



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 02:23 AM EDT

PDB ID : 2QJY
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

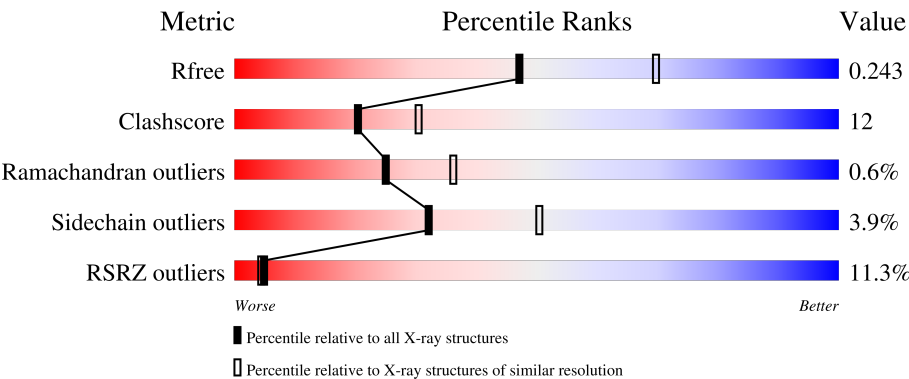
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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	<div><div>2%</div><div>77%</div><div>17%</div><div>.</div><div>.</div></div>
1	D	445	<div><div>2%</div><div>77%</div><div>18%</div><div>.</div><div>.</div></div>
1	G	445	<div><div>6%</div><div>75%</div><div>20%</div><div>.</div><div>.</div></div>
1	J	445	<div><div>7%</div><div>73%</div><div>21%</div><div>.</div><div>.</div></div>
1	M	445	<div><div>10%</div><div>72%</div><div>23%</div><div>.</div><div>.</div></div>

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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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	UQ2	A	1101	-	-	-	X
8	UQ2	J	1104	-	-	-	X
8	UQ2	M	1105	-	-	-	X

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 (three-letter code: 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

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- The diagram illustrates the chemical structure of a Heme (HEM) molecule. At the center is an iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The structure is labeled with various side chains and atoms, including C1A, C2A, C3A, C4A, C1B, C2B, C3B, C4B, C1C, C2C, C3C, C4C, C1D, C2D, C3D, C4D, C1E, C2E, C3E, C4E, C1F, C2F, C3F, C4F, C1G, C2G, C3G, C4G, C1H, C2H, C3H, C4H, C1I, C2I, C3I, C4I, C1J, C2J, C3J, C4J, C1K, C2K, C3K, C4K, C1L, C2L, C3L, C4L, C1M, C2M, C3M, C4M, C1N, C2N, C3N, C4N, C1O, C2O, C3O, C4O, C1P, C2P, C3P, C4P, C1Q, C2Q, C3Q, C4Q, C1R, C2R, C3R, C4R, C1S, C2S, C3S, C4S, C1T, C2T, C3T, C4T, C1U, C2U, C3U, C4U, C1V, C2V, C3V, C4V, C1W, C2W, C3W, C4W, C1X, C2X, C3X, C4X, C1Y, C2Y, C3Y, C4Y, C1Z, C2Z, C3Z, C4Z, C1AA, C2AA, C3AA, C4AA, C1AB, C2AB, C3AB, C4AB, C1AC, C2AC, C3AC, C4AC, C1AD, C2AD, C3AD, C4AD, C1AE, C2AE, C3AE, C4AE, C1AF, C2AF, C3AF, C4AF, C1AG, C2AG, C3AG, C4AG, C1AH, C2AH, C3AH, C4AH, C1AI, C2AI, C3AI, C4AI, C1AJ, C2AJ, C3AJ, C4AJ, C1AK, C2AK, C3AK, C4AK, C1AL, C2AL, C3AL, C4AL, C1AM, C2AM, C3AM, C4AM, C1AN, C2AN, C3AN, C4AN, C1AO, C2AO, C3AO, C4AO, C1AP, C2AP, C3AP, C4AP, C1AQ, C2AQ, C3AQ, C4AQ, 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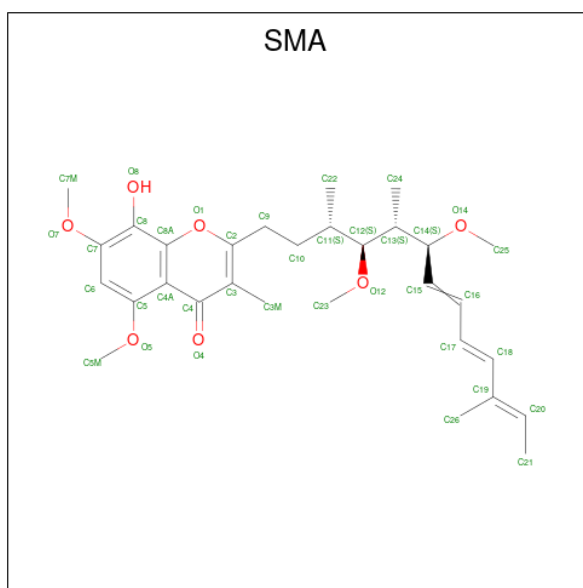
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
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5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0



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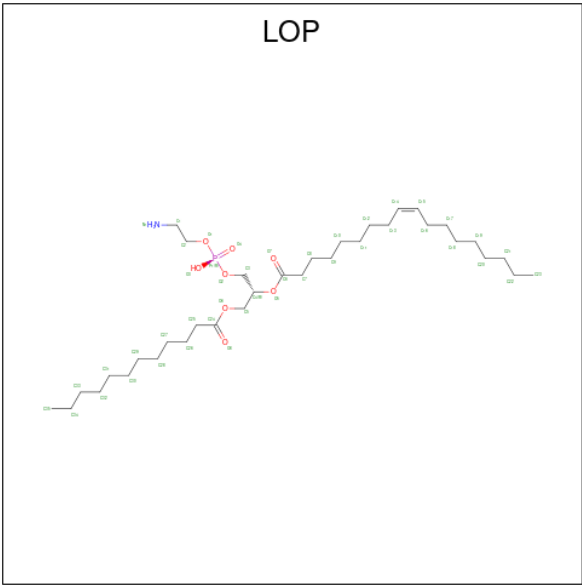
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	M	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 (three-letter code: SMA) (formula: $C_{30}H_{42}O_7$).



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 (three-letter code: LOP) (formula: C₃₅H₆₈NO₈P).



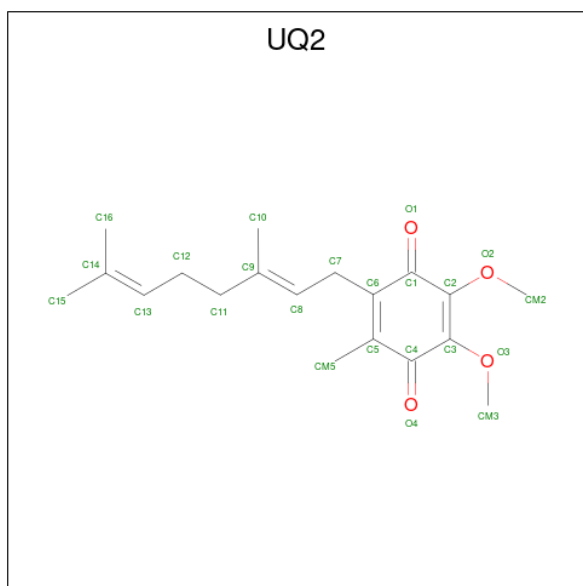
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
7	D	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
7	G	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
7	J	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
7	M	1	Total	C	N	O	P	0	0
			45	35	1	8	1		

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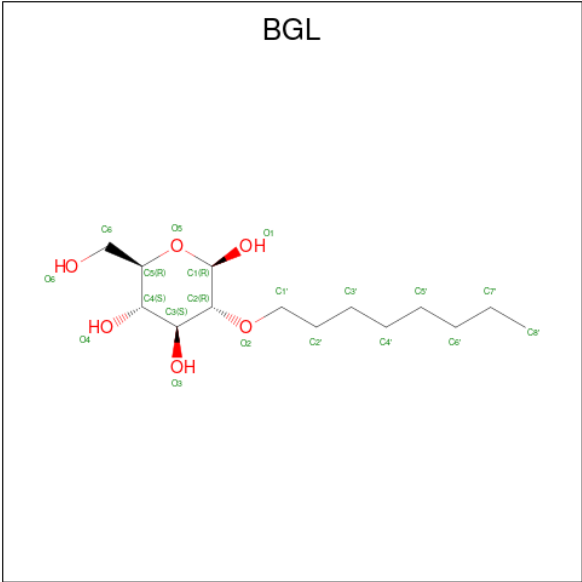
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	P	1	Total	C	N	O	P	0	0
			45	35	1	8	1		

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



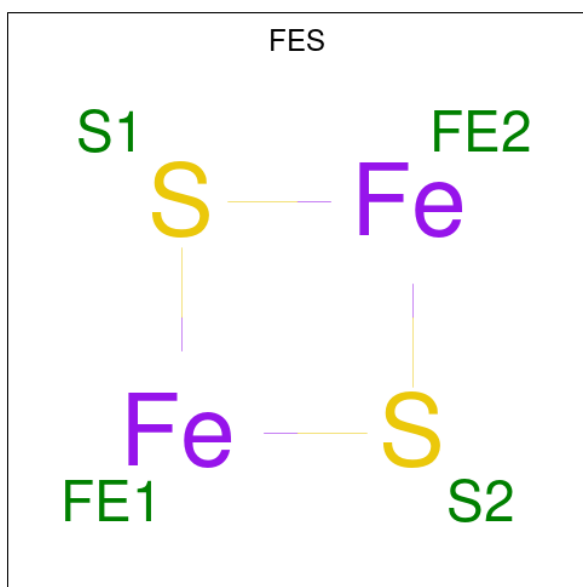
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			23	19	4		
8	D	1	Total	C	O	0	0
			23	19	4		
8	G	1	Total	C	O	0	0
			23	19	4		
8	J	1	Total	C	O	0	0
			23	19	4		
8	M	1	Total	C	O	0	0
			23	19	4		
8	P	1	Total	C	O	0	0
			23	19	4		

- Molecule 9 is 2-O-octyl-beta-D-glucopyranose (three-letter code: 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 (three-letter code: 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 (three-letter code: 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 (three-letter code: NA) (formula: Na).

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

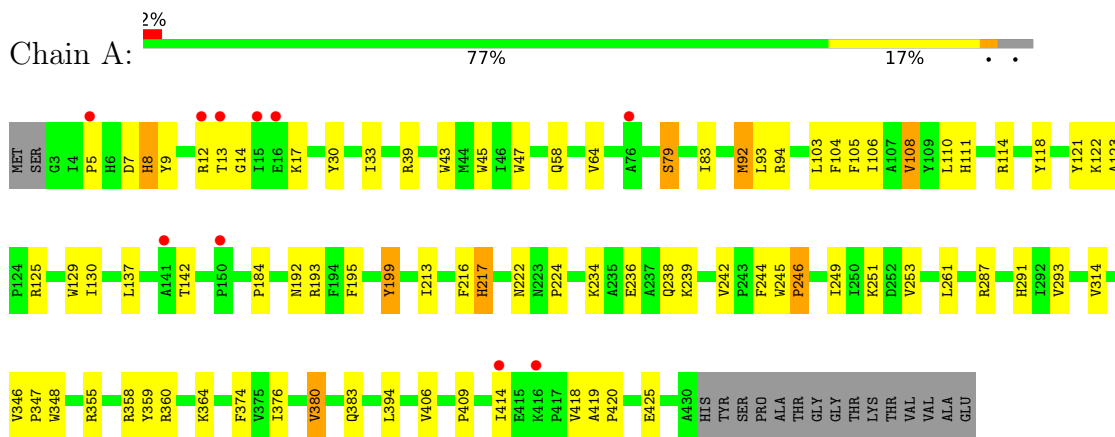
- Molecule 13 is water.

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

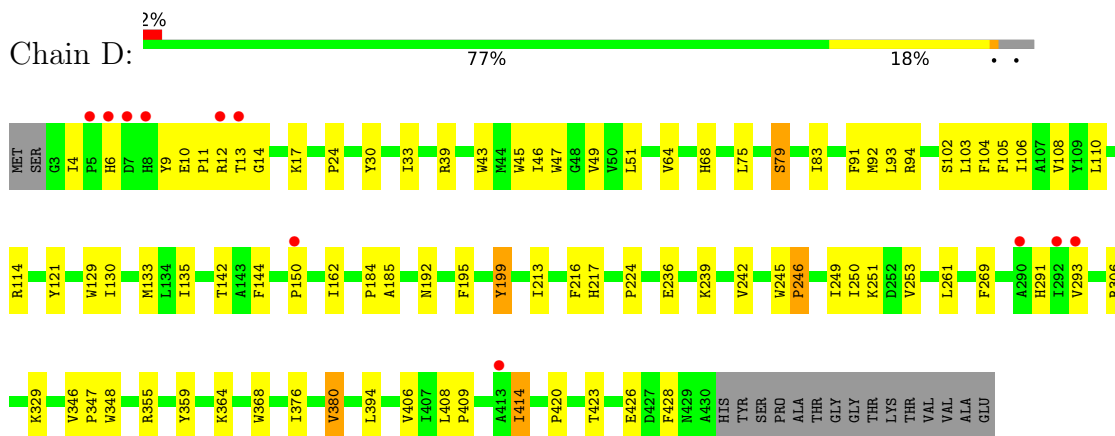
3 Residue-property plots [i](#)

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.

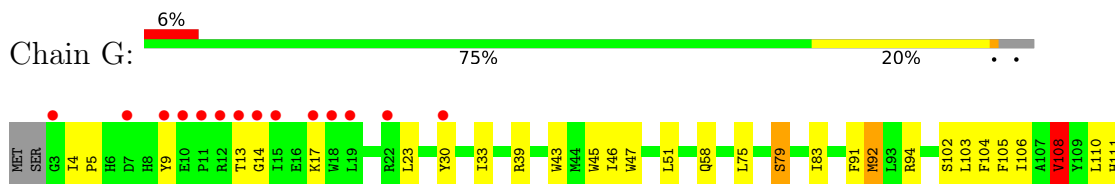
• Molecule 1: Cytochrome b

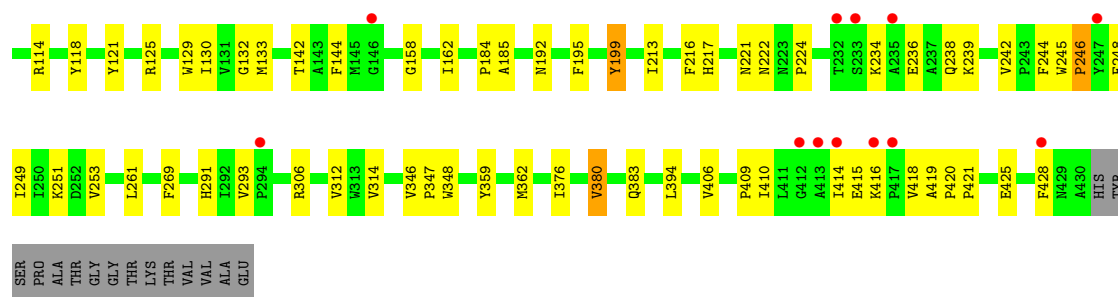


• Molecule 1: Cytochrome b



• Molecule 1: Cytochrome b





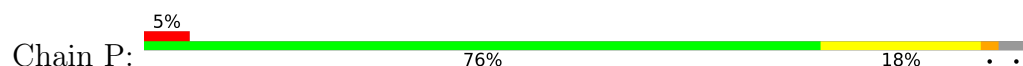
• Molecule 1: Cytochrome b

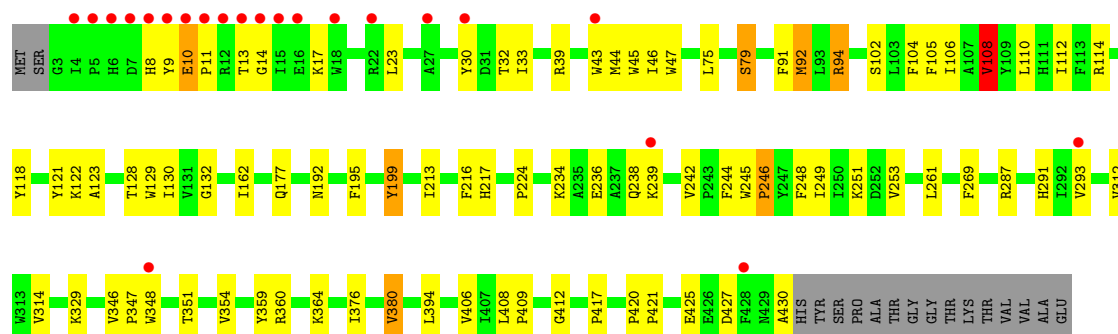


• Molecule 1: Cytochrome b

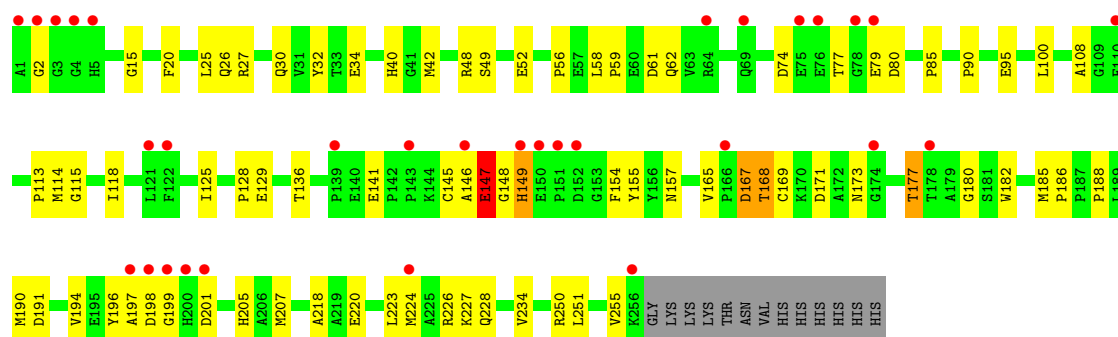


• Molecule 1: Cytochrome b

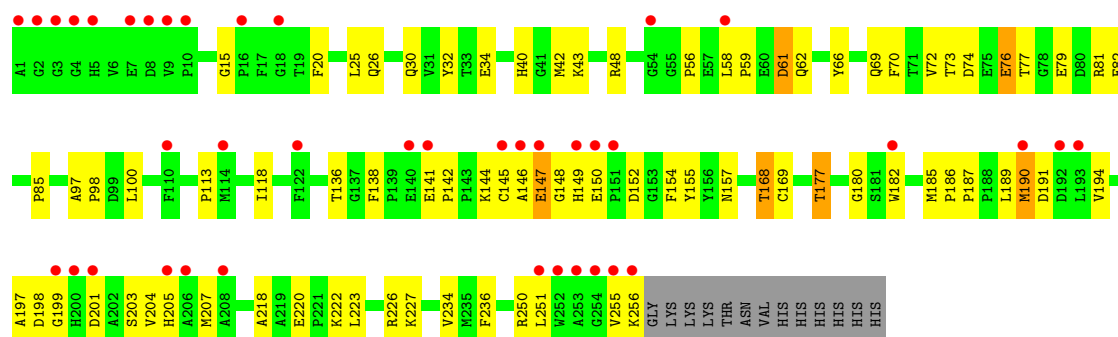




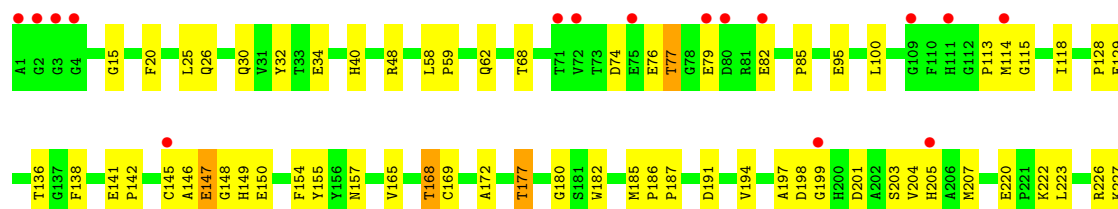
- Molecule 2: Cytochrome c1

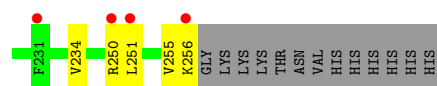


- Molecule 2: Cytochrome c1

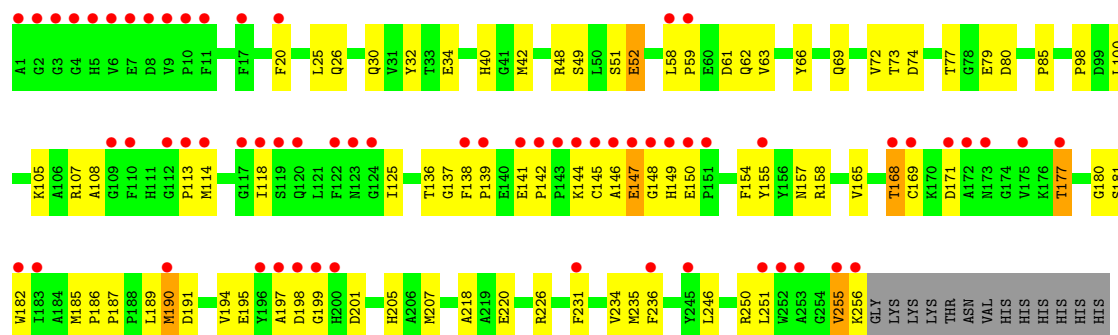


- Molecule 2: Cytochrome c1

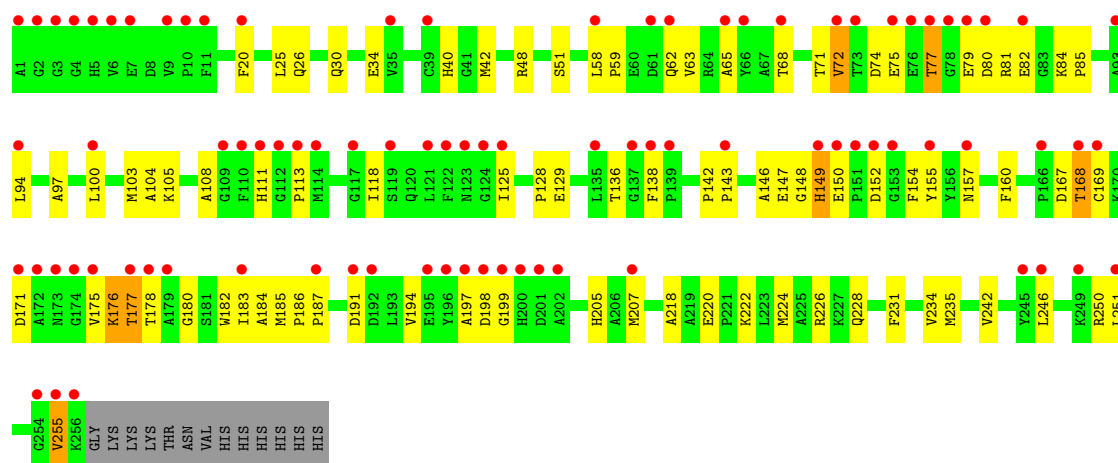




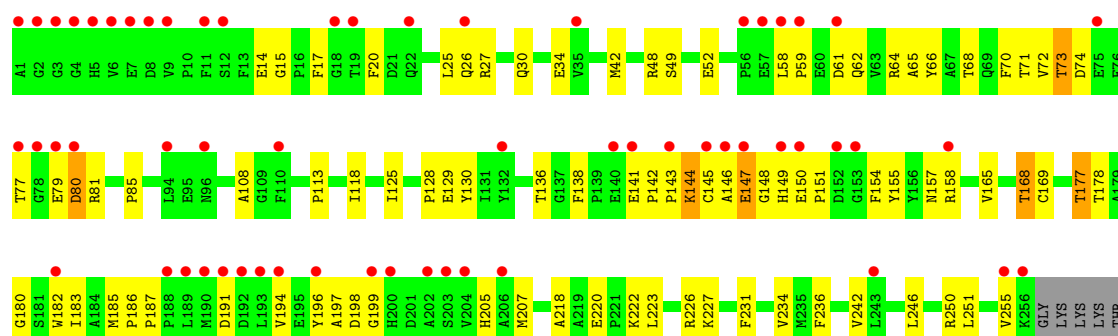
• Molecule 2: Cytochrome c1



• Molecule 2: Cytochrome c1




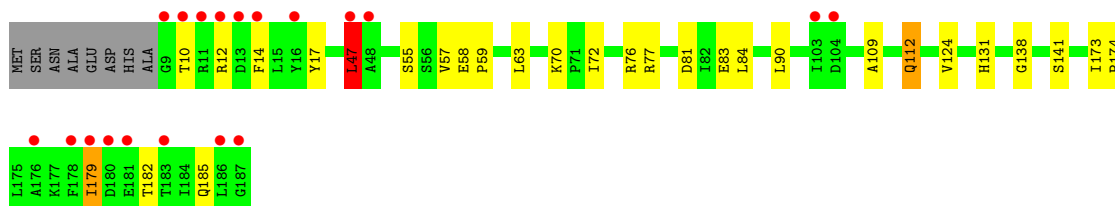
• Molecule 2: Cytochrome c1




ASN
VAL
HIS
HIS
HIS
HIS
HIS

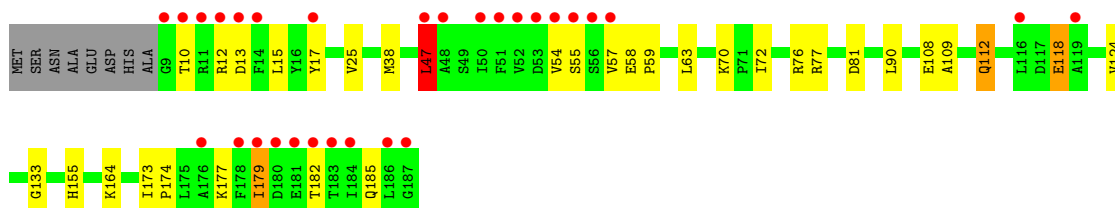
- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain C: 




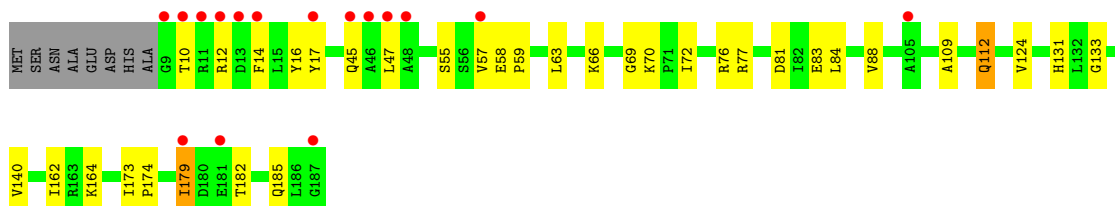
- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain F: 




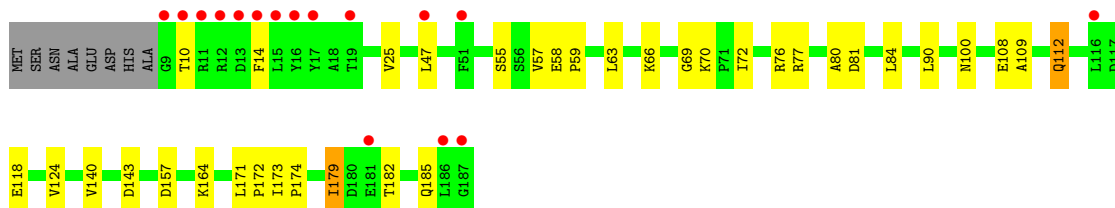
- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain I: 



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

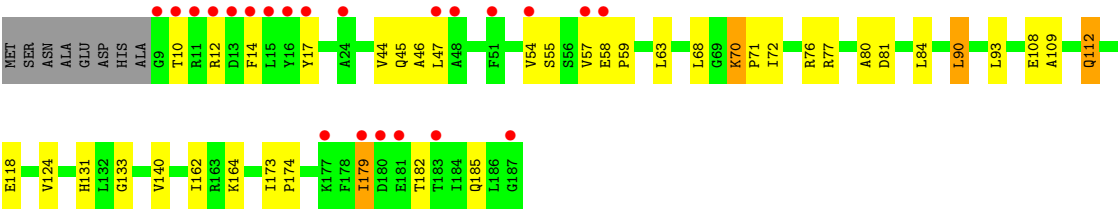
Chain L: 



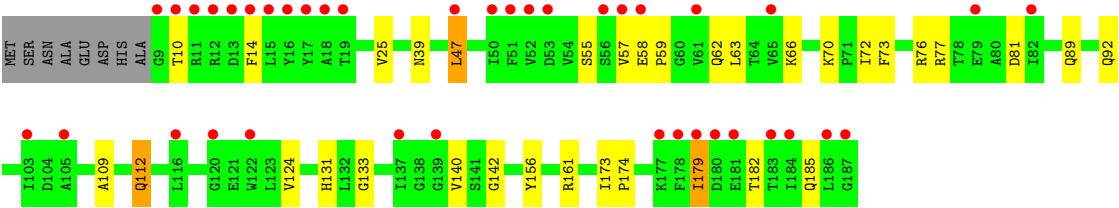
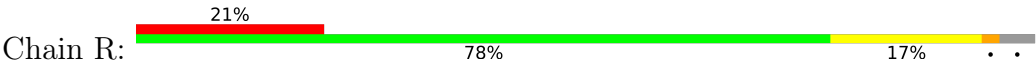
- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain O: 





● 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 47.10 – 2.35	Depositor EDS
% Data completeness (in resolution range)	93.7 (18.00-2.40) 91.9 (47.10-2.35)	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 0.229 , 0.243	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)	0.36 , 60.8	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: CL, SR, NA, HEM, LOP, SMA, BGL, UQ2, FES

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	0.39	0/3570	0.66	0/4897
1	D	0.39	0/3570	0.66	0/4897
1	G	0.38	0/3570	0.66	1/4897 (0.0%)
1	J	0.40	0/3570	0.66	0/4897
1	M	0.38	0/3570	0.65	0/4897
1	P	0.38	0/3570	0.65	1/4897 (0.0%)
2	B	0.37	0/2010	0.67	0/2733
2	E	0.36	0/2010	0.68	0/2733
2	H	0.37	0/2010	0.68	0/2733
2	K	0.36	0/2010	0.67	0/2733
2	N	0.36	0/2010	0.67	0/2733
2	Q	0.35	0/2010	0.66	0/2733
3	C	0.38	0/1370	0.74	1/1866 (0.1%)
3	F	0.39	0/1370	0.74	2/1866 (0.1%)
3	I	0.39	0/1370	0.76	1/1866 (0.1%)
3	L	0.38	0/1370	0.72	1/1866 (0.1%)
3	O	0.38	0/1370	0.72	1/1866 (0.1%)
3	R	0.38	0/1370	0.73	2/1866 (0.1%)
All	All	0.38	0/41700	0.68	10/56976 (0.0%)

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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	47	LEU	CA-CB-CG	7.62	132.83	115.30
3	R	47	LEU	CA-CB-CG	7.10	131.63	115.30
3	C	47	LEU	CA-CB-CG	6.99	131.38	115.30
3	L	47	LEU	CA-CB-CG	6.49	130.22	115.30
1	P	108	VAL	CB-CA-C	-5.59	100.78	111.40
1	G	108	VAL	CB-CA-C	-5.29	101.34	111.40
3	O	133	GLY	N-CA-C	5.21	126.12	113.10
3	R	133	GLY	N-CA-C	5.13	125.94	113.10
3	I	133	GLY	N-CA-C	5.12	125.89	113.10
3	F	133	GLY	N-CA-C	5.00	125.60	113.10

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	70	0
1	D	3440	0	3428	81	0
1	G	3440	0	3428	91	0
1	J	3440	0	3428	96	0
1	M	3440	0	3428	95	0
1	P	3440	0	3428	78	0
2	B	1953	0	1848	65	0
2	E	1953	0	1848	89	0
2	H	1953	0	1848	71	0
2	K	1953	0	1848	70	0
2	N	1953	0	1848	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Q	1953	0	1848	78	0
3	C	1340	0	1303	26	0
3	F	1340	0	1303	27	0
3	I	1340	0	1303	27	0
3	L	1340	0	1303	25	0
3	O	1340	0	1303	27	0
3	R	1340	0	1303	26	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	8	0
5	E	43	0	30	1	0
5	G	86	0	60	9	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	8	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	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	G	23	0	26	3	0
8	J	23	0	26	1	0
8	M	23	0	26	2	0
8	P	23	0	26	4	0
9	B	20	0	28	1	0
9	E	20	0	28	3	0
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	1025	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 12.

