



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 07:12 am BST

PDB ID : 6MQ6
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 : 2018-10-09
Resolution : 3.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

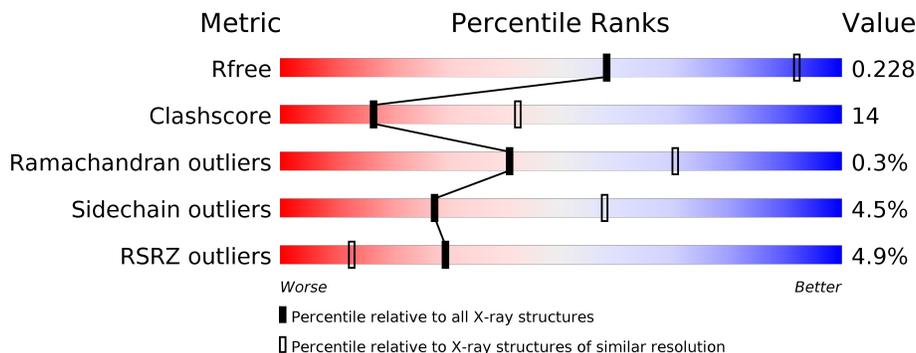
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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	
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	B	505	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6114 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
			Total	C	N	O	S			
1	A	371	2943	1892	501	533	17	0	0	0
1	B	366	2915	1878	496	524	17	0	0	0

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

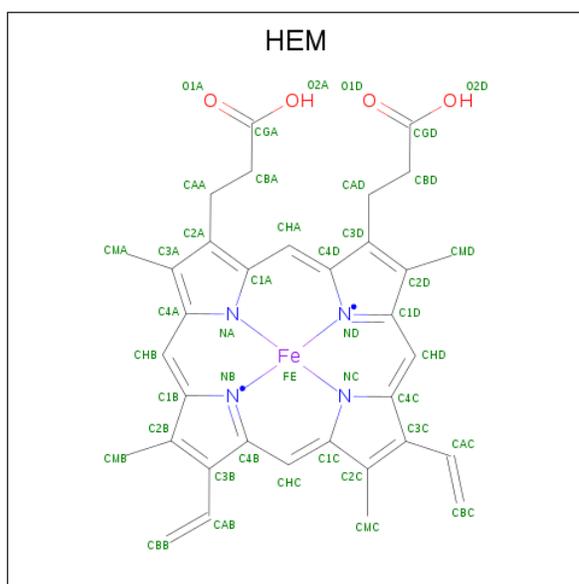
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Chain	Residue	Modelled	Actual	Comment	Reference
A	428	THR	-	expression tag	UNP P14902
A	429	GLY	-	expression tag	UNP P14902
A	430	HIS	-	expression tag	UNP P14902
A	431	HIS	-	expression tag	UNP P14902
A	432	HIS	-	expression tag	UNP P14902
A	433	HIS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

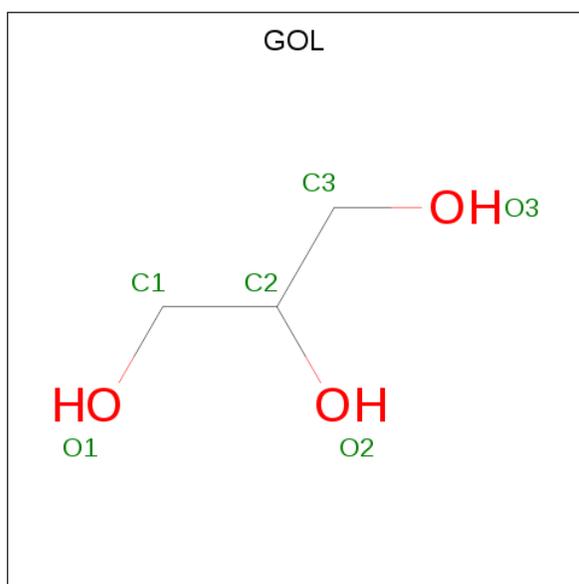
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



