



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 09:06 AM BST

PDB ID : 4EJH  
Title : Human Cytochrome P450 2A13 in complex with 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone (NNK)  
Authors : DeVore, N.M.; Scott, E.E.  
Deposited on : 2012-04-06  
Resolution : 2.35 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 : 2.13.1  
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) : 2.13.1

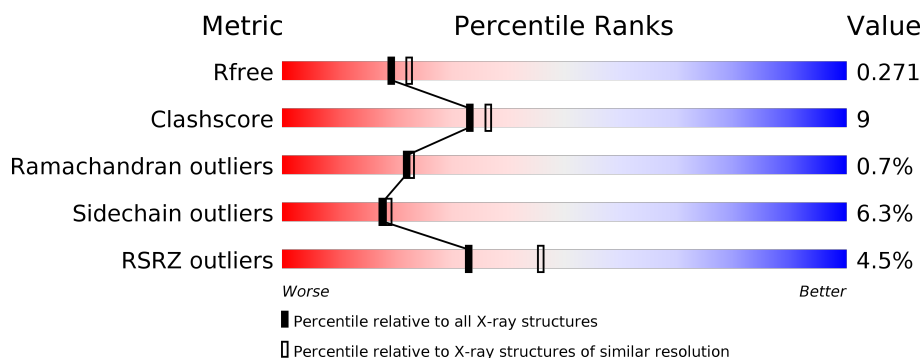
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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>13%</div> <div>• •</div> </div>
1	B	476	<div> <div>79%</div> <div>17%</div> <div>• •</div> </div>
1	C	476	<div> <div>82%</div> <div>14%</div> <div>• •</div> </div>
1	D	476	<div> <div>81%</div> <div>15%</div> <div>• •</div> </div>
1	E	476	<div> <div>2%</div> <div>76%</div> <div>20%</div> <div>• •</div> </div>
1	F	476	<div> <div>7%</div> <div>71%</div> <div>24%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	476	
1	H	476	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	0QA	F	502	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30804 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 2A13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	8	2	0
			3777	2430	653	676	18			
1	B	464	Total	C	N	O	S	0	1	0
			3771	2426	653	674	18			
1	C	464	Total	C	N	O	S	0	2	0
			3776	2429	653	676	18			
1	D	464	Total	C	N	O	S	0	1	0
			3771	2426	653	674	18			
1	E	464	Total	C	N	O	S	0	1	0
			3771	2426	653	674	18			
1	F	464	Total	C	N	O	S	0	1	0
			3771	2426	653	674	18			
1	G	463	Total	C	N	O	S	0	0	0
			3737	2404	642	673	18			
1	H	459	Total	C	N	O	S	0	1	0
			3723	2396	640	669	18			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	INITIATING METHIONINE	UNP Q16696
A	24	ALA	-	EXPRESSION TAG	UNP Q16696
A	25	LYS	-	EXPRESSION TAG	UNP Q16696
A	26	LYS	-	EXPRESSION TAG	UNP Q16696
A	27	THR	-	EXPRESSION TAG	UNP Q16696
A	28	SER	-	EXPRESSION TAG	UNP Q16696
A	29	SER	-	EXPRESSION TAG	UNP Q16696
A	30	LYS	-	EXPRESSION TAG	UNP Q16696
A	495	HIS	-	EXPRESSION TAG	UNP Q16696
A	496	HIS	-	EXPRESSION TAG	UNP Q16696
A	497	HIS	-	EXPRESSION TAG	UNP Q16696
A	498	HIS	-	EXPRESSION TAG	UNP Q16696
B	23	MET	-	INITIATING METHIONINE	UNP Q16696

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Chain	Residue	Modelled	Actual	Comment	Reference
B	24	ALA	-	EXPRESSION TAG	UNP Q16696
B	25	LYS	-	EXPRESSION TAG	UNP Q16696
B	26	LYS	-	EXPRESSION TAG	UNP Q16696
B	27	THR	-	EXPRESSION TAG	UNP Q16696
B	28	SER	-	EXPRESSION TAG	UNP Q16696
B	29	SER	-	EXPRESSION TAG	UNP Q16696
B	30	LYS	-	EXPRESSION TAG	UNP Q16696
B	495	HIS	-	EXPRESSION TAG	UNP Q16696
B	496	HIS	-	EXPRESSION TAG	UNP Q16696
B	497	HIS	-	EXPRESSION TAG	UNP Q16696
B	498	HIS	-	EXPRESSION TAG	UNP Q16696
C	23	MET	-	INITIATING METHIONINE	UNP Q16696
C	24	ALA	-	EXPRESSION TAG	UNP Q16696
C	25	LYS	-	EXPRESSION TAG	UNP Q16696
C	26	LYS	-	EXPRESSION TAG	UNP Q16696
C	27	THR	-	EXPRESSION TAG	UNP Q16696
C	28	SER	-	EXPRESSION TAG	UNP Q16696
C	29	SER	-	EXPRESSION TAG	UNP Q16696
C	30	LYS	-	EXPRESSION TAG	UNP Q16696
C	495	HIS	-	EXPRESSION TAG	UNP Q16696
C	496	HIS	-	EXPRESSION TAG	UNP Q16696
C	497	HIS	-	EXPRESSION TAG	UNP Q16696
C	498	HIS	-	EXPRESSION TAG	UNP Q16696
D	23	MET	-	INITIATING METHIONINE	UNP Q16696
D	24	ALA	-	EXPRESSION TAG	UNP Q16696
D	25	LYS	-	EXPRESSION TAG	UNP Q16696
D	26	LYS	-	EXPRESSION TAG	UNP Q16696
D	27	THR	-	EXPRESSION TAG	UNP Q16696
D	28	SER	-	EXPRESSION TAG	UNP Q16696
D	29	SER	-	EXPRESSION TAG	UNP Q16696
D	30	LYS	-	EXPRESSION TAG	UNP Q16696
D	495	HIS	-	EXPRESSION TAG	UNP Q16696
D	496	HIS	-	EXPRESSION TAG	UNP Q16696
D	497	HIS	-	EXPRESSION TAG	UNP Q16696
D	498	HIS	-	EXPRESSION TAG	UNP Q16696
E	23	MET	-	INITIATING METHIONINE	UNP Q16696
E	24	ALA	-	EXPRESSION TAG	UNP Q16696
E	25	LYS	-	EXPRESSION TAG	UNP Q16696
E	26	LYS	-	EXPRESSION TAG	UNP Q16696
E	27	THR	-	EXPRESSION TAG	UNP Q16696
E	28	SER	-	EXPRESSION TAG	UNP Q16696
E	29	SER	-	EXPRESSION TAG	UNP Q16696

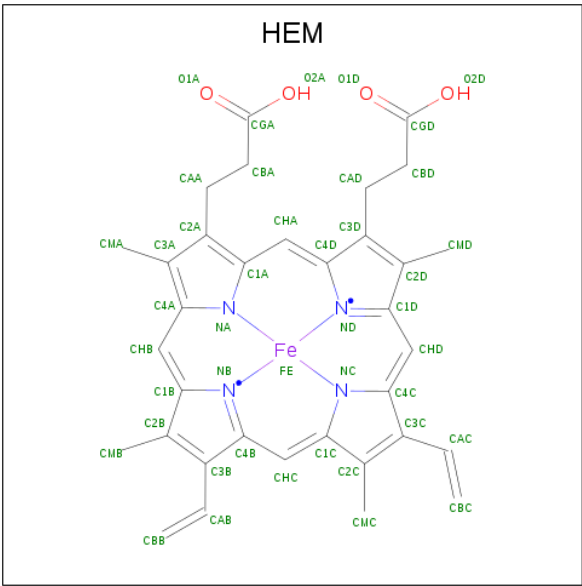
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Chain	Residue	Modelled	Actual	Comment	Reference
E	30	LYS	-	EXPRESSION TAG	UNP Q16696
E	495	HIS	-	EXPRESSION TAG	UNP Q16696
E	496	HIS	-	EXPRESSION TAG	UNP Q16696
E	497	HIS	-	EXPRESSION TAG	UNP Q16696
E	498	HIS	-	EXPRESSION TAG	UNP Q16696
F	23	MET	-	INITIATING METHIONINE	UNP Q16696
F	24	ALA	-	EXPRESSION TAG	UNP Q16696
F	25	LYS	-	EXPRESSION TAG	UNP Q16696
F	26	LYS	-	EXPRESSION TAG	UNP Q16696
F	27	THR	-	EXPRESSION TAG	UNP Q16696
F	28	SER	-	EXPRESSION TAG	UNP Q16696
F	29	SER	-	EXPRESSION TAG	UNP Q16696
F	30	LYS	-	EXPRESSION TAG	UNP Q16696
F	495	HIS	-	EXPRESSION TAG	UNP Q16696
F	496	HIS	-	EXPRESSION TAG	UNP Q16696
F	497	HIS	-	EXPRESSION TAG	UNP Q16696
F	498	HIS	-	EXPRESSION TAG	UNP Q16696
G	23	MET	-	INITIATING METHIONINE	UNP Q16696
G	24	ALA	-	EXPRESSION TAG	UNP Q16696
G	25	LYS	-	EXPRESSION TAG	UNP Q16696
G	26	LYS	-	EXPRESSION TAG	UNP Q16696
G	27	THR	-	EXPRESSION TAG	UNP Q16696
G	28	SER	-	EXPRESSION TAG	UNP Q16696
G	29	SER	-	EXPRESSION TAG	UNP Q16696
G	30	LYS	-	EXPRESSION TAG	UNP Q16696
G	495	HIS	-	EXPRESSION TAG	UNP Q16696
G	496	HIS	-	EXPRESSION TAG	UNP Q16696
G	497	HIS	-	EXPRESSION TAG	UNP Q16696
G	498	HIS	-	EXPRESSION TAG	UNP Q16696
H	23	MET	-	INITIATING METHIONINE	UNP Q16696
H	24	ALA	-	EXPRESSION TAG	UNP Q16696
H	25	LYS	-	EXPRESSION TAG	UNP Q16696
H	26	LYS	-	EXPRESSION TAG	UNP Q16696
H	27	THR	-	EXPRESSION TAG	UNP Q16696
H	28	SER	-	EXPRESSION TAG	UNP Q16696
H	29	SER	-	EXPRESSION TAG	UNP Q16696
H	30	LYS	-	EXPRESSION TAG	UNP Q16696
H	495	HIS	-	EXPRESSION TAG	UNP Q16696
H	496	HIS	-	EXPRESSION TAG	UNP Q16696
H	497	HIS	-	EXPRESSION TAG	UNP Q16696
H	498	HIS	-	EXPRESSION TAG	UNP Q16696

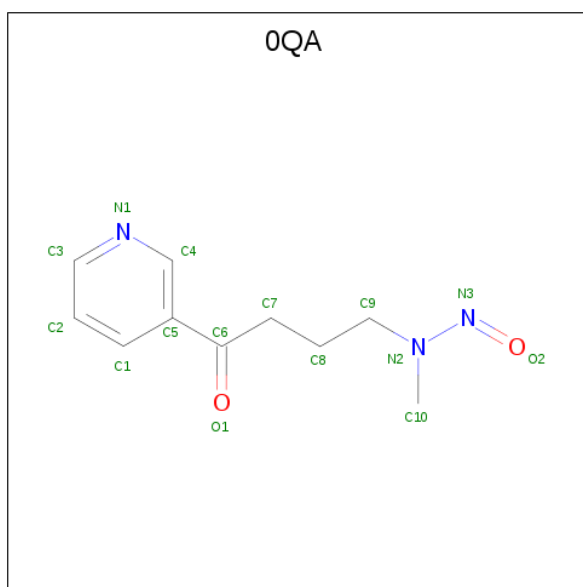
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: 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
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 4-[methyl(nitroso)amino]-1-(pyridin-3-yl)butan-1-one (three-letter code: 0QA) (formula: C<sub>10</sub>H<sub>13</sub>N<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	10	3	2		
3	B	1	Total	C	N	O	0	0
			15	10	3	2		
3	C	1	Total	C	N	O	0	0
			15	10	3	2		
3	D	1	Total	C	N	O	0	0
			15	10	3	2		
3	E	1	Total	C	N	O	0	0
			15	10	3	2		
3	F	1	Total	C	N	O	0	0
			15	10	3	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		

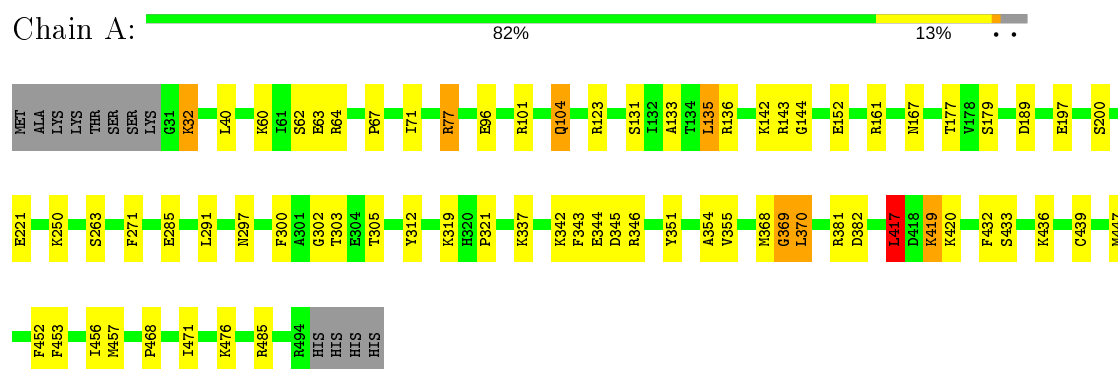
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	56	Total	O	0	0
			56	56		
5	B	39	Total	O	0	0
			39	39		
5	C	71	Total	O	0	0
			71	71		
5	D	49	Total	O	0	0
			49	49		
5	E	13	Total	O	0	0
			13	13		
5	F	11	Total	O	0	0
			11	11		
5	G	12	Total	O	0	0
			12	12		
5	H	10	Total	O	0	0
			10	10		

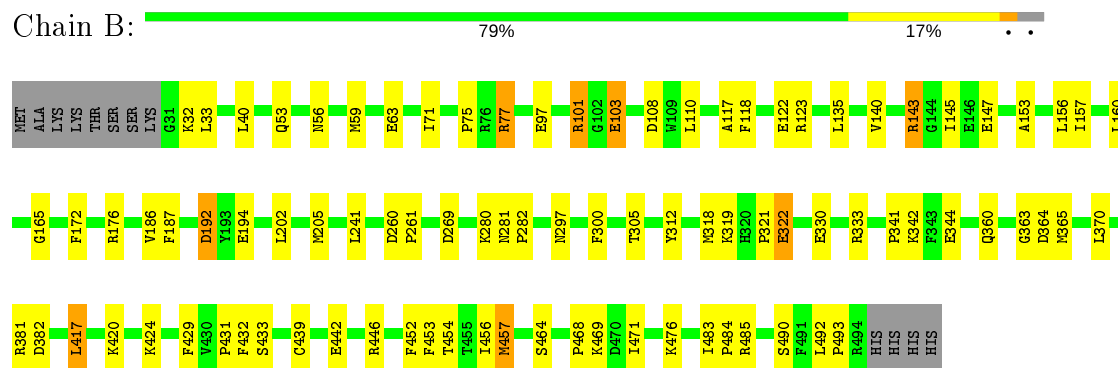
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

