



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:51 am BST

PDB ID : 3T3Q  
Title : Human Cytochrome P450 2A6 I208S/I300F/G301A/S369G in complex with  
Pilocarpine  
Authors : DeVore, N.M.; Scott, E.E.  
Deposited on : 2011-07-25  
Resolution : 2.10 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

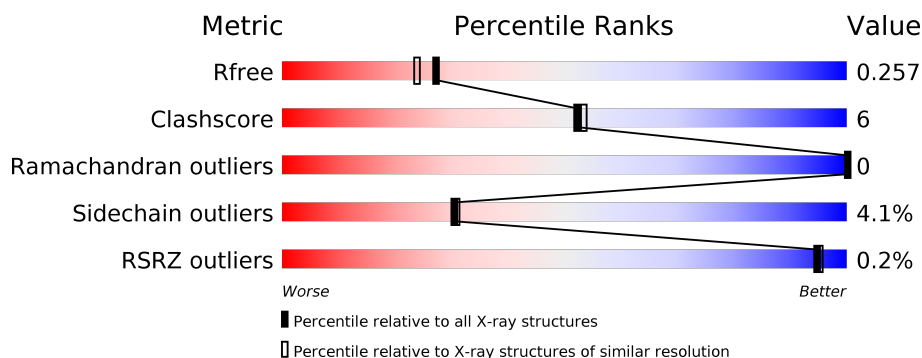
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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>82%</div> <div>14%</div> <div>••</div> </div>
1	B	476	<div> <div>87%</div> <div>10%</div> <div>••</div> </div>
1	C	476	<div> <div>86%</div> <div>11%</div> <div>••</div> </div>
1	D	476	<div> <div>87%</div> <div>9%</div> <div>••</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15809 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	463	Total	C	N	O	S	0	4	0
			3786	2428	660	680	18			
1	B	463	Total	C	N	O	S	0	1	0
			3758	2412	651	677	18			
1	C	463	Total	C	N	O	S	0	3	0
			3771	2420	654	679	18			
1	D	463	Total	C	N	O	S	0	1	0
			3758	2412	651	677	18			

There are 60 discrepancies between the modelled and reference sequences:

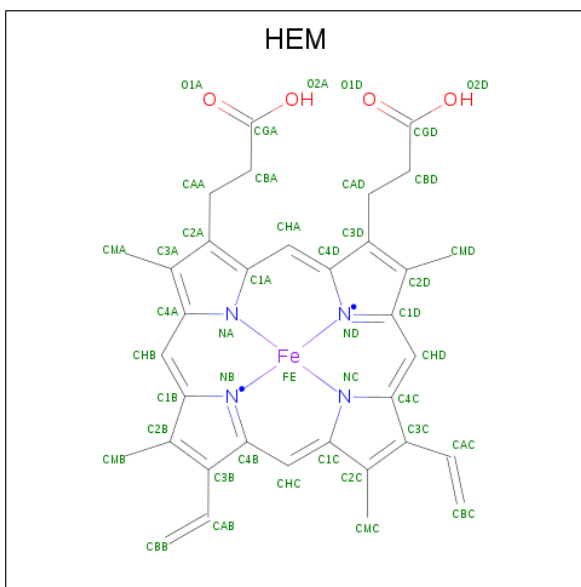
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	EXPRESSION TAG	UNP P11509
A	24	ALA	-	EXPRESSION TAG	UNP P11509
A	25	LYS	-	EXPRESSION TAG	UNP P11509
A	26	LYS	-	EXPRESSION TAG	UNP P11509
A	27	THR	-	EXPRESSION TAG	UNP P11509
A	28	SER	-	EXPRESSION TAG	UNP P11509
A	208	SER	ILE	ENGINEERED MUTATION	UNP P11509
A	300	PHE	ILE	ENGINEERED MUTATION	UNP P11509
A	301	ALA	GLY	ENGINEERED MUTATION	UNP P11509
A	369	GLY	SER	ENGINEERED MUTATION	UNP P11509
A	392	TYR	PHE	SEE REMARK 999	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	-	EXPRESSION TAG	UNP P11509
B	24	ALA	-	EXPRESSION TAG	UNP P11509
B	25	LYS	-	EXPRESSION TAG	UNP P11509
B	26	LYS	-	EXPRESSION TAG	UNP P11509
B	27	THR	-	EXPRESSION TAG	UNP P11509
B	28	SER	-	EXPRESSION TAG	UNP P11509

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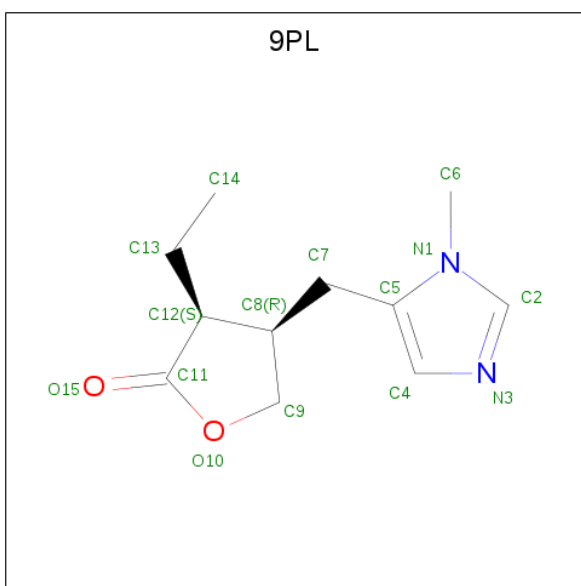
Chain	Residue	Modelled	Actual	Comment	Reference
B	208	SER	ILE	ENGINEERED MUTATION	UNP P11509
B	300	PHE	ILE	ENGINEERED MUTATION	UNP P11509
B	301	ALA	GLY	ENGINEERED MUTATION	UNP P11509
B	369	GLY	SER	ENGINEERED MUTATION	UNP P11509
B	392	TYR	PHE	SEE REMARK 999	UNP P11509
B	495	HIS	-	EXPRESSION TAG	UNP P11509
B	496	HIS	-	EXPRESSION TAG	UNP P11509
B	497	HIS	-	EXPRESSION TAG	UNP P11509
B	498	HIS	-	EXPRESSION TAG	UNP P11509
C	23	MET	-	EXPRESSION TAG	UNP P11509
C	24	ALA	-	EXPRESSION TAG	UNP P11509
C	25	LYS	-	EXPRESSION TAG	UNP P11509
C	26	LYS	-	EXPRESSION TAG	UNP P11509
C	27	THR	-	EXPRESSION TAG	UNP P11509
C	28	SER	-	EXPRESSION TAG	UNP P11509
C	208	SER	ILE	ENGINEERED MUTATION	UNP P11509
C	300	PHE	ILE	ENGINEERED MUTATION	UNP P11509
C	301	ALA	GLY	ENGINEERED MUTATION	UNP P11509
C	369	GLY	SER	ENGINEERED MUTATION	UNP P11509
C	392	TYR	PHE	SEE REMARK 999	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	-	EXPRESSION TAG	UNP P11509
D	24	ALA	-	EXPRESSION TAG	UNP P11509
D	25	LYS	-	EXPRESSION TAG	UNP P11509
D	26	LYS	-	EXPRESSION TAG	UNP P11509
D	27	THR	-	EXPRESSION TAG	UNP P11509
D	28	SER	-	EXPRESSION TAG	UNP P11509
D	208	SER	ILE	ENGINEERED MUTATION	UNP P11509
D	300	PHE	ILE	ENGINEERED MUTATION	UNP P11509
D	301	ALA	GLY	ENGINEERED MUTATION	UNP P11509
D	369	GLY	SER	ENGINEERED MUTATION	UNP P11509
D	392	TYR	PHE	SEE REMARK 999	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 PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 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 (3S,4R)-3-ethyl-4-[(1-methyl-1H-imidazol-5-yl)methyl]dihydrofuran-2(3H)-one (three-letter code: 9PL) (formula:  $C_{11}H_{16}N_2O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	11	2	2		
3	B	1	Total	C	N	O	0	0
			15	11	2	2		
3	C	1	Total	C	N	O	0	0
			15	11	2	2		
3	D	1	Total	C	N	O	0	0
			15	11	2	2		

