



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:43 AM UTC

PDB ID : 2QJY / pdb_00002qjy
Title : Crystal structure of rhodobacter sphaeroides double mutant with stigmatellin and UQ2
Authors : Esser, L.; Xia, D.
Deposited on : 2007-07-09
Resolution : 2.40 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:

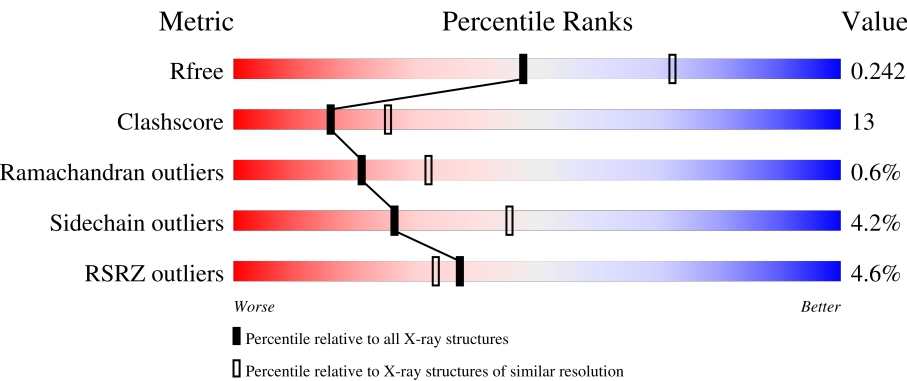
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	445	% 72%21% . .
1	D	445	% 70%24% . .
1	G	445	2% 70%23% . .
1	J	445	3% 68%25% . . .
1	M	445	2% 67%26% . .

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Mol	Chain	Length	Quality of chain
1	P	445	
2	B	269	
2	E	269	
2	H	269	
2	K	269	
2	N	269	
2	Q	269	
3	C	187	
3	F	187	
3	I	187	
3	L	187	
3	O	187	
3	R	187	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 42656 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3440	2322	548	555	15			
1	D	428	Total	C	N	O	S	0	0	0
			3440	2322	548	555	15			
1	G	428	Total	C	N	O	S	0	0	0
			3440	2322	548	555	15			
1	J	428	Total	C	N	O	S	0	0	0
			3440	2322	548	555	15			
1	M	428	Total	C	N	O	S	0	0	0
			3440	2322	548	555	15			
1	P	428	Total	C	N	O	S	0	0	0
			3440	2322	548	555	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	287	ARG	SER	engineered mutation	UNP Q02761
D	287	ARG	SER	engineered mutation	UNP Q02761
G	287	ARG	SER	engineered mutation	UNP Q02761
J	287	ARG	SER	engineered mutation	UNP Q02761
M	287	ARG	SER	engineered mutation	UNP Q02761
P	287	ARG	SER	engineered mutation	UNP Q02761

- Molecule 2 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	256	Total	C	N	O	S	0	0	0
			1953	1240	326	374	13			
2	E	256	Total	C	N	O	S	0	0	0
			1953	1240	326	374	13			
2	H	256	Total	C	N	O	S	0	0	0
			1953	1240	326	374	13			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	256	Total 1953	C 1240	N 326	O 374	S 13	0	0	0
2	N	256	Total 1953	C 1240	N 326	O 374	S 13	0	0	0
2	Q	256	Total 1953	C 1240	N 326	O 374	S 13	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	264	HIS	-	expression tag	UNP Q3IY11
B	265	HIS	-	expression tag	UNP Q3IY11
B	266	HIS	-	expression tag	UNP Q3IY11
B	267	HIS	-	expression tag	UNP Q3IY11
B	268	HIS	-	expression tag	UNP Q3IY11
B	269	HIS	-	expression tag	UNP Q3IY11
E	264	HIS	-	expression tag	UNP Q3IY11
E	265	HIS	-	expression tag	UNP Q3IY11
E	266	HIS	-	expression tag	UNP Q3IY11
E	267	HIS	-	expression tag	UNP Q3IY11
E	268	HIS	-	expression tag	UNP Q3IY11
E	269	HIS	-	expression tag	UNP Q3IY11
H	264	HIS	-	expression tag	UNP Q3IY11
H	265	HIS	-	expression tag	UNP Q3IY11
H	266	HIS	-	expression tag	UNP Q3IY11
H	267	HIS	-	expression tag	UNP Q3IY11
H	268	HIS	-	expression tag	UNP Q3IY11
H	269	HIS	-	expression tag	UNP Q3IY11
K	264	HIS	-	expression tag	UNP Q3IY11
K	265	HIS	-	expression tag	UNP Q3IY11
K	266	HIS	-	expression tag	UNP Q3IY11
K	267	HIS	-	expression tag	UNP Q3IY11
K	268	HIS	-	expression tag	UNP Q3IY11
K	269	HIS	-	expression tag	UNP Q3IY11
N	264	HIS	-	expression tag	UNP Q3IY11
N	265	HIS	-	expression tag	UNP Q3IY11
N	266	HIS	-	expression tag	UNP Q3IY11
N	267	HIS	-	expression tag	UNP Q3IY11
N	268	HIS	-	expression tag	UNP Q3IY11
N	269	HIS	-	expression tag	UNP Q3IY11
Q	264	HIS	-	expression tag	UNP Q3IY11
Q	265	HIS	-	expression tag	UNP Q3IY11

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	266	HIS	-	expression tag	UNP Q3IY11
Q	267	HIS	-	expression tag	UNP Q3IY11
Q	268	HIS	-	expression tag	UNP Q3IY11
Q	269	HIS	-	expression tag	UNP Q3IY11

- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	F	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	I	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	L	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	O	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	R	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	135	SER	VAL	engineered mutation	UNP Q02762
F	135	SER	VAL	engineered mutation	UNP Q02762
I	135	SER	VAL	engineered mutation	UNP Q02762
L	135	SER	VAL	engineered mutation	UNP Q02762
O	135	SER	VAL	engineered mutation	UNP Q02762
R	135	SER	VAL	engineered mutation	UNP Q02762

- Molecule 4 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

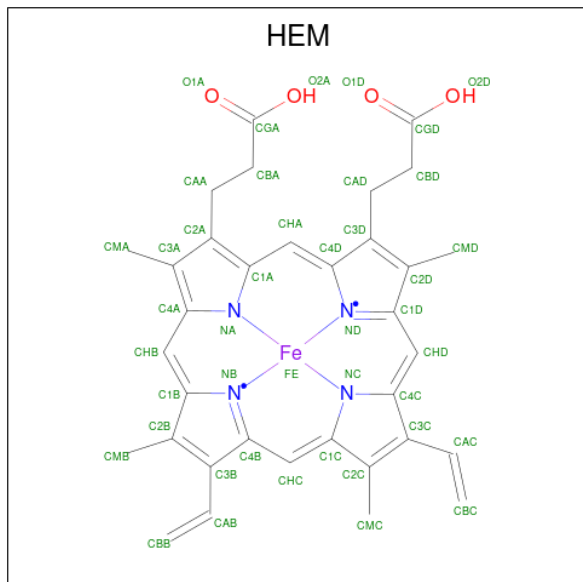
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Sr	0	0
			1	1		
4	B	1	Total	Sr	0	0
			1	1		
4	E	1	Total	Sr	0	0
			1	1		
4	G	1	Total	Sr	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total 1 Sr 1	0	0
4	K	1	Total 1 Sr 1	0	0
4	M	1	Total 1 Sr 1	0	0
4	N	1	Total 1 Sr 1	0	0
4	Q	1	Total 1 Sr 1	0	0

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



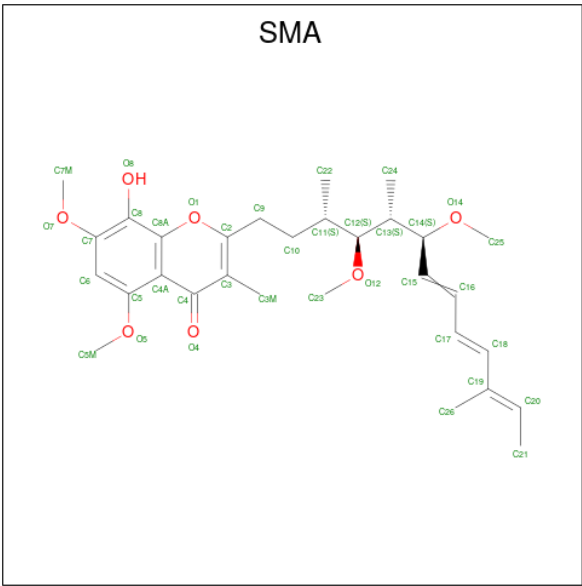
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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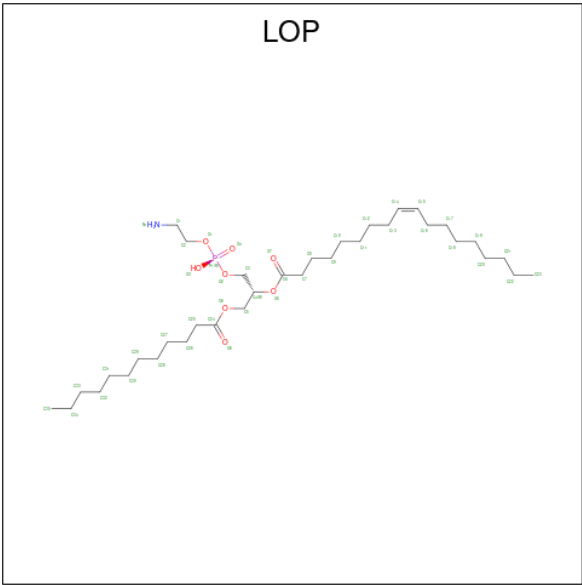
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is STIGMATELLIN A (CCD ID: SMA) (formula: C₃₀H₄₂O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			37	30	7		
6	D	1	Total	C	O	0	0
			37	30	7		
6	G	1	Total	C	O	0	0
			37	30	7		
6	J	1	Total	C	O	0	0
			37	30	7		
6	M	1	Total	C	O	0	0
			37	30	7		
6	P	1	Total	C	O	0	0
			37	30	7		

- Molecule 7 is (1R)-2-{[(R)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(DODECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOATE (CCD ID: LOP) (formula: C₃₅H₆₈NO₈P).



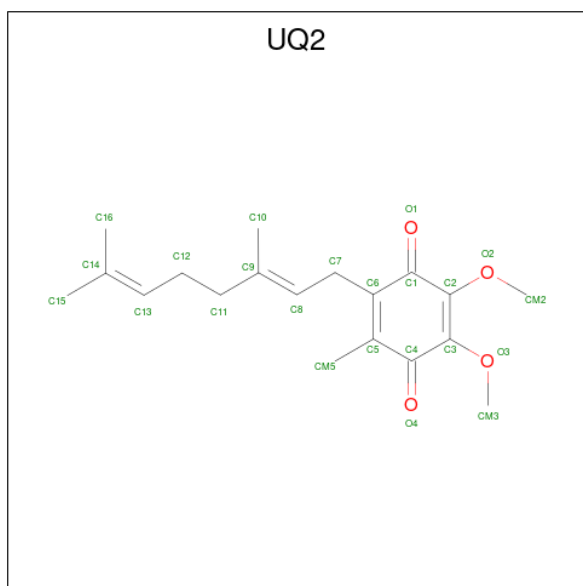
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
7	D	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
7	G	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
7	J	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
7	M	1	Total	C	N	O	P	0	0
			45	35	1	8	1		

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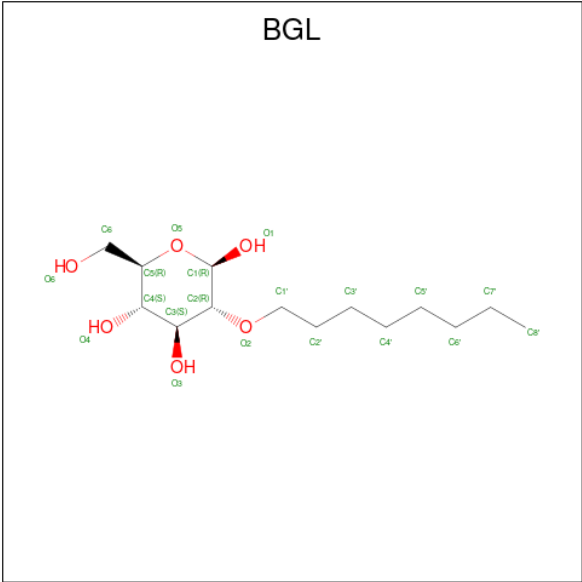
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	P	1	Total	C	N	O	P	0	0
			45	35	1	8	1		

- Molecule 8 is UBIQUINONE-2 (CCD ID: UQ2) (formula: $C_{19}H_{26}O_4$).



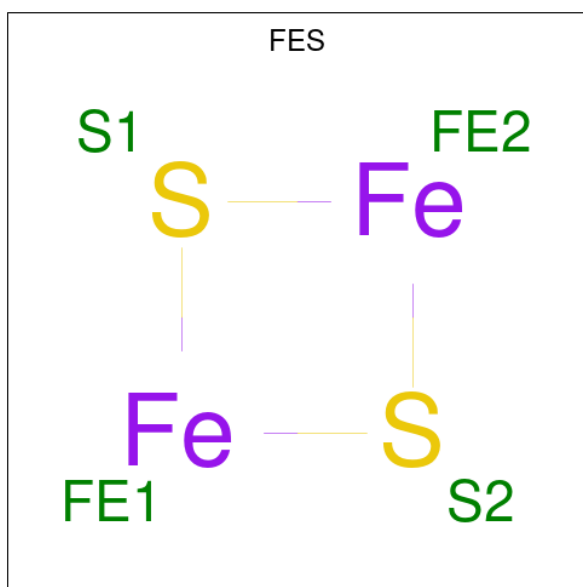
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			23	19	4		
8	D	1	Total	C	O	0	0
			23	19	4		
8	G	1	Total	C	O	0	0
			23	19	4		
8	J	1	Total	C	O	0	0
			23	19	4		
8	M	1	Total	C	O	0	0
			23	19	4		
8	P	1	Total	C	O	0	0
			23	19	4		

- Molecule 9 is 2-O-octyl-beta-D-glucopyranose (CCD ID: BGL) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			20	14	6		
9	E	1	Total	C	O	0	0
			20	14	6		
9	G	1	Total	C	O	0	0
			20	14	6		
9	K	1	Total	C	O	0	0
			20	14	6		
9	N	1	Total	C	O	0	0
			20	14	6		
9	P	1	Total	C	O	0	0
			20	14	6		

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	Fe	S	0	0
			4	2	2		
10	F	1	Total	Fe	S	0	0
			4	2	2		
10	I	1	Total	Fe	S	0	0
			4	2	2		
10	L	1	Total	Fe	S	0	0
			4	2	2		
10	O	1	Total	Fe	S	0	0
			4	2	2		
10	R	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 11 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	I	1	Total	Cl	0	0
			1	1		
11	R	1	Total	Cl	0	0
			1	1		

- Molecule 12 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	R	1	Total	Na	0	0
			1	1		

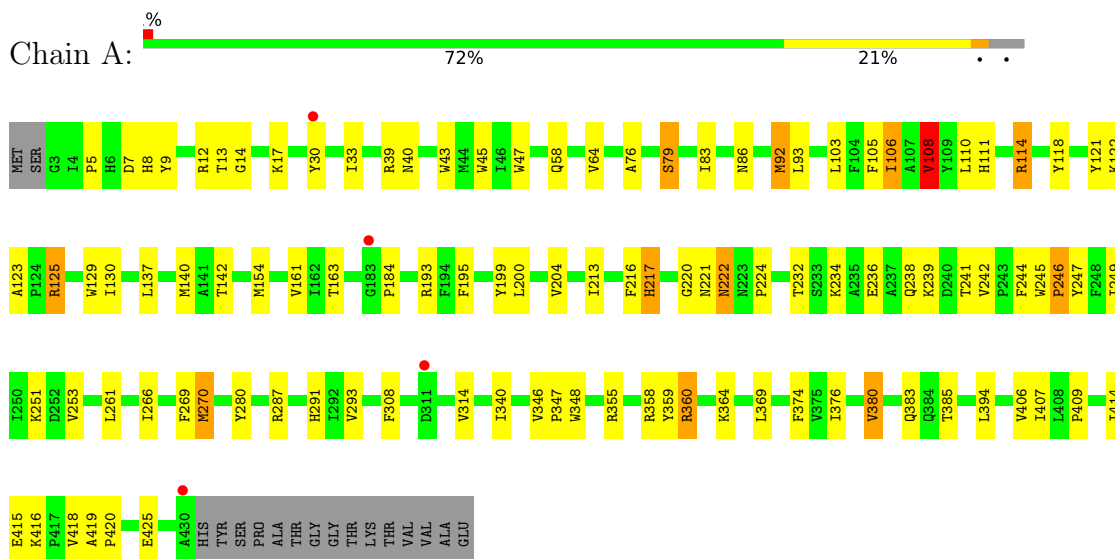
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	73	Total 73	O 73	0	0
13	B	19	Total 19	O 19	0	0
13	C	47	Total 47	O 47	0	0
13	D	64	Total 64	O 64	0	0
13	E	14	Total 14	O 14	0	0
13	F	36	Total 36	O 36	0	0
13	G	68	Total 68	O 68	0	0
13	H	35	Total 35	O 35	0	0
13	I	42	Total 42	O 42	0	0
13	J	55	Total 55	O 55	0	0
13	K	17	Total 17	O 17	0	0
13	L	42	Total 42	O 42	0	0
13	M	34	Total 34	O 34	0	0
13	N	11	Total 11	O 11	0	0
13	O	41	Total 41	O 41	0	0
13	P	60	Total 60	O 60	0	0
13	Q	16	Total 16	O 16	0	0
13	R	24	Total 24	O 24	0	0

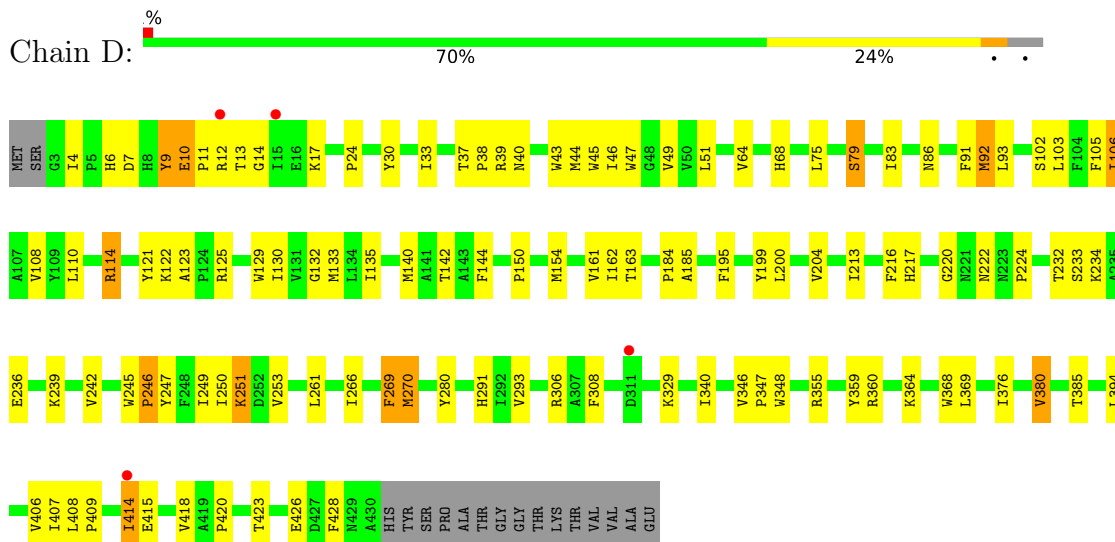
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cytochrome b



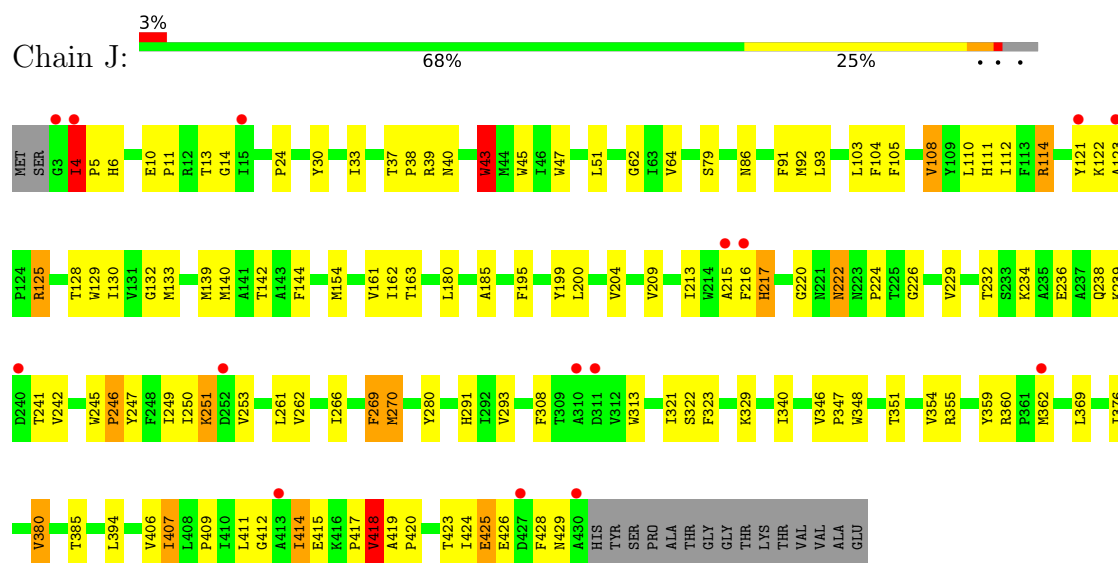
• Molecule 1: Cytochrome b



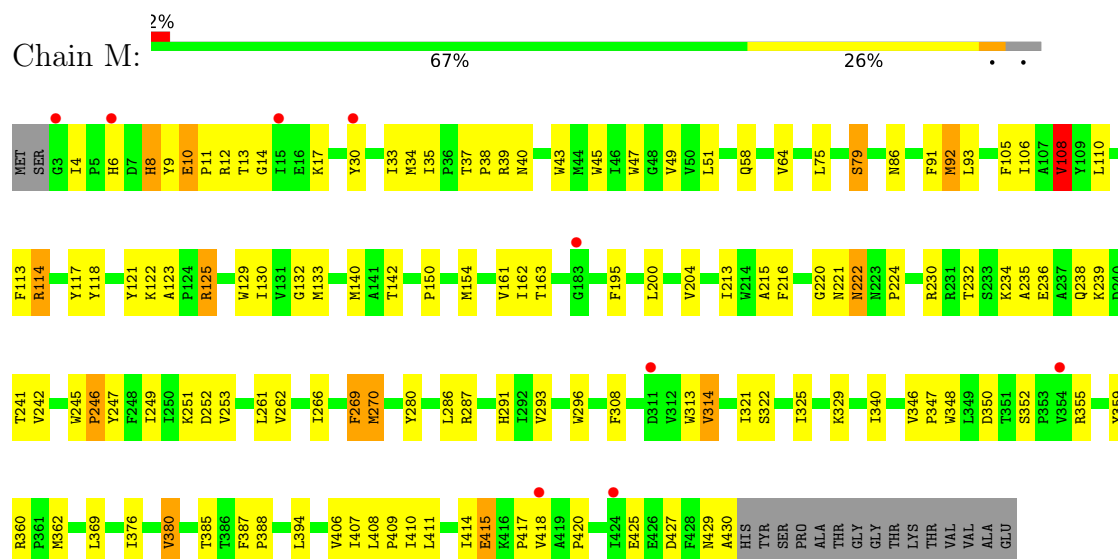
• Molecule 1: Cytochrome b

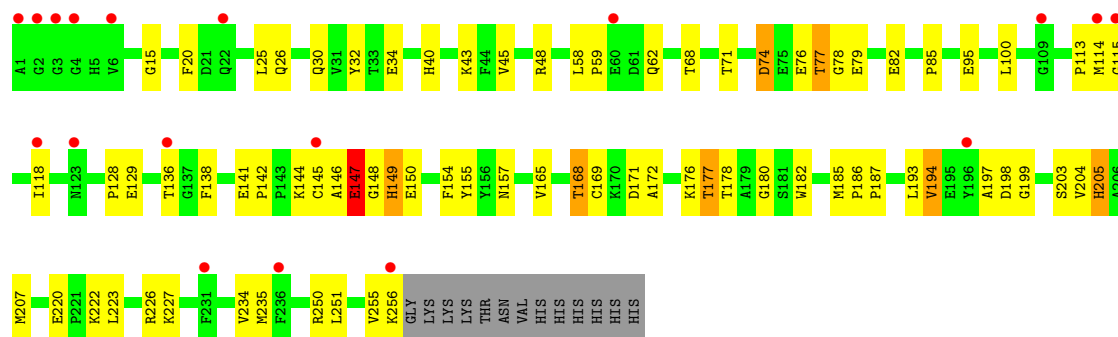


- Molecule 1: Cytochrome b

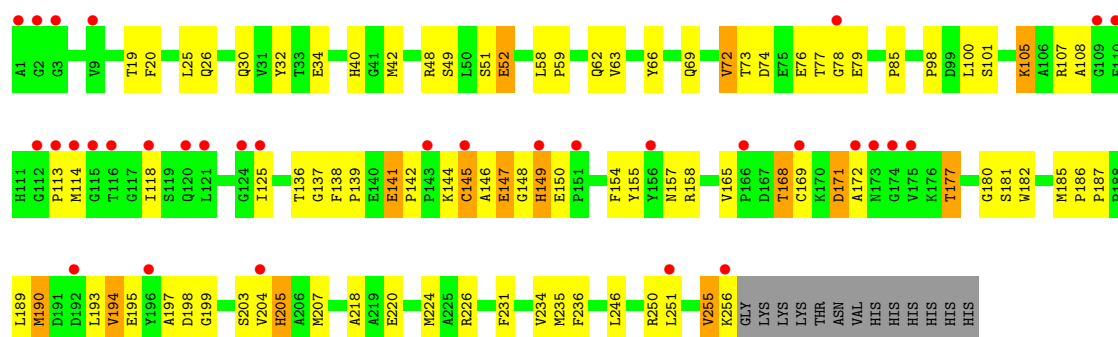


- Molecule 1: Cytochrome b

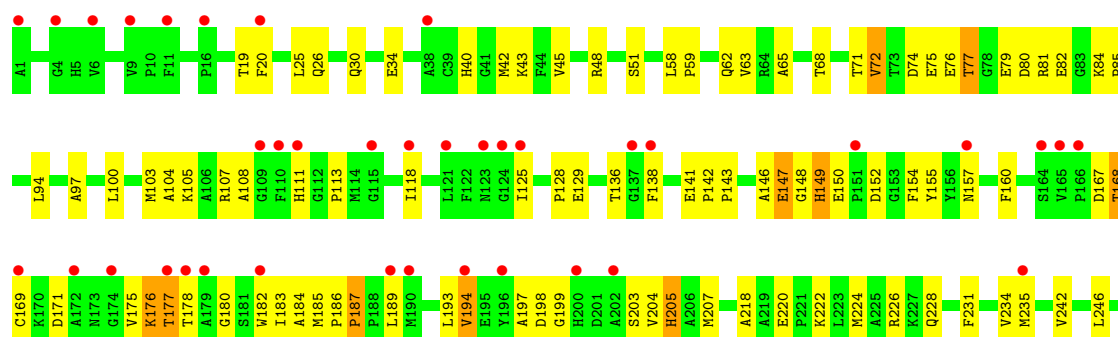




• Molecule 2: Cytochrome c1

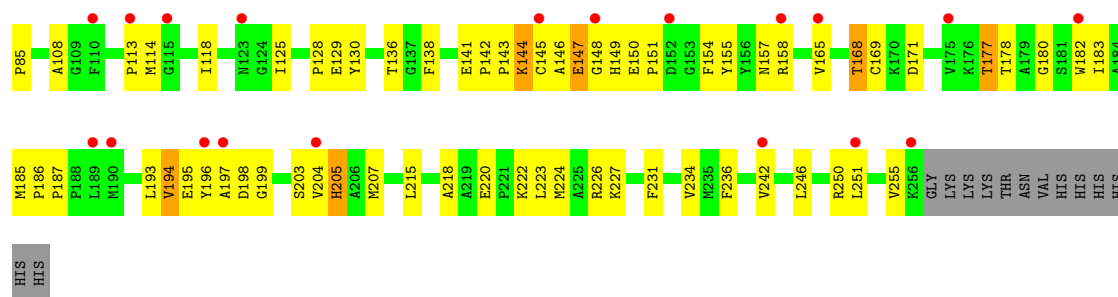


• Molecule 2: Cytochrome c1

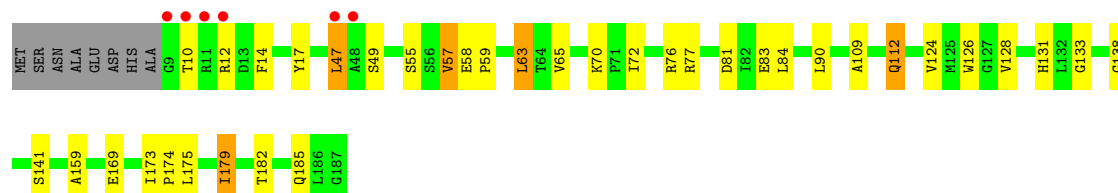
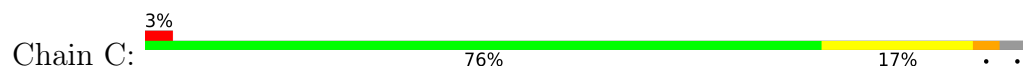


• Molecule 2: Cytochrome c1

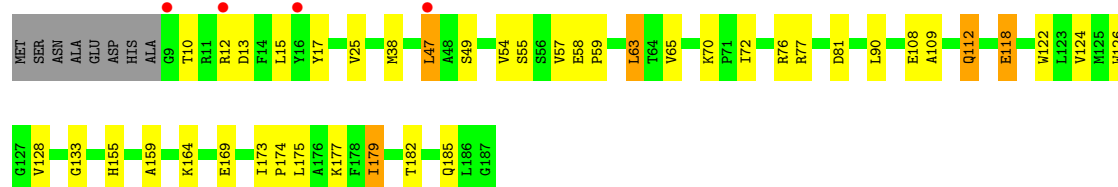




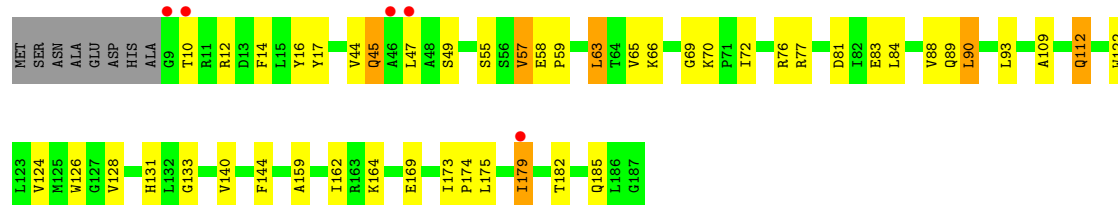
- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



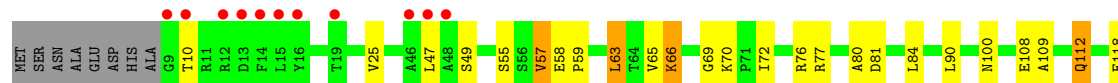
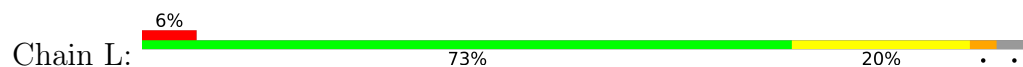
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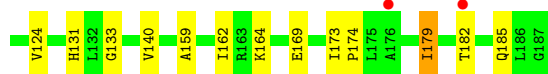
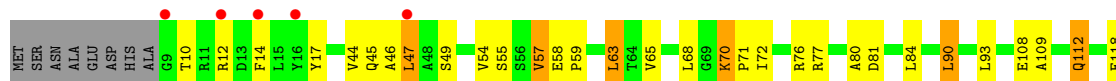
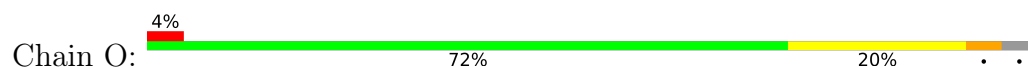


- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

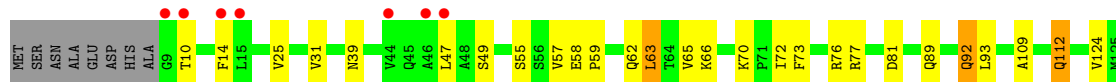
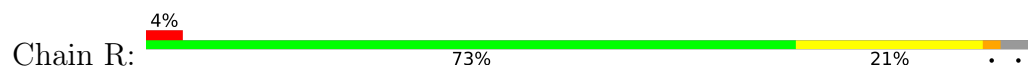




- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	351.89Å 147.04Å 161.31Å 90.00° 104.25° 90.00°	Depositor
Resolution (Å)	18.00 – 2.40 18.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.7 (18.00-2.40) 93.1 (18.00-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.34Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.251 0.225 , 0.242	Depositor DCC
R_{free} test set	9798 reflections (1.70%)	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	42656	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.94% 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: FES, HEM, SMA, SR, NA, UQ2, CL, LOP, BGL

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	0.47	0/3570	1.03	28/4897 (0.6%)
1	D	0.48	0/3570	1.03	26/4897 (0.5%)
1	G	0.47	0/3570	1.04	31/4897 (0.6%)
1	J	0.48	0/3570	1.04	29/4897 (0.6%)
1	M	0.45	0/3570	1.03	29/4897 (0.6%)
1	P	0.47	0/3570	1.03	31/4897 (0.6%)
2	B	0.44	0/2010	1.03	6/2733 (0.2%)
2	E	0.43	0/2010	1.02	7/2733 (0.3%)
2	H	0.45	0/2010	1.02	7/2733 (0.3%)
2	K	0.42	0/2010	1.01	6/2733 (0.2%)
2	N	0.41	0/2010	1.02	7/2733 (0.3%)
2	Q	0.43	0/2010	0.99	3/2733 (0.1%)
3	C	0.46	0/1370	1.05	6/1866 (0.3%)
3	F	0.48	0/1370	1.05	6/1866 (0.3%)
3	I	0.51	1/1370 (0.1%)	1.14	13/1866 (0.7%)
3	L	0.47	0/1370	1.03	6/1866 (0.3%)
3	O	0.46	0/1370	1.04	5/1866 (0.3%)
3	R	0.45	0/1370	1.05	7/1866 (0.4%)
All	All	0.46	1/41700 (0.0%)	1.03	253/56976 (0.4%)

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
2	B	0	1
2	E	0	1
2	H	0	1
2	K	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	44	VAL	CA-C	5.01	1.59	1.52

All (253) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	44	VAL	N-CA-C	14.17	123.85	110.53
3	O	133	GLY	N-CA-C	9.60	126.12	114.69
3	R	133	GLY	N-CA-C	9.45	125.94	114.69
3	I	133	GLY	N-CA-C	9.41	125.89	114.69
3	F	133	GLY	N-CA-C	9.17	125.60	114.69
1	J	313	TRP	N-CA-C	8.97	121.13	111.36
3	C	133	GLY	N-CA-C	8.96	125.35	114.69
3	L	133	GLY	N-CA-C	8.93	125.31	114.69
1	G	9	TYR	N-CA-C	8.66	122.45	110.24
1	P	108	VAL	CB-CA-C	-8.29	100.78	112.22
1	J	4	ILE	N-CA-C	8.15	116.60	109.02
1	G	108	VAL	CB-CA-C	-7.88	101.34	112.22
3	F	169	GLU	N-CA-C	7.74	119.77	108.86
3	I	169	GLU	N-CA-C	7.63	119.62	108.86
3	I	93	LEU	N-CA-C	7.61	122.41	110.32
3	O	169	GLU	N-CA-C	7.59	119.56	108.86
1	P	10	GLU	CA-C-N	7.54	128.72	119.98
1	P	10	GLU	C-N-CA	7.54	128.72	119.98
3	L	169	GLU	N-CA-C	7.50	119.44	108.86
3	C	169	GLU	N-CA-C	7.50	119.44	108.86
2	K	78	GLY	N-CA-C	-7.41	105.62	115.40
3	R	169	GLU	N-CA-C	7.38	119.26	108.86
2	H	144	LYS	N-CA-C	7.36	119.30	111.28
1	G	407	ILE	N-CA-C	7.29	118.02	110.36
2	B	78	GLY	N-CA-C	-7.29	106.16	115.42
1	M	407	ILE	N-CA-C	7.25	117.97	110.36
1	D	407	ILE	N-CA-C	7.14	117.86	110.36
1	J	125	ARG	N-CA-C	7.14	120.54	112.97
1	M	125	ARG	N-CA-C	7.08	120.86	112.93
2	K	105	LYS	N-CA-C	-7.00	105.67	114.56
1	G	200	LEU	N-CA-C	6.99	118.69	111.14
1	M	108	VAL	CB-CA-C	-6.90	102.70	112.22
2	N	43	LYS	N-CA-C	6.90	121.31	112.34
1	A	125	ARG	N-CA-C	6.87	120.62	112.93
2	K	76	GLU	N-CA-C	-6.86	103.94	112.72
1	P	125	ARG	N-CA-C	6.79	120.53	112.93
2	K	193	LEU	N-CA-C	-6.76	105.03	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	200	LEU	N-CA-C	6.75	118.42	111.14
2	Q	193	LEU	N-CA-C	-6.74	105.06	113.28
1	M	313	TRP	N-CA-C	6.74	118.63	111.28
1	D	125	ARG	N-CA-C	6.73	120.47	112.93
2	E	193	LEU	N-CA-C	-6.73	105.07	113.28
2	N	193	LEU	N-CA-C	-6.70	105.07	113.18
1	M	321	ILE	CB-CA-C	-6.70	103.26	112.04
3	R	93	LEU	N-CA-C	6.67	120.93	110.32
2	B	193	LEU	N-CA-C	-6.66	105.16	113.28
1	G	125	ARG	N-CA-C	6.61	120.33	112.93
2	H	193	LEU	N-CA-C	-6.61	105.18	113.18
2	H	43	LYS	N-CA-C	6.61	120.93	112.34
1	J	200	LEU	N-CA-C	6.57	118.23	111.14
1	J	407	ILE	N-CA-C	6.55	117.23	110.36
1	P	200	LEU	N-CA-C	6.51	118.17	111.14
1	J	415	GLU	N-CA-C	6.50	120.09	110.48
1	P	232	THR	N-CA-C	6.46	119.14	111.71
1	D	200	LEU	N-CA-C	6.45	118.11	111.14
2	B	75	GLU	N-CA-C	6.44	120.40	112.54
1	P	407	ILE	N-CA-C	6.42	117.10	110.36
1	A	232	THR	N-CA-C	6.40	119.07	111.71
1	G	232	THR	N-CA-C	6.36	119.02	111.71
1	M	232	THR	N-CA-C	6.36	119.02	111.71
1	J	232	THR	N-CA-C	6.35	119.01	111.71
1	D	232	THR	N-CA-C	6.34	119.01	111.71
2	Q	43	LYS	N-CA-C	6.30	120.53	112.34
1	A	200	LEU	N-CA-C	6.30	117.94	111.14
1	G	220	GLY	N-CA-C	-6.29	104.86	112.48
1	D	308	PHE	N-CA-C	6.26	119.45	108.56
1	A	269	PHE	N-CA-C	6.22	121.15	113.50
1	A	163	THR	N-CA-C	-6.22	105.18	112.89
1	A	308	PHE	N-CA-C	6.21	119.37	108.56
1	P	163	THR	N-CA-C	-6.21	105.20	112.89
1	M	270	MET	CA-C-N	6.20	125.88	119.56
1	M	270	MET	C-N-CA	6.20	125.88	119.56
1	P	308	PHE	N-CA-C	6.13	119.23	108.56
1	A	270	MET	CA-C-N	6.11	125.79	119.56
1	A	270	MET	C-N-CA	6.11	125.79	119.56
1	G	270	MET	CA-C-N	6.10	125.78	119.56
1	G	270	MET	C-N-CA	6.10	125.78	119.56
1	M	220	GLY	N-CA-C	-6.06	105.15	112.48
1	M	10	GLU	CA-C-N	6.06	127.01	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	10	GLU	C-N-CA	6.06	127.01	119.98
1	P	270	MET	CA-C-N	6.06	125.74	119.56
1	P	270	MET	C-N-CA	6.06	125.74	119.56
1	J	308	PHE	N-CA-C	6.04	119.06	108.56
1	M	308	PHE	N-CA-C	6.03	119.05	108.56
1	A	407	ILE	N-CA-C	6.02	117.48	110.62
1	P	220	GLY	N-CA-C	-6.02	105.20	112.48
1	D	220	GLY	N-CA-C	-6.01	105.21	112.48
1	D	415	GLU	N-CA-C	5.99	119.35	110.48
1	A	220	GLY	N-CA-C	-5.99	105.23	112.48
1	P	360	ARG	CA-C-N	5.99	125.70	119.05
1	P	360	ARG	C-N-CA	5.99	125.70	119.05
1	A	40	ASN	N-CA-C	5.99	120.20	113.02
1	J	270	MET	CA-C-N	5.97	125.65	119.56
1	J	270	MET	C-N-CA	5.97	125.65	119.56
1	P	414	ILE	N-CA-C	5.97	120.56	113.22
1	G	269	PHE	N-CA-C	5.96	120.83	113.50
1	D	270	MET	CA-C-N	5.96	125.64	119.56
1	D	270	MET	C-N-CA	5.96	125.64	119.56
1	J	220	GLY	N-CA-C	-5.96	105.27	112.48
1	M	415	GLU	N-CA-C	5.94	119.28	110.48
1	D	40	ASN	N-CA-C	5.94	120.15	113.02
1	M	269	PHE	N-CA-C	5.94	120.81	113.50
1	P	204	VAL	N-CA-C	-5.93	104.95	110.53
1	M	360	ARG	CA-C-N	5.92	125.63	119.05
1	M	360	ARG	C-N-CA	5.92	125.63	119.05
1	G	204	VAL	N-CA-C	-5.92	104.96	110.53
2	B	76	GLU	N-CA-C	-5.91	106.10	113.55
1	J	269	PHE	N-CA-C	5.88	120.74	113.50
2	E	89	PHE	CA-C-N	-5.87	114.70	120.52
2	E	89	PHE	C-N-CA	-5.87	114.70	120.52
1	M	204	VAL	N-CA-C	-5.85	104.81	110.72
1	M	40	ASN	N-CA-C	5.81	119.99	113.02
1	G	308	PHE	N-CA-C	5.80	118.66	108.56
1	G	40	ASN	N-CA-C	5.80	119.98	113.02
1	D	269	PHE	N-CA-C	5.79	120.62	113.50
3	I	45	GLN	N-CA-C	5.79	123.12	110.80
1	D	9	TYR	N-CA-C	5.78	118.39	110.24
1	A	161	VAL	N-CA-C	5.77	116.55	110.72
1	J	418	VAL	N-CA-C	-5.76	103.70	110.21
1	M	222	ASN	N-CA-C	-5.76	102.00	110.52
1	A	86	ASN	N-CA-C	5.75	120.31	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	415	GLU	N-CA-C	5.73	118.96	110.48
1	D	86	ASN	N-CA-C	5.73	120.28	113.12
1	M	163	THR	N-CA-C	-5.72	105.56	112.54
1	J	369	LEU	N-CA-C	-5.72	105.13	111.36
1	P	40	ASN	N-CA-C	5.71	119.87	113.02
1	A	241	THR	N-CA-C	5.70	118.54	109.65
1	G	10	GLU	CA-C-N	5.70	125.63	119.76
1	G	10	GLU	C-N-CA	5.70	125.63	119.76
1	G	86	ASN	N-CA-C	5.70	120.24	113.12
1	D	222	ASN	N-CA-C	-5.69	102.09	110.52
1	A	222	ASN	N-CA-C	-5.69	102.10	110.52
1	G	163	THR	N-CA-C	-5.69	105.60	112.54
1	M	161	VAL	N-CA-C	5.69	115.88	110.53
3	O	49	SER	N-CA-C	-5.67	100.43	109.23
1	J	40	ASN	N-CA-C	5.67	119.83	113.02
1	G	360	ARG	CA-C-N	5.67	125.34	119.05
1	G	360	ARG	C-N-CA	5.67	125.34	119.05
1	D	161	VAL	N-CA-C	5.66	116.44	110.72
2	H	45	VAL	N-CA-C	5.65	114.10	107.77
1	J	86	ASN	N-CA-C	5.63	120.16	113.12
1	P	269	PHE	N-CA-C	5.63	120.42	113.50
1	J	163	THR	N-CA-C	-5.62	105.68	112.54
3	I	44	VAL	CA-C-N	5.62	132.27	121.54
3	I	44	VAL	C-N-CA	5.62	132.27	121.54
1	G	241	THR	N-CA-C	5.62	118.41	109.65
1	A	415	GLU	N-CA-C	5.61	119.06	110.20
1	P	222	ASN	N-CA-C	-5.61	102.22	110.52
1	J	360	ARG	CA-C-N	5.60	125.27	119.05
1	J	360	ARG	C-N-CA	5.60	125.27	119.05
1	J	222	ASN	N-CA-C	-5.59	102.25	110.52
1	J	241	THR	N-CA-C	5.58	118.35	109.65
2	H	71	THR	N-CA-C	-5.57	100.63	109.76
1	G	222	ASN	N-CA-C	-5.56	102.29	110.52
1	G	161	VAL	N-CA-C	5.55	116.33	110.72
2	N	187	PRO	CA-C-N	-5.55	112.90	119.84
2	N	187	PRO	C-N-CA	-5.55	112.90	119.84
1	J	321	ILE	CB-CA-C	-5.54	104.78	112.04
3	F	49	SER	N-CA-C	-5.54	100.65	109.23
1	M	418	VAL	N-CA-C	-5.54	103.95	110.21
1	D	163	THR	N-CA-C	-5.52	105.80	112.54
1	A	108	VAL	CB-CA-C	-5.52	103.32	112.26
1	J	251	LYS	N-CA-C	-5.51	105.17	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	204	VAL	N-CA-C	-5.51	105.15	110.72
2	H	74	ASP	N-CA-C	5.51	118.31	110.10
1	P	241	THR	N-CA-C	5.51	118.24	109.65
2	N	45	VAL	N-CA-C	5.51	113.94	107.77
2	Q	45	VAL	N-CA-C	5.48	113.91	107.77
3	O	159	ALA	N-CA-C	-5.46	105.43	113.61
1	D	360	ARG	CA-C-N	5.45	125.10	119.05
1	D	360	ARG	C-N-CA	5.45	125.10	119.05
1	D	280	TYR	N-CA-C	-5.44	106.52	112.72
1	M	241	THR	N-CA-C	5.43	118.12	109.65
1	M	369	LEU	N-CA-C	-5.42	105.45	111.36
3	I	122	TRP	N-CA-C	5.42	117.83	107.75
3	R	49	SER	N-CA-C	-5.42	100.83	109.23
2	N	141	GLU	CA-C-N	5.42	125.96	120.38
2	N	141	GLU	C-N-CA	5.42	125.96	120.38
1	A	360	ARG	CA-C-N	5.42	125.06	119.05
1	A	360	ARG	C-N-CA	5.42	125.06	119.05
1	A	247	TYR	N-CA-C	5.41	117.60	111.11
1	A	204	VAL	N-CA-C	-5.40	105.27	110.72
3	I	49	SER	N-CA-C	-5.40	100.86	109.23
1	G	369	LEU	N-CA-C	-5.39	105.48	111.36
3	R	159	ALA	N-CA-C	-5.37	105.55	113.61
1	J	204	VAL	N-CA-C	-5.36	105.30	110.72
1	G	114	ARG	N-CA-C	-5.36	105.44	111.28
1	P	355	ARG	N-CA-C	5.36	116.98	111.03
1	A	369	LEU	N-CA-C	-5.35	105.53	111.36
1	A	416	LYS	CA-C-N	5.34	125.10	119.76
1	A	416	LYS	C-N-CA	5.34	125.10	119.76
1	D	418	VAL	N-CA-C	-5.34	104.17	110.21
1	A	114	ARG	N-CA-C	-5.33	105.36	111.07
3	F	122	TRP	N-CA-C	5.33	117.66	107.75
1	P	416	LYS	CA-C-N	5.31	125.47	119.90
1	P	416	LYS	C-N-CA	5.31	125.47	119.90
3	L	159	ALA	N-CA-C	-5.31	105.65	113.61
1	P	114	ARG	N-CA-C	-5.30	105.40	111.07
1	D	247	TYR	N-CA-C	5.30	117.47	111.11
1	G	325	ILE	CB-CA-C	-5.29	105.11	112.04
1	J	161	VAL	N-CA-C	5.29	116.06	110.72
1	G	280	TYR	N-CA-C	-5.28	106.70	112.72
2	K	141	GLU	CA-C-N	5.28	125.82	120.38
2	K	141	GLU	C-N-CA	5.28	125.82	120.38
2	E	141	GLU	CA-C-N	5.28	125.82	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	141	GLU	C-N-CA	5.28	125.82	120.38
3	C	49	SER	N-CA-C	-5.27	101.06	109.23
1	D	369	LEU	N-CA-C	-5.26	105.62	111.36
1	M	114	ARG	N-CA-C	-5.24	105.57	111.28
2	E	103	MET	N-CA-C	5.23	117.38	111.11
1	J	280	TYR	N-CA-C	-5.22	106.77	112.72
3	I	175	LEU	N-CA-C	-5.20	102.22	109.96
3	L	49	SER	N-CA-C	-5.18	101.19	109.23
1	J	247	TYR	N-CA-C	5.18	117.32	111.11
3	L	175	LEU	N-CA-C	-5.17	102.25	109.96
1	D	251	LYS	N-CA-C	-5.17	105.65	111.28
3	O	57	VAL	N-CA-C	5.16	115.20	107.51
3	R	175	LEU	N-CA-C	-5.15	102.29	109.96
1	G	247	TYR	N-CA-C	5.14	117.28	111.11
1	G	106	ILE	N-CA-C	-5.14	105.38	110.62
1	D	114	ARG	N-CA-C	-5.14	105.58	111.07
1	M	86	ASN	N-CA-C	5.13	119.54	113.12
1	A	106	ILE	CB-CA-C	-5.13	105.31	111.88
2	H	78	GLY	N-CA-C	-5.13	108.15	115.64
1	P	369	LEU	N-CA-C	-5.13	105.77	111.36
3	C	159	ALA	N-CA-C	-5.12	105.92	113.61
1	M	247	TYR	N-CA-C	5.12	117.25	111.11
1	A	280	TYR	N-CA-C	-5.11	106.90	112.72
1	J	114	ARG	N-CA-C	-5.10	105.61	111.07
1	A	76	ALA	N-CA-C	5.09	117.22	111.11
2	E	45	VAL	N-CA-C	5.09	113.47	107.77
1	M	280	TYR	N-CA-C	-5.08	106.92	112.72
3	L	57	VAL	N-CA-C	5.07	115.07	107.51
1	P	247	TYR	N-CA-C	5.07	117.20	111.11
1	P	86	ASN	N-CA-C	5.07	119.46	113.12
3	I	144	PHE	N-CA-C	5.07	118.94	112.26
1	P	108	VAL	N-CA-CB	5.07	118.18	110.58
3	I	159	ALA	N-CA-C	-5.06	106.01	113.61
2	B	216	MET	N-CA-C	-5.06	105.84	111.36
3	F	159	ALA	N-CA-C	-5.05	106.03	113.61
1	J	414	ILE	N-CA-C	5.05	119.43	113.22
1	P	76	ALA	N-CA-C	5.05	117.17	111.11
2	B	45	VAL	N-CA-C	5.05	113.43	107.77
1	G	416	LYS	CA-C-N	5.04	125.20	119.90
1	G	416	LYS	C-N-CA	5.04	125.20	119.90
3	I	57	VAL	N-CA-C	5.04	115.01	107.51
3	R	31	VAL	N-CA-C	5.04	115.26	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	175	LEU	N-CA-C	-5.03	102.47	109.96
1	P	161	VAL	N-CA-C	5.01	115.78	110.72
3	C	175	LEU	N-CA-C	-5.01	102.49	109.96
3	C	57	VAL	N-CA-C	5.01	114.97	107.51
1	P	418	VAL	N-CA-C	-5.01	104.55	110.21
1	D	106	ILE	N-CA-C	-5.00	105.52	110.62

