



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2020 – 07:27 pm BST

PDB ID : 2Z3T  
Title : Crystal Structure of Substrate Free Cytochrome P450 StaP (CYP245A1)  
Authors : Makino, M.; Sugimoto, H.; Shiro, Y.; Asamizu, S.; Onaka, H.; Nagano, S.  
Deposited on : 2007-06-06  
Resolution : 1.90 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.

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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

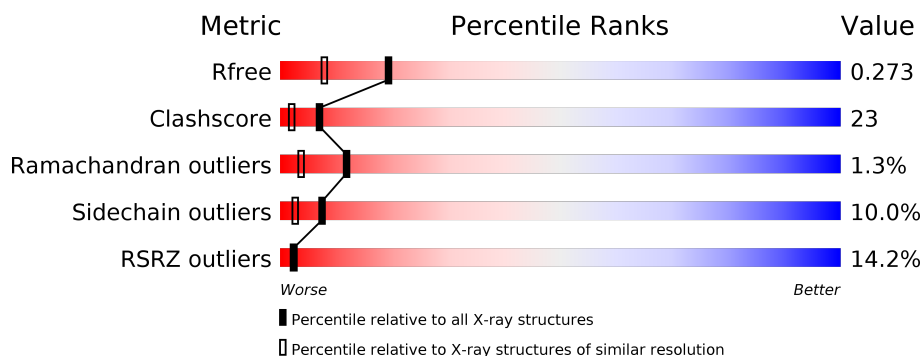
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	<div> <div>17%</div> <div> <div>54%</div> <div>31%</div> <div>6%</div> <div>9%</div> </div> </div>
1	B	425	<div> <div>9%</div> <div> <div>55%</div> <div>28%</div> <div>6%</div> <div>12%</div> </div> </div>
1	C	425	<div> <div>15%</div> <div> <div>52%</div> <div>32%</div> <div>6%</div> <div>10%</div> </div> </div>
1	D	425	<div> <div>10%</div> <div> <div>53%</div> <div>31%</div> <div>• •</div> <div>11%</div> </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
4	EDO	B	1209	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12642 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			3029	1908	563	553	5			
1	B	376	Total	C	N	O	S	0	0	0
			2962	1869	548	540	5			
1	C	383	Total	C	N	O	S	0	0	0
			3017	1900	561	551	5			
1	D	379	Total	C	N	O	S	0	0	0
			2980	1880	551	544	5			

There are 32 discrepancies between the modelled and reference sequences:

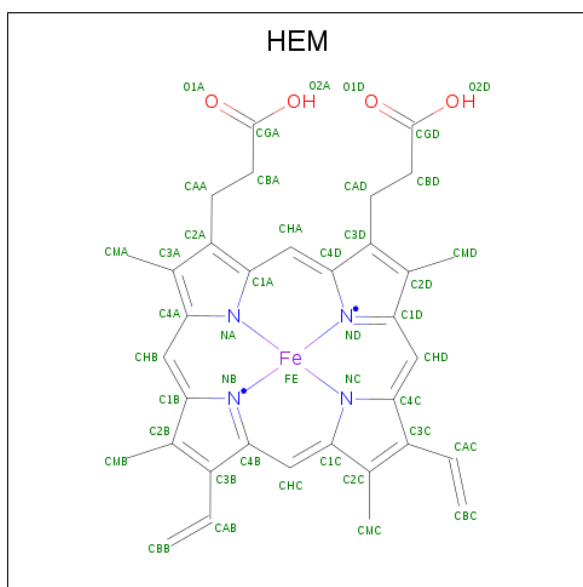
Chain	Residue	Modelled	Actual	Comment	Reference
A	418	LEU	-	CLONING ARTIFACT	UNP Q83WG3
A	419	GLU	-	CLONING ARTIFACT	UNP Q83WG3
A	420	HIS	-	EXPRESSION TAG	UNP Q83WG3
A	421	HIS	-	EXPRESSION TAG	UNP Q83WG3
A	422	HIS	-	EXPRESSION TAG	UNP Q83WG3
A	423	HIS	-	EXPRESSION TAG	UNP Q83WG3
A	424	HIS	-	EXPRESSION TAG	UNP Q83WG3
A	425	HIS	-	EXPRESSION TAG	UNP Q83WG3
B	418	LEU	-	CLONING ARTIFACT	UNP Q83WG3
B	419	GLU	-	CLONING ARTIFACT	UNP Q83WG3
B	420	HIS	-	EXPRESSION TAG	UNP Q83WG3
B	421	HIS	-	EXPRESSION TAG	UNP Q83WG3
B	422	HIS	-	EXPRESSION TAG	UNP Q83WG3
B	423	HIS	-	EXPRESSION TAG	UNP Q83WG3
B	424	HIS	-	EXPRESSION TAG	UNP Q83WG3
B	425	HIS	-	EXPRESSION TAG	UNP Q83WG3
C	418	LEU	-	CLONING ARTIFACT	UNP Q83WG3
C	419	GLU	-	CLONING ARTIFACT	UNP Q83WG3
C	420	HIS	-	EXPRESSION TAG	UNP Q83WG3
C	421	HIS	-	EXPRESSION TAG	UNP Q83WG3
C	422	HIS	-	EXPRESSION TAG	UNP Q83WG3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	423	HIS	-	EXPRESSION TAG	UNP Q83WG3
C	424	HIS	-	EXPRESSION TAG	UNP Q83WG3
C	425	HIS	-	EXPRESSION TAG	UNP Q83WG3
D	418	LEU	-	CLONING ARTIFACT	UNP Q83WG3
D	419	GLU	-	CLONING ARTIFACT	UNP Q83WG3
D	420	HIS	-	EXPRESSION TAG	UNP Q83WG3
D	421	HIS	-	EXPRESSION TAG	UNP Q83WG3
D	422	HIS	-	EXPRESSION TAG	UNP Q83WG3
D	423	HIS	-	EXPRESSION TAG	UNP Q83WG3
D	424	HIS	-	EXPRESSION TAG	UNP Q83WG3
D	425	HIS	-	EXPRESSION TAG	UNP Q83WG3

