



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 2, 2025 – 12:50 am BST

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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

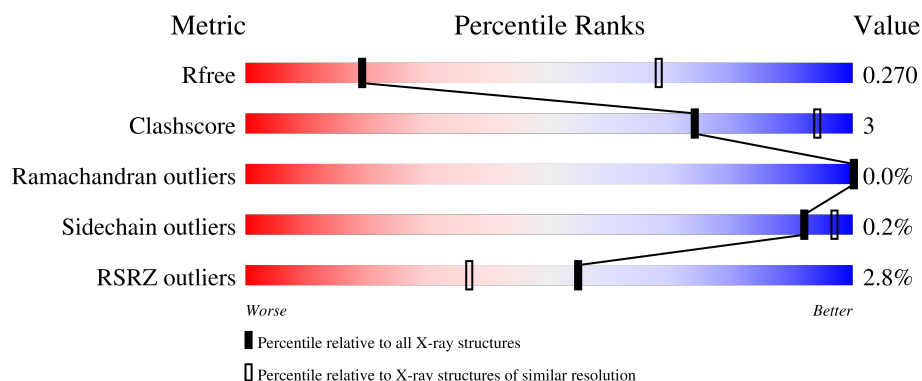
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	164625	1094 (3.56-3.44)
Clashscore	180529	1045 (3.54-3.46)
Ramachandran outliers	177936	1032 (3.54-3.46)
Sidechain outliers	177891	1033 (3.54-3.46)
RSRZ outliers	164620	1093 (3.56-3.44)

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  $\geq 3$ , 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> <div>3%</div> <div>96%</div> <div>.</div> </div>
1	N	444	<div> <div>4%</div> <div>97%</div> <div>.</div> </div>
2	B	423	<div> <div>2%</div> <div>96%</div> <div>.</div> </div>
2	O	423	<div> <div>4%</div> <div>94%</div> <div>6%</div> <div>.</div> </div>
3	C	372	<div> <div>%</div> <div>96%</div> <div>.</div> </div>

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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
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
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
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
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			

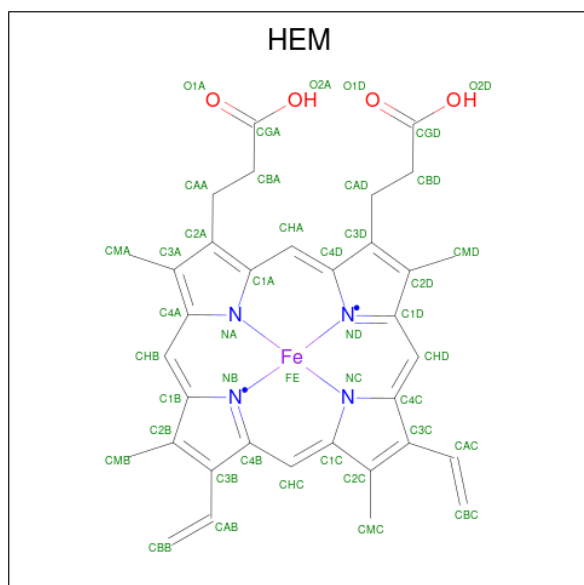
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9.

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.

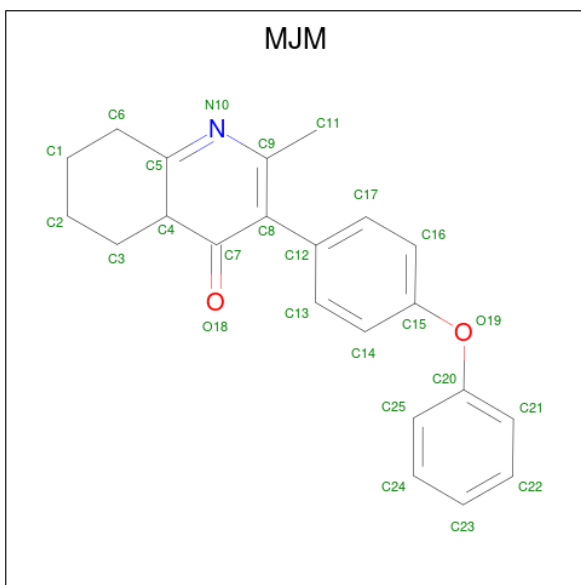
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	22	Total 159	C 103	N 29	O 27	0	0	0
10	X	22	Total 159	C 103	N 29	O 27	12	0	0

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



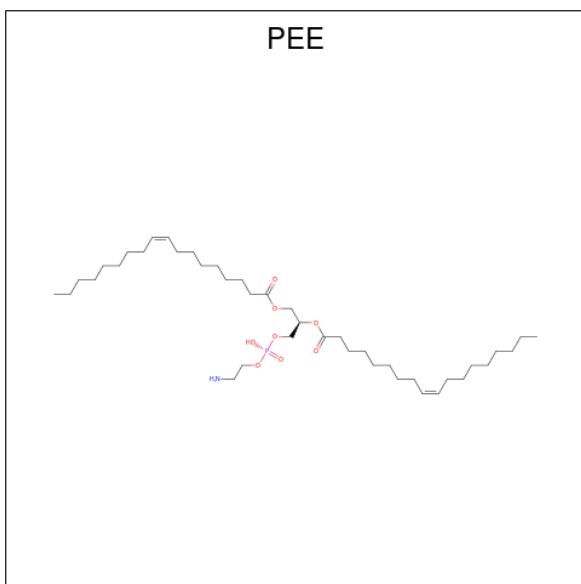
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
11	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
11	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
11	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
11	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 12 is (4a*S*)-2-methyl-3-(4-phenoxyphenyl)-5,6,7,8-tetrahydroquinolin-4(4a*H*)-one (CCD ID: MJM) (formula: C<sub>22</sub>H<sub>21</sub>NO<sub>2</sub>).



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

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



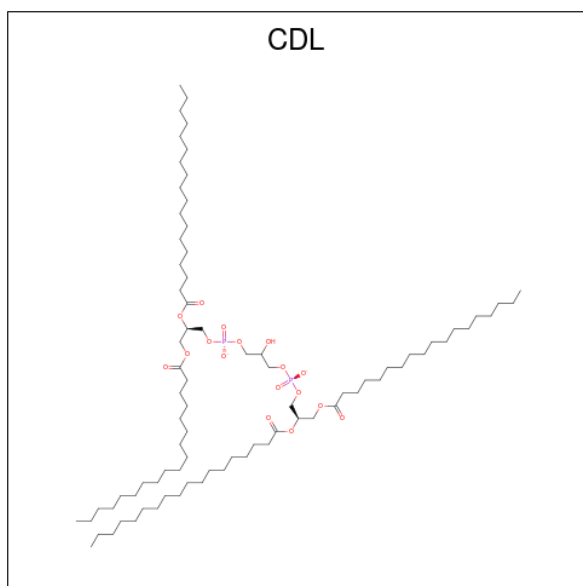
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	N	O	P	0	0
			28	19	1	7	1		

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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		



- [illegible]

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

- 
- Diagram illustrating the structure of a ferredoxin (FES) molecule, showing a square planar arrangement of two iron (Fe) and two sulfur (S) atoms. The atoms are labeled S1, FE2, FE1, and S2 in green. The bonds are colored yellow and purple.

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

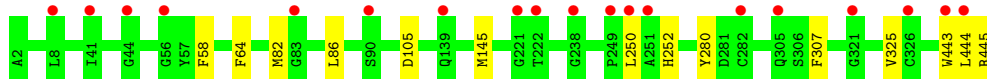
### 3 Residue-property plots

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

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



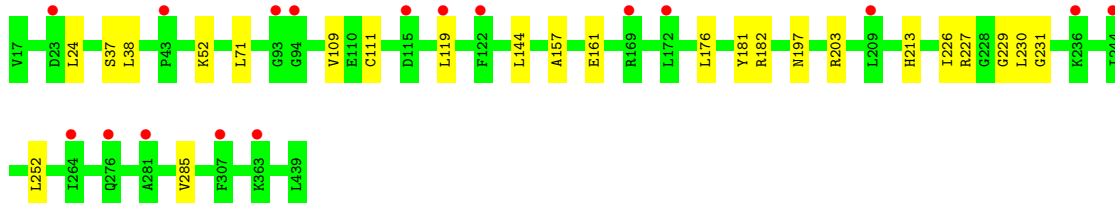
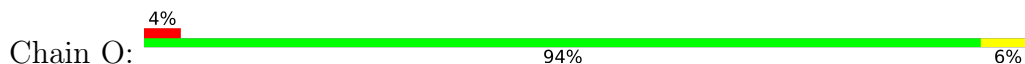
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



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



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



- Molecule 3: Cytochrome b

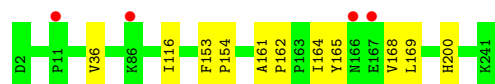




- Molecule 3: Cytochrome b



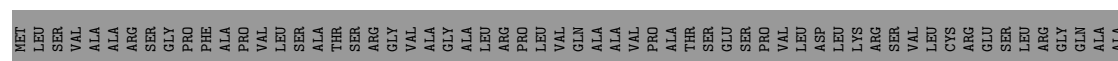
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



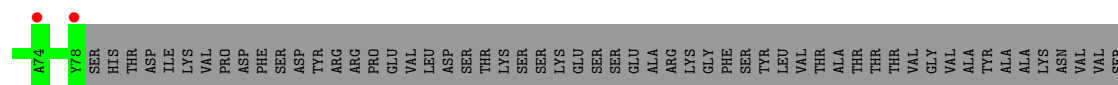
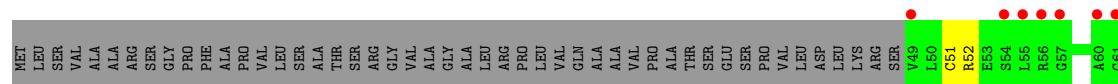
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

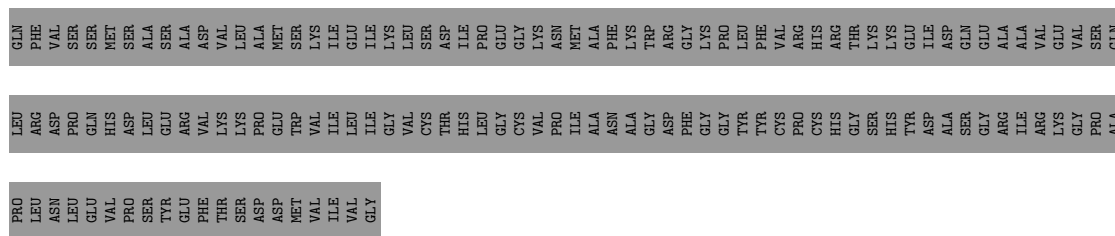


- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

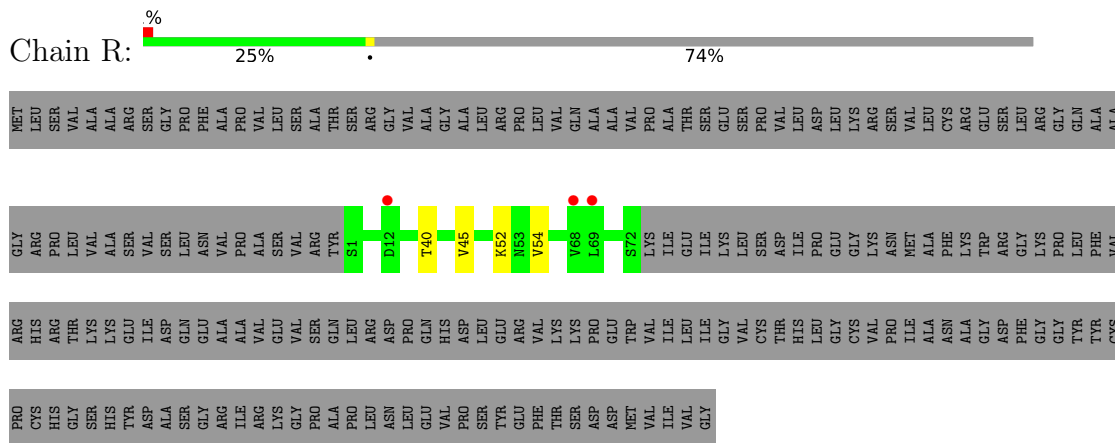


- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

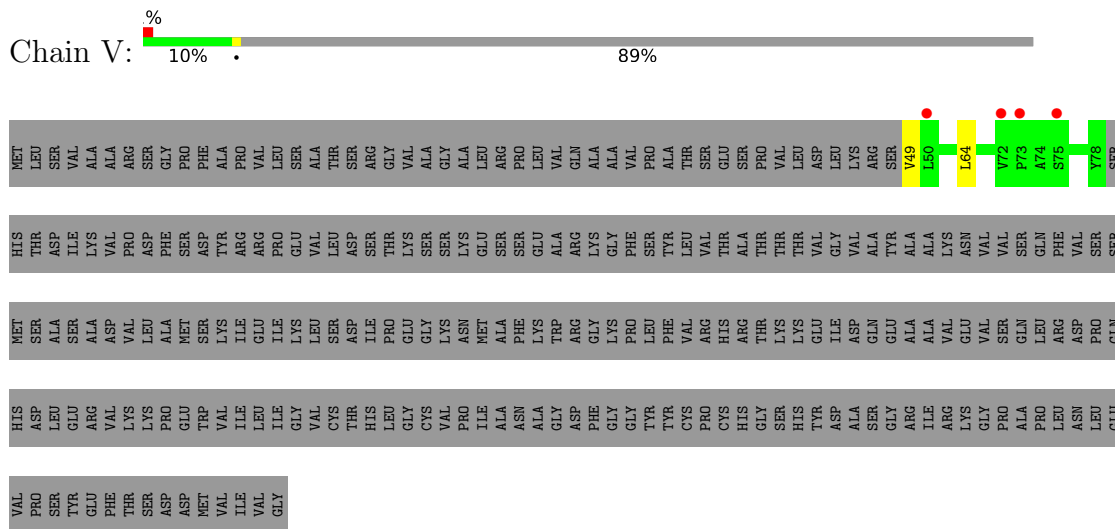




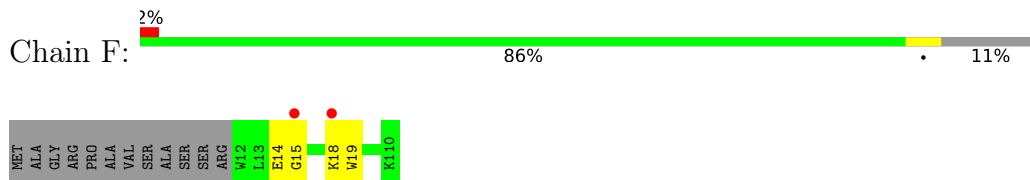
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



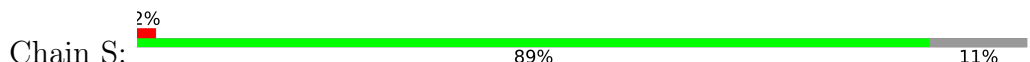
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

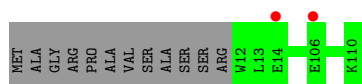


- Molecule 6: Cytochrome b-c1 complex subunit 7



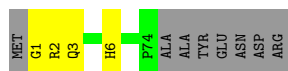
- Molecule 6: Cytochrome b-c1 complex subunit 7





- Molecule 7: Cytochrome b-c1 complex subunit 8

Chain G: 85% 5% 10%



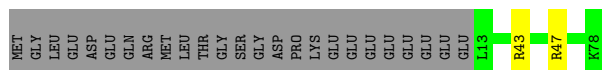
- Molecule 7: Cytochrome b-c1 complex subunit 8

Chain T: 4% 94% . .



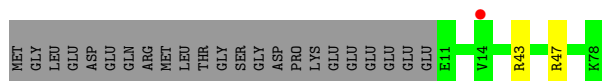
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain H: 70% . 27%



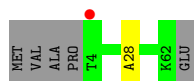
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain U: % 73% . 25%



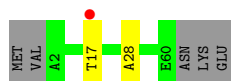
- Molecule 9: Cytochrome b-c1 complex subunit 9

Chain J: 2% 91% . 8%

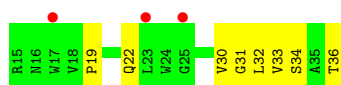


- Molecule 9: Cytochrome b-c1 complex subunit 9

Chain W: 2% 89% . 8%



- 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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.248 , 0.268 0.250 , 0.270	Depositor DCC
$R_{free}$ test set	4365 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.7	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 53.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.096 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	31648	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, PEE, HEC, FES, HEM, MJM

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	0.35	0/3512	0.60	0/4766
1	N	0.37	0/3512	0.60	0/4766
2	B	0.36	0/3232	0.56	0/4386
2	O	0.36	0/3232	0.56	0/4386
3	C	0.37	1/3051 (0.0%)	0.53	0/4177
3	P	0.37	0/3051	0.53	0/4177
4	D	0.36	0/1972	0.58	0/2676
4	Q	0.41	1/1972 (0.1%)	0.59	1/2676 (0.0%)
5	E	0.37	0/1553	0.61	0/2100
5	I	0.49	0/223	0.82	0/302
5	R	0.35	0/548	0.53	0/741
5	V	0.41	0/223	0.73	0/302
6	F	0.36	0/889	0.58	0/1191
6	S	0.36	0/889	0.57	0/1191
7	G	0.40	0/644	0.62	0/871
7	T	0.40	0/699	0.61	0/946
8	H	0.34	0/544	0.59	0/729
8	U	0.34	0/562	0.61	0/753
9	J	0.37	0/504	0.55	0/678
9	W	0.37	0/500	0.56	0/675
10	K	0.46	0/163	0.56	0/225
10	X	0.69	1/163 (0.6%)	0.56	0/225
All	All	0.37	3/31638 (0.0%)	0.58	1/42939 (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	-8.75	1.34	1.53
10	X	17	TRP	CB-CG	7.05	1.62	1.50
3	C	183	PHE	CG-CD2	-5.48	1.30	1.38



All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	241	LYS	CB-CA-C	-5.13	100.14	110.40

