



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 06:52 pm BST

PDB ID : 3T3S
Title : Human Cytochrome P450 2A13 in complex with Pilocarpine
Authors : DeVore, N.M.; Scott, E.E.
Deposited on : 2011-07-25
Resolution : 3.00 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

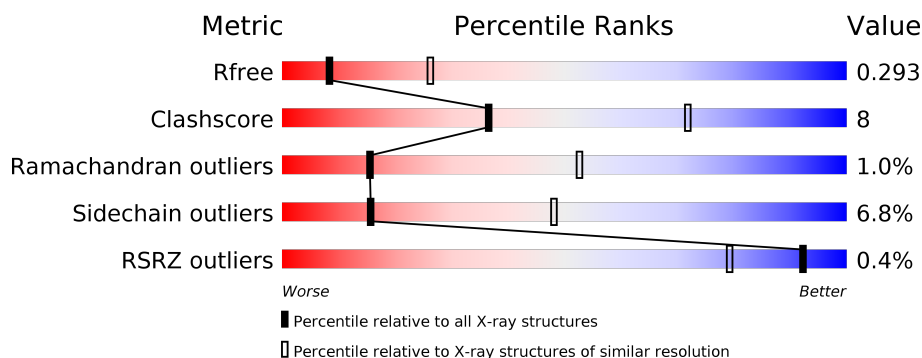
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 ≥ 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>76%</div> <div>19%</div> <div>• •</div> </div>
1	B	476	<div> <div>72%</div> <div>23%</div> <div>• •</div> </div>
1	C	476	<div> <div>79%</div> <div>17%</div> <div>• •</div> </div>
1	D	476	<div> <div>81%</div> <div>15%</div> <div>• •</div> </div>
1	E	476	<div> <div>78%</div> <div>18%</div> <div>• •</div> </div>
1	F	476	<div> <div>75%</div> <div>21%</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	9PL	C	1	-	-	X	-
3	9PL	E	1	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30483 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	0	0	0
			3759	2419	650	672	18			
1	B	464	Total	C	N	O	S	0	0	0
			3763	2421	650	674	18			
1	C	464	Total	C	N	O	S	0	0	0
			3755	2416	649	672	18			
1	D	464	Total	C	N	O	S	0	0	0
			3763	2421	650	674	18			
1	E	464	Total	C	N	O	S	0	0	0
			3755	2416	649	672	18			
1	F	464	Total	C	N	O	S	0	0	0
			3747	2407	650	672	18			
1	G	464	Total	C	N	O	S	0	0	0
			3743	2407	646	672	18			
1	H	464	Total	C	N	O	S	0	0	0
			3732	2396	648	670	18			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	EXPRESSION TAG	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	-	EXPRESSION TAG	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	-	EXPRESSION TAG	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	-	EXPRESSION TAG	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	-	EXPRESSION TAG	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

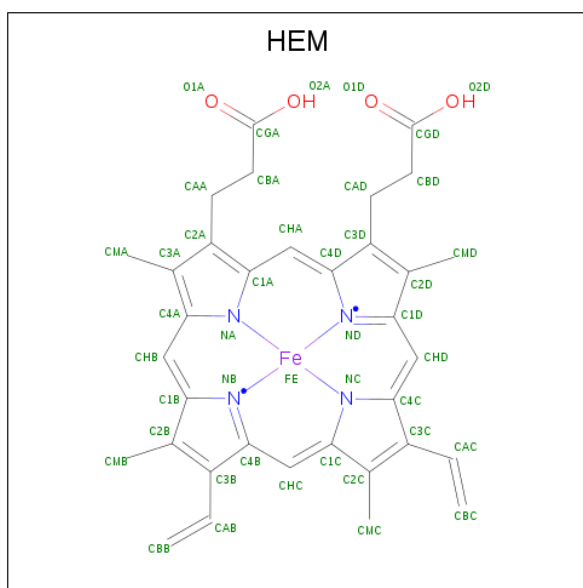
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Chain	Residue	Modelled	Actual	Comment	Reference
E	30	LYS	-	EXPRESSION TAG	UNP Q16696
E	495	HIS	-	EXPRESSION TAG	UNP Q16696
E	496	HIS	-	EXPRESSION TAG	UNP Q16696
E	497	HIS	-	EXPRESSION TAG	UNP Q16696
E	498	HIS	-	EXPRESSION TAG	UNP Q16696
F	23	MET	-	EXPRESSION TAG	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	-	EXPRESSION TAG	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	-	EXPRESSION TAG	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

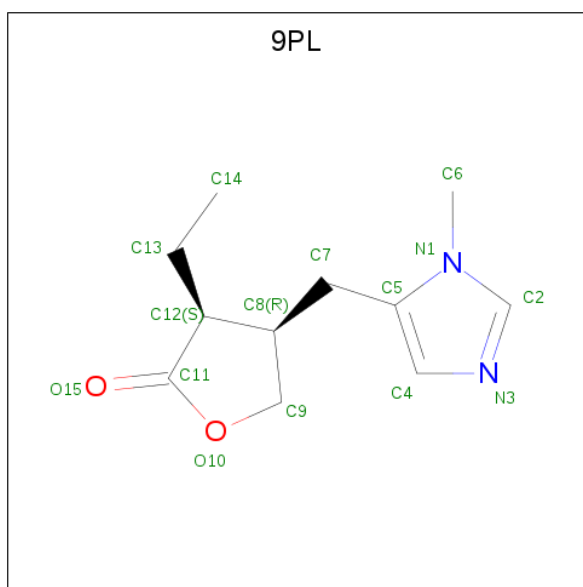
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
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 (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		
3	E	1	Total	C	N	O	0	0
			15	11	2	2		
3	F	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	5	Total	O	0	0
			5	5		
4	C	4	Total	O	0	0
			4	4		
4	D	5	Total	O	0	0
			5	5		
4	E	8	Total	O	0	0
			8	8		
4	G	1	Total	O	0	0
			1	1		

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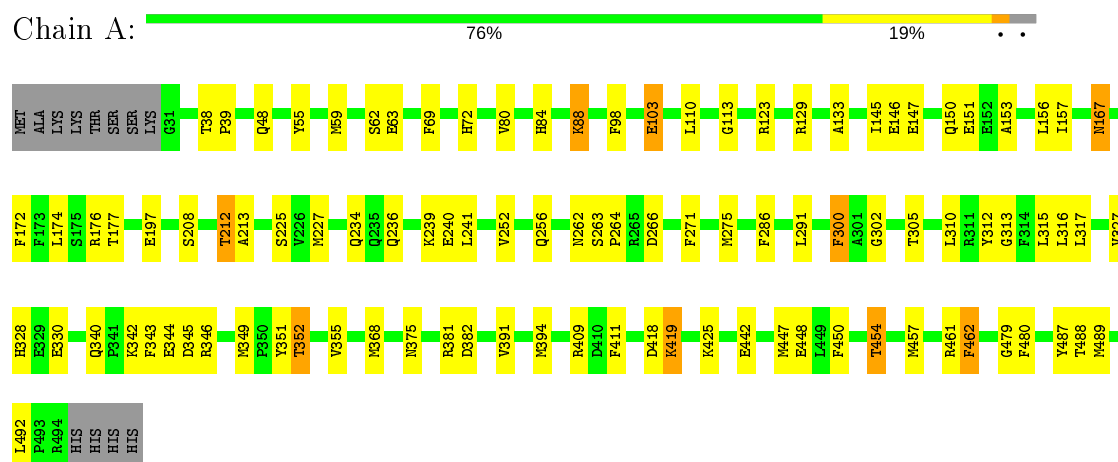
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	4	Total	O	0	0
			4	4		

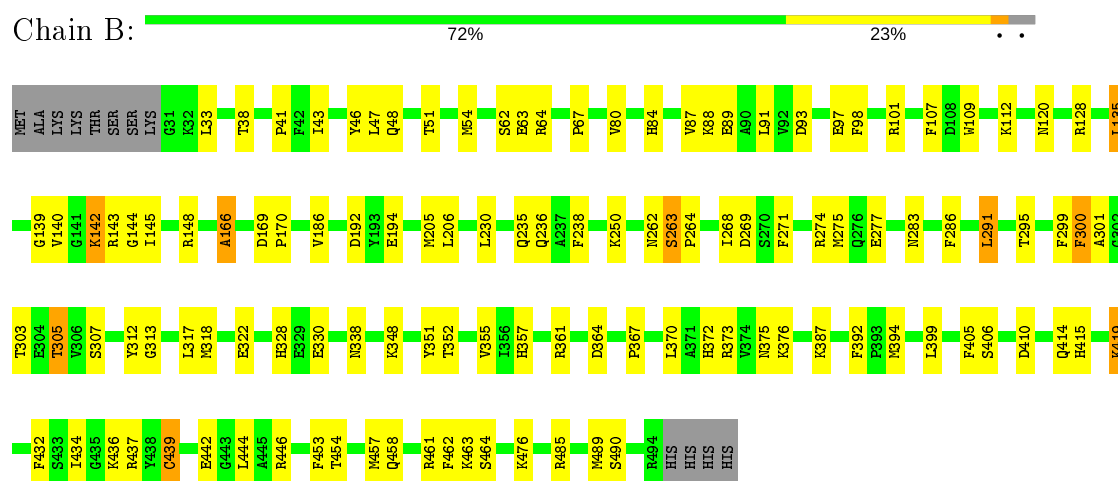
3 Residue-property plots

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.

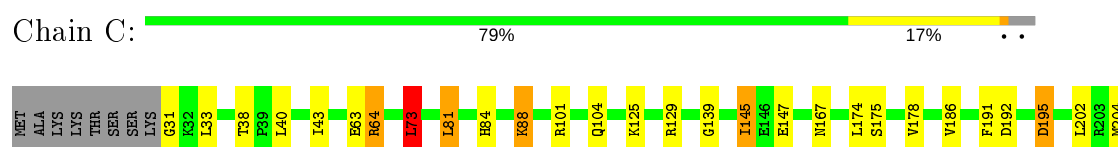
• Molecule 1: Cytochrome P450 2A13

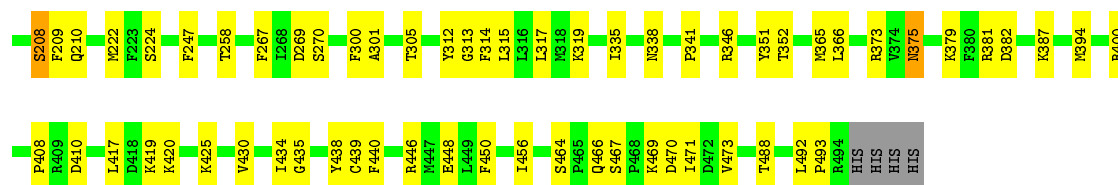


• Molecule 1: Cytochrome P450 2A13

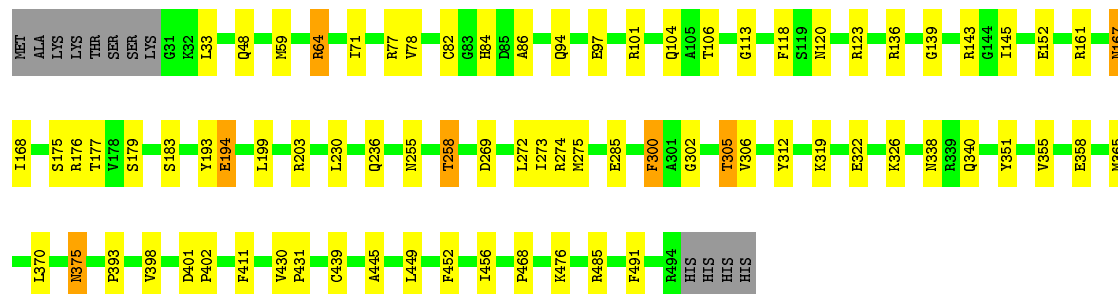
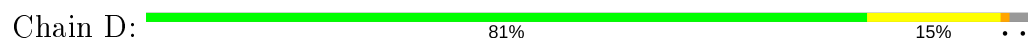


• Molecule 1: Cytochrome P450 2A13

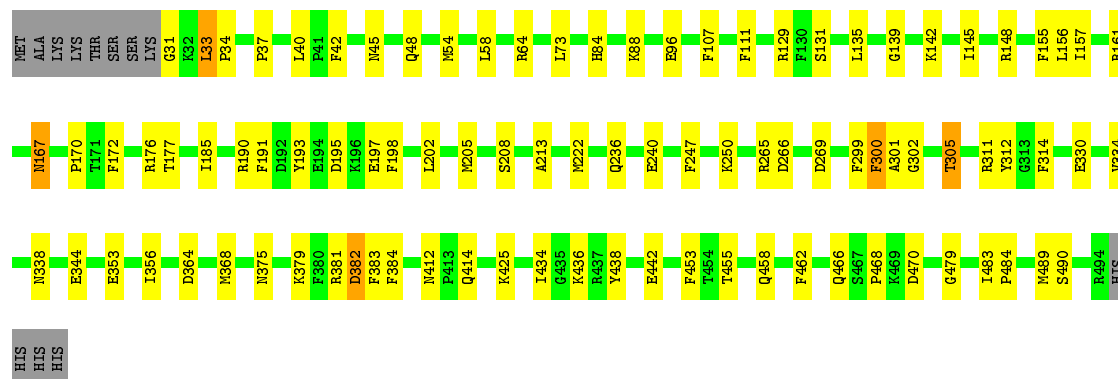
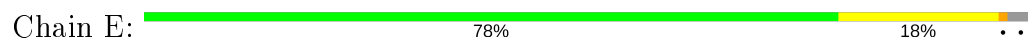




