



## Full wwPDB EM Validation Report ⓘ

May 12, 2025 – 01:42 PM EDT

PDB ID : 9BPB / pdb\_00009bpb  
EMDB ID : EMD-44770  
Title : Tethered respiratory III2IV2 supercomplex from *Saccharomyces cerevisiae*  
Authors : Eldeeb, M.H.; Carlstrom, A.; Berndtsson, J.; Ott, M.; Fontanesi, F.  
Deposited on : 2024-05-07  
Resolution : 2.57 Å (reported)  
Based on initial model : 6YMX

This is a Full wwPDB EM 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/EMValidationReportHelp>  
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:

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

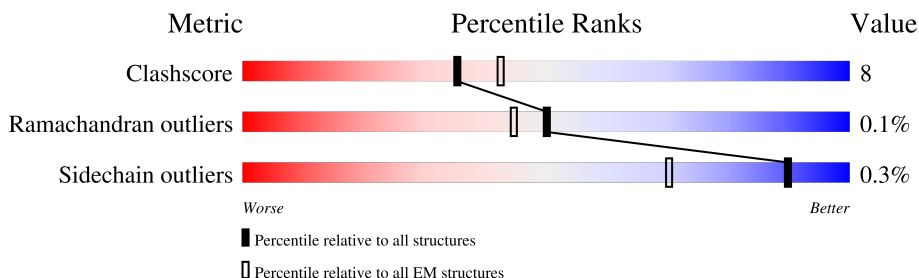
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.57 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	457	
1	K	457	
2	B	368	
2	L	368	
3	C	385	
3	M	385	
4	D	309	
4	N	309	

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Mol	Chain	Length	Quality of chain
5	E	215	
5	O	215	
6	F	147	
6	P	147	
7	G	183	
7	Q	183	
8	H	94	
8	R	94	
9	I	66	
9	S	66	
10	J	77	
10	T	77	
11	a	534	
11	m	534	
12	b	251	
12	n	251	
13	c	269	
13	o	269	
14	d	155	
14	p	155	
15	e	153	
15	q	153	
16	f	148	
16	r	148	
17	g	60	

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Mol	Chain	Length	Quality of chain
17	s	60	
18	i	59	
18	u	59	
19	j	83	
19	v	83	
20	k	129	
20	w	129	
21	l	66	
21	x	66	

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
31	FES	E	301	-	-	X	-
31	FES	O	301	-	-	X	-

## 2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 61288 atoms, of which 460 are hydrogens and 0 are deuteriums.

In the tables below, 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					AltConf	Trace
1	A	430	Total	C	N	O	S	0	0
			3339	2107	575	651	6		
1	K	430	Total	C	N	O	S	0	0
			3339	2107	575	651	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		
2	L	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	383	Total	C	N	O	S	0	0
			3071	2071	480	499	21		
3	M	383	Total	C	N	O	S	0	0
			3071	2071	480	499	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	245	Total	C	N	O	S	0	0
			1941	1237	337	359	8		
4	N	245	Total	C	N	O	S	0	0
			1941	1237	337	359	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		
5	O	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	74	Total	C	N	O	S	0	0
			624	391	108	123	2		
6	P	74	Total	C	N	O	S	0	0
			624	391	108	123	2		

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 7, mitochondrial, Cytochrome c oxidase subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	125	Total	C	N	O	S	0	0
			1008	647	171	188	2		
7	Q	125	Total	C	N	O	S	0	0
			1008	647	171	188	2		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	128	GLY	-	linker	UNP P00128
G	129	GLY	-	linker	UNP P00128
G	130	GLY	-	linker	UNP P00128
G	131	GLY	-	linker	UNP P00128
Q	128	GLY	-	linker	UNP P00128
Q	129	GLY	-	linker	UNP P00128
Q	130	GLY	-	linker	UNP P00128
Q	131	GLY	-	linker	UNP P00128

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	92	Total	C	N	O	S	0	0
			764	505	129	128	2		
8	R	92	Total	C	N	O	S	0	0
			764	505	129	128	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	53	Total	C	N	O	0	0
			436	291	73	72		
9	S	53	Total	C	N	O	0	0
			436	291	73	72		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	45	Total	C	N	O	S	0	0
			352	233	58	59	2		
10	T	45	Total	C	N	O	S	0	0
			352	233	58	59	2		

- Molecule 11 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a	534	Total	C	N	O	S	0	0
			4161	2778	649	712	22		
11	m	534	Total	C	N	O	S	0	0
			4161	2778	649	712	22		

- Molecule 12 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	b	236	Total	C	N	O	S	0	0
			1888	1242	286	350	10		
12	n	236	Total	C	N	O	S	0	0
			1888	1242	286	350	10		

- Molecule 13 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	c	269	Total	C	N	O	S	0	0
			2146	1430	344	357	15		
13	o	269	Total	C	N	O	S	0	0
			2146	1430	344	357	15		

- Molecule 14 is a protein called Cytochrome c oxidase subunit 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	d	119	Total	C	N	O	S	0	0
			898	565	149	179	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	p	119	Total	C	N	O	S	0	0
			898	565	149	179	5		

- Molecule 15 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	e	128	Total	C	N	O	S	0	0
			1008	639	175	190	4		
15	q	128	Total	C	N	O	S	0	0
			1008	639	175	190	4		

- Molecule 16 is a protein called Cytochrome c oxidase subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	f	98	Total	C	N	O	S	0	0
			819	528	133	157	1		
16	r	98	Total	C	N	O	S	0	0
			819	528	133	157	1		

- Molecule 17 is a protein called Cytochrome c oxidase subunit 7, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	g	55	Total	C	N	O	0	0
			456	310	77	69		
17	s	55	Total	C	N	O	0	0
			456	310	77	69		

- Molecule 18 is a protein called Cytochrome c oxidase subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	i	49	Total	C	N	O	S	0	0
			404	269	68	64	3		
18	u	49	Total	C	N	O	S	0	0
			404	269	68	64	3		

- Molecule 19 is a protein called Cytochrome c oxidase subunit 12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	j	74	Total	C	N	O	S	0	0
			621	400	106	110	5		
19	v	74	Total	C	N	O	S	0	0
			621	400	106	110	5		



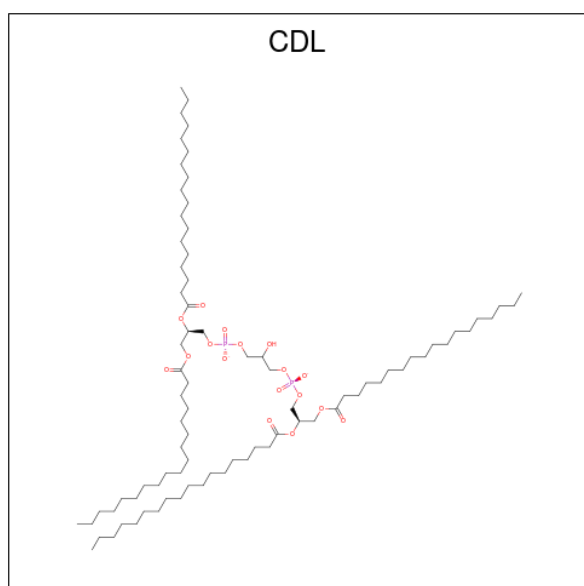
- Molecule 20 is a protein called Cytochrome c oxidase subunit 13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	k	110	Total	C	N	O	S	0	0
			911	591	158	159	3		
20	w	110	Total	C	N	O	S	0	0
			911	591	158	159	3		

- Molecule 21 is a protein called Cytochrome c oxidase subunit 26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	l	36	Total	C	N	O	S	0	0
			293	199	47	46	1		
21	x	36	Total	C	N	O	S	0	0
			293	199	47	46	1		

- Molecule 22 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



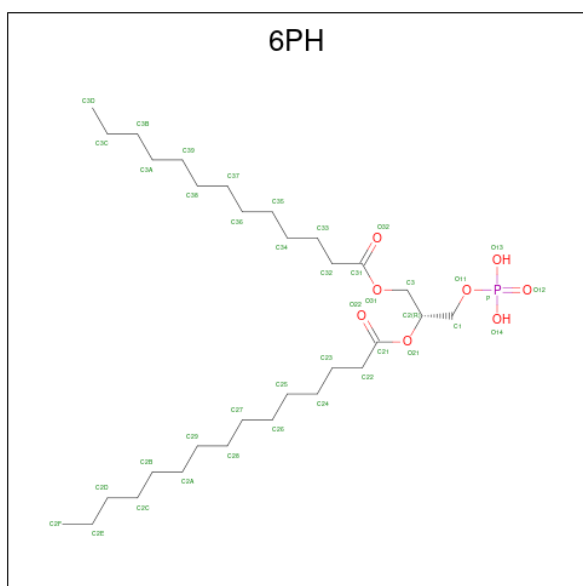
Mol	Chain	Residues	Atoms				AltConf
22	A	1	Total	C	O	P	0
			55	36	17	2	
22	D	1	Total	C	O	P	0
			60	41	17	2	
22	E	1	Total	C	O	P	0
			42	25	15	2	
22	H	1	Total	C	O	P	0
			53	34	17	2	
22	K	1	Total	C	O	P	0
			55	36	17	2	

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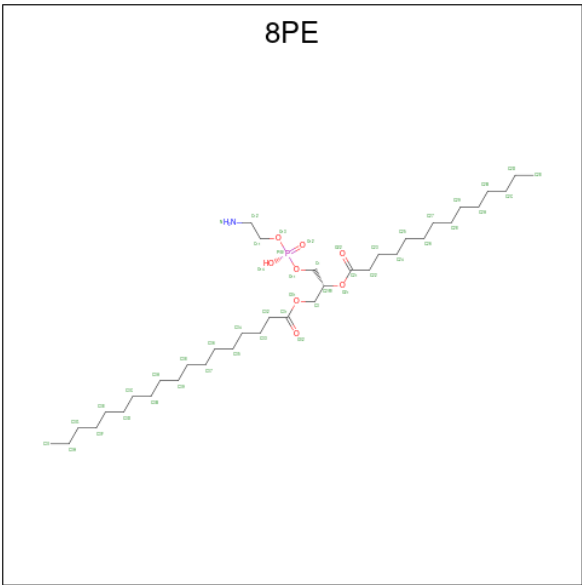
Mol	Chain	Residues	Atoms				AltConf
22	N	1	Total	C	O	P	0
			60	41	17	2	
22	O	1	Total	C	O	P	0
			42	25	15	2	
22	R	1	Total	C	O	P	0
			53	34	17	2	

- Molecule 23 is (1R)-2-(phosphonoxy)-1-[(tridecanoyloxy)methyl]ethyl pentadecanoate (CCD ID: 6PH) (formula: C<sub>31</sub>H<sub>61</sub>O<sub>8</sub>P).



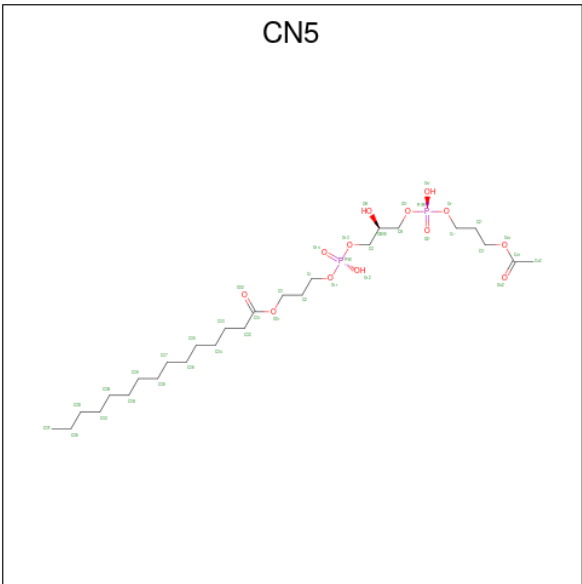
Mol	Chain	Residues	Atoms				AltConf
23	C	1	Total	C	O	P	0
			40	31	8	1	
23	M	1	Total	C	O	P	0
			40	31	8	1	

- Molecule 24 is (2R)-3-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(tetradecanoyloxy)propyl octadecanoate (CCD ID: 8PE) (formula: C<sub>37</sub>H<sub>74</sub>NO<sub>8</sub>P).



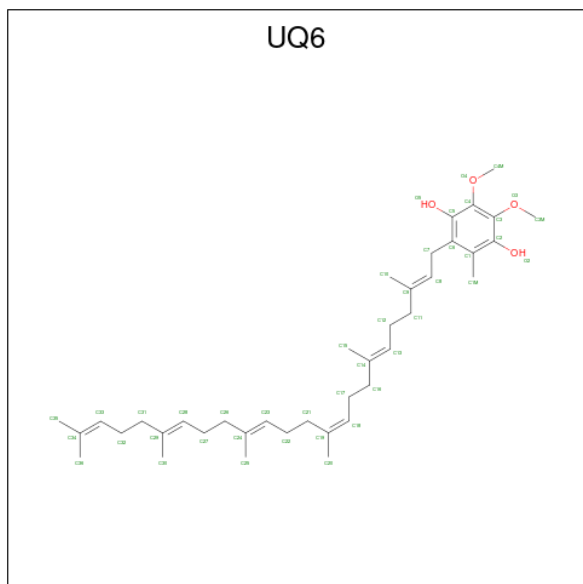
Mol	Chain	Residues	Atoms					AltConf
24	C	1	Total	C	N	O	P	0
			26	16	1	8	1	
24	M	1	Total	C	N	O	P	0
			26	16	1	8	1	

- Molecule 25 is (5S,11R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-4,6,10,12,16-pentaoxa-5,11-di phosphaoctadec-1-yl pentadecanoate (CCD ID: CN5) (formula: C<sub>26</sub>H<sub>52</sub>O<sub>13</sub>P<sub>2</sub>).



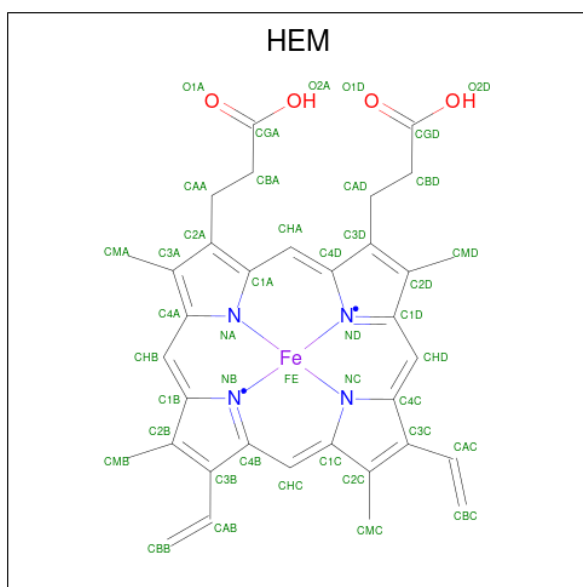
Mol	Chain	Residues	Atoms				AltConf
25	C	1	Total	C	O	P	0
			32	17	13	2	

- Molecule 26 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXAENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (CCD ID: UQ6) (formula:  $C_{39}H_{60}O_4$ ).



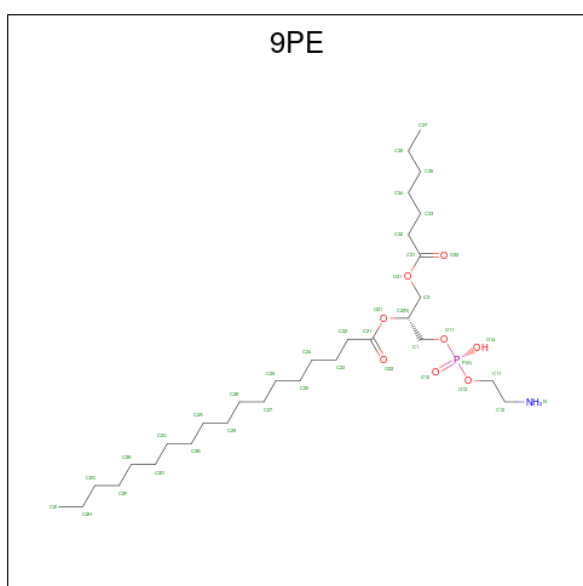
Mol	Chain	Residues	Atoms				AltConf
26	C	1	Total	C	H	O	0
			56	22	30	4	
26	C	1	Total	C	O		0
			43	39	4		
26	M	1	Total	C	H	O	0
			56	22	30	4	
26	M	1	Total	C	O		0
			43	39	4		

- Molecule 27 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



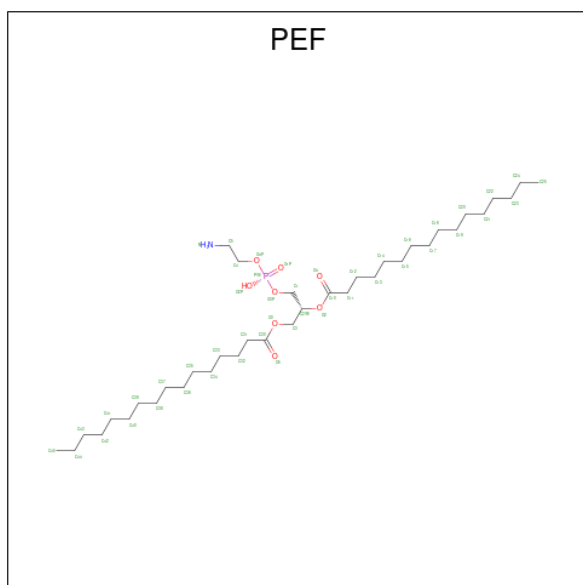
Mol	Chain	Residues	Atoms						AltConf
27	C	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0
27	C	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0
27	M	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0
27	M	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0

- Molecule 28 is (1R)-2-[[[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy]-1-[(heptanoyloxy)methyl]ethyl octadecanoate (CCD ID: 9PE) (formula: C<sub>30</sub>H<sub>60</sub>NO<sub>8</sub>P).



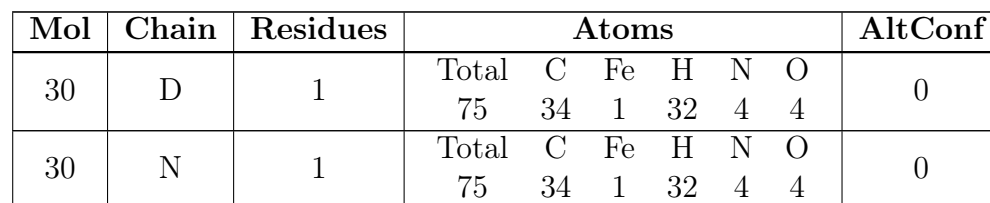
Mol	Chain	Residues	Atoms					AltConf
28	C	1	Total	C	N	O	P	0
			33	23	1	8	1	
28	M	1	Total	C	N	O	P	0
			33	23	1	8	1	

- Molecule 29 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula:  $C_{37}H_{74}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
29	D	1	Total	C	N	O	P	0
			40	30	1	8	1	
29	J	1	Total	C	N	O	P	0
			29	19	1	8	1	
29	a	1	Total	C	N	O	P	0
			43	33	1	8	1	
29	N	1	Total	C	N	O	P	0
			40	30	1	8	1	
29	T	1	Total	C	N	O	P	0
			29	19	1	8	1	
29	m	1	Total	C	N	O	P	0
			43	33	1	8	1	

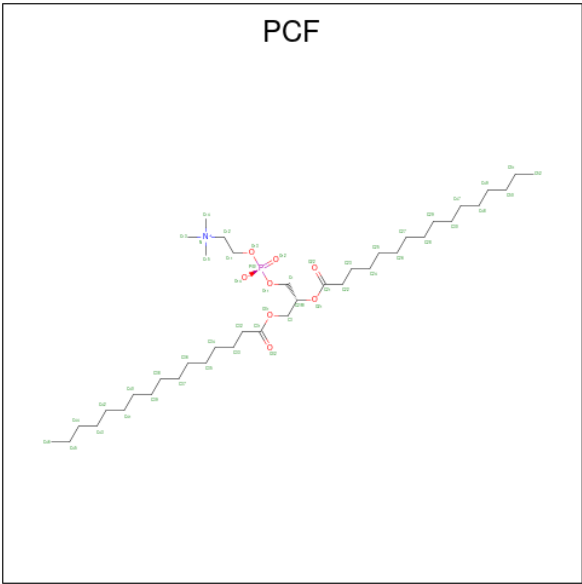
- Molecule 30 is HEME C (CCD ID: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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- 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 text. The bonds are colored yellow and purple.

Mol	Chain	Residues	Atoms			AltConf
31	E	1	Total 4	Fe 2	S 2	0
31	O	1	Total 4	Fe 2	S 2	0

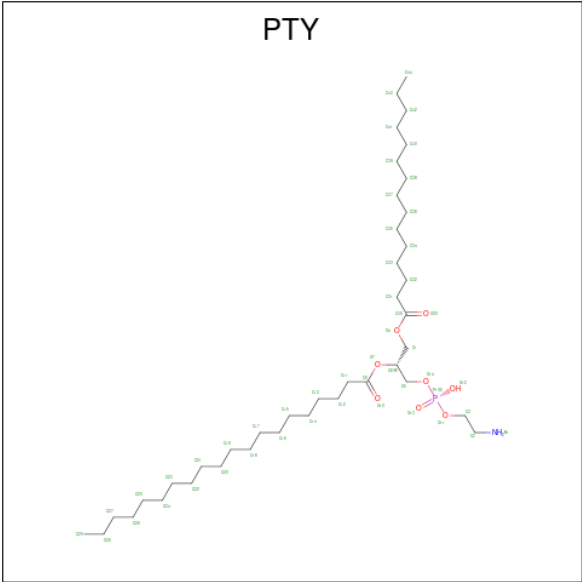
- Molecule 32 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (CCD ID: PCF) (formula: C<sub>40</sub>H<sub>80</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
32	H	1	Total	C	N	O	P	0
			32	22	1	8	1	
32	I	1	Total	C	N	O	P	0
			32	22	1	8	1	
32	k	1	Total	C	N	O	P	0
			43	33	1	8	1	
32	l	1	Total	C	N	O	P	0
			37	27	1	8	1	
32	R	1	Total	C	N	O	P	0
			32	22	1	8	1	
32	S	1	Total	C	N	O	P	0
			32	22	1	8	1	
32	w	1	Total	C	N	O	P	0
			43	33	1	8	1	
32	x	1	Total	C	N	O	P	0
			37	27	1	8	1	

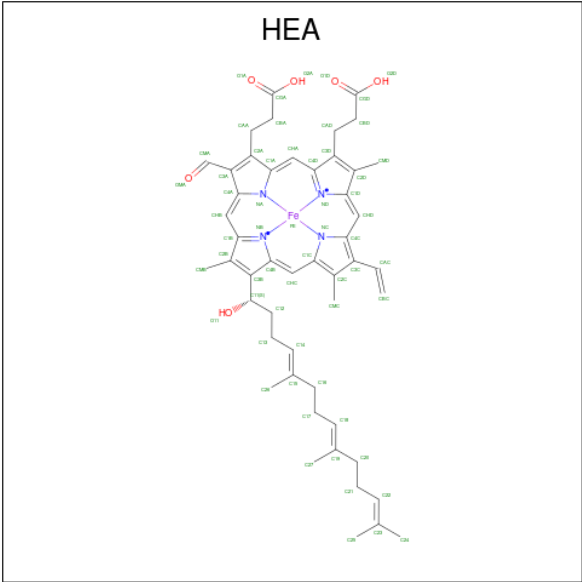
- Molecule 33 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C<sub>40</sub>H<sub>80</sub>NO<sub>8</sub>P).





Mol	Chain	Residues	Atoms					AltConf
33	I	1	Total	C	N	O	P	0
			32	22	1	8	1	
33	a	1	Total	C	N	O	P	0
			32	22	1	8	1	
33	b	1	Total	C	N	O	P	0
			34	24	1	8	1	
33	b	1	Total	C	N	O	P	0
			35	25	1	8	1	
33	c	1	Total	C	N	O	P	0
			40	30	1	8	1	
33	S	1	Total	C	N	O	P	0
			32	22	1	8	1	
33	m	1	Total	C	N	O	P	0
			32	22	1	8	1	
33	n	1	Total	C	N	O	P	0
			34	24	1	8	1	
33	n	1	Total	C	N	O	P	0
			35	25	1	8	1	
33	o	1	Total	C	N	O	P	0
			40	30	1	8	1	

- Molecule 34 is HEME-A (CCD ID: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms						AltConf
34	a	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
34	a	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
34	m	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
34	m	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	

- Molecule 35 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

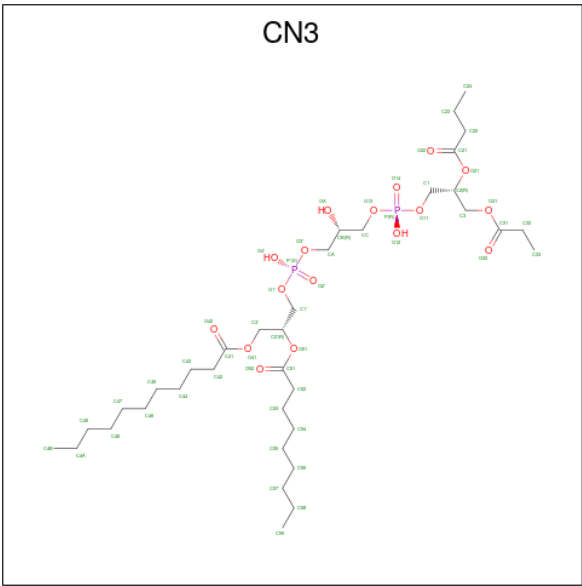
Mol	Chain	Residues	Atoms		AltConf
35	a	1	Total	Cu	0
			1	1	
35	m	1	Total	Cu	0
			1	1	

- Molecule 36 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
36	a	1	Total	Ca	0
			1	1	
36	m	1	Total	Ca	0
			1	1	

- Molecule 37 is (2R,5S,11R,14R)-5,8,11-trihydroxy-2-(nonanoyloxy)-5,11-dioxido-16-oxo-14-[(propanoyloxy)methyl]-4,6,10,12,15-pentaoxa-5,11-diphosphanadec-1-yl undecanoate

(CCD ID: CN3) (formula: C<sub>36</sub>H<sub>68</sub>O<sub>17</sub>P<sub>2</sub>).

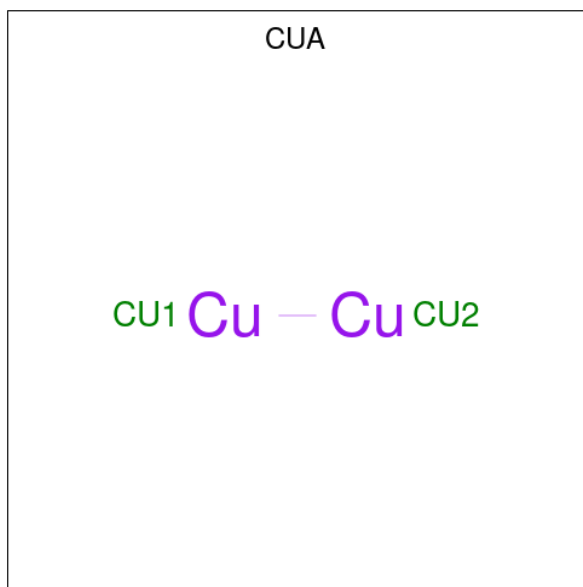


Mol	Chain	Residues	Atoms				AltConf
37	a	1	Total	C	O	P	0
			46	27	17	2	
37	m	1	Total	C	O	P	0
			46	27	17	2	

- Molecule 38 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
38	b	1	Total	Mg	0
			1	1	
38	n	1	Total	Mg	0
			1	1	

- Molecule 39 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu<sub>2</sub>).



Mol	Chain	Residues	Atoms		AltConf
39	b	1	Total 2	Cu 2	0
39	n	1	Total 2	Cu 2	0

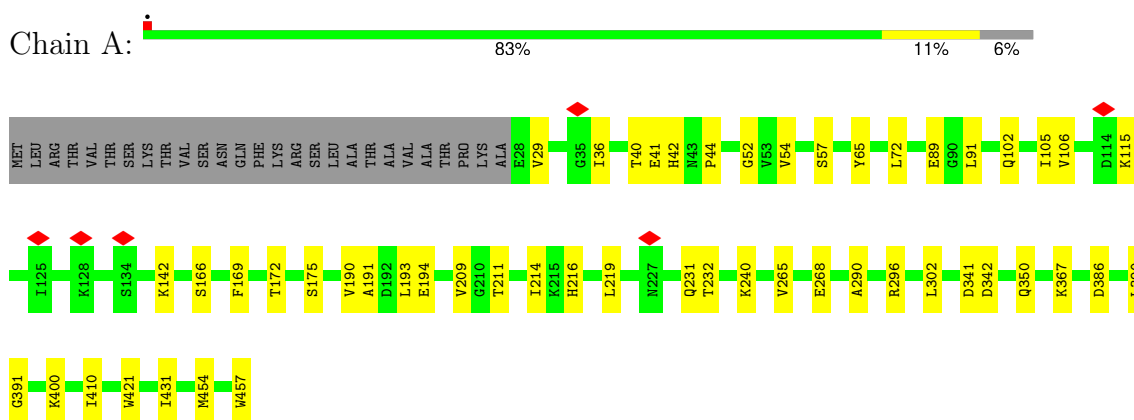
- Molecule 40 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
40	d	1	Total 1	Zn 1	0
40	p	1	Total 1	Zn 1	0

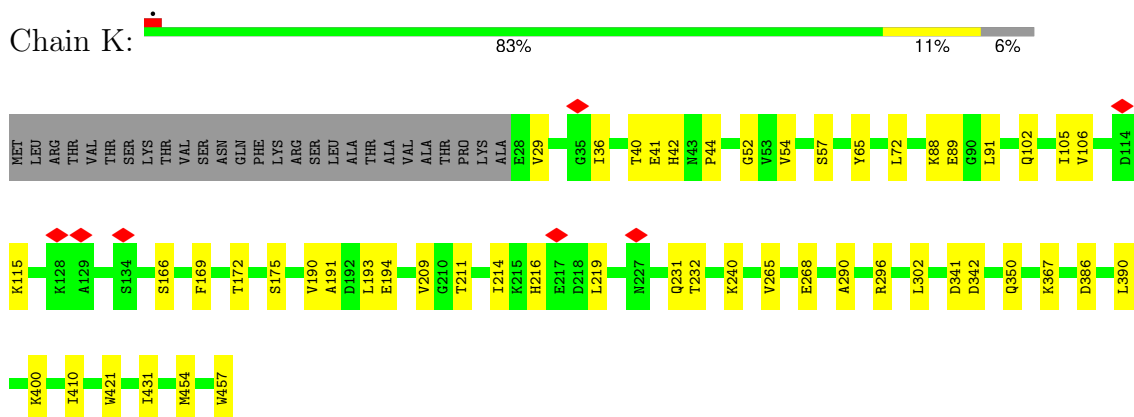
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

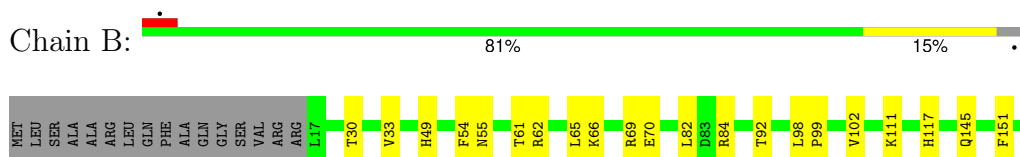
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

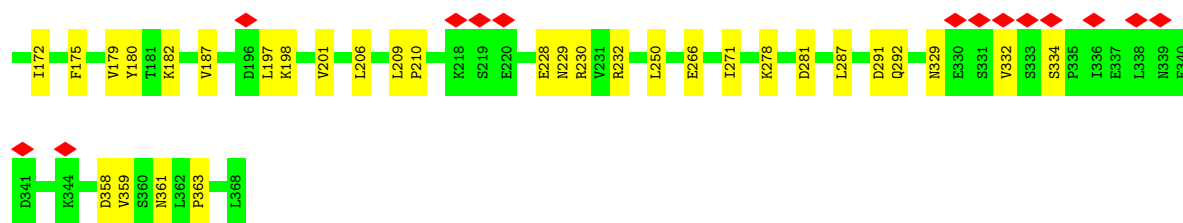


- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



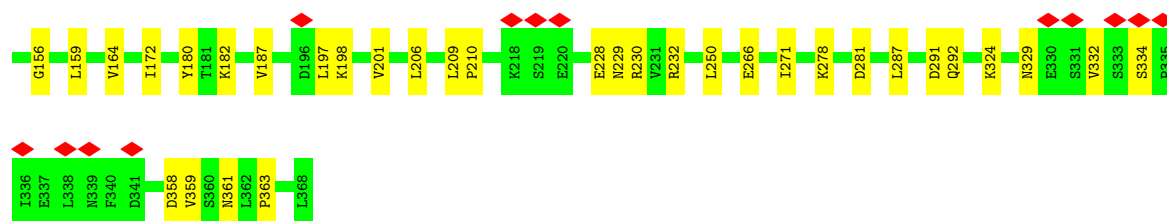
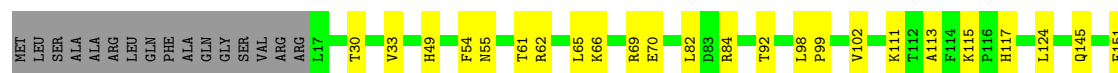
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial





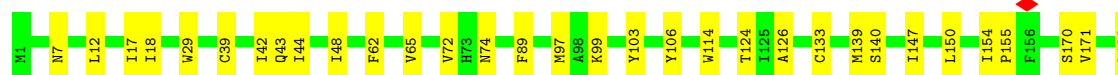
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain L: 80% 15%



- Molecule 3: Cytochrome b

Chain C: 82% 17%

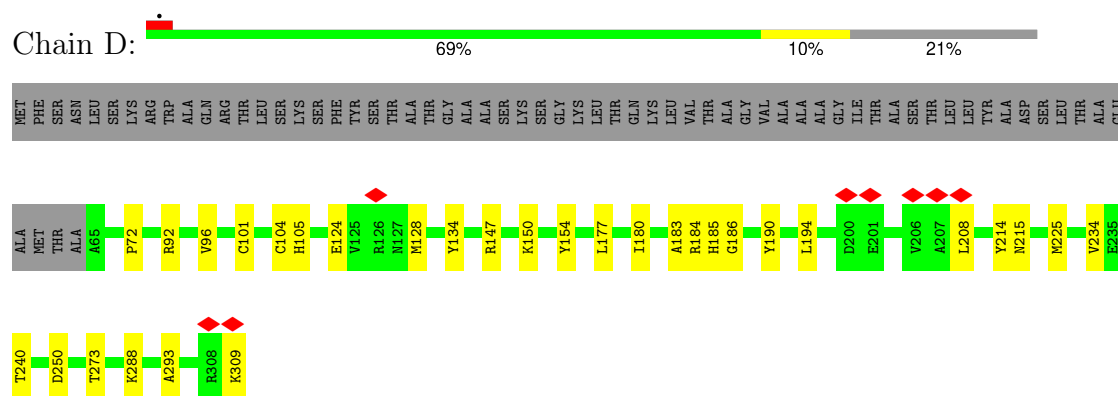


- Molecule 3: Cytochrome b

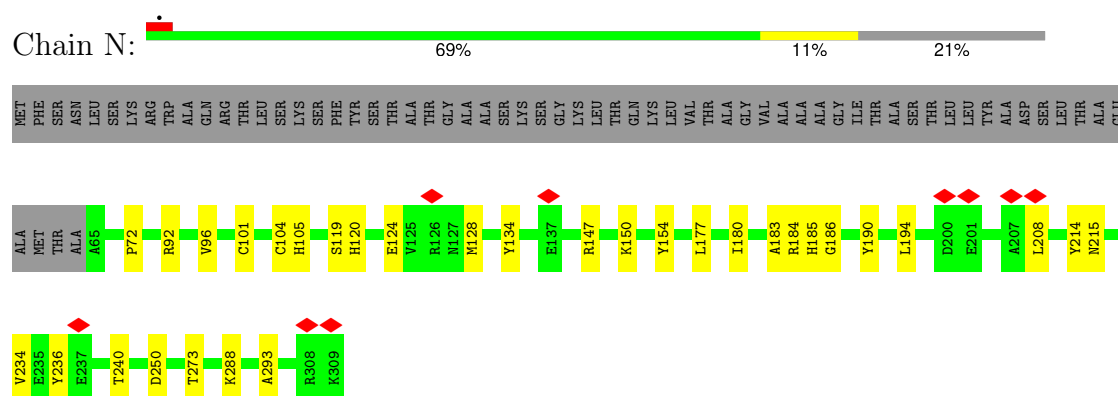
Chain M: 81% 18%



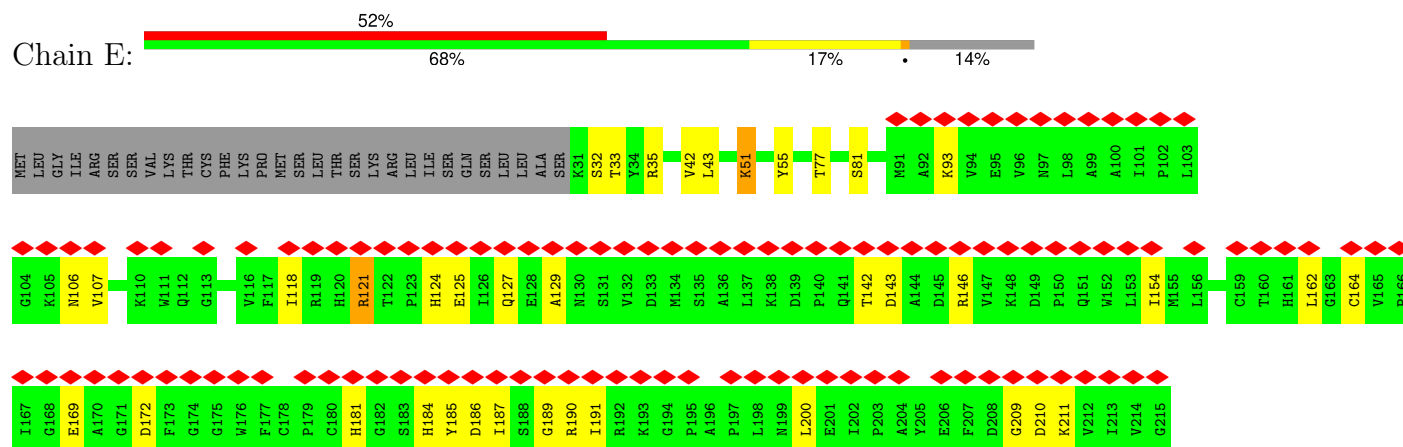
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



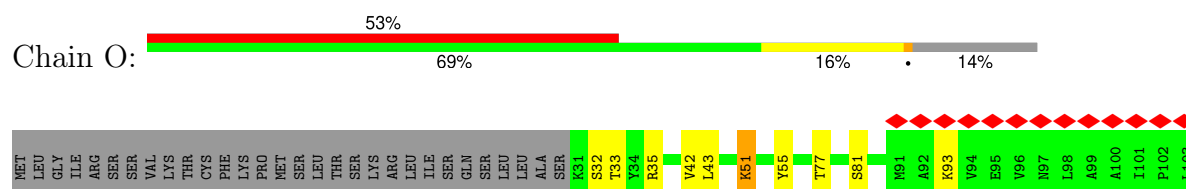
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



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



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




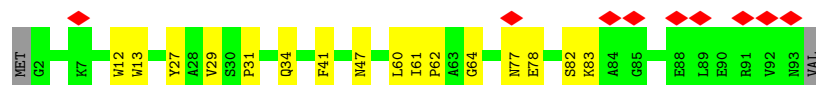





VAL  
LYS  
GLY  
ARG  
LYS  
THR  
PRO  
TYR  
ALA  
LEU  
SER  
HIS  
PHE  
GLY  
PHE  
PHE  
PHE  
ALA  
ILE  
GLY  
PHE  
ALA  
ALA  
VAL  
PRO  
PHE  
VAL  
VAL  
ALA  
CYS  
TYR  
VAL  
GLN  
LEU  
LYS  
LYS  
SER  
GLY  
ALA  
PHE

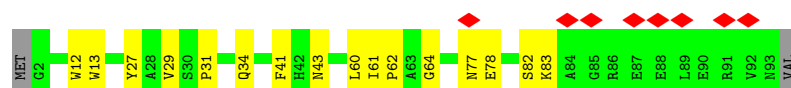
- Molecule 8: Cytochrome b-c1 complex subunit 8, mitochondrial

Chain H: 



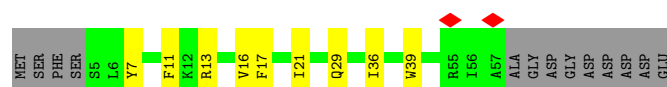
- Molecule 8: Cytochrome b-c1 complex subunit 8, mitochondrial

Chain R: 



- Molecule 9: Cytochrome b-c1 complex subunit 9, mitochondrial

Chain I: 



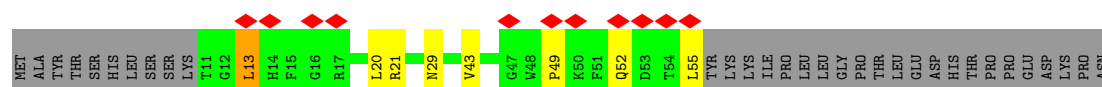
- Molecule 9: Cytochrome b-c1 complex subunit 9, mitochondrial

Chain S: 



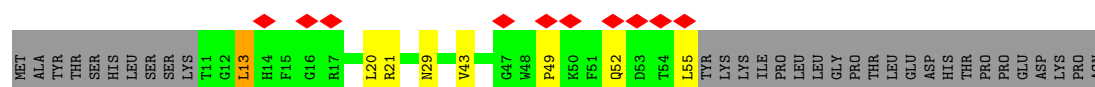
- Molecule 10: Cytochrome b-c1 complex subunit 10, mitochondrial

Chain J: 

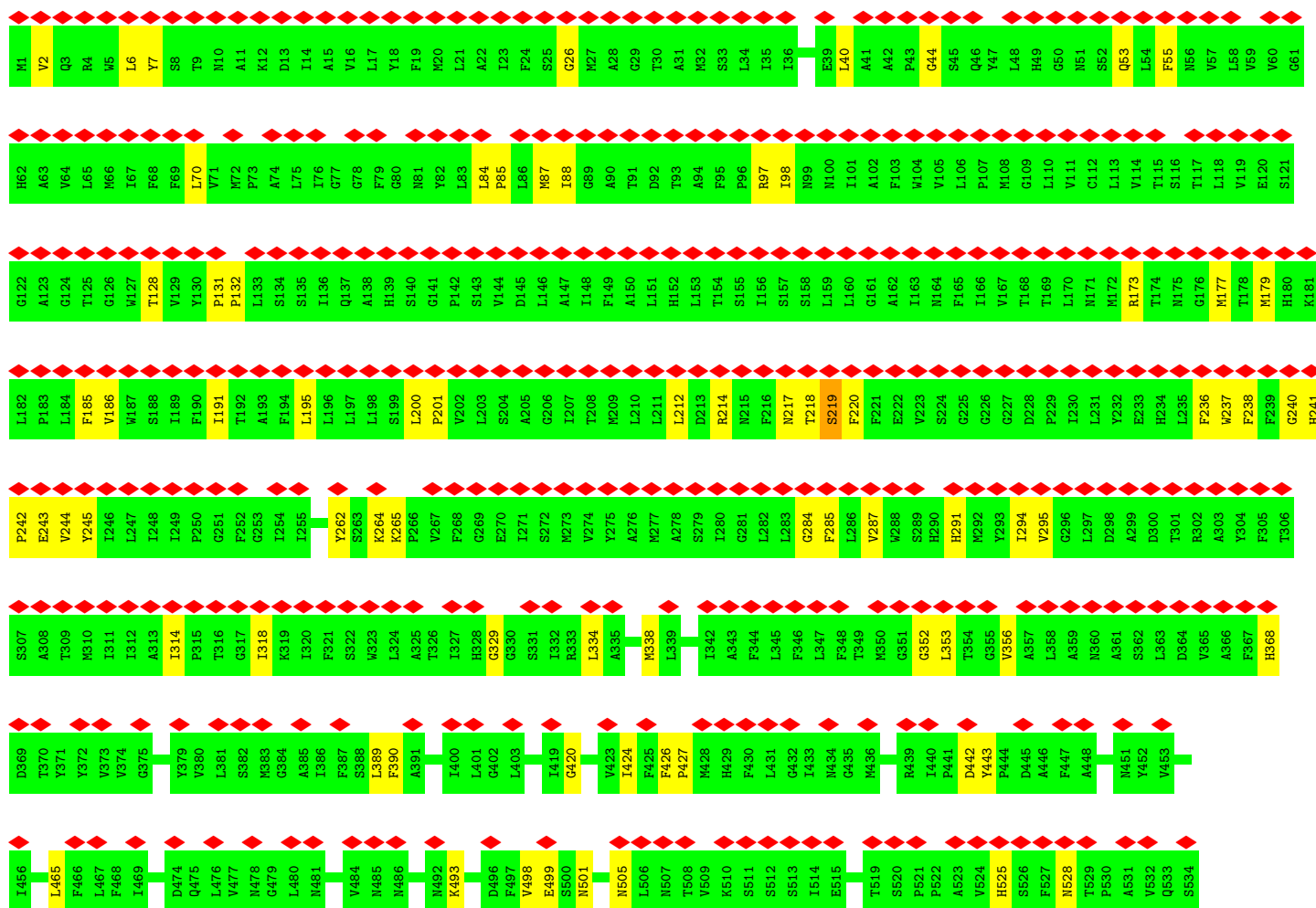
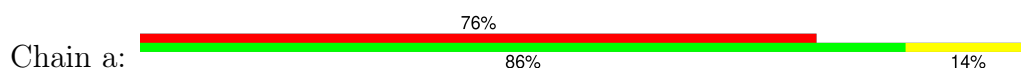


- Molecule 10: Cytochrome b-c1 complex subunit 10, mitochondrial

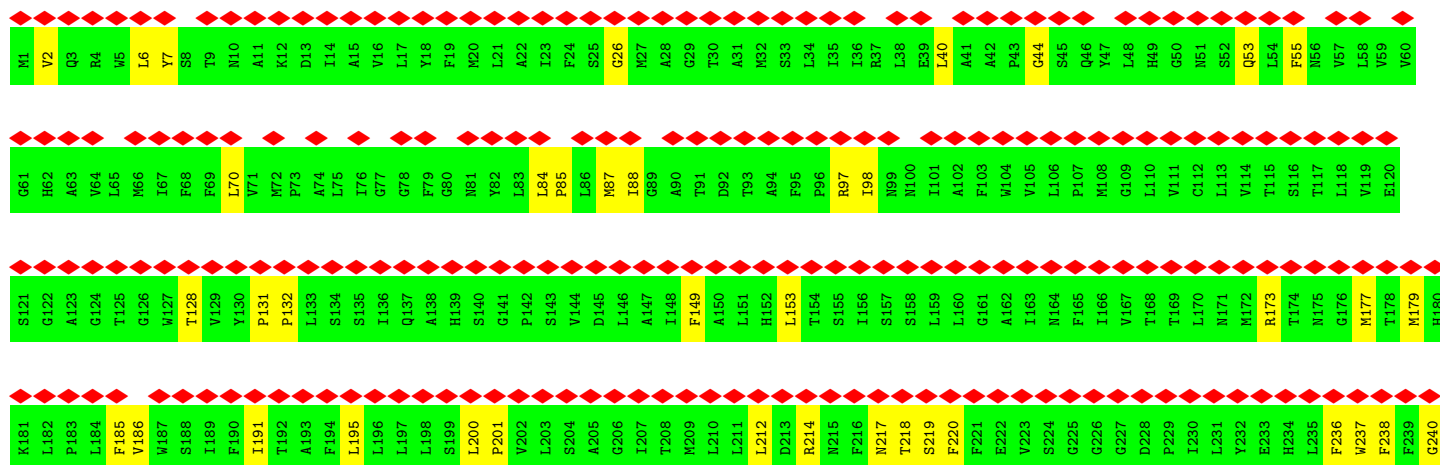
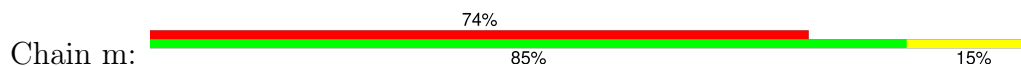
Chain T: 

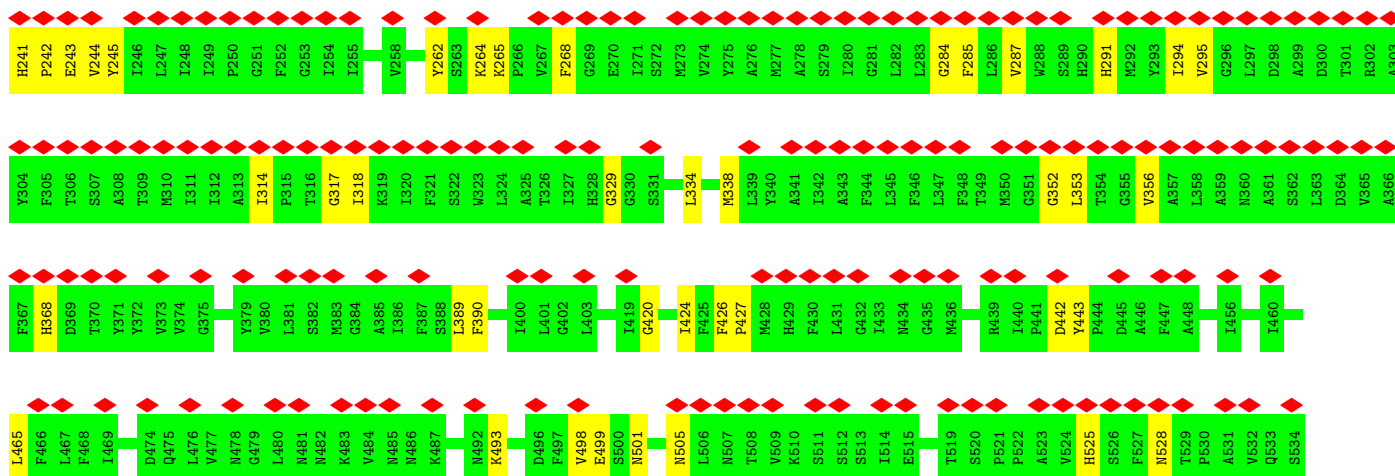


- Molecule 11: Cytochrome c oxidase subunit 1

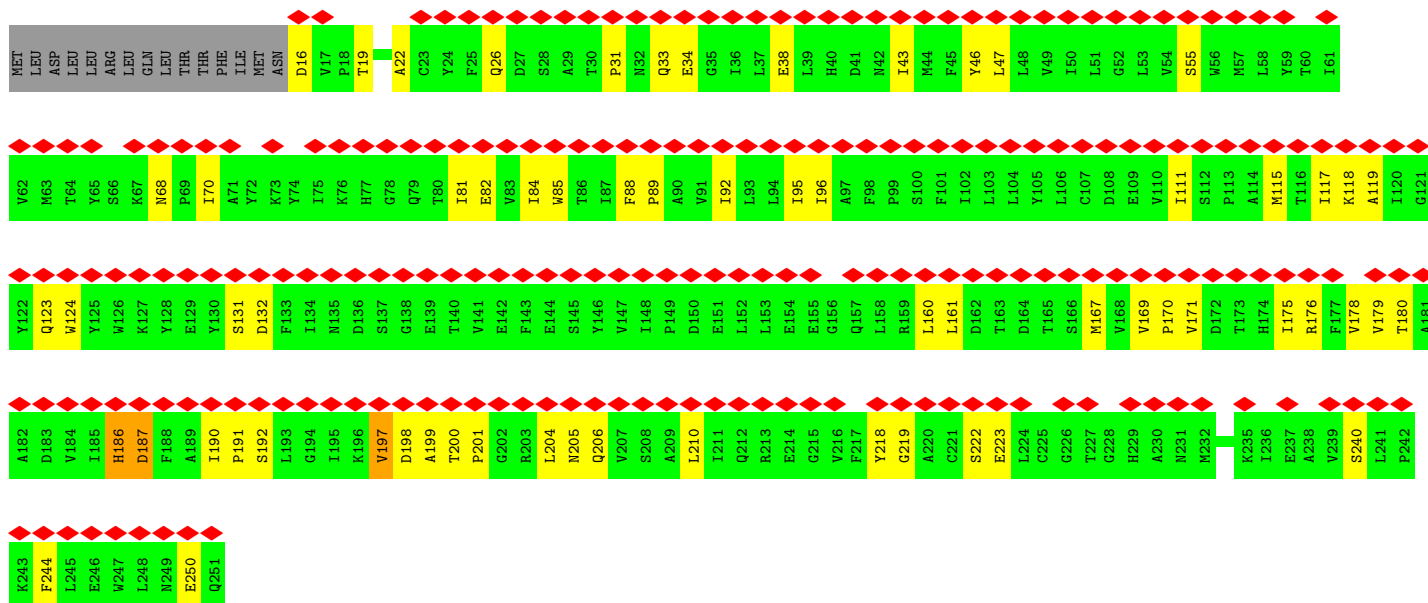
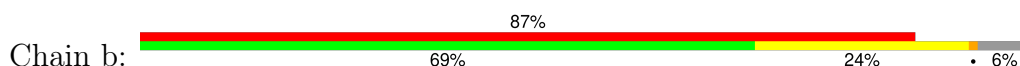


