



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 06:19 AM BST

PDB ID : 5VEU  
Title : Human Cytochrome P450 3A5 (CYP3A5)  
Authors : Hsu, M.-H.; Johnson, E.F.  
Deposited on : 2017-04-05  
Resolution : 2.91 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

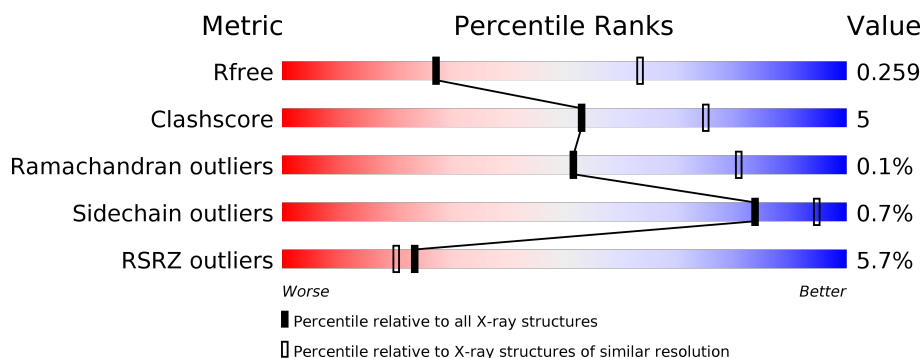
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	480	<div> <div>3%</div> <div>85% 11% .</div> </div>
1	B	480	<div> <div>4%</div> <div>80% 15% 5%</div> </div>
1	C	480	<div> <div>2%</div> <div>86% 11% ..</div> </div>
1	D	480	<div> <div>2%</div> <div>80% 16% .</div> </div>
1	E	480	<div> <div>14%</div> <div>78% 14% . 8%</div> </div>
1	F	480	<div> <div>8%</div> <div>80% 15% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	480	<div><div>%</div><div><div></div><div>83%</div><div>12%</div><div>5%</div></div></div>
1	H	480	<div><div>2%</div><div><div></div><div>81%</div><div>15%</div><div></div></div></div>
1	I	480	<div><div>3%</div><div><div></div><div>85%</div><div>12%</div><div></div></div></div>
1	J	480	<div><div>5%</div><div><div></div><div>79%</div><div>16%</div><div>5%</div></div></div>
1	K	480	<div><div>3%</div><div><div></div><div>83%</div><div>12%</div><div>5%</div></div></div>
1	L	480	<div><div>20%</div><div><div></div><div>80%</div><div>13%</div><div>7%</div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 44740 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 3A5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	0	0
			3714	2413	616	668	17			
1	B	458	Total	C	N	O	S	0	0	0
			3679	2391	609	662	17			
1	C	469	Total	C	N	O	S	0	0	0
			3773	2448	627	681	17			
1	D	459	Total	C	N	O	S	0	0	0
			3687	2395	610	665	17			
1	E	441	Total	C	N	O	S	0	0	0
			3540	2310	577	636	17			
1	F	456	Total	C	N	O	S	0	0	0
			3661	2381	604	659	17			
1	G	455	Total	C	N	O	S	0	0	0
			3651	2374	602	658	17			
1	H	459	Total	C	N	O	S	0	0	0
			3687	2395	610	665	17			
1	I	464	Total	C	N	O	S	0	0	0
			3732	2423	619	673	17			
1	J	458	Total	C	N	O	S	0	0	0
			3679	2391	609	662	17			
1	K	458	Total	C	N	O	S	0	0	0
			3681	2392	609	663	17			
1	L	448	Total	C	N	O	S	0	0	0
			3590	2339	588	646	17			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	MET	-	initiating methionine	UNP P20815
A	23	ALA	-	expression tag	UNP P20815
A	498	HIS	-	expression tag	UNP P20815
A	499	HIS	-	expression tag	UNP P20815
A	500	HIS	-	expression tag	UNP P20815

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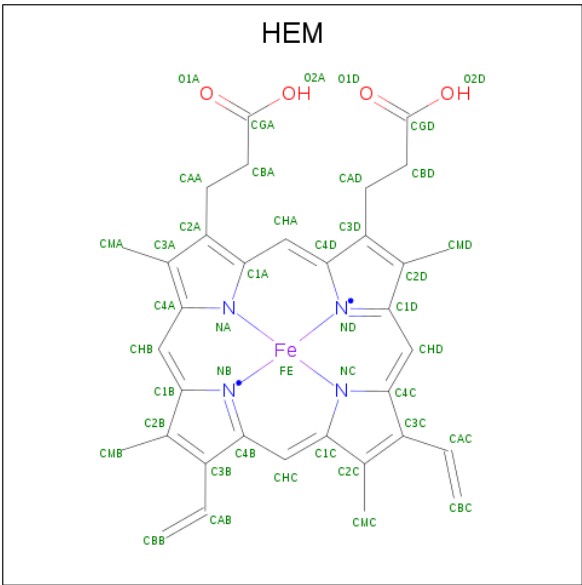
Chain	Residue	Modelled	Actual	Comment	Reference
A	501	HIS	-	expression tag	UNP P20815
B	22	MET	-	initiating methionine	UNP P20815
B	23	ALA	-	expression tag	UNP P20815
B	498	HIS	-	expression tag	UNP P20815
B	499	HIS	-	expression tag	UNP P20815
B	500	HIS	-	expression tag	UNP P20815
B	501	HIS	-	expression tag	UNP P20815
C	22	MET	-	initiating methionine	UNP P20815
C	23	ALA	-	expression tag	UNP P20815
C	498	HIS	-	expression tag	UNP P20815
C	499	HIS	-	expression tag	UNP P20815
C	500	HIS	-	expression tag	UNP P20815
C	501	HIS	-	expression tag	UNP P20815
D	22	MET	-	initiating methionine	UNP P20815
D	23	ALA	-	expression tag	UNP P20815
D	498	HIS	-	expression tag	UNP P20815
D	499	HIS	-	expression tag	UNP P20815
D	500	HIS	-	expression tag	UNP P20815
D	501	HIS	-	expression tag	UNP P20815
E	22	MET	-	initiating methionine	UNP P20815
E	23	ALA	-	expression tag	UNP P20815
E	498	HIS	-	expression tag	UNP P20815
E	499	HIS	-	expression tag	UNP P20815
E	500	HIS	-	expression tag	UNP P20815
E	501	HIS	-	expression tag	UNP P20815
F	22	MET	-	initiating methionine	UNP P20815
F	23	ALA	-	expression tag	UNP P20815
F	498	HIS	-	expression tag	UNP P20815
F	499	HIS	-	expression tag	UNP P20815
F	500	HIS	-	expression tag	UNP P20815
F	501	HIS	-	expression tag	UNP P20815
G	22	MET	-	initiating methionine	UNP P20815
G	23	ALA	-	expression tag	UNP P20815
G	498	HIS	-	expression tag	UNP P20815
G	499	HIS	-	expression tag	UNP P20815
G	500	HIS	-	expression tag	UNP P20815
G	501	HIS	-	expression tag	UNP P20815
H	22	MET	-	initiating methionine	UNP P20815
H	23	ALA	-	expression tag	UNP P20815
H	498	HIS	-	expression tag	UNP P20815
H	499	HIS	-	expression tag	UNP P20815
H	500	HIS	-	expression tag	UNP P20815

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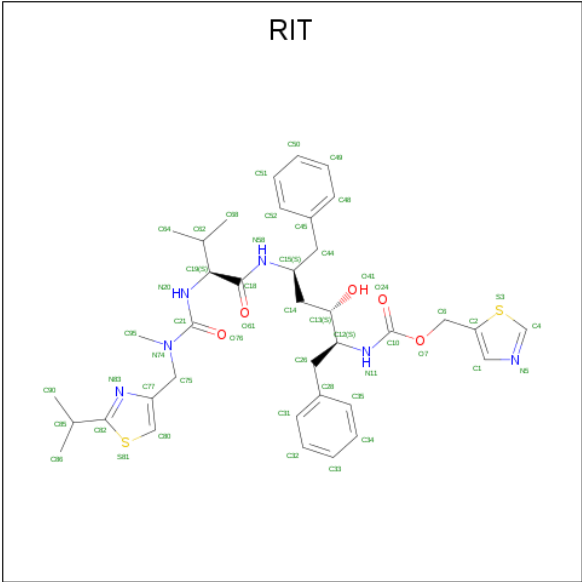
Chain	Residue	Modelled	Actual	Comment	Reference
H	501	HIS	-	expression tag	UNP P20815
I	22	MET	-	initiating methionine	UNP P20815
I	23	ALA	-	expression tag	UNP P20815
I	498	HIS	-	expression tag	UNP P20815
I	499	HIS	-	expression tag	UNP P20815
I	500	HIS	-	expression tag	UNP P20815
I	501	HIS	-	expression tag	UNP P20815
J	22	MET	-	initiating methionine	UNP P20815
J	23	ALA	-	expression tag	UNP P20815
J	498	HIS	-	expression tag	UNP P20815
J	499	HIS	-	expression tag	UNP P20815
J	500	HIS	-	expression tag	UNP P20815
J	501	HIS	-	expression tag	UNP P20815
K	22	MET	-	initiating methionine	UNP P20815
K	23	ALA	-	expression tag	UNP P20815
K	498	HIS	-	expression tag	UNP P20815
K	499	HIS	-	expression tag	UNP P20815
K	500	HIS	-	expression tag	UNP P20815
K	501	HIS	-	expression tag	UNP P20815
L	22	MET	-	initiating methionine	UNP P20815
L	23	ALA	-	expression tag	UNP P20815
L	498	HIS	-	expression tag	UNP P20815
L	499	HIS	-	expression tag	UNP P20815
L	500	HIS	-	expression tag	UNP P20815
L	501	HIS	-	expression tag	UNP P20815

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
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
2	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is RITONAVIR (three-letter code: RIT) (formula: C<sub>37</sub>H<sub>48</sub>N<sub>6</sub>O<sub>5</sub>S<sub>2</sub>).



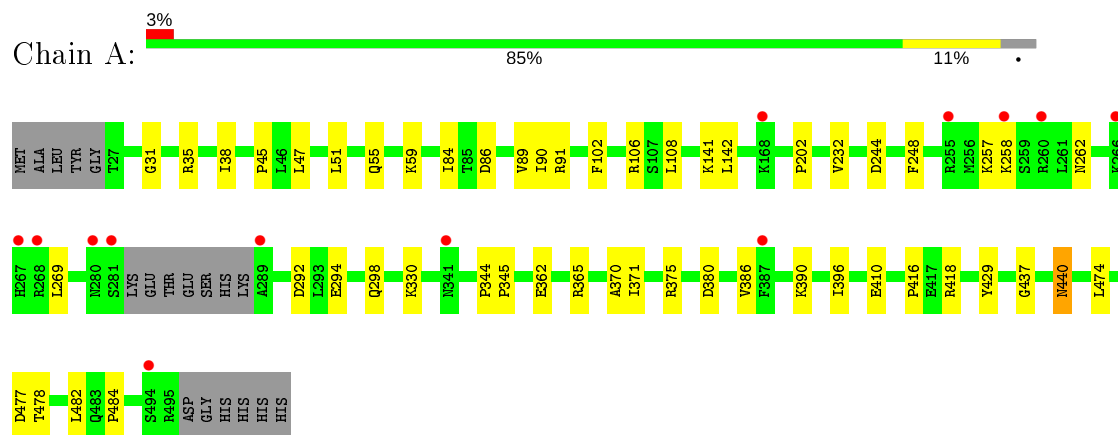
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			50	37	6	5	2		
3	B	1	Total	C	N	O	S	0	0
			50	37	6	5	2		
3	H	1	Total	C	N	O	S	0	0
			50	37	6	5	2		



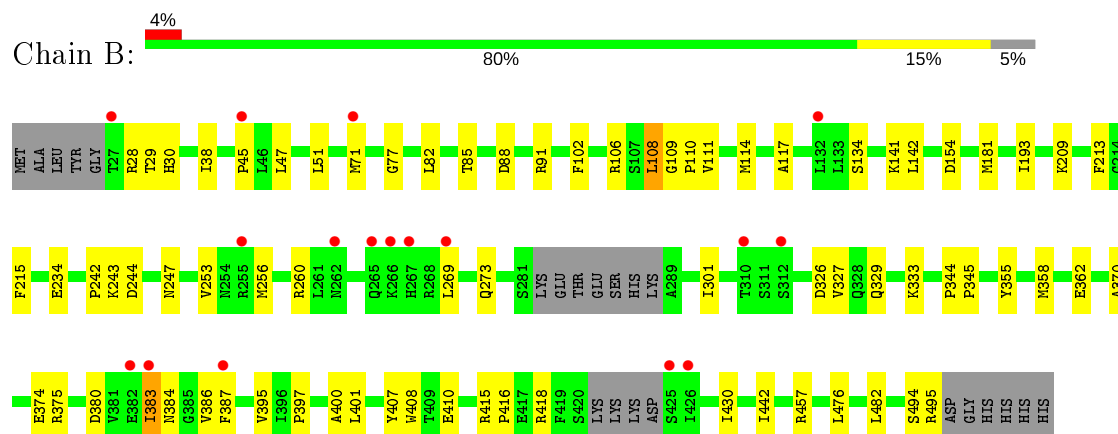
### 3 Residue-property plots [i](#)

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.

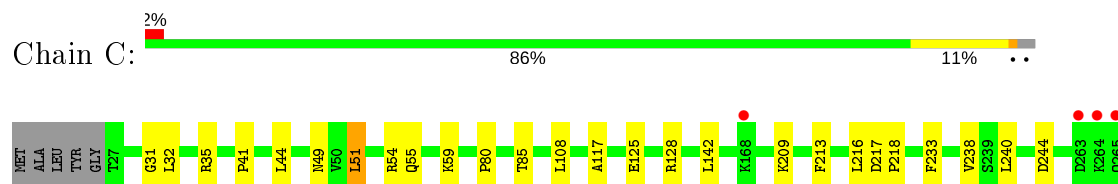
#### • Molecule 1: Cytochrome P450 3A5

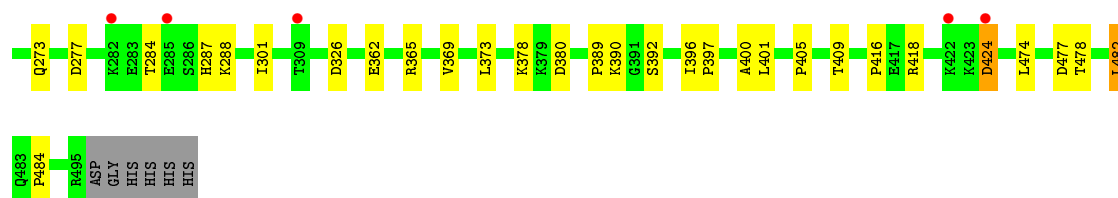


#### • Molecule 1: Cytochrome P450 3A5

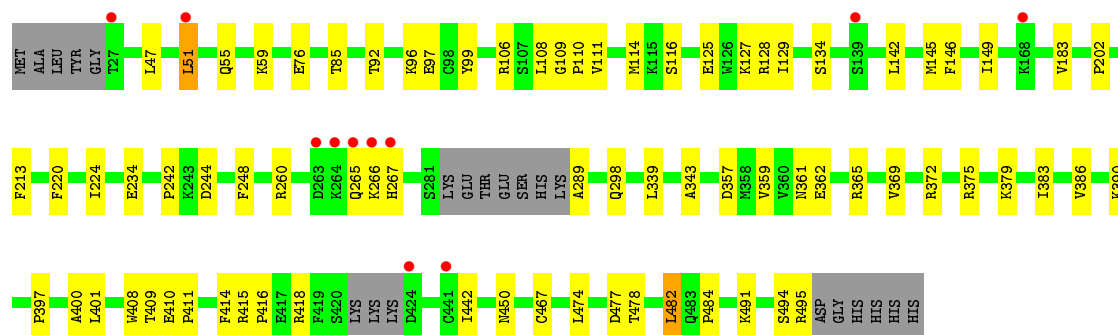
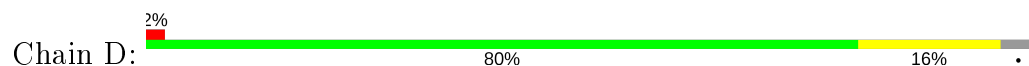


#### • Molecule 1: Cytochrome P450 3A5

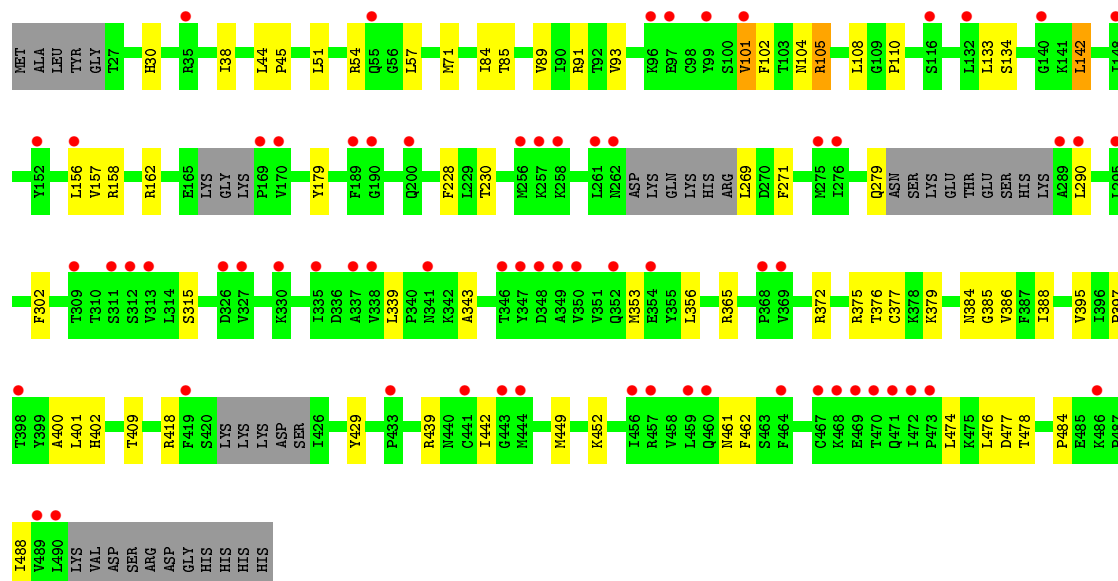
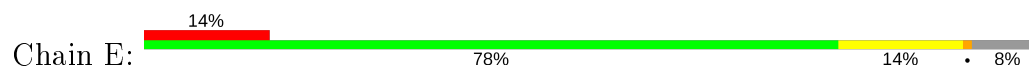




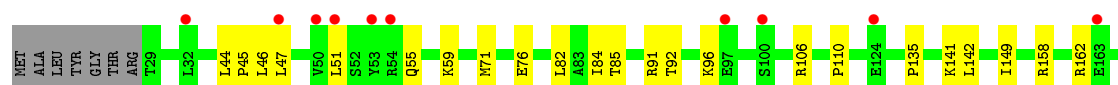
• Molecule 1: Cytochrome P450 3A5

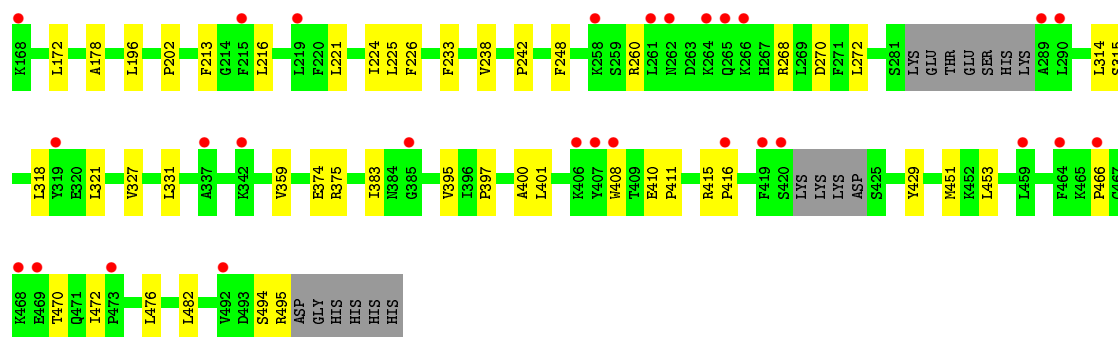


• Molecule 1: Cytochrome P450 3A5

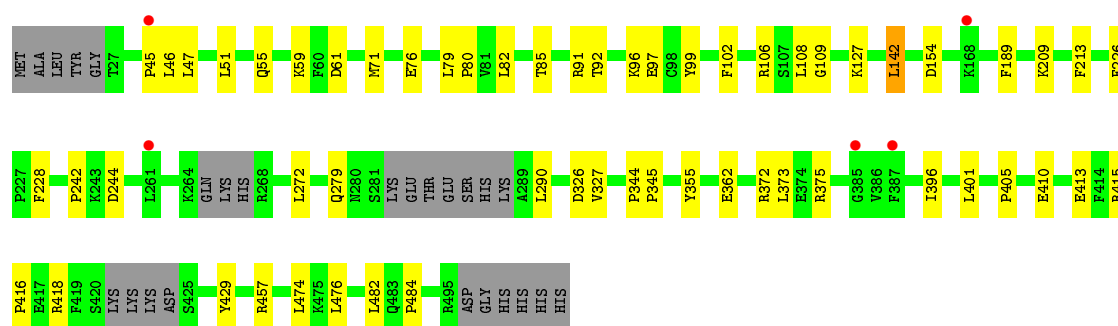
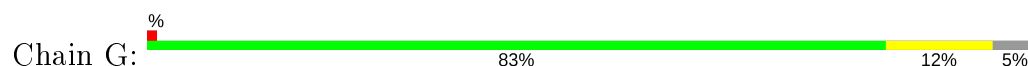


• Molecule 1: Cytochrome P450 3A5

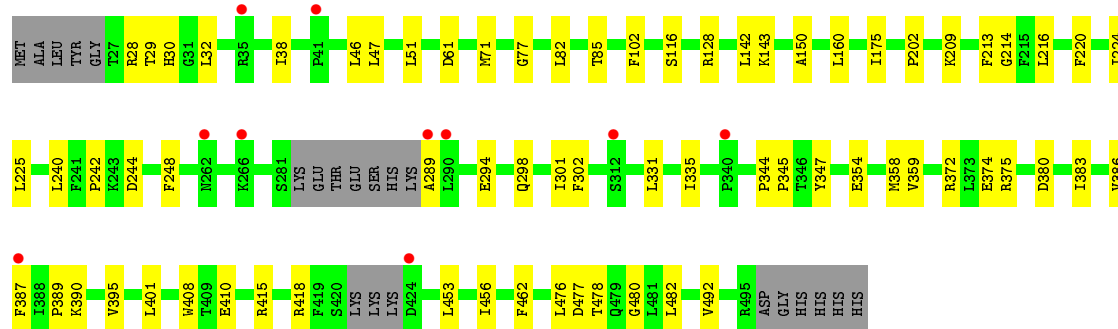
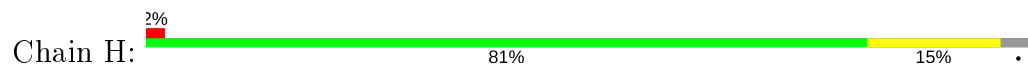