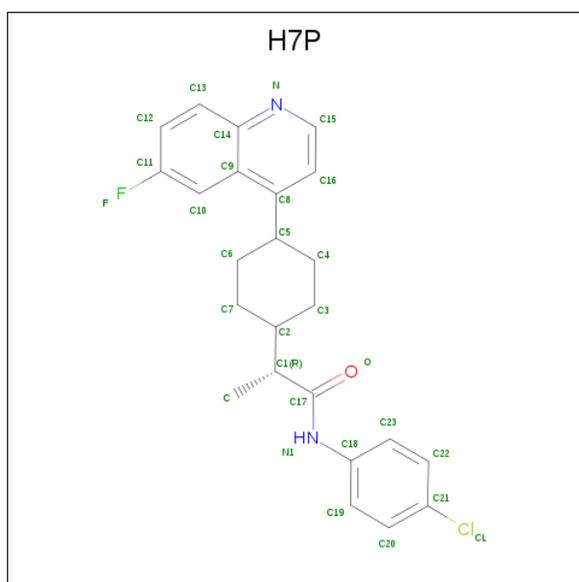
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	6	3	3	0	0
3	A	1	6	3	3	0	0

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

- Molecule 4 is (2R)-N-(4-chlorophenyl)-2-[cis-4-(6-fluoroquinolin-4-yl)cyclohexyl]propanamide (three-letter code: H7P) (formula: $C_{24}H_{24}ClFN_2O$) (labeled as "Ligand of Interest" by author).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	70	Total 70	O 70	0	0
5	B	78	Total 78	O 78	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.33Å 96.41Å 129.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.00 – 3.05 28.99 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.00-3.05) 99.8 (28.99-3.05)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 3.05Å)	Xtrriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.184 , 0.229 0.191 , 0.228	Depositor DCC
R_{free} test set	1094 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å ²)	105.2	Xtrriage
Anisotropy	0.032	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 67.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6114	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0/3011	0.42	0/4073
1	B	0.24	0/2983	0.42	0/4034
All	All	0.25	0/5994	0.42	0/8107

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	2
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	ARG	Sidechain
1	B	105	ARG	Sidechain
1	B	77	ARG	Sidechain

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	2943	0	2953	42	0
1	B	2915	0	2933	121	0
2	A	43	0	30	5	0
3	A	12	0	16	0	0
3	B	24	0	32	17	0
4	B	29	0	0	6	0
5	A	70	0	0	1	0
5	B	78	0	0	4	0
All	All	6114	0	5964	169	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 14.

The worst 5 of 169 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:346:HIS:NE2	3:B:505:GOL:H12	1.34	1.38
1:B:346:HIS:NE2	3:B:505:GOL:C1	2.14	1.11
1:B:264:ALA:HB2	3:B:505:GOL:H11	1.49	0.94
1:B:346:HIS:CE1	3:B:505:GOL:H12	2.05	0.90
1:B:346:HIS:NE2	3:B:505:GOL:H32	1.87	0.88

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%)	345 (94%)	21 (6%)	1 (0%)	41 70
1	B	362/425 (85%)	340 (94%)	21 (6%)	1 (0%)	41 70
All	All	729/850 (86%)	685 (94%)	42 (6%)	2 (0%)	41 70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	PRO
1	B	104	PRO

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	321/368 (87%)	309 (96%)	12 (4%)	34 64
1	B	318/368 (86%)	301 (95%)	17 (5%)	22 51
All	All	639/736 (87%)	610 (96%)	29 (4%)	27 58

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	51	GLU
1	B	99	VAL
1	B	384	LEU
1	B	57	GLU
1	B	115	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	113	GLN
1	B	189	GLN
1	B	280	GLN
1	B	29	GLN
1	B	290	GLN

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
3	GOL	A	503	-	5,5,5	0.26	0	5,5,5	0.26	0
3	GOL	B	503	-	5,5,5	0.30	0	5,5,5	0.14	0
3	GOL	A	502	-	5,5,5	0.29	0	5,5,5	0.21	0
3	GOL	B	504	-	5,5,5	0.28	0	5,5,5	0.21	0
2	HEM	A	501	1,5	27,50,50	0.84	2 (7%)	17,82,82	1.05	0
4	H7P	B	501	-	32,32,32	1.45	5 (15%)	45,45,45	1.33	6 (13%)
3	GOL	B	502	-	5,5,5	0.26	0	5,5,5	0.23	0
3	GOL	B	505	-	5,5,5	0.30	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
3	GOL	A	503	-	-	2/4/4/4	-
3	GOL	B	503	-	-	2/4/4/4	-
3	GOL	A	502	-	-	2/4/4/4	-
3	GOL	B	504	-	-	2/4/4/4	-
2	HEM	A	501	1,5	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	H7P	B	501	-	-	3/16/26/26	0/4/4/4
3	GOL	B	502	-	-	2/4/4/4	-
3	GOL	B	505	-	-	2/4/4/4	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	H7P	C9-C14	3.87	1.48	1.42
4	B	501	H7P	C8-C9	3.86	1.49	1.43
4	B	501	H7P	C18-N1	-2.82	1.35	1.41
4	B	501	H7P	C21-CL	2.45	1.79	1.74
2	A	501	HEM	C3B-C2B	-2.39	1.37	1.40