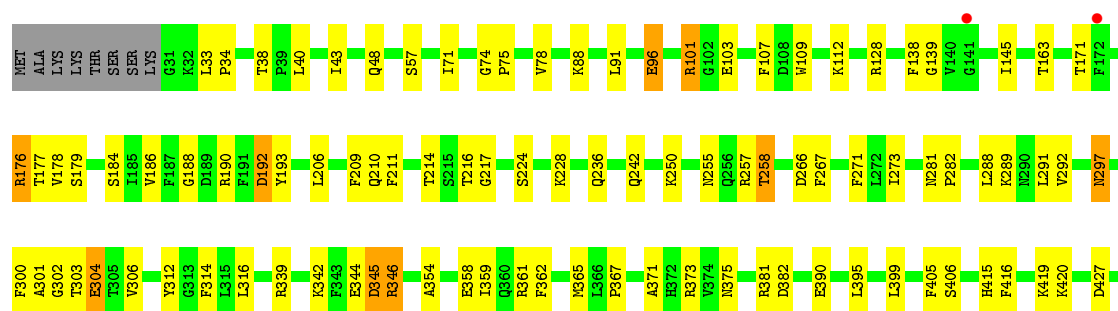
• Molecule 1: Cytochrome P450 2A13



• Molecule 1: Cytochrome P450 2A13



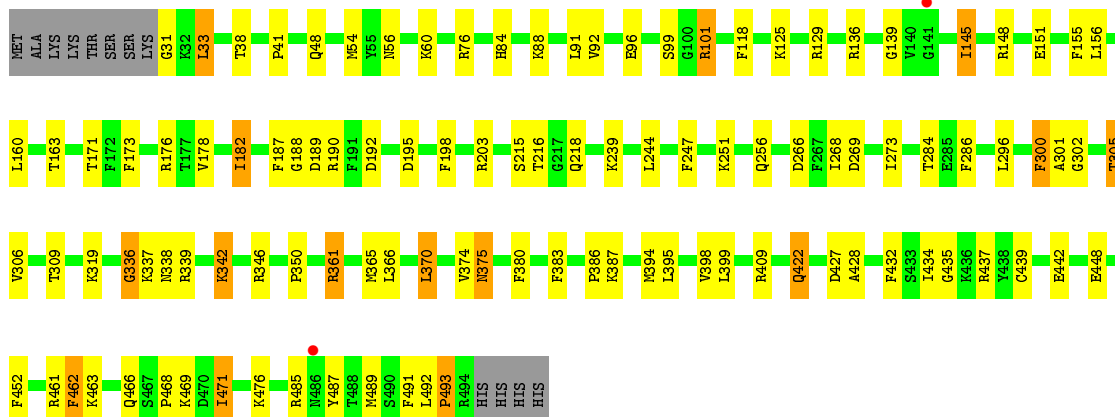
• Molecule 1: Cytochrome P450 2A13





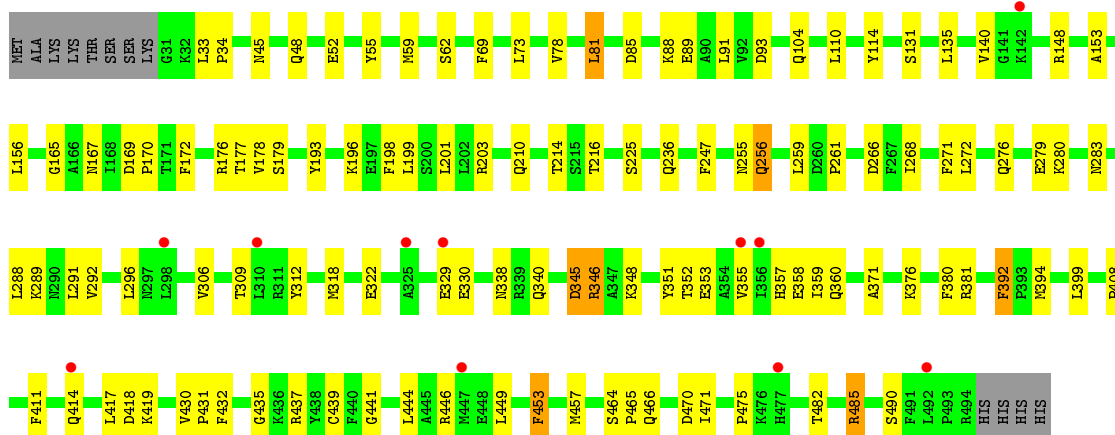
• Molecule 1: Cytochrome P450 2A13

Chain G: 74% 20%



• Molecule 1: Cytochrome P450 2A13

Chain H: 2% 73% 23%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.50Å 119.86Å 154.87Å 101.01° 101.72° 93.59°	Depositor
Resolution (Å)	102.88 – 3.00 102.87 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (102.88-3.00) 98.3 (102.87-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 3.01Å)	Xtriage
Refinement program	REFMAC 6.1.13	Depositor
R, R_{free}	0.213 , 0.303 0.217 , 0.293	Depositor DCC
R_{free} test set	4826 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	62.1	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	30483	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, 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	0.58	1/3856 (0.0%)	0.66	0/5193
1	B	0.49	0/3860	0.67	2/5198 (0.0%)
1	C	0.50	0/3852	0.64	3/5189 (0.1%)
1	D	0.50	0/3860	0.64	0/5198
1	E	0.46	0/3852	0.60	0/5189
1	F	0.48	0/3843	0.58	0/5176
1	G	0.47	0/3840	0.60	0/5174
1	H	0.47	0/3828	0.59	0/5159
All	All	0.49	1/30791 (0.0%)	0.62	5/41476 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	448	GLU	CD-OE1	-5.12	1.20	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	LEU	CA-CB-CG	5.95	128.98	115.30
1	C	73	LEU	CA-CB-CG	5.37	127.64	115.30
1	C	81	LEU	CA-CB-CG	5.35	127.60	115.30
1	C	33	LEU	CA-CB-CG	5.06	126.94	115.30
1	B	230	LEU	CA-CB-CG	5.03	126.86	115.30

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	3759	0	3724	51	0
1	B	3763	0	3728	78	0
1	C	3755	0	3713	56	0
1	D	3763	0	3728	50	0
1	E	3755	0	3713	54	0
1	F	3747	0	3699	56	0
1	G	3743	0	3684	59	0
1	H	3732	0	3664	61	0
2	A	43	0	30	3	0
2	B	43	0	30	3	0
2	C	43	0	30	10	0
2	D	43	0	30	13	0
2	E	43	0	30	5	0
2	F	43	0	30	6	0
2	G	43	0	30	5	0
2	H	43	0	30	5	0
3	A	15	0	15	3	0
3	B	15	0	16	6	0
3	C	15	0	16	12	0
3	D	15	0	16	4	0
3	E	15	0	16	8	0
3	F	15	0	16	2	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	4	0	0	1	0
4	D	5	0	0	1	0
4	E	8	0	0	1	0
4	G	1	0	0	1	0
4	H	4	0	0	1	0
All	All	30483	0	29988	479	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 8.

