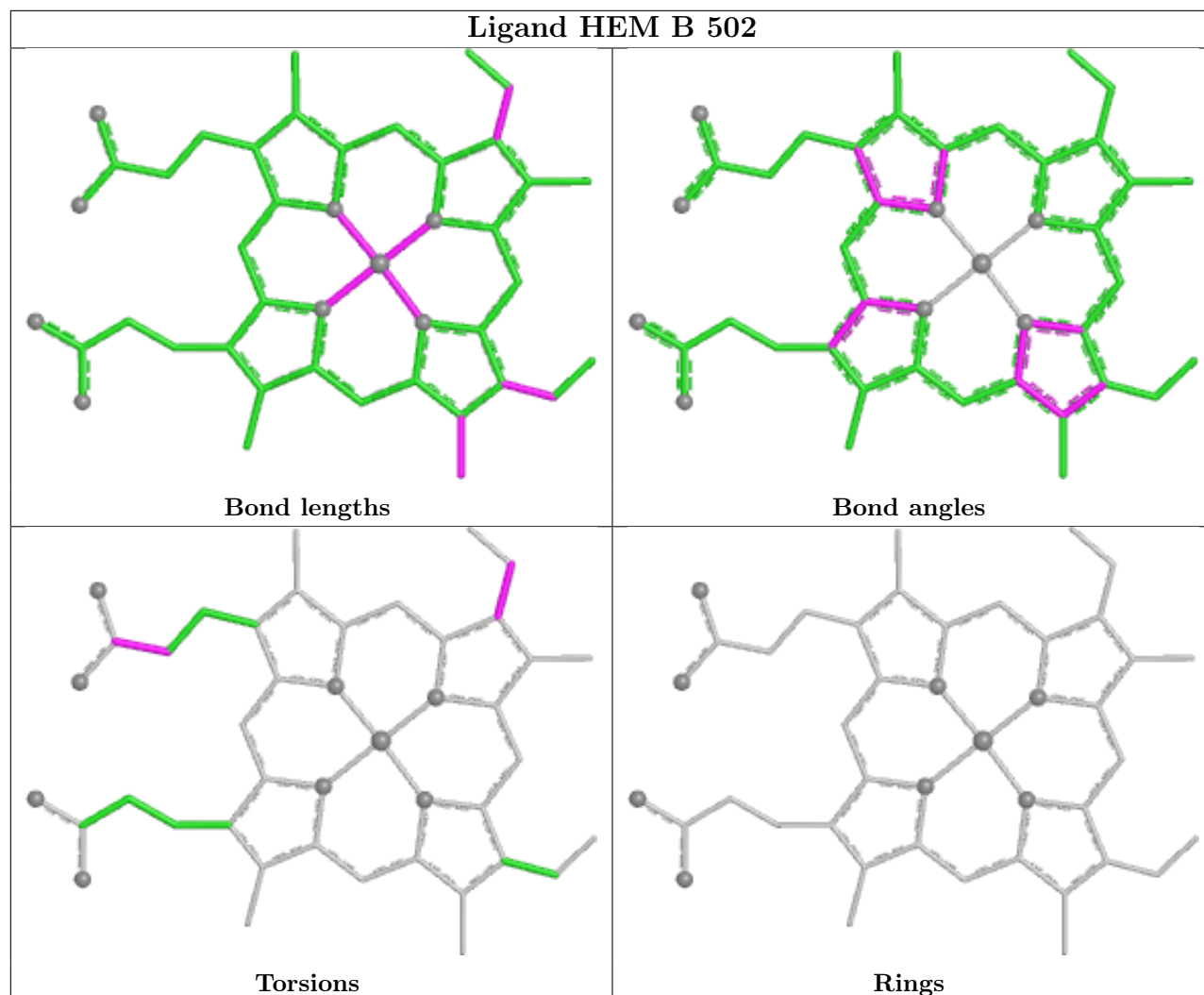
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	HEM	2	0
4	B	503[A]	UCH	1	0
4	A	505[B]	UCH	1	0
3	B	502	HEM	2	0
5	B	506[B]	PHE	3	0
4	B	505[B]	UCH	1	0
5	B	504[A]	PHE	1	0
5	A	504[A]	PHE	1	0

