



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 12:10 pm BST

PDB ID : 6AZU  
Title : Holo IDO1 crystal structure  
Authors : Lewis, H.A.; Yan, C.  
Deposited on : 2017-09-13  
Resolution : 2.82 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

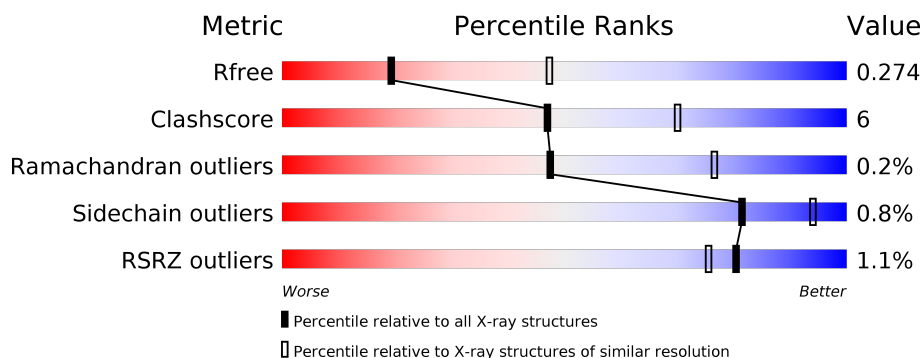
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.82 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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	402	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>8%</div> </div> </div>
1	B	402	<div> <div></div> <div>79%</div> <div>12%</div> <div>9%</div> </div>
1	C	402	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>11%</div> <div>9%</div> </div> </div>
1	D	402	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>8%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10993 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	370	Total	C	N	O	S	0	0	0
			2730	1777	458	479	16			
1	B	366	Total	C	N	O	S	0	0	0
			2709	1763	455	475	16			
1	C	366	Total	C	N	O	S	0	0	0
			2686	1746	449	475	16			
1	D	370	Total	C	N	O	S	0	0	0
			2676	1736	450	474	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	-	expression tag	UNP P14902
A	3	SER	-	expression tag	UNP P14902
A	4	HIS	-	expression tag	UNP P14902
B	2	GLY	-	expression tag	UNP P14902
B	3	SER	-	expression tag	UNP P14902
B	4	HIS	-	expression tag	UNP P14902
C	2	GLY	-	expression tag	UNP P14902
C	3	SER	-	expression tag	UNP P14902
C	4	HIS	-	expression tag	UNP P14902
D	2	GLY	-	expression tag	UNP P14902
D	3	SER	-	expression tag	UNP P14902
D	4	HIS	-	expression tag	UNP P14902

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).




Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

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 ( $\text{RSRZ} > 2$ ). 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.

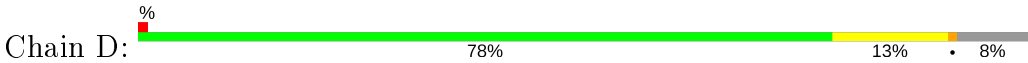
- Chain A:
- 
- 78% 14% 8%
- GLY SER HIS MET GLU ASN SER TRP THR ILE K12 K13 A24 L25 P28 L62 L78 A79 R80 L81 V82 L103 P104 S115 E119 L120 V125 Y126 A127 D128 L131 T144 L165 S176 K179 Q191 E192 R193 D194 T195 L196 L197 A204 S205 C206
- L207 E208 V213 F214 E215 Q216 N222 P223 W237 E258 G262 G265 Q266 S267 S268 V269 F270 Q271 D274 V275 Q280 A283 G284 G285 G286 P301 L310 E311 S312 L347 K352 I356 P357 A358 S359 Q360 GLN PRO LYS GLU ASN LYS THR SER GLU ASP
- PRO SER LYS LEU GLU ALA LYS GLY THR GLY G381 M385 L388 K401 GLU GLY

- [illegible]

- Chain C: 
- GLY  
SER  
HIS  
MET  
GLU  
ASN  
SER  
TRP  
THR  
ILE  
S12  
I17  
E51  
R80  
L81  
V82  
M88  
A89  
Y90  
H96  
G97  
P104  
I123  
L124  
V125  
Y126  
A127  
L131  
Y145  
F152  
R155  
K161  
A174  
A175  
S176  
A177  
K178  
K179  
V180  
M188  
R193  
D194  
L201
- C206  
F214  
H218  
Q242  
L247  
V248  
Y249  
S267  
S268  
V269  
F270  
D274  
V275  
Q281  
THR  
ALA  
GLY  
GLY  
G286  
R296  
M299  
E311  
R317  
F318  
F319  
V320  
G324  
D325  
A326  
E330  
Y345  
I356  
Q360  
GLN  
PRO  
LYS  
GLU  
ASN  
LYS  
THR  
SER  
GLU  
ASP

SER	LYS	LEU	GLU	ALA	LYS	GLY	THR	GLY	G381	K401	GLU	GLY
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● Molecule 1: Indoleamine 2,3-dioxygenase 1



GLY	SER	HIS	MET	GLU	ASN	SER	TRP	THR	ILE	S12	L25	P26	Q29	E30	D38	L62	L78	V82	T87	M88	V91	H96	G97	D98	V99	R100	L103	V109	P110	L118	I123	L124	V125	Y126	A127	D128	C129	V130	L131	V134	T144	M148			
L151	F152	L165	L168	L169	A174	I178	R193	Q212	V213	F214	H215	F226	P241	G262	S263	A264	G265	Q266	S267	S268	V269	F270	Q271	D274	Q281	T282	A283	F291	M295	V320	A326	G327	L328	L355	Q360	GLN	PRO	LYS	GLU	ASN	LYS	THR			
SER	GLU	ASP	PRO	SER	LYS	LEU	GLU	ALA	LYS	GLY	THR	G381	M385	T394	K401	GLU	GLY																												

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.11Å 177.51Å 101.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.02 – 2.82 34.02 – 2.82	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.02-2.82) 99.8 (34.02-2.82)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.211 , 0.272 0.214 , 0.274	Depositor DCC
$R_{free}$ test set	2666 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.2	Xtriage
Anisotropy	0.872	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 73.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10993	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.86% 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: HEM, SO4

