



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 12:47 am BST

PDB ID : 2FDV  
Title : Microsomal P450 2A6 with the inhibitor N-Methyl(5-(pyridin-3-yl)furan-2-yl)methanamine bound  
Authors : Yano, J.K.; Stout, C.D.; Johnson, E.F.  
Deposited on : 2005-12-14  
Resolution : 1.65 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](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.

---

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

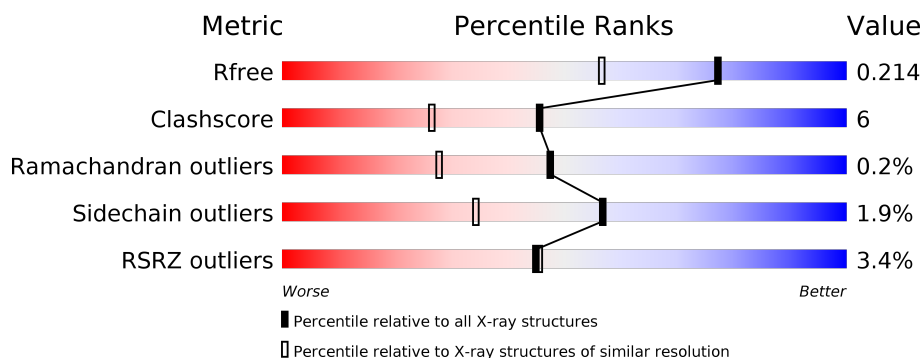
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	476	<div> <div>2%</div> <div>88% 9% .</div> </div>
1	B	476	<div> <div>4%</div> <div>85% 12% ..</div> </div>
1	C	476	<div> <div>2%</div> <div>86% 11% ..</div> </div>
1	D	476	<div> <div>5%</div> <div>84% 13% ..</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	C	2004	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16747 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 Cytochrome P450 2A6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3760	2414	650	678	18			
1	B	465	Total	C	N	O	S	0	0	0
			3767	2418	653	678	18			
1	C	464	Total	C	N	O	S	0	0	0
			3751	2408	648	677	18			
1	D	464	Total	C	N	O	S	0	0	0
			3751	2408	648	677	18			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	CLONING ARTIFACT	UNP P11509
A	24	ALA	-	CLONING ARTIFACT	UNP P11509
A	25	LYS	-	CLONING ARTIFACT	UNP P11509
A	26	LYS	-	CLONING ARTIFACT	UNP P11509
A	27	THR	-	CLONING ARTIFACT	UNP P11509
A	28	SER	-	CLONING ARTIFACT	UNP P11509
A	495	HIS	-	EXPRESSION TAG	UNP P11509
A	496	HIS	-	EXPRESSION TAG	UNP P11509
A	497	HIS	-	EXPRESSION TAG	UNP P11509
A	498	HIS	-	EXPRESSION TAG	UNP P11509
B	23	MET	-	CLONING ARTIFACT	UNP P11509
B	24	ALA	-	CLONING ARTIFACT	UNP P11509
B	25	LYS	-	CLONING ARTIFACT	UNP P11509
B	26	LYS	-	CLONING ARTIFACT	UNP P11509
B	27	THR	-	CLONING ARTIFACT	UNP P11509
B	28	SER	-	CLONING ARTIFACT	UNP P11509
B	495	HIS	-	EXPRESSION TAG	UNP P11509
B	496	HIS	-	EXPRESSION TAG	UNP P11509
B	497	HIS	-	EXPRESSION TAG	UNP P11509
B	498	HIS	-	EXPRESSION TAG	UNP P11509
C	23	MET	-	CLONING ARTIFACT	UNP P11509

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	24	ALA	-	CLONING ARTIFACT	UNP P11509
C	25	LYS	-	CLONING ARTIFACT	UNP P11509
C	26	LYS	-	CLONING ARTIFACT	UNP P11509
C	27	THR	-	CLONING ARTIFACT	UNP P11509
C	28	SER	-	CLONING ARTIFACT	UNP P11509
C	495	HIS	-	EXPRESSION TAG	UNP P11509
C	496	HIS	-	EXPRESSION TAG	UNP P11509
C	497	HIS	-	EXPRESSION TAG	UNP P11509
C	498	HIS	-	EXPRESSION TAG	UNP P11509
D	23	MET	-	CLONING ARTIFACT	UNP P11509
D	24	ALA	-	CLONING ARTIFACT	UNP P11509
D	25	LYS	-	CLONING ARTIFACT	UNP P11509
D	26	LYS	-	CLONING ARTIFACT	UNP P11509
D	27	THR	-	CLONING ARTIFACT	UNP P11509
D	28	SER	-	CLONING ARTIFACT	UNP P11509
D	495	HIS	-	EXPRESSION TAG	UNP P11509
D	496	HIS	-	EXPRESSION TAG	UNP P11509
D	497	HIS	-	EXPRESSION TAG	UNP P11509
D	498	HIS	-	EXPRESSION TAG	UNP P11509

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



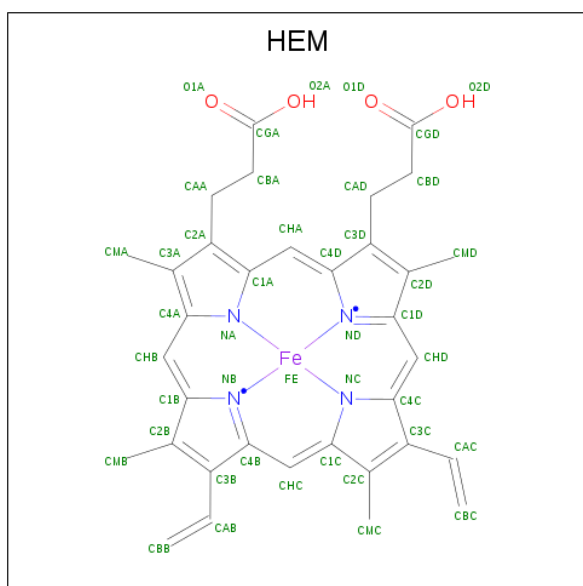
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