• Molecule 11: Cytochrome c oxidase subunit 1

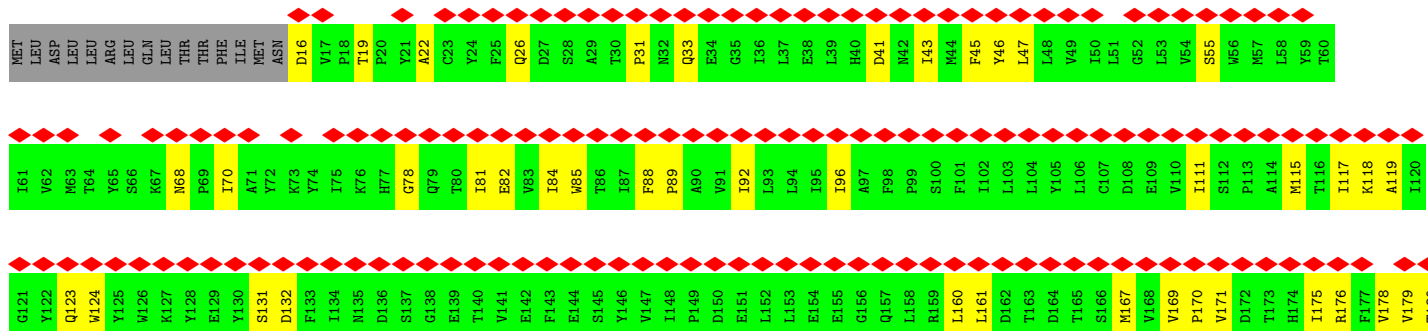
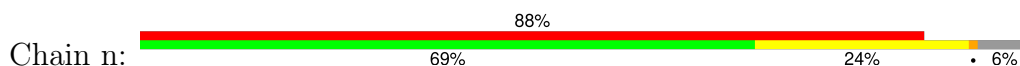




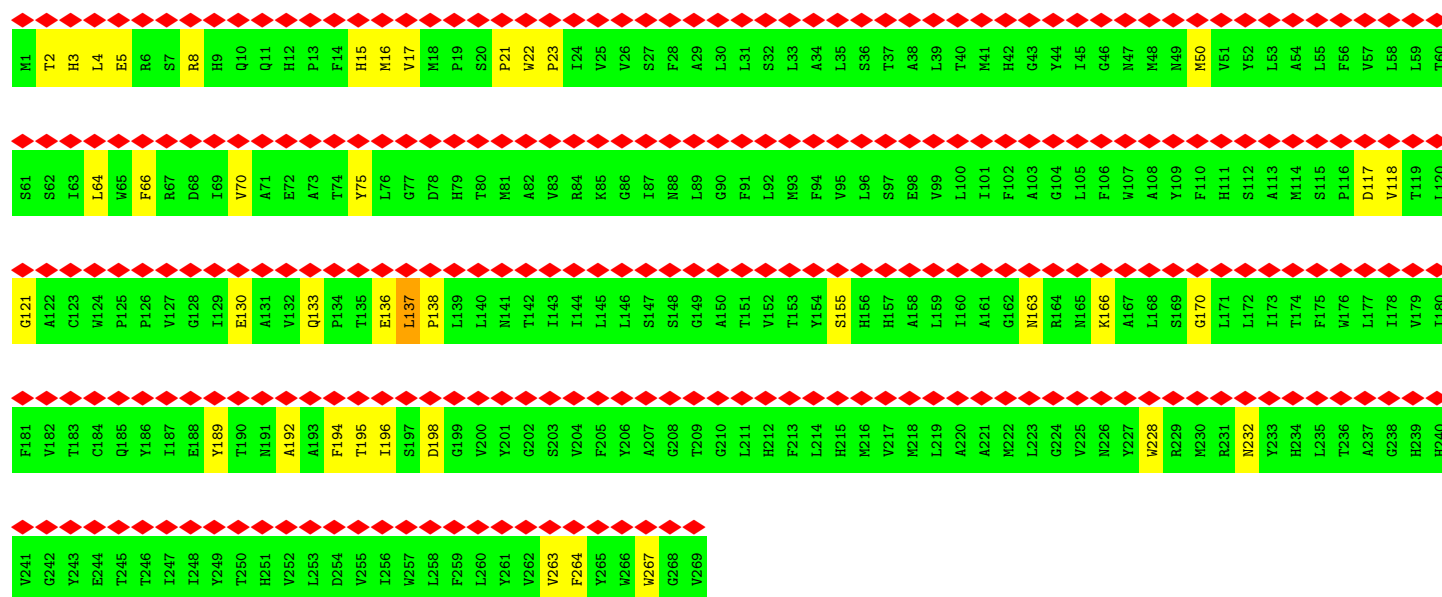
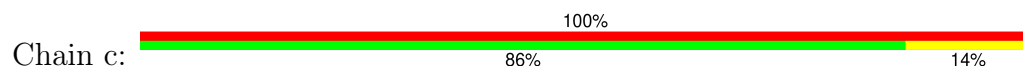
• Molecule 12: Cytochrome c oxidase subunit 2



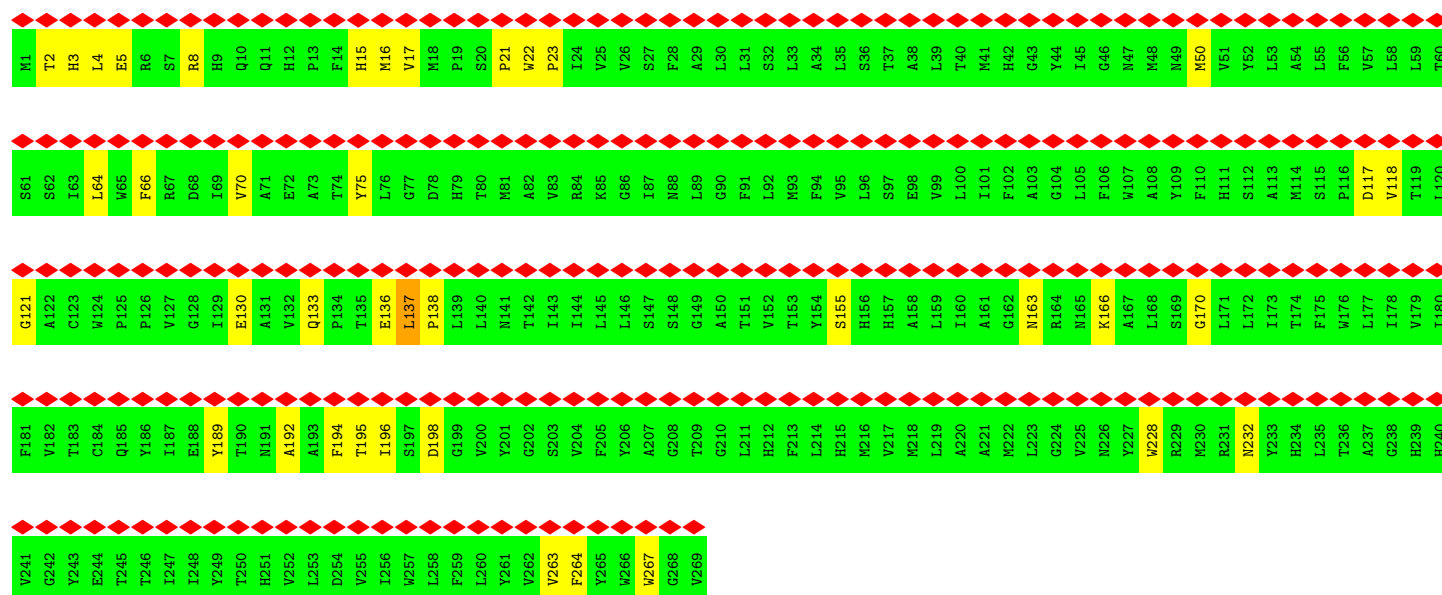
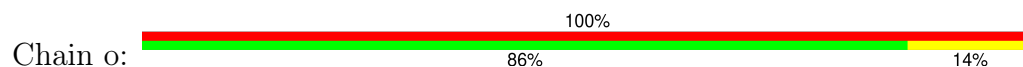
• Molecule 12: Cytochrome c oxidase subunit 2



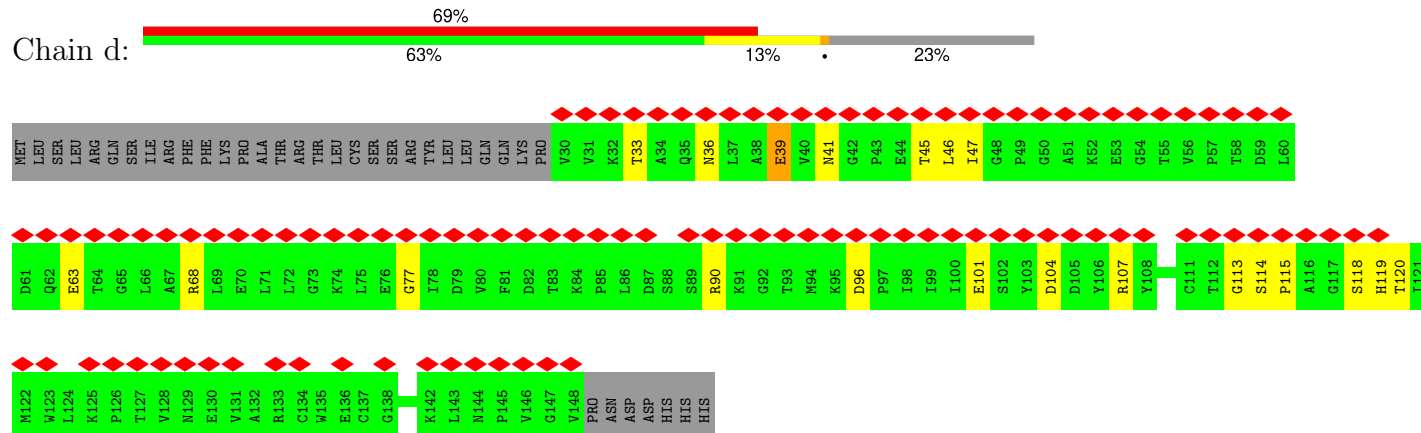
- Molecule 13: Cytochrome c oxidase subunit 3



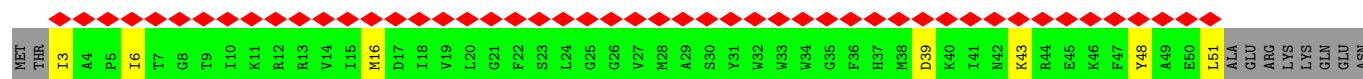
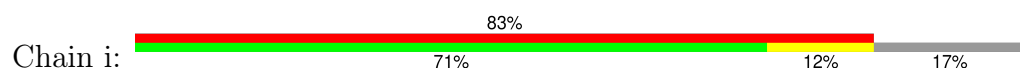
- Molecule 13: Cytochrome c oxidase subunit 3



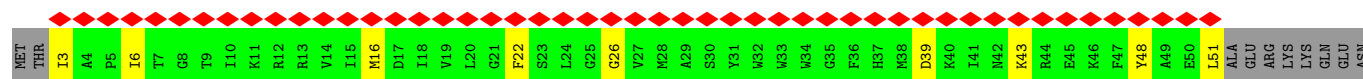
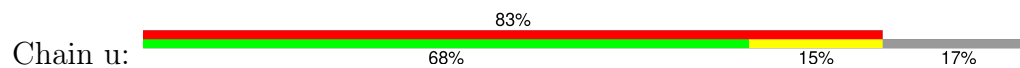
- Molecule 14: Cytochrome c oxidase subunit 4, mitochondrial



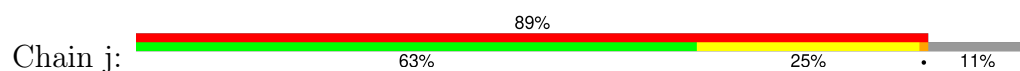




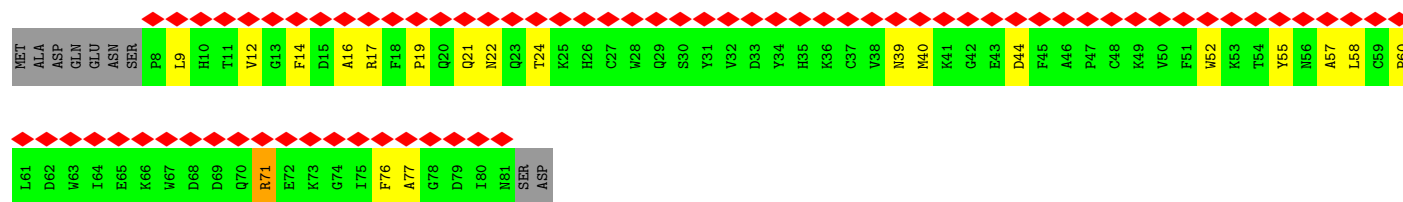
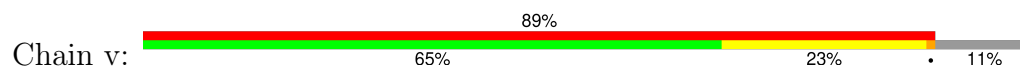
- Molecule 18: Cytochrome c oxidase subunit 9, mitochondrial



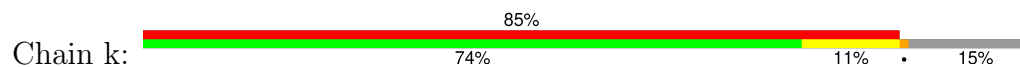
- Molecule 19: Cytochrome c oxidase subunit 12, mitochondrial



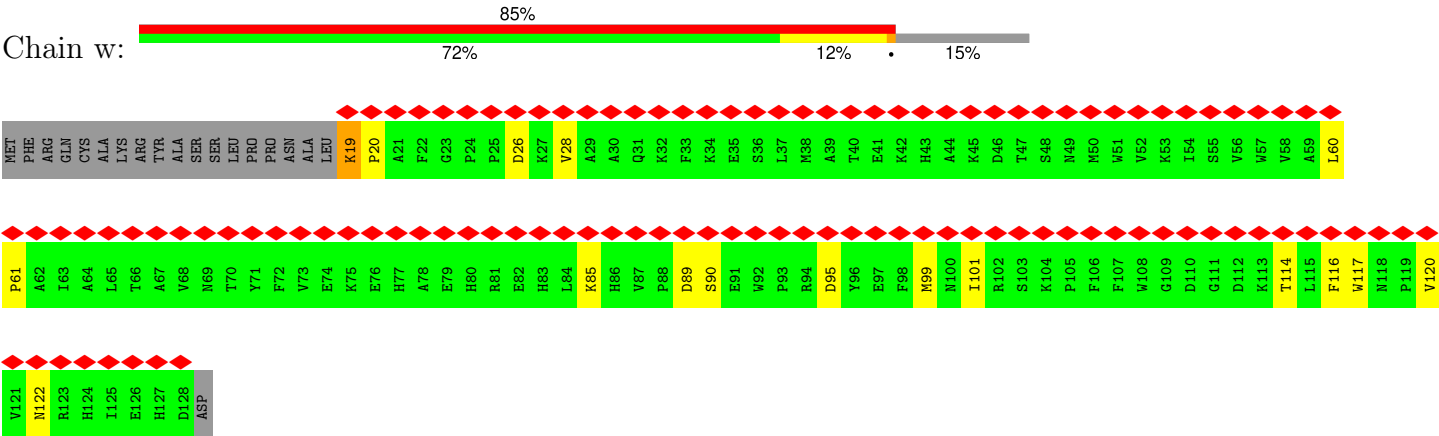
- Molecule 19: Cytochrome c oxidase subunit 12, mitochondrial



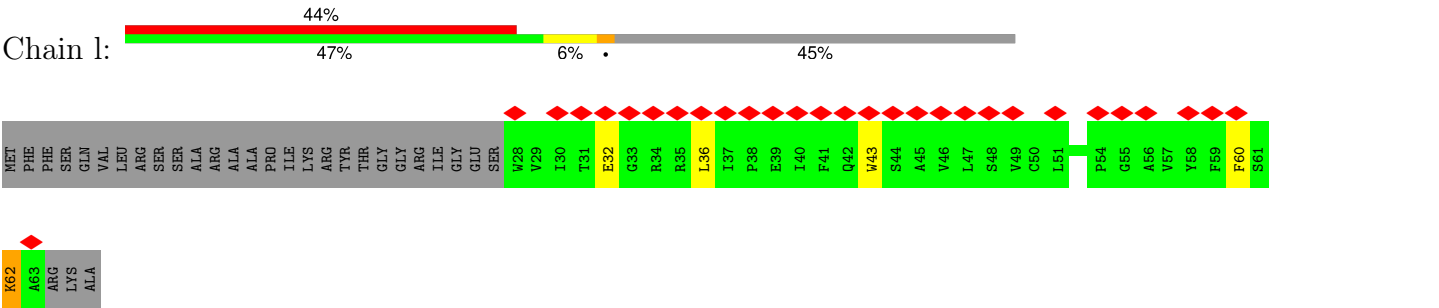
- Molecule 20: Cytochrome c oxidase subunit 13, mitochondrial



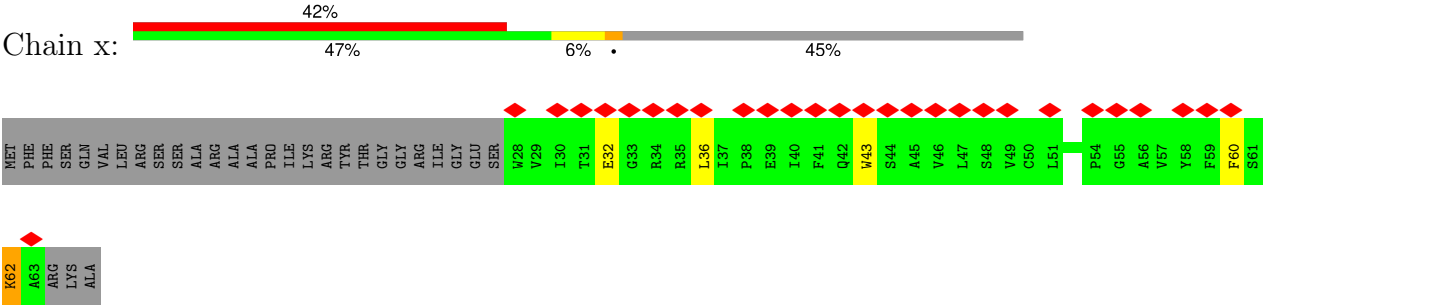
- Molecule 20: Cytochrome c oxidase subunit 13, mitochondrial



• Molecule 21: Cytochrome c oxidase subunit 26, mitochondrial



• Molecule 21: Cytochrome c oxidase subunit 26, mitochondrial





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	47746	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	55.452	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.231	Depositor
Minimum map value	-2.069	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.082	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	508.05, 508.05, 508.05	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.129, 1.129, 1.129	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FES, HEC, CUA, 6PH, UQ6, PTY, CA, CU, MG, 9PE, CN5, 8PE, ZN, PEF, CDL, HEA, CN3, HEM, PCF

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	0.22	0/3400	0.43	0/4608
1	K	0.22	0/3400	0.43	0/4608
2	B	0.17	0/2781	0.39	0/3764
2	L	0.17	0/2781	0.39	0/3764
3	C	0.32	0/3173	0.57	1/4330 (0.0%)
3	M	0.32	0/3173	0.57	1/4330 (0.0%)
4	D	0.27	0/2002	0.49	0/2724
4	N	0.27	0/2002	0.49	0/2724
5	E	0.58	0/1444	0.92	3/1957 (0.2%)
5	O	0.58	0/1444	0.92	3/1957 (0.2%)
6	F	0.13	0/638	0.36	0/858
6	P	0.13	0/638	0.36	0/858
7	G	0.34	0/1029	0.64	0/1396
7	Q	0.34	0/1029	0.64	0/1396
8	H	0.19	0/795	0.44	0/1076
8	R	0.19	0/795	0.44	0/1076
9	I	0.15	0/449	0.33	0/605
9	S	0.15	0/449	0.33	0/605
10	J	0.24	0/363	0.50	0/491
10	T	0.24	0/363	0.50	0/491
11	a	0.26	0/4289	0.46	1/5857 (0.0%)
11	m	0.26	0/4289	0.46	1/5857 (0.0%)
12	b	0.41	0/1940	0.59	0/2653
12	n	0.41	0/1940	0.59	0/2653
13	c	0.24	0/2218	0.40	0/3036
13	o	0.24	0/2218	0.40	0/3036
14	d	0.28	0/915	0.56	1/1244 (0.1%)
14	p	0.28	0/915	0.56	1/1244 (0.1%)
15	e	0.29	0/1032	0.50	1/1396 (0.1%)
15	q	0.29	0/1032	0.50	1/1396 (0.1%)
16	f	0.12	0/836	0.30	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	r	0.12	0/836	0.30	0/1131
17	g	0.13	0/472	0.29	0/645
17	s	0.13	0/472	0.29	0/645
18	i	0.17	0/416	0.32	0/559
18	u	0.17	0/416	0.32	0/559
19	j	0.33	0/643	0.54	0/871
19	v	0.33	0/643	0.54	0/871
20	k	0.29	0/944	0.58	0/1282
20	w	0.29	0/944	0.58	0/1282
21	l	0.44	0/304	0.90	1/415 (0.2%)
21	x	0.44	0/304	0.90	1/415 (0.2%)
All	All	0.29	0/60166	0.52	16/81796 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
11	a	0	1
11	m	0	1
19	j	0	1
19	v	0	1
All	All	0	4

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	l	62	LYS	N-CA-C	-10.84	99.47	111.28
21	x	62	LYS	N-CA-C	-10.84	99.47	111.28
14	d	39	GLU	N-CA-C	-6.21	105.35	113.17
14	p	39	GLU	N-CA-C	-6.21	105.35	113.17
3	C	312	VAL	N-CA-C	-6.16	106.50	112.29
3	M	312	VAL	N-CA-C	-6.16	106.50	112.29
15	e	36	SER	N-CA-C	-5.92	105.32	112.54
15	q	36	SER	N-CA-C	-5.92	105.32	112.54
11	a	291	HIS	N-CA-C	-5.91	105.83	113.16
11	m	291	HIS	N-CA-C	-5.91	105.83	113.16
5	E	93	LYS	CA-C-N	-5.76	115.59	123.14
5	E	93	LYS	C-N-CA	-5.76	115.59	123.14
5	O	93	LYS	CA-C-N	-5.76	115.59	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	93	LYS	C-N-CA	-5.76	115.59	123.14
5	E	121	ARG	N-CA-C	5.50	118.61	110.46
5	O	121	ARG	N-CA-C	5.50	118.61	110.46

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	a	214	ARG	Sidechain
19	j	71	ARG	Sidechain
11	m	214	ARG	Sidechain
19	v	71	ARG	Sidechain

## 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	3339	0	3318	32	0
1	K	3339	0	3318	32	0
2	B	2735	0	2774	42	0
2	L	2735	0	2774	45	0
3	C	3071	0	3106	62	0
3	M	3071	0	3106	60	0
4	D	1941	0	1869	35	0
4	N	1941	0	1869	34	0
5	E	1411	0	1388	31	0
5	O	1411	0	1388	30	0
6	F	624	0	581	11	0
6	P	624	0	581	11	0
7	G	1008	0	1018	24	0
7	Q	1008	0	1018	23	0
8	H	764	0	725	12	0
8	R	764	0	725	12	0
9	I	436	0	431	6	0
9	S	436	0	431	6	0
10	J	352	0	346	7	0
10	T	352	0	346	7	0

