



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:16 PM UTC

PDB ID : 4U8U / pdb_00004u8u
Title : The Crystallographic structure of the giant hemoglobin from *Glossoscolex paulistus* at 3.2 Å resolution.
Authors : Bachega, J.F.R.; Maluf, F.V.; Andi, B.; D'Muniz Pereira, H.; Carazzollea, M.F.; Orville, A.; Tabak, M.; Garratt, R.C.; Horjales, E.
Deposited on : 2014-08-04
Resolution : 3.20 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

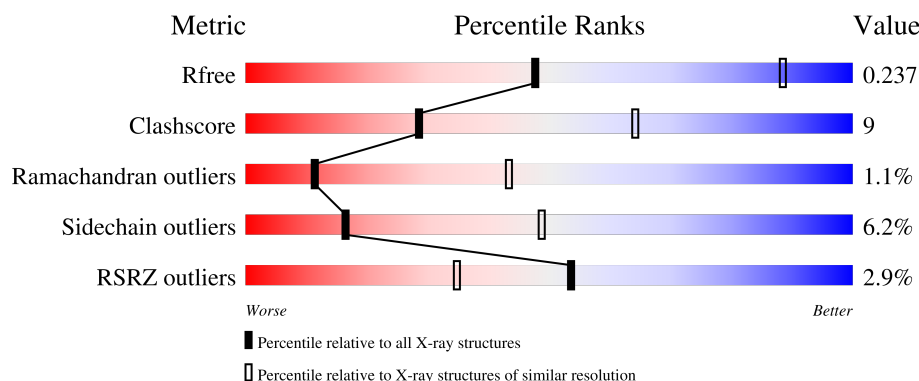
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 of 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	150	7% 68% 25% 5% ..
1	E	150	5% 71% 21% 6% .
1	I	150	6% 75% 19% 5% .
1	P	150	8% 72% 22% 5% .

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Mol	Chain	Length	Quality of chain
1	T	150	
1	X	150	
1	e	150	
1	i	150	
1	m	150	
2	B	142	
2	F	142	
2	J	142	
2	Q	142	
2	U	142	
2	Y	142	
2	f	142	
2	j	142	
2	n	142	
3	C	151	
3	G	151	
3	K	151	
3	R	151	
3	V	151	
3	Z	151	
3	g	151	
3	k	151	
3	o	151	
4	D	141	
4	H	141	

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Mol	Chain	Length	Quality of chain
4	L	141	80% 19% .
4	S	141	79% 20% .
4	W	141	4% 79% 18% .
4	a	141	82% 17% .
4	h	141	78% 21% .
4	l	141	82% 17% .
4	p	141	79% 20% .
5	M	224	2% 79% 18% ..
5	b	224	3% 80% 18% .
5	q	224	2% 79% 19% ..
6	N	236	3% 78% 11% . 7%
6	c	236	3% 75% 14% . 7%
6	r	236	75% 14% . 7%
7	O	218	84% 11% . .
7	d	218	84% 11% . .
7	s	218	87% 8% . .

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 59163 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 Globin a chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	148	Total	C	N	O	S	0	0	0
			1200	762	218	216	4			
1	E	148	Total	C	N	O	S	0	0	0
			1200	762	218	216	4			
1	I	148	Total	C	N	O	S	0	0	0
			1200	762	218	216	4			
1	P	148	Total	C	N	O	S	0	0	0
			1200	762	218	216	4			
1	T	148	Total	C	N	O	S	0	0	0
			1200	762	218	216	4			
1	X	148	Total	C	N	O	S	0	0	0
			1200	762	218	216	4			
1	e	148	Total	C	N	O	S	0	0	0
			1200	762	218	216	4			
1	i	148	Total	C	N	O	S	0	0	0
			1200	762	218	216	4			
1	m	148	Total	C	N	O	S	0	0	0
			1200	762	218	216	4			

- Molecule 2 is a protein called Globin b Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	142	Total	C	N	O	S	0	0	0
			1148	727	215	203	3			
2	F	142	Total	C	N	O	S	0	0	0
			1148	727	215	203	3			
2	J	142	Total	C	N	O	S	0	0	0
			1148	727	215	203	3			
2	Q	142	Total	C	N	O	S	0	0	0
			1148	727	215	203	3			
2	U	142	Total	C	N	O	S	0	0	0
			1148	727	215	203	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	142	Total	C	N	O	S	0	0	0
			1148	727	215	203	3			
2	f	142	Total	C	N	O	S	0	0	0
			1148	727	215	203	3			
2	j	142	Total	C	N	O	S	0	0	0
			1148	727	215	203	3			
2	n	142	Total	C	N	O	S	0	0	0
			1148	727	215	203	3			

- Molecule 3 is a protein called Globin c Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	151	Total	C	N	O	S	0	0	0
			1180	750	205	219	6			
3	G	151	Total	C	N	O	S	0	0	0
			1180	750	205	219	6			
3	K	151	Total	C	N	O	S	0	0	0
			1180	750	205	219	6			
3	R	151	Total	C	N	O	S	0	0	0
			1180	750	205	219	6			
3	V	151	Total	C	N	O	S	0	0	0
			1180	750	205	219	6			
3	Z	151	Total	C	N	O	S	0	0	0
			1180	750	205	219	6			
3	g	151	Total	C	N	O	S	0	0	0
			1180	750	205	219	6			
3	k	151	Total	C	N	O	S	0	0	0
			1180	750	205	219	6			
3	o	151	Total	C	N	O	S	0	0	0
			1189	755	208	220	6			

- Molecule 4 is a protein called Globin d Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	141	Total	C	N	O	S	0	0	0
			1140	734	199	204	3			
4	H	141	Total	C	N	O	S	0	0	0
			1140	734	199	204	3			
4	L	141	Total	C	N	O	S	0	0	0
			1140	734	199	204	3			
4	S	141	Total	C	N	O	S	0	0	0
			1140	734	199	204	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	W	141	Total	C	N	O	S	0	0	0
			1140	734	199	204	3			
4	a	141	Total	C	N	O	S	0	0	0
			1140	734	199	204	3			
4	h	141	Total	C	N	O	S	0	0	0
			1140	734	199	204	3			
4	l	141	Total	C	N	O	S	0	0	0
			1140	734	199	204	3			
4	p	141	Total	C	N	O	S	0	0	0
			1140	734	199	204	3			

- Molecule 5 is a protein called Linker L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	M	222	Total	C	N	O	S	0	0	0
			1754	1092	315	337	10			
5	b	222	Total	C	N	O	S	0	0	0
			1754	1092	315	337	10			
5	q	222	Total	C	N	O	S	0	0	0
			1754	1092	315	337	10			

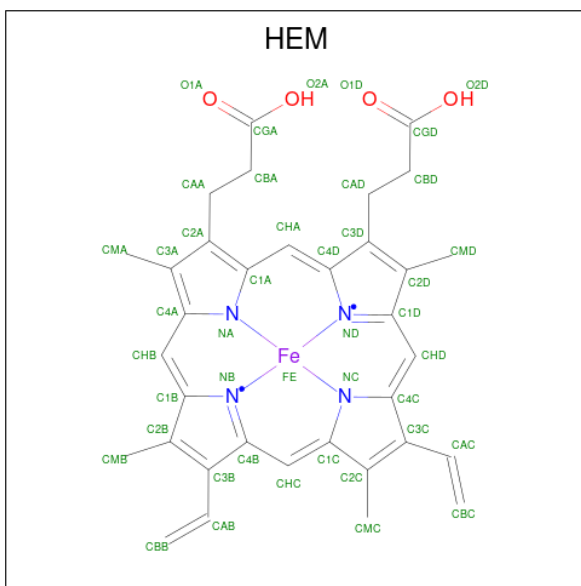
- Molecule 6 is a protein called Linker L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	N	219	Total	C	N	O	S	0	0	0
			1713	1060	326	317	10			
6	c	219	Total	C	N	O	S	0	0	0
			1713	1060	326	317	10			
6	r	219	Total	C	N	O	S	0	0	0
			1713	1060	326	317	10			

- Molecule 7 is a protein called Linker L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	O	213	Total	C	N	O	S	0	0	0
			1686	1044	297	337	8			
7	d	213	Total	C	N	O	S	0	0	0
			1686	1044	297	337	8			
7	s	213	Total	C	N	O	S	0	0	0
			1686	1044	297	337	8			

- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:

$$\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4).$$


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
8	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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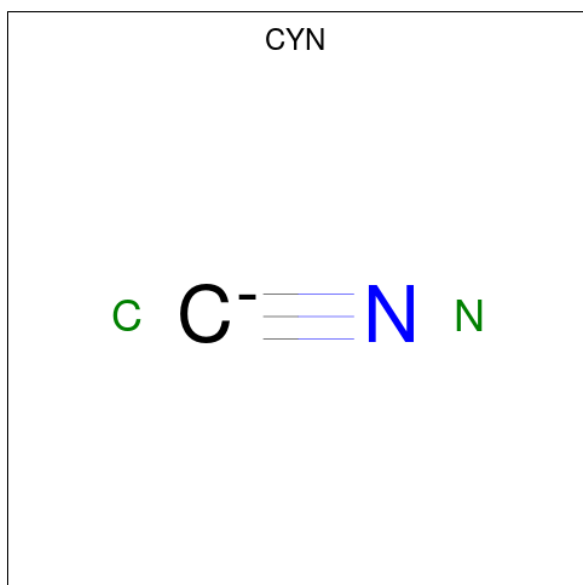
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	R	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	S	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	T	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	U	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	W	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	X	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	Y	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	Z	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	a	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	f	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	g	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	h	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	i	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	j	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	k	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	l	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	m	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	n	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	o	1	Total	C	Fe	N	O	
			43	34	1	4	4	
8	p	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 9 is CYANIDE ION (CCD ID: CYN) (formula: CN).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	N		
			2	1	1	0	0
9	B	1	Total	C	N		
			2	1	1	0	0
9	C	1	Total	C	N		
			2	1	1	0	0
9	D	1	Total	C	N		
			2	1	1	0	0
9	E	1	Total	C	N		
			2	1	1	0	0
9	F	1	Total	C	N		
			2	1	1	0	0
9	G	1	Total	C	N		
			2	1	1	0	0
9	H	1	Total	C	N		
			2	1	1	0	0
9	I	1	Total	C	N		
			2	1	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	J	1	Total	C	N	0	0
			2	1	1		
9	K	1	Total	C	N	0	0
			2	1	1		
9	L	1	Total	C	N	0	0
			2	1	1		
9	P	1	Total	C	N	0	0
			2	1	1		
9	Q	1	Total	C	N	0	0
			2	1	1		
9	R	1	Total	C	N	0	0
			2	1	1		
9	S	1	Total	C	N	0	0
			2	1	1		
9	T	1	Total	C	N	0	0
			2	1	1		
9	U	1	Total	C	N	0	0
			2	1	1		
9	V	1	Total	C	N	0	0
			2	1	1		
9	W	1	Total	C	N	0	0
			2	1	1		
9	X	1	Total	C	N	0	0
			2	1	1		
9	Y	1	Total	C	N	0	0
			2	1	1		
9	Z	1	Total	C	N	0	0
			2	1	1		
9	a	1	Total	C	N	0	0
			2	1	1		
9	e	1	Total	C	N	0	0
			2	1	1		
9	f	1	Total	C	N	0	0
			2	1	1		
9	g	1	Total	C	N	0	0
			2	1	1		
9	h	1	Total	C	N	0	0
			2	1	1		
9	i	1	Total	C	N	0	0
			2	1	1		
9	j	1	Total	C	N	0	0
			2	1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	k	1	Total C N 2 1 1	0	0
9	l	1	Total C N 2 1 1	0	0
9	m	1	Total C N 2 1 1	0	0
9	n	1	Total C N 2 1 1	0	0
9	o	1	Total C N 2 1 1	0	0
9	p	1	Total C N 2 1 1	0	0

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	M	1	Total Ca 1 1	0	0
10	N	1	Total Ca 1 1	0	0
10	O	1	Total Ca 1 1	0	0
10	b	1	Total Ca 1 1	0	0
10	c	1	Total Ca 1 1	0	0
10	d	1	Total Ca 1 1	0	0
10	q	1	Total Ca 1 1	0	0
10	r	1	Total Ca 1 1	0	0
10	s	1	Total Ca 1 1	0	0

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

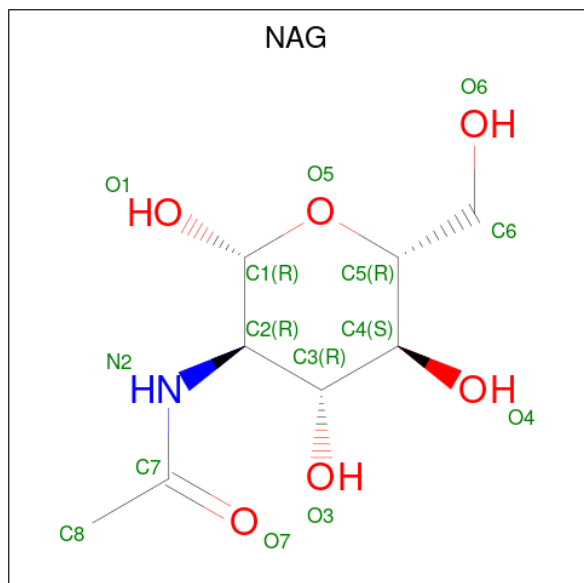
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	O	2	Total Zn 2 2	0	0
11	c	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	d	2	Total	Zn	0	0
			2	2		
11	s	1	Total	Zn	0	0
			1	1		

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	O	1	Total	C	N	O	0	0
			14	8	1	5		
12	d	1	Total	C	N	O	0	0
			14	8	1	5		
12	s	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	O	1	Total	O	0	0
			1	1		
13	c	1	Total	O	0	0
			1	1		
13	d	2	Total	O	0	0
			2	2		
13	r	1	Total	O	0	0
			1	1		

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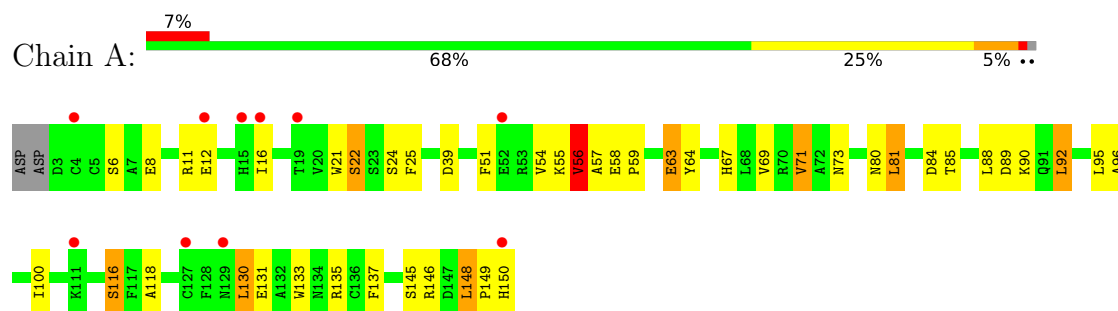
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	s	1	Total	O	0	0
			1	1		

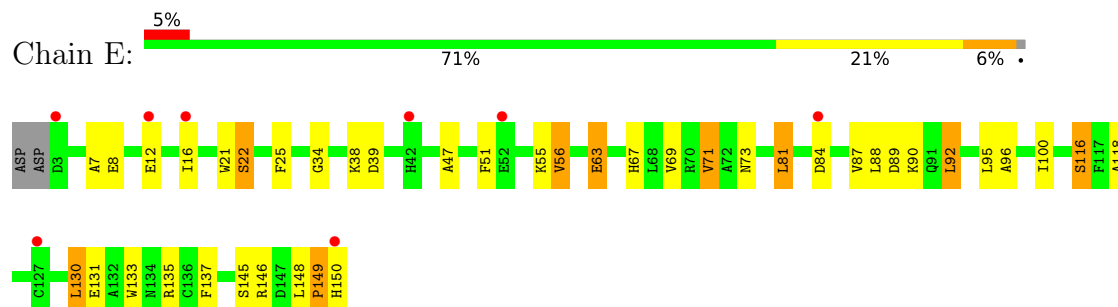
3 Residue-property plots [i](#)

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.

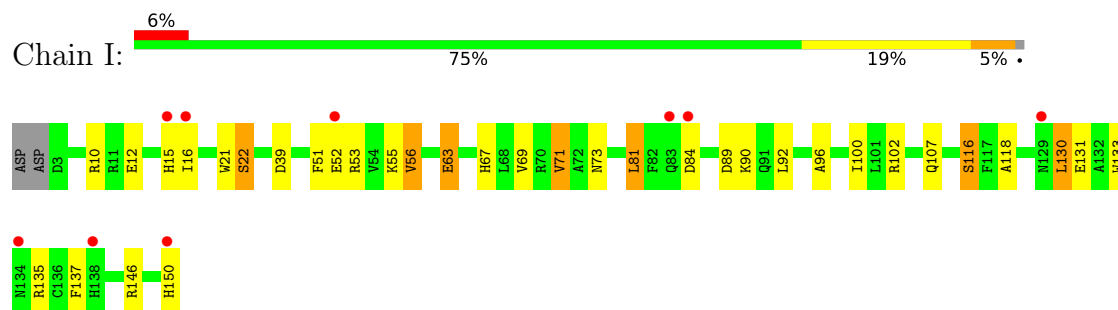
- Molecule 1: Globin a chain



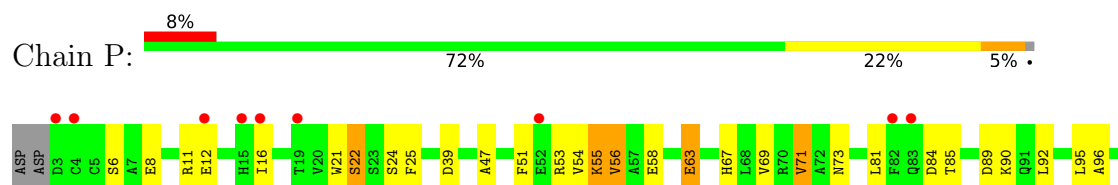
- Molecule 1: Globin a chain

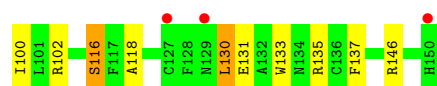


- Molecule 1: Globin a chain

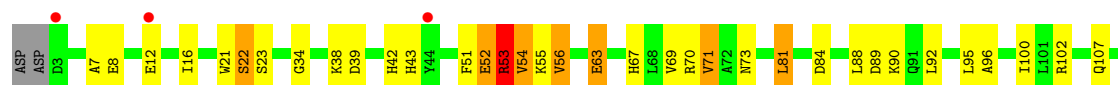


- Molecule 1: Globin a chain

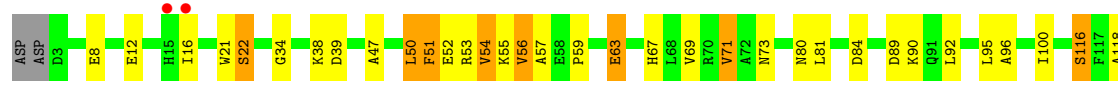




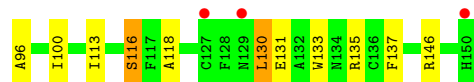
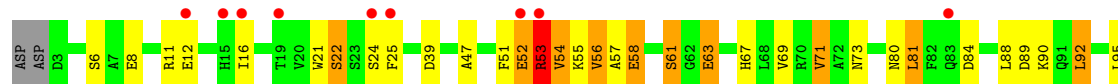
- Molecule 1: Globin a chain



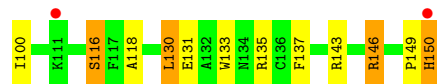
- Molecule 1: Globin a chain



- Molecule 1: Globin a chain

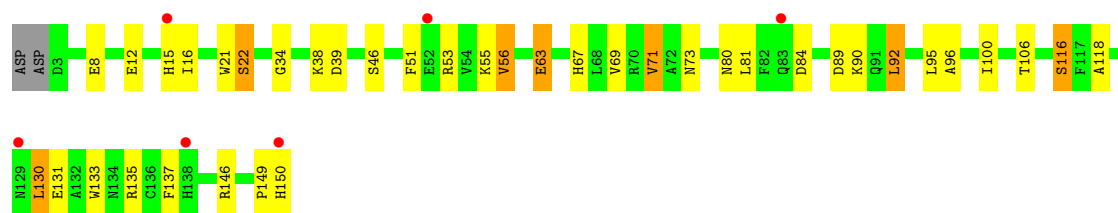


- Molecule 1: Globin a chain

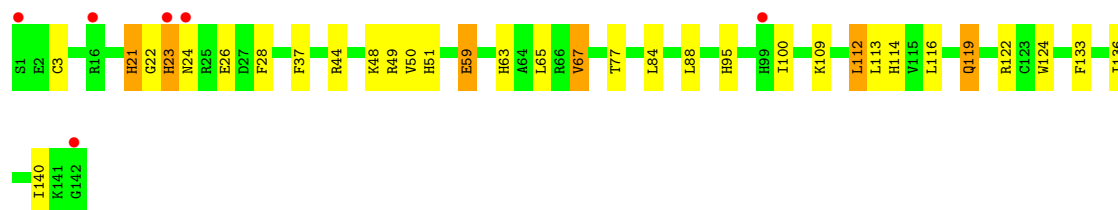
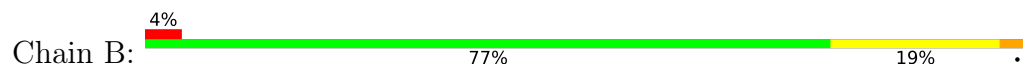


- Molecule 1: Globin a chain

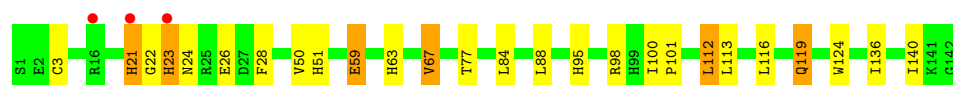
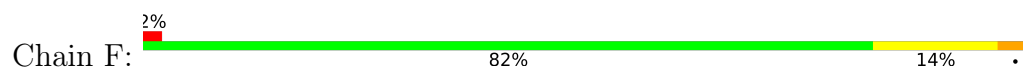




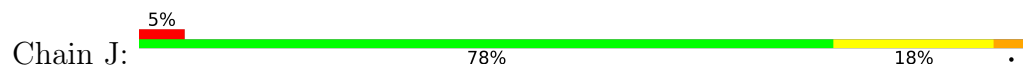
● Molecule 2: Globin b Chain



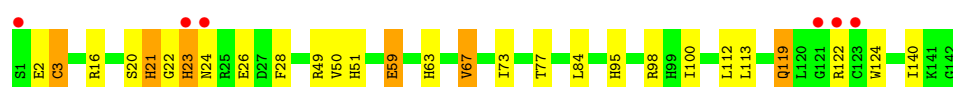
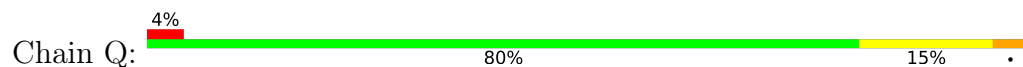
● Molecule 2: Globin b Chain



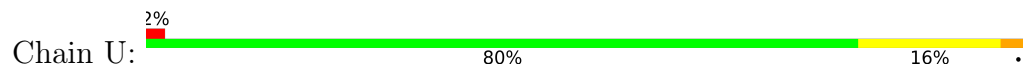
● Molecule 2: Globin b Chain



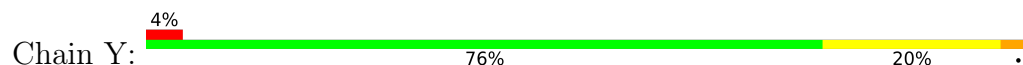
● Molecule 2: Globin b Chain



● Molecule 2: Globin b Chain

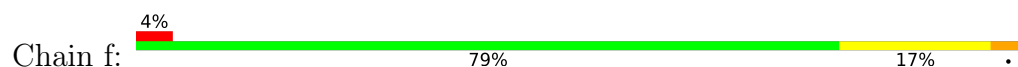


● Molecule 2: Globin b Chain

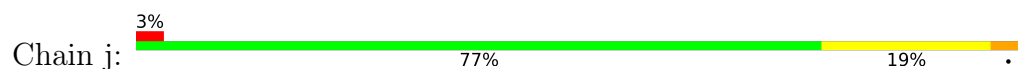




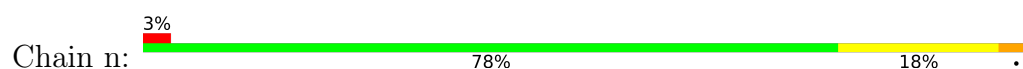
• Molecule 2: Globin b Chain



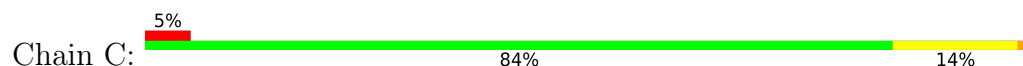
• Molecule 2: Globin b Chain



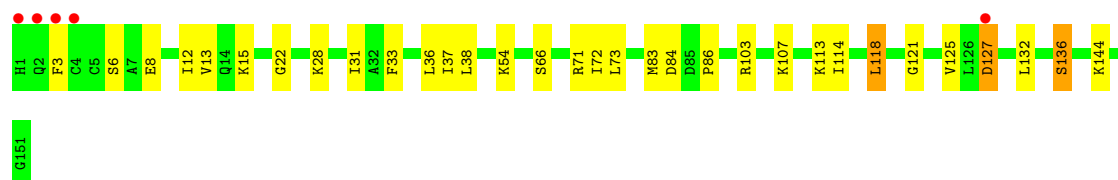
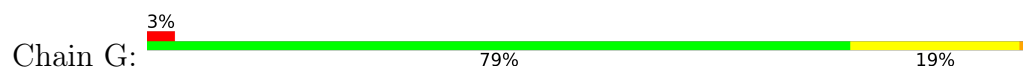
• Molecule 2: Globin b Chain



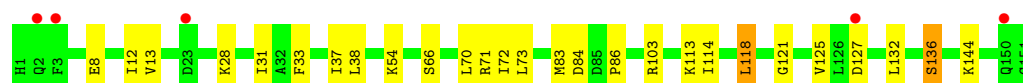
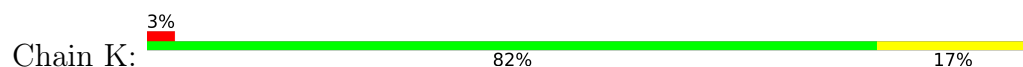
• Molecule 3: Globin c Chain



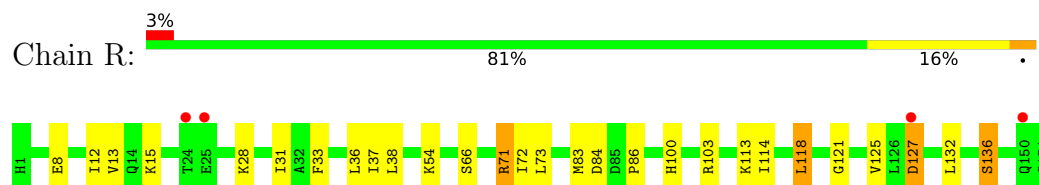
• Molecule 3: Globin c Chain



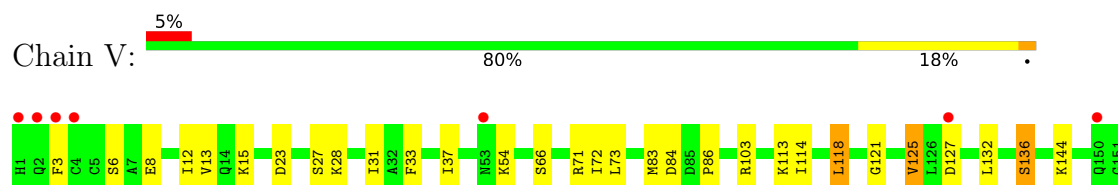
• Molecule 3: Globin c Chain



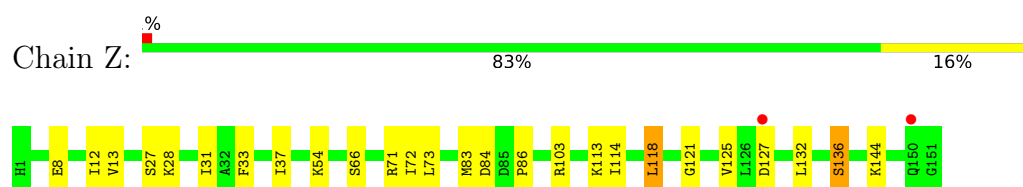
- Molecule 3: Globin c Chain



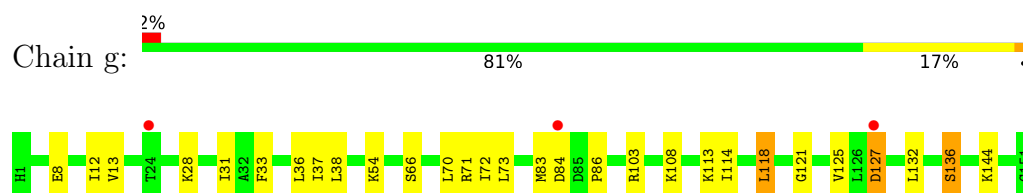
- Molecule 3: Globin c Chain



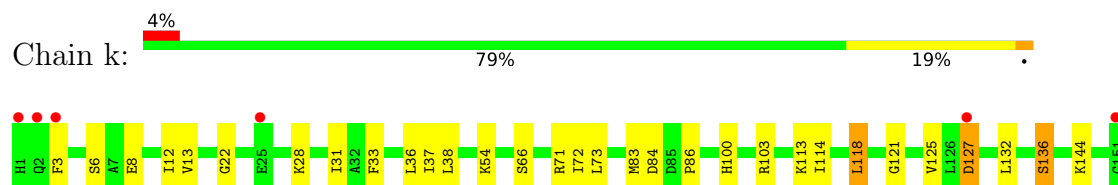
- Molecule 3: Globin c Chain



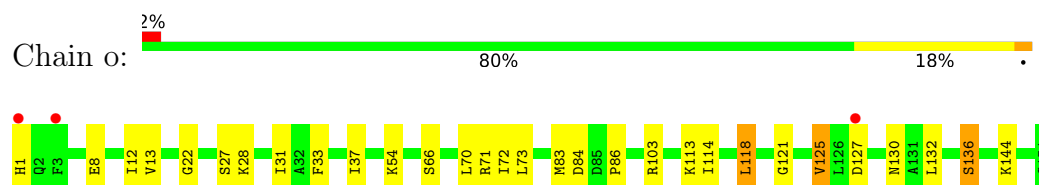
- Molecule 3: Globin c Chain



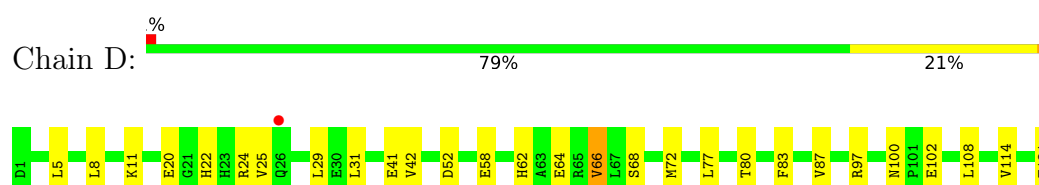
- Molecule 3: Globin c Chain



- Molecule 3: Globin c Chain

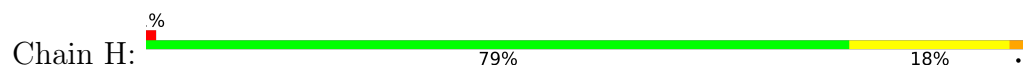


- Molecule 4: Globin d Chain

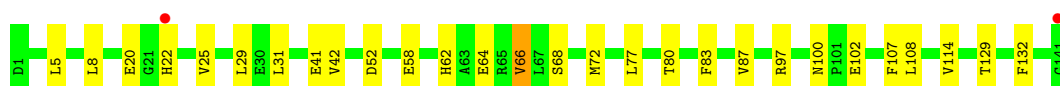
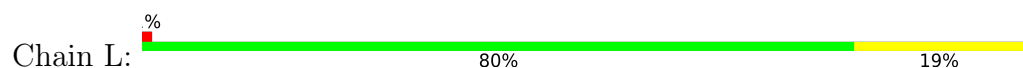




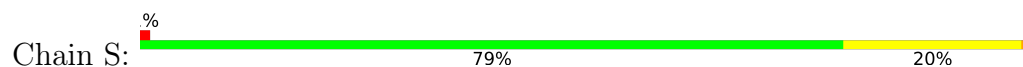
- Molecule 4: Globin d Chain



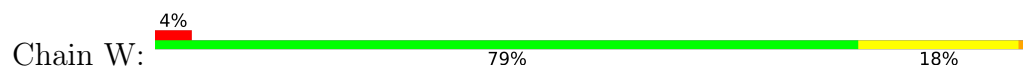
- Molecule 4: Globin d Chain



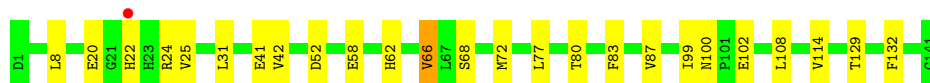
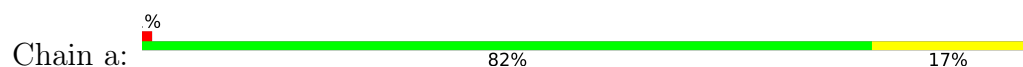
- Molecule 4: Globin d Chain



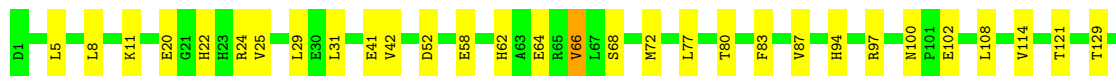
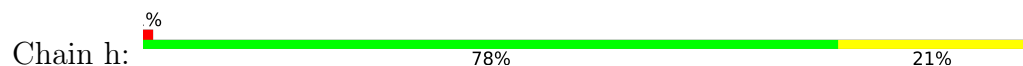
- Molecule 4: Globin d Chain



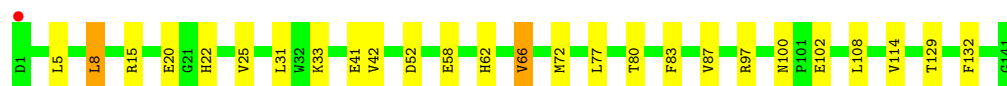
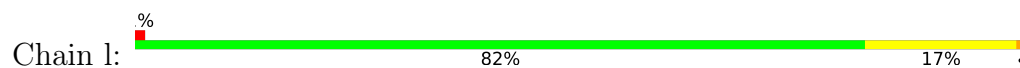
- Molecule 4: Globin d Chain



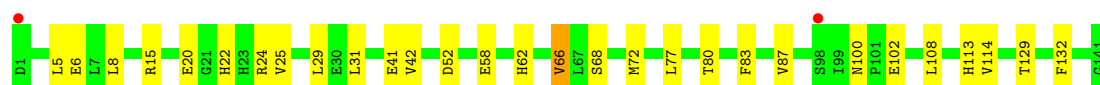
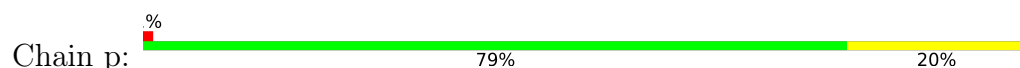
- Molecule 4: Globin d Chain



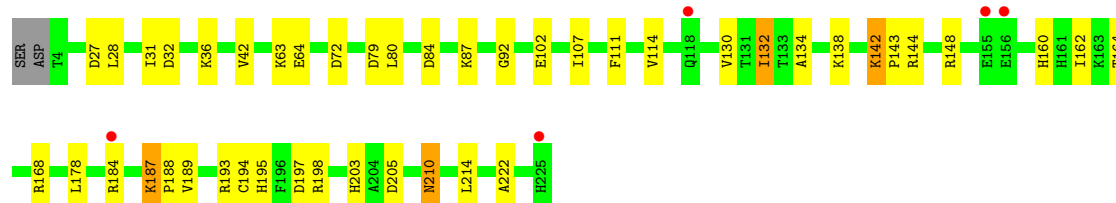
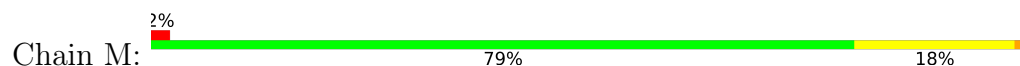
- Molecule 4: Globin d Chain



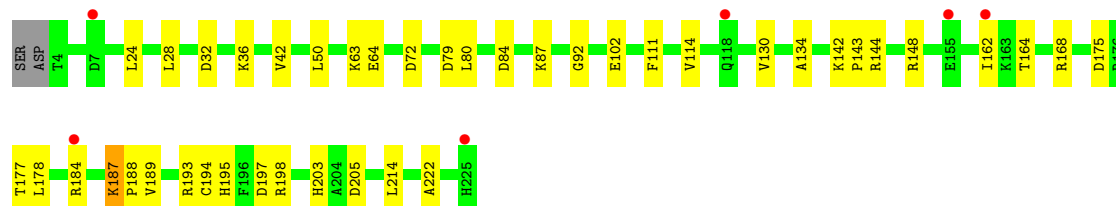
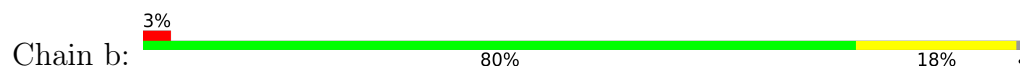
- Molecule 4: Globin d Chain



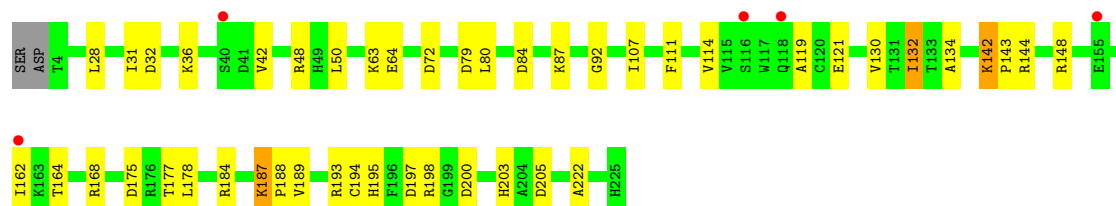
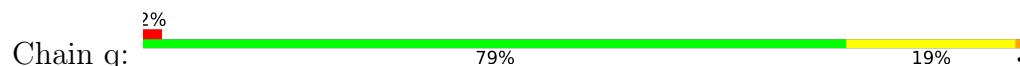
- Molecule 5: Linker L1



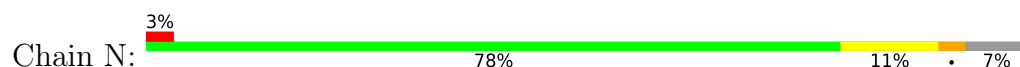
- Molecule 5: Linker L1



- Molecule 5: Linker L1

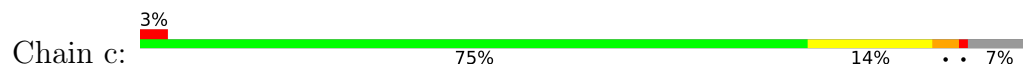


- Molecule 6: Linker L2

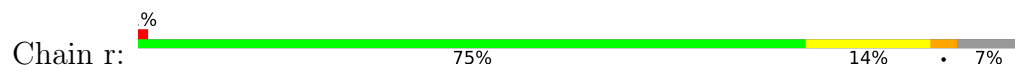




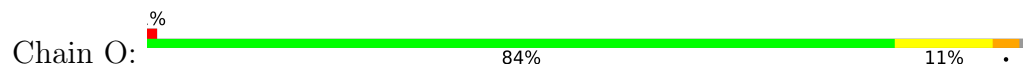
• Molecule 6: Linker L2



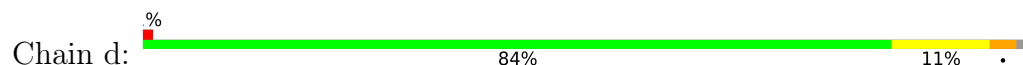
• Molecule 6: Linker L2



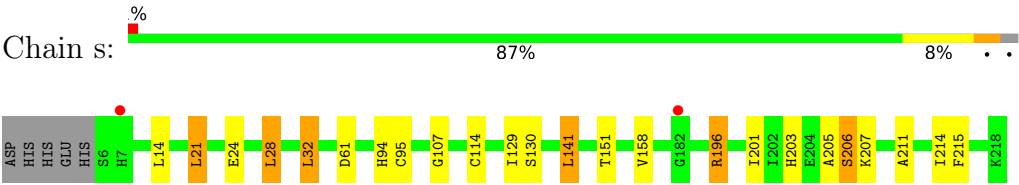
• Molecule 7: Linker L3



• Molecule 7: Linker L3



• Molecule 7: Linker L3



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	272.68Å 319.90Å 333.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.66 – 3.20 49.66 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.66-3.20) 94.1 (49.66-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.215 , 0.235 0.217 , 0.237	Depositor DCC
R_{free} test set	11885 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	59163	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.39% 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: NAG, CYN, CA, ZN, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.61	1/1231 (0.1%)	0.84	1/1665 (0.1%)
1	E	0.40	0/1231	0.79	1/1665 (0.1%)
1	I	0.44	0/1231	0.95	5/1665 (0.3%)
1	P	0.40	0/1231	0.79	1/1665 (0.1%)
1	T	0.59	0/1231	0.81	1/1665 (0.1%)
1	X	0.79	1/1231 (0.1%)	0.90	4/1665 (0.2%)
1	e	0.69	0/1231	0.88	5/1665 (0.3%)
1	i	0.77	2/1231 (0.2%)	0.90	2/1665 (0.1%)
1	m	0.45	0/1231	0.81	1/1665 (0.1%)
2	B	0.39	0/1181	0.81	1/1600 (0.1%)
2	F	0.40	0/1181	0.81	1/1600 (0.1%)
2	J	0.38	0/1181	0.79	3/1600 (0.2%)
2	Q	0.39	0/1181	0.81	1/1600 (0.1%)
2	U	0.40	0/1181	0.80	1/1600 (0.1%)
2	Y	0.38	0/1181	0.80	1/1600 (0.1%)
2	f	0.39	0/1181	0.81	1/1600 (0.1%)
2	j	0.38	0/1181	0.81	2/1600 (0.1%)
2	n	0.39	0/1181	0.80	1/1600 (0.1%)
3	C	0.34	0/1203	0.78	0/1622
3	G	0.35	0/1203	0.78	0/1622
3	K	0.34	0/1203	0.78	0/1622
3	R	0.35	0/1203	0.78	0/1622
3	V	0.34	0/1203	0.77	0/1622
3	Z	0.34	0/1203	0.78	0/1622
3	g	0.34	0/1203	0.77	0/1622
3	k	0.33	0/1203	0.78	0/1622
3	o	0.34	0/1213	0.78	0/1635
4	D	0.35	0/1172	0.74	1/1584 (0.1%)
4	H	0.36	0/1172	0.75	1/1584 (0.1%)
4	L	0.35	0/1172	0.75	1/1584 (0.1%)
4	S	0.34	0/1172	0.74	1/1584 (0.1%)
4	W	0.36	0/1172	0.75	1/1584 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	a	0.37	0/1172	0.76	1/1584 (0.1%)
4	h	0.35	0/1172	0.74	1/1584 (0.1%)
4	l	0.34	0/1172	0.75	1/1584 (0.1%)
4	p	0.35	0/1172	0.75	1/1584 (0.1%)
5	M	0.51	2/1793 (0.1%)	0.84	5/2421 (0.2%)
5	b	0.45	0/1793	0.84	4/2421 (0.2%)
5	q	0.43	0/1793	0.83	2/2421 (0.1%)
6	N	0.41	0/1748	0.80	0/2357
6	c	0.41	0/1748	0.80	0/2357
6	r	0.43	0/1748	0.80	0/2357
7	O	0.41	0/1723	0.79	0/2328
7	d	0.43	0/1723	0.79	0/2328
7	s	0.41	0/1723	0.79	0/2328
All	All	0.43	6/58885 (0.0%)	0.80	53/79570 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	O	0	1
7	d	0	1
7	s	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	210	ASN	CG-ND2	-8.46	1.15	1.33
1	X	51	PHE	CA-C	-6.75	1.45	1.53
5	M	210	ASN	CG-OD1	-6.21	1.11	1.23
1	i	52	GLU	CA-C	-5.60	1.47	1.53
1	A	148	LEU	C-O	-5.44	1.18	1.24
1	i	51	PHE	CA-C	-5.32	1.47	1.53

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	10	ARG	NE-CZ-NH2	12.96	130.87	119.20
1	I	10	ARG	NE-CZ-NH1	-12.81	108.69	121.50
1	X	52	GLU	N-CA-C	-10.13	101.24	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	10	ARG	CD-NE-CZ	9.61	137.85	124.40
2	Q	67	VAL	CB-CA-C	-7.20	102.48	111.70
2	B	67	VAL	CB-CA-C	-7.14	102.56	111.70
2	f	67	VAL	CB-CA-C	-7.02	102.72	111.70
2	j	67	VAL	CB-CA-C	-7.00	102.75	111.70
4	D	66	VAL	CB-CA-C	-6.86	102.92	111.70
2	F	67	VAL	CB-CA-C	-6.84	102.94	111.70
2	J	67	VAL	CB-CA-C	-6.77	103.03	111.70
4	p	66	VAL	CB-CA-C	-6.75	103.06	111.70
2	Y	67	VAL	CB-CA-C	-6.74	103.07	111.70
4	h	66	VAL	CB-CA-C	-6.71	103.11	111.70
4	W	66	VAL	CB-CA-C	-6.69	103.13	111.70
2	U	67	VAL	CB-CA-C	-6.68	103.15	111.70
5	q	142	LYS	CA-C-N	-6.66	114.04	120.83
5	q	142	LYS	C-N-CA	-6.66	114.04	120.83
4	l	66	VAL	CB-CA-C	-6.64	103.21	111.70
4	L	66	VAL	CB-CA-C	-6.63	103.21	111.70
5	M	142	LYS	CA-C-N	-6.57	114.12	120.83
5	M	142	LYS	C-N-CA	-6.57	114.12	120.83
2	n	67	VAL	CB-CA-C	-6.56	103.30	111.70
5	b	142	LYS	CA-C-N	-6.52	114.18	120.83
5	b	142	LYS	C-N-CA	-6.52	114.18	120.83
4	H	66	VAL	CB-CA-C	-6.51	103.36	111.70
4	S	66	VAL	CB-CA-C	-6.48	103.41	111.70
4	a	66	VAL	CB-CA-C	-6.44	103.46	111.70
1	i	71	VAL	CB-CA-C	-6.41	103.80	111.81
1	E	71	VAL	CB-CA-C	-6.40	103.81	111.81
1	m	71	VAL	CB-CA-C	-6.31	103.92	111.81
1	e	71	VAL	CB-CA-C	-6.21	104.05	111.81
1	X	71	VAL	CB-CA-C	-6.20	104.06	111.81
1	A	71	VAL	CB-CA-C	-6.16	104.11	111.81
1	P	71	VAL	CB-CA-C	-6.12	104.15	111.81
1	T	71	VAL	CB-CA-C	-6.08	104.21	111.81
1	e	56	VAL	CB-CA-C	-6.01	102.84	112.16
1	I	71	VAL	CB-CA-C	-5.95	104.37	111.81
1	X	56	VAL	CB-CA-C	-5.93	102.97	112.16
1	e	52	GLU	CB-CA-C	-5.41	99.65	110.42
1	e	56	VAL	N-CA-C	-5.32	104.40	111.05
1	I	10	ARG	CB-CG-CD	5.28	123.45	111.30
5	M	210	ASN	OD1-CG-ND2	-5.25	117.35	122.60
5	b	102	GLU	CA-C-N	5.24	123.54	120.24
5	b	102	GLU	C-N-CA	5.24	123.54	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	j	5	VAL	N-CA-C	-5.19	105.65	110.53
1	i	52	GLU	N-CA-C	-5.18	104.65	111.96
1	X	54	VAL	CB-CA-C	-5.16	105.60	112.46
5	M	102	GLU	CA-C-N	5.05	123.42	120.24
5	M	102	GLU	C-N-CA	5.05	123.42	120.24
2	J	80	GLN	CA-C-N	5.04	125.31	119.47
2	J	80	GLN	C-N-CA	5.04	125.31	119.47
1	e	54	VAL	N-CA-C	5.02	116.99	111.77