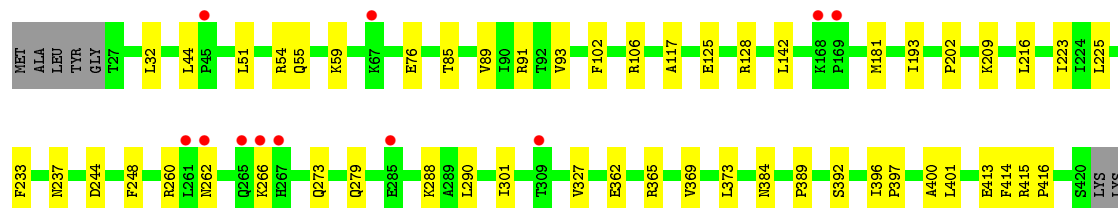
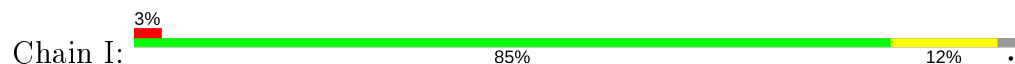
• Molecule 1: Cytochrome P450 3A5



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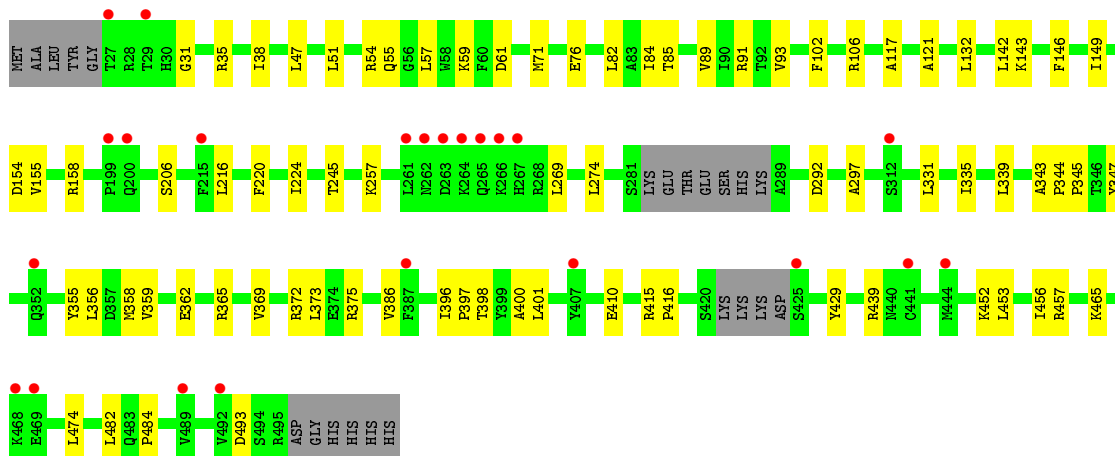
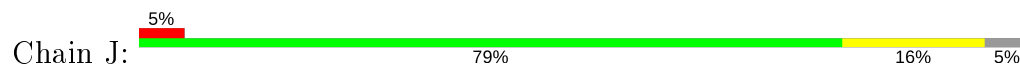


• Molecule 1: Cytochrome P450 3A5

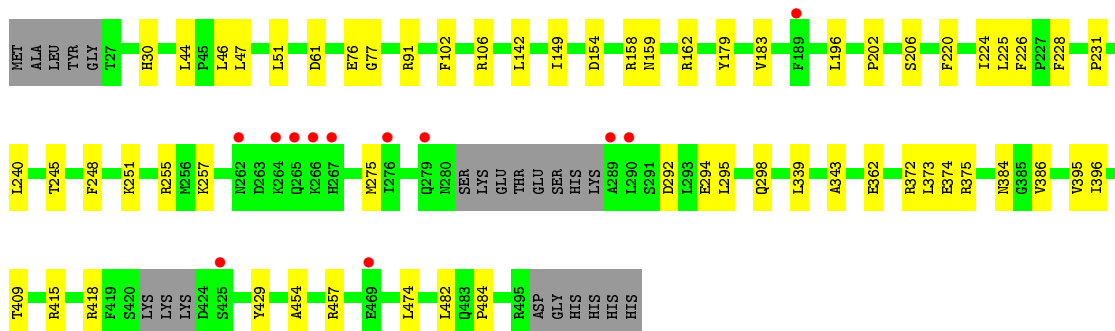
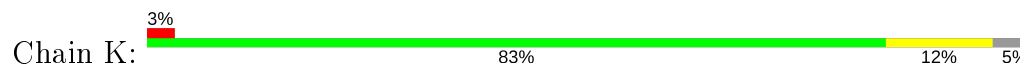




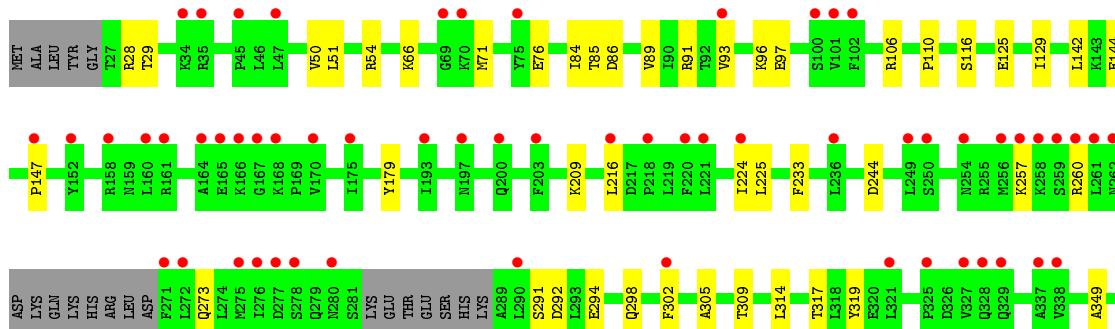
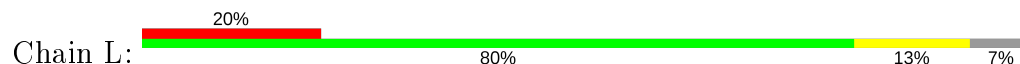
● Molecule 1: Cytochrome P450 3A5

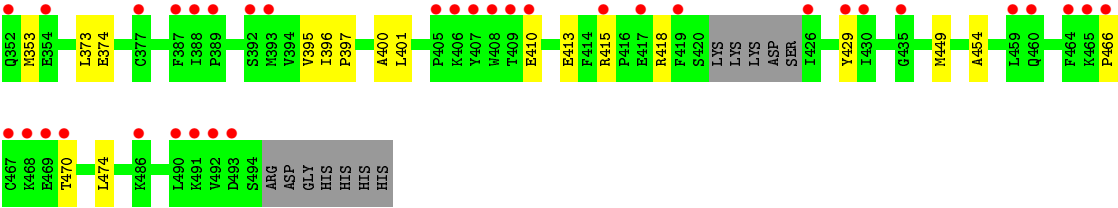


● Molecule 1: Cytochrome P450 3A5



● Molecule 1: Cytochrome P450 3A5





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.99Å 198.38Å 234.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.16 – 2.91 39.16 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.16-2.91) 99.7 (39.16-2.91)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.214 , 0.258 0.216 , 0.259	Depositor DCC
$R_{free}$ test set	7550 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.7	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.7	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	0.93	EDS
Total number of atoms	44740	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.26	0/3803	0.42	0/5148
1	B	0.26	0/3767	0.42	0/5101
1	C	0.26	0/3864	0.43	0/5230
1	D	0.25	0/3775	0.42	0/5112
1	E	0.25	0/3625	0.42	0/4912
1	F	0.25	0/3749	0.41	0/5077
1	G	0.26	0/3737	0.41	0/5060
1	H	0.25	0/3775	0.41	0/5112
1	I	0.26	0/3822	0.42	0/5175
1	J	0.25	0/3767	0.41	0/5101
1	K	0.25	0/3769	0.41	0/5104
1	L	0.24	0/3676	0.41	0/4980
All	All	0.25	0/45129	0.42	0/61112

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	3714	0	3810	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3679	0	3766	56	0
1	C	3773	0	3868	33	0
1	D	3687	0	3770	41	0
1	E	3540	0	3618	36	0
1	F	3661	0	3746	42	0
1	G	3651	0	3737	35	0
1	H	3687	0	3770	41	0
1	I	3732	0	3819	34	0
1	J	3679	0	3766	42	0
1	K	3681	0	3765	34	0
1	L	3590	0	3674	36	0
2	A	43	0	30	3	0
2	B	43	0	30	3	0
2	C	43	0	30	2	0
2	D	43	0	30	3	0
2	E	43	0	30	5	0
2	F	43	0	30	3	0
2	G	43	0	30	2	0
2	H	43	0	30	6	0
2	I	43	0	30	2	0
2	J	43	0	30	2	0
2	K	43	0	30	2	0
2	L	43	0	30	3	0
3	A	50	0	48	5	0
3	B	50	0	48	16	0
3	H	50	0	48	11	0
All	All	44740	0	45613	485	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 5.