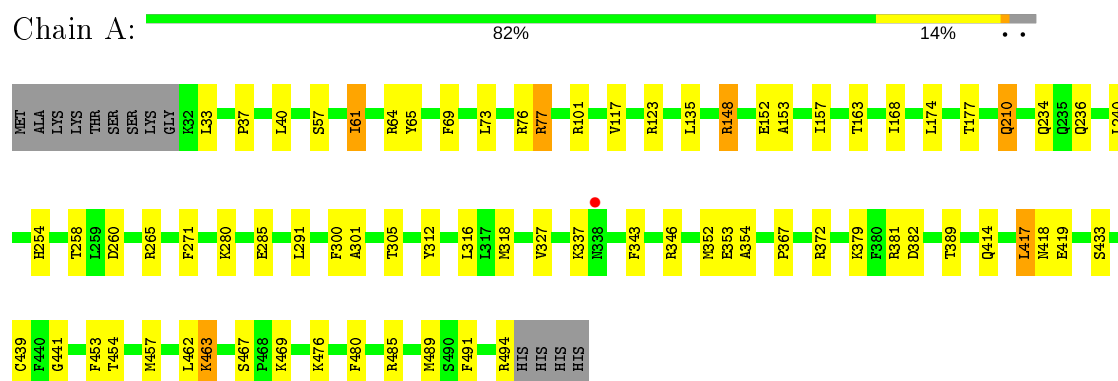
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	142	Total	O	0	0
			142	142		
4	B	139	Total	O	0	0
			139	139		
4	C	106	Total	O	0	0
			106	106		
4	D	117	Total	O	0	0
			117	117		

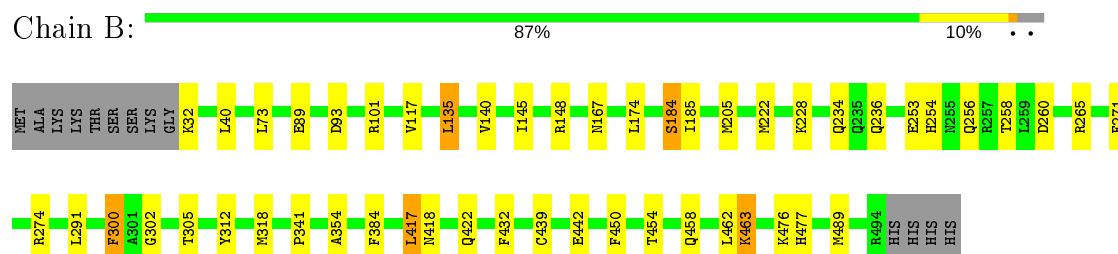
### 3 Residue-property plots [i](#)

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.

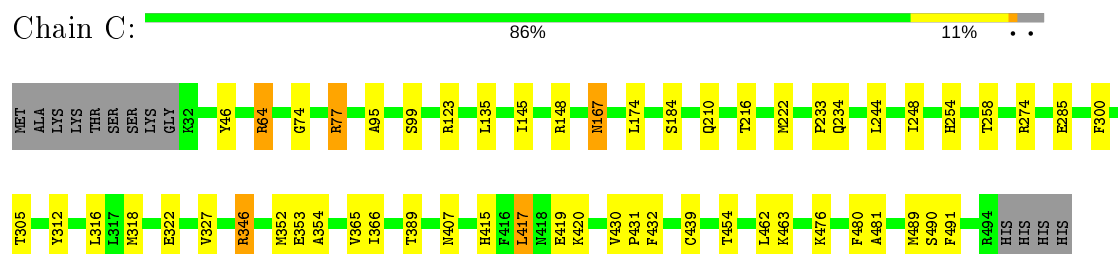
#### • Molecule 1: Cytochrome P450 2A6



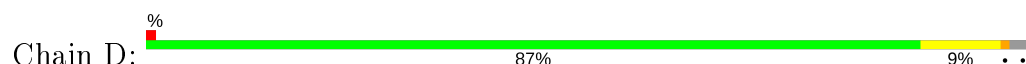
#### • Molecule 1: Cytochrome P450 2A6

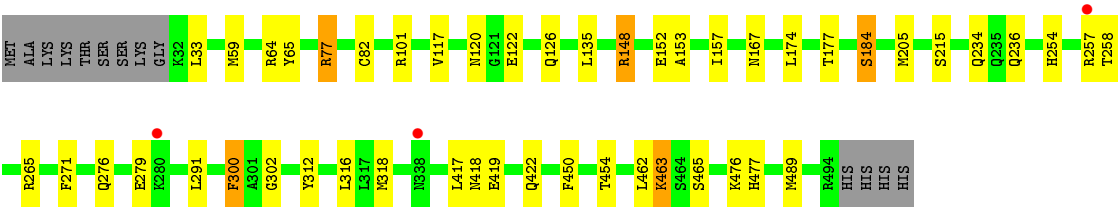


#### • Molecule 1: Cytochrome P450 2A6



#### • 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, $\alpha$ , $\beta$ , $\gamma$	70.95Å 159.84Å 103.86Å 90.00° 91.79° 90.00°	Depositor
Resolution (Å)	63.32 – 2.10 63.32 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.2 (63.32-2.10) 94.2 (63.32-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.211 , 0.257 0.212 , 0.257	Depositor DCC
$R_{free}$ test set	6402 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.8	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 38.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15809	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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, 9PL

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	0/3881	0.58	0/5225
1	B	0.46	0/3850	0.56	0/5185
1	C	0.46	0/3869	0.56	0/5210
1	D	0.46	0/3850	0.59	0/5185
All	All	0.46	0/15450	0.57	0/20805

There are no bond length outliers.

There are no bond angle outliers.

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	3786	0	3767	47	0
1	B	3758	0	3735	35	0
1	C	3771	0	3752	43	0
1	D	3758	0	3735	41	0
2	A	43	0	30	6	0
2	B	43	0	30	2	0
2	C	43	0	30	2	0
2	D	43	0	30	2	0
3	A	15	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	15	0	16	0	0
3	C	15	0	16	2	0
3	D	15	0	16	1	0
4	A	142	0	0	1	0
4	B	139	0	0	0	0
4	C	106	0	0	1	0
4	D	117	0	0	0	0
All	All	15809	0	15173	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 6.