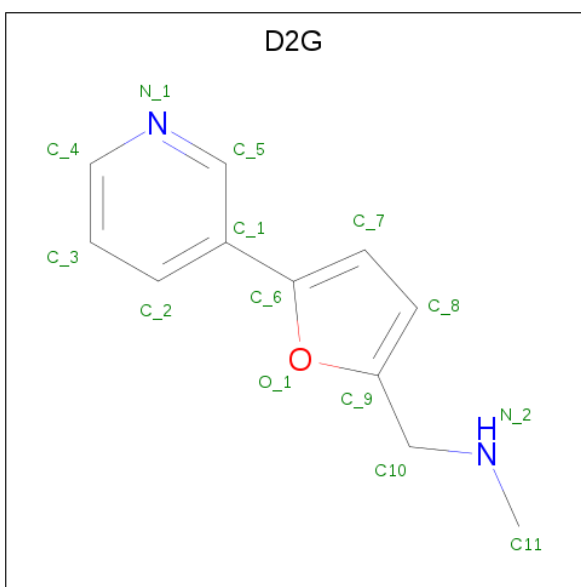
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



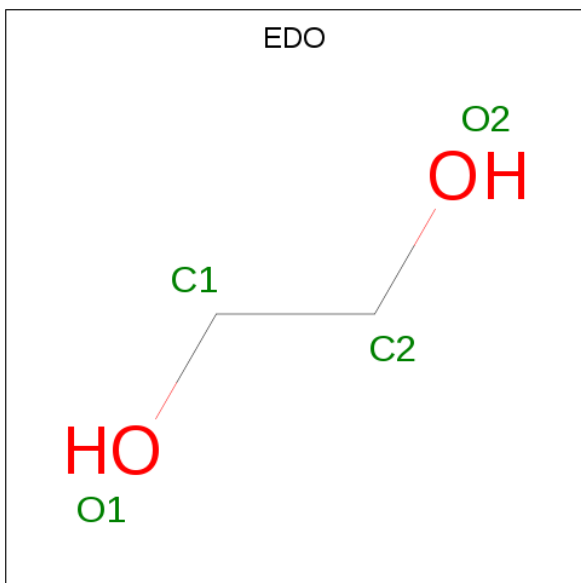
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is N-METHYL(5-(PYRIDIN-3-YL)FURAN-2-YL)METHANAMINE (three-letter code: D2G) (formula:  $C_{11}H_{12}N_2O$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	11	2	1		
4	B	1	Total	C	N	O	0	0
			14	11	2	1		
4	C	1	Total	C	N	O	0	0
			14	11	2	1		
4	D	1	Total	C	N	O	0	0
			14	11	2	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

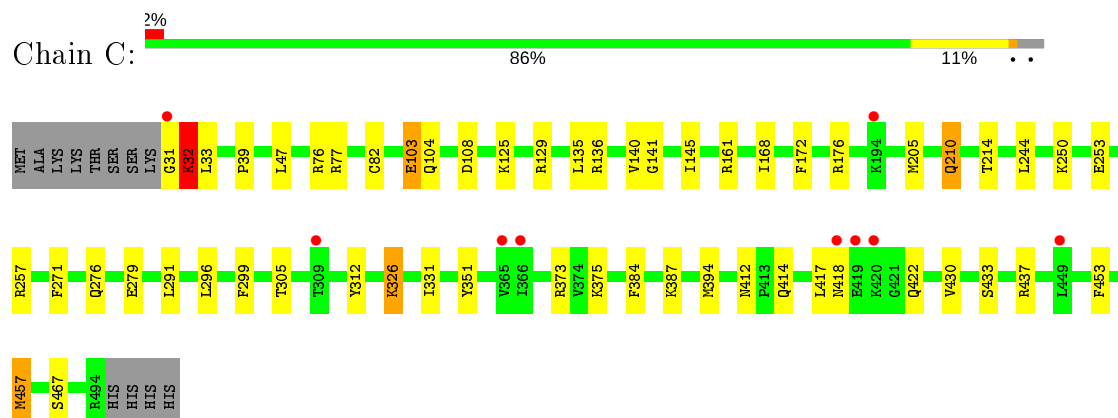
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	411	Total O 411 411	0	0
6	B	255	Total O 255 255	0	0
6	C	417	Total O 417 417	0	0
6	D	354	Total O 354 354	0	0

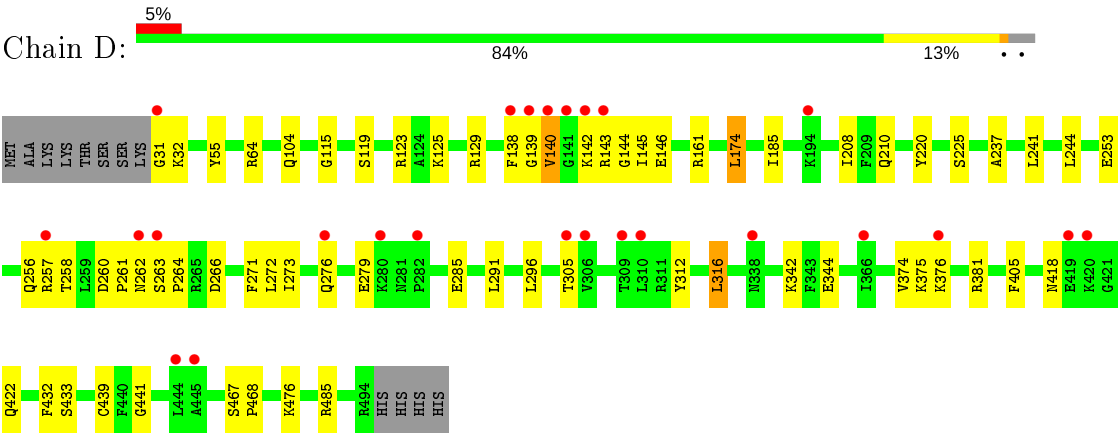




- Molecule 1: Cytochrome P450 2A6



● Molecule 1: Cytochrome P450 2A6



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.93Å 157.43Å 103.90Å 90.00° 92.21° 90.00°	Depositor
Resolution (Å)	33.80 – 1.65 33.80 – 1.60	Depositor EDS
% Data completeness (in resolution range)	88.0 (33.80-1.65) 89.2 (33.80-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 1.60Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.188 , 0.220 0.184 , 0.214	Depositor DCC
$R_{free}$ test set	13799 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.0	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 54.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16747	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, SO4, D2G, EDO

