



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 09:57 am BST

PDB ID : 6PZ1
Title : Crystal Structure of human Indoleamine 2,3-Dioxygenase 1 in complex with PF-06840003 in Active Site and Si site
Authors : Pham, K.N.; Lewis-Ballester, A.; Yeh, S.R.
Deposited on : 2019-07-31
Resolution : 2.65 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 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)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

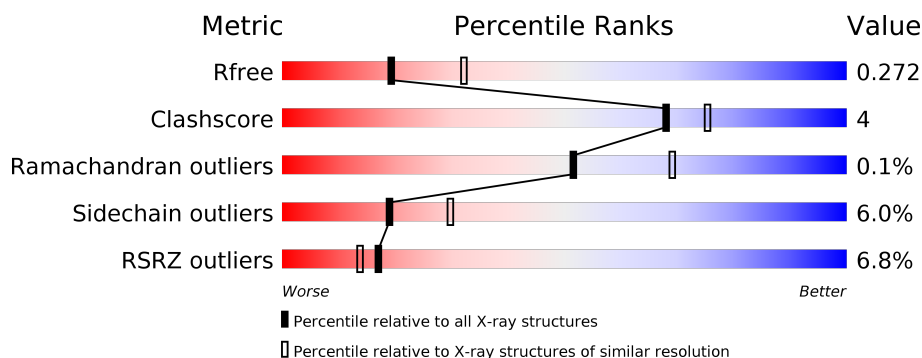
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 on 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	<div> <div>7%</div> <div> <div></div> <div>76%</div> <div>12%</div> <div>12%</div> </div> </div>
1	B	425	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>11%</div> <div>11%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6317 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	376	Total	C	N	O	S	0	0	0
			2977	1914	509	537	17			
1	B	377	Total	C	N	O	S	0	0	0
			2985	1919	509	540	17			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	initiating methionine	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

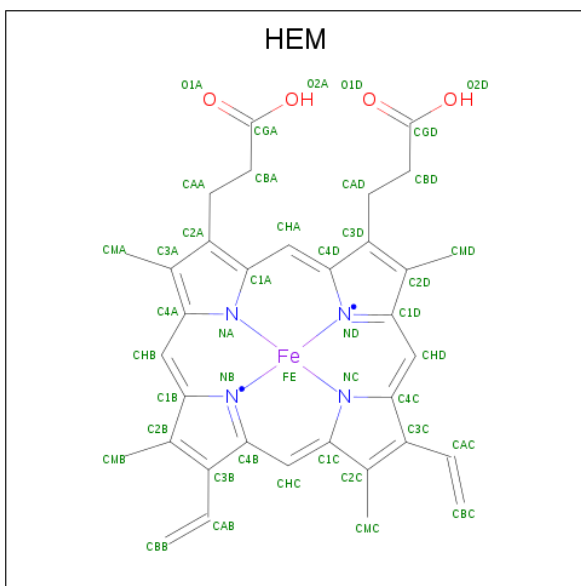
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Chain	Residue	Modelled	Actual	Comment	Reference
A	428	THR	-	expression tag	UNP P14902
A	429	GLY	-	expression tag	UNP P14902
A	430	HIS	-	expression tag	UNP P14902
A	431	HIS	-	expression tag	UNP P14902
A	432	HIS	-	expression tag	UNP P14902
A	433	HIS	-	expression tag	UNP P14902
A	434	HIS	-	expression tag	UNP P14902
A	435	HIS	-	expression tag	UNP P14902
B	11	MET	-	initiating methionine	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

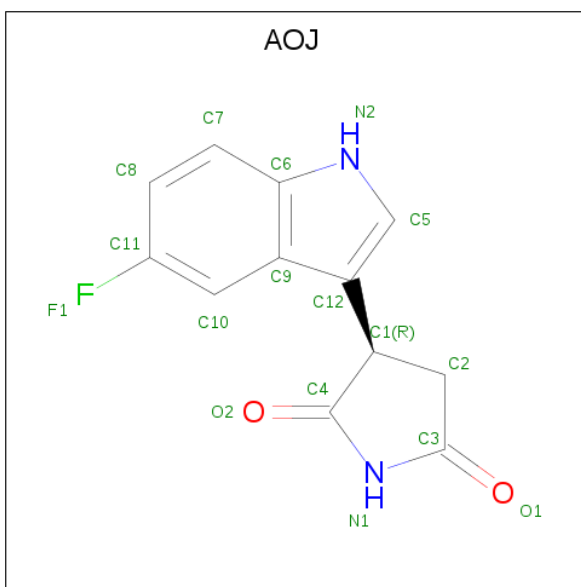
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: C₃₄H₃₂FeN₄O₄) (labeled as "Ligand of Interest" by author).



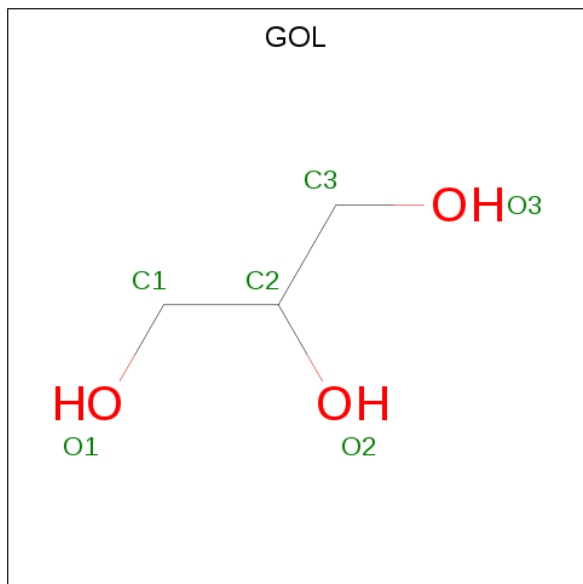
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is (3R)-3-(5-fluoro-1H-indol-3-yl)pyrrolidine-2,5-dione (three-letter code: AOJ) (formula: C₁₂H₉FN₂O₂) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			17	12	1	2	2		
3	B	1	Total	C	F	N	O	0	0
			17	12	1	2	2		
3	B	1	Total	C	F	N	O	0	0
			17	12	1	2	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

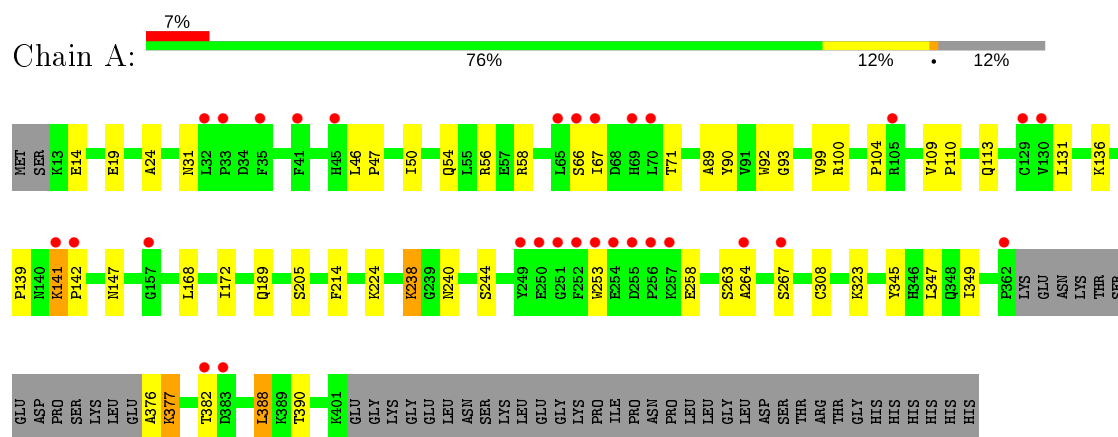
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	89	Total	O	0	0
			89	89		
5	B	99	Total	O	0	0
			99	99		

