



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 06:49 PM EDT

PDB ID : 5MNS
Title : Structural and functional characterization of OleP in complex with 6DEB in sodium formate
Authors : Parisi, G.; Savino, C.; Montemiglio, L.C.; Vallone, B.
Deposited on : 2016-12-13
Resolution : 2.62 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

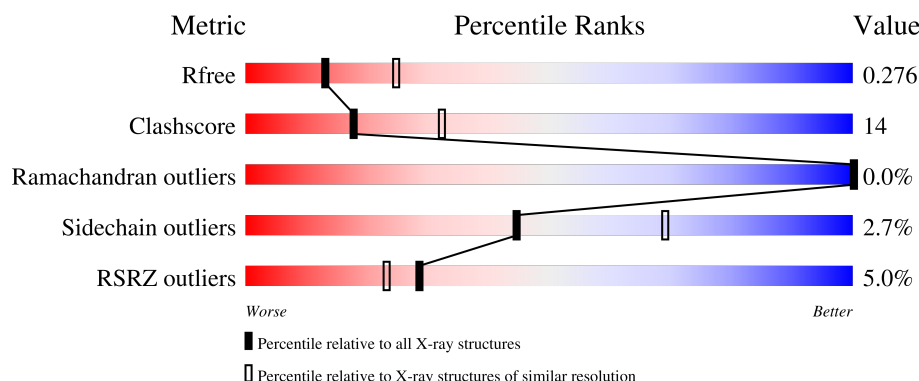
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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	407	 2% 78% 18% ..
1	B	407	 % 81% 15% ..
1	C	407	 % 83% 13% ..
1	D	407	 2% 72% 24% ..
1	E	407	 7% 78% 18% ..

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Mol	Chain	Length	Quality of chain
1	F	407	<div><div></div><div>16%</div><div></div><div>72%</div><div></div><div>22%</div><div></div><div></div></div>

2 Entry composition [i](#)

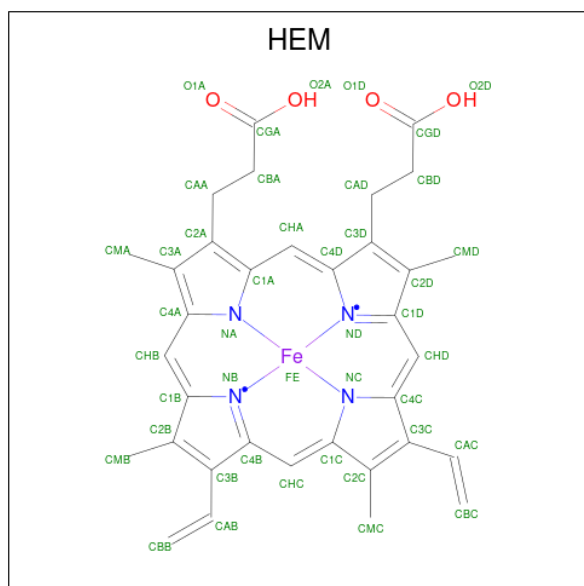
There are 4 unique types of molecules in this entry. The entry contains 19457 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 P-450.

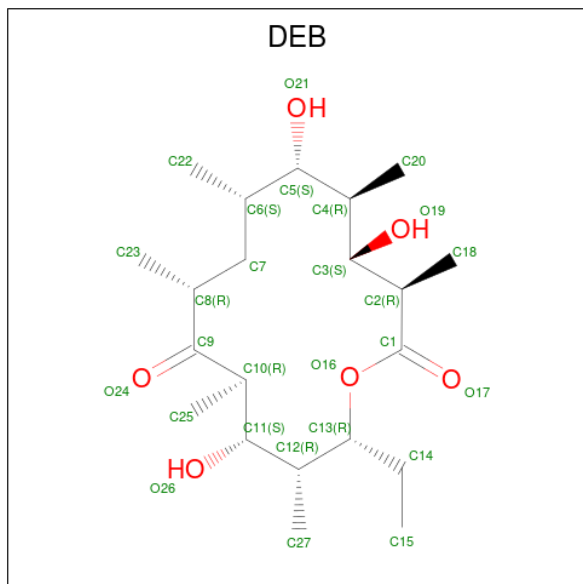
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			3077	1937	552	575	13			
1	B	395	Total	C	N	O	S	0	2	0
			3094	1947	556	578	13			
1	C	395	Total	C	N	O	S	0	0	0
			3077	1937	552	575	13			
1	D	395	Total	C	N	O	S	0	0	0
			3077	1937	552	575	13			
1	E	395	Total	C	N	O	S	0	1	0
			3085	1942	555	575	13			
1	F	393	Total	C	N	O	S	0	0	0
			3062	1928	550	571	13			

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



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

- Molecule 3 is 6-DEOXYERYTHRONOLIDE B (three-letter code: DEB) (formula: $C_{21}H_{38}O_6$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C O	0	0
			27	21 6		
3	B	1	Total	C O	0	0
			27	21 6		
3	C	1	Total	C O	0	0
			27	21 6		
3	D	1	Total	C O	0	0
			27	21 6		
3	E	1	Total	C O	0	0
			27	21 6		
3	F	1	Total	C O	0	0
			27	21 6		

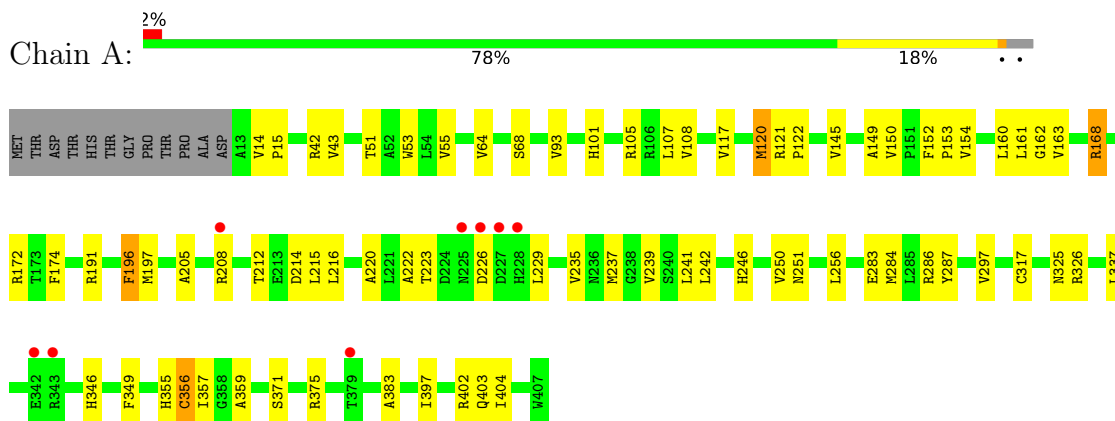
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	89	Total 89	O 89	0	0
4	B	126	Total 126	O 126	0	0
4	C	184	Total 184	O 184	0	0
4	D	56	Total 56	O 56	0	0
4	E	53	Total 53	O 53	0	0
4	F	57	Total 57	O 57	0	0

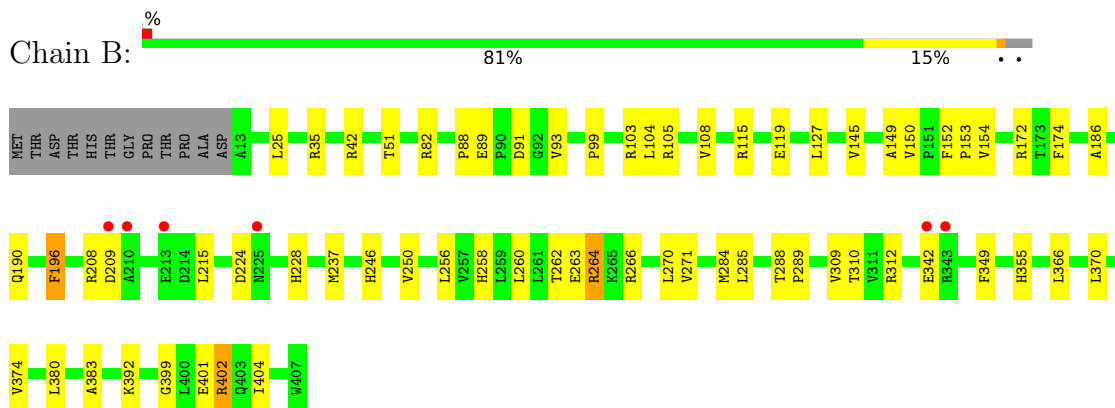
3 Residue-property plots [i](#)

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

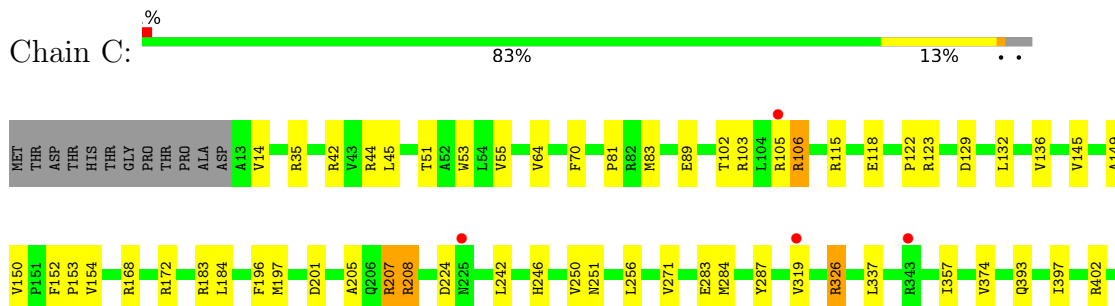
• Molecule 1: Cytochrome P-450



• Molecule 1: Cytochrome P-450



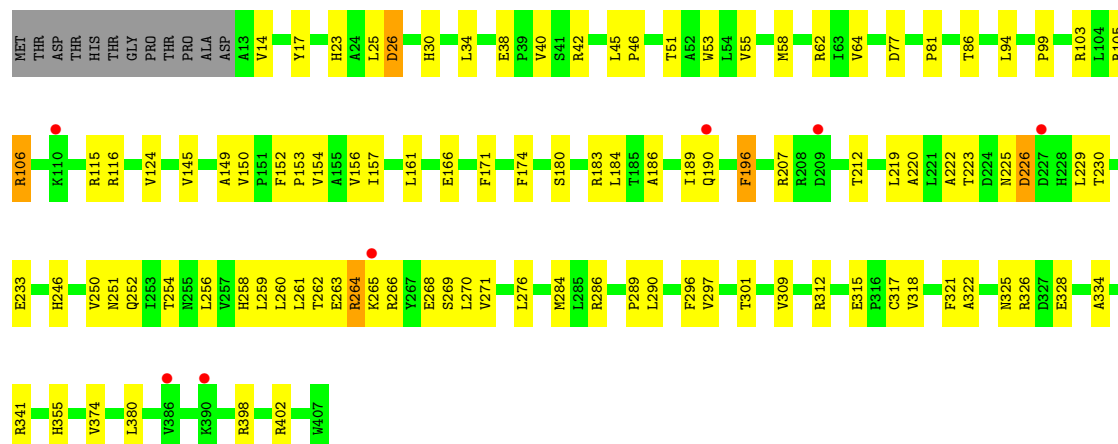
• Molecule 1: Cytochrome P-450




W407

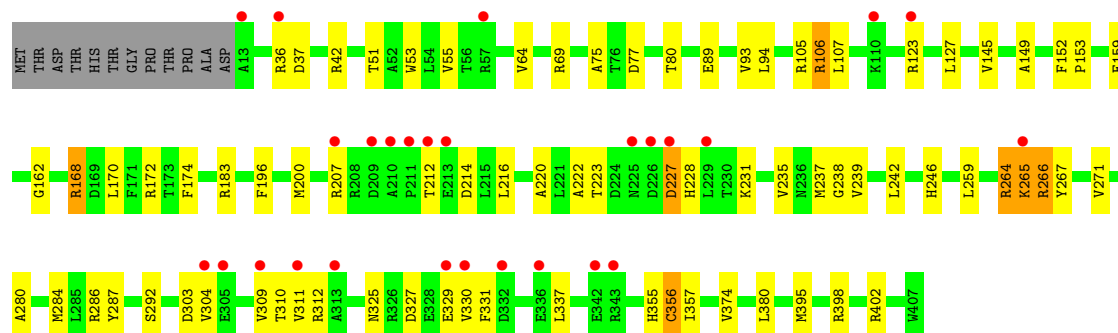
- Molecule 1: Cytochrome P-450

Chain D:  2% 72% 24%



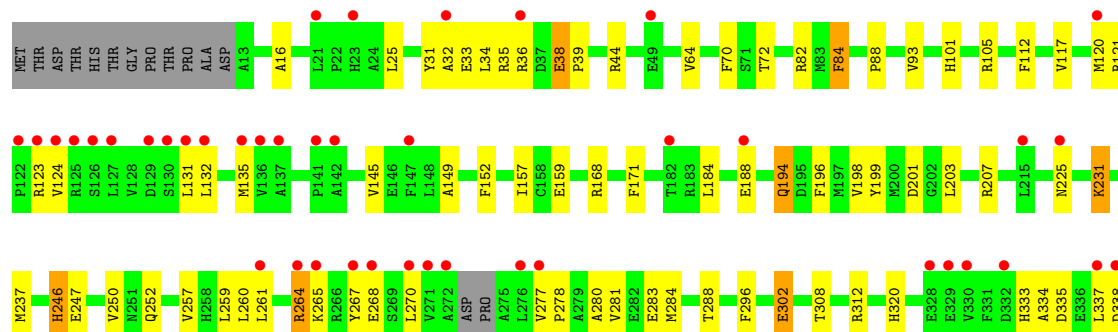
- Molecule 1: Cytochrome P-450

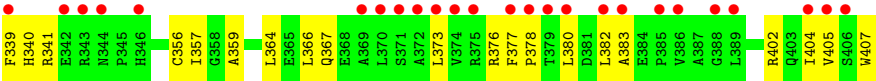
Chain E:  7% 78% 18%



- Molecule 1: Cytochrome P-450

Chain F:  16% 72% 22%





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	247.60Å 110.80Å 159.10Å 90.00° 129.60° 90.00°	Depositor
Resolution (Å)	120.00 – 2.62 47.91 – 2.62	Depositor EDS
% Data completeness (in resolution range)	99.6 (120.00-2.62) 99.7 (47.91-2.62)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.208 , 0.258 0.234 , 0.276	Depositor DCC
R_{free} test set	4932 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19457	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.57 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.4422e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: DEB, 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	0.50	0/3144	0.72	0/4284
1	B	0.50	0/3164	0.74	0/4310
1	C	0.51	0/3144	0.74	2/4284 (0.0%)
1	D	0.51	0/3144	0.75	1/4284 (0.0%)
1	E	0.49	0/3155	0.74	1/4298 (0.0%)
1	F	0.48	0/3127	0.74	0/4258
All	All	0.50	0/18878	0.74	4/25718 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	26	ASP	N-CA-C	-5.44	96.32	111.00
1	C	103	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	C	123	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	E	266	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3077	0	3056	75	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3094	0	3074	65	0
1	C	3077	0	3056	49	0
1	D	3077	0	3056	95	1
1	E	3085	0	3070	109	0
1	F	3062	0	3044	118	1
2	A	43	0	30	6	0
2	B	43	0	30	4	0
2	C	43	0	30	2	0
2	D	43	0	30	4	0
2	E	43	0	30	12	0
2	F	43	0	30	4	0
3	A	27	0	38	0	0
3	B	27	0	38	1	0
3	C	27	0	38	0	0
3	D	27	0	38	1	0
3	E	27	0	38	0	0
3	F	27	0	38	0	0
4	A	89	0	0	0	0
4	B	126	0	0	3	1
4	C	184	0	0	6	0
4	D	56	0	0	5	0
4	E	53	0	0	1	0
4	F	57	0	0	4	0
All	All	19457	0	18764	511	3

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 14.

