



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:13 AM UTC

PDB ID : 5NMI / pdb_00005nmi
Title : Cytochrome bc1 bound to the inhibitor MJM170
Authors : Capper, N.J.; Antonyuk, S.V.; Hasnain, S.S.
Deposited on : 2017-04-05
Resolution : 3.50 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)
Xtrriage (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

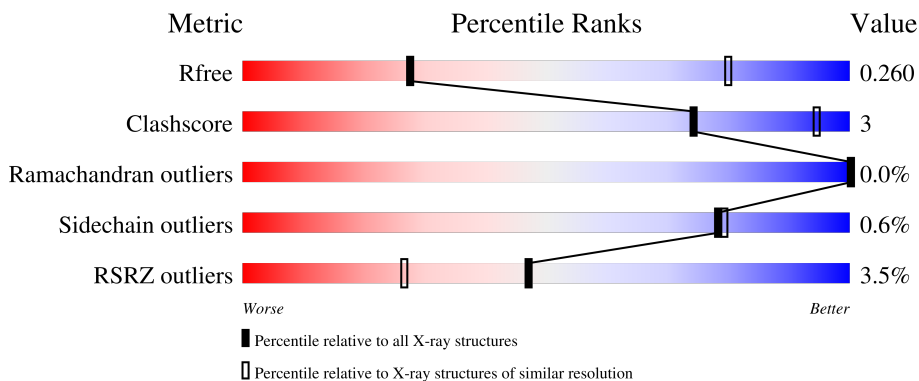
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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.



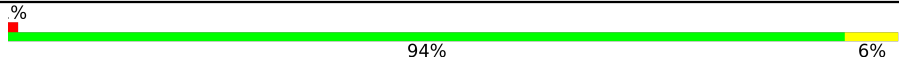
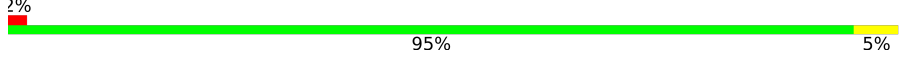
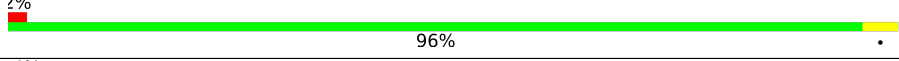


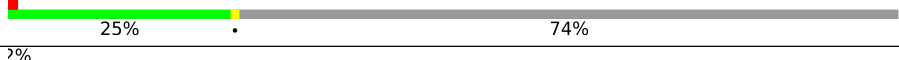

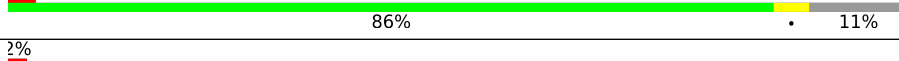
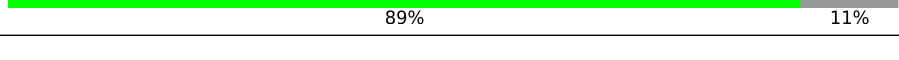
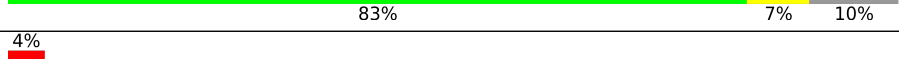
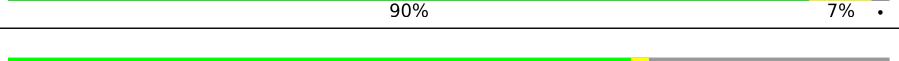
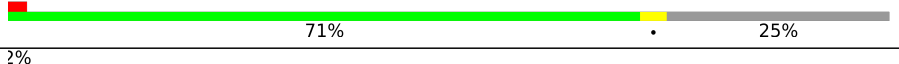

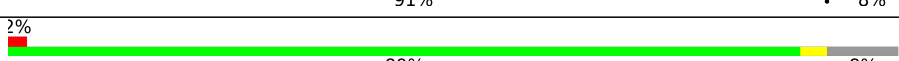
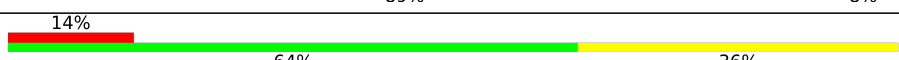
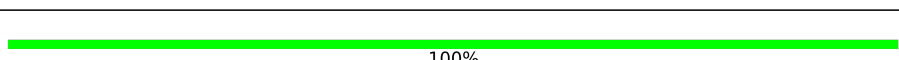

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	444	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 95%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 2px;"></div> </div> <p style="text-align: center;">95%</p>
1	N	444	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 96%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: yellow; margin-right: 2px;"></div> </div> <p style="text-align: center;">96%</p>
2	B	423	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 96%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: yellow; margin-right: 2px;"></div> </div> <p style="text-align: center;">96%</p>
2	O	423	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 94%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 2px;"></div> </div> <p style="text-align: center;">94%</p>
3	C	372	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 96%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 4%; height: 10px; background-color: yellow; margin-right: 2px;"></div> </div> <p style="text-align: center;">96%</p>

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Mol	Chain	Length	Quality of chain
3	P	372	
4	D	240	
4	Q	240	
5	E	274	
5	I	274	
5	R	274	
5	V	274	
6	F	111	
6	S	111	
7	G	82	
7	T	82	
8	H	91	
8	U	91	
9	J	64	
9	W	64	
10	K	22	
10	X	22	

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
12	MJM	C	503	X	-	-	-
12	MJM	P	404	X	-	-	-
13	PEE	D	502	X	-	-	-
13	PEE	E	502	X	-	-	-
13	PEE	R	201	X	-	-	-
13	PEE	R	202	X	-	-	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 31648 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	444	Total	C	N	O	S	48	0	0
			3440	2148	607	665	20			
1	N	444	Total	C	N	O	S	45	0	0
			3440	2148	607	665	20			

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	423	Total	C	N	O	S	27	0	0
			3172	1993	562	610	7			
2	O	423	Total	C	N	O	S	8	0	0
			3172	1993	562	610	7			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	372	Total	C	N	O	S	0	0	0
			2954	1984	460	492	18			
3	P	372	Total	C	N	O	S	0	0	0
			2954	1984	460	492	18			

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	240	Total	C	N	O	S	0	0	0
			1913	1222	329	347	15			
4	Q	240	Total	C	N	O	S	5	0	0
			1913	1222	329	347	15			

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1519	957	263	291	8			
5	I	30	Total	C	N	O	S	9	0	0
			221	137	44	39	1			
5	R	72	Total	C	N	O	S	0	0	0
			540	335	90	113	2			
5	V	30	Total	C	N	O	S	0	0	0
			221	137	44	39	1			

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	99	Total	C	N	O	S	0	0	0
			870	553	157	158	2			
6	S	99	Total	C	N	O	S	4	0	0
			870	553	157	158	2			

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	74	Total	C	N	O	S	0	0	0
			623	407	117	98	1			
7	T	80	Total	C	N	O	S	0	0	0
			677	439	127	110	1			

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	66	Total	C	N	O	S	3	0	0
			539	327	98	109	5			
8	U	68	Total	C	N	O	S	0	0	0
			557	337	100	115	5			

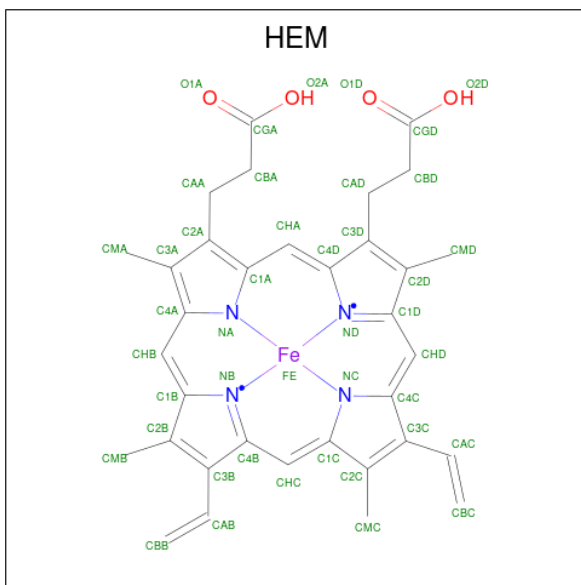
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	J	59	Total	C	N	O	0	0	0
			492	322	86	84			
9	W	59	Total	C	N	O	0	0	0
			487	320	84	83			

- Molecule 10 is a protein called ARG-ASN-TRP-VAL-PRO-THR-ALA-GLN-LEU-TRP-GLY-ALA-VAL-GLY-ALA-VAL-GLY-LEU-VAL-SER-ALA-THR.

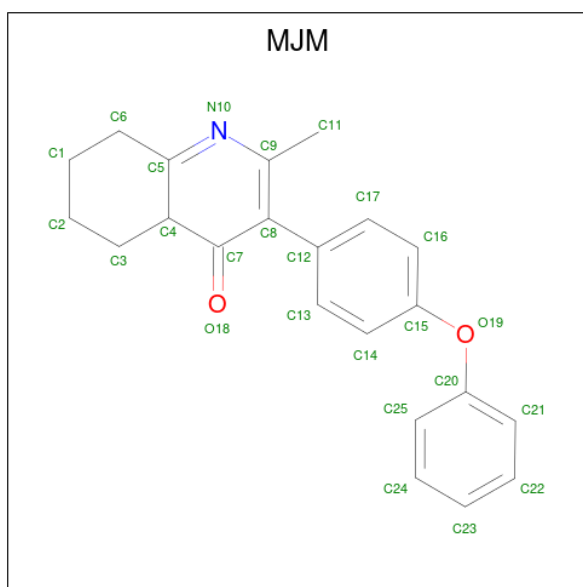
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	22	Total	C	N	O	0	0	0
			159	103	29	27			
10	X	22	Total	C	N	O	12	0	0
			159	103	29	27			

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



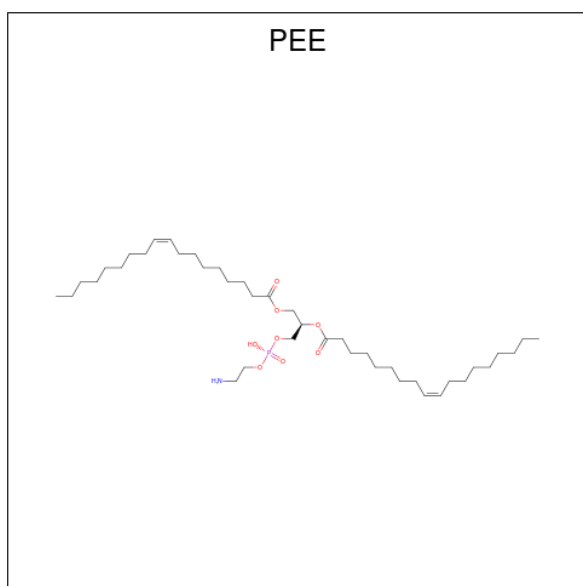
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
11	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
11	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
11	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
11	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 12 is (4aS)-2-methyl-3-(4-phenoxyphenyl)-5,6,7,8-tetrahydroquinolin-4(4aH)-one (CCD ID: MJM) (formula: $C_{22}H_{21}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
12	C	1	25	22	1	2	0	0
12	P	1	25	22	1	2	0	0

- Molecule 13 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



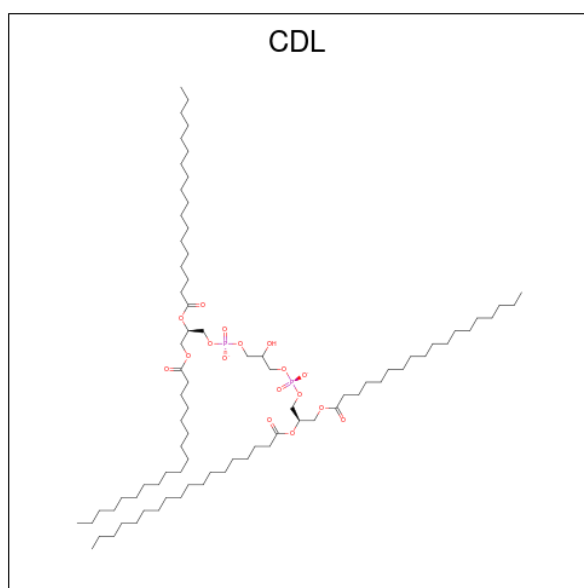
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
13	C	1	28	19	1	7	1	0	0

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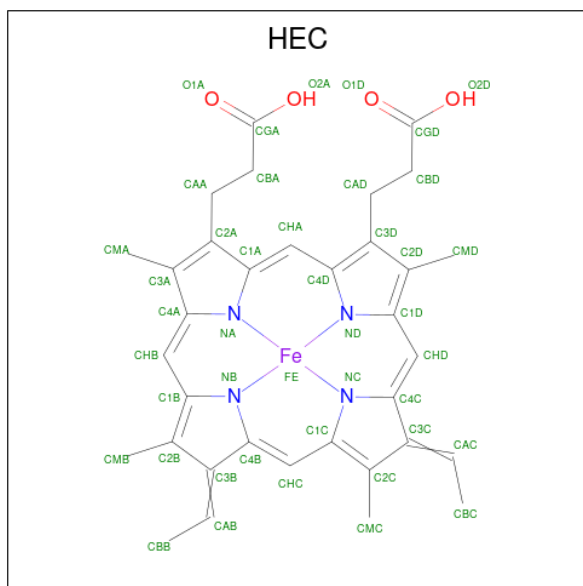
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	D	1	Total	C	N	O	P	0	0
			42	32	1	8	1		
13	E	1	Total	C	N	O	P	0	0
			29	19	1	8	1		
13	P	1	Total	C	N	O	P	0	0
			38	28	1	8	1		
13	R	1	Total	C	N	O	P	0	0
			34	24	1	8	1		
13	R	1	Total	C	N	O	P	0	0
			24	14	1	8	1		

- Molecule 14 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



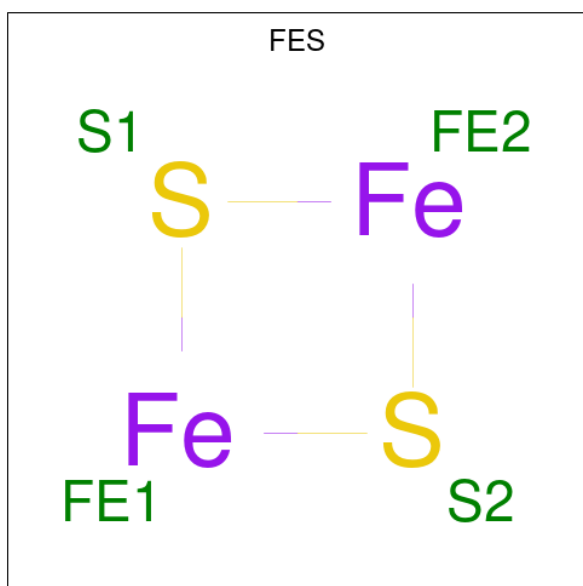
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total	C	O	P	0	0
			42	23	17	2		
14	C	1	Total	C	O	P	0	0
			37	18	17	2		
14	D	1	Total	C	O	P	0	0
			44	27	15	2		
14	P	1	Total	C	O	P	0	0
			42	27	13	2		
14	P	1	Total	C	O	P	0	0
			46	28	16	2		
14	P	1	Total	C	O	P	0	0
			38	19	17	2		

- Molecule 15 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
15	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
15	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

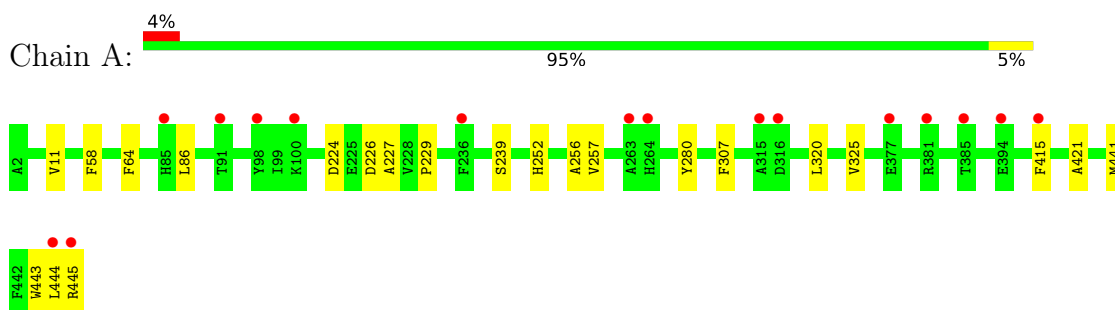


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
16	E	1	Total	Fe	S	0	0
			4	2	2		

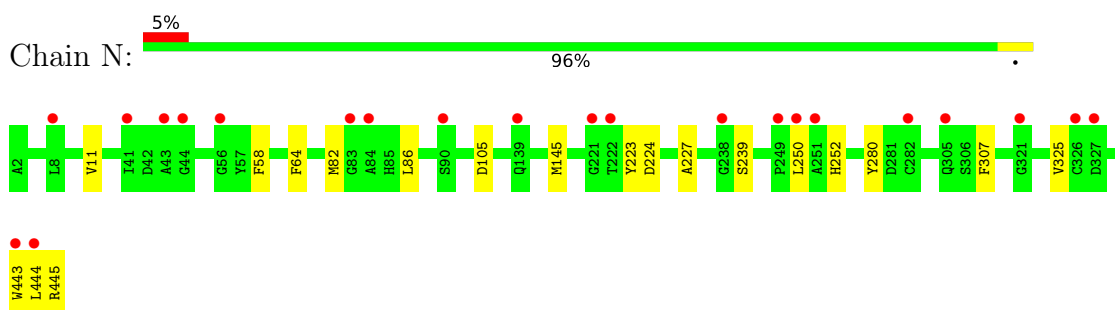
3 Residue-property plots [i](#)

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

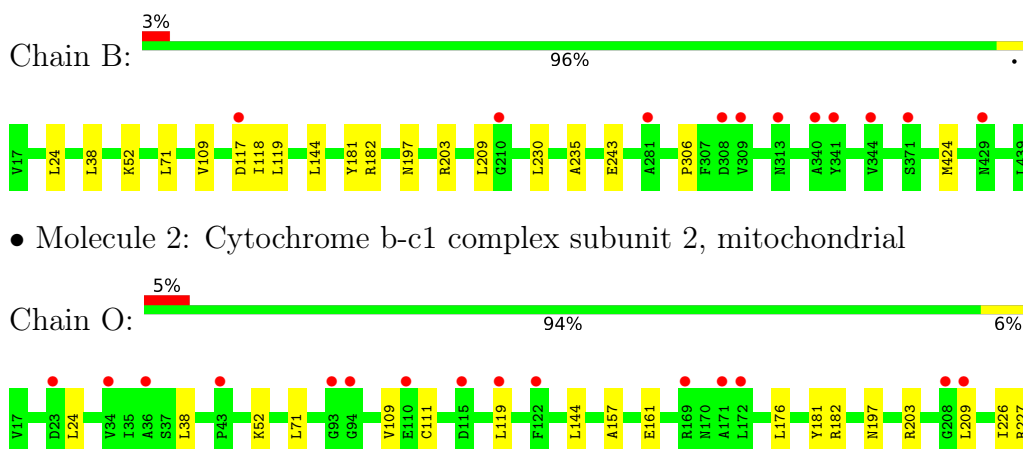
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



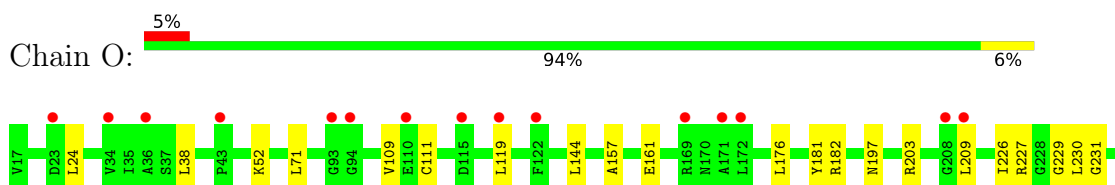
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

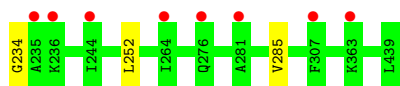


- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

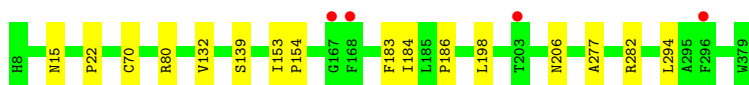


- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

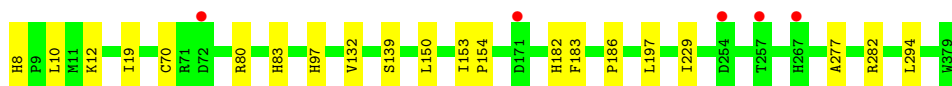




- Molecule 3: Cytochrome b



- Molecule 3: Cytochrome b



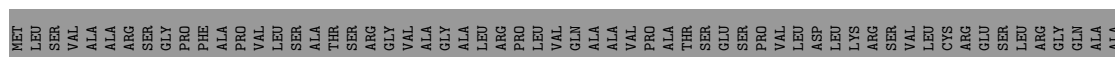
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



- Molecule 4: Cytochrome c1, heme protein, mitochondrial

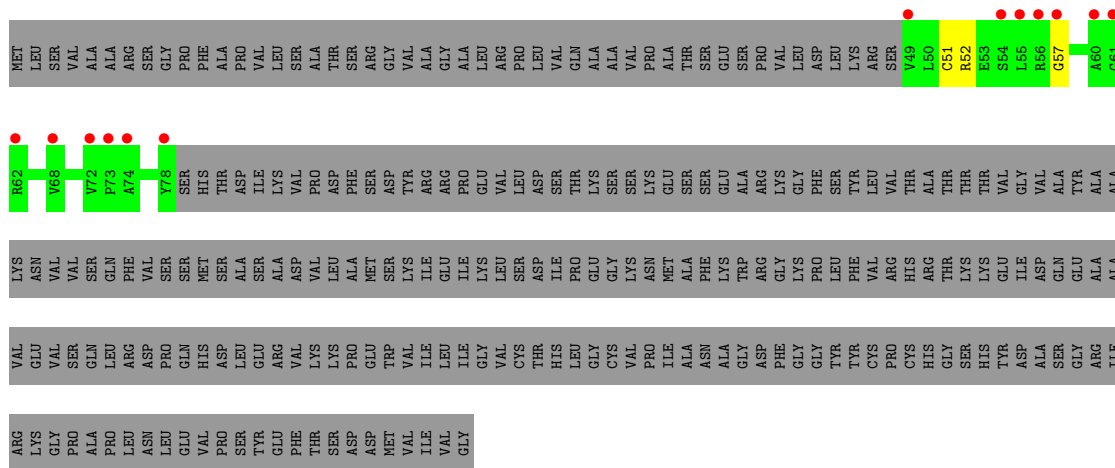


- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

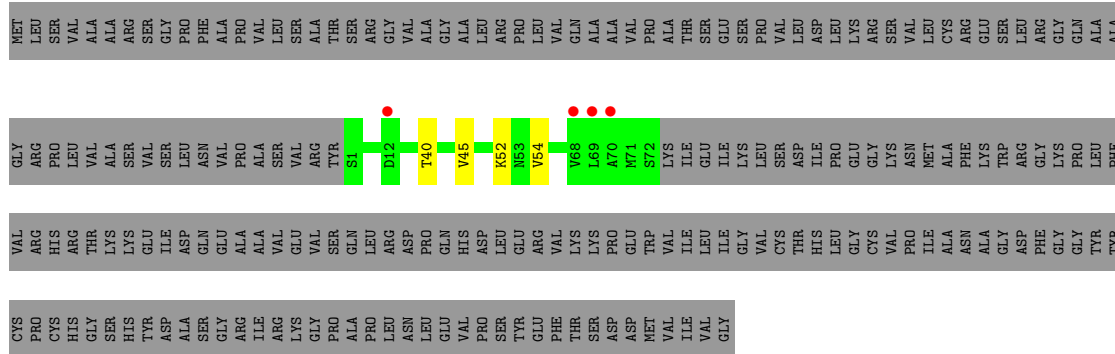


- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

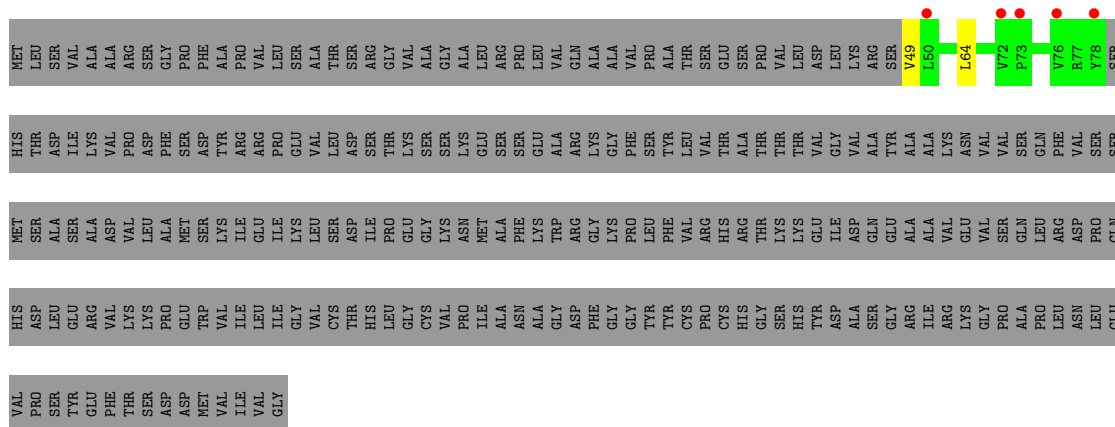




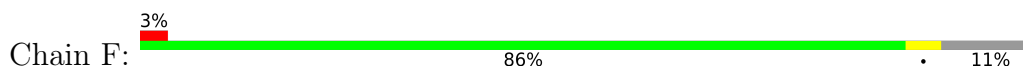
● Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