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	O	94	HIS	Peptide
7	d	94	HIS	Peptide
7	s	94	HIS	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1200	0	1155	51	0
1	E	1200	0	1155	32	0
1	I	1200	0	1155	26	0
1	P	1200	0	1155	35	1
1	T	1200	0	1155	58	0
1	X	1200	0	1153	39	0
1	e	1200	0	1150	51	0
1	i	1200	0	1155	61	1
1	m	1200	0	1155	37	0
2	B	1148	0	1103	38	0
2	F	1148	0	1103	18	0
2	J	1148	0	1103	22	0
2	Q	1148	0	1103	25	0
2	U	1148	0	1103	24	0
2	Y	1148	0	1103	26	0
2	f	1148	0	1103	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	j	1148	0	1103	21	0
2	n	1148	0	1103	23	0
3	C	1180	0	1182	14	0
3	G	1180	0	1182	20	1
3	K	1180	0	1182	18	0
3	R	1180	0	1182	19	0
3	V	1180	0	1182	21	0
3	Z	1180	0	1182	15	0
3	g	1180	0	1182	22	0
3	k	1180	0	1182	20	0
3	o	1189	0	1193	22	0
4	D	1140	0	1105	21	0
4	H	1140	0	1105	22	0
4	L	1140	0	1105	19	0
4	S	1140	0	1105	19	0
4	W	1140	0	1105	20	1
4	a	1140	0	1105	16	0
4	h	1140	0	1105	23	0
4	l	1140	0	1105	18	0
4	p	1140	0	1105	21	0
5	M	1754	0	1631	34	0
5	b	1754	0	1631	30	0
5	q	1754	0	1631	30	0
6	N	1713	0	1628	18	0
6	c	1713	0	1628	24	0
6	r	1713	0	1628	21	0
7	O	1686	0	1565	20	0
7	d	1686	0	1565	18	0
7	s	1686	0	1565	15	0
8	A	43	0	30	1	0
8	B	43	0	30	8	0
8	C	43	0	30	1	0
8	D	43	0	30	2	0
8	E	43	0	30	3	0
8	F	43	0	30	6	0
8	G	43	0	30	0	0
8	H	43	0	30	3	0
8	I	43	0	30	2	0
8	J	43	0	30	7	0
8	K	43	0	30	0	0
8	L	43	0	30	3	0
8	P	43	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	Q	43	0	30	7	0
8	R	43	0	30	2	0
8	S	43	0	30	4	0
8	T	43	0	30	2	0
8	U	43	0	30	9	0
8	V	43	0	30	0	0
8	W	43	0	30	3	0
8	X	43	0	30	4	0
8	Y	43	0	30	6	0
8	Z	43	0	30	0	0
8	a	43	0	30	2	0
8	e	43	0	30	5	0
8	f	43	0	30	6	0
8	g	43	0	30	1	0
8	h	43	0	30	4	0
8	i	43	0	30	6	0
8	j	43	0	30	6	0
8	k	43	0	30	2	0
8	l	43	0	30	2	0
8	m	43	0	30	5	0
8	n	43	0	30	6	0
8	o	43	0	30	0	0
8	p	43	0	30	1	0
9	A	2	0	0	0	0
9	B	2	0	0	1	0
9	C	2	0	0	0	0
9	D	2	0	0	0	0
9	E	2	0	0	0	0
9	F	2	0	0	1	0
9	G	2	0	0	0	0
9	H	2	0	0	0	0
9	I	2	0	0	0	0
9	J	2	0	0	0	0
9	K	2	0	0	0	0
9	L	2	0	0	0	0
9	P	2	0	0	0	0
9	Q	2	0	0	1	0
9	R	2	0	0	0	0
9	S	2	0	0	0	0
9	T	2	0	0	0	0
9	U	2	0	0	1	0
9	V	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	W	2	0	0	0	0
9	X	2	0	0	0	0
9	Y	2	0	0	0	0
9	Z	2	0	0	0	0
9	a	2	0	0	0	0
9	e	2	0	0	0	0
9	f	2	0	0	1	0
9	g	2	0	0	0	0
9	h	2	0	0	0	0
9	i	2	0	0	0	0
9	j	2	0	0	1	0
9	k	2	0	0	0	0
9	l	2	0	0	0	0
9	m	2	0	0	0	0
9	n	2	0	0	0	0
9	o	2	0	0	0	0
9	p	2	0	0	0	0
10	M	1	0	0	0	0
10	N	1	0	0	0	0
10	O	1	0	0	0	0
10	b	1	0	0	0	0
10	c	1	0	0	0	0
10	d	1	0	0	0	0
10	q	1	0	0	0	0
10	r	1	0	0	0	0
10	s	1	0	0	0	0
11	O	2	0	0	0	0
11	c	1	0	0	0	0
11	d	2	0	0	0	0
11	s	1	0	0	0	0
12	O	14	0	13	0	0
12	d	14	0	13	0	0
12	s	14	0	13	0	0
13	O	1	0	0	0	0
13	c	1	0	0	0	0
13	d	2	0	0	0	0
13	r	1	0	0	0	0
13	s	1	0	0	0	0
All	All	59163	0	56500	1017	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (1017) 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:T:55:LYS:CD	1:T:63:GLU:HG3	1.17	1.58
1:T:55:LYS:HD2	1:T:63:GLU:CG	1.09	1.52
1:T:55:LYS:NZ	1:T:63:GLU:CD	1.73	1.47
1:e:52:GLU:CG	1:e:53:ARG:N	1.71	1.35
1:T:55:LYS:NZ	1:T:63:GLU:OE2	1.67	1.20
1:T:55:LYS:HD2	1:T:63:GLU:HG2	1.18	1.18
1:T:55:LYS:CE	1:T:63:GLU:HG3	1.75	1.15
1:e:55:LYS:HG3	1:e:63:GLU:HG3	1.15	1.14
1:i:50:LEU:N	1:i:50:LEU:HD23	1.51	1.13
1:I:55:LYS:HD2	1:I:63:GLU:CG	1.79	1.12
1:T:55:LYS:HZ1	1:T:63:GLU:CD	1.45	1.12
1:m:55:LYS:HD2	1:m:63:GLU:CG	1.80	1.11
1:E:55:LYS:HD2	1:E:63:GLU:CG	1.81	1.11
1:i:52:GLU:O	1:i:55:LYS:N	1.83	1.11
1:i:53:ARG:NH2	8:i:201:HEM:O2D	1.87	1.07
1:e:52:GLU:HG2	1:e:53:ARG:N	1.62	1.07
1:i:52:GLU:O	1:i:54:VAL:N	1.87	1.07
1:X:55:LYS:HG3	1:X:63:GLU:HG3	1.28	1.06
1:T:55:LYS:CD	1:T:63:GLU:CG	1.93	1.04
1:e:52:GLU:HG3	1:e:53:ARG:CA	1.86	1.04
1:I:55:LYS:CD	1:I:63:GLU:HG3	1.88	1.02
1:E:55:LYS:CD	1:E:63:GLU:HG3	1.90	1.01
1:m:55:LYS:CD	1:m:63:GLU:HG3	1.89	1.00
1:E:55:LYS:HD2	1:E:63:GLU:HG3	0.99	0.99
1:P:55:LYS:HD2	1:P:63:GLU:HG3	1.43	0.98
1:P:55:LYS:CD	1:P:63:GLU:HG3	1.94	0.97
1:I:55:LYS:HD2	1:I:63:GLU:HG3	0.97	0.96
1:m:55:LYS:HD2	1:m:63:GLU:HG3	0.98	0.96
1:X:150:HIS:CD2	1:X:150:HIS:H	1.71	0.94
1:e:52:GLU:HG3	1:e:53:ARG:N	1.23	0.94
1:X:51:PHE:HB2	1:X:56:VAL:CG2	1.99	0.93
1:T:55:LYS:HZ2	1:T:63:GLU:CD	1.52	0.92
1:X:150:HIS:H	1:X:150:HIS:HD2	1.11	0.92
1:i:150:HIS:CD2	1:i:150:HIS:H	1.86	0.92
1:T:55:LYS:CE	1:T:63:GLU:CD	2.44	0.90
1:A:54:VAL:O	1:A:55:LYS:HB2	1.73	0.87
1:T:55:LYS:CE	1:T:63:GLU:CG	2.42	0.87
1:A:12:GLU:OE1	5:M:210:ASN:ND2	2.07	0.87
2:B:48:LYS:NZ	2:f:48:LYS:NZ	2.22	0.86
1:A:55:LYS:C	1:A:57:ALA:H	1.81	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:55:LYS:CG	1:e:63:GLU:HG3	2.04	0.86
1:i:61:SER:HB2	1:i:63:GLU:HG2	1.57	0.86
1:X:51:PHE:HB2	1:X:56:VAL:HG22	1.57	0.85
2:B:48:LYS:HZ1	2:f:48:LYS:HZ1	1.25	0.84
1:A:51:PHE:O	1:A:56:VAL:CG2	2.24	0.84
1:e:55:LYS:HG3	1:e:63:GLU:CG	2.03	0.83
1:i:150:HIS:H	1:i:150:HIS:HD2	1.27	0.83
5:q:72:ASP:OD1	7:s:196:ARG:NH1	2.12	0.83
1:A:55:LYS:HG3	1:A:63:GLU:HG3	1.60	0.83
1:i:52:GLU:C	1:i:54:VAL:N	2.34	0.82
1:i:61:SER:O	1:i:63:GLU:N	2.13	0.82
1:X:150:HIS:CD2	1:X:150:HIS:N	2.47	0.81
2:F:140:ILE:HD12	8:F:201:HEM:HBB2	1.61	0.81
1:m:12:GLU:OE1	7:s:206:SER:OG	1.98	0.80
1:T:51:PHE:O	1:T:56:VAL:CG2	2.29	0.80
5:q:79:ASP:HB3	5:q:144:ARG:HH22	1.47	0.79
5:M:72:ASP:OD1	7:O:196:ARG:NH1	2.16	0.79
1:i:52:GLU:C	1:i:54:VAL:H	1.90	0.79
1:P:8:GLU:OE2	3:V:6:SER:OG	2.01	0.78
1:i:61:SER:O	1:i:62:GLY:C	2.23	0.78
1:A:51:PHE:HB2	1:A:56:VAL:HG21	1.65	0.77
5:b:79:ASP:HB3	5:b:144:ARG:HH22	1.48	0.77
1:X:12:GLU:OE1	7:d:206:SER:OG	2.00	0.77
1:A:51:PHE:O	1:A:56:VAL:HG23	1.84	0.77
2:Q:24:ASN:ND2	2:Q:119:GLN:OE1	2.18	0.76
1:A:55:LYS:C	1:A:57:ALA:N	2.38	0.76
2:f:24:ASN:ND2	2:f:119:GLN:OE1	2.19	0.76
6:r:151:ARG:HG3	6:r:151:ARG:HH11	1.50	0.76
2:B:48:LYS:NZ	2:f:48:LYS:HZ1	1.82	0.75
1:T:55:LYS:CG	1:T:63:GLU:HG3	2.14	0.75
5:M:79:ASP:HB3	5:M:144:ARG:HH22	1.48	0.75
6:c:151:ARG:HH11	6:c:151:ARG:HG3	1.52	0.75
6:N:151:ARG:HG3	6:N:151:ARG:HH11	1.51	0.75
2:U:140:ILE:HD12	8:U:201:HEM:HBB2	1.69	0.74
5:b:72:ASP:OD1	7:d:196:ARG:NH1	2.20	0.74
1:A:54:VAL:O	1:A:55:LYS:CB	2.30	0.73
1:i:52:GLU:O	1:i:53:ARG:C	2.29	0.73
1:i:150:HIS:CD2	1:i:150:HIS:N	2.57	0.73
2:j:140:ILE:HD12	8:j:201:HEM:HBB2	1.69	0.73
2:U:24:ASN:ND2	2:U:119:GLN:OE1	2.21	0.73
2:B:24:ASN:ND2	2:B:119:GLN:OE1	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:61:SER:HB2	1:e:63:GLU:HG2	1.71	0.72
2:f:140:ILE:HD12	8:f:201:HEM:HBB2	1.69	0.72
3:Z:86:PRO:HG3	6:c:129:LEU:HD13	1.72	0.72
1:i:53:ARG:HH21	8:i:201:HEM:CGD	2.02	0.72
2:Y:24:ASN:ND2	2:Y:119:GLN:OE1	2.22	0.72
2:j:24:ASN:ND2	2:j:119:GLN:OE1	2.22	0.72
2:n:24:ASN:ND2	2:n:119:GLN:OE1	2.21	0.72
2:J:24:ASN:ND2	2:J:119:GLN:OE1	2.23	0.71
2:J:122:ARG:HD3	7:O:207:LYS:HZ3	1.55	0.71
2:F:24:ASN:ND2	2:F:119:GLN:OE1	2.23	0.71
1:I:12:GLU:OE1	7:O:206:SER:OG	2.08	0.71
1:i:49:GLY:C	1:i:50:LEU:HD23	2.13	0.71
1:m:69:VAL:HG12	4:p:72:MET:HE3	1.72	0.71
7:O:201:ILE:HB	7:O:211:ALA:HB3	1.74	0.70
2:B:48:LYS:HZ1	2:f:48:LYS:NZ	1.83	0.70
2:J:122:ARG:HD3	7:O:207:LYS:NZ	2.07	0.70
1:X:51:PHE:HB2	1:X:56:VAL:HG21	1.73	0.70
2:B:140:ILE:HD12	8:B:201:HEM:HBB2	1.72	0.70
1:E:90:LYS:HZ3	4:H:58:GLU:HG3	1.56	0.70
1:I:69:VAL:HG12	4:L:72:MET:HE3	1.74	0.70
7:d:201:ILE:HB	7:d:211:ALA:HB3	1.74	0.70
1:A:51:PHE:HB2	1:A:56:VAL:CG2	2.23	0.69
1:E:69:VAL:HG12	4:H:72:MET:HE3	1.74	0.69
7:s:201:ILE:HB	7:s:211:ALA:HB3	1.75	0.69
4:p:108:LEU:HD21	4:p:129:THR:HG22	1.75	0.68
2:Y:122:ARG:HD3	7:d:207:LYS:NZ	2.08	0.68
4:D:108:LEU:HD21	4:D:129:THR:HG22	1.76	0.68
4:H:108:LEU:HD21	4:H:129:THR:HG22	1.75	0.68
1:A:69:VAL:HG12	4:D:72:MET:HE3	1.77	0.67
1:P:55:LYS:CG	1:P:63:GLU:HG3	2.23	0.67
3:K:86:PRO:HG3	6:N:129:LEU:HD13	1.77	0.67
1:P:11:ARG:NH1	3:V:8:GLU:HG3	2.10	0.67
1:i:8:GLU:CD	3:o:8:GLU:HB2	2.19	0.67
2:Y:49:ARG:NH1	8:Y:201:HEM:O1D	2.28	0.67
4:l:108:LEU:HD21	4:l:129:THR:HG22	1.77	0.67
4:W:108:LEU:HD21	4:W:129:THR:HG22	1.77	0.67
1:T:55:LYS:NZ	1:T:63:GLU:CG	2.57	0.67
2:Q:51:HIS:CG	2:Q:59:GLU:HG3	2.30	0.66
2:Y:140:ILE:HD12	8:Y:201:HEM:HBB2	1.78	0.66
1:e:51:PHE:HB2	1:e:56:VAL:CG2	2.26	0.66
3:o:86:PRO:HG3	6:r:129:LEU:HD13	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:HIS:CG	2:B:59:GLU:HG3	2.31	0.66
4:S:108:LEU:HD21	4:S:129:THR:HG22	1.78	0.66
4:a:108:LEU:HD21	4:a:129:THR:HG22	1.78	0.66
1:e:6:SER:HB3	3:k:3:PHE:HA	1.78	0.65
4:h:108:LEU:HD21	4:h:129:THR:HG22	1.78	0.65
1:T:54:VAL:HG23	1:T:54:VAL:O	1.95	0.65
1:m:149:PRO:C	1:m:150:HIS:O	2.31	0.65
2:n:51:HIS:CG	2:n:59:GLU:HG3	2.31	0.65
2:f:51:HIS:CG	2:f:59:GLU:HG3	2.31	0.65
1:i:69:VAL:HG12	4:l:72:MET:HE3	1.77	0.65
3:G:22:GLY:HA3	4:H:15:ARG:NH1	2.12	0.65
1:I:90:LYS:HZ3	4:L:58:GLU:HG3	1.61	0.65
4:L:108:LEU:HD21	4:L:129:THR:HG22	1.78	0.65
2:F:51:HIS:CG	2:F:59:GLU:HG3	2.31	0.65
1:T:51:PHE:O	1:T:56:VAL:HG23	1.97	0.65
1:A:55:LYS:O	1:A:57:ALA:N	2.29	0.64
1:T:42:HIS:CE1	1:m:106:THR:HG21	2.32	0.64
1:T:51:PHE:HB2	1:T:56:VAL:HG21	1.79	0.64
1:T:52:GLU:O	1:T:54:VAL:N	2.30	0.64
1:e:51:PHE:CB	1:e:56:VAL:HG22	2.27	0.64
2:j:51:HIS:CG	2:j:59:GLU:HG3	2.32	0.64
2:n:95:HIS:HE1	8:n:201:HEM:NA	1.92	0.64
2:J:51:HIS:CG	2:J:59:GLU:HG3	2.33	0.64
1:T:8:GLU:CD	3:Z:8:GLU:HB2	2.23	0.64
1:X:51:PHE:CB	1:X:56:VAL:HG22	2.28	0.64
2:U:51:HIS:CG	2:U:59:GLU:HG3	2.32	0.64
1:e:52:GLU:HG3	1:e:53:ARG:HA	1.79	0.63
2:n:140:ILE:HD12	8:n:201:HEM:HBB2	1.80	0.63
6:N:151:ARG:HG3	6:N:151:ARG:NH1	2.11	0.63
6:N:232:LEU:O	6:N:234:GLY:N	2.32	0.63
2:U:100:ILE:HG23	8:U:201:HEM:HAC	1.79	0.63
2:Y:51:HIS:CG	2:Y:59:GLU:HG3	2.32	0.63
6:c:151:ARG:HG3	6:c:151:ARG:NH1	2.12	0.63
1:e:69:VAL:HG12	4:h:72:MET:HE3	1.80	0.63
1:X:69:VAL:HG12	4:a:72:MET:HE3	1.81	0.63
1:E:149:PRO:O	1:E:150:HIS:C	2.40	0.62
4:l:83:PHE:O	4:l:87:VAL:HG23	1.99	0.62
1:P:11:ARG:HH12	3:V:8:GLU:HG3	1.65	0.62
4:p:83:PHE:O	4:p:87:VAL:HG23	1.99	0.62
6:c:232:LEU:O	6:c:234:GLY:N	2.31	0.62
2:n:49:ARG:NH1	8:n:201:HEM:O1D	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:51:PHE:CB	1:e:56:VAL:CG2	2.77	0.62
1:e:52:GLU:CG	1:e:53:ARG:CA	2.62	0.62
1:E:90:LYS:NZ	4:H:58:GLU:HG3	2.13	0.62
1:e:51:PHE:HB2	1:e:56:VAL:HG21	1.82	0.62
2:n:122:ARG:HD3	7:s:207:LYS:NZ	2.14	0.62
2:B:95:HIS:HE1	8:B:201:HEM:NA	1.97	0.62
4:W:83:PHE:O	4:W:87:VAL:HG23	2.00	0.62
4:a:83:PHE:O	4:a:87:VAL:HG23	2.00	0.62
5:b:198:ARG:HD2	6:c:79:TYR:CZ	2.36	0.61
1:E:8:GLU:CD	3:K:8:GLU:HB2	2.26	0.61
1:A:12:GLU:CD	5:M:210:ASN:ND2	2.59	0.61
1:A:51:PHE:C	1:A:56:VAL:CG2	2.73	0.61
1:E:145:SER:O	1:E:148:LEU:HB2	2.00	0.61
1:I:90:LYS:NZ	4:L:58:GLU:HG3	2.15	0.61
1:i:54:VAL:O	1:i:55:LYS:HB2	2.01	0.61
1:P:55:LYS:HG3	1:P:63:GLU:HG3	1.82	0.61
8:Q:201:HEM:C1D	9:Q:202:CYN:N	2.54	0.60
1:T:7:ALA:HB3	3:Z:8:GLU:HB3	1.82	0.60
6:r:232:LEU:O	6:r:234:GLY:N	2.33	0.60
2:j:21:HIS:O	2:j:23:HIS:N	2.33	0.60
1:A:6:SER:HB3	3:G:3:PHE:HA	1.82	0.60
1:m:90:LYS:HZ3	4:p:58:GLU:HG3	1.67	0.60
2:J:21:HIS:O	2:J:23:HIS:N	2.33	0.60
1:P:6:SER:HB3	3:V:3:PHE:HA	1.83	0.60
2:f:23:HIS:HD2	5:q:63:LYS:HG2	1.66	0.60
6:r:151:ARG:HG3	6:r:151:ARG:NH1	2.11	0.60
1:i:51:PHE:CB	1:i:56:VAL:HG22	2.32	0.60
1:e:52:GLU:O	1:e:55:LYS:N	2.28	0.60
2:f:100:ILE:HG23	8:f:201:HEM:HAC	1.83	0.59
1:P:69:VAL:HG12	4:S:72:MET:HE3	1.83	0.59
1:m:53:ARG:NH2	8:m:201:HEM:O2D	2.35	0.59
1:T:69:VAL:HG12	4:W:72:MET:HE3	1.83	0.59
2:U:21:HIS:O	2:U:23:HIS:N	2.34	0.59
8:X:201:HEM:HBD1	8:X:201:HEM:HHA	1.83	0.59
5:b:198:ARG:HG3	5:b:203:HIS:HB2	1.84	0.59
4:D:83:PHE:O	4:D:87:VAL:HG23	2.02	0.59
4:h:83:PHE:O	4:h:87:VAL:HG23	2.03	0.59
1:i:90:LYS:HZ3	4:l:58:GLU:HG3	1.67	0.59
2:J:100:ILE:HG23	8:J:201:HEM:HAC	1.83	0.59
4:L:83:PHE:O	4:L:87:VAL:HG23	2.02	0.59
5:M:198:ARG:HG3	5:M:203:HIS:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:21:HIS:O	2:n:23:HIS:N	2.33	0.59
4:H:83:PHE:O	4:H:87:VAL:HG23	2.02	0.59
1:e:8:GLU:OE2	3:k:6:SER:OG	2.16	0.59
5:q:63:LYS:HE3	5:q:64:GLU:H	1.67	0.59
2:Q:21:HIS:O	2:Q:23:HIS:N	2.34	0.59
7:s:129:ILE:HG12	7:s:141:LEU:HD22	1.85	0.59
1:A:90:LYS:NZ	4:D:58:GLU:HG3	2.17	0.58
5:M:63:LYS:HE3	5:M:64:GLU:H	1.68	0.58
1:i:55:LYS:HG2	1:i:63:GLU:HG3	1.86	0.58
1:A:51:PHE:CB	1:A:56:VAL:CG2	2.81	0.58
2:n:100:ILE:HG23	8:n:201:HEM:HAC	1.86	0.58
5:q:198:ARG:HG3	5:q:203:HIS:HB2	1.84	0.58
1:i:52:GLU:HA	1:i:56:VAL:HG23	1.84	0.58
4:S:83:PHE:O	4:S:87:VAL:HG23	2.03	0.58
7:d:129:ILE:HG12	7:d:141:LEU:HD22	1.86	0.58
2:f:21:HIS:O	2:f:23:HIS:N	2.34	0.58
2:B:48:LYS:HZ2	2:f:48:LYS:NZ	2.02	0.57
2:Q:100:ILE:HG23	8:Q:201:HEM:HAC	1.84	0.57
2:Q:140:ILE:HD12	8:Q:201:HEM:HBB2	1.85	0.57
6:N:188:LEU:HB2	6:N:200:VAL:HG13	1.86	0.57
2:Y:21:HIS:O	2:Y:23:HIS:N	2.34	0.57
2:B:100:ILE:HG23	8:B:201:HEM:HAC	1.87	0.57
4:H:97:ARG:CZ	8:H:201:HEM:HAD2	2.35	0.57
5:b:63:LYS:HE3	5:b:64:GLU:H	1.67	0.57
1:m:90:LYS:NZ	4:p:58:GLU:HG3	2.20	0.57
2:Y:95:HIS:HE1	8:Y:201:HEM:C4A	2.21	0.57
2:j:95:HIS:HE1	8:j:201:HEM:NA	1.99	0.57
4:D:31:LEU:HA	4:D:114:VAL:HG21	1.87	0.57
2:J:140:ILE:HD12	8:J:201:HEM:HBB2	1.87	0.57
1:P:53:ARG:NH2	8:P:201:HEM:O2D	2.38	0.57
2:U:95:HIS:HE1	8:U:201:HEM:NA	1.96	0.57
2:n:95:HIS:HE1	8:n:201:HEM:C4A	2.23	0.57
2:F:21:HIS:O	2:F:23:HIS:N	2.33	0.56
5:M:168:ARG:NH1	5:M:184:ARG:HG3	2.20	0.56
1:T:43:HIS:HD2	1:m:46:SER:OG	1.88	0.56
1:T:107:GLN:OE1	1:T:150:HIS:ND1	2.37	0.56
1:e:47:ALA:HB1	8:e:201:HEM:HBC1	1.87	0.56
4:L:31:LEU:HA	4:L:114:VAL:HG21	1.88	0.56
1:T:42:HIS:HE1	1:m:106:THR:HG21	1.70	0.56
2:Q:23:HIS:CD2	5:b:63:LYS:HE2	2.40	0.56
2:n:50:VAL:HG21	2:n:63:HIS:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:36:LEU:HD22	4:D:5:LEU:HD21	1.87	0.56
2:B:23:HIS:HD2	5:M:63:LYS:HG2	1.70	0.56
7:O:129:ILE:HG12	7:O:141:LEU:HD22	1.87	0.56
1:A:21:TRP:CD1	1:A:22:SER:H	2.24	0.56
1:P:21:TRP:CD1	1:P:22:SER:H	2.24	0.56
1:T:21:TRP:CD1	1:T:22:SER:H	2.24	0.56
5:b:168:ARG:NH1	5:b:184:ARG:HG3	2.21	0.56
1:i:61:SER:C	1:i:63:GLU:N	2.61	0.56
4:h:31:LEU:HA	4:h:114:VAL:HG21	1.88	0.56
5:q:168:ARG:NH1	5:q:184:ARG:HG3	2.21	0.56
1:E:21:TRP:CD1	1:E:22:SER:H	2.24	0.55
6:c:188:LEU:HB2	6:c:200:VAL:HG13	1.88	0.55
4:l:31:LEU:HA	4:l:114:VAL:HG21	1.87	0.55
8:k:201:HEM:HBD2	8:k:201:HEM:HHA	1.88	0.55
2:Y:95:HIS:HE1	8:Y:201:HEM:NA	1.94	0.55
1:i:59:PRO:C	1:i:60:ASP:OD1	2.49	0.55
2:j:100:ILE:HG23	8:j:201:HEM:HAC	1.88	0.55
1:A:90:LYS:HZ3	4:D:58:GLU:HG3	1.70	0.55
2:U:63:HIS:O	2:U:67:VAL:HG23	2.07	0.55
4:W:31:LEU:HA	4:W:114:VAL:HG21	1.88	0.55
6:r:188:LEU:HB2	6:r:200:VAL:HG13	1.88	0.55
2:Q:95:HIS:HE1	8:Q:201:HEM:NA	2.01	0.55
8:f:201:HEM:C1D	9:f:202:CYN:N	2.75	0.55
2:j:95:HIS:HE1	8:j:201:HEM:C4A	2.24	0.55
1:I:21:TRP:CD1	1:I:22:SER:H	2.25	0.55
1:T:52:GLU:O	1:T:53:ARG:C	2.47	0.55
1:e:90:LYS:NZ	4:h:58:GLU:HG3	2.21	0.55
2:f:95:HIS:HE1	8:f:201:HEM:NA	2.01	0.55
2:U:50:VAL:HG21	2:U:63:HIS:HB2	1.89	0.55
1:m:21:TRP:CD1	1:m:22:SER:H	2.24	0.55
1:A:55:LYS:CG	1:A:63:GLU:HG3	2.34	0.55
1:T:55:LYS:HE3	1:T:63:GLU:HG3	1.83	0.55
4:a:31:LEU:HA	4:a:114:VAL:HG21	1.88	0.55
1:X:21:TRP:CD1	1:X:22:SER:H	2.25	0.54
4:a:62:HIS:O	4:a:66:VAL:HG23	2.06	0.54
2:f:50:VAL:HG21	2:f:63:HIS:HB2	1.90	0.54
8:B:201:HEM:C1D	9:B:202:CYN:N	2.76	0.54
4:H:31:LEU:HA	4:H:114:VAL:HG21	1.89	0.54
1:e:21:TRP:CD1	1:e:22:SER:H	2.24	0.54
2:J:95:HIS:HE1	8:J:201:HEM:C4A	2.25	0.54
5:M:198:ARG:HD2	6:N:79:TYR:CZ	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:ARG:NH1	8:B:201:HEM:O1D	2.41	0.54
1:i:21:TRP:CD1	1:i:22:SER:H	2.24	0.54
1:i:51:PHE:HB2	1:i:56:VAL:CG2	2.38	0.54
2:Y:63:HIS:O	2:Y:67:VAL:HG23	2.08	0.54
2:F:63:HIS:O	2:F:67:VAL:HG23	2.08	0.54
1:X:145:SER:O	1:X:148:LEU:HB2	2.08	0.54
2:n:63:HIS:O	2:n:67:VAL:HG23	2.07	0.54
2:J:50:VAL:HG21	2:J:63:HIS:HB2	1.90	0.54
1:T:90:LYS:HZ3	4:W:58:GLU:HG3	1.72	0.54
2:n:122:ARG:HD3	7:s:207:LYS:HZ3	1.70	0.54
4:p:31:LEU:HA	4:p:114:VAL:HG21	1.90	0.54
5:q:198:ARG:HD2	6:r:79:TYR:CZ	2.43	0.54
2:F:100:ILE:HG23	8:F:201:HEM:HAC	1.90	0.54
1:T:39:ASP:OD1	1:T:116:SER:HB3	2.08	0.54
2:Y:50:VAL:HG21	2:Y:63:HIS:HB2	1.90	0.54
5:b:195:HIS:CE1	5:b:197:ASP:HB3	2.43	0.54
1:X:150:HIS:HD2	1:X:150:HIS:N	1.93	0.53
6:c:77:GLY:H	6:c:80:ASP:HB3	1.73	0.53
5:q:195:HIS:CE1	5:q:197:ASP:HB3	2.44	0.53
1:A:54:VAL:C	1:A:55:LYS:CG	2.75	0.53
2:J:63:HIS:O	2:J:67:VAL:HG23	2.08	0.53
2:Q:50:VAL:HG21	2:Q:63:HIS:HB2	1.90	0.53
6:N:31:LEU:HD23	7:O:21:LEU:HD13	1.90	0.53
2:Q:63:HIS:O	2:Q:67:VAL:HG23	2.09	0.53
2:f:63:HIS:O	2:f:67:VAL:HG23	2.08	0.53
3:o:22:GLY:HA3	4:p:15:ARG:NH1	2.24	0.53
5:M:195:HIS:CE1	5:M:197:ASP:HB3	2.44	0.53
4:S:31:LEU:HA	4:S:114:VAL:HG21	1.89	0.53
4:S:97:ARG:CZ	8:S:201:HEM:HAD2	2.38	0.53
2:B:63:HIS:O	2:B:67:VAL:HG23	2.08	0.53
1:i:51:PHE:CB	1:i:56:VAL:CG2	2.85	0.53
1:e:25:PHE:CE2	3:g:28:LYS:HG2	2.44	0.53
2:B:21:HIS:O	2:B:23:HIS:N	2.34	0.53
1:E:137:PHE:CZ	8:E:201:HEM:HBB1	2.43	0.53
1:X:47:ALA:O	1:X:50:LEU:HD12	2.08	0.53
1:X:149:PRO:O	1:X:150:HIS:C	2.50	0.53
1:i:90:LYS:NZ	4:l:58:GLU:HG3	2.23	0.53
2:F:95:HIS:HE1	8:F:201:HEM:NA	2.00	0.53
1:T:51:PHE:O	1:T:56:VAL:HG22	2.08	0.53
2:U:102:ASP:OD1	3:g:108:LYS:NZ	2.42	0.53
2:j:63:HIS:O	2:j:67:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:72:ASP:OD2	7:d:216:HIS:NE2	2.37	0.52
2:Y:76:SER:HB3	3:Z:27:SER:HB3	1.91	0.52
2:j:50:VAL:HG21	2:j:63:HIS:HB2	1.91	0.52
6:r:77:GLY:H	6:r:80:ASP:HB3	1.74	0.52
2:B:50:VAL:HG21	2:B:63:HIS:HB2	1.91	0.52
6:r:31:LEU:HD23	7:s:21:LEU:HD13	1.90	0.52
1:A:51:PHE:CB	1:A:56:VAL:HG22	2.40	0.52
1:X:54:VAL:O	1:X:54:VAL:HG23	2.09	0.52
6:N:77:GLY:H	6:N:80:ASP:HB3	1.74	0.52
2:Y:122:ARG:HD3	7:d:207:LYS:HZ3	1.71	0.52
3:R:36:LEU:HD22	4:S:5:LEU:HD21	1.91	0.52
6:c:126:ASP:O	6:c:128:LEU:N	2.43	0.52
2:F:50:VAL:HG21	2:F:63:HIS:HB2	1.91	0.52
1:I:39:ASP:OD1	1:I:116:SER:HB3	2.10	0.52
1:T:52:GLU:C	1:T:54:VAL:N	2.66	0.52
4:h:108:LEU:HB2	4:h:132:PHE:CE2	2.45	0.52
2:B:48:LYS:HZ2	2:f:48:LYS:HZ2	1.55	0.52
2:J:95:HIS:HE1	8:J:201:HEM:NA	2.00	0.52
6:c:31:LEU:HD23	7:d:21:LEU:HD13	1.92	0.52
2:f:95:HIS:HE1	8:f:201:HEM:C4A	2.28	0.52
1:m:39:ASP:OD1	1:m:116:SER:HB3	2.10	0.52
5:M:111:PHE:HB3	5:M:222:ALA:HB1	1.92	0.51
1:X:51:PHE:CB	1:X:56:VAL:CG2	2.76	0.51
3:g:31:ILE:HD13	3:g:66:SER:HB3	1.91	0.51
4:D:97:ARG:CZ	8:D:201:HEM:HAD2	2.40	0.51
2:Q:49:ARG:NH1	8:Q:201:HEM:O1D	2.42	0.51
1:i:7:ALA:HB3	3:o:8:GLU:HB3	1.93	0.51
5:M:87:LYS:HE3	5:M:92:GLY:HA3	1.92	0.51
1:X:51:PHE:HZ	8:X:201:HEM:HBC2	1.76	0.51
1:A:145:SER:O	1:A:148:LEU:HB2	2.09	0.51
2:Q:23:HIS:HD2	5:b:63:LYS:HG2	1.74	0.51
1:T:118:ALA:HB1	1:T:130:LEU:HD21	1.93	0.51
3:g:114:ILE:O	3:g:118:LEU:HB2	2.10	0.51
5:M:160:HIS:HA	5:b:148:ARG:HH21	1.75	0.51
6:N:177:GLY:HA3	6:N:187:VAL:O	2.10	0.51
1:X:145:SER:HA	1:X:148:LEU:HD12	1.92	0.51
5:b:50:LEU:HD21	6:c:57:LEU:HB3	1.92	0.51
1:e:11:ARG:NH1	3:k:8:GLU:HG3	2.25	0.51
2:Q:95:HIS:HE1	8:Q:201:HEM:C4A	2.27	0.51
4:S:108:LEU:HB2	4:S:132:PHE:CE2	2.46	0.51
2:U:28:PHE:CD1	2:U:119:GLN:HG3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:HIS:CD2	5:M:63:LYS:HE2	2.45	0.51
4:D:108:LEU:HB2	4:D:132:PHE:CE2	2.45	0.51
6:c:177:GLY:HA3	6:c:187:VAL:O	2.11	0.51
3:o:31:ILE:HD13	3:o:66:SER:HB3	1.92	0.51
1:T:67:HIS:O	1:T:71:VAL:HG23	2.11	0.51
5:b:87:LYS:HE3	5:b:92:GLY:HA3	1.92	0.51
5:q:87:LYS:HE3	5:q:92:GLY:HA3	1.92	0.51
3:R:31:ILE:HD13	3:R:66:SER:HB3	1.93	0.51
3:V:8:GLU:O	3:V:12:ILE:HG12	2.12	0.51
3:V:31:ILE:HD13	3:V:66:SER:HB3	1.92	0.51
1:e:58:GLU:O	1:e:61:SER:OG	2.29	0.51
1:E:118:ALA:HB1	1:E:130:LEU:HD21	1.93	0.50
4:W:108:LEU:HB2	4:W:132:PHE:CE2	2.47	0.50
4:p:62:HIS:O	4:p:66:VAL:HG23	2.11	0.50
5:q:111:PHE:HB3	5:q:222:ALA:HB1	1.93	0.50
1:A:8:GLU:OE2	3:G:6:SER:OG	2.22	0.50
3:R:127:ASP:OD2	4:S:121:THR:HG21	2.12	0.50
6:r:177:GLY:HA3	6:r:187:VAL:O	2.11	0.50
3:C:114:ILE:O	3:C:118:LEU:HB2	2.11	0.50
1:E:95:LEU:HD21	8:E:201:HEM:HMB2	1.93	0.50
2:F:95:HIS:HE1	8:F:201:HEM:C4A	2.29	0.50
3:G:114:ILE:O	3:G:118:LEU:HB2	2.11	0.50
4:H:108:LEU:HB2	4:H:132:PHE:CE2	2.46	0.50
1:P:39:ASP:OD1	1:P:116:SER:HB3	2.11	0.50
4:W:42:VAL:HG13	8:W:201:HEM:HBC1	1.93	0.50
3:Z:114:ILE:O	3:Z:118:LEU:HB2	2.11	0.50
5:b:111:PHE:HB3	5:b:222:ALA:HB1	1.94	0.50
6:r:38:LEU:HD23	7:s:28:LEU:HD13	1.92	0.50
1:A:25:PHE:CE2	3:C:28:LYS:HG2	2.47	0.50
1:X:39:ASP:OD1	1:X:116:SER:HB3	2.11	0.50
1:i:59:PRO:O	1:i:60:ASP:OD1	2.30	0.50
1:A:57:ALA:C	1:A:58:GLU:HG3	2.36	0.50
5:M:198:ARG:HH21	5:M:205:ASP:HB2	1.76	0.50
3:R:114:ILE:O	3:R:118:LEU:HB2	2.11	0.50
1:T:95:LEU:HD21	8:T:201:HEM:HMB2	1.92	0.50
1:i:55:LYS:O	1:i:58:GLU:O	2.29	0.50
1:A:51:PHE:O	1:A:56:VAL:HG22	2.10	0.50
4:S:42:VAL:HG13	8:S:201:HEM:HBC1	1.94	0.50
3:V:114:ILE:O	3:V:118:LEU:HB2	2.12	0.50
1:X:149:PRO:O	1:X:150:HIS:O	2.30	0.50
2:B:28:PHE:CD1	2:B:119:GLN:HG3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:l:108:LEU:HB2	4:l:132:PHE:CE2	2.47	0.50
2:n:77:THR:O	2:n:84:LEU:HB2	2.12	0.50
3:o:114:ILE:O	3:o:118:LEU:HB2	2.12	0.50
5:q:198:ARG:HH21	5:q:205:ASP:HB2	1.76	0.50
4:H:100:ASN:OD1	4:H:102:GLU:HG2	2.12	0.50
2:B:48:LYS:NZ	2:f:48:LYS:HZ2	2.03	0.49
1:E:67:HIS:O	1:E:71:VAL:HG23	2.12	0.49
1:i:61:SER:O	1:i:64:TYR:N	2.45	0.49
3:k:8:GLU:O	3:k:12:ILE:HG12	2.12	0.49
2:F:28:PHE:CD1	2:F:119:GLN:HG3	2.47	0.49
4:H:62:HIS:O	4:H:66:VAL:HG23	2.12	0.49
2:J:49:ARG:NH1	8:J:201:HEM:O1D	2.45	0.49
3:Z:31:ILE:HD13	3:Z:66:SER:HB3	1.94	0.49
7:s:107:GLY:HA2	7:s:215:PHE:HA	1.94	0.49
5:M:72:ASP:OD2	7:O:216:HIS:NE2	2.40	0.49
1:i:51:PHE:HB2	1:i:56:VAL:HG21	1.93	0.49
1:m:149:PRO:O	1:m:150:HIS:O	2.29	0.49
1:I:67:HIS:O	1:I:71:VAL:HG23	2.12	0.49
8:R:201:HEM:HBD2	8:R:201:HEM:HHA	1.93	0.49
3:K:114:ILE:O	3:K:118:LEU:HB2	2.11	0.49
1:T:55:LYS:CD	1:T:63:GLU:HG2	2.04	0.49
6:c:118:PHE:HB3	6:c:230:VAL:HB	1.95	0.49
1:i:67:HIS:O	1:i:71:VAL:HG23	2.12	0.49
3:R:33:PHE:CE2	3:R:37:ILE:HD11	2.48	0.49
2:f:23:HIS:CD2	5:q:63:LYS:HE2	2.47	0.49
1:A:149:PRO:O	1:A:150:HIS:O	2.30	0.49
1:E:149:PRO:O	1:E:150:HIS:O	2.29	0.49
3:k:114:ILE:O	3:k:118:LEU:HB2	2.12	0.49
1:T:137:PHE:CZ	8:T:201:HEM:HBB1	2.47	0.49
4:W:62:HIS:O	4:W:66:VAL:HG23	2.13	0.49
1:e:96:ALA:O	1:e:100:ILE:HG13	2.13	0.49
3:g:36:LEU:HD22	4:h:5:LEU:HD21	1.94	0.49
4:h:42:VAL:HG13	8:h:201:HEM:HBC1	1.94	0.49
5:b:198:ARG:HH21	5:b:205:ASP:HB2	1.78	0.49
1:i:149:PRO:O	1:i:150:HIS:O	2.30	0.49
1:A:55:LYS:O	1:A:56:VAL:C	2.56	0.49
1:T:90:LYS:NZ	4:W:58:GLU:HG3	2.26	0.49
2:U:95:HIS:HE1	8:U:201:HEM:C4A	2.30	0.49
2:j:49:ARG:NH1	8:j:201:HEM:O1D	2.46	0.49
3:k:31:ILE:HD13	3:k:66:SER:HB3	1.94	0.49
3:k:33:PHE:CE2	3:k:37:ILE:HD11	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:p:108:LEU:HB2	4:p:132:PHE:CE2	2.47	0.49
5:q:134:ALA:HB3	5:q:148:ARG:HB2	1.94	0.49
1:A:39:ASP:OD1	1:A:116:SER:HB3	2.13	0.48
3:C:31:ILE:HD13	3:C:66:SER:HB3	1.94	0.48
3:G:31:ILE:HD13	3:G:66:SER:HB3	1.94	0.48
1:P:118:ALA:HB1	1:P:130:LEU:HD21	1.95	0.48
4:S:62:HIS:O	4:S:66:VAL:HG23	2.13	0.48
2:n:28:PHE:CD1	2:n:119:GLN:HG3	2.48	0.48
6:r:118:PHE:HB3	6:r:230:VAL:HB	1.95	0.48
1:I:107:GLN:CD	1:I:150:HIS:HD1	2.20	0.48
2:Y:100:ILE:HG23	8:Y:201:HEM:HAC	1.94	0.48
4:l:62:HIS:O	4:l:66:VAL:HG23	2.13	0.48
3:K:31:ILE:HD13	3:K:66:SER:HB3	1.95	0.48
2:Y:122:ARG:HD3	7:d:207:LYS:HZ2	1.78	0.48
4:a:108:LEU:HB2	4:a:132:PHE:CE2	2.47	0.48
1:e:67:HIS:O	1:e:71:VAL:HG23	2.14	0.48
5:M:134:ALA:HB3	5:M:148:ARG:HB2	1.95	0.48
7:O:107:GLY:HA2	7:O:215:PHE:HA	1.94	0.48
1:P:67:HIS:O	1:P:71:VAL:HG23	2.13	0.48
2:Y:77:THR:O	2:Y:84:LEU:HB2	2.14	0.48
1:e:53:ARG:HE	1:e:53:ARG:HB3	1.44	0.48
4:h:94:HIS:HE1	8:h:201:HEM:C4A	2.31	0.48
1:m:118:ALA:HB1	1:m:130:LEU:HD21	1.95	0.48
1:m:149:PRO:O	1:m:150:HIS:C	2.54	0.48
1:T:53:ARG:HD2	1:T:53:ARG:O	2.13	0.48
4:l:33:LYS:HE2	4:p:113:HIS:ND1	2.28	0.48
1:m:67:HIS:O	1:m:71:VAL:HG23	2.14	0.48
1:m:106:THR:HG22	1:m:149:PRO:HB2	1.94	0.48
1:E:39:ASP:OD1	1:E:116:SER:HB3	2.13	0.48
1:I:118:ALA:HB1	1:I:130:LEU:HD21	1.95	0.48
2:f:23:HIS:HD2	5:q:63:LYS:CG	2.26	0.48
3:C:127:ASP:OD2	4:D:121:THR:HG21	2.14	0.48
1:P:54:VAL:C	1:P:55:LYS:CG	2.83	0.48
3:o:8:GLU:O	3:o:12:ILE:HG12	2.14	0.48
4:p:42:VAL:HG13	8:p:201:HEM:HBC1	1.96	0.48
5:q:168:ARG:HH11	5:q:184:ARG:HG3	1.79	0.48
2:U:98:ARG:CZ	8:U:201:HEM:HAD2	2.43	0.48
1:e:39:ASP:OD1	1:e:116:SER:HB3	2.13	0.48
2:j:28:PHE:CD1	2:j:119:GLN:HG3	2.49	0.48
1:m:12:GLU:O	1:m:16:ILE:HG13	2.13	0.48
3:K:33:PHE:CE2	3:K:37:ILE:HD11	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:126:ASP:O	6:N:128:LEU:N	2.46	0.48
2:Q:28:PHE:CD1	2:Q:119:GLN:HG3	2.48	0.48
7:d:107:GLY:HA2	7:d:215:PHE:HA	1.95	0.48
5:M:31:ILE:HD12	6:N:35:LEU:HD22	1.96	0.48
1:T:51:PHE:CB	1:T:56:VAL:HG21	2.44	0.48
3:V:33:PHE:CE2	3:V:37:ILE:HD11	2.49	0.48
5:b:28:LEU:HD21	7:d:24:GLU:HB3	1.96	0.48
5:b:134:ALA:HB3	5:b:148:ARG:HB2	1.96	0.48
1:e:51:PHE:HB3	1:e:56:VAL:HG22	1.95	0.48
2:f:28:PHE:CD1	2:f:119:GLN:HG3	2.49	0.48
2:f:49:ARG:NH1	8:f:201:HEM:O1D	2.47	0.48
1:i:118:ALA:HB1	1:i:130:LEU:HD21	1.95	0.48
1:A:80:ASN:HB3	4:D:24:ARG:NH2	2.29	0.47
4:L:62:HIS:O	4:L:66:VAL:HG23	2.13	0.47
1:X:90:LYS:HZ3	4:a:58:GLU:HG3	1.79	0.47
1:i:39:ASP:OD1	1:i:116:SER:HB3	2.13	0.47
1:m:51:PHE:O	1:m:56:VAL:HG22	2.14	0.47
6:r:126:ASP:O	6:r:128:LEU:N	2.46	0.47
2:B:95:HIS:HE1	8:B:201:HEM:C4A	2.32	0.47
2:B:122:ARG:HG2	5:M:193:ARG:HH22	1.79	0.47
1:E:7:ALA:HB3	3:K:8:GLU:HB3	1.97	0.47
4:H:42:VAL:HG13	8:H:201:HEM:HBC1	1.95	0.47
1:X:67:HIS:O	1:X:71:VAL:HG23	2.13	0.47
2:Y:28:PHE:CD1	2:Y:119:GLN:HG3	2.49	0.47
3:Z:8:GLU:O	3:Z:12:ILE:HG12	2.14	0.47
1:e:90:LYS:HZ3	4:h:58:GLU:HG3	1.79	0.47
1:i:95:LEU:HD21	8:i:201:HEM:HMB2	1.96	0.47
4:L:42:VAL:HG13	8:L:201:HEM:HBC1	1.95	0.47
5:M:168:ARG:HH11	5:M:184:ARG:HG3	1.78	0.47
6:N:118:PHE:HB3	6:N:230:VAL:HB	1.95	0.47
4:h:62:HIS:O	4:h:66:VAL:HG23	2.15	0.47
1:i:51:PHE:CZ	8:i:201:HEM:HBC2	2.50	0.47
3:G:8:GLU:O	3:G:12:ILE:HG12	2.13	0.47
1:X:90:LYS:NZ	4:a:58:GLU:HG3	2.30	0.47
4:l:97:ARG:CZ	8:l:201:HEM:HAD2	2.44	0.47
1:I:21:TRP:HD1	1:I:22:SER:H	1.63	0.47
1:I:96:ALA:O	1:I:100:ILE:HG13	2.15	0.47
2:J:28:PHE:CD1	2:J:119:GLN:HG3	2.49	0.47
1:X:12:GLU:O	1:X:16:ILE:HG13	2.14	0.47
5:b:24:LEU:HD22	6:c:35:LEU:HD12	1.96	0.47
6:c:231:HIS:CE1	6:c:233:GLN:HG2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:k:127:ASP:OD1	3:k:127:ASP:N	2.36	0.47
1:A:67:HIS:O	1:A:71:VAL:HG23	2.15	0.47
2:B:23:HIS:HD2	5:M:63:LYS:CG	2.28	0.47
1:P:54:VAL:O	1:P:55:LYS:HB2	2.14	0.47
1:A:118:ALA:HB1	1:A:130:LEU:HD21	1.95	0.47
2:J:77:THR:O	2:J:84:LEU:HB2	2.14	0.47
4:L:108:LEU:HB2	4:L:132:PHE:CE2	2.49	0.47
1:X:118:ALA:HB1	1:X:130:LEU:HD21	1.96	0.47
5:b:168:ARG:HH11	5:b:184:ARG:HG3	1.78	0.47
7:d:117:ARG:O	7:d:149:LYS:NZ	2.44	0.47
1:e:118:ALA:HB1	1:e:130:LEU:HD21	1.95	0.47
3:g:8:GLU:O	3:g:12:ILE:HG12	2.15	0.47
4:h:94:HIS:CE1	8:h:201:HEM:C4A	3.03	0.47
1:T:43:HIS:CD2	1:m:46:SER:OG	2.66	0.47
4:a:42:VAL:HG13	8:a:201:HEM:HBC1	1.96	0.47
1:A:55:LYS:HG3	1:A:63:GLU:CG	2.39	0.47
2:J:49:ARG:HD3	8:J:201:HEM:O2D	2.15	0.47
3:K:8:GLU:O	3:K:12:ILE:HG12	2.14	0.47
1:P:51:PHE:O	1:P:56:VAL:HG22	2.15	0.47
2:U:102:ASP:OD2	3:g:108:LYS:NZ	2.42	0.47
2:B:77:THR:O	2:B:84:LEU:HB2	2.15	0.47
1:E:51:PHE:O	1:E:56:VAL:HG22	2.15	0.47
3:G:33:PHE:CE2	3:G:37:ILE:HD11	2.50	0.47
5:M:63:LYS:HA	5:M:63:LYS:HD2	1.73	0.47
1:X:96:ALA:O	1:X:100:ILE:HG13	2.15	0.47
3:R:8:GLU:O	3:R:12:ILE:HG12	2.14	0.46
1:X:21:TRP:HD1	1:X:22:SER:H	1.63	0.46
3:C:33:PHE:CE2	3:C:37:ILE:HD11	2.50	0.46
2:J:21:HIS:C	2:J:23:HIS:H	2.23	0.46
1:P:96:ALA:O	1:P:100:ILE:HG13	2.15	0.46
2:U:49:ARG:HD3	8:U:201:HEM:O2D	2.15	0.46
3:Z:33:PHE:CE2	3:Z:37:ILE:HD11	2.50	0.46
1:i:51:PHE:HZ	8:i:201:HEM:HBC2	1.81	0.46
2:n:49:ARG:HH11	8:n:201:HEM:CGD	2.29	0.46
5:q:31:ILE:HD12	6:r:35:LEU:HD22	1.98	0.46
1:A:24:SER:O	4:D:11:LYS:HE3	2.15	0.46
1:I:12:GLU:O	1:I:16:ILE:HG13	2.15	0.46
1:X:55:LYS:HG3	1:X:63:GLU:CG	2.20	0.46
6:N:218:LEU:HD12	6:N:223:HIS:HB3	1.97	0.46
6:N:231:HIS:CE1	6:N:233:GLN:HG2	2.50	0.46
1:T:54:VAL:O	1:T:55:LYS:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:54:LYS:HD2	3:G:103:ARG:HH22	1.81	0.46
4:S:94:HIS:HE1	8:S:201:HEM:C4A	2.33	0.46
1:T:51:PHE:C	1:T:56:VAL:CG2	2.89	0.46
1:A:12:GLU:O	1:A:16:ILE:HG13	2.16	0.46
4:D:62:HIS:O	4:D:66:VAL:HG23	2.15	0.46
1:E:21:TRP:HD1	1:E:22:SER:H	1.62	0.46
1:P:12:GLU:O	1:P:16:ILE:HG13	2.16	0.46
1:i:96:ALA:O	1:i:100:ILE:HG13	2.16	0.46
4:l:42:VAL:HG13	8:l:201:HEM:HBC1	1.98	0.46
1:m:51:PHE:CZ	8:m:201:HEM:HBC2	2.51	0.46
2:n:21:HIS:C	2:n:23:HIS:H	2.23	0.46
3:g:33:PHE:CE2	3:g:37:ILE:HD11	2.50	0.46
3:C:8:GLU:O	3:C:12:ILE:HG12	2.15	0.46
1:E:131:GLU:HB3	1:E:135:ARG:NH1	2.31	0.46
5:M:178:LEU:HB3	5:M:194:CYS:HB2	1.97	0.46
6:N:38:LEU:HD23	7:O:28:LEU:HD13	1.96	0.46
1:P:131:GLU:HB3	1:P:135:ARG:NH1	2.31	0.46
2:Q:77:THR:O	2:Q:84:LEU:HB2	2.16	0.46
2:Q:122:ARG:HG2	5:b:193:ARG:HH22	1.81	0.46
2:U:77:THR:O	2:U:84:LEU:HB2	2.15	0.46
2:Q:23:HIS:HD2	5:b:63:LYS:CG	2.28	0.46
3:g:54:LYS:HD2	3:g:103:ARG:HH22	1.81	0.46
1:i:137:PHE:CZ	8:i:201:HEM:HBB1	2.51	0.46
3:k:54:LYS:HD2	3:k:103:ARG:HH22	1.80	0.46
1:I:51:PHE:O	1:I:56:VAL:HG22	2.16	0.45
1:T:21:TRP:HD1	1:T:22:SER:H	1.62	0.45
3:g:38:LEU:HD23	3:g:38:LEU:HA	1.72	0.45
1:m:21:TRP:HD1	1:m:22:SER:H	1.63	0.45
1:A:21:TRP:HD1	1:A:22:SER:H	1.63	0.45
2:F:98:ARG:HG2	2:F:98:ARG:HH11	1.81	0.45
3:G:38:LEU:HD23	3:G:38:LEU:HA	1.73	0.45
1:e:51:PHE:HZ	8:e:201:HEM:HBC2	1.80	0.45
1:i:21:TRP:HD1	1:i:22:SER:H	1.63	0.45
1:i:55:LYS:O	1:i:56:VAL:C	2.58	0.45
3:k:38:LEU:HD23	3:k:38:LEU:HA	1.73	0.45
1:A:131:GLU:HB3	1:A:135:ARG:NH1	2.31	0.45
1:P:8:GLU:OE2	3:V:6:SER:CB	2.64	0.45
1:T:23:SER:OG	3:V:23:ASP:OD2	2.34	0.45
5:b:178:LEU:HB3	5:b:194:CYS:HB2	1.97	0.45
1:e:21:TRP:HD1	1:e:22:SER:H	1.63	0.45
3:o:33:PHE:CE2	3:o:37:ILE:HD11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:r:218:LEU:HD12	6:r:223:HIS:HB3	1.98	0.45
1:A:96:ALA:O	1:A:100:ILE:HG13	2.15	0.45
4:D:72:MET:HE2	4:D:72:MET:HB3	1.79	0.45
5:M:32:ASP:OD2	5:M:36:LYS:HE3	2.17	0.45
3:K:28:LYS:HB2	3:K:28:LYS:HE2	1.76	0.45
4:S:100:ASN:OD1	4:S:102:GLU:HG2	2.17	0.45
1:T:63:GLU:HA	4:W:85:ALA:HB1	1.99	0.45
3:V:132:LEU:O	3:V:136:SER:HB2	2.17	0.45
3:Z:54:LYS:HD2	3:Z:103:ARG:HH22	1.82	0.45
1:P:54:VAL:O	1:P:55:LYS:CB	2.64	0.45
1:e:12:GLU:O	1:e:16:ILE:HG13	2.17	0.45
1:m:96:ALA:O	1:m:100:ILE:HG13	2.16	0.45
1:P:25:PHE:CE2	3:R:28:LYS:HG2	2.52	0.45
2:Q:21:HIS:C	2:Q:23:HIS:H	2.24	0.45
3:R:28:LYS:HB2	3:R:28:LYS:HE2	1.75	0.45
3:g:8:GLU:HB2	1:m:8:GLU:CD	2.42	0.45
1:i:58:GLU:O	1:i:61:SER:OG	2.30	0.45
2:j:21:HIS:C	2:j:23:HIS:H	2.24	0.45
4:h:97:ARG:CZ	8:h:201:HEM:HAD2	2.47	0.45
1:i:60:ASP:OD1	1:i:60:ASP:N	2.44	0.45
3:o:54:LYS:HD2	3:o:103:ARG:HH22	1.82	0.45
3:K:84:ASP:O	3:K:86:PRO:HD3	2.17	0.45
3:V:15:LYS:HB2	3:V:15:LYS:HE3	1.84	0.45
1:e:25:PHE:CD2	3:g:28:LYS:HG2	2.51	0.45
3:g:132:LEU:O	3:g:136:SER:HB2	2.17	0.45
2:j:77:THR:O	2:j:84:LEU:HB2	2.17	0.45
8:F:201:HEM:C4D	9:F:202:CYN:N	2.85	0.45
3:R:132:LEU:O	3:R:136:SER:HB2	2.17	0.45
1:T:12:GLU:O	1:T:16:ILE:HG13	2.17	0.45
1:T:96:ALA:O	1:T:100:ILE:HG13	2.16	0.45
3:o:144:LYS:HE2	3:o:144:LYS:HB2	1.73	0.45
1:A:51:PHE:HB3	1:A:56:VAL:HG22	1.99	0.44
5:M:84:ASP:HB3	5:M:143:PRO:HG3	1.99	0.44
2:Q:122:ARG:HD3	5:b:214:LEU:HD21	1.99	0.44
3:V:54:LYS:HD2	3:V:103:ARG:HH22	1.82	0.44
5:b:32:ASP:OD2	5:b:36:LYS:HE3	2.17	0.44
3:k:22:GLY:HA3	4:l:15:ARG:NH1	2.33	0.44
3:R:8:GLU:HB2	1:X:8:GLU:CD	2.42	0.44
3:Z:144:LYS:HB2	3:Z:144:LYS:HE2	1.73	0.44
3:g:127:ASP:OD2	4:h:121:THR:HG21	2.17	0.44
5:q:178:LEU:HB3	5:q:194:CYS:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:GLU:OE2	5:M:210:ASN:ND2	2.50	0.44
1:A:133:TRP:CZ2	1:A:137:PHE:HD2	2.34	0.44
1:E:12:GLU:O	1:E:16:ILE:HG13	2.18	0.44
1:X:131:GLU:HB3	1:X:135:ARG:NH1	2.33	0.44
6:c:84:ILE:HD13	6:c:84:ILE:HA	1.77	0.44
1:P:25:PHE:CD2	3:R:28:LYS:HG2	2.52	0.44
1:P:90:LYS:NZ	4:S:58:GLU:HG3	2.33	0.44
5:b:214:LEU:HD23	5:b:214:LEU:HA	1.74	0.44
1:A:11:ARG:NH1	3:G:8:GLU:HG3	2.31	0.44
1:A:81:LEU:HD11	4:D:64:GLU:HG2	1.99	0.44
2:B:48:LYS:CE	2:f:48:LYS:HZ1	2.31	0.44
3:C:84:ASP:O	3:C:86:PRO:HD3	2.17	0.44
1:E:96:ALA:O	1:E:100:ILE:HG13	2.17	0.44
3:G:15:LYS:HB2	3:G:15:LYS:HE3	1.84	0.44
5:M:28:LEU:HD21	7:O:24:GLU:HB3	2.00	0.44
2:U:76:SER:HB3	3:V:27:SER:HB3	2.00	0.44
2:U:98:ARG:HG2	2:U:98:ARG:HH11	1.83	0.44
3:V:121:GLY:O	3:V:125:VAL:HG22	2.18	0.44
2:Y:21:HIS:C	2:Y:23:HIS:H	2.24	0.44
2:f:77:THR:O	2:f:84:LEU:HB2	2.17	0.44
4:p:29:LEU:HD12	4:p:29:LEU:HA	1.88	0.44
3:C:28:LYS:HB2	3:C:28:LYS:HE2	1.76	0.44
3:K:125:VAL:HG13	4:L:5:LEU:HD22	2.00	0.44
1:P:95:LEU:HD21	8:P:201:HEM:HMB2	2.00	0.44
4:W:100:ASN:OD1	4:W:102:GLU:HG2	2.18	0.44
1:X:80:ASN:HB3	4:a:24:ARG:NH2	2.33	0.44
1:e:131:GLU:HB3	1:e:135:ARG:NH1	2.32	0.44
1:e:133:TRP:CZ2	1:e:137:PHE:HD2	2.36	0.44
1:i:51:PHE:HB3	1:i:56:VAL:HG22	2.00	0.44
3:o:132:LEU:O	3:o:136:SER:HB2	2.17	0.44
4:H:29:LEU:HD12	4:H:29:LEU:HA	1.83	0.44
6:N:76:CYS:O	6:N:100:HIS:ND1	2.51	0.44
2:U:21:HIS:C	2:U:23:HIS:H	2.24	0.44
2:U:102:ASP:CG	3:g:108:LYS:NZ	2.75	0.44
6:c:38:LEU:HD23	7:d:28:LEU:HD13	2.00	0.44
6:c:48:ILE:O	7:d:35:ARG:NH1	2.50	0.44
4:D:108:LEU:HB2	4:D:132:PHE:CD2	2.53	0.44
1:E:25:PHE:CE2	4:H:11:LYS:HE2	2.53	0.44
4:H:72:MET:HE2	4:H:72:MET:HB3	1.80	0.44
3:R:54:LYS:HD2	3:R:103:ARG:HH22	1.82	0.44
1:i:12:GLU:O	1:i:16:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:o:84:ASP:O	3:o:86:PRO:HD3	2.18	0.44
2:F:112:LEU:HD22	2:F:116:LEU:HG	2.00	0.44
4:H:108:LEU:HB2	4:H:132:PHE:CD2	2.53	0.44
1:e:51:PHE:CZ	8:e:201:HEM:HBC2	2.53	0.44
1:i:150:HIS:HD2	1:i:150:HIS:N	2.04	0.44
4:D:42:VAL:HG13	8:D:201:HEM:HBC1	2.00	0.43
4:D:100:ASN:OD1	4:D:102:GLU:HG2	2.17	0.43
3:G:121:GLY:O	3:G:125:VAL:HG22	2.18	0.43
2:J:98:ARG:CZ	8:J:201:HEM:HAD2	2.48	0.43
1:P:85:THR:HG21	3:V:132:LEU:H	1.83	0.43
2:Y:112:LEU:HD22	2:Y:116:LEU:HG	2.00	0.43
1:e:95:LEU:HD21	8:e:201:HEM:HMB2	2.00	0.43
3:g:28:LYS:HE2	3:g:28:LYS:HB2	1.75	0.43
8:g:201:HEM:HBD2	8:g:201:HEM:HHA	1.99	0.43
1:i:133:TRP:CZ2	1:i:137:PHE:HD2	2.36	0.43
1:m:92:LEU:HD12	1:m:92:LEU:HA	1.91	0.43
2:B:48:LYS:HZ1	2:f:48:LYS:CE	2.31	0.43
3:K:54:LYS:HD2	3:K:103:ARG:HH22	1.83	0.43
1:P:24:SER:O	4:S:11:LYS:HE3	2.18	0.43
6:c:218:LEU:HD12	6:c:223:HIS:HB3	1.99	0.43
4:p:68:SER:O	4:p:72:MET:HG3	2.19	0.43
3:G:13:VAL:HB	3:G:83:MET:HE1	2.01	0.43
1:T:52:GLU:C	1:T:54:VAL:H	2.25	0.43
1:T:102:ARG:HA	1:T:102:ARG:HD3	1.87	0.43
4:W:29:LEU:HD12	4:W:29:LEU:HA	1.86	0.43
3:Z:121:GLY:O	3:Z:125:VAL:HG22	2.18	0.43
4:h:29:LEU:HD12	4:h:29:LEU:HA	1.87	0.43
1:i:81:LEU:HD21	1:i:87:VAL:HG12	2.00	0.43
4:l:8:LEU:HD12	4:l:8:LEU:HA	1.89	0.43
4:l:72:MET:HE2	4:l:72:MET:HB3	1.80	0.43
1:m:16:ILE:HG12	7:s:205:ALA:HB1	2.00	0.43
2:n:76:SER:HB3	3:o:27:SER:HB3	2.00	0.43
1:A:59:PRO:HA	1:A:64:TYR:CD2	2.54	0.43
3:K:121:GLY:O	3:K:125:VAL:HG22	2.18	0.43
2:U:100:ILE:CG2	8:U:201:HEM:HAC	2.47	0.43
4:W:107:PHE:CE2	8:W:201:HEM:HAB	2.53	0.43
1:i:10:ARG:NH1	3:o:130:ASN:HD21	2.16	0.43
3:o:28:LYS:HB2	3:o:28:LYS:HE2	1.76	0.43
3:G:132:LEU:O	3:G:136:SER:HB2	2.18	0.43
4:L:29:LEU:HD12	4:L:29:LEU:HA	1.86	0.43
5:M:187:LYS:O	5:M:189:VAL:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:144:LYS:HE2	3:V:144:LYS:HB2	1.74	0.43
3:Z:28:LYS:HE2	3:Z:28:LYS:HB2	1.76	0.43
2:f:100:ILE:HA	2:f:101:PRO:HD2	1.91	0.43
3:g:13:VAL:HB	3:g:83:MET:HE1	2.01	0.43
4:l:100:ASN:OD1	4:l:102:GLU:HG2	2.18	0.43
1:m:51:PHE:HZ	8:m:201:HEM:HBC2	1.82	0.43
3:C:132:LEU:O	3:C:136:SER:HB2	2.18	0.43
8:C:201:HEM:HBD2	8:C:201:HEM:HHA	2.01	0.43
2:F:21:HIS:C	2:F:23:HIS:H	2.24	0.43
3:K:132:LEU:O	3:K:136:SER:HB2	2.18	0.43
4:S:94:HIS:CE1	8:S:201:HEM:C4A	3.05	0.43
1:e:24:SER:O	4:h:11:LYS:HE3	2.19	0.43
1:e:80:ASN:HB3	4:h:24:ARG:NH2	2.33	0.43
4:h:108:LEU:HB2	4:h:132:PHE:CD2	2.54	0.43
1:m:133:TRP:CZ2	1:m:137:PHE:HD2	2.37	0.43
5:q:63:LYS:HD2	5:q:63:LYS:HA	1.74	0.43
1:P:47:ALA:HB1	8:P:201:HEM:HBC1	2.01	0.43
1:e:11:ARG:HH12	3:k:8:GLU:HG3	1.83	0.43
1:e:88:LEU:O	1:e:92:LEU:HB2	2.19	0.43
3:g:121:GLY:O	3:g:125:VAL:HG22	2.19	0.43
3:o:125:VAL:CG1	4:p:5:LEU:HD22	2.48	0.43
4:D:29:LEU:HD12	4:D:29:LEU:HA	1.87	0.43
1:E:92:LEU:HD12	1:E:92:LEU:HA	1.92	0.43
1:T:131:GLU:HB3	1:T:135:ARG:NH1	2.33	0.43
4:W:108:LEU:HB2	4:W:132:PHE:CD2	2.54	0.43
3:g:84:ASP:O	3:g:86:PRO:HD3	2.18	0.43
1:i:149:PRO:C	1:i:150:HIS:O	2.62	0.43
4:l:108:LEU:HB2	4:l:132:PHE:CD2	2.54	0.43
3:K:144:LYS:HB2	3:K:144:LYS:HE2	1.74	0.43
8:U:201:HEM:C4D	9:U:202:CYN:N	2.86	0.43
5:b:175:ASP:HB3	5:b:177:THR:OG1	2.19	0.43
2:B:49:ARG:HH11	8:B:201:HEM:CGD	2.31	0.43
2:F:77:THR:O	2:F:84:LEU:HB2	2.18	0.43
1:P:21:TRP:HD1	1:P:22:SER:H	1.62	0.43
3:R:13:VAL:HB	3:R:83:MET:HE1	2.01	0.43
1:T:12:GLU:OE1	6:c:218:LEU:HD13	2.19	0.43
3:V:13:VAL:HB	3:V:83:MET:HE1	2.01	0.43
3:Z:13:VAL:HB	3:Z:83:MET:HE1	2.01	0.43
3:Z:84:ASP:O	3:Z:86:PRO:HD3	2.19	0.43
1:e:113:ILE:HD13	8:e:201:HEM:HBB2	2.00	0.43
6:r:155:ARG:NH2	6:r:174:ASP:OD2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:LEU:HD21	2:B:136:ILE:HG23	2.01	0.42
3:C:54:LYS:HD2	3:C:103:ARG:HH22	1.83	0.42
1:E:131:GLU:HB3	1:E:135:ARG:HH12	1.83	0.42
1:P:8:GLU:CD	3:V:8:GLU:HB2	2.44	0.42
1:T:34:GLY:O	1:T:38:LYS:HG3	2.19	0.42
1:X:51:PHE:CZ	8:X:201:HEM:HBC2	2.54	0.42
2:Y:49:ARG:HH11	8:Y:201:HEM:CGD	2.32	0.42
2:Y:65:LEU:HD23	2:Y:65:LEU:HA	1.90	0.42
1:e:55:LYS:O	1:e:56:VAL:C	2.61	0.42
4:L:72:MET:HE2	4:L:72:MET:HB3	1.79	0.42
5:M:187:LYS:O	5:M:189:VAL:HG23	2.20	0.42
1:P:133:TRP:CZ2	1:P:137:PHE:HD2	2.36	0.42
1:e:54:VAL:O	1:e:55:LYS:C	2.61	0.42
1:e:81:LEU:HD11	4:h:64:GLU:HG2	2.00	0.42
3:o:70:LEU:HD23	3:o:70:LEU:HA	1.87	0.42
1:I:131:GLU:HB3	1:I:135:ARG:NH1	2.33	0.42
1:e:55:LYS:C	1:e:57:ALA:N	2.72	0.42
4:h:100:ASN:OD1	4:h:102:GLU:HG2	2.19	0.42
1:i:92:LEU:HD12	1:i:92:LEU:HA	1.92	0.42
1:i:143:ARG:NH1	1:i:146:ARG:HH11	2.17	0.42
3:k:13:VAL:HB	3:k:83:MET:HE1	2.01	0.42
1:I:15:HIS:ND1	7:O:205:ALA:O	2.52	0.42
4:L:68:SER:O	4:L:72:MET:HG3	2.19	0.42
1:P:131:GLU:HB3	1:P:135:ARG:HH12	1.85	0.42
1:T:133:TRP:CZ2	1:T:137:PHE:HD2	2.37	0.42
6:c:155:ARG:NH2	6:c:174:ASP:OD2	2.52	0.42
6:r:76:CYS:O	6:r:100:HIS:ND1	2.53	0.42
1:I:133:TRP:CZ2	1:I:137:PHE:HD2	2.38	0.42
3:k:132:LEU:O	3:k:136:SER:HB2	2.19	0.42
1:m:95:LEU:HD21	8:m:201:HEM:HMB2	2.01	0.42
5:q:175:ASP:HB3	5:q:177:THR:OG1	2.20	0.42
3:C:13:VAL:HB	3:C:83:MET:HE1	2.01	0.42
2:J:112:LEU:HD22	2:J:116:LEU:HG	2.02	0.42
4:L:20:GLU:HB3	4:L:22:HIS:CE1	2.55	0.42
7:O:22:THR:HG23	7:d:19:LEU:HD22	2.00	0.42
7:O:28:LEU:HD22	7:O:32:LEU:HD22	2.02	0.42
3:R:121:GLY:O	3:R:125:VAL:HG22	2.20	0.42
7:d:28:LEU:HD22	7:d:32:LEU:HD22	2.02	0.42
1:i:58:GLU:HA	1:i:59:PRO:HD2	1.90	0.42
1:i:131:GLU:HB3	1:i:135:ARG:NH1	2.33	0.42
3:o:125:VAL:HG13	4:p:5:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:q:84:ASP:HB3	5:q:143:PRO:HG3	2.00	0.42
1:A:88:LEU:O	1:A:92:LEU:HB2	2.20	0.42
3:R:38:LEU:HA	3:R:38:LEU:HD23	1.73	0.42
3:V:84:ASP:O	3:V:86:PRO:HD3	2.20	0.42
4:W:8:LEU:HD12	4:W:8:LEU:HA	1.87	0.42
5:b:84:ASP:HB3	5:b:143:PRO:HG3	2.02	0.42
1:m:15:HIS:ND1	7:s:205:ALA:O	2.53	0.42
1:I:15:HIS:CG	7:O:206:SER:HA	2.55	0.42
2:Q:16:ARG:O	2:Q:20:SER:OG	2.37	0.42
2:Q:73:ILE:HD11	3:R:71:ARG:HA	2.02	0.42
3:R:84:ASP:O	3:R:86:PRO:HD3	2.19	0.42
4:S:108:LEU:HB2	4:S:132:PHE:CD2	2.54	0.42
4:W:97:ARG:CZ	8:W:201:HEM:HAD2	2.49	0.42
3:g:127:ASP:OD1	3:g:127:ASP:N	2.37	0.42
3:k:36:LEU:HD22	4:l:5:LEU:HD21	2.01	0.42
5:q:32:ASP:OD2	5:q:36:LYS:HE3	2.19	0.42
2:B:122:ARG:HD3	5:M:214:LEU:HD21	2.02	0.42
1:I:102:ARG:HD3	1:I:102:ARG:HA	1.87	0.42
1:I:137:PHE:CZ	8:I:201:HEM:HBB1	2.55	0.42
1:T:131:GLU:HB3	1:T:135:ARG:HH12	1.85	0.42
4:a:20:GLU:HB3	4:a:22:HIS:CE1	2.55	0.42
5:b:187:LYS:O	5:b:189:VAL:N	2.52	0.42
1:e:51:PHE:HB2	1:e:56:VAL:HG22	1.94	0.42
3:g:144:LYS:HB2	3:g:144:LYS:HE2	1.73	0.42
1:A:95:LEU:HD21	8:A:201:HEM:HMB2	2.01	0.42
1:X:95:LEU:HD21	8:X:201:HEM:HMB2	2.01	0.42
2:f:98:ARG:HG2	2:f:98:ARG:HH11	1.85	0.42
3:g:70:LEU:HD23	3:g:70:LEU:HA	1.86	0.42
1:i:10:ARG:HH12	3:o:130:ASN:HD21	1.68	0.42
8:j:201:HEM:C4D	9:j:202:CYN:N	2.88	0.42
5:q:107:ILE:HA	5:q:132:ILE:HG22	2.02	0.42
6:r:234:GLY:O	6:r:235:HIS:HB3	2.20	0.42
7:s:28:LEU:HD22	7:s:32:LEU:HD22	2.01	0.42
2:F:88:LEU:HD21	2:F:136:ILE:HG23	2.02	0.41
2:J:88:LEU:HD21	2:J:136:ILE:HG23	2.02	0.41
3:K:125:VAL:CG1	4:L:5:LEU:HD22	2.50	0.41
4:a:108:LEU:HB2	4:a:132:PHE:CD2	2.55	0.41
4:l:20:GLU:HB3	4:l:22:HIS:CE1	2.55	0.41
2:F:50:VAL:CG2	2:F:63:HIS:HB2	2.50	0.41
4:H:77:LEU:HD12	4:H:77:LEU:HA	1.91	0.41
3:K:13:VAL:HB	3:K:83:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:100:ASN:OD1	4:L:102:GLU:HG2	2.20	0.41
7:O:107:GLY:HA2	7:O:214:ILE:O	2.20	0.41
4:S:68:SER:O	4:S:72:MET:HG3	2.20	0.41
2:U:140:ILE:CD1	8:U:201:HEM:HBB2	2.46	0.41
3:Z:132:LEU:O	3:Z:136:SER:HB2	2.20	0.41
7:d:203:HIS:C	7:d:205:ALA:H	2.28	0.41
3:k:100:HIS:HE1	8:k:201:HEM:C4A	2.38	0.41
4:p:72:MET:HB3	4:p:72:MET:HE2	1.79	0.41
7:s:203:HIS:C	7:s:205:ALA:H	2.27	0.41
2:B:112:LEU:HD22	2:B:116:LEU:HG	2.02	0.41
1:E:34:GLY:O	1:E:38:LYS:HG3	2.20	0.41
1:E:81:LEU:HD23	1:E:88:LEU:HA	2.02	0.41
3:G:28:LYS:HE2	3:G:28:LYS:HB2	1.76	0.41
4:p:100:ASN:OD1	4:p:102:GLU:HG2	2.20	0.41
2:B:48:LYS:NZ	2:f:48:LYS:CE	2.83	0.41
2:B:65:LEU:HD23	2:B:65:LEU:HA	1.93	0.41
1:E:12:GLU:OE1	6:N:218:LEU:HD13	2.21	0.41
1:E:81:LEU:HD21	1:E:87:VAL:HG12	2.03	0.41
3:G:127:ASP:OD1	3:G:127:ASP:N	2.35	0.41
4:S:29:LEU:HD12	4:S:29:LEU:HA	1.87	0.41
2:U:50:VAL:CG2	2:U:63:HIS:HB2	2.49	0.41
1:X:133:TRP:CZ2	1:X:137:PHE:HD2	2.37	0.41
4:a:99:ILE:HG23	8:a:201:HEM:HAC	2.01	0.41
1:m:131:GLU:HB3	1:m:135:ARG:NH1	2.34	0.41
2:n:98:ARG:HG2	2:n:98:ARG:HH11	1.85	0.41
4:p:20:GLU:HB3	4:p:22:HIS:CE1	2.54	0.41
5:q:28:LEU:HD21	7:s:24:GLU:HB3	2.01	0.41
1:A:85:THR:HG21	3:G:132:LEU:H	1.85	0.41
2:J:65:LEU:HD23	2:J:65:LEU:HA	1.94	0.41
4:L:97:ARG:CZ	8:L:201:HEM:HAD2	2.50	0.41
1:X:34:GLY:O	1:X:38:LYS:HG3	2.21	0.41
4:a:68:SER:O	4:a:72:MET:HG3	2.20	0.41
1:i:81:LEU:HD23	1:i:88:LEU:HA	2.01	0.41
3:k:28:LYS:HE2	3:k:28:LYS:HB2	1.77	0.41
7:s:107:GLY:HA2	7:s:214:ILE:O	2.20	0.41
2:B:48:LYS:CE	2:f:48:LYS:NZ	2.83	0.41
4:D:68:SER:O	4:D:72:MET:HG3	2.21	0.41
1:T:70:ARG:HD3	4:W:86:GLN:OE1	2.20	0.41
4:W:20:GLU:HB3	4:W:22:HIS:CE1	2.55	0.41
6:c:234:GLY:O	6:c:235:HIS:HB3	2.20	0.41
3:k:84:ASP:O	3:k:86:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:29:ALA:HB1	2:n:64:ALA:HB1	2.02	0.41
2:n:112:LEU:HD22	2:n:116:LEU:HG	2.01	0.41
2:B:114:HIS:NE2	5:M:138:LYS:HG3	2.36	0.41
4:H:20:GLU:HB3	4:H:22:HIS:CE1	2.56	0.41
2:J:50:VAL:CG2	2:J:63:HIS:HB2	2.50	0.41
3:K:38:LEU:HD23	3:K:38:LEU:HA	1.73	0.41
4:L:107:PHE:CE2	8:L:201:HEM:HAB	2.56	0.41
6:c:28:LEU:HD23	6:c:28:LEU:HA	1.90	0.41
4:h:72:MET:HB3	4:h:72:MET:HE2	1.79	0.41
1:m:137:PHE:CZ	8:m:201:HEM:HBB1	2.56	0.41
4:p:108:LEU:HB2	4:p:132:PHE:CD2	2.55	0.41
5:q:48:ARG:NH1	5:q:200:ASP:OD2	2.54	0.41
4:D:20:GLU:HB3	4:D:22:HIS:CE1	2.56	0.41
3:R:100:HIS:CD2	8:R:201:HEM:NC	2.89	0.41
4:S:20:GLU:HB3	4:S:22:HIS:CE1	2.56	0.41
1:T:51:PHE:CB	1:T:56:VAL:CG2	2.98	0.41
2:Y:29:ALA:HB1	2:Y:64:ALA:HB1	2.03	0.41
5:b:168:ARG:HH12	5:b:184:ARG:HH11	1.69	0.41
1:e:92:LEU:HD12	1:e:92:LEU:HA	1.89	0.41
4:h:68:SER:O	4:h:72:MET:HG3	2.21	0.41
2:j:88:LEU:HD21	2:j:136:ILE:HG23	2.02	0.41
2:j:136:ILE:O	2:j:140:ILE:HG13	2.21	0.41
2:n:50:VAL:CG2	2:n:63:HIS:HB2	2.49	0.41
3:o:121:GLY:O	3:o:125:VAL:HG22	2.21	0.41
1:A:131:GLU:HB3	1:A:135:ARG:HH12	1.85	0.41
2:B:100:ILE:CG2	8:B:201:HEM:HAC	2.50	0.41
1:E:133:TRP:CZ2	1:E:137:PHE:HD2	2.37	0.41
1:I:81:LEU:HD11	4:L:64:GLU:HG2	2.03	0.41
5:M:107:ILE:HA	5:M:132:ILE:HG22	2.02	0.41
6:N:84:ILE:HD13	6:N:84:ILE:HA	1.77	0.41
7:O:13:LYS:HD2	7:O:13:LYS:HA	1.79	0.41
1:P:21:TRP:CD1	1:P:22:SER:N	2.89	0.41
2:Q:98:ARG:HG2	2:Q:98:ARG:HH11	1.86	0.41
4:a:72:MET:HE2	4:a:72:MET:HB3	1.77	0.41
4:a:100:ASN:OD1	4:a:102:GLU:HG2	2.20	0.41
1:e:131:GLU:HB3	1:e:135:ARG:HH12	1.86	0.41
2:f:88:LEU:HD21	2:f:136:ILE:HG23	2.01	0.41
2:j:16:ARG:O	2:j:20:SER:OG	2.37	0.41
2:j:51:HIS:ND1	2:j:59:GLU:HG3	2.36	0.41
3:k:121:GLY:O	3:k:125:VAL:HG22	2.20	0.41
1:m:80:ASN:HB3	4:p:24:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:150:HIS:H	1:m:150:HIS:CD2	2.39	0.41
5:q:168:ARG:HH12	5:q:184:ARG:HH11	1.69	0.41
4:H:94:HIS:HE1	8:H:201:HEM:C4A	2.39	0.41
1:I:51:PHE:CZ	8:I:201:HEM:HBC2	2.55	0.41
7:O:117:ARG:O	7:O:149:LYS:NZ	2.46	0.41
3:V:28:LYS:HB2	3:V:28:LYS:HE2	1.77	0.41
1:m:34:GLY:O	1:m:38:LYS:HG3	2.21	0.41
5:q:142:LYS:N	5:q:143:PRO:HD3	2.36	0.41
1:A:21:TRP:CD1	1:A:22:SER:N	2.89	0.40
2:B:37:PHE:HB3	2:B:44:ARG:NH1	2.36	0.40
1:E:47:ALA:HB1	8:E:201:HEM:HBC1	2.02	0.40
1:I:16:ILE:HG12	7:O:205:ALA:HB1	2.02	0.40
1:I:53:ARG:HD2	1:I:53:ARG:O	2.21	0.40
5:M:142:LYS:N	5:M:143:PRO:HD3	2.36	0.40
1:P:102:ARG:HA	1:P:102:ARG:HD3	1.86	0.40
2:Q:50:VAL:CG2	2:Q:63:HIS:HB2	2.50	0.40
1:T:81:LEU:HD23	1:T:88:LEU:HA	2.03	0.40
2:Y:16:ARG:O	2:Y:20:SER:OG	2.38	0.40
2:Y:50:VAL:CG2	2:Y:63:HIS:HB2	2.51	0.40
5:b:187:LYS:O	5:b:189:VAL:HG23	2.21	0.40
2:f:16:ARG:O	2:f:20:SER:OG	2.39	0.40
2:j:98:ARG:HH11	2:j:98:ARG:HG2	1.84	0.40
2:n:16:ARG:O	2:n:20:SER:OG	2.39	0.40
3:o:13:VAL:HB	3:o:83:MET:HE1	2.02	0.40
5:q:187:LYS:O	5:q:189:VAL:N	2.53	0.40
6:r:21:LEU:HD12	6:r:21:LEU:HA	1.96	0.40
1:A:25:PHE:CD2	3:C:28:LYS:HG2	2.56	0.40
3:G:84:ASP:O	3:G:86:PRO:HD3	2.20	0.40
3:G:144:LYS:HE2	3:G:144:LYS:HB2	1.73	0.40
2:J:29:ALA:HB1	2:J:64:ALA:HB1	2.02	0.40
3:K:70:LEU:HA	3:K:70:LEU:HD23	1.86	0.40
4:W:68:SER:O	4:W:72:MET:HG3	2.22	0.40
1:X:131:GLU:HB3	1:X:135:ARG:HH12	1.86	0.40
2:Y:109:LYS:HB2	2:Y:133:PHE:CE1	2.56	0.40
2:f:50:VAL:CG2	2:f:63:HIS:HB2	2.50	0.40
2:n:100:ILE:HA	2:n:101:PRO:HD2	1.92	0.40
5:q:50:LEU:HD21	6:r:57:LEU:HB3	2.03	0.40
5:q:119:ALA:O	5:q:121:GLU:N	2.49	0.40
6:r:124:TRP:CE3	6:r:226:ALA:HB2	2.56	0.40
2:B:50:VAL:CG2	2:B:63:HIS:HB2	2.52	0.40
2:B:109:LYS:HB2	2:B:133:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:15:LYS:HB2	3:C:15:LYS:HE3	1.85	0.40
1:E:81:LEU:HD11	4:H:64:GLU:HG2	2.03	0.40
2:F:98:ARG:CZ	8:F:201:HEM:HAD2	2.51	0.40
2:F:100:ILE:HA	2:F:101:PRO:HD2	1.91	0.40
2:Q:2:GLU:HG2	2:Q:3:CYS:H	1.86	0.40
2:U:29:ALA:HB1	2:U:64:ALA:HB1	2.03	0.40
2:U:100:ILE:HA	2:U:101:PRO:HD2	1.89	0.40
1:X:95:LEU:HD12	1:X:95:LEU:HA	1.93	0.40
2:Y:100:ILE:HA	2:Y:101:PRO:HD2	1.90	0.40
7:d:107:GLY:HA2	7:d:214:ILE:O	2.20	0.40
2:f:113:LEU:HD12	2:f:113:LEU:HA	1.90	0.40
2:f:122:ARG:HG2	5:q:193:ARG:HH22	1.87	0.40
4:h:20:GLU:HB3	4:h:22:HIS:CE1	2.56	0.40
1:i:131:GLU:HB3	1:i:135:ARG:HH12	1.87	0.40
2:j:50:VAL:CG2	2:j:63:HIS:HB2	2.50	0.40
3:G:36:LEU:HD22	4:H:5:LEU:HD21	2.04	0.40
5:M:27:ASP:O	5:M:31:ILE:HG13	2.21	0.40
7:O:203:HIS:C	7:O:205:ALA:H	2.28	0.40
2:Y:98:ARG:HH11	2:Y:98:ARG:HG2	1.87	0.40
1:i:34:GLY:O	1:i:38:LYS:HG3	2.21	0.40
2:j:109:LYS:HB2	2:j:133:PHE:CE1	2.56	0.40
3:o:22:GLY:HA3	4:p:15:ARG:HH12	1.86	0.40
2:B:21:HIS:C	2:B:23:HIS:H	2.25	0.40
4:H:8:LEU:HD12	4:H:8:LEU:HA	1.90	0.40
2:Q:49:ARG:HH11	8:Q:201:HEM:CGD	2.34	0.40
2:Q:51:HIS:ND1	2:Q:59:GLU:HG3	2.37	0.40
3:R:15:LYS:HB2	3:R:15:LYS:HE3	1.84	0.40
4:W:74:ILE:O	4:W:77:LEU:HB2	2.22	0.40
1:X:57:ALA:C	1:X:59:PRO:HD3	2.46	0.40
6:c:76:CYS:O	6:c:100:HIS:ND1	2.54	0.40
6:c:124:TRP:CE3	6:c:226:ALA:HB2	2.57	0.40
2:j:37:PHE:HB3	2:j:44:ARG:NH1	2.37	0.40
3:k:144:LYS:HB2	3:k:144:LYS:HE2	1.74	0.40
6:r:51:GLU:O	6:r:55:LYS:HG3	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:107:LYS:NZ	1:P:58:GLU:OE2[2_555]	1.95	0.25
4:W:100:ASN:ND2	1:i:52:GLU:OE2[8_444]	2.19	0.01