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	20	0
1	N	3440	0	3337	13	0
2	B	3172	0	3152	9	0
2	O	3172	0	3152	20	0
3	C	2954	0	3010	29	0
3	P	2954	0	3010	32	0
4	D	1913	0	1860	10	0
4	Q	1913	0	1860	5	0
5	E	1519	0	1503	21	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3	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	1	0
15	Q	43	0	31	1	0
16	E	4	0	0	0	0
All	All	31648	0	31218	190	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 (190) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:G:1:GLY:C	7:G:2:ARG:HG2	2.09	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
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
10:K:19:PRO:HA	10:K:22:GLN:CD	2.16	0.66
3:C:183:PHE:HE2	3:P:183:PHE:CD1	2.09	0.65
2:O:197:ASN:C	2:O:230:LEU:HD12	2.17	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
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
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
4:D:116:ILE:HG12	15:D:501:HEC:HMA3	1.82	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:CD1	2.74	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:I:51:CYS:SG	5:I:52:ARG:N	2.76	0.56
5:E:155:GLY:C	5:E:156:TYR:CG	2.79	0.56
1:N:82:MET:CE	1:N:105:ASP:HB3	2.36	0.55
7:G:1:GLY:C	7:G:2:ARG:CG	2.74	0.55
10:K:32:LEU:O	10:K:36:THR:C	2.45	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
10:K:19:PRO:C	10:K:22:GLN:HG2	2.35	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
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
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
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
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:116:ILE:HG12	15:Q:501:HEC:HMA3	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:P:406:CDL:H521	14:P:406:CDL:C73	2.48	0.44
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
4:D:36:VAL:CG2	4:D:169:LEU:HD23	2.48	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
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:O:37:SER:HG	2:O:213:HIS:CG	2.39	0.41
4:Q:161:ALA:O	4:Q:162:PRO:C	2.58	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
1:N:145:MET:HE1	1:N:250:LEU:O	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	44	75
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	366 (100%)	2 (0%)	86	93
1	N	368/368 (100%)	366 (100%)	2 (0%)	86	93
2	B	332/332 (100%)	332 (100%)	0	100	100
2	O	332/332 (100%)	332 (100%)	0	100	100
3	C	320/320 (100%)	320 (100%)	0	100	100
3	P	320/320 (100%)	320 (100%)	0	100	100
4	D	205/205 (100%)	205 (100%)	0	100	100
4	Q	205/205 (100%)	205 (100%)	0	100	100
5	E	168/228 (74%)	167 (99%)	1 (1%)	84	91
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	S	91/99 (92%)	91 (100%)	0	100	100
7	G	66/72 (92%)	66 (100%)	0	100	100
7	T	71/72 (99%)	71 (100%)	0	100	100
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%)	3299 (100%)	5 (0%)	92	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	PHE
1	A	443	TRP
5	E	156	TYR
1	N	58	PHE
1	N	443	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry

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
11	HEM	P	402	3	41,50,50	1.45	7 (17%)	45,82,82	1.90	13 (28%)
14	CDL	D	503	-	42,42,99	1.02	2 (4%)	44,51,111	1.00	2 (4%)
11	HEM	C	501	3	41,50,50	1.37	6 (14%)	45,82,82	1.79	12 (26%)
15	HEC	D	501	4	32,50,50	2.19	11 (34%)	24,82,82	2.08	7 (29%)
12	MJM	C	503	-	27,28,28	1.58	2 (7%)	30,39,39	1.02	2 (6%)
11	HEM	P	403	3	41,50,50	1.39	5 (12%)	45,82,82	1.69	10 (22%)
14	CDL	P	406	-	45,45,99	1.14	3 (6%)	50,56,111	1.49	7 (14%)
15	HEC	Q	501	4	32,50,50	2.17	7 (21%)	24,82,82	2.20	6 (25%)
14	CDL	P	401	-	41,41,99	1.01	2 (4%)	45,50,111	1.19	3 (6%)
11	HEM	C	502	3	41,50,50	1.40	6 (14%)	45,82,82	1.66	8 (17%)
16	FES	E	501	5	0,4,4	-	-	-	-	-
13	PEE	E	502	-	28,28,50	1.16	2 (7%)	31,33,55	1.13	2 (6%)
14	CDL	P	407	-	37,37,99	1.35	4 (10%)	43,49,111	1.24	2 (4%)
14	CDL	C	506	-	36,36,99	1.36	4 (11%)	42,48,111	1.45	4 (9%)
13	PEE	R	201	-	33,33,50	1.33	3 (9%)	36,38,55	1.26	5 (13%)
13	PEE	P	405	-	37,37,50	1.20	4 (10%)	40,42,55	0.62	0
12	MJM	P	404	-	27,28,28	1.58	2 (7%)	30,39,39	1.24	3 (10%)
13	PEE	C	504	-	27,27,50	1.16	2 (7%)	29,31,55	0.56	0
13	PEE	D	502	-	41,41,50	4.15	7 (17%)	44,46,55	3.20	8 (18%)
13	PEE	R	202	-	23,23,50	1.24	2 (8%)	26,28,55	1.10	3 (11%)
14	CDL	C	505	-	41,41,99	1.48	4 (9%)	47,53,111	1.54	5 (10%)

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
11	HEM	P	402	3	-	5/12/54/54	-
14	CDL	D	503	-	-	18/48/48/110	-
11	HEM	C	501	3	-	5/12/54/54	-
15	HEC	D	501	4	-	4/10/54/54	-
12	MJM	C	503	-	1/1/5/5	0/8/35/35	0/4/4/4
11	HEM	P	403	3	-	4/12/54/54	-
14	CDL	P	406	-	-	25/55/55/110	-
15	HEC	Q	501	4	-	4/10/54/54	-
14	CDL	P	401	-	-	22/48/48/110	-
11	HEM	C	502	3	-	4/12/54/54	-
16	FES	E	501	5	-	-	0/1/1/1
13	PEE	E	502	-	1/1/4/8	13/32/32/54	-
14	CDL	P	407	-	-	20/45/45/110	-
14	CDL	C	506	-	-	22/44/44/110	-
13	PEE	R	201	-	1/1/4/8	15/37/37/54	-
13	PEE	P	405	-	-	11/41/41/54	-
12	MJM	P	404	-	1/1/5/5	0/8/35/35	0/4/4/4
13	PEE	C	504	-	-	10/30/30/54	-
13	PEE	D	502	-	1/1/4/8	18/45/45/54	-
13	PEE	R	202	-	1/1/4/8	8/27/27/54	-
14	CDL	C	505	-	-	28/49/49/110	-

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	502	PEE	O2-C2	-19.41	0.97	1.46
13	D	502	PEE	C1-C2	16.21	2.00	1.50
15	Q	501	HEC	C2B-C3B	6.22	1.47	1.40
15	D	501	HEC	C2B-C3B	5.91	1.46	1.40
15	D	501	HEC	C3C-C2C	5.58	1.46	1.40
15	Q	501	HEC	C3C-C2C	5.50	1.46	1.40
12	P	404	MJM	C5-N10	5.13	1.36	1.28
14	C	506	CDL	OB6-CB5	5.11	1.46	1.35
14	C	505	CDL	OA6-CA5	5.01	1.46	1.35
12	C	503	MJM	C5-N10	4.96	1.36	1.28
14	P	407	CDL	OB6-CB5	4.81	1.46	1.35
14	C	505	CDL	OA8-CA7	4.74	1.47	1.33
12	C	503	MJM	C8-C9	4.69	1.49	1.38
12	P	404	MJM	C8-C9	4.62	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	R	201	PEE	O3-C30	4.49	1.46	1.33
11	P	402	HEM	C1B-NB	-4.40	1.32	1.40
15	D	501	HEC	C3C-C4C	4.40	1.51	1.43
14	P	401	CDL	OB8-CB7	4.35	1.46	1.33
14	C	505	CDL	OB6-CB5	4.32	1.45	1.35
15	Q	501	HEC	C3C-C4C	4.27	1.50	1.43
14	P	406	CDL	OA8-CA7	4.25	1.45	1.33
14	P	407	CDL	OA6-CA5	4.23	1.46	1.34
14	D	503	CDL	OB6-CB5	4.17	1.46	1.34
14	D	503	CDL	OB8-CB7	4.11	1.45	1.33
11	C	502	HEM	C1B-NB	-4.08	1.33	1.40
13	D	502	PEE	O3-C30	4.03	1.45	1.33
13	R	201	PEE	O2-C10	4.01	1.45	1.34
13	E	502	PEE	O3-C30	4.01	1.45	1.33
11	P	403	HEM	C1B-NB	-3.98	1.33	1.40
13	R	202	PEE	O2-C10	3.88	1.45	1.34
14	P	401	CDL	OB6-CB5	3.86	1.45	1.34
14	P	406	CDL	OA6-CA5	3.78	1.45	1.34
13	R	202	PEE	O3-C30	3.76	1.44	1.33
13	E	502	PEE	O2-C10	3.75	1.44	1.34
14	P	406	CDL	OB6-CB5	3.74	1.44	1.34
13	D	502	PEE	O2-C10	3.68	1.44	1.34
13	D	502	PEE	C39-C38	3.68	1.53	1.31
14	C	506	CDL	OA6-CA5	3.61	1.44	1.34
13	D	502	PEE	C19-C18	3.61	1.52	1.28
11	C	501	HEM	C1B-NB	-3.60	1.34	1.40
13	R	201	PEE	C19-C18	3.58	1.52	1.28
11	P	403	HEM	C4D-ND	-3.35	1.34	1.40
11	P	402	HEM	C4D-ND	-3.26	1.34	1.40
13	C	504	PEE	O3-C30	3.14	1.42	1.33
11	C	501	HEM	FE-NB	3.03	2.11	1.96
11	P	402	HEM	C4B-NB	-3.01	1.32	1.38
13	P	405	PEE	O3-C30	2.97	1.42	1.33
13	P	405	PEE	P-O1P	2.96	1.61	1.50
11	C	502	HEM	FE-NB	2.94	2.11	1.96
13	P	405	PEE	O2-C10	2.93	1.42	1.34
15	D	501	HEC	C3D-C2D	2.78	1.45	1.37
15	Q	501	HEC	C3D-C2D	2.78	1.45	1.37
11	P	402	HEM	FE-NB	2.72	2.10	1.96
15	D	501	HEC	C2A-C3A	2.71	1.45	1.37
11	C	502	HEM	C4D-ND	-2.71	1.35	1.40
11	C	501	HEM	C4B-NB	-2.65	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	P	407	CDL	OB8-CB7	2.64	1.46	1.33
11	P	403	HEM	FE-NB	2.63	2.09	1.96
11	P	403	HEM	C4B-NB	-2.61	1.33	1.38
11	C	501	HEM	C4D-ND	-2.59	1.35	1.40
14	C	506	CDL	OA8-CA7	2.54	1.45	1.33
13	C	504	PEE	P-O1P	2.47	1.59	1.50
14	P	407	CDL	OA8-CA7	2.47	1.45	1.33
14	C	506	CDL	OB8-CB7	2.45	1.45	1.33
14	C	505	CDL	OB8-CB7	2.43	1.45	1.33
11	C	502	HEM	C3B-C4B	2.41	1.49	1.44
15	D	501	HEC	C3A-C4A	2.40	1.48	1.42
11	C	501	HEM	CHB-C1B	2.40	1.41	1.35
15	Q	501	HEC	C2A-C3A	2.36	1.44	1.37
15	D	501	HEC	C4B-C3B	2.35	1.47	1.43
13	P	405	PEE	C22-C21	-2.34	1.35	1.51
11	C	502	HEM	CHB-C1B	2.28	1.40	1.35
15	Q	501	HEC	CAA-C2A	-2.28	1.48	1.52
15	D	501	HEC	C1D-CHD	2.28	1.47	1.41
15	Q	501	HEC	C3A-C4A	2.21	1.47	1.42
13	D	502	PEE	C3-C2	-2.20	1.44	1.50
11	P	402	HEM	C4D-C3D	2.13	1.48	1.45
11	C	501	HEM	C3B-C4B	2.12	1.49	1.44
15	D	501	HEC	C2A-C1A	2.11	1.47	1.42
11	C	502	HEM	C4B-NB	-2.09	1.34	1.38
11	P	403	HEM	O2D-CGD	-2.06	1.23	1.30
11	P	402	HEM	C1D-C2D	2.06	1.48	1.44
15	D	501	HEC	C1B-CHB	2.04	1.46	1.41
11	P	402	HEM	CHB-C1B	2.03	1.40	1.35
15	D	501	HEC	C4D-CHA	2.02	1.46	1.41

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	502	PEE	O2-C2-C3	15.35	163.99	108.40
13	D	502	PEE	O3-C3-C2	-8.52	83.62	108.43
13	D	502	PEE	C3-C2-C1	-8.27	92.24	111.79
14	C	505	CDL	CB4-OB6-CB5	-5.59	107.47	117.90
14	C	505	CDL	OB6-CB5-C51	5.40	121.03	111.09
11	P	403	HEM	C1B-NB-C4B	5.24	110.48	105.07
14	C	506	CDL	OB6-CB5-C51	5.23	120.71	111.09
15	Q	501	HEC	CMB-C2B-C3B	5.14	131.87	125.82
14	P	401	CDL	OB6-CB5-C51	5.06	122.40	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	502	PEE	O2-C10-C11	5.00	122.28	111.50
15	Q	501	HEC	C1D-C2D-C3D	-4.80	103.66	107.00
15	D	501	HEC	C1D-C2D-C3D	-4.69	103.73	107.00
14	P	406	CDL	OB6-CB5-C51	4.68	121.58	111.50
14	P	407	CDL	OB6-CB5-C51	4.68	119.69	111.09
11	P	402	HEM	C1B-NB-C4B	4.66	109.88	105.07
14	P	406	CDL	CB4-OB6-CB5	-4.60	106.46	117.79
15	D	501	HEC	CMB-C2B-C3B	4.51	131.12	125.82
11	P	402	HEM	CHC-C4B-NB	4.49	129.30	124.43
11	C	502	HEM	C1B-NB-C4B	4.37	109.59	105.07
11	P	402	HEM	CHD-C1D-ND	4.27	129.07	124.43
11	C	501	HEM	C1B-NB-C4B	4.20	109.42	105.07
13	R	201	PEE	O2-C10-C11	4.20	120.55	111.50
15	Q	501	HEC	CBD-CAD-C3D	-4.17	105.50	112.62
11	P	403	HEM	CHD-C1D-ND	4.09	128.87	124.43
11	P	403	HEM	CHC-C4B-NB	3.98	128.76	124.43
12	P	404	MJM	C11-C9-N10	3.97	118.80	112.53
14	D	503	CDL	OB6-CB5-C51	3.94	119.99	111.50
14	C	506	CDL	OA6-CA5-C11	3.85	121.53	110.80
11	C	501	HEM	CHC-C4B-NB	3.81	128.57	124.43
11	C	501	HEM	CMD-C2D-C1D	3.58	130.49	125.04
11	C	502	HEM	CHC-C4B-NB	3.57	128.31	124.43
11	C	502	HEM	CHD-C1D-ND	3.57	128.31	124.43
11	P	402	HEM	CHD-C1D-C2D	-3.56	119.42	124.98
13	E	502	PEE	O2-C10-C11	3.44	118.91	111.50
14	P	407	CDL	OA6-CA5-C11	3.44	118.91	111.50
13	D	502	PEE	O2-C10-O4	-3.41	115.45	123.70
11	C	501	HEM	CHD-C1D-ND	3.36	128.08	124.43
15	Q	501	HEC	CAA-CBA-CGA	-3.29	104.54	113.76
14	C	505	CDL	OA6-CA5-C11	3.29	117.14	111.09
11	C	502	HEM	C4B-C3B-C2B	-3.29	104.50	107.11
12	C	503	MJM	C11-C9-N10	3.28	117.70	112.53
11	P	402	HEM	CMD-C2D-C1D	3.26	130.01	125.04
11	C	501	HEM	CBA-CAA-C2A	-3.23	107.11	112.62
11	C	502	HEM	CHD-C1D-C2D	-3.19	119.99	124.98
14	P	406	CDL	OA6-CA5-C11	3.17	119.64	110.80
15	D	501	HEC	CAA-CBA-CGA	-3.13	104.98	113.76
15	D	501	HEC	CBD-CAD-C3D	-3.10	107.34	112.62
12	C	503	MJM	C5-N10-C9	3.04	123.85	118.61
14	C	505	CDL	OB6-CB5-OB7	-3.00	117.01	122.96
11	P	403	HEM	CHA-C4D-ND	2.97	128.05	124.38
11	P	402	HEM	C4B-CHC-C1C	2.96	126.47	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	P	406	CDL	OB6-CB5-OB7	-2.95	116.58	123.70
11	P	402	HEM	CBA-CAA-C2A	-2.92	107.64	112.62
11	C	501	HEM	CHD-C1D-C2D	-2.84	120.55	124.98
15	Q	501	HEC	CMC-C2C-C3C	2.82	129.13	125.82
14	P	401	CDL	OB6-CB5-OB7	-2.79	116.96	123.70
15	Q	501	HEC	C4C-C3C-C2C	-2.77	103.36	106.35
12	P	404	MJM	C5-N10-C9	2.76	123.37	118.61
14	P	406	CDL	OA8-CA7-C31	2.73	120.48	111.91
14	C	506	CDL	OA6-CA5-OA7	-2.67	117.25	123.70
13	D	502	PEE	O3-C30-C31	2.67	120.29	111.91
11	C	501	HEM	CAD-C3D-C4D	2.67	129.32	124.66
15	D	501	HEC	C4C-C3C-C2C	-2.64	103.50	106.35
11	P	403	HEM	CHD-C1D-C2D	-2.63	120.86	124.98
11	C	502	HEM	C4B-CHC-C1C	2.62	126.02	122.56
15	D	501	HEC	CMC-C2C-C3C	2.61	128.89	125.82
11	C	501	HEM	C4B-C3B-C2B	-2.60	105.05	107.11
13	R	201	PEE	C3-O3-C30	2.55	126.55	117.12
11	P	402	HEM	CAD-C3D-C4D	2.54	129.09	124.66
13	E	502	PEE	O3-C30-C31	2.51	119.78	111.91
11	C	502	HEM	CHA-C4D-ND	2.49	127.46	124.38
11	C	502	HEM	CHA-C4D-C3D	-2.45	120.74	125.33
13	R	202	PEE	O3-C30-C31	2.44	119.55	111.91
13	R	202	PEE	O2-C10-C11	2.41	117.52	110.80
13	R	201	PEE	O2-C10-O4	-2.39	117.92	123.70
14	P	406	CDL	OA6-CA4-CA3	2.38	117.01	108.40
11	C	501	HEM	C4B-CHC-C1C	2.37	125.69	122.56
14	D	503	CDL	OB8-CB7-C71	2.30	119.14	111.91
13	D	502	PEE	C17-C18-C19	-2.28	111.35	126.84
13	R	201	PEE	C17-C18-C19	-2.28	111.36	126.84
14	C	505	CDL	OA8-CA7-C31	2.27	119.03	111.91
15	D	501	HEC	CBA-CAA-C2A	2.26	116.41	112.60
14	P	401	CDL	CB6-OB8-CB7	2.24	125.43	117.12
11	C	501	HEM	CMC-C2C-C3C	2.24	128.86	124.68
13	R	201	PEE	O3-C30-C31	2.23	118.92	111.91
11	C	501	HEM	C3C-C4C-NC	-2.22	106.75	110.94
11	P	402	HEM	CHA-C4D-C3D	-2.20	121.19	125.33
11	P	403	HEM	CHA-C4D-C3D	-2.20	121.20	125.33
13	R	202	PEE	O3-C30-O5	-2.19	118.06	123.59
11	P	402	HEM	CHA-C4D-ND	2.18	127.08	124.38
11	P	403	HEM	C3C-C4C-NC	-2.17	106.84	110.94
14	P	406	CDL	OA8-CA7-OA9	-2.15	118.16	123.59
14	C	506	CDL	CA6-OA8-CA7	2.13	122.46	117.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	P	402	HEM	CMC-C2C-C3C	2.12	128.65	124.68
11	P	402	HEM	C4B-C3B-C2B	-2.09	105.46	107.11
12	P	404	MJM	C20-O19-C15	2.07	123.65	118.80
11	P	403	HEM	CBA-CAA-C2A	-2.06	109.10	112.62
11	P	402	HEM	O2D-CGD-CBD	2.04	120.58	114.03
11	P	403	HEM	C4A-C3A-C2A	2.04	108.41	107.00
11	C	501	HEM	O2D-CGD-CBD	2.04	120.57	114.03
13	D	502	PEE	C2-O2-C10	-2.01	112.84	117.79
11	P	403	HEM	CHB-C1B-NB	2.01	126.86	124.38

