



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:09 am BST

PDB ID : 6DPQ  
Title : Mapping the binding trajectory of a suicide inhibitor in human indoleamine 2,3-dioxygenase 1  
Authors : Pham, K.N.; Yeh, S.R.  
Deposited on : 2018-06-09  
Resolution : 2.94 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](mailto: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.

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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

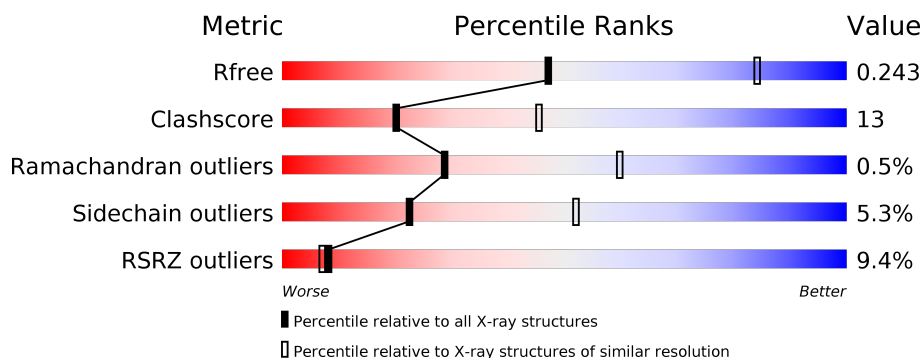
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.94 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	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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  $\geq 3$ , 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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	503	-	-	-	X
3	GOL	B	502	-	-	-	X
4	H7P	B	501	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6074 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	1890	501	531	17			
1	B	365	Total	C	N	O	S	0	0	0
			2907	1874	495	521	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

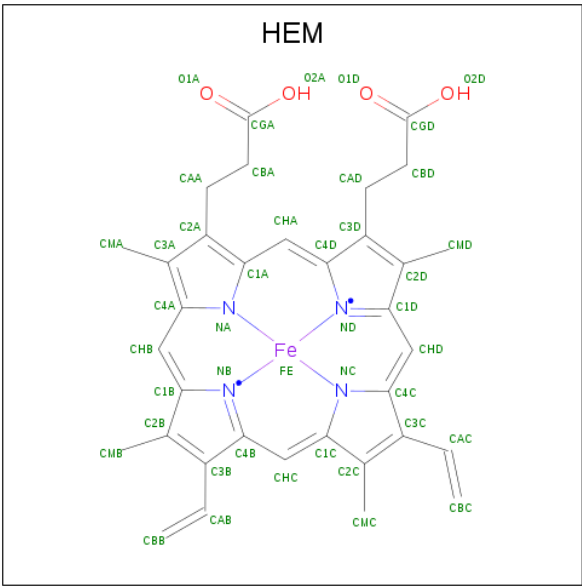
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Chain	Residue	Modelled	Actual	Comment	Reference
A	428	THR	-	expression tag	UNP P14902
A	429	GLY	-	expression tag	UNP P14902
A	430	HIS	-	expression tag	UNP P14902
A	431	HIS	-	expression tag	UNP P14902
A	432	HIS	-	expression tag	UNP P14902
A	433	HIS	-	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

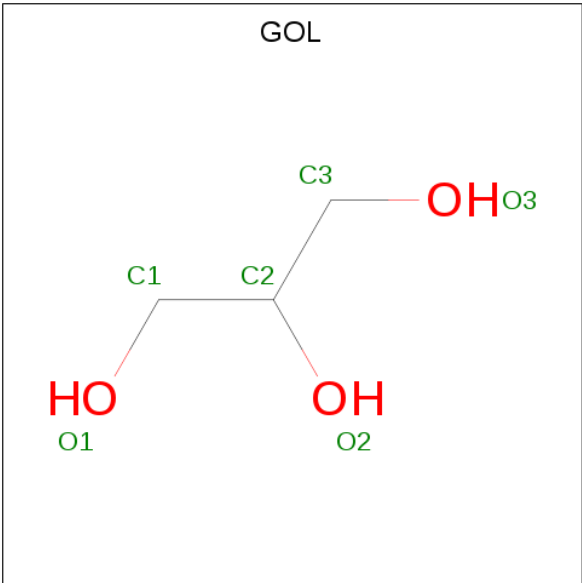
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



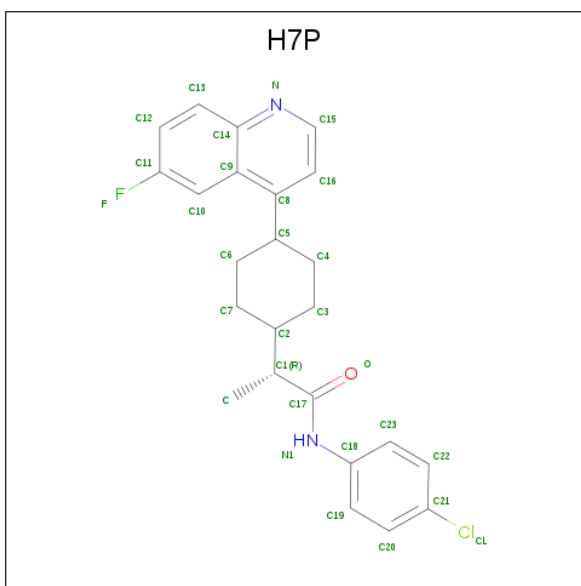
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 4 is (2R)-N-(4-chlorophenyl)-2-[cis-4-(6-fluoroquinolin-4-yl)cyclohexyl]propanamide (three-letter code: H7P) (formula: C<sub>24</sub>H<sub>24</sub>ClFN<sub>2</sub>O).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	B	1	Total	C	Cl	F	N	O		0	0
			29	24	1	1	2	1			

