



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:04 AM UTC

PDB ID : 3MK7 / pdb_00003mk7
Title : The structure of CBB3 cytochrome oxidase
Authors : Buschmann, S.; Warkentin, E.; Michel, H.; Ermler, U.
Deposited on : 2010-04-14
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

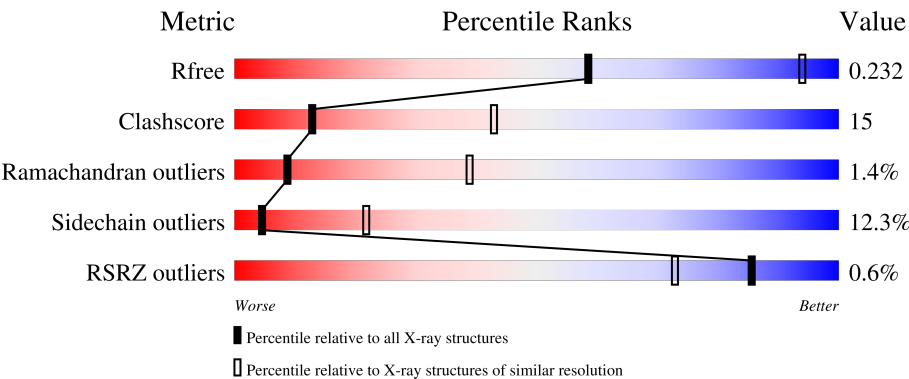
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	474	62%31%5%.
1	D	474	63%31%..
1	G	474	61%32%5%.
1	K	474	%65%29%..
2	B	203	63%30%...

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Mol	Chain	Length	Quality of chain
2	E	203	
2	H	203	
2	L	203	
3	C	311	
3	F	311	
3	I	311	
3	M	311	
4	U	30	
4	X	30	
4	Y	30	
4	Z	30	

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
11	FC6	C	323	-	-	X	-
11	FC6	F	323	-	-	X	-
11	FC6	I	323	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 31690 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 c oxidase, cbb3-type, subunit N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	0	0	0
			3683	2461	593	607	22			
1	D	463	Total	C	N	O	S	0	0	0
			3663	2450	590	601	22			
1	G	465	Total	C	N	O	S	0	0	0
			3676	2457	592	605	22			
1	K	465	Total	C	N	O	S	0	0	0
			3676	2457	592	605	22			

- Molecule 2 is a protein called Cytochrome c oxidase, cbb3-type, subunit O.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	197	Total	C	N	O	S	0	0	0
			1548	981	268	289	10			
2	E	197	Total	C	N	O	S	0	0	0
			1548	981	268	289	10			
2	H	197	Total	C	N	O	S	0	0	0
			1548	981	268	289	10			
2	L	197	Total	C	N	O	S	0	0	0
			1548	981	268	289	10			

- Molecule 3 is a protein called Cytochrome c oxidase, cbb3-type, subunit P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	303	Total	C	N	O	S	0	0	0
			2312	1483	391	427	11			
3	F	303	Total	C	N	O	S	0	0	0
			2312	1483	391	427	11			
3	I	303	Total	C	N	O	S	0	0	0
			2312	1483	391	427	11			
3	M	303	Total	C	N	O	S	0	0	0
			2312	1483	391	427	11			

- | Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|---------|---------|---------|---------|---------|-------|
| 4 | U | 30 | Total
150 | C
90 | N
30 | O
30 | 0 | 0 | 0 |
| 4 | X | 30 | Total
150 | C
90 | N
30 | O
30 | 0 | 0 | 0 |
| 4 | Y | 30 | Total
150 | C
90 | N
30 | O
30 | 0 | 0 | 0 |
| 4 | Z | 30 | Total
150 | C
90 | N
30 | O
30 | 0 | 0 | 0 |

- # HEM

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	K	1	Total	C	Fe	N	O	
			43	34	1	4	4	
5	K	1	Total	C	Fe	N	O	
			43	34	1	4	4	

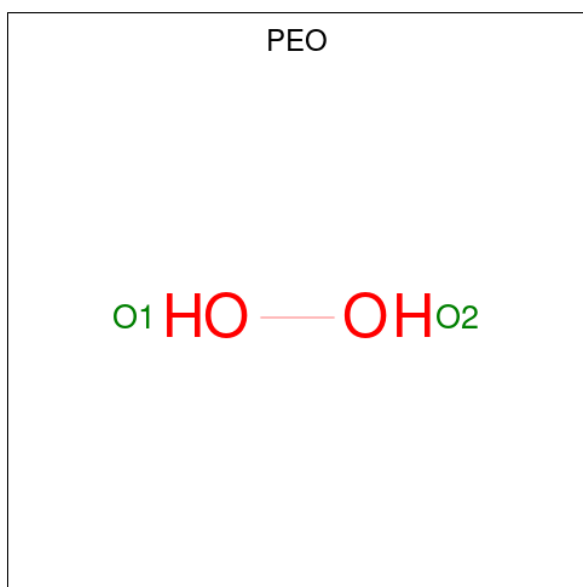
- Molecule 6 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cu		
			1	1	0	0
6	D	1	Total	Cu		
			1	1	0	0
6	G	1	Total	Cu		
			1	1	0	0
6	K	1	Total	Cu		
			1	1	0	0

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

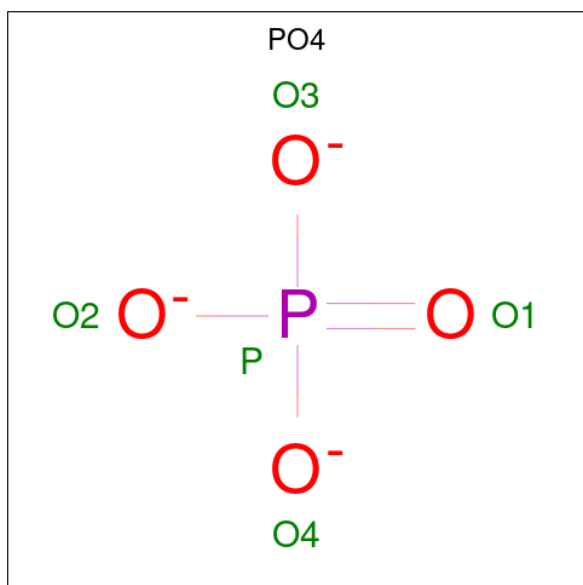
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca		
			1	1	0	0
7	B	1	Total	Ca		
			1	1	0	0
7	D	1	Total	Ca		
			1	1	0	0
7	E	1	Total	Ca		
			1	1	0	0
7	G	2	Total	Ca		
			2	2	0	0
7	K	2	Total	Ca		
			2	2	0	0

- Molecule 8 is HYDROGEN PEROXIDE (CCD ID: PEO) (formula: H₂O₂).



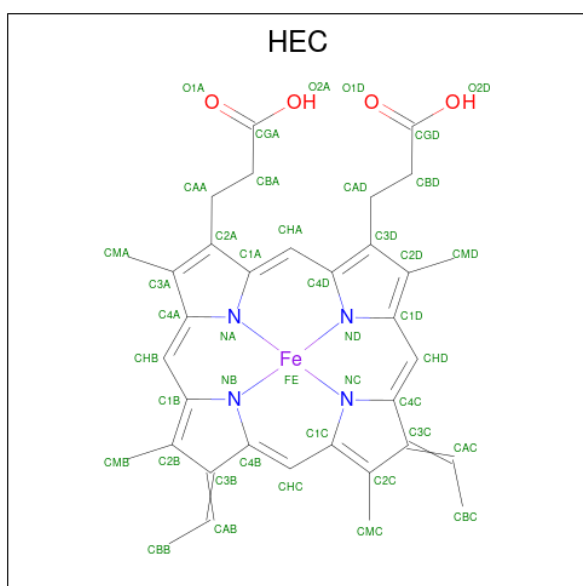
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O 2 2	0	0
8	D	1	Total O 2 2	0	0
8	G	1	Total O 2 2	0	0
8	K	1	Total O 2 2	0	0

- Molecule 9 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total 5	O 4	P 1	0	0
9	D	1	Total 5	O 4	P 1	0	0
9	G	1	Total 5	O 4	P 1	0	0
9	K	1	Total 5	O 4	P 1	0	0

- Molecule 10 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



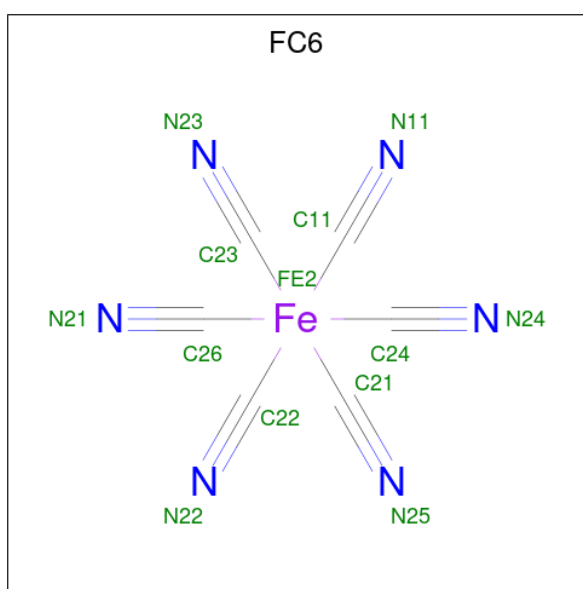
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	I	1	Total	C	Fe	N	O	
			43	34	1	4	4	
10	L	1	Total	C	Fe	N	O	
			43	34	1	4	4	
10	M	1	Total	C	Fe	N	O	
			43	34	1	4	4	
10	M	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 11 is HEXACYANOFERRATE(3-) (CCD ID: FC6) (formula: C_6FeN_6).

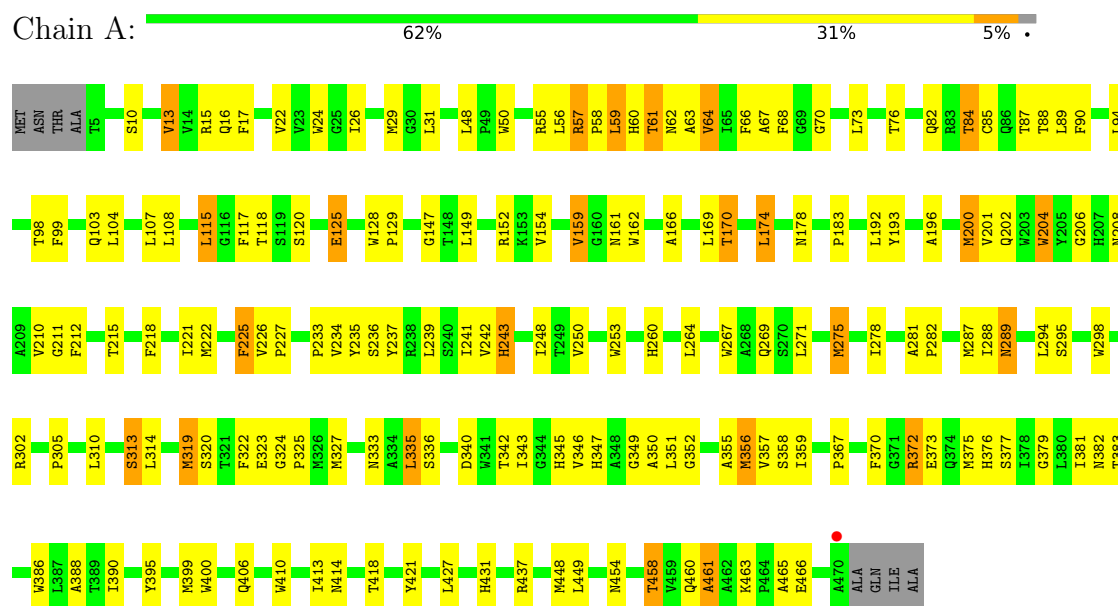


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	Fe	N		
			13	6	1	6	0	0
11	F	1	Total	C	Fe	N		
			13	6	1	6	0	0
11	I	1	Total	C	Fe	N		
			13	6	1	6	0	0
11	M	1	Total	C	Fe	N		
			13	6	1	6	0	0

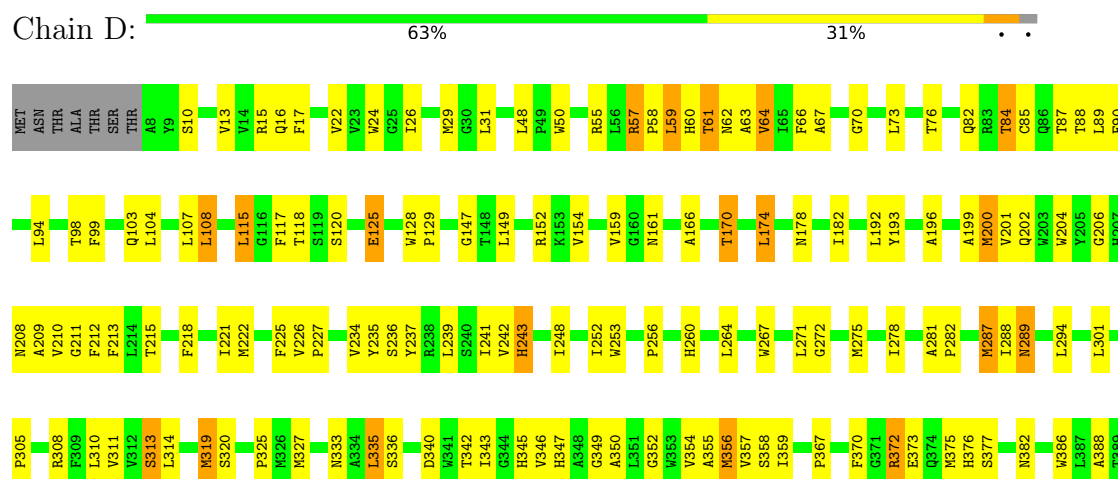
3 Residue-property plots

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 c oxidase, cbb3-type, subunit N



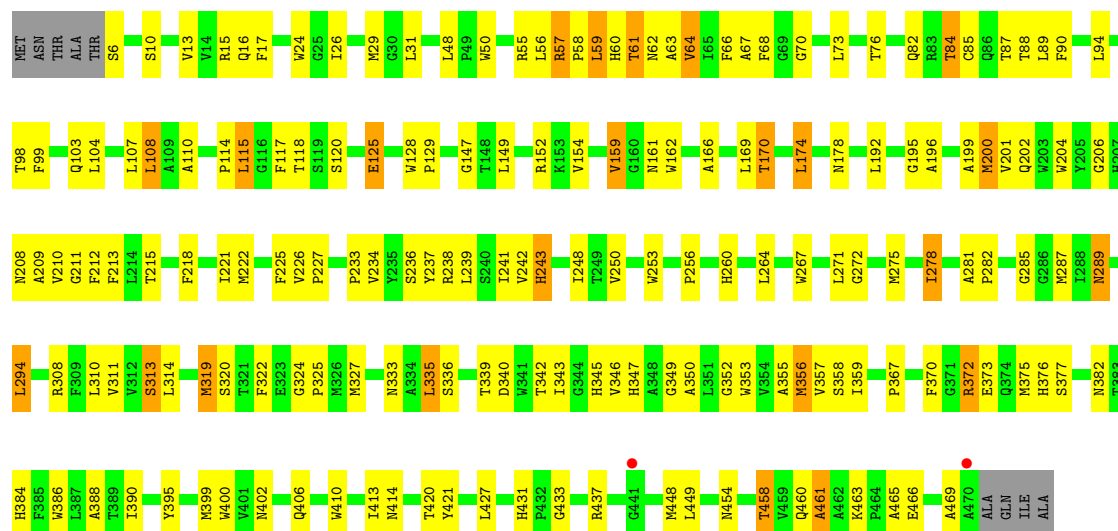
- Molecule 1: Cytochrome c oxidase, cbb3-type, subunit N





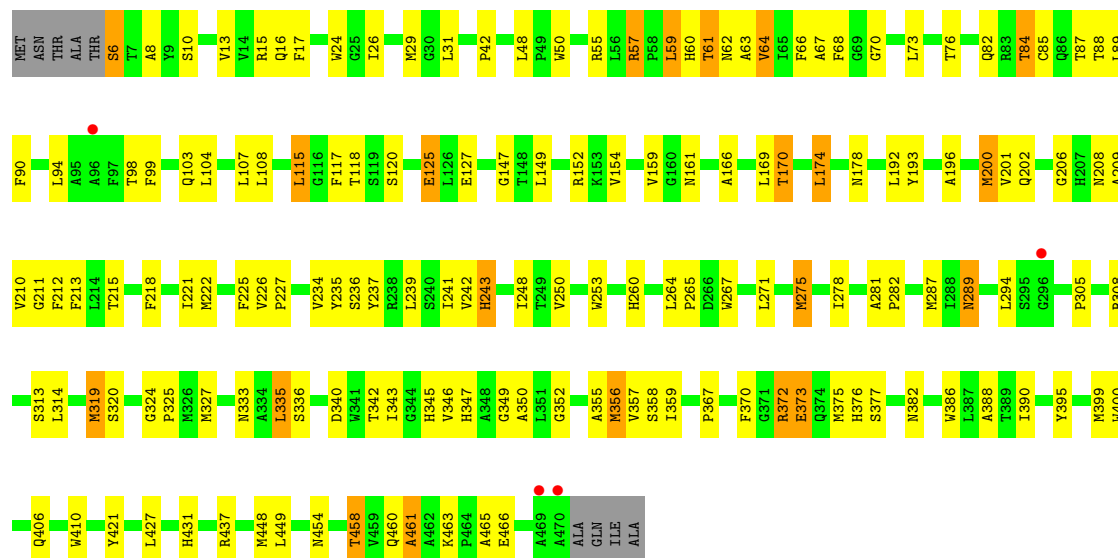
- Molecule 1: Cytochrome c oxidase, cbb3-type, subunit N

Chain G: 61% 32% 5%



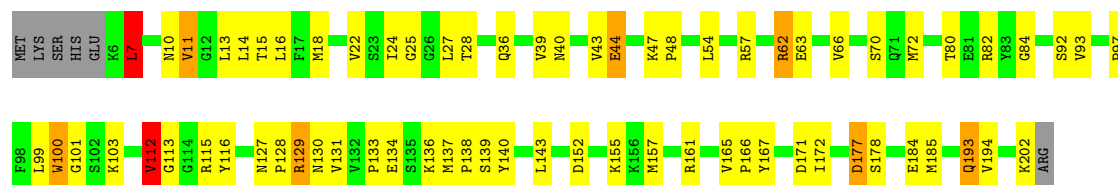
- Molecule 1: Cytochrome c oxidase, cbb3-type, subunit N

Chain K: 65% 29% 6%



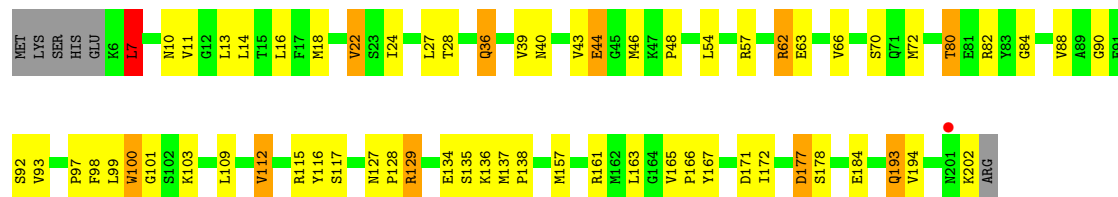
- Molecule 2: Cytochrome c oxidase, cbb3-type, subunit O

Chain B: 63% 30% 7%



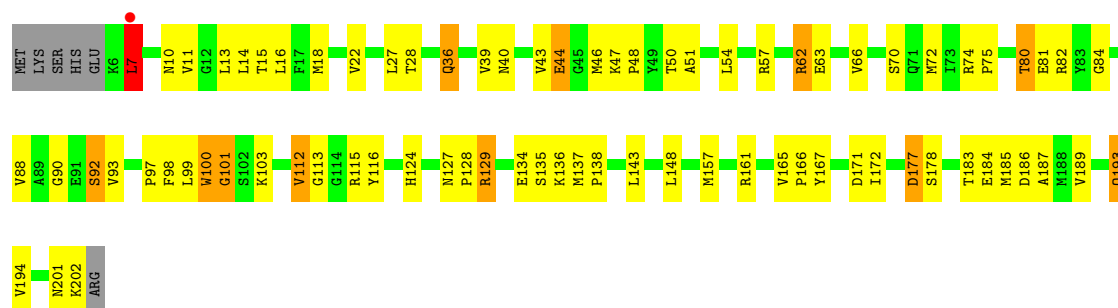
- Molecule 2: Cytochrome c oxidase, cbb3-type, subunit O

Chain E: 65% 27% 5%



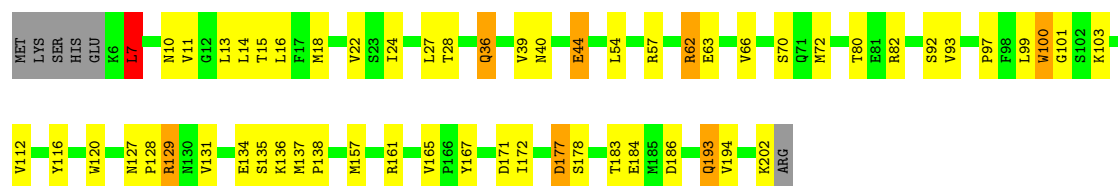
- Molecule 2: Cytochrome c oxidase, cbb3-type, subunit O

Chain H: 59% 33% 5%



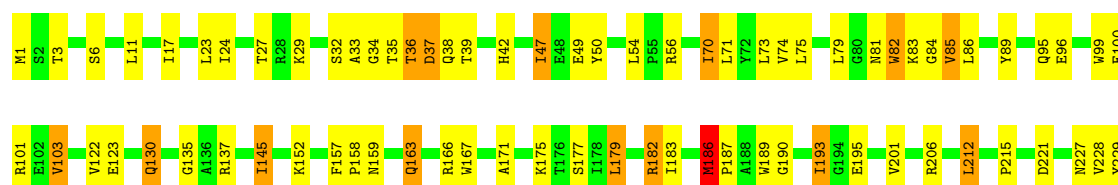
- Molecule 2: Cytochrome c oxidase, cbb3-type, subunit O

Chain L: 68% 25%



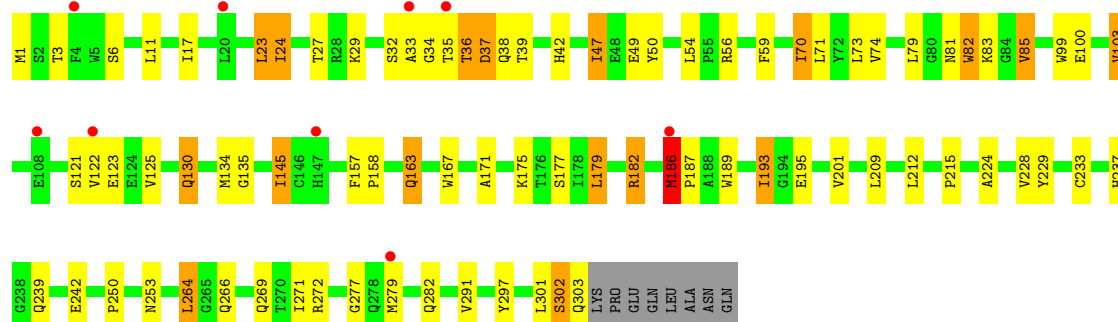
- Molecule 3: Cytochrome c oxidase, cbb3-type, subunit P

Chain C: 66% 25% 5%

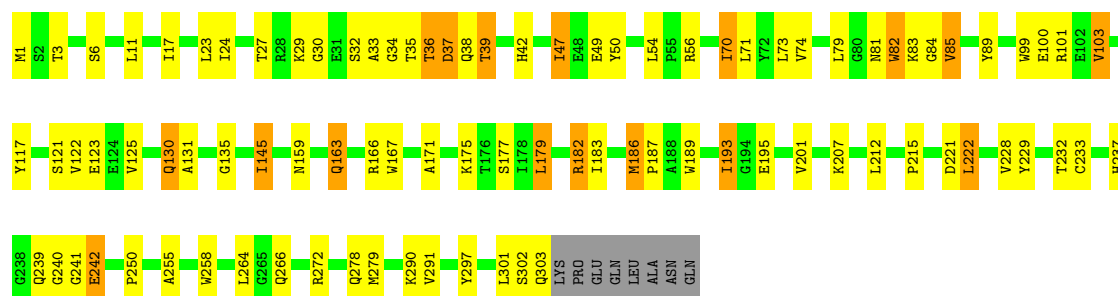




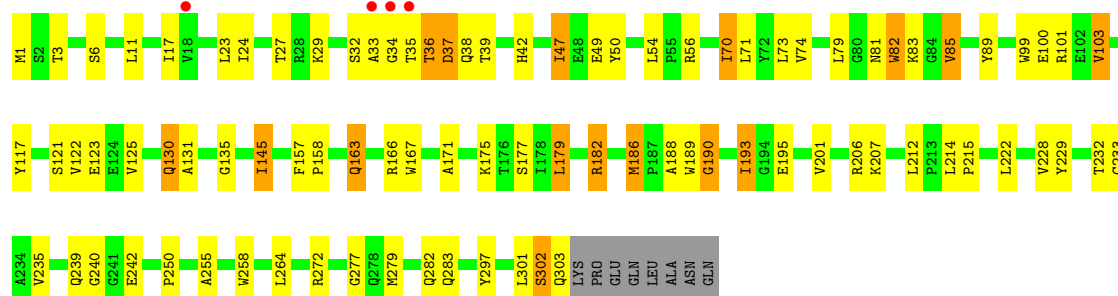
- Molecule 3: Cytochrome c oxidase, cbb3-type, subunit P



- Molecule 3: Cytochrome c oxidase, cbb3-type, subunit P

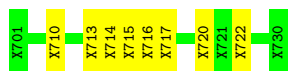


- Molecule 3: Cytochrome c oxidase, cbb3-type, subunit P



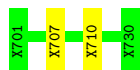
- Molecule 4: 30-mer peptide





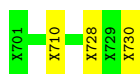
- Molecule 4: 30-mer peptide

Chain X: 93% 7%



- Molecule 4: 30-mer peptide

Chain Y: 90% 10%



- Molecule 4: 30-mer peptide

Chain Z: 80% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	136.47Å 279.93Å 175.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.20 15.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (15.00-3.20) 97.4 (15.00-3.20)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0046	Depositor
R, R_{free}	0.189 , 0.223 0.198 , 0.232	Depositor DCC
R_{free} test set	6720 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	87.0	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 73.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	31690	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, PEO, FC6, CA, HEC, CU, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.72	0/3811	0.93	4/5210 (0.1%)
1	D	0.49	0/3791	0.87	0/5182
1	G	0.64	1/3804 (0.0%)	0.91	2/5200 (0.0%)
1	K	0.57	2/3804 (0.1%)	0.88	1/5200 (0.0%)
2	B	0.83	0/1584	1.03	5/2146 (0.2%)
2	E	0.58	0/1584	0.93	1/2146 (0.0%)
2	H	0.77	1/1584 (0.1%)	1.03	3/2146 (0.1%)
2	L	0.65	0/1584	0.96	1/2146 (0.0%)
3	C	0.79	0/2374	1.03	7/3225 (0.2%)
3	F	0.55	0/2374	0.93	2/3225 (0.1%)
3	I	0.71	0/2374	0.98	1/3225 (0.0%)
3	M	0.81	1/2374 (0.0%)	1.04	0/3225
All	All	0.67	5/31042 (0.0%)	0.95	27/42276 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	101	GLY	C-O	6.58	1.29	1.23
1	K	6	SER	CB-OG	-6.16	1.29	1.42
3	M	188	ALA	CA-CB	-5.80	1.45	1.53
1	K	6	SER	CA-CB	5.64	1.64	1.53
1	G	469	ALA	CA-C	5.06	1.54	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	100	TRP	CA-C-N	-8.84	113.52	122.27
2	H	100	TRP	C-N-CA	-8.84	113.52	122.27
2	H	100	TRP	N-CA-C	-8.10	99.33	110.35
2	B	100	TRP	CA-C-N	-6.71	112.70	121.96
2	B	100	TRP	C-N-CA	-6.71	112.70	121.96
1	A	322	PHE	N-CA-C	-6.62	104.13	112.93
2	B	100	TRP	N-CA-C	-6.55	101.44	110.35
1	A	204	TRP	N-CA-C	-6.28	104.35	111.07
3	C	276	ASN	N-CA-C	6.13	117.94	109.54
3	C	84	GLY	N-CA-C	6.01	118.94	112.33
2	E	100	TRP	N-CA-C	-5.97	102.23	110.35
3	I	84	GLY	N-CA-C	5.75	118.65	112.33
2	L	100	TRP	N-CA-C	-5.70	102.60	110.35
1	G	322	PHE	N-CA-C	-5.65	105.49	112.72
1	G	204	TRP	N-CA-C	-5.48	105.22	111.14
3	C	212	LEU	CA-C-N	-5.42	115.00	120.31
3	C	212	LEU	C-N-CA	-5.42	115.00	120.31
3	C	186	MET	CB-CA-C	-5.28	104.01	110.08
1	K	127	GLU	N-CA-C	5.21	116.82	110.41
2	B	131	VAL	CB-CA-C	-5.12	106.56	111.06
1	A	225	PHE	N-CA-C	5.10	116.92	111.36
3	F	186	MET	CA-C-N	-5.08	115.34	120.21
3	F	186	MET	C-N-CA	-5.08	115.34	120.21
2	B	130	ASN	N-CA-C	5.06	117.53	111.71
1	A	381	ILE	N-CA-C	-5.05	105.50	111.00
3	C	279	MET	CA-C-N	5.04	124.95	119.76
3	C	279	MET	C-N-CA	5.04	124.95	119.76

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	112	VAL	Peptide

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	3683	0	3663	132	0
1	D	3663	0	3644	131	0
1	G	3676	0	3656	133	0
1	K	3676	0	3656	122	0
2	B	1548	0	1526	53	0
2	E	1548	0	1526	52	0
2	H	1548	0	1526	59	0
2	L	1548	0	1526	42	0
3	C	2312	0	2237	68	1
3	F	2312	0	2237	67	0
3	I	2312	0	2237	69	1
3	M	2312	0	2237	64	0
4	U	150	0	33	6	0
4	X	150	0	33	2	0
4	Y	150	0	33	4	0
4	Z	150	0	35	4	0
5	A	86	0	60	11	0
5	D	86	0	60	12	0
5	G	86	0	60	13	0
5	K	86	0	60	12	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
6	G	1	0	0	0	0
6	K	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
7	G	2	0	0	0	0
7	K	2	0	0	0	0
8	A	2	0	0	0	0
8	D	2	0	0	0	0
8	G	2	0	0	0	0
8	K	2	0	0	0	0
9	A	5	0	0	0	0
9	D	5	0	0	0	0
9	G	5	0	0	0	0
9	K	5	0	0	0	0
10	B	43	0	30	3	0
10	C	86	0	60	8	0
10	E	43	0	30	2	0
10	F	86	0	60	15	0
10	H	43	0	30	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	I	86	0	60	5	0
10	L	43	0	30	2	0
10	M	86	0	60	8	0
11	C	13	0	0	4	0
11	F	13	0	0	10	0
11	I	13	0	0	6	0
11	M	13	0	0	3	0
All	All	31690	0	30405	939	1

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 15.