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	32	TYR	Sidechain
2	E	32	TYR	Sidechain
2	H	32	TYR	Sidechain
2	K	32	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3440	0	3428	74	0
1	D	3440	0	3428	90	0
1	G	3440	0	3428	96	0
1	J	3440	0	3428	103	0
1	M	3440	0	3428	99	0
1	P	3440	0	3428	82	0
2	B	1953	0	1848	70	0
2	E	1953	0	1848	90	0
2	H	1953	0	1848	74	0
2	K	1953	0	1848	76	0
2	N	1953	0	1848	87	0
2	Q	1953	0	1848	86	0
3	C	1340	0	1303	27	0
3	F	1340	0	1303	28	0
3	I	1340	0	1303	29	0
3	L	1340	0	1303	27	0
3	O	1340	0	1303	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R	1340	0	1303	28	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	Q	1	0	0	0	0
5	A	86	0	60	7	0
5	B	43	0	30	1	0
5	D	86	0	60	9	0
5	E	43	0	30	1	0
5	G	86	0	60	10	0
5	H	43	0	30	1	0
5	J	86	0	60	15	0
5	K	43	0	30	2	0
5	M	86	0	60	9	0
5	N	43	0	30	3	0
5	P	86	0	60	7	0
5	Q	43	0	30	2	0
6	A	37	0	42	0	0
6	D	37	0	42	0	0
6	G	37	0	42	0	0
6	J	37	0	42	1	0
6	M	37	0	42	0	0
6	P	37	0	42	1	0
7	A	45	0	67	6	0
7	D	45	0	67	2	0
7	G	45	0	67	3	0
7	J	45	0	67	1	0
7	M	45	0	67	3	0
7	P	45	0	67	2	0
8	A	23	0	26	2	0
8	D	23	0	26	2	0
8	G	23	0	26	2	0
8	J	23	0	26	1	0
8	M	23	0	26	2	0
8	P	23	0	26	2	0
9	B	20	0	28	1	0
9	E	20	0	28	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	G	20	0	28	2	0
9	K	20	0	28	2	0
9	N	20	0	28	1	0
9	P	20	0	28	2	0
10	C	4	0	0	0	0
10	F	4	0	0	0	0
10	I	4	0	0	0	0
10	L	4	0	0	0	0
10	O	4	0	0	0	0
10	R	4	0	0	0	0
11	I	1	0	0	0	0
11	R	1	0	0	0	0
12	R	1	0	0	0	0
13	A	73	0	0	1	0
13	B	19	0	0	2	0
13	C	47	0	0	0	0
13	D	64	0	0	4	0
13	E	14	0	0	1	0
13	F	36	0	0	0	0
13	G	68	0	0	2	0
13	H	35	0	0	3	0
13	I	42	0	0	0	0
13	J	55	0	0	3	0
13	K	17	0	0	0	0
13	L	42	0	0	1	0
13	M	34	0	0	1	0
13	N	11	0	0	1	0
13	O	41	0	0	1	0
13	P	60	0	0	1	0
13	Q	16	0	0	1	0
13	R	24	0	0	2	0
All	All	42656	0	40992	1093	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (1093) 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)
2:Q:144:LYS:HA	2:Q:144:LYS:HZ3	1.06	1.14
2:K:139:PRO:HG3	2:K:158:ARG:HH11	1.14	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:77:THR:HG22	2:N:79:GLU:H	1.25	1.02
2:K:194:VAL:HB	2:K:207:MET:HE3	1.42	1.01
2:Q:144:LYS:HA	2:Q:144:LYS:NZ	1.75	1.01
2:B:194:VAL:HB	2:B:207:MET:HE3	1.42	1.01
2:B:250:ARG:HD3	3:C:12:ARG:HG2	1.41	1.01
2:Q:194:VAL:HB	2:Q:207:MET:HE3	1.41	1.01
2:N:194:VAL:HB	2:N:207:MET:HE3	1.41	1.00
2:K:74:ASP:HB3	2:K:77:THR:HB	1.42	0.99
2:H:194:VAL:HB	2:H:207:MET:HE3	1.41	0.98
2:E:194:VAL:HB	2:E:207:MET:HE3	1.42	0.97
2:K:144:LYS:O	2:K:147:GLU:HG3	1.66	0.95
2:Q:223:LEU:HD21	2:Q:227:LYS:HE3	1.45	0.95
2:N:74:ASP:HB3	2:N:77:THR:HB	1.48	0.94
1:D:142:THR:HG21	5:D:502:HEM:HBB2	1.50	0.94
1:A:195:PHE:HE2	1:D:195:PHE:HE2	1.18	0.92
2:E:144:LYS:O	2:E:147:GLU:HG3	1.71	0.90
1:M:329:LYS:HE3	3:R:131:HIS:O	1.70	0.90
2:H:77:THR:HG22	2:H:79:GLU:H	1.36	0.89
2:N:138:PHE:CD2	2:N:187:PRO:HG3	2.07	0.89
2:E:236:PHE:HE2	3:F:25:VAL:HG12	1.37	0.88
1:M:410:ILE:HG23	1:M:414:ILE:HD12	1.57	0.87
1:M:12:ARG:O	1:M:17:LYS:HE2	1.74	0.86
1:A:142:THR:HG21	5:A:502:HEM:HBB2	1.55	0.86
1:M:195:PHE:HE2	1:P:195:PHE:HE2	1.20	0.85
2:K:42:MET:HE1	2:K:218:ALA:CB	2.07	0.85
2:N:142:PRO:HG2	2:N:150:GLU:OE2	1.77	0.85
2:E:223:LEU:HD21	2:E:227:LYS:HE3	1.58	0.85
2:B:250:ARG:HG2	3:C:12:ARG:HD3	1.58	0.85
1:J:424:ILE:HG13	13:J:1157:HOH:O	1.76	0.84
1:G:195:PHE:HE2	1:J:195:PHE:HE2	1.22	0.84
1:G:410:ILE:HG23	1:G:414:ILE:HD12	1.58	0.84
1:G:248:PHE:CD1	1:G:251:LYS:HD3	2.13	0.83
2:K:139:PRO:HG3	2:K:158:ARG:NH1	1.92	0.83
2:Q:149:HIS:CD2	2:Q:168:THR:HG21	2.13	0.83
2:E:149:HIS:CD2	2:E:168:THR:HG21	2.14	0.83
2:E:236:PHE:CE2	3:F:25:VAL:HG12	2.14	0.82
2:N:77:THR:HG22	2:N:79:GLU:N	1.95	0.82
1:D:135:ILE:HG21	5:D:501:HEM:HAB	1.61	0.81
1:G:9:TYR:HB2	1:G:30:TYR:CD2	2.14	0.81
2:E:15:GLY:H	9:E:1042:BGL:H5	1.46	0.81
1:D:246:PRO:HG2	2:E:251:LEU:HD21	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:138:PHE:CD2	2:E:187:PRO:HG3	2.18	0.79
2:K:138:PHE:CD2	2:K:187:PRO:HG3	2.17	0.79
1:G:248:PHE:HD1	1:G:251:LYS:HD3	1.46	0.79
2:K:149:HIS:CD2	2:K:168:THR:HG21	2.18	0.79
2:H:95:GLU:HG2	13:H:327:HOH:O	1.82	0.78
2:E:74:ASP:HB3	2:E:77:THR:HB	1.64	0.78
2:E:250:ARG:HG3	2:E:250:ARG:HH11	1.45	0.78
1:J:4:ILE:N	1:J:4:ILE:HD12	1.99	0.78
2:N:74:ASP:CB	2:N:77:THR:HB	2.14	0.77
2:Q:77:THR:HG22	2:Q:79:GLU:HB2	1.65	0.77
2:K:77:THR:HG22	2:K:79:GLU:H	1.50	0.77
3:O:131:HIS:O	1:P:329:LYS:HE3	1.84	0.77
2:B:42:MET:HE1	2:B:218:ALA:CB	2.14	0.76
2:H:250:ARG:NH1	3:I:12:ARG:HB2	2.00	0.76
2:H:77:THR:HG22	2:H:79:GLU:N	2.00	0.76
2:N:231:PHE:O	2:N:235:MET:HG2	1.84	0.76
2:K:42:MET:HE1	2:K:218:ALA:HB1	1.67	0.75
1:P:239:LYS:HE2	1:P:425:GLU:OE2	1.86	0.75
1:M:13:THR:O	1:M:17:LYS:HG3	1.87	0.75
2:N:183:ILE:HG23	2:N:185:MET:H	1.52	0.75
2:H:250:ARG:CZ	3:I:12:ARG:HB2	2.17	0.75
1:M:105:PHE:HA	1:M:108:VAL:HG22	1.69	0.74
1:G:239:LYS:HE2	1:G:425:GLU:OE2	1.87	0.74
1:G:261:LEU:HD11	2:H:234:VAL:HG13	1.69	0.74
1:D:12:ARG:O	1:D:17:LYS:HE2	1.88	0.74
1:P:9:TYR:HB2	1:P:30:TYR:CD2	2.23	0.74
1:M:4:ILE:HD12	1:M:4:ILE:H	1.53	0.74
2:N:40:HIS:ND1	2:N:97:ALA:HB1	2.03	0.73
1:G:4:ILE:HD12	1:G:4:ILE:H	1.49	0.73
1:A:9:TYR:HB2	1:A:30:TYR:CD2	2.23	0.73
2:E:77:THR:CG2	2:E:79:GLU:HB2	2.19	0.73
2:Q:223:LEU:CD2	2:Q:227:LYS:HE3	2.18	0.73
2:Q:138:PHE:CD2	2:Q:187:PRO:HG3	2.24	0.73
1:J:4:ILE:HD12	1:J:4:ILE:H	1.53	0.72
1:M:91:PHE:CD1	2:N:222:LYS:HG2	2.24	0.72
5:M:502:HEM:HMC1	5:M:502:HEM:HBC2	1.71	0.72
1:J:428:PHE:CE1	2:K:256:LYS:HD2	2.24	0.72
1:D:92:MET:HE1	2:E:226:ARG:HG3	1.70	0.72
1:M:9:TYR:HB2	1:M:30:TYR:CD2	2.24	0.72
1:D:213:ILE:HA	1:D:216:PHE:CE2	2.25	0.72
1:P:44:MET:HE3	7:P:1026:LOP:H92	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:142:THR:HG21	5:G:502:HEM:HBB2	1.70	0.72
1:P:213:ILE:HA	1:P:216:PHE:CE2	2.25	0.72
1:P:287:ARG:HG2	1:P:287:ARG:HH11	1.53	0.72
1:M:213:ILE:HA	1:M:216:PHE:CE2	2.26	0.71
1:J:213:ILE:HA	1:J:216:PHE:CE2	2.25	0.71
1:A:213:ILE:HA	1:A:216:PHE:CE2	2.26	0.71
3:C:47:LEU:HD23	3:C:47:LEU:O	1.91	0.71
1:G:213:ILE:HA	1:G:216:PHE:CE2	2.26	0.70
2:Q:59:PRO:HD2	2:Q:62:GLN:NE2	2.06	0.70
2:N:59:PRO:HD2	2:N:62:GLN:NE2	2.06	0.70
1:J:239:LYS:HE2	1:J:425:GLU:OE1	1.90	0.70
1:G:130:ILE:HD11	1:G:348:TRP:HH2	1.57	0.70
1:G:246:PRO:HG2	2:H:251:LEU:HD21	1.74	0.70
1:A:261:LEU:HD11	2:B:234:VAL:HG13	1.71	0.70
1:D:261:LEU:HD11	2:E:234:VAL:HG13	1.73	0.70
3:C:84:LEU:HD23	3:L:84:LEU:HD23	1.74	0.70
1:M:376:ILE:O	1:M:380:VAL:HG22	1.92	0.70
3:F:47:LEU:HD23	3:F:47:LEU:O	1.92	0.69
2:H:59:PRO:HD2	2:H:62:GLN:NE2	2.07	0.69
1:J:428:PHE:CZ	2:K:256:LYS:HB2	2.27	0.69
2:N:194:VAL:HB	2:N:207:MET:CE	2.21	0.69
1:P:130:ILE:HD11	1:P:348:TRP:HH2	1.57	0.69
2:K:59:PRO:HD2	2:K:62:GLN:NE2	2.06	0.69
1:M:269:PHE:HB3	9:N:1045:BGL:H1'2	1.75	0.69
1:A:130:ILE:HD11	1:A:348:TRP:HH2	1.56	0.69
2:E:59:PRO:HD2	2:E:62:GLN:NE2	2.07	0.69
1:J:130:ILE:HD11	1:J:348:TRP:HH2	1.57	0.69
3:F:112:GLN:H	3:F:112:GLN:NE2	1.91	0.69
1:M:8:HIS:CD2	1:M:8:HIS:H	2.09	0.69
1:A:287:ARG:HG2	1:A:287:ARG:HH11	1.57	0.69
2:B:59:PRO:HD2	2:B:62:GLN:NE2	2.07	0.69
1:P:91:PHE:CD1	2:Q:222:LYS:HG2	2.28	0.69
2:E:77:THR:HG22	2:E:79:GLU:H	1.58	0.69
5:A:501:HEM:HMC2	5:A:501:HEM:HBC2	1.75	0.68
2:E:42:MET:HE1	2:E:218:ALA:CB	2.23	0.68
1:A:374:PHE:HD2	7:A:1021:LOP:H321	1.57	0.68
2:N:40:HIS:CE1	2:N:97:ALA:HB1	2.28	0.68
1:A:376:ILE:O	1:A:380:VAL:HG22	1.93	0.68
1:D:130:ILE:HD11	1:D:348:TRP:HH2	1.57	0.68
1:J:376:ILE:O	1:J:380:VAL:HG22	1.92	0.68
1:P:261:LEU:HD11	2:Q:234:VAL:HG13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:376:ILE:O	1:P:380:VAL:HG22	1.92	0.68
1:D:376:ILE:O	1:D:380:VAL:HG22	1.93	0.68
1:G:376:ILE:O	1:G:380:VAL:HG22	1.93	0.68
1:A:92:MET:HE1	2:B:226:ARG:HG3	1.74	0.68
2:K:49:SER:HA	2:K:52:GLU:HG3	1.76	0.68
3:O:118:GLU:CD	3:O:118:GLU:H	2.02	0.68
1:M:130:ILE:HD11	1:M:348:TRP:HH2	1.57	0.68
1:A:105:PHE:HA	1:A:108:VAL:HG22	1.76	0.67
3:C:70:LYS:HE3	1:D:184:PRO:O	1.95	0.67
1:J:104:PHE:O	1:J:108:VAL:HG22	1.94	0.67
1:G:103:LEU:HD13	7:G:1023:LOP:H211	1.76	0.67
2:H:250:ARG:CZ	3:I:12:ARG:CB	2.72	0.67
1:M:230:ARG:HA	13:M:528:HOH:O	1.94	0.67
1:P:43:TRP:CZ3	1:P:251:LYS:HE3	2.30	0.67
2:B:74:ASP:HB3	2:B:77:THR:HB	1.76	0.66
1:M:118:TYR:OH	7:M:1025:LOP:H31	1.96	0.66
1:J:62:GLY:C	5:J:502:HEM:HAC	2.20	0.66
2:N:138:PHE:HD2	2:N:187:PRO:HG3	1.56	0.66
2:Q:194:VAL:HB	2:Q:207:MET:CE	2.22	0.66
1:A:246:PRO:HG2	2:B:251:LEU:HD21	1.76	0.66
1:M:261:LEU:HD11	2:N:234:VAL:HG13	1.78	0.66
3:O:118:GLU:CD	3:O:118:GLU:N	2.54	0.66
2:E:77:THR:HG22	2:E:79:GLU:N	2.11	0.65
3:L:112:GLN:H	3:L:112:GLN:NE2	1.93	0.65
1:M:142:THR:HG21	5:M:502:HEM:HBB2	1.76	0.65
1:A:125:ARG:CZ	1:A:222:ASN:HB2	2.25	0.65
2:N:224:MET:O	2:N:228:GLN:HG3	1.95	0.65
1:D:39:ARG:HH12	2:E:255:VAL:CG1	2.09	0.65
2:K:105:LYS:HD3	2:K:220:GLU:HG2	1.78	0.65
2:K:194:VAL:HB	2:K:207:MET:CE	2.23	0.65
1:J:199:TYR:HA	5:J:502:HEM:HBC2	1.78	0.65
2:Q:20:PHE:HB3	2:Q:25:LEU:HD11	1.78	0.65
2:B:26:GLN:HG2	2:B:58:LEU:HD21	1.79	0.65
2:H:20:PHE:HB3	2:H:25:LEU:HD11	1.79	0.65
1:M:39:ARG:HG2	1:M:242:VAL:HG13	1.79	0.65
1:D:39:ARG:HG2	1:D:242:VAL:HG13	1.78	0.65
2:E:26:GLN:HG2	2:E:58:LEU:HD21	1.79	0.65
1:J:24:PRO:HA	13:J:1105:HOH:O	1.96	0.65
1:P:39:ARG:HG2	1:P:242:VAL:HG13	1.78	0.65
3:R:112:GLN:H	3:R:112:GLN:NE2	1.95	0.65
1:J:91:PHE:CE2	1:J:92:MET:HE2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:26:GLN:HG2	2:K:58:LEU:HD21	1.79	0.65
1:M:92:MET:HE1	2:N:226:ARG:HG3	1.79	0.64
3:C:112:GLN:H	3:C:112:GLN:NE2	1.95	0.64
1:G:105:PHE:HA	1:G:108:VAL:HG22	1.78	0.64
1:J:105:PHE:HA	1:J:108:VAL:HG23	1.78	0.64
2:Q:128:PRO:HG2	2:Q:129:GLU:OE1	1.98	0.64
2:H:74:ASP:HB3	2:H:77:THR:HB	1.80	0.64
2:K:20:PHE:HB3	2:K:25:LEU:HD11	1.80	0.64
1:M:105:PHE:HA	1:M:108:VAL:CG2	2.26	0.64
1:J:180:LEU:HD22	6:J:1004:SMA:H26	1.78	0.64
2:N:20:PHE:HB3	2:N:25:LEU:HD11	1.78	0.64
2:N:26:GLN:HG2	2:N:58:LEU:HD21	1.80	0.64
1:D:103:LEU:HD13	7:D:1022:LOP:H201	1.79	0.64
2:H:194:VAL:HB	2:H:207:MET:CE	2.23	0.64
2:H:26:GLN:HG2	2:H:58:LEU:HD21	1.80	0.64
1:P:217:HIS:NE2	8:P:1106:UQ2:O4	2.31	0.64
2:Q:61:ASP:HA	2:Q:64:ARG:NH1	2.12	0.64
3:I:112:GLN:H	3:I:112:GLN:NE2	1.96	0.64
1:G:39:ARG:HG2	1:G:242:VAL:HG13	1.78	0.64
1:A:33:ILE:HG13	1:A:245:TRP:HB2	1.79	0.64
2:Q:26:GLN:HG2	2:Q:58:LEU:HD21	1.80	0.63
1:J:125:ARG:CZ	1:J:222:ASN:HB2	2.28	0.63
1:J:428:PHE:HZ	2:K:256:LYS:HB2	1.63	0.63
1:J:39:ARG:HG2	1:J:242:VAL:HG13	1.78	0.63
1:P:246:PRO:HG2	2:Q:251:LEU:HD21	1.80	0.63
1:A:39:ARG:HG2	1:A:242:VAL:HG13	1.79	0.63
1:D:33:ILE:HG13	1:D:245:TRP:HB2	1.79	0.63
1:G:33:ILE:HG13	1:G:245:TRP:HB2	1.80	0.63
2:K:142:PRO:HG2	2:K:150:GLU:OE2	1.98	0.63
2:E:250:ARG:HD3	3:F:12:ARG:HB3	1.80	0.63
2:E:20:PHE:HB3	2:E:25:LEU:HD11	1.81	0.63
1:P:33:ILE:HG13	1:P:245:TRP:HB2	1.81	0.63
2:H:142:PRO:HG2	2:H:150:GLU:OE2	1.98	0.63
3:I:131:HIS:O	1:J:329:LYS:HE3	1.99	0.63
2:K:66:TYR:O	2:K:69:GLN:HG2	1.98	0.63
1:P:39:ARG:HH12	2:Q:255:VAL:CG1	2.11	0.62
1:M:117:TYR:CE2	7:M:1025:LOP:H32	2.34	0.62
1:G:39:ARG:HH12	2:H:255:VAL:CG1	2.11	0.62
1:J:33:ILE:HG13	1:J:245:TRP:HB2	1.80	0.62
1:M:132:GLY:C	5:M:501:HEM:HBC2	2.25	0.62
1:J:103:LEU:HD13	7:J:1024:LOP:H211	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:269:PHE:HB3	9:G:1043:BGL:H1'2	1.81	0.62
1:J:4:ILE:H	1:J:4:ILE:CD1	2.12	0.62
2:B:20:PHE:HB3	2:B:25:LEU:HD11	1.81	0.62
1:D:43:TRP:CZ3	1:D:251:LYS:HG2	2.35	0.62
1:D:269:PHE:HB3	9:E:1042:BGL:H1'2	1.80	0.62
2:B:194:VAL:HB	2:B:207:MET:CE	2.24	0.61
2:K:108:ALA:HA	2:K:125:ILE:HG22	1.83	0.61
1:A:374:PHE:CD2	7:A:1021:LOP:H321	2.35	0.61
1:G:199:TYR:CD2	5:G:502:HEM:HBC1	2.35	0.61
1:D:24:PRO:HA	13:D:1103:HOH:O	2.01	0.61
1:D:10:GLU:OE2	1:D:11:PRO:HD2	2.00	0.61
1:M:33:ILE:HG13	1:M:245:TRP:HB2	1.81	0.61
3:O:47:LEU:HD23	3:O:47:LEU:O	2.00	0.61
2:E:72:VAL:HG12	2:E:73:THR:N	2.16	0.61
2:N:171:ASP:OD2	2:N:175:VAL:HB	2.01	0.61
2:B:167:ASP:OD1	2:B:167:ASP:N	2.28	0.61
3:C:83:GLU:OE1	3:C:83:GLU:HA	2.00	0.61
2:H:256:LYS:O	2:H:256:LYS:HG2	2.00	0.61
2:K:189:LEU:O	2:K:190:MET:HB2	2.00	0.60
1:P:105:PHE:HA	1:P:108:VAL:HG22	1.82	0.60
1:A:39:ARG:HH12	2:B:255:VAL:CG1	2.15	0.60
2:B:129:GLU:OE1	2:B:129:GLU:N	2.27	0.60
2:N:142:PRO:CG	2:N:150:GLU:OE2	2.49	0.60
3:O:112:GLN:H	3:O:112:GLN:NE2	1.99	0.60
2:B:149:HIS:CD2	2:B:168:THR:HG21	2.37	0.60
1:G:306:ARG:HG3	13:G:1156:HOH:O	2.01	0.60
3:L:80:ALA:O	3:L:84:LEU:HG	2.01	0.60
2:B:250:ARG:HD3	3:C:12:ARG:CG	2.26	0.60
2:N:71:THR:CG2	2:N:80:ASP:HB3	2.32	0.59
2:H:77:THR:HG21	2:H:79:GLU:HB2	1.83	0.59
1:A:103:LEU:HD13	7:A:1021:LOP:H211	1.84	0.59
1:J:425:GLU:HG3	1:J:429:ASN:HD21	1.67	0.59
1:P:406:VAL:O	1:P:409:PRO:HD2	2.01	0.59
1:A:287:ARG:HG2	1:A:287:ARG:NH1	2.16	0.59
2:B:56:PRO:HD2	13:B:1044:HOH:O	2.01	0.59
2:E:223:LEU:CD2	2:E:227:LYS:HE3	2.30	0.59
2:Q:129:GLU:OE1	2:Q:129:GLU:N	2.36	0.59
2:K:77:THR:HG22	2:K:79:GLU:N	2.16	0.59
2:E:144:LYS:HE2	2:E:144:LYS:HA	1.84	0.59
1:J:144:PHE:HD1	13:J:1113:HOH:O	1.86	0.58
2:Q:77:THR:CG2	2:Q:79:GLU:HB2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:406:VAL:O	1:G:409:PRO:HD2	2.02	0.58
1:M:221:ASN:HD21	8:M:1105:UQ2:H3M1	1.68	0.58
1:M:4:ILE:HD12	1:M:4:ILE:N	2.18	0.58
2:Q:77:THR:C	2:Q:79:GLU:H	2.11	0.58
3:O:10:THR:HG22	3:O:10:THR:O	2.04	0.58
1:A:92:MET:CE	2:B:226:ARG:HG3	2.33	0.58
1:D:68:HIS:ND1	13:D:1105:HOH:O	2.32	0.58
1:D:91:PHE:CE2	1:D:92:MET:HE3	2.39	0.58
1:D:249:ILE:O	1:D:253:VAL:HG23	2.04	0.58
3:I:55:SER:HB3	3:I:182:THR:OG1	2.04	0.58
3:R:10:THR:O	3:R:10:THR:HG22	2.04	0.58
1:A:249:ILE:O	1:A:253:VAL:HG23	2.04	0.57
2:E:194:VAL:HB	2:E:207:MET:CE	2.24	0.57
1:D:43:TRP:CH2	1:D:251:LYS:HG2	2.39	0.57
1:J:351:THR:OG1	1:J:412:GLY:HA3	2.04	0.57
2:Q:114:MET:HE3	2:Q:114:MET:HA	1.85	0.57
3:L:55:SER:HB3	3:L:182:THR:OG1	2.04	0.57
2:N:19:THR:HB	2:N:224:MET:HE3	1.87	0.57
3:O:55:SER:HB3	3:O:182:THR:OG1	2.04	0.57
3:F:55:SER:HB3	3:F:182:THR:OG1	2.04	0.57
1:M:39:ARG:HH12	2:N:255:VAL:CG1	2.17	0.57
3:C:55:SER:HB3	3:C:182:THR:OG1	2.05	0.57
1:D:91:PHE:HE2	1:D:92:MET:HE3	1.69	0.57
3:F:10:THR:HG22	3:F:10:THR:O	2.04	0.57
2:K:51:SER:OG	2:K:63:VAL:HG21	2.05	0.57
1:D:105:PHE:HA	1:D:108:VAL:HG22	1.86	0.57
1:J:105:PHE:HA	1:J:108:VAL:CG2	2.35	0.57
1:J:261:LEU:HD11	2:K:234:VAL:HG13	1.87	0.57
2:N:71:THR:HG22	2:N:80:ASP:HB3	1.87	0.57
1:G:199:TYR:CE2	5:G:502:HEM:HBC1	2.40	0.57
2:Q:49:SER:HA	2:Q:52:GLU:HG3	1.87	0.56
3:R:55:SER:HB3	3:R:182:THR:OG1	2.05	0.56
1:A:114:ARG:C	1:A:114:ARG:HD2	2.30	0.56
1:J:114:ARG:HD2	1:J:114:ARG:C	2.31	0.56
1:M:411:LEU:O	1:M:415:GLU:HG2	2.04	0.56
1:A:5:PRO:HB2	1:A:234:LYS:HA	1.87	0.56
3:C:10:THR:O	3:C:10:THR:HG22	2.05	0.56
1:D:406:VAL:O	1:D:409:PRO:HD2	2.05	0.56
1:G:158:GLY:O	1:G:162:ILE:HD12	2.04	0.56
1:G:248:PHE:HA	1:G:251:LYS:HG2	1.87	0.56
3:I:10:THR:HG22	3:I:10:THR:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:10:THR:HG22	3:L:10:THR:O	2.05	0.56
5:M:502:HEM:HMC1	5:M:502:HEM:CBC	2.36	0.56
2:N:138:PHE:CE1	2:N:157:ASN:ND2	2.73	0.56
1:P:114:ARG:HD2	1:P:114:ARG:C	2.31	0.56
2:H:77:THR:CG2	2:H:79:GLU:HB2	2.36	0.56
1:J:5:PRO:HB2	1:J:234:LYS:HA	1.86	0.56
1:J:246:PRO:HG2	2:K:251:LEU:HD21	1.86	0.56
1:M:125:ARG:CZ	1:M:222:ASN:HB2	2.35	0.56
2:Q:72:VAL:HG12	2:Q:73:THR:N	2.21	0.56
1:D:217:HIS:NE2	8:D:1102:UQ2:O4	2.26	0.56
1:P:351:THR:OG1	1:P:412:GLY:HA3	2.05	0.56
1:A:12:ARG:O	1:A:17:LYS:HE2	2.05	0.56
1:A:359:TYR:CD2	1:A:420:PRO:HB3	2.41	0.56
2:B:145:CYS:O	2:B:168:THR:OG1	2.21	0.56
1:M:114:ARG:C	1:M:114:ARG:HD2	2.31	0.56
2:N:220:GLU:OE2	2:N:226:ARG:NH1	2.39	0.56
1:G:184:PRO:O	3:L:70:LYS:HE3	2.05	0.56
2:Q:81:ARG:HG3	2:Q:81:ARG:HH11	1.70	0.56
1:G:114:ARG:HD2	1:G:114:ARG:C	2.30	0.56
3:C:131:HIS:O	1:D:329:LYS:HE3	2.06	0.56
1:P:43:TRP:HZ3	1:P:251:LYS:HE3	1.69	0.56
1:D:114:ARG:HD2	1:D:114:ARG:C	2.31	0.56
1:G:383:GLN:HE22	2:H:115:GLY:HA3	1.71	0.56
1:J:249:ILE:O	1:J:253:VAL:HG23	2.06	0.55
2:N:42:MET:HE1	2:N:218:ALA:CB	2.35	0.55
1:P:236:GLU:HA	1:P:239:LYS:CD	2.36	0.55
1:J:199:TYR:CD2	5:J:502:HEM:HBC1	2.42	0.55
1:J:132:GLY:C	5:J:501:HEM:HBC2	2.31	0.55
1:D:144:PHE:CD1	1:D:162:ILE:HD12	2.40	0.55
2:K:114:MET:O	2:K:114:MET:HG2	2.05	0.55
1:A:358:ARG:HH21	7:A:1021:LOP:H21	1.71	0.55
1:G:4:ILE:HD12	1:G:4:ILE:N	2.19	0.55
1:P:199:TYR:CD2	5:P:502:HEM:HBC1	2.41	0.55
2:E:56:PRO:HD2	13:E:1045:HOH:O	2.06	0.55
1:A:58:GLN:CB	5:A:502:HEM:HAB	2.37	0.55
2:B:250:ARG:CD	3:C:12:ARG:HG2	2.28	0.55
1:D:13:THR:HG22	1:D:14:GLY:N	2.22	0.55
1:P:287:ARG:HG2	1:P:287:ARG:NH1	2.21	0.55
1:A:195:PHE:CE2	1:D:195:PHE:HE2	2.10	0.55
2:B:27:ARG:HD2	2:B:196:TYR:CE2	2.42	0.55
2:Q:246:LEU:O	2:Q:250:ARG:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:MET:CE	2:E:226:ARG:HG3	2.35	0.55
1:M:246:PRO:HG2	2:N:251:LEU:HD21	1.88	0.54
1:P:244:PHE:CE1	8:P:1106:UQ2:H2M2	2.42	0.54
3:R:89:GLN:O	3:R:92:GLN:HB2	2.07	0.54
2:Q:66:TYR:CE1	2:Q:70:PHE:HE2	2.24	0.54
1:D:359:TYR:CD2	1:D:420:PRO:HB3	2.43	0.54
2:E:169:CYS:O	2:E:177:THR:HB	2.06	0.54
2:E:142:PRO:HG2	2:E:150:GLU:OE2	2.07	0.54
2:H:146:ALA:O	2:H:148:GLY:N	2.41	0.54
1:J:226:GLY:HA2	1:J:355:ARG:HD2	1.89	0.54
1:M:249:ILE:O	1:M:253:VAL:HG23	2.07	0.54
1:P:406:VAL:C	1:P:409:PRO:HD2	2.33	0.54
2:B:141:GLU:O	2:B:141:GLU:HG3	2.07	0.54
1:D:13:THR:HG22	1:D:14:GLY:H	1.72	0.54
2:E:250:ARG:CD	3:F:12:ARG:HB3	2.36	0.54
1:G:185:ALA:HB2	3:L:70:LYS:HG3	1.87	0.54
1:G:249:ILE:O	1:G:253:VAL:HG23	2.06	0.54
1:P:269:PHE:HB3	9:P:1046:BGL:H1'2	1.89	0.54
2:Q:169:CYS:O	2:Q:177:THR:HB	2.08	0.54
2:B:42:MET:CE	2:B:218:ALA:CB	2.85	0.54
2:B:169:CYS:O	2:B:177:THR:HB	2.08	0.54
1:M:362:MET:CB	1:M:411:LEU:HD21	2.38	0.54
1:A:5:PRO:HB3	1:A:234:LYS:HG2	1.90	0.54
1:A:13:THR:HG22	1:A:14:GLY:N	2.22	0.54
2:N:128:PRO:HG2	2:N:129:GLU:OE1	2.08	0.54
1:G:13:THR:HG22	1:G:14:GLY:H	1.73	0.54
1:M:8:HIS:CD2	1:M:8:HIS:N	2.73	0.54
1:M:122:LYS:O	1:M:123:ALA:C	2.51	0.54
1:P:249:ILE:O	1:P:253:VAL:HG23	2.07	0.54
2:Q:236:PHE:CE1	3:R:25:VAL:CG1	2.90	0.54
2:E:66:TYR:O	2:E:69:GLN:HG2	2.07	0.54
1:A:195:PHE:HE2	1:D:195:PHE:CE2	2.10	0.53
2:B:128:PRO:HG2	2:B:129:GLU:OE1	2.08	0.53
1:D:346:VAL:HG12	1:D:347:PRO:HD3	1.90	0.53
1:A:13:THR:O	1:A:17:LYS:HG3	2.08	0.53
2:B:149:HIS:CE1	2:B:168:THR:HG21	2.43	0.53
1:G:13:THR:HG22	1:G:14:GLY:N	2.23	0.53
2:N:146:ALA:O	2:N:148:GLY:N	2.40	0.53
3:O:90:LEU:HD11	3:O:108:GLU:HB3	1.90	0.53
1:P:112:ILE:HG12	5:P:501:HEM:HAC	1.90	0.53
1:A:217:HIS:NE2	8:A:1101:UQ2:O4	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:146:ALA:O	2:K:148:GLY:N	2.41	0.53
1:M:13:THR:HG22	1:M:14:GLY:N	2.24	0.53
1:M:234:LYS:O	1:M:238:GLN:HG3	2.09	0.53
2:Q:146:ALA:O	2:Q:148:GLY:N	2.41	0.53
1:A:13:THR:HG22	1:A:14:GLY:H	1.72	0.53
1:J:13:THR:HG22	1:J:14:GLY:N	2.23	0.53
2:B:49:SER:HA	2:B:52:GLU:HG3	1.89	0.53
2:B:146:ALA:O	2:B:148:GLY:N	2.41	0.53
2:E:66:TYR:CE1	2:E:70:PHE:HE2	2.26	0.53
1:M:346:VAL:HG12	1:M:347:PRO:HD3	1.91	0.53
1:M:362:MET:HB2	1:M:411:LEU:HD21	1.91	0.53
2:E:81:ARG:HG3	2:E:81:ARG:HH11	1.74	0.53
1:G:58:GLN:CB	5:G:502:HEM:HAB	2.38	0.53
1:J:13:THR:HG22	1:J:14:GLY:H	1.73	0.53
2:Q:144:LYS:HZ3	2:Q:144:LYS:CA	1.97	0.53
1:A:184:PRO:O	3:F:70:LYS:HE3	2.08	0.53
1:D:39:ARG:NH1	2:E:255:VAL:CG1	2.72	0.53
1:G:33:ILE:HG13	1:G:245:TRP:CB	2.39	0.53
2:N:169:CYS:O	2:N:177:THR:HB	2.08	0.53
1:P:199:TYR:CE2	5:P:502:HEM:HBC1	2.44	0.53
2:Q:142:PRO:HB3	2:Q:150:GLU:OE2	2.09	0.53
1:D:9:TYR:HB2	1:D:30:TYR:CD2	2.44	0.52
1:D:199:TYR:CZ	5:D:502:HEM:HBC1	2.43	0.52
1:J:428:PHE:CZ	2:K:256:LYS:HD2	2.43	0.52
2:K:169:CYS:O	2:K:177:THR:HB	2.09	0.52
2:E:40:HIS:ND1	2:E:97:ALA:HB1	2.23	0.52
2:H:128:PRO:HG2	2:H:129:GLU:OE1	2.09	0.52
1:J:346:VAL:HG12	1:J:347:PRO:HD3	1.90	0.52
2:K:77:THR:HG22	2:K:79:GLU:CB	2.40	0.52
1:P:13:THR:HG22	1:P:14:GLY:N	2.23	0.52
1:P:33:ILE:HG13	1:P:245:TRP:CB	2.39	0.52
2:B:220:GLU:OE2	2:B:226:ARG:NH1	2.43	0.52
2:E:189:LEU:O	2:E:190:MET:HB2	2.10	0.52
1:J:234:LYS:O	1:J:238:GLN:HG3	2.09	0.52
1:M:13:THR:HG22	1:M:14:GLY:H	1.74	0.52
1:M:352:SER:HB2	1:M:415:GLU:OE2	2.09	0.52
1:A:33:ILE:HG13	1:A:245:TRP:CB	2.39	0.52
2:E:146:ALA:O	2:E:148:GLY:N	2.43	0.52
2:K:74:ASP:HB3	2:K:77:THR:CB	2.29	0.52
1:P:346:VAL:HG12	1:P:347:PRO:HD3	1.90	0.52
2:B:77:THR:C	2:B:79:GLU:H	2.16	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:HIS:ND1	2:B:205:HIS:C	2.68	0.52
3:C:84:LEU:CD2	3:L:84:LEU:HD23	2.39	0.52
1:D:33:ILE:HG13	1:D:245:TRP:CB	2.39	0.52
1:G:144:PHE:CD1	1:G:162:ILE:HD13	2.43	0.52
1:G:217:HIS:NE2	8:G:1103:UQ2:O4	2.36	0.52
1:J:199:TYR:CE2	5:J:502:HEM:HBC1	2.45	0.52
1:M:33:ILE:HG13	1:M:245:TRP:CB	2.39	0.52
3:C:70:LYS:HG3	1:D:185:ALA:HB2	1.92	0.52
1:D:150:PRO:HG3	5:D:502:HEM:O2D	2.10	0.52
2:E:74:ASP:CB	2:E:77:THR:HB	2.35	0.52
1:J:229:VAL:HG22	1:J:424:ILE:HD12	1.92	0.52
3:O:80:ALA:O	3:O:84:LEU:HG	2.09	0.52
1:P:32:THR:HG23	1:P:217:HIS:HE1	1.74	0.52
2:B:171:ASP:OD1	2:B:173:ASN:N	2.37	0.52
2:E:250:ARG:CZ	3:F:12:ARG:HG2	2.40	0.52
1:J:269:PHE:HB3	9:K:1044:BGL:H1'2	1.92	0.52
2:K:185:MET:HB2	5:K:301:HEM:C1D	2.45	0.52
1:P:13:THR:HG22	1:P:14:GLY:H	1.74	0.52
1:G:346:VAL:HG12	1:G:347:PRO:HD3	1.91	0.52
2:K:42:MET:CE	2:K:218:ALA:HB1	2.38	0.52
1:M:236:GLU:HA	1:M:239:LYS:CD	2.40	0.52
1:M:236:GLU:HA	1:M:239:LYS:HD3	1.92	0.52
1:M:58:GLN:CB	5:M:502:HEM:HAB	2.39	0.52
1:P:39:ARG:NH1	2:Q:255:VAL:CG1	2.72	0.52
1:A:346:VAL:HG12	1:A:347:PRO:HD3	1.91	0.51
2:E:77:THR:C	2:E:79:GLU:H	2.17	0.51
1:G:195:PHE:CE2	1:J:195:PHE:HE2	2.13	0.51
2:H:114:MET:O	2:H:114:MET:HG2	2.10	0.51
1:J:33:ILE:HG13	1:J:245:TRP:CB	2.39	0.51
2:N:160:PHE:CE2	2:N:183:ILE:HG13	2.44	0.51
2:N:205:HIS:ND1	2:N:205:HIS:C	2.69	0.51
1:A:154:MET:HE2	1:A:154:MET:HA	1.93	0.51
2:E:77:THR:HG22	2:E:79:GLU:HB2	1.92	0.51
1:J:142:THR:HG21	5:J:502:HEM:HBB2	1.92	0.51
2:E:205:HIS:ND1	2:E:205:HIS:C	2.68	0.51
2:H:205:HIS:ND1	2:H:205:HIS:C	2.69	0.51
2:B:224:MET:O	2:B:228:GLN:HG3	2.11	0.51
1:G:125:ARG:NE	1:G:222:ASN:HB2	2.25	0.51
2:H:250:ARG:CZ	3:I:12:ARG:HB3	2.40	0.51
2:E:42:MET:CE	2:E:218:ALA:CB	2.89	0.51
1:G:132:GLY:C	5:G:501:HEM:HBC2	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:501:HEM:HBB2	5:D:501:HEM:CMB	2.41	0.51
2:H:169:CYS:O	2:H:177:THR:HB	2.11	0.51
2:K:40:HIS:HE1	2:K:98:PRO:HD2	1.76	0.51
1:G:125:ARG:HD2	13:G:1118:HOH:O	2.11	0.50
2:Q:66:TYR:CE1	2:Q:70:PHE:CE2	3.00	0.50
2:H:220:GLU:OE2	2:H:226:ARG:NH1	2.44	0.50
2:H:250:ARG:NH1	3:I:12:ARG:CB	2.73	0.50
1:J:39:ARG:HH12	2:K:255:VAL:CG1	2.25	0.50
1:M:133:MET:N	5:M:501:HEM:HBC2	2.27	0.50
1:G:5:PRO:HB3	1:G:234:LYS:HG2	1.93	0.50
1:A:383:GLN:HE22	2:B:115:GLY:HA3	1.76	0.50
1:G:154:MET:HA	1:G:154:MET:HE2	1.94	0.50
1:D:91:PHE:CD1	2:E:222:LYS:HG2	2.46	0.50
2:Q:205:HIS:ND1	2:Q:205:HIS:C	2.69	0.50
2:B:108:ALA:HA	2:B:125:ILE:HG22	1.93	0.50
1:G:92:MET:HE1	2:H:226:ARG:HG3	1.92	0.50
2:K:205:HIS:ND1	2:K:205:HIS:C	2.68	0.50
2:N:176:LYS:O	2:N:176:LYS:HD3	2.11	0.50
3:C:57:VAL:HG22	3:C:63:LEU:HD13	1.94	0.50
2:E:66:TYR:CE1	2:E:70:PHE:CE2	2.99	0.50
1:P:94:ARG:C	1:P:94:ARG:HD3	2.37	0.50
1:P:312:VAL:HG12	1:P:314:VAL:HG12	1.94	0.50
3:I:70:LYS:HE3	1:J:185:ALA:HB2	1.92	0.50
1:M:125:ARG:NH1	1:M:222:ASN:HB2	2.27	0.50
2:N:149:HIS:CD2	2:N:168:THR:HG21	2.46	0.50
2:Q:236:PHE:CE1	3:R:25:VAL:HG12	2.46	0.50
1:D:92:MET:HE1	2:E:226:ARG:CG	2.40	0.50
2:E:42:MET:CE	2:E:218:ALA:HB1	2.42	0.50
2:H:149:HIS:CE1	2:H:168:THR:HG21	2.47	0.50
1:P:11:PRO:HB2	1:P:17:LYS:HG2	1.94	0.50
1:G:236:GLU:HA	1:G:239:LYS:HG3	1.92	0.49
2:H:154:PHE:HB3	2:H:182:TRP:HB3	1.94	0.49
3:L:157:ASP:HB2	13:L:505:HOH:O	2.12	0.49
1:A:266:ILE:HD12	1:A:270:MET:HE2	1.94	0.49
2:E:40:HIS:CE1	2:E:97:ALA:HB1	2.47	0.49
2:Q:220:GLU:OE2	2:Q:226:ARG:NH1	2.45	0.49
3:R:70:LYS:HB2	3:R:70:LYS:NZ	2.27	0.49
2:B:171:ASP:OD1	2:B:171:ASP:C	2.56	0.49
1:G:5:PRO:CB	1:G:234:LYS:HG2	2.42	0.49
2:H:76:GLU:O	2:H:77:THR:C	2.55	0.49
2:K:234:VAL:HG12	2:K:235:MET:HE2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:128:THR:HG21	5:P:501:HEM:HBD1	1.94	0.49
1:J:236:GLU:HA	1:J:239:LYS:CD	2.41	0.49
2:K:236:PHE:CE1	3:L:25:VAL:HG12	2.47	0.49
2:N:143:PRO:HG3	2:N:178:THR:CG2	2.42	0.49
1:P:248:PHE:CD1	1:P:251:LYS:HD3	2.48	0.49
1:P:354:VAL:HG21	1:P:417:PRO:CB	2.42	0.49
3:C:59:PRO:HD3	3:C:76:ARG:NH1	2.28	0.49
2:K:154:PHE:HB3	2:K:182:TRP:HB3	1.94	0.49
2:N:149:HIS:CG	2:N:168:THR:HG21	2.47	0.49
2:Q:151:PRO:HD2	2:Q:182:TRP:CD1	2.47	0.49
1:D:43:TRP:HA	1:D:43:TRP:CE3	2.48	0.49
1:M:235:ALA:O	1:M:239:LYS:HG3	2.13	0.49
2:N:183:ILE:HG23	2:N:185:MET:N	2.24	0.49
3:F:57:VAL:HG22	3:F:63:LEU:HD13	1.95	0.49
1:G:266:ILE:HD12	1:G:270:MET:HE2	1.95	0.49
3:R:59:PRO:HD3	3:R:76:ARG:NH1	2.28	0.49
3:F:118:GLU:CD	3:F:118:GLU:N	2.70	0.49
1:M:92:MET:CE	2:N:226:ARG:HG3	2.42	0.49
1:J:266:ILE:HD12	1:J:270:MET:HE2	1.95	0.49
2:K:49:SER:HA	2:K:52:GLU:CG	2.43	0.49
1:G:362:MET:N	1:G:415:GLU:OE2	2.45	0.49
2:K:231:PHE:O	2:K:235:MET:HG2	2.13	0.49
1:A:92:MET:HE1	2:B:226:ARG:CG	2.41	0.48
1:D:39:ARG:HH12	2:E:255:VAL:HG12	1.76	0.48
1:P:32:THR:HG23	1:P:217:HIS:CE1	2.48	0.48
1:D:102:SER:O	1:D:106:ILE:HG13	2.13	0.48
2:H:250:ARG:NH1	3:I:16:TYR:CZ	2.81	0.48
1:M:406:VAL:O	1:M:409:PRO:HD2	2.12	0.48
1:D:4:ILE:HD12	1:D:4:ILE:N	2.28	0.48
2:N:197:ALA:C	2:N:199:GLY:H	2.22	0.48
3:I:59:PRO:HD3	3:I:76:ARG:NH1	2.28	0.48
2:K:145:CYS:O	2:K:168:THR:OG1	2.28	0.48
1:P:132:GLY:C	5:P:501:HEM:HBC2	2.38	0.48
2:Q:130:TYR:OH	5:Q:301:HEM:O2A	2.17	0.48
3:R:57:VAL:HG22	3:R:63:LEU:HD13	1.94	0.48
1:D:154:MET:HE2	1:D:154:MET:HA	1.94	0.48
1:D:266:ILE:HD12	1:D:270:MET:HE2	1.94	0.48
1:G:125:ARG:CZ	1:G:222:ASN:HB2	2.43	0.48
1:G:406:VAL:C	1:G:409:PRO:HD2	2.38	0.48
9:G:1043:BGL:H5	2:H:15:GLY:H	1.77	0.48
2:N:72:VAL:O	2:N:80:ASP:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:184:ALA:HB3	5:N:301:HEM:HBD2	1.95	0.48
2:B:149:HIS:NE2	2:B:168:THR:HG21	2.28	0.48
3:F:47:LEU:O	3:F:47:LEU:CD2	2.61	0.48
1:G:39:ARG:NH1	2:H:255:VAL:CG1	2.76	0.48
1:J:154:MET:HE2	1:J:154:MET:HA	1.96	0.48
1:G:58:GLN:HB3	5:G:502:HEM:HAB	1.95	0.48
1:G:105:PHE:HA	1:G:108:VAL:CG2	2.44	0.48
1:J:91:PHE:HE2	1:J:92:MET:CE	2.26	0.48
1:J:355:ARG:HG3	1:J:355:ARG:HH11	1.79	0.48
3:L:57:VAL:HG22	3:L:63:LEU:HD13	1.94	0.48
2:N:154:PHE:HB3	2:N:182:TRP:HB3	1.95	0.48
3:F:90:LEU:HD11	3:F:108:GLU:HB3	1.95	0.48
1:M:51:LEU:HB3	5:M:501:HEM:HMB1	1.96	0.48
2:N:42:MET:CE	2:N:218:ALA:CB	2.91	0.48
2:Q:73:THR:HG23	2:Q:80:ASP:OD1	2.13	0.48
1:G:312:VAL:HG12	1:G:314:VAL:HG12	1.96	0.48
1:M:346:VAL:CG1	1:M:347:PRO:HD3	2.44	0.48
1:P:91:PHE:CE2	1:P:92:MET:HE3	2.48	0.48
2:E:72:VAL:CG1	2:E:73:THR:N	2.76	0.48
3:I:57:VAL:HG22	3:I:63:LEU:HD13	1.95	0.48
3:L:59:PRO:HD3	3:L:76:ARG:NH1	2.29	0.48
3:L:90:LEU:HD11	3:L:108:GLU:HB3	1.96	0.48
1:M:266:ILE:HD12	1:M:270:MET:HE2	1.96	0.48
2:N:74:ASP:CG	2:N:77:THR:HB	2.39	0.48
2:N:108:ALA:HA	2:N:125:ILE:O	2.14	0.48
2:Q:185:MET:HB2	5:Q:301:HEM:C1D	2.49	0.48
2:Q:197:ALA:C	2:Q:199:GLY:H	2.21	0.48
1:D:43:TRP:O	1:D:46:ILE:HG12	2.14	0.47
1:J:51:LEU:HB3	5:J:501:HEM:HMB1	1.96	0.47
3:O:59:PRO:HD3	3:O:76:ARG:NH1	2.29	0.47
2:Q:81:ARG:HG3	2:Q:81:ARG:NH1	2.29	0.47
2:Q:141:GLU:H	2:Q:141:GLU:HG2	1.49	0.47
1:A:236:GLU:HA	1:A:239:LYS:HD3	1.97	0.47
1:G:346:VAL:CG1	1:G:347:PRO:HD3	2.44	0.47
2:K:42:MET:HE2	2:K:101:SER:HA	1.95	0.47
1:M:4:ILE:H	1:M:4:ILE:CD1	2.24	0.47
1:M:425:GLU:O	1:M:429:ASN:ND2	2.47	0.47
1:P:43:TRP:HA	1:P:43:TRP:CE3	2.49	0.47
1:D:246:PRO:CG	2:E:251:LEU:HD21	2.41	0.47
2:E:142:PRO:CG	2:E:150:GLU:OE2	2.62	0.47
3:F:59:PRO:HD3	3:F:76:ARG:NH1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:248:PHE:CE1	1:G:251:LYS:HD3	2.48	0.47
3:I:66:LYS:HE2	3:I:69:GLY:HA2	1.96	0.47
2:K:197:ALA:C	2:K:199:GLY:H	2.23	0.47
1:M:6:HIS:ND1	1:M:6:HIS:C	2.71	0.47
1:P:346:VAL:CG1	1:P:347:PRO:HD3	2.44	0.47
1:A:346:VAL:CG1	1:A:347:PRO:HD3	2.45	0.47
2:B:42:MET:CE	2:B:218:ALA:HB1	2.45	0.47
2:E:40:HIS:HE1	2:E:98:PRO:HD2	1.79	0.47
3:I:84:LEU:O	3:I:88:VAL:HG23	2.14	0.47
1:J:91:PHE:CE2	1:J:92:MET:CE	2.97	0.47
2:K:220:GLU:OE2	2:K:226:ARG:NH1	2.48	0.47
1:M:43:TRP:CZ3	1:M:251:LYS:HE2	2.50	0.47
1:M:154:MET:HE2	1:M:154:MET:HA	1.95	0.47
3:O:57:VAL:HG22	3:O:63:LEU:HD13	1.95	0.47
2:Q:19:THR:CG2	2:Q:224:MET:HE3	2.45	0.47
3:R:62:GLN:NE2	3:R:73:PHE:CD1	2.83	0.47
1:A:360:ARG:O	1:A:364:LYS:HG3	2.14	0.47
1:M:10:GLU:HA	1:M:11:PRO:HD3	1.70	0.47
2:N:103:MET:C	2:N:105:LYS:H	2.21	0.47
1:P:177:GLN:NE2	13:P:611:HOH:O	2.40	0.47
1:P:266:ILE:HD12	1:P:270:MET:HE2	1.96	0.47
1:A:43:TRP:CZ3	1:A:251:LYS:HE3	2.50	0.47
1:D:346:VAL:CG1	1:D:347:PRO:HD3	2.44	0.47
1:J:407:ILE:O	1:J:411:LEU:HG	2.14	0.47
1:M:113:PHE:HB3	7:M:1025:LOP:H261	1.95	0.47
2:Q:236:PHE:CE1	3:R:25:VAL:HG11	2.49	0.47
1:A:199:TYR:CD2	5:A:502:HEM:HBC1	2.50	0.47
1:G:39:ARG:HD3	1:G:428:PHE:CD2	2.50	0.47
1:J:217:HIS:NE2	8:J:1104:UQ2:O4	2.46	0.47
1:J:346:VAL:CG1	1:J:347:PRO:HD3	2.44	0.47
3:O:47:LEU:HD23	3:O:47:LEU:C	2.39	0.47
1:A:118:TYR:OH	7:A:1021:LOP:H32	2.15	0.47
1:D:423:THR:OG1	1:D:426:GLU:HB2	2.14	0.47
2:N:157:ASN:O	2:N:180:GLY:HA3	2.15	0.47
1:J:128:THR:HG21	5:J:501:HEM:HBD1	1.97	0.47
1:M:92:MET:CE	1:M:92:MET:HA	2.45	0.47
1:M:195:PHE:HE2	1:P:195:PHE:CE2	2.12	0.47
2:Q:157:ASN:O	2:Q:180:GLY:HA3	2.15	0.47
2:Q:226:ARG:HD3	13:Q:672:HOH:O	2.14	0.47
1:A:123:ALA:O	1:A:355:ARG:NH1	2.48	0.47
5:A:501:HEM:HMC2	5:A:501:HEM:CBC	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:43:TRP:HA	1:G:43:TRP:CE3	2.50	0.47
2:E:185:MET:HB2	5:E:301:HEM:C1D	2.50	0.46
2:K:77:THR:HG22	2:K:79:GLU:HG3	1.97	0.46
3:L:66:LYS:HD3	3:L:69:GLY:HA2	1.96	0.46
1:M:30:TYR:HA	1:M:33:ILE:HG22	1.97	0.46
3:O:47:LEU:HG	3:O:68:LEU:HD21	1.97	0.46
1:D:406:VAL:C	1:D:409:PRO:HD2	2.40	0.46
2:E:76:GLU:O	2:E:77:THR:C	2.57	0.46
1:G:30:TYR:HA	1:G:33:ILE:HG22	1.98	0.46
1:J:30:TYR:HA	1:J:33:ILE:HG22	1.97	0.46
1:M:106:ILE:HG13	1:M:296:TRP:CH2	2.50	0.46
1:M:410:ILE:HG23	1:M:414:ILE:CD1	2.37	0.46
2:Q:145:CYS:O	2:Q:168:THR:OG1	2.26	0.46
1:A:39:ARG:NH1	2:B:255:VAL:CG1	2.79	0.46
1:A:234:LYS:O	1:A:238:GLN:HG3	2.16	0.46
2:B:147:GLU:OE1	2:B:147:GLU:HA	2.14	0.46
1:M:49:VAL:HG21	1:M:252:ASP:OD2	2.15	0.46
2:N:81:ARG:NH1	2:N:84:LYS:HG3	2.30	0.46
1:P:122:LYS:O	1:P:123:ALA:C	2.58	0.46
9:P:1046:BGL:H5	2:Q:15:GLY:H	1.81	0.46
3:R:39:ASN:HB3	13:R:676:HOH:O	2.14	0.46
1:D:30:TYR:HA	1:D:33:ILE:HG22	1.98	0.46
1:D:269:PHE:HB3	9:E:1042:BGL:O1	2.15	0.46
2:N:155:TYR:CZ	2:N:186:PRO:HB3	2.50	0.46
3:O:58:GLU:N	3:O:58:GLU:CD	2.74	0.46
1:A:30:TYR:HA	1:A:33:ILE:HG22	1.98	0.46
2:B:155:TYR:CZ	2:B:186:PRO:HB3	2.51	0.46
3:I:58:GLU:N	3:I:58:GLU:CD	2.73	0.46
1:J:354:VAL:HG21	1:J:417:PRO:CB	2.46	0.46
1:J:414:ILE:O	1:J:414:ILE:CG2	2.62	0.46
2:Q:154:PHE:C	2:Q:155:TYR:CD1	2.94	0.46
1:A:122:LYS:O	1:A:123:ALA:C	2.59	0.46
2:B:165:VAL:CG1	2:B:169:CYS:HB2	2.46	0.46
1:D:4:ILE:O	1:D:6:HIS:HD2	1.99	0.46
1:D:51:LEU:CD2	1:D:108:VAL:HG13	2.46	0.46
1:G:244:PHE:CE1	8:G:1103:UQ2:H2M2	2.51	0.46
2:H:165:VAL:CG1	2:H:169:CYS:HB2	2.45	0.46
2:K:155:TYR:CZ	2:K:186:PRO:HB3	2.51	0.46
1:M:359:TYR:CD2	1:M:420:PRO:HB3	2.51	0.46
2:B:90:PRO:HA	13:B:1046:HOH:O	2.15	0.46
1:G:111:HIS:CD2	5:G:501:HEM:NC	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:234:LYS:O	1:G:238:GLN:HG3	2.15	0.46
2:Q:154:PHE:HB3	2:Q:182:TRP:HB3	1.98	0.46
2:Q:223:LEU:HD21	2:Q:227:LYS:CE	2.32	0.46
3:R:58:GLU:CD	3:R:58:GLU:N	2.73	0.46
2:E:144:LYS:HE2	2:E:144:LYS:CA	2.46	0.46
1:G:43:TRP:CZ3	1:G:251:LYS:HE3	2.49	0.46
2:H:113:PRO:O	2:H:114:MET:HB3	2.16	0.46
3:I:131:HIS:O	1:J:329:LYS:CE	2.64	0.46
1:J:236:GLU:HA	1:J:239:LYS:HD3	1.98	0.46
1:J:362:MET:HE1	1:J:414:ILE:HG22	1.97	0.46
2:K:77:THR:HG22	2:K:79:GLU:CG	2.46	0.46
2:K:157:ASN:O	2:K:180:GLY:HA3	2.16	0.46
2:K:246:LEU:O	2:K:250:ARG:HG2	2.16	0.46
3:L:58:GLU:N	3:L:58:GLU:CD	2.73	0.46
1:M:58:GLN:HB3	5:M:502:HEM:HAB	1.96	0.46
1:P:154:MET:HE2	1:P:154:MET:HA	1.97	0.46
2:Q:72:VAL:CG1	2:Q:73:THR:N	2.79	0.46
3:F:58:GLU:CD	3:F:58:GLU:N	2.74	0.46
2:H:149:HIS:N	2:H:149:HIS:CD2	2.83	0.46
1:J:122:LYS:O	1:J:123:ALA:C	2.59	0.46
2:K:77:THR:CG2	2:K:79:GLU:HB2	2.46	0.46
2:Q:27:ARG:HD2	2:Q:196:TYR:CE2	2.51	0.46
3:C:90:LEU:HB2	2:H:172:ALA:HB1	1.98	0.45
1:P:30:TYR:HA	1:P:33:ILE:HG22	1.98	0.45
2:E:155:TYR:CZ	2:E:186:PRO:HB3	2.51	0.45
2:H:155:TYR:CZ	2:H:186:PRO:HB3	2.51	0.45
2:H:197:ALA:C	2:H:199:GLY:H	2.23	0.45
1:J:291:HIS:O	1:J:293:VAL:HG23	2.16	0.45
1:J:322:SER:O	1:J:323:PHE:HB2	2.16	0.45
1:P:291:HIS:O	1:P:293:VAL:HG23	2.16	0.45
2:Q:155:TYR:CZ	2:Q:186:PRO:HB3	2.51	0.45
1:A:244:PHE:CE1	8:A:1101:UQ2:H2M3	2.51	0.45
1:A:291:HIS:O	1:A:293:VAL:HG23	2.16	0.45
2:B:154:PHE:C	2:B:155:TYR:CD1	2.94	0.45
3:C:58:GLU:CD	3:C:58:GLU:N	2.73	0.45
2:E:40:HIS:HB3	2:E:100:LEU:HG	1.98	0.45
2:E:145:CYS:O	2:E:168:THR:OG1	2.27	0.45
2:N:154:PHE:C	2:N:155:TYR:CD1	2.94	0.45
2:Q:77:THR:C	2:Q:79:GLU:N	2.73	0.45
2:B:77:THR:HG22	2:B:79:GLU:CG	2.47	0.45
2:E:42:MET:HE1	2:E:218:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:250:ARG:HG3	2:E:250:ARG:NH1	2.23	0.45
2:E:250:ARG:NH2	3:F:15:LEU:HD22	2.31	0.45
1:G:125:ARG:HH21	1:G:221:ASN:C	2.23	0.45
2:H:250:ARG:NH1	3:I:16:TYR:CE1	2.84	0.45
1:M:150:PRO:HG3	5:M:502:HEM:O2D	2.16	0.45
2:N:152:ASP:C	2:N:152:ASP:OD1	2.59	0.45
2:Q:236:PHE:HE1	3:R:25:VAL:HG11	1.81	0.45
1:A:58:GLN:HB3	5:A:502:HEM:HAB	1.98	0.45
2:B:197:ALA:C	2:B:199:GLY:H	2.24	0.45
2:E:141:GLU:O	2:E:141:GLU:HG3	2.16	0.45
2:E:157:ASN:O	2:E:180:GLY:HA3	2.16	0.45
1:G:418:VAL:CG1	1:G:419:ALA:N	2.80	0.45
2:E:146:ALA:O	2:E:147:GLU:C	2.59	0.45
2:E:154:PHE:C	2:E:155:TYR:CD1	2.94	0.45
2:E:197:ALA:C	2:E:199:GLY:H	2.23	0.45
1:G:23:LEU:HD13	1:J:215:ALA:HA	1.98	0.45
1:G:428:PHE:CE1	2:H:256:LYS:HD3	2.51	0.45
2:H:157:ASN:O	2:H:180:GLY:HA3	2.16	0.45
2:H:185:MET:HB2	5:H:301:HEM:C1D	2.52	0.45
2:H:203:SER:O	2:H:204:VAL:C	2.60	0.45
1:J:209:VAL:HG22	5:J:501:HEM:HBB2	1.98	0.45
2:K:154:PHE:C	2:K:155:TYR:CD1	2.94	0.45
1:M:291:HIS:O	1:M:293:VAL:HG23	2.16	0.45
2:N:48:ARG:HB3	2:N:85:PRO:O	2.17	0.45
2:B:77:THR:HG22	2:B:79:GLU:HB2	1.99	0.45
2:E:203:SER:O	2:E:204:VAL:C	2.60	0.45
2:H:68:THR:HG23	2:H:82:GLU:OE1	2.16	0.45
1:J:6:HIS:ND1	1:J:6:HIS:C	2.75	0.45
3:L:118:GLU:N	3:L:118:GLU:CD	2.75	0.45
1:M:415:GLU:O	1:M:417:PRO:HD3	2.17	0.45
2:N:77:THR:CG2	2:N:79:GLU:HB2	2.46	0.45
2:N:250:ARG:HH11	3:O:12:ARG:HA	1.80	0.45
1:P:118:TYR:OH	7:P:1026:LOP:H32	2.17	0.45
2:Q:42:MET:HE2	2:Q:218:ALA:HB1	1.99	0.45
1:D:51:LEU:HD21	1:D:108:VAL:HG13	1.98	0.45
2:H:48:ARG:HB3	2:H:85:PRO:O	2.17	0.45
1:P:162:ILE:CG2	6:P:1006:SMA:H21	2.46	0.45
3:R:142:GLY:HA3	13:R:691:HOH:O	2.16	0.45
2:B:157:ASN:O	2:B:180:GLY:HA3	2.17	0.45
1:G:13:THR:O	1:G:17:LYS:HG3	2.17	0.45
1:G:291:HIS:O	1:G:293:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:154:PHE:C	2:H:155:TYR:CD1	2.95	0.45
2:Q:19:THR:HB	2:Q:224:MET:HE3	1.98	0.45
1:D:44:MET:HE3	7:D:1022:LOP:H92	1.99	0.45
2:E:250:ARG:HH11	2:E:250:ARG:CG	2.19	0.45
1:G:118:TYR:OH	7:G:1023:LOP:H32	2.15	0.45
2:N:51:SER:OG	2:N:63:VAL:HG21	2.17	0.45
1:D:291:HIS:O	1:D:293:VAL:HG23	2.16	0.44
1:G:47:TRP:CZ2	1:G:110:LEU:HD13	2.53	0.44
2:K:203:SER:O	2:K:204:VAL:C	2.60	0.44
1:P:102:SER:O	1:P:106:ILE:HG13	2.16	0.44
1:G:121:TYR:HB3	1:G:129:TRP:CE3	2.53	0.44
1:G:416:LYS:HA	1:G:416:LYS:HD3	1.63	0.44
1:D:47:TRP:CZ2	1:D:110:LEU:HD13	2.53	0.44
1:G:106:ILE:HD12	7:G:1023:LOP:H212	1.99	0.44
2:H:235:MET:HA	2:H:235:MET:HE2	1.99	0.44
2:K:144:LYS:C	2:K:147:GLU:HG3	2.38	0.44
2:K:171:ASP:CG	2:K:172:ALA:N	2.75	0.44
1:A:418:VAL:CG1	1:A:419:ALA:N	2.80	0.44
2:B:223:LEU:CD2	2:B:227:LYS:HD2	2.46	0.44
2:H:138:PHE:CD2	2:H:187:PRO:HG3	2.51	0.44
3:I:14:PHE:O	3:I:17:TYR:HB3	2.17	0.44
1:J:130:ILE:HD11	1:J:348:TRP:CH2	2.46	0.44
1:J:209:VAL:CG2	5:J:501:HEM:HBB2	2.48	0.44
2:N:203:SER:O	2:N:204:VAL:C	2.61	0.44
3:R:140:VAL:O	3:R:140:VAL:HG12	2.16	0.44
1:A:47:TRP:CZ2	1:A:110:LEU:HD13	2.53	0.44
1:G:428:PHE:CZ	2:H:256:LYS:HB3	2.52	0.44
2:H:146:ALA:O	2:H:147:GLU:C	2.60	0.44
1:J:406:VAL:O	1:J:409:PRO:HD2	2.18	0.44
1:M:39:ARG:NH1	2:N:255:VAL:CG1	2.80	0.44
1:P:427:ASP:O	1:P:430:ALA:HB3	2.18	0.44
2:Q:17:PHE:CE1	2:Q:231:PHE:CZ	3.04	0.44
2:K:236:PHE:HE1	3:L:25:VAL:CG1	2.30	0.44
1:A:121:TYR:HB3	1:A:129:TRP:CE3	2.52	0.44
1:A:125:ARG:HH21	1:A:221:ASN:C	2.26	0.44
1:G:133:MET:SD	5:G:501:HEM:HBC1	2.58	0.44
2:K:146:ALA:O	2:K:147:GLU:C	2.60	0.44
3:O:47:LEU:O	3:O:47:LEU:CD2	2.64	0.44
2:Q:48:ARG:HB3	2:Q:85:PRO:O	2.17	0.44
1:A:8:HIS:CD2	1:A:8:HIS:H	2.36	0.44
2:B:113:PRO:HD2	2:B:118:ILE:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:SER:O	2:B:204:VAL:C	2.59	0.44
1:D:49:VAL:HG23	8:D:1102:UQ2:H2M3	1.99	0.44
2:K:144:LYS:HA	2:K:147:GLU:HG3	1.99	0.44
3:L:143:ASP:OD2	3:L:164:LYS:NZ	2.51	0.44
1:M:387:PHE:CE1	1:M:388:PRO:HB3	2.53	0.44
2:Q:74:ASP:HB3	2:Q:77:THR:HB	2.00	0.44
2:B:19:THR:HB	2:B:224:MET:HE3	2.00	0.43
1:D:121:TYR:HB3	1:D:129:TRP:CE3	2.53	0.43
2:H:222:LYS:HB2	13:H:347:HOH:O	2.18	0.43
1:M:425:GLU:HG2	1:M:429:ASN:HD21	1.82	0.43
1:A:106:ILE:HD12	7:A:1021:LOP:H212	1.99	0.43
2:B:15:GLY:H	9:B:1041:BGL:H1	1.82	0.43
2:E:113:PRO:HD2	2:E:118:ILE:HB	2.00	0.43
1:G:132:GLY:O	5:G:501:HEM:HMC3	2.18	0.43
3:I:12:ARG:H	3:I:12:ARG:HG2	1.60	0.43
1:J:226:GLY:CA	1:J:355:ARG:HD2	2.49	0.43
2:N:111:HIS:HE1	13:N:552:HOH:O	2.00	0.43
1:P:10:GLU:HA	1:P:11:PRO:HD3	1.69	0.43
1:P:248:PHE:HD1	1:P:251:LYS:HD3	1.82	0.43
2:Q:146:ALA:O	2:Q:147:GLU:C	2.60	0.43
3:R:77:ARG:HB3	3:R:81:ASP:HB2	2.00	0.43
1:G:92:MET:CE	1:G:92:MET:HA	2.47	0.43
2:H:223:LEU:HD21	2:H:227:LYS:CE	2.49	0.43
1:J:43:TRP:HE3	1:J:43:TRP:HA	1.83	0.43
3:L:118:GLU:CD	3:L:118:GLU:H	2.27	0.43
2:B:146:ALA:O	2:B:147:GLU:C	2.59	0.43
2:E:34:GLU:OE1	2:E:194:VAL:HG22	2.19	0.43
1:J:262:VAL:HG13	9:K:1044:BGL:H8'1	1.99	0.43
2:K:48:ARG:HB3	2:K:85:PRO:O	2.17	0.43
1:M:195:PHE:CE2	1:P:195:PHE:HE2	2.12	0.43
2:N:146:ALA:O	2:N:147:GLU:C	2.61	0.43
1:P:105:PHE:HA	1:P:108:VAL:CG2	2.48	0.43
5:P:502:HEM:CBC	5:P:502:HEM:HHD	2.48	0.43
2:B:144:LYS:O	2:B:145:CYS:C	2.61	0.43
3:C:84:LEU:HD23	3:C:84:LEU:HA	1.81	0.43
1:D:355:ARG:CD	13:D:1155:HOH:O	2.66	0.43
3:I:179:ILE:HD13	3:I:179:ILE:HA	1.74	0.43
2:K:40:HIS:HB3	2:K:100:LEU:HG	2.00	0.43
2:K:141:GLU:HA	2:K:142:PRO:HD3	1.76	0.43
1:P:43:TRP:HA	1:P:43:TRP:HE3	1.84	0.43
3:R:10:THR:O	3:R:14:PHE:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:62:GLN:NE2	3:R:73:PHE:CG	2.87	0.43
2:H:141:GLU:HG2	13:H:338:HOH:O	2.19	0.43
2:N:149:HIS:CD2	2:N:168:THR:OG1	2.70	0.43
3:O:140:VAL:O	3:O:140:VAL:HG12	2.17	0.43
1:P:359:TYR:CD2	1:P:420:PRO:HB3	2.53	0.43
2:H:77:THR:HG23	2:H:79:GLU:OE2	2.19	0.43
1:J:43:TRP:HA	1:J:43:TRP:CE3	2.54	0.43
8:M:1105:UQ2:H3M3	8:M:1105:UQ2:H2M2	2.01	0.43
1:P:47:TRP:CZ2	1:P:110:LEU:HD13	2.53	0.43
2:Q:144:LYS:NZ	2:Q:147:GLU:OE1	2.51	0.43
1:A:105:PHE:HA	1:A:108:VAL:CG2	2.45	0.43
2:B:34:GLU:OE1	2:B:194:VAL:HG22	2.18	0.43
2:B:155:TYR:CD1	2:B:155:TYR:N	2.87	0.43
1:J:359:TYR:CD2	1:J:420:PRO:HB3	2.54	0.43
2:K:155:TYR:CD1	2:K:155:TYR:N	2.87	0.43
2:K:165:VAL:CG1	2:K:169:CYS:HB2	2.48	0.43
1:M:427:ASP:O	1:M:430:ALA:HB3	2.18	0.43
1:P:92:MET:HA	1:P:92:MET:HE2	2.01	0.43
1:P:360:ARG:O	1:P:364:LYS:HG3	2.19	0.43
1:A:45:TRP:CZ3	1:A:224:PRO:HG3	2.53	0.43
3:C:14:PHE:O	3:C:17:TYR:HB3	2.18	0.43
2:E:144:LYS:HD3	2:E:147:GLU:OE2	2.18	0.43
2:E:220:GLU:OE2	2:E:226:ARG:NH1	2.52	0.43
1:G:45:TRP:CZ3	1:G:224:PRO:HG3	2.54	0.43
2:H:155:TYR:CD1	2:H:155:TYR:N	2.87	0.43
1:J:47:TRP:CZ2	1:J:110:LEU:HD13	2.53	0.43
1:J:121:TYR:HB3	1:J:129:TRP:CE3	2.53	0.43
2:K:113:PRO:HD2	2:K:118:ILE:HB	2.01	0.43
3:L:77:ARG:HB3	3:L:81:ASP:HB2	2.01	0.43
2:N:74:ASP:C	2:N:76:GLU:H	2.27	0.43
1:P:45:TRP:CZ3	1:P:224:PRO:HG3	2.54	0.43
1:A:406:VAL:O	1:A:409:PRO:HD2	2.19	0.43
1:G:306:ARG:NH2	1:G:383:GLN:O	2.40	0.43
1:J:45:TRP:CZ3	1:J:224:PRO:HG3	2.54	0.43
1:J:111:HIS:CD2	5:J:501:HEM:NC	2.87	0.43
1:M:47:TRP:CZ2	1:M:110:LEU:HD13	2.53	0.43
2:N:34:GLU:OE1	2:N:194:VAL:HG22	2.19	0.43
3:R:59:PRO:HD3	3:R:76:ARG:HH11	1.83	0.43
1:A:140:MET:HE1	1:A:340:ILE:HD13	2.01	0.42
1:D:428:PHE:CZ	2:E:256:LYS:HB2	2.53	0.42
5:D:501:HEM:HBC2	5:D:501:HEM:HMC2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:155:TYR:CD1	2:E:155:TYR:N	2.86	0.42
2:K:107:ARG:HH21	5:K:301:HEM:CGA	2.32	0.42
3:L:59:PRO:HD3	3:L:76:ARG:HH11	1.84	0.42
1:M:10:GLU:OE2	1:M:11:PRO:HD2	2.19	0.42
1:M:350:ASP:HB2	1:M:408:LEU:HD13	2.01	0.42
3:O:44:VAL:C	3:O:46:ALA:H	2.27	0.42
2:B:48:ARG:HB3	2:B:85:PRO:O	2.19	0.42
3:C:59:PRO:HD3	3:C:76:ARG:HH11	1.84	0.42
3:C:138:GLY:O	3:C:141:SER:OG	2.32	0.42
1:D:79:SER:O	1:D:83:ILE:HG13	2.20	0.42
2:H:34:GLU:OE1	2:H:194:VAL:HG22	2.19	0.42
2:N:42:MET:HE2	2:N:218:ALA:HB1	2.00	0.42
2:Q:34:GLU:OE1	2:Q:194:VAL:HG22	2.19	0.42
2:Q:42:MET:CE	2:Q:218:ALA:CB	2.97	0.42
2:Q:171:ASP:OD1	2:Q:171:ASP:C	2.61	0.42
1:A:79:SER:O	1:A:83:ILE:HG13	2.19	0.42
1:D:133:MET:SD	5:D:501:HEM:HBC1	2.59	0.42
1:G:91:PHE:CD1	2:H:222:LYS:HG2	2.54	0.42
1:M:123:ALA:O	1:M:355:ARG:NH1	2.53	0.42
2:N:189:LEU:C	2:N:204:VAL:HG22	2.44	0.42
3:R:124:VAL:O	3:R:173:ILE:HG23	2.19	0.42
2:B:185:MET:HB2	5:B:301:HEM:C1D	2.54	0.42
1:J:112:ILE:HG12	5:J:501:HEM:HAC	2.00	0.42
2:K:34:GLU:OE1	2:K:194:VAL:HG22	2.19	0.42
1:M:394:LEU:HD23	1:M:394:LEU:HA	1.89	0.42
3:R:179:ILE:HD13	3:R:179:ILE:HA	1.74	0.42
2:B:42:MET:HE1	2:B:218:ALA:HB2	1.98	0.42
1:D:236:GLU:HA	1:D:239:LYS:HD2	2.02	0.42
1:G:387:PHE:CD1	1:G:387:PHE:C	2.98	0.42
2:H:113:PRO:HD2	2:H:118:ILE:HB	2.00	0.42
3:L:124:VAL:O	3:L:173:ILE:HG23	2.20	0.42
3:C:126:TRP:C	3:C:128:VAL:H	2.28	0.42
1:M:121:TYR:HB3	1:M:129:TRP:CE3	2.54	0.42
3:C:179:ILE:CG1	3:C:185:GLN:HE21	2.33	0.42
1:D:45:TRP:CZ3	1:D:224:PRO:HG3	2.54	0.42
2:E:236:PHE:CE2	3:F:25:VAL:CG1	2.95	0.42
1:G:394:LEU:HD23	1:G:394:LEU:HA	1.89	0.42
3:I:126:TRP:C	3:I:128:VAL:H	2.27	0.42
1:J:418:VAL:CG1	1:J:419:ALA:N	2.83	0.42
2:Q:183:ILE:HG12	2:Q:185:MET:H	1.85	0.42
1:D:39:ARG:NH1	2:E:255:VAL:HG12	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:MET:HE1	1:D:340:ILE:HD13	2.00	0.42
1:G:140:MET:HE1	1:G:340:ILE:HD13	2.02	0.42
3:I:59:PRO:HD3	3:I:76:ARG:HH11	1.84	0.42
1:J:4:ILE:HA	1:J:5:PRO:HD3	1.88	0.42
2:N:68:THR:HG23	2:N:82:GLU:HB3	2.01	0.42
2:N:155:TYR:CD1	2:N:155:TYR:N	2.87	0.42
2:N:250:ARG:NH1	3:O:12:ARG:HA	2.33	0.42
1:P:37:THR:O	1:P:38:PRO:C	2.62	0.42
1:P:121:TYR:HB3	1:P:129:TRP:CE3	2.54	0.42
2:Q:42:MET:HE1	2:Q:218:ALA:CB	2.49	0.42
2:Q:155:TYR:CD1	2:Q:155:TYR:N	2.87	0.42
3:R:179:ILE:CG1	3:R:185:GLN:HE21	2.33	0.42
1:G:92:MET:CE	2:H:226:ARG:HG3	2.50	0.42
1:G:359:TYR:CD2	1:G:420:PRO:HB3	2.55	0.42
1:J:108:VAL:HG21	1:J:139:MET:HE1	2.02	0.42
1:M:105:PHE:O	1:M:108:VAL:HG23	2.20	0.42
1:M:215:ALA:HA	1:P:23:LEU:HD13	2.01	0.42
1:M:239:LYS:HE2	1:M:425:GLU:OE2	2.20	0.42
2:N:94:LEU:HD22	5:N:301:HEM:HAC	2.01	0.42
1:P:234:LYS:O	1:P:238:GLN:HG3	2.19	0.42
2:Q:165:VAL:CG1	2:Q:169:CYS:HB2	2.50	0.42
1:A:291:HIS:CE1	2:B:2:GLY:HA2	2.54	0.42
1:D:92:MET:HA	1:D:92:MET:HE2	2.02	0.42
1:D:364:LYS:O	1:D:368:TRP:HD1	2.02	0.42
2:E:30:GLN:HG2	2:E:34:GLU:OE2	2.20	0.42
2:E:250:ARG:NH1	2:E:250:ARG:CG	2.82	0.42
3:F:13:ASP:O	3:F:17:TYR:HD2	2.02	0.42
3:F:77:ARG:HB3	3:F:81:ASP:HB2	2.01	0.42
1:G:102:SER:O	1:G:106:ILE:HG13	2.20	0.42
2:H:145:CYS:O	2:H:168:THR:OG1	2.28	0.42
3:I:77:ARG:HB3	3:I:81:ASP:HB2	2.01	0.42
1:J:108:VAL:CG2	1:J:139:MET:HE1	2.50	0.42
2:K:72:VAL:CG1	2:K:73:THR:N	2.83	0.42
3:L:179:ILE:HD13	3:L:179:ILE:HA	1.74	0.42
1:M:45:TRP:CZ3	1:M:224:PRO:HG3	2.54	0.42
1:M:262:VAL:O	1:M:266:ILE:HG12	2.20	0.42
1:M:362:MET:HB3	1:M:411:LEU:HD21	2.02	0.42
2:N:143:PRO:HG3	2:N:178:THR:HG21	2.02	0.42
2:Q:42:MET:HE3	2:Q:215:LEU:CD2	2.50	0.42
3:L:179:ILE:CG1	3:L:185:GLN:HE21	2.33	0.41
1:M:239:LYS:HB3	1:M:425:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:314:VAL:H	1:M:314:VAL:HG23	1.63	0.41
2:N:20:PHE:CB	2:N:25:LEU:HD11	2.48	0.41
3:R:126:TRP:C	3:R:128:VAL:H	2.28	0.41
1:A:355:ARG:HD3	13:A:1122:HOH:O	2.19	0.41
2:B:40:HIS:HB3	2:B:100:LEU:HG	2.02	0.41
3:C:77:ARG:HB3	3:C:81:ASP:HB2	2.02	0.41
2:E:48:ARG:HB3	2:E:85:PRO:O	2.19	0.41
2:E:154:PHE:HB3	2:E:182:TRP:HB3	2.01	0.41
3:F:124:VAL:O	3:F:173:ILE:HG23	2.20	0.41
1:G:39:ARG:HH12	2:H:255:VAL:HG12	1.82	0.41
2:H:141:GLU:HA	2:H:142:PRO:HD3	1.87	0.41
3:I:89:GLN:O	3:I:90:LEU:C	2.63	0.41
1:M:34:MET:O	1:M:35:ILE:C	2.63	0.41
2:N:160:PHE:CG	2:N:183:ILE:HD12	2.55	0.41
3:O:44:VAL:O	3:O:46:ALA:N	2.53	0.41
1:P:394:LEU:HA	1:P:394:LEU:HD23	1.89	0.41
2:B:19:THR:CG2	2:B:224:MET:HE3	2.50	0.41
1:D:135:ILE:CG2	5:D:501:HEM:HAB	2.42	0.41
1:D:261:LEU:CD1	2:E:234:VAL:HG13	2.46	0.41
2:H:171:ASP:C	2:H:171:ASP:OD1	2.62	0.41
3:I:124:VAL:O	3:I:173:ILE:HG23	2.19	0.41
2:K:48:ARG:HG3	2:K:48:ARG:HH11	1.86	0.41
2:N:94:LEU:CD2	5:N:301:HEM:HAC	2.49	0.41
1:A:111:HIS:CD2	5:A:501:HEM:NC	2.89	0.41
1:D:233:SER:O	1:D:234:LYS:C	2.62	0.41
1:D:394:LEU:HD23	1:D:394:LEU:HA	1.90	0.41
1:D:408:LEU:HD23	1:D:408:LEU:HA	1.89	0.41
3:I:162:ILE:HD11	3:I:164:LYS:O	2.21	0.41
1:M:92:MET:HA	1:M:92:MET:HE3	2.01	0.41
1:M:322:SER:O	1:M:325:ILE:HD12	2.21	0.41
2:N:42:MET:HE1	2:N:218:ALA:HB2	2.03	0.41
2:N:113:PRO:HD2	2:N:118:ILE:HB	2.02	0.41
3:O:124:VAL:O	3:O:173:ILE:HG23	2.20	0.41
1:P:408:LEU:HD23	1:P:408:LEU:HA	1.91	0.41
2:Q:20:PHE:CB	2:Q:25:LEU:HD11	2.48	0.41
2:Q:203:SER:O	2:Q:204:VAL:C	2.60	0.41
3:C:47:LEU:O	3:C:47:LEU:CD2	2.63	0.41
2:E:189:LEU:O	2:E:190:MET:CB	2.68	0.41
2:H:30:GLN:HG2	2:H:34:GLU:OE2	2.20	0.41
1:J:140:MET:HE1	1:J:340:ILE:HD13	2.01	0.41
2:N:176:LYS:HG2	2:N:178:THR:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:77:ARG:HB3	3:O:81:ASP:HB2	2.01	0.41
1:P:132:GLY:HA3	5:P:501:HEM:HBC2	2.02	0.41
2:Q:149:HIS:CG	2:Q:168:THR:HG21	2.53	0.41
1:D:306:ARG:HG3	13:D:1150:HOH:O	2.19	0.41
1:J:10:GLU:HA	1:J:11:PRO:HD3	1.87	0.41
1:J:262:VAL:O	1:J:266:ILE:HG12	2.21	0.41
2:K:30:GLN:HG2	2:K:34:GLU:OE2	2.21	0.41
2:N:143:PRO:HG3	2:N:178:THR:HG22	2.03	0.41
2:Q:48:ARG:HH11	2:Q:48:ARG:HG3	1.86	0.41
3:R:70:LYS:HB2	3:R:70:LYS:HZ3	1.84	0.41
1:J:199:TYR:CG	5:J:502:HEM:HBC1	2.56	0.41
1:J:250:ILE:HD12	2:K:251:LEU:CD2	2.51	0.41
3:O:162:ILE:HD11	3:O:164:LYS:O	2.20	0.41
1:P:354:VAL:HG21	1:P:417:PRO:HB2	2.03	0.41
2:Q:30:GLN:HG2	2:Q:34:GLU:OE2	2.21	0.41
2:Q:223:LEU:HD23	2:Q:223:LEU:C	2.45	0.41
2:Q:242:VAL:O	2:Q:246:LEU:HG	2.21	0.41
1:A:239:LYS:HE2	1:A:425:GLU:OE1	2.21	0.41
1:D:122:LYS:O	1:D:123:ALA:C	2.64	0.41
3:F:126:TRP:C	3:F:128:VAL:H	2.29	0.41
1:G:51:LEU:HB3	5:G:501:HEM:HMB1	2.03	0.41
1:J:37:THR:O	1:J:38:PRO:C	2.63	0.41
1:J:43:TRP:CZ3	1:J:251:LYS:HD3	2.55	0.41
1:J:64:VAL:HG11	1:J:93:LEU:HD13	2.02	0.41
1:J:133:MET:N	5:J:501:HEM:HBC2	2.36	0.41
2:N:48:ARG:HH11	2:N:48:ARG:HG3	1.86	0.41
3:O:54:VAL:O	3:O:54:VAL:HG13	2.20	0.41
1:A:130:ILE:HD11	1:A:348:TRP:CH2	2.46	0.41
2:B:30:GLN:HG2	2:B:34:GLU:OE2	2.20	0.41
2:B:77:THR:HG22	2:B:79:GLU:HG3	2.02	0.41
3:C:124:VAL:O	3:C:173:ILE:HG23	2.21	0.41
1:D:37:THR:O	1:D:38:PRO:C	2.64	0.41
1:D:132:GLY:C	5:D:501:HEM:HBC2	2.46	0.41
1:D:250:ILE:HD12	2:E:251:LEU:CD2	2.50	0.41
2:H:129:GLU:OE1	2:H:129:GLU:N	2.42	0.41
2:H:223:LEU:HD21	2:H:227:LYS:HE3	2.03	0.41
1:J:51:LEU:HD13	5:J:501:HEM:C3B	2.55	0.41
2:K:19:THR:HB	2:K:224:MET:HE3	2.03	0.41
2:K:189:LEU:O	2:K:190:MET:CB	2.69	0.41
3:L:171:LEU:HA	3:L:172:PRO:HD3	1.95	0.41
1:M:37:THR:O	1:M:38:PRO:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:64:VAL:HG11	1:M:93:LEU:HD13	2.03	0.41
1:M:75:LEU:O	1:M:79:SER:HB3	2.21	0.41
2:N:40:HIS:HB3	2:N:100:LEU:HG	2.02	0.41
2:N:103:MET:C	2:N:105:LYS:N	2.78	0.41
1:P:130:ILE:HD11	1:P:348:TRP:CH2	2.47	0.41
1:A:193:ARG:NH1	3:F:38:MET:HG2	2.36	0.41
2:B:77:THR:HG22	2:B:79:GLU:CB	2.51	0.41
2:E:61:ASP:OD1	2:E:61:ASP:N	2.53	0.41
3:F:54:VAL:O	3:F:54:VAL:HG13	2.20	0.41
1:G:75:LEU:O	1:G:79:SER:HB3	2.21	0.41
2:H:74:ASP:CB	2:H:77:THR:HB	2.51	0.41
3:I:179:ILE:CG1	3:I:185:GLN:HE21	2.33	0.41
1:J:425:GLU:HG3	1:J:429:ASN:ND2	2.33	0.41
2:N:242:VAL:O	2:N:246:LEU:HG	2.21	0.41
1:P:43:TRP:O	1:P:46:ILE:HG12	2.20	0.41
1:P:287:ARG:NH1	1:P:287:ARG:CG	2.83	0.41
2:Q:53:PRO:HA	2:Q:57:GLU:CD	2.46	0.41
2:Q:113:PRO:HD2	2:Q:118:ILE:HB	2.03	0.41
1:A:64:VAL:HG11	1:A:93:LEU:HD13	2.02	0.40
2:B:154:PHE:HB3	2:B:182:TRP:HB3	2.03	0.40
1:D:236:GLU:O	1:D:239:LYS:HB2	2.20	0.40
1:G:37:THR:O	1:G:38:PRO:C	2.63	0.40
1:G:43:TRP:O	1:G:46:ILE:HG12	2.22	0.40
2:H:40:HIS:HB3	2:H:100:LEU:HG	2.03	0.40
2:H:250:ARG:NH2	3:I:12:ARG:HB2	2.35	0.40
1:M:106:ILE:HG13	1:M:296:TRP:CZ2	2.56	0.40
3:O:59:PRO:HD3	3:O:76:ARG:HH11	1.85	0.40
3:O:93:LEU:HB3	13:O:574:HOH:O	2.20	0.40
3:O:179:ILE:CG1	3:O:185:GLN:HE21	2.33	0.40
2:Q:108:ALA:HA	2:Q:125:ILE:O	2.20	0.40
3:R:156:TYR:HA	3:R:161:ARG:O	2.21	0.40
1:D:64:VAL:HG11	1:D:93:LEU:HD13	2.02	0.40
2:E:234:VAL:HG12	2:E:235:MET:HE2	2.01	0.40
3:F:59:PRO:HD3	3:F:76:ARG:HH11	1.86	0.40
1:M:140:MET:HE1	1:M:340:ILE:HD13	2.03	0.40
1:M:286:LEU:HD21	3:R:66:LYS:HB2	2.04	0.40
2:Q:143:PRO:HG3	2:Q:178:THR:CG2	2.52	0.40
1:D:75:LEU:O	1:D:79:SER:HB3	2.21	0.40
3:F:155:HIS:CD2	3:F:164:LYS:HD3	2.56	0.40
3:F:179:ILE:CG1	3:F:185:GLN:HE21	2.33	0.40
1:G:79:SER:O	1:G:83:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:130:ILE:HD11	1:G:348:TRP:CH2	2.46	0.40
1:G:261:LEU:CD1	2:H:234:VAL:HG13	2.44	0.40
2:H:176:LYS:NZ	2:H:178:THR:O	2.53	0.40
1:J:43:TRP:HH2	1:J:251:LYS:HG2	1.86	0.40
2:N:30:GLN:HG2	2:N:34:GLU:OE2	2.21	0.40
3:O:70:LYS:HB3	3:O:71:PRO:HD2	2.02	0.40
1:A:394:LEU:HD23	1:A:394:LEU:HA	1.90	0.40
2:B:113:PRO:O	2:B:114:MET:HB2	2.21	0.40
2:Q:65:ALA:O	2:Q:68:THR:HB	2.22	0.40
1:D:414:ILE:O	1:D:414:ILE:HG23	2.22	0.40
2:E:141:GLU:HA	2:E:142:PRO:HD3	1.77	0.40
2:E:171:ASP:OD1	2:E:171:ASP:C	2.64	0.40
2:E:250:ARG:HD3	3:F:12:ARG:CG	2.51	0.40
1:J:394:LEU:HD23	1:J:394:LEU:HA	1.90	0.40
1:J:423:THR:OG1	1:J:426:GLU:HB2	2.22	0.40
2:K:113:PRO:O	2:K:114:MET:HB3	2.21	0.40
2:K:137:GLY:O	2:K:139:PRO:HD3	2.20	0.40
3:L:100:ASN:HA	3:L:173:ILE:HB	2.03	0.40
3:L:126:TRP:C	3:L:128:VAL:H	2.28	0.40
2:N:40:HIS:HD1	2:N:97:ALA:HB1	1.83	0.40
2:N:65:ALA:O	2:N:68:THR:HB	2.22	0.40
2:N:105:LYS:C	2:N:107:ARG:H	2.29	0.40
1:P:75:LEU:O	1:P:79:SER:HB3	2.21	0.40
1:P:140:MET:HE1	1:P:340:ILE:HD13	2.03	0.40
2:Q:141:GLU:HA	2:Q:142:PRO:HD3	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	426/445 (96%)	412 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	426/445 (96%)	413 (97%)	13 (3%)	0	100	100
1	G	426/445 (96%)	412 (97%)	14 (3%)	0	100	100
1	J	426/445 (96%)	407 (96%)	18 (4%)	1 (0%)	43	58
1	M	426/445 (96%)	407 (96%)	19 (4%)	0	100	100
1	P	426/445 (96%)	408 (96%)	18 (4%)	0	100	100
2	B	254/269 (94%)	233 (92%)	18 (7%)	3 (1%)	10	16
2	E	254/269 (94%)	231 (91%)	20 (8%)	3 (1%)	10	16
2	H	254/269 (94%)	233 (92%)	18 (7%)	3 (1%)	10	16
2	K	254/269 (94%)	231 (91%)	18 (7%)	5 (2%)	6	7
2	N	254/269 (94%)	229 (90%)	20 (8%)	5 (2%)	6	7
2	Q	254/269 (94%)	231 (91%)	21 (8%)	2 (1%)	16	25
3	C	177/187 (95%)	163 (92%)	13 (7%)	1 (1%)	21	32
3	F	177/187 (95%)	161 (91%)	15 (8%)	1 (1%)	21	32
3	I	177/187 (95%)	162 (92%)	12 (7%)	3 (2%)	7	10
3	L	177/187 (95%)	161 (91%)	14 (8%)	2 (1%)	11	18
3	O	177/187 (95%)	162 (92%)	12 (7%)	3 (2%)	7	10
3	R	177/187 (95%)	161 (91%)	15 (8%)	1 (1%)	21	32
All	All	5142/5406 (95%)	4817 (94%)	292 (6%)	33 (1%)	21	32