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	146/150 (97%)	141 (97%)	3 (2%)	2 (1%)	9	39
1	E	146/150 (97%)	140 (96%)	4 (3%)	2 (1%)	9	39
1	I	146/150 (97%)	142 (97%)	3 (2%)	1 (1%)	18	52
1	P	146/150 (97%)	142 (97%)	3 (2%)	1 (1%)	18	52
1	T	146/150 (97%)	141 (97%)	3 (2%)	2 (1%)	9	39
1	X	146/150 (97%)	139 (95%)	6 (4%)	1 (1%)	18	52
1	e	146/150 (97%)	140 (96%)	4 (3%)	2 (1%)	9	39
1	i	146/150 (97%)	136 (93%)	7 (5%)	3 (2%)	5	31
1	m	146/150 (97%)	142 (97%)	3 (2%)	1 (1%)	18	52
2	B	140/142 (99%)	132 (94%)	5 (4%)	3 (2%)	5	31
2	F	140/142 (99%)	133 (95%)	4 (3%)	3 (2%)	5	31
2	J	140/142 (99%)	132 (94%)	5 (4%)	3 (2%)	5	31
2	Q	140/142 (99%)	132 (94%)	5 (4%)	3 (2%)	5	31
2	U	140/142 (99%)	133 (95%)	4 (3%)	3 (2%)	5	31
2	Y	140/142 (99%)	132 (94%)	5 (4%)	3 (2%)	5	31
2	f	140/142 (99%)	132 (94%)	5 (4%)	3 (2%)	5	31
2	j	140/142 (99%)	132 (94%)	5 (4%)	3 (2%)	5	31
2	n	140/142 (99%)	132 (94%)	5 (4%)	3 (2%)	5	31
3	C	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
3	G	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
3	K	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
3	R	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
3	V	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
3	Z	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
3	g	149/151 (99%)	145 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	k	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
3	o	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
4	D	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
4	H	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
4	L	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
4	S	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
4	W	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
4	a	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
4	h	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
4	l	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
4	p	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
5	M	220/224 (98%)	208 (94%)	10 (4%)	2 (1%)	14	47
5	b	220/224 (98%)	208 (94%)	10 (4%)	2 (1%)	14	47
5	q	220/224 (98%)	207 (94%)	11 (5%)	2 (1%)	14	47
6	N	217/236 (92%)	198 (91%)	11 (5%)	8 (4%)	2	18
6	c	217/236 (92%)	199 (92%)	10 (5%)	8 (4%)	2	18
6	r	217/236 (92%)	198 (91%)	11 (5%)	8 (4%)	2	18
7	O	211/218 (97%)	199 (94%)	10 (5%)	2 (1%)	14	47
7	d	211/218 (97%)	200 (95%)	9 (4%)	2 (1%)	14	47
7	s	211/218 (97%)	199 (94%)	10 (5%)	2 (1%)	14	47
All	All	7110/7290 (98%)	6781 (95%)	251 (4%)	78 (1%)	11	43

All (78) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	N	19	PRO
6	N	76	CYS
6	N	233	GLN
6	N	235	HIS
6	c	19	PRO
6	c	76	CYS
6	c	233	GLN
6	c	235	HIS
1	e	53	ARG
1	i	53	ARG

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Mol	Chain	Res	Type
6	r	19	PRO
6	r	76	CYS
6	r	233	GLN
6	r	235	HIS
2	B	21	HIS
2	B	22	GLY
2	F	21	HIS
2	F	22	GLY
2	J	21	HIS
2	J	22	GLY
7	O	95	CYS
2	Q	21	HIS
2	Q	22	GLY
1	T	53	ARG
2	U	21	HIS
2	U	22	GLY
2	Y	21	HIS
2	Y	22	GLY
2	f	21	HIS
2	f	22	GLY
1	i	62	GLY
2	j	21	HIS
2	j	22	GLY
2	n	21	HIS
2	n	22	GLY
7	s	95	CYS
5	M	188	PRO
6	N	192	ALA
6	N	195	ASP
6	N	234	GLY
5	b	188	PRO
6	c	192	ALA
6	c	195	ASP
6	c	234	GLY
7	d	95	CYS
5	q	188	PRO
6	r	192	ALA
6	r	195	ASP
1	A	22	SER
1	E	22	SER
2	F	23	HIS
1	I	22	SER

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Mol	Chain	Res	Type
6	N	127	CYS
1	P	22	SER
1	T	22	SER
2	U	23	HIS
1	X	22	SER
6	c	127	CYS
1	e	22	SER
2	f	23	HIS
1	i	22	SER
2	j	23	HIS
1	m	22	SER
6	r	127	CYS
6	r	234	GLY
2	B	23	HIS
2	J	23	HIS
2	Q	23	HIS
2	Y	23	HIS
2	n	23	HIS
7	s	114	CYS
1	A	56	VAL
1	E	149	PRO
5	M	187	LYS
7	O	114	CYS
5	b	187	LYS
7	d	114	CYS
5	q	187	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	129/131 (98%)	119 (92%)	10 (8%)	11	41
1	E	129/131 (98%)	119 (92%)	10 (8%)	11	41
1	I	129/131 (98%)	118 (92%)	11 (8%)	10	37
1	P	129/131 (98%)	118 (92%)	11 (8%)	10	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	T	129/131 (98%)	116 (90%)	13 (10%)	7	30
1	X	129/131 (98%)	117 (91%)	12 (9%)	8	33
1	e	129/131 (98%)	117 (91%)	12 (9%)	8	33
1	i	129/131 (98%)	112 (87%)	17 (13%)	4	19
1	m	129/131 (98%)	119 (92%)	10 (8%)	11	41
2	B	117/117 (100%)	110 (94%)	7 (6%)	17	50
2	F	117/117 (100%)	110 (94%)	7 (6%)	17	50
2	J	117/117 (100%)	110 (94%)	7 (6%)	17	50
2	Q	117/117 (100%)	110 (94%)	7 (6%)	17	50
2	U	117/117 (100%)	110 (94%)	7 (6%)	17	50
2	Y	117/117 (100%)	110 (94%)	7 (6%)	17	50
2	f	117/117 (100%)	110 (94%)	7 (6%)	17	50
2	j	117/117 (100%)	110 (94%)	7 (6%)	17	50
2	n	117/117 (100%)	110 (94%)	7 (6%)	17	50
3	C	128/130 (98%)	121 (94%)	7 (6%)	19	52
3	G	128/130 (98%)	121 (94%)	7 (6%)	19	52
3	K	128/130 (98%)	121 (94%)	7 (6%)	19	52
3	R	128/130 (98%)	121 (94%)	7 (6%)	19	52
3	V	128/130 (98%)	120 (94%)	8 (6%)	16	48
3	Z	128/130 (98%)	121 (94%)	7 (6%)	19	52
3	g	128/130 (98%)	121 (94%)	7 (6%)	19	52
3	k	128/130 (98%)	121 (94%)	7 (6%)	19	52
3	o	130/130 (100%)	121 (93%)	9 (7%)	14	45
4	D	120/120 (100%)	114 (95%)	6 (5%)	22	55
4	H	120/120 (100%)	114 (95%)	6 (5%)	22	55
4	L	120/120 (100%)	114 (95%)	6 (5%)	22	55
4	S	120/120 (100%)	114 (95%)	6 (5%)	22	55
4	W	120/120 (100%)	114 (95%)	6 (5%)	22	55
4	a	120/120 (100%)	114 (95%)	6 (5%)	22	55
4	h	120/120 (100%)	114 (95%)	6 (5%)	22	55
4	l	120/120 (100%)	114 (95%)	6 (5%)	22	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	p	120/120 (100%)	113 (94%)	7 (6%)	18	51
5	M	185/194 (95%)	178 (96%)	7 (4%)	29	62
5	b	185/194 (95%)	179 (97%)	6 (3%)	34	65
5	q	185/194 (95%)	178 (96%)	7 (4%)	29	62
6	N	181/205 (88%)	170 (94%)	11 (6%)	17	49
6	c	181/205 (88%)	170 (94%)	11 (6%)	17	49
6	r	181/205 (88%)	170 (94%)	11 (6%)	17	49
7	O	187/193 (97%)	176 (94%)	11 (6%)	18	50
7	d	187/193 (97%)	176 (94%)	11 (6%)	18	50
7	s	187/193 (97%)	176 (94%)	11 (6%)	18	50
All	All	6107/6258 (98%)	5731 (94%)	376 (6%)	16	49

All (376) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	VAL
1	A	63	GLU
1	A	73	ASN
1	A	81	LEU
1	A	84	ASP
1	A	89	ASP
1	A	92	LEU
1	A	116	SER
1	A	130	LEU
1	A	146	ARG
2	B	3	CYS
2	B	26	GLU
2	B	59	GLU
2	B	112	LEU
2	B	113	LEU
2	B	119	GLN
2	B	124	TRP
3	C	71	ARG
3	C	72	ILE
3	C	73	LEU
3	C	113	LYS
3	C	118	LEU
3	C	127	ASP

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Mol	Chain	Res	Type
3	C	136	SER
4	D	8	LEU
4	D	25	VAL
4	D	41	GLU
4	D	52	ASP
4	D	77	LEU
4	D	80	THR
1	E	56	VAL
1	E	63	GLU
1	E	73	ASN
1	E	81	LEU
1	E	84	ASP
1	E	89	ASP
1	E	92	LEU
1	E	116	SER
1	E	130	LEU
1	E	146	ARG
2	F	3	CYS
2	F	26	GLU
2	F	59	GLU
2	F	112	LEU
2	F	113	LEU
2	F	119	GLN
2	F	124	TRP
3	G	71	ARG
3	G	72	ILE
3	G	73	LEU
3	G	113	LYS
3	G	118	LEU
3	G	127	ASP
3	G	136	SER
4	H	8	LEU
4	H	25	VAL
4	H	41	GLU
4	H	52	ASP
4	H	77	LEU
4	H	80	THR
1	I	52	GLU
1	I	56	VAL
1	I	63	GLU
1	I	73	ASN
1	I	81	LEU

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Mol	Chain	Res	Type
1	I	84	ASP
1	I	89	ASP
1	I	92	LEU
1	I	116	SER
1	I	130	LEU
1	I	146	ARG
2	J	3	CYS
2	J	26	GLU
2	J	59	GLU
2	J	112	LEU
2	J	113	LEU
2	J	119	GLN
2	J	124	TRP
3	K	71	ARG
3	K	72	ILE
3	K	73	LEU
3	K	113	LYS
3	K	118	LEU
3	K	127	ASP
3	K	136	SER
4	L	8	LEU
4	L	25	VAL
4	L	41	GLU
4	L	52	ASP
4	L	77	LEU
4	L	80	THR
5	M	42	VAL
5	M	80	LEU
5	M	114	VAL
5	M	130	VAL
5	M	132	ILE
5	M	162	ILE
5	M	164	THR
6	N	20	ARG
6	N	84	ILE
6	N	105	ASP
6	N	126	ASP
6	N	127	CYS
6	N	129	LEU
6	N	131	SER
6	N	191	ILE
6	N	200	VAL

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Mol	Chain	Res	Type
6	N	233	GLN
6	N	235	HIS
7	O	14	LEU
7	O	21	LEU
7	O	28	LEU
7	O	32	LEU
7	O	61	ASP
7	O	130	SER
7	O	141	LEU
7	O	151	THR
7	O	158	VAL
7	O	196	ARG
7	O	206	SER
1	P	55	LYS
1	P	56	VAL
1	P	63	GLU
1	P	73	ASN
1	P	81	LEU
1	P	84	ASP
1	P	89	ASP
1	P	92	LEU
1	P	116	SER
1	P	130	LEU
1	P	146	ARG
2	Q	3	CYS
2	Q	26	GLU
2	Q	59	GLU
2	Q	112	LEU
2	Q	113	LEU
2	Q	119	GLN
2	Q	124	TRP
3	R	71	ARG
3	R	72	ILE
3	R	73	LEU
3	R	113	LYS
3	R	118	LEU
3	R	127	ASP
3	R	136	SER
4	S	8	LEU
4	S	25	VAL
4	S	41	GLU
4	S	52	ASP

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Mol	Chain	Res	Type
4	S	77	LEU
4	S	80	THR
1	T	52	GLU
1	T	53	ARG
1	T	54	VAL
1	T	56	VAL
1	T	63	GLU
1	T	73	ASN
1	T	81	LEU
1	T	84	ASP
1	T	89	ASP
1	T	92	LEU
1	T	116	SER
1	T	130	LEU
1	T	146	ARG
2	U	3	CYS
2	U	26	GLU
2	U	59	GLU
2	U	112	LEU
2	U	113	LEU
2	U	119	GLN
2	U	124	TRP
3	V	71	ARG
3	V	72	ILE
3	V	73	LEU
3	V	113	LYS
3	V	118	LEU
3	V	125	VAL
3	V	127	ASP
3	V	136	SER
4	W	8	LEU
4	W	25	VAL
4	W	41	GLU
4	W	52	ASP
4	W	77	LEU
4	W	80	THR
1	X	50	LEU
1	X	53	ARG
1	X	63	GLU
1	X	73	ASN
1	X	81	LEU
1	X	84	ASP

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Mol	Chain	Res	Type
1	X	89	ASP
1	X	92	LEU
1	X	116	SER
1	X	130	LEU
1	X	146	ARG
1	X	150	HIS
2	Y	3	CYS
2	Y	26	GLU
2	Y	59	GLU
2	Y	112	LEU
2	Y	113	LEU
2	Y	119	GLN
2	Y	124	TRP
3	Z	71	ARG
3	Z	72	ILE
3	Z	73	LEU
3	Z	113	LYS
3	Z	118	LEU
3	Z	127	ASP
3	Z	136	SER
4	a	8	LEU
4	a	25	VAL
4	a	41	GLU
4	a	52	ASP
4	a	77	LEU
4	a	80	THR
5	b	42	VAL
5	b	80	LEU
5	b	114	VAL
5	b	130	VAL
5	b	162	ILE
5	b	164	THR
6	c	20	ARG
6	c	84	ILE
6	c	105	ASP
6	c	126	ASP
6	c	127	CYS
6	c	129	LEU
6	c	131	SER
6	c	191	ILE
6	c	200	VAL
6	c	233	GLN

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Mol	Chain	Res	Type
6	c	235	HIS
7	d	14	LEU
7	d	21	LEU
7	d	28	LEU
7	d	32	LEU
7	d	61	ASP
7	d	130	SER
7	d	141	LEU
7	d	151	THR
7	d	158	VAL
7	d	196	ARG
7	d	206	SER
1	e	53	ARG
1	e	58	GLU
1	e	61	SER
1	e	63	GLU
1	e	73	ASN
1	e	81	LEU
1	e	84	ASP
1	e	89	ASP
1	e	92	LEU
1	e	116	SER
1	e	130	LEU
1	e	146	ARG
2	f	3	CYS
2	f	26	GLU
2	f	59	GLU
2	f	112	LEU
2	f	113	LEU
2	f	119	GLN
2	f	124	TRP
3	g	71	ARG
3	g	72	ILE
3	g	73	LEU
3	g	113	LYS
3	g	118	LEU
3	g	127	ASP
3	g	136	SER
4	h	8	LEU
4	h	25	VAL
4	h	41	GLU
4	h	52	ASP

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Mol	Chain	Res	Type
4	h	77	LEU
4	h	80	THR
1	i	50	LEU
1	i	52	GLU
1	i	53	ARG
1	i	55	LYS
1	i	56	VAL
1	i	58	GLU
1	i	61	SER
1	i	63	GLU
1	i	73	ASN
1	i	81	LEU
1	i	84	ASP
1	i	89	ASP
1	i	92	LEU
1	i	116	SER
1	i	130	LEU
1	i	146	ARG
1	i	150	HIS
2	j	3	CYS
2	j	26	GLU
2	j	59	GLU
2	j	112	LEU
2	j	113	LEU
2	j	119	GLN
2	j	124	TRP
3	k	71	ARG
3	k	72	ILE
3	k	73	LEU
3	k	113	LYS
3	k	118	LEU
3	k	127	ASP
3	k	136	SER
4	l	8	LEU
4	l	25	VAL
4	l	41	GLU
4	l	52	ASP
4	l	77	LEU
4	l	80	THR
1	m	56	VAL
1	m	63	GLU
1	m	73	ASN

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Mol	Chain	Res	Type
1	m	81	LEU
1	m	84	ASP
1	m	89	ASP
1	m	92	LEU
1	m	116	SER
1	m	130	LEU
1	m	146	ARG
2	n	3	CYS
2	n	26	GLU
2	n	59	GLU
2	n	112	LEU
2	n	113	LEU
2	n	119	GLN
2	n	124	TRP
3	o	1	HIS
3	o	71	ARG
3	o	72	ILE
3	o	73	LEU
3	o	113	LYS
3	o	118	LEU
3	o	125	VAL
3	o	127	ASP
3	o	136	SER
4	p	6	GLU
4	p	8	LEU
4	p	25	VAL
4	p	41	GLU
4	p	52	ASP
4	p	77	LEU
4	p	80	THR
5	q	42	VAL
5	q	80	LEU
5	q	114	VAL
5	q	130	VAL
5	q	132	ILE
5	q	162	ILE
5	q	164	THR
6	r	20	ARG
6	r	84	ILE
6	r	105	ASP
6	r	126	ASP
6	r	127	CYS

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Mol	Chain	Res	Type
6	r	129	LEU
6	r	131	SER
6	r	191	ILE
6	r	200	VAL
6	r	233	GLN
6	r	235	HIS
7	s	14	LEU
7	s	21	LEU
7	s	28	LEU
7	s	32	LEU
7	s	61	ASP
7	s	130	SER
7	s	141	LEU
7	s	151	THR
7	s	158	VAL
7	s	196	ARG
7	s	206	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	HIS
2	B	23	HIS
2	B	63	HIS
1	E	138	HIS
2	F	63	HIS
4	H	89	HIS
1	I	138	HIS
2	J	63	HIS
5	M	65	HIS
5	M	195	HIS
6	N	24	ASN
6	N	93	HIS
6	N	180	ASN
6	N	215	HIS
6	N	227	ASN
6	N	231	HIS
7	O	15	ASN
7	O	209	HIS
1	P	67	HIS
1	P	138	HIS
2	Q	23	HIS

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Mol	Chain	Res	Type
2	Q	63	HIS
1	T	43	HIS
1	T	138	HIS
2	U	63	HIS
4	W	125	GLN
1	X	86	GLN
1	X	138	HIS
1	X	150	HIS
4	a	62	HIS
5	b	195	HIS
6	c	93	HIS
6	c	125	HIS
6	c	180	ASN
6	c	231	HIS
1	e	138	HIS
2	f	23	HIS
2	f	63	HIS
1	i	138	HIS
1	i	150	HIS
2	j	63	HIS
4	l	89	HIS
1	m	138	HIS
1	m	150	HIS
5	q	225	HIS
6	r	24	ASN
6	r	93	HIS
6	r	125	HIS
6	r	180	ASN
7	s	15	ASN
7	s	113	HIS
7	s	209	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 90 ligands modelled in this entry, 15 are monoatomic - leaving 75 for Mogul analysis.

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
9	CYN	R	202	-	1,1,1	0.34	0	-		
8	HEM	F	201	9,2	50,50,50	2.19	10 (20%)	67,82,82	1.74	17 (25%)
8	HEM	S	201	4	50,50,50	2.19	11 (22%)	67,82,82	1.77	15 (22%)
9	CYN	h	202	-	1,1,1	0.31	0	-		
8	HEM	Z	201	3	50,50,50	2.19	11 (22%)	67,82,82	1.71	13 (19%)
12	NAG	O	304	7	14,14,15	0.39	0	17,19,21	1.80	3 (17%)
9	CYN	X	202	-	1,1,1	0.31	0	-		
9	CYN	I	202	-	1,1,1	0.31	0	-		
9	CYN	W	202	8	1,1,1	0.30	0	-		
9	CYN	G	202	8	1,1,1	0.31	0	-		
8	HEM	E	201	1	50,50,50	2.26	10 (20%)	67,82,82	1.86	14 (20%)
9	CYN	H	202	-	1,1,1	0.31	0	-		
9	CYN	l	202	-	1,1,1	0.33	0	-		
9	CYN	K	202	-	1,1,1	0.30	0	-		
9	CYN	j	202	8	1,1,1	0.29	0	-		
9	CYN	A	202	-	1,1,1	0.29	0	-		
9	CYN	T	202	-	1,1,1	0.32	0	-		
9	CYN	p	202	8	1,1,1	0.29	0	-		
8	HEM	V	201	9,3	50,50,50	2.22	9 (18%)	67,82,82	1.76	13 (19%)
9	CYN	F	202	8	1,1,1	0.29	0	-		
8	HEM	H	201	4	50,50,50	2.15	11 (22%)	67,82,82	1.70	14 (20%)
9	CYN	S	202	-	1,1,1	0.32	0	-		
8	HEM	G	201	9,3	50,50,50	2.22	10 (20%)	67,82,82	1.79	15 (22%)
8	HEM	h	201	4	50,50,50	2.21	11 (22%)	67,82,82	1.71	14 (20%)
8	HEM	T	201	1	50,50,50	2.30	10 (20%)	67,82,82	1.84	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	CYN	P	202	-	1,1,1	0.30	0	-		
9	CYN	f	202	8	1,1,1	0.28	0	-		
8	HEM	e	201	9,1	50,50,50	2.27	10 (20%)	67,82,82	1.95	20 (29%)
8	HEM	W	201	9,4	50,50,50	2.23	10 (20%)	67,82,82	1.80	17 (25%)
8	HEM	Q	201	2	50,50,50	2.18	10 (20%)	67,82,82	1.79	17 (25%)
8	HEM	R	201	3	50,50,50	2.15	11 (22%)	67,82,82	1.72	13 (19%)
9	CYN	D	202	-	1,1,1	0.31	0	-		
8	HEM	i	201	1	50,50,50	2.32	8 (16%)	67,82,82	1.83	17 (25%)
9	CYN	E	202	-	1,1,1	0.30	0	-		
9	CYN	o	202	8	1,1,1	0.31	0	-		
8	HEM	f	201	9,2	50,50,50	2.18	9 (18%)	67,82,82	1.77	17 (25%)
8	HEM	U	201	9,2	50,50,50	2.23	9 (18%)	67,82,82	1.78	17 (25%)
8	HEM	C	201	3	50,50,50	2.10	10 (20%)	67,82,82	1.66	14 (20%)
9	CYN	B	202	8	1,1,1	0.27	0	-		
9	CYN	V	202	8	1,1,1	0.29	0	-		
9	CYN	n	202	8	1,1,1	0.30	0	-		
9	CYN	m	202	8	1,1,1	0.30	0	-		
12	NAG	d	304	7	14,14,15	0.42	0	17,19,21	1.20	2 (11%)
9	CYN	k	202	8	1,1,1	0.29	0	-		
8	HEM	A	201	1	50,50,50	2.21	10 (20%)	67,82,82	1.91	17 (25%)
8	HEM	P	201	1	50,50,50	2.31	10 (20%)	67,82,82	1.91	19 (28%)
8	HEM	a	201	9,4	50,50,50	2.21	9 (18%)	67,82,82	1.76	18 (26%)
8	HEM	p	201	9,4	50,50,50	2.23	11 (22%)	67,82,82	1.87	17 (25%)
8	HEM	D	201	4	50,50,50	2.20	10 (20%)	67,82,82	1.72	13 (19%)
8	HEM	L	201	4	50,50,50	2.18	10 (20%)	67,82,82	1.82	16 (23%)
9	CYN	e	202	8	1,1,1	0.30	0	-		
8	HEM	Y	201	9,2	50,50,50	2.30	10 (20%)	67,82,82	1.81	16 (23%)
9	CYN	g	202	-	1,1,1	0.33	0	-		
9	CYN	J	202	8	1,1,1	0.29	0	-		
8	HEM	X	201	1	50,50,50	2.26	10 (20%)	67,82,82	1.95	16 (23%)
8	HEM	m	201	9,1	50,50,50	2.31	10 (20%)	67,82,82	2.02	16 (23%)
9	CYN	i	202	-	1,1,1	0.33	0	-		
8	HEM	I	201	1	50,50,50	2.24	10 (20%)	67,82,82	1.85	17 (25%)
9	CYN	U	202	8	1,1,1	0.30	0	-		
8	HEM	g	201	3	50,50,50	2.13	10 (20%)	67,82,82	1.71	13 (19%)
8	HEM	k	201	9,3	50,50,50	2.30	10 (20%)	67,82,82	1.81	16 (23%)
8	HEM	j	201	9,2	50,50,50	2.21	11 (22%)	67,82,82	1.78	17 (25%)
8	HEM	l	201	4	50,50,50	2.20	10 (20%)	67,82,82	1.74	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	HEM	o	201	9,3	50,50,50	2.21	11 (22%)	67,82,82	1.73	13 (19%)
9	CYN	C	202	-	1,1,1	0.34	0	-		
9	CYN	L	202	-	1,1,1	0.31	0	-		
12	NAG	s	303	7	14,14,15	0.48	0	17,19,21	1.34	2 (11%)
8	HEM	B	201	9,2	50,50,50	2.22	11 (22%)	67,82,82	1.79	16 (23%)
8	HEM	n	201	9,2	50,50,50	2.26	10 (20%)	67,82,82	1.81	21 (31%)
9	CYN	a	202	8	1,1,1	0.29	0	-		
8	HEM	K	201	3	50,50,50	2.23	13 (26%)	67,82,82	1.75	14 (20%)
9	CYN	Z	202	-	1,1,1	0.30	0	-		
9	CYN	Y	202	8	1,1,1	0.30	0	-		
9	CYN	Q	202	-	1,1,1	0.25	0	-		
8	HEM	J	201	9,2	50,50,50	2.26	10 (20%)	67,82,82	1.85	17 (25%)

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
8	HEM	F	201	9,2	-	8/14/54/54	-
8	HEM	S	201	4	-	8/14/54/54	-
8	HEM	Z	201	3	-	5/14/54/54	-
12	NAG	O	304	7	-	0/6/23/26	0/1/1/1
8	HEM	E	201	1	-	6/14/54/54	-
8	HEM	V	201	9,3	-	8/14/54/54	-
8	HEM	H	201	4	-	6/14/54/54	-
8	HEM	G	201	9,3	-	6/14/54/54	-
8	HEM	h	201	4	-	8/14/54/54	-
8	HEM	T	201	1	-	6/14/54/54	-
8	HEM	e	201	9,1	-	8/14/54/54	-
8	HEM	W	201	9,4	-	8/14/54/54	-
8	HEM	Q	201	2	-	8/14/54/54	-
8	HEM	R	201	3	-	6/14/54/54	-
8	HEM	i	201	1	-	6/14/54/54	-
8	HEM	f	201	9,2	-	6/14/54/54	-
8	HEM	U	201	9,2	-	6/14/54/54	-
8	HEM	C	201	3	-	8/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	d	304	7	-	0/6/23/26	0/1/1/1
8	HEM	A	201	1	-	6/14/54/54	-
8	HEM	P	201	1	-	7/14/54/54	-
8	HEM	a	201	9,4	-	8/14/54/54	-
8	HEM	p	201	9,4	-	8/14/54/54	-
8	HEM	D	201	4	-	6/14/54/54	-
8	HEM	L	201	4	-	10/14/54/54	-
8	HEM	Y	201	9,2	-	9/14/54/54	-
8	HEM	X	201	1	-	7/14/54/54	-
8	HEM	m	201	9,1	-	6/14/54/54	-
8	HEM	I	201	1	-	4/14/54/54	-
8	HEM	g	201	3	-	6/14/54/54	-
8	HEM	k	201	9,3	-	6/14/54/54	-
8	HEM	j	201	9,2	-	8/14/54/54	-
8	HEM	l	201	4	-	8/14/54/54	-
8	HEM	o	201	9,3	-	6/14/54/54	-
12	NAG	s	303	7	-	0/6/23/26	0/1/1/1
8	HEM	B	201	9,2	-	8/14/54/54	-
8	HEM	n	201	9,2	-	7/14/54/54	-
8	HEM	K	201	3	-	6/14/54/54	-
8	HEM	J	201	9,2	-	6/14/54/54	-