All (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:A:77[A]:ARG:HG2	1:A:77[A]:ARG:HH11	1.01	1.11
1:C:77[A]:ARG:HG2	1:C:77[A]:ARG:HH11	1.05	1.08
1:C:318:MET:HE1	1:C:489:MET:HB2	1.38	1.01
1:B:318:MET:HE1	1:B:489:MET:HB2	1.44	0.96
1:A:318:MET:HE1	1:A:489:MET:HB2	1.52	0.92
1:D:318:MET:HE1	1:D:489:MET:HB2	1.49	0.92
1:C:77[A]:ARG:CG	1:C:77[A]:ARG:HH11	1.81	0.91
1:A:77[A]:ARG:HG2	1:A:77[A]:ARG:NH1	1.83	0.89
1:C:77[A]:ARG:NH1	1:C:77[A]:ARG:HG2	1.88	0.88
1:C:74:GLY:H	1:C:222:MET:HE3	1.36	0.87
1:A:77[A]:ARG:CG	1:A:77[A]:ARG:HH11	1.84	0.86
1:D:302:GLY:HA2	2:D:500:HEM:HMC2	1.58	0.86
1:A:61:ILE:HD11	1:A:69:PHE:CD1	2.11	0.84
1:A:318:MET:HE3	1:A:462:LEU:HB3	1.61	0.83
1:B:318:MET:HE3	1:B:462:LEU:HB3	1.62	0.81
1:D:101:ARG:H	1:D:120:ASN:HD21	1.30	0.80
1:D:318:MET:HE3	1:D:489:MET:HE3	1.64	0.78
1:C:74:GLY:N	1:C:222:MET:HE3	1.98	0.77
1:B:32:LYS:HB3	1:B:384:PHE:HB3	1.67	0.76
1:D:318:MET:HE3	1:D:462:LEU:HB3	1.68	0.75
2:C:500:HEM:HBB2	2:C:500:HEM:HMB2	1.69	0.74
1:C:64:ARG:CG	1:C:64:ARG:HH11	2.01	0.74
1:D:101:ARG:H	1:D:120:ASN:ND2	1.85	0.74
1:D:318:MET:HE3	1:D:489:MET:CE	2.19	0.72
1:D:77:ARG:HG2	1:D:77:ARG:HH11	1.54	0.71
2:A:500:HEM:HBB2	2:A:500:HEM:HMB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:MET:HE3	1:C:489:MET:HE3	1.78	0.66
1:D:276:GLN:HA	1:D:279:GLU:HG2	1.78	0.66
1:D:148:ARG:HH11	1:D:184:SER:HB3	1.59	0.66
1:C:352:MET:HE3	1:C:454:THR:HG22	1.78	0.65
1:C:254:HIS:O	1:C:258:THR:HG22	1.96	0.65
1:C:407:ASN:H	1:C:415:HIS:HE1	1.46	0.63
1:A:33:LEU:HD21	1:A:77[A]:ARG:HD2	1.79	0.63
1:C:318:MET:HE3	1:C:489:MET:CE	2.27	0.63
1:B:318:MET:HE3	1:B:489:MET:HE3	1.81	0.62
1:D:318:MET:CE	1:D:489:MET:CE	2.78	0.61
1:A:352:MET:HE3	1:A:454:THR:HG22	1.81	0.61
1:B:318:MET:CE	1:B:462:LEU:HB3	2.31	0.61
1:C:77[A]:ARG:NH1	1:C:77[A]:ARG:CG	2.51	0.60
1:A:258:THR:HG23	1:A:265:ARG:HH22	1.66	0.60
1:A:77[A]:ARG:HH12	1:A:389:THR:HG23	1.67	0.60
1:D:77:ARG:CG	1:D:77:ARG:HH11	2.14	0.60
1:A:318:MET:CE	1:A:462:LEU:HB3	2.32	0.60
1:C:77[A]:ARG:HH12	1:C:389:THR:HG23	1.67	0.59
1:A:254:HIS:O	1:A:258:THR:HG22	2.02	0.58
1:D:302:GLY:HA2	2:D:500:HEM:CMC	2.29	0.58
1:A:343:PHE:O	1:A:346:ARG:HB2	2.04	0.57
1:C:327:VAL:HG13	1:C:352:MET:HE2	1.86	0.57
1:D:254:HIS:O	1:D:258:THR:HG22	2.04	0.57
1:B:167:ASN:HB2	1:C:167:ASN:HB3	1.87	0.55
1:D:148:ARG:NH1	1:D:184:SER:HB3	2.20	0.55
1:D:101:ARG:N	1:D:120:ASN:HD21	2.03	0.55
1:B:253:GLU:HA	1:B:256:GLN:HE21	1.71	0.55
1:D:318:MET:CE	1:D:462:LEU:HB3	2.37	0.55
1:C:327:VAL:HG13	1:C:352:MET:CE	2.37	0.54
2:C:500:HEM:HBB2	2:C:500:HEM:CMB	2.37	0.54
1:D:450:PHE:O	1:D:454:THR:HG23	2.08	0.54
1:A:271:PHE:HB3	1:A:291:LEU:HD13	1.89	0.54
1:C:489:MET:HE1	1:C:491:PHE:CZ	2.42	0.54
1:C:148[A]:ARG:HD3	1:C:184:SER:CB	2.39	0.53
1:D:64[A]:ARG:HD3	1:D:65:TYR:CE2	2.44	0.53
1:D:318:MET:CE	1:D:489:MET:HE3	2.35	0.53
1:D:476:LYS:HD2	1:D:477:HIS:NE2	2.24	0.53
1:C:95:ALA:O	1:C:99:SER:HB3	2.08	0.53
1:B:101:ARG:CD	1:B:117:VAL:O	2.56	0.53
1:B:89:GLU:O	1:B:93:ASP:HB2	2.09	0.53
1:A:163:THR:HG21	1:A:168:ILE:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:CYS:HB2	2:A:500:HEM:NA	2.24	0.52
1:A:148[B]:ARG:NH1	1:A:152:GLU:OE2	2.41	0.52
1:C:476:LYS:HD3	4:C:519:HOH:O	2.10	0.52
1:A:61:ILE:HD11	1:A:69:PHE:CE1	2.44	0.52
1:D:318:MET:CE	1:D:489:MET:HE2	2.39	0.52
1:B:354:ALA:HB2	1:B:417:LEU:HD13	1.91	0.52
1:A:37:PRO:HD3	1:A:61:ILE:HD13	1.90	0.52
1:B:148[A]:ARG:HH11	1:B:184:SER:HB3	1.75	0.52
1:B:318:MET:HE3	1:B:489:MET:CE	2.40	0.52
1:C:64:ARG:HG2	1:C:64:ARG:HH11	1.71	0.52
2:B:500:HEM:HBB2	2:B:500:HEM:HMB1	1.92	0.52
1:A:433:SER:HB3	2:A:500:HEM:HBA1	1.92	0.51
1:A:77[A]:ARG:NH1	1:A:389:THR:HG23	2.24	0.51
1:A:318:MET:HE3	1:A:489:MET:HE3	1.93	0.51
1:B:450:PHE:O	1:B:454:THR:HG23	2.11	0.51
1:C:244:LEU:O	1:C:248:ILE:HG12	2.10	0.51
1:C:346:ARG:HG3	1:C:353:GLU:OE1	2.10	0.51
1:D:476:LYS:HD2	1:D:477:HIS:CD2	2.46	0.50
1:A:489:MET:HE1	1:A:491:PHE:CZ	2.46	0.50
1:B:258:THR:HG23	1:B:265:ARG:HH12	1.77	0.49
1:B:32:LYS:HB3	1:B:384:PHE:CB	2.41	0.49
1:C:64:ARG:HG3	1:C:64:ARG:HH11	1.73	0.49
1:D:148:ARG:HD2	1:D:184:SER:CB	2.42	0.49
1:B:271:PHE:HB3	1:B:291:LEU:HD13	1.95	0.49
1:A:367:PRO:HD2	1:A:480:PHE:O	2.13	0.49
1:C:46:TYR:HB2	1:C:222:MET:CE	2.42	0.49
1:C:123:ARG:HA	1:C:285:GLU:HG3	1.95	0.48
1:D:101:ARG:CD	1:D:117:VAL:O	2.62	0.48
1:C:463:LYS:HB3	1:C:490:SER:HB2	1.94	0.48
1:D:122:GLU:OE1	1:D:126:GLN:NE2	2.47	0.48
1:C:216:THR:HG21	1:C:233:PRO:HG2	1.95	0.47
1:D:257:ARG:O	1:D:257:ARG:HG2	2.14	0.47
1:B:101:ARG:HD3	1:B:117:VAL:O	2.13	0.47
1:B:205:MET:HE2	1:B:300:PHE:HA	1.97	0.47
1:A:101:ARG:NH2	2:A:500:HEM:O2A	2.40	0.47
1:D:271:PHE:CD2	1:D:291:LEU:HB2	2.50	0.47
1:A:152:GLU:HG3	1:A:177:THR:HG23	1.97	0.46
1:D:419:GLU:H	1:D:419:GLU:CD	2.19	0.46
1:B:73:LEU:HB3	1:B:222:MET:HG2	1.97	0.46
1:B:476:LYS:HE2	1:B:477:HIS:NE2	2.31	0.46
1:C:480:PHE:HZ	3:C:501:9PL:H7A	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:489:MET:HE1	1:C:491:PHE:CE2	2.51	0.46
1:D:101:ARG:HD2	1:D:117:VAL:O	2.16	0.45
1:A:476:LYS:HB2	1:A:485:ARG:HA	1.97	0.45
1:A:381:ARG:O	1:A:382:ASP:HB2	2.17	0.45
2:A:500:HEM:CMB	2:A:500:HEM:HBB2	2.43	0.45
1:B:205:MET:CE	1:B:300:PHE:HA	2.47	0.45
1:C:318:MET:HE3	1:C:462:LEU:HB3	1.98	0.45
1:B:167:ASN:HB2	1:C:167:ASN:CB	2.47	0.45
1:C:430:VAL:N	1:C:431:PRO:CD	2.80	0.45
1:C:64:ARG:CG	1:C:64:ARG:NH1	2.69	0.45
1:A:318:MET:HE2	1:A:463:LYS:N	2.32	0.45
1:B:254:HIS:O	1:B:258:THR:HG22	2.17	0.45
1:D:117:VAL:HG11	3:D:501:9PL:H9A	1.99	0.45
1:A:236:GLN:O	1:A:240:LEU:HG	2.17	0.44
1:A:327:VAL:HG13	1:A:352:MET:CE	2.46	0.44
1:C:354:ALA:HB2	1:C:417:LEU:HD13	1.99	0.44
1:B:302:GLY:HA2	2:B:500:HEM:HMC2	2.00	0.44
1:A:453:PHE:O	1:A:457:MET:HG2	2.18	0.43
1:B:418:ASN:HB2	1:B:422:GLN:H	1.82	0.43
1:B:271:PHE:CD2	1:B:291:LEU:HB2	2.54	0.43
1:D:318:MET:HE2	1:D:463:LYS:N	2.33	0.43
1:C:74:GLY:H	1:C:222:MET:CE	2.18	0.43
1:D:77:ARG:NH1	1:D:77:ARG:HG2	2.29	0.43
1:A:123:ARG:HA	1:A:285:GLU:HG3	2.01	0.43
1:C:432:PHE:HB3	1:C:439:CYS:HB3	2.00	0.43
1:B:318:MET:CE	1:B:489:MET:CE	2.97	0.43
1:D:418:ASN:HD22	1:D:422:GLN:HB2	1.82	0.43
1:A:101:ARG:CD	1:A:117:VAL:O	2.67	0.43
1:A:57:SER:O	1:A:61:ILE:HG23	2.19	0.43
1:C:64:ARG:NH1	1:C:64:ARG:HG2	2.33	0.43
1:D:318:MET:HE1	1:D:489:MET:HE2	2.01	0.43
1:B:418:ASN:HD22	1:B:422:GLN:HB2	1.84	0.43
1:A:210:GLN:HB2	1:A:210:GLN:HE21	1.58	0.42
1:B:140:VAL:HA	1:B:145:ILE:HG21	2.00	0.42
1:A:354:ALA:HB2	1:A:417:LEU:HD13	2.01	0.42
1:D:59:MET:CE	1:D:82:CYS:SG	3.07	0.42
1:A:73:LEU:O	1:A:76:ARG:HB2	2.19	0.42
1:B:135:LEU:HD12	1:B:185:ILE:HG21	2.02	0.42
1:B:318:MET:HE2	1:B:463:LYS:N	2.35	0.42
1:C:148[A]:ARG:HD3	1:C:184:SER:HB2	2.00	0.42
1:A:101:ARG:NH2	1:A:372:ARG:HD3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:LYS:NZ	1:A:494:ARG:HB2	2.34	0.42
1:A:153:ALA:O	1:A:157:ILE:HG12	2.19	0.41
1:B:341:PRO:HD3	1:B:458:GLN:OE1	2.20	0.41
1:C:145:ILE:HD12	1:C:148[A]:ARG:HD2	2.02	0.41
1:B:432:PHE:CD2	1:B:442:GLU:HG3	2.56	0.41
1:D:205:MET:CE	1:D:300:PHE:HA	2.50	0.41
1:A:301:ALA:HB2	3:A:501:9PL:H12	2.04	0.40
1:C:365:VAL:O	1:C:481:ALA:HA	2.21	0.40
1:D:153:ALA:O	1:D:157:ILE:HG12	2.22	0.40
1:D:258:THR:HG23	1:D:265:ARG:HH12	1.86	0.40
1:A:327:VAL:HG13	1:A:352:MET:HE1	2.03	0.40
1:A:414:GLN:NE2	4:A:593:HOH:O	2.54	0.40
1:A:77[A]:ARG:CG	1:A:77[A]:ARG:NH1	2.54	0.40
1:B:432:PHE:HB3	1:B:439:CYS:HB3	2.03	0.40
1:C:366:ILE:HD11	3:C:501:9PL:H6B	2.03	0.40
1:A:441:GLY:HA3	2:A:500:HEM:C3C	2.56	0.40
1:B:148[A]:ARG:HD3	1:B:184:SER:HB3	2.04	0.40
1:D:167:ASN:HD21	1:D:465:SER:HB3	1.86	0.40
1:A:64[A]:ARG:HD3	1:A:65:TYR:CE2	2.57	0.40
1:D:152:GLU:HG3	1:D:177:THR:HG23	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	465/476 (98%)	454 (98%)	11 (2%)	0	100	100
1	B	462/476 (97%)	450 (97%)	12 (3%)	0	100	100
1	C	464/476 (98%)	450 (97%)	14 (3%)	0	100	100
1	D	462/476 (97%)	449 (97%)	13 (3%)	0	100	100
All	All	1853/1904 (97%)	1803 (97%)	50 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	414/421 (98%)	390 (94%)	24 (6%)	20	17
1	B	411/421 (98%)	397 (97%)	14 (3%)	37	39
1	C	413/421 (98%)	395 (96%)	18 (4%)	28	28
1	D	411/421 (98%)	397 (97%)	14 (3%)	37	39
All	All	1649/1684 (98%)	1579 (96%)	70 (4%)	30	30