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 (236) 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-O2P
13	E	502	PEE	C4-O4P-P-O3P
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	C11-CA5-OA6-CA4
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	506	CDL	O1-C1-CB2-OB2
14	C	506	CDL	CA2-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
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	OB7-CB5-OB6-CB4
14	C	506	CDL	C51-CB5-OB6-CB4
14	D	503	CDL	CA2-OA2-PA1-OA3
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-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	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
14	P	406	CDL	CB2-OB2-PB2-OB4
14	P	406	CDL	C51-CB5-OB6-CB4
14	P	407	CDL	CA3-OA5-PA1-OA3
14	P	407	CDL	CB3-OB5-PB2-OB3
14	P	407	CDL	C51-CB5-OB6-CB4
14	C	505	CDL	C51-CB5-OB6-CB4
14	C	505	CDL	OB7-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	C	505	CDL	OB9-CB7-OB8-CB6
14	C	506	CDL	C71-CB7-OB8-CB6
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	P	407	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
14	D	503	CDL	C71-CB7-OB8-CB6
14	P	406	CDL	C31-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	R	201	PEE	C10-C11-C12-C13
13	R	201	PEE	C30-C31-C32-C33
13	D	502	PEE	C4-O4P-P-O3P
14	C	506	CDL	CA3-OA5-PA1-OA2
14	C	506	CDL	CB3-OB5-PB2-OB2
14	D	503	CDL	CB3-OB5-PB2-OB2
14	P	401	CDL	CA2-OA2-PA1-OA5
14	P	401	CDL	CB3-OB5-PB2-OB2
14	P	406	CDL	CA2-OA2-PA1-OA5
14	P	406	CDL	CB2-OB2-PB2-OB5
14	P	407	CDL	CA3-OA5-PA1-OA2
14	P	407	CDL	CB3-OB5-PB2-OB2
13	E	502	PEE	C31-C30-O3-C3
13	P	405	PEE	C12-C13-C14-C15
14	P	407	CDL	C11-CA5-OA6-CA4
13	C	504	PEE	C12-C13-C14-C15
14	P	406	CDL	CA3-CA4-OA6-CA5
14	P	407	CDL	OA7-CA5-OA6-CA4
13	D	502	PEE	C16-C17-C18-C19
14	D	503	CDL	O1-C1-CB2-OB2
13	D	502	PEE	C13-C14-C15-C16
14	P	406	CDL	C31-C32-C33-C34
13	P	405	PEE	C19-C20-C21-C22
13	E	502	PEE	O5-C30-O3-C3
13	E	502	PEE	C11-C10-O2-C2
14	D	503	CDL	C72-C73-C74-C75
13	R	201	PEE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
13	R	201	PEE	C13-C14-C15-C16
14	P	401	CDL	C71-C72-C73-C74
13	E	502	PEE	O4-C10-O2-C2
13	P	405	PEE	C33-C34-C35-C36
13	R	202	PEE	O4-C10-O2-C2
14	P	401	CDL	C58-C59-C60-C61
13	R	202	PEE	C31-C32-C33-C34
13	P	405	PEE	C13-C14-C15-C16
13	R	202	PEE	C11-C10-O2-C2
13	D	502	PEE	O3P-C1-C2-O2
13	C	504	PEE	C13-C14-C15-C16
13	D	502	PEE	C33-C34-C35-C36
13	C	504	PEE	C10-C11-C12-C13
14	C	505	CDL	CA2-OA2-PA1-OA5
14	D	503	CDL	CA2-OA2-PA1-OA5
14	C	506	CDL	OB5-CB3-CB4-CB6
14	P	406	CDL	OB5-CB3-CB4-CB6
13	D	502	PEE	C11-C12-C13-C14
13	D	502	PEE	C42-C43-C44-C45
14	C	505	CDL	CA3-CA4-CA6-OA8
14	D	503	CDL	CB3-CB4-CB6-OB8
14	P	401	CDL	C51-C52-C53-C54
13	D	502	PEE	C15-C16-C17-C18
13	P	405	PEE	C20-C21-C22-C23
14	C	505	CDL	C32-C33-C34-C35
13	E	502	PEE	C13-C14-C15-C16
14	P	407	CDL	OB5-CB3-CB4-OB6
13	E	502	PEE	C33-C34-C35-C36
14	P	406	CDL	C72-C71-CB7-OB8
14	C	505	CDL	OA5-CA3-CA4-CA6
14	C	506	CDL	OA5-CA3-CA4-CA6
14	P	407	CDL	CA3-CA4-CA6-OA8
14	D	503	CDL	CA3-OA5-PA1-OA2
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	C	505	CDL	OB5-CB3-CB4-CB6
14	D	503	CDL	C75-C76-C77-C78

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Mol	Chain	Res	Type	Atoms
13	P	405	PEE	C35-C36-C37-C38
14	P	401	CDL	C73-C74-C75-C76
14	C	505	CDL	CB3-CB4-CB6-OB8
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	OA6-CA4-CA6-OA8
14	C	505	CDL	OB6-CB4-CB6-OB8
14	C	506	CDL	OB6-CB4-CB6-OB8
14	C	506	CDL	C31-CA7-OA8-CA6
13	R	202	PEE	C1-O3P-P-O4P
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	CB3-OB5-PB2-OB4
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
14	P	407	CDL	OB5-CB3-CB4-CB6
13	R	201	PEE	C5-C4-O4P-P
14	P	406	CDL	OB5-CB3-CB4-OB6
14	P	407	CDL	OA5-CA3-CA4-OA6
14	P	406	CDL	O1-C1-CB2-OB2
14	C	505	CDL	C34-C35-C36-C37
14	P	407	CDL	OA6-CA4-CA6-OA8
14	P	406	CDL	C71-CB7-OB8-CB6
13	D	502	PEE	C31-C32-C33-C34
13	C	504	PEE	O5-C30-C31-C32
13	D	502	PEE	C3-C2-O2-C10
11	P	402	HEM	C3D-CAD-CBD-CGD
14	C	506	CDL	OA6-CA4-CA6-OA8
13	C	504	PEE	C4-O4P-P-O3P
13	E	502	PEE	C1-O3P-P-O4P
14	D	503	CDL	CB2-OB2-PB2-OB5
13	C	504	PEE	C16-C17-C18-C19
14	D	503	CDL	CA2-C1-CB2-OB2
14	D	503	CDL	C71-C72-C73-C74
11	C	501	HEM	CAD-CBD-CGD-O1D
11	P	402	HEM	CAD-CBD-CGD-O1D
13	P	405	PEE	C16-C17-C18-C19
11	P	403	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
13	R	201	PEE	C15-C16-C17-C18
14	P	406	CDL	C52-C51-CB5-OB6
14	P	401	CDL	CA3-OA5-PA1-OA4
11	C	502	HEM	CAA-CBA-CGA-O2A
11	P	403	HEM	CAD-CBD-CGD-O2D
11	C	502	HEM	CAA-CBA-CGA-O1A
11	P	403	HEM	CAD-CBD-CGD-O1D
13	R	201	PEE	C3-C2-O2-C10
14	C	505	CDL	CA3-CA4-OA6-CA5
13	C	504	PEE	O3-C30-C31-C32
13	R	201	PEE	O3-C30-C31-C32
11	C	501	HEM	CAD-CBD-CGD-O2D
11	C	501	HEM	C3D-CAD-CBD-CGD
11	P	402	HEM	CAD-CBD-CGD-O2D
14	P	401	CDL	C59-C60-C61-C62
11	P	403	HEM	CAA-CBA-CGA-O2A
13	R	202	PEE	C2-C1-O3P-P
14	C	505	CDL	C32-C31-CA7-OA8
13	R	201	PEE	C16-C17-C18-C19
11	C	502	HEM	CAD-CBD-CGD-O2D
11	P	402	HEM	CAA-CBA-CGA-O2A
14	C	505	CDL	OB5-CB3-CB4-OB6
11	C	501	HEM	CAA-CBA-CGA-O2A
15	D	501	HEC	CAA-CBA-CGA-O2A
14	P	407	CDL	OA5-CA3-CA4-CA6
14	C	506	CDL	OA9-CA7-OA8-CA6
14	P	401	CDL	C57-C58-C59-C60
11	C	501	HEM	CAA-CBA-CGA-O1A
11	P	402	HEM	CAA-CBA-CGA-O1A
15	Q	501	HEC	CAA-CBA-CGA-O2A
15	Q	501	HEC	CAD-CBD-CGD-O1D
13	C	504	PEE	O2-C10-C11-C12
13	E	502	PEE	C12-C13-C14-C15
11	C	502	HEM	CAD-CBD-CGD-O1D
14	C	506	CDL	CB3-CB4-CB6-OB8
15	D	501	HEC	CAD-CBD-CGD-O1D
15	D	501	HEC	CAD-CBD-CGD-O2D
15	D	501	HEC	CAA-CBA-CGA-O1A
15	Q	501	HEC	CAA-CBA-CGA-O1A
13	P	405	PEE	O3-C30-C31-C32
13	D	502	PEE	C38-C39-C40-C41
14	P	406	CDL	C12-C11-CA5-OA6

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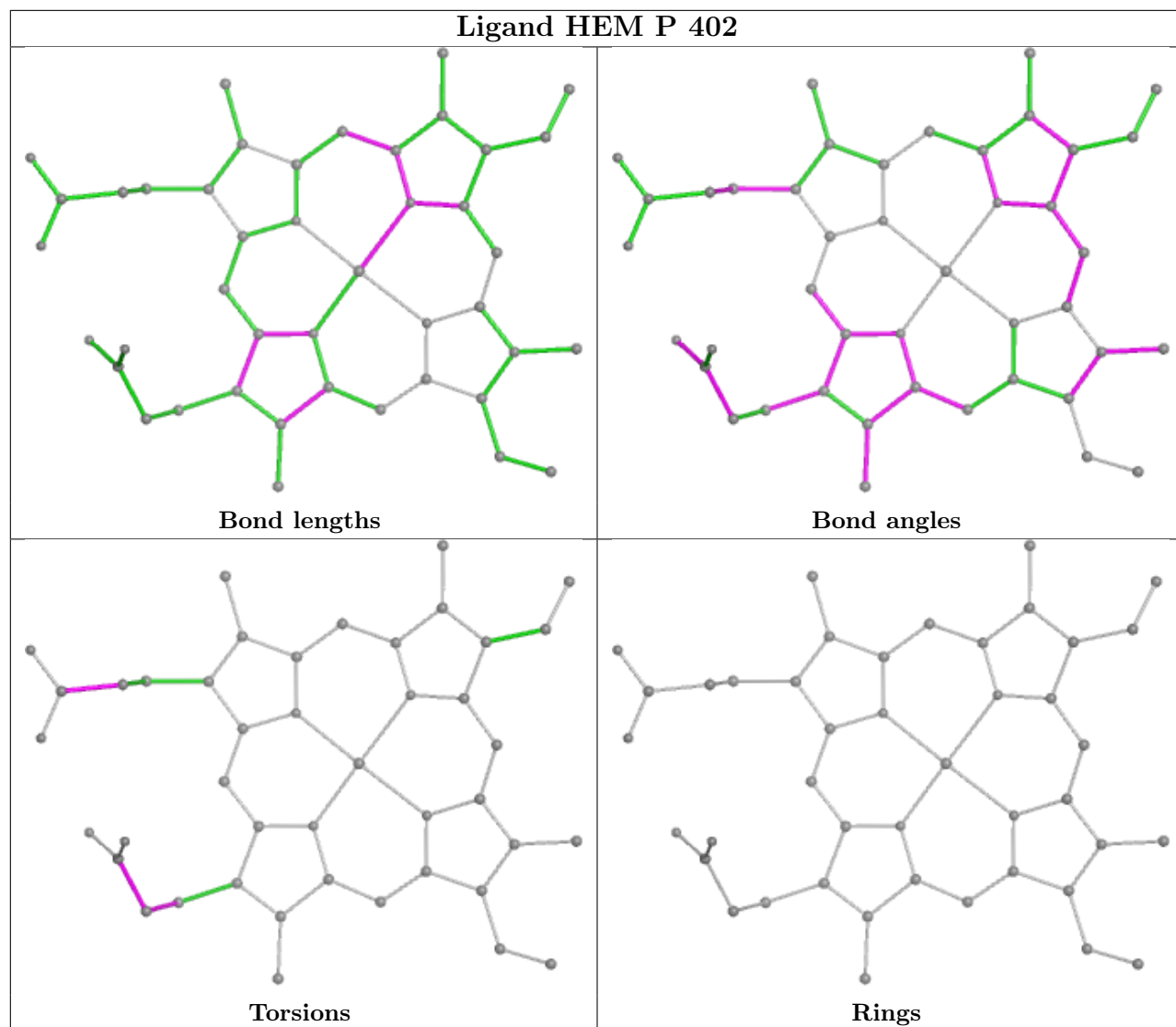
Mol	Chain	Res	Type	Atoms
15	Q	501	HEC	CAD-CBD-CGD-O2D
14	P	401	CDL	CA3-OA5-PA1-OA2
13	D	502	PEE	C5-C4-O4P-P
13	R	201	PEE	C1-C2-O2-C10
14	P	406	CDL	C12-C11-CA5-OA7
13	C	504	PEE	C17-C18-C19-C20
13	P	405	PEE	O5-C30-C31-C32

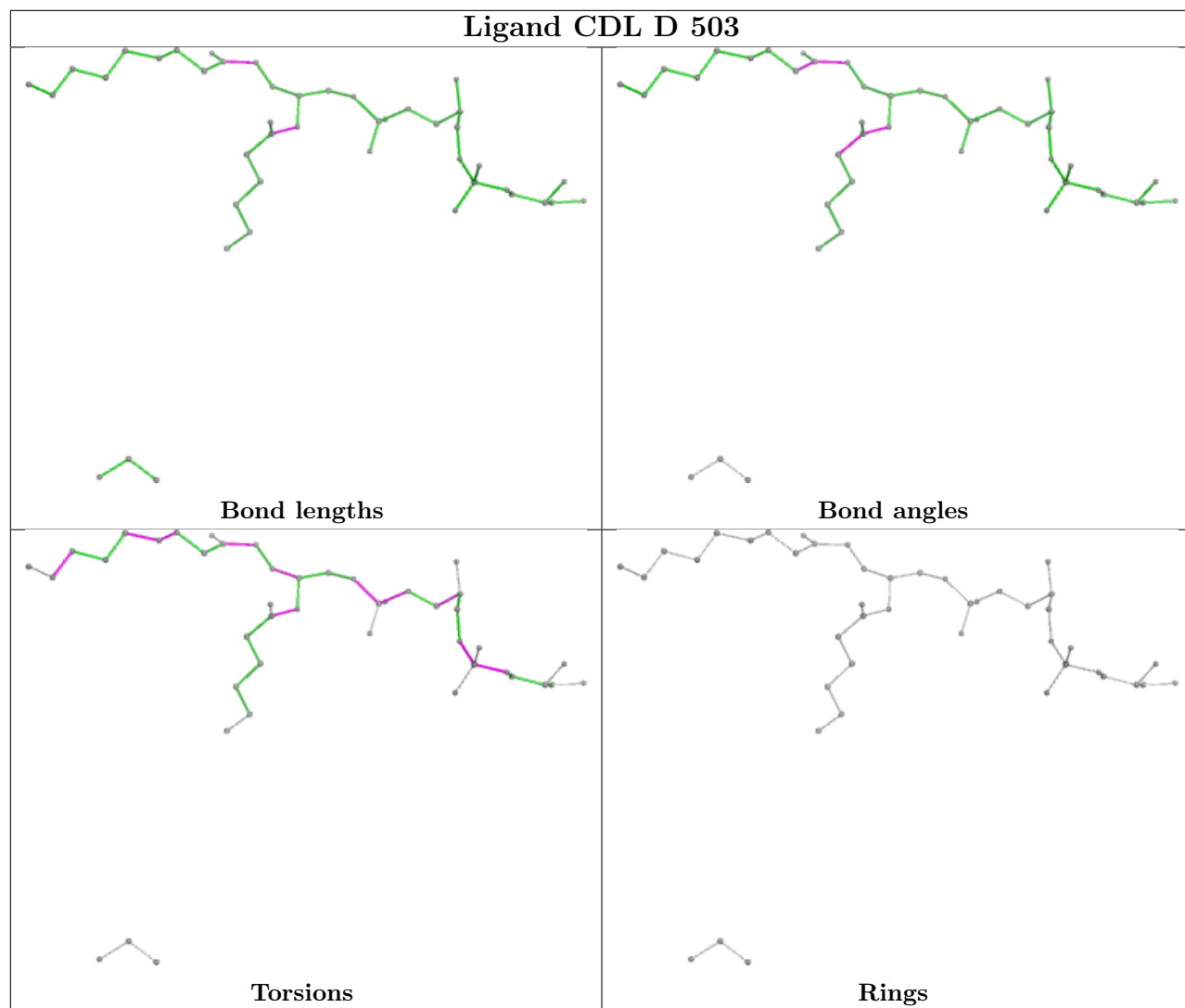
There are no ring outliers.