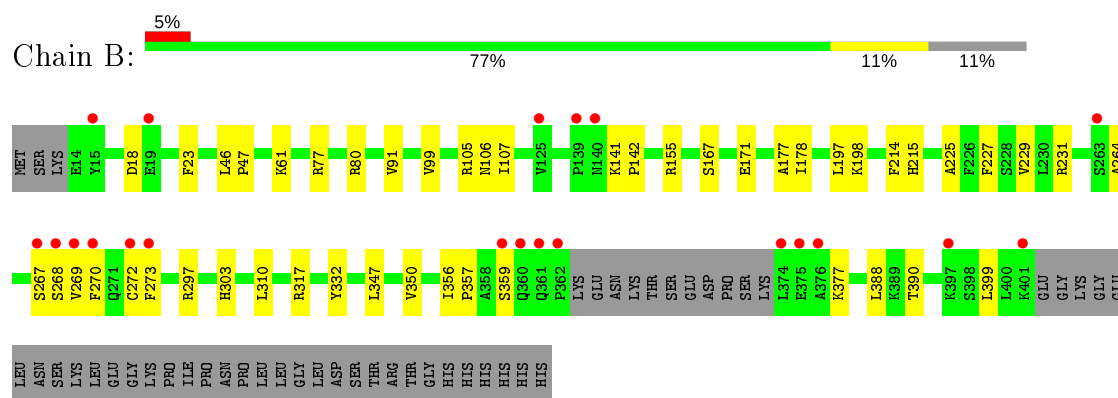
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Indoleamine 2,3-dioxygenase 1



• 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	87.48 Å 97.86 Å 131.97 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.65 39.30 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.00-2.65) 99.7 (39.30-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.65 Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.220 , 0.270 0.225 , 0.272	Depositor DCC
R_{free} test set	1671 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	78.0	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6317	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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: GOL, AOJ, 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	0.66	0/3046	0.73	0/4119
1	B	0.65	0/3054	0.72	0/4131
All	All	0.65	0/6100	0.73	0/8250

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	2977	0	2996	22	0
1	B	2985	0	3000	20	0
2	A	43	0	30	2	0
2	B	43	0	30	4	0
3	A	17	0	0	1	0
3	B	34	0	0	0	0
4	A	6	0	8	1	0
4	B	24	0	32	2	0
5	A	89	0	0	0	0
5	B	99	0	0	0	0
All	All	6317	0	6096	46	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 4.

All (46) 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:317:ARG:HD2	1:B:332:TYR:OH	1.97	0.65
1:B:269:VAL:HG13	1:B:270:PHE:CD1	2.32	0.65
2:B:501:HEM:HBB2	2:B:501:HEM:HMB2	1.77	0.65
2:A:501:HEM:HMB2	2:A:501:HEM:HBB2	1.77	0.64
1:A:89:ALA:O	1:A:93:GLY:HA2	2.02	0.59
1:B:167:SER:HA	2:B:501:HEM:HBC2	1.86	0.57
1:A:56:ARG:HH21	1:A:93:GLY:HA3	1.71	0.56
1:B:268:SER:OG	1:B:303:HIS:HB3	2.09	0.53
1:B:264:ALA:HB3	2:B:501:HEM:C1D	2.45	0.52
1:A:92:TRP:HH2	1:A:240:ASN:ND2	2.09	0.51
1:A:264:ALA:O	1:A:267:SER:HB3	2.11	0.51
1:A:147:ASN:O	1:A:147:ASN:CG	2.50	0.50
1:B:356:ILE:HB	1:B:357:PRO:HD3	1.95	0.49
1:B:225:ALA:O	1:B:229:VAL:HB	2.15	0.46
1:B:390:THR:HG21	4:B:504:GOL:H11	1.97	0.46
1:A:109:VAL:N	1:A:110:PRO:HD2	2.31	0.45
1:B:227:PHE:O	1:B:231:ARG:NH1	2.41	0.45
1:A:67:ILE:HD13	1:A:113:GLN:HB3	1.98	0.45
1:A:238:LYS:HG3	1:A:258:GLU:HB3	1.99	0.45
1:A:347:LEU:HD21	1:A:388:LEU:HB3	2.00	0.44
1:B:177:ALA:HB3	1:B:273:PHE:HZ	1.82	0.44
1:A:24:ALA:HA	1:A:131:LEU:HD22	2.00	0.43
1:B:171:GLU:OE1	1:B:267:SER:OG	2.31	0.43
1:B:178:ILE:HD11	1:B:269:VAL:HG23	2.01	0.43
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.48	0.42
1:B:267:SER:HB3	1:B:270:PHE:CD2	2.54	0.42
1:B:91:VAL:O	1:B:99:VAL:HA	2.19	0.42
1:A:56:ARG:HH11	1:A:100:ARG:NE	2.18	0.42
1:A:136:LYS:HG3	1:A:139:PRO:HA	2.02	0.42
1:A:390:THR:HG21	4:A:503:GOL:H2	2.02	0.41
1:A:92:TRP:HH2	1:A:240:ASN:HD21	1.67	0.41
1:B:46:LEU:N	1:B:47:PRO:CD	2.84	0.41
1:A:141:LYS:HD2	1:A:142:PRO:HD3	2.02	0.41
1:B:23:PHE:HD2	1:B:269:VAL:HB	1.85	0.41
2:A:501:HEM:CMB	2:A:501:HEM:HBB2	2.49	0.41
1:B:141:LYS:HB3	1:B:142:PRO:HD2	2.03	0.41
1:A:263:SER:HA	3:A:502:AOJ:C10	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:LEU:HD23	4:B:507:GOL:H11	2.03	0.40
1:A:168:LEU:O	1:A:172:ILE:HG12	2.21	0.40
1:A:345:TYR:CE2	1:A:349:ILE:HD11	2.56	0.40
1:A:376:ALA:O	1:A:377:LYS:HB2	2.21	0.40
1:B:350:VAL:HG21	1:B:388:LEU:HD13	2.04	0.40
1:B:350:VAL:HG21	1:B:388:LEU:CD1	2.52	0.40
1:A:46:LEU:N	1:A:47:PRO:CD	2.84	0.40
1:A:90:TYR:CE1	1:A:104:PRO:HD3	2.57	0.40
1:A:388:LEU:HD12	1:A:388:LEU:HA	1.96	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	372/425 (88%)	345 (93%)	26 (7%)	1 (0%)	41	56
1	B	373/425 (88%)	356 (95%)	17 (5%)	0	100	100
All	All	745/850 (88%)	701 (94%)	43 (6%)	1 (0%)	51	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	LYS