All (479) 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:305:THR:HG21	3:C:1:9PL:H2	1.37	1.05
1:B:305:THR:HG23	3:B:1:9PL:H6B	1.45	0.97
1:C:305:THR:CG2	3:C:1:9PL:H2	1.97	0.95
1:D:64:ARG:CG	1:D:64:ARG:HH11	1.81	0.93
1:B:166:ALA:O	1:B:490:SER:HB3	1.69	0.92
1:E:462:PHE:HD1	1:E:489:MET:HE1	1.35	0.90
1:E:305:THR:CG2	3:E:1:9PL:H2	2.06	0.86
1:E:305:THR:HG21	3:E:1:9PL:H2	1.59	0.85
1:D:161:ARG:HH11	1:D:161:ARG:HG3	1.38	0.85
1:G:31:GLY:HA2	4:G:1:HOH:O	1.76	0.85
1:C:31:GLY:HA2	4:C:12:HOH:O	1.78	0.83
1:B:107:PHE:CZ	3:B:1:9PL:H14	2.14	0.82
1:C:209:PHE:HE1	3:C:1:9PL:H14B	1.45	0.82
1:C:439:CYS:HB2	2:C:500:HEM:C1A	2.16	0.81
1:C:366:LEU:HD21	3:C:1:9PL:H6B	1.60	0.81
1:F:176:ARG:HB2	1:F:176:ARG:HH11	1.44	0.80
1:D:64:ARG:HG2	1:D:64:ARG:HH11	1.45	0.80
1:B:305:THR:CG2	3:B:1:9PL:H6B	2.13	0.79
1:E:167:ASN:HD22	1:E:490:SER:HB3	1.49	0.77
1:A:330:GLU:OE1	1:A:352:THR:HG22	1.86	0.76
1:G:375:ASN:O	1:G:387:LYS:HB2	1.86	0.76
1:C:440:PHE:CZ	2:C:500:HEM:HMD2	2.21	0.76
1:B:107:PHE:CE2	3:B:1:9PL:H14	2.23	0.74
3:D:1:9PL:H6	3:D:1:9PL:H14B	1.70	0.74
1:C:175:SER:HB3	1:C:202:LEU:HD22	1.70	0.74
1:E:462:PHE:HD1	1:E:489:MET:CE	2.01	0.74
1:F:109:TRP:O	1:F:112:LYS:HE3	1.87	0.73
1:F:211:PHE:O	1:F:214:THR:HG22	1.89	0.72
1:B:186:VAL:CG1	1:B:295:THR:CG2	2.68	0.72
1:G:139:GLY:O	1:G:145:ILE:HB	1.89	0.72
1:G:96:GLU:O	1:G:375:ASN:ND2	2.24	0.71
1:C:440:PHE:CZ	2:C:500:HEM:CMD	2.73	0.71
1:B:186:VAL:HG13	1:B:295:THR:HG23	1.72	0.71
1:B:330:GLU:OE1	1:B:352:THR:HG23	1.91	0.70
1:E:161:ARG:HG2	1:E:161:ARG:HH11	1.56	0.70
1:E:462:PHE:CD1	1:E:489:MET:HE1	2.24	0.70
1:E:302:GLY:HA2	2:E:500:HEM:HMC2	1.71	0.70
1:F:206:LEU:O	1:F:210:GLN:HG2	1.93	0.69
1:H:485:ARG:HG2	1:H:485:ARG:HH11	1.56	0.69
1:B:84:HIS:NE2	1:B:88:LYS:HE2	2.06	0.69
1:C:191:PHE:HZ	1:C:247:PHE:HZ	1.42	0.68
1:E:167:ASN:ND2	1:E:490:SER:HB3	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:THR:O	1:B:307:SER:HB2	1.94	0.67
1:F:78:VAL:HG22	1:F:390:GLU:HB2	1.75	0.67
1:B:186:VAL:CG1	1:B:295:THR:HG23	2.25	0.67
1:A:212:THR:HB	1:A:480:PHE:HB3	1.76	0.67
1:B:264:PRO:HB3	1:B:269:ASP:HB3	1.75	0.67
1:C:381:ARG:O	1:C:382:ASP:HB2	1.94	0.66
1:D:94:GLN:HG2	1:D:97:GLU:OE1	1.95	0.66
1:B:462:PHE:HD1	1:B:489:MET:HE1	1.58	0.66
1:D:370:LEU:HD13	2:D:500:HEM:HAA1	1.76	0.66
1:F:186:VAL:HA	1:F:267:PHE:HB3	1.78	0.66
1:D:33:LEU:HD21	1:D:77:ARG:HD2	1.76	0.66
1:F:271:PHE:HB3	1:F:291:LEU:HD13	1.79	0.65
1:C:209:PHE:HE1	3:C:1:9PL:C14	2.10	0.65
1:C:191:PHE:HZ	1:C:247:PHE:CZ	2.14	0.65
1:H:172:PHE:HB3	1:H:176:ARG:NH2	2.11	0.65
2:D:500:HEM:HHA	2:D:500:HEM:CBA	2.27	0.65
1:C:435:GLY:O	1:C:438:TYR:HD2	1.81	0.64
1:B:47:LEU:HD21	1:E:40:LEU:HD21	1.78	0.64
1:H:355:VAL:O	1:H:359:ILE:HD12	1.98	0.64
1:F:178:VAL:HG11	1:F:306:VAL:HB	1.80	0.64
1:G:462:PHE:HD1	1:G:491:PHE:CE2	2.16	0.64
1:A:262:ASN:OD1	1:B:436:LYS:HE3	1.98	0.64
1:D:64:ARG:HG3	1:D:64:ARG:HH11	1.62	0.64
1:F:214:THR:HG23	1:F:217:GLY:H	1.63	0.64
2:F:500:HEM:HBA2	2:F:500:HEM:HHA	1.79	0.63
1:A:344:GLU:C	1:A:346:ARG:H	2.02	0.63
1:E:139:GLY:O	1:E:145:ILE:HB	1.98	0.63
1:G:336:GLY:O	1:G:338:ASN:N	2.31	0.63
1:G:54:MET:HG3	1:G:218:GLN:OE1	1.97	0.63
1:C:439:CYS:HB2	2:C:500:HEM:NA	2.13	0.63
1:H:255:ASN:HD22	1:H:268:ILE:HB	1.64	0.63
2:D:500:HEM:HHA	2:D:500:HEM:HBA1	1.79	0.62
2:E:500:HEM:HMB2	2:E:500:HEM:HBB2	1.79	0.62
1:E:64:ARG:NH2	4:E:21:HOH:O	2.32	0.62
1:A:227:MET:O	1:A:234:GLN:NE2	2.31	0.62
1:C:375:ASN:ND2	1:C:375:ASN:H	1.98	0.62
1:H:358:GLU:HG3	1:H:411:PHE:CE1	2.35	0.62
1:E:37:PRO:HB3	1:E:48:GLN:OE1	2.00	0.61
1:G:394:MET:O	1:G:398:VAL:HG23	2.00	0.61
1:G:487:TYR:CD1	1:G:489:MET:HG2	2.35	0.61
1:B:462:PHE:HD1	1:B:489:MET:CE	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:381:ARG:O	1:E:382:ASP:HB2	2.01	0.61
1:F:405:PHE:HD2	1:F:415:HIS:HB3	1.66	0.60
1:A:418:ASP:HB2	1:A:419:LYS:HE2	1.83	0.60
2:C:500:HEM:ND	3:C:1:9PL:H4	2.16	0.60
1:H:430:VAL:N	1:H:431:PRO:HD3	2.17	0.60
1:A:349:MET:HB3	1:A:352:THR:CG2	2.32	0.60
1:H:353:GLU:O	1:H:357:HIS:HB2	2.01	0.60
1:A:275:MET:HG2	1:A:286:PHE:O	2.00	0.60
1:G:462:PHE:HD1	1:G:491:PHE:HE2	1.48	0.60
1:B:186:VAL:HG11	1:B:295:THR:HG22	1.84	0.60
1:B:264:PRO:CB	1:B:269:ASP:HB3	2.31	0.59
1:B:186:VAL:HG11	1:B:295:THR:CG2	2.31	0.59
1:C:375:ASN:ND2	1:C:375:ASN:N	2.49	0.59
1:D:64:ARG:CG	1:D:64:ARG:NH1	2.51	0.59
1:B:140:VAL:CG1	1:B:444:LEU:HB2	2.33	0.59
1:D:375:ASN:OD1	1:D:375:ASN:N	2.36	0.59
1:B:462:PHE:HB3	1:B:489:MET:HE3	1.83	0.59
1:A:110:LEU:HB2	1:A:241:LEU:HD13	1.84	0.59
1:B:405:PHE:HB3	1:B:415:HIS:CD2	2.37	0.59
1:A:302:GLY:HA2	2:A:500:HEM:HMC2	1.84	0.59
1:B:62:SER:C	1:B:64:ARG:H	2.06	0.59
1:A:349:MET:HB3	1:A:352:THR:HG23	1.83	0.58
1:D:179:SER:O	1:D:183:SER:OG	2.20	0.58
1:G:487:TYR:HD1	1:G:489:MET:HG2	1.68	0.58
1:H:201:LEU:HD11	1:H:247:PHE:CE2	2.38	0.58
1:B:275:MET:HG2	1:B:286:PHE:O	2.03	0.58
1:H:475:PRO:HB3	1:H:482:THR:HG23	1.85	0.58
1:D:64:ARG:NH1	1:D:64:ARG:HG3	2.18	0.58
1:D:123:ARG:HA	1:D:285:GLU:HG3	1.85	0.58
1:E:33:LEU:HD12	1:E:34:PRO:HD2	1.84	0.58
1:G:462:PHE:CD1	1:G:491:PHE:HE2	2.21	0.57
1:E:54:MET:O	1:E:58:LEU:HG	2.04	0.57
1:C:305:THR:HG21	3:C:1:9PL:C2	2.24	0.57
1:A:167:ASN:OD1	1:A:488:THR:HB	2.05	0.57
1:C:209:PHE:CE1	3:C:1:9PL:H14B	2.34	0.57
1:G:366:LEU:HD12	2:G:500:HEM:CHB	2.35	0.56
1:C:125:LYS:O	1:C:129:ARG:HB2	2.05	0.56
1:D:305:THR:HG22	1:D:365:MET:HG3	1.86	0.56
1:F:101:ARG:NH1	1:F:371:ALA:O	2.37	0.56
1:F:271:PHE:CD2	1:F:291:LEU:HB2	2.40	0.56
1:C:301:ALA:HB2	3:C:1:9PL:H9A	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:MET:HE2	1:B:300:PHE:HA	1.87	0.56
1:C:375:ASN:HD22	1:C:375:ASN:N	2.04	0.56
1:F:460:PHE:CD1	1:F:491:PHE:HB3	2.41	0.56
1:B:364:ASP:O	1:B:367:PRO:HD3	2.06	0.56
1:E:353:GLU:HA	1:E:356:ILE:HD12	1.89	0.55
1:E:96:GLU:OE1	1:E:436:LYS:HD2	2.06	0.55
2:G:500:HEM:HHA	2:G:500:HEM:HBA2	1.88	0.55
1:H:351:TYR:HD1	1:H:417:LEU:HD11	1.72	0.55
1:B:357:HIS:CE1	1:B:446:ARG:NH2	2.75	0.55
1:F:316:LEU:HD21	1:F:362:PHE:CE2	2.41	0.55
1:C:204:MET:O	1:C:208:SER:HB2	2.06	0.55
1:H:256:GLN:OE1	1:H:272:LEU:HD21	2.06	0.54
1:E:205:MET:HE2	1:E:300:PHE:HA	1.88	0.54
1:F:288:LEU:O	1:F:292:VAL:HG23	2.07	0.54
1:H:346:ARG:HH12	1:H:446:ARG:HH21	1.56	0.54
1:B:313:GLY:O	1:B:317:LEU:HG	2.08	0.54
1:D:476:LYS:HB2	1:D:485:ARG:HA	1.89	0.54
1:E:45:ASN:HD22	1:E:48:GLN:HE22	1.55	0.54
1:H:414:GLN:OE1	1:H:417:LEU:HD12	2.07	0.54
1:C:439:CYS:HB2	2:C:500:HEM:CHA	2.37	0.54
1:E:305:THR:HG21	3:E:1:9PL:C2	2.32	0.54
1:C:400:ARG:O	1:C:408:PRO:HB3	2.07	0.53
1:D:175:SER:O	1:D:179:SER:HB2	2.07	0.53
1:E:107:PHE:O	1:E:111:PHE:HD1	1.90	0.53
1:H:399:LEU:HD21	1:H:431:PRO:HG3	1.90	0.53
1:B:463:LYS:HG3	1:B:464:SER:N	2.23	0.53
1:H:131:SER:O	1:H:135:LEU:HD13	2.08	0.53
1:A:208:SER:OG	1:A:240:GLU:HG3	2.07	0.53
1:E:265:ARG:HB2	1:E:269:ASP:OD1	2.09	0.53
1:B:166:ALA:O	1:B:490:SER:CB	2.52	0.53
3:C:1:9PL:H14B	3:C:1:9PL:H6	1.91	0.53
1:G:92:VAL:HG23	1:G:434:ILE:HD12	1.90	0.53
1:E:172:PHE:O	1:E:176:ARG:HG2	2.09	0.53
1:F:40:LEU:HD12	1:F:43:ILE:HD11	1.90	0.52
1:H:179:SER:HG	1:H:198:PHE:HZ	1.57	0.52
1:C:373:ARG:HG3	1:C:373:ARG:HH11	1.74	0.52
1:F:303:THR:HG22	1:F:304:GLU:N	2.25	0.52
1:G:448:GLU:O	1:G:452:PHE:HB2	2.09	0.52
1:H:318:MET:SD	1:H:464:SER:OG	2.67	0.52
1:B:462:PHE:CD1	1:B:489:MET:HE1	2.42	0.52
1:D:101:ARG:NH2	2:D:500:HEM:O2A	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:ILE:HG22	1:D:78:VAL:HB	1.90	0.52
1:G:187:PHE:HB3	1:G:268:ILE:HD12	1.91	0.52
1:D:161:ARG:HG3	1:D:161:ARG:NH1	2.16	0.52
1:C:209:PHE:CE1	3:C:1:9PL:C14	2.92	0.52
1:G:339:ARG:HH12	1:G:342:LYS:CD	2.22	0.52
1:B:419:LYS:HD3	1:B:419:LYS:H	1.74	0.52
1:C:101:ARG:NH2	2:C:500:HEM:O2D	2.43	0.52
3:E:1:9PL:H6	3:E:1:9PL:H14B	1.91	0.52
1:H:439:CYS:HB2	2:H:500:HEM:NA	2.24	0.51
1:F:439:CYS:HB2	2:F:500:HEM:C1A	2.45	0.51
1:H:78:VAL:HG11	1:H:392:PHE:CD2	2.45	0.51
1:C:319:LYS:HD3	1:C:471:ILE:HB	1.92	0.51
2:E:500:HEM:ND	3:E:1:9PL:H4	2.25	0.51
1:G:125:LYS:O	1:G:129:ARG:HB3	2.11	0.51
1:G:192:ASP:HB3	1:G:195:ASP:HB2	1.93	0.51
1:E:197:GLU:OE1	1:E:247:PHE:HE1	1.93	0.51
1:F:302:GLY:HA2	2:F:500:HEM:HMC2	1.91	0.51
1:G:395:LEU:O	1:G:399:LEU:HG	2.11	0.51
1:A:450:PHE:O	1:A:454:THR:OG1	2.28	0.51
1:C:440:PHE:CZ	2:C:500:HEM:HMD1	2.45	0.51
1:H:81:LEU:O	1:H:394:MET:HB2	2.11	0.51
1:A:462:PHE:HB3	1:A:489:MET:CE	2.41	0.51
1:B:453:PHE:O	1:B:457:MET:HG3	2.11	0.51
1:E:176:ARG:HD2	1:E:193:TYR:CD1	2.46	0.51
1:A:252:VAL:O	1:A:256:GLN:HB2	2.11	0.51
1:A:55:TYR:CE2	1:A:59:MET:HG3	2.46	0.50
1:C:381:ARG:O	1:C:382:ASP:CB	2.59	0.50
1:F:257:ARG:O	1:F:258:THR:HG23	2.12	0.50
1:E:157:ILE:HD11	1:E:455:THR:O	2.11	0.50
1:F:447:MET:O	1:F:451:LEU:HB2	2.12	0.50
1:B:432:PHE:HB3	1:B:439:CYS:HB3	1.94	0.50
2:D:500:HEM:C4D	3:D:1:9PL:H4	2.46	0.49
1:G:398:VAL:O	1:G:428:ALA:HB1	2.12	0.49
1:A:457:MET:HG2	1:A:462:PHE:CZ	2.47	0.49
1:C:174:LEU:HD21	1:C:314:PHE:HE1	1.77	0.49
1:D:439:CYS:HB2	2:D:500:HEM:NA	2.27	0.49
1:B:476:LYS:HB2	1:B:485:ARG:HA	1.93	0.49
1:D:230:LEU:HD23	1:G:41:PRO:HB2	1.95	0.49
1:D:351:TYR:O	1:D:355:VAL:HG23	2.13	0.49
1:D:358:GLU:HG3	1:D:411:PHE:CE1	2.47	0.49
1:E:213:ALA:HA	1:E:479:GLY:HA3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:314:PHE:CD2	1:F:314:PHE:N	2.79	0.49
1:F:33:LEU:HG	1:F:34:PRO:HD2	1.94	0.49
1:B:140:VAL:HG13	1:B:444:LEU:HB2	1.95	0.49
1:B:454:THR:O	1:B:458:GLN:HB2	2.13	0.49
1:A:300:PHE:CD2	3:A:1:9PL:H14A	2.48	0.49
1:D:161:ARG:HH11	1:D:161:ARG:CG	2.17	0.49
1:E:208:SER:HB2	1:E:240:GLU:HG3	1.95	0.49
1:F:381:ARG:O	1:F:382:ASP:HB2	2.12	0.49
1:H:167:ASN:HD21	1:H:465:PRO:HG3	1.76	0.49
1:B:262:ASN:O	1:B:263:SER:HB3	2.13	0.49
2:D:500:HEM:HBB2	2:D:500:HEM:CMB	2.42	0.49
1:G:296:LEU:O	1:G:300:PHE:HB2	2.12	0.49
1:H:309:THR:HG21	1:H:360:GLN:HG2	1.95	0.49
1:D:305:THR:HG22	1:D:365:MET:CG	2.42	0.48
1:D:445:ALA:O	1:D:449:LEU:HB2	2.13	0.48
1:E:301:ALA:HB2	3:E:1:9PL:H8	1.94	0.48
1:H:62:SER:HB3	1:H:69:PHE:CE2	2.47	0.48
1:E:34:PRO:HD3	1:E:383:PHE:HB3	1.95	0.48
1:E:84:HIS:NE2	1:E:88:LYS:HE2	2.28	0.48
1:H:441:GLY:HA2	2:H:500:HEM:HBC2	1.94	0.48
1:A:457:MET:HG2	1:A:462:PHE:HZ	1.78	0.48
1:F:314:PHE:HD2	1:F:314:PHE:N	2.11	0.48
1:A:153:ALA:O	1:A:157:ILE:HG12	2.14	0.48
1:A:343:PHE:CE1	1:A:447:MET:HA	2.48	0.48
1:B:375:ASN:O	1:B:387:LYS:HG3	2.13	0.48
1:F:456:ILE:O	1:F:460:PHE:HB2	2.13	0.48
1:B:120:ASN:HD21	1:B:373:ARG:HD2	1.79	0.48
1:A:129:ARG:NH1	1:B:277:GLU:O	2.47	0.48
1:B:361:ARG:HA	1:B:399:LEU:HD22	1.95	0.48
1:D:139:GLY:C	1:D:145:ILE:HG12	2.33	0.48
1:H:355:VAL:HG12	1:H:355:VAL:O	2.14	0.48
1:B:268:ILE:HG23	1:B:291:LEU:HD11	1.95	0.47
1:B:87:VAL:HG12	1:B:434:ILE:HD11	1.96	0.47
1:D:269:ASP:O	1:D:273:ILE:HG13	2.14	0.47
1:F:405:PHE:CD2	1:F:415:HIS:HB3	2.48	0.47
1:H:176:ARG:HD2	1:H:193:TYR:CE2	2.49	0.47
1:G:432:PHE:HB3	1:G:439:CYS:HB3	1.96	0.47
1:H:172:PHE:O	1:H:176:ARG:HG3	2.15	0.47
3:C:1:9PL:H13	3:C:1:9PL:H7	1.73	0.47
1:D:152:GLU:HG3	1:D:177:THR:CG2	2.45	0.47
1:D:84:HIS:HA	1:D:398:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:PHE:CG	1:A:291:LEU:HD13	2.49	0.47
2:F:500:HEM:CBA	2:F:500:HEM:HHA	2.44	0.47
1:G:91:LEU:O	1:G:435:GLY:HA3	2.14	0.47
1:H:91:LEU:O	1:H:435:GLY:CA	2.63	0.47
2:A:500:HEM:HMB2	2:A:500:HEM:HBB2	1.96	0.47
1:C:351:TYR:CD1	1:C:417:LEU:HD11	2.50	0.47
1:B:250:LYS:O	1:B:250:LYS:HG2	2.14	0.47
1:G:448:GLU:O	1:G:452:PHE:HD2	1.98	0.47
1:F:184:SER:O	1:F:188:GLY:HA2	2.15	0.46
1:H:430:VAL:N	1:H:431:PRO:CD	2.78	0.46
1:H:110:LEU:HD21	1:H:296:LEU:HD21	1.96	0.46
1:A:84:HIS:CE1	1:A:88:LYS:HE2	2.50	0.46
1:B:301:ALA:HA	3:B:1:9PL:H6A	1.96	0.46
1:B:97:GLU:HG3	1:B:376:LYS:HE3	1.98	0.46
1:B:67:PRO:HG3	1:C:63:GLU:O	2.15	0.46
1:C:375:ASN:O	1:C:387:LYS:HG3	2.15	0.46
3:E:1:9PL:H13	3:E:1:9PL:H7	1.73	0.46
1:E:205:MET:CE	1:E:300:PHE:HA	2.46	0.46
1:H:288:LEU:O	1:H:292:VAL:HG23	2.16	0.46
1:D:167:ASN:HA	1:D:167:ASN:HD22	1.58	0.46
1:E:156:LEU:HB2	1:E:177:THR:HG21	1.98	0.46
1:F:301:ALA:HB2	3:F:1:9PL:H9A	1.97	0.46
1:H:432:PHE:HA	2:H:500:HEM:HHB	1.96	0.46
1:B:439:CYS:HB2	2:B:500:HEM:NA	2.31	0.46
1:C:139:GLY:O	1:C:145:ILE:HB	2.15	0.46
1:H:114:TYR:CE1	1:H:289:LYS:HE3	2.50	0.46
1:A:381:ARG:O	1:A:382:ASP:HB2	2.15	0.46
1:H:453:PHE:O	1:H:457:MET:HB2	2.16	0.46
1:D:168:ILE:HD11	1:D:491:PHE:CE1	2.51	0.45
1:G:76:ARG:H	1:G:76:ARG:HG3	1.55	0.45
1:A:327:VAL:HG13	1:A:352:THR:HB	1.97	0.45
1:D:430:VAL:N	1:D:431:PRO:CD	2.80	0.45
1:C:40:LEU:HD12	1:C:43:ILE:HD11	1.98	0.45
1:F:439:CYS:HB2	2:F:500:HEM:NA	2.30	0.45
1:B:109:TRP:CH2	1:B:238:PHE:HB3	2.51	0.45
3:D:1:9PL:H7	3:D:1:9PL:H13	1.75	0.45
1:A:146:GLU:O	1:A:150:GLN:HB2	2.17	0.45
1:C:305:THR:HB	2:C:500:HEM:CAB	2.46	0.45
1:E:156:LEU:HD22	1:E:177:THR:HG21	1.98	0.45
1:A:133:ALA:HB1	1:B:274:ARG:HH21	1.82	0.45
1:G:476:LYS:HB2	1:G:485:ARG:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:LEU:HD13	1:A:411:PHE:CE1	2.52	0.45
1:B:107:PHE:CE2	3:B:1:9PL:C14	2.98	0.45
1:E:202:LEU:HA	1:E:205:MET:HB2	1.99	0.45
1:B:98:PHE:O	1:B:372:HIS:ND1	2.46	0.45
1:D:452:PHE:O	1:D:456:ILE:HG13	2.16	0.45
1:F:96:GLU:OE1	1:F:96:GLU:HA	2.17	0.45
1:D:101:ARG:HB3	1:D:120:ASN:ND2	2.32	0.44
1:D:152:GLU:HG3	1:D:177:THR:HG23	1.99	0.44
1:E:131:SER:O	1:E:135:LEU:HB2	2.18	0.44
1:G:432:PHE:CD2	1:G:442:GLU:HG3	2.52	0.44
1:H:432:PHE:HA	2:H:500:HEM:CHB	2.46	0.44
1:A:351:TYR:O	1:A:355:VAL:HG23	2.17	0.44
1:E:381:ARG:O	1:E:382:ASP:CB	2.65	0.44
1:F:344:GLU:C	1:F:346:ARG:H	2.20	0.44
1:G:339:ARG:HH12	1:G:342:LYS:HD2	1.82	0.44
1:D:101:ARG:HB3	1:D:120:ASN:HD21	1.82	0.44
1:F:448:GLU:O	1:F:452:PHE:HB2	2.16	0.44
1:G:182:ILE:HG13	1:G:302:GLY:HA3	1.99	0.44
1:A:103:GLU:H	1:A:103:GLU:HG2	1.66	0.44
1:B:109:TRP:O	1:B:112:LYS:HE2	2.18	0.44
1:H:432:PHE:HB3	1:H:439:CYS:HB3	1.99	0.44
1:B:405:PHE:HB3	1:B:415:HIS:HD2	1.80	0.44
1:F:342:LYS:HD2	1:F:344:GLU:OE1	2.18	0.44
1:F:354:ALA:HB1	1:F:416:PHE:HB2	2.00	0.44
1:G:188:GLY:N	1:G:266:ASP:OD2	2.50	0.44
2:G:500:HEM:CMB	2:G:500:HEM:HBB2	2.48	0.44
1:H:91:LEU:O	1:H:435:GLY:HA3	2.18	0.44
1:B:62:SER:C	1:B:64:ARG:N	2.69	0.44
1:D:101:ARG:NH1	2:D:500:HEM:O2A	2.48	0.44
1:E:142:LYS:HE2	1:G:422:GLN:NE2	2.33	0.44
1:H:178:VAL:HG11	1:H:306:VAL:HB	1.99	0.44
1:A:263:SER:HA	1:A:264:PRO:HD3	1.77	0.44
1:A:98:PHE:CE2	1:A:391:VAL:HG21	2.52	0.44
1:E:466:GLN:OE1	1:H:203:ARG:NH2	2.51	0.44
1:H:33:LEU:HG	1:H:34:PRO:HD2	1.99	0.44
1:H:89:GLU:O	1:H:93:ASP:HB2	2.18	0.44
1:A:84:HIS:NE2	1:A:88:LYS:HE2	2.33	0.43
1:D:176:ARG:NH1	1:D:199:LEU:HD13	2.33	0.43
1:F:361:ARG:HA	1:F:399:LEU:HD13	1.99	0.43
1:F:103:GLU:HG3	1:F:373:ARG:HH22	1.83	0.43
1:B:442:GLU:O	1:B:446:ARG:HG3	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:LYS:HD2	1:D:468:PRO:O	2.18	0.43
2:A:500:HEM:CMB	2:A:500:HEM:HBB2	2.48	0.43
1:C:178:VAL:HG13	1:C:448:GLU:OE1	2.17	0.43
1:D:306:VAL:HG23	2:D:500:HEM:HAB	2.00	0.43
1:F:74:GLY:HA3	1:F:75:PRO:HD2	1.90	0.43
1:A:305:THR:OG1	3:A:1:9PL:H2	2.18	0.43
1:C:73:LEU:HB3	1:C:222:MET:HG2	2.00	0.43
1:H:199:LEU:HD21	1:H:203:ARG:HH21	1.83	0.43
1:E:205:MET:HE3	1:E:299:PHE:CE2	2.53	0.43
1:G:101:ARG:NH2	2:G:500:HEM:O2D	2.51	0.43
1:B:41:PRO:O	1:B:43:ILE:N	2.44	0.43
1:G:319:LYS:HA	1:G:471:ILE:HD12	2.01	0.43
1:H:153:ALA:HA	1:H:156:LEU:HB3	1.99	0.43
1:H:259:LEU:O	1:H:261:PRO:HD3	2.19	0.43
1:H:437:ARG:O	2:H:500:HEM:HBA2	2.18	0.43
1:A:63:GLU:O	1:A:63:GLU:HG2	2.18	0.43
1:B:101:ARG:NH2	2:B:500:HEM:O2D	2.51	0.43
1:C:305:THR:HG22	1:C:365:MET:CG	2.48	0.43
1:E:176:ARG:HB2	1:E:198:PHE:HE2	1.84	0.43
1:G:99:SER:O	1:G:437:ARG:HD2	2.19	0.43
1:D:194:GLU:HB2	4:D:499:HOH:O	2.19	0.43
1:D:139:GLY:O	1:D:145:ILE:HG12	2.18	0.43
3:A:1:9PL:H14B	3:A:1:9PL:H6	2.01	0.43
1:A:213:ALA:HA	1:A:479:GLY:HA3	1.99	0.43
1:C:84:HIS:O	1:C:88:LYS:HB2	2.19	0.43
1:F:359:ILE:HD13	1:F:453:PHE:CZ	2.54	0.43
1:G:173:PHE:HA	1:G:176:ARG:HE	1.84	0.43
1:G:301:ALA:O	1:G:305:THR:OG1	2.34	0.43
1:G:305:THR:HG22	1:G:365:MET:HG2	2.00	0.43
1:B:51:THR:HA	1:B:54:MET:HG2	2.01	0.42
1:E:330:GLU:O	1:E:334:VAL:HG23	2.19	0.42
1:F:107:PHE:CZ	3:F:1:9PL:H14	2.54	0.42
1:H:276:GLN:HA	1:H:279:GLU:OE2	2.19	0.42
1:H:338:ASN:HA	4:H:16:HOH:O	2.19	0.42
1:B:328:HIS:CE1	1:B:461:ARG:HB3	2.54	0.42
1:E:73:LEU:HB3	1:E:222:MET:HG2	2.02	0.42
1:C:464:SER:C	1:C:466:GLN:H	2.22	0.42
1:E:302:GLY:HA2	2:E:500:HEM:CMC	2.44	0.42
1:E:31:GLY:C	1:E:384:PHE:HB2	2.39	0.42
1:F:192:ASP:CG	1:F:193:TYR:N	2.73	0.42
1:G:492:LEU:HA	1:G:493:PRO:HD3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ILE:HD12	1:A:145:ILE:HA	1.82	0.42
1:D:136:ARG:HH11	1:D:136:ARG:HG3	1.85	0.42
1:E:314:PHE:HE2	1:E:453:PHE:CE2	2.37	0.42
1:A:315:LEU:HD13	1:A:487:TYR:CD2	2.54	0.42
1:A:344:GLU:C	1:A:346:ARG:N	2.69	0.42
1:C:186:VAL:HA	1:C:267:PHE:HB3	2.02	0.42
1:C:456:ILE:HG22	1:C:456:ILE:O	2.20	0.42
1:D:370:LEU:HD22	2:D:500:HEM:HBA2	2.02	0.42
1:F:281:ASN:HA	1:F:282:PRO:HD3	1.90	0.42
1:G:339:ARG:HH12	1:G:342:LYS:HD3	1.85	0.42
1:G:466:GLN:OE1	1:G:471:ILE:HG23	2.19	0.42
1:H:345:ASP:N	1:H:345:ASP:OD1	2.52	0.42
1:B:91:LEU:HD23	1:B:434:ILE:HG13	2.01	0.42
1:E:412:ASN:HD21	1:E:414:GLN:HB2	1.85	0.42
1:G:269:ASP:O	1:G:273:ILE:HD12	2.19	0.42
1:G:462:PHE:CD1	1:G:491:PHE:CE2	3.01	0.42
1:G:366:LEU:HD12	2:G:500:HEM:HHB	2.00	0.42
1:C:335:ILE:HD13	1:C:341:PRO:HB3	2.02	0.42
1:D:113:GLY:HA2	1:D:118:PHE:O	2.20	0.42
1:F:209:PHE:CE2	1:F:304:GLU:HG2	2.55	0.42
1:F:358:GLU:OE1	1:F:358:GLU:HA	2.19	0.42
1:F:302:GLY:HA2	2:F:500:HEM:CMC	2.49	0.42
1:B:351:TYR:O	1:B:355:VAL:HG23	2.20	0.42
1:D:302:GLY:HA2	2:D:500:HEM:HMC2	2.02	0.42
2:E:500:HEM:C4D	3:E:1:9PL:H4	2.55	0.42
1:F:342:LYS:O	1:F:345:ASP:HB2	2.20	0.42
1:G:33:LEU:HD11	1:G:386:PRO:HD2	2.02	0.42
1:H:346:ARG:C	1:H:348:LYS:H	2.23	0.42
1:A:172:PHE:O	1:A:176:ARG:HG3	2.20	0.42
1:B:89:GLU:HA	1:B:93:ASP:HB2	2.00	0.42
1:C:346:ARG:HG2	1:C:450:PHE:CE2	2.55	0.42
1:F:176:ARG:NH1	1:F:176:ARG:HB2	2.24	0.42
2:D:500:HEM:CHA	2:D:500:HEM:CBA	2.93	0.42
1:E:161:ARG:HH11	1:E:161:ARG:CG	2.27	0.42
1:F:303:THR:O	1:F:304:GLU:C	2.58	0.42
1:F:242:GLN:OE1	1:F:242:GLN:HA	2.20	0.41
1:H:169:ASP:HA	1:H:170:PRO:HD3	1.75	0.41
1:H:466:GLN:HG3	1:H:471:ILE:HG12	2.02	0.41
1:B:462:PHE:N	1:B:462:PHE:CD2	2.87	0.41
1:H:199:LEU:O	1:H:203:ARG:HG3	2.20	0.41
1:A:313:GLY:O	1:A:317:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ARG:NH1	1:B:437:ARG:HA	2.36	0.41
2:D:500:HEM:HBB2	2:D:500:HEM:HMB2	2.02	0.41
1:H:45:ASN:HD22	1:H:48:GLN:NE2	2.18	0.41
1:B:142:LYS:HG2	1:B:144:GLY:H	1.86	0.41
1:C:192:ASP:HB3	1:C:195:ASP:HB2	2.02	0.41
1:C:315:LEU:HG	1:C:473:VAL:HG12	2.02	0.41
1:H:371:ALA:HB2	1:H:392:PHE:CE1	2.55	0.41
1:A:156:LEU:HD13	1:A:177:THR:OG1	2.19	0.41
1:B:80:VAL:HG22	1:B:392:PHE:HB2	2.01	0.41
1:C:373:ARG:HG3	1:C:373:ARG:NH1	2.34	0.41
1:D:401:ASP:HA	1:D:402:PRO:HD2	1.90	0.41
1:G:380:PHE:O	1:G:383:PHE:HB2	2.21	0.41
1:B:169:ASP:HA	1:B:170:PRO:HD3	1.80	0.41
1:C:430:VAL:HG23	1:C:430:VAL:O	2.21	0.41
1:F:71:ILE:HD12	1:F:71:ILE:HA	1.92	0.41
1:B:112:LYS:HB2	1:B:112:LYS:HE3	1.94	0.41
1:C:313:GLY:O	1:C:317:LEU:HG	2.20	0.41
1:C:366:LEU:HD12	2:C:500:HEM:C3A	2.56	0.41
1:D:300:PHE:CD2	3:D:1:9PL:H14A	2.55	0.41
1:G:148:ARG:HH22	1:G:190:ARG:HD2	1.85	0.41
1:H:210:GLN:O	1:H:214:THR:HG23	2.21	0.41
1:B:205:MET:HE3	1:B:299:PHE:CE2	2.56	0.41
1:G:350:PRO:HB2	1:G:422:GLN:HA	2.02	0.41
1:H:165:GLY:O	1:H:490:SER:HB2	2.21	0.41
1:G:178:VAL:HG11	1:G:306:VAL:HB	2.03	0.41
1:E:129:ARG:NH2	1:G:427:ASP:OD1	2.43	0.41
1:H:55:TYR:CZ	1:H:59:MET:HG3	2.55	0.41
1:B:235:GLN:HA	1:B:238:PHE:CD2	2.56	0.41
1:C:420:LYS:HD3	1:C:420:LYS:HA	1.94	0.41
1:D:82:CYS:O	1:D:86:ALA:HB3	2.21	0.41
1:E:483:ILE:HA	1:E:484:PRO:HD2	1.90	0.41
1:H:380:PHE:CE2	1:H:381:ARG:HD2	2.55	0.41
1:H:140:VAL:HG22	1:H:444:LEU:HD13	2.03	0.41
1:A:328:HIS:HE1	1:A:461:ARG:HB3	1.86	0.41
1:A:461:ARG:CZ	1:A:492:LEU:HD11	2.50	0.41
1:B:457:MET:HG2	1:B:462:PHE:CZ	2.56	0.41
1:E:161:ARG:NH1	1:E:161:ARG:CG	2.84	0.41
1:F:224:SER:O	1:F:228:LYS:HG2	2.21	0.41
1:G:118:PHE:CE2	1:G:370:LEU:CD1	3.04	0.41
1:G:156:LEU:O	1:G:160:LEU:HG	2.21	0.41
1:B:139:GLY:O	1:B:145:ILE:HB	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:492:LEU:HA	1:C:493:PRO:HD3	1.95	0.40
1:C:64:ARG:HG3	1:C:64:ARG:O	2.21	0.40
1:E:33:LEU:HA	1:E:34:PRO:HD3	1.94	0.40
1:F:395:LEU:O	1:F:399:LEU:HG	2.21	0.40
1:G:244:LEU:HB3	1:G:296:LEU:HD11	2.03	0.40
1:G:361:ARG:HG2	1:G:399:LEU:HB3	2.02	0.40
1:H:271:PHE:CG	1:H:291:LEU:HD13	2.56	0.40
1:A:113:GLY:O	1:A:123:ARG:NH2	2.53	0.40
1:A:174:LEU:HD22	1:A:310:LEU:HD13	2.02	0.40
1:A:69:PHE:CZ	1:A:80:VAL:HB	2.56	0.40
1:F:297:ASN:HD22	1:F:297:ASN:HA	1.70	0.40
1:G:203:ARG:CG	1:G:203:ARG:HH11	2.33	0.40
1:B:370:LEU:HD13	2:B:500:HEM:HAA1	2.03	0.40
1:G:247:PHE:O	1:G:251:LYS:HG2	2.22	0.40
1:G:284:THR:OG1	1:G:286:PHE:HD2	2.04	0.40
1:A:39:PRO:HG3	1:A:72:HIS:CE1	2.56	0.40
1:B:135:LEU:O	1:B:140:VAL:HG23	2.21	0.40
1:E:170:PRO:HG3	1:E:489:MET:HG2	2.04	0.40
1:F:139:GLY:HA3	1:F:145:ILE:HB	2.04	0.40
1:G:284:THR:HG23	1:G:286:PHE:H	1.86	0.40
1:H:485:ARG:HG2	1:H:485:ARG:NH1	2.32	0.40
1:A:317:LEU:HD13	1:A:457:MET:HE3	2.03	0.40
1:B:271:PHE:CD2	1:B:291:LEU:HB2	2.57	0.40
1:B:457:MET:HG2	1:B:462:PHE:CE2	2.57	0.40
1:D:272:LEU:O	1:D:275:MET:HB2	2.22	0.40
1:F:271:PHE:CE2	1:F:291:LEU:HB2	2.56	0.40
1:F:346:ARG:HH11	1:F:446:ARG:NH2	2.19	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	462/476 (97%)	445 (96%)	15 (3%)	2 (0%)	34	72
1	B	462/476 (97%)	423 (92%)	31 (7%)	8 (2%)	9	39
1	C	462/476 (97%)	420 (91%)	39 (8%)	3 (1%)	25	64
1	D	462/476 (97%)	421 (91%)	39 (8%)	2 (0%)	34	72
1	E	462/476 (97%)	429 (93%)	25 (5%)	8 (2%)	9	39
1	F	462/476 (97%)	406 (88%)	49 (11%)	7 (2%)	10	42
1	G	462/476 (97%)	424 (92%)	31 (7%)	7 (2%)	10	42
1	H	462/476 (97%)	396 (86%)	65 (14%)	1 (0%)	47	82
All	All	3696/3808 (97%)	3364 (91%)	294 (8%)	38 (1%)	15	53

