



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5WN8 / pdb_00005wn8
Title : Structural Insights into Substrate and Inhibitor Binding Sites in Human Indoleamine 2,3-Dioxygenase 1
Authors : Lewis-Ballester, A.; Pham, K.N.; Batabyal, D.; Karkashon, S.; Bonanno, J.B.; Poulos, T.L.; Yeh, S.R.
Deposited on : 2017-07-31
Resolution : 2.50 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

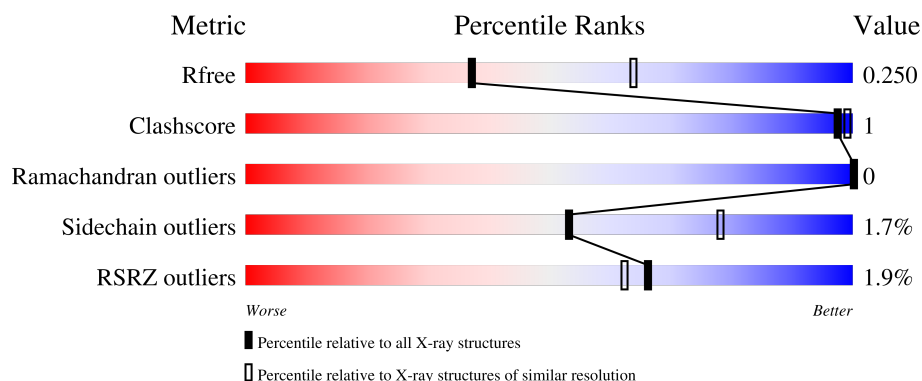
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	425	
1	B	425	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6164 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	371	Total	C	N	O	S	0	0	0
			2939	1889	500	533	17			
1	B	370	Total	C	N	O	S	0	0	0
			2941	1892	501	531	17			

There are 66 discrepancies between the modelled and reference sequences:

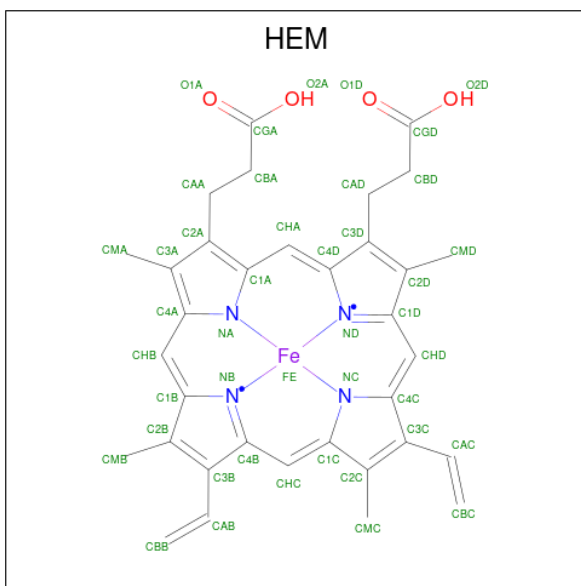
Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	expression tag	UNP P14902
A	404	LYS	-	expression tag	UNP P14902
A	405	GLY	-	expression tag	UNP P14902
A	406	GLU	-	expression tag	UNP P14902
A	407	LEU	-	expression tag	UNP P14902
A	408	ASN	-	expression tag	UNP P14902
A	409	SER	-	expression tag	UNP P14902
A	410	LYS	-	expression tag	UNP P14902
A	411	LEU	-	expression tag	UNP P14902
A	412	GLU	-	expression tag	UNP P14902
A	413	GLY	-	expression tag	UNP P14902
A	414	LYS	-	expression tag	UNP P14902
A	415	PRO	-	expression tag	UNP P14902
A	416	ILE	-	expression tag	UNP P14902
A	417	PRO	-	expression tag	UNP P14902
A	418	ASN	-	expression tag	UNP P14902
A	419	PRO	-	expression tag	UNP P14902
A	420	LEU	-	expression tag	UNP P14902
A	421	LEU	-	expression tag	UNP P14902
A	422	GLY	-	expression tag	UNP P14902
A	423	LEU	-	expression tag	UNP P14902
A	424	ASP	-	expression tag	UNP P14902
A	425	SER	-	expression tag	UNP P14902
A	426	THR	-	expression tag	UNP P14902
A	427	ARG	-	expression tag	UNP P14902