All (939) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ILE:HD11	1:A:448:MET:HE1	1.32	1.10
11:F:323:FC6:N24	3:I:215:PRO:HB3	1.66	1.10
1:K:359:ILE:HD11	1:K:448:MET:HE1	1.33	1.10
1:D:359:ILE:HD11	1:D:448:MET:HE1	1.28	1.10
1:G:359:ILE:HD11	1:G:448:MET:HE1	1.36	1.02
1:G:166:ALA:O	1:G:170:THR:HG22	1.58	1.02
11:C:323:FC6:N24	3:M:215:PRO:HB3	1.73	1.02
3:F:193:ILE:HD11	3:F:228:VAL:HG11	1.40	1.01
3:C:186:MET:HG2	10:C:321:HEC:ND	1.76	1.00
2:B:193:GLN:HA	2:B:193:GLN:HE21	1.25	0.99
1:D:359:ILE:HD11	1:D:448:MET:CE	1.91	0.99
3:C:186:MET:HG2	10:C:321:HEC:C4D	1.92	0.99
1:A:166:ALA:O	1:A:170:THR:HG22	1.62	0.98
1:D:166:ALA:O	1:D:170:THR:HG22	1.63	0.98
2:H:193:GLN:HE21	2:H:193:GLN:HA	1.30	0.97
1:K:166:ALA:O	1:K:170:THR:HG22	1.65	0.97
1:A:281:ALA:HB3	1:A:282:PRO:HD3	1.46	0.97
3:M:186:MET:HG2	10:M:321:HEC:ND	1.78	0.96
1:A:359:ILE:HD11	1:A:448:MET:CE	1.94	0.96
1:A:76:THR:HG21	1:A:221:ILE:HG12	1.48	0.96
5:A:502:HEM:HHC	5:A:502:HEM:HBB2	1.47	0.95
1:G:281:ALA:HB3	1:G:282:PRO:HD3	1.48	0.95
1:G:359:ILE:HD11	1:G:448:MET:CE	1.96	0.95
3:F:186:MET:HG2	10:F:321:HEC:C4D	1.97	0.95
5:D:502:HEM:HHC	5:D:502:HEM:HBB2	1.48	0.94
3:F:186:MET:HG2	10:F:321:HEC:ND	1.82	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:THR:HG21	1:D:221:ILE:HG12	1.50	0.93
3:M:186:MET:HG2	10:M:321:HEC:C4D	1.98	0.92
1:K:29:MET:HE1	1:K:448:MET:HE3	1.53	0.91
1:K:359:ILE:HD11	1:K:448:MET:CE	1.99	0.91
1:G:24:TRP:HE1	1:G:103:GLN:HE22	1.20	0.90
1:K:76:THR:HG21	1:K:221:ILE:HG12	1.54	0.90
3:I:193:ILE:HD11	3:I:228:VAL:HG11	1.51	0.89
1:D:24:TRP:HE1	1:D:103:GLN:HE22	1.16	0.89
1:A:335:LEU:HD22	4:U:710:UNK:CB	2.02	0.89
3:F:167:TRP:CE2	3:F:182:ARG:HG2	2.08	0.89
1:A:24:TRP:HE1	1:A:103:GLN:HE22	1.21	0.88
2:E:193:GLN:HE21	2:E:193:GLN:HA	1.35	0.88
3:I:167:TRP:CE2	3:I:182:ARG:HG2	2.08	0.88
2:L:193:GLN:HA	2:L:193:GLN:HE21	1.38	0.88
3:M:193:ILE:HD11	3:M:228:VAL:HG11	1.52	0.88
3:C:167:TRP:CE2	3:C:182:ARG:HG2	2.10	0.87
1:A:29:MET:HE1	1:A:448:MET:HE3	1.54	0.87
3:M:167:TRP:CE2	3:M:182:ARG:HG2	2.10	0.86
5:G:502:HEM:HBB2	5:G:502:HEM:HHC	1.55	0.86
3:I:186:MET:HG2	10:I:321:HEC:C4D	1.94	0.85
1:K:24:TRP:HE1	1:K:103:GLN:HE22	1.22	0.84
1:G:29:MET:HE1	1:G:448:MET:HE3	1.58	0.84
3:C:193:ILE:HD11	3:C:228:VAL:HG11	1.60	0.84
1:K:281:ALA:HB3	1:K:282:PRO:HD3	1.60	0.84
1:D:29:MET:HE1	1:D:448:MET:HE3	1.58	0.83
1:D:281:ALA:HB3	1:D:282:PRO:HD3	1.60	0.83
3:C:215:PRO:HB3	11:M:323:FC6:N24	1.94	0.83
1:G:76:THR:HG21	1:G:221:ILE:HG12	1.59	0.82
5:K:502:HEM:HHC	5:K:502:HEM:HBB2	1.61	0.82
2:E:116:TYR:HE2	3:F:145:ILE:HG21	1.45	0.82
1:K:335:LEU:HD22	4:Z:710:UNK:CB	2.10	0.82
1:A:10:SER:H	1:A:82:GLN:HE22	1.28	0.81
1:G:10:SER:H	1:G:82:GLN:HE22	1.27	0.80
1:D:10:SER:H	1:D:82:GLN:HE22	1.29	0.80
1:G:170:THR:HG21	1:G:212:PHE:CD2	2.16	0.80
5:K:502:HEM:HBC2	5:K:502:HEM:HHD	1.65	0.78
1:G:335:LEU:HD22	4:Y:710:UNK:CB	2.14	0.78
1:D:85:CYS:HB2	1:D:152:ARG:HB2	1.65	0.77
1:K:85:CYS:HB2	1:K:152:ARG:HB2	1.66	0.77
1:A:63:ALA:O	1:A:67:ALA:HB3	1.84	0.77
3:I:207:LYS:HD3	3:I:222:LEU:HD21	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:85:CYS:HB2	1:G:152:ARG:HB2	1.67	0.77
1:G:325:PRO:HD3	5:G:501:HEM:HBB2	1.68	0.75
1:K:10:SER:H	1:K:82:GLN:HE22	1.35	0.75
1:A:170:THR:HG21	1:A:212:PHE:CD2	2.22	0.74
1:D:170:THR:HG21	1:D:212:PHE:CD2	2.23	0.74
5:G:502:HEM:HBC2	5:G:502:HEM:HHD	1.68	0.74
1:K:170:THR:HG21	1:K:212:PHE:CD2	2.22	0.74
3:F:215:PRO:HB3	11:I:323:FC6:N24	2.02	0.74
1:A:85:CYS:HB2	1:A:152:ARG:HB2	1.68	0.73
1:D:335:LEU:HD22	4:X:710:UNK:CB	2.18	0.73
5:A:502:HEM:HBC2	5:A:502:HEM:HHD	1.70	0.73
5:D:502:HEM:HBC2	5:D:502:HEM:HHD	1.71	0.73
1:A:325:PRO:HD3	5:A:501:HEM:HBB2	1.71	0.72
2:E:62:ARG:HH22	2:E:184:GLU:CD	1.96	0.72
1:D:63:ALA:O	1:D:67:ALA:HB3	1.88	0.72
1:G:355:ALA:O	1:G:359:ILE:HG12	1.90	0.72
1:D:325:PRO:HD3	5:D:501:HEM:HBB2	1.72	0.71
1:G:63:ALA:O	1:G:67:ALA:HB3	1.90	0.71
2:B:128:PRO:HD2	2:B:129:ARG:HH21	1.55	0.71
3:M:17:ILE:HG21	3:M:70:ILE:HD11	1.72	0.71
2:E:116:TYR:CE2	3:F:145:ILE:HG21	2.24	0.71
2:L:57:ARG:NH2	2:L:97:PRO:O	2.23	0.71
2:L:72:MET:HE3	2:L:100:TRP:CD2	2.24	0.71
1:K:31:LEU:HD11	1:K:59:LEU:HD13	1.72	0.71
1:A:61:THR:HG22	1:A:62:ASN:HD22	1.55	0.70
2:B:7:LEU:HA	2:B:10:ASN:HD22	1.57	0.70
3:F:17:ILE:HG21	3:F:70:ILE:HD11	1.73	0.70
2:B:57:ARG:NH2	2:B:97:PRO:O	2.25	0.70
1:K:63:ALA:O	1:K:67:ALA:HB3	1.91	0.69
1:K:325:PRO:HD3	5:K:501:HEM:HBB2	1.73	0.69
1:K:319:MET:HE1	1:K:400:TRP:HZ2	1.58	0.69
3:C:189:TRP:O	3:C:193:ILE:HG22	1.92	0.69
1:G:253:TRP:CH2	2:H:28:THR:HG21	2.27	0.69
1:D:31:LEU:HD11	1:D:59:LEU:HD13	1.75	0.68
1:D:319:MET:HE1	1:D:400:TRP:HZ2	1.58	0.68
2:H:157:MET:HE3	2:H:167:TYR:CD2	2.28	0.68
2:E:157:MET:HE3	2:E:167:TYR:CD2	2.29	0.68
3:F:229:TYR:HE1	3:F:239:GLN:HA	1.58	0.68
3:C:195:GLU:OE2	3:C:272:ARG:NH1	2.27	0.68
1:K:421:TYR:O	2:L:82:ARG:NH2	2.27	0.68
2:H:72:MET:HE3	2:H:100:TRP:CD2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:17:ILE:HG21	3:I:70:ILE:HD11	1.76	0.67
1:K:64:VAL:HG11	5:K:502:HEM:C4C	2.28	0.67
1:G:352:GLY:O	1:G:356:MET:HG3	1.93	0.67
2:H:57:ARG:NH2	2:H:97:PRO:O	2.27	0.67
1:A:340:ASP:H	1:A:406:GLN:HE22	1.42	0.67
2:B:72:MET:HE3	2:B:100:TRP:CD2	2.29	0.67
1:A:349:GLY:HA3	5:A:501:HEM:HAC	1.76	0.67
2:L:62:ARG:HH22	2:L:184:GLU:CD	2.01	0.67
2:E:44:GLU:HB3	2:E:202:LYS:HB2	1.77	0.67
1:D:355:ALA:O	1:D:359:ILE:HG12	1.94	0.66
3:M:195:GLU:OE2	3:M:272:ARG:NH1	2.29	0.66
1:G:61:THR:HG22	1:G:62:ASN:HD22	1.59	0.66
1:G:64:VAL:HG11	5:G:502:HEM:C4C	2.31	0.66
2:H:116:TYR:HE2	3:I:145:ILE:HG21	1.61	0.66
1:D:253:TRP:CH2	2:E:28:THR:HG21	2.31	0.66
3:I:279:MET:HB2	10:I:322:HEC:C4D	2.25	0.66
1:K:355:ALA:O	1:K:359:ILE:HG12	1.95	0.66
1:D:356:MET:CE	1:D:388:ALA:HB1	2.26	0.66
3:I:36:THR:O	3:I:37:ASP:HB2	1.93	0.66
2:E:72:MET:HE3	2:E:100:TRP:CD2	2.31	0.66
1:K:349:GLY:HA3	5:K:501:HEM:HAC	1.78	0.66
2:B:62:ARG:HH22	2:B:184:GLU:CD	2.04	0.66
1:K:61:THR:HG22	1:K:62:ASN:HD22	1.61	0.65
3:M:229:TYR:HE1	3:M:239:GLN:HA	1.60	0.65
1:D:17:PHE:CZ	1:D:99:PHE:HA	2.31	0.65
1:G:10:SER:N	1:G:82:GLN:HE22	1.94	0.65
2:H:7:LEU:HA	2:H:10:ASN:HD22	1.61	0.65
1:A:76:THR:HG21	1:A:221:ILE:CG1	2.23	0.65
1:G:347:HIS:HA	1:G:350:ALA:HB3	1.78	0.65
3:C:17:ILE:HG21	3:C:70:ILE:HD11	1.78	0.65
1:G:356:MET:CE	1:G:388:ALA:HB1	2.27	0.65
2:H:44:GLU:HB3	2:H:202:LYS:HB2	1.78	0.65
2:H:62:ARG:HH22	2:H:184:GLU:CD	2.05	0.65
3:M:130:GLN:HE21	3:M:130:GLN:HA	1.61	0.65
1:D:352:GLY:O	1:D:356:MET:HG3	1.97	0.65
1:A:355:ALA:O	1:A:359:ILE:HG12	1.97	0.65
1:A:31:LEU:HD11	1:A:59:LEU:HD13	1.77	0.65
3:C:189:TRP:CZ2	10:C:321:HEC:HMC2	2.32	0.65
3:F:189:TRP:CZ2	10:F:321:HEC:HMC2	2.32	0.65
2:H:157:MET:HE1	2:H:171:ASP:HB3	1.77	0.65
2:E:7:LEU:HA	2:E:10:ASN:HD22	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:PHE:CZ	1:A:99:PHE:HA	2.33	0.64
1:A:253:TRP:CH2	2:B:28:THR:HG21	2.31	0.64
3:I:189:TRP:O	3:I:193:ILE:HG22	1.96	0.64
2:L:7:LEU:HA	2:L:10:ASN:HD22	1.60	0.64
3:M:36:THR:O	3:M:37:ASP:HB2	1.96	0.64
3:F:36:THR:O	3:F:37:ASP:HB2	1.97	0.64
1:K:253:TRP:CH2	2:L:28:THR:HG21	2.32	0.64
1:K:340:ASP:H	1:K:406:GLN:HE22	1.44	0.64
2:B:44:GLU:HB3	2:B:202:LYS:HB2	1.80	0.64
1:A:82:GLN:NE2	1:A:89:LEU:H	1.96	0.64
1:A:421:TYR:O	2:B:82:ARG:NH2	2.31	0.64
3:C:279:MET:HB2	10:C:322:HEC:C4D	2.27	0.64
1:G:319:MET:HE1	1:G:400:TRP:HZ2	1.62	0.64
1:K:352:GLY:O	1:K:356:MET:HG3	1.98	0.64
2:L:44:GLU:HB3	2:L:202:LYS:HB2	1.79	0.64
1:D:327:MET:HE1	1:D:345:HIS:CG	2.33	0.64
1:K:367:PRO:HD3	1:K:375:MET:HE3	1.80	0.64
2:H:193:GLN:HA	2:H:193:GLN:NE2	2.09	0.64
2:B:62:ARG:NH1	2:B:63:GLU:OE2	2.28	0.63
3:I:183:ILE:HG12	3:I:278:GLN:HG2	1.80	0.63
1:K:356:MET:CE	1:K:388:ALA:HB1	2.29	0.63
1:K:386:TRP:O	1:K:390:ILE:HG12	1.99	0.63
1:A:327:MET:HE1	1:A:345:HIS:CG	2.34	0.63
1:D:76:THR:HG21	1:D:221:ILE:CG1	2.24	0.63
2:B:116:TYR:HE2	3:C:145:ILE:HG21	1.63	0.63
2:E:128:PRO:HD2	2:E:129:ARG:HH21	1.63	0.63
1:D:10:SER:N	1:D:82:GLN:HE22	1.95	0.63
2:E:57:ARG:NH2	2:E:97:PRO:O	2.31	0.63
2:H:157:MET:HE2	2:H:172:ILE:HG13	1.81	0.63
3:C:229:TYR:HE1	3:C:239:GLN:HA	1.62	0.63
1:D:386:TRP:O	1:D:390:ILE:HG12	1.99	0.63
1:G:386:TRP:O	1:G:390:ILE:HG12	1.98	0.63
3:C:36:THR:O	3:C:37:ASP:HB2	1.98	0.63
3:F:195:GLU:OE2	3:F:272:ARG:NH1	2.30	0.63
3:F:193:ILE:HD11	3:F:228:VAL:CG1	2.24	0.63
2:B:157:MET:HE3	2:B:167:TYR:CD2	2.34	0.63
1:K:10:SER:N	1:K:82:GLN:HE22	1.97	0.63
1:D:64:VAL:HG11	5:D:502:HEM:C4C	2.34	0.62
1:G:17:PHE:CZ	1:G:99:PHE:HA	2.34	0.62
1:A:399:MET:HE2	1:A:399:MET:HA	1.82	0.62
1:D:82:GLN:NE2	1:D:89:LEU:H	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:PRO:HD3	1:D:375:MET:HE3	1.81	0.62
2:L:14:LEU:HG	2:L:18:MET:HE2	1.80	0.62
3:I:130:GLN:HE21	3:I:130:GLN:HA	1.62	0.62
2:L:62:ARG:NH1	2:L:63:GLU:OE2	2.32	0.62
2:L:116:TYR:HE2	3:M:145:ILE:HG21	1.63	0.62
1:A:10:SER:N	1:A:82:GLN:HE22	1.97	0.62
3:I:266:GLN:NE2	11:I:323:FC6:N11	2.47	0.62
3:M:279:MET:HB2	10:M:322:HEC:C4D	2.29	0.62
3:C:130:GLN:HE21	3:C:130:GLN:HA	1.63	0.62
3:F:189:TRP:O	3:F:193:ILE:HG22	1.99	0.62
3:F:279:MET:HB2	10:F:322:HEC:C4D	2.30	0.62
1:A:346:VAL:HG22	5:A:501:HEM:C2D	2.34	0.62
1:D:421:TYR:O	2:E:82:ARG:NH2	2.33	0.62
2:E:157:MET:HE1	2:E:171:ASP:HB3	1.80	0.62
1:A:178:ASN:HD22	1:A:201:VAL:HG12	1.65	0.62
1:K:82:GLN:NE2	1:K:89:LEU:H	1.98	0.62
1:A:319:MET:HE1	1:A:400:TRP:HZ2	1.65	0.61
1:D:359:ILE:CD1	1:D:448:MET:HE1	2.19	0.61
2:E:14:LEU:HG	2:E:18:MET:HE2	1.82	0.61
1:G:349:GLY:HA3	5:G:501:HEM:HAC	1.81	0.61
1:K:76:THR:HG21	1:K:221:ILE:CG1	2.29	0.61
1:A:372:ARG:NH1	1:A:461:ALA:HB1	2.14	0.61
1:A:356:MET:CE	1:A:388:ALA:HB1	2.29	0.61
2:B:138:PRO:HD3	10:B:211:HEC:HBC3	1.81	0.61
2:H:128:PRO:HD2	2:H:129:ARG:HH21	1.65	0.61
2:H:138:PRO:HD3	10:H:211:HEC:HBC3	1.82	0.61
2:B:14:LEU:HG	2:B:18:MET:HE2	1.82	0.61
3:C:277:GLY:HA3	10:C:322:HEC:O1D	2.01	0.61
1:D:347:HIS:HA	1:D:350:ALA:HB3	1.82	0.61
1:G:234:VAL:HB	3:I:49:GLU:HB3	1.82	0.61
1:A:352:GLY:O	1:A:356:MET:HG3	2.00	0.61
3:M:74:VAL:O	3:M:82:TRP:CZ3	2.53	0.61
1:D:82:GLN:HE21	1:D:89:LEU:H	1.48	0.61
1:D:349:GLY:HA3	5:D:501:HEM:HAC	1.82	0.61
1:K:17:PHE:CZ	1:K:99:PHE:HA	2.36	0.61
1:A:64:VAL:HG11	5:A:502:HEM:C4C	2.36	0.61
3:F:130:GLN:HA	3:F:130:GLN:HE21	1.65	0.61
1:K:340:ASP:H	1:K:406:GLN:NE2	1.99	0.61
3:I:229:TYR:HE1	3:I:239:GLN:HA	1.66	0.60
1:K:239:LEU:O	1:K:243:HIS:HB3	2.01	0.60
1:A:431:HIS:HD2	2:B:136:LYS:NZ	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:SER:H	1:D:82:GLN:NE2	1.99	0.60
1:D:372:ARG:NH1	1:D:461:ALA:HB1	2.16	0.60
2:B:157:MET:HE1	2:B:171:ASP:HB3	1.83	0.60
1:G:239:LEU:HD23	1:G:289:ASN:HD22	1.66	0.60
1:A:222:MET:HG3	1:A:314:LEU:HD21	1.83	0.60
1:G:31:LEU:HD11	1:G:59:LEU:HD13	1.81	0.60
1:G:359:ILE:CD1	1:G:448:MET:HE1	2.24	0.60
1:K:222:MET:HG3	1:K:314:LEU:HD21	1.83	0.60
1:A:281:ALA:HB3	1:A:282:PRO:CD	2.26	0.60
2:E:116:TYR:HE2	3:F:145:ILE:CG2	2.11	0.60
3:F:189:TRP:HZ2	10:F:321:HEC:HMC2	1.66	0.60
1:G:372:ARG:NH1	1:G:461:ALA:HB1	2.16	0.60
1:K:343:ILE:HG12	5:K:502:HEM:HBA2	1.84	0.60
2:B:193:GLN:HE21	2:B:193:GLN:CA	2.08	0.60
3:C:189:TRP:HZ2	10:C:321:HEC:HMC2	1.67	0.60
3:I:195:GLU:OE2	3:I:272:ARG:NH1	2.35	0.60
1:K:82:GLN:HE21	1:K:89:LEU:H	1.49	0.60
3:C:32:SER:O	3:C:34:GLY:N	2.35	0.60
11:F:323:FC6:C24	3:I:215:PRO:HB3	2.27	0.59
2:H:62:ARG:NH1	2:H:63:GLU:OE2	2.33	0.59
3:M:73:LEU:HD22	3:M:79:LEU:HG	1.84	0.59
1:A:82:GLN:HE21	1:A:89:LEU:H	1.50	0.59
1:A:239:LEU:HD23	1:A:289:ASN:HD22	1.66	0.59
1:A:340:ASP:H	1:A:406:GLN:NE2	1.99	0.59
2:E:80:THR:HG21	3:F:99:TRP:HZ2	1.67	0.59
1:K:29:MET:CE	1:K:448:MET:HE3	2.30	0.59
1:A:239:LEU:O	1:A:243:HIS:HB3	2.03	0.59
1:G:367:PRO:HD3	1:G:375:MET:HE3	1.84	0.59
2:L:157:MET:HE3	2:L:167:TYR:CD2	2.38	0.59
3:F:73:LEU:HD22	3:F:79:LEU:HG	1.85	0.59
1:K:454:ASN:O	1:K:458:THR:HG23	2.03	0.59
1:G:82:GLN:NE2	1:G:89:LEU:H	2.00	0.59
1:G:76:THR:HG21	1:G:221:ILE:CG1	2.32	0.59
2:L:157:MET:HE1	2:L:171:ASP:HB3	1.84	0.59
1:D:335:LEU:HD13	4:X:707:UNK:HA	1.85	0.58
2:L:128:PRO:HD2	2:L:129:ARG:HH21	1.68	0.58
1:G:178:ASN:HD22	1:G:201:VAL:HG12	1.69	0.58
2:H:14:LEU:HG	2:H:18:MET:HE2	1.83	0.58
3:I:73:LEU:HD22	3:I:79:LEU:HG	1.85	0.58
3:I:189:TRP:CZ2	10:I:321:HEC:HMC2	2.38	0.58
1:K:6:SER:C	1:K:8:ALA:H	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:62:ARG:HG3	2:L:63:GLU:N	2.19	0.58
1:D:356:MET:HE1	1:D:388:ALA:CB	2.34	0.58
3:F:74:VAL:O	3:F:82:TRP:CZ3	2.57	0.58
1:A:359:ILE:CD1	1:A:448:MET:HE1	2.21	0.58
3:C:215:PRO:HG3	11:M:323:FC6:C21	2.34	0.58
3:C:74:VAL:O	3:C:82:TRP:CZ3	2.57	0.57
3:M:207:LYS:HD3	3:M:222:LEU:HD21	1.85	0.57
3:C:242:GLU:CD	3:C:242:GLU:H	2.11	0.57
1:D:340:ASP:H	1:D:406:GLN:NE2	2.02	0.57
1:K:347:HIS:HA	1:K:350:ALA:HB3	1.85	0.57
1:A:386:TRP:O	1:A:390:ILE:HG12	2.03	0.57
1:A:233:PRO:HG2	3:C:50:TYR:CZ	2.39	0.57
2:E:138:PRO:HD3	10:E:211:HEC:HBC3	1.85	0.57
1:G:346:VAL:HG22	5:G:501:HEM:C2D	2.39	0.57
1:A:367:PRO:HD3	1:A:375:MET:HE3	1.87	0.57
3:I:266:GLN:HG2	11:I:323:FC6:C22	2.34	0.57
1:K:174:LEU:HD21	1:K:208:ASN:HB3	1.86	0.57
1:A:281:ALA:CB	1:A:282:PRO:HD3	2.29	0.57
1:D:431:HIS:HD2	2:E:136:LYS:NZ	2.03	0.57
1:K:227:PRO:HB2	3:M:47:ILE:HD12	1.87	0.57
1:K:356:MET:HE1	1:K:388:ALA:CB	2.35	0.57
1:D:340:ASP:H	1:D:406:GLN:HE22	1.52	0.57
3:I:74:VAL:O	3:I:82:TRP:CZ3	2.58	0.57
3:I:242:GLU:CD	3:I:242:GLU:H	2.12	0.57
1:G:239:LEU:O	1:G:243:HIS:HB3	2.05	0.56
1:A:418:THR:OG1	3:C:137:ARG:HD2	2.05	0.56
2:B:177:ASP:OD1	2:B:177:ASP:N	2.38	0.56
1:D:61:THR:HG22	1:D:62:ASN:HD22	1.69	0.56
1:G:342:THR:O	1:G:346:VAL:HG23	2.05	0.56
2:L:138:PRO:HD3	10:L:211:HEC:HBC3	1.87	0.56
1:A:13:VAL:HA	1:A:16:GLN:HE21	1.69	0.56
1:G:82:GLN:HE21	1:G:88:THR:HA	1.71	0.56
1:K:13:VAL:HA	1:K:16:GLN:HE21	1.70	0.56
1:D:239:LEU:HD23	1:D:289:ASN:HD22	1.70	0.56
3:M:239:GLN:OE1	3:M:239:GLN:N	2.36	0.56
1:D:346:VAL:HG22	5:D:501:HEM:C2D	2.39	0.56
3:F:187:PRO:HG2	3:F:189:TRP:CZ2	2.40	0.56
1:G:327:MET:HE1	1:G:345:HIS:CG	2.41	0.56
3:C:6:SER:OG	3:C:81:ASN:HB2	2.06	0.56
2:E:117:SER:H	10:F:322:HEC:HBC1	1.72	0.55
2:E:193:GLN:HA	2:E:193:GLN:NE2	2.13	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:10:SER:H	1:G:82:GLN:NE2	1.98	0.55
3:I:38:GLN:O	3:I:50:TYR:HD2	1.88	0.55
3:M:189:TRP:CZ2	10:M:321:HEC:HMC2	2.41	0.55
1:A:234:VAL:HB	3:C:49:GLU:HB3	1.87	0.55
1:D:62:ASN:HD21	1:D:125:GLU:HG3	1.72	0.55
1:G:343:ILE:HG12	5:G:502:HEM:HBA2	1.88	0.55
1:K:367:PRO:CD	1:K:375:MET:HE3	2.37	0.55
1:G:115:LEU:HB3	1:G:117:PHE:CE2	2.42	0.55
1:G:237:TYR:CE2	1:G:241:ILE:HD11	2.41	0.55
3:M:277:GLY:HA3	10:M:322:HEC:O1D	2.06	0.55
1:D:76:THR:HG23	1:D:225:PHE:HE1	1.72	0.55
1:D:239:LEU:O	1:D:243:HIS:HB3	2.06	0.55
2:L:72:MET:HE3	2:L:100:TRP:CE2	2.41	0.55
3:M:38:GLN:O	3:M:50:TYR:HD2	1.89	0.55
1:D:227:PRO:HB2	3:F:47:ILE:HD12	1.88	0.55
1:A:82:GLN:HE21	1:A:88:THR:HA	1.72	0.55
1:A:335:LEU:CD2	4:U:710:UNK:CB	2.82	0.55
1:D:174:LEU:HD21	1:D:208:ASN:HB3	1.88	0.55
1:G:222:MET:HG3	1:G:314:LEU:HD21	1.89	0.55
1:K:239:LEU:HD23	1:K:289:ASN:HD22	1.72	0.55
1:G:82:GLN:HE21	1:G:89:LEU:H	1.55	0.55
1:G:281:ALA:HB3	1:G:282:PRO:CD	2.28	0.55
2:H:157:MET:CE	2:H:171:ASP:HB3	2.36	0.55
1:G:356:MET:HE1	1:G:388:ALA:CB	2.36	0.54
1:K:327:MET:HE1	1:K:345:HIS:CG	2.42	0.54
1:K:375:MET:HA	1:K:375:MET:HE2	1.89	0.54
1:A:10:SER:H	1:A:82:GLN:NE2	2.01	0.54
2:B:62:ARG:HG3	2:B:63:GLU:N	2.23	0.54
1:D:234:VAL:HB	3:F:49:GLU:HB3	1.88	0.54
1:K:399:MET:HE2	1:K:399:MET:HA	1.90	0.54
1:D:399:MET:HE2	1:D:399:MET:HA	1.88	0.54
3:C:186:MET:HG2	10:C:321:HEC:CHA	2.36	0.54
1:D:222:MET:HG3	1:D:314:LEU:HD21	1.88	0.54
3:F:6:SER:OG	3:F:81:ASN:HB2	2.06	0.54
11:F:323:FC6:C21	3:I:215:PRO:HG3	2.38	0.54
1:G:10:SER:HB2	1:G:88:THR:HG23	1.88	0.54
1:G:319:MET:HE1	1:G:400:TRP:CZ2	2.43	0.54
1:K:234:VAL:HB	3:M:49:GLU:HB3	1.90	0.54
2:B:157:MET:HE2	2:B:172:ILE:HG13	1.88	0.54
1:D:13:VAL:HA	1:D:16:GLN:HE21	1.72	0.54
1:G:211:GLY:O	1:G:215:THR:HB	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:10:SER:H	1:K:82:GLN:NE2	2.03	0.54
1:K:149:LEU:HD21	1:K:161:ASN:HD22	1.73	0.54
1:K:319:MET:HE1	1:K:400:TRP:CZ2	2.41	0.54
1:K:431:HIS:HD2	2:L:136:LYS:NZ	2.04	0.54
2:H:116:TYR:CE2	3:I:145:ILE:HG21	2.41	0.54
3:I:6:SER:OG	3:I:81:ASN:HB2	2.08	0.54
1:A:319:MET:HE1	1:A:400:TRP:CZ2	2.41	0.54
3:C:135:GLY:HA3	3:C:297:TYR:HB2	1.90	0.54
3:F:32:SER:O	3:F:34:GLY:N	2.41	0.54
1:K:237:TYR:CE2	1:K:241:ILE:HD11	2.42	0.54
11:C:323:FC6:C24	3:M:215:PRO:HB3	2.35	0.53
1:D:84:THR:CG2	1:D:161:ASN:HD21	2.21	0.53
3:F:266:GLN:NE2	11:F:323:FC6:N11	2.56	0.53
1:G:375:MET:HE2	1:G:375:MET:HA	1.90	0.53
3:I:32:SER:O	3:I:34:GLY:N	2.40	0.53
1:A:375:MET:HA	1:A:375:MET:HE2	1.90	0.53
3:F:266:GLN:HG3	11:F:323:FC6:N22	2.24	0.53
1:A:55:ARG:NH2	2:B:62:ARG:HD2	2.23	0.53
1:D:454:ASN:O	1:D:458:THR:HG23	2.08	0.53
5:D:502:HEM:HBB2	5:D:502:HEM:CHC	2.29	0.53
3:F:135:GLY:HA3	3:F:297:TYR:HB2	1.89	0.53
1:G:421:TYR:O	2:H:82:ARG:NH2	2.41	0.53
3:M:32:SER:O	3:M:34:GLY:N	2.41	0.53
1:A:61:THR:HG22	1:A:62:ASN:ND2	2.23	0.53
3:I:167:TRP:CD2	3:I:182:ARG:HG2	2.42	0.53
1:K:178:ASN:HD22	1:K:201:VAL:HG12	1.73	0.53
2:L:177:ASP:OD1	2:L:177:ASP:N	2.42	0.53
2:B:57:ARG:NH1	2:B:99:LEU:HD12	2.23	0.53
3:C:239:GLN:OE1	3:C:239:GLN:N	2.40	0.53
1:K:346:VAL:HG22	5:K:501:HEM:C2D	2.43	0.53
1:K:372:ARG:NH1	1:K:461:ALA:HB1	2.23	0.53
1:D:82:GLN:HE21	1:D:88:THR:HA	1.74	0.53
1:G:454:ASN:O	1:G:458:THR:HG23	2.08	0.53
2:E:70:SER:HA	2:E:101:GLY:HA3	1.91	0.53
1:A:395:TYR:CZ	1:A:437:ARG:HD2	2.45	0.52
3:C:227:ASN:OD1	2:H:201:ASN:HB2	2.09	0.52
1:G:356:MET:HE1	1:G:388:ALA:HB1	1.91	0.52
1:K:10:SER:HB2	1:K:88:THR:HG23	1.91	0.52
3:F:38:GLN:O	3:F:50:TYR:HD2	1.92	0.52
3:F:167:TRP:CD2	3:F:182:ARG:HG2	2.45	0.52
3:F:186:MET:HG2	10:F:321:HEC:CHA	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:122:VAL:HB	3:I:171:ALA:HB1	1.91	0.52
1:G:13:VAL:HA	1:G:16:GLN:HE21	1.73	0.52
3:M:189:TRP:HZ2	10:M:321:HEC:HMC2	1.75	0.52
3:M:242:GLU:CD	3:M:242:GLU:H	2.18	0.52
1:A:66:PHE:O	1:A:70:GLY:HA3	2.09	0.52
2:B:157:MET:HE1	2:B:171:ASP:C	2.34	0.52
3:C:189:TRP:CZ3	3:C:232:THR:HG21	2.45	0.52
2:E:161:ARG:HA	2:E:165:VAL:O	2.10	0.52
2:L:157:MET:CE	2:L:171:ASP:HB3	2.39	0.52
1:A:29:MET:CE	1:A:448:MET:HE3	2.33	0.52
1:A:90:PHE:CD1	1:A:147:GLY:HA3	2.45	0.52
1:G:281:ALA:CB	1:G:282:PRO:HD3	2.31	0.52
3:I:239:GLN:OE1	3:I:239:GLN:N	2.39	0.52
1:A:211:GLY:O	1:A:215:THR:HB	2.09	0.52
2:E:157:MET:CE	2:E:171:ASP:HB3	2.39	0.52
1:G:395:TYR:CZ	1:G:437:ARG:HD2	2.45	0.52
2:H:161:ARG:HA	2:H:165:VAL:O	2.09	0.52
1:D:367:PRO:CD	1:D:375:MET:HE3	2.40	0.52
2:E:62:ARG:HG3	2:E:63:GLU:N	2.24	0.52
2:H:62:ARG:HG3	2:H:63:GLU:N	2.24	0.52
1:A:84:THR:CG2	1:A:161:ASN:HD21	2.23	0.52
2:B:193:GLN:HA	2:B:193:GLN:NE2	2.06	0.52
1:G:202:GLN:O	1:G:206:GLY:N	2.35	0.52
2:H:116:TYR:HE2	3:I:145:ILE:CG2	2.22	0.52
2:L:193:GLN:HA	2:L:193:GLN:NE2	2.17	0.52
2:E:63:GLU:OE1	2:E:63:GLU:HA	2.10	0.52
10:H:211:HEC:HMB3	10:H:211:HEC:HBB3	1.92	0.52
1:D:61:THR:HG22	1:D:62:ASN:N	2.25	0.51
2:E:62:ARG:NH1	2:E:63:GLU:OE2	2.38	0.51
3:C:73:LEU:HD22	3:C:79:LEU:HG	1.92	0.51
1:G:227:PRO:HB2	3:I:47:ILE:HD12	1.92	0.51
2:E:177:ASP:OD1	2:E:177:ASP:N	2.44	0.51
1:G:26:ILE:HD12	1:G:449:LEU:HD23	1.92	0.51
1:G:174:LEU:HD21	1:G:208:ASN:HB3	1.92	0.51
3:I:187:PRO:HG2	3:I:189:TRP:CZ2	2.44	0.51
3:M:189:TRP:O	3:M:190:GLY:C	2.52	0.51
2:H:63:GLU:HA	2:H:63:GLU:OE1	2.10	0.51
3:I:177:SER:HA	3:I:182:ARG:HD2	1.92	0.51
1:A:356:MET:HE3	1:A:388:ALA:HB1	1.92	0.51
3:M:122:VAL:HB	3:M:171:ALA:HB1	1.92	0.51
3:M:193:ILE:HD11	3:M:228:VAL:CG1	2.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:GLN:O	2:B:40:ASN:ND2	2.43	0.51
1:D:149:LEU:HD21	1:D:161:ASN:HD22	1.76	0.51
1:G:149:LEU:HD21	1:G:161:ASN:HD22	1.75	0.51
3:C:215:PRO:HG3	11:M:323:FC6:N25	2.25	0.51
1:D:319:MET:HE1	1:D:400:TRP:CZ2	2.41	0.51
3:F:242:GLU:CD	3:F:242:GLU:H	2.19	0.51
1:G:377:SER:H	1:G:454:ASN:HD21	1.58	0.51
3:M:99:TRP:O	3:M:103:VAL:HG23	2.10	0.51
1:A:10:SER:HB2	1:A:88:THR:HG23	1.92	0.51
1:D:211:GLY:O	1:D:215:THR:HB	2.10	0.51
1:D:410:TRP:O	2:E:82:ARG:NH1	2.42	0.51
2:L:116:TYR:CE2	3:M:145:ILE:HG21	2.45	0.51
2:L:129:ARG:HD3	2:L:135:SER:O	2.11	0.51
1:D:375:MET:HE2	1:D:375:MET:HA	1.93	0.51
1:G:399:MET:HA	1:G:399:MET:HE2	1.93	0.51
3:I:302:SER:O	3:I:303:GLN:HB3	2.11	0.51
1:K:356:MET:HE1	1:K:388:ALA:HB1	1.91	0.51
2:L:116:TYR:HE2	3:M:145:ILE:CG2	2.24	0.51
1:A:367:PRO:CD	1:A:375:MET:HE3	2.42	0.50
2:B:157:MET:CE	2:B:171:ASP:HB3	2.41	0.50
1:D:10:SER:HB2	1:D:88:THR:HG23	1.91	0.50
1:D:178:ASN:HD22	1:D:201:VAL:HG12	1.75	0.50
1:A:15:ARG:HG2	1:A:370:PHE:CZ	2.47	0.50
1:A:410:TRP:O	2:B:82:ARG:NH1	2.42	0.50
3:C:163:GLN:HE21	3:C:163:GLN:HA	1.77	0.50
1:A:174:LEU:HD21	1:A:208:ASN:HB3	1.93	0.50
1:A:356:MET:HE1	1:A:388:ALA:CB	2.41	0.50
1:A:377:SER:H	1:A:454:ASN:HD21	1.60	0.50
1:A:454:ASN:O	1:A:458:THR:HG23	2.11	0.50
2:L:161:ARG:HA	2:L:165:VAL:O	2.11	0.50
2:B:70:SER:HA	2:B:101:GLY:HA3	1.93	0.50
2:E:72:MET:HE3	2:E:100:TRP:CE2	2.46	0.50
3:C:183:ILE:HG12	3:C:278:GLN:HG2	1.92	0.50