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	338	ASN
1	F	304	GLU
1	G	336	GLY
1	G	337	LYS
1	G	375	ASN
1	B	166	ALA
1	C	195	ASP
1	C	394	MET
1	D	258	THR
1	E	338	ASN
1	E	364	ASP
1	A	394	MET
1	B	394	MET
1	B	439	CYS
1	E	382	ASP
1	F	190	ARG
1	F	192	ASP
1	F	345	ASP
1	G	468	PRO
1	B	46	TYR
1	B	142	LYS
1	C	338	ASN
1	E	195	ASP
1	E	468	PRO
1	F	266	ASP
1	G	84	HIS
1	H	408	PRO

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Mol	Chain	Res	Type
1	B	63	GLU
1	B	263	SER
1	G	171	THR
1	A	345	ASP
1	B	338	ASN
1	E	42	PHE
1	E	344	GLU
1	F	258	THR
1	F	406	SER
1	G	493	PRO
1	E	33	LEU

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	407/419 (97%)	380 (93%)	27 (7%)	16	49
1	B	408/419 (97%)	387 (95%)	21 (5%)	24	60
1	C	406/419 (97%)	377 (93%)	29 (7%)	14	46
1	D	408/419 (97%)	386 (95%)	22 (5%)	22	57
1	E	406/419 (97%)	384 (95%)	22 (5%)	22	57
1	F	404/419 (96%)	370 (92%)	34 (8%)	11	38
1	G	403/419 (96%)	369 (92%)	34 (8%)	11	38
1	H	400/419 (96%)	368 (92%)	32 (8%)	12	40
All	All	3242/3352 (97%)	3021 (93%)	221 (7%)	16	48

All (221) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	THR
1	A	48	GLN
1	A	62	SER
1	A	88	LYS

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Mol	Chain	Res	Type
1	A	103	GLU
1	A	147	GLU
1	A	151	GLU
1	A	167	ASN
1	A	197	GLU
1	A	212	THR
1	A	225	SER
1	A	236	GLN
1	A	239	LYS
1	A	266	ASP
1	A	300	PHE
1	A	312	TYR
1	A	340	GLN
1	A	342	LYS
1	A	352	THR
1	A	368	MET
1	A	375	ASN
1	A	409	ARG
1	A	419	LYS
1	A	425	LYS
1	A	442	GLU
1	A	454	THR
1	A	462	PHE
1	B	38	THR
1	B	48	GLN
1	B	135	LEU
1	B	143	ARG
1	B	148	ARG
1	B	192	ASP
1	B	194	GLU
1	B	206	LEU
1	B	236	GLN
1	B	283	ASN
1	B	291	LEU
1	B	300	PHE
1	B	305	THR
1	B	312	TYR
1	B	318	MET
1	B	322	GLU
1	B	348	LYS
1	B	406	SER
1	B	410	ASP

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Mol	Chain	Res	Type
1	B	414	GLN
1	B	419	LYS
1	C	38	THR
1	C	64	ARG
1	C	73	LEU
1	C	81	LEU
1	C	88	LYS
1	C	104	GLN
1	C	145	ILE
1	C	147	GLU
1	C	167	ASN
1	C	208	SER
1	C	210	GLN
1	C	224	SER
1	C	258	THR
1	C	269	ASP
1	C	270	SER
1	C	300	PHE
1	C	312	TYR
1	C	352	THR
1	C	375	ASN
1	C	379	LYS
1	C	410	ASP
1	C	419	LYS
1	C	425	LYS
1	C	434	ILE
1	C	446	ARG
1	C	467	SER
1	C	469	LYS
1	C	470	ASP
1	C	488	THR
1	D	48	GLN
1	D	59	MET
1	D	64	ARG
1	D	104	GLN
1	D	106	THR
1	D	143	ARG
1	D	167	ASN
1	D	193	TYR
1	D	194	GLU
1	D	203	ARG
1	D	236	GLN

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Mol	Chain	Res	Type
1	D	255	ASN
1	D	258	THR
1	D	274	ARG
1	D	300	PHE
1	D	305	THR
1	D	312	TYR
1	D	322	GLU
1	D	326	LYS
1	D	340	GLN
1	D	375	ASN
1	D	393	PRO
1	E	148	ARG
1	E	155	PHE
1	E	167	ASN
1	E	185	ILE
1	E	190	ARG
1	E	191	PHE
1	E	236	GLN
1	E	250	LYS
1	E	266	ASP
1	E	300	PHE
1	E	305	THR
1	E	311	ARG
1	E	312	TYR
1	E	368	MET
1	E	375	ASN
1	E	379	LYS
1	E	425	LYS
1	E	434	ILE
1	E	438	TYR
1	E	442	GLU
1	E	458	GLN
1	E	470	ASP
1	F	38	THR
1	F	48	GLN
1	F	57	SER
1	F	88	LYS
1	F	91	LEU
1	F	96	GLU
1	F	101	ARG
1	F	128	ARG
1	F	138	PHE

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Mol	Chain	Res	Type
1	F	163	THR
1	F	171	THR
1	F	176	ARG
1	F	177	THR
1	F	179	SER
1	F	216	THR
1	F	236	GLN
1	F	250	LYS
1	F	255	ASN
1	F	273	ILE
1	F	289	LYS
1	F	297	ASN
1	F	300	PHE
1	F	312	TYR
1	F	339	ARG
1	F	346	ARG
1	F	365	MET
1	F	367	PRO
1	F	375	ASN
1	F	419	LYS
1	F	420	LYS
1	F	427	ASP
1	F	451	LEU
1	F	454	THR
1	F	470	ASP
1	G	33	LEU
1	G	38	THR
1	G	48	GLN
1	G	56	ASN
1	G	60	LYS
1	G	88	LYS
1	G	101	ARG
1	G	136	ARG
1	G	145	ILE
1	G	151	GLU
1	G	155	PHE
1	G	163	THR
1	G	182	ILE
1	G	189	ASP
1	G	198	PHE
1	G	215	SER
1	G	216	THR