All (485) 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:B:106:ARG:NH1	3:B:602:RIT:H683	1.96	0.81
3:H:602:RIT:H141	3:H:602:RIT:H48	1.61	0.81
1:B:106:ARG:NH1	3:B:602:RIT:C68	2.46	0.79
1:A:38:ILE:HD11	1:A:386:VAL:HG21	1.64	0.79
1:B:117:ALA:HB1	1:B:301:ILE:HG13	1.67	0.76
1:D:410:GLU:OE1	1:D:415:ARG:NH2	2.19	0.76
1:H:408:TRP:HE3	1:H:418:ARG:HD3	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:PRO:HG2	1:L:216:LEU:HB3	1.66	0.75
1:E:38:ILE:HD11	1:E:386:VAL:HG11	1.69	0.75
1:H:301:ILE:HD13	3:H:602:RIT:H34	1.68	0.75
1:J:369:VAL:HA	1:J:482:LEU:HB2	1.69	0.75
1:B:88:ASP:OD1	1:B:91:ARG:NH1	2.20	0.74
1:F:213:PHE:HE2	1:F:242:PRO:HG3	1.52	0.74
1:G:413:GLU:OE1	1:G:415:ARG:NH2	2.23	0.72
1:C:54:ARG:HD2	1:C:216:LEU:HD11	1.70	0.71
1:L:28:ARG:HG3	1:L:29:THR:HG23	1.73	0.71
1:B:374:GLU:HG2	1:B:395:VAL:HG22	1.72	0.71
1:I:474:LEU:HD11	1:I:484:PRO:HB3	1.72	0.71
1:K:47:LEU:HD13	1:K:225:LEU:HD21	1.72	0.71
1:A:55:GLN:HB3	1:A:59:LYS:HD3	1.73	0.70
1:C:474:LEU:HD11	1:C:484:PRO:HB3	1.72	0.69
1:G:209:LYS:NZ	1:G:244:ASP:OD2	2.25	0.69
1:H:28:ARG:HG3	1:H:29:THR:HG23	1.75	0.69
1:F:76:GLU:OE1	1:F:106:ARG:NH2	2.26	0.68
1:B:408:TRP:HE3	1:B:418:ARG:HD3	1.59	0.68
1:E:409:THR:O	1:E:418:ARG:NH2	2.26	0.68
1:B:111:VAL:HG12	1:B:114:MET:HB2	1.76	0.68
1:C:128:ARG:HB3	1:C:288:LYS:HB2	1.77	0.67
1:C:369:VAL:HA	1:C:482:LEU:HB2	1.75	0.67
1:I:128:ARG:HB3	1:I:288:LYS:HB2	1.76	0.67
1:H:301:ILE:CD1	3:H:602:RIT:H34	2.25	0.67
1:D:142:LEU:HA	1:D:145:MET:HE2	1.78	0.66
1:C:373:LEU:HB2	1:C:396:ILE:HB	1.77	0.66
1:I:32:LEU:HD21	1:I:389:PRO:HG3	1.79	0.65
1:I:260:ARG:HH21	1:I:266:LYS:HE2	1.61	0.65
1:B:410:GLU:OE1	1:B:415:ARG:NH2	2.25	0.64
1:H:374:GLU:HG2	1:H:395:VAL:HG12	1.80	0.64
1:A:474:LEU:HD11	1:A:484:PRO:HB3	1.80	0.64
3:H:602:RIT:C48	3:H:602:RIT:H141	2.27	0.64
1:B:85:THR:HB	1:B:401:LEU:HD21	1.79	0.64
1:H:209:LYS:NZ	1:H:244:ASP:OD2	2.28	0.63
1:L:76:GLU:OE1	1:L:106:ARG:NH2	2.31	0.63
1:I:413:GLU:OE1	1:I:415:ARG:NH2	2.32	0.63
1:E:474:LEU:HD11	1:E:484:PRO:HB3	1.81	0.62
1:C:209:LYS:NZ	1:C:244:ASP:OD2	2.31	0.62
1:J:84:ILE:HD12	1:J:89:VAL:HG12	1.81	0.62
1:F:260:ARG:HE	1:F:272:LEU:HD23	1.64	0.62
1:B:301:ILE:CD1	3:B:602:RIT:H35	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:155:VAL:HG13	1:J:158:ARG:HH21	1.64	0.62
1:H:408:TRP:CE3	1:H:418:ARG:HD3	2.35	0.61
1:G:474:LEU:HD11	1:G:484:PRO:HB3	1.82	0.61
2:C:601:HEM:HMC2	2:C:601:HEM:HBC2	1.83	0.61
1:D:474:LEU:HD11	1:D:484:PRO:HB3	1.83	0.61
1:F:397:PRO:HB2	1:F:400:ALA:HB3	1.83	0.61
1:C:44:LEU:HD12	1:C:51:LEU:HD23	1.81	0.61
1:I:362:GLU:HG3	1:I:416:PRO:HA	1.83	0.61
1:B:209:LYS:NZ	1:B:244:ASP:OD2	2.34	0.61
1:L:410:GLU:OE1	1:L:415:ARG:NH2	2.32	0.61
1:G:476:LEU:HD23	1:G:482:LEU:HD11	1.83	0.60
2:I:601:HEM:HMC2	2:I:601:HEM:HBC2	1.83	0.60
2:D:601:HEM:HMC2	2:D:601:HEM:HBC2	1.83	0.60
1:E:105:ARG:HH11	2:E:601:HEM:HAA1	1.67	0.60
1:L:413:GLU:O	1:L:418:ARG:NH2	2.35	0.60
1:B:28:ARG:HG3	1:B:29:THR:HG23	1.84	0.60
1:C:32:LEU:HD21	1:C:389:PRO:HG3	1.82	0.60
1:F:375:ARG:NH2	2:F:601:HEM:O1A	2.27	0.60
1:G:55:GLN:HB3	1:G:59:LYS:HD3	1.84	0.60
1:K:474:LEU:HD11	1:K:484:PRO:HB3	1.83	0.60
1:B:106:ARG:NH1	3:B:602:RIT:H681	2.16	0.60
2:J:601:HEM:HBC2	2:J:601:HEM:HMC2	1.83	0.60
1:D:47:LEU:HG	1:D:51:LEU:HD23	1.84	0.59
1:E:279:GLN:NE2	1:E:290:LEU:O	2.35	0.59
1:K:362:GLU:OE2	1:K:418:ARG:NH1	2.32	0.59
1:A:362:GLU:HG3	1:A:416:PRO:HA	1.84	0.59
3:B:602:RIT:H141	3:B:602:RIT:C48	2.31	0.59
1:J:362:GLU:HG3	1:J:416:PRO:HA	1.85	0.59
2:L:601:HEM:HMC2	2:L:601:HEM:HBC2	1.85	0.59
1:B:383:ILE:HG22	1:B:384:ASN:H	1.68	0.59
1:D:55:GLN:HB3	1:D:59:LYS:HD3	1.85	0.59
2:A:601:HEM:HBB2	2:A:601:HEM:HMB2	1.85	0.59
2:K:601:HEM:HMC2	2:K:601:HEM:HBC2	1.83	0.59
1:F:45:PRO:HG2	1:H:216:LEU:HB3	1.85	0.58
1:H:410:GLU:OE1	1:H:415:ARG:NH2	2.36	0.58
2:E:601:HEM:HBC2	2:E:601:HEM:HMC2	1.86	0.58
1:J:71:MET:HE3	1:J:82:LEU:HD11	1.85	0.58
1:J:85:THR:HB	1:J:401:LEU:HD21	1.85	0.58
1:G:154:ASP:OD1	1:G:457:ARG:NH1	2.37	0.58
1:H:375:ARG:NH2	2:H:601:HEM:O1A	2.30	0.58
3:A:602:RIT:H141	3:A:602:RIT:H48	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:VAL:HG22	1:D:114:MET:HB2	1.86	0.58
1:D:213:PHE:HE2	1:D:242:PRO:HG3	1.68	0.58
1:E:302:PHE:CD2	2:E:601:HEM:HBC1	2.39	0.58
1:C:362:GLU:HG3	1:C:416:PRO:HA	1.86	0.57
1:A:386:VAL:HG12	1:G:405:PRO:HG2	1.85	0.57
1:J:362:GLU:OE2	1:J:365:ARG:NE	2.27	0.57
1:B:215:PHE:HE2	3:B:602:RIT:H752	1.69	0.57
1:B:355:TYR:HD2	1:B:358:MET:HE3	1.70	0.57
2:F:601:HEM:HBC2	2:F:601:HEM:HMC2	1.85	0.57
1:H:47:LEU:HG	1:H:225:LEU:HD21	1.85	0.57
2:B:601:HEM:HMB2	2:B:601:HEM:HBB2	1.87	0.57
2:C:601:HEM:HMB2	2:C:601:HEM:HBB2	1.86	0.57
2:G:601:HEM:HMC2	2:G:601:HEM:HBC2	1.87	0.57
3:A:602:RIT:C48	3:A:602:RIT:H141	2.35	0.57
1:B:213:PHE:HE2	1:B:242:PRO:HG3	1.69	0.57
1:B:494:SER:OG	1:B:495:ARG:NH1	2.37	0.57
1:J:474:LEU:HD11	1:J:484:PRO:HB3	1.86	0.57
2:K:601:HEM:HMB2	2:K:601:HEM:HBB2	1.87	0.56
2:B:601:HEM:HBC2	2:B:601:HEM:HMC2	1.87	0.56
1:F:466:PRO:HB3	1:F:470:THR:HG21	1.87	0.56
1:L:374:GLU:HG2	1:L:395:VAL:HG22	1.88	0.56
1:A:90:ILE:HG23	1:A:396:ILE:HG12	1.87	0.56
2:D:601:HEM:HBB2	2:D:601:HEM:HMB1	1.86	0.56
2:G:601:HEM:HMB2	2:G:601:HEM:HBB2	1.86	0.56
1:G:71:MET:HE3	1:G:82:LEU:HD11	1.88	0.56
1:D:375:ARG:NH2	2:D:601:HEM:O1A	2.28	0.56
1:F:410:GLU:OE1	1:F:415:ARG:NH2	2.38	0.56
2:J:601:HEM:HBB2	2:J:601:HEM:HMB2	1.86	0.56
1:F:85:THR:HB	1:F:401:LEU:HD21	1.88	0.56
2:I:601:HEM:HMB2	2:I:601:HEM:HBB2	1.87	0.56
1:J:47:LEU:HD13	1:K:47:LEU:HD21	1.87	0.56
2:A:601:HEM:HMC2	2:A:601:HEM:HBC2	1.86	0.55
1:E:157:VAL:HG21	1:E:461:ASN:HD22	1.71	0.55
1:B:38:ILE:HD11	1:B:386:VAL:HG21	1.87	0.55
1:I:262:ASN:HD21	1:I:266:LYS:HD2	1.71	0.55
1:H:128:ARG:NH1	1:H:289:ALA:O	2.39	0.55
2:L:601:HEM:HBB2	2:L:601:HEM:HMB2	1.89	0.55
2:H:601:HEM:HBB2	2:H:601:HEM:HMB2	1.89	0.55
1:G:47:LEU:HD22	1:G:51:LEU:HD21	1.89	0.55
2:F:601:HEM:HBB2	2:F:601:HEM:HMB2	1.88	0.55
2:H:601:HEM:CHA	3:H:602:RIT:H50	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:TRP:CE3	1:B:418:ARG:HD3	2.42	0.54
1:E:339:LEU:HB3	1:E:343:ALA:HB3	1.88	0.54
1:K:154:ASP:OD1	1:K:457:ARG:NH1	2.41	0.54
1:G:189:PHE:HD1	1:G:272:LEU:HB2	1.72	0.54
1:F:44:LEU:HD12	1:F:51:LEU:HD23	1.89	0.54
1:H:480:GLY:HA2	3:H:602:RIT:H953	1.90	0.54
3:B:602:RIT:C77	3:B:602:RIT:H20	2.20	0.54
1:I:76:GLU:OE2	1:I:106:ARG:NH2	2.41	0.54
2:E:601:HEM:HMB2	2:E:601:HEM:HBB2	1.90	0.54
1:D:339:LEU:HB3	1:D:343:ALA:HB3	1.89	0.53
1:B:370:ALA:HB2	3:B:602:RIT:H51	1.91	0.53
1:J:339:LEU:HB3	1:J:343:ALA:HB3	1.89	0.53
1:D:362:GLU:OE2	1:D:365:ARG:NE	2.35	0.53
1:G:79:LEU:HD12	1:G:80:PRO:HD2	1.91	0.53
1:B:71:MET:HG2	1:B:82:LEU:HD11	1.91	0.52
1:A:45:PRO:HG2	1:I:216:LEU:HB3	1.91	0.52
1:B:108:LEU:H	1:B:108:LEU:HD13	1.74	0.52
1:J:154:ASP:OD1	1:J:457:ARG:NH1	2.37	0.52
1:K:409:THR:O	1:K:418:ARG:NH2	2.41	0.52
1:L:209:LYS:NZ	1:L:244:ASP:OD2	2.37	0.52
1:C:273:GLN:NE2	1:C:277:ASP:OD1	2.40	0.52
1:J:355:TYR:HD2	1:J:358:MET:HE3	1.75	0.52
1:K:61:ASP:OD1	1:K:372:ARG:NH2	2.43	0.52
1:C:380:ASP:OD1	1:C:390:LYS:N	2.42	0.52
1:H:331:LEU:HD22	1:H:359:VAL:HG21	1.93	0.51
1:J:331:LEU:HD22	1:J:359:VAL:HG21	1.92	0.51
1:C:213:PHE:HE1	1:C:240:LEU:HD12	1.75	0.51
1:A:47:LEU:HD11	1:I:225:LEU:HD11	1.92	0.51
1:A:380:ASP:OD1	1:A:390:LYS:N	2.42	0.51
1:C:397:PRO:HB2	1:C:400:ALA:HB3	1.92	0.51
1:B:253:VAL:HA	1:B:256:MET:HE2	1.92	0.51
1:A:330:LYS:NZ	1:C:405:PRO:O	2.31	0.51
1:F:233:PHE:HB3	1:F:238:VAL:HB	1.91	0.51
1:F:408:TRP:HB2	1:F:411:PRO:HB3	1.91	0.51
1:D:467:CYS:HB3	1:D:491:LYS:HG3	1.92	0.51
1:J:38:ILE:HD11	1:J:386:VAL:HG11	1.93	0.51
1:J:55:GLN:HB3	1:J:59:LYS:HD3	1.92	0.51
1:I:209:LYS:NZ	1:I:244:ASP:OD2	2.32	0.51
1:E:101:VAL:HG12	1:E:379:LYS:HG2	1.93	0.51
1:D:362:GLU:HG3	1:D:416:PRO:HA	1.93	0.51
1:H:380:ASP:OD1	1:H:390:LYS:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:257:LYS:NZ	1:L:292:ASP:OD1	2.44	0.51
1:D:369:VAL:HA	1:D:482:LEU:HB2	1.92	0.51
1:G:362:GLU:HG3	1:G:416:PRO:HA	1.93	0.51
1:L:50:VAL:HG21	1:L:224:ILE:HD13	1.93	0.51
1:F:331:LEU:HD22	1:F:359:VAL:HG21	1.94	0.50
1:B:47:LEU:HD21	1:L:225:LEU:HD11	1.92	0.50
1:D:116:SER:O	1:D:298:GLN:NE2	2.41	0.50
1:L:466:PRO:HB3	1:L:470:THR:HG21	1.93	0.50
1:J:220:PHE:CE2	1:J:224:ILE:HD11	2.47	0.50
1:G:61:ASP:OD1	1:G:372:ARG:NH2	2.43	0.50
1:G:415:ARG:O	1:G:418:ARG:HG2	2.11	0.50
1:H:32:LEU:HD11	1:H:389:PRO:HG3	1.94	0.50
1:L:86:ASP:HB3	1:L:89:VAL:HB	1.94	0.50
1:B:397:PRO:HB2	1:B:400:ALA:HB3	1.93	0.50
1:F:327:VAL:HG11	1:F:416:PRO:HG2	1.93	0.50
1:F:91:ARG:HG3	1:F:429:TYR:CZ	2.47	0.50
1:I:397:PRO:HB2	1:I:400:ALA:HB3	1.94	0.50
1:J:61:ASP:OD1	1:J:372:ARG:NH2	2.44	0.50
1:B:301:ILE:CD1	3:B:602:RIT:C35	2.90	0.49
1:C:51:LEU:O	1:C:54:ARG:HG3	2.13	0.49
1:K:384:ASN:H	1:K:386:VAL:HG22	1.77	0.49
1:L:125:GLU:O	1:L:129:ILE:HG12	2.12	0.49
1:D:149:ILE:HD13	1:D:450:ASN:HB3	1.94	0.49
1:L:291:SER:H	1:L:294:GLU:HB2	1.77	0.49
1:A:141:LYS:NZ	1:A:269:LEU:HG	2.27	0.49
1:G:213:PHE:HE2	1:G:242:PRO:HG3	1.77	0.49
1:G:373:LEU:HB2	1:G:396:ILE:HB	1.94	0.49
1:F:55:GLN:HB3	1:F:59:LYS:HD3	1.94	0.49
1:K:339:LEU:HB3	1:K:343:ALA:HB3	1.93	0.49
1:L:302:PHE:CD2	2:L:601:HEM:HBC1	2.47	0.49
3:B:602:RIT:N11	3:B:602:RIT:H48	2.27	0.49
1:F:149:ILE:HG22	1:F:453:LEU:HD22	1.95	0.49
1:G:102:PHE:HB3	1:G:375:ARG:HB3	1.93	0.49
1:C:41:PRO:HB2	1:C:49:ASN:ND2	2.28	0.49
1:J:143:LYS:HG2	1:J:347:TYR:CG	2.48	0.48
1:A:294:GLU:O	1:A:298:GLN:HG2	2.14	0.48
1:I:91:ARG:HG3	1:I:429:TYR:CZ	2.49	0.48
1:B:215:PHE:CE2	3:B:602:RIT:H752	2.48	0.48
1:D:409:THR:O	1:D:418:ARG:NH2	2.47	0.48
1:H:354:GLU:O	1:H:358:MET:HG3	2.13	0.48
1:L:260:ARG:HH12	1:L:273:GLN:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:GLU:HG3	1:B:416:PRO:HA	1.94	0.48
1:C:80:PRO:HG2	1:C:392:SER:HB3	1.95	0.48
1:D:359:VAL:HG13	1:D:414:PHE:HZ	1.78	0.48
1:H:61:ASP:OD2	1:H:372:ARG:HD3	2.14	0.48
1:J:149:ILE:HG22	1:J:453:LEU:HD22	1.96	0.48
1:B:102:PHE:HB3	1:B:375:ARG:HB3	1.95	0.48
1:D:357:ASP:O	1:D:361:ASN:ND2	2.46	0.48
1:K:158:ARG:HE	1:K:162:ARG:HH21	1.60	0.48
1:D:397:PRO:HB2	1:D:400:ALA:HB3	1.96	0.48
1:F:158:ARG:HH21	1:F:162:ARG:HH22	1.61	0.48
1:H:150:ALA:HA	1:H:453:LEU:HD21	1.96	0.48
1:B:141:LYS:NZ	1:B:269:LEU:HG	2.29	0.48
1:E:377:CYS:SG	1:E:388:ILE:HD11	2.54	0.48
1:K:206:SER:HB3	1:K:245:THR:HG23	1.96	0.48
1:G:91:ARG:HG3	1:G:429:TYR:CZ	2.49	0.48
1:B:109:GLY:O	1:B:111:VAL:HG23	2.13	0.48
1:E:133:LEU:HD22	1:E:271:PHE:HE1	1.78	0.48
1:F:268:ARG:HH11	1:F:270:ASP:HB3	1.78	0.48
1:J:91:ARG:HG3	1:J:429:TYR:OH	2.13	0.48
1:K:220:PHE:CE2	1:K:224:ILE:HD11	2.48	0.48
1:L:110:PRO:HG3	1:L:233:PHE:HD2	1.78	0.47
1:H:294:GLU:O	1:H:298:GLN:HG2	2.14	0.47
1:K:159:ASN:ND2	1:K:196:LEU:O	2.47	0.47
1:H:202:PRO:HB2	1:H:248:PHE:CZ	2.50	0.47
1:I:362:GLU:OE2	1:I:365:ARG:NE	2.40	0.47
1:A:102:PHE:HB3	1:A:375:ARG:HB3	1.95	0.47
1:J:102:PHE:HB3	1:J:375:ARG:HB3	1.96	0.47
1:B:30:HIS:NE2	1:B:77:GLY:O	2.42	0.47
1:C:117:ALA:HB1	1:C:301:ILE:HG13	1.97	0.47
1:J:257:LYS:NZ	1:J:292:ASP:OD1	2.48	0.47
1:H:160:LEU:HD13	1:H:175:ILE:HD13	1.96	0.47
1:K:91:ARG:HG3	1:K:429:TYR:CZ	2.50	0.47
1:L:51:LEU:O	1:L:54:ARG:HG2	2.14	0.47
1:C:362:GLU:OE2	1:C:365:ARG:NE	2.45	0.47
1:C:85:THR:HB	1:C:401:LEU:HD21	1.97	0.47
1:I:260:ARG:HD3	1:I:273:GLN:OE1	2.15	0.47
1:J:31:GLY:O	1:J:35:ARG:HG2	2.15	0.47
1:D:477:ASP:OD1	1:D:478:THR:N	2.48	0.47
2:H:601:HEM:C1D	3:H:602:RIT:H1	2.49	0.47
1:J:410:GLU:OE1	1:J:415:ARG:NH2	2.48	0.47
1:L:373:LEU:HB2	1:L:396:ILE:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:LEU:HD12	1:D:109:GLY:H	1.80	0.46
1:D:110:PRO:HA	1:D:234:GLU:OE1	2.16	0.46
1:E:110:PRO:HD3	1:E:230:THR:HG23	1.97	0.46
1:C:216:LEU:HB3	1:G:45:PRO:HG2	1.97	0.46
1:L:96:LYS:HG2	1:L:97:GLU:HG3	1.97	0.46
1:E:356:LEU:HD21	1:E:452:LYS:HB3	1.96	0.46
1:L:319:TYR:CZ	1:L:474:LEU:HB2	2.50	0.46
1:L:84:ILE:HD12	1:L:89:VAL:HG12	1.97	0.46
1:B:329:GLN:HG2	1:B:333:LYS:HE3	1.97	0.46
2:B:601:HEM:CAA	3:B:602:RIT:H50	2.46	0.46
3:H:602:RIT:O61	3:H:602:RIT:H441	2.14	0.46
1:I:223:ILE:HD11	1:I:233:PHE:HD2	1.80	0.46
1:C:409:THR:O	1:C:418:ARG:NH1	2.48	0.46
1:D:128:ARG:HH21	1:D:289:ALA:N	2.12	0.46
1:I:202:PRO:HB2	1:I:248:PHE:CZ	2.50	0.46
1:K:257:LYS:NZ	1:K:292:ASP:OD1	2.49	0.46
1:H:38:ILE:HD11	1:H:386:VAL:HG21	1.98	0.46
1:H:214:GLY:HA2	3:H:602:RIT:C95	2.45	0.46
1:A:477:ASP:OD1	1:A:478:THR:N	2.48	0.46
1:A:371:ILE:HG13	1:A:482:LEU:HD21	1.98	0.46
1:A:370:ALA:HB2	3:A:602:RIT:C51	2.45	0.46
1:F:110:PRO:HG3	1:F:233:PHE:HB2	1.97	0.46
1:F:92:THR:HA	1:F:96:LYS:HB3	1.98	0.46
1:G:142:LEU:HA	1:G:142:LEU:HD13	1.84	0.46
1:C:55:GLN:HB2	1:C:59:LYS:HE3	1.98	0.46
1:E:384:ASN:HB3	1:E:385:GLY:H	1.62	0.46
1:I:51:LEU:O	1:I:54:ARG:HG3	2.15	0.46
1:A:232:VAL:HG22	1:E:228:PHE:HD1	1.80	0.45
1:B:243:LYS:O	1:B:247:ASN:ND2	2.38	0.45
1:H:477:ASP:OD1	1:H:478:THR:N	2.49	0.45
1:B:301:ILE:HD13	3:B:602:RIT:H34	1.98	0.45
1:B:326:ASP:OD1	1:B:327:VAL:N	2.49	0.45
1:C:284:THR:HG23	1:C:287:HIS:H	1.81	0.45
1:D:85:THR:HB	1:D:401:LEU:HD21	1.98	0.45
1:A:31:GLY:O	1:A:35:ARG:HB2	2.16	0.45
1:F:476:LEU:HD23	1:F:482:LEU:HD11	1.98	0.45
1:H:213:PHE:HE2	1:H:242:PRO:HG3	1.81	0.45
1:L:91:ARG:HG3	1:L:429:TYR:OH	2.16	0.45
1:C:477:ASP:OD1	1:C:478:THR:N	2.49	0.45
1:G:279:GLN:HG2	1:G:290:LEU:O	2.17	0.45
1:H:85:THR:HB	1:H:401:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:117:ALA:HB2	1:J:297:ALA:HB1	1.98	0.45
1:K:102:PHE:HB3	1:K:375:ARG:HB3	1.98	0.45
1:K:415:ARG:O	1:K:418:ARG:HG2	2.16	0.45
1:E:156:LEU:HD13	1:E:179:TYR:HB2	1.99	0.45
1:D:265:GLN:HG3	1:D:266:LYS:HG3	1.98	0.45
1:J:132:LEU:O	1:J:274:LEU:HD21	2.15	0.45
1:J:373:LEU:HB2	1:J:396:ILE:HB	1.99	0.45
1:J:397:PRO:HB2	1:J:400:ALA:HB3	1.98	0.45
1:A:362:GLU:OE2	1:A:365:ARG:NE	2.30	0.45
1:F:216:LEU:HA	1:F:221:LEU:HD22	1.99	0.45
1:B:181:MET:HG3	1:B:193:ILE:HD11	1.99	0.45
1:B:260:ARG:NH1	1:B:273:GLN:HB2	2.32	0.45
1:I:89:VAL:HG22	1:I:384:ASN:HB2	1.99	0.45
1:K:294:GLU:O	1:K:298:GLN:HG2	2.16	0.45
1:L:349:ALA:O	1:L:353:MET:HG3	2.17	0.45
1:E:158:ARG:HG2	1:E:162:ARG:HH21	1.82	0.44
1:E:142:LEU:HD12	1:E:449:MET:SD	2.57	0.44
1:F:318:LEU:HD23	1:F:321:LEU:HD12	1.98	0.44
1:F:494:SER:HB3	1:F:495:ARG:NH1	2.32	0.44
1:I:482:LEU:HD12	1:I:482:LEU:HA	1.86	0.44
1:C:233:PHE:HB3	1:C:238:VAL:HB	1.99	0.44
1:H:71:MET:HE2	1:H:82:LEU:HD11	1.98	0.44
1:I:262:ASN:ND2	1:I:266:LYS:HD2	2.32	0.44
1:L:314:LEU:O	1:L:317:THR:OG1	2.30	0.44
1:B:110:PRO:HA	1:B:234:GLU:OE1	2.17	0.44
1:E:91:ARG:HG3	1:E:429:TYR:OH	2.17	0.44
1:F:221:LEU:O	1:F:225:LEU:HG	2.18	0.44
1:I:44:LEU:HD12	1:I:51:LEU:HD23	2.00	0.44
1:C:326:ASP:OD1	1:C:326:ASP:N	2.49	0.44
1:G:410:GLU:HB3	1:G:413:GLU:HG3	2.00	0.44
1:J:465:LYS:NZ	1:J:493:ASP:OD2	2.45	0.44
1:A:202:PRO:HB2	1:A:248:PHE:CZ	2.53	0.44
1:B:380:ASP:HB3	1:B:387:PHE:CZ	2.53	0.44
1:B:106:ARG:HD3	3:B:602:RIT:H641	2.00	0.44
1:D:220:PHE:CE2	1:D:224:ILE:HD11	2.53	0.44
1:K:179:TYR:CZ	1:K:454:ALA:HB2	2.53	0.44
1:E:93:VAL:HA	1:E:102:PHE:CD2	2.53	0.44
1:H:30:HIS:NE2	1:H:77:GLY:O	2.50	0.44
1:E:71:MET:HG2	1:E:84:ILE:HG22	2.00	0.43
1:G:96:LYS:HG2	1:G:97:GLU:HG3	2.00	0.43
1:A:437:GLY:O	1:A:440:ASN:ND2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:47:LEU:HD21	1:K:46:LEU:HD23	1.99	0.43
1:D:494:SER:HB3	1:D:495:ARG:NH1	2.33	0.43
1:F:46:LEU:HD11	1:F:226:PHE:HE1	1.84	0.43
1:G:362:GLU:OE2	1:G:418:ARG:HD2	2.18	0.43
1:K:149:ILE:HG12	1:K:183:VAL:HG13	2.00	0.43
1:G:228:PHE:HB2	1:K:231:PRO:HB2	2.00	0.43
1:B:326:ASP:N	1:B:326:ASP:OD1	2.51	0.43
1:C:31:GLY:O	1:C:35:ARG:HG3	2.18	0.43
1:A:108:LEU:HD12	1:A:108:LEU:HA	1.88	0.43
1:E:365:ARG:NH1	1:E:402:HIS:O	2.51	0.43
1:E:397:PRO:HB2	1:E:400:ALA:HB3	1.99	0.43
1:I:389:PRO:HG2	1:I:392:SER:OG	2.19	0.43
1:J:76:GLU:OE1	1:J:106:ARG:NH2	2.51	0.43
1:L:179:TYR:CE2	1:L:454:ALA:HB2	2.53	0.43
1:D:134:SER:HA	1:D:442:ILE:HD11	2.01	0.43
1:E:372:ARG:HD2	1:E:395:VAL:HG13	2.01	0.43
1:F:470:THR:HG22	1:F:472:ILE:HG13	2.01	0.43
1:I:117:ALA:HB1	1:I:301:ILE:HG13	2.01	0.43
1:J:91:ARG:HG3	1:J:429:TYR:CZ	2.54	0.43
1:L:142:LEU:HD12	1:L:449:MET:SD	2.59	0.43
1:C:244:ASP:N	1:C:244:ASP:OD1	2.52	0.43
1:D:99:TYR:HD1	1:D:127:LYS:HE2	1.84	0.43
1:F:71:MET:HB3	1:F:71:MET:HE2	1.85	0.43
1:F:47:LEU:HA	1:F:225:LEU:HD22	1.99	0.43
1:B:355:TYR:CD2	1:B:358:MET:HE3	2.51	0.43
1:D:379:LYS:HA	1:D:390:LYS:HG3	2.00	0.43
1:L:85:THR:HB	1:L:401:LEU:HD21	2.01	0.43
1:L:84:ILE:HD11	1:L:93:VAL:HG21	2.01	0.43
1:J:51:LEU:O	1:J:54:ARG:HG2	2.19	0.43
1:K:226:PHE:HB3	1:K:228:PHE:CZ	2.54	0.43
1:D:92:THR:HG23	1:D:96:LYS:HD3	2.01	0.42
1:E:30:HIS:NE2	1:E:45:PRO:O	2.52	0.42
1:F:314:LEU:HG	1:F:451:MET:HG2	2.00	0.42
1:A:410:GLU:O	1:A:418:ARG:NH2	2.52	0.42
1:E:84:ILE:HD12	1:E:89:VAL:HG12	2.01	0.42
1:I:93:VAL:HG13	1:I:102:PHE:CG	2.54	0.42
1:J:335:ILE:HD13	1:J:456:ILE:HA	2.01	0.42
2:H:601:HEM:CHA	3:H:602:RIT:C50	2.96	0.42
1:J:269:LEU:HA	1:J:269:LEU:HD12	1.84	0.42
1:B:301:ILE:HD12	3:B:602:RIT:H35	2.01	0.42
1:E:375:ARG:NH2	2:E:601:HEM:O1A	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:220:PHE:CE2	1:H:224:ILE:HD11	2.54	0.42
1:H:302:PHE:CD2	2:H:601:HEM:HBC1	2.55	0.42
1:J:93:VAL:HG13	1:J:102:PHE:CG	2.53	0.42
1:L:116:SER:O	1:L:298:GLN:NE2	2.42	0.42
2:A:601:HEM:C1A	3:A:602:RIT:H50	2.54	0.42
1:B:407:TYR:CE1	1:B:430:ILE:HG13	2.55	0.42
1:G:85:THR:HB	1:G:401:LEU:HD21	2.01	0.42
1:I:125:GLU:OE1	1:I:128:ARG:NH2	2.45	0.42
1:I:369:VAL:HA	1:I:482:LEU:HB2	2.00	0.42
1:I:373:LEU:HB2	1:I:396:ILE:HB	2.02	0.42
1:D:408:TRP:HB2	1:D:411:PRO:HB3	2.01	0.42
1:K:202:PRO:HB2	1:K:248:PHE:CZ	2.54	0.42
1:D:260:ARG:NH1	1:D:267:HIS:HA	2.34	0.42
1:G:326:ASP:OD1	1:G:326:ASP:N	2.53	0.42
1:H:335:ILE:HD13	1:H:456:ILE:HA	2.02	0.42
1:H:143:LYS:HE2	1:H:347:TYR:CE2	2.55	0.42
1:J:121:ALA:O	1:J:439:ARG:NH1	2.44	0.42
1:J:206:SER:HB3	1:J:245:THR:HG23	2.02	0.42
1:A:344:PRO:HA	1:A:345:PRO:HD3	1.90	0.42
1:E:315:SER:HB3	1:E:488:ILE:HD12	2.02	0.42
1:F:172:LEU:HD23	1:F:315:SER:HA	2.01	0.42
1:G:327:VAL:HG13	1:G:355:TYR:OH	2.19	0.42
1:H:102:PHE:HB3	1:H:375:ARG:HB3	2.01	0.42
1:I:327:VAL:HG11	1:I:414:PHE:HE2	1.85	0.42
1:K:220:PHE:HB2	1:K:240:LEU:HD11	2.01	0.42
1:K:373:LEU:HB2	1:K:396:ILE:HB	2.02	0.42
1:A:244:ASP:N	1:A:244:ASP:OD1	2.51	0.42
1:A:258:LYS:O	1:A:262:ASN:ND2	2.50	0.42
1:B:38:ILE:HD11	1:B:386:VAL:HG11	2.01	0.42
1:C:125:GLU:OE2	1:C:288:LYS:NZ	2.43	0.42
1:E:104:ASN:HA	1:E:439:ARG:NH1	2.35	0.42
1:L:260:ARG:NH1	1:L:273:GLN:HB2	2.34	0.42
1:L:397:PRO:HB2	1:L:400:ALA:HB3	2.02	0.42
1:D:125:GLU:O	1:D:129:ILE:HG12	2.19	0.42
1:F:221:LEU:HA	1:F:224:ILE:HD12	2.02	0.42
1:G:108:LEU:HD12	1:G:109:GLY:H	1.85	0.42
1:H:301:ILE:CD1	3:H:602:RIT:C34	2.97	0.42
1:L:71:MET:HE3	1:L:71:MET:HB3	1.92	0.42
1:A:257:LYS:NZ	1:A:292:ASP:OD1	2.53	0.41
1:B:362:GLU:OE2	1:B:418:ARG:NH1	2.52	0.41
1:E:477:ASP:OD1	1:E:478:THR:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:THR:HB	1:E:401:LEU:HD21	2.02	0.41
1:F:84:ILE:O	1:F:397:PRO:HD2	2.20	0.41
1:F:82:LEU:HD23	1:F:383:ILE:HD11	2.00	0.41
1:G:344:PRO:HA	1:G:345:PRO:HD3	1.88	0.41
1:G:76:GLU:OE1	1:G:106:ARG:NH2	2.52	0.41
1:H:344:PRO:HA	1:H:345:PRO:HD3	1.88	0.41
1:K:482:LEU:HA	1:K:482:LEU:HD12	1.87	0.41
3:B:602:RIT:H142	3:B:602:RIT:H643	2.02	0.41
1:F:158:ARG:HE	1:F:162:ARG:NH2	2.19	0.41
1:L:144:GLU:O	1:L:147:PRO:HD2	2.20	0.41
1:A:370:ALA:HB2	3:A:602:RIT:H51	2.02	0.41
1:E:105:ARG:HA	1:E:375:ARG:HA	2.01	0.41
1:E:44:LEU:HD22	1:E:51:LEU:HD23	2.03	0.41
1:F:221:LEU:HD21	1:H:46:LEU:HD22	2.01	0.41
1:H:476:LEU:HD23	1:H:482:LEU:HD11	2.02	0.41
1:I:279:GLN:HG2	1:I:290:LEU:O	2.21	0.41
1:B:154:ASP:OD1	1:B:457:ARG:NH1	2.53	0.41
1:C:213:PHE:CE1	1:C:240:LEU:HD12	2.53	0.41
1:H:462:PHE:HB3	1:H:492:VAL:HG23	2.03	0.41
1:K:44:LEU:HD22	1:K:51:LEU:HD23	2.01	0.41
1:L:66:LYS:HE2	1:L:66:LYS:HB3	1.87	0.41
1:D:96:LYS:HG2	1:D:97:GLU:HG3	2.03	0.41
1:E:134:SER:HA	1:E:442:ILE:HD11	2.02	0.41
1:F:482:LEU:HA	1:F:482:LEU:HD12	1.86	0.41
1:I:223:ILE:HD11	1:I:233:PHE:CD2	2.55	0.41
1:K:374:GLU:HG2	1:K:395:VAL:HG22	2.02	0.41
1:F:135:PRO:O	1:F:141:LYS:HD2	2.21	0.41
1:F:374:GLU:HG2	1:F:395:VAL:HG22	2.03	0.41
1:J:57:LEU:HD12	1:J:57:LEU:HA	1.91	0.41
1:K:251:LYS:O	1:K:255:ARG:HG3	2.21	0.41
1:K:46:LEU:HG	1:K:225:LEU:HD22	2.01	0.41
1:K:275:MET:HE3	1:K:295:LEU:HG	2.03	0.41
1:C:378:LYS:O	1:C:390:LYS:HG3	2.21	0.41
1:I:55:GLN:HG3	1:I:59:LYS:HD3	2.03	0.41
1:A:91:ARG:HG3	1:A:429:TYR:CZ	2.55	0.41
1:B:47:LEU:HG	1:B:51:LEU:CD2	2.51	0.41
1:B:482:LEU:HA	1:B:482:LEU:HD12	1.80	0.41
1:D:76:GLU:OE1	1:D:106:ARG:NH2	2.54	0.41
1:J:356:LEU:HD21	1:J:452:LYS:HB3	2.03	0.41
1:F:178:ALA:HB1	1:F:196:LEU:HA	2.03	0.41
1:L:305:ALA:O	1:L:309:THR:OG1	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:PRO:HB3	1:G:46:LEU:HD13	2.03	0.41
1:E:157:VAL:HG23	1:E:462:PHE:CE2	2.56	0.41
1:G:99:TYR:HD1	1:G:127:LYS:HE2	1.86	0.41
1:H:383:ILE:O	1:H:386:VAL:HG22	2.20	0.41
1:I:181:MET:HG3	1:I:193:ILE:HD11	2.03	0.41
1:K:76:GLU:OE1	1:K:106:ARG:NH2	2.54	0.41
1:K:30:HIS:HE1	1:K:77:GLY:O	2.04	0.41
1:D:202:PRO:HB2	1:D:248:PHE:CZ	2.56	0.40
1:G:226:PHE:HB3	1:G:228:PHE:CZ	2.56	0.40
1:I:85:THR:HB	1:I:401:LEU:HD21	2.03	0.40
1:D:213:PHE:CE2	1:D:242:PRO:HG3	2.53	0.40
1:D:183:VAL:HG11	1:D:450:ASN:HD22	1.87	0.40
1:A:84:ILE:HD12	1:A:89:VAL:HG12	2.03	0.40
1:B:134:SER:HA	1:B:442:ILE:HD11	2.04	0.40
1:D:244:ASP:OD1	1:D:244:ASP:N	2.54	0.40
1:H:116:SER:O	1:H:298:GLN:NE2	2.45	0.40
1:A:371:ILE:HG13	1:A:482:LEU:CD2	2.51	0.40
1:B:213:PHE:CE2	1:B:242:PRO:HG3	2.53	0.40
1:E:105:ARG:O	1:E:376:THR:OG1	2.30	0.40
1:F:202:PRO:HB2	1:F:248:PHE:CZ	2.56	0.40
1:J:396:ILE:O	1:J:398:THR:N	2.55	0.40
1:A:86:ASP:O	1:A:90:ILE:HG13	2.21	0.40
1:B:244:ASP:OD1	1:B:244:ASP:N	2.54	0.40
1:B:344:PRO:HA	1:B:345:PRO:HD3	1.88	0.40
1:D:383:ILE:O	1:D:386:VAL:HG22	2.21	0.40
1:G:92:THR:HA	1:G:96:LYS:HB3	2.04	0.40
1:J:344:PRO:HA	1:J:345:PRO:HD3	1.90	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	458/480 (95%)	441 (96%)	17 (4%)	0	100	100
1	B	452/480 (94%)	430 (95%)	21 (5%)	1 (0%)	47	77
1	C	467/480 (97%)	449 (96%)	17 (4%)	1 (0%)	47	77
1	D	453/480 (94%)	432 (95%)	21 (5%)	0	100	100
1	E	431/480 (90%)	412 (96%)	18 (4%)	1 (0%)	47	77
1	F	450/480 (94%)	431 (96%)	19 (4%)	0	100	100
1	G	447/480 (93%)	432 (97%)	15 (3%)	0	100	100
1	H	453/480 (94%)	436 (96%)	17 (4%)	0	100	100
1	I	460/480 (96%)	441 (96%)	19 (4%)	0	100	100
1	J	452/480 (94%)	434 (96%)	18 (4%)	0	100	100
1	K	452/480 (94%)	432 (96%)	20 (4%)	0	100	100
1	L	440/480 (92%)	424 (96%)	16 (4%)	0	100	100
All	All	5415/5760 (94%)	5194 (96%)	218 (4%)	3 (0%)	51	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	424	ASP
1	B	383	ILE
1	E	353	MET