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	61	ILE
1	A	77[A]	ARG
1	A	77[B]	ARG
1	A	135	LEU
1	A	148[A]	ARG
1	A	148[B]	ARG
1	A	174	LEU
1	A	210	GLN
1	A	234	GLN
1	A	260	ASP
1	A	280	LYS
1	A	300	PHE
1	A	305	THR
1	A	312	TYR
1	A	316	LEU
1	A	353	GLU
1	A	379	LYS
1	A	417	LEU
1	A	418	ASN
1	A	419	GLU
1	A	463	LYS

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Mol	Chain	Res	Type
1	A	467	SER
1	A	469	LYS
1	B	40	LEU
1	B	135	LEU
1	B	174	LEU
1	B	184	SER
1	B	228	LYS
1	B	234	GLN
1	B	236	GLN
1	B	260	ASP
1	B	274	ARG
1	B	300	PHE
1	B	305	THR
1	B	312	TYR
1	B	417	LEU
1	B	463	LYS
1	C	64	ARG
1	C	77[A]	ARG
1	C	77[B]	ARG
1	C	135	LEU
1	C	167	ASN
1	C	174	LEU
1	C	210	GLN
1	C	234	GLN
1	C	274	ARG
1	C	300	PHE
1	C	305	THR
1	C	312	TYR
1	C	316	LEU
1	C	322	GLU
1	C	346	ARG
1	C	417	LEU
1	C	419	GLU
1	C	420	LYS
1	D	33	LEU
1	D	77	ARG
1	D	135	LEU
1	D	148	ARG
1	D	174	LEU
1	D	184	SER
1	D	215	SER
1	D	234	GLN

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Mol	Chain	Res	Type
1	D	236	GLN
1	D	300	PHE
1	D	312	TYR
1	D	316	LEU
1	D	417	LEU
1	D	463	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	414	GLN
1	B	56	ASN
1	B	236	GLN
1	B	256	GLN
1	B	340	GLN
1	B	407	ASN
1	C	340	GLN
1	C	415	HIS
1	C	477	HIS
1	D	120	ASN
1	D	126	GLN
1	D	236	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	9PL	D	501	2	13,16,16	1.38	1 (7%)	16,22,22	1.82	3 (18%)
3	9PL	A	501	2	13,16,16	1.45	1 (7%)	16,22,22	1.94	4 (25%)
3	9PL	C	501	2	13,16,16	1.41	1 (7%)	16,22,22	1.97	4 (25%)
3	9PL	B	501	2	13,16,16	1.32	1 (7%)	16,22,22	1.86	4 (25%)
2	HEM	D	500	1,3	27,50,50	2.24	6 (22%)	17,82,82	1.66	4 (23%)
2	HEM	C	500	1,3	27,50,50	2.11	5 (18%)	17,82,82	1.89	4 (23%)
2	HEM	A	500	1,3	27,50,50	2.13	6 (22%)	17,82,82	1.47	3 (17%)
2	HEM	B	500	1,3	27,50,50	2.15	6 (22%)	17,82,82	1.56	4 (23%)