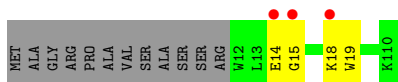


● Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

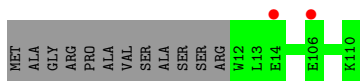
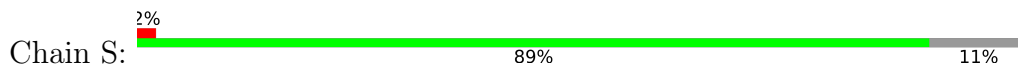


● Molecule 6: Cytochrome b-c1 complex subunit 7

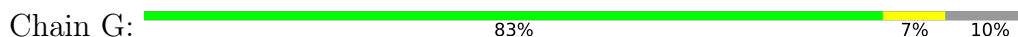




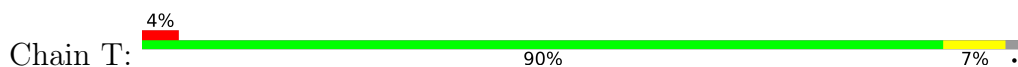
- Molecule 6: Cytochrome b-c1 complex subunit 7



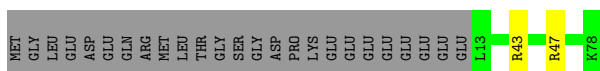
- Molecule 7: Cytochrome b-c1 complex subunit 8



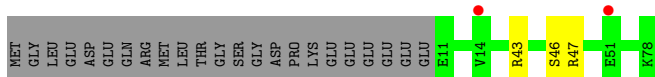
- Molecule 7: Cytochrome b-c1 complex subunit 8



- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



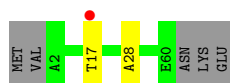
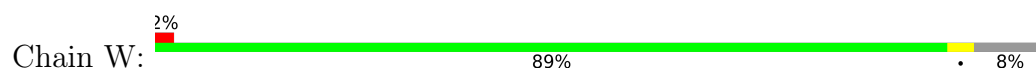
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



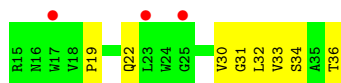
- Molecule 9: Cytochrome b-c1 complex subunit 9



- Molecule 9: Cytochrome b-c1 complex subunit 9



• Molecule 10: ARG-ASN-TRP-VAL-PRO-THR-ALA-GLN-LEU-TRP-GLY-ALA-VAL-GLY-ALA-VAL-GLY-LEU-VAL-SER-ALA-THR



• Molecule 10: ARG-ASN-TRP-VAL-PRO-THR-ALA-GLN-LEU-TRP-GLY-ALA-VAL-GLY-ALA-VAL-GLY-LEU-VAL-SER-ALA-THR



There are no outlier residues recorded for this chain.

4 Data and refinement statistics i

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	129.48Å 129.48Å 720.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	64.74 – 3.50 64.74 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (64.74-3.50) 99.5 (64.74-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.49Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.248 , 0.268 (Not available) , 0.260	Depositor DCC
R_{free} test set	4344 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	78.7	Xtrriage
Anisotropy	0.335	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	0.096 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	31648	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.82% 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: HEC, MJM, FES, HEM, PEE, CDL

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	0/3512	0.88	3/4766 (0.1%)
1	N	0.53	0/3512	0.87	3/4766 (0.1%)
2	B	0.53	1/3232 (0.0%)	0.82	0/4386
2	O	0.52	0/3232	0.83	1/4386 (0.0%)
3	C	0.53	0/3051	0.89	0/4177
3	P	0.54	0/3051	0.89	0/4177
4	D	0.52	0/1972	0.81	0/2676
4	Q	0.56	1/1972 (0.1%)	0.83	1/2676 (0.0%)
5	E	0.56	0/1553	0.84	0/2100
5	I	0.79	1/223 (0.4%)	1.05	3/302 (1.0%)
5	R	0.52	0/548	0.89	0/741
5	V	0.62	0/223	0.78	0/302
6	F	0.49	0/889	0.80	0/1191
6	S	0.49	0/889	0.79	0/1191
7	G	0.55	0/644	0.85	1/871 (0.1%)
7	T	0.57	0/699	0.89	2/946 (0.2%)
8	H	0.50	0/544	0.88	0/729
8	U	0.49	0/562	0.93	1/753 (0.1%)
9	J	0.49	0/504	0.89	0/678
9	W	0.51	0/500	0.90	0/675
10	K	0.67	0/163	0.93	0/225
10	X	0.71	0/163	0.90	0/225
All	All	0.53	3/31638 (0.0%)	0.86	15/42939 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	241	LYS	CA-CB	-9.37	1.34	1.53
5	I	57	GLY	C-N	-7.09	1.23	1.33
2	B	235	ALA	C-N	-5.63	1.25	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	ASP	N-CA-C	-10.43	100.10	112.92
1	N	227	ALA	O-C-N	8.40	130.56	122.00
1	A	226	ASP	CA-C-N	-8.12	109.55	122.79
1	A	226	ASP	C-N-CA	-8.12	109.55	122.79
1	N	223	TYR	N-CA-C	7.68	122.00	109.94
5	I	57	GLY	CA-C-N	-6.13	110.10	120.58
5	I	57	GLY	C-N-CA	-6.13	110.10	120.58
1	N	224	ASP	N-CA-C	-5.67	106.58	112.93
2	O	234	GLY	N-CA-C	5.66	118.07	110.43
5	I	57	GLY	O-C-N	5.55	129.48	122.43
8	U	46	SER	N-CA-C	5.24	118.94	112.54
4	Q	241	LYS	CB-CA-C	-5.24	100.14	110.10
7	T	50	PRO	N-CA-C	5.08	116.90	110.70
7	T	34	ILE	N-CA-CB	5.04	113.67	110.50
7	G	50	PRO	N-CA-C	5.04	116.84	110.70

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	3440	0	3337	21	0
1	N	3440	0	3337	15	0
2	B	3172	0	3152	9	0
2	O	3172	0	3152	19	0
3	C	2954	0	3010	29	0
3	P	2954	0	3010	32	0
4	D	1913	0	1860	11	0
4	Q	1913	0	1860	5	0
5	E	1519	0	1503	22	0
5	I	221	0	234	2	0
5	R	540	0	534	5	0
5	V	221	0	234	5	0
6	F	870	0	864	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	S	870	0	864	0	0
7	G	623	0	631	7	0
7	T	677	0	673	2	0
8	H	539	0	524	1	0
8	U	557	0	536	2	0
9	J	492	0	494	1	0
9	W	487	0	487	2	0
10	K	159	0	159	11	0
10	X	159	0	159	0	0
11	C	86	0	60	15	0
11	P	86	0	60	14	0
12	C	25	0	0	0	0
12	P	25	0	0	1	0
13	C	28	0	32	0	0
13	D	42	0	57	5	0
13	E	29	0	32	1	0
13	P	38	0	50	0	0
13	R	58	0	64	4	0
14	C	79	0	46	1	0
14	D	44	0	40	0	0
14	P	126	0	101	3	0
15	D	43	0	31	0	0
15	Q	43	0	31	0	0
16	E	4	0	0	0	0
All	All	31648	0	31218	194	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (194) 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)
13:D:502:PEE:C1	13:D:502:PEE:C2	2.00	1.39
3:C:183:PHE:CE1	11:C:501:HEM:HBC1	1.89	1.08
3:C:183:PHE:CD2	3:P:183:PHE:CD1	2.44	1.06
2:O:197:ASN:O	2:O:230:LEU:HD12	1.62	0.98
3:C:183:PHE:CE2	3:P:183:PHE:CD1	2.55	0.94
11:C:501:HEM:HMC1	11:C:501:HEM:HBC2	1.48	0.93
3:C:183:PHE:HD2	3:P:183:PHE:CD1	1.85	0.92
13:D:502:PEE:C1	13:D:502:PEE:C3	2.51	0.88
3:C:183:PHE:CD1	11:C:501:HEM:CBC	2.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:402:HEM:HMC1	11:P:402:HEM:HBC2	1.56	0.87
3:C:183:PHE:CE2	3:P:183:PHE:HD1	1.91	0.87
7:G:3:GLN:OE1	7:G:6:HIS:ND1	2.10	0.84
1:A:320:LEU:HG	1:A:415:PHE:CZ	2.13	0.83
1:A:257:VAL:HG22	1:A:415:PHE:CE1	2.14	0.82
1:A:320:LEU:HG	1:A:415:PHE:HZ	1.43	0.82
3:P:19:ILE:HG21	14:P:406:CDL:H111	1.60	0.82
1:N:145:MET:HB2	1:N:252:HIS:CE1	2.14	0.82
7:G:1:GLY:O	7:G:2:ARG:CG	2.28	0.81
2:B:197:ASN:HB3	2:B:230:LEU:HD12	1.62	0.81
2:O:52:LYS:O	2:O:203:ARG:NH2	2.14	0.80
3:C:183:PHE:HD2	3:P:183:PHE:CE1	1.99	0.80
3:C:183:PHE:HD1	11:C:501:HEM:CAC	1.93	0.80
2:B:52:LYS:O	2:B:203:ARG:NH2	2.15	0.78
7:G:1:GLY:C	7:G:2:ARG:HG2	2.09	0.78
3:P:8:HIS:NE2	3:P:12:LYS:HE3	1.98	0.78
5:E:153:PHE:CE2	5:E:172:ARG:HG3	2.20	0.77
3:C:183:PHE:CE1	11:C:501:HEM:CBC	2.67	0.76
3:C:183:PHE:CD1	11:C:501:HEM:CAC	2.69	0.76
7:G:1:GLY:O	7:G:2:ARG:HG2	1.85	0.74
5:E:153:PHE:CD2	5:E:172:ARG:HG3	2.23	0.73
3:P:153:ILE:HG23	3:P:154:PRO:HD2	1.70	0.73
3:P:8:HIS:NE2	3:P:12:LYS:CE	2.51	0.73
1:N:145:MET:HB3	1:N:252:HIS:ND1	2.03	0.73
11:P:403:HEM:HBC2	11:P:403:HEM:HMC2	1.72	0.71
3:C:183:PHE:CD1	11:C:501:HEM:HBC1	2.24	0.71
3:C:183:PHE:HE2	3:P:183:PHE:HD1	1.35	0.71
10:K:19:PRO:HA	10:K:22:GLN:CD	2.16	0.70
2:O:197:ASN:C	2:O:230:LEU:HD12	2.17	0.70
1:A:320:LEU:CD2	1:A:415:PHE:CE2	2.76	0.69
1:N:145:MET:CB	1:N:252:HIS:CE1	2.76	0.68
1:A:227:ALA:O	1:A:229:PRO:HD3	1.94	0.68
1:A:320:LEU:HD21	1:A:415:PHE:CE2	2.30	0.67
10:K:19:PRO:O	10:K:22:GLN:HG2	1.94	0.67
7:G:1:GLY:O	7:G:2:ARG:HG3	1.95	0.67
1:N:145:MET:HE1	1:N:250:LEU:O	1.94	0.66
3:C:183:PHE:HE2	3:P:183:PHE:CD1	2.09	0.65
5:E:155:GLY:C	5:E:156:TYR:CD1	2.74	0.65
1:A:252:HIS:CD2	1:A:325:VAL:HG22	2.33	0.64
3:C:15:ASN:ND2	14:C:505:CDL:OA9	2.32	0.63
5:E:157:TYR:CD1	5:E:164:HIS:CD2	2.87	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:501:HEM:HBC2	11:C:501:HEM:CMC	2.24	0.63
1:N:145:MET:HB2	1:N:252:HIS:HE1	1.60	0.63
3:P:153:ILE:CG2	3:P:154:PRO:HD2	2.29	0.63
4:D:165:TYR:O	4:D:168:VAL:HG13	1.99	0.62
4:Q:204:MET:HE2	13:R:201:PEE:H3	1.79	0.62
1:A:444:LEU:HB2	1:A:445:ARG:O	1.99	0.62
3:C:183:PHE:HE1	11:C:501:HEM:HBC1	1.62	0.61
5:E:81:ILE:HD13	5:E:87:MET:HE2	1.83	0.61
4:D:168:VAL:HG23	4:D:169:LEU:HG	1.83	0.61
8:H:43:ARG:O	8:H:47:ARG:HG2	2.02	0.60
1:A:64:PHE:CE2	1:A:86:LEU:HG	2.36	0.60
1:A:320:LEU:CG	1:A:415:PHE:CZ	2.83	0.60
5:E:155:GLY:C	5:E:156:TYR:CG	2.79	0.60
10:K:31:GLY:O	10:K:34:SER:HB3	2.02	0.60
3:C:183:PHE:HD1	11:C:501:HEM:HAC	1.63	0.60
7:G:1:GLY:C	7:G:2:ARG:CG	2.74	0.60
10:K:32:LEU:O	10:K:36:THR:C	2.45	0.60
5:E:155:GLY:O	5:E:156:TYR:CG	2.55	0.59
1:A:444:LEU:N	1:A:445:ARG:HA	2.17	0.59
5:E:157:TYR:CZ	5:E:162:GLY:HA2	2.39	0.58
1:N:145:MET:CB	1:N:252:HIS:ND1	2.67	0.58
2:O:229:GLY:O	2:O:230:LEU:HB2	2.02	0.58
1:N:252:HIS:CD2	1:N:325:VAL:HG13	2.39	0.57
3:P:183:PHE:CE2	11:P:402:HEM:HBC1	2.40	0.57
1:N:64:PHE:CE2	1:N:86:LEU:HG	2.40	0.56
1:A:444:LEU:CB	1:A:445:ARG:O	2.54	0.56
1:N:82:MET:CE	1:N:105:ASP:HB3	2.36	0.55
2:B:117:ASP:OD1	2:B:118:ILE:N	2.40	0.55
1:N:445:ARG:HB3	9:W:17:THR:OG1	2.07	0.54
3:C:22:PRO:HG3	7:G:2:ARG:O	2.07	0.54
5:E:157:TYR:HD1	5:E:164:HIS:CD2	2.25	0.54
3:P:182:HIS:O	3:P:186:PRO:HD2	2.08	0.54
5:E:157:TYR:CE1	5:E:162:GLY:HA2	2.43	0.53
2:O:111:CYS:HB3	2:O:119:LEU:HD22	1.89	0.53
11:C:502:HEM:HMC2	11:C:502:HEM:HBC2	1.91	0.53
5:E:153:PHE:HE2	5:E:172:ARG:HG3	1.73	0.53
3:C:153:ILE:HG23	3:C:154:PRO:HD2	1.91	0.53
1:A:257:VAL:CG2	1:A:415:PHE:CE1	2.88	0.52
2:O:109:VAL:HB	2:O:119:LEU:HD23	1.90	0.52
3:P:8:HIS:NE2	3:P:12:LYS:HE2	2.23	0.52
10:K:19:PRO:C	10:K:22:GLN:HG2	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:402:HEM:HBC2	11:P:402:HEM:CMC	2.33	0.52
1:A:320:LEU:CD2	1:A:415:PHE:CZ	2.92	0.51
10:K:19:PRO:HA	10:K:22:GLN:NE2	2.25	0.51
3:C:183:PHE:CE2	3:P:183:PHE:HB3	2.46	0.51
3:P:182:HIS:CD2	11:P:402:HEM:C4C	2.97	0.51
1:A:257:VAL:CG2	1:A:415:PHE:CD1	2.94	0.51
11:P:403:HEM:HMA1	12:P:404:MJM:C13	2.41	0.51
2:O:226:ILE:O	2:O:227:ARG:HG3	2.11	0.50
3:P:150:LEU:O	3:P:153:ILE:HG12	2.11	0.50
2:O:111:CYS:SG	2:O:119:LEU:HD22	2.51	0.50
5:E:153:PHE:HE2	5:E:172:ARG:CG	2.25	0.50
2:B:306:PRO:HA	5:I:52:ARG:HB3	1.93	0.50
5:R:54:VAL:HG22	13:R:201:PEE:H17	1.94	0.49
10:K:19:PRO:HA	10:K:22:GLN:HG2	1.94	0.49
5:I:51:CYS:SG	5:I:52:ARG:N	2.76	0.49
3:P:277:ALA:HB1	3:P:294:LEU:HD12	1.94	0.49
3:C:184:ILE:HB	3:P:183:PHE:HE1	1.77	0.49
5:E:153:PHE:CE2	5:E:172:ARG:CG	2.94	0.49
5:E:37:TYR:CE1	13:E:502:PEE:H9	2.47	0.48
3:C:277:ALA:HB1	3:C:294:LEU:HD12	1.95	0.48
4:D:153:PHE:CD1	4:D:154:PRO:HD2	2.48	0.48
11:P:403:HEM:HHA	11:P:403:HEM:HBD1	1.95	0.48
10:K:31:GLY:O	10:K:34:SER:N	2.47	0.47
1:A:257:VAL:HG21	1:A:415:PHE:CD1	2.49	0.47
2:O:252:LEU:HD11	5:V:49:VAL:CG1	2.44	0.47
5:E:155:GLY:O	5:E:156:TYR:CD2	2.68	0.47
13:D:502:PEE:C1	13:D:502:PEE:O2	2.42	0.47
10:K:34:SER:O	5:R:52:LYS:HD2	2.15	0.47
5:E:76:ILE:HG22	5:E:194:ILE:HG12	1.97	0.47
5:E:86:ASN:OD1	5:E:156:TYR:HE2	1.98	0.47
4:Q:3:LEU:H	4:Q:156:GLN:HE22	1.63	0.47
4:Q:153:PHE:CD1	4:Q:154:PRO:HD2	2.49	0.46
1:N:86:LEU:HD23	2:O:285:VAL:HG13	1.96	0.46
4:D:165:TYR:H	4:D:168:VAL:HG13	1.80	0.46
6:F:15:GLY:O	6:F:18:LYS:N	2.49	0.46
2:B:243:GLU:HA	2:B:424:MET:O	2.16	0.46
10:K:19:PRO:HA	10:K:22:GLN:CG	2.46	0.46
4:Q:161:ALA:O	4:Q:162:PRO:C	2.58	0.46
2:O:176:LEU:HD23	5:V:64:LEU:HD12	1.99	0.45
5:R:54:VAL:HG22	13:R:201:PEE:C13	2.45	0.45
13:D:502:PEE:O3	13:D:502:PEE:H13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:78:GLU:HA	8:U:47:ARG:NH2	2.32	0.45
7:T:3:GLN:O	7:T:7:LEU:HG	2.17	0.45
3:C:184:ILE:HB	3:P:183:PHE:CE1	2.52	0.45
1:N:145:MET:HE2	1:N:252:HIS:CG	2.51	0.45
3:P:197:LEU:HD21	11:P:403:HEM:CMA	2.47	0.45
3:C:183:PHE:CD1	11:C:501:HEM:HAC	2.48	0.45
6:F:15:GLY:O	6:F:19:TRP:N	2.44	0.44
2:O:176:LEU:HD23	5:V:64:LEU:CD1	2.48	0.44
3:P:97:HIS:CD2	11:P:403:HEM:C1C	3.05	0.44
4:D:43:MET:HE1	4:D:189:PHE:HE2	1.82	0.44
10:K:30:VAL:O	10:K:33:VAL:HB	2.17	0.44
4:D:161:ALA:HB1	4:D:162:PRO:HD2	1.98	0.44
4:Q:161:ALA:HB1	4:Q:162:PRO:HD2	1.99	0.44
11:C:501:HEM:HMC1	11:C:501:HEM:CBC	2.35	0.44
4:D:164:ILE:HA	4:D:168:VAL:HG11	1.99	0.44
3:C:206:ASN:HB3	11:C:502:HEM:O2D	2.17	0.44
4:D:200:HIS:NE2	13:D:502:PEE:O2P	2.40	0.44
8:U:43:ARG:O	8:U:47:ARG:HG3	2.18	0.44
14:P:406:CDL:H521	14:P:406:CDL:C73	2.48	0.44
1:A:415:PHE:O	1:A:441:MET:HE3	2.17	0.43
3:P:182:HIS:HE1	11:P:402:HEM:C1B	2.35	0.43
1:A:280:TYR:HB3	1:A:307:PHE:CE2	2.54	0.43
1:A:256:ALA:O	1:A:421:ALA:N	2.51	0.43
4:D:165:TYR:H	4:D:168:VAL:CG1	2.31	0.43
3:C:70:CYS:SG	3:C:80:ARG:HD3	2.59	0.43
1:N:145:MET:HE2	1:N:252:HIS:ND1	2.32	0.43
4:D:36:VAL:CG2	4:D:169:LEU:HD23	2.48	0.43
4:D:169:LEU:C	4:D:169:LEU:HD12	2.43	0.43
1:N:280:TYR:HB3	1:N:307:PHE:CE2	2.54	0.43
1:N:444:LEU:N	1:N:444:LEU:HD12	2.33	0.43
5:R:40:THR:HG21	13:R:202:PEE:O2P	2.19	0.42
3:P:83:HIS:HE1	11:P:402:HEM:C1C	2.37	0.42
3:P:132:VAL:HA	3:P:139:SER:HB2	2.02	0.42
1:A:257:VAL:HG22	1:A:415:PHE:CD1	2.54	0.42
3:C:132:VAL:HA	3:C:139:SER:HB2	2.02	0.42
3:P:70:CYS:SG	3:P:80:ARG:HD3	2.59	0.42
3:C:186:PRO:HG2	11:C:501:HEM:HMC3	2.02	0.42
5:E:157:TYR:OH	5:E:162:GLY:HA2	2.20	0.42
2:O:24:LEU:HD12	2:O:38:LEU:HB2	2.01	0.42
2:O:111:CYS:HB3	2:O:119:LEU:CD2	2.49	0.42
5:E:81:ILE:N	5:E:82:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:14:GLU:O	6:F:18:LYS:N	2.50	0.41
2:B:109:VAL:HB	2:B:119:LEU:HD12	2.02	0.41
2:O:181:TYR:CE2	2:O:182:ARG:HG2	2.55	0.41
3:P:97:HIS:HD2	11:P:403:HEM:C1C	2.38	0.41
2:O:157:ALA:HA	5:V:64:LEU:CD2	2.50	0.41
2:O:161:GLU:OE1	5:V:64:LEU:HD21	2.20	0.41
3:P:97:HIS:CD2	11:P:403:HEM:NC	2.88	0.41
3:P:197:LEU:HD21	11:P:403:HEM:HMA2	2.03	0.41
5:E:77:LYS:HE2	5:E:89:PHE:CZ	2.56	0.41
2:B:181:TYR:CE2	2:B:182:ARG:HG2	2.55	0.41
2:B:24:LEU:HD12	2:B:38:LEU:HB2	2.03	0.41
2:B:71:LEU:CD1	2:B:144:LEU:HB3	2.51	0.41
3:P:229:ILE:CD1	14:P:406:CDL:H722	2.51	0.41
2:O:111:CYS:CB	2:O:119:LEU:HD22	2.50	0.41
5:R:45:VAL:HG13	9:W:28:ALA:HA	2.03	0.41
5:E:99:ARG:HD2	5:E:156:TYR:OH	2.20	0.40
2:O:71:LEU:CD1	2:O:144:LEU:HB3	2.52	0.40
3:C:183:PHE:O	3:C:183:PHE:CG	2.75	0.40
3:C:198:LEU:HD22	3:P:10:LEU:CD1	2.51	0.40
5:E:45:VAL:HG13	9:J:28:ALA:HA	2.02	0.40
1:A:252:HIS:HD2	1:A:325:VAL:HG22	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	442/444 (100%)	422 (96%)	20 (4%)	0	100	100
1	N	442/444 (100%)	417 (94%)	25 (6%)	0	100	100
2	B	421/423 (100%)	396 (94%)	25 (6%)	0	100	100
2	O	421/423 (100%)	393 (93%)	27 (6%)	1 (0%)	43	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	370/372 (100%)	356 (96%)	14 (4%)	0	100	100
3	P	370/372 (100%)	356 (96%)	14 (4%)	0	100	100
4	D	238/240 (99%)	227 (95%)	11 (5%)	0	100	100
4	Q	238/240 (99%)	228 (96%)	10 (4%)	0	100	100
5	E	194/274 (71%)	182 (94%)	12 (6%)	0	100	100
5	I	28/274 (10%)	24 (86%)	4 (14%)	0	100	100
5	R	70/274 (26%)	70 (100%)	0	0	100	100
5	V	28/274 (10%)	26 (93%)	2 (7%)	0	100	100
6	F	97/111 (87%)	95 (98%)	2 (2%)	0	100	100
6	S	97/111 (87%)	96 (99%)	1 (1%)	0	100	100
7	G	72/82 (88%)	66 (92%)	6 (8%)	0	100	100
7	T	78/82 (95%)	71 (91%)	7 (9%)	0	100	100
8	H	64/91 (70%)	63 (98%)	1 (2%)	0	100	100
8	U	66/91 (72%)	66 (100%)	0	0	100	100
9	J	57/64 (89%)	54 (95%)	3 (5%)	0	100	100
9	W	57/64 (89%)	54 (95%)	3 (5%)	0	100	100
10	K	20/22 (91%)	19 (95%)	1 (5%)	0	100	100
10	X	20/22 (91%)	20 (100%)	0	0	100	100
All	All	3890/4794 (81%)	3701 (95%)	188 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	O	231	GLY