### 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	419/434 (96%)	415 (99%)	4 (1%)	76	91
1	B	415/434 (96%)	412 (99%)	3 (1%)	84	95
1	C	426/434 (98%)	420 (99%)	6 (1%)	67	88
1	D	416/434 (96%)	412 (99%)	4 (1%)	76	91
1	E	399/434 (92%)	391 (98%)	8 (2%)	55	81
1	F	413/434 (95%)	412 (100%)	1 (0%)	93	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	412/434 (95%)	411 (100%)	1 (0%)	93	98
1	H	416/434 (96%)	412 (99%)	4 (1%)	76	91
1	I	421/434 (97%)	419 (100%)	2 (0%)	88	96
1	J	415/434 (96%)	412 (99%)	3 (1%)	84	95
1	K	415/434 (96%)	414 (100%)	1 (0%)	93	98
1	L	405/434 (93%)	405 (100%)	0	100	100
All	All	4972/5208 (96%)	4935 (99%)	37 (1%)	84	95

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	106	ARG
1	A	142	LEU
1	A	440	ASN
1	B	108	LEU
1	B	142	LEU
1	B	476	LEU
1	C	51	LEU
1	C	108	LEU
1	C	142	LEU
1	C	217	ASP
1	C	424	ASP
1	C	482	LEU
1	D	51	LEU
1	D	146	PHE
1	D	372	ARG
1	D	482	LEU
1	E	54	ARG
1	E	57	LEU
1	E	101	VAL
1	E	105	ARG
1	E	108	LEU
1	E	142	LEU
1	E	269	LEU
1	E	476	LEU
1	F	142	LEU
1	G	142	LEU
1	H	51	LEU
1	H	142	LEU

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Mol	Chain	Res	Type
1	H	240	LEU
1	H	387	PHE
1	I	142	LEU
1	I	237	ASN
1	J	142	LEU
1	J	146	PHE
1	J	216	LEU
1	K	142	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	460	GLN
1	H	265	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

15 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	J	601	1	27,50,50	1.73	4 (14%)	17,82,82	1.51	2 (11%)
2	HEM	H	601	1,3	27,50,50	1.81	4 (14%)	17,82,82	1.99	5 (29%)
2	HEM	C	601	1	27,50,50	1.74	5 (18%)	17,82,82	1.43	1 (5%)
3	RIT	B	602	2	48,53,53	0.50	1 (2%)	55,71,71	0.76	3 (5%)
2	HEM	A	601	1,3	27,50,50	1.75	4 (14%)	17,82,82	1.51	3 (17%)
2	HEM	G	601	1	27,50,50	1.74	4 (14%)	17,82,82	1.47	3 (17%)
2	HEM	E	601	1	27,50,50	1.74	4 (14%)	17,82,82	1.53	4 (23%)
2	HEM	K	601	1	27,50,50	1.72	4 (14%)	17,82,82	1.54	3 (17%)
2	HEM	D	601	1	27,50,50	1.74	4 (14%)	17,82,82	1.53	5 (29%)
2	HEM	I	601	1	27,50,50	1.74	5 (18%)	17,82,82	1.45	3 (17%)
3	RIT	H	602	2	48,53,53	0.53	1 (2%)	55,71,71	1.03	4 (7%)
3	RIT	A	602	2	48,53,53	0.50	1 (2%)	55,71,71	0.90	3 (5%)
2	HEM	L	601	1	27,50,50	1.72	4 (14%)	17,82,82	1.52	2 (11%)
2	HEM	B	601	1,3	27,50,50	1.76	4 (14%)	17,82,82	1.50	4 (23%)
2	HEM	F	601	1	27,50,50	1.73	4 (14%)	17,82,82	1.51	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	J	601	1	-	0/6/54/54	-
2	HEM	H	601	1,3	-	1/6/54/54	-
2	HEM	C	601	1	-	0/6/54/54	-
3	RIT	B	602	2	-	11/49/53/53	0/4/4/4
2	HEM	A	601	1,3	-	0/6/54/54	-
2	HEM	G	601	1	-	0/6/54/54	-
2	HEM	E	601	1	-	0/6/54/54	-
2	HEM	K	601	1	-	0/6/54/54	-
2	HEM	D	601	1	-	0/6/54/54	-
2	HEM	I	601	1	-	0/6/54/54	-
3	RIT	H	602	2	-	10/49/53/53	0/4/4/4
3	RIT	A	602	2	-	5/49/53/53	0/4/4/4
2	HEM	L	601	1	-	0/6/54/54	-
2	HEM	B	601	1,3	-	0/6/54/54	-
2	HEM	F	601	1	-	0/6/54/54	-



All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	601	HEM	C3C-CAC	4.06	1.56	1.47
2	H	601	HEM	C3B-C2B	-4.02	1.34	1.40
2	I	601	HEM	C3C-CAC	3.98	1.56	1.47
2	B	601	HEM	C3C-CAC	3.91	1.55	1.47
2	F	601	HEM	C3C-CAC	3.90	1.55	1.47
2	G	601	HEM	C3B-CAB	3.90	1.55	1.47
2	G	601	HEM	C3C-CAC	3.89	1.55	1.47
2	B	601	HEM	C3B-CAB	3.88	1.55	1.47
2	E	601	HEM	C3C-CAC	3.87	1.55	1.47
2	H	601	HEM	C3C-C2C	-3.86	1.35	1.40
2	E	601	HEM	C3B-CAB	3.86	1.55	1.47
2	A	601	HEM	C3B-CAB	3.85	1.55	1.47
2	C	601	HEM	C3C-CAC	3.85	1.55	1.47
2	D	601	HEM	C3B-CAB	3.83	1.55	1.47
2	J	601	HEM	C3C-CAC	3.83	1.55	1.47
2	I	601	HEM	C3B-CAB	3.83	1.55	1.47
2	L	601	HEM	C3C-CAC	3.83	1.55	1.47
2	J	601	HEM	C3B-CAB	3.82	1.55	1.47
2	K	601	HEM	C3C-CAC	3.81	1.55	1.47
2	L	601	HEM	C3B-CAB	3.81	1.55	1.47
2	A	601	HEM	C3C-CAC	3.80	1.55	1.47
2	D	601	HEM	C3C-CAC	3.79	1.55	1.47
2	A	601	HEM	C3B-C2B	-3.78	1.35	1.40
2	B	601	HEM	C3B-C2B	-3.78	1.35	1.40
2	K	601	HEM	C3B-CAB	3.77	1.55	1.47
2	C	601	HEM	C3B-CAB	3.77	1.55	1.47
2	C	601	HEM	C3C-C2C	-3.77	1.35	1.40
2	F	601	HEM	C3B-CAB	3.77	1.55	1.47
2	D	601	HEM	C3C-C2C	-3.76	1.35	1.40
2	B	601	HEM	C3C-C2C	-3.74	1.35	1.40
2	K	601	HEM	C3C-C2C	-3.72	1.35	1.40
2	A	601	HEM	C3C-C2C	-3.71	1.35	1.40
2	J	601	HEM	C3B-C2B	-3.71	1.35	1.40
2	D	601	HEM	C3B-C2B	-3.71	1.35	1.40
2	J	601	HEM	C3C-C2C	-3.70	1.35	1.40
2	H	601	HEM	C3B-CAB	3.70	1.55	1.47
2	L	601	HEM	C3B-C2B	-3.69	1.35	1.40
2	F	601	HEM	C3C-C2C	-3.67	1.35	1.40
2	G	601	HEM	C3B-C2B	-3.67	1.35	1.40
2	G	601	HEM	C3C-C2C	-3.67	1.35	1.40
2	E	601	HEM	C3C-C2C	-3.64	1.35	1.40
2	E	601	HEM	C3B-C2B	-3.64	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	601	HEM	C3B-C2B	-3.63	1.35	1.40
2	I	601	HEM	C3C-C2C	-3.62	1.35	1.40
2	L	601	HEM	C3C-C2C	-3.62	1.35	1.40
2	C	601	HEM	C3B-C2B	-3.62	1.35	1.40
2	K	601	HEM	C3B-C2B	-3.61	1.35	1.40
2	I	601	HEM	C3B-C2B	-3.59	1.35	1.40
3	B	602	RIT	C2-S3	-2.69	1.68	1.73
3	A	602	RIT	C2-S3	-2.65	1.68	1.73
3	H	602	RIT	C2-S3	-2.57	1.68	1.73
2	I	601	HEM	CAA-C2A	2.03	1.55	1.52
2	C	601	HEM	CAA-C2A	2.01	1.55	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	601	HEM	CAA-CBA-CGA	-5.75	103.02	112.67
3	A	602	RIT	C77-C75-N74	-3.66	107.33	113.60
3	H	602	RIT	C26-C12-C13	-3.49	105.81	111.65
3	H	602	RIT	C77-C75-N74	-3.43	107.72	113.60
3	B	602	RIT	C14-C15-C44	3.26	116.52	112.42
2	B	601	HEM	CAA-CBA-CGA	-2.55	108.39	112.67
3	H	602	RIT	C19-N20-C21	-2.52	117.39	122.39
2	H	601	HEM	CMC-C2C-C3C	2.49	129.33	124.68
2	H	601	HEM	CMB-C2B-C3B	2.45	129.26	124.68
2	H	601	HEM	CAD-CBD-CGD	-2.45	108.56	112.67
2	F	601	HEM	CMB-C2B-C3B	2.42	129.21	124.68
2	D	601	HEM	CAA-CBA-CGA	-2.42	108.62	112.67
2	H	601	HEM	CMD-C2D-C1D	-2.41	124.75	128.46
2	E	601	HEM	CMC-C2C-C3C	2.37	129.12	124.68
2	K	601	HEM	CMB-C2B-C3B	2.31	129.00	124.68
2	I	601	HEM	CMB-C2B-C3B	2.30	128.97	124.68
2	L	601	HEM	CMC-C2C-C3C	2.28	128.95	124.68
2	K	601	HEM	CMD-C2D-C1D	-2.26	124.98	128.46
2	L	601	HEM	CMB-C2B-C3B	2.26	128.90	124.68
2	B	601	HEM	CMC-C2C-C3C	2.25	128.89	124.68
3	A	602	RIT	C14-C15-C44	-2.25	109.59	112.42
2	A	601	HEM	CMB-C2B-C3B	2.24	128.87	124.68
2	F	601	HEM	CMC-C2C-C3C	2.23	128.85	124.68
3	A	602	RIT	C26-C12-C13	-2.22	107.92	111.65
2	E	601	HEM	CMB-C2B-C3B	2.21	128.82	124.68
2	K	601	HEM	CMC-C2C-C3C	2.20	128.80	124.68
2	C	601	HEM	CMB-C2B-C3B	2.19	128.78	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	601	HEM	CMB-C2B-C3B	2.19	128.77	124.68
2	J	601	HEM	CMC-C2C-C3C	2.18	128.76	124.68
2	D	601	HEM	CMC-C2C-C3C	2.18	128.76	124.68
2	A	601	HEM	CMC-C2C-C3C	2.18	128.75	124.68
2	A	601	HEM	CMD-C2D-C1D	-2.17	125.12	128.46
2	J	601	HEM	CMB-C2B-C3B	2.17	128.74	124.68
2	D	601	HEM	CMB-C2B-C3B	2.16	128.72	124.68
2	E	601	HEM	CMD-C2D-C1D	-2.14	125.18	128.46
2	B	601	HEM	CMB-C2B-C3B	2.11	128.62	124.68
2	F	601	HEM	CMD-C2D-C1D	-2.10	125.24	128.46
3	B	602	RIT	C75-C77-C80	-2.09	126.47	129.62
2	G	601	HEM	CMC-C2C-C3C	2.09	128.59	124.68
2	I	601	HEM	CAA-CBA-CGA	-2.09	109.16	112.67
2	B	601	HEM	CMD-C2D-C1D	-2.09	125.25	128.46
2	F	601	HEM	CAA-CBA-CGA	-2.07	109.20	112.67
3	H	602	RIT	C13-C12-N11	2.06	113.89	109.92
2	G	601	HEM	CMD-C2D-C1D	-2.05	125.31	128.46
2	D	601	HEM	C1D-C2D-C3D	2.04	108.42	107.00
2	I	601	HEM	CMC-C2C-C3C	2.03	128.47	124.68
2	D	601	HEM	CMD-C2D-C1D	-2.02	125.36	128.46
2	E	601	HEM	CAA-CBA-CGA	-2.02	109.29	112.67
3	B	602	RIT	C26-C12-C13	-2.01	108.28	111.65

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	RIT	C12-C13-C14-C15
3	B	602	RIT	C13-C14-C15-C44
3	H	602	RIT	C12-C13-C14-C15
3	H	602	RIT	N83-C82-C85-C86
3	A	602	RIT	N58-C18-C19-C62
3	A	602	RIT	O61-C18-C19-C62
3	B	602	RIT	C14-C15-N58-C18
3	B	602	RIT	C13-C14-C15-N58
3	H	602	RIT	O61-C18-C19-C62
3	H	602	RIT	C13-C14-C15-C44
3	H	602	RIT	C44-C15-N58-C18
3	H	602	RIT	N58-C18-C19-C62
3	H	602	RIT	O41-C13-C14-C15
3	H	602	RIT	C13-C14-C15-N58
3	B	602	RIT	C14-C15-C44-C45

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Mol	Chain	Res	Type	Atoms
3	A	602	RIT	C62-C19-N20-C21
3	B	602	RIT	C77-C75-N74-C95
3	A	602	RIT	C77-C75-N74-C95
2	H	601	HEM	C4D-C3D-CAD-CBD
3	B	602	RIT	C19-C18-N58-C15
3	B	602	RIT	C77-C75-N74-C21
3	H	602	RIT	C77-C75-N74-C21
3	B	602	RIT	C12-C26-C28-C31
3	B	602	RIT	O61-C18-N58-C15
3	B	602	RIT	C12-C26-C28-C35
3	A	602	RIT	C14-C15-N58-C18
3	H	602	RIT	C77-C75-N74-C95

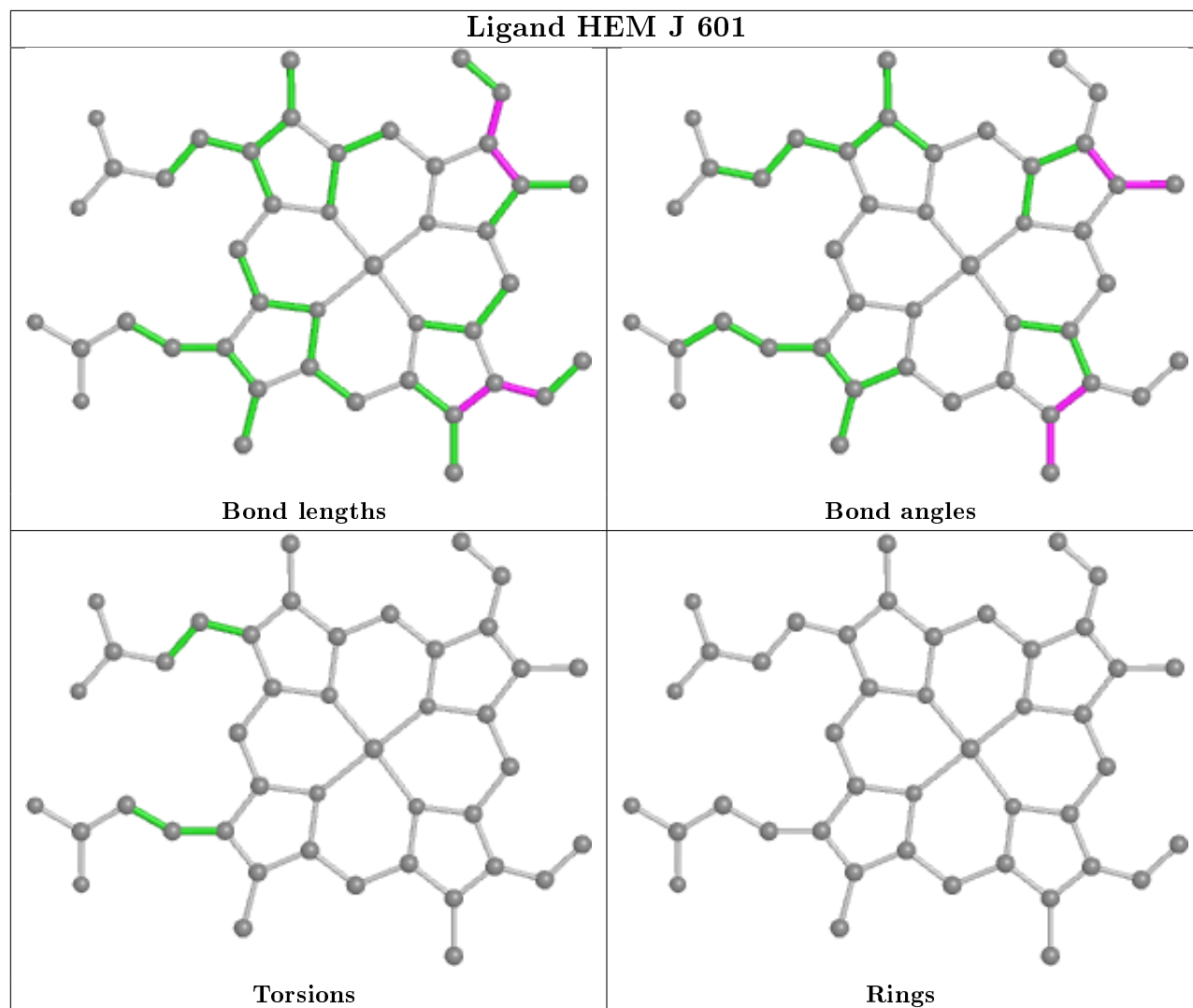
There are no ring outliers.