All (511) 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:E:356:CYS:SG	2:E:501:HEM:FE	0.96	1.56
1:A:42:ARG:HH11	1:A:51:THR:CG2	1.30	1.44
1:E:123:ARG:NH1	1:E:127:LEU:HD12	1.42	1.35
1:E:356:CYS:SG	2:E:501:HEM:ND	2.00	1.34
1:E:42:ARG:HD2	1:E:51:THR:OG1	1.34	1.25
1:A:42:ARG:NH1	1:A:51:THR:HG21	1.48	1.25
1:E:356:CYS:SG	2:E:501:HEM:NA	2.09	1.25
1:C:207:ARG:NH2	4:C:601:HOH:O	1.70	1.23
1:A:42:ARG:NH1	1:A:51:THR:CG2	1.97	1.22
1:F:283:GLU:HG3	1:F:337:LEU:CD1	1.73	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:GLY:HA3	1:E:207:ARG:HH12	1.10	1.17
1:A:42:ARG:HH11	1:A:51:THR:HG23	1.02	1.15
1:D:150:VAL:O	1:D:153:PRO:HD2	1.50	1.12
1:D:45:LEU:HD12	1:D:81:PRO:CB	1.81	1.11
1:F:337:LEU:HD21	1:F:339:PHE:HE1	1.14	1.10
1:D:264:ARG:NH2	1:D:380:LEU:O	1.87	1.08
1:D:186:ALA:O	1:D:190:GLN:HG3	1.54	1.08
1:B:209:ASP:OD1	1:F:302:GLU:HG3	1.52	1.07
2:E:501:HEM:HHC	2:E:501:HEM:HBB2	1.38	1.05
1:D:45:LEU:HD12	1:D:81:PRO:HB2	1.34	1.04
1:E:207:ARG:NH2	1:E:214:ASP:CB	2.20	1.04
1:F:337:LEU:HD21	1:F:339:PHE:CE1	1.92	1.03
1:F:337:LEU:CD2	1:F:339:PHE:HE1	1.72	1.03
1:B:256:LEU:CD2	1:B:284:MET:HB3	1.88	1.02
1:E:106[A]:ARG:HH21	1:E:106[A]:ARG:HG2	1.20	1.02
1:E:106[B]:ARG:HG2	1:E:106[B]:ARG:NH1	1.59	1.02
1:E:106[B]:ARG:HH11	1:E:106[B]:ARG:CG	1.72	1.02
1:E:123:ARG:HH12	1:E:127:LEU:CD1	1.71	1.01
1:E:207:ARG:NH2	1:E:216:LEU:HB2	1.75	1.01
1:E:220:ALA:O	1:E:223:THR:HG22	1.58	1.01
1:E:183:ARG:HH11	1:E:395:MET:HG3	1.26	0.99
1:E:106[A]:ARG:HH21	1:E:106[A]:ARG:CG	1.75	0.99
1:F:337:LEU:CD2	1:F:339:PHE:CE1	2.45	0.98
1:B:309:VAL:HG22	1:C:122:PRO:HB3	1.46	0.97
1:F:283:GLU:HG3	1:F:337:LEU:HD12	1.46	0.97
1:F:101:HIS:HD2	4:F:616:HOH:O	1.45	0.97
1:E:123:ARG:HH12	1:E:127:LEU:HD12	0.94	0.96
1:D:297:VAL:HG22	1:D:318:VAL:HG22	1.48	0.95
1:C:105:ARG:NE	4:C:602:HOH:O	1.99	0.95
1:A:105:ARG:NH2	1:A:355:HIS:O	2.00	0.95
1:E:106[B]:ARG:HG2	1:E:106[B]:ARG:HH11	0.78	0.94
1:E:207:ARG:HH22	1:E:214:ASP:HB3	1.34	0.93
1:B:264:ARG:NH1	1:B:380:LEU:O	2.02	0.92
1:E:69:ARG:HE	1:E:304:VAL:HG22	1.33	0.92
1:E:123:ARG:NH2	1:E:159:GLU:OE2	2.03	0.91
1:E:123:ARG:NH1	1:E:127:LEU:CD1	2.30	0.91
1:E:123:ARG:CZ	1:E:127:LEU:HD12	1.99	0.91
1:E:356:CYS:SG	2:E:501:HEM:NB	2.44	0.90
1:E:200:MET:CE	1:E:238:GLY:C	2.40	0.90
1:E:200:MET:HE1	1:E:238:GLY:C	1.93	0.89
1:F:283:GLU:HG3	1:F:337:LEU:HD11	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:356:CYS:SG	2:E:501:HEM:NC	2.47	0.87
1:A:42:ARG:NH1	1:A:51:THR:HG23	1.76	0.87
1:E:207:ARG:NH2	1:E:214:ASP:HB3	1.88	0.87
1:E:36:ARG:NH1	1:E:37:ASP:OD1	2.07	0.87
1:B:42[A]:ARG:NH1	1:B:51:THR:OG1	2.06	0.86
1:E:42:ARG:CD	1:E:51:THR:OG1	2.22	0.85
1:E:183:ARG:NH1	1:E:395:MET:HG3	1.91	0.85
1:E:207:ARG:NH2	1:E:214:ASP:HB2	1.92	0.84
1:F:135:MET:CE	1:F:407:TRP:CZ3	2.60	0.84
1:B:256:LEU:CD2	1:B:284:MET:CB	2.55	0.83
1:D:45:LEU:HD12	1:D:81:PRO:HB3	1.59	0.83
1:B:256:LEU:HD23	1:B:284:MET:HB3	1.60	0.83
1:E:123:ARG:NE	1:E:159:GLU:OE2	2.12	0.82
1:D:186:ALA:O	1:D:190:GLN:CG	2.27	0.82
2:E:501:HEM:HMC1	2:E:501:HEM:HBC2	1.61	0.82
1:F:277:VAL:HG22	1:F:278:PRO:HD3	1.61	0.82
1:E:200:MET:HE1	1:E:238:GLY:O	1.80	0.82
1:D:42:ARG:NH2	1:D:53:TRP:CZ2	2.47	0.81
1:E:162:GLY:HA3	1:E:207:ARG:NH1	1.94	0.81
1:D:297:VAL:HG13	1:D:317:CYS:O	1.81	0.81
1:D:166:GLU:HG2	1:E:227:ASP:OD2	1.80	0.80
1:E:309:VAL:HG12	1:E:310:THR:N	1.96	0.80
1:E:242:LEU:O	1:E:246:HIS:HD2	1.64	0.80
1:E:123:ARG:CZ	1:E:159:GLU:OE2	2.30	0.80
1:F:267:TYR:OH	1:F:373:LEU:O	2.00	0.79
1:D:42:ARG:NH2	1:D:53:TRP:CE2	2.46	0.79
1:F:101:HIS:CD2	4:F:616:HOH:O	2.24	0.78
1:E:200:MET:HE3	1:E:239:VAL:N	1.98	0.78
1:D:220:ALA:O	1:D:223:THR:OG1	2.01	0.78
1:F:264:ARG:NH2	1:F:380:LEU:O	2.17	0.77
1:F:34:LEU:O	1:F:38:GLU:O	2.03	0.77
1:A:122:PRO:HB3	1:D:309:VAL:HG12	1.66	0.77
1:B:105:ARG:NH2	1:B:355:HIS:O	2.17	0.76
1:F:260:LEU:HD21	1:F:270:LEU:HD11	1.67	0.76
1:C:45:LEU:HD12	1:C:81:PRO:CB	2.15	0.76
1:A:42:ARG:HH12	1:A:51:THR:HG21	1.49	0.75
1:B:256:LEU:HD22	1:B:284:MET:CB	2.17	0.75
1:D:149:ALA:O	1:D:153:PRO:HG2	1.86	0.75
1:E:200:MET:HE3	1:E:238:GLY:C	2.08	0.75
1:B:309:VAL:HG22	1:C:122:PRO:CB	2.16	0.75
1:E:42:ARG:HD2	1:E:51:THR:HG1	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:135:MET:HE3	1:F:407:TRP:CZ3	2.22	0.74
1:F:277:VAL:CG2	1:F:278:PRO:HD3	2.17	0.74
1:B:208:ARG:NE	1:B:224:ASP:OD1	2.17	0.74
1:C:42:ARG:HD3	1:C:53:TRP:CH2	2.22	0.74
1:C:45:LEU:HD12	1:C:81:PRO:HB2	1.68	0.74
1:F:246:HIS:HE1	4:F:603:HOH:O	1.71	0.74
1:B:108:VAL:HG22	1:B:215:LEU:HD22	1.69	0.73
1:E:356:CYS:SG	2:E:501:HEM:C4D	2.81	0.73
1:D:321:PHE:O	4:D:601:HOH:O	2.06	0.73
1:E:69:ARG:NE	1:E:304:VAL:HG22	2.04	0.73
1:D:297:VAL:HG22	1:D:318:VAL:CG2	2.17	0.72
1:D:166:GLU:HG2	1:E:227:ASP:CG	2.09	0.72
1:E:162:GLY:CA	1:E:207:ARG:HH12	1.98	0.72
1:F:260:LEU:CD2	1:F:270:LEU:HD11	2.20	0.72
1:A:108:VAL:HG23	1:A:215:LEU:CD2	2.20	0.71
1:F:39:PRO:HG3	1:F:308:THR:CG2	2.20	0.70
1:F:135:MET:HE2	1:F:407:TRP:CZ3	2.26	0.70
1:B:392:LYS:HG2	1:B:401:GLU:HG3	1.73	0.70
1:A:122:PRO:HB3	1:D:309:VAL:CG1	2.21	0.70
1:E:356:CYS:SG	2:E:501:HEM:C1A	2.85	0.70
1:F:280:ALA:O	1:F:284:MET:HG3	1.92	0.69
1:F:34:LEU:O	1:F:38:GLU:C	2.31	0.69
1:D:166:GLU:HG2	1:E:227:ASP:OD1	1.92	0.68
1:D:265:LYS:HA	1:D:268:GLU:OE2	1.93	0.68
1:B:42[A]:ARG:HD3	1:C:118:GLU:OE2	1.94	0.68
1:B:209:ASP:HB2	1:F:302:GLU:OE2	1.93	0.68
1:F:120:MET:O	1:F:124:VAL:HG23	1.94	0.68
1:B:309:VAL:CG2	1:C:122:PRO:HB3	2.21	0.68
1:A:108:VAL:HG23	1:A:215:LEU:HD22	1.75	0.67
1:A:168:ARG:HG2	1:A:172:ARG:HG3	1.77	0.67
1:F:194:GLN:O	1:F:198:VAL:HG23	1.93	0.67
1:C:242:LEU:O	1:C:246:HIS:HD2	1.76	0.67
1:C:208:ARG:NH2	1:C:224:ASP:OD1	2.27	0.67
1:E:183:ARG:NH1	1:E:395:MET:CG	2.57	0.67
1:E:309:VAL:CG1	1:E:310:THR:N	2.58	0.66
1:A:42:ARG:CD	1:A:53:TRP:CE3	2.79	0.66
1:A:356:CYS:SG	2:A:501:HEM:C1A	2.82	0.66
1:E:106[A]:ARG:CG	1:E:106[A]:ARG:NH2	2.42	0.66
1:E:329:GLU:HG2	4:E:651:HOH:O	1.95	0.66
1:B:370:LEU:O	1:B:374:VAL:HG23	1.97	0.65
1:A:42:ARG:HD3	1:A:53:TRP:CH2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:260:LEU:HD22	1:F:270:LEU:CD1	2.26	0.65
1:F:337:LEU:HD23	1:F:339:PHE:CE1	2.30	0.65
1:F:39:PRO:HG3	1:F:308:THR:HG21	1.77	0.64
1:F:260:LEU:HD22	1:F:270:LEU:HD12	1.79	0.64
1:E:183:ARG:HH11	1:E:395:MET:CG	2.05	0.64
1:E:266:ARG:HD3	1:E:337:LEU:HD23	1.79	0.64
2:E:501:HEM:HBB2	2:E:501:HEM:CHC	2.17	0.64
1:B:383:ALA:HB3	1:B:404:ILE:HG22	1.80	0.64
2:E:501:HEM:HBC2	2:E:501:HEM:CMC	2.28	0.64
1:F:93:VAL:CG2	1:F:237:MET:SD	2.86	0.64
2:B:501:HEM:HMC1	2:B:501:HEM:HBC2	1.78	0.64
1:B:89:GLU:HG3	1:B:91:ASP:H	1.63	0.63
1:E:123:ARG:NH1	1:E:127:LEU:HB2	2.14	0.63
1:B:99:PRO:HB2	1:B:103:ARG:NH1	2.13	0.63
1:C:183:ARG:NH2	1:C:393:GLN:O	2.31	0.63
1:E:183:ARG:NH1	1:E:395:MET:SD	2.71	0.63
1:E:53:TRP:CD1	1:E:311:VAL:HG22	2.34	0.62
1:A:122:PRO:CB	1:D:309:VAL:HG12	2.28	0.62
1:D:106:ARG:CG	1:D:106:ARG:HH11	2.12	0.62
1:C:55:VAL:HB	1:C:319:VAL:HG22	1.82	0.62
1:C:208:ARG:NE	1:C:208:ARG:HA	2.15	0.62
1:A:42:ARG:HD3	1:A:53:TRP:CZ3	2.35	0.61
1:D:153:PRO:HG2	1:D:250:VAL:HG22	1.82	0.61
1:F:283:GLU:CG	1:F:337:LEU:HD12	2.28	0.61
2:A:501:HEM:HBB2	2:A:501:HEM:HMB2	1.81	0.61
1:D:30:HIS:O	1:D:34:LEU:HD12	2.00	0.61
1:D:219:LEU:O	1:D:223:THR:HG23	1.99	0.61
1:D:14:VAL:HG11	1:D:42:ARG:HG3	1.82	0.61
1:B:256:LEU:HD12	1:B:366:LEU:HD22	1.83	0.61
1:A:42:ARG:HD2	1:A:53:TRP:CE3	2.36	0.61
1:C:145:VAL:HA	1:C:149:ALA:HB3	1.83	0.61
1:E:170:LEU:HD22	1:E:174:PHE:CZ	2.36	0.61
1:D:150:VAL:C	1:D:153:PRO:HD2	2.21	0.60
1:D:297:VAL:HG23	4:D:639:HOH:O	2.01	0.60
1:F:32:ALA:O	1:F:36:ARG:NH1	2.34	0.60
1:D:270:LEU:HD23	1:D:276:LEU:HD23	1.84	0.60
1:D:180:SER:OG	1:D:189:ILE:HD11	2.01	0.60
1:F:135:MET:CE	1:F:407:TRP:CH2	2.84	0.60
1:A:108:VAL:CG2	1:A:215:LEU:HD22	2.32	0.59
1:D:246:HIS:O	1:D:250:VAL:HG23	2.01	0.59
2:D:501:HEM:HBB2	2:D:501:HEM:HMB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:260:LEU:CD2	1:F:270:LEU:CD1	2.80	0.59
1:F:123:ARG:NH2	1:F:159:GLU:HG3	2.17	0.59
1:E:242:LEU:O	1:E:246:HIS:CD2	2.51	0.59
1:F:338:ASP:OD1	1:F:340:HIS:ND1	2.34	0.59
1:C:42:ARG:HD3	1:C:53:TRP:CZ2	2.37	0.59
1:D:149:ALA:O	1:D:153:PRO:CG	2.50	0.59
1:F:377:PHE:N	1:F:378:PRO:HD3	2.17	0.59
1:D:286:ARG:HG3	1:D:325:ASN:HB3	1.84	0.59
1:B:209:ASP:CG	1:F:302:GLU:HG3	2.21	0.59
1:F:383:ALA:HB3	1:F:404:ILE:HG22	1.83	0.58
1:B:25:LEU:HD22	1:B:288:THR:HG23	1.85	0.58
1:E:123:ARG:NH2	1:E:127:LEU:HD12	2.18	0.58
1:E:168:ARG:O	1:E:172:ARG:HG3	2.04	0.58
1:F:145:VAL:HA	1:F:149:ALA:HB3	1.86	0.58
1:F:380:LEU:HD11	1:F:405:VAL:HG11	1.85	0.58
1:F:246:HIS:O	1:F:250:VAL:HG23	2.04	0.58
1:B:309:VAL:HG12	1:B:310:THR:N	2.19	0.57
1:F:39:PRO:CG	1:F:308:THR:HG21	2.35	0.57
1:E:330:VAL:HG13	1:E:331:PHE:CD2	2.39	0.57
2:F:501:HEM:HMB2	2:F:501:HEM:HBB2	1.86	0.57
1:A:212:THR:OG1	1:A:214:ASP:OD1	2.21	0.57
1:D:106:ARG:HH11	1:D:106:ARG:HG3	1.69	0.57
1:D:166:GLU:CG	1:E:227:ASP:OD2	2.52	0.57
1:D:264:ARG:O	1:D:264:ARG:HG2	2.03	0.57
1:A:161:LEU:O	1:A:216:LEU:HG	2.05	0.57
1:A:42:ARG:HD3	1:A:53:TRP:CZ2	2.40	0.56
1:D:251:ASN:O	1:D:254:THR:OG1	2.17	0.56
1:C:45:LEU:HD12	1:C:81:PRO:HB3	1.86	0.56
1:E:123:ARG:HH12	1:E:127:LEU:CG	2.19	0.56
1:E:309:VAL:CG1	1:E:310:THR:H	2.18	0.56
1:C:42:ARG:HD3	1:C:53:TRP:CZ3	2.41	0.56
1:F:264:ARG:HD3	1:F:268:GLU:HG3	1.86	0.56
1:A:42:ARG:CD	1:A:53:TRP:CZ3	2.89	0.56
1:A:55:VAL:HG21	1:A:64:VAL:HG21	1.87	0.56
1:F:39:PRO:HG3	1:F:308:THR:HG23	1.88	0.56
1:D:86:THR:HG22	4:D:618:HOH:O	2.05	0.56
1:B:256:LEU:HD22	1:B:284:MET:HB2	1.87	0.56
1:E:264:ARG:NH2	1:E:380:LEU:O	2.39	0.55
1:D:219:LEU:O	1:D:222:ALA:HB3	2.06	0.55
1:F:39:PRO:HG2	1:F:308:THR:OG1	2.07	0.55
1:A:220:ALA:O	1:A:223:THR:HG22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220:ALA:O	1:E:223:THR:CG2	2.46	0.55
1:F:123:ARG:HH22	1:F:159:GLU:HG3	1.71	0.55
1:D:183:ARG:HB3	1:D:184:LEU:HD13	1.89	0.55
1:D:260:LEU:O	1:D:264:ARG:HA	2.06	0.54
1:E:327:ASP:HB3	1:E:330:VAL:HG12	1.89	0.54
1:F:39:PRO:CG	1:F:308:THR:CG2	2.84	0.54
1:A:117:VAL:O	1:A:120:MET:HG3	2.07	0.54
1:F:264:ARG:HH21	1:F:264:ARG:HG3	1.73	0.54
1:F:135:MET:HE3	1:F:407:TRP:CH2	2.42	0.54
1:F:277:VAL:CG2	1:F:278:PRO:CD	2.85	0.54
1:B:103:ARG:NH2	1:B:228:HIS:CD2	2.76	0.54
1:D:145:VAL:HA	1:D:149:ALA:HB3	1.89	0.54
1:D:229:LEU:N	1:D:229:LEU:HD12	2.23	0.54
1:B:115:ARG:NH1	1:B:119:GLU:HG3	2.22	0.54
1:F:264:ARG:HH21	1:F:264:ARG:CG	2.21	0.54
1:A:160:LEU:HG	1:A:215:LEU:HD12	1.90	0.54
1:E:207:ARG:HH21	1:E:216:LEU:HB2	1.66	0.54
1:B:103:ARG:HH21	1:B:228:HIS:CG	2.26	0.54
1:B:392:LYS:HG2	1:B:401:GLU:CG	2.38	0.54
1:F:84:PHE:CE1	1:F:88:PRO:HG3	2.42	0.54
1:B:42[A]:ARG:NH1	1:B:51:THR:HG21	2.22	0.54
1:F:31:TYR:CE2	1:F:320:HIS:CE1	2.96	0.53
1:C:42:ARG:CD	1:C:53:TRP:CZ3	2.90	0.53
1:E:309:VAL:HG12	1:E:310:THR:H	1.73	0.53
2:F:501:HEM:HMC2	2:F:501:HEM:HBC2	1.89	0.53
1:F:338:ASP:HB3	1:F:341:ARG:HG3	1.91	0.53
1:A:287:TYR:O	1:A:326:ARG:NH1	2.41	0.53
1:B:127:LEU:HD23	1:B:152:PHE:HD1	1.72	0.53
1:D:23:HIS:O	1:D:26:ASP:HB2	2.08	0.53
1:F:64:VAL:HA	1:F:70:PHE:CE2	2.42	0.53
1:A:197:MET:CE	1:A:235:VAL:CG1	2.87	0.53
1:D:252:GLN:HE22	1:D:290:LEU:HB2	1.74	0.53
1:B:127:LEU:HD23	1:B:152:PHE:CD1	2.43	0.53
1:C:45:LEU:HD22	1:C:83:MET:SD	2.49	0.53
1:F:376:ARG:O	1:F:377:PHE:HD1	1.90	0.53
1:D:105:ARG:HD2	2:D:501:HEM:O2D	2.09	0.53
1:A:246:HIS:O	1:A:250:VAL:HG23	2.08	0.52
1:E:280:ALA:O	1:E:284:MET:HG3	2.09	0.52
1:F:135:MET:HE2	1:F:407:TRP:CH2	2.43	0.52
1:A:197:MET:HE3	1:A:235:VAL:HG11	1.90	0.52
1:F:283:GLU:CG	1:F:337:LEU:CD1	2.68	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:MET:SD	1:A:235:VAL:HG12	2.50	0.52
1:C:42:ARG:HD2	1:C:53:TRP:CE3	2.44	0.52
1:D:157:ILE:HG13	1:D:161:LEU:CD1	2.40	0.52
1:E:105:ARG:HD3	1:E:357:ILE:HD12	1.91	0.52
1:E:77:ASP:HB3	1:E:80:THR:HG23	1.92	0.52
1:E:145:VAL:HA	1:E:149:ALA:HB3	1.91	0.52
1:A:205:ALA:O	1:A:208:ARG:HG3	2.09	0.52
2:D:501:HEM:HBC2	2:D:501:HEM:HMC2	1.91	0.52
1:F:277:VAL:HG23	1:F:278:PRO:N	2.24	0.52
1:D:184:LEU:CD1	1:D:184:LEU:N	2.73	0.51
1:A:93:VAL:HG12	2:A:501:HEM:O1D	2.10	0.51
1:B:258:HIS:O	1:B:262:THR:HG23	2.09	0.51
1:B:260:LEU:HG	1:B:284:MET:HE1	1.91	0.51
1:E:55:VAL:HG21	1:E:64:VAL:HG21	1.92	0.51
1:B:103:ARG:HD3	1:B:228:HIS:ND1	2.25	0.51
1:A:162:GLY:O	1:A:216:LEU:HD12	2.11	0.51
1:A:256:LEU:HD22	1:A:284:MET:HB3	1.91	0.51
1:D:106:ARG:CG	1:D:106:ARG:NH1	2.73	0.51
1:E:106[A]:ARG:NH2	1:E:106[A]:ARG:HG3	2.23	0.51
1:C:197:MET:O	1:C:201:ASP:HB2	2.09	0.51
1:E:106[B]:ARG:NH1	1:E:106[B]:ARG:CG	2.44	0.51
1:A:42:ARG:HD3	1:A:53:TRP:CE2	2.46	0.51
1:E:287:TYR:CG	1:E:337:LEU:HD13	2.45	0.51
1:F:33:GLU:HA	1:F:36:ARG:NH1	2.25	0.51
1:D:256:LEU:HD22	1:D:284:MET:HB3	1.92	0.51
1:E:207:ARG:CZ	1:E:214:ASP:OD2	2.59	0.51
1:A:42:ARG:HD3	1:A:53:TRP:CE3	2.46	0.51
1:A:42:ARG:HG2	1:A:53:TRP:CZ3	2.46	0.51
1:E:123:ARG:NH2	1:E:159:GLU:CD	2.63	0.50
1:F:34:LEU:HB3	1:F:38:GLU:O	2.11	0.50
1:C:105:ARG:HH12	1:C:357:ILE:HB	1.76	0.50
1:B:82:ARG:HD3	1:B:88:PRO:HD3	1.93	0.50
1:B:150:VAL:O	1:B:154:VAL:HG13	2.11	0.50
1:E:75:ALA:HA	1:E:80:THR:HG21	1.92	0.50
1:D:258:HIS:CD2	1:D:262:THR:HG23	2.47	0.50
1:F:264:ARG:HD3	1:F:268:GLU:CG	2.42	0.50
1:D:166:GLU:CB	1:E:227:ASP:OD2	2.60	0.50
1:C:14:VAL:O	1:C:44:ARG:NH1	2.43	0.50
1:F:82:ARG:HD2	1:F:84:PHE:CD1	2.47	0.50
1:E:207:ARG:HD3	1:E:212:THR:OG1	2.11	0.50
1:F:84:PHE:HE1	1:F:88:PRO:HG3	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:132:LEU:HD21	1:F:373:LEU:HD23	1.94	0.50
1:A:150:VAL:O	1:A:154:VAL:HG23	2.11	0.50
1:F:16:ALA:HA	1:F:44:ARG:HG3	1.93	0.50
1:F:264:ARG:NH1	1:F:378:PRO:O	2.45	0.50
1:F:337:LEU:CD2	1:F:339:PHE:CZ	2.95	0.50
1:F:84:PHE:HB2	4:F:609:HOH:O	2.11	0.49
1:A:145:VAL:HA	1:A:149:ALA:HB3	1.94	0.49
1:A:222:ALA:O	1:A:226:ASP:HB2	2.12	0.49
1:D:258:HIS:CD2	1:D:262:THR:CG2	2.95	0.49
1:E:231:LYS:O	1:E:235:VAL:HG23	2.12	0.49
1:F:33:GLU:HA	1:F:36:ARG:CZ	2.43	0.49
1:B:256:LEU:HD22	1:B:284:MET:SD	2.52	0.49
1:C:251:ASN:HD22	1:C:397:ILE:HD12	1.76	0.49
1:E:220:ALA:C	1:E:223:THR:HG22	2.29	0.49
1:D:42:ARG:HD2	1:D:51:THR:OG1	2.12	0.49
1:F:252:GLN:HB3	1:F:366:LEU:HD21	1.95	0.49
1:A:107:LEU:HD13	1:A:229:LEU:HD12	1.95	0.49
1:A:108:VAL:CG2	1:A:215:LEU:CD2	2.90	0.49
1:C:64:VAL:HA	1:C:70:PHE:CE2	2.48	0.49
1:D:45:LEU:CD1	1:D:81:PRO:HB2	2.25	0.49
1:D:99:PRO:O	1:D:103:ARG:HG3	2.12	0.49
1:F:117:VAL:HG13	1:F:364:LEU:HD22	1.95	0.49
1:A:163:VAL:HG22	1:A:216:LEU:HD11	1.93	0.49
1:D:40:VAL:HG12	1:D:53:TRP:CE3	2.48	0.49
1:F:376:ARG:C	1:F:378:PRO:HD3	2.34	0.49
1:D:258:HIS:NE2	1:D:262:THR:HG21	2.28	0.48
1:F:121:ARG:HG3	1:F:364:LEU:CD1	2.43	0.48
1:F:334:ALA:O	1:F:335:ASP:CB	2.60	0.48
1:B:263:GLU:HB2	1:B:266:ARG:HD2	1.95	0.48
1:D:174:PHE:HB3	1:D:196:PHE:CD2	2.49	0.48
1:F:184:LEU:HD22	1:F:188:GLU:OE1	2.14	0.48
1:A:174:PHE:HB3	1:A:196:PHE:CD2	2.49	0.48
1:B:152:PHE:HB3	1:B:153:PRO:HD3	1.96	0.48
1:D:42:ARG:NH2	1:D:53:TRP:NE1	2.60	0.48
1:D:328:GLU:OE1	1:D:334:ALA:HB3	2.14	0.48
1:B:309:VAL:CG1	1:B:310:THR:N	2.76	0.48
1:D:322:ALA:O	1:D:326:ARG:HG2	2.13	0.48
1:B:172:ARG:HD2	4:B:662:HOH:O	2.13	0.48
1:C:105:ARG:NH1	1:C:357:ILE:HB	2.28	0.48
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.95	0.48
1:E:264:ARG:O	1:E:267:TYR:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:LEU:CD2	1:B:152:PHE:HD1	2.26	0.48
1:A:42:ARG:CD	1:A:53:TRP:CD2	2.97	0.48
1:A:287:TYR:CG	1:A:337:LEU:HD23	2.49	0.48
1:F:105:ARG:HD2	1:F:357:ILE:HD12	1.95	0.48
1:A:121:ARG:N	1:A:122:PRO:CD	2.77	0.48
1:B:42[A]:ARG:NH1	1:B:51:THR:CG2	2.77	0.48
1:C:287:TYR:O	1:C:326:ARG:NH1	2.46	0.48
1:F:93:VAL:CG1	2:F:501:HEM:O2D	2.62	0.47
1:F:264:ARG:HD3	1:F:268:GLU:OE2	2.13	0.47
1:F:277:VAL:HG23	1:F:278:PRO:CD	2.44	0.47
1:D:152:PHE:CE1	1:D:156:VAL:HG21	2.49	0.47
1:F:34:LEU:C	1:F:38:GLU:O	2.51	0.47
1:A:297:VAL:HG13	1:A:317:CYS:O	2.14	0.47
1:D:184:LEU:N	1:D:184:LEU:HD12	2.29	0.47
1:F:117:VAL:CG1	1:F:364:LEU:HD22	2.44	0.47
1:F:264:ARG:HD3	1:F:268:GLU:CD	2.35	0.47
1:A:242:LEU:O	1:A:246:HIS:HD2	1.97	0.47
1:B:154:VAL:HG12	1:B:246:HIS:HB2	1.96	0.47
1:C:89:GLU:HB3	4:C:663:HOH:O	2.15	0.47
1:C:42:ARG:CD	1:C:53:TRP:CE3	2.98	0.47
1:C:256:LEU:HD22	1:C:284:MET:HB3	1.97	0.47
1:D:219:LEU:HA	1:D:222:ALA:HB3	1.96	0.47
1:E:36:ARG:NH1	1:E:37:ASP:CG	2.67	0.47
1:E:292:SER:HA	1:E:398:ARG:HE	1.80	0.47
1:F:131:LEU:CD1	1:F:152:PHE:HB2	2.45	0.47
1:D:124:VAL:HG13	1:D:152:PHE:CZ	2.50	0.46
1:F:82:ARG:HG2	1:F:82:ARG:HH11	1.80	0.46
1:A:150:VAL:CG1	1:A:168:ARG:HH11	2.28	0.46
1:D:325:ASN:CB	4:D:601:HOH:O	2.62	0.46
1:F:377:PHE:N	1:F:378:PRO:CD	2.78	0.46
1:D:152:PHE:CE1	1:D:156:VAL:CG2	2.98	0.46
1:B:246:HIS:O	1:B:250:VAL:HG23	2.16	0.46
1:C:150:VAL:O	1:C:154:VAL:HG23	2.15	0.46
1:D:25:LEU:HA	1:D:289:PRO:HG2	1.97	0.46
1:D:105:ARG:NH1	1:D:355:HIS:O	2.29	0.46
1:D:259:LEU:O	1:D:266:ARG:NH1	2.49	0.46
1:E:286:ARG:NH1	1:E:325:ASN:O	2.46	0.46
1:F:334:ALA:O	1:F:335:ASP:HB2	2.15	0.46
1:F:376:ARG:O	1:F:377:PHE:CD1	2.69	0.46
1:B:288:THR:HG23	1:B:289:PRO:HD2	1.98	0.46
1:F:281:VAL:HG21	1:F:367:GLN:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:ALA:O	1:D:153:PRO:CD	2.64	0.46
1:C:105:ARG:HH22	1:C:357:ILE:HA	1.81	0.46
1:C:183:ARG:HD2	4:C:753:HOH:O	2.15	0.45
1:D:225:ASN:OD1	1:D:226:ASP:N	2.49	0.45
1:A:42:ARG:HD3	1:A:53:TRP:CD2	2.51	0.45
1:C:246:HIS:O	1:C:250:VAL:HG23	2.16	0.45
1:A:402:ARG:HG2	1:A:403:GLN:N	2.30	0.45
1:D:286:ARG:CG	1:D:325:ASN:HB3	2.47	0.45
1:F:264:ARG:O	1:F:265:LYS:C	2.55	0.45
1:E:106[A]:ARG:HG2	1:E:106[A]:ARG:NH2	2.03	0.45
1:E:227:ASP:OD2	1:E:228:HIS:CE1	2.70	0.45
1:E:264:ARG:O	1:E:265:LYS:C	2.55	0.45
1:A:371:SER:HB3	1:A:375:ARG:NH2	2.31	0.45
1:D:183:ARG:C	1:D:184:LEU:HD12	2.36	0.45
1:F:261:LEU:HB3	1:F:382:LEU:HG	1.98	0.45
1:C:35:ARG:NH2	4:C:604:HOH:O	2.30	0.45
1:C:132:LEU:O	1:C:136:VAL:HG13	2.16	0.45
1:E:207:ARG:CD	1:E:212:THR:OG1	2.65	0.45
1:F:277:VAL:O	1:F:280:ALA:HB3	2.17	0.45
1:B:256:LEU:CD1	1:B:366:LEU:HD22	2.47	0.44
1:C:205:ALA:O	1:C:208:ARG:HB2	2.17	0.44
1:F:283:GLU:HG3	1:F:337:LEU:CG	2.42	0.44
1:C:172:ARG:HD2	4:C:609:HOH:O	2.17	0.44
1:A:121:ARG:HB3	1:A:122:PRO:HD3	1.98	0.44
1:A:383:ALA:HB3	1:A:404:ILE:HG22	1.99	0.44
1:B:93:VAL:HG11	2:B:501:HEM:CGD	2.48	0.44
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	2.00	0.44
1:C:183:ARG:HG3	1:C:184:LEU:HG	1.98	0.44
1:E:355:HIS:O	1:E:356:CYS:C	2.55	0.44
1:F:337:LEU:HD21	1:F:339:PHE:CZ	2.47	0.44
1:D:55:VAL:HG21	1:D:64:VAL:HG21	1.99	0.44
1:A:14:VAL:CG1	1:A:15:PRO:CD	2.96	0.44
1:B:174:PHE:HB3	1:B:196:PHE:CD2	2.53	0.44
1:D:261:LEU:HD23	1:D:261:LEU:HA	1.77	0.44
1:D:325:ASN:N	4:D:601:HOH:O	2.19	0.44
1:E:93:VAL:CG1	1:E:237:MET:SD	3.06	0.44
1:B:145:VAL:HA	1:B:149:ALA:HB3	2.01	0.43
1:D:166:GLU:HB3	1:E:227:ASP:OD2	2.16	0.43
1:F:259:LEU:HB2	1:F:284:MET:CE	2.47	0.43
1:F:380:LEU:HD11	1:F:405:VAL:CG1	2.48	0.43
1:B:392:LYS:HG3	1:B:399:GLY:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:VAL:HA	1:D:374:VAL:HG13	2.00	0.43
1:F:356:CYS:HB3	1:F:359:ALA:HB2	2.00	0.43
1:D:154:VAL:HG13	1:D:171:PHE:HZ	1.82	0.43
1:E:207:ARG:HH21	1:E:214:ASP:HB2	1.79	0.43
1:B:145:VAL:HG21	1:B:402:ARG:HA	2.00	0.43
1:E:123:ARG:HH12	1:E:127:LEU:HB2	1.82	0.43
1:A:349:PHE:CE1	1:A:359:ALA:HA	2.53	0.43
1:F:264:ARG:NH2	1:F:264:ARG:CG	2.78	0.43
1:F:277:VAL:HG23	1:F:278:PRO:HD3	1.99	0.43
1:A:42:ARG:HD2	1:A:53:TRP:CD2	2.53	0.43
1:C:283:GLU:HG3	1:C:337:LEU:CD2	2.48	0.43
1:F:246:HIS:CE1	1:F:247:GLU:HG2	2.53	0.43
1:A:105:ARG:HD3	1:A:357:ILE:HD12	2.01	0.43
1:D:17:TYR:O	1:D:46:PRO:HD3	2.19	0.43
1:E:36:ARG:HG3	1:E:37:ASP:N	2.33	0.43
1:A:93:VAL:CG1	2:A:501:HEM:CGD	2.97	0.43
1:B:186:ALA:O	1:B:190:GLN:HB2	2.19	0.43
2:D:501:HEM:HBB2	2:D:501:HEM:CMB	2.49	0.43
1:E:93:VAL:HG11	1:E:237:MET:SD	2.59	0.43
1:E:200:MET:CE	1:E:238:GLY:O	2.52	0.43
1:B:93:VAL:HG12	2:B:501:HEM:O1D	2.19	0.42
1:C:42:ARG:HH21	1:C:51:THR:HB	1.84	0.42
1:D:229:LEU:HD12	1:D:229:LEU:H	1.83	0.42
1:E:152:PHE:HB3	1:E:153:PRO:HD3	2.00	0.42
1:F:25:LEU:HD13	1:F:288:THR:HG23	2.00	0.42
1:F:72:THR:HB	1:F:296:PHE:CE2	2.54	0.42
1:A:93:VAL:HG12	2:A:501:HEM:CGD	2.49	0.42
1:D:264:ARG:HD3	1:D:268:GLU:OE1	2.20	0.42
1:A:108:VAL:HG21	1:A:241:LEU:HD11	2.01	0.42
1:B:270:LEU:C	1:B:374:VAL:HG11	2.39	0.42
1:C:271:VAL:HA	1:C:374:VAL:HG13	2.01	0.42
1:D:94:LEU:HG	1:D:296:PHE:CD1	2.54	0.42
1:F:257:VAL:HG12	1:F:261:LEU:HD12	2.00	0.42
1:E:36:ARG:CZ	1:E:37:ASP:OD1	2.65	0.42
1:B:35:ARG:NH2	4:B:604:HOH:O	2.51	0.42
1:D:25:LEU:H	1:D:398:ARG:HH11	1.67	0.42
1:F:93:VAL:HG11	2:F:501:HEM:O2D	2.20	0.42
1:F:112:PHE:HB3	1:F:357:ILE:O	2.19	0.42
1:A:197:MET:CE	1:A:235:VAL:HG12	2.50	0.42
1:B:215:LEU:HD23	1:B:215:LEU:HA	1.93	0.42
1:D:58:MET:HE2	1:D:62:ARG:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:PHE:CZ	1:A:239:VAL:HG13	2.55	0.42
3:B:502:DEB:H221	3:B:502:DEB:H8	1.80	0.42
1:D:157:ILE:HG13	1:D:161:LEU:HD12	2.02	0.42
1:D:230:THR:HG23	1:D:233:GLU:OE1	2.19	0.42
1:B:285:LEU:HD13	1:B:349:PHE:CE2	2.55	0.42
1:F:199:TYR:CZ	1:F:203:LEU:HD11	2.54	0.42
1:A:93:VAL:CG2	1:A:237:MET:SD	3.08	0.41
1:B:312:ARG:NH2	1:C:129:ASP:OD2	2.53	0.41
1:D:53:TRP:NE1	1:D:315:GLU:OE2	2.33	0.41
1:D:207:ARG:HD2	1:D:212:THR:CG2	2.49	0.41
1:E:266:ARG:CD	1:E:337:LEU:HD23	2.48	0.41
2:E:501:HEM:HHC	2:E:501:HEM:CBB	2.26	0.41
1:F:32:ALA:HA	1:F:35:ARG:NH1	2.34	0.41
1:B:93:VAL:CG2	1:B:237:MET:SD	3.08	0.41
1:C:55:VAL:HG21	1:C:64:VAL:HG21	2.02	0.41
1:F:168:ARG:HA	1:F:171:PHE:CZ	2.55	0.41
1:C:208:ARG:NE	1:C:208:ARG:CA	2.78	0.41
1:E:259:LEU:HB2	1:E:284:MET:CE	2.50	0.41
1:A:14:VAL:HG12	1:A:43:VAL:HA	2.02	0.41
1:A:283:GLU:HG3	1:A:337:LEU:HD22	2.02	0.41
1:C:152:PHE:HB3	1:C:153:PRO:HD3	2.02	0.41
1:D:266:ARG:O	1:D:269:SER:OG	2.36	0.41
1:A:93:VAL:HG13	1:A:101:HIS:CD2	2.56	0.41
1:C:42:ARG:HG2	1:C:53:TRP:CZ3	2.56	0.41
1:B:104:LEU:HD21	4:B:669:HOH:O	2.19	0.41
1:B:271:VAL:HA	1:B:374:VAL:HG12	2.02	0.41
1:C:102:THR:O	1:C:106:ARG:CG	2.69	0.41
1:F:82:ARG:HD2	1:F:84:PHE:CE1	2.55	0.41
1:F:121:ARG:HG3	1:F:364:LEU:HD11	2.01	0.41
2:B:501:HEM:HMB1	2:B:501:HEM:HBB2	2.02	0.41
1:F:131:LEU:HD12	1:F:152:PHE:HB2	2.01	0.41
1:F:264:ARG:CD	1:F:268:GLU:HG3	2.49	0.41
1:A:251:ASN:ND2	1:A:397:ILE:HD12	2.36	0.41
1:A:286:ARG:HG2	1:A:325:ASN:HB3	2.03	0.41
2:C:501:HEM:HBB2	2:C:501:HEM:HMB2	2.02	0.41
1:D:106:ARG:O	1:D:106:ARG:HG2	2.21	0.41
1:E:107:LEU:HD22	1:E:222:ALA:CB	2.50	0.41
1:E:207:ARG:CZ	1:E:214:ASP:CG	2.89	0.41
1:E:259:LEU:HB2	1:E:284:MET:HE1	2.03	0.41
1:F:93:VAL:HG21	1:F:237:MET:SD	2.59	0.41
1:B:309:VAL:HG12	1:B:310:THR:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:LEU:HD21	3:D:502:DEB:O26	2.20	0.41
1:F:157:ILE:HG21	1:F:246:HIS:HB3	2.02	0.40
1:A:152:PHE:HB3	1:A:153:PRO:HD3	2.03	0.40
1:B:342:GLU:H	1:B:342:GLU:HG3	1.72	0.40
1:A:14:VAL:HG13	1:A:15:PRO:CD	2.51	0.40
1:A:93:VAL:HG21	1:A:237:MET:SD	2.61	0.40
1:F:337:LEU:HD23	1:F:339:PHE:CZ	2.57	0.40
1:E:93:VAL:HG23	1:E:94:LEU:N	2.36	0.40
1:E:271:VAL:HA	1:E:374:VAL:HG13	2.02	0.40