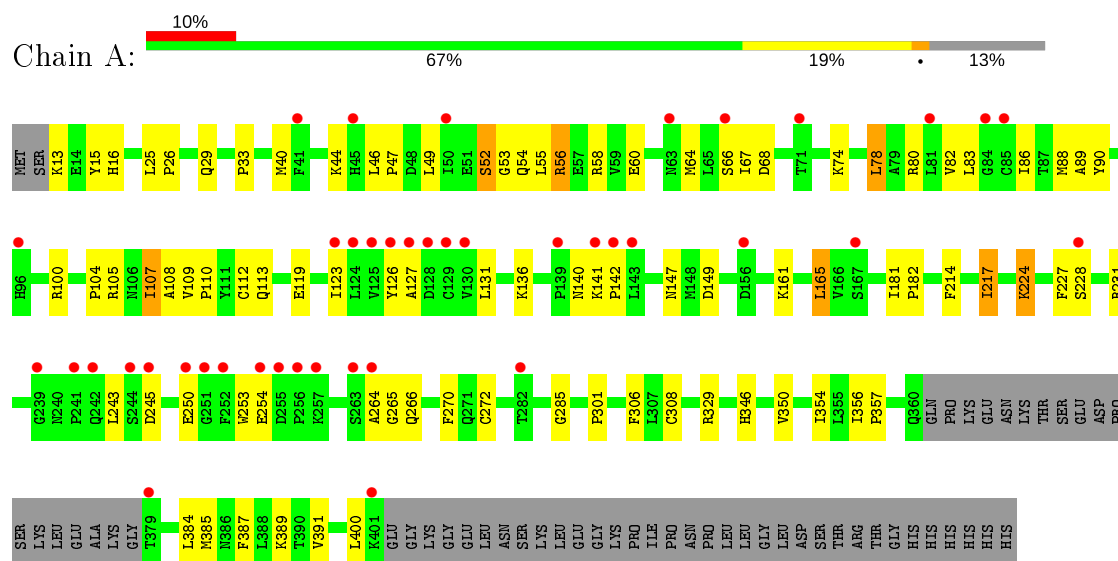
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	52	Total	O	0	0
			52	52		
5	B	68	Total	O	0	0
			68	68		

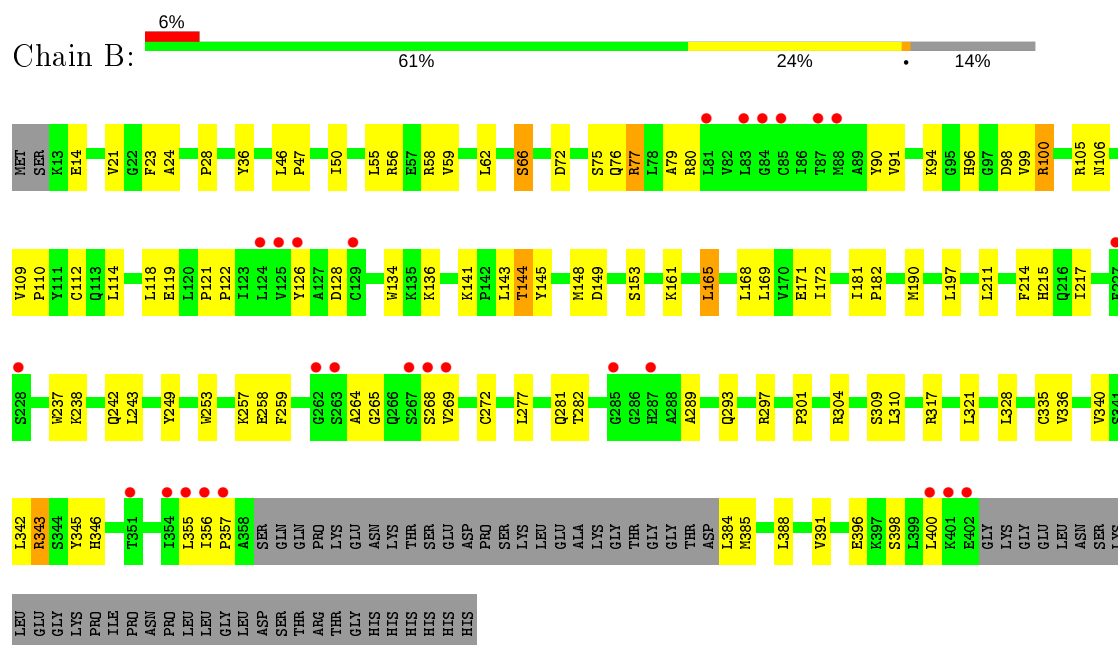
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	85.60 Å 96.56 Å 130.76 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.36 – 2.94 29.36 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.36-2.94) 99.9 (29.36-2.94)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 2.95 Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, $R_{free}$	0.191 , 0.240 0.198 , 0.243	Depositor DCC
$R_{free}$ test set	1145 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	100.7	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 65.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6074	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, H7P, 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	0.25	0/3007	0.42	0/4068
1	B	0.25	0/2975	0.42	0/4023
All	All	0.25	0/5982	0.42	0/8091

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	56	ARG	Sidechain
1	B	100	ARG	Sidechain
1	B	297	ARG	Sidechain
1	B	77	ARG	Sidechain

## 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	2949	55	0
1	B	2907	0	2929	83	0
2	A	43	0	30	8	0
3	A	18	0	24	0	0
3	B	18	0	24	3	0
4	B	29	0	0	20	0
5	A	52	0	0	2	0
5	B	68	0	0	4	0
All	All	6074	0	5956	149	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 13.