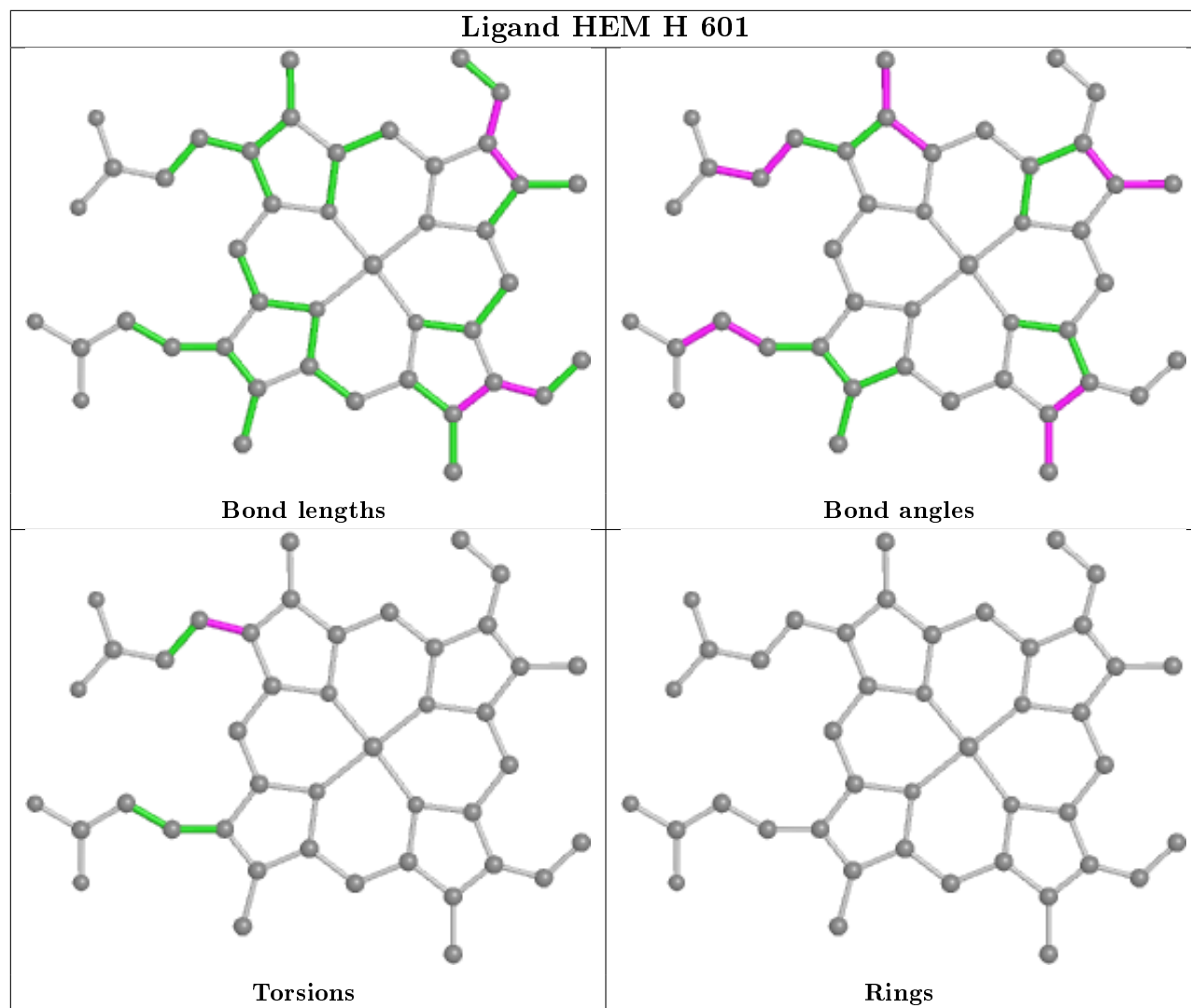
15 monomers are involved in 63 short contacts:

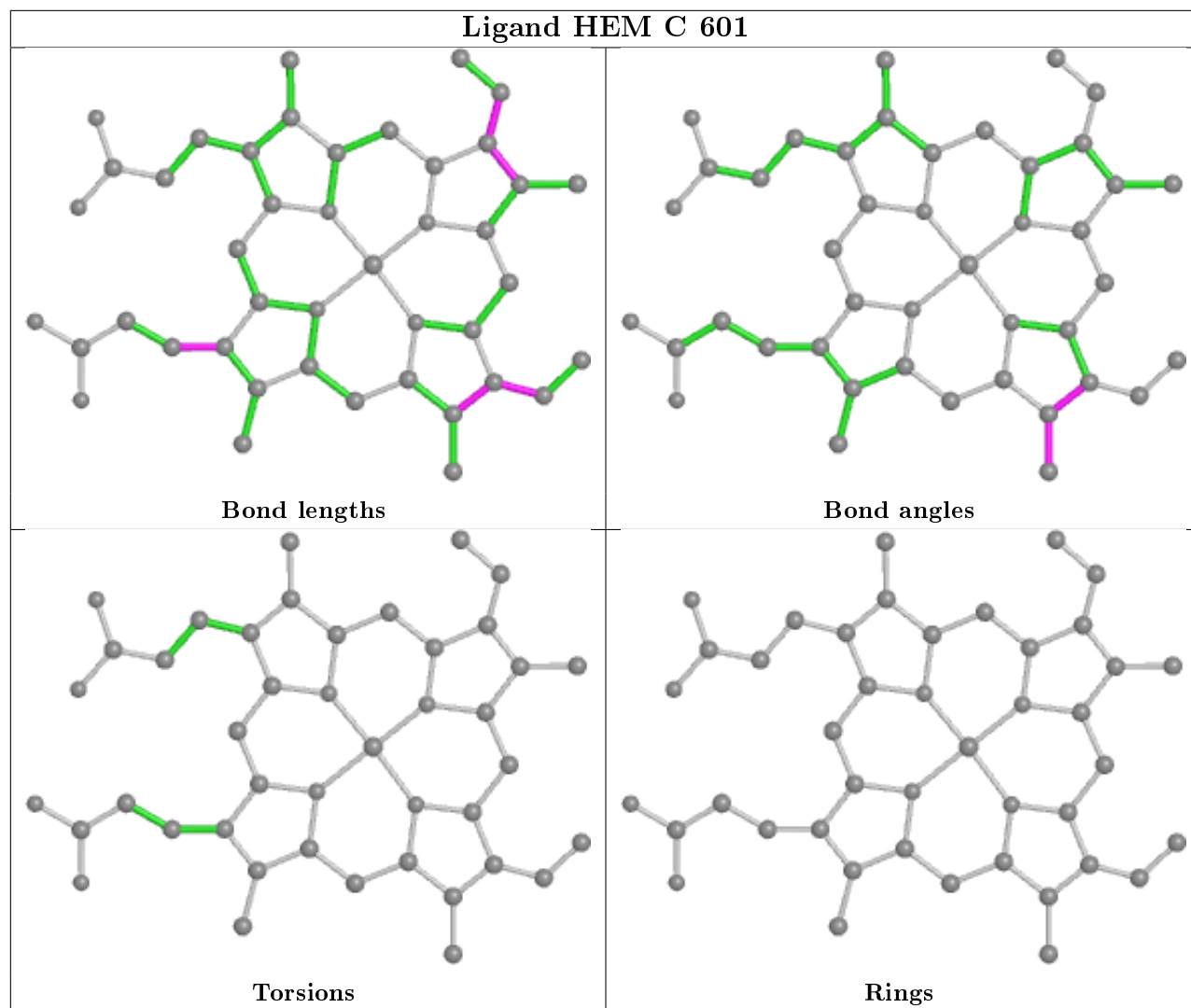
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	601	HEM	2	0
2	H	601	HEM	6	0
2	C	601	HEM	2	0
3	B	602	RIT	16	0
2	A	601	HEM	3	0
2	G	601	HEM	2	0
2	E	601	HEM	5	0
2	K	601	HEM	2	0
2	D	601	HEM	3	0
2	I	601	HEM	2	0
3	H	602	RIT	11	0
3	A	602	RIT	5	0
2	L	601	HEM	3	0
2	B	601	HEM	3	0
2	F	601	HEM	3	0

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

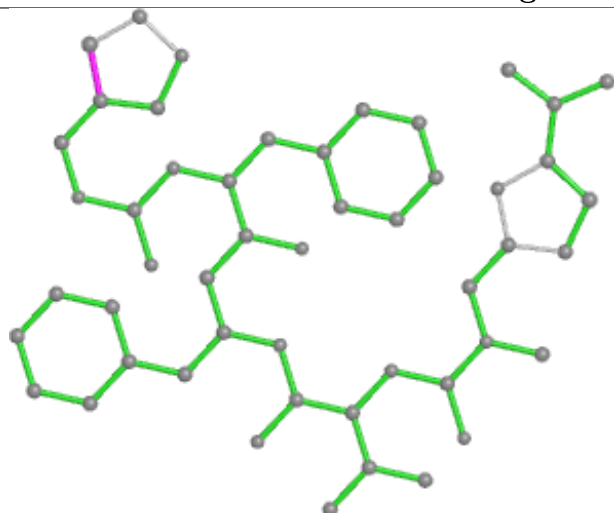
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