5.3.2 Protein sidechains [i](#)

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	368/368 (100%)	364 (99%)	4 (1%)	65	74
1	N	368/368 (100%)	364 (99%)	4 (1%)	65	74
2	B	332/332 (100%)	331 (100%)	1 (0%)	86	83
2	O	332/332 (100%)	331 (100%)	1 (0%)	86	83
3	C	320/320 (100%)	319 (100%)	1 (0%)	86	83
3	P	320/320 (100%)	319 (100%)	1 (0%)	86	83
4	D	205/205 (100%)	204 (100%)	1 (0%)	81	80
4	Q	205/205 (100%)	203 (99%)	2 (1%)	68	75
5	E	168/228 (74%)	166 (99%)	2 (1%)	63	73
5	I	24/228 (10%)	24 (100%)	0	100	100
5	R	62/228 (27%)	62 (100%)	0	100	100
5	V	24/228 (10%)	24 (100%)	0	100	100
6	F	91/99 (92%)	91 (100%)	0	100	100
6	S	91/99 (92%)	91 (100%)	0	100	100
7	G	66/72 (92%)	65 (98%)	1 (2%)	57	71
7	T	71/72 (99%)	70 (99%)	1 (1%)	59	71
8	H	63/85 (74%)	63 (100%)	0	100	100
8	U	65/85 (76%)	65 (100%)	0	100	100
9	J	50/54 (93%)	50 (100%)	0	100	100
9	W	49/54 (91%)	49 (100%)	0	100	100
10	K	15/15 (100%)	15 (100%)	0	100	100
10	X	15/15 (100%)	15 (100%)	0	100	100
All	All	3304/4012 (82%)	3285 (99%)	19 (1%)	78	79

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	A	58	PHE
1	A	239	SER
1	A	443	TRP
2	B	209	LEU
3	C	282	ARG
4	D	36	VAL
5	E	62	MET

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Mol	Chain	Res	Type
5	E	156	TYR
7	G	45	ILE
1	N	11	VAL
1	N	58	PHE
1	N	239	SER
1	N	443	TRP
2	O	209	LEU
3	P	282	ARG
4	Q	36	VAL
4	Q	214	LEU
7	T	45	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	118	GLN
1	A	165	GLN
1	A	213	GLN
1	A	215	HIS
1	A	264	HIS
1	A	308	GLN
1	A	311	ASN
2	B	104	ASN
2	B	222	GLN
2	B	313	ASN
3	C	16	ASN
4	D	31	GLN
4	D	105	ASN
4	D	106	ASN
5	E	108	GLN
5	E	116	GLN
5	E	164	HIS
6	F	38	HIS
6	F	79	GLN
7	G	12	HIS
9	J	57	HIS
10	K	16	ASN
1	N	21	ASN
1	N	87	ASN
1	N	118	GLN
1	N	136	GLN

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Mol	Chain	Res	Type
1	N	213	GLN
1	N	215	HIS
1	N	264	HIS
1	N	311	ASN
1	N	328	HIS
1	N	418	GLN
2	O	104	ASN
2	O	222	GLN
2	O	313	ASN
2	O	343	GLN
4	Q	31	GLN
4	Q	106	ASN
4	Q	225	HIS
5	R	57	GLN
6	S	38	HIS
6	S	79	GLN
7	T	12	HIS
9	W	57	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](#)

21 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
15	HEC	D	501	4	46,50,50	2.55	23 (50%)	58,82,82	2.11	21 (36%)
14	CDL	C	506	-	36,36,99	1.38	4 (11%)	42,48,111	1.43	4 (9%)
13	PEE	D	502	-	41,41,50	4.27	7 (17%)	44,46,55	3.23	9 (20%)
15	HEC	Q	501	4	46,50,50	2.52	22 (47%)	58,82,82	2.15	26 (44%)
13	PEE	R	201	-	33,33,50	1.34	3 (9%)	36,38,55	1.26	5 (13%)
13	PEE	E	502	-	28,28,50	1.17	2 (7%)	31,33,55	1.15	3 (9%)
14	CDL	P	407	-	37,37,99	1.37	4 (10%)	43,49,111	1.27	2 (4%)
14	CDL	P	406	-	45,45,99	1.14	3 (6%)	50,56,111	1.48	7 (14%)
16	FES	E	501	5	0,4,4	-	-	-	-	-
13	PEE	R	202	-	23,23,50	1.24	2 (8%)	26,28,55	1.07	2 (7%)
11	HEM	P	402	3	50,50,50	1.71	7 (14%)	67,82,82	1.49	9 (13%)
13	PEE	C	504	-	27,27,50	1.17	2 (7%)	29,31,55	0.57	0
11	HEM	C	502	3	50,50,50	1.64	8 (16%)	67,82,82	1.35	7 (10%)
14	CDL	D	503	-	42,42,99	1.02	2 (4%)	45,51,111	1.01	2 (4%)
11	HEM	P	403	3	50,50,50	1.64	8 (16%)	67,82,82	1.48	10 (14%)
14	CDL	P	401	-	41,41,99	1.01	2 (4%)	45,50,111	1.20	3 (6%)
14	CDL	C	505	-	41,41,99	1.50	4 (9%)	47,53,111	1.60	6 (12%)
12	MJM	P	404	-	27,28,28	1.34	1 (3%)	28,39,39	1.31	3 (10%)
13	PEE	P	405	-	37,37,50	1.23	4 (10%)	40,42,55	0.68	1 (2%)
11	HEM	C	501	3	50,50,50	1.62	7 (14%)	67,82,82	1.43	11 (16%)
12	MJM	C	503	-	27,28,28	1.32	1 (3%)	28,39,39	1.05	2 (7%)

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
15	HEC	D	501	4	-	4/14/54/54	-
14	CDL	C	506	-	-	22/44/44/110	-
13	PEE	D	502	-	1/1/4/8	17/45/45/54	-
15	HEC	Q	501	4	-	4/14/54/54	-
13	PEE	R	201	-	1/1/4/8	15/37/37/54	-
13	PEE	E	502	-	1/1/4/8	12/32/32/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CDL	P	407	-	-	20/45/45/110	-
14	CDL	P	406	-	-	24/55/55/110	-
16	FES	E	501	5	-	-	0/1/1/1
13	PEE	R	202	-	1/1/4/8	7/27/27/54	-
11	HEM	P	402	3	-	5/14/54/54	-
13	PEE	C	504	-	-	9/30/30/54	-
11	HEM	C	502	3	-	4/14/54/54	-
14	CDL	D	503	-	-	17/48/48/110	-
11	HEM	P	403	3	-	4/14/54/54	-
14	CDL	P	401	-	-	21/48/48/110	-
14	CDL	C	505	-	-	28/49/49/110	-
12	MJM	P	404	-	1/1/5/5	0/8/35/35	0/4/4/4
13	PEE	P	405	-	-	11/41/41/54	-
12	MJM	C	503	-	1/1/5/5	0/8/35/35	0/4/4/4
11	HEM	C	501	3	-	5/14/54/54	-

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	502	PEE	O2-C2	-20.66	0.97	1.46
13	D	502	PEE	C1-C2	15.85	2.00	1.50
11	C	501	HEM	FE-NB	5.50	2.11	1.94
11	C	502	HEM	FE-NB	5.37	2.11	1.94
14	C	506	CDL	OB6-CB5	5.22	1.46	1.35
12	P	404	MJM	C5-N10	5.13	1.36	1.28
14	C	505	CDL	OA6-CA5	5.12	1.46	1.35
15	D	501	HEC	CAC-C3C	5.03	1.51	1.35
11	P	402	HEM	FE-NB	5.00	2.10	1.94
15	Q	501	HEC	CAC-C3C	5.00	1.51	1.35
12	C	503	MJM	C5-N10	4.96	1.36	1.28
14	P	407	CDL	OB6-CB5	4.91	1.46	1.35
11	P	403	HEM	FE-NB	4.86	2.09	1.94
14	C	505	CDL	OA8-CA7	4.75	1.47	1.33
11	P	402	HEM	FE-NC	4.65	2.10	1.95
11	C	502	HEM	FE-NC	4.58	2.10	1.95
15	Q	501	HEC	CHD-C4C	4.50	1.47	1.38
13	R	201	PEE	O3-C30	4.50	1.46	1.33
15	D	501	HEC	CHD-C4C	4.45	1.47	1.38
14	C	505	CDL	OB6-CB5	4.41	1.45	1.35
11	C	501	HEM	FE-NC	4.37	2.09	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	P	401	CDL	OB8-CB7	4.36	1.46	1.33
11	P	402	HEM	C1B-NB	-4.35	1.32	1.40
15	D	501	HEC	CAB-C3B	4.30	1.49	1.35
14	P	406	CDL	OA8-CA7	4.26	1.45	1.33
14	P	407	CDL	OA6-CA5	4.23	1.46	1.34
14	D	503	CDL	OB6-CB5	4.18	1.46	1.34
11	P	403	HEM	FE-NC	4.16	2.08	1.95
15	D	501	HEC	C2A-C3A	4.14	1.45	1.36
14	D	503	CDL	OB8-CB7	4.12	1.45	1.33
15	D	501	HEC	CHC-C4B	4.04	1.46	1.38
13	D	502	PEE	O3-C30	4.04	1.45	1.33
11	C	502	HEM	C1B-NB	-4.03	1.33	1.40
13	E	502	PEE	O3-C30	4.02	1.45	1.33
13	R	201	PEE	O2-C10	4.02	1.45	1.34
15	D	501	HEC	CHA-C1A	3.99	1.46	1.38
11	P	403	HEM	C1B-NB	-3.93	1.33	1.40
15	D	501	HEC	CHB-C4A	3.91	1.46	1.38
15	Q	501	HEC	CAB-C3B	3.91	1.47	1.35
13	R	202	PEE	O2-C10	3.89	1.45	1.34
14	P	401	CDL	OB6-CB5	3.86	1.45	1.34
15	D	501	HEC	C4B-NB	-3.85	1.32	1.39
15	Q	501	HEC	C1D-ND	-3.79	1.32	1.39
14	P	406	CDL	OA6-CA5	3.79	1.45	1.34
15	Q	501	HEC	CHC-C4B	3.78	1.45	1.38
13	D	502	PEE	C39-C38	3.77	1.53	1.31
13	R	202	PEE	O3-C30	3.76	1.44	1.33
15	Q	501	HEC	C4B-NB	-3.76	1.32	1.39
13	E	502	PEE	O2-C10	3.75	1.44	1.34
14	P	406	CDL	OB6-CB5	3.74	1.44	1.34
15	Q	501	HEC	C4A-NA	-3.70	1.32	1.39
13	D	502	PEE	C19-C18	3.69	1.52	1.29
13	D	502	PEE	O2-C10	3.68	1.44	1.34
15	Q	501	HEC	C2A-C3A	3.66	1.44	1.36
13	R	201	PEE	C19-C18	3.66	1.52	1.29
14	C	506	CDL	OA6-CA5	3.62	1.44	1.34
15	Q	501	HEC	CHA-C1A	3.60	1.45	1.38
15	Q	501	HEC	C1B-NB	-3.56	1.32	1.39
15	Q	501	HEC	CHB-C4A	3.55	1.45	1.38
11	C	501	HEM	C1B-NB	-3.55	1.34	1.40
15	D	501	HEC	CHD-C1D	3.52	1.47	1.39
15	D	501	HEC	C1C-NC	-3.48	1.33	1.39
15	Q	501	HEC	C1A-NA	-3.40	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	D	501	HEC	C1A-NA	-3.38	1.33	1.39
15	Q	501	HEC	C4C-NC	-3.30	1.33	1.39
11	P	403	HEM	C4D-ND	-3.30	1.34	1.40
15	D	501	HEC	C4D-ND	-3.23	1.33	1.39
15	Q	501	HEC	C1C-NC	-3.23	1.33	1.39
15	D	501	HEC	CHB-C1B	3.23	1.46	1.39
11	P	402	HEM	C4D-ND	-3.21	1.34	1.40
15	D	501	HEC	CHA-C4D	3.20	1.46	1.39
11	P	402	HEM	C4B-NB	-3.18	1.32	1.38
11	C	501	HEM	C1C-C2C	-3.15	1.39	1.45
13	C	504	PEE	O3-C30	3.14	1.42	1.33
15	Q	501	HEC	CHB-C1B	3.11	1.46	1.39
15	Q	501	HEC	CHD-C1D	3.10	1.46	1.39
13	P	405	PEE	P-O1P	3.05	1.61	1.50
15	D	501	HEC	C1D-ND	-2.99	1.34	1.39
13	P	405	PEE	O3-C30	2.97	1.42	1.33
15	D	501	HEC	C1B-NB	-2.97	1.34	1.39
13	P	405	PEE	O2-C10	2.93	1.42	1.34
11	P	402	HEM	C1C-C2C	-2.89	1.39	1.45
15	D	501	HEC	C3C-C4C	2.88	1.51	1.46
15	Q	501	HEC	CHC-C1C	2.84	1.45	1.39
15	Q	501	HEC	CHA-C4D	2.83	1.45	1.39
11	C	501	HEM	C4B-NB	-2.81	1.33	1.38
15	Q	501	HEC	C4D-ND	-2.78	1.34	1.39
11	P	403	HEM	C4B-NB	-2.76	1.33	1.38
15	Q	501	HEC	C3C-C4C	2.74	1.50	1.46
15	D	501	HEC	C4A-NA	-2.71	1.34	1.39
14	P	407	CDL	OB8-CB7	2.71	1.46	1.33
15	D	501	HEC	C4C-NC	-2.70	1.34	1.39
11	P	403	HEM	C1C-C2C	-2.70	1.40	1.45
15	D	501	HEC	CHC-C1C	2.70	1.45	1.39
15	D	501	HEC	C3D-C2D	2.69	1.45	1.38
15	Q	501	HEC	C3D-C2D	2.69	1.45	1.38
13	P	405	PEE	C22-C21	-2.68	1.35	1.51
11	C	502	HEM	C4D-ND	-2.66	1.35	1.40
14	C	506	CDL	OA8-CA7	2.61	1.45	1.33
13	C	504	PEE	P-O1P	2.56	1.59	1.50
11	C	501	HEM	C4D-ND	-2.54	1.35	1.40
14	P	407	CDL	OA8-CA7	2.53	1.45	1.33
14	C	506	CDL	OB8-CB7	2.52	1.45	1.33
14	C	505	CDL	OB8-CB7	2.49	1.45	1.33
11	C	502	HEM	C3B-C4B	2.46	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	502	HEM	C4B-NB	-2.22	1.34	1.38
13	D	502	PEE	C3-C2	-2.19	1.44	1.50
11	P	402	HEM	C4D-C3D	2.16	1.48	1.45
11	C	501	HEM	C3B-C4B	2.16	1.49	1.44
11	P	403	HEM	O2D-CGD	-2.12	1.23	1.30
15	D	501	HEC	C1D-C2D	2.12	1.48	1.43
11	C	502	HEM	C1D-ND	-2.10	1.34	1.38
15	D	501	HEC	C1C-C2C	2.10	1.48	1.43
15	Q	501	HEC	C1D-C2D	2.02	1.47	1.43
11	C	502	HEM	C1C-C2C	-2.01	1.41	1.45
11	P	403	HEM	C1D-ND	-2.01	1.34	1.38

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	502	PEE	O2-C2-C3	15.51	163.99	108.34
13	D	502	PEE	O3-C3-C2	-8.59	83.62	108.40
13	D	502	PEE	C3-C2-C1	-8.38	92.24	111.78
14	C	505	CDL	CB4-OB6-CB5	-5.87	107.47	117.85
14	C	505	CDL	OB6-CB5-C51	5.58	121.03	111.09
14	C	506	CDL	OB6-CB5-C51	5.39	120.71	111.09
15	D	501	HEC	C2A-C1A-NA	5.08	115.22	110.32
14	P	401	CDL	OB6-CB5-C51	5.05	122.40	111.48
13	D	502	PEE	O2-C10-C11	4.99	122.28	111.48
15	Q	501	HEC	C2A-C1A-NA	4.91	115.06	110.32
14	P	407	CDL	OB6-CB5-C51	4.83	119.69	111.09
14	P	406	CDL	CB4-OB6-CB5	-4.74	106.46	117.80
15	Q	501	HEC	C3D-C4D-ND	4.70	115.37	110.15
14	P	406	CDL	OB6-CB5-C51	4.67	121.58	111.48
15	D	501	HEC	C3D-C4D-ND	4.59	115.24	110.15
15	D	501	HEC	C2C-C1C-NC	4.58	117.48	110.14
11	P	402	HEM	CHC-C4B-NB	4.54	129.30	124.42
11	P	403	HEM	C1B-NB-C4B	4.45	110.48	105.21
11	P	402	HEM	CHD-C1D-ND	4.32	129.07	124.42
12	P	404	MJM	C11-C9-N10	4.25	118.80	112.45
13	R	201	PEE	O2-C10-C11	4.19	120.55	111.48
11	P	403	HEM	CHD-C1D-ND	4.13	128.87	124.42
11	P	403	HEM	CHC-C4B-NB	4.03	128.76	124.42
15	Q	501	HEC	C2C-C1C-NC	3.96	116.49	110.14
11	P	402	HEM	C1B-NB-C4B	3.95	109.88	105.21
14	D	503	CDL	OB6-CB5-C51	3.93	119.99	111.48
11	C	501	HEM	CHC-C4B-NB	3.86	128.57	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Q	501	HEC	C2B-C1B-NB	3.72	116.11	110.14
11	C	502	HEM	C1B-NB-C4B	3.70	109.59	105.21
15	Q	501	HEC	CMA-C3A-C4A	3.68	131.21	124.73
11	C	502	HEM	CHC-C4B-NB	3.61	128.31	124.42
11	C	502	HEM	CHD-C1D-ND	3.61	128.31	124.42
11	C	501	HEM	C1B-NB-C4B	3.55	109.42	105.21
11	P	402	HEM	CHD-C1D-C2D	-3.55	119.42	125.03
15	Q	501	HEC	C4A-C3A-C2A	-3.54	101.72	106.97
13	D	502	PEE	O2-C10-O4	-3.53	115.45	123.70
15	D	501	HEC	C2B-C1B-NB	3.52	115.79	110.14
12	C	503	MJM	C11-C9-N10	3.52	117.70	112.45
11	C	501	HEM	CMD-C2D-C1D	3.49	130.49	125.03
15	Q	501	HEC	CAA-CBA-CGA	-3.44	104.54	113.67
15	D	501	HEC	C4A-C3A-C2A	-3.44	101.87	106.97
13	E	502	PEE	O2-C10-C11	3.43	118.91	111.48
14	P	407	CDL	OA6-CA5-C11	3.43	118.91	111.48
11	C	501	HEM	CHD-C1D-ND	3.40	128.08	124.42
14	C	505	CDL	OA6-CA5-C11	3.39	117.14	111.09
11	P	403	HEM	C3B-C4B-NB	-3.39	107.03	109.47
15	D	501	HEC	CMA-C3A-C4A	3.37	130.66	124.73
15	Q	501	HEC	C3A-C4A-NA	3.35	115.83	109.64
15	D	501	HEC	CAA-CBA-CGA	-3.27	104.98	113.67
15	D	501	HEC	C3A-C4A-NA	3.22	115.59	109.64
15	Q	501	HEC	C4D-C3D-C2D	-3.21	101.89	106.87
11	C	502	HEM	CHD-C1D-C2D	-3.19	119.99	125.03
11	P	402	HEM	CMD-C2D-C1D	3.18	130.01	125.03
14	C	505	CDL	OB6-CB5-OB7	-3.10	117.01	122.99
14	P	406	CDL	OB6-CB5-OB7	-3.05	116.58	123.70
12	C	503	MJM	C5-N10-C9	3.04	123.85	118.61
11	C	502	HEM	C4B-C3B-C2B	-3.02	104.50	107.28
11	P	403	HEM	CHA-C4D-ND	2.98	128.05	124.37
15	D	501	HEC	C4D-C3D-C2D	-2.94	102.31	106.87
15	D	501	HEC	CMC-C2C-C1C	2.92	129.87	125.42
15	D	501	HEC	CMD-C2D-C1D	2.92	129.86	125.42
15	Q	501	HEC	CHA-C1A-C2A	-2.89	120.30	124.86
14	C	506	CDL	OA6-CA5-C11	2.89	121.53	110.93
14	P	401	CDL	OB6-CB5-OB7	-2.88	116.96	123.70
11	C	501	HEM	CHD-C1D-C2D	-2.84	120.55	125.03
14	P	406	CDL	OA8-CA7-C31	2.83	120.48	111.83
13	D	502	PEE	O3-C30-C31	2.77	120.29	111.83
12	P	404	MJM	C5-N10-C9	2.76	123.37	118.61
14	C	506	CDL	OA6-CA5-OA7	-2.76	117.25	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Q	501	HEC	C1D-C2D-C3D	-2.76	103.66	106.82
15	D	501	HEC	C1A-C2A-C3A	-2.72	103.53	107.11
15	D	501	HEC	CHC-C1C-C2C	-2.71	119.55	127.43
15	Q	501	HEC	CHC-C1C-C2C	-2.70	119.59	127.43
15	D	501	HEC	C1D-C2D-C3D	-2.70	103.73	106.82
15	Q	501	HEC	CHB-C1B-C2B	-2.68	119.65	127.43
15	Q	501	HEC	C2D-C1D-ND	2.67	114.43	110.14
15	D	501	HEC	CHA-C1A-C2A	-2.66	120.66	124.86
11	C	501	HEM	CAD-C3D-C4D	2.65	129.32	124.70
15	Q	501	HEC	C1A-C2A-C3A	-2.64	103.63	107.11
11	P	403	HEM	CHD-C1D-C2D	-2.64	120.86	125.03
15	Q	501	HEC	CMD-C2D-C1D	2.61	129.39	125.42
13	E	502	PEE	O3-C30-C31	2.61	119.78	111.83
13	R	201	PEE	C3-O3-C30	2.58	126.55	117.12
11	P	403	HEM	C4C-NC-C1C	2.55	109.98	105.82
15	Q	501	HEC	CBD-CAD-C3D	-2.54	105.50	112.53
13	R	202	PEE	O3-C30-C31	2.53	119.55	111.83
11	P	402	HEM	CAD-C3D-C4D	2.52	129.09	124.70
11	C	502	HEM	CHA-C4D-ND	2.50	127.46	124.37
15	D	501	HEC	CHB-C1B-C2B	-2.50	120.18	127.43
13	R	201	PEE	O2-C10-O4	-2.47	117.92	123.70
15	D	501	HEC	CHA-C4D-C3D	-2.46	119.92	125.30
11	C	502	HEM	CHA-C4D-C3D	-2.43	120.74	125.23
11	C	501	HEM	C4B-C3B-C2B	-2.42	105.05	107.28
15	Q	501	HEC	CMC-C2C-C1C	2.42	129.10	125.42
14	P	406	CDL	OA6-CA4-CA3	2.41	117.01	108.34
14	D	503	CDL	OB8-CB7-C71	2.40	119.14	111.83
14	P	406	CDL	OA6-CA5-C11	2.37	119.64	110.93
15	Q	501	HEC	CHA-C4D-C3D	-2.36	120.13	125.30
14	C	505	CDL	OA8-CA7-C31	2.36	119.03	111.83
13	R	201	PEE	O3-C30-C31	2.32	118.92	111.83
15	Q	501	HEC	CAD-C3D-C4D	2.29	129.41	124.94
14	P	401	CDL	CB6-OB8-CB7	2.27	125.43	117.12
15	Q	501	HEC	CMB-C2B-C3B	2.26	131.87	126.55
13	R	202	PEE	O3-C30-O5	-2.23	118.06	123.63
15	Q	501	HEC	CHB-C4A-C3A	-2.22	120.86	125.49
11	P	403	HEM	C4C-CHD-C1D	-2.22	121.29	126.02
11	P	402	HEM	CHA-C4D-ND	2.19	127.08	124.37
11	P	402	HEM	CHA-C4D-C3D	-2.19	121.19	125.23
14	P	406	CDL	OA8-CA7-OA9	-2.19	118.16	123.63
11	P	403	HEM	CHA-C4D-C3D	-2.18	121.20	125.23
14	C	506	CDL	CA6-OA8-CA7	2.18	122.46	117.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	D	501	HEC	CHB-C4A-C3A	-2.18	120.96	125.49
15	Q	501	HEC	CBB-CAB-C3B	-2.18	123.08	127.43
11	C	501	HEM	C4C-NC-C1C	2.18	109.37	105.82
15	Q	501	HEC	CAA-C2A-C1A	2.16	129.24	124.85
12	P	404	MJM	C20-O19-C15	2.13	123.65	118.78
15	D	501	HEC	CAA-C2A-C1A	2.13	129.18	124.85
13	P	405	PEE	C23-C22-C21	2.13	127.72	113.36
15	D	501	HEC	C2D-C1D-ND	2.11	113.53	110.14
13	D	502	PEE	C17-C18-C19	-2.10	111.35	126.65
13	R	201	PEE	C17-C18-C19	-2.10	111.36	126.65
11	P	402	HEM	O2D-CGD-CBD	2.08	120.58	114.00
11	C	501	HEM	O2D-CGD-CBD	2.08	120.57	114.00
13	D	502	PEE	C2-O2-C10	-2.07	112.84	117.80
15	D	501	HEC	CAD-C3D-C4D	2.06	128.97	124.94
15	Q	501	HEC	CHD-C1D-C2D	-2.05	121.48	127.43
15	Q	501	HEC	CBC-CAC-C3C	2.03	131.49	127.43
11	P	403	HEM	CHB-C1B-NB	2.02	126.86	124.37
11	C	501	HEM	CHC-C1C-NC	2.01	126.65	124.45
14	C	505	CDL	OA8-CA6-CA4	2.01	114.20	108.40
13	D	502	PEE	C40-C39-C38	-2.01	109.76	124.83
13	E	502	PEE	O2-C10-O4	-2.01	119.00	123.70
11	C	501	HEM	CHA-C4D-ND	2.01	126.85	124.37