1:K:42:PRO:HG3	2:L:136:LYS:HD2	1.93	0.50
3:M:6:SER:OG	3:M:81:ASN:HB2	2.11	0.50
3:M:135:GLY:HA3	3:M:297:TYR:HB2	1.93	0.50
1:D:343:ILE:HG12	5:D:502:HEM:HBA2	1.92	0.50
2:H:88:VAL:HG12	2:H:90:GLY:H	1.76	0.50
1:A:310:LEU:O	1:A:313:SER:HB3	2.11	0.50
3:C:240:GLY:C	3:C:242:GLU:OE1	2.55	0.50
1:G:242:VAL:HG22	3:I:27:THR:OG1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:367:PRO:CD	1:G:375:MET:HE3	2.42	0.50
1:K:267:TRP:HE1	2:L:36:GLN:HE22	1.60	0.50
2:E:36:GLN:O	2:E:40:ASN:ND2	2.45	0.49
3:I:189:TRP:HZ2	10:I:321:HEC:HMC2	1.74	0.49
3:C:166:ARG:NH2	3:C:250:PRO:HG3	2.27	0.49
2:E:193:GLN:HE21	2:E:193:GLN:CA	2.18	0.49
3:F:302:SER:O	3:F:303:GLN:HB3	2.11	0.49
3:I:135:GLY:HA3	3:I:297:TYR:HB2	1.93	0.49
1:K:218:PHE:CD2	1:K:221:ILE:HD12	2.47	0.49
3:C:122:VAL:HB	3:C:171:ALA:HB1	1.94	0.49
2:E:137:MET:HB2	10:E:211:HEC:C1D	2.42	0.49
3:F:266:GLN:HG3	11:F:323:FC6:C22	2.42	0.49
1:K:395:TYR:CZ	1:K:437:ARG:HD2	2.48	0.49
2:L:70:SER:HA	2:L:101:GLY:HA3	1.93	0.49
3:F:122:VAL:HB	3:F:171:ALA:HB1	1.95	0.49
1:A:61:THR:HG22	1:A:62:ASN:N	2.26	0.49
1:D:237:TYR:CE2	1:D:241:ILE:HD11	2.47	0.49
1:K:82:GLN:HE21	1:K:88:THR:HA	1.77	0.49
1:A:196:ALA:HB3	2:B:39:VAL:HB	1.95	0.49
2:E:157:MET:HE2	2:E:172:ILE:HG13	1.93	0.49
11:F:323:FC6:N24	3:I:215:PRO:CB	2.58	0.49
1:K:372:ARG:HH11	1:K:372:ARG:HB2	1.78	0.49
1:A:57:ARG:NH1	5:A:502:HEM:O2A	2.45	0.49
1:A:235:TYR:O	1:A:289:ASN:ND2	2.46	0.49
2:E:129:ARG:HD3	2:E:135:SER:O	2.13	0.49
2:H:157:MET:HE1	2:H:171:ASP:C	2.38	0.48
1:A:200:MET:HG3	1:A:264:LEU:HD11	1.95	0.48
1:A:347:HIS:HA	1:A:350:ALA:HB3	1.95	0.48
2:L:36:GLN:O	2:L:40:ASN:ND2	2.46	0.48
1:A:13:VAL:HA	1:A:16:GLN:NE2	2.29	0.48
2:B:72:MET:HE3	2:B:100:TRP:CE2	2.48	0.48
1:G:84:THR:CG2	1:G:161:ASN:HD21	2.25	0.48
1:G:94:LEU:O	1:G:98:THR:HG23	2.13	0.48
1:K:281:ALA:HB3	1:K:282:PRO:CD	2.39	0.48
2:B:80:THR:HA	2:B:84:GLY:O	2.13	0.48
2:H:57:ARG:NH1	2:H:99:LEU:HD12	2.28	0.48
1:A:115:LEU:HB3	1:A:117:PHE:CE2	2.49	0.48
2:B:127:ASN:C	2:B:127:ASN:HD22	2.21	0.48
3:C:167:TRP:CD2	3:C:182:ARG:HG2	2.48	0.48
1:G:15:ARG:HG2	1:G:370:PHE:CZ	2.48	0.48
1:K:460:GLN:O	1:K:461:ALA:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:229:TYR:CD2	3:M:233:CYS:HB2	2.48	0.48
4:U:715:UNK:O	4:U:716:UNK:C	2.61	0.48
1:A:76:THR:HG23	1:A:225:PHE:HE1	1.78	0.48
2:B:128:PRO:HD2	2:B:129:ARG:NH2	2.27	0.48
1:D:356:MET:HE1	1:D:388:ALA:HB1	1.89	0.48
2:H:72:MET:HE3	2:H:100:TRP:CE2	2.48	0.48
2:H:81:GLU:OE1	3:I:290:LYS:NZ	2.41	0.48
3:M:166:ARG:NH2	3:M:250:PRO:HG3	2.29	0.48
1:D:90:PHE:CD1	1:D:147:GLY:HA3	2.48	0.48
1:D:372:ARG:HH11	1:D:372:ARG:HB2	1.78	0.48
1:D:395:TYR:CZ	1:D:437:ARG:HD2	2.49	0.48
1:G:233:PRO:HG2	3:I:50:TYR:CZ	2.48	0.48
1:G:410:TRP:O	2:H:82:ARG:NH1	2.45	0.48
2:L:157:MET:HE2	2:L:172:ILE:HG13	1.96	0.48
1:G:76:THR:HG23	1:G:225:PHE:HE1	1.78	0.48
2:H:177:ASP:OD1	2:H:177:ASP:N	2.47	0.48
3:M:177:SER:HA	3:M:182:ARG:HD2	1.95	0.48
1:A:343:ILE:HG12	5:A:502:HEM:HBA2	1.96	0.48
2:E:116:TYR:HA	10:F:322:HEC:HBC3	1.96	0.47
1:G:431:HIS:HD2	2:H:136:LYS:NZ	2.12	0.47
2:H:193:GLN:HE21	2:H:193:GLN:CA	2.14	0.47
1:K:84:THR:CG2	1:K:161:ASN:HD21	2.26	0.47
2:L:157:MET:HE1	2:L:171:ASP:C	2.39	0.47
1:G:61:THR:HG22	1:G:62:ASN:ND2	2.28	0.47
1:G:340:ASP:H	1:G:406:GLN:NE2	2.12	0.47
3:I:163:GLN:HE21	3:I:163:GLN:HA	1.79	0.47
1:K:76:THR:HG23	1:K:225:PHE:HE1	1.77	0.47
1:D:55:ARG:NH2	2:E:62:ARG:HD2	2.29	0.47
1:D:242:VAL:HG22	3:F:27:THR:OG1	2.14	0.47
1:A:26:ILE:HD12	1:A:449:LEU:HD23	1.96	0.47
1:A:169:LEU:HD11	2:B:15:THR:HG23	1.96	0.47
1:D:66:PHE:O	1:D:70:GLY:HA3	2.15	0.47
1:K:90:PHE:CD1	1:K:147:GLY:HA3	2.49	0.47
1:A:242:VAL:HG22	3:C:27:THR:OG1	2.14	0.47
3:C:99:TRP:O	3:C:103:VAL:HG23	2.15	0.47
3:I:266:GLN:HG3	11:I:323:FC6:N22	2.29	0.47
1:K:26:ILE:HD12	1:K:449:LEU:HD23	1.96	0.47
1:K:209:ALA:O	1:K:213:PHE:CB	2.63	0.47
1:K:342:THR:O	1:K:346:VAL:HG23	2.14	0.47
2:H:70:SER:HA	2:H:101:GLY:HA3	1.96	0.47
3:I:229:TYR:CD2	3:I:233:CYS:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:169:LEU:HD11	2:L:15:THR:HG23	1.95	0.47
1:K:196:ALA:HB3	2:L:39:VAL:HB	1.96	0.47
1:A:237:TYR:CE2	1:A:241:ILE:HD11	2.49	0.47
3:C:215:PRO:CD	3:C:264:LEU:HD12	2.44	0.47
1:G:62:ASN:HD21	1:G:125:GLU:HG3	1.80	0.47
1:K:125:GLU:H	1:K:125:GLU:HG2	1.42	0.47
1:K:211:GLY:O	1:K:215:THR:HB	2.14	0.47
3:M:232:THR:O	3:M:235:VAL:HG23	2.14	0.47
10:M:321:HEC:HMB3	10:M:321:HEC:HBB3	1.96	0.47
1:A:250:VAL:HG13	1:A:275:MET:HE2	1.96	0.47
3:C:38:GLN:O	3:C:50:TYR:HD2	1.97	0.47
3:C:89:TYR:CD1	3:C:101:ARG:NH1	2.83	0.47
1:G:128:TRP:CG	1:G:129:PRO:HD3	2.50	0.47
3:I:193:ILE:HD11	3:I:228:VAL:CG1	2.36	0.47
2:E:157:MET:HE1	2:E:171:ASP:C	2.40	0.47
1:G:226:VAL:HB	1:G:227:PRO:HD3	1.96	0.47
1:G:356:MET:HE3	1:G:388:ALA:HB1	1.97	0.47
1:K:193:TYR:CE1	1:K:201:VAL:HG11	2.49	0.47
3:M:206:ARG:HD3	3:M:214:LEU:HD23	1.96	0.47
1:G:169:LEU:HD11	2:H:15:THR:HG23	1.97	0.47
3:I:179:LEU:HD23	3:I:291:VAL:HG11	1.96	0.47
1:A:60:HIS:O	1:A:64:VAL:HB	2.15	0.46
1:A:346:VAL:HG22	5:A:501:HEM:C3D	2.50	0.46
2:B:161:ARG:HA	2:B:165:VAL:O	2.15	0.46
1:K:235:TYR:O	1:K:289:ASN:ND2	2.47	0.46
1:K:242:VAL:HG22	3:M:27:THR:OG1	2.16	0.46
1:K:376:HIS:CB	1:K:458:THR:HG22	2.45	0.46
3:M:177:SER:OG	3:M:182:ARG:NH1	2.44	0.46
4:Y:728:UNK:C	4:Y:730:UNK:H	2.28	0.46
1:D:346:VAL:HG22	5:D:501:HEM:C3D	2.49	0.46
2:E:57:ARG:NH1	2:E:99:LEU:HD12	2.30	0.46
3:F:177:SER:HA	3:F:182:ARG:HD2	1.98	0.46
1:K:6:SER:C	1:K:8:ALA:N	2.73	0.46
2:B:128:PRO:HD3	2:B:139:SER:HA	1.97	0.46
1:K:64:VAL:HG11	5:K:502:HEM:CHD	2.45	0.46
1:A:202:GLN:O	1:A:206:GLY:N	2.44	0.46
1:A:226:VAL:HB	1:A:227:PRO:HD3	1.96	0.46
2:B:48:PRO:HG3	2:B:166:PRO:HD2	1.96	0.46
3:C:177:SER:HA	3:C:182:ARG:HD2	1.97	0.46
1:D:15:ARG:HG2	1:D:370:PHE:CZ	2.51	0.46
1:D:26:ILE:HD12	1:D:449:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:376:HIS:CB	1:G:458:THR:HG22	2.46	0.46
3:I:99:TRP:O	3:I:103:VAL:HG23	2.15	0.46
1:K:115:LEU:HB3	1:K:117:PHE:CE2	2.50	0.46
1:G:218:PHE:HA	1:G:221:ILE:HG13	1.97	0.46
10:I:321:HEC:HBB3	10:I:321:HEC:HMB3	1.98	0.46
1:A:342:THR:O	1:A:346:VAL:HG23	2.16	0.46
2:H:127:ASN:C	2:H:127:ASN:HD22	2.24	0.46
1:K:377:SER:H	1:K:454:ASN:HD21	1.63	0.46
1:A:128:TRP:CG	1:A:129:PRO:HD3	2.50	0.46
1:A:149:LEU:HD21	1:A:161:ASN:HD22	1.81	0.46
3:C:206:ARG:NH1	3:C:262:SER:O	2.48	0.46
1:D:281:ALA:HB3	1:D:282:PRO:CD	2.39	0.46
3:I:130:GLN:HE21	3:I:130:GLN:CA	2.24	0.46
3:I:266:GLN:CG	11:I:323:FC6:C22	2.93	0.46
3:M:167:TRP:NE1	3:M:182:ARG:HG2	2.30	0.46
3:F:266:GLN:HG2	11:F:323:FC6:C23	2.45	0.46
1:G:372:ARG:HH11	1:G:372:ARG:HB2	1.80	0.46
2:L:57:ARG:NH1	2:L:99:LEU:HD12	2.30	0.46
3:M:212:LEU:HA	3:M:212:LEU:HD23	1.66	0.46
1:K:202:GLN:O	1:K:206:GLY:N	2.44	0.45
1:A:125:GLU:H	1:A:125:GLU:HG2	1.39	0.45
1:A:218:PHE:CD2	1:A:221:ILE:HD12	2.52	0.45
1:G:90:PHE:CD1	1:G:147:GLY:HA3	2.51	0.45
2:L:127:ASN:HD22	2:L:127:ASN:C	2.23	0.45
3:M:74:VAL:O	3:M:82:TRP:HZ3	1.98	0.45
2:B:47:LYS:HE2	3:I:221:ASP:OD2	2.16	0.45
2:B:129:ARG:HB2	2:B:129:ARG:CZ	2.46	0.45
1:D:356:MET:HE3	1:D:388:ALA:HB1	1.97	0.45
1:D:413:ILE:HG22	1:D:414:ASN:O	2.16	0.45
3:I:167:TRP:NE1	3:I:182:ARG:HG2	2.32	0.45
1:K:335:LEU:HD13	4:Z:707:UNK:HA	1.98	0.45
3:M:121:SER:O	3:M:125:VAL:HG23	2.16	0.45
1:A:367:PRO:HG3	1:A:375:MET:HE3	1.97	0.45
2:B:63:GLU:OE1	2:B:63:GLU:HA	2.16	0.45
1:D:125:GLU:H	1:D:125:GLU:HG2	1.44	0.45
1:D:226:VAL:HB	1:D:227:PRO:HD3	1.97	0.45
1:G:250:VAL:HG11	1:G:278:ILE:HG22	1.99	0.45
1:K:57:ARG:NH1	5:K:502:HEM:O2A	2.50	0.45
1:D:218:PHE:CD2	1:D:221:ILE:HD12	2.52	0.45
1:G:339:THR:HG22	1:G:410:TRP:CZ3	2.52	0.45
1:K:61:THR:HG22	1:K:62:ASN:ND2	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:346:VAL:HG22	5:K:501:HEM:C3D	2.52	0.45
4:U:715:UNK:C	4:U:717:UNK:N	2.79	0.45
3:C:229:TYR:CD2	3:C:233:CYS:HB2	2.52	0.45
1:D:209:ALA:O	1:D:213:PHE:CB	2.64	0.45
1:K:60:HIS:O	1:K:64:VAL:HB	2.17	0.45
1:K:227:PRO:HB2	3:M:47:ILE:CD1	2.45	0.45
1:A:58:PRO:HA	1:A:61:THR:HB	1.97	0.45
3:C:37:ASP:HB3	3:C:38:GLN:H	1.65	0.45
11:C:323:FC6:N25	3:M:215:PRO:HG3	2.30	0.45
1:D:13:VAL:HA	1:D:16:GLN:NE2	2.32	0.45
3:F:167:TRP:NE1	3:F:182:ARG:HG2	2.31	0.45
1:G:58:PRO:HA	1:G:61:THR:HB	1.99	0.45
3:M:130:GLN:HA	3:M:130:GLN:NE2	2.30	0.45
2:B:43:VAL:O	2:B:44:GLU:C	2.59	0.45
1:G:413:ILE:HG22	1:G:414:ASN:O	2.17	0.45
3:M:167:TRP:CD2	3:M:182:ARG:HG2	2.50	0.45
1:D:200:MET:HG3	1:D:264:LEU:HD11	1.98	0.45
2:H:48:PRO:HG3	2:H:166:PRO:HD2	1.98	0.45
3:I:85:VAL:O	3:I:85:VAL:CG1	2.64	0.45
2:L:127:ASN:C	2:L:127:ASN:ND2	2.73	0.45
3:M:282:GLN:HG3	10:M:322:HEC:HBB2	1.98	0.45
1:A:319:MET:HG3	1:A:320:SER:N	2.29	0.45
1:G:55:ARG:NH2	2:H:62:ARG:HD2	2.32	0.45
1:K:410:TRP:O	2:L:82:ARG:NH1	2.50	0.45
1:A:460:GLN:O	1:A:461:ALA:C	2.60	0.44
1:G:308:ARG:NH1	1:G:382:ASN:HD21	2.15	0.44
1:G:460:GLN:O	1:G:461:ALA:C	2.60	0.44
3:M:189:TRP:O	3:M:193:ILE:HG22	2.17	0.44
1:A:94:LEU:O	1:A:98:THR:HG23	2.18	0.44
1:A:376:HIS:CB	1:A:458:THR:HG22	2.46	0.44
3:C:85:VAL:O	3:C:85:VAL:CG1	2.64	0.44
1:D:202:GLN:O	1:D:206:GLY:N	2.44	0.44
3:F:179:LEU:HD23	3:F:291:VAL:HG11	1.98	0.44
3:F:237:HIS:HE1	3:F:250:PRO:HD2	1.82	0.44
1:G:402:ASN:OD1	1:G:433:GLY:HA3	2.17	0.44
3:I:121:SER:O	3:I:125:VAL:HG23	2.17	0.44
3:M:302:SER:O	3:M:303:GLN:HB3	2.16	0.44
2:B:127:ASN:C	2:B:127:ASN:ND2	2.75	0.44
3:C:212:LEU:HA	3:C:212:LEU:HD23	1.69	0.44
1:D:58:PRO:HA	1:D:61:THR:HB	1.99	0.44
1:G:340:ASP:H	1:G:406:GLN:HE22	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:GLY:HA3	5:A:501:HEM:C1B	2.52	0.44
2:B:137:MET:HG3	10:B:211:HEC:NC	2.33	0.44
1:D:376:HIS:CB	1:D:458:THR:HG22	2.48	0.44
1:K:376:HIS:HB2	1:K:458:THR:HG22	2.00	0.44
3:C:187:PRO:HG2	3:C:189:TRP:CZ2	2.52	0.44
1:D:174:LEU:HD12	1:D:204:TRP:CZ2	2.52	0.44
3:F:130:GLN:HE21	3:F:130:GLN:CA	2.28	0.44
1:G:29:MET:CE	1:G:448:MET:HE3	2.38	0.44
3:I:130:GLN:HA	3:I:130:GLN:NE2	2.31	0.44
3:M:255:ALA:HA	3:M:258:TRP:CD2	2.53	0.44
1:D:342:THR:O	1:D:346:VAL:HG23	2.17	0.44
2:E:127:ASN:HD22	2:E:127:ASN:C	2.25	0.44
3:F:264:LEU:HB2	11:I:323:FC6:N25	2.32	0.44
1:K:94:LEU:O	1:K:98:THR:HG23	2.17	0.44
1:K:367:PRO:HG3	1:K:375:MET:HE3	2.00	0.44
1:D:24:TRP:NE1	1:D:103:GLN:HE22	1.99	0.44
1:D:235:TYR:O	1:D:289:ASN:ND2	2.51	0.44
3:F:229:TYR:CD2	3:F:233:CYS:HB2	2.52	0.44
11:F:323:FC6:N25	3:I:215:PRO:HG3	2.33	0.44
1:G:346:VAL:HG22	5:G:501:HEM:C3D	2.51	0.44
1:D:94:LEU:O	1:D:98:THR:HG23	2.17	0.44
1:G:64:VAL:O	1:G:68:PHE:HB3	2.18	0.44
1:G:200:MET:HG3	1:G:264:LEU:HD11	2.00	0.44
1:K:260:HIS:HB2	1:K:333:ASN:OD1	2.18	0.44
1:D:115:LEU:HB3	1:D:117:PHE:CE2	2.52	0.44
1:D:196:ALA:HB3	2:E:39:VAL:HB	1.98	0.44
1:D:377:SER:H	1:D:454:ASN:HD21	1.65	0.44
1:G:66:PHE:O	1:G:70:GLY:HA3	2.18	0.44
2:H:137:MET:HB2	10:H:211:HEC:C1D	2.48	0.44
3:I:189:TRP:CZ3	3:I:232:THR:HG21	2.52	0.44
1:K:64:VAL:O	1:K:68:PHE:HB3	2.18	0.44
1:G:57:ARG:NH1	5:G:502:HEM:O2A	2.51	0.43
1:G:209:ALA:O	1:G:213:PHE:CB	2.66	0.43
1:K:218:PHE:HA	1:K:221:ILE:HG13	1.99	0.43
1:K:356:MET:HE1	1:K:388:ALA:HB3	2.00	0.43
3:M:163:GLN:HE21	3:M:163:GLN:HA	1.81	0.43
1:D:260:HIS:HB2	1:D:333:ASN:OD1	2.17	0.43
1:D:372:ARG:CZ	1:D:461:ALA:HB1	2.48	0.43
2:E:127:ASN:C	2:E:127:ASN:ND2	2.76	0.43
3:F:282:GLN:HG3	10:F:322:HEC:HBB2	2.00	0.43
1:G:376:HIS:HB2	1:G:458:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:240:GLY:C	3:I:242:GLU:OE1	2.61	0.43
1:K:13:VAL:HA	1:K:16:GLN:NE2	2.31	0.43
3:M:179:LEU:HD22	3:M:283:GLN:HB2	2.00	0.43
3:F:271:ILE:HG12	10:F:321:HEC:HMB1	1.99	0.43
1:G:196:ALA:HB3	2:H:39:VAL:HB	2.00	0.43
1:G:218:PHE:CD2	1:G:221:ILE:HD12	2.54	0.43
1:G:267:TRP:HE1	2:H:36:GLN:HE22	1.65	0.43
1:G:310:LEU:O	1:G:313:SER:HB3	2.18	0.43
5:G:502:HEM:HBB2	5:G:502:HEM:CHC	2.34	0.43
2:H:112:VAL:O	2:H:113:GLY:C	2.61	0.43
3:M:240:GLY:C	3:M:242:GLU:OE1	2.61	0.43
1:A:372:ARG:CZ	1:A:461:ALA:HB1	2.48	0.43
3:C:130:GLN:HA	3:C:130:GLN:NE2	2.33	0.43
1:G:399:MET:HE3	1:G:437:ARG:HB2	2.00	0.43
1:K:226:VAL:HB	1:K:227:PRO:HD3	2.00	0.43
1:A:260:HIS:HB2	1:A:333:ASN:OD1	2.18	0.43
1:A:267:TRP:HE1	2:B:36:GLN:HE22	1.65	0.43
1:A:372:ARG:HH11	1:A:372:ARG:HB2	1.83	0.43
3:C:189:TRP:CH2	3:C:232:THR:CG2	3.02	0.43
1:D:182:ILE:HD12	2:E:163:LEU:HG	2.01	0.43
1:D:227:PRO:HB2	3:F:47:ILE:CD1	2.48	0.43
5:D:502:HEM:HHC	5:D:502:HEM:CBB	2.36	0.43
1:G:238:ARG:HH22	3:I:30:GLY:C	2.25	0.43
2:H:50:THR:O	2:H:51:ALA:C	2.62	0.43
1:K:264:LEU:HD12	1:K:265:PRO:HD2	1.99	0.43
1:G:239:LEU:HD23	1:G:289:ASN:ND2	2.33	0.43
3:I:47:ILE:H	3:I:47:ILE:HG12	1.62	0.43
1:A:305:PRO:HB3	1:A:382:ASN:HD22	1.83	0.43
10:C:321:HEC:HHD	10:C:321:HEC:HBC2	2.00	0.43
11:C:323:FC6:C21	3:M:215:PRO:HG3	2.48	0.43
1:D:308:ARG:NH1	1:D:382:ASN:HD21	2.17	0.43
2:E:116:TYR:CE2	3:F:145:ILE:CG2	2.95	0.43
1:G:195:GLY:HA2	2:H:92:SER:HB2	2.00	0.43
2:H:36:GLN:O	2:H:40:ASN:ND2	2.51	0.43
3:M:117:TYR:CE1	3:M:131:ALA:HB2	2.54	0.43
1:A:295:SER:HA	1:A:298:TRP:NE1	2.34	0.43
1:A:323:GLU:HG2	1:A:327:MET:HE2	2.01	0.43
1:A:351:LEU:O	1:A:355:ALA:HB3	2.19	0.43
2:B:116:TYR:HE2	3:C:145:ILE:CG2	2.28	0.43
3:C:159:ASN:OD1	3:C:159:ASN:C	2.62	0.43
1:D:460:GLN:O	1:D:461:ALA:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:127:ASN:C	2:H:127:ASN:ND2	2.76	0.43
1:K:61:THR:HG22	1:K:62:ASN:N	2.34	0.43
1:K:64:VAL:HG21	5:K:502:HEM:C2C	2.53	0.43
1:K:66:PHE:O	1:K:70:GLY:HA3	2.18	0.43
1:A:152:ARG:HH12	2:B:11:VAL:CG2	2.32	0.43
1:A:413:ILE:HG22	1:A:414:ASN:O	2.19	0.43
1:D:305:PRO:HB3	1:D:382:ASN:HD22	1.84	0.43
3:I:37:ASP:HB3	3:I:38:GLN:H	1.69	0.43
3:C:255:ALA:HA	3:C:258:TRP:CD2	2.54	0.43
1:D:256:PRO:HB2	1:D:272:GLY:HA3	2.00	0.43
1:K:250:VAL:HG13	1:K:275:MET:HE2	2.00	0.43
1:A:227:PRO:HB2	3:C:47:ILE:HD12	2.01	0.42
1:D:108:LEU:HD12	1:D:108:LEU:HA	1.93	0.42
3:F:269:GLN:HG2	11:F:323:FC6:N24	2.34	0.42
2:H:124:HIS:HE1	10:H:211:HEC:C1A	2.32	0.42
1:A:193:TYR:CE1	1:A:201:VAL:HG11	2.54	0.42
3:C:157:PHE:HA	3:C:158:PRO:HD3	1.79	0.42
1:D:399:MET:HE3	1:D:437:ARG:HB2	2.01	0.42
1:K:356:MET:HE3	1:K:388:ALA:HB1	1.99	0.42
1:A:64:VAL:O	1:A:68:PHE:HB3	2.19	0.42
1:D:128:TRP:CG	1:D:129:PRO:HD3	2.55	0.42
3:F:130:GLN:HA	3:F:130:GLN:NE2	2.34	0.42
1:G:64:VAL:HG21	5:G:502:HEM:C2C	2.54	0.42
2:H:129:ARG:HD3	2:H:135:SER:O	2.19	0.42
2:H:143:LEU:HB2	2:H:185:MET:HE2	2.00	0.42
2:H:189:VAL:O	2:H:193:GLN:HG2	2.19	0.42
1:K:62:ASN:HD21	1:K:125:GLU:HG3	1.83	0.42
4:U:713:UNK:O	4:U:714:UNK:C	2.66	0.42
4:Z:720:UNK:C	4:Z:722:UNK:H	2.33	0.42
1:D:60:HIS:O	1:D:64:VAL:HB	2.19	0.42
1:D:193:TYR:CE1	1:D:201:VAL:HG11	2.54	0.42
1:D:267:TRP:HE1	2:E:36:GLN:HE22	1.67	0.42
3:F:47:ILE:H	3:F:47:ILE:HG12	1.62	0.42
3:F:209:LEU:O	3:F:253:ASN:HA	2.20	0.42
1:G:13:VAL:HA	1:G:16:GLN:NE2	2.34	0.42
1:G:61:THR:HG22	1:G:62:ASN:N	2.34	0.42
1:K:200:MET:HG3	1:K:264:LEU:HD11	2.01	0.42
1:A:84:THR:HG21	1:A:161:ASN:HD21	1.84	0.42
2:B:140:TYR:CE1	10:B:211:HEC:HBB2	2.54	0.42
3:C:221:ASP:OD2	2:H:47:LYS:HE2	2.19	0.42
1:G:60:HIS:O	1:G:64:VAL:HB	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:227:PRO:HB2	3:I:47:ILE:CD1	2.50	0.42
1:G:256:PRO:HB2	1:G:272:GLY:HA3	2.00	0.42
1:K:319:MET:HG3	1:K:320:SER:N	2.30	0.42
1:A:379:GLY:O	1:A:383:THR:HG23	2.20	0.42
1:G:294:LEU:HD22	1:G:311:VAL:HG21	2.01	0.42
2:H:183:THR:O	2:H:186:ASP:HB2	2.19	0.42
4:Y:728:UNK:C	4:Y:730:UNK:N	2.83	0.42
1:A:159:VAL:HA	1:A:162:TRP:CD2	2.55	0.42
3:C:152:LYS:O	3:C:159:ASN:HB2	2.19	0.42
3:C:240:GLY:HA3	3:C:242:GLU:OE1	2.20	0.42
1:D:356:MET:HE1	1:D:388:ALA:HB3	2.00	0.42
3:F:99:TRP:O	3:F:103:VAL:HG23	2.19	0.42
3:F:121:SER:O	3:F:125:VAL:HG23	2.19	0.42
3:F:189:TRP:CD1	10:F:321:HEC:HBB2	2.55	0.42
1:K:15:ARG:HG2	1:K:370:PHE:CZ	2.55	0.42
1:K:373:GLU:CD	1:K:373:GLU:H	2.26	0.42
2:B:25:GLY:HA2	2:B:28:THR:HG22	2.02	0.42
1:D:22:VAL:O	1:D:26:ILE:HG12	2.19	0.42
1:D:218:PHE:HA	1:D:221:ILE:HG13	2.02	0.42
1:D:252:ILE:HD11	2:E:22:VAL:HG22	2.02	0.42
2:E:48:PRO:HG3	2:E:166:PRO:HD2	2.02	0.42
3:F:277:GLY:HA3	10:F:322:HEC:O1D	2.19	0.42
1:G:325:PRO:CD	5:G:501:HEM:HBB2	2.44	0.42
4:U:720:UNK:C	4:U:722:UNK:N	2.83	0.42
2:B:112:VAL:O	2:B:113:GLY:C	2.61	0.42
1:G:199:ALA:HA	2:H:98:PHE:CZ	2.54	0.42
3:I:159:ASN:OD1	3:I:159:ASN:C	2.62	0.42
3:M:37:ASP:HB3	3:M:38:GLN:H	1.68	0.42
1:A:128:TRP:CE2	1:A:183:PRO:HB3	2.55	0.42
1:A:239:LEU:HD23	1:A:289:ASN:ND2	2.33	0.42
1:A:376:HIS:HB2	1:A:458:THR:HG22	2.01	0.42
3:F:85:VAL:O	3:F:85:VAL:CG1	2.68	0.42
3:F:157:PHE:HA	3:F:158:PRO:HD3	1.81	0.42
3:F:224:ALA:O	3:F:228:VAL:HG23	2.19	0.42
1:G:359:ILE:HD12	1:G:384:HIS:HE1	1.85	0.42
3:I:241:GLY:N	3:I:242:GLU:OE1	2.53	0.42
3:C:167:TRP:NE1	3:C:182:ARG:HG2	2.34	0.41
1:D:76:THR:CG2	1:D:221:ILE:HG12	2.36	0.41
3:F:24:ILE:HD12	3:F:59:PHE:CD2	2.55	0.41
2:H:43:VAL:O	2:H:46:MET:HB3	2.19	0.41
2:L:183:THR:O	2:L:186:ASP:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:MET:HE1	1:A:388:ALA:HB3	2.02	0.41
3:C:179:LEU:HD22	3:C:283:GLN:HB2	2.02	0.41
1:G:170:THR:HG21	1:G:212:PHE:CE2	2.54	0.41
1:G:335:LEU:CD2	4:Y:710:UNK:CB	2.92	0.41
2:L:120:TRP:NE1	2:L:131:VAL:HG11	2.35	0.41
2:B:129:ARG:O	2:B:133:PRO:HA	2.20	0.41
3:C:47:ILE:H	3:C:47:ILE:HG12	1.60	0.41
1:D:287:MET:HG3	1:D:288:ILE:N	2.35	0.41
1:D:418:THR:HG23	3:F:134:MET:HE3	2.02	0.41
2:E:80:THR:HA	2:E:84:GLY:O	2.19	0.41
2:E:109:LEU:O	2:E:112:VAL:HG22	2.20	0.41
3:F:212:LEU:HD23	3:F:212:LEU:HA	1.86	0.41
1:G:56:LEU:HD23	1:G:56:LEU:HA	1.90	0.41
3:I:89:TYR:HA	3:I:101:ARG:HH12	1.85	0.41
1:A:287:MET:HG3	1:A:288:ILE:N	2.35	0.41
3:C:240:GLY:CA	3:C:242:GLU:OE1	2.68	0.41
1:D:243:HIS:HD2	1:D:282:PRO:O	2.03	0.41
1:D:319:MET:HG3	1:D:320:SER:N	2.31	0.41
3:I:255:ALA:HA	3:I:258:TRP:CD2	2.55	0.41
1:K:237:TYR:CZ	1:K:241:ILE:HD11	2.56	0.41
1:D:29:MET:CE	1:D:448:MET:HE3	2.40	0.41
1:K:454:ASN:O	1:K:458:THR:CG2	2.66	0.41
3:M:130:GLN:HE21	3:M:130:GLN:CA	2.23	0.41
1:A:376:HIS:HB3	1:A:454:ASN:ND2	2.35	0.41
3:F:250:PRO:HG3	10:F:321:HEC:HBA1	2.02	0.41
1:G:110:ALA:O	1:G:114:PRO:HD2	2.21	0.41
1:G:367:PRO:HG3	1:G:375:MET:HE3	2.02	0.41
3:M:47:ILE:H	3:M:47:ILE:HG12	1.62	0.41
1:A:29:MET:SD	1:A:448:MET:HG3	2.60	0.41
1:A:174:LEU:HD12	1:A:204:TRP:CZ2	2.56	0.41
1:D:84:THR:HG21	1:D:161:ASN:HD21	1.85	0.41
1:D:199:ALA:HA	2:E:98:PHE:CZ	2.55	0.41
1:G:319:MET:HG3	1:G:320:SER:N	2.32	0.41
1:G:414:ASN:HD21	1:G:420:THR:HG23	1.86	0.41
1:K:55:ARG:NH2	2:L:62:ARG:HD2	2.35	0.41
2:L:15:THR:HA	2:L:18:MET:HE3	2.03	0.41
3:M:85:VAL:O	3:M:85:VAL:CG1	2.69	0.41
1:A:218:PHE:HA	1:A:221:ILE:HG13	2.02	0.41
3:C:179:LEU:HD23	3:C:291:VAL:HG11	2.02	0.41
1:D:64:VAL:HG11	5:D:502:HEM:CHD	2.51	0.41
1:D:170:THR:HB	2:E:22:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:43:VAL:O	2:E:46:MET:HB3	2.21	0.41
10:F:321:HEC:HHD	10:F:321:HEC:HBC2	2.03	0.41
1:G:159:VAL:HA	1:G:162:TRP:CD2	2.55	0.41
1:G:324:GLY:HA3	5:G:501:HEM:C1B	2.55	0.41
1:K:324:GLY:HA3	5:K:501:HEM:C1B	2.56	0.41
2:L:137:MET:HB2	10:L:211:HEC:C1D	2.51	0.41
1:A:64:VAL:HG21	5:A:502:HEM:C2C	2.55	0.41
1:A:84:THR:HG21	1:A:161:ASN:ND2	2.35	0.41
1:A:269:GLN:NE2	3:C:95:GLN:HE22	2.19	0.41
2:B:143:LEU:HB2	2:B:185:MET:HE2	2.02	0.41
2:B:152:ASP:HA	2:B:155:LYS:HE3	2.02	0.41
1:D:57:ARG:NH1	5:D:502:HEM:O2A	2.54	0.41
3:F:239:GLN:OE1	3:F:239:GLN:N	2.49	0.41
2:H:15:THR:HA	2:H:18:MET:HE3	2.03	0.41
2:H:43:VAL:O	2:H:44:GLU:C	2.63	0.41
2:H:74:ARG:HA	2:H:75:PRO:HD3	1.86	0.41
1:K:209:ALA:O	1:K:213:PHE:HB3	2.21	0.41
1:K:243:HIS:HD2	1:K:282:PRO:O	2.03	0.41
1:K:281:ALA:CB	1:K:282:PRO:HD3	2.42	0.41
1:K:305:PRO:HB3	1:K:382:ASN:HD22	1.86	0.41
4:Z:726:UNK:C	4:Z:728:UNK:N	2.82	0.41
3:C:74:VAL:O	3:C:82:TRP:HZ3	2.01	0.41
3:C:189:TRP:O	3:C:190:GLY:C	2.64	0.41
1:D:242:VAL:HG13	3:F:23:LEU:HD13	2.03	0.41
1:D:327:MET:HE3	1:D:327:MET:HB2	1.95	0.41
2:H:80:THR:HA	2:H:84:GLY:O	2.21	0.41
3:I:166:ARG:NH2	3:I:250:PRO:HG3	2.36	0.41
3:I:212:LEU:HA	3:I:212:LEU:HD23	1.84	0.41
1:K:305:PRO:O	1:K:308:ARG:HB2	2.20	0.41
1:A:22:VAL:O	1:A:26:ILE:HG12	2.21	0.40
1:D:376:HIS:HB2	1:D:458:THR:HG22	2.03	0.40
2:E:88:VAL:HG12	2:E:90:GLY:H	1.86	0.40
3:M:89:TYR:CD1	3:M:101:ARG:NH1	2.88	0.40
1:D:301:LEU:HD21	1:D:311:VAL:HG21	2.04	0.40
1:G:108:LEU:HD12	1:G:108:LEU:HA	1.90	0.40
3:F:163:GLN:HE21	3:F:163:GLN:HA	1.86	0.40
1:G:285:GLY:O	1:G:289:ASN:HB2	2.22	0.40
1:G:349:GLY:O	1:G:353:TRP:HB3	2.22	0.40
3:I:117:TYR:CE1	3:I:131:ALA:HB2	2.56	0.40
3:M:157:PHE:HA	3:M:158:PRO:HD3	1.83	0.40
1:A:56:LEU:HD23	1:A:56:LEU:HA	1.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:GLN:HE21	2:B:36:GLN:HB2	1.75	0.40
3:C:75:LEU:HD22	3:C:86:LEU:HD12	2.03	0.40
10:F:321:HEC:HBB3	10:F:321:HEC:HMB3	2.04	0.40
1:G:260:HIS:HB2	1:G:333:ASN:OD1	2.21	0.40
3:M:79:LEU:O	3:M:82:TRP:HB2	2.20	0.40
1:D:84:THR:HG21	1:D:161:ASN:ND2	2.36	0.40
1:D:218:PHE:CZ	1:D:354:VAL:HG13	2.57	0.40
1:D:310:LEU:O	1:D:313:SER:HB3	2.21	0.40
1:G:458:THR:O	1:G:461:ALA:CB	2.70	0.40
2:H:148:LEU:HD11	2:H:187:ALA:HB2	2.03	0.40
3:I:237:HIS:HE1	3:I:250:PRO:HD2	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:34:GLY:CA	3:I:39:THR:OG1[1_556]	2.10	0.10