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	0.46	0/2796	0.61	1/3813 (0.0%)
1	B	0.49	0/2774	0.63	0/3779
1	C	0.43	0/2751	0.61	0/3751
1	D	0.44	0/2742	0.61	0/3742
All	All	0.45	0/11063	0.62	1/15085 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	LEU	CA-CB-CG	5.65	128.29	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2730	0	2512	34	0
1	B	2709	0	2471	31	0
1	C	2686	0	2429	30	0
1	D	2676	0	2377	34	0
2	A	43	0	30	3	0
2	B	43	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	43	0	30	3	0
2	D	43	0	30	2	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
All	All	10993	0	9909	130	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (130) 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:C:51:GLU:HG2	1:C:155:ARG:HH21	1.34	0.93
1:C:194:ASP:OD2	1:D:193:ARG:NH2	2.18	0.76
1:B:80:ARG:NH2	1:B:121:PRO:O	2.19	0.76
1:C:176:SER:HA	1:C:179:LYS:HE2	1.66	0.76
1:A:193:ARG:HH12	1:A:197:LEU:HD12	1.55	0.72
1:D:88:MET:HE1	1:D:123:ILE:HG13	1.72	0.71
1:C:88:MET:HE1	1:C:123:ILE:HG13	1.73	0.70
1:C:275:VAL:HG13	1:C:311:GLU:HG3	1.74	0.67
1:A:280:GLN:NE2	1:B:293:GLN:OE1	2.28	0.67
2:A:501:HEM:HBB2	2:A:501:HEM:HMB1	1.77	0.66
1:B:275:VAL:HG13	1:B:311:GLU:HG3	1.77	0.66
1:A:275:VAL:HG13	1:A:311:GLU:HG3	1.77	0.64
1:D:124:LEU:HD21	1:D:129:CYS:HB3	1.78	0.64
1:A:385:MET:HE2	1:A:385:MET:HA	1.81	0.62
1:D:262:GLY:O	1:D:264:ALA:N	2.28	0.61
1:A:119:GLU:HB2	1:A:301:PRO:HG3	1.82	0.61
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.84	0.60
1:B:88:MET:HE1	1:B:123:ILE:HG13	1.84	0.60
1:C:267:SER:OG	1:C:269:VAL:HG12	2.01	0.60
1:B:271:GLN:HA	1:B:274:ASP:HB2	1.85	0.59
1:C:188:MET:HG2	1:C:193:ARG:HH12	1.67	0.59
1:B:88:MET:HE3	1:B:124:LEU:H	1.69	0.57
1:C:90:TYR:CE2	1:C:104:PRO:HD3	2.40	0.57
1:D:165:LEU:O	1:D:169:LEU:HD12	2.05	0.57
1:C:127:ALA:HA	1:C:131:LEU:HD12	1.87	0.56
1:A:214:PHE:HD2	1:A:214:PHE:O	1.89	0.55
1:B:176:SER:HA	1:B:179:LYS:HE2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:SER:HA	1:C:17:ILE:H	1.73	0.53
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.89	0.53
2:C:501:HEM:HMB1	2:C:501:HEM:HBB2	1.91	0.53
1:C:51:GLU:HG2	1:C:155:ARG:NH2	2.16	0.52
1:A:176:SER:HA	1:A:179:LYS:HE3	1.91	0.52
1:D:134:TRP:CD1	1:D:168:LEU:HD11	2.45	0.52
1:A:204:ALA:O	1:A:208:GLU:HG3	2.10	0.51
1:A:25:LEU:HD23	1:A:28:PRO:HB3	1.92	0.51
1:C:176:SER:HB3	1:C:206:CYS:SG	2.50	0.51
1:A:176:SER:HB3	1:A:206:CYS:SG	2.50	0.51
1:C:356:ILE:HG22	1:C:360:GLN:OE1	2.11	0.51
2:A:501:HEM:CMB	2:A:501:HEM:HBB2	2.41	0.50
1:C:80:ARG:HH21	1:C:125:VAL:HG22	1.75	0.50
1:D:30:GLU:HA	1:D:151:LEU:HD21	1.91	0.50
1:D:82:VAL:HG12	1:D:152:PHE:CZ	2.45	0.50
1:A:80:ARG:NH2	1:A:128:ASP:OD2	2.38	0.50
1:B:385:MET:HA	1:B:385:MET:HE2	1.94	0.50
1:D:127:ALA:HA	1:D:131:LEU:HD12	1.93	0.50
1:D:97:GLY:O	1:D:99:VAL:N	2.45	0.49
1:C:218:HIS:NE2	1:C:345:TYR:OH	2.44	0.48
1:B:177:ALA:HB2	1:B:206:CYS:HB2	1.95	0.48
1:B:212:GLN:O	1:B:215:HIS:HB2	2.13	0.48
1:D:29:GLN:O	1:D:78:LEU:HD12	2.14	0.48
1:A:262:GLY:O	1:A:266:GLN:HG3	2.13	0.48
1:B:262:GLY:O	1:B:266:GLN:HG3	2.13	0.48
1:C:326:ALA:O	1:C:330:GLU:HB2	2.14	0.48
1:D:271:GLN:HA	1:D:274:ASP:HB2	1.95	0.48
1:A:271:GLN:HA	1:A:274:ASP:HB2	1.96	0.47
1:D:174:ALA:O	1:D:178:ILE:HG13	2.15	0.47
1:D:38:ASP:HB3	1:D:62:LEU:HD11	1.95	0.47
1:C:218:HIS:HE2	1:C:345:TYR:HH	1.62	0.47
1:D:109:VAL:HB	1:D:110:PRO:HD3	1.95	0.47
1:A:311:GLU:HG2	1:B:293:GLN:NE2	2.30	0.47
1:B:222:ASN:OD1	1:B:225:ALA:N	2.36	0.47
1:A:267:SER:OG	1:A:269:VAL:HG12	2.15	0.47
1:B:119:GLU:HB2	1:B:301:PRO:HG3	1.96	0.47
1:B:237:TRP:HB3	1:B:243:LEU:HD22	1.97	0.46