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	147	GLU
2	E	147	GLU
2	E	190	MET
2	H	77	THR
2	H	147	GLU
2	K	147	GLU
2	K	190	MET
2	N	147	GLU
2	Q	147	GLU
2	B	198	ASP
2	E	198	ASP
2	H	198	ASP
2	K	198	ASP
2	N	198	ASP

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Mol	Chain	Res	Type
2	Q	198	ASP
2	B	190	MET
3	C	109	ALA
3	F	109	ALA
3	I	109	ALA
1	J	43	TRP
3	L	109	ALA
2	N	75	GLU
3	O	109	ALA
3	R	109	ALA
3	I	45	GLN
2	K	145	CYS
3	O	45	GLN
2	N	104	ALA
3	O	90	LEU
3	I	140	VAL
2	K	255	VAL
2	N	255	VAL
3	L	140	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	353/366 (96%)	342 (97%)	11 (3%)	35	57
1	D	353/366 (96%)	345 (98%)	8 (2%)	44	66
1	G	353/366 (96%)	345 (98%)	8 (2%)	44	66
1	J	353/366 (96%)	342 (97%)	11 (3%)	35	57
1	M	353/366 (96%)	343 (97%)	10 (3%)	38	60
1	P	353/366 (96%)	345 (98%)	8 (2%)	44	66
2	B	203/215 (94%)	191 (94%)	12 (6%)	18	31
2	E	203/215 (94%)	191 (94%)	12 (6%)	18	31
2	H	203/215 (94%)	196 (97%)	7 (3%)	32	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	203/215 (94%)	192 (95%)	11 (5%)	20	35
2	N	203/215 (94%)	193 (95%)	10 (5%)	22	39
2	Q	203/215 (94%)	189 (93%)	14 (7%)	14	24
3	C	138/144 (96%)	131 (95%)	7 (5%)	21	37
3	F	138/144 (96%)	129 (94%)	9 (6%)	15	27
3	I	138/144 (96%)	129 (94%)	9 (6%)	15	27
3	L	138/144 (96%)	130 (94%)	8 (6%)	18	32
3	O	138/144 (96%)	128 (93%)	10 (7%)	13	23
3	R	138/144 (96%)	130 (94%)	8 (6%)	18	32
All	All	4164/4350 (96%)	3991 (96%)	173 (4%)	26	45

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	79	SER
1	A	92	MET
1	A	108	VAL
1	A	137	LEU
1	A	217	HIS
1	A	246	PRO
1	A	314	VAL
1	A	380	VAL
1	A	385	THR
1	A	414	ILE
2	B	61	ASP
2	B	73	THR
2	B	95	GLU
2	B	136	THR
2	B	147	GLU
2	B	149	HIS
2	B	167	ASP
2	B	168	THR
2	B	177	THR
2	B	188	PRO
2	B	194	VAL
2	B	205	HIS
3	C	47	LEU
3	C	63	LEU

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Mol	Chain	Res	Type
3	C	65	VAL
3	C	72	ILE
3	C	112	GLN
3	C	174	PRO
3	C	179	ILE
1	D	7	ASP
1	D	10	GLU
1	D	79	SER
1	D	92	MET
1	D	246	PRO
1	D	380	VAL
1	D	385	THR
1	D	414	ILE
2	E	43	LYS
2	E	61	ASP
2	E	76	GLU
2	E	82	GLU
2	E	136	THR
2	E	141	GLU
2	E	152	ASP
2	E	168	THR
2	E	177	THR
2	E	194	VAL
2	E	195	GLU
2	E	205	HIS
3	F	47	LEU
3	F	63	LEU
3	F	65	VAL
3	F	72	ILE
3	F	112	GLN
3	F	118	GLU
3	F	174	PRO
3	F	177	LYS
3	F	179	ILE
1	G	4	ILE
1	G	79	SER
1	G	92	MET
1	G	108	VAL
1	G	246	PRO
1	G	380	VAL
1	G	385	THR
1	G	421	PRO

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Mol	Chain	Res	Type
2	H	136	THR
2	H	147	GLU
2	H	149	HIS
2	H	168	THR
2	H	177	THR
2	H	194	VAL
2	H	205	HIS
3	I	47	LEU
3	I	63	LEU
3	I	65	VAL
3	I	72	ILE
3	I	83	GLU
3	I	90	LEU
3	I	112	GLN
3	I	174	PRO
3	I	179	ILE
1	J	4	ILE
1	J	43	TRP
1	J	79	SER
1	J	108	VAL
1	J	162	ILE
1	J	217	HIS
1	J	246	PRO
1	J	380	VAL
1	J	385	THR
1	J	418	VAL
1	J	425	GLU
2	K	52	GLU
2	K	72	VAL
2	K	136	THR
2	K	149	HIS
2	K	168	THR
2	K	171	ASP
2	K	177	THR
2	K	181	SER
2	K	194	VAL
2	K	195	GLU
2	K	205	HIS
3	L	47	LEU
3	L	63	LEU
3	L	65	VAL
3	L	66	LYS

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Mol	Chain	Res	Type
3	L	72	ILE
3	L	112	GLN
3	L	174	PRO
3	L	179	ILE
1	M	8	HIS
1	M	79	SER
1	M	92	MET
1	M	108	VAL
1	M	162	ILE
1	M	246	PRO
1	M	287	ARG
1	M	314	VAL
1	M	380	VAL
1	M	385	THR
2	N	72	VAL
2	N	77	THR
2	N	136	THR
2	N	149	HIS
2	N	167	ASP
2	N	168	THR
2	N	176	LYS
2	N	177	THR
2	N	194	VAL
2	N	205	HIS
3	O	14	PHE
3	O	17	TYR
3	O	47	LEU
3	O	63	LEU
3	O	65	VAL
3	O	70	LYS
3	O	72	ILE
3	O	112	GLN
3	O	174	PRO
3	O	179	ILE
1	P	10	GLU
1	P	79	SER
1	P	92	MET
1	P	108	VAL
1	P	246	PRO
1	P	380	VAL
1	P	418	VAL
1	P	421	PRO