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	1.07	2/3851 (0.1%)	0.98	6/5186 (0.1%)
1	B	0.94	1/3860 (0.0%)	0.93	4/5200 (0.1%)
1	C	1.08	3/3842 (0.1%)	0.97	4/5175 (0.1%)
1	D	1.05	4/3842 (0.1%)	0.95	5/5175 (0.1%)
All	All	1.04	10/15395 (0.1%)	0.96	19/20736 (0.1%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	103	GLU	CG-CD	7.62	1.63	1.51
1	D	237	ALA	CA-CB	5.81	1.64	1.52
1	C	82	CYS	CB-SG	5.42	1.91	1.82
1	A	103	GLU	CD-OE1	5.39	1.31	1.25
1	B	221	GLU	CG-CD	5.19	1.59	1.51

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ASP	CB-CG-OD2	7.25	124.83	118.30
1	B	352	MET	CG-SD-CE	-6.24	90.21	100.20
1	D	64	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	D	381	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	C	104	GLN	N-CA-C	-6.01	94.78	111.00

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	3760	0	3747	37	0
1	B	3767	0	3745	54	0
1	C	3751	0	3734	50	0
1	D	3751	0	3734	54	0
2	A	15	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	43	0	30	4	0
3	B	43	0	30	1	0
3	C	43	0	30	1	0
3	D	43	0	30	2	0
4	A	14	0	11	2	0
4	B	14	0	11	2	0
4	C	14	0	11	1	0
4	D	14	0	11	2	0
5	A	4	0	6	0	0
5	C	20	0	30	9	0
5	D	4	0	6	0	0
6	A	411	0	0	4	0
6	B	255	0	0	9	0
6	C	417	0	0	10	0
6	D	354	0	0	2	0
All	All	16747	0	15166	196	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.

The worst 5 of 196 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:108:ASP:HA	5:C:2004:EDO:H22	1.22	1.11
5:C:2004:EDO:H11	6:C:2808:HOH:O	1.58	1.04
1:C:108:ASP:CA	5:C:2004:EDO:H22	1.91	0.99
1:B:176:ARG:HD3	1:B:198:PHE:CE2	2.00	0.96
1:C:453:PHE:O	1:C:457:MET:HG2	1.71	0.91

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	463/476 (97%)	453 (98%)	10 (2%)	0	100	100
1	B	463/476 (97%)	451 (97%)	12 (3%)	0	100	100
1	C	462/476 (97%)	453 (98%)	8 (2%)	1 (0%)	47	28
1	D	462/476 (97%)	448 (97%)	12 (3%)	2 (0%)	34	16
All	All	1850/1904 (97%)	1805 (98%)	42 (2%)	3 (0%)	47	28

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	32	LYS
1	D	140	VAL
1	D	261	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	412/422 (98%)	405 (98%)	7 (2%)	60	39
1	B	413/422 (98%)	402 (97%)	11 (3%)	44	19
1	C	411/422 (97%)	403 (98%)	8 (2%)	57	34
1	D	411/422 (97%)	406 (99%)	5 (1%)	71	53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1647/1688 (98%)	1616 (98%)	31 (2%)	57 34

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	417	LEU
1	B	495	HIS
1	D	312	TYR
1	B	419	GLU
1	C	32	LYS

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

Mol	Chain	Res	Type
1	B	126	GLN
1	B	466	GLN
1	D	320	HIS
1	D	422	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 ⓘ

20 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	HEM	B	500	1,4	27,50,50	1.51	4 (14%)	17,82,82	1.34	1 (5%)
2	SO4	B	2506	-	4,4,4	0.59	0	6,6,6	0.36	0
3	HEM	D	500	1,4	27,50,50	1.69	5 (18%)	17,82,82	1.56	2 (11%)
3	HEM	C	500	1,4	27,50,50	1.62	6 (22%)	17,82,82	1.56	2 (11%)
2	SO4	A	2502	-	4,4,4	0.52	0	6,6,6	0.22	0
3	HEM	A	500	1,4	27,50,50	1.69	7 (25%)	17,82,82	1.18	1 (5%)
2	SO4	C	2508	-	4,4,4	0.49	0	6,6,6	0.15	0
5	EDO	D	2007	-	3,3,3	0.51	0	2,2,2	1.20	0
4	D2G	D	501	3	12,15,15	1.72	3 (25%)	11,19,19	1.95	2 (18%)
5	EDO	C	2001	-	3,3,3	1.39	0	2,2,2	0.16	0
4	D2G	B	501	3	12,15,15	1.79	4 (33%)	11,19,19	1.99	4 (36%)
5	EDO	C	2005	-	3,3,3	1.40	0	2,2,2	0.37	0
5	EDO	C	2006	-	3,3,3	0.88	0	2,2,2	0.45	0
4	D2G	C	501	3	12,15,15	1.68	2 (16%)	11,19,19	1.87	2 (18%)
5	EDO	C	2004	-	3,3,3	1.45	0	2,2,2	1.07	0
2	SO4	A	2504	-	4,4,4	0.49	0	6,6,6	0.27	0
5	EDO	C	2002	-	3,3,3	0.47	0	2,2,2	0.72	0
2	SO4	A	2503	-	4,4,4	0.55	0	6,6,6	0.12	0
5	EDO	A	2003	-	3,3,3	1.78	1 (33%)	2,2,2	0.33	0
4	D2G	A	501	3	12,15,15	1.62	2 (16%)	11,19,19	1.82	2 (18%)