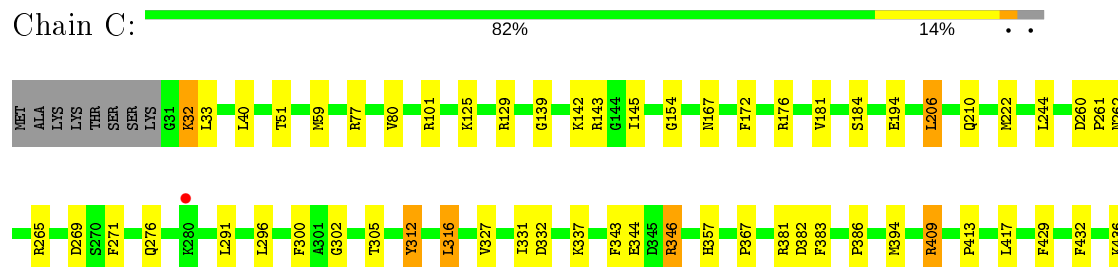
#### • Molecule 1: Cytochrome P450 2A13



#### • Molecule 1: Cytochrome P450 2A13



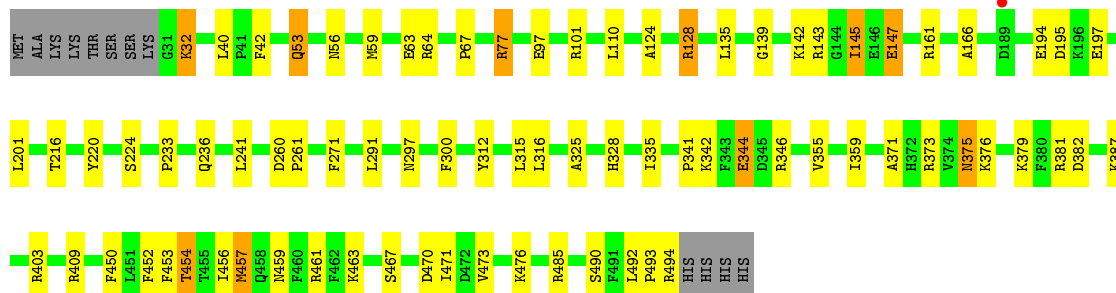
#### • Molecule 1: Cytochrome P450 2A13





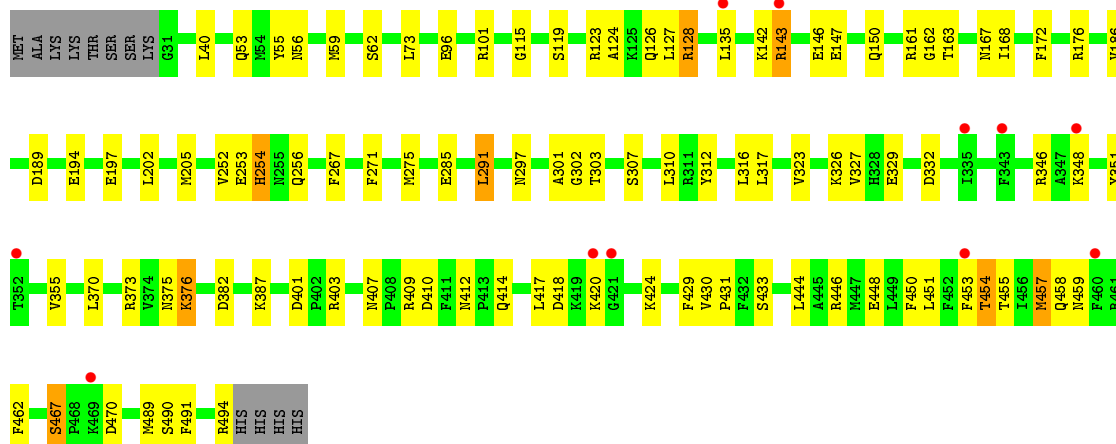
• Molecule 1: Cytochrome P450 2A13

Chain D: 81% 15%



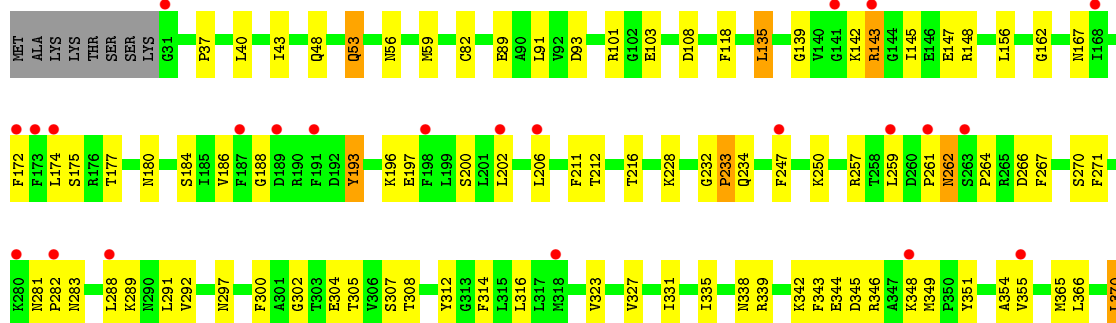
• Molecule 1: Cytochrome P450 2A13

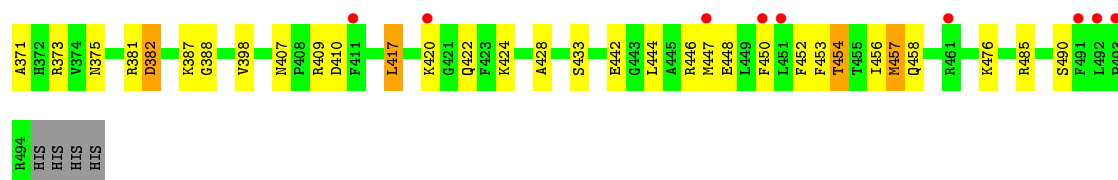
Chain E: 2% 76% 20%



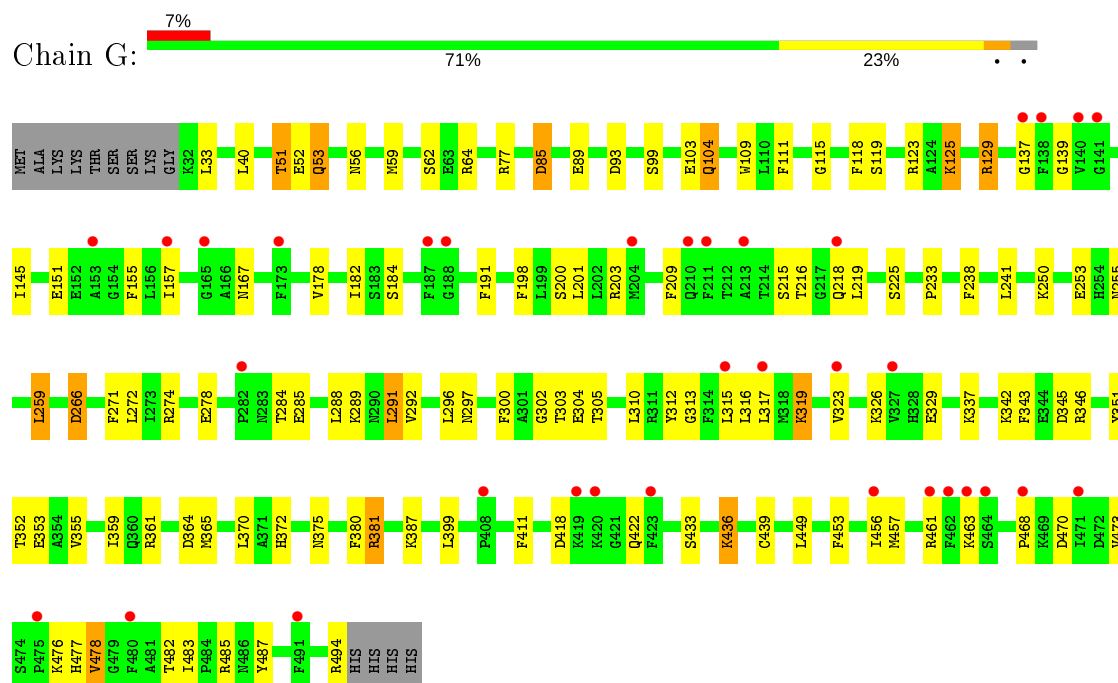
• Molecule 1: Cytochrome P450 2A13

Chain F: 7% 71% 24%

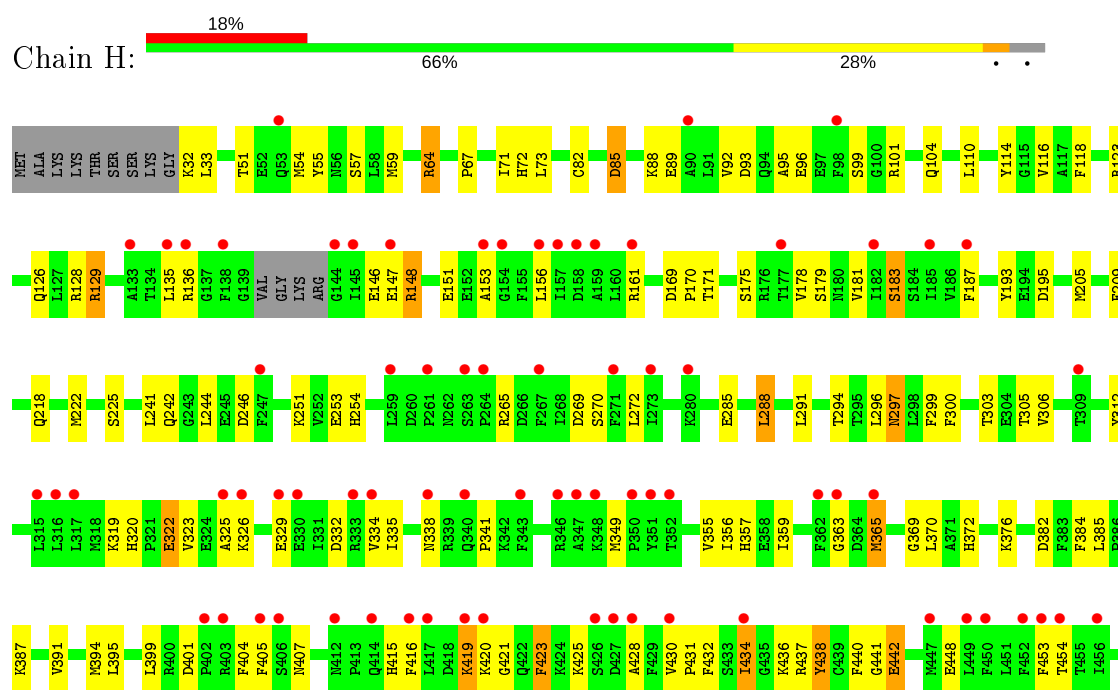


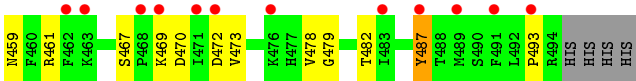


- Molecule 1: Cytochrome P450 2A13



- Molecule 1: Cytochrome P450 2A13





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.68Å 119.27Å 153.66Å 100.59° 101.86° 93.56°	Depositor
Resolution (Å)	69.77 – 2.35 69.77 – 2.35	Depositor EDS
% Data completeness (in resolution range)	97.5 (69.77-2.35) 97.5 (69.77-2.35)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 2.34Å)	Xtriage
Refinement program	REFMAC 6.1.13	Depositor
R, $R_{free}$	0.214 , 0.273 0.214 , 0.271	Depositor DCC
$R_{free}$ test set	9958 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.3	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	30804	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.85% 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: GOL, 0QA, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.01	2/3880 (0.1%)	0.90	1/5224 (0.0%)
1	B	0.99	3/3871 (0.1%)	0.88	4/5212 (0.1%)
1	C	1.04	4/3879 (0.1%)	0.89	2/5223 (0.0%)
1	D	0.99	1/3871 (0.0%)	0.87	1/5212 (0.0%)
1	E	0.85	0/3871	0.79	0/5212
1	F	0.80	0/3871	0.76	1/5212 (0.0%)
1	G	0.82	0/3834	0.81	0/5170
1	H	0.77	0/3822	0.75	1/5149 (0.0%)
All	All	0.92	10/30899 (0.0%)	0.83	10/41614 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	473	VAL	CB-CG2	5.94	1.65	1.52
1	C	383	PHE	CE2-CZ	5.37	1.47	1.37
1	B	63	GLU	CG-CD	5.28	1.59	1.51
1	B	322	GLU	CG-CD	5.24	1.59	1.51
1	A	133	ALA	CA-CB	5.20	1.63	1.52
1	C	429	PHE	CE1-CZ	5.20	1.47	1.37
1	C	80	VAL	CB-CG2	5.09	1.63	1.52
1	D	97	GLU	CD-OE1	5.06	1.31	1.25
1	A	104	GLN	CG-CD	5.05	1.62	1.51
1	B	103	GLU	CB-CG	-5.01	1.42	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	123	ARG	NE-CZ-NH1	-5.97	117.31	120.30
1	C	143	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	H	288	LEU	CA-CB-CG	5.86	128.78	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	143	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	F	316	LEU	CA-CB-CG	5.79	128.63	115.30
1	A	417	LEU	CA-CB-CG	5.33	127.55	115.30
1	B	33	LEU	CA-CB-CG	5.29	127.45	115.30
1	B	417	LEU	CA-CB-CG	5.25	127.38	115.30
1	B	269	ASP	CB-CG-OD2	5.23	123.00	118.30
1	D	195	ASP	CB-CG-OD2	5.15	122.94	118.30

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	3777	0	3747	50	0
1	B	3771	0	3741	47	0
1	C	3776	0	3745	53	0
1	D	3771	0	3741	56	0
1	E	3771	0	3741	55	0
1	F	3771	0	3741	78	0
1	G	3737	0	3670	85	0
1	H	3723	0	3668	81	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0
2	C	43	0	30	3	0
2	D	43	0	30	2	0
2	E	43	0	30	3	0
2	F	43	0	30	9	0
2	G	43	0	30	6	0
2	H	43	0	30	6	0
3	A	15	0	13	4	0
3	B	15	0	13	5	0
3	C	15	0	13	4	0
3	D	15	0	13	5	0
3	E	15	0	13	3	0
3	F	15	0	13	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	6	0	8	2	0
4	H	6	0	8	0	0
5	A	56	0	0	0	0
5	B	39	0	0	3	0
5	C	71	0	0	4	0
5	D	49	0	0	3	0
5	E	13	0	0	0	0
5	F	11	0	0	0	0
5	G	12	0	0	1	0
5	H	10	0	0	0	0
All	All	30804	0	30128	524	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 9.