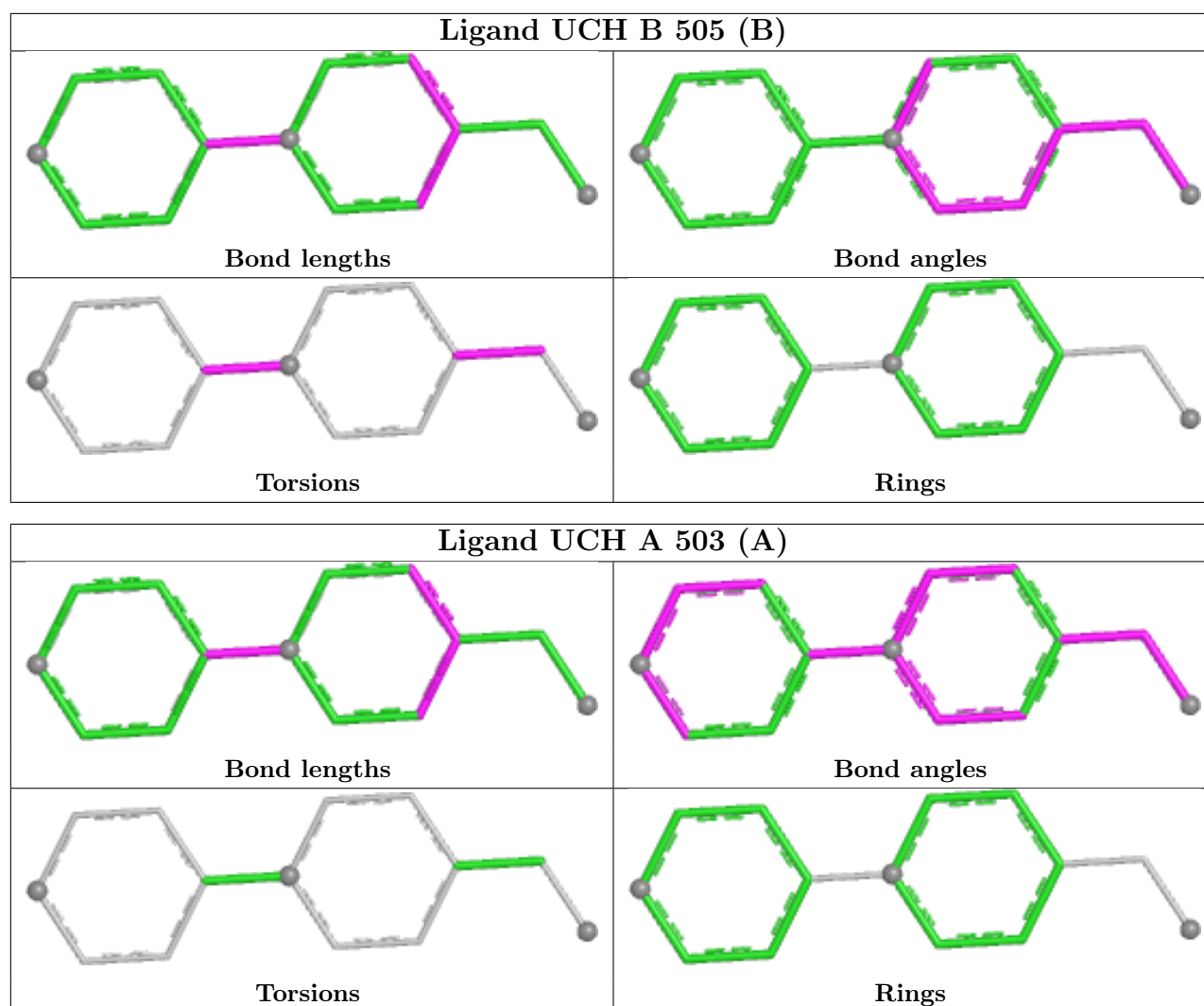
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	447/465 (96%)	0.58	29 (6%) 25 21	17, 30, 60, 81	0
1	B	448/465 (96%)	0.69	35 (7%) 19 15	16, 32, 60, 79	0
All	All	895/930 (96%)	0.63	64 (7%) 21 17	16, 31, 60, 81	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	227	GLY	6.2
1	A	227	GLY	4.9
1	B	231	ASP	4.5
1	B	224	LYS	4.4
1	A	264	ALA	4.1
1	B	288	GLN	3.6
1	A	196	PRO	3.4
1	A	209	ILE	3.3
1	A	177	MET	3.2
1	A	267	GLU	3.1
1	A	226	SER	3.1
1	A	230	SER	3.1
1	B	220	ILE	3.1
1	B	198	TYR	3.0
1	B	182	ASP	2.9
1	A	228	GLU	2.9
1	B	180	ALA	2.9
1	B	226	SER	2.8
1	A	236	HIS	2.8
1	A	175	THR	2.7
1	B	387	GLN	2.7
1	B	174	ILE	2.7
1	B	191	ALA	2.7
1	B	108	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	135	ALA	2.7
1	A	220	ILE	2.6
1	A	211	VAL	2.6
1	A	169	GLN	2.6
1	A	174	ILE	2.5
1	B	267	GLU	2.5
1	A	231	ASP	2.5
1	B	266	HIS	2.5
1	B	330	ALA	2.5
1	A	428	ASN	2.4
1	A	221	ALA	2.4
1	B	270	SER	2.4
1	B	234	LEU	2.4
1	B	13	GLU	2.4
1	A	208	ASP	2.4
1	B	196	PRO	2.4
1	B	264	ALA	2.4
1	B	136	ASP	2.3
1	B	202	LYS	2.3
1	A	170	PRO	2.3
1	B	401	ILE	2.3
1	B	104	LEU	2.3
1	B	437	LEU	2.2
1	B	381	ASN	2.2
1	A	182	ASP	2.2
1	B	228	GLU	2.2
1	A	185	MET	2.2
1	A	266	HIS	2.2
1	A	224	LYS	2.1
1	B	201	ASN	2.1
1	A	352	GLU	2.1
1	A	254	ILE	2.1
1	A	135	ALA	2.1
1	B	154	GLY	2.1
1	B	23	ASP	2.0
1	B	203	ARG	2.0
1	B	170	PRO	2.0
1	A	431	LEU	2.0
1	B	230	SER	2.0
1	A	263	ILE	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](#)