2:D:501:HEM:HBC2	2:D:501:HEM:HMC1	1.97	0.46
1:A:125:VAL:HG12	1:A:127:ALA:H	1.80	0.46
1:D:212:GLN:O	1:D:215:HIS:HB2	2.15	0.46
1:D:134:TRP:CG	1:D:168:LEU:HD11	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:LYS:HD3	1:B:353:TYR:CE1	2.51	0.46
1:D:25:LEU:HA	1:D:26:PRO:HD3	1.78	0.46
1:D:126:TYR:CB	1:D:266:GLN:HB2	2.46	0.45
1:A:356:ILE:HB	1:A:357:PRO:HD3	1.98	0.45
1:A:312:SER:O	1:B:297:ARG:HG2	2.16	0.45
1:B:349:ILE:HA	1:B:349:ILE:HD13	1.85	0.45
1:B:124:LEU:HD21	1:B:129:CYS:HB3	1.99	0.45
1:A:115:SER:HB3	1:A:120:LEU:O	2.17	0.44
1:D:100:ARG:HD3	1:D:100:ARG:HA	1.73	0.44
1:A:213:VAL:O	1:A:216:GLN:HB2	2.16	0.44
1:D:118:LEU:HD23	1:D:118:LEU:HA	1.72	0.44
1:D:263:SER:HA	1:D:266:GLN:OE1	2.18	0.44
1:D:267:SER:OG	1:D:269:VAL:HG12	2.17	0.44
1:D:144:THR:O	1:D:148:MET:HG3	2.17	0.44
1:A:269:VAL:HG13	1:A:270:PHE:CD1	2.53	0.44
1:C:82:VAL:HG12	1:C:152:PHE:CZ	2.53	0.44
1:A:24:ALA:HA	1:A:131:LEU:HD22	2.00	0.44
1:B:82:VAL:HG12	1:B:152:PHE:CZ	2.52	0.44
1:B:78:LEU:O	1:B:82:VAL:HG13	2.17	0.43
1:C:296:ARG:HA	1:C:299:MET:SD	2.58	0.43
1:C:356:ILE:O	1:C:360:GLN:HG2	2.18	0.43
1:D:355:LEU:HD11	1:D:385:MET:CG	2.47	0.43
1:B:24:ALA:HA	1:B:131:LEU:HD22	2.00	0.43
1:C:174:ALA:O	1:C:178:ILE:HG13	2.18	0.43
1:B:80:ARG:NH1	1:B:128:ASP:OD2	2.51	0.43
1:C:270:PHE:O	1:C:274:ASP:HB2	2.18	0.43
1:D:226:PHE:CZ	2:D:501:HEM:HMB3	2.53	0.43
1:D:320:VAL:HG22	1:D:328:LEU:HB3	1.99	0.43
1:B:127:ALA:HA	1:B:131:LEU:HD12	1.99	0.43
1:A:222:ASN:HA	1:A:223:PRO:HD3	1.88	0.43
1:A:311:GLU:HG2	1:B:293:GLN:HE21	1.84	0.43
1:C:201:LEU:HD23	1:C:201:LEU:HA	1.74	0.43
1:D:281:GLN:HA	1:D:394:THR:HG21	1.99	0.43
1:C:317:ARG:HA	1:C:320:VAL:HG22	2.00	0.42
1:C:214:PHE:HZ	2:C:501:HEM:HHC	1.84	0.42
1:A:78:LEU:O	1:A:82:VAL:HG13	2.19	0.42
1:B:121:PRO:HG2	1:B:298:TYR:CD2	2.54	0.42
1:B:23:PHE:O	1:B:131:LEU:HD13	2.20	0.42
1:A:357:PRO:C	1:A:359:SER:H	2.22	0.42
1:C:180:VAL:O	1:C:180:VAL:HG12	2.20	0.42
1:D:126:TYR:HB2	1:D:266:GLN:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LEU:HA	1:A:104:PRO:HD3	1.96	0.41
1:D:269:VAL:HG13	1:D:270:PHE:CD1	2.55	0.41
1:D:291:PHE:O	1:D:295:MET:HG2	2.19	0.41
1:A:237:TRP:O	1:A:258:GLU:HG2	2.20	0.41
1:B:80:ARG:HD3	1:B:128:ASP:OD1	2.20	0.41
1:A:265:GLY:HA2	2:A:501:HEM:C4D	2.56	0.41
1:B:90:TYR:CE2	1:B:104:PRO:HD3	2.55	0.41
1:A:223:PRO:HG3	1:A:352:LYS:HE2	2.02	0.41
1:C:12:SER:HB2	1:C:17:ILE:O	2.20	0.41
1:D:87:THR:HG23	1:D:103:LEU:HD13	2.02	0.41
1:C:193:ARG:HD2	1:C:319:PHE:CZ	2.56	0.41
1:C:247:LEU:HD23	1:C:249:TYR:CZ	2.55	0.41
1:A:347:LEU:HD21	1:A:388:LEU:HB2	2.03	0.41
1:D:214:PHE:O	1:D:214:PHE:HD2	2.03	0.41
1:C:145:TYR:OH	1:C:161:LYS:HG2	2.21	0.41
1:B:56:ARG:HD3	1:B:100:ARG:CZ	2.50	0.41
1:A:192:GLU:HB3	1:A:195:THR:OG1	2.21	0.40
1:A:165:LEU:HD23	1:A:165:LEU:HA	1.77	0.40
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.82	0.40
1:B:181:ILE:HD13	1:B:276:LEU:HD22	2.04	0.40
1:D:91:VAL:O	1:D:99:VAL:HA	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	366/402 (91%)	350 (96%)	14 (4%)	2 (0%)	29	59
1	B	360/402 (90%)	349 (97%)	11 (3%)	0	100	100
1	C	360/402 (90%)	347 (96%)	13 (4%)	0	100	100
1	D	366/402 (91%)	352 (96%)	13 (4%)	1 (0%)	41	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1452/1608 (90%)	1398 (96%)	51 (4%)	3 (0%)	47 76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	263	SER
1	A	13	LYS
1	A	285	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	245/348 (70%)	242 (99%)	3 (1%)	71 91
1	B	240/348 (69%)	237 (99%)	3 (1%)	69 90
1	C	237/348 (68%)	237 (100%)	0	100 100
1	D	227/348 (65%)	225 (99%)	2 (1%)	78 93
All	All	949/1392 (68%)	941 (99%)	8 (1%)	81 94