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	9PL	D	501	2	-	2/6/19/19	0/2/2/2
3	9PL	A	501	2	-	2/6/19/19	0/2/2/2
3	9PL	C	501	2	-	3/6/19/19	0/2/2/2
3	9PL	B	501	2	-	2/6/19/19	0/2/2/2
2	HEM	D	500	1,3	-	0/6/54/54	-
2	HEM	C	500	1,3	-	0/6/54/54	-
2	HEM	A	500	1,3	-	0/6/54/54	-
2	HEM	B	500	1,3	-	0/6/54/54	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C3D-C2D	5.54	1.54	1.37
2	D	500	HEM	C3D-C2D	5.44	1.53	1.37
2	B	500	HEM	C3D-C2D	5.25	1.53	1.37
2	C	500	HEM	C3D-C2D	5.21	1.53	1.37
2	D	500	HEM	C3C-C2C	-4.94	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	9PL	O10-C11	4.70	1.45	1.35
3	C	501	9PL	O10-C11	4.52	1.45	1.35
2	B	500	HEM	C3C-C2C	-4.41	1.34	1.40
3	D	501	9PL	O10-C11	4.40	1.44	1.35
2	C	500	HEM	C3B-C2B	-4.35	1.34	1.40
3	B	501	9PL	O10-C11	4.34	1.44	1.35
2	C	500	HEM	C3C-CAC	4.10	1.56	1.47
2	D	500	HEM	C3C-CAC	4.00	1.56	1.47
2	B	500	HEM	C3B-CAB	3.92	1.55	1.47
2	A	500	HEM	C3C-CAC	3.89	1.55	1.47
2	C	500	HEM	C3C-C2C	-3.81	1.35	1.40
2	A	500	HEM	C3C-C2C	-3.79	1.35	1.40
2	A	500	HEM	C3B-CAB	3.77	1.55	1.47
2	B	500	HEM	C3C-CAC	3.69	1.55	1.47
2	D	500	HEM	C3B-CAB	3.69	1.55	1.47
2	A	500	HEM	C3B-C2B	-3.64	1.35	1.40
2	B	500	HEM	C3B-C2B	-3.60	1.35	1.40
2	C	500	HEM	C3B-CAB	3.59	1.55	1.47
2	D	500	HEM	C3B-C2B	-3.54	1.35	1.40
2	B	500	HEM	CAA-C2A	2.28	1.55	1.52
2	D	500	HEM	CAA-C2A	2.17	1.55	1.52
2	A	500	HEM	CAA-C2A	2.07	1.55	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	9PL	C9-C8-C12	5.35	109.83	101.44
3	A	501	9PL	C9-C8-C12	5.29	109.74	101.44
2	C	500	HEM	CBA-CAA-C2A	-5.09	103.10	112.49
3	B	501	9PL	C9-C8-C12	5.00	109.28	101.44
3	D	501	9PL	C9-C8-C12	4.88	109.09	101.44
2	D	500	HEM	C1D-C2D-C3D	-3.54	104.53	107.00
3	A	501	9PL	O15-C11-C12	-3.09	124.56	128.83
3	D	501	9PL	O15-C11-C12	-2.78	124.99	128.83
2	B	500	HEM	CBA-CAA-C2A	-2.70	107.50	112.49
2	A	500	HEM	CBA-CAA-C2A	-2.70	107.51	112.49
2	C	500	HEM	CMA-C3A-C4A	-2.64	124.40	128.46
3	C	501	9PL	C5-C7-C8	-2.63	108.35	114.25
2	C	500	HEM	CAD-CBD-CGD	-2.59	108.33	112.67
3	B	501	9PL	O15-C11-C12	-2.55	125.30	128.83
2	D	500	HEM	CMA-C3A-C4A	-2.54	124.56	128.46
2	D	500	HEM	CBA-CAA-C2A	-2.53	107.81	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	HEM	CAD-CBD-CGD	-2.41	108.62	112.67
3	A	501	9PL	N3-C2-N1	-2.38	108.72	112.26
3	D	501	9PL	N3-C2-N1	-2.32	108.81	112.26
3	C	501	9PL	N3-C2-N1	-2.30	108.84	112.26
2	C	500	HEM	CMB-C2B-C3B	2.27	128.93	124.68
2	B	500	HEM	CMA-C3A-C4A	-2.26	125.00	128.46
3	A	501	9PL	O10-C11-O15	2.25	123.75	121.42
2	A	500	HEM	C1D-C2D-C3D	-2.23	105.44	107.00
3	C	501	9PL	O15-C11-C12	-2.21	125.78	128.83
3	B	501	9PL	N3-C2-N1	-2.20	108.99	112.26
2	A	500	HEM	CMB-C2B-C3B	2.15	128.70	124.68
2	D	500	HEM	CMD-C2D-C3D	2.08	128.87	124.94
2	B	500	HEM	C1D-C2D-C3D	-2.07	105.55	107.00
3	B	501	9PL	C5-C7-C8	-2.07	109.62	114.25

There are no chirality outliers.

All (9) torsion outliers are listed below:

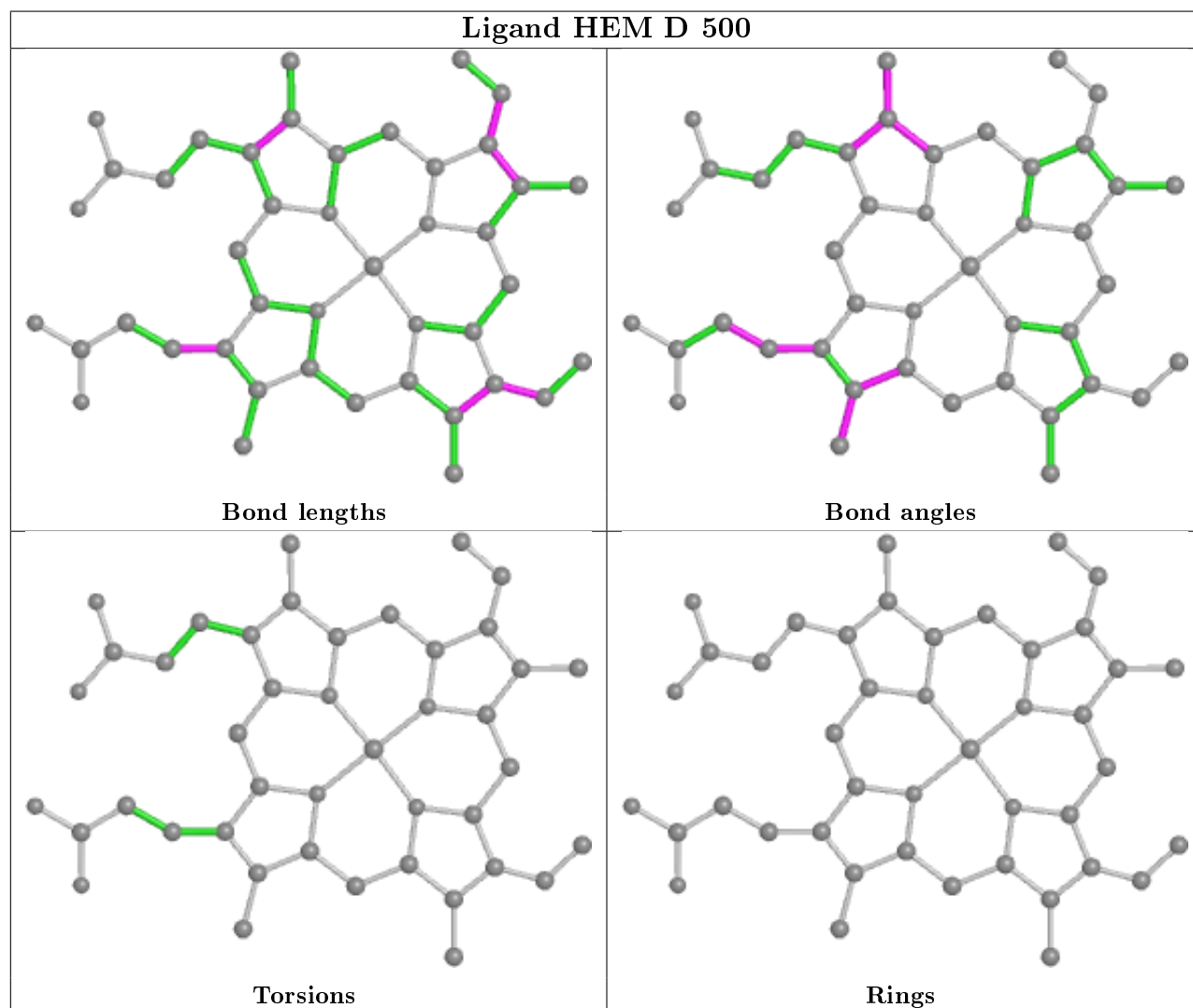
Mol	Chain	Res	Type	Atoms
3	A	501	9PL	C11-C12-C13-C14
3	D	501	9PL	C11-C12-C13-C14
3	B	501	9PL	C11-C12-C13-C14
3	C	501	9PL	C5-C7-C8-C9
3	B	501	9PL	C5-C7-C8-C9
3	D	501	9PL	N1-C5-C7-C8
3	A	501	9PL	N1-C5-C7-C8
3	C	501	9PL	N1-C5-C7-C8
3	C	501	9PL	C11-C12-C13-C14