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	324/368 (88%)	303 (94%)	21 (6%)	17	26
1	B	325/368 (88%)	307 (94%)	18 (6%)	21	33
All	All	649/736 (88%)	610 (94%)	39 (6%)	19	30

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	19	GLU
1	A	31	ASN
1	A	50	ILE
1	A	54	GLN
1	A	58	ARG
1	A	66	SER
1	A	71	THR
1	A	99	VAL
1	A	141	LYS
1	A	189	GLN
1	A	205	SER
1	A	214	PHE
1	A	224	LYS
1	A	238	LYS
1	A	244	SER
1	A	253	TRP
1	A	308	CYS
1	A	323	LYS
1	A	382	THR
1	A	388	LEU
1	B	18	ASP
1	B	61	LYS
1	B	77	ARG
1	B	80	ARG
1	B	105	ARG
1	B	106	ASN
1	B	107	ILE
1	B	155	ARG
1	B	197	LEU
1	B	198	LYS
1	B	214	PHE
1	B	215	HIS
1	B	272	CYS

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Mol	Chain	Res	Type
1	B	297	ARG
1	B	347	LEU
1	B	359	SER
1	B	377	LYS
1	B	399	LEU

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

Mol	Chain	Res	Type
1	A	191	GLN
1	A	305	ASN
1	A	386	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

10 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	$\# Z > 2$
4	GOL	A	503	-	5,5,5	0.10	0	5,5,5	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AOJ	B	502	-	17,19,19	2.13	5 (29%)	19,28,28	1.95	5 (26%)
4	GOL	B	507	-	5,5,5	0.10	0	5,5,5	0.28	0
2	HEM	B	501	1	27,50,50	0.84	2 (7%)	17,82,82	0.92	0
3	AOJ	B	503	-	17,19,19	2.15	5 (29%)	19,28,28	2.01	7 (36%)
4	GOL	B	505	-	5,5,5	0.10	0	5,5,5	0.28	0
4	GOL	B	506	-	5,5,5	0.10	0	5,5,5	0.27	0
3	AOJ	A	502	-	17,19,19	2.08	5 (29%)	19,28,28	1.93	5 (26%)
2	HEM	A	501	1	27,50,50	0.83	2 (7%)	17,82,82	1.18	2 (11%)
4	GOL	B	504	-	5,5,5	0.10	0	5,5,5	0.28	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
4	GOL	A	503	-	-	2/4/4/4	-
3	AOJ	B	502	-	-	0/0/16/16	0/3/3/3
4	GOL	B	507	-	-	2/4/4/4	-
2	HEM	B	501	1	-	0/6/54/54	-
3	AOJ	B	503	-	-	0/0/16/16	0/3/3/3
4	GOL	B	505	-	-	2/4/4/4	-
4	GOL	B	506	-	-	0/4/4/4	-
3	AOJ	A	502	-	-	0/0/16/16	0/3/3/3
2	HEM	A	501	1	-	0/6/54/54	-
4	GOL	B	504	-	-	2/4/4/4	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	AOJ	C12-C9	6.08	1.47	1.40
3	B	503	AOJ	C12-C9	5.79	1.47	1.40
3	A	502	AOJ	C12-C9	5.73	1.47	1.40
3	B	503	AOJ	C4-N1	-3.87	1.32	1.37
3	A	502	AOJ	C4-N1	-3.20	1.33	1.37
3	B	502	AOJ	C4-N1	-2.99	1.33	1.37
3	B	503	AOJ	C3-N1	-2.78	1.33	1.37
3	A	502	AOJ	C3-N1	-2.78	1.33	1.37
3	B	502	AOJ	C3-N1	-2.62	1.33	1.37
2	B	501	HEM	C4D-C3D	2.45	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	AOJ	C10-C11	2.40	1.40	1.36
3	B	503	AOJ	C10-C11	2.32	1.39	1.36
3	A	502	AOJ	C10-C11	2.30	1.39	1.36
2	A	501	HEM	C3B-C2B	-2.22	1.37	1.40
3	B	502	AOJ	C9-C6	2.17	1.48	1.42
2	A	501	HEM	C4D-C3D	2.11	1.47	1.42
3	A	502	AOJ	C9-C6	2.10	1.48	1.42
3	B	503	AOJ	C9-C6	2.06	1.48	1.42
2	B	501	HEM	C3B-C2B	-2.02	1.37	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	AOJ	C12-C9-C6	-4.95	101.68	106.83
3	A	502	AOJ	C12-C9-C6	-4.89	101.74	106.83
3	B	503	AOJ	C12-C9-C6	-4.73	101.91	106.83
3	B	502	AOJ	C1-C2-C3	-3.68	102.55	105.58
3	B	503	AOJ	O1-C3-C2	-3.32	122.01	126.39
3	A	502	AOJ	C1-C2-C3	-3.20	102.95	105.58
3	A	502	AOJ	C10-C9-C6	2.66	121.90	118.26
3	B	503	AOJ	C10-C9-C6	2.64	121.87	118.26
2	A	501	HEM	CAA-CBA-CGA	-2.60	108.31	112.67
3	B	503	AOJ	O1-C3-N1	2.56	128.45	125.00
3	B	503	AOJ	C7-C8-C11	2.52	121.62	118.74
3	A	502	AOJ	C7-C8-C11	2.51	121.61	118.74
3	B	502	AOJ	C10-C9-C6	2.45	121.61	118.26
3	B	502	AOJ	C7-C8-C11	2.40	121.49	118.74
3	B	503	AOJ	C2-C1-C4	-2.40	102.47	103.64
3	B	502	AOJ	C12-C1-C4	2.36	118.26	112.14
3	B	503	AOJ	C1-C2-C3	-2.21	103.76	105.58
2	A	501	HEM	C1D-C2D-C3D	-2.06	105.56	107.00
3	A	502	AOJ	O1-C3-C2	-2.03	123.71	126.39

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	GOL	O1-C1-C2-C3
4	B	507	GOL	C1-C2-C3-O3
4	B	504	GOL	C1-C2-C3-O3
4	A	503	GOL	O1-C1-C2-O2
4	B	507	GOL	O2-C2-C3-O3