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	214	PHE
1	A	356	ILE
1	B	64	MET
1	B	214	PHE
1	B	323	LYS
1	D	169	LEU
1	D	214	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	280	GLN
1	A	293	GLN
1	B	293	GLN
1	C	212	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	SO4	A	502	-	4,4,4	0.11	0	6,6,6	0.18	0
2	HEM	C	501	1	27,50,50	2.19	8 (29%)	17,82,82	1.66	4 (23%)
2	HEM	A	501	1	27,50,50	2.20	8 (29%)	17,82,82	1.90	7 (41%)
3	SO4	C	502	-	4,4,4	0.17	0	6,6,6	0.21	0
3	SO4	B	502	-	4,4,4	0.15	0	6,6,6	0.09	0
3	SO4	D	502	-	4,4,4	0.12	0	6,6,6	0.22	0
2	HEM	D	501	1	27,50,50	2.14	7 (25%)	17,82,82	1.70	4 (23%)
2	HEM	B	501	1	27,50,50	2.19	7 (25%)	17,82,82	1.46	5 (29%)

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	C	501	1	-	3/6/54/54	-
2	HEM	D	501	1	-	2/6/54/54	-
2	HEM	A	501	1	-	4/6/54/54	-
2	HEM	B	501	1	-	0/6/54/54	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	C3D-C2D	5.24	1.53	1.37
2	C	501	HEM	C3D-C2D	5.12	1.52	1.37
2	B	501	HEM	C3D-C2D	4.84	1.52	1.37
2	B	501	HEM	C3B-C2B	-4.58	1.34	1.40
2	A	501	HEM	C3D-C2D	4.43	1.50	1.37
2	A	501	HEM	C3C-C2C	-4.34	1.34	1.40
2	A	501	HEM	C3B-C2B	-4.18	1.34	1.40
2	C	501	HEM	C3B-C2B	-4.18	1.34	1.40
2	D	501	HEM	C3C-C2C	-4.12	1.34	1.40
2	B	501	HEM	C3C-CAC	3.92	1.55	1.47
2	D	501	HEM	C3B-CAB	3.91	1.55	1.47
2	C	501	HEM	C3B-CAB	3.85	1.55	1.47
2	A	501	HEM	C1D-ND	3.79	1.44	1.36
2	B	501	HEM	C3B-CAB	3.77	1.55	1.47
2	C	501	HEM	C3C-CAC	3.75	1.55	1.47
2	B	501	HEM	C3C-C2C	-3.73	1.35	1.40
2	D	501	HEM	C3B-C2B	-3.71	1.35	1.40
2	C	501	HEM	C3C-C2C	-3.68	1.35	1.40
2	A	501	HEM	C3C-CAC	3.20	1.54	1.47
2	D	501	HEM	C3C-CAC	3.11	1.54	1.47
2	A	501	HEM	C3B-CAB	3.05	1.54	1.47
2	C	501	HEM	CAA-C2A	2.83	1.56	1.52
2	A	501	HEM	C4B-NB	2.57	1.41	1.36
2	A	501	HEM	CAA-C2A	2.56	1.55	1.52
2	D	501	HEM	CAA-C2A	2.49	1.55	1.52
2	B	501	HEM	C1D-ND	2.46	1.41	1.36
2	B	501	HEM	CAA-C2A	2.33	1.55	1.52
2	C	501	HEM	CMC-C2C	2.15	1.56	1.51
2	C	501	HEM	C1D-ND	2.13	1.40	1.36
2	D	501	HEM	C1D-ND	2.04	1.40	1.36



All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	HEM	CBA-CAA-C2A	3.66	119.24	112.49
2	A	501	HEM	CMA-C3A-C4A	-3.56	123.00	128.46
2	A	501	HEM	CBA-CAA-C2A	3.25	118.49	112.49
2	B	501	HEM	CBD-CAD-C3D	-3.06	106.83	112.48
2	D	501	HEM	CMA-C3A-C4A	-3.02	123.82	128.46
2	C	501	HEM	CBD-CAD-C3D	-2.71	107.49	112.48
2	A	501	HEM	CMB-C2B-C3B	2.67	129.68	124.68
2	D	501	HEM	CMB-C2B-C3B	2.58	129.50	124.68
2	B	501	HEM	CAD-CBD-CGD	2.52	116.90	112.67
2	C	501	HEM	CMC-C2C-C3C	2.48	129.32	124.68
2	D	501	HEM	CBD-CAD-C3D	-2.47	107.92	112.48
2	A	501	HEM	CBD-CAD-C3D	-2.43	108.00	112.48
2	A	501	HEM	C1D-C2D-C3D	-2.39	105.33	107.00
2	C	501	HEM	CMA-C3A-C4A	-2.33	124.89	128.46
2	B	501	HEM	CMC-C2C-C3C	2.25	128.90	124.68
2	B	501	HEM	CMA-C3A-C4A	-2.19	125.09	128.46
2	B	501	HEM	C4A-C3A-C2A	2.14	108.49	107.00
2	D	501	HEM	C1D-C2D-C3D	-2.11	105.53	107.00
2	A	501	HEM	C4A-C3A-C2A	2.11	108.46	107.00
2	A	501	HEM	CAA-CBA-CGA	2.10	116.20	112.67

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	HEM	C1A-C2A-CAA-CBA
2	C	501	HEM	C3A-C2A-CAA-CBA
2	A	501	HEM	C1A-C2A-CAA-CBA
2	A	501	HEM	C3A-C2A-CAA-CBA
2	D	501	HEM	C1A-C2A-CAA-CBA
2	D	501	HEM	C3A-C2A-CAA-CBA
2	A	501	HEM	C3D-CAD-CBD-CGD
2	A	501	HEM	C2A-CAA-CBA-CGA
2	C	501	HEM	C2A-CAA-CBA-CGA

There are no ring outliers.