13 monomers are involved in 44 short contacts:

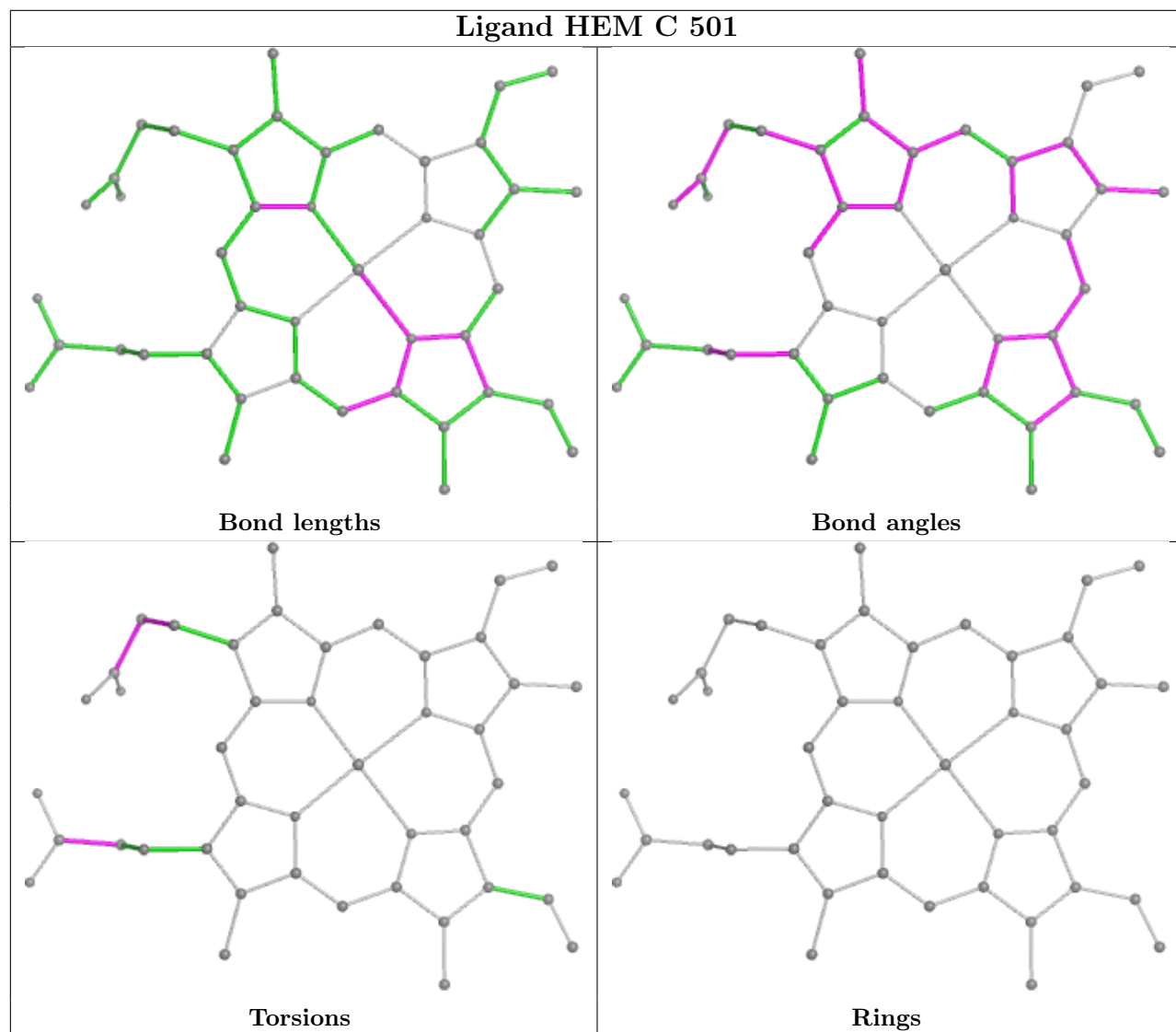
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	P	402	HEM	6	0
11	C	501	HEM	13	0
15	D	501	HEC	1	0
11	P	403	HEM	8	0
14	P	406	CDL	3	0
15	Q	501	HEC	1	0
11	C	502	HEM	2	0
13	E	502	PEE	1	0
13	R	201	PEE	2	0
12	P	404	MJM	1	0
13	D	502	PEE	5	0
13	R	202	PEE	1	0
14	C	505	CDL	1	0

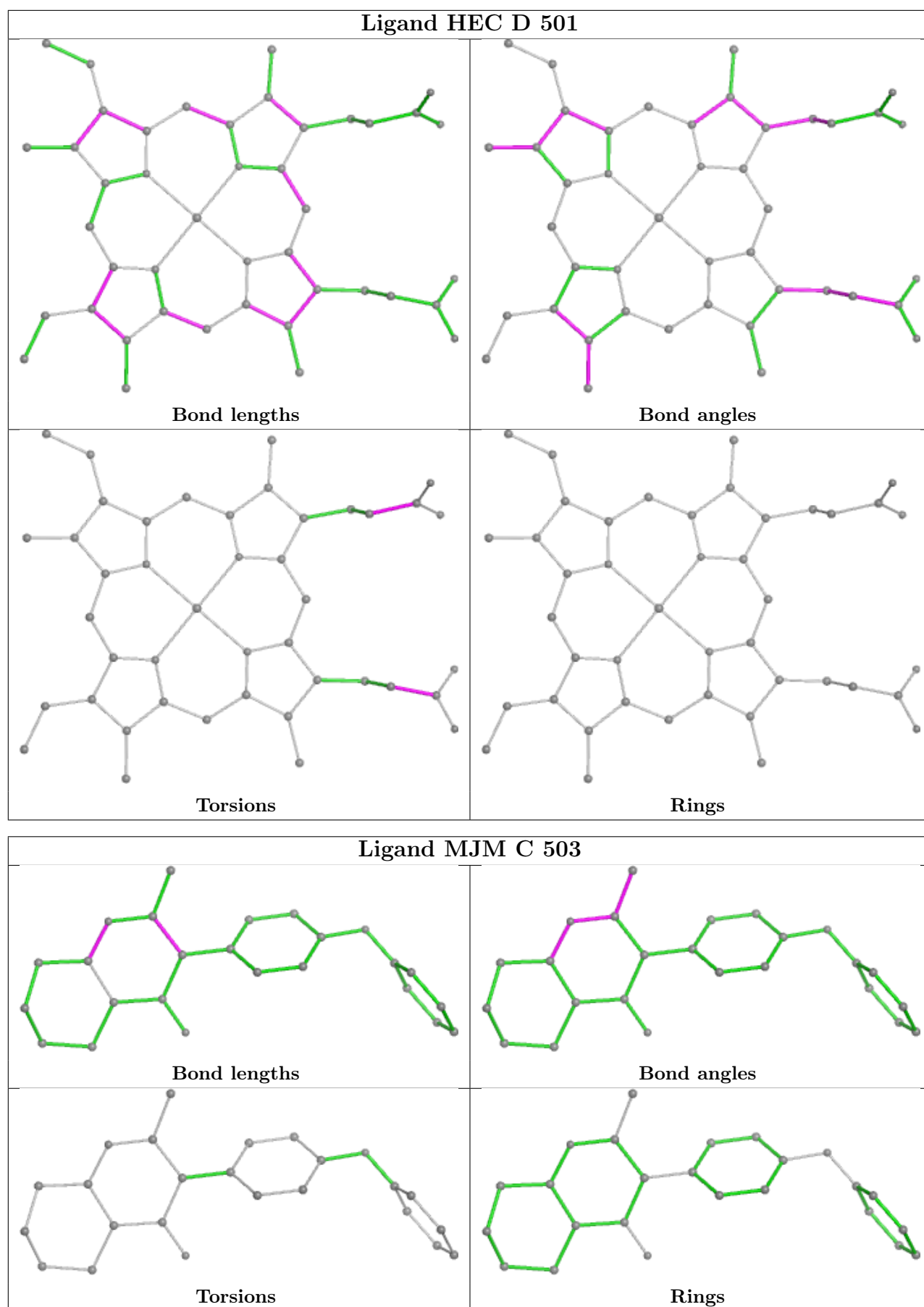
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