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Mol	Chain	Res	Type
2	Q	14	GLU
2	Q	43	LYS
2	Q	71	THR
2	Q	73	THR
2	Q	76	GLU
2	Q	80	ASP
2	Q	136	THR
2	Q	144	LYS
2	Q	158	ARG
2	Q	168	THR
2	Q	177	THR
2	Q	194	VAL
2	Q	195	GLU
2	Q	205	HIS
3	R	47	LEU
3	R	63	LEU
3	R	65	VAL
3	R	72	ILE
3	R	92	GLN
3	R	112	GLN
3	R	174	PRO
3	R	179	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	8	HIS
1	A	383	GLN
1	A	429	ASN
2	B	22	GLN
2	B	23	HIS
2	B	62	GLN
2	B	149	HIS
2	B	161	GLN
2	B	228	GLN
3	C	36	ASN
3	C	39	ASN
3	C	89	GLN
3	C	112	GLN
3	C	185	GLN
1	D	6	HIS

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Mol	Chain	Res	Type
1	D	383	GLN
2	E	5	HIS
2	E	22	GLN
2	E	23	HIS
2	E	62	GLN
2	E	149	HIS
2	E	228	GLN
3	F	36	ASN
3	F	45	GLN
3	F	89	GLN
3	F	112	GLN
3	F	185	GLN
1	G	383	GLN
2	H	22	GLN
2	H	23	HIS
2	H	62	GLN
2	H	149	HIS
3	I	36	ASN
3	I	39	ASN
3	I	112	GLN
3	I	185	GLN
1	J	177	GLN
1	J	221	ASN
1	J	383	GLN
1	J	429	ASN
2	K	22	GLN
2	K	62	GLN
2	K	149	HIS
2	K	228	GLN
3	L	36	ASN
3	L	39	ASN
3	L	112	GLN
3	L	185	GLN
1	M	8	HIS
1	M	174	HIS
1	M	177	GLN
1	M	221	ASN
1	M	291	HIS
1	M	383	GLN
1	M	429	ASN
2	N	22	GLN
2	N	23	HIS

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Mol	Chain	Res	Type
2	N	62	GLN
2	N	149	HIS
2	N	228	GLN
2	N	248	ASN
3	O	36	ASN
3	O	39	ASN
3	O	112	GLN
3	O	185	GLN
1	P	8	HIS
1	P	221	ASN
1	P	291	HIS
1	P	383	GLN
2	Q	22	GLN
2	Q	62	GLN
2	Q	149	HIS
3	R	36	ASN
3	R	39	ASN
3	R	45	GLN
3	R	112	GLN
3	R	185	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 60 ligands modelled in this entry, 12 are monoatomic - leaving 48 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
5	HEM	N	301	2	50,50,50	1.34	3 (6%)	67,82,82	1.10	3 (4%)
5	HEM	K	301	2	50,50,50	1.33	3 (6%)	67,82,82	1.07	3 (4%)
6	SMA	A	1001	-	38,38,38	2.12	10 (26%)	47,52,52	1.91	14 (29%)
5	HEM	D	501	1	50,50,50	1.24	2 (4%)	67,82,82	1.03	3 (4%)
7	LOP	P	1026	-	44,44,44	0.62	0	47,49,49	1.18	5 (10%)
5	HEM	E	301	2	50,50,50	1.29	4 (8%)	67,82,82	1.04	3 (4%)
5	HEM	A	502	1	50,50,50	1.31	3 (6%)	67,82,82	1.04	3 (4%)
7	LOP	A	1021	-	44,44,44	0.63	0	47,49,49	1.17	6 (12%)
8	UQ2	D	1102	-	23,23,23	1.44	5 (21%)	30,31,31	1.17	2 (6%)
9	BGL	E	1042	-	20,20,20	1.03	1 (5%)	24,25,25	0.95	1 (4%)
10	FES	I	200	3	0,4,4	-	-	-	-	-
5	HEM	M	502	1	50,50,50	1.27	4 (8%)	67,82,82	1.00	3 (4%)
10	FES	R	200	3	0,4,4	-	-	-	-	-
5	HEM	P	502	1	50,50,50	1.25	3 (6%)	67,82,82	1.03	4 (5%)
8	UQ2	A	1101	-	23,23,23	1.57	6 (26%)	30,31,31	1.19	2 (6%)
9	BGL	G	1043	-	20,20,20	1.32	1 (5%)	24,25,25	0.75	0
8	UQ2	J	1104	-	23,23,23	1.31	4 (17%)	30,31,31	1.19	3 (10%)
6	SMA	P	1006	-	38,38,38	2.03	9 (23%)	47,52,52	2.09	14 (29%)
7	LOP	D	1022	-	44,44,44	0.71	0	47,49,49	1.17	5 (10%)
9	BGL	N	1045	-	20,20,20	1.33	1 (5%)	24,25,25	0.73	0
9	BGL	P	1046	-	20,20,20	1.18	1 (5%)	24,25,25	0.92	1 (4%)
6	SMA	D	1002	-	38,38,38	2.00	9 (23%)	47,52,52	1.89	12 (25%)
5	HEM	J	501	1	50,50,50	1.32	4 (8%)	67,82,82	1.03	3 (4%)
5	HEM	G	502	1	50,50,50	1.33	4 (8%)	67,82,82	1.05	3 (4%)
5	HEM	P	501	1	50,50,50	1.27	4 (8%)	67,82,82	1.04	3 (4%)
10	FES	C	200	3	0,4,4	-	-	-	-	-
5	HEM	Q	301	2	50,50,50	1.30	3 (6%)	67,82,82	1.04	3 (4%)
5	HEM	J	502	1	50,50,50	1.34	4 (8%)	67,82,82	1.05	3 (4%)
9	BGL	B	1041	-	20,20,20	1.05	1 (5%)	24,25,25	0.87	1 (4%)
7	LOP	J	1024	-	44,44,44	0.65	0	47,49,49	1.24	6 (12%)
7	LOP	G	1023	-	44,44,44	0.72	0	47,49,49	1.16	4 (8%)
6	SMA	M	1005	-	38,38,38	2.07	9 (23%)	47,52,52	1.89	10 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	HEM	M	501	1	50,50,50	1.24	4 (8%)	67,82,82	1.01	3 (4%)
5	HEM	G	501	1	50,50,50	1.29	4 (8%)	67,82,82	1.01	3 (4%)
6	SMA	J	1004	-	38,38,38	1.99	9 (23%)	47,52,52	1.72	9 (19%)
10	FES	L	200	3	0,4,4	-	-	-	-	-
5	HEM	B	301	2	50,50,50	1.36	4 (8%)	67,82,82	1.05	3 (4%)
7	LOP	M	1025	-	44,44,44	0.70	0	47,49,49	1.16	3 (6%)
9	BGL	K	1044	-	20,20,20	1.00	1 (5%)	24,25,25	1.11	2 (8%)
10	FES	O	200	3	0,4,4	-	-	-	-	-
10	FES	F	200	3	0,4,4	-	-	-	-	-
5	HEM	A	501	1	50,50,50	1.27	3 (6%)	67,82,82	1.02	3 (4%)
8	UQ2	M	1105	-	23,23,23	1.54	5 (21%)	30,31,31	1.16	3 (10%)
8	UQ2	P	1106	-	23,23,23	1.63	5 (21%)	30,31,31	1.22	5 (16%)
5	HEM	H	301	2	50,50,50	1.29	3 (6%)	67,82,82	1.11	3 (4%)
8	UQ2	G	1103	-	23,23,23	1.52	5 (21%)	30,31,31	1.09	1 (3%)
5	HEM	D	502	1	50,50,50	1.23	4 (8%)	67,82,82	1.02	3 (4%)
6	SMA	G	1003	-	38,38,38	2.08	10 (26%)	47,52,52	1.82	11 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	N	301	2	-	8/14/54/54	-
5	HEM	K	301	2	-	8/14/54/54	-
6	SMA	A	1001	-	-	5/34/34/34	0/2/2/2
5	HEM	D	501	1	-	3/14/54/54	-
7	LOP	P	1026	-	-	8/48/48/48	-
5	HEM	E	301	2	-	9/14/54/54	-
5	HEM	A	502	1	-	7/14/54/54	-
7	LOP	A	1021	-	-	12/48/48/48	-
8	UQ2	D	1102	-	-	2/15/39/39	0/1/1/1
9	BGL	E	1042	-	-	0/11/31/31	0/1/1/1
10	FES	I	200	3	-	-	0/1/1/1
5	HEM	M	502	1	-	7/14/54/54	-
10	FES	R	200	3	-	-	0/1/1/1
5	HEM	P	502	1	-	5/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	UQ2	A	1101	-	-	6/15/39/39	0/1/1/1
9	BGL	G	1043	-	-	0/11/31/31	0/1/1/1
8	UQ2	J	1104	-	-	0/15/39/39	0/1/1/1
6	SMA	P	1006	-	-	7/34/34/34	0/2/2/2
7	LOP	D	1022	-	-	4/48/48/48	-
9	BGL	N	1045	-	-	0/11/31/31	0/1/1/1
9	BGL	P	1046	-	-	0/11/31/31	0/1/1/1
6	SMA	D	1002	-	-	6/34/34/34	0/2/2/2
5	HEM	J	501	1	-	4/14/54/54	-
5	HEM	G	502	1	-	9/14/54/54	-
5	HEM	P	501	1	-	6/14/54/54	-
10	FES	C	200	3	-	-	0/1/1/1
5	HEM	Q	301	2	-	7/14/54/54	-
5	HEM	J	502	1	-	8/14/54/54	-
9	BGL	B	1041	-	-	0/11/31/31	0/1/1/1
7	LOP	J	1024	-	-	10/48/48/48	-
7	LOP	G	1023	-	-	11/48/48/48	-
6	SMA	M	1005	-	-	8/34/34/34	0/2/2/2
5	HEM	M	501	1	-	6/14/54/54	-
5	HEM	G	501	1	-	6/14/54/54	-
6	SMA	J	1004	-	-	2/34/34/34	0/2/2/2
10	FES	L	200	3	-	-	0/1/1/1
5	HEM	B	301	2	-	8/14/54/54	-
7	LOP	M	1025	-	-	4/48/48/48	-
9	BGL	K	1044	-	-	0/11/31/31	0/1/1/1
10	FES	O	200	3	-	-	0/1/1/1
10	FES	F	200	3	-	-	0/1/1/1
5	HEM	A	501	1	-	3/14/54/54	-
8	UQ2	M	1105	-	-	2/15/39/39	0/1/1/1
8	UQ2	P	1106	-	-	4/15/39/39	0/1/1/1
5	HEM	H	301	2	-	8/14/54/54	-
8	UQ2	G	1103	-	-	5/15/39/39	0/1/1/1
5	HEM	D	502	1	-	8/14/54/54	-
6	SMA	G	1003	-	-	5/34/34/34	0/2/2/2

All (155) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	1003	SMA	O5-C5	7.24	1.48	1.37
6	A	1001	SMA	O5-C5	6.96	1.48	1.37
6	J	1004	SMA	O5-C5	6.64	1.47	1.37
6	D	1002	SMA	O5-C5	6.55	1.47	1.37
6	M	1005	SMA	O7-C7	6.53	1.47	1.37
6	A	1001	SMA	O7-C7	6.40	1.47	1.37
6	M	1005	SMA	O5-C5	6.17	1.47	1.37
6	P	1006	SMA	O5-C5	6.05	1.47	1.37
6	J	1004	SMA	O7-C7	5.77	1.46	1.37
6	G	1003	SMA	O7-C7	5.43	1.46	1.37
6	P	1006	SMA	O7-C7	5.23	1.45	1.37
5	K	301	HEM	CBB-CAB	5.14	1.55	1.30
6	D	1002	SMA	O7-C7	5.06	1.45	1.37
5	H	301	HEM	CBB-CAB	5.01	1.54	1.30
5	B	301	HEM	CBC-CAC	4.99	1.54	1.30
5	Q	301	HEM	CBB-CAB	4.95	1.54	1.30
5	H	301	HEM	CBC-CAC	4.95	1.54	1.30
5	N	301	HEM	CBB-CAB	4.89	1.53	1.30
5	E	301	HEM	CBB-CAB	4.89	1.53	1.30
5	B	301	HEM	CBB-CAB	4.88	1.53	1.30
5	Q	301	HEM	CBC-CAC	4.87	1.53	1.30
5	K	301	HEM	CBC-CAC	4.87	1.53	1.30
5	N	301	HEM	CBC-CAC	4.87	1.53	1.30
5	E	301	HEM	CBC-CAC	4.79	1.53	1.30
5	G	501	HEM	CBC-CAC	4.76	1.53	1.30
5	P	502	HEM	CBB-CAB	4.76	1.53	1.30
5	D	501	HEM	CBC-CAC	4.72	1.53	1.30
5	A	501	HEM	CBB-CAB	4.69	1.52	1.30
5	J	502	HEM	CBB-CAB	4.66	1.52	1.30
5	J	501	HEM	CBC-CAC	4.66	1.52	1.30
5	A	501	HEM	CBC-CAC	4.59	1.52	1.30
5	J	501	HEM	CBB-CAB	4.58	1.52	1.30
5	P	501	HEM	CBB-CAB	4.56	1.52	1.30
5	M	502	HEM	CBC-CAC	4.55	1.52	1.30
5	A	502	HEM	CBB-CAB	4.55	1.52	1.30
5	G	501	HEM	CBB-CAB	4.54	1.52	1.30
5	A	502	HEM	CBC-CAC	4.54	1.52	1.30
5	D	501	HEM	CBB-CAB	4.53	1.52	1.30
5	M	501	HEM	CBC-CAC	4.52	1.52	1.30
5	M	501	HEM	CBB-CAB	4.50	1.52	1.30
5	P	501	HEM	CBC-CAC	4.49	1.52	1.30
5	G	502	HEM	CBB-CAB	4.49	1.51	1.30
5	D	502	HEM	CBB-CAB	4.46	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	1043	BGL	C1-C2	4.45	1.56	1.52
5	M	502	HEM	CBB-CAB	4.44	1.51	1.30
5	D	502	HEM	CBC-CAC	4.35	1.51	1.30
9	N	1045	BGL	C1-C2	4.31	1.56	1.52
5	P	502	HEM	CBC-CAC	4.30	1.51	1.30
5	G	502	HEM	CBC-CAC	4.15	1.50	1.30
5	J	502	HEM	CAC-C3C	-4.08	1.36	1.47
8	G	1103	UQ2	C6-C5	3.91	1.42	1.35
8	P	1106	UQ2	C6-C5	3.89	1.42	1.35
6	A	1001	SMA	O8-C8	3.87	1.45	1.36
5	J	502	HEM	CBC-CAC	3.77	1.48	1.30
9	P	1046	BGL	C1-C2	3.66	1.55	1.52
6	P	1006	SMA	C3-C4	-3.64	1.39	1.47
9	B	1041	BGL	C1-C2	3.56	1.55	1.52
8	M	1105	UQ2	C6-C5	3.52	1.41	1.35
8	M	1105	UQ2	C7-C8	3.50	1.56	1.50
8	A	1101	UQ2	C7-C8	3.46	1.56	1.50
6	M	1005	SMA	O8-C8	3.41	1.44	1.36
9	E	1042	BGL	C1-C2	3.41	1.55	1.52
6	D	1002	SMA	C7-C8	-3.35	1.35	1.40
6	D	1002	SMA	O8-C8	3.35	1.44	1.36
6	P	1006	SMA	O8-C8	3.32	1.44	1.36
6	J	1004	SMA	O8-C8	3.27	1.44	1.36
8	D	1102	UQ2	C6-C5	3.26	1.41	1.35
8	P	1106	UQ2	C7-C8	3.25	1.55	1.50
8	P	1106	UQ2	C7-C6	3.25	1.57	1.51
6	G	1003	SMA	O8-C8	3.23	1.44	1.36
8	A	1101	UQ2	C6-C5	3.22	1.41	1.35
5	G	502	HEM	CAC-C3C	-3.16	1.38	1.47
8	G	1103	UQ2	C7-C8	3.16	1.55	1.50
5	N	301	HEM	CAC-C3C	-3.15	1.39	1.47
6	P	1006	SMA	C7-C8	-2.99	1.36	1.40
6	P	1006	SMA	C4A-C4	-2.94	1.39	1.46
8	D	1102	UQ2	C7-C8	2.91	1.55	1.50
8	J	1104	UQ2	C6-C5	2.85	1.40	1.35
5	A	502	HEM	CAB-C3B	-2.84	1.39	1.47
6	D	1002	SMA	C4A-C4	-2.84	1.39	1.46
5	J	501	HEM	CAB-C3B	-2.82	1.39	1.47
8	J	1104	UQ2	C7-C8	2.82	1.55	1.50
6	A	1001	SMA	C3-C4	-2.82	1.41	1.47
5	M	502	HEM	CAB-C3B	-2.80	1.39	1.47
5	B	301	HEM	CAC-C3C	-2.77	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1002	SMA	C3-C2	2.75	1.39	1.34
9	K	1044	BGL	C1-C2	2.69	1.55	1.52
6	J	1004	SMA	C3-C4	-2.64	1.41	1.47
6	M	1005	SMA	C3-C4	-2.63	1.41	1.47
8	D	1102	UQ2	O3-C3	2.62	1.43	1.36
6	J	1004	SMA	C7-C8	-2.58	1.36	1.40
8	G	1103	UQ2	O3-C3	2.58	1.43	1.36
5	P	502	HEM	CAC-C3C	-2.56	1.40	1.47
8	A	1101	UQ2	O2-C2	2.56	1.42	1.36
6	G	1003	SMA	C7-C8	-2.56	1.37	1.40
6	M	1005	SMA	C20-C19	2.56	1.35	1.33
8	G	1103	UQ2	O2-C2	2.55	1.42	1.36
6	D	1002	SMA	C3-C4	-2.55	1.41	1.47
6	G	1003	SMA	C20-C19	2.54	1.35	1.33
8	M	1105	UQ2	C7-C6	2.53	1.56	1.51
6	A	1001	SMA	C4A-C4	-2.53	1.40	1.46
6	G	1003	SMA	C4A-C4	-2.52	1.40	1.46
5	Q	301	HEM	CAB-C3B	-2.49	1.40	1.47
6	D	1002	SMA	O5-C5M	2.49	1.49	1.42
8	P	1106	UQ2	O3-C3	2.47	1.42	1.36
5	A	501	HEM	CAB-C3B	-2.47	1.40	1.47
6	J	1004	SMA	C4A-C4	-2.45	1.40	1.46
6	M	1005	SMA	O1-C2	2.44	1.39	1.36
5	B	301	HEM	CAB-C3B	-2.44	1.40	1.47
6	G	1003	SMA	C3-C4	-2.42	1.42	1.47
5	D	502	HEM	CAC-C3C	-2.41	1.40	1.47
6	D	1002	SMA	O12-C12	2.40	1.48	1.42
5	J	502	HEM	CAB-C3B	-2.40	1.41	1.47
8	G	1103	UQ2	C7-C6	2.39	1.55	1.51
6	M	1005	SMA	C7-C8	-2.39	1.37	1.40
5	M	501	HEM	CAC-C3C	-2.38	1.41	1.47
6	A	1001	SMA	C20-C19	2.38	1.35	1.33
8	D	1102	UQ2	O2-C2	2.38	1.42	1.36
5	E	301	HEM	CAC-C3C	-2.37	1.41	1.47
6	P	1006	SMA	O12-C12	2.37	1.48	1.42
5	M	501	HEM	CAB-C3B	-2.36	1.41	1.47
6	A	1001	SMA	C7-C8	-2.35	1.37	1.40
6	A	1001	SMA	C3-C2	2.34	1.39	1.34
8	M	1105	UQ2	O3-C3	2.34	1.42	1.36
8	A	1101	UQ2	C7-C6	2.33	1.55	1.51
8	P	1106	UQ2	O2-C2	2.30	1.42	1.36
6	J	1004	SMA	C3-C2	2.29	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	501	HEM	CAC-C3C	-2.26	1.41	1.47
6	G	1003	SMA	C8-C8A	-2.25	1.36	1.39
5	M	502	HEM	CAC-C3C	-2.24	1.41	1.47
6	G	1003	SMA	O12-C12	2.23	1.48	1.42
5	H	301	HEM	CAC-C3C	-2.22	1.41	1.47
8	J	1104	UQ2	O3-C3	2.21	1.42	1.36
5	G	502	HEM	CAB-C3B	-2.21	1.41	1.47
5	D	502	HEM	CAB-C3B	-2.20	1.41	1.47
6	M	1005	SMA	C4A-C4	-2.17	1.41	1.46
5	P	501	HEM	CAB-C3B	-2.17	1.41	1.47
6	M	1005	SMA	C3-C2	2.16	1.38	1.34
6	A	1001	SMA	C24-C13	2.15	1.57	1.53
6	P	1006	SMA	O5-C5M	2.14	1.48	1.42
5	K	301	HEM	CAC-C3C	-2.14	1.41	1.47
8	M	1105	UQ2	C8-C9	2.12	1.38	1.33
5	J	501	HEM	CAC-C3C	-2.10	1.41	1.47
5	G	501	HEM	CAB-C3B	-2.08	1.41	1.47
5	E	301	HEM	CAB-C3B	-2.08	1.41	1.47
8	J	1104	UQ2	O2-C2	2.07	1.41	1.36
6	G	1003	SMA	C3-C2	2.06	1.38	1.34
8	A	1101	UQ2	C8-C9	2.06	1.37	1.33
5	G	501	HEM	CAC-C3C	-2.06	1.41	1.47
8	A	1101	UQ2	O3-C3	2.06	1.41	1.36
6	J	1004	SMA	O5-C5M	2.05	1.48	1.42
6	J	1004	SMA	C8-C8A	-2.03	1.36	1.39
6	A	1001	SMA	C8-C8A	-2.01	1.36	1.39
8	D	1102	UQ2	C7-C6	2.00	1.55	1.51
6	P	1006	SMA	O1-C2	2.00	1.39	1.36

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	1006	SMA	C14-C15-C16	6.09	138.23	125.88
6	P	1006	SMA	O7-C7-C8	4.96	119.71	114.53
6	M	1005	SMA	C5M-O5-C5	-4.94	110.27	117.51
6	A	1001	SMA	O5-C5-C4A	4.79	122.63	115.84
6	A	1001	SMA	O7-C7-C8	4.55	119.29	114.53
6	D	1002	SMA	O5-C5-C4A	4.43	122.12	115.84
6	M	1005	SMA	O5-C5-C4A	4.35	122.01	115.84
6	G	1003	SMA	O5-C5-C4A	4.24	121.85	115.84
6	G	1003	SMA	O1-C2-C9	4.14	118.91	110.12
6	M	1005	SMA	O7-C7-C8	4.14	118.86	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	1006	SMA	O1-C2-C9	4.08	118.78	110.12
6	A	1001	SMA	O1-C2-C9	4.04	118.69	110.12
6	D	1002	SMA	C5M-O5-C5	-4.02	111.61	117.51
6	J	1004	SMA	O5-C5-C4A	4.01	121.53	115.84
6	P	1006	SMA	O5-C5-C4A	3.94	121.43	115.84
6	M	1005	SMA	O1-C2-C9	3.92	118.43	110.12
6	P	1006	SMA	C5M-O5-C5	-3.91	111.78	117.51
6	J	1004	SMA	C5M-O5-C5	-3.90	111.79	117.51
6	J	1004	SMA	O7-C7-C8	3.89	118.60	114.53
6	J	1004	SMA	C9-C10-C11	-3.86	107.25	114.46
5	J	502	HEM	CBC-CAC-C3C	-3.84	108.32	127.53
6	D	1002	SMA	O1-C2-C9	3.84	118.27	110.12
6	G	1003	SMA	O7-C7-C8	3.79	118.49	114.53
6	J	1004	SMA	O1-C2-C9	3.77	118.12	110.12
6	D	1002	SMA	O7-C7-C8	3.73	118.43	114.53
7	J	1024	LOP	O5-C6-C7	3.70	119.49	111.48
6	A	1001	SMA	O5-C5-C6	-3.69	117.72	124.08
5	G	502	HEM	CBC-CAC-C3C	-3.66	109.25	127.53
6	A	1001	SMA	C5M-O5-C5	-3.65	112.16	117.51
6	G	1003	SMA	C5M-O5-C5	-3.54	112.31	117.51
6	G	1003	SMA	C14-C15-C16	3.54	133.06	125.88
5	K	301	HEM	CBB-CAB-C3B	-3.54	109.86	127.53
5	H	301	HEM	CBB-CAB-C3B	-3.53	109.87	127.53
5	H	301	HEM	C3B-C4B-NB	3.51	111.99	109.47
5	E	301	HEM	CBB-CAB-C3B	-3.50	110.04	127.53
5	B	301	HEM	CBB-CAB-C3B	-3.50	110.06	127.53
5	J	501	HEM	CBB-CAB-C3B	-3.47	110.16	127.53
5	D	502	HEM	CBB-CAB-C3B	-3.47	110.17	127.53
9	K	1044	BGL	C1'-O2-C2	-3.47	106.31	114.02
5	N	301	HEM	CBC-CAC-C3C	-3.47	110.20	127.53
5	Q	301	HEM	CBB-CAB-C3B	-3.46	110.24	127.53
5	B	301	HEM	CBC-CAC-C3C	-3.45	110.31	127.53
5	A	502	HEM	CBB-CAB-C3B	-3.43	110.38	127.53
5	P	501	HEM	CBC-CAC-C3C	-3.42	110.45	127.53
5	N	301	HEM	CBB-CAB-C3B	-3.41	110.46	127.53
5	K	301	HEM	CBC-CAC-C3C	-3.41	110.47	127.53
5	H	301	HEM	CBC-CAC-C3C	-3.40	110.54	127.53
5	J	501	HEM	CBC-CAC-C3C	-3.37	110.67	127.53
5	E	301	HEM	CBC-CAC-C3C	-3.37	110.68	127.53
5	Q	301	HEM	CBC-CAC-C3C	-3.37	110.68	127.53
5	M	501	HEM	CBB-CAB-C3B	-3.37	110.71	127.53
5	A	502	HEM	CBC-CAC-C3C	-3.36	110.72	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	502	HEM	CBB-CAB-C3B	-3.36	110.74	127.53
5	G	502	HEM	CBB-CAB-C3B	-3.36	110.75	127.53
6	D	1002	SMA	C17-C18-C19	-3.35	117.17	126.36
5	G	501	HEM	CBC-CAC-C3C	-3.34	110.81	127.53
5	M	501	HEM	CBC-CAC-C3C	-3.31	110.98	127.53
5	G	501	HEM	CBB-CAB-C3B	-3.30	111.02	127.53
5	J	502	HEM	CBB-CAB-C3B	-3.28	111.13	127.53
5	P	501	HEM	CBB-CAB-C3B	-3.28	111.14	127.53
5	M	502	HEM	CBC-CAC-C3C	-3.28	111.15	127.53
5	P	502	HEM	CBC-CAC-C3C	-3.28	111.15	127.53
5	A	501	HEM	CBB-CAB-C3B	-3.23	111.39	127.53
6	D	1002	SMA	C9-C10-C11	-3.21	108.47	114.46
5	D	502	HEM	CBC-CAC-C3C	-3.21	111.51	127.53
5	P	502	HEM	CBB-CAB-C3B	-3.20	111.54	127.53
5	D	501	HEM	CBC-CAC-C3C	-3.17	111.70	127.53
5	A	501	HEM	CBC-CAC-C3C	-3.13	111.88	127.53
6	A	1001	SMA	C9-C10-C11	-3.13	108.61	114.46
5	D	501	HEM	CBB-CAB-C3B	-3.12	111.92	127.53
7	A	1021	LOP	O5-C6-C7	3.03	118.03	111.48
5	N	301	HEM	C3B-C4B-NB	3.01	111.63	109.47
9	P	1046	BGL	C1'-O2-C2	-3.01	107.34	114.02
6	D	1002	SMA	O5-C5-C6	-2.99	118.94	124.08
6	P	1006	SMA	C7M-O7-C7	-2.98	113.14	117.51
7	G	1023	LOP	O5-C6-C7	2.98	117.93	111.48
6	P	1006	SMA	C9-C10-C11	-2.97	108.92	114.46
6	G	1003	SMA	C9-C10-C11	-2.94	108.97	114.46
7	G	1023	LOP	C19-C18-C17	-2.94	99.52	114.37
6	M	1005	SMA	O5-C5-C6	-2.93	119.02	124.08
5	G	502	HEM	C3B-C4B-NB	2.93	111.57	109.47
7	M	1025	LOP	O5-C6-C7	2.91	117.77	111.48
6	M	1005	SMA	C17-C18-C19	-2.90	118.41	126.36
7	D	1022	LOP	O5-C6-C7	2.87	117.69	111.48
9	E	1042	BGL	C1'-O2-C2	-2.87	107.65	114.02
6	D	1002	SMA	C14-C15-C16	2.86	131.68	125.88
6	M	1005	SMA	C7M-O7-C7	-2.85	113.33	117.51
7	D	1022	LOP	C27-C26-C25	-2.84	102.69	113.13
8	A	1101	UQ2	C10-C9-C11	2.84	120.15	115.23
6	M	1005	SMA	C14-C15-C16	2.83	131.62	125.88
7	A	1021	LOP	C19-C18-C17	-2.82	100.09	114.37
5	E	301	HEM	C3B-C4B-NB	2.80	111.48	109.47
5	P	501	HEM	C3B-C4B-NB	2.79	111.47	109.47
6	P	1006	SMA	C13-C14-C15	2.78	118.13	112.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	502	HEM	C3B-C4B-NB	2.78	111.46	109.47
5	G	501	HEM	C3B-C4B-NB	2.78	111.46	109.47
7	J	1024	LOP	O6-C24-C25	2.77	120.29	111.83
5	D	501	HEM	C3B-C4B-NB	2.75	111.44	109.47
5	J	502	HEM	C3B-C4B-NB	2.74	111.43	109.47
5	B	301	HEM	C3B-C4B-NB	2.72	111.42	109.47
6	G	1003	SMA	O1-C2-C3	-2.72	119.42	121.81
6	D	1002	SMA	O1-C2-C3	-2.71	119.43	121.81
6	D	1002	SMA	C7M-O7-C7	-2.70	113.55	117.51
7	P	1026	LOP	C9-C8-C7	-2.70	103.22	113.13
5	P	502	HEM	C3B-C4B-NB	2.69	111.40	109.47
7	G	1023	LOP	C21-C20-C19	-2.67	100.87	114.37
6	A	1001	SMA	O1-C2-C3	-2.66	119.48	121.81
7	P	1026	LOP	C27-C26-C25	-2.65	103.37	113.13
6	J	1004	SMA	C7M-O7-C7	-2.64	113.65	117.51
6	G	1003	SMA	C7M-O7-C7	-2.62	113.67	117.51
7	G	1023	LOP	O6-C24-C25	2.61	119.79	111.83
5	M	501	HEM	C3B-C4B-NB	2.61	111.34	109.47
5	Q	301	HEM	C3B-C4B-NB	2.61	111.34	109.47
5	K	301	HEM	C3B-C4B-NB	2.59	111.33	109.47
6	A	1001	SMA	C7M-O7-C7	-2.57	113.75	117.51
6	M	1005	SMA	O1-C2-C3	-2.56	119.56	121.81
9	B	1041	BGL	C1'-O2-C2	-2.56	108.33	114.02
5	A	501	HEM	C3B-C4B-NB	2.56	111.31	109.47
8	P	1106	UQ2	C8-C7-C6	2.54	118.35	112.08
6	P	1006	SMA	O5-C5-C6	-2.54	119.69	124.08
8	J	1104	UQ2	C10-C9-C11	2.54	119.64	115.23
8	A	1101	UQ2	C7-C8-C9	-2.54	122.46	126.83
6	G	1003	SMA	C26-C19-C18	2.53	121.96	118.09
6	G	1003	SMA	O5-C5-C6	-2.53	119.72	124.08
6	J	1004	SMA	O1-C2-C3	-2.53	119.59	121.81
6	J	1004	SMA	C17-C18-C19	-2.53	119.44	126.36
7	M	1025	LOP	C21-C20-C19	-2.53	101.60	114.37
7	M	1025	LOP	C19-C18-C17	-2.51	101.67	114.37
7	D	1022	LOP	O6-C24-C25	2.50	119.46	111.83
5	J	501	HEM	C3B-C4B-NB	2.50	111.26	109.47
7	D	1022	LOP	C19-C18-C17	-2.48	101.81	114.37
6	P	1006	SMA	C26-C19-C18	2.47	121.86	118.09
7	P	1026	LOP	O5-C6-C7	2.47	116.82	111.48
8	M	1105	UQ2	C10-C9-C11	2.46	119.49	115.23
5	A	502	HEM	C3B-C4B-NB	2.44	111.22	109.47
8	D	1102	UQ2	C10-C9-C11	2.42	119.43	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1021	LOP	C21-C20-C19	-2.41	102.16	114.37
7	P	1026	LOP	O6-C24-C25	2.41	119.17	111.83
8	J	1104	UQ2	C7-C6-C5	-2.40	120.78	124.89
7	J	1024	LOP	C19-C18-C17	-2.38	102.34	114.37
6	J	1004	SMA	O5-C5-C6	-2.37	119.99	124.08
6	P	1006	SMA	O7-C7-C6	-2.36	120.01	124.08
8	M	1105	UQ2	C7-C8-C9	-2.31	122.84	126.83
9	K	1044	BGL	C3'-C2'-C1'	-2.31	103.43	113.47
6	P	1006	SMA	C17-C18-C19	-2.28	120.11	126.36
6	M	1005	SMA	C9-C10-C11	-2.26	110.24	114.46
8	P	1106	UQ2	C10-C9-C11	2.23	119.10	115.23
7	A	1021	LOP	C31-C30-C29	-2.23	103.10	114.37
8	D	1102	UQ2	C7-C8-C9	-2.21	123.02	126.83
6	D	1002	SMA	C26-C19-C18	2.21	121.46	118.09
7	A	1021	LOP	C29-C28-C27	-2.21	103.21	114.37
7	J	1024	LOP	C21-C20-C19	-2.20	103.25	114.37
6	G	1003	SMA	C17-C18-C19	-2.19	120.34	126.36
7	J	1024	LOP	C29-C28-C27	-2.18	103.35	114.37
8	J	1104	UQ2	CM5-C5-C6	-2.17	120.88	124.45
5	P	502	HEM	CAC-C3C-C4C	2.17	130.00	124.82
5	D	502	HEM	C3B-C4B-NB	2.16	111.02	109.47
6	A	1001	SMA	C17-C18-C19	-2.15	120.46	126.36
6	A	1001	SMA	C13-C14-C15	-2.15	107.48	112.11
6	P	1006	SMA	O1-C2-C3	-2.14	119.93	121.81
6	A	1001	SMA	C3M-C3-C2	-2.13	120.12	123.28
8	P	1106	UQ2	C5-C6-C1	-2.12	117.56	119.62
6	D	1002	SMA	C3M-C3-C2	-2.12	120.14	123.28
7	P	1026	LOP	C19-C18-C17	-2.12	103.67	114.37
6	A	1001	SMA	C3M-C3-C4	2.10	120.54	116.68
8	G	1103	UQ2	C7-C8-C9	-2.09	123.22	126.83
6	P	1006	SMA	C17-C16-C15	-2.09	110.32	124.25
6	A	1001	SMA	C14-C15-C16	-2.08	121.67	125.88
8	P	1106	UQ2	C7-C8-C9	-2.08	123.25	126.83
6	A	1001	SMA	C16-C17-C18	-2.08	119.74	124.65
7	J	1024	LOP	C27-C26-C25	-2.06	105.55	113.13
7	A	1021	LOP	O6-C24-C25	2.06	118.12	111.83
8	M	1105	UQ2	C8-C7-C6	2.04	117.12	112.08
7	D	1022	LOP	P1-O1-C2	-2.03	111.57	121.26
8	P	1106	UQ2	C3-C4-C5	2.03	122.11	118.10

There are no chirality outliers.

All (221) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	502	HEM	C2B-C3B-CAB-CBB
5	A	502	HEM	C4B-C3B-CAB-CBB
5	D	502	HEM	C2B-C3B-CAB-CBB
5	D	502	HEM	C4B-C3B-CAB-CBB
5	E	301	HEM	C2C-C3C-CAC-CBC
5	G	502	HEM	C2B-C3B-CAB-CBB
5	J	501	HEM	C2B-C3B-CAB-CBB
5	J	501	HEM	C2C-C3C-CAC-CBC
5	J	501	HEM	C4C-C3C-CAC-CBC
5	J	502	HEM	C2B-C3B-CAB-CBB
5	J	502	HEM	C2C-C3C-CAC-CBC
5	K	301	HEM	C2C-C3C-CAC-CBC
5	M	501	HEM	C2B-C3B-CAB-CBB
5	M	501	HEM	C2C-C3C-CAC-CBC
5	M	502	HEM	C2B-C3B-CAB-CBB
5	N	301	HEM	C2C-C3C-CAC-CBC
5	P	501	HEM	C2C-C3C-CAC-CBC
5	P	501	HEM	C4C-C3C-CAC-CBC
6	G	1003	SMA	C13-C14-C15-C16
6	M	1005	SMA	C13-C14-C15-C16
6	P	1006	SMA	C13-C14-C15-C16
7	A	1021	LOP	C2-O1-P1-O2
7	A	1021	LOP	C2-O1-P1-O3
7	A	1021	LOP	C2-O1-P1-O4
7	G	1023	LOP	C2-O1-P1-O2
7	G	1023	LOP	C2-O1-P1-O3
7	G	1023	LOP	C2-O1-P1-O4
7	J	1024	LOP	C2-O1-P1-O2
7	J	1024	LOP	C2-O1-P1-O3
7	J	1024	LOP	C3-O2-P1-O1
7	J	1024	LOP	C3-O2-P1-O3
7	P	1026	LOP	C2-O1-P1-O2
7	P	1026	LOP	C2-O1-P1-O3
7	P	1026	LOP	C2-O1-P1-O4
8	P	1106	UQ2	C1-C6-C7-C8
8	A	1101	UQ2	C9-C11-C12-C13
8	G	1103	UQ2	C9-C11-C12-C13
8	A	1101	UQ2	C12-C11-C9-C8
6	G	1003	SMA	C9-C10-C11-C22
6	M	1005	SMA	C6-C5-O5-C5M
7	G	1023	LOP	O5-C4-C5-O6
6	M	1005	SMA	C4A-C5-O5-C5M
6	A	1001	SMA	C4A-C5-O5-C5M

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Mol	Chain	Res	Type	Atoms
6	A	1001	SMA	C6-C5-O5-C5M
6	P	1006	SMA	C9-C10-C11-C22
6	A	1001	SMA	C9-C10-C11-C22
6	P	1006	SMA	C8-C7-O7-C7M
6	M	1005	SMA	C11-C10-C9-C2
6	J	1004	SMA	C6-C5-O5-C5M
6	D	1002	SMA	C9-C10-C11-C22
8	P	1106	UQ2	C5-C6-C7-C8
8	A	1101	UQ2	C12-C11-C9-C10
5	E	301	HEM	C2B-C3B-CAB-CBB
5	G	501	HEM	C2B-C3B-CAB-CBB
5	G	501	HEM	C2C-C3C-CAC-CBC
5	G	502	HEM	C2C-C3C-CAC-CBC
5	H	301	HEM	C2C-C3C-CAC-CBC
5	N	301	HEM	C2B-C3B-CAB-CBB
5	P	501	HEM	C2B-C3B-CAB-CBB
5	Q	301	HEM	C2C-C3C-CAC-CBC
5	G	502	HEM	C4B-C3B-CAB-CBB
5	J	501	HEM	C4B-C3B-CAB-CBB
5	J	502	HEM	C4C-C3C-CAC-CBC
5	M	501	HEM	C4B-C3B-CAB-CBB
5	M	501	HEM	C4C-C3C-CAC-CBC
5	M	502	HEM	C4B-C3B-CAB-CBB
7	G	1023	LOP	C3-C4-C5-O6
6	J	1004	SMA	C4A-C5-O5-C5M
7	G	1023	LOP	O2-C3-C4-O5
7	G	1023	LOP	C17-C18-C19-C20
6	M	1005	SMA	C9-C10-C11-C22
7	A	1021	LOP	C17-C18-C19-C20
7	J	1024	LOP	C17-C18-C19-C20
6	D	1002	SMA	C11-C10-C9-C2
6	D	1002	SMA	O14-C14-C15-C16
7	D	1022	LOP	C17-C18-C19-C20
7	A	1021	LOP	O5-C4-C5-O6
8	P	1106	UQ2	C9-C11-C12-C13
5	A	501	HEM	C2B-C3B-CAB-CBB
5	B	301	HEM	C2B-C3B-CAB-CBB
5	B	301	HEM	C2C-C3C-CAC-CBC
5	D	501	HEM	C2C-C3C-CAC-CBC
5	H	301	HEM	C2B-C3B-CAB-CBB
5	K	301	HEM	C2B-C3B-CAB-CBB
5	Q	301	HEM	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
6	A	1001	SMA	C15-C14-O14-C25
8	D	1102	UQ2	C4-C3-O3-CM3
8	P	1106	UQ2	C4-C3-O3-CM3
5	E	301	HEM	C4B-C3B-CAB-CBB
5	G	502	HEM	C4C-C3C-CAC-CBC
5	K	301	HEM	C4C-C3C-CAC-CBC
5	N	301	HEM	C4B-C3B-CAB-CBB
5	N	301	HEM	C4C-C3C-CAC-CBC
8	A	1101	UQ2	C1-C6-C7-C8
8	G	1103	UQ2	C1-C6-C7-C8
8	M	1105	UQ2	C1-C6-C7-C8
6	D	1002	SMA	C13-C14-C15-C16
6	P	1006	SMA	C6-C7-O7-C7M
7	G	1023	LOP	O2-C3-C4-C5
7	A	1021	LOP	C3-C4-C5-O6
6	D	1002	SMA	C4A-C5-O5-C5M
6	G	1003	SMA	O14-C14-C15-C16
6	M	1005	SMA	O14-C14-C15-C16
8	A	1101	UQ2	C1-C2-O2-CM2
6	P	1006	SMA	C6-C5-O5-C5M
7	J	1024	LOP	C3-O2-P1-O4
7	M	1025	LOP	C3-O2-P1-O4
6	D	1002	SMA	C6-C5-O5-C5M
8	G	1103	UQ2	C4-C3-O3-CM3
7	M	1025	LOP	C14-C15-C16-C17
8	G	1103	UQ2	C5-C6-C7-C8
8	A	1101	UQ2	C3-C2-O2-CM2
5	B	301	HEM	C4B-C3B-CAB-CBB
5	E	301	HEM	C4C-C3C-CAC-CBC
5	H	301	HEM	C4B-C3B-CAB-CBB
5	J	502	HEM	C4B-C3B-CAB-CBB
5	K	301	HEM	C4B-C3B-CAB-CBB
5	Q	301	HEM	C4C-C3C-CAC-CBC
6	P	1006	SMA	C4A-C5-O5-C5M
5	K	301	HEM	CAA-CBA-CGA-O2A
6	M	1005	SMA	C24-C13-C14-C15
5	E	301	HEM	CAD-CBD-CGD-O2D
5	B	301	HEM	CAD-CBD-CGD-O1D
5	J	502	HEM	CAA-CBA-CGA-O1A
5	D	502	HEM	CAA-CBA-CGA-O2A
5	J	502	HEM	CAA-CBA-CGA-O2A
5	M	502	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
8	G	1103	UQ2	C2-C3-O3-CM3
5	B	301	HEM	CAD-CBD-CGD-O2D
5	G	501	HEM	CAA-CBA-CGA-O1A
5	A	501	HEM	CAA-CBA-CGA-O2A
5	A	502	HEM	CAD-CBD-CGD-O2D
5	D	501	HEM	CAA-CBA-CGA-O1A
5	E	301	HEM	CAA-CBA-CGA-O2A
5	P	502	HEM	CAA-CBA-CGA-O1A
5	D	502	HEM	C3D-CAD-CBD-CGD
5	M	502	HEM	C3D-CAD-CBD-CGD
5	E	301	HEM	CAD-CBD-CGD-O1D
5	M	502	HEM	CAA-CBA-CGA-O2A
7	J	1024	LOP	O5-C4-C5-O6
5	D	502	HEM	CAD-CBD-CGD-O1D
5	G	502	HEM	CAD-CBD-CGD-O1D
5	H	301	HEM	CAA-CBA-CGA-O2A
5	K	301	HEM	CAA-CBA-CGA-O1A
5	A	501	HEM	CAA-CBA-CGA-O1A
5	J	502	HEM	CAD-CBD-CGD-O1D
5	M	502	HEM	CAD-CBD-CGD-O1D
5	Q	301	HEM	CAA-CBA-CGA-O2A
7	P	1026	LOP	C17-C18-C19-C20
5	P	502	HEM	CAA-CBA-CGA-O2A
5	A	502	HEM	CAD-CBD-CGD-O1D
5	D	501	HEM	CAA-CBA-CGA-O2A
5	M	502	HEM	CAD-CBD-CGD-O2D
5	D	502	HEM	CAA-CBA-CGA-O1A
5	G	502	HEM	C3D-CAD-CBD-CGD
7	P	1026	LOP	C27-C28-C29-C30
5	D	502	HEM	CAD-CBD-CGD-O2D
5	E	301	HEM	CAA-CBA-CGA-O1A
5	H	301	HEM	CAD-CBD-CGD-O2D
5	B	301	HEM	CAA-CBA-CGA-O2A
5	M	501	HEM	CAA-CBA-CGA-O2A
6	P	1006	SMA	C11-C10-C9-C2
5	G	501	HEM	CAA-CBA-CGA-O2A
5	J	502	HEM	CAD-CBD-CGD-O2D
7	P	1026	LOP	C14-C15-C16-C17
5	G	502	HEM	CAD-CBD-CGD-O2D
7	A	1021	LOP	C12-C13-C14-C15
5	K	301	HEM	CAD-CBD-CGD-O2D
5	Q	301	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
7	D	1022	LOP	C15-C16-C17-C18
5	M	501	HEM	CAA-CBA-CGA-O1A
5	N	301	HEM	CAD-CBD-CGD-O2D
5	E	301	HEM	C4D-C3D-CAD-CBD
5	D	502	HEM	C2C-C3C-CAC-CBC
5	P	502	HEM	C2B-C3B-CAB-CBB
5	H	301	HEM	CAA-CBA-CGA-O1A
7	D	1022	LOP	C14-C15-C16-C17
7	G	1023	LOP	C12-C13-C14-C15
7	M	1025	LOP	C12-C13-C14-C15
7	P	1026	LOP	C12-C13-C14-C15
5	B	301	HEM	CAA-CBA-CGA-O1A
5	P	502	HEM	CAD-CBD-CGD-O1D
5	H	301	HEM	CAD-CBD-CGD-O1D
5	P	502	HEM	CAD-CBD-CGD-O2D
5	G	502	HEM	CAA-CBA-CGA-O2A
5	G	502	HEM	CAA-CBA-CGA-O1A
5	N	301	HEM	CAD-CBD-CGD-O1D
5	K	301	HEM	CAD-CBD-CGD-O1D
5	A	502	HEM	C4C-C3C-CAC-CBC
5	B	301	HEM	C4C-C3C-CAC-CBC
5	G	501	HEM	C4B-C3B-CAB-CBB
5	G	501	HEM	C4C-C3C-CAC-CBC
5	H	301	HEM	C4C-C3C-CAC-CBC
5	P	501	HEM	C4B-C3B-CAB-CBB
5	Q	301	HEM	C4B-C3B-CAB-CBB
5	A	502	HEM	CAA-CBA-CGA-O2A
5	A	502	HEM	CAA-CBA-CGA-O1A
7	J	1024	LOP	C12-C13-C14-C15
7	J	1024	LOP	C14-C15-C16-C17
7	A	1021	LOP	O2-C3-C4-C5
8	D	1102	UQ2	C2-C3-O3-CM3
7	D	1022	LOP	C12-C13-C14-C15
7	P	1026	LOP	C30-C31-C32-C33
6	M	1005	SMA	C24-C13-C14-O14
5	P	501	HEM	CAA-CBA-CGA-O1A
5	P	501	HEM	CAA-CBA-CGA-O2A
7	A	1021	LOP	O6-C24-C25-C26
7	A	1021	LOP	O5-C6-C7-C8
7	G	1023	LOP	O5-C6-C7-C8
6	G	1003	SMA	C11-C10-C9-C2
6	G	1003	SMA	C4A-C5-O5-C5M

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Mol	Chain	Res	Type	Atoms
5	N	301	HEM	CAA-CBA-CGA-O2A
7	M	1025	LOP	O6-C24-C25-C26
8	M	1105	UQ2	C4-C3-O3-CM3
7	G	1023	LOP	O7-C6-C7-C8
5	N	301	HEM	CAA-CBA-CGA-O1A
7	A	1021	LOP	C14-C15-C16-C17
7	A	1021	LOP	O8-C24-C25-C26
6	A	1001	SMA	C11-C10-C9-C2
5	Q	301	HEM	CAD-CBD-CGD-O2D
7	J	1024	LOP	O6-C24-C25-C26

There are no ring outliers.