4 monomers are involved in 9 short contacts:

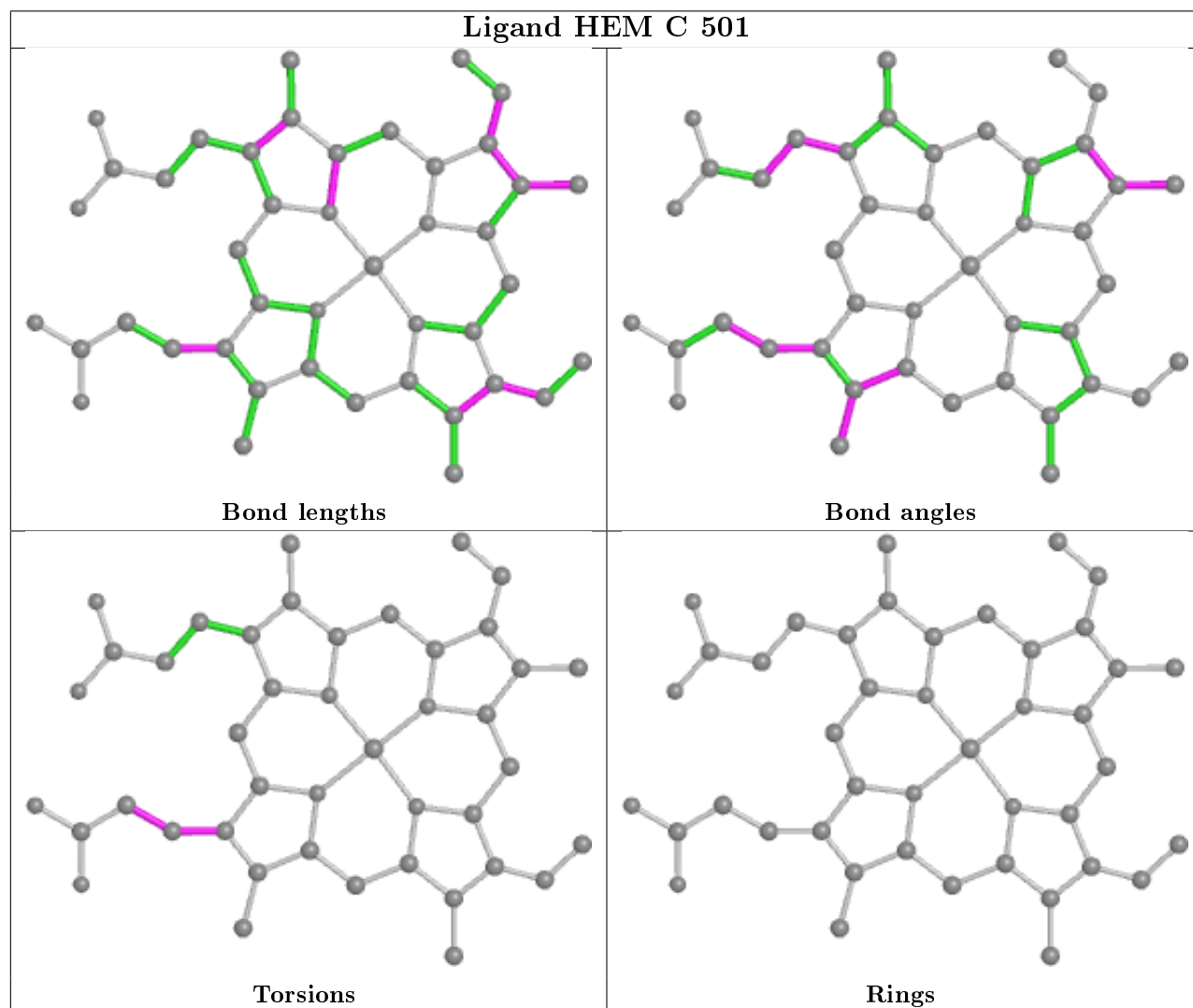
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	HEM	3	0