All (149) 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:56:ARG:NH1	1:B:98:ASP:O	1.86	1.08
1:B:264:ALA:HB3	4:B:501:H7P:C11	1.92	0.99
1:B:346:HIS:NE2	4:B:501:H7P:C9	2.25	0.99
1:B:264:ALA:CB	4:B:501:H7P:C11	2.40	0.98
1:B:343:ARG:HD3	1:B:391:VAL:HG12	1.46	0.94
1:B:346:HIS:NE2	4:B:501:H7P:C10	2.31	0.94
1:B:56:ARG:NH2	1:B:90:TYR:O	2.03	0.91
1:B:46:LEU:O	1:B:50:ILE:HG13	1.76	0.86
2:A:501:HEM:HBB2	2:A:501:HEM:HMB1	1.60	0.83
1:A:161:LYS:O	1:A:165:LEU:HB2	1.83	0.79
1:B:346:HIS:CE1	4:B:501:H7P:C11	2.66	0.78
1:B:214:PHE:O	1:B:217:ILE:HG22	1.85	0.77
1:A:67:ILE:CD1	1:A:113:GLN:HB2	2.17	0.74
1:B:80:ARG:NH1	1:B:121:PRO:O	2.17	0.73
4:B:501:H7P:C15	5:B:604:HOH:O	2.37	0.71
1:B:161:LYS:O	1:B:165:LEU:HB2	1.90	0.71
1:B:346:HIS:CE1	1:B:388:LEU:HD21	2.25	0.71
1:B:215:HIS:HD2	1:B:345:TYR:CZ	2.09	0.71
1:B:128:ASP:OD1	5:B:601:HOH:O	2.08	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ALA:CB	4:B:501:H7P:C10	2.70	0.69
1:A:29:GLN:HG2	1:A:74:LYS:HB3	1.75	0.68
1:B:119:GLU:HB2	1:B:301:PRO:HG3	1.74	0.68
4:B:501:H7P:C10	4:B:501:H7P:C4	2.72	0.67
2:A:501:HEM:CMB	2:A:501:HEM:HBB2	2.25	0.67
4:B:501:H7P:C7	4:B:501:H7P:N1	2.57	0.67
1:B:264:ALA:HB2	4:B:501:H7P:C10	2.24	0.67
1:B:355:LEU:HD11	1:B:385:MET:CE	2.25	0.66
1:B:136:LYS:HE2	1:B:141:LYS:O	1.96	0.66
1:B:321:LEU:HD21	1:B:400:LEU:HD22	1.77	0.66
1:B:346:HIS:CE1	4:B:501:H7P:C10	2.80	0.65
1:A:78:LEU:HD12	1:A:78:LEU:O	1.98	0.62
4:B:501:H7P:C6	4:B:501:H7P:N1	2.63	0.62
1:B:126:TYR:OH	1:B:171:GLU:OE1	2.15	0.62
1:B:264:ALA:HB3	4:B:501:H7P:C12	2.29	0.61
1:B:317:ARG:NH1	1:B:398:SER:O	2.35	0.59
1:B:59:VAL:O	1:B:62:LEU:HB2	2.02	0.59
1:B:144:THR:O	1:B:148:MET:HG3	2.03	0.59
1:B:122:PRO:HB2	1:B:249:TYR:CE2	2.38	0.59
1:A:49:LEU:HB3	1:A:55:LEU:HB2	1.83	0.59
1:A:46:LEU:N	1:A:47:PRO:CD	2.67	0.58
1:B:336:VAL:O	1:B:340:VAL:HG23	2.05	0.57
1:B:264:ALA:HB2	4:B:501:H7P:C11	2.33	0.57
1:B:46:LEU:N	1:B:47:PRO:HD2	2.19	0.57
1:B:56:ARG:NH2	1:B:100:ARG:HG2	2.19	0.56
1:B:355:LEU:HD11	1:B:385:MET:HE1	1.88	0.56
1:A:52:SER:OG	1:A:53:GLY:N	2.39	0.55
1:B:76:GLN:HG2	1:B:114:LEU:HD11	1.89	0.54
1:A:385:MET:O	1:A:389:LYS:HG3	2.08	0.54
1:B:76:GLN:HB3	1:B:118:LEU:HD11	1.89	0.54
1:B:281:GLN:O	1:B:289:ALA:HA	2.07	0.54
1:B:36:TYR:OH	1:B:66:SER:O	2.20	0.54
1:A:40:MET:O	1:A:44:LYS:HB2	2.08	0.54
1:A:105:ARG:HG2	1:A:250:GLU:C	2.28	0.54
1:A:67:ILE:CD1	1:A:113:GLN:CB	2.84	0.54
1:A:86:ILE:HG21	1:A:107:ILE:HD11	1.89	0.53
1:B:343:ARG:HD3	1:B:391:VAL:CG1	2.32	0.53
1:B:72:ASP:O	1:B:76:GLN:NE2	2.42	0.53
1:A:67:ILE:HD11	1:A:113:GLN:HB2	1.91	0.52
1:B:238:LYS:O	3:B:502:GOL:O3	2.27	0.52
1:B:181:ILE:N	1:B:182:PRO:CD	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:LEU:C	1:B:55:LEU:HD13	2.31	0.51
1:A:13:LYS:HG2	1:A:16:HIS:HA	1.91	0.51
4:B:501:H7P:C17	4:B:501:H7P:C4	2.88	0.51
1:B:214:PHE:O	1:B:214:PHE:CD1	2.64	0.50
1:A:254:GLU:H	1:A:254:GLU:CD	2.14	0.50
1:B:346:HIS:NE2	4:B:501:H7P:C14	2.75	0.50
1:B:21:VAL:HB	1:B:24:ALA:HB3	1.94	0.50
1:B:238:LYS:HA	1:B:258:GLU:HB3	1.93	0.50
1:A:227:PHE:O	1:A:231:ARG:NH1	2.44	0.50
1:B:143:LEU:HD22	1:B:148:MET:HE1	1.94	0.50
4:B:501:H7P:C23	4:B:501:H7P:O	2.57	0.50
1:B:264:ALA:HB3	4:B:501:H7P:F	2.01	0.49
1:A:119:GLU:HB2	1:A:301:PRO:HG3	1.94	0.49
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.43	0.49
1:A:108:ALA:O	1:A:112:CYS:HB2	2.13	0.49
1:B:119:GLU:O	1:B:304:ARG:NH2	2.43	0.49
1:A:56:ARG:HH21	1:A:100:ARG:HG2	1.77	0.48