38 monomers are involved in 108 short contacts:

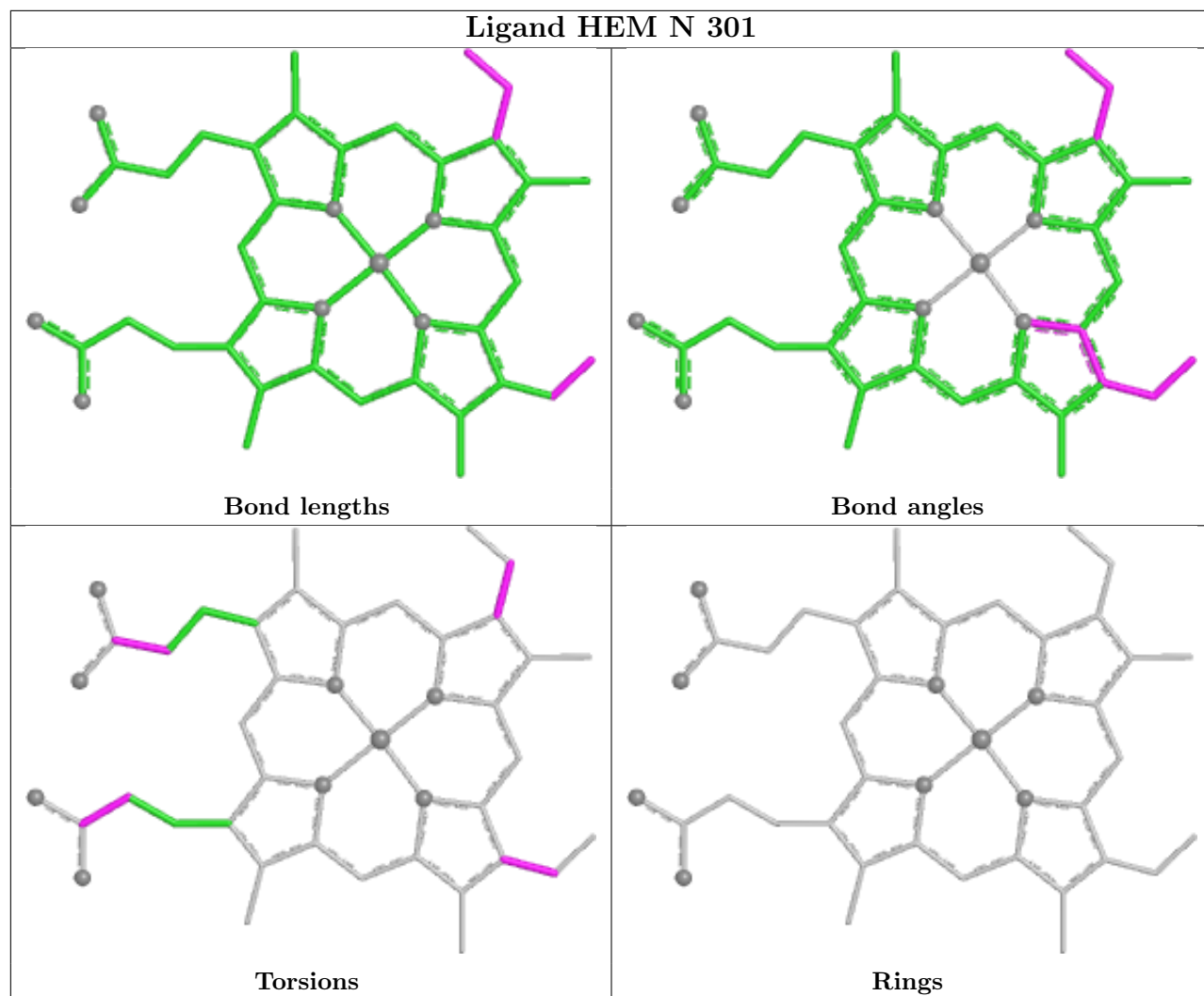
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	N	301	HEM	3	0
5	K	301	HEM	2	0
5	D	501	HEM	6	0
7	P	1026	LOP	2	0
5	E	301	HEM	1	0
5	A	502	HEM	4	0
7	A	1021	LOP	6	0
8	D	1102	UQ2	2	0
9	E	1042	BGL	3	0
5	M	502	HEM	6	0
5	P	502	HEM	3	0
8	A	1101	UQ2	2	0
9	G	1043	BGL	2	0
8	J	1104	UQ2	1	0
6	P	1006	SMA	1	0
7	D	1022	LOP	2	0
9	N	1045	BGL	1	0
9	P	1046	BGL	2	0
5	J	501	HEM	9	0
5	G	502	HEM	5	0
5	P	501	HEM	4	0
5	Q	301	HEM	2	0
5	J	502	HEM	6	0
9	B	1041	BGL	1	0
7	J	1024	LOP	1	0
7	G	1023	LOP	3	0
5	M	501	HEM	3	0

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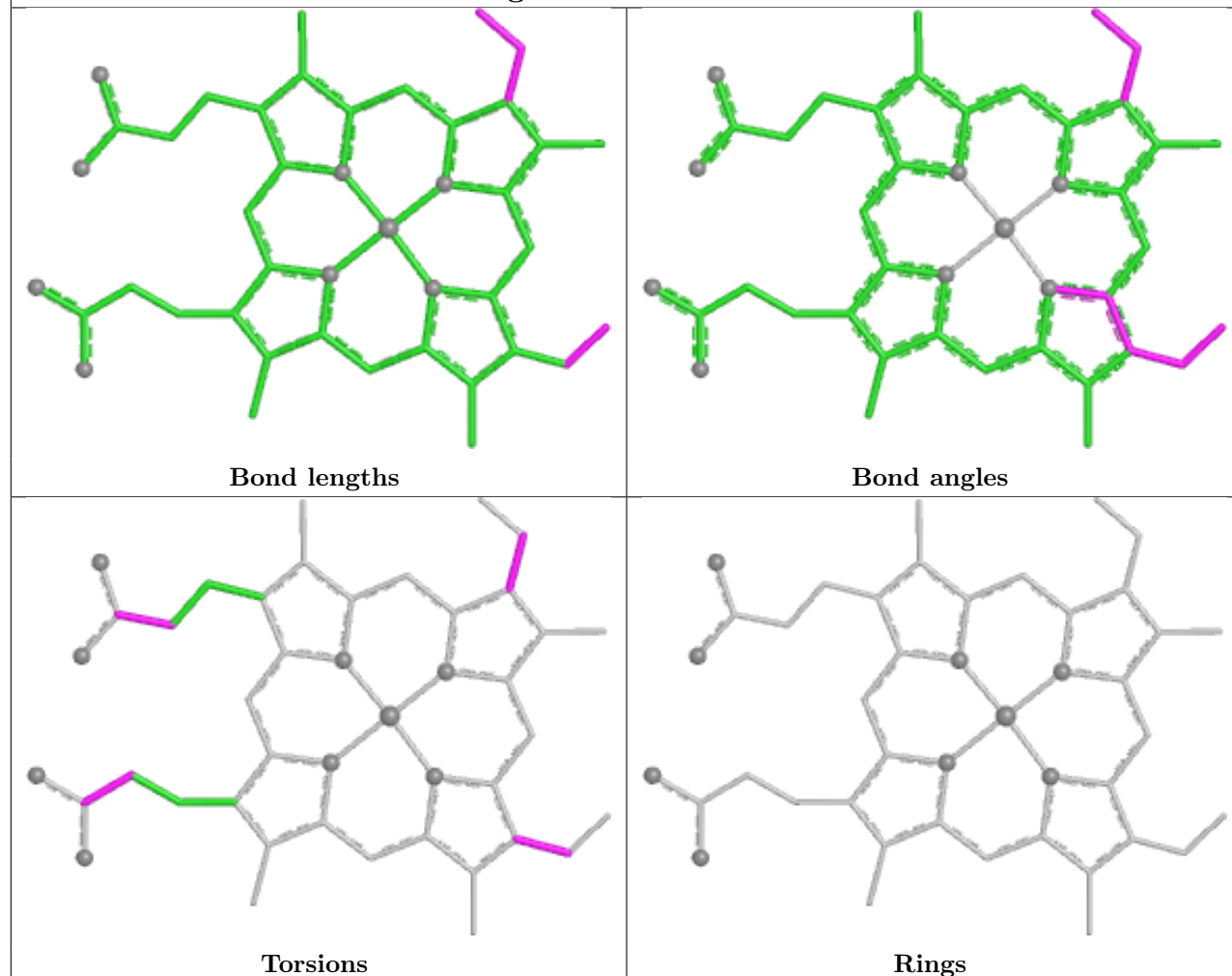
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	501	HEM	5	0
6	J	1004	SMA	1	0
5	B	301	HEM	1	0
7	M	1025	LOP	3	0
9	K	1044	BGL	2	0
5	A	501	HEM	3	0
8	M	1105	UQ2	2	0
8	P	1106	UQ2	2	0
5	H	301	HEM	1	0
8	G	1103	UQ2	2	0
5	D	502	HEM	3	0

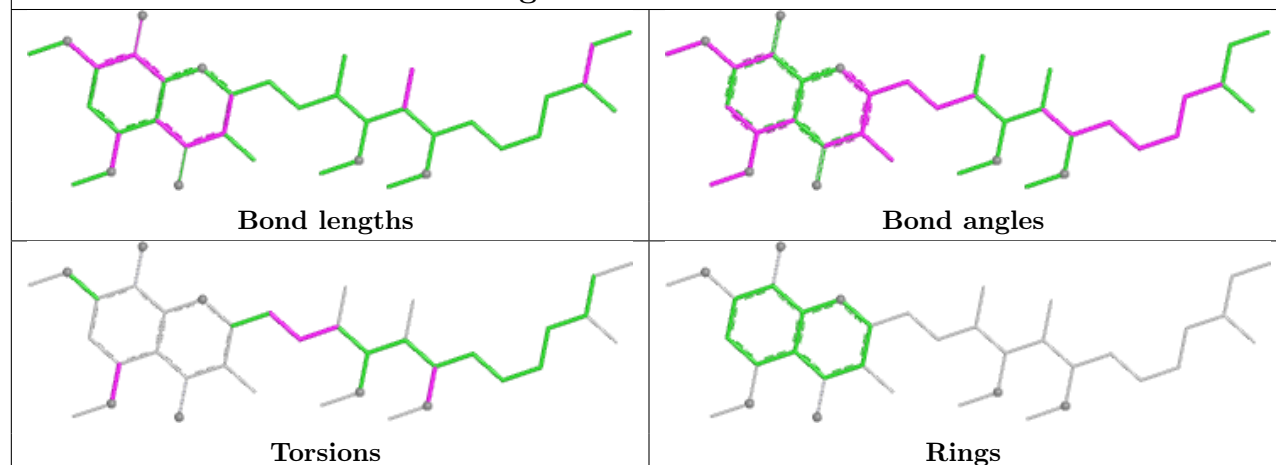
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

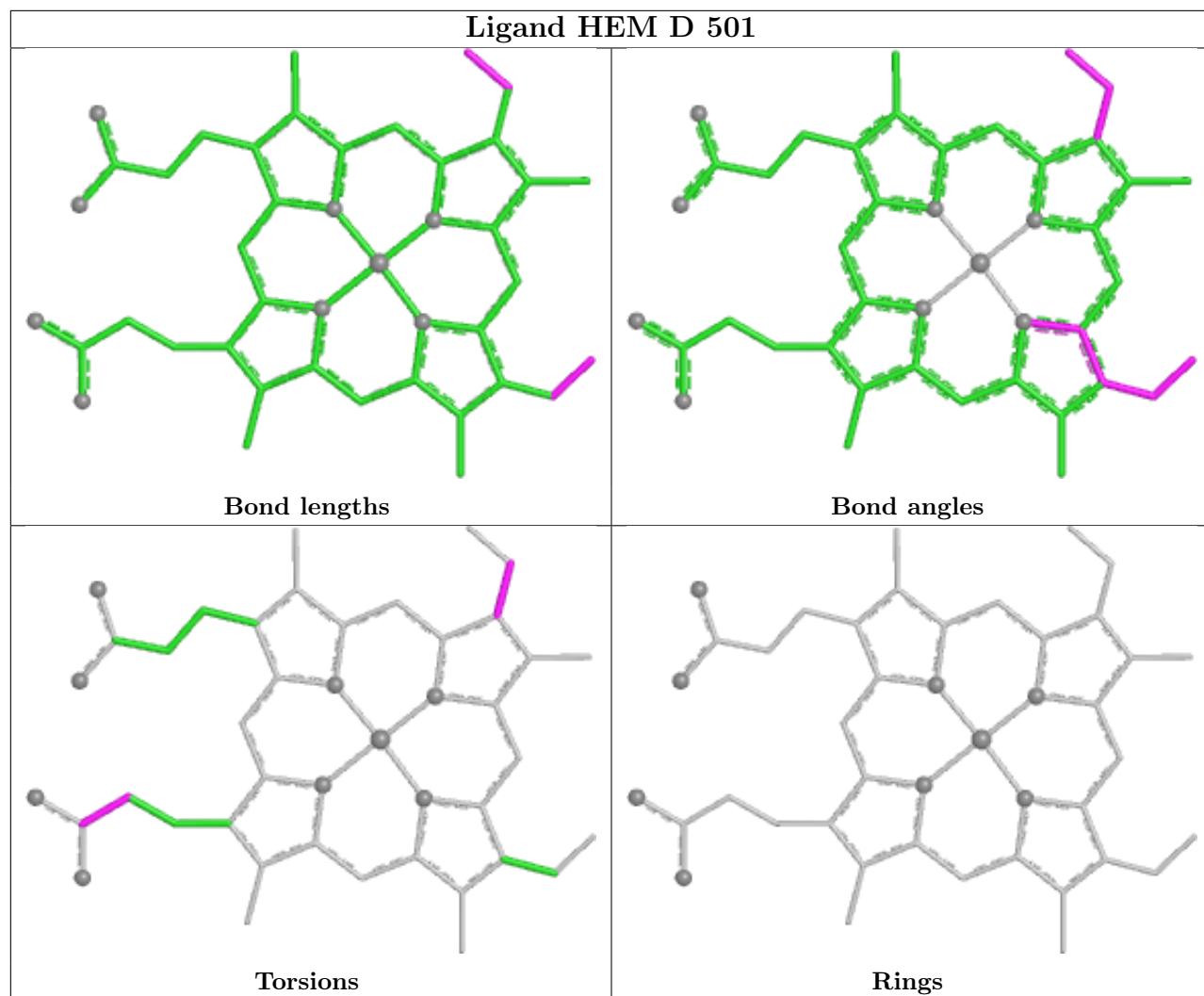


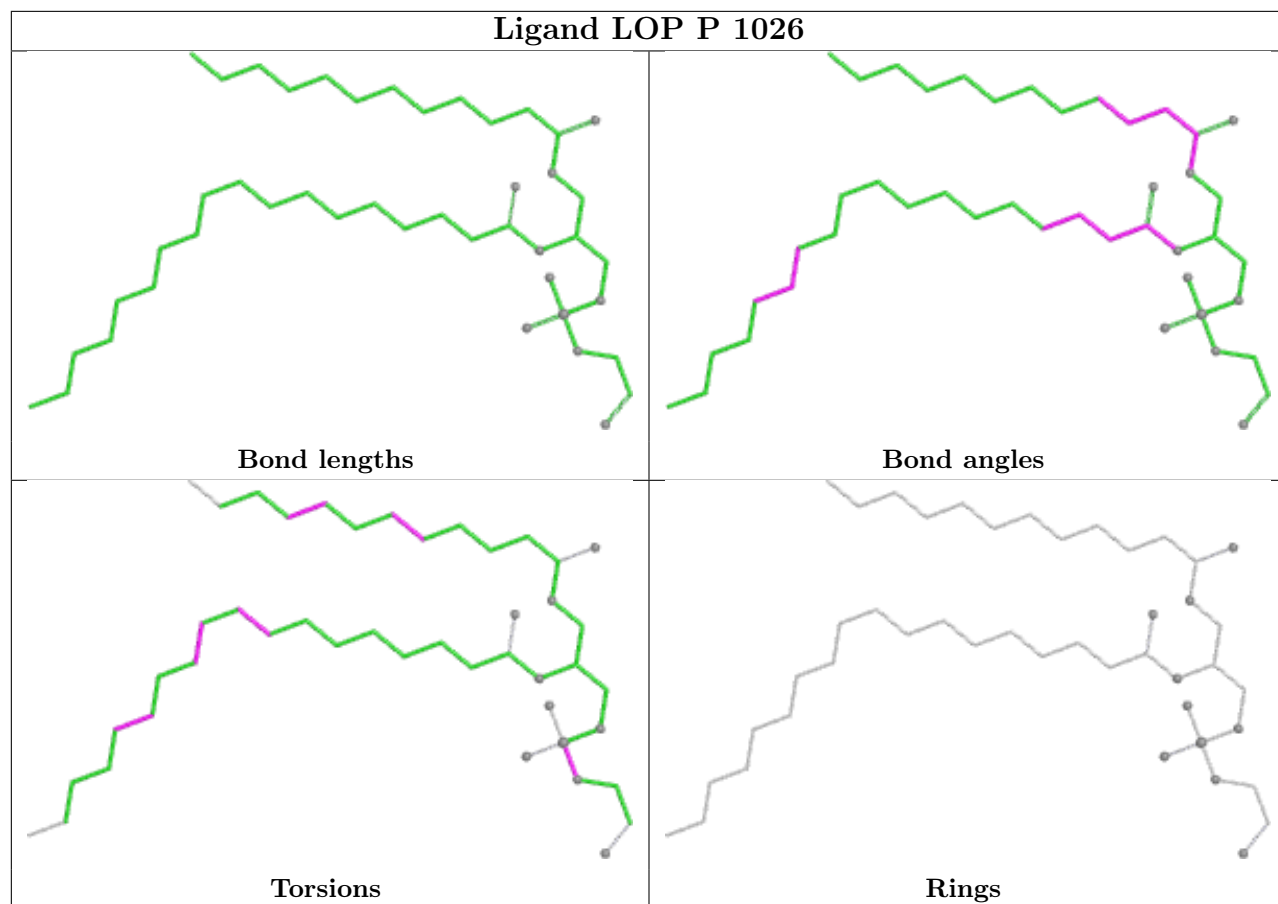
Ligand HEM K 301

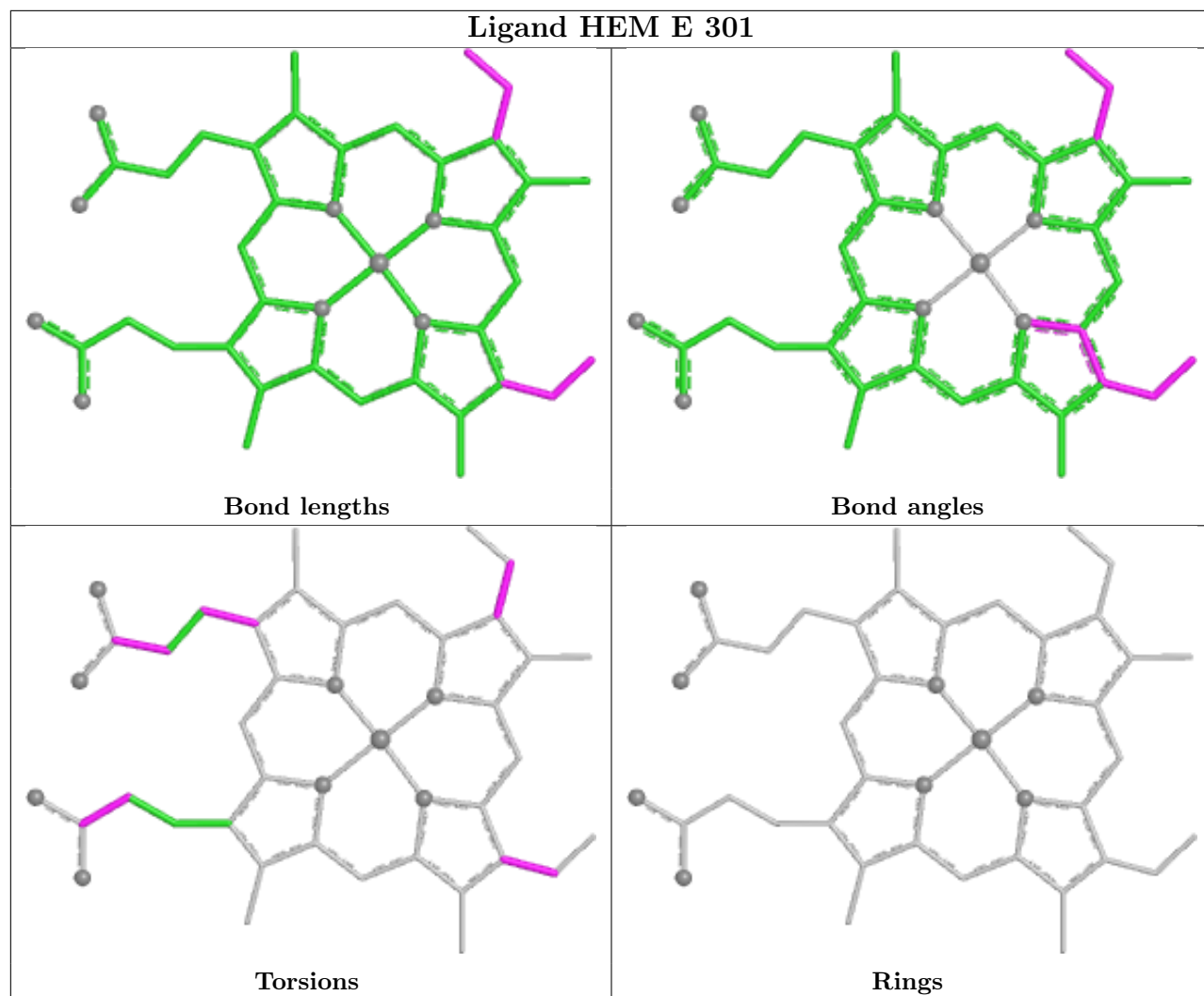


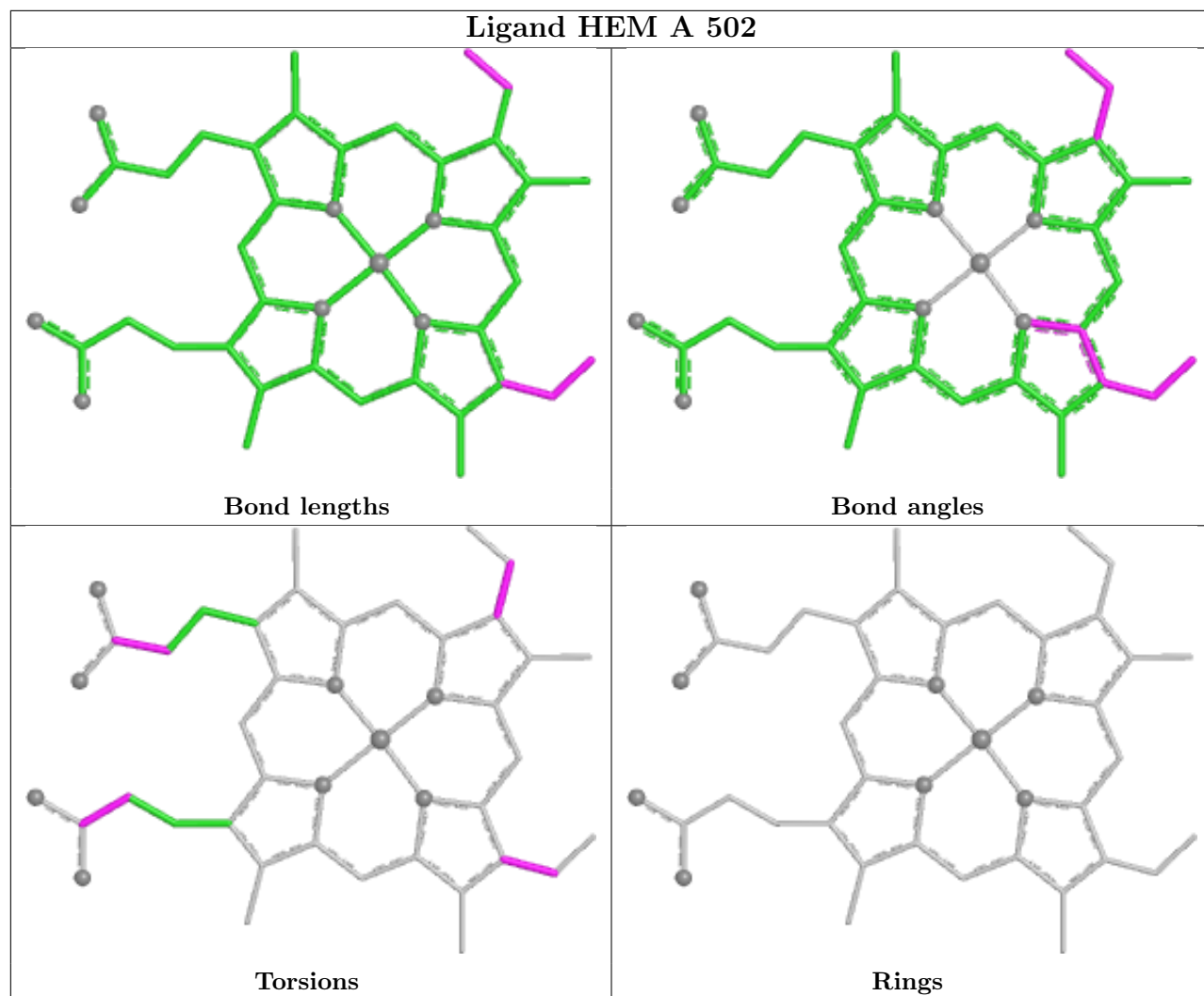
Ligand SMA A 1001

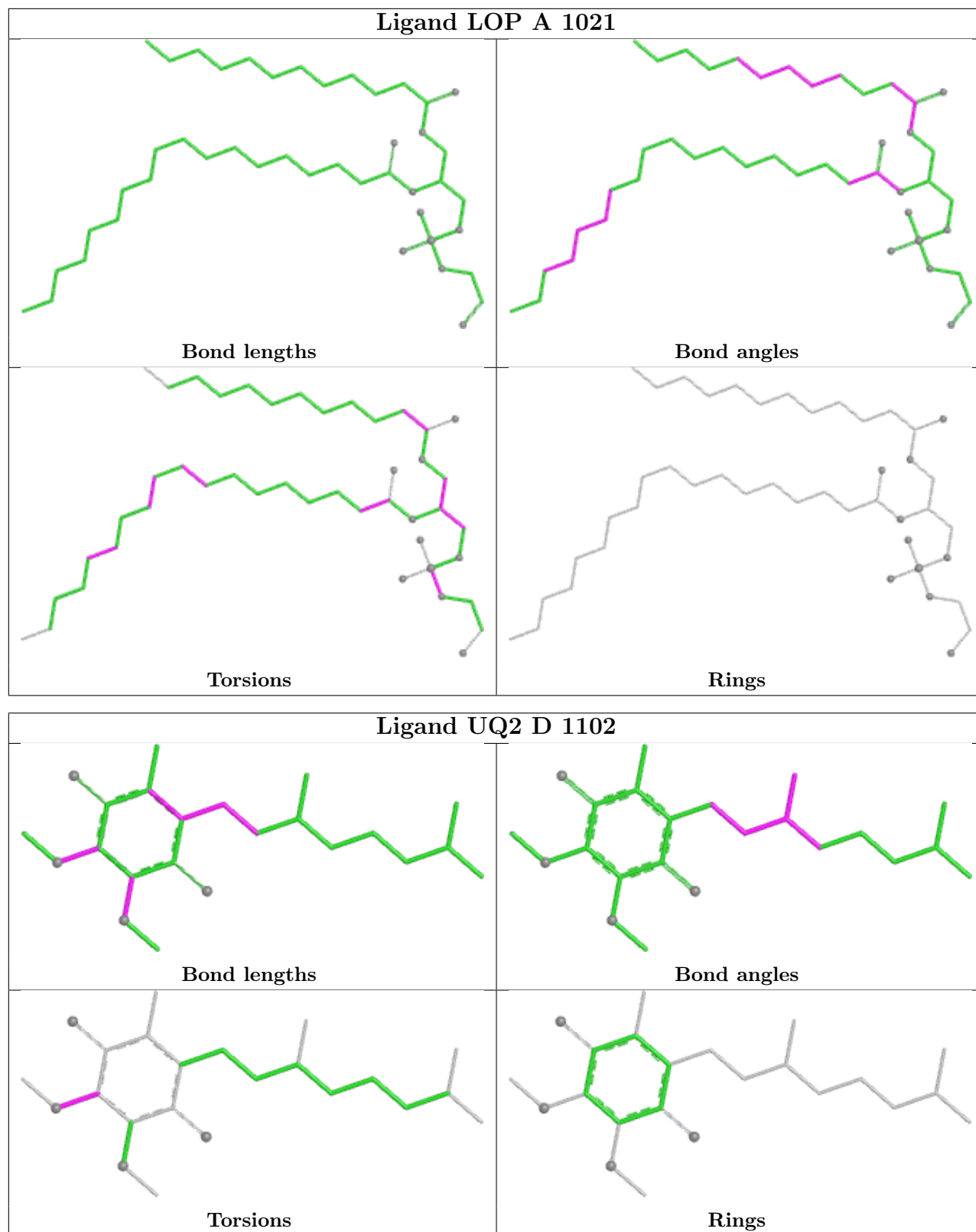




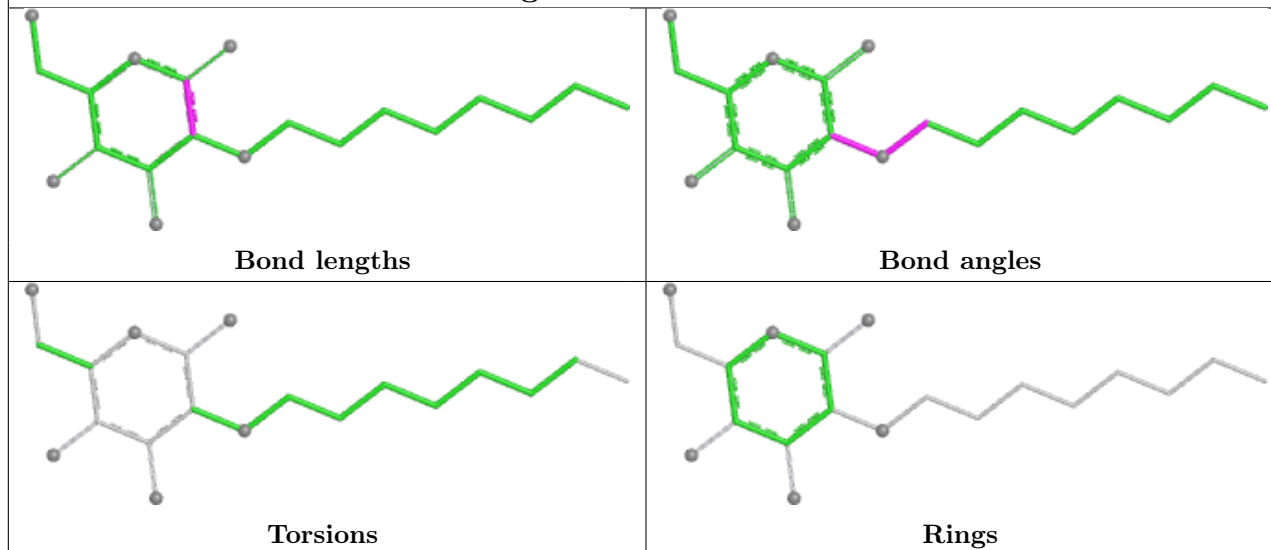




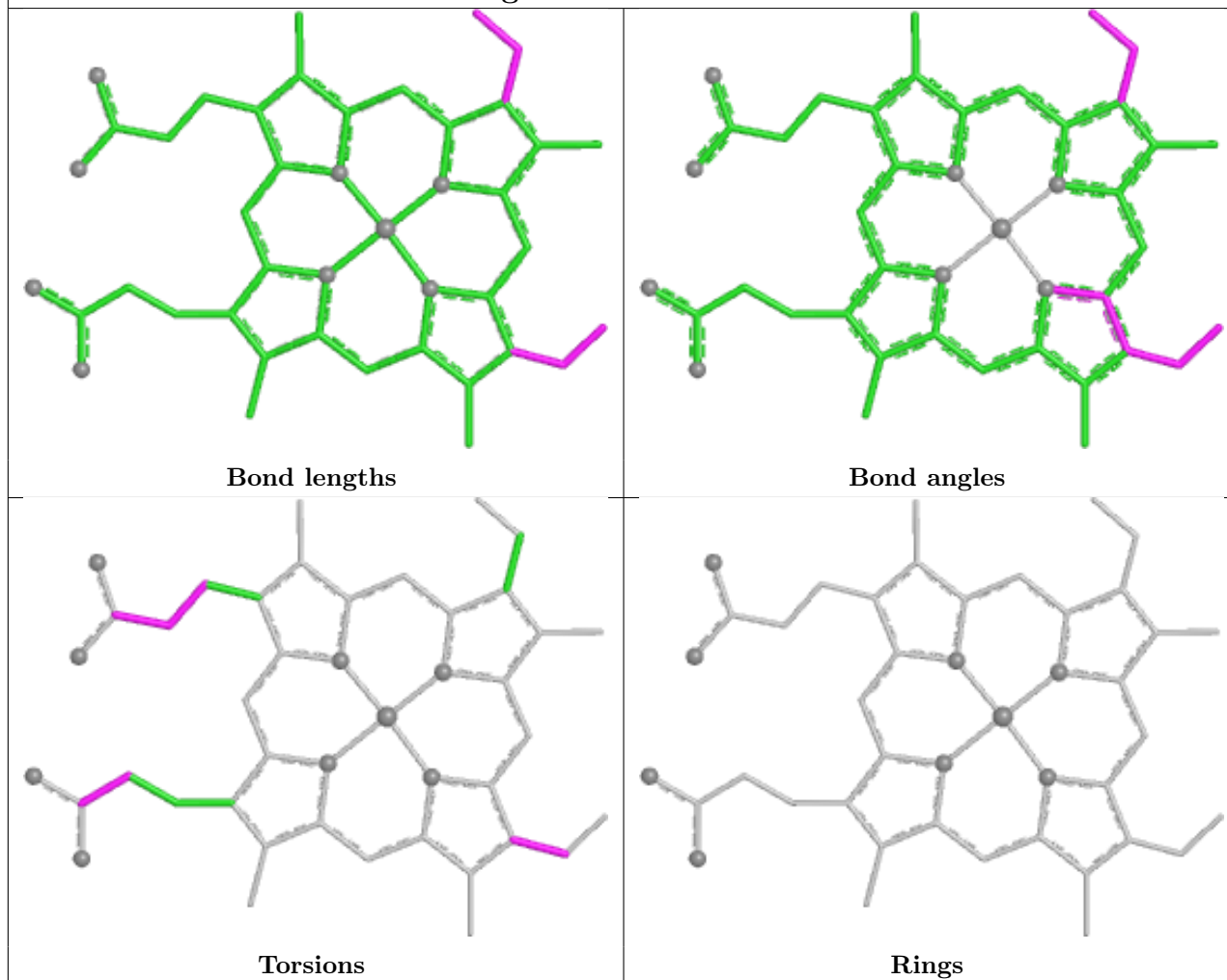


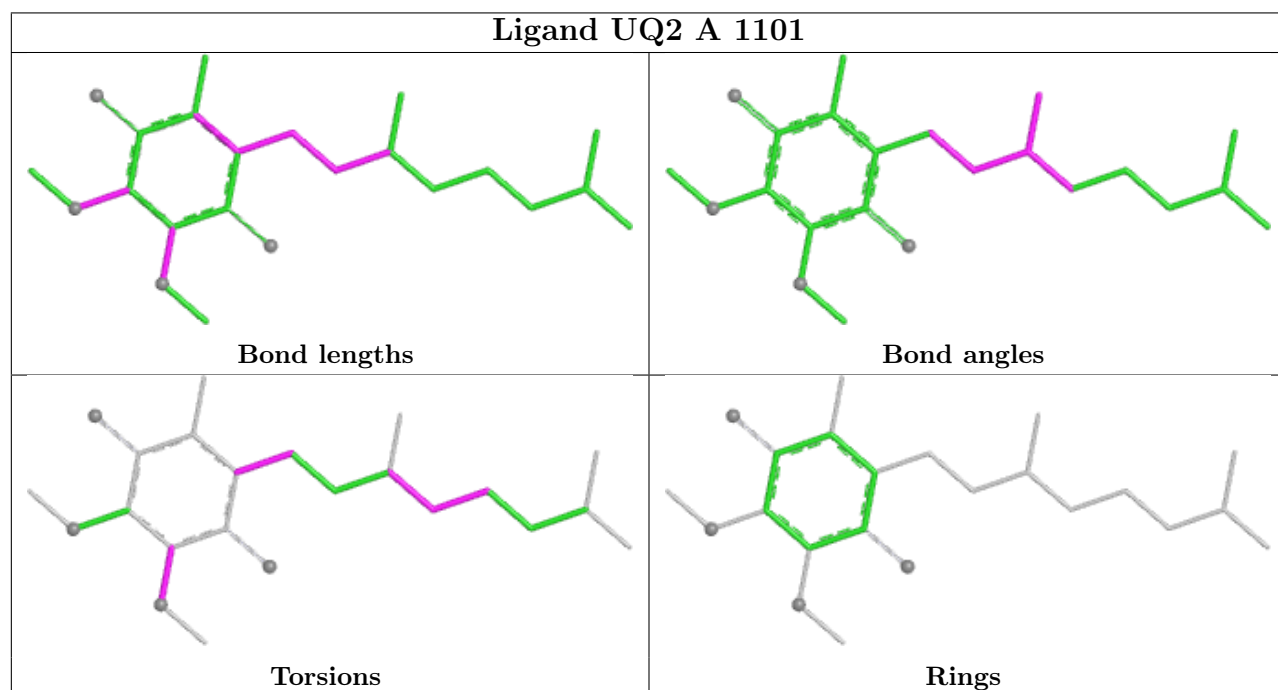
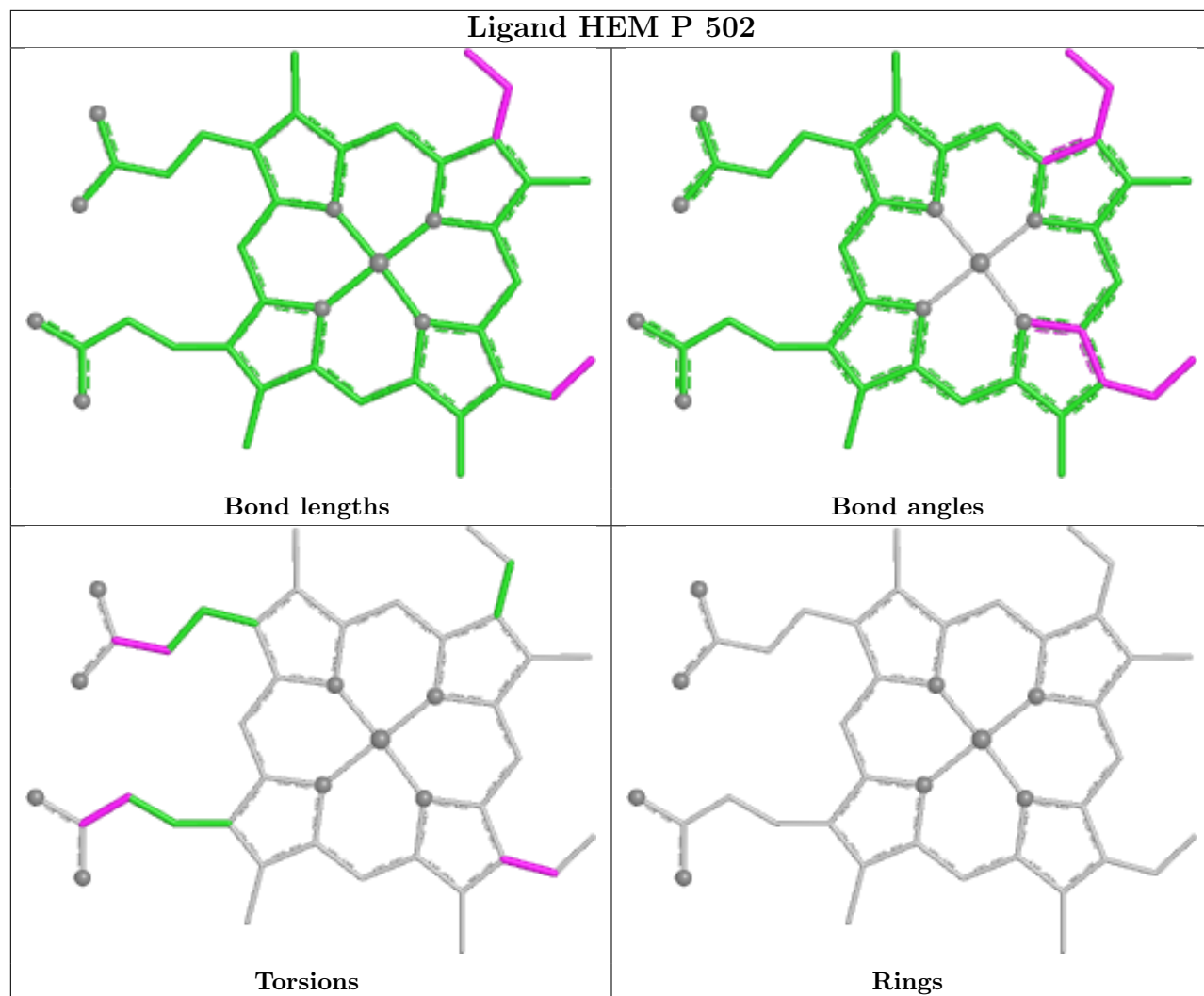


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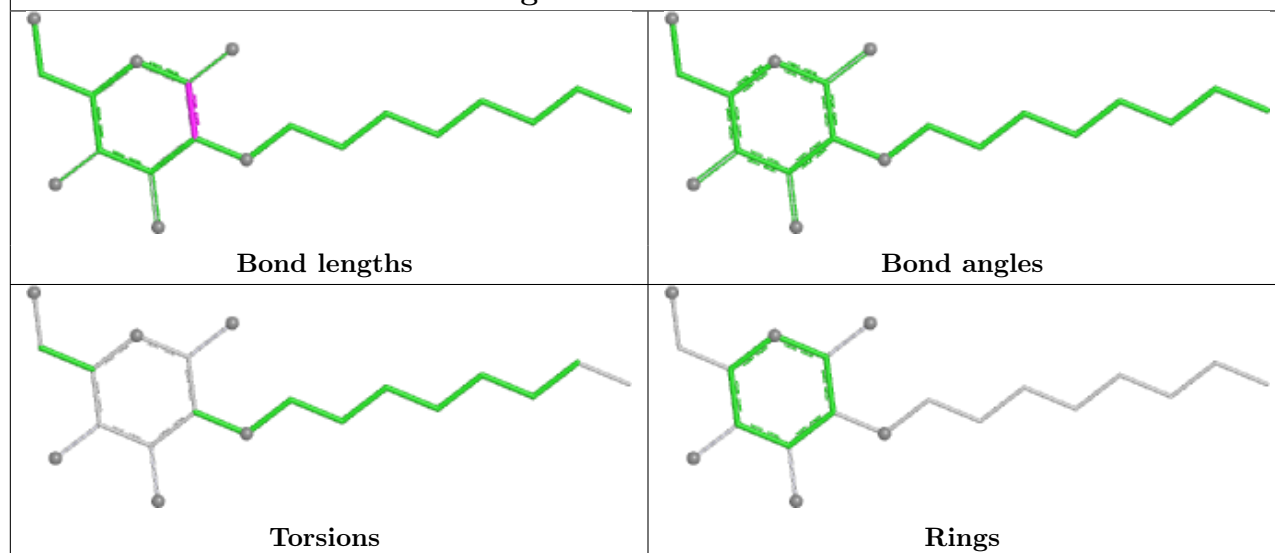


Ligand HEM M 502

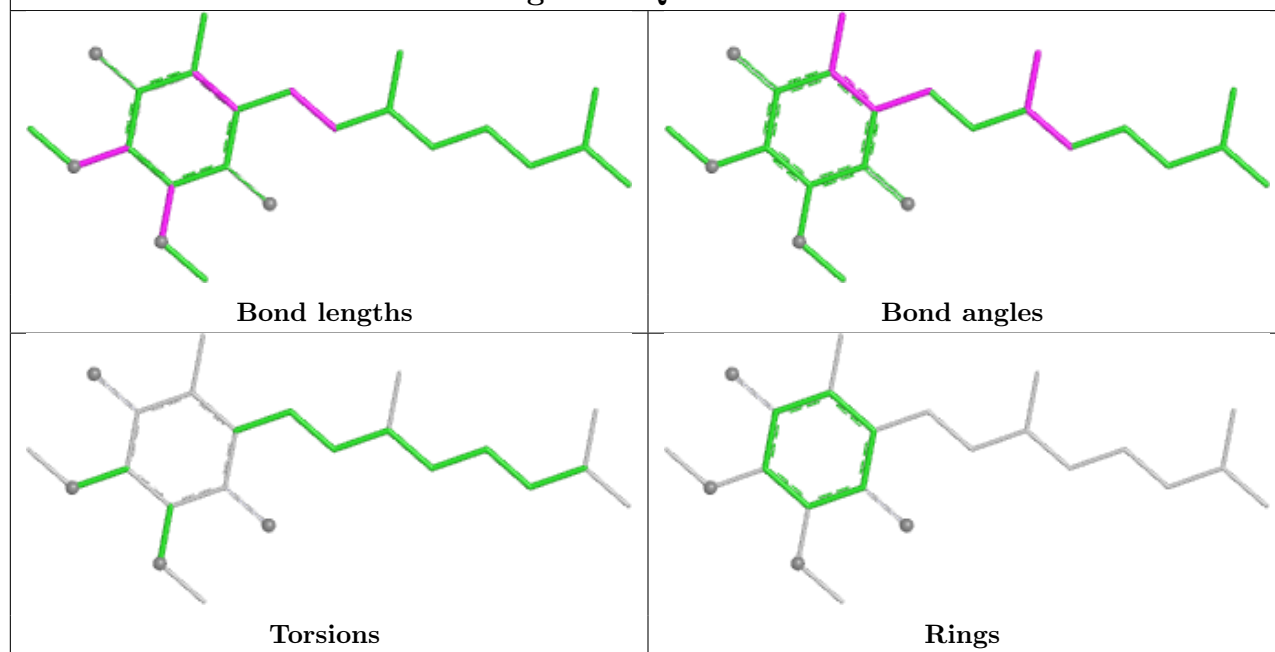


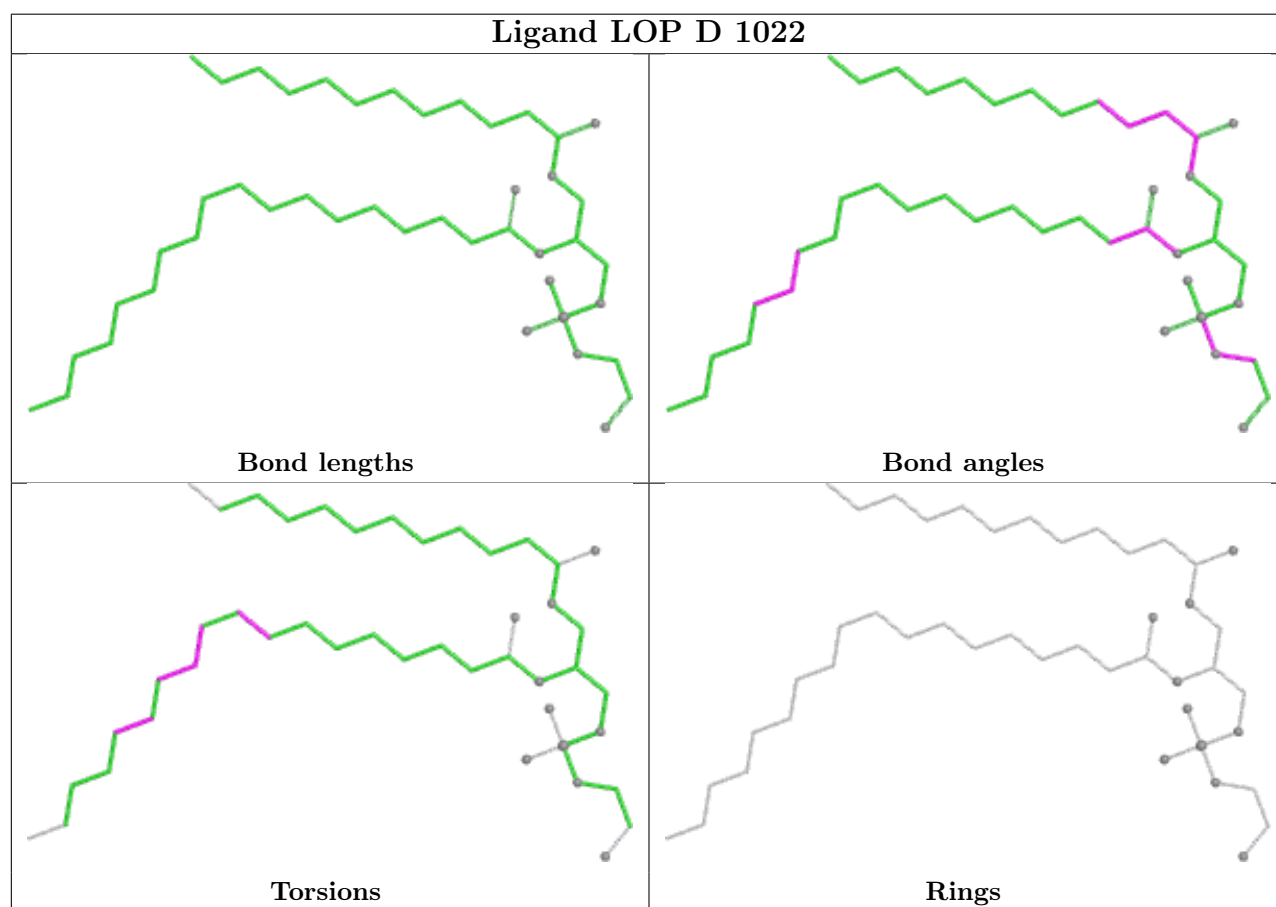
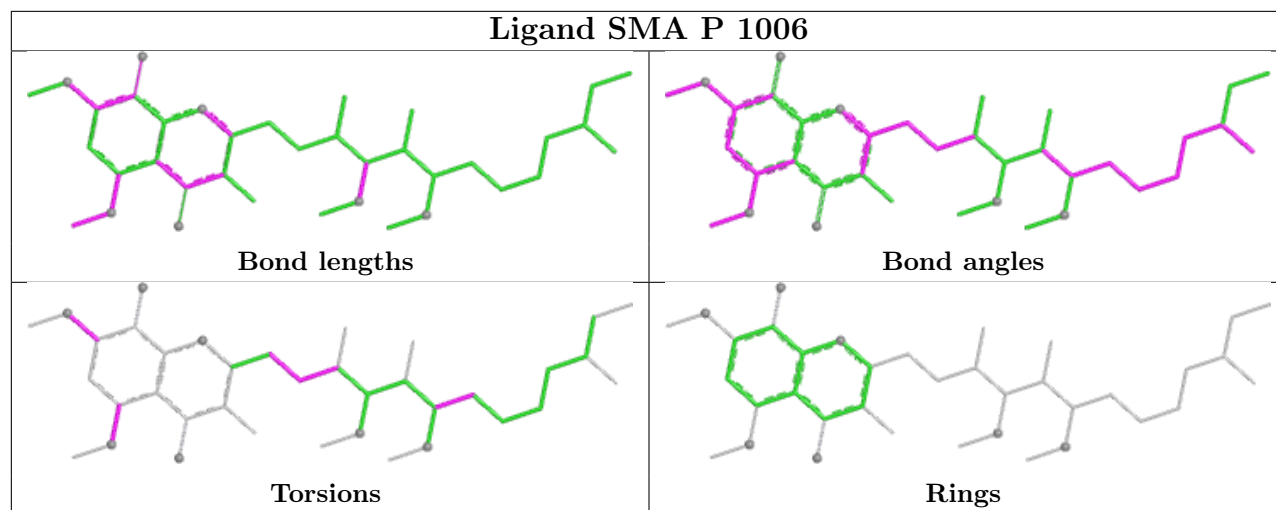