All (1025) 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
2:N:77:THR:HG22	2:N:79:GLU:H	1.25	1.02
2:Q:144:LYS:HA	2:Q:144:LYS:NZ	1.75	1.01
2:B:250:ARG:HD3	3:C:12:ARG:HG2	1.41	1.01
2:K:74:ASP:HB3	2:K:77:THR:HB	1.42	0.99
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
1:J:428:PHE:CE1	2:K:256:LYS:HD2	2.24	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: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
2:N:194:VAL:HB	2:N:207:MET:CE	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:239:LYS:HE2	1:J:425:GLU:OE1	1.90	0.70
1:D:92:MET:HE1	2:E:226:ARG:HG3	1.72	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
2:Q:194:VAL:HB	2:Q:207:MET:CE	2.22	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
2:N:194:VAL:HB	2:N:207:MET:HE3	1.72	0.69
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
1:P:130:ILE:HD11	1:P:348:TRP:HH2	1.57	0.69
2:H:194:VAL:HB	2:H:207:MET:CE	2.23	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
2:K:194:VAL:HB	2:K:207:MET:CE	2.23	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
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
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
2:K:49:SER:HA	2:K:52:GLU:HG3	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:194:VAL:HB	2:E:207:MET:CE	2.24	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
2:N:138:PHE:HD2	2:N:187:PRO:HG3	1.56	0.66
2:B:194:VAL:HB	2:B:207:MET:CE	2.24	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
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
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
2:K:26:GLN:HG2	2:K:58:LEU:HD21	1.79	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:O:118:GLU:CD	3:O:118:GLU:H	2.02	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:J:103:LEU:HD13	7:J:1024:LOP:H211	1.82	0.62
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
1:J:62:GLY:C	5:J:502:HEM:HAC	2.20	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
2:K:194:VAL:HB	2:K:207:MET:HE1	1.81	0.61
3:O:118:GLU:CD	3:O:118:GLU:N	2.54	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:91:PHE:CE2	1:D:92:MET:HE3	2.37	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
2:H:194:VAL:HB	2:H:207:MET:HE1	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:194:VAL:HB	2:B:207:MET:HE3	1.85	0.59
2:Q:194:VAL:HB	2:Q:207:MET:HE1	1.83	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:K:42:MET:HE2	2:K:218:ALA:HB1	1.85	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
8:P:1106:UQ2:H5M1	8:P:1106:UQ2:C8	2.33	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
2:Q:194:VAL:HB	2:Q:207:MET:HE3	1.84	0.58
1:D:91:PHE:HE2	1:D:92:MET:HE3	1.68	0.58
1:G:406:VAL:O	1:G:409:PRO:HD2	2.02	0.58
2:Q:42:MET:HE2	2:Q:218:ALA:HB1	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:E:194:VAL:HB	2:E:207:MET:HE1	1.85	0.57
3:L:55:SER:HB3	3:L:182:THR:OG1	2.04	0.57
3:O:55:SER:HB3	3:O:182:THR:OG1	2.04	0.57
1:A:92:MET:HE1	2:B:226:ARG:HG3	1.86	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
2:B:42:MET:HE2	2:B:218:ALA:HB1	1.86	0.57
3:C:55:SER:HB3	3:C:182:THR:OG1	2.05	0.57
3:F:10:THR:HG22	3:F:10:THR:O	2.04	0.57
1:M:132:GLY:C	5:M:501:HEM:HBC2	2.25	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
2:E:42:MET:HE2	2:E:218:ALA:HB1	1.86	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: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
2:B:42:MET:HE1	2:B:218:ALA:CB	2.35	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
3:L:10:THR:HG22	3:L:10:THR:O	2.05	0.56
2:N:138:PHE:CE1	2:N:157:ASN:ND2	2.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:N:42:MET:HE2	2:N:218:ALA:HB1	1.88	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
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: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
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:D:144:PHE:CD1	1:D:162:ILE:HD12	2.40	0.55
2:E:194:VAL:HB	2:E:207:MET:HE3	1.88	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
2:K:194:VAL:HB	2:K:207:MET:HE3	1.89	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:E:42:MET:HE1	2:E:218:ALA:CB	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:H:194:VAL:HB	2:H:207:MET:HE3	1.87	0.55
2:Q:246:LEU:O	2:Q:250:ARG:HG2	2.07	0.55
1:D:92:MET:CE	2:E:226:ARG:HG3	2.35	0.55
1:G:92:MET:HE2	1:G:92:MET:HA	1.89	0.55
2:B:194:VAL:HB	2:B:207:MET:HE1	1.88	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:42:MET:CE	2:B:218:ALA:CB	2.85	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: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: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
1:J:91:PHE:CE2	1:J:92:MET:HE2	2.43	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:42:MET:CE	2:K:218:ALA:HB1	2.38	0.53
2:Q:77:THR:C	2:Q:79:GLU:H	2.11	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:114:ARG:C	1:A:114:ARG:HD2	2.30	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
1:J:114:ARG:HD2	1:J:114:ARG:C	2.31	0.52
1:J:132:GLY:C	5:J:501:HEM:HBC2	2.31	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:P:114:ARG:HD2	1:P:114:ARG:C	2.31	0.52
1:A:346:VAL:HG12	1:A:347:PRO:HD3	1.91	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
1:M:114:ARG:C	1:M:114:ARG:HD2	2.31	0.51
2:N:160:PHE:CE2	2:N:183:ILE:HG13	2.44	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
1:G:114:ARG:HD2	1:G:114:ARG:C	2.30	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
1:D:114:ARG:HD2	1:D:114:ARG:C	2.31	0.51
2:E:42:MET:CE	2:E:218:ALA:CB	2.89	0.51
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
2:K:42:MET:HE1	2:K:218:ALA:CB	2.41	0.51
1:G:125:ARG:HD2	13:G:1118:HOH:O	2.11	0.50
1:M:92:MET:CE	2:N:226:ARG:HG3	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:91:PHE:CD1	2:E:222:LYS:HG2	2.46	0.50
2:B:108:ALA:HA	2:B:125:ILE:HG22	1.93	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: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
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
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
1:G:5:PRO:CB	1:G:234:LYS:HG2	2.42	0.49
1:P:128:THR:HG21	5:P:501:HEM:HBD1	1.94	0.49
1:P:406:VAL:C	1:P:409:PRO:HD2	2.33	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:D:92:MET:HE1	2:E:226:ARG:CG	2.41	0.49
1:M:122:LYS:O	1:M:123:ALA:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:R:59:PRO:HD3	3:R:76:ARG:NH1	2.28	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: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
8:G:1103:UQ2:H5M1	8:G:1103:UQ2:C8	2.43	0.48
3:I:59:PRO:HD3	3:I:76:ARG:NH1	2.28	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:G:125:ARG:CZ	1:G:222:ASN:HB2	2.43	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
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: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
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
2:N:108:ALA:HA	2:N:125:ILE:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:185:MET:HB2	5:Q:301:HEM:C1D	2.49	0.48
2:B:77:THR:C	2:B:79:GLU:H	2.16	0.47
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
1:P:92:MET:HA	1:P:92:MET:HE2	1.96	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
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
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
1:J:91:PHE:CE2	1:J:92:MET:CE	2.97	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: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
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
3:O:57:VAL:HG22	3:O:63:LEU:HD13	1.95	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
2:B:205:HIS:ND1	2:B:205:HIS:C	2.68	0.47
1:M:10:GLU:HA	1:M:11:PRO:HD3	1.70	0.47
1:P:177:GLN:NE2	13:P:611:HOH:O	2.40	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:92:MET:HE1	2:N:226:ARG:HG3	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:414:ILE:O	1:J:414:ILE:CG2	2.62	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:E:77:THR:C	2:E:79:GLU:H	2.17	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
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
2:N:205:HIS:ND1	2:N:205:HIS:C	2.69	0.46
3:O:47:LEU:HG	3:O:68:LEU:HD21	1.97	0.46
2:E:205:HIS:ND1	2:E:205:HIS:C	2.68	0.46
1:G:30:TYR:HA	1:G:33:ILE:HG22	1.98	0.46
2:H:205:HIS:ND1	2:H:205:HIS:C	2.69	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:42:MET:CE	2:B:218:ALA:HB1	2.45	0.46
2:B:147:GLU:OE1	2:B:147:GLU:HA	2.14	0.46
1:G:132:GLY:C	5:G:501:HEM:HBC2	2.35	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
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
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
1:J:354:VAL:HG21	1:J:417:PRO:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:234:LYS:O	1:G:238:GLN:HG3	2.15	0.46
2:N:194:VAL:HB	2:N:207:MET:HE1	1.94	0.46
2:Q:154:PHE:HB3	2:Q:182:TRP:HB3	1.98	0.46
8:P:1106:UQ2:H5M1	8:P:1106:UQ2:H8	1.98	0.46
2:Q:223:LEU:HD21	2:Q:227:LYS:CE	2.32	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:322:SER:O	1:J:323:PHE:HB2	2.16	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
1:M:58:GLN:HB3	5:M:502:HEM:HAB	1.96	0.46
2:Q:72:VAL:CG1	2:Q:73:THR:N	2.79	0.46
2:H:149:HIS:N	2:H:149:HIS:CD2	2.83	0.46
2:K:77:THR:CG2	2:K:79:GLU:HB2	2.46	0.46
1:P:92:MET:HE2	1:P:92:MET:CA	2.44	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
1:J:291:HIS:O	1:J:293:VAL:HG23	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
2:Q:205:HIS:ND1	2:Q:205:HIS:C	2.69	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:205:HIS:ND1	2:K:205:HIS:C	2.68	0.45
2:B:77:THR:HG22	2:B:79:GLU:CG	2.47	0.45
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
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
1:P:94:ARG:C	1:P:94:ARG:HD3	2.37	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: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
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
1:J:209:VAL:HG22	5:J:501:HEM:HBB2	1.98	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:H:68:THR:HG23	2:H:82:GLU:OE1	2.16	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
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
2:Q:42:MET:HE2	2:Q:218:ALA:CB	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
2:B:171:ASP:OD1	2:B:171:ASP:C	2.56	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
2:E:250:ARG:HH11	2:E:250:ARG:CG	2.19	0.45
3:F:118:GLU:CD	3:F:118:GLU:N	2.70	0.45
1:G:118:TYR:OH	7:G:1023:LOP:H32	2.15	0.45
2:H:76:GLU:O	2:H:77:THR:C	2.55	0.45
2:N:42:MET:HE1	2:N:218:ALA:CB	2.47	0.45
2:N:51:SER:OG	2:N:63:VAL:HG21	2.17	0.45
3:O:140:VAL:HG12	3:O:140:VAL:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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:P:132:GLY:C	5:P:501:HEM:HBC2	2.38	0.44
1:A:121:TYR:HB3	1:A:129:TRP:CE3	2.52	0.44
1:G:133:MET:SD	5:G:501:HEM:HBC1	2.58	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
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:N:197:ALA:C	2:N:199:GLY:H	2.22	0.44
2:Q:74:ASP:HB3	2:Q:77:THR:HB	2.00	0.44
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
3:I:12:ARG:H	3:I:12:ARG:HG2	1.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:R:77:ARG:HB3	3:R:81:ASP:HB2	2.00	0.43
1:G:406:VAL:C	1:G:409:PRO:HD2	2.38	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
2:E:34:GLU:OE1	2:E:194:VAL:HG22	2.19	0.43
1:G:92:MET:HA	1:G:92:MET:CE	2.47	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
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
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
1:P:44:MET:CE	7:P:1026:LOP:H92	2.48	0.43
3:R:10:THR:O	3:R:14:PHE:HB3	2.18	0.43
3:R:62:GLN:NE2	3:R:73:PHE:CG	2.87	0.43
1:A:92:MET:HA	1:A:92:MET:HE2	2.01	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
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
2:Q:197:ALA:C	2:Q:199:GLY:H	2.21	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:N	2:B:155:TYR:CD1	2.87	0.43
1:J:359:TYR:CD2	1:J:420:PRO:HB3	2.54	0.43
2:K:42:MET:CE	2:K:218:ALA:CB	2.97	0.43
2:K:155:TYR:N	2:K:155:TYR:CD1	2.87	0.43
2:K:165:VAL:CG1	2:K:169:CYS:HB2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:427:ASP:O	1:M:430:ALA:HB3	2.18	0.43
2:N:74:ASP:CG	2:N:77:THR:HB	2.39	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
1:M:92:MET:HA	1:M:92:MET:HE2	2.00	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:6:HIS:ND1	1:M:6:HIS:C	2.71	0.43
1:M:47:TRP:CZ2	1:M:110:LEU:HD13	2.53	0.43
5:M:502:HEM:HBC2	5:M:502:HEM:CMC	2.49	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: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
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
2:N:103:MET:C	2:N:105:LYS:H	2.21	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:K:197:ALA:C	2:K:199:GLY:H	2.23	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
1:D:236:GLU:HA	1:D:239:LYS:HD2	2.02	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:O:47:LEU:HD23	3:O:47:LEU:C	2.39	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
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
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:121:TYR:HB3	1:P:129:TRP:CE3	2.54	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
3:L:58:GLU:N	3:L:58:GLU:CD	2.73	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:364:LYS:O	1:D:368:TRP:HD1	2.02	0.42
1:D:406:VAL:C	1:D:409:PRO:HD2	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:30:GLN:HG2	2:E:34:GLU:OE2	2.20	0.42
2:E:76:GLU:O	2:E:77:THR:C	2.57	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
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
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
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
1:P:122:LYS:O	1:P:123:ALA:C	2.58	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:58:GLU:N	3:I:58:GLU:CD	2.73	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
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
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
3:O:58:GLU:N	3:O:58:GLU:CD	2.74	0.41
1:A:111:HIS:CD2	5:A:501:HEM:NC	2.89	0.41
1:A:122:LYS:O	1:A:123:ALA:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:162:ILE:HD11	3:I:164:LYS:O	2.21	0.41
1:M:322:SER:O	1:M:325:ILE:HD12	2.21	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
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
2:N:176:LYS:HG2	2:N:178:THR:O	2.19	0.41
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
2:Q:154:PHE:C	2:Q:155:TYR:CD1	2.94	0.41
3:R:58:GLU:CD	3:R:58:GLU:N	2.73	0.41
2:H:197:ALA:C	2:H:199:GLY:H	2.23	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
2:N:42:MET:HE2	2:N:218:ALA:CB	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: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
3:F:58:GLU:CD	3:F:58:GLU:N	2.74	0.41
1:G:51:LEU:HB3	5:G:501:HEM:HMB1	2.03	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:122:LYS:O	1:J:123:ALA:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:GLU:CD	3:C:58:GLU:N	2.73	0.41
3:C:124:VAL:O	3:C:173:ILE:HG23	2.21	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: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: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
1:P:130:ILE:HD11	1:P:348:TRP:CH2	2.47	0.41
2:Q:77:THR:C	2:Q:79:GLU:N	2.73	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:B:154:PHE:C	2:B:155:TYR:CD1	2.94	0.41
2:E:61:ASP:OD1	2:E:61:ASP:N	2.53	0.41
3:F:54:VAL:HG13	3:F:54:VAL:O	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:154:PHE:C	2:N:155:TYR:CD1	2.94	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: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:43:TRP:O	1:G:46:ILE:HG12	2.22	0.40
1:G:92:MET:HE1	2:H:226:ARG:HG3	2.03	0.40
1:G:125:ARG:HH21	1:G:221:ASN:C	2.23	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
2:N:152:ASP:OD1	2:N:152:ASP:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:156:TYR:HA	3:R:161:ARG:O	2.21	0.40
2:B:197:ALA:C	2:B:199:GLY:H	2.24	0.40
1:D:64:VAL:HG11	1:D:93:LEU:HD13	2.02	0.40
2:E:154:PHE:C	2:E:155:TYR:CD1	2.94	0.40
3:F:59:PRO:HD3	3:F:76:ARG:HH11	1.86	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
2:E:146:ALA:O	2:E:147:GLU:C	2.59	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
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:203:SER:O	2:H:204:VAL:C	2.60	0.40
1:J:43:TRP:HH2	1:J:251:LYS:HG2	1.86	0.40
2:K:154:PHE:C	2:K:155:TYR:CD1	2.94	0.40
1:M:122:LYS:HZ1	1:M:360:ARG:NH1	2.19	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:E:203:SER:O	2:E:204:VAL:C	2.60	0.40
1:J:6:HIS:ND1	1:J:6:HIS:C	2.75	0.40
3:L:118:GLU:N	3:L:118:GLU:CD	2.75	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:197:ALA:C	2:E:199:GLY:H	2.23	0.40
2:E:250:ARG:HD3	3:F:12:ARG:CG	2.51	0.40
2:H:154:PHE:C	2:H:155:TYR:CD1	2.95	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
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
1:P:75:LEU:O	1:P:79:SER:HB3	2.21	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
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%)	47	62
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%)	13	19
2	E	254/269 (94%)	231 (91%)	20 (8%)	3 (1%)	13	19
2	H	254/269 (94%)	233 (92%)	18 (7%)	3 (1%)	13	19
2	K	254/269 (94%)	231 (91%)	18 (7%)	5 (2%)	7	9
2	N	254/269 (94%)	229 (90%)	20 (8%)	5 (2%)	7	9
2	Q	254/269 (94%)	231 (91%)	21 (8%)	2 (1%)	19	29
3	C	177/187 (95%)	163 (92%)	13 (7%)	1 (1%)	25	36
3	F	177/187 (95%)	161 (91%)	15 (8%)	1 (1%)	25	36
3	I	177/187 (95%)	162 (92%)	12 (7%)	3 (2%)	9	11
3	L	177/187 (95%)	161 (91%)	14 (8%)	2 (1%)	14	20
3	O	177/187 (95%)	162 (92%)	12 (7%)	3 (2%)	9	11
3	R	177/187 (95%)	161 (91%)	15 (8%)	1 (1%)	25	36
All	All	5142/5406 (95%)	4817 (94%)	292 (6%)	33 (1%)	25	36

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

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Mol	Chain	Res	Type
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
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%)	338 (96%)	15 (4%)	30	47
1	D	353/366 (96%)	345 (98%)	8 (2%)	50	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	353/366 (96%)	343 (97%)	10 (3%)	43	63
1	J	353/366 (96%)	342 (97%)	11 (3%)	40	60
1	M	353/366 (96%)	340 (96%)	13 (4%)	34	53
1	P	353/366 (96%)	341 (97%)	12 (3%)	37	56
2	B	203/215 (94%)	191 (94%)	12 (6%)	19	32
2	E	203/215 (94%)	193 (95%)	10 (5%)	25	40
2	H	203/215 (94%)	197 (97%)	6 (3%)	41	61
2	K	203/215 (94%)	192 (95%)	11 (5%)	22	36
2	N	203/215 (94%)	194 (96%)	9 (4%)	28	45
2	Q	203/215 (94%)	193 (95%)	10 (5%)	25	40
3	C	138/144 (96%)	133 (96%)	5 (4%)	35	54
3	F	138/144 (96%)	131 (95%)	7 (5%)	24	39
3	I	138/144 (96%)	132 (96%)	6 (4%)	29	46
3	L	138/144 (96%)	133 (96%)	5 (4%)	35	54
3	O	138/144 (96%)	131 (95%)	7 (5%)	24	39
3	R	138/144 (96%)	133 (96%)	5 (4%)	35	54
All	All	4164/4350 (96%)	4002 (96%)	162 (4%)	32	50

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	8	HIS
1	A	79	SER
1	A	92	MET
1	A	94	ARG
1	A	104	PHE
1	A	108	VAL
1	A	137	LEU
1	A	192	ASN
1	A	199	TYR
1	A	217	HIS
1	A	246	PRO
1	A	314	VAL
1	A	380	VAL
1	A	414	ILE

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Mol	Chain	Res	Type
2	B	61	ASP
2	B	80	ASP
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	191	ASP
2	B	201	ASP
3	C	47	LEU
3	C	72	ILE
3	C	112	GLN
3	C	174	PRO
3	C	179	ILE
1	D	79	SER
1	D	94	ARG
1	D	104	PHE
1	D	192	ASN
1	D	199	TYR
1	D	246	PRO
1	D	380	VAL
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	152	ASP
2	E	168	THR
2	E	177	THR
2	E	191	ASP
2	E	201	ASP
3	F	47	LEU
3	F	72	ILE
3	F	112	GLN
3	F	118	GLU
3	F	174	PRO
3	F	177	LYS
3	F	179	ILE

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Mol	Chain	Res	Type
1	G	79	SER
1	G	92	MET
1	G	94	ARG
1	G	104	PHE
1	G	108	VAL
1	G	192	ASN
1	G	199	TYR
1	G	246	PRO
1	G	380	VAL
1	G	421	PRO
2	H	136	THR
2	H	147	GLU
2	H	168	THR
2	H	177	THR
2	H	191	ASP
2	H	201	ASP
3	I	47	LEU
3	I	72	ILE
3	I	83	GLU
3	I	112	GLN
3	I	174	PRO
3	I	179	ILE
1	J	43	TRP
1	J	79	SER
1	J	94	ARG
1	J	104	PHE
1	J	108	VAL
1	J	192	ASN
1	J	199	TYR
1	J	217	HIS
1	J	246	PRO
1	J	380	VAL
1	J	425	GLU
2	K	52	GLU
2	K	61	ASP
2	K	80	ASP
2	K	136	THR
2	K	168	THR
2	K	171	ASP
2	K	177	THR
2	K	181	SER
2	K	191	ASP

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Mol	Chain	Res	Type
2	K	195	GLU
2	K	201	ASP
3	L	14	PHE
3	L	72	ILE
3	L	112	GLN
3	L	174	PRO
3	L	179	ILE
1	M	6	HIS
1	M	8	HIS
1	M	79	SER
1	M	92	MET
1	M	94	ARG
1	M	104	PHE
1	M	108	VAL
1	M	162	ILE
1	M	192	ASN
1	M	199	TYR
1	M	246	PRO
1	M	287	ARG
1	M	380	VAL
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	191	ASP
3	O	14	PHE
3	O	17	TYR
3	O	70	LYS
3	O	72	ILE
3	O	112	GLN
3	O	174	PRO
3	O	179	ILE
1	P	8	HIS
1	P	10	GLU
1	P	79	SER
1	P	92	MET
1	P	94	ARG
1	P	104	PHE

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Mol	Chain	Res	Type
1	P	108	VAL
1	P	192	ASN
1	P	199	TYR
1	P	246	PRO
1	P	380	VAL
1	P	421	PRO
2	Q	14	GLU
2	Q	71	THR
2	Q	73	THR
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	191	ASP
3	R	47	LEU
3	R	72	ILE
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 (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	192	ASN
1	A	383	GLN
1	A	429	ASN
2	B	22	GLN
2	B	62	GLN
2	B	149	HIS
2	B	228	GLN
3	C	36	ASN
3	C	39	ASN
3	C	112	GLN
3	C	185	GLN
1	D	6	HIS
1	D	192	ASN
1	D	383	GLN
2	E	5	HIS
2	E	22	GLN

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Mol	Chain	Res	Type
2	E	62	GLN
2	E	149	HIS
2	E	228	GLN
3	F	36	ASN
3	F	39	ASN
3	F	45	GLN
3	F	89	GLN
3	F	112	GLN
3	F	185	GLN
1	G	192	ASN
1	G	383	GLN
2	H	22	GLN
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	192	ASN
1	J	221	ASN
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	177	GLN
1	M	192	ASN
1	M	221	ASN
1	M	383	GLN
1	M	429	ASN
2	N	22	GLN
2	N	62	GLN
2	N	149	HIS
2	N	228	GLN
3	O	36	ASN
3	O	39	ASN

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Mol	Chain	Res	Type
3	O	112	GLN
3	O	185	GLN
1	P	8	HIS
1	P	192	ASN
1	P	221	ASN
1	P	383	GLN
2	Q	22	GLN
2	Q	62	GLN
2	Q	149	HIS
2	Q	228	GLN
3	R	36	ASN
3	R	39	ASN
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 monosaccharides 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
8	UQ2	M	1105	-	23,23,23	1.57	5 (21%)	28,31,31	1.16	2 (7%)
9	BGL	B	1041	-	20,20,20	1.03	1 (5%)	24,25,25	0.87	1 (4%)
5	HEM	J	502	1	27,50,50	1.91	7 (25%)	17,82,82	0.99	0
7	LOP	J	1024	-	44,44,44	0.64	0	47,49,49	1.23	6 (12%)
10	FES	O	200	3	0,4,4	-	-	-	-	-
6	SMA	A	1001	-	35,38,38	2.00	6 (17%)	46,52,52	2.00	11 (23%)
5	HEM	H	301	2	27,50,50	1.70	6 (22%)	17,82,82	1.17	1 (5%)
5	HEM	M	501	1	27,50,50	1.62	6 (22%)	17,82,82	0.94	0
5	HEM	A	502	1	27,50,50	1.80	7 (25%)	17,82,82	1.04	0
9	BGL	N	1045	-	20,20,20	1.30	1 (5%)	24,25,25	0.74	0
5	HEM	J	501	1	27,50,50	1.74	6 (22%)	17,82,82	0.87	0
5	HEM	P	502	1	27,50,50	1.71	5 (18%)	17,82,82	1.15	0
8	UQ2	J	1104	-	23,23,23	1.32	4 (17%)	28,31,31	1.13	2 (7%)
6	SMA	P	1006	-	35,38,38	1.92	8 (22%)	46,52,52	2.28	14 (30%)
5	HEM	D	501	1	27,50,50	1.47	4 (14%)	17,82,82	1.06	1 (5%)
5	HEM	A	501	1	27,50,50	1.56	4 (14%)	17,82,82	1.11	0
5	HEM	K	301	2	27,50,50	1.63	5 (18%)	17,82,82	1.04	0
5	HEM	P	501	1	27,50,50	1.66	5 (18%)	17,82,82	0.85	0
9	BGL	K	1044	-	20,20,20	0.99	1 (5%)	24,25,25	1.09	2 (8%)
5	HEM	E	301	2	27,50,50	1.63	6 (22%)	17,82,82	0.98	0
10	FES	F	200	3	0,4,4	-	-	-	-	-
9	BGL	P	1046	-	20,20,20	1.15	1 (5%)	24,25,25	0.92	1 (4%)
10	FES	C	200	3	0,4,4	-	-	-	-	-
7	LOP	A	1021	-	44,44,44	0.62	0	47,49,49	1.17	5 (10%)
6	SMA	J	1004	-	35,38,38	1.88	4 (11%)	46,52,52	1.91	8 (17%)
5	HEM	B	301	2	27,50,50	1.81	6 (22%)	17,82,82	1.01	0
7	LOP	M	1025	-	44,44,44	0.68	0	47,49,49	1.15	3 (6%)
7	LOP	P	1026	-	44,44,44	0.61	0	47,49,49	1.17	5 (10%)
5	HEM	G	501	1	27,50,50	1.59	5 (18%)	17,82,82	0.87	0
8	UQ2	D	1102	-	23,23,23	1.45	5 (21%)	28,31,31	1.18	2 (7%)
10	FES	R	200	3	0,4,4	-	-	-	-	-
5	HEM	D	502	1	27,50,50	1.67	5 (18%)	17,82,82	1.05	0
7	LOP	D	1022	-	44,44,44	0.70	0	47,49,49	1.17	5 (10%)
5	HEM	G	502	1	27,50,50	1.89	6 (22%)	17,82,82	1.08	0
6	SMA	D	1002	-	35,38,38	1.89	6 (17%)	46,52,52	2.01	11 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BGL	E	1042	-	20,20,20	1.01	1 (5%)	24,25,25	0.95	1 (4%)
9	BGL	G	1043	-	20,20,20	1.29	1 (5%)	24,25,25	0.76	0
8	UQ2	G	1103	-	23,23,23	1.54	5 (21%)	28,31,31	1.09	1 (3%)
6	SMA	M	1005	-	35,38,38	2.00	6 (17%)	46,52,52	2.00	11 (23%)
5	HEM	N	301	2	27,50,50	1.71	6 (22%)	17,82,82	1.01	0
8	UQ2	P	1106	-	23,23,23	1.67	5 (21%)	28,31,31	1.20	4 (14%)
10	FES	L	200	3	0,4,4	-	-	-	-	-
7	LOP	G	1023	-	44,44,44	0.70	0	47,49,49	1.16	4 (8%)
8	UQ2	A	1101	-	23,23,23	1.59	5 (21%)	28,31,31	1.17	2 (7%)
10	FES	I	200	3	0,4,4	-	-	-	-	-
6	SMA	G	1003	-	35,38,38	1.97	7 (20%)	46,52,52	1.98	11 (23%)
5	HEM	Q	301	2	27,50,50	1.63	4 (14%)	17,82,82	1.02	0
5	HEM	M	502	1	27,50,50	1.70	5 (18%)	17,82,82	1.02	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	UQ2	M	1105	-	-	2/15/39/39	0/1/1/1
9	BGL	B	1041	-	-	0/11/31/31	0/1/1/1
5	HEM	J	502	1	-	0/6/54/54	-
7	LOP	J	1024	-	-	10/48/48/48	-
10	FES	O	200	3	-	-	0/1/1/1
6	SMA	A	1001	-	-	4/33/34/34	0/2/2/2
5	HEM	H	301	2	-	0/6/54/54	-
5	HEM	M	501	1	-	0/6/54/54	-
5	HEM	A	502	1	-	0/6/54/54	-
9	BGL	N	1045	-	-	0/11/31/31	0/1/1/1
5	HEM	J	501	1	-	0/6/54/54	-
5	HEM	P	502	1	-	0/6/54/54	-
8	UQ2	J	1104	-	-	0/15/39/39	0/1/1/1
6	SMA	P	1006	-	-	6/33/34/34	0/2/2/2
5	HEM	D	501	1	-	0/6/54/54	-
5	HEM	A	501	1	-	0/6/54/54	-
5	HEM	K	301	2	-	0/6/54/54	-
5	HEM	P	501	1	-	0/6/54/54	-
9	BGL	K	1044	-	-	0/11/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	E	301	2	-	0/6/54/54	-
10	FES	F	200	3	-	-	0/1/1/1
9	BGL	P	1046	-	-	0/11/31/31	0/1/1/1
10	FES	C	200	3	-	-	0/1/1/1
7	LOP	A	1021	-	-	12/48/48/48	-
6	SMA	J	1004	-	-	2/33/34/34	0/2/2/2
5	HEM	B	301	2	-	0/6/54/54	-
7	LOP	M	1025	-	-	6/48/48/48	-
7	LOP	P	1026	-	-	10/48/48/48	-
5	HEM	G	501	1	-	0/6/54/54	-
8	UQ2	D	1102	-	-	2/15/39/39	0/1/1/1
10	FES	R	200	3	-	-	0/1/1/1
5	HEM	D	502	1	-	0/6/54/54	-
7	LOP	D	1022	-	-	5/48/48/48	-
5	HEM	G	502	1	-	0/6/54/54	-
6	SMA	D	1002	-	-	6/33/34/34	0/2/2/2
9	BGL	E	1042	-	-	0/11/31/31	0/1/1/1
9	BGL	G	1043	-	-	0/11/31/31	0/1/1/1
8	UQ2	G	1103	-	-	5/15/39/39	0/1/1/1
6	SMA	M	1005	-	-	8/33/34/34	0/2/2/2
5	HEM	N	301	2	-	0/6/54/54	-
8	UQ2	P	1106	-	-	4/15/39/39	0/1/1/1
10	FES	L	200	3	-	-	0/1/1/1
7	LOP	G	1023	-	-	11/48/48/48	-
8	UQ2	A	1101	-	-	6/15/39/39	0/1/1/1
10	FES	I	200	3	-	-	0/1/1/1
6	SMA	G	1003	-	-	5/33/34/34	0/2/2/2
5	HEM	Q	301	2	-	0/6/54/54	-
5	HEM	M	502	1	-	0/6/54/54	-

All (170) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	1003	SMA	O5-C5	6.84	1.48	1.36
6	M	1005	SMA	O7-C7	6.65	1.47	1.37
6	A	1001	SMA	O5-C5	6.59	1.48	1.36
6	A	1001	SMA	O7-C7	6.52	1.47	1.37
6	J	1004	SMA	O5-C5	6.31	1.47	1.36
6	D	1002	SMA	O5-C5	6.22	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	1004	SMA	O7-C7	5.88	1.46	1.37
6	M	1005	SMA	O5-C5	5.88	1.47	1.36
6	P	1006	SMA	O5-C5	5.77	1.47	1.36
6	G	1003	SMA	O7-C7	5.54	1.46	1.37
5	J	502	HEM	C3C-CAC	-5.52	1.36	1.47
6	P	1006	SMA	O7-C7	5.33	1.45	1.37
6	D	1002	SMA	O7-C7	5.16	1.45	1.37
9	G	1043	BGL	C1-C2	4.35	1.56	1.52
5	G	502	HEM	C3C-CAC	-4.32	1.38	1.47
5	N	301	HEM	C3C-CAC	-4.30	1.39	1.47
9	N	1045	BGL	C1-C2	4.22	1.56	1.52
5	A	502	HEM	C3B-CAB	-3.99	1.39	1.47
5	J	501	HEM	C3B-CAB	-3.96	1.39	1.47
5	P	502	HEM	C3C-C2C	-3.94	1.34	1.40
5	M	502	HEM	C3B-CAB	-3.93	1.39	1.47
5	G	502	HEM	C3C-C2C	-3.92	1.34	1.40
5	K	301	HEM	CBB-CAB	3.89	1.55	1.29
8	G	1103	UQ2	C6-C5	3.84	1.42	1.35
8	P	1106	UQ2	C6-C5	3.82	1.42	1.35
5	B	301	HEM	C3C-CAC	-3.81	1.40	1.47
5	H	301	HEM	CBB-CAB	3.79	1.54	1.29
5	B	301	HEM	CBC-CAC	3.78	1.54	1.29
5	Q	301	HEM	CBB-CAB	3.75	1.54	1.29
5	H	301	HEM	CBC-CAC	3.75	1.54	1.29
8	M	1105	UQ2	C7-C8	3.74	1.56	1.50
5	N	301	HEM	CBB-CAB	3.71	1.53	1.29
5	E	301	HEM	CBB-CAB	3.70	1.53	1.29
5	B	301	HEM	CBB-CAB	3.70	1.53	1.29
5	Q	301	HEM	CBC-CAC	3.69	1.53	1.29
5	K	301	HEM	CBC-CAC	3.69	1.53	1.29
8	A	1101	UQ2	C7-C8	3.69	1.56	1.50
5	N	301	HEM	CBC-CAC	3.69	1.53	1.29
8	P	1106	UQ2	C7-C6	3.67	1.57	1.51
5	E	301	HEM	CBC-CAC	3.63	1.53	1.29
5	G	501	HEM	CBC-CAC	3.61	1.53	1.29
5	P	502	HEM	CBB-CAB	3.61	1.53	1.29
5	G	502	HEM	C3B-C2B	-3.59	1.35	1.40
9	P	1046	BGL	C1-C2	3.58	1.55	1.52
5	D	501	HEM	CBC-CAC	3.58	1.53	1.29
5	A	501	HEM	CBB-CAB	3.56	1.52	1.29
5	J	502	HEM	CBB-CAB	3.54	1.52	1.29
5	J	501	HEM	CBC-CAC	3.54	1.52	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	502	HEM	C3C-CAC	-3.54	1.40	1.47
5	Q	301	HEM	C3B-CAB	-3.53	1.40	1.47
5	A	501	HEM	C3B-CAB	-3.50	1.40	1.47
5	A	501	HEM	CBC-CAC	3.49	1.52	1.29
9	B	1041	BGL	C1-C2	3.48	1.55	1.52
5	J	501	HEM	CBB-CAB	3.48	1.52	1.29
8	P	1106	UQ2	C7-C8	3.47	1.55	1.50
5	P	501	HEM	CBB-CAB	3.47	1.52	1.29
6	D	1002	SMA	C7-C8	-3.46	1.35	1.40
5	M	502	HEM	CBC-CAC	3.46	1.52	1.29
5	B	301	HEM	C3B-CAB	-3.46	1.40	1.47
5	A	502	HEM	CBB-CAB	3.46	1.52	1.29
5	G	501	HEM	CBB-CAB	3.46	1.52	1.29
8	M	1105	UQ2	C6-C5	3.45	1.41	1.35
5	A	502	HEM	CBC-CAC	3.45	1.52	1.29
5	D	501	HEM	CBB-CAB	3.45	1.52	1.29
5	M	501	HEM	CBC-CAC	3.44	1.52	1.29
5	M	501	HEM	CBB-CAB	3.42	1.52	1.29
5	P	501	HEM	CBC-CAC	3.42	1.52	1.29
5	J	502	HEM	C3B-CAB	-3.41	1.41	1.47
5	G	502	HEM	CBB-CAB	3.41	1.51	1.29
5	D	502	HEM	CBB-CAB	3.39	1.51	1.29
5	M	502	HEM	CBB-CAB	3.38	1.51	1.29
8	G	1103	UQ2	C7-C8	3.37	1.55	1.50
5	M	501	HEM	C3B-CAB	-3.36	1.41	1.47
5	M	502	HEM	C3B-C2B	-3.36	1.35	1.40
5	D	502	HEM	C3C-CAC	-3.34	1.40	1.47
9	E	1042	BGL	C1-C2	3.34	1.55	1.52
5	A	502	HEM	C3C-C2C	-3.34	1.35	1.40
5	D	502	HEM	CBC-CAC	3.32	1.51	1.29
5	M	501	HEM	C3C-CAC	-3.31	1.41	1.47
5	E	301	HEM	C3C-CAC	-3.29	1.41	1.47
5	P	502	HEM	CBC-CAC	3.28	1.51	1.29
5	D	502	HEM	C3B-C2B	-3.26	1.35	1.40
8	D	1102	UQ2	C6-C5	3.20	1.41	1.35
5	G	502	HEM	CBC-CAC	3.17	1.50	1.29
8	A	1101	UQ2	C6-C5	3.16	1.41	1.35
5	G	502	HEM	C3B-CAB	-3.16	1.41	1.47
5	D	502	HEM	C3B-CAB	-3.15	1.41	1.47
5	P	501	HEM	C3C-CAC	-3.15	1.41	1.47
5	A	502	HEM	C3B-C2B	-3.13	1.36	1.40
5	M	502	HEM	C3C-CAC	-3.12	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	501	HEM	C3B-CAB	-3.11	1.41	1.47
8	D	1102	UQ2	C7-C8	3.10	1.55	1.50
5	H	301	HEM	C3C-CAC	-3.09	1.41	1.47
6	P	1006	SMA	C7-C8	-3.09	1.36	1.40
6	A	1001	SMA	O8-C8	3.03	1.45	1.35
5	J	502	HEM	C3C-C2C	-3.03	1.36	1.40
6	M	1005	SMA	O1-C2	3.03	1.39	1.35
8	J	1104	UQ2	C7-C8	3.00	1.55	1.50
5	G	501	HEM	C3B-CAB	-2.99	1.41	1.47
5	E	301	HEM	C3B-CAB	-2.99	1.41	1.47
5	K	301	HEM	C3C-CAC	-2.98	1.41	1.47
5	J	501	HEM	C3B-C2B	-2.93	1.36	1.40
5	J	501	HEM	C3C-CAC	-2.93	1.41	1.47
5	P	501	HEM	C3C-C2C	-2.93	1.36	1.40
5	J	502	HEM	CBC-CAC	2.90	1.48	1.29
5	G	501	HEM	C3C-CAC	-2.88	1.41	1.47
5	H	301	HEM	C3B-CAB	-2.88	1.42	1.47
8	M	1105	UQ2	C7-C6	2.87	1.56	1.51
5	B	301	HEM	C3B-C2B	-2.85	1.36	1.40
8	J	1104	UQ2	C6-C5	2.80	1.40	1.35
5	H	301	HEM	C3B-C2B	-2.79	1.36	1.40
5	P	502	HEM	C3B-CAB	-2.78	1.42	1.47
5	D	501	HEM	C3B-CAB	-2.78	1.42	1.47
6	M	1005	SMA	O8-C8	2.72	1.44	1.35
8	G	1103	UQ2	C7-C6	2.72	1.55	1.51
6	P	1006	SMA	O1-C2	2.68	1.39	1.35
6	D	1002	SMA	O8-C8	2.68	1.44	1.35
5	K	301	HEM	C3B-C2B	-2.67	1.36	1.40
6	J	1004	SMA	C7-C8	-2.67	1.36	1.40
5	Q	301	HEM	C3C-CAC	-2.66	1.42	1.47
6	P	1006	SMA	O8-C8	2.66	1.44	1.35
8	A	1101	UQ2	C7-C6	2.65	1.55	1.51
9	K	1044	BGL	C1-C2	2.64	1.55	1.52
5	N	301	HEM	C3B-CAB	-2.64	1.42	1.47
5	G	501	HEM	C3B-C2B	-2.64	1.36	1.40
6	G	1003	SMA	O1-C2	2.64	1.39	1.35
6	G	1003	SMA	C7-C8	-2.64	1.37	1.40
6	J	1004	SMA	O8-C8	2.62	1.44	1.35
5	A	502	HEM	C3C-CAC	-2.61	1.42	1.47
6	G	1003	SMA	O8-C8	2.60	1.44	1.35
8	D	1102	UQ2	O3-C3	2.55	1.43	1.36
5	J	501	HEM	C3C-C2C	-2.52	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	1103	UQ2	O3-C3	2.51	1.43	1.36
5	M	501	HEM	C3B-C2B	-2.50	1.36	1.40
5	D	501	HEM	C3C-CAC	-2.49	1.42	1.47
8	A	1101	UQ2	O2-C2	2.49	1.42	1.36
8	G	1103	UQ2	O2-C2	2.48	1.42	1.36
5	K	301	HEM	C3B-CAB	-2.47	1.42	1.47
5	J	502	HEM	C3B-C2B	-2.47	1.36	1.40
6	M	1005	SMA	C7-C8	-2.46	1.37	1.40
5	N	301	HEM	C3B-C2B	-2.45	1.37	1.40
5	E	301	HEM	C3B-C2B	-2.43	1.37	1.40
6	A	1001	SMA	C7-C8	-2.42	1.37	1.40
8	P	1106	UQ2	O3-C3	2.40	1.42	1.36
5	M	501	HEM	C3C-C2C	-2.36	1.37	1.40
6	D	1002	SMA	O5-C5M	2.34	1.49	1.42
5	E	301	HEM	C3C-C2C	-2.32	1.37	1.40
6	D	1002	SMA	O12-C12	2.32	1.48	1.42
8	D	1102	UQ2	O2-C2	2.31	1.42	1.36
5	J	502	HEM	C1A-NA	2.29	1.40	1.36
5	N	301	HEM	C3C-C2C	-2.29	1.37	1.40
6	P	1006	SMA	O12-C12	2.29	1.48	1.42
8	D	1102	UQ2	C7-C6	2.28	1.55	1.51
8	M	1105	UQ2	O3-C3	2.27	1.42	1.36
5	B	301	HEM	C3C-C2C	-2.26	1.37	1.40
6	M	1005	SMA	C20-C19	2.25	1.35	1.33
5	A	501	HEM	C3C-CAC	-2.25	1.43	1.47
6	G	1003	SMA	C20-C19	2.23	1.35	1.33
8	P	1106	UQ2	O2-C2	2.23	1.42	1.36
6	P	1006	SMA	O1-C8A	2.16	1.40	1.36
6	G	1003	SMA	O12-C12	2.15	1.48	1.42
8	J	1104	UQ2	O3-C3	2.14	1.42	1.36
5	H	301	HEM	C3C-C2C	-2.13	1.37	1.40
5	A	502	HEM	CAA-C2A	2.11	1.55	1.52
6	A	1001	SMA	C24-C13	2.10	1.57	1.53
6	A	1001	SMA	C20-C19	2.09	1.35	1.33
8	M	1105	UQ2	C8-C9	2.07	1.38	1.33
6	P	1006	SMA	O5-C5M	2.01	1.48	1.42
8	A	1101	UQ2	C8-C9	2.01	1.37	1.33
8	J	1104	UQ2	O2-C2	2.00	1.41	1.36