All (524) 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:32:LYS:HD2	1:C:33:LEU:H	1.09	1.07
1:D:381:ARG:O	1:D:382:ASP:HB2	1.55	1.03
1:D:143:ARG:HH12	1:D:147:GLU:HB2	1.22	1.03
3:B:502:OQA:O1	3:B:502:OQA:H5	1.58	0.99
1:A:77:ARG:HG2	1:A:77:ARG:HH11	1.26	0.98
3:F:502:OQA:O1	3:F:502:OQA:H1	1.64	0.97
1:B:77:ARG:HG2	1:B:77:ARG:HH11	1.31	0.95
1:C:59:MET:CE	1:C:394:MET:HE2	1.99	0.91
1:D:341:PRO:HG3	1:D:454:THR:HG22	1.54	0.90
1:E:172:PHE:O	1:E:176:ARG:HG3	1.72	0.89
1:C:32:LYS:HD2	1:C:33:LEU:N	1.89	0.86
1:D:77:ARG:HG2	1:D:77:ARG:HH11	1.40	0.86
1:D:143:ARG:NH1	1:D:147:GLU:HB2	1.91	0.85
1:C:125:LYS:HE2	1:C:129:ARG:HH22	1.39	0.85
1:G:216:THR:HG21	1:G:233:PRO:HG2	1.56	0.85
1:C:59:MET:CE	1:C:394:MET:CE	2.56	0.84
1:A:381:ARG:O	1:A:382:ASP:HB2	1.79	0.83
1:G:53:GLN:OE1	1:G:53:GLN:HA	1.77	0.82
1:A:342:LYS:HE3	1:A:344:GLU:OE1	1.80	0.81
1:F:139:GLY:O	1:F:145:ILE:HB	1.81	0.81
1:E:450:PHE:O	1:E:454:THR:HB	1.82	0.80
1:F:433:SER:HB3	2:F:501:HEM:HBA1	1.64	0.79
1:B:165:GLY:O	1:B:490:SER:HB2	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:476:LYS:HG3	1:G:477:HIS:H	1.47	0.78
1:H:187:PHE:CE1	1:H:251:LYS:HB3	2.20	0.77
1:F:271:PHE:CD2	1:F:291:LEU:HB2	2.19	0.77
1:C:327:VAL:HG11	1:C:457:MET:CE	2.15	0.76
1:C:305:THR:HG21	3:C:502:0QA:O2	1.86	0.75
1:F:262:ASN:O	1:F:264:PRO:HD3	1.85	0.75
1:H:73:LEU:HB3	1:H:222:MET:HG2	1.67	0.75
1:D:452:PHE:O	1:D:456:ILE:HD12	1.87	0.74
1:A:77:ARG:HH11	1:A:77:ARG:CG	1.99	0.74
1:C:327:VAL:HG11	1:C:457:MET:HE2	1.70	0.73
3:D:502:0QA:O1	3:D:502:0QA:H5	1.88	0.73
1:G:182:ILE:HD11	1:G:302:GLY:HA3	1.70	0.73
1:D:143:ARG:HH12	1:D:147:GLU:CB	2.00	0.73
1:C:32:LYS:CD	1:C:33:LEU:H	1.96	0.72
1:A:142:LYS:HG3	1:A:143:ARG:N	2.04	0.72
3:C:502:0QA:O1	3:C:502:0QA:H5	1.88	0.72
1:C:59:MET:HE1	1:C:394:MET:CE	2.19	0.72
1:D:381:ARG:O	1:D:382:ASP:CB	2.27	0.72
1:H:320:HIS:HB3	1:H:323:VAL:HG22	1.72	0.71
1:B:77:ARG:CG	1:B:77:ARG:HH11	2.00	0.71
1:A:433:SER:HB3	2:A:501:HEM:HBA1	1.73	0.70
1:F:174:LEU:HD21	1:F:314:PHE:HE1	1.56	0.70
1:H:114:TYR:CE1	1:H:123:ARG:NH1	2.59	0.70
1:F:271:PHE:CE2	1:F:291:LEU:HB2	2.27	0.70
3:A:502:0QA:H5	3:A:502:0QA:O1	1.89	0.69
1:E:376:LYS:HA	1:E:387:LYS:HG3	1.73	0.69
1:A:342:LYS:HG3	1:A:344:GLU:HG3	1.74	0.69
1:H:178:VAL:HG11	1:H:306:VAL:HB	1.74	0.69
1:B:143:ARG:O	1:B:147:GLU:HG2	1.92	0.69
1:H:407:ASN:O	1:H:415:HIS:NE2	2.25	0.69
2:H:501:HEM:HBB2	2:H:501:HEM:HMB1	1.75	0.68
1:G:109:TRP:CH2	1:G:238:PHE:HB3	2.28	0.68
1:H:441:GLY:HA3	2:H:501:HEM:C3C	2.29	0.68
1:H:372:HIS:O	1:H:391:VAL:N	2.23	0.68
1:E:205:MET:HE1	1:E:303:THR:HG21	1.76	0.67
1:H:92:VAL:HG23	1:H:434:ILE:HG13	1.76	0.67
1:G:315:LEU:HB2	1:G:487:TYR:CE2	2.29	0.67
1:C:59:MET:HE1	1:C:394:MET:HE2	1.73	0.67
1:C:265:ARG:HB2	1:C:269:ASP:OD1	1.94	0.67
1:C:453:PHE:O	1:C:457:MET:HG2	1.93	0.67
1:F:302:GLY:HA2	2:F:501:HEM:HMC2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:478:VAL:O	1:G:478:VAL:HG12	1.94	0.67
1:C:125:LYS:CE	1:C:129:ARG:HH22	2.08	0.67
1:A:60:LYS:HG3	1:D:403:ARG:NH2	2.10	0.66
1:F:407:ASN:HB3	1:F:410:ASP:HB2	1.77	0.66
1:H:54:MET:HB2	1:H:479:GLY:HA2	1.78	0.66
2:D:501:HEM:C4D	3:D:502:0QA:H1	2.28	0.66
1:F:297:ASN:HA	3:F:502:0QA:N1	2.11	0.66
1:D:341:PRO:CG	1:D:454:THR:HG22	2.26	0.66
1:B:122:GLU:HA	1:B:122:GLU:OE2	1.97	0.65
1:E:302:GLY:HA2	2:E:501:HEM:HMC2	1.79	0.65
1:F:323:VAL:O	1:F:327:VAL:HG23	1.96	0.65
1:F:433:SER:CB	2:F:501:HEM:HBA1	2.26	0.65
1:F:450:PHE:O	1:F:454:THR:HB	1.96	0.65
1:H:179:SER:O	1:H:183:SER:HB2	1.97	0.65
1:C:139:GLY:HA2	1:C:142:LYS:HD2	1.78	0.64
1:F:288:LEU:O	1:F:292:VAL:HG23	1.97	0.64
1:A:381:ARG:O	1:A:382:ASP:CB	2.42	0.64
1:D:409:ARG:HG2	5:D:631:HOH:O	1.98	0.64
1:E:453:PHE:O	1:E:457:MET:HB2	1.97	0.64
1:D:166:ALA:O	1:D:490:SER:HB3	1.98	0.64
1:D:53:GLN:HG3	1:D:56:ASN:HB2	1.80	0.64
1:E:297:ASN:HA	3:E:502:0QA:N1	2.13	0.64
1:C:453:PHE:O	1:C:457:MET:CG	2.46	0.64
2:G:501:HEM:HBB2	2:G:501:HEM:HMB2	1.78	0.64
1:C:77:ARG:NH2	1:C:386:PRO:HG2	2.13	0.63
1:E:301:ALA:HA	3:E:502:0QA:H3	1.80	0.63
1:E:332:ASP:OD2	1:E:494:ARG:NH2	2.28	0.63
1:F:118:PHE:HE2	1:F:370:LEU:HD11	1.63	0.63
1:F:345:ASP:O	1:F:349:MET:HG3	1.98	0.63
1:F:145:ILE:HD12	1:F:148:ARG:HB3	1.81	0.63
2:E:501:HEM:HMB1	2:E:501:HEM:HBB2	1.81	0.63
1:G:355:VAL:O	1:G:359:ILE:HG12	1.98	0.63
1:D:143:ARG:HH11	1:D:143:ARG:HG3	1.64	0.62
1:F:448:GLU:O	1:F:452:PHE:CD2	2.51	0.62
1:H:372:HIS:NE2	2:H:501:HEM:O1A	2.29	0.62
1:C:77:ARG:HH22	1:C:386:PRO:HG2	1.64	0.62
1:D:77:ARG:CG	1:D:77:ARG:HH11	2.11	0.62
1:F:216:THR:HG21	1:F:233:PRO:HG2	1.81	0.62
1:A:342:LYS:HG3	1:A:344:GLU:CG	2.30	0.61
1:D:375:ASN:O	1:D:387:LYS:HG3	2.00	0.61
1:G:476:LYS:HG3	1:G:477:HIS:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:104:GLN:NE2	1:H:118:PHE:CE1	2.69	0.61
1:E:53:GLN:HG3	1:E:56:ASN:HB2	1.81	0.61
1:G:33:LEU:HD21	1:G:77:ARG:HD2	1.82	0.61
3:C:502:0QA:O1	3:C:502:0QA:C9	2.48	0.61
3:D:502:0QA:C9	3:D:502:0QA:O1	2.48	0.61
1:E:205:MET:CE	1:E:303:THR:HG21	2.30	0.61
1:H:146:GLU:C	1:H:148:ARG:H	2.05	0.61
1:C:59:MET:HE3	1:C:394:MET:CE	2.31	0.60
1:F:343:PHE:CE1	1:F:447:MET:HA	2.37	0.60
1:G:365:MET:HA	1:G:365:MET:CE	2.32	0.60
1:H:363:GLY:O	1:H:365:MET:CE	2.49	0.60
1:F:174:LEU:HD21	1:F:314:PHE:CE1	2.37	0.59
1:D:379:LYS:HD3	5:D:640:HOH:O	2.02	0.59
1:F:308:THR:HB	1:F:365:MET:CE	2.32	0.59
1:A:179:SER:HB2	1:A:303:THR:HG23	1.83	0.59
1:D:341:PRO:HG3	1:D:454:THR:CG2	2.30	0.59
1:D:342:LYS:HE2	1:D:344:GLU:OE1	2.02	0.59
1:H:432:PHE:CG	1:H:442:GLU:HG3	2.37	0.59
1:F:375:ASN:O	1:F:387:LYS:HG3	2.02	0.59
1:F:40:LEU:HD22	1:F:43:ILE:HD11	1.85	0.59
1:C:172:PHE:O	1:C:176:ARG:HG3	2.02	0.59
1:G:215:SER:N	4:G:502:GOL:O3	2.28	0.59
1:B:77:ARG:NH1	5:B:612:HOH:O	2.35	0.58
1:G:285:GLU:HA	1:G:285:GLU:OE1	2.03	0.58
1:A:297:ASN:HA	3:A:502:0QA:N1	2.18	0.58
1:G:123:ARG:HA	1:G:285:GLU:HG3	1.86	0.58
1:A:142:LYS:HG3	1:A:144:GLY:H	1.68	0.58
1:D:220:TYR:CZ	1:D:224:SER:HB2	2.39	0.58
1:F:420:LYS:HE2	1:F:422:GLN:HE21	1.68	0.58
1:A:197:GLU:O	1:A:200:SER:HB3	2.04	0.57
1:H:129:ARG:HG3	1:H:129:ARG:HH11	1.68	0.57
1:G:125:LYS:O	1:G:129:ARG:HB2	2.05	0.57
1:F:305:THR:HA	1:F:365:MET:CE	2.34	0.57
1:H:363:GLY:O	1:H:365:MET:HE2	2.05	0.57
1:F:308:THR:HB	1:F:365:MET:HE1	1.86	0.57
1:G:209:PHE:HE2	1:G:300:PHE:HD1	1.52	0.57
1:B:77:ARG:HG2	1:B:77:ARG:NH1	2.11	0.57
1:C:332:ASP:CG	1:C:494:ARG:HH22	2.08	0.57
1:G:178:VAL:HG11	1:G:303:THR:O	2.05	0.57
2:C:501:HEM:C4D	3:C:502:0QA:H1	2.33	0.56
1:C:210:GLN:HG3	1:C:483:ILE:HG13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:LYS:HG2	1:E:143:ARG:HH22	1.70	0.56
1:F:373:ARG:HD3	1:F:388:GLY:HA2	1.86	0.56
1:G:315:LEU:HB2	1:G:487:TYR:HE2	1.68	0.56
1:F:143:ARG:O	1:F:147:GLU:HG2	2.05	0.56
1:G:375:ASN:O	1:G:387:LYS:HG3	2.06	0.56
1:H:51:THR:HG23	1:H:218:GLN:HB2	1.88	0.56
1:D:476:LYS:NZ	5:D:604:HOH:O	2.38	0.56
1:F:381:ARG:O	1:F:382:ASP:HB2	2.04	0.56
1:H:372:HIS:HE1	1:H:437:ARG:HB2	1.70	0.56
1:G:151:GLU:O	1:G:155:PHE:HD2	1.88	0.56
1:A:468:PRO:HA	1:A:471:ILE:HD12	1.87	0.56
1:D:124:ALA:O	1:D:128:ARG:HB2	2.06	0.56
1:H:382:ASP:OD1	1:H:382:ASP:N	2.39	0.56
1:H:114:TYR:HE1	1:H:123:ARG:NH1	2.03	0.56
1:F:476:LYS:HB2	1:F:485:ARG:HA	1.87	0.55
1:G:278:GLU:HG2	1:G:284:THR:OG1	2.05	0.55
1:B:453:PHE:O	1:B:457:MET:HB2	2.06	0.55
1:G:178:VAL:CG1	1:G:303:THR:HA	2.36	0.55
1:H:401:ASP:HB3	1:H:404:PHE:HB2	1.88	0.55
1:G:319:LYS:HE2	1:G:473:VAL:HG22	1.88	0.55
1:H:104:GLN:NE2	1:H:118:PHE:HE1	2.04	0.55
1:G:215:SER:HB3	4:G:502:GOL:O3	2.05	0.55
1:E:142:LYS:HG2	1:E:143:ARG:NH2	2.22	0.55
1:A:77:ARG:NH1	1:A:77:ARG:HG2	2.08	0.54
1:G:361:ARG:NH1	1:G:399:LEU:O	2.37	0.54
1:H:95:ALA:O	1:H:99:SER:HB3	2.07	0.54
1:A:142:LYS:CG	1:A:144:GLY:H	2.21	0.54
1:D:355:VAL:O	1:D:359:ILE:HG13	2.08	0.54
1:H:355:VAL:O	1:H:359:ILE:HG12	2.08	0.54
1:A:123:ARG:HA	1:A:285:GLU:HG3	1.89	0.54
1:F:448:GLU:O	1:F:452:PHE:HD2	1.91	0.54
1:C:59:MET:CE	1:C:394:MET:HE3	2.37	0.54
1:B:101:ARG:HD2	1:B:117:ALA:O	2.08	0.54
1:F:103:GLU:HB2	1:F:108:ASP:OD2	2.08	0.54
1:F:89:GLU:O	1:F:93:ASP:HB2	2.08	0.54
1:G:139:GLY:CA	1:G:145:ILE:HG12	2.38	0.54
1:E:253:GLU:HA	1:E:256:GLN:HG3	1.90	0.53
1:G:453:PHE:O	1:G:457:MET:HG3	2.08	0.53
1:G:478:VAL:HG22	1:G:482:THR:HG23	1.89	0.53
1:E:101:ARG:CZ	1:E:370:LEU:HD23	2.38	0.53
1:E:254:HIS:C	1:E:254:HIS:ND1	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:444:LEU:O	1:E:448:GLU:HG3	2.09	0.53
1:F:354:ALA:HB2	1:F:417:LEU:HD13	1.90	0.53
1:A:419:LYS:HB2	1:A:420:LYS:HE2	1.89	0.53
1:F:259:LEU:O	1:F:261:PRO:HD3	2.08	0.53
1:H:407:ASN:H	1:H:415:HIS:HE1	1.56	0.53
1:G:139:GLY:HA2	1:G:145:ILE:HG12	1.90	0.53
1:A:67:PRO:HG3	1:D:63:GLU:O	2.09	0.53
2:F:501:HEM:ND	3:F:502:OQA:C10	2.71	0.53
1:H:101:ARG:NH1	2:H:501:HEM:O2A	2.42	0.53
1:F:53:GLN:HG3	1:F:56:ASN:OD1	2.09	0.52
1:G:433:SER:HB3	2:G:501:HEM:HBA1	1.91	0.52
1:A:104:GLN:NE2	1:A:221:GLU:OE2	2.43	0.52
1:C:244:LEU:HB3	1:C:296:LEU:HD11	1.92	0.52
3:B:502:OQA:O1	3:B:502:OQA:C9	2.44	0.52
1:G:288:LEU:O	1:G:292:VAL:HG23	2.09	0.52
1:G:461:ARG:HB3	1:G:494:ARG:HD3	1.91	0.52
1:B:321:PRO:HD2	1:B:322:GLU:OE2	2.10	0.52
1:F:271:PHE:HB3	1:F:291:LEU:HD13	1.90	0.52
1:F:373:ARG:NH1	1:F:388:GLY:O	2.43	0.52
1:G:316:LEU:O	1:G:317:LEU:HB2	2.10	0.52
1:D:110:LEU:HD22	1:D:241:LEU:HB3	1.92	0.52
1:E:123:ARG:O	1:E:127:LEU:HG	2.08	0.52
1:C:181:VAL:O	1:C:184:SER:HB2	2.09	0.52
3:F:502:OQA:O1	3:F:502:OQA:C10	2.49	0.52
1:H:265:ARG:HB2	1:H:269:ASP:OD2	2.09	0.52
1:C:271:PHE:CE2	1:C:291:LEU:HB2	2.45	0.51
1:G:439:CYS:HB2	2:G:501:HEM:NA	2.25	0.51
1:A:381:ARG:HB3	1:D:64[B]:ARG:HH21	1.74	0.51
1:H:322:GLU:O	1:H:325:ALA:HB3	2.10	0.51
1:A:271:PHE:CD2	1:A:291:LEU:HB2	2.45	0.51
1:G:99:SER:HB2	1:G:436:LYS:HB3	1.92	0.51
1:H:469:LYS:HG3	1:H:469:LYS:O	2.10	0.51
1:H:96:GLU:HA	1:H:96:GLU:OE1	2.10	0.51
1:F:118:PHE:CE2	1:F:370:LEU:HD11	2.44	0.51
1:F:327:VAL:O	1:F:331:ILE:HG13	2.11	0.51
2:H:501:HEM:HBB2	2:H:501:HEM:CMB	2.38	0.51
1:B:432:PHE:HB3	1:B:439:CYS:HB3	1.93	0.51
1:C:476:LYS:HB2	1:C:485:ARG:HA	1.92	0.51
1:A:342:LYS:HG2	1:A:345:ASP:OD2	2.11	0.51
1:B:442:GLU:OE1	1:B:446:ARG:NE	2.41	0.51
1:H:341:PRO:HG2	1:H:454:THR:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:180:ASN:ND2	1:F:193:TYR:HE1	2.09	0.51
1:E:462:PHE:HB3	1:E:489:MET:HE3	1.93	0.51
1:H:305:THR:HA	1:H:365:MET:HG3	1.92	0.51
1:A:161:ARG:HG2	1:A:161:ARG:HH11	1.76	0.50
1:B:305:THR:HG21	3:B:502:0QA:O2	2.11	0.50
1:G:259:LEU:HD21	1:G:272:LEU:HB3	1.94	0.50
1:F:142:LYS:HE3	1:F:143:ARG:NH2	2.25	0.50
2:D:501:HEM:HMB2	2:D:501:HEM:HBB2	1.93	0.50
1:F:180:ASN:HD22	1:F:193:TYR:HE1	1.58	0.50
1:C:332:ASP:OD2	1:C:494:ARG:NH2	2.38	0.50
1:G:104:GLN:HE21	1:G:104:GLN:N	2.10	0.50
1:C:327:VAL:HG11	1:C:457:MET:HE3	1.94	0.50
1:F:211:PHE:CE1	1:F:233:PRO:HB2	2.47	0.50
1:C:59:MET:HE1	1:C:394:MET:HE3	1.90	0.50
1:F:211:PHE:HE1	1:F:233:PRO:HB2	1.77	0.50
1:G:476:LYS:CG	1:G:477:HIS:H	2.17	0.50
1:E:161:ARG:O	1:E:163:THR:N	2.45	0.49
1:E:412:ASN:OD1	1:E:414:GLN:HB2	2.11	0.49
1:B:452:PHE:O	1:B:456:ILE:HD12	2.12	0.49
1:H:187:PHE:CE1	1:H:251:LYS:CB	2.94	0.49
1:H:55:TYR:CE2	1:H:59:MET:HG2	2.47	0.49
1:B:297:ASN:HD22	3:B:502:0QA:C4	2.25	0.49
1:H:55:TYR:CE2	1:H:59:MET:CG	2.95	0.49
1:B:318:MET:SD	1:B:464:SER:HB3	2.52	0.49
1:D:161:ARG:NH2	1:D:459:ASN:OD1	2.44	0.49
1:E:375:ASN:O	1:E:387:LYS:HE2	2.13	0.49
3:A:502:0QA:C9	3:A:502:0QA:O1	2.49	0.49
1:B:172:PHE:O	1:B:176:ARG:HG3	2.12	0.49
1:C:51:THR:HG22	1:C:222:MET:CE	2.43	0.49
1:E:124:ALA:O	1:E:128:ARG:HB2	2.12	0.49
1:H:244:LEU:HB3	1:H:296:LEU:HD11	1.95	0.49
1:B:110:LEU:HD22	1:B:241:LEU:HB3	1.95	0.48
1:A:101:ARG:NH1	1:A:370:LEU:HB3	2.27	0.48
1:A:453:PHE:HD2	1:A:457:MET:CE	2.25	0.48
1:A:60:LYS:HG3	1:D:403:ARG:HH21	1.75	0.48
2:F:501:HEM:ND	3:F:502:0QA:H3	2.28	0.48
1:G:313:GLY:HA2	1:G:359:ILE:HD12	1.96	0.48
1:H:288:LEU:O	1:H:291:LEU:HB3	2.12	0.48
1:G:255:ASN:ND2	1:G:266:ASP:OD1	2.46	0.48