- 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 IMIDAZOLE (three-letter code: IMD) (formula:  $C_3H_5N_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			5	3	2		
3	B	1	Total	C	N	0	0
			5	3	2		
3	C	1	Total	C	N	0	0
			5	3	2		
3	D	1	Total	C	N	0	0
			5	3	2		

- Molecule 4 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
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

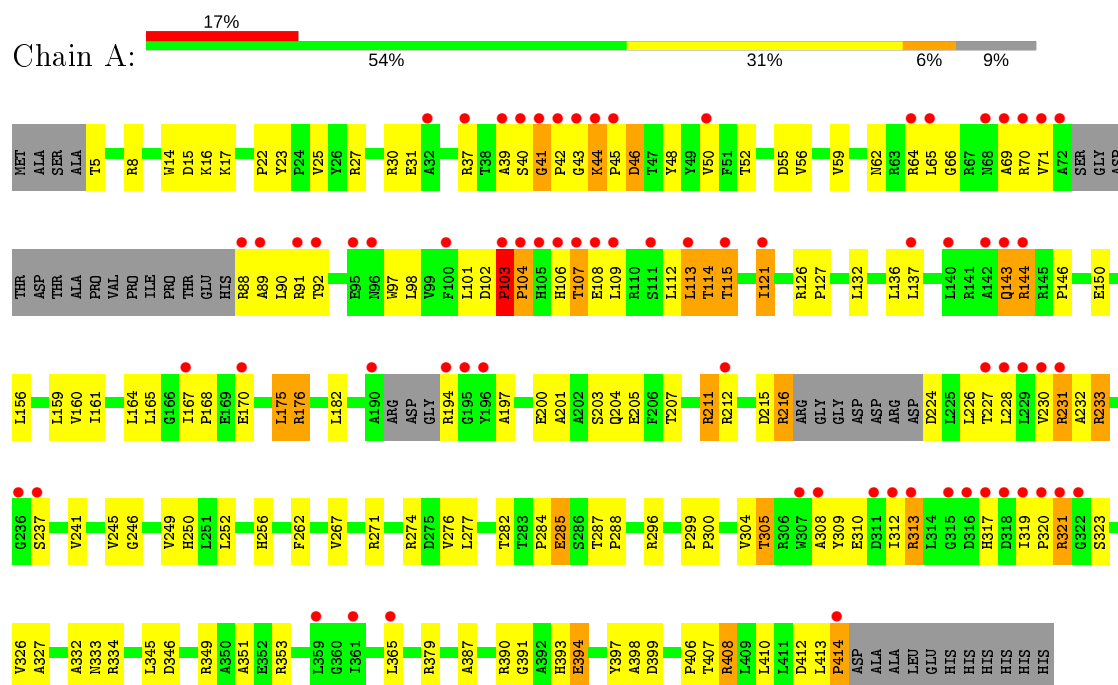
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	125	Total O 125 125	0	0
5	B	107	Total O 107 107	0	0
5	C	92	Total O 92 92	0	0
5	D	102	Total O 102 102	0	0

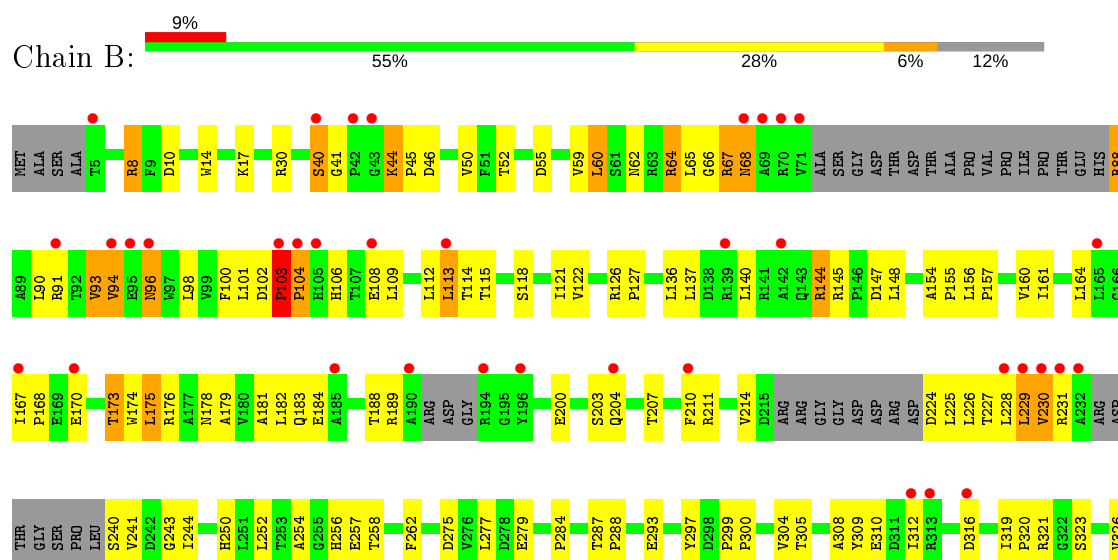
### 3 Residue-property plots [i](#)