All (114) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	1006	SMA	C14-C15-C16	6.44	138.23	125.61
6	G	1003	SMA	O1-C2-C9	5.90	118.91	111.91
6	P	1006	SMA	O1-C2-C9	5.79	118.78	111.91
6	A	1001	SMA	O1-C2-C9	5.71	118.69	111.91
6	J	1004	SMA	C9-C10-C11	-5.55	107.25	114.72
6	M	1005	SMA	O1-C2-C9	5.50	118.43	111.91
6	D	1002	SMA	O1-C2-C9	5.37	118.27	111.91
6	M	1005	SMA	C5M-O5-C5	-5.34	110.27	117.75
6	J	1004	SMA	O1-C2-C9	5.23	118.12	111.91
6	P	1006	SMA	O7-C7-C8	5.13	119.71	114.54
6	A	1001	SMA	O7-C7-C8	4.71	119.29	114.54
6	D	1002	SMA	C9-C10-C11	-4.64	108.47	114.72
6	A	1001	SMA	O5-C5-C4A	4.58	122.63	115.89
6	A	1001	SMA	C9-C10-C11	-4.53	108.61	114.72
6	D	1002	SMA	C5M-O5-C5	-4.39	111.61	117.75
6	P	1006	SMA	C9-C10-C11	-4.31	108.92	114.72
6	M	1005	SMA	O7-C7-C8	4.28	118.86	114.54
6	G	1003	SMA	C9-C10-C11	-4.27	108.97	114.72
6	P	1006	SMA	C5M-O5-C5	-4.26	111.78	117.75
6	J	1004	SMA	C5M-O5-C5	-4.25	111.79	117.75
6	D	1002	SMA	O5-C5-C4A	4.24	122.12	115.89
6	M	1005	SMA	O5-C5-C4A	4.16	122.01	115.89
6	G	1003	SMA	O5-C5-C4A	4.05	121.85	115.89
6	J	1004	SMA	O7-C7-C8	4.03	118.60	114.54
6	A	1001	SMA	C5M-O5-C5	-3.99	112.16	117.75
6	G	1003	SMA	O7-C7-C8	3.92	118.49	114.54
6	G	1003	SMA	C5M-O5-C5	-3.88	112.31	117.75
6	D	1002	SMA	O7-C7-C8	3.86	118.43	114.54
6	J	1004	SMA	O5-C5-C4A	3.83	121.53	115.89
6	G	1003	SMA	C14-C15-C16	3.81	133.06	125.61
6	P	1006	SMA	O5-C5-C4A	3.77	121.43	115.89
7	J	1024	LOP	O5-C6-C7	3.71	119.49	111.50
9	K	1044	BGL	C1'-O2-C2	-3.36	106.31	114.32
6	M	1005	SMA	C9-C10-C11	-3.32	110.24	114.72
6	D	1002	SMA	C17-C18-C19	-3.29	117.17	126.42
6	A	1001	SMA	O5-C5-C6	-3.15	117.72	123.34
6	D	1002	SMA	C14-C15-C16	3.10	131.68	125.61
6	M	1005	SMA	C14-C15-C16	3.07	131.62	125.61
7	A	1021	LOP	O5-C6-C7	3.03	118.03	111.50
7	G	1023	LOP	O5-C6-C7	2.98	117.93	111.50
6	P	1006	SMA	C4-C3-C2	2.96	119.87	116.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	1023	LOP	C19-C18-C17	-2.94	99.52	114.42
9	P	1046	BGL	C1'-O2-C2	-2.93	107.34	114.32
7	D	1022	LOP	C27-C26-C25	-2.92	102.69	113.19
6	P	1006	SMA	C7M-O7-C7	-2.91	113.14	117.53
7	M	1025	LOP	O5-C6-C7	2.91	117.77	111.50
8	A	1101	UQ2	C10-C9-C11	2.90	120.15	115.27
7	D	1022	LOP	O5-C6-C7	2.87	117.69	111.50
6	D	1002	SMA	C4-C3-C2	2.86	119.77	116.63
6	G	1003	SMA	C4-C3-C2	2.85	119.75	116.63
6	M	1005	SMA	C17-C18-C19	-2.85	118.41	126.42
7	A	1021	LOP	C19-C18-C17	-2.82	100.09	114.42
6	J	1004	SMA	C4-C3-C2	2.81	119.70	116.63
9	E	1042	BGL	C1'-O2-C2	-2.80	107.65	114.32
6	M	1005	SMA	C7M-O7-C7	-2.78	113.33	117.53
7	P	1026	LOP	C9-C8-C7	-2.77	103.22	113.19
6	P	1006	SMA	O1-C8A-C8	2.76	119.59	116.12
6	P	1006	SMA	C13-C14-C15	2.75	118.13	112.13
7	P	1026	LOP	C27-C26-C25	-2.73	103.37	113.19
7	J	1024	LOP	O6-C24-C25	2.67	120.29	111.91
7	G	1023	LOP	C21-C20-C19	-2.67	100.87	114.42
6	D	1002	SMA	C7M-O7-C7	-2.64	113.55	117.53
6	M	1005	SMA	C4-C3-C2	2.60	119.48	116.63
8	A	1101	UQ2	C7-C8-C9	-2.60	122.46	126.79
8	J	1104	UQ2	C10-C9-C11	2.60	119.64	115.27
6	J	1004	SMA	C7M-O7-C7	-2.57	113.65	117.53
6	G	1003	SMA	C7M-O7-C7	-2.56	113.67	117.53
7	M	1025	LOP	C21-C20-C19	-2.53	101.60	114.42
7	M	1025	LOP	C19-C18-C17	-2.51	101.67	114.42
9	B	1041	BGL	C1'-O2-C2	-2.51	108.33	114.32
7	G	1023	LOP	O6-C24-C25	2.51	119.79	111.91
8	M	1105	UQ2	C10-C9-C11	2.51	119.49	115.27
6	A	1001	SMA	C7M-O7-C7	-2.50	113.75	117.53
7	D	1022	LOP	C19-C18-C17	-2.48	101.81	114.42
6	J	1004	SMA	C17-C18-C19	-2.48	119.44	126.42
6	D	1002	SMA	O5-C5-C6	-2.47	118.94	123.34
8	D	1102	UQ2	C10-C9-C11	2.47	119.43	115.27
7	P	1026	LOP	O5-C6-C7	2.47	116.82	111.50
6	G	1003	SMA	C26-C19-C18	2.46	121.96	118.08
6	M	1005	SMA	O5-C5-C6	-2.42	119.02	123.34
7	A	1021	LOP	C21-C20-C19	-2.42	102.16	114.42
7	D	1022	LOP	O6-C24-C25	2.41	119.46	111.91
6	P	1006	SMA	C26-C19-C18	2.40	121.86	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	1006	SMA	O7-C7-C6	-2.39	120.01	124.12
7	J	1024	LOP	C19-C18-C17	-2.38	102.34	114.42
8	M	1105	UQ2	C7-C8-C9	-2.37	122.84	126.79
8	P	1106	UQ2	C8-C7-C6	2.34	118.35	112.05
7	P	1026	LOP	O6-C24-C25	2.31	119.17	111.91
6	A	1001	SMA	C4-C3-C2	2.30	119.15	116.63
8	P	1106	UQ2	C10-C9-C11	2.28	119.10	115.27
9	K	1044	BGL	C3'-C2'-C1'	-2.27	103.43	113.49
8	D	1102	UQ2	C7-C8-C9	-2.27	123.02	126.79
6	P	1006	SMA	C17-C18-C19	-2.24	120.11	126.42
7	A	1021	LOP	C31-C30-C29	-2.23	103.10	114.42
7	A	1021	LOP	C29-C28-C27	-2.21	103.21	114.42
7	J	1024	LOP	C21-C20-C19	-2.20	103.25	114.42
7	J	1024	LOP	C29-C28-C27	-2.18	103.35	114.42
6	G	1003	SMA	C17-C18-C19	-2.16	120.34	126.42
8	J	1104	UQ2	CM5-C5-C6	-2.16	120.88	124.40
5	D	501	HEM	CMB-C2B-C3B	2.16	128.71	124.68
8	P	1106	UQ2	C5-C6-C1	-2.15	117.56	119.58
5	H	301	HEM	C3B-C4B-NB	2.15	111.99	109.21
6	D	1002	SMA	C26-C19-C18	2.15	121.46	118.08
8	G	1103	UQ2	C7-C8-C9	-2.14	123.22	126.79
6	A	1001	SMA	C13-C14-C15	-2.13	107.48	112.13
7	J	1024	LOP	C27-C26-C25	-2.13	105.55	113.19
8	P	1106	UQ2	C7-C8-C9	-2.12	123.25	126.79
6	A	1001	SMA	C17-C18-C19	-2.12	120.46	126.42
7	P	1026	LOP	C19-C18-C17	-2.12	103.67	114.42
6	M	1005	SMA	O1-C8A-C8	2.08	118.73	116.12
6	P	1006	SMA	O5-C5-C6	-2.05	119.69	123.34
7	D	1022	LOP	P1-O1-C2	-2.03	111.57	121.59
6	G	1003	SMA	O5-C5-C6	-2.03	119.72	123.34
6	A	1001	SMA	C14-C15-C16	-2.01	121.67	125.61

There are no chirality outliers.

All (104) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1001	SMA	C4A-C5-O5-C5M
6	M	1005	SMA	C4A-C5-O5-C5M
6	M	1005	SMA	C6-C5-O5-C5M
6	P	1006	SMA	C13-C14-C15-C16
7	A	1021	LOP	C2-O1-P1-O2
7	A	1021	LOP	C2-O1-P1-O3

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Mol	Chain	Res	Type	Atoms
7	A	1021	LOP	C2-O1-P1-O4
7	G	1023	LOP	C2-O1-P1-O3
7	G	1023	LOP	C2-O1-P1-O4
7	J	1024	LOP	C2-O1-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	P	1106	UQ2	C5-C6-C7-C8
6	A	1001	SMA	C6-C5-O5-C5M
6	J	1004	SMA	C4A-C5-O5-C5M
8	A	1101	UQ2	C9-C11-C12-C13
8	G	1103	UQ2	C9-C11-C12-C13
6	J	1004	SMA	C6-C5-O5-C5M
6	G	1003	SMA	C9-C10-C11-C22
7	G	1023	LOP	O5-C4-C5-O6
8	A	1101	UQ2	C12-C11-C9-C8
7	G	1023	LOP	C2-O1-P1-O2
7	J	1024	LOP	C2-O1-P1-O2
7	J	1024	LOP	C3-O2-P1-O1
6	A	1001	SMA	C9-C10-C11-C22
6	P	1006	SMA	C9-C10-C11-C22
6	P	1006	SMA	C8-C7-O7-C7M
6	D	1002	SMA	C4A-C5-O5-C5M
6	D	1002	SMA	C9-C10-C11-C22
8	A	1101	UQ2	C12-C11-C9-C10
6	M	1005	SMA	C11-C10-C9-C2
6	P	1006	SMA	C4A-C5-O5-C5M
6	D	1002	SMA	C6-C5-O5-C5M
6	P	1006	SMA	C6-C5-O5-C5M
7	G	1023	LOP	C3-C4-C5-O6
7	G	1023	LOP	C17-C18-C19-C20
8	G	1103	UQ2	C1-C6-C7-C8
7	G	1023	LOP	O2-C3-C4-O5
7	A	1021	LOP	C17-C18-C19-C20
6	M	1005	SMA	C9-C10-C11-C22
7	J	1024	LOP	C17-C18-C19-C20
7	D	1022	LOP	C17-C18-C19-C20
7	A	1021	LOP	O5-C4-C5-O6
8	P	1106	UQ2	C9-C11-C12-C13
8	D	1102	UQ2	C4-C3-O3-CM3
8	P	1106	UQ2	C4-C3-O3-CM3

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Mol	Chain	Res	Type	Atoms
7	A	1021	LOP	C3-C4-C5-O6
6	G	1003	SMA	C4A-C5-O5-C5M
6	P	1006	SMA	C6-C7-O7-C7M
6	D	1002	SMA	O14-C14-C15-C16
6	G	1003	SMA	O14-C14-C15-C16
6	M	1005	SMA	O14-C14-C15-C16
7	J	1024	LOP	C3-O2-P1-O3
7	J	1024	LOP	C3-O2-P1-O4
7	G	1023	LOP	O2-C3-C4-C5
8	A	1101	UQ2	C1-C2-O2-CM2
6	A	1001	SMA	C15-C14-O14-C25
8	G	1103	UQ2	C5-C6-C7-C8
8	G	1103	UQ2	C4-C3-O3-CM3
8	A	1101	UQ2	C1-C6-C7-C8
8	M	1105	UQ2	C1-C6-C7-C8
7	D	1022	LOP	C2-O1-P1-O2
7	M	1025	LOP	C3-O2-P1-O1
6	D	1002	SMA	C13-C14-C15-C16
6	G	1003	SMA	C13-C14-C15-C16
8	A	1101	UQ2	C3-C2-O2-CM2
6	D	1002	SMA	C11-C10-C9-C2
6	M	1005	SMA	C24-C13-C14-C15
7	M	1025	LOP	C14-C15-C16-C17
7	P	1026	LOP	C17-C18-C19-C20
8	G	1103	UQ2	C2-C3-O3-CM3
7	P	1026	LOP	C27-C28-C29-C30
7	J	1024	LOP	O5-C4-C5-O6
6	G	1003	SMA	C6-C5-O5-C5M
7	A	1021	LOP	C12-C13-C14-C15
6	M	1005	SMA	C13-C14-C15-C16
7	P	1026	LOP	C14-C15-C16-C17
7	P	1026	LOP	C12-C13-C14-C15
7	D	1022	LOP	C15-C16-C17-C18
7	P	1026	LOP	C30-C31-C32-C33
7	D	1022	LOP	C14-C15-C16-C17
7	G	1023	LOP	C12-C13-C14-C15
7	J	1024	LOP	C14-C15-C16-C17
7	M	1025	LOP	C12-C13-C14-C15
7	A	1021	LOP	O2-C3-C4-C5
6	M	1005	SMA	C24-C13-C14-O14
7	A	1021	LOP	O5-C6-C7-C8
7	A	1021	LOP	O6-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
7	G	1023	LOP	O5-C6-C7-C8
7	J	1024	LOP	C12-C13-C14-C15
8	D	1102	UQ2	C2-C3-O3-CM3
8	M	1105	UQ2	C4-C3-O3-CM3
7	D	1022	LOP	C12-C13-C14-C15
7	M	1025	LOP	O6-C24-C25-C26
7	G	1023	LOP	O7-C6-C7-C8
7	M	1025	LOP	C3-O2-P1-O4
7	A	1021	LOP	O8-C24-C25-C26
7	A	1021	LOP	C14-C15-C16-C17
7	J	1024	LOP	O5-C6-C7-C8
7	M	1025	LOP	O8-C24-C25-C26
7	P	1026	LOP	O5-C6-C7-C8
7	P	1026	LOP	O7-C6-C7-C8

There are no ring outliers.

38 monomers are involved in 107 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	1105	UQ2	2	0
9	B	1041	BGL	1	0
5	J	502	HEM	6	0
7	J	1024	LOP	1	0
5	H	301	HEM	1	0
5	M	501	HEM	3	0
5	A	502	HEM	4	0
9	N	1045	BGL	1	0
5	J	501	HEM	9	0
5	P	502	HEM	3	0
8	J	1104	UQ2	1	0
6	P	1006	SMA	1	0
5	D	501	HEM	5	0
5	A	501	HEM	3	0
5	K	301	HEM	2	0
5	P	501	HEM	4	0
9	K	1044	BGL	2	0
5	E	301	HEM	1	0
9	P	1046	BGL	2	0
7	A	1021	LOP	6	0
6	J	1004	SMA	1	0
5	B	301	HEM	1	0
7	M	1025	LOP	3	0

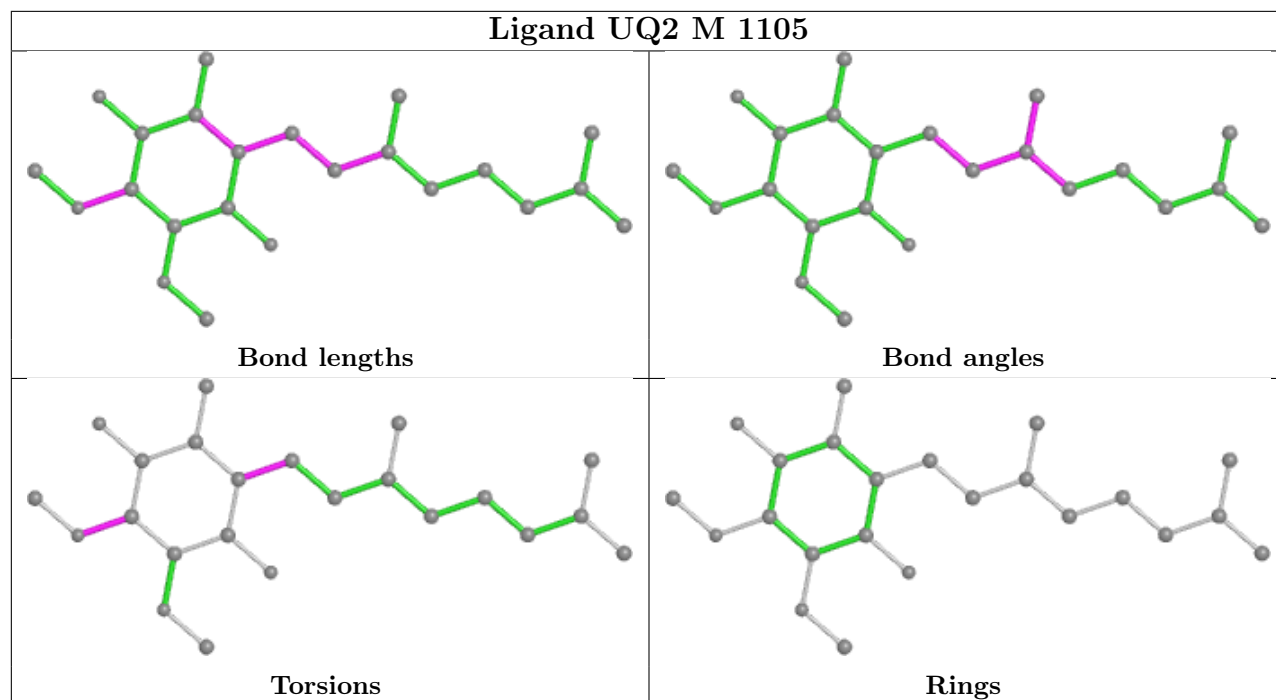
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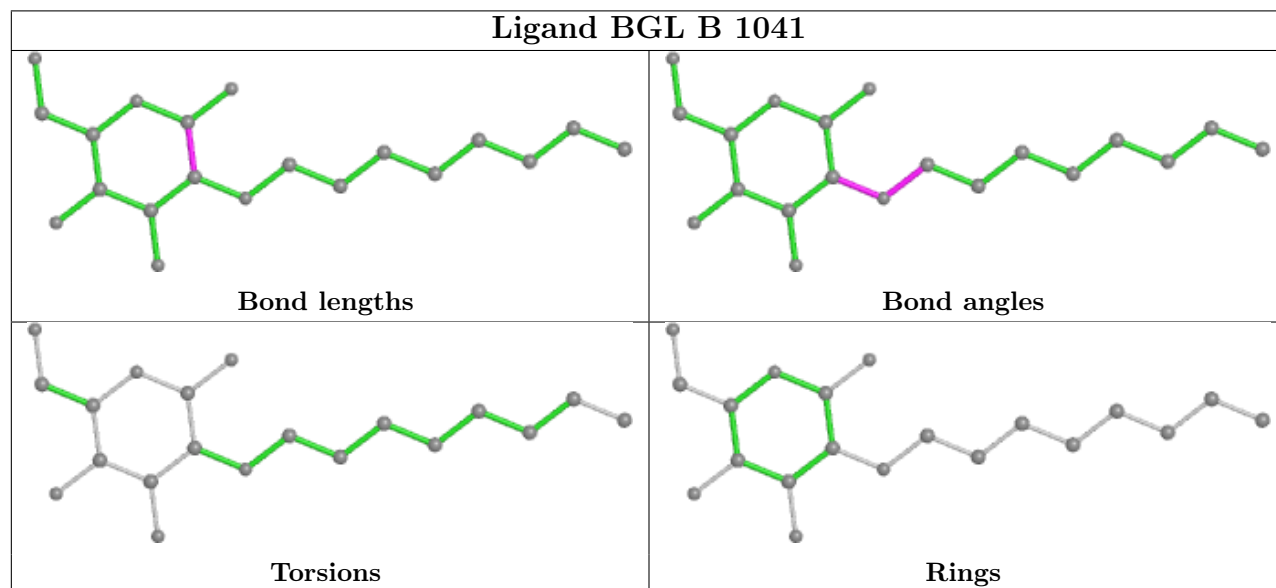
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	P	1026	LOP	2	0
5	G	501	HEM	4	0
8	D	1102	UQ2	2	0
5	D	502	HEM	3	0
7	D	1022	LOP	1	0
5	G	502	HEM	5	0
9	E	1042	BGL	3	0
9	G	1043	BGL	2	0
8	G	1103	UQ2	3	0
5	N	301	HEM	3	0
8	P	1106	UQ2	4	0
7	G	1023	LOP	3	0
8	A	1101	UQ2	2	0
5	Q	301	HEM	2	0
5	M	502	HEM	5	0

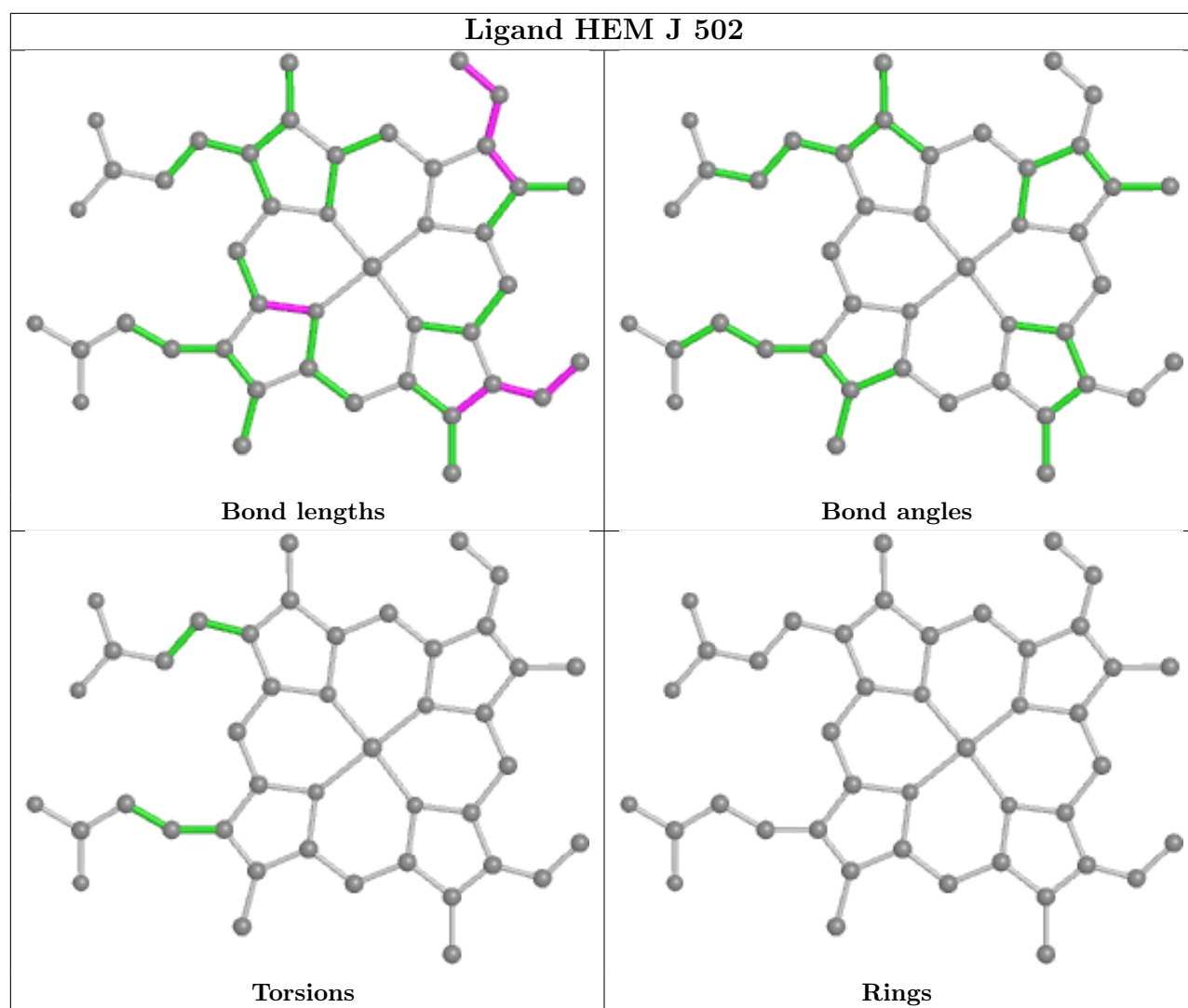
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

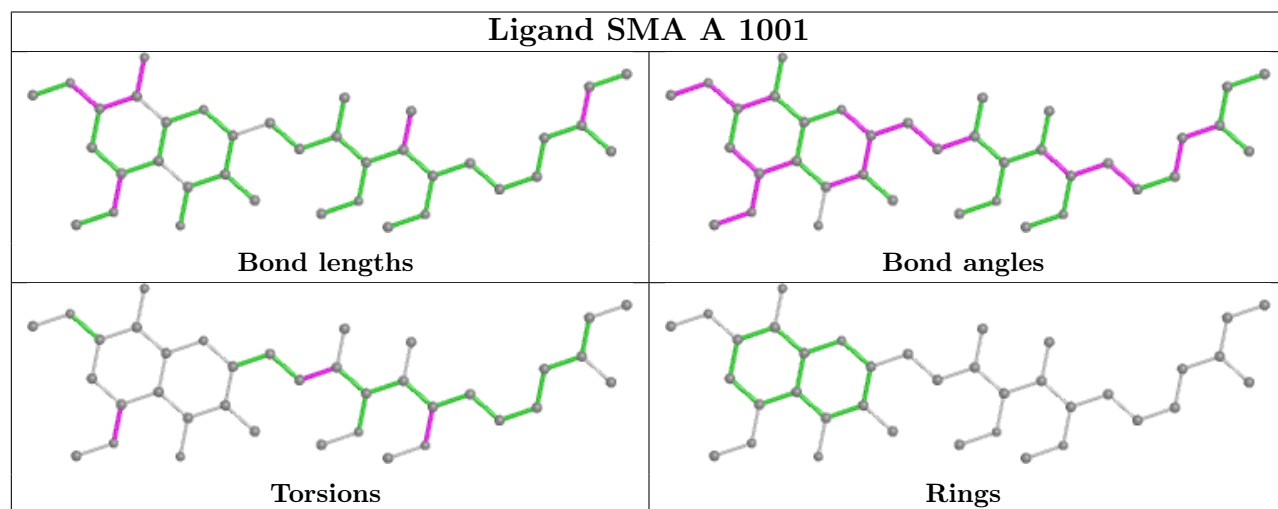
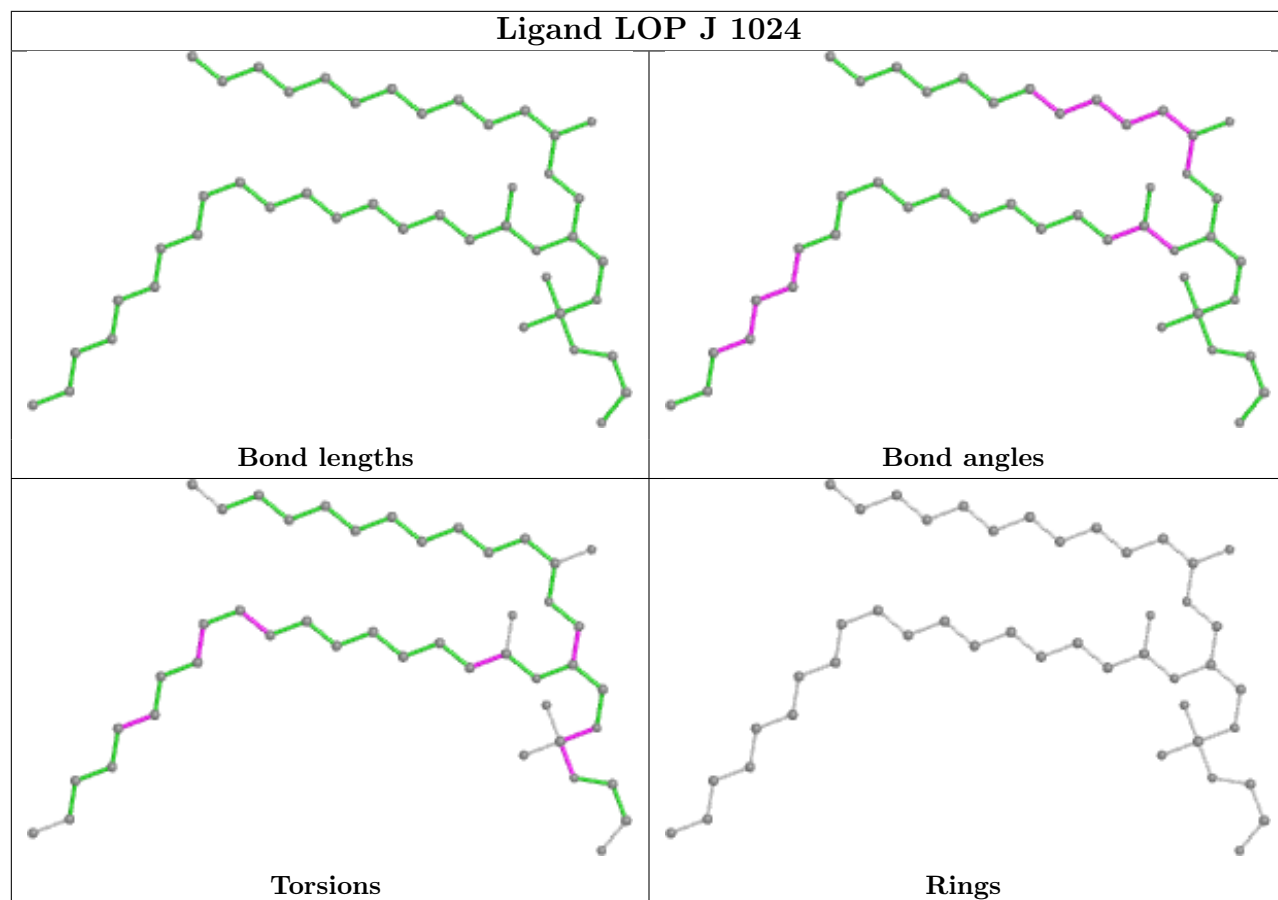
Ligand UQ2 M 1105