1:A:127:ALA:HA	1:A:131:LEU:HD12	1.95	0.48
1:B:94:LYS:HG3	3:B:503:GOL:H12	1.96	0.48
1:A:29:GLN:O	1:A:78:LEU:HD22	2.14	0.48
1:A:54:GLN:O	1:A:58:ARG:HB2	2.14	0.48
1:B:190:MET:HG3	5:B:665:HOH:O	2.13	0.47
1:B:282:THR:HG23	1:B:293:GLN:HG2	1.97	0.47
1:B:215:HIS:HA	1:B:345:TYR:OH	2.14	0.47
1:B:282:THR:CG2	1:B:282:THR:O	2.62	0.47
1:B:109:VAL:HB	1:B:110:PRO:CD	2.45	0.47
1:A:346:HIS:O	1:A:350:VAL:HG23	2.14	0.47
1:A:80:ARG:NH1	1:A:123:ILE:O	2.47	0.47
2:A:501:HEM:HMB1	2:A:501:HEM:CBB	2.41	0.47
1:B:168:LEU:O	1:B:172:ILE:HG13	2.14	0.46
1:B:346:HIS:CE1	4:B:501:H7P:C12	2.98	0.46
1:B:98:ASP:HB3	3:B:503:GOL:O1	2.15	0.46
1:A:112:CYS:SG	1:A:253:TRP:CZ3	3.06	0.46
1:A:67:ILE:HD12	1:A:113:GLN:HB2	1.95	0.46
1:B:72:ASP:O	1:B:75:SER:OG	2.33	0.45
1:A:126:TYR:CD1	1:A:264:ALA:HA	2.50	0.45
1:A:329:ARG:HG2	1:A:400:LEU:HD23	1.97	0.45
1:B:384:LEU:HD11	5:B:667:HOH:O	2.17	0.45
1:B:277:LEU:HD11	1:B:335:CYS:HB3	1.97	0.45
1:A:105:ARG:HG2	1:A:250:GLU:O	2.16	0.45
1:A:136:LYS:HE2	1:A:141:LYS:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LEU:N	1:A:47:PRO:HD2	2.31	0.45
1:A:265:GLY:HA2	2:A:501:HEM:C3D	2.52	0.45
1:B:215:HIS:HD2	1:B:345:TYR:CE1	2.33	0.45
1:A:224:LYS:O	1:A:228:SER:OG	2.26	0.45
1:A:356:ILE:HB	1:A:357:PRO:HD3	1.98	0.45
1:B:211:LEU:HD13	1:B:342:LEU:HD23	1.99	0.44
1:B:264:ALA:HA	4:B:501:H7P:C23	2.48	0.44
1:A:165:LEU:HA	1:A:165:LEU:HD22	1.80	0.44
1:B:23:PHE:CE2	1:B:268:SER:HB2	2.53	0.44
1:A:90:TYR:CE2	1:A:104:PRO:HD3	2.52	0.44
1:B:356:ILE:HG22	1:B:357:PRO:HD3	1.98	0.44
1:A:49:LEU:HD23	1:A:55:LEU:HA	1.99	0.44
1:B:14:GLU:OE2	1:B:14:GLU:HA	2.16	0.44
1:B:301:PRO:HA	1:B:304:ARG:NH1	2.33	0.43
1:B:310:LEU:HD23	1:B:310:LEU:HA	1.86	0.43
1:B:289:ALA:O	1:B:293:GLN:HG3	2.19	0.43
1:A:387:PHE:O	1:A:391:VAL:HG23	2.18	0.43
1:A:15:TYR:HB3	1:A:306:PHE:HB2	2.01	0.43
1:B:79:ALA:HB3	1:B:114:LEU:HD21	2.01	0.42
2:A:501:HEM:HBC2	2:A:501:HEM:HMC1	2.01	0.42
1:B:197:LEU:HD23	1:B:328:LEU:HD23	2.00	0.42
1:A:67:ILE:HD12	1:A:113:GLN:CB	2.49	0.42
1:A:126:TYR:HB2	1:A:266:GLN:HB2	2.02	0.42
1:B:282:THR:O	1:B:282:THR:HG22	2.20	0.42
1:A:181:ILE:HB	1:A:182:PRO:HD3	2.02	0.42
1:A:384:LEU:HD11	2:A:501:HEM:HMA3	2.02	0.42
1:A:217:ILE:HD11	2:A:501:HEM:HAB	2.02	0.42
1:A:55:LEU:HD21	1:A:89:ALA:HB1	2.01	0.41
1:A:82:VAL:HG12	1:A:83:LEU:N	2.34	0.41
1:A:270:PHE:N	5:A:606:HOH:O	2.52	0.41
1:A:25:LEU:HA	1:A:26:PRO:HD3	1.90	0.41
1:A:64:MET:HG2	1:A:64:MET:O	2.20	0.41
1:B:28:PRO:HD3	1:B:134:TRP:CZ2	2.56	0.41
1:A:181:ILE:N	1:A:182:PRO:HD2	2.36	0.41
1:B:253:TRP:CE3	1:B:257:LYS:HG3	2.55	0.41
1:B:23:PHE:HD2	1:B:269:VAL:HG23	1.85	0.41
1:B:91:VAL:O	1:B:99:VAL:HA	2.20	0.41
1:A:127:ALA:O	1:A:131:LEU:HB2	2.20	0.41
1:A:109:VAL:N	1:A:110:PRO:HD2	2.34	0.41
1:A:78:LEU:HD12	1:A:78:LEU:C	2.41	0.41
1:B:165:LEU:HD23	1:B:165:LEU:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:TYR:CD1	1:B:145:TYR:C	2.95	0.40
1:B:112:CYS:SG	1:B:249:TYR:CD2	3.14	0.40
1:A:147:ASN:O	1:A:147:ASN:CG	2.60	0.40
1:B:122:PRO:HD2	1:B:259:PHE:CE2	2.57	0.40
1:B:165:LEU:O	1:B:169:LEU:HG	2.21	0.40
1:A:270:PHE:HB2	5:A:635:HOH:O	2.20	0.40
1:B:77:ARG:HG3	1:B:77:ARG:HH11	1.87	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%)	341 (93%)	23 (6%)	3 (1%)	19	49
1	B	361/425 (85%)	338 (94%)	22 (6%)	1 (0%)	41	69
All	All	728/850 (86%)	679 (93%)	45 (6%)	4 (0%)	29	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	PRO
1	A	142	PRO
1	B	265	GLY
1	A	285	GLY