All (366) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	l	201	HEM	C3D-C2D	8.28	1.54	1.36
8	J	201	HEM	C3D-C2D	8.25	1.54	1.36
8	p	201	HEM	C3D-C2D	8.24	1.54	1.36
8	W	201	HEM	C3D-C2D	8.16	1.54	1.36
8	D	201	HEM	C3D-C2D	8.15	1.54	1.36
8	U	201	HEM	C3D-C2D	8.14	1.54	1.36
8	S	201	HEM	C3D-C2D	8.13	1.54	1.36
8	H	201	HEM	C3D-C2D	8.12	1.54	1.36
8	Y	201	HEM	C3D-C2D	8.11	1.54	1.36
8	n	201	HEM	C3D-C2D	8.08	1.54	1.36
8	h	201	HEM	C3D-C2D	8.08	1.54	1.36
8	k	201	HEM	C3D-C2D	8.07	1.54	1.36
8	j	201	HEM	C3D-C2D	8.07	1.54	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	X	201	HEM	C3D-C2D	8.03	1.54	1.36
8	i	201	HEM	C3D-C2D	7.98	1.54	1.36
8	F	201	HEM	C3D-C2D	7.97	1.54	1.36
8	T	201	HEM	C3D-C2D	7.96	1.53	1.36
8	a	201	HEM	C3D-C2D	7.95	1.53	1.36
8	P	201	HEM	C3D-C2D	7.95	1.53	1.36
8	L	201	HEM	C3D-C2D	7.89	1.53	1.36
8	Z	201	HEM	C3D-C2D	7.87	1.53	1.36
8	V	201	HEM	C3D-C2D	7.86	1.53	1.36
8	I	201	HEM	C3D-C2D	7.84	1.53	1.36
8	o	201	HEM	C3D-C2D	7.84	1.53	1.36
8	Q	201	HEM	C3D-C2D	7.83	1.53	1.36
8	G	201	HEM	C3D-C2D	7.82	1.53	1.36
8	R	201	HEM	C3D-C2D	7.82	1.53	1.36
8	K	201	HEM	C3D-C2D	7.81	1.53	1.36
8	e	201	HEM	C3D-C2D	7.80	1.53	1.36
8	m	201	HEM	C3D-C2D	7.80	1.53	1.36
8	g	201	HEM	C3D-C2D	7.79	1.53	1.36
8	B	201	HEM	C3D-C2D	7.76	1.53	1.36
8	A	201	HEM	C3D-C2D	7.73	1.53	1.36
8	E	201	HEM	C3D-C2D	7.71	1.53	1.36
8	f	201	HEM	C3D-C2D	7.66	1.53	1.36
8	C	201	HEM	C3D-C2D	7.57	1.53	1.36
8	e	201	HEM	FE-NB	6.82	2.15	1.94
8	G	201	HEM	FE-NB	6.46	2.14	1.94
8	Y	201	HEM	FE-NC	6.44	2.16	1.95
8	m	201	HEM	FE-ND	6.43	2.14	1.94
8	P	201	HEM	FE-NB	6.42	2.14	1.94
8	i	201	HEM	FE-NB	6.35	2.14	1.94
8	k	201	HEM	FE-NB	6.21	2.14	1.94
8	o	201	HEM	FE-NB	6.20	2.14	1.94
8	E	201	HEM	FE-NB	6.17	2.13	1.94
8	h	201	HEM	FE-NB	6.17	2.13	1.94
8	T	201	HEM	FE-NB	5.99	2.13	1.94
8	i	201	HEM	FE-NC	5.93	2.14	1.95
8	I	201	HEM	FE-ND	5.88	2.13	1.94
8	W	201	HEM	FE-NB	5.84	2.12	1.94
8	A	201	HEM	FE-NB	5.78	2.12	1.94
8	U	201	HEM	FE-NB	5.59	2.12	1.94
8	Y	201	HEM	FE-ND	5.58	2.12	1.94
8	V	201	HEM	FE-NB	5.51	2.11	1.94
8	n	201	HEM	FE-NC	5.49	2.13	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	K	201	HEM	FE-NB	5.48	2.11	1.94
8	B	201	HEM	FE-NB	5.48	2.11	1.94
8	S	201	HEM	FE-NB	5.45	2.11	1.94
8	X	201	HEM	FE-NB	5.41	2.11	1.94
8	D	201	HEM	FE-NB	5.40	2.11	1.94
8	a	201	HEM	FE-NB	5.39	2.11	1.94
8	T	201	HEM	FE-ND	5.38	2.11	1.94
8	B	201	HEM	FE-ND	5.34	2.11	1.94
8	E	201	HEM	FE-NC	5.27	2.12	1.95
8	F	201	HEM	FE-NB	5.24	2.11	1.94
8	l	201	HEM	FE-ND	5.23	2.11	1.94
8	n	201	HEM	FE-ND	5.19	2.10	1.94
8	Q	201	HEM	FE-ND	5.19	2.10	1.94
8	X	201	HEM	FE-ND	5.19	2.10	1.94
8	K	201	HEM	CBC-CAC	5.17	1.55	1.30
8	V	201	HEM	CBC-CAC	5.16	1.55	1.30
8	J	201	HEM	FE-NC	5.14	2.12	1.95
8	G	201	HEM	CBC-CAC	5.14	1.55	1.30
8	k	201	HEM	CBC-CAC	5.14	1.55	1.30
8	Z	201	HEM	CBC-CAC	5.13	1.55	1.30
8	p	201	HEM	FE-NB	5.13	2.10	1.94
8	o	201	HEM	CBC-CAC	5.11	1.55	1.30
8	g	201	HEM	CBC-CAC	5.09	1.54	1.30
8	a	201	HEM	CBB-CAB	5.09	1.54	1.30
8	F	201	HEM	CBC-CAC	5.09	1.54	1.30
8	J	201	HEM	CBB-CAB	5.09	1.54	1.30
8	n	201	HEM	CBC-CAC	5.08	1.54	1.30
8	j	201	HEM	FE-NB	5.08	2.10	1.94
8	p	201	HEM	CBB-CAB	5.08	1.54	1.30
8	J	201	HEM	CBC-CAC	5.07	1.54	1.30
8	i	201	HEM	CBC-CAC	5.07	1.54	1.30
8	h	201	HEM	CBB-CAB	5.07	1.54	1.30
8	j	201	HEM	CBC-CAC	5.07	1.54	1.30
8	F	201	HEM	CBB-CAB	5.07	1.54	1.30
8	Y	201	HEM	CBB-CAB	5.06	1.54	1.30
8	E	201	HEM	CBB-CAB	5.06	1.54	1.30
8	n	201	HEM	CBB-CAB	5.06	1.54	1.30
8	I	201	HEM	CBC-CAC	5.06	1.54	1.30
8	E	201	HEM	CBC-CAC	5.06	1.54	1.30
8	l	201	HEM	CBB-CAB	5.06	1.54	1.30
8	A	201	HEM	CBC-CAC	5.06	1.54	1.30
8	D	201	HEM	CBB-CAB	5.06	1.54	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	R	201	HEM	CBC-CAC	5.05	1.54	1.30
8	m	201	HEM	CBC-CAC	5.05	1.54	1.30
8	B	201	HEM	CBB-CAB	5.05	1.54	1.30
8	L	201	HEM	CBB-CAB	5.05	1.54	1.30
8	j	201	HEM	CBB-CAB	5.05	1.54	1.30
8	o	201	HEM	CBB-CAB	5.05	1.54	1.30
8	X	201	HEM	CBC-CAC	5.04	1.54	1.30
8	e	201	HEM	CBC-CAC	5.04	1.54	1.30
8	C	201	HEM	CBC-CAC	5.04	1.54	1.30
8	S	201	HEM	CBB-CAB	5.04	1.54	1.30
8	Q	201	HEM	CBB-CAB	5.03	1.54	1.30
8	k	201	HEM	CBB-CAB	5.03	1.54	1.30
8	P	201	HEM	CBC-CAC	5.03	1.54	1.30
8	T	201	HEM	CBC-CAC	5.03	1.54	1.30
8	R	201	HEM	CBB-CAB	5.03	1.54	1.30
8	W	201	HEM	CBB-CAB	5.02	1.54	1.30
8	B	201	HEM	CBC-CAC	5.02	1.54	1.30
8	U	201	HEM	CBB-CAB	5.02	1.54	1.30
8	G	201	HEM	CBB-CAB	5.02	1.54	1.30
8	f	201	HEM	CBC-CAC	5.02	1.54	1.30
8	U	201	HEM	CBC-CAC	5.02	1.54	1.30
8	m	201	HEM	FE-NB	5.01	2.10	1.94
8	f	201	HEM	CBB-CAB	5.01	1.54	1.30
8	H	201	HEM	FE-NB	5.01	2.10	1.94
8	Z	201	HEM	CBB-CAB	5.01	1.54	1.30
8	V	201	HEM	CBB-CAB	5.01	1.54	1.30
8	X	201	HEM	CBB-CAB	5.01	1.54	1.30
8	i	201	HEM	CBB-CAB	5.00	1.54	1.30
8	D	201	HEM	CBC-CAC	5.00	1.54	1.30
8	g	201	HEM	CBB-CAB	5.00	1.54	1.30
8	Q	201	HEM	CBC-CAC	4.99	1.54	1.30
8	Y	201	HEM	CBC-CAC	4.99	1.54	1.30
8	K	201	HEM	CBB-CAB	4.99	1.54	1.30
8	H	201	HEM	CBB-CAB	4.98	1.54	1.30
8	P	201	HEM	CBB-CAB	4.97	1.54	1.30
8	I	201	HEM	CBB-CAB	4.97	1.54	1.30
8	T	201	HEM	CBB-CAB	4.97	1.54	1.30
8	m	201	HEM	CBB-CAB	4.96	1.54	1.30
8	m	201	HEM	FE-NC	4.95	2.11	1.95
8	a	201	HEM	CBC-CAC	4.95	1.54	1.30
8	H	201	HEM	CBC-CAC	4.94	1.54	1.30
8	Z	201	HEM	FE-NB	4.94	2.10	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	201	HEM	CBB-CAB	4.94	1.54	1.30
8	C	201	HEM	CBB-CAB	4.94	1.54	1.30
8	S	201	HEM	CBC-CAC	4.93	1.54	1.30
8	e	201	HEM	CBB-CAB	4.93	1.54	1.30
8	l	201	HEM	CBC-CAC	4.93	1.54	1.30
8	W	201	HEM	CBC-CAC	4.93	1.54	1.30
8	p	201	HEM	CBC-CAC	4.91	1.54	1.30
8	L	201	HEM	CBC-CAC	4.91	1.54	1.30
8	h	201	HEM	CBC-CAC	4.91	1.54	1.30
8	F	201	HEM	FE-NC	4.84	2.11	1.95
8	C	201	HEM	FE-NB	4.84	2.09	1.94
8	f	201	HEM	FE-ND	4.82	2.09	1.94
8	g	201	HEM	FE-NB	4.80	2.09	1.94
8	W	201	HEM	FE-NA	4.79	2.11	1.95
8	L	201	HEM	FE-ND	4.78	2.09	1.94
8	L	201	HEM	FE-NB	4.78	2.09	1.94
8	Z	201	HEM	FE-ND	4.72	2.09	1.94
8	I	201	HEM	FE-NC	4.72	2.10	1.95
8	R	201	HEM	FE-NB	4.72	2.09	1.94
8	J	201	HEM	FE-ND	4.71	2.09	1.94
8	f	201	HEM	FE-NB	4.61	2.09	1.94
8	k	201	HEM	FE-NC	4.60	2.10	1.95
8	a	201	HEM	FE-NC	4.59	2.10	1.95
8	i	201	HEM	FE-ND	4.53	2.08	1.94
8	p	201	HEM	FE-NA	4.51	2.10	1.95
8	k	201	HEM	FE-ND	4.50	2.08	1.94
8	P	201	HEM	FE-NC	4.50	2.10	1.95
8	J	201	HEM	FE-NB	4.49	2.08	1.94
8	f	201	HEM	FE-NC	4.49	2.10	1.95
8	C	201	HEM	FE-ND	4.47	2.08	1.94
8	a	201	HEM	FE-ND	4.46	2.08	1.94
8	l	201	HEM	FE-NB	4.45	2.08	1.94
8	A	201	HEM	FE-NC	4.44	2.09	1.95
8	V	201	HEM	FE-ND	4.42	2.08	1.94
8	E	201	HEM	FE-ND	4.41	2.08	1.94
8	U	201	HEM	FE-NC	4.39	2.09	1.95
8	K	201	HEM	FE-ND	4.29	2.08	1.94
8	g	201	HEM	FE-ND	4.29	2.08	1.94
8	n	201	HEM	FE-NB	4.29	2.08	1.94
8	Q	201	HEM	FE-NB	4.28	2.08	1.94
8	p	201	HEM	FE-ND	4.28	2.08	1.94
8	D	201	HEM	FE-NA	4.27	2.09	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	201	HEM	FE-ND	4.25	2.08	1.94
8	K	201	HEM	FE-NA	4.23	2.09	1.95
8	Z	201	HEM	FE-NA	4.22	2.09	1.95
8	h	201	HEM	FE-NA	4.21	2.09	1.95
8	V	201	HEM	FE-NA	4.20	2.09	1.95
8	j	201	HEM	FE-NC	4.18	2.09	1.95
8	G	201	HEM	FE-NC	4.17	2.08	1.95
8	Q	201	HEM	FE-NC	4.12	2.08	1.95
8	R	201	HEM	FE-ND	4.12	2.07	1.94
8	S	201	HEM	FE-ND	4.08	2.07	1.94
8	B	201	HEM	FE-NC	4.05	2.08	1.95
8	e	201	HEM	FE-NC	4.03	2.08	1.95
8	X	201	HEM	FE-NC	4.02	2.08	1.95
8	e	201	HEM	FE-NA	4.00	2.08	1.95
8	j	201	HEM	FE-ND	3.99	2.07	1.94
8	I	201	HEM	FE-NB	3.98	2.07	1.94
8	T	201	HEM	FE-NC	3.92	2.08	1.95
8	o	201	HEM	FE-NC	3.86	2.07	1.95
8	D	201	HEM	FE-ND	3.85	2.06	1.94
8	L	201	HEM	FE-NA	3.79	2.07	1.95
8	A	201	HEM	FE-ND	3.75	2.06	1.94
8	H	201	HEM	FE-ND	3.75	2.06	1.94
8	W	201	HEM	FE-ND	3.75	2.06	1.94
8	P	201	HEM	FE-NA	3.73	2.07	1.95
8	H	201	HEM	FE-NA	3.68	2.07	1.95
8	o	201	HEM	FE-NA	3.68	2.07	1.95
8	S	201	HEM	FE-NC	3.68	2.07	1.95
8	Y	201	HEM	FE-NB	3.64	2.06	1.94
8	T	201	HEM	FE-NA	3.61	2.07	1.95
8	e	201	HEM	FE-ND	3.58	2.05	1.94
8	U	201	HEM	FE-NA	3.57	2.06	1.95
8	j	201	HEM	FE-NA	3.54	2.06	1.95
8	U	201	HEM	FE-ND	3.52	2.05	1.94
8	G	201	HEM	FE-ND	3.51	2.05	1.94
8	R	201	HEM	FE-NA	3.44	2.06	1.95
8	K	201	HEM	FE-NC	3.43	2.06	1.95
8	R	201	HEM	FE-NC	3.42	2.06	1.95
8	k	201	HEM	FE-NA	3.40	2.06	1.95
8	g	201	HEM	FE-NC	3.37	2.06	1.95
8	I	201	HEM	FE-NA	3.30	2.06	1.95
8	l	201	HEM	FE-NA	3.24	2.05	1.95
8	V	201	HEM	FE-NC	3.22	2.05	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	h	201	HEM	FE-ND	3.22	2.04	1.94
8	A	201	HEM	FE-NA	3.22	2.05	1.95
8	p	201	HEM	FE-NC	3.14	2.05	1.95
8	C	201	HEM	FE-NA	3.14	2.05	1.95
8	L	201	HEM	FE-NC	3.12	2.05	1.95
8	F	201	HEM	FE-ND	3.05	2.04	1.94
8	X	201	HEM	FE-NA	3.05	2.05	1.95
8	Q	201	HEM	CAB-C3B	3.04	1.55	1.47
8	h	201	HEM	CAB-C3B	3.03	1.55	1.47
8	n	201	HEM	CAB-C3B	3.03	1.55	1.47
8	J	201	HEM	CAB-C3B	3.02	1.55	1.47
8	U	201	HEM	CAB-C3B	3.00	1.55	1.47
8	a	201	HEM	CAB-C3B	3.00	1.55	1.47
8	G	201	HEM	FE-NA	2.99	2.05	1.95
8	D	201	HEM	FE-NC	2.99	2.05	1.95
8	R	201	HEM	CAC-C3C	2.98	1.55	1.47
8	Y	201	HEM	CAB-C3B	2.96	1.55	1.47
8	C	201	HEM	CAC-C3C	2.96	1.55	1.47
8	H	201	HEM	CAB-C3B	2.96	1.55	1.47
8	F	201	HEM	CAB-C3B	2.96	1.55	1.47
8	l	201	HEM	CAB-C3B	2.96	1.55	1.47
8	k	201	HEM	CAC-C3C	2.95	1.55	1.47
8	G	201	HEM	CAC-C3C	2.94	1.55	1.47
8	p	201	HEM	CAB-C3B	2.93	1.55	1.47
8	D	201	HEM	CAB-C3B	2.92	1.55	1.47
8	S	201	HEM	CAB-C3B	2.92	1.55	1.47
8	o	201	HEM	FE-ND	2.91	2.03	1.94
8	J	201	HEM	FE-NA	2.91	2.04	1.95
8	V	201	HEM	CAC-C3C	2.90	1.55	1.47
8	o	201	HEM	CAC-C3C	2.90	1.55	1.47
8	j	201	HEM	CAB-C3B	2.90	1.55	1.47
8	L	201	HEM	CAB-C3B	2.90	1.55	1.47
8	f	201	HEM	CAB-C3B	2.89	1.55	1.47
8	T	201	HEM	CAC-C3C	2.88	1.55	1.47
8	W	201	HEM	CAB-C3B	2.87	1.55	1.47
8	K	201	HEM	CAC-C3C	2.87	1.55	1.47
8	B	201	HEM	CAB-C3B	2.86	1.55	1.47
8	H	201	HEM	FE-NC	2.86	2.04	1.95
8	E	201	HEM	CAB-C3B	2.84	1.55	1.47
8	Z	201	HEM	CAC-C3C	2.83	1.55	1.47
8	F	201	HEM	FE-NA	2.83	2.04	1.95
8	T	201	HEM	CAB-C3B	2.82	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	X	201	HEM	CAC-C3C	2.82	1.54	1.47
8	P	201	HEM	CAB-C3B	2.80	1.54	1.47
8	I	201	HEM	CAC-C3C	2.80	1.54	1.47
8	m	201	HEM	CAC-C3C	2.79	1.54	1.47
8	i	201	HEM	CAB-C3B	2.79	1.54	1.47
8	g	201	HEM	CAC-C3C	2.79	1.54	1.47
8	E	201	HEM	CAC-C3C	2.78	1.54	1.47
8	e	201	HEM	CAC-C3C	2.77	1.54	1.47
8	X	201	HEM	CAB-C3B	2.76	1.54	1.47
8	G	201	HEM	CAB-C3B	2.75	1.54	1.47
8	P	201	HEM	CAC-C3C	2.74	1.54	1.47
8	S	201	HEM	FE-NA	2.74	2.04	1.95
8	K	201	HEM	CAB-C3B	2.72	1.54	1.47
8	A	201	HEM	CAB-C3B	2.72	1.54	1.47
8	A	201	HEM	CAC-C3C	2.72	1.54	1.47
8	m	201	HEM	CAB-C3B	2.71	1.54	1.47
8	l	201	HEM	CAC-C3C	2.71	1.54	1.47
8	j	201	HEM	CAC-C3C	2.71	1.54	1.47
8	l	201	HEM	FE-NC	2.71	2.04	1.95
8	e	201	HEM	CAB-C3B	2.71	1.54	1.47
8	o	201	HEM	CAB-C3B	2.71	1.54	1.47
8	k	201	HEM	CAB-C3B	2.70	1.54	1.47
8	f	201	HEM	FE-NA	2.70	2.04	1.95
8	g	201	HEM	CAB-C3B	2.70	1.54	1.47
8	i	201	HEM	CAC-C3C	2.68	1.54	1.47
8	R	201	HEM	CAB-C3B	2.68	1.54	1.47
8	n	201	HEM	FE-NA	2.67	2.04	1.95
8	f	201	HEM	CAC-C3C	2.67	1.54	1.47
8	U	201	HEM	CAC-C3C	2.67	1.54	1.47
8	Q	201	HEM	FE-NA	2.66	2.03	1.95
8	H	201	HEM	CAC-C3C	2.64	1.54	1.47
8	I	201	HEM	CAB-C3B	2.64	1.54	1.47
8	Z	201	HEM	FE-NC	2.63	2.03	1.95
8	B	201	HEM	CAC-C3C	2.63	1.54	1.47
8	V	201	HEM	CAB-C3B	2.62	1.54	1.47
8	C	201	HEM	CAB-C3B	2.62	1.54	1.47
8	Z	201	HEM	CAB-C3B	2.62	1.54	1.47
8	S	201	HEM	CAC-C3C	2.61	1.54	1.47
8	n	201	HEM	CAC-C3C	2.60	1.54	1.47
8	Y	201	HEM	CAC-C3C	2.57	1.54	1.47
8	Q	201	HEM	CAC-C3C	2.56	1.54	1.47
8	a	201	HEM	FE-NA	2.55	2.03	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	201	HEM	CAC-C3C	2.55	1.54	1.47
8	F	201	HEM	CAC-C3C	2.54	1.54	1.47
8	p	201	HEM	CAC-C3C	2.52	1.54	1.47
8	W	201	HEM	CAC-C3C	2.50	1.54	1.47
8	D	201	HEM	CAC-C3C	2.50	1.54	1.47
8	g	201	HEM	FE-NA	2.47	2.03	1.95
8	L	201	HEM	CAC-C3C	2.46	1.54	1.47
8	h	201	HEM	FE-NC	2.46	2.03	1.95
8	C	201	HEM	FE-NC	2.46	2.03	1.95
8	a	201	HEM	CAC-C3C	2.45	1.53	1.47
8	h	201	HEM	CAC-C3C	2.41	1.53	1.47
8	m	201	HEM	FE-NA	2.40	2.03	1.95
8	W	201	HEM	FE-NC	2.27	2.02	1.95
8	R	201	HEM	C2A-C3A	-2.21	1.33	1.38
8	g	201	HEM	C2A-C3A	-2.17	1.33	1.38
8	h	201	HEM	CMB-C2B	2.15	1.55	1.50
8	K	201	HEM	CMC-C2C	2.11	1.55	1.50
8	C	201	HEM	C2A-C3A	-2.10	1.33	1.38
8	p	201	HEM	CMB-C2B	2.10	1.55	1.50
8	m	201	HEM	CMD-C2D	2.09	1.55	1.50
8	B	201	HEM	FE-NA	2.07	2.02	1.95
8	h	201	HEM	C2A-C3A	-2.06	1.33	1.38
8	T	201	HEM	CMB-C2B	2.05	1.55	1.50
8	l	201	HEM	CMB-C2B	2.05	1.55	1.50
8	Y	201	HEM	CMB-C2B	2.05	1.55	1.50
8	H	201	HEM	CMB-C2B	2.05	1.55	1.50
8	k	201	HEM	CMD-C2D	2.05	1.55	1.50
8	J	201	HEM	CMB-C2B	2.04	1.55	1.50
8	o	201	HEM	CMA-C3A	2.04	1.55	1.50
8	R	201	HEM	CMC-C2C	2.04	1.55	1.50
8	G	201	HEM	CMB-C2B	2.04	1.55	1.50
8	E	201	HEM	FE-NA	2.04	2.01	1.95
8	I	201	HEM	CMD-C2D	2.04	1.54	1.50
8	B	201	HEM	C2A-C3A	-2.04	1.33	1.38
8	o	201	HEM	CMD-C2D	2.03	1.54	1.50
8	S	201	HEM	CMC-C2C	2.03	1.54	1.50
8	j	201	HEM	CMD-C2D	2.03	1.54	1.50
8	e	201	HEM	CMA-C3A	2.03	1.54	1.50
8	B	201	HEM	CMB-C2B	2.03	1.54	1.50
8	K	201	HEM	CMB-C2B	2.03	1.54	1.50
8	j	201	HEM	CMC-C2C	2.02	1.54	1.50
8	L	201	HEM	CMD-C2D	2.02	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	X	201	HEM	CMD-C2D	2.02	1.54	1.50
8	p	201	HEM	CMD-C2D	2.02	1.54	1.50
8	W	201	HEM	CMB-C2B	2.02	1.54	1.50
8	A	201	HEM	CMA-C3A	2.02	1.54	1.50
8	F	201	HEM	CMC-C2C	2.02	1.54	1.50
8	K	201	HEM	CMA-C3A	2.02	1.54	1.50
8	S	201	HEM	CMB-C2B	2.01	1.54	1.50
8	Z	201	HEM	C2A-C3A	-2.01	1.33	1.38
8	P	201	HEM	CMA-C3A	2.01	1.54	1.50
8	Y	201	HEM	CMC-C2C	2.01	1.54	1.50
8	K	201	HEM	CMD-C2D	2.01	1.54	1.50
8	n	201	HEM	CMC-C2C	2.01	1.54	1.50
8	D	201	HEM	CMB-C2B	2.01	1.54	1.50
8	Z	201	HEM	CMD-C2D	2.00	1.54	1.50
8	E	201	HEM	C2A-C3A	-2.00	1.33	1.38
8	H	201	HEM	CMC-C2C	2.00	1.54	1.50
8	Q	201	HEM	CMA-C3A	2.00	1.54	1.50

All (574) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	e	201	HEM	C4D-ND-C1D	6.54	112.95	105.21
8	P	201	HEM	C4D-ND-C1D	6.52	112.92	105.21
8	E	201	HEM	C4D-ND-C1D	6.38	112.76	105.21
8	i	201	HEM	C4D-ND-C1D	6.33	112.70	105.21
8	A	201	HEM	C4D-ND-C1D	6.31	112.69	105.21
8	T	201	HEM	C4D-ND-C1D	6.29	112.66	105.21
8	m	201	HEM	C4D-ND-C1D	6.16	112.50	105.21
8	X	201	HEM	C4D-ND-C1D	6.12	112.46	105.21
8	G	201	HEM	C4D-ND-C1D	6.12	112.45	105.21
8	p	201	HEM	C4D-ND-C1D	6.11	112.44	105.21
8	J	201	HEM	C4D-ND-C1D	6.10	112.43	105.21
8	n	201	HEM	C4D-ND-C1D	6.09	112.42	105.21
8	B	201	HEM	C4D-ND-C1D	6.03	112.34	105.21
8	S	201	HEM	C4D-ND-C1D	6.02	112.34	105.21
8	k	201	HEM	C4D-ND-C1D	6.01	112.32	105.21
8	h	201	HEM	C4D-ND-C1D	6.00	112.32	105.21
8	o	201	HEM	C4D-ND-C1D	6.00	112.31	105.21
8	W	201	HEM	C4D-ND-C1D	5.99	112.31	105.21
8	K	201	HEM	C4D-ND-C1D	5.97	112.28	105.21
8	Y	201	HEM	C4D-ND-C1D	5.94	112.24	105.21
8	a	201	HEM	C4D-ND-C1D	5.93	112.23	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	201	HEM	C4D-ND-C1D	5.91	112.21	105.21
8	U	201	HEM	C4D-ND-C1D	5.91	112.20	105.21
8	j	201	HEM	C4D-ND-C1D	5.90	112.19	105.21
8	F	201	HEM	C4D-ND-C1D	5.87	112.16	105.21
8	I	201	HEM	C4D-ND-C1D	5.78	112.05	105.21
8	Q	201	HEM	C4D-ND-C1D	5.78	112.05	105.21
8	l	201	HEM	C4D-ND-C1D	5.73	112.00	105.21
8	L	201	HEM	C4D-ND-C1D	5.72	111.98	105.21
8	f	201	HEM	C4D-ND-C1D	5.72	111.98	105.21
8	V	201	HEM	C4D-ND-C1D	5.69	111.95	105.21
8	H	201	HEM	C4D-ND-C1D	5.68	111.93	105.21
8	R	201	HEM	C4D-ND-C1D	5.63	111.88	105.21
8	Z	201	HEM	C4D-ND-C1D	5.53	111.75	105.21
8	g	201	HEM	C4D-ND-C1D	5.47	111.68	105.21
8	C	201	HEM	C4D-ND-C1D	5.33	111.52	105.21
8	m	201	HEM	CAD-C3D-C4D	4.97	133.36	124.70
12	O	304	NAG	C1-O5-C5	4.86	118.70	112.19
8	X	201	HEM	CAD-C3D-C4D	4.71	132.90	124.70
8	L	201	HEM	CBC-CAC-C3C	-4.32	105.93	127.53
8	a	201	HEM	CBC-CAC-C3C	-4.27	106.17	127.53
8	I	201	HEM	C3B-C4B-NB	-4.26	106.41	109.47
8	h	201	HEM	CBC-CAC-C3C	-4.23	106.40	127.53
8	e	201	HEM	C3B-C4B-NB	-4.18	106.47	109.47
8	p	201	HEM	CBC-CAC-C3C	-4.15	106.79	127.53
8	F	201	HEM	CBC-CAC-C3C	-4.05	107.31	127.53
8	W	201	HEM	CBC-CAC-C3C	-4.04	107.34	127.53
8	P	201	HEM	C3B-C4B-NB	-4.01	106.59	109.47
8	l	201	HEM	CHC-C1C-NC	3.97	128.78	124.45
8	Y	201	HEM	CBC-CAC-C3C	-3.96	107.72	127.53
12	s	303	NAG	C2-N2-C7	-3.92	117.64	122.90
8	B	201	HEM	CHC-C1C-NC	3.92	128.72	124.45
8	D	201	HEM	CBC-CAC-C3C	-3.91	108.00	127.53
8	I	201	HEM	CBB-CAB-C3B	-3.87	108.17	127.53
8	L	201	HEM	CHD-C4C-NC	3.87	128.67	124.45
8	n	201	HEM	CBC-CAC-C3C	-3.87	108.18	127.53
8	J	201	HEM	CBC-CAC-C3C	-3.87	108.21	127.53
8	m	201	HEM	C3B-C4B-NB	-3.86	106.69	109.47
8	W	201	HEM	CHC-C1C-NC	3.83	128.62	124.45
8	H	201	HEM	CBC-CAC-C3C	-3.83	108.40	127.53
8	l	201	HEM	CBC-CAC-C3C	-3.82	108.43	127.53
8	m	201	HEM	CBB-CAB-C3B	-3.82	108.43	127.53
8	F	201	HEM	CHA-C4D-ND	3.81	129.08	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	201	HEM	CHC-C1C-NC	3.81	128.60	124.45
8	A	201	HEM	C3B-C4B-NB	-3.80	106.74	109.47
8	S	201	HEM	CBC-CAC-C3C	-3.80	108.56	127.53
8	S	201	HEM	CHC-C1C-NC	3.79	128.58	124.45
8	p	201	HEM	CHA-C4D-ND	3.77	129.04	124.37
8	A	201	HEM	CBB-CAB-C3B	-3.77	108.71	127.53
8	e	201	HEM	CBB-CAB-C3B	-3.76	108.72	127.53
8	Q	201	HEM	CHD-C4C-NC	3.76	128.54	124.45
8	Q	201	HEM	CBC-CAC-C3C	-3.73	108.87	127.53
8	J	201	HEM	CHA-C4D-ND	3.73	128.98	124.37
8	Z	201	HEM	CBB-CAB-C3B	-3.72	108.93	127.53
8	T	201	HEM	CBB-CAB-C3B	-3.72	108.95	127.53
8	V	201	HEM	CBB-CAB-C3B	-3.71	108.98	127.53
8	h	201	HEM	CHC-C1C-NC	3.71	128.49	124.45
8	A	201	HEM	CBC-CAC-C3C	-3.68	109.12	127.53
8	i	201	HEM	CBC-CAC-C3C	-3.67	109.21	127.53
8	B	201	HEM	CBC-CAC-C3C	-3.66	109.22	127.53
8	f	201	HEM	CBC-CAC-C3C	-3.66	109.24	127.53
8	J	201	HEM	CHD-C4C-NC	3.65	128.43	124.45
8	j	201	HEM	CHA-C4D-ND	3.65	128.88	124.37
8	k	201	HEM	C3B-C4B-NB	-3.65	106.85	109.47
8	U	201	HEM	CHA-C4D-ND	3.64	128.87	124.37
8	m	201	HEM	CHC-C1C-NC	3.63	128.41	124.45
8	T	201	HEM	C3B-C4B-NB	-3.61	106.87	109.47
8	V	201	HEM	C3B-C4B-NB	-3.61	106.87	109.47
8	X	201	HEM	CBC-CAC-C3C	-3.61	109.47	127.53
8	m	201	HEM	CHD-C1D-ND	3.61	128.31	124.42
8	k	201	HEM	CAD-C3D-C4D	3.60	130.98	124.70
8	H	201	HEM	CHC-C1C-NC	3.60	128.37	124.45
8	j	201	HEM	CBC-CAC-C3C	-3.59	109.58	127.53
8	m	201	HEM	CAD-C3D-C2D	-3.59	121.14	127.87
8	i	201	HEM	CBB-CAB-C3B	-3.58	109.63	127.53
8	f	201	HEM	CHD-C4C-NC	3.58	128.35	124.45
8	U	201	HEM	CBC-CAC-C3C	-3.58	109.64	127.53
8	X	201	HEM	CBB-CAB-C3B	-3.58	109.65	127.53
8	P	201	HEM	CBB-CAB-C3B	-3.57	109.69	127.53
8	Z	201	HEM	C3B-C4B-NB	-3.57	106.91	109.47
8	B	201	HEM	CHD-C4C-NC	3.56	128.33	124.45
8	X	201	HEM	CHD-C1D-ND	3.53	128.22	124.42
8	l	201	HEM	CHD-C4C-NC	3.53	128.29	124.45
8	W	201	HEM	CHD-C4C-NC	3.52	128.29	124.45
8	R	201	HEM	C3B-C4B-NB	-3.52	106.94	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	201	HEM	CBB-CAB-C3B	-3.51	110.01	127.53
8	J	201	HEM	CHC-C1C-NC	3.50	128.27	124.45
8	H	201	HEM	CHD-C4C-NC	3.50	128.26	124.45
8	P	201	HEM	CBC-CAC-C3C	-3.50	110.05	127.53
8	o	201	HEM	C3B-C4B-NB	-3.48	106.97	109.47
8	K	201	HEM	CBB-CAB-C3B	-3.48	110.15	127.53
8	E	201	HEM	CBC-CAC-C3C	-3.47	110.16	127.53
8	k	201	HEM	CBB-CAB-C3B	-3.47	110.17	127.53
8	D	201	HEM	CHC-C1C-NC	3.47	128.23	124.45
8	C	201	HEM	C3B-C4B-NB	-3.46	106.98	109.47
8	g	201	HEM	CBB-CAB-C3B	-3.46	110.26	127.53
8	X	201	HEM	C3B-C4B-NB	-3.45	106.99	109.47
8	o	201	HEM	CBB-CAB-C3B	-3.44	110.36	127.53
8	e	201	HEM	CBC-CAC-C3C	-3.43	110.39	127.53
8	K	201	HEM	C3B-C4B-NB	-3.42	107.01	109.47
8	Z	201	HEM	CBC-CAC-C3C	-3.42	110.45	127.53
8	p	201	HEM	CHD-C4C-NC	3.41	128.17	124.45
8	X	201	HEM	CHD-C4C-NC	3.40	128.16	124.45
8	a	201	HEM	CHD-C4C-NC	3.40	128.16	124.45
8	g	201	HEM	CAD-C3D-C4D	3.40	130.62	124.70
8	V	201	HEM	CBC-CAC-C3C	-3.40	110.55	127.53
8	g	201	HEM	CBC-CAC-C3C	-3.39	110.57	127.53
8	G	201	HEM	C3B-C4B-NB	-3.39	107.03	109.47
12	O	304	NAG	C2-N2-C7	-3.39	118.36	122.90
8	Q	201	HEM	CHC-C1C-NC	3.39	128.14	124.45
8	n	201	HEM	CHC-C1C-NC	3.38	128.13	124.45
8	j	201	HEM	CHC-C1C-NC	3.37	128.12	124.45
8	k	201	HEM	CBC-CAC-C3C	-3.35	110.80	127.53
8	C	201	HEM	CBB-CAB-C3B	-3.33	110.88	127.53
8	X	201	HEM	C3B-C2B-C1B	3.33	108.91	106.41
8	I	201	HEM	CBC-CAC-C3C	-3.32	110.91	127.53
8	Y	201	HEM	C3B-C4B-NB	-3.32	107.08	109.47
8	C	201	HEM	CHC-C1C-NC	3.32	128.07	124.45
8	L	201	HEM	CHA-C4D-ND	3.31	128.46	124.37
8	U	201	HEM	CHC-C1C-NC	3.31	128.06	124.45
8	T	201	HEM	CHC-C1C-NC	3.31	128.06	124.45
8	E	201	HEM	C3B-C4B-NB	-3.31	107.09	109.47
8	e	201	HEM	CHC-C1C-NC	3.30	128.05	124.45
8	m	201	HEM	CBC-CAC-C3C	-3.30	111.06	127.53
8	T	201	HEM	CBC-CAC-C3C	-3.29	111.07	127.53
12	d	304	NAG	C1-O5-C5	3.29	116.60	112.19
8	n	201	HEM	CHD-C4C-NC	3.29	128.03	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	201	HEM	CBB-CAB-C3B	-3.29	111.11	127.53
8	H	201	HEM	CHA-C4D-ND	3.28	128.42	124.37
8	P	201	HEM	C3B-C2B-C1B	3.27	108.87	106.41
8	A	201	HEM	CHC-C1C-NC	3.26	128.01	124.45
8	K	201	HEM	CBC-CAC-C3C	-3.26	111.23	127.53
8	A	201	HEM	CHD-C4C-NC	3.26	128.00	124.45
8	Y	201	HEM	CHD-C4C-NC	3.25	127.99	124.45
8	D	201	HEM	CHA-C4D-ND	3.25	128.39	124.37
8	I	201	HEM	CHD-C1D-ND	3.25	127.92	124.42
8	R	201	HEM	CBB-CAB-C3B	-3.24	111.33	127.53
8	S	201	HEM	CHD-C4C-NC	3.23	127.97	124.45
8	a	201	HEM	C3B-C2B-C1B	3.23	108.84	106.41
8	f	201	HEM	C3B-C4B-NB	-3.23	107.15	109.47
8	Y	201	HEM	CHC-C1C-NC	3.22	127.96	124.45
8	G	201	HEM	CBC-CAC-C3C	-3.22	111.43	127.53
8	E	201	HEM	CHC-C1C-NC	3.22	127.96	124.45
8	h	201	HEM	CHD-C4C-NC	3.22	127.96	124.45
8	i	201	HEM	C3B-C4B-NB	-3.21	107.16	109.47
8	p	201	HEM	CHC-C1C-NC	3.21	127.95	124.45
8	m	201	HEM	C3B-C2B-C1B	3.20	108.81	106.41
8	W	201	HEM	C3B-C2B-C1B	3.20	108.81	106.41
8	U	201	HEM	CHD-C4C-NC	3.18	127.92	124.45
8	Y	201	HEM	CHA-C4D-ND	3.17	128.29	124.37
8	G	201	HEM	CAA-CBA-CGA	-3.16	105.27	113.67
8	A	201	HEM	CHA-C4D-ND	3.16	128.28	124.37
8	J	201	HEM	CHD-C1D-ND	3.16	127.82	124.42
8	p	201	HEM	CAD-CBD-CGD	-3.15	105.30	113.67
8	R	201	HEM	CHD-C1D-ND	3.15	127.81	124.42
8	i	201	HEM	C2A-C1A-NA	-3.15	106.66	110.15
8	W	201	HEM	C4C-C3C-C2C	3.14	109.54	106.81
8	L	201	HEM	C3B-C2B-C1B	3.14	108.77	106.41
8	E	201	HEM	C2A-C1A-NA	-3.14	106.67	110.15
8	D	201	HEM	CHD-C4C-NC	3.13	127.86	124.45
8	J	201	HEM	C3B-C4B-NB	-3.12	107.22	109.47
8	E	201	HEM	CHD-C1D-ND	3.12	127.78	124.42
8	f	201	HEM	CHC-C1C-NC	3.11	127.84	124.45
8	a	201	HEM	C4C-C3C-C2C	3.11	109.51	106.81
8	g	201	HEM	C3B-C4B-NB	-3.11	107.23	109.47
8	j	201	HEM	CHD-C4C-NC	3.11	127.83	124.45
8	W	201	HEM	CHA-C4D-ND	3.10	128.20	124.37
8	f	201	HEM	CBB-CAB-C3B	-3.08	112.15	127.53
8	A	201	HEM	C3B-C2B-C1B	3.08	108.72	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	o	201	HEM	CBC-CAC-C3C	-3.07	112.19	127.53
8	T	201	HEM	C2A-C1A-NA	-3.07	106.75	110.15
8	I	201	HEM	C3B-C2B-C1B	3.06	108.71	106.41
8	a	201	HEM	CBB-CAB-C3B	-3.06	112.24	127.53
8	I	201	HEM	C1B-NB-C4B	3.05	108.81	105.21
12	O	304	NAG	C4-C3-C2	-3.05	106.56	111.02
8	Z	201	HEM	CHD-C4C-NC	3.04	127.77	124.45
8	B	201	HEM	C2A-C1A-NA	-3.04	106.78	110.15
8	e	201	HEM	CHD-C4C-NC	3.04	127.76	124.45
8	X	201	HEM	CAD-C3D-C2D	-3.03	122.20	127.87
8	n	201	HEM	C3B-C2B-C1B	3.02	108.68	106.41
8	h	201	HEM	CHA-C4D-ND	3.02	128.10	124.37
8	R	201	HEM	CAA-CBA-CGA	-3.00	105.70	113.67
8	F	201	HEM	CHD-C4C-NC	3.00	127.72	124.45
8	U	201	HEM	C3B-C4B-NB	-3.00	107.31	109.47
8	m	201	HEM	C1B-NB-C4B	3.00	108.76	105.21
8	L	201	HEM	CBB-CAB-C3B	-3.00	112.55	127.53
8	V	201	HEM	CHD-C4C-NC	2.99	127.71	124.45
8	R	201	HEM	CAD-C3D-C4D	2.99	129.91	124.70
8	i	201	HEM	CHC-C1C-NC	2.99	127.71	124.45
8	Y	201	HEM	CHD-C1D-ND	2.98	127.63	124.42
8	W	201	HEM	CBB-CAB-C3B	-2.98	112.62	127.53
8	P	201	HEM	CHD-C1D-ND	2.98	127.63	124.42
8	K	201	HEM	CHD-C4C-NC	2.98	127.70	124.45
8	A	201	HEM	CHD-C1D-ND	2.98	127.63	124.42
8	p	201	HEM	C4C-C3C-C2C	2.98	109.40	106.81
8	e	201	HEM	C1B-NB-C4B	2.98	108.73	105.21
8	m	201	HEM	C2A-C1A-NA	-2.98	106.85	110.15
8	F	201	HEM	C3B-C2B-C1B	2.97	108.64	106.41
8	p	201	HEM	C3B-C4B-NB	-2.97	107.33	109.47
8	B	201	HEM	CBB-CAB-C3B	-2.97	112.70	127.53
8	L	201	HEM	C4C-C3C-C2C	2.96	109.39	106.81
8	p	201	HEM	CBB-CAB-C3B	-2.96	112.73	127.53
8	k	201	HEM	CHB-C1B-NB	2.96	128.03	124.37
8	j	201	HEM	C3B-C4B-NB	-2.96	107.34	109.47
8	V	201	HEM	CAD-C3D-C4D	2.96	129.85	124.70
8	G	201	HEM	CHD-C4C-NC	2.95	127.67	124.45
8	Q	201	HEM	C4C-C3C-C2C	2.95	109.37	106.81
8	e	201	HEM	C3B-C2B-C1B	2.95	108.62	106.41
8	n	201	HEM	CBB-CAB-C3B	-2.93	112.87	127.53
8	j	201	HEM	CBB-CAB-C3B	-2.92	112.91	127.53
8	S	201	HEM	CBB-CAB-C3B	-2.92	112.92	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	g	201	HEM	CHC-C1C-NC	2.92	127.64	124.45
8	i	201	HEM	CHD-C1D-ND	2.92	127.57	124.42
8	l	201	HEM	C4C-C3C-C2C	2.92	109.35	106.81
8	m	201	HEM	CHD-C4C-NC	2.92	127.63	124.45
8	Y	201	HEM	C3B-C2B-C1B	2.91	108.60	106.41
8	n	201	HEM	CHA-C4D-ND	2.91	127.97	124.37
8	U	201	HEM	C4C-C3C-C2C	2.91	109.34	106.81
8	F	201	HEM	CHC-C1C-NC	2.91	127.62	124.45
8	P	201	HEM	CHC-C1C-NC	2.91	127.62	124.45
8	S	201	HEM	C4C-C3C-C2C	2.90	109.33	106.81
8	k	201	HEM	C3B-C2B-C1B	2.90	108.59	106.41
8	J	201	HEM	CBB-CAB-C3B	-2.90	113.05	127.53
8	l	201	HEM	C3B-C2B-C1B	2.90	108.58	106.41
8	Q	201	HEM	C3B-C4B-NB	-2.89	107.39	109.47
8	D	201	HEM	CBB-CAB-C3B	-2.89	113.08	127.53
8	n	201	HEM	CHD-C1D-ND	2.89	127.53	124.42
8	Y	201	HEM	CBB-CAB-C3B	-2.89	113.10	127.53
8	k	201	HEM	CHD-C1D-ND	2.89	127.53	124.42
8	E	201	HEM	C3D-C4D-ND	-2.88	107.01	110.17
8	h	201	HEM	CBB-CAB-C3B	-2.88	113.13	127.53
8	h	201	HEM	C3B-C2B-C1B	2.87	108.57	106.41
8	Z	201	HEM	C3B-C2B-C1B	2.87	108.57	106.41
8	f	201	HEM	CHD-C1D-ND	2.87	127.51	124.42
8	J	201	HEM	C3B-C2B-C1B	2.86	108.56	106.41
8	S	201	HEM	C3B-C2B-C1B	2.86	108.56	106.41
8	p	201	HEM	C3B-C2B-C1B	2.86	108.56	106.41
8	a	201	HEM	CHA-C4D-ND	2.85	127.90	124.37
8	U	201	HEM	C3B-C2B-C1B	2.85	108.55	106.41
8	h	201	HEM	C4C-C3C-C2C	2.85	109.28	106.81
8	Y	201	HEM	C1B-NB-C4B	2.84	108.58	105.21
8	j	201	HEM	C3B-C2B-C1B	2.84	108.55	106.41
8	K	201	HEM	C3B-C2B-C1B	2.84	108.55	106.41
8	j	201	HEM	CHD-C1D-ND	2.84	127.48	124.42
8	F	201	HEM	CHD-C1D-ND	2.84	127.48	124.42
8	H	201	HEM	C4C-C3C-C2C	2.84	109.28	106.81
8	L	201	HEM	C3B-C4B-NB	-2.83	107.44	109.47
8	g	201	HEM	CHD-C4C-NC	2.83	127.53	124.45
8	H	201	HEM	C3B-C2B-C1B	2.82	108.53	106.41
8	G	201	HEM	C3B-C2B-C1B	2.82	108.53	106.41
8	I	201	HEM	CHC-C1C-NC	2.82	127.53	124.45
8	R	201	HEM	CBC-CAC-C3C	-2.82	113.43	127.53
12	d	304	NAG	C2-N2-C7	-2.82	119.12	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	201	HEM	CHA-C4D-ND	2.82	127.85	124.37
8	D	201	HEM	C3B-C4B-NB	-2.82	107.45	109.47
8	P	201	HEM	C1B-NB-C4B	2.81	108.53	105.21
8	V	201	HEM	C3B-C2B-C1B	2.80	108.52	106.41
8	D	201	HEM	C3B-C2B-C1B	2.80	108.51	106.41
8	p	201	HEM	CHB-C1B-NB	2.80	127.83	124.37
8	e	201	HEM	CHD-C1D-ND	2.79	127.42	124.42
8	i	201	HEM	C3B-C2B-C1B	2.79	108.50	106.41
8	G	201	HEM	CHB-C1B-NB	2.79	127.82	124.37
8	e	201	HEM	CHB-C1B-NB	2.79	127.81	124.37
8	F	201	HEM	C4C-C3C-C2C	2.79	109.23	106.81
8	J	201	HEM	C1B-NB-C4B	2.78	108.50	105.21
8	K	201	HEM	CHB-C1B-NB	2.78	127.80	124.37
8	o	201	HEM	CHB-C1B-NB	2.77	127.80	124.37
8	J	201	HEM	C4C-C3C-C2C	2.77	109.22	106.81
8	T	201	HEM	CHD-C1D-ND	2.77	127.40	124.42
8	C	201	HEM	CBC-CAC-C3C	-2.76	113.72	127.53
8	Y	201	HEM	CHB-C1B-NB	2.76	127.78	124.37
8	Q	201	HEM	C3B-C2B-C1B	2.75	108.48	106.41
8	n	201	HEM	C3B-C4B-NB	-2.75	107.49	109.47
8	n	201	HEM	C2A-C1A-NA	-2.75	107.10	110.15
8	V	201	HEM	CHD-C1D-ND	2.74	127.37	124.42
8	D	201	HEM	C4C-C3C-C2C	2.74	109.19	106.81
8	o	201	HEM	C3B-C2B-C1B	2.74	108.47	106.41
8	Q	201	HEM	C2A-C1A-NA	-2.74	107.11	110.15
8	Y	201	HEM	C2A-C1A-NA	-2.73	107.12	110.15
8	Q	201	HEM	CHA-C4D-ND	2.73	127.75	124.37
8	C	201	HEM	CAD-C3D-C4D	2.73	129.45	124.70
8	l	201	HEM	CHA-C4D-ND	2.72	127.73	124.37
8	k	201	HEM	C1B-NB-C4B	2.71	108.41	105.21
8	o	201	HEM	CHD-C4C-NC	2.70	127.39	124.45
8	V	201	HEM	C2A-C1A-NA	-2.70	107.16	110.15
8	n	201	HEM	C4C-C3C-C2C	2.70	109.15	106.81
8	A	201	HEM	C1B-NB-C4B	2.69	108.39	105.21
8	K	201	HEM	CAD-C3D-C4D	2.69	129.38	124.70
8	T	201	HEM	C1B-NB-C4B	2.69	108.39	105.21
8	Z	201	HEM	CHC-C1C-NC	2.68	127.38	124.45
8	l	201	HEM	CBB-CAB-C3B	-2.68	114.12	127.53
8	X	201	HEM	C1B-NB-C4B	2.68	108.38	105.21
8	S	201	HEM	C2A-C1A-NA	-2.68	107.18	110.15
8	U	201	HEM	CBB-CAB-C3B	-2.67	114.16	127.53
8	k	201	HEM	C2A-C1A-NA	-2.67	107.19	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	f	201	HEM	C1B-NB-C4B	2.67	108.37	105.21
8	P	201	HEM	CHB-C1B-NB	2.66	127.66	124.37
8	W	201	HEM	CAD-CBD-CGD	-2.66	106.60	113.67
8	g	201	HEM	CHD-C1D-ND	2.66	127.28	124.42
8	e	201	HEM	C2A-C1A-NA	-2.66	107.20	110.15
8	Q	201	HEM	CBB-CAB-C3B	-2.65	114.27	127.53
8	F	201	HEM	CBB-CAB-C3B	-2.65	114.27	127.53
8	n	201	HEM	C1B-NB-C4B	2.65	108.34	105.21
8	G	201	HEM	CHD-C1D-ND	2.65	127.27	124.42
8	P	201	HEM	CHD-C4C-NC	2.64	127.33	124.45
8	H	201	HEM	CBB-CAB-C3B	-2.64	114.31	127.53
8	T	201	HEM	CHD-C4C-NC	2.64	127.33	124.45
8	L	201	HEM	C1B-NB-C4B	2.63	108.32	105.21
8	W	201	HEM	CHB-C1B-NB	2.63	127.62	124.37
8	I	201	HEM	C2A-C1A-NA	-2.63	107.23	110.15
8	G	201	HEM	CHC-C1C-NC	2.63	127.31	124.45
8	Z	201	HEM	CHD-C1D-ND	2.62	127.24	124.42
8	e	201	HEM	CAD-C3D-C4D	2.62	129.26	124.70
8	f	201	HEM	C2A-C1A-NA	-2.61	107.25	110.15
8	P	201	HEM	C2A-C1A-NA	-2.61	107.26	110.15
8	G	201	HEM	C2A-C1A-NA	-2.61	107.26	110.15
8	A	201	HEM	C3D-C4D-ND	-2.61	107.31	110.17
8	Z	201	HEM	C1B-NB-C4B	2.60	108.29	105.21
8	E	201	HEM	C3B-C2B-C1B	2.60	108.36	106.41
8	f	201	HEM	CHA-C4D-ND	2.60	127.58	124.37
8	V	201	HEM	CHB-C1B-NB	2.59	127.58	124.37
8	j	201	HEM	C2A-C1A-NA	-2.59	107.28	110.15
8	p	201	HEM	C1B-NB-C4B	2.59	108.28	105.21
8	a	201	HEM	C3B-C4B-NB	-2.59	107.61	109.47
8	T	201	HEM	C3B-C2B-C1B	2.59	108.36	106.41
8	U	201	HEM	CHC-C4B-NB	2.59	127.21	124.42
8	A	201	HEM	CHB-C1B-NB	2.59	127.57	124.37
8	o	201	HEM	CHC-C1C-NC	2.59	127.27	124.45
8	J	201	HEM	CHB-C1B-NB	2.58	127.56	124.37
8	j	201	HEM	C1B-NB-C4B	2.58	108.26	105.21
8	A	201	HEM	C2A-C1A-NA	-2.58	107.29	110.15
8	Q	201	HEM	CHD-C1D-ND	2.57	127.19	124.42
8	K	201	HEM	C1B-NB-C4B	2.56	108.24	105.21
8	g	201	HEM	CHB-C1B-NB	2.56	127.53	124.37
8	V	201	HEM	C1B-NB-C4B	2.56	108.24	105.21
8	L	201	HEM	CHB-C1B-NB	2.56	127.53	124.37
8	X	201	HEM	CHC-C1C-NC	2.55	127.23	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	f	201	HEM	C3B-C2B-C1B	2.55	108.33	106.41
8	X	201	HEM	CHB-C1B-NB	2.55	127.52	124.37
8	E	201	HEM	CAD-C3D-C4D	2.55	129.13	124.70
8	i	201	HEM	C3D-C4D-ND	-2.54	107.38	110.17
8	V	201	HEM	CHC-C1C-NC	2.54	127.22	124.45
8	o	201	HEM	C1B-NB-C4B	2.54	108.22	105.21
8	G	201	HEM	CAD-CBD-CGD	-2.54	106.93	113.67
8	U	201	HEM	C2A-C1A-NA	-2.54	107.33	110.15
8	B	201	HEM	C3B-C4B-NB	-2.53	107.65	109.47
8	Q	201	HEM	C1B-NB-C4B	2.53	108.20	105.21
8	f	201	HEM	CHC-C4B-NB	2.53	127.14	124.42
8	D	201	HEM	C1B-NB-C4B	2.52	108.20	105.21
8	g	201	HEM	C3B-C2B-C1B	2.52	108.31	106.41
8	R	201	HEM	CHB-C1B-NB	2.52	127.48	124.37
8	T	201	HEM	C3D-C4D-ND	-2.51	107.42	110.17
8	j	201	HEM	C4C-C3C-C2C	2.51	108.99	106.81
12	s	303	NAG	C1-O5-C5	2.51	115.55	112.19
8	i	201	HEM	CHD-C4C-NC	2.51	127.18	124.45
8	k	201	HEM	CHC-C1C-NC	2.50	127.18	124.45
8	G	201	HEM	CAD-C3D-C4D	2.50	129.05	124.70
8	G	201	HEM	C1B-NB-C4B	2.49	108.16	105.21
8	P	201	HEM	C4C-C3C-C2C	2.49	108.97	106.81
8	o	201	HEM	CHD-C1D-ND	2.48	127.09	124.42
8	I	201	HEM	CAD-C3D-C4D	2.48	129.02	124.70
8	f	201	HEM	CAD-CBD-CGD	-2.48	107.09	113.67
8	Y	201	HEM	CHC-C4B-NB	2.47	127.08	124.42
8	a	201	HEM	CHC-C1C-NC	2.47	127.14	124.45
8	a	201	HEM	C1B-NB-C4B	2.47	108.13	105.21
8	m	201	HEM	C3D-C4D-ND	-2.47	107.46	110.17
8	U	201	HEM	C1B-NB-C4B	2.47	108.13	105.21
8	B	201	HEM	C4C-C3C-C2C	2.47	108.95	106.81
8	J	201	HEM	C2A-C1A-NA	-2.46	107.42	110.15
8	F	201	HEM	C2A-C1A-NA	-2.46	107.42	110.15
8	X	201	HEM	C2A-C1A-NA	-2.46	107.42	110.15
8	m	201	HEM	C3C-C2C-C1C	2.46	109.37	107.05
8	m	201	HEM	C2B-C1B-NB	-2.45	107.02	109.84
8	k	201	HEM	CAA-CBA-CGA	-2.45	107.17	113.67
8	Z	201	HEM	CAD-C3D-C4D	2.45	128.97	124.70
8	n	201	HEM	CHC-C4B-NB	2.45	127.06	124.42
8	e	201	HEM	C3D-C4D-ND	-2.44	107.50	110.17
8	E	201	HEM	CHD-C4C-NC	2.43	127.10	124.45
8	T	201	HEM	CAD-C3D-C4D	2.43	128.94	124.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Y	201	HEM	C4C-C3C-C2C	2.43	108.92	106.81
8	D	201	HEM	CHB-C1B-NB	2.43	127.37	124.37
8	P	201	HEM	C3D-C4D-ND	-2.42	107.52	110.17
8	k	201	HEM	CHD-C4C-NC	2.42	127.09	124.45
8	I	201	HEM	C2B-C1B-NB	-2.42	107.06	109.84
8	f	201	HEM	C4C-C3C-C2C	2.42	108.91	106.81
8	Z	201	HEM	CHB-C1B-NB	2.42	127.36	124.37
8	K	201	HEM	CAD-CBD-CGD	-2.42	107.26	113.67
8	S	201	HEM	CHB-C1B-NB	2.41	127.35	124.37
8	X	201	HEM	C2B-C1B-NB	-2.41	107.06	109.84
8	K	201	HEM	CHD-C1D-ND	2.41	127.02	124.42
8	B	201	HEM	CHD-C1D-ND	2.41	127.02	124.42
8	a	201	HEM	C2A-C1A-NA	-2.41	107.48	110.15
8	T	201	HEM	CMC-C2C-C3C	-2.40	122.62	128.43
8	n	201	HEM	CHB-C1B-NB	2.39	127.33	124.37
8	I	201	HEM	CHB-C1B-NB	2.39	127.33	124.37
8	e	201	HEM	C2D-C1D-ND	-2.39	107.14	109.90
8	C	201	HEM	CHD-C4C-NC	2.39	127.05	124.45
8	U	201	HEM	CHB-C1B-NB	2.39	127.32	124.37
8	l	201	HEM	CHD-C1D-ND	2.39	126.99	124.42
8	R	201	HEM	CHC-C1C-NC	2.38	127.05	124.45
8	i	201	HEM	C1B-NB-C4B	2.38	108.03	105.21
8	j	201	HEM	CAD-CBD-CGD	-2.38	107.36	113.67
8	a	201	HEM	CHB-C1B-NB	2.38	127.31	124.37
8	i	201	HEM	CAD-C3D-C4D	2.37	128.83	124.70
8	P	201	HEM	CAD-C3D-C4D	2.37	128.82	124.70
8	E	201	HEM	C1B-NB-C4B	2.37	108.01	105.21
8	B	201	HEM	CAD-C3D-C4D	2.36	128.82	124.70
8	S	201	HEM	C3B-C4B-NB	-2.36	107.77	109.47
8	e	201	HEM	C2B-C1B-NB	-2.35	107.14	109.84
8	W	201	HEM	C1B-NB-C4B	2.35	107.99	105.21
8	P	201	HEM	C2D-C1D-ND	-2.34	107.19	109.90
8	e	201	HEM	CAD-CBD-CGD	-2.34	107.46	113.67
8	Q	201	HEM	CHB-C1B-NB	2.34	127.26	124.37
8	l	201	HEM	CHB-C1B-NB	2.33	127.25	124.37
8	L	201	HEM	C2B-C1B-NB	-2.33	107.16	109.84
8	C	201	HEM	CMD-C2D-C1D	2.33	128.67	125.03
8	K	201	HEM	CAA-CBA-CGA	-2.32	107.50	113.67
8	R	201	HEM	C1B-NB-C4B	2.32	107.95	105.21
8	R	201	HEM	C3B-C2B-C1B	2.32	108.15	106.41
8	I	201	HEM	CHA-C4D-ND	2.31	127.22	124.37
8	j	201	HEM	CHB-C1B-NB	2.31	127.22	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	h	201	HEM	C1B-NB-C4B	2.30	107.94	105.21
8	Q	201	HEM	CAA-CBA-CGA	-2.30	107.56	113.67
8	h	201	HEM	CHB-C1B-NB	2.30	127.22	124.37
8	h	201	HEM	CHD-C1D-ND	2.29	126.89	124.42
8	e	201	HEM	CHA-C4D-ND	2.29	127.20	124.37
8	H	201	HEM	CHC-C4B-NB	2.29	126.89	124.42
8	o	201	HEM	CHA-C4D-ND	2.29	127.20	124.37
8	P	201	HEM	C2B-C1B-NB	-2.28	107.22	109.84
8	C	201	HEM	C1B-NB-C4B	2.28	107.91	105.21
8	F	201	HEM	CHC-C4B-NB	2.28	126.88	124.42
8	D	201	HEM	CHC-C4B-NB	2.28	126.88	124.42
8	g	201	HEM	CAA-CBA-CGA	-2.28	107.63	113.67
8	E	201	HEM	CAD-CBD-CGD	-2.27	107.63	113.67
8	H	201	HEM	CHD-C1D-ND	2.27	126.87	124.42
8	S	201	HEM	CHD-C1D-ND	2.27	126.86	124.42
8	p	201	HEM	CHD-C1D-ND	2.27	126.86	124.42
8	l	201	HEM	C1B-NB-C4B	2.26	107.89	105.21
8	S	201	HEM	C1B-NB-C4B	2.25	107.87	105.21
8	g	201	HEM	C1B-NB-C4B	2.25	107.87	105.21
8	H	201	HEM	CHB-C1B-NB	2.24	127.14	124.37
8	m	201	HEM	CHB-C1B-NB	2.24	127.14	124.37
8	Q	201	HEM	CAD-CBD-CGD	-2.24	107.73	113.67
8	G	201	HEM	C3D-C4D-ND	-2.23	107.72	110.17
8	B	201	HEM	C3B-C2B-C1B	2.23	108.08	106.41
8	F	201	HEM	C1B-NB-C4B	2.23	107.85	105.21
8	L	201	HEM	CAD-CBD-CGD	-2.23	107.76	113.67
8	K	201	HEM	CHC-C1C-NC	2.22	126.87	124.45
8	l	201	HEM	C2A-C1A-NA	-2.22	107.69	110.15
8	o	201	HEM	C2A-C1A-NA	-2.21	107.69	110.15
8	W	201	HEM	C2B-C1B-NB	-2.21	107.30	109.84
8	R	201	HEM	C2A-C1A-NA	-2.21	107.70	110.15
8	J	201	HEM	CHC-C4B-NB	2.21	126.80	124.42
8	B	201	HEM	C1B-NB-C4B	2.21	107.82	105.21
8	l	201	HEM	CBA-CAA-C2A	-2.20	106.44	112.53
8	e	201	HEM	C4C-C3C-C2C	2.20	108.72	106.81
8	E	201	HEM	C3C-C2C-C1C	2.20	109.13	107.05
8	F	201	HEM	CHB-C1B-NB	2.19	127.08	124.37
8	H	201	HEM	C1B-NB-C4B	2.19	107.80	105.21
8	I	201	HEM	C3C-C2C-C1C	2.19	109.12	107.05
8	D	201	HEM	C2A-C1A-NA	-2.19	107.72	110.15
8	B	201	HEM	CAD-CBD-CGD	-2.18	107.88	113.67
8	P	201	HEM	CHC-C4B-NB	2.18	126.77	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	201	HEM	CAD-CBD-CGD	-2.18	107.89	113.67
8	F	201	HEM	CAD-CBD-CGD	-2.18	107.89	113.67
8	A	201	HEM	C2B-C1B-NB	-2.17	107.35	109.84
8	a	201	HEM	CAD-CBD-CGD	-2.16	107.93	113.67
8	p	201	HEM	C2A-C1A-NA	-2.16	107.76	110.15
8	Q	201	HEM	CHC-C4B-NB	2.16	126.74	124.42
8	a	201	HEM	CMC-C2C-C3C	-2.15	123.22	128.43
8	Z	201	HEM	C2A-C1A-NA	-2.15	107.77	110.15
8	L	201	HEM	CHD-C1D-ND	2.15	126.73	124.42
8	T	201	HEM	CAA-CBA-CGA	-2.14	107.98	113.67
8	J	201	HEM	CMC-C2C-C3C	-2.14	123.24	128.43
8	C	201	HEM	CAD-CBD-CGD	-2.14	107.99	113.67
8	p	201	HEM	C4C-NC-C1C	2.13	109.30	105.82
8	f	201	HEM	CHB-C1B-NB	2.13	127.00	124.37
8	n	201	HEM	C3D-C4D-ND	-2.13	107.84	110.17
8	J	201	HEM	C2D-C1D-ND	-2.13	107.44	109.90
8	h	201	HEM	C2A-C1A-NA	-2.13	107.79	110.15
8	B	201	HEM	CMD-C2D-C1D	2.13	128.35	125.03
8	I	201	HEM	CHD-C4C-NC	2.12	126.77	124.45
8	e	201	HEM	CHC-C4B-NB	2.12	126.71	124.42
8	j	201	HEM	CHC-C4B-NB	2.12	126.70	124.42
8	W	201	HEM	C2D-C1D-ND	-2.12	107.45	109.90
8	P	201	HEM	CHA-C4D-ND	2.12	126.98	124.37
8	g	201	HEM	C2A-C1A-NA	-2.12	107.80	110.15
8	i	201	HEM	CHB-C1B-NB	2.11	126.98	124.37
8	i	201	HEM	C4C-C3C-C2C	2.11	108.65	106.81
8	W	201	HEM	C3B-C4B-NB	-2.11	107.95	109.47
8	L	201	HEM	C2A-C1A-NA	-2.11	107.81	110.15
8	n	201	HEM	C3A-C4A-NA	-2.11	106.76	110.14
8	W	201	HEM	CHD-C1D-ND	2.11	126.69	124.42
8	A	201	HEM	C4C-C3C-C2C	2.11	108.64	106.81
8	n	201	HEM	CMC-C2C-C3C	-2.11	123.33	128.43
8	a	201	HEM	C3A-C4A-NA	-2.10	106.77	110.14
8	k	201	HEM	CAD-C3D-C2D	-2.10	123.93	127.87
8	I	201	HEM	C3D-C4D-ND	-2.10	107.87	110.17
8	F	201	HEM	C3A-C4A-NA	-2.10	106.77	110.14
8	W	201	HEM	C2A-C1A-NA	-2.10	107.82	110.15
8	A	201	HEM	C2D-C1D-ND	-2.09	107.48	109.90
8	S	201	HEM	CHC-C4B-NB	2.09	126.67	124.42
8	F	201	HEM	C3B-C4B-NB	-2.09	107.97	109.47
8	J	201	HEM	C2B-C1B-NB	-2.09	107.44	109.84
8	C	201	HEM	C3B-C2B-C1B	2.08	107.97	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	201	HEM	CHC-C4B-NB	2.08	126.66	124.42
8	k	201	HEM	C3C-C2C-C1C	2.08	109.02	107.05
8	H	201	HEM	C2A-C1A-NA	-2.08	107.84	110.15
8	l	201	HEM	C4C-NC-C1C	2.08	109.21	105.82
8	n	201	HEM	CAD-CBD-CGD	-2.07	108.16	113.67
8	h	201	HEM	C3B-C4B-NB	-2.07	107.98	109.47
8	I	201	HEM	CHC-C4B-NB	2.07	126.65	124.42
8	C	201	HEM	CAA-CBA-CGA	-2.07	108.18	113.67
8	k	201	HEM	C2B-C1B-NB	-2.07	107.47	109.84
8	p	201	HEM	C2D-C1D-ND	-2.07	107.52	109.90
8	Y	201	HEM	CMC-C2C-C3C	-2.06	123.44	128.43
8	F	201	HEM	CMC-C2C-C3C	-2.06	123.44	128.43
8	B	201	HEM	C3A-C4A-NA	-2.06	106.84	110.14
8	o	201	HEM	C4C-C3C-C2C	2.06	108.60	106.81
8	j	201	HEM	C2B-C1B-NB	-2.06	107.48	109.84
8	R	201	HEM	CAD-CBD-CGD	-2.06	108.21	113.67
8	C	201	HEM	CHB-C1B-NB	2.05	126.91	124.37
8	a	201	HEM	C2B-C1B-NB	-2.05	107.48	109.84
8	j	201	HEM	C3A-C4A-NA	-2.05	106.86	110.14
8	i	201	HEM	CAA-CBA-CGA	-2.05	108.24	113.67
8	X	201	HEM	C2D-C1D-ND	-2.04	107.54	109.90
8	Z	201	HEM	C2B-C1B-NB	-2.04	107.50	109.84
8	X	201	HEM	C3A-C4A-NA	-2.04	106.87	110.14
8	S	201	HEM	C2D-C1D-ND	-2.04	107.55	109.90
8	n	201	HEM	C4A-NA-C1A	2.03	109.14	105.82
8	p	201	HEM	CMC-C2C-C3C	-2.03	123.51	128.43
8	B	201	HEM	CHA-C1A-NA	2.03	127.54	123.86
8	V	201	HEM	C2B-C1B-NB	-2.03	107.51	109.84
8	n	201	HEM	C2B-C1B-NB	-2.03	107.51	109.84
8	f	201	HEM	C3A-C4A-NA	-2.03	106.89	110.14
8	i	201	HEM	C3C-C2C-C1C	2.02	108.96	107.05
8	C	201	HEM	C2A-C1A-NA	-2.02	107.91	110.15
8	h	201	HEM	CMC-C2C-C3C	-2.02	123.54	128.43
8	K	201	HEM	C3D-C4D-ND	-2.02	107.96	110.17
8	Y	201	HEM	C2B-C1B-NB	-2.02	107.52	109.84
8	Q	201	HEM	CMC-C2C-C3C	-2.01	123.55	128.43
8	a	201	HEM	CHD-C1D-ND	2.01	126.59	124.42
8	W	201	HEM	C4C-NC-C1C	2.01	109.10	105.82
8	a	201	HEM	C2D-C1D-ND	-2.01	107.58	109.90
8	U	201	HEM	CAD-CBD-CGD	-2.01	108.33	113.67
8	U	201	HEM	CHD-C1D-ND	2.01	126.59	124.42
8	n	201	HEM	C4A-C3A-C2A	2.01	109.12	106.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	201	HEM	C4C-NC-C1C	2.01	109.09	105.82
8	i	201	HEM	C4A-NA-C1A	2.01	109.09	105.82
8	H	201	HEM	CAD-CBD-CGD	-2.00	108.35	113.67
8	U	201	HEM	C2D-C1D-ND	-2.00	107.59	109.90
8	U	201	HEM	C3A-C4A-NA	-2.00	106.93	110.14
8	e	201	HEM	C4C-NC-C1C	2.00	109.08	105.82
8	f	201	HEM	C3D-C4D-ND	-2.00	107.98	110.17

There are no chirality outliers.