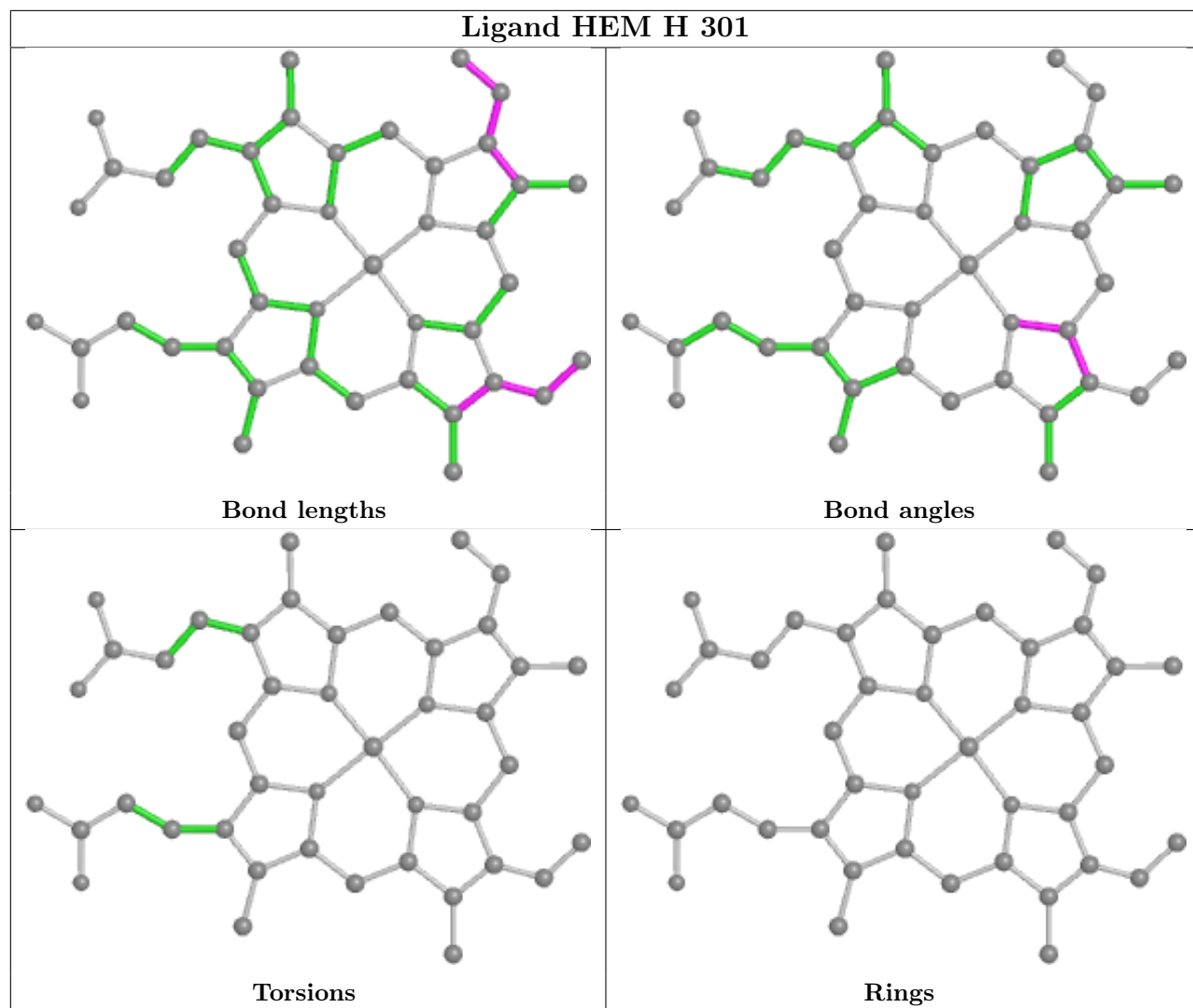


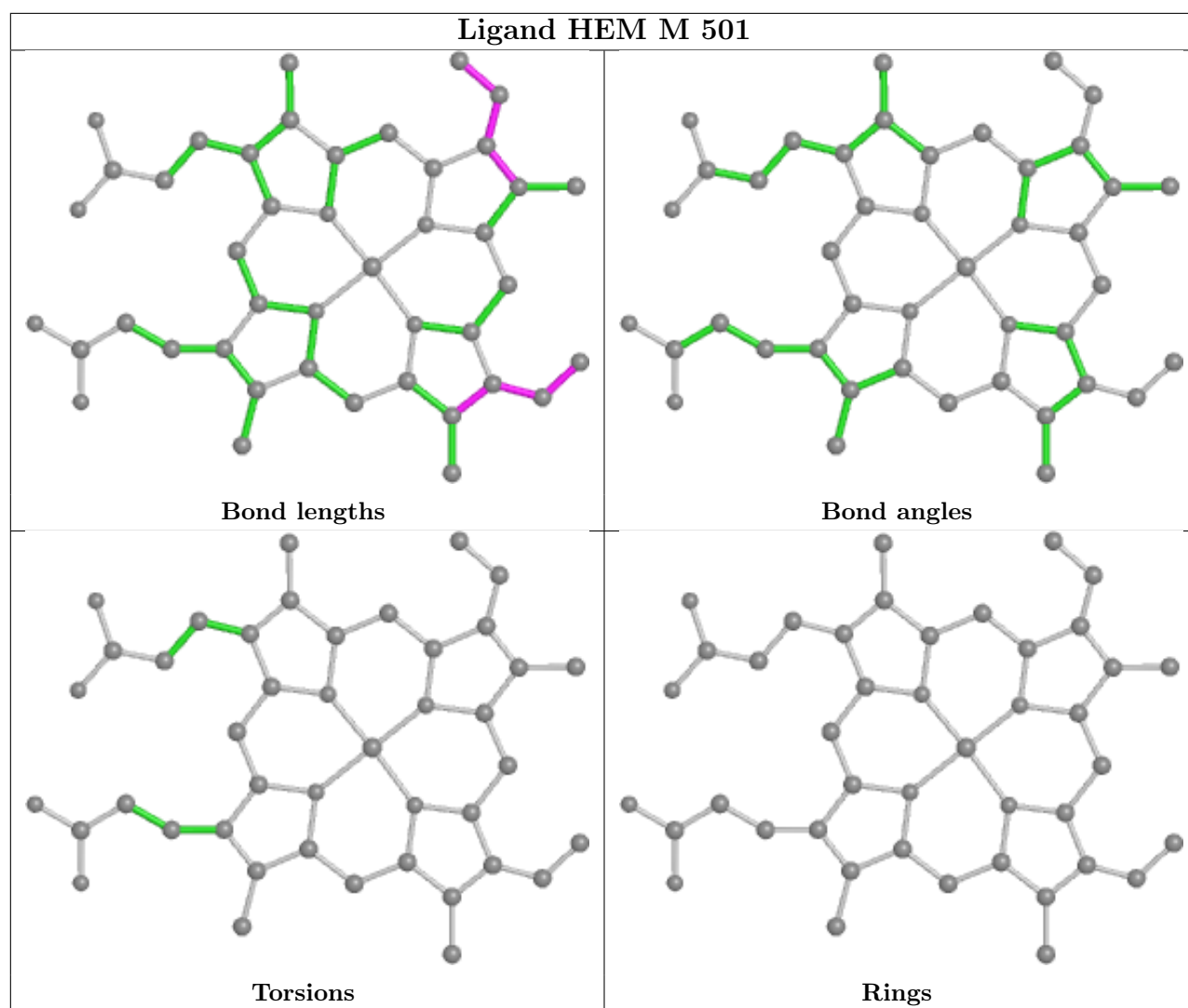
Ligand BGL B 1041

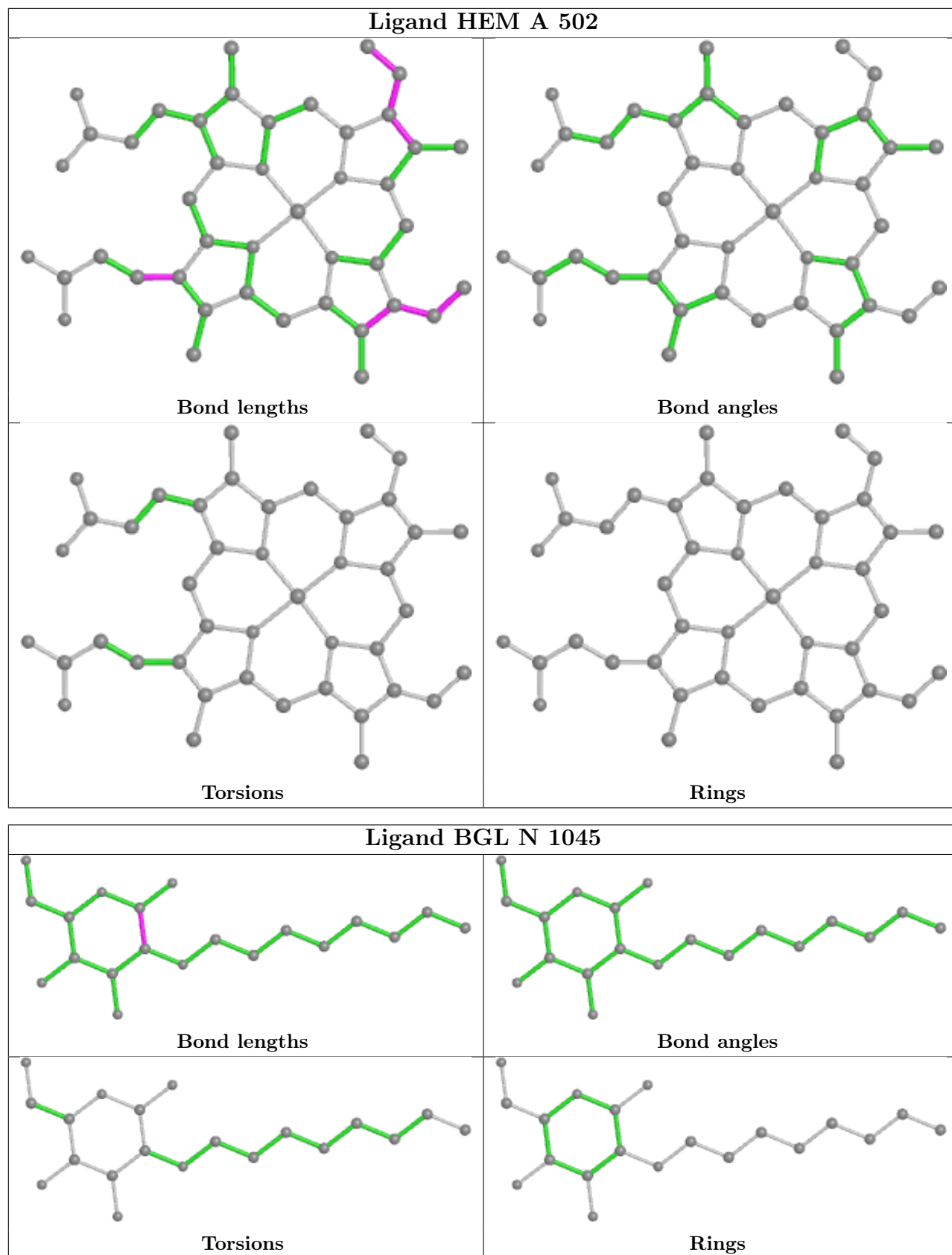


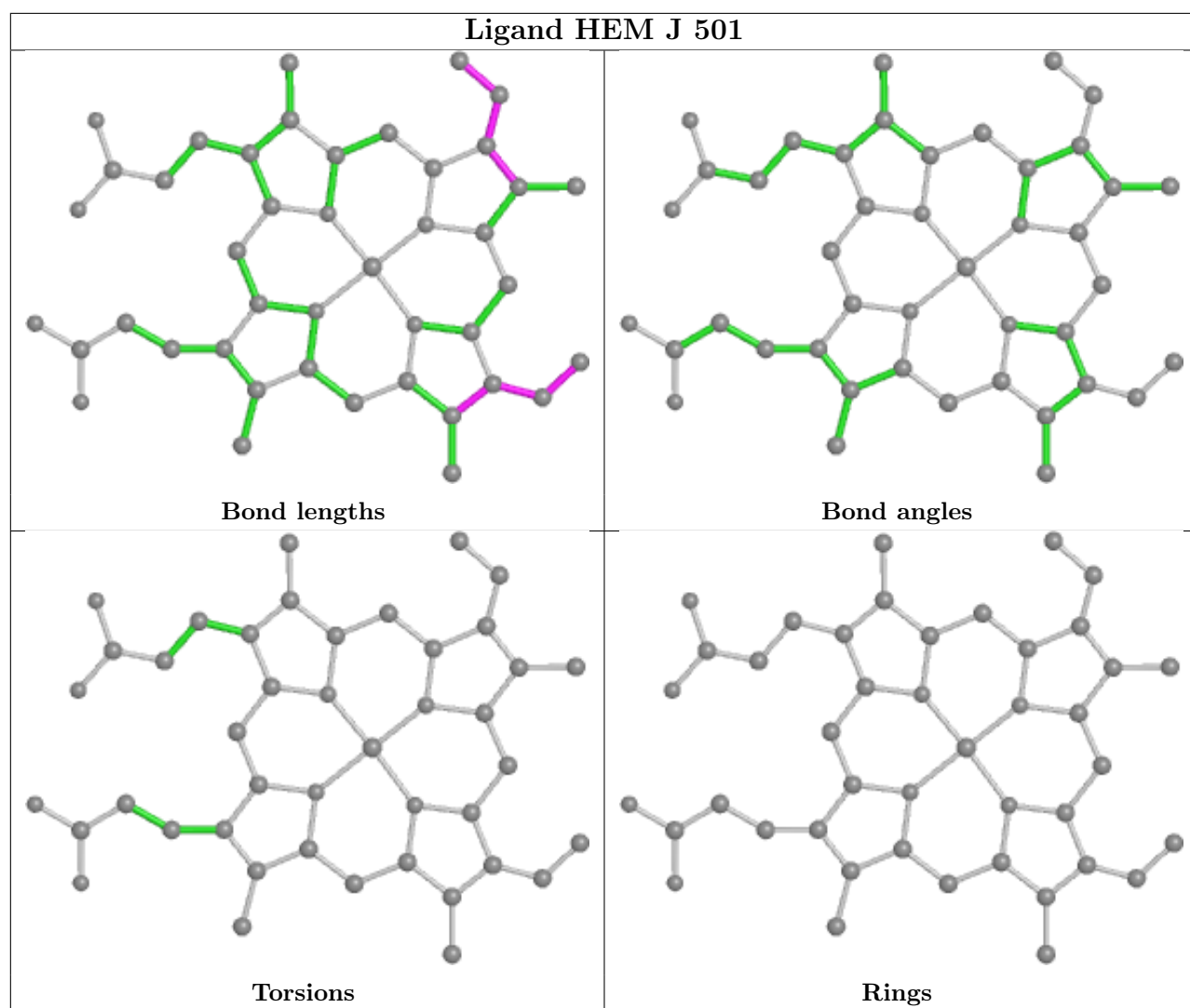


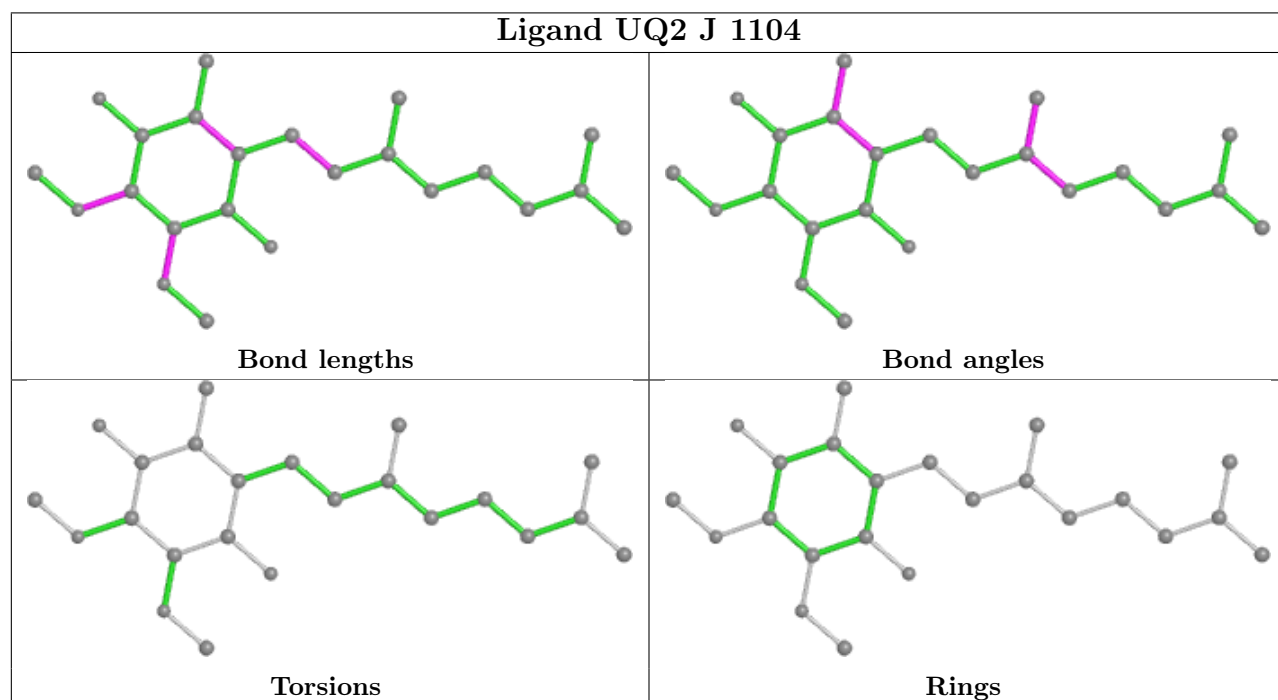
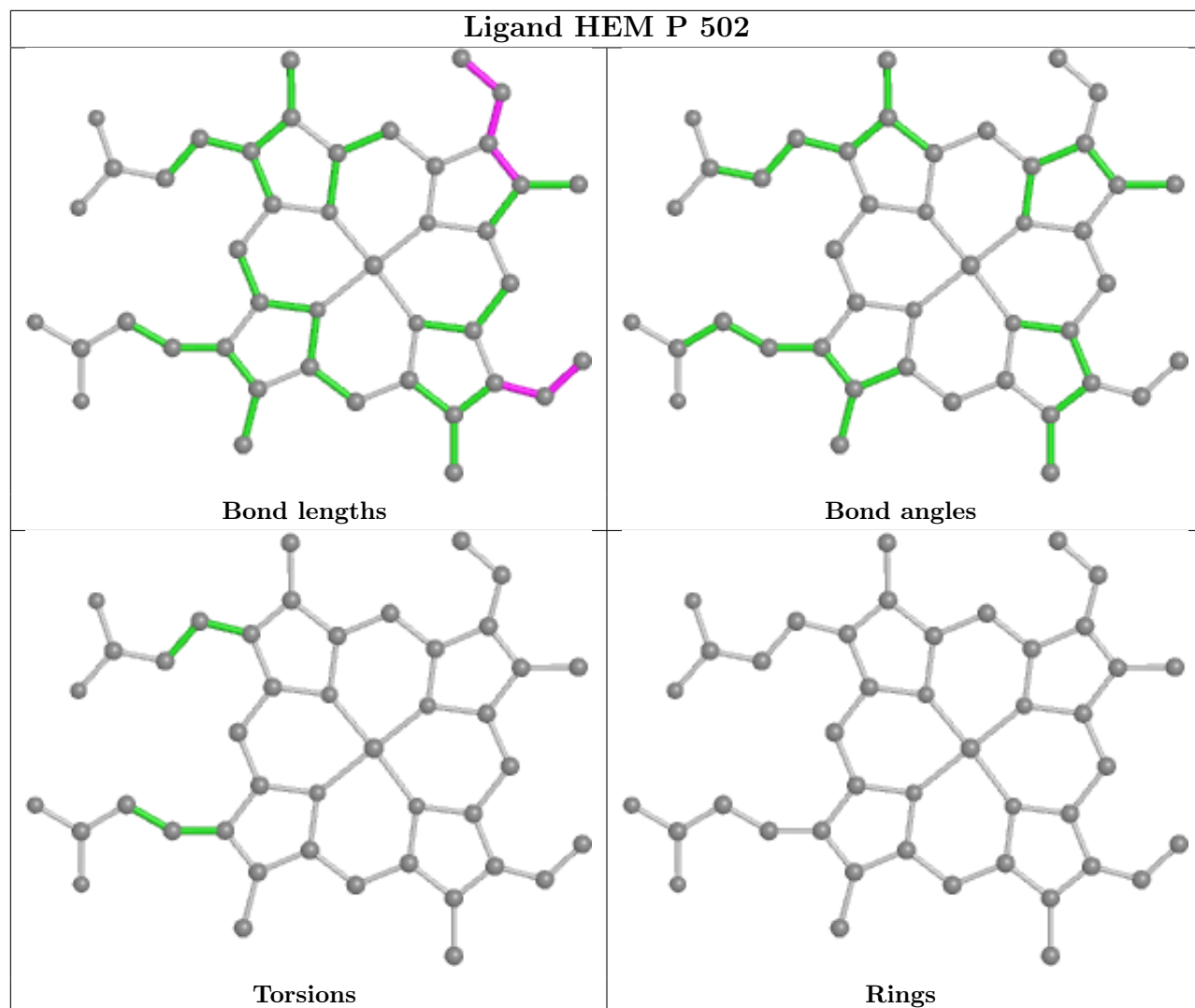


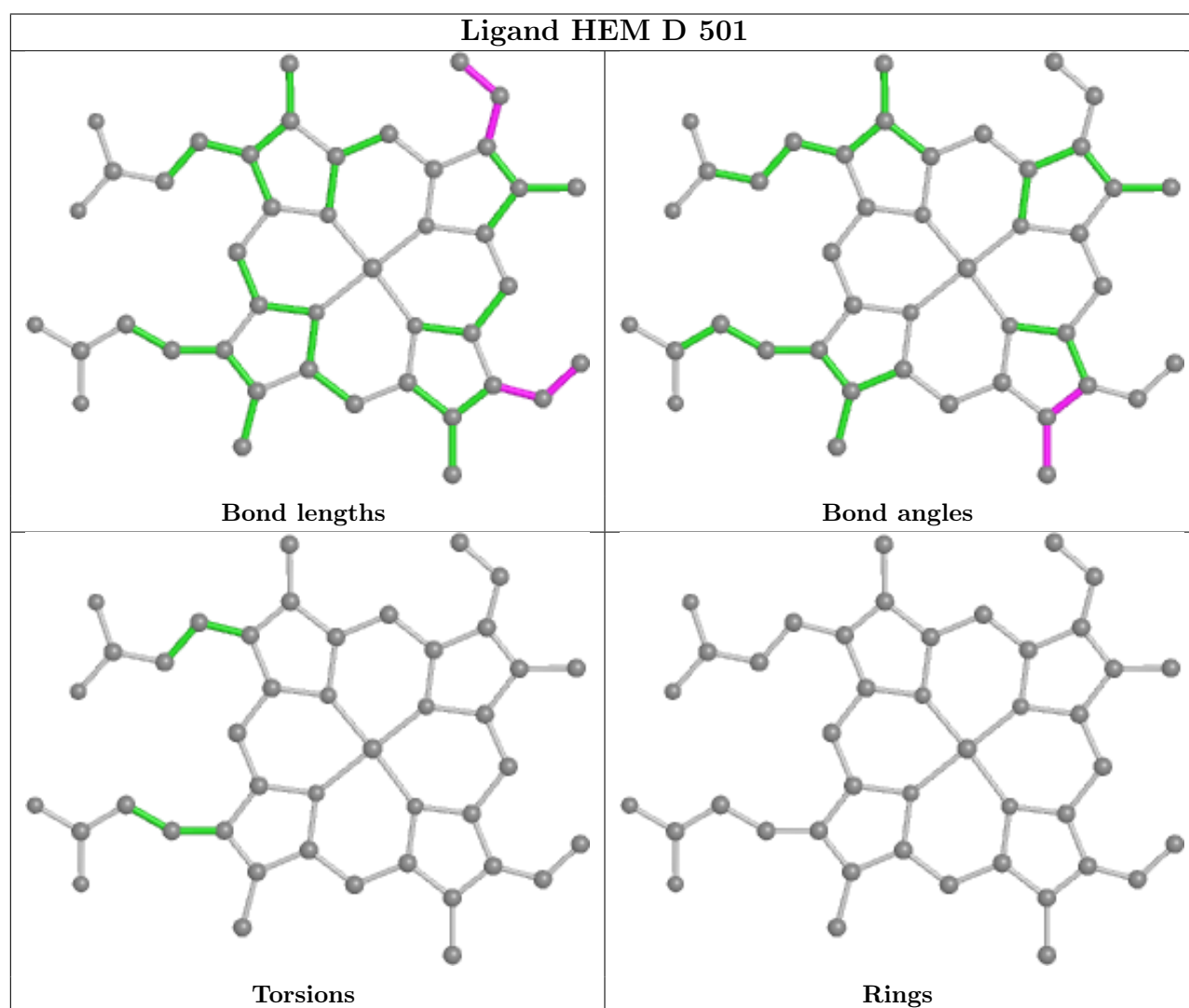
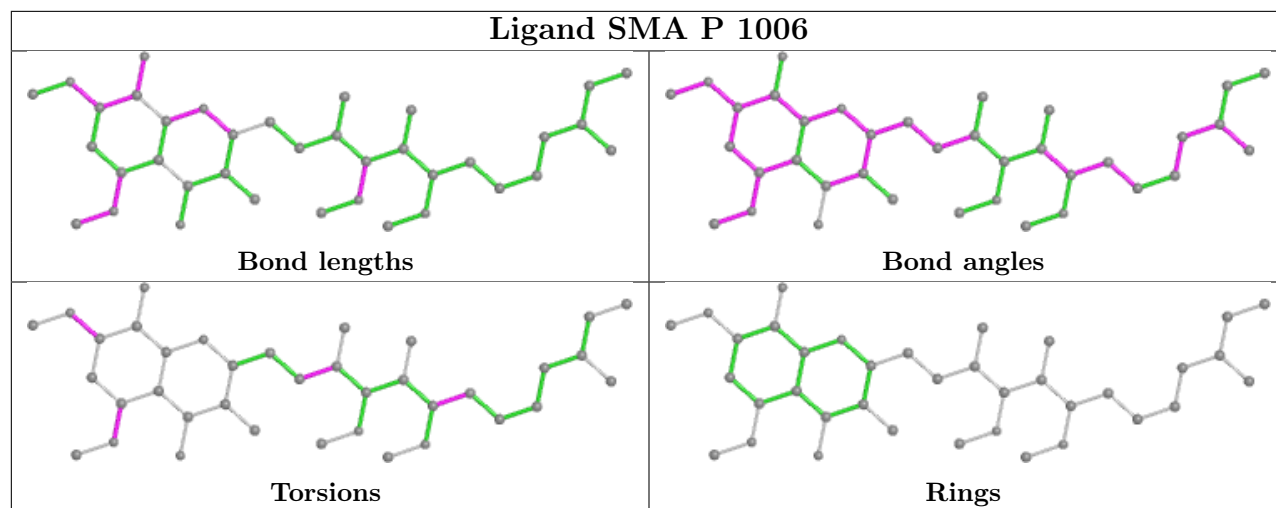


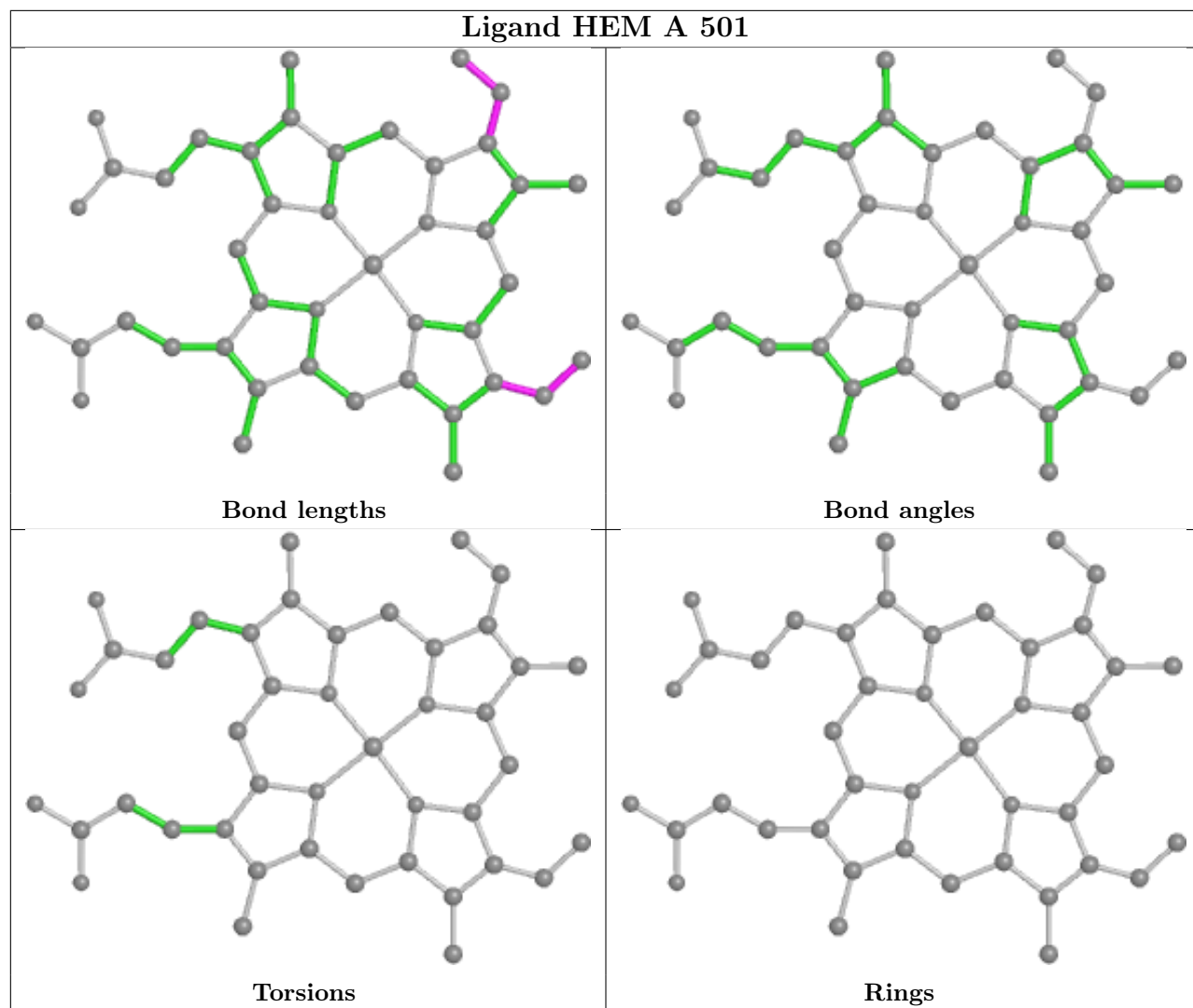


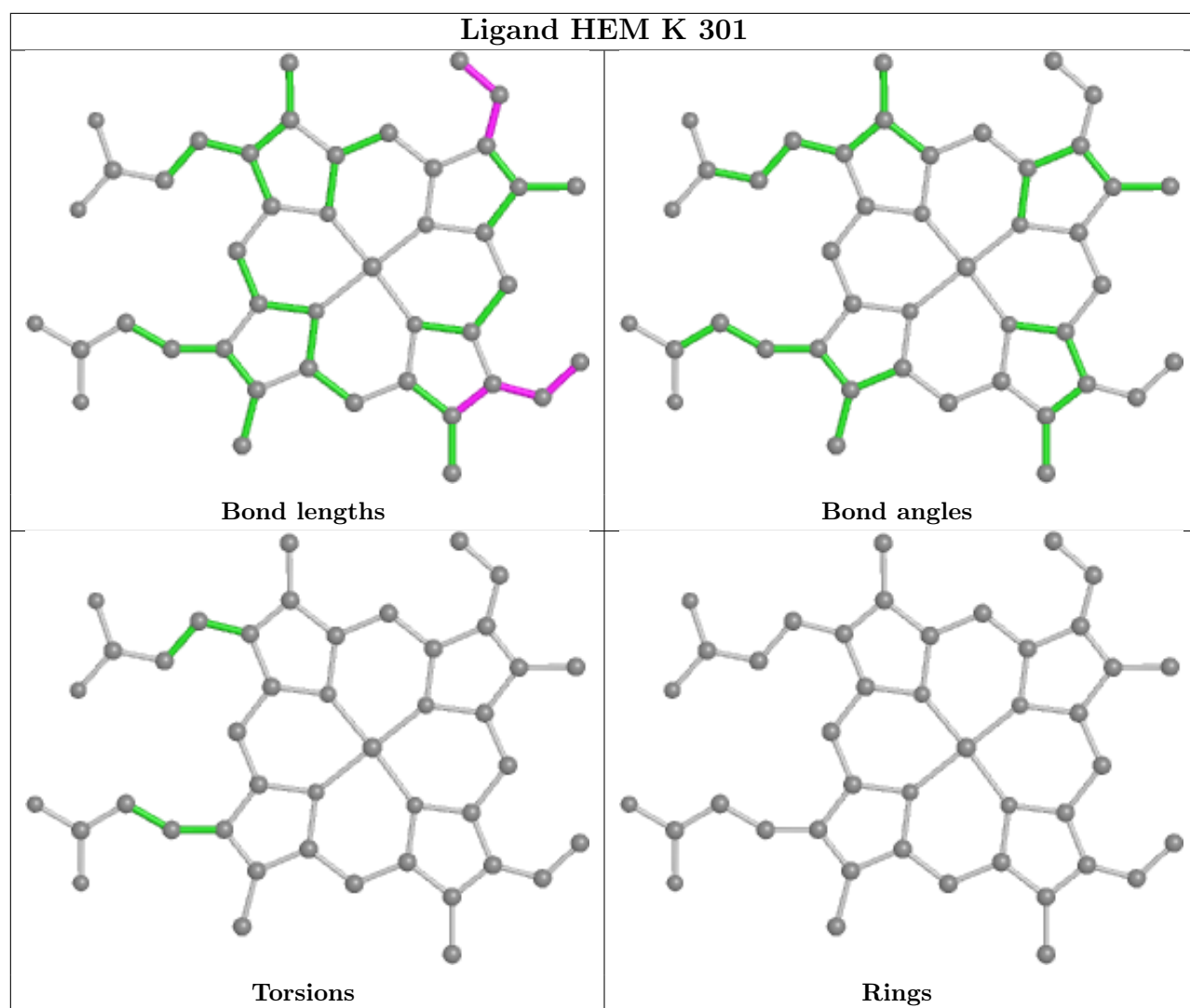


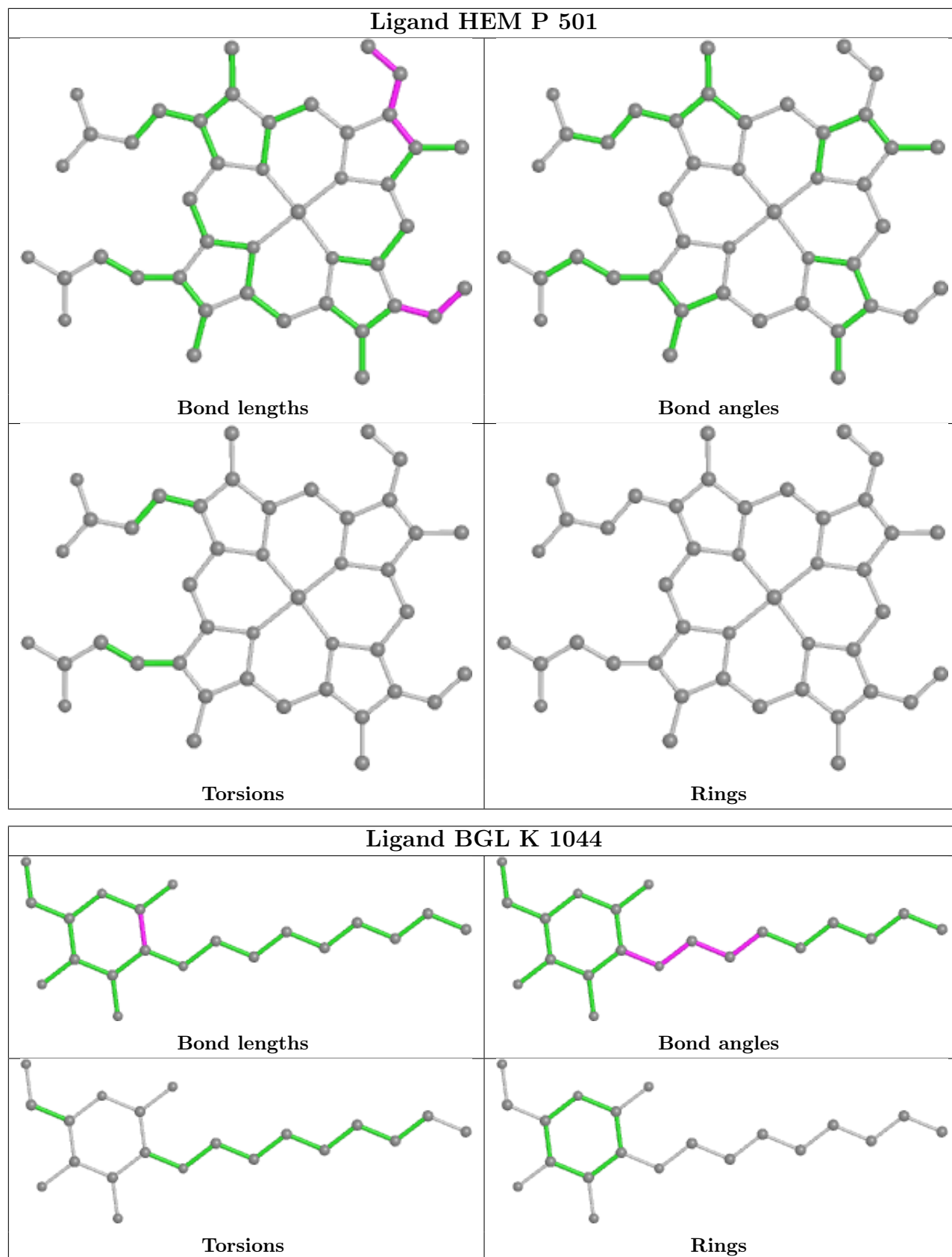


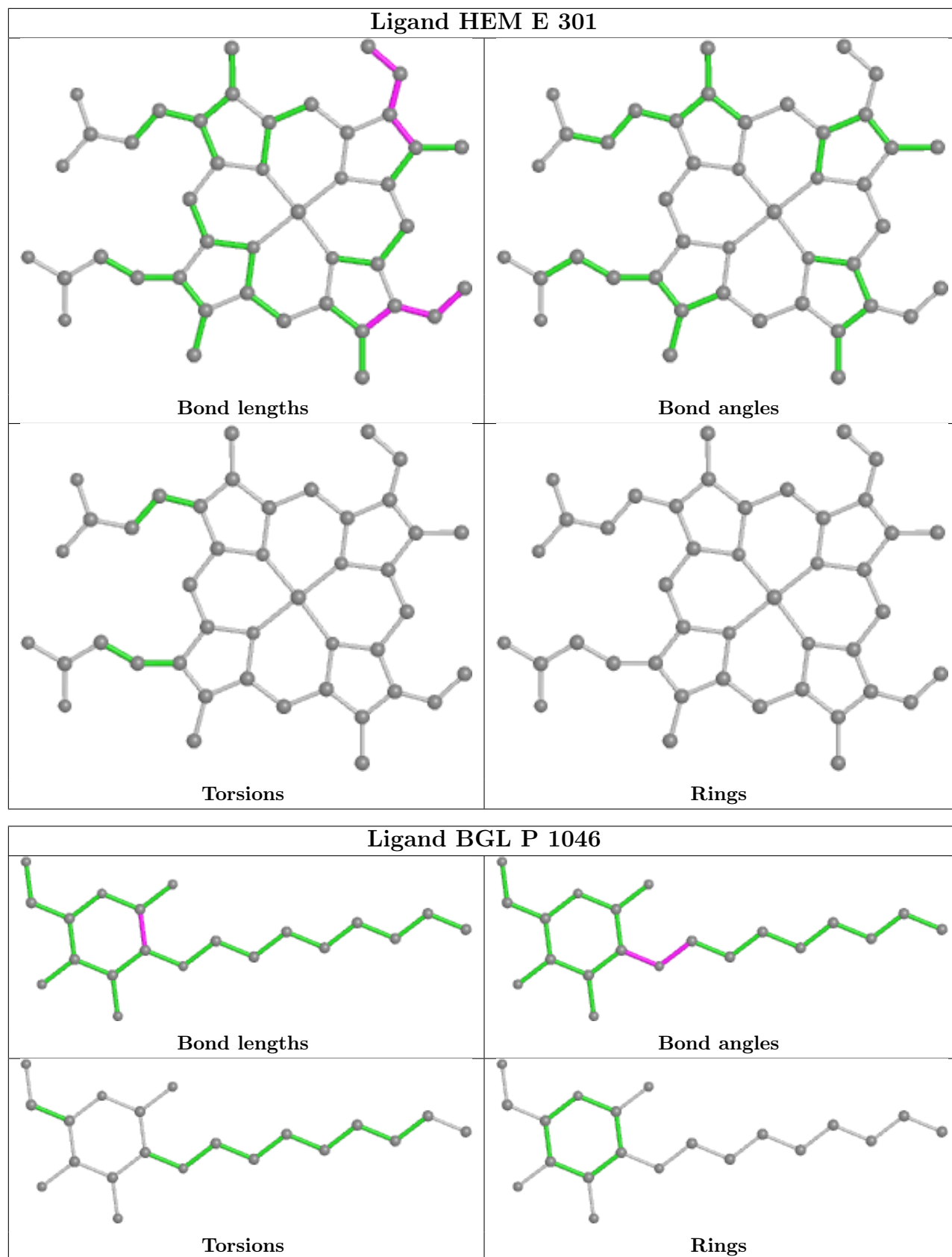


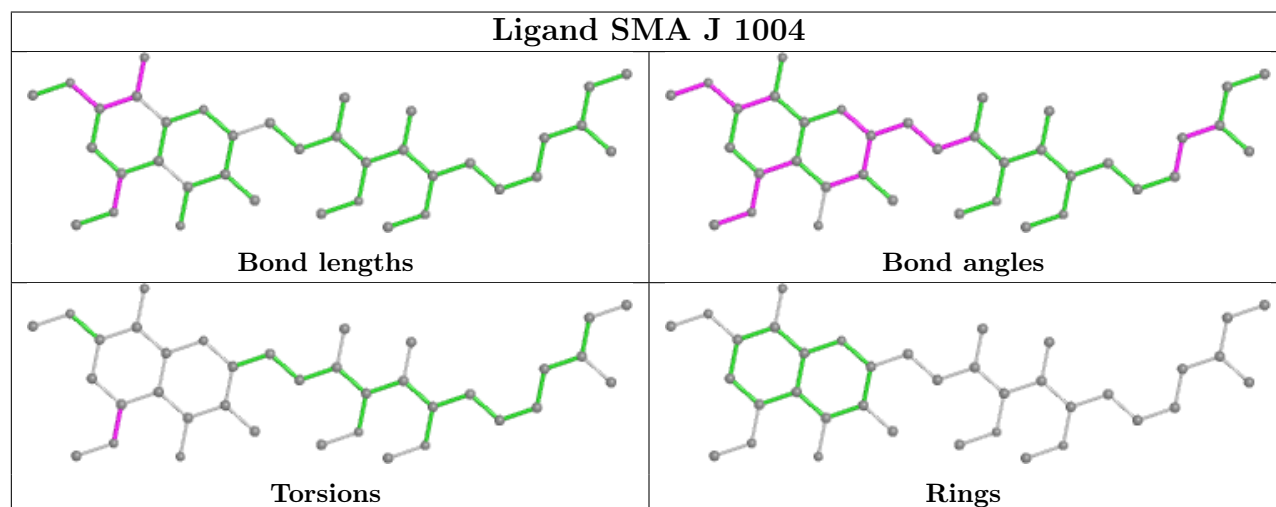
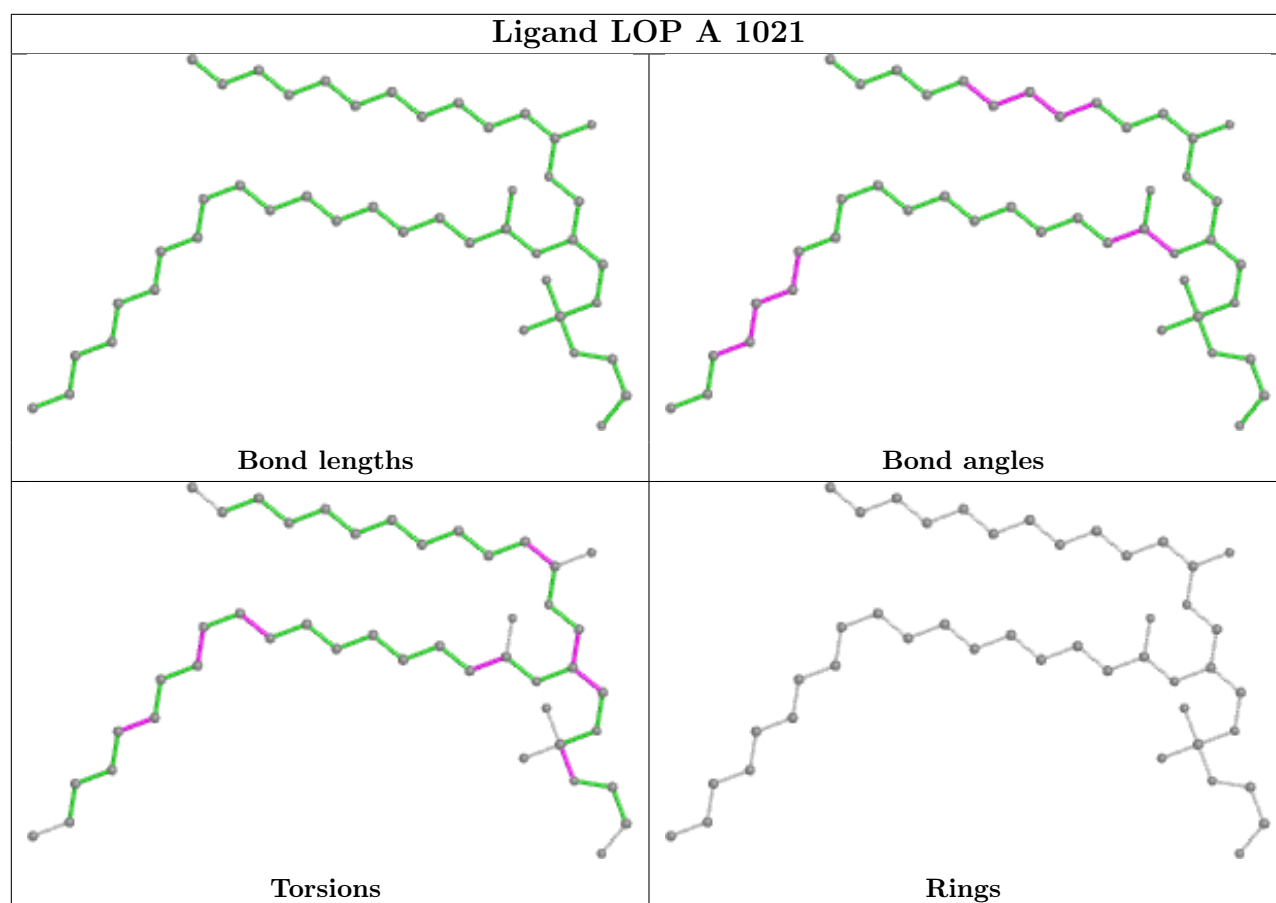