1:E:375:ASN:O	1:E:387:LYS:HG3	2.13	0.48
1:E:332:ASP:CG	1:E:494:ARG:HH22	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:SER:O	1:A:135:LEU:HB2	2.13	0.48
1:C:206:LEU:O	1:C:210:GLN:HB2	2.12	0.48
1:C:453:PHE:O	1:C:457:MET:HG3	2.14	0.48
1:D:197:GLU:O	1:D:201:LEU:HG	2.14	0.48
1:F:381:ARG:O	1:F:382:ASP:CB	2.61	0.48
1:F:351:TYR:O	1:F:355:VAL:HG23	2.14	0.48
1:G:317:LEU:HD23	1:G:323:VAL:HG23	1.96	0.48
1:A:63:GLU:O	1:D:67:PRO:HG3	2.14	0.47
1:A:319:LYS:C	1:A:321:PRO:HD3	2.33	0.47
1:B:360:GLN:HG2	5:B:633:HOH:O	2.13	0.47
1:H:51:THR:HG23	1:H:218:GLN:CB	2.44	0.47
1:B:381:ARG:O	1:B:382:ASP:HB2	2.14	0.47
1:F:188:GLY:N	1:F:266:ASP:HB3	2.29	0.47
1:H:175:SER:O	1:H:179:SER:HB3	2.14	0.47
1:A:32:LYS:HD2	1:A:32:LYS:HA	1.52	0.47
1:D:101:ARG:O	1:D:373:ARG:HG2	2.15	0.47
1:F:398:VAL:HG12	1:F:428:ALA:HB1	1.97	0.47
1:H:187:PHE:CE1	1:H:251:LYS:HD3	2.50	0.47
1:D:315:LEU:HG	1:D:473:VAL:HG12	1.97	0.47
1:H:187:PHE:HE1	1:H:251:LYS:HB3	1.73	0.47
1:A:432:PHE:HB3	1:A:439:CYS:HB3	1.96	0.47
1:E:418:ASP:OD1	1:E:420:LYS:HB2	2.14	0.47
1:G:418:ASP:OD1	1:G:422:GLN:HB2	2.14	0.47
1:H:363:GLY:O	1:H:365:MET:HE1	2.13	0.47
1:A:152:GLU:HG3	1:A:177:THR:HG23	1.96	0.47
1:D:77:ARG:HG2	1:D:77:ARG:NH1	2.18	0.47
1:G:104:GLN:OE1	1:G:118:PHE:CE1	2.68	0.47
1:A:161:ARG:HG2	1:A:161:ARG:NH1	2.30	0.47
1:D:467:SER:HB3	1:D:470:ASP:OD2	2.15	0.47
1:D:297:ASN:HA	3:D:502:OQA:N1	2.30	0.47
1:C:302:GLY:HA2	2:C:501:HEM:HMC2	1.97	0.47
1:E:348:LYS:HB2	1:E:348:LYS:HE2	1.61	0.47
1:E:401:ASP:OD2	1:E:403:ARG:HG2	2.15	0.47
1:F:206:LEU:HD13	1:F:304:GLU:OE1	2.15	0.47
1:G:111:PHE:CG	1:G:118:PHE:CD2	3.03	0.47
1:A:271:PHE:CE2	1:A:291:LEU:HB2	2.50	0.46
1:H:369:GLY:O	1:H:370:LEU:HD12	2.15	0.46
1:B:118:PHE:HE2	1:B:370:LEU:HD11	1.79	0.46
1:F:424:LYS:HE2	1:F:424:LYS:HB3	1.54	0.46
1:H:405:PHE:HB3	1:H:415:HIS:CE1	2.50	0.46
1:G:209:PHE:CE1	1:G:304:GLU:HG2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:VAL:HA	1:B:145:ILE:HG21	1.97	0.46
1:F:305:THR:HA	1:F:365:MET:HE1	1.96	0.46
1:D:143:ARG:HG3	1:D:143:ARG:NH1	2.27	0.46
1:H:357:HIS:HB3	1:H:416:PHE:CZ	2.49	0.46
1:A:351:TYR:O	1:A:355:VAL:HG23	2.16	0.46
1:C:473:VAL:HG22	5:C:605:HOH:O	2.15	0.46
1:D:145:ILE:HA	1:D:145:ILE:HD12	1.75	0.46
1:F:156:LEU:HB2	1:F:177:THR:HG21	1.97	0.46
1:G:64:ARG:HB3	1:G:64:ARG:NH2	2.30	0.46
1:H:209:PHE:CZ	1:H:300:PHE:HD1	2.34	0.46
1:B:281:ASN:HA	1:B:282:PRO:HD2	1.79	0.46
1:F:37:PRO:HB2	1:F:48:GLN:NE2	2.30	0.46
1:F:59:MET:HE1	1:F:82:CYS:SG	2.55	0.46
1:G:182:ILE:HD11	1:G:302:GLY:CA	2.43	0.46
1:H:73:LEU:CB	1:H:222:MET:HG2	2.42	0.46
1:A:305:THR:HG23	3:A:502:OQA:H3	1.97	0.46
1:F:197:GLU:O	1:F:200:SER:HB3	2.15	0.46
1:D:341:PRO:CB	1:D:454:THR:HG21	2.46	0.46
1:E:302:GLY:HA2	2:E:501:HEM:CMC	2.45	0.46
1:G:111:PHE:CD2	1:G:118:PHE:HD2	2.33	0.46
1:C:343:PHE:O	1:C:346:ARG:HB2	2.16	0.46
1:F:305:THR:HG22	1:F:365:MET:HE2	1.98	0.46
1:H:430:VAL:N	1:H:431:PRO:HD3	2.31	0.46
1:F:331:ILE:HG23	1:F:335:ILE:HD12	1.97	0.45
1:H:175:SER:O	1:H:179:SER:CB	2.64	0.45
1:H:423:PHE:CE1	1:H:425:LYS:HG3	2.52	0.45
1:B:330:GLU:HG2	1:B:333:ARG:NH2	2.31	0.45
1:D:476:LYS:HB2	1:D:485:ARG:HA	1.98	0.45
1:G:103:GLU:C	1:G:104:GLN:HE21	2.19	0.45
1:B:341:PRO:HG2	1:B:454:THR:HG22	1.98	0.45
1:G:64:ARG:CZ	1:G:64:ARG:HB3	2.46	0.45
1:H:399:LEU:HD23	1:H:428:ALA:O	2.17	0.45
1:E:326:LYS:HD2	1:E:351:TYR:CZ	2.52	0.45
1:E:454:THR:HG22	1:E:455:THR:N	2.32	0.45
1:E:59:MET:O	1:E:62:SER:HB3	2.17	0.45
1:B:433:SER:HB3	2:B:501:HEM:HBA1	1.99	0.45
1:C:409:ARG:HB3	1:C:409:ARG:HE	1.68	0.45
2:F:501:HEM:NA	3:F:502:OQA:H2	2.32	0.45
1:G:111:PHE:CG	1:G:118:PHE:HD2	2.35	0.45
1:G:145:ILE:HD13	1:G:145:ILE:HA	1.83	0.45
1:D:32:LYS:HA	1:D:32:LYS:HD2	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:442:GLU:O	1:F:446:ARG:HG3	2.17	0.45
1:A:136:ARG:O	1:A:142:LYS:HE3	2.17	0.45
1:C:409:ARG:HG2	5:C:630:HOH:O	2.15	0.45
1:E:168:ILE:HD11	1:E:491:PHE:CD1	2.52	0.45
1:G:51:THR:HG23	1:G:218:GLN:HB2	1.99	0.45
1:G:271:PHE:CE1	1:G:291:LEU:HB2	2.51	0.45
1:A:368:MET:O	1:A:369:GLY:C	2.55	0.45
1:B:342:LYS:HE2	1:B:344:GLU:OE1	2.16	0.45
1:E:252:VAL:O	1:E:256:GLN:HG3	2.17	0.45
1:H:461:ARG:NH1	1:H:493:PRO:O	2.47	0.45
1:H:423:PHE:C	1:H:423:PHE:CD1	2.90	0.45
1:G:370:LEU:HD12	1:G:370:LEU:HA	1.81	0.44
1:H:67:PRO:HA	1:H:82:CYS:HB2	1.99	0.44
1:B:53:GLN:HG2	1:B:56:ASN:OD1	2.16	0.44
1:D:271:PHE:CD2	1:D:291:LEU:HB2	2.51	0.44
1:D:335:ILE:HD13	1:D:341:PRO:HB3	1.99	0.44
1:F:172:PHE:HA	1:F:175:SER:OG	2.16	0.44
1:A:452:PHE:O	1:A:456:ILE:HD12	2.17	0.44
1:G:365:MET:HE2	1:G:365:MET:HA	1.99	0.44
1:H:123:ARG:HA	1:H:285:GLU:HG3	1.99	0.44
1:A:142:LYS:HG3	1:A:143:ARG:H	1.79	0.44
1:B:260:ASP:HA	1:B:261:PRO:HD2	1.81	0.44
1:D:139:GLY:O	1:D:145:ILE:HB	2.18	0.44
1:G:157:ILE:HD11	1:G:456:ILE:HA	1.98	0.44
1:G:310:LEU:HD23	1:G:453:PHE:CE2	2.53	0.44
1:H:89:GLU:O	1:H:93:ASP:HB2	2.17	0.44
1:E:202:LEU:HA	1:E:205:MET:HE2	1.98	0.44
1:G:478:VAL:O	1:G:478:VAL:CG1	2.65	0.44
1:H:487:TYR:C	1:H:487:TYR:CD1	2.91	0.44
1:C:367:PRO:HD2	1:C:480:PHE:O	2.18	0.44
1:F:186:VAL:HA	1:F:267:PHE:CB	2.48	0.44
1:C:271:PHE:CG	1:C:291:LEU:HD13	2.52	0.44
1:C:312:TYR:O	1:C:316:LEU:HD22	2.18	0.44
1:F:302:GLY:HA2	2:F:501:HEM:CMC	2.47	0.44
1:G:380:PHE:O	1:G:381:ARG:C	2.56	0.44
1:G:85:ASP:HB3	1:G:381:ARG:HH12	1.83	0.44
1:F:232:GLY:O	1:F:234:GLN:N	2.51	0.44
1:G:191:PHE:CD2	1:G:198:PHE:CD1	3.06	0.44
1:G:271:PHE:CD1	1:G:291:LEU:HB2	2.52	0.44
1:G:365:MET:CA	1:G:365:MET:HE2	2.45	0.44
1:B:103:GLU:HB2	1:B:108:ASP:OD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:197:GLU:OE1	1:F:247:PHE:CE1	2.71	0.44
1:E:101:ARG:NH2	1:E:370:LEU:HD23	2.33	0.43
1:H:128:ARG:NH2	1:H:438:TYR:CD2	2.85	0.43
1:H:441:GLY:HA3	2:H:501:HEM:CAC	2.48	0.43
1:B:192:ASP:C	1:B:194:GLU:H	2.20	0.43
1:E:291:LEU:O	1:E:291:LEU:HD12	2.18	0.43
1:A:476:LYS:HB2	1:A:485:ARG:HA	2.01	0.43
1:E:451:LEU:HD23	1:E:451:LEU:HA	1.86	0.43
1:C:444:LEU:O	1:C:448:GLU:HG3	2.19	0.43
1:A:343:PHE:CE1	1:A:447:MET:HA	2.53	0.43
1:E:115:GLY:O	1:E:119:SER:HB3	2.19	0.43
1:G:449:LEU:O	1:G:453:PHE:HB2	2.17	0.43
1:H:116:VAL:CG1	1:H:294:THR:HG23	2.47	0.43
1:H:116:VAL:HG12	1:H:294:THR:HG23	2.01	0.43
1:B:202:LEU:HD23	1:B:205:MET:CE	2.48	0.43
1:E:351:TYR:O	1:E:355:VAL:HG23	2.18	0.43
1:F:135:LEU:HA	1:F:135:LEU:HD12	1.82	0.43
1:H:161:ARG:HH22	1:H:459:ASN:HD22	1.65	0.43
1:H:64:ARG:HB2	1:H:64:ARG:HE	1.70	0.43
1:C:154:GLY:HA3	5:C:650:HOH:O	2.18	0.43
1:D:453:PHE:O	1:D:457:MET:HB2	2.19	0.43
1:H:55:TYR:CE2	1:H:59:MET:HG3	2.53	0.43
1:C:432:PHE:HB3	1:C:439:CYS:HB3	2.00	0.43
1:E:407:ASN:HB3	1:E:410:ASP:HB2	2.01	0.43
1:F:175:SER:HB2	1:F:202:LEU:HD22	2.01	0.43
1:H:440:PHE:CD1	1:H:440:PHE:C	2.92	0.43
1:C:51:THR:HG22	1:C:222:MET:HE3	2.00	0.42
1:C:260:ASP:HA	1:C:261:PRO:HD2	1.92	0.42
1:G:296:LEU:HD12	1:G:296:LEU:HA	1.81	0.42
1:B:145:ILE:HA	1:B:145:ILE:HD12	1.72	0.42
1:B:186:VAL:HG23	1:B:187:PHE:CD1	2.54	0.42
1:C:357:HIS:NE2	1:C:446:ARG:NH2	2.67	0.42
1:D:471:ILE:HG22	1:D:473:VAL:HG13	2.01	0.42
1:F:452:PHE:O	1:F:456:ILE:HG13	2.20	0.42
1:B:59:MET:CE	1:B:59:MET:HA	2.50	0.42
1:D:325:ALA:O	1:D:328:HIS:HB2	2.19	0.42
1:D:492:LEU:HA	1:D:493:PRO:HD3	1.81	0.42
1:E:317:LEU:HD13	1:E:457:MET:CE	2.49	0.42
1:E:467:SER:O	1:E:470:ASP:HB2	2.20	0.42
1:G:53:GLN:HB3	1:G:56:ASN:HB2	2.01	0.42
1:F:59:MET:CE	1:F:82:CYS:SG	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:305:THR:HG22	1:G:365:MET:HG3	2.00	0.42
1:H:394:MET:O	1:H:395:LEU:C	2.57	0.42
1:B:319:LYS:HD2	1:B:468:PRO:O	2.19	0.42
1:B:476:LYS:HB2	1:B:485:ARG:HA	2.01	0.42
1:A:436:LYS:HE2	1:C:262:ASN:OD1	2.19	0.42
1:C:381:ARG:O	1:C:382:ASP:HB2	2.20	0.42
1:D:216:THR:HG21	1:D:233:PRO:HG2	2.01	0.42
1:F:344:GLU:C	1:F:346:ARG:H	2.22	0.42
1:G:411:PHE:O	1:G:411:PHE:CD2	2.72	0.42
1:G:89:GLU:O	1:G:93:ASP:HB2	2.19	0.42
1:H:153:ALA:HA	1:H:156:LEU:HB3	2.02	0.42
1:D:341:PRO:CB	1:D:454:THR:CG2	2.98	0.42
1:F:300:PHE:CD2	3:F:502:0QA:C2	3.02	0.42
1:B:429:PHE:CZ	1:B:431:PRO:HG3	2.55	0.42
1:G:323:VAL:HG21	1:G:411:PHE:HE2	1.84	0.42
1:G:487:TYR:CD1	1:G:487:TYR:C	2.93	0.42
1:H:356:ILE:HG12	1:H:453:PHE:HD2	1.85	0.42
1:A:77:ARG:NH1	1:A:77:ARG:CG	2.73	0.42
1:B:363:GLY:O	1:B:364:ASP:C	2.58	0.42
1:B:71:ILE:HA	1:B:71:ILE:HD12	1.92	0.42
1:E:310:LEU:HD23	1:E:453:PHE:CE1	2.55	0.42
3:E:502:0QA:H6	3:E:502:0QA:H2	1.63	0.42
1:G:59:MET:O	1:G:62:SER:HB3	2.20	0.42
1:A:71:ILE:HA	1:A:71:ILE:HD12	1.93	0.42
1:E:96:GLU:O	1:E:375:ASN:ND2	2.52	0.42
1:G:343:PHE:CE2	1:G:346:ARG:NH2	2.88	0.42
1:F:281:ASN:OD1	1:F:282:PRO:HD2	2.20	0.42
2:F:501:HEM:C4D	3:F:502:0QA:C10	3.03	0.42
1:G:302:GLY:HA2	2:G:501:HEM:CMC	2.50	0.42
1:D:59:MET:HA	1:D:59:MET:CE	2.50	0.41
1:G:288:LEU:O	1:G:291:LEU:HB3	2.20	0.41
1:H:73:LEU:HB3	1:H:222:MET:CG	2.44	0.41
1:E:271:PHE:O	1:E:275:MET:HG3	2.21	0.41
1:H:71:ILE:HG13	1:H:72:HIS:N	2.35	0.41
1:C:167:ASN:ND2	1:C:488:THR:OG1	2.45	0.41
1:E:146:GLU:O	1:E:150:GLN:HG3	2.19	0.41
2:F:501:HEM:C1A	3:F:502:0QA:H2	2.55	0.41
1:G:477:HIS:HB2	1:G:483:ILE:HD12	2.02	0.41
1:B:153:ALA:O	1:B:157:ILE:HG12	2.21	0.41
1:B:424:LYS:HB3	1:B:424:LYS:HE3	1.90	0.41
1:B:75:PRO:HA	5:B:603:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:143:ARG:O	1:E:147:GLU:HG2	2.20	0.41
1:E:186:VAL:HA	1:E:267:PHE:HB3	2.03	0.41
1:F:143:ARG:H	1:F:143:ARG:NE	2.18	0.41
1:H:299:PHE:O	1:H:303:THR:HB	2.20	0.41
1:A:453:PHE:CD2	1:A:457:MET:CE	3.03	0.41
1:B:341:PRO:CG	1:B:454:THR:HG22	2.50	0.41
1:B:483:ILE:HA	1:B:484:PRO:HD2	1.90	0.41
1:C:101:ARG:NH1	2:C:501:HEM:O2A	2.48	0.41
1:C:331:ILE:CD1	1:C:457:MET:HB2	2.50	0.41
1:D:291:LEU:O	1:D:291:LEU:HD12	2.20	0.41
1:E:429:PHE:CZ	1:E:431:PRO:HG3	2.56	0.41
1:E:55:TYR:CD2	1:E:55:TYR:C	2.93	0.41
1:F:420:LYS:HE2	1:F:422:GLN:NE2	2.34	0.41
1:H:116:VAL:HB	1:H:294:THR:HG23	2.03	0.41
1:A:302:GLY:HA2	2:A:501:HEM:HMC2	2.02	0.41
1:C:436:LYS:NZ	5:C:631:HOH:O	2.52	0.41
1:D:101:ARG:HD3	1:D:371:ALA:O	2.20	0.41
1:H:146:GLU:C	1:H:148:ARG:N	2.73	0.41
1:B:492:LEU:HA	1:B:493:PRO:HD3	1.92	0.41
1:G:250:LYS:CE	5:G:605:HOH:O	2.69	0.41
1:D:461:ARG:HB3	1:D:494:ARG:HD2	2.03	0.41
3:D:502:0QA:H10	3:D:502:0QA:H8	1.78	0.41
1:E:323:VAL:O	1:E:327:VAL:HG23	2.21	0.41
1:E:430:VAL:N	1:E:431:PRO:CD	2.83	0.41
1:F:335:ILE:HA	1:F:339:ARG:NH2	2.36	0.41
1:H:178:VAL:CG1	1:H:306:VAL:HB	2.47	0.41
1:H:169:ASP:HA	1:H:170:PRO:HD3	1.89	0.41
1:A:354:ALA:HB2	1:A:417:LEU:HD13	2.03	0.41
1:F:453:PHE:O	1:F:457:MET:HB2	2.20	0.40
1:G:297:ASN:HA	1:G:297:ASN:HD22	1.66	0.40
1:G:351:TYR:O	1:G:355:VAL:HG23	2.21	0.40
1:G:433:SER:CB	2:G:501:HEM:HBA1	2.51	0.40
1:H:110:LEU:HD22	1:H:241:LEU:HB3	2.03	0.40
1:H:297:ASN:HA	1:H:297:ASN:HD22	1.58	0.40
1:B:156:LEU:O	1:B:160:LEU:HG	2.21	0.40
3:B:502:0QA:H1	3:B:502:0QA:H6	1.62	0.40
1:D:260:ASP:HA	1:D:261:PRO:HD3	1.87	0.40
1:D:341:PRO:CG	1:D:454:THR:CG2	2.96	0.40
1:F:444:LEU:O	1:F:448:GLU:HG3	2.21	0.40
1:G:352:THR:O	1:G:353:GLU:C	2.58	0.40
1:G:372:HIS:NE2	2:G:501:HEM:O1A	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:384:PHE:C	1:H:385:LEU:HD23	2.42	0.40
1:E:123:ARG:HA	1:E:285:GLU:HG3	2.03	0.40
1:F:53:GLN:CG	1:F:56:ASN:OD1	2.69	0.40
1:G:115:GLY:O	1:G:119:SER:HB3	2.21	0.40
1:G:200:SER:O	1:G:203:ARG:HB3	2.20	0.40
1:D:450:PHE:O	1:D:454:THR:HB	2.21	0.40
1:F:101:ARG:HD3	1:F:371:ALA:O	2.21	0.40
1:H:181:VAL:HG11	1:H:448:GLU:OE2	2.21	0.40
1:E:458:GLN:OE1	1:E:459:ASN:ND2	2.54	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	464/476 (98%)	439 (95%)	24 (5%)	1 (0%)	47	56
1	B	463/476 (97%)	445 (96%)	18 (4%)	0	100	100
1	C	464/476 (98%)	443 (96%)	20 (4%)	1 (0%)	47	56
1	D	463/476 (97%)	444 (96%)	18 (4%)	1 (0%)	47	56
1	E	463/476 (97%)	434 (94%)	28 (6%)	1 (0%)	47	56
1	F	463/476 (97%)	413 (89%)	44 (10%)	6 (1%)	12	10
1	G	461/476 (97%)	417 (90%)	36 (8%)	8 (2%)	9	7
1	H	456/476 (96%)	396 (87%)	53 (12%)	7 (2%)	10	8
All	All	3697/3808 (97%)	3431 (93%)	241 (6%)	25 (1%)	22	23