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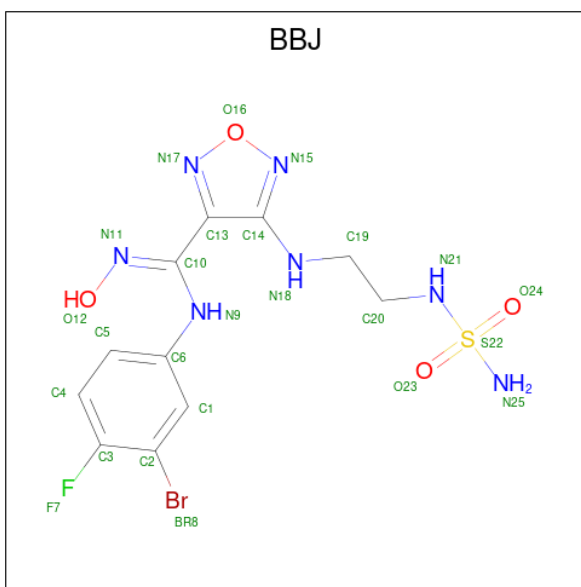
Chain	Residue	Modelled	Actual	Comment	Reference
A	428	THR	-	expression tag	UNP P14902
A	429	GLY	-	expression tag	UNP P14902
A	430	HIS	-	expression tag	UNP P14902
A	431	HIS	-	expression tag	UNP P14902
A	432	HIS	-	expression tag	UNP P14902
A	433	HIS	-	expression tag	UNP P14902
A	434	HIS	-	expression tag	UNP P14902
A	435	HIS	-	expression tag	UNP P14902
B	11	MET	-	expression tag	UNP P14902
B	404	LYS	-	expression tag	UNP P14902
B	405	GLY	-	expression tag	UNP P14902
B	406	GLU	-	expression tag	UNP P14902
B	407	LEU	-	expression tag	UNP P14902
B	408	ASN	-	expression tag	UNP P14902
B	409	SER	-	expression tag	UNP P14902
B	410	LYS	-	expression tag	UNP P14902
B	411	LEU	-	expression tag	UNP P14902
B	412	GLU	-	expression tag	UNP P14902
B	413	GLY	-	expression tag	UNP P14902
B	414	LYS	-	expression tag	UNP P14902
B	415	PRO	-	expression tag	UNP P14902
B	416	ILE	-	expression tag	UNP P14902
B	417	PRO	-	expression tag	UNP P14902
B	418	ASN	-	expression tag	UNP P14902
B	419	PRO	-	expression tag	UNP P14902
B	420	LEU	-	expression tag	UNP P14902
B	421	LEU	-	expression tag	UNP P14902
B	422	GLY	-	expression tag	UNP P14902
B	423	LEU	-	expression tag	UNP P14902
B	424	ASP	-	expression tag	UNP P14902
B	425	SER	-	expression tag	UNP P14902
B	426	THR	-	expression tag	UNP P14902
B	427	ARG	-	expression tag	UNP P14902
B	428	THR	-	expression tag	UNP P14902
B	429	GLY	-	expression tag	UNP P14902
B	430	HIS	-	expression tag	UNP P14902
B	431	HIS	-	expression tag	UNP P14902
B	432	HIS	-	expression tag	UNP P14902
B	433	HIS	-	expression tag	UNP P14902
B	434	HIS	-	expression tag	UNP P14902
B	435	HIS	-	expression tag	UNP P14902

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:

$$\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4).$$


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

- Molecule 3 is N-(3-bromo-4-fluorophenyl)-N'-hydroxy-4-[[2-(sulfamoylamino)ethyl]amino]-1,2,5-oxadiazole-3-carboximidamide (CCD ID: BBJ) (formula: C₁₁H₁₃BrFN₇O₄S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	Br	C	F	N	O	S	0	0
			25	1	11	1	7	4	1		
3	B	1	Total	Br	C	F	N	O	S	0	0
			25	1	11	1	7	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	76	Total	O	0	0
			76	76		
4	B	72	Total	O	0	0
			72	72		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.73Å 97.78Å 128.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.69 – 2.50 29.69 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.69-2.50) 99.8 (29.69-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.213 , 0.252 0.216 , 0.250	Depositor DCC
R_{free} test set	1928 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	71.6	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6164	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BBJ, 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	0.56	0/3007	0.84	0/4069
1	B	0.53	0/3009	0.82	0/4069
All	All	0.55	0/6016	0.83	0/8138

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2939	0	2942	2	0
1	B	2941	0	2956	5	0
2	A	43	0	30	1	0
2	B	43	0	30	1	0
3	A	25	0	0	2	0
3	B	25	0	0	3	0
4	A	76	0	0	0	0
4	B	72	0	0	0	0
All	All	6164	0	5958	9	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 1.

All (9) 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:A:234:LEU:HD22	3:A:502:BBJ:BR8	2.58	0.59
1:B:262:GLY:HA3	3:B:502:BBJ:BR8	2.60	0.57
2:B:501:HEM:HBB2	2:B:501:HEM:HMB1	1.85	0.56
2:A:501:HEM:HBB2	2:A:501:HEM:HMB1	1.94	0.48
1:B:215:HIS:HD2	1:B:345:TYR:CZ	2.35	0.44
1:B:280:GLN:HE21	1:B:280:GLN:HA	1.83	0.43
1:B:234:LEU:HD22	3:B:502:BBJ:BR8	2.75	0.42
1:B:163:PHE:CZ	3:B:502:BBJ:C5	3.05	0.40
1:A:129:CYS:SG	3:A:502:BBJ:BR8	3.35	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	367/425 (86%)	359 (98%)	8 (2%)	0	100	100
1	B	366/425 (86%)	353 (96%)	13 (4%)	0	100	100
All	All	733/850 (86%)	712 (97%)	21 (3%)	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	320/368 (87%)	314 (98%)	6 (2%)	50	76
1	B	321/368 (87%)	316 (98%)	5 (2%)	55	79
All	All	641/736 (87%)	630 (98%)	11 (2%)	53	78