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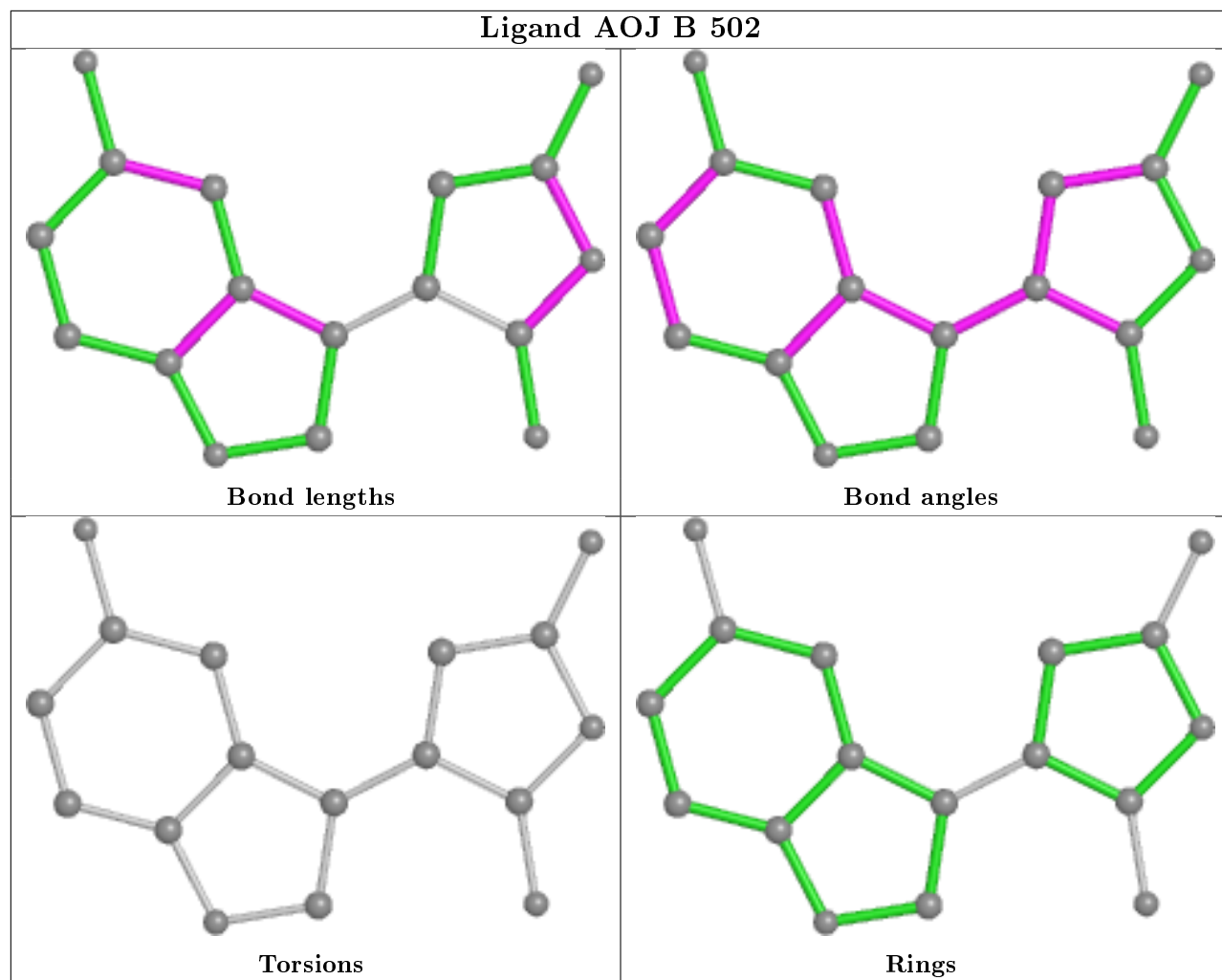
Mol	Chain	Res	Type	Atoms
4	B	504	GOL	O2-C2-C3-O3
4	B	505	GOL	O1-C1-C2-O2
4	B	505	GOL	O1-C1-C2-C3

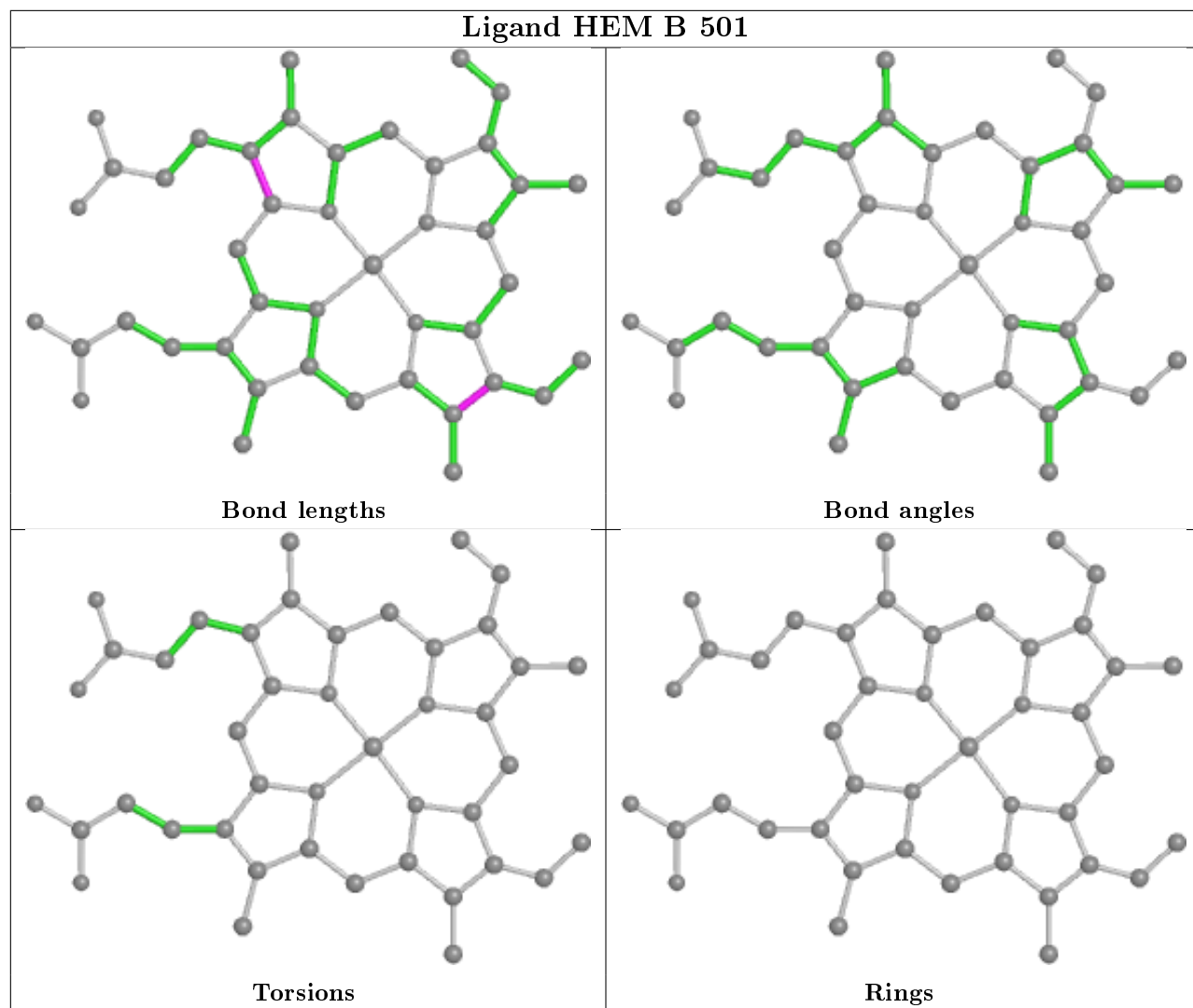
There are no ring outliers.