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Mol	Chain	Res	Type
1	G	239	LYS
1	G	256	GLN
1	G	300	PHE
1	G	305	THR
1	G	309	THR
1	G	342	LYS
1	G	346	ARG
1	G	361	ARG
1	G	370	LEU
1	G	374	VAL
1	G	409	ARG
1	G	422	GLN
1	G	461	ARG
1	G	462	PHE
1	G	463	LYS
1	G	469	LYS
1	G	471	ILE
1	H	52	GLU
1	H	73	LEU
1	H	81	LEU
1	H	85	ASP
1	H	88	LYS
1	H	104	GLN
1	H	148	ARG
1	H	177	THR
1	H	196	LYS
1	H	216	THR
1	H	225	SER
1	H	236	GLN
1	H	256	GLN
1	H	266	ASP
1	H	280	LYS
1	H	283	ASN
1	H	312	TYR
1	H	322	GLU
1	H	329	GLU
1	H	330	GLU
1	H	340	GLN
1	H	345	ASP
1	H	346	ARG
1	H	352	THR
1	H	376	LYS

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Mol	Chain	Res	Type
1	H	392	PHE
1	H	418	ASP
1	H	419	LYS
1	H	449	LEU
1	H	453	PHE
1	H	470	ASP
1	H	485	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	328	HIS
1	A	375	ASN
1	A	459	ASN
1	B	297	ASN
1	B	328	HIS
1	B	415	HIS
1	C	210	GLN
1	C	218	GLN
1	C	297	ASN
1	C	375	ASN
1	D	48	GLN
1	D	72	HIS
1	D	120	ASN
1	D	167	ASN
1	D	255	ASN
1	D	283	ASN
1	D	412	ASN
1	E	48	GLN
1	E	167	ASN
1	E	297	ASN
1	E	340	GLN
1	E	412	ASN
1	E	414	GLN
1	F	283	ASN
1	F	297	ASN
1	F	375	ASN
1	G	48	GLN
1	G	94	GLN
1	G	422	GLN
1	H	45	ASN

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Mol	Chain	Res	Type
1	H	48	GLN
1	H	120	ASN
1	H	167	ASN
1	H	412	ASN
1	H	458	GLN
1	H	459	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

14 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	C	500	1,3	27,50,50	2.17	5 (18%)	17,82,82	1.86	4 (23%)
2	HEM	E	500	1,3	27,50,50	2.60	8 (29%)	17,82,82	1.51	4 (23%)
2	HEM	B	500	1,3	27,50,50	2.21	6 (22%)	17,82,82	1.69	5 (29%)
2	HEM	G	500	1	27,50,50	2.61	13 (48%)	17,82,82	2.21	6 (35%)
2	HEM	D	500	1,3	27,50,50	2.21	7 (25%)	17,82,82	1.52	3 (17%)
3	9PL	B	1	2	13,16,16	1.69	2 (15%)	16,22,22	2.56	6 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	9PL	A	1	2	13,16,16	1.58	2 (15%)	16,22,22	3.20	7 (43%)
3	9PL	D	1	2	13,16,16	1.44	1 (7%)	16,22,22	2.72	8 (50%)
3	9PL	C	1	2	13,16,16	1.46	1 (7%)	16,22,22	2.56	7 (43%)
3	9PL	F	1	2	13,16,16	1.42	1 (7%)	16,22,22	2.29	5 (31%)
3	9PL	E	1	2	13,16,16	1.44	1 (7%)	16,22,22	2.57	7 (43%)
2	HEM	F	500	1,3	27,50,50	2.28	8 (29%)	17,82,82	1.84	5 (29%)
2	HEM	H	500	1	27,50,50	2.53	10 (37%)	17,82,82	1.56	3 (17%)
2	HEM	A	500	1,3	27,50,50	2.23	8 (29%)	17,82,82	1.68	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
2	HEM	C	500	1,3	-	0/6/54/54	-
2	HEM	E	500	1,3	-	0/6/54/54	-
2	HEM	B	500	1,3	-	1/6/54/54	-
2	HEM	G	500	1	-	2/6/54/54	-
2	HEM	D	500	1,3	-	2/6/54/54	-
3	9PL	B	1	2	-	3/6/19/19	0/2/2/2
3	9PL	A	1	2	-	3/6/19/19	0/2/2/2
3	9PL	D	1	2	-	4/6/19/19	0/2/2/2
3	9PL	C	1	2	-	4/6/19/19	0/2/2/2
3	9PL	F	1	2	-	1/6/19/19	0/2/2/2
3	9PL	E	1	2	-	4/6/19/19	0/2/2/2
2	HEM	F	500	1,3	-	2/6/54/54	-
2	HEM	H	500	1	-	0/6/54/54	-
2	HEM	A	500	1,3	-	1/6/54/54	-

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	500	HEM	C3C-CAC	6.34	1.60	1.47
2	H	500	HEM	C3B-CAB	5.81	1.59	1.47
2	G	500	HEM	C3D-C2D	5.75	1.54	1.37
2	H	500	HEM	C3C-C2C	-5.59	1.32	1.40
2	F	500	HEM	C3D-C2D	5.56	1.54	1.37
2	E	500	HEM	C3D-C2D	5.52	1.54	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C3D-C2D	5.26	1.53	1.37
2	B	500	HEM	C3D-C2D	5.15	1.52	1.37
2	E	500	HEM	C3B-CAB	5.14	1.58	1.47
2	D	500	HEM	C3D-C2D	5.05	1.52	1.37
2	G	500	HEM	C3B-C2B	-4.87	1.33	1.40
2	D	500	HEM	C3C-C2C	-4.86	1.33	1.40
2	H	500	HEM	C3D-C2D	4.84	1.52	1.37
2	C	500	HEM	C3D-C2D	4.83	1.52	1.37
2	B	500	HEM	C3C-C2C	-4.79	1.33	1.40
3	F	1	9PL	O10-C11	4.62	1.45	1.35
2	G	500	HEM	C3C-C2C	-4.61	1.34	1.40
2	C	500	HEM	C3C-C2C	-4.52	1.34	1.40
3	C	1	9PL	O10-C11	4.46	1.45	1.35
3	E	1	9PL	O10-C11	4.43	1.44	1.35
3	D	1	9PL	O10-C11	4.38	1.44	1.35
2	G	500	HEM	C3C-CAC	4.38	1.56	1.47
2	H	500	HEM	CAA-C2A	4.32	1.58	1.52
2	E	500	HEM	C3C-C2C	-4.30	1.34	1.40
2	A	500	HEM	C3C-CAC	4.29	1.56	1.47
2	F	500	HEM	C3B-CAB	4.25	1.56	1.47
2	D	500	HEM	C3C-CAC	4.24	1.56	1.47
2	C	500	HEM	C3B-C2B	-4.23	1.34	1.40
2	C	500	HEM	C3B-CAB	4.21	1.56	1.47
2	C	500	HEM	C3C-CAC	4.17	1.56	1.47
3	B	1	9PL	C7-C5	4.14	1.56	1.50
2	B	500	HEM	C3B-CAB	4.14	1.56	1.47
2	B	500	HEM	C3C-CAC	4.10	1.56	1.47
2	B	500	HEM	C3B-C2B	-4.07	1.34	1.40
2	D	500	HEM	C3B-C2B	-3.97	1.34	1.40
2	A	500	HEM	C3C-C2C	-3.96	1.34	1.40
2	E	500	HEM	C3B-C2B	-3.96	1.34	1.40
2	A	500	HEM	C3B-CAB	3.90	1.55	1.47
3	A	1	9PL	O10-C11	3.90	1.43	1.35
2	F	500	HEM	C3C-C2C	-3.82	1.35	1.40
2	F	500	HEM	C3B-C2B	-3.73	1.35	1.40
2	F	500	HEM	C3C-CAC	3.64	1.55	1.47
2	A	500	HEM	C3B-C2B	-3.41	1.35	1.40
2	G	500	HEM	CMD-C2D	3.37	1.58	1.51
2	G	500	HEM	CAD-C3D	3.34	1.58	1.52
2	H	500	HEM	CMA-C3A	3.30	1.58	1.51
2	G	500	HEM	CAA-C2A	3.24	1.56	1.52
2	E	500	HEM	CMC-C2C	3.21	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	HEM	C3B-CAB	3.17	1.54	1.47
3	B	1	9PL	O10-C11	3.17	1.42	1.35
2	F	500	HEM	CMB-C2B	3.12	1.59	1.51
3	A	1	9PL	C7-C5	2.94	1.55	1.50
2	E	500	HEM	CMD-C2D	2.91	1.57	1.51
2	F	500	HEM	CAA-C2A	2.91	1.56	1.52
2	A	500	HEM	CAA-C2A	2.88	1.56	1.52
2	G	500	HEM	C3B-CAB	2.81	1.53	1.47
2	H	500	HEM	CAD-C3D	2.79	1.57	1.52
2	H	500	HEM	CMB-C2B	2.58	1.57	1.51
2	G	500	HEM	CMC-C2C	2.58	1.57	1.51
2	H	500	HEM	C3B-C2B	-2.56	1.36	1.40
2	G	500	HEM	C1C-C2C	2.54	1.48	1.42
2	H	500	HEM	C3C-CAC	2.48	1.52	1.47
2	A	500	HEM	C1D-ND	2.40	1.41	1.36
2	A	500	HEM	C4B-NB	2.36	1.41	1.36
2	D	500	HEM	CAD-C3D	2.31	1.56	1.52
2	G	500	HEM	C1A-NA	2.30	1.40	1.36
2	B	500	HEM	C1D-ND	2.28	1.40	1.36
2	F	500	HEM	C1D-ND	2.14	1.40	1.36
2	G	500	HEM	C1D-ND	2.14	1.40	1.36
2	H	500	HEM	C1B-C2B	2.08	1.47	1.42
2	D	500	HEM	CMC-C2C	2.03	1.56	1.51
2	G	500	HEM	C4B-NB	2.02	1.40	1.36
2	E	500	HEM	C1B-C2B	2.02	1.47	1.42

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	9PL	C9-C8-C12	7.41	113.06	101.44
3	E	1	9PL	C9-C8-C12	6.55	111.71	101.44
3	C	1	9PL	C9-C8-C12	6.53	111.68	101.44
3	A	1	9PL	C5-C7-C8	-6.24	100.26	114.25
3	F	1	9PL	C9-C8-C12	6.24	111.22	101.44
3	D	1	9PL	C9-C8-C12	5.98	110.81	101.44
3	B	1	9PL	C14-C13-C12	-5.44	101.36	113.47
2	C	500	HEM	CAA-CBA-CGA	-5.38	103.65	112.67
3	B	1	9PL	C5-C7-C8	-5.17	102.67	114.25
3	B	1	9PL	C9-C8-C12	4.99	109.26	101.44
2	G	500	HEM	CAA-CBA-CGA	-4.81	104.60	112.67
3	D	1	9PL	C5-C7-C8	-4.80	103.49	114.25
3	A	1	9PL	C7-C8-C9	4.61	119.15	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	9PL	C7-C8-C12	4.28	124.64	114.74
2	G	500	HEM	C1D-C2D-C3D	-4.17	104.09	107.00
2	H	500	HEM	CAD-CBD-CGD	-4.12	105.76	112.67
3	C	1	9PL	C5-C7-C8	-4.11	105.04	114.25
3	E	1	9PL	C5-C7-C8	-4.09	105.09	114.25
2	G	500	HEM	C4A-C3A-C2A	4.04	109.81	107.00
2	A	500	HEM	C4A-C3A-C2A	4.03	109.80	107.00
3	D	1	9PL	C7-C8-C9	4.00	118.29	112.67
2	F	500	HEM	C4A-C3A-C2A	3.93	109.73	107.00
2	B	500	HEM	CMA-C3A-C4A	-3.66	122.83	128.46
2	E	500	HEM	C1D-C2D-C3D	-3.66	104.45	107.00
2	F	500	HEM	CBD-CAD-C3D	-3.56	105.92	112.48
3	E	1	9PL	C6-N1-C5	3.23	128.74	124.44
3	C	1	9PL	C6-N1-C5	3.23	128.74	124.44
3	F	1	9PL	C5-C7-C8	-3.17	107.15	114.25
3	F	1	9PL	O15-C11-C12	-3.14	124.49	128.83
3	D	1	9PL	O10-C11-O15	3.07	124.60	121.42
2	H	500	HEM	C1D-C2D-C3D	-3.04	104.88	107.00
3	B	1	9PL	C7-C8-C12	3.04	121.76	114.74
2	G	500	HEM	CMA-C3A-C4A	-2.94	123.95	128.46
3	D	1	9PL	C6-N1-C5	2.91	128.31	124.44
2	C	500	HEM	CBD-CAD-C3D	-2.88	107.18	112.48
3	E	1	9PL	O15-C11-C12	-2.80	124.97	128.83
3	C	1	9PL	O15-C11-C12	-2.77	125.00	128.83
2	D	500	HEM	CAA-CBA-CGA	-2.70	108.14	112.67
3	A	1	9PL	C14-C13-C12	-2.69	107.47	113.47
2	F	500	HEM	CMA-C3A-C4A	-2.66	124.38	128.46
2	C	500	HEM	CAD-CBD-CGD	-2.66	108.21	112.67
2	A	500	HEM	C1D-C2D-C3D	-2.59	105.19	107.00
2	A	500	HEM	CBA-CAA-C2A	2.55	117.20	112.49
3	A	1	9PL	O10-C9-C8	-2.55	100.91	105.37
2	F	500	HEM	C1D-C2D-C3D	-2.47	105.28	107.00
3	D	1	9PL	O15-C11-C12	-2.45	125.45	128.83
2	G	500	HEM	CBA-CAA-C2A	2.44	116.98	112.49
2	B	500	HEM	CMA-C3A-C2A	2.42	129.50	124.94
2	G	500	HEM	C4C-C3C-C2C	-2.41	105.21	106.90
2	D	500	HEM	CMB-C2B-C3B	2.40	129.17	124.68
2	E	500	HEM	C4A-C3A-C2A	2.37	108.64	107.00
3	B	1	9PL	C6-N1-C5	2.36	127.59	124.44
3	F	1	9PL	C6-N1-C5	2.35	127.58	124.44
2	H	500	HEM	C4C-C3C-C2C	2.35	108.54	106.90
2	B	500	HEM	CAA-CBA-CGA	-2.33	108.76	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	9PL	C7-C8-C12	2.31	120.07	114.74
2	F	500	HEM	CAD-CBD-CGD	-2.30	108.81	112.67
3	A	1	9PL	C8-C12-C11	-2.30	98.76	102.45
2	E	500	HEM	CMD-C2D-C3D	2.24	129.17	124.94
3	C	1	9PL	C14-C13-C12	-2.24	108.48	113.47
3	E	1	9PL	C14-C13-C12	-2.22	108.52	113.47
2	D	500	HEM	CBD-CAD-C3D	2.20	116.53	112.48
3	B	1	9PL	C9-O10-C11	2.16	112.25	110.28
3	E	1	9PL	C7-C8-C9	2.16	115.70	112.67
2	B	500	HEM	CAD-CBD-CGD	-2.14	109.08	112.67
3	C	1	9PL	C7-C8-C9	2.14	115.67	112.67
3	F	1	9PL	C7-C8-C12	2.10	119.59	114.74
2	A	500	HEM	C4C-C3C-C2C	2.10	108.36	106.90
2	E	500	HEM	CMA-C3A-C4A	-2.09	125.25	128.46
2	C	500	HEM	C1D-C2D-C3D	-2.08	105.55	107.00
2	B	500	HEM	CMC-C2C-C3C	2.07	128.55	124.68
3	E	1	9PL	O10-C11-O15	2.01	123.50	121.42
3	C	1	9PL	O10-C11-O15	2.01	123.50	121.42
3	D	1	9PL	N3-C2-N1	-2.00	109.28	112.26