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	346	ARG

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Mol	Chain	Res	Type
1	G	364	ASP
1	G	468	PRO
1	A	369	GLY
1	E	162	GLY
1	F	338	ASN
1	G	137	GLY
1	G	225	SER
1	G	337	LYS
1	H	85	ASP
1	H	419	LYS
1	G	345	ASP
1	G	381	ARG
1	H	147	GLU
1	H	193	TYR
1	D	42	PHE
1	F	212	THR
1	F	382	ASP
1	H	171	THR
1	H	322	GLU
1	F	162	GLY
1	F	193	TYR
1	H	421	GLY
1	F	233	PRO
1	G	478	VAL

### 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	410/419 (98%)	391 (95%)	19 (5%)	27	32
1	B	409/419 (98%)	392 (96%)	17 (4%)	30	36
1	C	410/419 (98%)	394 (96%)	16 (4%)	32	40
1	D	409/419 (98%)	388 (95%)	21 (5%)	24	27
1	E	409/419 (98%)	380 (93%)	29 (7%)	14	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	409/419 (98%)	383 (94%)	26 (6%)	17	18
1	G	403/419 (96%)	375 (93%)	28 (7%)	15	15
1	H	403/419 (96%)	354 (88%)	49 (12%)	5	4
All	All	3262/3352 (97%)	3057 (94%)	205 (6%)	18	19

All (205) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	40	LEU
1	A	62	SER
1	A	64[A]	ARG
1	A	64[B]	ARG
1	A	77	ARG
1	A	96	GLU
1	A	135	LEU
1	A	167	ASN
1	A	189	ASP
1	A	250	LYS
1	A	263	SER
1	A	300	PHE
1	A	312	TYR
1	A	337	LYS
1	A	346	ARG
1	A	370	LEU
1	A	417	LEU
1	A	419	LYS
1	B	32	LYS
1	B	40	LEU
1	B	77	ARG
1	B	97	GLU
1	B	101	ARG
1	B	135	LEU
1	B	143	ARG
1	B	192	ASP
1	B	280	LYS
1	B	300	PHE
1	B	312	TYR
1	B	365	MET
1	B	417	LEU
1	B	420	LYS

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Mol	Chain	Res	Type
1	B	457	MET
1	B	469	LYS
1	B	471	ILE
1	C	32	LYS
1	C	40	LEU
1	C	145	ILE
1	C	194	GLU
1	C	206	LEU
1	C	276	GLN
1	C	300	PHE
1	C	312	TYR
1	C	316	LEU
1	C	337	LYS
1	C	344	GLU
1	C	409	ARG
1	C	413	PRO
1	C	417	LEU
1	C	457	MET
1	C	469	LYS
1	D	32	LYS
1	D	40	LEU
1	D	53	GLN
1	D	77	ARG
1	D	128	ARG
1	D	135	LEU
1	D	142	LYS
1	D	145	ILE
1	D	147	GLU
1	D	194	GLU
1	D	236	GLN
1	D	300	PHE
1	D	312	TYR
1	D	316	LEU
1	D	344	GLU
1	D	346	ARG
1	D	375	ASN
1	D	376	LYS
1	D	454	THR
1	D	457	MET
1	D	463	LYS
1	E	40	LEU
1	E	73	LEU

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Mol	Chain	Res	Type
1	E	126	GLN
1	E	128	ARG
1	E	135	LEU
1	E	143	ARG
1	E	167	ASN
1	E	189	ASP
1	E	194	GLU
1	E	197	GLU
1	E	254	HIS
1	E	291	LEU
1	E	307	SER
1	E	312	TYR
1	E	316	LEU
1	E	329	GLU
1	E	346	ARG
1	E	373	ARG
1	E	376	LYS
1	E	382	ASP
1	E	409	ARG
1	E	417	LEU
1	E	424	LYS
1	E	433	SER
1	E	446	ARG
1	E	454	THR
1	E	457	MET
1	E	467	SER
1	E	490	SER
1	F	53	GLN
1	F	91	LEU
1	F	135	LEU
1	F	143	ARG
1	F	167	ASN
1	F	184	SER
1	F	196	LYS
1	F	228	LYS
1	F	250	LYS
1	F	257	ARG
1	F	262	ASN
1	F	270	SER
1	F	283	ASN
1	F	289	LYS
1	F	307	SER

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Mol	Chain	Res	Type
1	F	312	TYR
1	F	342	LYS
1	F	348	LYS
1	F	366	LEU
1	F	370	LEU
1	F	409	ARG
1	F	417	LEU
1	F	454	THR
1	F	457	MET
1	F	458	GLN
1	F	490	SER
1	G	40	LEU
1	G	51	THR
1	G	52	GLU
1	G	53	GLN
1	G	85	ASP
1	G	104	GLN
1	G	125	LYS
1	G	129	ARG
1	G	167	ASN
1	G	184	SER
1	G	201	LEU
1	G	219	LEU
1	G	241	LEU
1	G	253	GLU
1	G	259	LEU
1	G	266	ASP
1	G	274	ARG
1	G	289	LYS
1	G	291	LEU
1	G	312	TYR
1	G	319	LYS
1	G	326	LYS
1	G	329	GLU
1	G	342	LYS
1	G	436	LYS
1	G	463	LYS
1	G	470	ASP
1	G	485	ARG
1	H	32	LYS
1	H	33	LEU
1	H	57	SER

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Mol	Chain	Res	Type
1	H	64	ARG
1	H	85	ASP
1	H	88	LYS
1	H	126	GLN
1	H	129	ARG
1	H	135	LEU
1	H	136	ARG
1	H	148	ARG
1	H	151	GLU
1	H	183	SER
1	H	195	ASP
1	H	205	MET
1	H	225	SER
1	H	242	GLN
1	H	246	ASP
1	H	253	GLU
1	H	254	HIS
1	H	270	SER
1	H	272	LEU
1	H	297	ASN
1	H	312	TYR
1	H	319	LYS
1	H	326	LYS
1	H	329	GLU
1	H	332	ASP
1	H	334	VAL
1	H	335	ILE
1	H	338	ASN
1	H	349	MET
1	H	365	MET
1	H	376	LYS
1	H	387	LYS
1	H	419	LYS
1	H	420	LYS
1	H	423	PHE
1	H	434	ILE
1	H	436	LYS
1	H	438	TYR
1	H	442	GLU
1	H	467	SER
1	H	470	ASP
1	H	472	ASP

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Mol	Chain	Res	Type
1	H	473	VAL
1	H	478	VAL
1	H	482	THR
1	H	487	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	167	ASN
1	D	236	GLN
1	E	210	GLN
1	F	283	ASN
1	F	422	GLN
1	G	104	GLN
1	G	126	GLN
1	G	255	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

16 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
2	HEM	E	501	1,3	27,50,50	2.21	7 (25%)	17,82,82	1.43	2 (11%)
2	HEM	G	501	1	27,50,50	2.36	7 (25%)	17,82,82	1.54	3 (17%)
3	0QA	B	502	-	13,15,15	0.60	0	14,18,18	1.96	5 (35%)
3	0QA	F	502	2	13,15,15	0.53	0	14,18,18	1.44	2 (14%)
2	HEM	D	501	1	27,50,50	2.40	11 (40%)	17,82,82	1.12	1 (5%)
2	HEM	F	501	1,3	27,50,50	2.22	8 (29%)	17,82,82	1.79	4 (23%)
3	0QA	C	502	2	13,15,15	0.61	0	14,18,18	1.53	4 (28%)
3	0QA	D	502	-	13,15,15	0.61	0	14,18,18	1.54	4 (28%)
2	HEM	B	501	1	27,50,50	2.58	12 (44%)	17,82,82	2.28	5 (29%)
4	GOL	G	502	-	5,5,5	0.58	0	5,5,5	0.53	0
2	HEM	C	501	1,3	27,50,50	2.44	8 (29%)	17,82,82	1.91	7 (41%)
3	0QA	E	502	2	13,15,15	0.71	0	14,18,18	1.55	3 (21%)
3	0QA	A	502	2	13,15,15	0.44	0	14,18,18	2.12	4 (28%)
2	HEM	H	501	1	27,50,50	2.20	6 (22%)	17,82,82	2.37	5 (29%)
4	GOL	H	502	-	5,5,5	1.24	1 (20%)	5,5,5	2.56	2 (40%)
2	HEM	A	501	1,3	27,50,50	2.32	9 (33%)	17,82,82	1.82	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	E	501	1,3	-	0/6/54/54	-
2	HEM	G	501	1	-	0/6/54/54	-
3	0QA	B	502	-	-	6/12/12/12	0/1/1/1
3	0QA	F	502	2	-	6/12/12/12	0/1/1/1
2	HEM	D	501	1	-	0/6/54/54	-
2	HEM	F	501	1,3	-	0/6/54/54	-
3	0QA	C	502	2	-	7/12/12/12	0/1/1/1
3	0QA	D	502	-	-	7/12/12/12	0/1/1/1
2	HEM	B	501	1	-	0/6/54/54	-
4	GOL	G	502	-	-	2/4/4/4	-
2	HEM	C	501	1,3	-	0/6/54/54	-
3	0QA	E	502	2	-	6/12/12/12	0/1/1/1
3	0QA	A	502	2	-	5/12/12/12	0/1/1/1
2	HEM	H	501	1	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	H	502	-	-	2/4/4/4	-
2	HEM	A	501	1,3	-	0/6/54/54	-

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3C-C2C	-6.01	1.32	1.40
2	C	501	HEM	C3D-C2D	5.90	1.55	1.37
2	G	501	HEM	C3D-C2D	5.73	1.54	1.37
2	D	501	HEM	C3C-C2C	-5.66	1.32	1.40
2	B	501	HEM	C3B-C2B	-5.57	1.32	1.40
2	A	501	HEM	C3C-C2C	-5.55	1.32	1.40
2	C	501	HEM	C3B-C2B	-5.54	1.32	1.40
2	E	501	HEM	C3D-C2D	5.38	1.53	1.37
2	H	501	HEM	C3D-C2D	5.37	1.53	1.37
2	A	501	HEM	C3D-C2D	5.19	1.53	1.37
2	G	501	HEM	C3C-C2C	-5.06	1.33	1.40
2	H	501	HEM	C3C-C2C	-4.99	1.33	1.40
2	F	501	HEM	C3D-C2D	4.82	1.51	1.37
2	C	501	HEM	C3C-C2C	-4.70	1.33	1.40
2	C	501	HEM	C3C-CAC	4.64	1.57	1.47
2	F	501	HEM	C3C-C2C	-4.51	1.34	1.40
2	E	501	HEM	C3C-CAC	4.51	1.57	1.47
2	A	501	HEM	C3B-C2B	-4.49	1.34	1.40
2	G	501	HEM	C3B-C2B	-4.44	1.34	1.40
2	F	501	HEM	C3B-C2B	-4.39	1.34	1.40
2	E	501	HEM	C3C-C2C	-4.34	1.34	1.40
2	D	501	HEM	C3B-C2B	-4.13	1.34	1.40
2	A	501	HEM	C3C-CAC	4.00	1.56	1.47
2	B	501	HEM	C3C-CAC	3.97	1.55	1.47
2	H	501	HEM	C3B-CAB	3.94	1.56	1.47
2	B	501	HEM	CAA-C2A	3.92	1.57	1.52
2	E	501	HEM	C3B-CAB	3.92	1.55	1.47
2	D	501	HEM	C3B-CAB	3.92	1.55	1.47
2	D	501	HEM	CMA-C3A	3.90	1.59	1.51
2	F	501	HEM	C3C-CAC	3.88	1.55	1.47
2	B	501	HEM	C3D-C2D	3.80	1.48	1.37
2	D	501	HEM	C3D-C2D	3.75	1.48	1.37
2	C	501	HEM	C3B-CAB	3.71	1.55	1.47
2	G	501	HEM	C3C-CAC	3.69	1.55	1.47
2	G	501	HEM	C3B-CAB	3.65	1.55	1.47
2	E	501	HEM	C3B-C2B	-3.61	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	CAA-C2A	3.51	1.57	1.52
2	B	501	HEM	CMD-C2D	3.42	1.58	1.51
2	D	501	HEM	C3C-CAC	3.35	1.54	1.47
2	H	501	HEM	C3C-CAC	3.30	1.54	1.47
2	F	501	HEM	CAA-C2A	3.26	1.56	1.52
2	F	501	HEM	C3B-CAB	3.23	1.54	1.47
2	H	501	HEM	C3B-C2B	-3.15	1.36	1.40
2	G	501	HEM	CAA-C2A	3.10	1.56	1.52
2	B	501	HEM	C3B-CAB	2.95	1.54	1.47
2	A	501	HEM	CMA-C3A	2.86	1.57	1.51
2	A	501	HEM	C3B-CAB	2.83	1.53	1.47
2	B	501	HEM	C4B-CHC	-2.73	1.33	1.41
2	A	501	HEM	CMB-C2B	2.56	1.57	1.51
2	C	501	HEM	CMA-C3A	2.44	1.56	1.51
2	B	501	HEM	C4A-CHB	-2.39	1.34	1.41
2	C	501	HEM	CAA-C2A	2.32	1.55	1.52
2	D	501	HEM	C1B-C2B	2.27	1.47	1.42
2	F	501	HEM	CMB-C2B	2.23	1.56	1.51
2	G	501	HEM	CMB-C2B	2.20	1.56	1.51
2	B	501	HEM	CMB-C2B	2.17	1.56	1.51
4	H	502	GOL	O2-C2	-2.16	1.36	1.43
2	E	501	HEM	CMA-C3A	2.15	1.56	1.51
2	A	501	HEM	CMD-C2D	2.14	1.56	1.51
2	D	501	HEM	C1C-C2C	2.12	1.47	1.42
2	E	501	HEM	CAA-C2A	2.12	1.55	1.52
2	B	501	HEM	CMC-C2C	2.11	1.56	1.51
2	B	501	HEM	C1D-CHD	-2.11	1.35	1.41
2	C	501	HEM	CMD-C2D	2.11	1.56	1.51
2	D	501	HEM	CMD-C2D	2.09	1.56	1.51
2	H	501	HEM	C1D-CHD	-2.09	1.35	1.41
2	D	501	HEM	C1D-CHD	-2.07	1.35	1.41
2	F	501	HEM	CMD-C2D	2.06	1.55	1.51
2	A	501	HEM	C1D-CHD	-2.06	1.35	1.41

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	501	HEM	CAA-CBA-CGA	-5.47	103.50	112.67
2	B	501	HEM	C1D-C2D-C3D	-5.39	103.25	107.00
2	B	501	HEM	CBD-CAD-C3D	-5.16	102.97	112.48
3	A	502	0QA	C8-C7-C6	-4.69	104.99	113.62
3	B	502	0QA	C8-C7-C6	-4.66	105.04	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	501	HEM	C1D-C2D-C3D	-4.65	103.76	107.00
4	H	502	GOL	O3-C3-C2	-4.51	88.56	110.20
2	A	501	HEM	CAA-CBA-CGA	-4.48	105.16	112.67
3	A	502	0QA	C9-C8-C7	-4.19	100.96	112.10
2	H	501	HEM	CBD-CAD-C3D	-4.07	104.98	112.48
2	C	501	HEM	C4C-C3C-C2C	3.98	109.68	106.90
2	E	501	HEM	CAA-CBA-CGA	-3.96	106.03	112.67
2	F	501	HEM	CAA-CBA-CGA	-3.85	106.20	112.67
3	D	502	0QA	C8-C7-C6	-3.60	106.99	113.62
3	C	502	0QA	C8-C7-C6	-3.60	107.00	113.62
2	H	501	HEM	CMB-C2B-C3B	3.43	131.09	124.68
2	F	501	HEM	C1D-C2D-C3D	-3.28	104.71	107.00
2	B	501	HEM	CAD-CBD-CGD	-3.20	107.30	112.67
4	H	502	GOL	O2-C2-C3	-3.13	95.33	109.12
2	G	501	HEM	CMA-C3A-C4A	-3.07	123.75	128.46
3	E	502	0QA	C5-C4-N1	-3.00	119.05	123.49
3	E	502	0QA	C3-N1-C4	2.95	121.96	116.85
3	B	502	0QA	C9-C8-C7	-2.91	104.36	112.10
3	E	502	0QA	C8-C7-C6	-2.80	108.46	113.62
2	A	501	HEM	CMA-C3A-C4A	-2.78	124.19	128.46
3	A	502	0QA	C3-N1-C4	2.76	121.63	116.85
3	F	502	0QA	C3-N1-C4	2.76	121.62	116.85
2	C	501	HEM	CBD-CAD-C3D	-2.76	107.39	112.48
2	F	501	HEM	CBD-CAD-C3D	-2.66	107.57	112.48
3	F	502	0QA	C8-C7-C6	-2.65	108.75	113.62
2	C	501	HEM	CMD-C2D-C3D	2.62	129.87	124.94
2	G	501	HEM	CMB-C2B-C3B	2.51	129.38	124.68
2	C	501	HEM	C1D-C2D-C3D	-2.51	105.25	107.00
2	F	501	HEM	C4C-C3C-C2C	2.48	108.63	106.90
2	B	501	HEM	CMD-C2D-C1D	2.45	132.23	128.46
3	A	502	0QA	C5-C4-N1	-2.44	119.88	123.49
2	A	501	HEM	C1D-C2D-C3D	-2.43	105.31	107.00
3	B	502	0QA	C5-C4-N1	-2.42	119.91	123.49
2	B	501	HEM	CAA-CBA-CGA	-2.42	108.61	112.67
3	B	502	0QA	C1-C5-C4	2.41	120.37	117.63
3	D	502	0QA	C1-C5-C4	2.37	120.31	117.63
3	C	502	0QA	C1-C5-C4	2.34	120.29	117.63
2	C	501	HEM	CMD-C2D-C1D	-2.34	124.87	128.46
3	C	502	0QA	C3-N1-C4	2.32	120.86	116.85
3	D	502	0QA	C3-N1-C4	2.32	120.85	116.85
2	D	501	HEM	C1D-C2D-C3D	-2.29	105.40	107.00
3	B	502	0QA	C3-N1-C4	2.29	120.81	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	HEM	CMB-C2B-C3B	2.24	128.87	124.68
2	H	501	HEM	CMD-C2D-C3D	2.20	129.10	124.94
2	C	501	HEM	CMB-C2B-C3B	2.15	128.69	124.68
2	C	501	HEM	C3C-C4C-NC	-2.13	106.92	110.94
2	A	501	HEM	C4C-C3C-C2C	2.11	108.37	106.90
3	C	502	0QA	C5-C4-N1	-2.10	120.39	123.49
3	D	502	0QA	C5-C4-N1	-2.10	120.39	123.49
2	G	501	HEM	CBA-CAA-C2A	2.03	116.23	112.49
2	A	501	HEM	C3C-C4C-NC	-2.03	107.11	110.94