All (3) 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)
4:B:723:HOH:O	4:B:723:HOH:O[2_656]	2.11	0.09
1:A:208:ARG:NH1	1:D:301:THR:OG1[4_445]	2.16	0.04
1:A:68:SER:OG	1:F:231:LYS:NZ[4_546]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	393/407 (97%)	383 (98%)	10 (2%)	0	100	100
1	B	395/407 (97%)	384 (97%)	11 (3%)	0	100	100
1	C	393/407 (97%)	380 (97%)	13 (3%)	0	100	100
1	D	393/407 (97%)	371 (94%)	22 (6%)	0	100	100
1	E	394/407 (97%)	378 (96%)	15 (4%)	1 (0%)	41	62
1	F	389/407 (96%)	372 (96%)	17 (4%)	0	100	100
All	All	2357/2442 (96%)	2268 (96%)	88 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	265	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	331/341 (97%)	325 (98%)	6 (2%)	59	79
1	B	333/341 (98%)	330 (99%)	3 (1%)	78	90
1	C	331/341 (97%)	323 (98%)	8 (2%)	49	72
1	D	331/341 (97%)	319 (96%)	12 (4%)	35	59
1	E	332/341 (97%)	321 (97%)	11 (3%)	38	62
1	F	329/341 (96%)	315 (96%)	14 (4%)	29	53
All	All	1987/2046 (97%)	1933 (97%)	54 (3%)	44	69