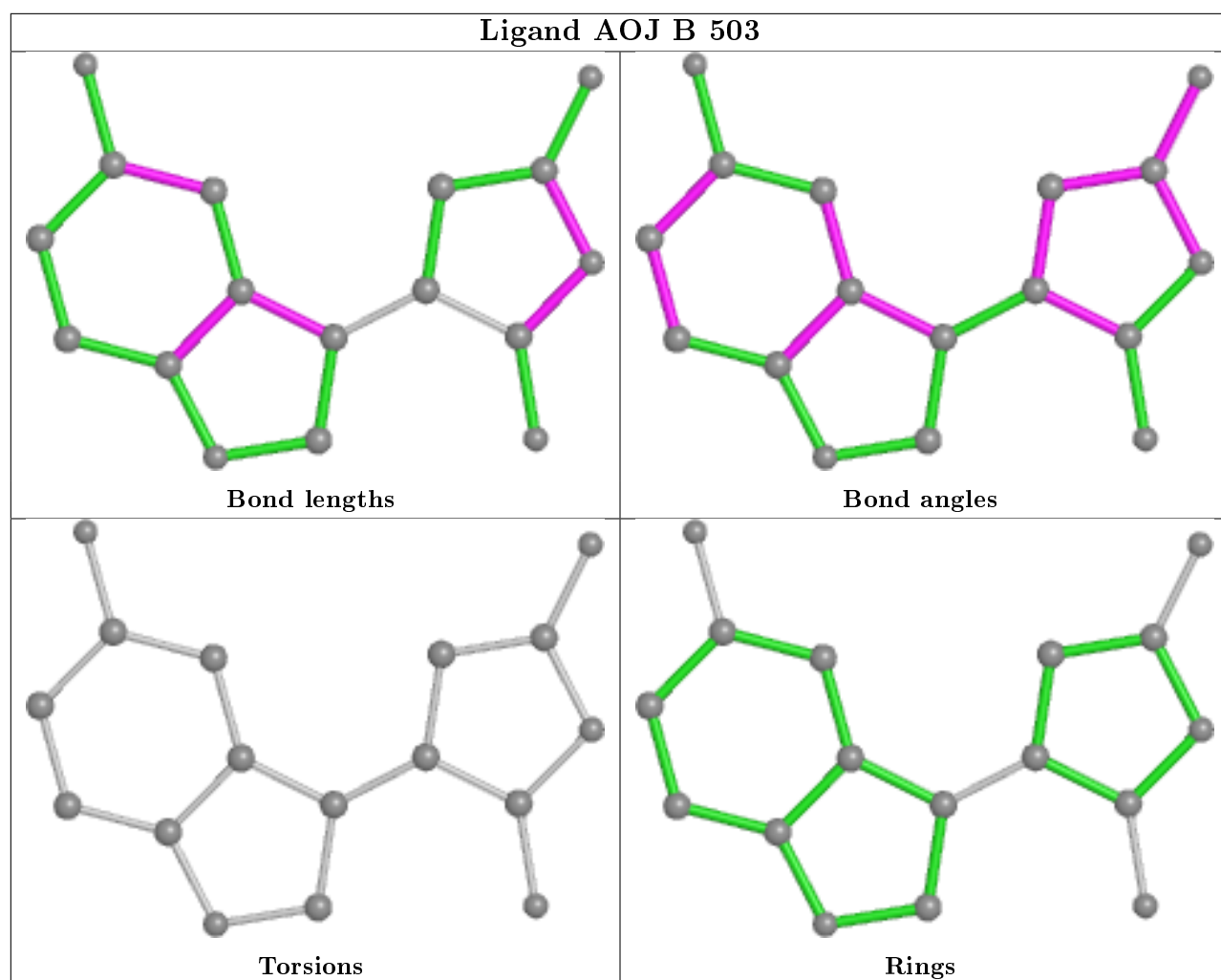
6 monomers are involved in 10 short contacts:

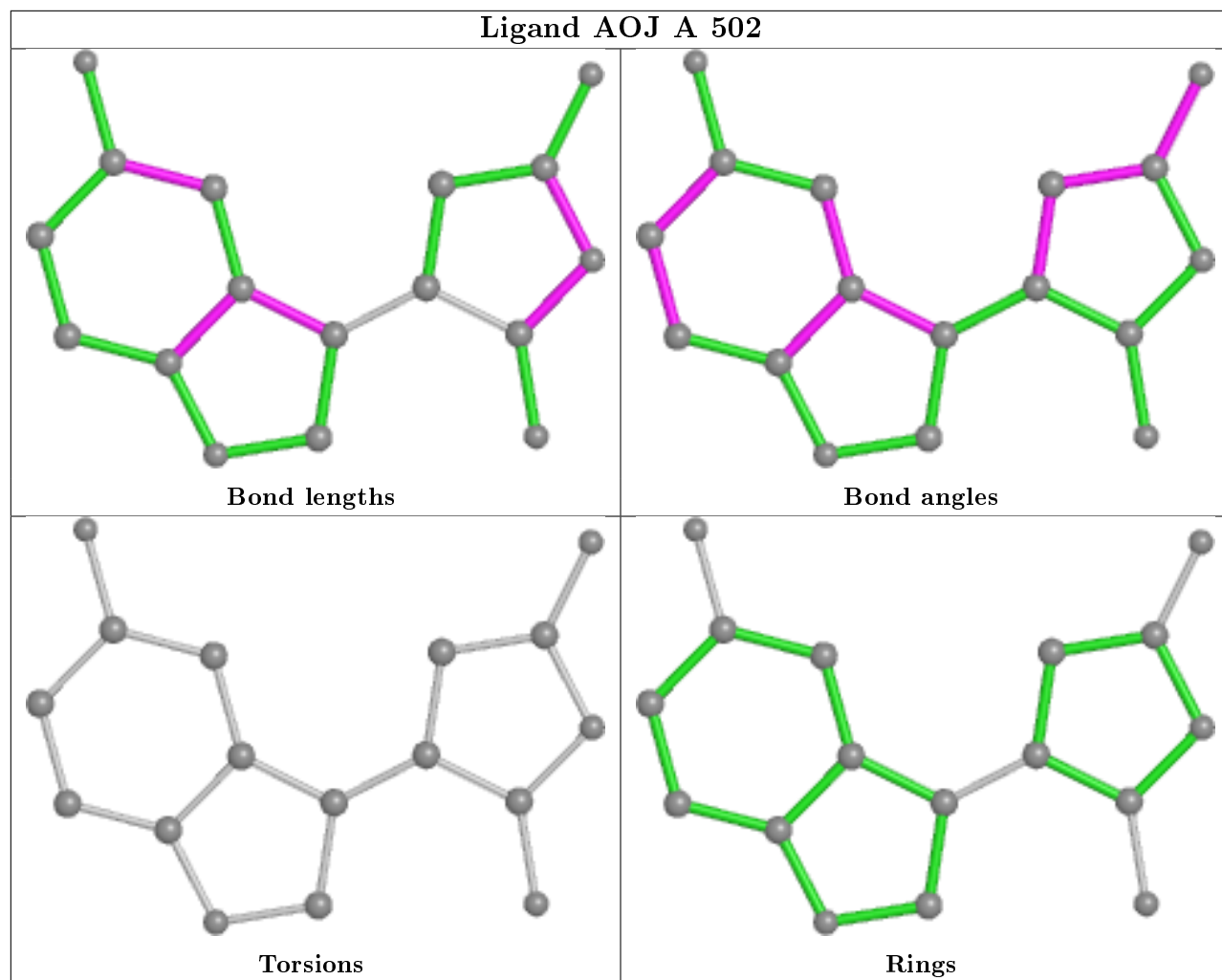
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	GOL	1	0
4	B	507	GOL	1	0
2	B	501	HEM	4	0
3	A	502	AOJ	1	0
2	A	501	HEM	2	0
4	B	504	GOL	1	0