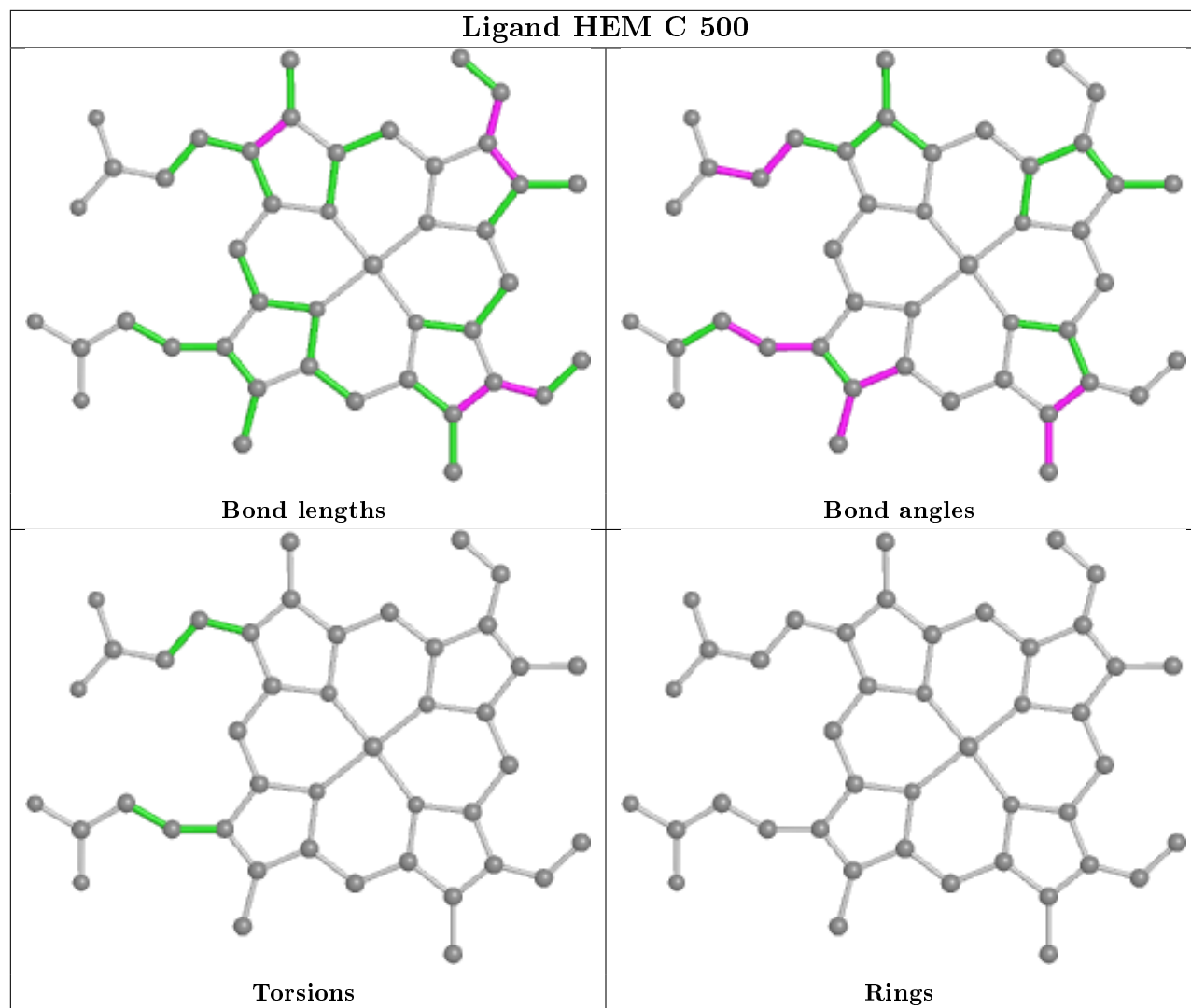
There are no ring outliers.

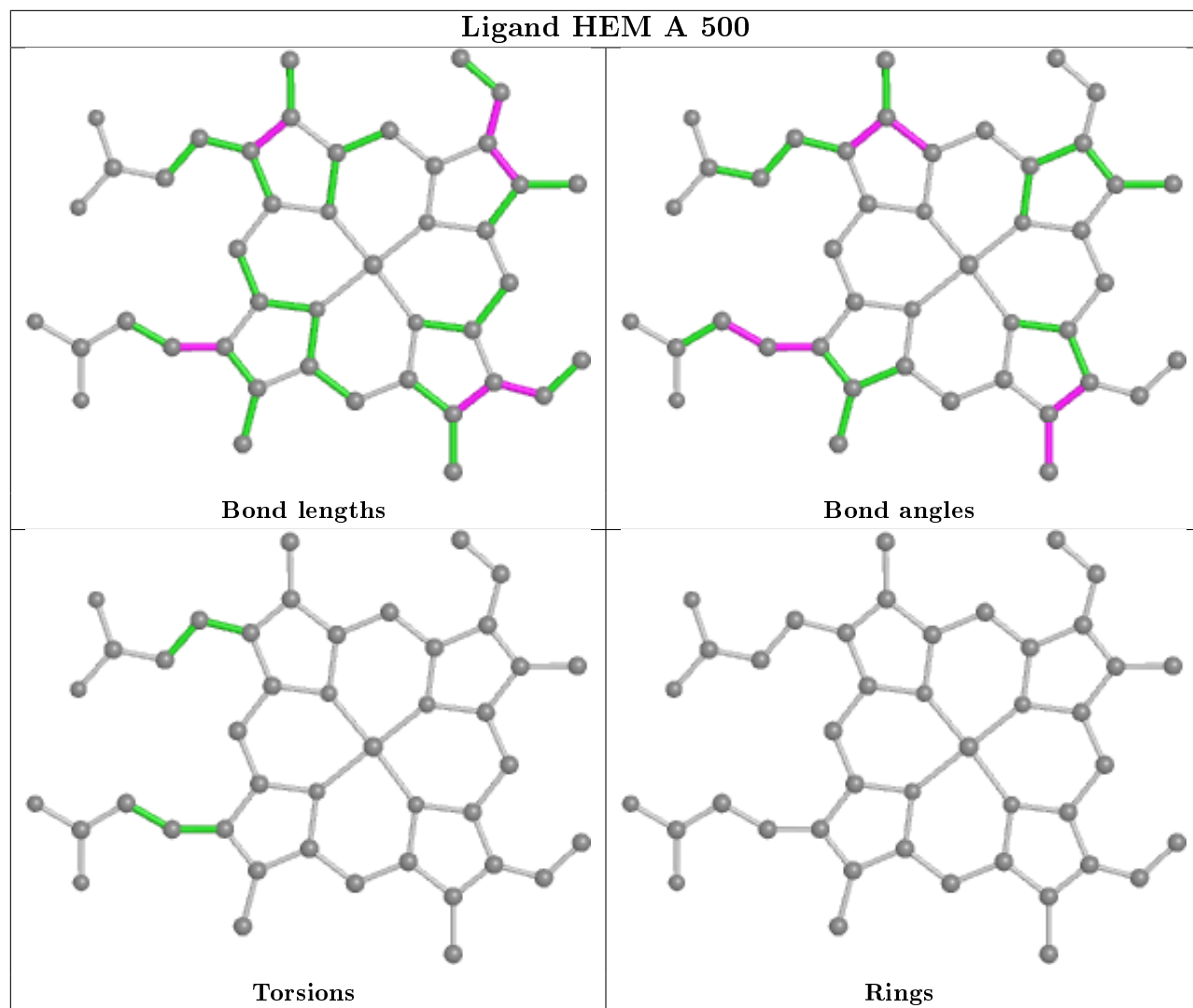
7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	9PL	1	0
3	A	501	9PL	1	0
3	C	501	9PL	2	0
2	D	500	HEM	2	0
2	C	500	HEM	2	0
2	A	500	HEM	6	0
2	B	500	HEM	2	0