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	HEM	B	500	1,4	-	0/6/54/54	-
3	HEM	A	500	1,4	-	0/6/54/54	-
3	HEM	D	500	1,4	-	0/6/54/54	-
3	HEM	C	500	1,4	-	0/6/54/54	-
5	EDO	C	2005	-	-	0/1/1/1	-
5	EDO	C	2004	-	-	0/1/1/1	-
5	EDO	D	2007	-	-	0/1/1/1	-
4	D2G	D	501	3	-	2/3/7/7	0/2/2/2
5	EDO	C	2001	-	-	1/1/1/1	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	D2G	B	501	3	-	2/3/7/7	0/2/2/2
5	EDO	C	2006	-	-	0/1/1/1	-
4	D2G	C	501	3	-	2/3/7/7	0/2/2/2
4	D2G	A	501	3	-	2/3/7/7	0/2/2/2
5	EDO	C	2002	-	-	1/1/1/1	-
5	EDO	A	2003	-	-	0/1/1/1	-

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	500	HEM	CMD-C2D	4.03	1.60	1.51
3	C	500	HEM	C3C-CAC	-3.77	1.40	1.47
3	D	500	HEM	C3C-CAC	-3.77	1.40	1.47
4	C	501	D2G	C10-C_9	-3.71	1.47	1.51
3	A	500	HEM	C3B-C2B	-3.53	1.35	1.40

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	D2G	C_7-C_6-C_1	4.60	133.07	128.77
4	A	501	D2G	C_7-C_6-C_1	4.30	132.79	128.77
4	D	501	D2G	C_7-C_6-C_1	4.23	132.73	128.77
4	B	501	D2G	C_7-C_6-C_1	4.09	132.60	128.77
3	D	500	HEM	CMB-C2B-C3B	3.79	131.78	124.68

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	501	D2G	C_5-C_1-C_6-C_7
4	D	501	D2G	C_9-C10-N_2-C11
4	B	501	D2G	C_5-C_1-C_6-C_7
4	B	501	D2G	C_9-C10-N_2-C11
4	C	501	D2G	C_5-C_1-C_6-C_7

There are no ring outliers.

11 monomers are involved in 24 short contacts:

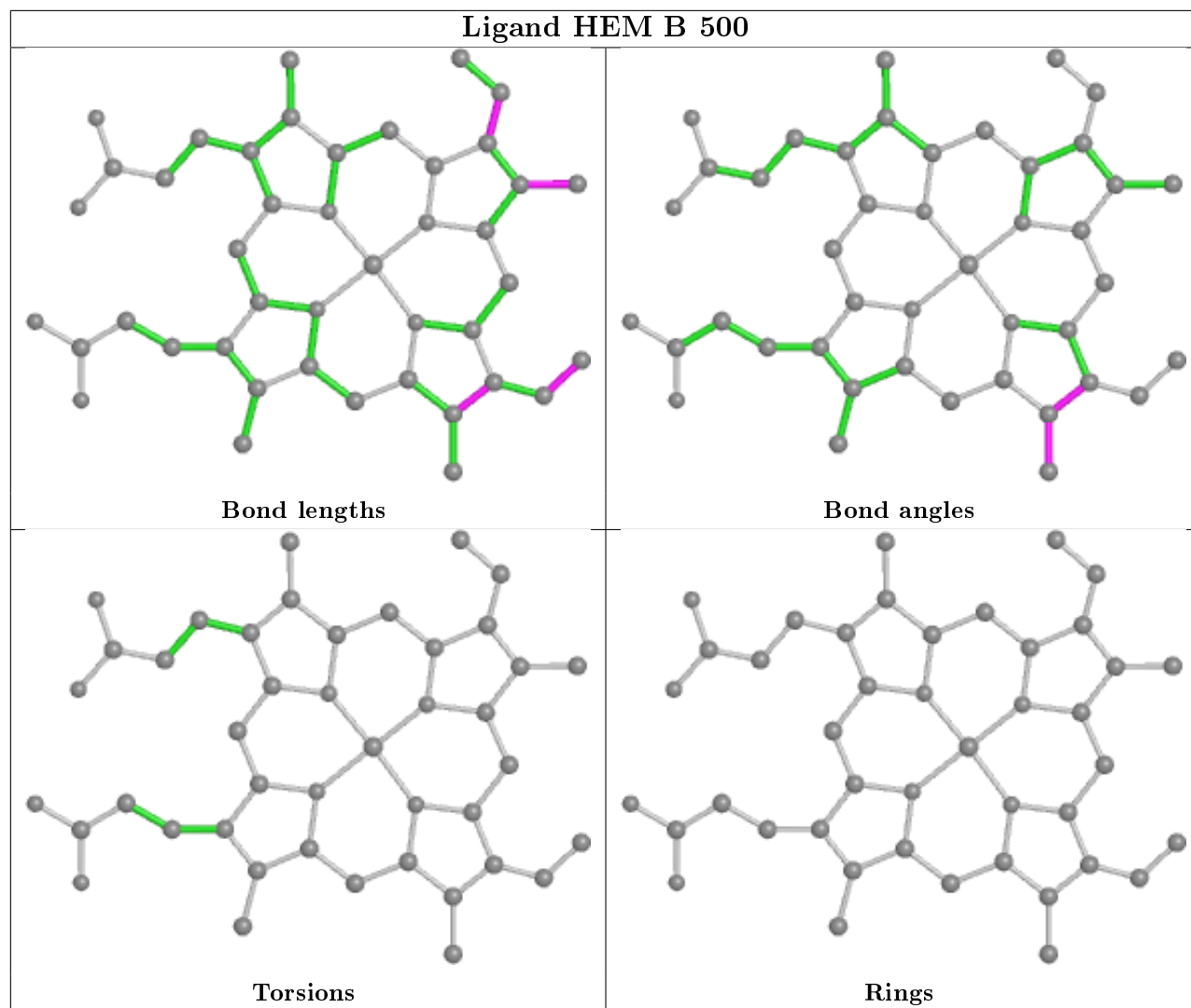
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	500	HEM	1	0