Ligand BGL G 1043

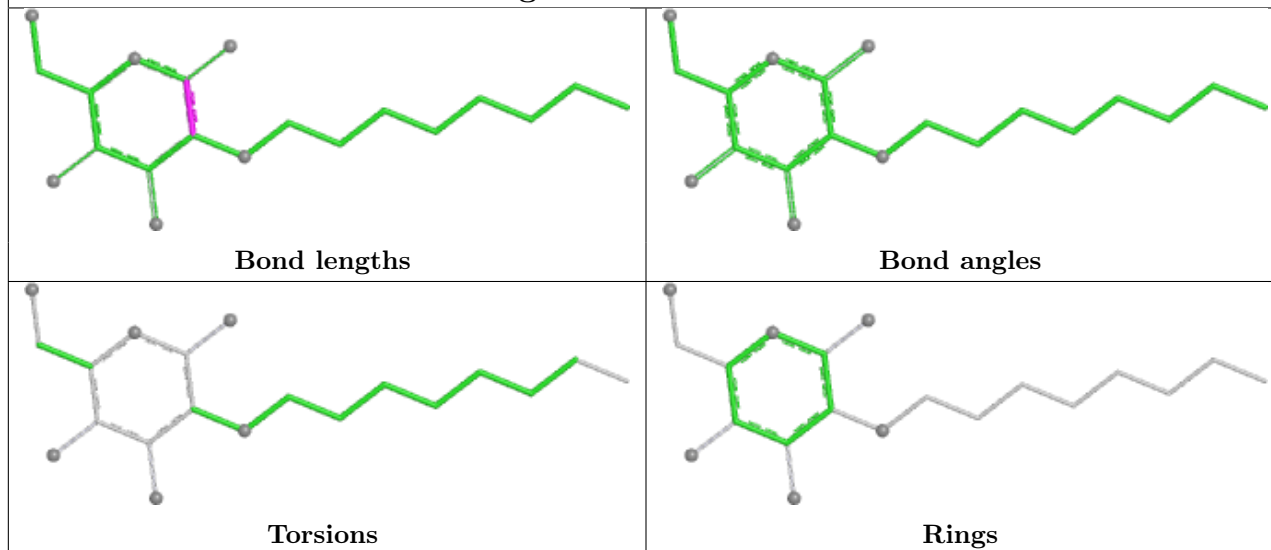


Ligand UQ2 J 1104

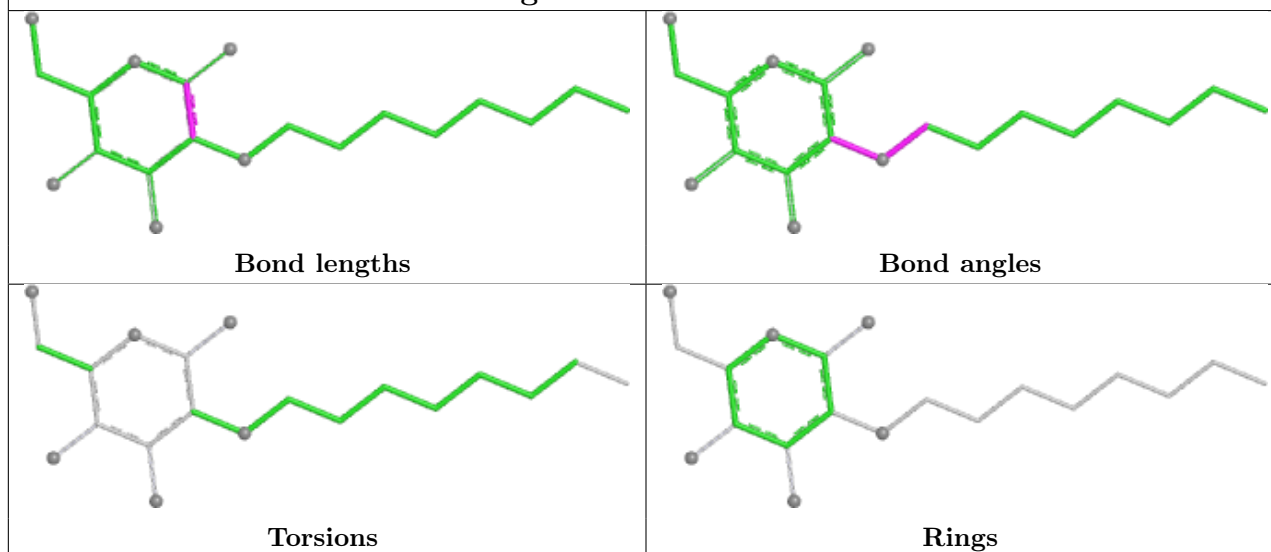




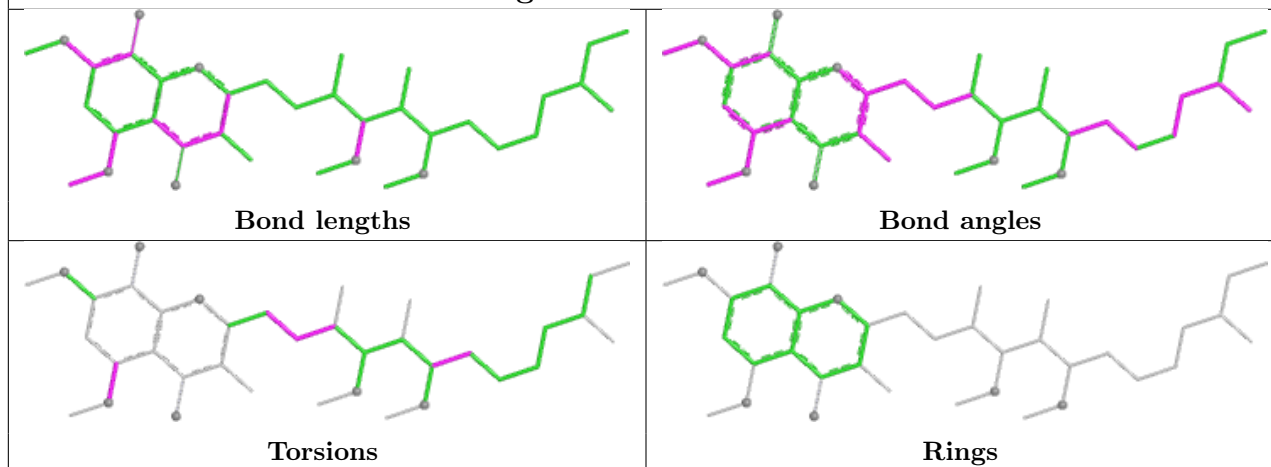
Ligand BGL N 1045

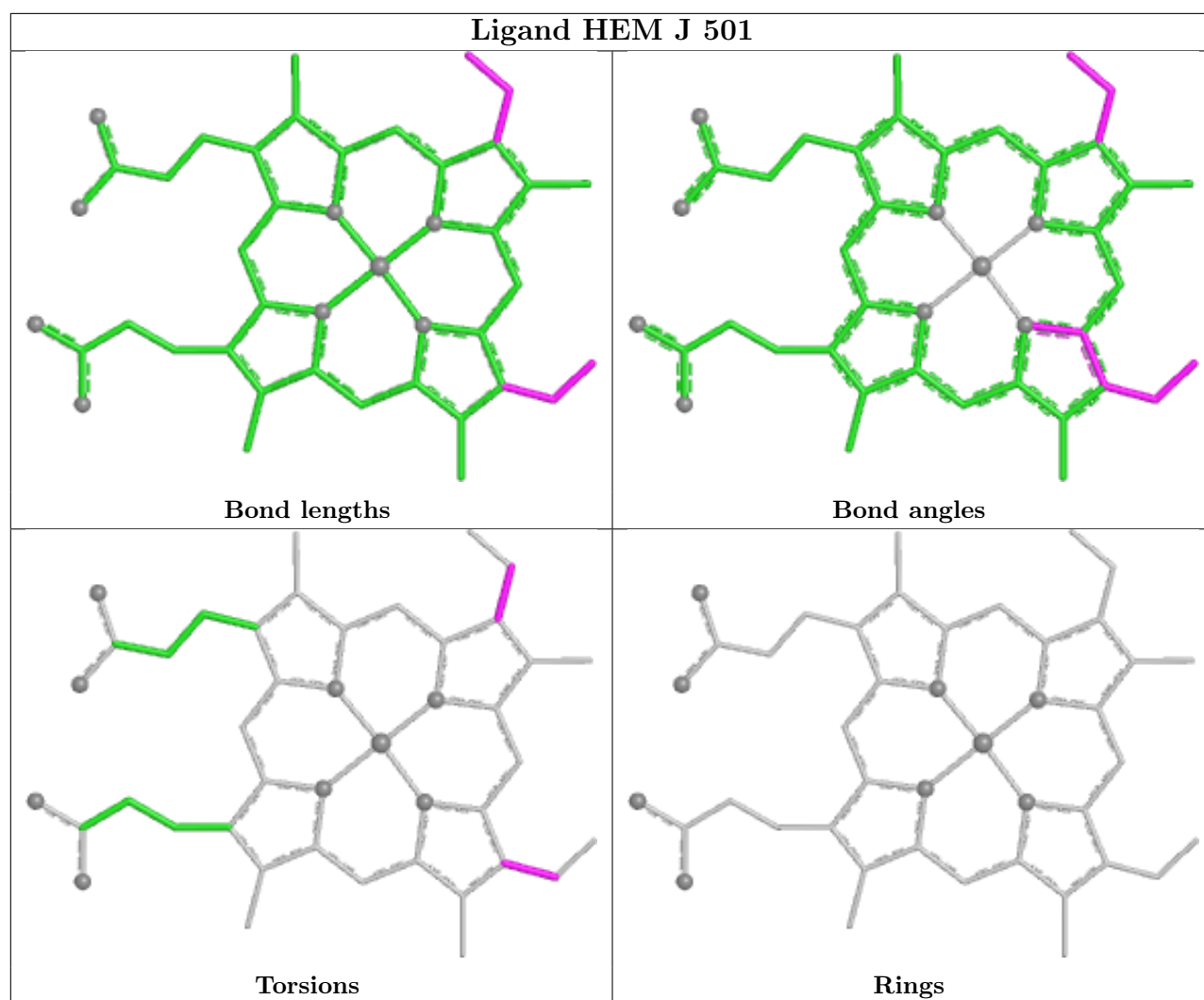


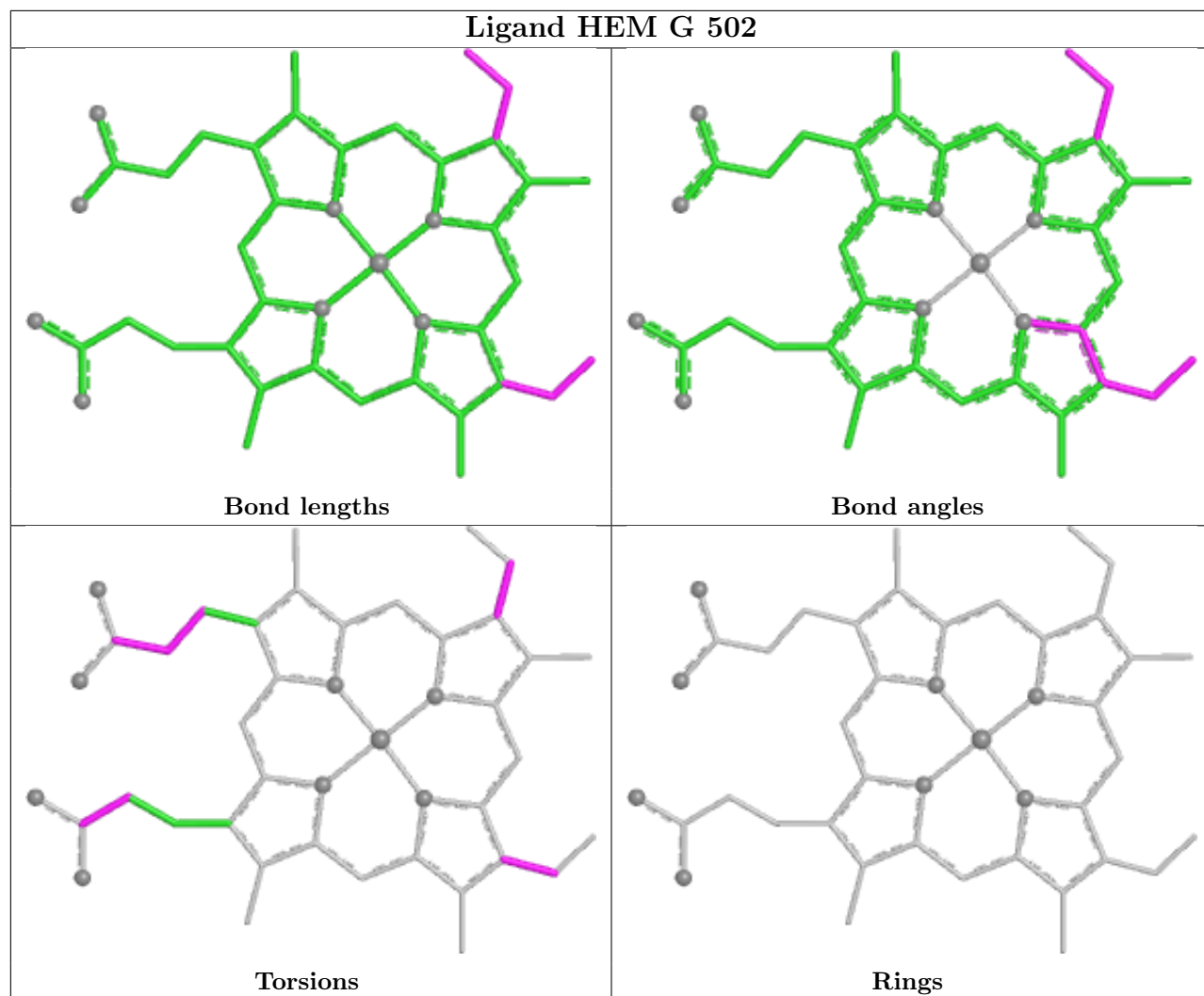
Ligand BGL P 1046

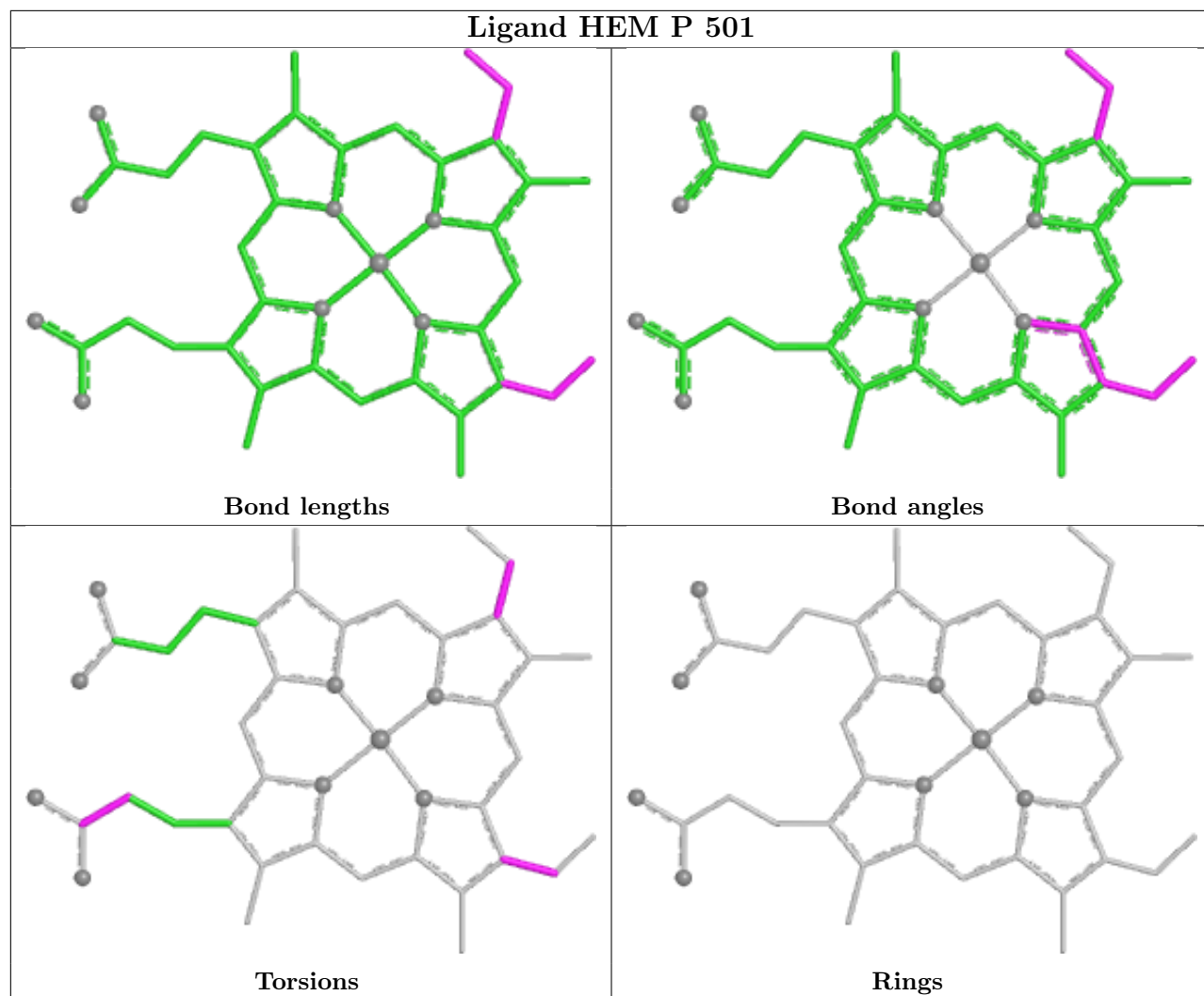


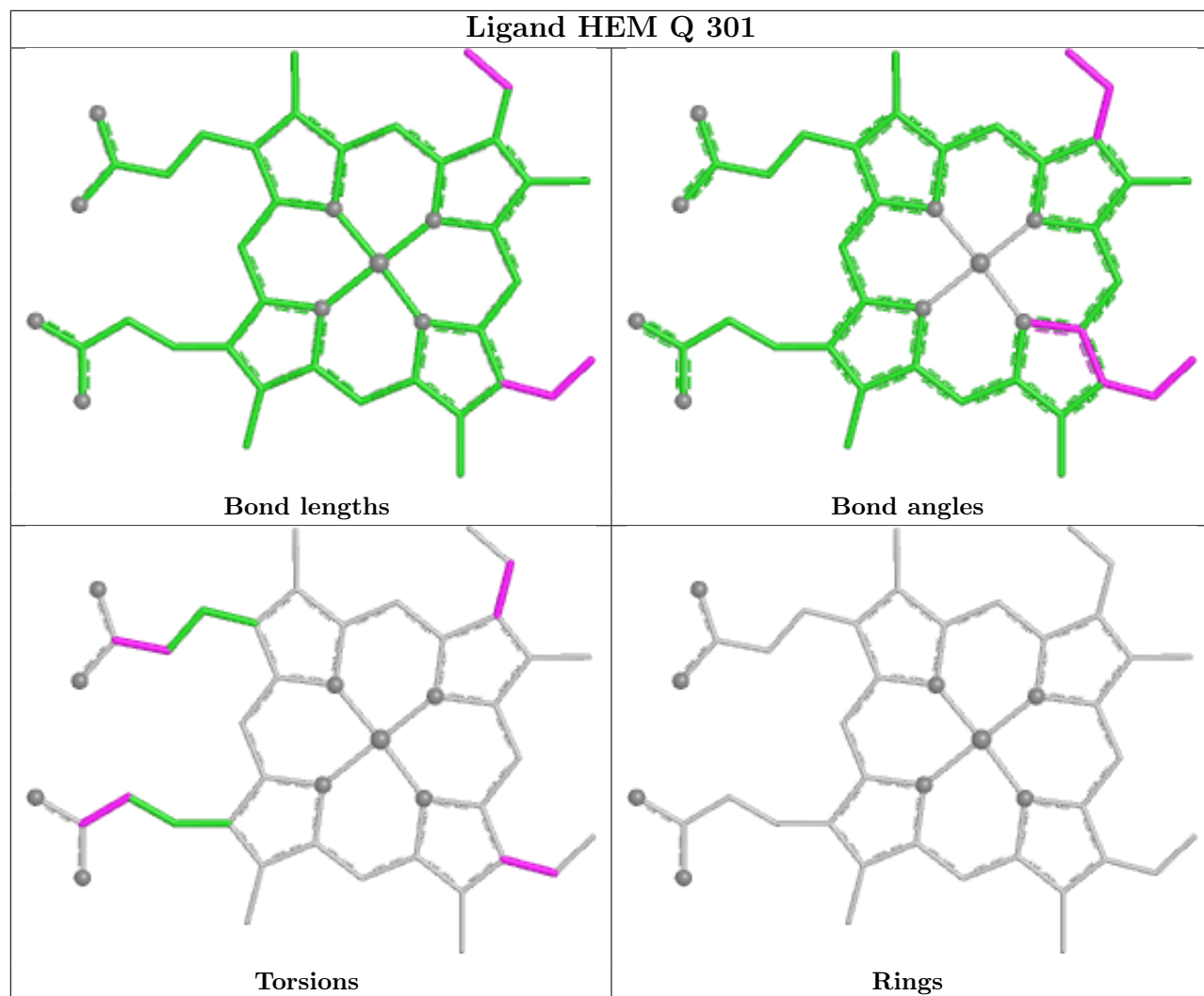
Ligand SMA D 1002



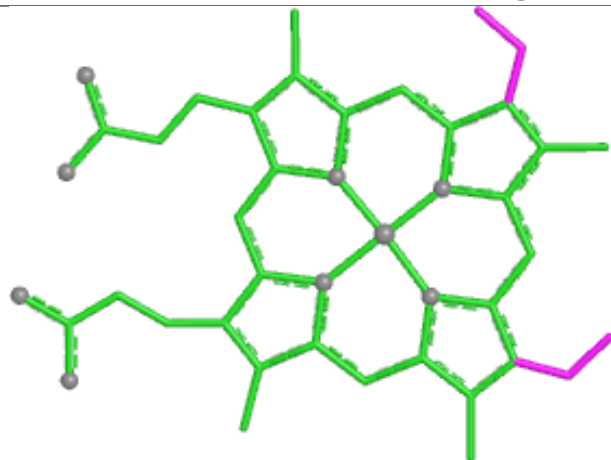




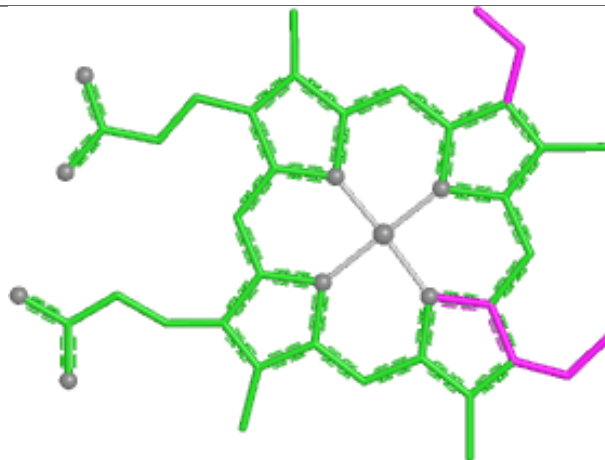




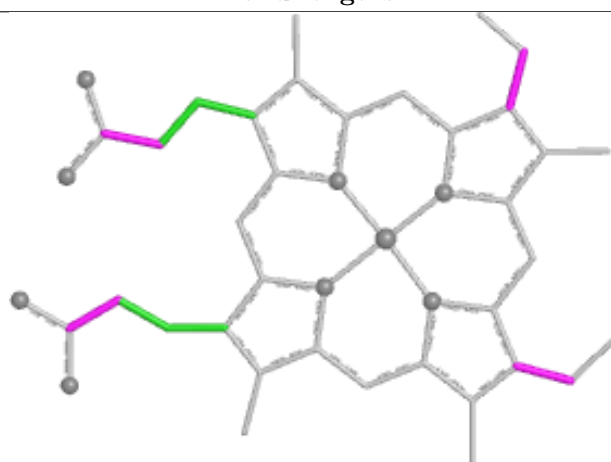
Ligand HEM J 502



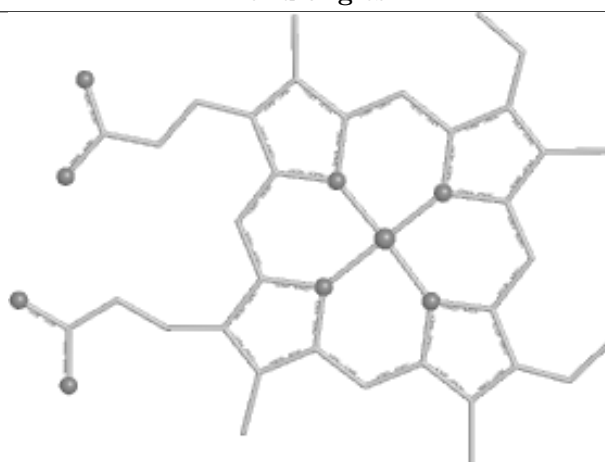
Bond lengths



Bond angles

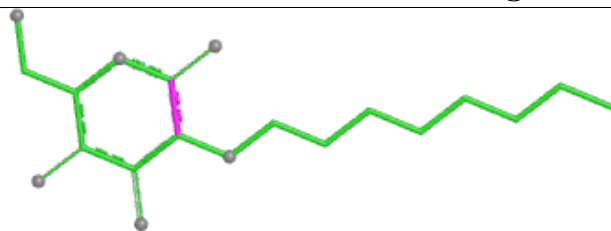


Torsions

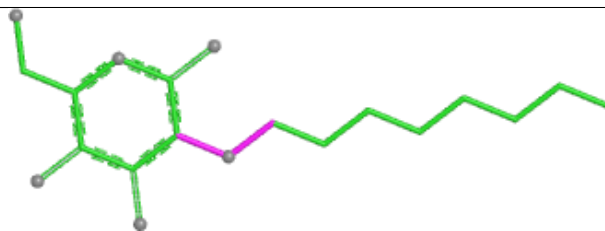


Rings

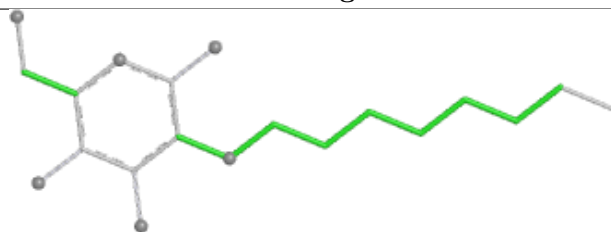
Ligand BGL B 1041



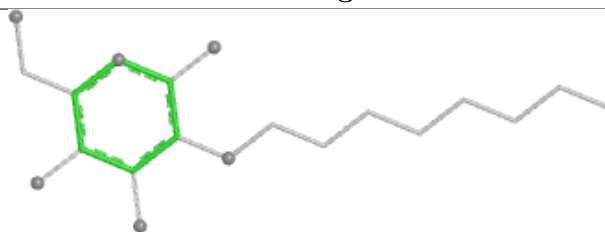
Bond lengths



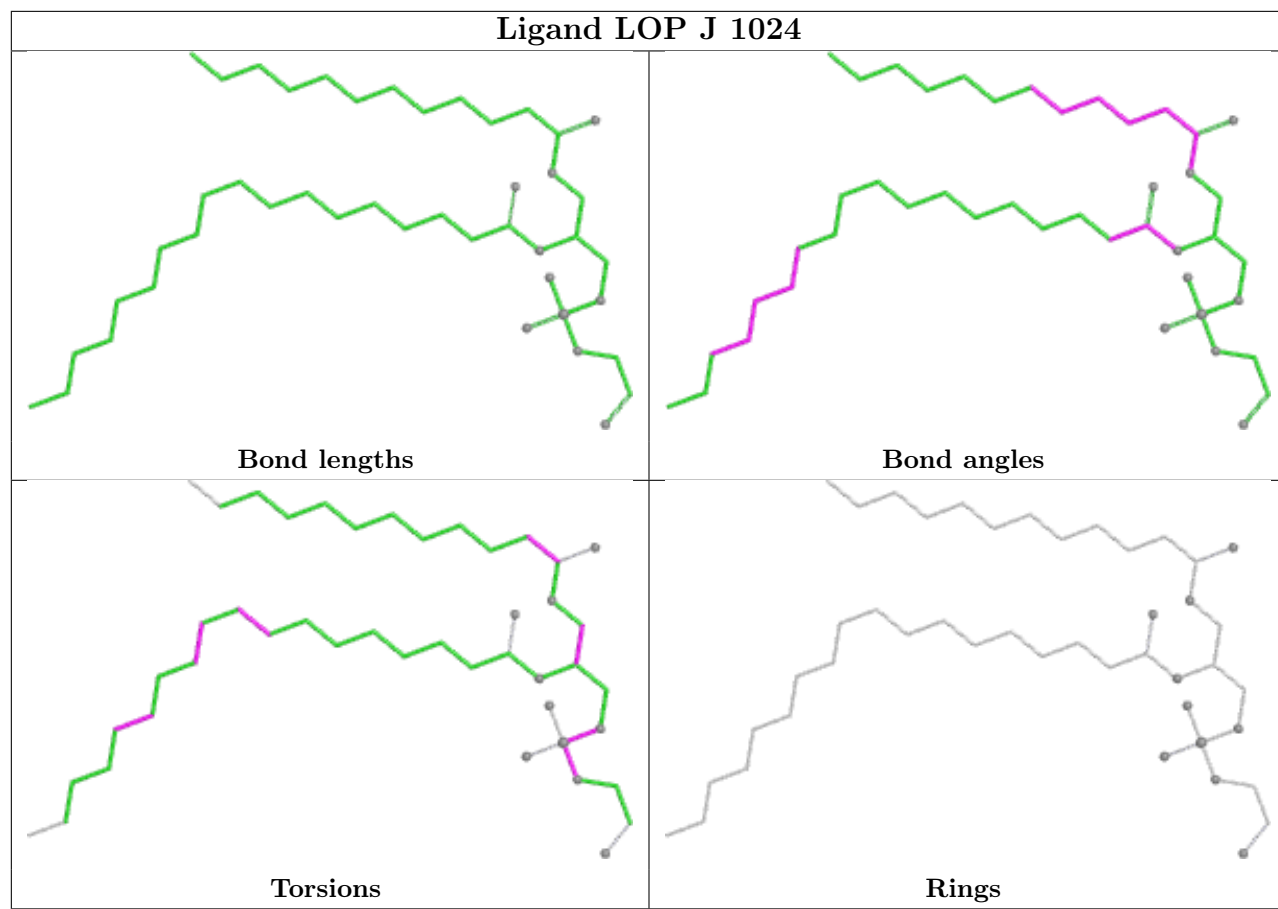
Bond angles

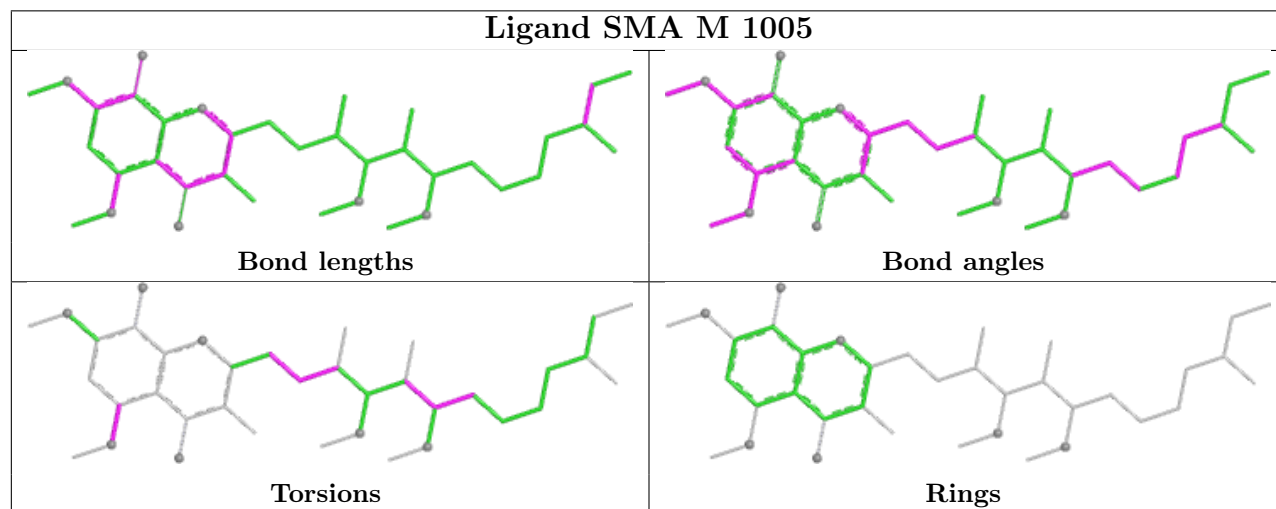
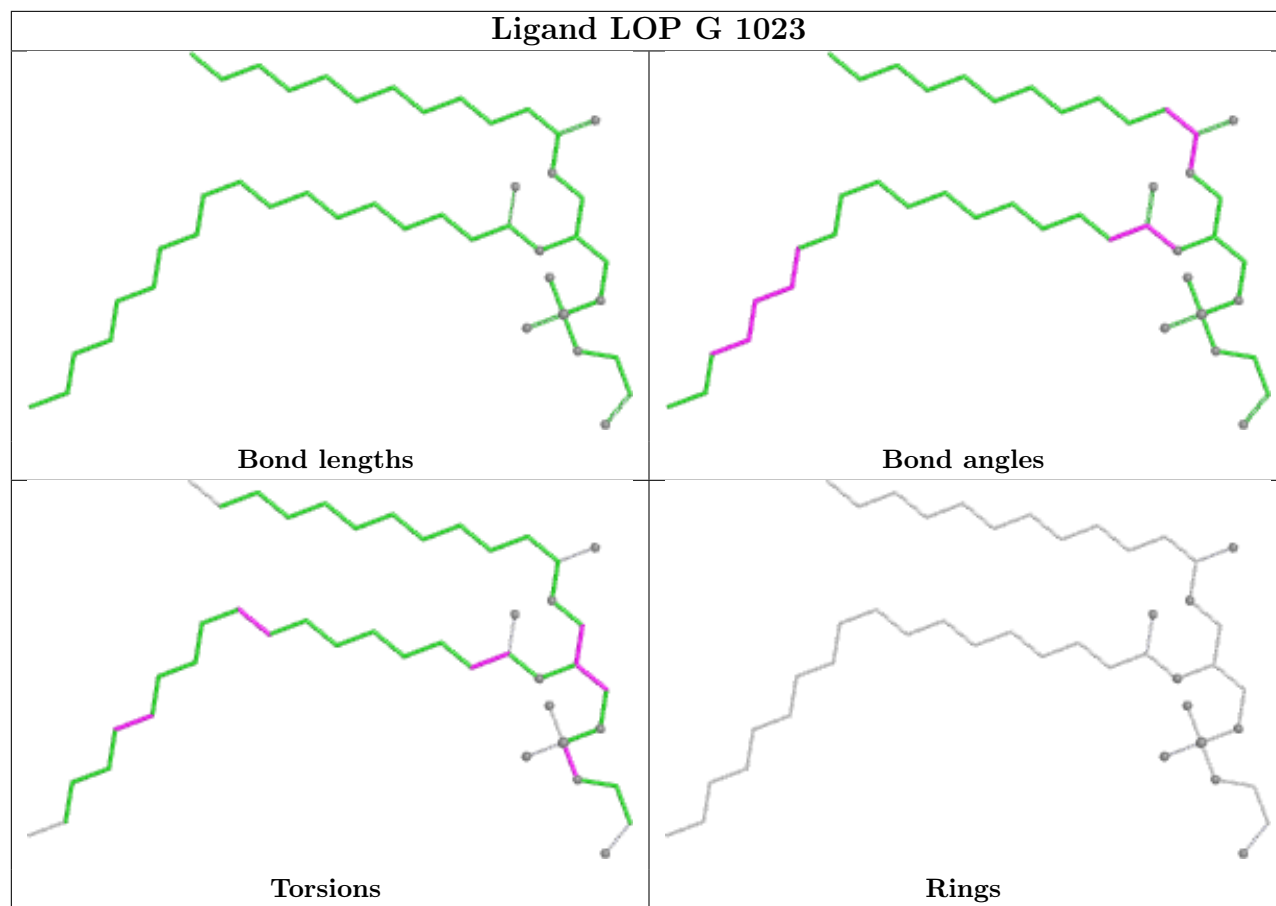