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	502	0QA	C9-N2-N3-O2
3	F	502	0QA	C8-C9-N2-C10
3	C	502	0QA	C9-N2-N3-O2
3	C	502	0QA	C8-C9-N2-N3
3	C	502	0QA	C6-C7-C8-C9
3	D	502	0QA	C9-N2-N3-O2
3	D	502	0QA	C8-C9-N2-N3
3	D	502	0QA	C6-C7-C8-C9
4	G	502	GOL	C1-C2-C3-O3
3	E	502	0QA	C10-N2-N3-O2
3	E	502	0QA	C9-N2-N3-O2
3	E	502	0QA	C8-C9-N2-C10
3	A	502	0QA	C10-N2-N3-O2
3	A	502	0QA	C8-C9-N2-N3
3	A	502	0QA	C6-C7-C8-C9
3	B	502	0QA	C10-N2-N3-O2
3	B	502	0QA	C8-C9-N2-N3
3	B	502	0QA	C6-C7-C8-C9
3	C	502	0QA	C7-C8-C9-N2
3	D	502	0QA	C7-C8-C9-N2
3	E	502	0QA	C7-C8-C9-N2
3	C	502	0QA	O1-C6-C7-C8
3	D	502	0QA	O1-C6-C7-C8
3	C	502	0QA	C5-C6-C7-C8
3	D	502	0QA	C5-C6-C7-C8
4	G	502	GOL	O2-C2-C3-O3
3	B	502	0QA	C5-C6-C7-C8
4	H	502	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	F	502	0QA	C7-C8-C9-N2
3	B	502	0QA	O1-C6-C7-C8
3	F	502	0QA	C8-C9-N2-N3
3	A	502	0QA	C5-C6-C7-C8
3	B	502	0QA	C7-C8-C9-N2
4	H	502	GOL	C1-C2-C3-O3
3	A	502	0QA	O1-C6-C7-C8
3	F	502	0QA	C5-C6-C7-C8
3	E	502	0QA	C5-C6-C7-C8
3	F	502	0QA	O1-C6-C7-C8
3	E	502	0QA	O1-C6-C7-C8
3	C	502	0QA	C8-C9-N2-C10
3	D	502	0QA	C8-C9-N2-C10

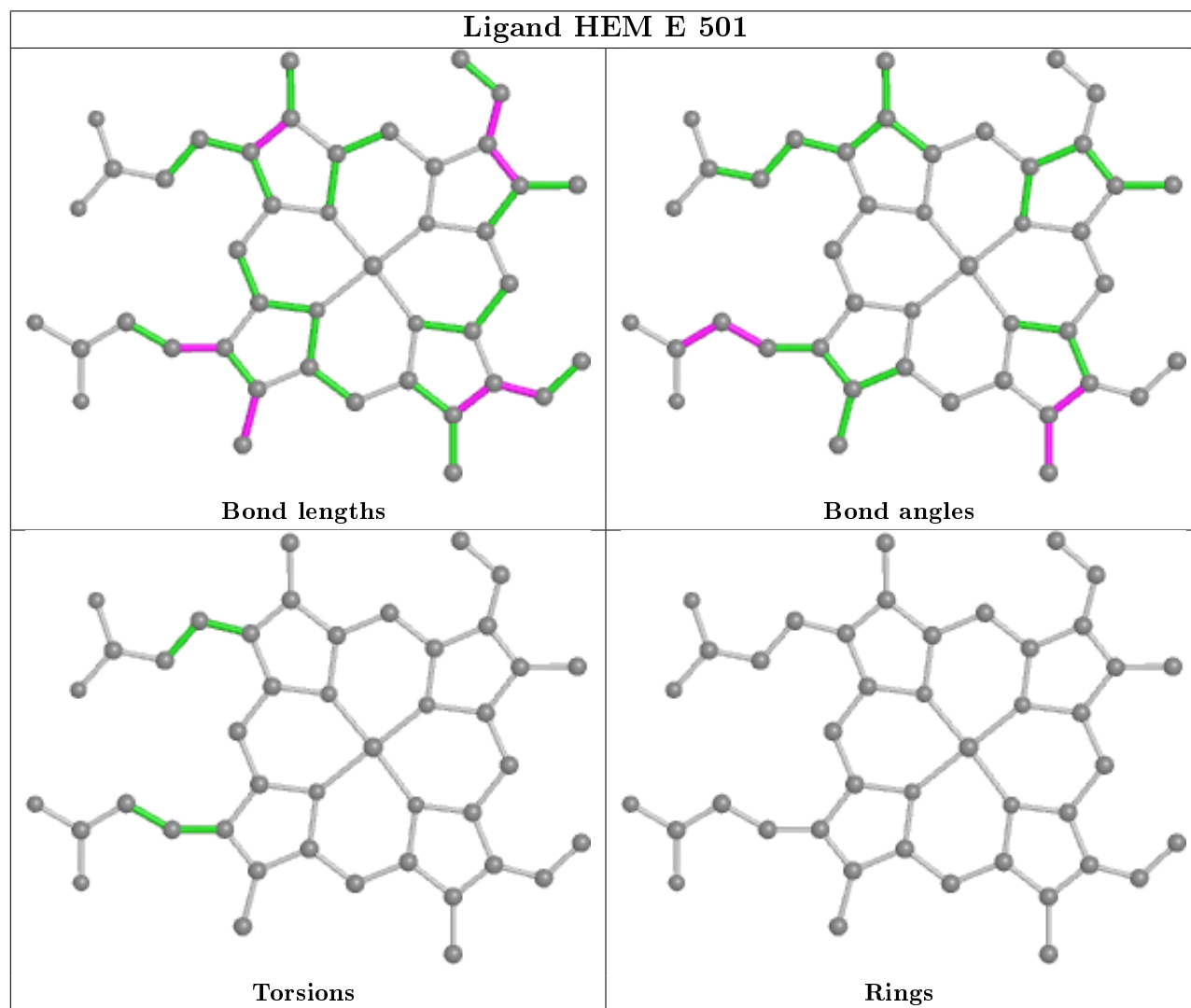
There are no ring outliers.

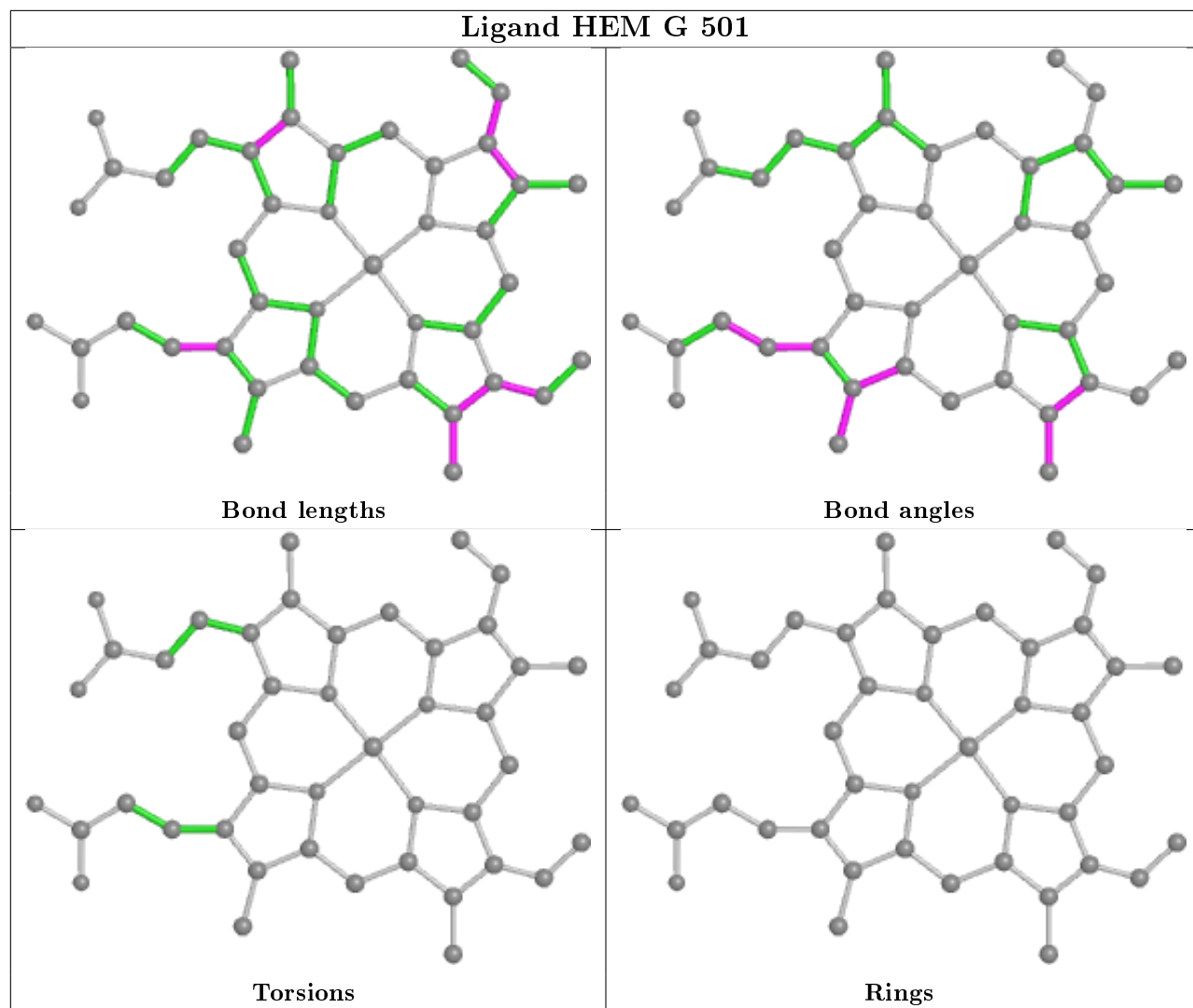
15 monomers are involved in 57 short contacts:

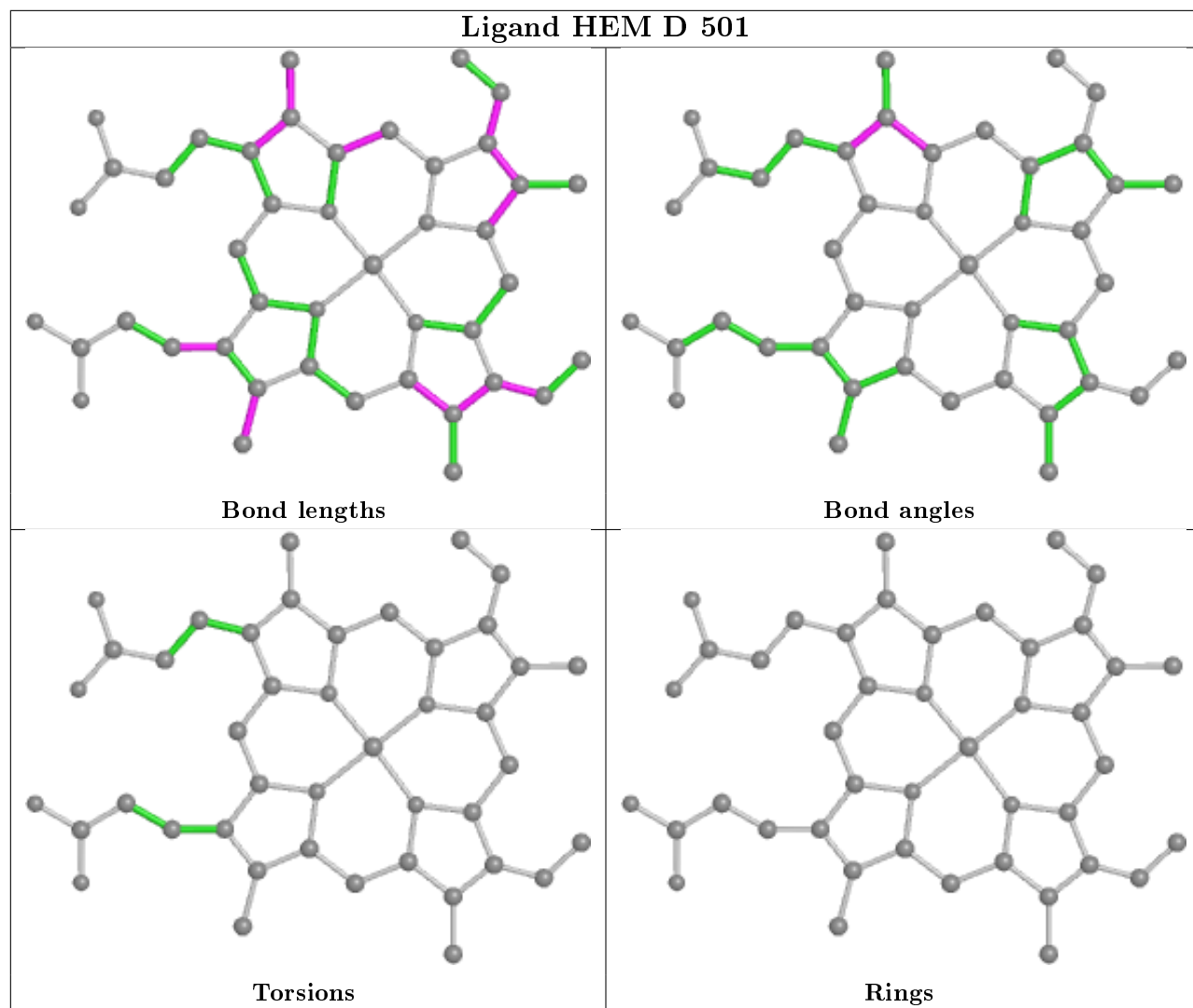
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	HEM	3	0
2	G	501	HEM	6	0
3	B	502	0QA	5	0
3	F	502	0QA	9	0
2	D	501	HEM	2	0
2	F	501	HEM	9	0
3	C	502	0QA	4	0
3	D	502	0QA	5	0
2	B	501	HEM	1	0
4	G	502	GOL	2	0
2	C	501	HEM	3	0
3	E	502	0QA	3	0
3	A	502	0QA	4	0
2	H	501	HEM	6	0
2	A	501	HEM	2	0

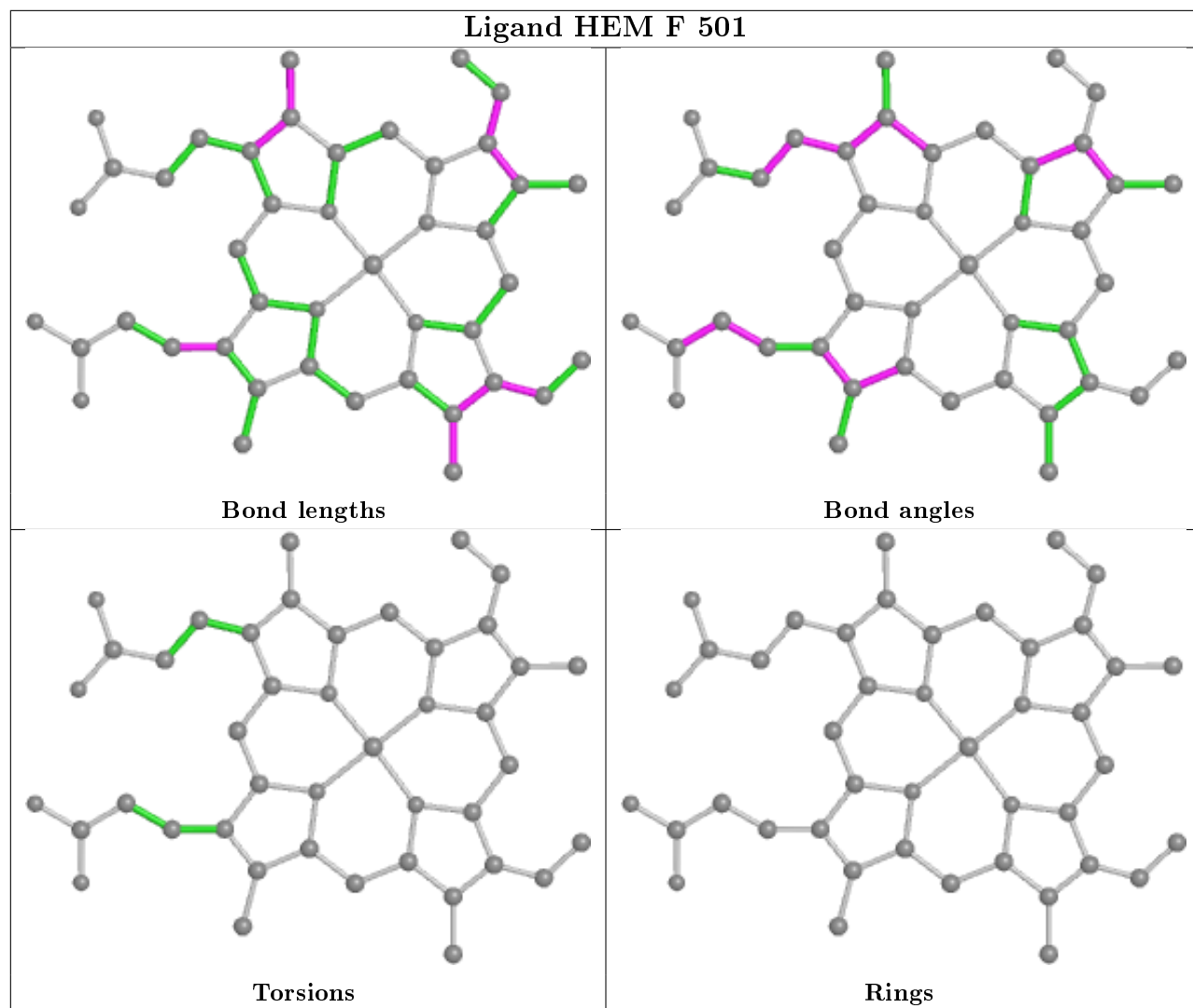
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