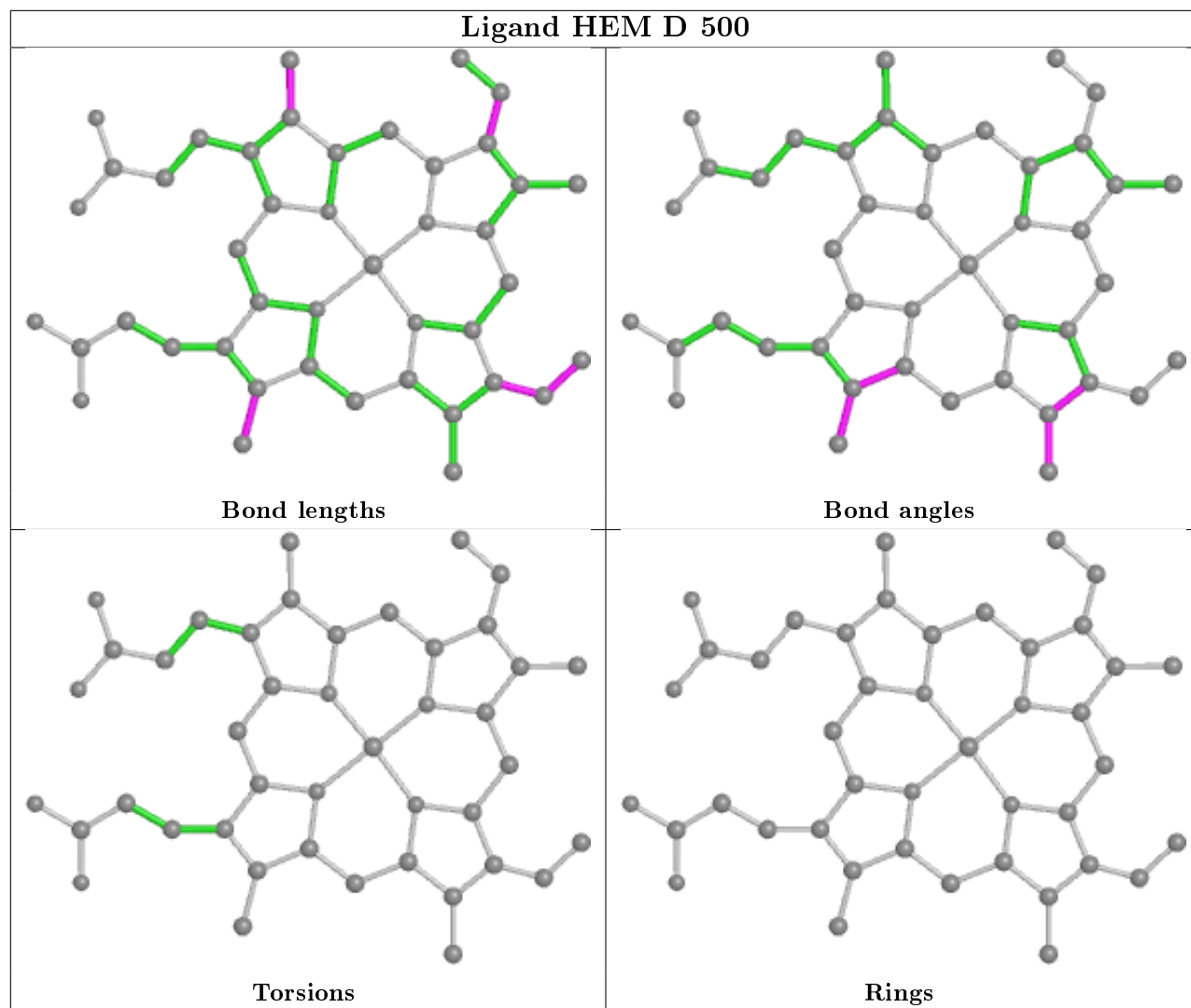
*Continued on next page...*

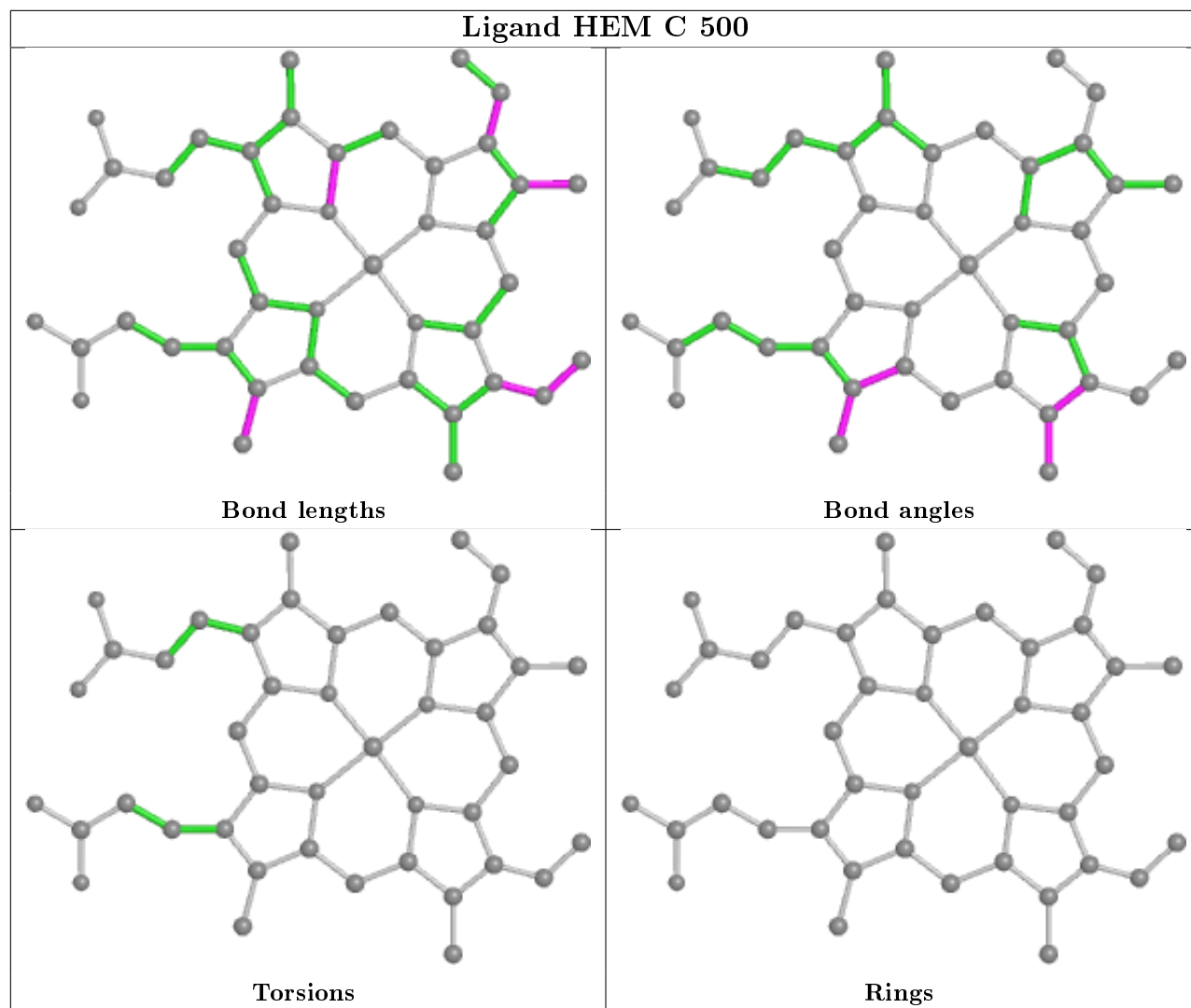
*Continued from previous page...*

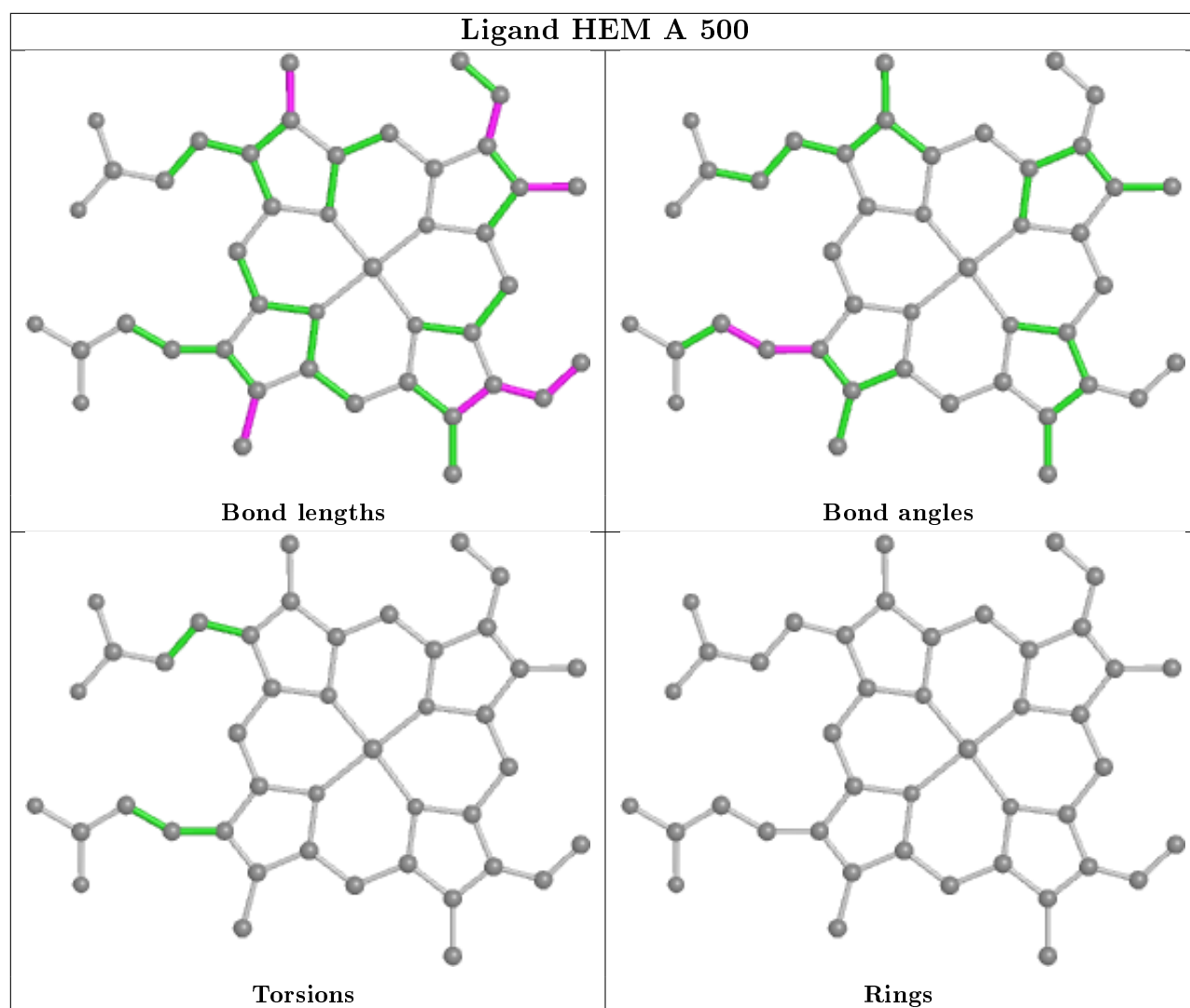
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	500	HEM	2	0
3	C	500	HEM	1	0
3	A	500	HEM	4	0
4	D	501	D2G	2	0
5	C	2001	EDO	1	0
4	B	501	D2G	2	0
5	C	2006	EDO	1	0
4	C	501	D2G	1	0
5	C	2004	EDO	7	0
4	A	501	D2G	2	0