*Continued on next page...*

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	a	4161	0	4192	71	0
11	m	4161	0	4192	72	0
12	b	1888	0	1866	58	0
12	n	1888	0	1866	56	0
13	c	2146	0	2137	37	0
13	o	2146	0	2137	37	0
14	d	898	0	891	13	0
14	p	898	0	891	14	0
15	e	1008	0	990	15	0
15	q	1008	0	990	15	0
16	f	819	0	801	13	0
16	r	819	0	801	13	0
17	g	456	0	481	3	0
17	s	456	0	481	3	0
18	i	404	0	408	5	0
18	u	404	0	408	6	0
19	j	621	0	573	18	0
19	v	621	0	573	17	0
20	k	911	0	876	16	0
20	w	911	0	876	17	0
21	l	293	0	291	5	0
21	x	293	0	291	5	0
22	A	55	0	54	2	0
22	D	60	0	64	5	0
22	E	42	0	35	6	0
22	H	53	0	50	3	0
22	K	55	0	54	2	0
22	N	60	0	64	3	0
22	O	42	0	35	6	0
22	R	53	0	50	1	0
23	C	40	0	59	2	0
23	M	40	0	59	2	0
24	C	26	0	25	0	0
24	M	26	0	25	0	0
25	C	32	0	29	0	0
26	C	69	30	89	12	0
26	M	69	30	89	12	0
27	C	86	60	60	9	0
27	M	86	60	60	9	0
28	C	33	0	42	1	0
28	M	33	0	42	1	0
29	D	40	0	53	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	J	29	0	31	1	0
29	N	40	0	53	3	0
29	T	29	0	31	1	0
29	a	43	0	62	2	0
29	m	43	0	62	1	0
30	D	43	32	32	16	0
30	N	43	32	32	16	0
31	E	4	0	0	4	0
31	O	4	0	0	4	0
32	H	32	0	38	3	0
32	I	32	0	38	0	0
32	R	32	0	38	3	0
32	S	32	0	38	0	0
32	k	43	0	60	12	0
32	l	37	0	48	2	0
32	w	43	0	60	12	0
32	x	37	0	48	1	0
33	I	32	0	37	2	0
33	S	32	0	37	2	0
33	a	32	0	37	9	0
33	b	69	0	84	4	0
33	c	40	0	53	1	0
33	m	32	0	37	9	0
33	n	69	0	84	4	0
33	o	40	0	53	1	0
34	a	120	108	108	9	0
34	m	120	108	108	10	0
35	a	1	0	0	0	0
35	m	1	0	0	0	0
36	a	1	0	0	0	0
36	m	1	0	0	0	0
37	a	46	0	42	0	0
37	m	46	0	42	0	0
38	b	1	0	0	0	0
38	n	1	0	0	0	0
39	b	2	0	0	0	0
39	n	2	0	0	0	0
40	d	1	0	0	0	0
40	p	1	0	0	0	0
All	All	60828	460	60555	939	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 8.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:b:16:ASP:N	12:b:192:SER:HG	1.53	1.04
12:n:16:ASP:N	12:n:192:SER:HG	1.55	1.03
11:a:353:LEU:HD12	12:b:47:LEU:HD22	1.51	0.93
11:m:353:LEU:HD12	12:n:47:LEU:HD22	1.51	0.93
4:N:104:CYS:SG	30:N:402:HEC:HAC	2.09	0.93
4:D:104:CYS:SG	30:D:402:HEC:HAC	2.09	0.92
13:o:195:THR:HG22	32:w:201:PCF:H133	1.52	0.90
13:c:195:THR:HG22	32:k:201:PCF:H133	1.52	0.90
3:M:210:LEU:HD12	7:Q:79:HIS:HD2	1.36	0.89
3:C:210:LEU:HD12	7:G:79:HIS:HD2	1.36	0.88
12:n:43:ILE:HG23	12:n:96:ILE:HD11	1.57	0.86
12:b:43:ILE:HG23	12:b:96:ILE:HD11	1.57	0.85
11:m:241:HIS:CE1	11:m:245:TYR:HE2	1.97	0.82
11:a:241:HIS:CE1	11:a:245:TYR:HE2	1.97	0.81
12:b:186:HIS:O	12:b:199:ALA:HB3	1.80	0.80
12:n:186:HIS:O	12:n:199:ALA:HB3	1.80	0.80
3:C:210:LEU:HD12	7:G:79:HIS:CD2	2.17	0.79
12:n:46:TYR:HB3	12:n:92:ILE:HD11	1.65	0.79
15:e:26:LEU:HD22	15:e:31:VAL:HG13	1.65	0.78
5:E:164:CYS:HB2	31:E:301:FES:S2	2.23	0.78
3:M:210:LEU:HD12	7:Q:79:HIS:CD2	2.17	0.78
5:O:164:CYS:HB2	31:O:301:FES:S2	2.23	0.78
12:b:46:TYR:HB3	12:b:92:ILE:HD11	1.65	0.78
15:q:26:LEU:HD22	15:q:31:VAL:HG13	1.65	0.77
11:a:88:ILE:HD11	11:a:186:VAL:HG11	1.65	0.77
11:m:88:ILE:HD11	11:m:186:VAL:HG11	1.65	0.77
3:C:7:ASN:HA	28:C:406:9PE:H12A	1.68	0.76
4:D:101:CYS:HB3	30:D:402:HEC:HAB	1.68	0.76
3:M:7:ASN:HA	28:M:405:9PE:H12A	1.68	0.76
4:N:101:CYS:HB3	30:N:402:HEC:HAB	1.68	0.76
4:N:104:CYS:SG	30:N:402:HEC:CAC	2.74	0.76
4:D:104:CYS:SG	30:D:402:HEC:CAC	2.74	0.75
1:A:29:VAL:HG22	1:A:41:GLU:HG2	1.69	0.75
3:C:375:ASN:HB3	7:G:8:ILE:HD12	1.70	0.74
11:a:241:HIS:NE2	11:a:245:TYR:HE2	1.86	0.74
3:M:375:ASN:HB3	7:Q:8:ILE:HD12	1.70	0.73
1:K:29:VAL:HG22	1:K:41:GLU:HG2	1.69	0.73
11:m:241:HIS:NE2	11:m:245:TYR:HE2	1.86	0.73
12:n:187:ASP:OD1	12:n:223:GLU:N	2.22	0.71
12:b:187:ASP:OD1	12:b:223:GLU:N	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:M:406:HEM:HMC1	27:M:406:HEM:HBC2	1.74	0.69
4:N:101:CYS:HB3	30:N:402:HEC:CAB	2.23	0.69
11:m:499:GLU:O	15:q:83:ARG:NH2	2.26	0.69
27:C:407:HEM:HMC1	27:C:407:HEM:HBC2	1.74	0.68
22:O:302:CDL:H522	22:O:302:CDL:HB61	1.75	0.68
3:M:310:ARG:HB3	7:Q:3:GLN:HB2	1.76	0.68
4:D:101:CYS:HB3	30:D:402:HEC:CAB	2.23	0.68
5:E:55:TYR:HB2	22:E:302:CDL:HA61	1.75	0.68
5:O:55:TYR:HB2	22:O:302:CDL:HA61	1.75	0.68
16:r:112:LYS:NZ	16:r:141:GLU:OE2	2.25	0.67
11:a:499:GLU:O	15:e:83:ARG:NH2	2.26	0.67
5:E:181:HIS:HB2	31:E:301:FES:S1	2.34	0.67
22:E:302:CDL:H522	22:E:302:CDL:HB61	1.75	0.67
5:O:181:HIS:HB2	31:O:301:FES:S1	2.34	0.67
3:C:310:ARG:HB3	7:G:3:GLN:HB2	1.76	0.67
3:C:318:PHE:CD1	7:G:38:TYR:HB3	2.30	0.67
5:E:55:TYR:HB2	22:E:302:CDL:H312	1.77	0.66
13:c:192:ALA:HB3	32:k:201:PCF:H153	1.78	0.66
11:m:87:MET:HE1	11:m:185:PHE:HB3	1.77	0.66
11:a:87:MET:HE1	11:a:185:PHE:HB3	1.77	0.66
13:o:192:ALA:HB3	32:w:201:PCF:H153	1.78	0.66
3:M:346:VAL:O	8:R:77:ASN:ND2	2.29	0.66
11:a:498:VAL:O	16:f:70:GLN:NE2	2.29	0.66
27:M:404:HEM:HBB2	27:M:404:HEM:HMB2	1.77	0.66
12:n:131:SER:HB2	19:v:57:ALA:HA	1.77	0.66
27:C:405:HEM:HBB2	27:C:405:HEM:HMB2	1.77	0.66
3:M:318:PHE:CD1	7:Q:38:TYR:HB3	2.30	0.66
5:O:55:TYR:HB2	22:O:302:CDL:H312	1.77	0.66
20:w:114:THR:HG22	20:w:117:TRP:HE3	1.62	0.65
12:b:131:SER:HB2	19:j:57:ALA:HA	1.77	0.65
19:j:16:ALA:O	19:j:17:ARG:HB3	1.97	0.65
4:N:225:MET:HE3	30:N:402:HEC:NC	2.12	0.65
12:n:16:ASP:O	12:n:26:GLN:NE2	2.29	0.65
20:k:114:THR:HG22	20:k:117:TRP:HE3	1.62	0.65
3:C:12:LEU:HD12	3:M:199:MET:HE1	1.79	0.65
33:a:604:PTY:N1	13:c:15:HIS:HD2	1.93	0.65
12:b:16:ASP:O	12:b:26:GLN:NE2	2.29	0.65
33:m:604:PTY:N1	13:o:15:HIS:HD2	1.93	0.65
3:C:42:ILE:HG12	29:D:401:PEF:H412	1.79	0.65
3:C:199:MET:HE1	3:M:12:LEU:HD12	1.79	0.65
33:a:604:PTY:H311	13:c:66:PHE:CE1	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:346:VAL:O	8:H:77:ASN:ND2	2.29	0.64
12:b:85:TRP:HA	12:b:88:PHE:HB3	1.78	0.64
11:m:498:VAL:O	16:r:70:GLN:NE2	2.29	0.64
33:m:604:PTY:H311	13:o:66:PHE:CE1	2.32	0.64
12:n:85:TRP:HA	12:n:88:PHE:HB3	1.78	0.64
1:A:65:TYR:CE1	15:e:37:ARG:HD2	2.33	0.64
4:D:225:MET:HE3	30:D:402:HEC:NC	2.12	0.64
1:K:29:VAL:HG21	1:K:400:LYS:HD2	1.79	0.64
1:A:29:VAL:HG21	1:A:400:LYS:HD2	1.79	0.64
5:E:210:ASP:O	5:E:211:LYS:HD2	1.97	0.64
3:M:42:ILE:HG12	29:N:401:PEF:H412	1.79	0.64
11:m:98:ILE:HG23	33:m:604:PTY:O12	1.98	0.64
1:K:65:TYR:CE1	15:q:37:ARG:HD2	2.33	0.64
5:O:210:ASP:O	5:O:211:LYS:HD2	1.97	0.64
1:A:89:GLU:HB3	1:A:115:LYS:HD3	1.80	0.63
10:T:13:LEU:HD22	10:T:21:ARG:HE	1.64	0.63
1:K:89:GLU:HB3	1:K:115:LYS:HD3	1.80	0.63
19:v:16:ALA:O	19:v:17:ARG:HB3	1.97	0.63
3:C:309:ASP:O	7:G:2:PRO:HG2	1.99	0.63
4:D:293:ALA:HB3	8:H:31:PRO:HB3	1.80	0.63
10:J:13:LEU:HD22	10:J:21:ARG:HE	1.64	0.63
1:K:72:LEU:HD23	1:K:193:LEU:HD21	1.81	0.63
19:v:39:ASN:OD1	19:v:40:MET:N	2.32	0.63
19:j:39:ASN:OD1	19:j:40:MET:N	2.32	0.62
11:m:498:VAL:HG11	16:r:73:LEU:HD23	1.81	0.62
1:A:41:GLU:HG3	1:A:390:LEU:HD22	1.81	0.62
3:M:133:CYS:HA	3:M:140:SER:HB2	1.80	0.62
11:a:70:LEU:HD11	34:a:601:HEA:H201	1.81	0.62
11:a:98:ILE:HG23	33:a:604:PTY:O12	1.98	0.62
15:q:65:THR:HG23	15:q:67:PRO:HG2	1.82	0.62
15:e:65:THR:HG23	15:e:67:PRO:HG2	1.82	0.62
3:C:201:LEU:HD21	26:C:408:UQ6:H3M2	1.81	0.62
3:M:201:LEU:HD21	26:M:407:UQ6:H3M2	1.81	0.62
3:M:309:ASP:O	7:Q:2:PRO:HG2	1.99	0.62
1:A:72:LEU:HD23	1:A:193:LEU:HD21	1.81	0.62
3:C:133:CYS:HA	3:C:140:SER:HB2	1.80	0.62
12:b:119:ALA:HB3	12:b:179:VAL:HG12	1.82	0.62
17:g:12:PHE:O	17:g:22:ARG:NH1	2.33	0.62
4:N:293:ALA:HB3	8:R:31:PRO:HB3	1.80	0.62
12:n:119:ALA:HB3	12:n:179:VAL:HG12	1.82	0.62
3:C:318:PHE:CE1	7:G:38:TYR:HB3	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:n:19:THR:HB	12:n:22:ALA:HB2	1.81	0.62
1:K:41:GLU:HG3	1:K:390:LEU:HD22	1.81	0.61
12:b:19:THR:HB	12:b:22:ALA:HB2	1.81	0.61
13:o:70:VAL:HG12	33:o:301:PTY:HC11	1.82	0.61
11:a:498:VAL:HG11	16:f:73:LEU:HD23	1.81	0.61
27:M:406:HEM:HBB2	27:M:406:HEM:HMB2	1.82	0.61
11:m:70:LEU:HD11	34:m:601:HEA:H201	1.81	0.61
17:s:12:PHE:O	17:s:22:ARG:NH1	2.33	0.61
1:A:290:ALA:O	1:A:296:ARG:NH1	2.33	0.61
27:C:407:HEM:HBB2	27:C:407:HEM:HMB2	1.82	0.61
12:b:19:THR:HG22	33:b:304:PTY:HN11	1.66	0.61
1:K:290:ALA:O	1:K:296:ARG:NH1	2.33	0.61
27:C:405:HEM:HAA2	26:C:408:UQ6:H3M2	1.83	0.61
11:m:501:ASN:O	11:m:505:ASN:ND2	2.33	0.61
13:o:263:VAL:HG13	13:o:264:PHE:HD1	1.65	0.61
16:f:112:LYS:NZ	16:f:141:GLU:OE2	2.25	0.60
2:L:250:LEU:HD22	2:L:278:LYS:HG2	1.83	0.60
13:c:189:TYR:O	32:k:201:PCF:H122	2.02	0.60
13:c:263:VAL:HG13	13:c:264:PHE:HD1	1.65	0.60
11:m:98:ILE:CG2	33:m:604:PTY:HC52	2.32	0.60
12:n:16:ASP:N	12:n:192:SER:OG	2.31	0.60
2:B:250:LEU:HD22	2:B:278:LYS:HG2	1.83	0.60
13:c:70:VAL:HG12	33:c:301:PTY:HC11	1.82	0.60
13:o:189:TYR:O	32:w:201:PCF:H122	2.02	0.60
3:C:170:SER:OG	3:C:171:VAL:N	2.35	0.60
1:K:166:SER:HA	1:K:175:SER:HB2	1.84	0.60
3:M:318:PHE:CE1	7:Q:38:TYR:HB3	2.35	0.60
11:a:98:ILE:CG2	33:a:604:PTY:HC52	2.32	0.59
12:b:187:ASP:CG	12:b:222:SER:HB2	2.27	0.59
32:H:102:PCF:H12	32:H:102:PCF:H143	1.84	0.59
12:n:19:THR:HG22	33:n:304:PTY:HN11	1.66	0.59
12:n:187:ASP:CG	12:n:222:SER:HB2	2.27	0.59
32:R:102:PCF:H143	32:R:102:PCF:H12	1.84	0.59
16:r:130:ASP:OD1	16:r:131:VAL:N	2.35	0.59
3:M:170:SER:OG	3:M:171:VAL:N	2.35	0.59
14:p:33:THR:HA	14:p:45:THR:O	2.03	0.59
16:f:130:ASP:OD1	16:f:131:VAL:N	2.35	0.59
11:m:241:HIS:O	11:m:244:VAL:HG22	2.03	0.59
11:a:501:ASN:O	11:a:505:ASN:ND2	2.33	0.59
27:M:404:HEM:HAA2	26:M:407:UQ6:H3M2	1.83	0.58
1:A:166:SER:HA	1:A:175:SER:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:j:71:ARG:HA	19:j:76:PHE:HB2	1.85	0.58
27:M:404:HEM:HBC2	27:M:404:HEM:HMC2	1.85	0.58
33:m:604:PTY:N1	13:o:15:HIS:CD2	2.72	0.58
14:d:33:THR:HA	14:d:45:THR:O	2.03	0.58
11:a:241:HIS:O	11:a:244:VAL:HG22	2.03	0.58
26:C:408:UQ6:H311	26:M:403:UQ6:C19	2.34	0.58
5:E:43:LEU:HD21	8:H:29:VAL:HG11	1.85	0.58
10:T:52:GLN:HA	10:T:55:LEU:HB2	1.86	0.58
2:B:230:ARG:NH2	2:B:363:PRO:O	2.37	0.58
3:C:228:LYS:HG3	4:D:288:LYS:HE3	1.86	0.58
19:v:71:ARG:HA	19:v:76:PHE:HB2	1.85	0.58
33:a:604:PTY:N1	13:c:15:HIS:CD2	2.72	0.57
4:D:72:PRO:HG3	6:F:135:ASP:HB3	1.86	0.57
3:M:228:LYS:HG3	4:N:288:LYS:HE3	1.86	0.57
5:O:43:LEU:HD21	8:R:29:VAL:HG11	1.85	0.57
11:m:442:ASP:OD2	12:n:160:LEU:HD11	2.04	0.57
2:B:61:THR:HB	2:B:111:LYS:HZ1	1.69	0.57
12:b:169:VAL:HG11	12:b:175:ILE:HD13	1.86	0.57
11:m:241:HIS:NE2	11:m:245:TYR:CE2	2.72	0.57
2:B:54:PHE:HE2	2:B:172:ILE:HD13	1.69	0.57
27:C:405:HEM:HBC2	27:C:405:HEM:HMC2	1.85	0.57
33:a:604:PTY:HN12	13:c:15:HIS:HD2	1.53	0.57
2:L:230:ARG:NH2	2:L:363:PRO:O	2.37	0.57
4:N:72:PRO:HG3	6:P:135:ASP:HB3	1.86	0.57
11:a:241:HIS:NE2	11:a:245:TYR:CE2	2.72	0.57
11:a:442:ASP:OD2	12:b:160:LEU:HD11	2.04	0.57
5:E:121:ARG:HD2	5:E:187:ILE:HG13	1.87	0.57
5:O:121:ARG:HD2	5:O:187:ILE:HG13	1.87	0.57
1:A:268:GLU:OE2	1:A:421:TRP:NE1	2.38	0.57
12:b:16:ASP:N	12:b:192:SER:OG	2.31	0.57
12:b:43:ILE:O	12:b:47:LEU:HG	2.05	0.57
15:q:66:GLU:N	15:q:67:PRO:HD2	2.19	0.57
4:D:273:THR:HG23	29:D:401:PEF:H112	1.87	0.57
10:J:52:GLN:HA	10:J:55:LEU:HB2	1.86	0.57
1:K:268:GLU:OE2	1:K:421:TRP:NE1	2.38	0.56
2:L:54:PHE:HE2	2:L:172:ILE:HD13	1.69	0.56
26:C:404:UQ6:C19	26:M:407:UQ6:H311	2.34	0.56
15:e:66:GLU:N	15:e:67:PRO:HD2	2.19	0.56
18:i:16:MET:HE1	21:l:32:GLU:HG3	1.86	0.56
2:L:61:THR:HB	2:L:111:LYS:HZ1	1.69	0.56
12:n:43:ILE:O	12:n:47:LEU:HG	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:n:84:ILE:O	12:n:88:PHE:N	2.38	0.56
13:o:192:ALA:O	32:w:201:PCF:H151	2.04	0.56
2:B:69:ARG:HG3	7:Q:120:LEU:HD13	1.88	0.56
32:H:102:PCF:H142	15:e:93:SER:OG	2.06	0.56
5:O:51:LYS:HG2	22:O:302:CDL:HA62	1.88	0.56
33:m:604:PTY:HN12	13:o:15:HIS:HD2	1.53	0.56
7:G:120:LEU:HD13	2:L:69:ARG:HG3	1.88	0.56
11:a:353:LEU:CD1	12:b:47:LEU:HD22	2.31	0.56
13:c:192:ALA:O	32:k:201:PCF:H151	2.04	0.56
12:n:169:VAL:HG11	12:n:175:ILE:HD13	1.86	0.56
12:n:191:PRO:HD3	12:n:219:GLY:HA2	1.88	0.56
18:u:16:MET:HE1	21:x:32:GLU:HG3	1.86	0.56
4:N:273:THR:HG23	29:N:401:PEF:H112	1.87	0.56
5:E:42:VAL:HG12	8:H:34:GLN:HB2	1.87	0.56
13:c:75:TYR:HA	17:g:9:GLN:HG2	1.88	0.56
7:Q:4:SER:OG	7:Q:5:PHE:N	2.38	0.56
16:f:65:ASP:OD1	16:f:68:GLU:N	2.38	0.56
4:D:134:TYR:OH	4:D:154:TYR:O	2.24	0.56
32:R:102:PCF:H142	15:q:93:SER:OG	2.06	0.55
20:w:114:THR:HG22	20:w:117:TRP:CE3	2.41	0.55
13:c:50:MET:HE1	17:g:40:ALA:HA	1.89	0.55
2:B:332:VAL:HG23	2:B:334:SER:H	1.72	0.55
13:c:117:ASP:OD1	13:c:118:VAL:N	2.40	0.55
5:O:42:VAL:HG12	8:R:34:GLN:HB2	1.87	0.55
5:E:186:ASP:OD2	5:E:190:ARG:NH2	2.40	0.55
2:L:84:ARG:HH11	2:L:159:LEU:HD13	1.72	0.55
12:b:191:PRO:HD3	12:b:219:GLY:HA2	1.88	0.55
3:M:150:LEU:HG	3:M:292:VAL:HG22	1.89	0.55
5:O:186:ASP:OD2	5:O:190:ARG:NH2	2.40	0.55
13:o:117:ASP:OD1	13:o:118:VAL:N	2.40	0.55
5:E:51:LYS:HG2	22:E:302:CDL:HA62	1.88	0.55
20:k:114:THR:HG22	20:k:117:TRP:CE3	2.41	0.55
13:o:75:TYR:HA	17:s:9:GLN:HG2	1.88	0.55
13:o:194:PHE:O	32:w:201:PCF:H152	2.07	0.55
4:D:180:ILE:HG12	30:D:402:HEC:CMA	2.38	0.55
3:M:201:LEU:HD21	26:M:407:UQ6:C3M	2.37	0.55
2:B:117:HIS:HB2	7:Q:62:ARG:HH11	1.72	0.54
13:o:195:THR:HG22	32:w:201:PCF:C13	2.33	0.54
19:j:52:TRP:HA	19:j:55:TYR:CE1	2.43	0.54
32:k:201:PCF:H262	32:k:201:PCF:H402	1.90	0.54
2:L:332:VAL:HG23	2:L:334:SER:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:185:TYR:HE1	5:O:191:ILE:HG22	1.72	0.54
3:C:150:LEU:HG	3:C:292:VAL:HG22	1.89	0.54
7:G:62:ARG:HH11	2:L:117:HIS:HB2	1.72	0.54
2:B:84:ARG:HH11	2:B:159:LEU:HD13	1.72	0.54
20:k:122:ASN:CG	32:k:201:PCF:H131	2.32	0.54
12:n:180:THR:HB	12:n:204:LEU:HD23	1.89	0.54
3:C:201:LEU:HD21	26:C:408:UQ6:C3M	2.37	0.54
3:C:247:SER:OG	3:C:250:THR:OG1	2.22	0.54
12:b:180:THR:HB	12:b:204:LEU:HD23	1.89	0.54
20:w:122:ASN:CG	32:w:201:PCF:H131	2.32	0.54
5:O:33:THR:O	8:R:27:TYR:OH	2.25	0.54
32:w:201:PCF:H262	32:w:201:PCF:H402	1.90	0.54
13:c:194:PHE:O	32:k:201:PCF:H152	2.07	0.54
12:n:178:VAL:HG21	19:v:58:LEU:HD12	1.89	0.54
11:a:241:HIS:CE1	11:a:245:TYR:CE2	2.88	0.54
3:C:210:LEU:CD1	7:G:79:HIS:HD2	2.16	0.53
1:K:209:VAL:HG23	1:K:390:LEU:HD23	1.90	0.53
4:N:134:TYR:OH	4:N:154:TYR:O	2.24	0.53
4:N:180:ILE:HG12	30:N:402:HEC:CMA	2.38	0.53
33:m:604:PTY:H311	13:o:66:PHE:HE1	1.73	0.53
1:A:214:ILE:HD12	1:A:219:LEU:HD12	1.90	0.53
6:F:78:LEU:HD13	6:F:142:LEU:HD13	1.90	0.53
34:a:601:HEA:HBC1	34:a:601:HEA:HMC1	1.90	0.53
7:G:4:SER:OG	7:G:5:PHE:N	2.38	0.53
11:a:420:GLY:O	11:a:424:ILE:HG13	2.08	0.53
13:c:198:ASP:HA	20:k:99:MET:O	2.08	0.53
13:o:50:MET:HE1	17:s:40:ALA:HA	1.89	0.53
12:b:84:ILE:O	12:b:88:PHE:N	2.38	0.53
4:N:101:CYS:CB	30:N:402:HEC:CAB	2.87	0.53
6:P:78:LEU:HD13	6:P:142:LEU:HD13	1.90	0.53
11:m:44:GLY:N	11:m:442:ASP:OD1	2.41	0.53
11:m:173:ARG:NH1	11:m:179:MET:SD	2.82	0.53
19:v:52:TRP:HA	19:v:55:TYR:CE1	2.43	0.53
4:D:92:ARG:NH1	4:D:250:ASP:OD2	2.42	0.53
22:D:403:CDL:H112	22:D:403:CDL:H532	1.90	0.53
5:E:185:TYR:HE1	5:E:191:ILE:HG22	1.72	0.53
8:H:60:LEU:O	8:H:64:GLY:N	2.42	0.53
12:n:68:ASN:ND2	12:n:70:ILE:O	2.41	0.53
3:C:230:LEU:HD13	23:C:401:6PH:H26	1.90	0.53
13:c:163:ASN:HD21	13:c:166:LYS:HD3	1.74	0.53
34:m:601:HEA:HMC1	34:m:601:HEA:HBC1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:w:122:ASN:OD1	32:w:201:PCF:H131	2.09	0.53
4:D:101:CYS:CB	30:D:402:HEC:CAB	2.87	0.53
12:b:68:ASN:ND2	12:b:70:ILE:O	2.41	0.53
12:b:81:ILE:HG13	12:b:85:TRP:CD1	2.44	0.53
16:f:117:ASN:HB2	16:f:120:GLN:HB2	1.91	0.53
1:K:214:ILE:HD12	1:K:219:LEU:HD12	1.90	0.53
3:M:230:LEU:HD13	23:M:401:6PH:H26	1.90	0.53
13:o:163:ASN:HD21	13:o:166:LYS:HD3	1.74	0.53
20:w:95:ASP:HB3	20:w:99:MET:HB3	1.90	0.53
1:A:169:PHE:O	1:A:172:THR:OG1	2.24	0.53
11:a:525:HIS:NE2	13:c:16:MET:HE1	2.24	0.53
12:b:178:VAL:HG21	19:j:58:LEU:HD12	1.89	0.53
20:k:122:ASN:OD1	32:k:201:PCF:H131	2.09	0.53
22:N:403:CDL:H112	22:N:403:CDL:H532	1.90	0.53
3:M:379:TYR:CE2	7:Q:12:GLY:HA3	2.44	0.53
8:R:60:LEU:O	8:R:64:GLY:N	2.42	0.53
20:k:85:LYS:HD3	20:k:120:VAL:HG22	1.92	0.52
11:m:420:GLY:O	11:m:424:ILE:HG13	2.08	0.52
13:o:198:ASP:HA	20:w:99:MET:O	2.08	0.52
1:A:209:VAL:HG23	1:A:390:LEU:HD23	1.90	0.52
1:A:211:THR:HG21	1:A:386:ASP:HB2	1.91	0.52
20:k:95:ASP:HB3	20:k:99:MET:HB3	1.90	0.52
5:O:124:HIS:O	5:O:127:GLN:NE2	2.42	0.52
11:m:241:HIS:CE1	11:m:245:TYR:CE2	2.88	0.52
11:a:173:ARG:NH1	11:a:179:MET:SD	2.82	0.52
4:N:92:ARG:NH1	4:N:250:ASP:OD2	2.42	0.52
3:C:72:VAL:CG1	5:E:81:SER:OG	2.58	0.52
9:I:13:ARG:HB2	9:I:16:VAL:HG22	1.91	0.52
3:M:72:VAL:CG1	5:O:81:SER:OG	2.58	0.52
3:M:247:SER:OG	3:M:250:THR:OG1	2.22	0.52
11:a:218:THR:HG22	13:c:196:ILE:HG13	1.91	0.52
21:l:60:PHE:CD2	32:l:101:PCF:H252	2.45	0.52
2:L:66:LYS:HE2	2:L:70:GLU:OE2	2.10	0.52
2:B:66:LYS:HE2	2:B:70:GLU:OE2	2.10	0.52
2:B:198:LYS:HA	2:B:201:VAL:HB	1.92	0.52
3:M:320:VAL:HB	7:Q:32:PHE:CE1	2.45	0.52
12:n:81:ILE:HG13	12:n:85:TRP:CD1	2.44	0.52
20:w:85:LYS:HD3	20:w:120:VAL:HG22	1.92	0.52
33:a:604:PTY:H311	13:c:66:PHE:HE1	1.73	0.52
9:S:13:ARG:HB2	9:S:16:VAL:HG22	1.91	0.52
16:r:65:ASP:OD1	16:r:68:GLU:N	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:m:40:LEU:O	11:m:443:TYR:OH	2.26	0.52
11:m:353:LEU:CD1	12:n:47:LEU:HD22	2.31	0.52
21:x:60:PHE:CD2	32:x:101:PCF:H252	2.45	0.52
3:C:320:VAL:HB	7:G:32:PHE:CE1	2.45	0.51
3:C:379:TYR:CE2	7:G:12:GLY:HA3	2.44	0.51
2:B:291:ASP:OD1	2:B:292:GLN:N	2.43	0.51
11:a:40:LEU:O	11:a:443:TYR:OH	2.26	0.51
2:L:291:ASP:OD1	2:L:292:GLN:N	2.43	0.51
3:C:89:PHE:HE2	3:C:124:THR:HG21	1.75	0.51
3:M:106:TYR:HB3	3:M:114:TRP:CD2	2.46	0.51
11:m:525:HIS:NE2	13:o:16:MET:HE1	2.24	0.51
14:p:77:GLY:HA3	20:w:26:ASP:H	1.75	0.51
3:C:106:TYR:HB3	3:C:114:TRP:CD2	2.46	0.51
4:D:105:HIS:NE2	30:D:402:HEC:ND	2.59	0.51
14:d:36:ASN:HB3	14:d:39:GLU:HG3	1.92	0.51
1:K:211:THR:HG21	1:K:386:ASP:HB2	1.91	0.51
11:m:218:THR:HG22	13:o:196:ILE:HG13	1.91	0.51
22:H:101:CDL:H522	22:H:101:CDL:OA7	2.11	0.51
13:c:133:GLN:HB3	13:c:136:GLU:HG2	1.92	0.51
4:N:101:CYS:HB3	30:N:402:HEC:HHC	1.93	0.51
13:c:137:LEU:HB3	13:c:138:PRO:HD3	1.93	0.51
5:E:33:THR:O	8:H:27:TYR:OH	2.25	0.51
13:c:228:TRP:CD1	13:c:232:ASN:HD22	2.29	0.51
3:M:62:PHE:O	3:M:65:VAL:HG22	2.11	0.51
13:o:133:GLN:HB3	13:o:136:GLU:HG2	1.92	0.51
16:r:85:PRO:HG3	18:u:3:ILE:HG13	1.93	0.51
4:D:225:MET:HE3	30:D:402:HEC:C1C	2.41	0.51
5:E:124:HIS:O	5:E:127:GLN:NE2	2.42	0.51
12:n:55:SER:HB3	21:x:43:TRP:HH2	1.76	0.51
13:o:137:LEU:HB3	13:o:138:PRO:HD3	1.93	0.51
12:b:55:SER:HB3	21:l:43:TRP:HH2	1.76	0.51
3:M:89:PHE:HE2	3:M:124:THR:HG21	1.75	0.51
14:p:36:ASN:HB3	14:p:39:GLU:HG3	1.92	0.51
14:d:77:GLY:HA3	20:k:26:ASP:H	1.75	0.51
2:L:182:LYS:N	2:L:210:PRO:O	2.36	0.51
10:T:13:LEU:HD11	10:T:20:LEU:HB3	1.93	0.51
33:m:604:PTY:HN12	13:o:15:HIS:CD2	2.28	0.51
2:B:164:VAL:HG21	2:L:232:ARG:NH2	2.26	0.50
2:B:182:LYS:N	2:B:210:PRO:O	2.36	0.50
12:b:33:GLN:HG2	12:b:192:SER:O	2.12	0.50
7:Q:3:GLN:NE2	7:Q:8:ILE:HG22	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:101:CDL:OA7	22:R:101:CDL:H522	2.11	0.50
16:r:117:ASN:HB2	16:r:120:GLN:HB2	1.91	0.50
3:C:62:PHE:O	3:C:65:VAL:HG22	2.11	0.50
33:a:604:PTY:HN12	13:c:15:HIS:CD2	2.28	0.50
14:d:63:GLU:HB3	14:d:68:ARG:HB2	1.94	0.50
2:B:98:LEU:HD11	2:B:197:LEU:HD13	1.94	0.50
4:D:101:CYS:HB3	30:D:402:HEC:HHC	1.93	0.50
5:E:125:GLU:HB3	5:E:187:ILE:HG21	1.94	0.50
16:f:85:PRO:HG3	18:i:3:ILE:HG13	1.93	0.50
2:L:98:LEU:HD11	2:L:197:LEU:HD13	1.94	0.50
12:n:33:GLN:HG2	12:n:192:SER:O	2.12	0.50
2:L:198:LYS:HA	2:L:201:VAL:HB	1.92	0.50
4:N:105:HIS:NE2	30:N:402:HEC:ND	2.59	0.50
13:o:228:TRP:CD1	13:o:232:ASN:HD22	2.29	0.50
12:n:250:GLU:N	12:n:250:GLU:OE1	2.45	0.50
2:B:232:ARG:NH2	2:L:164:VAL:HG21	2.26	0.50
13:c:121:GLY:HA2	19:j:77:ALA:HB1	1.93	0.50
4:N:225:MET:HE3	30:N:402:HEC:C1C	2.41	0.50
5:O:164:CYS:CB	31:O:301:FES:S2	2.97	0.50
3:C:362:TYR:O	3:C:367:VAL:HG23	2.12	0.50
2:L:228:GLU:HG2	2:L:229:ASN:N	2.27	0.50
12:n:187:ASP:OD1	12:n:187:ASP:N	2.45	0.50
12:n:118:LYS:HE3	19:v:60:PRO:HA	1.94	0.50
3:M:210:LEU:CD1	7:Q:79:HIS:HD2	2.16	0.49
14:p:63:GLU:HB3	14:p:68:ARG:HB2	1.94	0.49
13:c:155:SER:HB2	13:c:170:GLY:HA3	1.94	0.49
7:G:3:GLN:NE2	7:G:8:ILE:HG22	2.27	0.49
12:b:250:GLU:N	12:b:250:GLU:OE1	2.45	0.49
22:A:501:CDL:OB7	22:A:501:CDL:HA21	2.13	0.49
10:J:13:LEU:HD11	10:J:20:LEU:HB3	1.93	0.49
1:K:367:LYS:NZ	1:K:410:ILE:O	2.45	0.49
22:K:501:CDL:HA21	22:K:501:CDL:OB7	2.13	0.49
13:o:121:GLY:HA2	19:v:77:ALA:HB1	1.93	0.49
20:w:19:LYS:N	20:w:20:PRO:CD	2.76	0.49
1:A:52:GLY:HA3	1:A:105:ILE:HD13	1.95	0.49
11:a:26:GLY:HA2	11:a:70:LEU:HD12	1.95	0.49
11:a:334:LEU:HD13	29:a:607:PEF:H112	1.95	0.49
20:k:19:LYS:N	20:k:20:PRO:CD	2.76	0.49
11:m:97:ARG:HH21	13:o:17:VAL:HG21	1.78	0.49
12:n:81:ILE:HG13	12:n:85:TRP:NE1	2.28	0.49
2:B:232:ARG:NH2	2:L:164:VAL:CG2	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:m:26:GLY:HA2	11:m:70:LEU:HD12	1.95	0.49
2:B:164:VAL:CG2	2:L:232:ARG:NH2	2.76	0.49
1:A:367:LYS:NZ	1:A:410:ILE:O	2.45	0.49
6:F:126:GLU:N	6:F:126:GLU:OE1	2.46	0.49
7:G:3:GLN:O	7:G:3:GLN:HG2	2.13	0.49
11:a:128:THR:HG22	11:a:236:PHE:CE2	2.48	0.49
12:b:81:ILE:HG13	12:b:85:TRP:NE1	2.28	0.49
11:m:128:THR:HG22	11:m:236:PHE:CE2	2.48	0.49
11:m:334:LEU:HD13	29:m:607:PEF:H112	1.95	0.49
20:w:116:PHE:O	32:w:201:PCF:H121	2.13	0.49
2:B:228:GLU:HG2	2:B:229:ASN:N	2.27	0.49
6:F:80:ASP:OD1	6:F:80:ASP:N	2.45	0.49
11:a:237:TRP:HE3	11:a:240:GLY:HA3	1.78	0.49
5:O:125:GLU:HB3	5:O:187:ILE:HG21	1.94	0.49
4:D:208:LEU:HD11	4:D:214:TYR:HB2	1.95	0.48
29:D:401:PEF:H52	5:E:77:THR:OG1	2.13	0.48
9:I:17:PHE:O	9:I:21:ILE:HG12	2.13	0.48
12:b:117:ILE:HG21	12:b:167:MET:HE1	1.95	0.48
14:d:101:GLU:O	14:d:107:ARG:NH1	2.46	0.48
4:N:208:LEU:HD11	4:N:214:TYR:HB2	1.95	0.48
11:m:70:LEU:HD11	34:m:601:HEA:C20	2.43	0.48
11:m:237:TRP:HE3	11:m:240:GLY:HA3	1.78	0.48
11:a:264:LYS:HG2	11:a:493:LYS:HE2	1.95	0.48
13:c:263:VAL:HG13	13:c:264:PHE:CD1	2.47	0.48
11:m:264:LYS:HG2	11:m:493:LYS:HE2	1.95	0.48
1:K:52:GLY:HA3	1:K:105:ILE:HD13	1.95	0.48
3:M:97:MET:HG2	27:M:404:HEM:CBC	2.43	0.48
3:M:362:TYR:O	3:M:367:VAL:HG23	2.12	0.48
9:S:17:PHE:O	9:S:21:ILE:HG12	2.13	0.48
12:n:117:ILE:HG21	12:n:167:MET:HE1	1.95	0.48
3:C:97:MET:HG2	27:C:405:HEM:CBC	2.43	0.48
34:a:603:HEA:HMC3	34:a:603:HEA:HBC1	1.95	0.48
14:d:90:ARG:NH2	14:d:96:ASP:O	2.45	0.48
4:N:105:HIS:CE1	4:N:177:LEU:HD21	2.49	0.48
7:Q:6:THR:HG22	7:Q:108:LEU:HD22	1.95	0.48
13:o:155:SER:HB2	13:o:170:GLY:HA3	1.94	0.48
4:D:186:GLY:HA3	4:D:190:TYR:HB2	1.96	0.48
13:c:195:THR:HG22	32:k:201:PCF:C13	2.33	0.48
2:L:201:VAL:HG13	2:L:206:LEU:HD11	1.96	0.48
3:M:331:PHE:O	3:M:335:LEU:N	2.41	0.48
11:m:352:GLY:O	11:m:356:VAL:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:p:90:ARG:NH2	14:p:96:ASP:O	2.45	0.48
14:p:113:GLY:HA3	14:p:118:SER:OG	2.13	0.48
22:D:403:CDL:HB61	22:D:403:CDL:H712	1.50	0.48
7:G:6:THR:HG22	7:G:108:LEU:HD22	1.95	0.48
12:b:118:LYS:HE3	19:j:60:PRO:HA	1.94	0.48
14:d:113:GLY:HA3	14:d:118:SER:OG	2.13	0.48
16:f:82:VAL:HG22	16:f:114:LYS:HG3	1.95	0.48
16:r:82:VAL:HG22	16:r:114:LYS:HG3	1.95	0.48
2:B:201:VAL:HG13	2:B:206:LEU:HD11	1.96	0.48
3:C:182:LEU:O	3:C:186:VAL:HG23	2.14	0.48
2:L:281:ASP:N	2:L:281:ASP:OD1	2.47	0.48
3:M:182:LEU:O	3:M:186:VAL:HG23	2.14	0.48
1:A:42:HIS:HD2	1:A:44:PRO:HD3	1.79	0.48
11:a:352:GLY:O	11:a:356:VAL:HG13	2.13	0.48
1:K:57:SER:O	1:K:102:GLN:HG3	2.14	0.48
7:Q:3:GLN:O	7:Q:3:GLN:HG2	2.13	0.48
2:B:98:LEU:HD21	2:B:197:LEU:HB2	1.94	0.48
11:a:97:ARG:HH21	13:c:17:VAL:HG21	1.78	0.48
11:a:265:LYS:HZ1	11:a:329:GLY:H	1.62	0.48
20:k:116:PHE:O	32:k:201:PCF:H121	2.13	0.48
5:O:172:ASP:OD2	5:O:184:HIS:NE2	2.47	0.48
4:D:105:HIS:CE1	4:D:177:LEU:HD21	2.49	0.48
1:K:42:HIS:HD2	1:K:44:PRO:HD3	1.79	0.48
1:K:231:GLN:HG3	1:K:232:THR:H	1.78	0.48
3:M:29:TRP:HB3	3:M:99:LYS:HG3	1.96	0.48
6:P:126:GLU:N	6:P:126:GLU:OE1	2.46	0.48
14:p:101:GLU:O	14:p:107:ARG:NH1	2.46	0.48
2:L:30:THR:HG22	2:L:92:THR:HG23	1.95	0.47
2:L:98:LEU:HD21	2:L:197:LEU:HB2	1.94	0.47
11:m:498:VAL:O	11:m:498:VAL:HG12	2.14	0.47
34:m:603:HEA:HMC3	34:m:603:HEA:HBC1	1.95	0.47
2:B:329:ASN:HA	2:B:332:VAL:HG22	1.96	0.47
15:e:53:LEU:HD13	15:e:72:VAL:HG12	1.96	0.47
1:A:231:GLN:HG3	1:A:232:THR:H	1.78	0.47
4:N:180:ILE:HG12	30:N:402:HEC:HMA3	1.96	0.47
29:N:401:PEF:H52	5:O:77:THR:OG1	2.13	0.47
4:D:96:VAL:HG12	4:D:234:VAL:HG11	1.96	0.47
1:A:57:SER:O	1:A:102:GLN:HG3	2.14	0.47
5:E:55:TYR:CB	22:E:302:CDL:HA61	2.42	0.47
11:a:295:VAL:HA	12:b:198:ASP:HB2	1.97	0.47
12:b:31:PRO:HD2	12:b:210:LEU:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:n:31:PRO:HD2	12:n:210:LEU:O	2.13	0.47
12:n:81:ILE:HG13	12:n:85:TRP:HE1	1.80	0.47
4:D:180:ILE:HG12	30:D:402:HEC:HMA3	1.96	0.47
5:E:172:ASP:OD2	5:E:184:HIS:NE2	2.47	0.47
5:E:186:ASP:OD1	5:E:190:ARG:N	2.47	0.47
6:F:109:GLN:HG2	6:F:114:TYR:CE2	2.50	0.47
10:J:13:LEU:HD21	10:J:21:ARG:H	1.80	0.47
22:O:302:CDL:HA61	22:O:302:CDL:H312	1.53	0.47
1:A:40:THR:HB	1:A:216:HIS:HD1	1.79	0.47
3:C:29:TRP:HB3	3:C:99:LYS:HG3	1.96	0.47
11:a:44:GLY:N	11:a:442:ASP:OD1	2.41	0.47
11:a:498:VAL:O	11:a:498:VAL:HG12	2.14	0.47
3:M:254:PRO:HD2	4:N:185:HIS:NE2	2.29	0.47
5:O:186:ASP:OD1	5:O:190:ARG:N	2.47	0.47
11:m:295:VAL:HA	12:n:198:ASP:HB2	1.97	0.47
34:m:603:HEA:H22	34:m:603:HEA:H261	1.96	0.47
14:p:114:SER:HB3	14:p:115:PRO:HD3	1.97	0.47
11:a:70:LEU:HD11	34:a:601:HEA:C20	2.43	0.47
4:N:96:VAL:HG12	4:N:234:VAL:HG11	1.96	0.47
11:m:217:ASN:ND2	20:w:101:ILE:O	2.46	0.47
3:C:199:MET:HE1	3:M:12:LEU:CD1	2.45	0.47
3:C:254:PRO:HD2	4:D:185:HIS:NE2	2.29	0.47
19:j:17:ARG:C	19:j:19:PRO:HD3	2.40	0.47
5:O:55:TYR:CB	22:O:302:CDL:HA61	2.42	0.47
15:q:53:LEU:HD13	15:q:72:VAL:HG12	1.96	0.47
11:a:53:GLN:C	11:a:55:PHE:H	2.23	0.47
11:a:528:ASN:HB3	14:d:104:ASP:OD2	2.15	0.47
4:N:186:GLY:HA3	4:N:190:TYR:HB2	1.96	0.47
10:T:13:LEU:HD21	10:T:21:ARG:H	1.80	0.47
2:B:30:THR:HG22	2:B:92:THR:HG23	1.95	0.46
3:C:12:LEU:CD1	3:M:199:MET:HE1	2.45	0.46
4:D:184:ARG:HE	30:D:402:HEC:CGA	2.27	0.46
2:L:329:ASN:HA	2:L:332:VAL:HG22	1.96	0.46
4:N:184:ARG:HE	30:N:402:HEC:CGA	2.27	0.46
13:o:263:VAL:HG13	13:o:264:PHE:CD1	2.47	0.46
34:a:603:HEA:H261	34:a:603:HEA:H22	1.96	0.46
12:b:81:ILE:HG13	12:b:85:TRP:HE1	1.80	0.46
2:B:206:LEU:HA	2:B:209:LEU:HG	1.97	0.46
2:B:229:ASN:OD1	2:B:230:ARG:N	2.48	0.46
5:E:164:CYS:CB	31:E:301:FES:S2	2.97	0.46
14:d:114:SER:HB3	14:d:115:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:371:SER:O	3:M:375:ASN:ND2	2.48	0.46
11:m:218:THR:C	11:m:220:PHE:H	2.23	0.46
12:b:170:PRO:HG3	12:b:244:PHE:CG	2.51	0.46
1:K:40:THR:HB	1:K:216:HIS:HD1	1.79	0.46
2:L:229:ASN:OD1	2:L:230:ARG:N	2.48	0.46
11:m:528:ASN:HB3	14:p:104:ASP:OD2	2.15	0.46
19:v:17:ARG:C	19:v:19:PRO:HD3	2.40	0.46
11:a:177:MET:HE3	11:a:177:MET:HB2	1.82	0.46
11:a:262:TYR:HB2	11:a:338:MET:HE2	1.98	0.46
12:b:132:ASP:OD1	12:b:132:ASP:N	2.47	0.46
2:L:206:LEU:HA	2:L:209:LEU:HG	1.97	0.46
6:P:109:GLN:HG2	6:P:114:TYR:CE2	2.50	0.46
3:C:371:SER:O	3:C:375:ASN:ND2	2.48	0.46
1:K:169:PHE:O	1:K:172:THR:OG1	2.24	0.46
5:E:32:SER:OG	5:E:35:ARG:HG3	2.16	0.46
2:L:358:ASP:OD2	2:L:361:ASN:ND2	2.46	0.46
11:a:318:ILE:HG23	12:b:85:TRP:HZ3	1.81	0.46
12:b:111:ILE:HA	19:j:14:PHE:HB2	1.97	0.46
23:M:401:6PH:H61	23:M:401:6PH:H2C	1.86	0.46
5:O:32:SER:OG	5:O:35:ARG:HG3	2.16	0.46
3:C:332:ASN:O	3:C:336:LEU:N	2.45	0.46
1:K:191:ALA:HB3	15:q:27:SER:HB3	1.98	0.46
3:M:332:ASN:O	3:M:336:LEU:N	2.45	0.46
11:m:53:GLN:C	11:m:55:PHE:H	2.23	0.46
2:B:230:ARG:HH11	2:B:359:VAL:HB	1.81	0.46
11:a:217:ASN:ND2	20:k:101:ILE:O	2.46	0.46
11:a:314:ILE:HD13	12:b:89:PRO:HB2	1.98	0.46
11:m:241:HIS:CD2	11:m:241:HIS:C	2.93	0.46
12:n:170:PRO:HG3	12:n:244:PHE:CG	2.51	0.46
11:a:191:ILE:O	11:a:195:LEU:HG	2.16	0.45
33:b:304:PTY:HC11	33:b:304:PTY:H311	1.55	0.45
4:N:194:LEU:HD12	4:N:215:ASN:ND2	2.32	0.45
6:P:80:ASP:OD1	6:P:80:ASP:N	2.45	0.45
1:A:191:ALA:HB3	15:e:27:SER:HB3	1.98	0.45
11:a:240:GLY:O	11:a:243:GLU:HB3	2.17	0.45
26:M:407:UQ6:H3M3	26:M:407:UQ6:O2	2.17	0.45
11:m:177:MET:HE3	11:m:177:MET:HB2	1.82	0.45
12:n:132:ASP:OD1	12:n:132:ASP:N	2.47	0.45
6:F:117:LEU:O	6:F:118:GLU:HG3	2.16	0.45
11:a:243:GLU:C	11:a:245:TYR:H	2.24	0.45
12:b:81:ILE:HG21	33:b:302:PTY:H112	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:230:ARG:HH11	2:L:359:VAL:HB	1.81	0.45
12:n:111:ILE:HA	19:v:14:PHE:HB2	1.97	0.45
2:L:99:PRO:O	2:L:102:VAL:HG12	2.17	0.45
11:m:195:LEU:HD22	11:m:285:PHE:HE1	1.81	0.45
11:m:262:TYR:HB2	11:m:338:MET:HE2	1.98	0.45
11:m:318:ILE:HG23	12:n:85:TRP:HZ3	1.81	0.45
3:C:221:MET:HE1	26:C:408:UQ6:C3	2.46	0.45
3:C:331:PHE:O	3:C:335:LEU:N	2.41	0.45
12:b:176:ARG:HH22	19:j:12:VAL:HB	1.81	0.45
11:m:191:ILE:O	11:m:195:LEU:HG	2.16	0.45
11:m:389:LEU:HG	34:m:601:HEA:C25	2.47	0.45
12:n:123:GLN:HG2	12:n:124:TRP:CD1	2.52	0.45
3:C:126:ALA:HB2	26:C:404:UQ6:O5	2.17	0.45
34:m:601:HEA:H273	34:m:601:HEA:H161	1.99	0.45
1:A:36:ILE:HD12	1:A:36:ILE:H	1.82	0.45
11:a:238:PHE:O	11:a:242:PRO:HG2	2.17	0.45
12:b:123:GLN:HG2	12:b:124:TRP:CD1	2.52	0.45
3:M:184:TYR:HD1	3:M:184:TYR:O	2.00	0.45
11:m:237:TRP:CE3	11:m:240:GLY:HA3	2.52	0.45
12:n:176:ARG:HH22	19:v:12:VAL:HB	1.81	0.45
6:F:104:ARG:HA	6:F:107:ILE:HG12	1.99	0.45
11:a:294:ILE:CD1	11:a:368:HIS:HD2	2.29	0.45
1:K:36:ILE:HD12	1:K:36:ILE:H	1.82	0.45
3:M:103:TYR:O	3:M:314:ARG:HG2	2.17	0.45
3:M:221:MET:HE1	26:M:407:UQ6:C3	2.46	0.45
12:n:81:ILE:HG21	33:n:302:PTY:H112	1.98	0.45
2:B:358:ASP:OD2	2:B:361:ASN:ND2	2.46	0.45
11:a:218:THR:C	11:a:220:PHE:H	2.23	0.45
5:O:129:ALA:O	5:O:190:ARG:NH2	2.50	0.45
6:P:117:LEU:O	6:P:118:GLU:HG3	2.16	0.45
11:m:240:GLY:O	11:m:243:GLU:HB3	2.17	0.45
13:o:22:TRP:CH2	13:o:64:LEU:HD23	2.52	0.45
2:B:55:ASN:OD1	2:B:180:TYR:OH	2.35	0.44
2:B:99:PRO:O	2:B:102:VAL:HG12	2.17	0.44
15:e:143:PRO:HB2	15:e:144:TRP:CE3	2.52	0.44
26:M:407:UQ6:H253	26:M:407:UQ6:H201	1.98	0.44
11:m:294:ILE:CD1	11:m:368:HIS:HD2	2.29	0.44
11:m:314:ILE:HD13	12:n:89:PRO:HB2	1.98	0.44
1:A:454:MET:O	22:A:501:CDL:PA1	2.75	0.44
11:a:195:LEU:HD22	11:a:285:PHE:HE1	1.81	0.44
12:b:81:ILE:HD13	33:b:302:PTY:H332	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:3:HIS:HB2	20:w:19:LYS:HE3	1.99	0.44
1:A:265:VAL:HG12	1:A:431:ILE:HG22	2.00	0.44
5:E:106:ASN:HD21	5:E:169:GLU:HG3	1.83	0.44
11:a:84:LEU:HB3	11:a:85:PRO:HD3	2.00	0.44
11:a:241:HIS:CD2	11:a:241:HIS:C	2.93	0.44
12:b:118:LYS:NZ	12:b:131:SER:HB3	2.32	0.44
12:b:131:SER:CB	19:j:57:ALA:HA	2.46	0.44
1:K:454:MET:O	22:K:501:CDL:PA1	2.75	0.44
2:L:55:ASN:OD1	2:L:180:TYR:OH	2.35	0.44
22:N:403:CDL:H1	7:Q:85:HIS:CD2	2.52	0.44
5:O:142:THR:OG1	5:O:143:ASP:N	2.50	0.44
6:P:77:GLN:OE1	6:P:77:GLN:N	2.51	0.44
9:S:39:TRP:CH2	33:S:101:PTY:H131	2.53	0.44
11:m:7:TYR:CZ	13:o:21:PRO:HB3	2.53	0.44
11:m:265:LYS:NZ	11:m:329:GLY:H	2.15	0.44
33:n:304:PTY:HC11	33:n:304:PTY:H311	1.55	0.44
2:B:145:GLN:OE1	2:B:229:ASN:ND2	2.51	0.44
4:D:194:LEU:HD12	4:D:215:ASN:ND2	2.32	0.44
14:d:46:LEU:O	14:d:68:ARG:NE	2.50	0.44
5:O:156:LEU:HD12	5:O:156:LEU:HA	1.88	0.44
5:O:162:LEU:HB2	31:O:301:FES:S2	2.58	0.44
11:m:243:GLU:C	11:m:245:TYR:H	2.24	0.44
16:r:115:VAL:HG11	16:r:121:TYR:HB2	1.99	0.44
11:a:97:ARG:HG2	13:c:23:PRO:HG3	2.00	0.44
1:K:302:LEU:HD13	1:K:350:GLN:HG3	1.98	0.44
27:M:406:HEM:HBB2	27:M:406:HEM:CMB	2.47	0.44
14:p:46:LEU:O	14:p:68:ARG:NE	2.50	0.44
3:C:367:VAL:O	3:C:371:SER:OG	2.29	0.44
26:C:408:UQ6:H3M3	26:C:408:UQ6:O2	2.17	0.44
22:D:403:CDL:H1	7:G:85:HIS:CD2	2.52	0.44
11:a:389:LEU:HG	34:a:601:HEA:C25	2.47	0.44
4:N:119:SER:OG	4:N:120:HIS:ND1	2.45	0.44
5:O:106:ASN:HD21	5:O:169:GLU:HG3	1.83	0.44
15:q:143:PRO:HB2	15:q:144:TRP:CE3	2.52	0.44
1:A:54:VAL:HG21	1:A:391:GLY:HA3	2.00	0.44
26:C:408:UQ6:H253	26:C:408:UQ6:H201	1.98	0.44
11:a:7:TYR:CZ	13:c:21:PRO:HB3	2.53	0.44
16:f:115:VAL:HG11	16:f:121:TYR:HB2	1.99	0.44
3:C:103:TYR:O	3:C:314:ARG:HG2	2.17	0.44
11:m:238:PHE:O	11:m:242:PRO:HG2	2.17	0.44
12:n:118:LYS:NZ	12:n:131:SER:HB3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:129:ALA:O	5:E:190:ARG:NH2	2.50	0.44
11:a:237:TRP:CE3	11:a:240:GLY:HA3	2.52	0.44
11:a:265:LYS:NZ	11:a:329:GLY:H	2.15	0.44
14:p:119:HIS:ND1	14:p:120:THR:O	2.46	0.44
1:A:302:LEU:HD13	1:A:350:GLN:HG3	1.98	0.43
6:F:77:GLN:OE1	6:F:77:GLN:N	2.51	0.43
12:b:34:GLU:O	12:b:38:GLU:N	2.44	0.43
13:c:22:TRP:CH2	13:c:64:LEU:HD23	2.52	0.43
15:e:65:THR:HG22	15:e:68:GLU:CD	2.43	0.43
1:K:265:VAL:HG12	1:K:431:ILE:HG22	2.00	0.43
2:L:98:LEU:N	2:L:99:PRO:HD2	2.33	0.43
3:M:39:CYS:O	3:M:43:GLN:HG2	2.18	0.43
3:M:126:ALA:HB2	26:M:403:UQ6:O5	2.17	0.43
11:m:84:LEU:HB3	11:m:85:PRO:HD3	2.00	0.43
16:r:118:GLU:N	16:r:118:GLU:OE1	2.51	0.43
5:E:162:LEU:HB2	31:E:301:FES:S2	2.58	0.43
11:a:525:HIS:CD2	13:c:16:MET:HE1	2.53	0.43
12:b:161:LEU:HG	12:b:218:TYR:CD1	2.54	0.43
1:K:54:VAL:HG21	1:K:391:GLY:HA3	2.00	0.43
2:L:49:HIS:HA	2:L:82:LEU:HD22	2.00	0.43
2:L:266:GLU:OE1	2:L:266:GLU:N	2.51	0.43
3:M:147:ILE:HG22	26:M:403:UQ6:O2	2.18	0.43
4:N:101:CYS:HA	30:N:402:HEC:HMC2	2.00	0.43
15:q:26:LEU:HD23	15:q:27:SER:N	2.33	0.43
2:B:49:HIS:HA	2:B:82:LEU:HD22	2.00	0.43
2:B:281:ASP:N	2:B:281:ASP:OD1	2.47	0.43
3:C:147:ILE:HG22	26:C:404:UQ6:O2	2.18	0.43
5:E:142:THR:OG1	5:E:143:ASP:N	2.50	0.43
11:a:98:ILE:HG23	33:a:604:PTY:HC52	2.00	0.43
12:b:200:THR:HA	12:b:201:PRO:HD3	1.92	0.43
15:e:26:LEU:HD23	15:e:27:SER:N	2.33	0.43
3:M:74:ASN:CB	5:O:77:THR:HG23	2.49	0.43
6:P:104:ARG:HA	6:P:107:ILE:HG12	1.99	0.43
11:m:2:VAL:O	11:m:6:LEU:HB2	2.17	0.43
11:m:525:HIS:CD2	13:o:16:MET:HE1	2.53	0.43
12:n:161:LEU:HG	12:n:218:TYR:CD1	2.54	0.43
12:n:205:ASN:HB3	19:v:21:GLN:HG2	2.00	0.43
16:r:122:LYS:HA	16:r:125:LEU:HB2	1.99	0.43
3:C:184:TYR:HD1	3:C:184:TYR:O	2.00	0.43
12:b:197:VAL:CG2	12:b:205:ASN:HB2	2.48	0.43
2:L:145:GLN:OE1	2:L:229:ASN:ND2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:44:ILE:O	3:M:48:ILE:HG12	2.17	0.43
11:m:287:VAL:HG23	11:m:287:VAL:O	2.19	0.43
20:w:85:LYS:HE3	20:w:85:LYS:HB2	1.86	0.43
3:C:44:ILE:O	3:C:48:ILE:HG12	2.17	0.43
3:C:74:ASN:CB	5:E:77:THR:HG23	2.49	0.43
9:I:39:TRP:CH2	33:I:101:PTY:H131	2.53	0.43
3:M:54:TYR:OH	3:M:134:CYS:O	2.37	0.43
11:m:97:ARG:HG2	13:o:23:PRO:HG3	2.00	0.43
12:n:131:SER:CB	19:v:57:ALA:HA	2.46	0.43
1:A:457:TRP:HA	10:J:29:ASN:HD21	1.84	0.43
3:C:367:VAL:N	3:C:368:PRO:HD2	2.34	0.43
4:D:101:CYS:HA	30:D:402:HEC:HMC2	2.00	0.43
11:a:287:VAL:HG23	11:a:287:VAL:O	2.19	0.43
16:f:118:GLU:N	16:f:118:GLU:OE1	2.51	0.43
1:K:341:ASP:OD1	1:K:342:ASP:N	2.52	0.43
12:n:197:VAL:CG2	12:n:205:ASN:HB2	2.48	0.43
2:B:62:ARG:HB2	2:B:66:LYS:HG2	2.01	0.43
3:C:39:CYS:O	3:C:43:GLN:HG2	2.18	0.43
3:C:297:ALA:O	3:C:301:VAL:HG23	2.19	0.43
29:D:401:PEF:H362	29:D:401:PEF:H332	1.75	0.43
11:a:2:VAL:O	11:a:6:LEU:HB2	2.17	0.43
34:a:601:HEA:H273	34:a:601:HEA:H161	1.99	0.43
10:T:49:PRO:HD3	29:T:101:PEF:H11	2.01	0.43
12:n:81:ILE:HD13	33:n:302:PTY:H332	1.99	0.43
2:B:65:LEU:HD21	7:Q:117:LYS:HD2	2.00	0.43
11:a:26:GLY:CA	11:a:70:LEU:HD12	2.49	0.43
32:l:101:PCF:H132	32:l:101:PCF:H112	1.84	0.43
1:K:457:TRP:HA	10:T:29:ASN:HD21	1.84	0.43
8:R:41:PHE:HD2	32:R:102:PCF:O12	2.02	0.43
15:q:46:GLN:O	15:q:49:ILE:HG22	2.19	0.43
8:H:12:TRP:CD1	8:H:13:TRP:H	2.36	0.43
11:a:131:PRO:HG2	11:a:132:PRO:HD3	2.00	0.43
19:j:44:ASP:N	19:j:44:ASP:OD1	2.51	0.43
11:m:131:PRO:HG2	11:m:132:PRO:HD3	2.00	0.43
15:q:65:THR:HG22	15:q:68:GLU:CD	2.43	0.43
20:w:26:ASP:C	20:w:28:VAL:H	2.26	0.43
2:B:54:PHE:CE2	2:B:172:ILE:HD13	2.51	0.43
4:D:180:ILE:HG12	30:D:402:HEC:HMA1	2.01	0.43
9:I:36:ILE:HD13	33:I:101:PTY:H181	2.01	0.43
1:K:190:VAL:O	1:K:194:GLU:HG2	2.19	0.43
3:M:297:ALA:O	3:M:301:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:m:212:LEU:HD21	32:w:201:PCF:H371	2.01	0.43
12:n:81:ILE:HG23	12:n:82:GLU:N	2.34	0.43
19:v:44:ASP:OD1	19:v:44:ASP:N	2.51	0.43
1:A:190:VAL:O	1:A:194:GLU:HG2	2.19	0.42
4:D:147:ARG:HH12	4:D:150:LYS:HG2	1.84	0.42
7:G:117:LYS:HD2	2:L:65:LEU:HD21	2.00	0.42
12:b:115:MET:HG2	19:j:9:LEU:HD23	2.01	0.42
14:d:41:ASN:HB2	14:d:45:THR:HG21	2.01	0.42
15:e:46:GLN:O	15:e:49:ILE:HG22	2.19	0.42
3:M:254:PRO:HD2	4:N:185:HIS:CE1	2.54	0.42
11:m:98:ILE:HG23	33:m:604:PTY:HC52	2.00	0.42
3:C:372:THR:HG23	7:G:3:GLN:NE2	2.34	0.42
27:C:407:HEM:HBB2	27:C:407:HEM:CMB	2.47	0.42
12:b:81:ILE:HG23	12:b:82:GLU:N	2.34	0.42
12:b:205:ASN:HB3	19:j:21:GLN:HG2	2.00	0.42
18:i:39:ASP:O	18:i:43:LYS:HG2	2.19	0.42
2:L:54:PHE:CE2	2:L:172:ILE:HD13	2.51	0.42
8:R:12:TRP:CD1	8:R:13:TRP:H	2.36	0.42
12:n:206:GLN:H	19:v:21:GLN:HG3	1.83	0.42
15:q:69:LYS:HD2	16:r:138:PRO:HG3	2.01	0.42
18:u:39:ASP:O	18:u:43:LYS:HG2	2.19	0.42
20:w:89:ASP:OD1	20:w:90:SER:N	2.49	0.42
3:C:254:PRO:HD2	4:D:185:HIS:CE1	2.54	0.42
8:H:41:PHE:HD2	32:H:102:PCF:O12	2.02	0.42
13:c:3:HIS:HB2	20:k:19:LYS:HE3	1.99	0.42
4:N:180:ILE:HG12	30:N:402:HEC:HMA1	2.01	0.42
9:S:36:ILE:HD13	33:S:101:PTY:H181	2.01	0.42
2:B:98:LEU:N	2:B:99:PRO:HD2	2.33	0.42
2:B:266:GLU:N	2:B:266:GLU:OE1	2.51	0.42
26:C:408:UQ6:H253	26:C:408:UQ6:C20	2.49	0.42
5:E:118:ILE:HG23	5:E:154:ILE:HG12	2.01	0.42
5:E:146:ARG:HH11	5:E:189:GLY:HA3	1.85	0.42
5:E:200:LEU:HD12	5:E:200:LEU:HA	1.87	0.42
9:I:7:TYR:CD1	9:I:11:PHE:HB2	2.54	0.42
12:b:206:GLN:H	19:j:21:GLN:HG3	1.83	0.42
14:d:119:HIS:ND1	14:d:120:THR:O	2.46	0.42
16:f:122:LYS:HA	16:f:125:LEU:HB2	1.99	0.42
3:M:367:VAL:N	3:M:368:PRO:HD2	2.34	0.42
11:m:353:LEU:O	11:m:356:VAL:HG22	2.19	0.42
13:o:130:GLU:OE1	13:o:130:GLU:N	2.49	0.42
2:L:54:PHE:CE2	2:L:172:ILE:HG21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:M:404:HEM:HBB2	27:M:404:HEM:CMB	2.48	0.42
12:n:171:VAL:HG22	12:n:240:SER:HA	2.02	0.42
1:A:341:ASP:OD1	1:A:342:ASP:N	2.52	0.42
12:b:171:VAL:HG22	12:b:240:SER:HA	2.02	0.42
14:p:41:ASN:HB2	14:p:45:THR:HG21	2.01	0.42
21:x:32:GLU:HB3	21:x:36:LEU:HD12	2.01	0.42
12:b:161:LEU:HD11	12:b:218:TYR:HB3	2.01	0.42
15:e:69:LYS:HD2	16:f:138:PRO:HG3	2.01	0.42
26:M:407:UQ6:H253	26:M:407:UQ6:C20	2.49	0.42
22:N:403:CDL:HB61	22:N:403:CDL:H712	1.50	0.42
11:m:26:GLY:CA	11:m:70:LEU:HD12	2.49	0.42
12:n:161:LEU:HD11	12:n:218:TYR:HB3	2.01	0.42
2:B:271:ILE:HD13	2:B:287:LEU:HD11	2.02	0.42
11:a:200:LEU:N	11:a:201:PRO:HD2	2.35	0.42
2:L:62:ARG:HB2	2:L:66:LYS:HG2	2.01	0.42
2:L:271:ILE:HD13	2:L:287:LEU:HD11	2.02	0.42
3:M:17:ILE:HG13	3:M:18:ILE:HG13	2.02	0.42
5:O:118:ILE:HG23	5:O:154:ILE:HG12	2.01	0.42
6:P:117:LEU:O	6:P:117:LEU:HD23	2.20	0.42
11:m:88:ILE:HG23	11:m:173:ARG:HG2	2.01	0.42
7:G:72:ALA:O	7:G:76:ILE:HG13	2.20	0.42
20:k:116:PHE:O	32:k:201:PCF:H132	2.20	0.42
2:L:324:LYS:HD3	2:L:324:LYS:HA	1.88	0.42
9:S:7:TYR:CD1	9:S:11:PHE:HB2	2.54	0.42
10:J:49:PRO:HD3	29:J:101:PEF:H11	2.01	0.42
3:M:372:THR:HG23	7:Q:3:GLN:NE2	2.34	0.42
4:N:147:ARG:HH12	4:N:150:LYS:HG2	1.84	0.42
6:P:92:LYS:HA	6:P:95:VAL:HG12	2.02	0.42
4:D:105:HIS:ND1	4:D:177:LEU:HD11	2.35	0.41
30:D:402:HEC:HMB1	30:D:402:HEC:CBB	2.51	0.41
6:F:92:LYS:HA	6:F:95:VAL:HG12	2.02	0.41
11:a:88:ILE:HG23	11:a:173:ARG:HG2	2.01	0.41
11:a:219:SER:O	11:a:219:SER:OG	2.38	0.41
13:c:130:GLU:OE1	13:c:130:GLU:N	2.49	0.41
13:c:263:VAL:HA	13:c:267:TRP:HB3	2.02	0.41
20:k:26:ASP:C	20:k:28:VAL:H	2.26	0.41
20:k:89:ASP:OD1	20:k:90:SER:N	2.49	0.41
2:B:54:PHE:CE2	2:B:172:ILE:HG21	2.54	0.41
3:C:312:VAL:O	7:G:49:ILE:HA	2.20	0.41
8:H:83:LYS:HB3	8:H:83:LYS:HE2	1.92	0.41
1:K:91:LEU:HD23	1:K:106:VAL:HG11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:151:PHE:O	2:L:156:GLY:HA3	2.20	0.41
3:M:139:MET:HE1	3:M:270:VAL:H	1.85	0.41
3:M:312:VAL:O	7:Q:49:ILE:HA	2.20	0.41
11:m:200:LEU:N	11:m:201:PRO:HD2	2.35	0.41
3:C:154:ILE:HA	3:C:155:PRO:HD3	1.94	0.41
23:C:401:6PH:H61	23:C:401:6PH:H2C	1.86	0.41
22:E:302:CDL:HA61	22:E:302:CDL:H312	1.53	0.41
11:m:390:PHE:CD1	34:m:601:HEA:H253	2.56	0.41
12:n:115:MET:HG2	19:v:9:LEU:HD23	2.01	0.41
3:C:139:MET:HE1	3:C:270:VAL:H	1.85	0.41
3:C:201:LEU:HD21	27:C:405:HEM:HAA2	2.02	0.41
3:C:312:VAL:O	7:G:49:ILE:HG23	2.20	0.41
3:C:320:VAL:HB	7:G:32:PHE:HE1	1.85	0.41
11:a:465:LEU:HD13	34:a:601:HEA:H272	2.02	0.41
3:M:201:LEU:HD21	27:M:404:HEM:HAA2	2.02	0.41
5:O:146:ARG:HH11	5:O:189:GLY:HA3	1.85	0.41
8:R:78:GLU:O	8:R:82:SER:HB3	2.21	0.41
14:p:46:LEU:O	14:p:47:ILE:C	2.63	0.41
1:A:91:LEU:HD23	1:A:106:VAL:HG11	2.01	0.41
3:C:89:PHE:CE2	3:C:124:THR:HG21	2.55	0.41
6:F:117:LEU:O	6:F:117:LEU:HD23	2.20	0.41
3:M:312:VAL:O	7:Q:49:ILE:HG23	2.20	0.41
7:Q:72:ALA:O	7:Q:76:ILE:HG13	2.20	0.41
8:R:61:ILE:HB	8:R:62:PRO:HD3	2.03	0.41
13:o:5:GLU:OE1	13:o:8:ARG:NH2	2.53	0.41
2:B:151:PHE:O	2:B:156:GLY:HA3	2.20	0.41
27:C:405:HEM:HBB2	27:C:405:HEM:CMB	2.48	0.41
11:a:353:LEU:O	11:a:356:VAL:HG22	2.19	0.41
20:k:85:LYS:HE3	20:k:85:LYS:HB2	1.86	0.41
21:l:32:GLU:HB3	21:l:36:LEU:HD12	2.01	0.41
2:L:61:THR:H	2:L:111:LYS:NZ	2.19	0.41
4:N:101:CYS:SG	30:N:402:HEC:CAB	3.09	0.41
4:N:236:TYR:CD2	4:N:240:THR:HB	2.56	0.41
7:Q:42:GLY:HA3	7:Q:77:ARG:NH2	2.36	0.41
20:w:116:PHE:O	32:w:201:PCF:H132	2.20	0.41
1:A:169:PHE:HB2	1:A:175:SER:HB3	2.02	0.41
11:a:212:LEU:HD21	32:k:201:PCF:H371	2.01	0.41
12:b:55:SER:CB	21:l:43:TRP:HH2	2.33	0.41
1:K:88:LYS:HE3	1:K:88:LYS:HB2	1.82	0.41
1:K:169:PHE:HB2	1:K:175:SER:HB3	2.02	0.41
2:L:113:ALA:HB1	2:L:115:LYS:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:89:GLU:HG2	6:P:90:GLU:N	2.36	0.41
11:m:268:PHE:HZ	12:n:78:GLY:HA3	1.85	0.41
20:w:60:LEU:HB3	20:w:61:PRO:HD3	2.02	0.41
29:a:607:PEF:H241	29:a:607:PEF:H212	1.84	0.41
12:b:187:ASP:OD1	12:b:222:SER:HB2	2.21	0.41
14:d:46:LEU:O	14:d:47:ILE:C	2.63	0.41
9:S:29:GLN:NE2	10:T:43:VAL:HG13	2.35	0.41
11:m:426:PHE:HB3	11:m:427:PRO:HD3	2.02	0.41
1:A:142:LYS:HB2	1:A:142:LYS:HE3	1.75	0.41
3:C:17:ILE:HG13	3:C:18:ILE:HG13	2.02	0.41
3:C:236:PHE:HD1	22:H:101:CDL:H371	1.86	0.41
3:C:254:PRO:O	4:D:183:ALA:HA	2.21	0.41
3:C:297:ALA:O	3:C:301:VAL:N	2.51	0.41
4:D:236:TYR:CD2	4:D:240:THR:HB	2.56	0.41
4:D:309:LYS:HA	4:D:309:LYS:HD3	1.85	0.41
5:E:209:GLY:O	5:E:210:ASP:HB3	2.21	0.41
6:F:89:GLU:HG2	6:F:90:GLU:N	2.36	0.41
7:G:42:GLY:HA3	7:G:77:ARG:NH2	2.36	0.41
8:H:78:GLU:O	8:H:82:SER:HB3	2.21	0.41
11:a:241:HIS:CD2	11:a:284:GLY:O	2.74	0.41
11:a:390:PHE:CD1	34:a:601:HEA:H253	2.56	0.41
13:c:2:THR:HG22	13:c:4:LEU:H	1.85	0.41
13:c:5:GLU:OE1	13:c:8:ARG:NH2	2.53	0.41
16:f:122:LYS:HD3	16:f:125:LEU:HD12	2.03	0.41
4:N:105:HIS:ND1	4:N:177:LEU:HD11	2.35	0.41
4:N:124:GLU:O	4:N:128:MET:HG3	2.21	0.41
30:N:402:HEC:CBB	30:N:402:HEC:HMB1	2.51	0.41
11:m:317:GLY:HA3	34:m:603:HEA:H202	2.02	0.41
11:m:465:LEU:HD13	34:m:601:HEA:H272	2.02	0.41
16:r:52:PHE:CE1	16:r:81:LEU:HD11	2.56	0.41
2:B:175:PHE:O	2:B:179:VAL:HG22	2.21	0.41
22:D:403:CDL:OB3	8:H:47:ASN:ND2	2.47	0.41
8:H:61:ILE:HB	8:H:62:PRO:HD3	2.03	0.41
19:j:22:ASN:OD1	19:j:24:THR:HG23	2.21	0.41
5:O:209:GLY:O	5:O:210:ASP:HB3	2.21	0.41
15:q:131:LYS:HE2	15:q:131:LYS:HB3	1.91	0.41
18:u:6:ILE:HD12	18:u:6:ILE:H	1.86	0.41
18:u:48:TYR:O	18:u:51:LEU:HB2	2.21	0.41
4:D:101:CYS:SG	30:D:402:HEC:CAB	3.09	0.40
4:D:124:GLU:O	4:D:128:MET:HG3	2.21	0.40
5:E:107:VAL:HB	5:E:118:ILE:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:29:GLN:NE2	10:J:43:VAL:HG13	2.35	0.40
1:K:240:LYS:HD3	15:q:40:ASN:ND2	2.36	0.40
13:o:263:VAL:HA	13:o:267:TRP:HB3	2.02	0.40
19:v:22:ASN:OD1	19:v:24:THR:HG23	2.21	0.40
2:B:61:THR:H	2:B:111:LYS:NZ	2.19	0.40
26:C:408:UQ6:H201	26:C:408:UQ6:C23	2.52	0.40
22:D:403:CDL:H322	22:H:101:CDL:OA6	2.22	0.40
11:a:426:PHE:HB3	11:a:427:PRO:HD3	2.02	0.40
2:L:84:ARG:NH1	2:L:159:LEU:HB2	2.37	0.40
3:M:254:PRO:O	4:N:183:ALA:HA	2.21	0.40
8:R:83:LYS:HB3	8:R:83:LYS:HE2	1.92	0.40
14:p:82:ASP:OD1	14:p:84:LYS:NZ	2.38	0.40
1:A:240:LYS:HD3	15:e:40:ASN:ND2	2.36	0.40
2:B:33:VAL:HG22	2:B:187:VAL:HG13	2.03	0.40
12:b:95:ILE:HD13	12:b:95:ILE:HA	1.94	0.40
2:L:33:VAL:HG22	2:L:187:VAL:HG13	2.03	0.40
3:M:112:THR:O	3:M:116:VAL:HG23	2.21	0.40
26:M:407:UQ6:H201	26:M:407:UQ6:C23	2.52	0.40
12:n:41:ASP:O	12:n:45:PHE:N	2.53	0.40
18:u:22:PHE:O	18:u:26:GLY:N	2.54	0.40
3:C:261:ASN:OD1	3:C:264:VAL:HG12	2.22	0.40
4:D:184:ARG:HD3	4:D:184:ARG:HA	1.83	0.40
15:e:114:ARG:HD2	15:e:114:ARG:HA	1.92	0.40
18:i:6:ILE:HD12	18:i:6:ILE:H	1.86	0.40
18:i:48:TYR:O	18:i:51:LEU:HB2	2.21	0.40
19:j:32:VAL:O	19:j:36:LYS:HG3	2.21	0.40
3:M:222:HIS:O	3:M:223:SER:OG	2.35	0.40
3:M:243:PHE:O	3:M:248:PRO:HA	2.21	0.40
11:m:241:HIS:CD2	11:m:284:GLY:O	2.74	0.40
12:n:55:SER:CB	21:x:43:TRP:HH2	2.33	0.40
13:o:2:THR:HG22	13:o:4:LEU:H	1.85	0.40
11:a:243:GLU:C	11:a:245:TYR:N	2.79	0.40
12:b:170:PRO:HG3	12:b:244:PHE:CD2	2.56	0.40
2:L:124:LEU:HA	2:L:124:LEU:HD23	1.84	0.40
3:M:89:PHE:CE2	3:M:124:THR:HG21	2.55	0.40
8:R:41:PHE:C	8:R:43:ASN:H	2.30	0.40
11:m:149:PHE:O	11:m:153:LEU:HG	2.22	0.40
11:m:243:GLU:C	11:m:245:TYR:N	2.79	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	428/457 (94%)	417 (97%)	11 (3%)	0	100	100
1	K	428/457 (94%)	417 (97%)	11 (3%)	0	100	100
2	B	350/368 (95%)	344 (98%)	6 (2%)	0	100	100
2	L	350/368 (95%)	344 (98%)	6 (2%)	0	100	100
3	C	381/385 (99%)	373 (98%)	8 (2%)	0	100	100
3	M	381/385 (99%)	373 (98%)	8 (2%)	0	100	100
4	D	243/309 (79%)	234 (96%)	9 (4%)	0	100	100
4	N	243/309 (79%)	234 (96%)	9 (4%)	0	100	100
5	E	183/215 (85%)	178 (97%)	5 (3%)	0	100	100
5	O	183/215 (85%)	178 (97%)	5 (3%)	0	100	100
6	F	72/147 (49%)	69 (96%)	3 (4%)	0	100	100
6	P	72/147 (49%)	69 (96%)	3 (4%)	0	100	100
7	G	123/183 (67%)	117 (95%)	6 (5%)	0	100	100
7	Q	123/183 (67%)	117 (95%)	6 (5%)	0	100	100
8	H	90/94 (96%)	83 (92%)	7 (8%)	0	100	100
8	R	90/94 (96%)	83 (92%)	7 (8%)	0	100	100
9	I	51/66 (77%)	50 (98%)	1 (2%)	0	100	100
9	S	51/66 (77%)	50 (98%)	1 (2%)	0	100	100
10	J	43/77 (56%)	41 (95%)	2 (5%)	0	100	100
10	T	43/77 (56%)	41 (95%)	2 (5%)	0	100	100
11	a	532/534 (100%)	506 (95%)	25 (5%)	1 (0%)	44	64
11	m	532/534 (100%)	506 (95%)	25 (5%)	1 (0%)	44	64
12	b	234/251 (93%)	221 (94%)	13 (6%)	0	100	100
12	n	234/251 (93%)	221 (94%)	13 (6%)	0	100	100
13	c	267/269 (99%)	261 (98%)	5 (2%)	1 (0%)	30	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	267/269 (99%)	261 (98%)	5 (2%)	1 (0%)	30	50
14	d	117/155 (76%)	108 (92%)	9 (8%)	0	100	100
14	p	117/155 (76%)	108 (92%)	9 (8%)	0	100	100
15	e	126/153 (82%)	120 (95%)	6 (5%)	0	100	100
15	q	126/153 (82%)	120 (95%)	6 (5%)	0	100	100
16	f	96/148 (65%)	95 (99%)	1 (1%)	0	100	100
16	r	96/148 (65%)	95 (99%)	1 (1%)	0	100	100
17	g	53/60 (88%)	53 (100%)	0	0	100	100
17	s	53/60 (88%)	53 (100%)	0	0	100	100
18	i	47/59 (80%)	44 (94%)	3 (6%)	0	100	100
18	u	47/59 (80%)	44 (94%)	3 (6%)	0	100	100
19	j	72/83 (87%)	68 (94%)	4 (6%)	0	100	100
19	v	72/83 (87%)	68 (94%)	4 (6%)	0	100	100
20	k	108/129 (84%)	98 (91%)	10 (9%)	0	100	100
20	w	108/129 (84%)	98 (91%)	10 (9%)	0	100	100
21	l	34/66 (52%)	32 (94%)	2 (6%)	0	100	100
21	x	34/66 (52%)	32 (94%)	2 (6%)	0	100	100
All	All	7300/8416 (87%)	7024 (96%)	272 (4%)	4 (0%)	50	69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	c	137	LEU
13	o	137	LEU
11	a	219	SER
11	m	219	SER