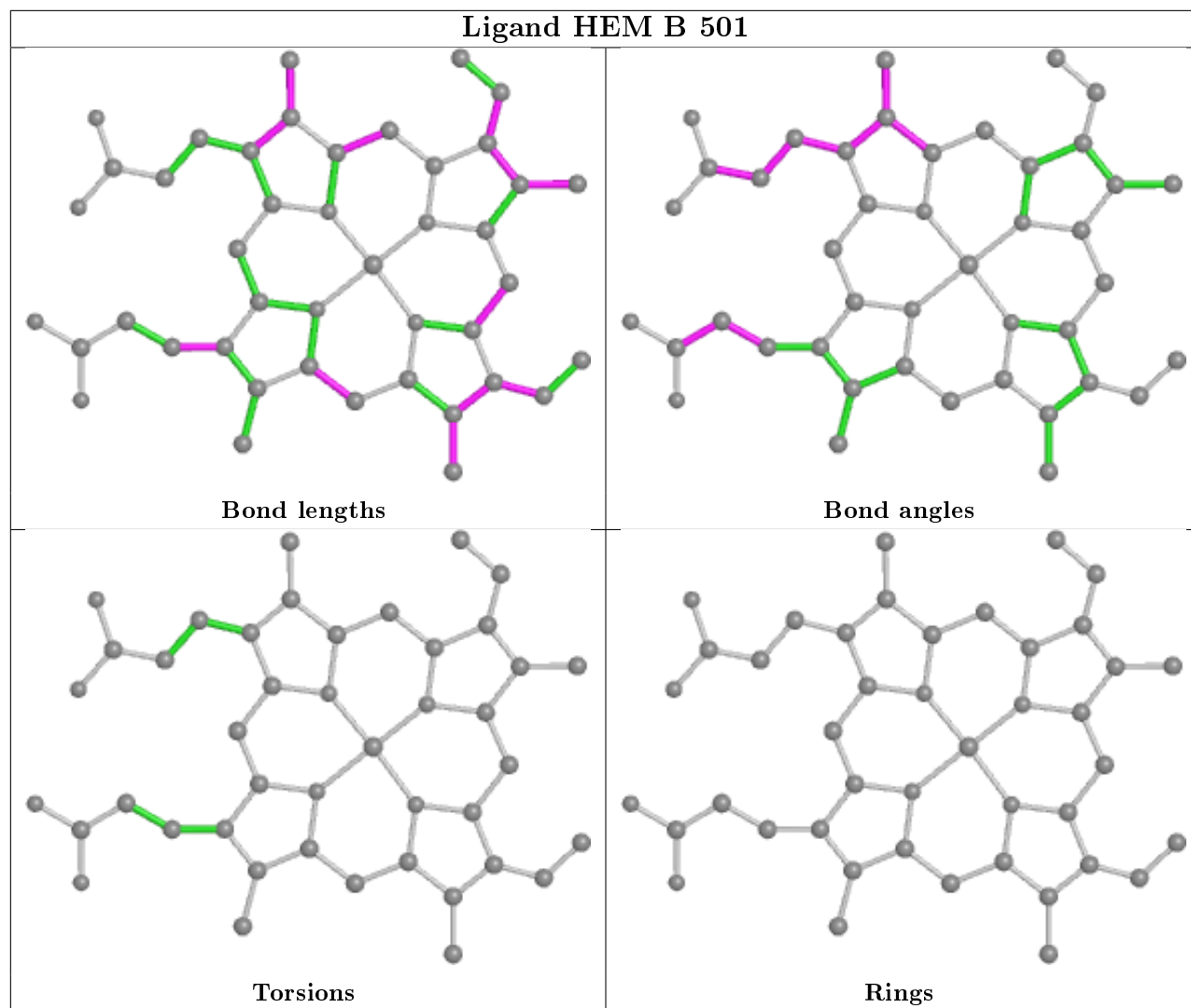
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



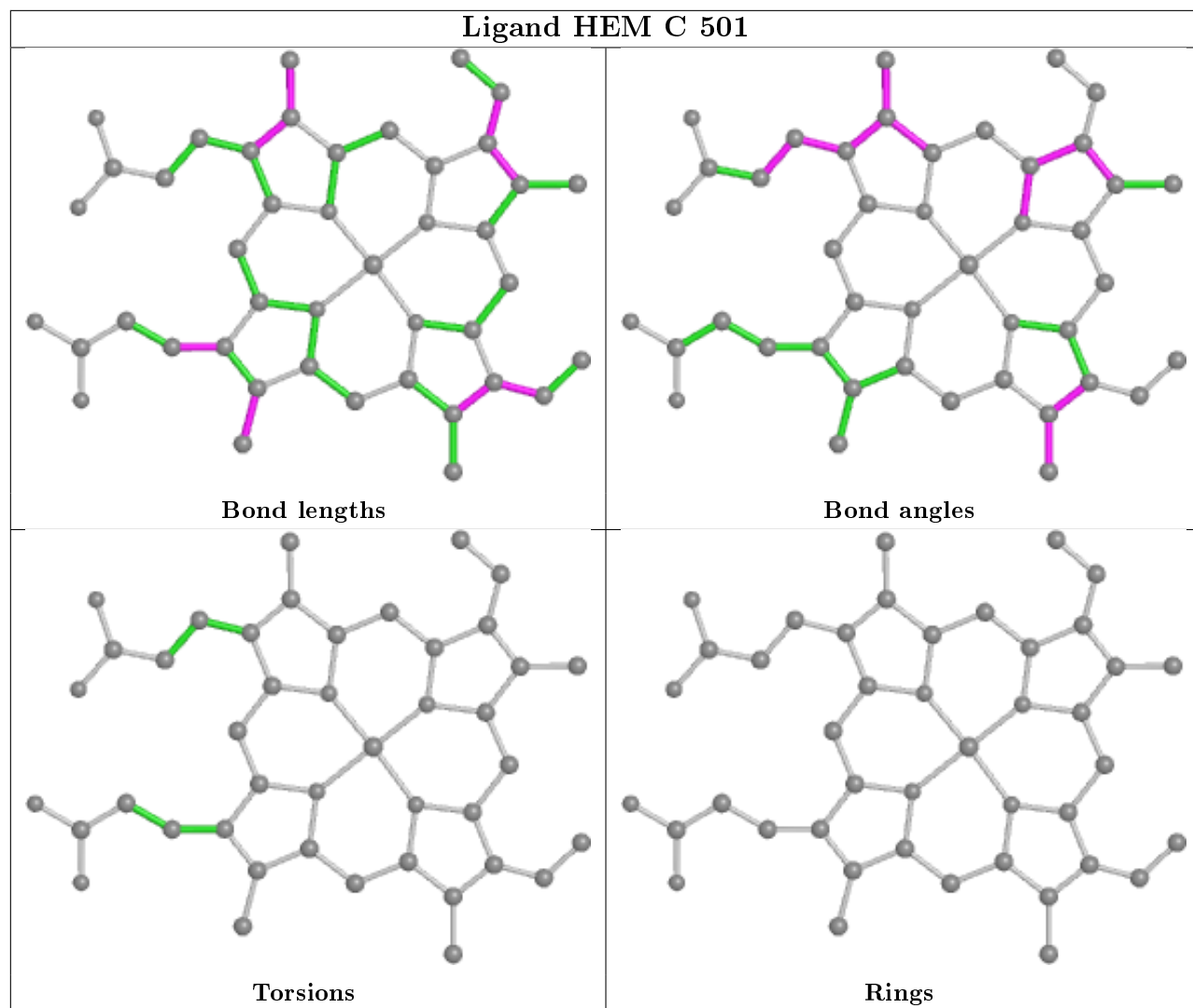


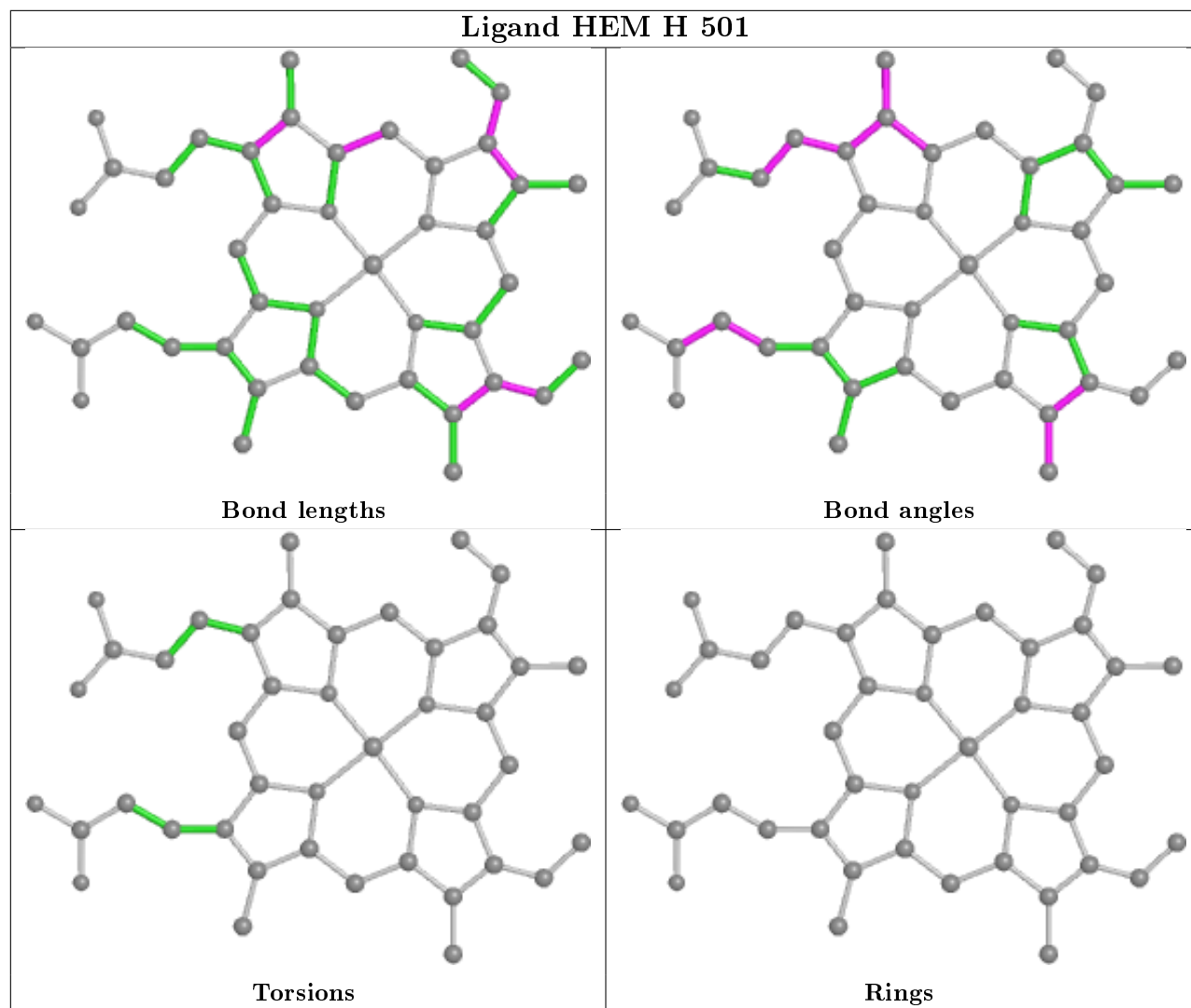


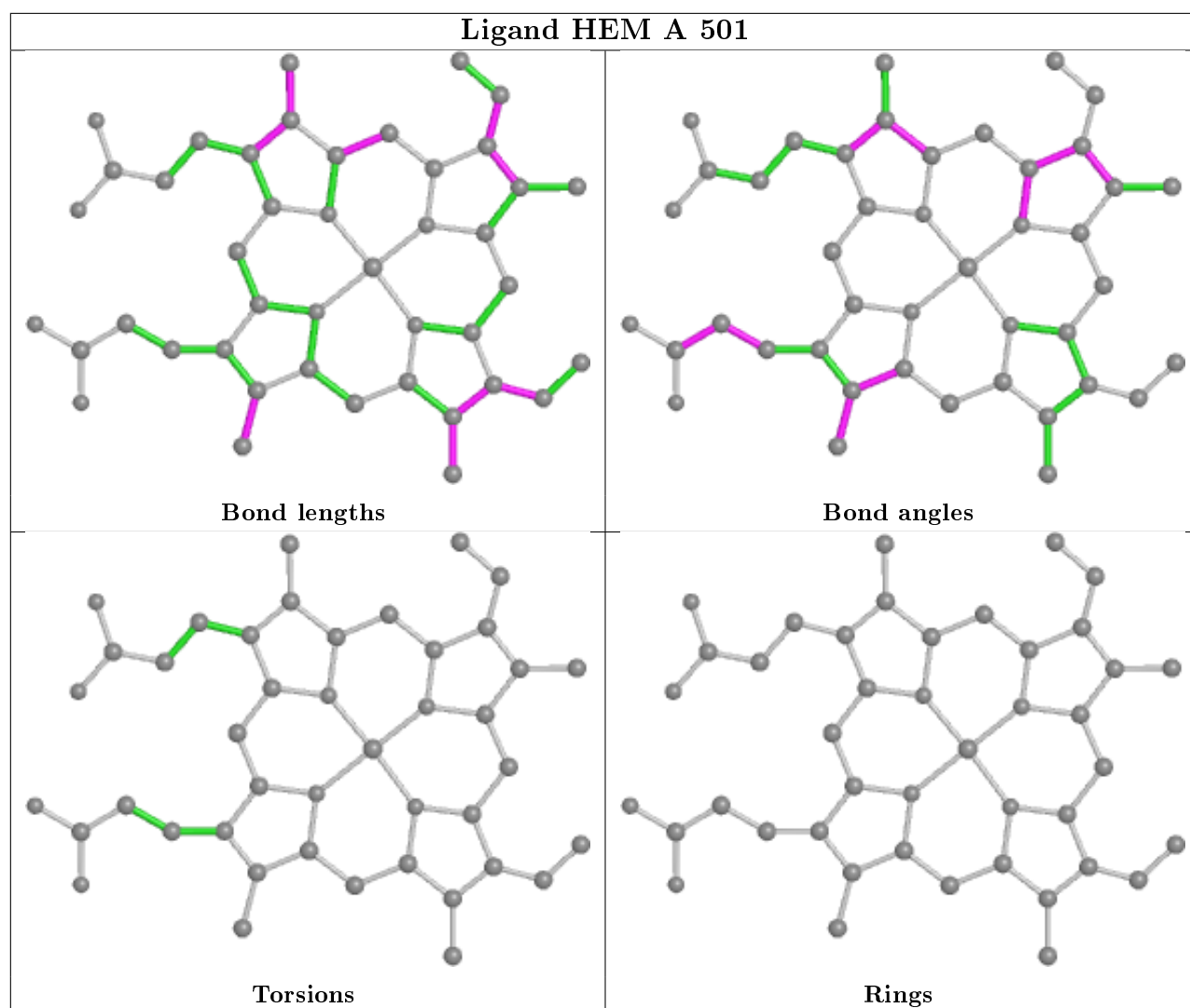












## 5.7 Other polymers [i](#)

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

### 6.1 Protein, DNA and RNA chains

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	464/476 (97%)	0.21	0	100	100	20, 35, 53, 63	0
1	B	464/476 (97%)	0.21	0	100	100	19, 35, 54, 62	0
1	C	464/476 (97%)	0.16	1 (0%)	95	97	19, 33, 48, 58	0
1	D	464/476 (97%)	0.19	1 (0%)	95	97	17, 35, 55, 63	0
1	E	464/476 (97%)	0.25	11 (2%)	59	68	27, 48, 70, 78	0
1	F	464/476 (97%)	0.63	32 (6%)	16	24	27, 60, 85, 91	0
1	G	463/476 (97%)	0.65	34 (7%)	15	22	29, 59, 78, 88	0
1	H	459/476 (96%)	1.01	86 (18%)	1	2	28, 71, 92, 96	0
All	All	3706/3808 (97%)	0.41	165 (4%)	33	46	17, 44, 81, 96	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	141	GLY	6.4
1	H	491	PHE	6.1
1	F	491	PHE	5.2
1	H	468	PRO	4.9
1	H	453	PHE	4.8
1	G	419	LYS	4.7
1	F	141	GLY	4.6
1	G	491	PHE	4.5
1	F	168	ILE	4.5
1	H	273	ILE	4.4
1	F	172	PHE	4.3
1	H	343	PHE	4.3
1	H	416	PHE	4.3
1	H	420	LYS	4.2
1	F	206	LEU	4.2
1	H	317	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	H	434	ILE	4.0
1	E	420	LYS	3.9
1	G	456	ILE	3.9
1	H	489	MET	3.8
1	H	454	THR	3.7
1	H	133	ALA	3.6
1	H	452	PHE	3.6
1	H	156	LEU	3.6
1	H	406	SER	3.6
1	H	428	ALA	3.5
1	H	450	PHE	3.4
1	G	165	GLY	3.4
1	H	154	GLY	3.4
1	H	153	ALA	3.4
1	G	317	LEU	3.4
1	H	259	LEU	3.4
1	H	449	LEU	3.3
1	G	471	ILE	3.3
1	F	355	VAL	3.3
1	H	347	ALA	3.2
1	H	267	PHE	3.2
1	G	282	PRO	3.2
1	G	157	ILE	3.1
1	F	247	PHE	3.1
1	G	420	LYS	3.1
1	H	316	LEU	3.1
1	H	261	PRO	3.1
1	H	462	PHE	3.1
1	G	468	PRO	3.1
1	H	136	ARG	3.1
1	H	159	ALA	3.1
1	F	143	ARG	3.0
1	E	343	PHE	3.0
1	G	462	PHE	3.0
1	F	451	LEU	3.0
1	H	315	LEU	2.9
1	H	426	SER	2.9
1	H	53	GLN	2.9
1	E	143	ARG	2.9
1	H	352	THR	2.9
1	F	492	LEU	2.9
1	H	362	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	288	LEU	2.9
1	G	173	PHE	2.9
1	H	330	GLU	2.8
1	E	135	LEU	2.8
1	H	350	PRO	2.8
1	H	405	PHE	2.8
1	G	323	VAL	2.8
1	H	351	TYR	2.8
1	H	412	ASN	2.8
1	G	188	GLY	2.7
1	H	334	VAL	2.7
1	H	333	ARG	2.7
1	F	261	PRO	2.7
1	H	263	SER	2.7
1	H	98	PHE	2.7
1	H	447	MET	2.7
1	H	427	ASP	2.7
1	H	161	ARG	2.7
1	H	271	PHE	2.7
1	F	461	ARG	2.7
1	F	191	PHE	2.7
1	G	140	VAL	2.7
1	H	483	ILE	2.7
1	H	430	VAL	2.7
1	G	464	SER	2.6
1	H	326	LYS	2.6
1	F	189	ASP	2.6
1	G	408	PRO	2.6
1	H	417	LEU	2.6
1	G	211	PHE	2.6
1	H	340	GLN	2.6
1	H	138	PHE	2.5
1	H	463	LYS	2.5
1	H	476	LYS	2.5
1	H	329	GLU	2.5
1	F	282	PRO	2.5
1	H	135	LEU	2.5
1	G	213	ALA	2.5
1	H	348	LYS	2.5
1	C	280	LYS	2.4
1	H	325	ALA	2.4
1	F	263	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	338	ASN	2.4
1	G	138	PHE	2.4
1	H	469	LYS	2.4
1	H	185	ILE	2.4
1	F	173	PHE	2.4
1	F	280	LYS	2.4
1	H	363	GLY	2.4
1	E	352	THR	2.4
1	G	218	GLN	2.4
1	H	187	PHE	2.4
1	H	145	ILE	2.3
1	F	202	LEU	2.3
1	G	480	PHE	2.3
1	G	475	PRO	2.3
1	F	174	LEU	2.3
1	H	177	THR	2.3
1	H	472	ASP	2.3
1	F	259	LEU	2.3
1	H	264	PRO	2.3
1	H	402	PRO	2.3
1	H	493	PRO	2.3
1	H	157	ILE	2.3
1	F	447	MET	2.3
1	F	450	PHE	2.3
1	G	423	PHE	2.3
1	H	419	LYS	2.3
1	D	189	ASP	2.2
1	H	280	LYS	2.2
1	F	411	PHE	2.2
1	G	153	ALA	2.2
1	H	182	ILE	2.2
1	F	420	LYS	2.2
1	H	403	ARG	2.2
1	G	327	VAL	2.2
1	H	471	ILE	2.2
1	G	461	ARG	2.2
1	G	204	MET	2.2
1	G	463	LYS	2.2
1	G	137	GLY	2.1
1	H	309	THR	2.1
1	H	158	ASP	2.1
1	E	421	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	144	GLY	2.1
1	E	348	LYS	2.1
1	H	487	TYR	2.1
1	H	456	ILE	2.1
1	F	187	PHE	2.1
1	F	198	PHE	2.1
1	E	335	ILE	2.1
1	E	453	PHE	2.1
1	E	460	PHE	2.1
1	F	348	LYS	2.1
1	H	247	PHE	2.1
1	F	493	PRO	2.1
1	H	147	GLU	2.1
1	H	365	MET	2.1
1	H	90	ALA	2.1
1	G	210	GLN	2.0
1	G	315	LEU	2.0
1	E	469	LYS	2.0
1	F	318	MET	2.0
1	H	414	GLN	2.0
1	H	346	ARG	2.0
1	F	31	GLY	2.0
1	G	187	PHE	2.0

## 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 monosaccharides 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.