All (249) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	201	HEM	C2B-C3B-CAB-CBB
8	A	201	HEM	C2C-C3C-CAC-CBC
8	A	201	HEM	C4C-C3C-CAC-CBC
8	B	201	HEM	C2B-C3B-CAB-CBB
8	B	201	HEM	C2C-C3C-CAC-CBC
8	B	201	HEM	C4C-C3C-CAC-CBC
8	C	201	HEM	C2B-C3B-CAB-CBB
8	D	201	HEM	C2C-C3C-CAC-CBC
8	D	201	HEM	C4C-C3C-CAC-CBC
8	E	201	HEM	C2B-C3B-CAB-CBB
8	E	201	HEM	C2C-C3C-CAC-CBC
8	F	201	HEM	C2B-C3B-CAB-CBB
8	F	201	HEM	C2C-C3C-CAC-CBC
8	F	201	HEM	C4C-C3C-CAC-CBC
8	G	201	HEM	C2B-C3B-CAB-CBB
8	H	201	HEM	C2C-C3C-CAC-CBC
8	H	201	HEM	C4C-C3C-CAC-CBC
8	I	201	HEM	C2B-C3B-CAB-CBB
8	I	201	HEM	C2C-C3C-CAC-CBC
8	J	201	HEM	C2C-C3C-CAC-CBC
8	J	201	HEM	C4C-C3C-CAC-CBC
8	K	201	HEM	C2B-C3B-CAB-CBB
8	K	201	HEM	C2C-C3C-CAC-CBC
8	L	201	HEM	C2B-C3B-CAB-CBB
8	L	201	HEM	C2C-C3C-CAC-CBC
8	P	201	HEM	C2B-C3B-CAB-CBB
8	P	201	HEM	C2C-C3C-CAC-CBC
8	Q	201	HEM	C2C-C3C-CAC-CBC
8	Q	201	HEM	C4C-C3C-CAC-CBC
8	R	201	HEM	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
8	S	201	HEM	C2C-C3C-CAC-CBC
8	S	201	HEM	C4C-C3C-CAC-CBC
8	T	201	HEM	C2B-C3B-CAB-CBB
8	T	201	HEM	C2C-C3C-CAC-CBC
8	T	201	HEM	C4C-C3C-CAC-CBC
8	U	201	HEM	C2C-C3C-CAC-CBC
8	U	201	HEM	C4C-C3C-CAC-CBC
8	V	201	HEM	C2B-C3B-CAB-CBB
8	W	201	HEM	C2B-C3B-CAB-CBB
8	W	201	HEM	C2C-C3C-CAC-CBC
8	W	201	HEM	C4C-C3C-CAC-CBC
8	X	201	HEM	C2B-C3B-CAB-CBB
8	X	201	HEM	C2C-C3C-CAC-CBC
8	X	201	HEM	C2D-C3D-CAD-CBD
8	X	201	HEM	C4D-C3D-CAD-CBD
8	Y	201	HEM	C2C-C3C-CAC-CBC
8	Y	201	HEM	C4C-C3C-CAC-CBC
8	Z	201	HEM	C2B-C3B-CAB-CBB
8	Z	201	HEM	C2C-C3C-CAC-CBC
8	a	201	HEM	C2B-C3B-CAB-CBB
8	a	201	HEM	C2C-C3C-CAC-CBC
8	a	201	HEM	C4C-C3C-CAC-CBC
8	e	201	HEM	C2B-C3B-CAB-CBB
8	e	201	HEM	C2C-C3C-CAC-CBC
8	e	201	HEM	C4C-C3C-CAC-CBC
8	f	201	HEM	C2B-C3B-CAB-CBB
8	f	201	HEM	C2C-C3C-CAC-CBC
8	f	201	HEM	C4C-C3C-CAC-CBC
8	g	201	HEM	C2B-C3B-CAB-CBB
8	g	201	HEM	C2C-C3C-CAC-CBC
8	h	201	HEM	C2C-C3C-CAC-CBC
8	h	201	HEM	C4C-C3C-CAC-CBC
8	i	201	HEM	C2B-C3B-CAB-CBB
8	i	201	HEM	C2C-C3C-CAC-CBC
8	j	201	HEM	C2B-C3B-CAB-CBB
8	j	201	HEM	C2C-C3C-CAC-CBC
8	j	201	HEM	C4C-C3C-CAC-CBC
8	k	201	HEM	C2B-C3B-CAB-CBB
8	k	201	HEM	C2D-C3D-CAD-CBD
8	l	201	HEM	C2C-C3C-CAC-CBC
8	l	201	HEM	C4C-C3C-CAC-CBC
8	m	201	HEM	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
8	m	201	HEM	C2C-C3C-CAC-CBC
8	m	201	HEM	C2D-C3D-CAD-CBD
8	m	201	HEM	C4D-C3D-CAD-CBD
8	n	201	HEM	C2C-C3C-CAC-CBC
8	n	201	HEM	C4C-C3C-CAC-CBC
8	o	201	HEM	C2B-C3B-CAB-CBB
8	o	201	HEM	C2C-C3C-CAC-CBC
8	p	201	HEM	C2C-C3C-CAC-CBC
8	p	201	HEM	C4C-C3C-CAC-CBC
8	k	201	HEM	C4D-C3D-CAD-CBD
8	H	201	HEM	C2D-C3D-CAD-CBD
8	U	201	HEM	C2D-C3D-CAD-CBD
8	l	201	HEM	C2D-C3D-CAD-CBD
8	g	201	HEM	C4D-C3D-CAD-CBD
8	l	201	HEM	C4D-C3D-CAD-CBD
8	g	201	HEM	C2D-C3D-CAD-CBD
8	H	201	HEM	C4D-C3D-CAD-CBD
8	R	201	HEM	C2D-C3D-CAD-CBD
8	U	201	HEM	C4D-C3D-CAD-CBD
8	D	201	HEM	C2D-C3D-CAD-CBD
8	D	201	HEM	C4D-C3D-CAD-CBD
8	R	201	HEM	C4D-C3D-CAD-CBD
8	S	201	HEM	C4D-C3D-CAD-CBD
8	p	201	HEM	C4D-C3D-CAD-CBD
8	C	201	HEM	C2C-C3C-CAC-CBC
8	D	201	HEM	C2B-C3B-CAB-CBB
8	G	201	HEM	C2C-C3C-CAC-CBC
8	H	201	HEM	C2B-C3B-CAB-CBB
8	J	201	HEM	C2B-C3B-CAB-CBB
8	Q	201	HEM	C2B-C3B-CAB-CBB
8	R	201	HEM	C2C-C3C-CAC-CBC
8	S	201	HEM	C2B-C3B-CAB-CBB
8	U	201	HEM	C2B-C3B-CAB-CBB
8	V	201	HEM	C2C-C3C-CAC-CBC
8	h	201	HEM	C2B-C3B-CAB-CBB
8	k	201	HEM	C2C-C3C-CAC-CBC
8	l	201	HEM	C2B-C3B-CAB-CBB
8	n	201	HEM	C2B-C3B-CAB-CBB
8	p	201	HEM	C2B-C3B-CAB-CBB
8	B	201	HEM	C4B-C3B-CAB-CBB
8	E	201	HEM	C4C-C3C-CAC-CBC
8	F	201	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
8	I	201	HEM	C4B-C3B-CAB-CBB
8	L	201	HEM	C4B-C3B-CAB-CBB
8	L	201	HEM	C4C-C3C-CAC-CBC
8	P	201	HEM	C4B-C3B-CAB-CBB
8	P	201	HEM	C4C-C3C-CAC-CBC
8	T	201	HEM	C4B-C3B-CAB-CBB
8	V	201	HEM	C4B-C3B-CAB-CBB
8	W	201	HEM	C4B-C3B-CAB-CBB
8	X	201	HEM	C4C-C3C-CAC-CBC
8	a	201	HEM	C4B-C3B-CAB-CBB
8	f	201	HEM	C4B-C3B-CAB-CBB
8	i	201	HEM	C4B-C3B-CAB-CBB
8	i	201	HEM	C4C-C3C-CAC-CBC
8	j	201	HEM	C4B-C3B-CAB-CBB
8	k	201	HEM	C4B-C3B-CAB-CBB
8	W	201	HEM	C4D-C3D-CAD-CBD
8	C	201	HEM	C4D-C3D-CAD-CBD
8	K	201	HEM	C4D-C3D-CAD-CBD
8	j	201	HEM	C4D-C3D-CAD-CBD
8	S	201	HEM	C2D-C3D-CAD-CBD
8	p	201	HEM	C2D-C3D-CAD-CBD
8	E	201	HEM	C4D-C3D-CAD-CBD
8	W	201	HEM	C2D-C3D-CAD-CBD
8	j	201	HEM	C2D-C3D-CAD-CBD
8	C	201	HEM	C2D-C3D-CAD-CBD
8	Y	201	HEM	C1A-C2A-CAA-CBA
8	K	201	HEM	C2D-C3D-CAD-CBD
8	Y	201	HEM	C2B-C3B-CAB-CBB
8	A	201	HEM	C4B-C3B-CAB-CBB
8	C	201	HEM	C4B-C3B-CAB-CBB
8	C	201	HEM	C4C-C3C-CAC-CBC
8	D	201	HEM	C4B-C3B-CAB-CBB
8	E	201	HEM	C4B-C3B-CAB-CBB
8	G	201	HEM	C4B-C3B-CAB-CBB
8	G	201	HEM	C4C-C3C-CAC-CBC
8	H	201	HEM	C4B-C3B-CAB-CBB
8	I	201	HEM	C4C-C3C-CAC-CBC
8	J	201	HEM	C4B-C3B-CAB-CBB
8	K	201	HEM	C4B-C3B-CAB-CBB
8	Q	201	HEM	C4B-C3B-CAB-CBB
8	R	201	HEM	C4B-C3B-CAB-CBB
8	R	201	HEM	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
8	S	201	HEM	C4B-C3B-CAB-CBB
8	U	201	HEM	C4B-C3B-CAB-CBB
8	V	201	HEM	C4C-C3C-CAC-CBC
8	X	201	HEM	C4B-C3B-CAB-CBB
8	Z	201	HEM	C4B-C3B-CAB-CBB
8	Z	201	HEM	C4C-C3C-CAC-CBC
8	e	201	HEM	C4B-C3B-CAB-CBB
8	g	201	HEM	C4B-C3B-CAB-CBB
8	g	201	HEM	C4C-C3C-CAC-CBC
8	m	201	HEM	C4B-C3B-CAB-CBB
8	m	201	HEM	C4C-C3C-CAC-CBC
8	n	201	HEM	C4B-C3B-CAB-CBB
8	o	201	HEM	C4B-C3B-CAB-CBB
8	p	201	HEM	C4B-C3B-CAB-CBB
8	E	201	HEM	C2D-C3D-CAD-CBD
8	G	201	HEM	C4D-C3D-CAD-CBD
8	T	201	HEM	C4D-C3D-CAD-CBD
8	i	201	HEM	C4D-C3D-CAD-CBD
8	h	201	HEM	C2D-C3D-CAD-CBD
8	h	201	HEM	C4D-C3D-CAD-CBD
8	i	201	HEM	C2D-C3D-CAD-CBD
8	G	201	HEM	C2D-C3D-CAD-CBD
8	T	201	HEM	C2D-C3D-CAD-CBD
8	X	201	HEM	C3D-CAD-CBD-CGD
8	K	201	HEM	C4C-C3C-CAC-CBC
8	Y	201	HEM	C4B-C3B-CAB-CBB
8	h	201	HEM	C4B-C3B-CAB-CBB
8	k	201	HEM	C4C-C3C-CAC-CBC
8	l	201	HEM	C4B-C3B-CAB-CBB
8	o	201	HEM	C4C-C3C-CAC-CBC
8	Q	201	HEM	CAD-CBD-CGD-O2D
8	L	201	HEM	C2D-C3D-CAD-CBD
8	e	201	HEM	C4D-C3D-CAD-CBD
8	Z	201	HEM	C3D-CAD-CBD-CGD
8	B	201	HEM	CAD-CBD-CGD-O2D
8	L	201	HEM	C4D-C3D-CAD-CBD
8	V	201	HEM	C4D-C3D-CAD-CBD
8	L	201	HEM	CAA-CBA-CGA-O1A
8	L	201	HEM	CAA-CBA-CGA-O2A
8	a	201	HEM	CAA-CBA-CGA-O1A
8	a	201	HEM	CAA-CBA-CGA-O2A
8	n	201	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
8	l	201	HEM	CAA-CBA-CGA-O2A
8	p	201	HEM	CAA-CBA-CGA-O2A
8	F	201	HEM	C2D-C3D-CAD-CBD
8	B	201	HEM	CAD-CBD-CGD-O1D
8	J	201	HEM	CAD-CBD-CGD-O2D
8	p	201	HEM	CAA-CBA-CGA-O1A
8	B	201	HEM	CAA-CBA-CGA-O2A
8	Q	201	HEM	CAD-CBD-CGD-O1D
8	V	201	HEM	C2D-C3D-CAD-CBD
8	e	201	HEM	C2D-C3D-CAD-CBD
8	P	201	HEM	CAD-CBD-CGD-O2D
8	l	201	HEM	CAA-CBA-CGA-O1A
8	o	201	HEM	CAD-CBD-CGD-O2D
8	W	201	HEM	CAA-CBA-CGA-O2A
8	n	201	HEM	CAD-CBD-CGD-O1D
8	Y	201	HEM	CAD-CBD-CGD-O2D
8	J	201	HEM	CAD-CBD-CGD-O1D
8	n	201	HEM	C1A-C2A-CAA-CBA
8	a	201	HEM	CAD-CBD-CGD-O2D
8	e	201	HEM	CAD-CBD-CGD-O2D
8	F	201	HEM	CAD-CBD-CGD-O2D
8	Y	201	HEM	C2D-C3D-CAD-CBD
8	S	201	HEM	CAA-CBA-CGA-O2A
8	V	201	HEM	CAD-CBD-CGD-O2D
8	Y	201	HEM	CAD-CBD-CGD-O1D
8	B	201	HEM	CAA-CBA-CGA-O1A
8	e	201	HEM	CAD-CBD-CGD-O1D
8	C	201	HEM	CAD-CBD-CGD-O2D
8	P	201	HEM	CAD-CBD-CGD-O1D
8	W	201	HEM	CAA-CBA-CGA-O1A
8	o	201	HEM	CAD-CBD-CGD-O1D
8	Y	201	HEM	C3A-C2A-CAA-CBA
8	F	201	HEM	CAD-CBD-CGD-O1D
8	A	201	HEM	CAD-CBD-CGD-O1D
8	V	201	HEM	CAD-CBD-CGD-O1D
8	C	201	HEM	CAD-CBD-CGD-O1D
8	L	201	HEM	CAD-CBD-CGD-O2D
8	S	201	HEM	CAA-CBA-CGA-O1A
8	f	201	HEM	CAD-CBD-CGD-O1D
8	A	201	HEM	CAD-CBD-CGD-O2D
8	F	201	HEM	C4D-C3D-CAD-CBD
8	a	201	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
8	f	201	HEM	CAD-CBD-CGD-O2D
8	Q	201	HEM	CAA-CBA-CGA-O2A
8	h	201	HEM	CAD-CBD-CGD-O2D
8	P	201	HEM	C4D-C3D-CAD-CBD
8	L	201	HEM	CAD-CBD-CGD-O1D
8	h	201	HEM	CAD-CBD-CGD-O1D
8	Q	201	HEM	CAA-CBA-CGA-O1A
8	j	201	HEM	C1A-C2A-CAA-CBA
8	j	201	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

37 monomers are involved in 122 short contacts:

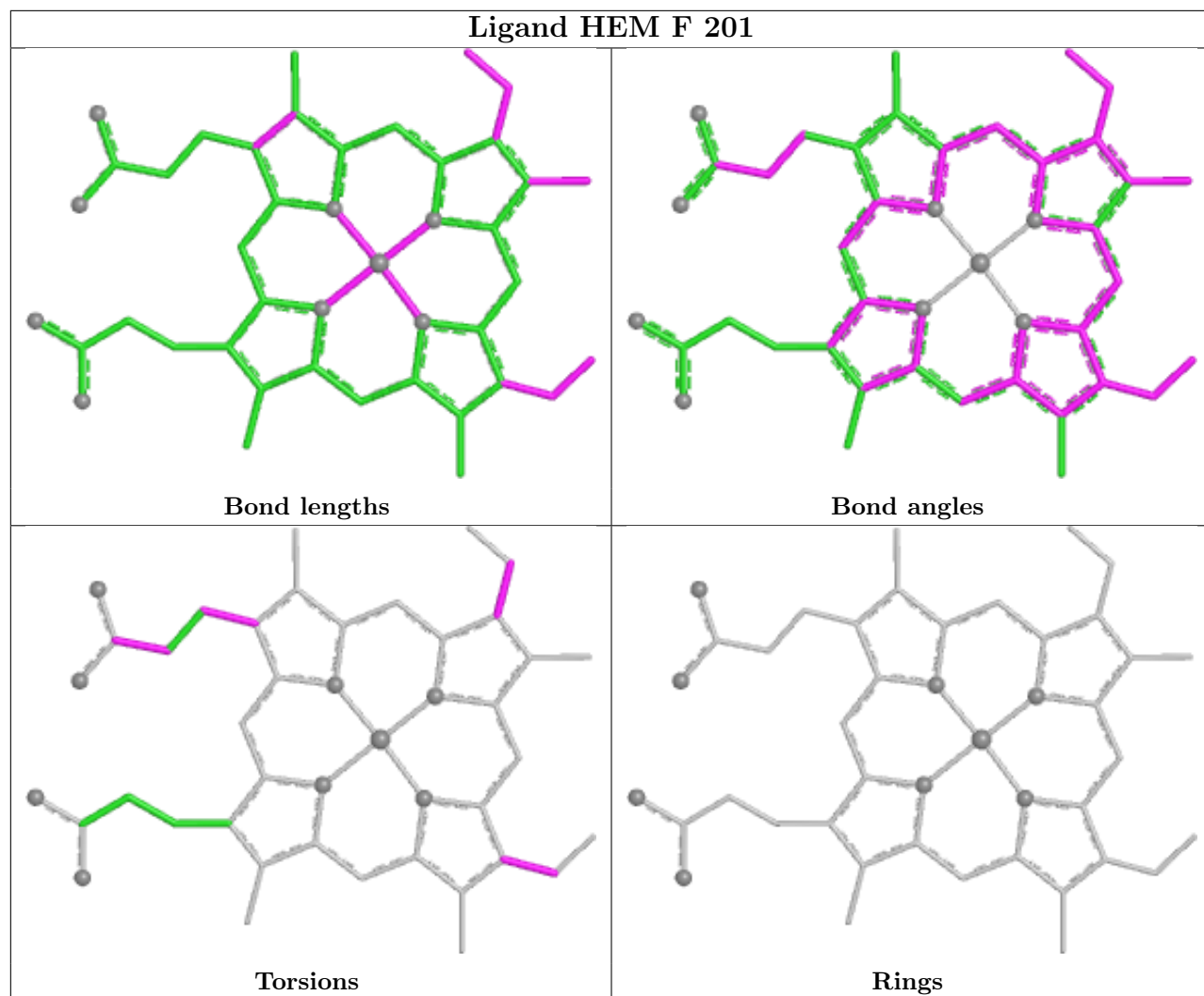
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	201	HEM	6	0
8	S	201	HEM	4	0
8	E	201	HEM	3	0
9	j	202	CYN	1	0
9	F	202	CYN	1	0
8	H	201	HEM	3	0
8	h	201	HEM	4	0
8	T	201	HEM	2	0
9	f	202	CYN	1	0
8	e	201	HEM	5	0
8	W	201	HEM	3	0
8	Q	201	HEM	7	0
8	R	201	HEM	2	0
8	i	201	HEM	6	0
8	f	201	HEM	6	0
8	U	201	HEM	9	0
8	C	201	HEM	1	0
9	B	202	CYN	1	0
8	A	201	HEM	1	0
8	P	201	HEM	3	0
8	a	201	HEM	2	0
8	p	201	HEM	1	0
8	D	201	HEM	2	0
8	L	201	HEM	3	0
8	Y	201	HEM	6	0
8	X	201	HEM	4	0
8	m	201	HEM	5	0
8	I	201	HEM	2	0

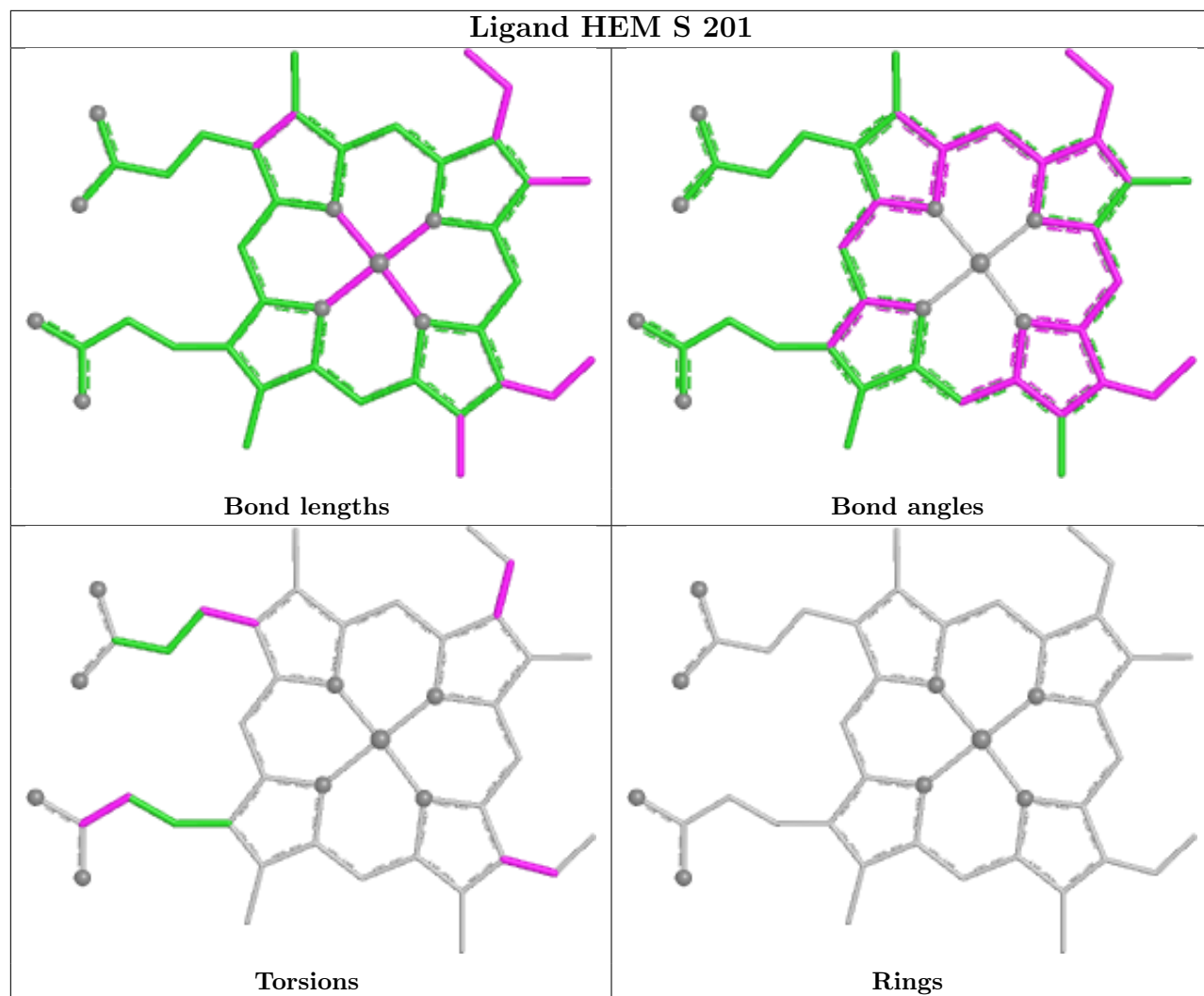
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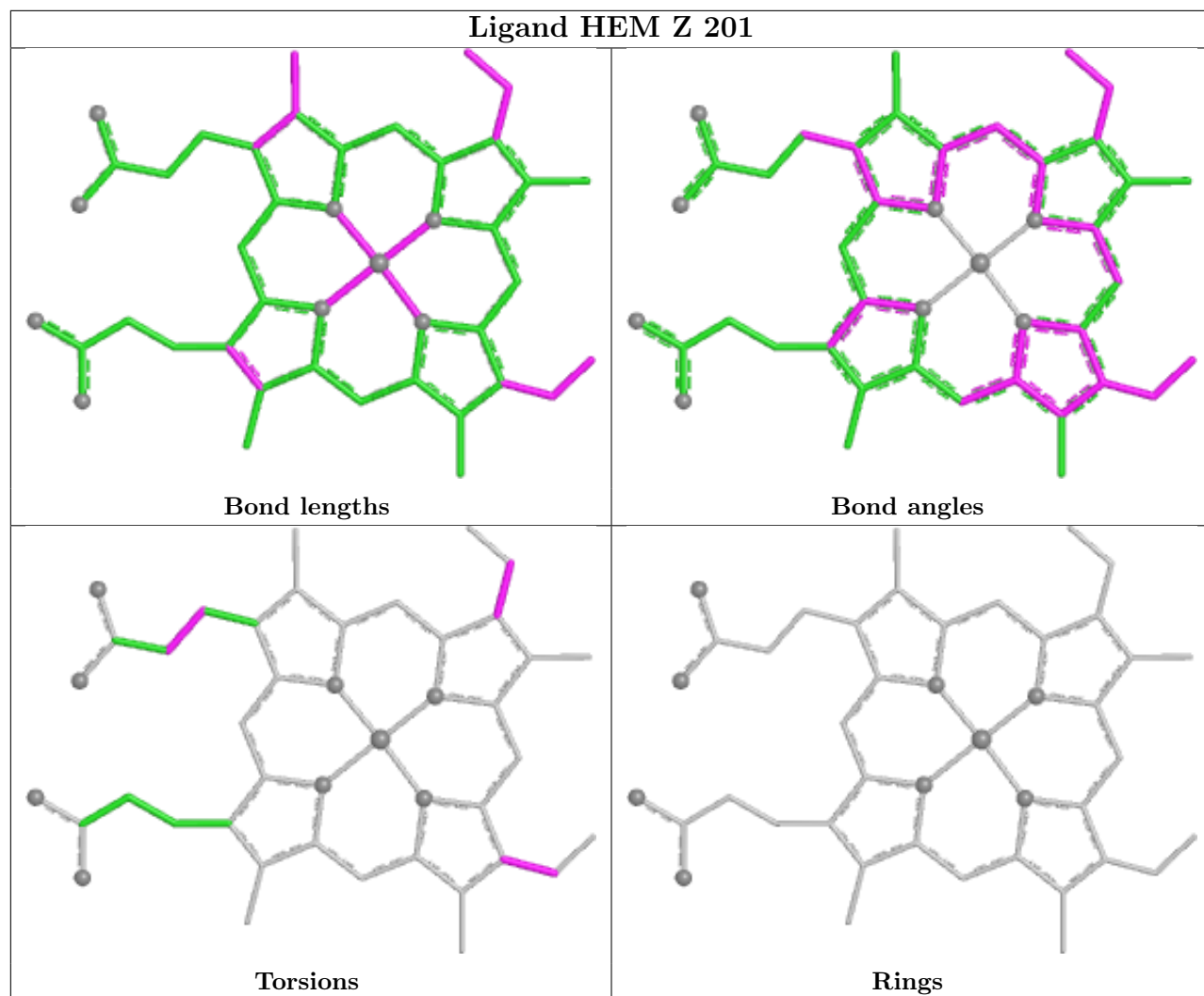
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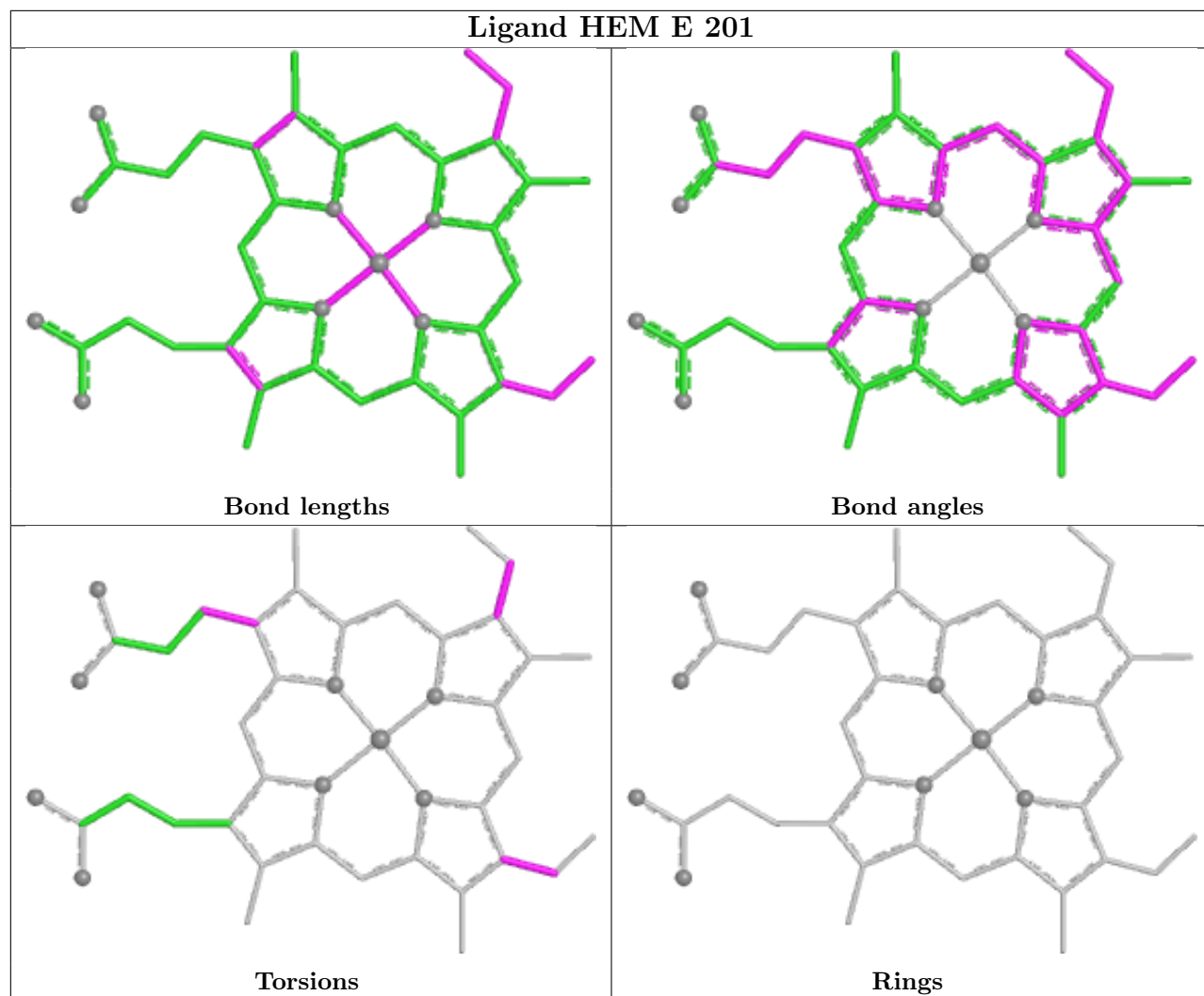
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	U	202	CYN	1	0
8	g	201	HEM	1	0
8	k	201	HEM	2	0
8	j	201	HEM	6	0
8	l	201	HEM	2	0
8	B	201	HEM	8	0
8	n	201	HEM	6	0
9	Q	202	CYN	1	0
8	J	201	HEM	7	0

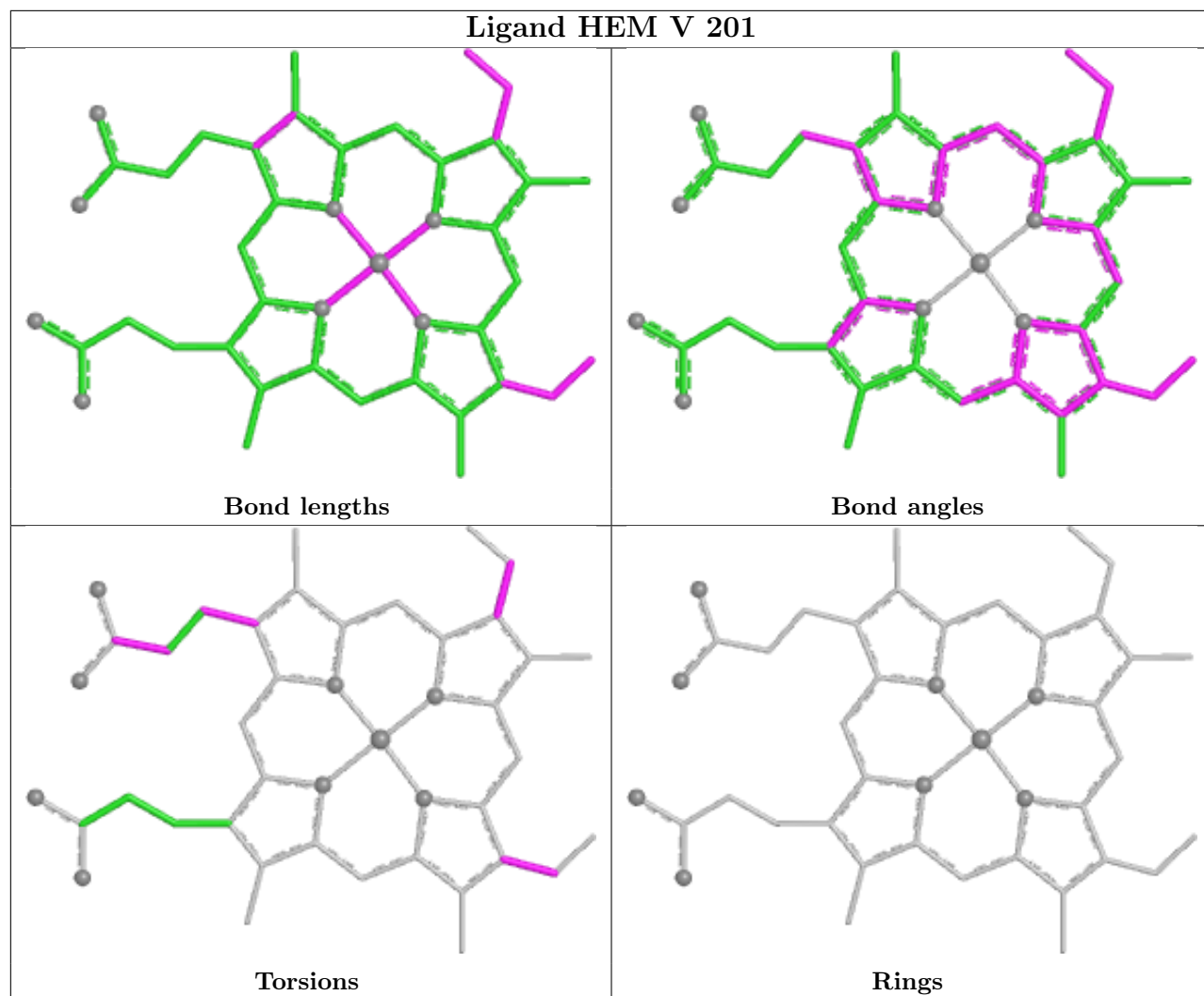
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