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	C	503	MJM	C4
12	P	404	MJM	C4
13	D	502	PEE	C2
13	E	502	PEE	C2
13	R	201	PEE	C2
13	R	202	PEE	C2

All (229) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	C	504	PEE	C4-O4P-P-O1P
13	D	502	PEE	C11-C10-O2-C2
13	D	502	PEE	O2-C2-C3-O3
13	D	502	PEE	C4-O4P-P-O3P
13	D	502	PEE	C4-O4P-P-O2P
13	E	502	PEE	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
13	E	502	PEE	C4-O4P-P-O2P
13	E	502	PEE	C4-O4P-P-O1P
13	E	502	PEE	O4P-C4-C5-N
13	P	405	PEE	C4-O4P-P-O1P
13	R	201	PEE	C11-C10-O2-C2
13	R	201	PEE	O4P-C4-C5-N
13	R	202	PEE	O4P-C4-C5-N
14	C	505	CDL	CA2-OA2-PA1-OA3
14	C	505	CDL	CA2-OA2-PA1-OA5
14	C	505	CDL	CB2-OB2-PB2-OB3
14	C	505	CDL	CB2-OB2-PB2-OB4
14	C	505	CDL	CB2-OB2-PB2-OB5
14	C	505	CDL	C51-CB5-OB6-CB4
14	C	506	CDL	O1-C1-CB2-OB2
14	C	506	CDL	CA2-C1-CB2-OB2
14	C	506	CDL	CA3-OA5-PA1-OA2
14	C	506	CDL	CA3-OA5-PA1-OA3
14	C	506	CDL	CA3-OA5-PA1-OA4
14	C	506	CDL	OA7-CA5-OA6-CA4
14	C	506	CDL	C11-CA5-OA6-CA4
14	C	506	CDL	CB3-OB5-PB2-OB2
14	C	506	CDL	C51-CB5-OB6-CB4
14	D	503	CDL	CA2-OA2-PA1-OA3
14	D	503	CDL	CA2-OA2-PA1-OA5
14	D	503	CDL	CB3-OB5-PB2-OB2
14	D	503	CDL	CB3-OB5-PB2-OB4
14	P	401	CDL	CA2-OA2-PA1-OA5
14	P	401	CDL	CA3-OA5-PA1-OA3
14	P	401	CDL	CB2-OB2-PB2-OB3
14	P	401	CDL	CB2-OB2-PB2-OB4
14	P	401	CDL	CB2-OB2-PB2-OB5
14	P	401	CDL	CB3-OB5-PB2-OB2
14	P	401	CDL	CB3-OB5-PB2-OB3
14	P	401	CDL	OB7-CB5-OB6-CB4
14	P	401	CDL	C51-CB5-OB6-CB4
14	P	406	CDL	CA2-OA2-PA1-OA3
14	P	406	CDL	CA2-OA2-PA1-OA4
14	P	406	CDL	CA2-OA2-PA1-OA5
14	P	406	CDL	CA3-OA5-PA1-OA2
14	P	406	CDL	CA3-OA5-PA1-OA3
14	P	406	CDL	CA3-OA5-PA1-OA4
14	P	406	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
14	P	406	CDL	CB2-OB2-PB2-OB4
14	P	406	CDL	CB2-OB2-PB2-OB5
14	P	406	CDL	C51-CB5-OB6-CB4
14	P	407	CDL	CA3-OA5-PA1-OA2
14	P	407	CDL	CA3-OA5-PA1-OA3
14	P	407	CDL	CB3-OB5-PB2-OB2
14	P	407	CDL	CB3-OB5-PB2-OB3
14	C	505	CDL	C11-CA5-OA6-CA4
14	C	505	CDL	OB7-CB5-OB6-CB4
14	C	506	CDL	OB7-CB5-OB6-CB4
14	P	407	CDL	C51-CB5-OB6-CB4
14	P	407	CDL	C71-CB7-OB8-CB6
14	P	407	CDL	OB9-CB7-OB8-CB6
14	P	406	CDL	OA9-CA7-OA8-CA6
13	D	502	PEE	O4-C10-O2-C2
13	R	201	PEE	O4-C10-O2-C2
14	D	503	CDL	OB7-CB5-OB6-CB4
14	P	406	CDL	OA7-CA5-OA6-CA4
14	P	406	CDL	OB7-CB5-OB6-CB4
13	R	202	PEE	C31-C30-O3-C3
14	D	503	CDL	C51-CB5-OB6-CB4
14	C	505	CDL	OA7-CA5-OA6-CA4
14	P	407	CDL	OB7-CB5-OB6-CB4
14	C	505	CDL	OB9-CB7-OB8-CB6
14	C	506	CDL	C71-CB7-OB8-CB6
14	D	503	CDL	C71-CB7-OB8-CB6
14	P	406	CDL	C31-CA7-OA8-CA6
14	P	407	CDL	OA9-CA7-OA8-CA6
14	C	505	CDL	C71-CB7-OB8-CB6
14	P	407	CDL	C31-CA7-OA8-CA6
14	C	505	CDL	O1-C1-CA2-OA2
14	C	505	CDL	O1-C1-CB2-OB2
14	P	401	CDL	O1-C1-CB2-OB2
13	R	202	PEE	O5-C30-O3-C3
14	D	503	CDL	OB9-CB7-OB8-CB6
14	C	505	CDL	CB2-C1-CA2-OA2
14	C	505	CDL	CA2-C1-CB2-OB2
14	C	506	CDL	OB9-CB7-OB8-CB6
13	D	502	PEE	C10-C11-C12-C13
13	P	405	PEE	C10-C11-C12-C13
13	E	502	PEE	C10-C11-C12-C13
13	E	502	PEE	C31-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
13	R	201	PEE	C10-C11-C12-C13
13	R	201	PEE	C30-C31-C32-C33
14	P	407	CDL	C11-CA5-OA6-CA4
13	D	502	PEE	C16-C17-C18-C19
14	P	407	CDL	OA7-CA5-OA6-CA4
14	D	503	CDL	O1-C1-CB2-OB2
14	P	406	CDL	CA3-CA4-OA6-CA5
13	C	504	PEE	C12-C13-C14-C15
13	P	405	PEE	C12-C13-C14-C15
13	E	502	PEE	O5-C30-O3-C3
13	E	502	PEE	C11-C10-O2-C2
13	D	502	PEE	C13-C14-C15-C16
14	P	406	CDL	C31-C32-C33-C34
13	E	502	PEE	O4-C10-O2-C2
13	R	201	PEE	C13-C14-C15-C16
13	R	202	PEE	C11-C10-O2-C2
13	R	202	PEE	O4-C10-O2-C2
13	P	405	PEE	C19-C20-C21-C22
13	P	405	PEE	C33-C34-C35-C36
13	C	504	PEE	C10-C11-C12-C13
13	D	502	PEE	O3P-C1-C2-O2
14	P	401	CDL	C58-C59-C60-C61
14	D	503	CDL	C72-C73-C74-C75
13	R	201	PEE	C32-C33-C34-C35
14	P	401	CDL	C71-C72-C73-C74
13	D	502	PEE	C33-C34-C35-C36
14	C	506	CDL	OB5-CB3-CB4-CB6
14	P	406	CDL	OB5-CB3-CB4-CB6
14	C	505	CDL	CA3-CA4-CA6-OA8
14	D	503	CDL	CB3-CB4-CB6-OB8
13	R	202	PEE	C31-C32-C33-C34
13	D	502	PEE	C15-C16-C17-C18
13	D	502	PEE	C11-C12-C13-C14
13	P	405	PEE	C13-C14-C15-C16
13	C	504	PEE	C13-C14-C15-C16
13	P	405	PEE	C20-C21-C22-C23
14	P	407	CDL	OB5-CB3-CB4-OB6
13	D	502	PEE	C42-C43-C44-C45
14	C	505	CDL	C32-C33-C34-C35
13	E	502	PEE	C13-C14-C15-C16
14	P	401	CDL	C51-C52-C53-C54
14	P	406	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
14	C	505	CDL	OA5-CA3-CA4-CA6
14	C	506	CDL	OA5-CA3-CA4-CA6
13	E	502	PEE	C33-C34-C35-C36
14	P	407	CDL	CA3-CA4-CA6-OA8
14	C	505	CDL	OA5-CA3-CA4-OA6
14	C	506	CDL	OB5-CB3-CB4-OB6
14	D	503	CDL	OB6-CB4-CB6-OB8
13	D	502	PEE	C32-C33-C34-C35
14	P	401	CDL	CA2-C1-CB2-OB2
14	P	406	CDL	CA2-C1-CB2-OB2
13	R	201	PEE	O3P-C1-C2-C3
14	P	401	CDL	C1-CB2-OB2-PB2
13	R	201	PEE	O3P-C1-C2-O2
14	C	506	CDL	OA5-CA3-CA4-OA6
14	C	505	CDL	CB3-CB4-CB6-OB8
13	R	201	PEE	C5-C4-O4P-P
14	C	505	CDL	OA6-CA4-CA6-OA8
14	C	505	CDL	OB6-CB4-CB6-OB8
14	C	506	CDL	OB6-CB4-CB6-OB8
14	D	503	CDL	C75-C76-C77-C78
14	C	506	CDL	C31-CA7-OA8-CA6
14	P	406	CDL	O1-C1-CB2-OB2
13	P	405	PEE	C35-C36-C37-C38
14	P	401	CDL	C73-C74-C75-C76
14	C	505	CDL	OB5-CB3-CB4-CB6
14	P	407	CDL	OB5-CB3-CB4-CB6
14	P	406	CDL	OB5-CB3-CB4-OB6
14	P	407	CDL	OA5-CA3-CA4-OA6
13	C	504	PEE	O5-C30-C31-C32
14	P	407	CDL	OA6-CA4-CA6-OA8
14	C	505	CDL	C34-C35-C36-C37
14	P	406	CDL	C71-CB7-OB8-CB6
14	C	505	CDL	CA2-OA2-PA1-OA4
14	C	506	CDL	CB3-OB5-PB2-OB3
14	D	503	CDL	CA2-OA2-PA1-OA4
14	D	503	CDL	CA3-OA5-PA1-OA2
14	P	401	CDL	CA2-OA2-PA1-OA3
14	P	401	CDL	CB3-OB5-PB2-OB4
14	P	407	CDL	CA3-OA5-PA1-OA4
14	P	407	CDL	CB3-OB5-PB2-OB4
13	D	502	PEE	C3-C2-O2-C10
13	D	502	PEE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
14	C	506	CDL	OA6-CA4-CA6-OA8
14	P	401	CDL	CA3-OA5-PA1-OA4
13	C	504	PEE	O3-C30-C31-C32
13	R	201	PEE	C15-C16-C17-C18
14	D	503	CDL	C71-C72-C73-C74
14	D	503	CDL	CA2-C1-CB2-OB2
13	C	504	PEE	C16-C17-C18-C19
11	P	403	HEM	CAA-CBA-CGA-O1A
13	R	201	PEE	C3-C2-O2-C10
14	C	505	CDL	CA3-CA4-OA6-CA5
14	P	406	CDL	C52-C51-CB5-OB6
11	C	502	HEM	CAA-CBA-CGA-O2A
11	C	502	HEM	CAA-CBA-CGA-O1A
11	P	402	HEM	CAD-CBD-CGD-O1D
13	P	405	PEE	C16-C17-C18-C19
11	P	403	HEM	CAD-CBD-CGD-O2D
11	P	402	HEM	C3D-CAD-CBD-CGD
11	P	403	HEM	CAD-CBD-CGD-O1D
11	C	501	HEM	CAD-CBD-CGD-O1D
13	R	201	PEE	O3-C30-C31-C32
14	P	401	CDL	C59-C60-C61-C62
11	C	502	HEM	CAD-CBD-CGD-O2D
15	D	501	HEC	CAA-CBA-CGA-O2A
14	C	505	CDL	OB5-CB3-CB4-OB6
14	C	505	CDL	C32-C31-CA7-OA8
11	C	501	HEM	CAD-CBD-CGD-O2D
11	P	403	HEM	CAA-CBA-CGA-O2A
11	P	402	HEM	CAA-CBA-CGA-O2A
13	R	201	PEE	C16-C17-C18-C19
11	C	501	HEM	CAA-CBA-CGA-O2A
11	P	402	HEM	CAA-CBA-CGA-O1A
14	P	407	CDL	OA5-CA3-CA4-CA6
15	Q	501	HEC	CAA-CBA-CGA-O2A
13	R	202	PEE	C2-C1-O3P-P
11	C	501	HEM	CAA-CBA-CGA-O1A
11	P	402	HEM	CAD-CBD-CGD-O2D
14	C	506	CDL	OA9-CA7-OA8-CA6
11	C	502	HEM	CAD-CBD-CGD-O1D
14	P	401	CDL	C57-C58-C59-C60
13	C	504	PEE	O2-C10-C11-C12
15	D	501	HEC	CAA-CBA-CGA-O1A
14	C	506	CDL	CB3-CB4-CB6-OB8

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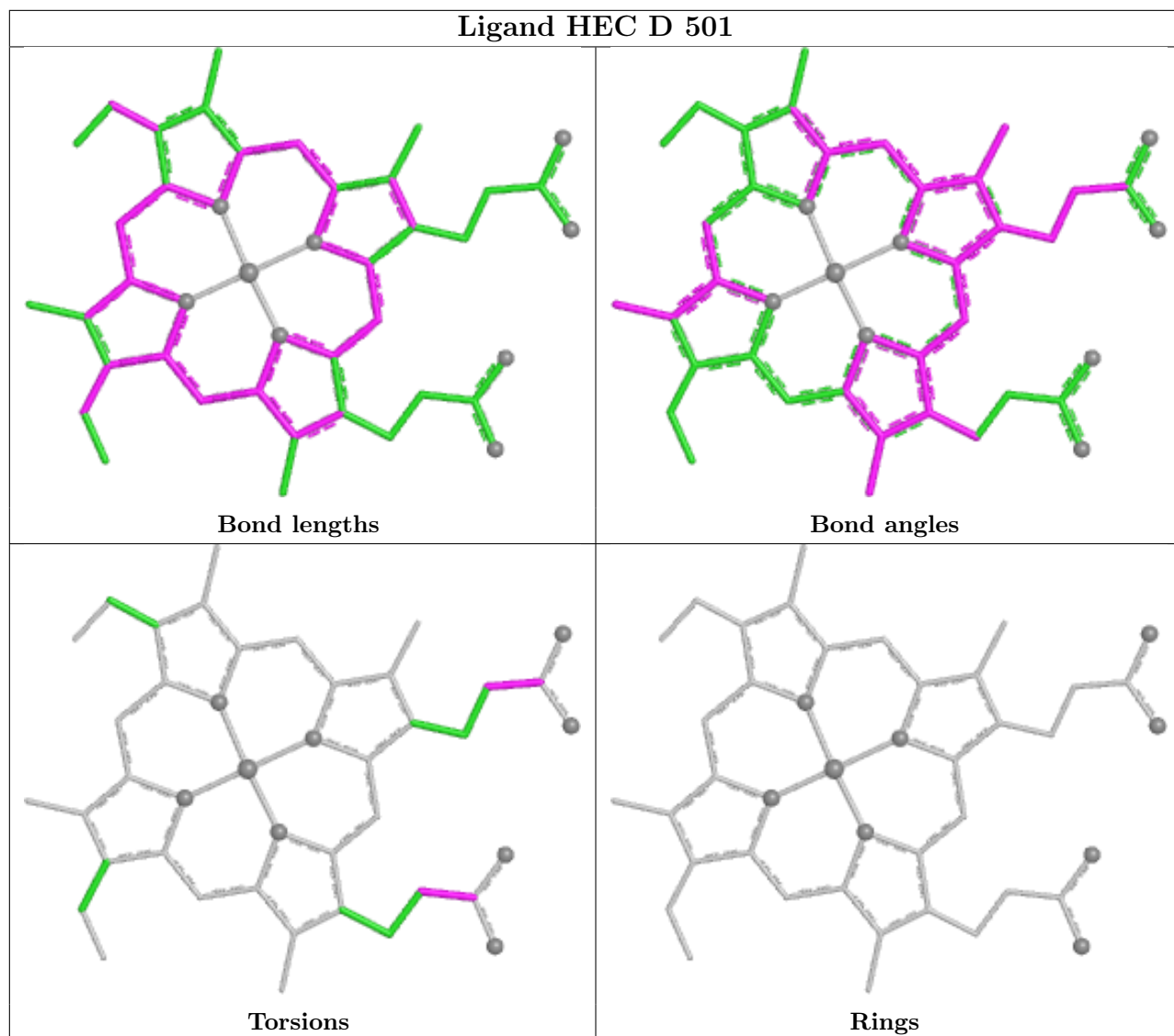
Mol	Chain	Res	Type	Atoms
11	C	501	HEM	C3D-CAD-CBD-CGD
13	E	502	PEE	C12-C13-C14-C15
15	Q	501	HEC	CAA-CBA-CGA-O1A
13	D	502	PEE	C38-C39-C40-C41
15	Q	501	HEC	CAD-CBD-CGD-O1D
15	D	501	HEC	CAD-CBD-CGD-O2D
15	D	501	HEC	CAD-CBD-CGD-O1D
13	P	405	PEE	O3-C30-C31-C32
13	R	201	PEE	C1-C2-O2-C10
14	P	406	CDL	C12-C11-CA5-OA6
15	Q	501	HEC	CAD-CBD-CGD-O2D
13	C	504	PEE	C17-C18-C19-C20
13	P	405	PEE	O5-C30-C31-C32

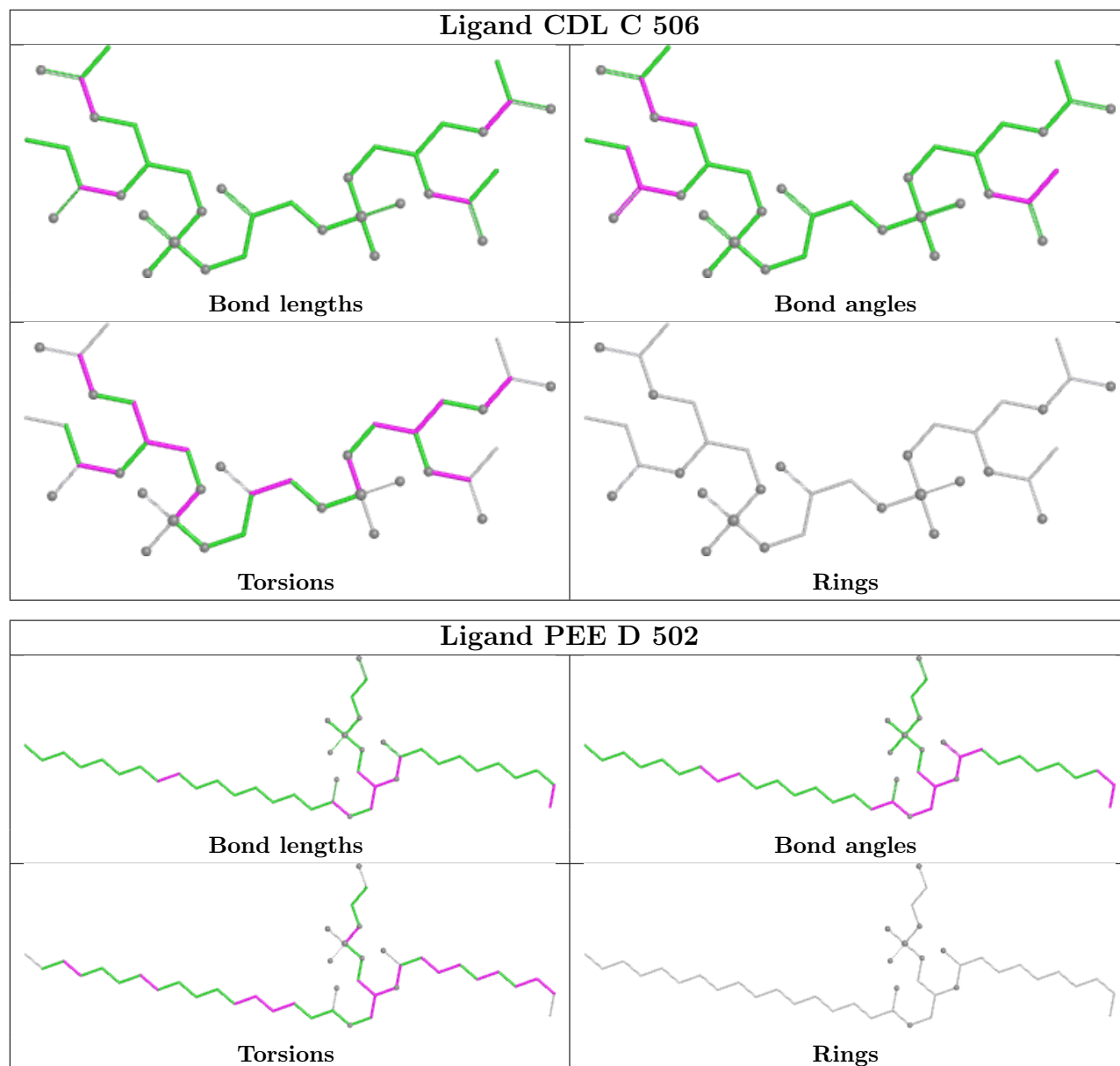
There are no ring outliers.