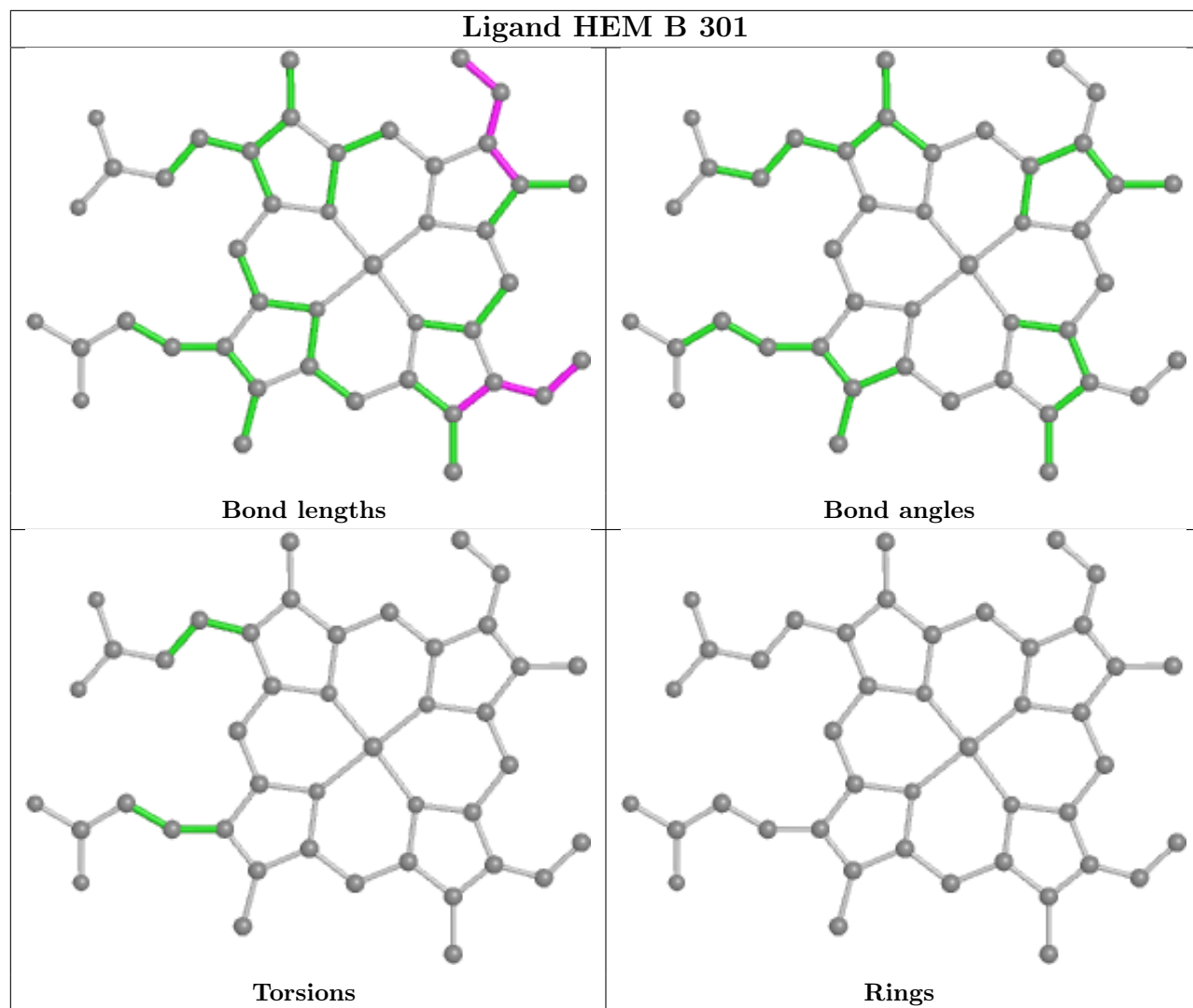


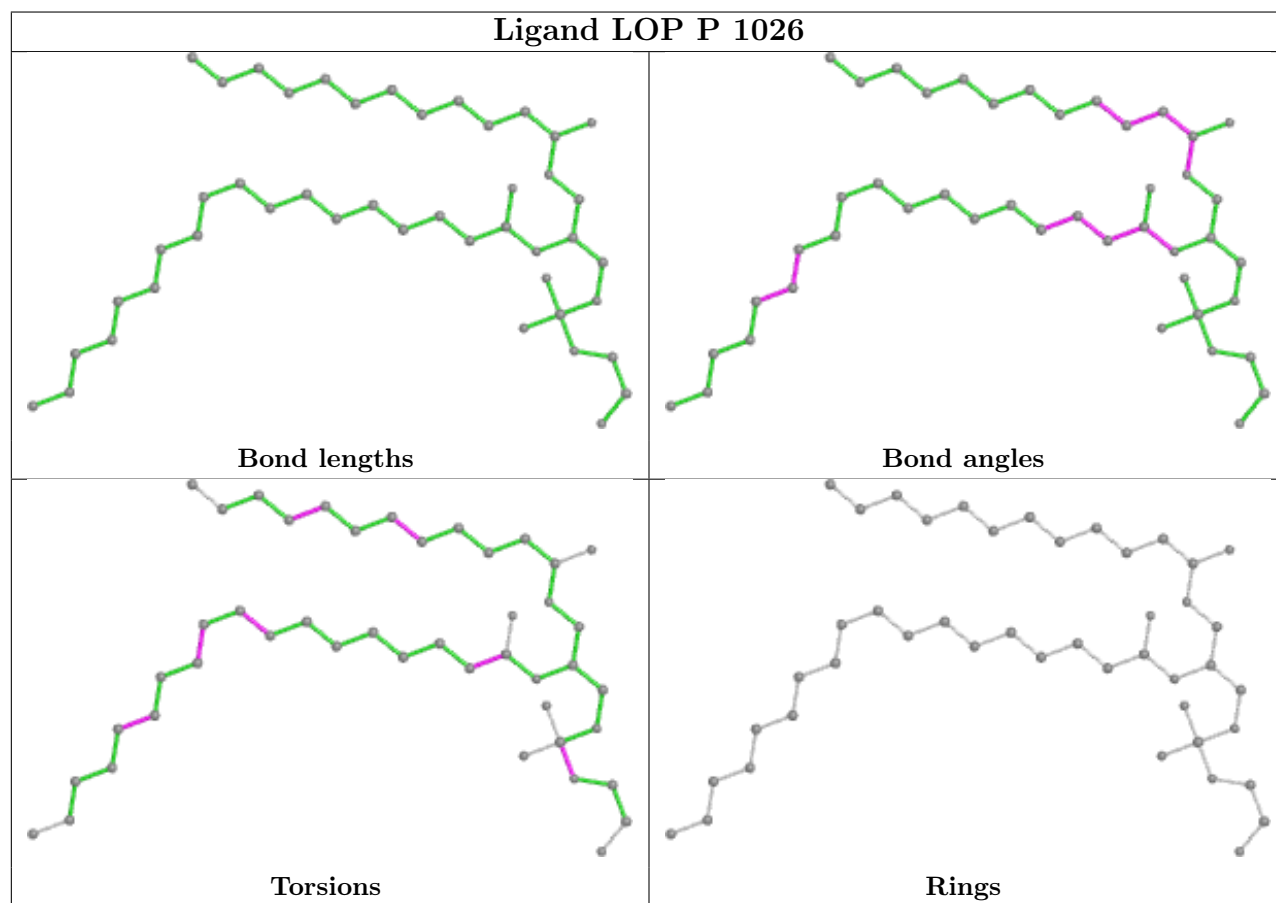
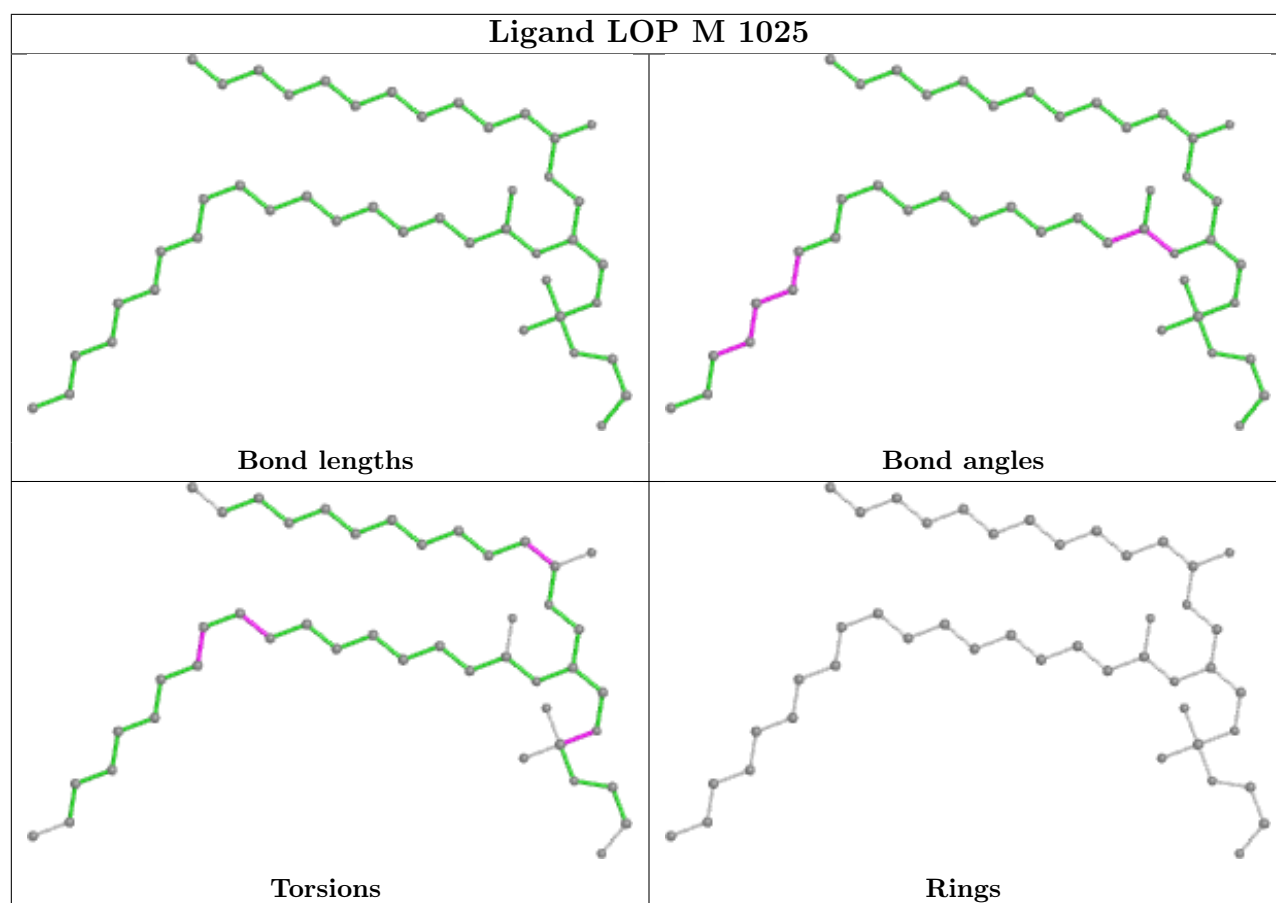


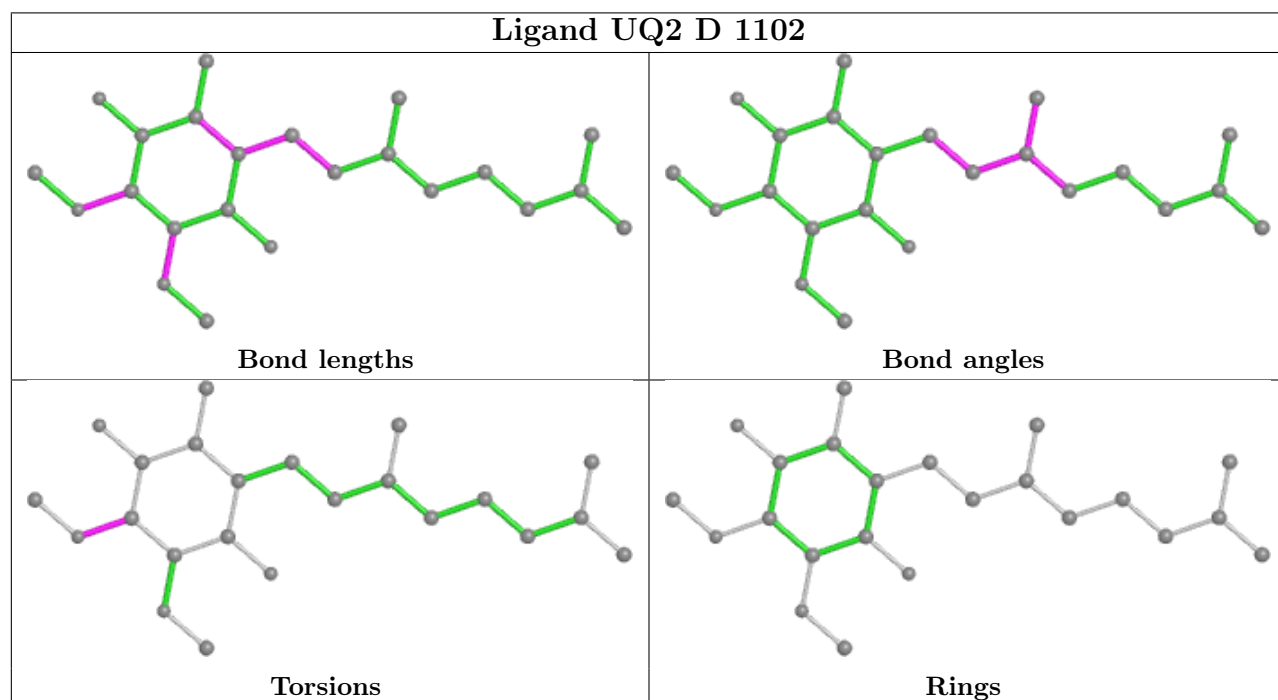
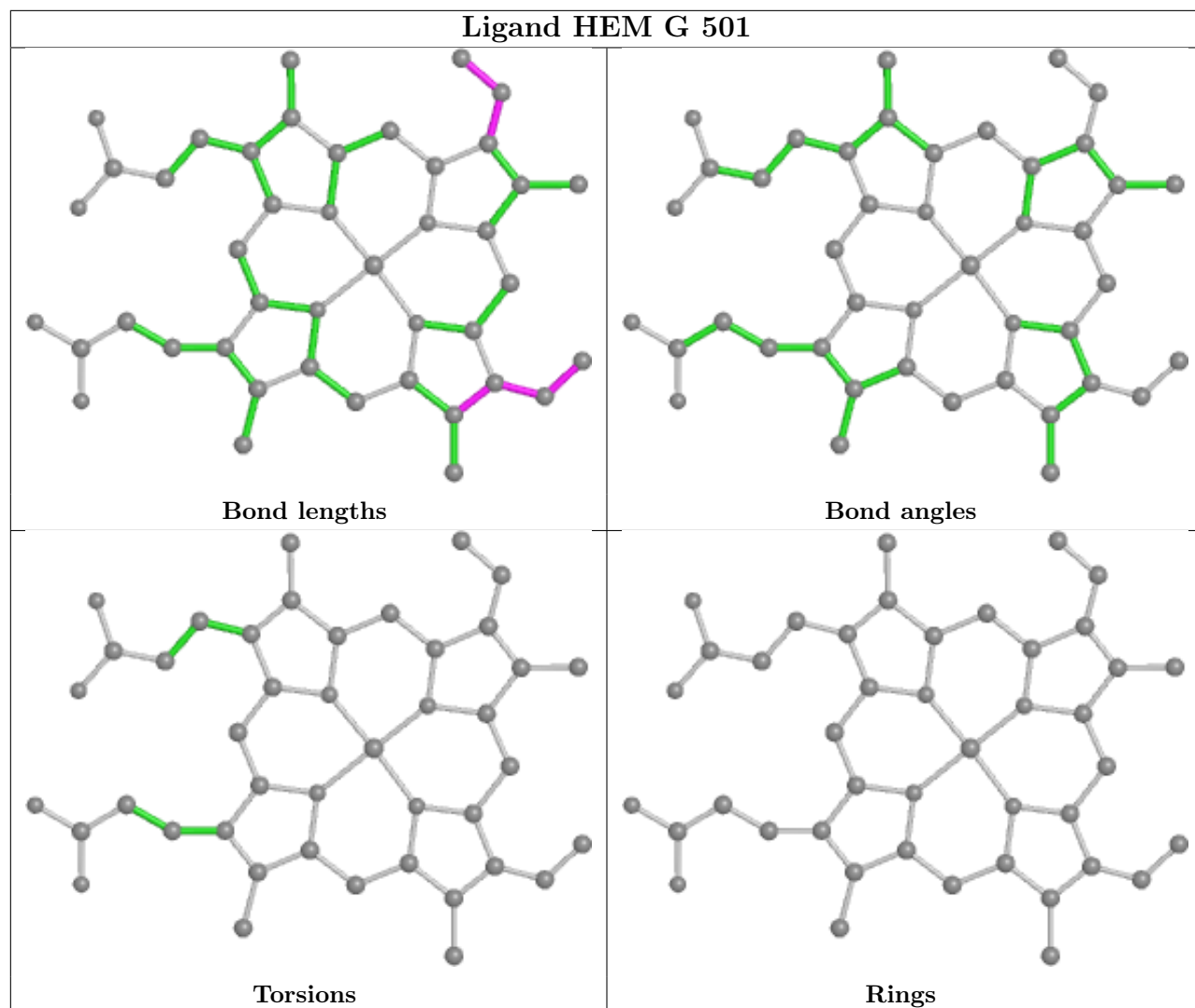


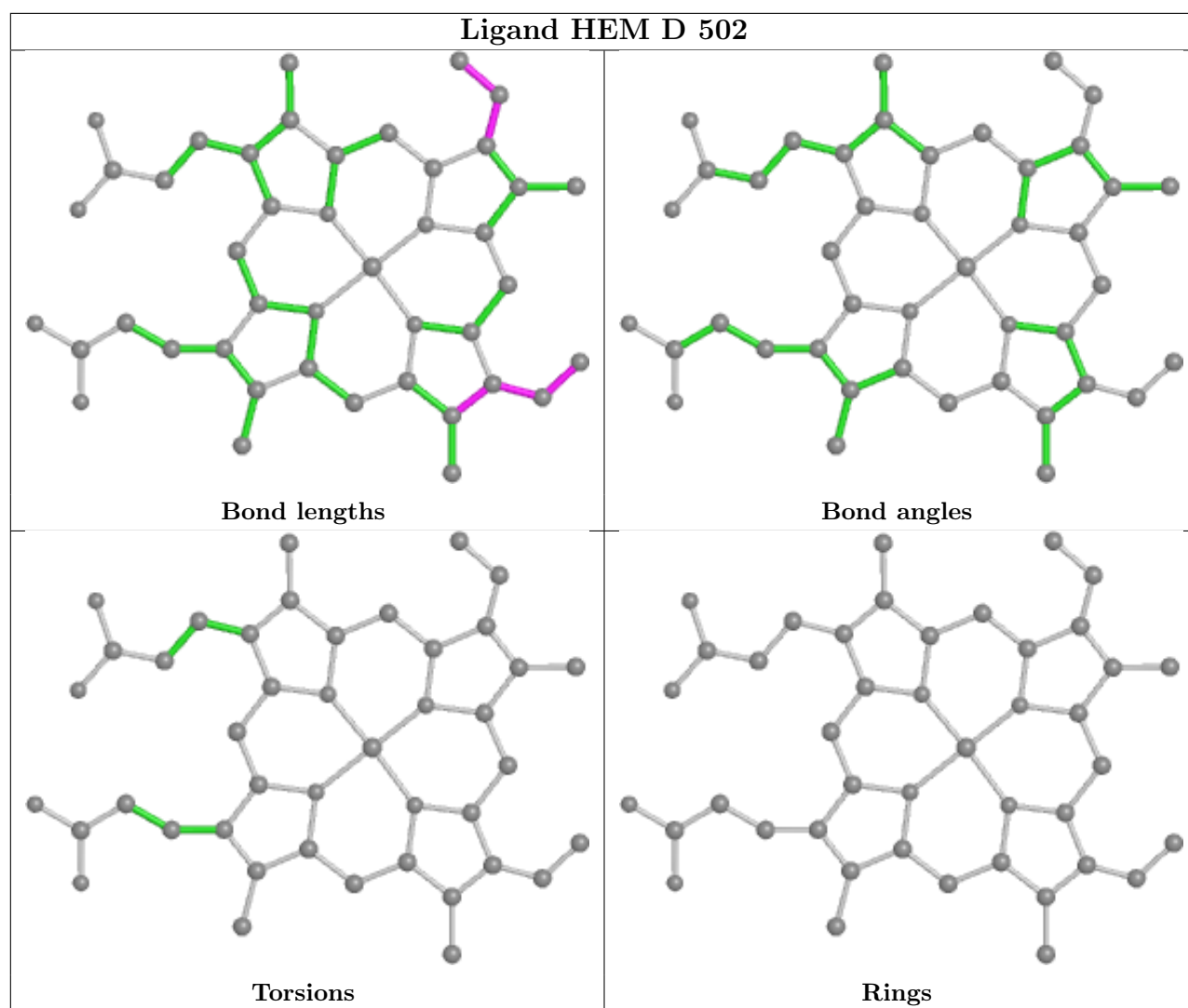


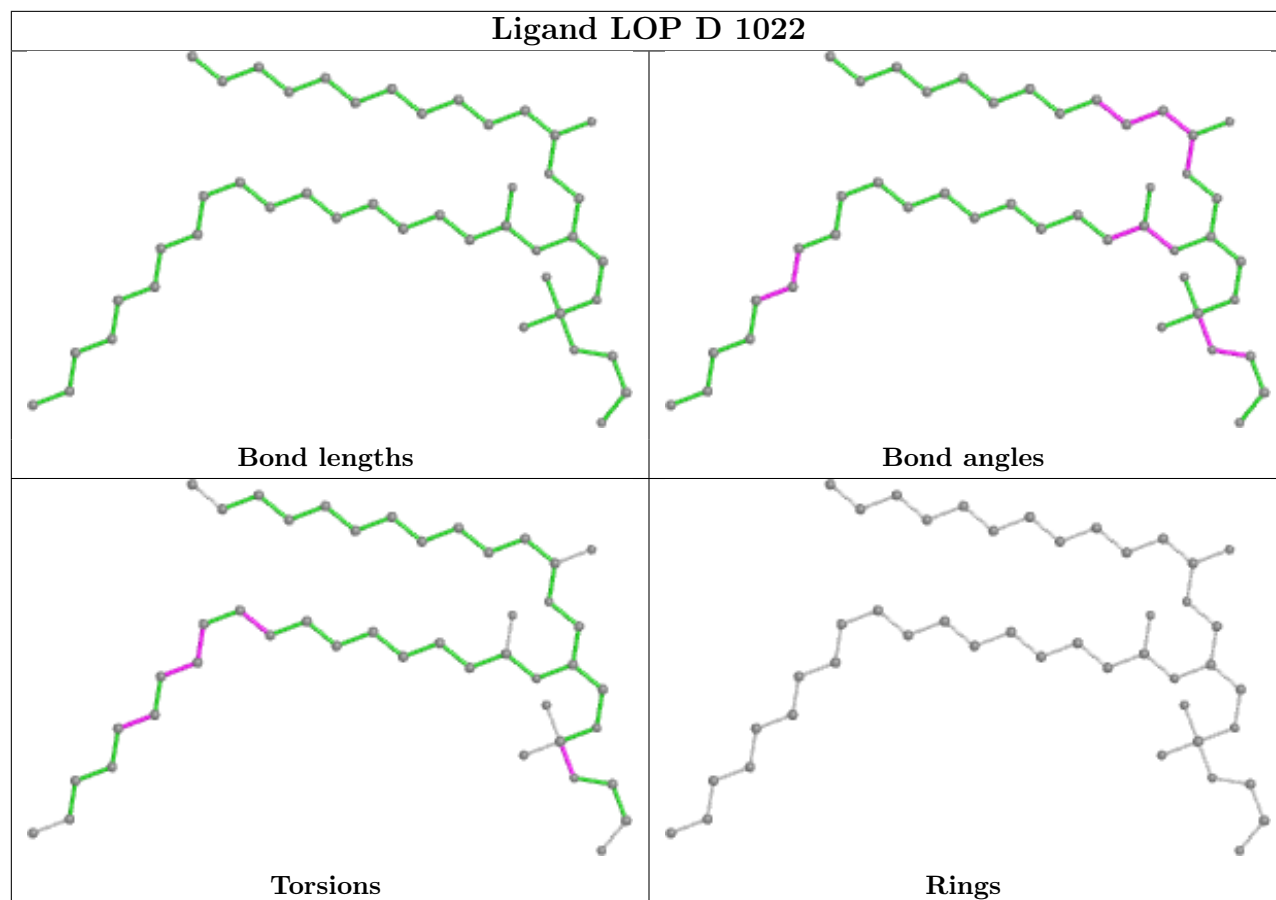


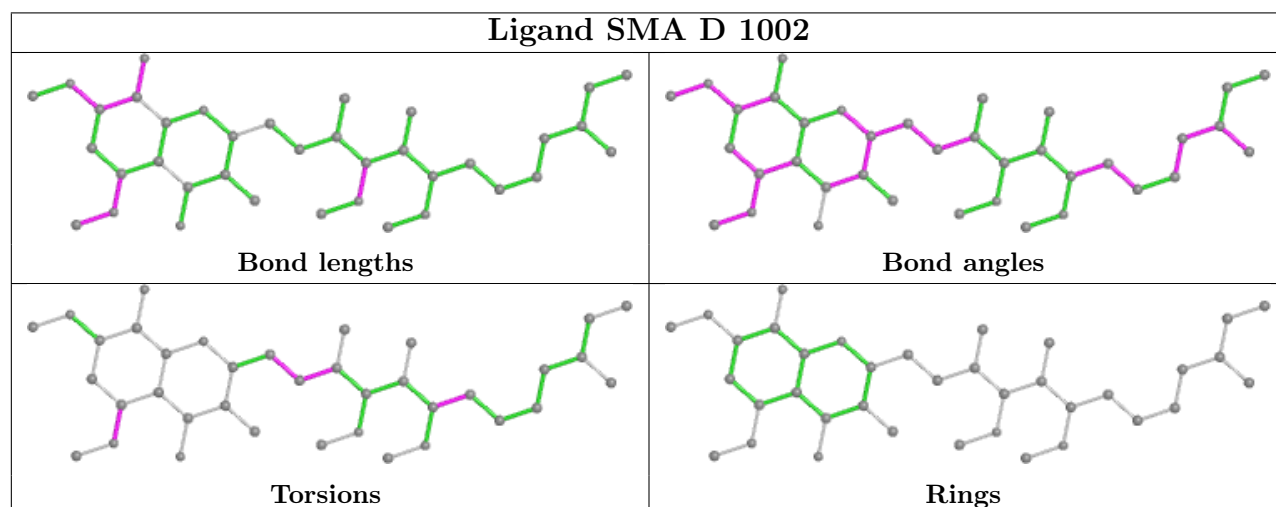
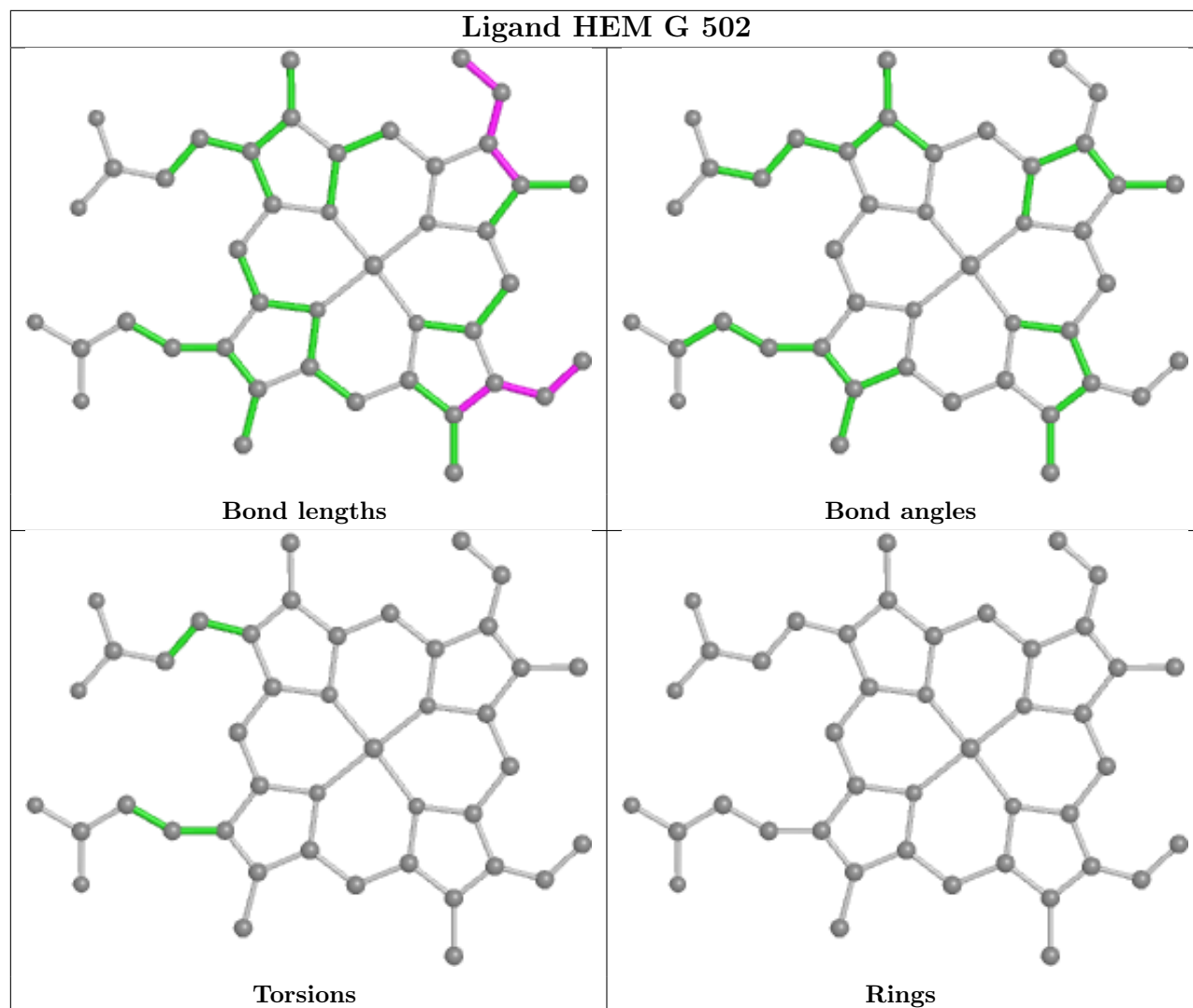


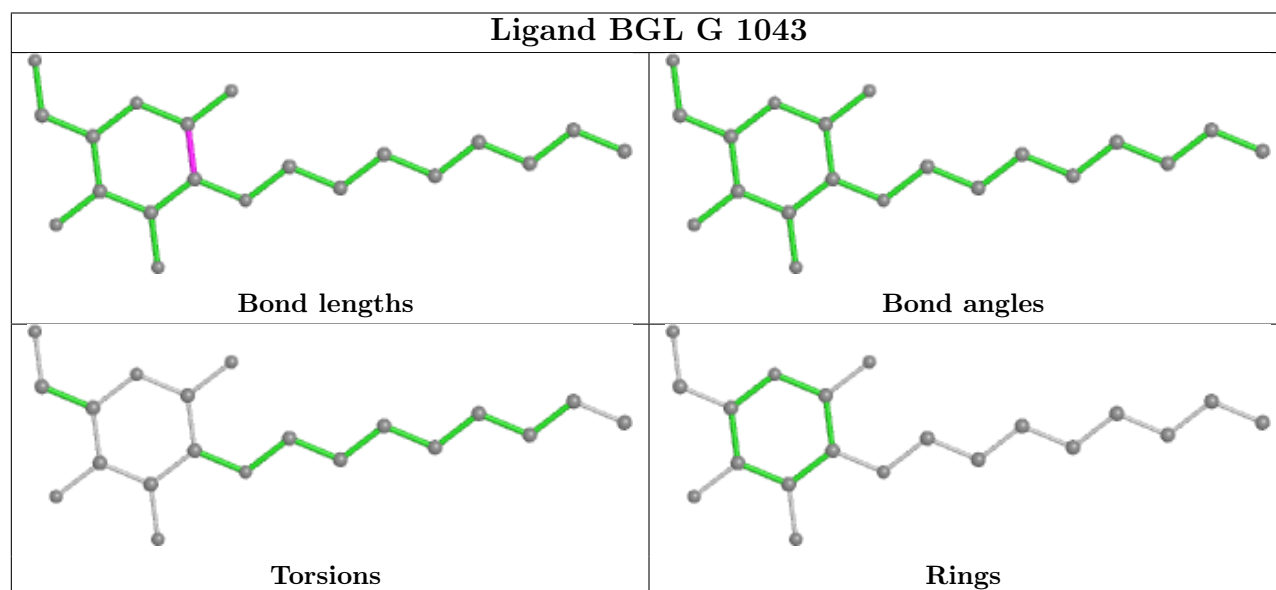
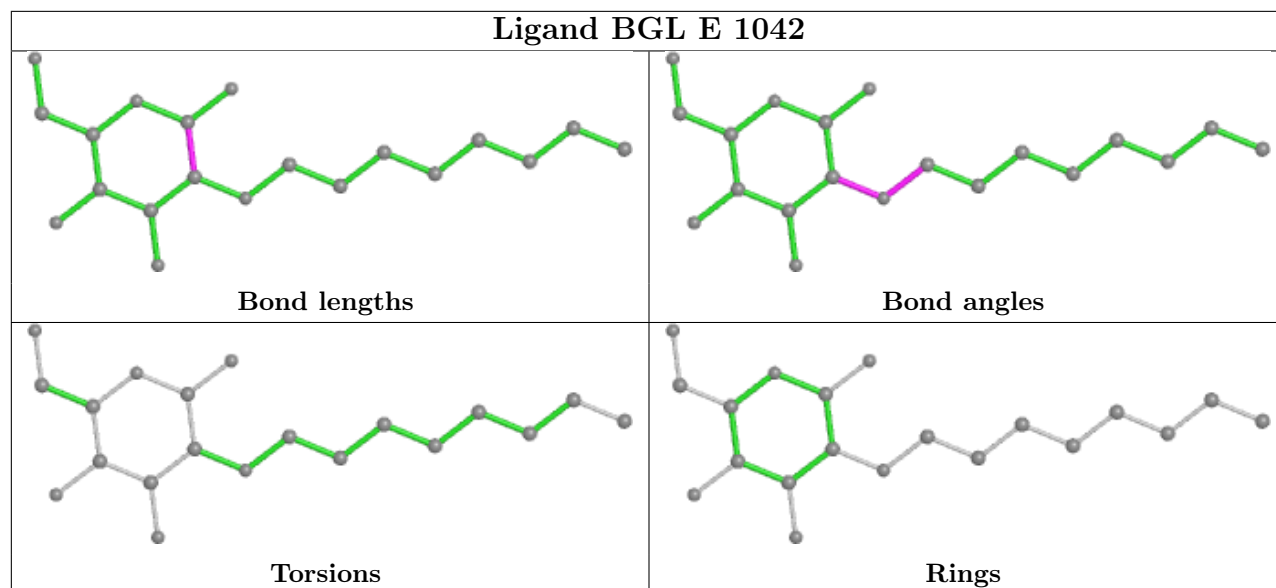




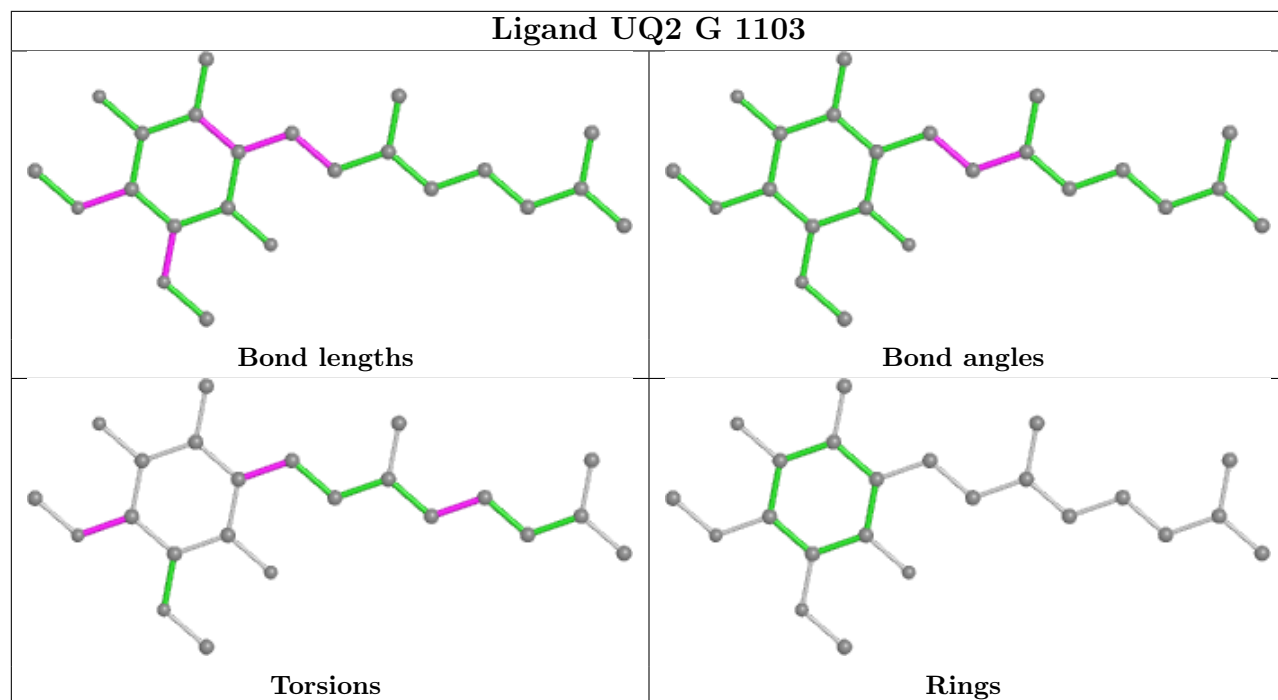




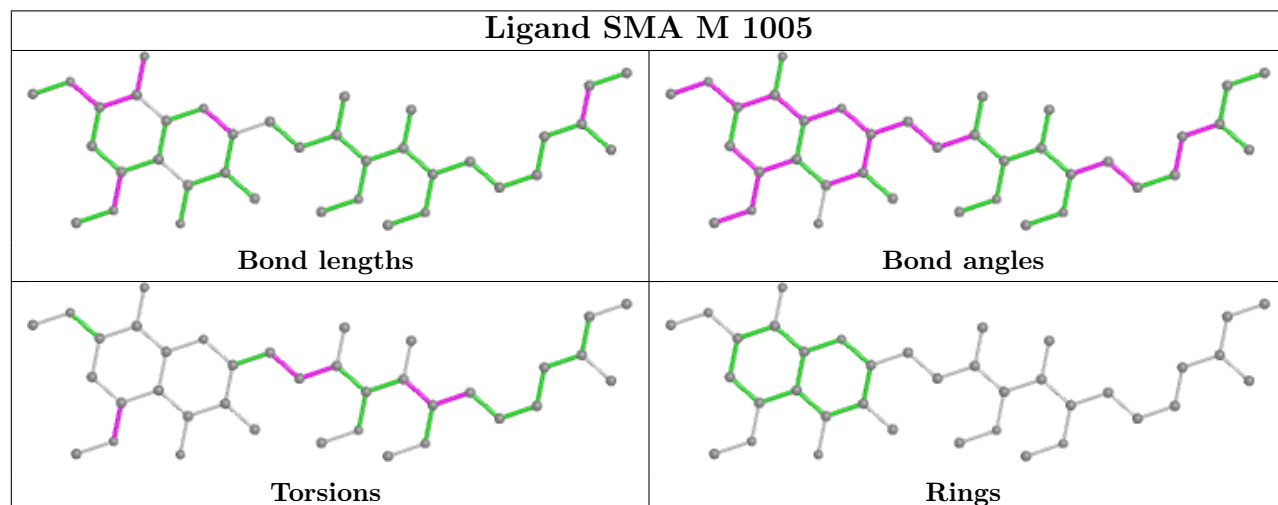


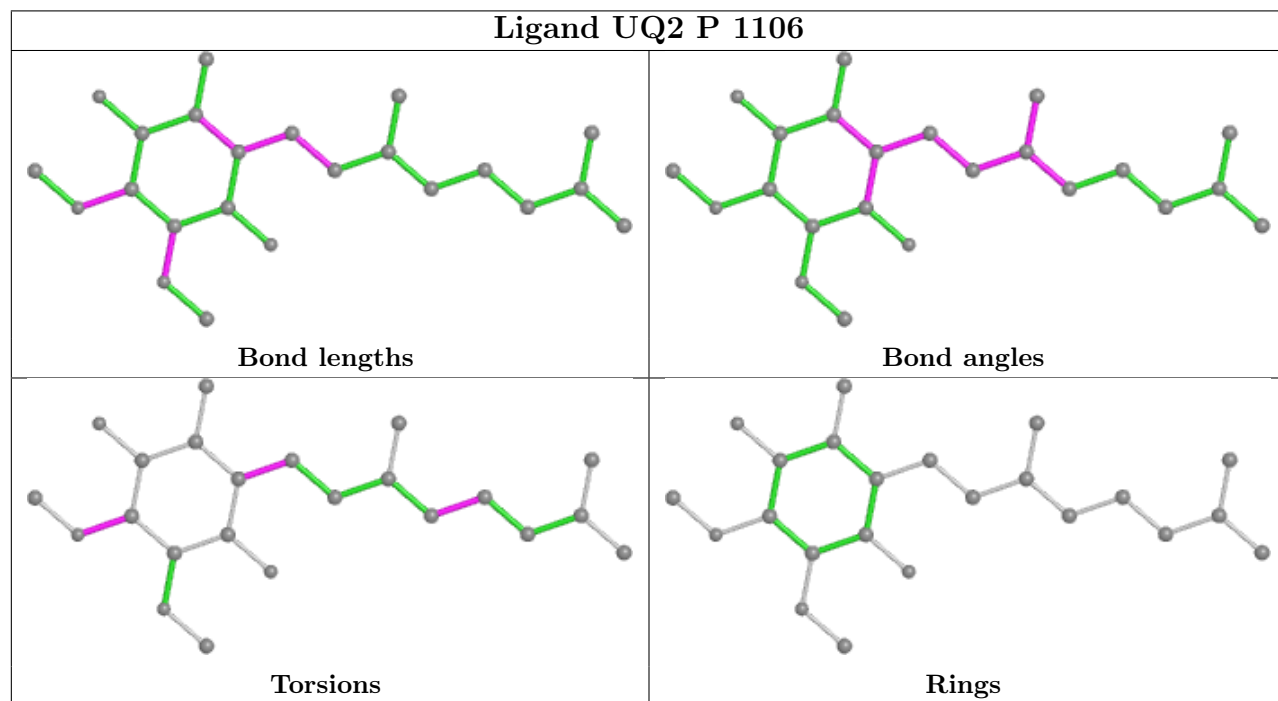
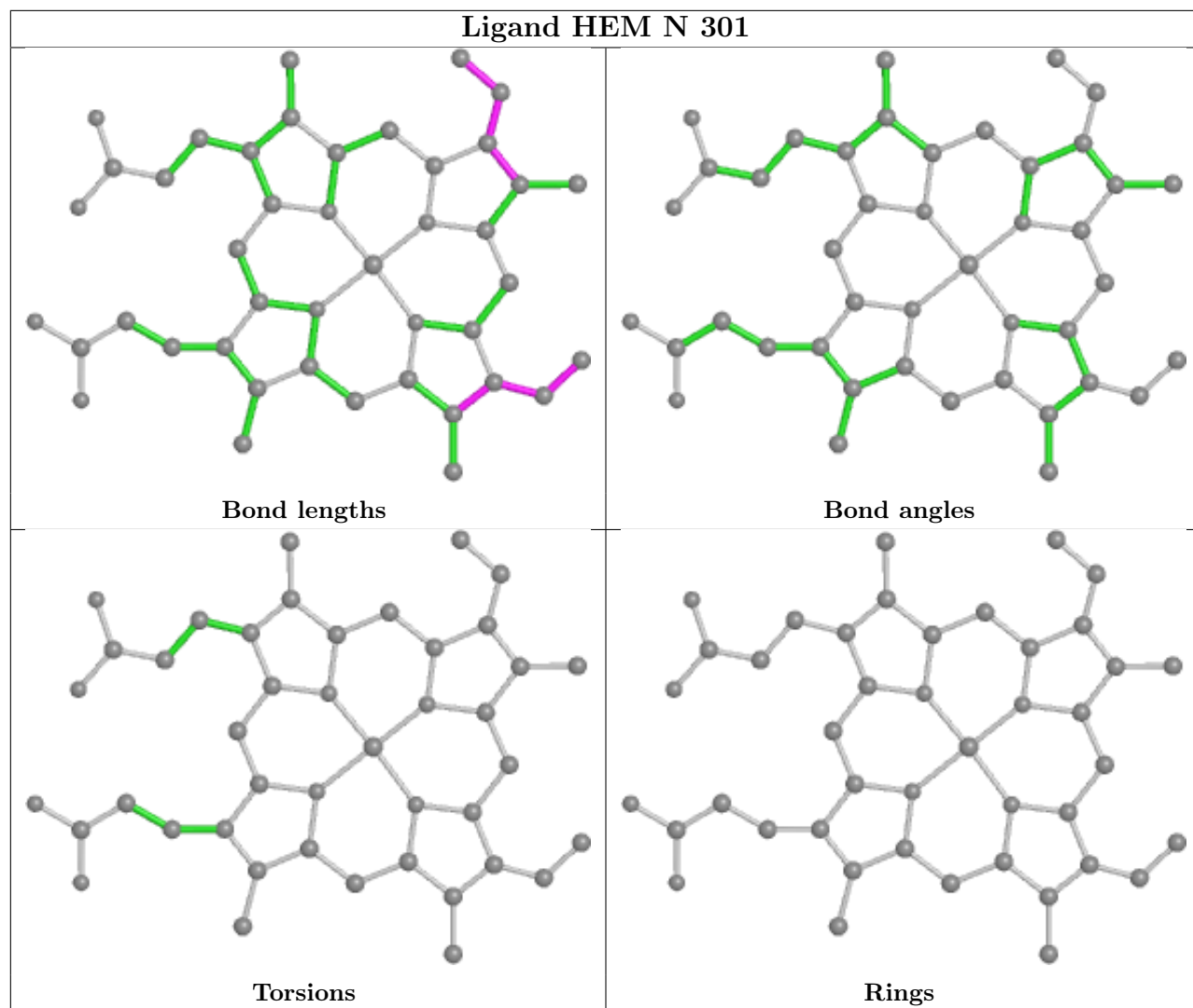