### 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%)	302 (94%)	18 (6%)	21	50
1	B	317/368 (86%)	301 (95%)	16 (5%)	24	54
All	All	637/736 (86%)	603 (95%)	34 (5%)	22	52

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	SER
1	A	60	GLU
1	A	66	SER
1	A	68	ASP
1	A	78	LEU
1	A	88	MET
1	A	107	ILE
1	A	140	ASN
1	A	149	ASP
1	A	165	LEU
1	A	214	PHE
1	A	217	ILE
1	A	224	LYS
1	A	243	LEU
1	A	245	ASP
1	A	272	CYS
1	A	308	CYS
1	A	354	ILE
1	B	58	ARG
1	B	66	SER
1	B	96	HIS
1	B	105	ARG
1	B	106	ASN
1	B	144	THR
1	B	149	ASP
1	B	153	SER
1	B	165	LEU
1	B	237	TRP
1	B	242	GLN
1	B	243	LEU
1	B	272	CYS
1	B	309	SER
1	B	343	ARG

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Mol	Chain	Res	Type
1	B	396	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	73	HIS
1	A	113	GLN
1	A	140	ASN
1	A	222	ASN
1	A	290	GLN
1	B	63	ASN
1	B	113	GLN
1	B	140	ASN
1	B	215	HIS

### 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](#)

8 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
2	HEM	A	501	1,5	27,50,50	0.86	2 (7%)	17,82,82	1.12	0
3	GOL	A	504	-	5,5,5	0.28	0	5,5,5	0.23	0
3	GOL	B	502	-	5,5,5	0.25	0	5,5,5	0.22	0
4	H7P	B	501	-	32,32,32	1.49	5 (15%)	45,45,45	1.60	7 (15%)
3	GOL	A	502	-	5,5,5	0.29	0	5,5,5	0.17	0
3	GOL	B	503	-	5,5,5	0.27	0	5,5,5	0.28	0
3	GOL	B	504	-	5,5,5	0.29	0	5,5,5	0.28	0
3	GOL	A	503	-	5,5,5	0.28	0	5,5,5	0.20	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
2	HEM	A	501	1,5	-	0/6/54/54	-
3	GOL	A	504	-	-	2/4/4/4	-
3	GOL	B	502	-	-	0/4/4/4	-
4	H7P	B	501	-	-	8/16/26/26	0/4/4/4
3	GOL	A	502	-	-	4/4/4/4	-
3	GOL	B	503	-	-	0/4/4/4	-
3	GOL	B	504	-	-	2/4/4/4	-
3	GOL	A	503	-	-	2/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	H7P	C8-C9	4.01	1.50	1.43
4	B	501	H7P	C9-C14	3.88	1.48	1.42
4	B	501	H7P	C18-N1	-3.25	1.35	1.41
2	A	501	HEM	C3B-C2B	-2.55	1.36	1.40
4	B	501	H7P	C21-CL	2.54	1.80	1.74
4	B	501	H7P	C10-C11	2.36	1.40	1.36
2	A	501	HEM	C4D-C3D	2.20	1.47	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	H7P	C7-C6-C5	4.81	119.56	110.52
4	B	501	H7P	C5-C8-C9	3.98	124.83	120.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	H7P	C18-N1-C17	-3.44	119.17	127.40
4	B	501	H7P	C15-N-C14	3.21	121.90	116.93
4	B	501	H7P	C9-C14-N	-2.68	119.98	122.83
4	B	501	H7P	C6-C7-C2	2.61	118.13	112.24
4	B	501	H7P	C16-C8-C5	-2.20	118.28	120.55