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	GLU
1	A	67	ILE
1	A	189	GLN
1	A	190	MET
1	A	214	PHE
1	A	400	LEU
1	B	94	LYS
1	B	98	ASP
1	B	280	GLN
1	B	337	LYS
1	B	385	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	96	HIS
1	A	220	HIS
1	A	242	GLN
1	A	280	GLN
1	A	293	GLN
1	A	313	ASN
1	A	360	GLN
1	B	16	HIS
1	B	63	ASN
1	B	215	HIS
1	B	216	GLN
1	B	220	HIS
1	B	242	GLN
1	B	280	GLN
1	B	290	GLN
1	B	313	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	BBJ	A	502	2	25,26,26	1.69	6 (24%)	32,36,36	3.14	10 (31%)
2	HEM	A	501	3,1	50,50,50	1.57	7 (14%)	67,82,82	1.63	14 (20%)
2	HEM	B	501	3,1	50,50,50	1.58	6 (12%)	67,82,82	1.48	11 (16%)
3	BBJ	B	502	2	25,26,26	1.77	6 (24%)	32,36,36	3.14	11 (34%)

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	BBJ	A	502	2	-	4/15/18/18	0/2/2/2
2	HEM	A	501	3,1	-	3/14/54/54	-
2	HEM	B	501	3,1	-	4/14/54/54	-
3	BBJ	B	502	2	-	5/15/18/18	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	FE-NB	5.08	2.10	1.94
2	B	501	HEM	FE-NB	5.07	2.10	1.94
2	A	501	HEM	FE-NC	4.46	2.09	1.95
3	A	502	BBJ	C10-N9	-4.45	1.27	1.36
3	B	502	BBJ	C10-N9	-4.40	1.27	1.36
2	B	501	HEM	FE-NC	4.20	2.09	1.95
3	B	502	BBJ	C13-C10	4.19	1.51	1.46
2	B	501	HEM	C1B-NB	-3.84	1.33	1.40
2	A	501	HEM	C1B-NB	-3.77	1.33	1.40
3	A	502	BBJ	C13-C10	3.72	1.50	1.46
3	B	502	BBJ	C13-C14	3.43	1.50	1.42
3	A	502	BBJ	C13-C14	3.04	1.49	1.42
2	A	501	HEM	C4D-ND	-2.77	1.35	1.40
3	B	502	BBJ	C14-N15	2.72	1.34	1.30
2	B	501	HEM	C4D-ND	-2.71	1.35	1.40
3	A	502	BBJ	C14-N15	2.68	1.34	1.30
3	A	502	BBJ	C10-N11	2.49	1.33	1.29
3	B	502	BBJ	C10-N11	2.32	1.32	1.29
2	B	501	HEM	C4B-NB	-2.32	1.34	1.38
2	A	501	HEM	C4B-NB	-2.30	1.34	1.38
2	A	501	HEM	C1C-C2C	-2.30	1.40	1.45
2	B	501	HEM	C3B-C4B	2.27	1.49	1.44
3	A	502	BBJ	O16-N15	-2.20	1.34	1.39
3	B	502	BBJ	O16-N15	-2.13	1.34	1.39
2	A	501	HEM	C3B-C4B	2.01	1.48	1.44

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	BBJ	O12-N11-C10	9.37	121.63	110.02
3	B	502	BBJ	O12-N11-C10	9.21	121.43	110.02
3	A	502	BBJ	C14-C13-N17	-9.16	103.50	108.98
3	B	502	BBJ	C14-C13-N17	-9.14	103.50	108.98
3	B	502	BBJ	N9-C10-N11	-6.80	113.39	124.28
3	A	502	BBJ	N9-C10-N11	-6.18	114.37	124.28
3	B	502	BBJ	N17-O16-N15	5.23	117.98	111.49
3	A	502	BBJ	N17-O16-N15	5.05	117.75	111.49
2	B	501	HEM	C1B-NB-C4B	4.20	110.19	105.21
2	A	501	HEM	C1B-NB-C4B	4.17	110.15	105.21
2	A	501	HEM	CHC-C4B-NB	4.09	128.83	124.42
3	A	502	BBJ	O16-N15-C14	-4.09	101.47	104.78
3	B	502	BBJ	O16-N15-C14	-4.05	101.50	104.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	CHC-C4B-NB	4.00	128.72	124.42
2	B	501	HEM	CHD-C1D-ND	3.73	128.44	124.42
3	A	502	BBJ	C13-C14-N15	3.61	111.29	109.08
2	A	501	HEM	CHD-C1D-ND	3.60	128.30	124.42
3	A	502	BBJ	C10-C13-N17	3.44	130.93	120.52
2	B	501	HEM	CHA-C4D-ND	3.41	128.59	124.37
2	A	501	HEM	CAC-C3C-C4C	3.38	132.90	124.82
3	B	502	BBJ	C13-C14-N15	3.36	111.14	109.08
3	B	502	BBJ	C10-C13-N17	3.31	130.54	120.52
2	A	501	HEM	CHA-C4D-ND	3.11	128.21	124.37
2	A	501	HEM	CHA-C4D-C3D	-2.94	119.81	125.23
2	B	501	HEM	CHD-C1D-C2D	-2.91	120.44	125.03
2	A	501	HEM	C4B-C3B-C2B	-2.88	104.63	107.28
3	A	502	BBJ	O23-S22-N21	2.82	113.32	106.64
2	B	501	HEM	CHA-C4D-C3D	-2.77	120.11	125.23
2	A	501	HEM	CMD-C2D-C1D	2.77	129.37	125.03
2	A	501	HEM	CHD-C1D-C2D	-2.72	120.73	125.03
3	B	502	BBJ	O24-S22-N21	2.68	112.98	106.64
2	B	501	HEM	CMD-C2D-C1D	2.63	129.15	125.03
2	B	501	HEM	C3B-C4B-NB	-2.50	107.67	109.47
2	A	501	HEM	CAC-C3C-C2C	-2.49	120.34	128.43
2	B	501	HEM	C4B-C3B-C2B	-2.36	105.11	107.28
3	B	502	BBJ	C13-C10-N9	2.33	128.08	118.48
3	A	502	BBJ	C10-C13-C14	-2.30	125.57	128.79
2	B	501	HEM	C1A-CHA-C4D	-2.19	121.11	126.25
3	A	502	BBJ	C13-C10-N9	2.18	127.46	118.48
2	A	501	HEM	C3B-C2B-C1B	2.10	107.99	106.41
2	A	501	HEM	CHB-C1B-NB	2.09	126.95	124.37
2	A	501	HEM	O2D-CGD-CBD	2.06	120.52	114.00
2	B	501	HEM	O2D-CGD-CBD	2.05	120.49	114.00
2	A	501	HEM	O2D-CGD-O1D	-2.05	118.05	123.33
3	B	502	BBJ	N18-C14-N15	-2.03	122.20	123.93
3	B	502	BBJ	C10-C13-C14	-2.03	125.95	128.79