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	H7P	C5-C8-C9	4.12	124.97	120.67
4	B	501	H7P	C15-N-C14	3.23	121.94	116.93
4	B	501	H7P	C9-C14-N	-2.74	119.91	122.83
4	B	501	H7P	C16-C8-C5	-2.42	118.05	120.55
4	B	501	H7P	C3-C2-C7	2.33	113.55	109.44

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

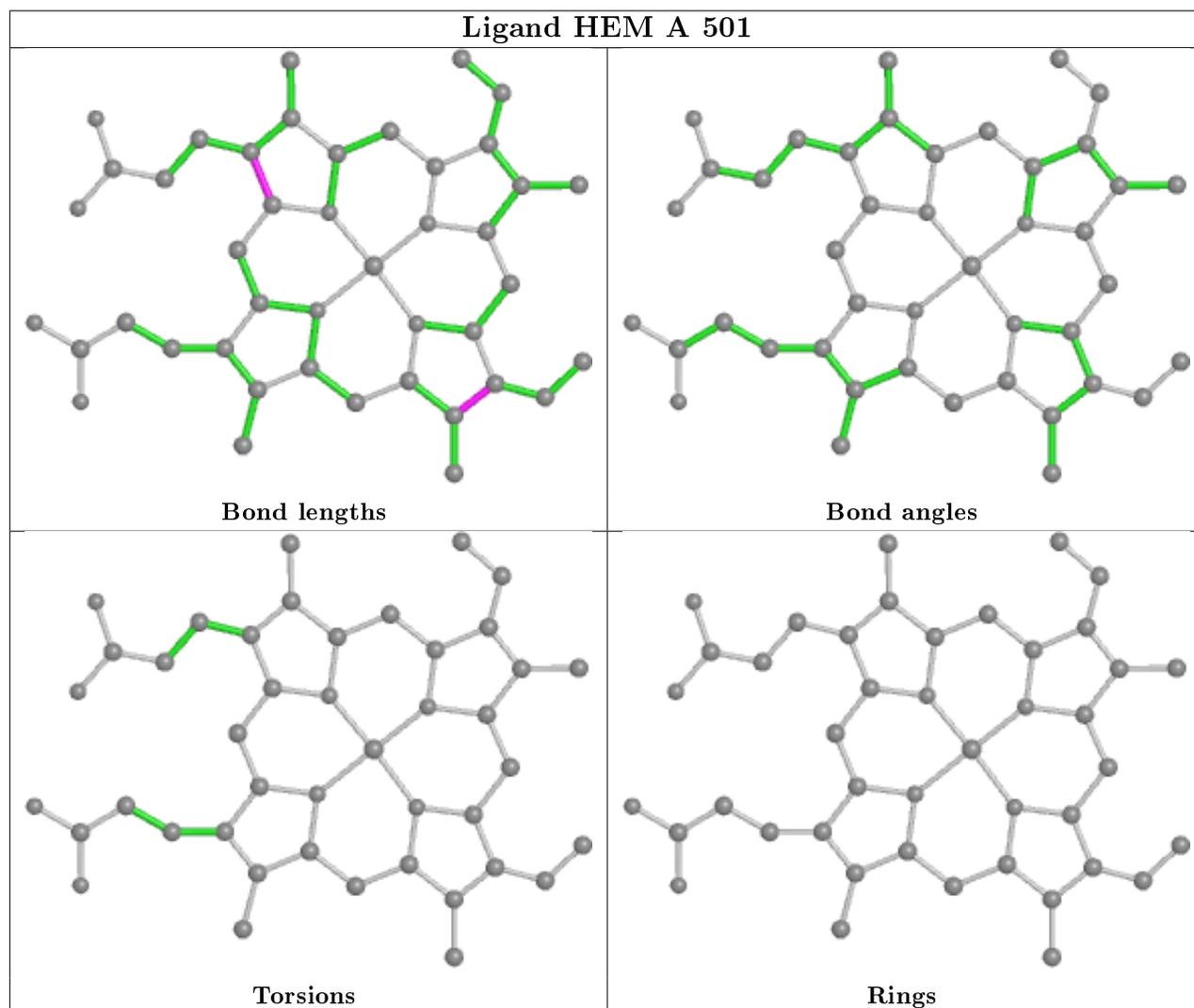
Mol	Chain	Res	Type	Atoms
3	B	503	GOL	O1-C1-C2-O2
3	B	503	GOL	O1-C1-C2-C3
3	B	504	GOL	O1-C1-C2-C3
4	B	501	H7P	C6-C5-C8-C9
4	B	501	H7P	C6-C5-C8-C16