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: Cytochrome P450



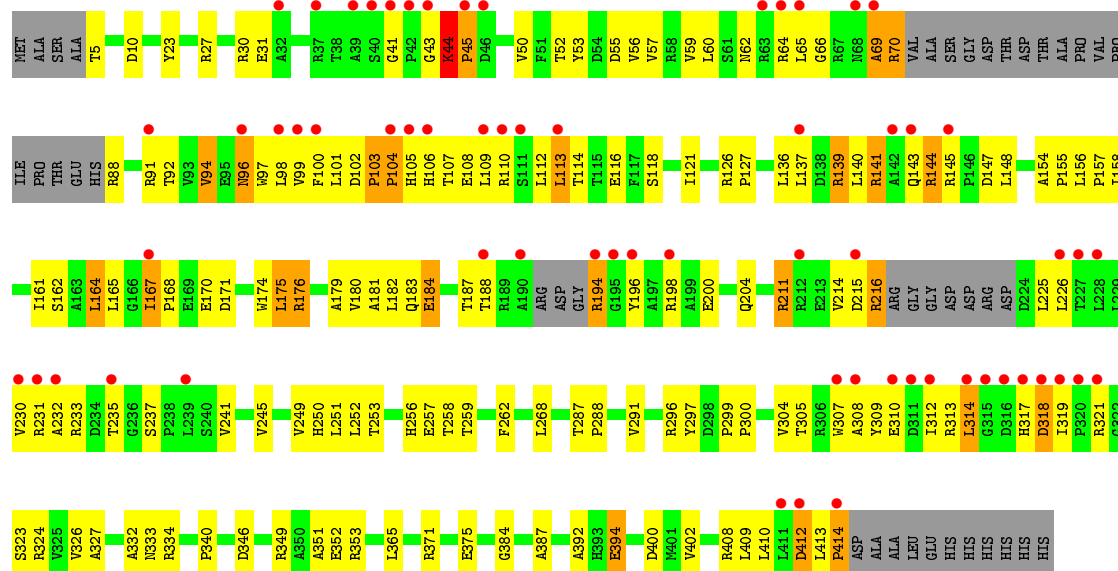
#### • Molecule 1: Cytochrome P450



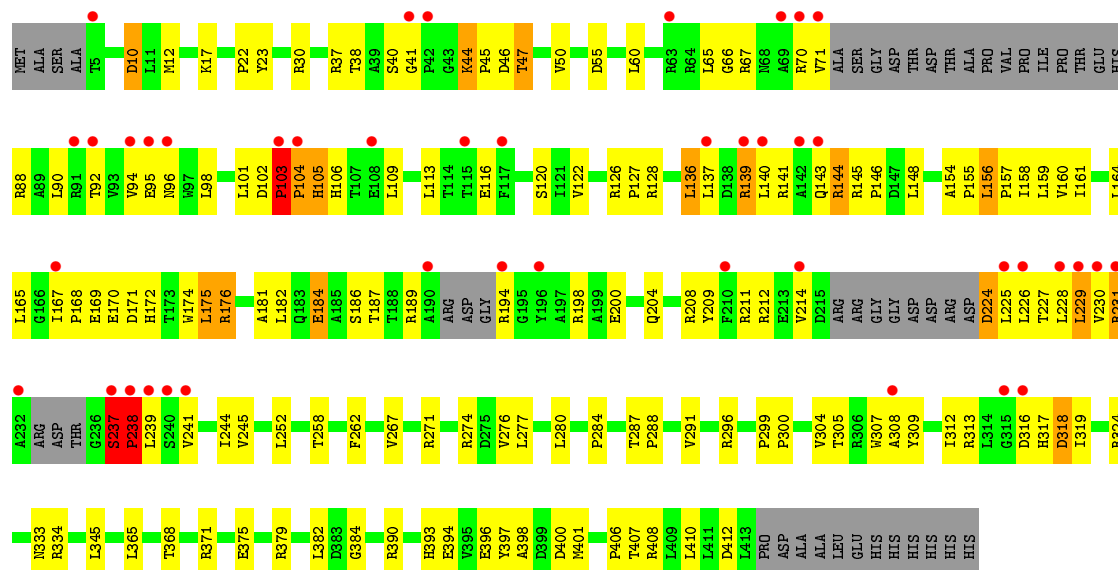




• Molecule 1: Cytochrome P450



• Molecule 1: Cytochrome P450



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.64Å 78.72Å 145.66Å 90.00° 107.92° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 19.92 – 1.91	Depositor EDS
% Data completeness (in resolution range)	79.0 (20.00-1.90) 88.0 (19.92-1.91)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.03	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 1.90Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.228 , 0.273 0.233 , 0.273	Depositor DCC
$R_{free}$ test set	5865 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.2	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 38.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.479 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.453 for -h,-k,h+l	Depositor
Outliers	7 of 131947 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12642	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 80.00 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.9289e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, IMD, 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	0.40	0/3094	0.73	1/4214 (0.0%)
1	B	0.39	0/3025	0.73	2/4119 (0.0%)
1	C	0.38	0/3082	0.73	2/4197 (0.0%)
1	D	0.41	0/3043	0.70	0/4143
All	All	0.39	0/12244	0.72	5/16673 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	43	GLY	N-CA-C	-9.56	89.19	113.10
1	C	44	LYS	N-CA-C	7.89	132.30	111.00
1	A	43	GLY	N-CA-C	-7.45	94.48	113.10
1	B	113	LEU	CA-CB-CG	6.88	131.13	115.30
1	B	413	LEU	C-N-CD	-5.39	108.74	120.60

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	3029	0	3029	134	0
1	B	2962	0	2960	133	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3017	0	3015	162	0
1	D	2980	0	2979	130	0
2	A	43	0	30	0	0
2	B	43	0	30	3	0
2	C	43	0	30	3	0
2	D	43	0	30	3	0
3	A	5	0	4	0	0
3	B	5	0	5	0	0
3	C	5	0	5	0	0
3	D	5	0	5	0	0
4	A	8	0	12	3	0
4	B	16	0	24	5	0
4	C	4	0	6	1	0
4	D	8	0	12	1	0
5	A	125	0	0	6	0
5	B	107	0	0	10	0
5	C	92	0	0	6	0
5	D	102	0	0	6	0
All	All	12642	0	12176	558	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 23.