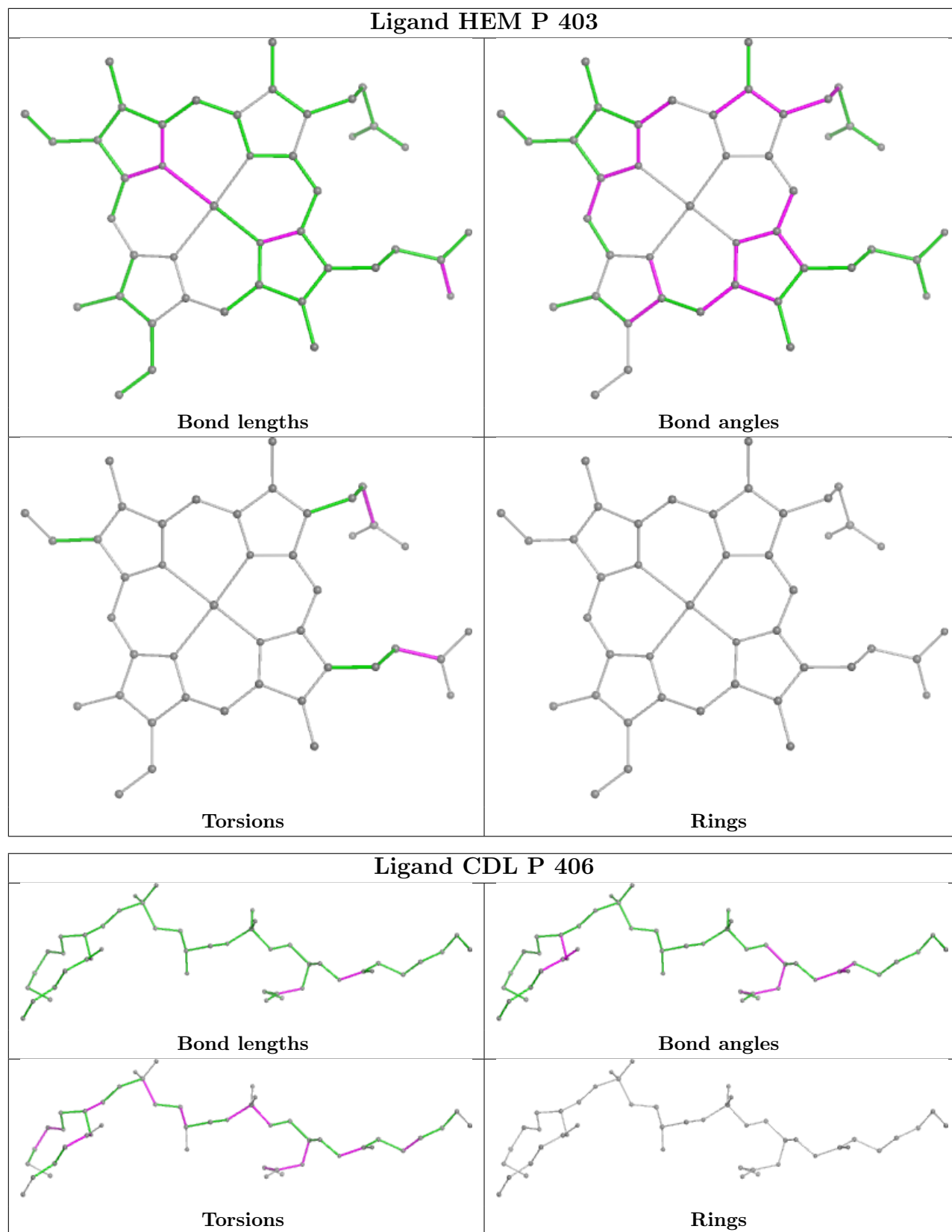


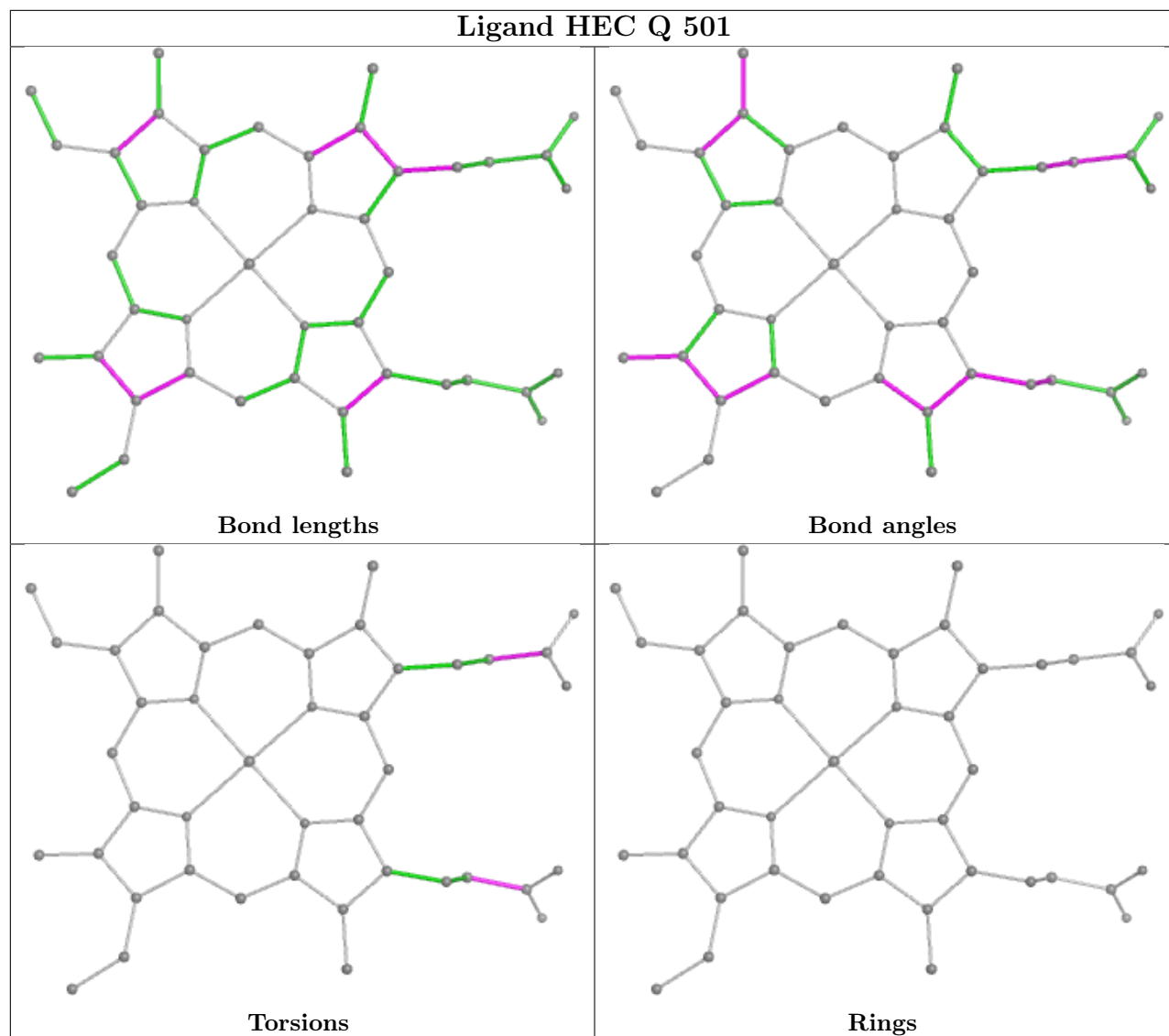


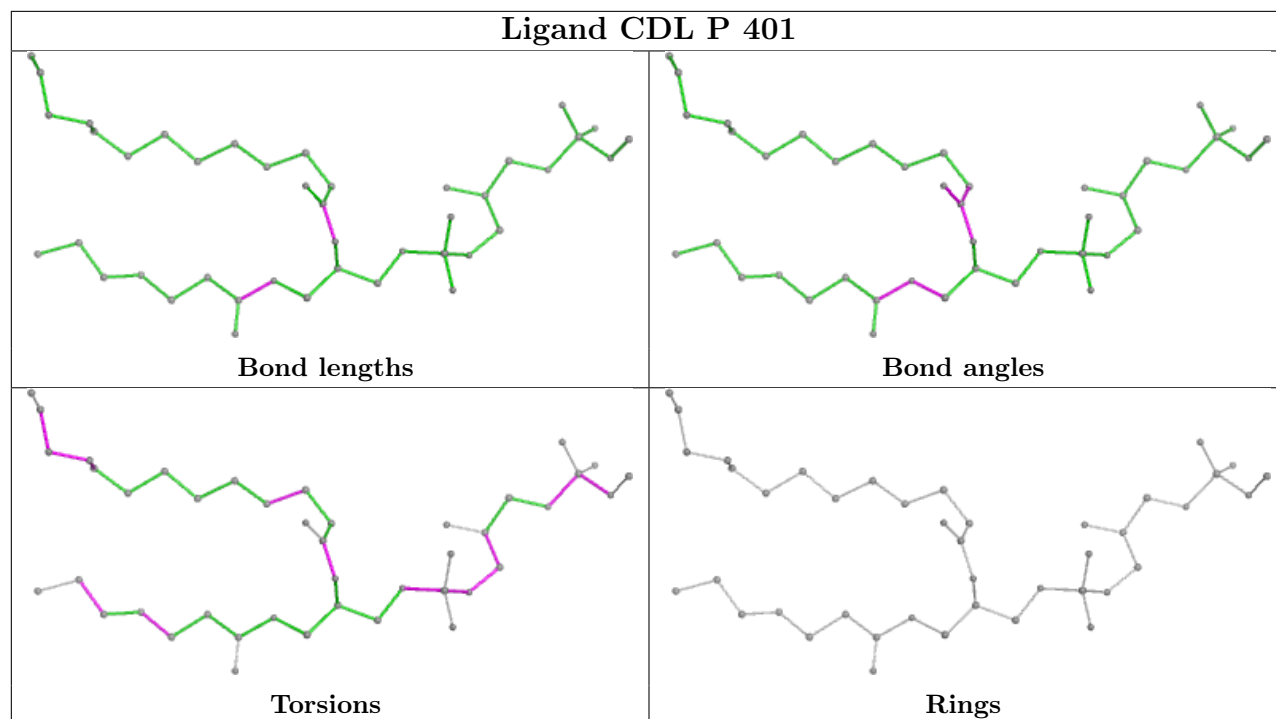


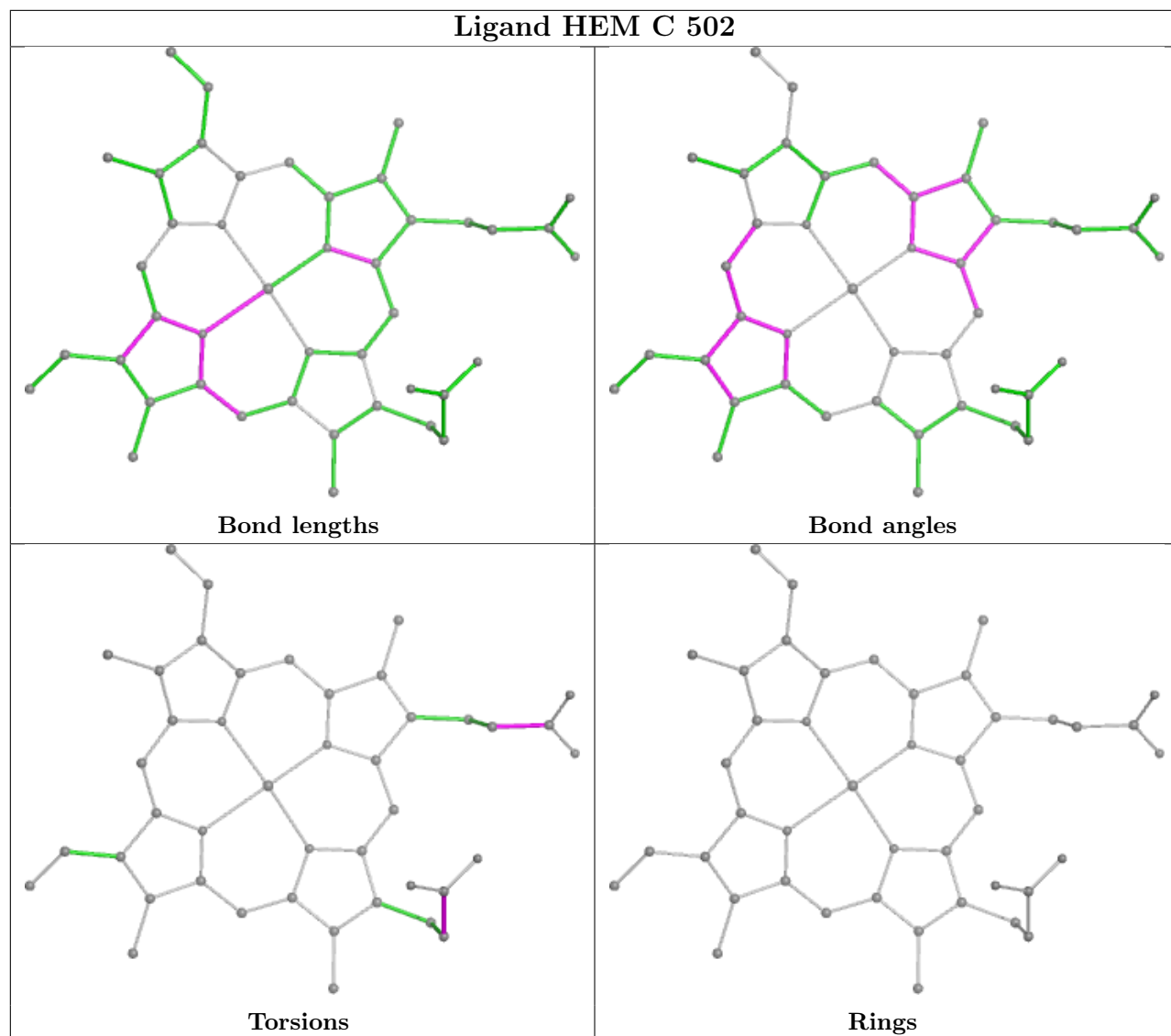


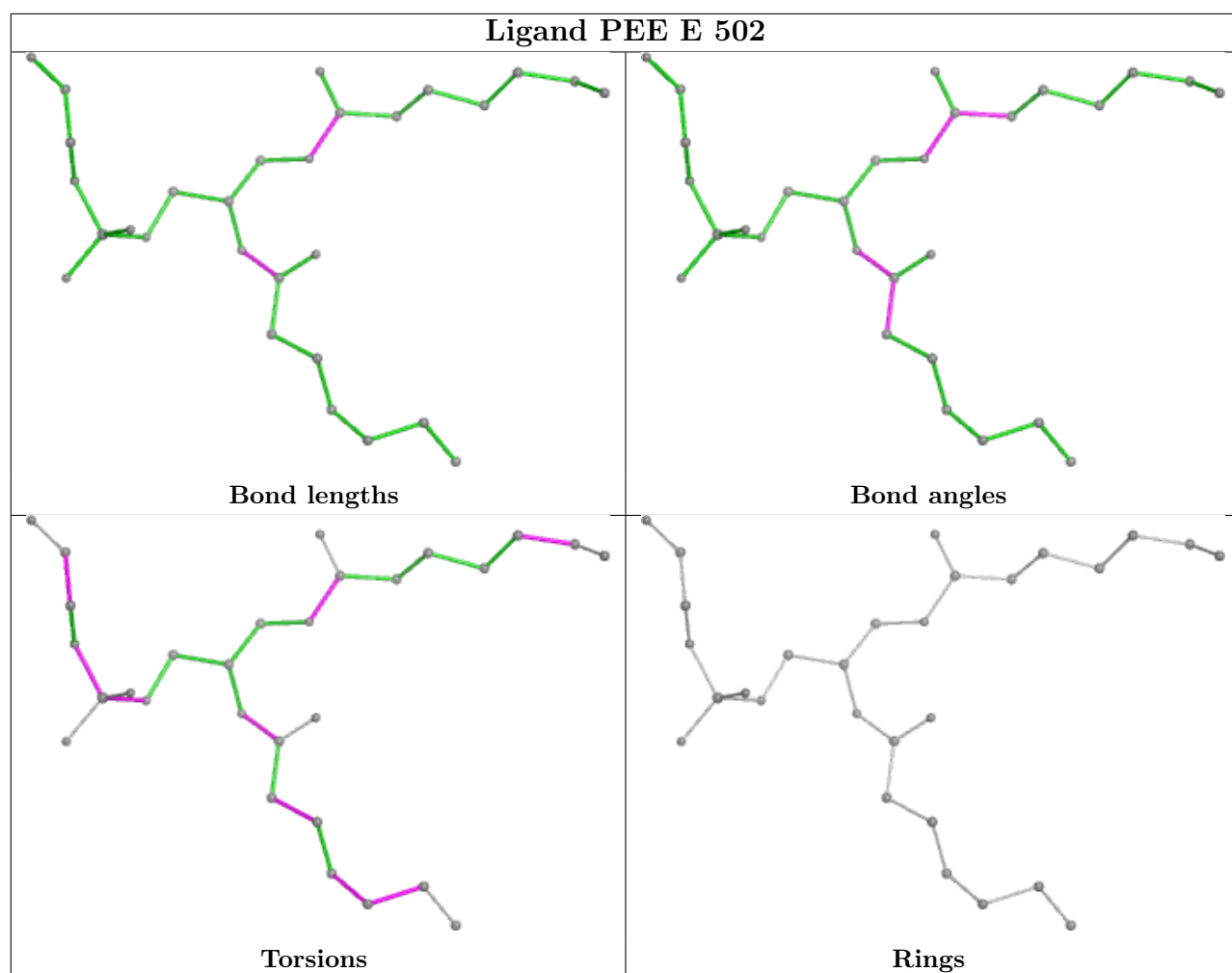


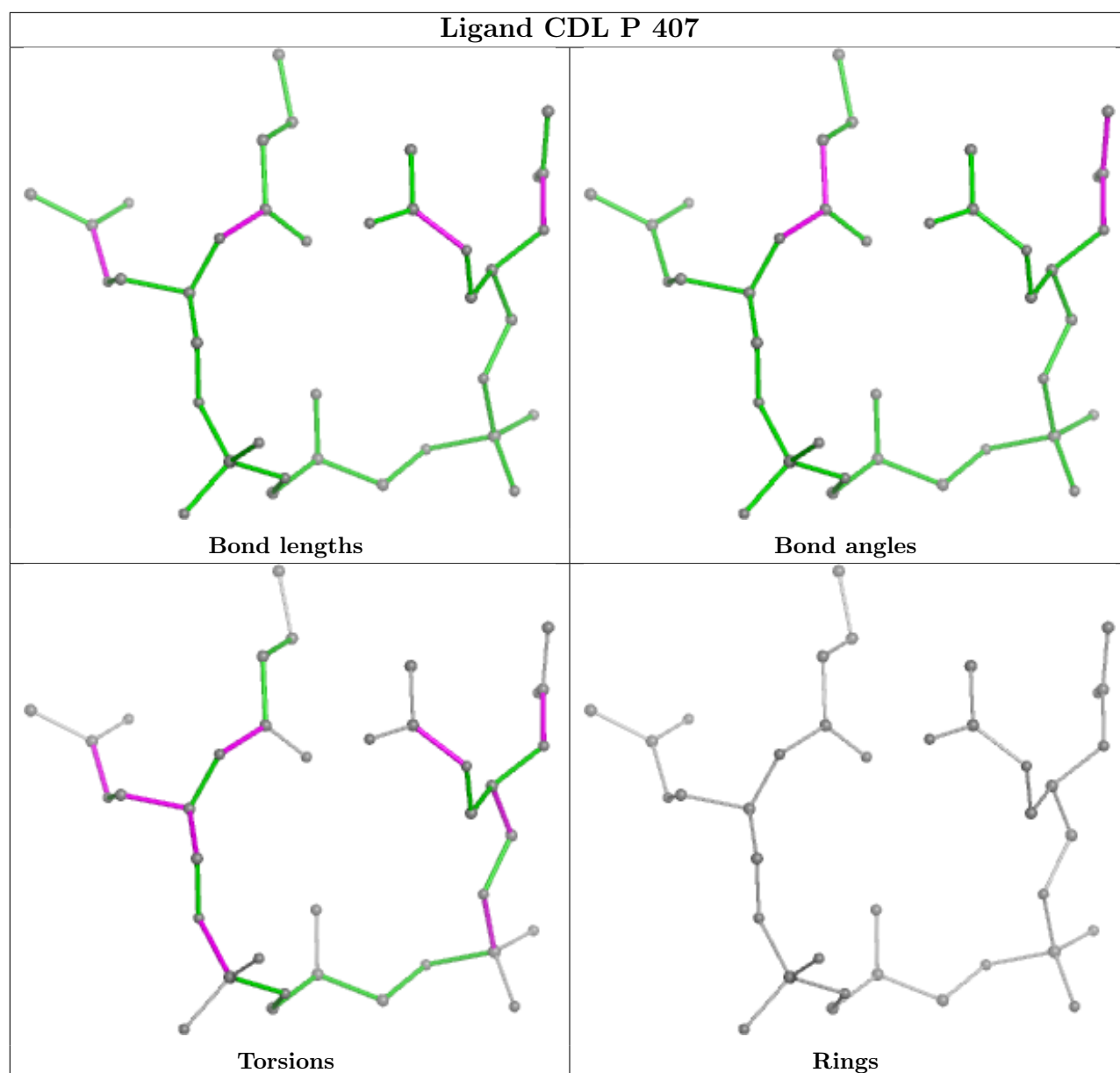




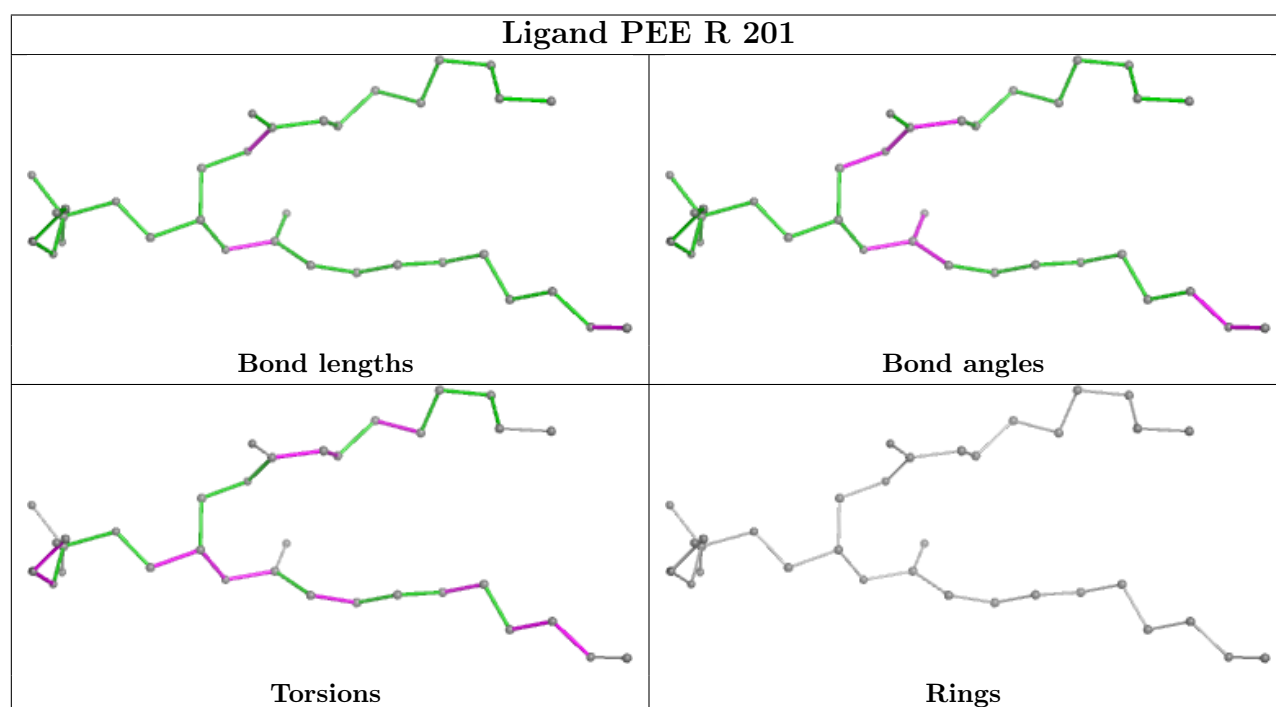
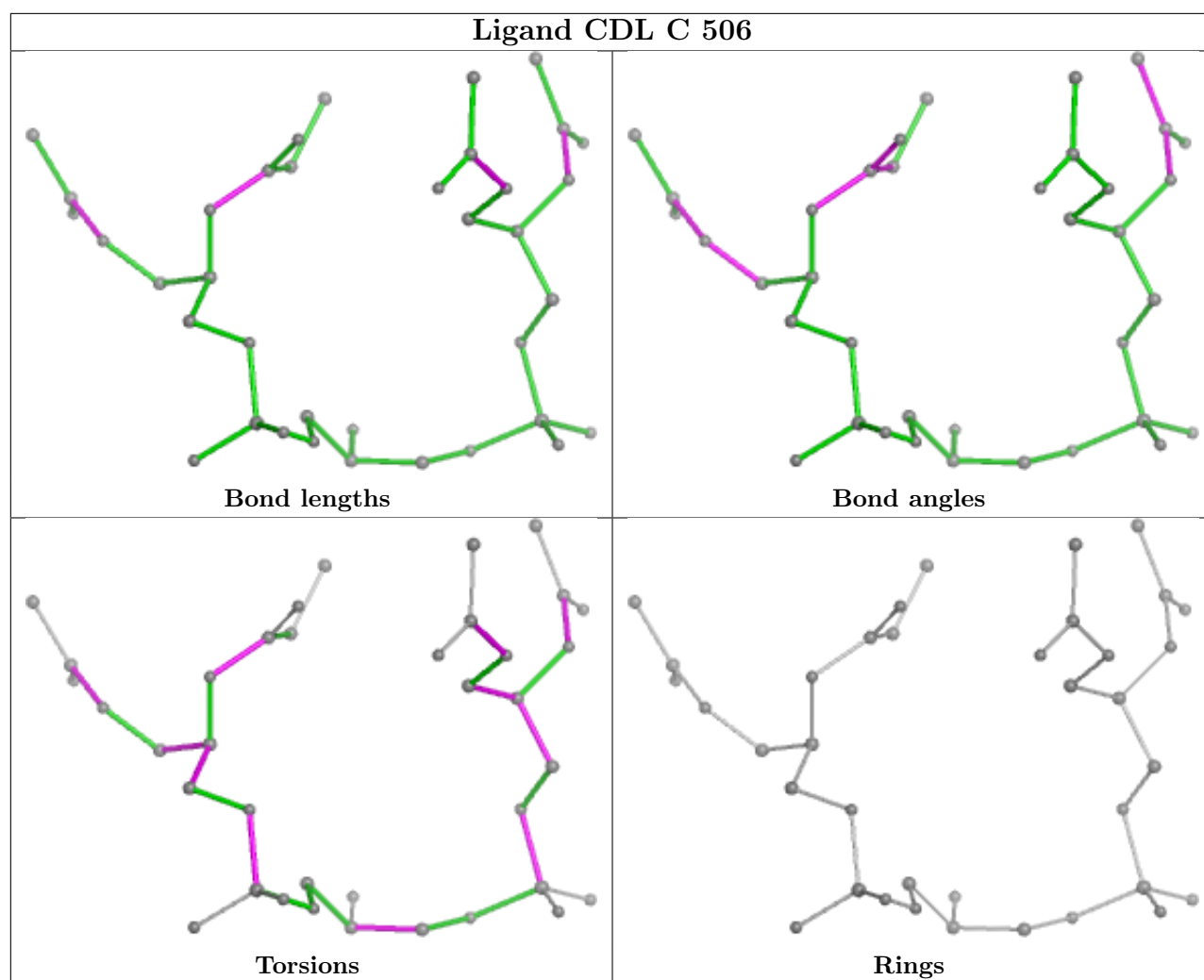