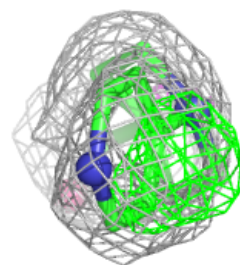
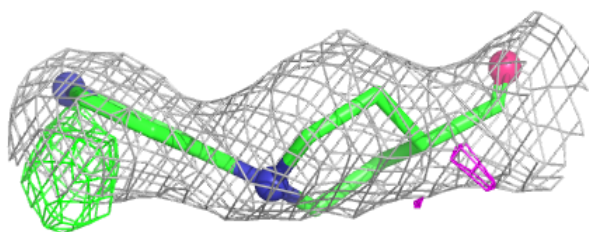
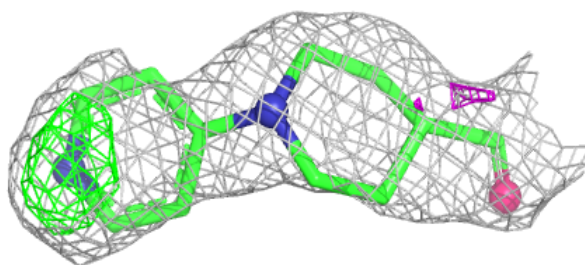
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	UCH	A	503[A]	14/15	0.65	0.22	21,29,32,32	14
5	PHE	B	506[B]	12/12	0.65	0.32	32,35,38,39	12
5	PHE	B	504[A]	12/12	0.67	0.21	30,32,37,37	12
5	PHE	A	506[B]	12/12	0.72	0.24	30,32,35,35	12
4	UCH	B	503[A]	14/15	0.75	0.21	27,32,36,36	14
5	PHE	A	504[A]	12/12	0.82	0.17	25,28,33,34	12
4	UCH	B	505[B]	14/15	0.84	0.16	32,35,36,37	14
4	UCH	A	505[B]	14/15	0.86	0.16	29,31,34,34	14
2	HOA	B	501	2/2	0.91	0.10	25,25,25,29	0
3	HEM	A	502	43/43	0.93	0.10	16,26,31,33	0
3	HEM	B	502	43/43	0.93	0.10	16,26,31,32	0
2	HOA	A	501	2/2	0.94	0.13	24,24,24,34	0