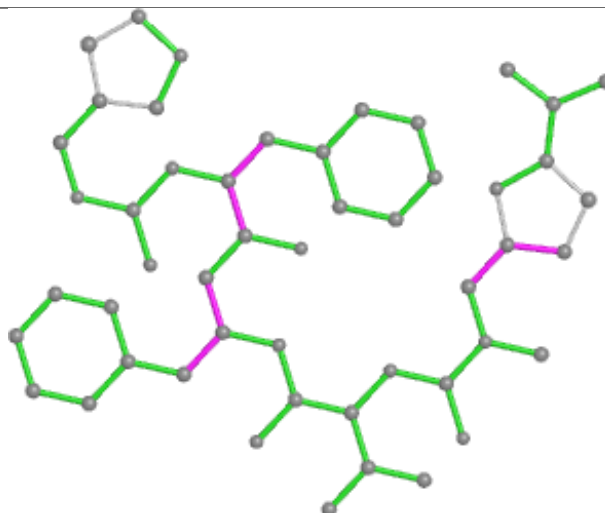




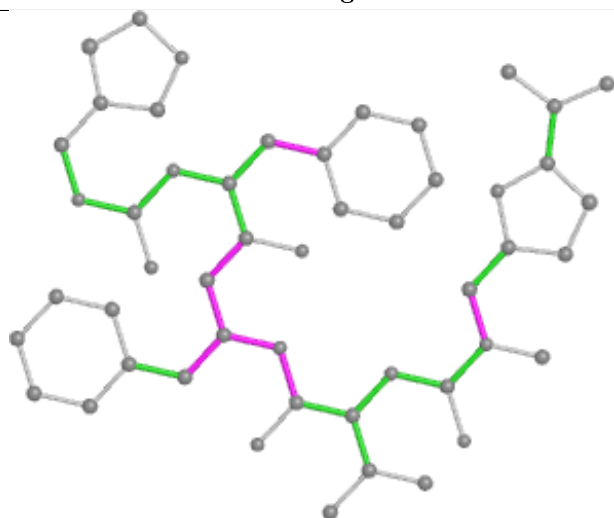
## Ligand RIT B 602



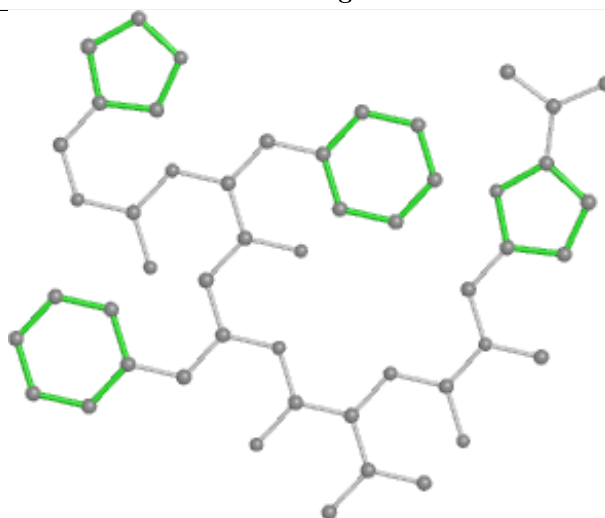
Bond lengths



Bond angles

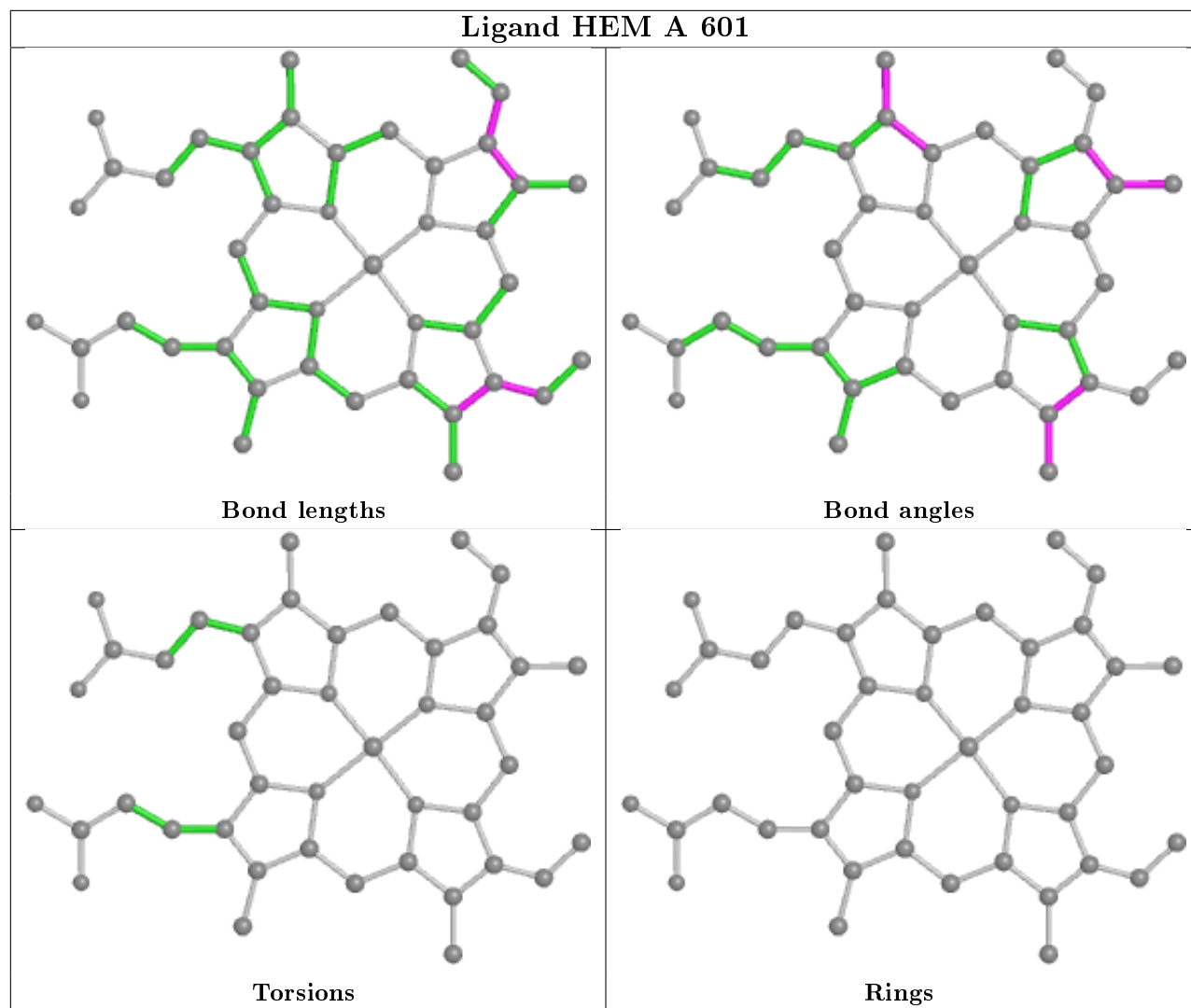


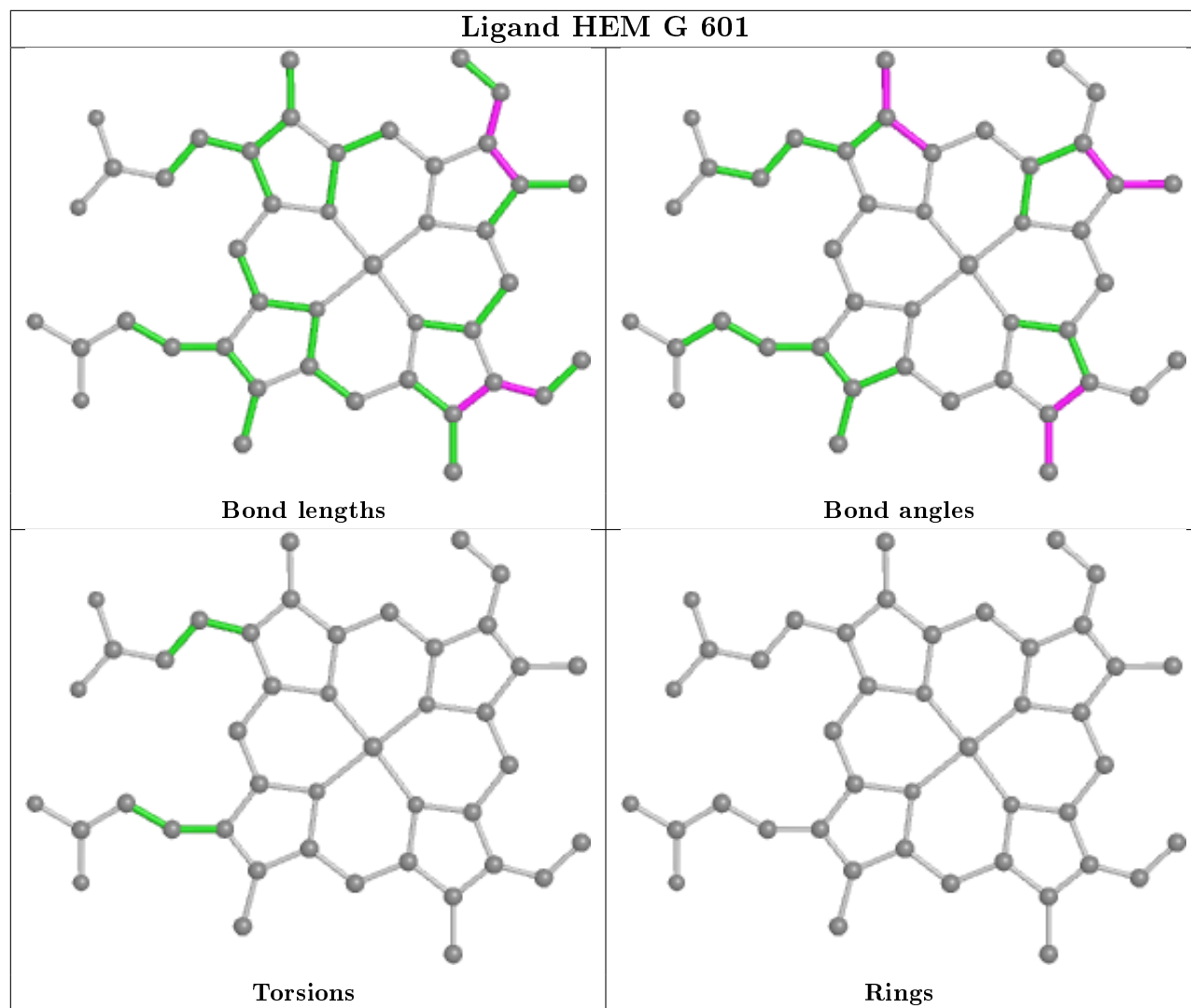
Torsions

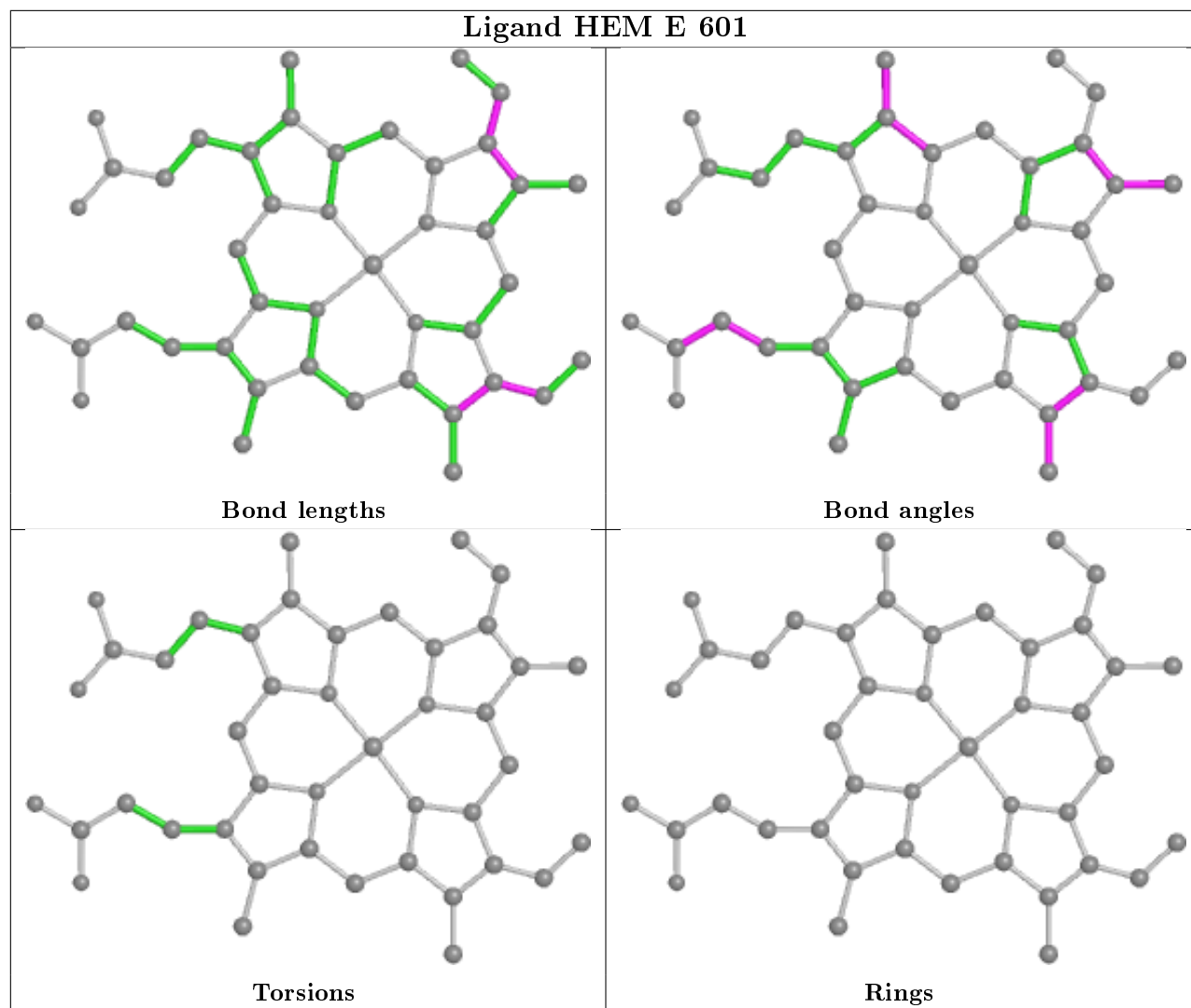


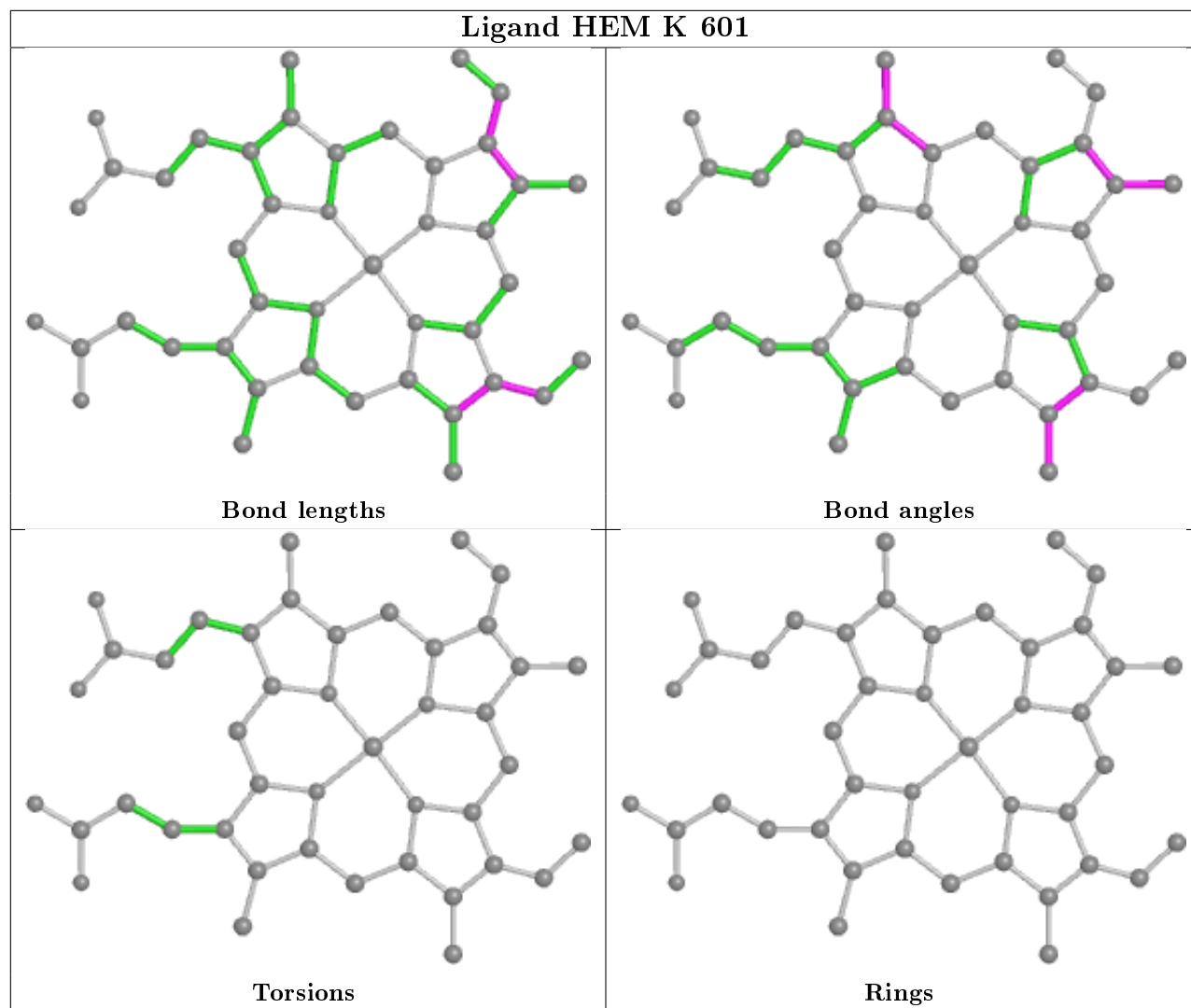
Rings

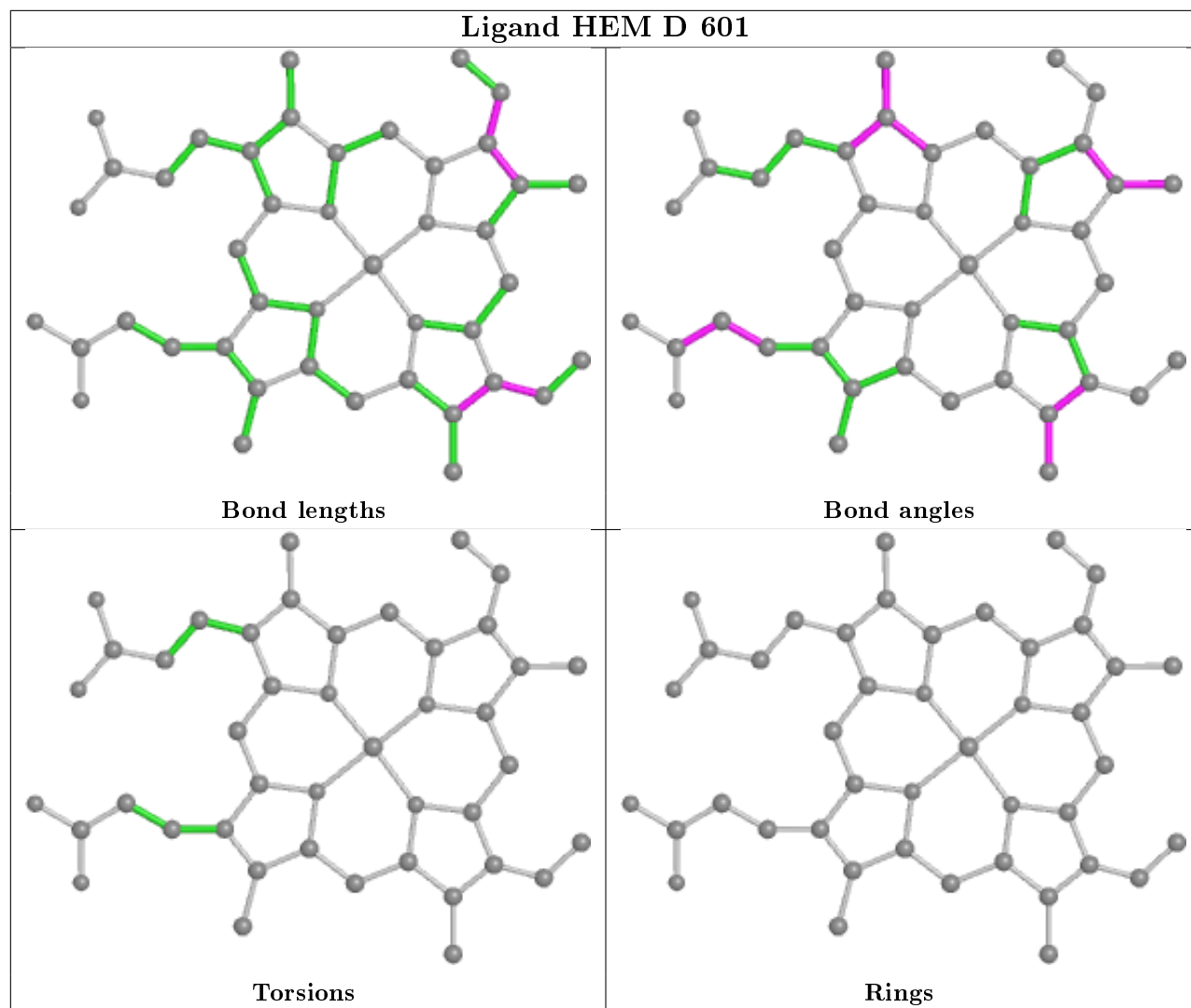


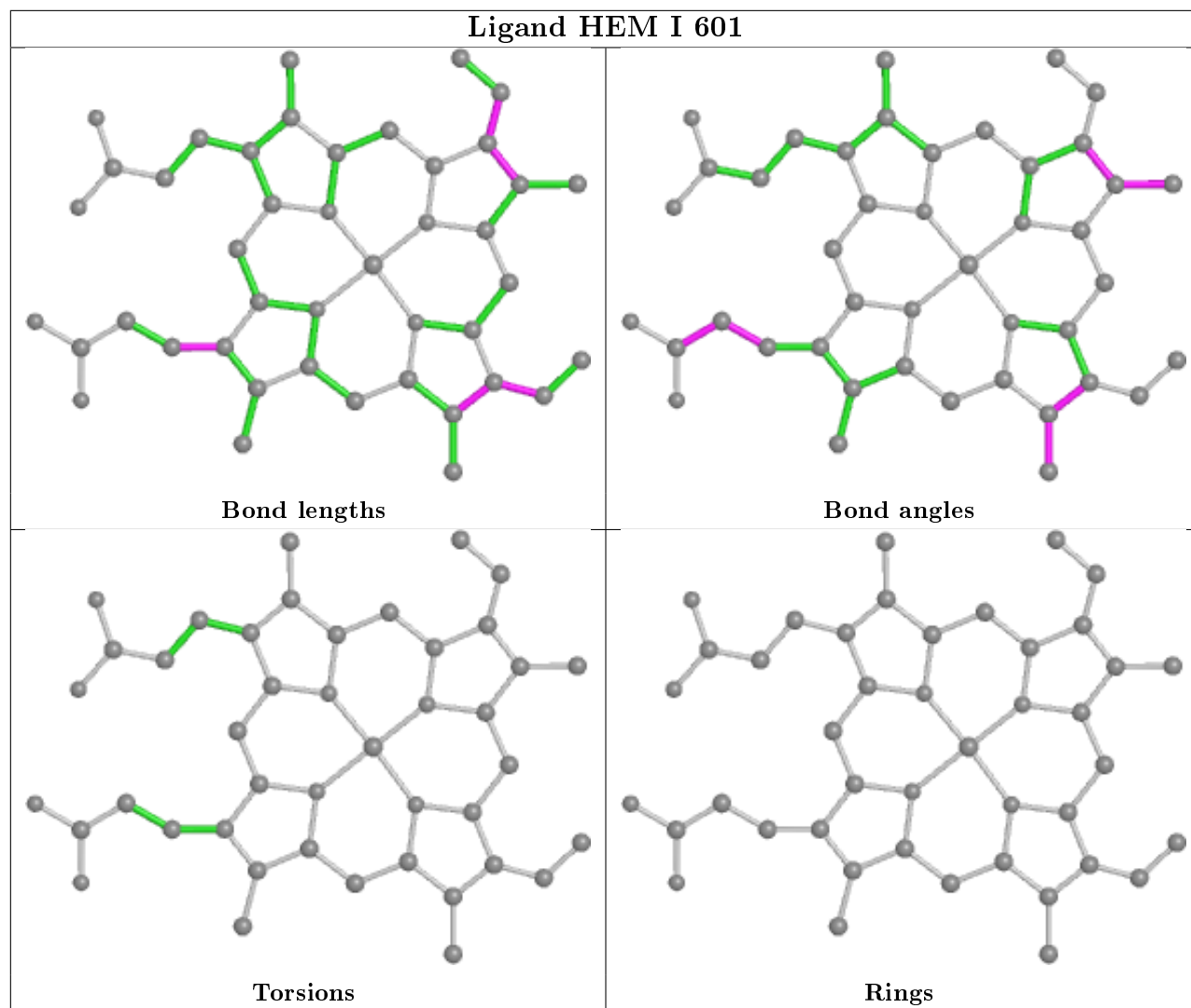




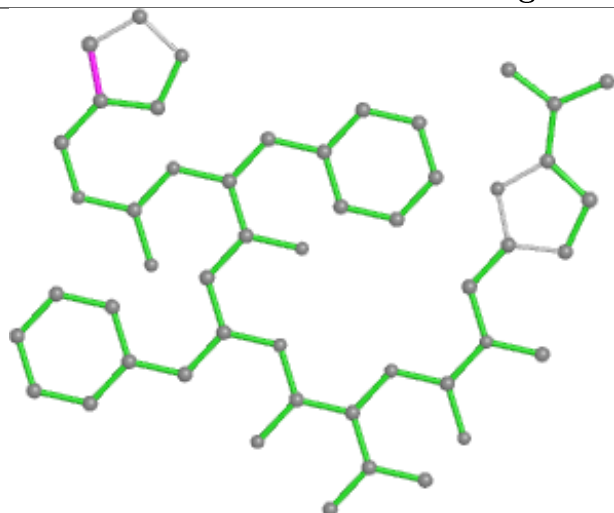




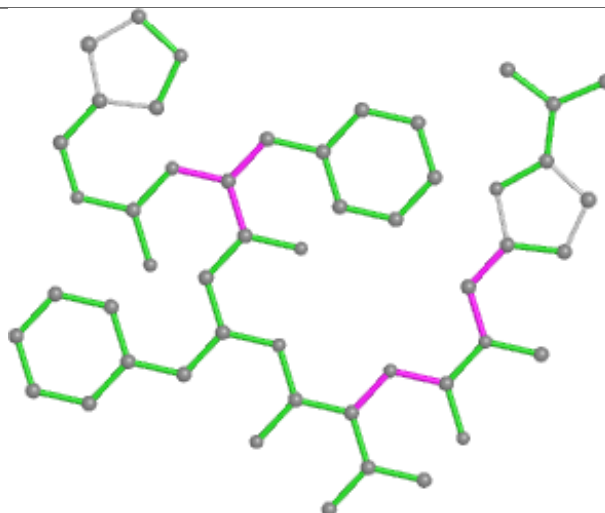




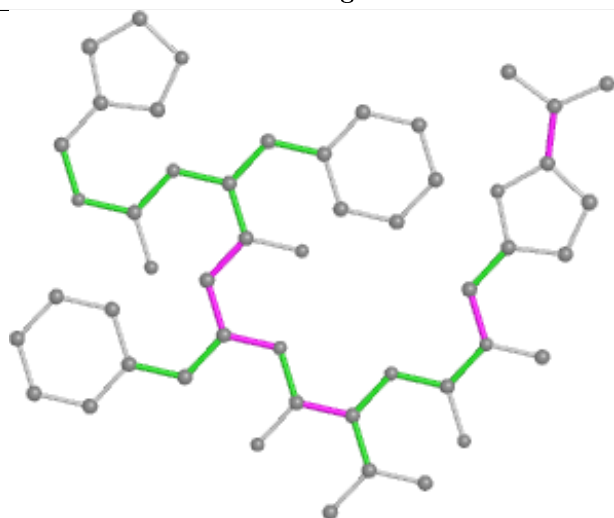
## Ligand RIT H 602



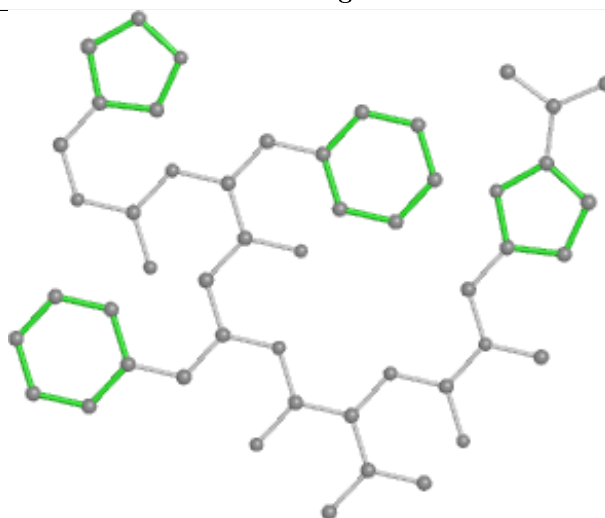
Bond lengths



Bond angles

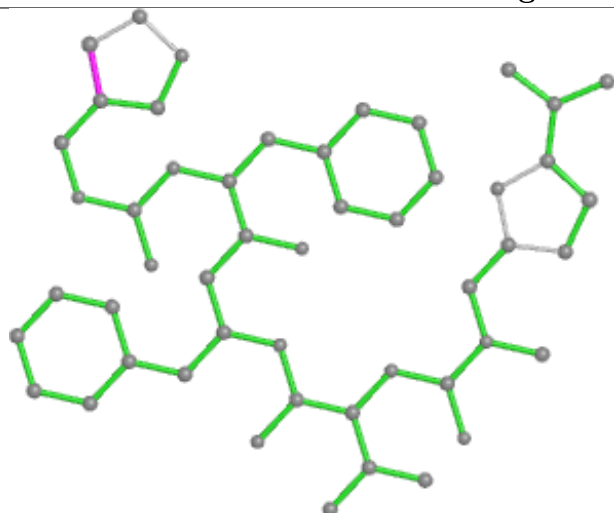


Torsions

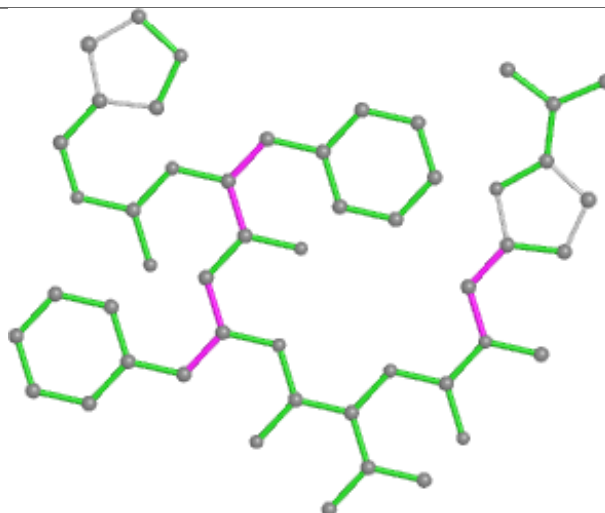


Rings

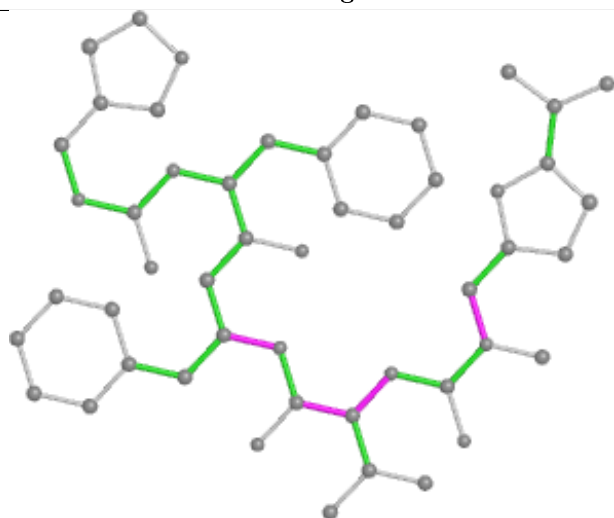
## Ligand RIT A 602



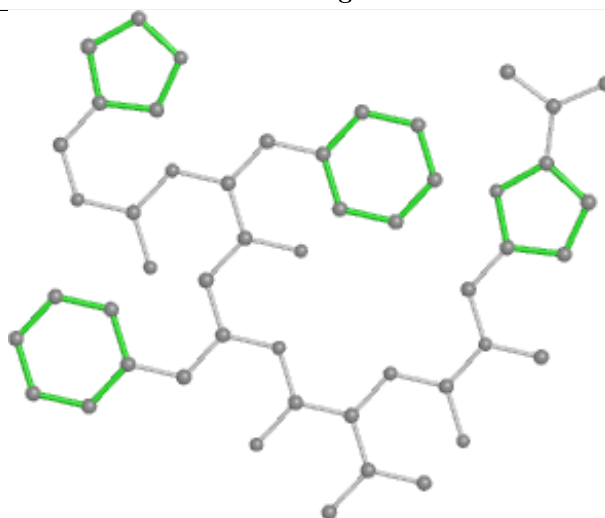
Bond lengths



Bond angles

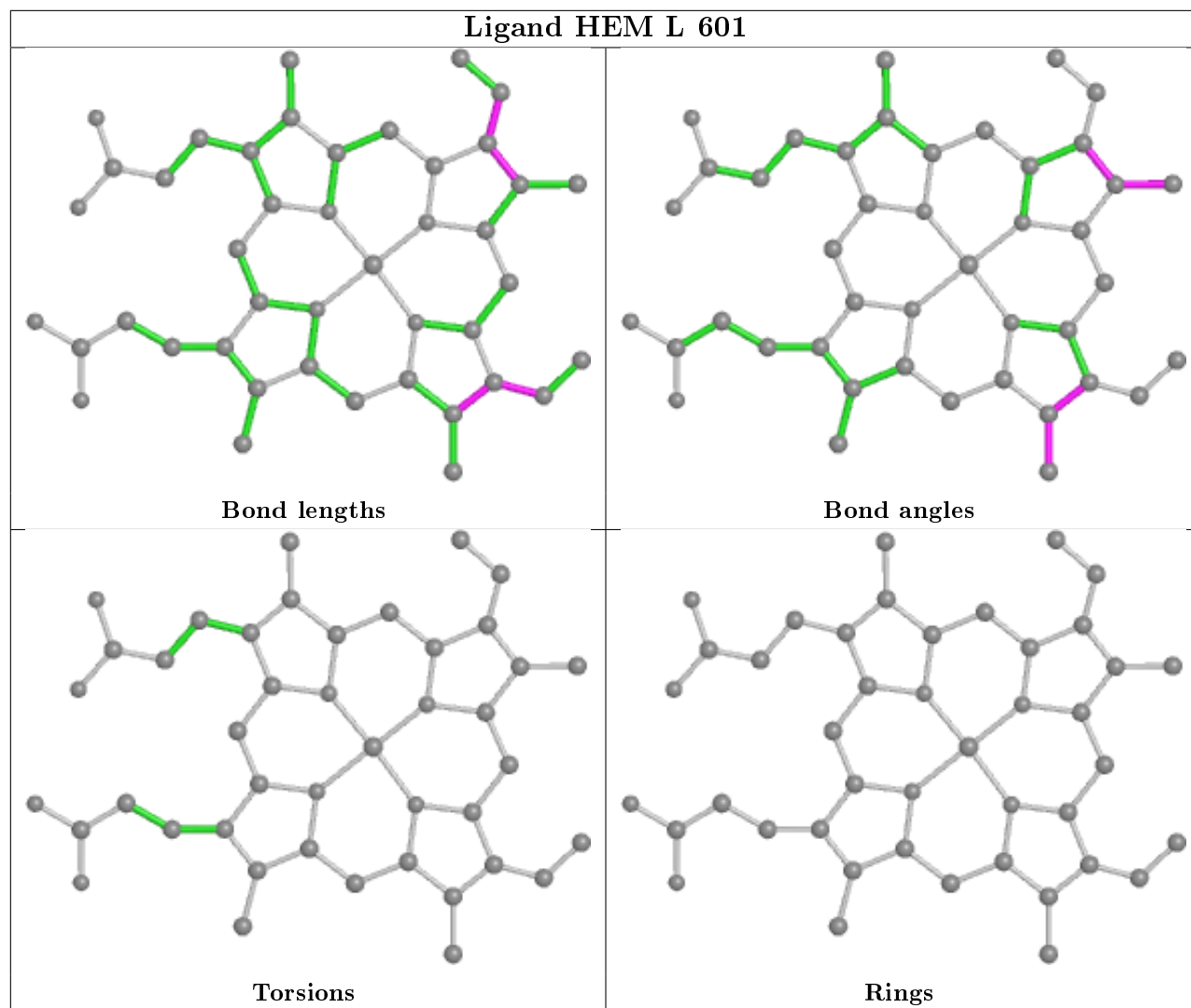


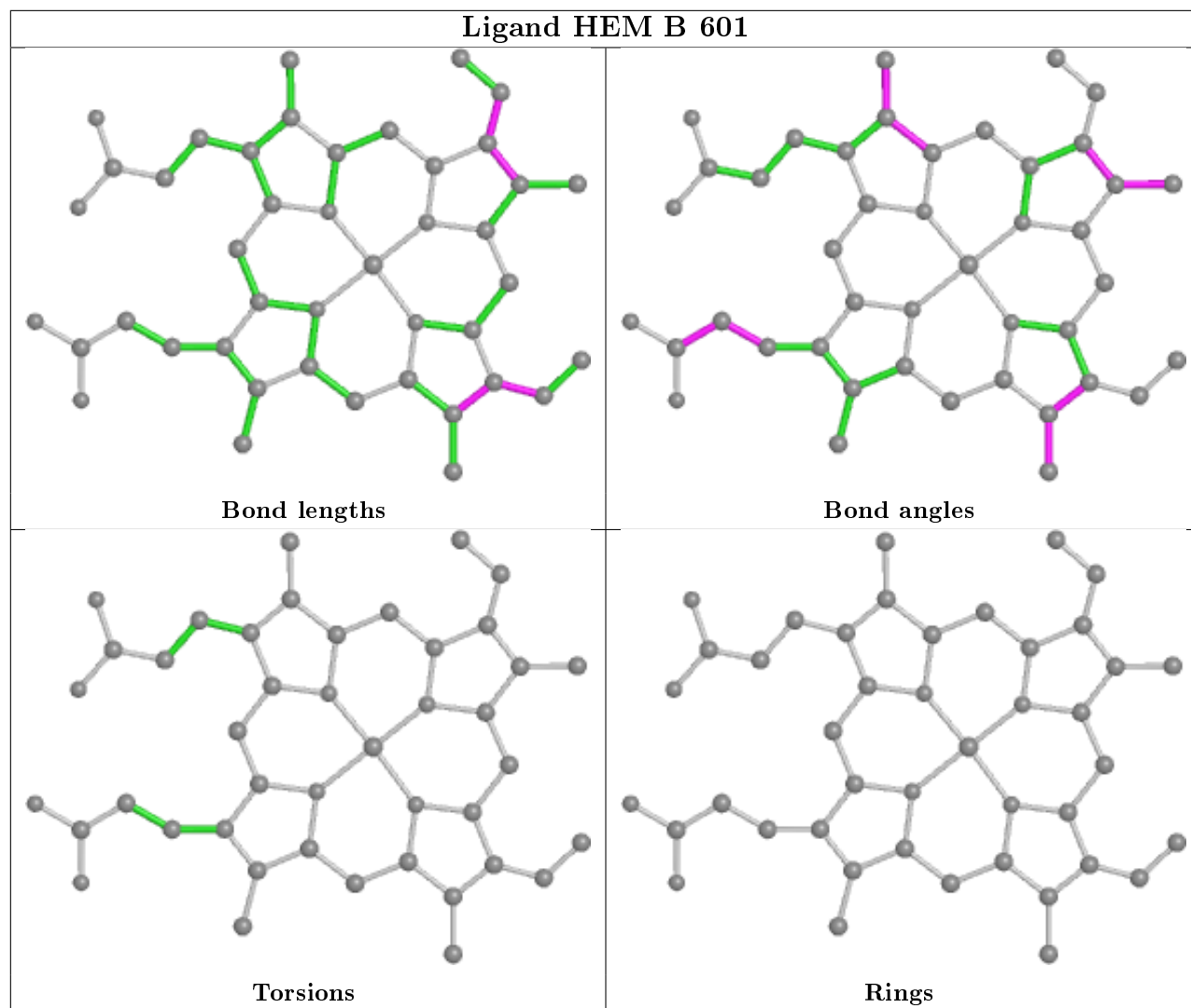
Torsions

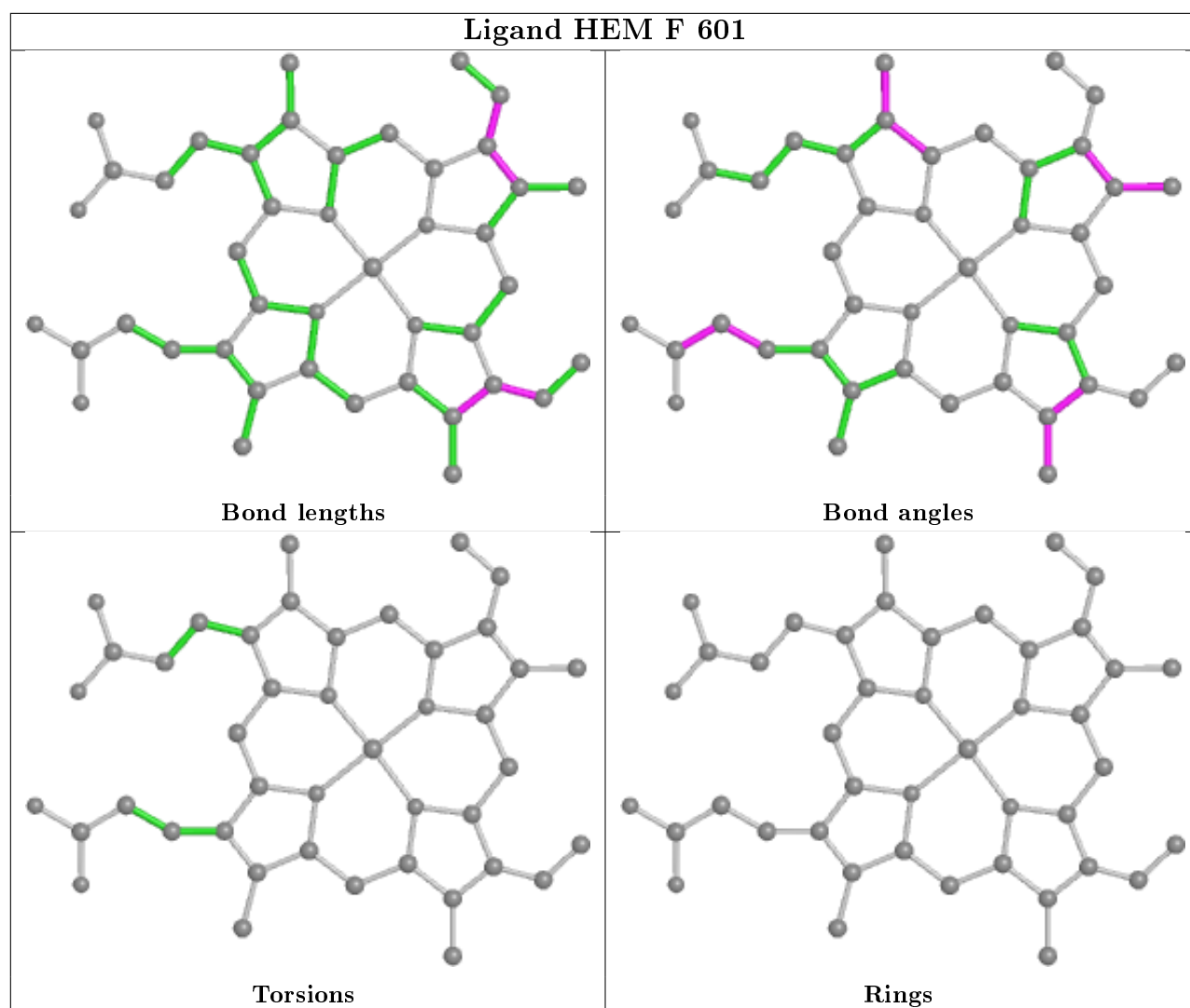


Rings









## 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	462/480 (96%)	-0.03	13 (2%)	53	50	31, 51, 83, 109	0
1	B	458/480 (95%)	0.26	17 (3%)	41	38	37, 63, 94, 129	0
1	C	469/480 (97%)	-0.03	9 (1%)	66	65	27, 45, 77, 111	0
1	D	459/480 (95%)	0.10	11 (2%)	59	57	35, 57, 85, 123	0
1	E	441/480 (91%)	0.96	68 (15%)	2	1	45, 100, 129, 141	0
1	F	456/480 (95%)	0.58	38 (8%)	11	9	55, 79, 111, 128	0
1	G	455/480 (94%)	0.02	5 (1%)	80	81	33, 56, 86, 109	0
1	H	459/480 (95%)	0.08	10 (2%)	62	60	40, 60, 84, 104	0
1	I	464/480 (96%)	0.09	12 (2%)	56	53	36, 54, 82, 123	0
1	J	458/480 (95%)	0.30	23 (5%)	28	25	31, 65, 94, 140	0
1	K	458/480 (95%)	0.09	12 (2%)	56	53	39, 60, 88, 133	0
1	L	448/480 (93%)	1.11	94 (20%)	1	0	64, 104, 135, 143	0
All	All	5487/5760 (95%)	0.29	312 (5%)	23	20	27, 63, 117, 143	0

All (312) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	377	CYS	6.2
1	L	257	LYS	6.2
1	E	338	VAL	6.0
1	J	265	GLN	6.0
1	E	489	VAL	6.0
1	J	27	THR	5.9
1	L	389	PRO	5.7
1	F	262	ASN	5.3
1	I	265	GLN	5.2
1	L	405	PRO	5.0
1	L	261	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
1	F	469	GLU	4.8
1	L	409	THR	4.8
1	E	490	LEU	4.7
1	F	407	TYR	4.7
1	E	326	ASP	4.7
1	F	473	PRO	4.7
1	E	459	LEU	4.6
1	J	266	LYS	4.6
1	L	491	LYS	4.5
1	J	492	VAL	4.5
1	L	465	LYS	4.5
1	F	416	PRO	4.4
1	E	352	GLN	4.4
1	L	387	PHE	4.4
1	E	290	LEU	4.3
1	L	464	PHE	4.3
1	E	258	LYS	4.3
1	L	486	LYS	4.2
1	L	276	ILE	4.2
1	L	419	PHE	4.1
1	C	168	LYS	4.1
1	L	275	MET	4.1
1	F	51	LEU	4.1
1	E	470	THR	4.0
1	E	190	GLY	4.0
1	E	460	GLN	4.0
1	E	327	VAL	4.0
1	L	410	GLU	4.0
1	C	265	GLN	4.0
1	L	216	LEU	3.9
1	D	27	THR	3.9
1	D	266	LYS	3.8
1	K	266	LYS	3.8
1	L	470	THR	3.8
1	B	425	SER	3.8
1	L	388	ILE	3.8
1	K	262	ASN	3.8
1	F	419	PHE	3.8
1	L	221	LEU	3.7
1	L	271	PHE	3.7
1	L	469	GLU	3.6
1	L	100	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	330	LYS	3.5
1	E	472	ILE	3.5
1	L	200	GLN	3.5
1	L	415	ARG	3.5
1	L	493	ASP	3.5
1	E	471	GLN	3.4
1	L	193	ILE	3.4
1	L	329	GLN	3.4
1	L	259	SER	3.4
1	L	468	LYS	3.4
1	E	354	GLU	3.4
1	C	263	ASP	3.4
1	H	387	PHE	3.4
1	L	407	TYR	3.4
1	E	341	ASN	3.3
1	J	199	PRO	3.3
1	E	443	GLY	3.3
1	B	267	HIS	3.3
1	L	467	CYS	3.3
1	B	27	THR	3.3
1	E	369	VAL	3.3
1	H	340	PRO	3.3
1	I	168	LYS	3.3
1	E	99	TYR	3.2
1	J	262	ASN	3.2
1	L	164	ALA	3.2
1	B	266	LYS	3.2
1	K	267	HIS	3.2
1	I	285	GLU	3.2
1	E	457	ARG	3.2
1	L	492	VAL	3.2
1	D	424	ASP	3.2
1	B	383	ILE	3.2
1	F	264	LYS	3.2
1	E	156	LEU	3.2
1	B	269	LEU	3.2
1	L	256	MET	3.2
1	L	408	TRP	3.1
1	L	168	LYS	3.1
1	F	266	LYS	3.1
1	F	53	TYR	3.1
1	J	425	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	L	236	LEU	3.1
1	L	35	ARG	3.1
1	C	285	GLU	3.1
1	F	459	LEU	3.0
1	L	220	PHE	3.0
1	L	45	PRO	3.0
1	F	100	SER	3.0
1	G	387	PHE	3.0
1	A	267	HIS	3.0
1	L	101	VAL	3.0
1	L	337	ALA	3.0
1	A	268	ARG	3.0
1	E	337	ALA	3.0
1	F	258	LYS	3.0
1	L	459	LEU	3.0
1	F	215	PHE	2.9
1	L	258	LYS	2.9
1	D	265	GLN	2.9
1	F	265	GLN	2.9
1	K	289	ALA	2.9
1	C	264	LYS	2.9
1	L	272	LEU	2.9
1	L	197	ASN	2.9
1	L	70	LYS	2.9
1	A	266	LYS	2.9
1	C	424	ASP	2.9
1	L	406	LYS	2.9
1	B	71	MET	2.9
1	A	255	ARG	2.8
1	E	312	SER	2.8
1	I	266	LYS	2.8
1	J	264	LYS	2.8