The worst 5 of 558 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:394:GLU:HG2	1:C:410:LEU:HB2	1.29	1.11
1:A:40:SER:OG	1:A:44:LYS:HA	1.55	1.05
1:D:116:GLU:HG2	1:D:225:LEU:HD13	1.34	1.04
1:B:413:LEU:HB2	1:B:414:PRO:C	1.83	0.98
1:C:313:ARG:HE	1:C:318:ASP:HB2	1.30	0.96

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	377/425 (89%)	357 (95%)	14 (4%)	6 (2%)	9	2
1	B	366/425 (86%)	350 (96%)	13 (4%)	3 (1%)	19	9
1	C	375/425 (88%)	358 (96%)	12 (3%)	5 (1%)	12	4
1	D	369/425 (87%)	351 (95%)	13 (4%)	5 (1%)	11	3
All	All	1487/1700 (88%)	1416 (95%)	52 (4%)	19 (1%)	12	4

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	PRO
1	C	45	PRO
1	C	103	PRO
1	D	103	PRO
1	A	44	LYS

### 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	316/347 (91%)	284 (90%)	32 (10%)	7	2
1	B	309/347 (89%)	276 (89%)	33 (11%)	6	2
1	C	315/347 (91%)	285 (90%)	30 (10%)	8	3
1	D	311/347 (90%)	281 (90%)	30 (10%)	8	3
All	All	1251/1388 (90%)	1126 (90%)	125 (10%)	7	3

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	241	VAL
1	C	92	THR
1	D	229	LEU

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Mol	Chain	Res	Type
1	B	323	SER
1	B	412	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	172	HIS
1	C	183	GLN
1	D	106	HIS
1	B	250	HIS
1	D	96	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

17 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	EDO	B	1206	-	3,3,3	0.50	0	2,2,2	0.39	0
3	IMD	A	501	2	3,5,5	0.65	0	4,5,5	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	A	1203	-	3,3,3	0.49	0	2,2,2	0.21	0
2	HEM	C	500	1,3	27,50,50	1.32	2 (7%)	17,82,82	1.36	2 (11%)
2	HEM	D	500	1,3	27,50,50	1.29	2 (7%)	17,82,82	1.47	3 (17%)
2	HEM	A	500	1,3	27,50,50	1.37	3 (11%)	17,82,82	1.44	2 (11%)
2	HEM	B	500	1,3	27,50,50	1.35	3 (11%)	17,82,82	1.22	1 (5%)
4	EDO	D	1201	-	3,3,3	0.49	0	2,2,2	0.38	0
4	EDO	A	1202	-	3,3,3	0.49	0	2,2,2	0.34	0
4	EDO	B	1204	-	3,3,3	0.49	0	2,2,2	0.32	0
3	IMD	B	501	2	3,5,5	0.67	0	4,5,5	1.00	0
4	EDO	B	1205	-	3,3,3	0.49	0	2,2,2	0.33	0
3	IMD	C	501	2	3,5,5	0.63	0	4,5,5	1.03	0
4	EDO	D	1208	-	3,3,3	0.49	0	2,2,2	0.32	0
4	EDO	B	1209	-	3,3,3	0.47	0	2,2,2	0.40	0
3	IMD	D	501	2	3,5,5	0.61	0	4,5,5	0.99	0
4	EDO	C	1207	-	3,3,3	0.48	0	2,2,2	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	1206	-	-	0/1/1/1	-
2	HEM	D	500	1,3	-	0/6/54/54	-
4	EDO	A	1203	-	-	0/1/1/1	-
2	HEM	C	500	1,3	-	0/6/54/54	-
4	EDO	A	1202	-	-	0/1/1/1	-
2	HEM	A	500	1,3	-	0/6/54/54	-
2	HEM	B	500	1,3	-	0/6/54/54	-
4	EDO	D	1201	-	-	0/1/1/1	-
3	IMD	A	501	2	-	-	0/1/1/1
4	EDO	B	1204	-	-	0/1/1/1	-
3	IMD	B	501	2	-	-	0/1/1/1
4	EDO	B	1205	-	-	0/1/1/1	-
3	IMD	C	501	2	-	-	0/1/1/1
4	EDO	D	1208	-	-	0/1/1/1	-
4	EDO	B	1209	-	-	0/1/1/1	-
3	IMD	D	501	2	-	-	0/1/1/1
4	EDO	C	1207	-	-	0/1/1/1	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	HEM	C4B-NB	3.14	1.42	1.36
2	B	500	HEM	C4B-NB	3.08	1.42	1.36
2	A	500	HEM	C4B-NB	3.05	1.42	1.36
2	D	500	HEM	C4B-NB	2.85	1.42	1.36
2	C	500	HEM	C3C-CAC	-2.73	1.42	1.47

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	HEM	C4C-C3C-C2C	-3.09	104.74	106.90
2	C	500	HEM	C4C-C3C-C2C	-3.00	104.80	106.90
2	A	500	HEM	C4C-C3C-C2C	-2.80	104.94	106.90
2	A	500	HEM	CAD-CBD-CGD	2.59	117.02	112.67
2	B	500	HEM	C4C-C3C-C2C	-2.52	105.14	106.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