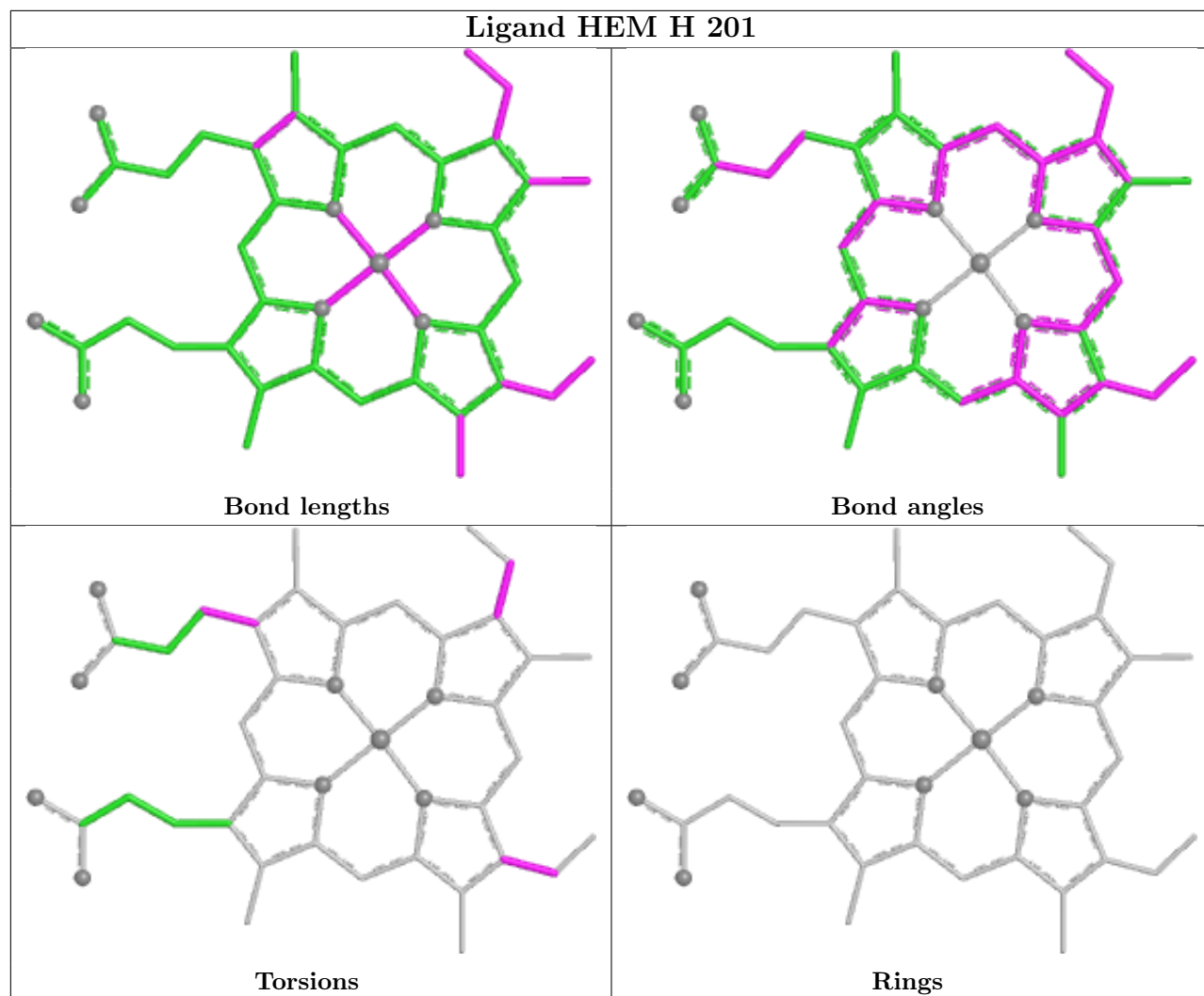


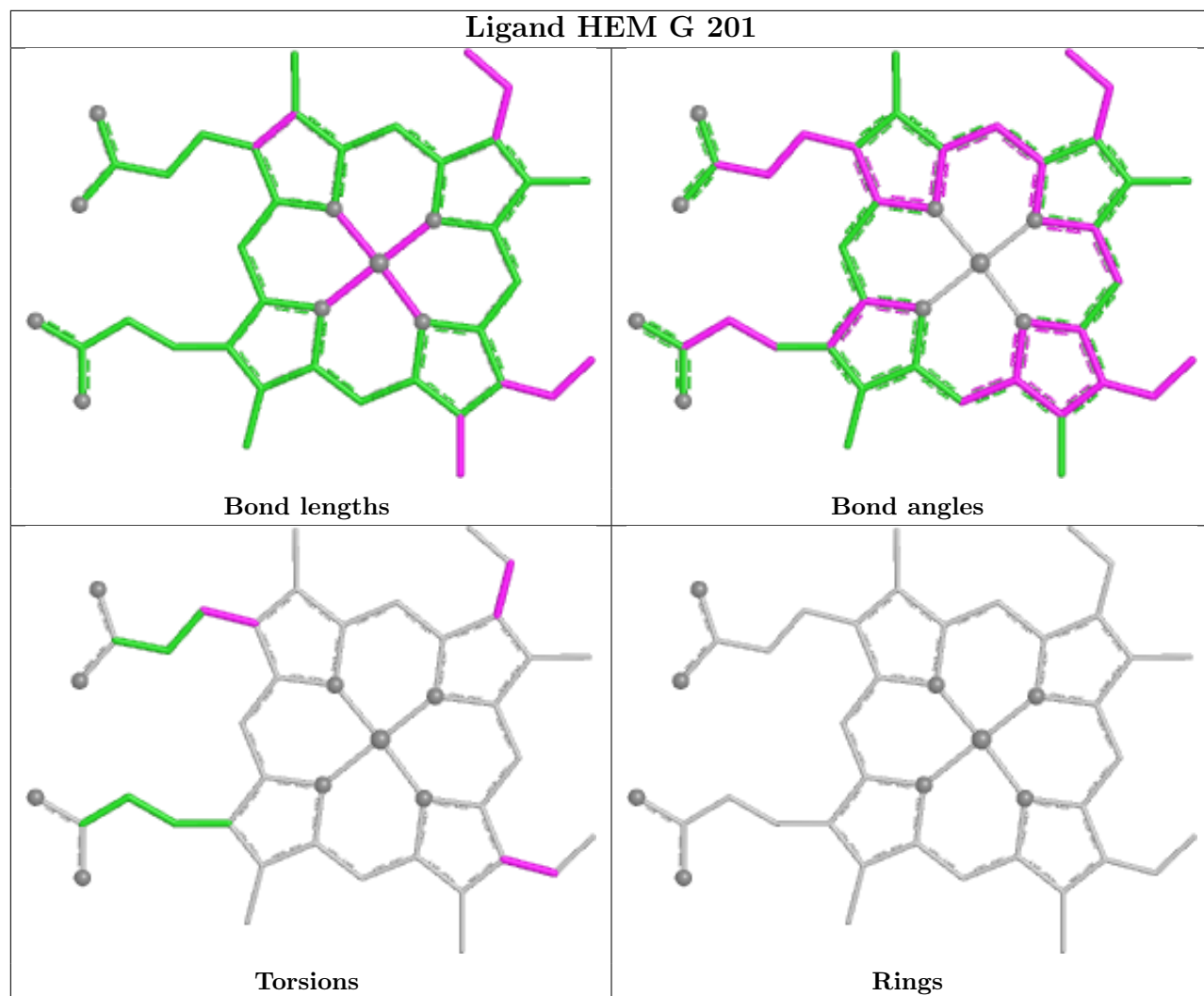


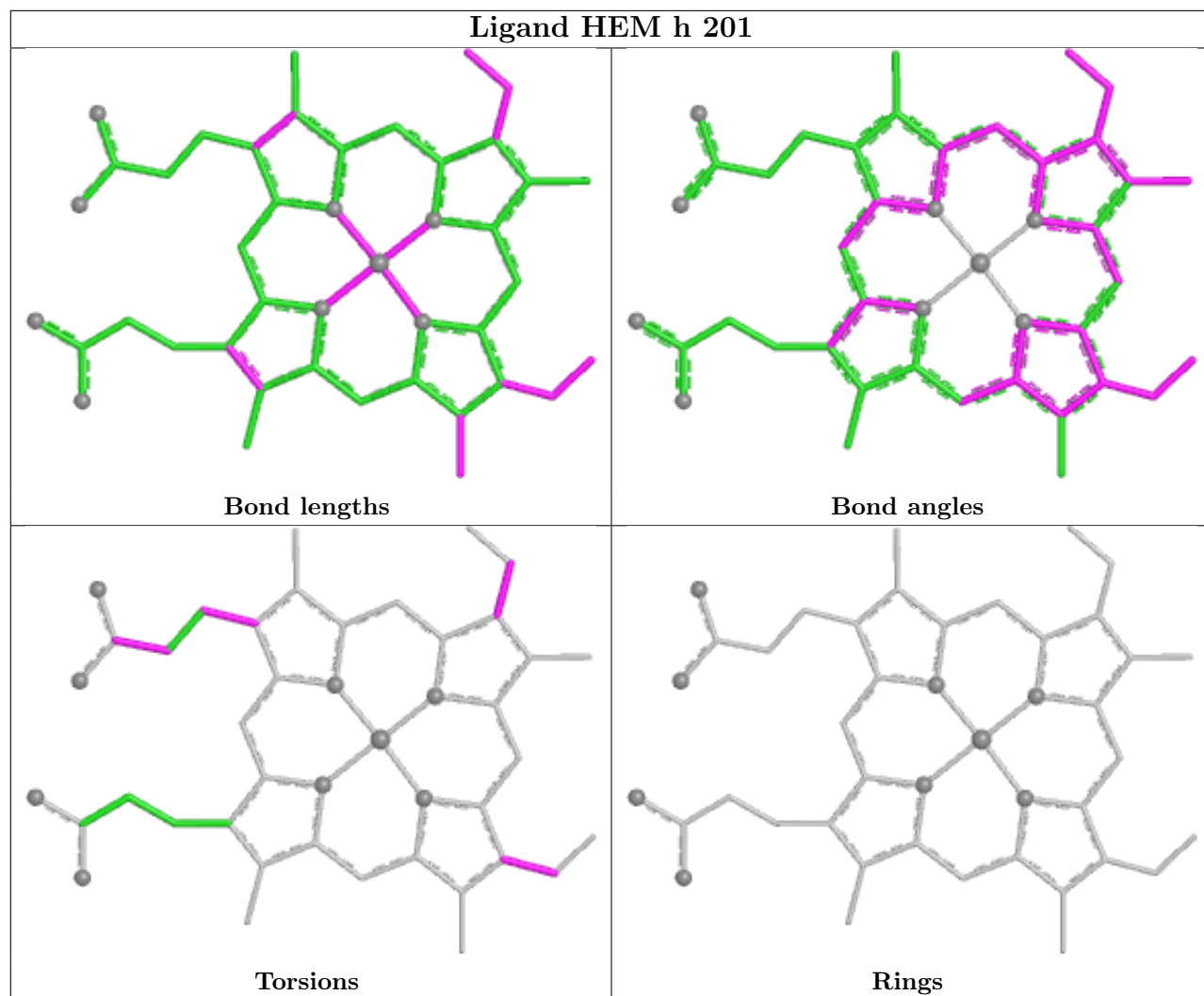


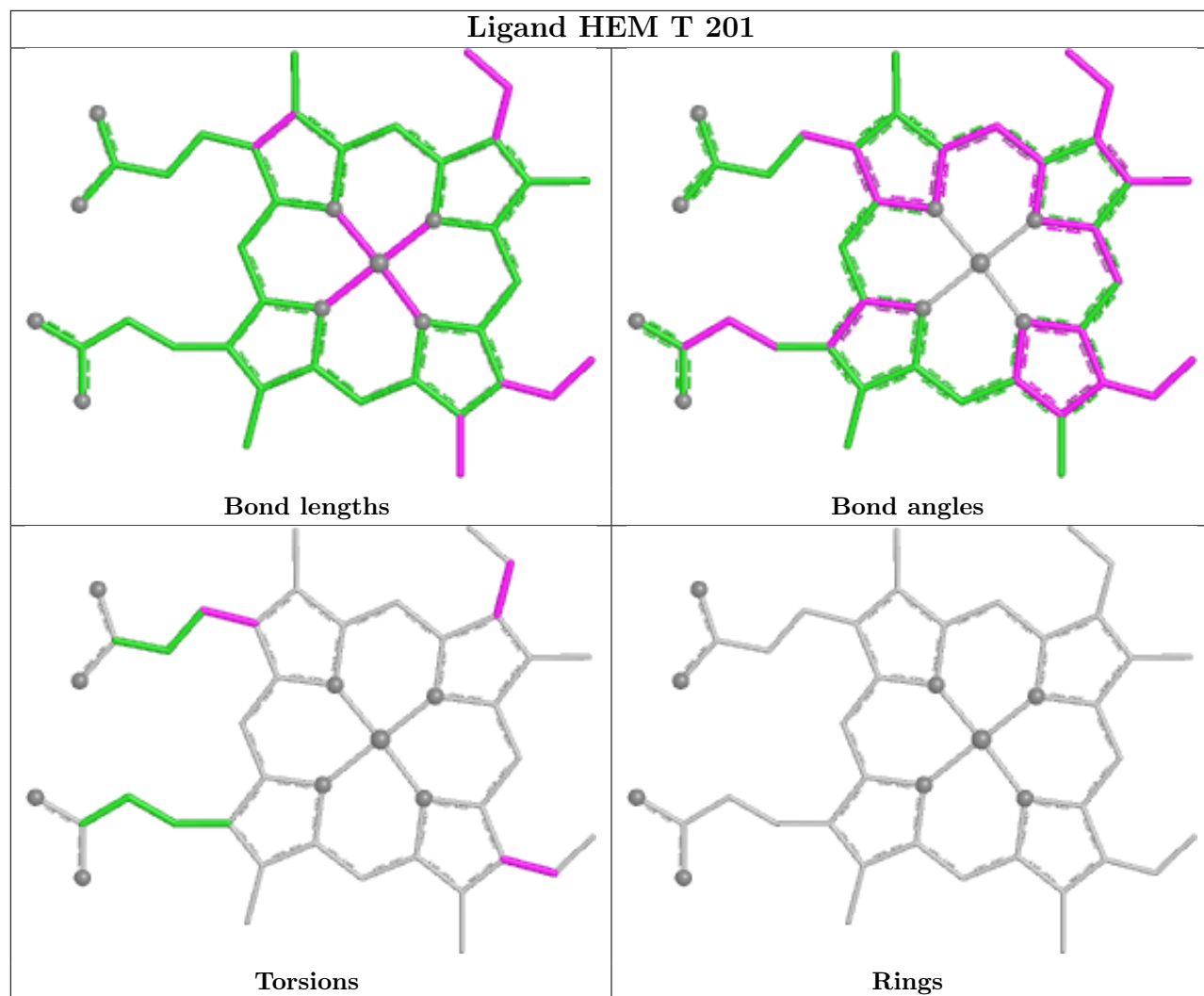




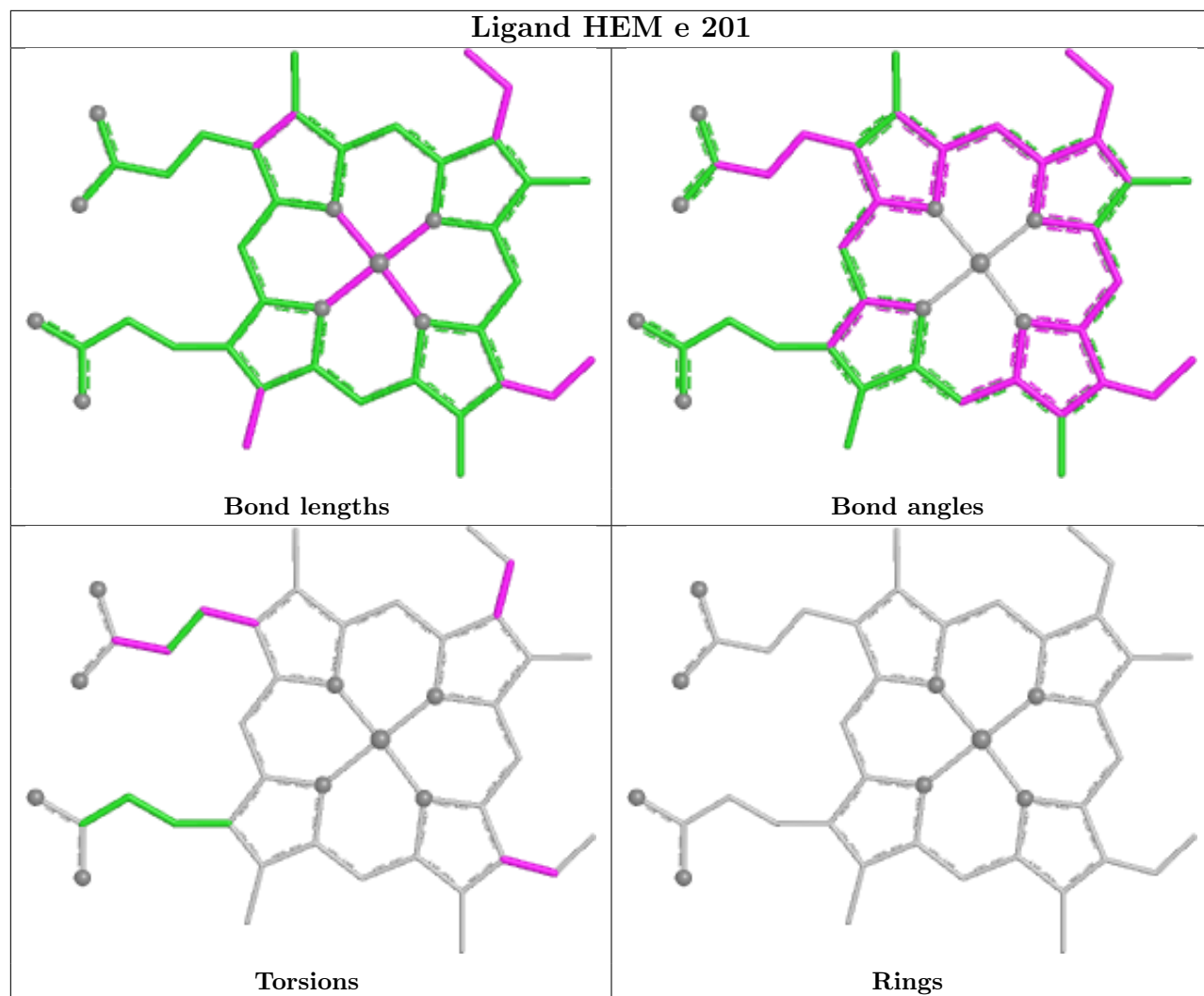




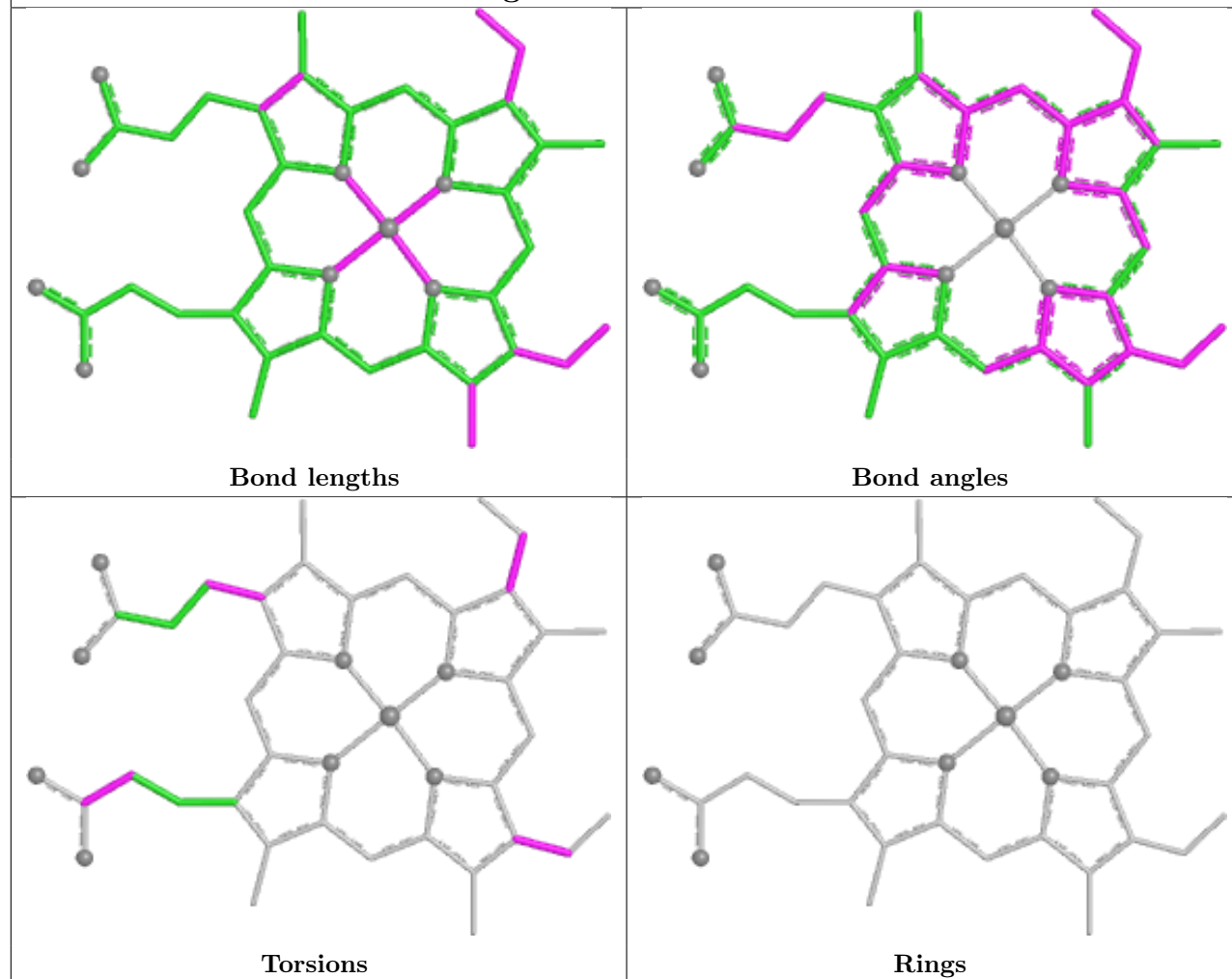


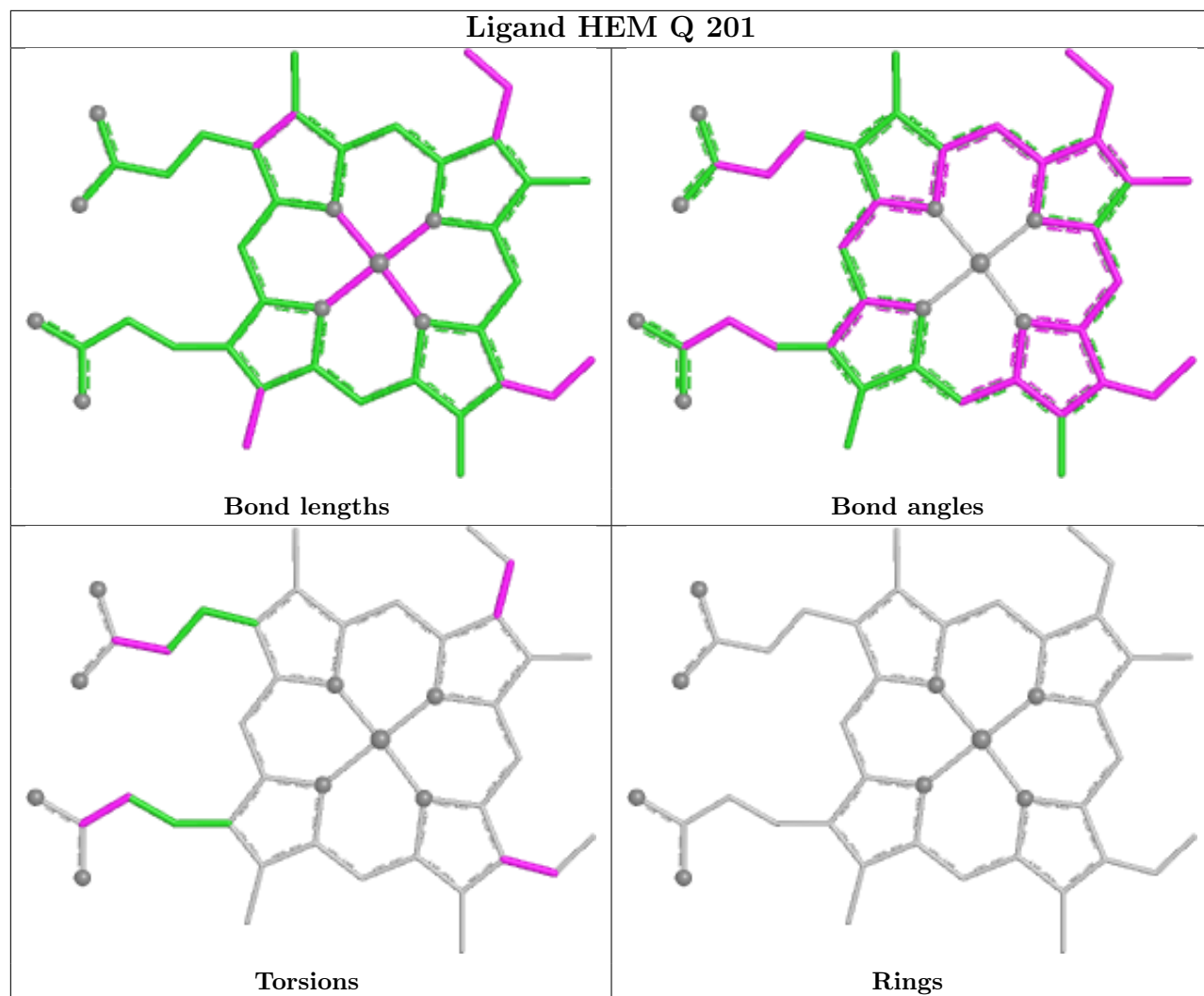


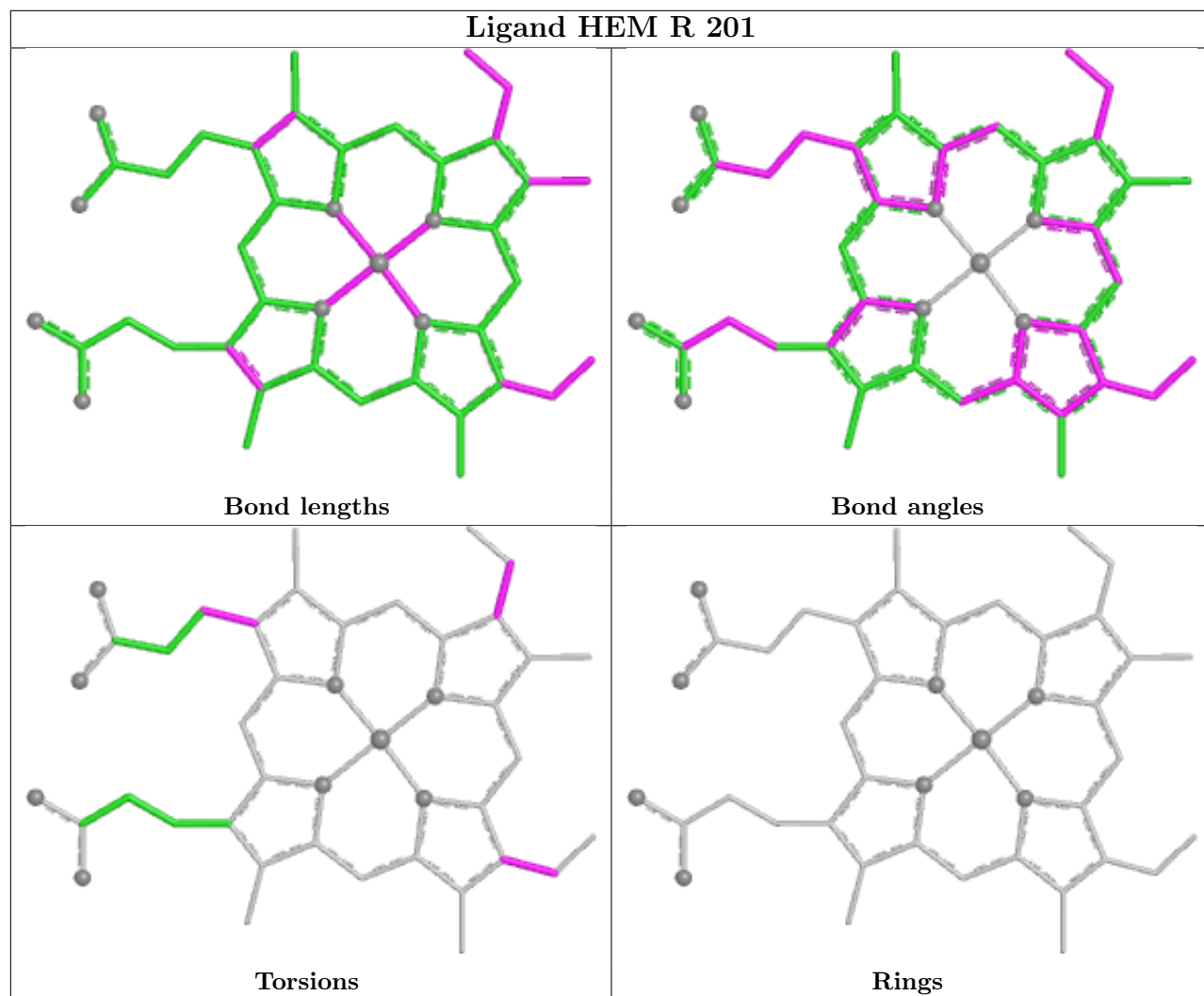
Ligand HEM e 201



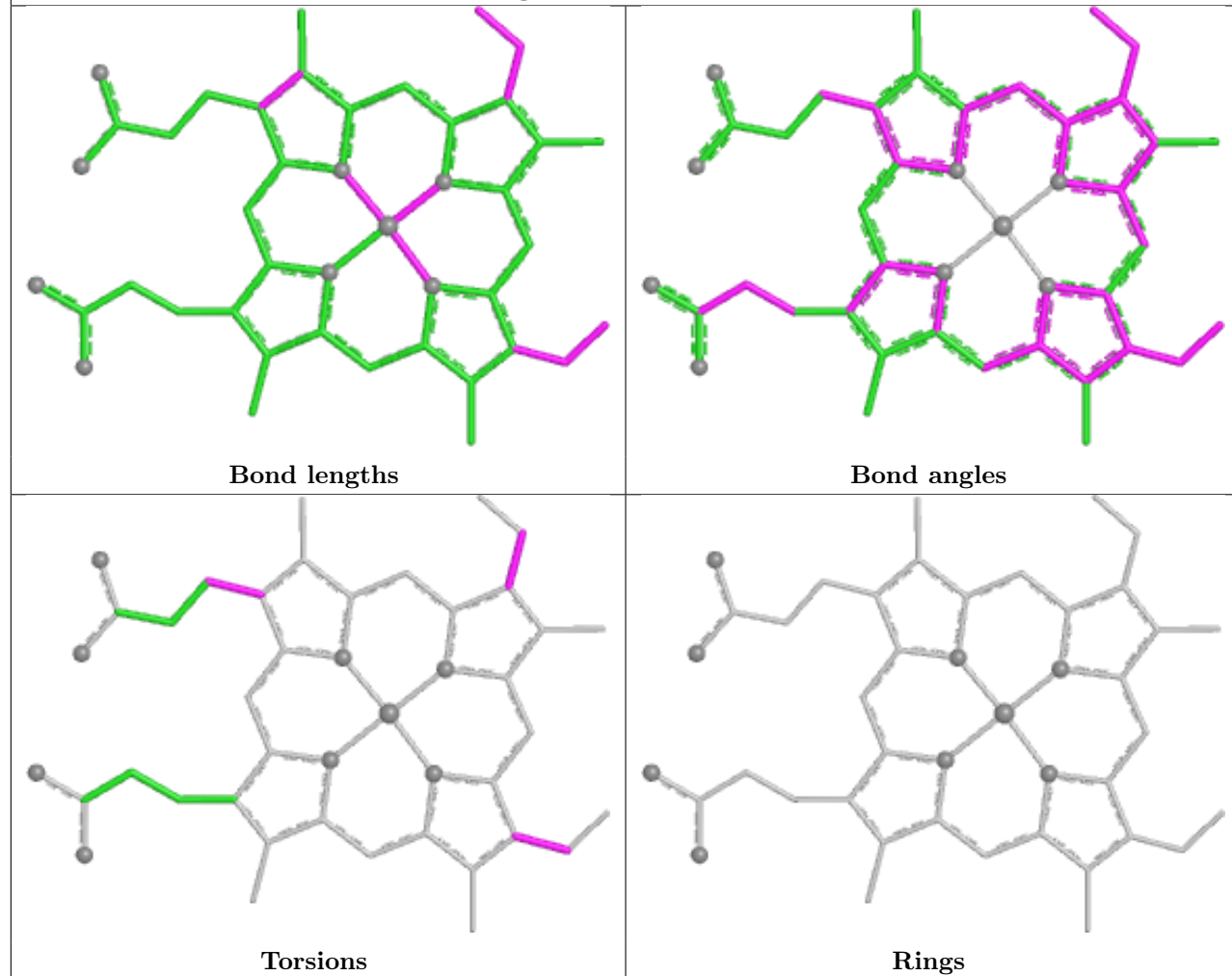
Ligand HEM W 201



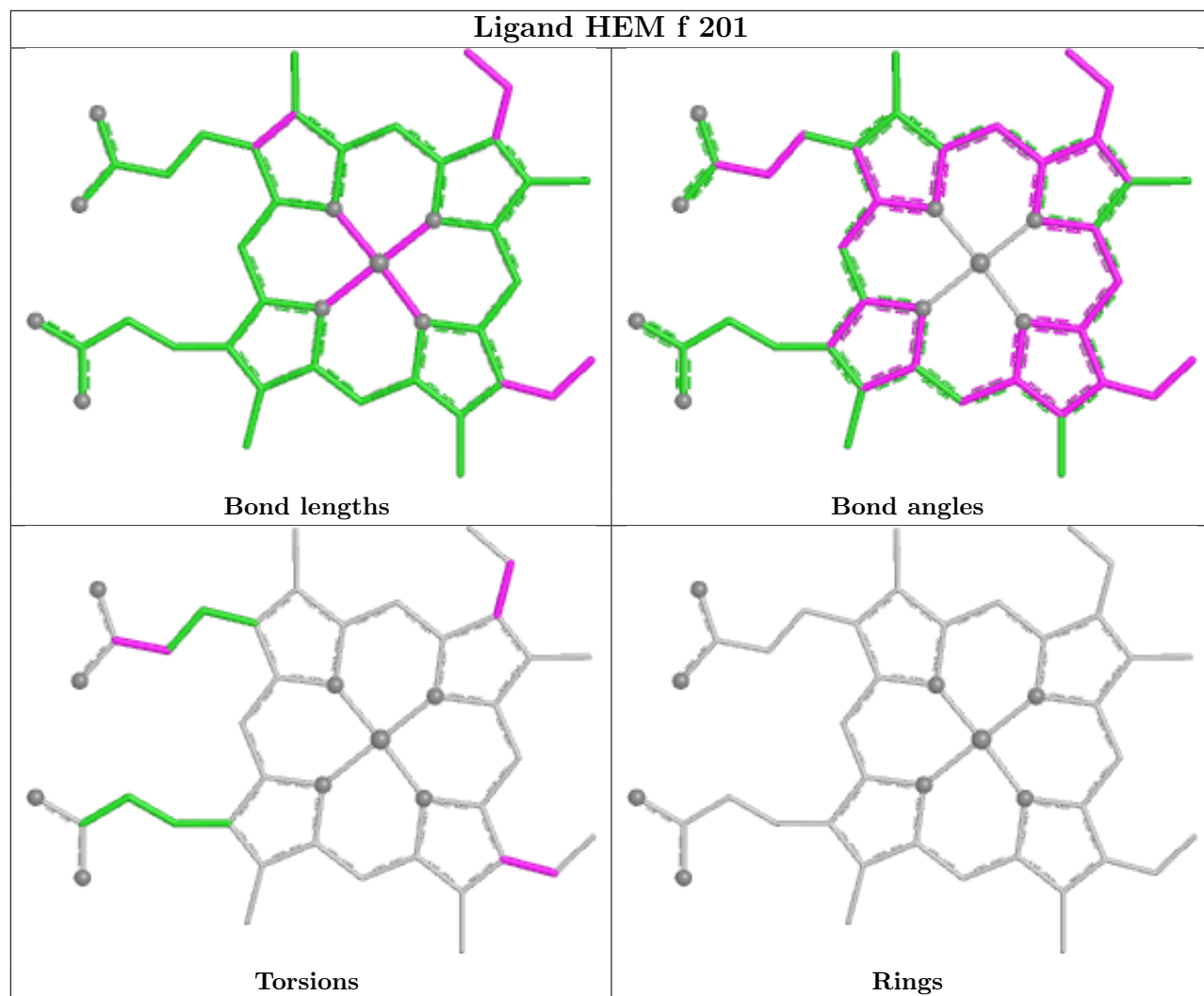


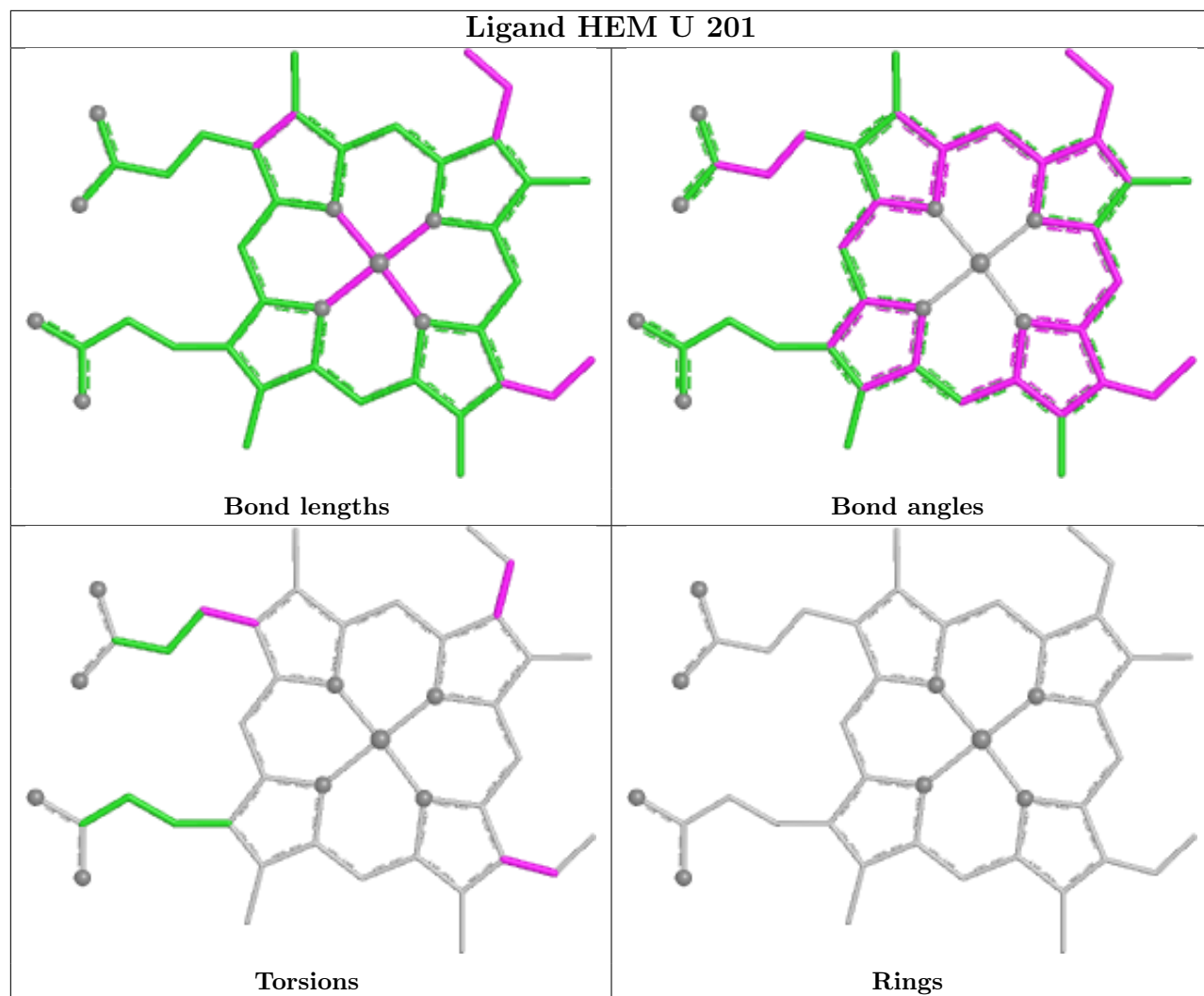


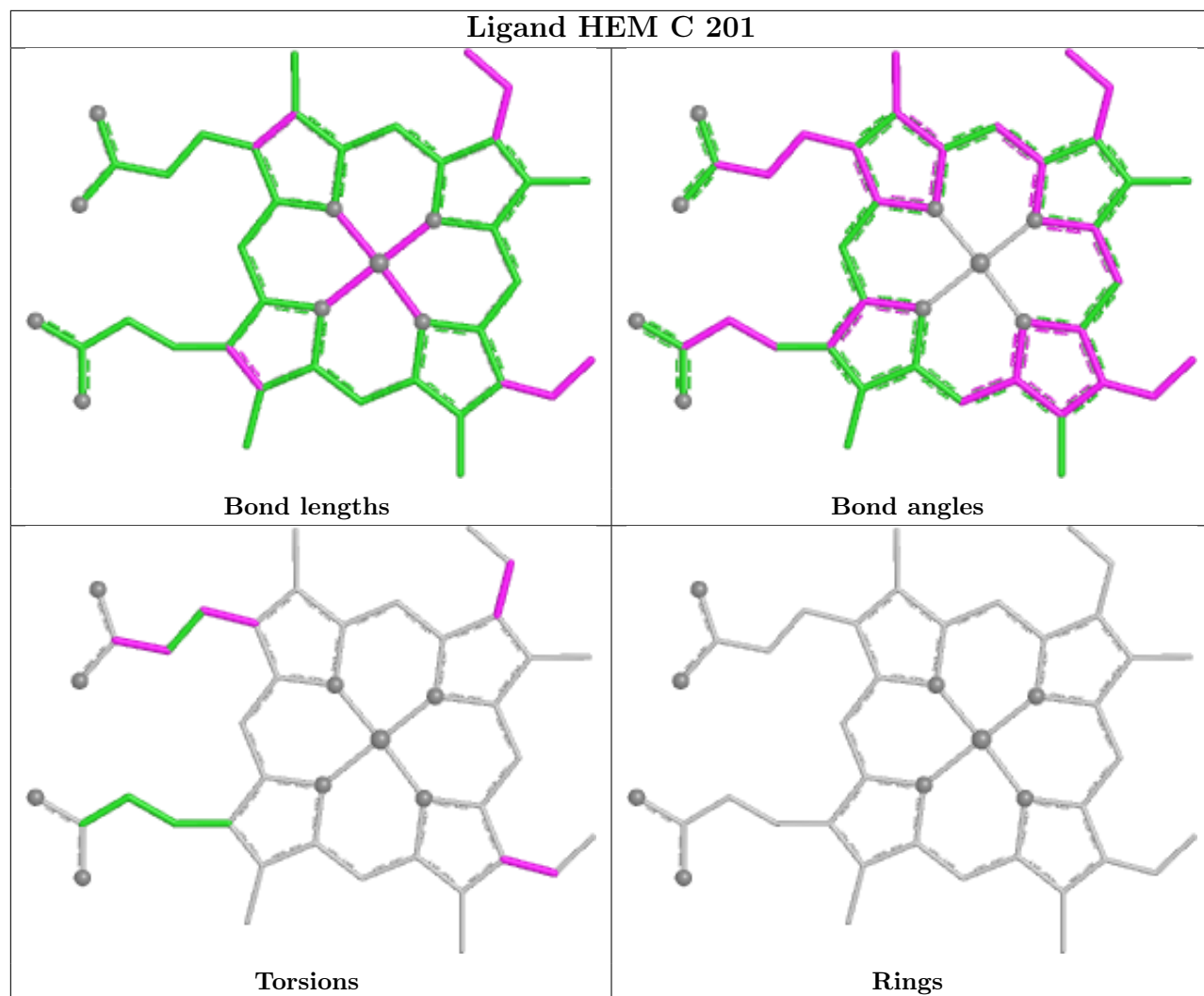
Ligand HEM i 201

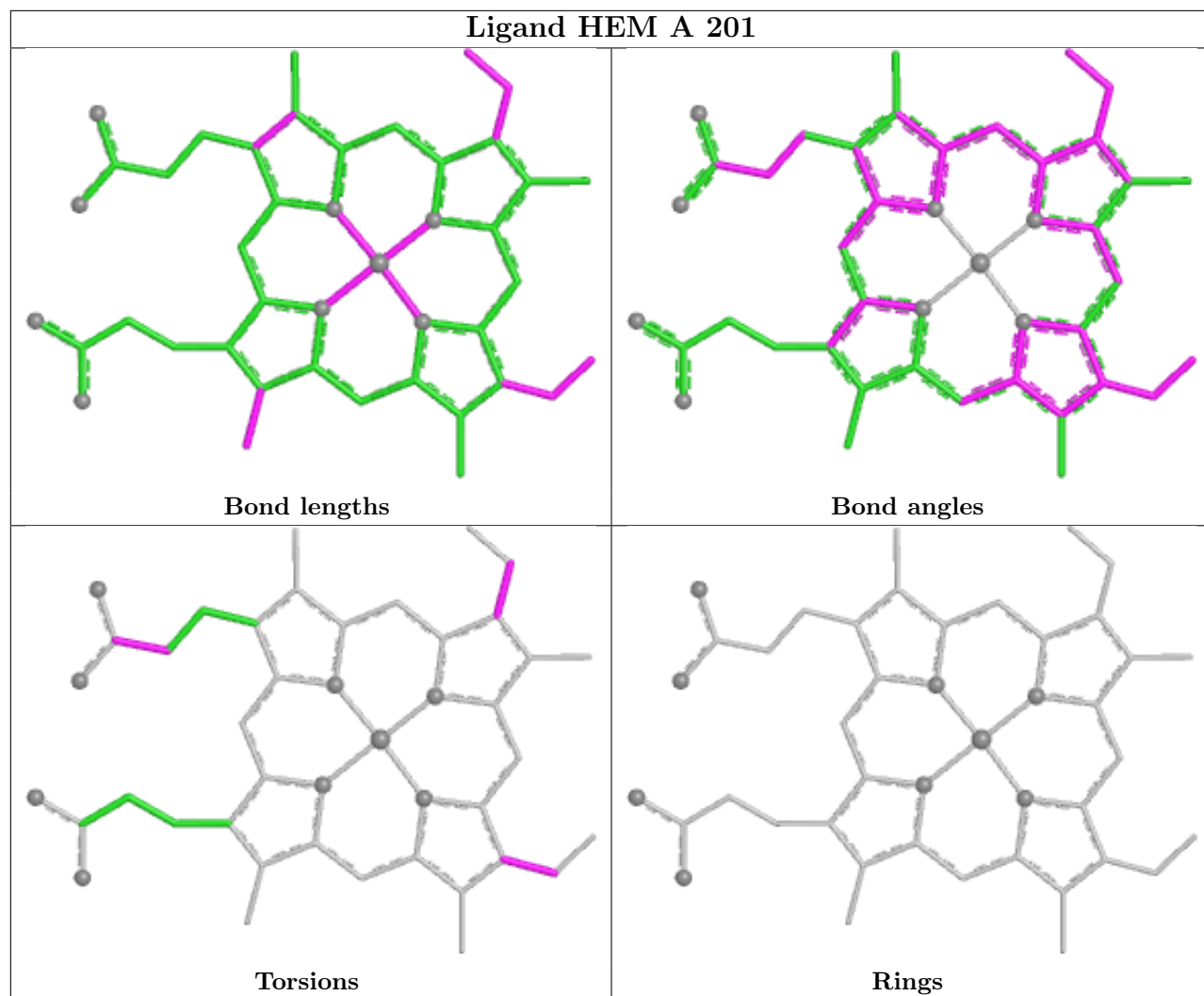


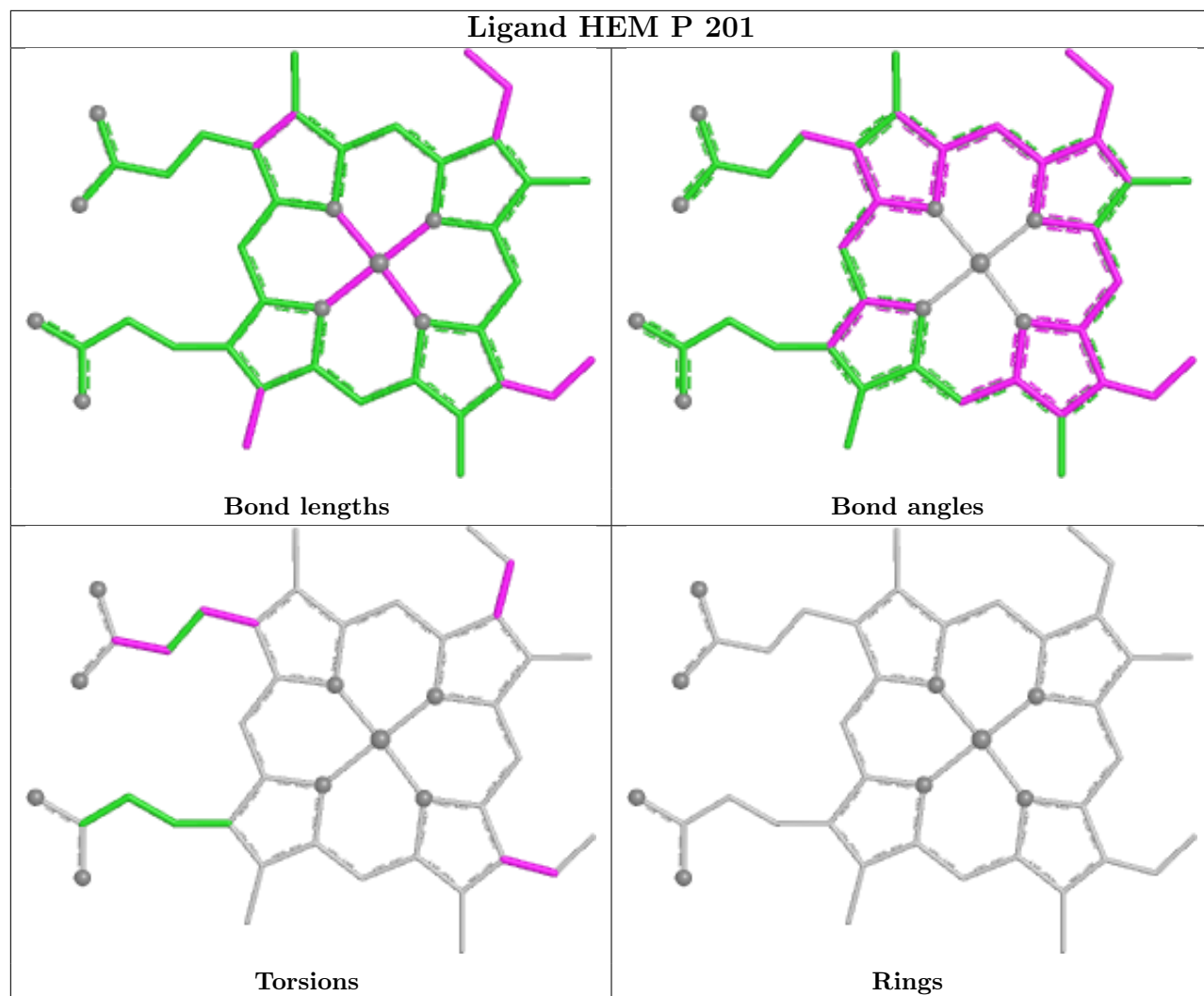
Ligand HEM f 201



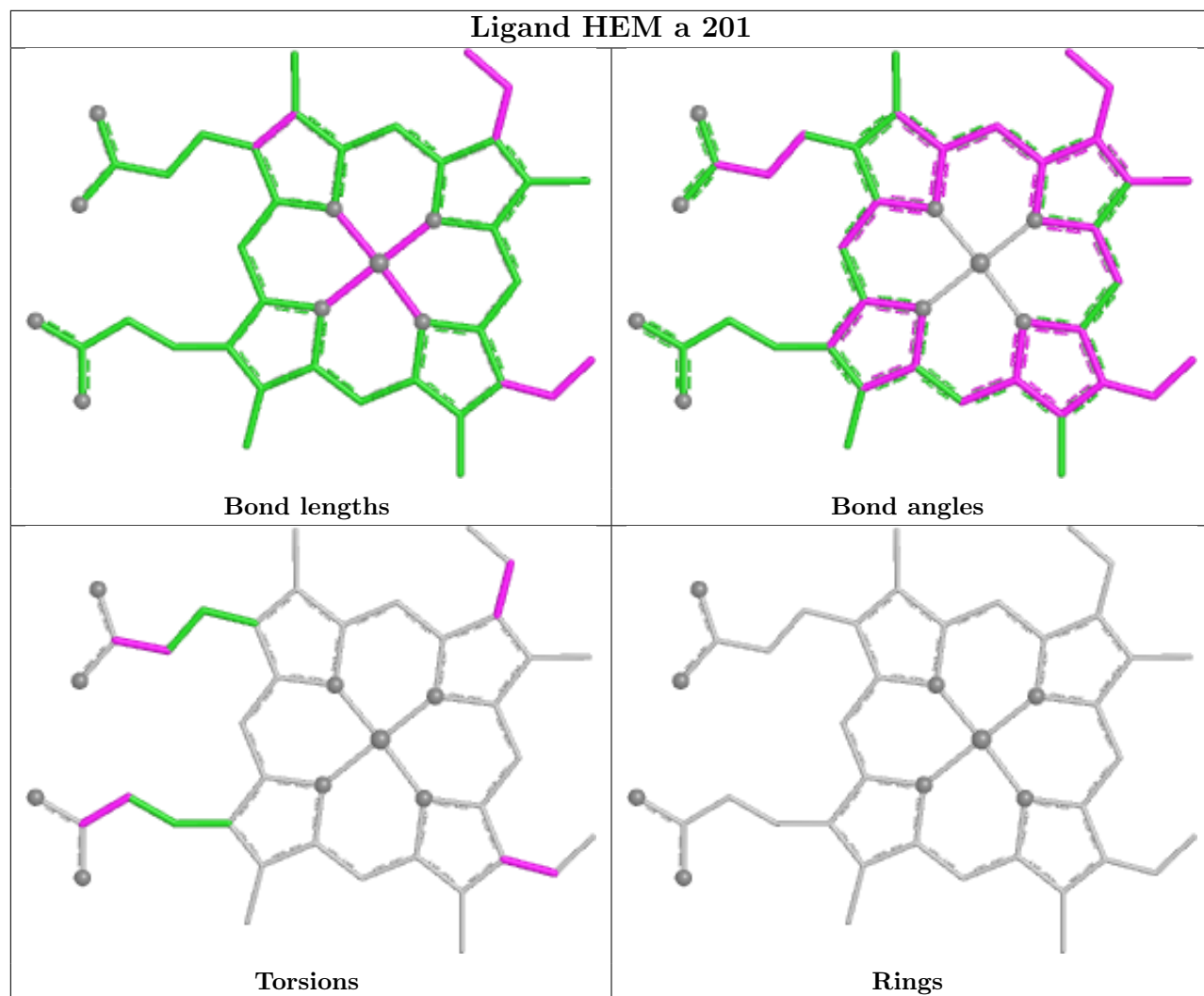


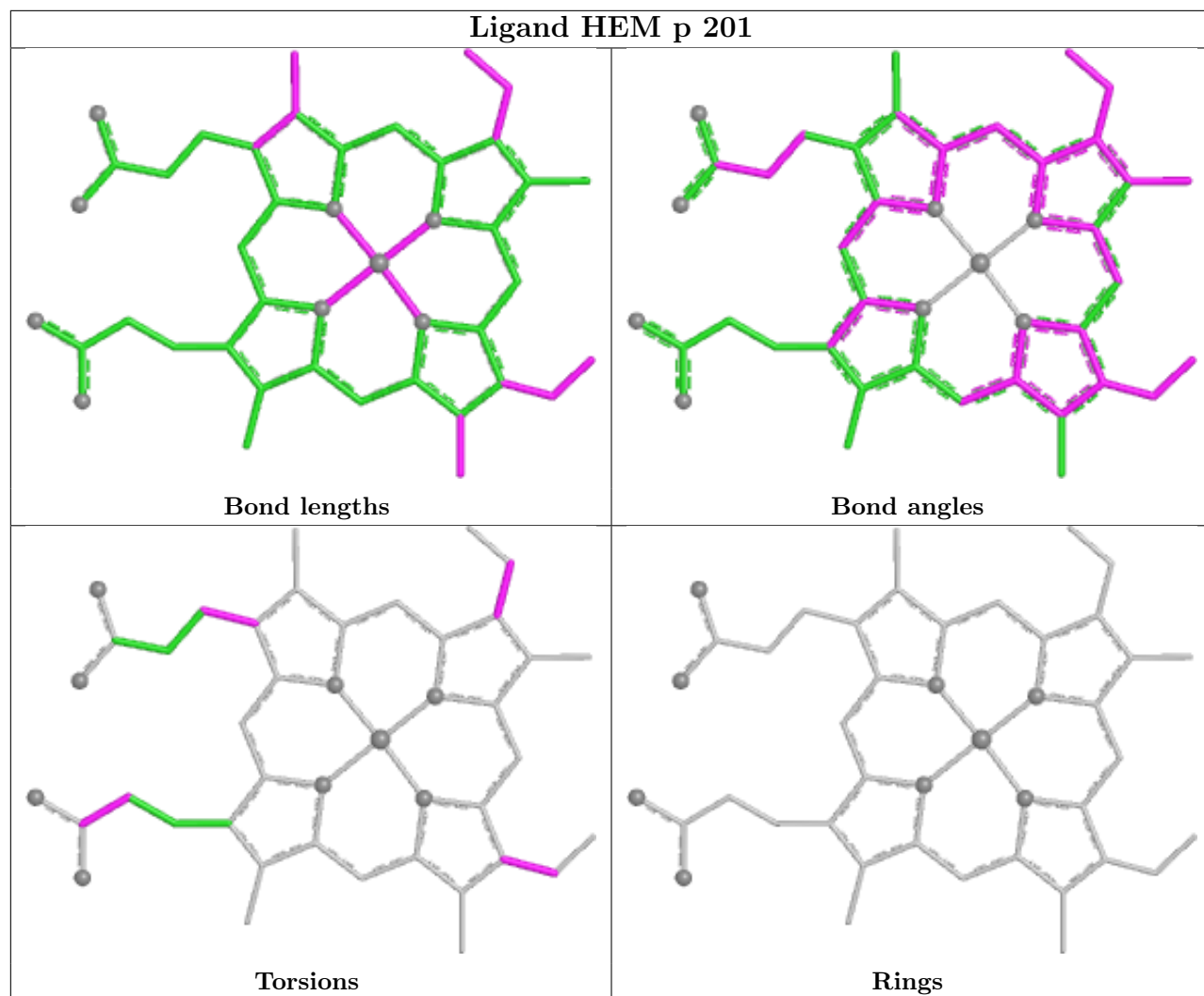


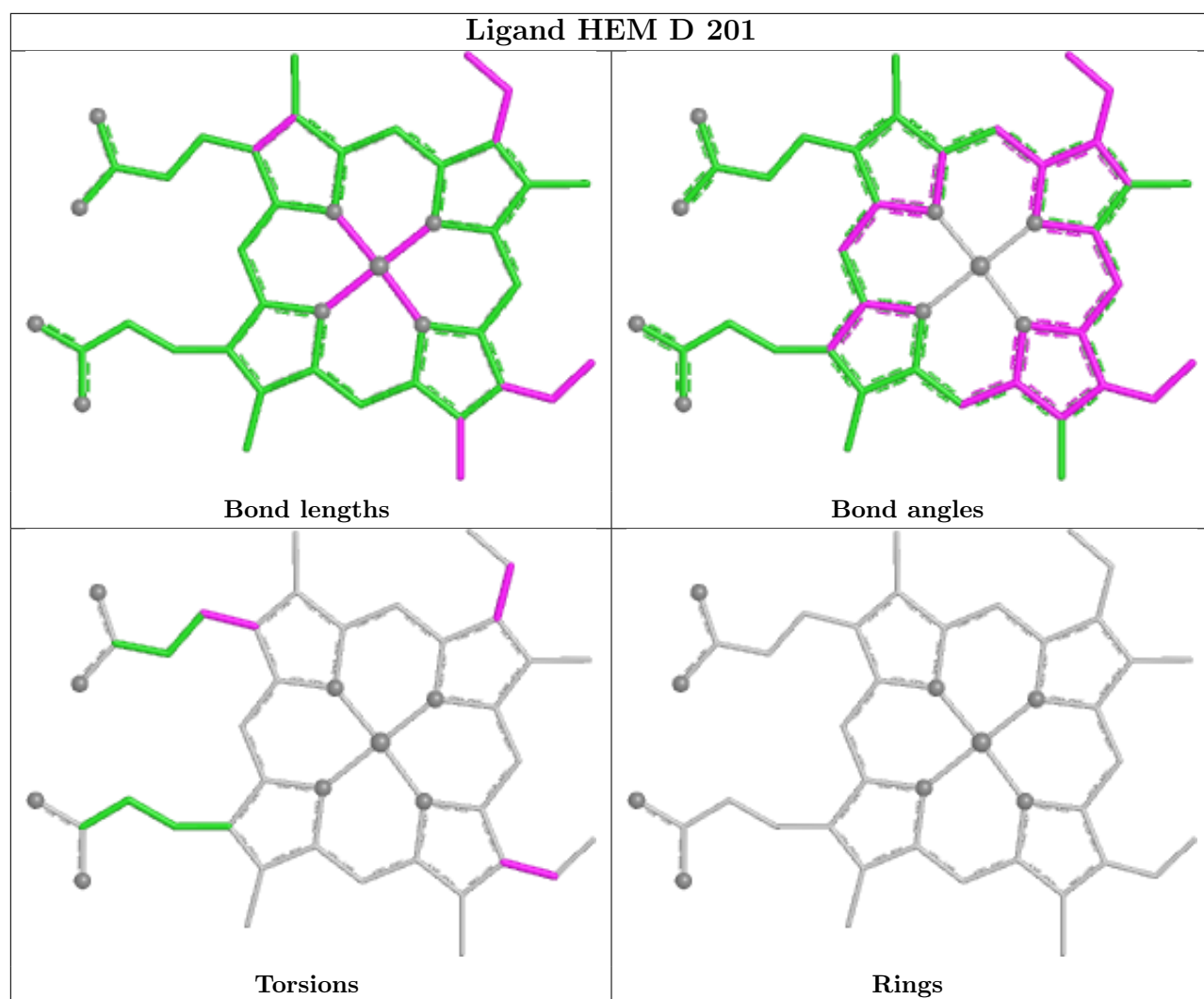


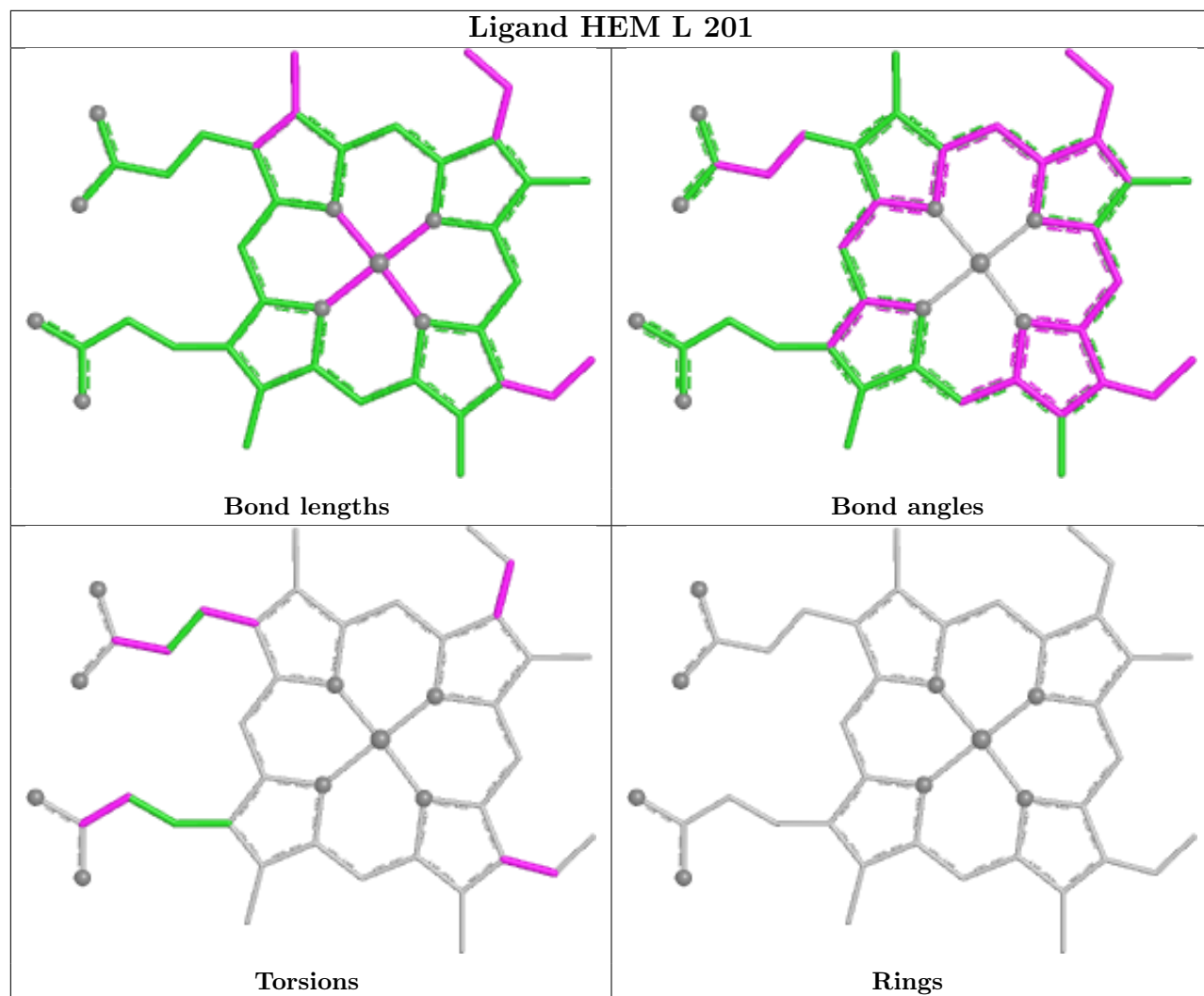


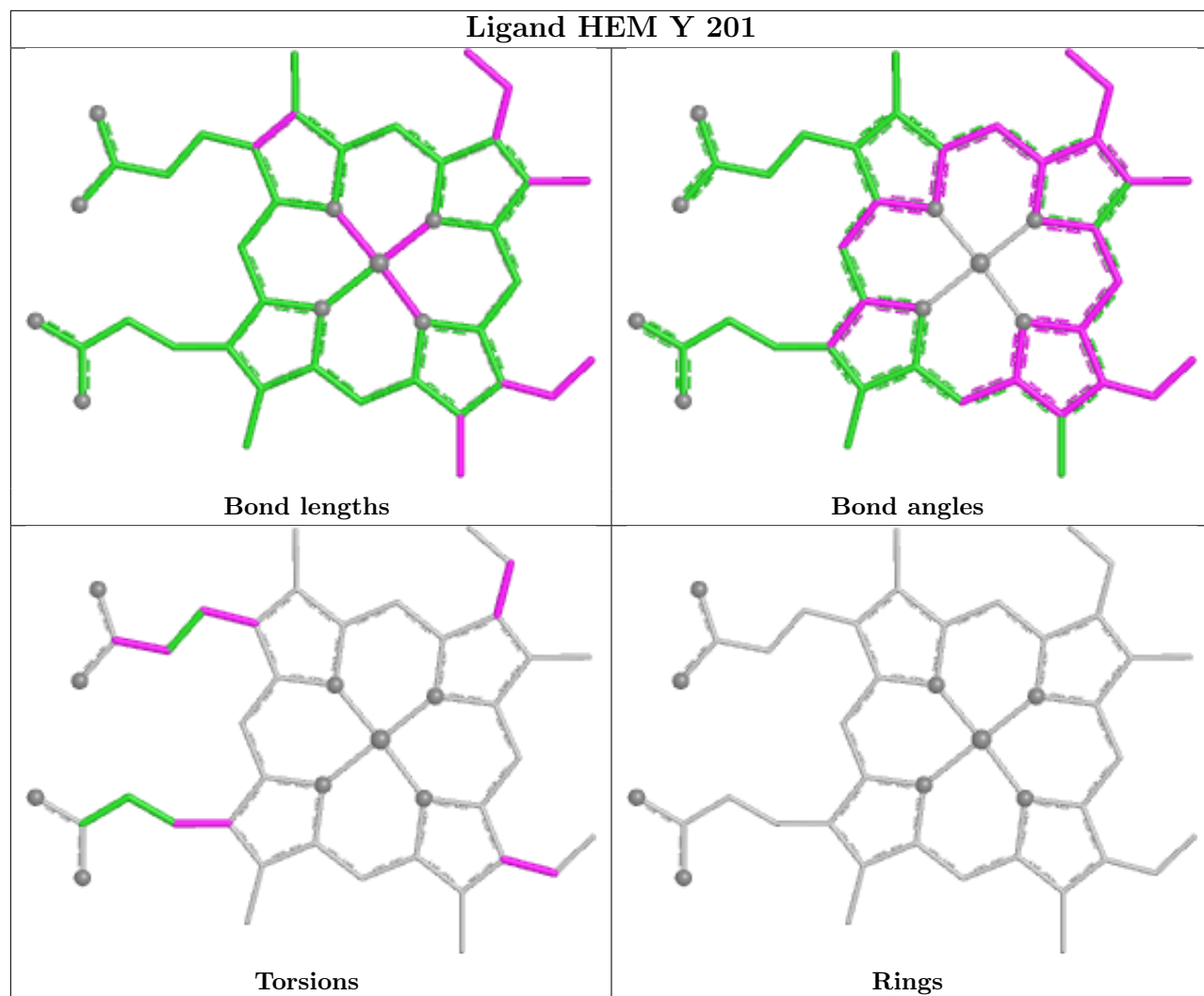
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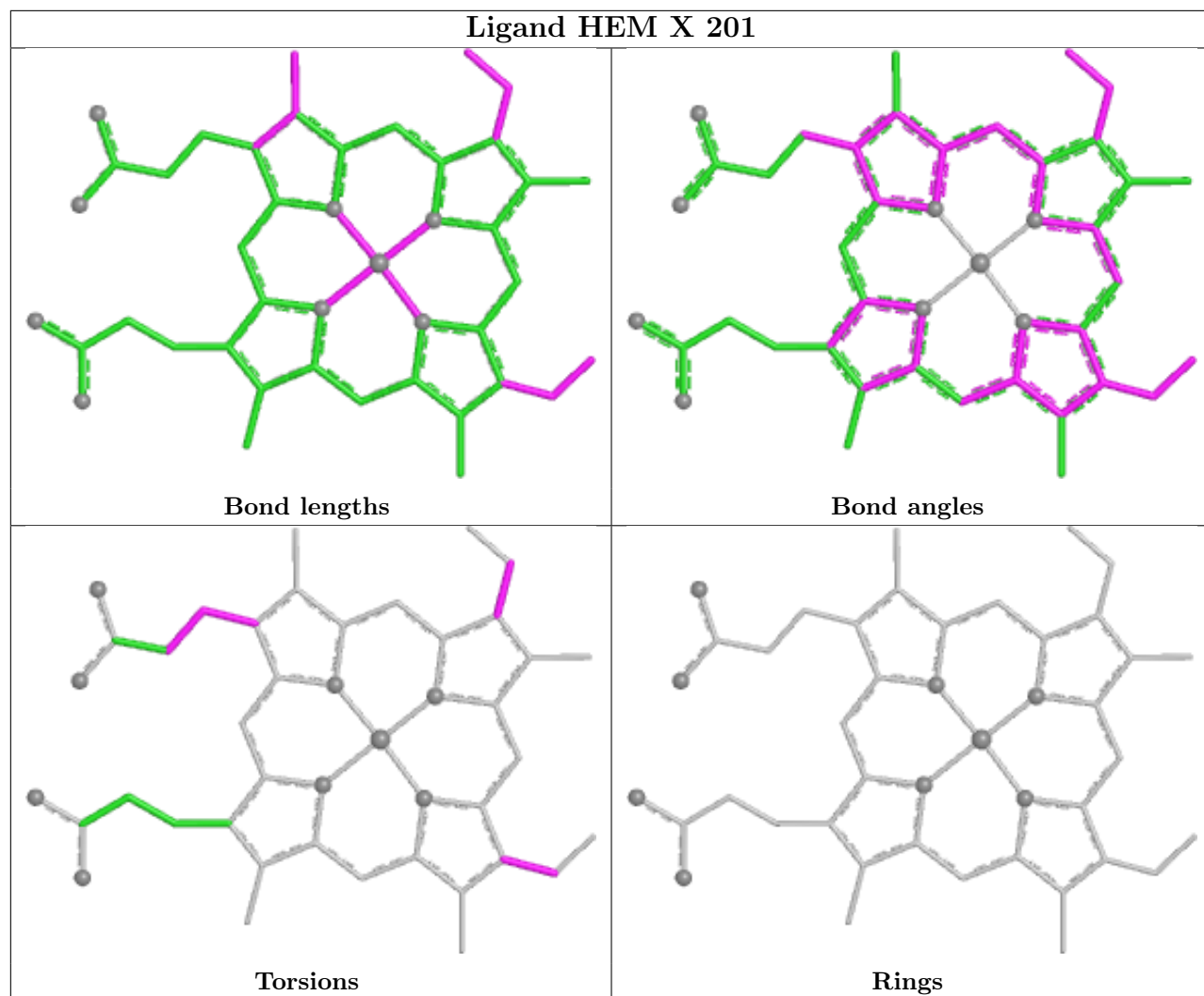