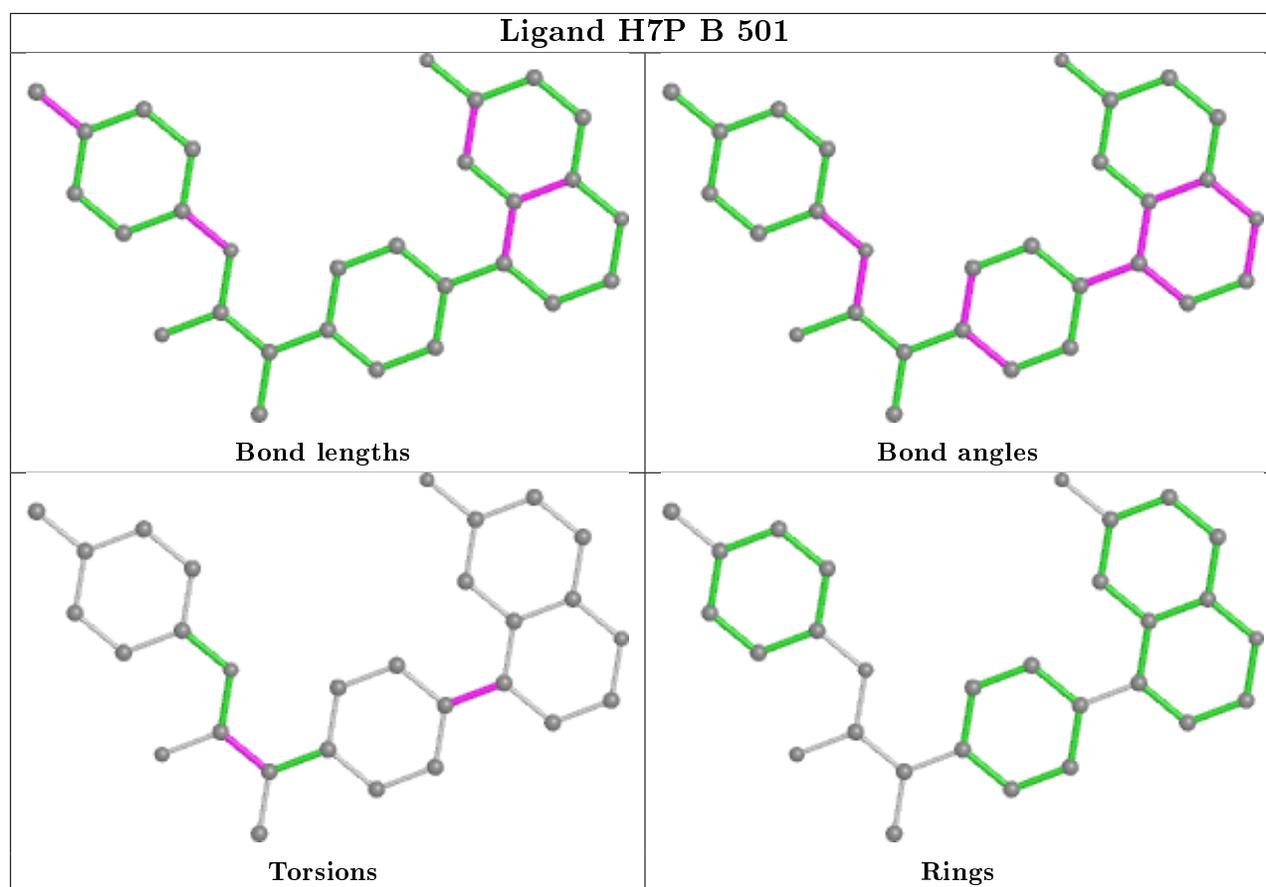
There are no ring outliers.