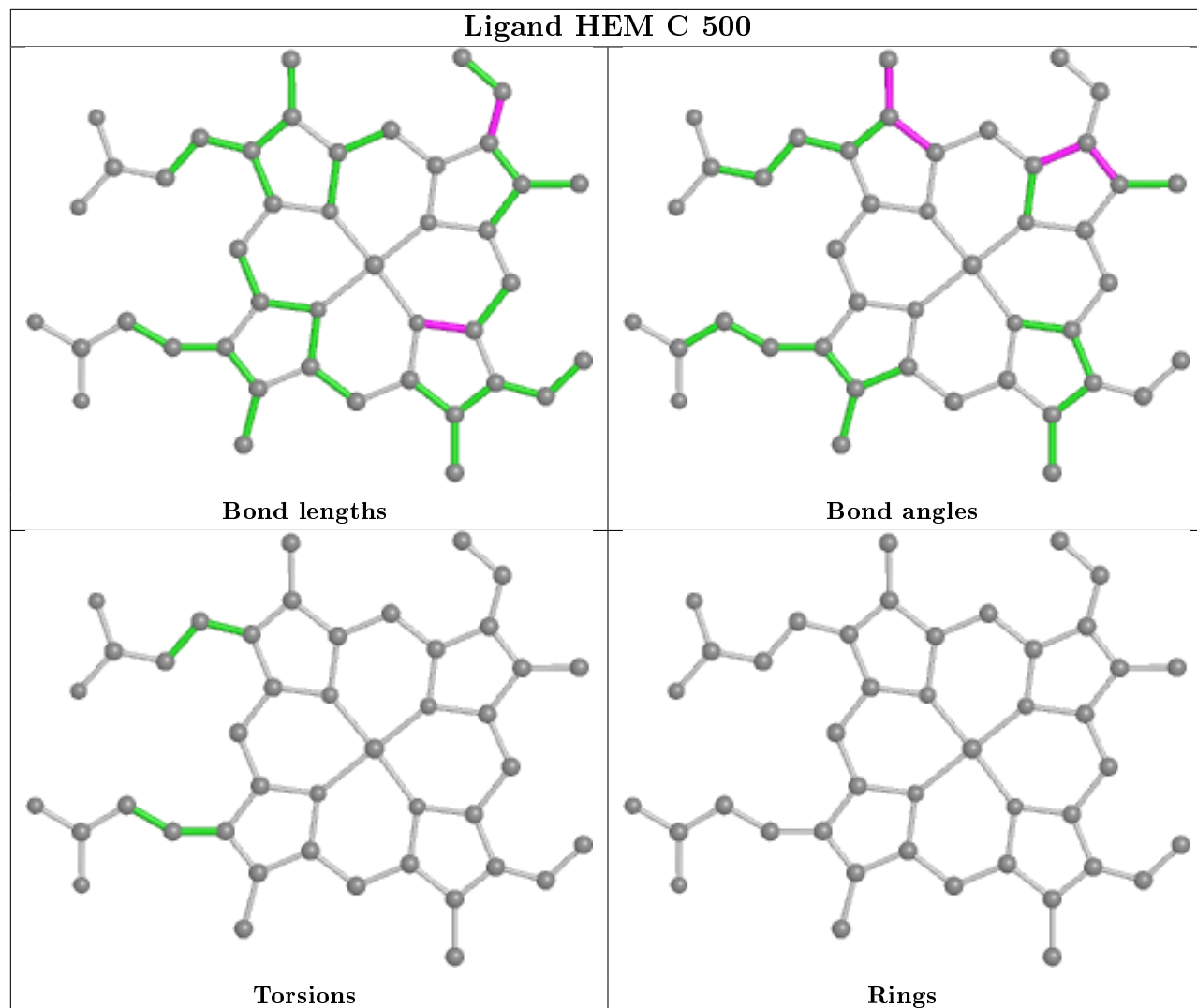
9 monomers are involved in 19 short contacts:

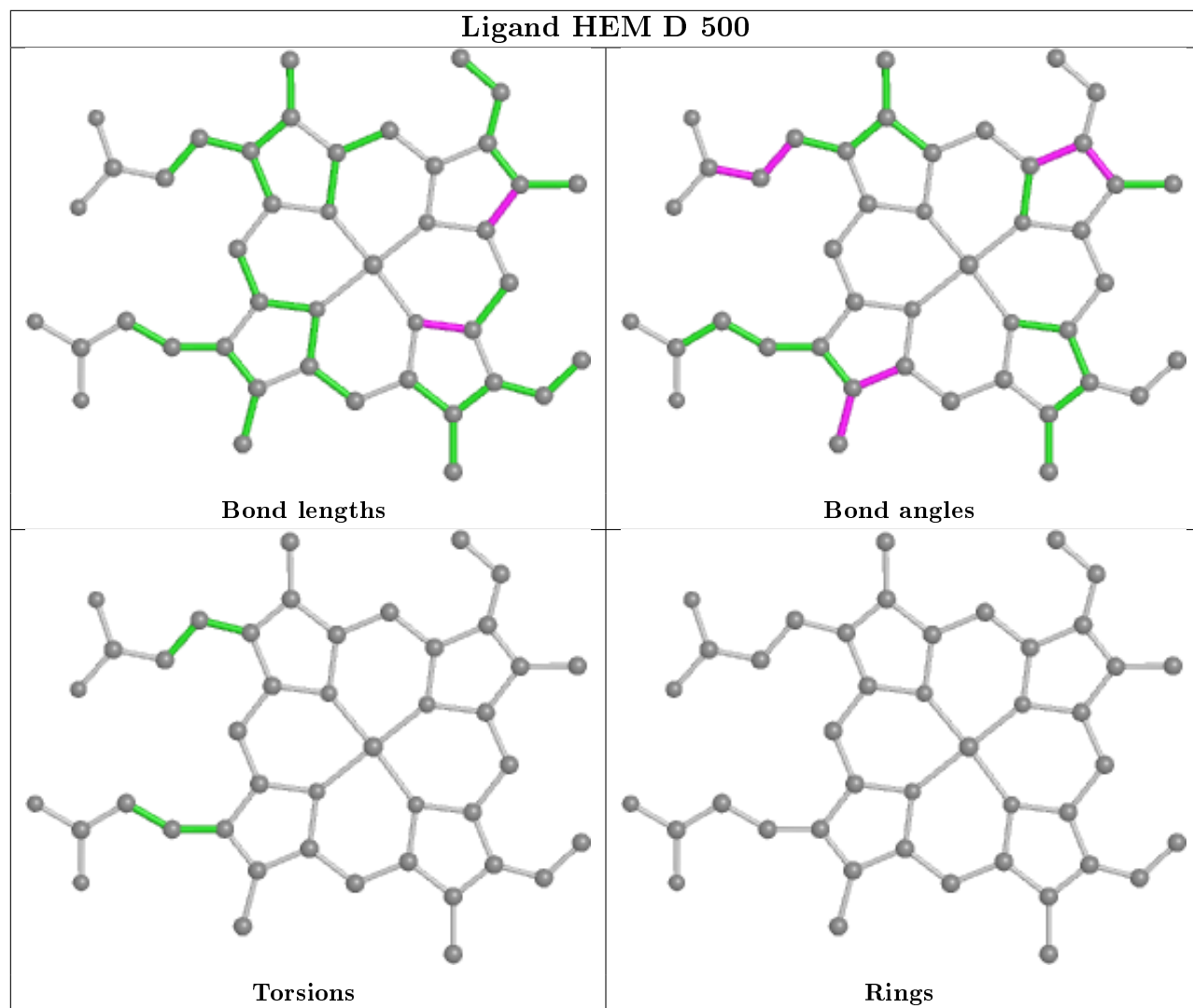
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1206	EDO	1	0
4	A	1203	EDO	1	0
2	C	500	HEM	3	0
2	D	500	HEM	3	0
2	B	500	HEM	3	0
4	A	1202	EDO	2	0
4	D	1208	EDO	1	0
4	B	1209	EDO	4	0
4	C	1207	EDO	1	0