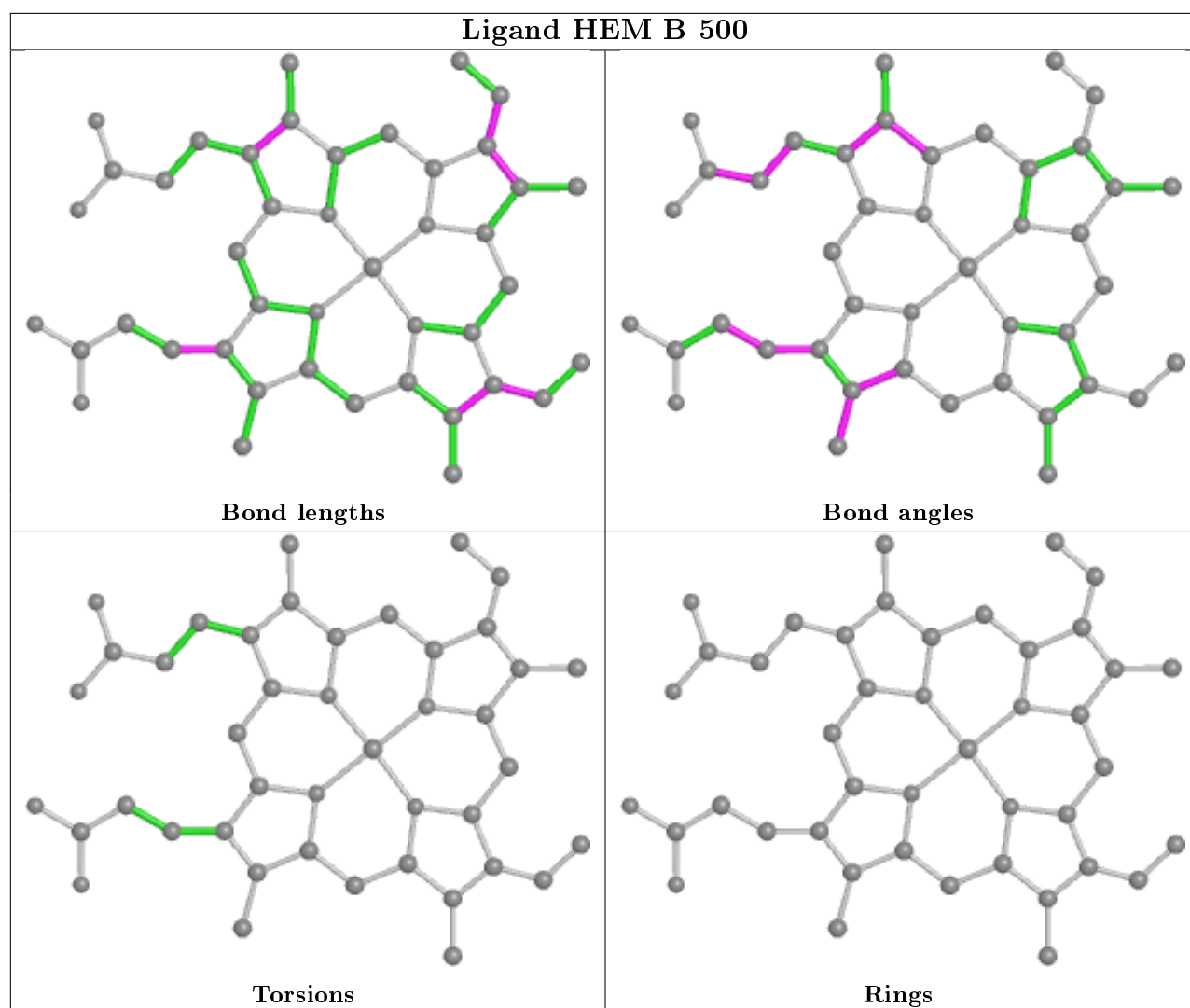
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	463/476 (97%)	-0.19	1 (0%) 95 95	21, 30, 43, 50	0
1	B	463/476 (97%)	-0.18	0 100 100	20, 30, 43, 50	0
1	C	463/476 (97%)	-0.16	0 100 100	20, 31, 44, 51	0
1	D	463/476 (97%)	-0.17	3 (0%) 89 91	21, 30, 44, 55	0
All	All	1852/1904 (97%)	-0.18	4 (0%) 95 95	20, 30, 44, 55	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	280	LYS	5.5
1	D	338	ASN	2.7
1	A	338	ASN	2.3
1	D	257	ARG	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 [i](#)

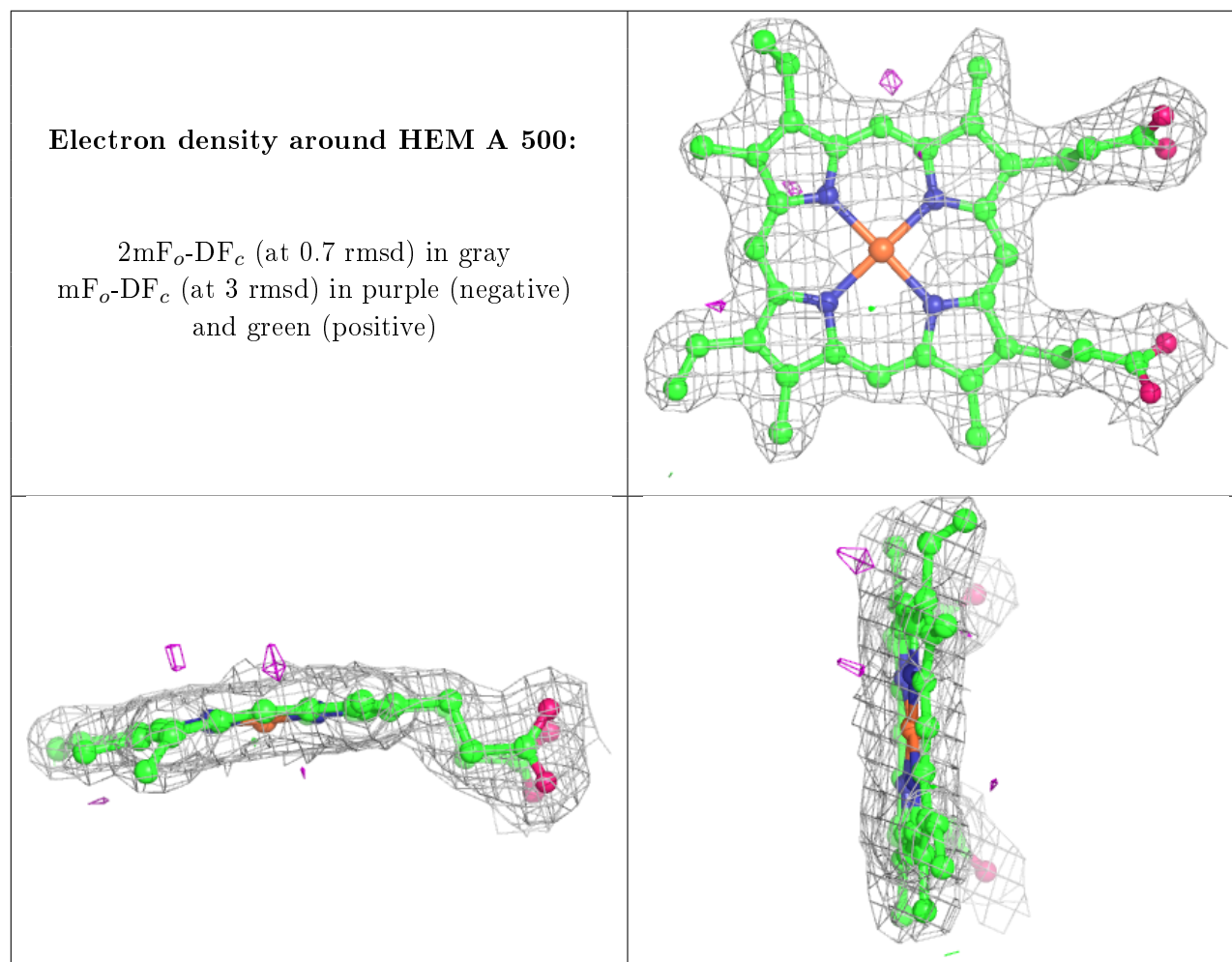
There are no carbohydrates in this entry.