3 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	5	0
4	B	501	H7P	6	0
3	B	505	GOL	17	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 [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%)	0.04	31 (8%) 11 4	72, 114, 172, 206	0
1	B	366/425 (86%)	-0.17	5 (1%) 75 53	73, 105, 147, 185	0
All	All	737/850 (86%)	-0.07	36 (4%) 29 13	72, 110, 167, 206	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	402	GLU	6.1
1	A	63	ASN	4.5
1	A	263	SER	4.4
1	A	142	PRO	4.0
1	A	129	CYS	3.7

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](#)

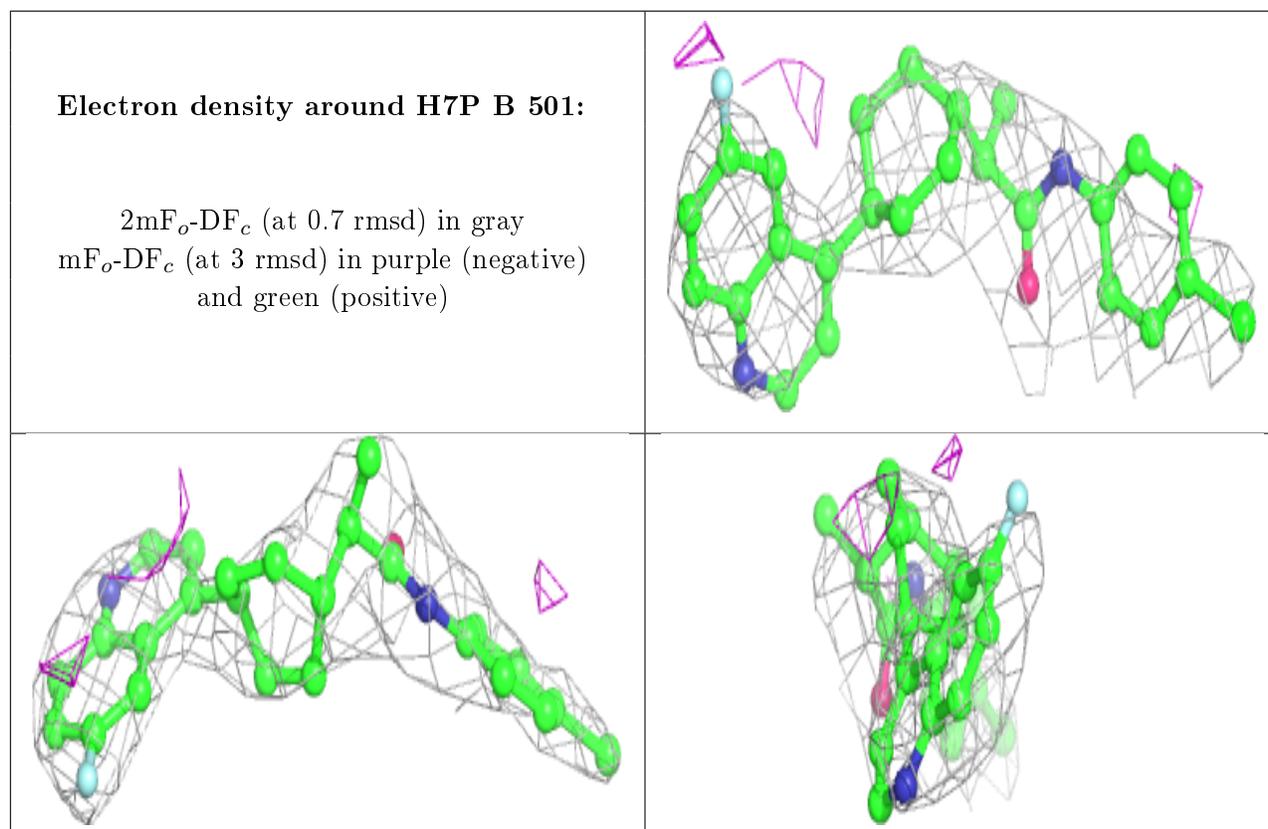
There are no carbohydrates in this entry.