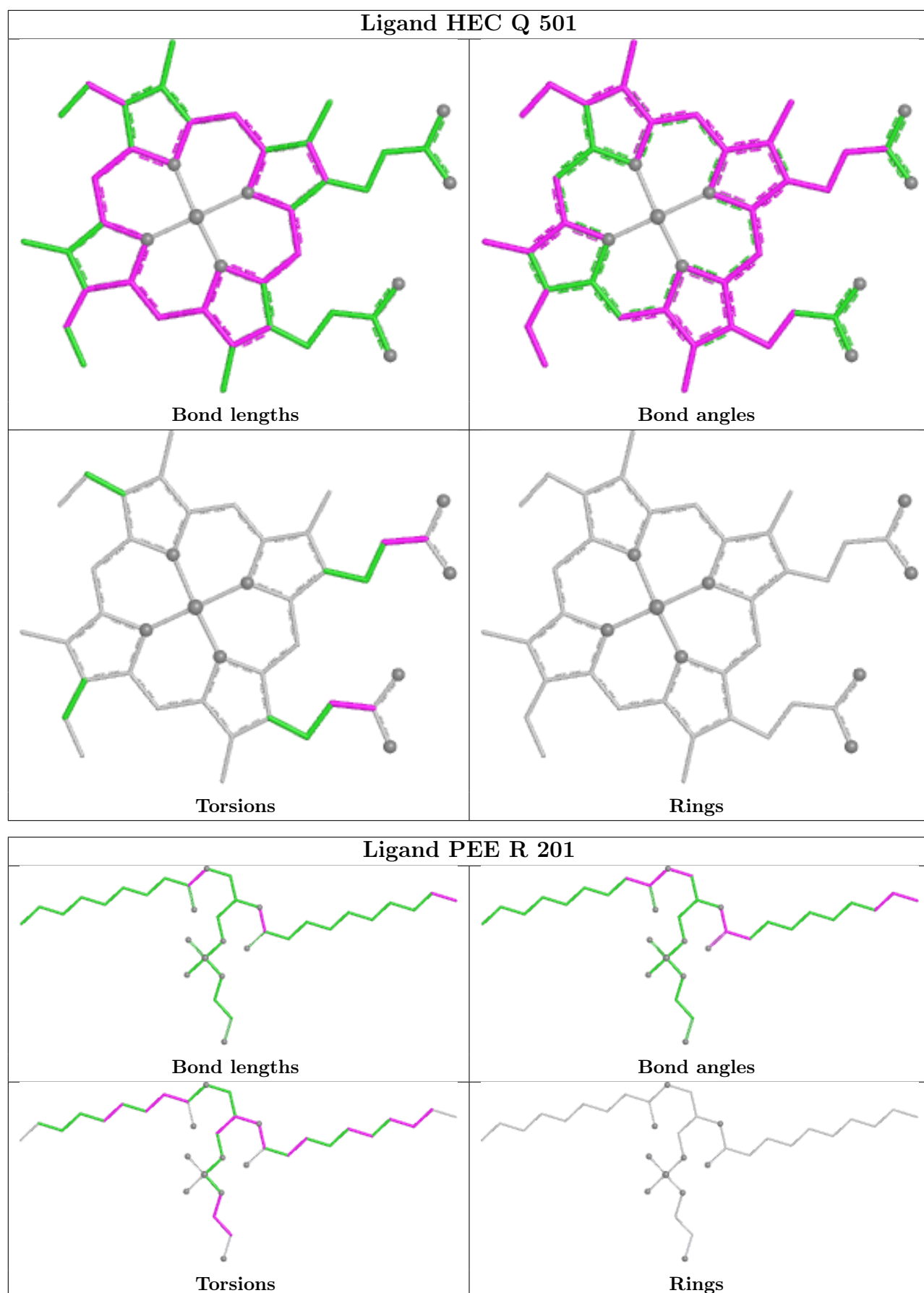
11 monomers are involved in 43 short contacts:

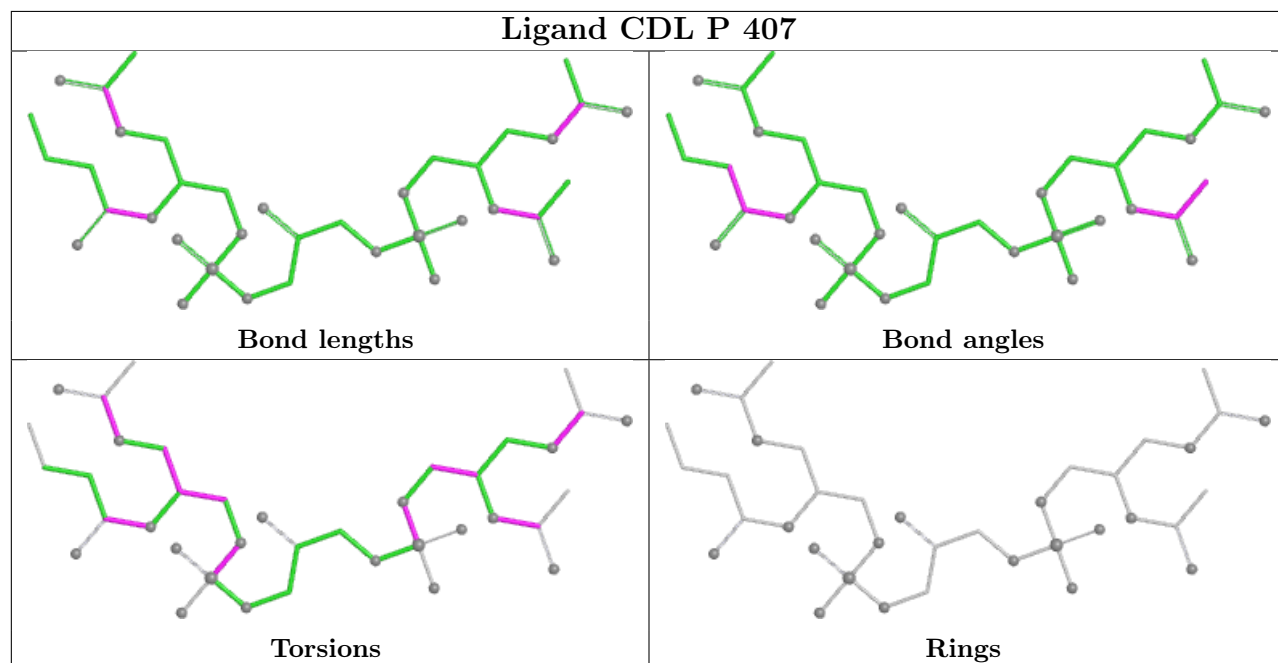
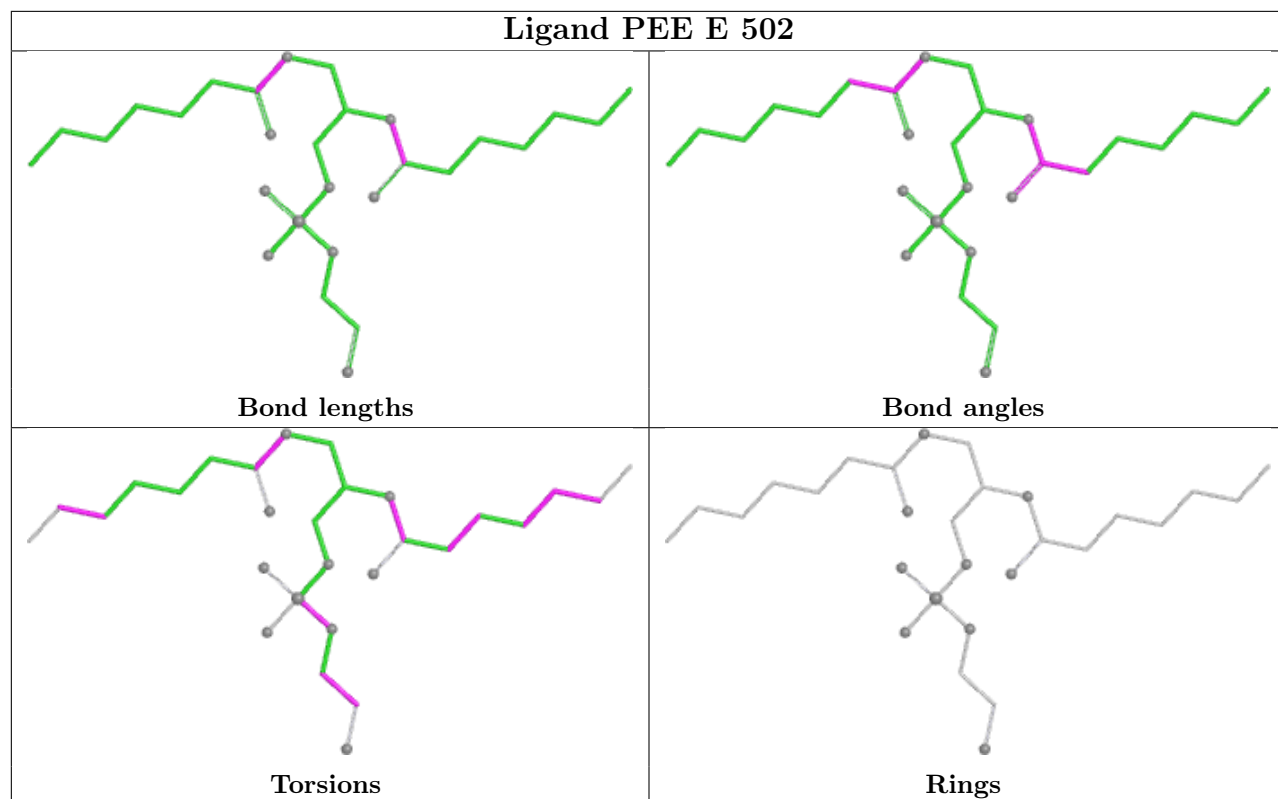
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	D	502	PEE	5	0
13	R	201	PEE	3	0
13	E	502	PEE	1	0
14	P	406	CDL	3	0
13	R	202	PEE	1	0
11	P	402	HEM	6	0
11	C	502	HEM	2	0
11	P	403	HEM	8	0
14	C	505	CDL	1	0
12	P	404	MJM	1	0
11	C	501	HEM	13	0

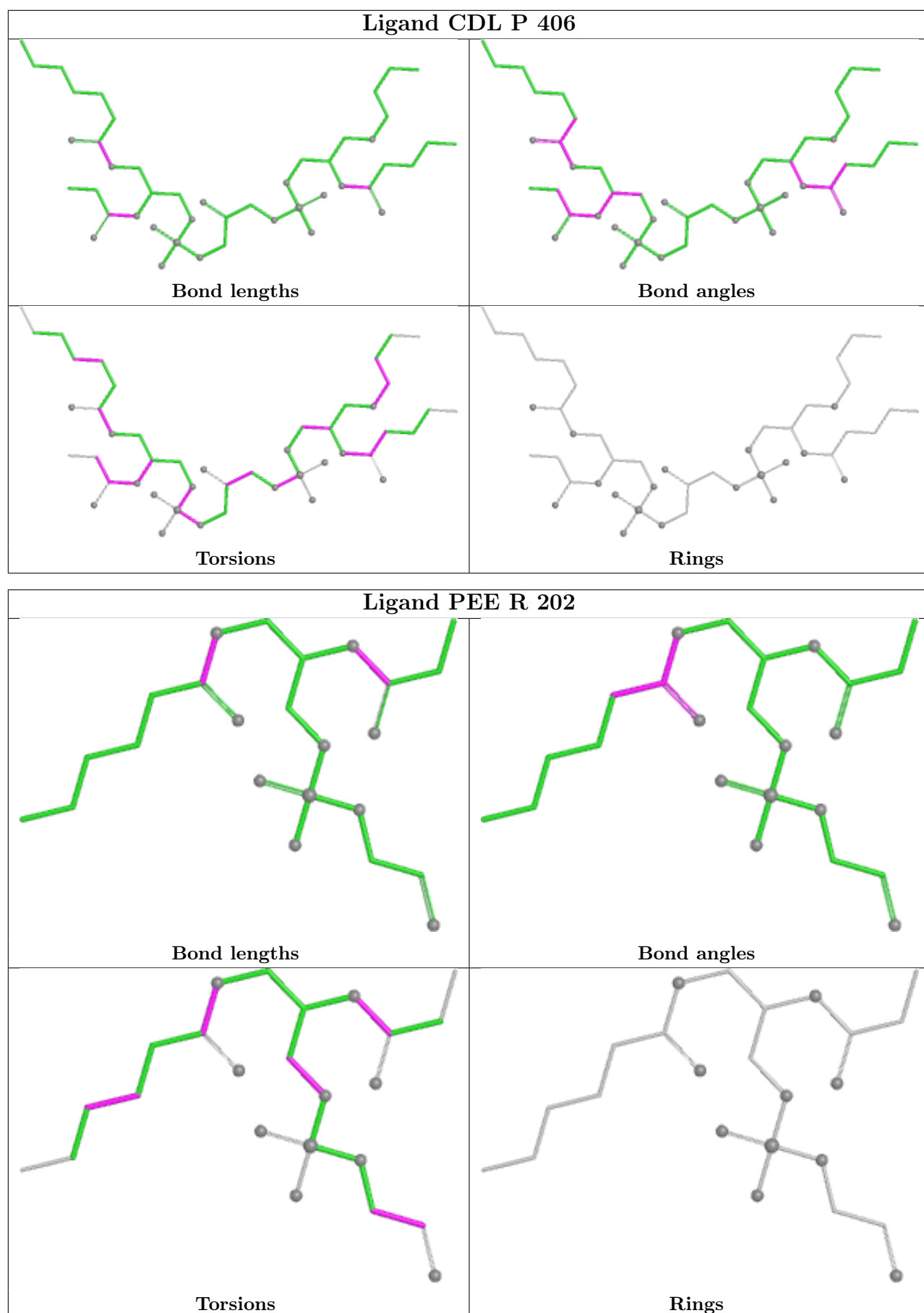
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