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	500	HEM	C1A-C2A-CAA-CBA
2	G	500	HEM	C3A-C2A-CAA-CBA
2	D	500	HEM	C1A-C2A-CAA-CBA
2	D	500	HEM	C3A-C2A-CAA-CBA
3	B	1	9PL	C5-C7-C8-C12
3	B	1	9PL	C11-C12-C13-C14
3	A	1	9PL	C5-C7-C8-C12
3	A	1	9PL	C11-C12-C13-C14
3	D	1	9PL	C5-C7-C8-C9
3	D	1	9PL	C5-C7-C8-C12
3	D	1	9PL	C8-C12-C13-C14
3	D	1	9PL	C11-C12-C13-C14
3	C	1	9PL	C5-C7-C8-C9
3	C	1	9PL	C5-C7-C8-C12
3	C	1	9PL	C11-C12-C13-C14
3	F	1	9PL	C5-C7-C8-C12
3	E	1	9PL	C5-C7-C8-C9
3	E	1	9PL	C5-C7-C8-C12

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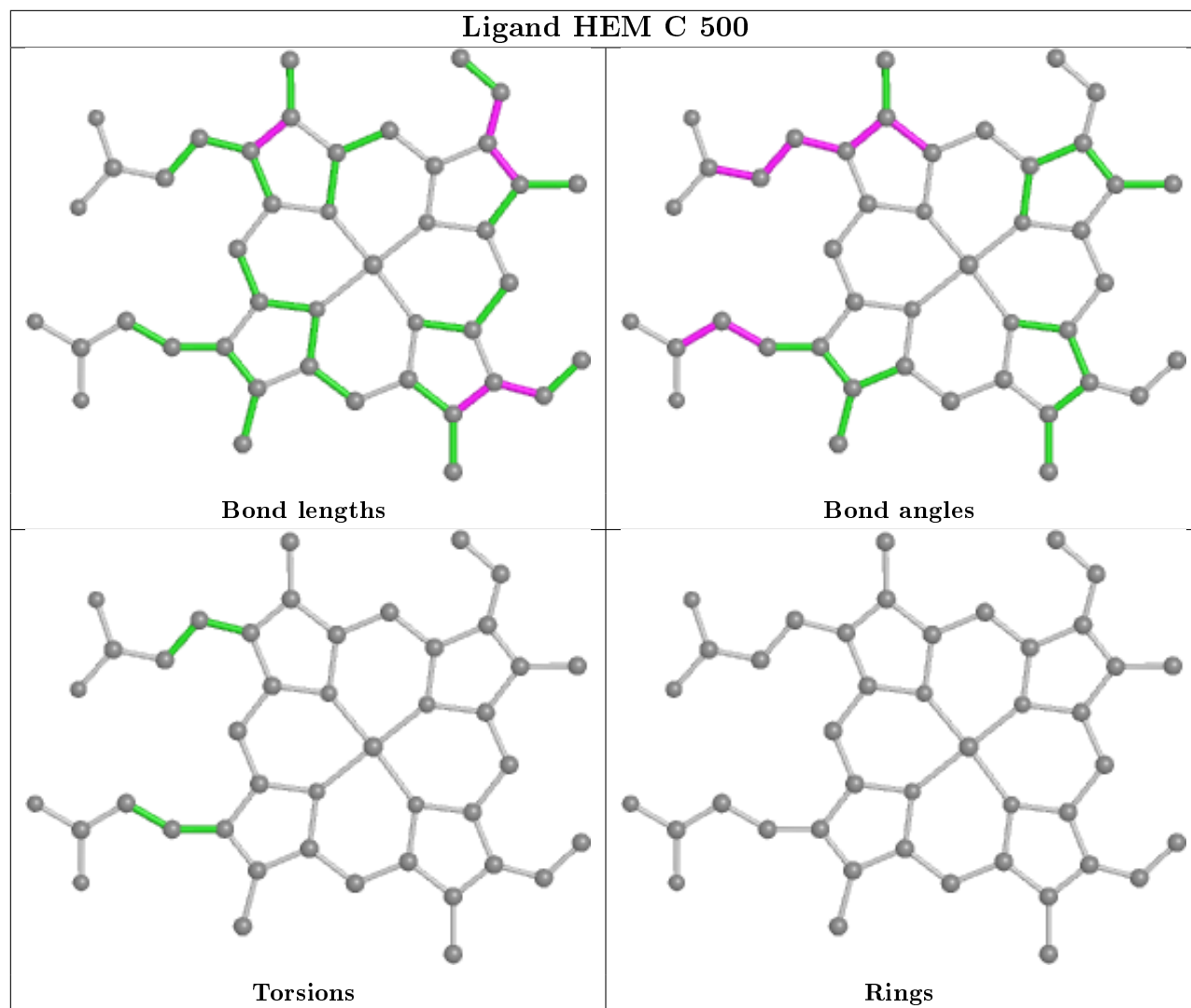
Mol	Chain	Res	Type	Atoms
3	E	1	9PL	C11-C12-C13-C14
2	F	500	HEM	C1A-C2A-CAA-CBA
2	F	500	HEM	C3A-C2A-CAA-CBA
3	B	1	9PL	C8-C12-C13-C14
3	A	1	9PL	C8-C12-C13-C14
3	C	1	9PL	C8-C12-C13-C14
3	E	1	9PL	C8-C12-C13-C14
2	A	500	HEM	C3A-C2A-CAA-CBA
2	B	500	HEM	C3D-CAD-CBD-CGD

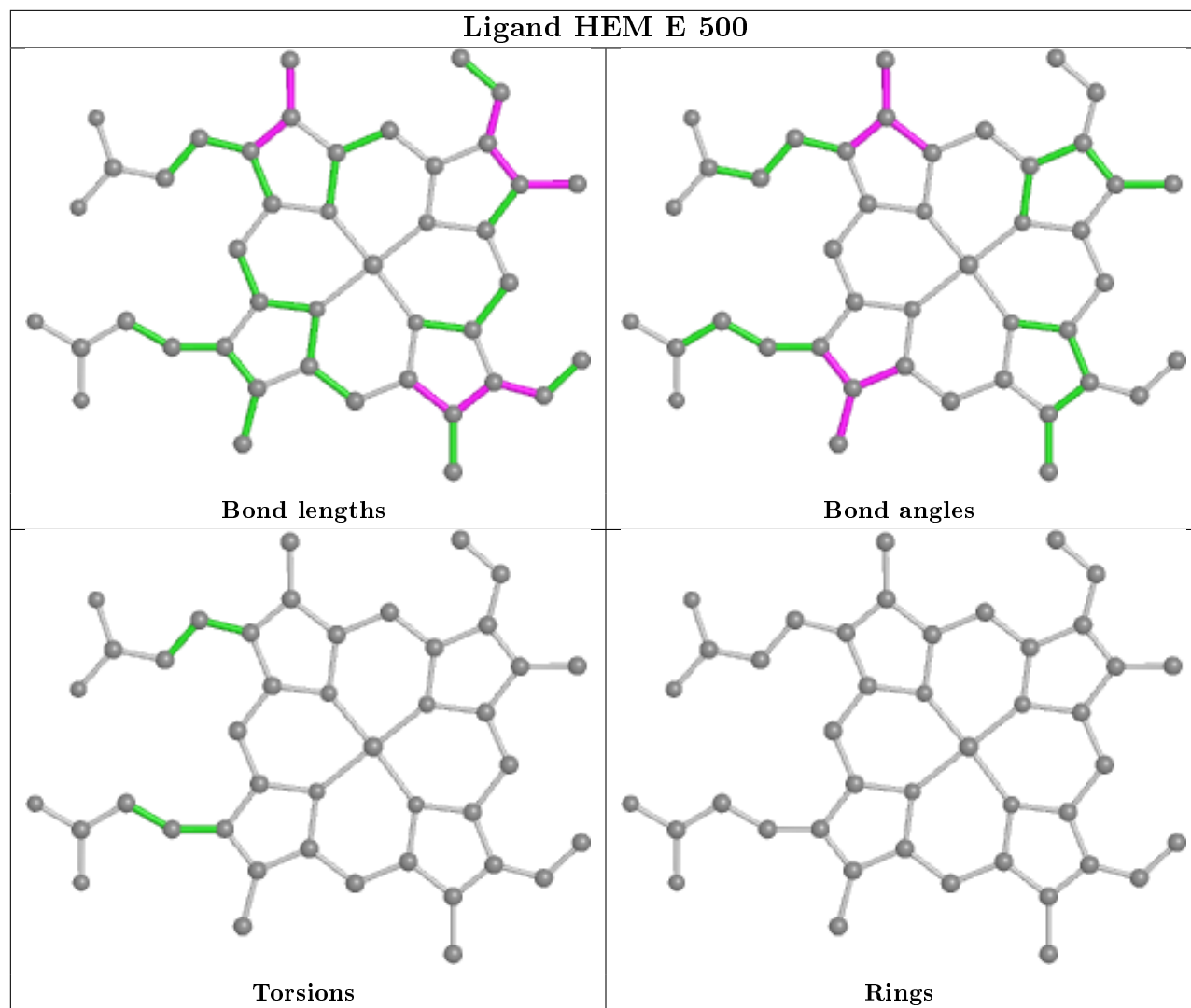
There are no ring outliers.

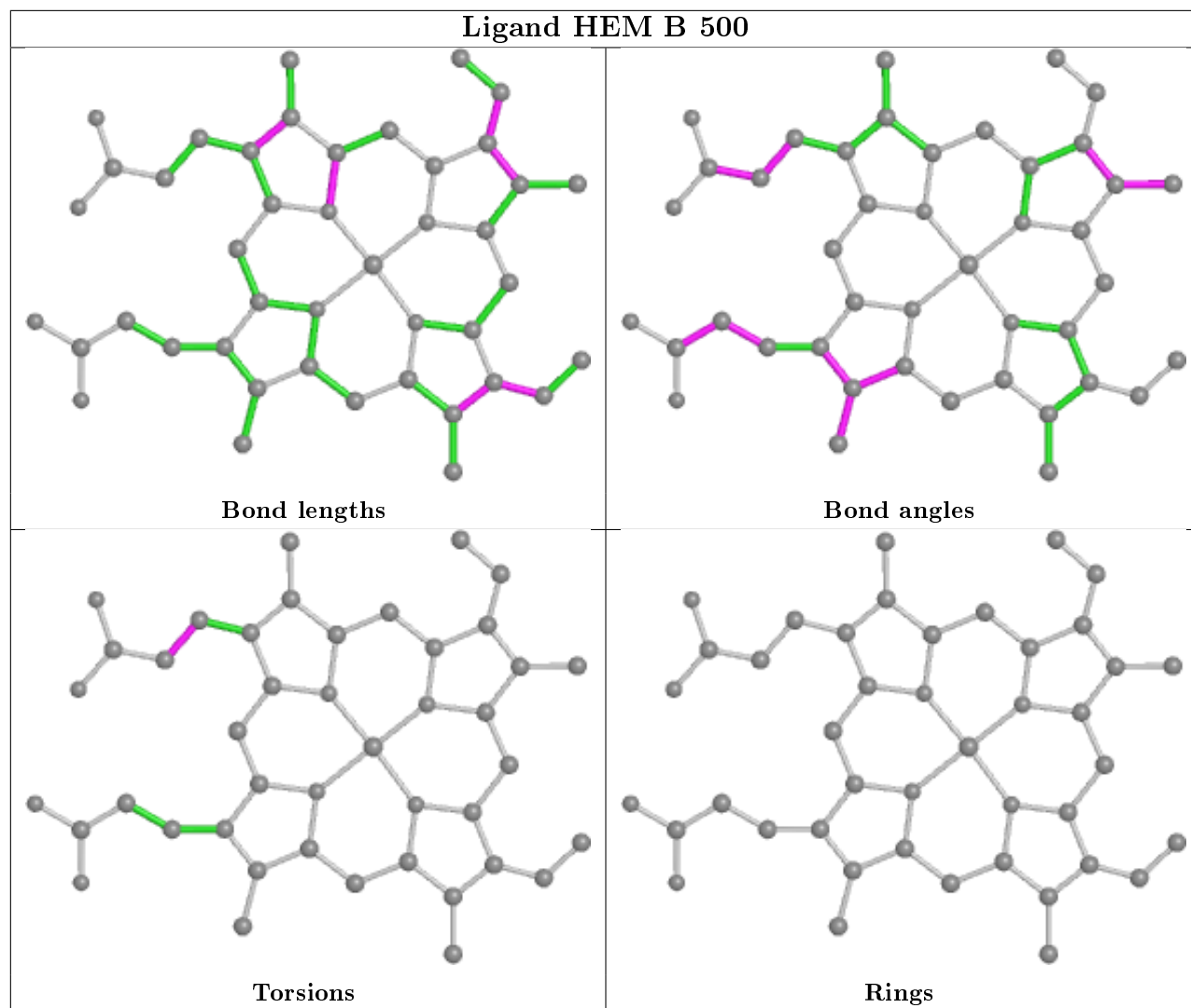
14 monomers are involved in 81 short contacts:

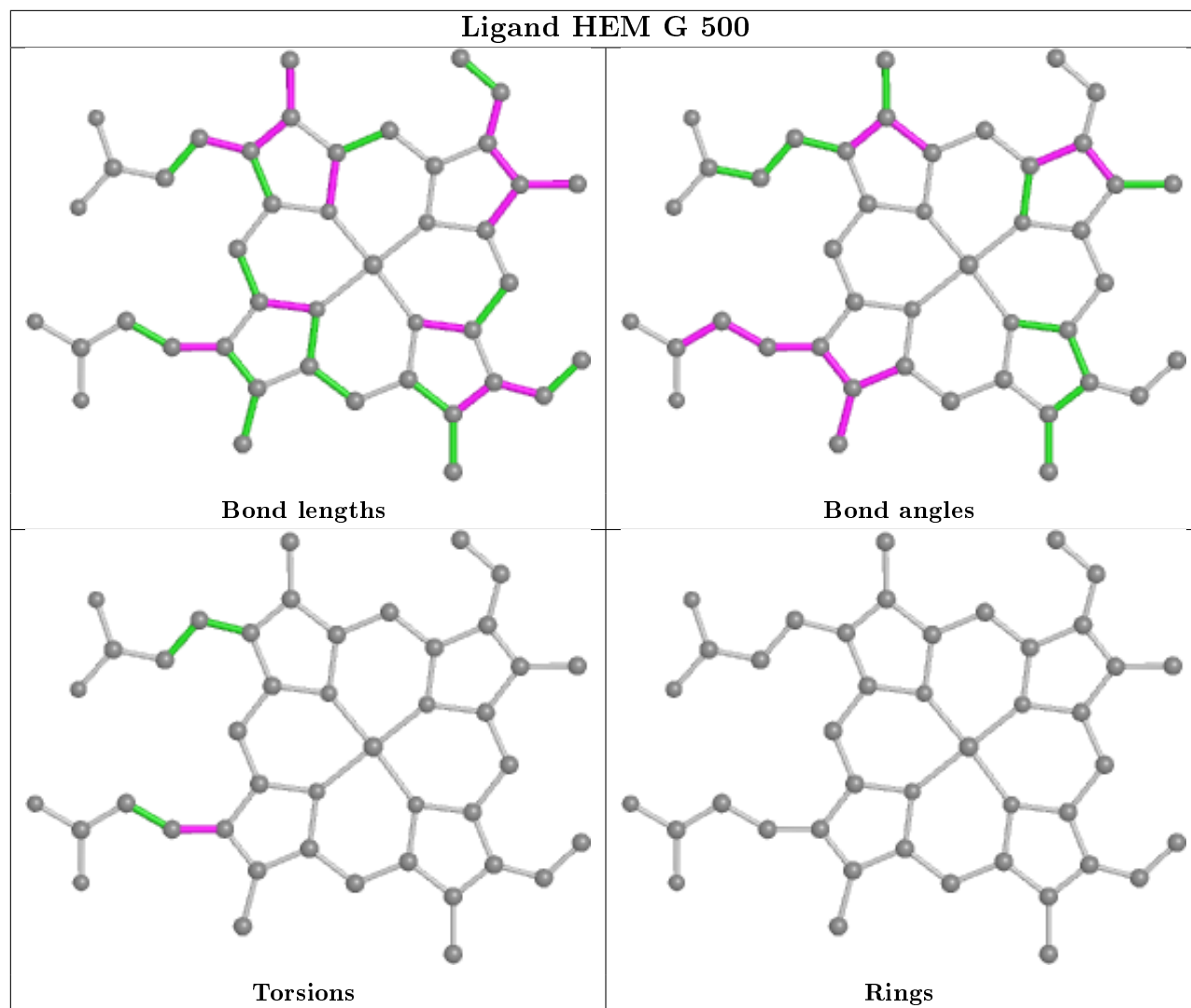
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	500	HEM	10	0
2	E	500	HEM	5	0
2	B	500	HEM	3	0
2	G	500	HEM	5	0
2	D	500	HEM	13	0
3	B	1	9PL	6	0
3	A	1	9PL	3	0
3	D	1	9PL	4	0
3	C	1	9PL	12	0
3	F	1	9PL	2	0
3	E	1	9PL	8	0
2	F	500	HEM	6	0
2	H	500	HEM	5	0
2	A	500	HEM	3	0