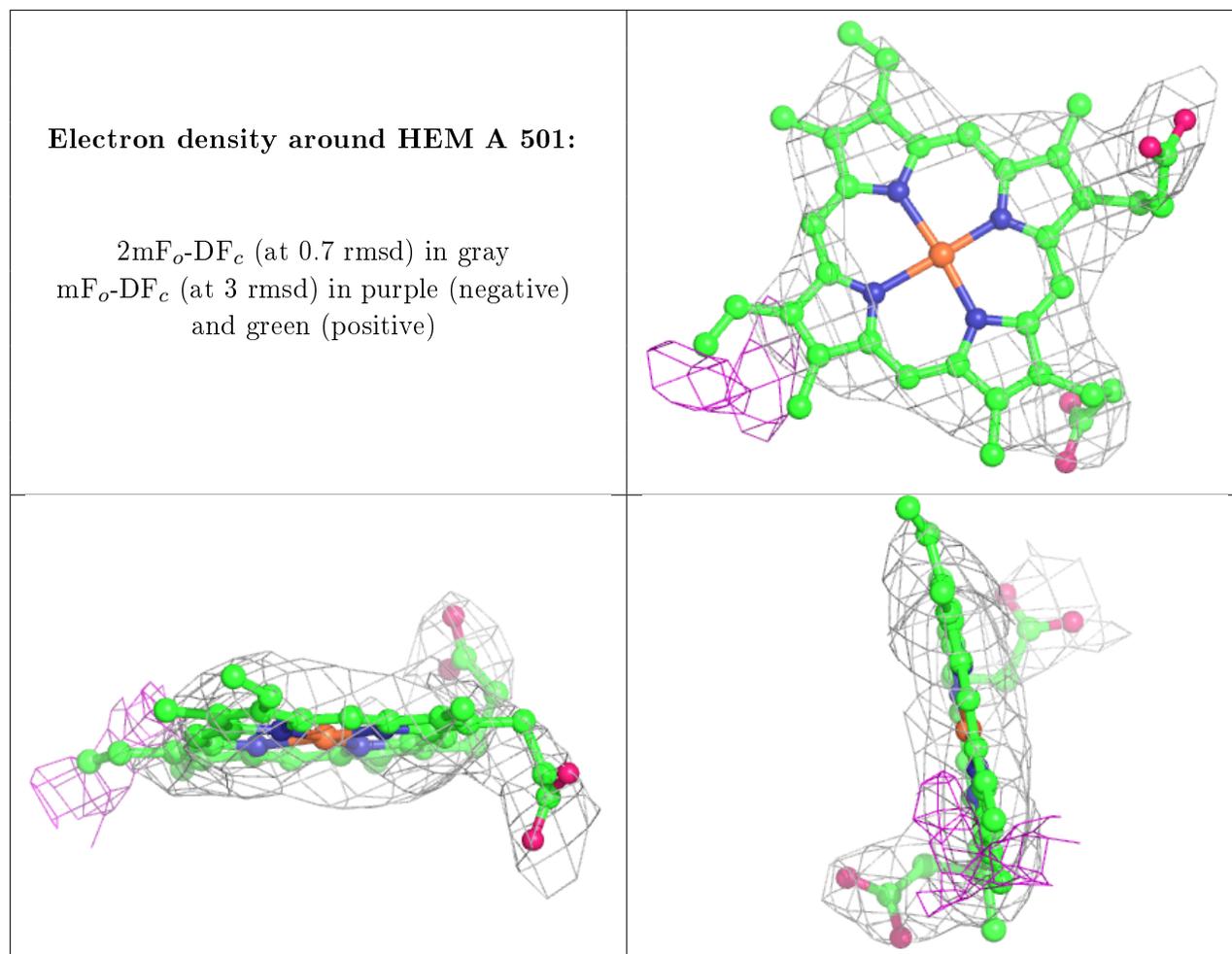
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
3	GOL	B	504	6/6	0.75	0.24	110,125,129,132	0
3	GOL	A	502	6/6	0.86	0.37	101,110,112,113	0
3	GOL	B	502	6/6	0.86	0.44	126,132,133,137	0
4	H7P	B	501	29/29	0.91	0.34	110,125,136,138	0
3	GOL	A	503	6/6	0.92	0.31	124,126,129,131	0
3	GOL	B	503	6/6	0.93	0.20	106,116,120,123	0
3	GOL	B	505	6/6	0.96	0.34	113,118,121,123	0
2	HEM	A	501	43/43	0.97	0.22	88,100,109,115	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.