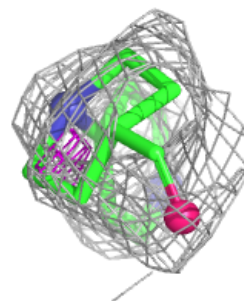
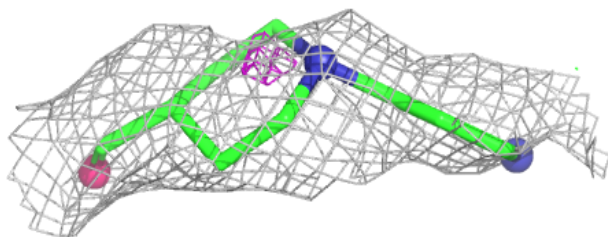
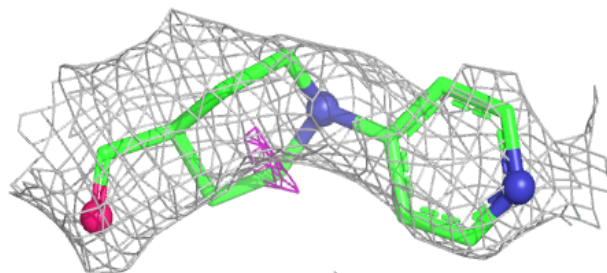
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UCH A 503 (A):

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

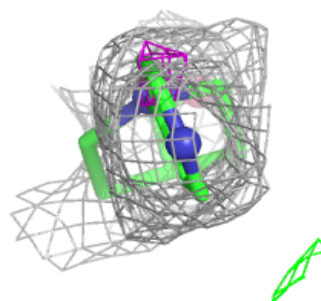
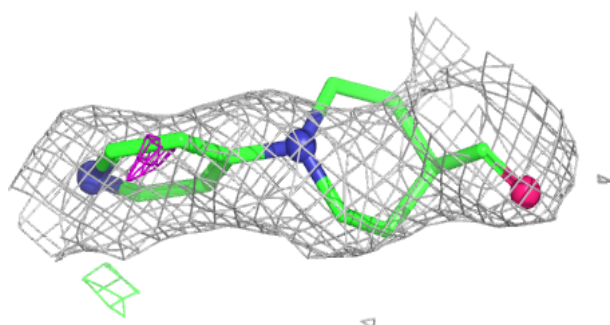
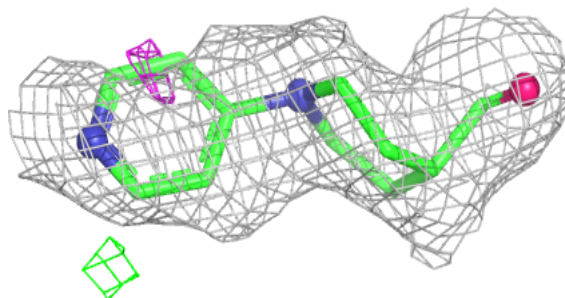
**Electron density around UCH B 503 (A):**