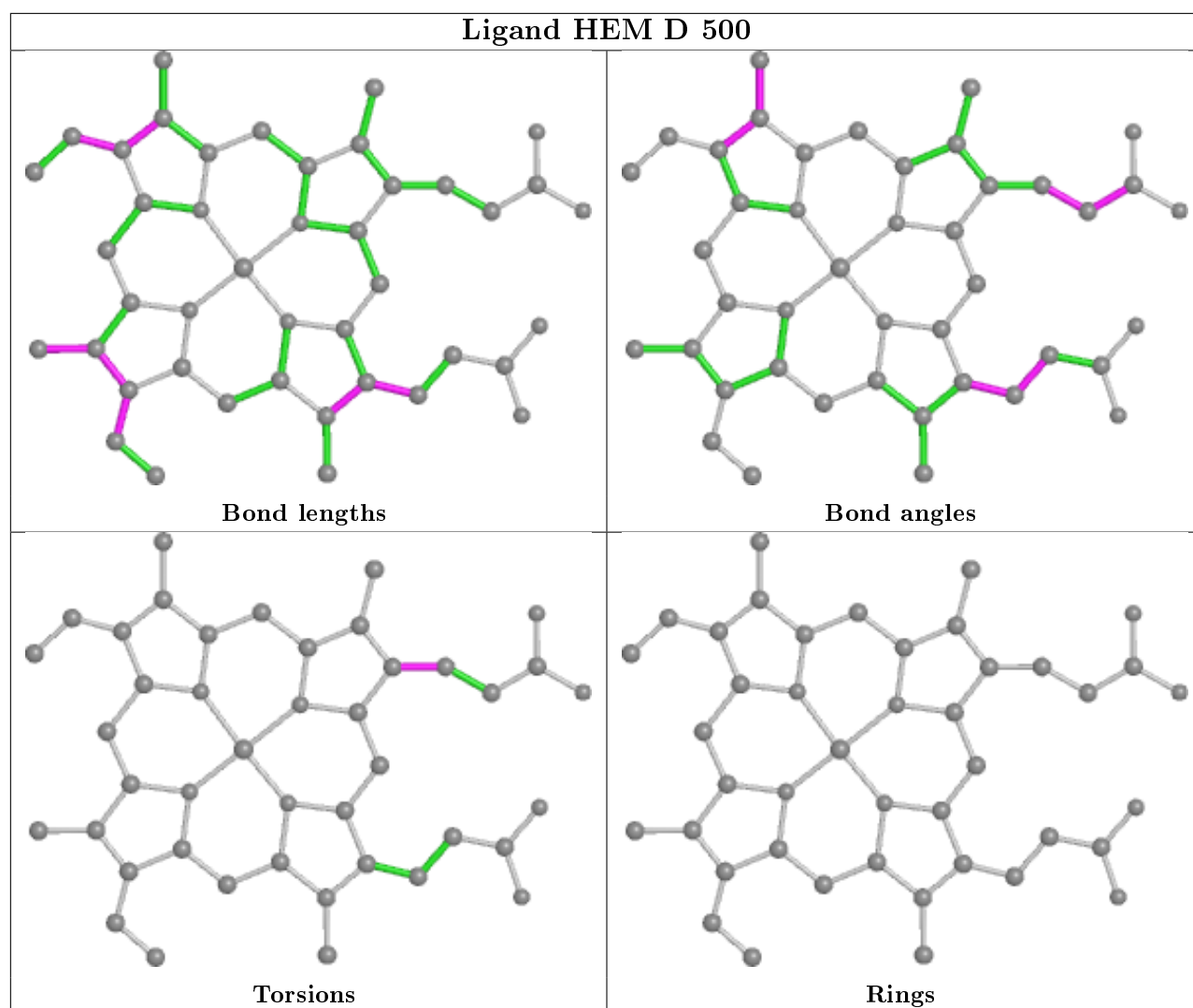
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

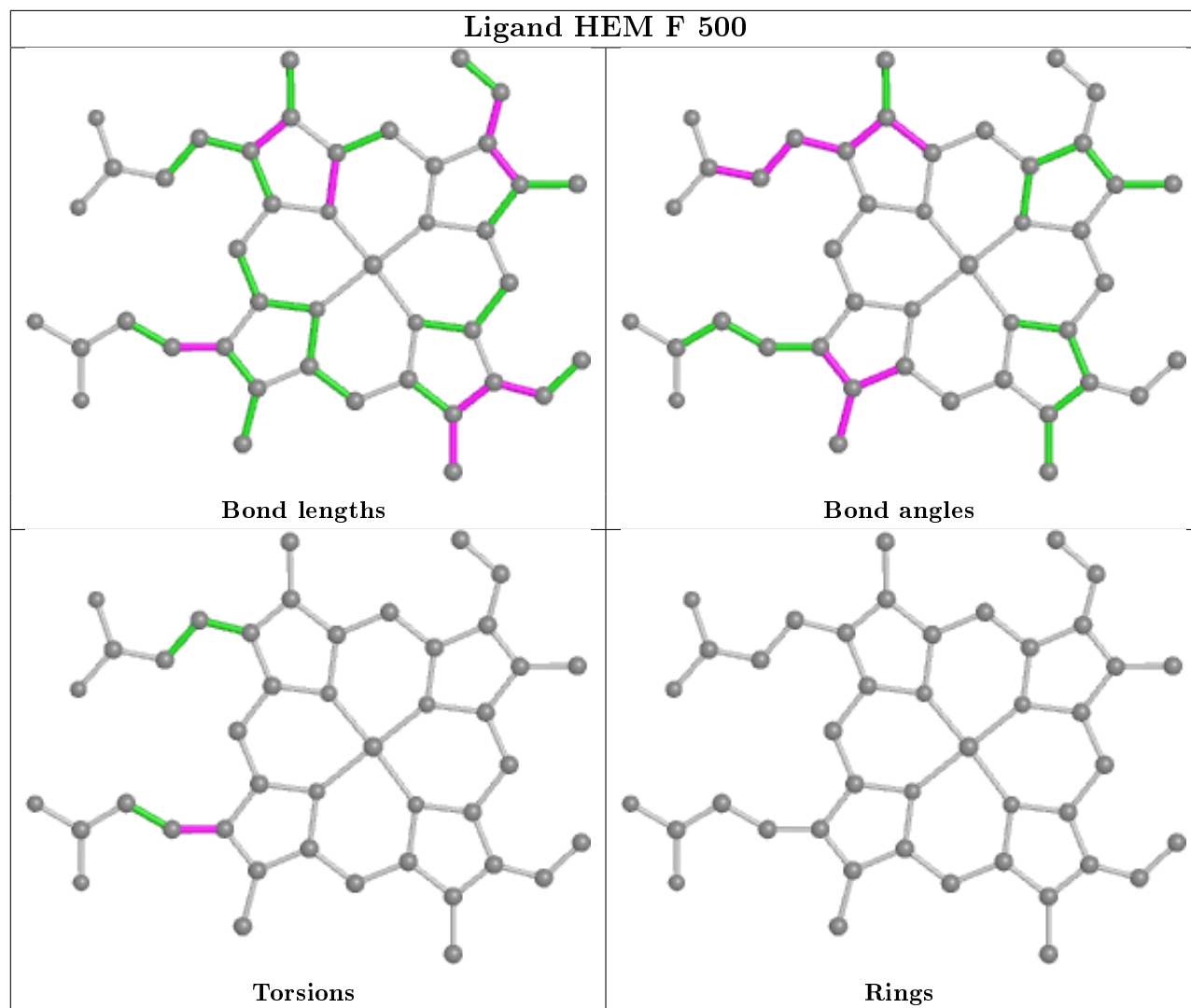


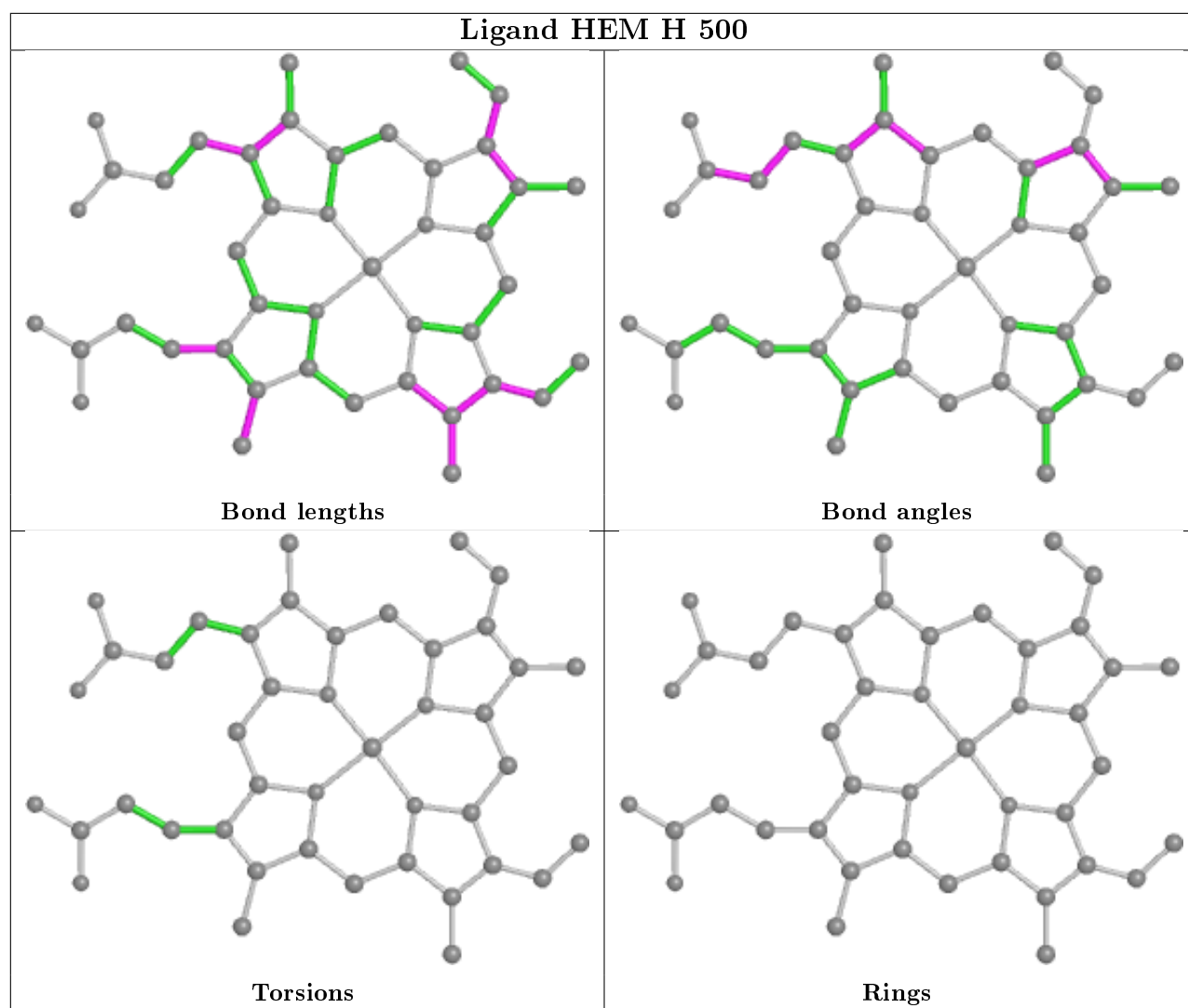


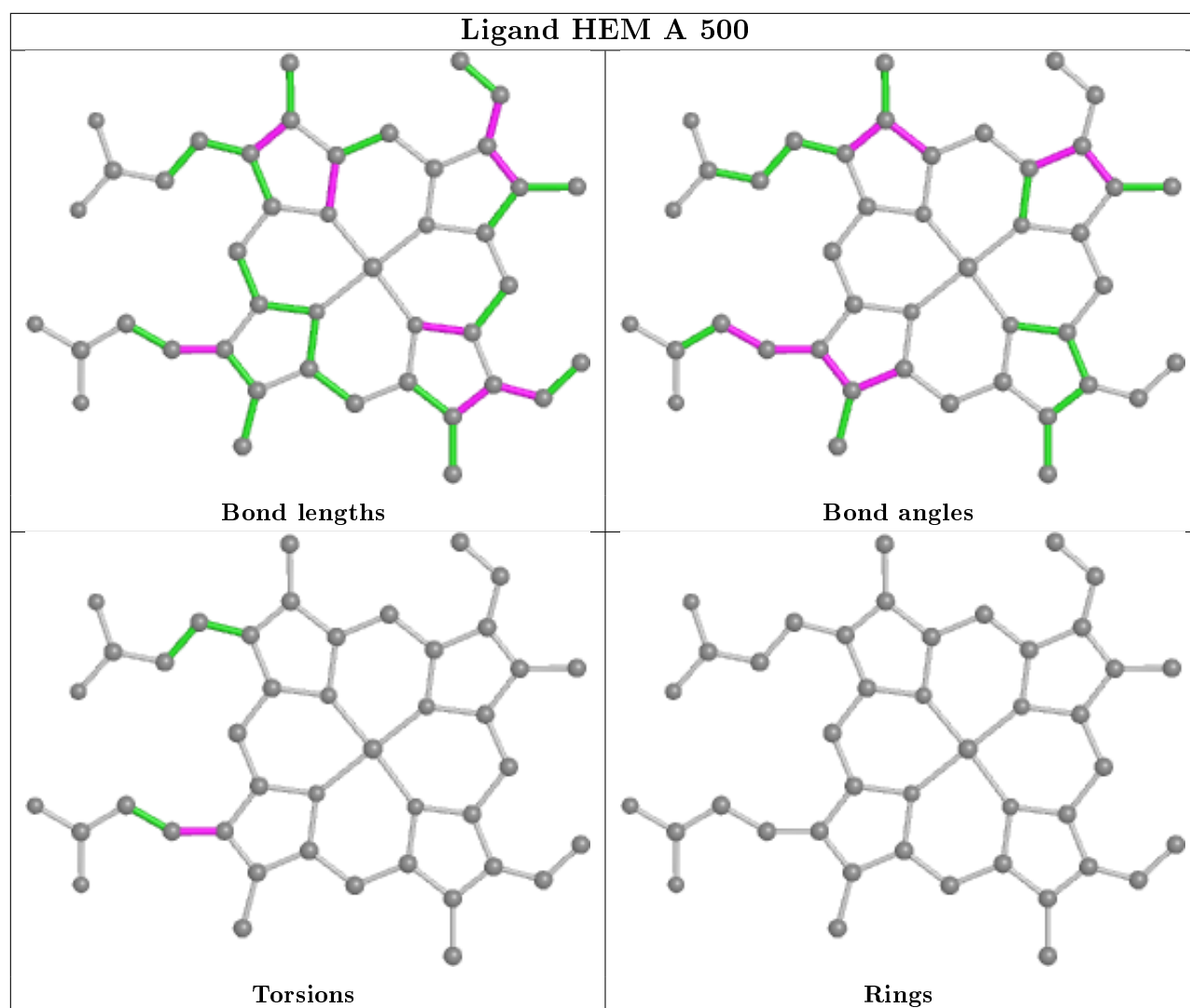












5.7 Other polymers [i](#)

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, 95th 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 ²)	Q<0.9
1	A	464/476 (97%)	-0.36	0 100 100	23, 38, 54, 60	0
1	B	464/476 (97%)	-0.29	0 100 100	24, 44, 64, 66	0
1	C	464/476 (97%)	-0.33	0 100 100	26, 45, 71, 76	0
1	D	464/476 (97%)	-0.34	0 100 100	22, 42, 62, 69	0
1	E	464/476 (97%)	-0.25	0 100 100	32, 60, 76, 82	0
1	F	464/476 (97%)	-0.16	2 (0%) 92 79	29, 67, 85, 93	0
1	G	464/476 (97%)	-0.14	2 (0%) 92 79	35, 67, 94, 98	0
1	H	464/476 (97%)	0.14	11 (2%) 59 30	40, 84, 101, 104	0
All	All	3712/3808 (97%)	-0.22	15 (0%) 92 79	22, 54, 91, 104	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	329	GLU	3.4
1	F	172	PHE	3.2
1	H	356	ILE	2.8
1	H	414	GLN	2.5
1	H	355	VAL	2.4
1	G	141	GLY	2.4
1	H	310	LEU	2.3
1	H	447	MET	2.2
1	G	486	ASN	2.2
1	H	477	HIS	2.2
1	H	492	LEU	2.2
1	F	141	GLY	2.2
1	H	298	LEU	2.1
1	H	325	ALA	2.1
1	H	142	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

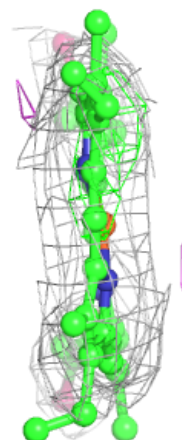
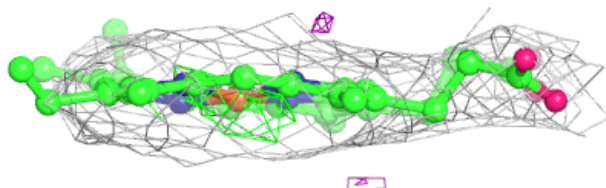
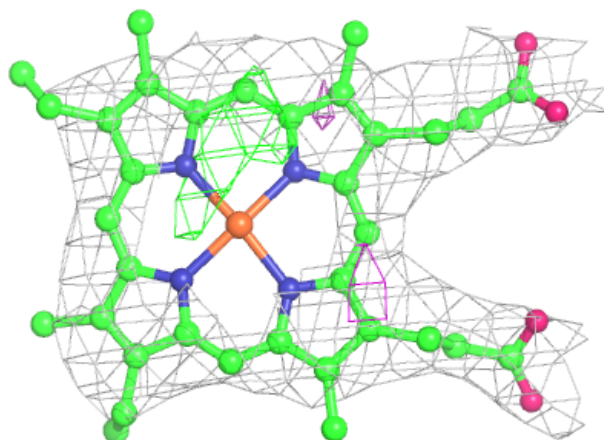
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	9PL	C	1	15/15	0.91	0.42	74,75,76,76	0
2	HEM	H	500	43/43	0.95	0.29	80,82,85,85	0
3	9PL	F	1	15/15	0.96	0.35	74,75,75,76	0
3	9PL	E	1	15/15	0.96	0.31	74,75,76,76	0
3	9PL	B	1	15/15	0.96	0.36	75,77,79,80	0
2	HEM	E	500	43/43	0.97	0.24	53,59,61,62	0
2	HEM	G	500	43/43	0.97	0.28	54,58,60,63	0
2	HEM	C	500	43/43	0.97	0.26	34,41,43,46	0
3	9PL	A	1	15/15	0.97	0.39	60,64,70,71	0
2	HEM	D	500	43/43	0.98	0.26	28,38,42,44	0
3	9PL	D	1	15/15	0.98	0.28	63,66,71,71	0
2	HEM	F	500	43/43	0.98	0.24	56,62,64,64	0
2	HEM	B	500	43/43	0.98	0.27	29,34,38,40	0
2	HEM	A	500	43/43	0.98	0.26	28,34,38,40	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.