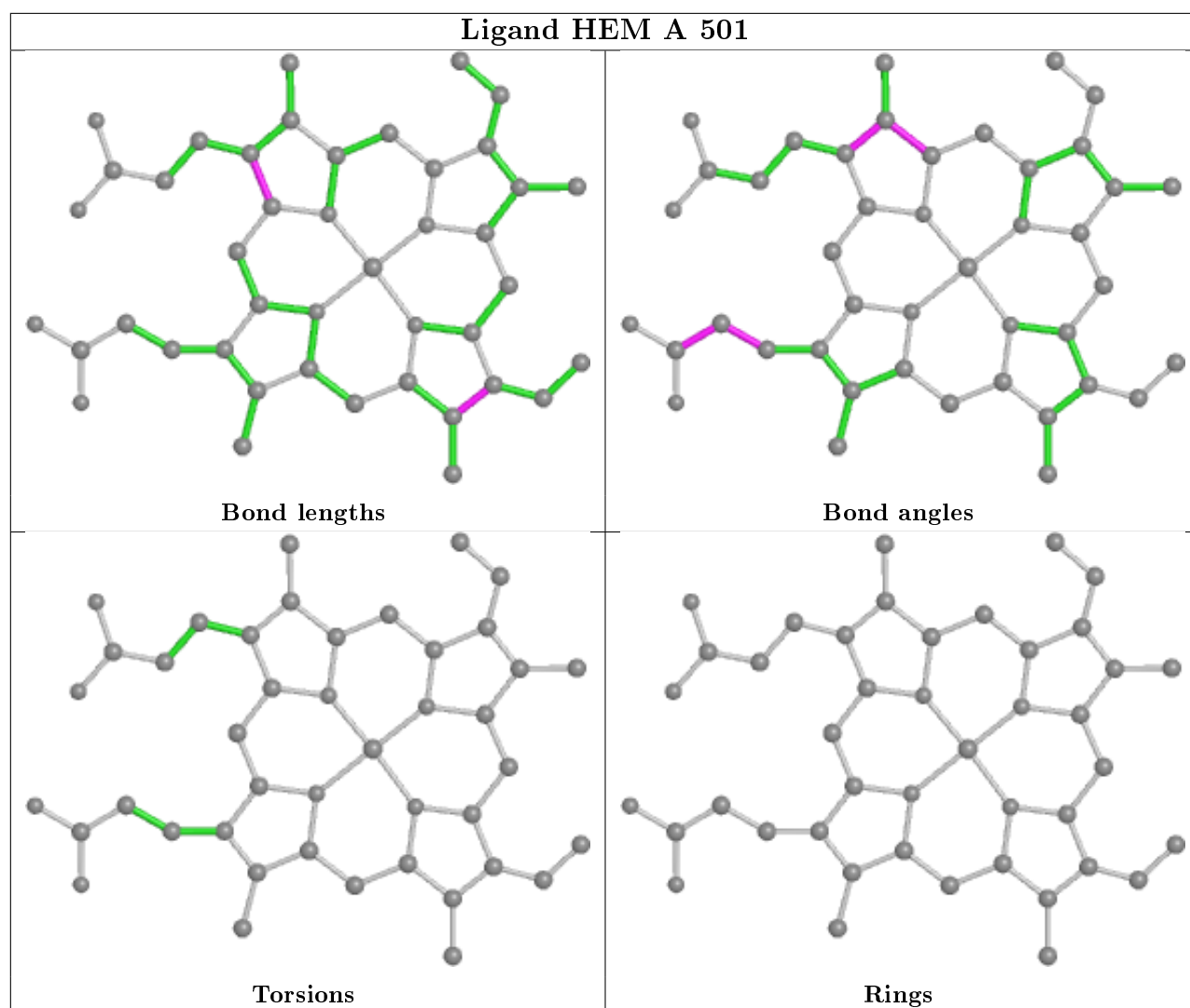
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	376/425 (88%)	0.59	30 (7%) 12 9	67, 91, 125, 136	0
1	B	377/425 (88%)	0.39	21 (5%) 24 21	65, 84, 107, 139	0
All	All	753/850 (88%)	0.49	51 (6%) 17 14	65, 87, 122, 139	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	376	ALA	5.0
1	B	401	LYS	4.9
1	A	251	GLY	4.7
1	A	383	ASP	4.5
1	A	362	PRO	4.5
1	B	362	PRO	4.4
1	A	257	LYS	4.4
1	B	374	LEU	4.2
1	A	142	PRO	4.1
1	A	252	PHE	4.0
1	A	33	PRO	3.7
1	B	139	PRO	3.6
1	A	35	PHE	3.6
1	B	375	GLU	3.4
1	A	264	ALA	3.3
1	A	249	TYR	3.3
1	A	250	GLU	3.3
1	A	105	ARG	3.3
1	B	360	GLN	3.2
1	A	45	HIS	3.1
1	A	129	CYS	3.1
1	A	141	LYS	3.1
1	B	267	SER	3.1
1	A	253	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	270	PHE	3.0
1	A	67	ILE	2.9
1	B	359	SER	2.9
1	A	69	HIS	2.8
1	A	254	GLU	2.8
1	A	130	VAL	2.8
1	B	273	PHE	2.7
1	B	272	CYS	2.6
1	B	263	SER	2.6
1	B	268	SER	2.6
1	A	256	PRO	2.5
1	A	65	LEU	2.5
1	B	125	VAL	2.5
1	B	361	GLN	2.4
1	B	19	GLU	2.4
1	A	255	ASP	2.4
1	B	269	VAL	2.4
1	B	15	TYR	2.4
1	A	267	SER	2.4
1	A	32	LEU	2.3
1	A	66	SER	2.3
1	A	41	PHE	2.2
1	B	140	ASN	2.2
1	B	397	LYS	2.2
1	A	70	LEU	2.1
1	A	157	GLY	2.1
1	A	382	THR	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 carbohydrates in this entry.