1	K	276	ILE	2.8
1	E	140	GLY	2.8
1	E	276	ILE	2.8
1	L	429	TYR	2.8
1	F	319	TYR	2.8
1	L	278	SER	2.8
1	F	289	ALA	2.8
1	J	200	GLN	2.8
1	L	460	GLN	2.8
1	A	168	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	417	GLU	2.7
1	E	261	LEU	2.7
1	B	265	GLN	2.7
1	J	468	LYS	2.7
1	E	189	PHE	2.7
1	B	132	LEU	2.7
1	J	489	VAL	2.7
1	L	327	VAL	2.7
1	L	490	LEU	2.7
1	L	166	LYS	2.7
1	F	466	PRO	2.7
1	F	163	GLU	2.7
1	E	256	MET	2.7
1	E	132	LEU	2.7
1	E	200	GLN	2.7
1	B	312	SER	2.7
1	E	346	THR	2.7
1	E	419	PHE	2.6
1	E	309	THR	2.6
1	L	170	VAL	2.6
1	J	469	GLU	2.6
1	G	261	LEU	2.6
1	F	54	ARG	2.6
1	E	473	PRO	2.6
1	L	102	PHE	2.6
1	F	385	GLY	2.6
1	J	407	TYR	2.6
1	L	392	SER	2.6
1	L	426	ILE	2.6
1	E	469	GLU	2.6
1	E	152	TYR	2.6
1	K	189	PHE	2.6
1	E	348	ASP	2.6
1	F	420	SER	2.6
1	E	349	ALA	2.6
1	A	341	ASN	2.6
1	E	468	LYS	2.5
1	F	464	PHE	2.5
1	E	486	LYS	2.5
1	F	342	LYS	2.5
1	I	67	LYS	2.5
1	E	262	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	387	PHE	2.5
1	L	203	PHE	2.5
1	E	347	TYR	2.5
1	K	279	GLN	2.5
1	E	116	SER	2.5
1	L	321	LEU	2.5
1	G	385	GLY	2.5
1	E	335	ILE	2.5
1	L	254	ASN	2.5
1	L	354	GLU	2.5
1	L	147	PRO	2.5
1	J	215	PHE	2.5
1	J	261	LEU	2.5
1	D	441	CYS	2.4
1	L	161	ARG	2.4
1	H	290	LEU	2.4
1	I	493	ASP	2.4
1	J	444	MET	2.4
1	A	289	ALA	2.4
1	C	282	LYS	2.4
1	A	280	ASN	2.4
1	B	262	ASN	2.4
1	E	289	ALA	2.4
1	B	382	GLU	2.4
1	L	250	SER	2.4
1	G	168	LYS	2.4
1	F	50	VAL	2.4
1	J	441	CYS	2.4
1	L	262	ASN	2.4
1	F	47	LEU	2.4
1	F	468	LYS	2.4
1	L	260	ARG	2.4
1	E	55	GLN	2.3
1	F	337	ALA	2.3
1	B	426	ILE	2.3
1	B	45	PRO	2.3
1	K	265	GLN	2.3
1	H	262	ASN	2.3
1	B	255	ARG	2.3
1	J	267	HIS	2.3
1	H	289	ALA	2.3
1	F	261	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	312	SER	2.3
1	L	175	ILE	2.3
1	E	398	THR	2.3
1	L	352	GLN	2.3
1	E	169	PRO	2.3
1	J	263	ASP	2.3
1	L	277	ASP	2.3
1	K	290	LEU	2.3
1	L	280	ASN	2.3
1	D	267	HIS	2.3
1	E	467	CYS	2.3
1	E	97	GLU	2.3
1	L	165	GLU	2.3
1	L	158	ARG	2.3
1	L	302	PHE	2.3
1	L	325	PRO	2.2
1	A	387	PHE	2.2
1	E	148	ILE	2.2
1	E	275	MET	2.2
1	E	295	LEU	2.2
1	L	69	GLY	2.2
1	E	444	MET	2.2
1	E	456	ILE	2.2
1	D	51	LEU	2.2
1	F	219	LEU	2.2
1	D	168	LYS	2.2
1	F	408	TRP	2.2
1	L	75	TYR	2.2
1	F	290	LEU	2.2
1	A	258	LYS	2.2
1	L	393	MET	2.2
1	L	93	VAL	2.2
1	H	424	ASP	2.2
1	I	262	ASN	2.2
1	A	281	SER	2.2
1	A	494	SER	2.2
1	B	387	PHE	2.2
1	L	34	LYS	2.2
1	E	368	PRO	2.2
1	F	492	VAL	2.2
1	L	338	VAL	2.2
1	L	167	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	45	PRO	2.2
1	J	352	GLN	2.2
1	H	266	LYS	2.2
1	L	435	GLY	2.2
1	G	45	PRO	2.2
1	I	169	PRO	2.2
1	D	263	ASP	2.1
1	L	430	ILE	2.1
1	C	309	THR	2.1
1	E	313	VAL	2.1
1	I	261	LEU	2.1
1	L	290	LEU	2.1
1	D	264	LYS	2.1
1	F	406	LYS	2.1
1	D	139	SER	2.1
1	E	101	VAL	2.1
1	E	441	CYS	2.1
1	K	425	SER	2.1
1	C	422	LYS	2.1
1	E	257	LYS	2.1
1	L	466	PRO	2.1
1	E	433	PRO	2.1
1	F	97	GLU	2.1
1	L	328	GLN	2.1
1	E	170	VAL	2.1
1	L	152	TYR	2.1
1	E	96	LYS	2.1
1	J	312	SER	2.1
1	K	264	LYS	2.1
1	L	249	LEU	2.1
1	B	310	THR	2.1
1	E	464	PHE	2.1
1	L	47	LEU	2.0
1	L	160	LEU	2.0
1	H	35	ARG	2.0
1	L	224	ILE	2.0
1	J	29	THR	2.0
1	K	469	GLU	2.0
1	H	41	PRO	2.0
1	I	267	HIS	2.0
1	E	35	ARG	2.0
1	F	124	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	309	THR	2.0
1	E	311	SER	2.0
1	A	260	ARG	2.0
1	E	350	VAL	2.0
1	F	32	LEU	2.0
1	F	168	LYS	2.0
1	L	218	PRO	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](#)

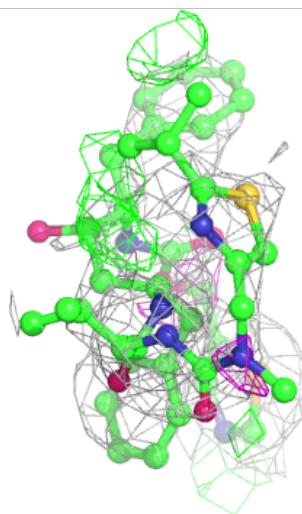
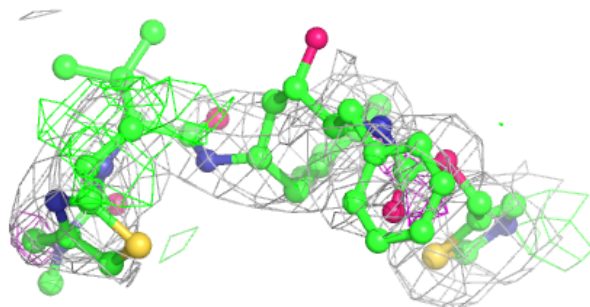
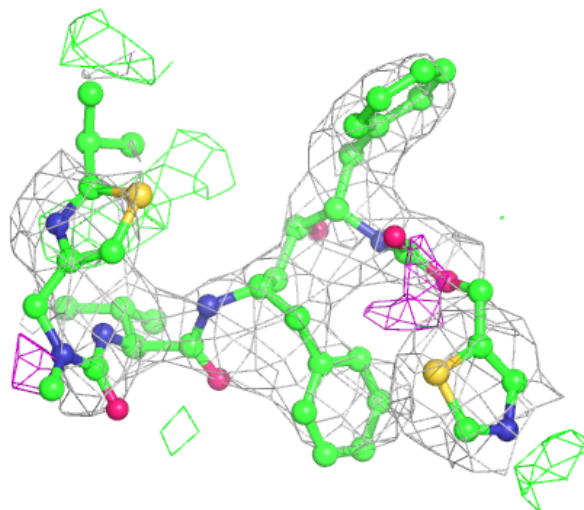
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	RIT	B	602	50/50	0.84	0.32	55,90,108,129	0
3	RIT	H	602	50/50	0.84	0.31	53,83,106,113	0
3	RIT	A	602	50/50	0.86	0.33	39,79,107,111	0
2	HEM	E	601	43/43	0.93	0.32	66,79,92,100	0
2	HEM	L	601	43/43	0.94	0.28	69,78,92,97	0
2	HEM	F	601	43/43	0.95	0.26	37,46,63,65	0
2	HEM	K	601	43/43	0.97	0.22	37,44,50,55	0
2	HEM	D	601	43/43	0.97	0.28	34,44,50,56	0
2	HEM	I	601	43/43	0.97	0.26	30,37,42,48	0
2	HEM	C	601	43/43	0.97	0.23	22,31,37,39	0
2	HEM	J	601	43/43	0.97	0.28	38,46,49,56	0
2	HEM	G	601	43/43	0.97	0.24	26,36,41,68	0
2	HEM	B	601	43/43	0.97	0.24	37,46,55,60	0
2	HEM	H	601	43/43	0.97	0.24	42,50,54,56	0
2	HEM	A	601	43/43	0.98	0.22	30,36,41,44	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.