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

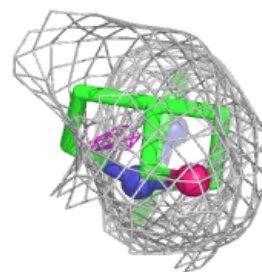
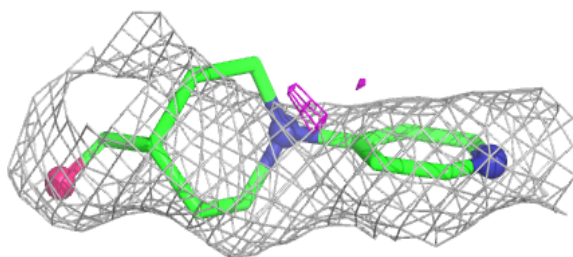
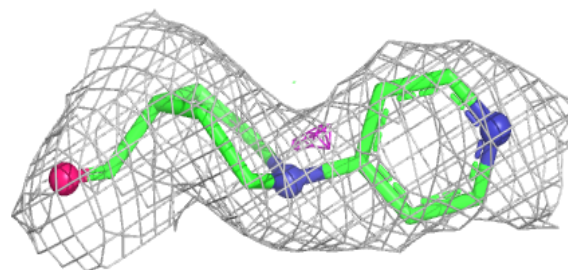


Electron density around UCH B 505 (B):

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

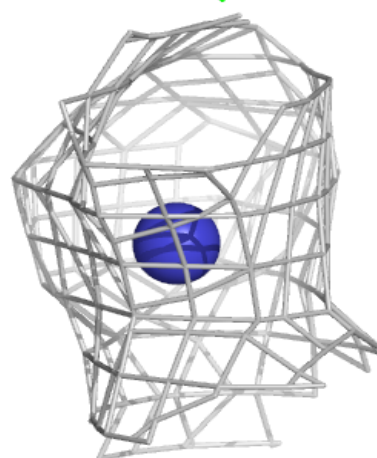
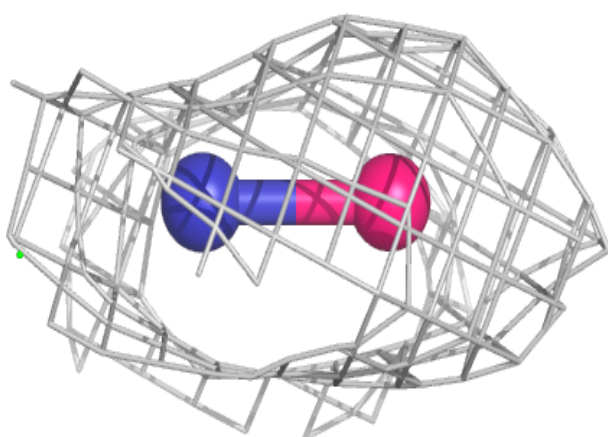
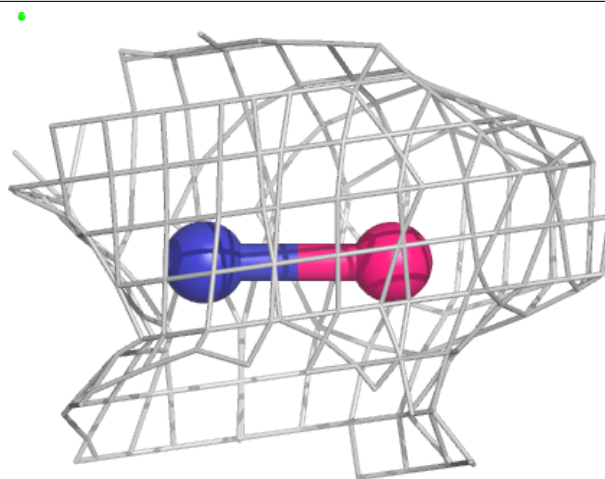
**Electron density around UCH A 505 (B):**