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	464/474 (98%)	432 (93%)	27 (6%)	5 (1%)	11	43
1	D	461/474 (97%)	430 (93%)	26 (6%)	5 (1%)	11	43
1	G	463/474 (98%)	428 (92%)	30 (6%)	5 (1%)	11	43
1	K	463/474 (98%)	430 (93%)	28 (6%)	5 (1%)	11	43
2	B	195/203 (96%)	185 (95%)	8 (4%)	2 (1%)	12	45
2	E	195/203 (96%)	186 (95%)	7 (4%)	2 (1%)	12	45
2	H	195/203 (96%)	184 (94%)	9 (5%)	2 (1%)	12	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	195/203 (96%)	185 (95%)	8 (4%)	2 (1%)	12	45
3	C	301/311 (97%)	276 (92%)	17 (6%)	8 (3%)	4	25
3	F	301/311 (97%)	276 (92%)	19 (6%)	6 (2%)	6	31
3	I	301/311 (97%)	276 (92%)	19 (6%)	6 (2%)	6	31
3	M	301/311 (97%)	274 (91%)	20 (7%)	7 (2%)	5	29
All	All	3835/3952 (97%)	3562 (93%)	218 (6%)	55 (1%)	9	39

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	461	ALA
1	A	465	ALA
2	B	44	GLU
3	C	29	LYS
3	C	33	ALA
3	C	37	ASP
1	D	461	ALA
1	D	465	ALA
2	E	44	GLU
3	F	29	LYS
3	F	33	ALA
3	F	37	ASP
1	G	461	ALA
1	G	465	ALA
2	H	44	GLU
3	I	29	LYS
3	I	33	ALA
3	I	37	ASP
1	K	461	ALA
1	K	465	ALA
2	L	44	GLU
3	M	29	LYS
3	M	33	ALA
3	M	37	ASP
3	C	36	THR
3	C	82	TRP
3	F	36	THR
3	F	82	TRP
3	I	36	THR
3	I	82	TRP

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Mol	Chain	Res	Type
3	M	36	THR
3	M	82	TRP
3	M	190	GLY
2	B	7	LEU
1	D	236	SER
2	E	7	LEU
1	G	236	SER
2	H	7	LEU
1	K	236	SER
2	L	7	LEU
3	C	42	HIS
3	F	42	HIS
3	I	42	HIS
3	M	42	HIS
1	A	236	SER
3	C	301	LEU
1	D	466	GLU
1	G	466	GLU
1	K	466	GLU
1	A	463	LYS
1	A	466	GLU
1	D	463	LYS
1	G	463	LYS
1	K	463	LYS
3	C	238	GLY

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	374/379 (99%)	331 (88%)	43 (12%)	5	24
1	D	371/379 (98%)	329 (89%)	42 (11%)	5	24
1	G	373/379 (98%)	330 (88%)	43 (12%)	5	24
1	K	373/379 (98%)	331 (89%)	42 (11%)	5	24
2	B	166/172 (96%)	145 (87%)	21 (13%)	4	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	166/172 (96%)	143 (86%)	23 (14%)	3	17
2	H	166/172 (96%)	144 (87%)	22 (13%)	4	19
2	L	166/172 (96%)	144 (87%)	22 (13%)	4	19
3	C	227/234 (97%)	196 (86%)	31 (14%)	3	18
3	F	227/234 (97%)	198 (87%)	29 (13%)	4	20
3	I	227/234 (97%)	197 (87%)	30 (13%)	4	19
3	M	227/234 (97%)	198 (87%)	29 (13%)	4	20
All	All	3063/3140 (98%)	2686 (88%)	377 (12%)	4	22

All (377) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	48	LEU
1	A	50	TRP
1	A	57	ARG
1	A	59	LEU
1	A	61	THR
1	A	64	VAL
1	A	73	LEU
1	A	84	THR
1	A	87	THR
1	A	104	LEU
1	A	107	LEU
1	A	108	LEU
1	A	115	LEU
1	A	118	THR
1	A	120	SER
1	A	125	GLU
1	A	154	VAL
1	A	159	VAL
1	A	170	THR
1	A	174	LEU
1	A	192	LEU
1	A	200	MET
1	A	210	VAL
1	A	243	HIS
1	A	248	ILE
1	A	271	LEU
1	A	275	MET

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Mol	Chain	Res	Type
1	A	278	ILE
1	A	289	ASN
1	A	294	LEU
1	A	302	ARG
1	A	313	SER
1	A	319	MET
1	A	335	LEU
1	A	336	SER
1	A	356	MET
1	A	357	VAL
1	A	358	SER
1	A	372	ARG
1	A	373	GLU
1	A	427	LEU
1	A	458	THR
2	B	7	LEU
2	B	11	VAL
2	B	13	LEU
2	B	16	LEU
2	B	22	VAL
2	B	24	ILE
2	B	27	LEU
2	B	54	LEU
2	B	62	ARG
2	B	66	VAL
2	B	92	SER
2	B	93	VAL
2	B	103	LYS
2	B	112	VAL
2	B	115	ARG
2	B	129	ARG
2	B	134	GLU
2	B	177	ASP
2	B	178	SER
2	B	193	GLN
2	B	194	VAL
3	C	1	MET
3	C	3	THR
3	C	11	LEU
3	C	23	LEU
3	C	24	ILE
3	C	35	THR

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Mol	Chain	Res	Type
3	C	39	THR
3	C	47	ILE
3	C	54	LEU
3	C	56	ARG
3	C	70	ILE
3	C	71	LEU
3	C	83	LYS
3	C	85	VAL
3	C	96	GLU
3	C	100	GLU
3	C	103	VAL
3	C	123	GLU
3	C	130	GLN
3	C	145	ILE
3	C	163	GLN
3	C	175	LYS
3	C	179	LEU
3	C	182	ARG
3	C	186	MET
3	C	193	ILE
3	C	201	VAL
3	C	251	LYS
3	C	264	LEU
3	C	301	LEU
3	C	302	SER
1	D	48	LEU
1	D	50	TRP
1	D	57	ARG
1	D	59	LEU
1	D	61	THR
1	D	64	VAL
1	D	73	LEU
1	D	84	THR
1	D	87	THR
1	D	104	LEU
1	D	107	LEU
1	D	108	LEU
1	D	115	LEU
1	D	118	THR
1	D	120	SER
1	D	125	GLU
1	D	154	VAL

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Mol	Chain	Res	Type
1	D	159	VAL
1	D	170	THR
1	D	174	LEU
1	D	192	LEU
1	D	200	MET
1	D	210	VAL
1	D	243	HIS
1	D	248	ILE
1	D	271	LEU
1	D	275	MET
1	D	278	ILE
1	D	287	MET
1	D	289	ASN
1	D	294	LEU
1	D	313	SER
1	D	319	MET
1	D	335	LEU
1	D	336	SER
1	D	356	MET
1	D	357	VAL
1	D	358	SER
1	D	372	ARG
1	D	373	GLU
1	D	427	LEU
1	D	458	THR
2	E	7	LEU
2	E	11	VAL
2	E	13	LEU
2	E	16	LEU
2	E	22	VAL
2	E	24	ILE
2	E	27	LEU
2	E	36	GLN
2	E	54	LEU
2	E	62	ARG
2	E	66	VAL
2	E	80	THR
2	E	92	SER
2	E	93	VAL
2	E	103	LYS
2	E	112	VAL
2	E	115	ARG

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Mol	Chain	Res	Type
2	E	129	ARG
2	E	134	GLU
2	E	177	ASP
2	E	178	SER
2	E	193	GLN
2	E	194	VAL
3	F	1	MET
3	F	3	THR
3	F	11	LEU
3	F	23	LEU
3	F	24	ILE
3	F	35	THR
3	F	39	THR
3	F	47	ILE
3	F	54	LEU
3	F	56	ARG
3	F	70	ILE
3	F	71	LEU
3	F	83	LYS
3	F	85	VAL
3	F	100	GLU
3	F	103	VAL
3	F	123	GLU
3	F	130	GLN
3	F	145	ILE
3	F	163	GLN
3	F	175	LYS
3	F	179	LEU
3	F	182	ARG
3	F	186	MET
3	F	193	ILE
3	F	201	VAL
3	F	264	LEU
3	F	301	LEU
3	F	302	SER
1	G	6	SER
1	G	48	LEU
1	G	50	TRP
1	G	57	ARG
1	G	59	LEU
1	G	61	THR
1	G	64	VAL

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Mol	Chain	Res	Type
1	G	73	LEU
1	G	84	THR
1	G	87	THR
1	G	104	LEU
1	G	107	LEU
1	G	108	LEU
1	G	115	LEU
1	G	118	THR
1	G	120	SER
1	G	125	GLU
1	G	154	VAL
1	G	159	VAL
1	G	170	THR
1	G	174	LEU
1	G	192	LEU
1	G	200	MET
1	G	210	VAL
1	G	243	HIS
1	G	248	ILE
1	G	271	LEU
1	G	275	MET
1	G	278	ILE
1	G	287	MET
1	G	289	ASN
1	G	294	LEU
1	G	313	SER
1	G	319	MET
1	G	335	LEU
1	G	336	SER
1	G	356	MET
1	G	357	VAL
1	G	358	SER
1	G	372	ARG
1	G	373	GLU
1	G	427	LEU
1	G	458	THR
2	H	7	LEU
2	H	11	VAL
2	H	13	LEU
2	H	16	LEU
2	H	22	VAL
2	H	27	LEU

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Mol	Chain	Res	Type
2	H	36	GLN
2	H	54	LEU
2	H	62	ARG
2	H	66	VAL
2	H	80	THR
2	H	92	SER
2	H	93	VAL
2	H	103	LYS
2	H	112	VAL
2	H	115	ARG
2	H	129	ARG
2	H	134	GLU
2	H	177	ASP
2	H	178	SER
2	H	193	GLN
2	H	194	VAL
3	I	1	MET
3	I	3	THR
3	I	11	LEU
3	I	23	LEU
3	I	24	ILE
3	I	35	THR
3	I	39	THR
3	I	47	ILE
3	I	54	LEU
3	I	56	ARG
3	I	70	ILE
3	I	71	LEU
3	I	83	LYS
3	I	85	VAL
3	I	100	GLU
3	I	103	VAL
3	I	123	GLU
3	I	130	GLN
3	I	145	ILE
3	I	163	GLN
3	I	175	LYS
3	I	179	LEU
3	I	182	ARG
3	I	186	MET
3	I	193	ILE
3	I	201	VAL

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Mol	Chain	Res	Type
3	I	222	LEU
3	I	242	GLU
3	I	264	LEU
3	I	301	LEU
1	K	48	LEU
1	K	50	TRP
1	K	57	ARG
1	K	59	LEU
1	K	61	THR
1	K	64	VAL
1	K	73	LEU
1	K	84	THR
1	K	87	THR
1	K	104	LEU
1	K	107	LEU
1	K	108	LEU
1	K	115	LEU
1	K	118	THR
1	K	120	SER
1	K	125	GLU
1	K	154	VAL
1	K	159	VAL
1	K	170	THR
1	K	174	LEU
1	K	192	LEU
1	K	200	MET
1	K	210	VAL
1	K	243	HIS
1	K	248	ILE
1	K	271	LEU
1	K	275	MET
1	K	278	ILE
1	K	287	MET
1	K	289	ASN
1	K	294	LEU
1	K	313	SER
1	K	319	MET
1	K	335	LEU
1	K	336	SER
1	K	356	MET
1	K	357	VAL
1	K	358	SER

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Mol	Chain	Res	Type
1	K	372	ARG
1	K	373	GLU
1	K	427	LEU
1	K	458	THR
2	L	7	LEU
2	L	11	VAL
2	L	13	LEU
2	L	16	LEU
2	L	22	VAL
2	L	24	ILE
2	L	27	LEU
2	L	36	GLN
2	L	54	LEU
2	L	62	ARG
2	L	66	VAL
2	L	80	THR
2	L	92	SER
2	L	93	VAL
2	L	103	LYS
2	L	112	VAL
2	L	129	ARG
2	L	134	GLU
2	L	177	ASP
2	L	178	SER
2	L	193	GLN
2	L	194	VAL
3	M	1	MET
3	M	3	THR
3	M	11	LEU
3	M	23	LEU
3	M	24	ILE
3	M	35	THR
3	M	39	THR
3	M	47	ILE
3	M	54	LEU
3	M	56	ARG
3	M	70	ILE
3	M	71	LEU
3	M	83	LYS
3	M	85	VAL
3	M	100	GLU
3	M	103	VAL

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Mol	Chain	Res	Type
3	M	123	GLU
3	M	130	GLN
3	M	145	ILE
3	M	163	GLN
3	M	175	LYS
3	M	179	LEU
3	M	182	ARG
3	M	186	MET
3	M	193	ILE
3	M	201	VAL
3	M	264	LEU
3	M	301	LEU
3	M	302	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (128) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	38	GLN
1	A	62	ASN
1	A	82	GLN
1	A	103	GLN
1	A	156	HIS
1	A	161	ASN
1	A	175	HIS
1	A	178	ASN
1	A	243	HIS
1	A	289	ASN
1	A	299	HIS
1	A	376	HIS
1	A	382	ASN
1	A	406	GLN
1	A	414	ASN
1	A	431	HIS
1	A	454	ASN
1	A	460	GLN
2	B	10	ASN
2	B	29	GLN
2	B	36	GLN
2	B	71	GLN
2	B	127	ASN
2	B	193	GLN

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Mol	Chain	Res	Type
3	C	42	HIS
3	C	95	GLN
3	C	98	GLN
3	C	105	GLN
3	C	130	GLN
3	C	141	ASN
3	C	163	GLN
3	C	273	HIS
3	C	292	HIS
1	D	16	GLN
1	D	62	ASN
1	D	82	GLN
1	D	103	GLN
1	D	161	ASN
1	D	175	HIS
1	D	178	ASN
1	D	243	HIS
1	D	289	ASN
1	D	299	HIS
1	D	376	HIS
1	D	382	ASN
1	D	406	GLN
1	D	414	ASN
1	D	431	HIS
1	D	454	ASN
1	D	460	GLN
2	E	10	ASN
2	E	29	GLN
2	E	36	GLN
2	E	127	ASN
2	E	193	GLN
3	F	105	GLN
3	F	130	GLN
3	F	163	GLN
3	F	227	ASN
3	F	268	GLN
3	F	282	GLN
3	F	292	HIS
1	G	16	GLN
1	G	62	ASN
1	G	82	GLN
1	G	103	GLN

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Mol	Chain	Res	Type
1	G	156	HIS
1	G	161	ASN
1	G	175	HIS
1	G	178	ASN
1	G	243	HIS
1	G	289	ASN
1	G	299	HIS
1	G	376	HIS
1	G	382	ASN
1	G	406	GLN
1	G	414	ASN
1	G	431	HIS
1	G	454	ASN
1	G	460	GLN
2	H	10	ASN
2	H	29	GLN
2	H	36	GLN
2	H	71	GLN
2	H	127	ASN
2	H	193	GLN
3	I	42	HIS
3	I	98	GLN
3	I	105	GLN
3	I	130	GLN
3	I	163	GLN
3	I	266	GLN
3	I	268	GLN
3	I	282	GLN
3	I	292	HIS
1	K	16	GLN
1	K	38	GLN
1	K	62	ASN
1	K	82	GLN
1	K	103	GLN
1	K	156	HIS
1	K	161	ASN
1	K	175	HIS
1	K	178	ASN
1	K	243	HIS
1	K	289	ASN
1	K	299	HIS
1	K	376	HIS

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Mol	Chain	Res	Type
1	K	382	ASN
1	K	406	GLN
1	K	414	ASN
1	K	431	HIS
1	K	454	ASN
1	K	460	GLN
2	L	10	ASN
2	L	29	GLN
2	L	36	GLN
2	L	71	GLN
2	L	193	GLN
3	M	98	GLN
3	M	105	GLN
3	M	130	GLN
3	M	163	GLN
3	M	268	GLN
3	M	276	ASN
3	M	282	GLN
3	M	292	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 44 ligands modelled in this entry, 12 are monoatomic - leaving 32 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	$\# Z > 2$
10	HEC	E	211	2	46,50,50	1.94	7 (15%)	58,82,82	1.89	6 (10%)
8	PEO	D	508	6,5	1,1,1	0.30	0	-		
8	PEO	K	508	6,5	1,1,1	0.29	0	-		
9	PO4	G	506	-	4,4,4	0.61	0	6,6,6	1.01	0
11	FC6	I	323	-	12,12,12	1.02	0	-		
10	HEC	L	211	2	46,50,50	1.94	7 (15%)	58,82,82	1.96	8 (13%)
11	FC6	F	323	-	12,12,12	1.03	0	-		
8	PEO	A	508	6,5	1,1,1	0.26	0	-		
10	HEC	C	322	3	46,50,50	1.90	8 (17%)	58,82,82	1.99	11 (18%)
11	FC6	M	323	-	12,12,12	1.24	2 (16%)	-		
5	HEM	K	502	7,1	50,50,50	1.83	10 (20%)	67,82,82	1.42	11 (16%)
5	HEM	D	502	7,1	50,50,50	1.80	8 (16%)	67,82,82	1.36	7 (10%)
10	HEC	B	211	2	46,50,50	1.94	7 (15%)	58,82,82	2.16	8 (13%)
10	HEC	I	322	3	46,50,50	1.90	6 (13%)	58,82,82	1.85	14 (24%)
5	HEM	K	501	7,1,8	50,50,50	1.86	10 (20%)	67,82,82	1.20	3 (4%)
10	HEC	F	321	3	46,50,50	1.85	6 (13%)	58,82,82	1.82	8 (13%)
11	FC6	C	323	-	12,12,12	1.27	1 (8%)	-		
5	HEM	A	501	8,1,7	50,50,50	1.79	11 (22%)	67,82,82	1.24	5 (7%)
10	HEC	C	321	3	46,50,50	1.95	7 (15%)	58,82,82	1.92	10 (17%)
9	PO4	K	506	-	4,4,4	0.75	0	6,6,6	0.85	0
10	HEC	I	321	3	46,50,50	1.95	7 (15%)	58,82,82	2.01	10 (17%)
5	HEM	G	502	7,1	50,50,50	1.74	9 (18%)	67,82,82	1.30	5 (7%)
10	HEC	M	322	3	46,50,50	1.97	8 (17%)	58,82,82	1.98	12 (20%)
5	HEM	G	501	7,1,8	50,50,50	1.82	9 (18%)	67,82,82	1.24	5 (7%)
9	PO4	D	506	-	4,4,4	0.77	0	6,6,6	0.70	0
10	HEC	F	322	3	46,50,50	1.90	9 (19%)	58,82,82	1.86	13 (22%)
10	HEC	H	211	2	46,50,50	1.99	10 (21%)	58,82,82	2.08	12 (20%)
9	PO4	A	506	-	4,4,4	0.85	0	6,6,6	1.20	1 (16%)
10	HEC	M	321	3	46,50,50	1.81	6 (13%)	58,82,82	2.29	9 (15%)
5	HEM	D	501	8,1,7	50,50,50	1.93	9 (18%)	67,82,82	1.21	4 (5%)
5	HEM	A	502	7,1	50,50,50	1.77	14 (28%)	67,82,82	1.47	11 (16%)
8	PEO	G	508	6,5	1,1,1	0.36	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
10	HEC	E	211	2	-	8/14/54/54	-
10	HEC	L	211	2	-	8/14/54/54	-
10	HEC	C	322	3	-	6/14/54/54	-
5	HEM	K	502	7,1	-	3/14/54/54	-
5	HEM	D	502	7,1	-	4/14/54/54	-
10	HEC	B	211	2	-	8/14/54/54	-
10	HEC	I	322	3	-	6/14/54/54	-
5	HEM	K	501	7,1,8	-	8/14/54/54	-
10	HEC	F	321	3	-	6/14/54/54	-
5	HEM	A	501	8,1,7	-	8/14/54/54	-
10	HEC	C	321	3	-	6/14/54/54	-
10	HEC	I	321	3	-	6/14/54/54	-
5	HEM	G	502	7,1	-	2/14/54/54	-
10	HEC	M	322	3	-	6/14/54/54	-
5	HEM	G	501	7,1,8	-	8/14/54/54	-
10	HEC	F	322	3	-	6/14/54/54	-
10	HEC	H	211	2	-	8/14/54/54	-
10	HEC	M	321	3	-	6/14/54/54	-
5	HEM	D	501	8,1,7	-	8/14/54/54	-
5	HEM	A	502	7,1	-	4/14/54/54	-

All (171) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	501	HEM	C3D-C2D	7.93	1.53	1.36
5	D	502	HEM	C3D-C2D	7.67	1.53	1.36
5	K	501	HEM	C3D-C2D	7.61	1.53	1.36
5	G	502	HEM	C3D-C2D	7.60	1.53	1.36
5	K	502	HEM	C3D-C2D	7.55	1.53	1.36
5	G	501	HEM	C3D-C2D	7.37	1.52	1.36
5	A	501	HEM	C3D-C2D	7.26	1.52	1.36
5	A	502	HEM	C3D-C2D	7.22	1.52	1.36
10	I	321	HEC	CAC-C3C	6.93	1.57	1.35
10	C	321	HEC	CAC-C3C	6.74	1.56	1.35
10	M	321	HEC	CAC-C3C	6.62	1.56	1.35
10	I	322	HEC	CAC-C3C	6.54	1.56	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	E	211	HEC	CAC-C3C	6.52	1.56	1.35
10	M	322	HEC	CAC-C3C	6.51	1.56	1.35
10	B	211	HEC	CAC-C3C	6.51	1.56	1.35
10	M	322	HEC	CAB-C3B	6.50	1.56	1.35
10	I	322	HEC	CAB-C3B	6.47	1.56	1.35
10	F	321	HEC	CAC-C3C	6.46	1.56	1.35
10	L	211	HEC	CAB-C3B	6.42	1.55	1.35
10	F	322	HEC	CAB-C3B	6.41	1.55	1.35
10	H	211	HEC	CAC-C3C	6.38	1.55	1.35
10	H	211	HEC	CAB-C3B	6.37	1.55	1.35
10	F	322	HEC	CAC-C3C	6.37	1.55	1.35
10	E	211	HEC	CAB-C3B	6.29	1.55	1.35
10	C	322	HEC	CAB-C3B	6.24	1.55	1.35
10	C	322	HEC	CAC-C3C	6.19	1.55	1.35
10	L	211	HEC	CAC-C3C	6.15	1.55	1.35
10	F	321	HEC	CAB-C3B	6.13	1.54	1.35
10	B	211	HEC	CAB-C3B	6.01	1.54	1.35
10	I	321	HEC	CAB-C3B	6.01	1.54	1.35
10	C	321	HEC	CAB-C3B	5.82	1.53	1.35
10	L	211	HEC	C3D-C2D	5.58	1.53	1.38
10	M	321	HEC	CAB-C3B	5.46	1.52	1.35
10	M	322	HEC	C3D-C2D	5.32	1.52	1.38
10	C	321	HEC	C3D-C2D	5.23	1.52	1.38
10	F	322	HEC	C3D-C2D	5.20	1.52	1.38
10	H	211	HEC	C3D-C2D	5.17	1.52	1.38
10	E	211	HEC	C3D-C2D	5.16	1.52	1.38
5	K	502	HEM	FE-NB	5.00	2.10	1.94
10	I	321	HEC	C3D-C2D	4.98	1.51	1.38
10	F	321	HEC	C3D-C2D	4.85	1.51	1.38
5	G	501	HEM	FE-ND	4.82	2.09	1.94
5	D	501	HEM	FE-ND	4.74	2.09	1.94
5	D	501	HEM	FE-NC	4.66	2.10	1.95
5	A	501	HEM	FE-NA	4.57	2.10	1.95
10	B	211	HEC	C3D-C2D	4.56	1.50	1.38
10	C	322	HEC	C3D-C2D	4.56	1.50	1.38
10	I	322	HEC	C3D-C2D	4.51	1.50	1.38
10	M	321	HEC	C3D-C2D	4.38	1.50	1.38
5	K	501	HEM	FE-ND	3.79	2.06	1.94
5	D	502	HEM	FE-NC	3.74	2.07	1.95
5	K	501	HEM	FE-NC	3.70	2.07	1.95
5	A	501	HEM	FE-NB	3.52	2.05	1.94
5	G	501	HEM	FE-NA	3.29	2.06	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	501	HEM	FE-NB	3.29	2.05	1.94
5	A	502	HEM	FE-NC	3.20	2.05	1.95
5	K	501	HEM	CAB-C3B	3.17	1.55	1.47
5	D	501	HEM	CAC-C3C	3.06	1.55	1.47
5	G	501	HEM	FE-NC	3.06	2.05	1.95
5	D	501	HEM	CAB-C3B	3.04	1.55	1.47
5	D	502	HEM	FE-ND	3.02	2.04	1.94
5	G	502	HEM	FE-NC	3.01	2.05	1.95
5	G	502	HEM	FE-ND	2.94	2.03	1.94
10	H	211	HEC	CMA-C3A	2.92	1.56	1.50
5	D	502	HEM	CAC-C3C	2.92	1.55	1.47
5	A	501	HEM	FE-ND	2.92	2.03	1.94
5	A	502	HEM	C3C-C2C	-2.90	1.31	1.37
5	D	501	HEM	FE-NB	2.90	2.03	1.94
5	K	502	HEM	FE-NA	2.88	2.04	1.95
10	B	211	HEC	C3C-C2C	-2.87	1.31	1.41
5	K	501	HEM	FE-NA	2.79	2.04	1.95
5	K	502	HEM	CAB-C3B	2.78	1.54	1.47
5	K	501	HEM	CAC-C3C	2.75	1.54	1.47
11	C	323	FC6	C26-FE2	-2.74	1.85	1.93
5	G	501	HEM	CAC-C3C	2.73	1.54	1.47
5	G	502	HEM	CAC-C3C	2.70	1.54	1.47
5	G	502	HEM	CMB-C2B	2.66	1.56	1.50
5	K	502	HEM	CAC-C3C	2.64	1.54	1.47
5	D	502	HEM	CMB-C2B	2.63	1.56	1.50
5	G	501	HEM	CAB-C3B	2.61	1.54	1.47
5	D	502	HEM	CAB-C3B	2.61	1.54	1.47
5	A	501	HEM	CAB-C3B	2.58	1.54	1.47
10	I	322	HEC	C3C-C2C	-2.57	1.32	1.41
5	D	502	HEM	C3C-C2C	-2.57	1.31	1.37
10	M	321	HEC	C3C-C2C	-2.53	1.32	1.41
5	G	501	HEM	FE-NB	2.52	2.02	1.94
10	C	321	HEC	C3B-C2B	-2.51	1.32	1.41
10	C	322	HEC	C3C-C2C	-2.49	1.32	1.41
5	G	502	HEM	C3C-C2C	-2.47	1.32	1.37
10	L	211	HEC	C3C-C2C	-2.46	1.32	1.41
10	F	321	HEC	CMB-C2B	2.44	1.55	1.50
10	E	211	HEC	C3C-C2C	-2.43	1.32	1.41
10	H	211	HEC	CMB-C2B	2.43	1.55	1.50
10	M	322	HEC	C2A-C3A	-2.41	1.31	1.36
10	H	211	HEC	C3C-C2C	-2.40	1.33	1.41
11	M	323	FC6	C22-FE2	-2.40	1.86	1.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	502	HEM	CMB-C2B	2.39	1.55	1.50
5	A	502	HEM	CMC-C2C	2.38	1.55	1.50
10	F	322	HEC	CMC-C2C	2.37	1.55	1.50
5	K	502	HEM	C3C-C2C	-2.37	1.32	1.37
5	A	502	HEM	CAC-C3C	2.37	1.53	1.47
10	E	211	HEC	CMB-C2B	2.36	1.55	1.50
10	B	211	HEC	C3B-C2B	-2.36	1.33	1.41
5	A	501	HEM	CAC-C3C	2.36	1.53	1.47
10	M	322	HEC	C3C-C2C	-2.35	1.33	1.41
11	M	323	FC6	C23-FE2	-2.35	1.86	1.93
5	G	502	HEM	CAB-C3B	2.33	1.53	1.47
10	L	211	HEC	C3B-C2B	-2.32	1.33	1.41
5	K	502	HEM	CMC-C2C	2.31	1.55	1.50
5	A	501	HEM	CMA-C3A	2.31	1.55	1.50
10	B	211	HEC	CMA-C3A	2.30	1.55	1.50
5	A	502	HEM	FE-NB	2.30	2.02	1.94
10	F	322	HEC	C3C-C2C	-2.29	1.33	1.41
10	B	211	HEC	CMB-C2B	2.29	1.55	1.50
5	A	501	HEM	CMC-C2C	2.28	1.55	1.50
10	M	322	HEC	C3B-C2B	-2.28	1.33	1.41
10	H	211	HEC	C1B-NB	-2.28	1.35	1.39
10	H	211	HEC	C3B-C2B	-2.27	1.33	1.41
5	K	502	HEM	FE-NC	2.26	2.02	1.95
10	F	321	HEC	C3B-C2B	-2.25	1.33	1.41
10	H	211	HEC	CHB-C1B	-2.23	1.34	1.39
10	C	321	HEC	CMC-C2C	2.22	1.55	1.50
10	C	322	HEC	C3B-C2B	-2.20	1.33	1.41
10	I	321	HEC	O1A-CGA	2.20	1.29	1.22
10	I	321	HEC	CHC-C4B	-2.19	1.34	1.38
10	F	322	HEC	CMA-C3A	2.19	1.55	1.50
10	I	321	HEC	C3C-C2C	-2.19	1.33	1.41
10	E	211	HEC	CMC-C2C	2.18	1.55	1.50
10	M	322	HEC	CMC-C2C	2.18	1.55	1.50
10	L	211	HEC	CMB-C2B	2.18	1.55	1.50
10	I	322	HEC	C3B-C2B	-2.18	1.33	1.41
5	A	502	HEM	FE-ND	2.17	2.01	1.94
5	A	502	HEM	C2A-C3A	-2.17	1.33	1.38
5	A	502	HEM	CAA-C2A	2.17	1.56	1.51
10	F	322	HEC	C3B-C2B	-2.16	1.33	1.41
10	I	321	HEC	CMA-C3A	2.16	1.55	1.50
10	E	211	HEC	C3B-C2B	-2.16	1.33	1.41
10	C	322	HEC	CMC-C2C	2.16	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	501	HEM	CMB-C2B	2.16	1.55	1.50
5	K	501	HEM	CMB-C2B	2.15	1.55	1.50
5	A	501	HEM	C2A-C3A	-2.14	1.33	1.38
5	A	502	HEM	C3B-C2B	-2.14	1.32	1.37
10	M	321	HEC	CMB-C2B	2.13	1.55	1.50
5	A	501	HEM	CMB-C2B	2.13	1.55	1.50
5	G	502	HEM	CMC-C2C	2.12	1.55	1.50
5	D	501	HEM	CMC-C2C	2.12	1.55	1.50
10	F	321	HEC	C3C-C2C	-2.12	1.34	1.41
10	C	322	HEC	CMA-C3A	2.11	1.55	1.50
10	F	322	HEC	CMD-C2D	2.11	1.55	1.50
10	M	321	HEC	C3B-C2B	-2.11	1.34	1.41
10	F	322	HEC	CMB-C2B	2.11	1.55	1.50
5	K	502	HEM	CMB-C2B	2.10	1.55	1.50
5	A	502	HEM	CAB-C3B	2.10	1.53	1.47
5	D	501	HEM	C2A-C3A	-2.10	1.33	1.38
10	M	322	HEC	CMB-C2B	2.10	1.55	1.50
5	A	502	HEM	O1A-CGA	2.10	1.29	1.22
5	G	501	HEM	CMA-C3A	2.09	1.55	1.50
5	K	501	HEM	C2A-C3A	-2.08	1.33	1.38
10	H	211	HEC	CMC-C2C	2.08	1.55	1.50
10	L	211	HEC	CMC-C2C	2.07	1.55	1.50
10	C	321	HEC	C3C-C2C	-2.07	1.34	1.41
5	K	502	HEM	CMA-C3A	2.06	1.55	1.50
10	C	321	HEC	CMB-C2B	2.06	1.55	1.50
5	G	501	HEM	C3C-C2C	-2.03	1.33	1.37
5	A	501	HEM	C3B-C2B	-2.02	1.33	1.37
10	C	322	HEC	C2A-C3A	-2.02	1.32	1.36
10	I	322	HEC	C4C-NC	-2.02	1.35	1.39
5	D	502	HEM	C2A-C3A	-2.01	1.33	1.38
5	K	501	HEM	CMD-C2D	2.01	1.54	1.50
5	G	502	HEM	O1A-CGA	2.00	1.28	1.22
5	A	502	HEM	CMD-C2D	2.00	1.54	1.50