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	MET
1	A	168	ARG
1	A	191	ARG
1	A	196	PHE
1	A	346	HIS
1	A	356	CYS
1	B	196	PHE
1	B	264	ARG
1	B	402	ARG
1	C	106	ARG
1	C	115	ARG
1	C	168	ARG
1	C	196	PHE
1	C	207	ARG
1	C	208	ARG
1	C	326	ARG

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Mol	Chain	Res	Type
1	C	402	ARG
1	D	38	GLU
1	D	77	ASP
1	D	106	ARG
1	D	115	ARG
1	D	116	ARG
1	D	196	PHE
1	D	226	ASP
1	D	263	GLU
1	D	264	ARG
1	D	312	ARG
1	D	341	ARG
1	D	402	ARG
1	E	89	GLU
1	E	106[A]	ARG
1	E	106[B]	ARG
1	E	168	ARG
1	E	196	PHE
1	E	227	ASP
1	E	264	ARG
1	E	303	ASP
1	E	312	ARG
1	E	356	CYS
1	E	402	ARG
1	F	38	GLU
1	F	84	PHE
1	F	194	GLN
1	F	196	PHE
1	F	201	ASP
1	F	207	ARG
1	F	225	ASN
1	F	231	LYS
1	F	246	HIS
1	F	264	ARG
1	F	302	GLU
1	F	312	ARG
1	F	333	HIS
1	F	402	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	HIS
1	B	246	HIS
1	C	206	GLN
1	C	246	HIS
1	D	246	HIS
1	D	252	GLN
1	E	246	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	DEB	A	502	-	27,27,27	1.13	1 (3%)	35,39,39	1.18	2 (5%)
3	DEB	F	502	-	27,27,27	1.12	1 (3%)	35,39,39	1.16	4 (11%)
2	HEM	A	501	-	41,50,50	1.39	7 (17%)	45,82,82	1.99	16 (35%)
2	HEM	D	501	1	41,50,50	1.47	5 (12%)	45,82,82	2.05	14 (31%)
2	HEM	B	501	1	41,50,50	1.35	6 (14%)	45,82,82	2.00	14 (31%)
3	DEB	C	502	-	27,27,27	1.10	1 (3%)	35,39,39	1.06	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DEB	D	502	-	27,27,27	1.16	1 (3%)	35,39,39	1.27	2 (5%)
2	HEM	F	501	1	41,50,50	1.36	5 (12%)	45,82,82	1.84	11 (24%)
2	HEM	E	501	-	41,50,50	1.78	14 (34%)	45,82,82	1.79	8 (17%)
3	DEB	E	502	-	27,27,27	1.52	4 (14%)	35,39,39	1.56	7 (20%)
3	DEB	B	502	-	27,27,27	1.55	3 (11%)	35,39,39	1.38	3 (8%)
2	HEM	C	501	1	41,50,50	1.40	6 (14%)	45,82,82	2.11	16 (35%)

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
3	DEB	A	502	-	-	7/50/50/50	0/1/1/1
3	DEB	F	502	-	-	10/50/50/50	0/1/1/1
2	HEM	A	501	-	-	2/12/54/54	-
2	HEM	D	501	1	-	5/12/54/54	-
2	HEM	B	501	1	-	2/12/54/54	-
3	DEB	C	502	-	-	10/50/50/50	0/1/1/1
3	DEB	D	502	-	-	8/50/50/50	0/1/1/1
2	HEM	F	501	1	-	0/12/54/54	-
2	HEM	E	501	-	-	1/12/54/54	-
3	DEB	E	502	-	-	6/50/50/50	0/1/1/1
3	DEB	B	502	-	-	8/50/50/50	0/1/1/1
2	HEM	C	501	1	-	2/12/54/54	-

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	DEB	O16-C1	5.54	1.47	1.34
3	D	502	DEB	O16-C1	5.46	1.47	1.34
3	F	502	DEB	O16-C1	5.20	1.46	1.34
2	E	501	HEM	C1B-NB	-4.82	1.32	1.40
2	D	501	HEM	C1B-NB	-4.79	1.32	1.40
3	C	502	DEB	O16-C1	4.70	1.45	1.34
2	E	501	HEM	C4D-ND	-4.50	1.32	1.40
3	B	502	DEB	O16-C13	-3.94	1.39	1.46
3	E	502	DEB	O16-C13	-3.71	1.39	1.46
2	B	501	HEM	C1B-NB	-3.69	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	C1B-NB	-3.53	1.34	1.40
2	B	501	HEM	C4B-NB	-3.51	1.31	1.38
3	B	502	DEB	O16-C1	3.41	1.42	1.34
2	F	501	HEM	C1B-NB	-3.40	1.34	1.40
2	A	501	HEM	C1B-NB	-3.36	1.34	1.40
3	E	502	DEB	O16-C1	3.35	1.42	1.34
2	F	501	HEM	FE-NB	3.30	2.13	1.96
2	D	501	HEM	C4D-ND	-3.23	1.34	1.40
2	D	501	HEM	C4B-NB	-3.19	1.32	1.38
2	C	501	HEM	C4D-ND	-3.17	1.34	1.40
2	E	501	HEM	C1D-ND	-3.08	1.32	1.38
2	F	501	HEM	C4D-ND	-3.08	1.35	1.40
2	B	501	HEM	C4D-ND	-2.86	1.35	1.40
2	A	501	HEM	C4B-NB	-2.86	1.32	1.38
3	B	502	DEB	C10-C9	-2.82	1.48	1.52
2	E	501	HEM	FE-ND	-2.81	1.83	1.96
2	E	501	HEM	C4B-NB	-2.79	1.33	1.38
2	C	501	HEM	C4B-NB	-2.72	1.33	1.38
2	D	501	HEM	FE-NB	2.69	2.10	1.96
2	E	501	HEM	C3D-C2D	-2.67	1.31	1.36
2	A	501	HEM	FE-NB	2.64	2.09	1.96
3	E	502	DEB	C10-C9	-2.60	1.48	1.52
2	C	501	HEM	FE-NB	2.58	2.09	1.96
2	E	501	HEM	C3C-C2C	-2.58	1.36	1.40
2	E	501	HEM	O2D-CGD	-2.54	1.22	1.30
2	A	501	HEM	C4D-ND	-2.50	1.36	1.40
2	D	501	HEM	C1D-ND	-2.44	1.33	1.38
2	C	501	HEM	C1D-ND	-2.42	1.33	1.38
2	F	501	HEM	CHB-C1B	2.41	1.41	1.35
2	B	501	HEM	FE-NB	2.35	2.08	1.96
2	B	501	HEM	C1D-ND	-2.34	1.34	1.38
2	C	501	HEM	CHB-C1B	2.33	1.40	1.35
2	E	501	HEM	C1B-C2B	-2.29	1.40	1.44
2	F	501	HEM	C3B-C4B	2.28	1.49	1.44
2	A	501	HEM	CHB-C1B	2.26	1.40	1.35
2	E	501	HEM	O2A-CGA	-2.17	1.23	1.30
2	E	501	HEM	C1A-CHA	-2.14	1.35	1.41
2	B	501	HEM	CHB-C1B	2.12	1.40	1.35
3	E	502	DEB	C10-C11	-2.07	1.49	1.53
2	E	501	HEM	FE-NB	2.06	2.07	1.96
2	A	501	HEM	C1D-ND	-2.05	1.34	1.38
2	E	501	HEM	C3B-C2B	-2.02	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C4D-C3D	2.01	1.48	1.45
2	E	501	HEM	C2C-C1C	-2.00	1.38	1.42

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	HEM	C1B-NB-C4B	5.89	111.16	105.07
2	C	501	HEM	CHC-C4B-NB	5.65	130.57	124.43
2	B	501	HEM	C1B-NB-C4B	5.46	110.72	105.07
2	A	501	HEM	C1B-NB-C4B	5.41	110.66	105.07
2	A	501	HEM	CHC-C4B-NB	5.19	130.07	124.43
2	B	501	HEM	CHC-C4B-NB	5.04	129.91	124.43
2	D	501	HEM	CHC-C4B-NB	4.70	129.54	124.43
2	E	501	HEM	CHC-C4B-NB	4.59	129.41	124.43
2	C	501	HEM	CBA-CAA-C2A	4.45	120.21	112.62
2	F	501	HEM	CHC-C4B-NB	4.42	129.23	124.43
2	D	501	HEM	C1B-NB-C4B	4.42	109.64	105.07
2	D	501	HEM	CBA-CAA-C2A	4.40	120.14	112.62
2	D	501	HEM	CHA-C4D-ND	4.11	129.46	124.38
3	D	502	DEB	O16-C1-C2	4.09	120.55	111.56
2	F	501	HEM	C1B-NB-C4B	4.08	109.29	105.07
2	F	501	HEM	CHD-C1D-ND	3.99	128.76	124.43
2	E	501	HEM	C1B-NB-C4B	3.95	109.16	105.07
2	D	501	HEM	CHD-C1D-ND	3.94	128.71	124.43
3	B	502	DEB	O16-C1-C2	3.82	119.94	111.56
2	B	501	HEM	CHD-C1D-ND	3.74	128.49	124.43
2	B	501	HEM	CHA-C4D-ND	3.74	129.00	124.38
3	F	502	DEB	O16-C1-C2	3.73	119.75	111.56
2	C	501	HEM	C4A-C3A-C2A	3.73	109.59	107.00
2	A	501	HEM	CBA-CAA-C2A	3.69	118.92	112.62
3	E	502	DEB	C11-C10-C9	-3.59	103.86	110.36
2	E	501	HEM	CHD-C1D-ND	3.58	128.32	124.43
2	E	501	HEM	CHB-C1B-NB	3.57	128.79	124.38
2	E	501	HEM	CHA-C4D-ND	3.55	128.76	124.38
2	A	501	HEM	CMD-C2D-C1D	3.39	130.21	125.04
2	A	501	HEM	C4A-C3A-C2A	3.32	109.31	107.00
2	F	501	HEM	CMD-C2D-C1D	3.24	129.97	125.04
2	B	501	HEM	CBA-CAA-C2A	3.18	118.04	112.62
3	E	502	DEB	C8-C9-C10	3.12	124.52	119.10
3	E	502	DEB	O16-C1-C2	3.05	118.26	111.56
2	C	501	HEM	CHD-C1D-ND	3.03	127.72	124.43
2	B	501	HEM	CHB-C1B-NB	2.99	128.08	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	HEM	CHA-C4D-C3D	-2.96	119.78	125.33
2	F	501	HEM	CHD-C1D-C2D	-2.93	120.40	124.98
3	A	502	DEB	O16-C1-C2	2.93	117.98	111.56
2	F	501	HEM	CHA-C4D-ND	2.87	127.92	124.38
2	B	501	HEM	CMD-C2D-C1D	2.83	129.35	125.04
3	A	502	DEB	C6-C5-C4	-2.83	111.89	116.27
2	C	501	HEM	CMD-C2D-C1D	2.82	129.34	125.04
2	D	501	HEM	CMD-C2D-C1D	2.82	129.33	125.04
2	D	501	HEM	CHD-C1D-C2D	-2.81	120.58	124.98
2	C	501	HEM	CHA-C4D-ND	2.80	127.83	124.38
2	A	501	HEM	O2A-CGA-O1A	-2.75	116.44	123.30
2	B	501	HEM	CHD-C1D-C2D	-2.66	120.83	124.98
3	B	502	DEB	C6-C5-C4	-2.64	112.18	116.27
2	C	501	HEM	O2A-CGA-O1A	-2.62	116.76	123.30
2	A	501	HEM	CMA-C3A-C4A	-2.59	124.48	128.46
2	A	501	HEM	CHD-C1D-ND	2.58	127.23	124.43
2	A	501	HEM	CHA-C4D-ND	2.54	127.52	124.38
2	C	501	HEM	CMC-C2C-C3C	2.52	129.40	124.68
2	D	501	HEM	CMA-C3A-C4A	-2.52	124.59	128.46
2	C	501	HEM	C4B-CHC-C1C	2.52	125.88	122.56
2	F	501	HEM	C4B-C3B-C2B	-2.52	105.12	107.11
2	D	501	HEM	CHB-C1B-NB	2.51	127.49	124.38
2	A	501	HEM	CHB-C1B-NB	2.49	127.46	124.38
2	F	501	HEM	CBA-CAA-C2A	2.48	116.86	112.62
2	B	501	HEM	C4B-CHC-C1C	2.48	125.83	122.56
2	C	501	HEM	CHD-C1D-C2D	-2.47	121.11	124.98
2	D	501	HEM	CMC-C2C-C3C	2.47	129.29	124.68
2	D	501	HEM	CHA-C4D-C3D	-2.46	120.71	125.33
3	F	502	DEB	O16-C13-C14	2.44	110.83	106.92
2	A	501	HEM	C4B-CHC-C1C	2.44	125.77	122.56
2	C	501	HEM	CHA-C4D-C3D	-2.41	120.80	125.33
2	E	501	HEM	CHD-C1D-C2D	-2.41	121.21	124.98
2	B	501	HEM	CHA-C4D-C3D	-2.41	120.81	125.33
2	D	501	HEM	CAD-CBD-CGD	-2.38	108.48	113.60
2	C	501	HEM	CAD-C3D-C4D	2.38	128.81	124.66
2	F	501	HEM	C4B-CHC-C1C	2.36	125.67	122.56
2	F	501	HEM	CAD-CBD-CGD	-2.35	108.55	113.60
2	F	501	HEM	O2A-CGA-O1A	-2.35	117.45	123.30
2	A	501	HEM	CHD-C1D-C2D	-2.29	121.40	124.98
2	C	501	HEM	CHB-C1B-NB	2.29	127.21	124.38
2	B	501	HEM	O2A-CGA-O1A	-2.29	117.60	123.30
2	A	501	HEM	CAD-C3D-C4D	2.28	128.64	124.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	HEM	O2A-CGA-CBA	2.26	121.30	114.03
2	B	501	HEM	CMC-C2C-C3C	2.25	128.89	124.68
2	B	501	HEM	O2D-CGD-CBD	2.23	121.18	114.03
2	D	501	HEM	C4D-ND-C1D	2.22	107.36	105.07
3	E	502	DEB	C22-C6-C5	-2.20	107.45	111.54
3	C	502	DEB	O16-C1-C2	2.20	116.38	111.56
2	A	501	HEM	CMC-C2C-C3C	2.16	128.71	124.68
3	F	502	DEB	O16-C1-O17	-2.15	119.91	123.94
2	E	501	HEM	CMD-C2D-C1D	2.11	128.25	125.04
3	E	502	DEB	O24-C9-C10	-2.10	117.61	120.60
2	B	501	HEM	O2A-CGA-CBA	2.08	120.72	114.03
2	A	501	HEM	O2A-CGA-CBA	2.07	120.69	114.03
3	C	502	DEB	O19-C3-C2	2.07	113.62	108.82
2	A	501	HEM	CHA-C4D-C3D	-2.06	121.47	125.33
2	D	501	HEM	C4B-CHC-C1C	2.05	125.27	122.56
3	D	502	DEB	O16-C13-C12	2.05	111.43	107.78
3	E	502	DEB	O16-C1-O17	-2.05	120.11	123.94
3	E	502	DEB	C6-C5-C4	-2.04	113.11	116.27
3	B	502	DEB	O16-C1-O17	-2.02	120.16	123.94
3	F	502	DEB	C22-C6-C5	-2.02	107.80	111.54
2	C	501	HEM	C4B-C3B-C2B	-2.01	105.52	107.11

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	DEB	C3-C4-C5-O21
3	A	502	DEB	C20-C4-C5-O21
3	C	502	DEB	C18-C2-C3-C4
3	D	502	DEB	C3-C4-C5-O21
3	E	502	DEB	C3-C4-C5-O21
3	B	502	DEB	C3-C4-C5-O21
3	C	502	DEB	C3-C4-C5-O21
3	F	502	DEB	C3-C4-C5-O21
3	D	502	DEB	C20-C4-C5-O21
3	A	502	DEB	C18-C2-C3-O19
3	B	502	DEB	C18-C2-C3-O19
3	C	502	DEB	C18-C2-C3-O19
3	F	502	DEB	C18-C2-C3-O19
3	E	502	DEB	C20-C4-C5-O21
3	B	502	DEB	C18-C2-C3-C4
3	F	502	DEB	C18-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	B	502	DEB	C20-C4-C5-O21
3	C	502	DEB	C20-C4-C5-O21
3	F	502	DEB	C20-C4-C5-O21
3	A	502	DEB	C20-C4-C5-C6
3	A	502	DEB	C3-C4-C5-C6
3	D	502	DEB	C18-C2-C3-O19
3	D	502	DEB	C3-C4-C5-C6
3	A	502	DEB	C18-C2-C3-C4
3	D	502	DEB	C18-C2-C3-C4
3	E	502	DEB	C18-C2-C3-C4
3	E	502	DEB	C3-C4-C5-C6
3	E	502	DEB	C18-C2-C3-O19
3	E	502	DEB	C20-C4-C5-C6
3	B	502	DEB	C20-C4-C5-C6
3	C	502	DEB	C20-C4-C5-C6
3	D	502	DEB	C20-C4-C5-C6
3	F	502	DEB	C20-C4-C5-C6
2	E	501	HEM	C4B-C3B-CAB-CBB
3	C	502	DEB	C3-C4-C5-C6
3	F	502	DEB	C3-C4-C5-C6
3	B	502	DEB	C3-C4-C5-C6
2	D	501	HEM	C3D-CAD-CBD-CGD
3	D	502	DEB	C23-C8-C9-O24
3	B	502	DEB	C1-C2-C3-C4
3	B	502	DEB	C1-C2-C3-O19
3	C	502	DEB	C1-C2-C3-C4
3	C	502	DEB	C1-C2-C3-O19
3	F	502	DEB	C1-C2-C3-C4
3	F	502	DEB	C1-C2-C3-O19
2	C	501	HEM	C4D-C3D-CAD-CBD
2	C	501	HEM	C2D-C3D-CAD-CBD
3	A	502	DEB	C23-C8-C9-O24
3	F	502	DEB	C2-C1-O16-C13
3	F	502	DEB	O17-C1-O16-C13
2	D	501	HEM	CAD-CBD-CGD-O2D
2	D	501	HEM	CAA-CBA-CGA-O2A
2	B	501	HEM	CAA-CBA-CGA-O2A
2	B	501	HEM	CAA-CBA-CGA-O1A
2	D	501	HEM	CAA-CBA-CGA-O1A
2	D	501	HEM	CAD-CBD-CGD-O1D
3	C	502	DEB	C2-C1-O16-C13
2	A	501	HEM	CAA-CBA-CGA-O2A

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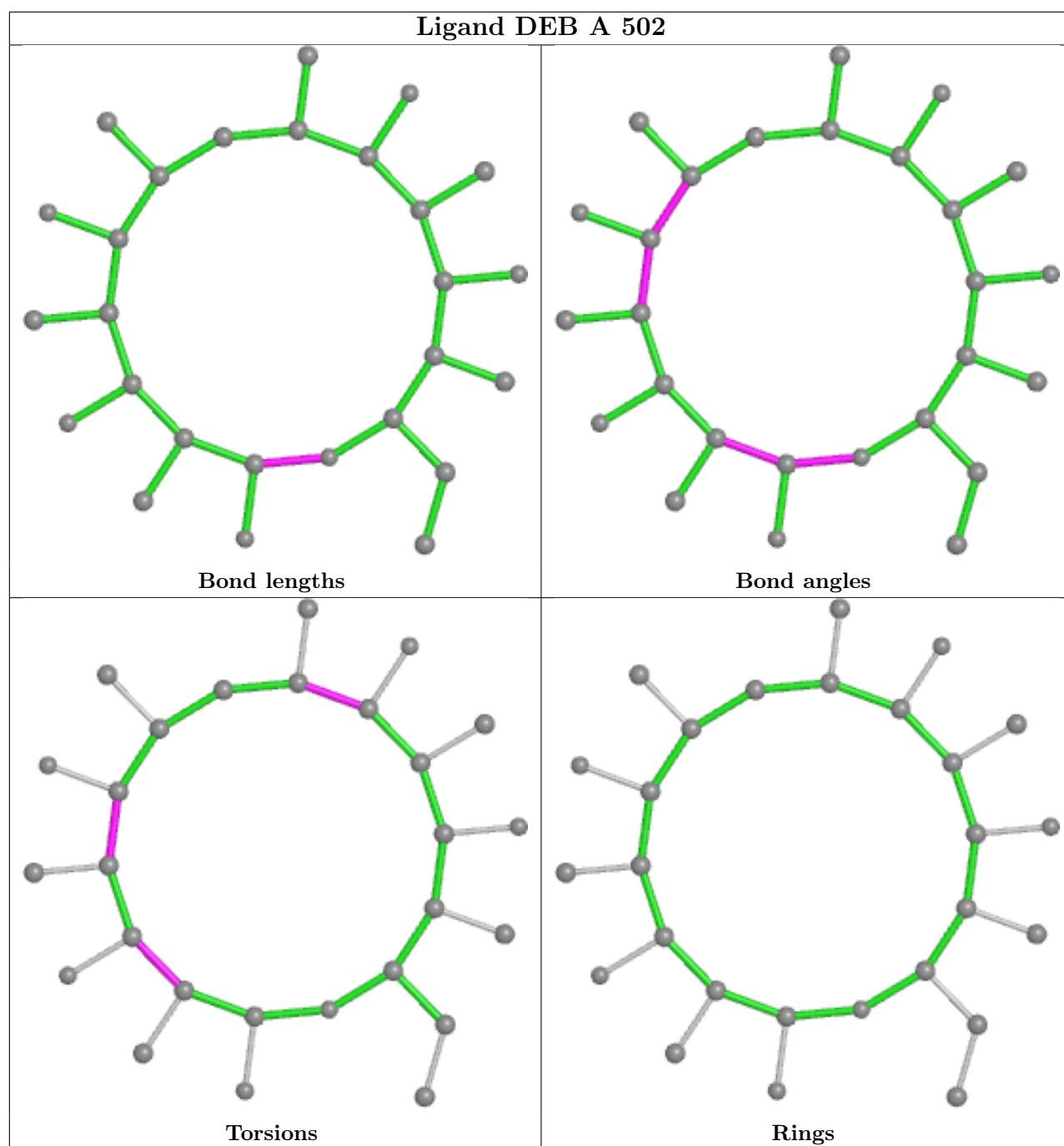
Mol	Chain	Res	Type	Atoms
2	A	501	HEM	CAA-CBA-CGA-O1A
3	D	502	DEB	C7-C8-C9-O24
3	C	502	DEB	O17-C1-O16-C13

There are no ring outliers.