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 [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	465/476 (97%)	-0.20	10 (2%) 62 63	16, 25, 41, 58	0
1	B	465/476 (97%)	0.15	19 (4%) 37 37	19, 31, 50, 67	0
1	C	464/476 (97%)	-0.19	9 (1%) 66 69	16, 24, 39, 56	0
1	D	464/476 (97%)	0.01	25 (5%) 25 24	16, 25, 50, 64	0
All	All	1858/1904 (97%)	-0.06	63 (3%) 45 45	16, 26, 45, 67	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	31	GLY	7.4
1	B	496	HIS	6.3
1	B	495	HIS	5.7
1	D	143	ARG	5.4
1	A	30	LYS	5.3

### 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.

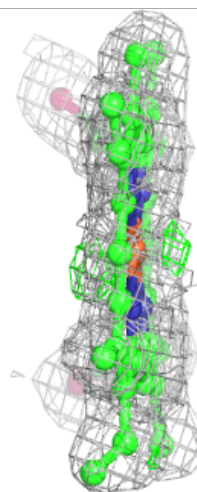
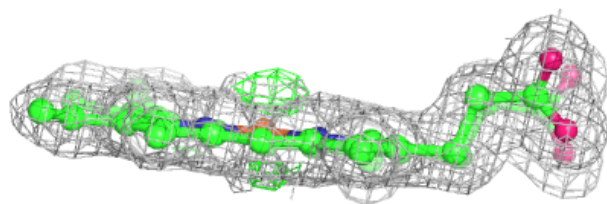
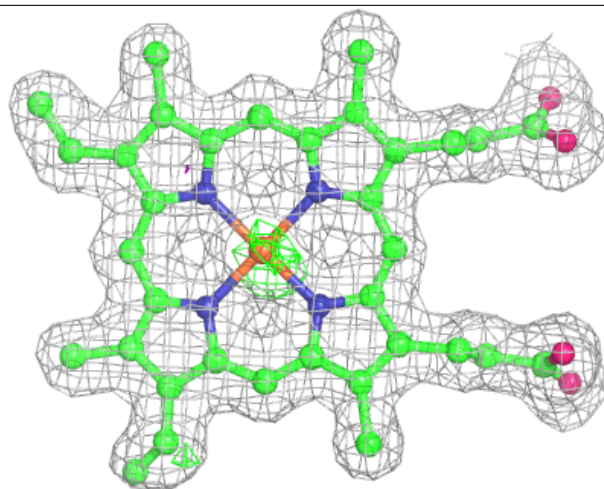
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	C	2002	4/4	0.81	0.23	33,35,36,39	0
5	EDO	C	2001	4/4	0.84	0.33	33,35,36,37	0
5	EDO	A	2003	4/4	0.85	0.31	34,34,35,36	0
5	EDO	D	2007	4/4	0.86	0.14	31,32,33,34	0
2	SO4	A	2504	5/5	0.88	0.25	50,51,53,55	0
5	EDO	C	2005	4/4	0.91	0.33	36,37,38,39	0
2	SO4	C	2508	5/5	0.92	0.13	62,62,63,65	0
2	SO4	B	2506	5/5	0.93	0.15	57,59,60,60	0
5	EDO	C	2006	4/4	0.93	0.17	34,35,36,37	0
2	SO4	A	2502	5/5	0.94	0.12	54,55,57,57	0
2	SO4	A	2503	5/5	0.95	0.19	56,56,57,58	0
5	EDO	C	2004	4/4	0.96	0.07	23,25,28,30	0
4	D2G	C	501	14/14	0.97	0.15	19,22,24,28	0
4	D2G	D	501	14/14	0.97	0.17	20,22,24,28	0
4	D2G	B	501	14/14	0.97	0.14	22,24,25,26	0
3	HEM	D	500	43/43	0.98	0.14	16,20,23,29	0
4	D2G	A	501	14/14	0.98	0.13	16,19,21,23	0
3	HEM	B	500	43/43	0.98	0.14	17,21,24,29	0
3	HEM	A	500	43/43	0.99	0.13	12,15,18,25	0
3	HEM	C	500	43/43	0.99	0.12	15,18,21,24	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.



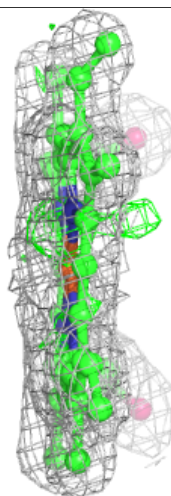
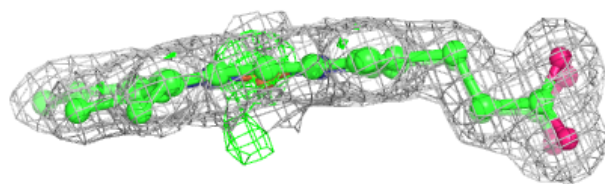
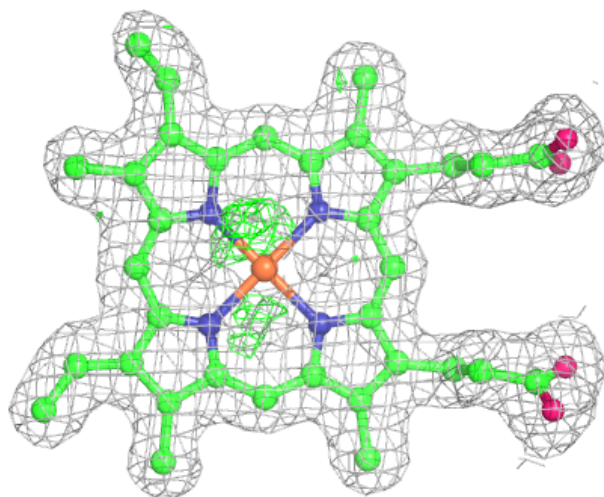
**Electron density around HEM D 500:**