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	504	GOL	O1-C1-C2-C3
4	B	501	H7P	C4-C5-C8-C9
4	B	501	H7P	C4-C5-C8-C16
3	A	502	GOL	O1-C1-C2-C3
3	A	502	GOL	C1-C2-C3-O3
3	B	504	GOL	O1-C1-C2-C3
3	A	504	GOL	O1-C1-C2-O2
3	A	502	GOL	O1-C1-C2-O2
3	A	502	GOL	O2-C2-C3-O3
3	A	503	GOL	O1-C1-C2-C3
4	B	501	H7P	C1-C17-N1-C18
3	B	504	GOL	O1-C1-C2-O2
4	B	501	H7P	C2-C1-C17-O
4	B	501	H7P	C-C1-C17-N1
4	B	501	H7P	O-C17-N1-C18
3	A	503	GOL	O1-C1-C2-O2
4	B	501	H7P	C2-C1-C17-N1
4	B	501	H7P	C19-C18-N1-C17

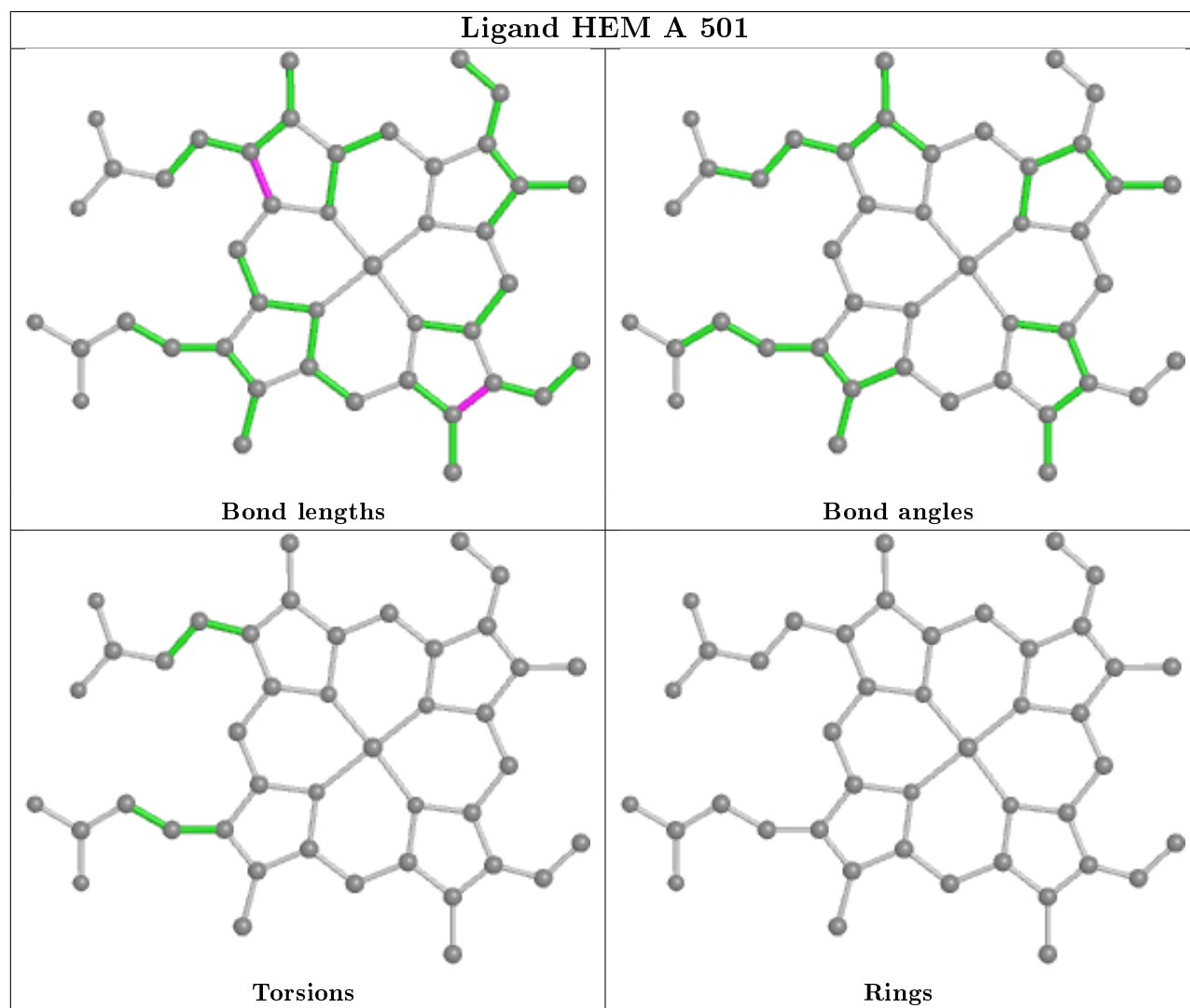
There are no ring outliers.