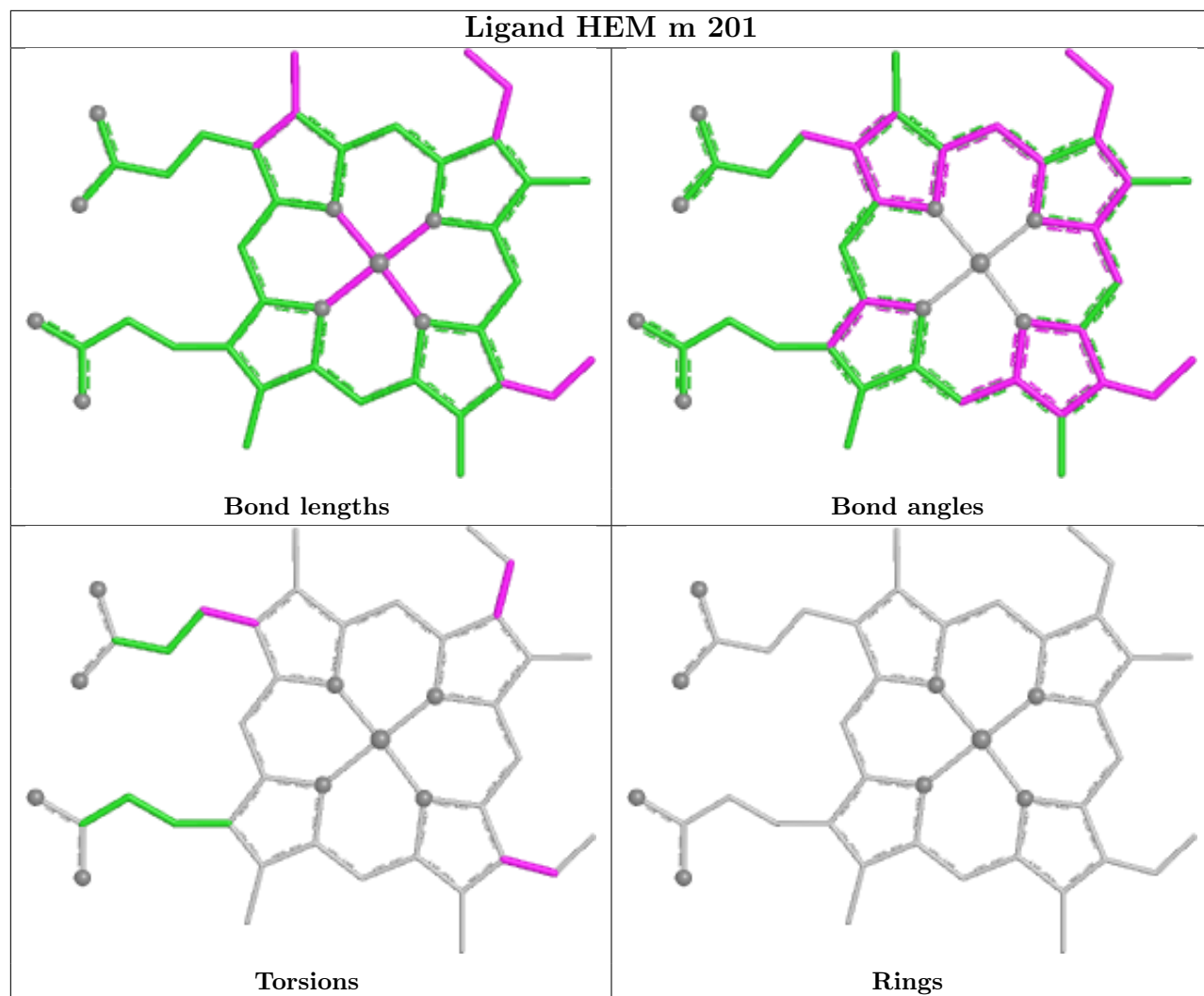




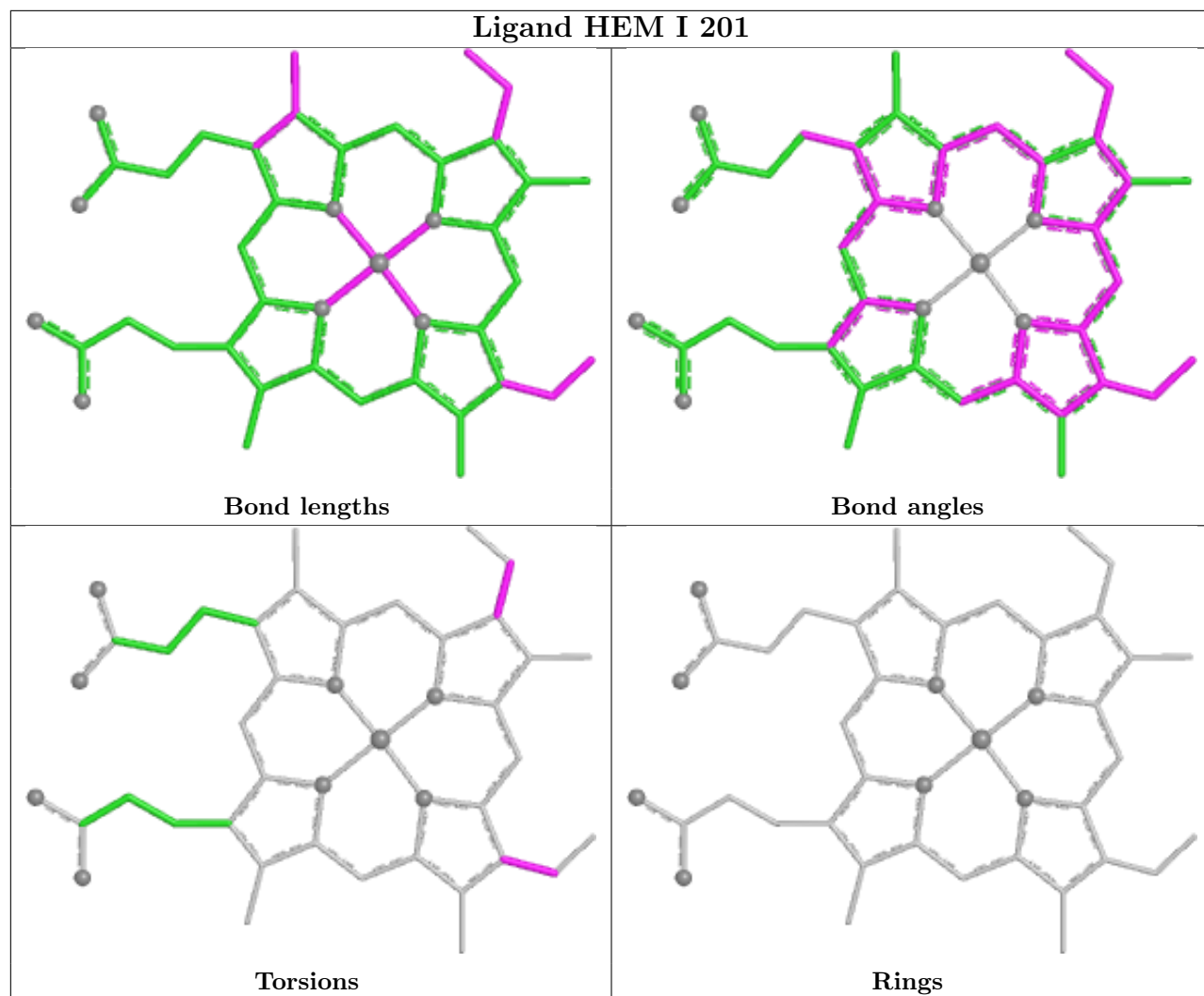


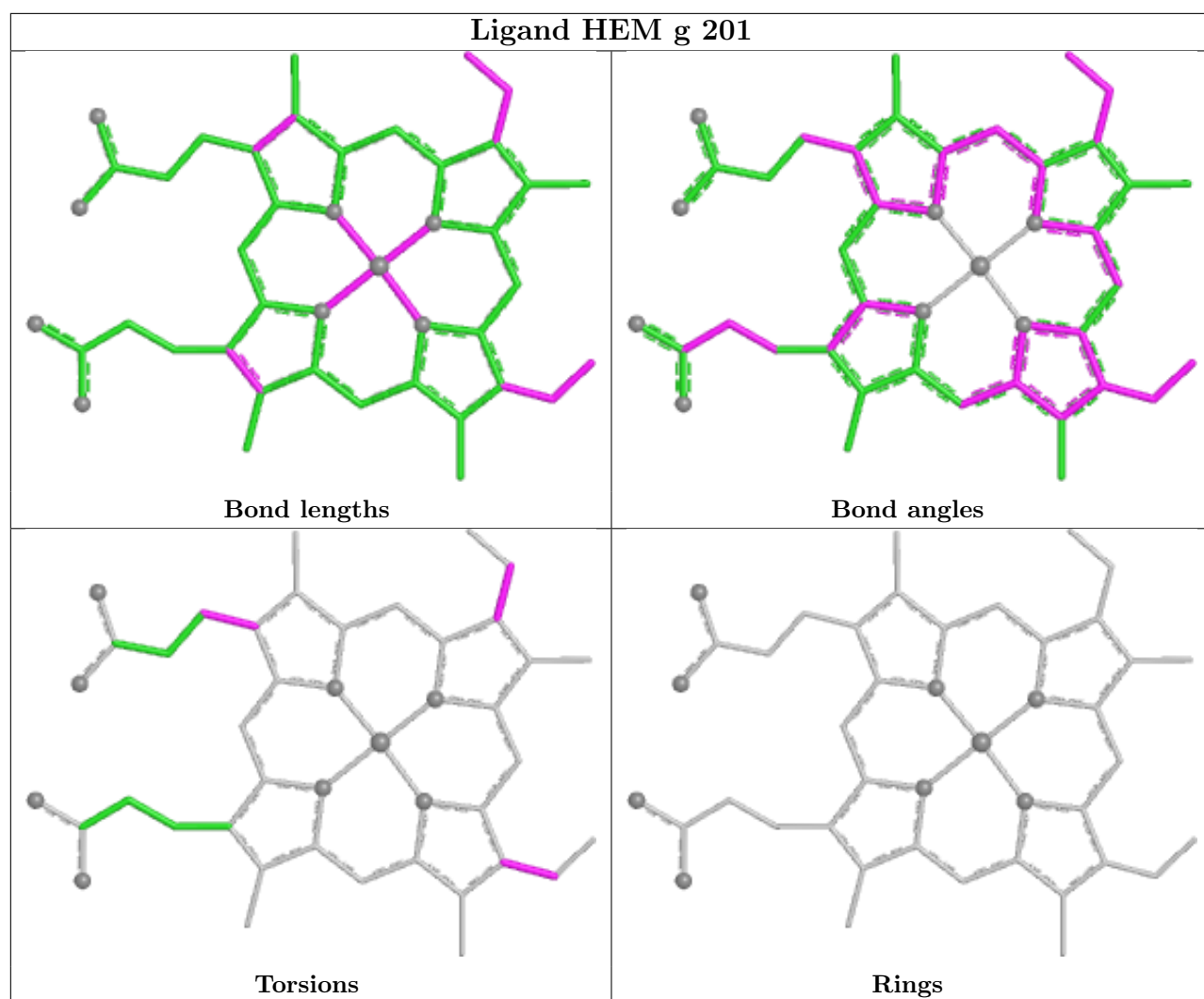


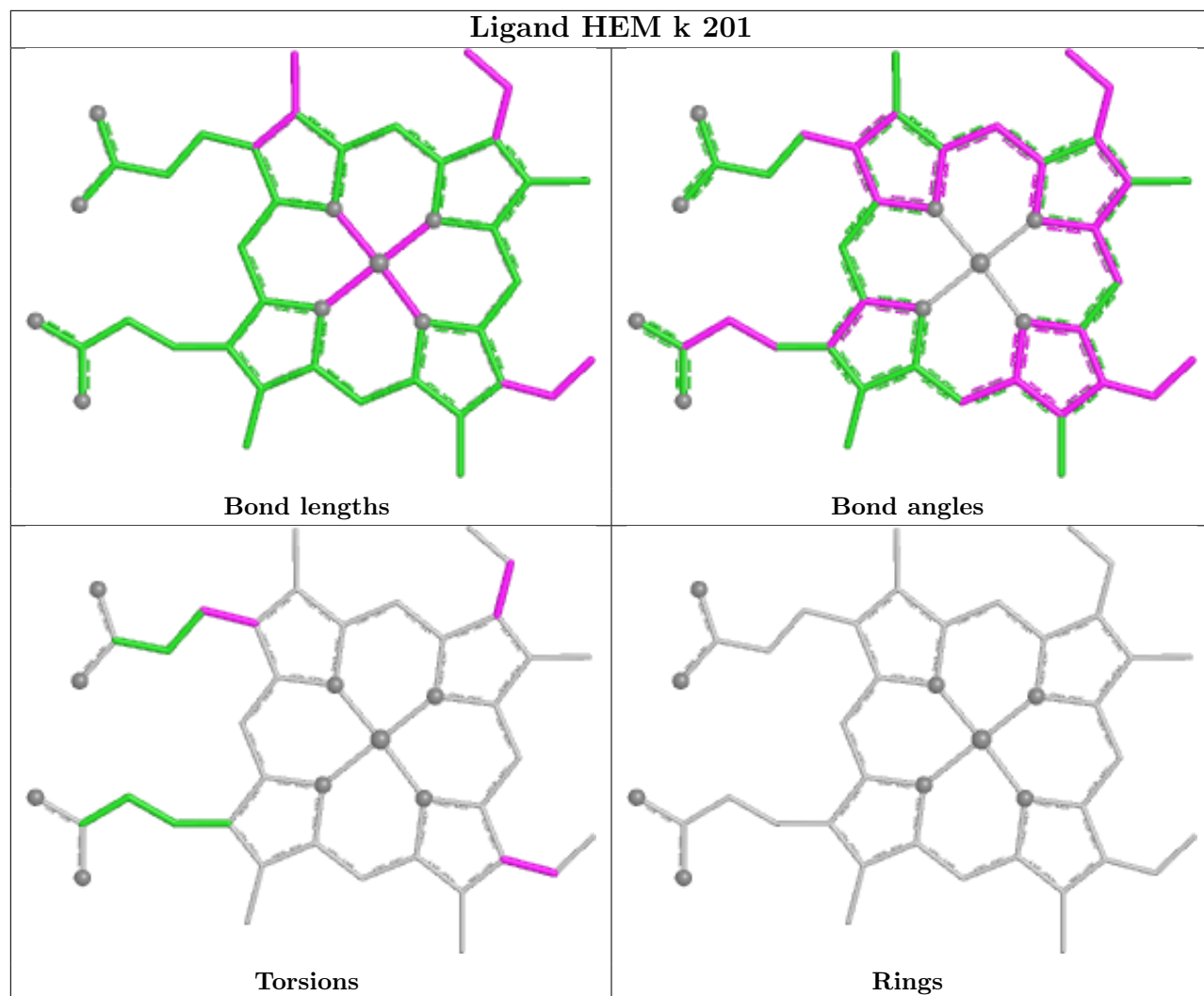




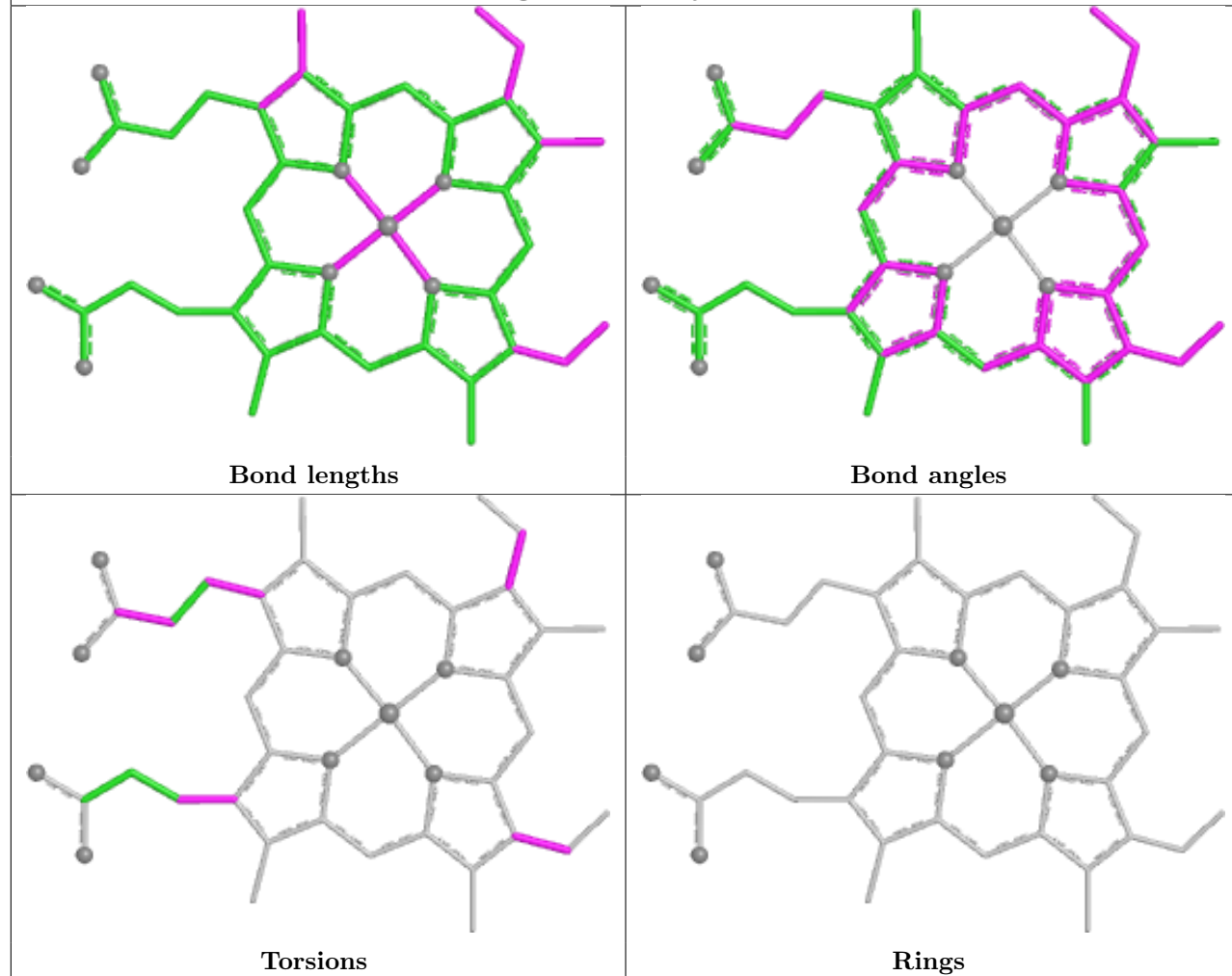
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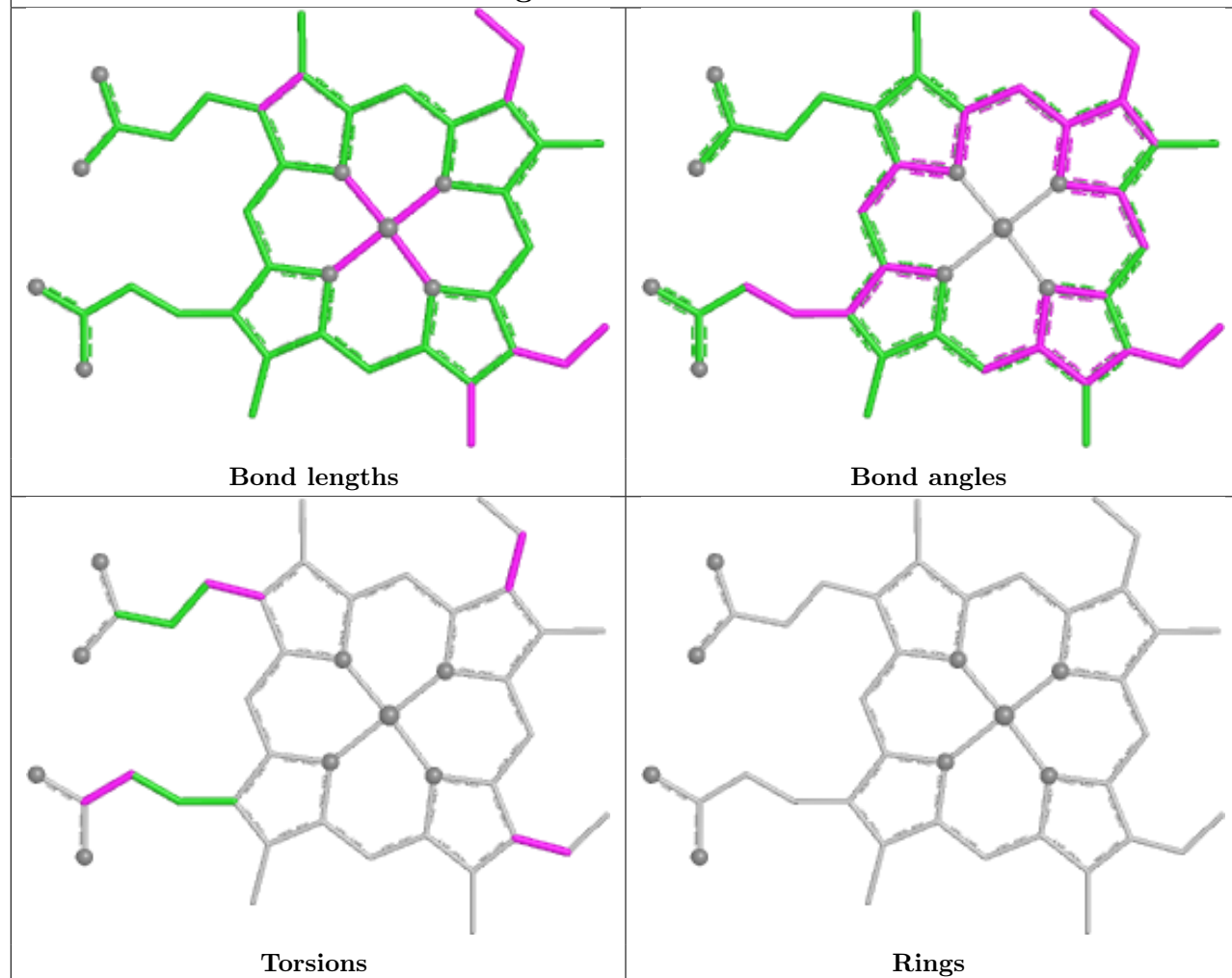




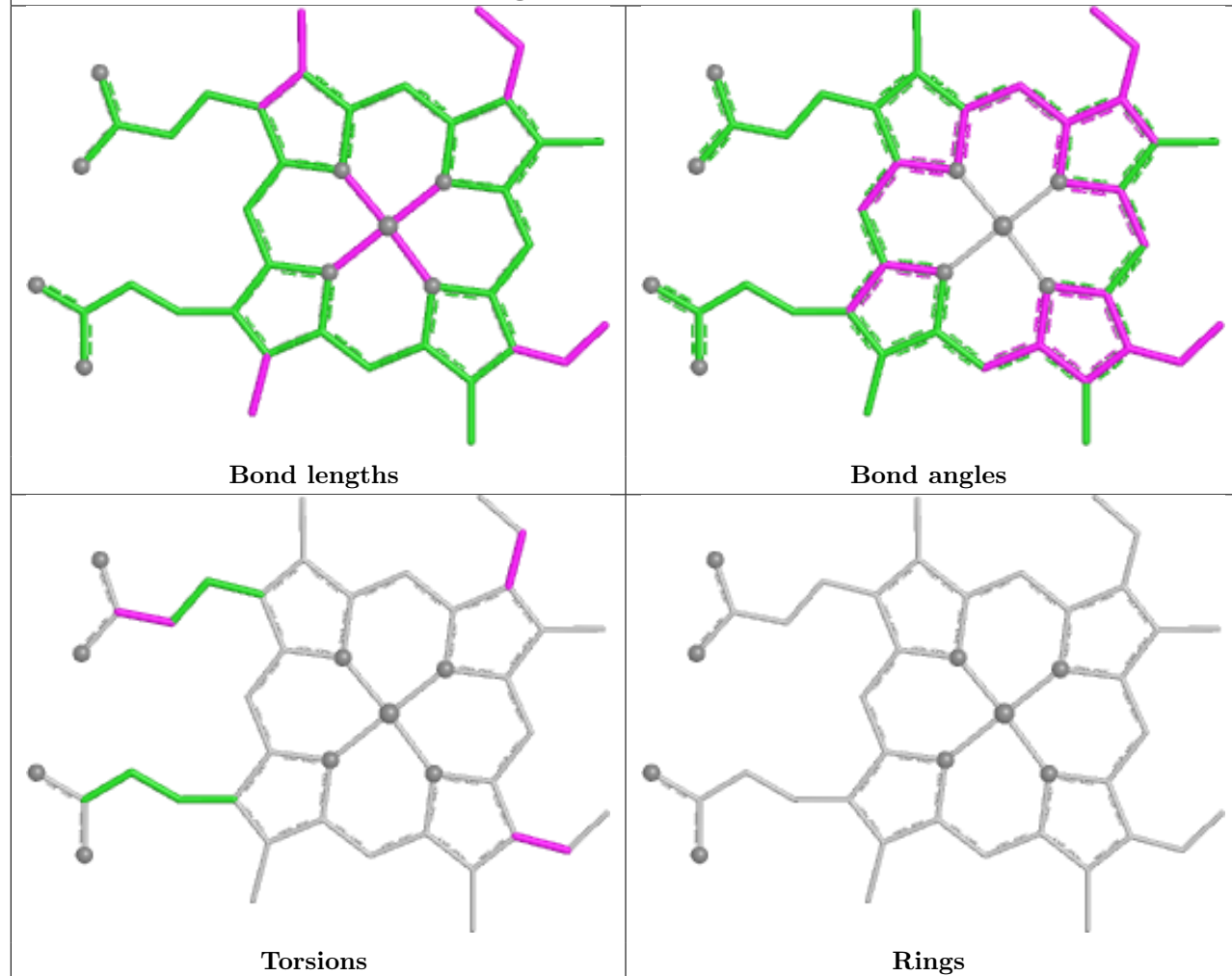
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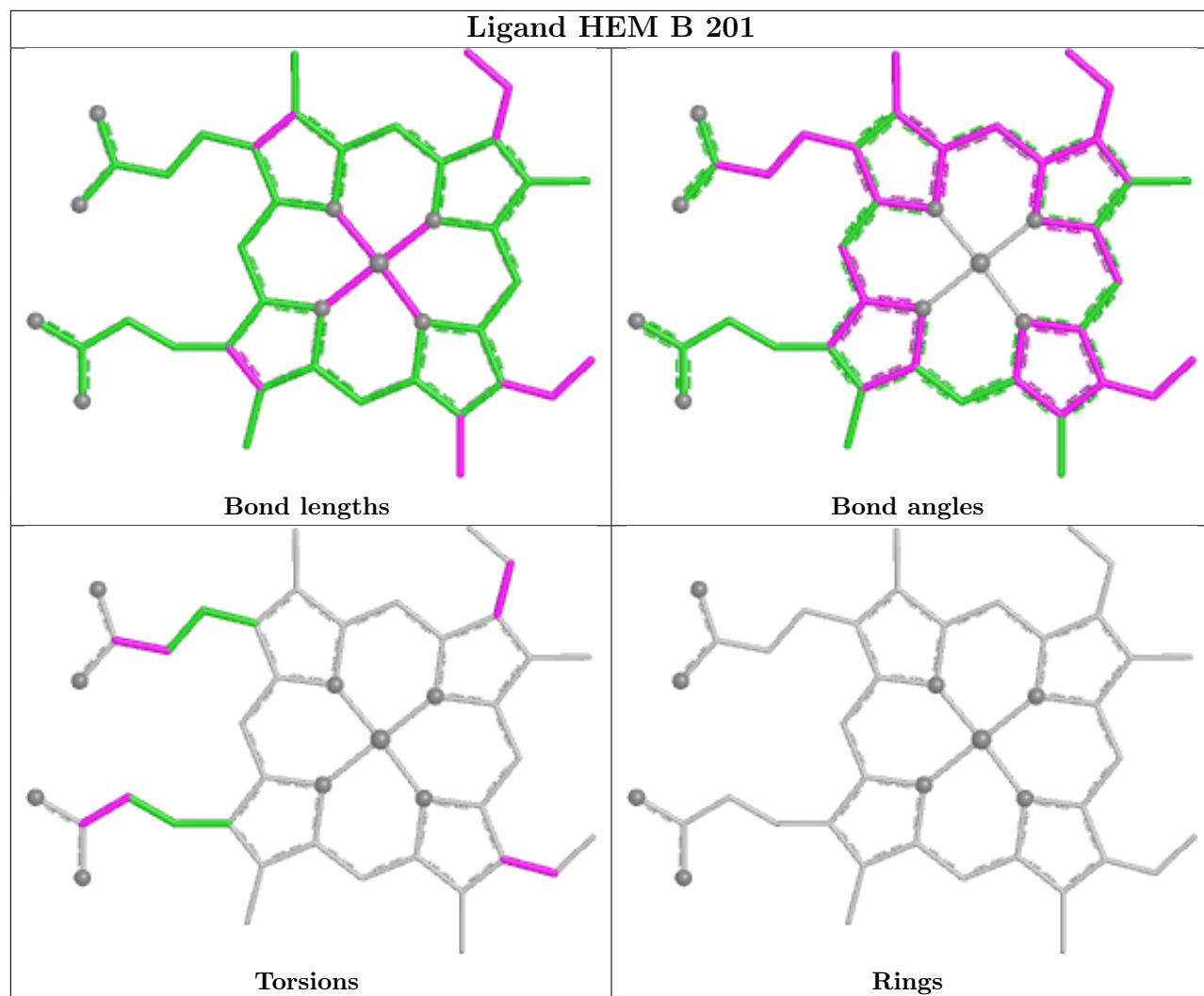


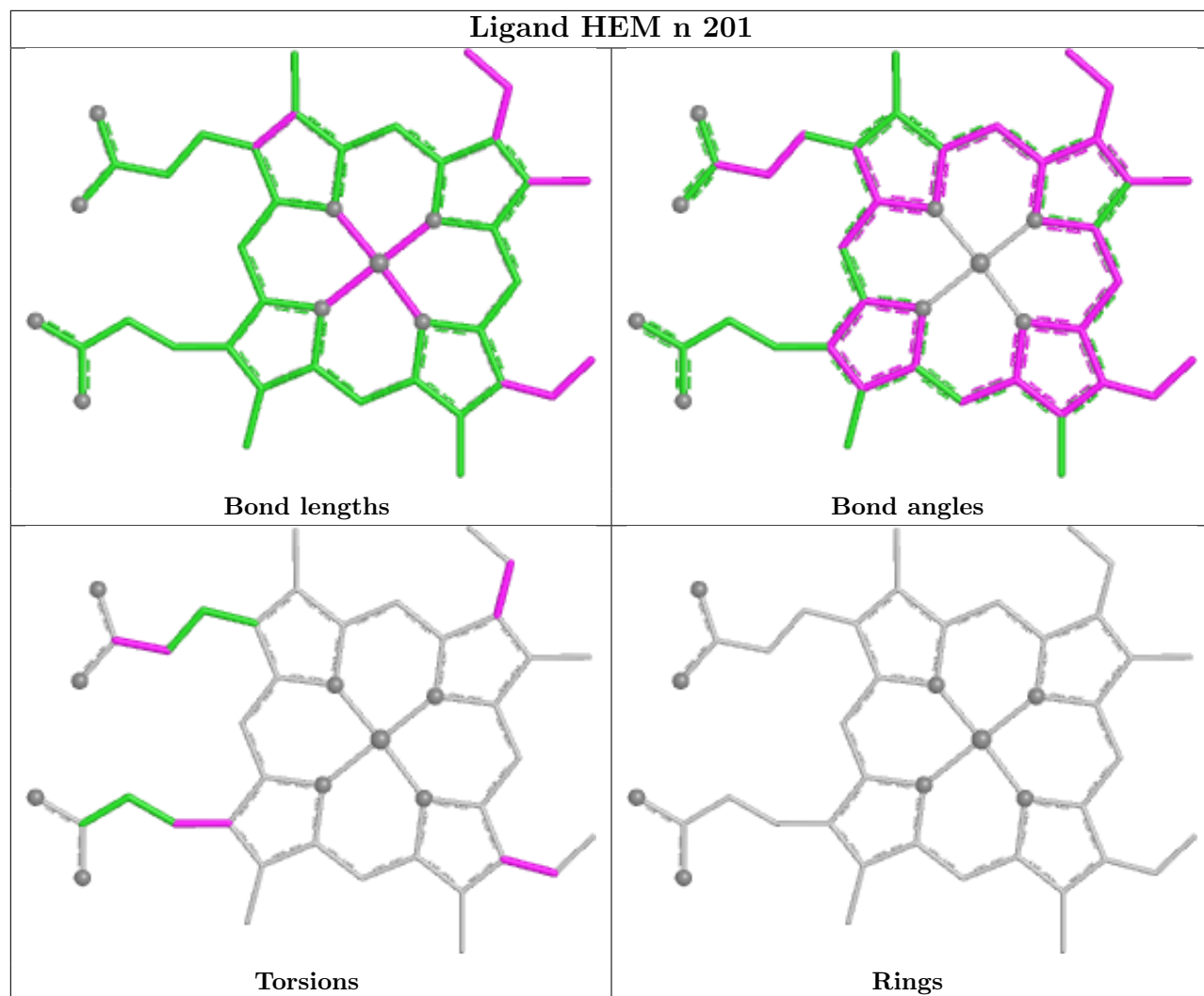
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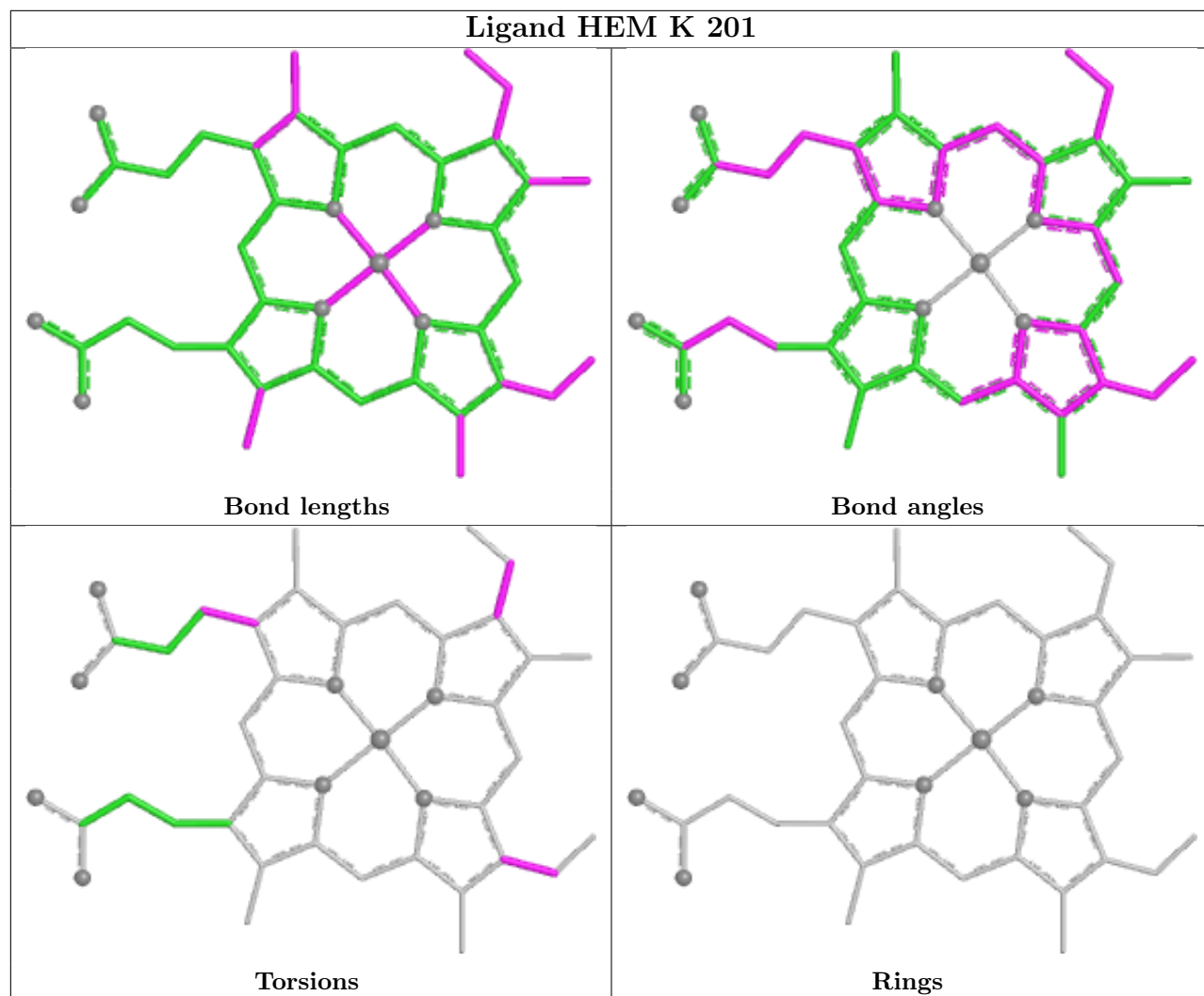
Ligand HEM o 201

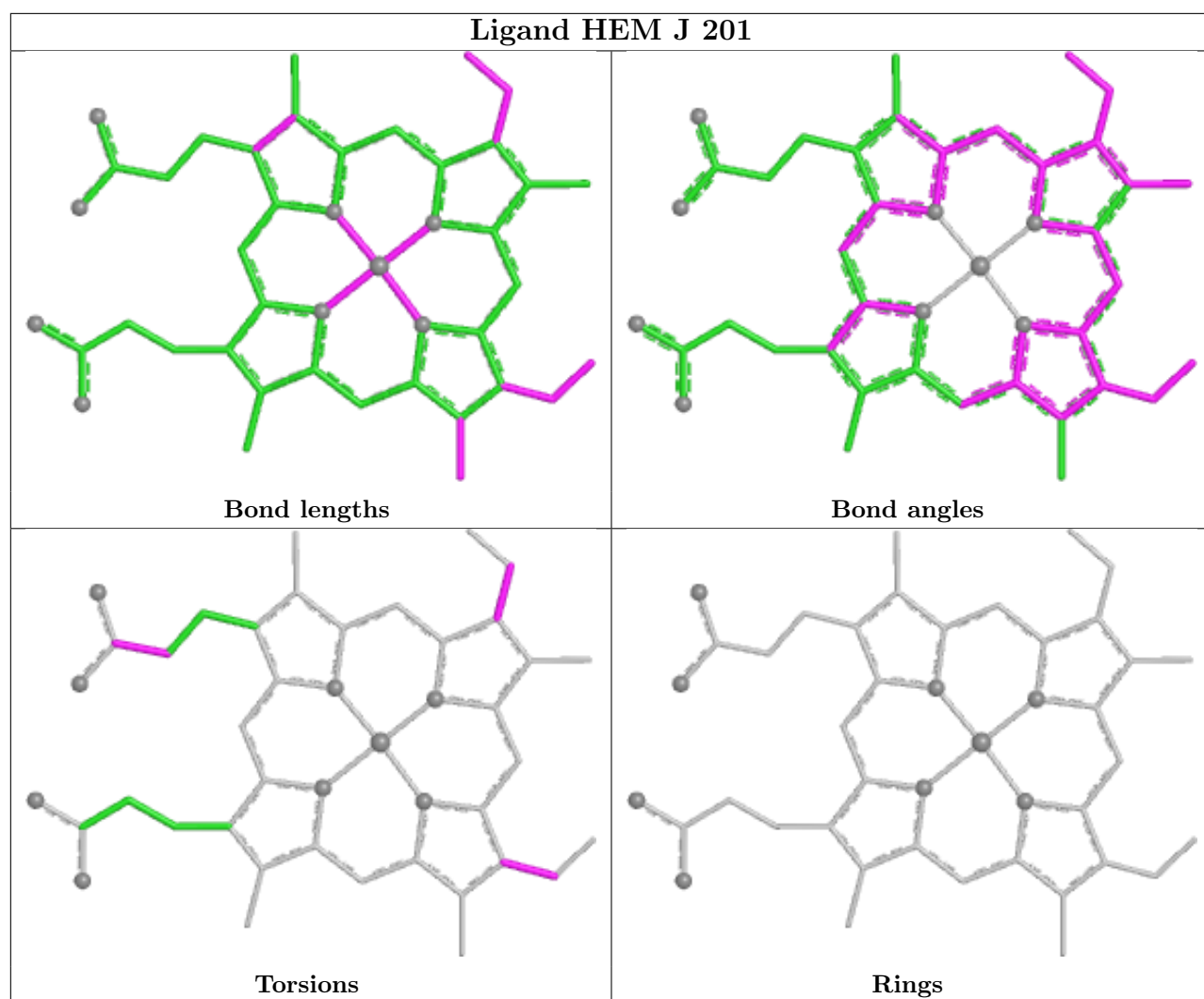






Ligand HEM K 201





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	148/150 (98%)	0.23	10 (6%) 23 15	11, 32, 58, 80	0
1	E	148/150 (98%)	0.16	8 (5%) 31 20	7, 28, 55, 74	0
1	I	148/150 (98%)	0.10	9 (6%) 27 17	6, 24, 54, 70	0
1	P	148/150 (98%)	0.38	12 (8%) 18 11	8, 34, 63, 78	0
1	T	148/150 (98%)	0.20	5 (3%) 48 30	8, 25, 50, 68	0
1	X	148/150 (98%)	-0.01	2 (1%) 73 54	6, 26, 55, 67	0
1	e	148/150 (98%)	0.43	12 (8%) 18 11	13, 40, 69, 84	0
1	i	148/150 (98%)	0.19	3 (2%) 65 45	8, 30, 55, 70	0
1	m	148/150 (98%)	0.18	6 (4%) 41 25	8, 25, 52, 73	0
2	B	142/142 (100%)	-0.07	6 (4%) 40 25	9, 23, 59, 88	0
2	F	142/142 (100%)	0.00	3 (2%) 63 43	7, 22, 54, 106	0
2	J	142/142 (100%)	-0.00	7 (4%) 35 22	6, 24, 62, 98	0
2	Q	142/142 (100%)	0.02	6 (4%) 40 25	7, 22, 64, 86	0
2	U	142/142 (100%)	-0.06	3 (2%) 63 43	5, 23, 53, 94	0
2	Y	142/142 (100%)	-0.02	5 (3%) 47 29	10, 26, 58, 95	0
2	f	142/142 (100%)	0.04	5 (3%) 47 29	5, 25, 63, 89	0
2	j	142/142 (100%)	-0.10	4 (2%) 55 35	6, 24, 53, 101	0
2	n	142/142 (100%)	-0.04	4 (2%) 55 35	6, 26, 58, 93	0
3	C	151/151 (100%)	0.06	7 (4%) 37 23	8, 27, 59, 92	0
3	G	151/151 (100%)	0.16	5 (3%) 49 30	9, 28, 66, 96	0
3	K	151/151 (100%)	0.15	5 (3%) 49 30	8, 36, 62, 85	0
3	R	151/151 (100%)	-0.00	4 (2%) 57 37	5, 27, 64, 88	0
3	V	151/151 (100%)	0.21	7 (4%) 37 23	8, 30, 71, 92	0
3	Z	151/151 (100%)	0.08	2 (1%) 75 55	9, 35, 65, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	g	151/151 (100%)	0.02	3 (1%) 65 45	6, 28, 57, 88	0
3	k	151/151 (100%)	0.18	6 (3%) 42 26	11, 35, 72, 98	0
3	o	151/151 (100%)	0.15	3 (1%) 65 45	10, 37, 70, 82	0
4	D	141/141 (100%)	-0.02	1 (0%) 84 69	6, 30, 61, 80	0
4	H	141/141 (100%)	0.06	2 (1%) 73 54	10, 24, 57, 81	0
4	L	141/141 (100%)	-0.02	2 (1%) 73 54	8, 26, 55, 83	0
4	S	141/141 (100%)	0.03	1 (0%) 84 69	13, 32, 62, 79	0
4	W	141/141 (100%)	0.10	6 (4%) 40 24	8, 30, 55, 79	0
4	a	141/141 (100%)	-0.06	1 (0%) 84 69	10, 33, 57, 82	0
4	h	141/141 (100%)	0.04	1 (0%) 84 69	10, 35, 69, 89	0
4	l	141/141 (100%)	-0.04	1 (0%) 84 69	10, 31, 61, 84	0
4	p	141/141 (100%)	0.06	2 (1%) 73 54	13, 29, 63, 77	0
5	M	222/224 (99%)	0.16	5 (2%) 61 41	6, 25, 65, 88	0
5	b	222/224 (99%)	0.19	6 (2%) 56 36	7, 25, 67, 89	0
5	q	222/224 (99%)	0.06	5 (2%) 61 41	7, 24, 70, 84	0
6	N	219/236 (92%)	0.06	6 (2%) 56 36	5, 23, 59, 88	0
6	c	219/236 (92%)	0.15	7 (3%) 50 31	5, 24, 56, 87	0
6	r	219/236 (92%)	-0.02	3 (1%) 73 54	4, 24, 59, 90	0
7	O	213/218 (97%)	0.11	3 (1%) 73 54	6, 24, 49, 84	0
7	d	213/218 (97%)	0.15	3 (1%) 73 54	4, 25, 55, 89	0
7	s	213/218 (97%)	0.08	2 (0%) 81 64	6, 23, 55, 85	0
All	All	7200/7290 (98%)	0.09	209 (2%) 53 35	4, 27, 62, 106	0

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	e	150	HIS	5.8
1	P	127	CYS	5.7
3	k	3	PHE	5.4
2	F	23	HIS	5.3
1	P	150	HIS	5.1
1	e	127	CYS	5.0
3	V	3	PHE	5.0
3	G	2	GLN	4.7
3	C	127	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
1	T	150	HIS	4.5
2	Q	24	ASN	4.5
1	A	127	CYS	4.4
4	p	98	SER	4.4
2	B	24	ASN	4.4
3	G	3	PHE	4.3
3	k	2	GLN	4.3
3	V	2	GLN	4.3
2	B	23	HIS	4.2
6	c	97	HIS	4.1
7	d	182	GLY	4.1
1	A	150	HIS	4.1
1	e	52	GLU	4.0
2	f	23	HIS	4.0
3	g	127	ASP	4.0
5	q	118	GLN	4.0
2	Y	23	HIS	3.9
7	O	182	GLY	3.9
1	P	15	HIS	3.8
1	P	52	GLU	3.8
1	e	15	HIS	3.8
2	n	23	HIS	3.7
2	J	21	HIS	3.7
2	Y	21	HIS	3.6
2	j	23	HIS	3.6
2	f	24	ASN	3.6
1	T	12	GLU	3.6
2	Y	99	HIS	3.6
6	N	97	HIS	3.5
2	f	142	GLY	3.5
2	U	23	HIS	3.5
1	I	150	HIS	3.5
3	K	127	ASP	3.5
2	j	21	HIS	3.4
6	r	194	ASP	3.4
2	Y	22	GLY	3.4
2	J	23	HIS	3.4
3	V	1	HIS	3.4
2	J	22	GLY	3.3
1	I	15	HIS	3.3
2	Q	23	HIS	3.3
5	M	118	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
3	G	4	CYS	3.2
3	G	1	HIS	3.2
2	n	21	HIS	3.2
1	P	19	THR	3.2
3	g	24	THR	3.2
6	N	233	GLN	3.2
1	e	129	ASN	3.1
1	E	150	HIS	3.1
1	e	12	GLU	3.1
4	W	1	ASP	3.1
1	E	127	CYS	3.1
6	c	194	ASP	3.1
3	K	3	PHE	3.0
5	b	155	GLU	3.0
3	o	3	PHE	3.0
1	i	12	GLU	3.0
3	G	127	ASP	3.0
3	Z	127	ASP	3.0
2	F	21	HIS	3.0
1	E	12	GLU	3.0
3	C	25	GLU	3.0
5	q	155	GLU	3.0
3	o	1	HIS	3.0
7	d	7	HIS	3.0
1	e	24	SER	3.0
1	m	83	GLN	3.0
2	Q	121	GLY	2.9
4	H	141	GLY	2.9
1	P	12	GLU	2.9
1	m	138	HIS	2.9
3	V	4	CYS	2.9
2	n	22	GLY	2.9
3	C	3	PHE	2.9
2	Q	123	CYS	2.8
6	c	235	HIS	2.8
3	o	127	ASP	2.8
1	m	150	HIS	2.8
1	A	19	THR	2.8
1	P	4	CYS	2.8
2	j	20	SER	2.8
2	J	99	HIS	2.7
2	Q	122	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
6	c	233	GLN	2.7
3	R	24	THR	2.7
1	I	83	GLN	2.7
2	J	16	ARG	2.7
1	P	129	ASN	2.7
6	N	193	GLN	2.7
4	W	141	GLY	2.7
1	E	42	HIS	2.7
6	c	195	ASP	2.7
5	b	118	GLN	2.6
5	b	162	ILE	2.6
1	A	52	GLU	2.6
1	E	52	GLU	2.6
1	e	53	ARG	2.6
2	U	21	HIS	2.6
7	O	7	HIS	2.6
1	A	4	CYS	2.6
1	X	16	ILE	2.6
4	W	98	SER	2.6
2	B	99	HIS	2.6
7	s	182	GLY	2.6
5	b	225	HIS	2.5
1	T	44	TYR	2.5
6	N	234	GLY	2.5
1	m	129	ASN	2.5
1	I	16	ILE	2.5
1	e	19	THR	2.5
1	A	15	HIS	2.5
3	k	1	HIS	2.5
2	Q	1	SER	2.5
1	A	129	ASN	2.5
3	R	127	ASP	2.5
1	e	25	PHE	2.5
3	C	24	THR	2.5
1	A	16	ILE	2.4
3	k	127	ASP	2.4
1	m	15	HIS	2.4
3	V	127	ASP	2.4
6	N	235	HIS	2.4
3	K	2	GLN	2.4
3	V	150	GLN	2.4
6	r	193	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
3	R	25	GLU	2.4
6	N	194	ASP	2.4
2	f	99	HIS	2.4
3	C	1	HIS	2.4
4	L	141	GLY	2.4
7	s	7	HIS	2.4
4	W	26	GLN	2.4
2	B	16	ARG	2.4
5	M	155	GLU	2.4
2	f	1	SER	2.4
1	I	84	ASP	2.4
1	i	150	HIS	2.3
1	P	83	GLN	2.3
3	R	150	GLN	2.3
4	D	26	GLN	2.3
1	A	12	GLU	2.3
2	J	26	GLU	2.3
1	P	16	ILE	2.3
6	c	18	ASP	2.3
1	A	111	LYS	2.3
5	M	184	ARG	2.3
1	T	138	HIS	2.3
7	O	180	ASP	2.3
6	c	193	GLN	2.3
1	I	129	ASN	2.3
3	V	53	ASN	2.3
3	K	23	ASP	2.3
3	K	150	GLN	2.3
3	Z	150	GLN	2.3
3	k	151	GLY	2.3
2	F	16	ARG	2.3
1	E	3	ASP	2.3
4	H	1	ASP	2.3
5	b	184	ARG	2.2
1	m	52	GLU	2.2
4	p	1	ASP	2.2
4	S	141	GLY	2.2
2	Y	16	ARG	2.2
1	E	16	ILE	2.2
4	h	141	GLY	2.2
4	L	22	HIS	2.2
5	q	40	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	n	16	ARG	2.2
2	B	142	GLY	2.2
1	P	82	PHE	2.2
1	T	3	ASP	2.2
5	q	162	ILE	2.1
4	W	96	GLU	2.1
4	a	22	HIS	2.1
1	e	83	GLN	2.1
2	j	1	SER	2.1
3	k	25	GLU	2.1
1	E	84	ASP	2.1
1	e	16	ILE	2.1
6	r	233	GLN	2.1
3	C	84	ASP	2.1
1	X	15	HIS	2.1
1	P	3	ASP	2.1
3	g	84	ASP	2.1
5	b	7	ASP	2.1
7	d	61	ASP	2.1
2	U	22	GLY	2.1
3	C	2	GLN	2.1
4	W	21	GLY	2.1
5	M	156	GLU	2.1
1	i	111	LYS	2.0
2	J	20	SER	2.0
5	q	116	SER	2.0
4	l	1	ASP	2.0
2	B	1	SER	2.0
1	I	134	ASN	2.0
1	I	138	HIS	2.0
5	M	225	HIS	2.0
1	I	52	GLU	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 oligosaccharides 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(Å ²)	Q<0.9
12	NAG	d	304	14/15	0.87	0.12	28,28,28,28	0
12	NAG	s	303	14/15	0.87	0.11	28,28,28,28	0
12	NAG	O	304	14/15	0.88	0.11	28,28,28,28	0
9	CYN	l	202	2/2	0.89	0.17	28,28,28,28	0
9	CYN	E	202	2/2	0.91	0.24	28,28,28,28	0
11	ZN	O	302	1/1	0.92	0.30	28,28,28,28	0
9	CYN	W	202	2/2	0.93	0.14	28,28,28,28	0
9	CYN	k	202	2/2	0.94	0.12	28,28,28,28	0
9	CYN	G	202	2/2	0.94	0.19	28,28,28,28	0
9	CYN	S	202	2/2	0.94	0.17	28,28,28,28	0
9	CYN	V	202	2/2	0.94	0.15	28,28,28,28	0
8	HEM	e	201	43/43	0.94	0.12	28,28,28,28	0
9	CYN	j	202	2/2	0.94	0.13	28,28,28,28	0
9	CYN	i	202	2/2	0.95	0.17	28,28,28,28	0
9	CYN	H	202	2/2	0.95	0.16	28,28,28,28	0
9	CYN	P	202	2/2	0.95	0.20	28,28,28,28	0
9	CYN	R	202	2/2	0.95	0.17	28,28,28,28	0
8	HEM	k	201	43/43	0.95	0.10	28,28,28,28	0
11	ZN	d	302	1/1	0.95	0.29	28,28,28,28	0
11	ZN	s	302	1/1	0.95	0.28	28,28,28,28	0
9	CYN	F	202	2/2	0.95	0.10	28,28,28,28	0
9	CYN	C	202	2/2	0.95	0.24	28,28,28,28	0
9	CYN	e	202	2/2	0.95	0.11	28,28,28,28	0
9	CYN	Z	202	2/2	0.96	0.09	28,28,28,28	0
8	HEM	T	201	43/43	0.96	0.10	28,28,28,28	0
9	CYN	g	202	2/2	0.96	0.14	28,28,28,28	0
8	HEM	p	201	43/43	0.96	0.11	28,28,28,28	0
9	CYN	B	202	2/2	0.96	0.11	28,28,28,28	0
8	HEM	V	201	43/43	0.96	0.11	28,28,28,28	0
9	CYN	D	202	2/2	0.96	0.14	28,28,28,28	0
9	CYN	m	202	2/2	0.96	0.12	28,28,28,28	0
9	CYN	o	202	2/2	0.96	0.11	28,28,28,28	0
9	CYN	p	202	2/2	0.96	0.17	28,28,28,28	0
9	CYN	T	202	2/2	0.96	0.12	28,28,28,28	0
9	CYN	U	202	2/2	0.96	0.12	28,28,28,28	0
8	HEM	G	201	43/43	0.96	0.10	28,28,28,28	0
8	HEM	i	201	43/43	0.96	0.10	28,28,28,28	0

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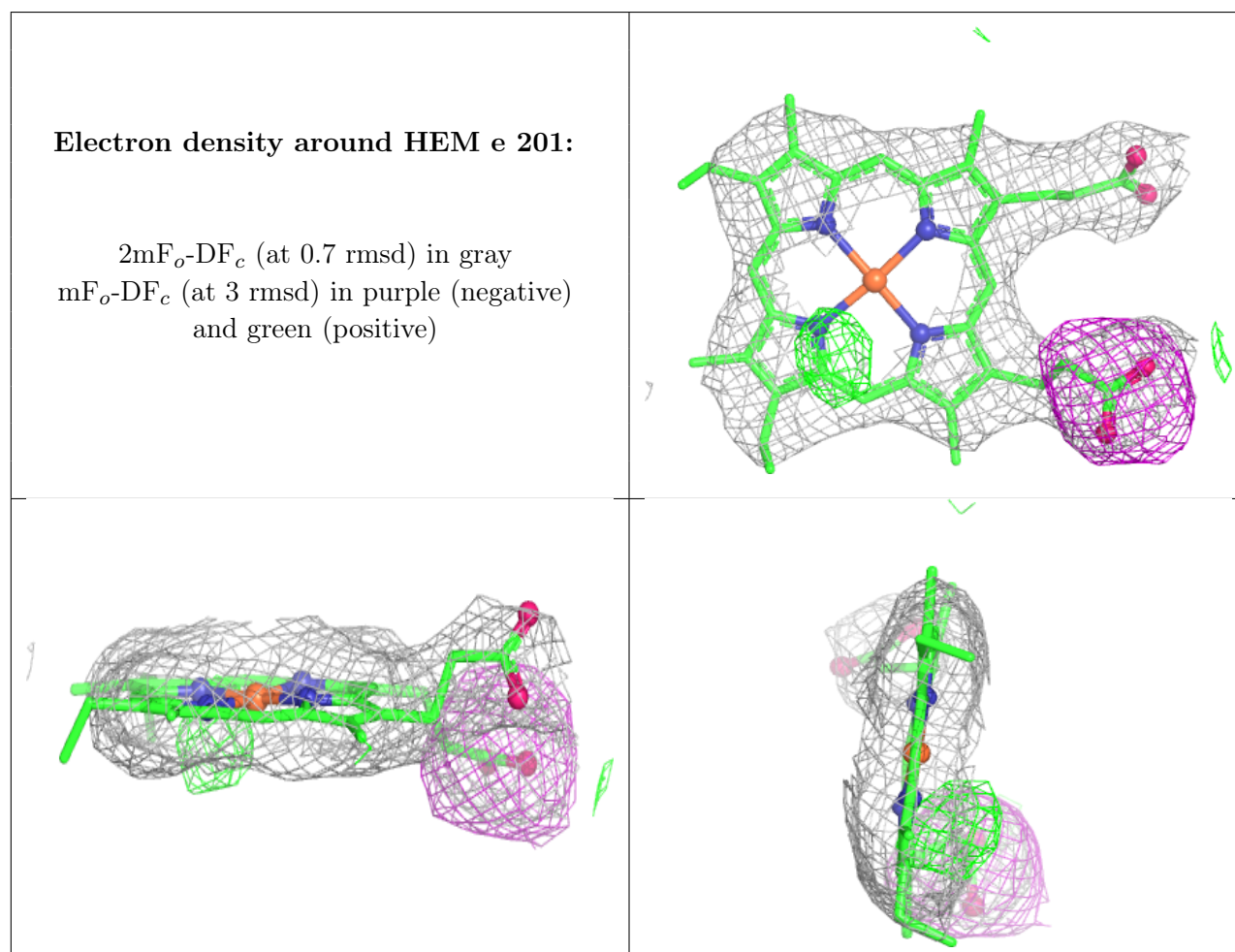
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	CYN	X	202	2/2	0.96	0.18	28,28,28,28	0
9	CYN	Y	202	2/2	0.96	0.11	28,28,28,28	0
8	HEM	Y	201	43/43	0.97	0.12	28,28,28,28	0
8	HEM	Z	201	43/43	0.97	0.09	28,28,28,28	0
8	HEM	A	201	43/43	0.97	0.09	28,28,28,28	0
8	HEM	f	201	43/43	0.97	0.11	28,28,28,28	0
8	HEM	h	201	43/43	0.97	0.10	28,28,28,28	0
8	HEM	H	201	43/43	0.97	0.11	28,28,28,28	0
8	HEM	j	201	43/43	0.97	0.11	28,28,28,28	0
8	HEM	I	201	43/43	0.97	0.10	28,28,28,28	0
8	HEM	m	201	43/43	0.97	0.10	28,28,28,28	0
8	HEM	n	201	43/43	0.97	0.10	28,28,28,28	0
8	HEM	o	201	43/43	0.97	0.08	28,28,28,28	0
8	HEM	J	201	43/43	0.97	0.11	28,28,28,28	0
9	CYN	A	202	2/2	0.97	0.10	28,28,28,28	0
8	HEM	L	201	43/43	0.97	0.12	28,28,28,28	0
8	HEM	P	201	43/43	0.97	0.10	28,28,28,28	0
8	HEM	Q	201	43/43	0.97	0.10	28,28,28,28	0
9	CYN	n	202	2/2	0.97	0.13	28,28,28,28	0
8	HEM	S	201	43/43	0.97	0.11	28,28,28,28	0
8	HEM	E	201	43/43	0.97	0.10	28,28,28,28	0
8	HEM	F	201	43/43	0.97	0.11	28,28,28,28	0
8	HEM	W	201	43/43	0.97	0.11	28,28,28,28	0
9	CYN	I	202	2/2	0.97	0.18	28,28,28,28	0
9	CYN	J	202	2/2	0.97	0.09	28,28,28,28	0
9	CYN	L	202	2/2	0.97	0.13	28,28,28,28	0
8	HEM	X	201	43/43	0.97	0.10	28,28,28,28	0
8	HEM	a	201	43/43	0.98	0.09	28,28,28,28	0
8	HEM	U	201	43/43	0.98	0.11	28,28,28,28	0
8	HEM	C	201	43/43	0.98	0.10	28,28,28,28	0
8	HEM	g	201	43/43	0.98	0.10	28,28,28,28	0
8	HEM	D	201	43/43	0.98	0.09	28,28,28,28	0
9	CYN	K	202	2/2	0.98	0.07	28,28,28,28	0
8	HEM	R	201	43/43	0.98	0.10	28,28,28,28	0
9	CYN	a	202	2/2	0.98	0.14	28,28,28,28	0
8	HEM	K	201	43/43	0.98	0.09	28,28,28,28	0
9	CYN	f	202	2/2	0.98	0.09	28,28,28,28	0
8	HEM	B	201	43/43	0.98	0.11	28,28,28,28	0
9	CYN	h	202	2/2	0.98	0.11	28,28,28,28	0
8	HEM	l	201	43/43	0.98	0.10	28,28,28,28	0
11	ZN	d	303	1/1	0.99	0.02	28,28,28,28	0
10	CA	b	301	1/1	0.99	0.04	28,28,28,28	0

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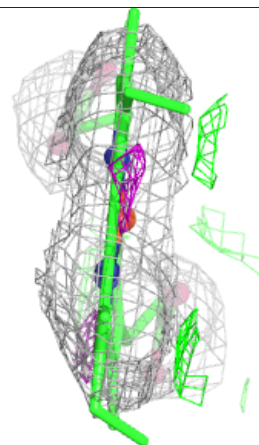
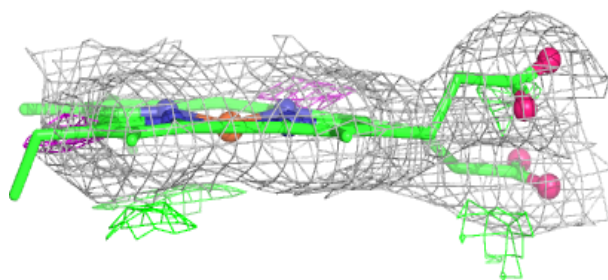
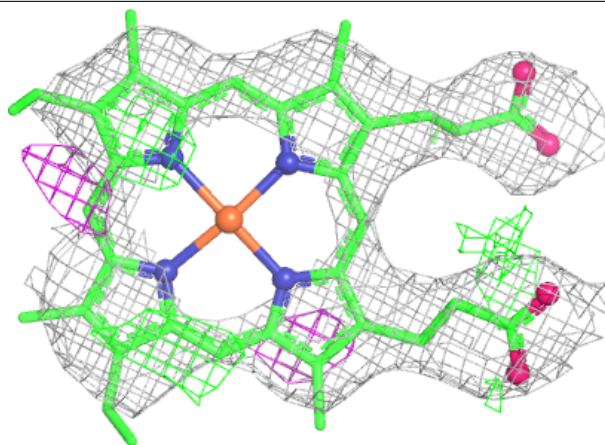
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	CA	q	301	1/1	0.99	0.03	28,28,28,28	0
9	CYN	Q	202	2/2	0.99	0.07	28,28,28,28	0
10	CA	N	301	1/1	0.99	0.04	28,28,28,28	0
11	ZN	O	303	1/1	1.00	0.02	28,28,28,28	0
11	ZN	c	302	1/1	1.00	0.01	28,28,28,28	0
10	CA	c	301	1/1	1.00	0.03	28,28,28,28	0
10	CA	d	301	1/1	1.00	0.02	28,28,28,28	0
10	CA	O	301	1/1	1.00	0.02	28,28,28,28	0
10	CA	r	301	1/1	1.00	0.02	28,28,28,28	0
10	CA	s	301	1/1	1.00	0.03	28,28,28,28	0
10	CA	M	301	1/1	1.00	0.03	28,28,28,28	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.