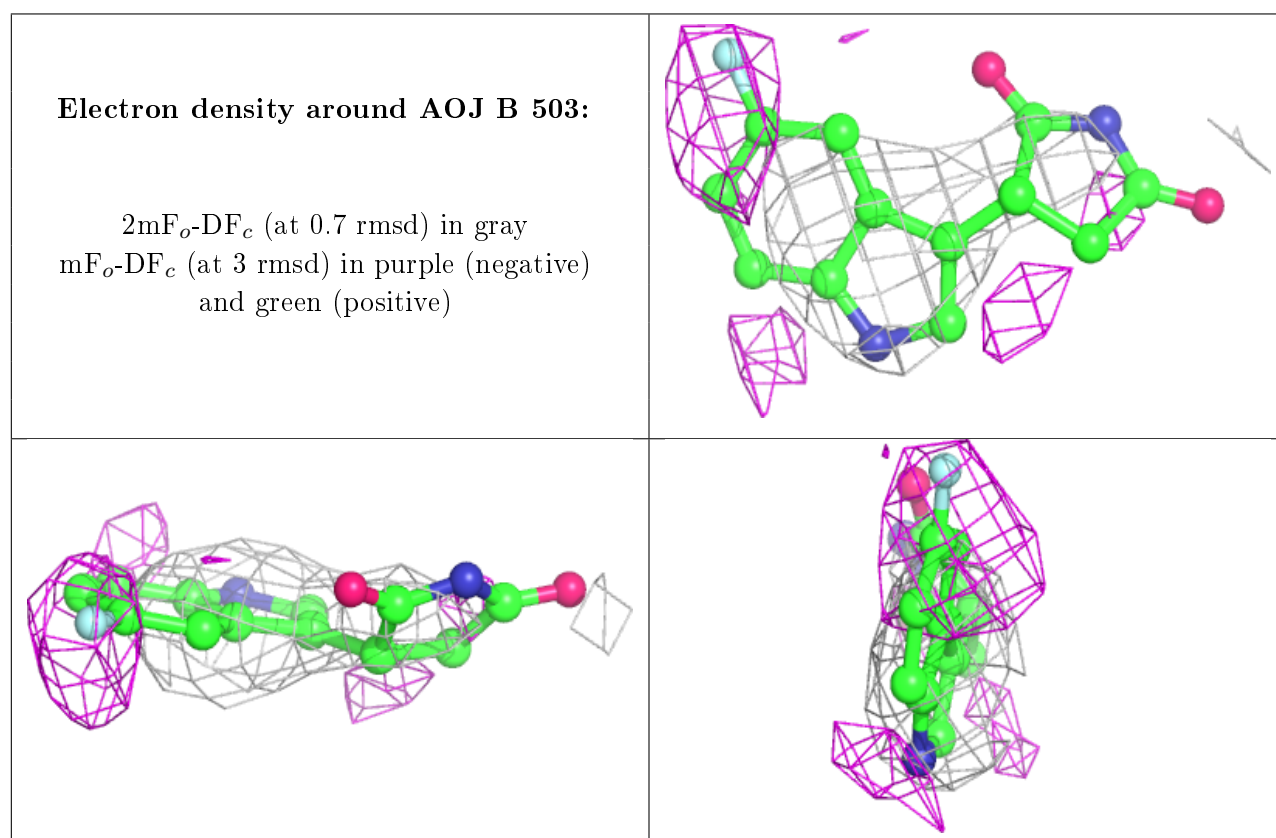
6.4 Ligands [i](#)

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.

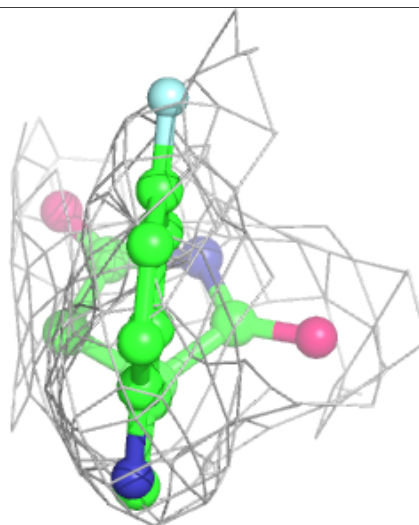
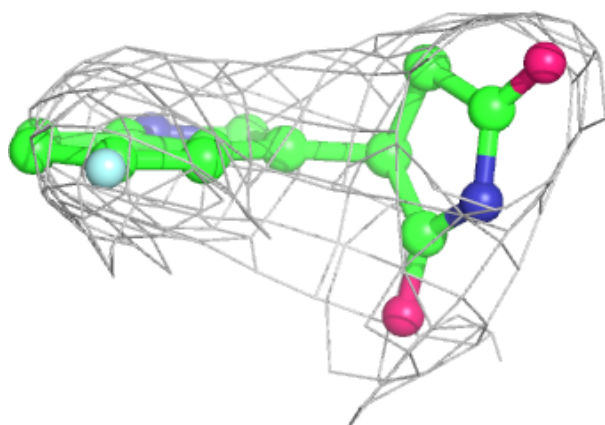
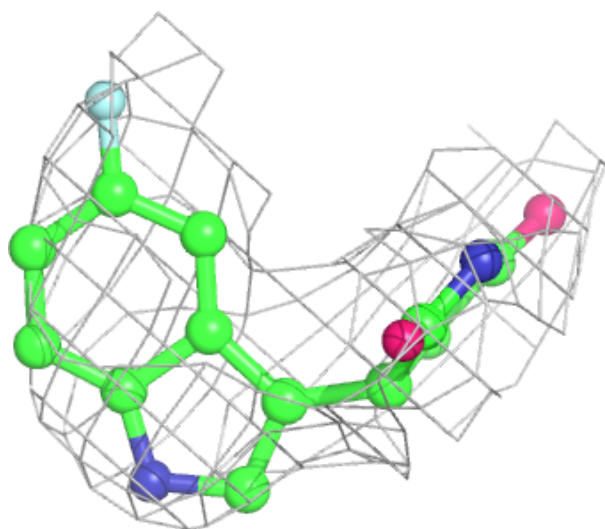
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	B	504	6/6	0.82	0.20	99,100,101,102	0
3	AOJ	B	503	17/17	0.85	0.56	126,130,138,140	0
4	GOL	B	506	6/6	0.87	0.26	77,78,79,80	0
4	GOL	A	503	6/6	0.88	0.25	101,102,103,103	0
4	GOL	B	505	6/6	0.89	0.17	82,83,86,88	0
4	GOL	B	507	6/6	0.90	0.27	113,114,114,114	0
3	AOJ	A	502	17/17	0.92	0.30	109,111,112,112	0
2	HEM	B	501	43/43	0.95	0.18	75,77,79,80	0
3	AOJ	B	502	17/17	0.95	0.16	70,72,74,74	0
2	HEM	A	501	43/43	0.97	0.23	70,74,76,78	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.