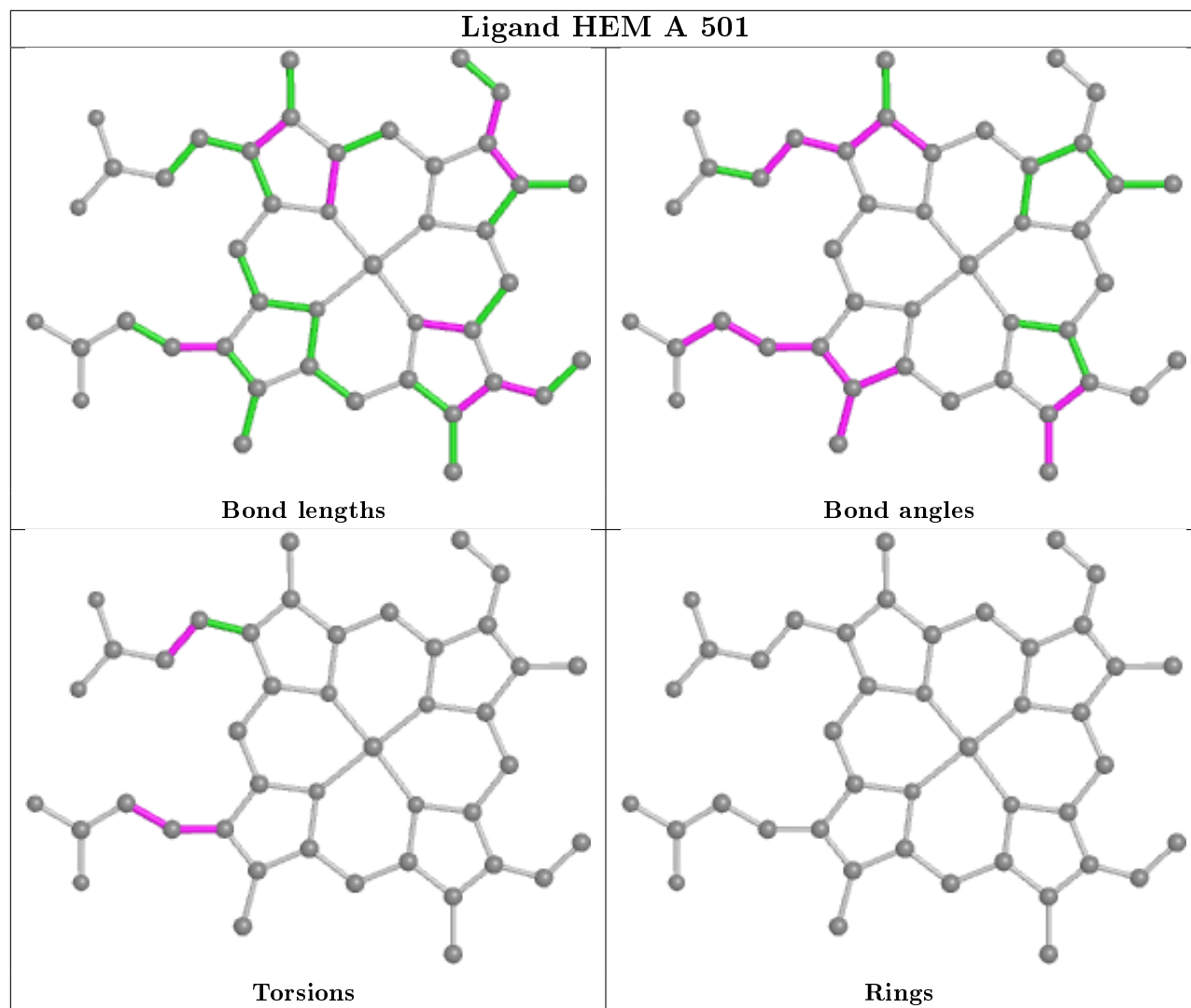
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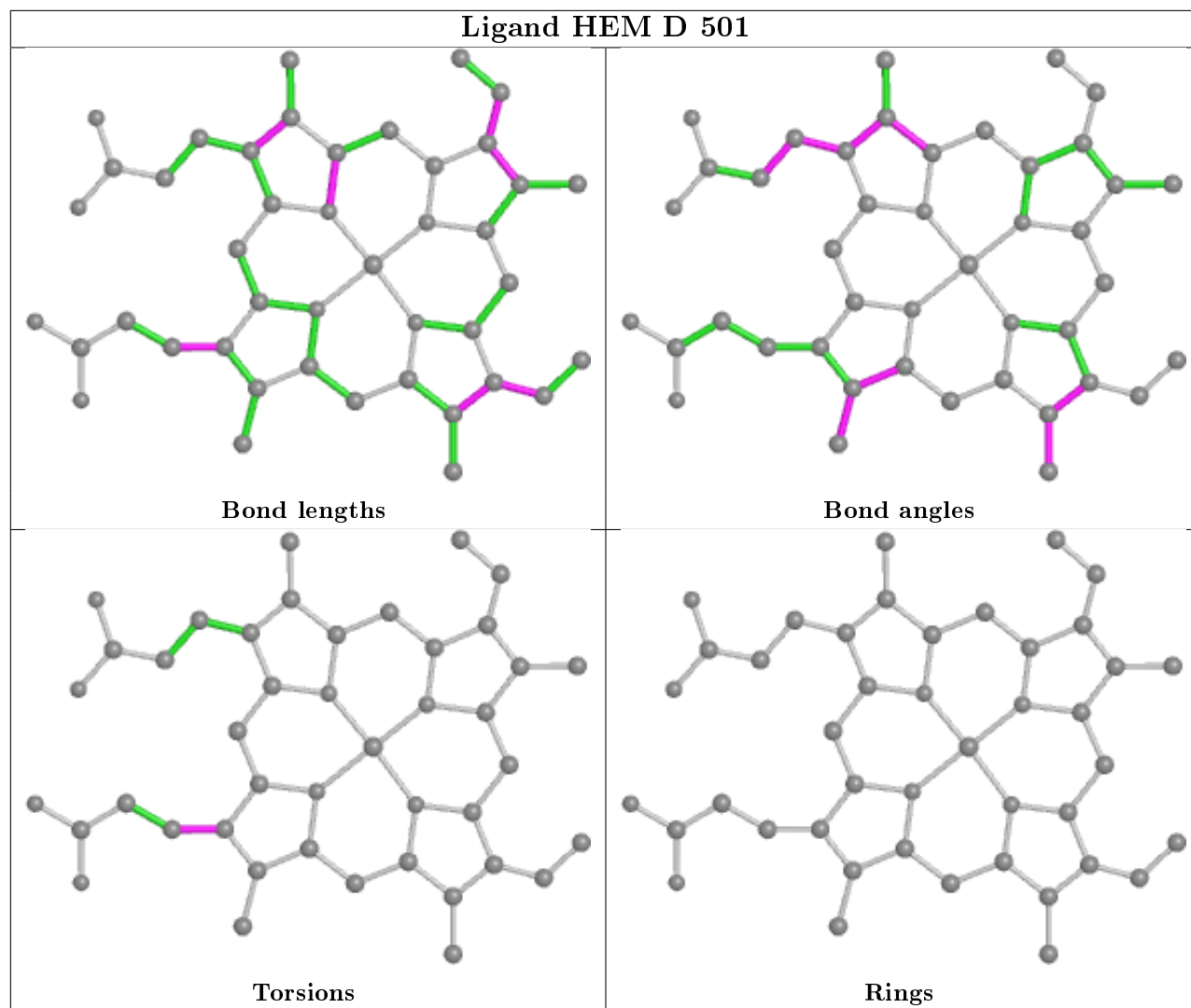
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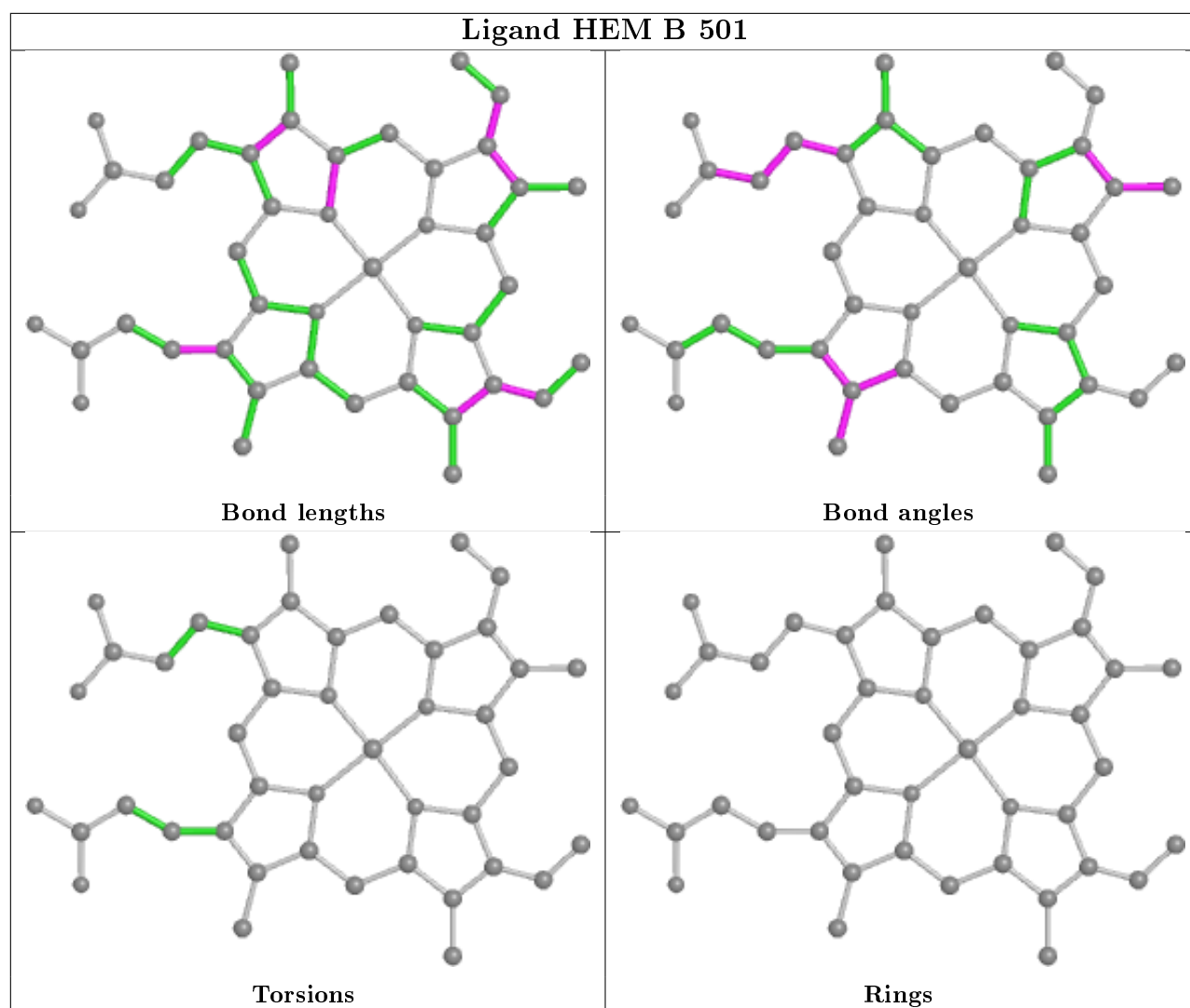
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	3	0
2	D	501	HEM	2	0
2	B	501	HEM	1	0