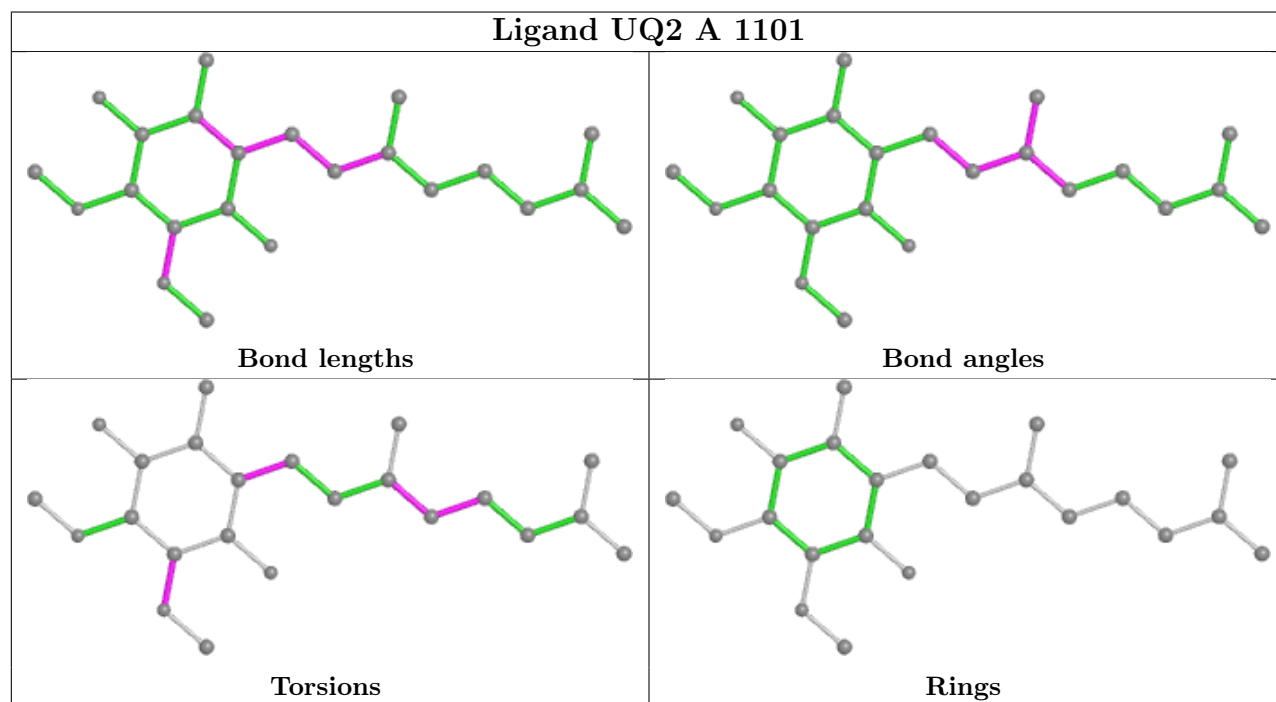
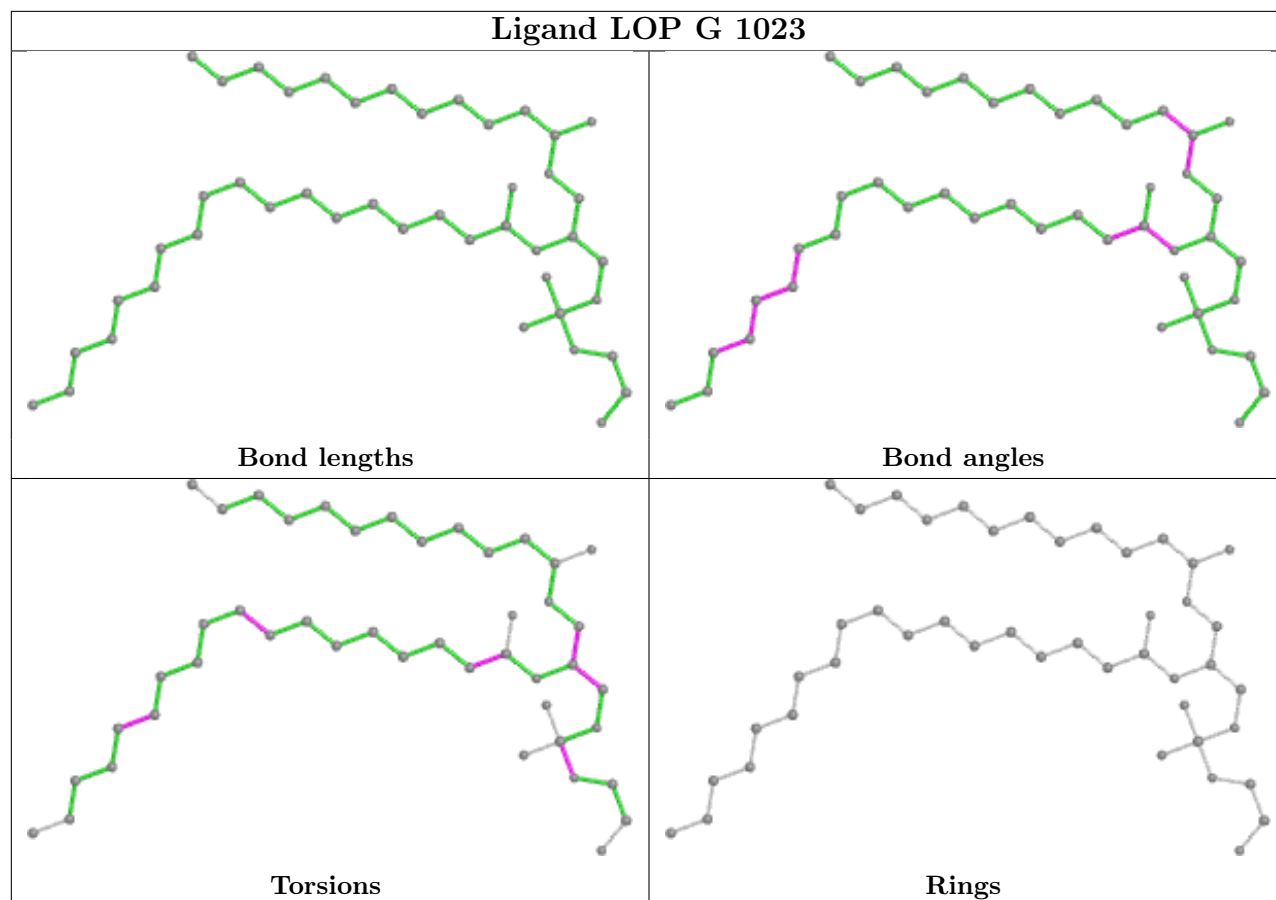
Ligand UQ2 G 1103



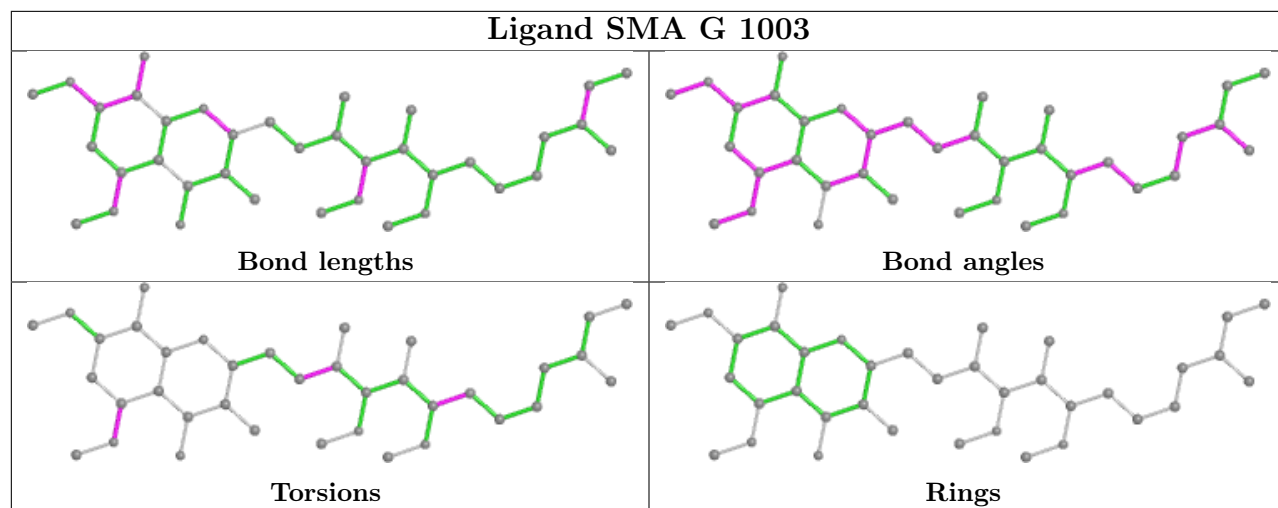
Ligand SMA M 1005



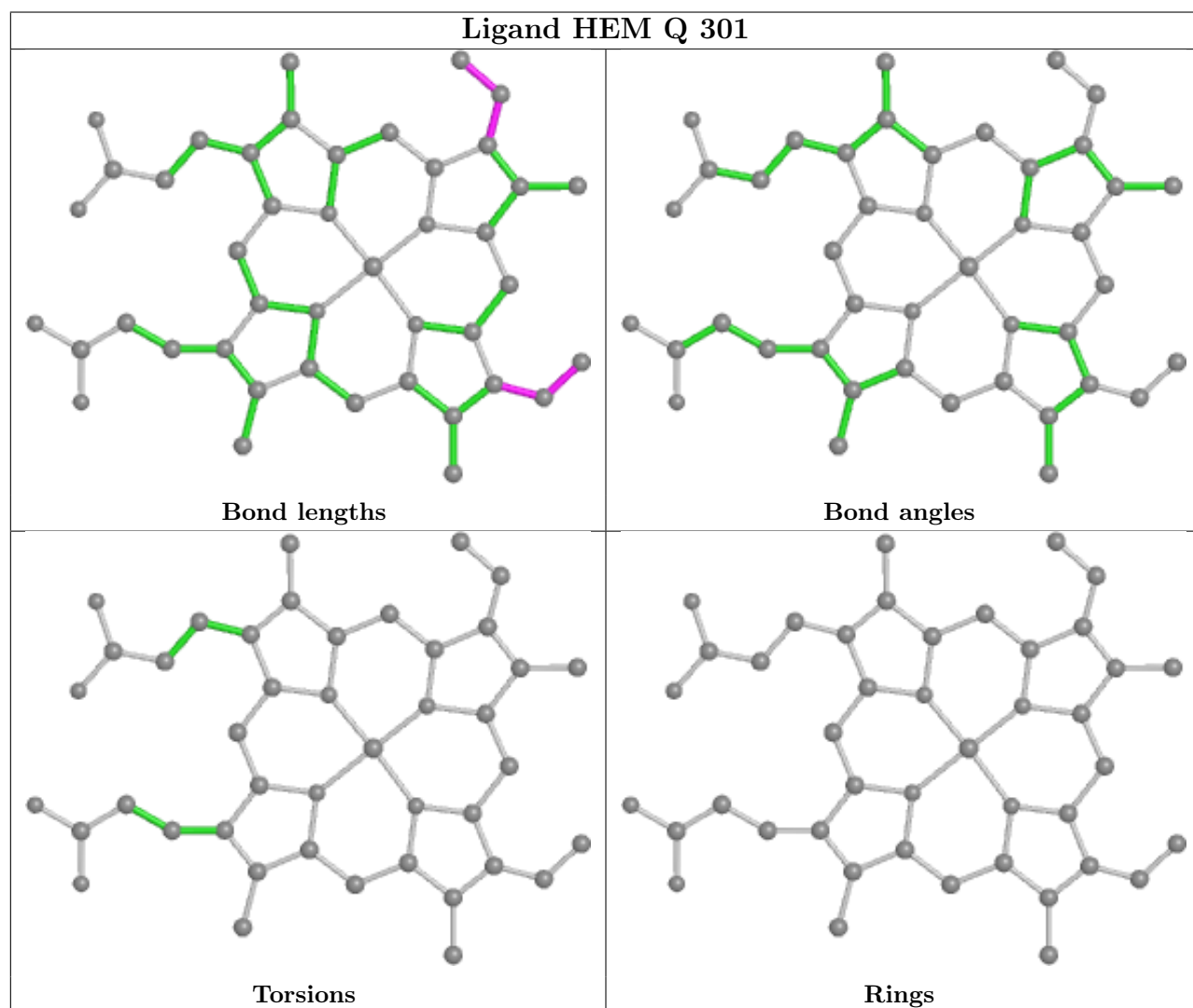


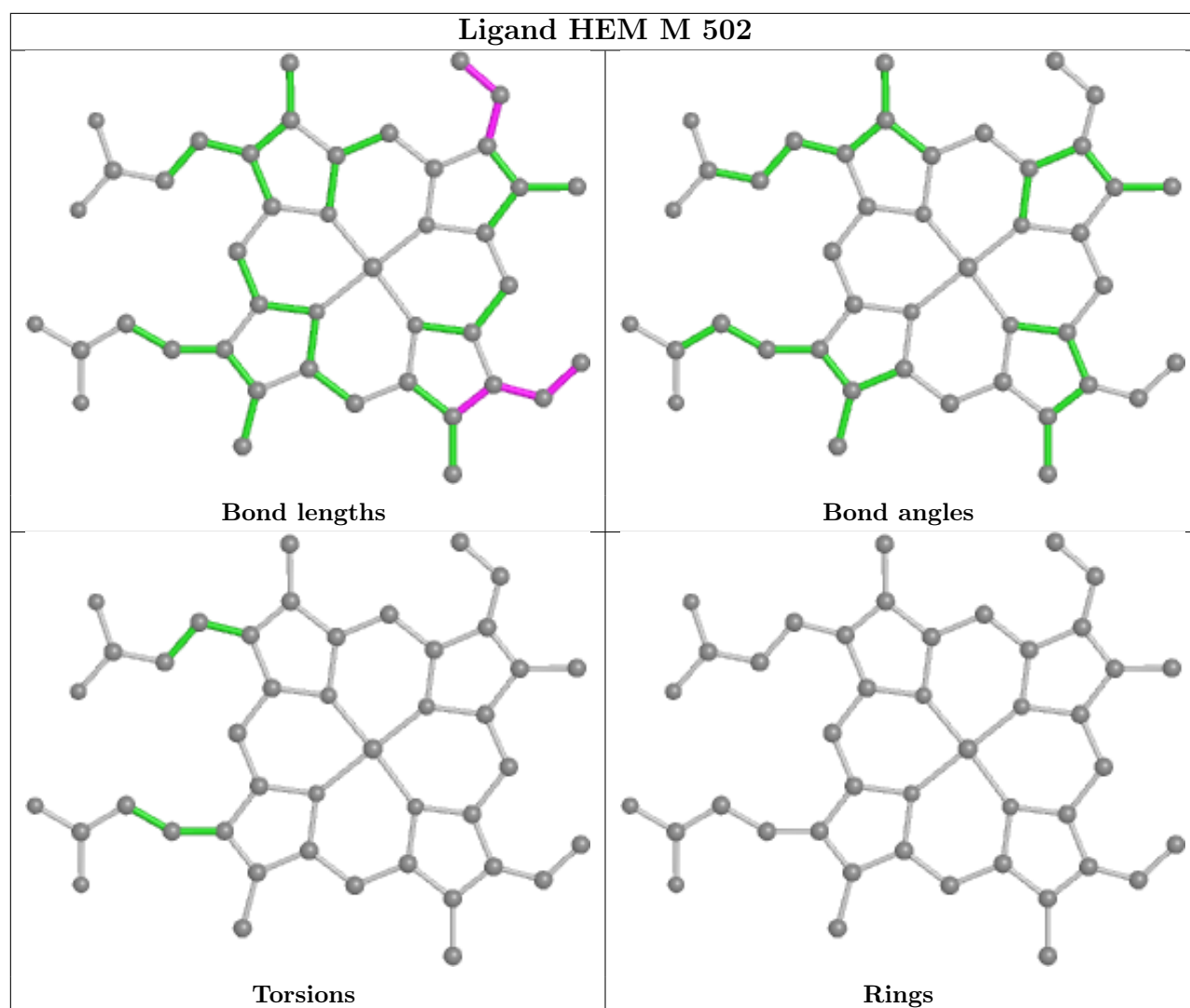


Ligand SMA G 1003



Ligand HEM Q 301





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%)	0.41	10 (2%) 60 58	35, 53, 90, 117	0
1	D	428/445 (96%)	0.34	11 (2%) 56 54	35, 53, 93, 124	0
1	G	428/445 (96%)	0.58	26 (6%) 21 20	35, 56, 100, 124	0
1	J	428/445 (96%)	0.64	30 (7%) 16 15	36, 62, 101, 125	0
1	M	428/445 (96%)	0.69	43 (10%) 7 6	38, 67, 107, 130	0
1	P	428/445 (96%)	0.49	22 (5%) 28 26	35, 56, 100, 127	0
2	B	256/269 (95%)	0.78	31 (12%) 4 3	47, 78, 112, 134	0
2	E	256/269 (95%)	0.91	40 (15%) 2 1	50, 80, 117, 133	0
2	H	256/269 (95%)	0.57	20 (7%) 13 11	40, 72, 113, 135	0
2	K	256/269 (95%)	1.29	64 (25%) 0 0	49, 87, 120, 136	0
2	N	256/269 (95%)	1.70	87 (33%) 0 0	59, 95, 121, 135	0
2	Q	256/269 (95%)	1.14	59 (23%) 0 0	51, 87, 119, 134	0
3	C	179/187 (95%)	0.68	19 (10%) 6 5	37, 59, 101, 139	0
3	F	179/187 (95%)	0.70	29 (16%) 1 1	38, 63, 102, 140	0
3	I	179/187 (95%)	0.53	16 (8%) 9 9	41, 58, 105, 139	0
3	L	179/187 (95%)	0.54	16 (8%) 9 9	37, 59, 104, 139	0
3	O	179/187 (95%)	0.74	22 (12%) 4 3	34, 64, 108, 138	0
3	R	179/187 (95%)	1.08	39 (21%) 0 0	46, 70, 108, 138	0
All	All	5178/5406 (95%)	0.72	584 (11%) 5 4	34, 66, 112, 140	0

All (584) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Q	2	GLY	17.9
2	E	3	GLY	17.8
3	C	9	GLY	17.7

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Mol	Chain	Res	Type	RSRZ
3	I	9	GLY	17.4
2	K	3	GLY	15.9
2	E	2	GLY	14.1
2	N	2	GLY	11.5
2	K	2	GLY	11.4
2	N	3	GLY	11.3
3	I	46	ALA	10.9
3	F	12	ARG	10.8
3	R	9	GLY	10.8
2	N	1	ALA	10.2
2	K	172	ALA	10.0
3	O	10	THR	10.0
3	O	9	GLY	9.8
3	O	12	ARG	9.7
3	C	10	THR	9.7
3	R	11	ARG	9.7
3	C	11	ARG	9.5
3	L	12	ARG	9.4
3	O	11	ARG	9.1
3	I	10	THR	8.9
2	N	4	GLY	8.8
3	O	16	TYR	8.7
2	E	1	ALA	8.6
3	C	12	ARG	8.3
2	N	199	GLY	8.2
2	K	4	GLY	8.0
2	N	109	GLY	7.8
3	O	179	ILE	7.7
3	L	10	THR	7.6
2	H	1	ALA	7.5
2	K	169	CYS	7.2
3	R	10	THR	7.1
2	K	114	MET	7.1
3	R	179	ILE	7.0
3	L	11	ARG	6.9
2	H	3	GLY	6.7
1	J	8	HIS	6.7
2	N	174	GLY	6.7
3	F	179	ILE	6.7
1	M	354	VAL	6.7
2	B	1	ALA	6.7
1	D	12	ARG	6.6

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Mol	Chain	Res	Type	RSRZ
2	K	145	CYS	6.6
2	N	122	PHE	6.3
2	Q	1	ALA	6.3
3	F	9	GLY	6.3
2	E	4	GLY	6.3
2	K	256	LYS	6.2
2	B	256	LYS	6.2
1	P	12	ARG	6.1
2	N	6	VAL	6.1
2	K	5	HIS	6.0
2	K	138	PHE	6.0
1	J	5	PRO	5.9
2	H	2	GLY	5.9
1	M	232	THR	5.9
3	I	47	LEU	5.9
3	F	187	GLY	5.8
3	R	184	ILE	5.8
3	F	10	THR	5.8
2	B	121	LEU	5.7
3	L	14	PHE	5.7
2	B	199	GLY	5.6
2	K	173	ASN	5.6
2	N	173	ASN	5.5
2	N	178	THR	5.5
3	R	12	ARG	5.5
1	J	7	ASP	5.5
2	K	143	PRO	5.4
3	L	19	THR	5.4
2	N	172	ALA	5.4
2	Q	255	VAL	5.4
2	B	4	GLY	5.3
2	E	199	GLY	5.3
2	N	110	PHE	5.3
1	M	5	PRO	5.3
2	K	6	VAL	5.2
1	M	417	PRO	5.2
1	M	416	LYS	5.2
2	N	200	HIS	5.2
3	C	179	ILE	5.2
1	M	359	TYR	5.2
2	N	198	ASP	5.1
2	B	2	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
2	Q	58	LEU	5.1
1	J	11	PRO	5.1
3	F	47	LEU	5.1
1	J	12	ARG	5.0
1	G	12	ARG	5.0
2	N	196	TYR	5.0
3	R	13	ASP	5.0
3	I	12	ARG	5.0
1	J	10	GLU	4.9
2	N	175	VAL	4.9
1	J	9	TYR	4.9
2	N	10	PRO	4.9
1	M	12	ARG	4.9
2	K	253	ALA	4.9
2	N	121	LEU	4.8
2	K	122	PHE	4.8
2	K	144	LYS	4.8
1	J	348	TRP	4.7
1	M	418	VAL	4.7
3	R	52	VAL	4.7
3	R	47	LEU	4.7
2	Q	5	HIS	4.7
2	Q	7	GLU	4.7
2	B	146	ALA	4.7
3	R	14	PHE	4.7
2	N	77	THR	4.7
1	M	15	ILE	4.6
3	I	179	ILE	4.6
3	R	17	TYR	4.6
2	N	201	ASP	4.6
2	K	124	GLY	4.6
1	J	362	MET	4.6
2	K	150	GLU	4.6
3	C	48	ALA	4.5
2	N	169	CYS	4.5
1	J	6	HIS	4.5
2	E	200	HIS	4.5
3	L	13	ASP	4.5
3	L	116	LEU	4.5
2	N	78	GLY	4.4
1	P	8	HIS	4.4
1	G	18	TRP	4.4

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Mol	Chain	Res	Type	RSRZ
2	K	9	VAL	4.4
3	O	15	LEU	4.4
2	Q	79	GLU	4.4
2	Q	152	ASP	4.4
2	Q	147	GLU	4.4
1	J	416	LYS	4.4
3	I	17	TYR	4.4
2	Q	190	MET	4.4
1	A	416	LYS	4.4
2	Q	204	VAL	4.4
2	N	152	ASP	4.3
2	K	11	PHE	4.3
2	N	256	LYS	4.3
3	O	187	GLY	4.3
3	R	187	GLY	4.3
1	G	15	ILE	4.3
2	Q	193	LEU	4.3
3	F	54	VAL	4.3
1	P	6	HIS	4.3
2	N	197	ALA	4.3
3	F	48	ALA	4.3
2	N	171	ASP	4.2
3	C	47	LEU	4.2
3	O	47	LEU	4.2
2	Q	110	PHE	4.2
2	K	110	PHE	4.2
2	N	123	ASN	4.2
3	I	11	ARG	4.2
3	O	13	ASP	4.2
2	H	109	GLY	4.2
3	L	9	GLY	4.2
2	Q	196	TYR	4.1
3	F	53	ASP	4.1
2	Q	9	VAL	4.1
2	N	149	HIS	4.1
2	B	200	HIS	4.1
2	N	111	HIS	4.1
1	P	5	PRO	4.0
2	K	171	ASP	4.0
2	K	149	HIS	4.0
2	K	118	ILE	4.0
2	N	7	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	5	HIS	4.0
1	G	416	LYS	4.0
2	Q	194	VAL	4.0
3	F	17	TYR	4.0
1	G	414	ILE	3.9
2	Q	80	ASP	3.9
2	Q	3	GLY	3.9
3	F	11	ARG	3.9
1	M	323	PHE	3.9
1	P	4	ILE	3.9
3	R	50	ILE	3.9
2	B	151	PRO	3.9
2	E	7	GLU	3.9
2	Q	35	VAL	3.9
2	N	202	ALA	3.8
2	E	251	LEU	3.8
2	E	140	GLU	3.8
3	F	186	LEU	3.8
3	L	181	GLU	3.8
2	N	153	GLY	3.8
3	R	181	GLU	3.8
2	B	143	PRO	3.8
2	N	192	ASP	3.7
3	L	15	LEU	3.7
1	D	13	THR	3.7
2	E	5	HIS	3.7
1	P	11	PRO	3.7
3	R	186	LEU	3.7
2	K	139	PRO	3.7
1	G	17	LYS	3.7
3	O	51	PHE	3.7
3	R	51	PHE	3.7
1	J	311	ASP	3.7
2	E	58	LEU	3.7
3	R	183	THR	3.7
2	B	149	HIS	3.7
2	Q	59	PRO	3.7
1	M	8	HIS	3.7
1	A	12	ARG	3.7
3	L	17	TYR	3.6
2	N	138	PHE	3.6
1	D	5	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	19	LEU	3.6
3	O	17	TYR	3.6
2	K	17	PHE	3.6
2	K	10	PRO	3.6
2	B	197	ALA	3.6
1	P	13	THR	3.5
1	M	365	ILE	3.5
3	O	14	PHE	3.5
2	N	255	VAL	3.5
2	K	112	GLY	3.5
2	E	149	HIS	3.5
3	R	116	LEU	3.5
1	P	7	ASP	3.5
2	N	82	GLU	3.5
3	R	178	PHE	3.5
3	F	183	THR	3.5
2	B	75	GLU	3.5
2	K	141	GLU	3.5
2	E	114	MET	3.4
2	Q	192	ASP	3.4
2	N	179	ALA	3.4
1	M	11	PRO	3.4
2	K	113	PRO	3.4
3	R	18	ALA	3.4
2	H	79	GLU	3.4
2	Q	78	GLY	3.4
1	G	13	THR	3.4
2	K	59	PRO	3.4
3	I	14	PHE	3.4
2	N	177	THR	3.4
1	J	4	ILE	3.3
1	M	428	PHE	3.3
2	B	122	PHE	3.3
1	P	30	TYR	3.3
3	I	48	ALA	3.3
1	M	234	LYS	3.3
2	B	79	GLU	3.3
1	M	233	SER	3.3
2	N	58	LEU	3.3
2	Q	191	ASP	3.3
2	Q	145	CYS	3.3
3	C	180	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
2	Q	57	GLU	3.3
2	B	150	GLU	3.3
1	M	414	ILE	3.3
2	Q	146	ALA	3.3
2	E	201	ASP	3.3
3	I	45	GLN	3.3
1	D	8	HIS	3.2
1	M	362	MET	3.2
3	C	181	GLU	3.2
1	G	14	GLY	3.2
2	Q	149	HIS	3.2
2	N	68	THR	3.2
1	J	365	ILE	3.2
2	N	125	ILE	3.2
2	H	114	MET	3.2
2	E	256	LYS	3.2
2	B	198	ASP	3.2
3	O	24	ALA	3.2
1	M	248	PHE	3.2
2	Q	11	PHE	3.2
2	E	182	TRP	3.2
2	E	205	HIS	3.2
2	Q	256	LYS	3.2
2	E	190	MET	3.2
2	K	175	VAL	3.2
2	N	66	TYR	3.2
2	K	197	ALA	3.2
2	N	39	CYS	3.2
2	E	10	PRO	3.1
2	N	151	PRO	3.1
2	Q	182	TRP	3.1
2	K	146	ALA	3.1
1	M	358	ARG	3.1
3	F	181	GLU	3.1
3	R	61	VAL	3.1
1	A	414	ILE	3.1
2	H	256	LYS	3.1
2	K	148	GLY	3.1
3	O	183	THR	3.1
1	G	9	TYR	3.1
2	E	141	GLU	3.1
2	K	7	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
2	N	79	GLU	3.1
2	H	199	GLY	3.1
1	D	292	ILE	3.1
2	N	139	PRO	3.1
1	M	13	THR	3.1
3	F	52	VAL	3.1
3	F	51	PHE	3.0
2	N	155	TYR	3.0
2	Q	8	ASP	3.0
2	K	190	MET	3.0
2	K	147	GLU	3.0
2	K	199	GLY	3.0
2	H	75	GLU	3.0
1	J	428	PHE	3.0
1	M	249	ILE	3.0
2	Q	4	GLY	3.0
3	C	187	GLY	3.0
2	N	72	VAL	3.0
1	D	7	ASP	3.0
2	N	246	LEU	3.0
2	Q	189	LEU	3.0
3	C	183	THR	3.0
2	B	3	GLY	3.0
2	K	120	GLN	3.0
1	G	10	GLU	3.0
1	G	30	TYR	3.0
2	E	193	LEU	3.0
2	K	142	PRO	3.0
2	E	8	ASP	2.9
3	I	13	ASP	2.9
3	I	187	GLY	2.9
2	N	245	TYR	2.9
1	M	242	VAL	2.9
2	Q	6	VAL	2.9
2	Q	200	HIS	2.9
2	H	251	LEU	2.9
2	Q	143	PRO	2.9
3	C	13	ASP	2.9
3	R	15	LEU	2.9
1	J	414	ILE	2.9
2	E	206	ALA	2.9
3	R	19	THR	2.9

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Mol	Chain	Res	Type	RSRZ
2	N	75	GLU	2.9
1	M	415	GLU	2.9
1	G	417	PRO	2.9
1	G	247	TYR	2.9
1	G	413	ALA	2.8
2	N	166	PRO	2.8
1	M	411	LEU	2.8
2	N	150	GLU	2.8
2	N	80	ASP	2.8
2	N	195	GLU	2.8
1	D	290	ALA	2.8
2	Q	94	LEU	2.8
2	Q	153	GLY	2.8
1	P	239	LYS	2.8
2	Q	56	PRO	2.8
3	C	104	ASP	2.8
2	E	255	VAL	2.7
2	N	249	LYS	2.7
3	R	58	GLU	2.7
1	J	30	TYR	2.7
2	Q	188	PRO	2.7
2	Q	199	GLY	2.7
1	M	419	ALA	2.7
2	K	231	PHE	2.7
2	E	151	PRO	2.7
1	P	14	GLY	2.7
2	H	72	VAL	2.7
2	E	122	PHE	2.7
2	N	100	LEU	2.7
2	N	9	VAL	2.7
3	C	16	TYR	2.7
1	G	11	PRO	2.7
2	E	252	TRP	2.7
1	M	348	TRP	2.7
1	A	13	THR	2.6
2	B	110	PHE	2.6
2	E	110	PHE	2.6
2	N	124	GLY	2.6
1	M	6	HIS	2.6
1	M	412	GLY	2.6
3	F	182	THR	2.6
2	Q	12	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	413	ALA	2.6
1	M	14	GLY	2.6
2	Q	96	ASN	2.6
3	L	187	GLY	2.6
1	M	413	ALA	2.6
2	N	11	PHE	2.6
3	O	181	GLU	2.6
3	F	13	ASP	2.6
3	O	180	ASP	2.6
3	L	47	LEU	2.6
3	F	14	PHE	2.6
3	F	184	ILE	2.6
3	R	82	ILE	2.6
2	K	182	TRP	2.6
2	N	119	SER	2.6
3	R	180	ASP	2.6
2	H	82	GLU	2.6
2	Q	140	GLU	2.5
3	C	103	ILE	2.5
3	F	55	SER	2.5
1	A	76	ALA	2.5
1	J	123	ALA	2.5
2	K	1	ALA	2.5
1	M	19	LEU	2.5
1	P	10	GLU	2.5
2	K	119	SER	2.5
1	J	124	PRO	2.5
2	E	16	PRO	2.5
3	R	65	VAL	2.5
2	N	5	HIS	2.5
1	M	387	PHE	2.5
2	N	114	MET	2.5
1	J	27	ALA	2.5
3	O	48	ALA	2.5
1	G	7	ASP	2.5
1	J	361	PRO	2.5
1	G	412	GLY	2.5
2	E	18	GLY	2.5
3	R	56	SER	2.5
3	C	178	PHE	2.5
2	N	61	ASP	2.5
2	B	139	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	K	251	LEU	2.4
3	R	57	VAL	2.4
1	J	172	ILE	2.4
1	P	428	PHE	2.4
2	N	113	PRO	2.4
1	J	237	ALA	2.4
2	E	253	ALA	2.4
2	Q	202	ALA	2.4
2	K	255	VAL	2.4
1	P	9	TYR	2.4
2	Q	61	ASP	2.4
2	K	236	PHE	2.4
2	Q	243	LEU	2.4
2	E	147	GLU	2.4
3	I	57	VAL	2.4
1	J	323	PHE	2.4
1	M	18	TRP	2.4
2	B	76	GLU	2.4
2	N	94	LEU	2.4
3	R	177	LYS	2.4
2	Q	18	GLY	2.4
2	K	252	TRP	2.4
2	K	58	LEU	2.4
2	E	9	VAL	2.4
2	H	250	ARG	2.4
2	Q	158	ARG	2.4
2	N	62	GLN	2.4
2	N	251	LEU	2.4
3	O	57	VAL	2.4
3	F	50	ILE	2.4
1	M	9	TYR	2.4
3	R	79	GLU	2.4
2	K	117	GLY	2.3
3	F	57	VAL	2.3
3	R	103	ILE	2.3
1	J	244	PHE	2.3
2	N	20	PHE	2.3
2	N	168	THR	2.3
1	P	22	ARG	2.3
2	N	207	MET	2.3
2	K	20	PHE	2.3
1	P	348	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
2	K	123	ASN	2.3
2	K	245	TYR	2.3
2	Q	141	GLU	2.3
3	L	186	LEU	2.3
1	P	293	VAL	2.3
2	N	35	VAL	2.3
1	G	22	ARG	2.3
1	M	237	ALA	2.3
2	N	112	GLY	2.3
3	F	176	ALA	2.3
1	G	232	THR	2.3
1	G	294	PRO	2.3
2	N	143	PRO	2.3
2	B	178	THR	2.3
1	M	197	LEU	2.3
2	B	64	ARG	2.3
2	B	174	GLY	2.3
2	B	69	GLN	2.3
2	K	183	ILE	2.3
2	K	8	ASP	2.3
2	H	145	CYS	2.3
2	Q	150	GLU	2.3
2	Q	206	ALA	2.2
1	P	16	GLU	2.2
2	K	177	THR	2.2
2	H	205	HIS	2.2
3	O	54	VAL	2.2
2	Q	75	GLU	2.2
2	N	65	ALA	2.2
3	R	105	ALA	2.2
2	K	168	THR	2.2
2	Q	132	TYR	2.2
1	M	7	ASP	2.2
2	B	78	GLY	2.2
3	F	180	ASP	2.2
3	I	181	GLU	2.2
2	E	145	CYS	2.2
1	P	15	ILE	2.2
2	H	231	PHE	2.2
3	L	51	PHE	2.2
2	N	135	LEU	2.2
3	R	122	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	428	PHE	2.2
2	H	71	THR	2.2
2	Q	22	GLN	2.2
3	C	14	PHE	2.2
3	F	116	LEU	2.2
3	L	16	TYR	2.2
3	F	56	SER	2.2
2	E	208	ALA	2.2
2	N	76	GLU	2.2
1	G	3	GLY	2.2
2	E	146	ALA	2.2
1	A	15	ILE	2.2
2	H	80	ASP	2.2
2	N	254	GLY	2.2
1	A	150	PRO	2.2
2	Q	203	SER	2.2
2	H	111	HIS	2.1
1	P	18	TRP	2.1
1	P	43	TRP	2.1
3	F	119	ALA	2.1
2	E	254	GLY	2.1
2	N	73	THR	2.1
1	J	170	PRO	2.1
1	A	141	ALA	2.1
1	D	293	VAL	2.1
2	K	109	GLY	2.1
2	Q	19	THR	2.1
1	M	292	ILE	2.1
2	N	183	ILE	2.1
3	R	137	ILE	2.1
1	D	6	HIS	2.1
2	K	155	TYR	2.1
3	C	176	ALA	2.1
1	M	325	ILE	2.1
2	N	187	PRO	2.1
1	G	235	ALA	2.1
2	Q	77	THR	2.1
1	J	18	TRP	2.1
1	G	233	SER	2.1
1	M	251	LYS	2.1
2	K	198	ASP	2.1
2	K	200	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
2	N	191	ASP	2.1
3	O	177	LYS	2.1
1	G	146	GLY	2.1
2	E	150	GLU	2.1
2	K	196	TYR	2.1
3	R	16	TYR	2.1
2	B	201	ASP	2.1
2	N	117	GLY	2.1
3	R	139	GLY	2.1
1	J	427	ASP	2.1
3	C	186	LEU	2.1
1	J	100	GLY	2.1
2	N	137	GLY	2.1
3	R	120	GLY	2.1
1	M	311	ASP	2.0
2	E	192	ASP	2.0
2	E	54	GLY	2.0
2	B	152	ASP	2.0
2	B	224	MET	2.0
1	A	5	PRO	2.0
2	B	166	PRO	2.0
2	N	93	ALA	2.0
3	O	58	GLU	2.0
1	D	150	PRO	2.0
1	M	43	TRP	2.0
2	K	151	PRO	2.0
1	P	27	ALA	2.0
2	Q	26	GLN	2.0
3	I	105	ALA	2.0
2	N	157	ASN	2.0
2	H	4	GLY	2.0
1	J	19	LEU	2.0
3	F	178	PHE	2.0
1	A	16	GLU	2.0
3	R	53	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	UQ2	J	1104	23/23	0.53	0.48	107,115,116,117	0
8	UQ2	D	1102	23/23	0.63	0.37	92,98,107,107	0
8	UQ2	M	1105	23/23	0.64	0.44	112,123,125,125	0
8	UQ2	A	1101	23/23	0.66	0.41	102,105,108,109	0
8	UQ2	G	1103	23/23	0.69	0.38	109,116,117,118	0
4	SR	Q	1016	1/1	0.70	0.08	137,137,137,137	0
8	UQ2	P	1106	23/23	0.70	0.32	101,104,107,108	0
9	BGL	N	1045	20/20	0.71	0.31	107,111,113,114	0
7	LOP	G	1023	45/45	0.77	0.28	88,102,112,113	0
4	SR	K	1014	1/1	0.77	0.11	145,145,145,145	0
9	BGL	G	1043	20/20	0.78	0.27	89,91,101,101	0
9	BGL	B	1041	20/20	0.79	0.23	87,97,101,102	0
4	SR	E	1012	1/1	0.79	0.04	138,138,138,138	0
4	SR	B	1011	1/1	0.79	0.04	132,132,132,132	0
7	LOP	M	1025	45/45	0.80	0.28	89,114,123,123	0
4	SR	G	1018	1/1	0.80	0.19	98,98,98,98	0
7	LOP	J	1024	45/45	0.82	0.36	93,113,125,126	0
7	LOP	P	1026	45/45	0.83	0.28	69,95,99,100	0
9	BGL	K	1044	20/20	0.86	0.20	95,99,101,101	0
4	SR	M	1019	1/1	0.86	0.08	154,154,154,154	0
7	LOP	D	1022	45/45	0.87	0.25	63,88,98,102	0
4	SR	H	1013	1/1	0.88	0.08	113,113,113,113	0
9	BGL	P	1046	20/20	0.88	0.26	87,93,95,95	0
7	LOP	A	1021	45/45	0.89	0.22	72,86,94,99	0
9	BGL	E	1042	20/20	0.90	0.20	80,85,102,102	0
11	CL	I	2004	1/1	0.93	0.16	67,67,67,67	0
6	SMA	D	1002	37/37	0.94	0.22	39,44,76,78	0
4	SR	N	1015	1/1	0.94	0.06	153,153,153,153	0
4	SR	A	1017	1/1	0.94	0.17	114,114,114,114	0
5	HEM	N	301	43/43	0.94	0.20	65,72,79,84	0
11	CL	R	2005	1/1	0.94	0.09	67,67,67,67	0
5	HEM	B	301	43/43	0.95	0.20	51,56,70,73	0