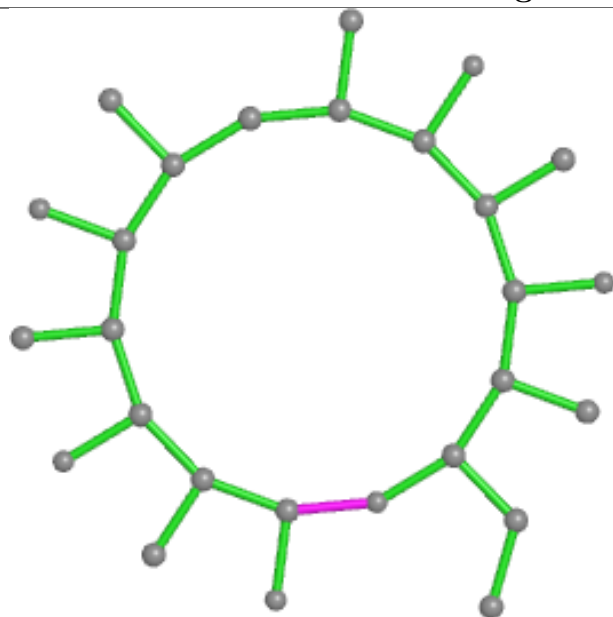
8 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	6	0
2	D	501	HEM	4	0
2	B	501	HEM	4	0
3	D	502	DEB	1	0
2	F	501	HEM	4	0
2	E	501	HEM	12	0
3	B	502	DEB	1	0
2	C	501	HEM	2	0

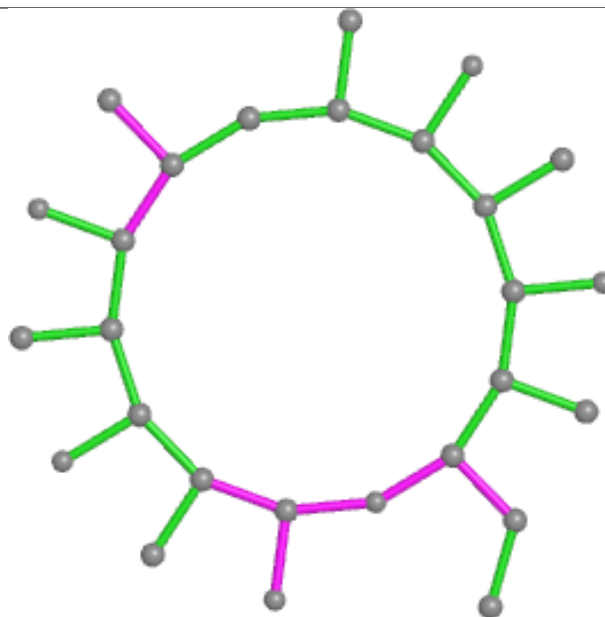
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