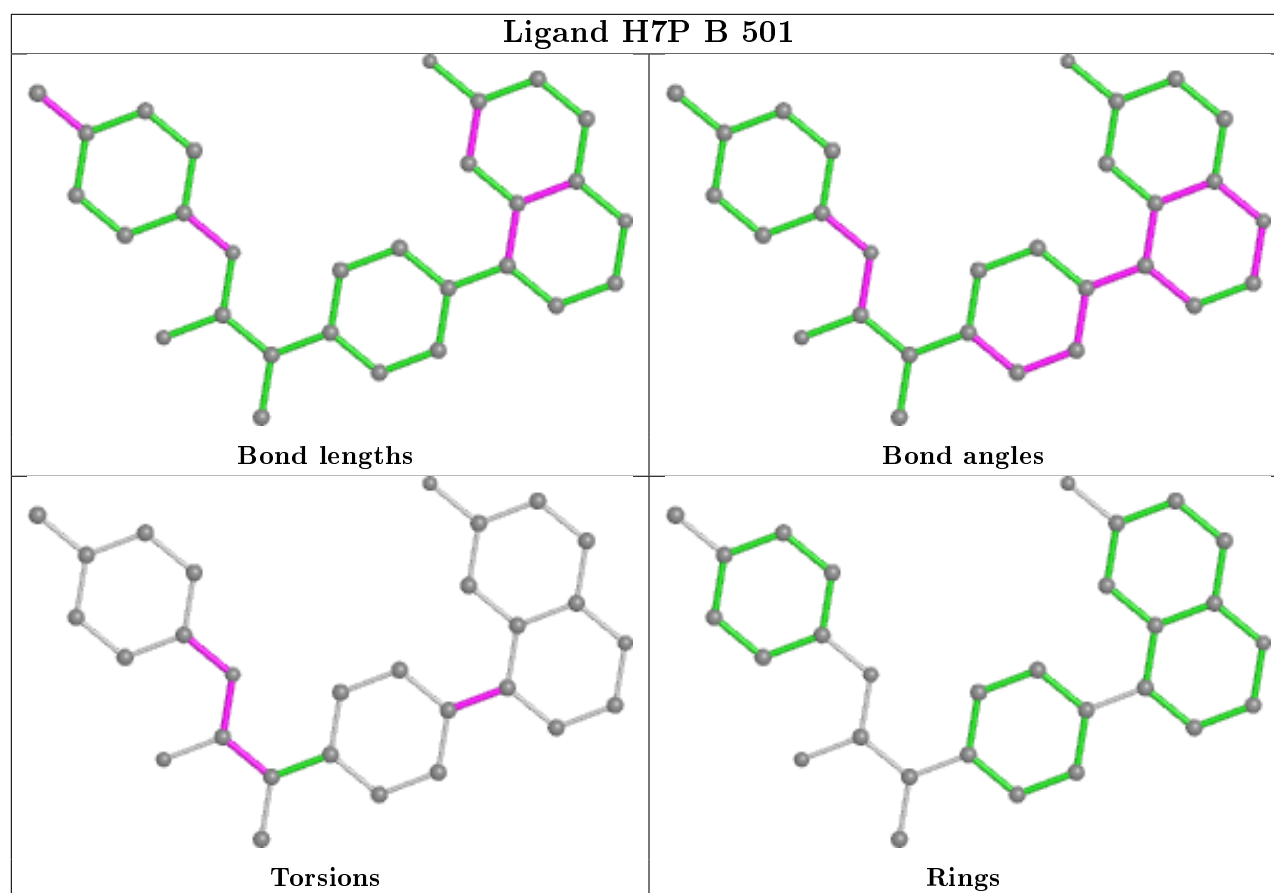
4 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	8	0
3	B	502	GOL	1	0
4	B	501	H7P	20	0
3	B	503	GOL	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	371/425 (87%)	0.31	42 (11%) 5 4	70, 116, 170, 197	0
1	B	365/425 (85%)	0.14	27 (7%) 14 12	75, 106, 145, 174	0
All	All	736/850 (86%)	0.23	69 (9%) 8 7	70, 109, 163, 197	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	241	PRO	5.6
1	A	142	PRO	5.2
1	A	129	CYS	4.8
1	B	84	GLY	4.7
1	B	85	CYS	4.6
1	A	244	SER	4.5
1	A	263	SER	4.4
1	A	84	GLY	4.3
1	A	255	ASP	4.2
1	A	125	VAL	4.0
1	B	228	SER	4.0
1	A	156	ASP	3.8
1	B	355	LEU	3.8
1	A	252	PHE	3.8
1	A	45	HIS	3.7
1	A	379	THR	3.6
1	A	264	ALA	3.5
1	A	250	GLU	3.4
1	B	129	CYS	3.3
1	A	85	CYS	3.3
1	A	128	ASP	3.3
1	B	267	SER	3.2
1	A	71	THR	3.2
1	B	124	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	400	LEU	3.1
1	B	269	VAL	3.1
1	B	227	PHE	3.1
1	B	88	MET	3.0
1	A	130	VAL	3.0
1	A	245	ASP	3.0
1	A	126	TYR	2.9
1	A	63	ASN	2.9
1	A	41	PHE	2.9
1	A	256	PRO	2.9
1	A	228	SER	2.8
1	A	141	LYS	2.8
1	B	87	THR	2.8
1	B	354	ILE	2.8
1	B	357	PRO	2.8
1	A	96	HIS	2.8
1	A	242	GLN	2.7
1	B	402	GLU	2.7
1	A	124	LEU	2.6
1	A	251	GLY	2.6
1	B	287	HIS	2.6
1	A	123	ILE	2.5
1	A	139	PRO	2.5
1	B	285	GLY	2.5
1	B	351	THR	2.5
1	A	282	THR	2.5
1	B	356	ILE	2.4
1	A	81	LEU	2.4
1	A	143	LEU	2.4
1	A	254	GLU	2.4
1	A	167	SER	2.4
1	B	262	GLY	2.3
1	B	401	LYS	2.3
1	A	401	LYS	2.2
1	B	81	LEU	2.2
1	B	125	VAL	2.2
1	B	268	SER	2.1
1	A	66	SER	2.1
1	B	83	LEU	2.1
1	A	50	ILE	2.1
1	A	127	ALA	2.1
1	A	239	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	257	LYS	2.1
1	B	126	TYR	2.0
1	B	263	SER	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, 95<sup>th</sup> 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.