Torsions

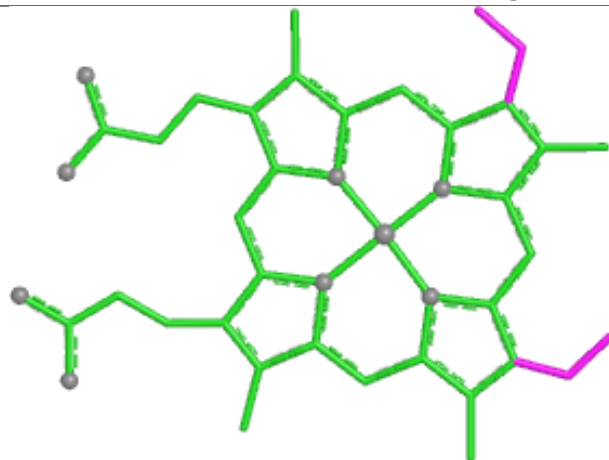


Rings

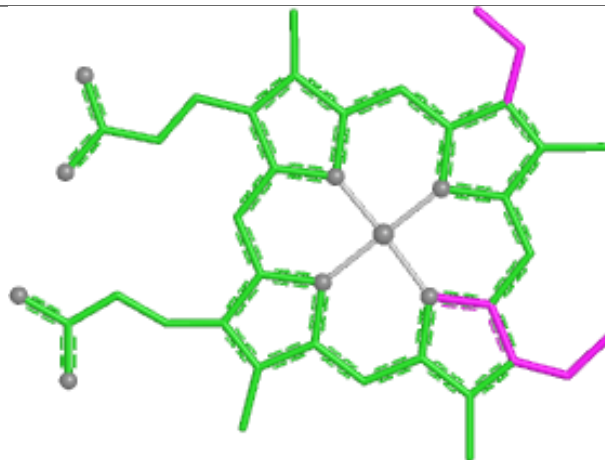




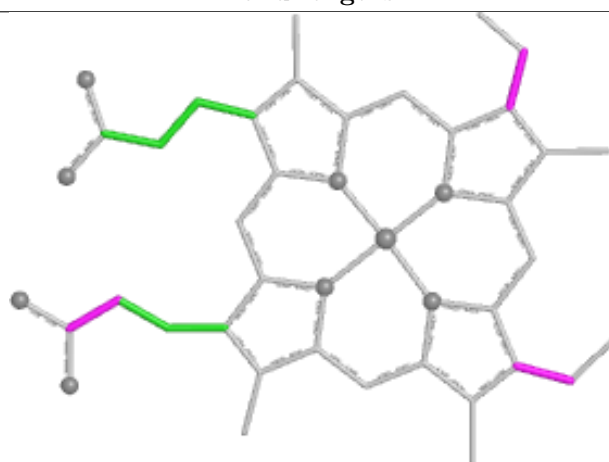
Ligand HEM M 501



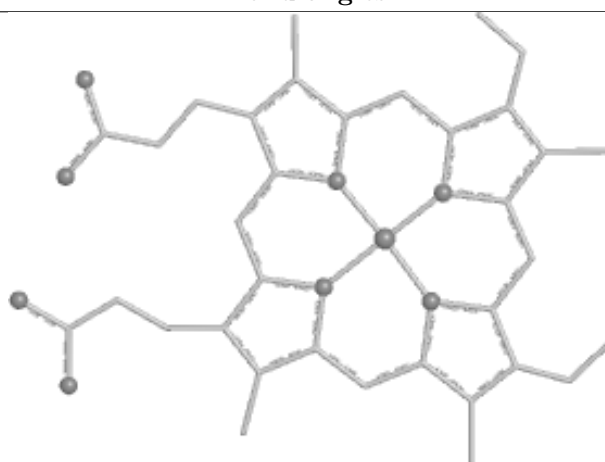
Bond lengths



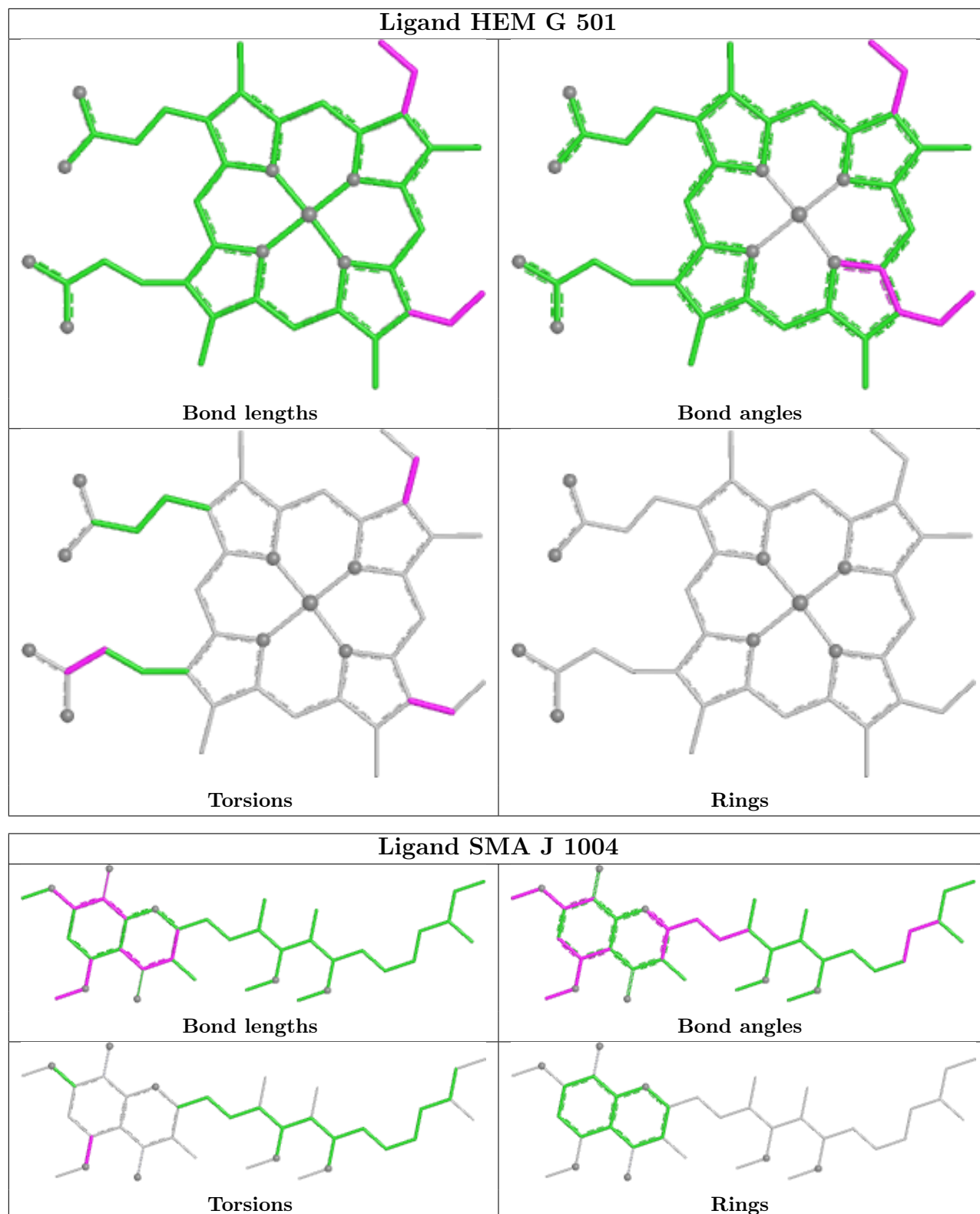
Bond angles

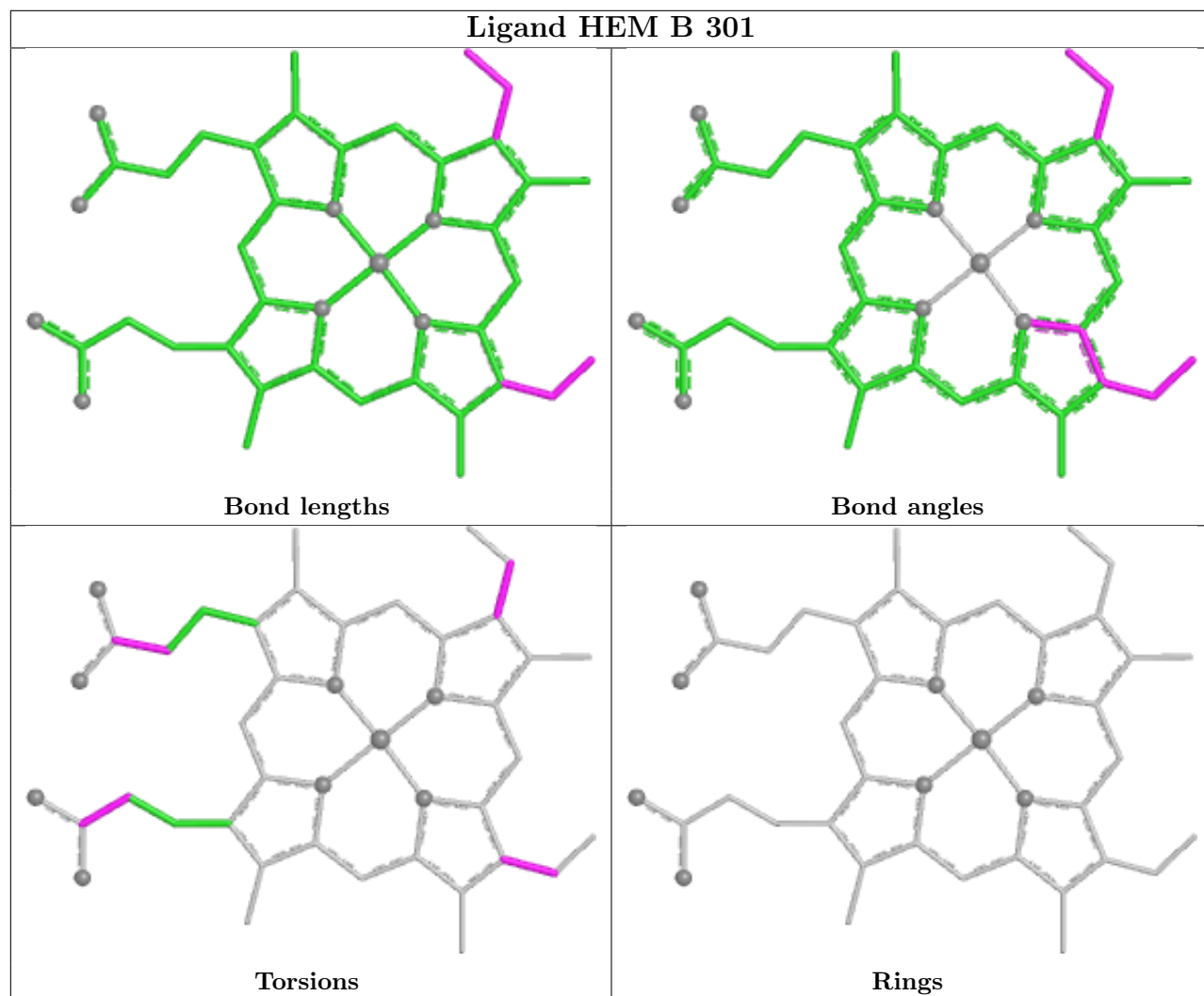


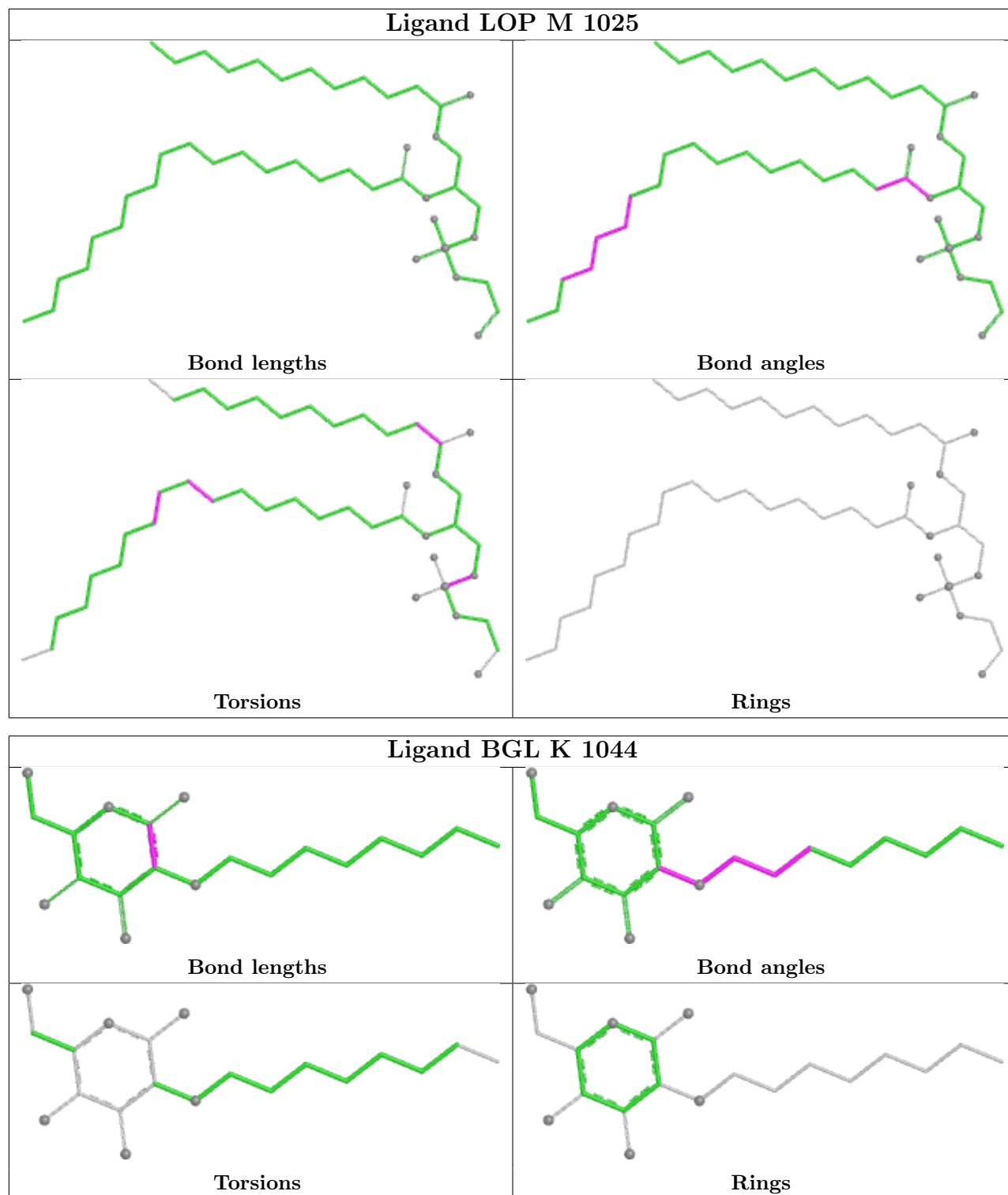
Torsions



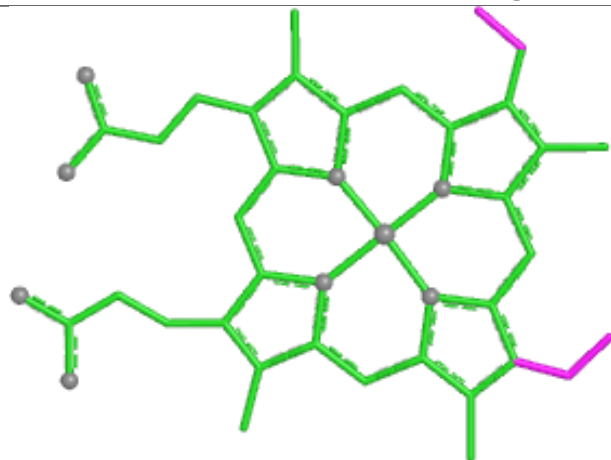
Rings



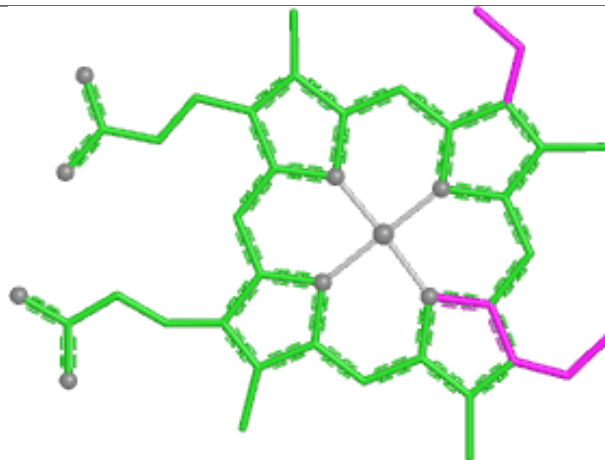




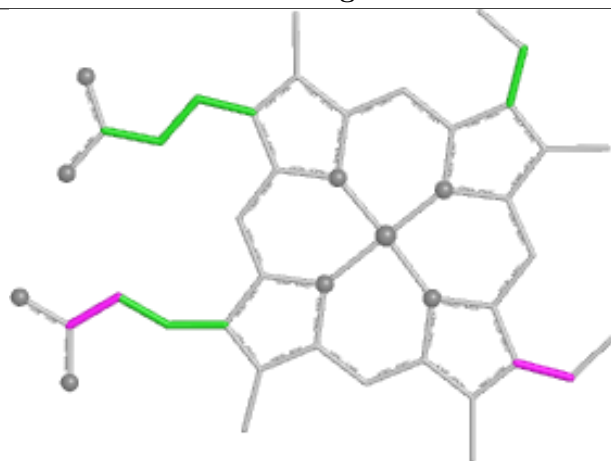
Ligand HEM A 501



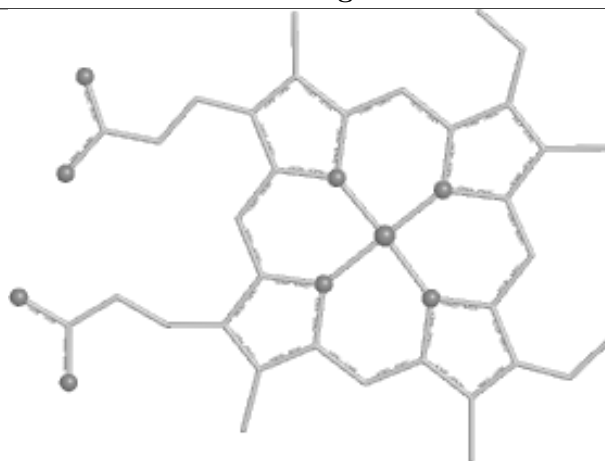
Bond lengths



Bond angles

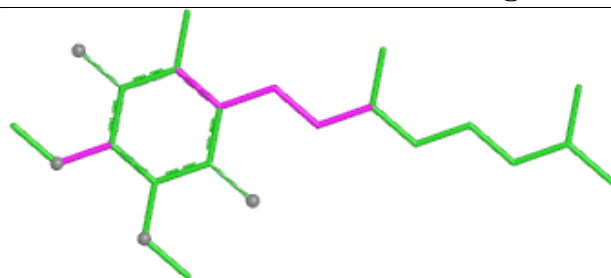


Torsions

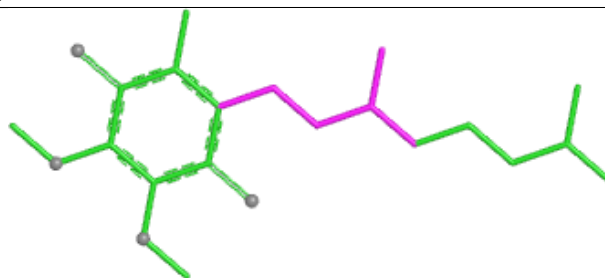


Rings

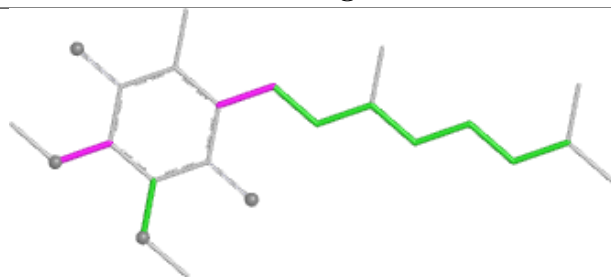
Ligand UQ2 M 1105



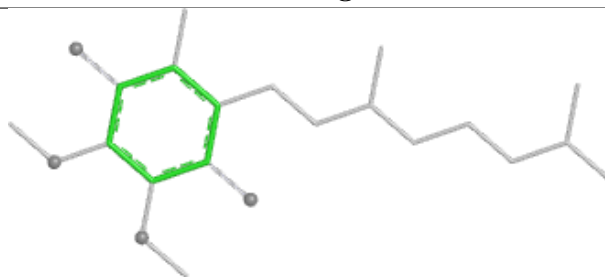
Bond lengths



Bond angles

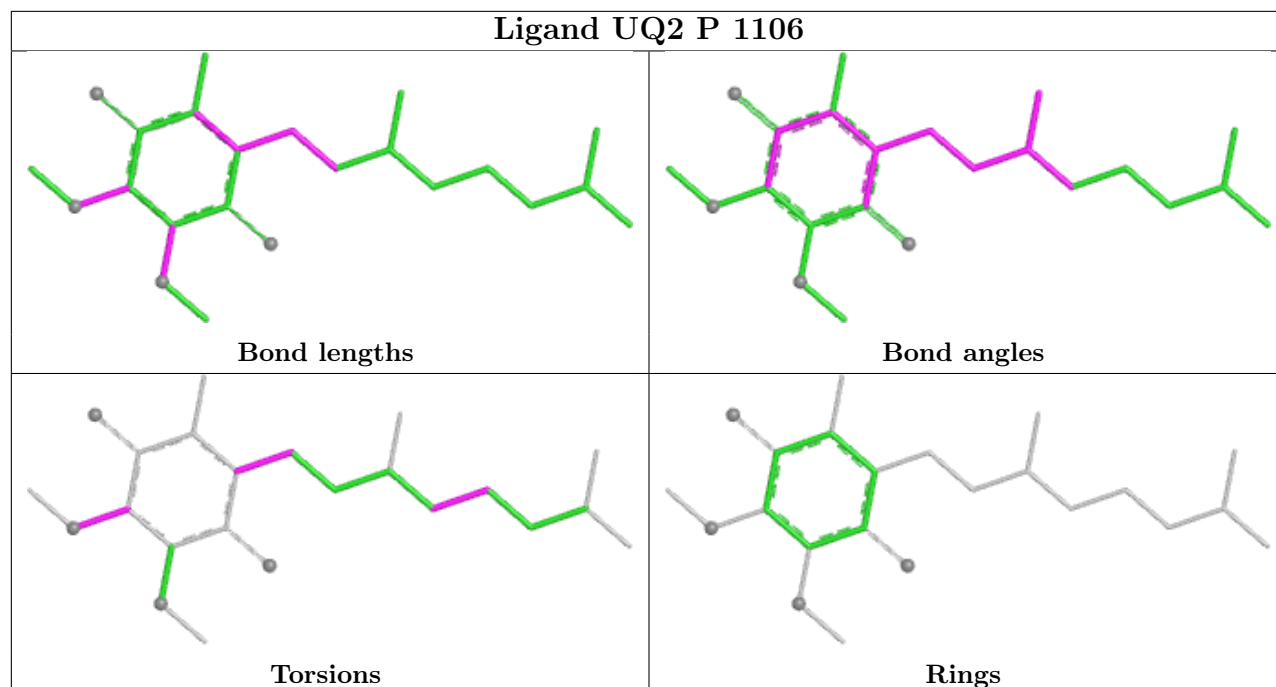


Torsions

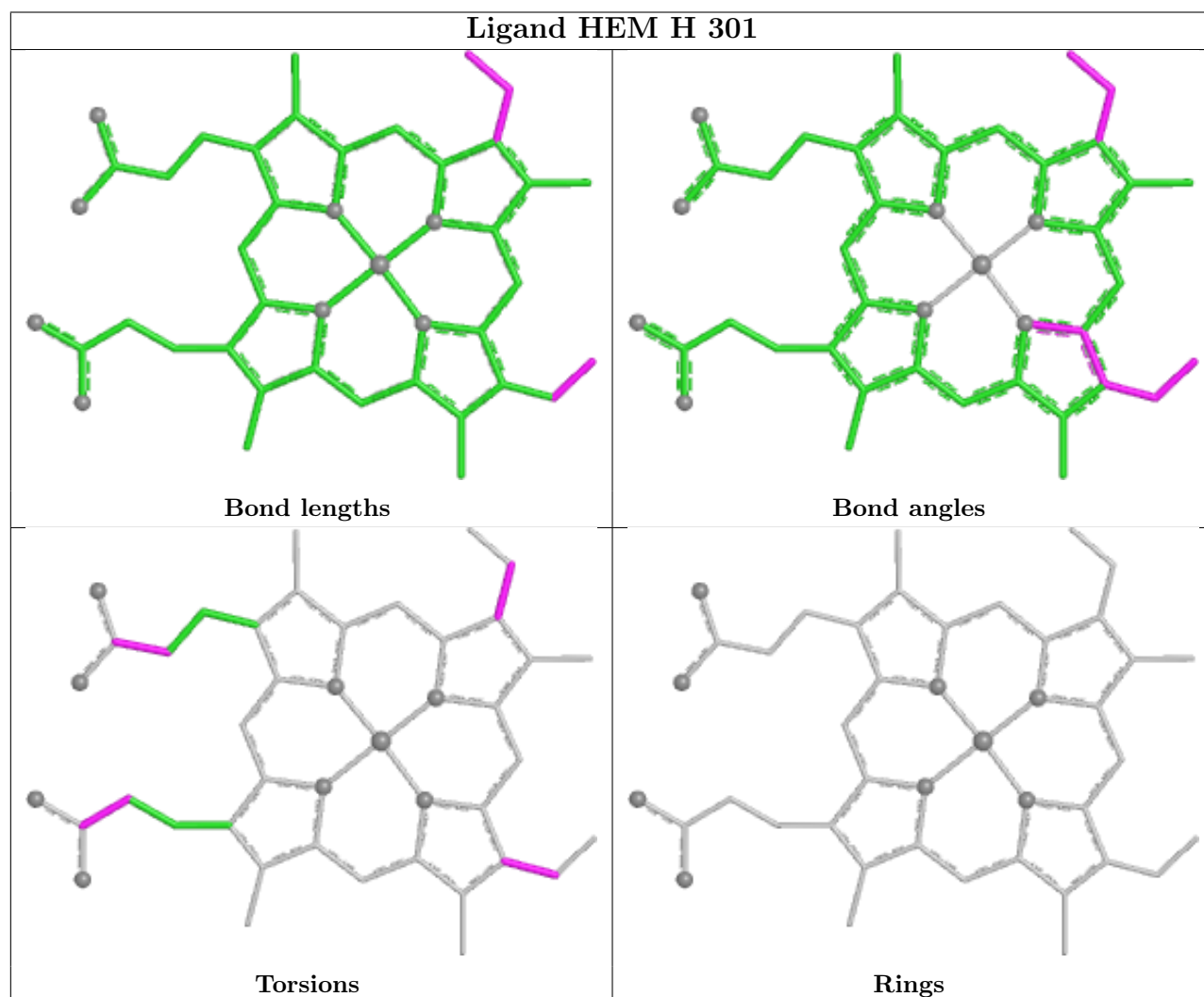


Rings

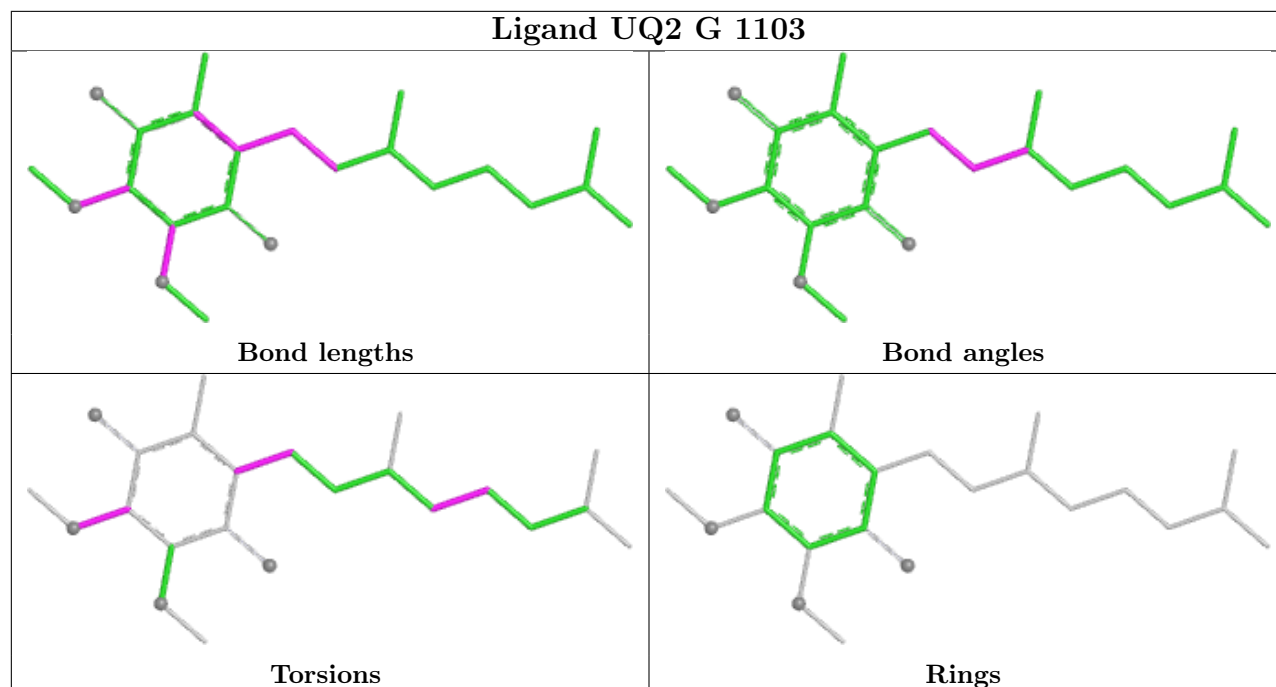
Ligand UQ2 P 1106



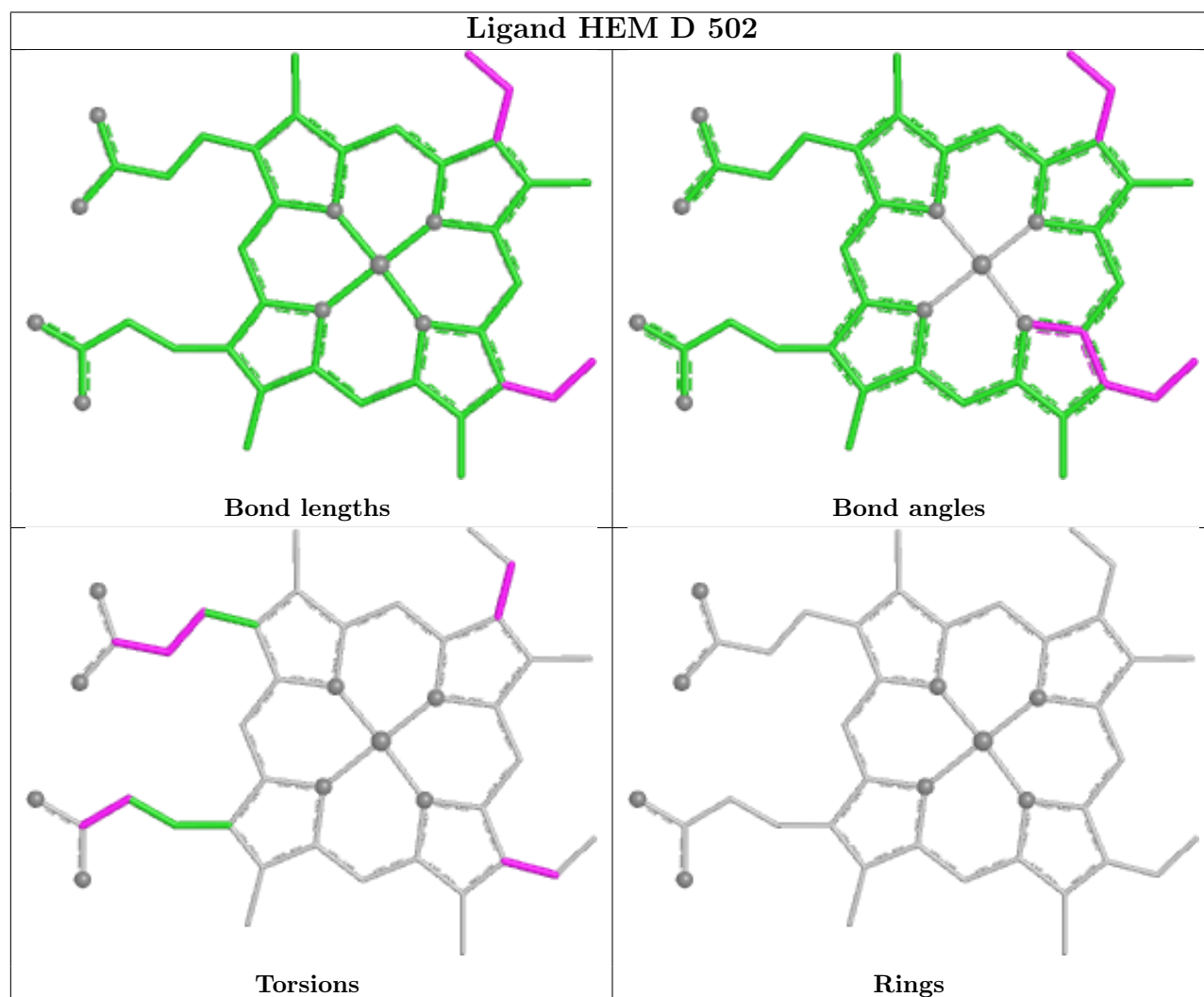
Ligand HEM H 301

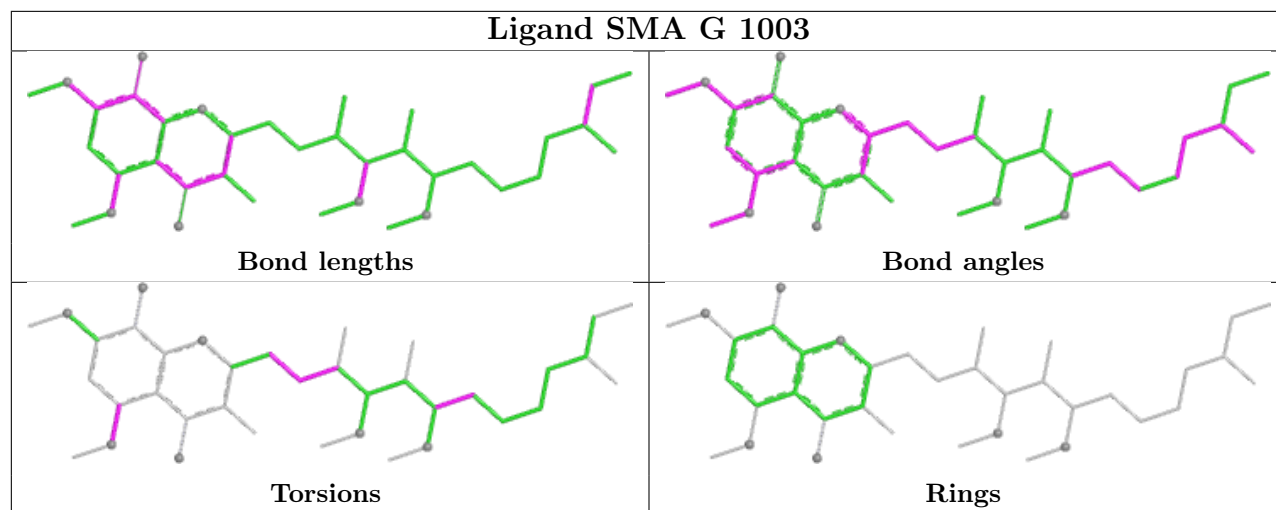


Ligand UQ2 G 1103



Ligand HEM D 502





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	428/445 (96%)	-0.02	4 (0%) 81 78	35, 53, 90, 117	0
1	D	428/445 (96%)	0.04	4 (0%) 81 78	35, 53, 93, 124	0
1	G	428/445 (96%)	0.20	8 (1%) 66 62	35, 56, 100, 124	0
1	J	428/445 (96%)	0.39	15 (3%) 47 43	36, 62, 101, 125	0
1	M	428/445 (96%)	0.41	9 (2%) 63 59	38, 67, 107, 130	0
1	P	428/445 (96%)	0.18	9 (2%) 63 59	35, 56, 100, 127	0
2	B	256/269 (95%)	0.62	12 (4%) 36 32	47, 78, 112, 134	0
2	E	256/269 (95%)	0.72	20 (7%) 19 15	50, 80, 117, 133	0
2	H	256/269 (95%)	0.58	18 (7%) 22 19	40, 72, 113, 135	0
2	K	256/269 (95%)	0.91	33 (12%) 7 5	49, 87, 120, 136	0
2	N	256/269 (95%)	1.12	39 (15%) 5 4	59, 95, 121, 135	0
2	Q	256/269 (95%)	0.90	24 (9%) 14 11	51, 87, 119, 134	0
3	C	179/187 (95%)	0.25	6 (3%) 48 44	37, 59, 101, 139	0
3	F	179/187 (95%)	0.26	4 (2%) 62 58	38, 63, 102, 140	0
3	I	179/187 (95%)	0.29	5 (2%) 55 51	41, 58, 105, 139	0
3	L	179/187 (95%)	0.29	12 (6%) 24 20	37, 59, 104, 139	0
3	O	179/187 (95%)	0.34	7 (3%) 43 39	34, 64, 108, 138	0
3	R	179/187 (95%)	0.65	7 (3%) 43 39	46, 70, 108, 138	0
All	All	5178/5406 (95%)	0.41	236 (4%) 37 33	34, 66, 112, 140	0

All (236) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	109	GLY	5.6
3	I	47	LEU	4.5
2	K	172	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
2	B	121	LEU	4.4
2	H	115	GLY	4.3
2	N	109	GLY	4.3
3	L	12	ARG	4.3
2	H	1	ALA	4.2
2	N	202	ALA	4.1
3	F	9	GLY	4.1
3	L	9	GLY	4.0
3	C	47	LEU	4.0
2	K	124	GLY	4.0
2	H	114	MET	3.9
2	K	114	MET	3.9
1	J	311	ASP	3.9
2	N	110	PHE	3.9
2	N	169	CYS	3.8
3	F	47	LEU	3.8
1	M	354	VAL	3.8
3	I	46	ALA	3.8
1	J	413	ALA	3.8
2	E	110	PHE	3.7
2	H	256	LYS	3.7
3	L	47	LEU	3.6
2	K	110	PHE	3.6
3	L	15	LEU	3.6
2	N	125	ILE	3.6
2	K	196	TYR	3.5
2	K	169	CYS	3.5
3	O	9	GLY	3.5
2	E	3	GLY	3.5
2	Q	110	PHE	3.5
1	G	3	GLY	3.4
2	N	179	ALA	3.4
2	Q	123	ASN	3.4
2	N	151	PRO	3.4
2	N	178	THR	3.4
1	A	30	TYR	3.3
3	L	14	PHE	3.3
2	E	115	GLY	3.3
3	C	9	GLY	3.3
2	N	164	SER	3.3
2	K	151	PRO	3.3
1	J	430	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
2	H	2	GLY	3.2
2	H	145	CYS	3.2
3	I	9	GLY	3.1
1	M	6	HIS	3.1
1	A	311	ASP	3.1
2	Q	251	LEU	3.1
2	E	4	GLY	3.1
3	F	12	ARG	3.1
2	H	3	GLY	3.1
2	K	121	LEU	3.0
1	G	311	ASP	3.0
2	N	115	GLY	3.0
2	K	256	LYS	3.0
2	K	120	GLN	3.0
2	K	125	ILE	3.0
1	M	3	GLY	3.0
2	K	115	GLY	3.0
2	K	118	ILE	2.9
2	N	6	VAL	2.9
2	N	1	ALA	2.9
2	N	121	LEU	2.9
1	P	3	GLY	2.9
2	B	118	ILE	2.9
3	I	10	THR	2.9
3	L	10	THR	2.9
2	B	110	PHE	2.9
2	Q	115	GLY	2.9
3	L	181	GLU	2.9
2	B	145	CYS	2.9
2	Q	145	CYS	2.9
2	K	175	VAL	2.9
1	D	311	ASP	2.9
2	Q	6	VAL	2.9
3	C	10	THR	2.9
3	R	47	LEU	2.9
1	P	311	ASP	2.9
2	N	190	MET	2.9
2	Q	242	VAL	2.8
1	M	311	ASP	2.8
3	L	46	ALA	2.8
2	Q	113	PRO	2.8
2	K	113	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	J	3	GLY	2.7
2	K	3	GLY	2.7
2	N	157	ASN	2.7
3	O	47	LEU	2.7
1	G	4	ILE	2.7
2	N	123	ASN	2.7
2	Q	175	VAL	2.7
2	B	256	LYS	2.7
2	N	177	THR	2.7
2	H	231	PHE	2.7
2	H	123	ASN	2.7
2	Q	204	VAL	2.7
2	B	190	MET	2.7
2	B	2	GLY	2.7
2	K	145	CYS	2.7
2	E	175	VAL	2.7
2	B	172	ALA	2.7
1	G	15	ILE	2.6
2	N	166	PRO	2.6
2	E	196	TYR	2.6
2	E	200	HIS	2.6
1	P	430	ALA	2.6
1	G	232	THR	2.6
2	N	182	TRP	2.5
2	Q	152	ASP	2.5
1	J	215	ALA	2.5
3	L	19	THR	2.5
3	F	16	TYR	2.5
1	J	216	PHE	2.5
2	N	172	ALA	2.5
2	Q	196	TYR	2.5
1	D	414	ILE	2.5
2	N	118	ILE	2.5
2	N	9	VAL	2.5
2	N	111	HIS	2.5
1	D	12	ARG	2.5
2	B	143	PRO	2.5
1	J	427	ASP	2.5
1	P	15	ILE	2.5
3	O	176	ALA	2.5
2	E	125	ILE	2.4
2	N	189	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	Q	182	TRP	2.4
2	N	256	LYS	2.4
1	M	424	ILE	2.4
1	M	30	TYR	2.4
3	O	16	TYR	2.4
2	K	116	THR	2.4
2	E	117	GLY	2.4
3	I	179	ILE	2.4
3	R	46	ALA	2.4
2	B	200	HIS	2.4
2	Q	58	LEU	2.4
2	Q	1	ALA	2.4
2	E	18	GLY	2.3
2	N	137	GLY	2.3
2	N	4	GLY	2.3
2	Q	148	GLY	2.3
2	E	201	ASP	2.3
1	A	430	ALA	2.3
1	G	310	ALA	2.3
2	E	1	ALA	2.3
2	Q	197	ALA	2.3
1	P	13	THR	2.3
2	K	174	GLY	2.3
1	M	418	VAL	2.3
2	E	145	CYS	2.3
1	J	123	ALA	2.3
3	O	12	ARG	2.3
1	P	232	THR	2.3
2	E	199	GLY	2.3
2	H	60	GLU	2.3
2	K	166	PRO	2.3
1	J	310	ALA	2.2
1	P	30	TYR	2.3
2	K	1	ALA	2.2
2	N	200	HIS	2.2
1	G	414	ILE	2.2
1	J	15	ILE	2.2
2	K	192	ASP	2.2
2	N	20	PHE	2.2
2	H	6	VAL	2.2
2	Q	158	ARG	2.2
2	K	2	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	K	112	GLY	2.2
2	N	174	GLY	2.2
2	K	251	LEU	2.2
3	R	15	LEU	2.2
2	K	143	PRO	2.2
2	E	2	GLY	2.2
1	D	15	ILE	2.2
2	E	118	ILE	2.2
2	Q	10	PRO	2.2
3	R	14	PHE	2.2
2	Q	190	MET	2.2
1	M	183	GLY	2.2
1	J	240	ASP	2.2
1	J	252	ASP	2.2
2	N	16	PRO	2.2
2	N	165	VAL	2.1
1	G	430	ALA	2.1
2	Q	189	LEU	2.1
3	R	9	GLY	2.1
3	L	16	TYR	2.1
3	C	12	ARG	2.1
2	Q	256	LYS	2.1
2	H	236	PHE	2.1
3	O	14	PHE	2.1
2	K	9	VAL	2.1
2	E	116	THR	2.1
3	O	182	THR	2.1
3	R	10	THR	2.1
2	H	118	ILE	2.1
1	J	362	MET	2.1
2	K	149	HIS	2.1
3	R	44	VAL	2.1
2	K	173	ASN	2.1
2	H	4	GLY	2.1
2	H	136	THR	2.1
2	N	124	GLY	2.1
2	H	196	TYR	2.1
2	E	6	VAL	2.1
2	N	138	PHE	2.1
2	E	251	LEU	2.1
1	A	183	GLY	2.1
2	K	78	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	4	ILE	2.1
1	M	15	ILE	2.1
1	J	121	TYR	2.1
2	N	196	TYR	2.1
2	H	22	GLN	2.0
2	K	204	VAL	2.0
2	N	11	PHE	2.0
2	N	38	ALA	2.0
3	C	11	ARG	2.0
3	C	48	ALA	2.0
2	B	4	GLY	2.0
2	K	109	GLY	2.0
1	P	11	PRO	2.0
2	N	194	VAL	2.0
2	Q	165	VAL	2.0
3	L	48	ALA	2.0
2	B	124	GLY	2.0
2	Q	2	GLY	2.0
1	P	4	ILE	2.0
2	E	151	PRO	2.0
2	N	235	MET	2.0
3	L	13	ASP	2.0
2	K	156	TYR	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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	UQ2	J	1104	23/23	0.57	0.27	107,115,116,117	0
8	UQ2	G	1103	23/23	0.65	0.29	109,116,117,118	0
8	UQ2	A	1101	23/23	0.66	0.25	102,105,108,109	0
8	UQ2	M	1105	23/23	0.68	0.26	112,123,125,125	0
8	UQ2	D	1102	23/23	0.69	0.25	92,98,107,107	0
8	UQ2	P	1106	23/23	0.71	0.25	101,104,107,108	0
9	BGL	N	1045	20/20	0.72	0.22	107,111,113,114	0
7	LOP	M	1025	45/45	0.73	0.20	89,114,123,123	0
7	LOP	J	1024	45/45	0.76	0.18	93,113,125,126	0
9	BGL	B	1041	20/20	0.77	0.22	87,97,101,102	0
9	BGL	K	1044	20/20	0.77	0.19	95,99,101,101	0
7	LOP	G	1023	45/45	0.77	0.19	88,102,112,113	0
9	BGL	P	1046	20/20	0.79	0.18	87,93,95,95	0
7	LOP	P	1026	45/45	0.80	0.18	69,95,99,100	0
9	BGL	G	1043	20/20	0.82	0.21	89,91,101,101	0
7	LOP	A	1021	45/45	0.84	0.16	72,86,94,99	0
9	BGL	E	1042	20/20	0.84	0.17	80,85,102,102	0
7	LOP	D	1022	45/45	0.84	0.15	63,88,98,102	0
4	SR	M	1019	1/1	0.87	0.07	154,154,154,154	0
4	SR	Q	1016	1/1	0.88	0.08	137,137,137,137	0
4	SR	A	1017	1/1	0.89	0.07	114,114,114,114	0
4	SR	N	1015	1/1	0.90	0.07	153,153,153,153	0
4	SR	B	1011	1/1	0.91	0.06	132,132,132,132	0
4	SR	K	1014	1/1	0.92	0.05	145,145,145,145	0
4	SR	G	1018	1/1	0.92	0.05	98,98,98,98	0
6	SMA	D	1002	37/37	0.93	0.10	39,44,76,78	0
6	SMA	A	1001	37/37	0.94	0.08	38,47,54,56	0
6	SMA	G	1003	37/37	0.94	0.09	35,43,60,65	0
6	SMA	M	1005	37/37	0.94	0.10	56,66,73,73	0
12	NA	R	2001	1/1	0.94	0.07	62,62,62,62	0
5	HEM	J	501	43/43	0.95	0.13	67,75,79,81	0
6	SMA	P	1006	37/37	0.95	0.09	34,45,76,77	0
11	CL	I	2004	1/1	0.95	0.08	67,67,67,67	0
11	CL	R	2005	1/1	0.95	0.14	67,67,67,67	0
6	SMA	J	1004	37/37	0.95	0.09	40,49,79,85	0
4	SR	H	1013	1/1	0.96	0.05	113,113,113,113	0
4	SR	E	1012	1/1	0.96	0.06	138,138,138,138	0
5	HEM	N	301	43/43	0.96	0.10	65,72,79,84	0
5	HEM	M	501	43/43	0.97	0.10	63,69,75,78	0
5	HEM	E	301	43/43	0.97	0.09	53,62,73,76	0
5	HEM	Q	301	43/43	0.97	0.08	56,65,73,78	0

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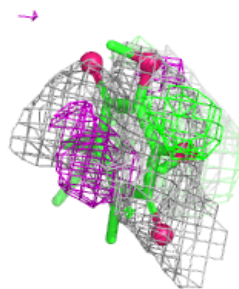
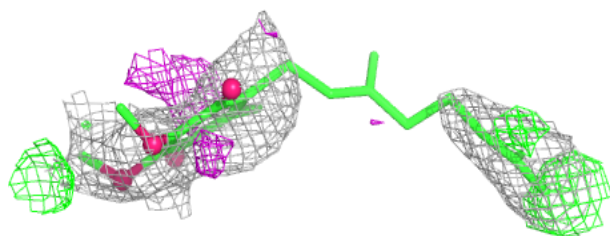
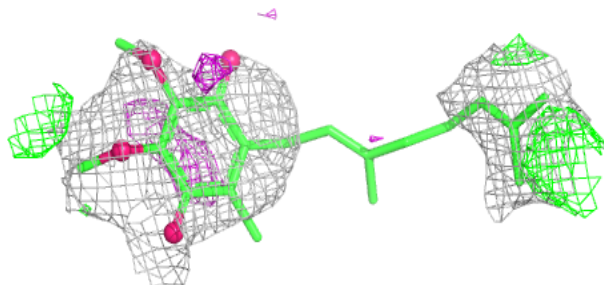
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	HEM	G	501	43/43	0.97	0.09	50,59,62,62	0
5	HEM	B	301	43/43	0.97	0.09	51,56,70,73	0
5	HEM	K	301	43/43	0.97	0.09	49,55,67,69	0
5	HEM	P	501	43/43	0.98	0.08	48,54,57,57	0
5	HEM	P	502	43/43	0.98	0.08	35,40,49,53	0
5	HEM	G	502	43/43	0.98	0.09	32,36,45,49	0
5	HEM	H	301	43/43	0.98	0.07	33,42,47,50	0
5	HEM	D	501	43/43	0.98	0.08	40,48,53,55	0
5	HEM	J	502	43/43	0.98	0.07	37,41,54,57	0
5	HEM	D	502	43/43	0.98	0.08	32,37,49,58	0
10	FES	O	200	4/4	0.98	0.04	42,43,43,43	0
5	HEM	A	502	43/43	0.98	0.09	32,37,49,49	0
5	HEM	M	502	43/43	0.98	0.08	47,49,59,63	0
5	HEM	A	501	43/43	0.98	0.07	43,47,51,53	0
10	FES	C	200	4/4	0.99	0.03	41,42,42,43	0
10	FES	R	200	4/4	0.99	0.04	55,57,58,58	0
10	FES	F	200	4/4	0.99	0.04	43,43,44,45	0
10	FES	I	200	4/4	0.99	0.04	47,48,48,48	0
10	FES	L	200	4/4	0.99	0.04	40,41,41,42	0

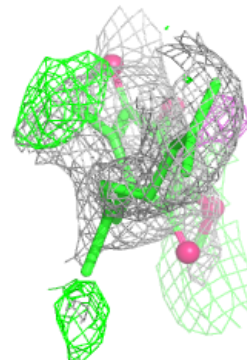
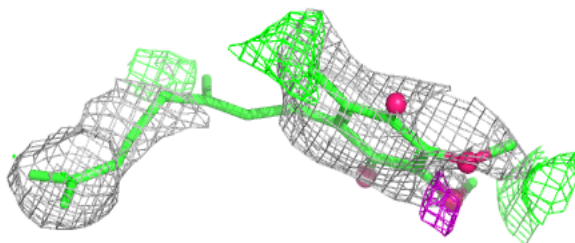
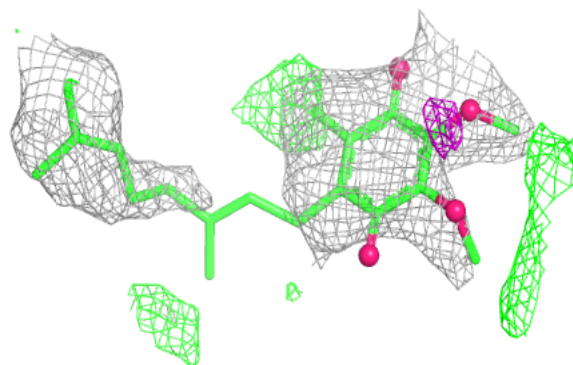
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around UQ2 J 1104:

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

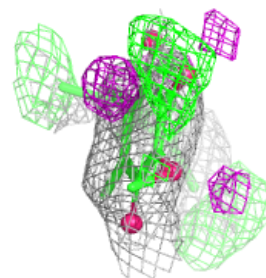
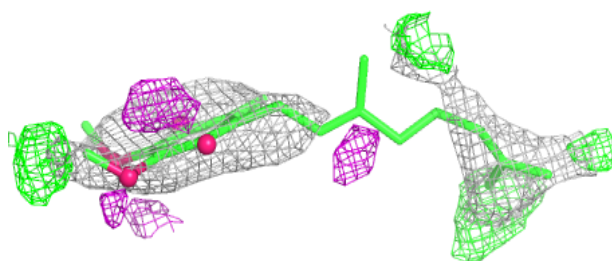
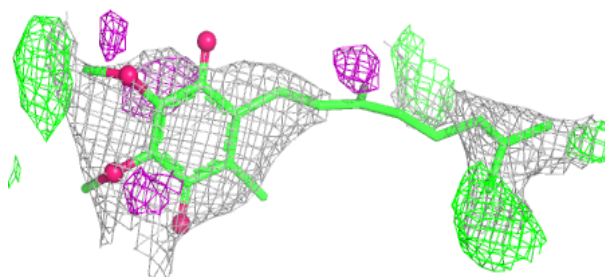
**Electron density around UQ2 G 1103:**

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

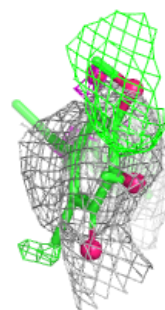
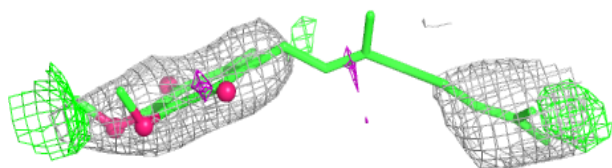
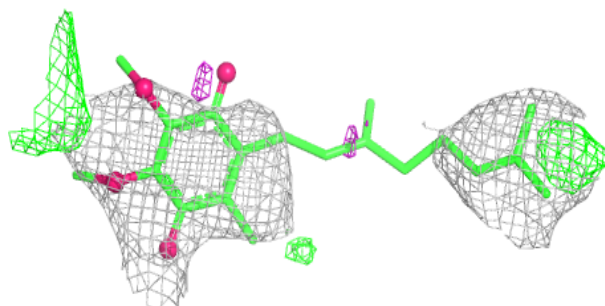


Electron density around UQ2 A 1101:

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

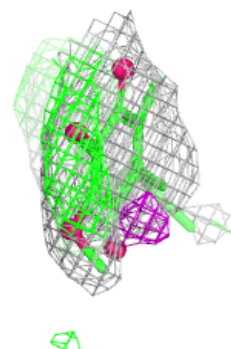
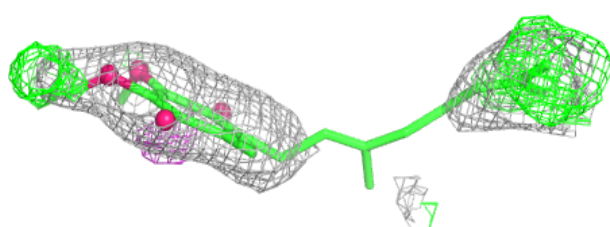
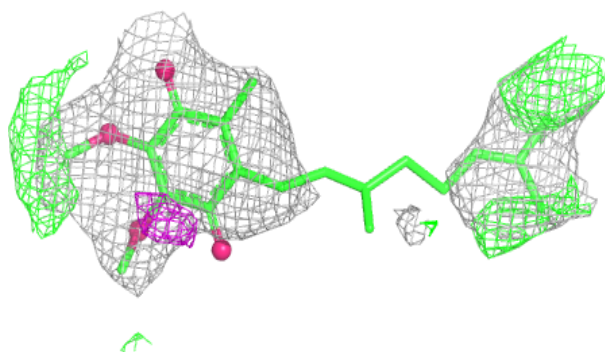
**Electron density around UQ2 M 1105:**

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

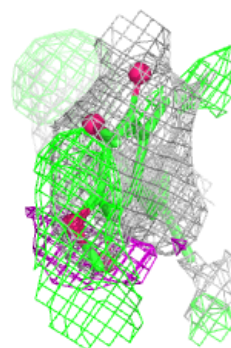
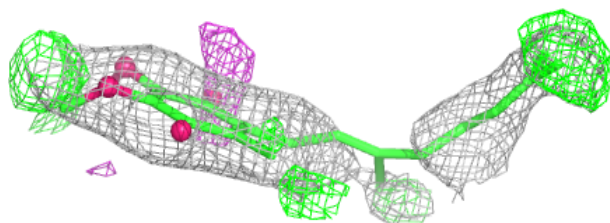
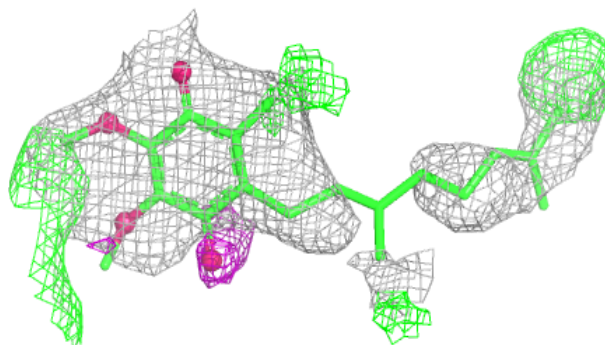


Electron density around UQ2 D 1102:

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

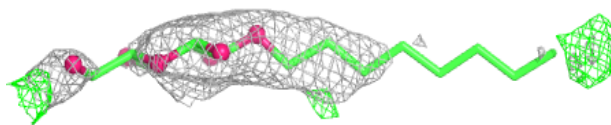
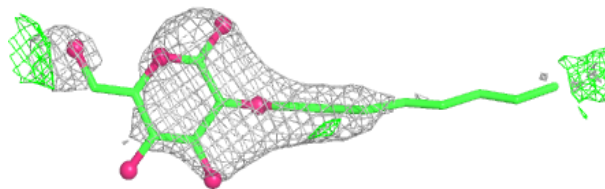
**Electron density around UQ2 P 1106:**

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

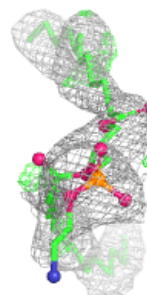
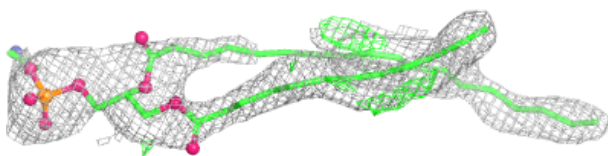
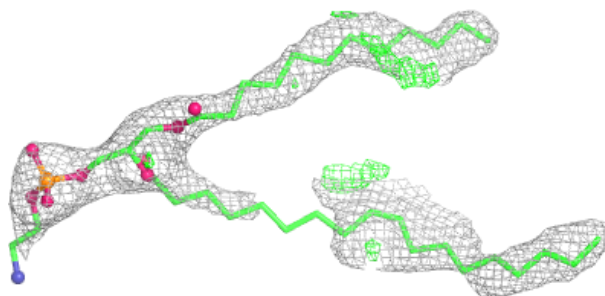


Electron density around BGL N 1045:

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

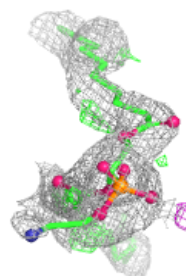
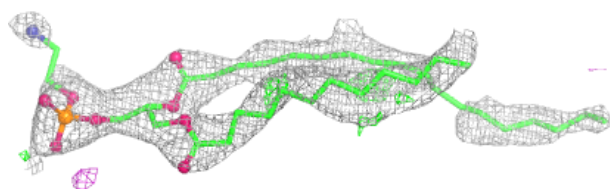
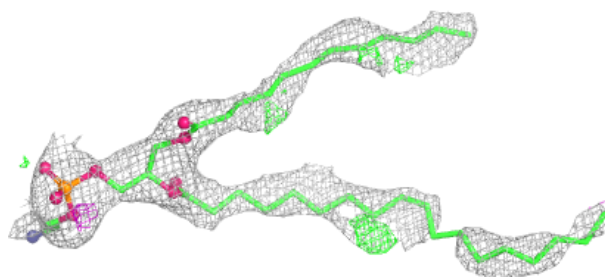
**Electron density around LOP M 1025:**

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

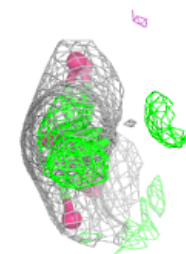
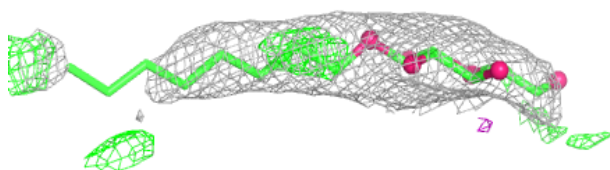
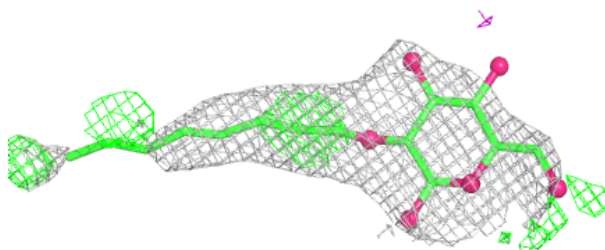


Electron density around LOP J 1024:

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

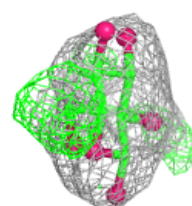
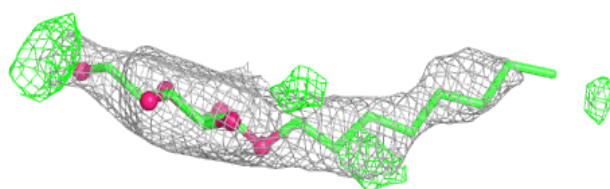
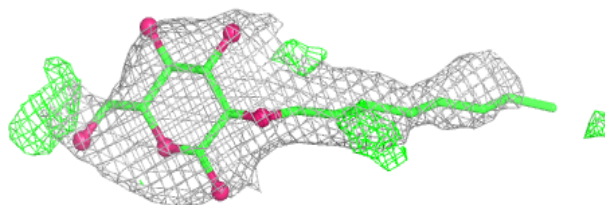
**Electron density around BGL B 1041:**

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

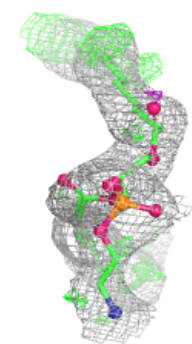
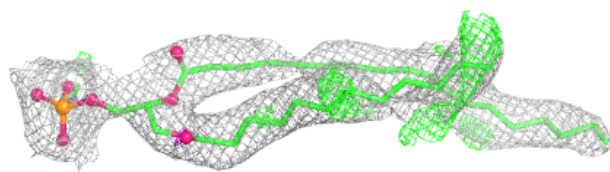
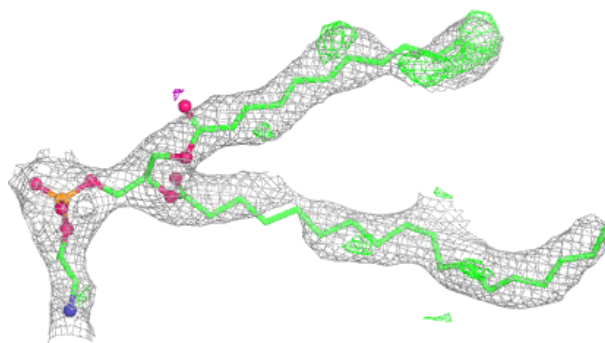


Electron density around BGL K 1044:

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

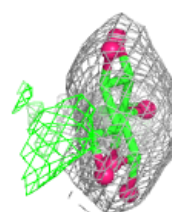
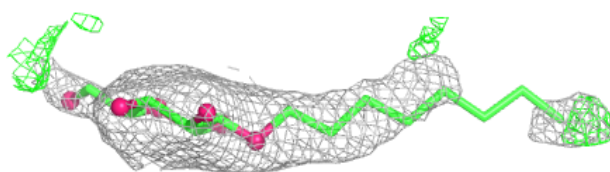
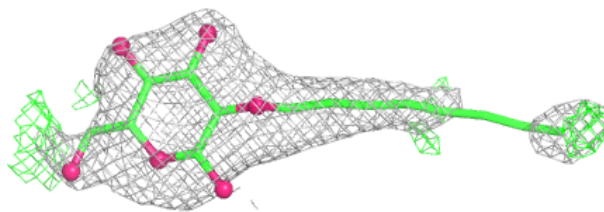
**Electron density around LOP G 1023:**

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

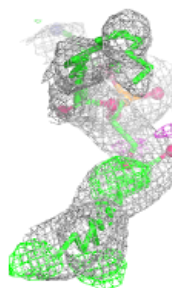
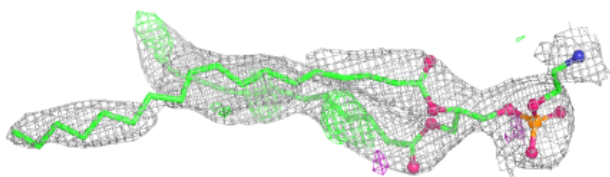
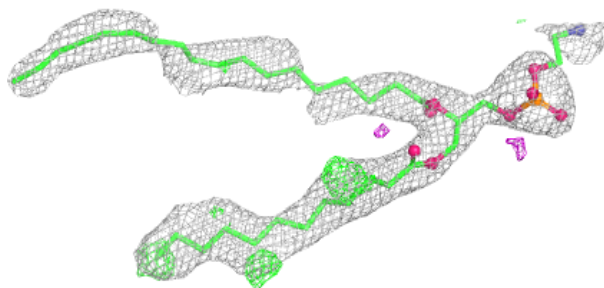