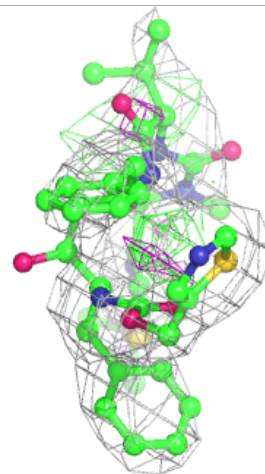
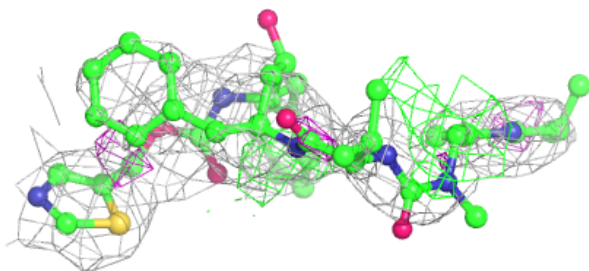
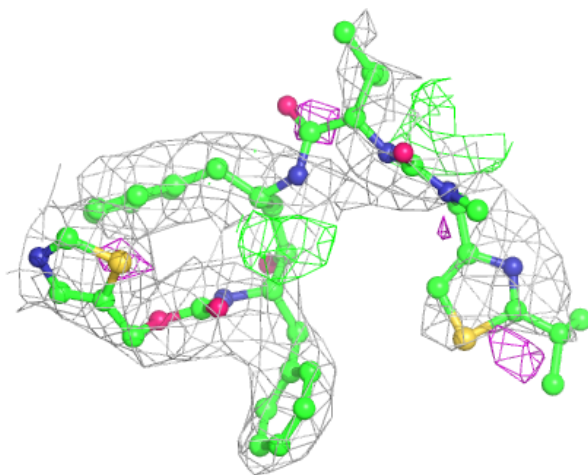
**Electron density around RIT B 602:**

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



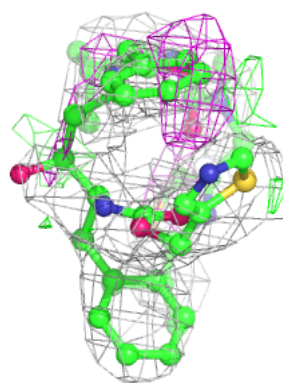
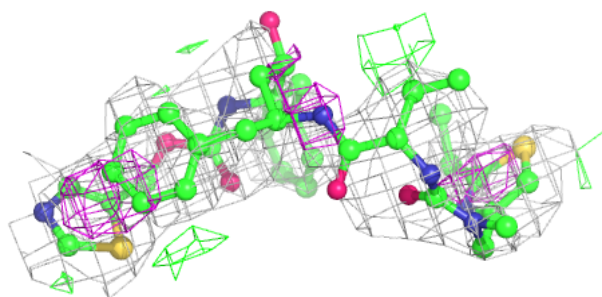
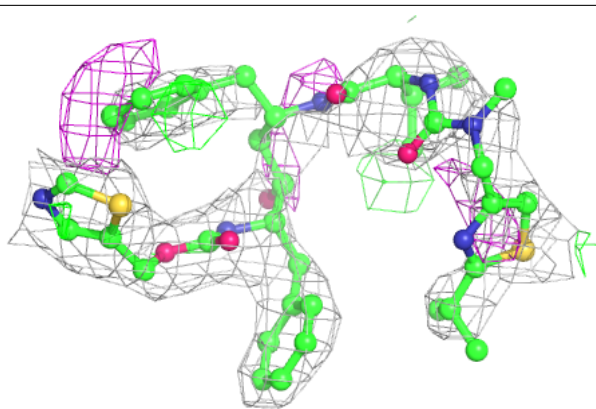
**Electron density around RIT H 602:**

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



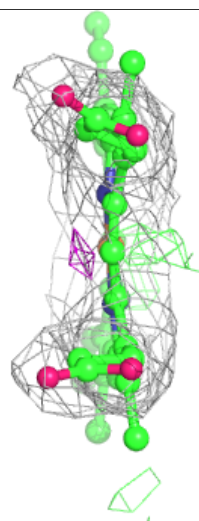
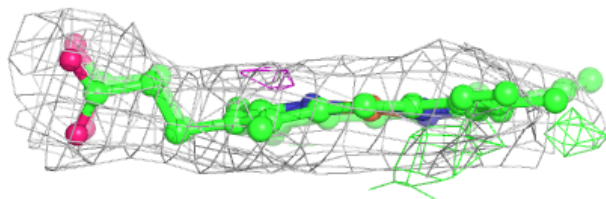
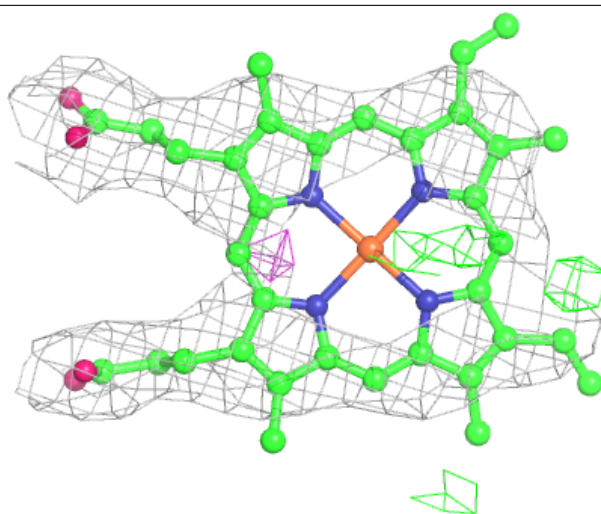
**Electron density around RIT A 602:**

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



**Electron density around HEM E 601:**

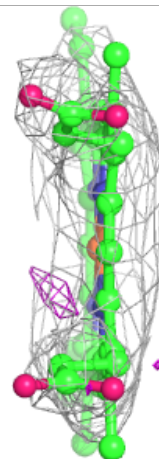
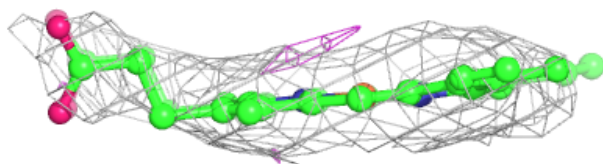
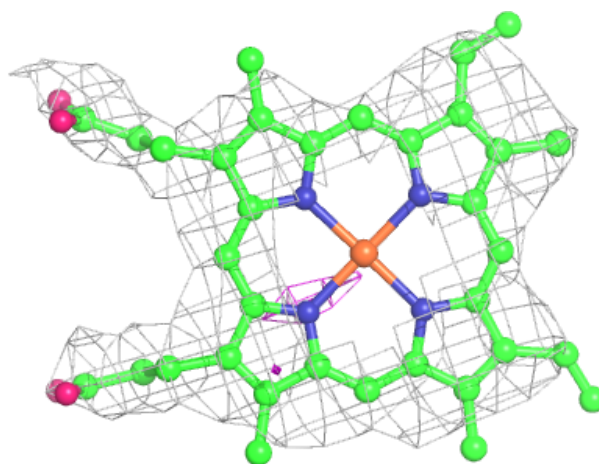
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





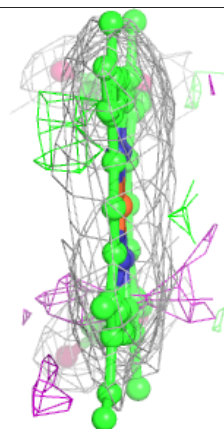
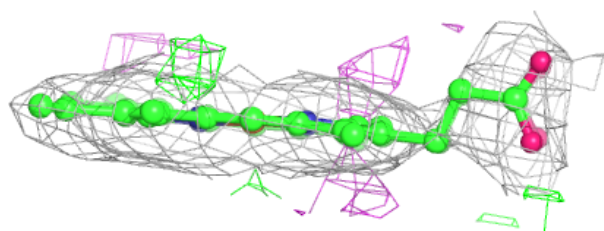
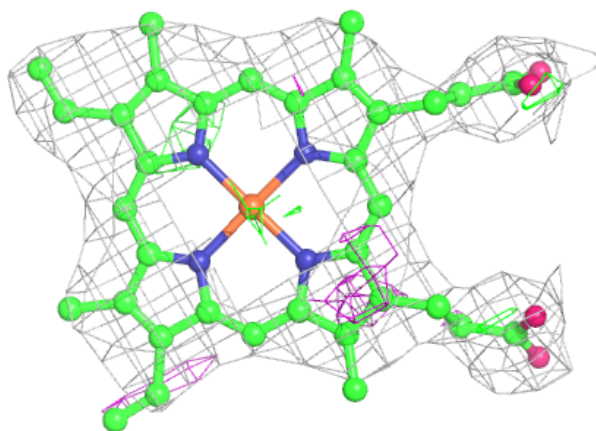
**Electron density around HEM L 601:**

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



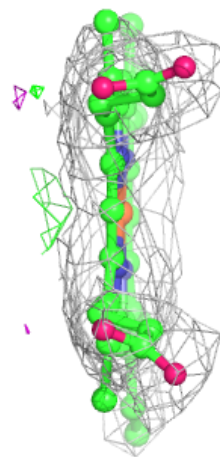
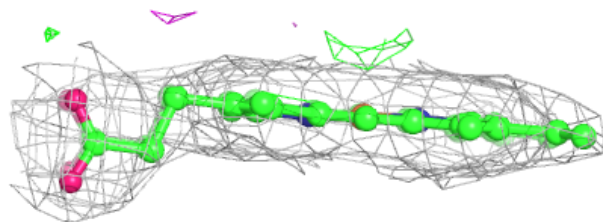
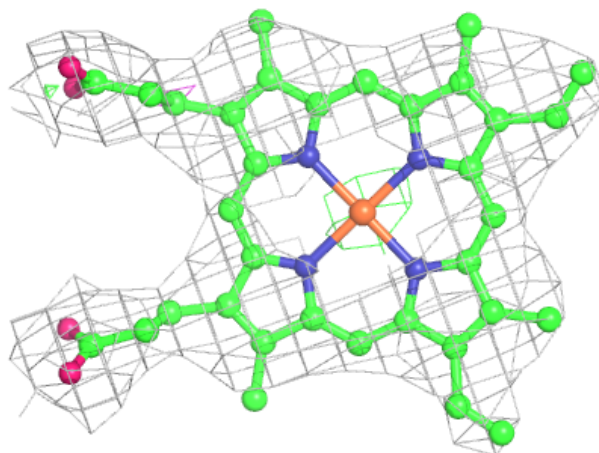
**Electron density around HEM F 601:**

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



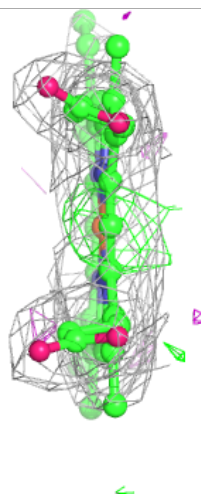
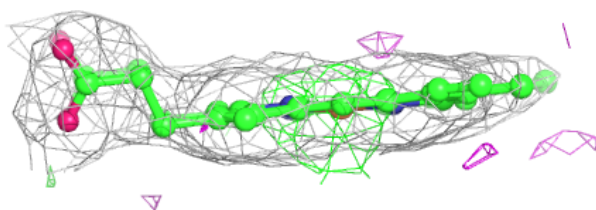
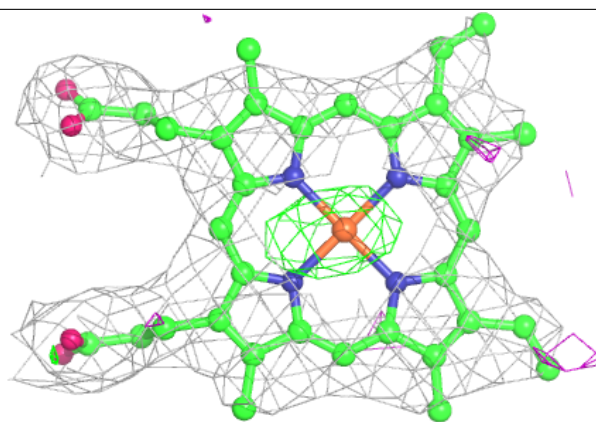
**Electron density around HEM K 601:**

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



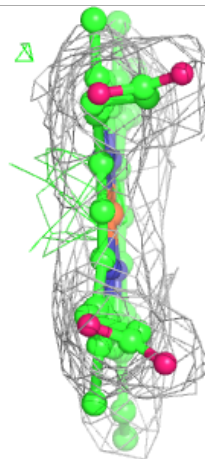
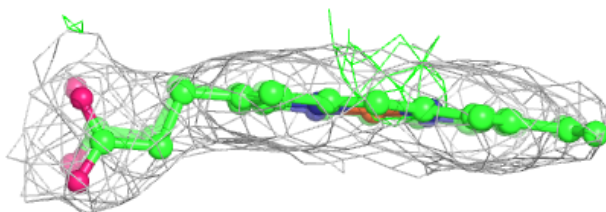
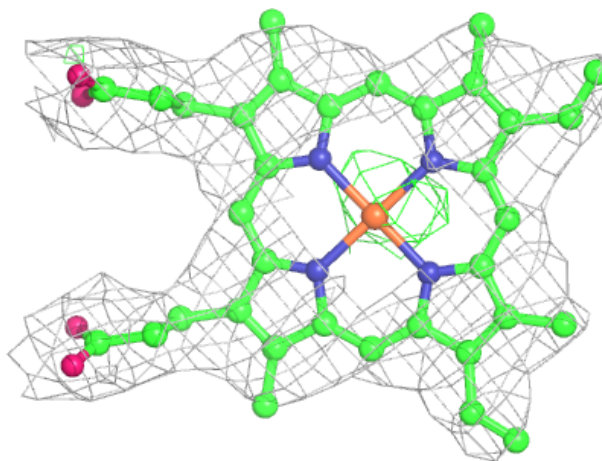
**Electron density around HEM D 601:**

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



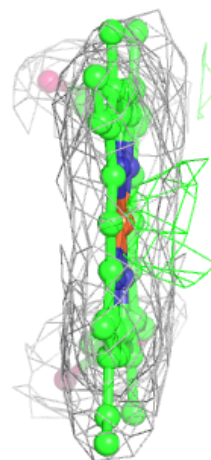
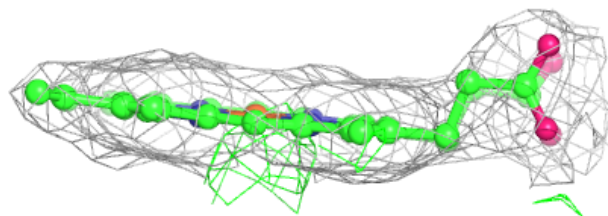
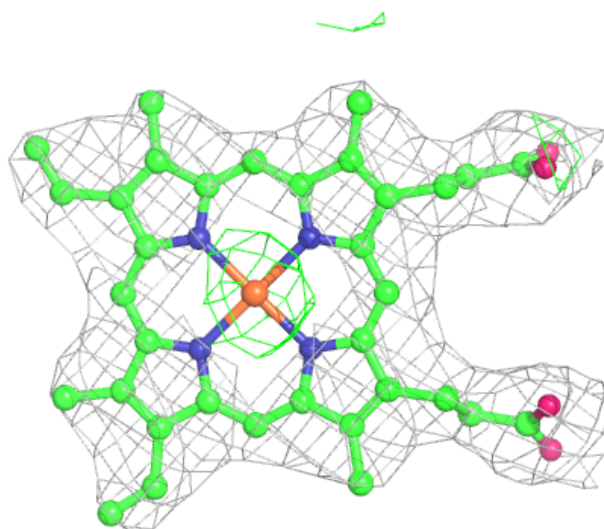
**Electron density around HEM I 601:**

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



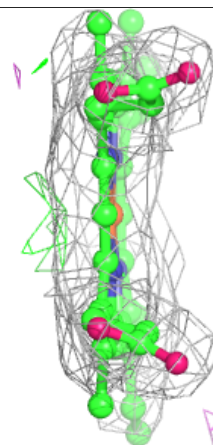
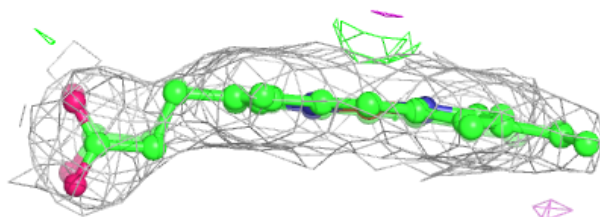
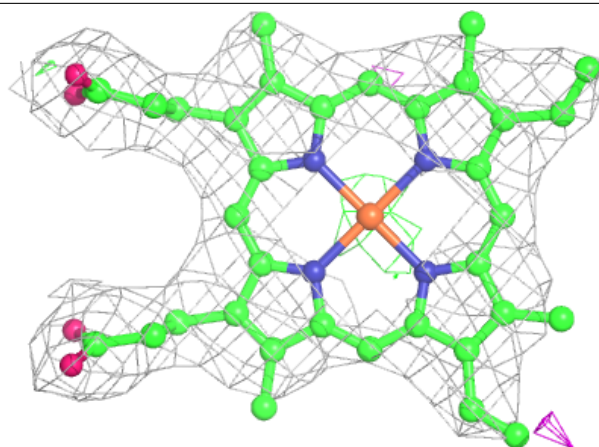
**Electron density around HEM C 601:**

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



**Electron density around HEM J 601:**

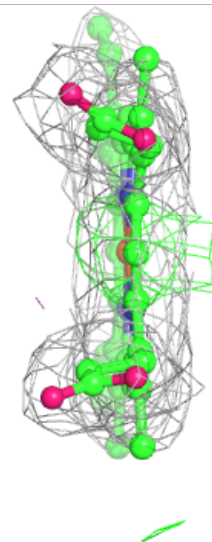
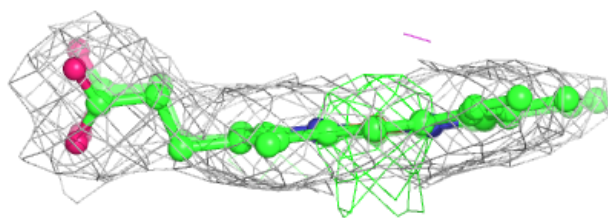
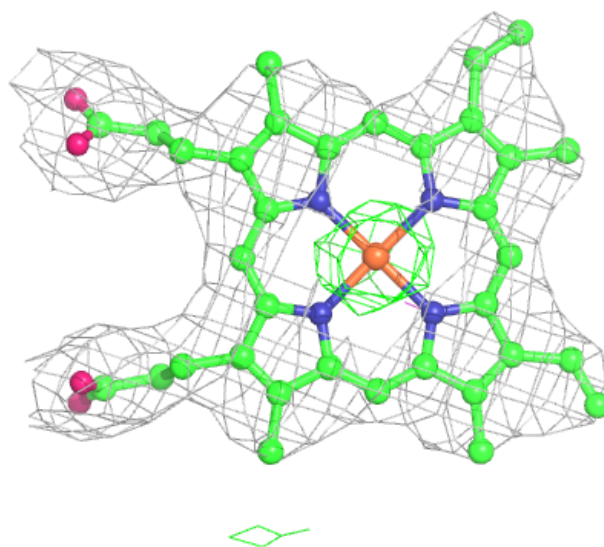
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEM G 601:**

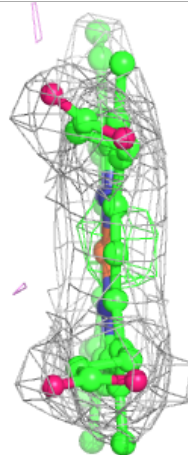
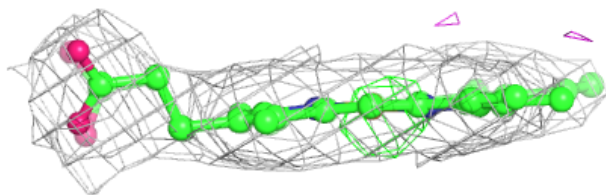
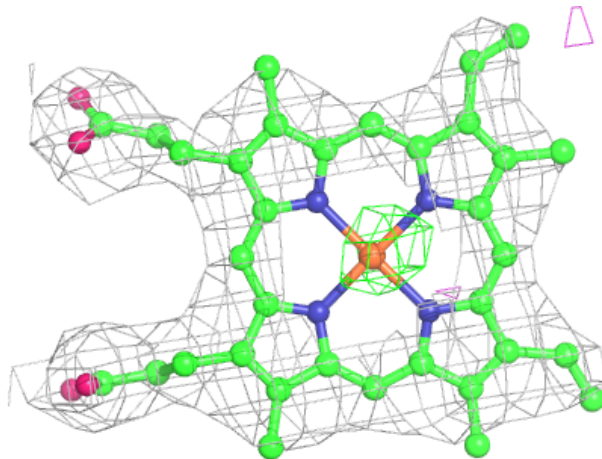
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





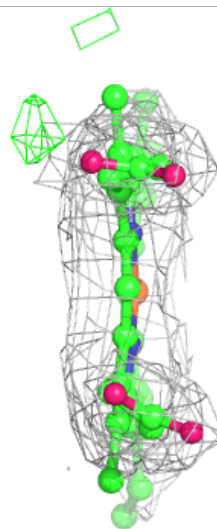
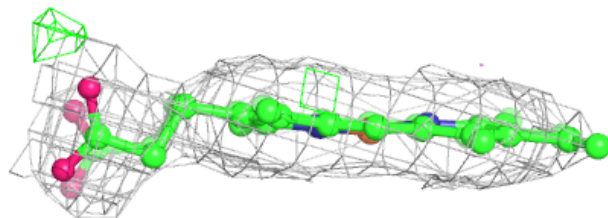
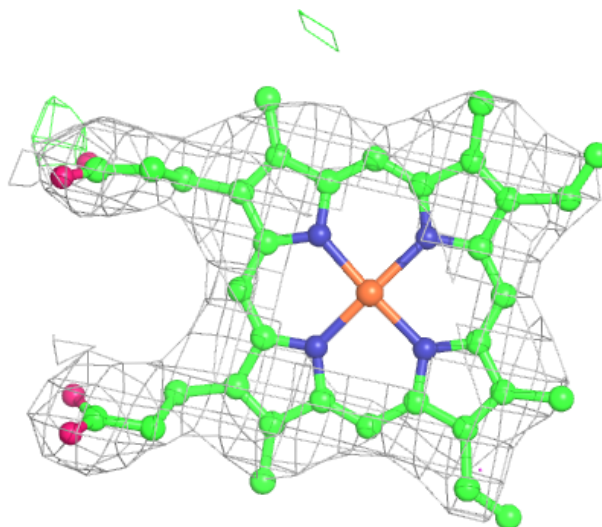
**Electron density around HEM B 601:**

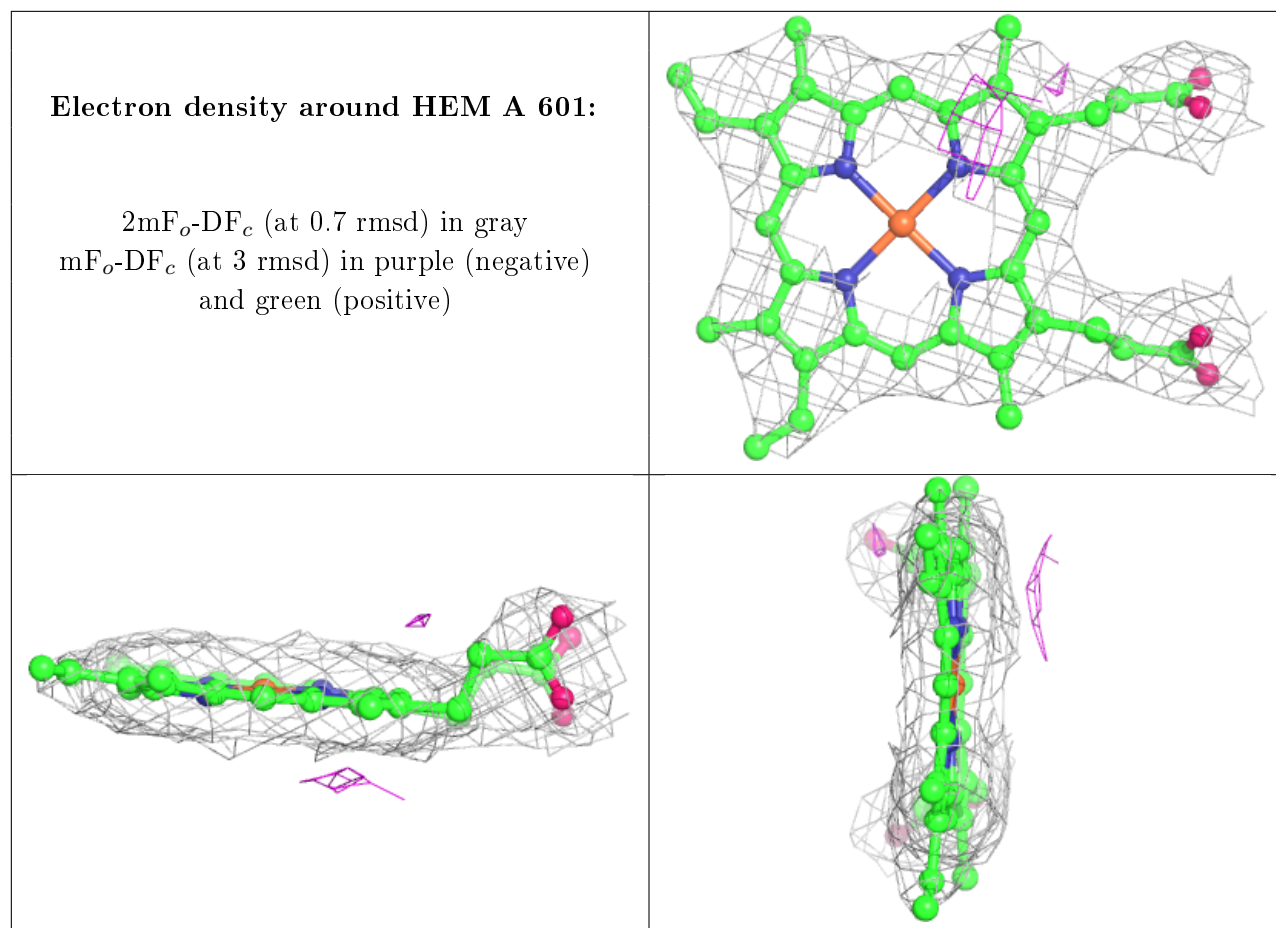
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM H 601:**

$2mF_o-DF_c$  (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.