### 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 PDB entries followed by that with respect to all EM entries.

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	370/393 (94%)	370 (100%)	0	100	100
1	K	370/393 (94%)	370 (100%)	0	100	100
2	B	301/313 (96%)	301 (100%)	0	100	100
2	L	301/313 (96%)	301 (100%)	0	100	100
3	C	335/338 (99%)	335 (100%)	0	100	100
3	M	336/338 (99%)	336 (100%)	0	100	100
4	D	204/251 (81%)	204 (100%)	0	100	100
4	N	204/251 (81%)	204 (100%)	0	100	100
5	E	151/179 (84%)	150 (99%)	1 (1%)	81	92
5	O	151/179 (84%)	150 (99%)	1 (1%)	81	92
6	F	67/131 (51%)	67 (100%)	0	100	100
6	P	67/131 (51%)	67 (100%)	0	100	100
7	G	108/153 (71%)	107 (99%)	1 (1%)	75	89
7	Q	108/153 (71%)	107 (99%)	1 (1%)	75	89
8	H	76/78 (97%)	76 (100%)	0	100	100
8	R	76/78 (97%)	76 (100%)	0	100	100
9	I	44/54 (82%)	44 (100%)	0	100	100
9	S	44/54 (82%)	44 (100%)	0	100	100
10	J	36/66 (54%)	35 (97%)	1 (3%)	38	63
10	T	35/66 (53%)	34 (97%)	1 (3%)	37	62
11	a	447/447 (100%)	447 (100%)	0	100	100
11	m	447/447 (100%)	447 (100%)	0	100	100
12	b	209/224 (93%)	205 (98%)	4 (2%)	52	74
12	n	209/224 (93%)	205 (98%)	4 (2%)	52	74
13	c	228/228 (100%)	228 (100%)	0	100	100
13	o	228/228 (100%)	228 (100%)	0	100	100
14	d	100/135 (74%)	100 (100%)	0	100	100
14	p	100/135 (74%)	100 (100%)	0	100	100
15	e	106/127 (84%)	106 (100%)	0	100	100
15	q	106/127 (84%)	106 (100%)	0	100	100
16	f	87/131 (66%)	87 (100%)	0	100	100
16	r	87/131 (66%)	87 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	g	48/51 (94%)	48 (100%)	0	100	100
17	s	48/51 (94%)	48 (100%)	0	100	100
18	i	41/50 (82%)	41 (100%)	0	100	100
18	u	41/50 (82%)	41 (100%)	0	100	100
19	j	66/74 (89%)	66 (100%)	0	100	100
19	v	66/74 (89%)	66 (100%)	0	100	100
20	k	97/113 (86%)	96 (99%)	1 (1%)	73	87
20	w	97/113 (86%)	96 (99%)	1 (1%)	73	87
21	l	30/53 (57%)	29 (97%)	1 (3%)	33	57
21	x	30/53 (57%)	29 (97%)	1 (3%)	33	57
All	All	6302/7178 (88%)	6284 (100%)	18 (0%)	90	97

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	51	LYS
7	G	8	ILE
10	J	13	LEU
12	b	186	HIS
12	b	187	ASP
12	b	190	ILE
12	b	197	VAL
20	k	19	LYS
21	l	62	LYS
5	O	51	LYS
7	Q	8	ILE
10	T	13	LEU
12	n	186	HIS
12	n	187	ASP
12	n	190	ILE
12	n	197	VAL
20	w	19	LYS
21	x	62	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	GLN
1	A	199	ASN
1	A	298	GLN
1	A	314	ASN
1	A	345	HIS
1	A	376	GLN
2	B	57	GLN
2	B	170	GLN
2	B	252	GLN
3	C	22	GLN
3	C	57	ASN
3	C	141	HIS
3	C	202	HIS
3	C	316	ASN
3	C	332	ASN
4	D	122	ASN
5	E	46	ASN
5	E	151	GLN
5	E	161	HIS
7	G	3	GLN
7	G	79	HIS
7	G	80	GLN
7	G	85	HIS
8	H	43	ASN
11	a	241	HIS
11	a	368	HIS
12	b	26	GLN
12	b	79	GLN
12	b	157	GLN
12	b	205	ASN
12	b	229	HIS
13	c	3	HIS
13	c	15	HIS
13	c	226	ASN
14	d	36	ASN
14	d	41	ASN
14	d	62	GLN
14	d	144	ASN
17	g	13	GLN
19	j	70	GLN
1	K	170	GLN
1	K	199	ASN
1	K	298	GLN

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Mol	Chain	Res	Type
1	K	314	ASN
1	K	345	HIS
1	K	376	GLN
2	L	57	GLN
2	L	170	GLN
2	L	252	GLN
2	L	258	ASN
3	M	22	GLN
3	M	57	ASN
3	M	84	ASN
3	M	141	HIS
3	M	202	HIS
3	M	316	ASN
3	M	332	ASN
4	N	122	ASN
5	O	46	ASN
5	O	151	GLN
5	O	161	HIS
7	Q	3	GLN
7	Q	79	HIS
7	Q	80	GLN
7	Q	85	HIS
8	R	43	ASN
11	m	241	HIS
11	m	368	HIS
12	n	26	GLN
12	n	79	GLN
12	n	157	GLN
12	n	205	ASN
12	n	229	HIS
13	o	3	HIS
13	o	15	HIS
13	o	226	ASN
14	p	36	ASN
14	p	41	ASN
14	p	62	GLN
14	p	144	ASN
17	s	13	GLN
19	v	70	GLN

### 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 ⓘ

Of 67 ligands modelled in this entry, 8 are monoatomic - leaving 59 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
22	CDL	O	302	-	41,41,99	0.37	0	46,51,111	0.50	0
39	CUA	n	303	12	0,1,1	-	-	-		
33	PTY	b	304	-	34,34,49	0.33	0	37,39,54	0.39	0
22	CDL	D	403	-	59,59,99	0.36	0	65,71,111	0.47	0
33	PTY	a	604	-	31,31,49	0.39	0	34,36,54	0.49	0
22	CDL	H	101	-	52,52,99	0.37	0	58,64,111	0.47	0
27	HEM	C	407	3	42,50,50	1.35	6 (14%)	46,82,82	1.84	12 (26%)
33	PTY	o	301	-	39,39,49	0.34	0	42,44,54	0.39	0
34	HEA	a	603	-	58,67,67	2.12	18 (31%)	63,103,103	2.42	26 (41%)
29	PEF	a	607	-	42,42,46	0.31	0	45,47,51	0.34	0
33	PTY	b	302	-	33,33,49	0.36	0	36,38,54	0.52	0
22	CDL	K	501	-	54,54,99	0.37	0	60,66,111	0.49	0
30	HEC	D	402	4	32,50,50	1.94	5 (15%)	30,82,82	2.91	11 (36%)
23	6PH	M	401	-	39,39,39	0.38	0	42,44,44	0.29	0
27	HEM	C	405	3	42,50,50	1.41	7 (16%)	46,82,82	1.71	11 (23%)
22	CDL	R	101	-	52,52,99	0.37	0	58,64,111	0.47	0
33	PTY	n	302	-	33,33,49	0.36	0	36,38,54	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	PTY	c	301	-	39,39,49	0.34	0	42,44,54	0.39	0
22	CDL	E	302	-	41,41,99	0.37	0	46,51,111	0.50	0
32	PCF	I	102	-	31,31,49	0.39	0	37,39,57	0.37	0
26	UQ6	C	408	-	43,43,43	0.24	0	54,55,55	0.62	1 (1%)
32	PCF	x	101	-	36,36,49	0.36	0	42,44,57	0.42	0
34	HEA	m	601	11	58,67,67	2.22	20 (34%)	63,103,103	2.27	20 (31%)
26	UQ6	M	407	-	43,43,43	0.24	0	54,55,55	0.62	1 (1%)
27	HEM	M	406	3	42,50,50	1.35	6 (14%)	46,82,82	1.84	12 (26%)
32	PCF	S	102	-	31,31,49	0.39	0	37,39,57	0.37	0
34	HEA	m	603	-	58,67,67	2.12	18 (31%)	63,103,103	2.42	26 (41%)
33	PTY	S	101	-	31,31,49	0.36	0	34,36,54	0.37	0
25	CN5	C	403	-	31,31,40	0.36	0	35,39,48	0.44	0
29	PEF	D	401	-	39,39,46	0.34	0	42,44,51	0.37	0
27	HEM	M	404	3	42,50,50	1.41	7 (16%)	46,82,82	1.71	11 (23%)
30	HEC	N	402	4	32,50,50	1.94	5 (15%)	30,82,82	2.91	11 (36%)
31	FES	E	301	-	0,4,4	-	-	-	-	-
37	CN3	a	606	-	45,45,54	0.38	0	51,57,66	0.43	0
32	PCF	l	101	-	36,36,49	0.36	0	42,44,57	0.42	0
23	6PH	C	401	-	39,39,39	0.38	0	42,44,44	0.29	0
32	PCF	k	201	-	42,42,49	0.37	0	48,50,57	0.38	0
29	PEF	m	607	-	42,42,46	0.31	0	45,47,51	0.34	0
33	PTY	m	604	-	31,31,49	0.39	0	34,36,54	0.49	0
29	PEF	J	101	-	28,28,46	0.39	0	31,33,51	0.50	0
33	PTY	n	304	-	34,34,49	0.33	0	37,39,54	0.39	0
34	HEA	a	601	11	58,67,67	2.22	20 (34%)	63,103,103	2.27	20 (31%)
26	UQ6	C	404	-	26,26,43	0.37	0	33,34,55	0.64	0
37	CN3	m	606	-	45,45,54	0.38	0	51,57,66	0.43	0
29	PEF	T	101	-	28,28,46	0.39	0	31,33,51	0.50	0
28	9PE	M	405	-	32,32,39	0.36	0	35,37,44	0.42	0
22	CDL	A	501	-	54,54,99	0.37	0	60,66,111	0.49	0
24	8PE	M	402	-	25,25,46	0.40	0	28,30,51	0.51	0
32	PCF	w	201	-	42,42,49	0.37	0	48,50,57	0.38	0
28	9PE	C	406	-	32,32,39	0.36	0	35,37,44	0.42	0
33	PTY	I	101	-	31,31,49	0.36	0	34,36,54	0.37	0
32	PCF	H	102	-	31,31,49	0.37	0	37,39,57	0.37	0
22	CDL	N	403	-	59,59,99	0.36	0	65,71,111	0.47	0
31	FES	O	301	-	0,4,4	-	-	-	-	-
39	CUA	b	303	12	0,1,1	-	-	-	-	-
24	8PE	C	402	-	25,25,46	0.40	0	28,30,51	0.51	0
29	PEF	N	401	-	39,39,46	0.34	0	42,44,51	0.37	0
32	PCF	R	102	-	31,31,49	0.37	0	37,39,57	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	UQ6	M	403	-	26,26,43	0.37	0	33,34,55	0.64	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CDL	O	302	-	-	16/49/49/110	-
33	PTY	b	304	-	-	12/38/38/53	-
22	CDL	D	403	-	-	25/70/70/110	-
33	PTY	a	604	-	-	11/35/35/53	-
22	CDL	H	101	-	-	13/63/63/110	-
27	HEM	C	407	3	-	5/12/54/54	-
33	PTY	o	301	-	-	10/43/43/53	-
34	HEA	a	603	-	-	8/32/76/76	-
29	PEF	a	607	-	-	12/46/46/50	-
33	PTY	b	302	-	-	7/37/37/53	-
22	CDL	K	501	-	-	10/64/64/110	-
30	HEC	D	402	4	-	1/10/54/54	-
23	6PH	M	401	-	-	26/41/41/41	-
27	HEM	C	405	3	-	0/12/54/54	-
22	CDL	R	101	-	-	13/63/63/110	-
33	PTY	n	302	-	-	7/37/37/53	-
33	PTY	c	301	-	-	10/43/43/53	-
22	CDL	E	302	-	-	16/49/49/110	-
32	PCF	I	102	-	-	4/35/35/53	-
26	UQ6	C	408	-	-	16/39/39/39	0/1/1/1
32	PCF	x	101	-	-	6/40/40/53	-
34	HEA	m	601	11	-	6/32/76/76	-
26	UQ6	M	407	-	-	16/39/39/39	0/1/1/1
27	HEM	M	406	3	-	5/12/54/54	-
32	PCF	S	102	-	-	4/35/35/53	-
34	HEA	m	603	-	-	8/32/76/76	-
33	PTY	S	101	-	-	6/35/35/53	-
25	CN5	C	403	-	-	7/35/35/44	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEF	D	401	-	-	12/43/43/50	-
27	HEM	M	404	3	-	0/12/54/54	-
30	HEC	N	402	4	-	1/10/54/54	-
37	CN3	a	606	-	-	10/56/56/65	-
31	FES	E	301	-	-	-	0/1/1/1
32	PCF	l	101	-	-	6/40/40/53	-
23	6PH	C	401	-	-	26/41/41/41	-
32	PCF	k	201	-	-	12/46/46/53	-
29	PEF	m	607	-	-	12/46/46/50	-
33	PTY	m	604	-	-	11/35/35/53	-
29	PEF	J	101	-	-	6/32/32/50	-
33	PTY	n	304	-	-	12/38/38/53	-
34	HEA	a	601	11	-	6/32/76/76	-
26	UQ6	C	404	-	-	9/19/19/39	0/1/1/1
37	CN3	m	606	-	-	10/56/56/65	-
29	PEF	T	101	-	-	6/32/32/50	-
28	9PE	M	405	-	-	4/36/36/43	-
22	CDL	A	501	-	-	10/64/64/110	-
24	8PE	M	402	-	-	6/29/29/50	-
32	PCF	w	201	-	-	12/46/46/53	-
28	9PE	C	406	-	-	4/36/36/43	-
33	PTY	I	101	-	-	6/35/35/53	-
32	PCF	H	102	-	-	11/35/35/53	-
22	CDL	N	403	-	-	25/70/70/110	-
31	FES	O	301	-	-	-	0/1/1/1
24	8PE	C	402	-	-	6/29/29/50	-
29	PEF	N	401	-	-	12/43/43/50	-
32	PCF	R	102	-	-	11/35/35/53	-
26	UQ6	M	403	-	-	9/19/19/39	0/1/1/1

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	D	402	HEC	C3C-C2C	-6.52	1.33	1.40
30	N	402	HEC	C3C-C2C	-6.52	1.33	1.40
34	a	601	HEA	C3B-C2B	5.56	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	m	601	HEA	C3B-C2B	5.56	1.47	1.34
34	a	603	HEA	CHC-C4B	5.53	1.48	1.34
34	m	603	HEA	CHC-C4B	5.53	1.48	1.34
34	a	601	HEA	C3A-C4A	5.40	1.49	1.41
34	m	601	HEA	C3A-C4A	5.40	1.49	1.41
34	a	601	HEA	CHC-C4B	5.30	1.47	1.34
34	m	601	HEA	CHC-C4B	5.30	1.47	1.34
30	D	402	HEC	C2B-C3B	-5.29	1.34	1.40
30	N	402	HEC	C2B-C3B	-5.29	1.34	1.40
34	a	601	HEA	C3A-C2A	5.28	1.47	1.40
34	m	601	HEA	C3A-C2A	5.28	1.47	1.40
34	a	603	HEA	C3B-C2B	5.16	1.46	1.34
34	m	603	HEA	C3B-C2B	5.16	1.46	1.34
34	a	601	HEA	C3C-C2C	5.10	1.47	1.40
34	m	601	HEA	C3C-C2C	5.10	1.47	1.40
34	a	601	HEA	CHD-C1D	5.09	1.47	1.34
34	m	601	HEA	CHD-C1D	5.09	1.47	1.34
34	a	603	HEA	CHD-C1D	4.97	1.46	1.34
34	m	603	HEA	CHD-C1D	4.97	1.46	1.34
34	a	603	HEA	C3C-C2C	4.85	1.46	1.40
34	m	603	HEA	C3C-C2C	4.85	1.46	1.40
34	a	601	HEA	C3D-C2D	4.58	1.46	1.36
34	m	601	HEA	C3D-C2D	4.58	1.46	1.36
34	a	603	HEA	C3A-C4A	4.49	1.48	1.41
34	m	603	HEA	C3A-C4A	4.49	1.48	1.41
34	a	603	HEA	C3A-C2A	4.46	1.46	1.40
34	m	603	HEA	C3A-C2A	4.46	1.46	1.40
34	a	603	HEA	C3D-C2D	4.28	1.46	1.36
34	m	603	HEA	C3D-C2D	4.28	1.46	1.36
27	C	405	HEM	C4D-ND	-3.82	1.33	1.40
27	M	404	HEM	C4D-ND	-3.82	1.33	1.40
27	C	405	HEM	C1B-NB	-3.65	1.33	1.40
27	M	404	HEM	C1B-NB	-3.65	1.33	1.40
30	D	402	HEC	CBC-CAC	-3.63	1.36	1.49
30	N	402	HEC	CBC-CAC	-3.63	1.36	1.49
27	C	407	HEM	C4D-ND	-3.37	1.34	1.40
27	M	406	HEM	C4D-ND	-3.37	1.34	1.40
27	C	407	HEM	C1B-NB	-3.34	1.34	1.40
27	M	406	HEM	C1B-NB	-3.34	1.34	1.40
34	a	603	HEA	C1D-ND	-2.92	1.35	1.40
34	m	603	HEA	C1D-ND	-2.92	1.35	1.40
34	a	603	HEA	C4B-C3B	2.86	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	m	603	HEA	C4B-C3B	2.86	1.49	1.44
34	a	601	HEA	C4B-NB	-2.79	1.35	1.40
34	m	601	HEA	C4B-NB	-2.79	1.35	1.40
34	a	601	HEA	C2A-C1A	2.69	1.48	1.42
34	m	601	HEA	C2A-C1A	2.69	1.48	1.42
34	a	601	HEA	C1D-ND	-2.67	1.35	1.40
34	m	601	HEA	C1D-ND	-2.67	1.35	1.40
34	a	603	HEA	C4B-NB	-2.66	1.35	1.40
34	m	603	HEA	C4B-NB	-2.66	1.35	1.40
27	C	407	HEM	C1D-ND	-2.64	1.33	1.38
27	M	406	HEM	C1D-ND	-2.64	1.33	1.38
34	a	603	HEA	C1C-CHC	2.62	1.48	1.41
34	m	603	HEA	C1C-CHC	2.62	1.48	1.41
34	a	603	HEA	C11-C3B	-2.60	1.48	1.51
34	m	603	HEA	C11-C3B	-2.60	1.48	1.51
27	C	405	HEM	C4B-NB	-2.59	1.33	1.38
27	M	404	HEM	C4B-NB	-2.59	1.33	1.38
34	a	601	HEA	FE-ND	2.46	2.11	1.98
34	m	601	HEA	FE-ND	2.46	2.11	1.98
30	D	402	HEC	CBB-CAB	-2.43	1.40	1.49
30	N	402	HEC	CBB-CAB	-2.43	1.40	1.49
27	C	407	HEM	C4B-NB	-2.41	1.34	1.38
27	M	406	HEM	C4B-NB	-2.41	1.34	1.38
34	a	601	HEA	C4B-C3B	2.39	1.48	1.44
34	m	601	HEA	C4B-C3B	2.39	1.48	1.44
34	a	601	HEA	FE-NB	2.37	2.11	1.98
34	m	601	HEA	FE-NB	2.37	2.11	1.98
27	C	405	HEM	FE-NB	2.36	2.11	1.98
27	M	404	HEM	FE-NB	2.36	2.11	1.98
34	a	603	HEA	C2A-C1A	2.36	1.47	1.42
34	m	603	HEA	C2A-C1A	2.36	1.47	1.42
34	a	601	HEA	C1C-CHC	2.36	1.47	1.41
34	m	601	HEA	C1C-CHC	2.36	1.47	1.41
34	a	603	HEA	FE-NB	2.34	2.11	1.98
34	m	603	HEA	FE-NB	2.34	2.11	1.98
34	a	603	HEA	FE-ND	2.34	2.11	1.98
34	m	603	HEA	FE-ND	2.34	2.11	1.98
34	a	601	HEA	C4C-CHD	2.32	1.47	1.41
34	m	601	HEA	C4C-CHD	2.32	1.47	1.41
27	C	407	HEM	FE-NB	2.26	2.10	1.98
27	M	406	HEM	FE-NB	2.26	2.10	1.98
34	a	601	HEA	C11-C3B	-2.24	1.48	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	m	601	HEA	C11-C3B	-2.24	1.48	1.51
34	a	603	HEA	C4D-ND	-2.24	1.34	1.38
34	m	603	HEA	C4D-ND	-2.24	1.34	1.38
27	C	405	HEM	C1D-ND	-2.21	1.34	1.38
27	M	404	HEM	C1D-ND	-2.21	1.34	1.38
34	a	603	HEA	C4C-CHD	2.21	1.47	1.41
34	m	603	HEA	C4C-CHD	2.21	1.47	1.41
34	a	601	HEA	C1D-C2D	2.18	1.48	1.44
34	m	601	HEA	C1D-C2D	2.18	1.48	1.44
34	a	601	HEA	C1B-C2B	2.16	1.48	1.44
34	m	601	HEA	C1B-C2B	2.16	1.48	1.44
34	a	601	HEA	CHB-C1B	2.16	1.47	1.40
34	m	601	HEA	CHB-C1B	2.16	1.47	1.40
30	D	402	HEC	C3D-C2D	-2.16	1.31	1.37
30	N	402	HEC	C3D-C2D	-2.16	1.31	1.37
27	C	405	HEM	CHB-C1B	2.13	1.39	1.34
27	M	404	HEM	CHB-C1B	2.13	1.39	1.34
27	C	407	HEM	CHB-C1B	2.12	1.39	1.34
27	M	406	HEM	CHB-C1B	2.12	1.39	1.34
34	a	601	HEA	C4D-C3D	2.09	1.48	1.45
34	m	601	HEA	C4D-C3D	2.09	1.48	1.45
27	C	405	HEM	FE-ND	-2.04	1.86	1.98
27	M	404	HEM	FE-ND	-2.04	1.86	1.98
34	a	603	HEA	C1B-NB	-2.03	1.34	1.38
34	m	603	HEA	C1B-NB	-2.03	1.34	1.38

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	402	HEC	CMB-C2B-C3B	6.99	134.04	125.82
30	N	402	HEC	CMB-C2B-C3B	6.99	134.04	125.82
30	D	402	HEC	CBC-CAC-C3C	-6.70	111.81	127.49
30	N	402	HEC	CBC-CAC-C3C	-6.70	111.81	127.49
34	a	601	HEA	C3D-C4D-ND	6.63	116.76	110.35
34	m	601	HEA	C3D-C4D-ND	6.63	116.76	110.35
34	a	603	HEA	C3D-C4D-ND	6.58	116.71	110.35
34	m	603	HEA	C3D-C4D-ND	6.58	116.71	110.35
30	D	402	HEC	CMB-C2B-C1B	-6.33	119.18	128.46
30	N	402	HEC	CMB-C2B-C1B	-6.33	119.18	128.46
34	a	603	HEA	C2B-C1B-NB	6.08	116.93	109.90
34	m	603	HEA	C2B-C1B-NB	6.08	116.93	109.90
30	D	402	HEC	CBB-CAB-C3B	-5.79	113.93	127.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	N	402	HEC	CBB-CAB-C3B	-5.79	113.93	127.49
34	a	601	HEA	C2D-C1D-ND	5.53	116.20	109.84
34	m	601	HEA	C2D-C1D-ND	5.53	116.20	109.84
34	a	603	HEA	C2D-C1D-ND	5.49	116.15	109.84
34	m	603	HEA	C2D-C1D-ND	5.49	116.15	109.84
34	a	601	HEA	C3B-C4B-NB	5.44	116.10	109.84
34	m	601	HEA	C3B-C4B-NB	5.44	116.10	109.84
34	a	601	HEA	C2B-C1B-NB	5.38	116.12	109.90
34	m	601	HEA	C2B-C1B-NB	5.38	116.12	109.90
27	C	407	HEM	CHC-C4B-NB	5.09	129.91	124.44
27	M	406	HEM	CHC-C4B-NB	5.09	129.91	124.44
34	a	603	HEA	C3B-C4B-NB	4.52	115.03	109.84
34	m	603	HEA	C3B-C4B-NB	4.52	115.03	109.84
27	C	405	HEM	CHC-C4B-NB	4.50	129.28	124.44
27	M	404	HEM	CHC-C4B-NB	4.50	129.28	124.44
34	a	603	HEA	CBA-CAA-C2A	-4.38	105.33	112.55
34	m	603	HEA	CBA-CAA-C2A	-4.38	105.33	112.55
34	a	603	HEA	C3C-C4C-NC	4.33	114.81	109.21
34	m	603	HEA	C3C-C4C-NC	4.33	114.81	109.21
34	a	603	HEA	C1D-C2D-C3D	-4.25	102.51	106.98
34	m	603	HEA	C1D-C2D-C3D	-4.25	102.51	106.98
34	a	601	HEA	C1D-C2D-C3D	-4.15	102.62	106.98
34	m	601	HEA	C1D-C2D-C3D	-4.15	102.62	106.98
34	a	601	HEA	C3C-C4C-NC	4.09	114.50	109.21
34	m	601	HEA	C3C-C4C-NC	4.09	114.50	109.21
27	C	407	HEM	CBA-CAA-C2A	-4.01	105.80	112.54
27	M	406	HEM	CBA-CAA-C2A	-4.01	105.80	112.54
34	a	603	HEA	C1B-C2B-C3B	-3.89	102.29	106.80
34	m	603	HEA	C1B-C2B-C3B	-3.89	102.29	106.80
27	C	405	HEM	CHA-C4D-ND	3.87	129.17	124.37
27	M	404	HEM	CHA-C4D-ND	3.87	129.17	124.37
34	a	603	HEA	CHB-C1B-C2B	-3.86	118.93	125.03
34	m	603	HEA	CHB-C1B-C2B	-3.86	118.93	125.03
27	C	405	HEM	CHD-C1D-ND	3.84	128.57	124.44
27	M	404	HEM	CHD-C1D-ND	3.84	128.57	124.44
34	a	601	HEA	C1B-C2B-C3B	-3.75	102.46	106.80
34	m	601	HEA	C1B-C2B-C3B	-3.75	102.46	106.80
30	D	402	HEC	C4C-C3C-C2C	3.71	110.36	106.35
30	N	402	HEC	C4C-C3C-C2C	3.71	110.36	106.35
30	D	402	HEC	O1D-CGD-CBD	-3.67	111.44	123.09
30	N	402	HEC	O1D-CGD-CBD	-3.67	111.44	123.09
27	C	407	HEM	CHD-C1D-ND	3.67	128.38	124.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	M	406	HEM	CHD-C1D-ND	3.67	128.38	124.44
27	C	407	HEM	CHA-C4D-ND	3.35	128.53	124.37
27	M	406	HEM	CHA-C4D-ND	3.35	128.53	124.37
27	C	407	HEM	C1B-NB-C4B	3.32	109.14	105.21
27	M	406	HEM	C1B-NB-C4B	3.32	109.14	105.21
34	a	601	HEA	C4D-C3D-C2D	-3.19	102.25	106.89
34	m	601	HEA	C4D-C3D-C2D	-3.19	102.25	106.89
30	D	402	HEC	CMD-C2D-C1D	-3.15	123.84	128.46
30	N	402	HEC	CMD-C2D-C1D	-3.15	123.84	128.46
34	a	603	HEA	CAD-CBD-CGD	-3.12	105.38	113.67
34	m	603	HEA	CAD-CBD-CGD	-3.12	105.38	113.67
34	a	603	HEA	C4D-C3D-C2D	-3.12	102.35	106.89
34	m	603	HEA	C4D-C3D-C2D	-3.12	102.35	106.89
34	a	601	HEA	CHA-C4D-C3D	-2.97	120.45	124.77
34	m	601	HEA	CHA-C4D-C3D	-2.97	120.45	124.77
27	C	407	HEM	CHB-C1B-NB	2.96	128.04	124.37
27	M	406	HEM	CHB-C1B-NB	2.96	128.04	124.37
34	a	601	HEA	C4B-C3B-C2B	-2.95	102.47	107.44
34	m	601	HEA	C4B-C3B-C2B	-2.95	102.47	107.44
34	a	603	HEA	CHA-C4D-C3D	-2.94	120.48	124.77
34	m	603	HEA	CHA-C4D-C3D	-2.94	120.48	124.77
34	a	601	HEA	CMC-C2C-C3C	2.85	130.38	124.68
34	m	601	HEA	CMC-C2C-C3C	2.85	130.38	124.68
27	C	405	HEM	CHB-C1B-NB	2.78	127.82	124.37
27	M	404	HEM	CHB-C1B-NB	2.78	127.82	124.37
34	a	603	HEA	CMC-C2C-C3C	2.69	130.06	124.68
34	m	603	HEA	CMC-C2C-C3C	2.69	130.06	124.68
34	a	603	HEA	C4B-C3B-C2B	-2.68	102.93	107.44
34	m	603	HEA	C4B-C3B-C2B	-2.68	102.93	107.44
34	a	601	HEA	CMD-C2D-C1D	2.68	129.22	125.03
34	m	601	HEA	CMD-C2D-C1D	2.68	129.22	125.03
34	a	603	HEA	CMD-C2D-C1D	2.66	129.19	125.03
34	m	603	HEA	CMD-C2D-C1D	2.66	129.19	125.03
34	a	603	HEA	C13-C12-C11	-2.66	110.15	114.39
34	m	603	HEA	C13-C12-C11	-2.66	110.15	114.39
34	a	601	HEA	CHB-C1B-C2B	-2.64	120.85	125.03
34	m	601	HEA	CHB-C1B-C2B	-2.64	120.85	125.03
30	D	402	HEC	CMA-C3A-C2A	2.63	129.90	124.94
30	N	402	HEC	CMA-C3A-C2A	2.63	129.90	124.94
27	C	405	HEM	CHA-C4D-C3D	-2.62	120.39	125.23
27	M	404	HEM	CHA-C4D-C3D	-2.62	120.39	125.23
27	C	407	HEM	CHD-C1D-C2D	-2.59	120.93	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	M	406	HEM	CHD-C1D-C2D	-2.59	120.93	125.03
30	D	402	HEC	CMC-C2C-C3C	2.59	128.87	125.82
30	N	402	HEC	CMC-C2C-C3C	2.59	128.87	125.82
34	a	603	HEA	C27-C19-C20	2.58	119.70	115.23
34	m	603	HEA	C27-C19-C20	2.58	119.70	115.23
34	a	601	HEA	C1D-ND-C4D	-2.57	102.16	105.21
34	m	601	HEA	C1D-ND-C4D	-2.57	102.16	105.21
27	C	405	HEM	C1B-NB-C4B	2.57	108.25	105.21
27	M	404	HEM	C1B-NB-C4B	2.57	108.25	105.21
34	a	603	HEA	C1D-ND-C4D	-2.50	102.25	105.21
34	m	603	HEA	C1D-ND-C4D	-2.50	102.25	105.21
30	D	402	HEC	O1A-CGA-CBA	-2.49	115.20	123.09
30	N	402	HEC	O1A-CGA-CBA	-2.49	115.20	123.09
27	C	407	HEM	O2D-CGD-CBD	2.45	121.75	114.00
27	M	406	HEM	O2D-CGD-CBD	2.45	121.75	114.00
34	a	603	HEA	CHD-C1D-C2D	-2.44	120.03	126.94
34	m	603	HEA	CHD-C1D-C2D	-2.44	120.03	126.94
34	a	601	HEA	CAD-C3D-C4D	2.43	128.93	124.70
34	m	601	HEA	CAD-C3D-C4D	2.43	128.93	124.70
34	a	601	HEA	CHD-C1D-C2D	-2.41	120.11	126.94
34	m	601	HEA	CHD-C1D-C2D	-2.41	120.11	126.94
27	C	405	HEM	CMC-C2C-C3C	2.40	129.49	124.68
27	M	404	HEM	CMC-C2C-C3C	2.40	129.49	124.68
34	a	601	HEA	CBA-CAA-C2A	-2.40	108.60	112.55
34	m	601	HEA	CBA-CAA-C2A	-2.40	108.60	112.55
27	C	405	HEM	CMD-C2D-C1D	2.40	128.78	125.03
27	M	404	HEM	CMD-C2D-C1D	2.40	128.78	125.03
27	C	407	HEM	C3B-C4B-NB	-2.36	107.77	109.47
27	M	406	HEM	C3B-C4B-NB	-2.36	107.77	109.47
34	a	601	HEA	CHC-C4B-C3B	-2.29	120.03	125.80
34	m	601	HEA	CHC-C4B-C3B	-2.29	120.03	125.80
27	C	405	HEM	C4B-C3B-C2B	-2.28	105.19	107.28
27	M	404	HEM	C4B-C3B-C2B	-2.28	105.19	107.28
27	C	407	HEM	CMD-C2D-C1D	2.25	128.55	125.03
27	M	406	HEM	CMD-C2D-C1D	2.25	128.55	125.03
34	a	601	HEA	CMB-C2B-C1B	2.25	128.55	125.03
34	m	601	HEA	CMB-C2B-C1B	2.25	128.55	125.03
27	C	407	HEM	CHA-C4D-C3D	-2.22	121.14	125.23
27	M	406	HEM	CHA-C4D-C3D	-2.22	121.14	125.23
34	a	603	HEA	CAD-C3D-C4D	2.16	128.46	124.70
34	m	603	HEA	CAD-C3D-C4D	2.16	128.46	124.70
34	a	603	HEA	CMB-C2B-C1B	2.12	128.35	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	m	603	HEA	CMB-C2B-C1B	2.12	128.35	125.03
34	a	603	HEA	C17-C18-C19	-2.09	122.83	127.62
34	m	603	HEA	C17-C18-C19	-2.09	122.83	127.62
34	a	603	HEA	O1A-CGA-CBA	-2.09	116.46	123.09
34	m	603	HEA	O1A-CGA-CBA	-2.09	116.46	123.09
34	a	601	HEA	C17-C18-C19	-2.07	122.89	127.62
34	m	601	HEA	C17-C18-C19	-2.07	122.89	127.62
34	a	603	HEA	C12-C11-C3B	-2.07	108.89	112.12
34	m	603	HEA	C12-C11-C3B	-2.07	108.89	112.12
27	C	407	HEM	CAD-C3D-C4D	2.06	128.28	124.70
27	M	406	HEM	CAD-C3D-C4D	2.06	128.28	124.70
27	C	405	HEM	O2A-CGA-CBA	2.06	120.50	114.00
27	M	404	HEM	O2A-CGA-CBA	2.06	120.50	114.00
34	a	603	HEA	C25-C23-C24	2.06	119.32	114.59
34	m	603	HEA	C25-C23-C24	2.06	119.32	114.59
27	C	405	HEM	CHD-C1D-C2D	-2.05	121.79	125.03
27	M	404	HEM	CHD-C1D-C2D	-2.05	121.79	125.03
30	D	402	HEC	CMC-C2C-C1C	-2.04	125.46	128.46
30	N	402	HEC	CMC-C2C-C1C	-2.04	125.46	128.46
26	C	408	UQ6	O3-C3-C2	2.04	123.39	119.00
26	M	407	UQ6	O3-C3-C2	2.04	123.39	119.00
34	a	603	HEA	C4B-NB-C1B	-2.02	102.81	105.21
34	m	603	HEA	C4B-NB-C1B	-2.02	102.81	105.21

There are no chirality outliers.

All (535) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	501	CDL	CB3-OB5-PB2-OB2
22	A	501	CDL	CB3-OB5-PB2-OB4
22	D	403	CDL	CA2-OA2-PA1-OA3
22	D	403	CDL	CA2-OA2-PA1-OA5
22	D	403	CDL	CA3-OA5-PA1-OA2
22	D	403	CDL	CA3-OA5-PA1-OA3
22	D	403	CDL	CA3-OA5-PA1-OA4
22	D	403	CDL	OB9-CB7-OB8-CB6
22	D	403	CDL	C71-CB7-OB8-CB6
22	E	302	CDL	CA2-OA2-PA1-OA4
22	E	302	CDL	CA2-OA2-PA1-OA5
22	E	302	CDL	CA3-OA5-PA1-OA3
22	E	302	CDL	CB3-OB5-PB2-OB2
22	E	302	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
22	E	302	CDL	C51-CB5-OB6-CB4
22	H	101	CDL	CA2-C1-CB2-OB2
22	K	501	CDL	CB3-OB5-PB2-OB2
22	K	501	CDL	CB3-OB5-PB2-OB4
22	N	403	CDL	CA2-OA2-PA1-OA3
22	N	403	CDL	CA2-OA2-PA1-OA5
22	N	403	CDL	CA3-OA5-PA1-OA2
22	N	403	CDL	CA3-OA5-PA1-OA3
22	N	403	CDL	CA3-OA5-PA1-OA4
22	N	403	CDL	OB9-CB7-OB8-CB6
22	N	403	CDL	C71-CB7-OB8-CB6
22	O	302	CDL	CA2-OA2-PA1-OA4
22	O	302	CDL	CA2-OA2-PA1-OA5
22	O	302	CDL	CA3-OA5-PA1-OA3
22	O	302	CDL	CB3-OB5-PB2-OB2
22	O	302	CDL	CB3-OB5-PB2-OB3
22	O	302	CDL	C51-CB5-OB6-CB4
22	R	101	CDL	CA2-C1-CB2-OB2
23	C	401	6PH	C1-O11-P-O12
23	C	401	6PH	C1-O11-P-O13
23	C	401	6PH	C1-O11-P-O14
23	M	401	6PH	C1-O11-P-O12
23	M	401	6PH	C1-O11-P-O13
23	M	401	6PH	C1-O11-P-O14
25	C	403	CN5	C1'-O1'-P'-O3'
25	C	403	CN5	C1'-O1'-P'-O4'
26	C	404	UQ6	C7-C8-C9-C10
26	C	404	UQ6	C7-C8-C9-C11
26	C	404	UQ6	C12-C13-C14-C15
26	C	404	UQ6	C12-C13-C14-C16
26	C	408	UQ6	C22-C23-C24-C25
26	C	408	UQ6	C22-C23-C24-C26
26	M	403	UQ6	C7-C8-C9-C10
26	M	403	UQ6	C7-C8-C9-C11
26	M	403	UQ6	C12-C13-C14-C15
26	M	403	UQ6	C12-C13-C14-C16
26	M	407	UQ6	C22-C23-C24-C25
26	M	407	UQ6	C22-C23-C24-C26
28	C	406	9PE	C11-O13-P-O14
28	M	405	9PE	C11-O13-P-O14
29	D	401	PEF	C11-C10-O2-C2
29	D	401	PEF	O4-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
29	D	401	PEF	C4-O4P-P-O3P
29	J	101	PEF	O4-C10-O2-C2
29	J	101	PEF	C4-O4P-P-O2P
29	N	401	PEF	C11-C10-O2-C2
29	N	401	PEF	O4-C10-O2-C2
29	N	401	PEF	C4-O4P-P-O3P
29	T	101	PEF	O4-C10-O2-C2
29	T	101	PEF	C4-O4P-P-O2P
32	H	102	PCF	C11-O13-P-O11
32	H	102	PCF	O32-C31-O31-C3
32	H	102	PCF	C32-C31-O31-C3
32	k	201	PCF	C11-O13-P-O11
32	k	201	PCF	C11-O13-P-O14
32	k	201	PCF	O13-C11-C12-N
32	l	101	PCF	C1-O11-P-O14
32	l	101	PCF	O13-C11-C12-N
32	R	102	PCF	C11-O13-P-O11
32	R	102	PCF	O32-C31-O31-C3
32	R	102	PCF	C32-C31-O31-C3
32	w	201	PCF	C11-O13-P-O11
32	w	201	PCF	C11-O13-P-O14
32	w	201	PCF	O13-C11-C12-N
32	x	101	PCF	C1-O11-P-O14
32	x	101	PCF	O13-C11-C12-N
33	I	101	PTY	C2-C3-O11-P1
33	a	604	PTY	C11-C8-O7-C6
33	a	604	PTY	C5-O14-P1-O11
33	b	304	PTY	C31-C30-O4-C1
33	b	304	PTY	O30-C30-O4-C1
33	b	304	PTY	C6-C5-O14-P1
33	b	304	PTY	C5-O14-P1-O13
33	c	301	PTY	O14-C5-C6-O7
33	S	101	PTY	C2-C3-O11-P1
33	m	604	PTY	C11-C8-O7-C6
33	m	604	PTY	C5-O14-P1-O11
33	n	304	PTY	C31-C30-O4-C1
33	n	304	PTY	O30-C30-O4-C1
33	n	304	PTY	C6-C5-O14-P1
33	n	304	PTY	C5-O14-P1-O13
33	o	301	PTY	O14-C5-C6-O7
37	a	606	CN3	C1-O11-P-O13
37	a	606	CN3	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
37	m	606	CN3	C1-O11-P-O13
37	m	606	CN3	C1-O11-P-O14
22	E	302	CDL	OA9-CA7-OA8-CA6
22	O	302	CDL	OA9-CA7-OA8-CA6
22	E	302	CDL	C31-CA7-OA8-CA6
22	O	302	CDL	C31-CA7-OA8-CA6
22	E	302	CDL	OB7-CB5-OB6-CB4
22	O	302	CDL	OB7-CB5-OB6-CB4
33	a	604	PTY	O10-C8-O7-C6
33	m	604	PTY	O10-C8-O7-C6
33	a	604	PTY	C31-C30-O4-C1
33	m	604	PTY	C31-C30-O4-C1
29	J	101	PEF	C11-C10-O2-C2
29	T	101	PEF	C11-C10-O2-C2
23	C	401	6PH	O32-C31-O31-C3
23	M	401	6PH	O32-C31-O31-C3
33	a	604	PTY	O30-C30-O4-C1
33	m	604	PTY	O30-C30-O4-C1
22	H	101	CDL	O1-C1-CB2-OB2
22	R	101	CDL	O1-C1-CB2-OB2
37	a	606	CN3	O3'-CA-CB-OA
37	m	606	CN3	O3'-CA-CB-OA
32	l	101	PCF	C22-C21-O21-C2
32	x	101	PCF	C22-C21-O21-C2
26	C	408	UQ6	C32-C33-C34-C36
26	M	407	UQ6	C32-C33-C34-C36
23	C	401	6PH	C32-C31-O31-C3
23	M	401	6PH	C32-C31-O31-C3
26	C	408	UQ6	C12-C11-C9-C10
26	C	408	UQ6	C25-C24-C26-C27
26	M	407	UQ6	C12-C11-C9-C10
26	M	407	UQ6	C25-C24-C26-C27
26	C	408	UQ6	C12-C11-C9-C8
26	C	408	UQ6	C23-C24-C26-C27
26	M	407	UQ6	C12-C11-C9-C8
26	M	407	UQ6	C23-C24-C26-C27
26	C	404	UQ6	C9-C11-C12-C13
26	M	403	UQ6	C9-C11-C12-C13
22	A	501	CDL	O1-C1-CA2-OA2
22	K	501	CDL	O1-C1-CA2-OA2
26	C	408	UQ6	C32-C33-C34-C35
26	M	407	UQ6	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
22	H	101	CDL	C71-CB7-OB8-CB6
22	R	101	CDL	C71-CB7-OB8-CB6
26	C	404	UQ6	C16-C17-C18-C19
26	M	403	UQ6	C16-C17-C18-C19
26	C	408	UQ6	C14-C16-C17-C18
26	M	407	UQ6	C14-C16-C17-C18
32	k	201	PCF	C11-C12-N-C15
32	w	201	PCF	C11-C12-N-C15
33	b	302	PTY	C11-C8-O7-C6
33	n	302	PTY	C11-C8-O7-C6
32	l	101	PCF	O22-C21-O21-C2
32	x	101	PCF	O22-C21-O21-C2
29	D	401	PEF	C30-C31-C32-C33
29	N	401	PEF	C30-C31-C32-C33
22	D	403	CDL	C11-CA5-OA6-CA4
22	N	403	CDL	C11-CA5-OA6-CA4
33	b	302	PTY	O10-C8-O7-C6
33	n	302	PTY	O10-C8-O7-C6
22	A	501	CDL	C1-CB2-OB2-PB2
22	E	302	CDL	CB4-CB3-OB5-PB2
22	K	501	CDL	C1-CB2-OB2-PB2
22	O	302	CDL	CB4-CB3-OB5-PB2
27	C	407	HEM	C3D-CAD-CBD-CGD
27	M	406	HEM	C3D-CAD-CBD-CGD
22	H	101	CDL	OB9-CB7-OB8-CB6
22	R	101	CDL	OB9-CB7-OB8-CB6
33	c	301	PTY	C11-C8-O7-C6
33	o	301	PTY	C11-C8-O7-C6
37	a	606	CN3	C52-C51-O51-C2'
37	m	606	CN3	C52-C51-O51-C2'
22	D	403	CDL	OA7-CA5-OA6-CA4
22	N	403	CDL	OA7-CA5-OA6-CA4
23	C	401	6PH	C28-C29-C2A-C2B
23	M	401	6PH	C28-C29-C2A-C2B
22	H	101	CDL	CB4-CB6-OB8-CB7
22	R	101	CDL	CB4-CB6-OB8-CB7
23	C	401	6PH	C32-C33-C34-C35
23	M	401	6PH	C32-C33-C34-C35
23	C	401	6PH	C27-C28-C29-C2A
23	M	401	6PH	C27-C28-C29-C2A
37	a	606	CN3	O52-C51-O51-C2'
37	m	606	CN3	O52-C51-O51-C2'

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Mol	Chain	Res	Type	Atoms
23	C	401	6PH	C25-C26-C27-C28
23	M	401	6PH	C25-C26-C27-C28
23	C	401	6PH	C24-C25-C26-C27
23	M	401	6PH	C24-C25-C26-C27
22	A	501	CDL	C51-CB5-OB6-CB4
22	K	501	CDL	C51-CB5-OB6-CB4
32	k	201	PCF	C22-C21-O21-C2
32	w	201	PCF	C22-C21-O21-C2
33	b	304	PTY	C11-C8-O7-C6
33	n	304	PTY	C11-C8-O7-C6
33	c	301	PTY	O10-C8-O7-C6
33	o	301	PTY	O10-C8-O7-C6
32	k	201	PCF	C11-C12-N-C14
32	w	201	PCF	C11-C12-N-C14
29	J	101	PEF	C10-C11-C12-C13
29	T	101	PEF	C10-C11-C12-C13
29	a	607	PEF	C10-C11-C12-C13
29	m	607	PEF	C10-C11-C12-C13
33	b	304	PTY	C8-C11-C12-C13
33	n	304	PTY	C8-C11-C12-C13
33	b	304	PTY	O10-C8-O7-C6
33	n	304	PTY	O10-C8-O7-C6
33	a	604	PTY	C12-C13-C14-C15
33	m	604	PTY	C12-C13-C14-C15
23	C	401	6PH	O21-C2-C3-O31
23	M	401	6PH	O21-C2-C3-O31
32	I	102	PCF	O21-C2-C3-O31
32	S	102	PCF	O21-C2-C3-O31
33	c	301	PTY	C31-C30-O4-C1
33	o	301	PTY	C31-C30-O4-C1
23	C	401	6PH	C33-C34-C35-C36
23	M	401	6PH	C33-C34-C35-C36
32	k	201	PCF	O22-C21-O21-C2
32	w	201	PCF	O22-C21-O21-C2
37	a	606	CN3	C22-C21-O21-C2
37	m	606	CN3	C22-C21-O21-C2
22	D	403	CDL	C56-C57-C58-C59
22	N	403	CDL	C56-C57-C58-C59
22	A	501	CDL	OB7-CB5-OB6-CB4
22	K	501	CDL	OB7-CB5-OB6-CB4
29	a	607	PEF	C16-C17-C18-C19
29	m	607	PEF	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	a	607	PEF	C11-C10-O2-C2
29	m	607	PEF	C11-C10-O2-C2
25	C	403	CN5	C32-C31-O31-C3
33	c	301	PTY	O30-C30-O4-C1
33	o	301	PTY	O30-C30-O4-C1
33	b	304	PTY	C14-C15-C16-C17
33	n	304	PTY	C14-C15-C16-C17
23	C	401	6PH	C34-C35-C36-C37
23	M	401	6PH	C34-C35-C36-C37
29	D	401	PEF	C15-C16-C17-C18
29	N	401	PEF	C15-C16-C17-C18
25	C	403	CN5	OA-CB-CC-O13
23	C	401	6PH	C2C-C2D-C2E-C2F
23	M	401	6PH	C2C-C2D-C2E-C2F
22	D	403	CDL	C31-CA7-OA8-CA6
22	N	403	CDL	C31-CA7-OA8-CA6
26	C	404	UQ6	C12-C11-C9-C10
26	M	403	UQ6	C12-C11-C9-C10
22	E	302	CDL	C1-CB2-OB2-PB2
22	O	302	CDL	C1-CB2-OB2-PB2
22	A	501	CDL	OA5-CA3-CA4-CA6
22	K	501	CDL	OA5-CA3-CA4-CA6
24	C	402	8PE	O11-C1-C2-C3
24	M	402	8PE	O11-C1-C2-C3
33	c	301	PTY	O14-C5-C6-C1
33	o	301	PTY	O14-C5-C6-C1
23	C	401	6PH	C3A-C3B-C3C-C3D
23	M	401	6PH	C3A-C3B-C3C-C3D
25	C	403	CN5	O32-C31-O31-C3
33	b	304	PTY	C17-C18-C19-C20
33	n	304	PTY	C17-C18-C19-C20
23	C	401	6PH	C1-C2-C3-O31
23	M	401	6PH	C1-C2-C3-O31
29	a	607	PEF	C1-C2-C3-O3
29	m	607	PEF	C1-C2-C3-O3
32	I	102	PCF	C1-C2-C3-O31
32	S	102	PCF	C1-C2-C3-O31
33	I	101	PTY	O4-C1-C6-C5
33	S	101	PTY	O4-C1-C6-C5
29	a	607	PEF	C13-C14-C15-C16
29	m	607	PEF	C13-C14-C15-C16
29	a	607	PEF	O4-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
29	m	607	PEF	O4-C10-O2-C2
22	D	403	CDL	OB5-CB3-CB4-OB6
22	N	403	CDL	OB5-CB3-CB4-OB6
32	H	102	PCF	O11-C1-C2-O21
32	k	201	PCF	O11-C1-C2-O21
32	R	102	PCF	O11-C1-C2-O21
32	w	201	PCF	O11-C1-C2-O21
32	l	101	PCF	C2-C1-O11-P
32	x	101	PCF	C2-C1-O11-P
28	C	406	9PE	C25-C26-C27-C28
28	M	405	9PE	C25-C26-C27-C28
26	C	404	UQ6	C12-C11-C9-C8
26	M	403	UQ6	C12-C11-C9-C8
23	C	401	6PH	C2B-C2C-C2D-C2E
23	M	401	6PH	C2B-C2C-C2D-C2E
33	c	301	PTY	C32-C33-C34-C35
33	o	301	PTY	C32-C33-C34-C35
33	b	304	PTY	C31-C32-C33-C34
33	n	304	PTY	C31-C32-C33-C34
32	k	201	PCF	C11-C12-N-C13
32	w	201	PCF	C11-C12-N-C13
22	H	101	CDL	C51-CB5-OB6-CB4
22	R	101	CDL	C51-CB5-OB6-CB4
37	a	606	CN3	O3'-CA-CB-CC
37	m	606	CN3	O3'-CA-CB-CC
23	C	401	6PH	C29-C2A-C2B-C2C
23	M	401	6PH	C29-C2A-C2B-C2C
22	D	403	CDL	OA5-CA3-CA4-CA6
22	E	302	CDL	OB5-CB3-CB4-CB6
22	N	403	CDL	OA5-CA3-CA4-CA6
22	O	302	CDL	OB5-CB3-CB4-CB6
29	D	401	PEF	C10-C11-C12-C13
29	N	401	PEF	C10-C11-C12-C13
22	D	403	CDL	CA7-C31-C32-C33
22	N	403	CDL	CA7-C31-C32-C33
37	a	606	CN3	O22-C21-O21-C2
37	m	606	CN3	O22-C21-O21-C2
22	D	403	CDL	OA5-CA3-CA4-OA6
22	E	302	CDL	OB5-CB3-CB4-OB6
22	N	403	CDL	OA5-CA3-CA4-OA6
22	O	302	CDL	OB5-CB3-CB4-OB6
33	a	604	PTY	O4-C1-C6-C5