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	BBJ	N11-C10-C13-C14
3	A	502	BBJ	C20-N21-S22-O24
3	B	502	BBJ	N11-C10-C13-C14
3	B	502	BBJ	C20-N21-S22-O23

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Mol	Chain	Res	Type	Atoms
3	A	502	BBJ	C20-N21-S22-O23
3	B	502	BBJ	C20-N21-S22-O24
2	A	501	HEM	CAA-CBA-CGA-O1A
2	B	501	HEM	CAD-CBD-CGD-O1D
3	B	502	BBJ	C19-C20-N21-S22
2	A	501	HEM	CAA-CBA-CGA-O2A
2	B	501	HEM	CAD-CBD-CGD-O2D
3	B	502	BBJ	N11-C10-C13-N17
3	A	502	BBJ	N18-C19-C20-N21
2	B	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	CAD-CBD-CGD-O2D
2	B	501	HEM	CAA-CBA-CGA-O1A

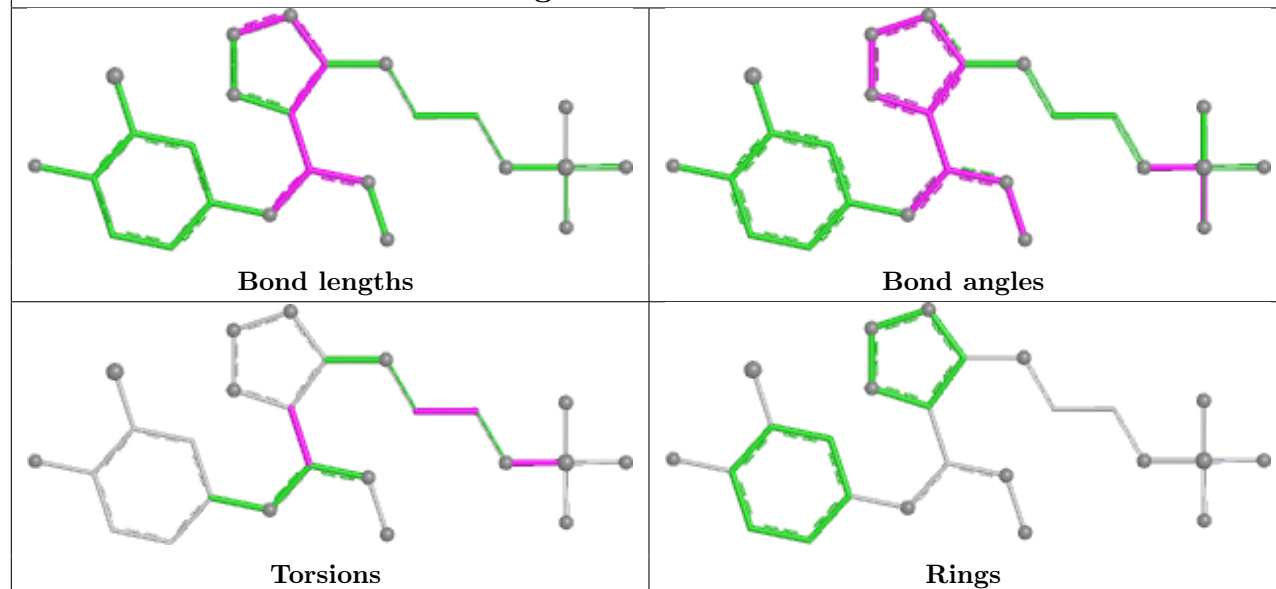
There are no ring outliers.