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	211	HEC	CBB-CAB-C3B	-11.24	104.97	127.43
10	M	321	HEC	CBB-CAB-C3B	-10.34	106.78	127.43
10	H	211	HEC	CBB-CAB-C3B	-9.89	107.66	127.43
10	E	211	HEC	CBB-CAB-C3B	-9.37	108.70	127.43
10	L	211	HEC	CBB-CAB-C3B	-9.19	109.06	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	321	HEC	CBB-CAB-C3B	-8.93	109.58	127.43
10	C	321	HEC	CBB-CAB-C3B	-8.51	110.42	127.43
10	C	322	HEC	CBC-CAC-C3C	-8.50	110.44	127.43
10	F	321	HEC	CBB-CAB-C3B	-8.49	110.47	127.43
10	M	321	HEC	CBC-CAC-C3C	-8.26	110.93	127.43
10	C	322	HEC	CBB-CAB-C3B	-7.98	111.48	127.43
10	M	322	HEC	CBB-CAB-C3B	-7.98	111.49	127.43
10	M	322	HEC	CBC-CAC-C3C	-7.82	111.80	127.43
10	F	322	HEC	CBC-CAC-C3C	-7.74	111.96	127.43
10	F	322	HEC	CBB-CAB-C3B	-7.43	112.58	127.43
10	H	211	HEC	CBC-CAC-C3C	-7.40	112.65	127.43
10	B	211	HEC	CBC-CAC-C3C	-7.25	112.95	127.43
10	I	322	HEC	CBB-CAB-C3B	-7.22	113.01	127.43
10	L	211	HEC	CBC-CAC-C3C	-7.10	113.24	127.43
10	E	211	HEC	CBC-CAC-C3C	-6.98	113.48	127.43
10	I	321	HEC	CBC-CAC-C3C	-6.86	113.72	127.43
10	I	322	HEC	CBC-CAC-C3C	-6.55	114.34	127.43
10	C	321	HEC	CBC-CAC-C3C	-6.49	114.46	127.43
10	F	321	HEC	CBC-CAC-C3C	-6.23	114.99	127.43
5	D	501	HEM	C4D-ND-C1D	5.41	111.61	105.21
5	K	501	HEM	C4D-ND-C1D	5.20	111.36	105.21
5	G	501	HEM	C4D-ND-C1D	4.91	111.02	105.21
5	D	502	HEM	C4D-ND-C1D	4.86	110.96	105.21
5	K	502	HEM	C4D-ND-C1D	4.76	110.84	105.21
5	G	502	HEM	C4D-ND-C1D	4.48	110.51	105.21
10	I	321	HEC	CAA-CBA-CGA	-4.47	101.80	113.67
5	A	502	HEM	C4D-ND-C1D	4.47	110.50	105.21
5	A	501	HEM	C4D-ND-C1D	4.46	110.48	105.21
10	F	321	HEC	CAA-CBA-CGA	-4.42	101.94	113.67
10	M	321	HEC	CAA-CBA-CGA	-4.36	102.09	113.67
10	C	321	HEC	CAA-CBA-CGA	-4.16	102.64	113.67
10	M	321	HEC	CHD-C4C-C3C	3.80	131.61	125.21
10	M	321	HEC	CHD-C4C-NC	-3.67	120.46	124.45
10	M	321	HEC	CHB-C4A-NA	3.60	128.37	124.45
5	A	501	HEM	CAD-CBD-CGD	-3.57	104.20	113.67
5	G	501	HEM	CAA-CBA-CGA	-3.52	104.34	113.67
10	I	322	HEC	CAD-CBD-CGD	-3.47	104.46	113.67
10	B	211	HEC	CAD-C3D-C4D	3.40	131.59	124.94
10	M	321	HEC	CBD-CAD-C3D	-3.37	103.23	112.53
10	M	322	HEC	CAA-CBA-CGA	-3.36	104.74	113.67
5	A	502	HEM	CMC-C2C-C1C	3.28	130.50	124.73
10	C	321	HEC	CBD-CAD-C3D	-3.27	103.49	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	321	HEC	CMC-C2C-C1C	-3.13	120.66	125.42
5	D	502	HEM	CBA-CAA-C2A	-3.12	103.92	112.53
5	G	502	HEM	CBA-CAA-C2A	-3.10	103.96	112.53
5	K	501	HEM	CAD-CBD-CGD	-3.06	105.55	113.67
10	C	322	HEC	CAA-CBA-CGA	-2.99	105.73	113.67
5	K	502	HEM	CBA-CAA-C2A	-2.95	104.38	112.53
10	C	322	HEC	CAD-C3D-C4D	2.94	130.69	124.94
10	B	211	HEC	CMC-C2C-C3C	-2.94	119.64	126.55
5	D	501	HEM	CAD-CBD-CGD	-2.87	106.04	113.67
10	M	322	HEC	O2D-CGD-CBD	2.86	123.03	114.00
5	A	501	HEM	O1A-CGA-CBA	-2.84	114.08	123.09
10	I	321	HEC	CHD-C4C-NC	-2.83	121.37	124.45
10	I	321	HEC	C4D-ND-C1D	2.83	110.43	105.82
5	A	502	HEM	CAC-C3C-C4C	2.81	131.53	124.82
5	K	501	HEM	CAA-CBA-CGA	-2.80	106.23	113.67
5	G	501	HEM	CAD-CBD-CGD	-2.80	106.23	113.67
10	I	321	HEC	CBD-CAD-C3D	-2.75	104.92	112.53
10	M	321	HEC	C4D-ND-C1D	2.73	110.27	105.82
10	F	321	HEC	C4D-ND-C1D	2.72	110.26	105.82
5	A	501	HEM	CAA-CBA-CGA	-2.69	106.54	113.67
10	M	322	HEC	O1D-CGD-CBD	-2.69	114.57	123.09
10	L	211	HEC	CBA-CAA-C2A	-2.67	105.16	112.53
5	D	502	HEM	O1A-CGA-CBA	-2.66	114.66	123.09
10	F	321	HEC	CHD-C4C-C3C	2.65	129.68	125.21
10	L	211	HEC	O1D-CGD-CBD	-2.65	114.68	123.09
10	C	321	HEC	C4D-ND-C1D	2.64	110.13	105.82
10	F	322	HEC	C4D-ND-C1D	2.64	110.13	105.82
10	C	322	HEC	O1A-CGA-CBA	-2.63	114.73	123.09
5	K	502	HEM	O1A-CGA-CBA	-2.63	114.76	123.09
10	I	321	HEC	CHD-C4C-C3C	2.61	129.61	125.21
10	H	211	HEC	CBA-CAA-C2A	-2.61	105.32	112.53
10	I	322	HEC	O1A-CGA-CBA	-2.60	114.84	123.09
10	I	322	HEC	O1D-CGD-CBD	-2.60	114.84	123.09
5	K	502	HEM	CMC-C2C-C1C	2.60	129.30	124.73
10	F	321	HEC	CBD-CAD-C3D	-2.59	105.36	112.53
10	C	322	HEC	CMC-C2C-C3C	-2.59	120.47	126.55
10	H	211	HEC	C4D-ND-C1D	2.59	110.04	105.82
5	A	502	HEM	CMC-C2C-C3C	-2.59	122.17	128.43
5	A	502	HEM	CAC-C3C-C2C	-2.58	120.03	128.43
10	E	211	HEC	C4D-ND-C1D	2.58	110.03	105.82
10	L	211	HEC	C4D-ND-C1D	2.58	110.02	105.82
10	L	211	HEC	CAD-C3D-C4D	2.55	129.93	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	211	HEC	CBA-CAA-C2A	-2.53	105.53	112.53
10	M	321	HEC	CMD-C2D-C1D	2.53	129.27	125.42
10	E	211	HEC	CBA-CAA-C2A	-2.53	105.55	112.53
10	C	321	HEC	CMC-C2C-C1C	-2.52	121.58	125.42
5	G	502	HEM	CAC-C3C-C4C	2.51	130.82	124.82
10	I	322	HEC	CAD-C3D-C4D	2.51	129.84	124.94
10	C	322	HEC	O1D-CGD-CBD	-2.50	115.16	123.09
5	D	502	HEM	CHD-C1D-ND	2.49	127.10	124.42
5	D	501	HEM	CAA-CBA-CGA	-2.49	107.07	113.67
5	A	502	HEM	O1A-CGA-CBA	-2.48	115.22	123.09
10	B	211	HEC	CMD-C2D-C1D	2.48	129.20	125.42
5	A	502	HEM	CBA-CAA-C2A	-2.47	105.69	112.53
5	K	502	HEM	C3B-C4B-NB	-2.47	107.69	109.47
10	H	211	HEC	CAD-C3D-C4D	2.47	129.76	124.94
5	K	502	HEM	CHD-C1D-ND	2.47	127.08	124.42
5	A	502	HEM	O2A-CGA-CBA	2.46	121.77	114.00
10	C	322	HEC	CBD-CAD-C3D	-2.45	105.76	112.53
5	A	501	HEM	O2A-CGA-CBA	2.44	121.70	114.00
10	B	211	HEC	O1A-CGA-CBA	-2.44	115.36	123.09
10	I	322	HEC	C2A-C1A-NA	-2.43	107.98	110.32
10	M	322	HEC	CBD-CAD-C3D	-2.42	105.85	112.53
5	D	502	HEM	O2A-CGA-CBA	2.40	121.59	114.00
10	M	322	HEC	C1D-C2D-C3D	-2.39	104.08	106.82
10	F	322	HEC	CHA-C1A-NA	2.38	127.04	124.45
10	C	321	HEC	CHD-C4C-C3C	2.36	129.19	125.21
10	H	211	HEC	CMC-C2C-C3C	-2.36	121.00	126.55
10	F	322	HEC	O1D-CGD-CBD	-2.35	115.63	123.09
10	H	211	HEC	CMC-C2C-C1C	-2.35	121.85	125.42
10	M	322	HEC	CAD-CBD-CGD	-2.34	107.47	113.67
10	C	321	HEC	CHD-C4C-NC	-2.33	121.91	124.45
10	H	211	HEC	CAD-CBD-CGD	-2.32	107.50	113.67
10	M	322	HEC	O1A-CGA-CBA	-2.32	115.74	123.09
10	I	321	HEC	CHB-C4A-NA	2.29	126.95	124.45
10	H	211	HEC	CMD-C2D-C1D	2.29	128.91	125.42
10	M	322	HEC	CAD-C3D-C4D	2.29	129.41	124.94
10	I	322	HEC	C4D-ND-C1D	2.28	109.55	105.82
10	I	322	HEC	CMD-C2D-C1D	2.28	128.89	125.42
5	A	502	HEM	CHD-C1D-ND	2.27	126.87	124.42
10	F	321	HEC	CMD-C2D-C1D	2.26	128.86	125.42
10	I	321	HEC	CMD-C2D-C1D	2.25	128.85	125.42
10	B	211	HEC	C4D-ND-C1D	2.24	109.48	105.82
5	G	502	HEM	CAC-C3C-C2C	-2.24	121.14	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	322	HEC	CHB-C4A-NA	2.24	126.89	124.45
5	G	501	HEM	O1A-CGA-CBA	-2.24	116.00	123.09
5	K	502	HEM	O2A-CGA-CBA	2.23	121.05	114.00
5	D	502	HEM	CAC-C3C-C4C	2.23	130.15	124.82
10	C	322	HEC	CMC-C2C-C1C	-2.23	122.03	125.42
10	I	322	HEC	CHA-C1A-NA	2.23	126.88	124.45
10	F	322	HEC	O2D-CGD-CBD	2.22	121.03	114.00
10	H	211	HEC	CHB-C4A-NA	2.22	126.87	124.45
10	E	211	HEC	CMC-C2C-C3C	-2.21	121.34	126.55
10	F	322	HEC	CAD-CBD-CGD	-2.20	107.82	113.67
5	K	502	HEM	CMC-C2C-C3C	-2.18	123.15	128.43
9	A	506	PO4	O2-P-O1	-2.18	103.25	110.95
10	M	322	HEC	CMC-C2C-C3C	-2.18	121.43	126.55
10	M	322	HEC	O2A-CGA-CBA	2.18	120.88	114.00
10	L	211	HEC	CMC-C2C-C3C	-2.18	121.43	126.55
10	I	322	HEC	CAA-CBA-CGA	-2.17	107.91	113.67
10	C	321	HEC	CMD-C2D-C1D	2.16	128.71	125.42
10	C	322	HEC	CAD-CBD-CGD	-2.16	107.93	113.67
5	G	502	HEM	O1A-CGA-CBA	-2.15	116.27	123.09
10	E	211	HEC	CHA-C1A-NA	2.14	126.78	124.45
10	F	322	HEC	CHB-C4A-NA	2.14	126.78	124.45
10	F	322	HEC	CAA-CBA-CGA	-2.13	108.03	113.67
5	K	502	HEM	CHA-C4D-ND	2.12	126.99	124.37
10	H	211	HEC	O1D-CGD-CBD	-2.12	116.37	123.09
10	C	321	HEC	CHC-C1C-NC	2.11	127.69	123.86
10	L	211	HEC	CHD-C1D-ND	2.11	127.69	123.86
10	F	322	HEC	CMC-C2C-C1C	-2.11	122.20	125.42
10	I	322	HEC	O2D-CGD-CBD	2.10	120.63	114.00
5	D	501	HEM	C1B-NB-C4B	2.08	107.67	105.21
10	F	322	HEC	CAD-C3D-C4D	2.08	128.99	124.94
5	A	502	HEM	CAA-CBA-CGA	2.07	119.17	113.67
10	I	322	HEC	CBD-CAD-C3D	-2.07	106.82	112.53
10	C	322	HEC	CMD-C2D-C1D	2.07	128.56	125.42
5	G	501	HEM	CMD-C2D-C1D	2.07	128.26	125.03
10	H	211	HEC	O1A-CGA-CBA	-2.06	116.57	123.09
5	A	502	HEM	CMD-C2D-C1D	2.06	128.25	125.03
10	F	321	HEC	CMC-C2C-C1C	-2.05	122.29	125.42
10	F	322	HEC	C2A-C1A-NA	-2.05	108.34	110.32
5	D	502	HEM	CMC-C2C-C1C	2.05	128.34	124.73
5	K	502	HEM	CAC-C3C-C2C	-2.05	121.77	128.43
5	K	502	HEM	CAC-C3C-C4C	2.04	129.70	124.82
10	F	322	HEC	CBD-CAD-C3D	-2.04	106.89	112.53

There are no chirality outliers.

All (125) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	HEM	C2C-C3C-CAC-CBC
5	D	501	HEM	C2C-C3C-CAC-CBC
5	G	501	HEM	C2C-C3C-CAC-CBC
5	K	501	HEM	C2C-C3C-CAC-CBC
10	B	211	HEC	C2B-C3B-CAB-CBB
10	B	211	HEC	C4B-C3B-CAB-CBB
10	B	211	HEC	C2C-C3C-CAC-CBC
10	B	211	HEC	C4C-C3C-CAC-CBC
10	C	321	HEC	C2B-C3B-CAB-CBB
10	C	321	HEC	C4B-C3B-CAB-CBB
10	C	321	HEC	C2C-C3C-CAC-CBC
10	C	321	HEC	C4C-C3C-CAC-CBC
10	C	322	HEC	C2B-C3B-CAB-CBB
10	C	322	HEC	C4B-C3B-CAB-CBB
10	C	322	HEC	C2C-C3C-CAC-CBC
10	C	322	HEC	C4C-C3C-CAC-CBC
10	E	211	HEC	C2B-C3B-CAB-CBB
10	E	211	HEC	C4B-C3B-CAB-CBB
10	E	211	HEC	C2C-C3C-CAC-CBC
10	E	211	HEC	C4C-C3C-CAC-CBC
10	F	321	HEC	C2B-C3B-CAB-CBB
10	F	321	HEC	C4B-C3B-CAB-CBB
10	F	321	HEC	C2C-C3C-CAC-CBC
10	F	321	HEC	C4C-C3C-CAC-CBC
10	F	322	HEC	C2B-C3B-CAB-CBB
10	F	322	HEC	C4B-C3B-CAB-CBB
10	F	322	HEC	C2C-C3C-CAC-CBC
10	H	211	HEC	C2B-C3B-CAB-CBB
10	H	211	HEC	C4B-C3B-CAB-CBB
10	H	211	HEC	C2C-C3C-CAC-CBC
10	H	211	HEC	C4C-C3C-CAC-CBC
10	I	321	HEC	C2B-C3B-CAB-CBB
10	I	321	HEC	C4B-C3B-CAB-CBB
10	I	321	HEC	C2C-C3C-CAC-CBC
10	I	321	HEC	C4C-C3C-CAC-CBC
10	I	322	HEC	C2B-C3B-CAB-CBB
10	I	322	HEC	C4B-C3B-CAB-CBB
10	I	322	HEC	C2C-C3C-CAC-CBC
10	L	211	HEC	C2B-C3B-CAB-CBB
10	L	211	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
10	L	211	HEC	C2C-C3C-CAC-CBC
10	L	211	HEC	C4C-C3C-CAC-CBC
10	M	321	HEC	C2B-C3B-CAB-CBB
10	M	321	HEC	C4B-C3B-CAB-CBB
10	M	321	HEC	C2C-C3C-CAC-CBC
10	M	321	HEC	C4C-C3C-CAC-CBC
10	M	322	HEC	C2B-C3B-CAB-CBB
10	M	322	HEC	C4B-C3B-CAB-CBB
10	M	322	HEC	C2C-C3C-CAC-CBC
5	A	502	HEM	C4B-C3B-CAB-CBB
5	D	502	HEM	C4B-C3B-CAB-CBB
5	A	501	HEM	C2B-C3B-CAB-CBB
5	D	501	HEM	C2B-C3B-CAB-CBB
5	K	501	HEM	C2B-C3B-CAB-CBB
5	A	501	HEM	C4C-C3C-CAC-CBC
5	A	502	HEM	C4C-C3C-CAC-CBC
5	D	501	HEM	C4C-C3C-CAC-CBC
5	D	502	HEM	C4C-C3C-CAC-CBC
5	G	501	HEM	C4C-C3C-CAC-CBC
5	G	502	HEM	C4B-C3B-CAB-CBB
5	G	502	HEM	C4C-C3C-CAC-CBC
5	K	501	HEM	C4C-C3C-CAC-CBC
5	K	502	HEM	C4B-C3B-CAB-CBB
5	K	502	HEM	C4C-C3C-CAC-CBC
10	F	322	HEC	C4C-C3C-CAC-CBC
10	I	322	HEC	C4C-C3C-CAC-CBC
10	M	322	HEC	C4C-C3C-CAC-CBC
5	A	501	HEM	C4B-C3B-CAB-CBB
5	K	501	HEM	C4B-C3B-CAB-CBB
10	C	321	HEC	CAA-CBA-CGA-O1A
10	F	322	HEC	CAD-CBD-CGD-O1D
10	I	322	HEC	CAD-CBD-CGD-O1D
10	F	321	HEC	CAA-CBA-CGA-O1A
10	M	322	HEC	CAD-CBD-CGD-O1D
10	H	211	HEC	CAD-CBD-CGD-O1D
10	B	211	HEC	CAA-CBA-CGA-O1A
10	E	211	HEC	CAD-CBD-CGD-O1D
10	F	322	HEC	CAD-CBD-CGD-O2D
10	I	321	HEC	CAA-CBA-CGA-O1A
10	C	322	HEC	CAD-CBD-CGD-O2D
10	L	211	HEC	CAD-CBD-CGD-O1D
10	M	321	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
10	M	322	HEC	CAD-CBD-CGD-O2D
10	I	322	HEC	CAD-CBD-CGD-O2D
10	B	211	HEC	CAD-CBD-CGD-O1D
10	C	322	HEC	CAD-CBD-CGD-O1D
10	M	321	HEC	CAA-CBA-CGA-O2A
10	B	211	HEC	CAA-CBA-CGA-O2A
10	L	211	HEC	CAD-CBD-CGD-O2D
10	B	211	HEC	CAD-CBD-CGD-O2D
10	E	211	HEC	CAD-CBD-CGD-O2D
10	I	321	HEC	CAA-CBA-CGA-O2A
10	F	321	HEC	CAA-CBA-CGA-O2A
10	H	211	HEC	CAD-CBD-CGD-O2D
5	A	501	HEM	CAD-CBD-CGD-O1D
10	C	321	HEC	CAA-CBA-CGA-O2A
10	H	211	HEC	CAA-CBA-CGA-O1A
5	A	501	HEM	CAA-CBA-CGA-O2A
5	A	501	HEM	CAD-CBD-CGD-O2D
5	G	501	HEM	CAA-CBA-CGA-O2A
5	K	501	HEM	CAA-CBA-CGA-O2A
5	K	501	HEM	CAD-CBD-CGD-O1D
5	G	501	HEM	C2B-C3B-CAB-CBB
5	K	501	HEM	CAD-CBD-CGD-O2D
5	D	501	HEM	CAA-CBA-CGA-O2A
5	D	501	HEM	C4B-C3B-CAB-CBB
5	G	501	HEM	C4B-C3B-CAB-CBB
5	G	501	HEM	CAD-CBD-CGD-O2D
10	E	211	HEC	CAA-CBA-CGA-O1A
5	D	501	HEM	CAA-CBA-CGA-O1A
5	G	501	HEM	CAD-CBD-CGD-O1D
5	D	501	HEM	CAD-CBD-CGD-O1D
5	G	501	HEM	CAA-CBA-CGA-O1A
5	A	501	HEM	CAA-CBA-CGA-O1A
5	D	501	HEM	CAD-CBD-CGD-O2D
10	H	211	HEC	CAA-CBA-CGA-O2A
5	A	502	HEM	CAD-CBD-CGD-O2D
5	D	502	HEM	CAD-CBD-CGD-O2D
10	L	211	HEC	CAA-CBA-CGA-O1A
5	K	501	HEM	CAA-CBA-CGA-O1A
10	E	211	HEC	CAA-CBA-CGA-O2A
5	A	502	HEM	CAD-CBD-CGD-O1D
10	L	211	HEC	CAA-CBA-CGA-O2A
5	D	502	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
5	K	502	HEM	CAA-CBA-CGA-O2A

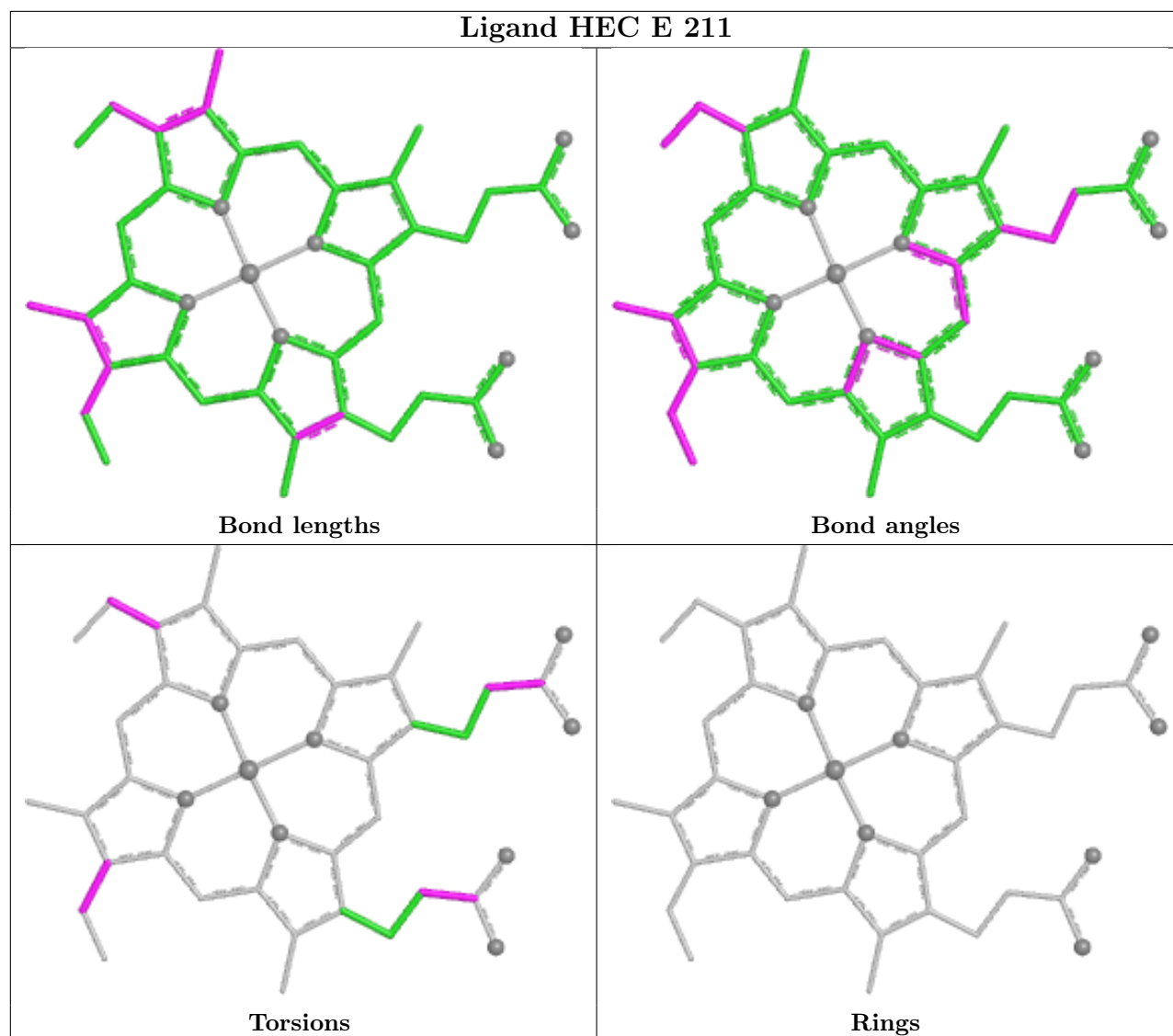
There are no ring outliers.

24 monomers are involved in 118 short contacts:

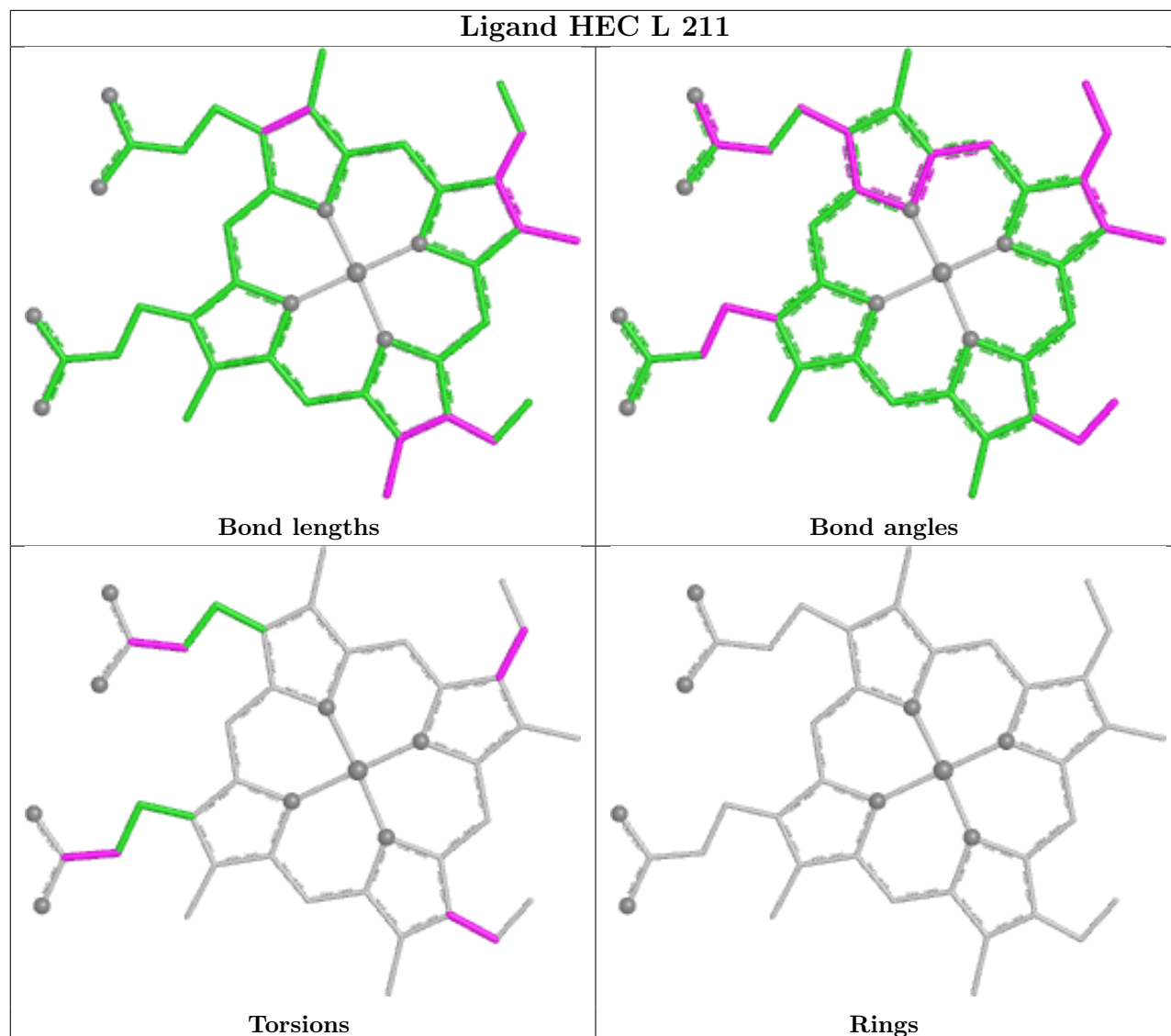
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	E	211	HEC	2	0
11	I	323	FC6	6	0
10	L	211	HEC	2	0
11	F	323	FC6	10	0
10	C	322	HEC	2	0
11	M	323	FC6	3	0
5	K	502	HEM	7	0
5	D	502	HEM	8	0
10	B	211	HEC	3	0
10	I	322	HEC	1	0
5	K	501	HEM	5	0
10	F	321	HEC	10	0
11	C	323	FC6	4	0
5	A	501	HEM	5	0
10	C	321	HEC	6	0
10	I	321	HEC	4	0
5	G	502	HEM	7	0
10	M	322	HEC	3	0
5	G	501	HEM	6	0
10	F	322	HEC	5	0
10	H	211	HEC	4	0
10	M	321	HEC	5	0
5	D	501	HEM	4	0
5	A	502	HEM	6	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

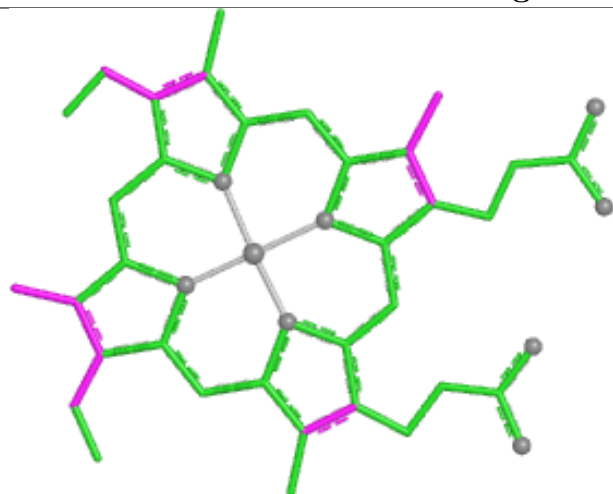
equivalents in the CSD to analyse the geometry.