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Mol	Chain	Res	Type	Atoms
33	m	604	PTY	O4-C1-C6-C5
33	b	302	PTY	C14-C15-C16-C17
33	n	302	PTY	C14-C15-C16-C17
24	C	402	8PE	C12-C11-O13-P
24	M	402	8PE	C12-C11-O13-P
32	k	201	PCF	C12-C11-O13-P
32	w	201	PCF	C12-C11-O13-P
22	D	403	CDL	OA6-CA4-CA6-OA8
22	N	403	CDL	OA6-CA4-CA6-OA8
33	I	101	PTY	O4-C1-C6-O7
33	S	101	PTY	O4-C1-C6-O7
23	C	401	6PH	C2A-C2B-C2C-C2D
23	M	401	6PH	C2A-C2B-C2C-C2D
32	H	102	PCF	C11-C12-N-C13
32	H	102	PCF	C11-C12-N-C15
32	R	102	PCF	C11-C12-N-C13
32	R	102	PCF	C11-C12-N-C15
28	C	406	9PE	O31-C31-C32-C33
28	M	405	9PE	O31-C31-C32-C33
29	D	401	PEF	C37-C38-C39-C40
29	N	401	PEF	C37-C38-C39-C40
25	C	403	CN5	CA-CB-CC-O13
33	c	301	PTY	C31-C32-C33-C34
33	o	301	PTY	C31-C32-C33-C34
22	D	403	CDL	OA9-CA7-OA8-CA6
22	N	403	CDL	OA9-CA7-OA8-CA6
23	C	401	6PH	C38-C39-C3A-C3B
23	M	401	6PH	C38-C39-C3A-C3B
32	k	201	PCF	O11-C1-C2-C3
32	w	201	PCF	O11-C1-C2-C3
22	H	101	CDL	OB7-CB5-OB6-CB4
22	R	101	CDL	OB7-CB5-OB6-CB4
23	C	401	6PH	C26-C27-C28-C29
23	M	401	6PH	C26-C27-C28-C29
29	D	401	PEF	C33-C34-C35-C36
29	N	401	PEF	C33-C34-C35-C36
22	A	501	CDL	OA5-CA3-CA4-OA6
22	K	501	CDL	OA5-CA3-CA4-OA6
24	C	402	8PE	O11-C1-C2-O21
24	M	402	8PE	O11-C1-C2-O21
23	C	401	6PH	C23-C24-C25-C26
23	M	401	6PH	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
26	C	408	UQ6	C4-C3-O3-C3M
26	M	407	UQ6	C4-C3-O3-C3M
29	a	607	PEF	O2-C2-C3-O3
29	m	607	PEF	O2-C2-C3-O3
33	a	604	PTY	O4-C1-C6-O7
33	m	604	PTY	O4-C1-C6-O7
23	C	401	6PH	C22-C23-C24-C25
23	M	401	6PH	C22-C23-C24-C25
22	E	302	CDL	CA2-OA2-PA1-OA3
22	E	302	CDL	CB3-OB5-PB2-OB4
22	H	101	CDL	CA2-OA2-PA1-OA3
22	O	302	CDL	CA2-OA2-PA1-OA3
22	O	302	CDL	CB3-OB5-PB2-OB4
22	R	101	CDL	CA2-OA2-PA1-OA3
29	D	401	PEF	C1-O3P-P-O1P
29	D	401	PEF	C4-O4P-P-O1P
29	J	101	PEF	C4-O4P-P-O3P
29	N	401	PEF	C1-O3P-P-O1P
29	N	401	PEF	C4-O4P-P-O1P
29	T	101	PEF	C4-O4P-P-O3P
32	H	102	PCF	C1-O11-P-O13
32	H	102	PCF	C11-O13-P-O12
32	l	101	PCF	C1-O11-P-O13
32	R	102	PCF	C1-O11-P-O13
32	R	102	PCF	C11-O13-P-O12
32	x	101	PCF	C1-O11-P-O13
33	a	604	PTY	C5-O14-P1-O13
33	b	302	PTY	C3-O11-P1-O13
33	m	604	PTY	C5-O14-P1-O13
33	n	302	PTY	C3-O11-P1-O13
34	a	601	HEA	O11-C11-C3B-C2B
34	m	601	HEA	O11-C11-C3B-C2B
37	a	606	CN3	C1-O11-P-O12
37	m	606	CN3	C1-O11-P-O12
22	A	501	CDL	CB4-CB3-OB5-PB2
22	E	302	CDL	C1-CA2-OA2-PA1
22	K	501	CDL	CB4-CB3-OB5-PB2
22	O	302	CDL	C1-CA2-OA2-PA1
33	I	101	PTY	C6-C5-O14-P1
33	S	101	PTY	C6-C5-O14-P1
22	D	403	CDL	CA6-CA4-OA6-CA5
22	N	403	CDL	CA6-CA4-OA6-CA5

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Mol	Chain	Res	Type	Atoms
28	C	406	9PE	O11-C1-C2-C3
28	M	405	9PE	O11-C1-C2-C3
24	C	402	8PE	O21-C2-C3-O31
24	M	402	8PE	O21-C2-C3-O31
33	c	301	PTY	C11-C12-C13-C14
33	o	301	PTY	C11-C12-C13-C14
34	a	603	HEA	C4D-C3D-CAD-CBD
34	m	603	HEA	C4D-C3D-CAD-CBD
33	a	604	PTY	C14-C15-C16-C17
33	m	604	PTY	C14-C15-C16-C17
24	C	402	8PE	C32-C33-C34-C35
24	M	402	8PE	C32-C33-C34-C35
22	D	403	CDL	OB7-CB5-OB6-CB4
22	N	403	CDL	OB7-CB5-OB6-CB4
34	a	603	HEA	CAD-CBD-CGD-O2D
34	m	603	HEA	CAD-CBD-CGD-O2D
32	H	102	PCF	C11-C12-N-C14
32	R	102	PCF	C11-C12-N-C14
26	C	404	UQ6	C14-C16-C17-C18
26	M	403	UQ6	C14-C16-C17-C18
25	C	403	CN5	C42-C41-O41-C3'
22	D	403	CDL	C72-C71-CB7-OB8
22	N	403	CDL	C72-C71-CB7-OB8
22	H	101	CDL	CB7-C71-C72-C73
22	R	101	CDL	CB7-C71-C72-C73
29	a	607	PEF	C33-C34-C35-C36
29	m	607	PEF	C33-C34-C35-C36
27	C	407	HEM	CAD-CBD-CGD-O1D
27	M	406	HEM	CAD-CBD-CGD-O1D
27	C	407	HEM	CAA-CBA-CGA-O2A
27	M	406	HEM	CAA-CBA-CGA-O2A
34	a	603	HEA	CAA-CBA-CGA-O1A
34	a	603	HEA	CAD-CBD-CGD-O1D
34	m	603	HEA	CAA-CBA-CGA-O1A
34	m	603	HEA	CAD-CBD-CGD-O1D
27	C	407	HEM	CAA-CBA-CGA-O1A
27	M	406	HEM	CAA-CBA-CGA-O1A
22	D	403	CDL	C51-CB5-OB6-CB4
22	N	403	CDL	C51-CB5-OB6-CB4
33	b	302	PTY	C8-C11-C12-C13
33	n	302	PTY	C8-C11-C12-C13
22	H	101	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
22	R	101	CDL	CA3-CA4-CA6-OA8
34	a	601	HEA	C19-C20-C21-C22
34	m	601	HEA	C19-C20-C21-C22
32	k	201	PCF	C28-C29-C30-C47
32	w	201	PCF	C28-C29-C30-C47
27	C	407	HEM	CAD-CBD-CGD-O2D
27	M	406	HEM	CAD-CBD-CGD-O2D
34	a	603	HEA	CAA-CBA-CGA-O2A
34	m	603	HEA	CAA-CBA-CGA-O2A
34	a	601	HEA	CAD-CBD-CGD-O2D
34	m	601	HEA	CAD-CBD-CGD-O2D
22	D	403	CDL	OB5-CB3-CB4-CB6
22	N	403	CDL	OB5-CB3-CB4-CB6
32	H	102	PCF	O11-C1-C2-C3
32	R	102	PCF	O11-C1-C2-C3
33	I	101	PTY	O14-C5-C6-C1
33	S	101	PTY	O14-C5-C6-C1
34	a	601	HEA	CAD-CBD-CGD-O1D
34	m	601	HEA	CAD-CBD-CGD-O1D
22	D	403	CDL	CA3-CA4-CA6-OA8
22	N	403	CDL	CA3-CA4-CA6-OA8
26	C	408	UQ6	C19-C21-C22-C23
26	M	407	UQ6	C19-C21-C22-C23
22	A	501	CDL	C14-C15-C16-C17
22	K	501	CDL	C14-C15-C16-C17
26	C	408	UQ6	C7-C8-C9-C10
26	M	407	UQ6	C7-C8-C9-C10
26	C	408	UQ6	C2-C3-O3-C3M
26	M	407	UQ6	C2-C3-O3-C3M
29	D	401	PEF	C34-C35-C36-C37
29	N	401	PEF	C34-C35-C36-C37
22	H	101	CDL	C33-C34-C35-C36
22	R	101	CDL	C33-C34-C35-C36
33	b	304	PTY	C18-C19-C20-C21
33	n	304	PTY	C18-C19-C20-C21
29	a	607	PEF	C32-C33-C34-C35
29	m	607	PEF	C32-C33-C34-C35
33	c	301	PTY	C35-C36-C37-C38
33	o	301	PTY	C35-C36-C37-C38
34	a	603	HEA	C3B-C11-C12-C13
34	m	603	HEA	C3B-C11-C12-C13
32	I	102	PCF	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
32	S	102	PCF	O13-C11-C12-N
32	H	102	PCF	C32-C33-C34-C35
32	R	102	PCF	C32-C33-C34-C35
32	I	102	PCF	C33-C34-C35-C36
32	S	102	PCF	C33-C34-C35-C36
33	b	302	PTY	C17-C18-C19-C20
33	n	302	PTY	C17-C18-C19-C20
29	a	607	PEF	C15-C16-C17-C18
29	m	607	PEF	C15-C16-C17-C18
33	a	604	PTY	C13-C14-C15-C16
33	m	604	PTY	C13-C14-C15-C16
34	a	603	HEA	C2D-C3D-CAD-CBD
34	m	603	HEA	C2D-C3D-CAD-CBD
33	b	302	PTY	C32-C33-C34-C35
33	n	302	PTY	C32-C33-C34-C35
29	D	401	PEF	C32-C33-C34-C35
29	N	401	PEF	C32-C33-C34-C35
23	C	401	6PH	O21-C21-C22-C23
23	M	401	6PH	O21-C21-C22-C23
24	C	402	8PE	C1-C2-C3-O31
24	M	402	8PE	C1-C2-C3-O31
23	C	401	6PH	C36-C37-C38-C39
23	M	401	6PH	C36-C37-C38-C39
30	D	402	HEC	CAD-CBD-CGD-O2D
30	N	402	HEC	CAD-CBD-CGD-O2D
22	D	403	CDL	C72-C71-CB7-OB9
22	N	403	CDL	C72-C71-CB7-OB9
22	D	403	CDL	CA3-CA4-OA6-CA5
22	H	101	CDL	CA3-CA4-OA6-CA5
22	N	403	CDL	CA3-CA4-OA6-CA5
22	R	101	CDL	CA3-CA4-OA6-CA5
29	J	101	PEF	C1-C2-O2-C10
29	T	101	PEF	C1-C2-O2-C10
33	b	304	PTY	C13-C14-C15-C16
33	n	304	PTY	C13-C14-C15-C16
26	C	408	UQ6	C11-C12-C13-C14
26	C	408	UQ6	C16-C17-C18-C19
26	M	407	UQ6	C11-C12-C13-C14
26	M	407	UQ6	C16-C17-C18-C19
37	a	606	CN3	C43-C44-C45-C46
37	m	606	CN3	C43-C44-C45-C46
22	H	101	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
22	R	101	CDL	OB5-CB3-CB4-OB6
34	a	603	HEA	O11-C11-C12-C13
34	m	603	HEA	O11-C11-C12-C13
23	C	401	6PH	O22-C21-C22-C23
23	M	401	6PH	O22-C21-C22-C23
29	a	607	PEF	C21-C22-C23-C24
29	m	607	PEF	C21-C22-C23-C24
34	a	601	HEA	CAA-CBA-CGA-O1A
34	m	601	HEA	CAA-CBA-CGA-O1A
34	a	601	HEA	O11-C11-C3B-C4B
34	m	601	HEA	O11-C11-C3B-C4B
26	C	408	UQ6	C12-C13-C14-C15
26	M	407	UQ6	C12-C13-C14-C15
29	a	607	PEF	C18-C19-C20-C21
29	m	607	PEF	C18-C19-C20-C21
33	I	101	PTY	O4-C30-C31-C32
33	S	101	PTY	O4-C30-C31-C32

There are no ring outliers.

50 monomers are involved in 207 short contacts:

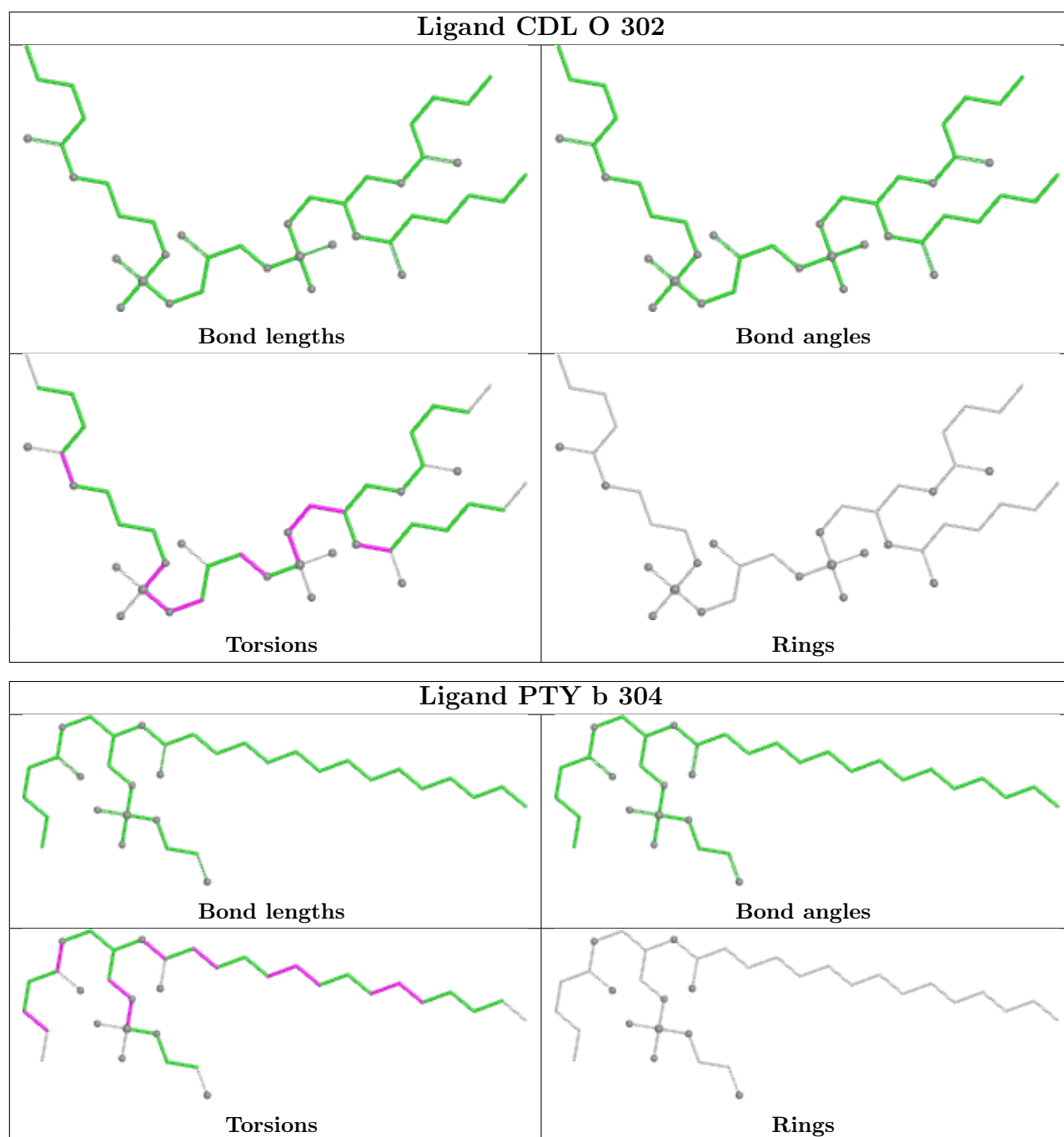
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	O	302	CDL	6	0
33	b	304	PTY	2	0
22	D	403	CDL	5	0
33	a	604	PTY	9	0
22	H	101	CDL	3	0
27	C	407	HEM	3	0
33	o	301	PTY	1	0
34	a	603	HEA	2	0
29	a	607	PEF	2	0
33	b	302	PTY	2	0
22	K	501	CDL	2	0
30	D	402	HEC	16	0
23	M	401	6PH	2	0
27	C	405	HEM	6	0
22	R	101	CDL	1	0
33	n	302	PTY	2	0
33	c	301	PTY	1	0
22	E	302	CDL	6	0
26	C	408	UQ6	9	0
32	x	101	PCF	1	0

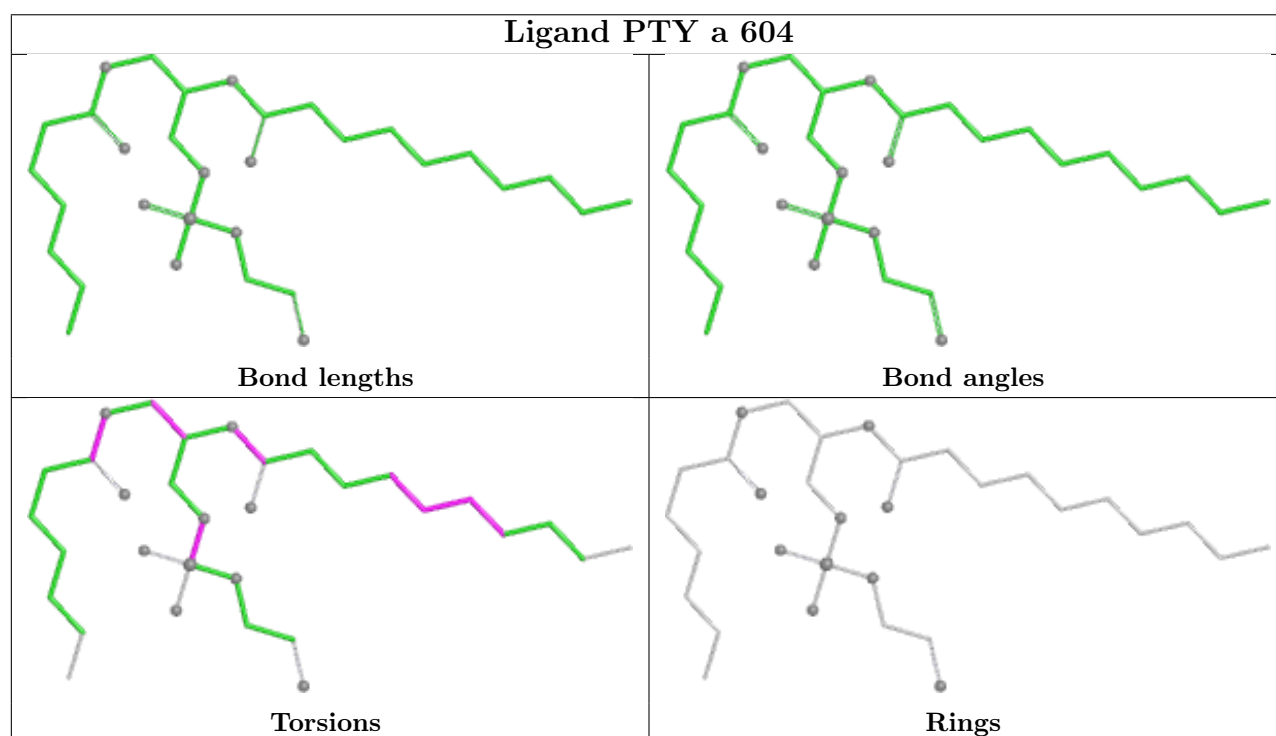
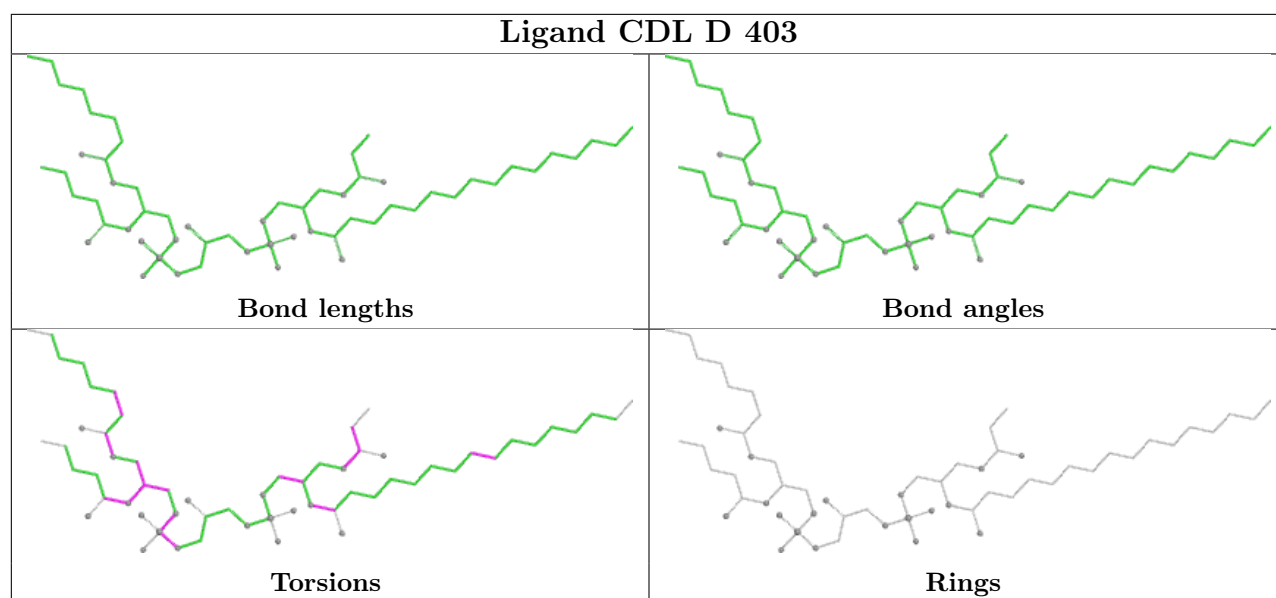
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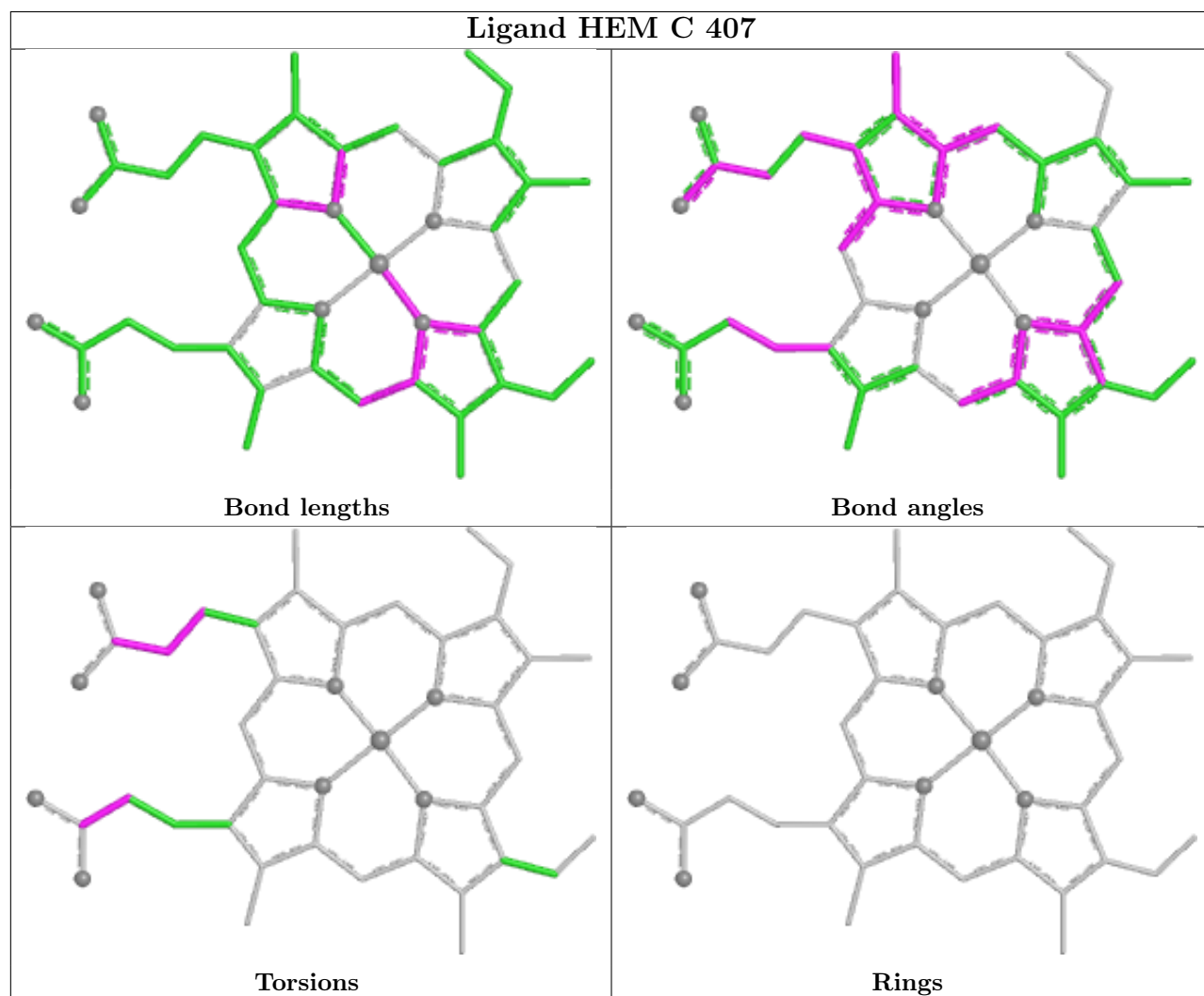
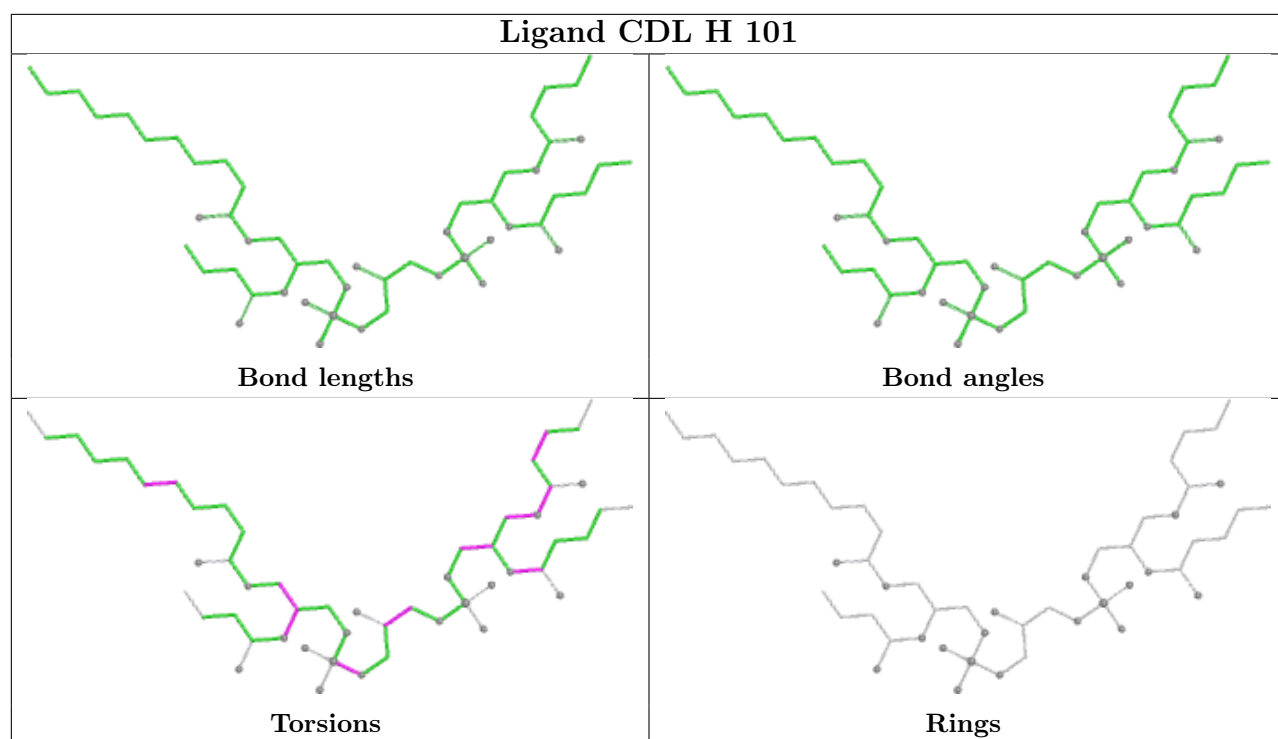
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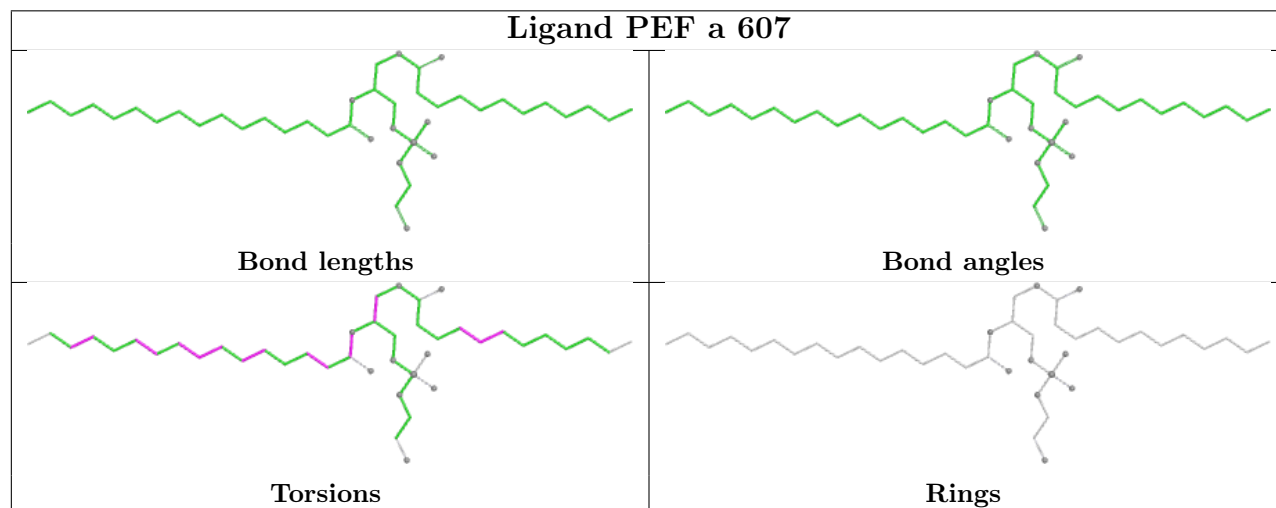
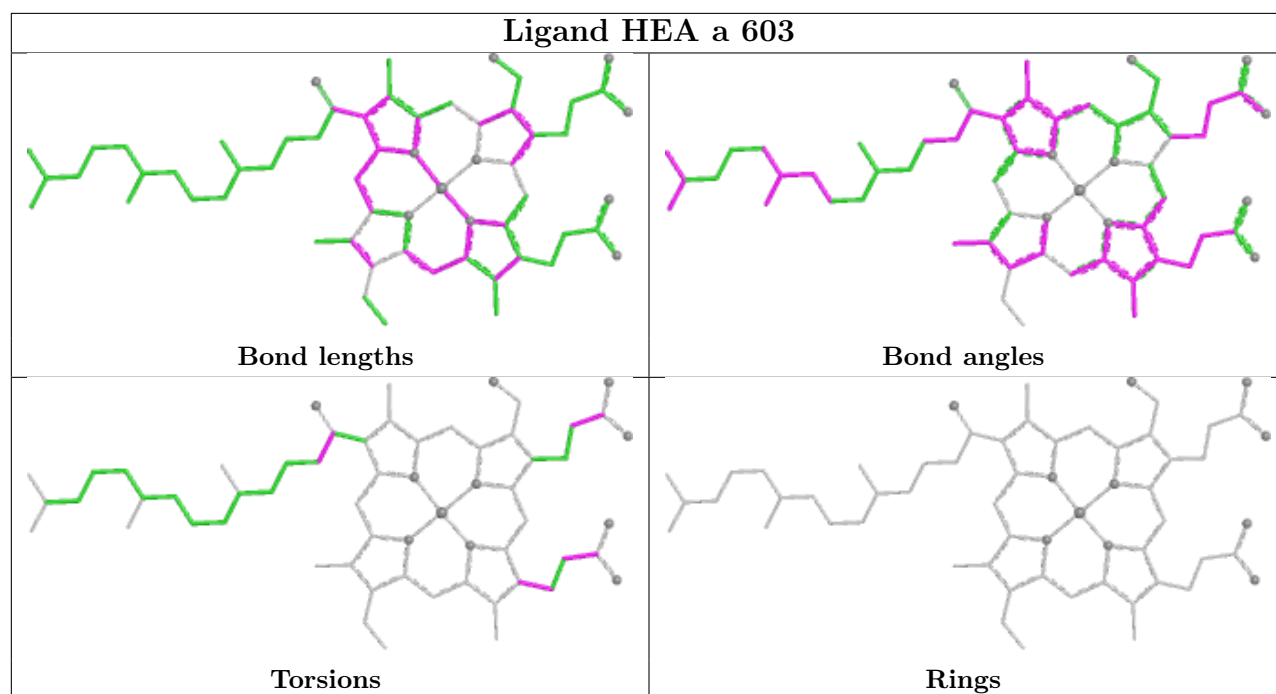
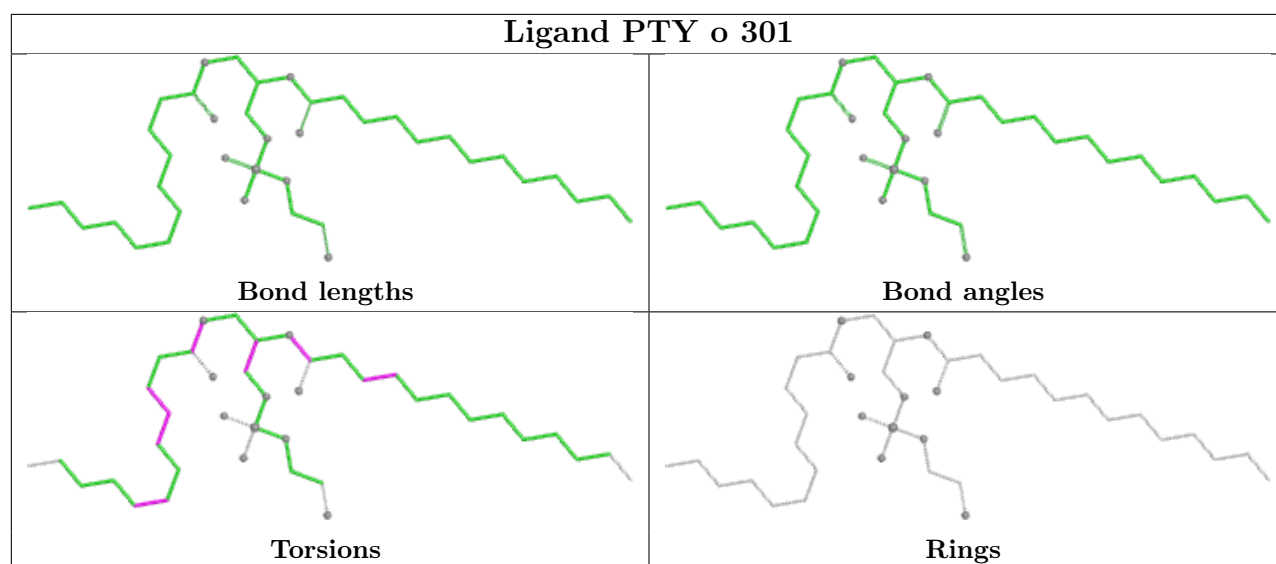
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	m	601	HEA	7	0
26	M	407	UQ6	9	0
27	M	406	HEM	3	0
34	m	603	HEA	3	0
33	S	101	PTY	2	0
29	D	401	PEF	4	0
27	M	404	HEM	6	0
30	N	402	HEC	16	0
31	E	301	FES	4	0
32	l	101	PCF	2	0
23	C	401	6PH	2	0
32	k	201	PCF	12	0
29	m	607	PEF	1	0
33	m	604	PTY	9	0
29	J	101	PEF	1	0
33	n	304	PTY	2	0
34	a	601	HEA	7	0
26	C	404	UQ6	3	0
29	T	101	PEF	1	0
28	M	405	9PE	1	0
22	A	501	CDL	2	0
32	w	201	PCF	12	0
28	C	406	9PE	1	0
33	I	101	PTY	2	0
32	H	102	PCF	3	0
22	N	403	CDL	3	0
31	O	301	FES	4	0
29	N	401	PEF	3	0
32	R	102	PCF	3	0
26	M	403	UQ6	3	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.

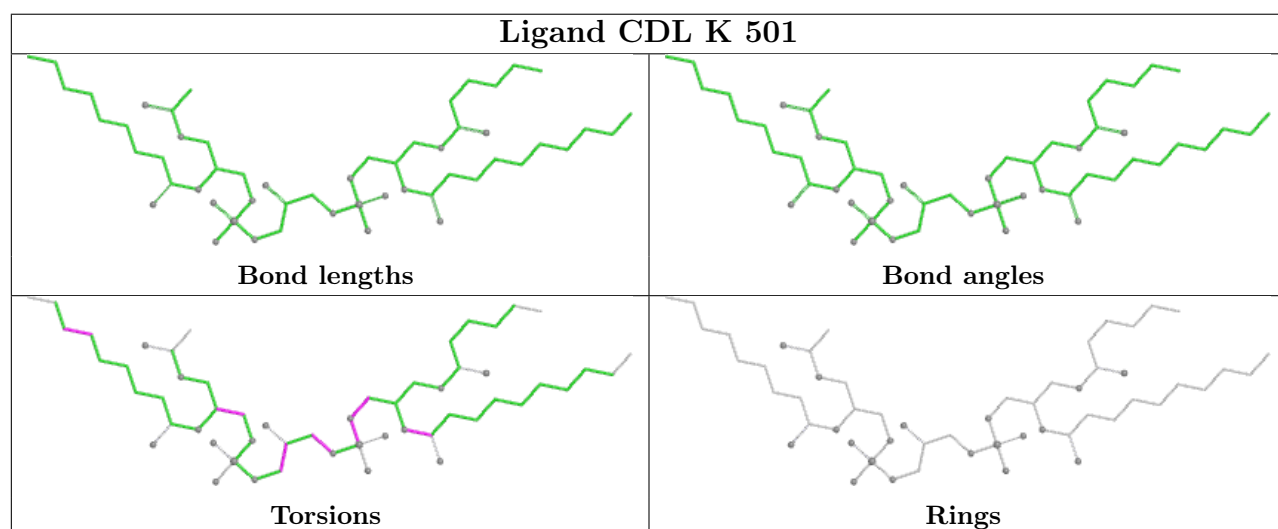
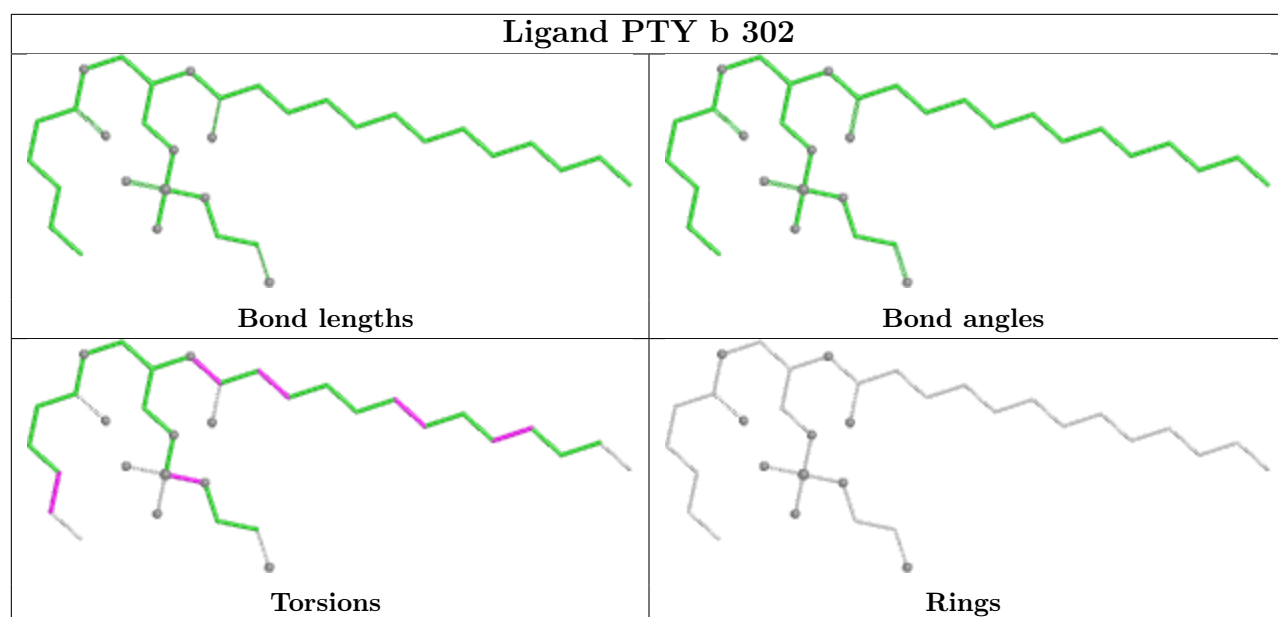


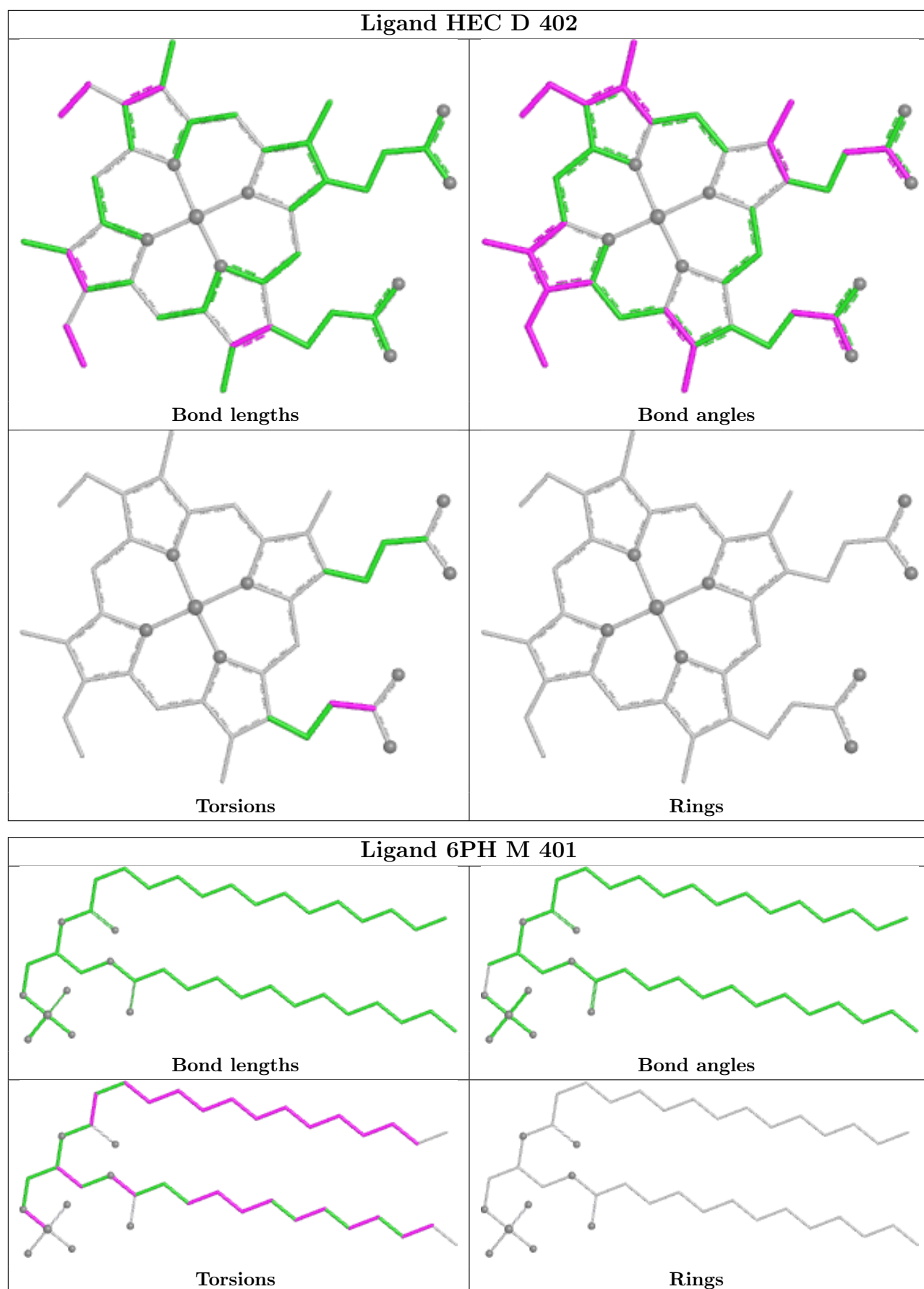


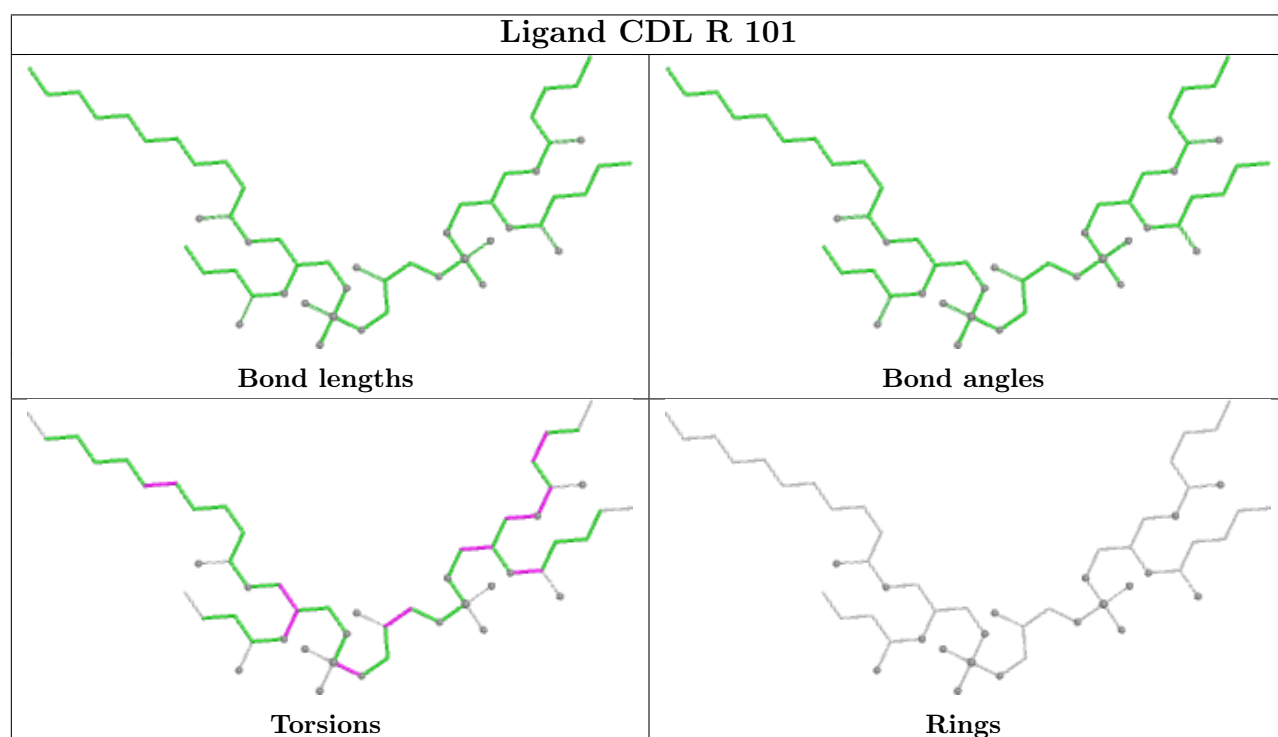
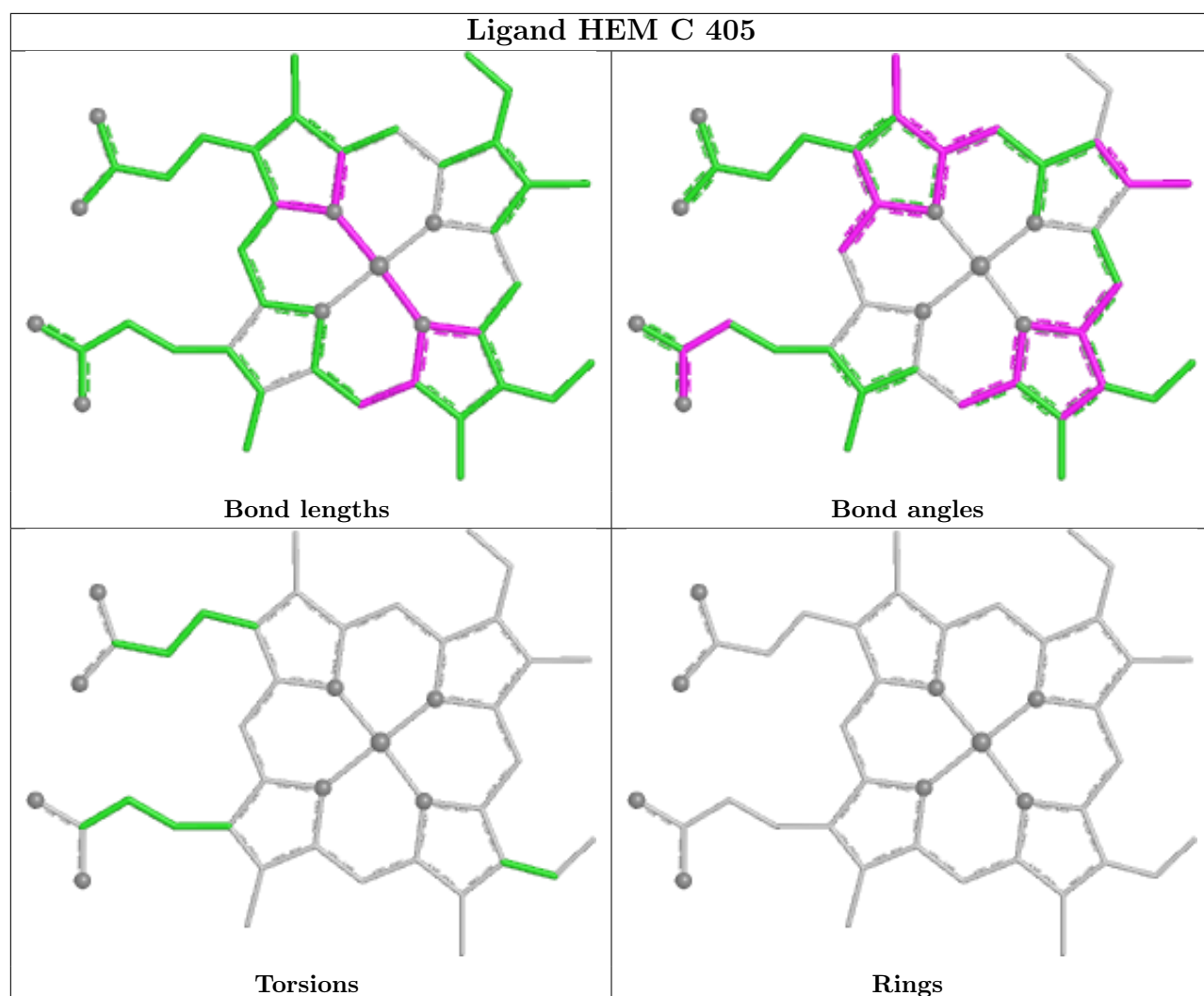