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 [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, 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	370/402 (92%)	-0.38	5 (1%) 75 69	28, 45, 74, 161	0
1	B	366/402 (91%)	-0.39	2 (0%) 91 88	28, 43, 68, 107	0
1	C	366/402 (91%)	-0.27	5 (1%) 75 69	29, 47, 75, 122	0
1	D	370/402 (92%)	-0.31	4 (1%) 80 75	31, 51, 77, 129	0
All	All	1472/1608 (91%)	-0.34	16 (1%) 80 75	28, 47, 74, 161	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	284	GLY	4.3
1	D	326	ALA	3.5
1	C	324	GLY	3.4
1	A	285	GLY	3.2
1	D	241	PRO	2.9
1	D	283	ALA	2.8
1	C	193	ARG	2.7
1	C	242	GLN	2.5
1	D	96	HIS	2.4
1	B	360	GLN	2.4
1	C	96	HIS	2.3
1	A	286	GLY	2.3
1	C	97	GLY	2.3
1	B	139	PRO	2.1
1	A	144	THR	2.1
1	A	283	ALA	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

There are no carbohydrates in this entry.

### 6.4 Ligands

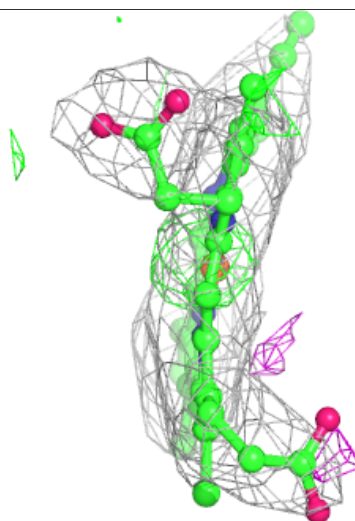
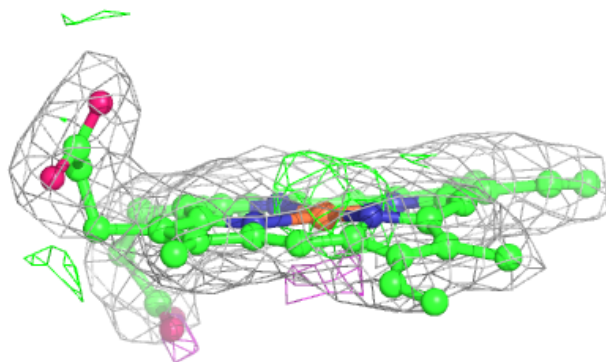
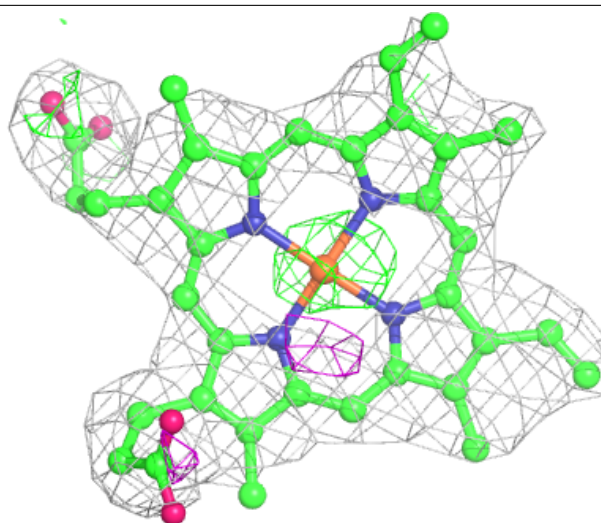
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	SO4	A	502	5/5	0.72	0.28	117,120,123,127	0
3	SO4	B	502	5/5	0.81	0.41	132,132,136,137	0
3	SO4	D	502	5/5	0.87	0.17	102,106,110,114	0
2	HEM	C	501	43/43	0.93	0.18	22,45,69,108	0
2	HEM	A	501	43/43	0.94	0.19	3,28,75,83	0
2	HEM	D	501	43/43	0.94	0.16	13,49,79,86	0
3	SO4	C	502	5/5	0.95	0.17	100,100,103,103	0
2	HEM	B	501	43/43	0.97	0.16	9,28,49,53	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 HEM C 501:**