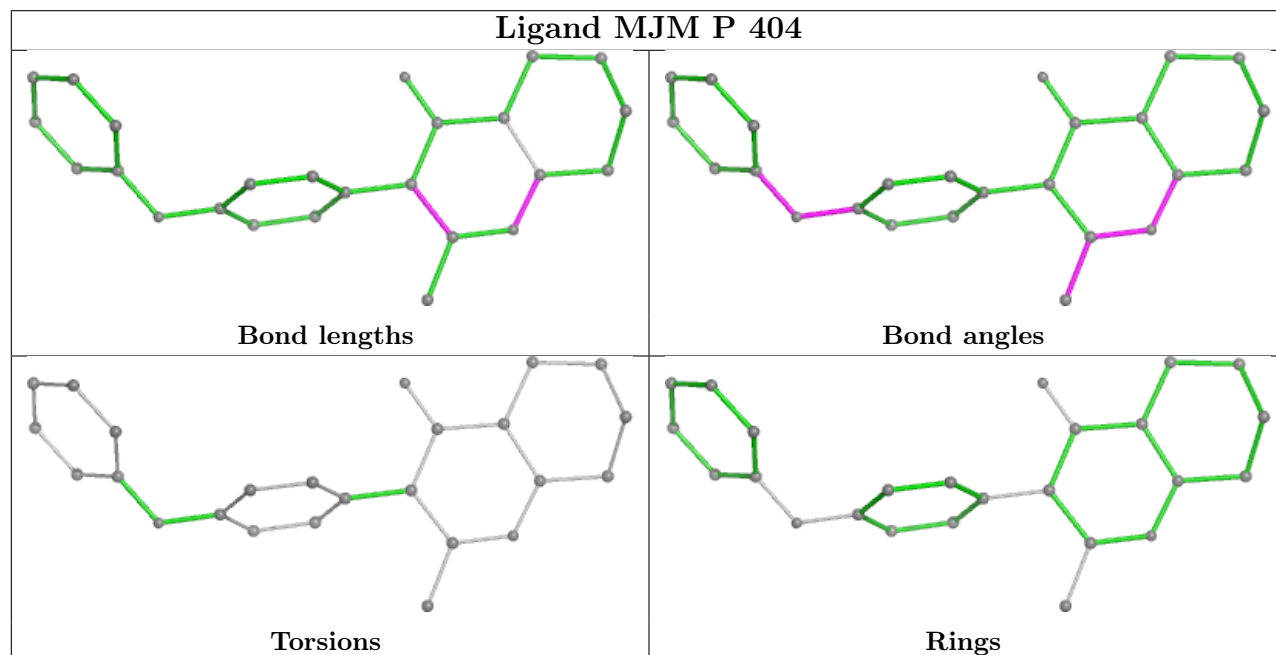
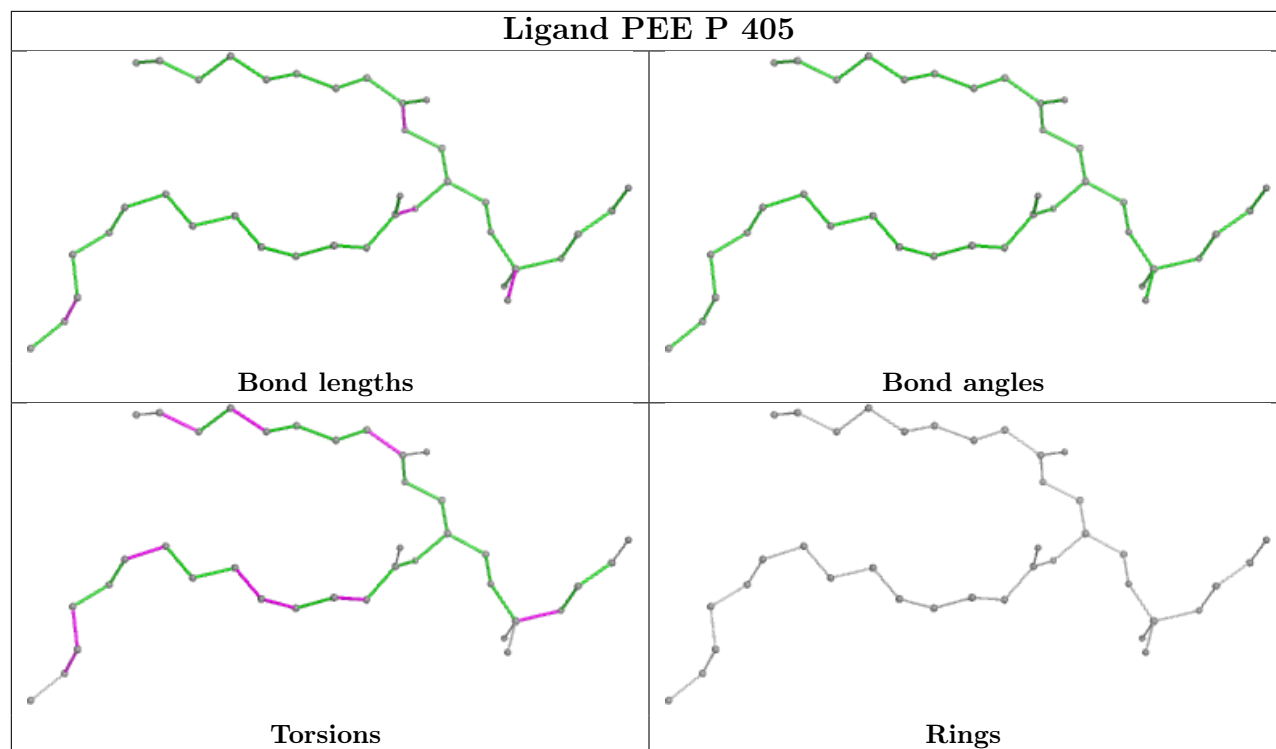


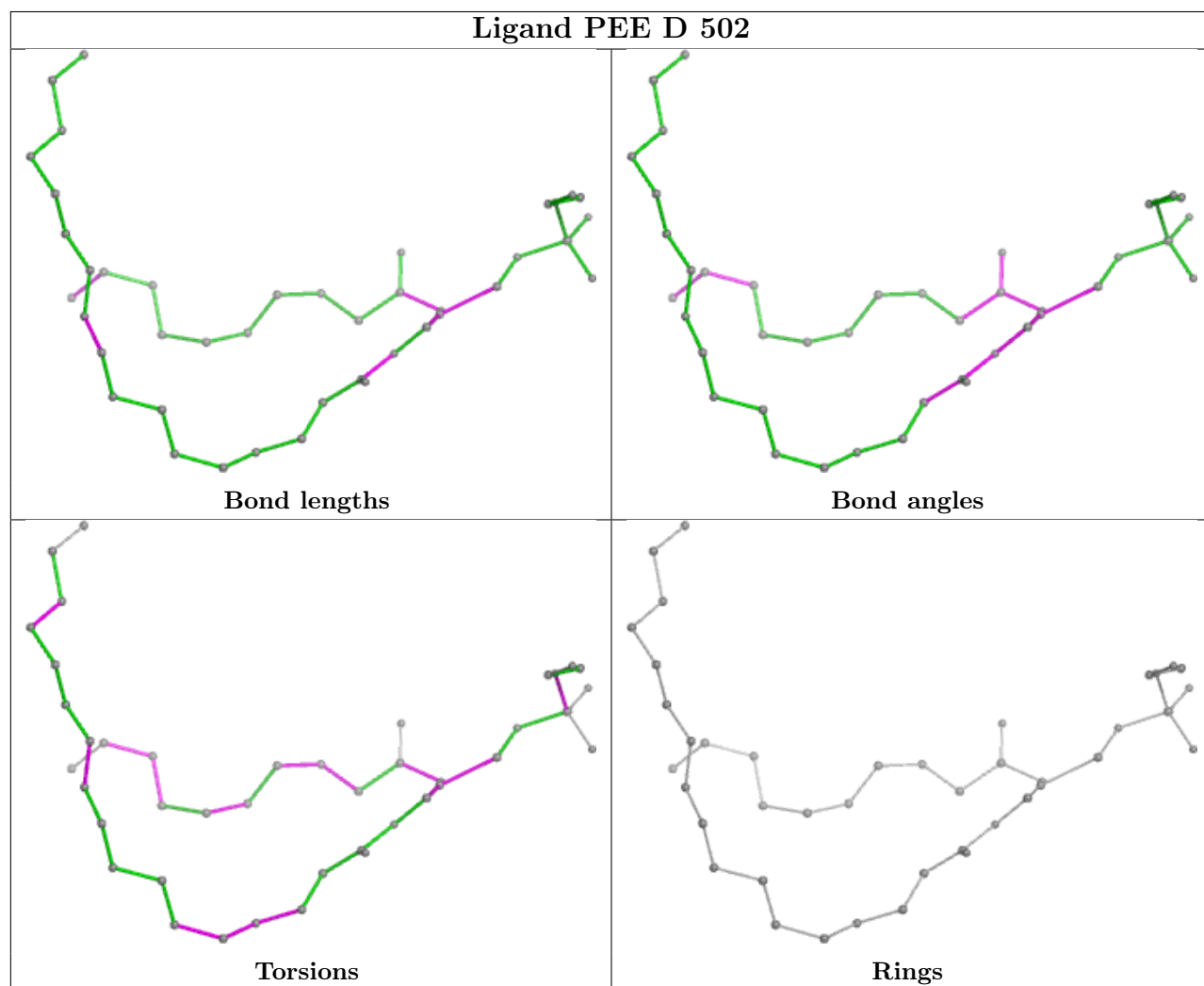
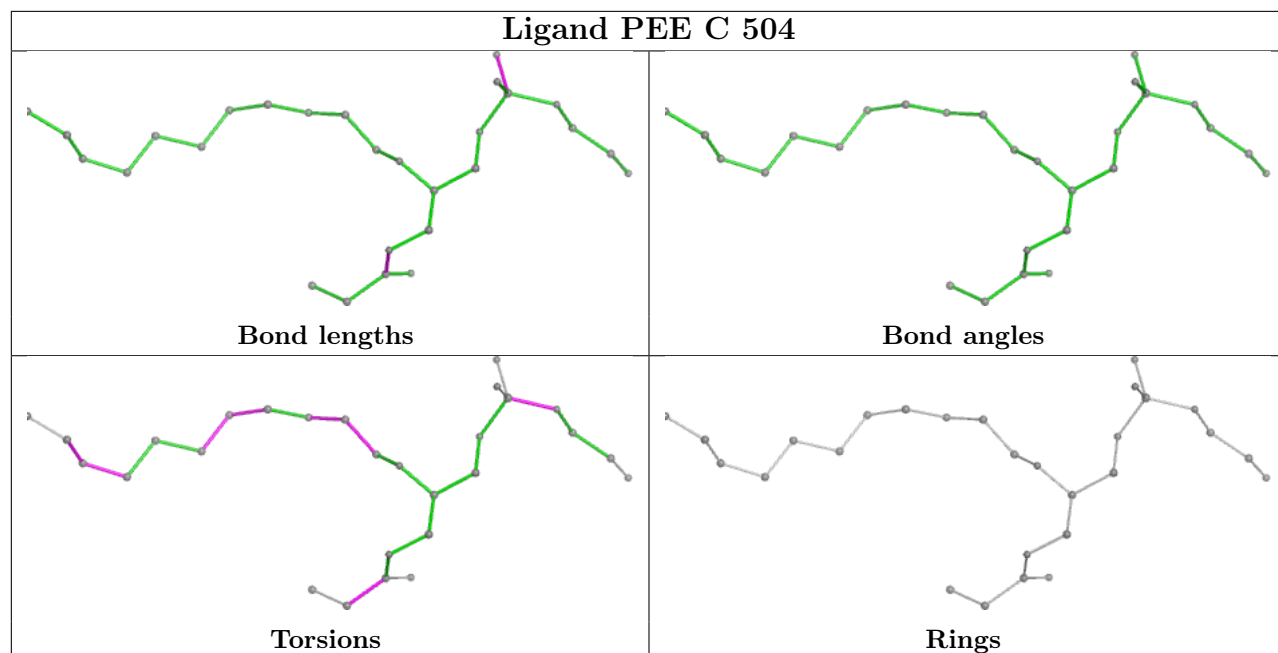




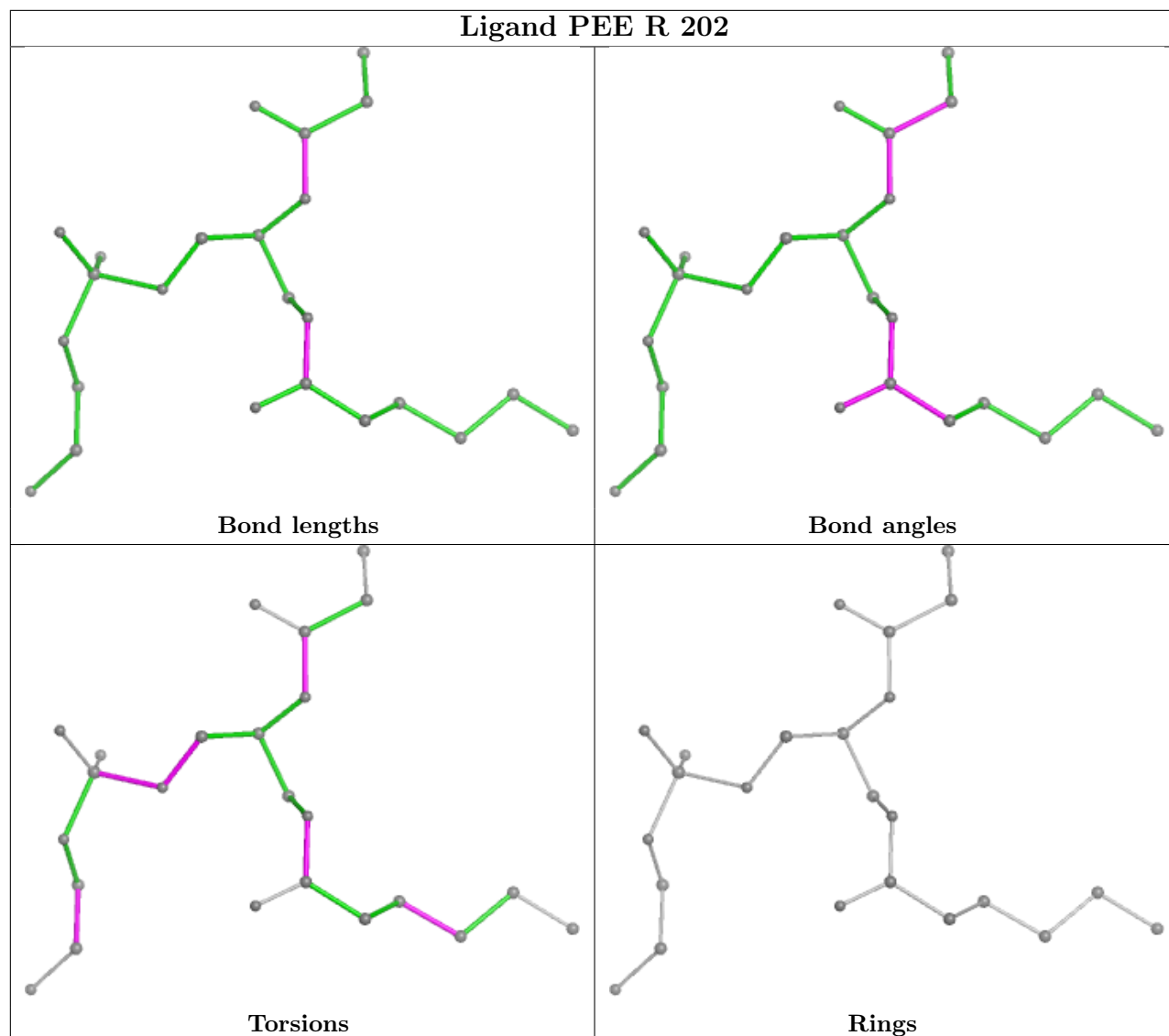




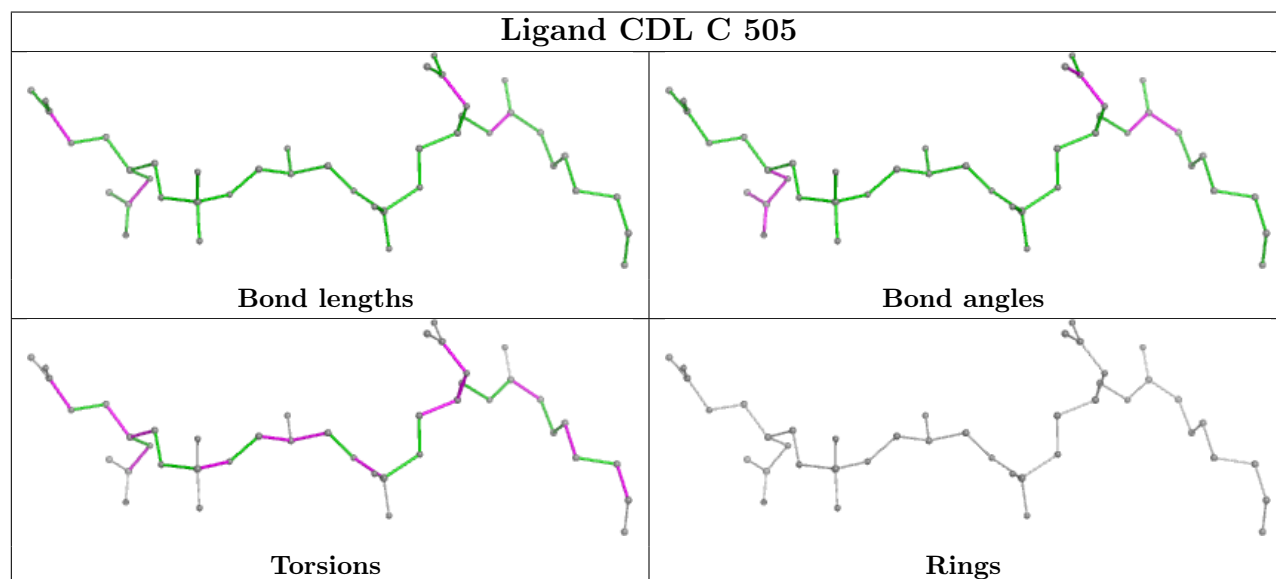




## Ligand PEE R 202



## Ligand CDL C 505



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	438/444 (98%)	0.08	14 (3%)	50	34	47, 92, 130, 166	0
1	N	439/444 (98%)	0.27	19 (4%)	40	27	56, 108, 152, 181	2 (0%)
2	B	418/423 (98%)	0.10	7 (1%)	69	49	64, 106, 143, 196	0
2	O	422/423 (99%)	0.36	17 (4%)	43	29	71, 115, 151, 203	0
3	C	372/372 (100%)	-0.18	4 (1%)	77	59	46, 73, 105, 141	0
3	P	372/372 (100%)	-0.17	4 (1%)	77	59	33, 62, 92, 127	0
4	D	240/240 (100%)	0.05	4 (1%)	69	49	56, 96, 132, 181	0
4	Q	240/240 (100%)	0.13	4 (1%)	69	49	52, 82, 120, 138	1 (0%)
5	E	196/274 (71%)	0.26	9 (4%)	38	27	48, 107, 143, 166	0
5	I	29/274 (10%)	1.73	9 (31%)	1	1	84, 130, 157, 166	0
5	R	72/274 (26%)	0.10	3 (4%)	41	28	55, 84, 118, 130	0
5	V	30/274 (10%)	1.09	4 (13%)	8	7	89, 132, 168, 208	0
6	F	99/111 (89%)	-0.02	2 (2%)	64	45	50, 78, 127, 141	0
6	S	99/111 (89%)	-0.03	2 (2%)	64	45	53, 81, 115, 128	1 (1%)
7	G	74/82 (90%)	-0.07	0	100	100	54, 85, 127, 147	0
7	T	80/82 (97%)	0.07	3 (3%)	44	30	57, 82, 129, 161	0
8	H	66/91 (72%)	0.23	0	100	100	68, 135, 156, 182	1 (1%)
8	U	68/91 (74%)	0.26	1 (1%)	71	53	64, 95, 126, 141	0
9	J	59/64 (92%)	-0.15	1 (1%)	69	49	57, 83, 123, 138	0
9	W	59/64 (92%)	-0.22	1 (1%)	69	49	60, 95, 126, 141	0
10	K	22/22 (100%)	1.07	3 (13%)	8	7	123, 151, 173, 200	0
10	X	22/22 (100%)	0.09	0	100	100	59, 128, 140, 155	2 (9%)
All	All	3916/4794 (81%)	0.11	111 (2%)	55	37	33, 93, 143, 208	7 (0%)