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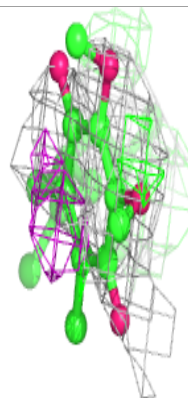
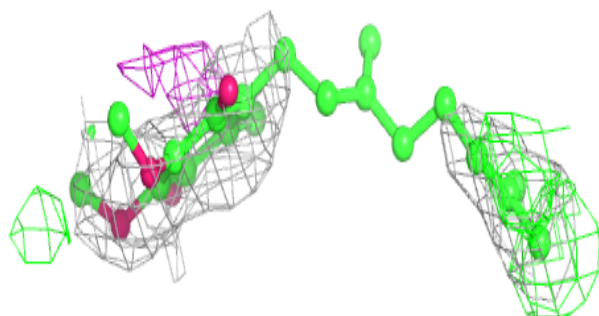
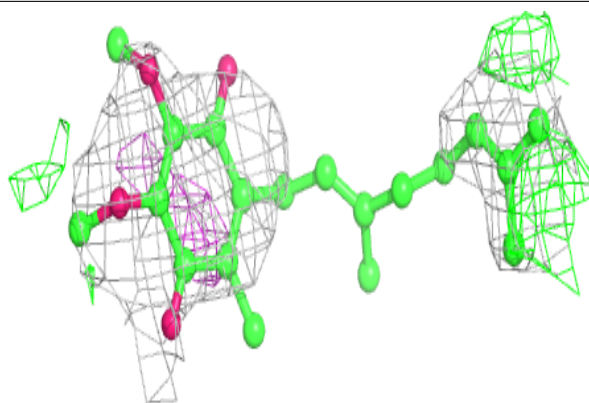
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	SMA	A	1001	37/37	0.95	0.21	38,47,54,56	0
5	HEM	J	501	43/43	0.95	0.18	67,75,79,81	0
6	SMA	J	1004	37/37	0.95	0.24	40,49,79,85	0
6	SMA	P	1006	37/37	0.95	0.22	34,45,76,77	0
12	NA	R	2001	1/1	0.95	0.10	62,62,62,62	0
5	HEM	H	301	43/43	0.96	0.17	33,42,47,50	0
6	SMA	M	1005	37/37	0.96	0.20	56,66,73,73	0
5	HEM	Q	301	43/43	0.96	0.15	56,65,73,78	0
5	HEM	E	301	43/43	0.96	0.17	53,62,73,76	0
5	HEM	K	301	43/43	0.96	0.17	49,55,67,69	0
6	SMA	G	1003	37/37	0.96	0.22	35,43,60,65	0
5	HEM	D	501	43/43	0.97	0.15	40,48,53,55	0
10	FES	I	200	4/4	0.97	0.17	47,48,48,48	0
5	HEM	G	501	43/43	0.97	0.17	50,59,62,62	0
5	HEM	M	501	43/43	0.97	0.18	63,69,75,78	0
5	HEM	D	502	43/43	0.97	0.22	32,37,49,58	0
5	HEM	G	502	43/43	0.98	0.23	32,36,45,49	0
5	HEM	A	502	43/43	0.98	0.25	32,37,49,49	0
5	HEM	M	502	43/43	0.98	0.21	47,49,59,63	0
5	HEM	A	501	43/43	0.98	0.18	43,47,51,53	0
10	FES	O	200	4/4	0.98	0.18	42,43,43,43	0
10	FES	R	200	4/4	0.98	0.15	55,57,58,58	0
5	HEM	P	501	43/43	0.98	0.16	48,54,57,57	0
5	HEM	P	502	43/43	0.98	0.24	35,40,49,53	0
5	HEM	J	502	43/43	0.98	0.22	37,41,54,57	0
10	FES	L	200	4/4	0.99	0.20	40,41,41,42	0
10	FES	F	200	4/4	0.99	0.18	43,43,44,45	0
10	FES	C	200	4/4	0.99	0.18	41,42,42,43	0

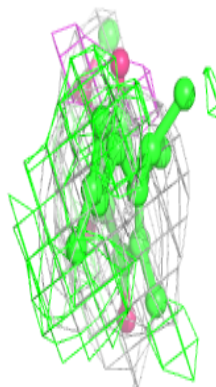
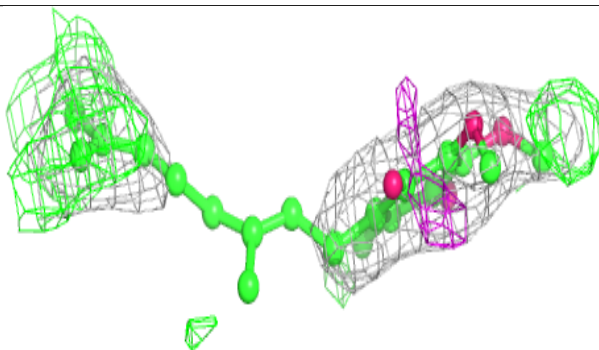
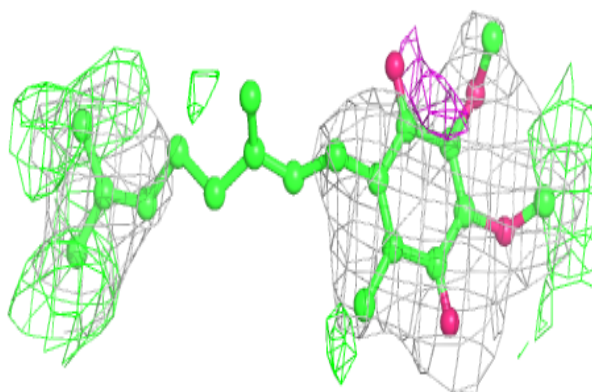
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

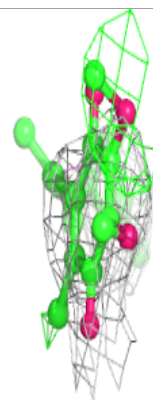
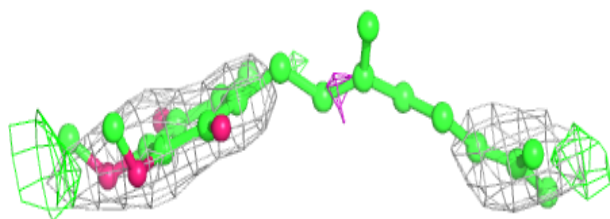
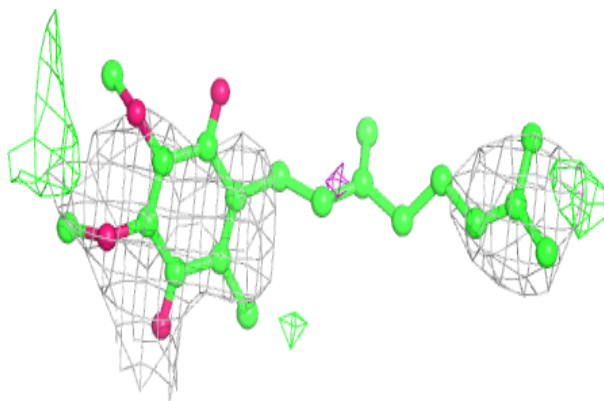
**Electron density around UQ2 D 1102:**

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

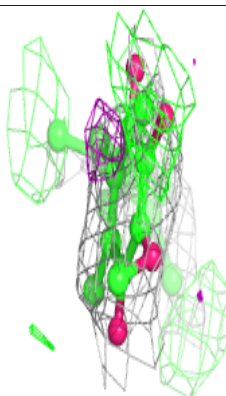
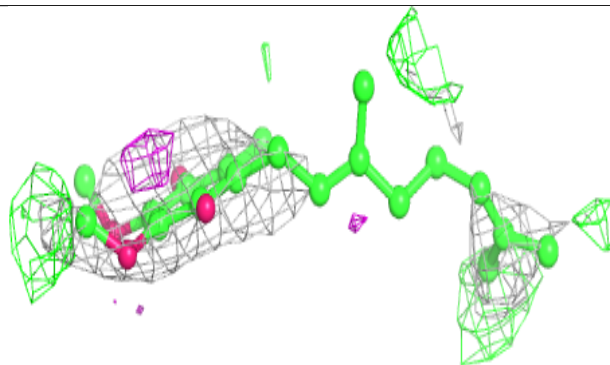
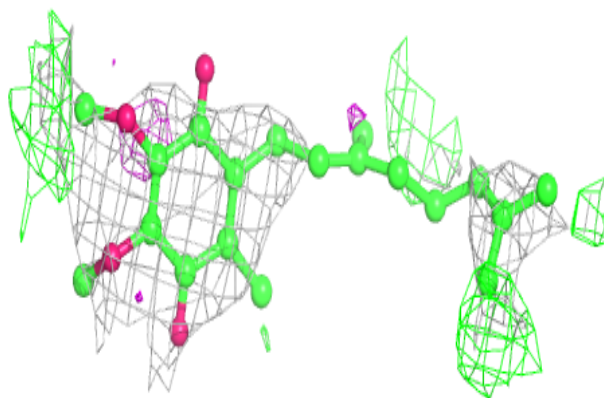


Electron density around UQ2 M 1105:

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

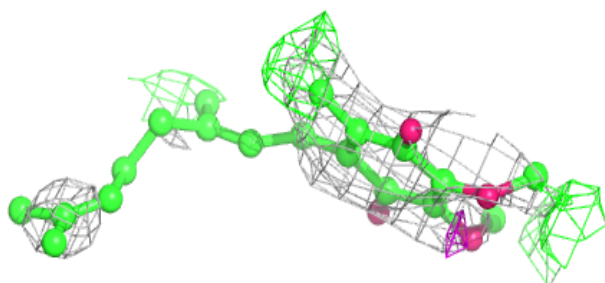
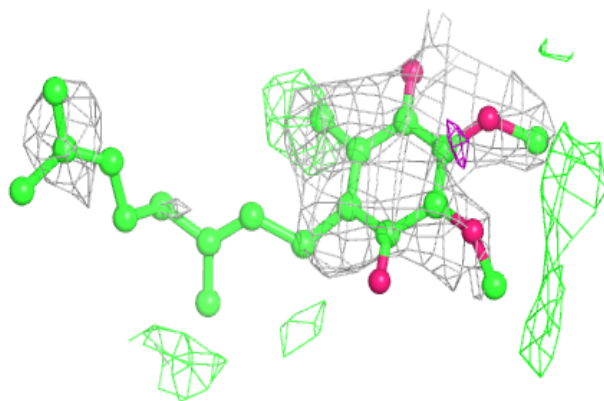
**Electron density around UQ2 A 1101:**

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

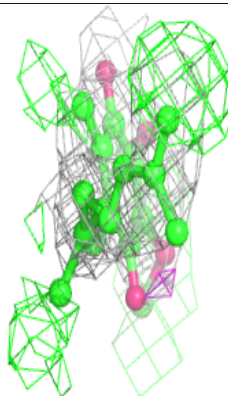
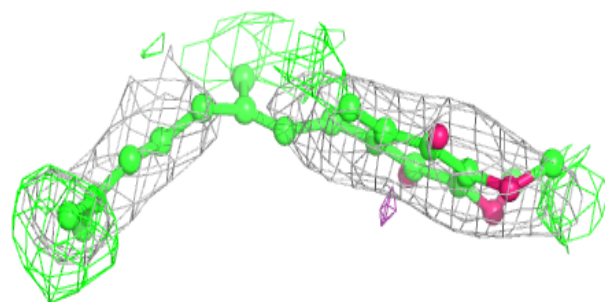
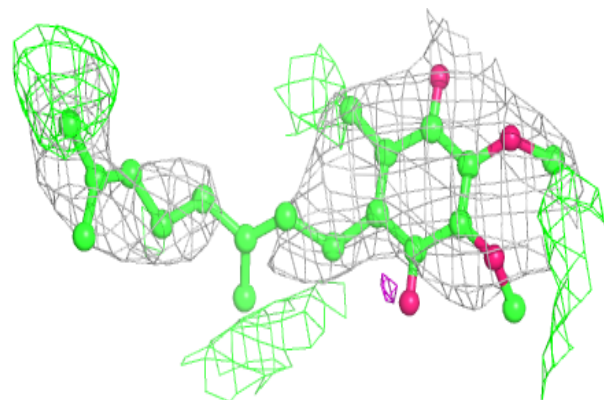


Electron density around UQ2 G 1103:

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

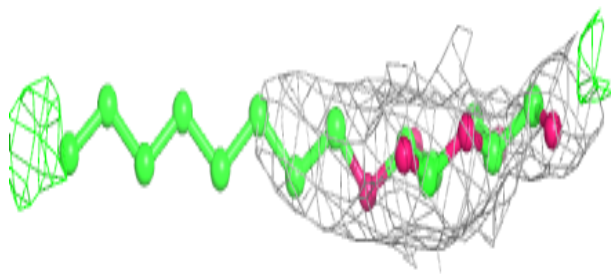
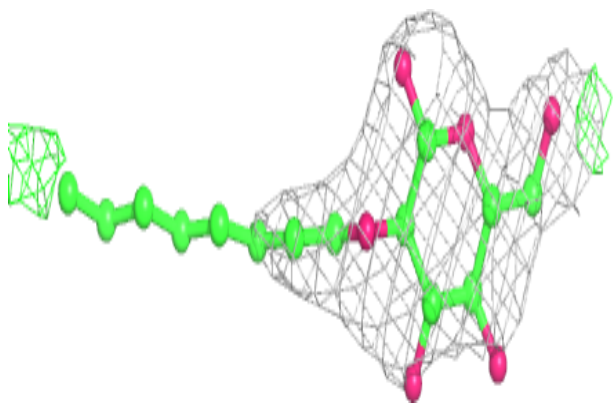
**Electron density around UQ2 P 1106:**

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

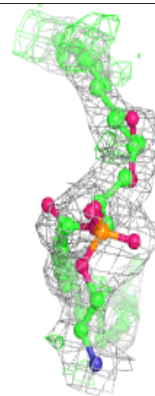
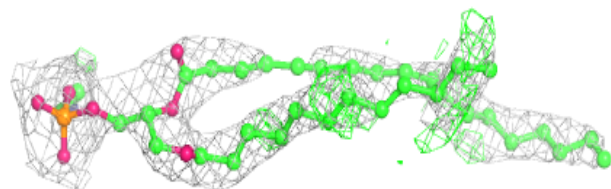
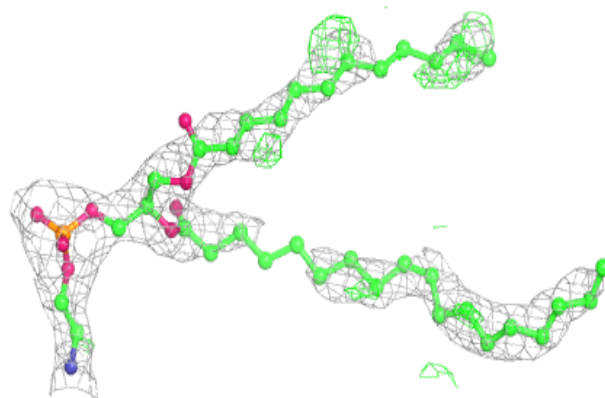


Electron density around BGL N 1045:

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

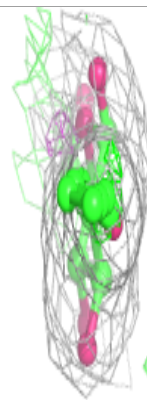
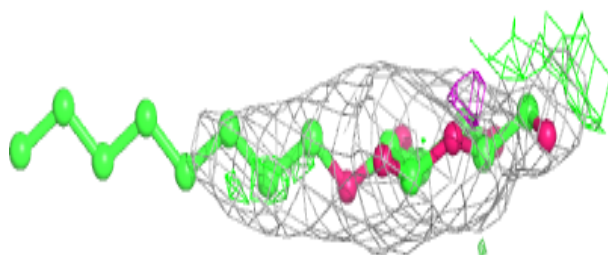
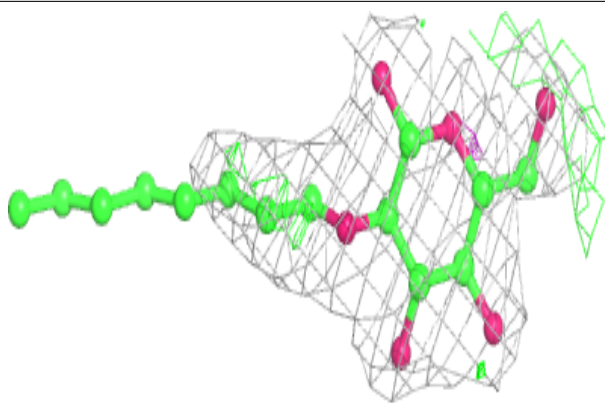
**Electron density around LOP G 1023:**

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

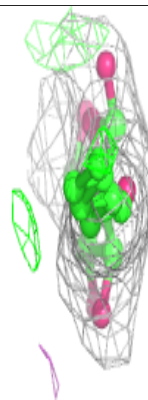
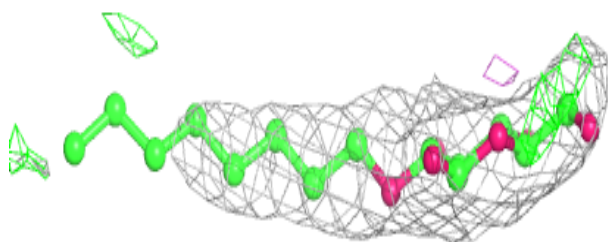
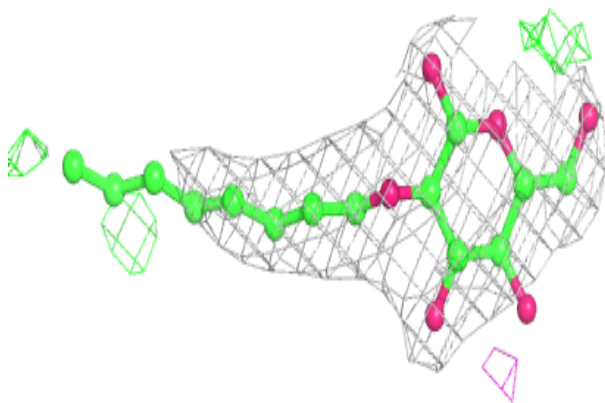


Electron density around BGL G 1043:

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

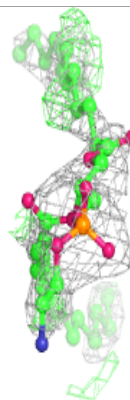
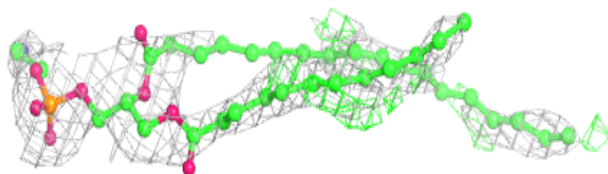
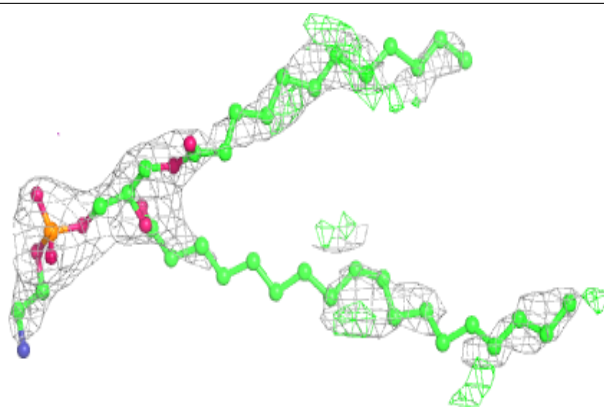
**Electron density around BGL B 1041:**

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

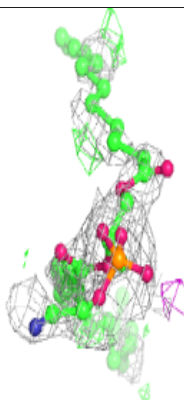
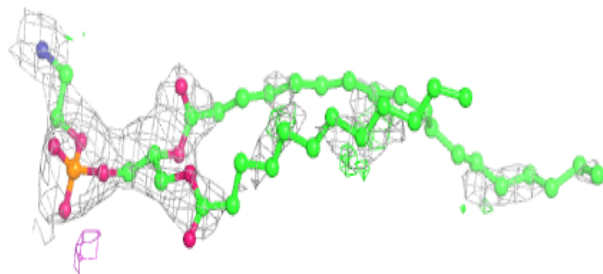
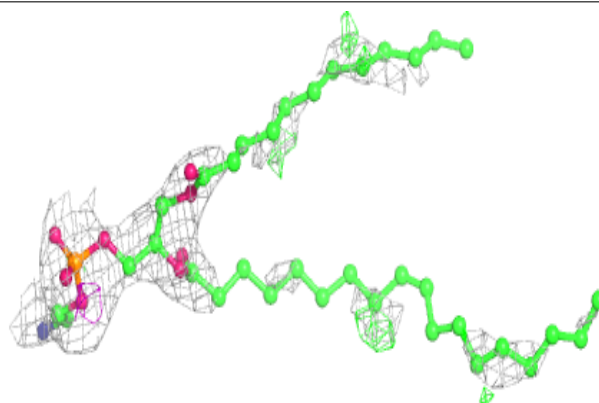


Electron density around LOP M 1025:

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

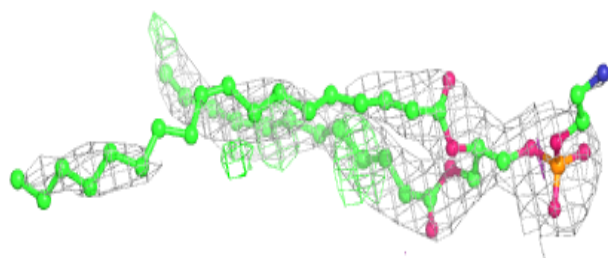
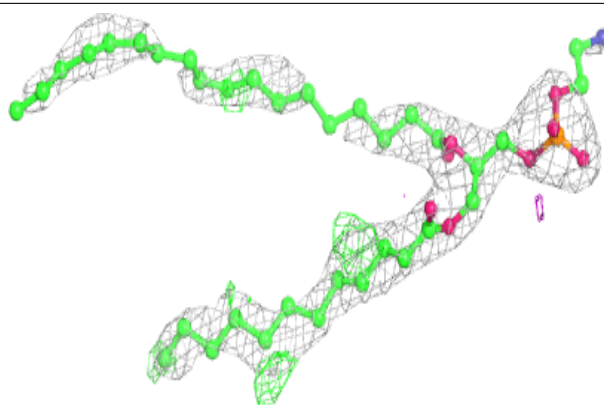
**Electron density around LOP J 1024:**

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

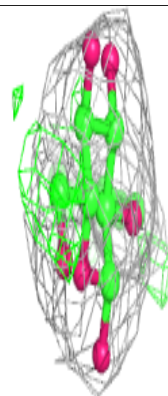
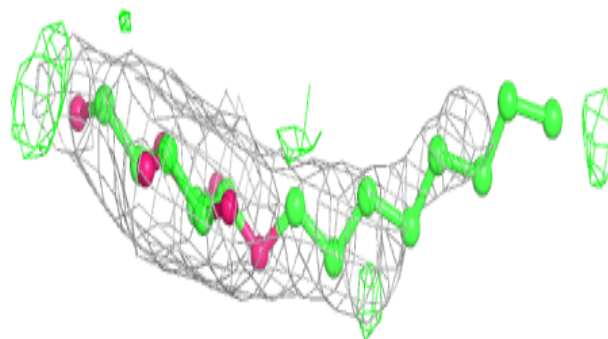
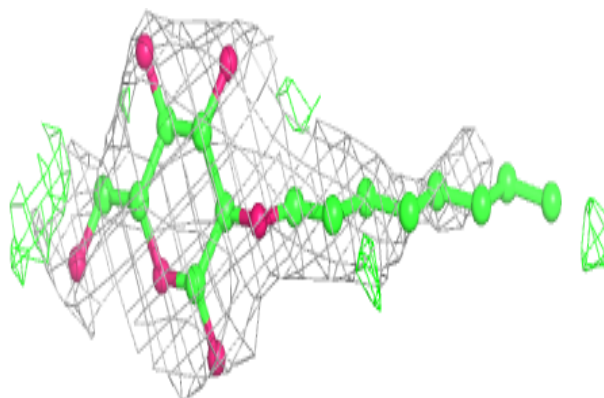


Electron density around LOP P 1026:

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

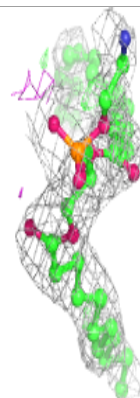
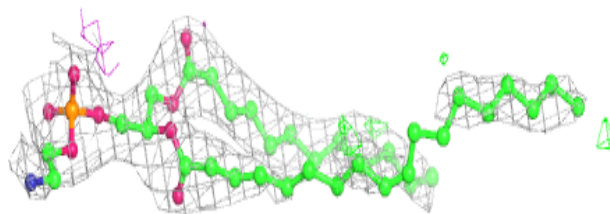
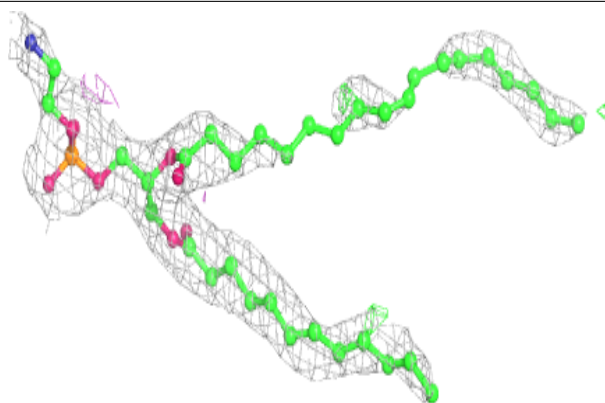
**Electron density around BGL K 1044:**

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

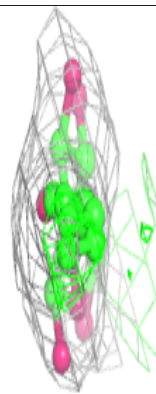
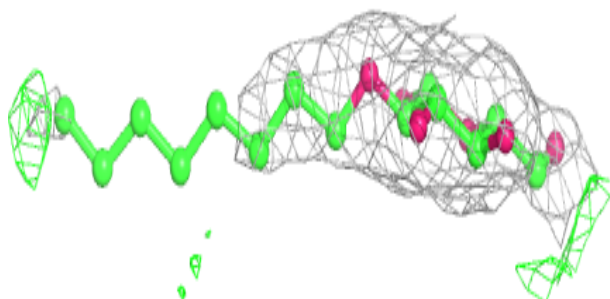
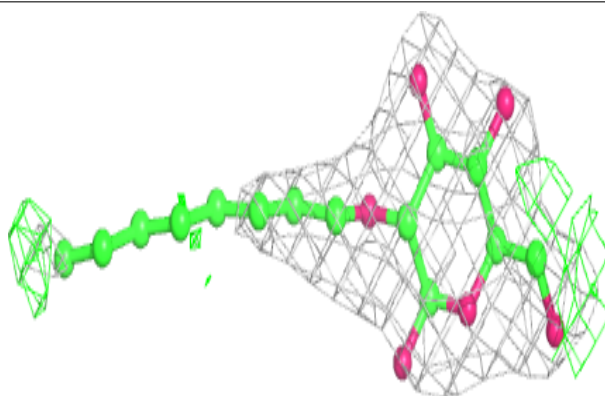


Electron density around LOP D 1022:

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

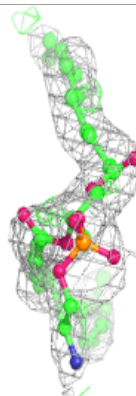
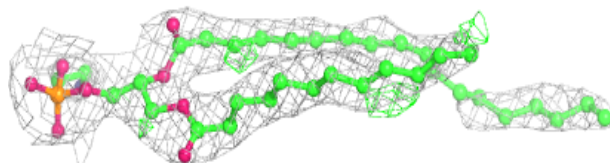
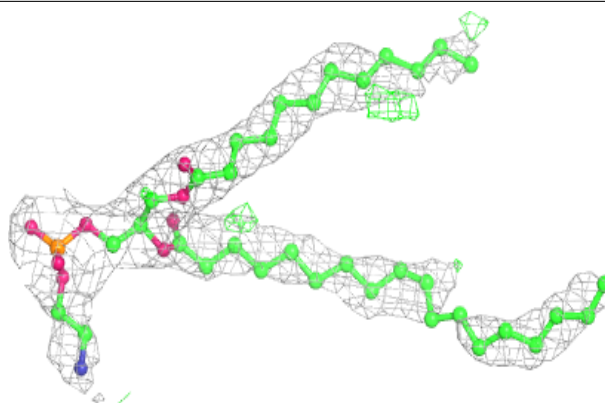
**Electron density around BGL P 1046:**

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

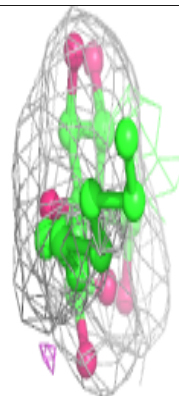
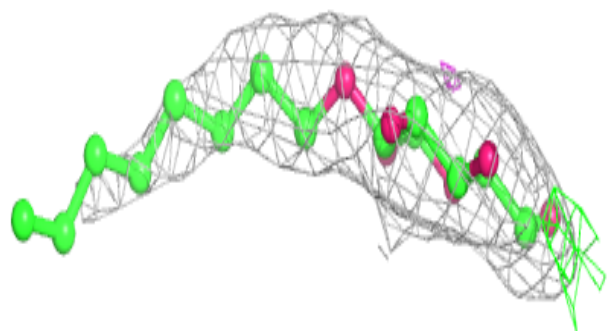
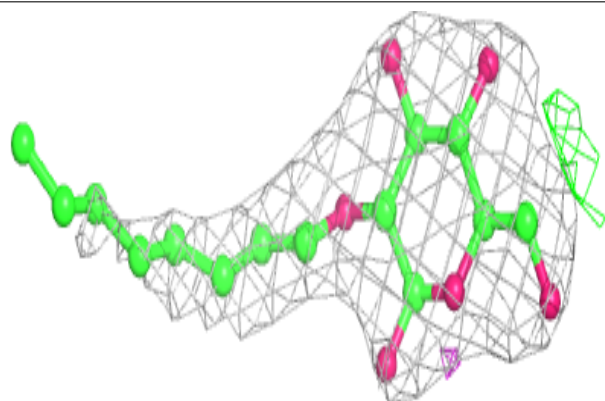


Electron density around LOP A 1021:

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

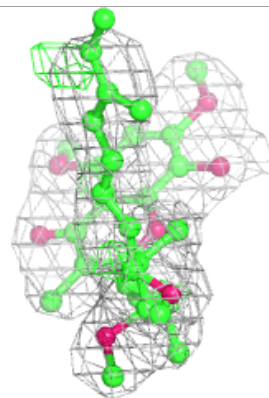
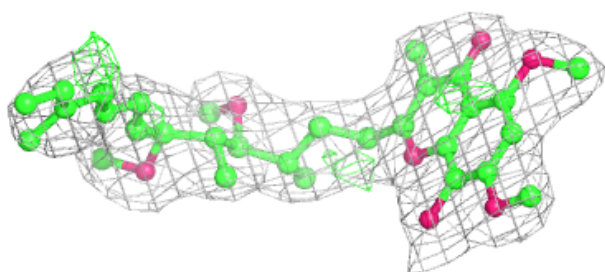
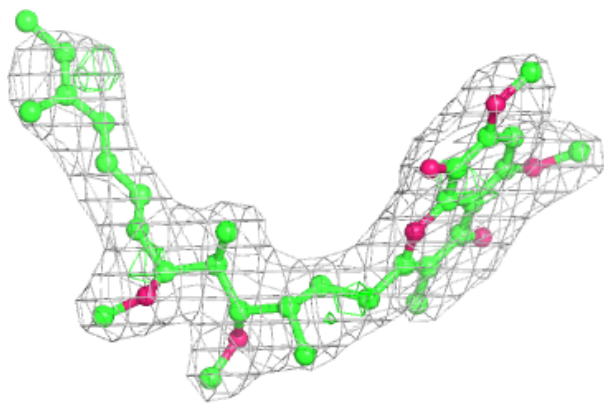
**Electron density around BGL E 1042:**

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

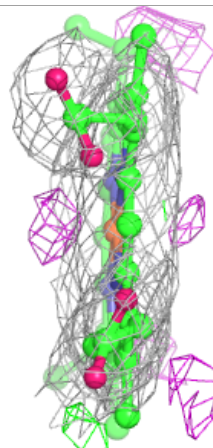
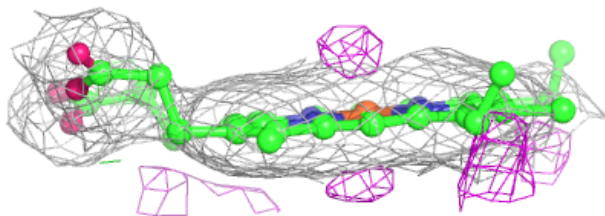
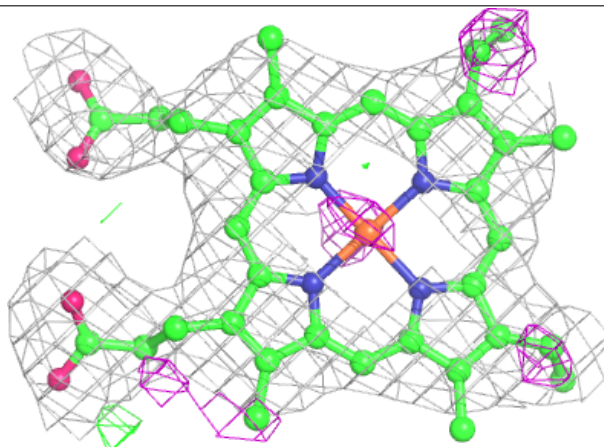


Electron density around SMA D 1002:

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

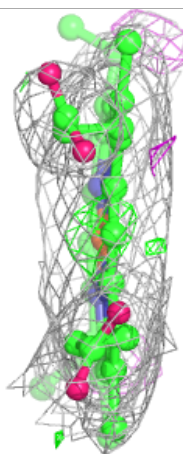
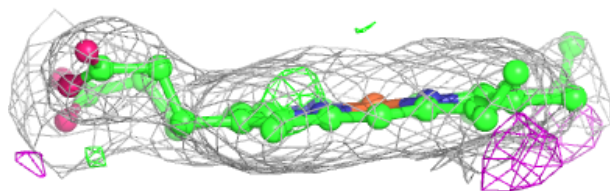
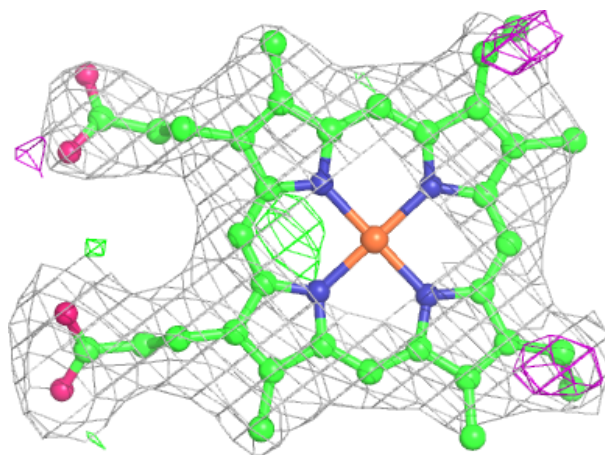
**Electron density around HEM N 301:**