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



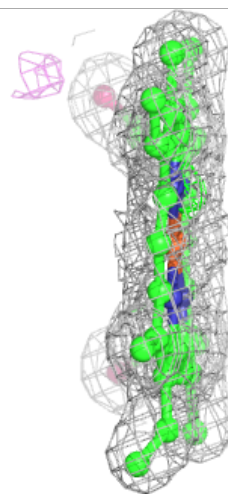
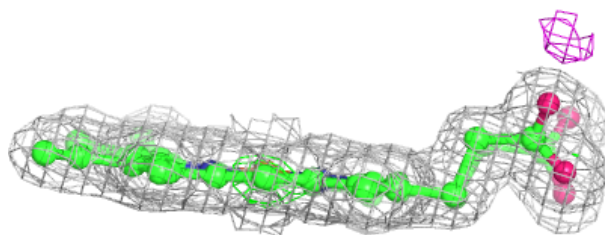
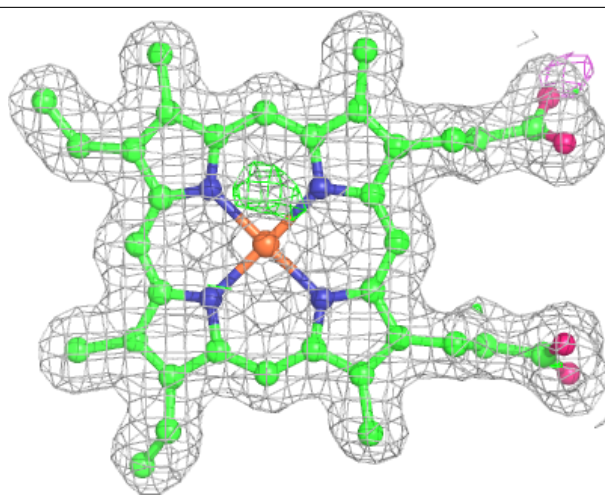
**Electron density around HEM B 500:**

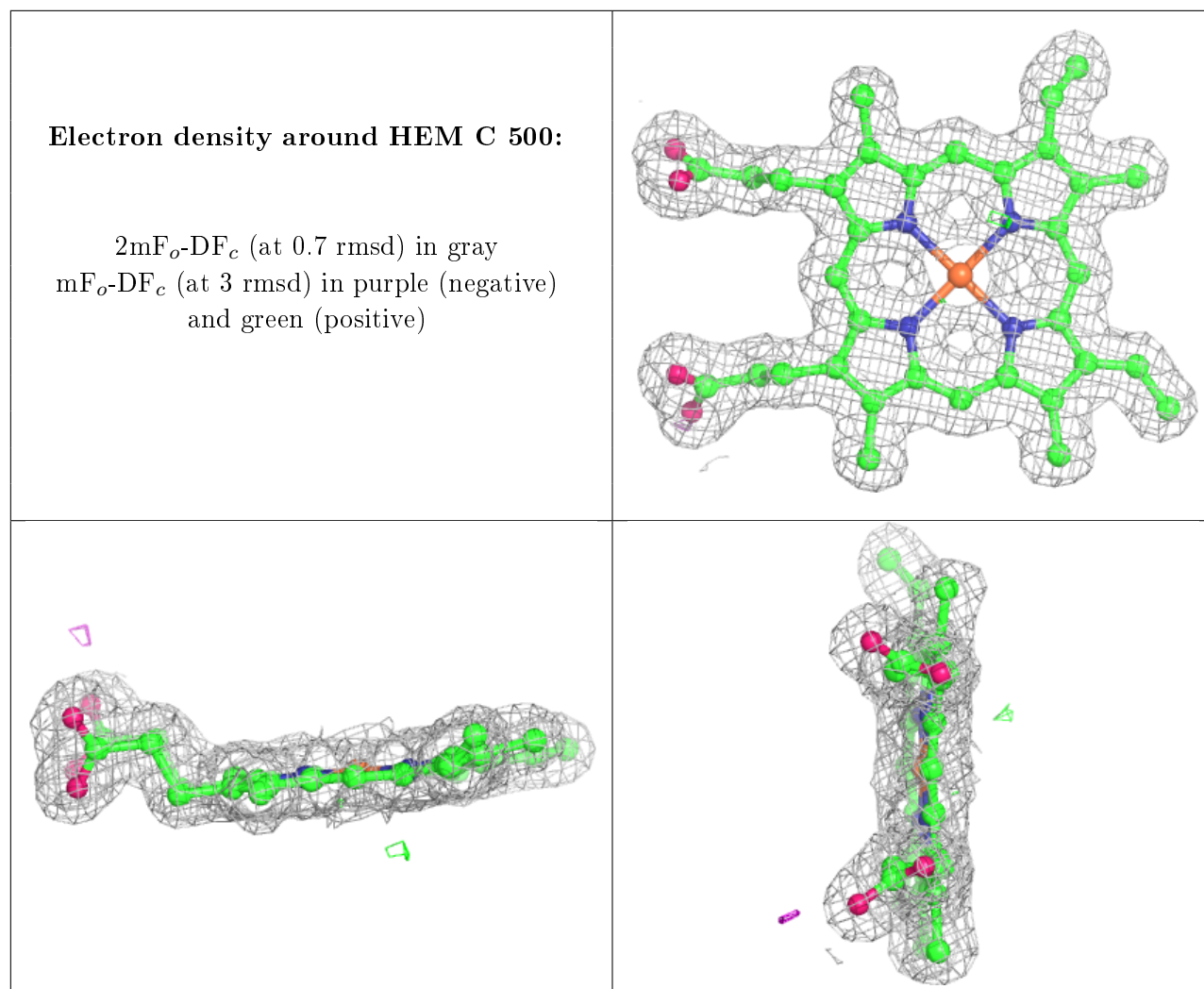
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM A 500:**

$2mF_o-DF_c$  (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.