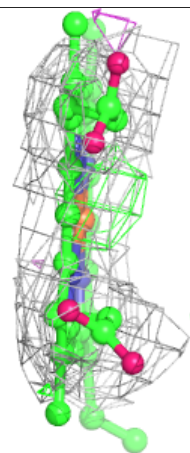
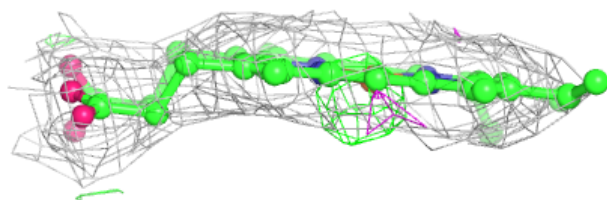
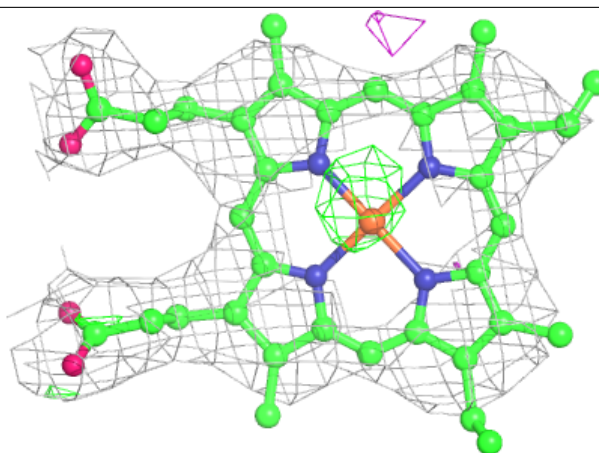
Electron density around HEM H 500:

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



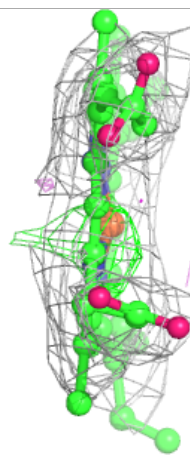
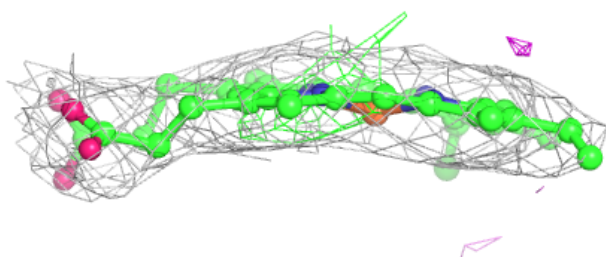
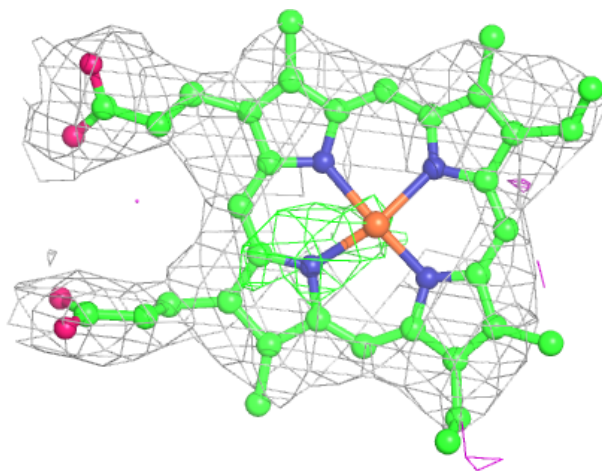
Electron density around HEM E 500:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



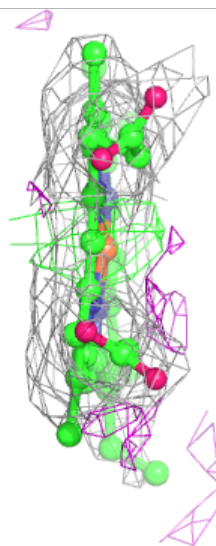
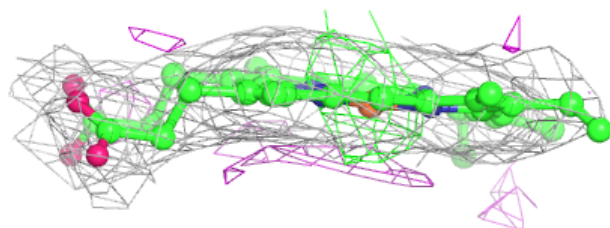
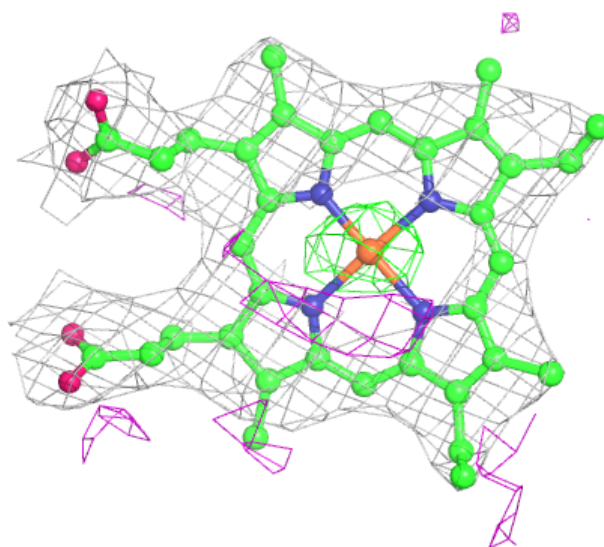
Electron density around HEM G 500:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



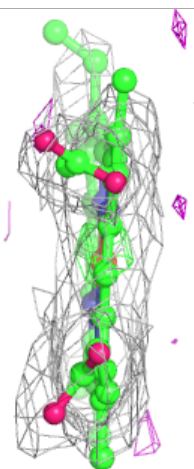
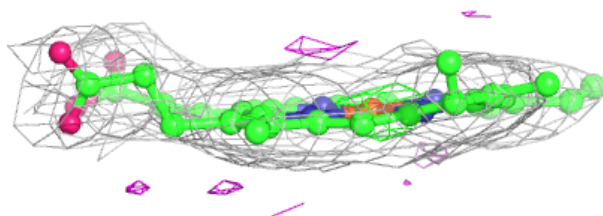
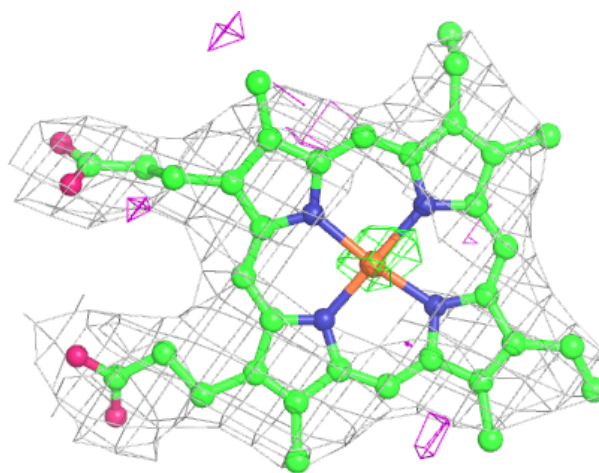
Electron density around HEM C 500:

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



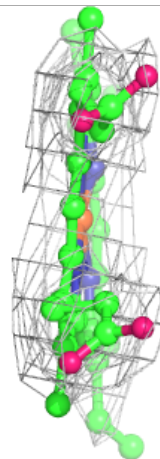
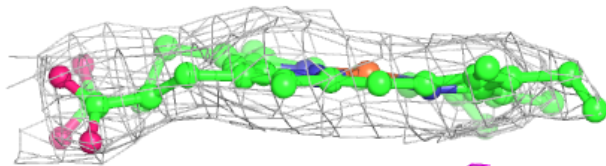
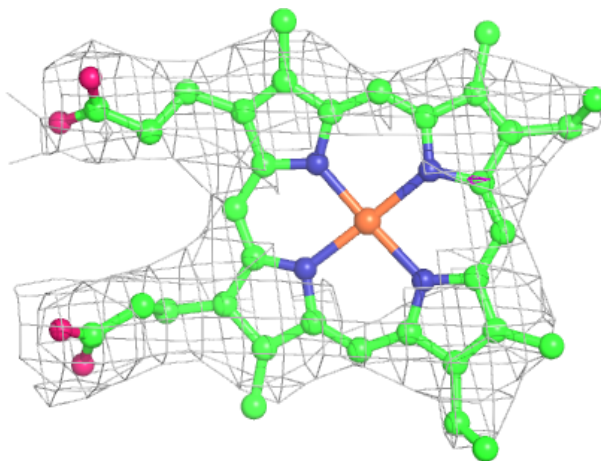
Electron density around HEM D 500:

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



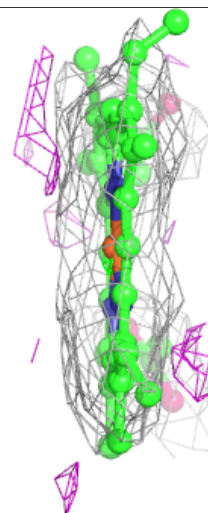
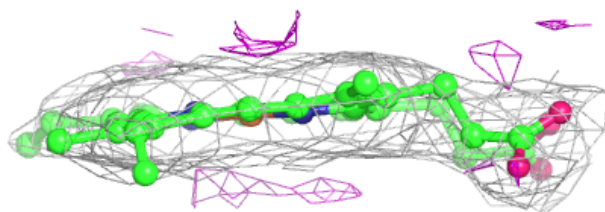
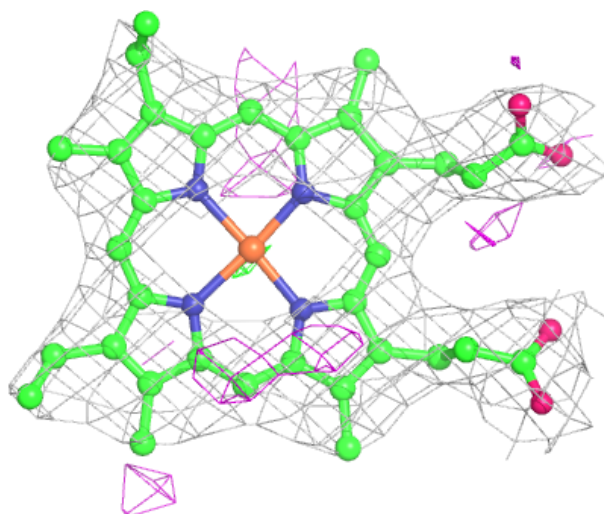
Electron density around HEM F 500:

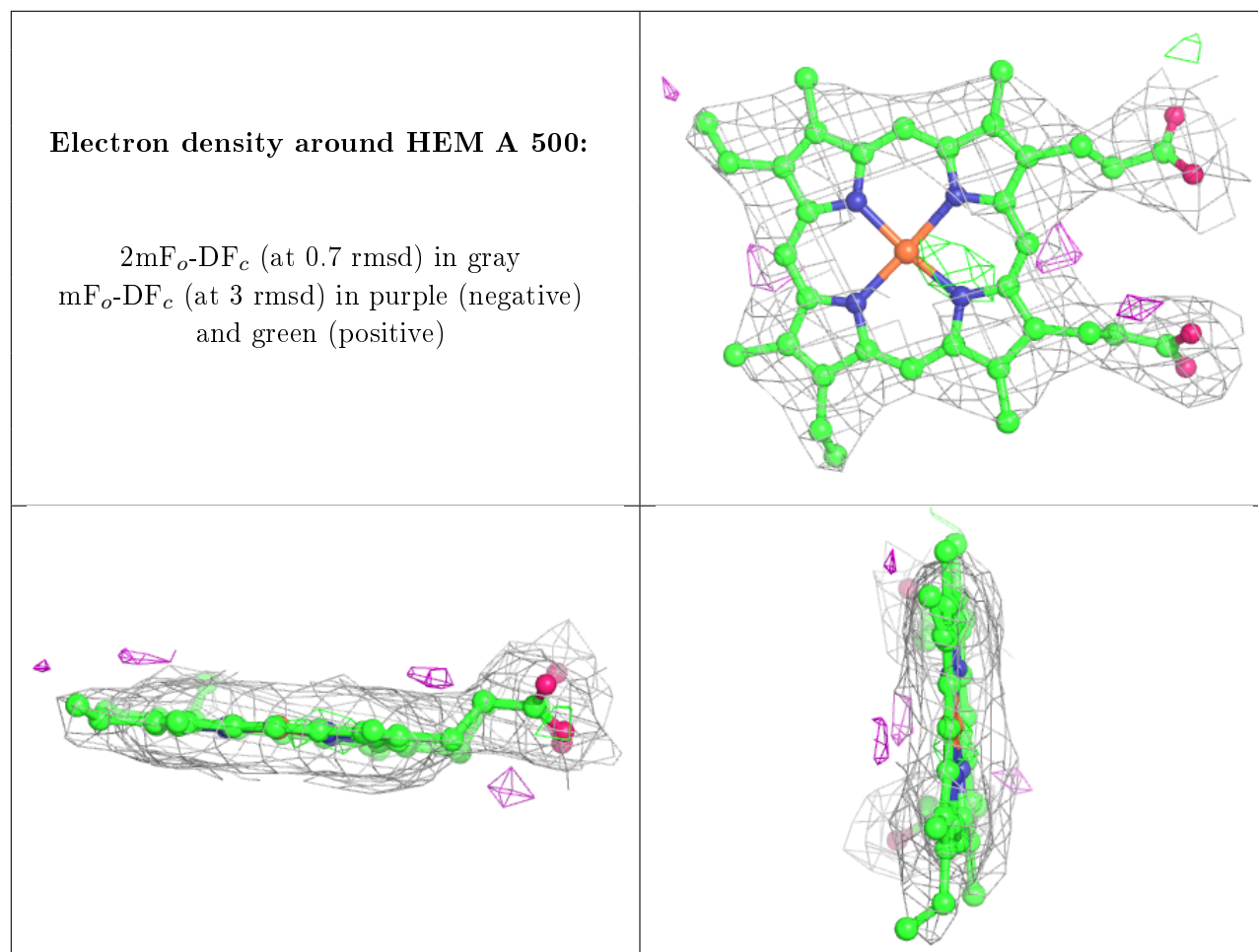
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 ⓘ

There are no such residues in this entry.