Electron density around BGL P 1046:

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

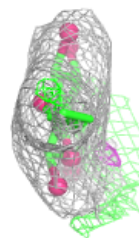
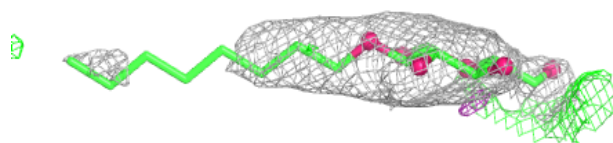
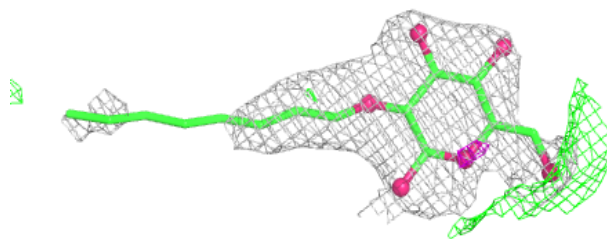
**Electron density around LOP P 1026:**

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

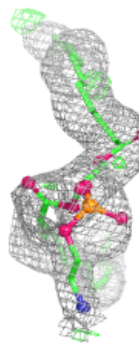
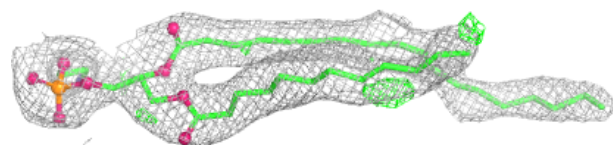
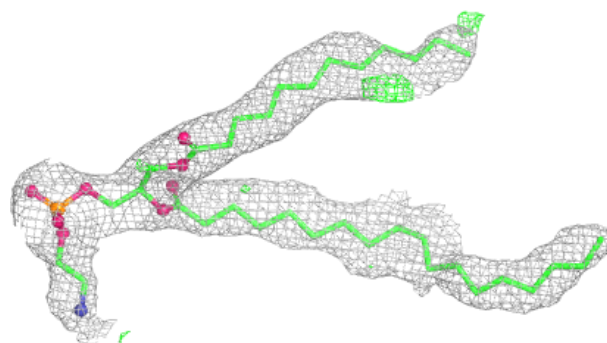


Electron density around BGL G 1043:

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

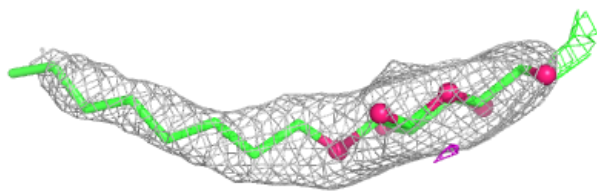
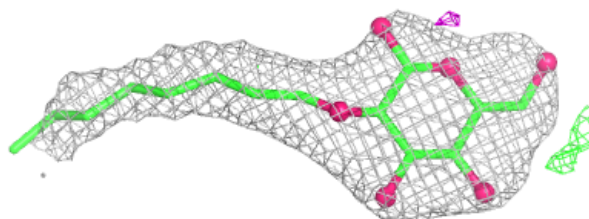
**Electron density around LOP A 1021:**

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

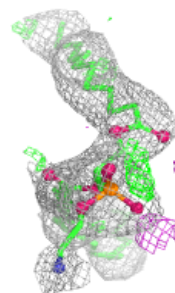
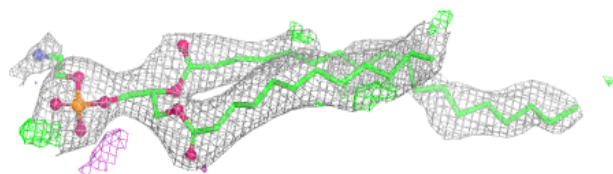
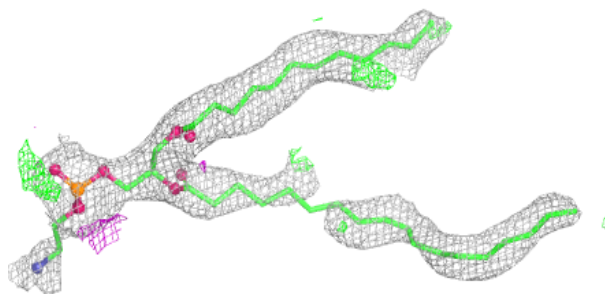


Electron density around BGL E 1042:

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

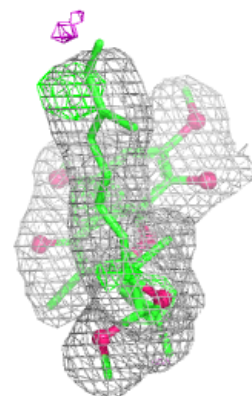
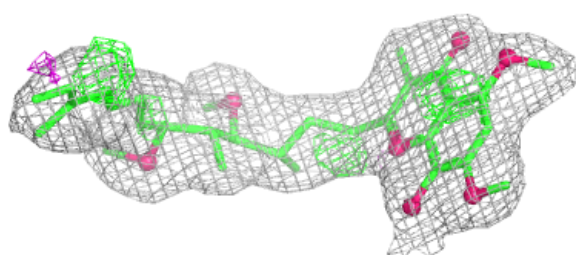
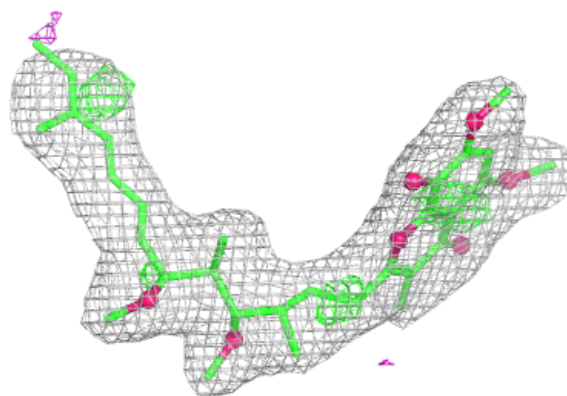
**Electron density around LOP D 1022:**

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

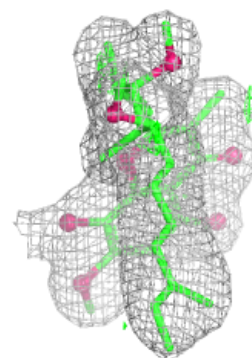
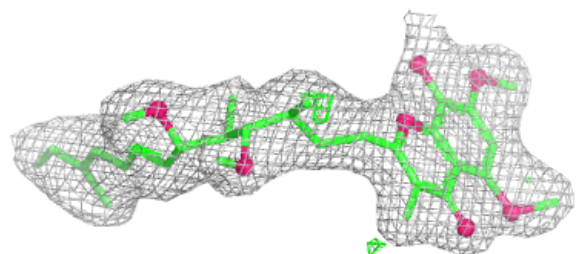
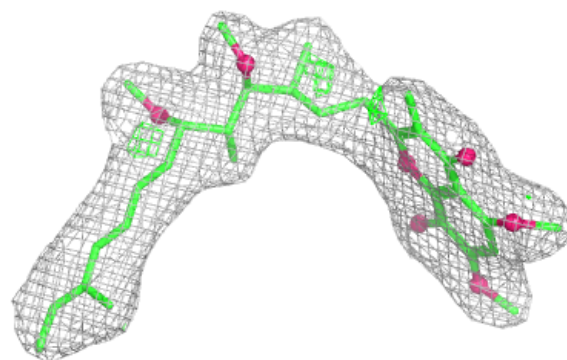


Electron density around SMA D 1002:

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

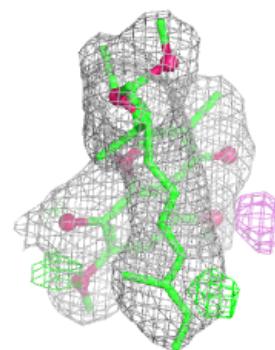
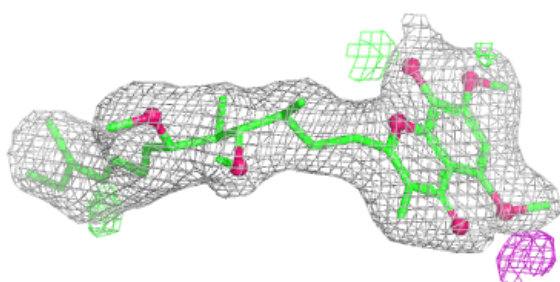
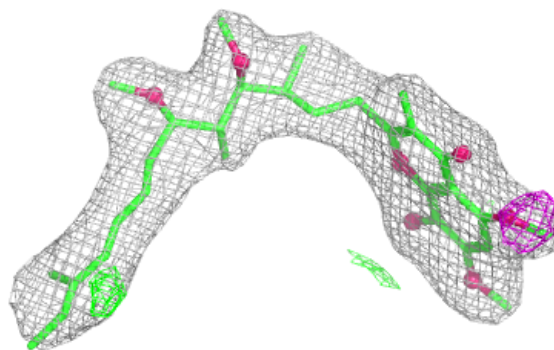
**Electron density around SMA A 1001:**

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

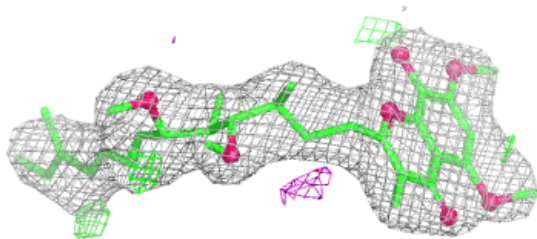
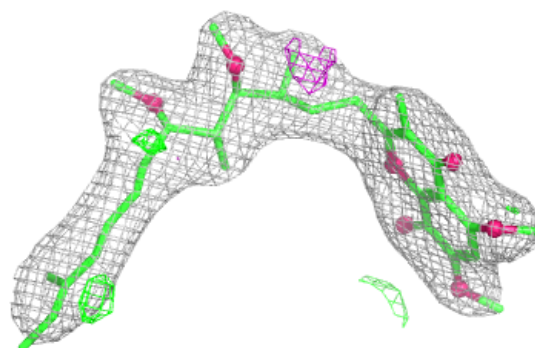


Electron density around SMA G 1003:

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

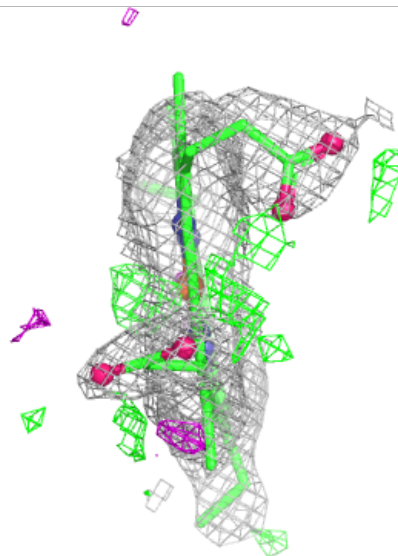
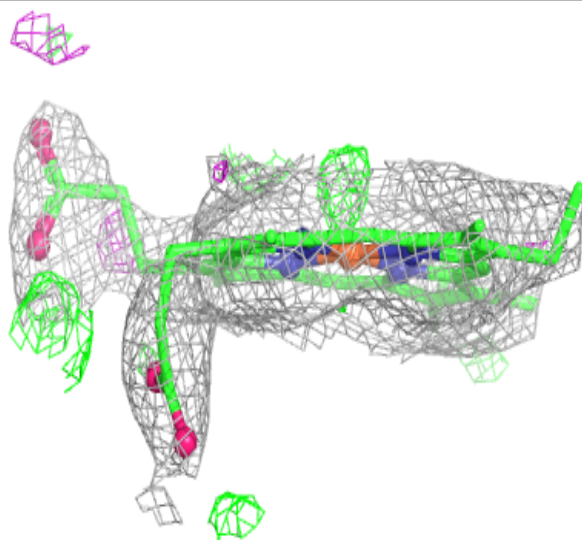
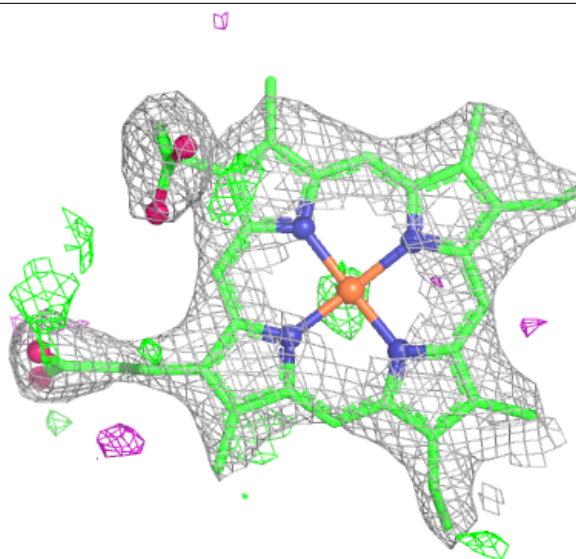
**Electron density around SMA M 1005:**

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



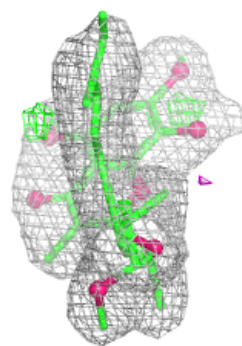
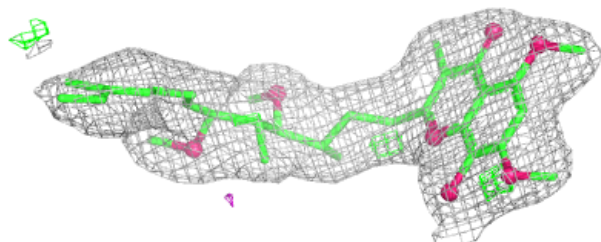
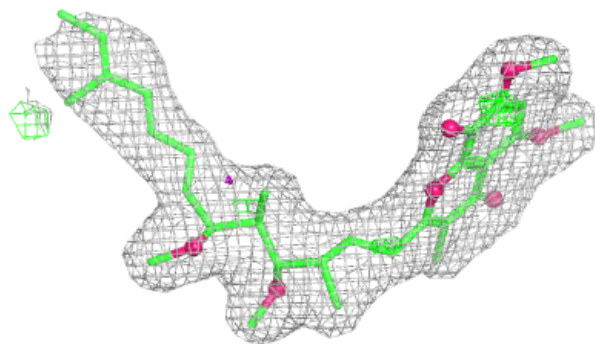
Electron density around HEM J 501:

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

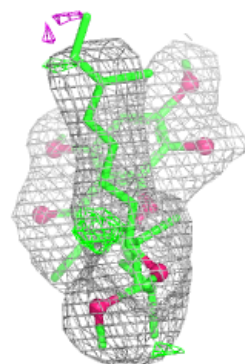
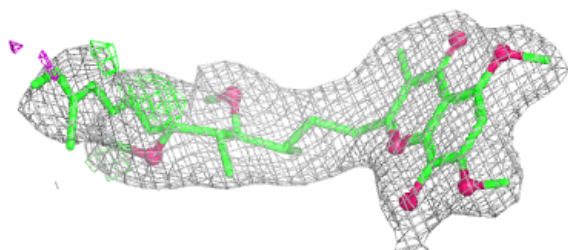
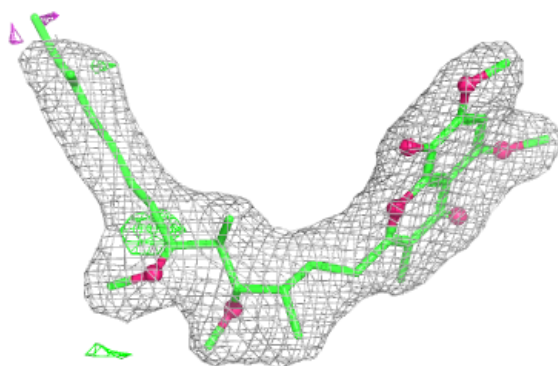


Electron density around SMA P 1006:

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

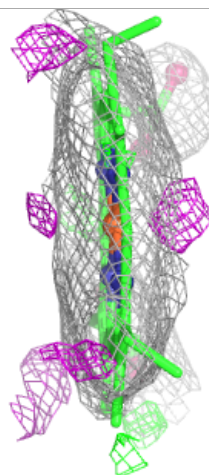
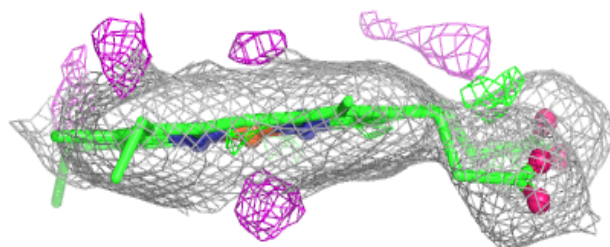
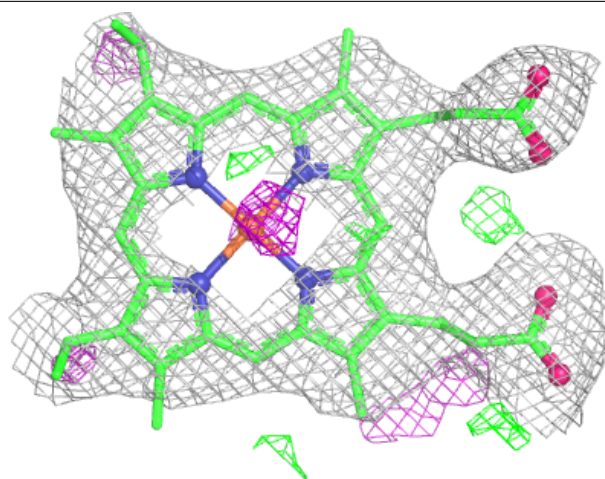
**Electron density around SMA J 1004:**

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



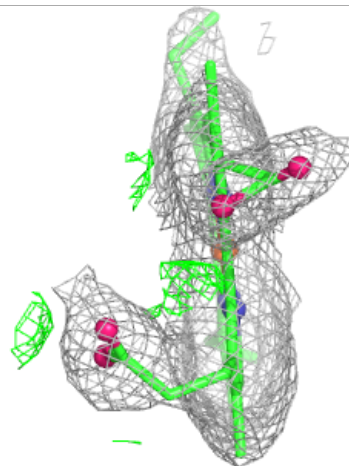
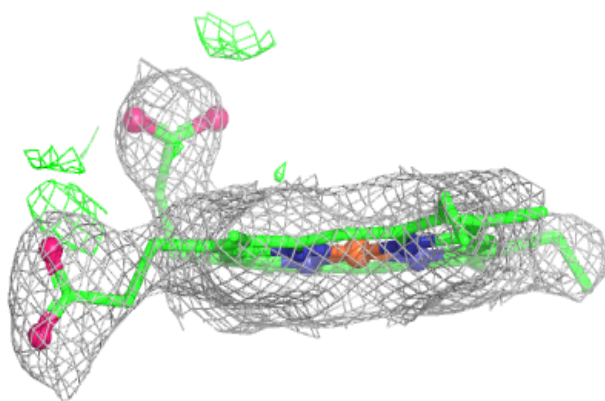
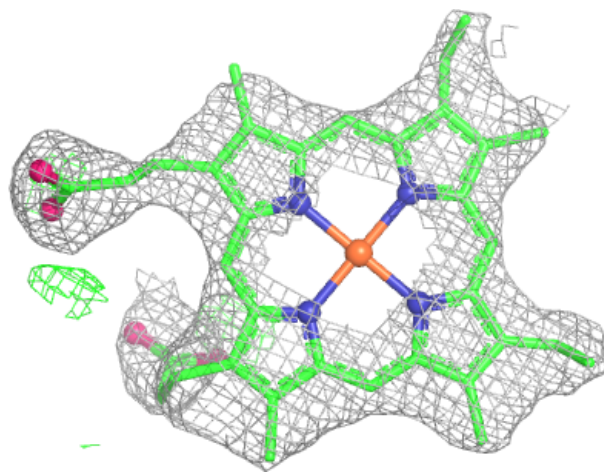
Electron density around HEM N 301:

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



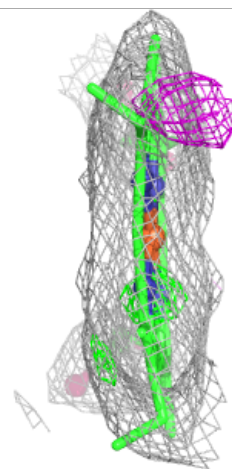
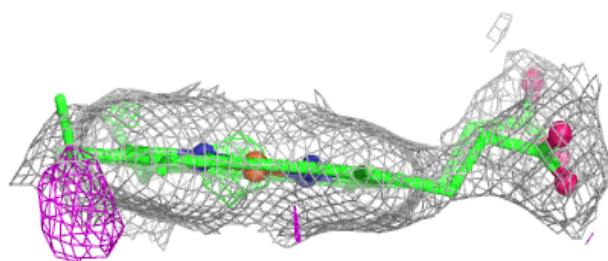
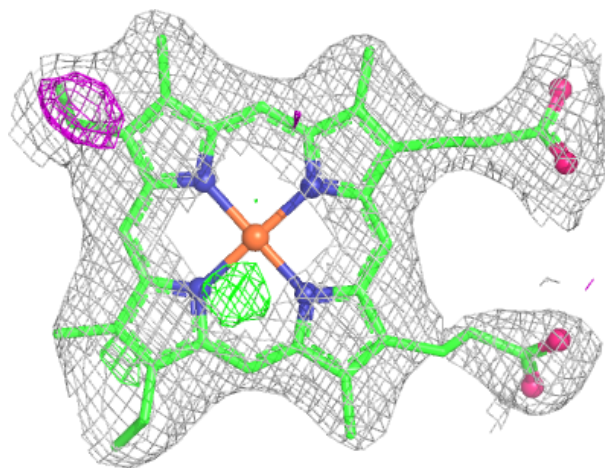
Electron density around HEM M 501:

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



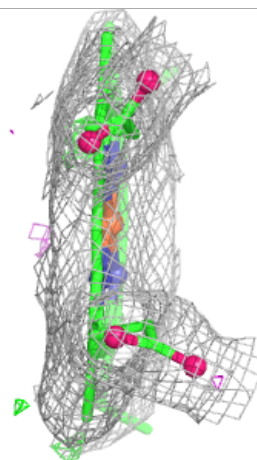
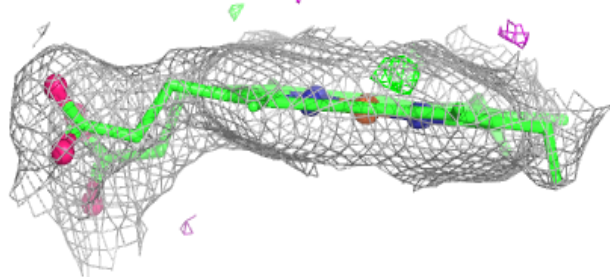
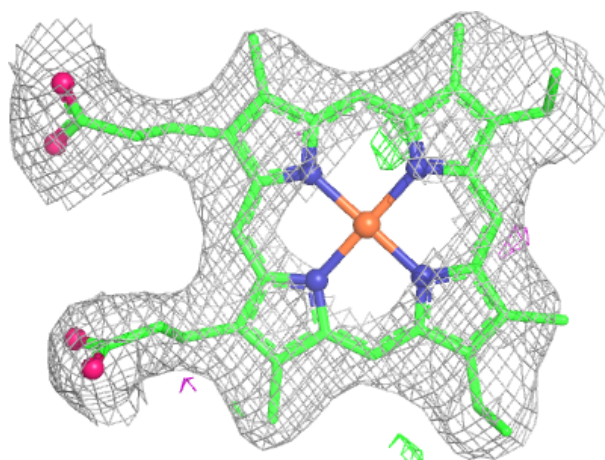
Electron density around HEM E 301:

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



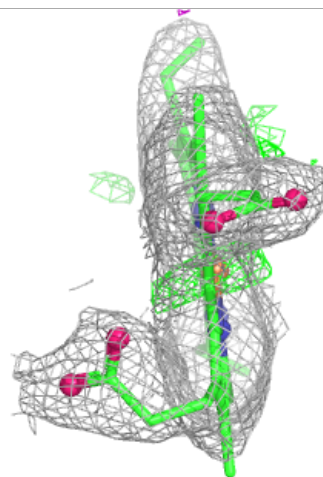
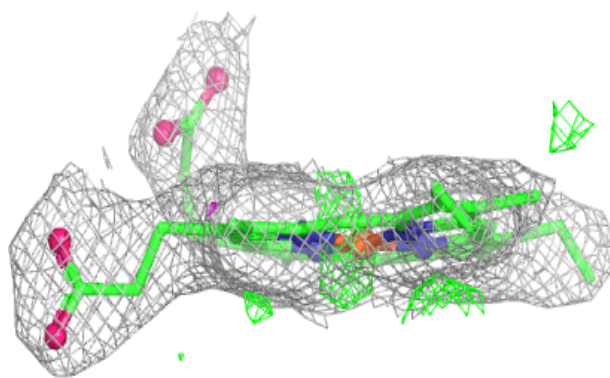
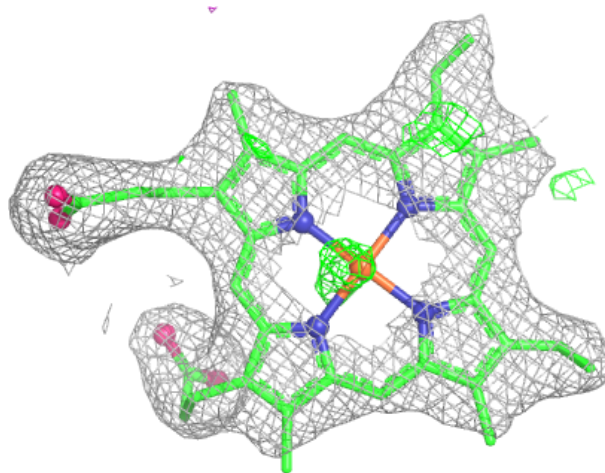
Electron density around HEM Q 301:

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



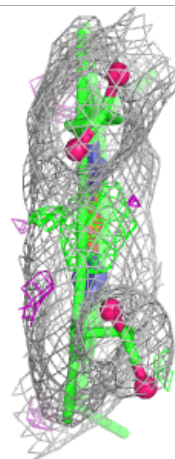
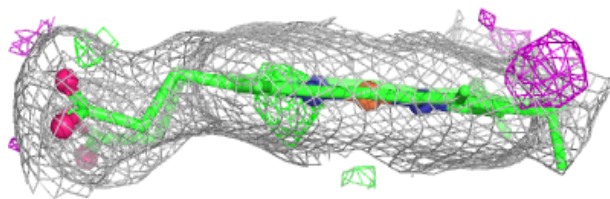
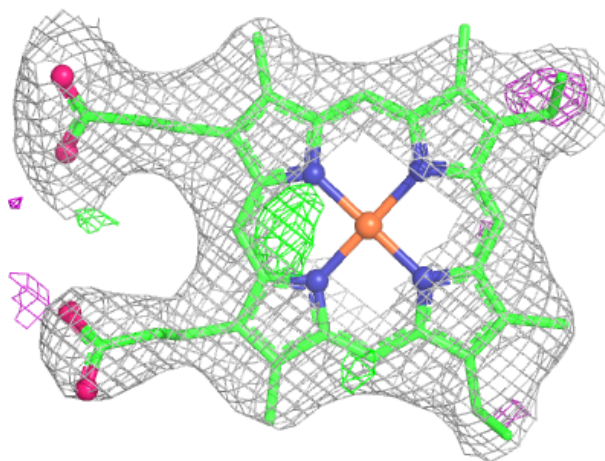
Electron density around HEM G 501:

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



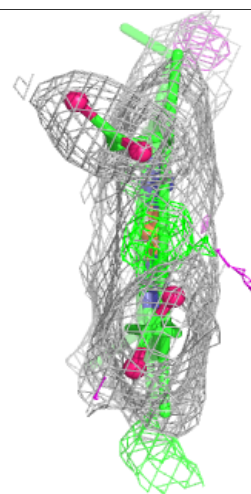
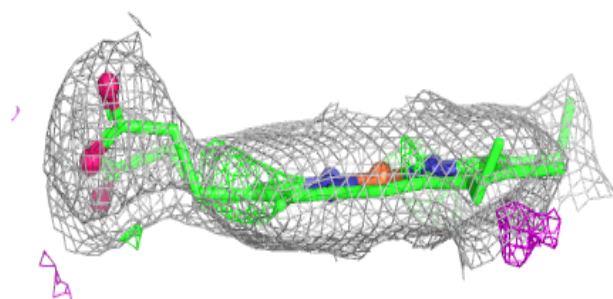
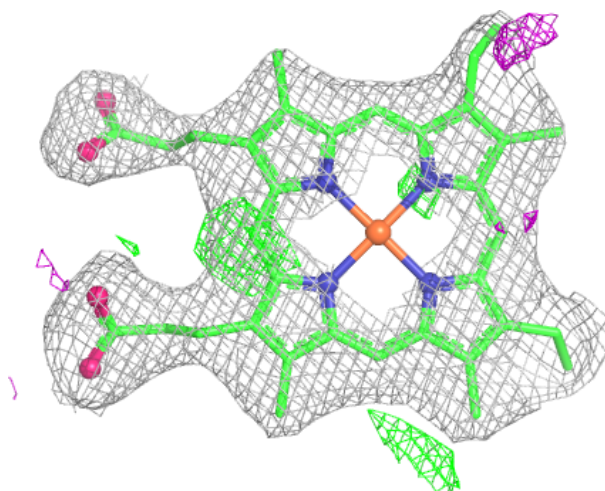
Electron density around HEM B 301:

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



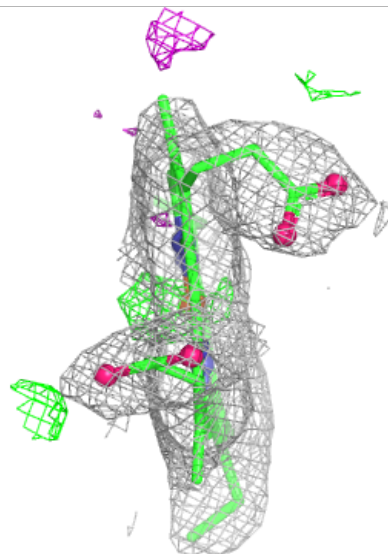
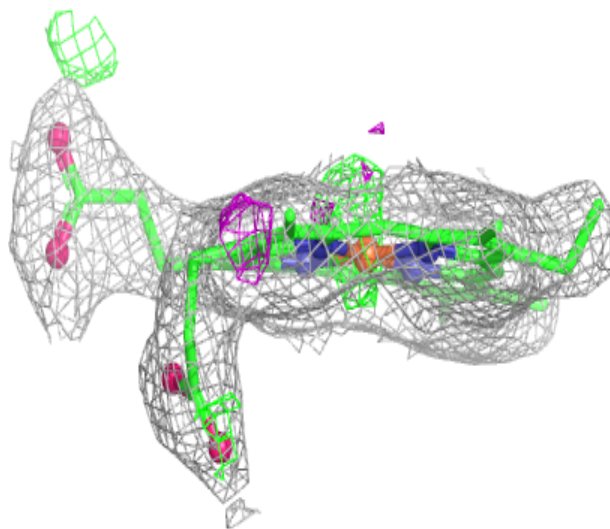
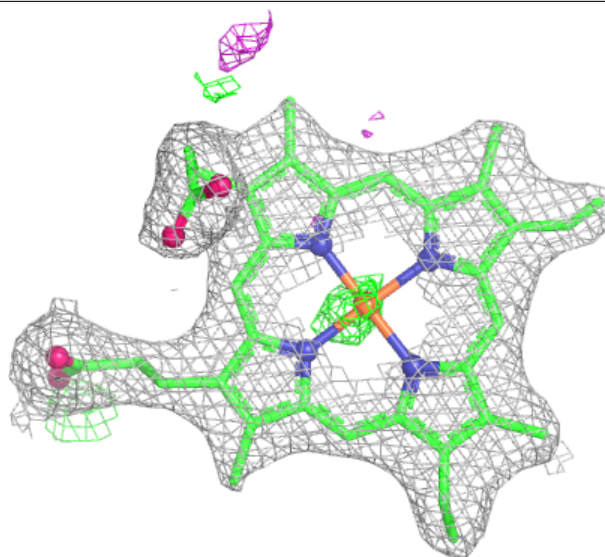
Electron density around HEM K 301:

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



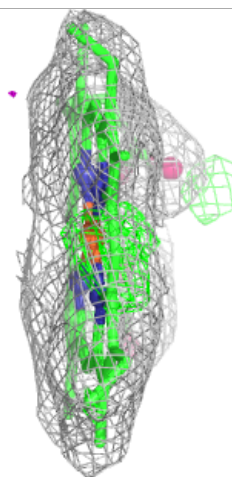
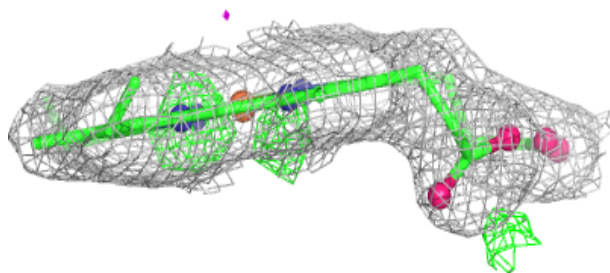
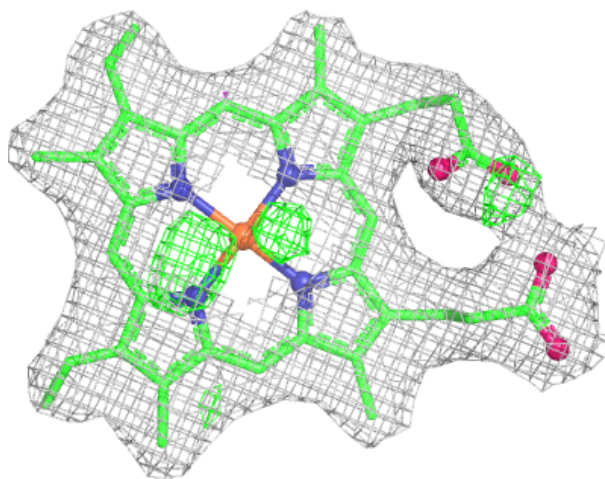
Electron density around HEM P 501:

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



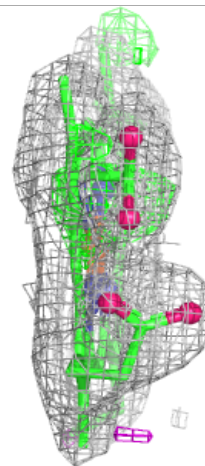
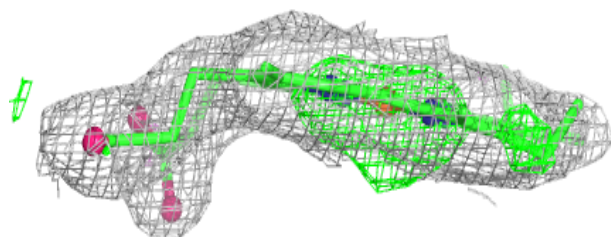
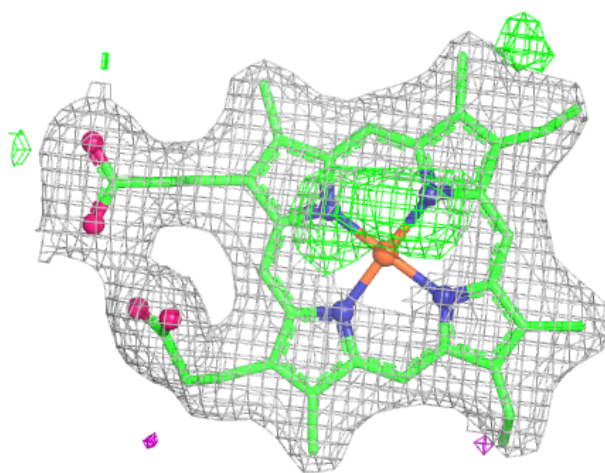
Electron density around HEM P 502:

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



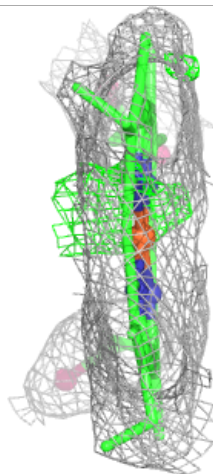
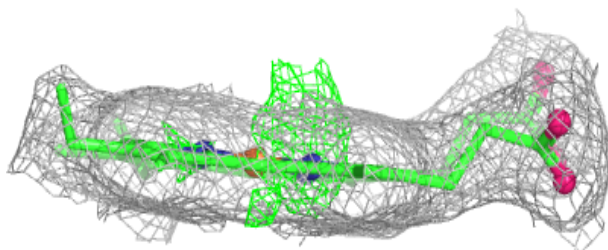
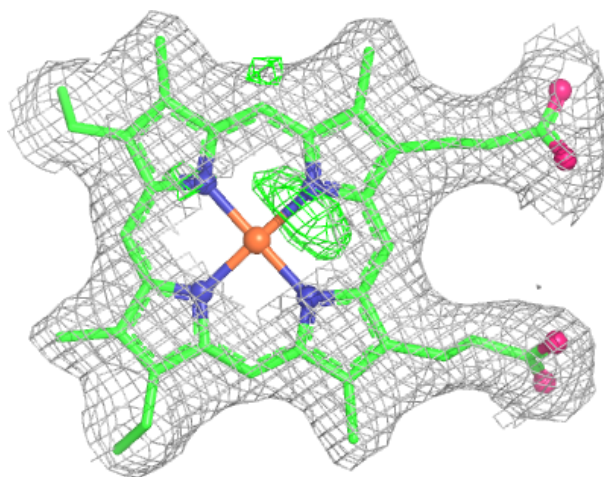
Electron density around HEM G 502:

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



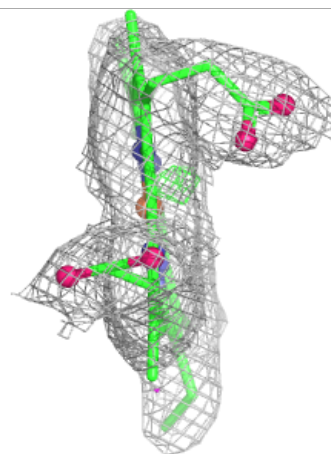
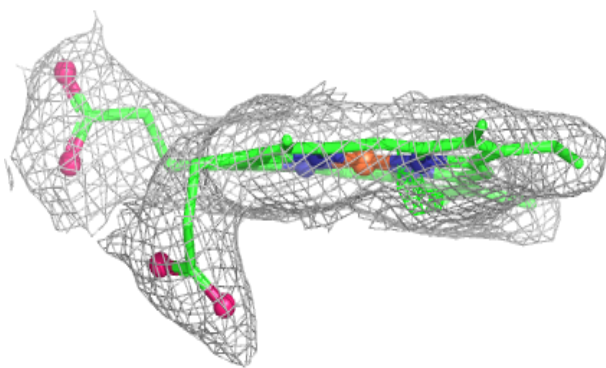
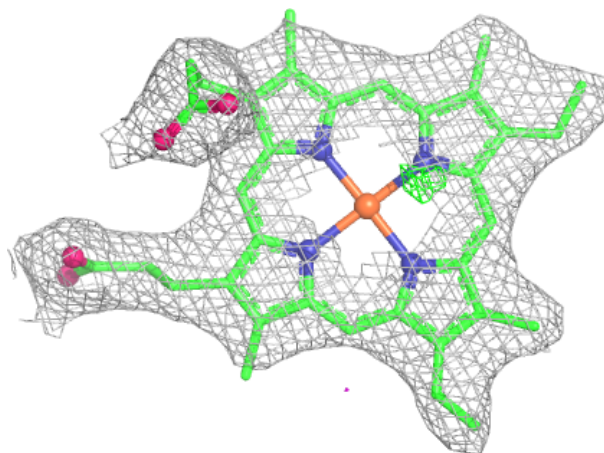
Electron density around HEM H 301:

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



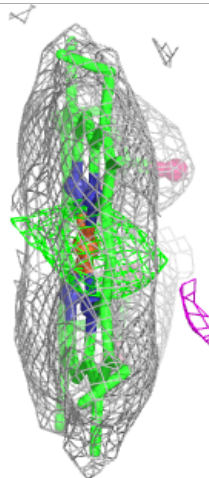
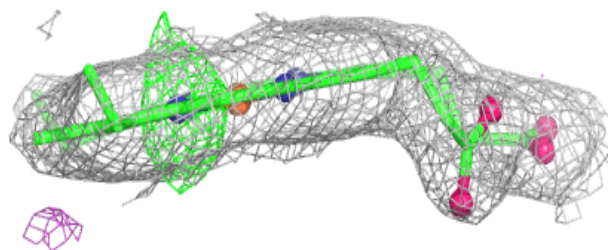
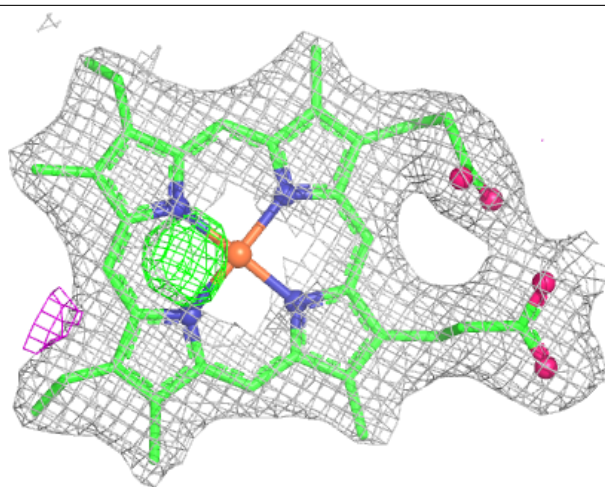
Electron density around HEM D 501:

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



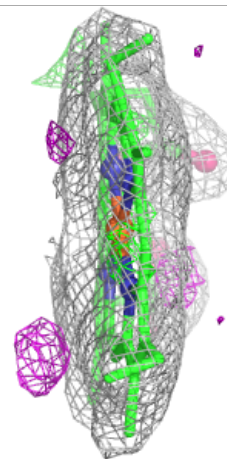
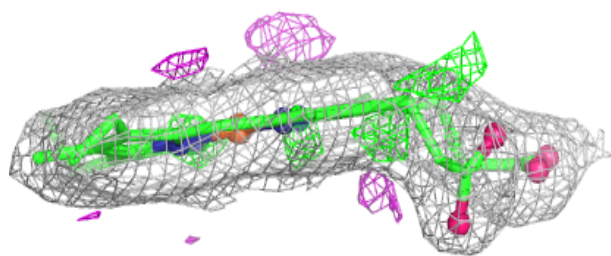
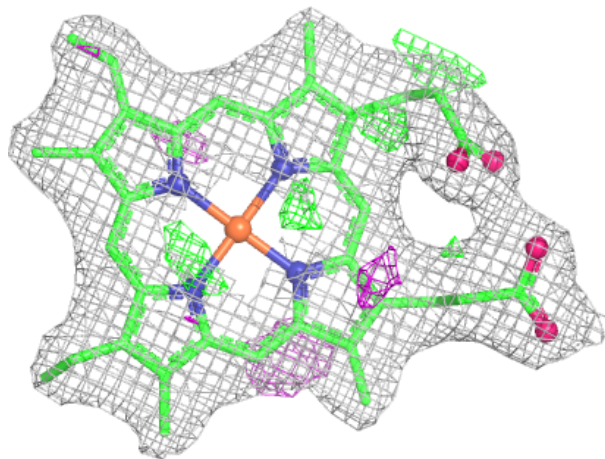
Electron density around HEM J 502:

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



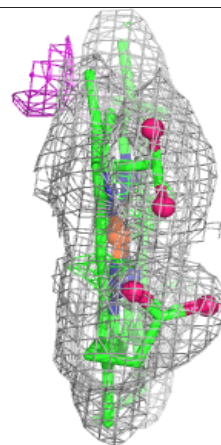
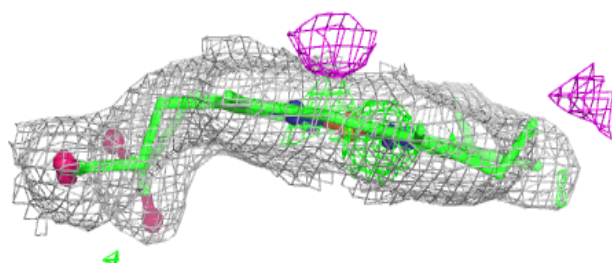
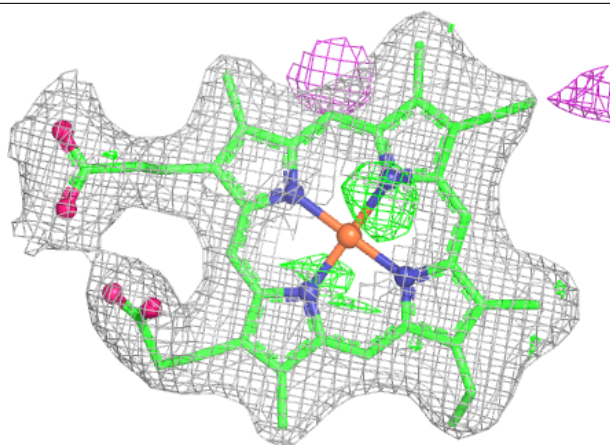
Electron density around HEM D 502:

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



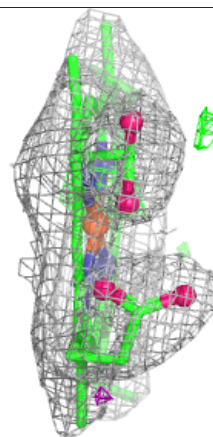
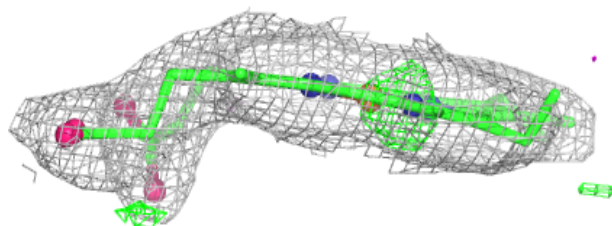
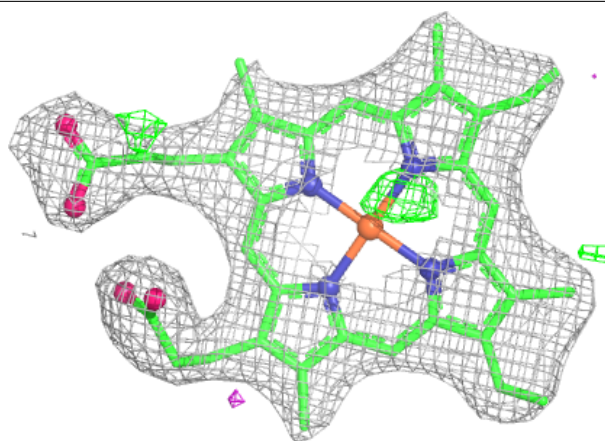
Electron density around HEM A 502:

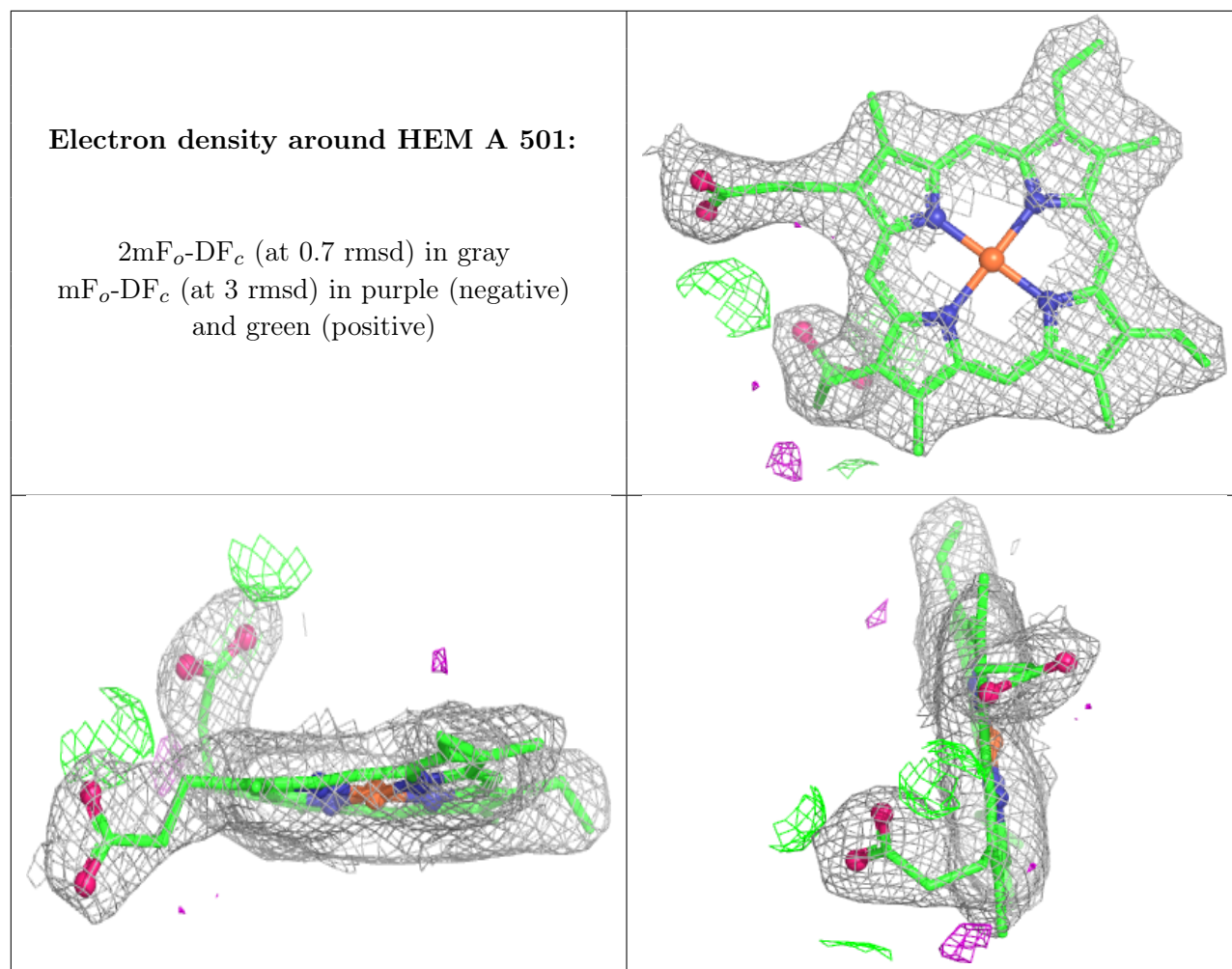
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM M 502:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.