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



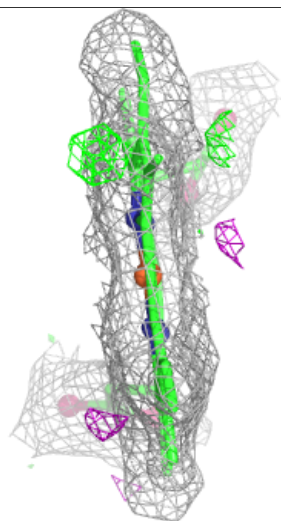
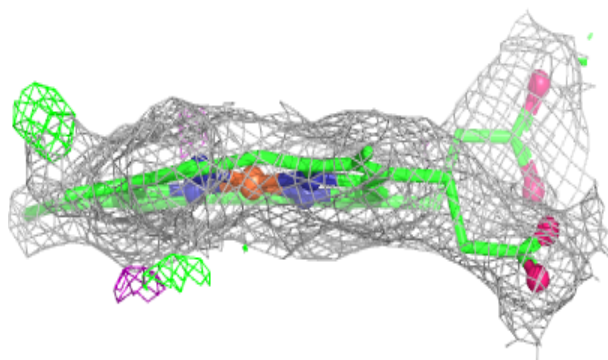
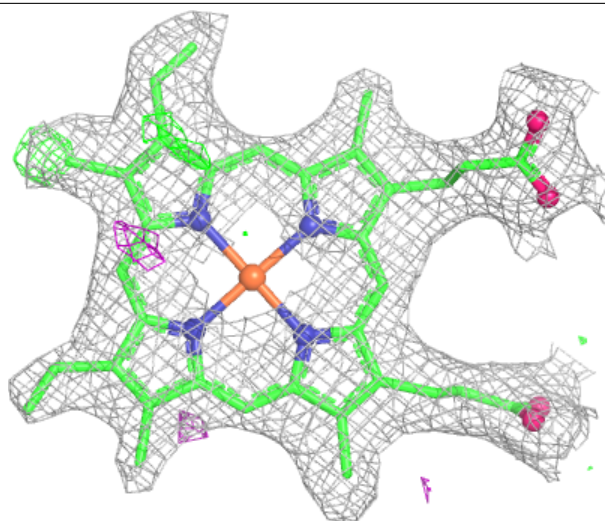
Electron density around HOA B 501:

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



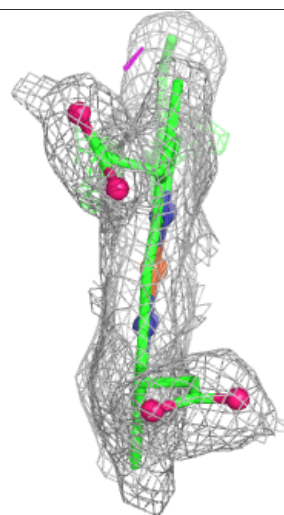
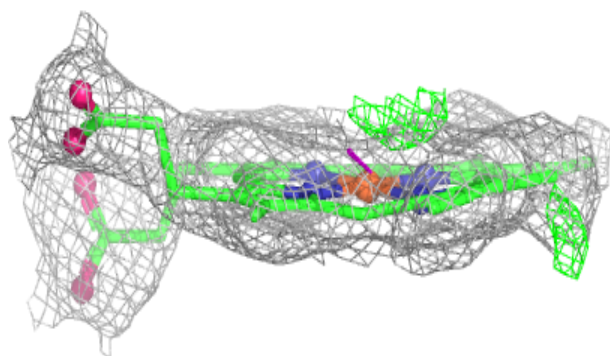
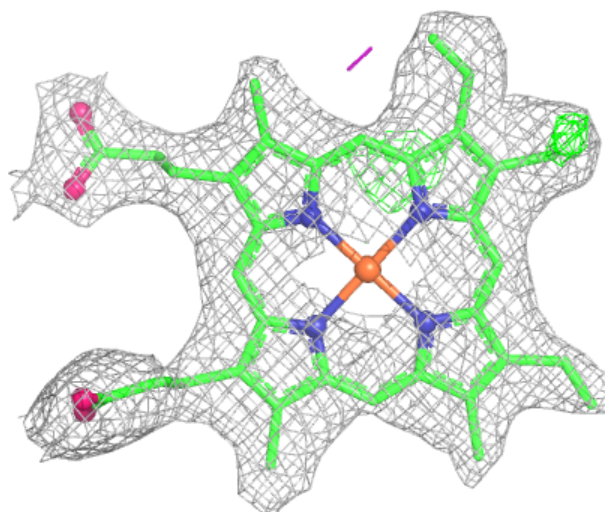
Electron density around HEM A 502:

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



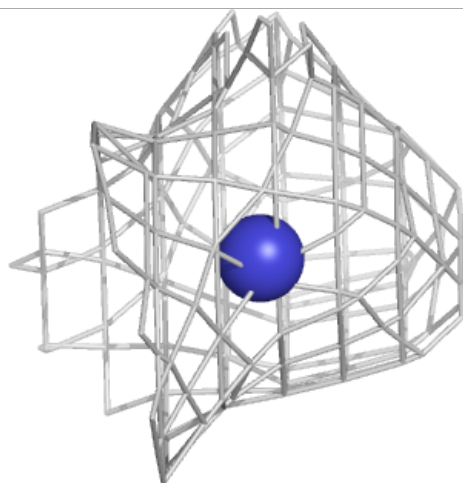
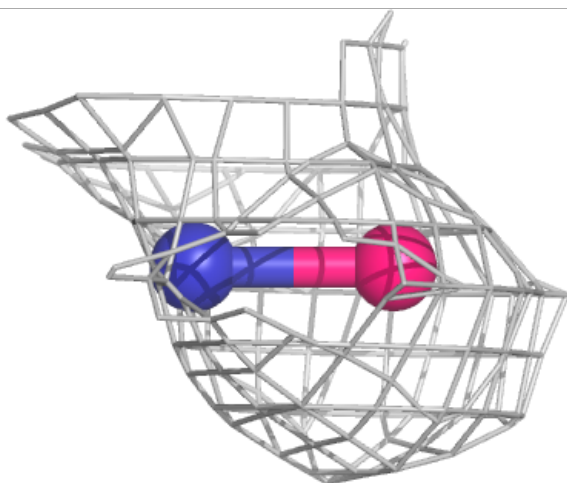
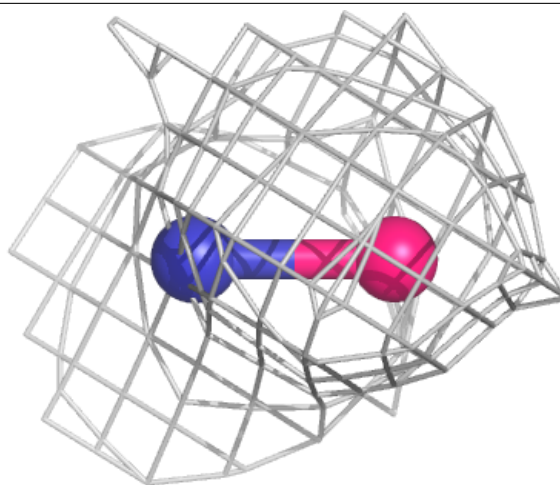
Electron density around HEM B 502:

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



Electron density around HOA 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.