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	I	54	SER	6.4
1	A	98	TYR	4.5
5	I	57	GLY	4.4
2	O	119	LEU	4.4
3	C	168	PHE	4.4
6	S	106	GLU	4.2
5	R	12	ASP	4.1
5	E	190	ASP	4.1
1	A	394	GLU	3.8
1	N	321	GLY	3.7
2	O	276	GLN	3.7
4	Q	178	THR	3.6
5	E	142	LEU	3.4
1	N	56	GLY	3.3
2	O	172	LEU	3.3
6	S	14	GLU	3.2
1	N	444	LEU	3.1
5	I	56	ARG	3.1
1	N	83	GLY	3.1
5	V	73	PRO	3.1
4	D	167	GLU	3.0
2	B	341	TYR	3.0
1	A	264	HIS	3.0
1	A	85	HIS	3.0
2	B	281	ALA	3.0
5	I	55	LEU	2.9
5	I	74	ALA	2.9
2	O	169	ARG	2.8
5	V	72	VAL	2.8
1	A	385	THR	2.8
5	E	72	SER	2.8
2	O	307	PHE	2.8
1	A	91	THR	2.8
1	N	90	SER	2.8
1	A	377	GLU	2.8
2	O	281	ALA	2.8
4	Q	4	GLU	2.7
2	O	244	ILE	2.7
1	N	222	THR	2.7
4	Q	167	GLU	2.7
8	U	14	VAL	2.7
5	I	61	GLY	2.7
1	A	381	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
5	I	49	VAL	2.6
6	F	15	GLY	2.6
4	D	86	LYS	2.6
1	A	315	ALA	2.6
5	E	132	TRP	2.6
1	N	305	GLN	2.6
5	E	27	GLU	2.6
10	K	17	TRP	2.6
5	R	69	LEU	2.5
1	N	249	PRO	2.5
5	R	68	VAL	2.5
1	N	221	GLY	2.5
1	N	282	CYS	2.5
2	B	117	ASP	2.5
5	E	81	ILE	2.5
4	Q	2	ASP	2.5
9	W	17	THR	2.4
6	F	18	LYS	2.4
5	V	50	LEU	2.4
1	A	444	LEU	2.4
1	A	100	LYS	2.4
1	N	443	TRP	2.4
2	O	43	PRO	2.3
3	P	267	HIS	2.3
7	T	73	ASN	2.3
1	N	326	CYS	2.3
2	B	344	VAL	2.3
2	B	371	SER	2.3
2	O	115	ASP	2.3
3	P	72	ASP	2.3
9	J	4	THR	2.3
1	A	415	PHE	2.3
3	C	296	PHE	2.3
3	P	257	THR	2.3
1	N	139	GLN	2.3
7	T	3	GLN	2.3
1	N	238	GLY	2.2
2	O	93	GLY	2.2
4	D	166	ASN	2.2
5	I	60	ALA	2.2
1	A	236	PHE	2.2
2	O	94	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
3	P	254	ASP	2.2
5	E	75	GLU	2.2
3	C	203	THR	2.2
5	E	143	GLY	2.2
5	I	78	TYR	2.2
1	N	41	ILE	2.2
5	E	77	LYS	2.2
1	N	44	GLY	2.1
2	B	210	GLY	2.1
10	K	23	LEU	2.1
3	C	167	GLY	2.1
1	N	250	LEU	2.1
2	O	209	LEU	2.1
2	O	264	ILE	2.1
5	V	75	SER	2.1
10	K	25	GLY	2.1
2	B	313	ASN	2.1
2	O	23	ASP	2.1
7	T	81	ARG	2.1
2	O	122	PHE	2.1
2	O	363	LYS	2.1
1	N	251	ALA	2.0
1	N	8	LEU	2.0
1	A	316	ASP	2.0
2	O	236	LYS	2.0
4	D	11	PRO	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](#)

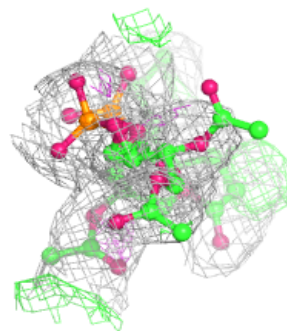
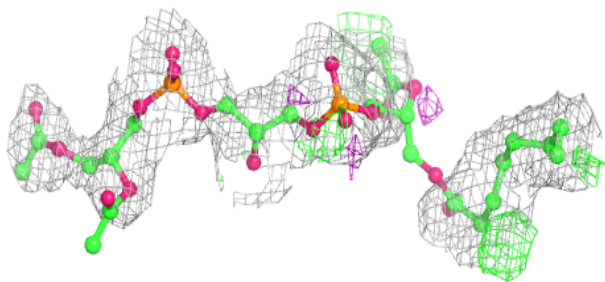
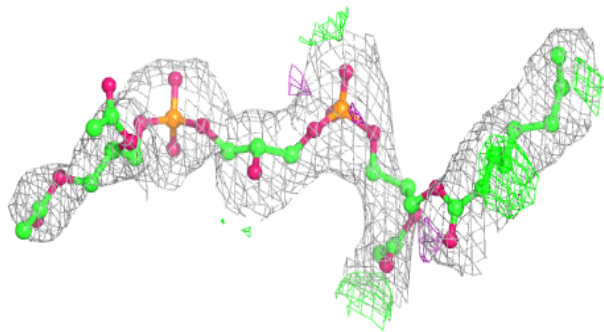
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	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
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

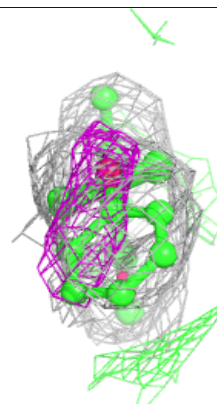
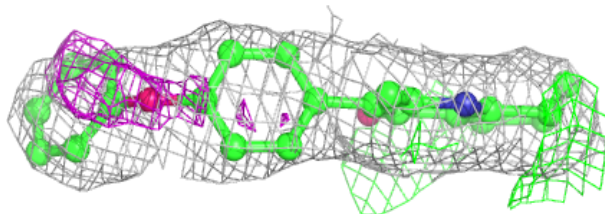
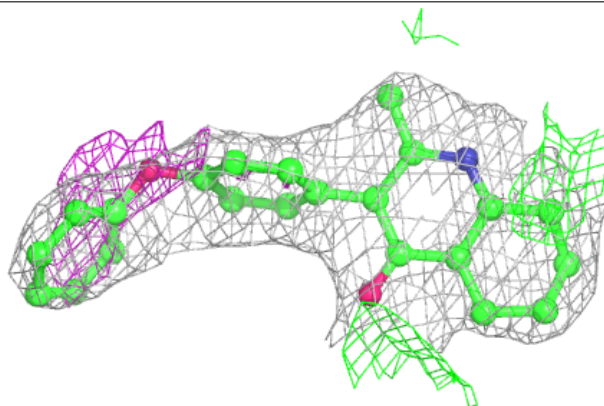
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around CDL C 505:**

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

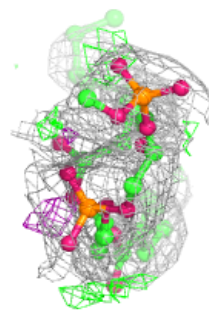
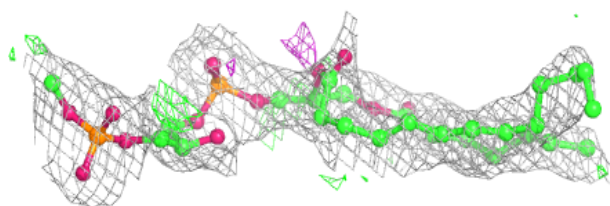
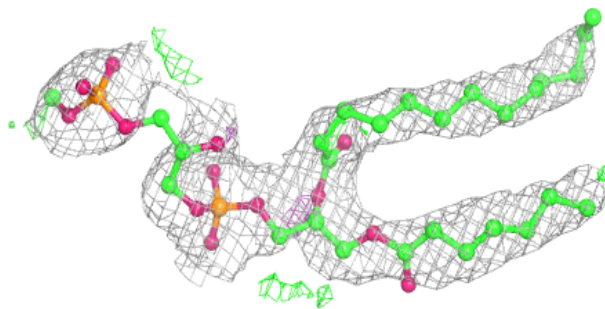
**Electron density around MJM P 404:**

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

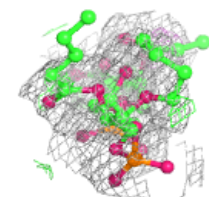
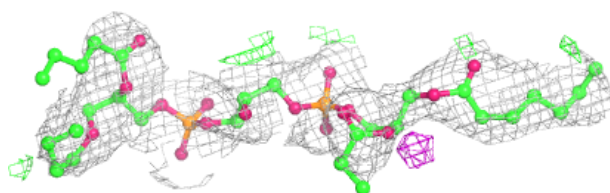
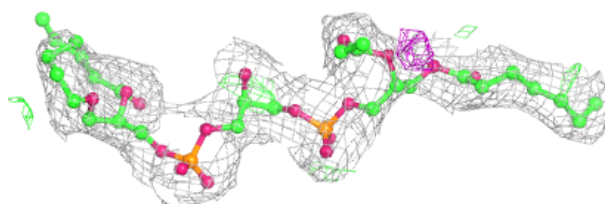


**Electron density around CDL P 401:**

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

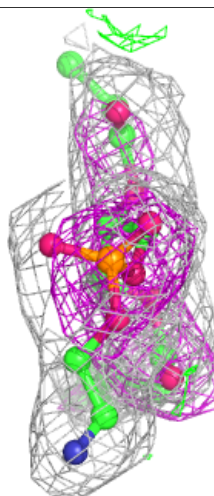
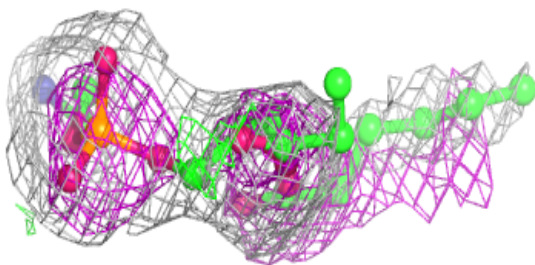
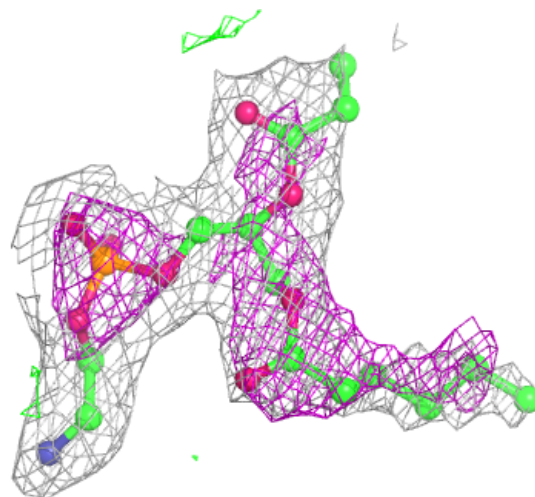
**Electron density around CDL P 406:**

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



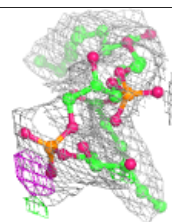
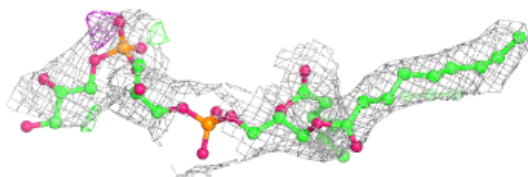
**Electron density around PEE R 202:**

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



**Electron density around CDL D 503:**

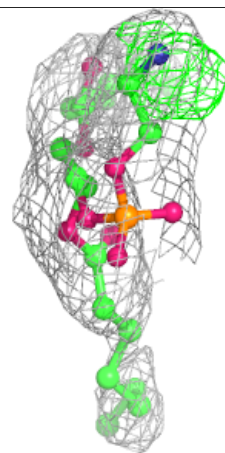
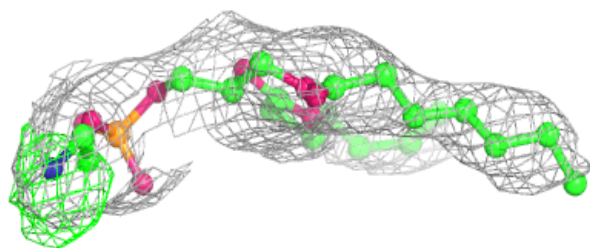
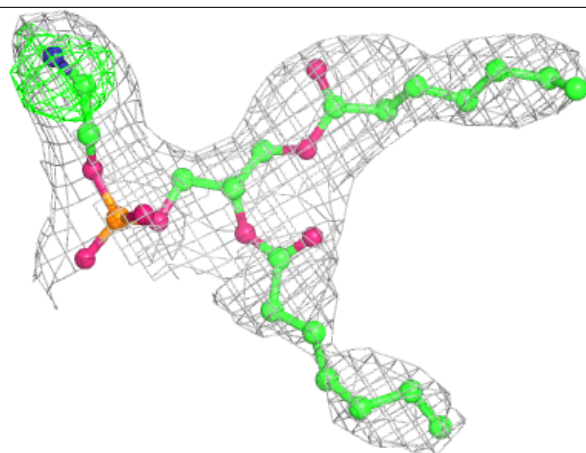
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



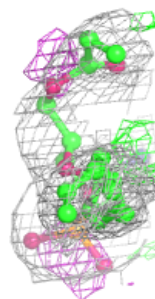
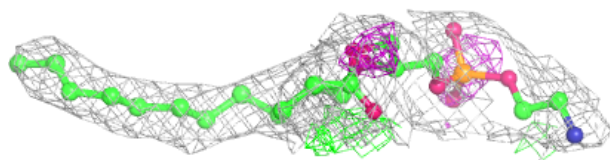
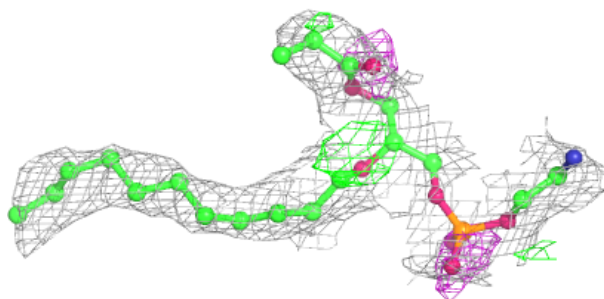


**Electron density around PEE E 502:**

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

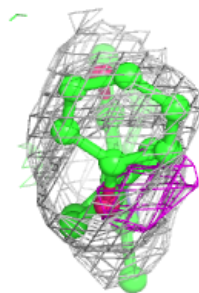
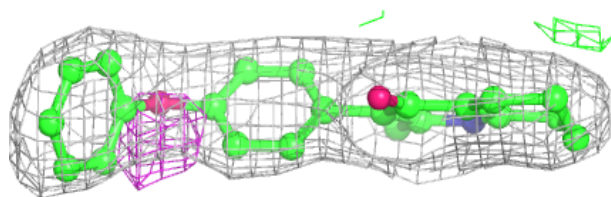
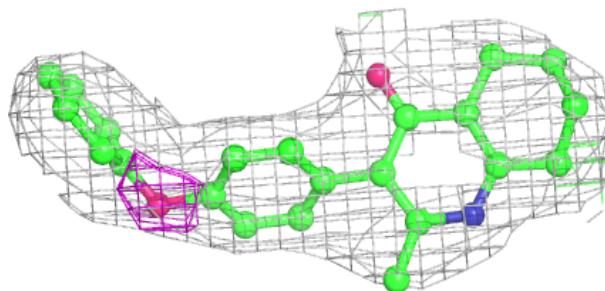
**Electron density around PEE C 504:**

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

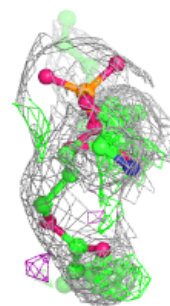
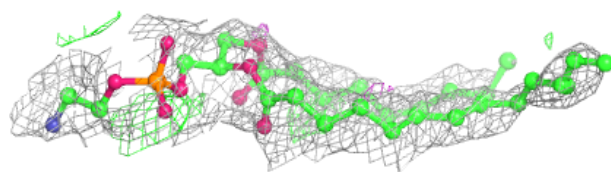
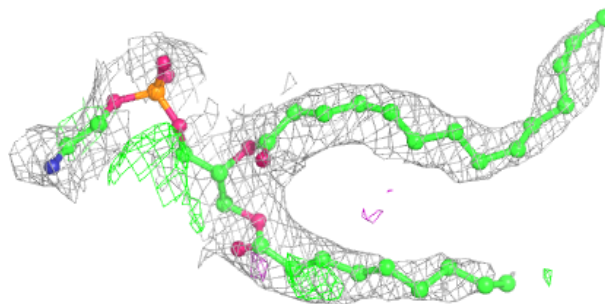


**Electron density around MJM C 503:**

$2mF_o-DF_c$  (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:**

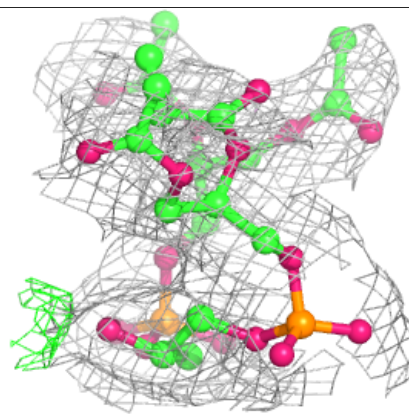
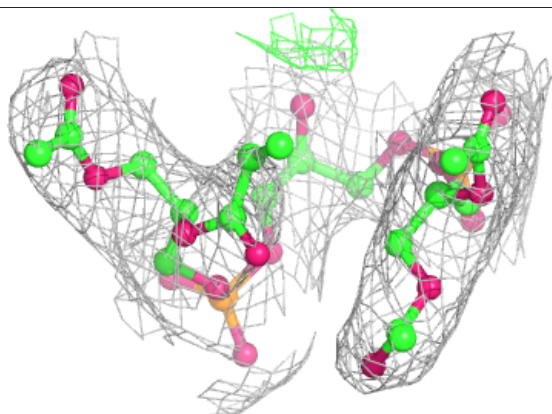
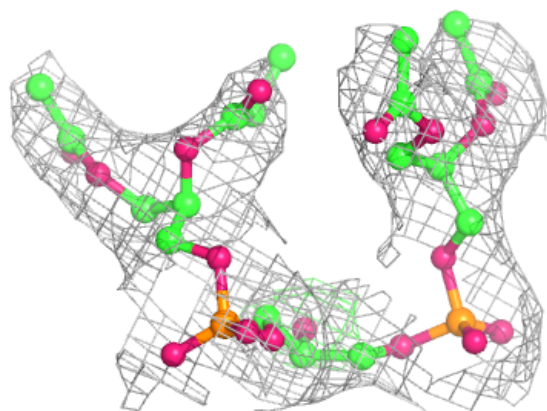
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