4 monomers are involved in 7 short contacts:

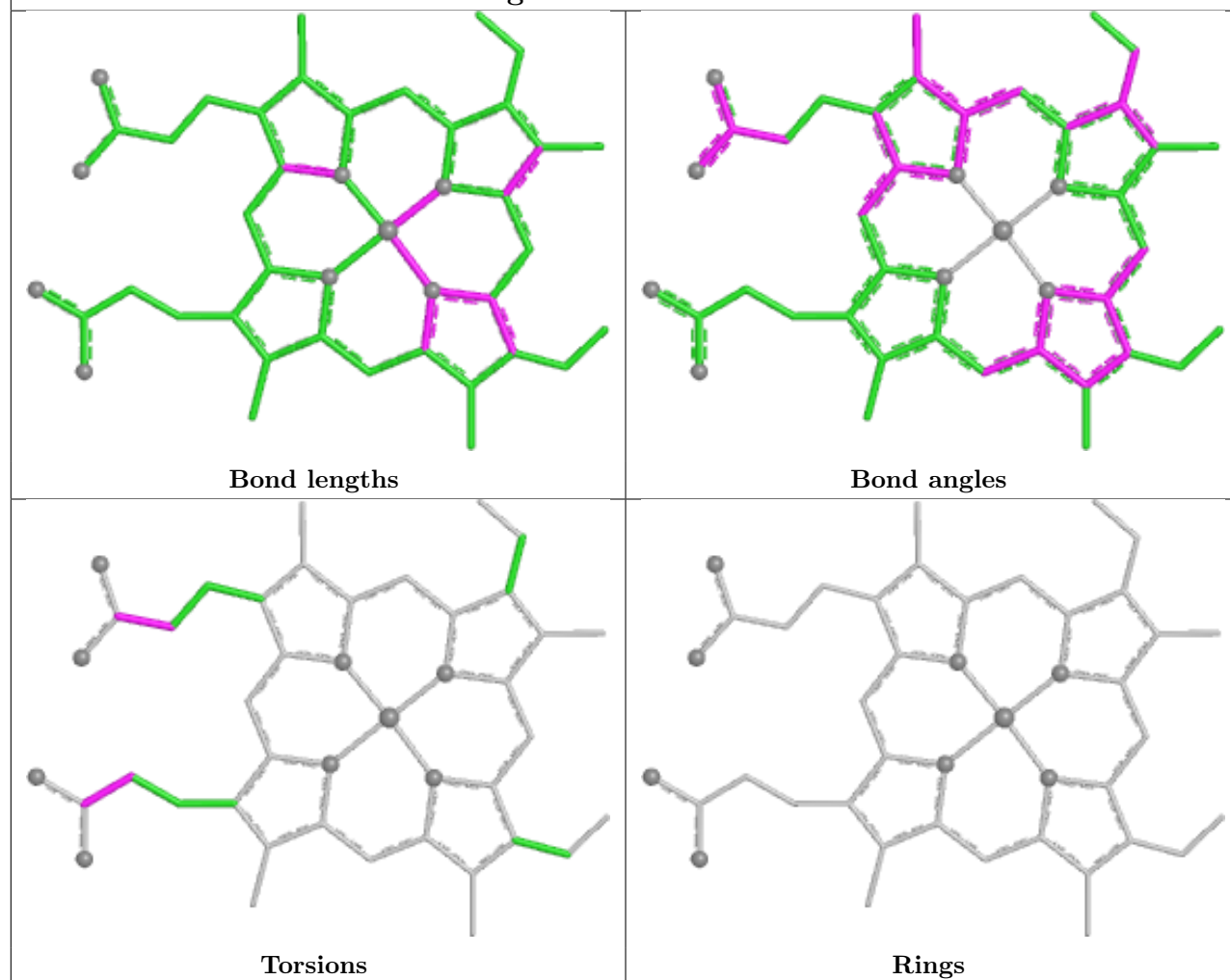
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	BBJ	2	0
2	A	501	HEM	1	0
2	B	501	HEM	1	0
3	B	502	BBJ	3	0