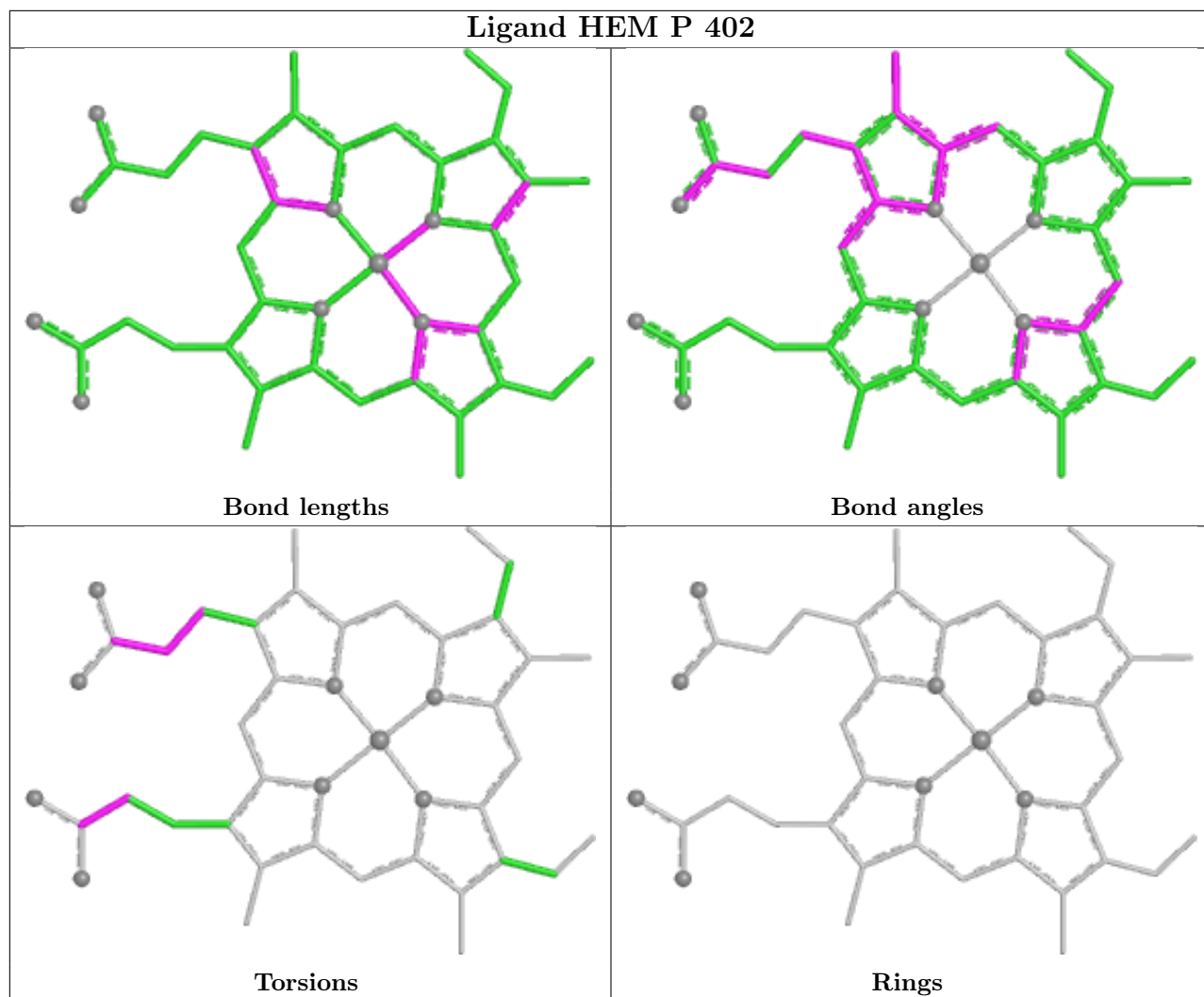


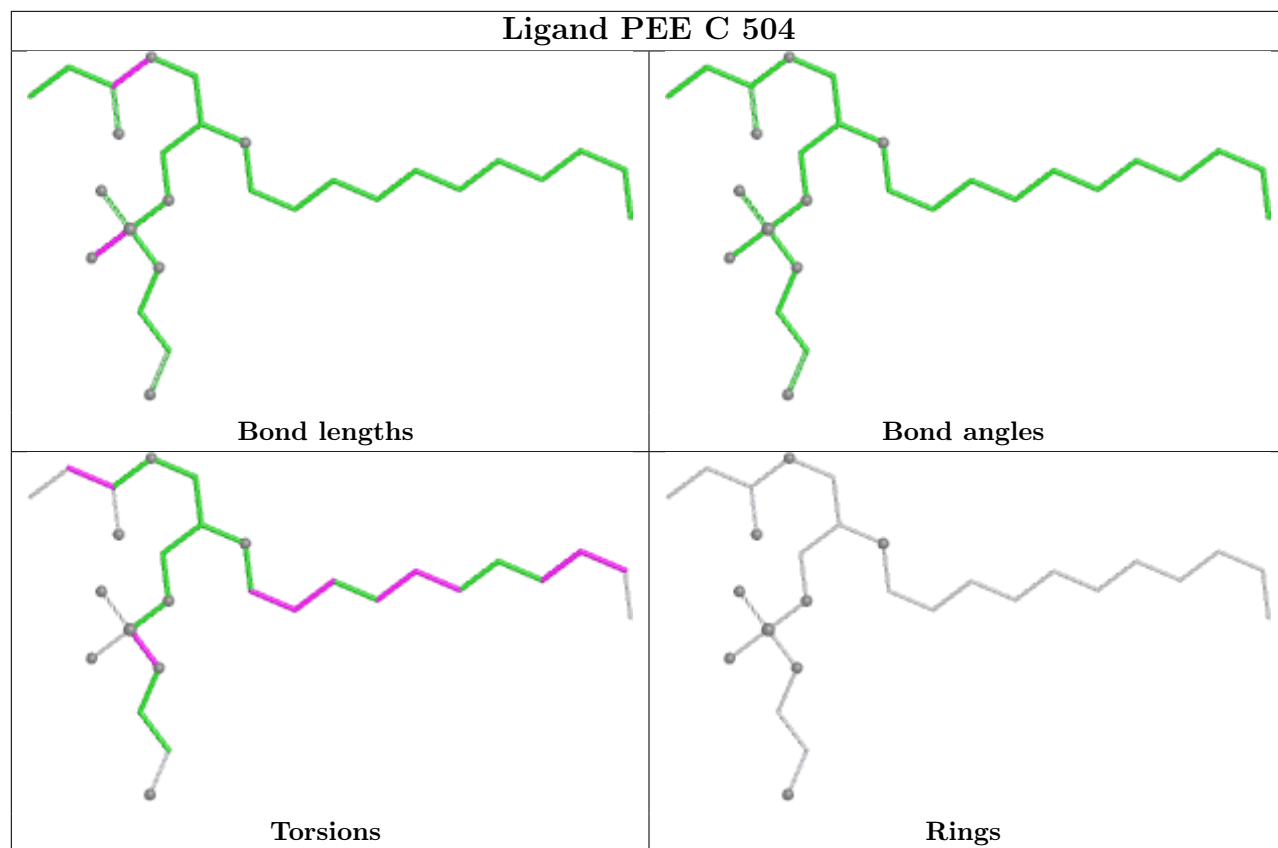


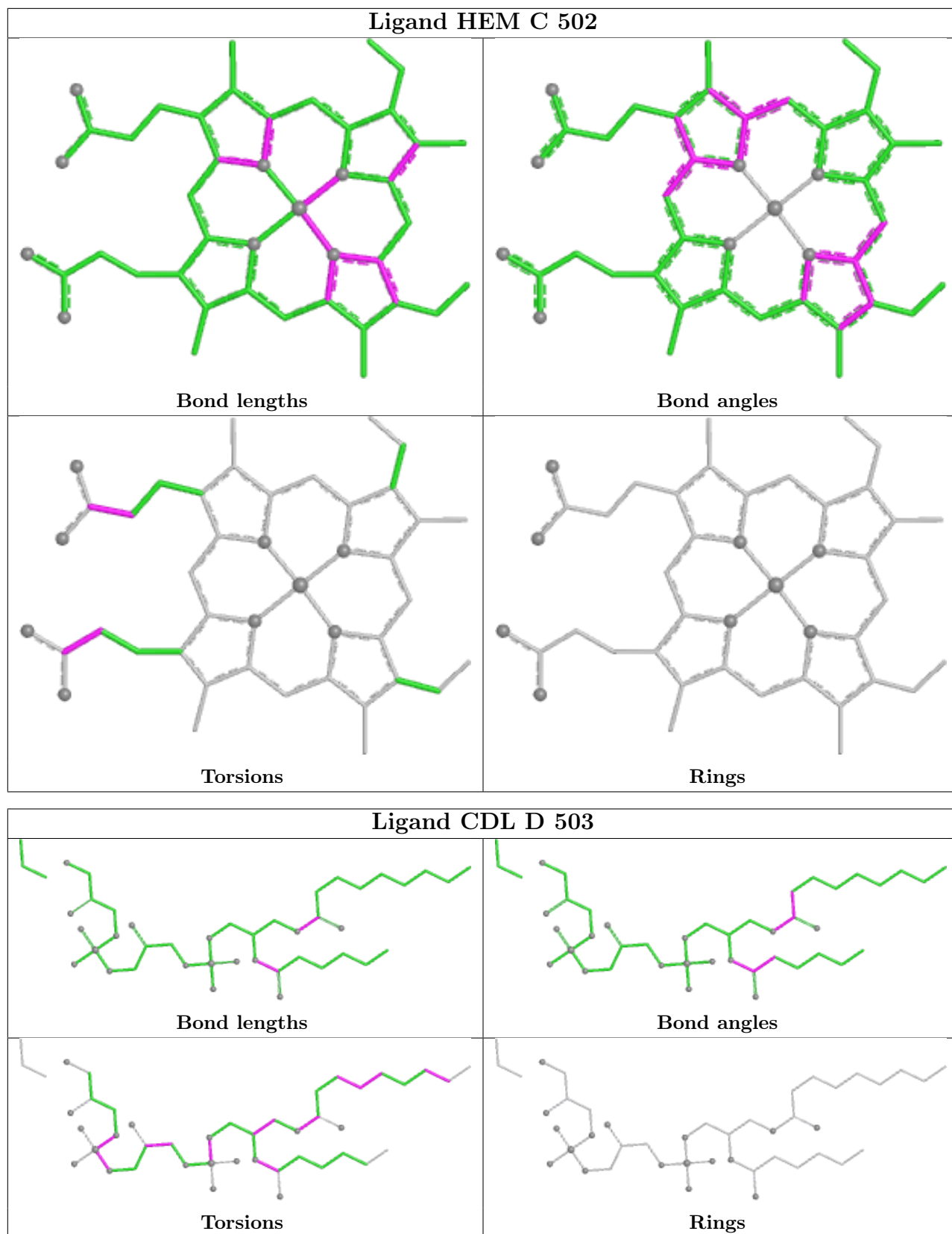


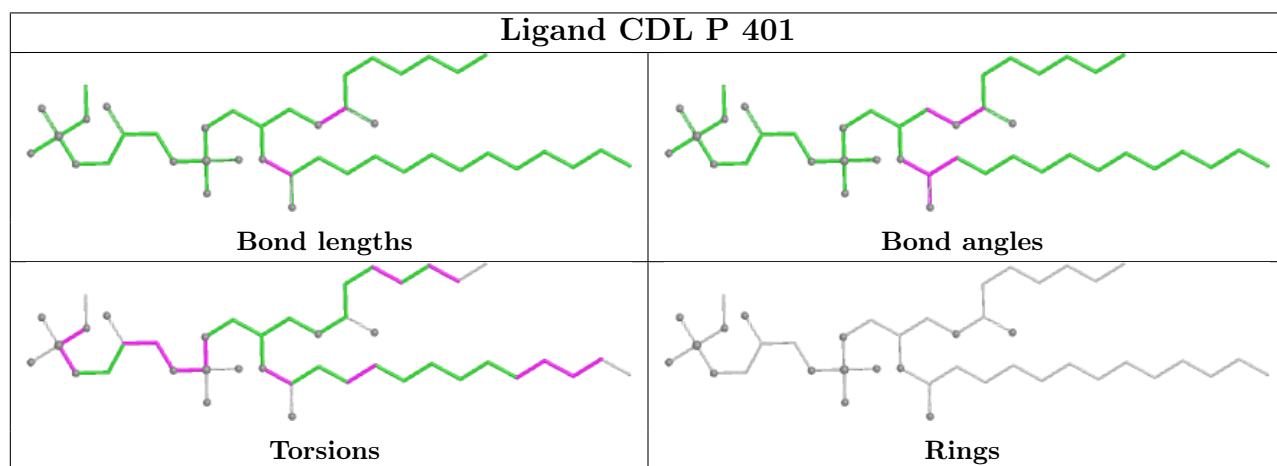
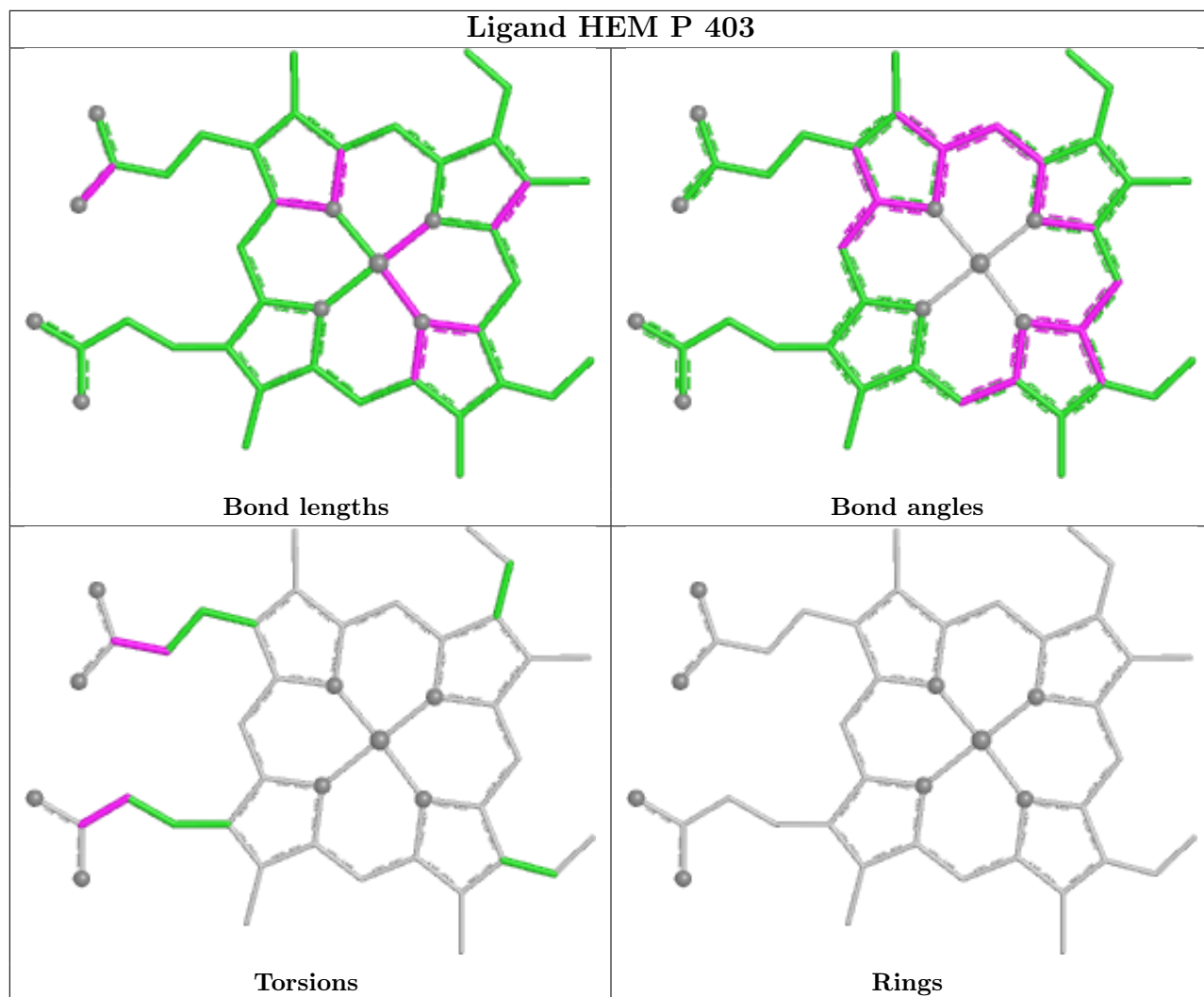


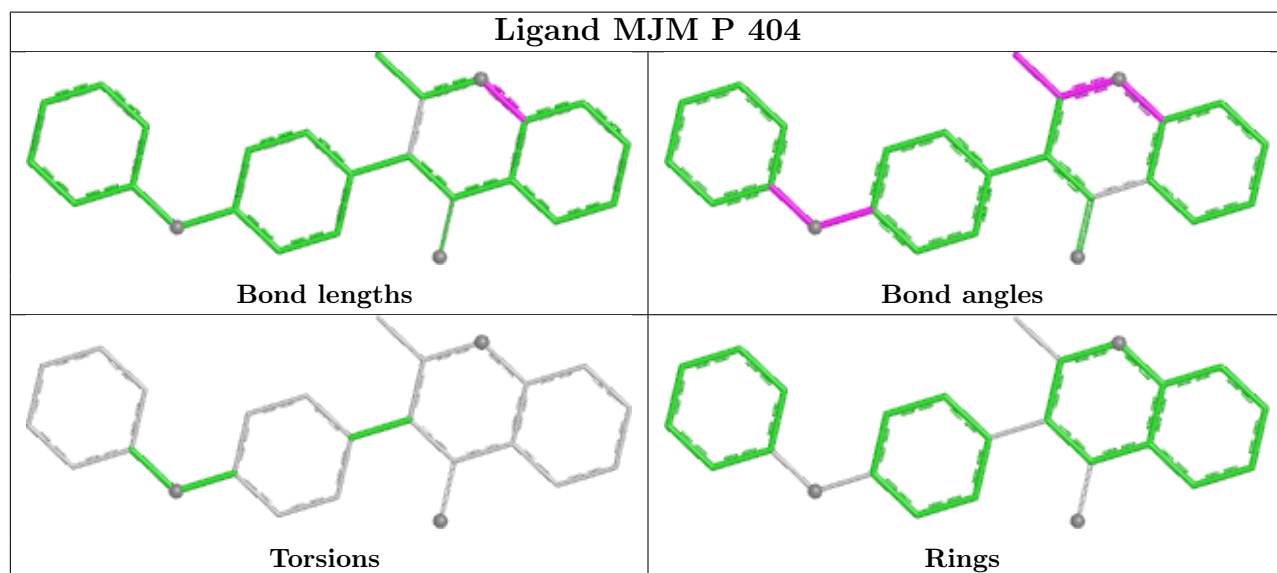
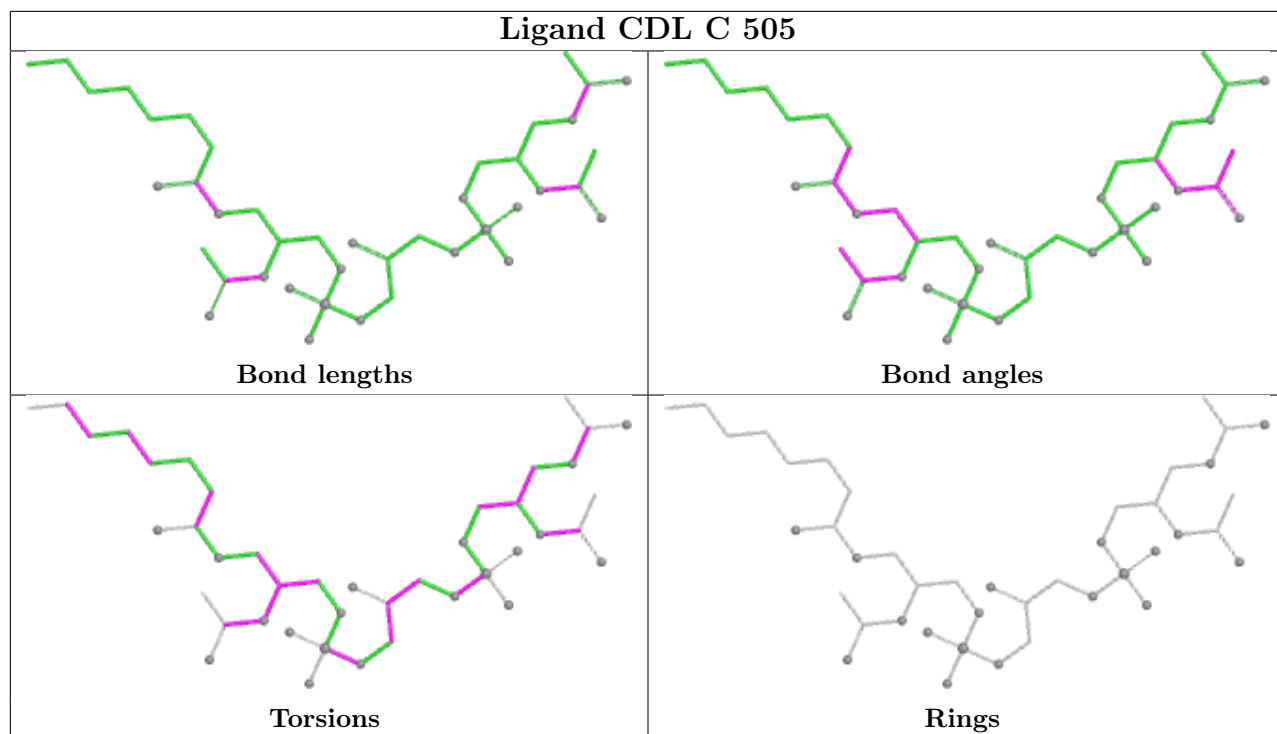


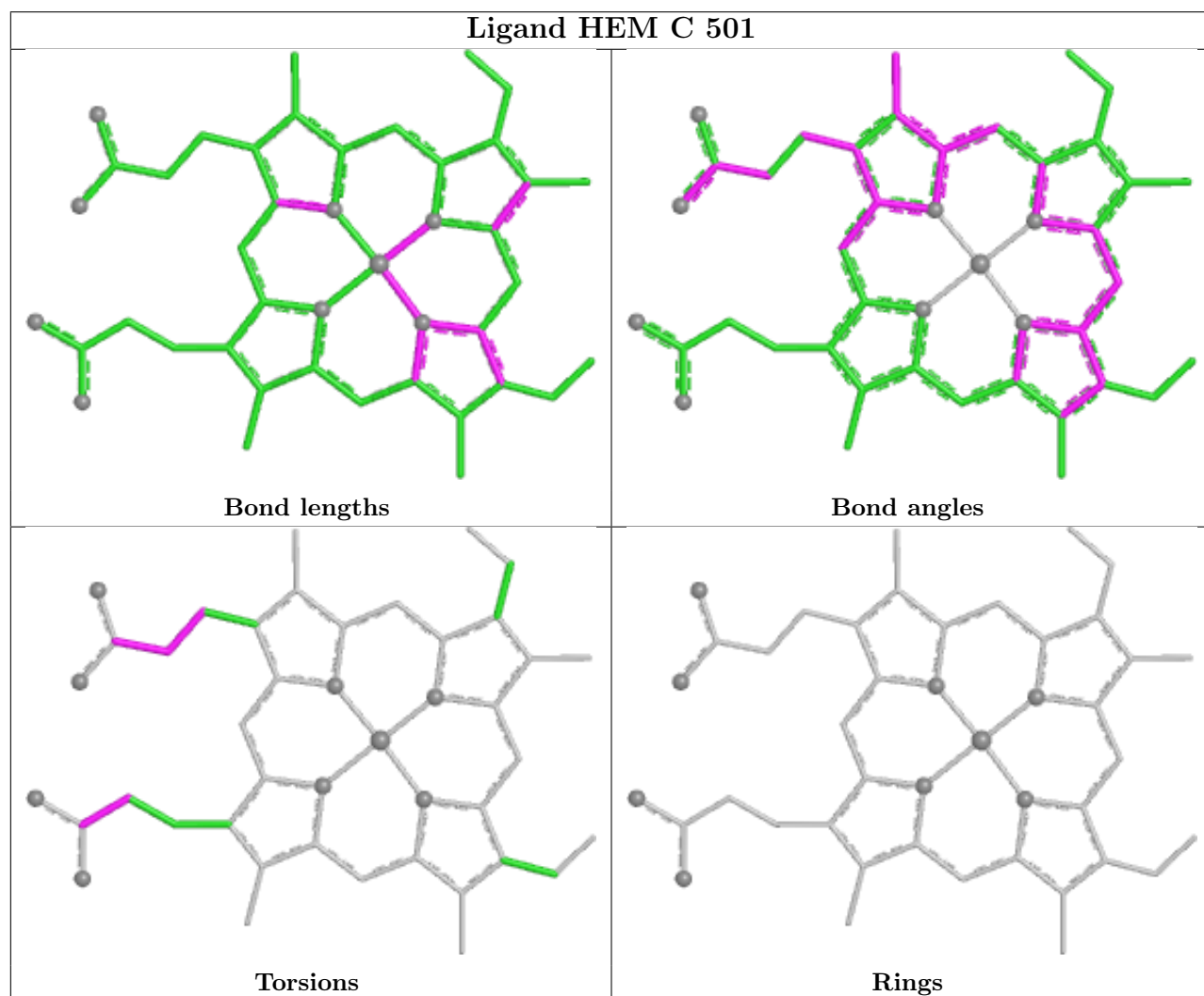
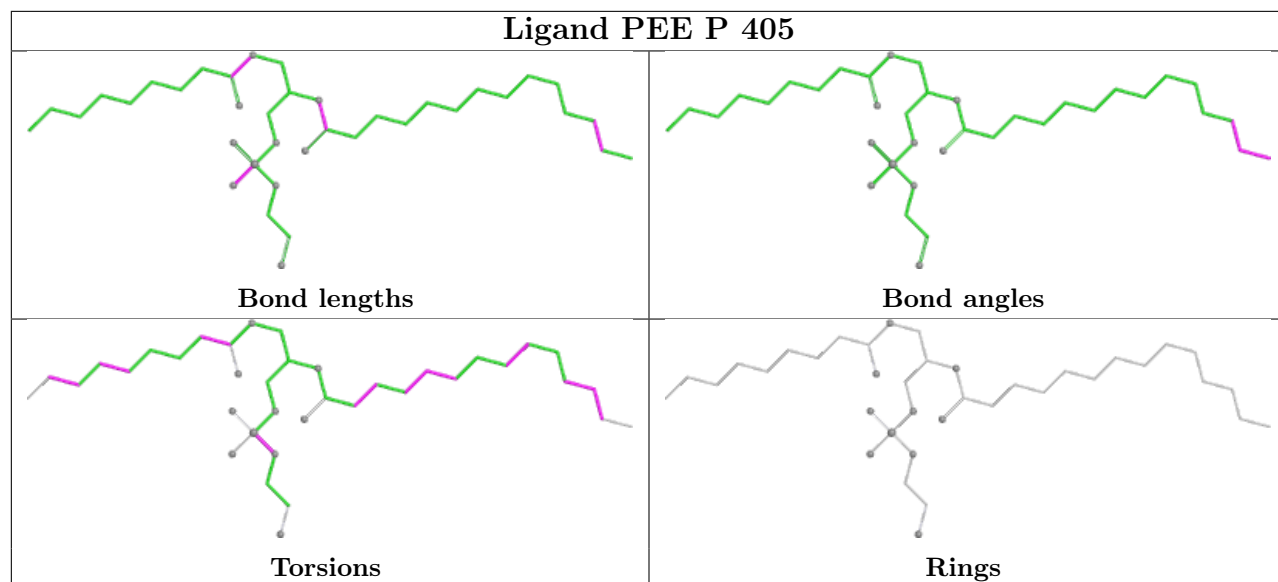


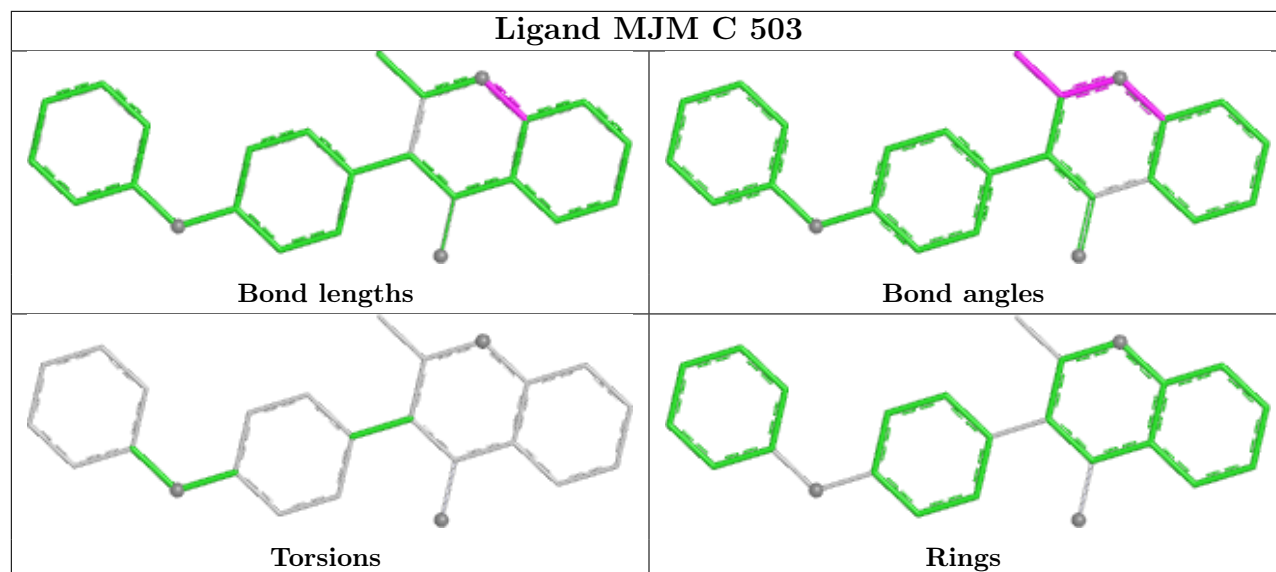












5.7 Other polymers [\(i\)](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	438/444 (98%)	0.24	16 (3%) 45 25	47, 92, 130, 166	0
1	N	439/444 (98%)	0.43	22 (5%) 34 19	56, 108, 152, 181	2 (0%)
2	B	418/423 (98%)	0.25	11 (2%) 57 33	64, 106, 143, 196	0
2	O	422/423 (99%)	0.52	23 (5%) 30 18	71, 115, 151, 203	0
3	C	372/372 (100%)	-0.02	4 (1%) 78 54	46, 73, 105, 141	0
3	P	372/372 (100%)	-0.00	5 (1%) 75 50	33, 62, 92, 127	0
4	D	240/240 (100%)	0.22	4 (1%) 69 43	56, 96, 132, 181	0
4	Q	240/240 (100%)	0.29	6 (2%) 58 35	52, 82, 120, 138	1 (0%)
5	E	196/274 (71%)	0.42	11 (5%) 30 17	48, 107, 143, 166	0
5	I	29/274 (10%)	1.88	13 (44%) 0 1	84, 130, 157, 166	0
5	R	72/274 (26%)	0.26	4 (5%) 30 17	55, 84, 118, 130	0
5	V	30/274 (10%)	1.24	5 (16%) 4 4	89, 132, 168, 208	0
6	F	99/111 (89%)	0.15	3 (3%) 52 30	50, 78, 127, 141	0
6	S	99/111 (89%)	0.14	2 (2%) 65 39	53, 81, 115, 128	1 (1%)
7	G	74/82 (90%)	0.10	0 100 100	54, 85, 127, 147	0
7	T	80/82 (97%)	0.24	3 (3%) 44 24	57, 82, 129, 161	0
8	H	66/91 (72%)	0.39	0 100 100	68, 135, 156, 182	1 (1%)
8	U	68/91 (74%)	0.43	2 (2%) 53 31	64, 95, 126, 141	0
9	J	59/64 (92%)	0.01	1 (1%) 69 43	57, 83, 123, 138	0
9	W	59/64 (92%)	-0.06	1 (1%) 69 43	60, 95, 126, 141	0
10	K	22/22 (100%)	1.23	3 (13%) 7 5	123, 151, 173, 200	0
10	X	22/22 (100%)	0.25	0 100 100	59, 128, 140, 155	2 (9%)
All	All	3916/4794 (81%)	0.27	139 (3%) 47 26	33, 93, 143, 208	7 (0%)