### 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.

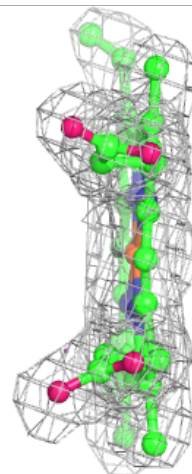
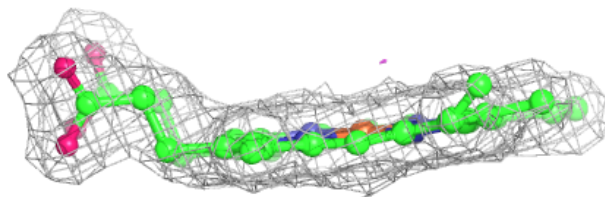
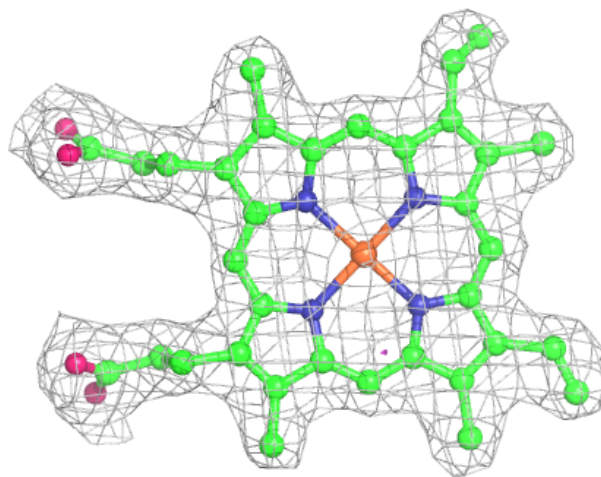
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	9PL	C	501	15/15	0.93	0.15	31,34,37,37	0
3	9PL	A	501	15/15	0.94	0.16	35,38,39,39	0
3	9PL	B	501	15/15	0.94	0.16	40,41,42,42	0
3	9PL	D	501	15/15	0.95	0.15	40,41,42,42	0
2	HEM	A	500	43/43	0.97	0.11	19,25,27,29	0
2	HEM	C	500	43/43	0.98	0.12	16,20,24,27	0
2	HEM	D	500	43/43	0.98	0.11	18,23,25,27	0
2	HEM	B	500	43/43	0.98	0.11	20,23,26,26	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.



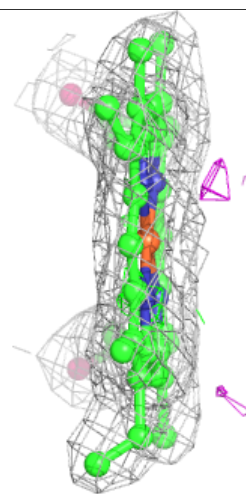
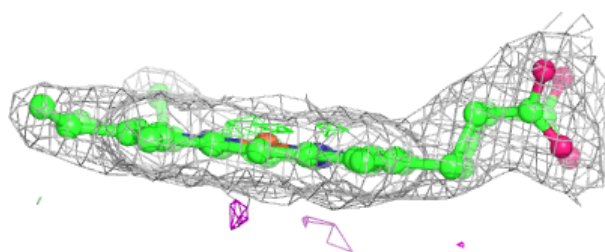
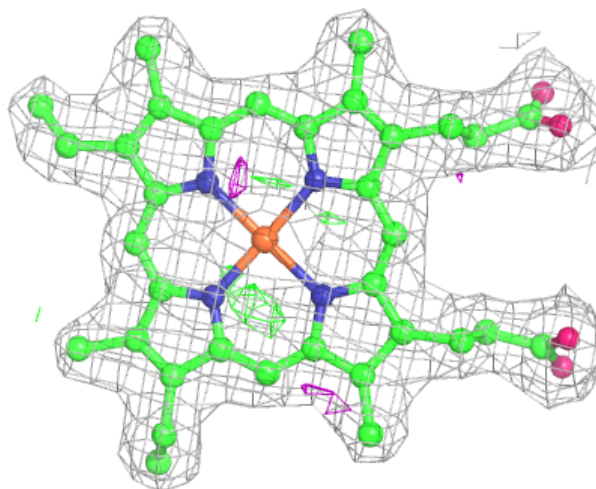
**Electron density around HEM C 500:**

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



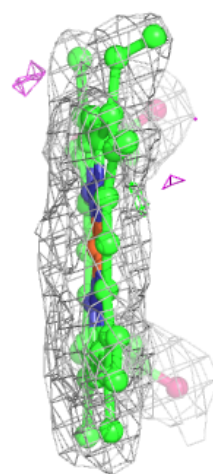
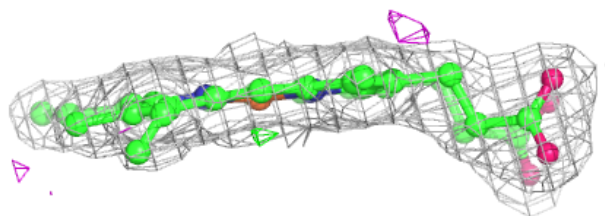
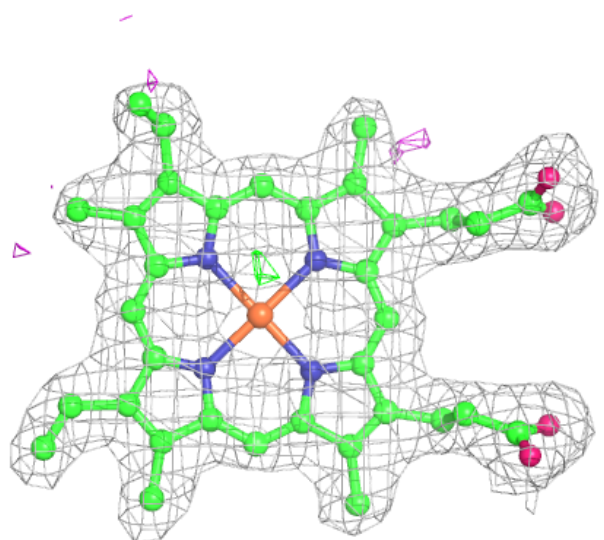
**Electron density around HEM D 500:**

$2mF_o-DF_c$  (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.