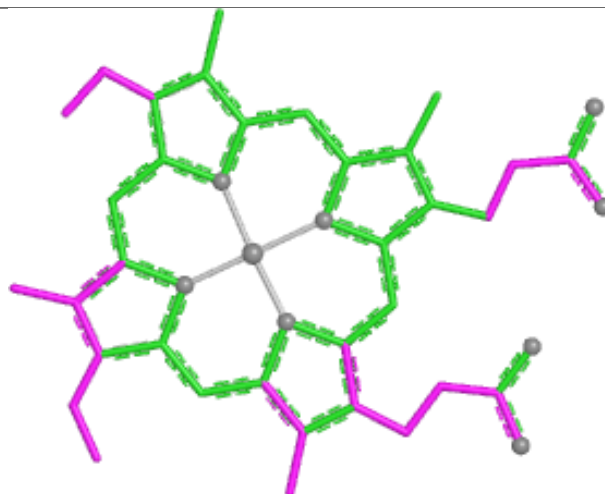
Ligand HEC L 211



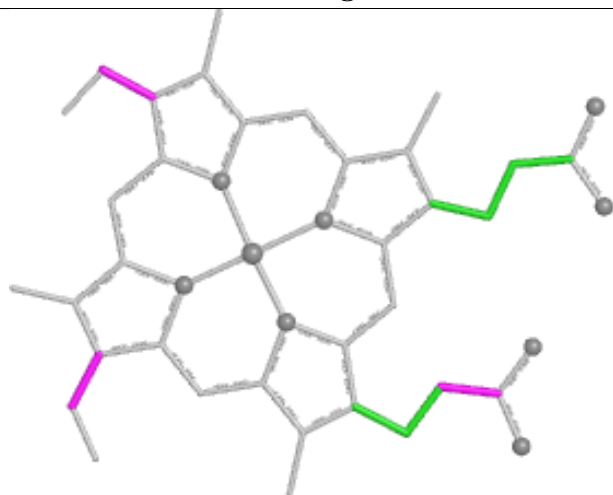
Ligand HEC C 322



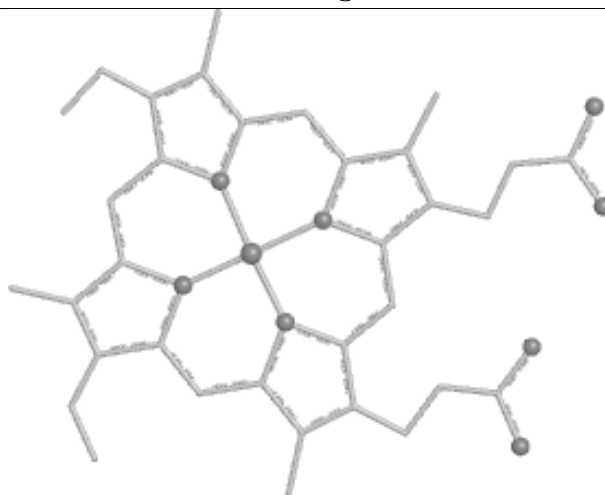
Bond lengths



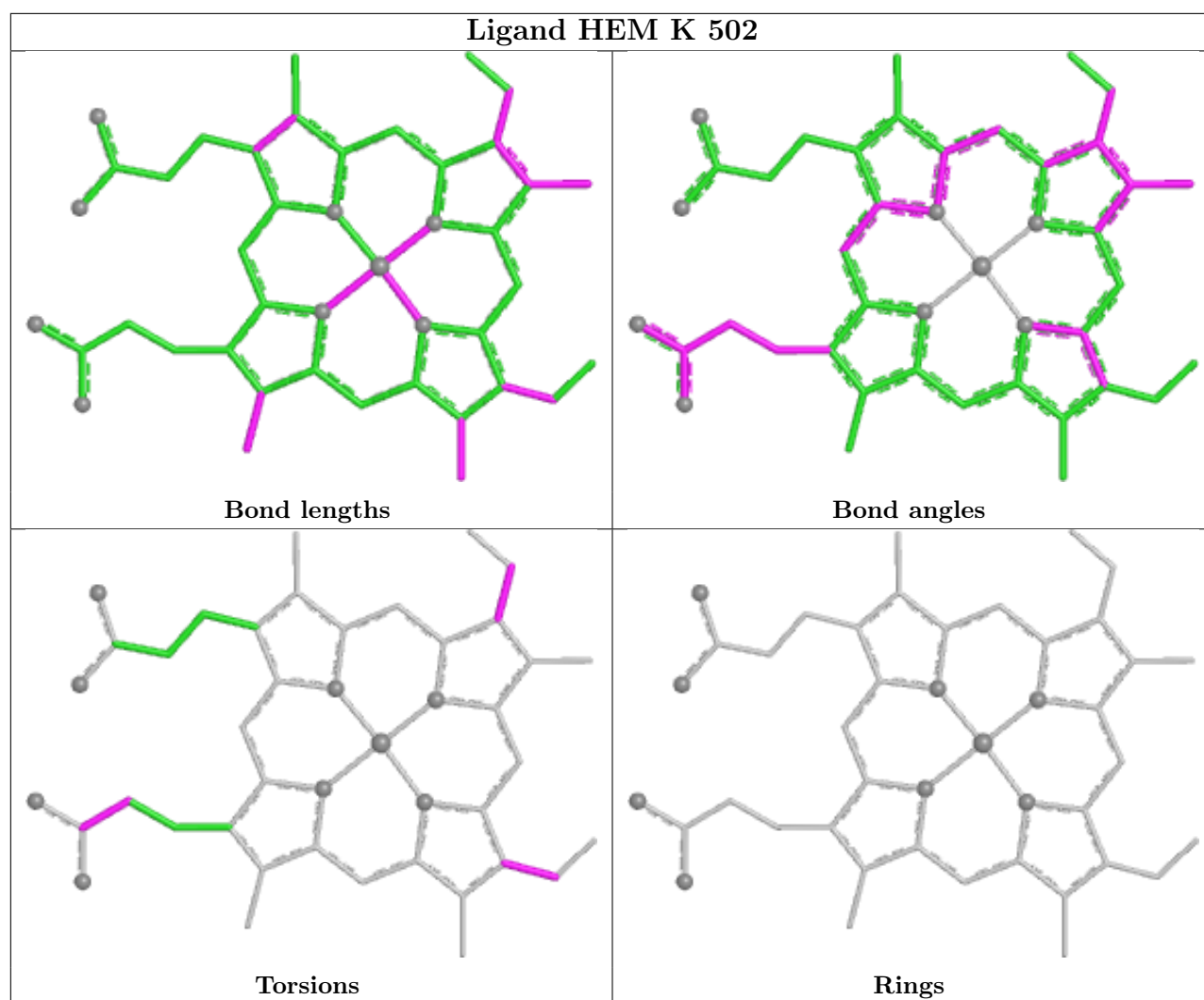
Bond angles

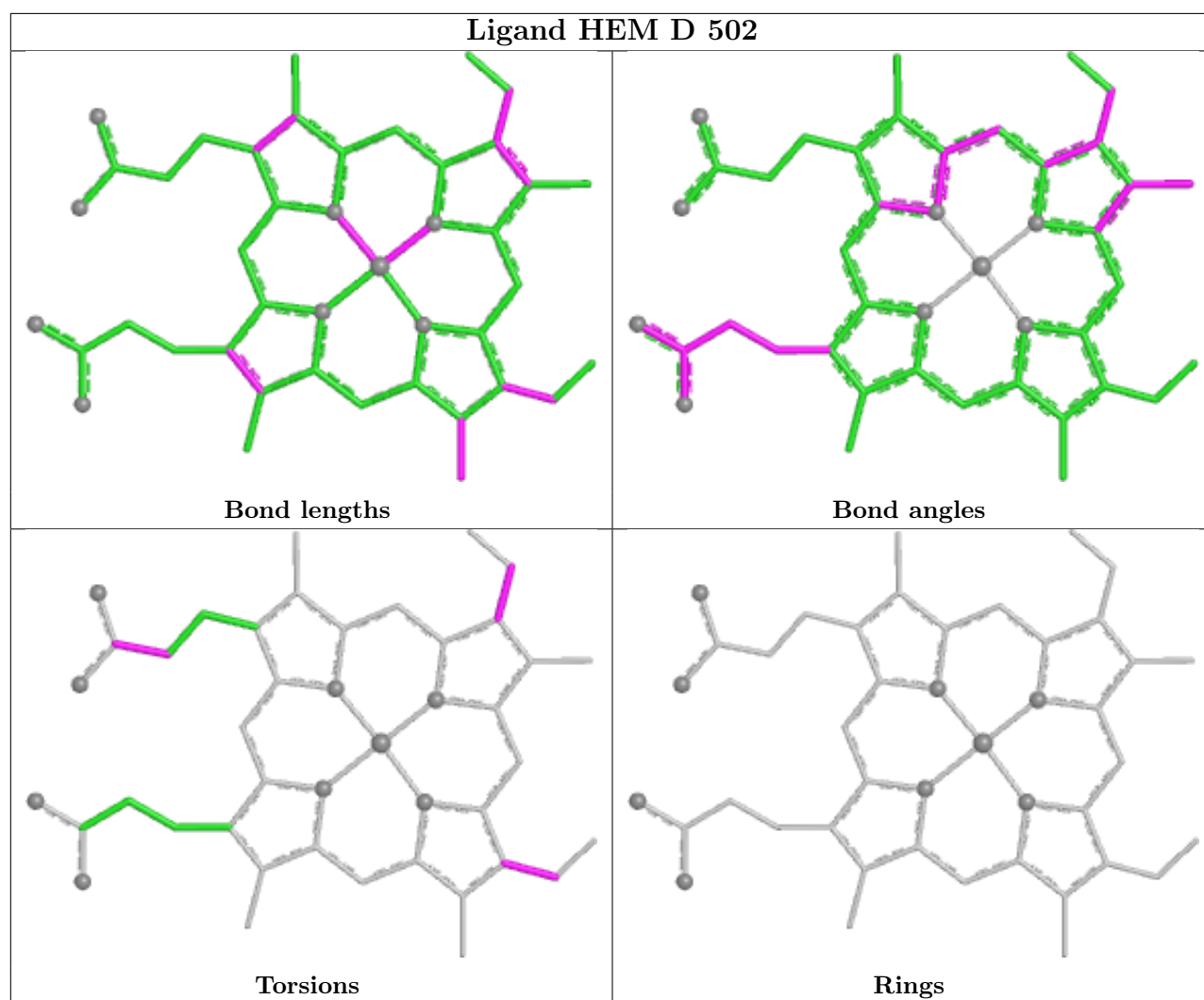


Torsions

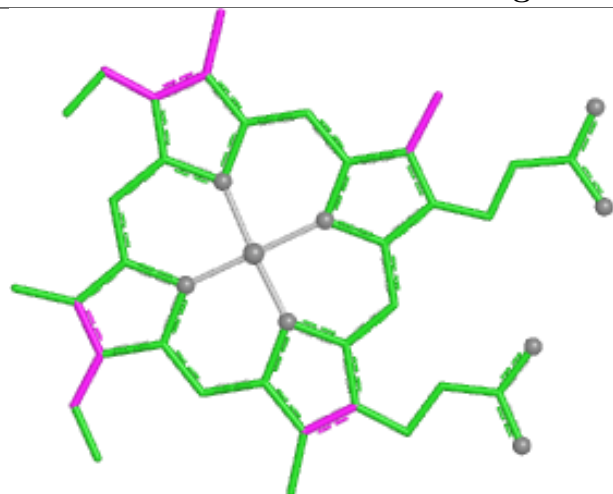


Rings

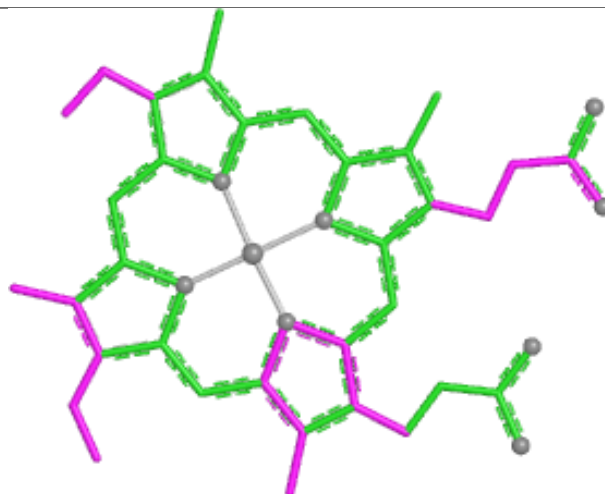




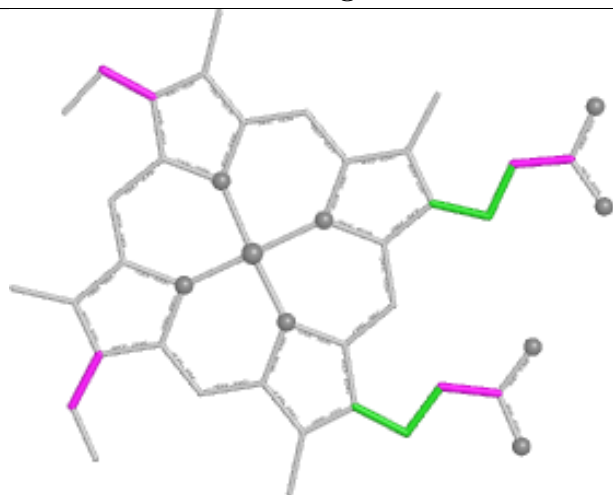
Ligand HEC B 211



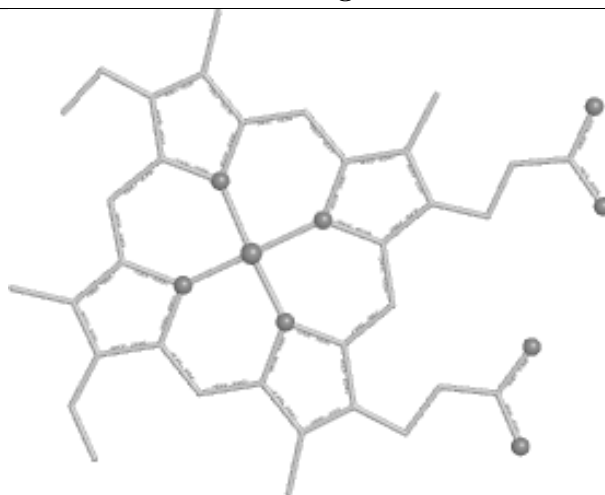
Bond lengths



Bond angles

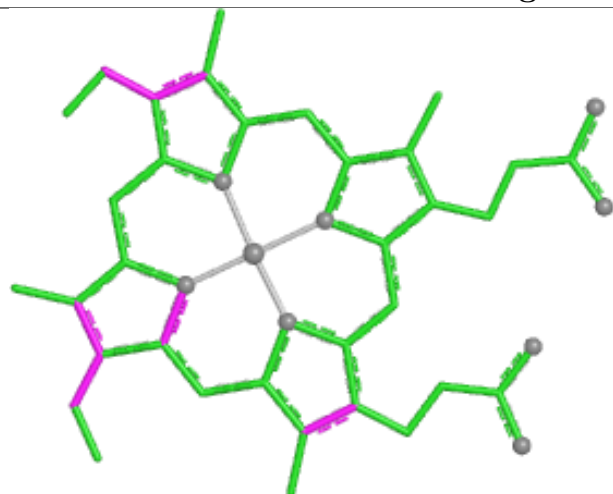


Torsions

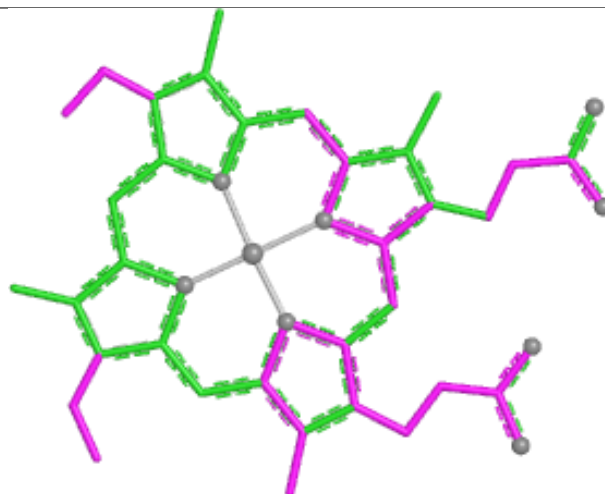


Rings

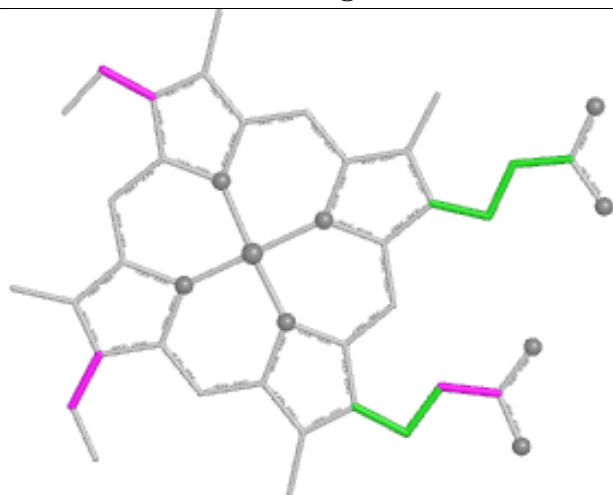
Ligand HEC I 322



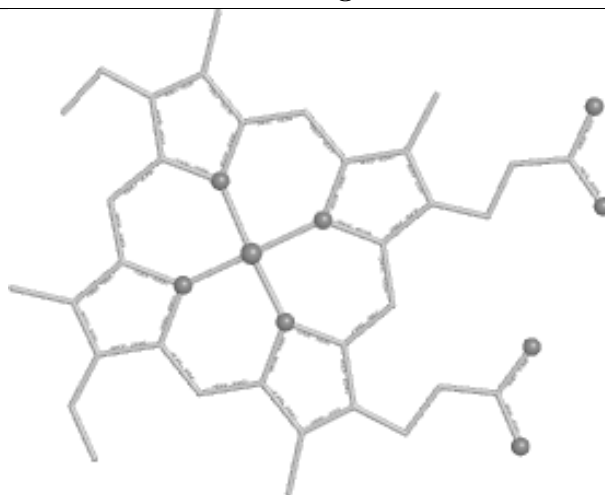
Bond lengths



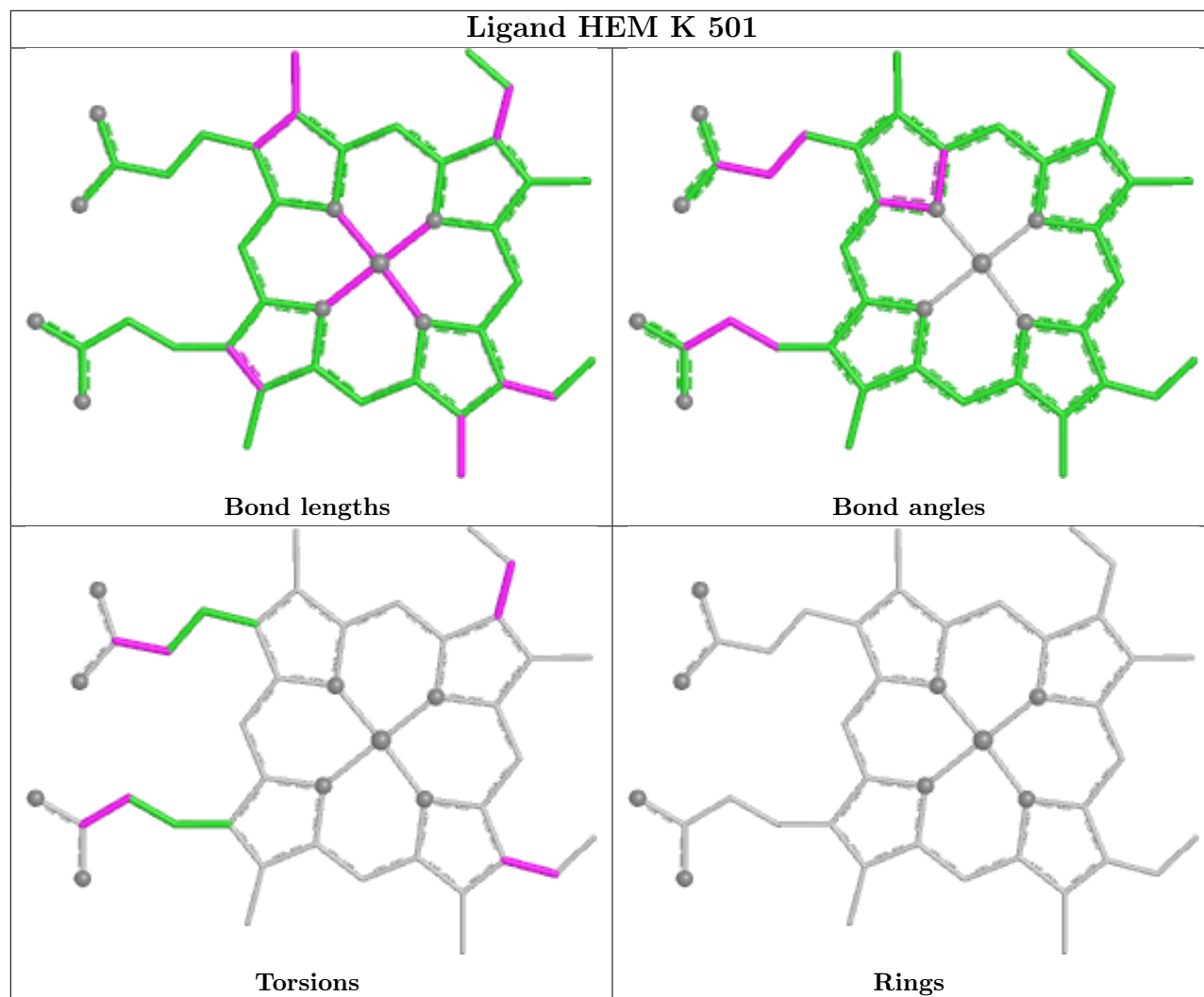
Bond angles



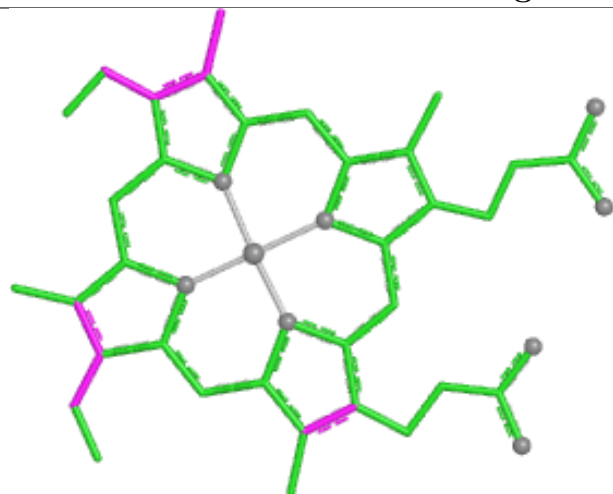
Torsions



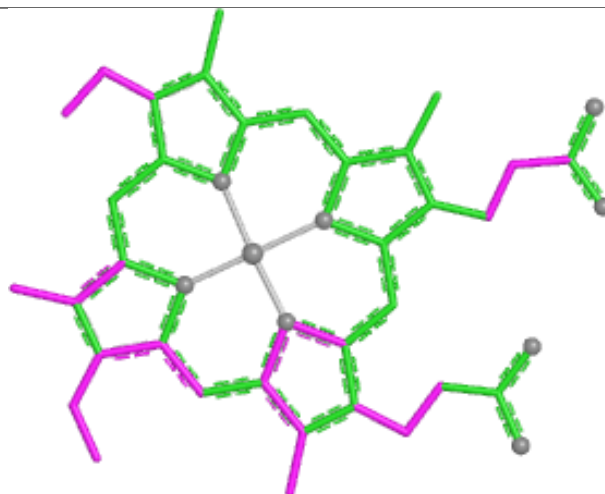
Rings



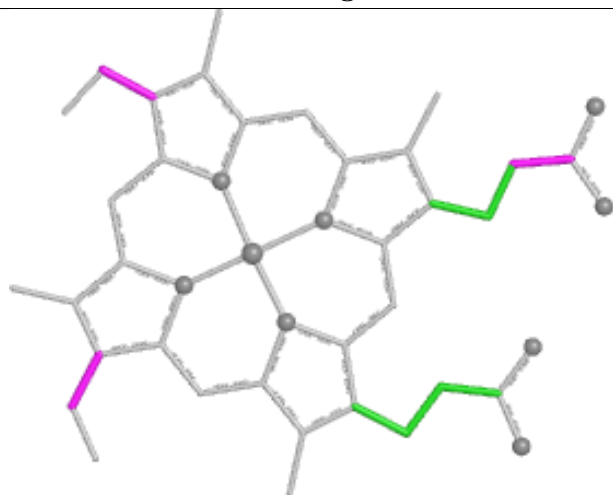
Ligand HEC F 321



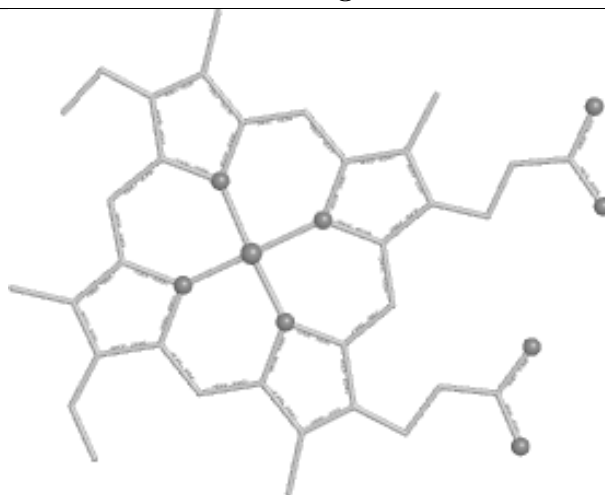
Bond lengths



Bond angles

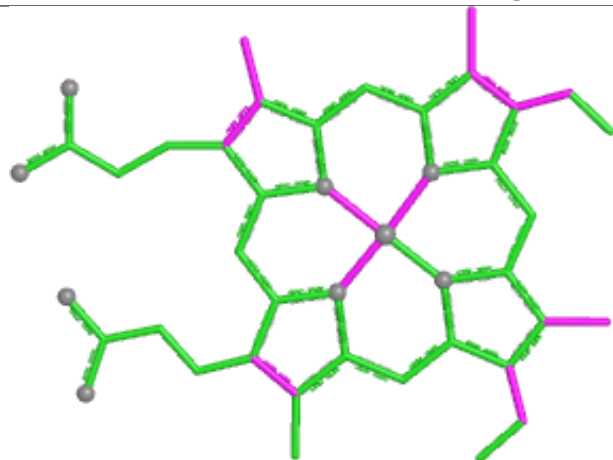


Torsions

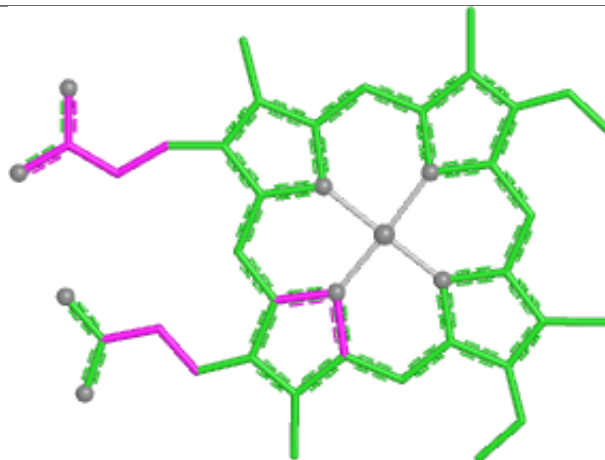


Rings

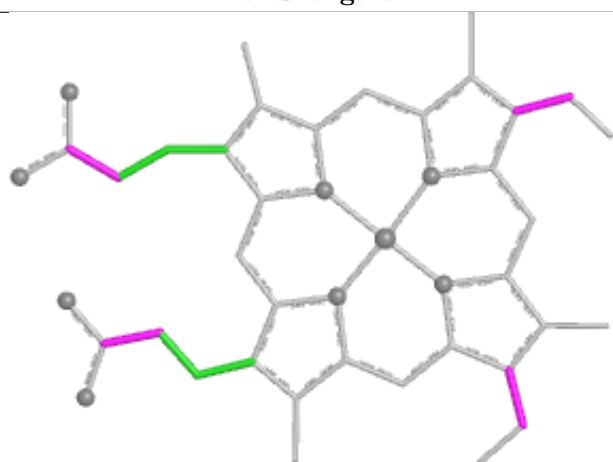
Ligand HEM A 501



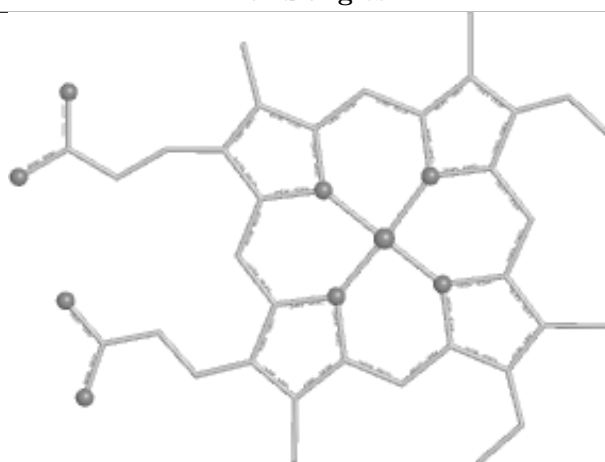
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Bond angles

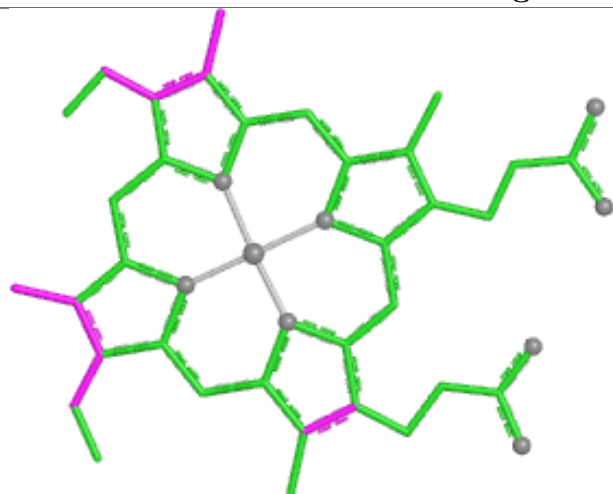


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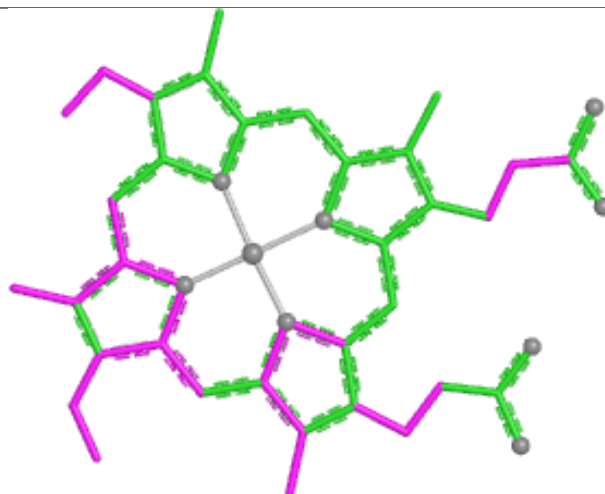


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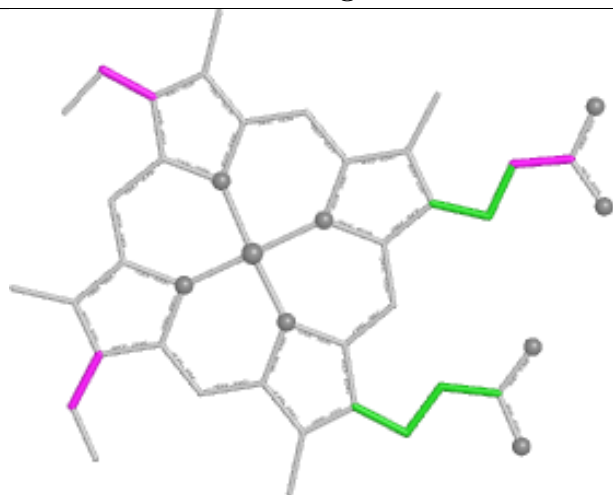
Ligand HEC C 321



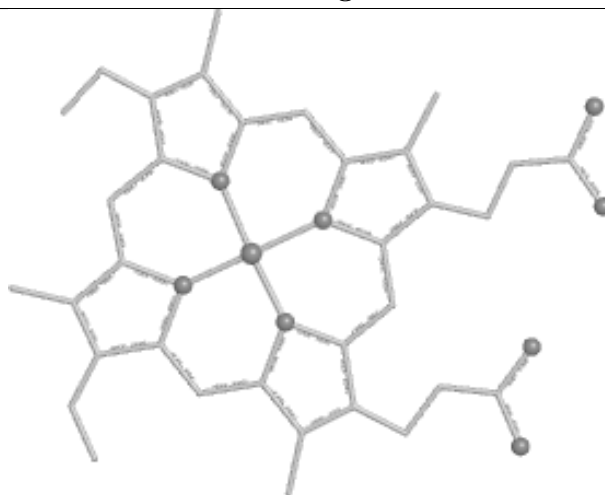
Bond lengths



Bond angles

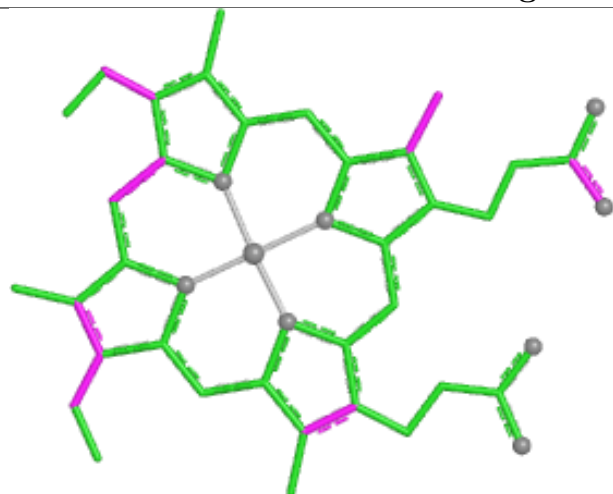


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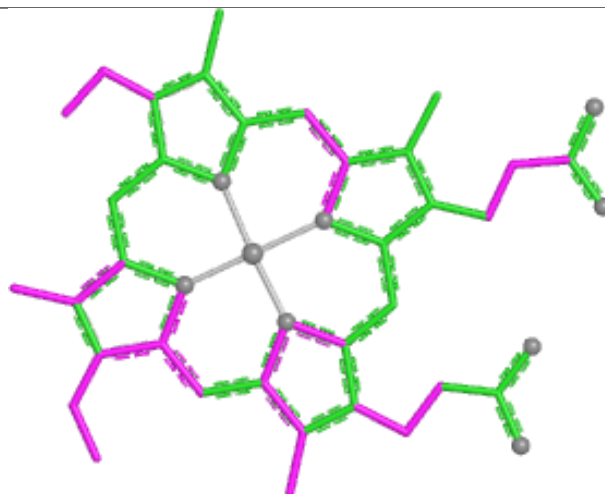


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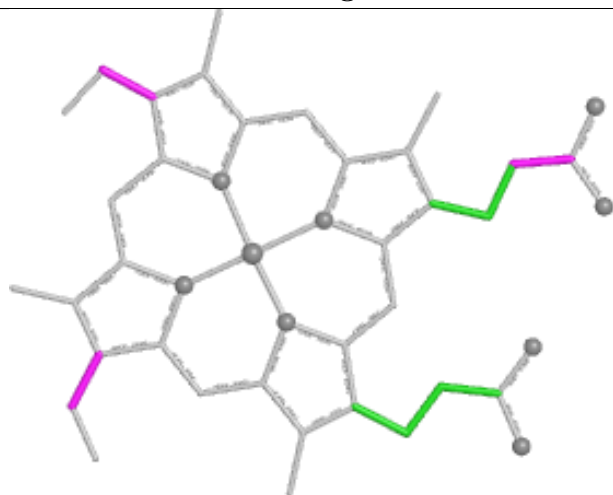
Ligand HEC I 321