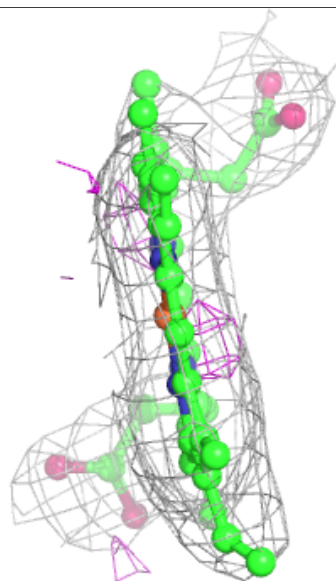
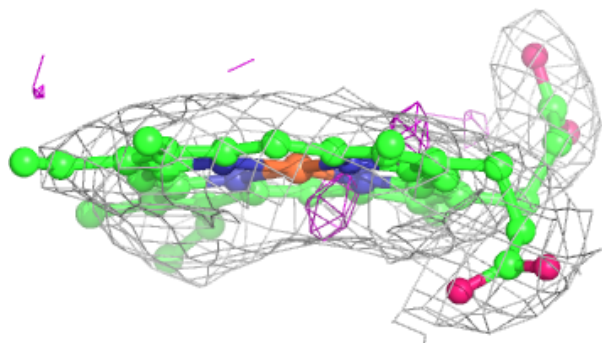
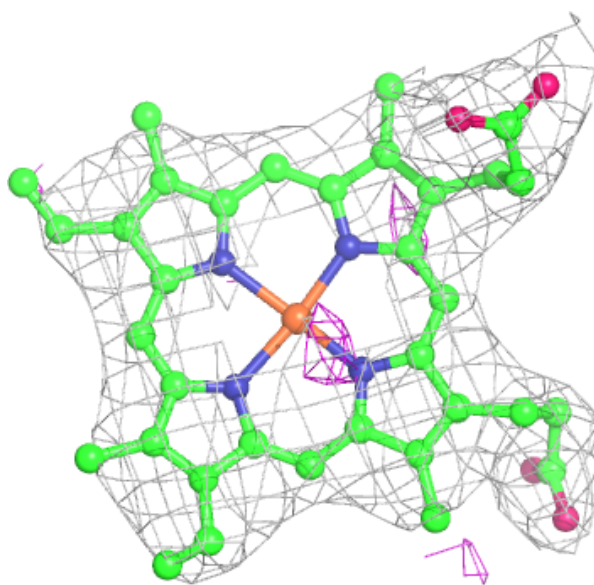
Electron density around AOJ A 502:

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



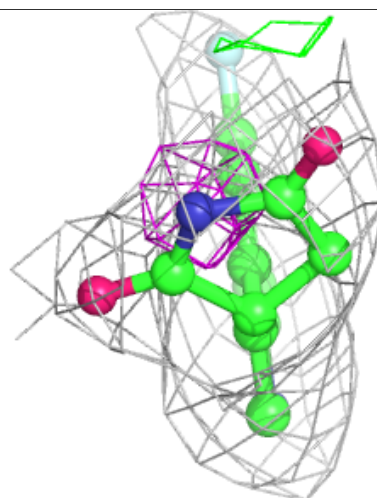
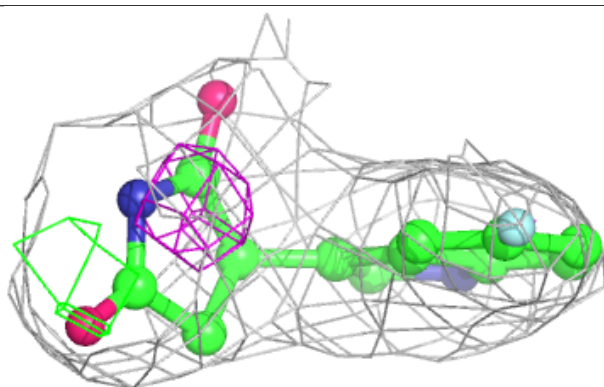
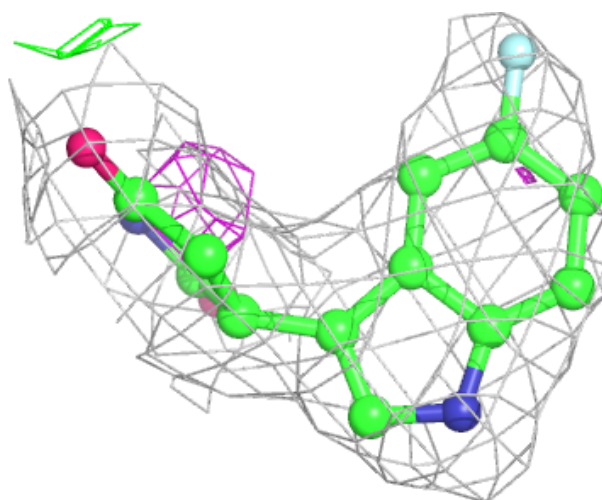
Electron density around HEM B 501:

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



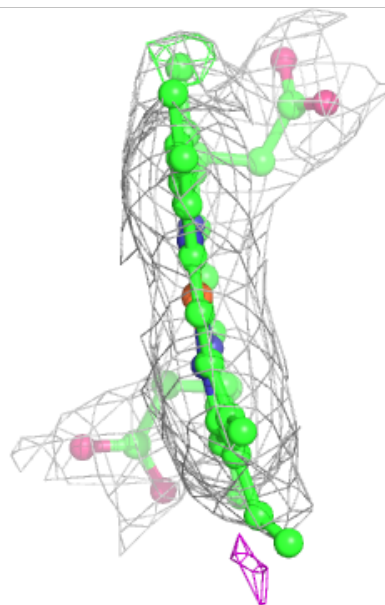
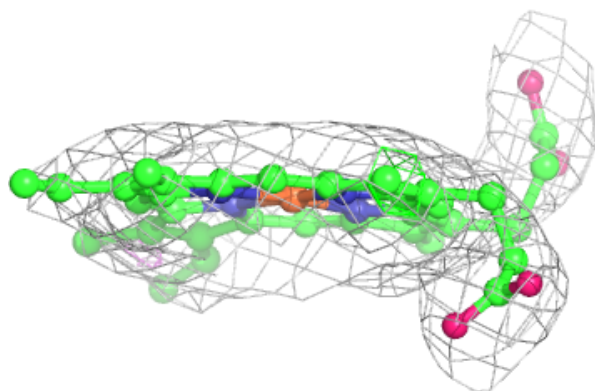
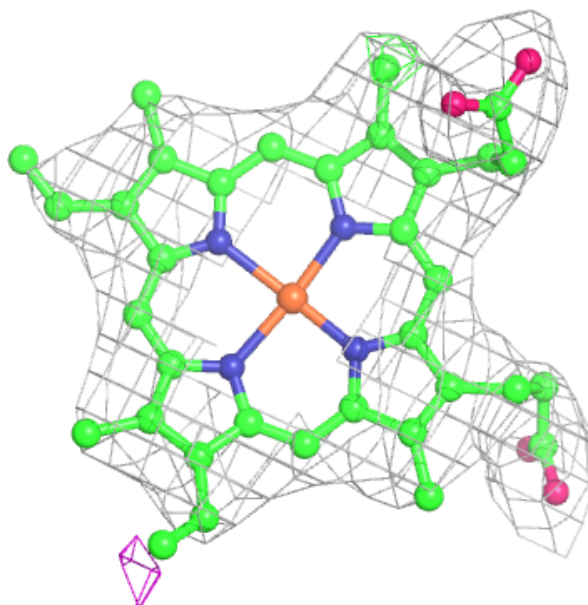
Electron density around AOJ B 502:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.