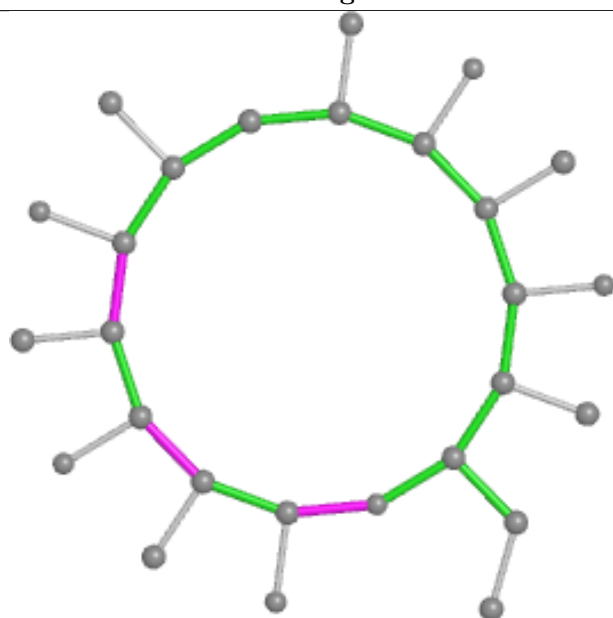
Ligand DEB F 502



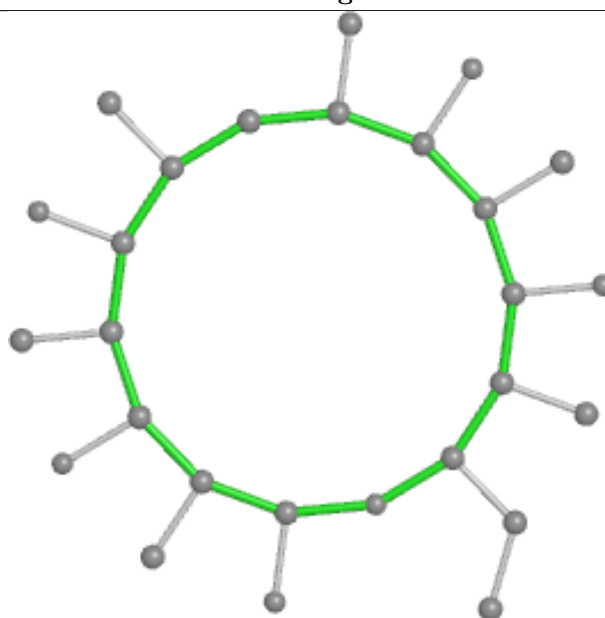
Bond lengths



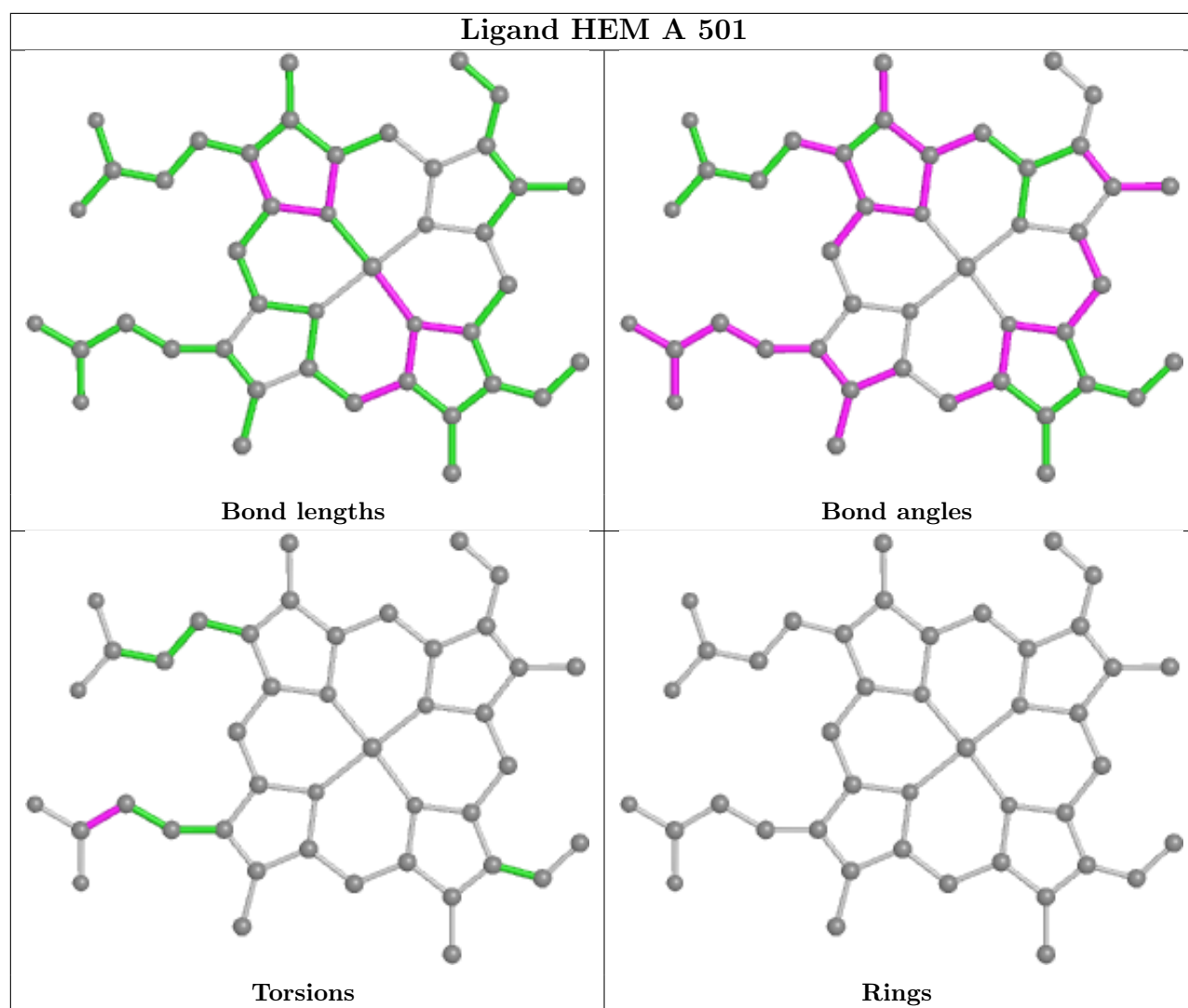
Bond angles

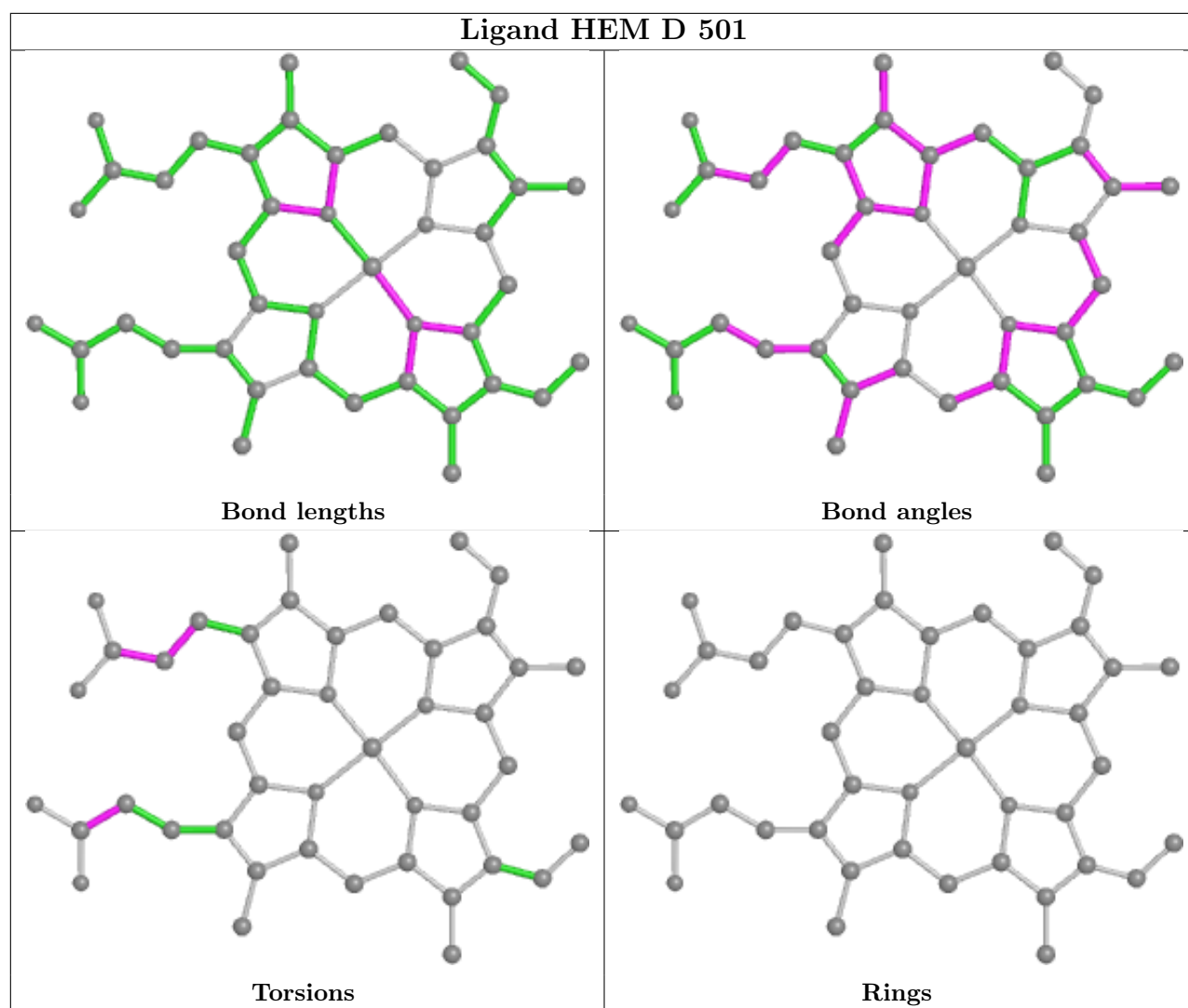


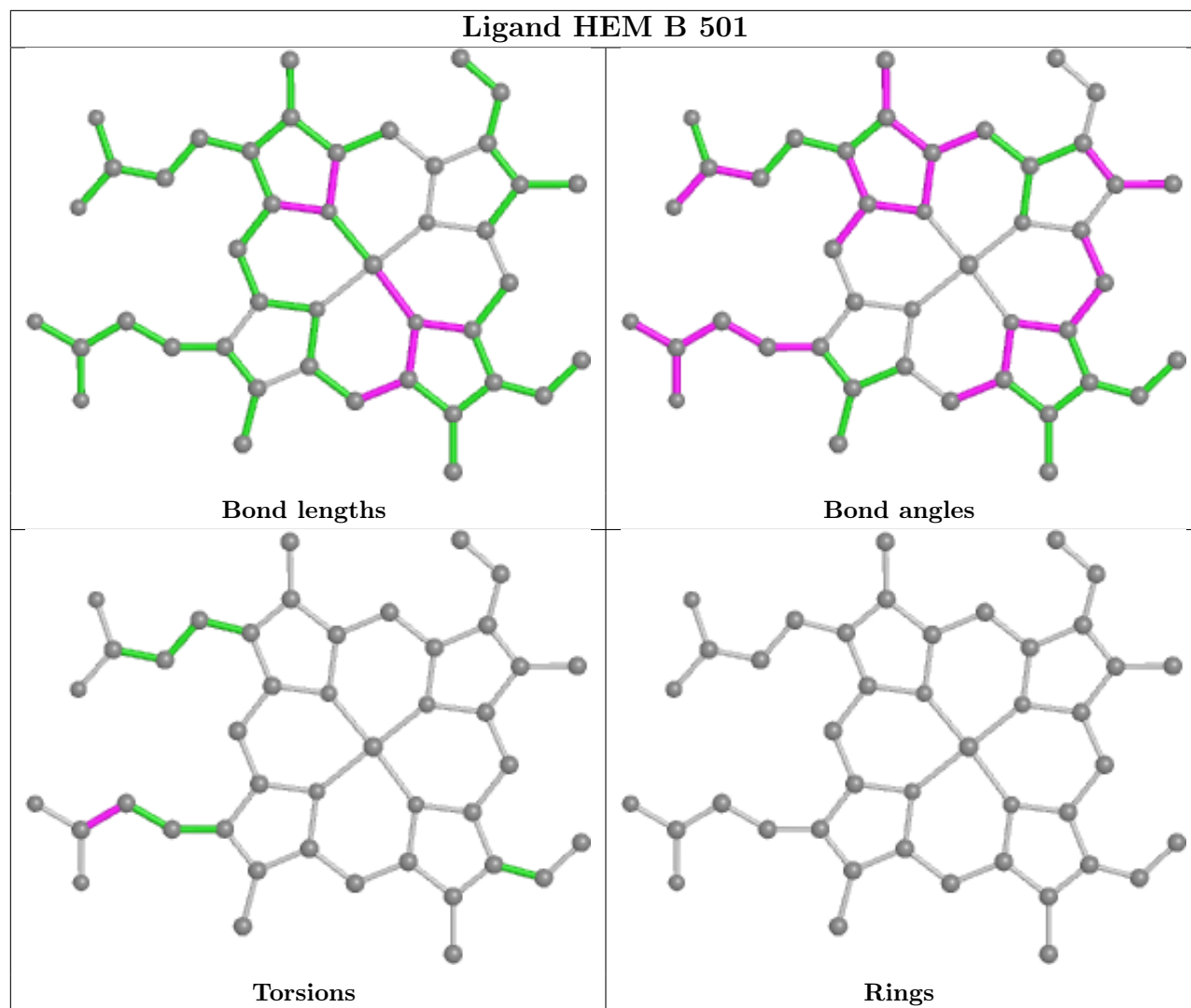
Torsions

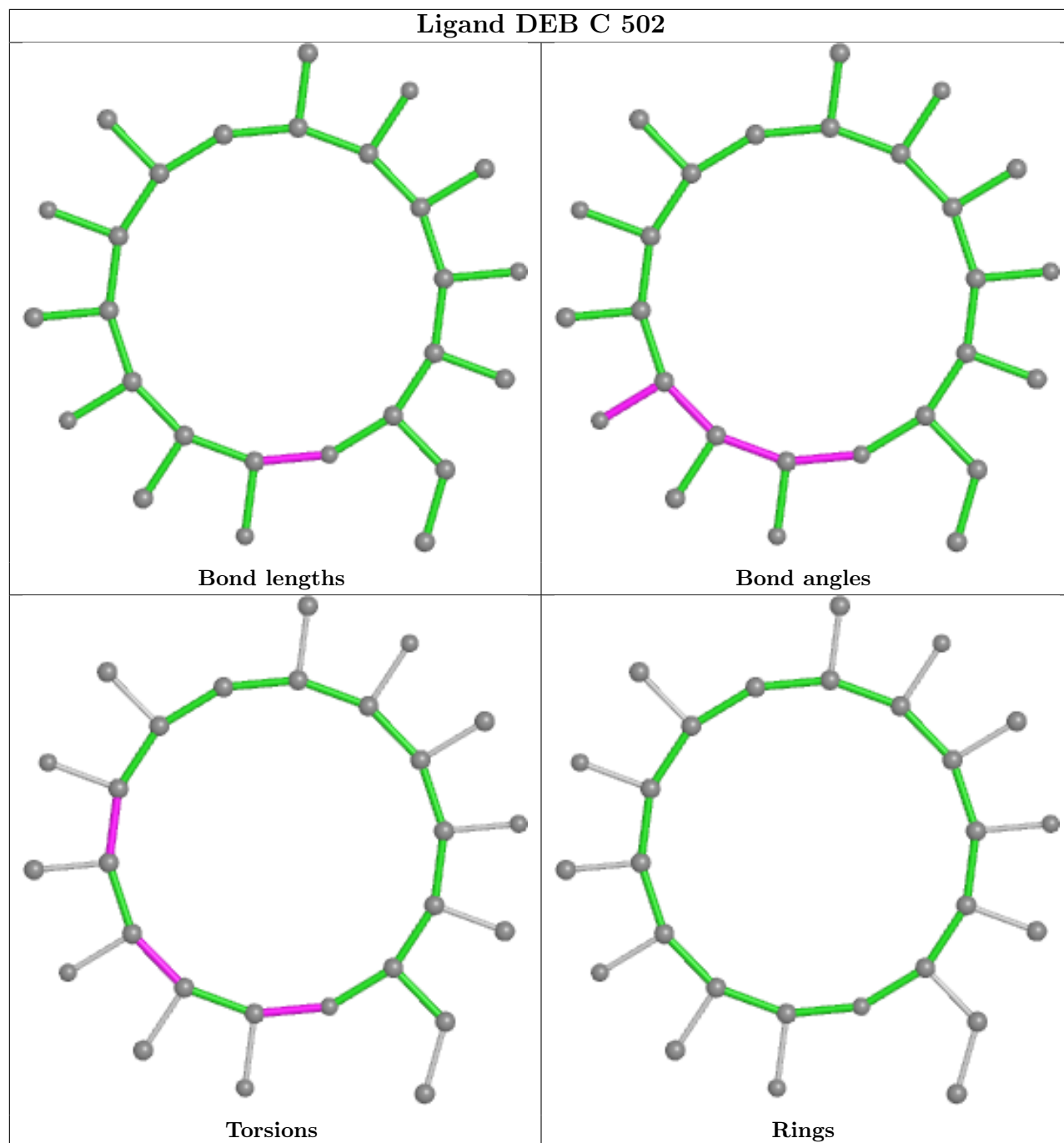


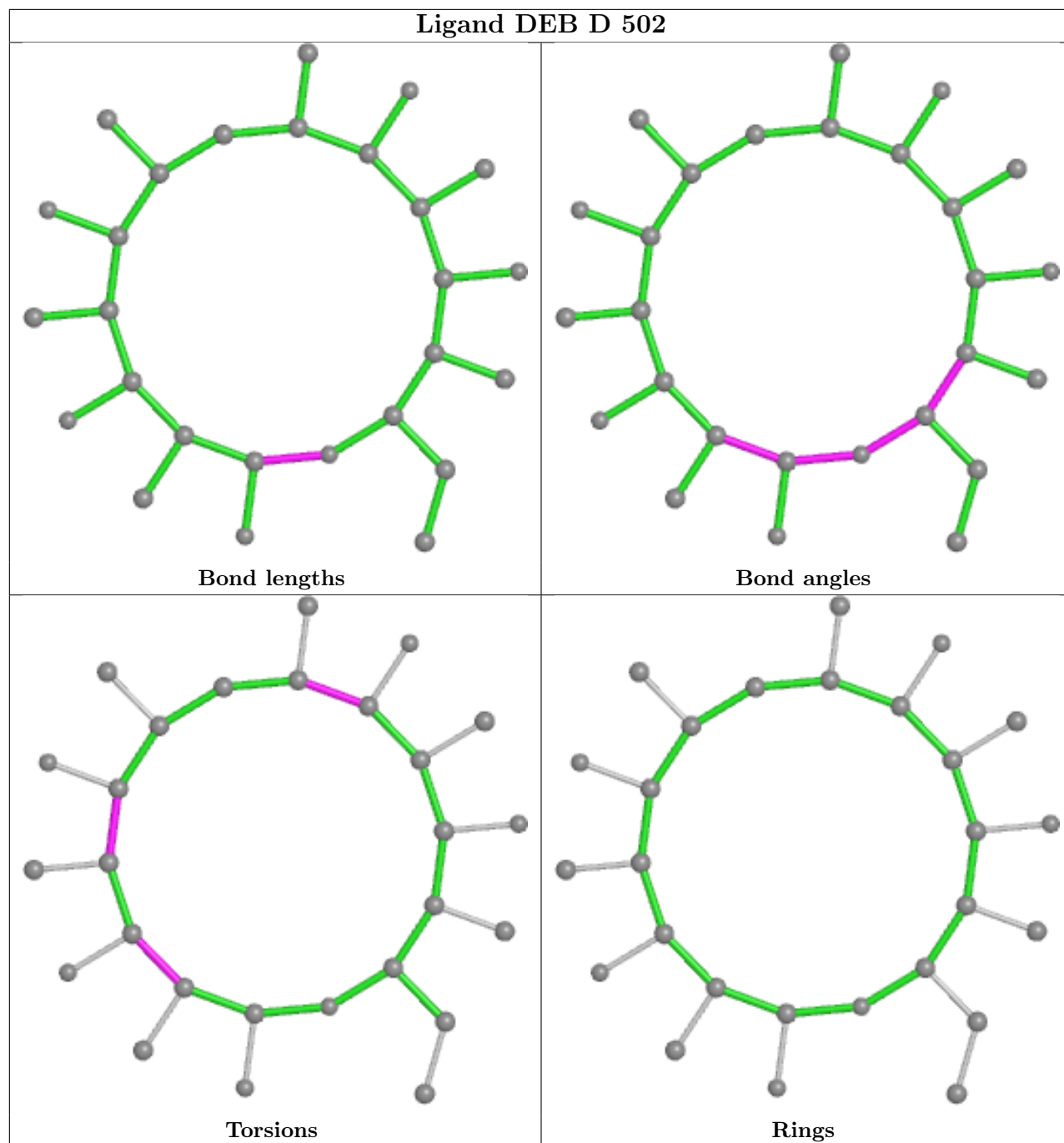
Rings

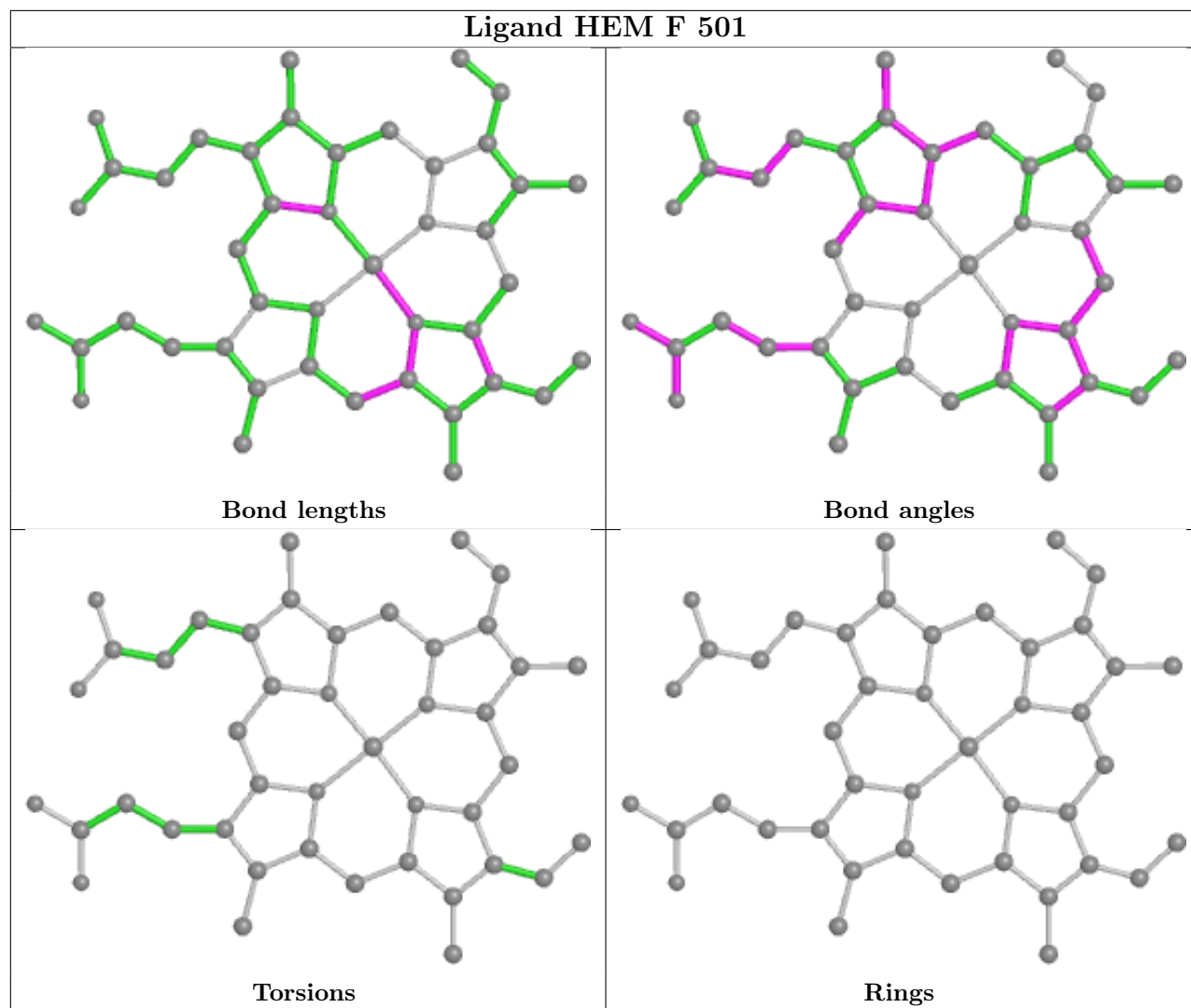


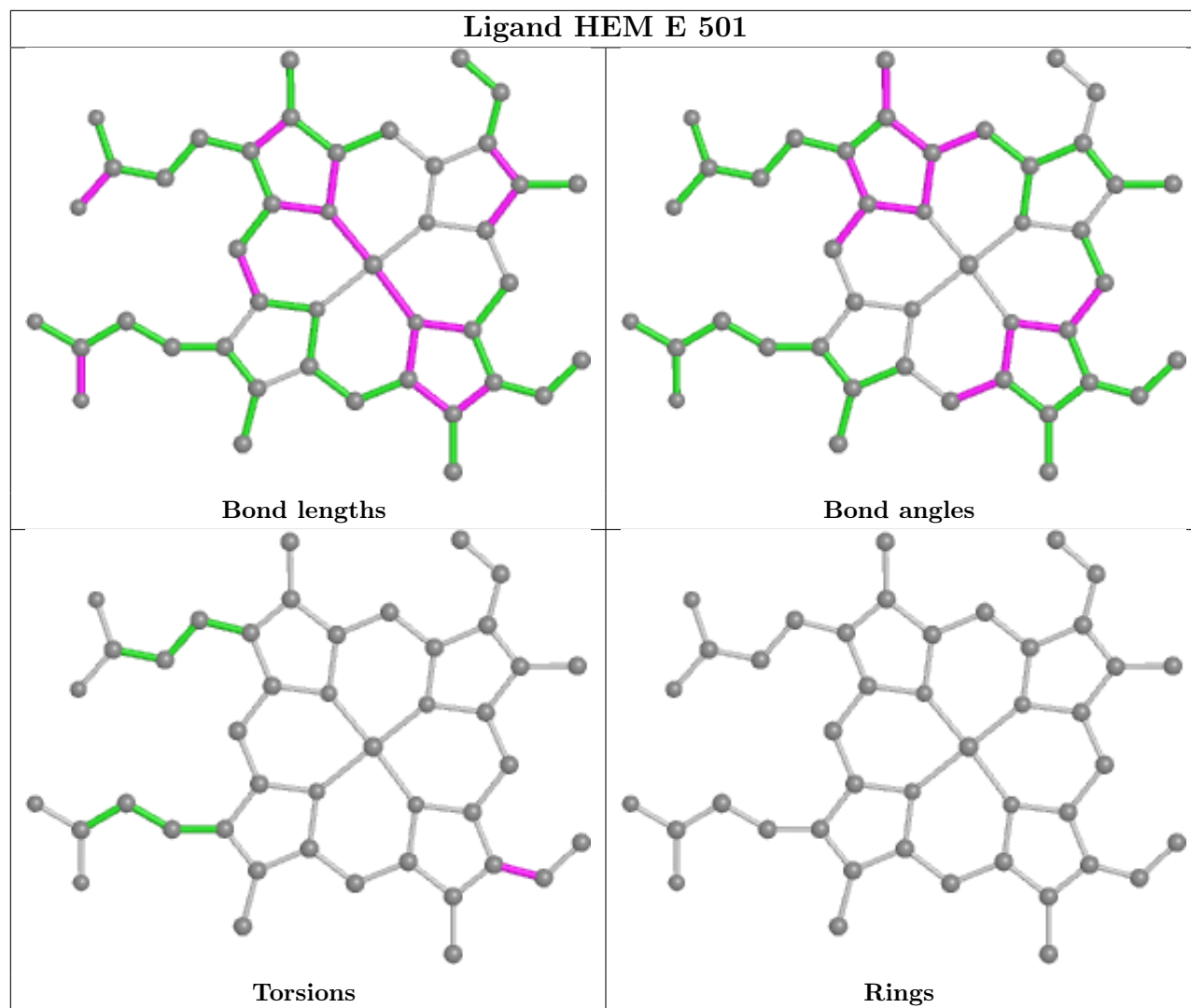




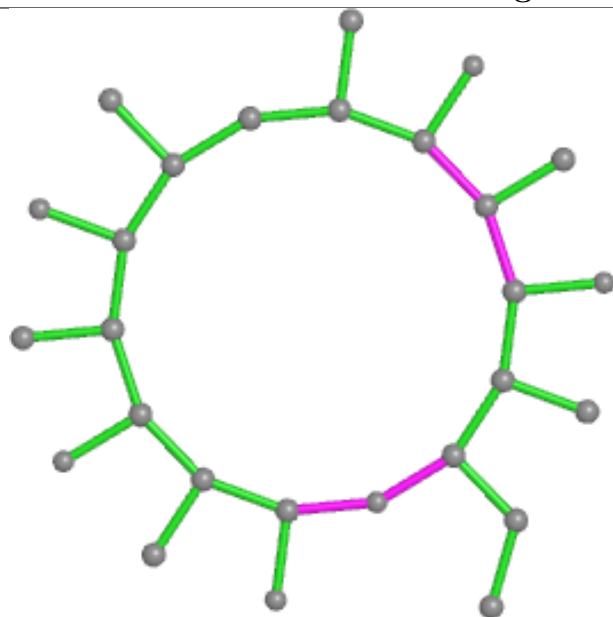




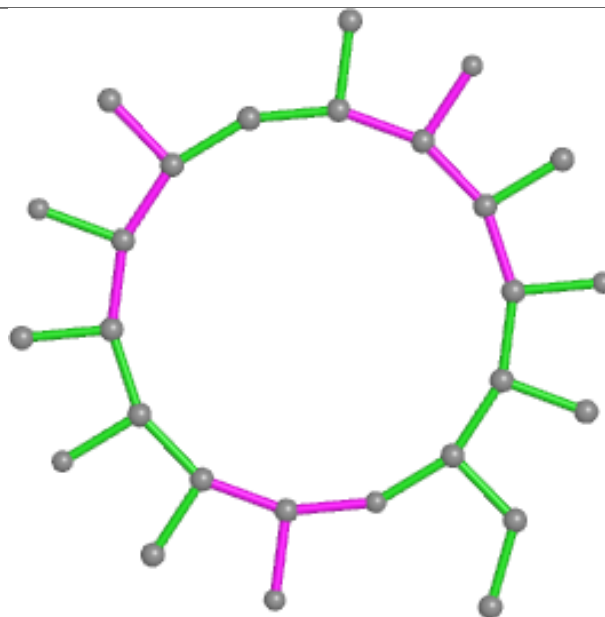




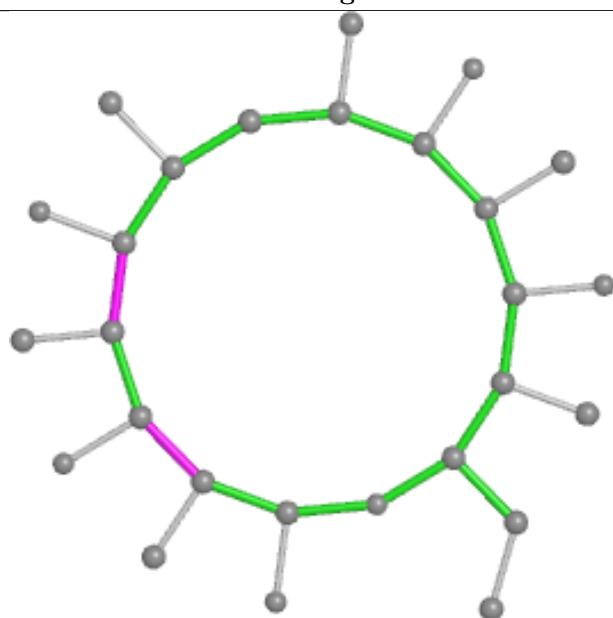
Ligand DEB E 502



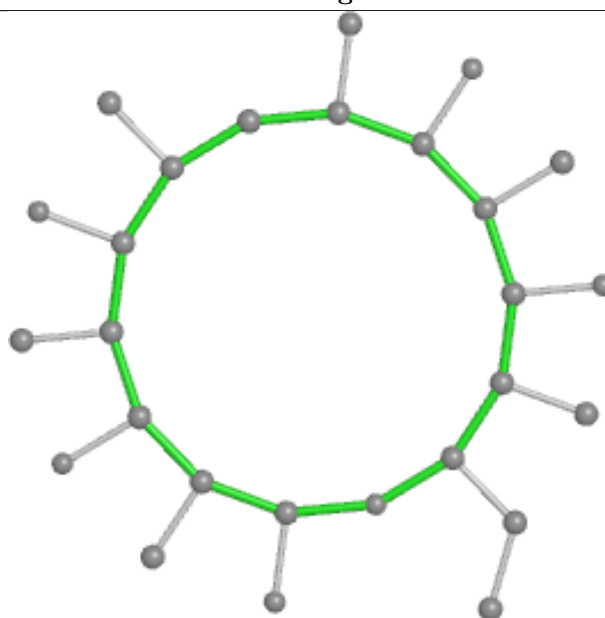
Bond lengths



Bond angles

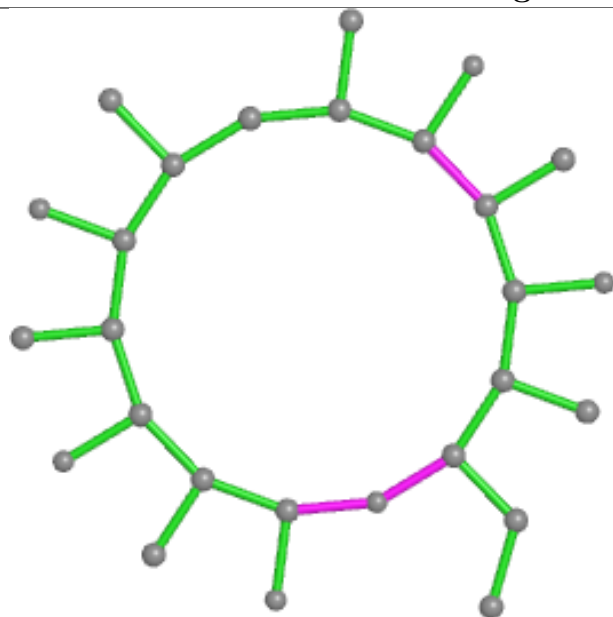


Torsions

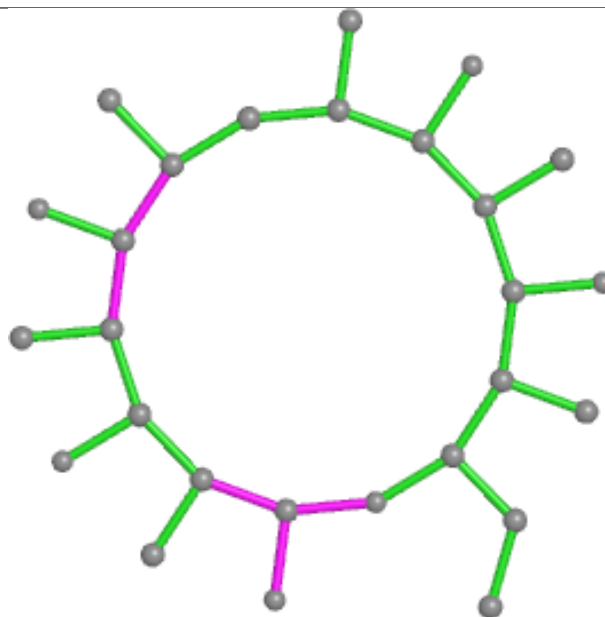


Rings

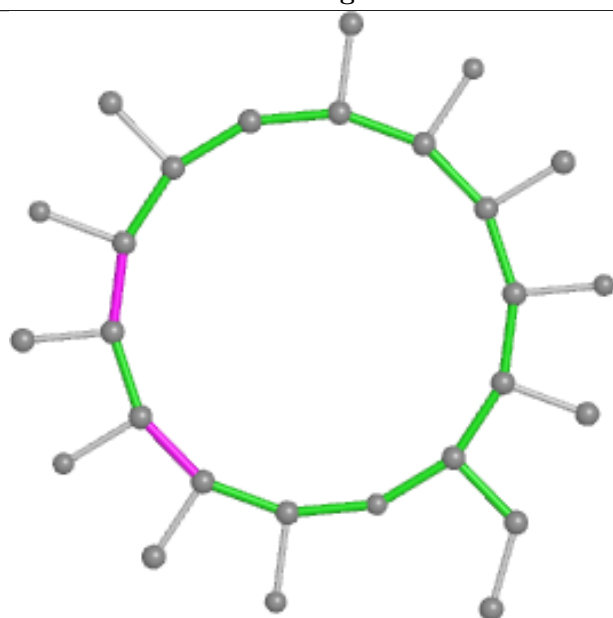
Ligand DEB B 502



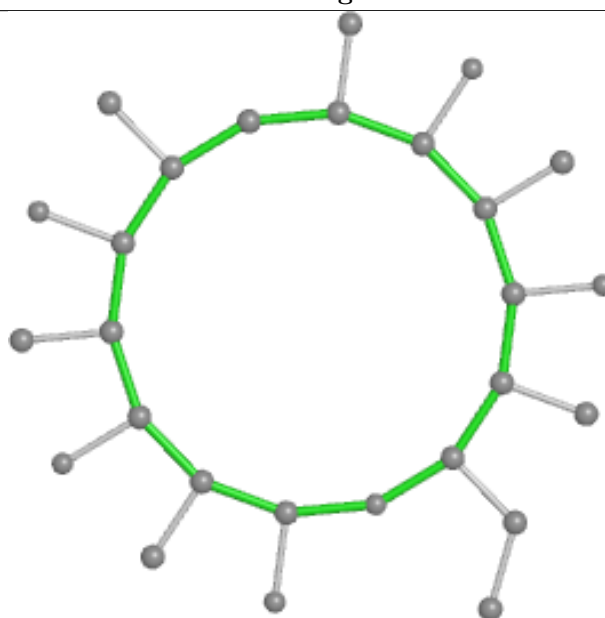
Bond lengths



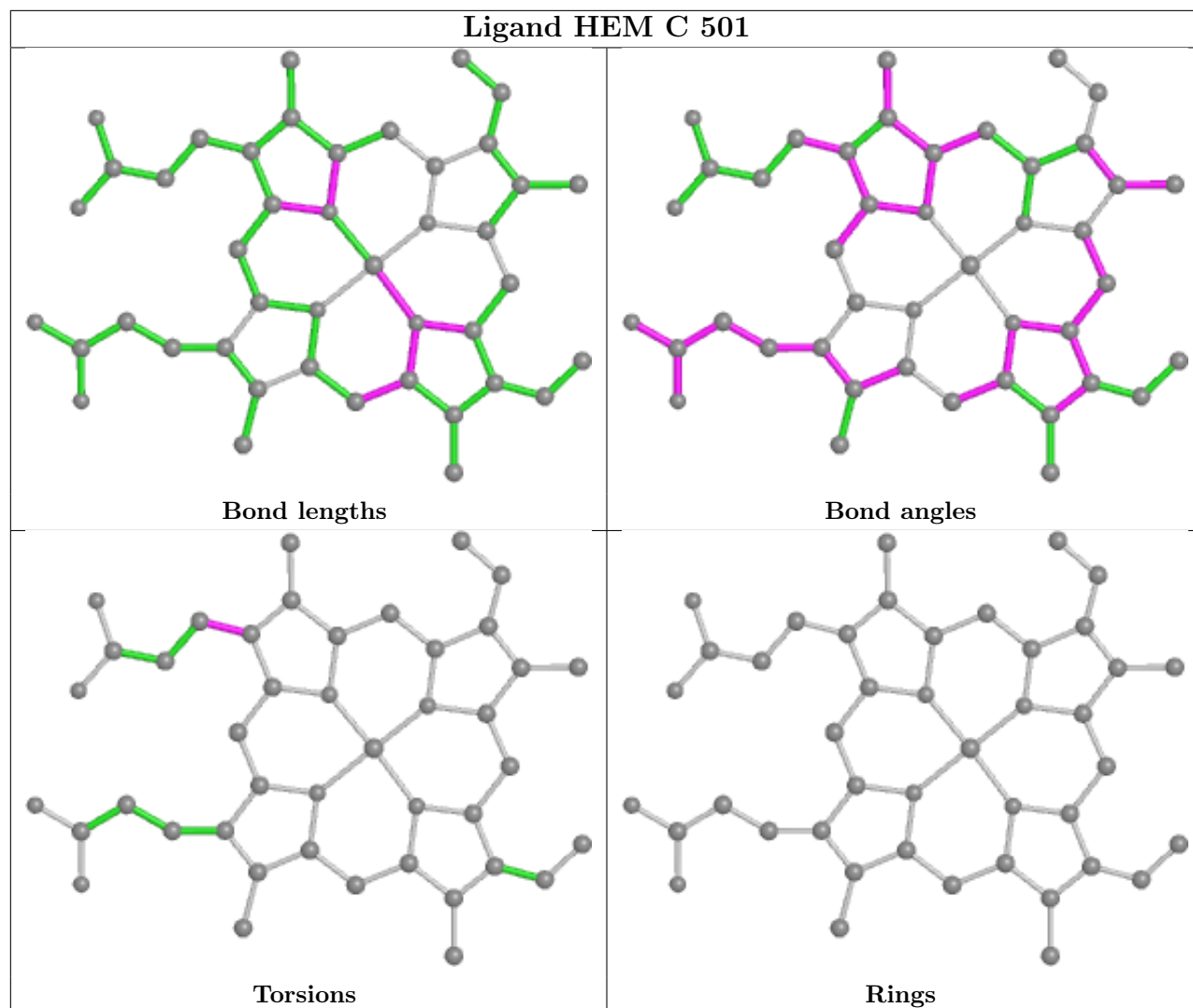
Bond angles



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	395/407 (97%)	-0.07	8 (2%) 65 60	26, 48, 75, 102	0
1	B	395/407 (97%)	-0.21	6 (1%) 73 70	25, 43, 66, 111	0
1	C	395/407 (97%)	-0.32	4 (1%) 82 80	24, 37, 54, 88	0
1	D	395/407 (97%)	0.11	7 (1%) 68 64	33, 58, 86, 121	0
1	E	395/407 (97%)	0.23	27 (6%) 17 13	37, 64, 93, 120	0
1	F	393/407 (96%)	0.68	67 (17%) 1 1	42, 72, 106, 121	0
All	All	2368/2442 (96%)	0.07	119 (5%) 28 23	24, 53, 91, 121	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	131	LEU	6.3
1	F	261	LEU	6.3
1	F	267	TYR	5.4
1	F	405	VAL	5.3
1	E	209	ASP	5.3
1	F	374	VAL	5.3
1	F	371	SER	5.2
1	F	125	ARG	5.1
1	A	343	ARG	5.0
1	F	377	PHE	4.9
1	F	404	ILE	4.8
1	B	209	ASP	4.8
1	F	379	THR	4.8
1	E	227	ASP	4.7
1	F	36	ARG	4.7
1	E	212	THR	4.7
1	F	276	LEU	4.6
1	F	270	LEU	4.6
1	F	23	HIS	4.6

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Mol	Chain	Res	Type	RSRZ
1	F	328	GLU	4.5
1	F	339	PHE	4.5
1	F	337	LEU	4.5
1	E	343	ARG	4.5
1	F	375	ARG	4.5
1	B	225	ASN	4.5
1	F	271	VAL	4.4
1	F	129	ASP	4.4
1	E	210	ALA	4.4
1	F	21	LEU	4.3
1	F	182	THR	4.3
1	D	227	ASP	4.0
1	F	141	PRO	4.0
1	F	372	ALA	4.0
1	F	380	LEU	4.0
1	F	343	ARG	3.9
1	A	208	ARG	3.9
1	A	228	HIS	3.8
1	E	213	GLU	3.8
1	E	265	LYS	3.7
1	E	305	GLU	3.7
1	F	342	GLU	3.7
1	B	343	ARG	3.6
1	F	124	VAL	3.6
1	A	227	ASP	3.5
1	E	336	GLU	3.5
1	F	123	ARG	3.5
1	A	225	ASN	3.5
1	C	343	ARG	3.5
1	F	225	ASN	3.5