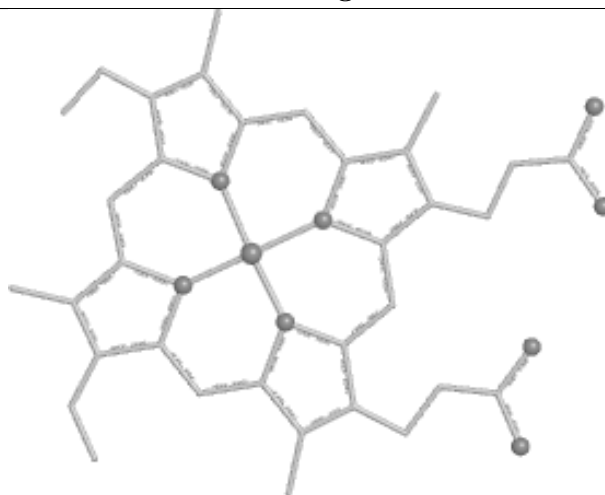
Bond lengths



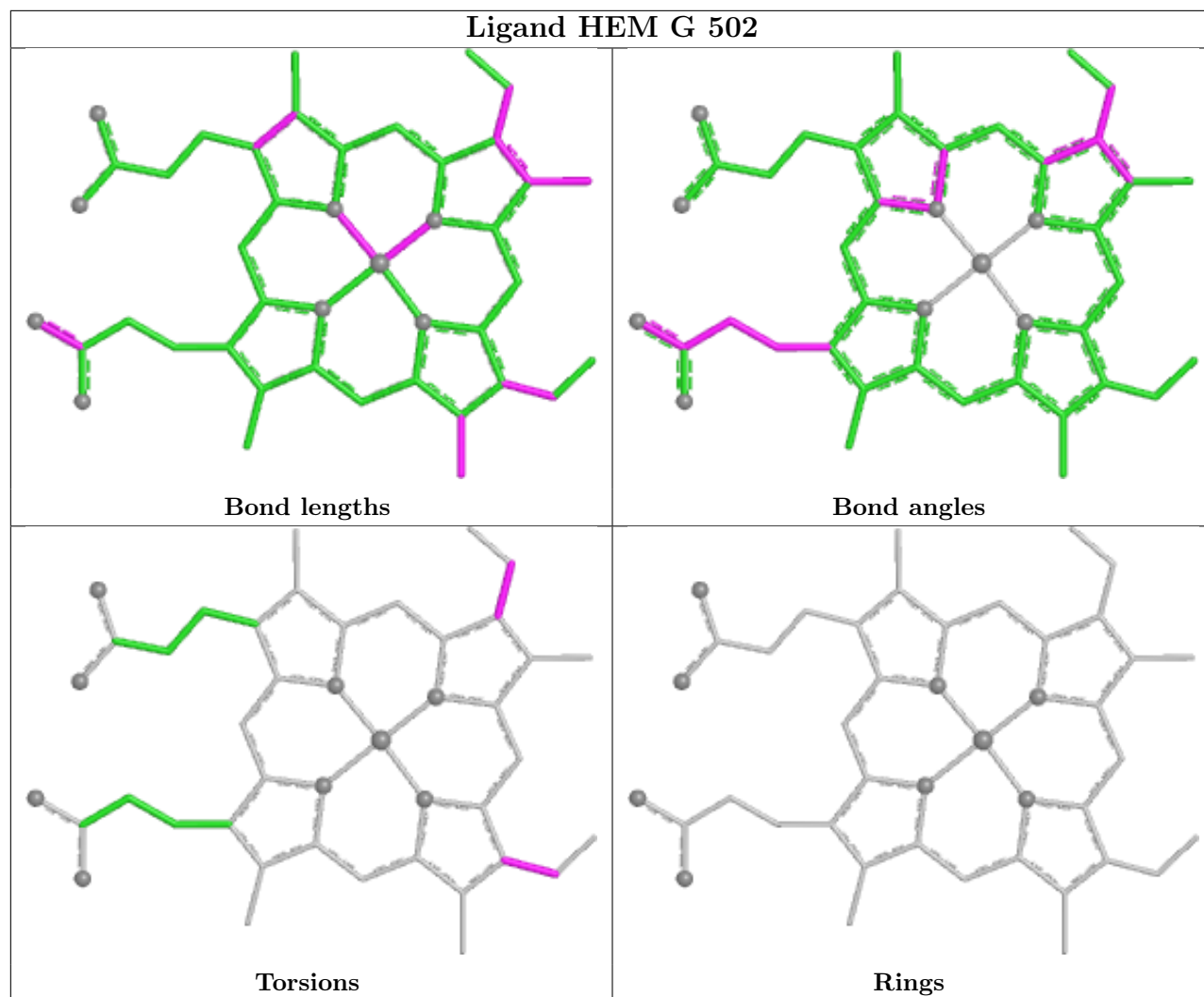
Bond angles



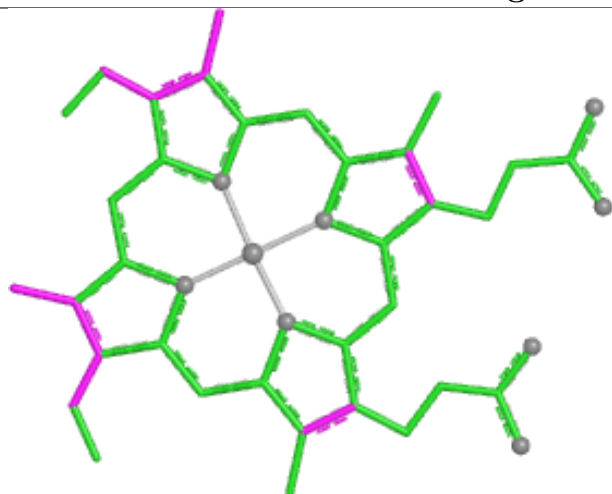
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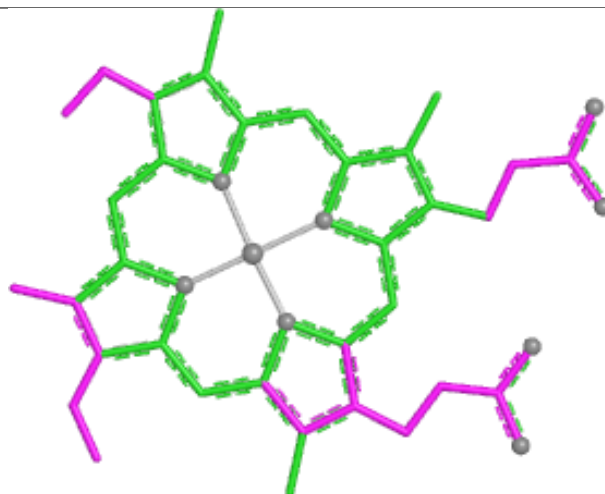
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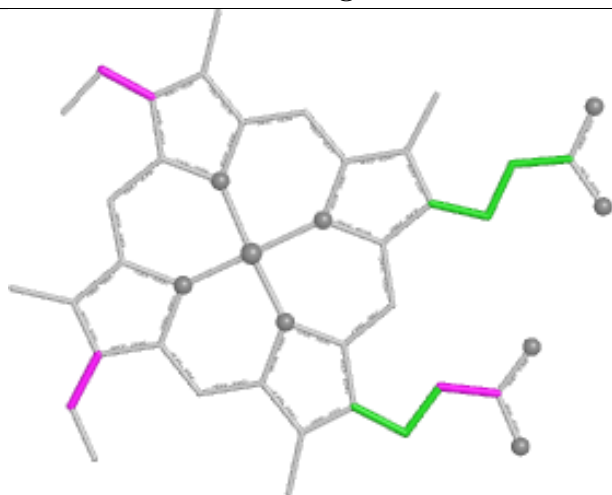
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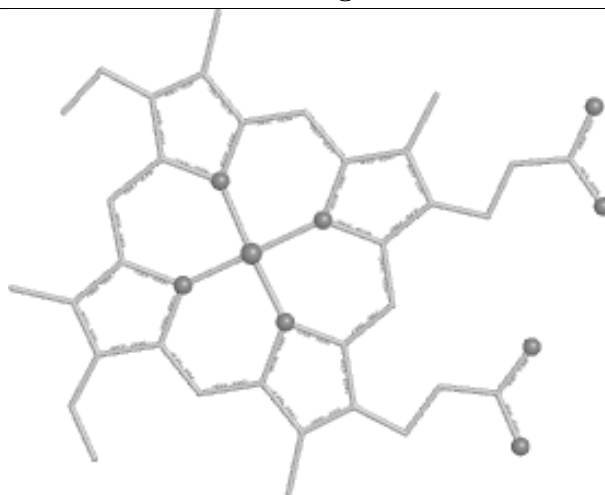
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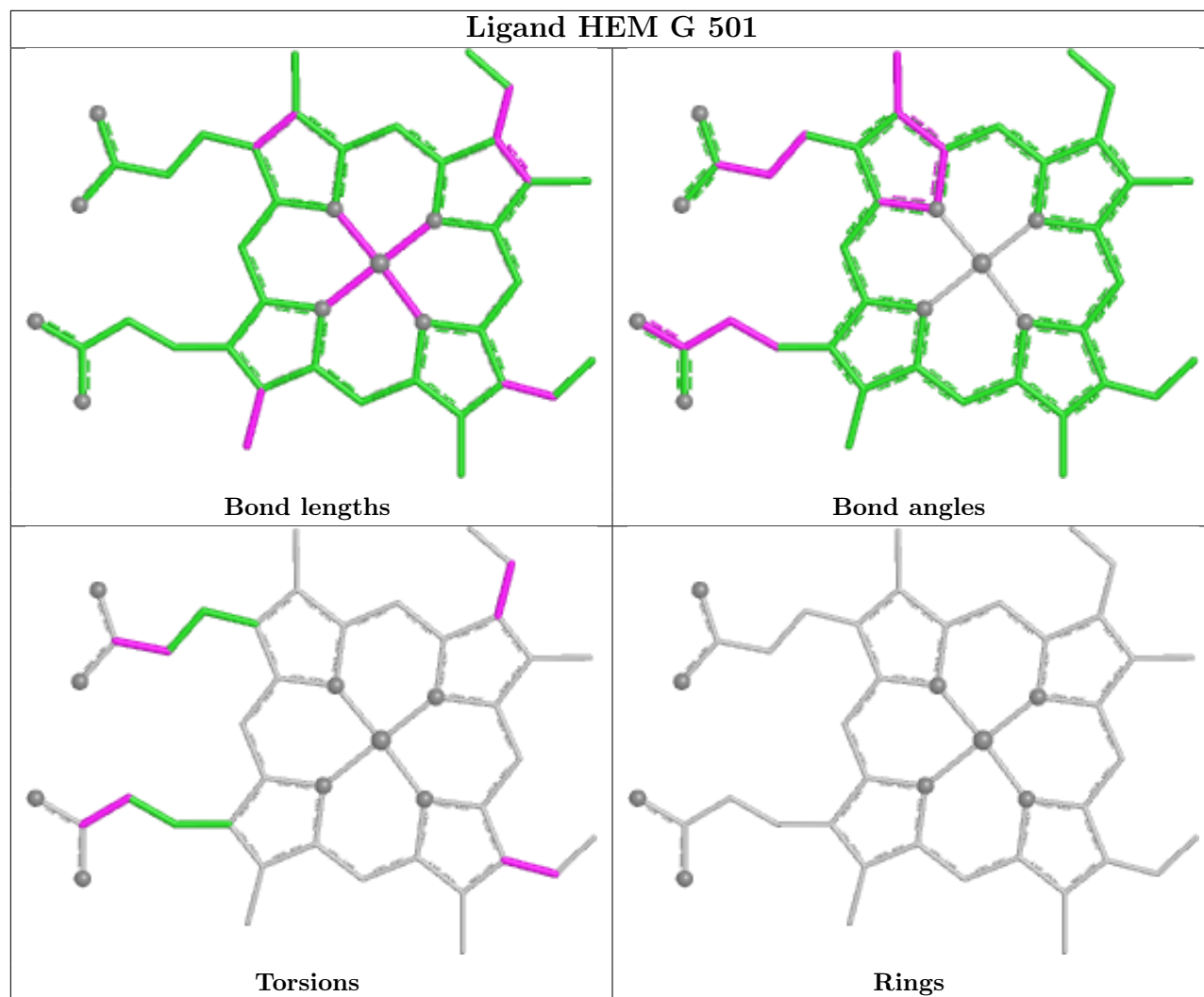
Bond angles



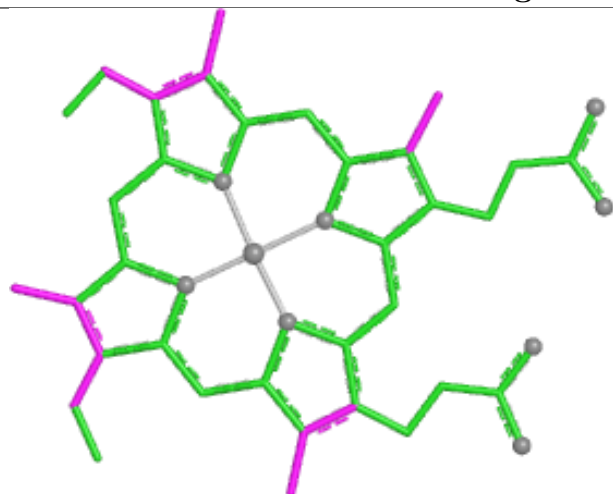
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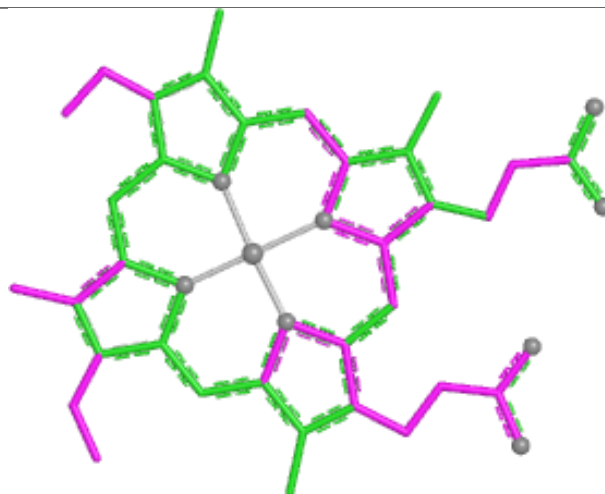
Rings



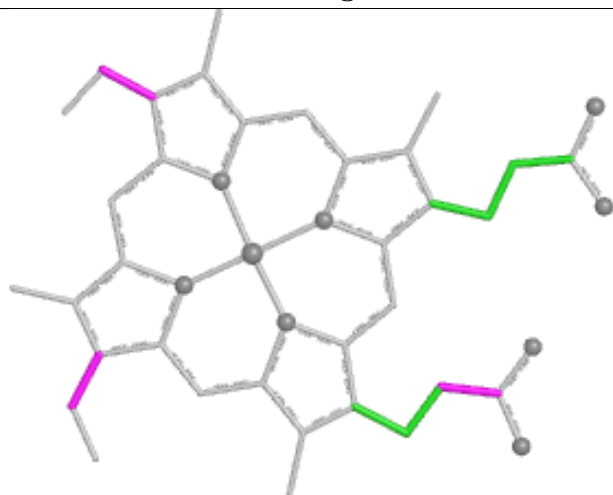
Ligand HEC F 322



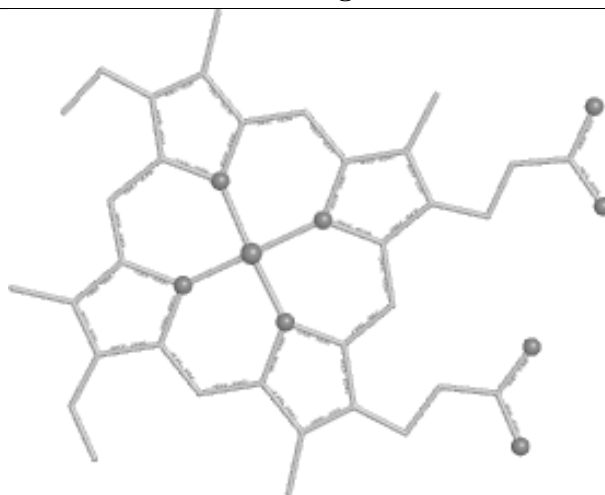
Bond lengths



Bond angles

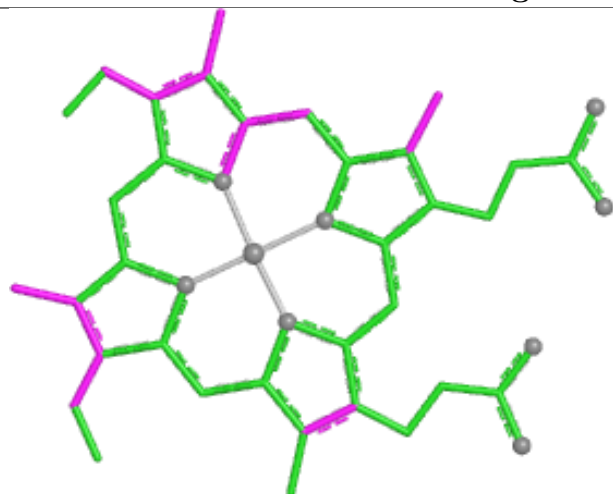


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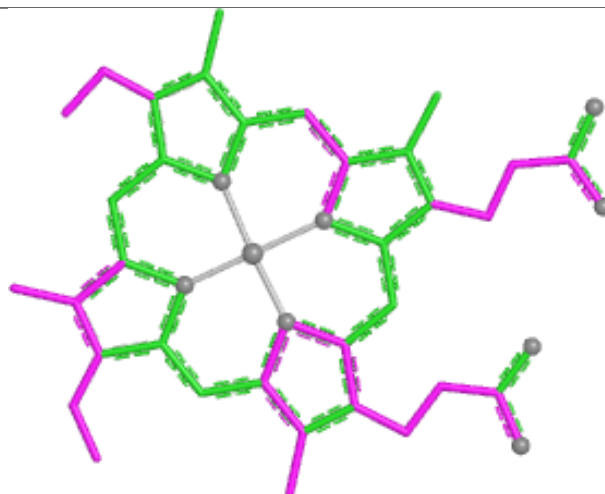


Rings

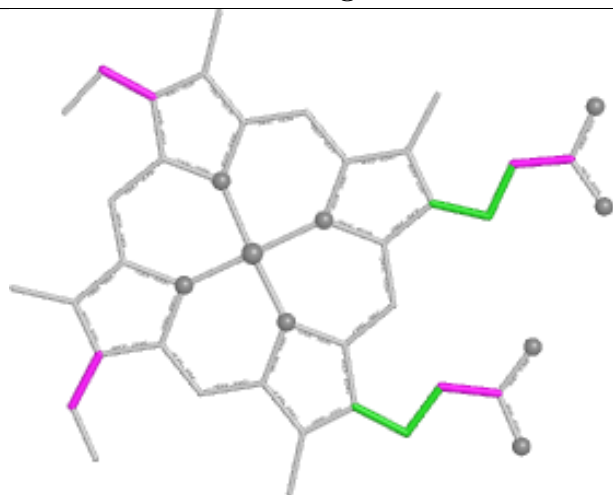
Ligand HEC H 211



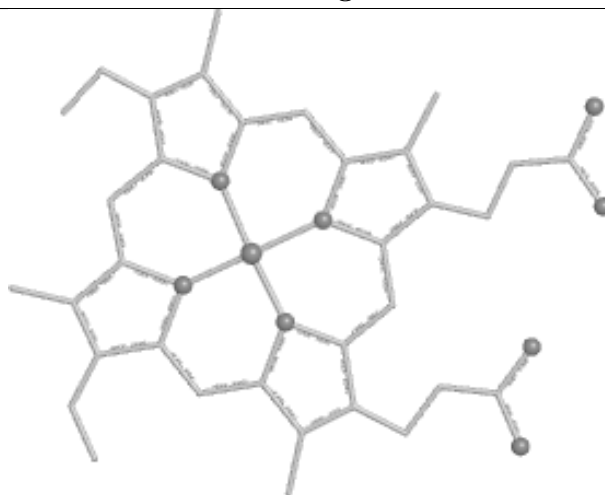
Bond lengths



Bond angles

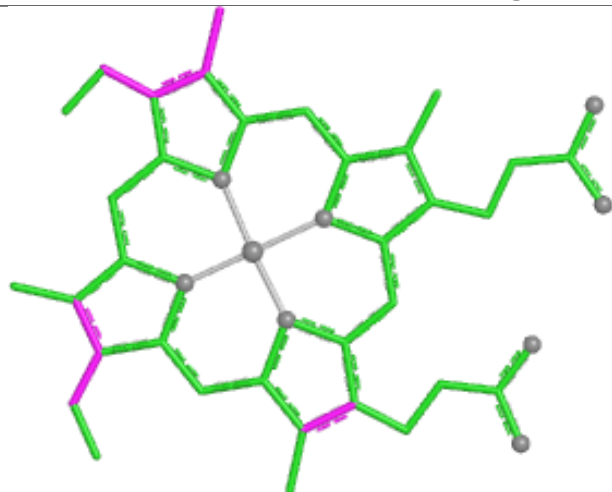


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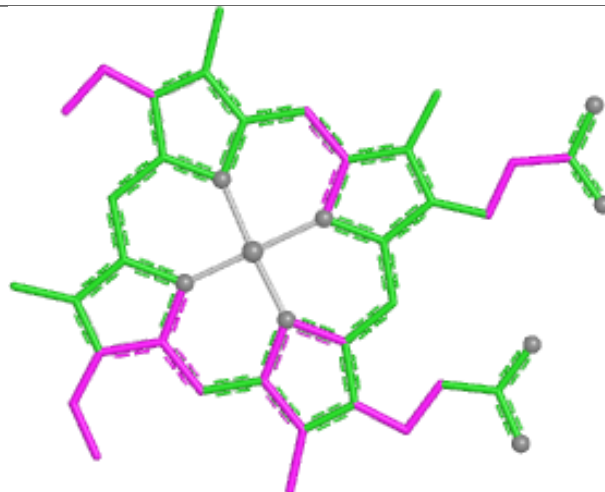


Rings

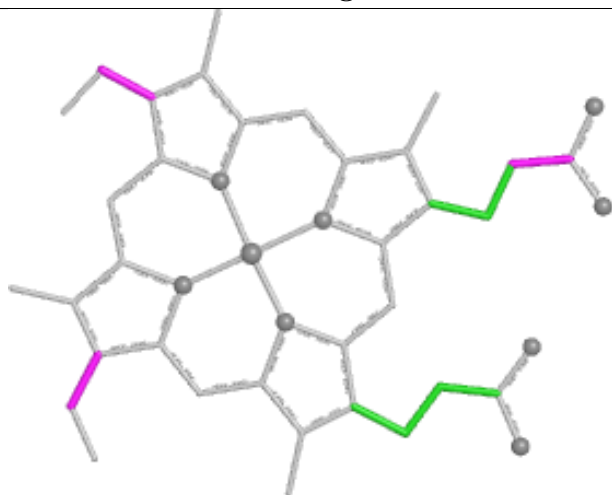
Ligand HEC M 321



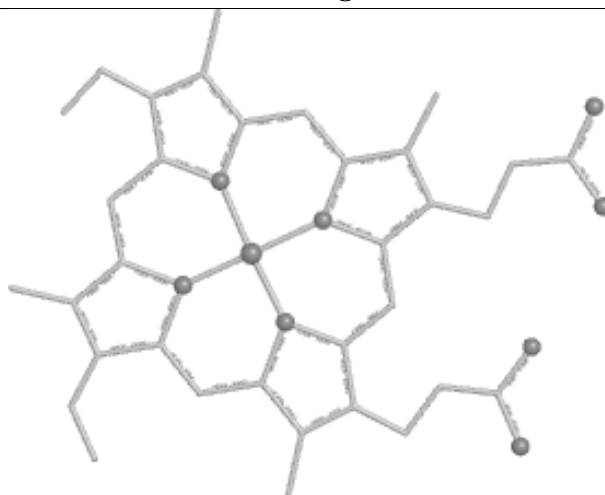
Bond lengths



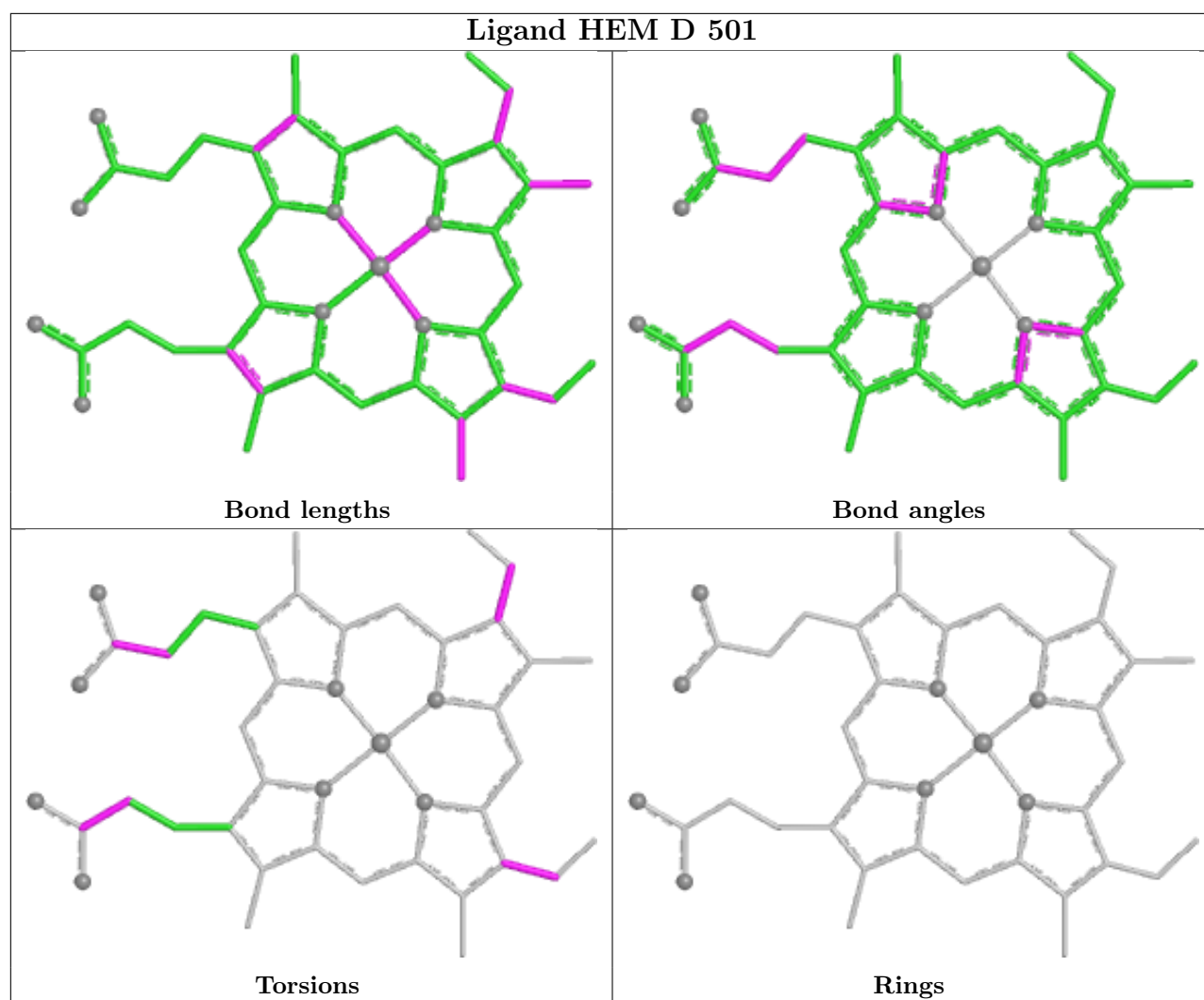
Bond angles

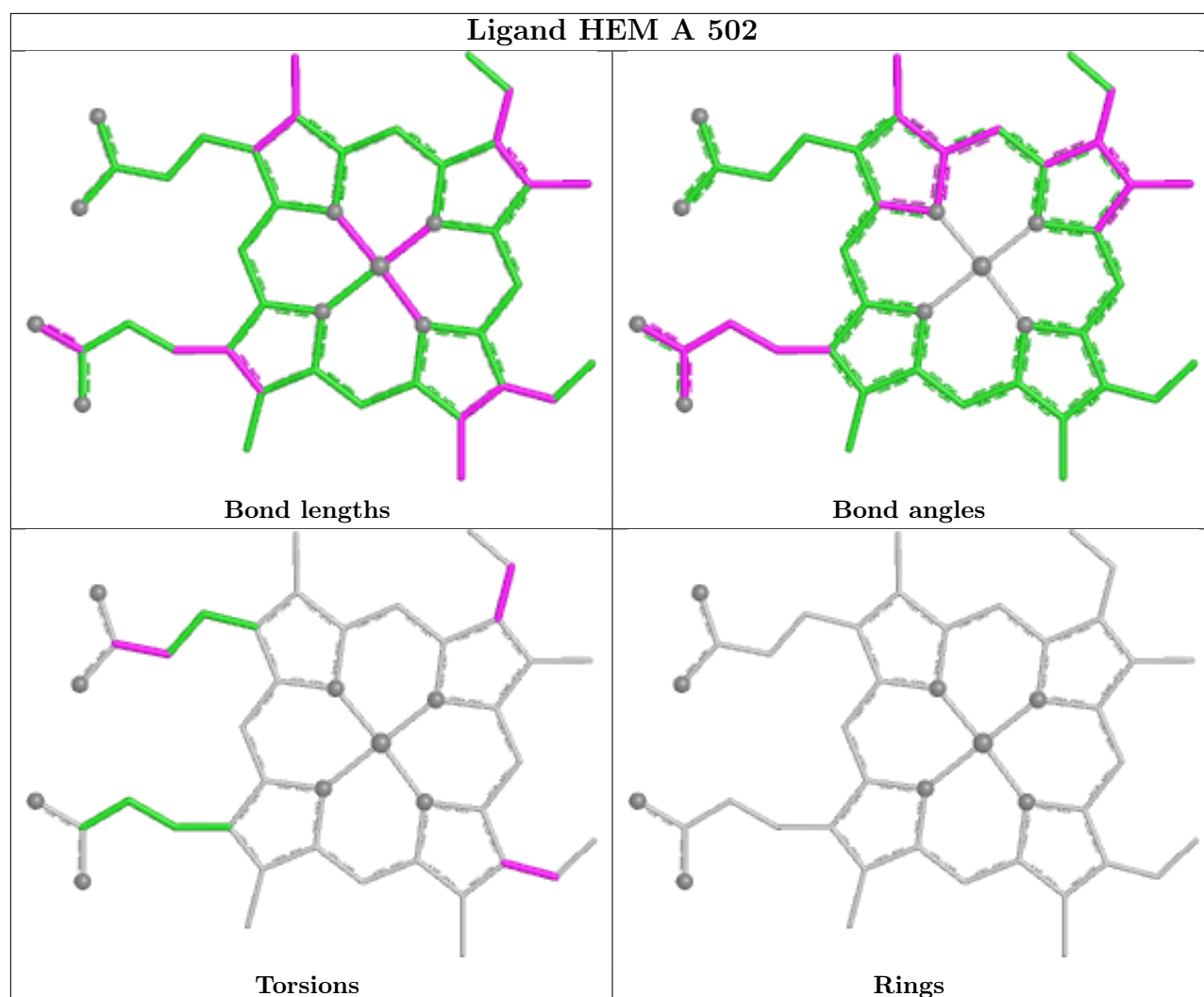


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	466/474 (98%)	-0.74	1 (0%) 91 85	44, 75, 127, 177	0
1	D	463/474 (97%)	-0.31	2 (0%) 88 79	73, 156, 249, 313	0
1	G	465/474 (98%)	-0.65	2 (0%) 88 79	54, 88, 133, 176	0
1	K	465/474 (98%)	-0.30	4 (0%) 81 64	64, 145, 232, 269	0
2	B	197/203 (97%)	-0.84	0 100 100	39, 64, 124, 172	0
2	E	197/203 (97%)	-0.29	1 (0%) 87 76	66, 140, 243, 290	0
2	H	197/203 (97%)	-0.70	1 (0%) 87 76	50, 78, 144, 200	0
2	L	197/203 (97%)	-0.43	0 100 100	51, 105, 244, 304	0
3	C	303/311 (97%)	-0.75	0 100 100	41, 77, 123, 179	0
3	F	303/311 (97%)	0.07	9 (2%) 52 33	71, 182, 279, 333	0
3	I	303/311 (97%)	-0.56	0 100 100	48, 100, 158, 209	0
3	M	303/311 (97%)	-0.45	4 (1%) 75 55	43, 81, 279, 345	0
4	U	0/30	-	-	-	-
4	X	0/30	-	-	-	-
4	Y	0/30	-	-	-	-
4	Z	0/30	-	-	-	-
All	All	3859/4072 (94%)	-0.49	24 (0%) 85 73	39, 103, 235, 345	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	470	ALA	5.1
1	K	470	ALA	5.0
1	D	469	ALA	4.0
3	F	33	ALA	3.3
3	M	33	ALA	2.9
1	K	469	ALA	2.9
1	K	296	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
3	M	35	THR	2.8
1	G	470	ALA	2.7
3	F	279	MET	2.5
1	G	441	GLY	2.5
3	F	4	PHE	2.4
2	H	7	LEU	2.4
3	F	108	GLU	2.3
3	F	122	VAL	2.3
1	A	470	ALA	2.3
1	K	96	ALA	2.3
3	M	18	VAL	2.3
3	F	147	HIS	2.1
2	E	201	ASN	2.1
3	F	20	LEU	2.0
3	F	186	MET	2.0
3	F	35	THR	2.0
3	M	34	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	PO4	D	506	5/5	0.81	0.09	177,178,188,191	0
9	PO4	G	506	5/5	0.89	0.23	27,29,32,35	0
11	FC6	F	323	13/13	0.89	0.24	37,40,42,46	13
11	FC6	I	323	13/13	0.89	0.26	52,57,68,80	13
7	CA	G	505	1/1	0.90	0.06	91,91,91,91	0
9	PO4	K	506	5/5	0.91	0.06	140,144,146,153	0

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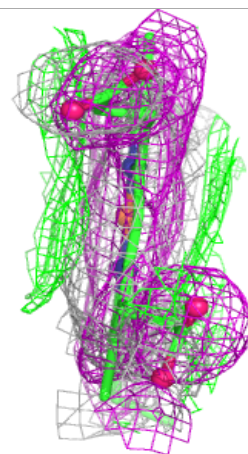
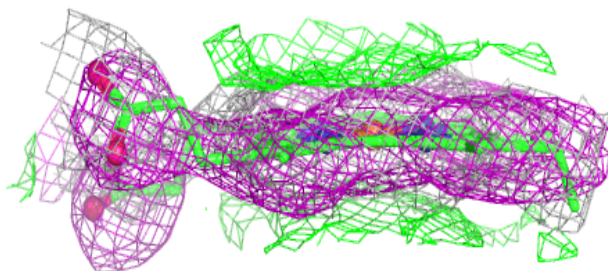
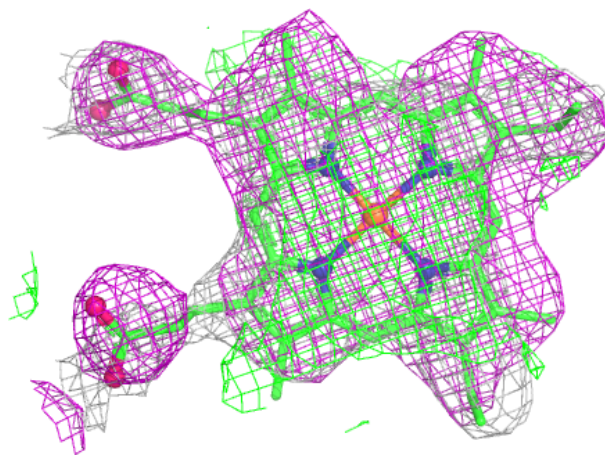
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	HEC	F	322	43/43	0.91	0.14	34,43,47,50	0
10	HEC	F	321	43/43	0.93	0.14	20,24,28,35	0
9	PO4	A	506	5/5	0.94	0.15	21,22,23,24	0
7	CA	D	505	1/1	0.94	0.06	138,138,138,138	0
7	CA	A	505	1/1	0.94	0.05	88,88,88,88	0
7	CA	K	505	1/1	0.94	0.05	133,133,133,133	0
11	FC6	C	323	13/13	0.96	0.16	33,39,46,55	13
5	HEM	K	501	43/43	0.96	0.13	117,127,147,153	0
10	HEC	E	211	43/43	0.96	0.09	16,18,27,32	0
8	PEO	K	508	2/2	0.97	0.12	130,130,130,135	0
7	CA	G	504	1/1	0.97	0.05	74,74,74,74	0
10	HEC	L	211	43/43	0.97	0.08	18,21,26,30	0
10	HEC	C	322	43/43	0.98	0.06	22,28,34,36	0
5	HEM	K	502	43/43	0.98	0.10	85,102,115,125	0
5	HEM	D	501	43/43	0.98	0.09	96,121,137,149	0
5	HEM	D	502	43/43	0.98	0.08	83,96,110,112	0
10	HEC	H	211	43/43	0.98	0.06	24,27,32,38	0
10	HEC	I	321	43/43	0.98	0.07	20,24,34,39	0
10	HEC	I	322	43/43	0.98	0.06	24,28,31,36	0
7	CA	E	504	1/1	0.98	0.05	105,105,105,105	0
5	HEM	G	502	43/43	0.98	0.07	56,61,70,83	0
5	HEM	A	502	43/43	0.98	0.08	43,52,61,72	0
10	HEC	C	321	43/43	0.98	0.06	21,27,36,44	0
11	FC6	M	323	13/13	0.98	0.10	28,30,38,39	13
10	HEC	B	211	43/43	0.99	0.05	25,28,35,46	0
8	PEO	G	508	2/2	0.99	0.04	71,71,71,74	0
7	CA	B	504	1/1	0.99	0.06	51,51,51,51	0
10	HEC	M	321	43/43	0.99	0.06	18,25,35,43	0
10	HEC	M	322	43/43	0.99	0.06	19,23,27,34	0
5	HEM	A	501	43/43	0.99	0.06	47,57,64,71	0
7	CA	K	504	1/1	0.99	0.02	99,99,99,99	0
5	HEM	G	501	43/43	0.99	0.07	56,71,81,89	0
8	PEO	D	508	2/2	0.99	0.06	133,133,133,141	0
6	CU	K	503	1/1	1.00	0.07	135,135,135,135	0
8	PEO	A	508	2/2	1.00	0.04	57,57,57,63	0
6	CU	A	503	1/1	1.00	0.03	59,59,59,59	0
6	CU	D	503	1/1	1.00	0.01	115,115,115,115	0
6	CU	G	503	1/1	1.00	0.01	77,77,77,77	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.