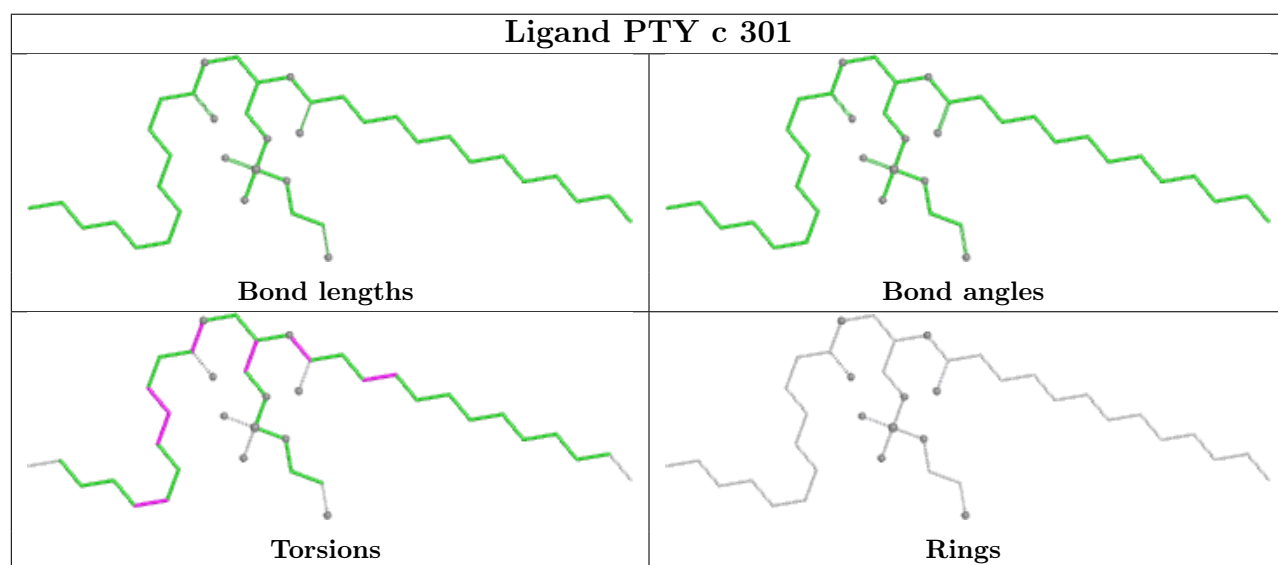
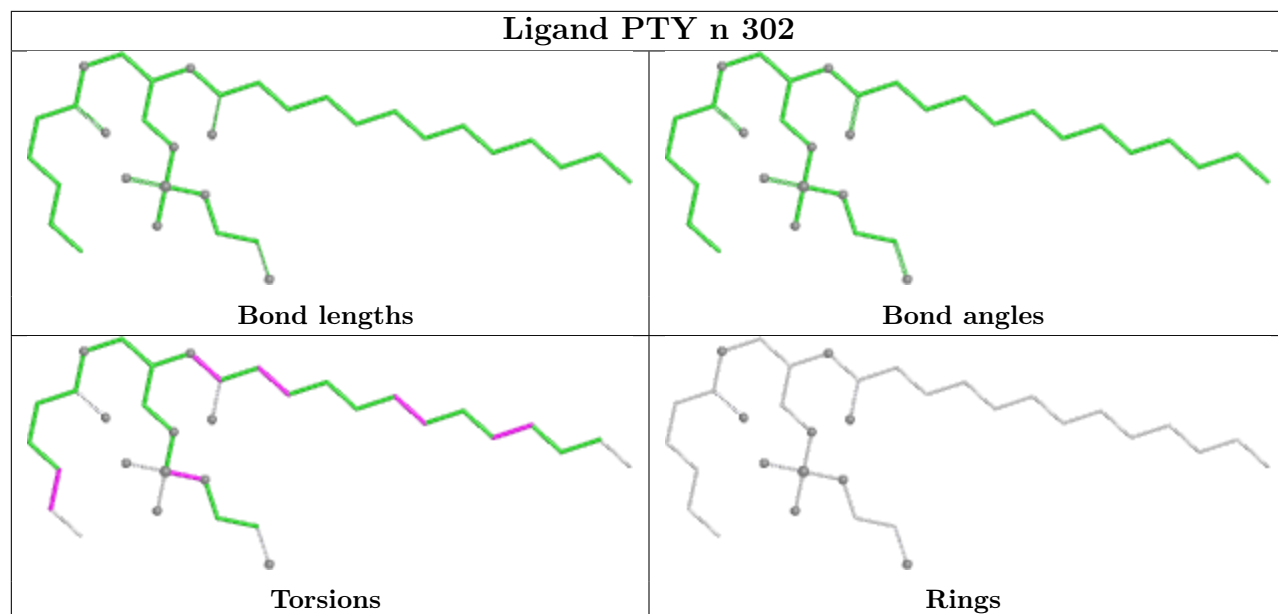


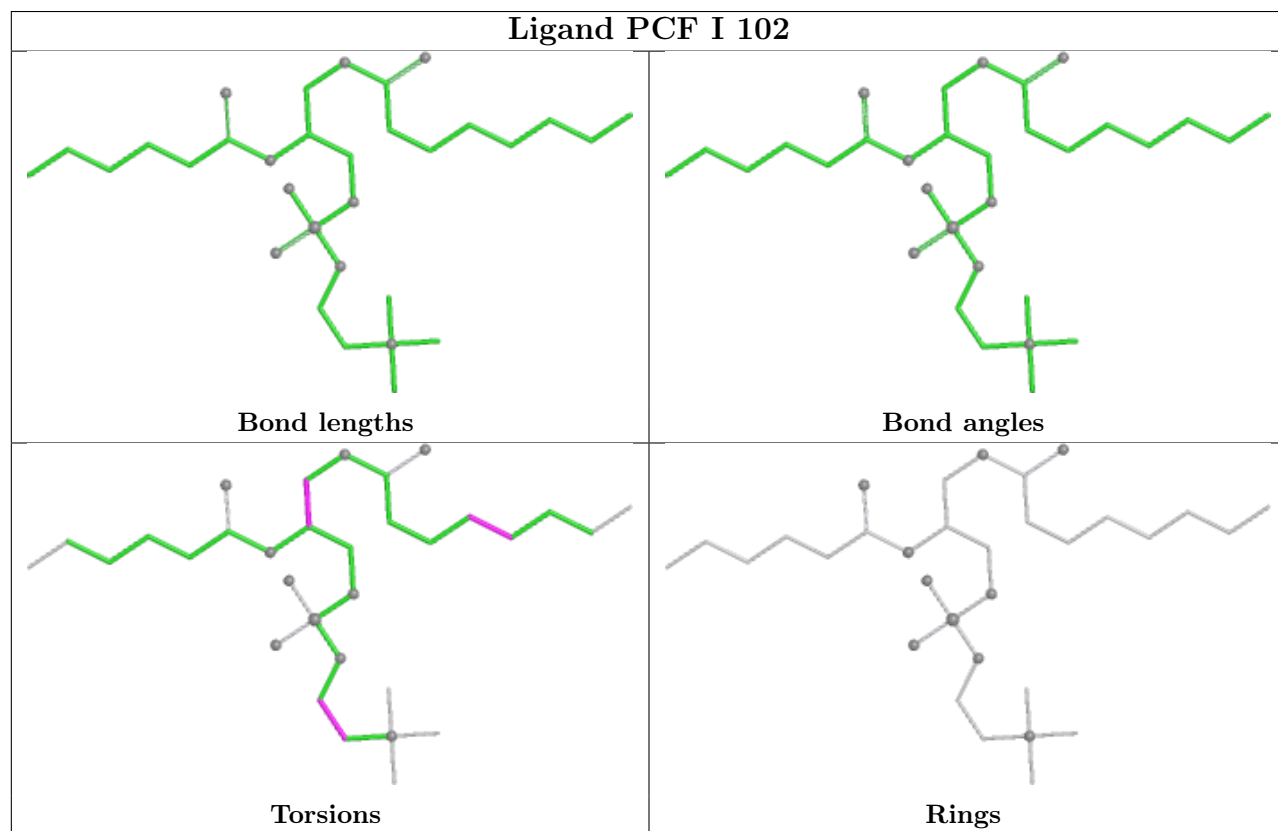
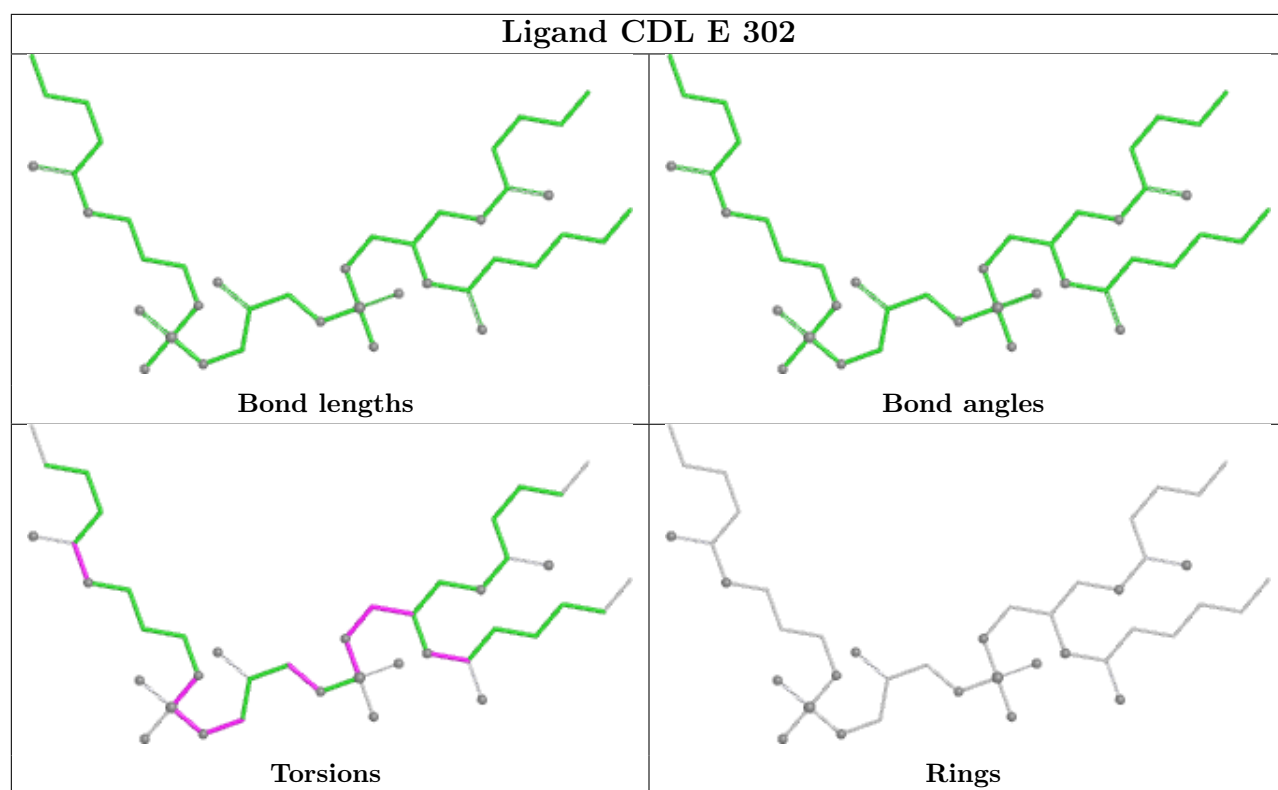


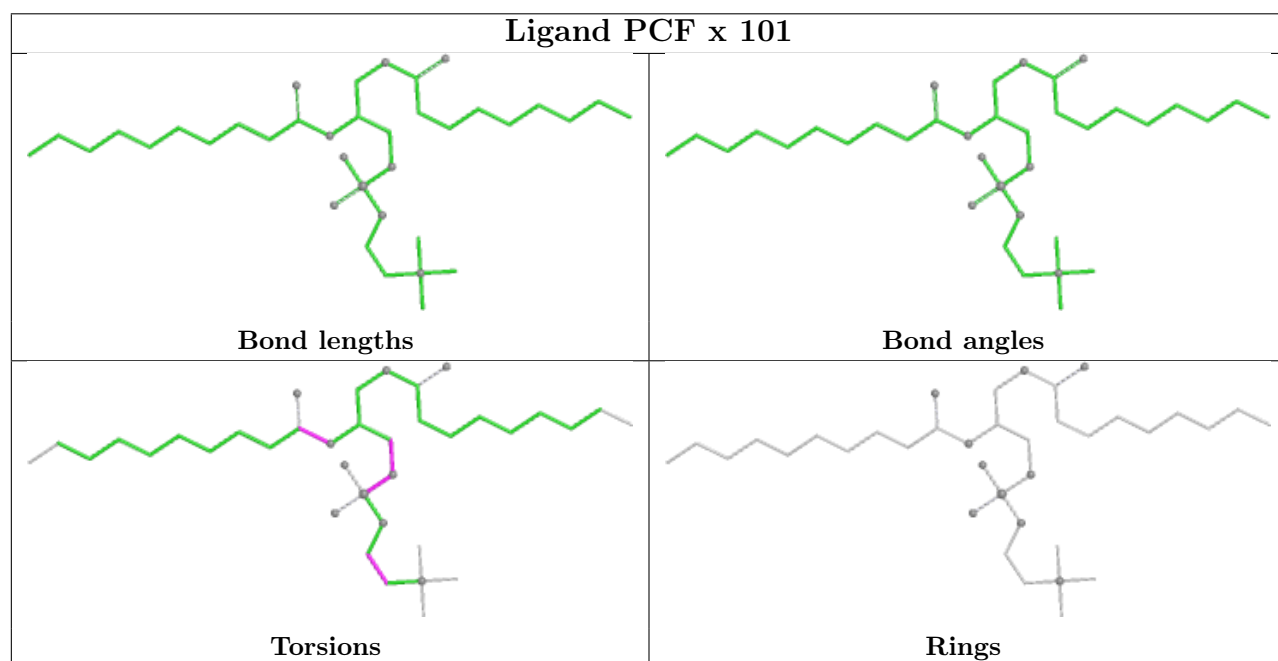
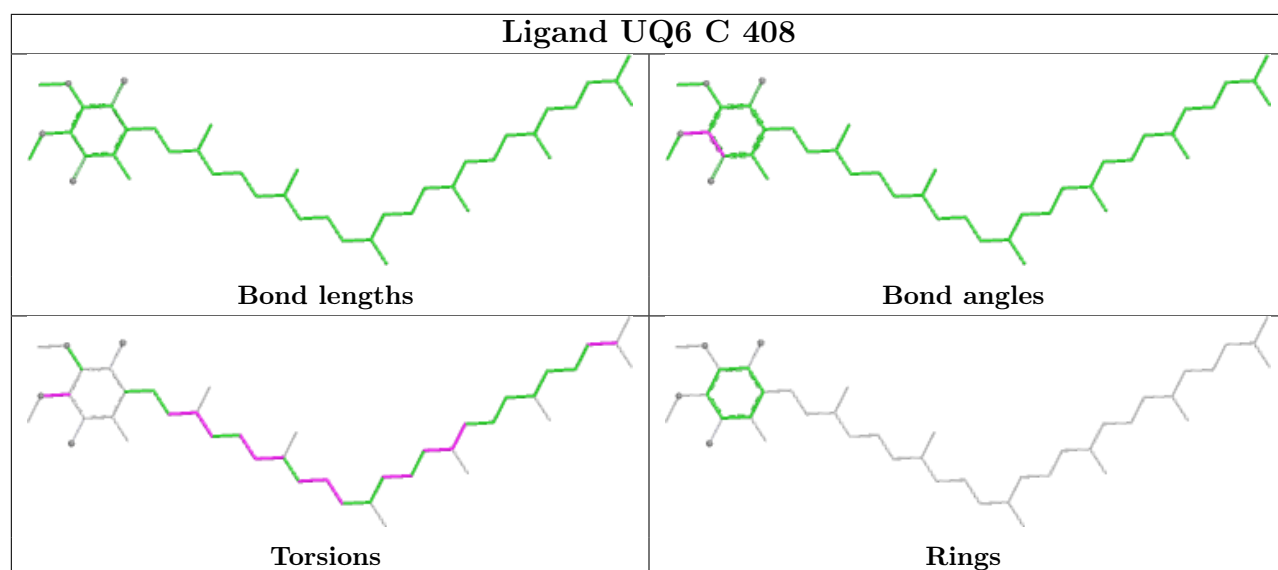


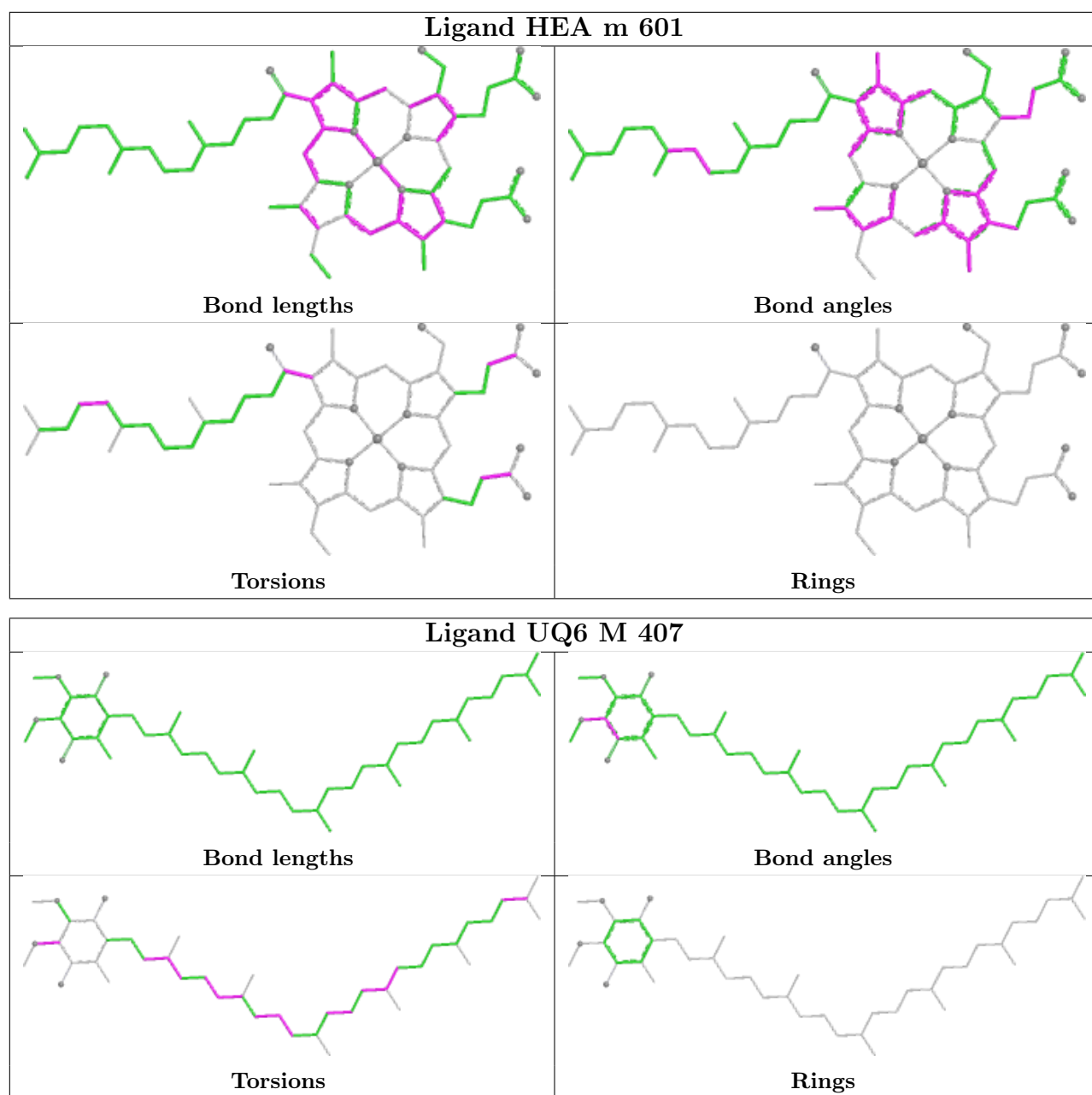


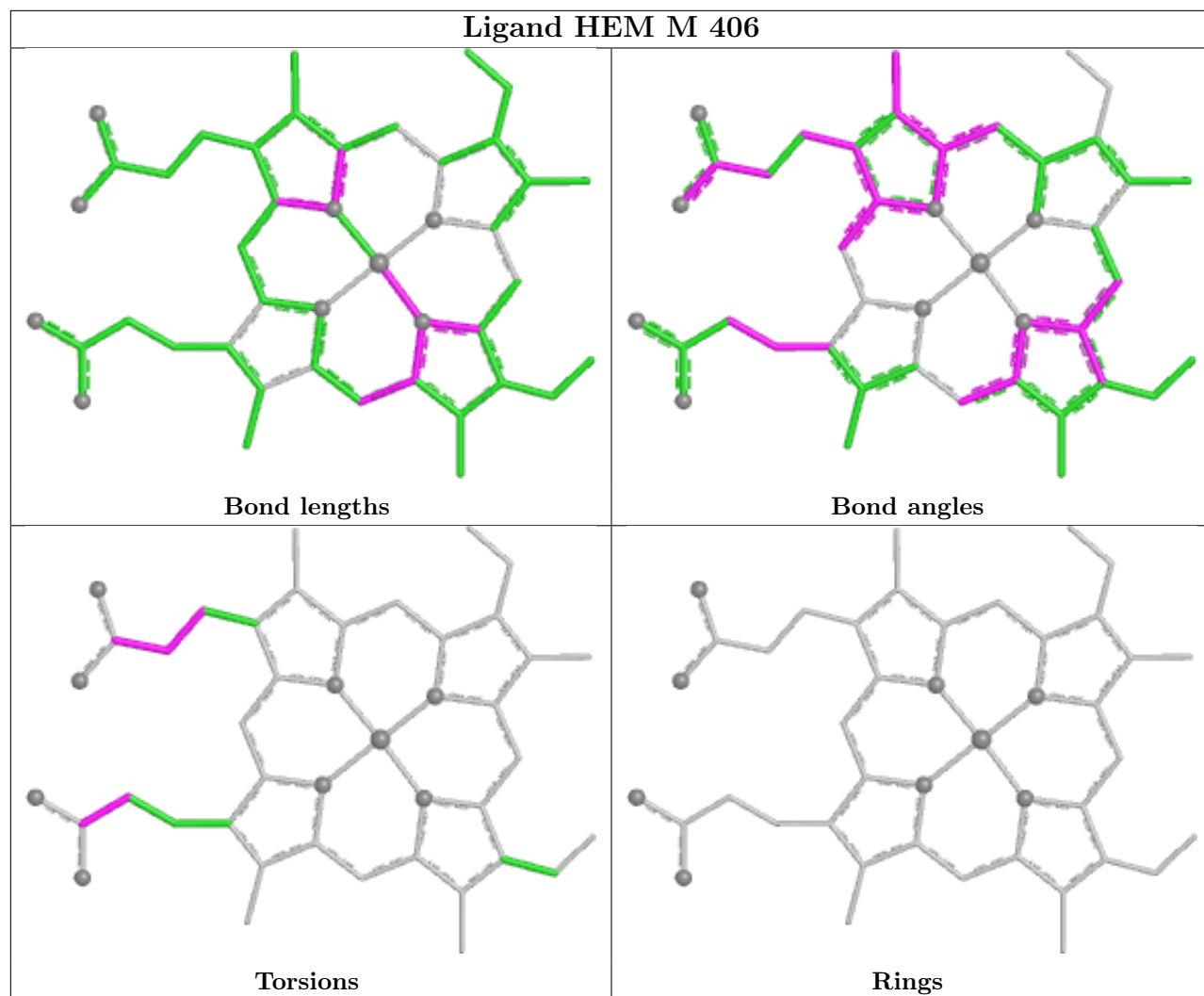




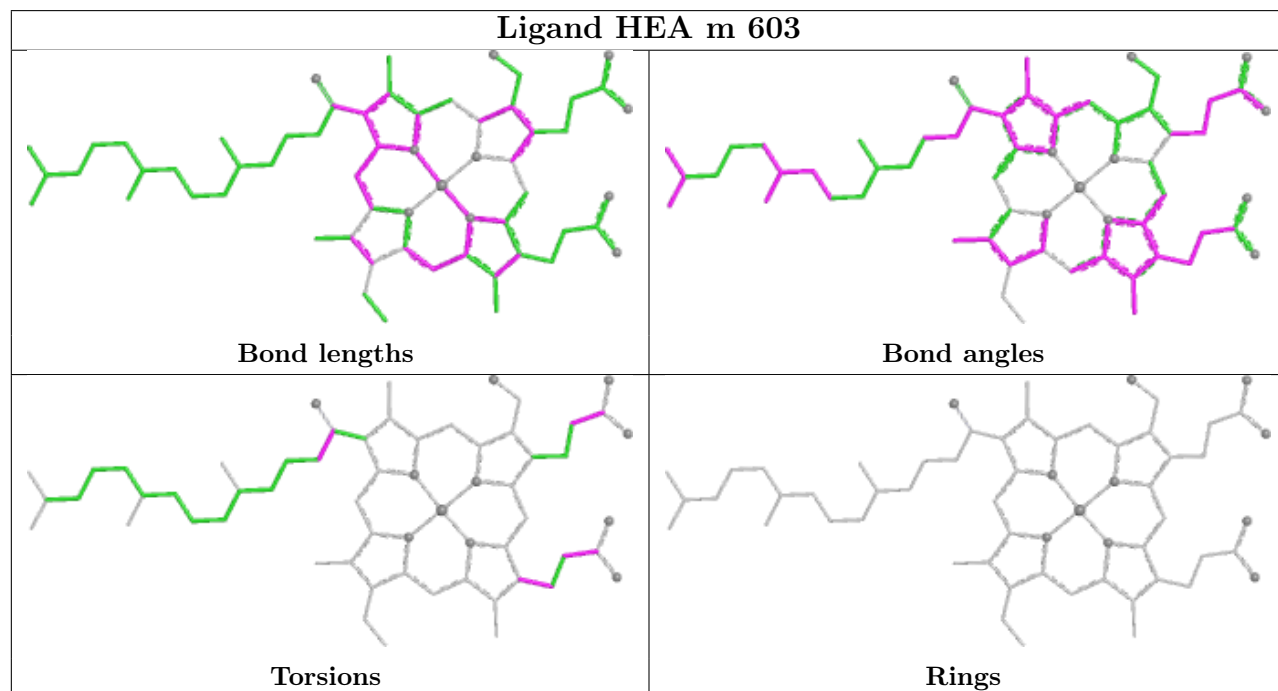
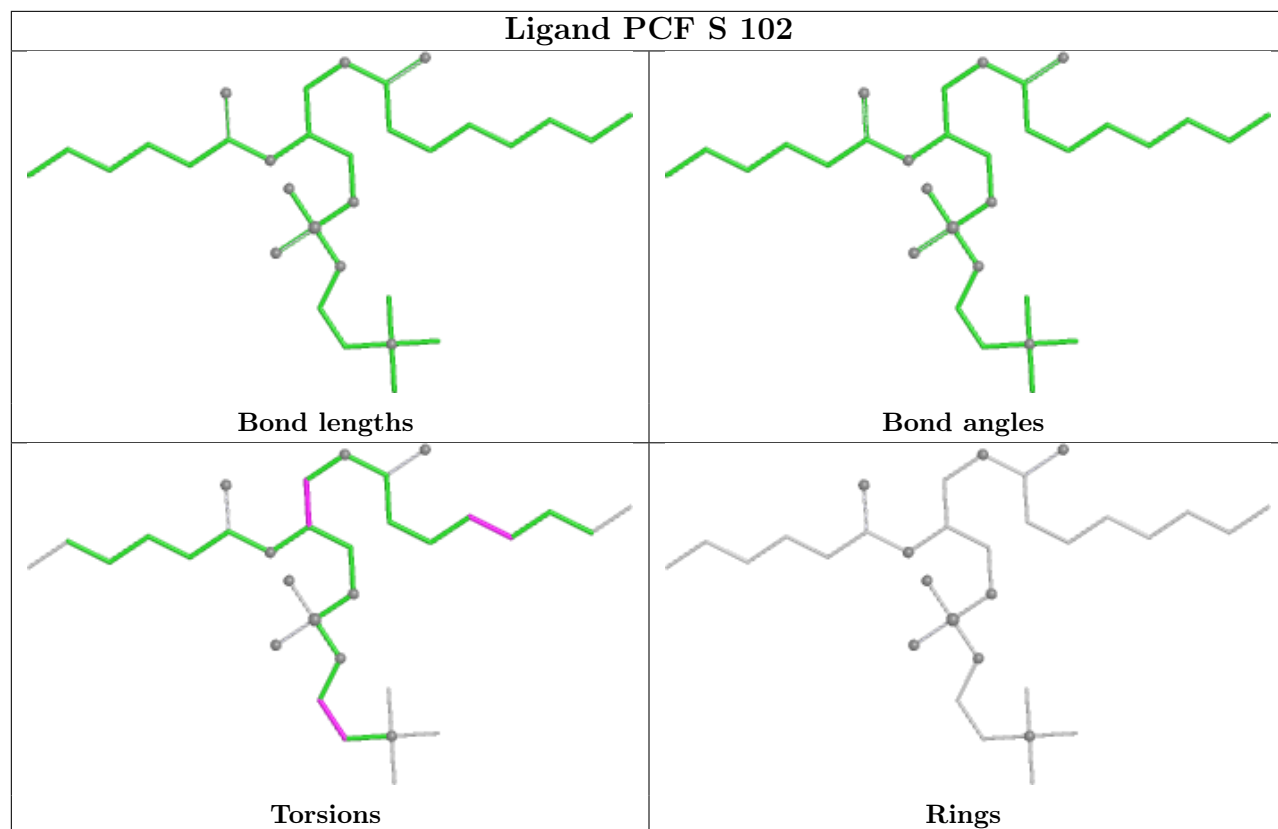


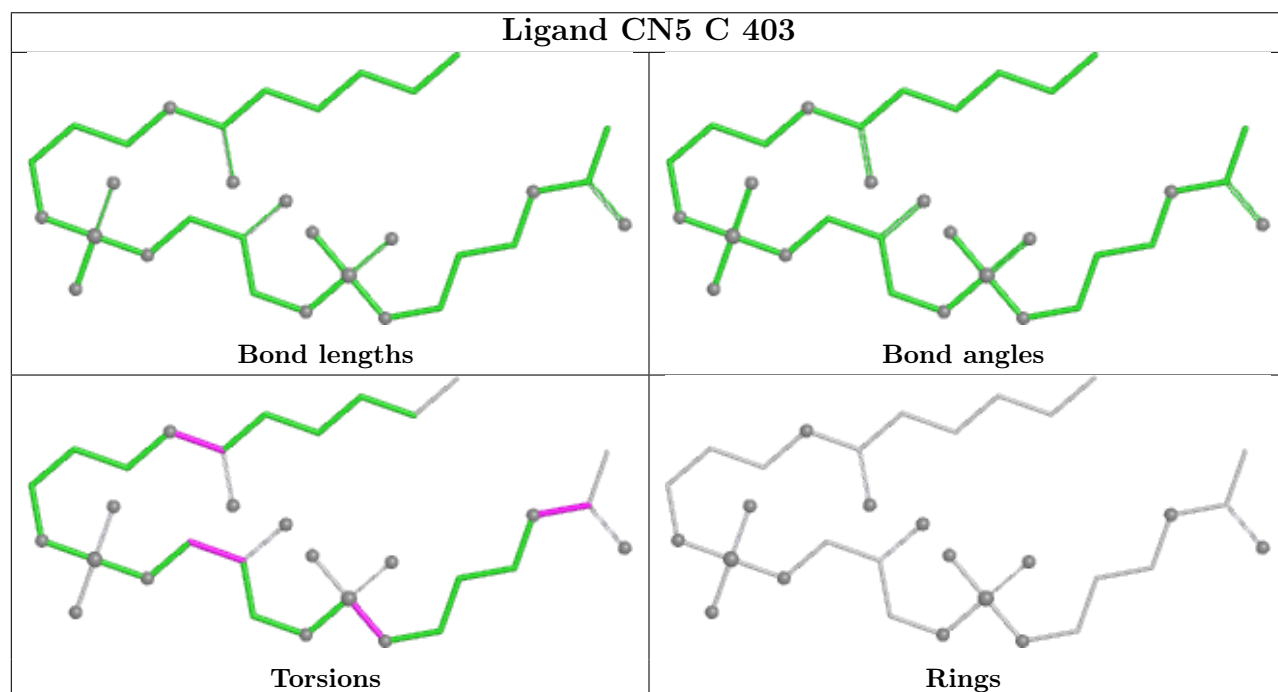
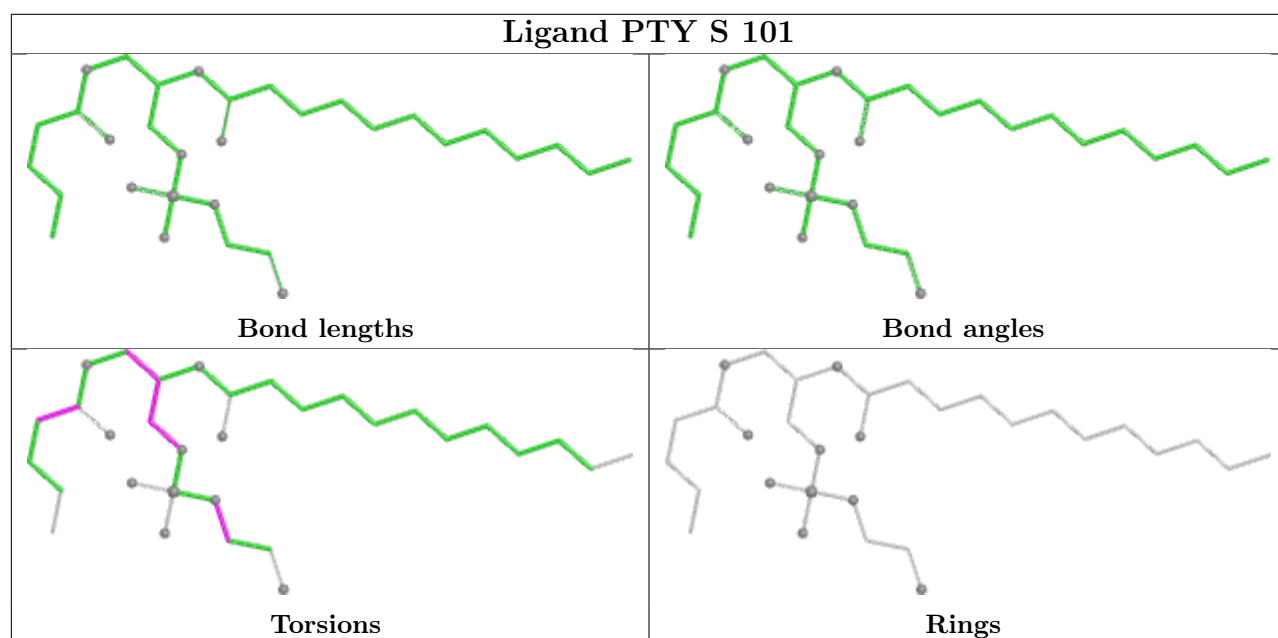


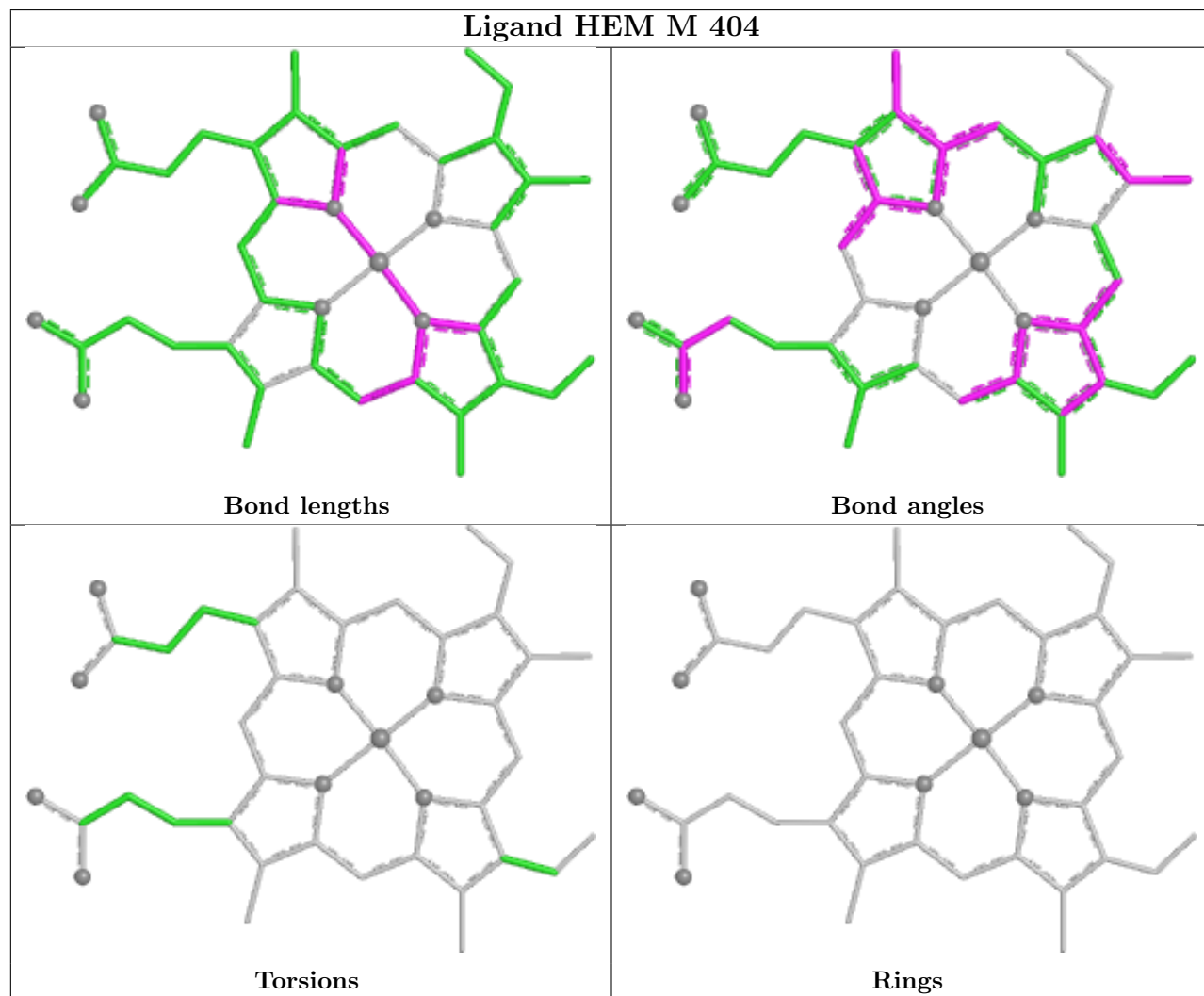
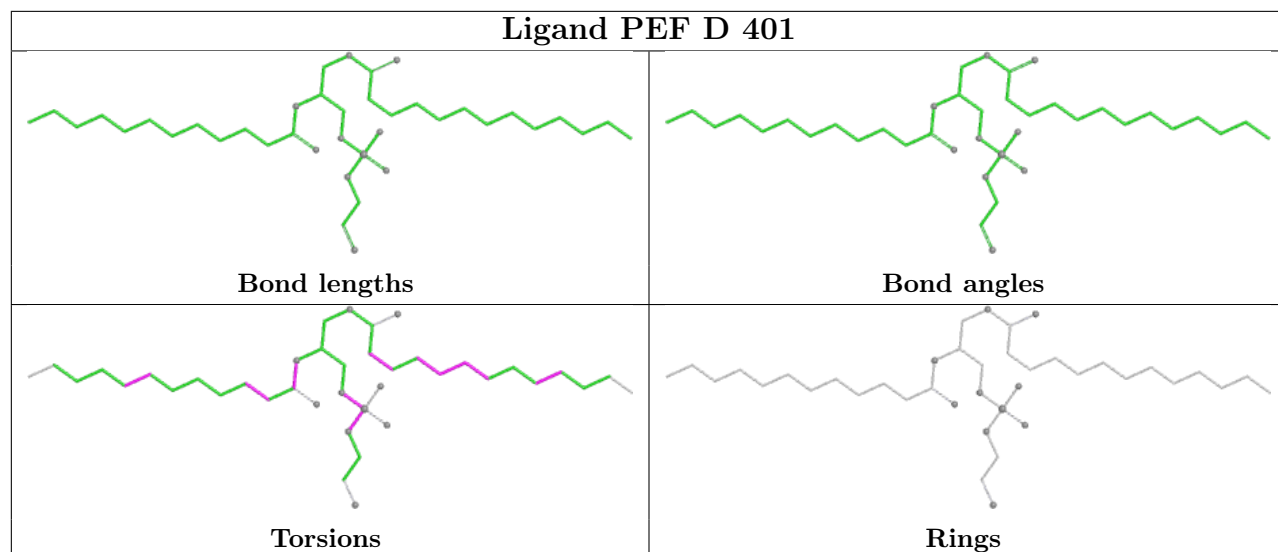


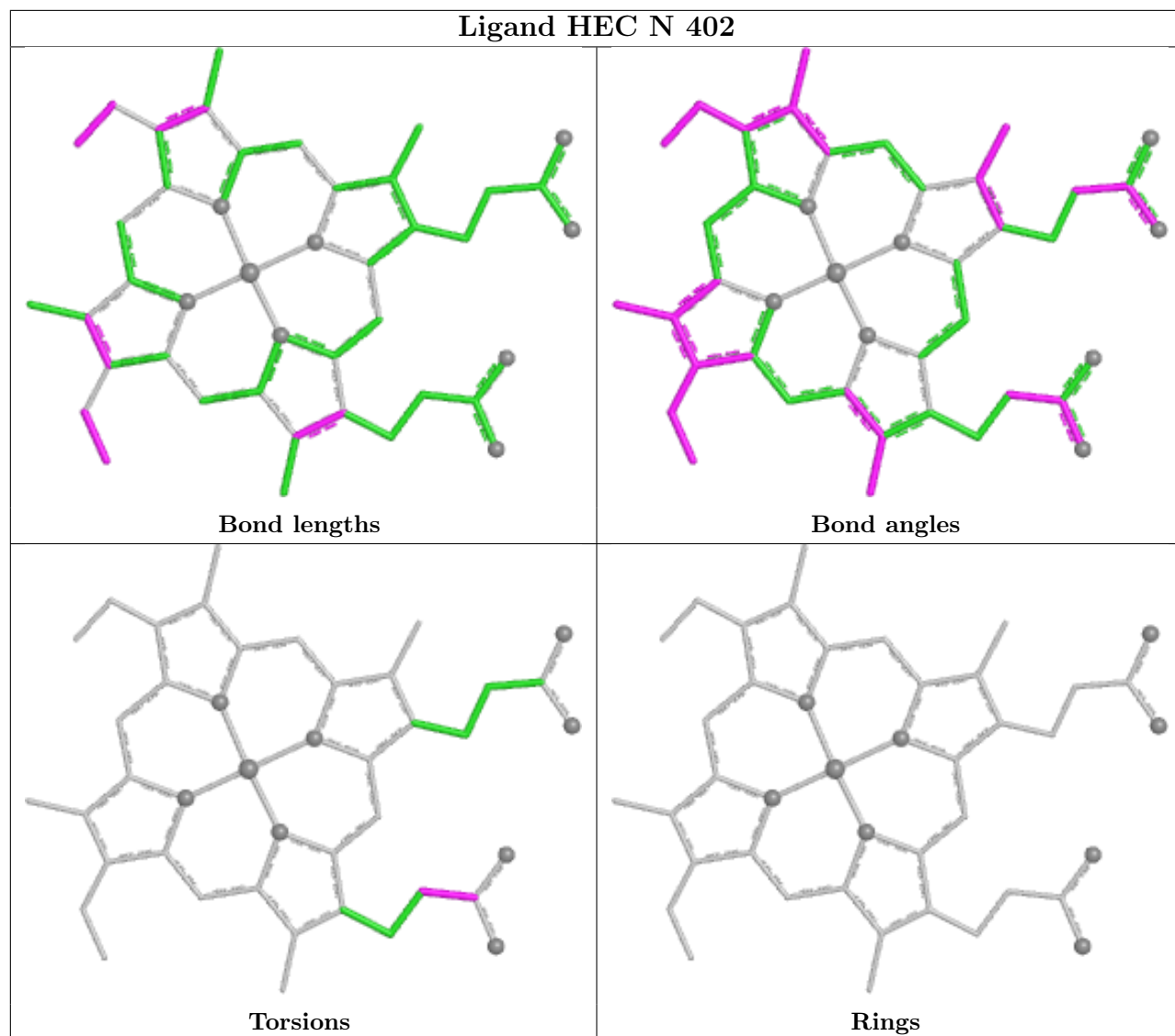


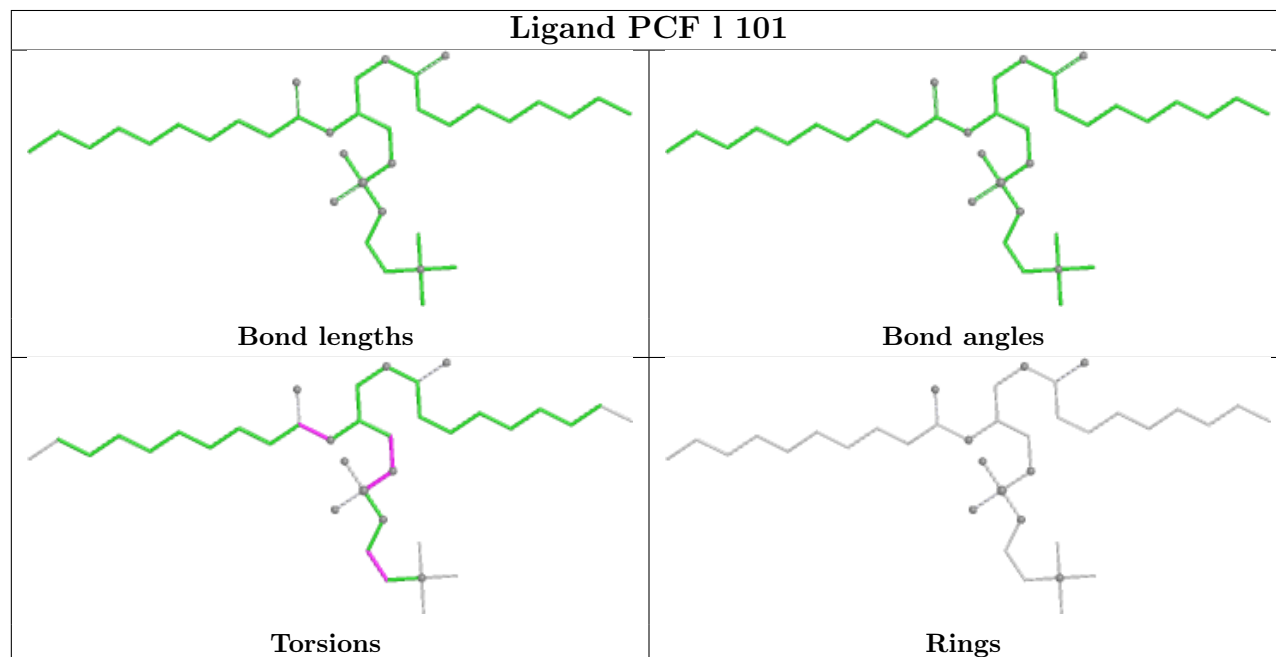
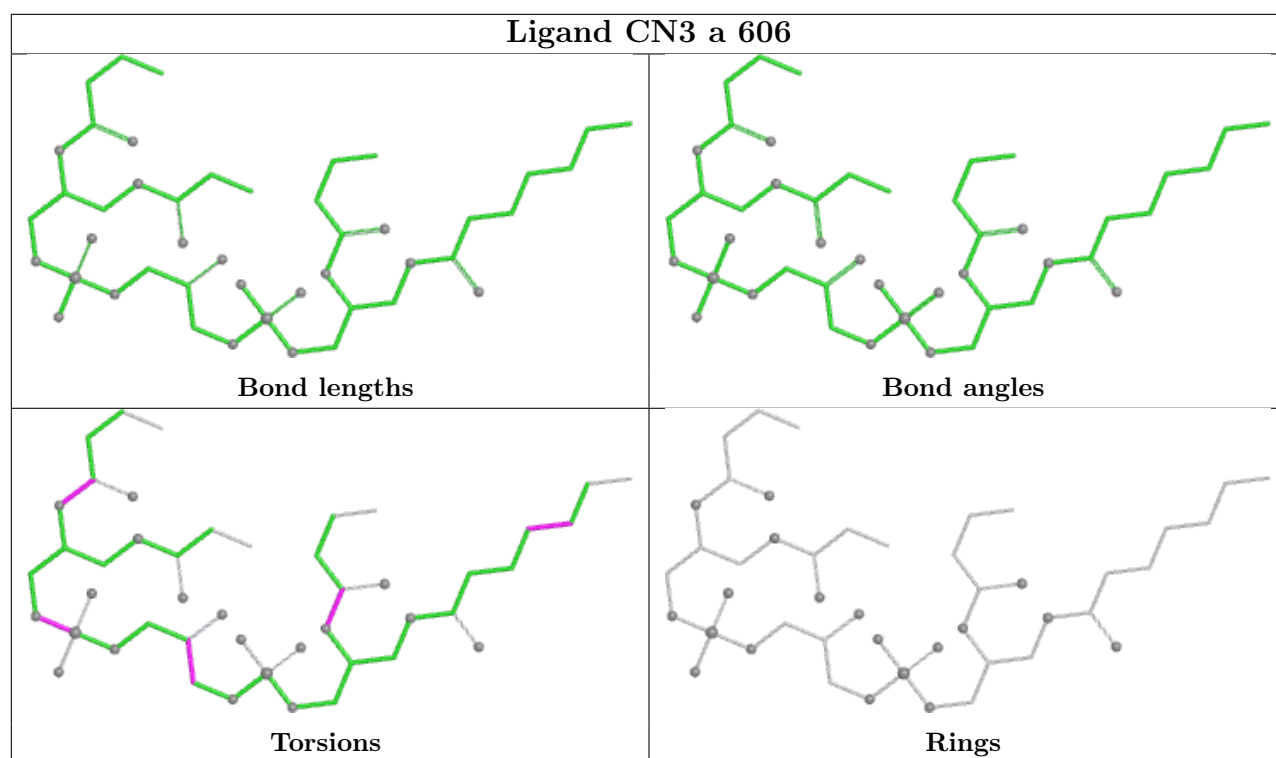