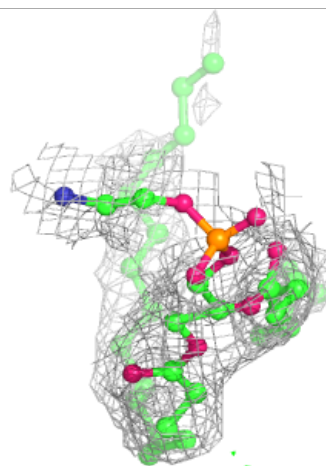
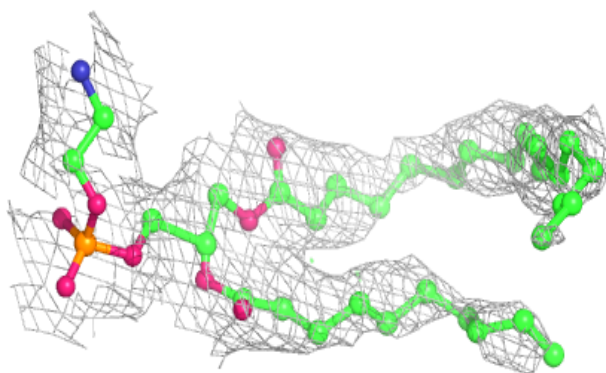
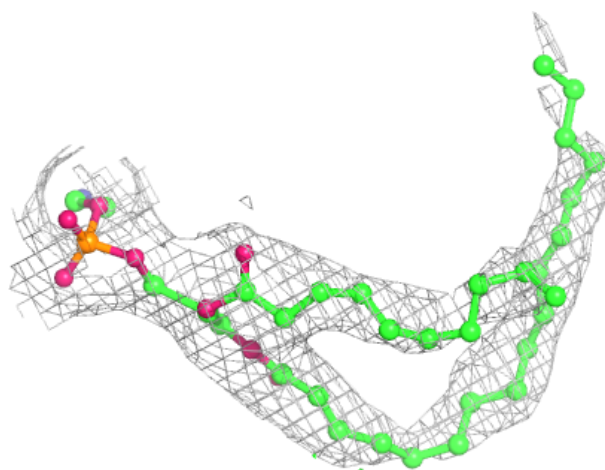
**Electron density around CDL C 506:**

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



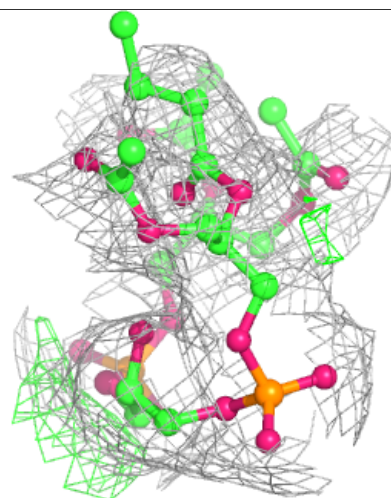
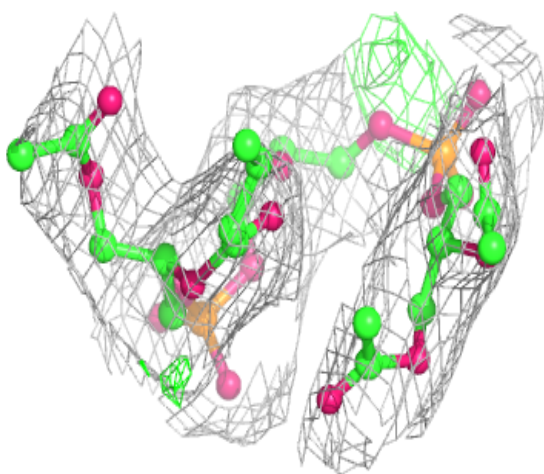
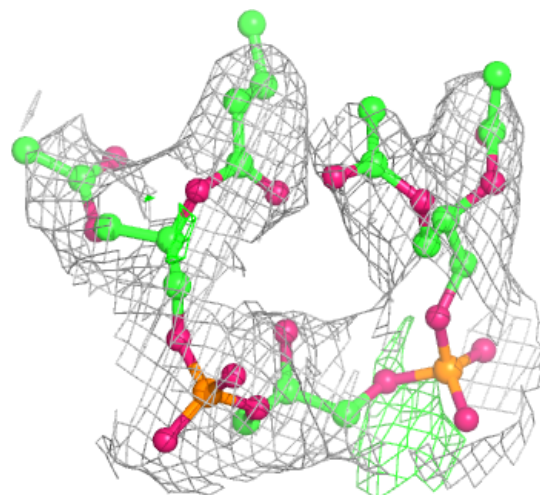
**Electron density around PEE D 502:**

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



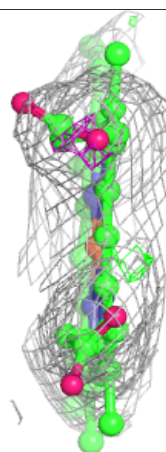
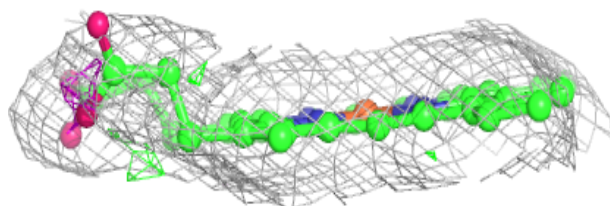
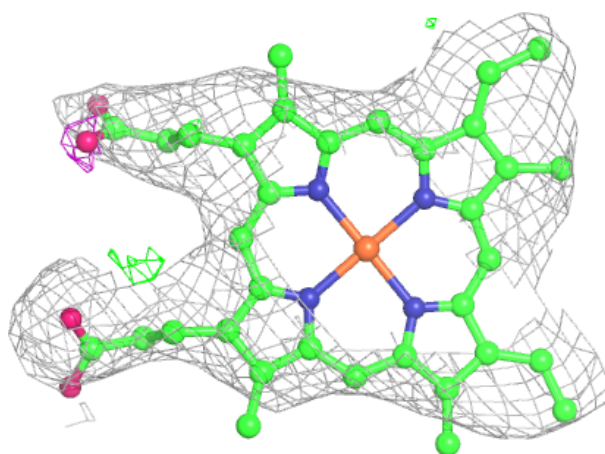
**Electron density around CDL P 407:**

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



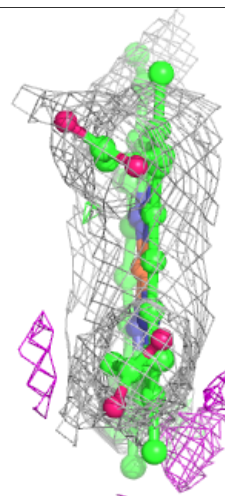
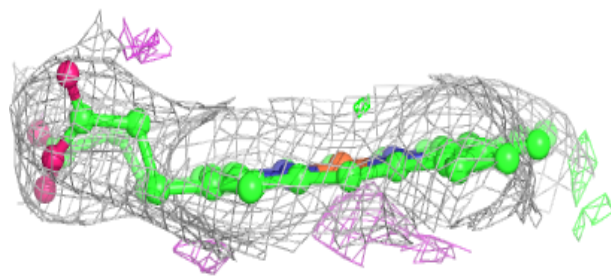
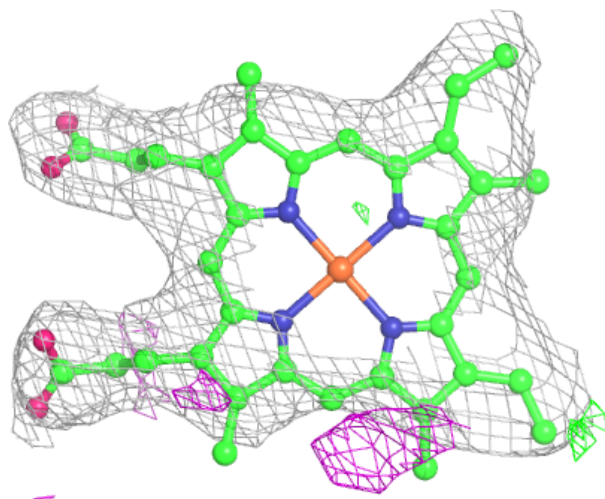
**Electron density around HEC D 501:**

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



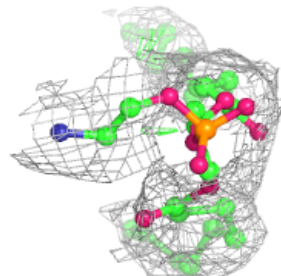
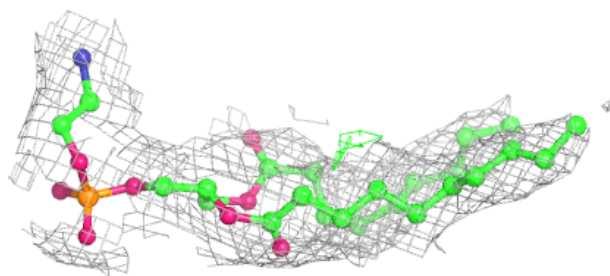
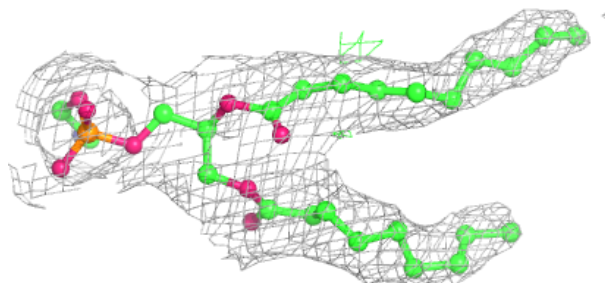
**Electron density around HEC Q 501:**

$2mF_o-DF_c$  (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:**

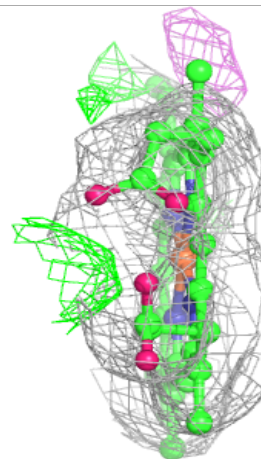
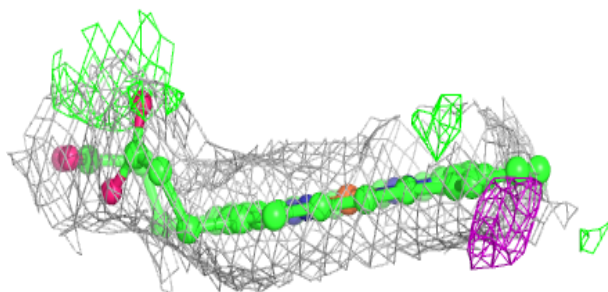
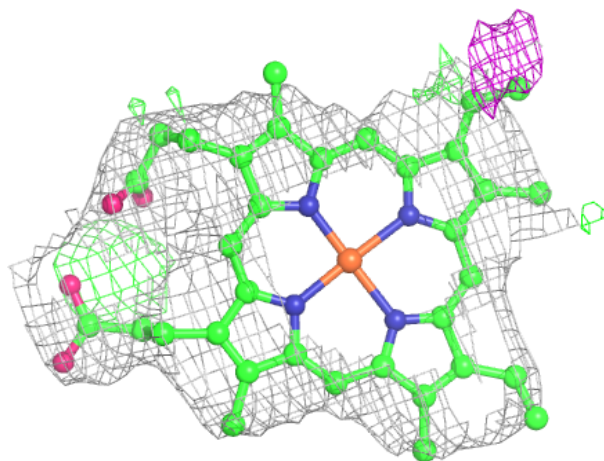
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





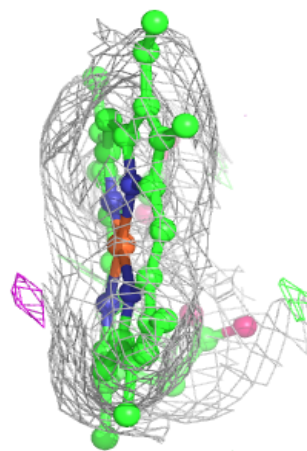
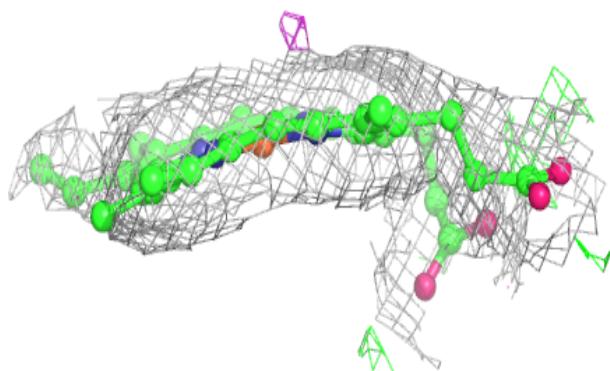
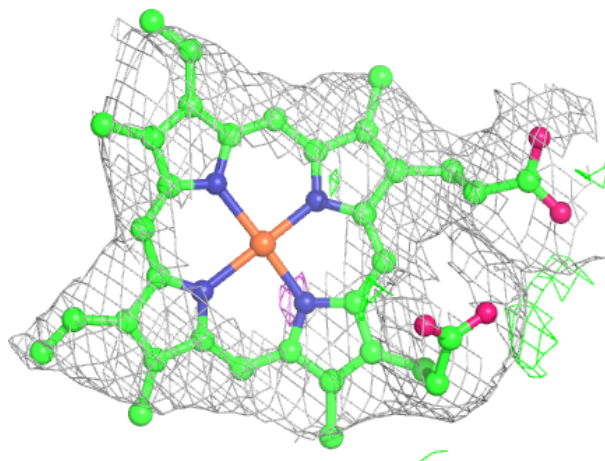
**Electron density around HEM C 501:**

$2mF_o-DF_c$  (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:**

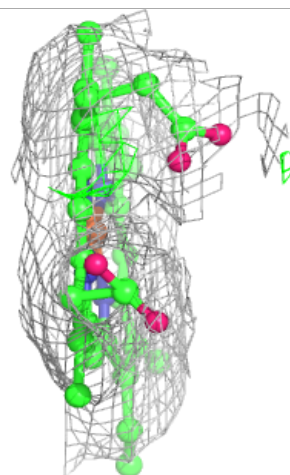
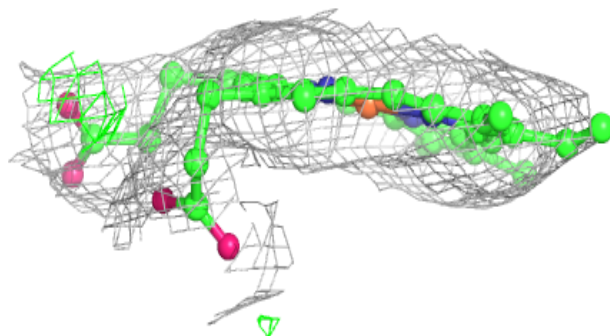
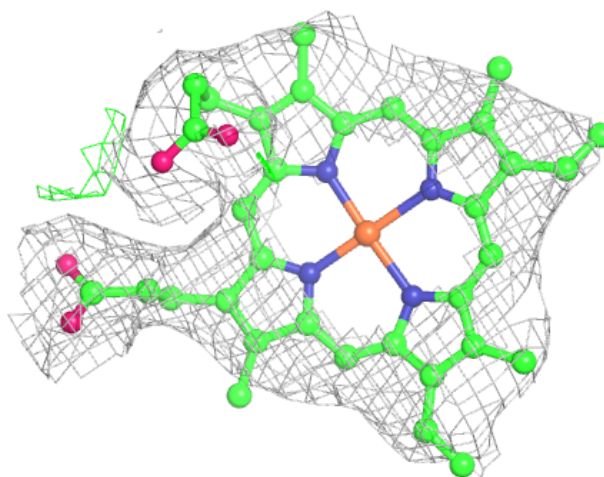
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





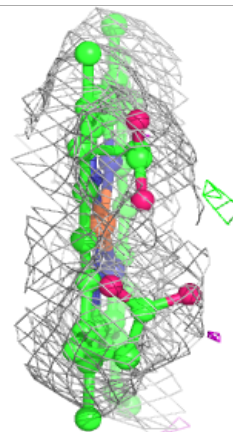
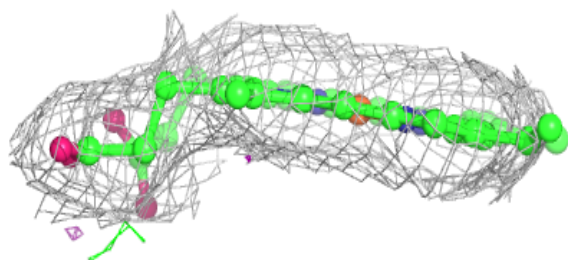
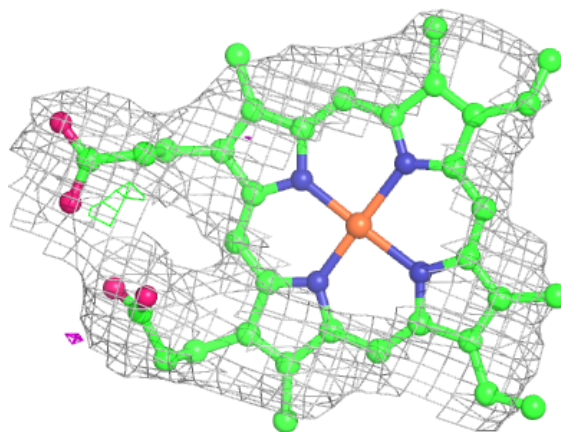
**Electron density around HEM C 502:**

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



**Electron density around HEM P 402:**

$2mF_o-DF_c$  (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.