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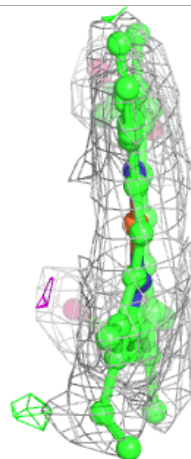
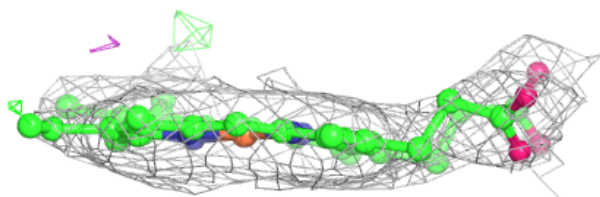
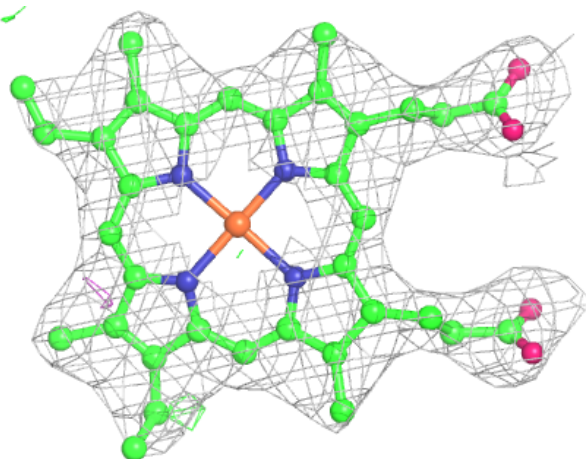
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	0QA	E	502	15/15	0.90	0.28	71,74,76,78	0
3	0QA	C	502	15/15	0.91	0.22	48,55,58,67	0
3	0QA	F	502	15/15	0.91	0.35	84,85,86,87	0
4	GOL	G	502	6/6	0.92	0.16	54,56,58,58	0
3	0QA	B	502	15/15	0.92	0.21	42,51,59,59	0
3	0QA	A	502	15/15	0.94	0.24	57,62,71,72	0
4	GOL	H	502	6/6	0.94	0.27	33,36,42,50	0
3	0QA	D	502	15/15	0.94	0.21	48,55,58,67	0
2	HEM	H	501	43/43	0.96	0.16	47,52,60,63	0
2	HEM	F	501	43/43	0.97	0.16	37,49,54,59	0
2	HEM	C	501	43/43	0.98	0.15	12,22,27,28	0
2	HEM	G	501	43/43	0.98	0.15	33,38,43,47	0
2	HEM	A	501	43/43	0.98	0.17	21,27,31,36	0
2	HEM	E	501	43/43	0.98	0.15	30,35,37,39	0
2	HEM	B	501	43/43	0.98	0.17	18,25,29,32	0
2	HEM	D	501	43/43	0.98	0.16	18,26,29,30	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.

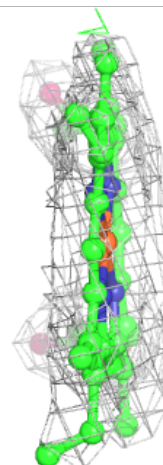
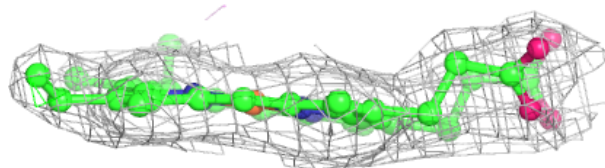
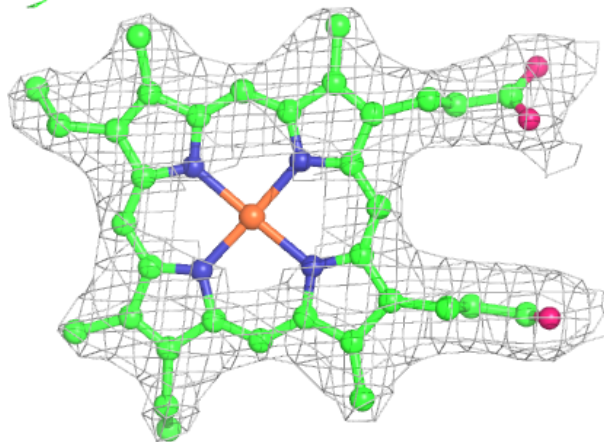
**Electron density around HEM H 501:**

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



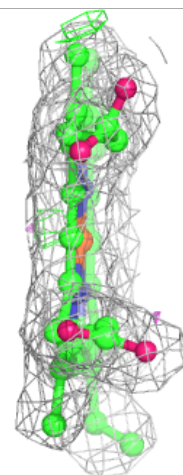
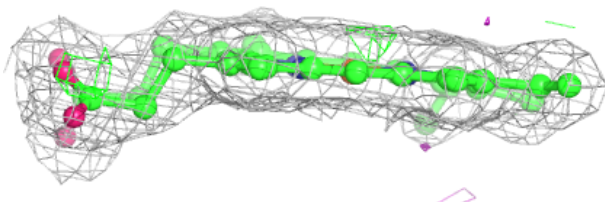
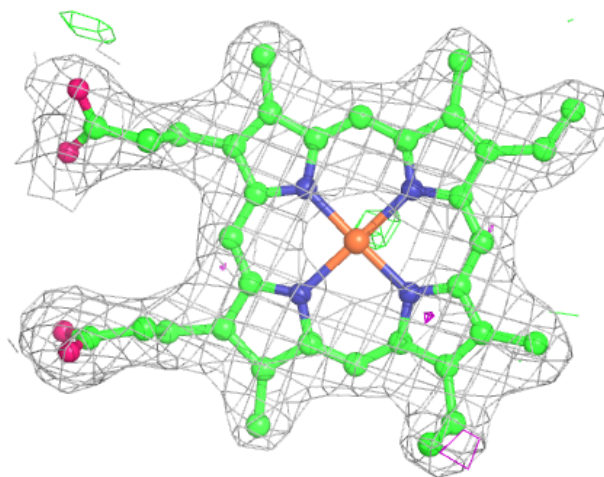
**Electron density around HEM F 501:**

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



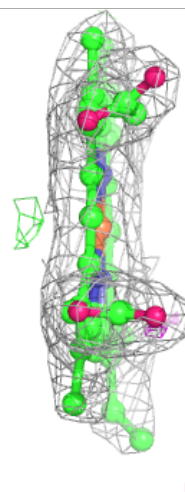
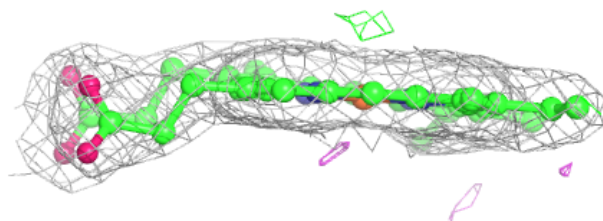
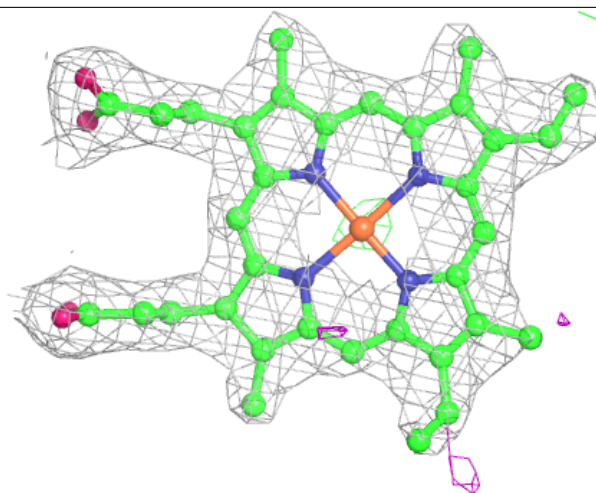
**Electron density around HEM C 501:**

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



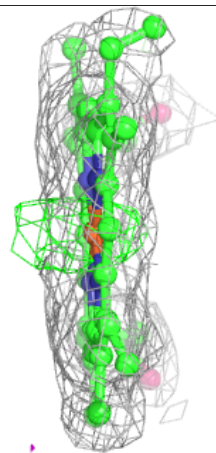
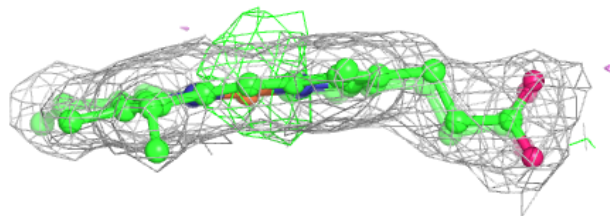
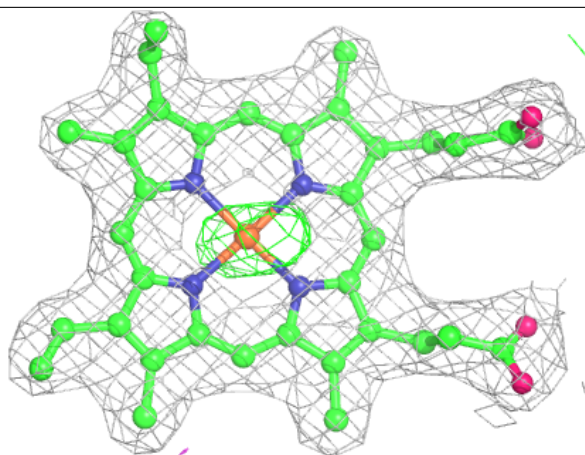
**Electron density around HEM G 501:**

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



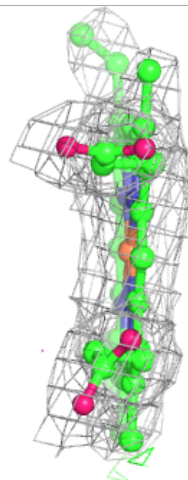
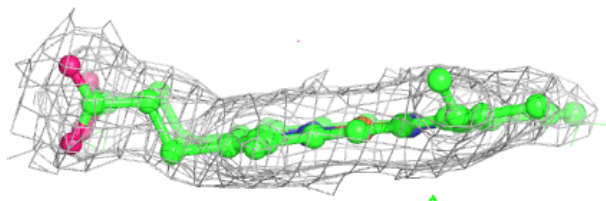
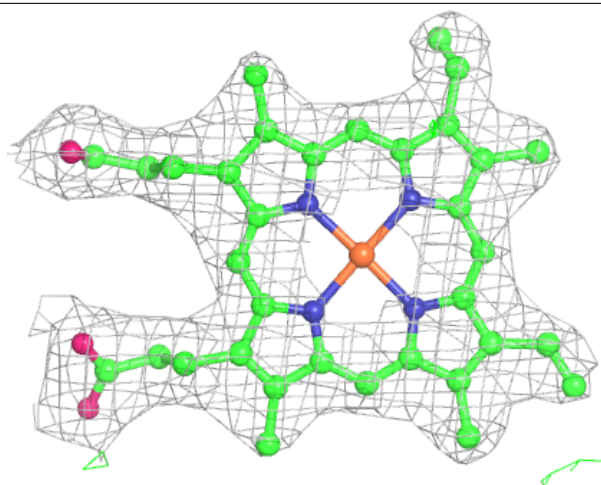
**Electron density around HEM A 501:**

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



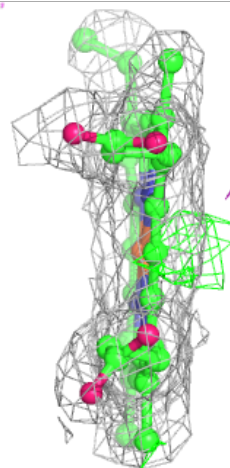
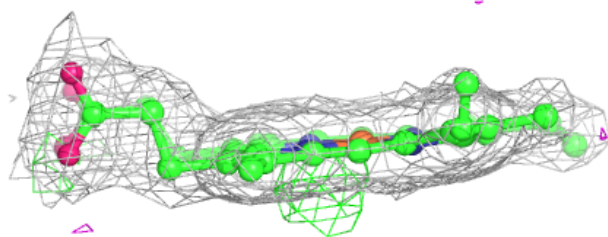
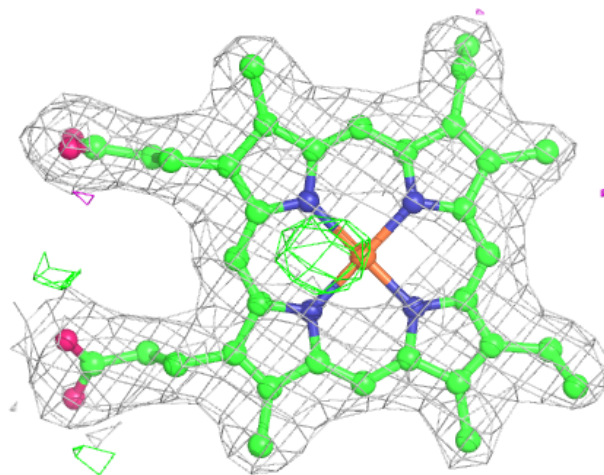
**Electron density around HEM E 501:**

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

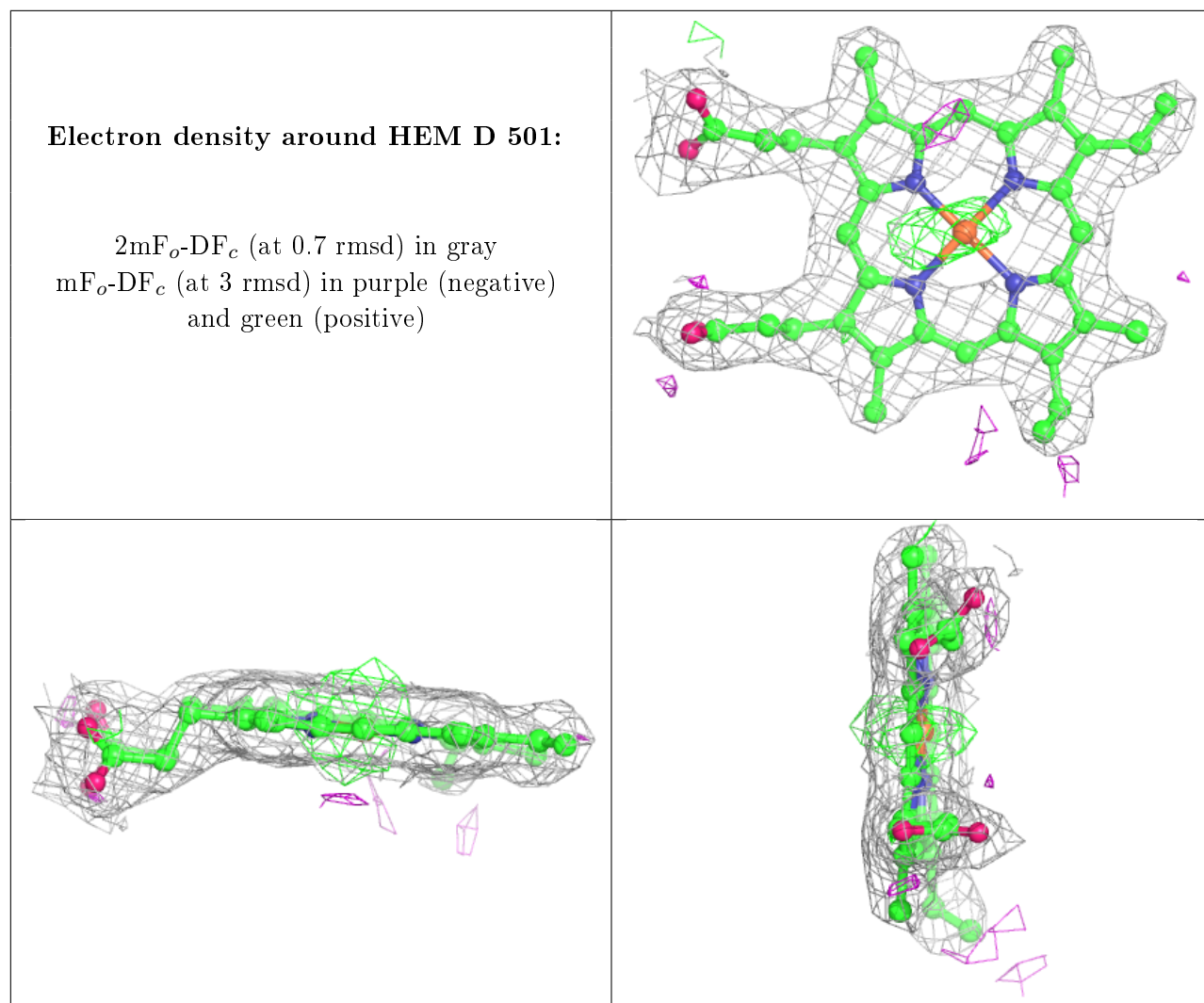


**Electron density around HEM B 501:**

$2mF_o-DF_c$  (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.