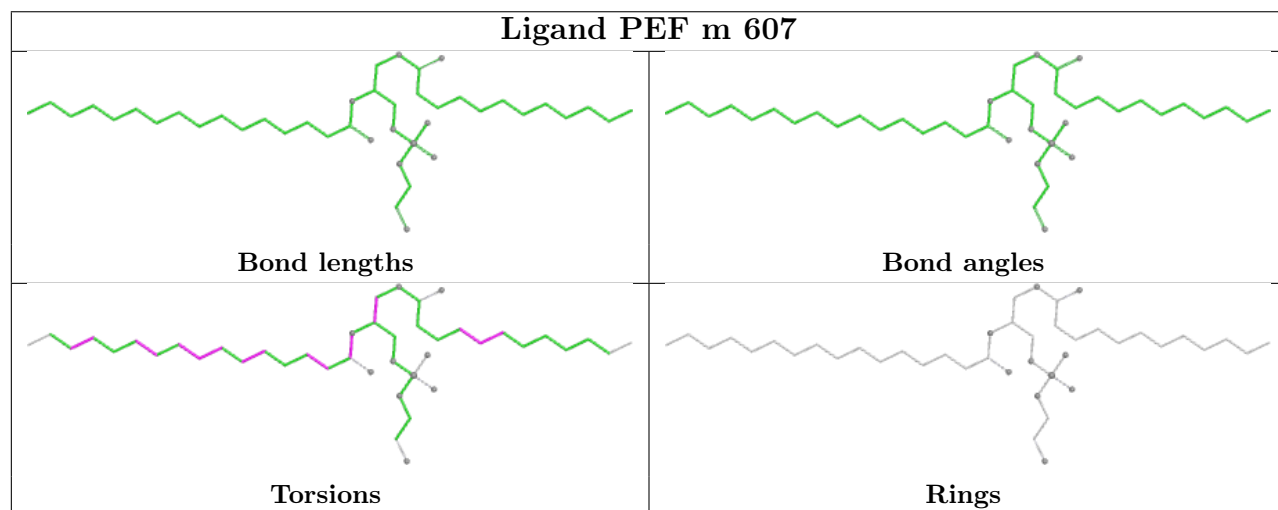
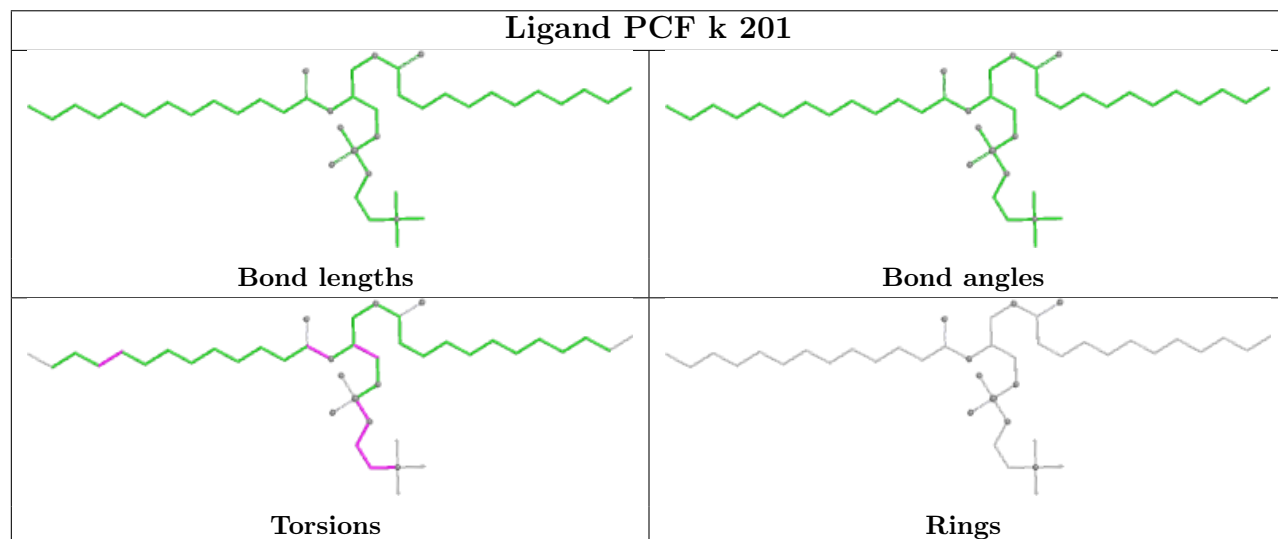
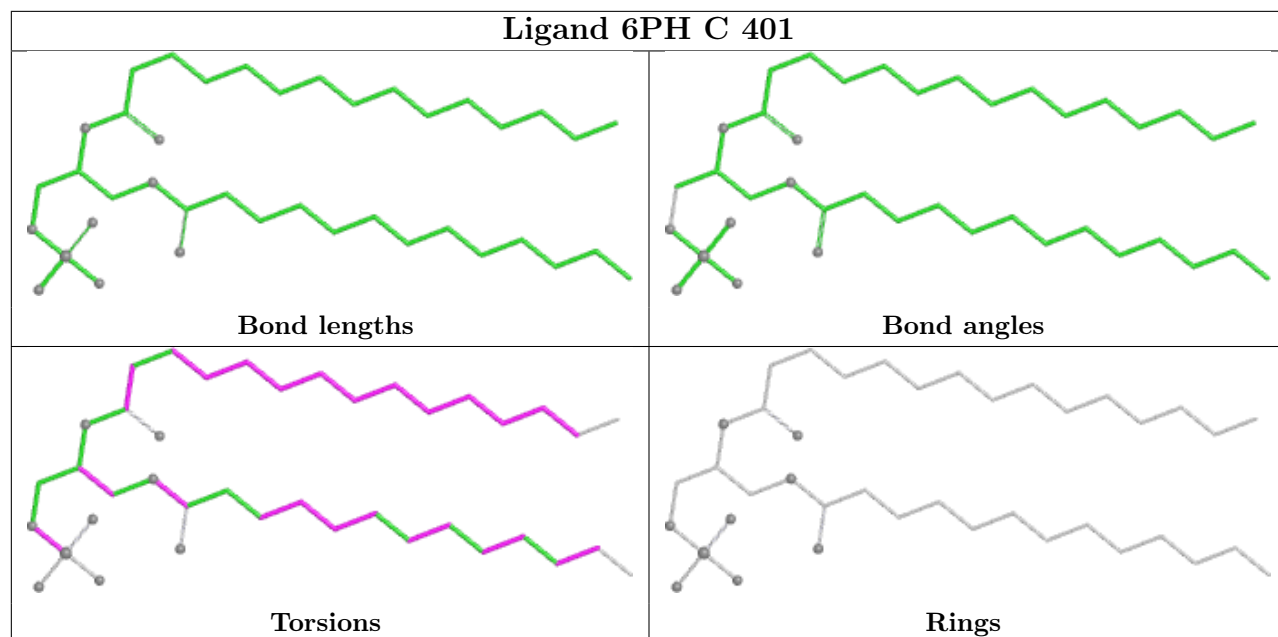


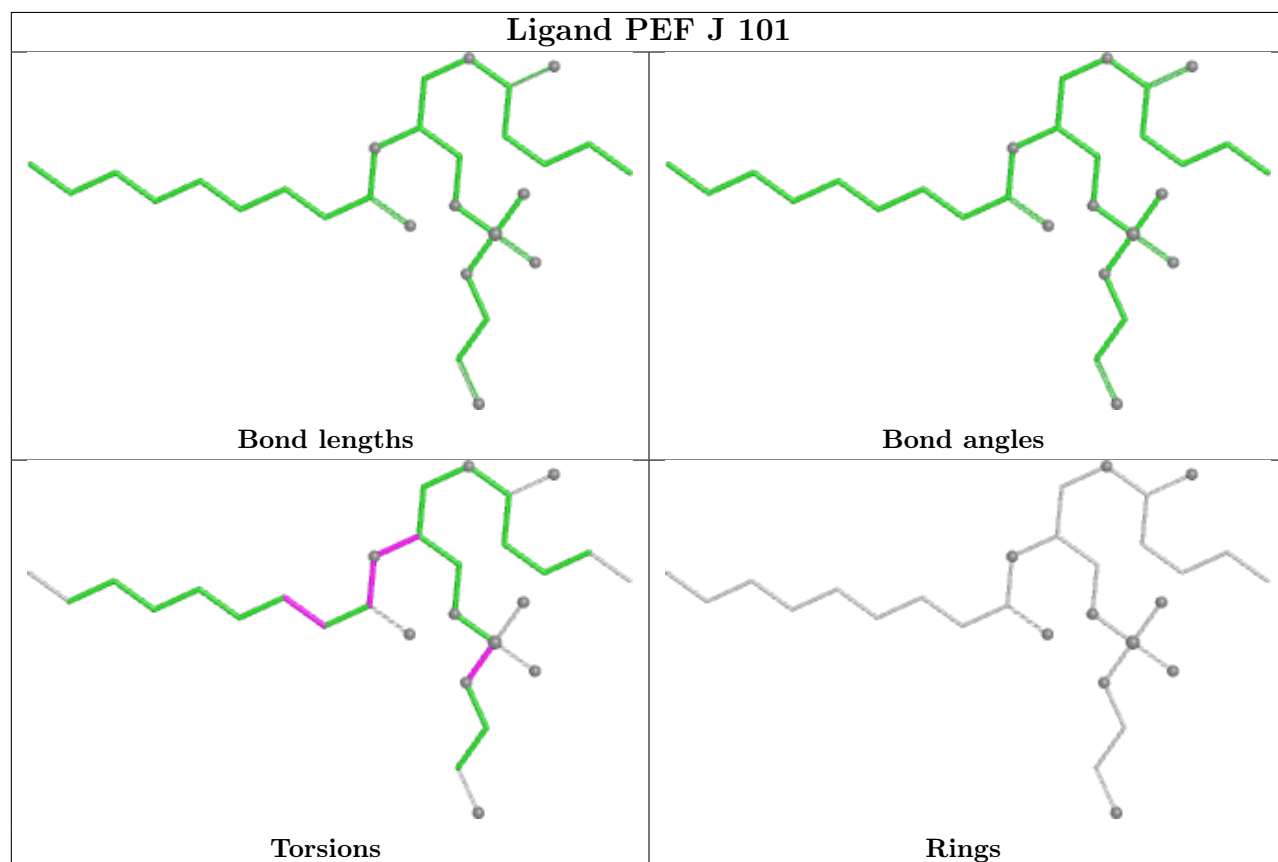
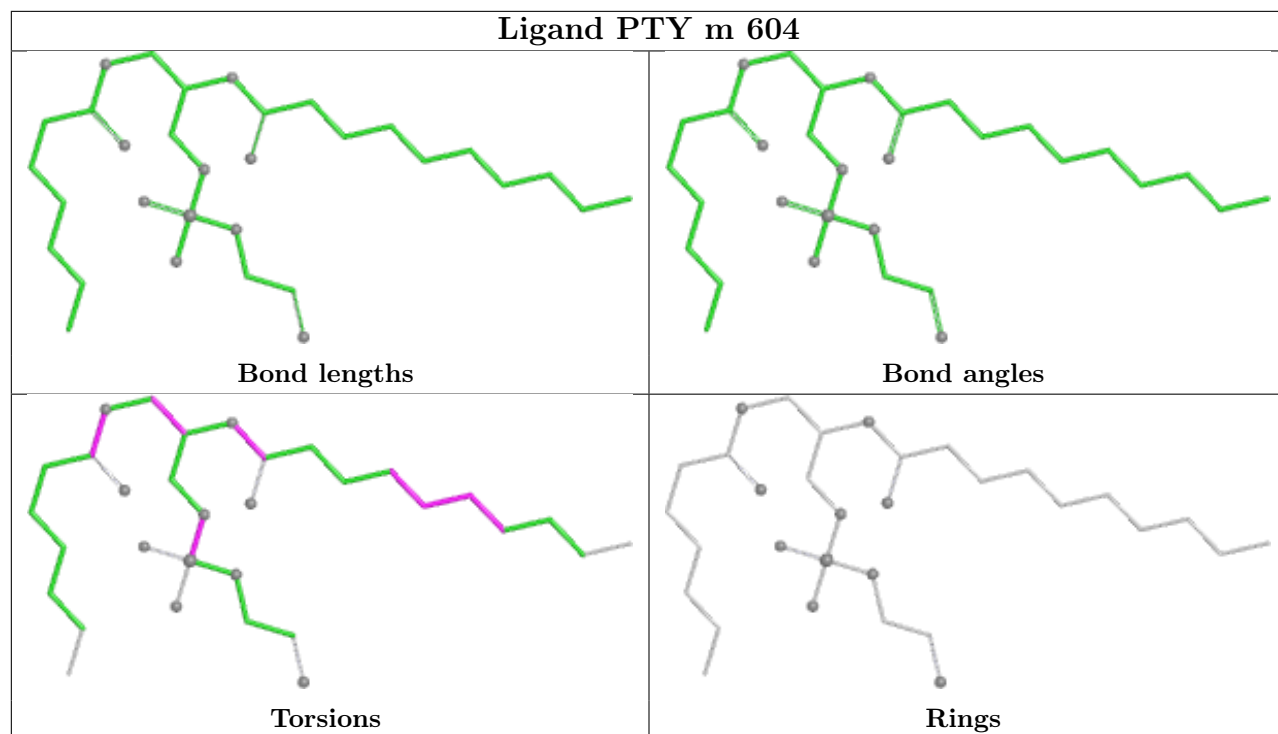


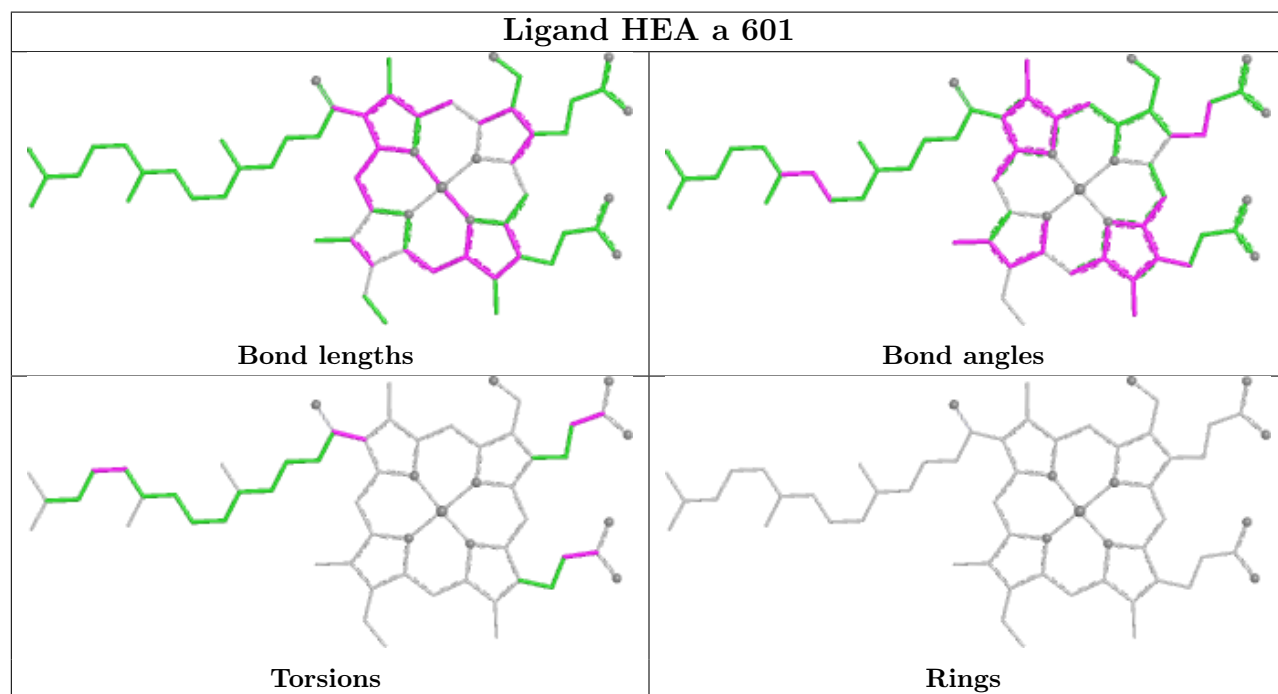
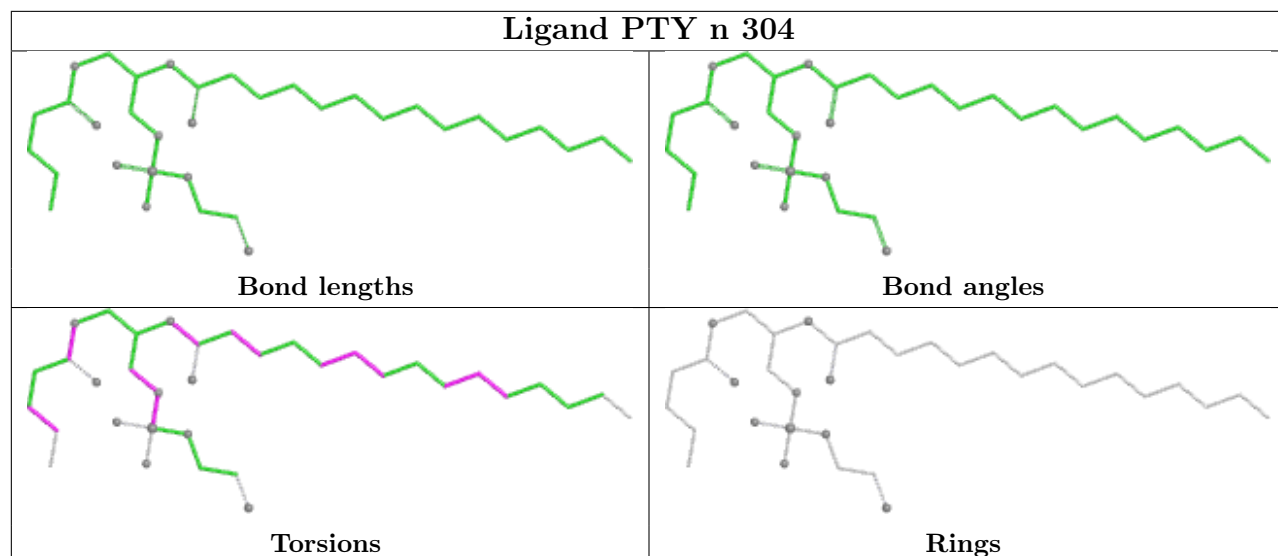




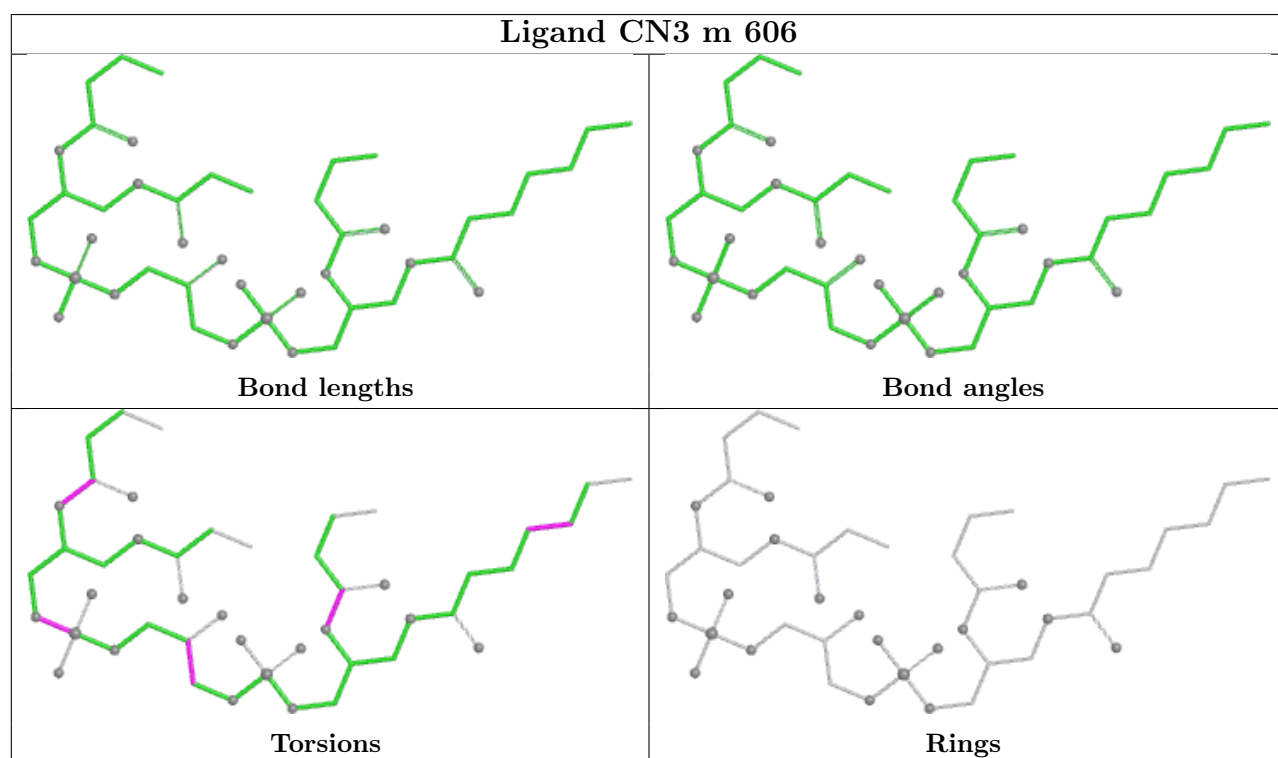
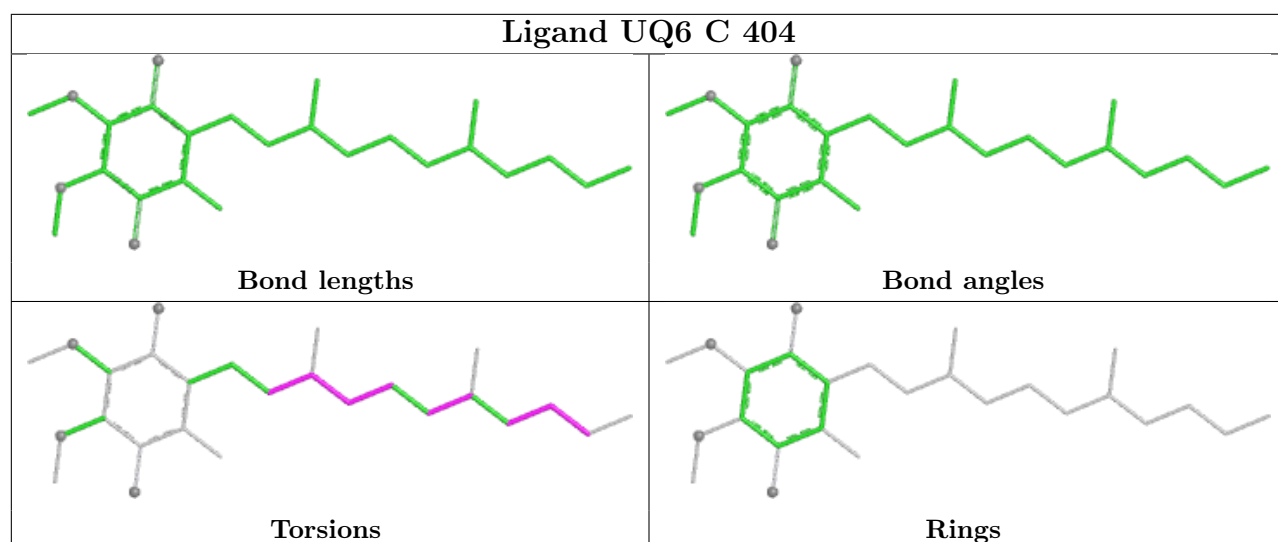


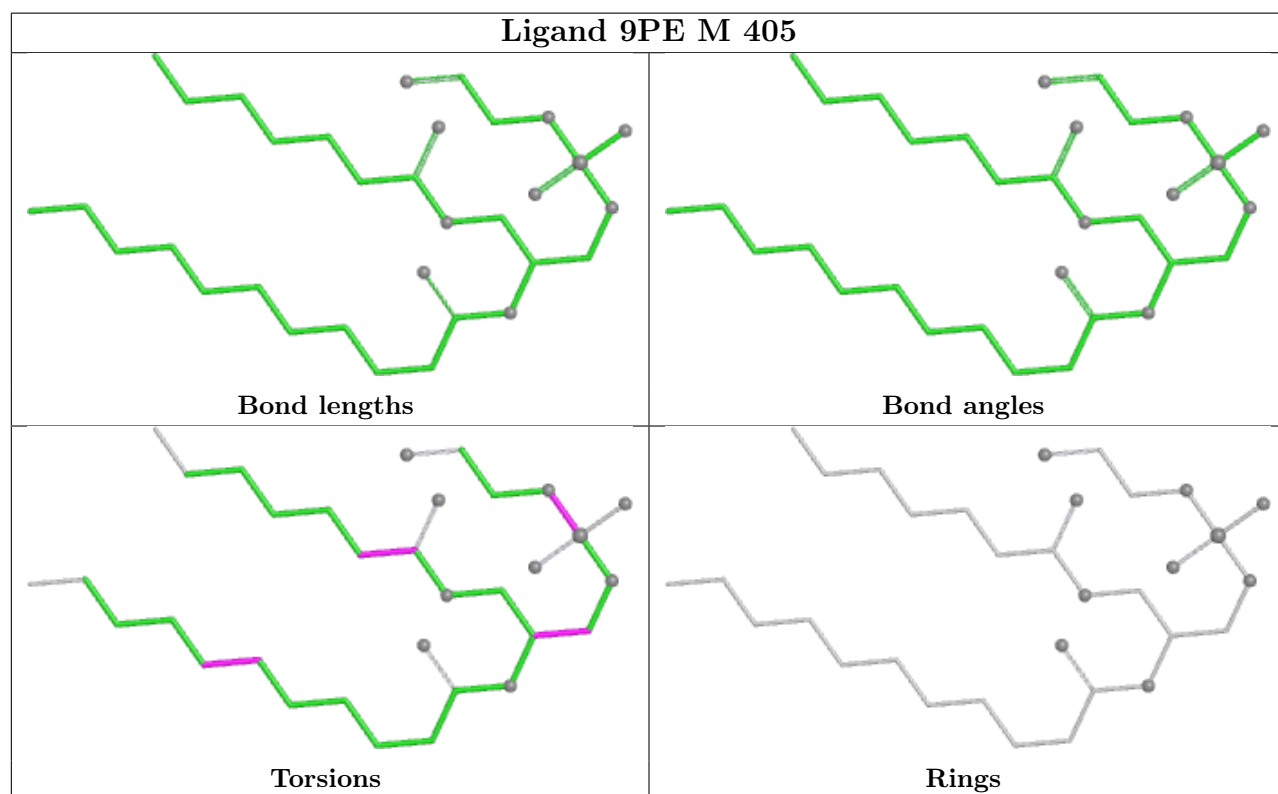
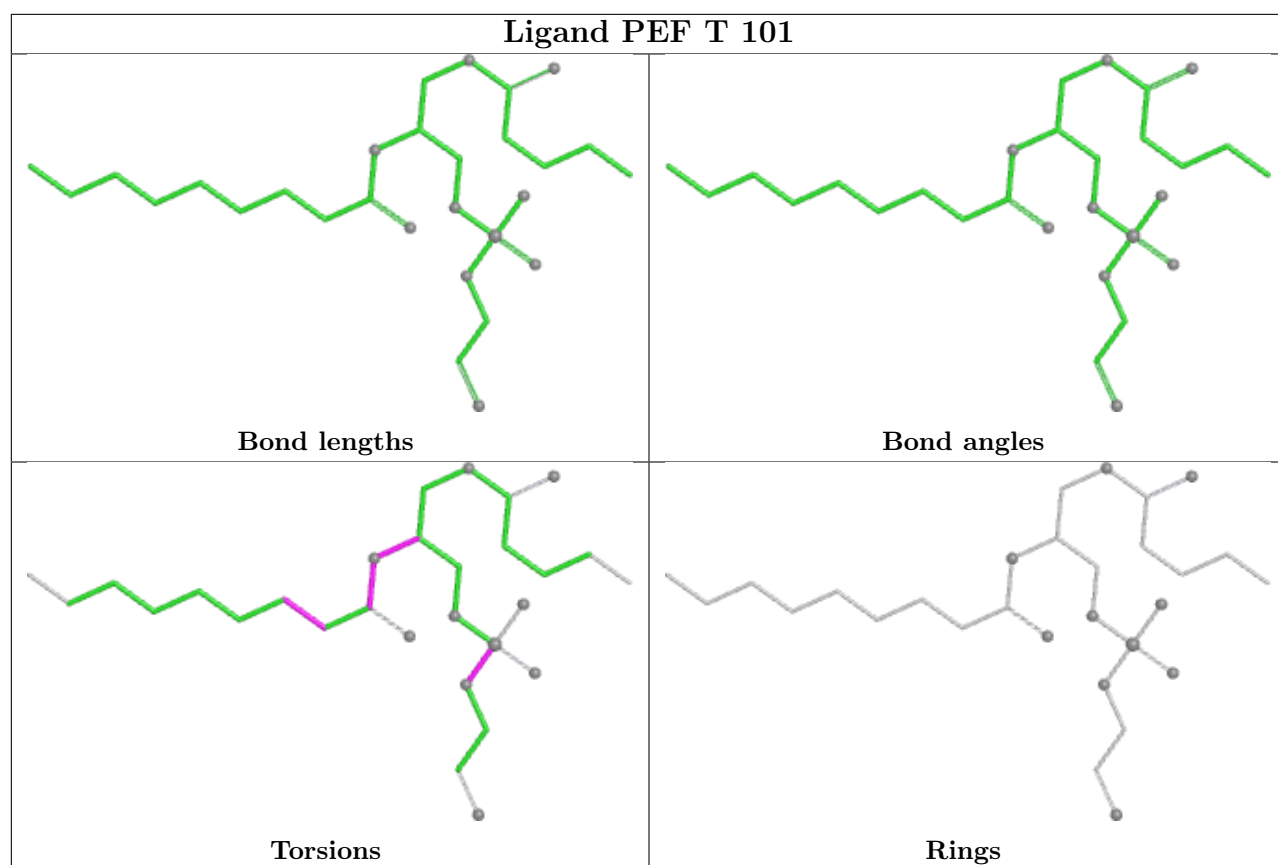


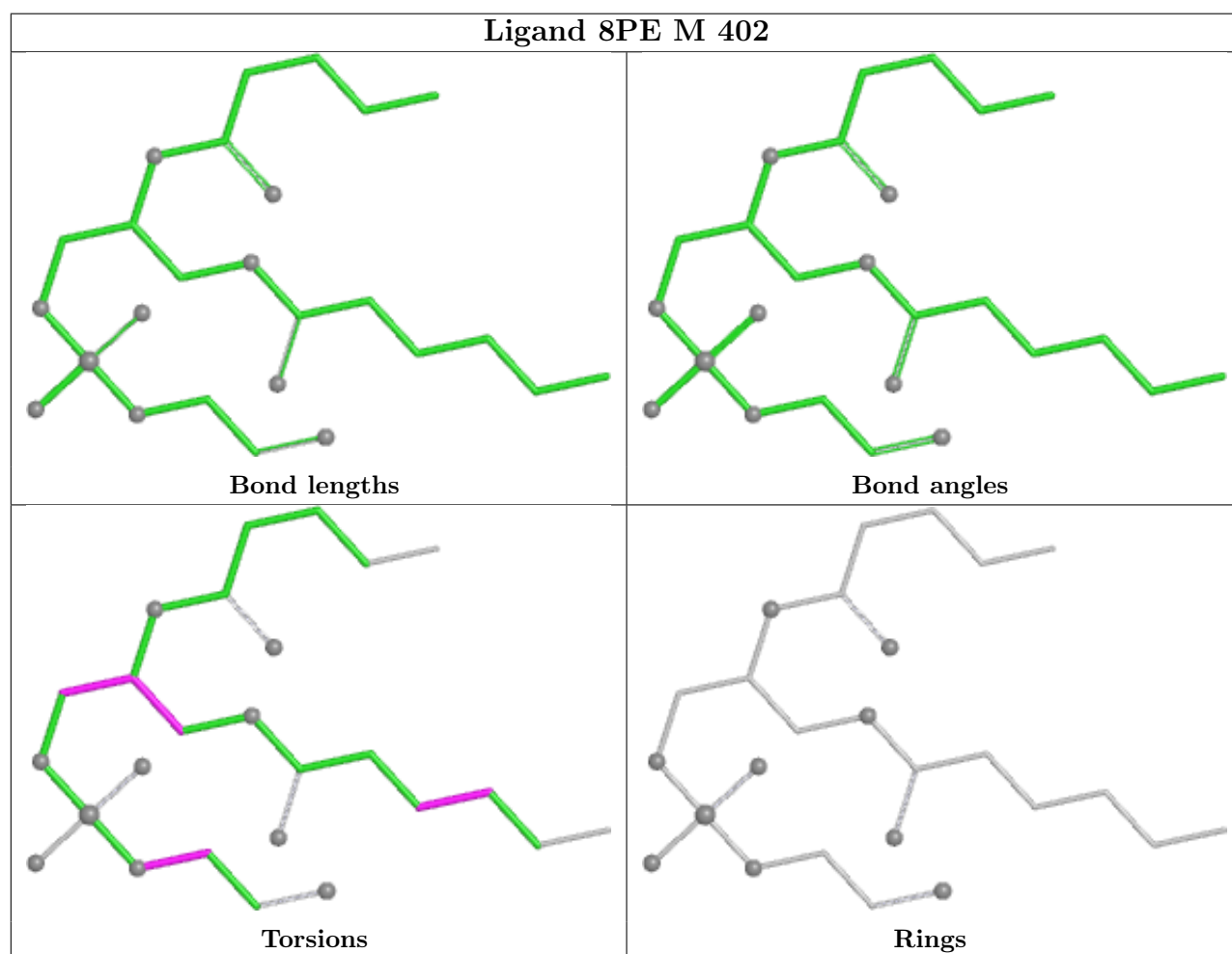
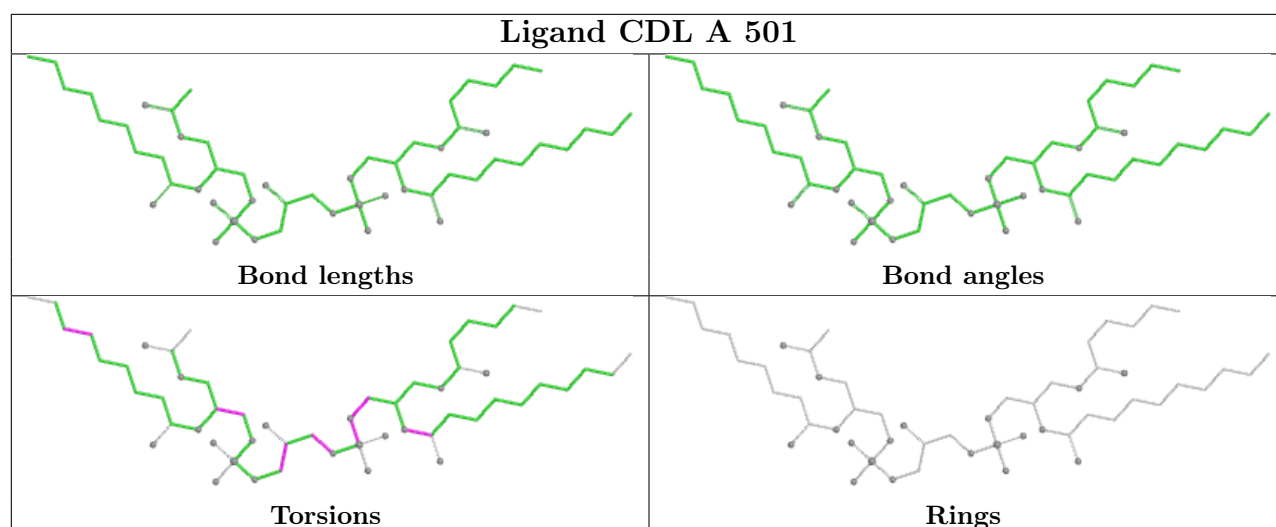


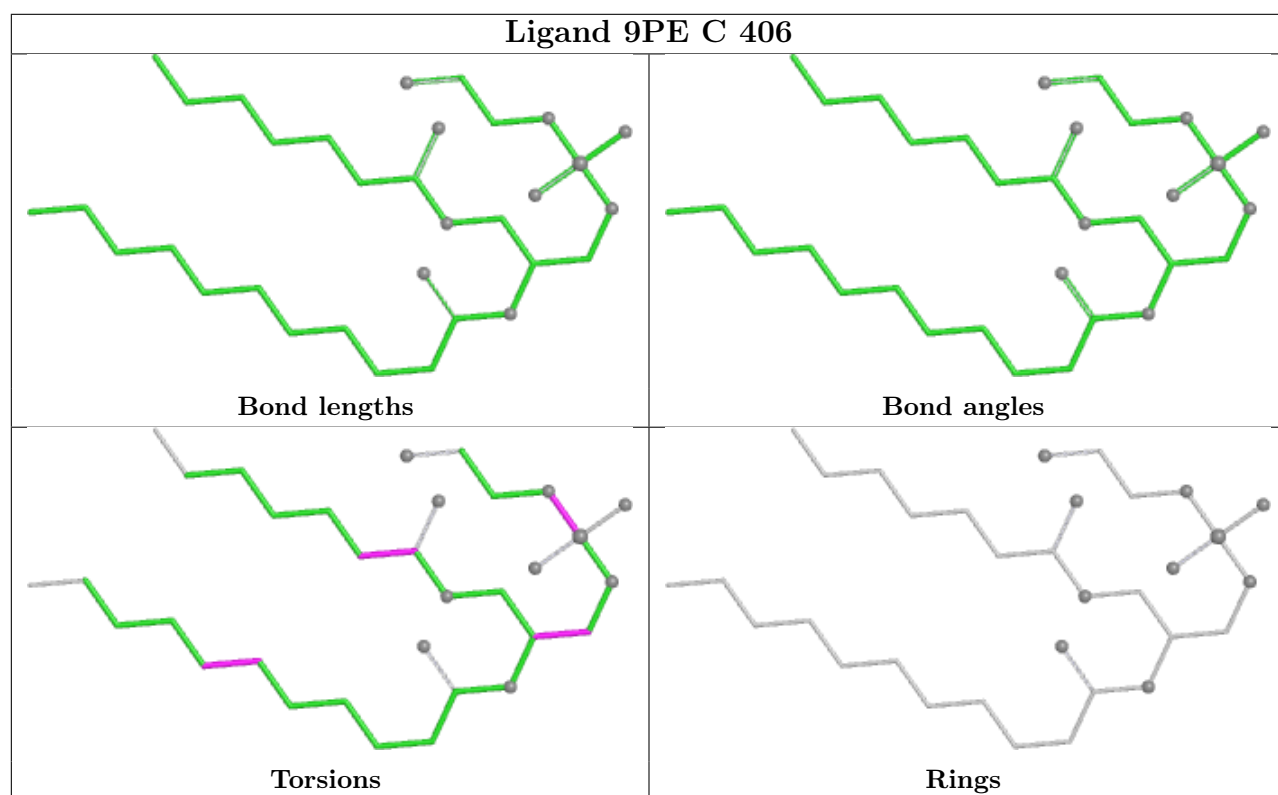
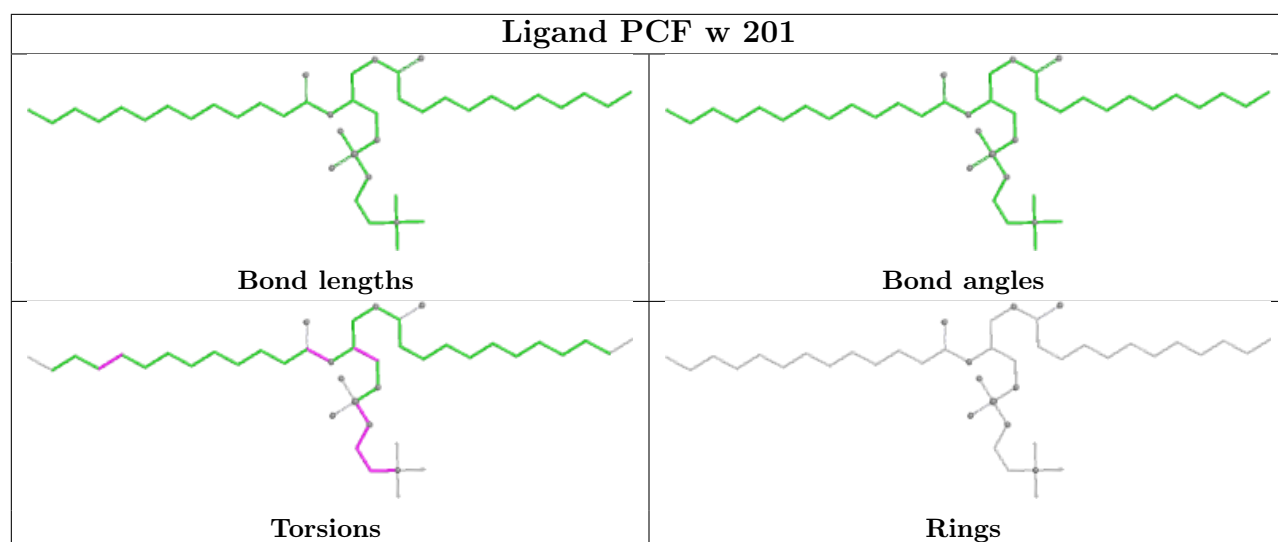


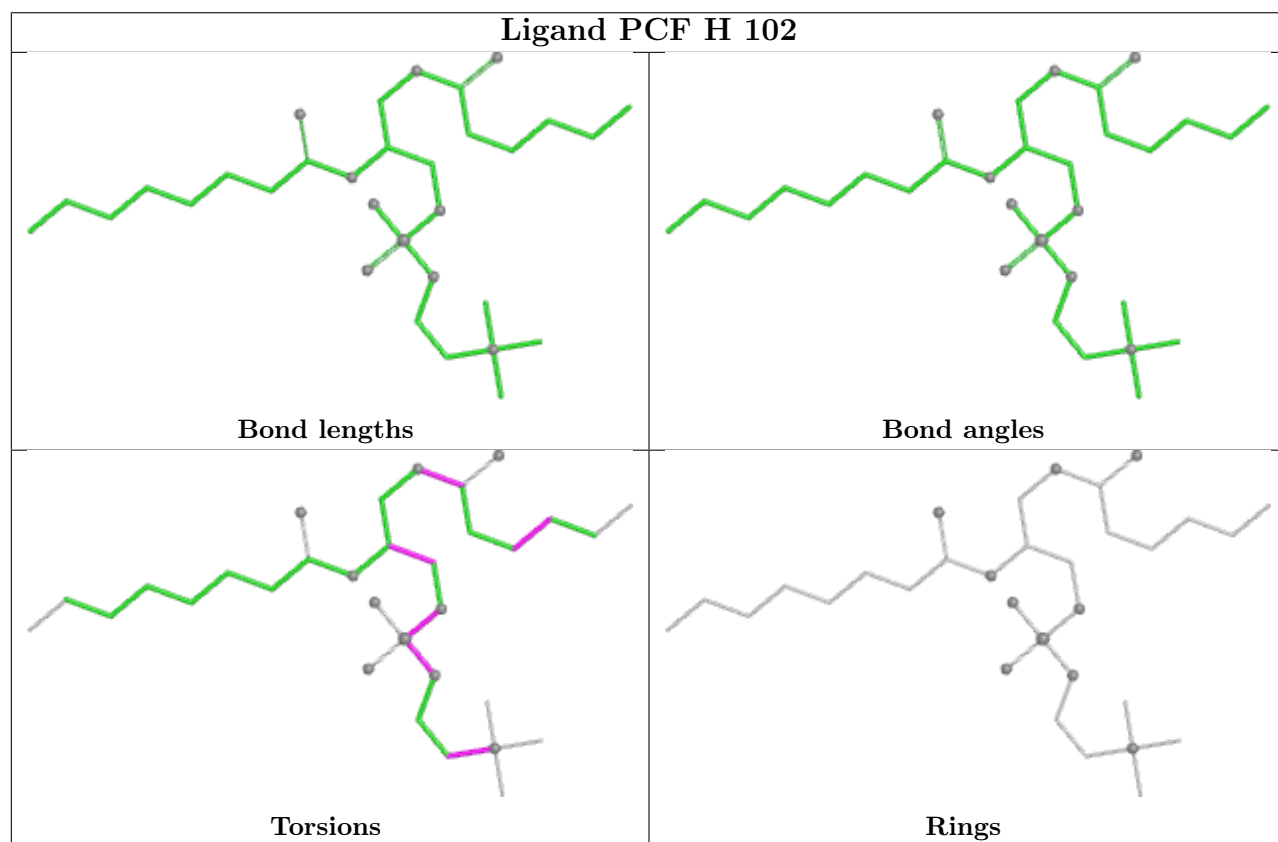
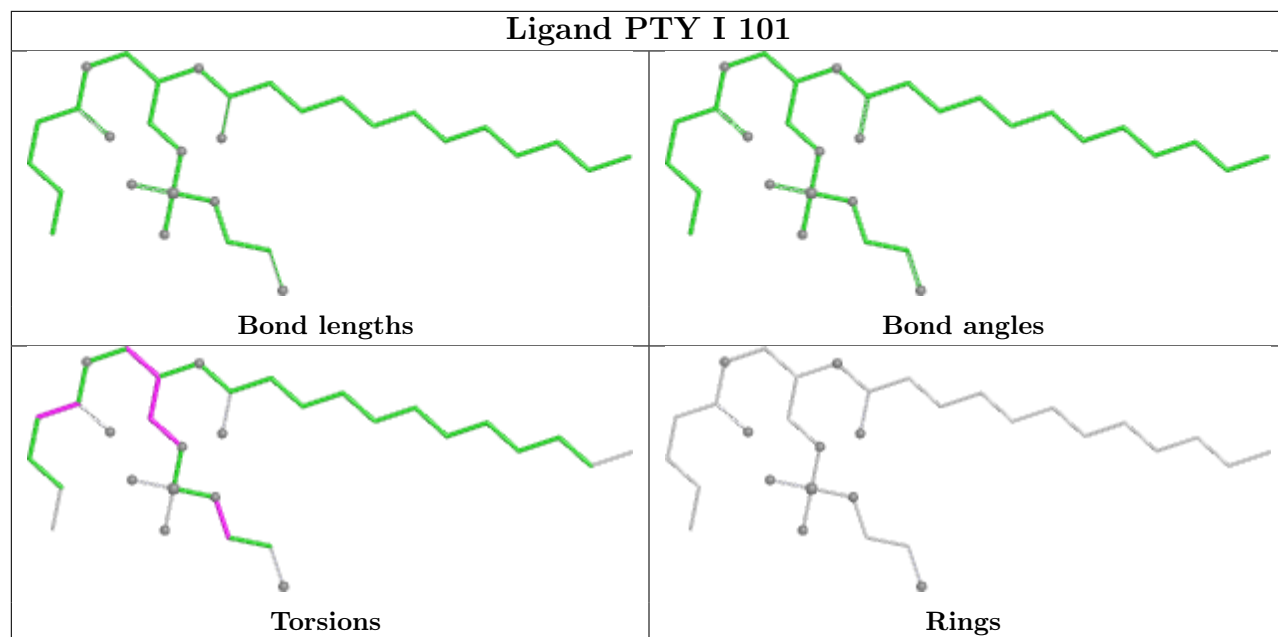


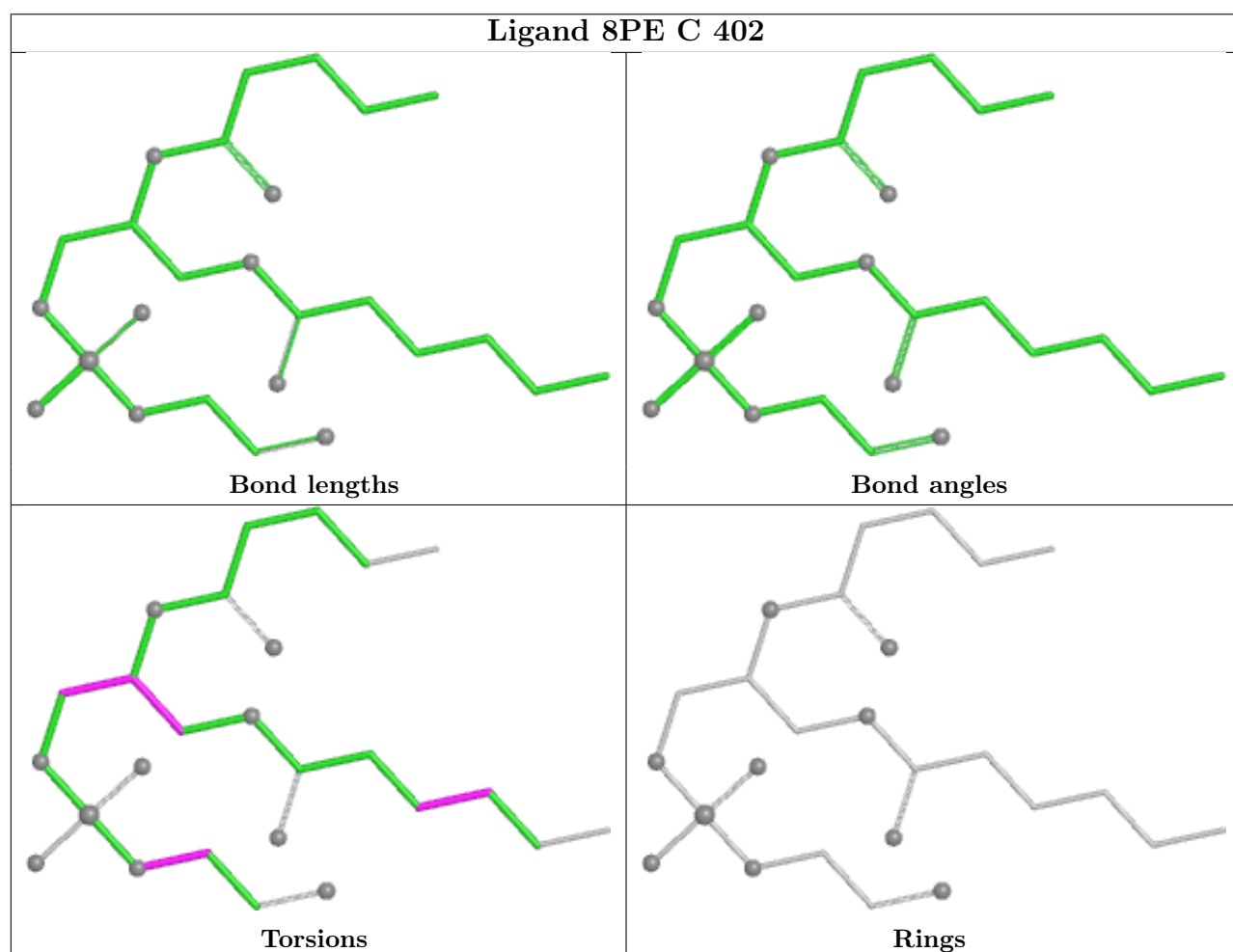
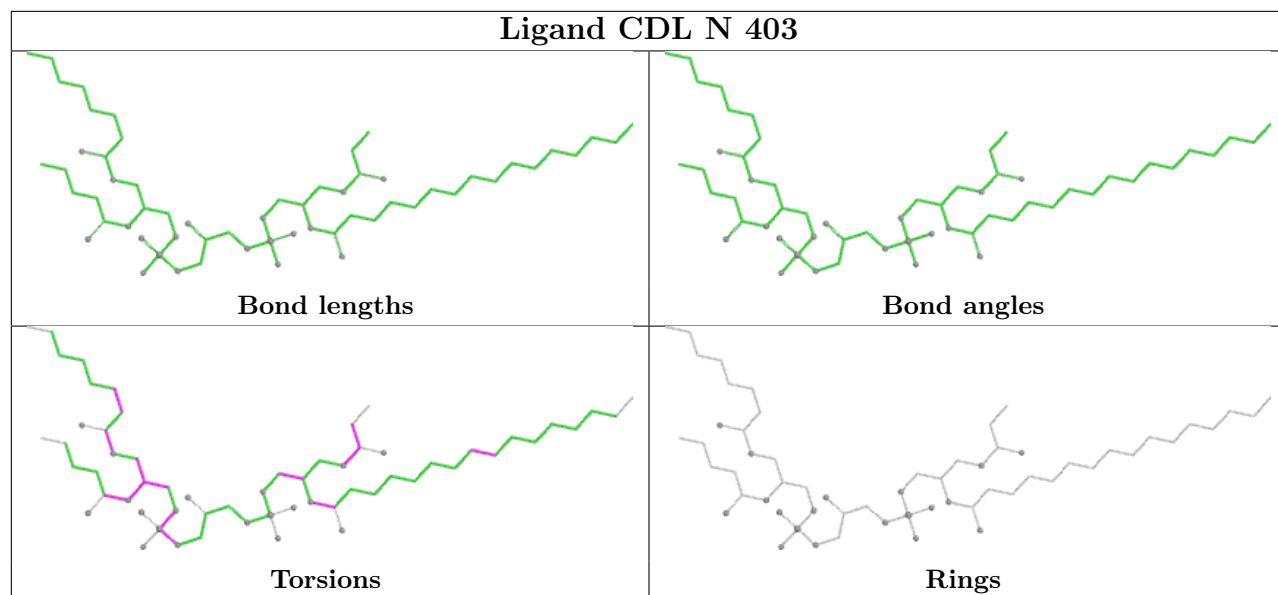