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	I	54	SER	5.9
1	A	98	TYR	4.9
5	I	57	GLY	4.6
3	C	168	PHE	4.5
6	S	106	GLU	4.4
2	O	119	LEU	4.4
5	R	12	ASP	4.3
5	E	190	ASP	4.3
1	A	394	GLU	4.0
1	N	321	GLY	3.9
2	O	276	GLN	3.7
4	Q	178	THR	3.5
1	N	56	GLY	3.5
5	E	142	LEU	3.4
6	S	14	GLU	3.4
5	I	56	ARG	3.4
2	B	341	TYR	3.4
2	O	172	LEU	3.3
1	N	83	GLY	3.3
1	A	264	HIS	3.3
4	D	167	GLU	3.3
1	A	85	HIS	3.3
5	V	73	PRO	3.2
2	B	281	ALA	3.2
1	N	444	LEU	3.2
5	I	74	ALA	3.1
2	O	169	ARG	3.1
5	V	72	VAL	3.0
5	I	55	LEU	3.0
1	A	377	GLU	3.0
8	U	14	VAL	3.0
2	O	281	ALA	3.0
4	Q	4	GLU	2.9
4	Q	167	GLU	2.9
2	O	307	PHE	2.9
5	E	132	TRP	2.9
1	A	381	ARG	2.9
5	I	49	VAL	2.9
5	I	61	GLY	2.9
10	K	17	TRP	2.9
1	N	282	CYS	2.9
6	F	15	GLY	2.8
2	O	244	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
5	E	27	GLU	2.8
1	A	315	ALA	2.8
1	A	385	THR	2.8
1	A	91	THR	2.8
5	R	68	VAL	2.8
4	D	86	LYS	2.8
1	N	222	THR	2.7
1	N	443	TRP	2.7
2	B	117	ASP	2.7
1	N	249	PRO	2.7
1	N	221	GLY	2.7
1	N	326	CYS	2.7
4	Q	2	ASP	2.7
1	N	305	GLN	2.6
3	P	267	HIS	2.6
5	E	72	SER	2.6
6	F	18	LYS	2.6
5	R	69	LEU	2.6
1	N	90	SER	2.6
5	E	81	ILE	2.5
1	A	100	LYS	2.5
2	B	344	VAL	2.5
2	O	115	ASP	2.5
3	P	72	ASP	2.5
2	O	43	PRO	2.5
5	I	78	TYR	2.5
5	V	50	LEU	2.5
1	A	444	LEU	2.5
9	W	17	THR	2.5
1	A	415	PHE	2.4
3	C	296	PHE	2.4
5	I	60	ALA	2.4
3	P	254	ASP	2.4
5	E	75	GLU	2.4
7	T	73	ASN	2.4
1	N	238	GLY	2.4
2	O	93	GLY	2.4
2	O	94	GLY	2.4
1	A	236	PHE	2.4
5	E	143	GLY	2.3
1	N	139	GLN	2.3
7	T	3	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
9	J	4	THR	2.3
5	E	77	LYS	2.3
1	N	44	GLY	2.3
2	B	210	GLY	2.3
4	D	166	ASN	2.3
3	P	257	THR	2.3
7	T	81	ARG	2.3
3	C	167	GLY	2.3
2	O	23	ASP	2.3
1	N	41	ILE	2.3
10	K	25	GLY	2.2
3	C	203	THR	2.2
1	N	251	ALA	2.2
2	B	309	VAL	2.2
1	A	316	ASP	2.2
2	O	122	PHE	2.2
2	O	363	LYS	2.2
5	I	62	ARG	2.2
5	I	72	VAL	2.2
10	K	23	LEU	2.2
1	N	327	ASP	2.2
1	N	250	LEU	2.2
5	V	78	TYR	2.2
5	I	68	VAL	2.2
2	O	171	ALA	2.2
2	O	235	ALA	2.2
3	P	171	ASP	2.2
5	R	70	ALA	2.2
1	A	445	ARG	2.2
2	B	371	SER	2.2
2	O	209	LEU	2.2
2	O	264	ILE	2.2
4	D	11	PRO	2.2
5	E	30	GLU	2.2
2	O	236	LYS	2.2
2	B	313	ASN	2.2
1	A	263	ALA	2.1
2	B	340	ALA	2.1
2	O	36	ALA	2.1
2	O	34	VAL	2.1
5	V	76	VAL	2.1
1	N	8	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	O	208	GLY	2.1
5	I	73	PRO	2.1
6	F	14	GLU	2.1
2	B	429	ASN	2.0
4	Q	154	PRO	2.0
4	Q	136	GLU	2.0
2	O	110	GLU	2.0
8	U	51	GLU	2.0
1	N	43	ALA	2.0
1	N	84	ALA	2.0
2	B	308	ASP	2.0
5	E	12	ASP	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.

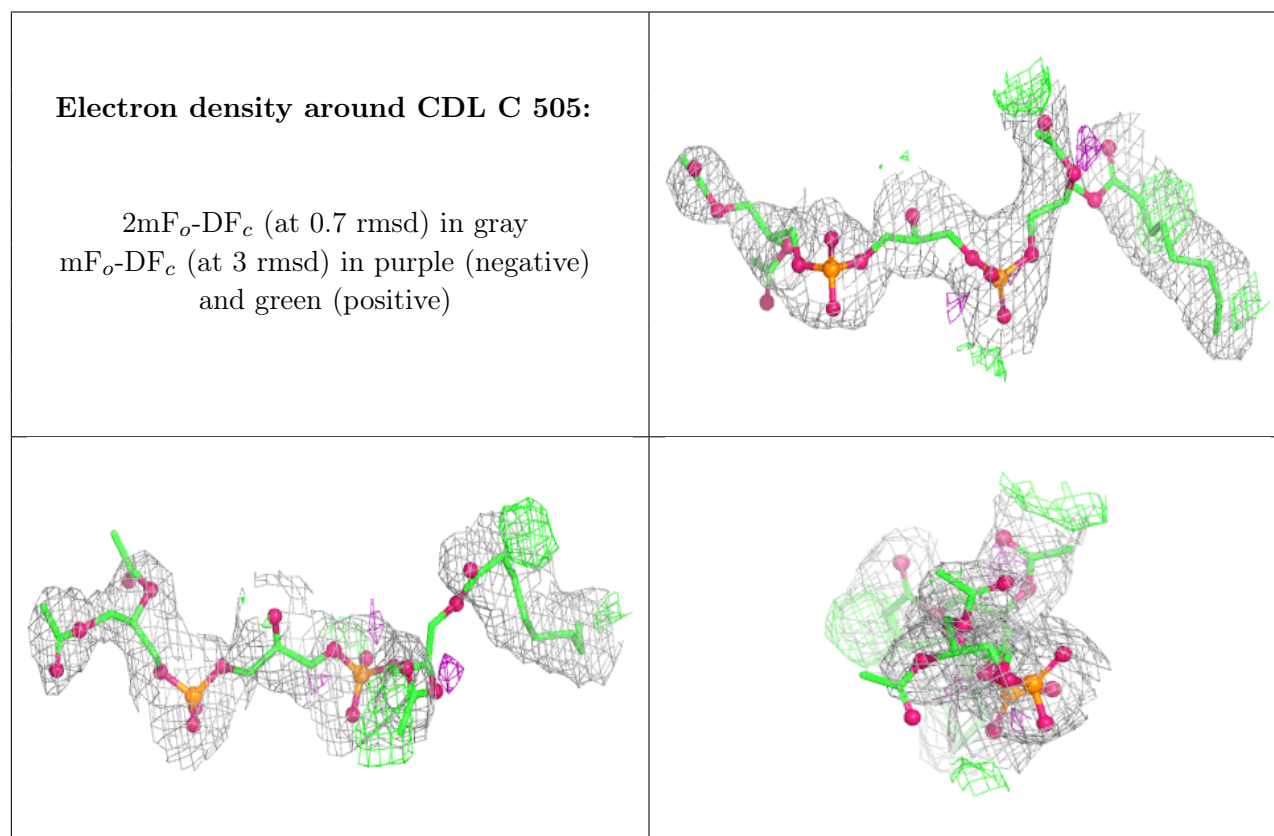
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	CDL	C	505	42/100	0.80	0.19	45,88,122,130	0
12	MJM	P	404	25/25	0.82	0.19	49,56,64,69	0
14	CDL	P	401	42/100	0.85	0.20	53,90,135,159	0
14	CDL	P	406	46/100	0.86	0.16	70,106,125,128	0
13	PEE	R	202	24/51	0.88	0.15	26,37,52,55	0
14	CDL	D	503	44/100	0.88	0.17	42,86,112,116	0
13	PEE	E	502	29/51	0.89	0.18	47,83,98,103	0
13	PEE	C	504	28/51	0.89	0.16	35,45,57,59	0
12	MJM	C	503	25/25	0.91	0.13	49,56,68,69	0
13	PEE	P	405	38/51	0.92	0.16	41,56,81,81	0
14	CDL	C	506	37/100	0.93	0.12	59,73,108,108	0

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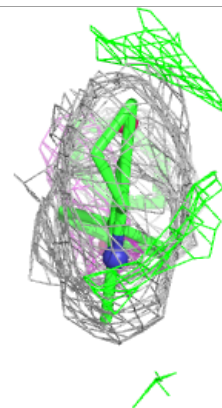
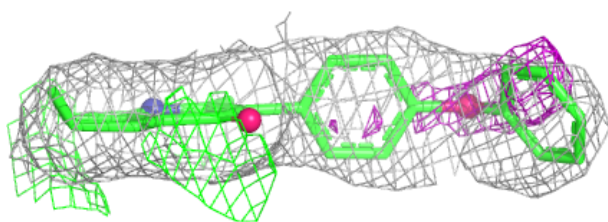
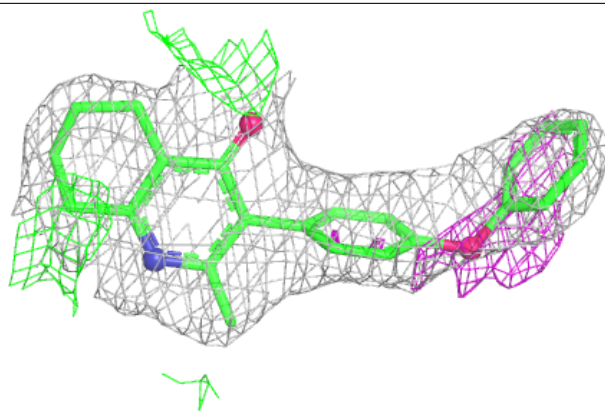
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	PEE	D	502	42/51	0.94	0.15	60,79,102,111	0
14	CDL	P	407	38/100	0.94	0.13	53,71,87,90	0
15	HEC	D	501	43/43	0.94	0.12	66,84,109,147	0
15	HEC	Q	501	43/43	0.95	0.14	59,79,111,145	0
13	PEE	R	201	34/51	0.96	0.12	57,78,91,101	0
11	HEM	C	501	43/43	0.96	0.11	51,59,77,90	0
16	FES	E	501	4/4	0.96	0.07	104,106,122,144	0
11	HEM	P	403	43/43	0.97	0.10	52,55,60,61	0
11	HEM	C	502	43/43	0.97	0.09	45,53,71,76	0
11	HEM	P	402	43/43	0.97	0.10	43,55,60,74	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.

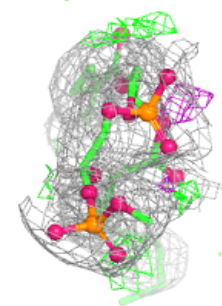
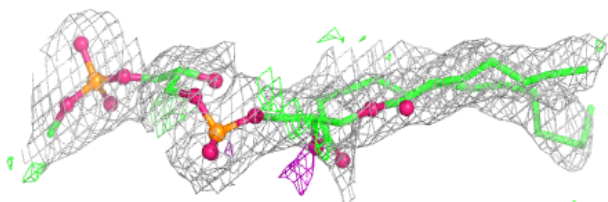
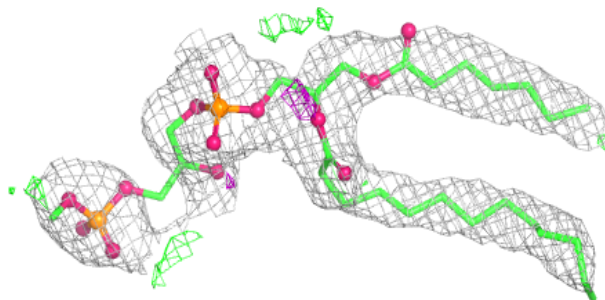


Electron density around MJM P 404:

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

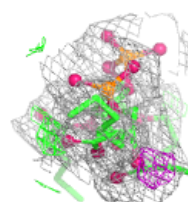
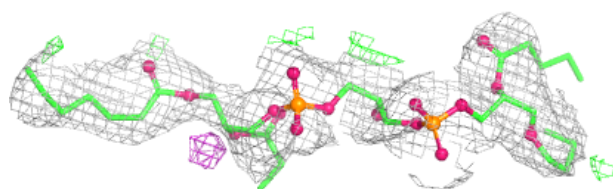
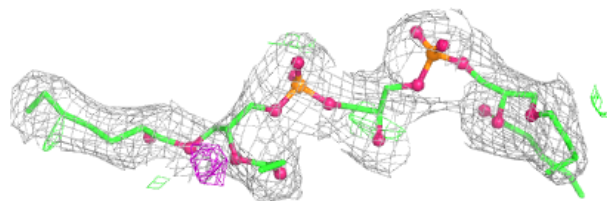
**Electron density around CDL P 401:**

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



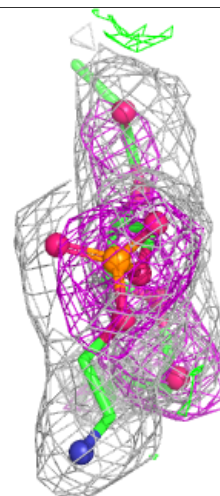
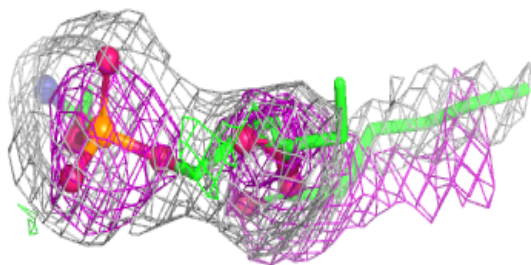
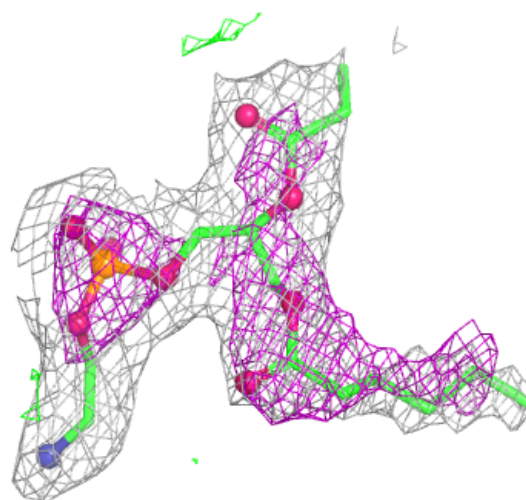
Electron density around CDL P 406:

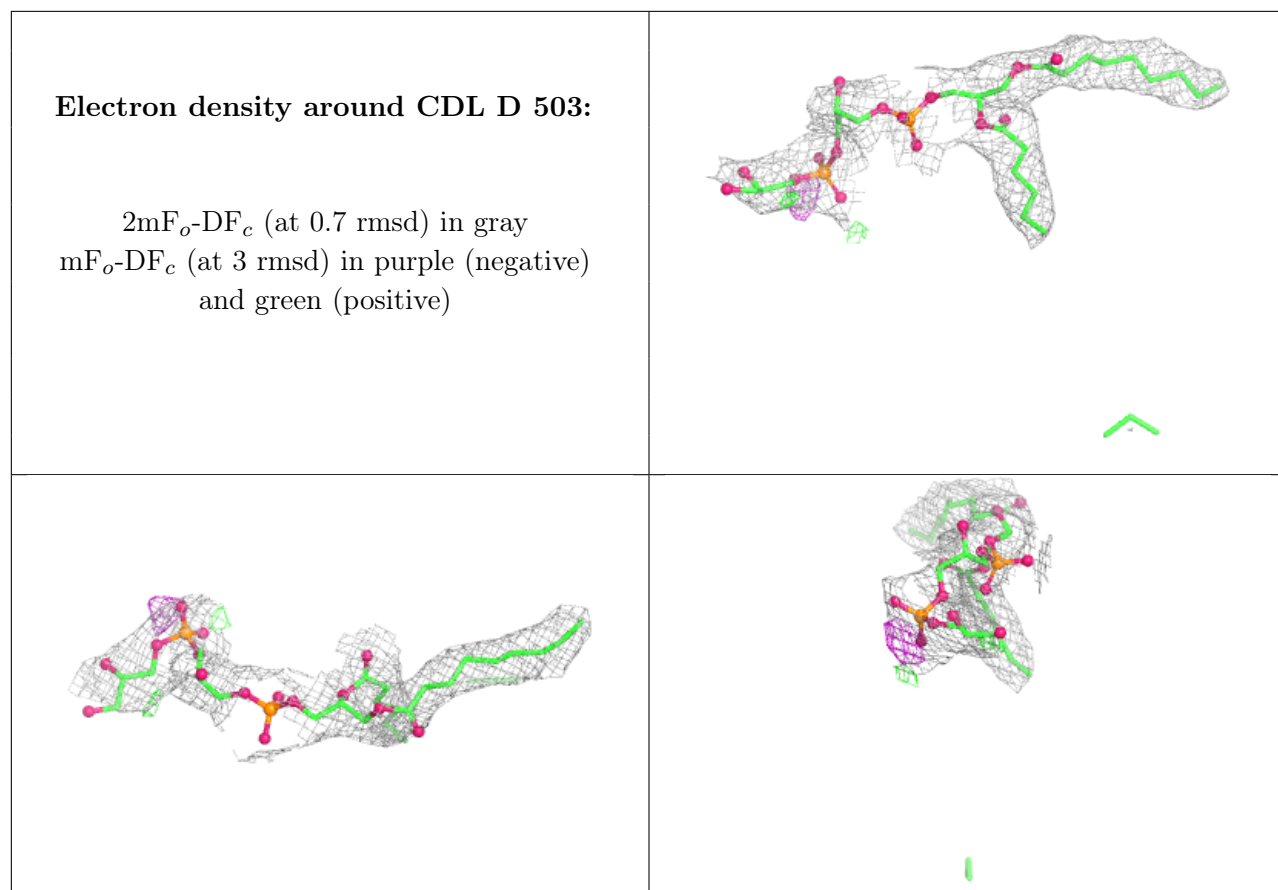
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PEE R 202:

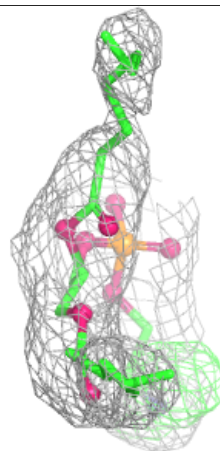
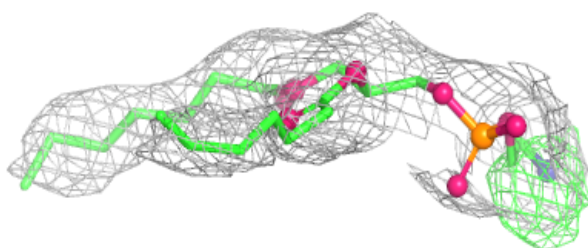
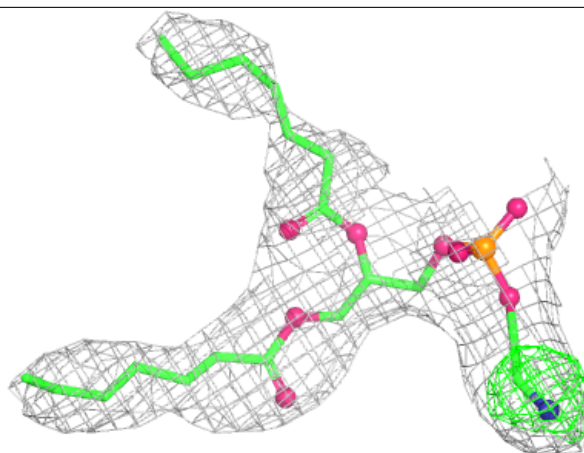
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



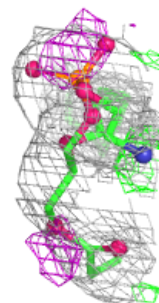
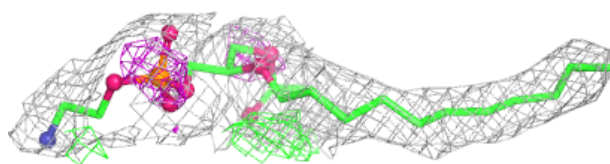
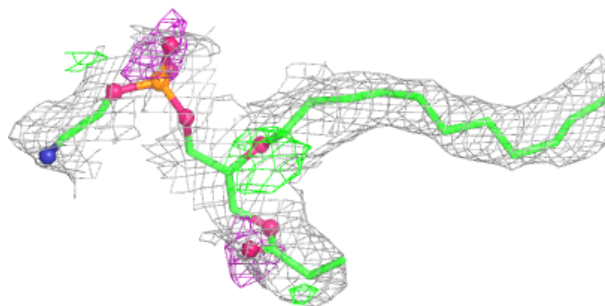


Electron density around PEE E 502:

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

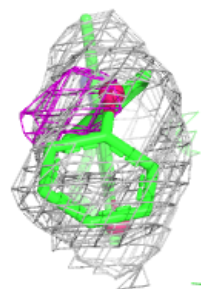
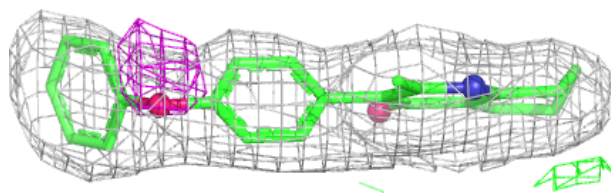
**Electron density around PEE C 504:**