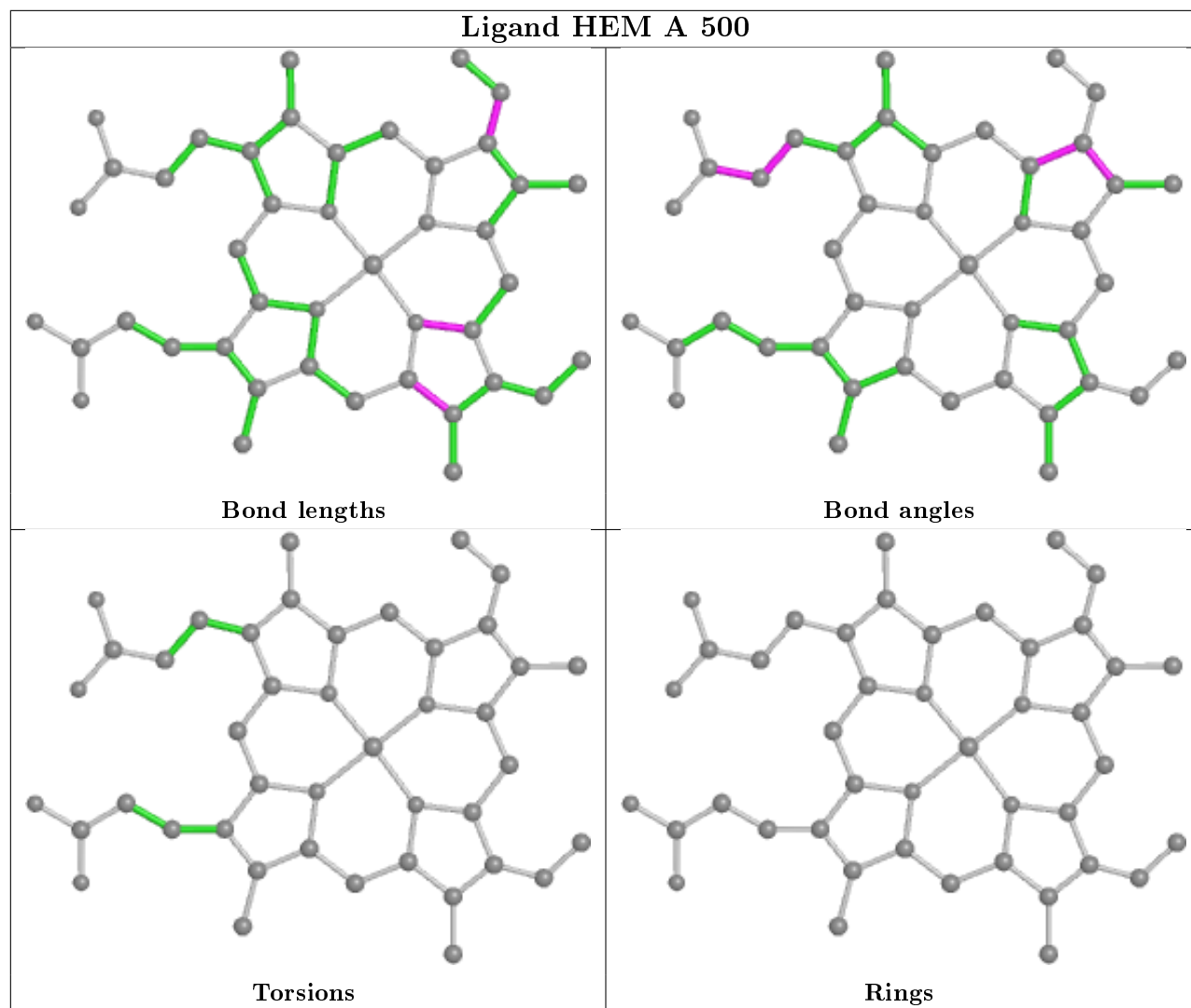
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