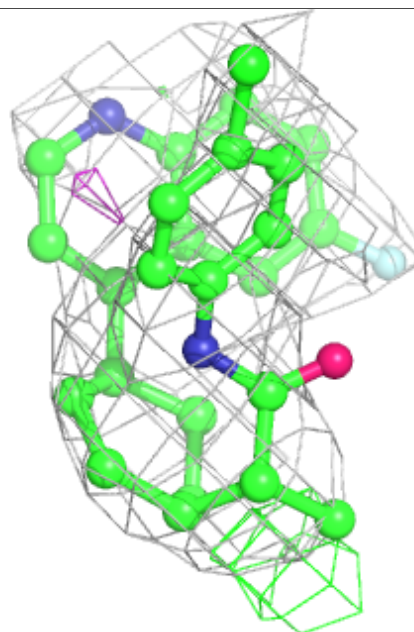
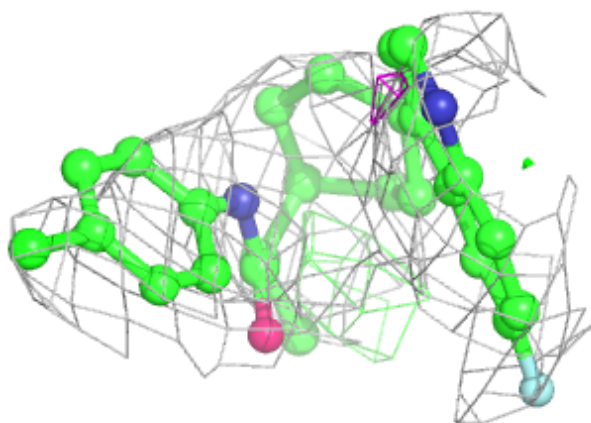
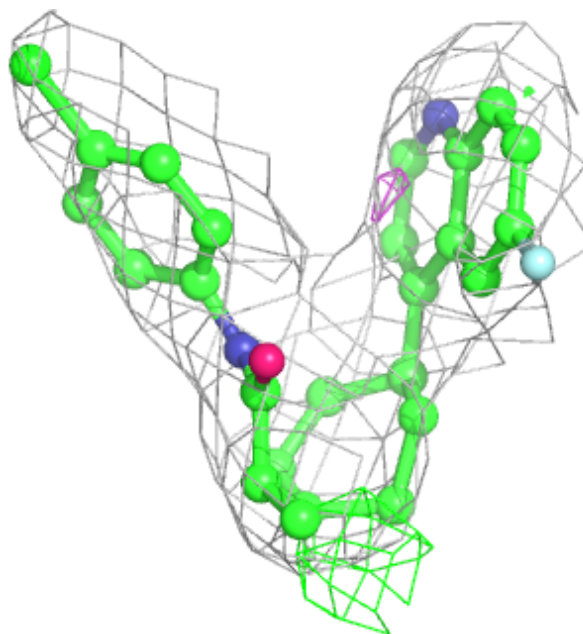
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	B	502	6/6	0.62	0.50	120,123,125,125	0
3	GOL	B	503	6/6	0.68	0.32	115,119,124,126	0
3	GOL	A	503	6/6	0.74	0.49	130,136,147,148	0
3	GOL	A	502	6/6	0.84	0.48	122,133,138,141	0
3	GOL	A	504	6/6	0.89	0.58	103,107,111,111	0
4	H7P	B	501	29/29	0.90	0.34	116,130,147,175	0
3	GOL	B	504	6/6	0.96	0.33	90,91,91,95	0
2	HEM	A	501	43/43	0.98	0.21	83,100,110,122	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.



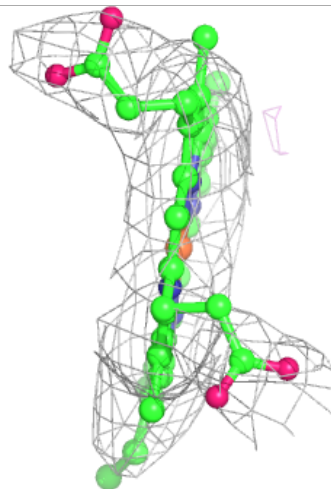
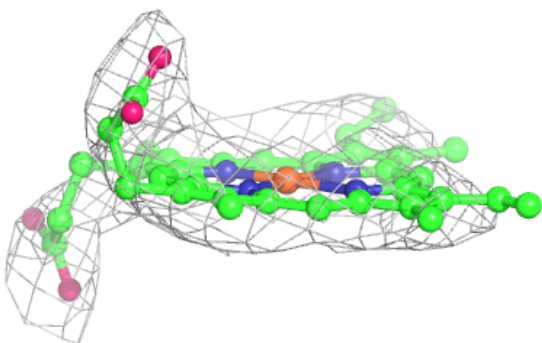
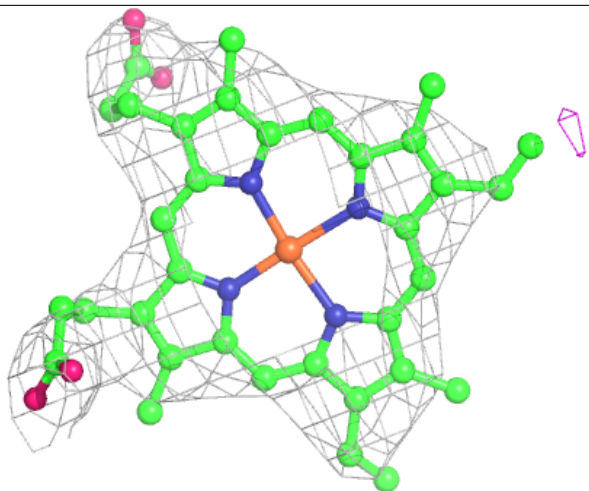
**Electron density around H7P B 501:**

$2mF_o-DF_c$  (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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.