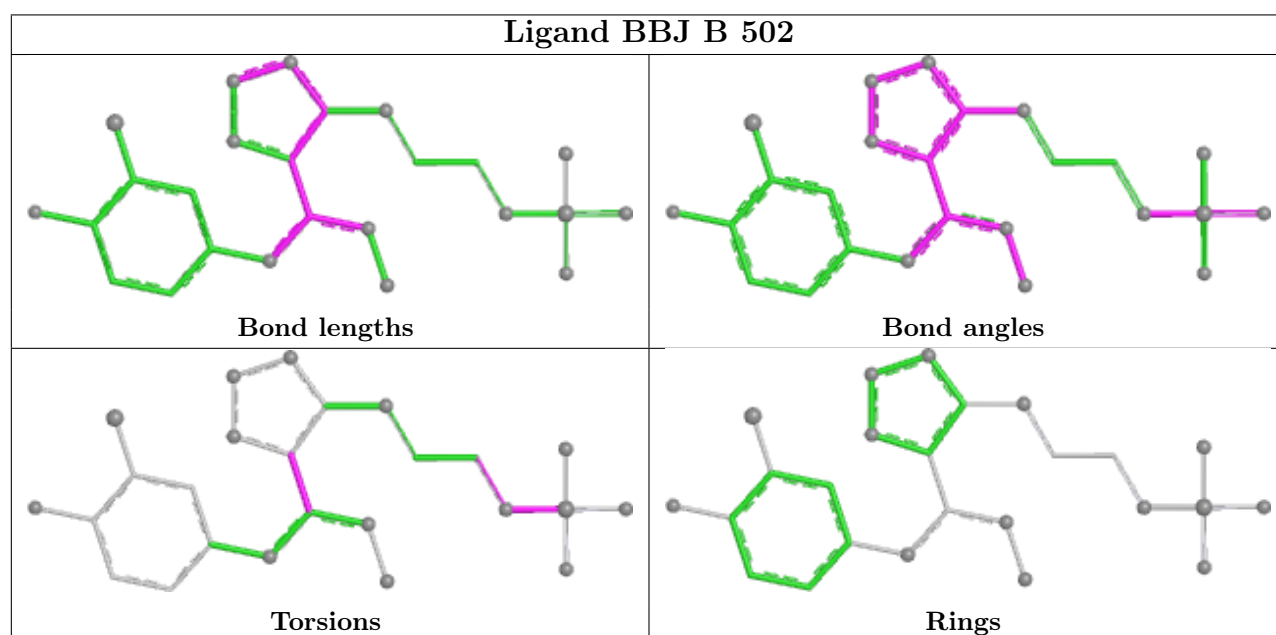
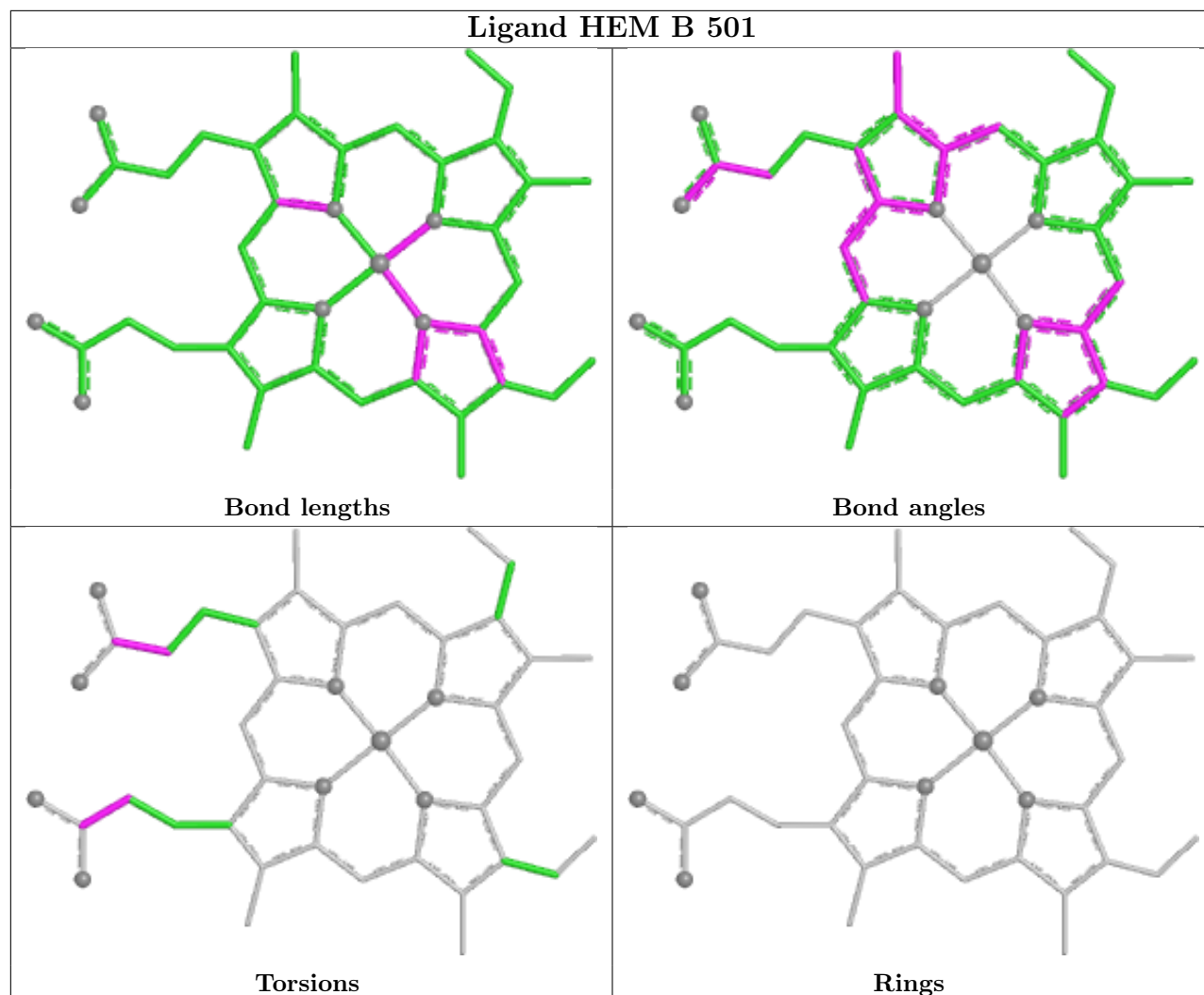
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand BBJ A 502