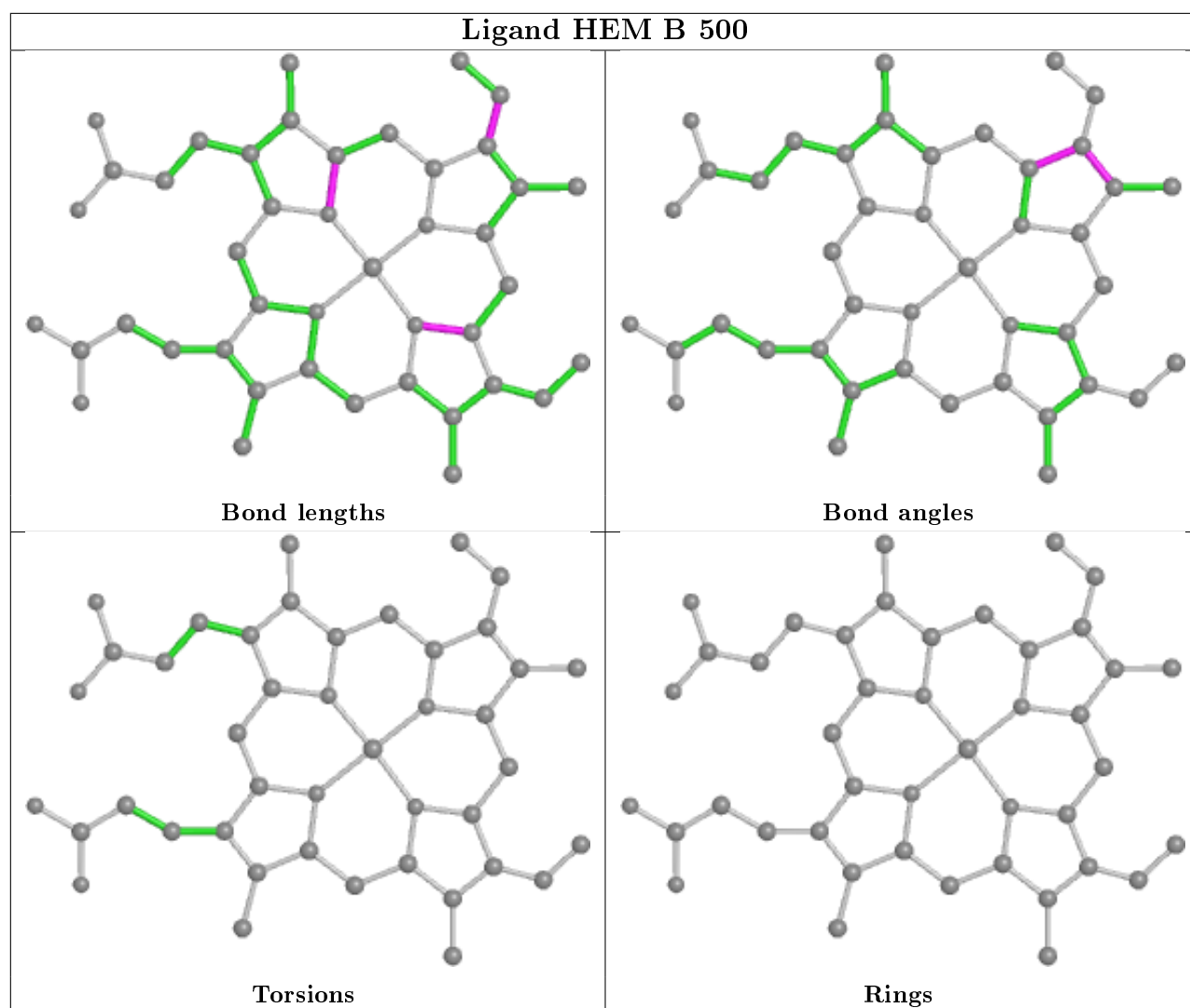


equivalents in the CSD to analyse the geometry.









## 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	385/425 (90%)	1.13	71 (18%) <b>1</b> <b>1</b>	17, 45, 77, 88	0
1	B	376/425 (88%)	0.81	39 (10%) <b>6</b> <b>7</b>	17, 39, 70, 80	0
1	C	383/425 (90%)	1.00	63 (16%) <b>1</b> <b>1</b>	20, 42, 74, 87	0
1	D	379/425 (89%)	0.84	43 (11%) <b>5</b> <b>5</b>	17, 37, 69, 86	0
All	All	1523/1700 (89%)	0.95	216 (14%) <b>2</b> <b>2</b>	17, 41, 73, 88	0

The worst 5 of 216 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	72	ALA	11.4
1	C	43	GLY	9.3
1	A	109	LEU	8.9
1	B	232	ALA	8.9
1	C	41	GLY	8.8

### 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](#)

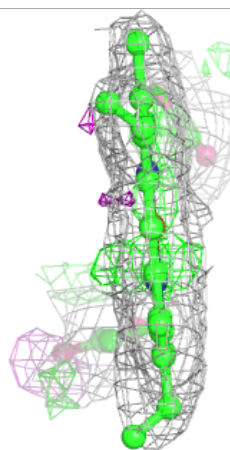
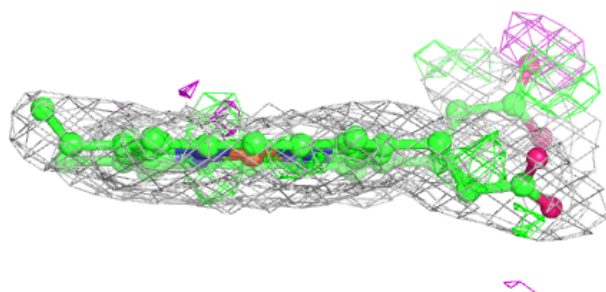
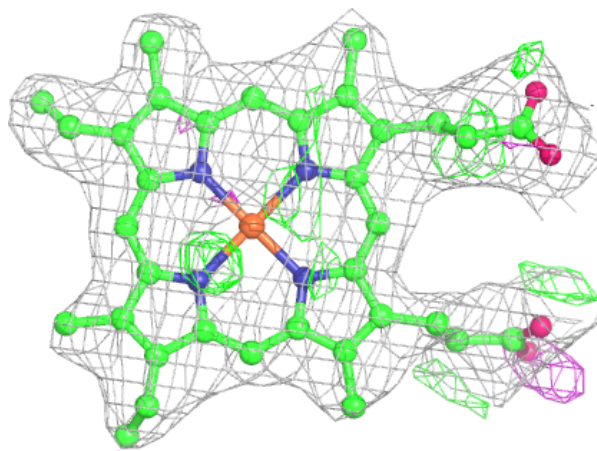
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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
4	EDO	C	1207	4/4	0.38	0.28	82,82,83,83	0
4	EDO	A	1202	4/4	0.63	0.22	39,41,43,45	0
4	EDO	D	1208	4/4	0.69	0.33	45,47,48,48	0
4	EDO	B	1204	4/4	0.76	0.38	44,44,45,45	0
4	EDO	A	1203	4/4	0.78	0.30	32,34,35,36	0
4	EDO	B	1209	4/4	0.79	0.23	44,44,45,46	0
4	EDO	B	1205	4/4	0.83	0.23	28,31,32,34	0
3	IMD	C	501	5/5	0.85	0.16	53,54,55,55	0
4	EDO	D	1201	4/4	0.85	0.16	34,34,35,36	0
3	IMD	D	501	5/5	0.86	0.20	56,56,57,58	0
4	EDO	B	1206	4/4	0.90	0.12	26,26,28,29	0
2	HEM	A	500	43/43	0.91	0.18	34,41,54,58	0
3	IMD	B	501	5/5	0.92	0.15	27,27,29,29	0
2	HEM	C	500	43/43	0.93	0.14	23,30,33,38	0
2	HEM	D	500	43/43	0.96	0.13	15,25,38,42	0
2	HEM	B	500	43/43	0.96	0.15	23,32,37,41	0
3	IMD	A	501	5/5	0.97	0.10	20,20,21,21	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.