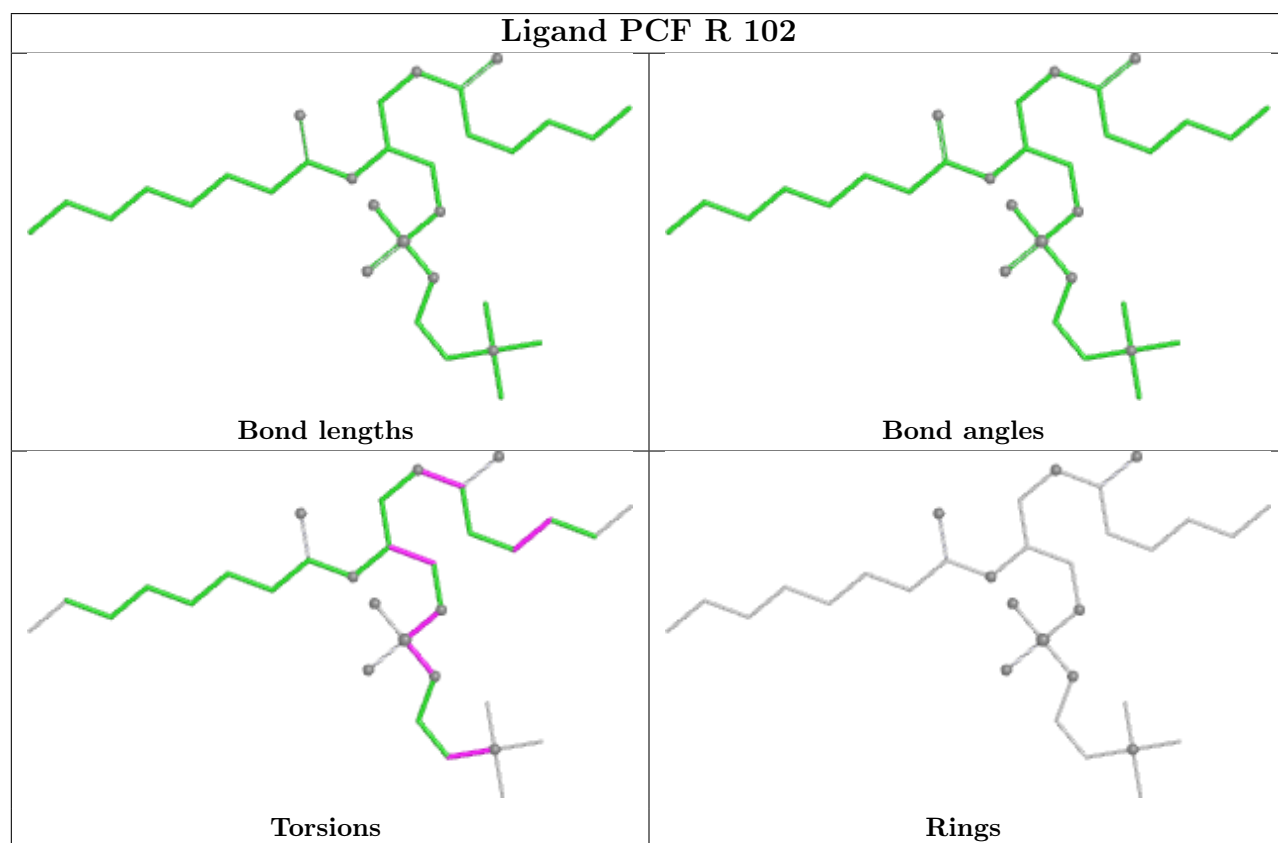
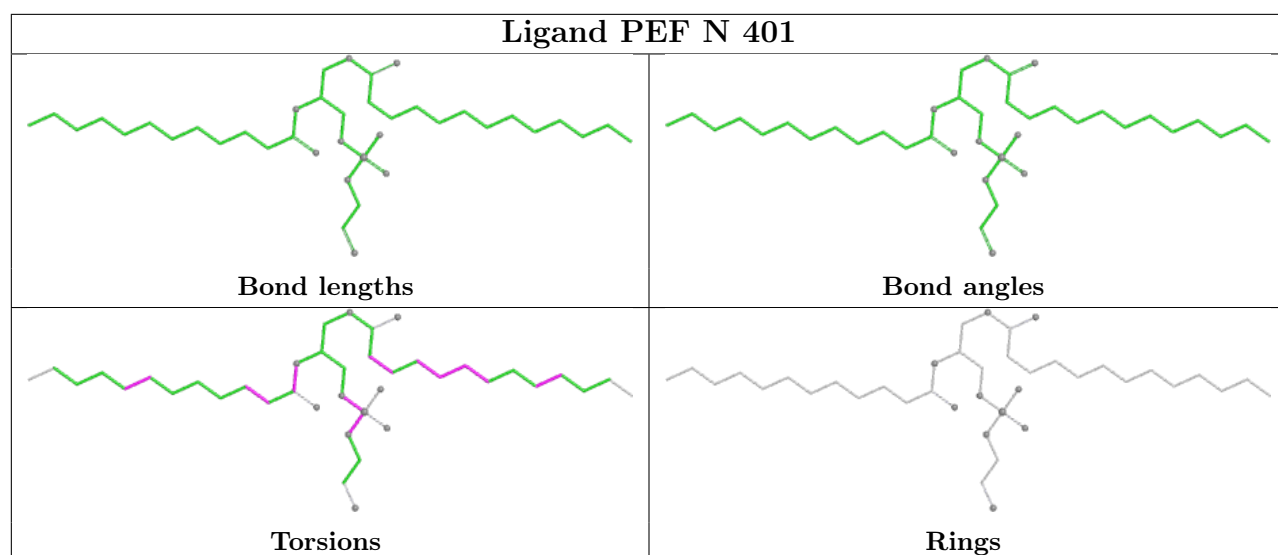


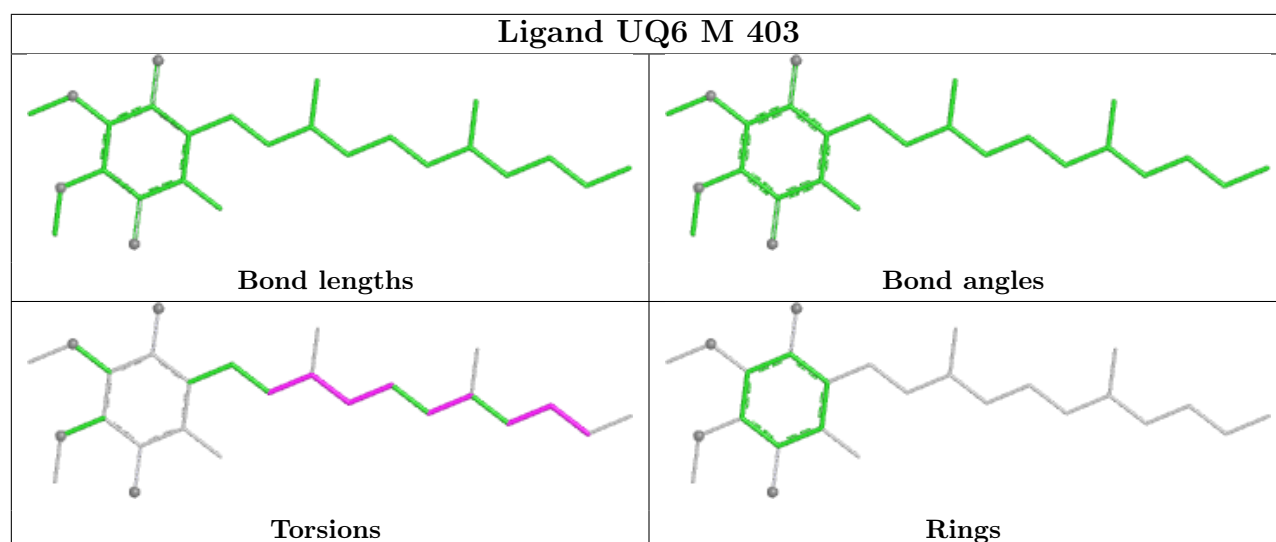












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



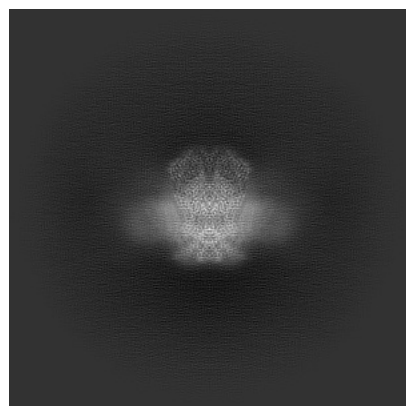
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44770. These allow visual inspection of the internal detail of the map and identification of artifacts.

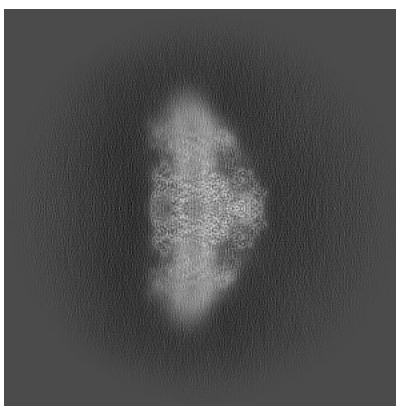
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

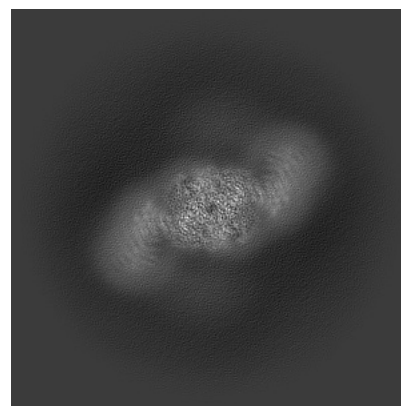
#### 6.1.1 Primary map



X

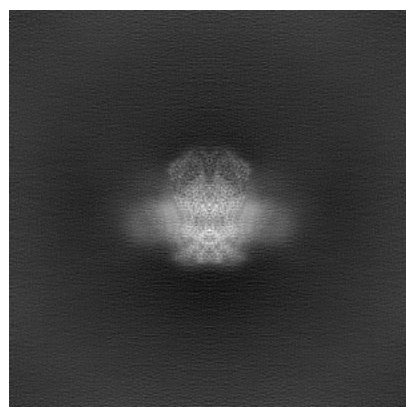


Y

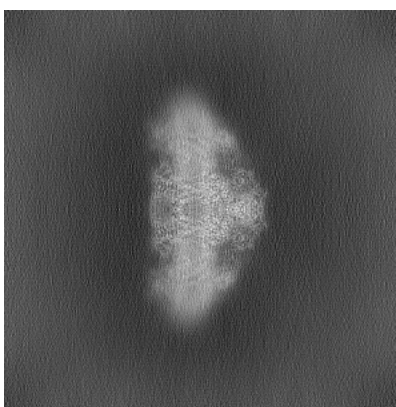


Z

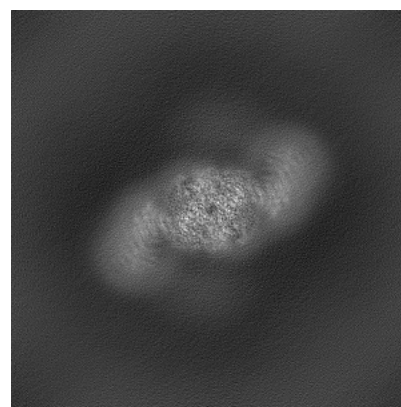
#### 6.1.2 Raw map



X



Y

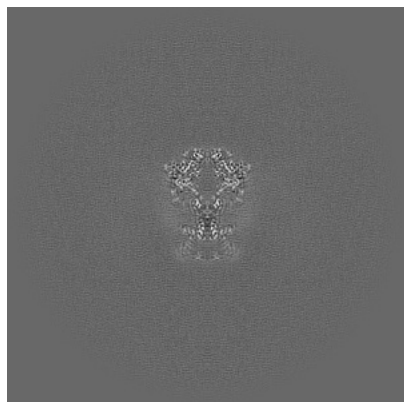


Z

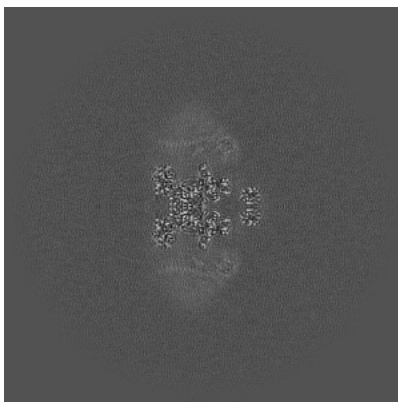
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

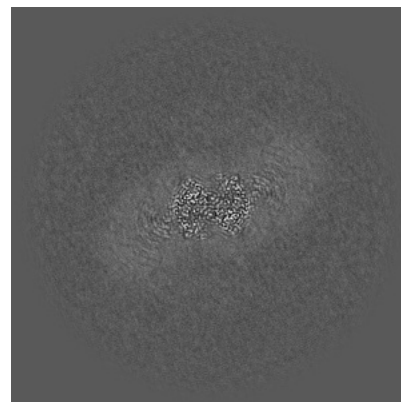
### 6.2.1 Primary map



X Index: 225

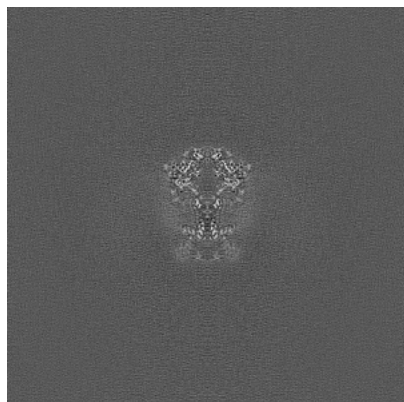


Y Index: 225

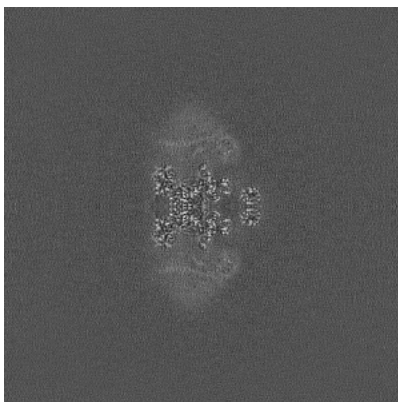


Z Index: 225

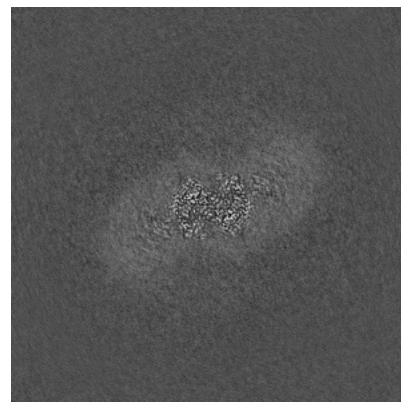
### 6.2.2 Raw map



X Index: 225



Y Index: 225

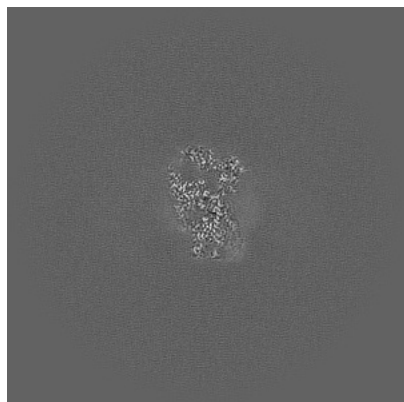


Z Index: 225

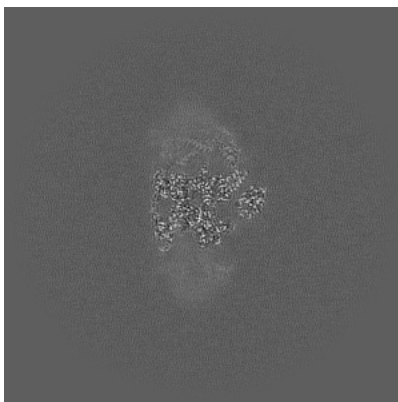
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

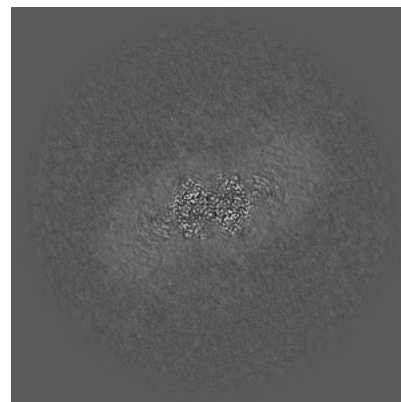
### 6.3.1 Primary map



X Index: 214

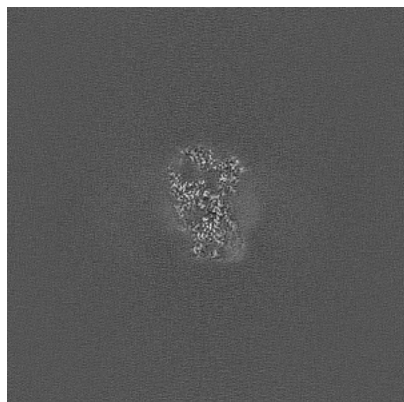


Y Index: 232

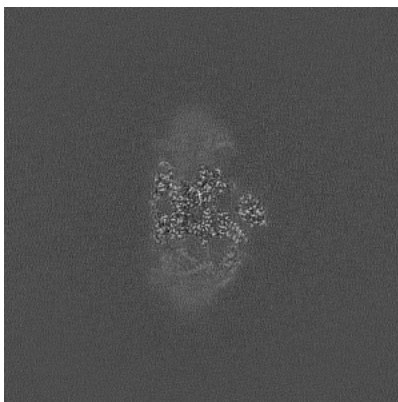


Z Index: 225

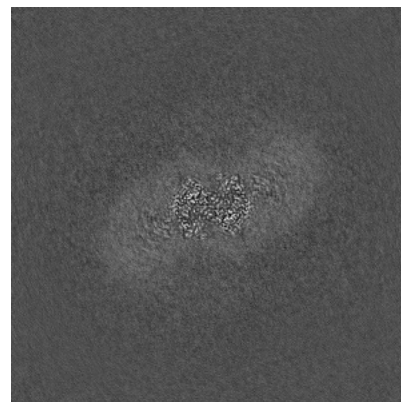
### 6.3.2 Raw map



X Index: 214



Y Index: 218



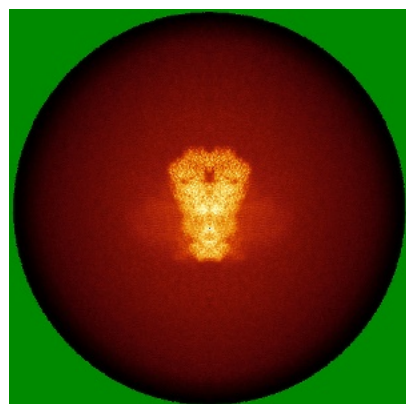
Z Index: 225

The images above show the largest variance slices of the map in three orthogonal directions.

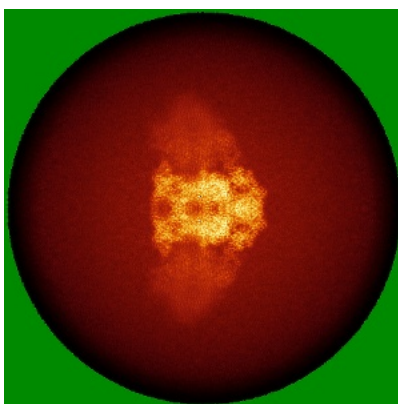


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

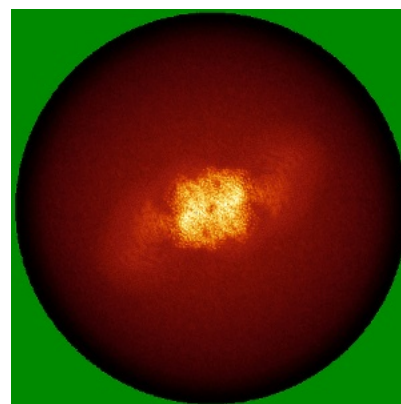
### 6.4.1 Primary map



X

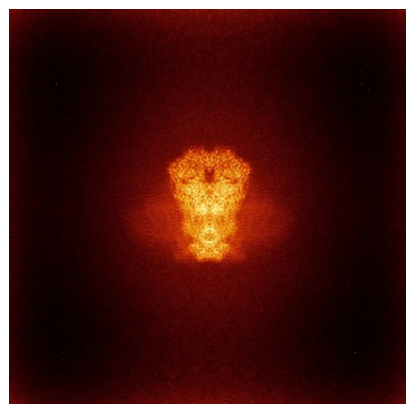


Y

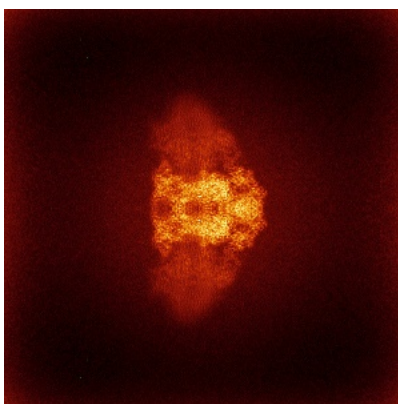


Z

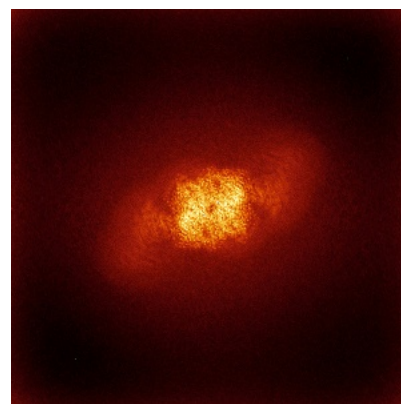
### 6.4.2 Raw map



X



Y

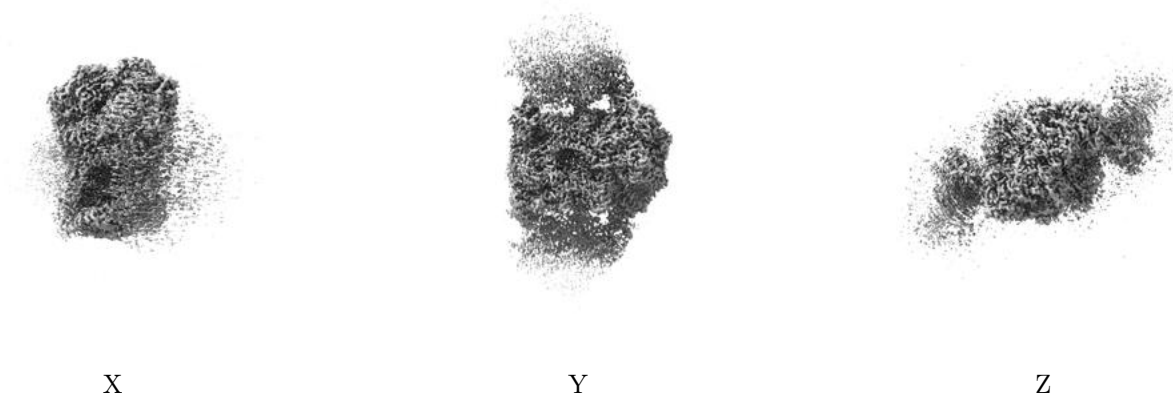


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

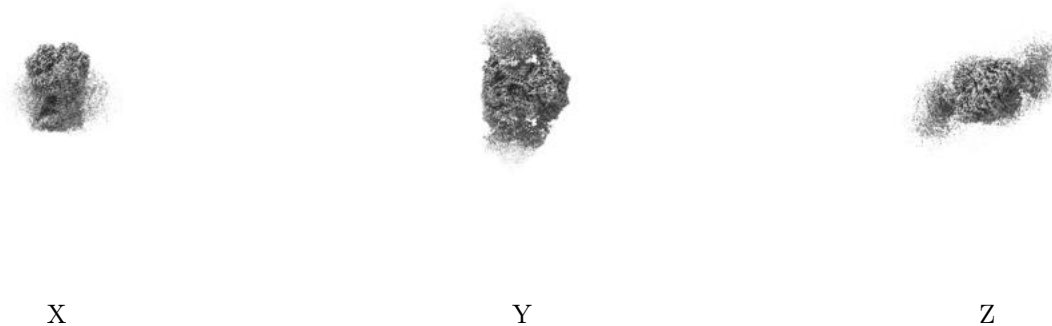
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

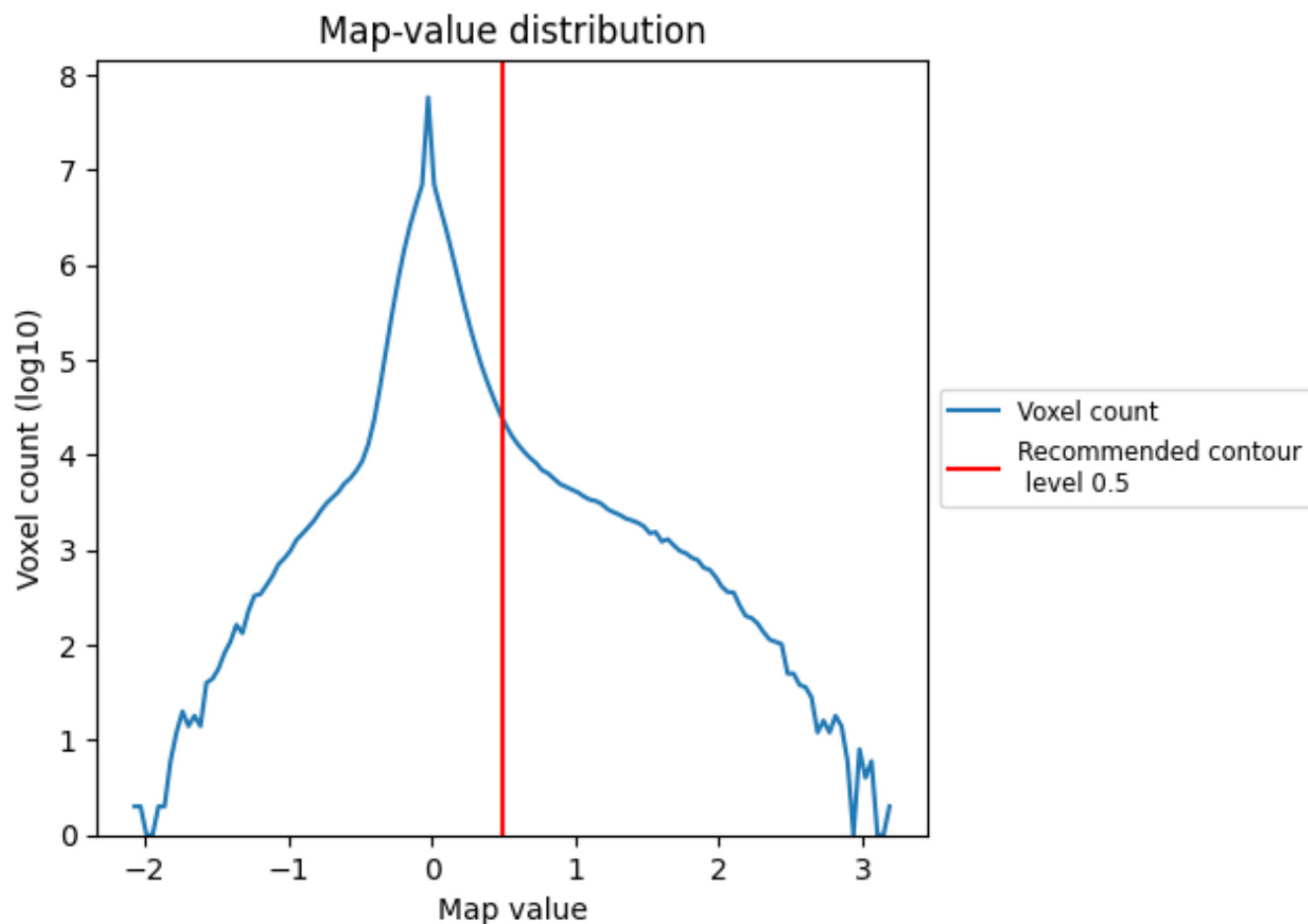
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

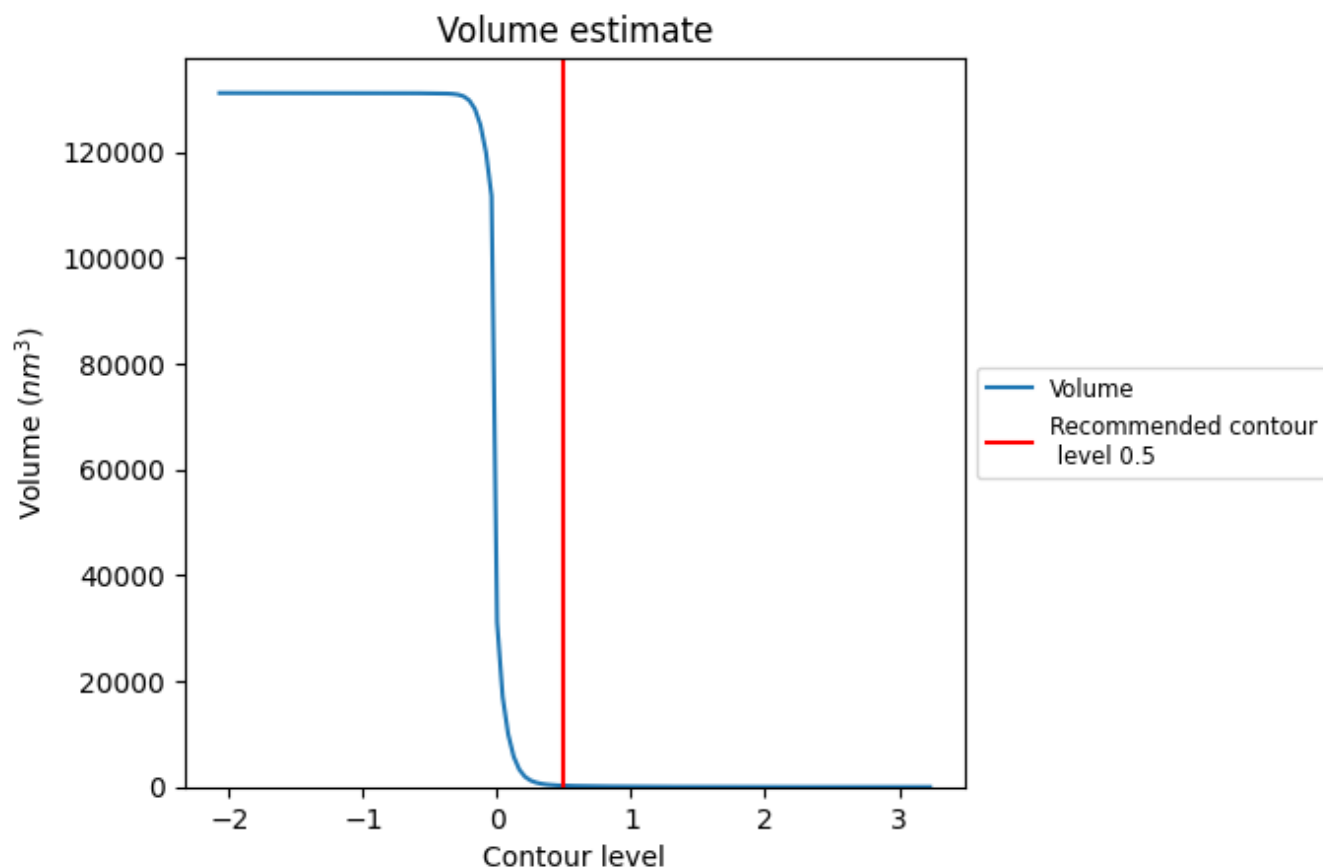
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

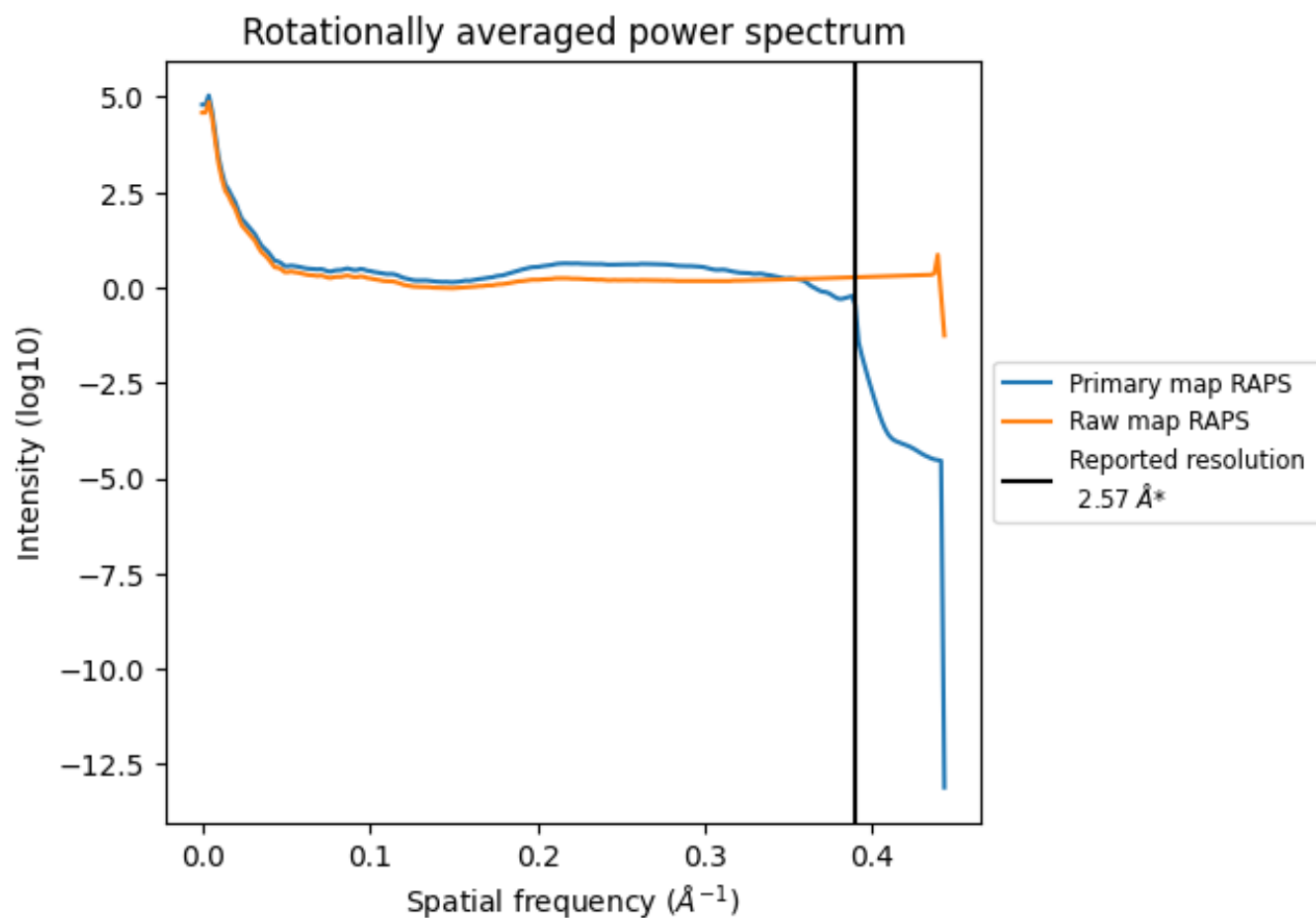
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 242  $\text{nm}^3$ ; this corresponds to an approximate mass of 219 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



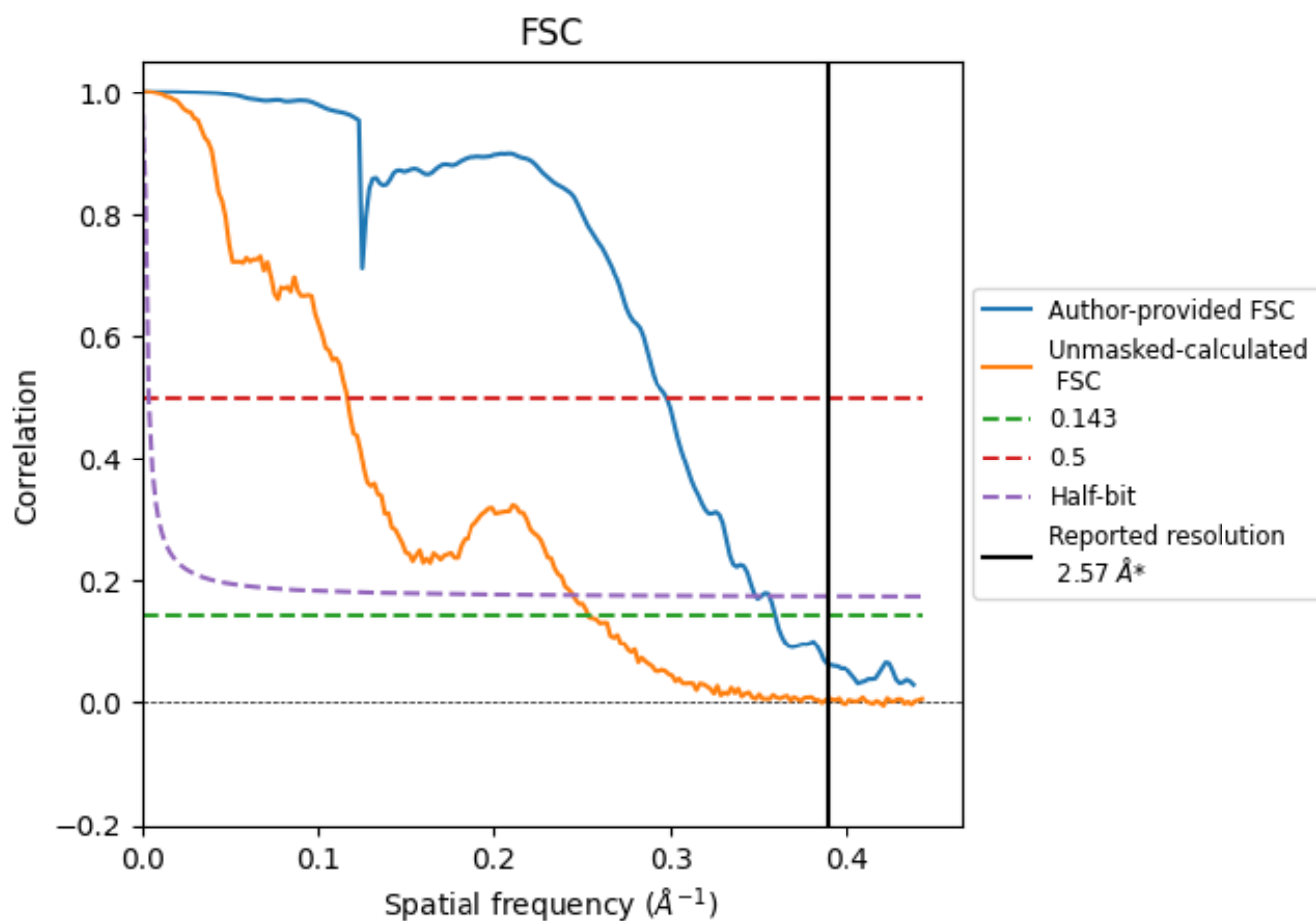
\*Reported resolution corresponds to spatial frequency of 0.389 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.389 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

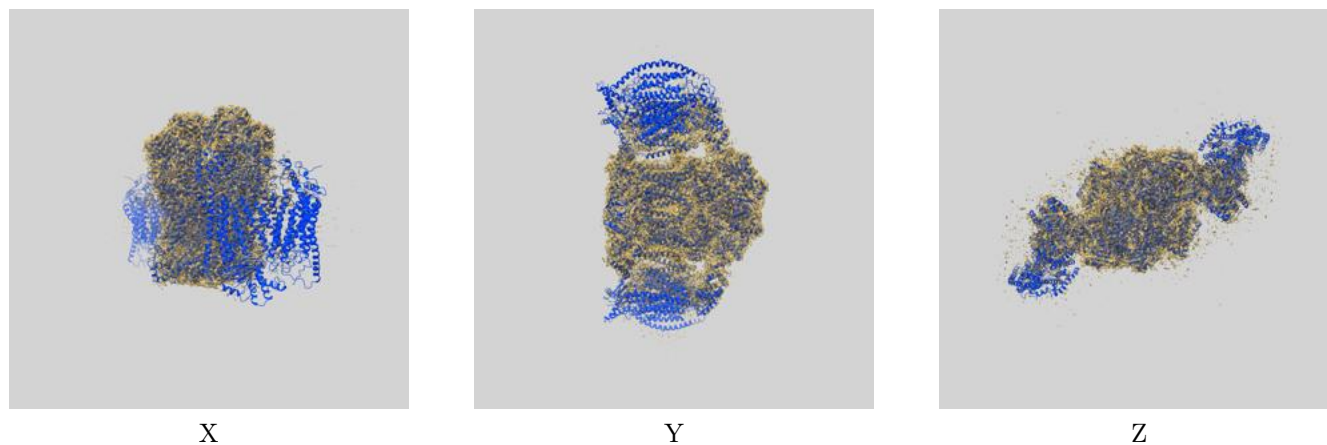
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.57	-	-
Author-provided FSC curve	2.78	3.36	2.87
Unmasked-calculated*	3.95	8.58	4.09

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.95 differs from the reported value 2.57 by more than 10 %

## 9 Map-model fit [i](#)

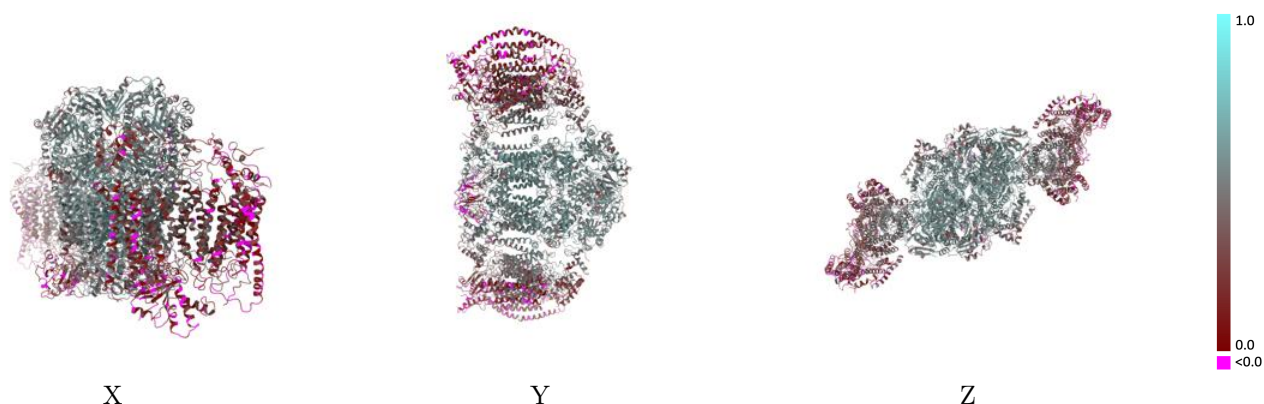
This section contains information regarding the fit between EMDB map EMD-44770 and PDB model 9BPB. Per-residue inclusion information can be found in section 3 on page 21.

### 9.1 Map-model overlay [i](#)



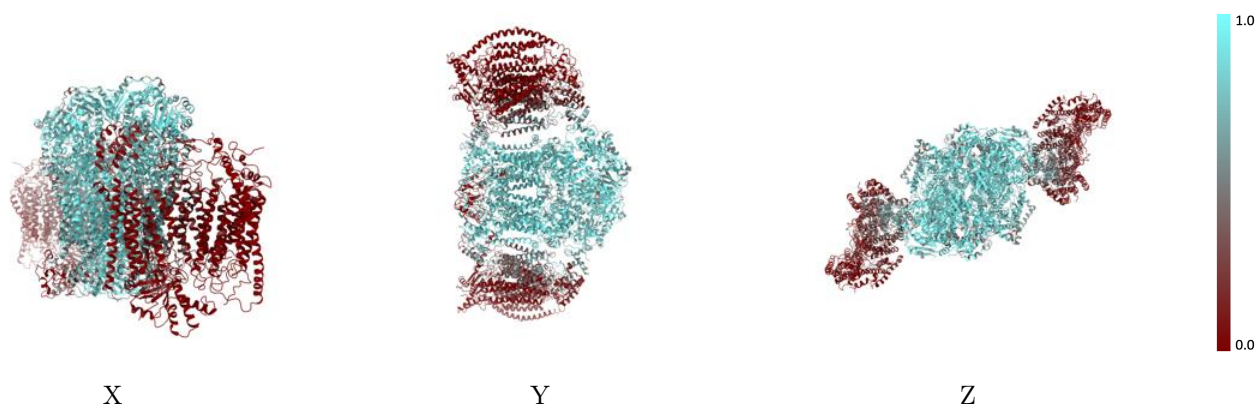
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



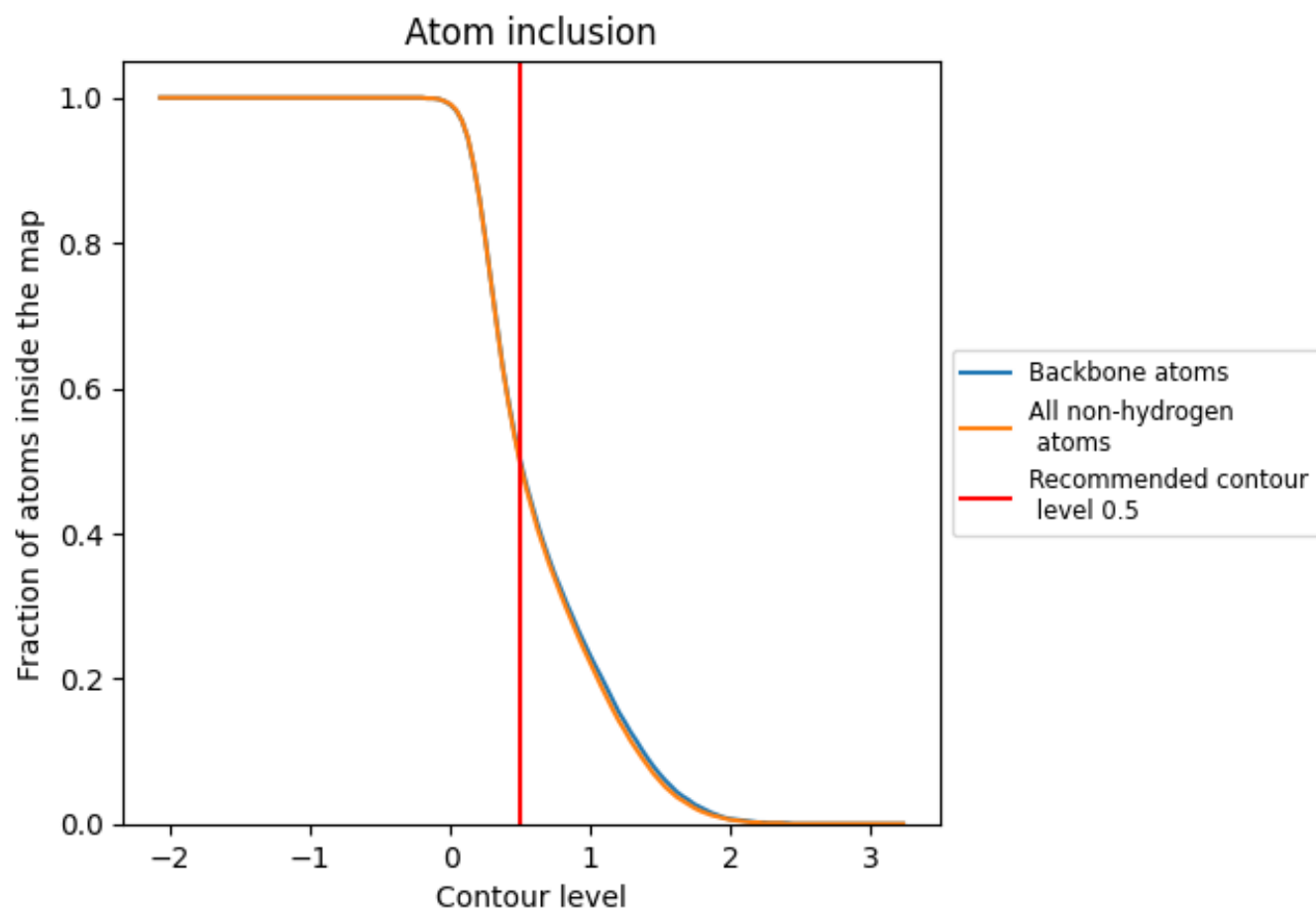
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

















The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4950	 0.4000
A	 0.8630	 0.5680
B	 0.8230	 0.5170
C	 0.8730	 0.5730
D	 0.8460	 0.5330
E	 0.3640	 0.2620
F	 0.5450	 0.3850
G	 0.7980	 0.5160
H	 0.7770	 0.5180
I	 0.8170	 0.5720
J	 0.5880	 0.4820
K	 0.8640	 0.5700
L	 0.8160	 0.5160
M	 0.8840	 0.5790
N	 0.8490	 0.5420
O	 0.3690	 0.2690
P	 0.5410	 0.3910
Q	 0.8220	 0.5310
R	 0.7870	 0.5240
S	 0.8250	 0.5750
T	 0.6020	 0.4800
a	 0.2470	 0.3670
b	 0.1120	 0.2250
c	 0.0190	 0.1780
d	 0.1220	 0.2240
e	 0.4680	 0.3950
f	 0.2000	 0.2730
g	 0.0090	 0.1430
i	 0.0710	 0.1490
j	 0.0050	 0.1020
k	 0.0030	 0.0890
l	 0.1890	 0.3040
m	 0.2580	 0.3800
n	 0.1080	 0.2310
o	 0.0190	 0.1870



*Continued on next page...*

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Chain	Atom inclusion	Q-score
p	 0.1300	 0.2430
q	 0.4700	 0.4030
r	 0.2250	 0.2850
s	 0.0070	 0.1450
u	 0.0460	 0.1510
v	 0.0050	 0.1070
w	 0.0020	 0.0900
x	 0.2140	 0.3120