1	F	373	LEU	3.5
1	F	272	ALA	3.4
1	B	342	GLU	3.3
1	E	311	VAL	3.3
1	E	313	ALA	3.3
1	F	132	LEU	3.3
1	F	329	GLU	3.2
1	F	130	SER	3.2
1	F	142	ALA	3.2
1	E	304	VAL	3.2
1	F	406	SER	3.1
1	D	386	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	342	GLU	3.1
1	F	268	GLU	3.0
1	F	126	SER	3.0
1	F	382	LEU	3.0
1	E	207	ARG	2.9
1	E	342	GLU	2.9
1	F	127	LEU	2.9
1	F	338	ASP	2.9
1	F	369	ALA	2.9
1	F	264	ARG	2.9
1	E	226	ASP	2.9
1	F	49	GLU	2.8
1	F	388	GLY	2.8
1	F	383	ALA	2.7
1	D	110	LYS	2.7
1	A	379	THR	2.7
1	D	265	LYS	2.7
1	E	309	VAL	2.7
1	F	332	ASP	2.7
1	F	265	LYS	2.6
1	D	390	LYS	2.6
1	E	36	ARG	2.6
1	F	277	VAL	2.6
1	E	329	GLU	2.6
1	C	319	VAL	2.5
1	E	211	PRO	2.5
1	E	13	ALA	2.4
1	F	215	LEU	2.4
1	C	225	ASN	2.4
1	F	188	GLU	2.4
1	F	136	VAL	2.4
1	F	385	PRO	2.4
1	E	332	ASP	2.4
1	C	105	ARG	2.4
1	F	344	ASN	2.4
1	E	123	ARG	2.4
1	F	32	ALA	2.3
1	F	346	HIS	2.3
1	E	225	ASN	2.3
1	A	226	ASP	2.3
1	F	386	VAL	2.3
1	F	378	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	110	LYS	2.1
1	D	190	GLN	2.1
1	F	120	MET	2.1
1	E	330	VAL	2.1
1	B	213	GLU	2.1
1	E	229	LEU	2.1
1	B	210	ALA	2.1
1	F	122	PRO	2.0
1	E	57	ARG	2.0
1	F	137	ALA	2.0
1	F	370	LEU	2.0
1	F	330	VAL	2.0
1	D	209	ASP	2.0
1	F	135	MET	2.0
1	F	147	PHE	2.0
1	F	389	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

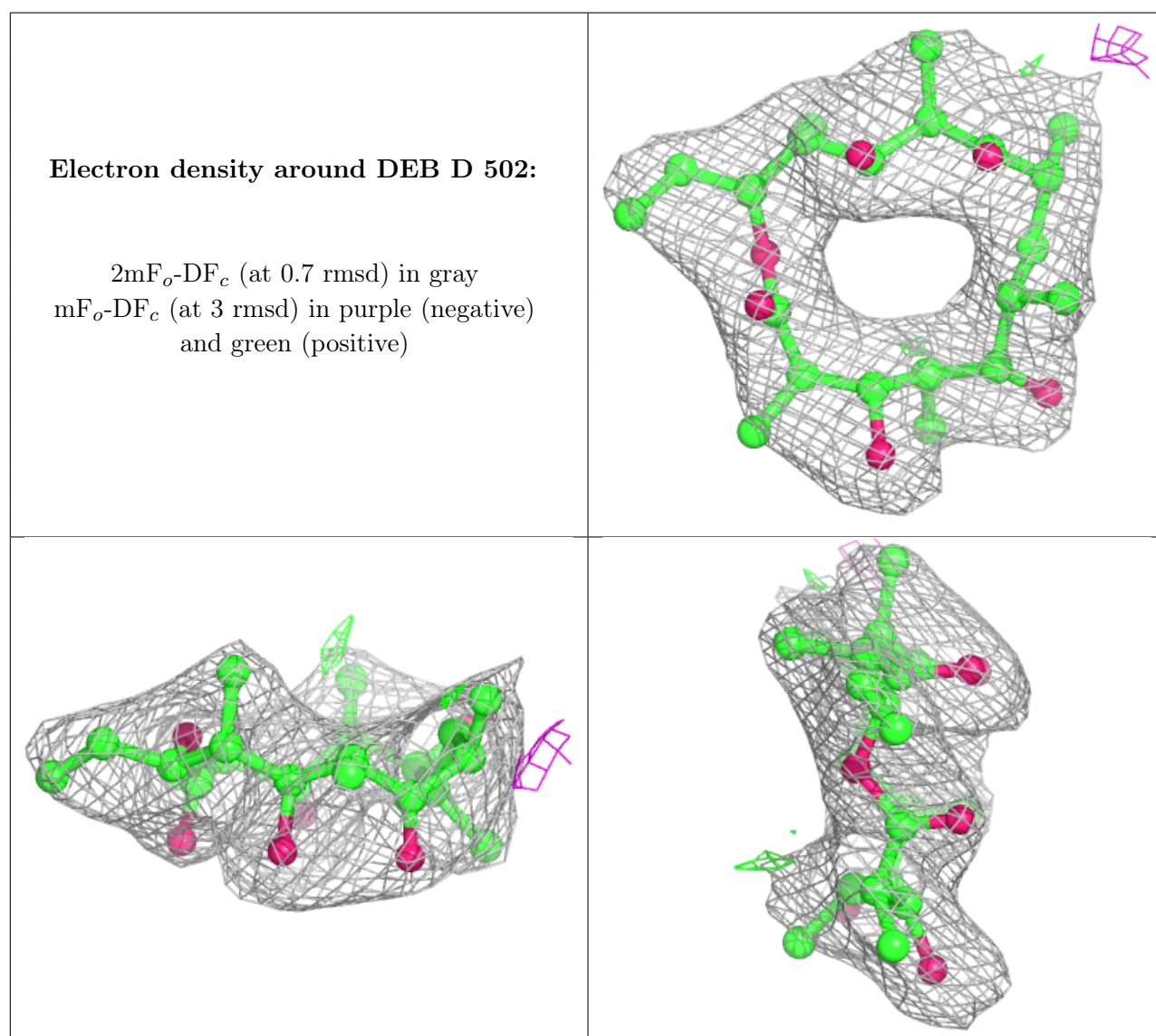
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	DEB	D	502	27/27	0.94	0.19	39,43,47,50	0
2	HEM	F	501	43/43	0.95	0.16	50,70,76,84	0
3	DEB	E	502	27/27	0.95	0.16	40,43,45,45	0
3	DEB	F	502	27/27	0.95	0.17	54,58,61,61	0
2	HEM	E	501	43/43	0.96	0.11	39,44,50,60	0
2	HEM	A	501	43/43	0.96	0.14	24,26,29,34	0
3	DEB	B	502	27/27	0.96	0.17	29,32,33,33	0

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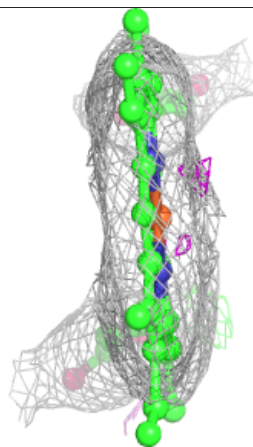
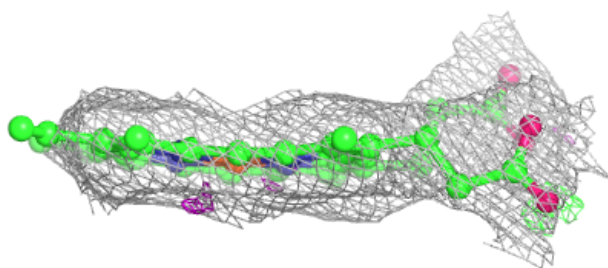
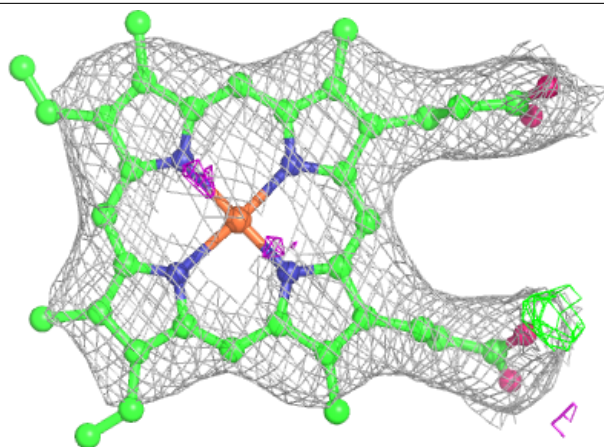
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	DEB	A	502	27/27	0.97	0.19	27,28,29,30	0
2	HEM	D	501	43/43	0.97	0.17	22,24,36,44	0
3	DEB	C	502	27/27	0.97	0.16	25,28,31,32	0
2	HEM	C	501	43/43	0.98	0.16	23,25,29,36	0
2	HEM	B	501	43/43	0.98	0.17	20,22,26,29	0

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



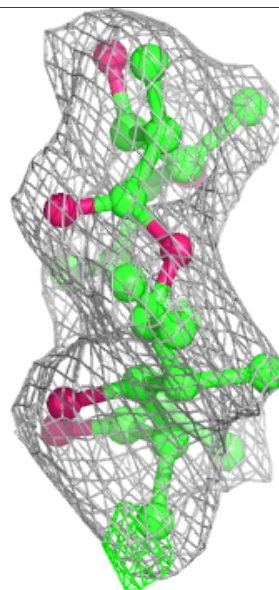
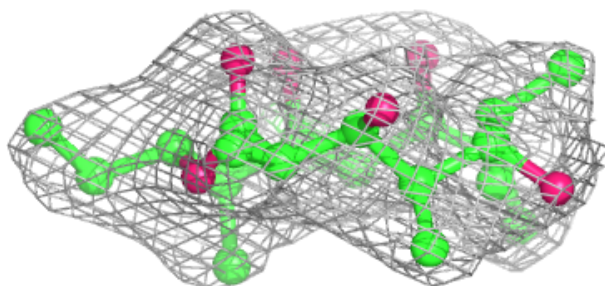
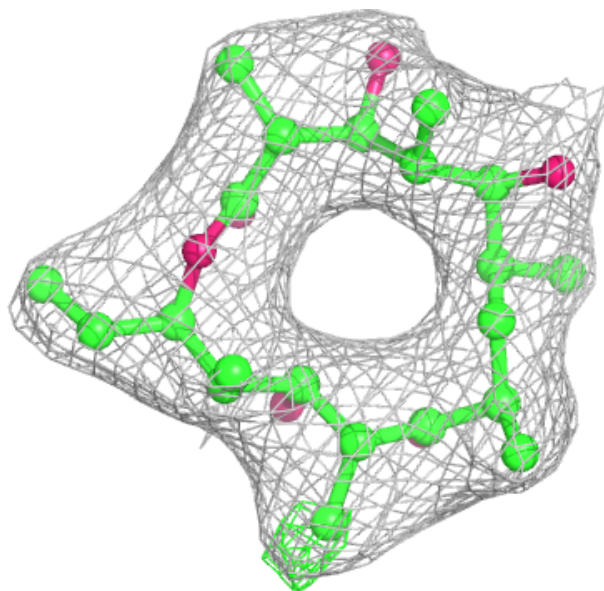
Electron density around HEM F 501:

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



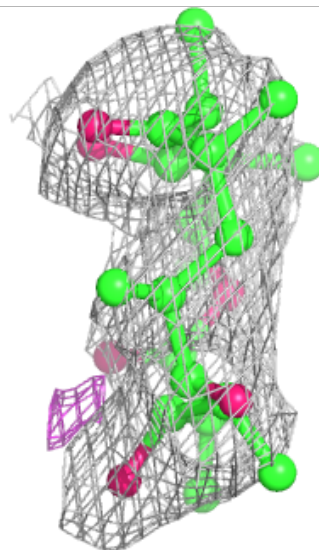
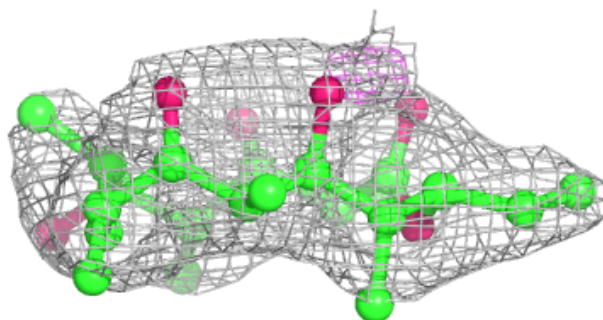
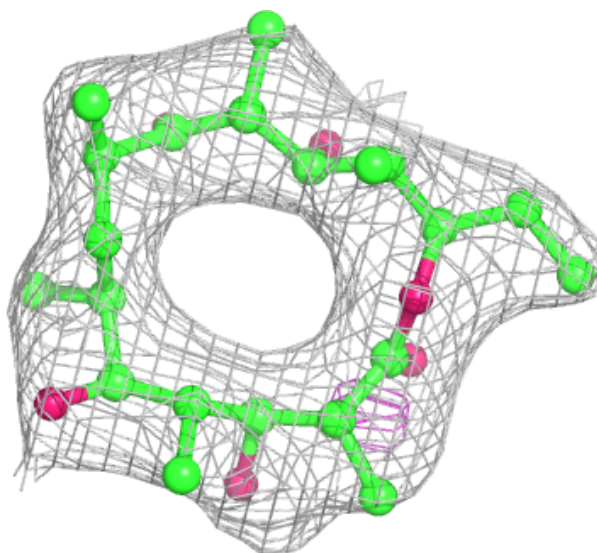
Electron density around DEB E 502:

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



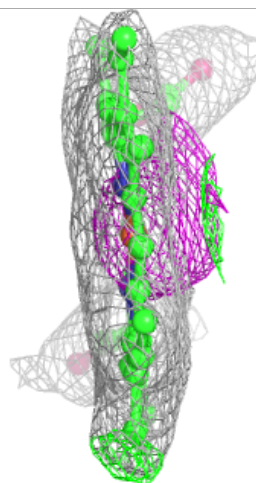
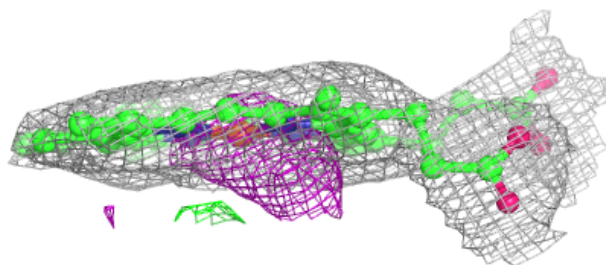
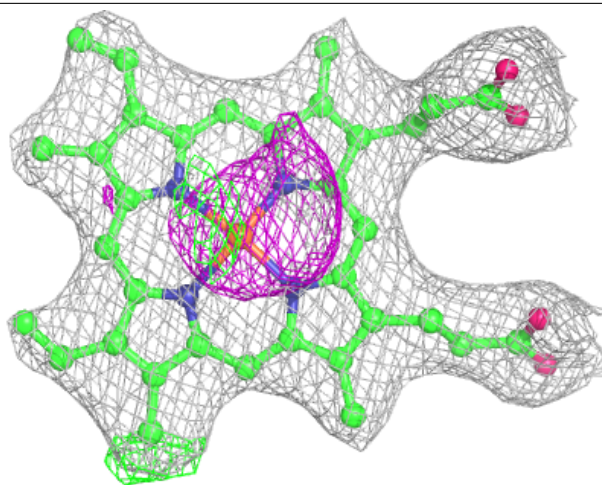
Electron density around DEB F 502:

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



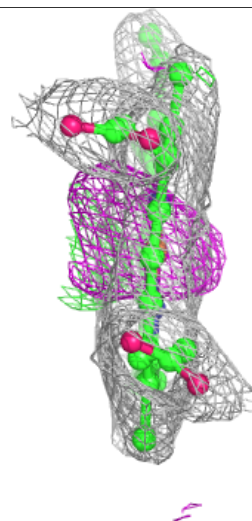
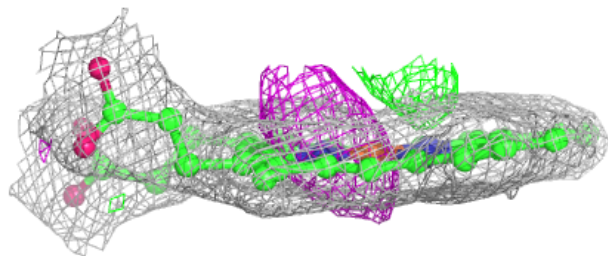
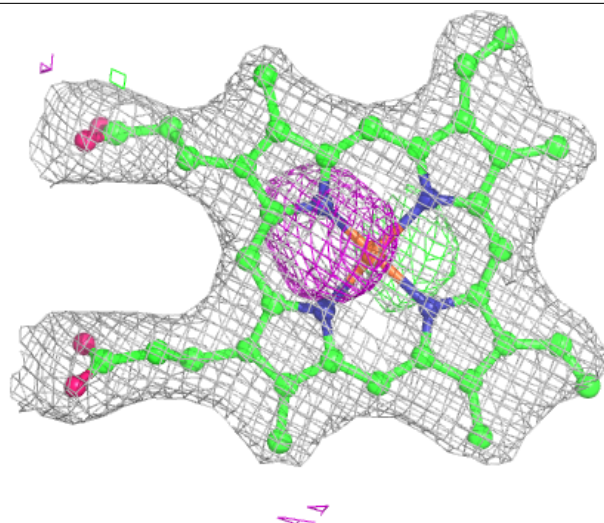
Electron density around HEM E 501:

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



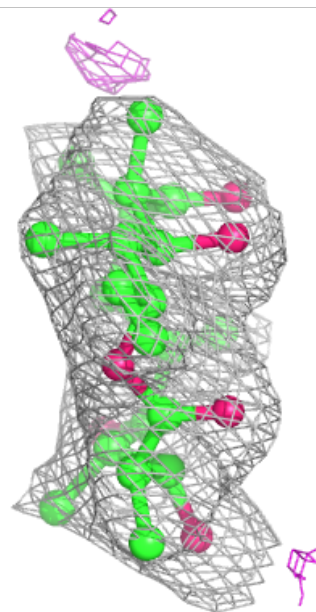
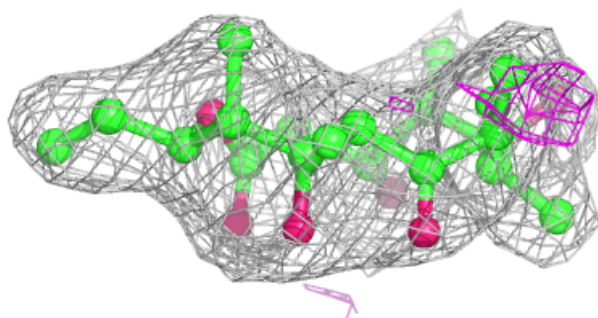
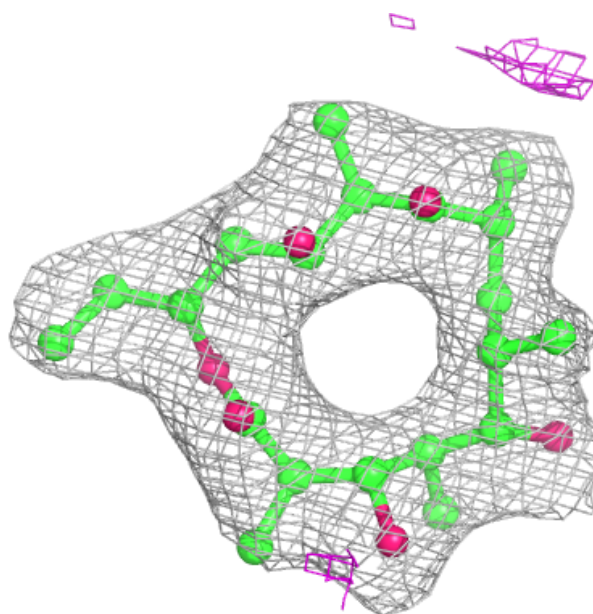
Electron density around HEM A 501:

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



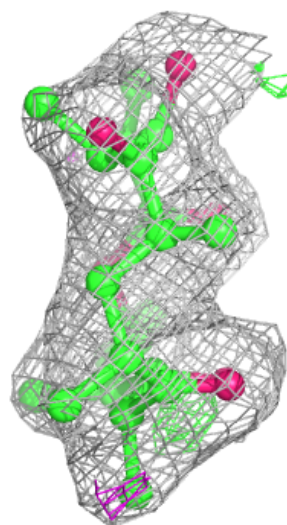
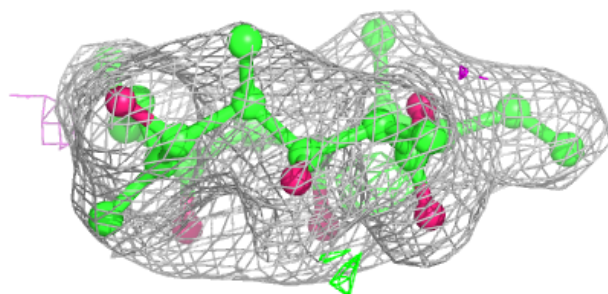
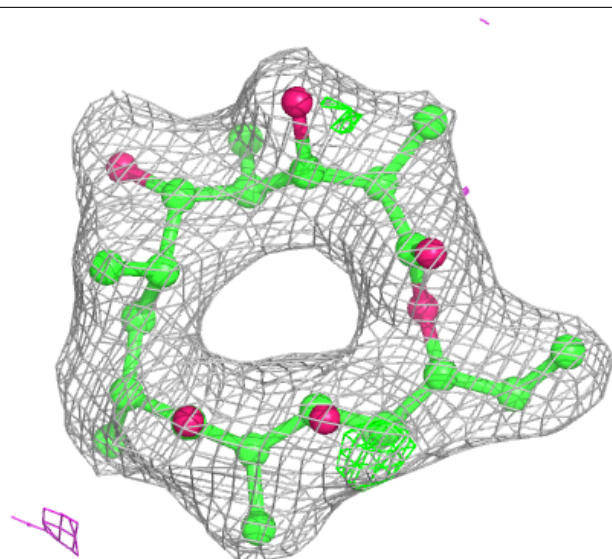
Electron density around DEB B 502:

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and green (positive)



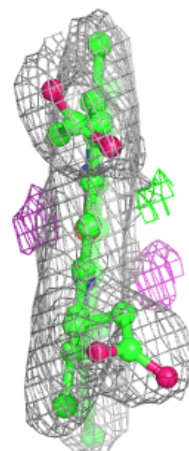
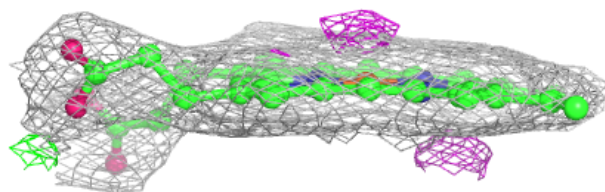
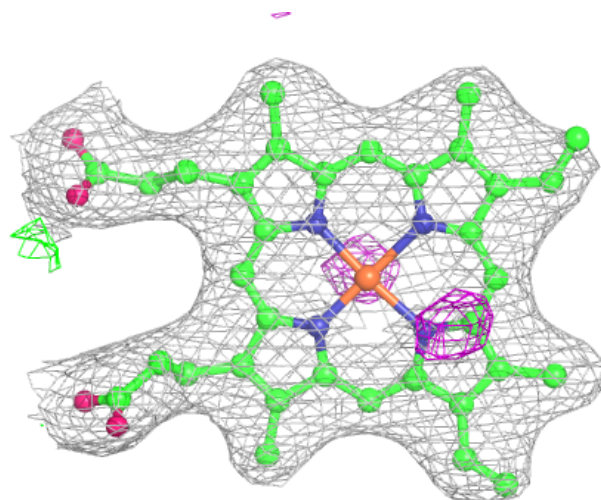
Electron density around DEB A 502:

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



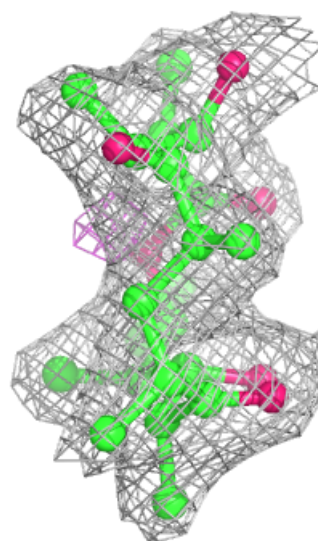
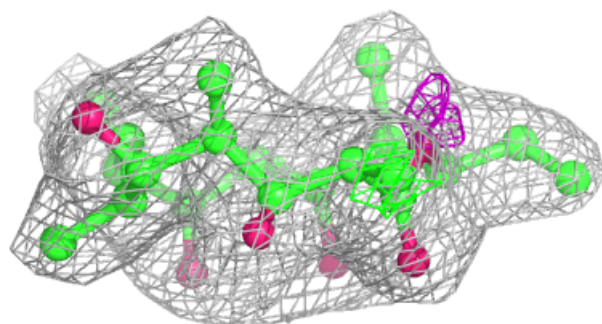
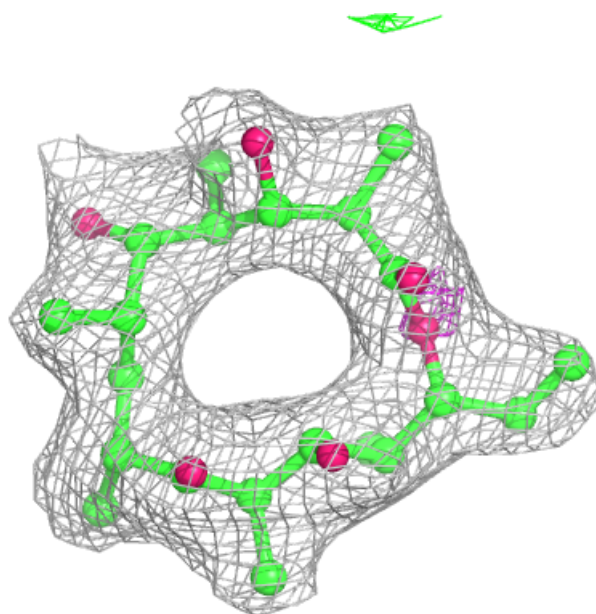
Electron density around HEM D 501:

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



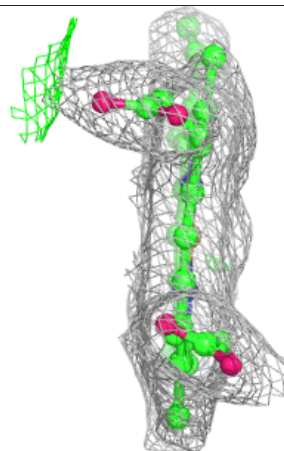
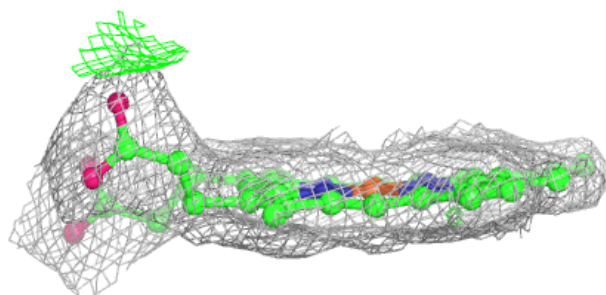
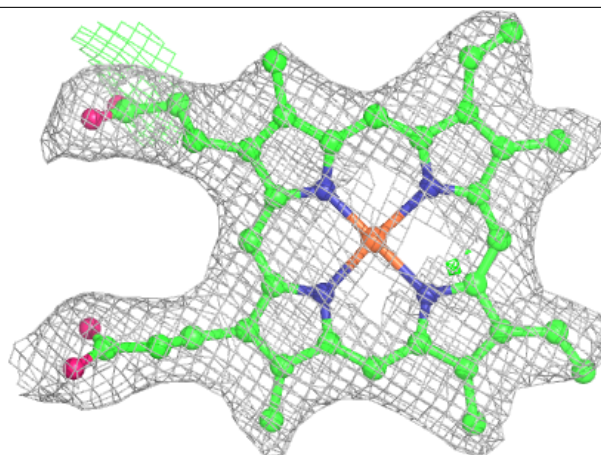
Electron density around DEB C 502:

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



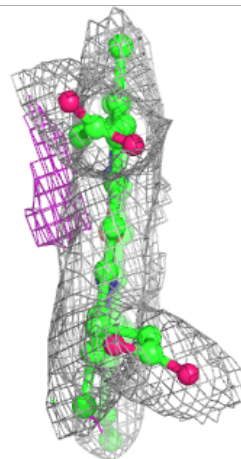
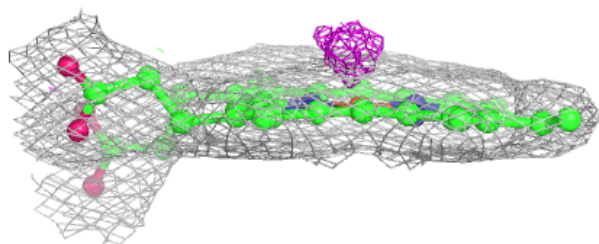
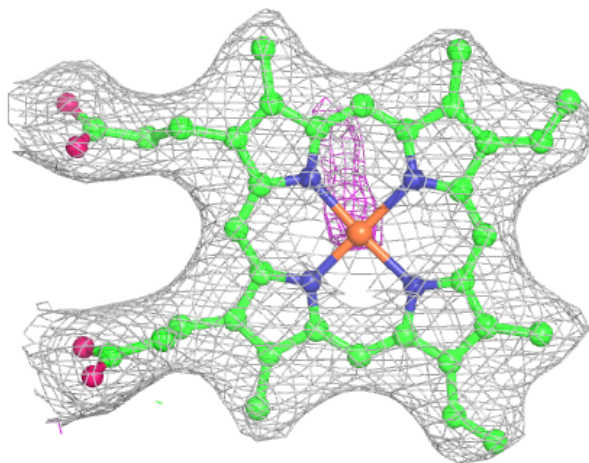
Electron density around HEM C 501:

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



Electron density around HEM B 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.