Ligand HEM A 501





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	371/425 (87%)	0.21	7 (1%) 66 62	58, 82, 114, 126	0
1	B	370/425 (87%)	0.14	7 (1%) 66 62	55, 76, 107, 138	0
All	All	741/850 (87%)	0.18	14 (1%) 66 62	55, 79, 112, 138	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	283	ALA	3.5
1	A	282	THR	2.9
1	A	249	TYR	2.8
1	B	286	GLY	2.6
1	A	283	ALA	2.5
1	B	381	GLY	2.5
1	A	26	PRO	2.4
1	B	401	LYS	2.3
1	A	41	PHE	2.3
1	B	294	ASP	2.2
1	B	287	HIS	2.2
1	A	62	LEU	2.2
1	A	284	GLY	2.2
1	B	285	GLY	2.1

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](#)

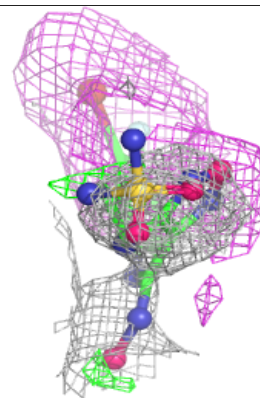
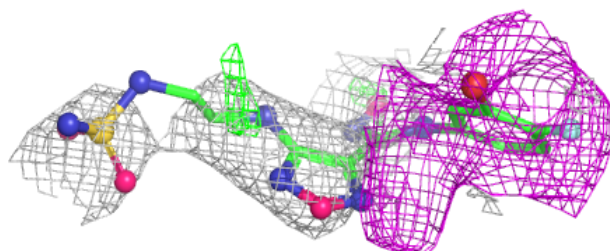
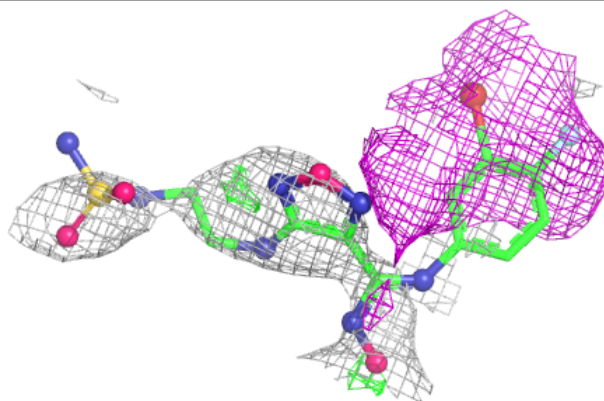
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BBJ	A	502	25/25	0.73	0.26	120,155,186,200	0
3	BBJ	B	502	25/25	0.82	0.16	105,119,151,154	0
2	HEM	A	501	43/43	0.98	0.08	64,69,77,84	0
2	HEM	B	501	43/43	0.98	0.09	66,71,84,92	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.

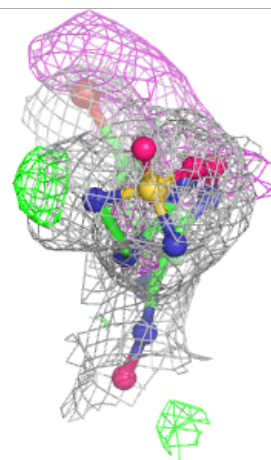
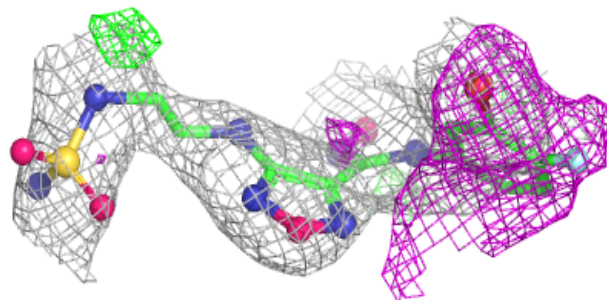
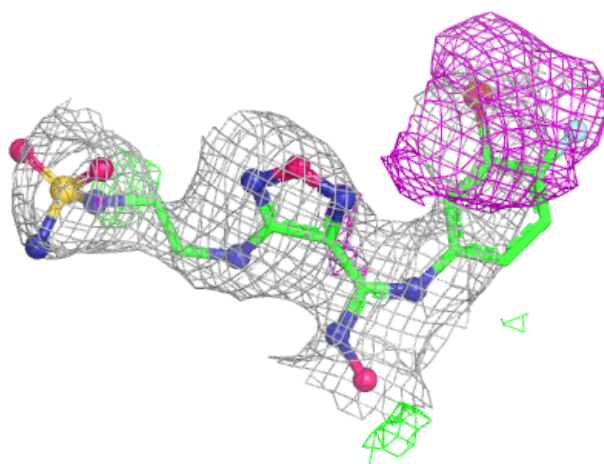
Electron density around BBJ A 502:

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



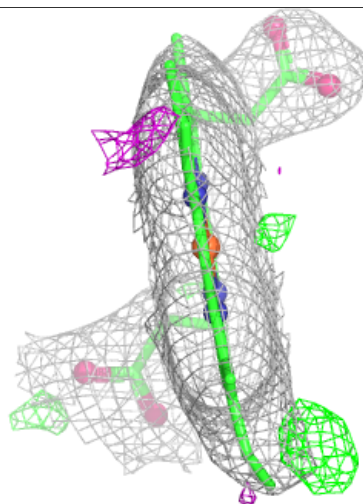
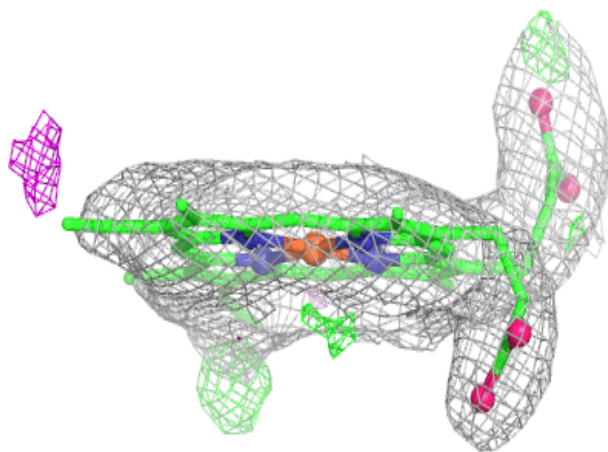
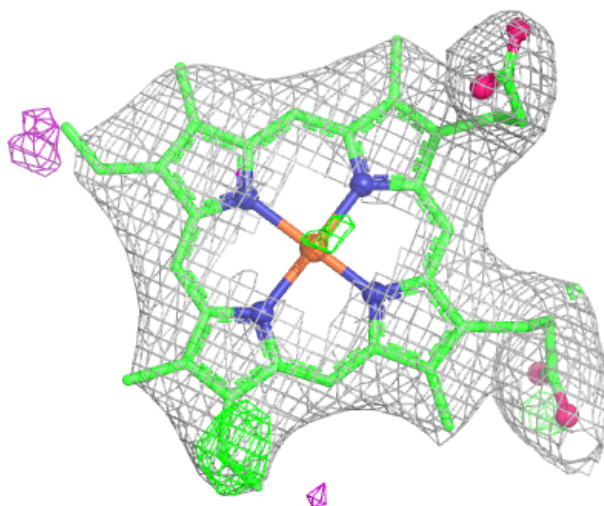
Electron density around BBJ B 502:

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



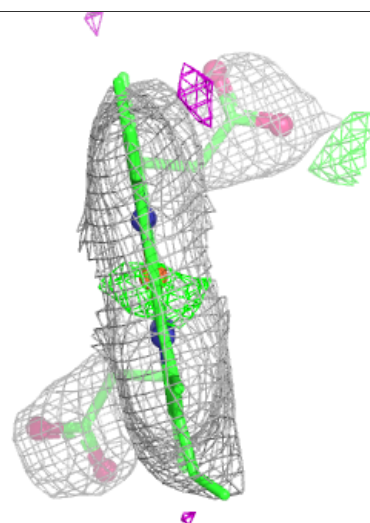
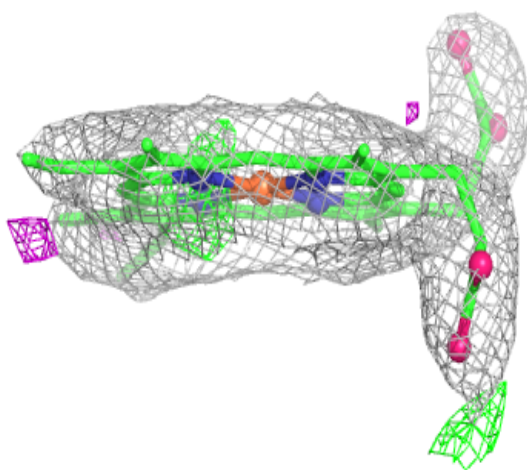
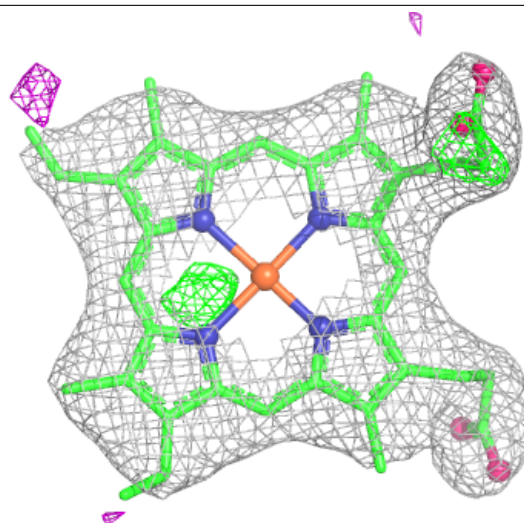
Electron density around HEM A 501:

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.