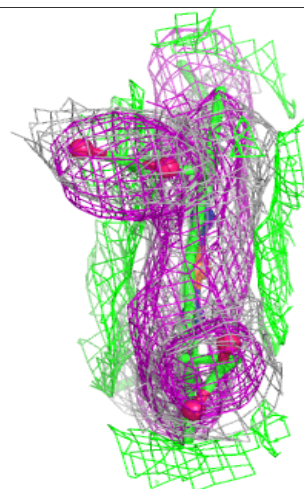
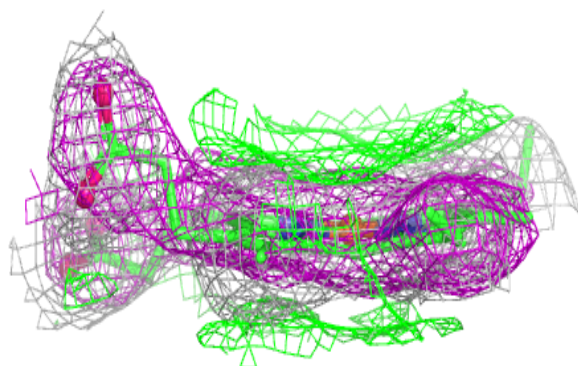
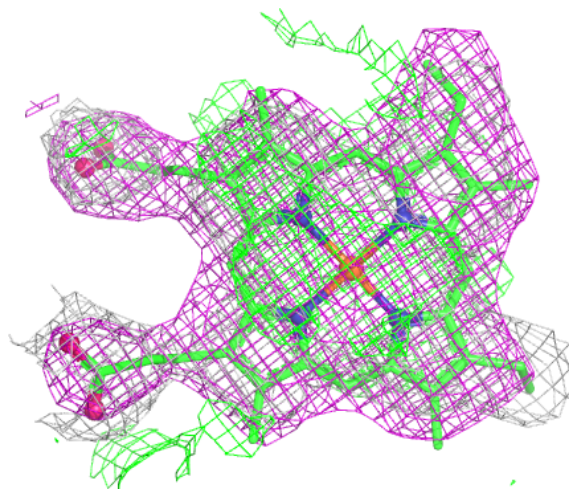
Electron density around HEC F 322:

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



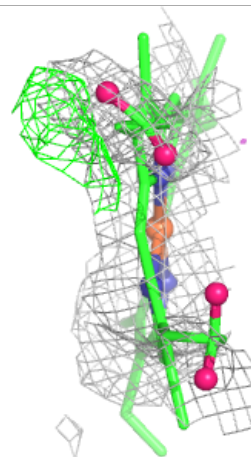
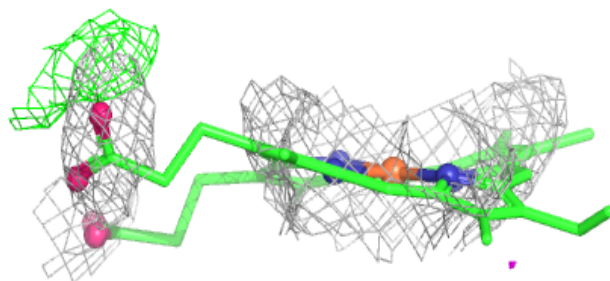
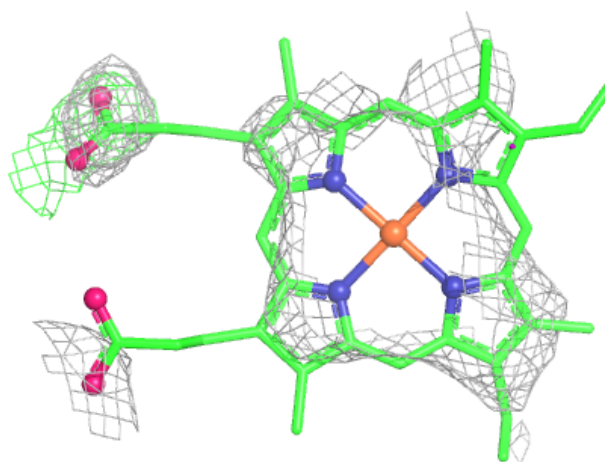
Electron density around HEC F 321:

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



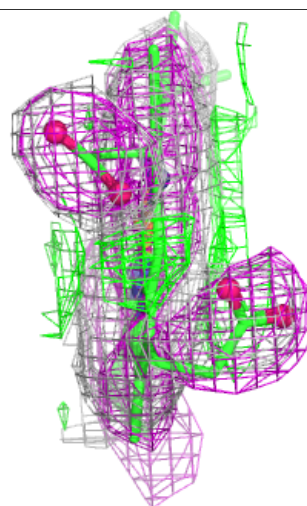
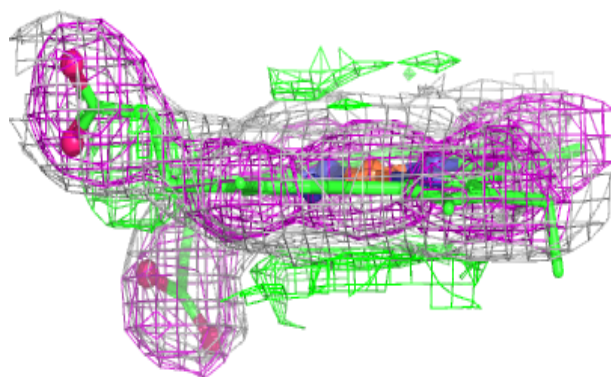
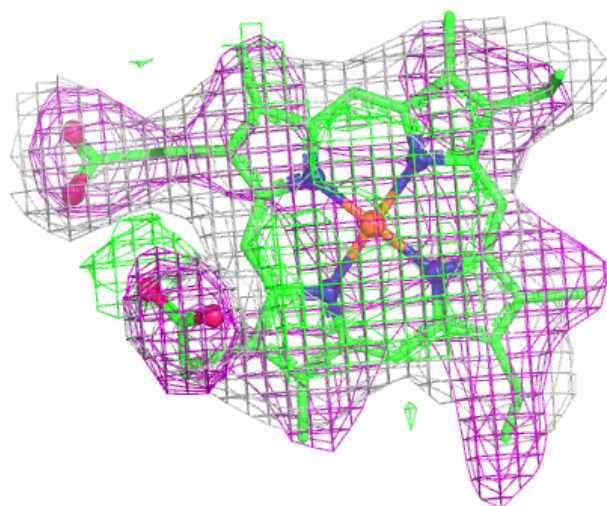
Electron density around HEM K 501:

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



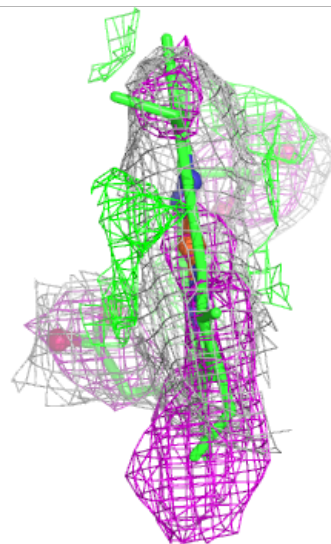
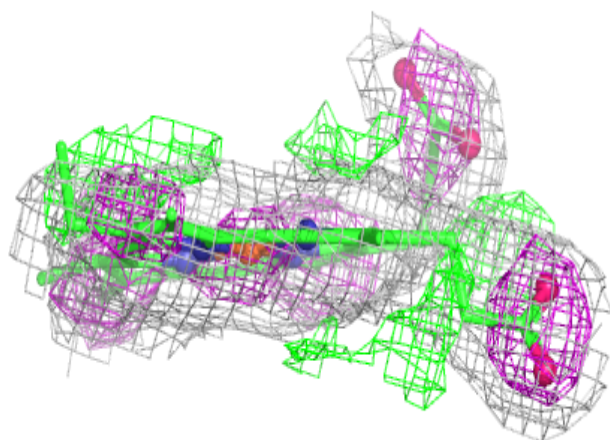
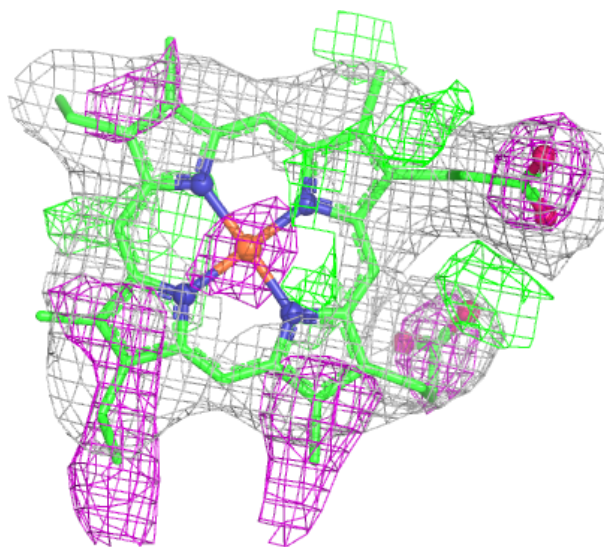
Electron density around HEC E 211:

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



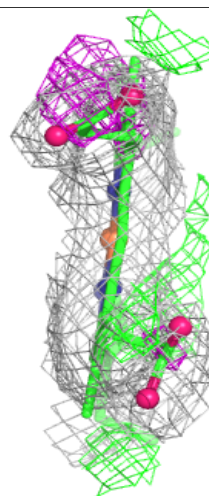
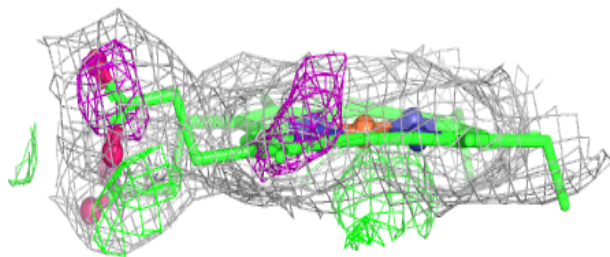
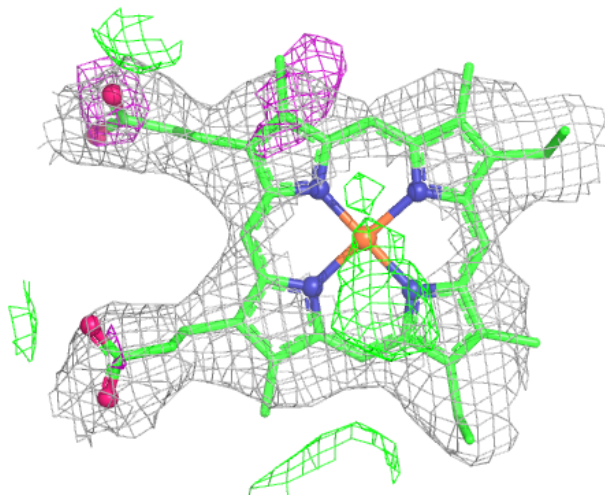
Electron density around HEC L 211:

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



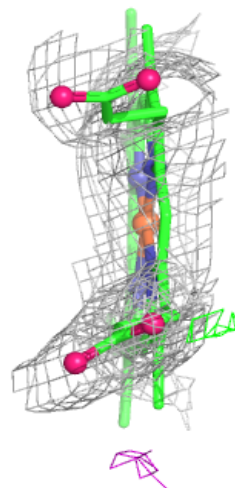
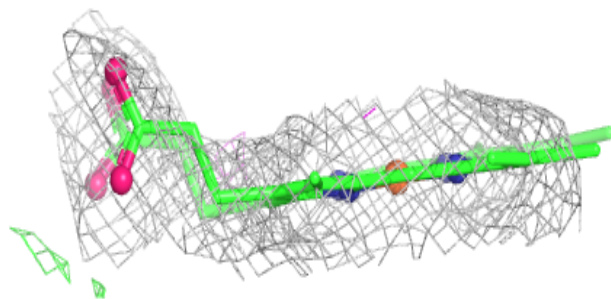
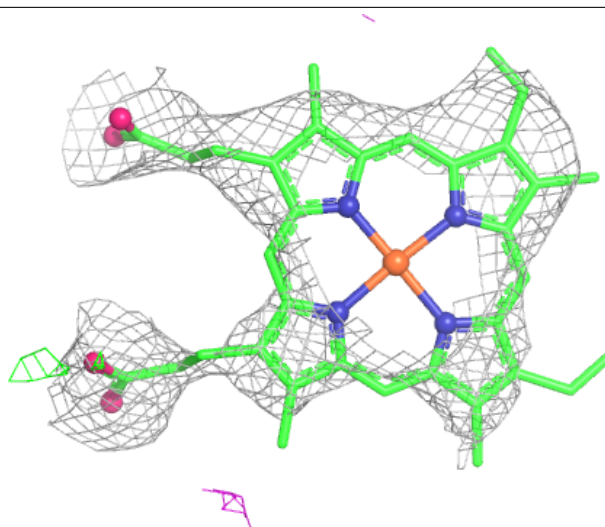
Electron density around HEC C 322:

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



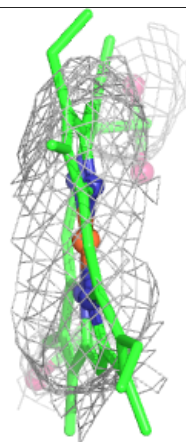
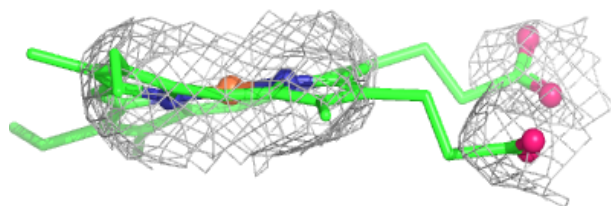
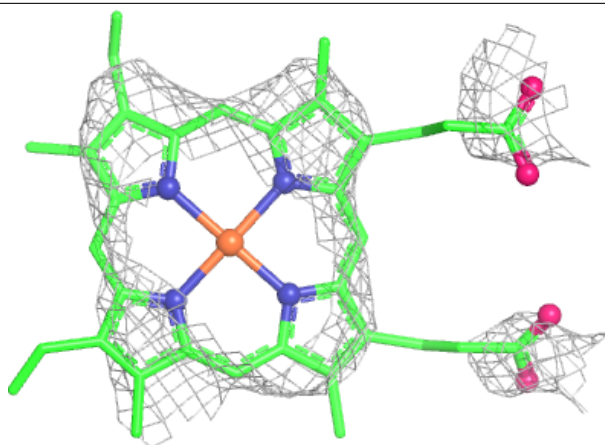
Electron density around HEM K 502:

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



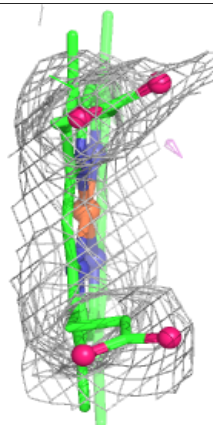
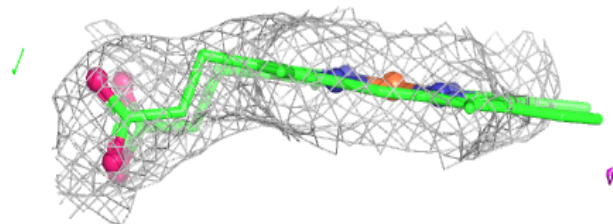
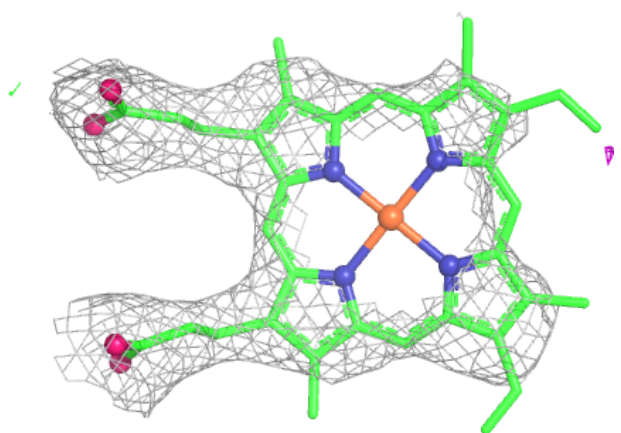
Electron density around HEM D 501:

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



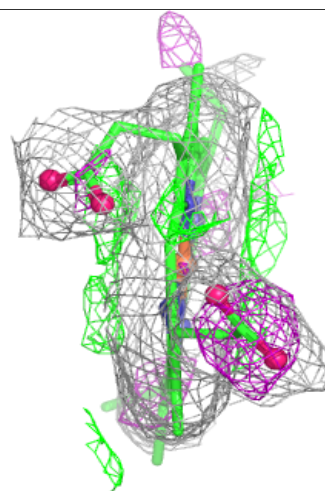
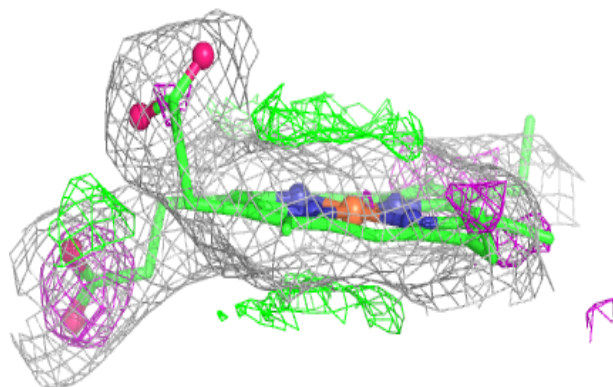
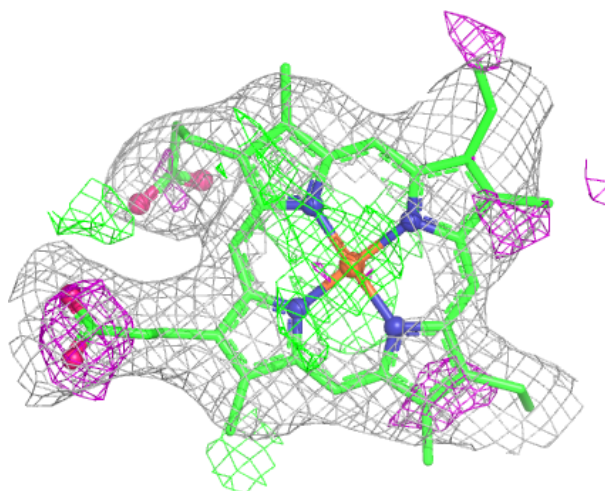
Electron density around HEM D 502:

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



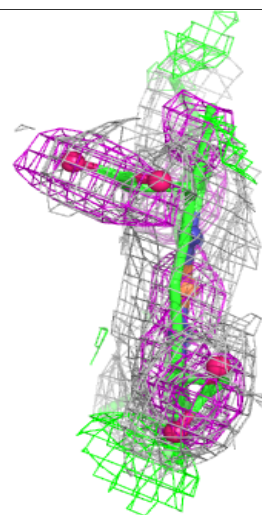
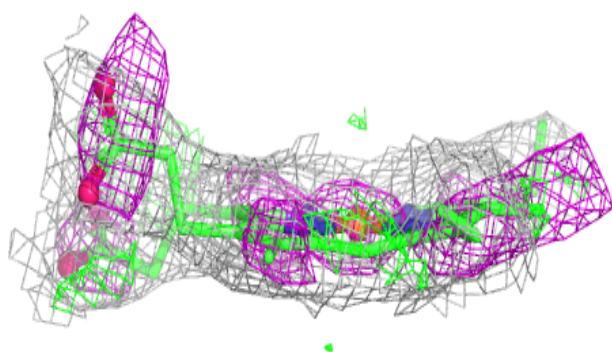
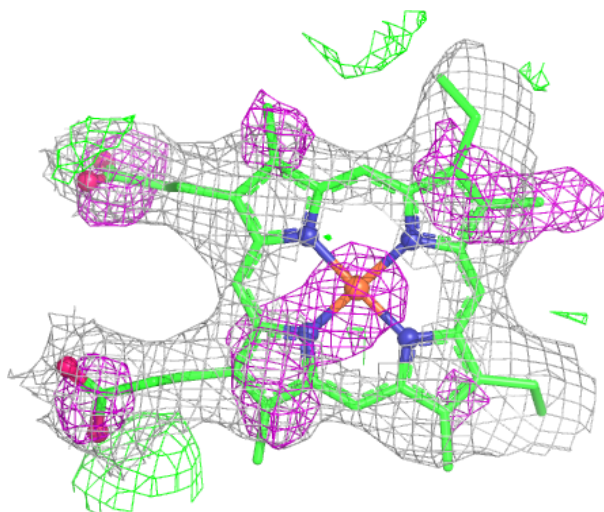
Electron density around HEC H 211:

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



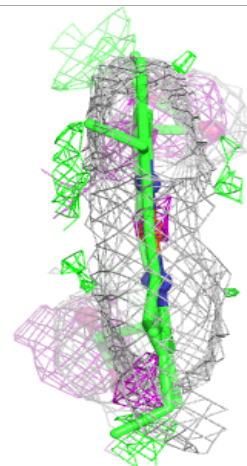
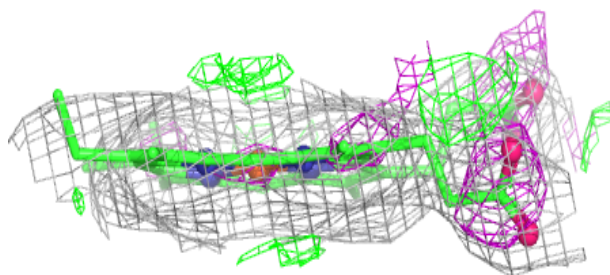
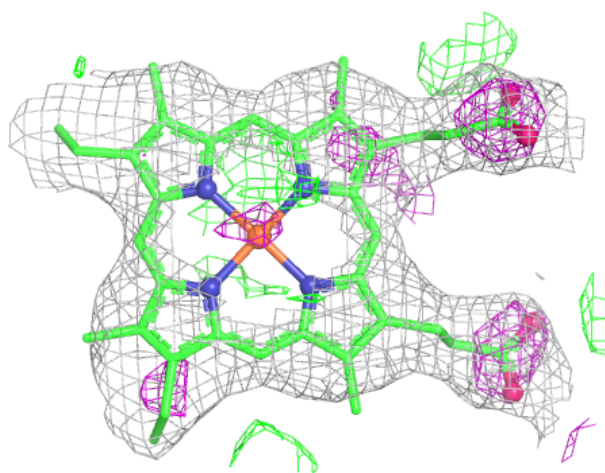
Electron density around HEC I 321:

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



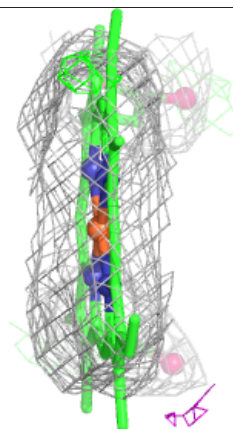
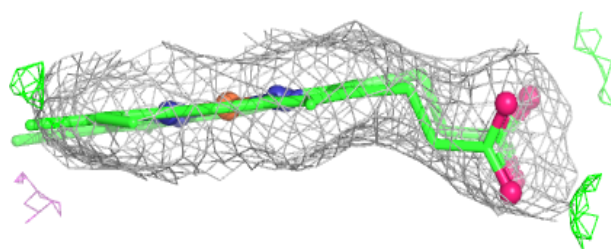
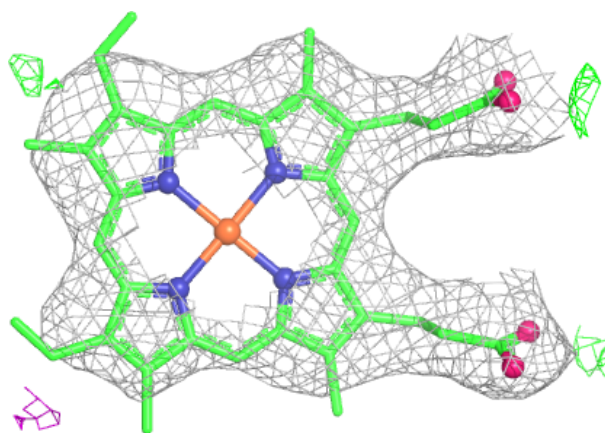
Electron density around HEC I 322:

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

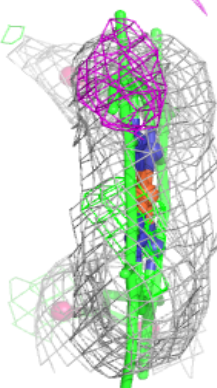
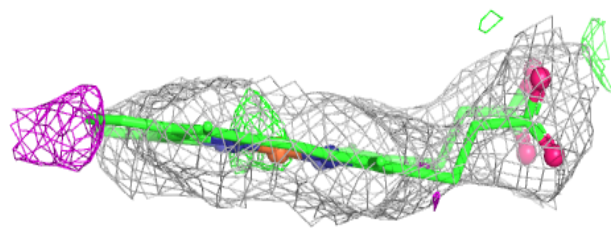
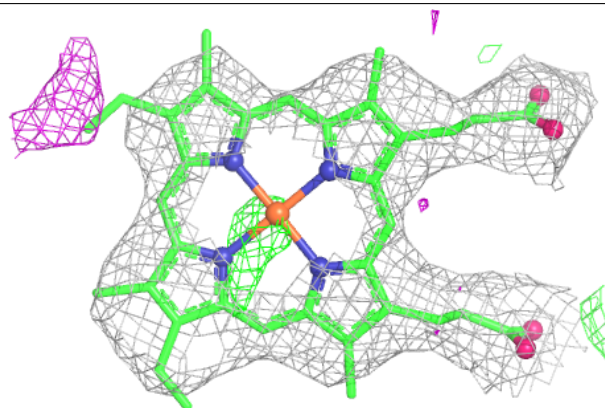


Electron density around HEM G 502:

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

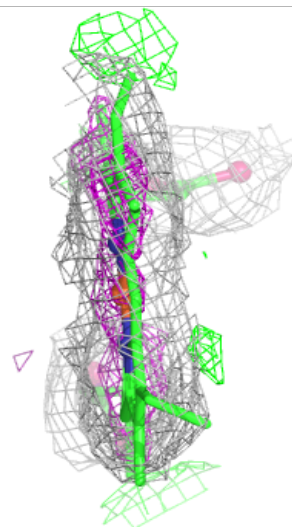
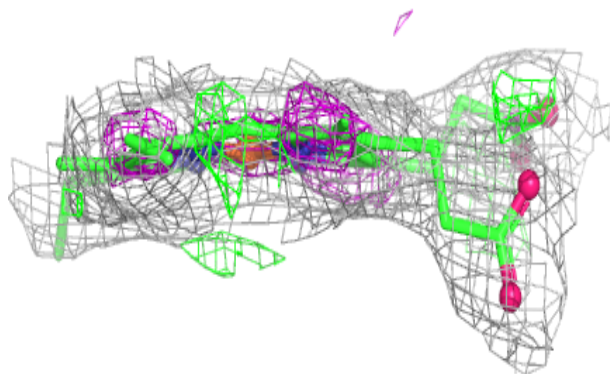
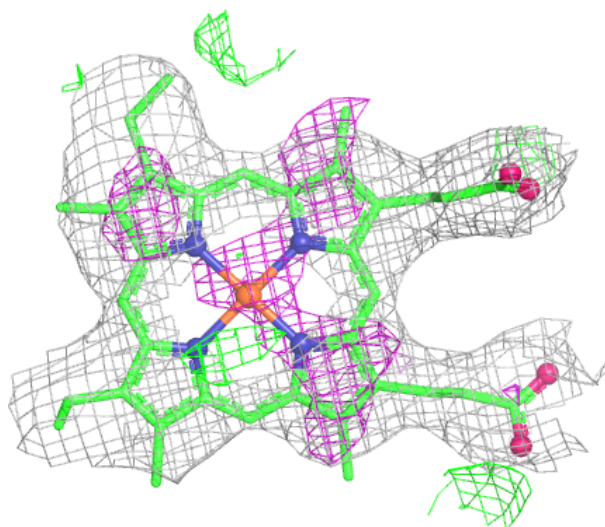
**Electron density around HEM A 502:**

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



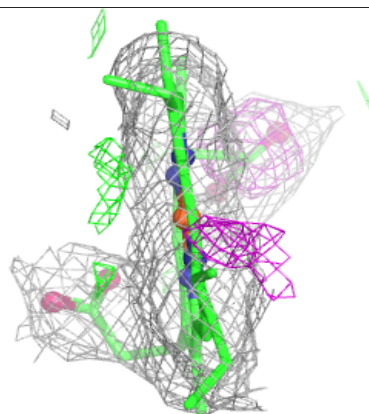
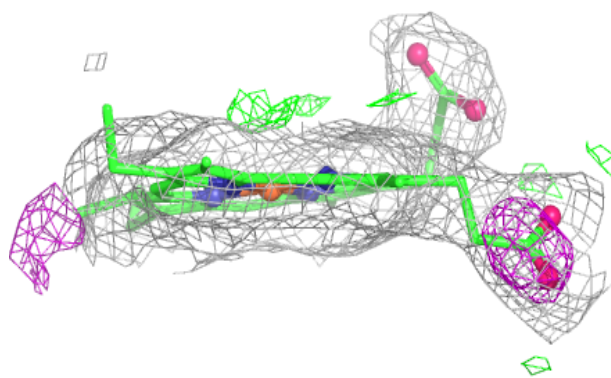
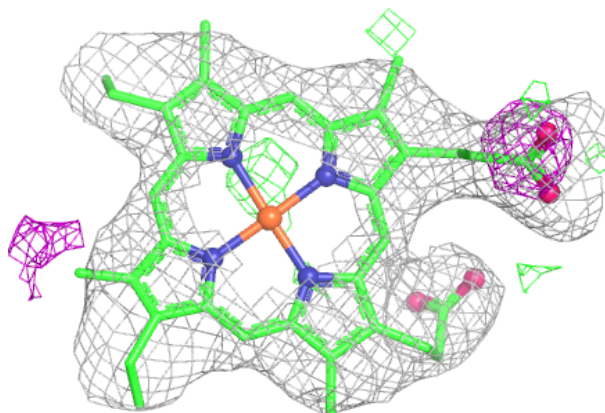
Electron density around HEC C 321:

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



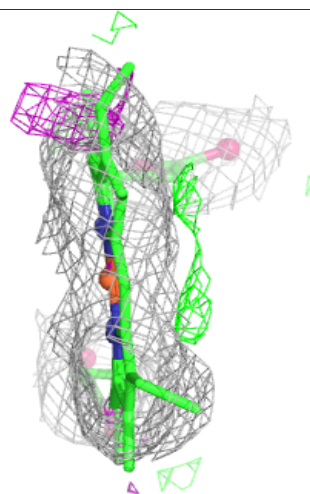
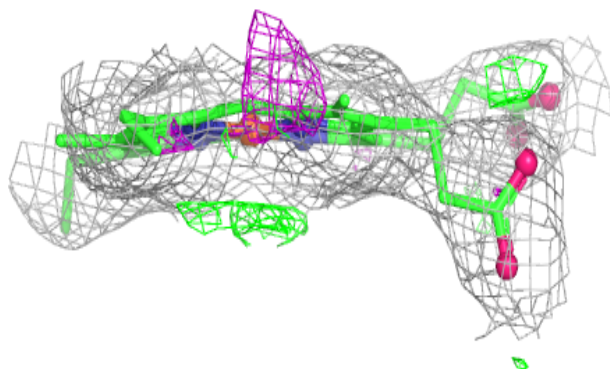
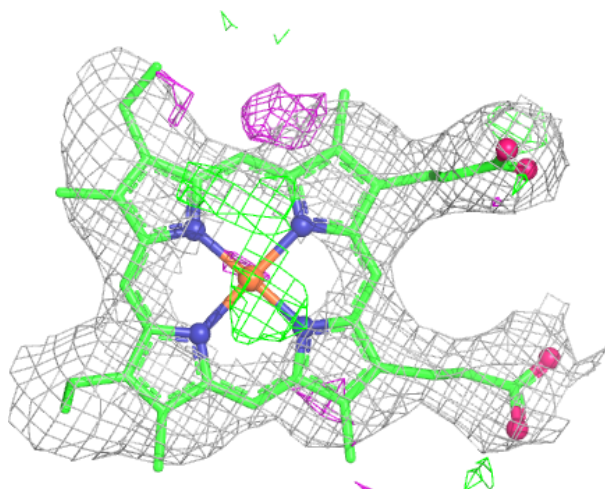
Electron density around HEC B 211:

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



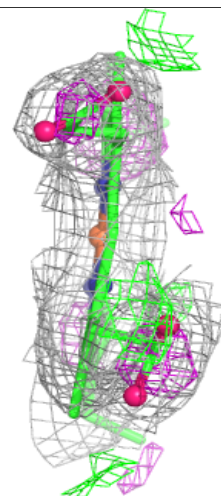
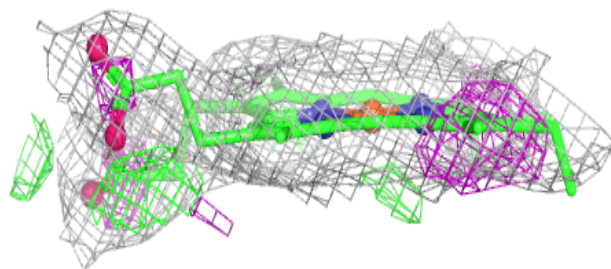
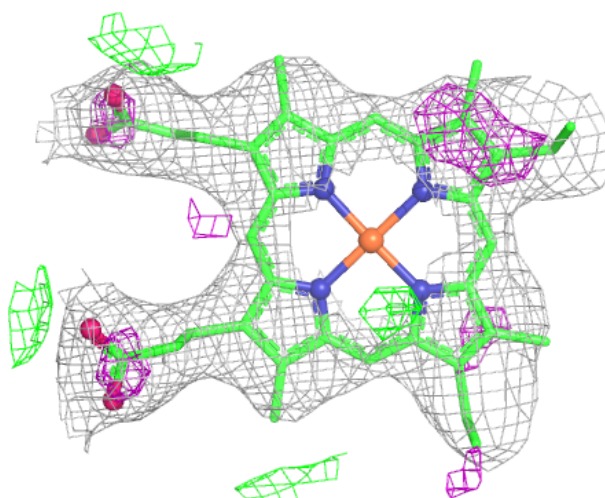
Electron density around HEC M 321:

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



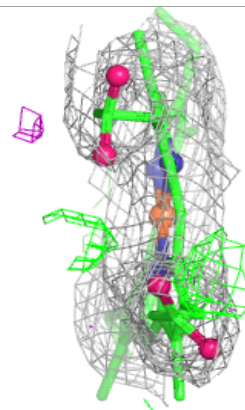
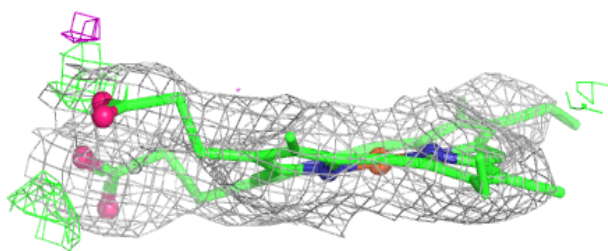
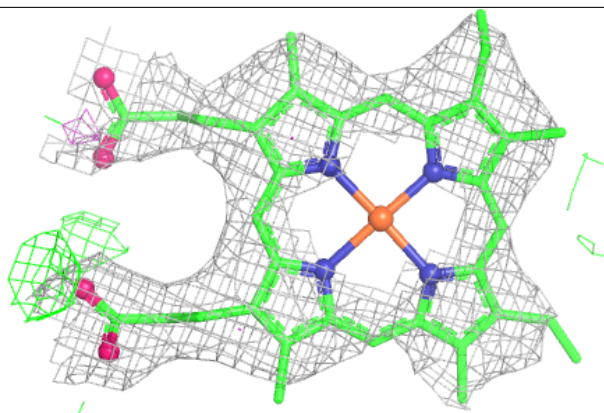
Electron density around HEC M 322:

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

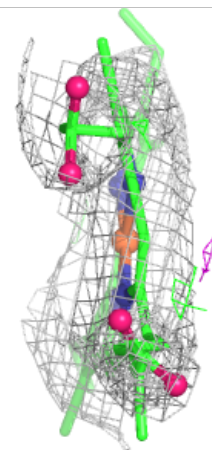
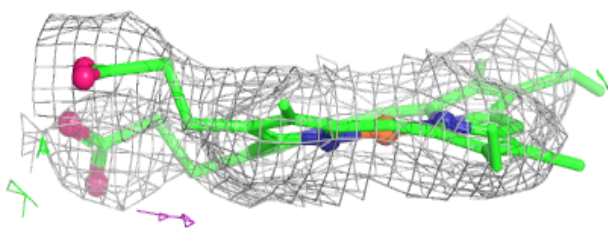
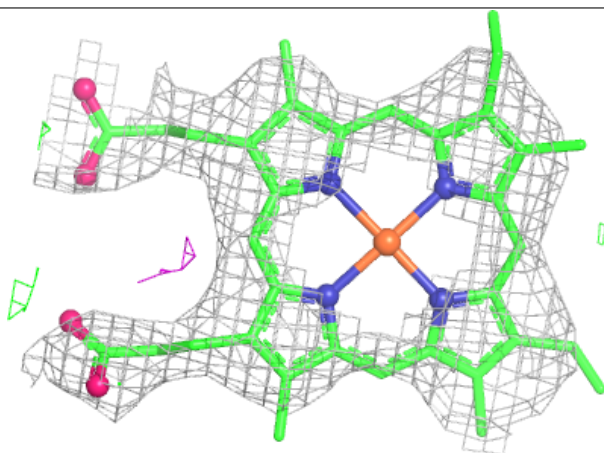


Electron density around HEM A 501:

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

**Electron density around HEM 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.