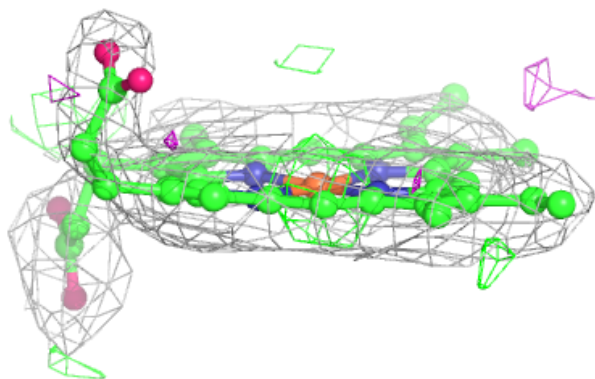
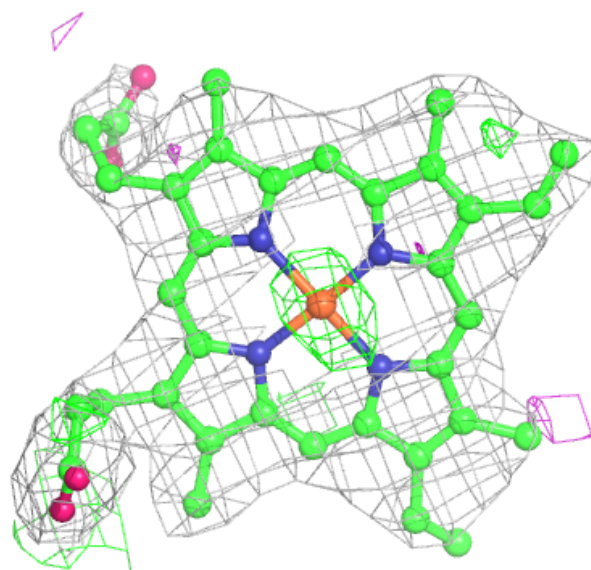
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





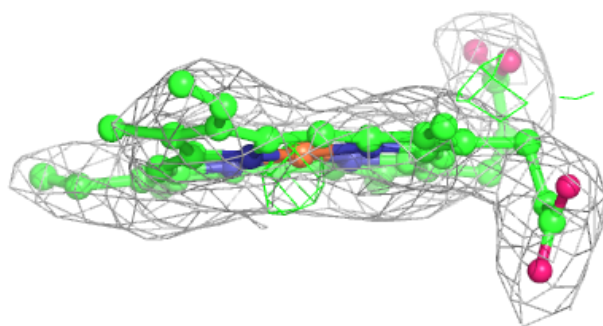
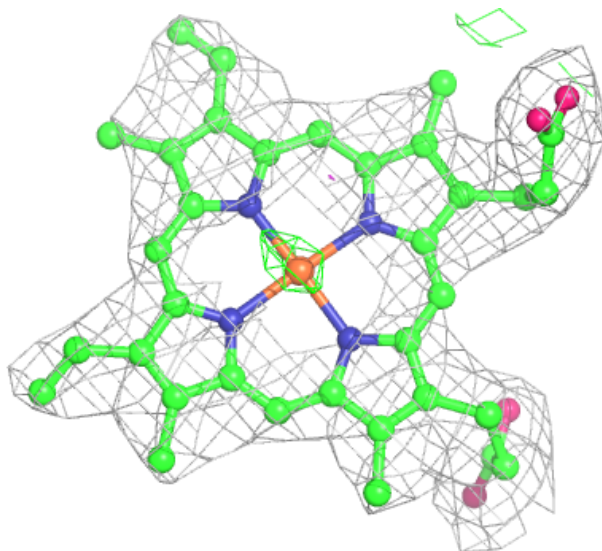
**Electron density around HEM A 501:**

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



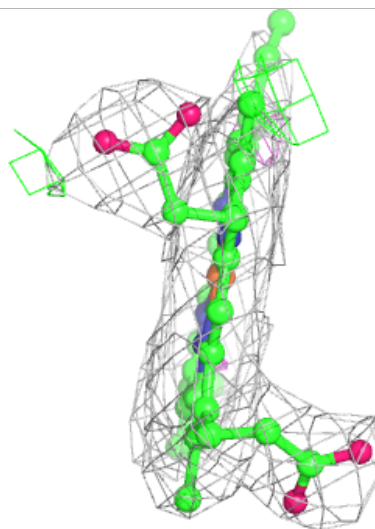
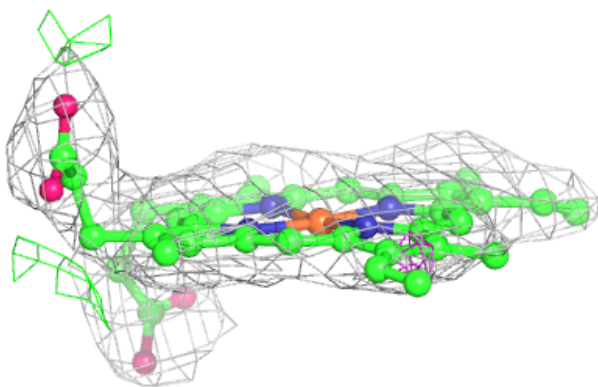
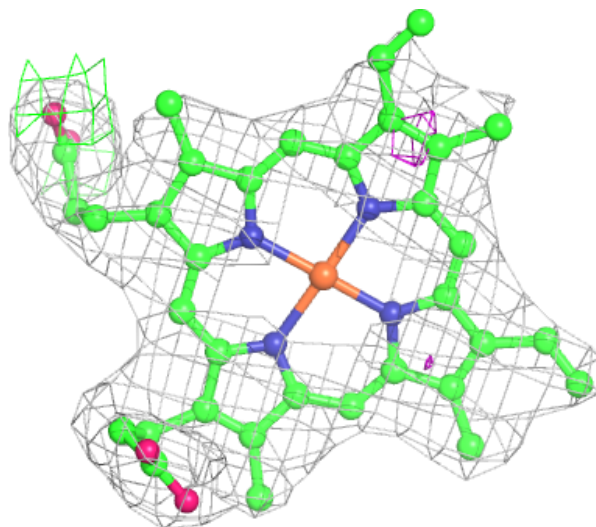
**Electron density around HEM D 501:**

$2mF_o-DF_c$  (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 ⓘ

There are no such residues in this entry.