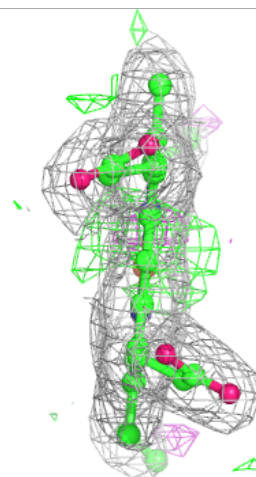
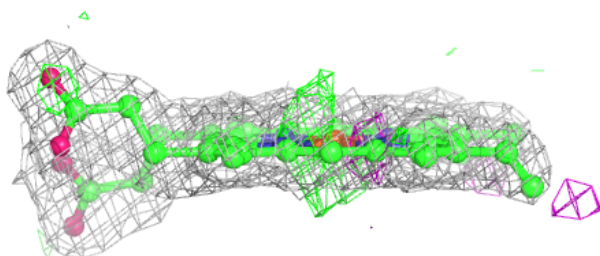
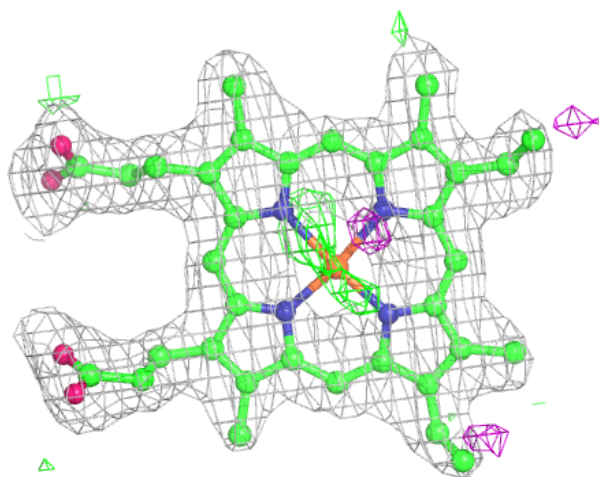
**Electron density around HEM A 500:**

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



**Electron density around HEM C 500:**

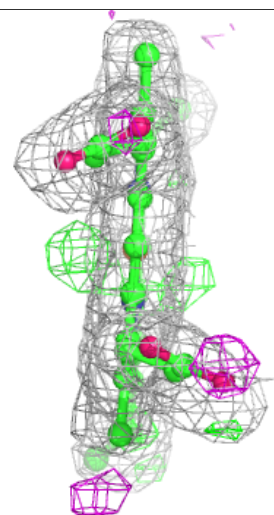
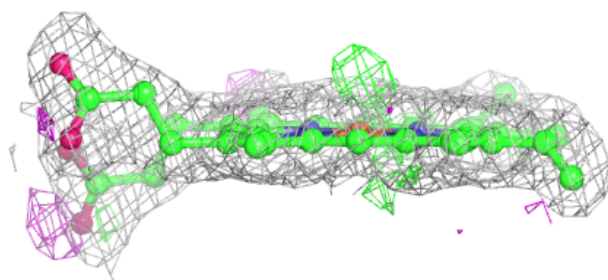
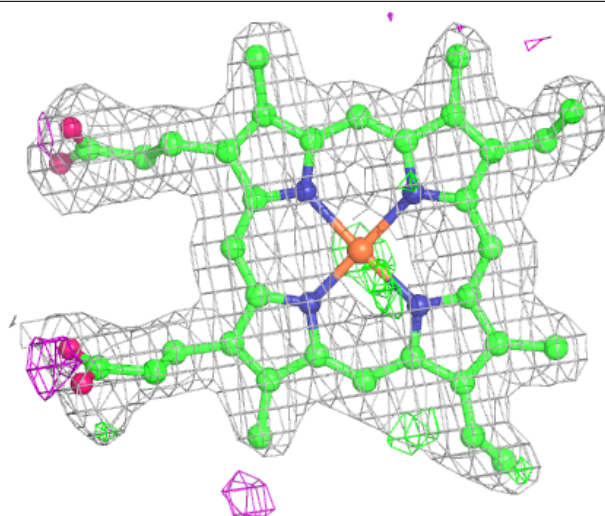
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





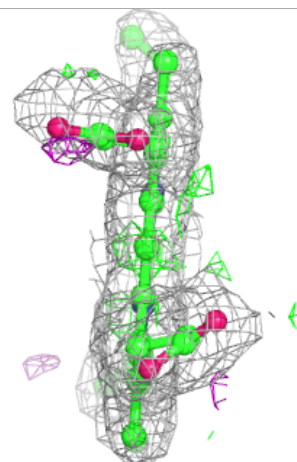
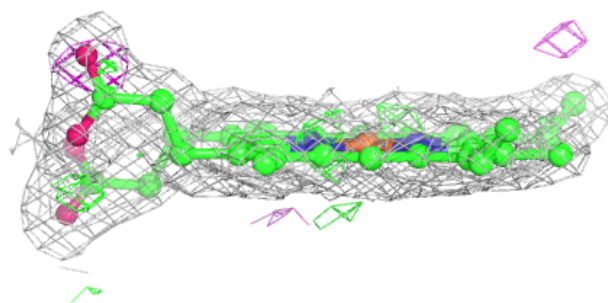
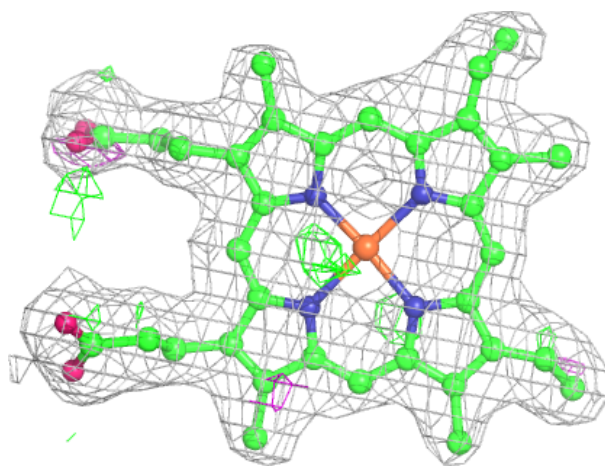
**Electron density around HEM D 500:**

$2mF_o-DF_c$  (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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.