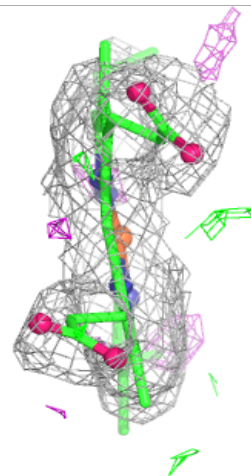
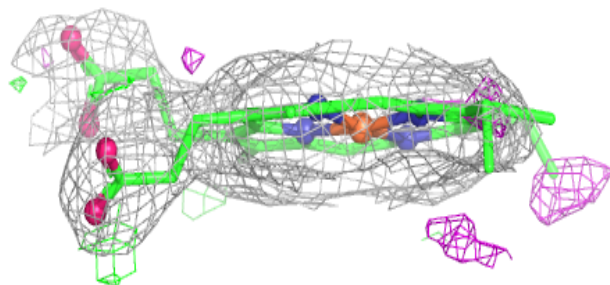
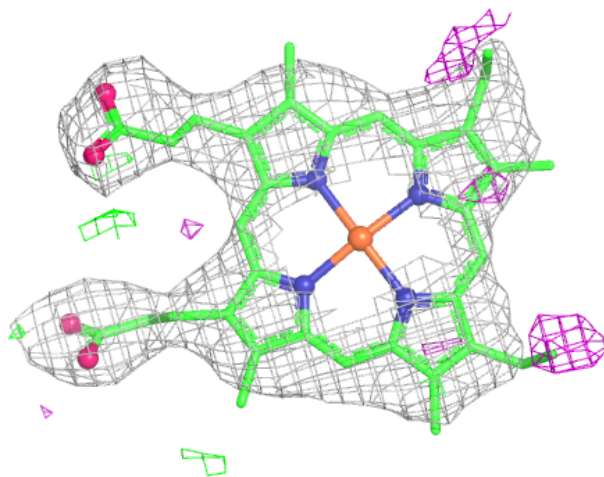
Electron density around HEM k 201:

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



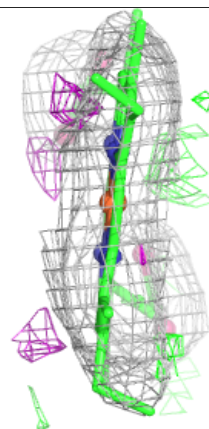
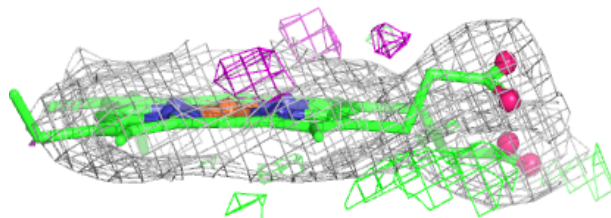
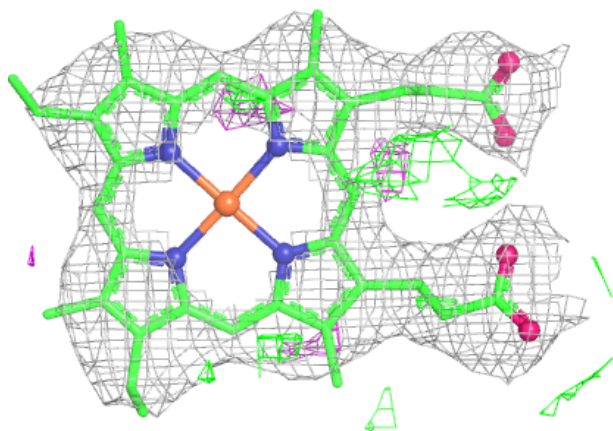
Electron density around HEM T 201:

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



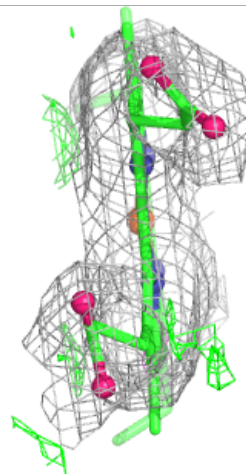
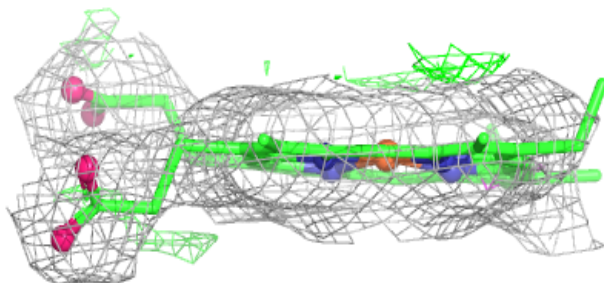
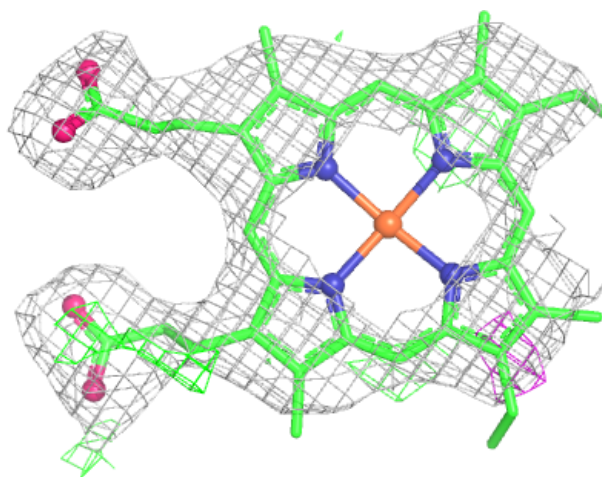
Electron density around HEM p 201:

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



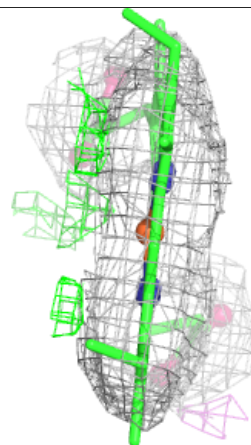
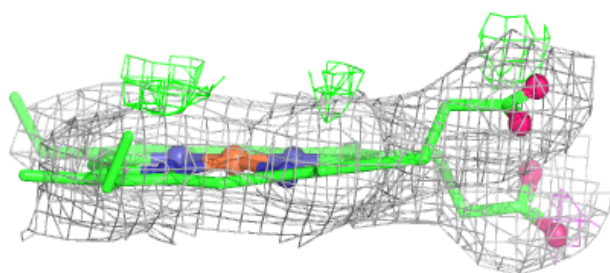
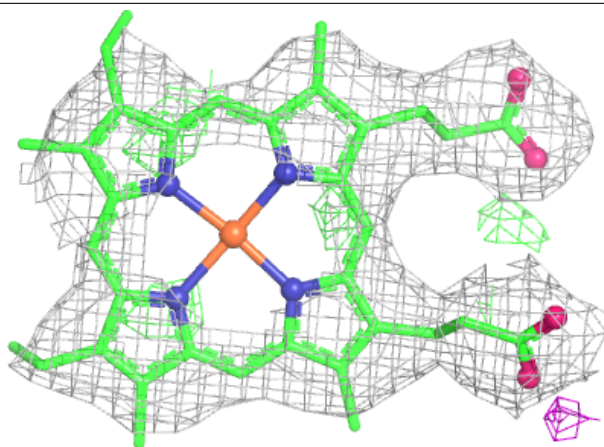
Electron density around HEM V 201:

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

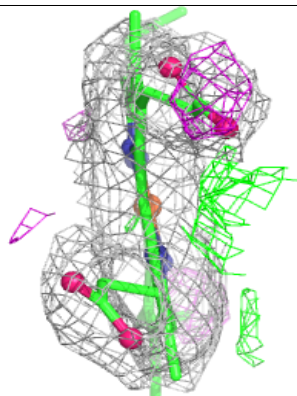
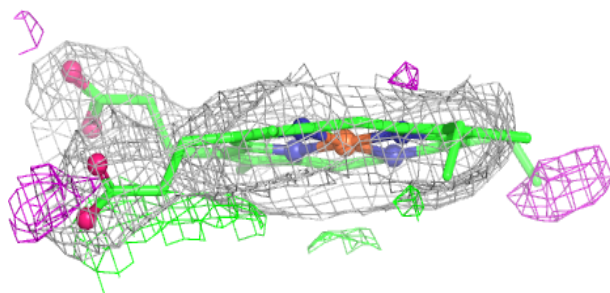
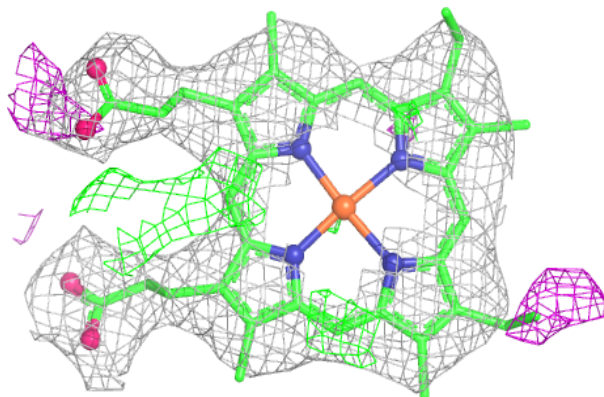


Electron density around HEM G 201:

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

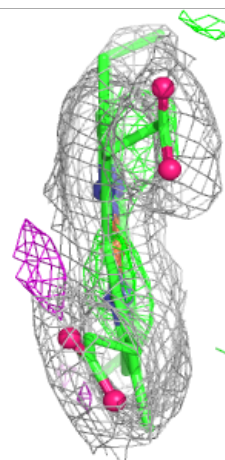
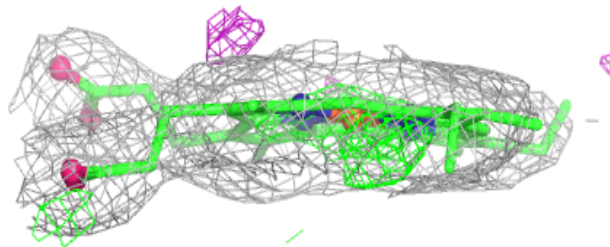
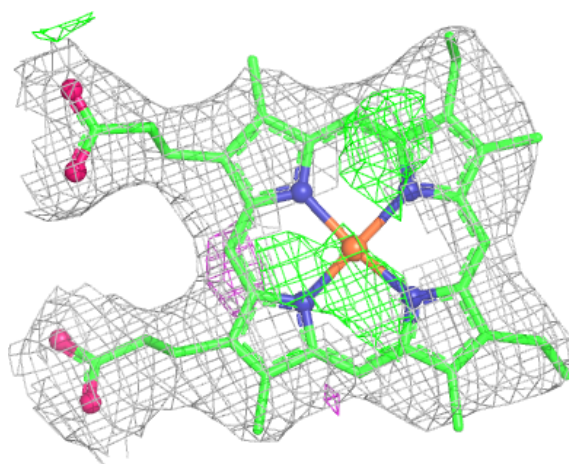
**Electron density around HEM i 201:**

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



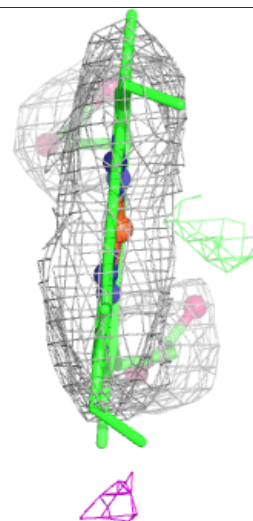
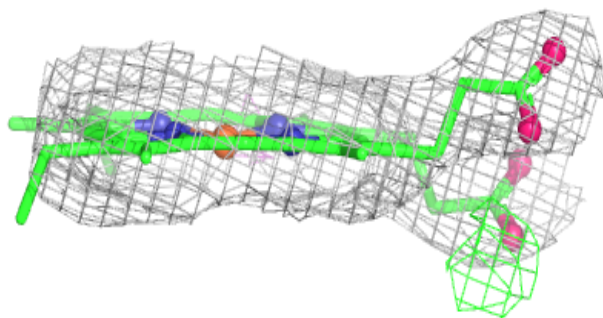
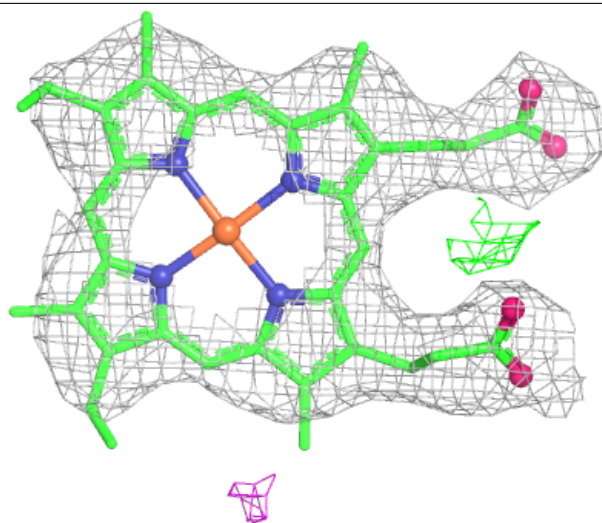
Electron density around HEM Y 201:

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



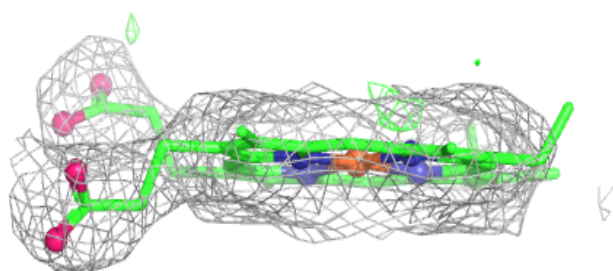
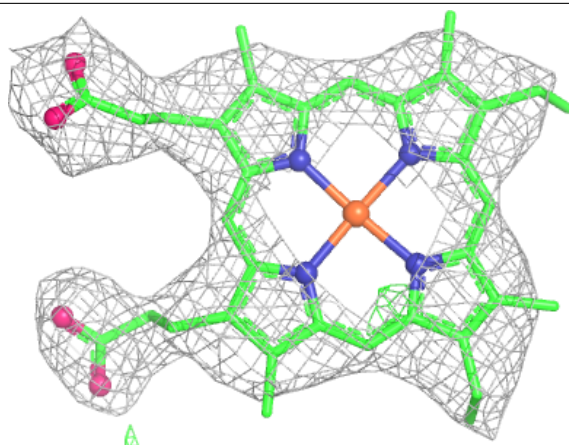
Electron density around HEM Z 201:

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



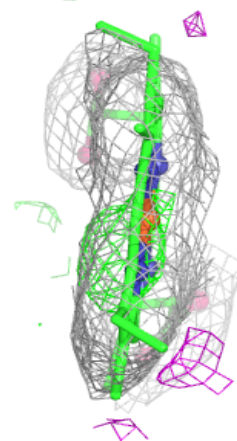
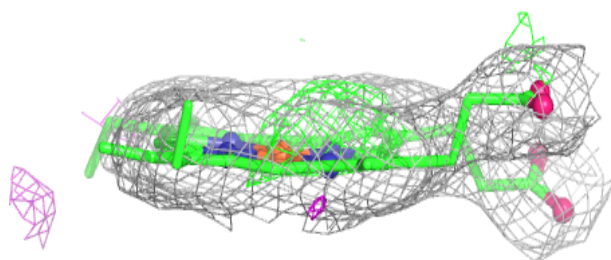
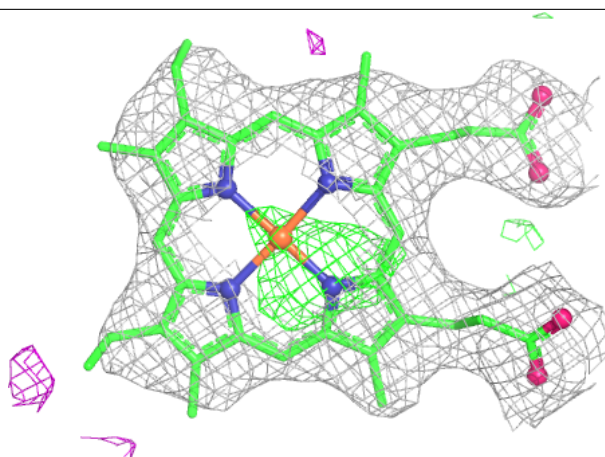
Electron density around HEM A 201:

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



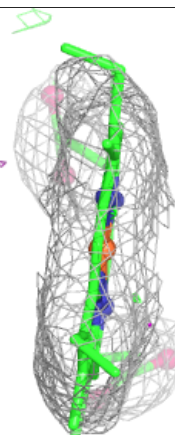
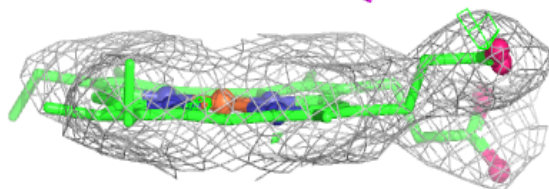
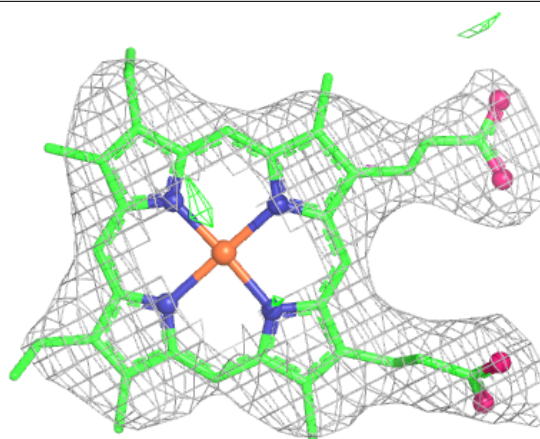
Electron density around HEM f 201:

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



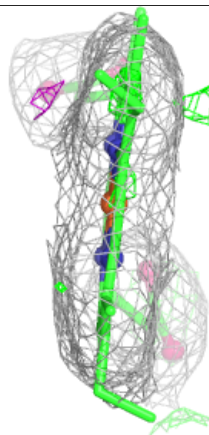
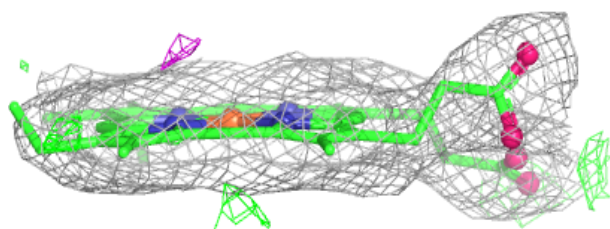
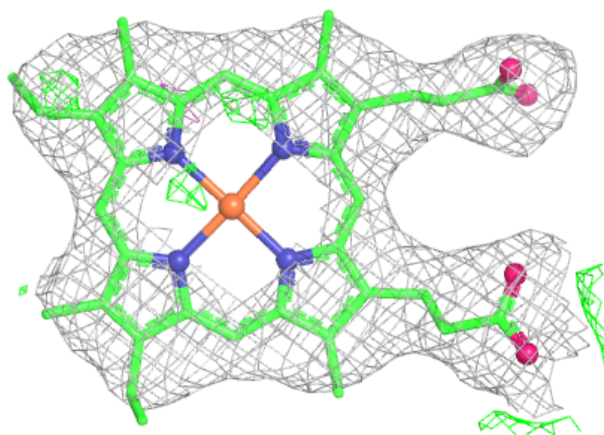
Electron density around HEM h 201:

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



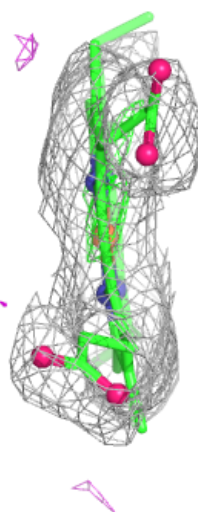
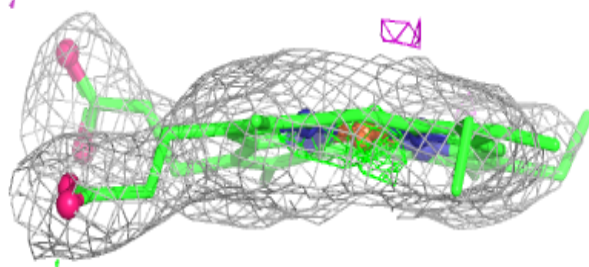
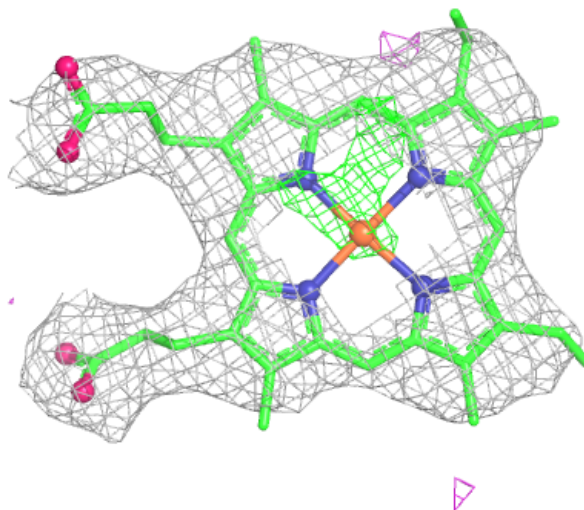
Electron density around HEM H 201:

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



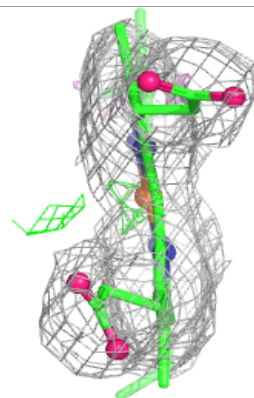
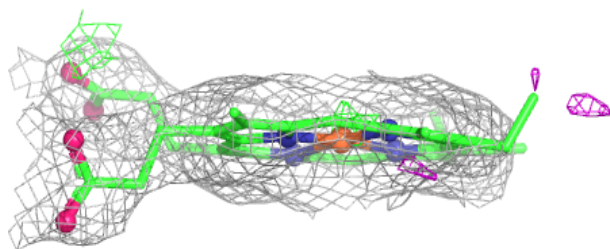
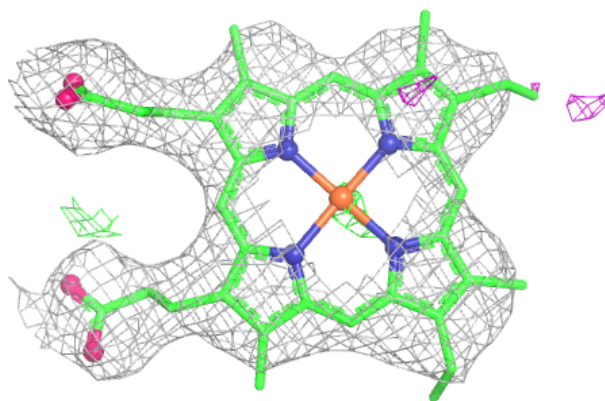
Electron density around HEM j 201:

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



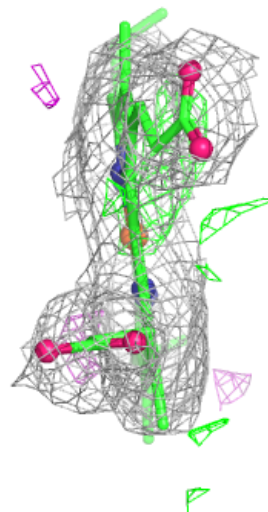
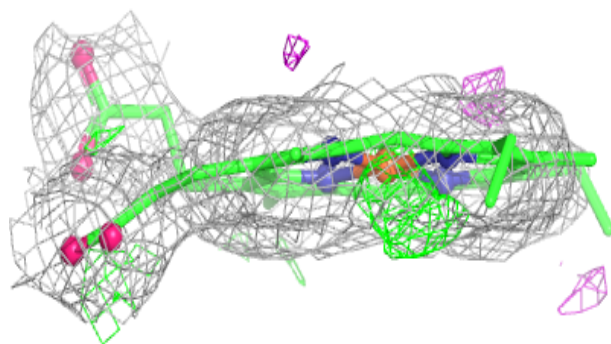
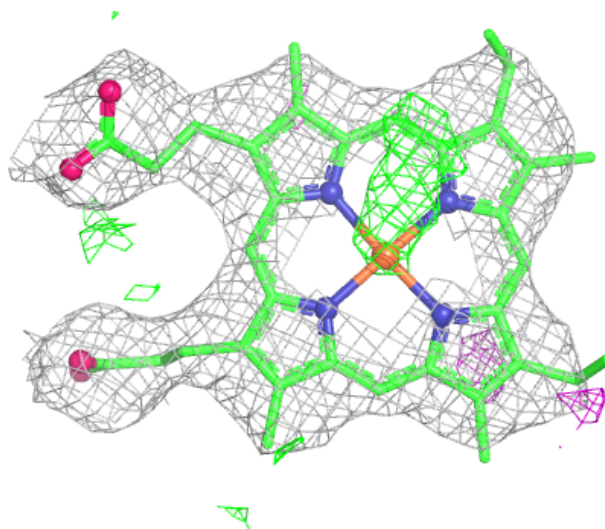
Electron density around HEM I 201:

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



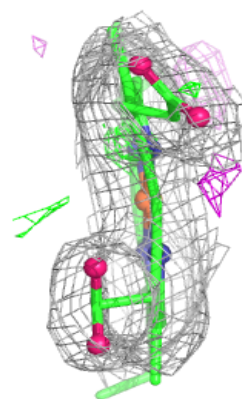
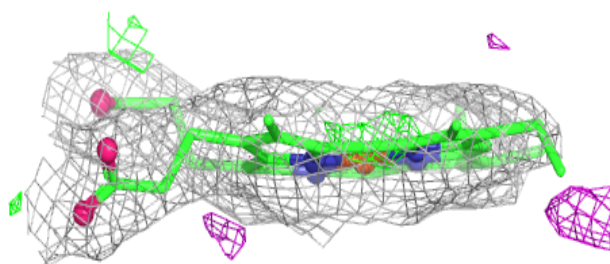
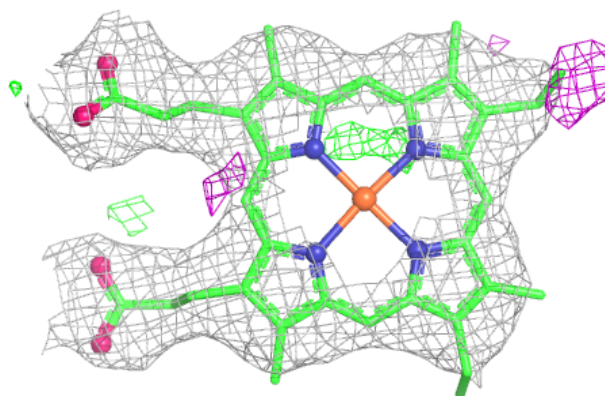
Electron density around HEM m 201:

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



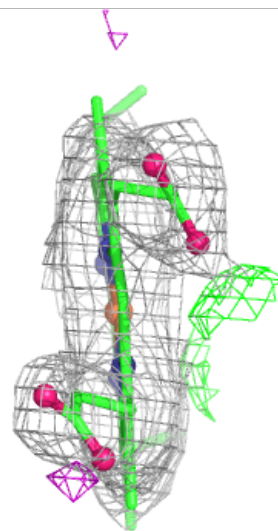
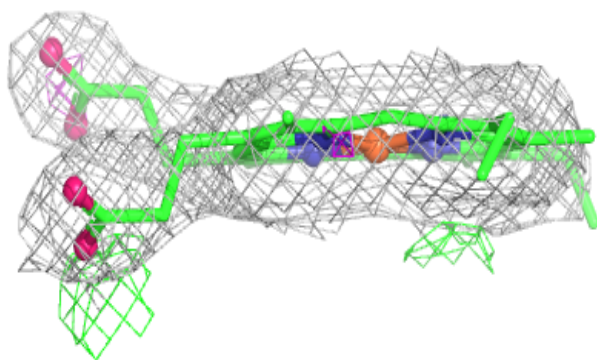
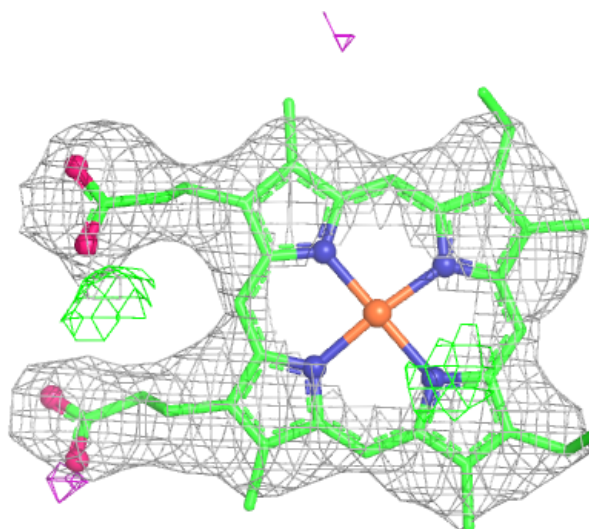
Electron density around HEM n 201:

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



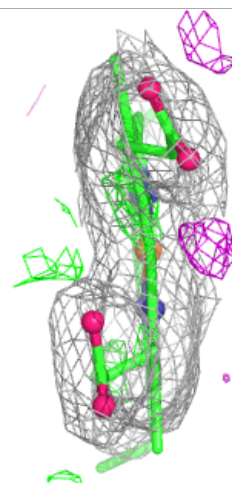
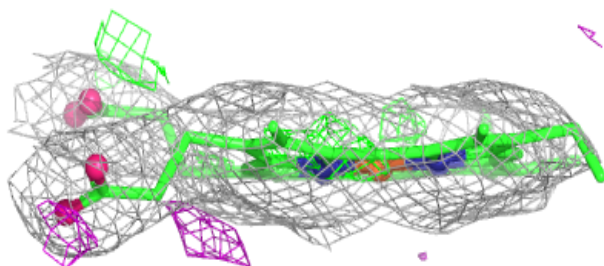
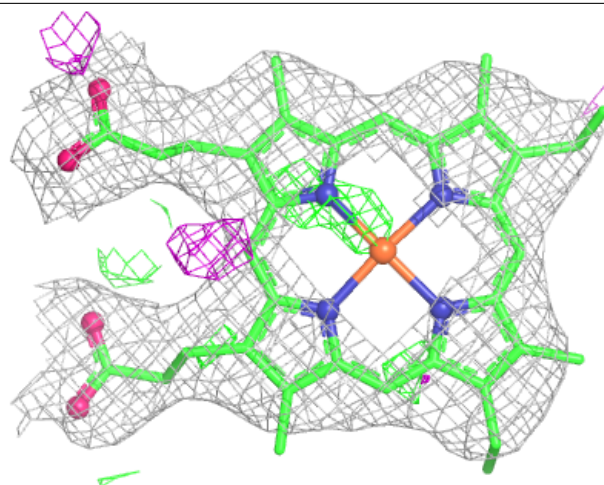
Electron density around HEM o 201:

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



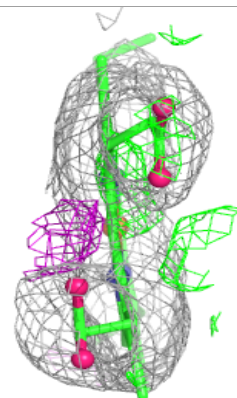
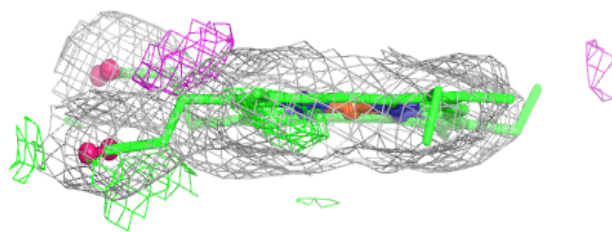
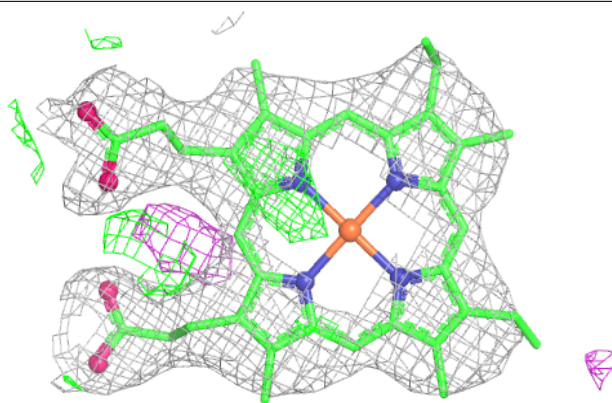
Electron density around HEM J 201:

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



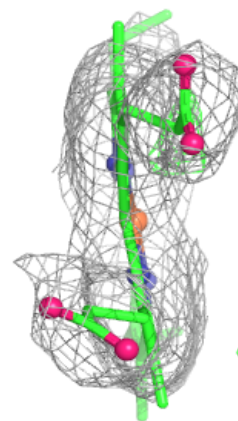
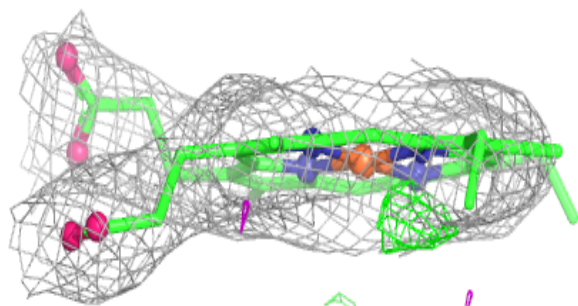
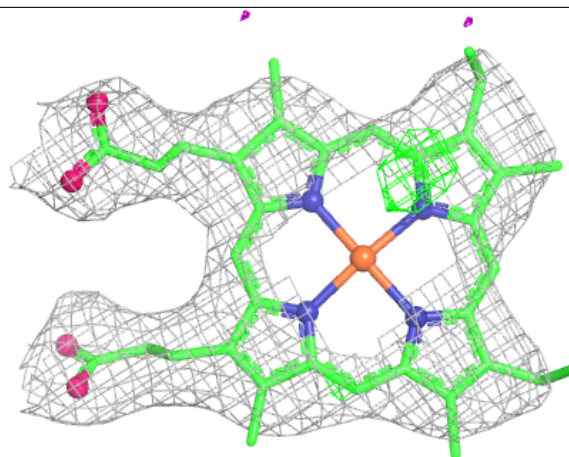
Electron density around HEM L 201:

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



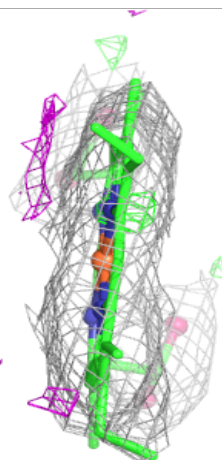
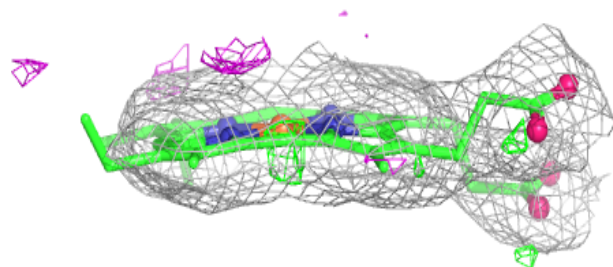
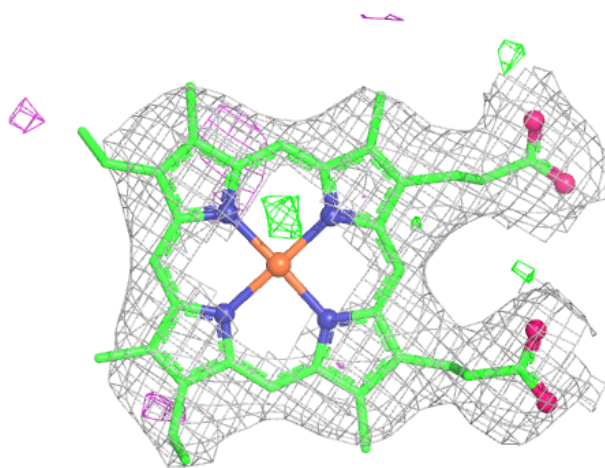
Electron density around HEM P 201:

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



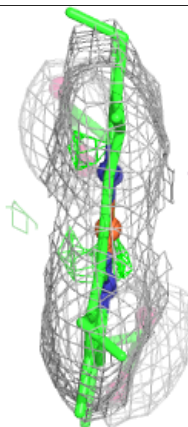
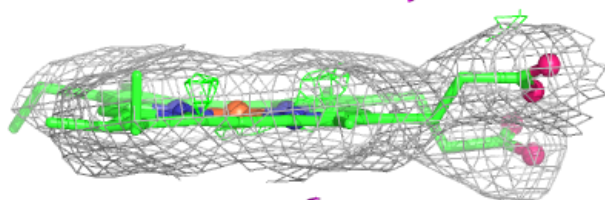
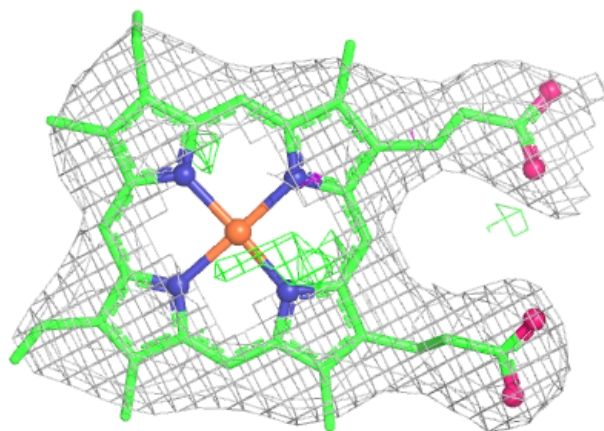
Electron density around HEM Q 201:

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

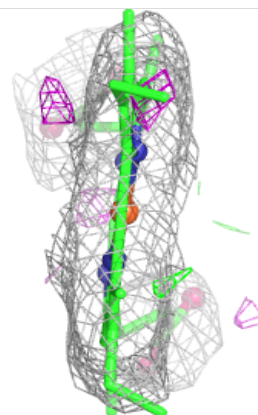
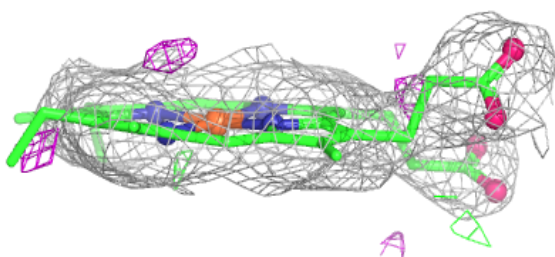
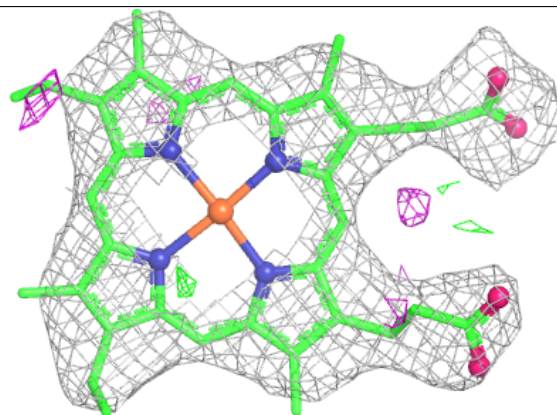


Electron density around HEM S 201:

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

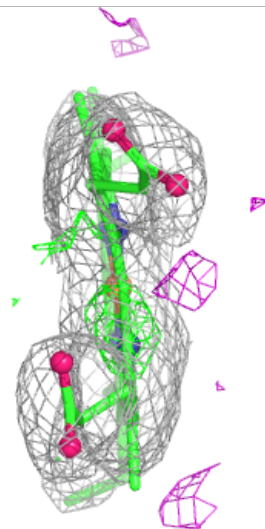
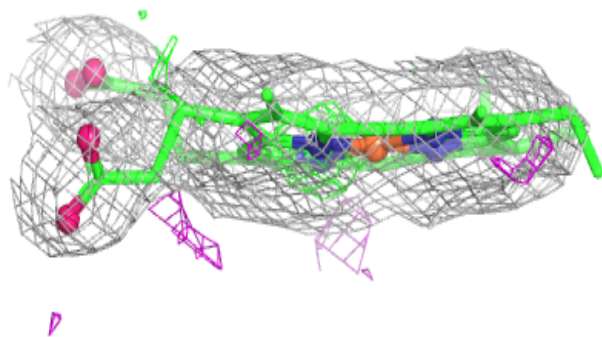
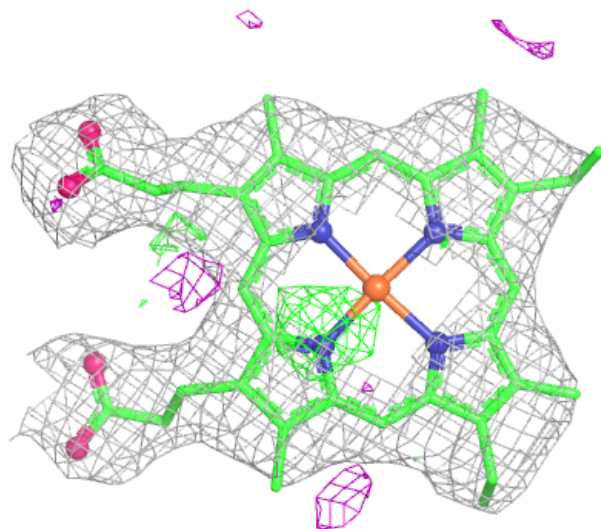
**Electron density around HEM E 201:**

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



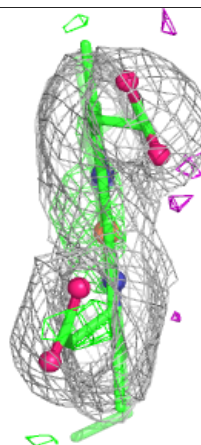
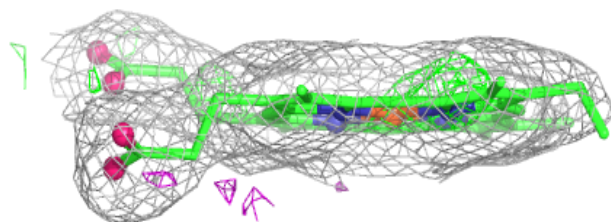
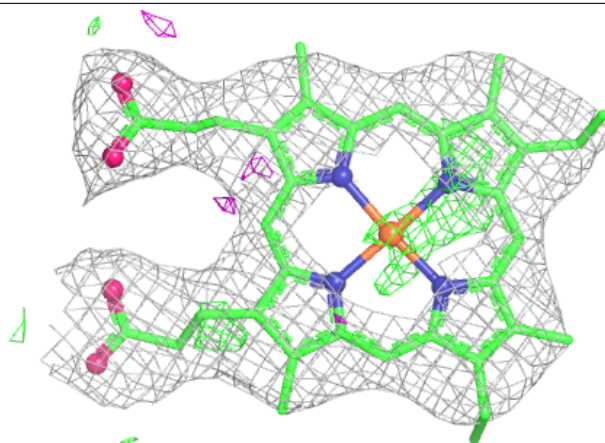
Electron density around HEM F 201:

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



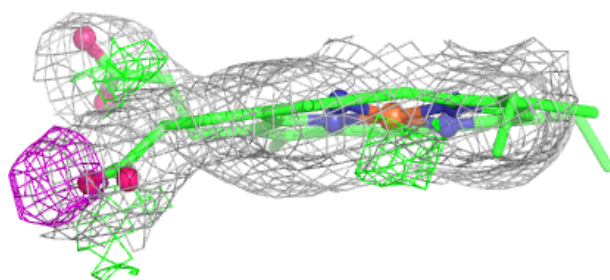
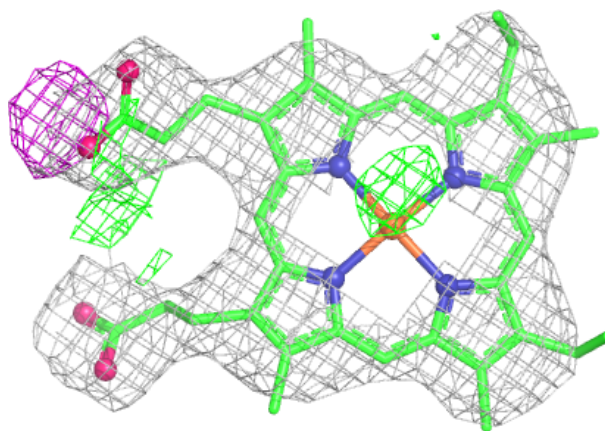
Electron density around HEM W 201:

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



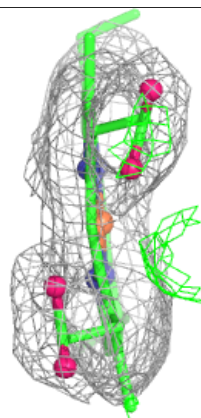
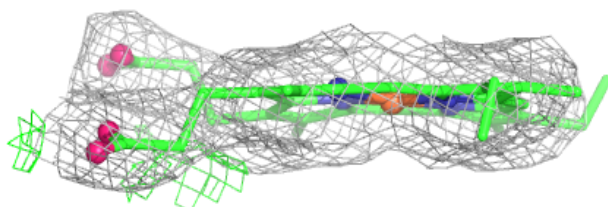
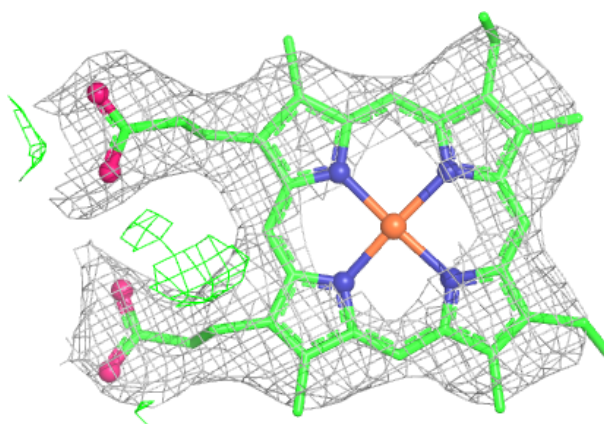
Electron density around HEM X 201:

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



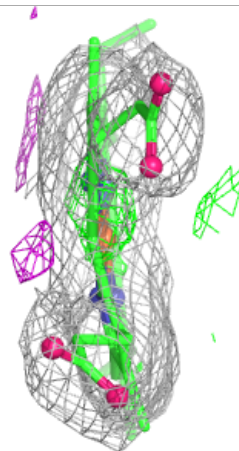
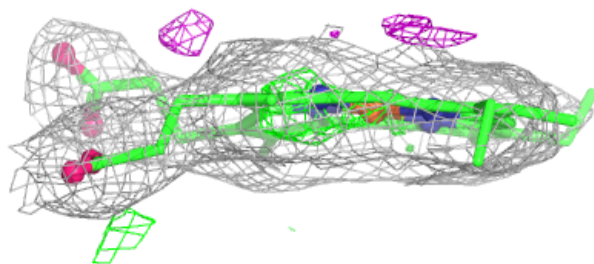
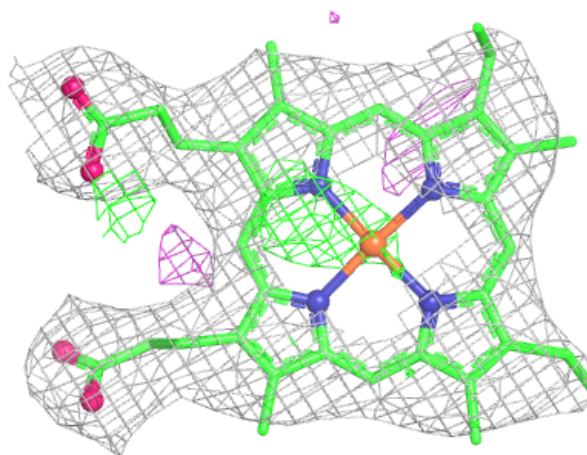
Electron density around HEM a 201:

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



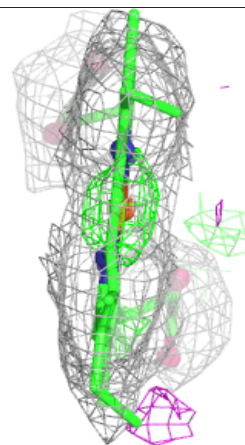
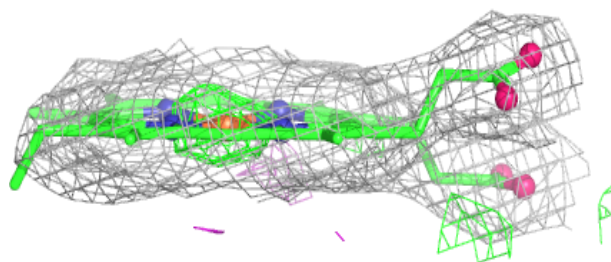
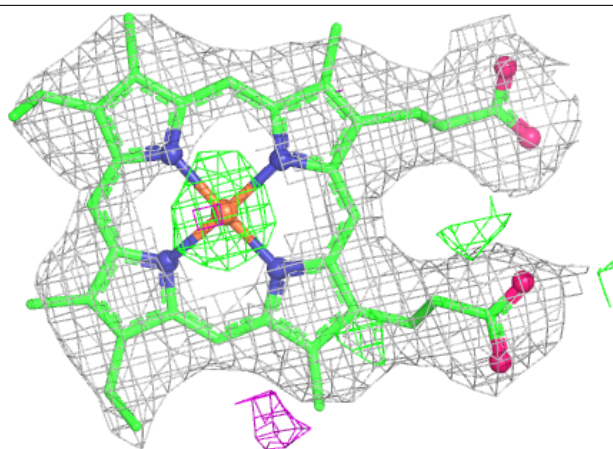
Electron density around HEM U 201:

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



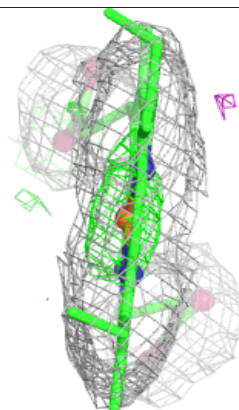
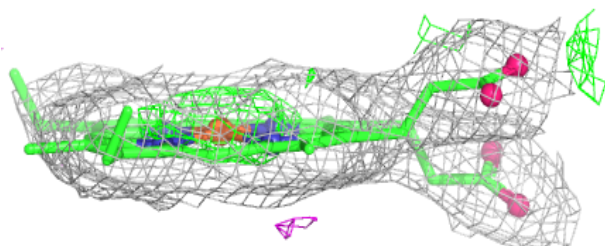
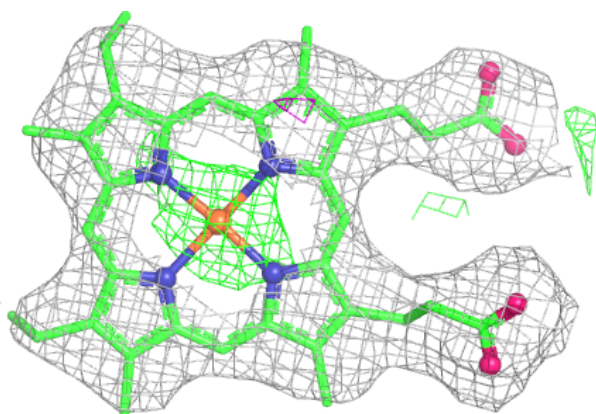
Electron density around HEM C 201:

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



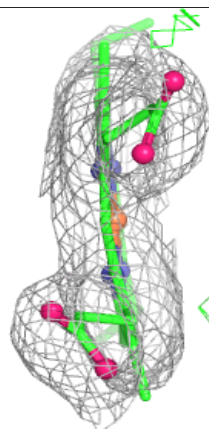
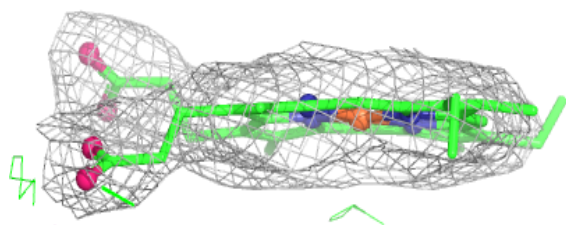
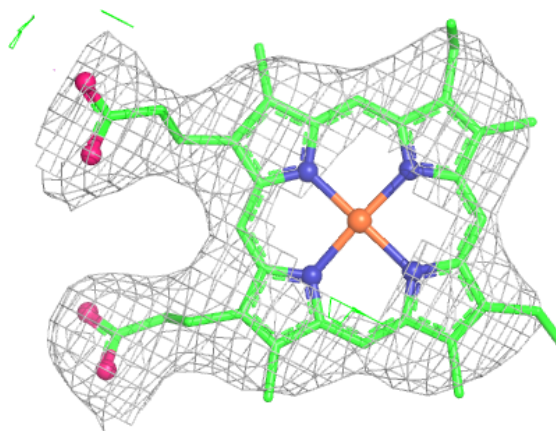
Electron density around HEM g 201:

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



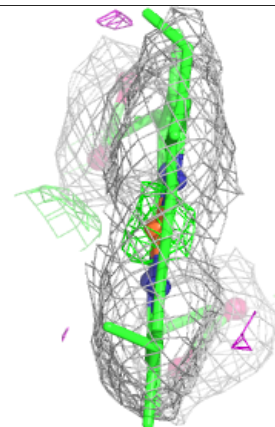
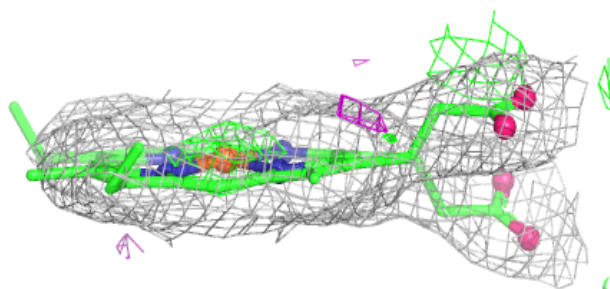
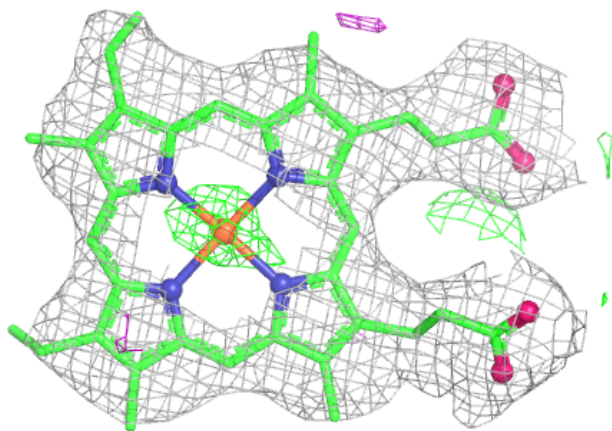
Electron density around HEM D 201:

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



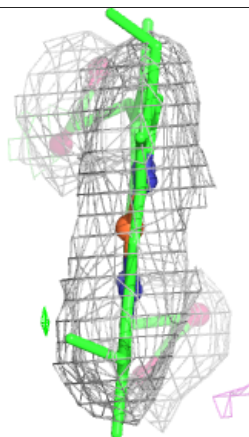
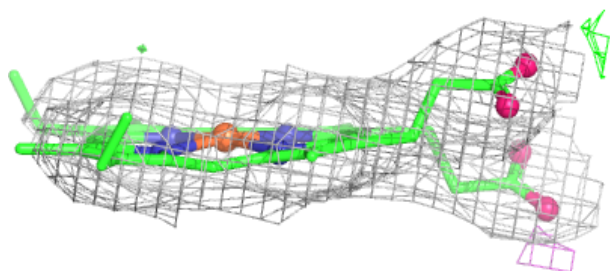
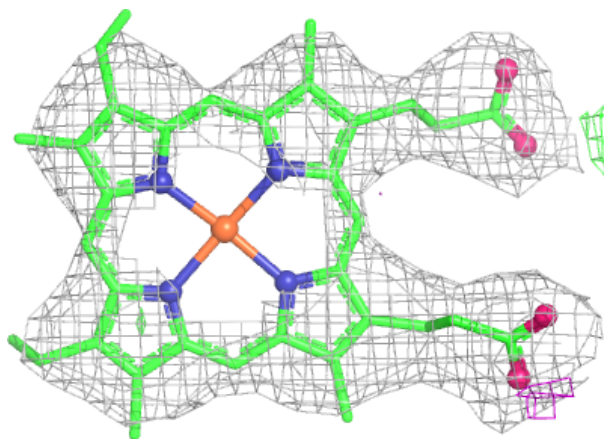
Electron density around HEM R 201:

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



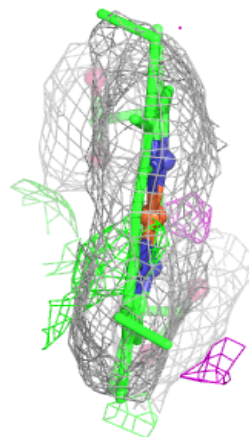
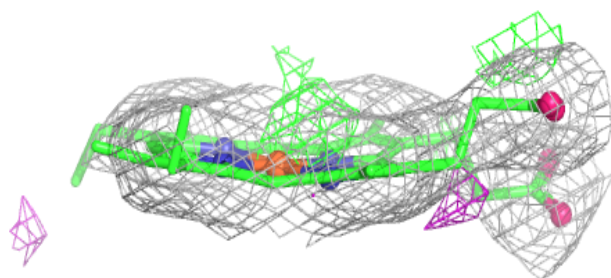
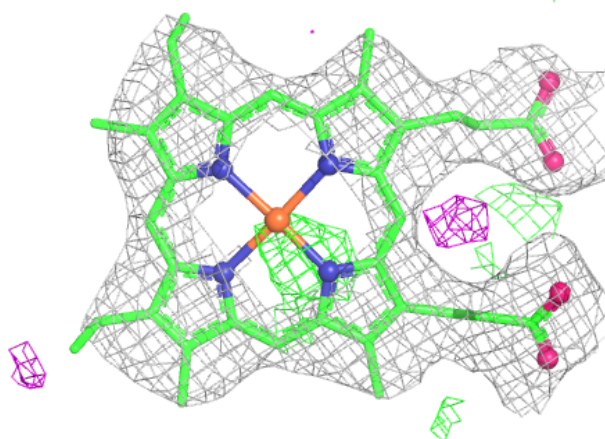
Electron density around HEM K 201:

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

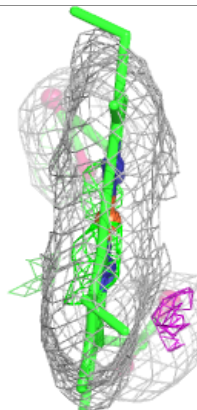
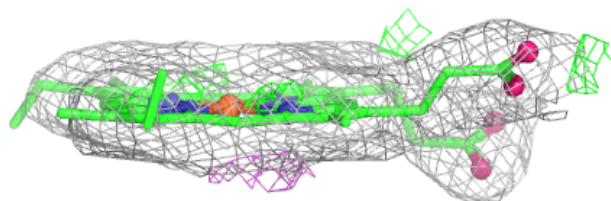
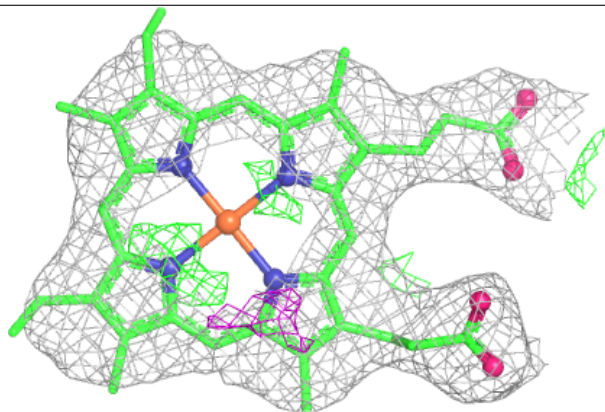


Electron density around HEM B 201:

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

**Electron density around HEM I 201:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.