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



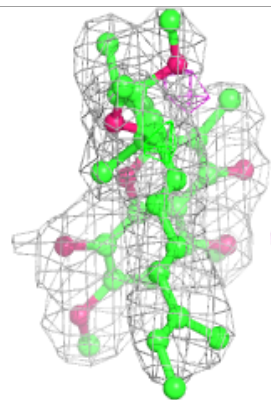
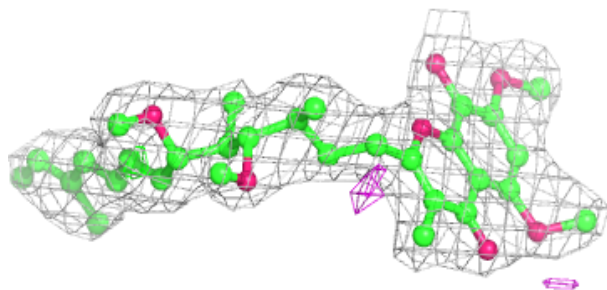
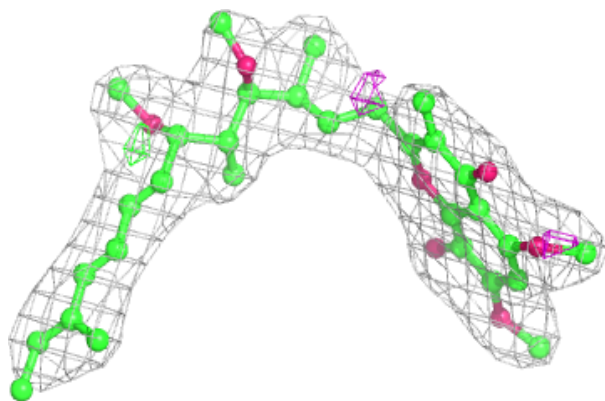
Electron density around HEM B 301:

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



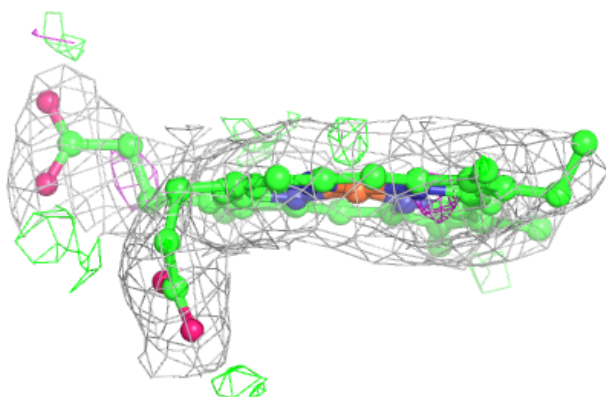
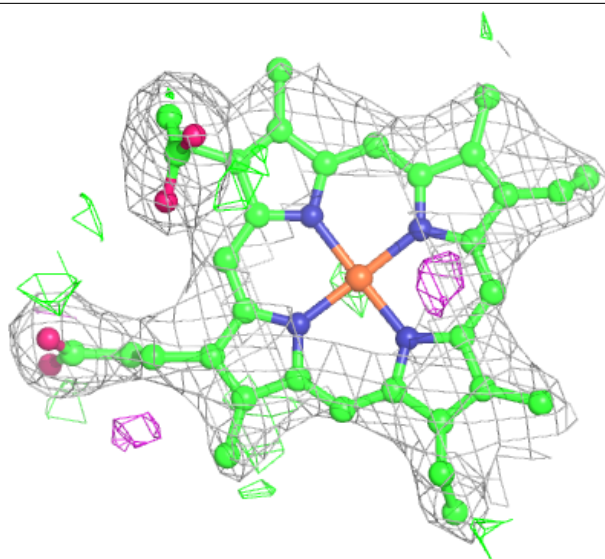
Electron density around SMA A 1001:

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



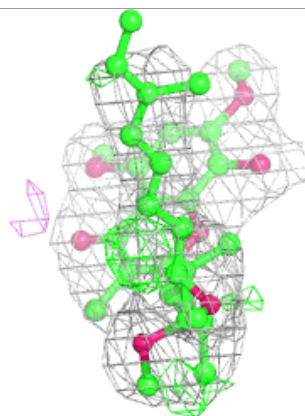
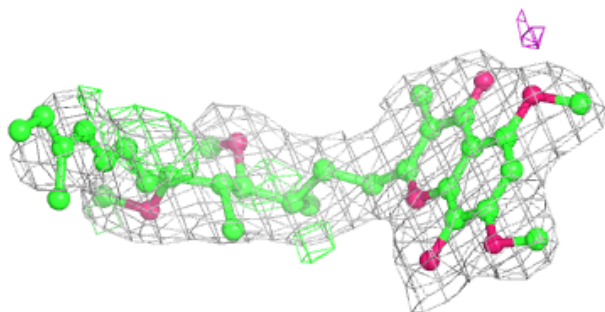
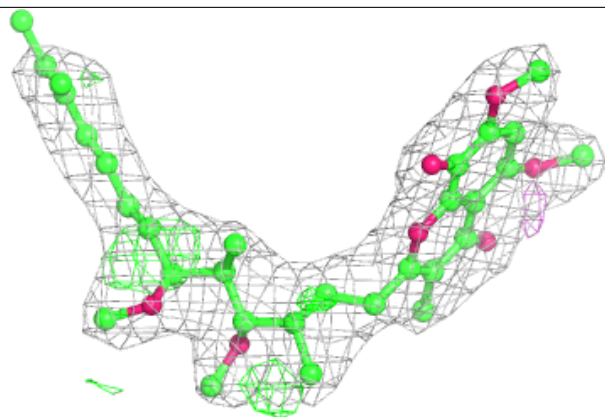
Electron density around HEM J 501:

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

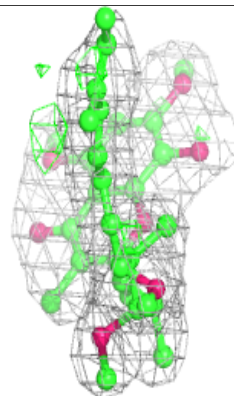
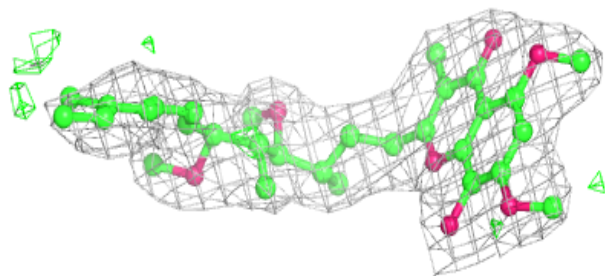
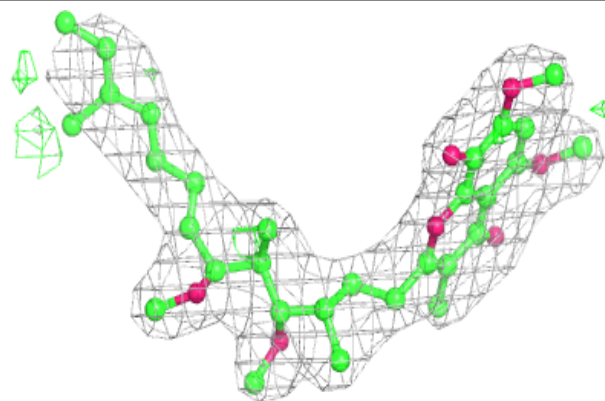


Electron density around SMA J 1004:

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

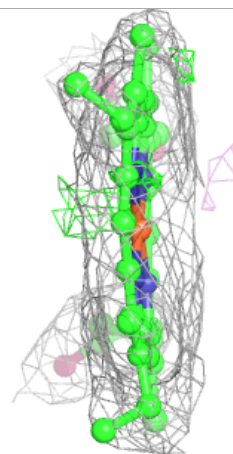
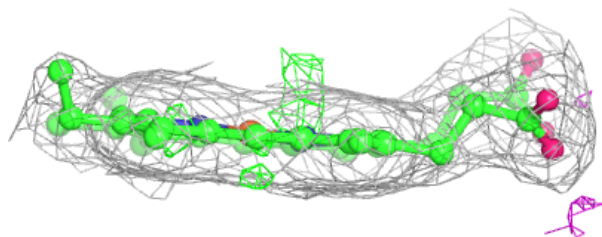
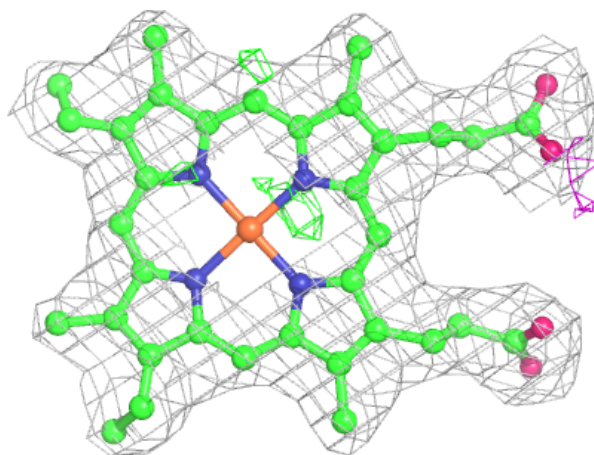
**Electron density around SMA P 1006:**

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



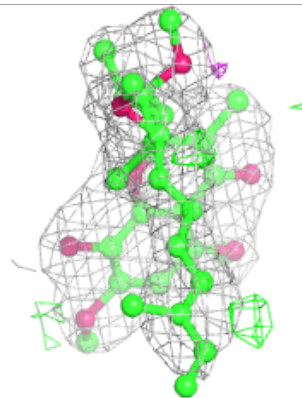
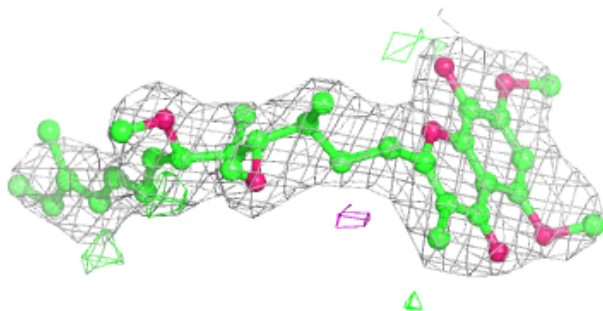
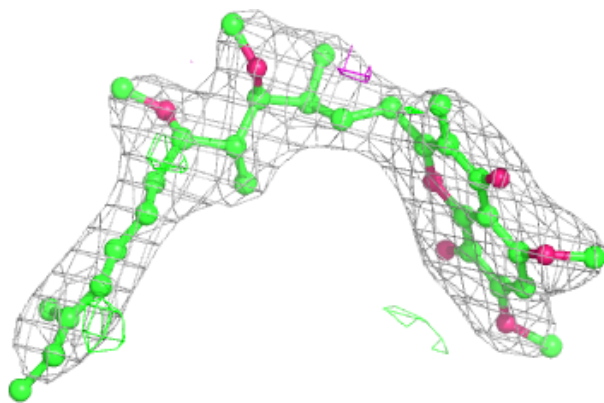
Electron density around HEM H 301:

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



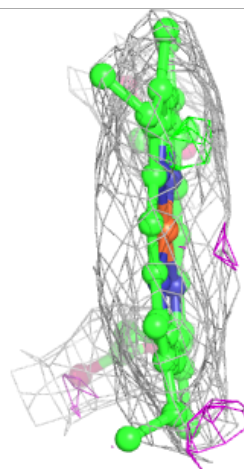
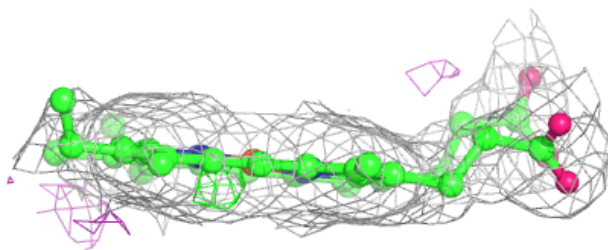
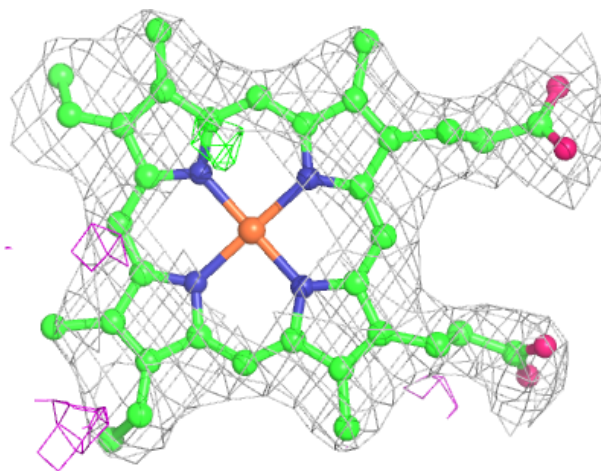
Electron density around SMA M 1005:

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



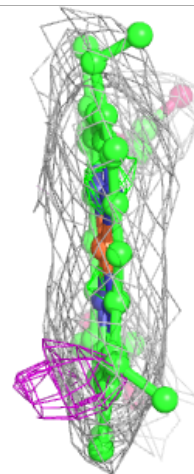
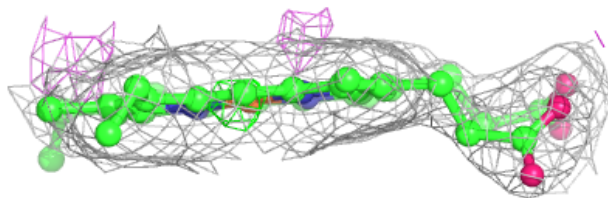
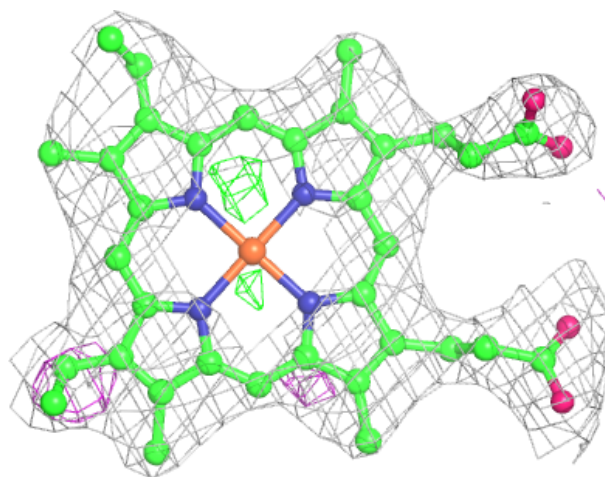
Electron density around HEM Q 301:

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



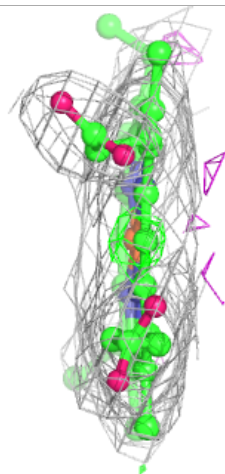
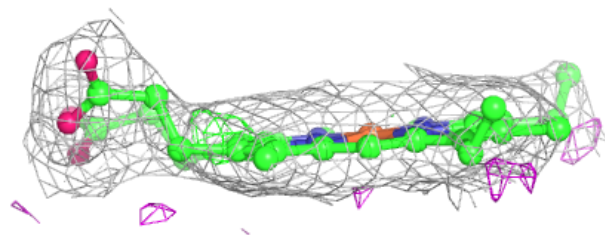
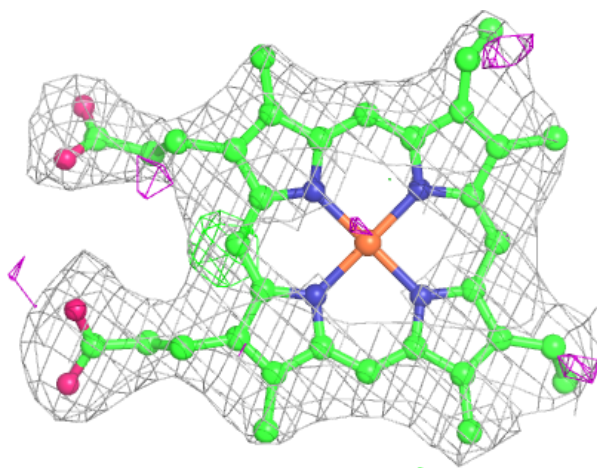
Electron density around HEM E 301:

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



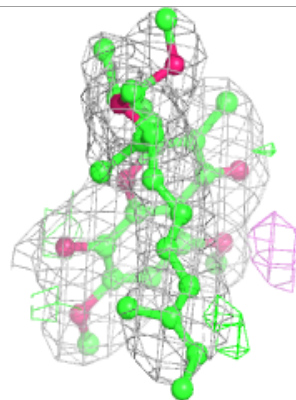
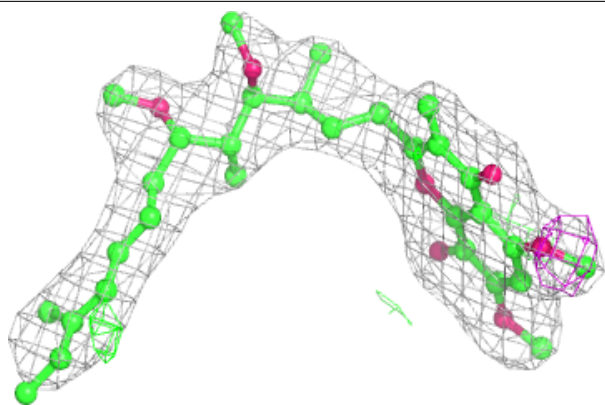
Electron density around HEM K 301:

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



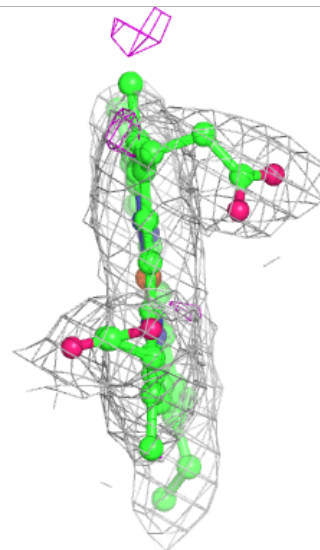
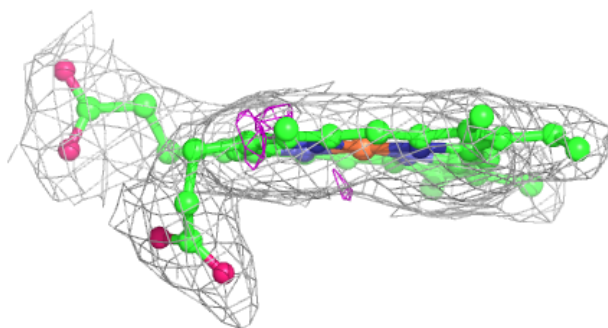
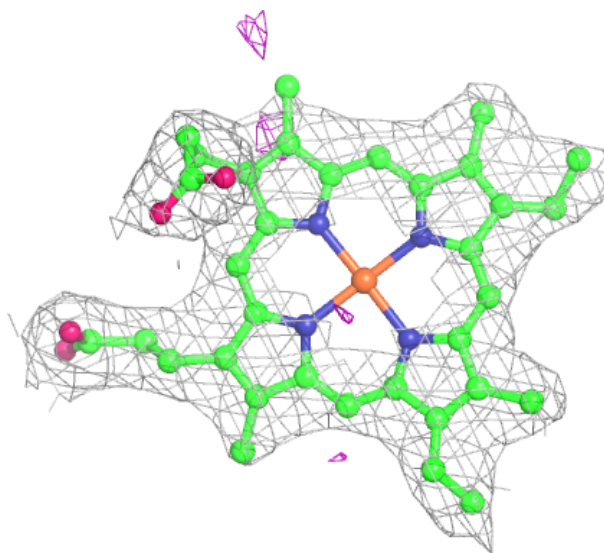
Electron density around SMA G 1003:

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



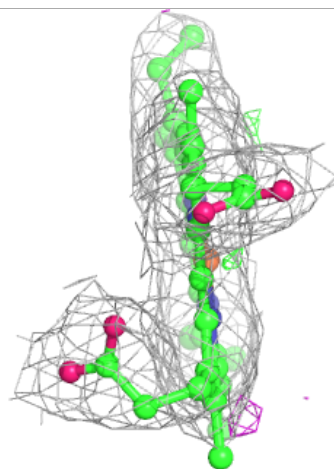
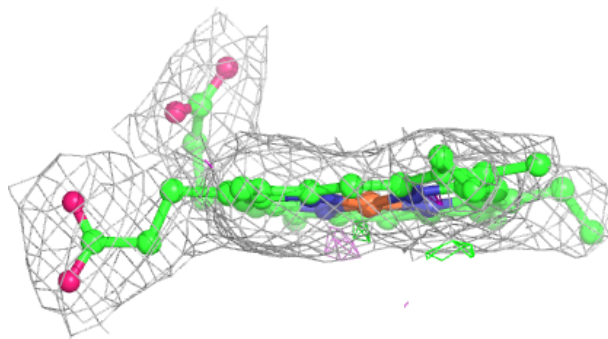
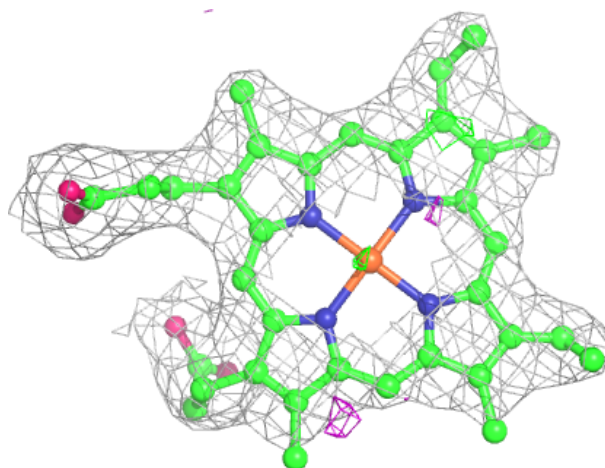
Electron density around HEM D 501:

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



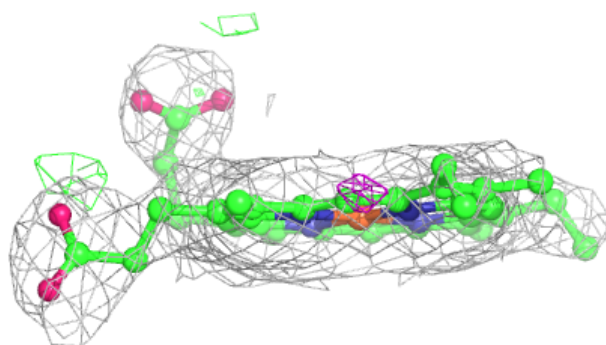
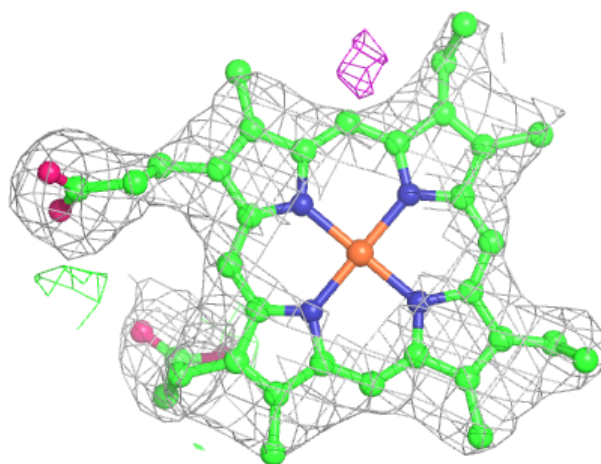
Electron density around HEM G 501:

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



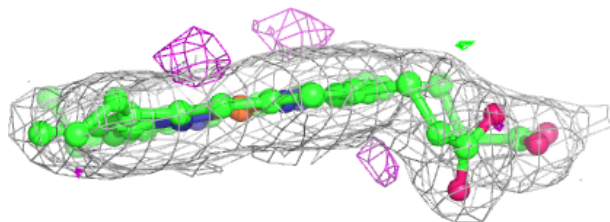
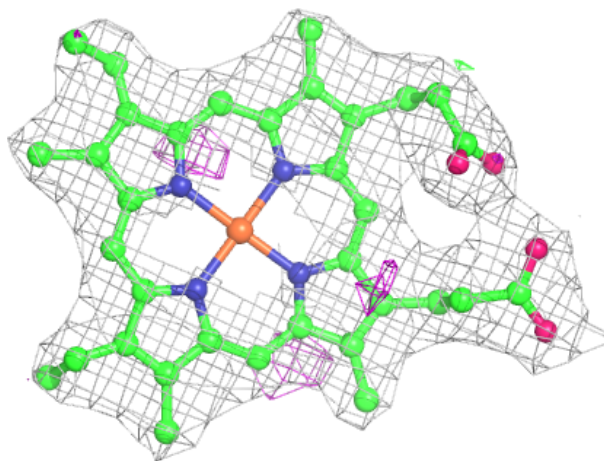
Electron density around HEM M 501:

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



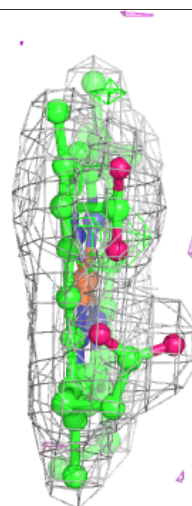
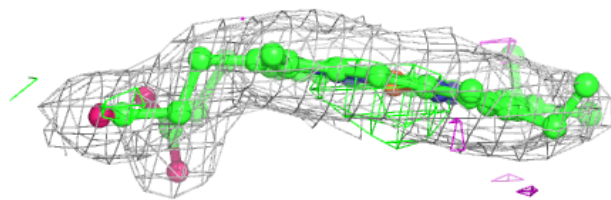
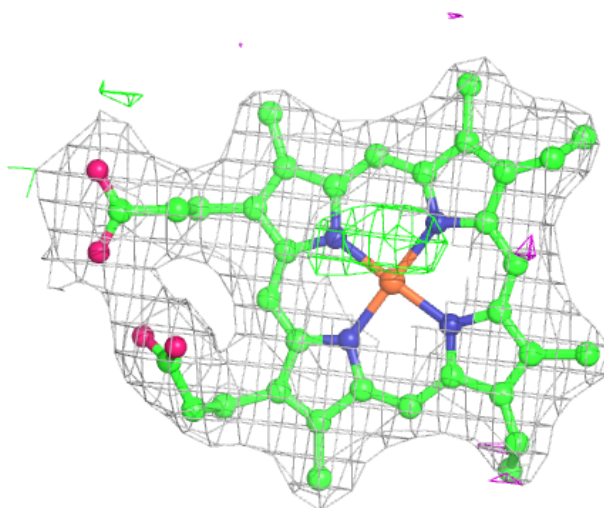
Electron density around HEM D 502:

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



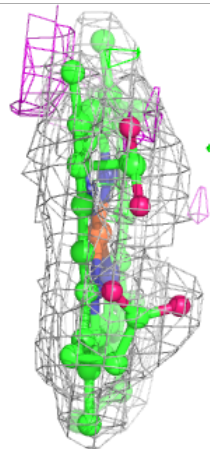
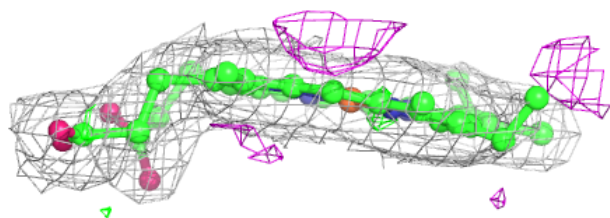
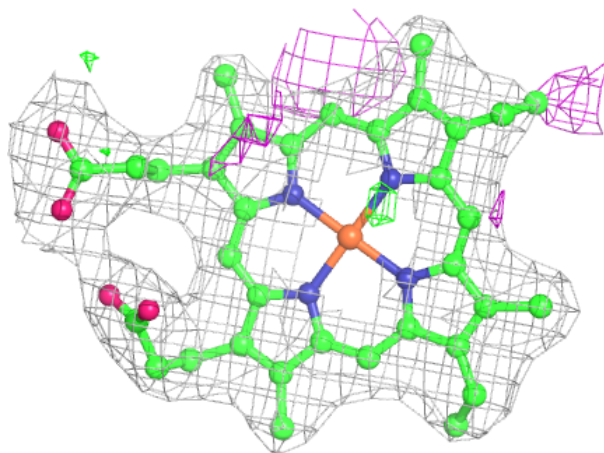
Electron density around HEM G 502:

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



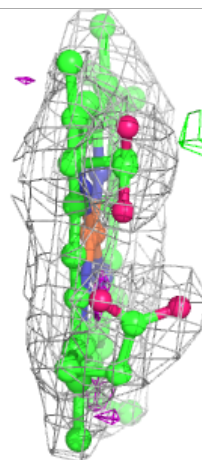
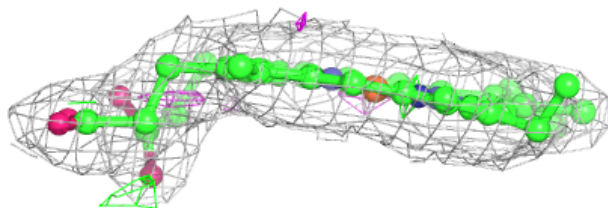
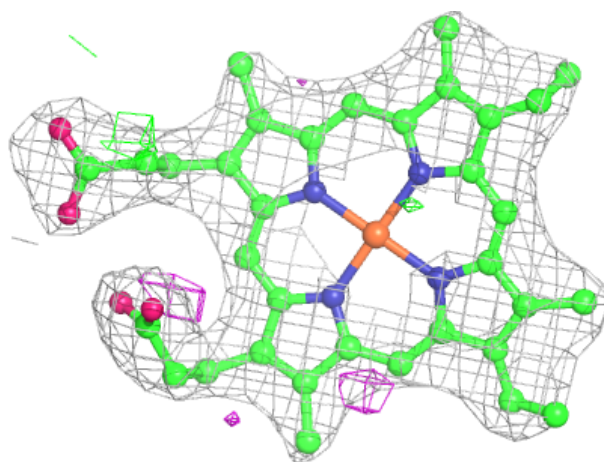
Electron density around HEM A 502:

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



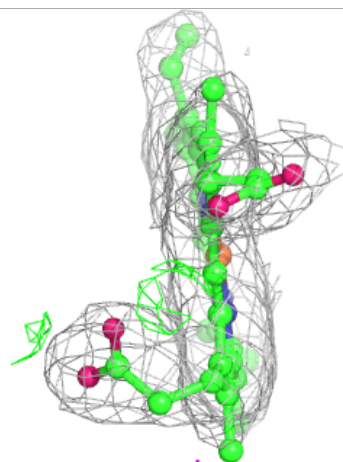
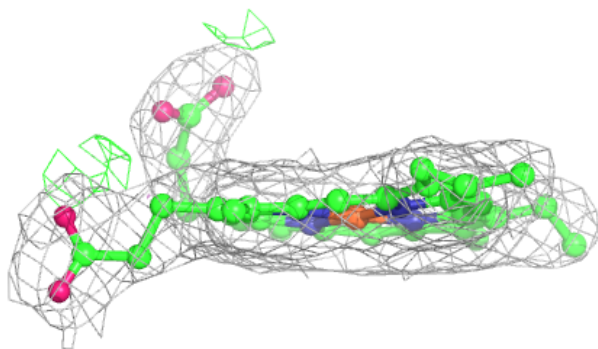
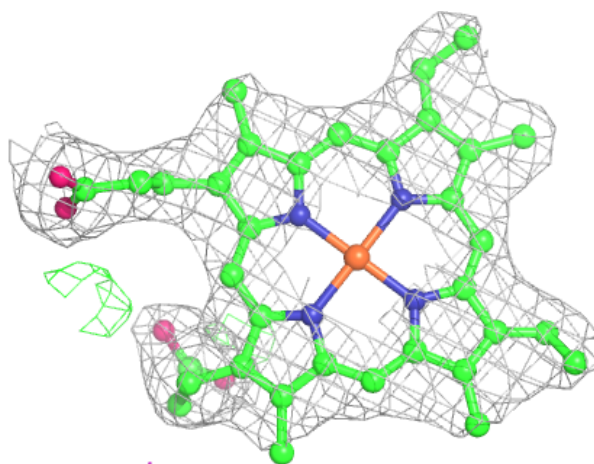
Electron density around HEM M 502:

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



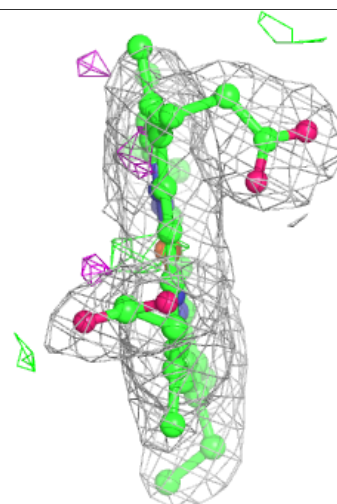
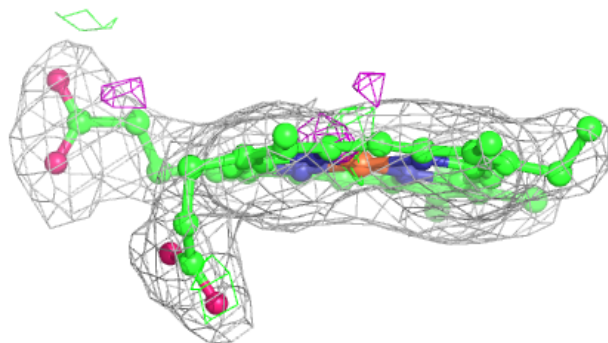
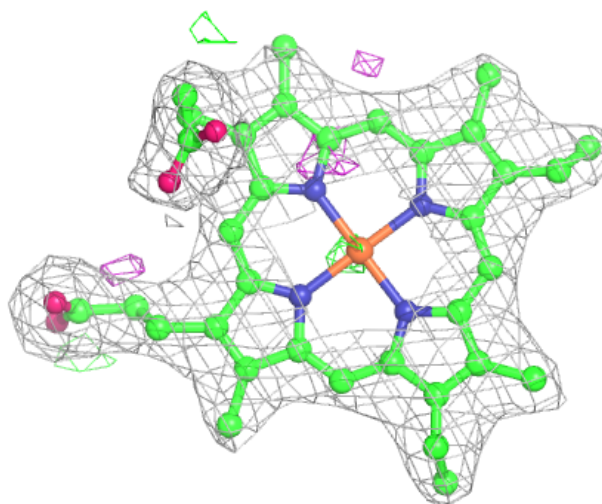
Electron density around HEM A 501:

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



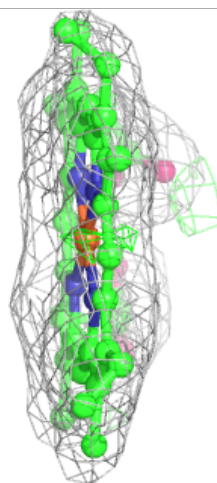
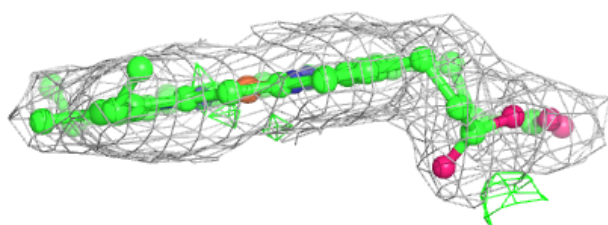
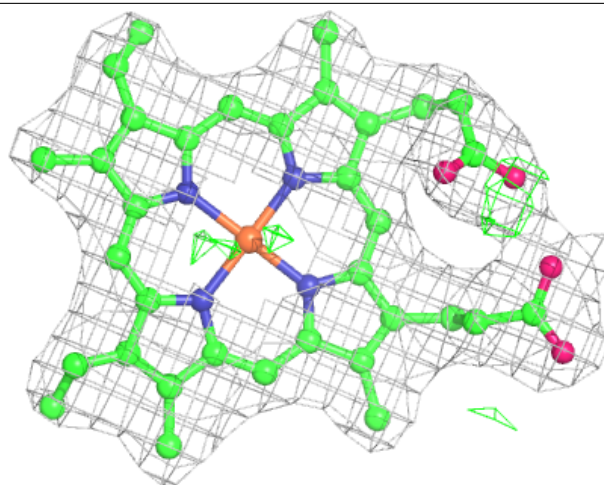
Electron density around HEM P 501:

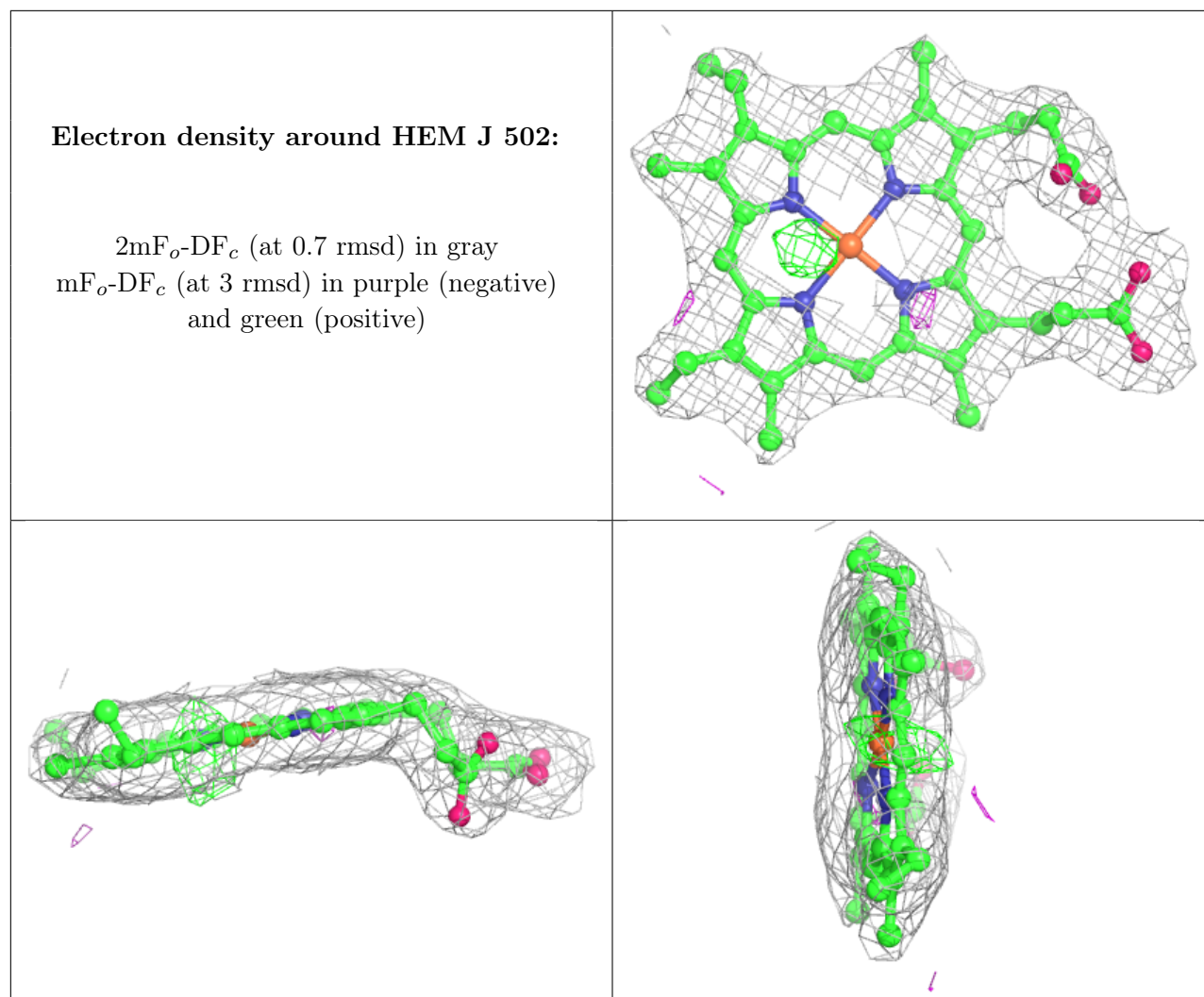
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.