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

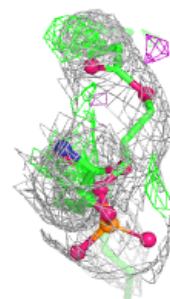
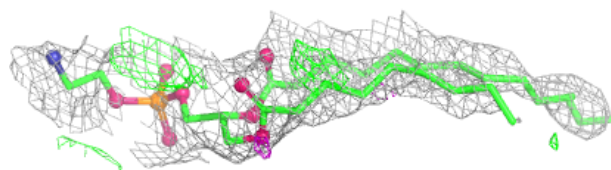
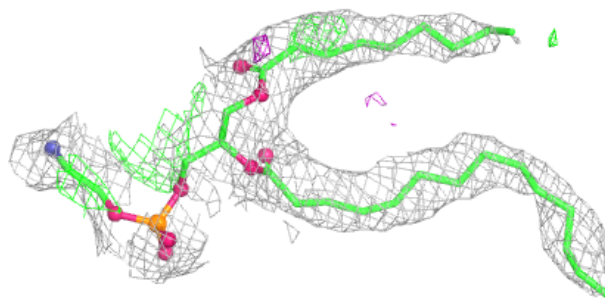


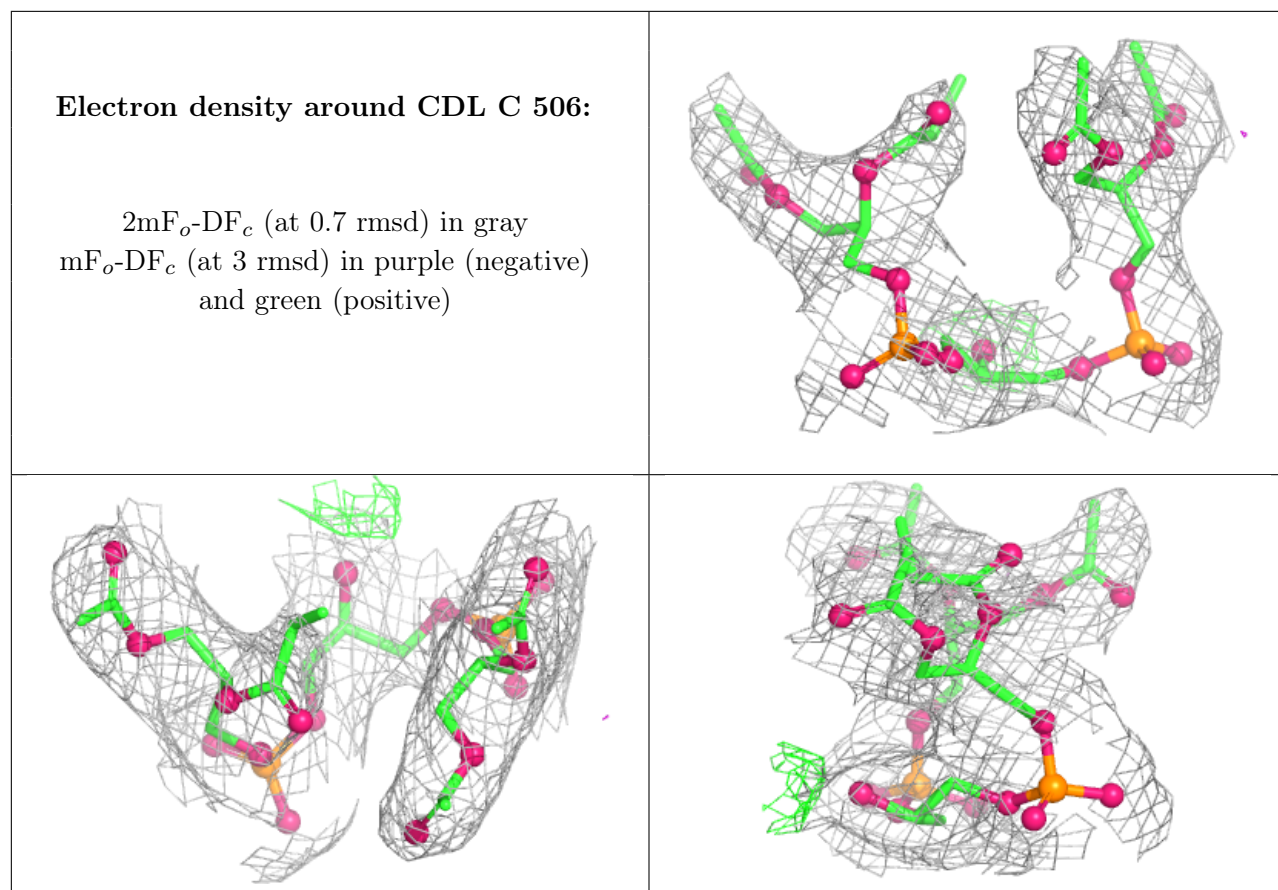
Electron density around MJM C 503:

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

**Electron density around PEE P 405:**

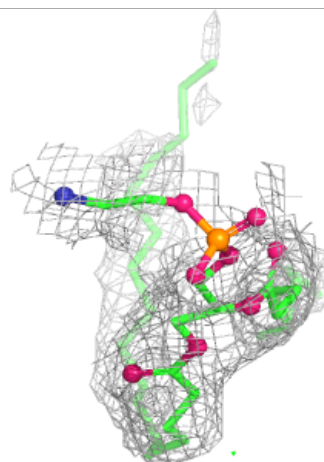
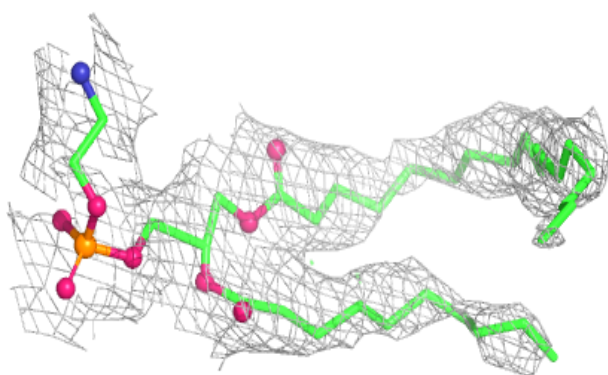
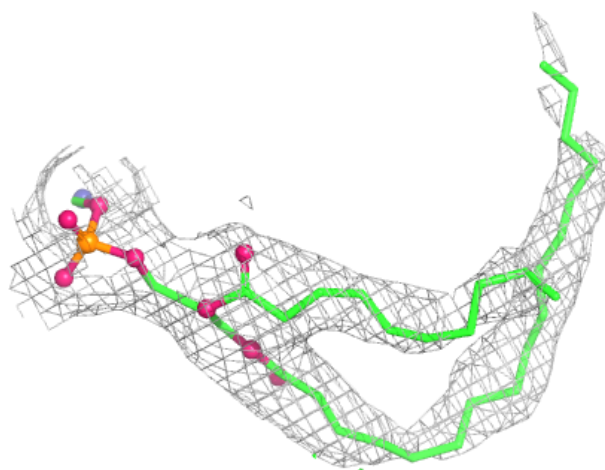
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





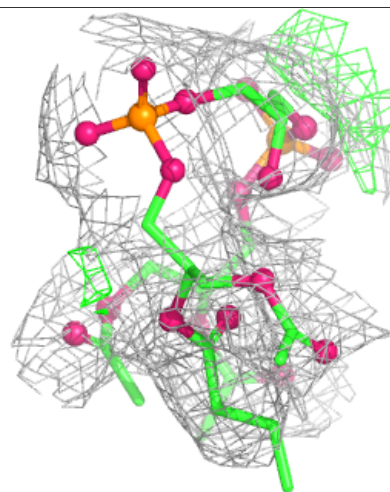
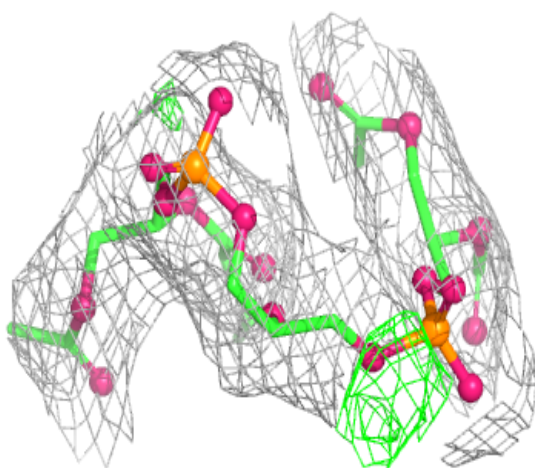
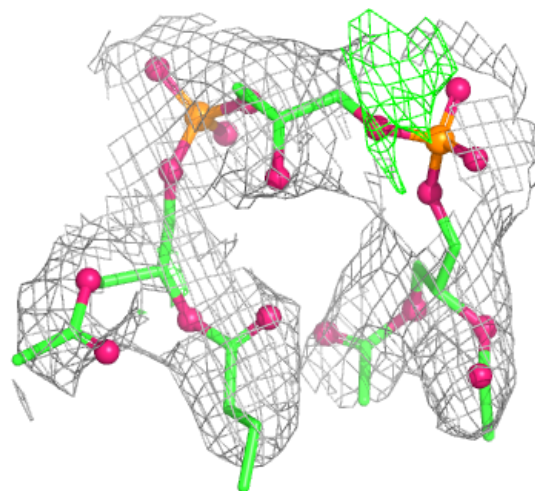
Electron density around PEE D 502:

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



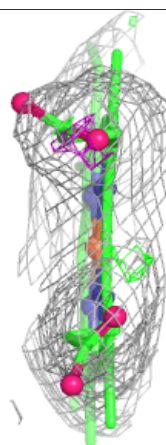
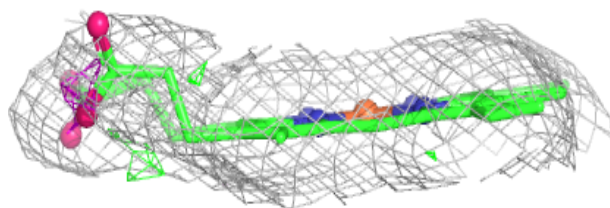
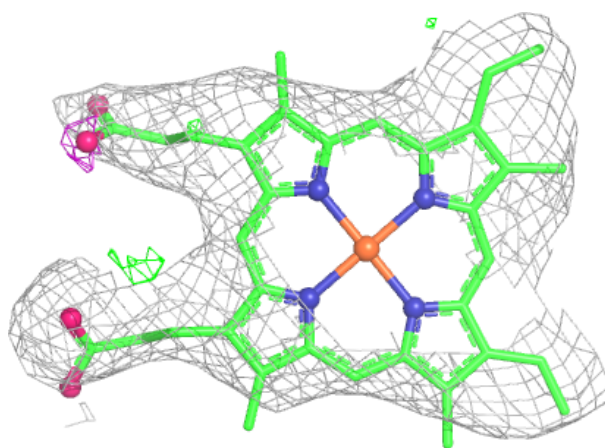
Electron density around CDL P 407:

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



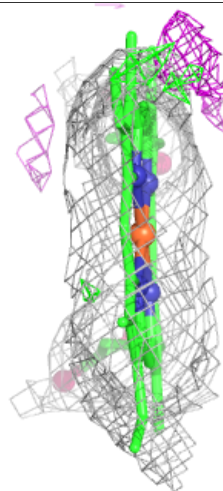
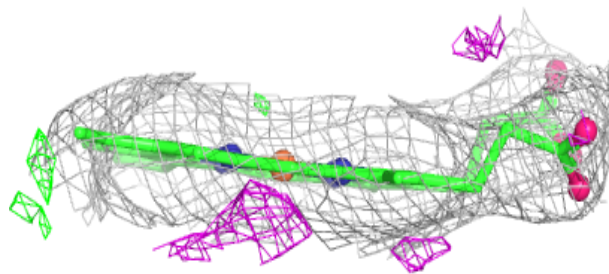
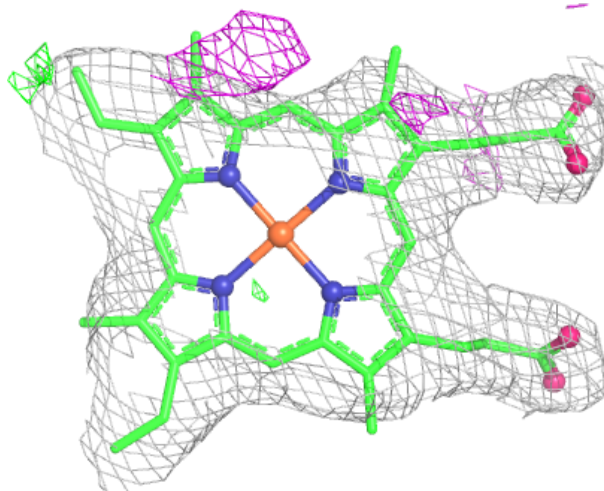
Electron density around HEC D 501:

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



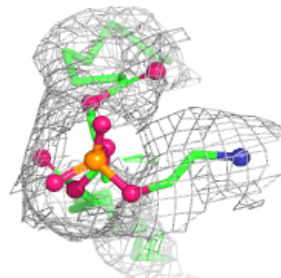
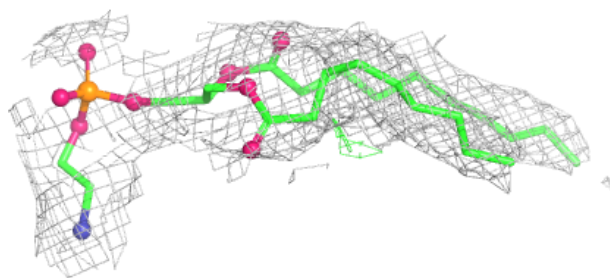
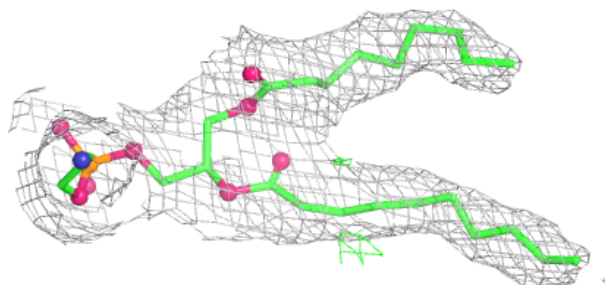
Electron density around HEC Q 501:

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



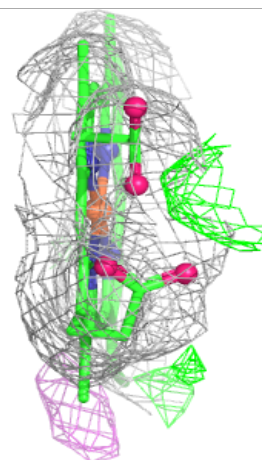
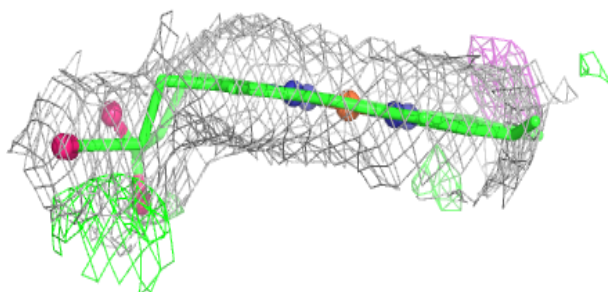
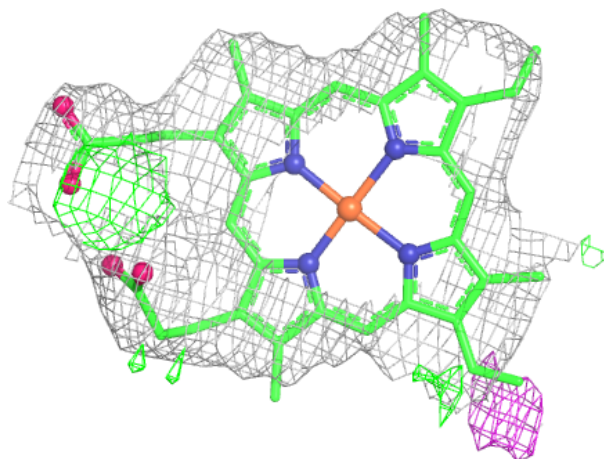
Electron density around PEE R 201:

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



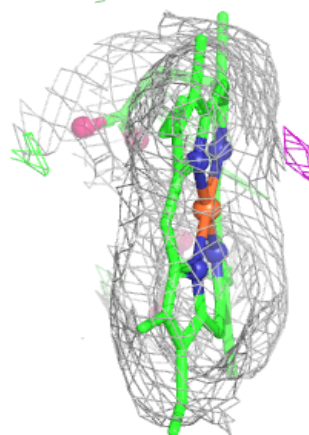
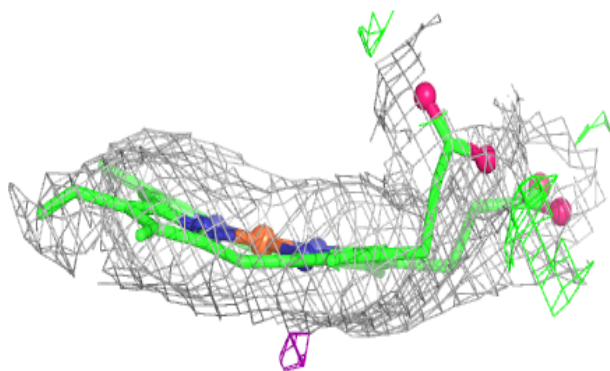
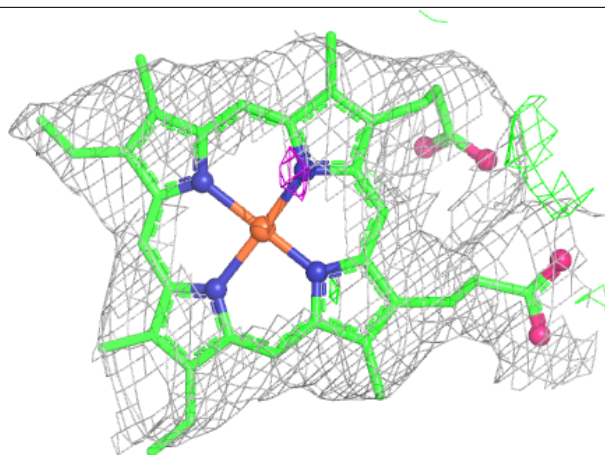
Electron density around HEM C 501:

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



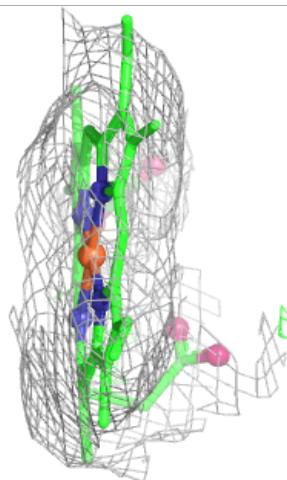
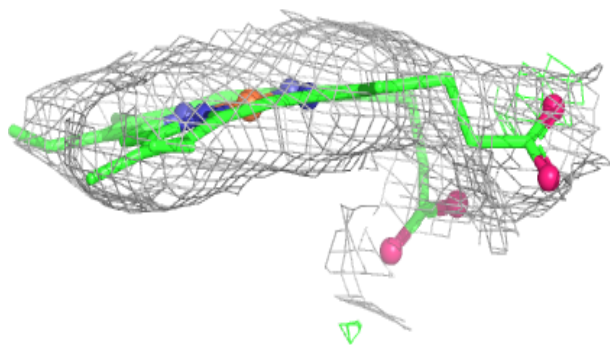
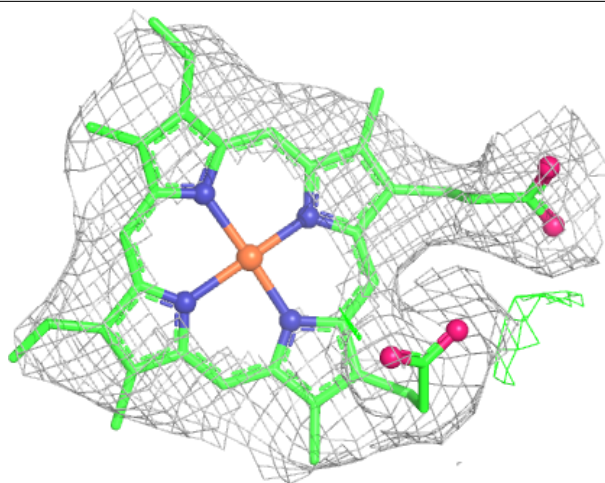
Electron density around HEM P 403:

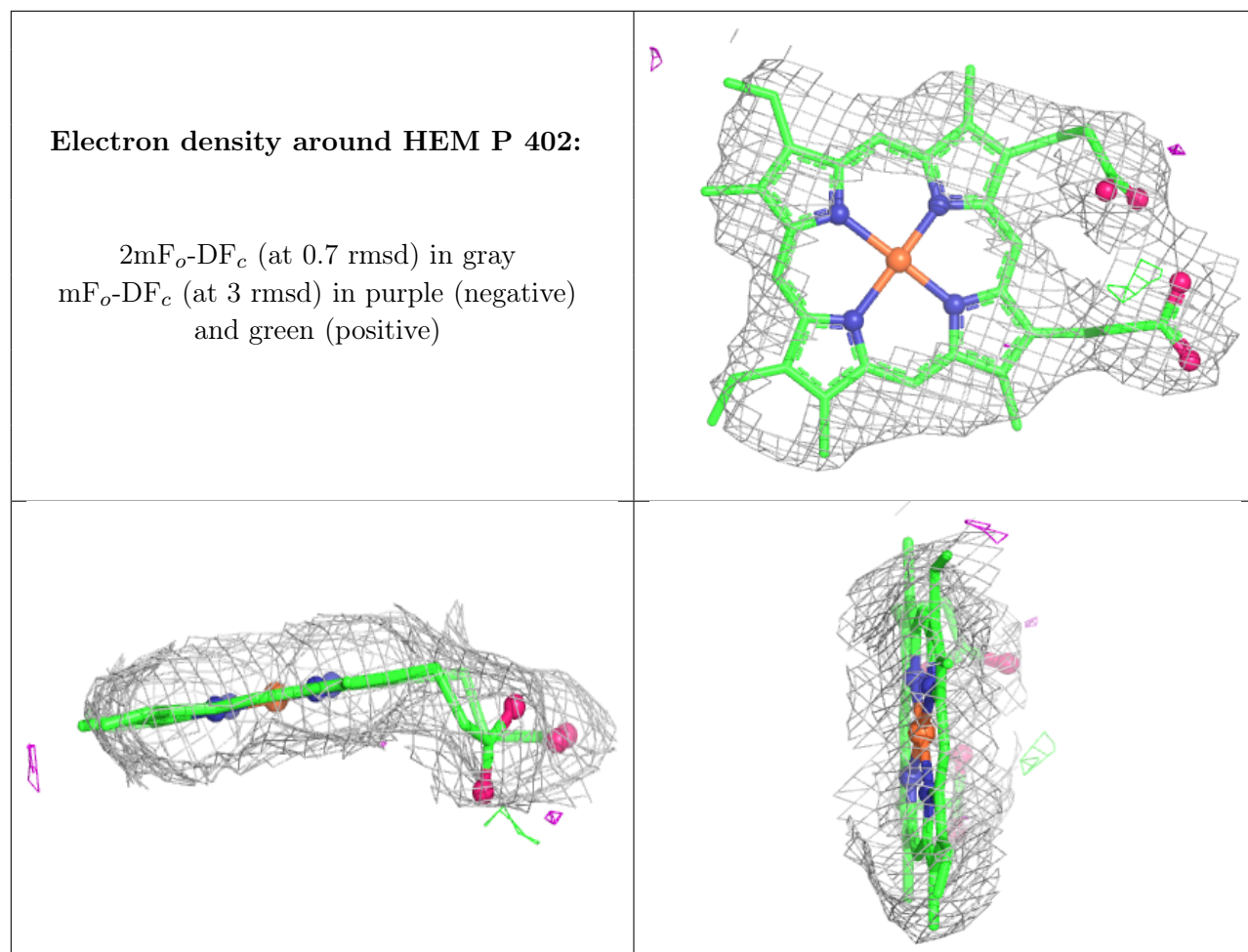
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 502:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.