



## Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 02:58 AM EST

PDB ID : 7RH7  
EMDB ID : EMD-24457  
Title : Mycobacterial CIII2CIV2 supercomplex, Telacebec (Q203) bound  
Authors : Di Trani, J.M.; Yanofsky, D.J.; Rubinstein, J.L.  
Deposited on : 2021-07-16  
Resolution : 3.00 Å(reported)

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.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
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) : 2.39

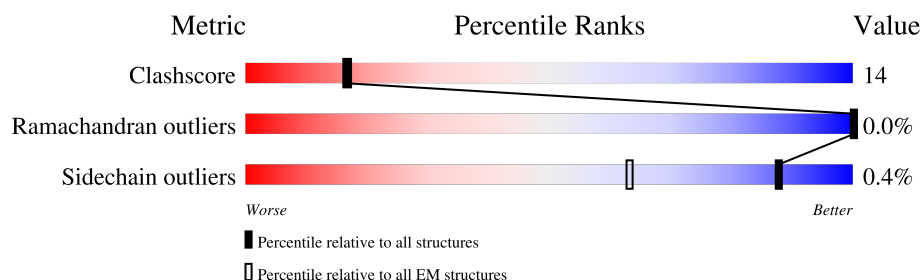
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 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	W	159	<div> <div>87%</div> <div>80%19%.</div> </div>
1	c	159	<div> <div>88%</div> <div>99%.</div> </div>
2	K	312	<div> <div>49%</div> <div>69%31%</div> </div>
2	Q	312	<div> <div>53%</div> <div>71%29%</div> </div>
3	L	552	<div> <div>9%</div> <div>66%34%</div> </div>
3	R	552	<div> <div>9%</div> <div>66%34%</div> </div>
4	S	203	<div> <div>32%</div> <div>80%20%</div> </div>
4	X	203	<div> <div>34%</div> <div>75%24%.</div> </div>

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Mol	Chain	Length	Quality of chain
5	T	139	
5	Z	139	
6	U	79	
6	a	79	
7	V	145	
7	b	145	
8	J	100	
8	P	100	
9	D	216	
9	G	216	
10	I	223	
10	O	223	
11	E	535	
11	F	535	
12	M	382	
12	Y	382	

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
17	CDL	T	202	-	-	X	-
17	CDL	X	302	-	-	X	-
17	CDL	Z	202	-	-	X	-
24	FES	Y	501	-	-	X	-

## 2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 95515 atoms, of which 46689 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 LpqE protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	W	158	Total	C	H	N	O	S	0	0
			2259	708	1110	192	248	1		
1	c	158	Total	C	H	N	O	S	0	0
			2259	708	1110	192	248	1		

- Molecule 2 is a protein called Cytochrome aa3 subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	Q	312	Total	C	H	N	O	S	0	0
			4857	1592	2392	412	451	10		
2	K	312	Total	C	H	N	O	S	0	0
			4857	1592	2392	412	451	10		

- Molecule 3 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	R	552	Total	C	H	N	O	S	0	0
			8717	2937	4347	695	712	26		
3	L	552	Total	C	H	N	O	S	0	0
			8716	2937	4346	695	712	26		

- Molecule 4 is a protein called Cytochrome aa3 subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	S	203	Total	C	H	N	O	S	0	0
			3108	1039	1548	253	260	8		
4	X	203	Total	C	H	N	O	S	0	0
			3108	1039	1548	253	260	8		

- Molecule 5 is a protein called Cytochrome c oxidase polypeptide 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	T	139	Total	C	H	N	O	S	0	0
			2135	719	1058	167	188	3		
5	Z	139	Total	C	H	N	O	S	0	0
			2135	719	1058	167	188	3		

- Molecule 6 is a protein called Cytochrome c oxidase subunit CtaJ.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	U	79	Total	C	H	N	O	S	0	0
			1167	381	576	107	101	2		
6	a	79	Total	C	H	N	O	S	0	0
			1167	381	576	107	101	2		

- Molecule 7 is a protein called Uncharacterized protein MSMEG\_4692/MSMEI\_4575.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	V	145	Total	C	H	N	O	S	0	0
			2093	658	1052	176	205	2		
7	b	145	Total	C	H	N	O	S	0	0
			2093	658	1052	176	205	2		

- Molecule 8 is a protein called Conserved transmembrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	P	92	Total	C	H	N	O	S	0	0
			1452	471	716	136	124	5		
8	J	92	Total	C	H	N	O	S	0	0
			1453	471	717	136	124	5		

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	1	MET	-	initiating methionine	UNP A0QVH4
P	2	SER	-	expression tag	UNP A0QVH4
P	3	SER	-	expression tag	UNP A0QVH4
P	4	THR	-	expression tag	UNP A0QVH4
P	5	GLN	-	expression tag	UNP A0QVH4
P	6	ASP	-	expression tag	UNP A0QVH4
P	7	ARG	-	expression tag	UNP A0QVH4
P	8	SER	-	expression tag	UNP A0QVH4
P	9	GLN	-	expression tag	UNP A0QVH4
P	10	LEU	-	expression tag	UNP A0QVH4
P	11	ASP	-	expression tag	UNP A0QVH4

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Chain	Residue	Modelled	Actual	Comment	Reference
P	12	PRO	-	expression tag	UNP A0QVH4
P	13	GLU	-	expression tag	UNP A0QVH4
P	14	GLU	-	expression tag	UNP A0QVH4
P	15	GLN	-	expression tag	UNP A0QVH4
P	16	PRO	-	expression tag	UNP A0QVH4
P	17	VAL	-	expression tag	UNP A0QVH4
J	1	MET	-	initiating methionine	UNP A0QVH4
J	2	SER	-	expression tag	UNP A0QVH4
J	3	SER	-	expression tag	UNP A0QVH4
J	4	THR	-	expression tag	UNP A0QVH4
J	5	GLN	-	expression tag	UNP A0QVH4
J	6	ASP	-	expression tag	UNP A0QVH4
J	7	ARG	-	expression tag	UNP A0QVH4
J	8	SER	-	expression tag	UNP A0QVH4
J	9	GLN	-	expression tag	UNP A0QVH4
J	10	LEU	-	expression tag	UNP A0QVH4
J	11	ASP	-	expression tag	UNP A0QVH4
J	12	PRO	-	expression tag	UNP A0QVH4
J	13	GLU	-	expression tag	UNP A0QVH4
J	14	GLU	-	expression tag	UNP A0QVH4
J	15	GLN	-	expression tag	UNP A0QVH4
J	16	PRO	-	expression tag	UNP A0QVH4
J	17	VAL	-	expression tag	UNP A0QVH4

- Molecule 9 is a protein called Superoxide dismutase [Cu-Zn].

Mol	Chain	Residues	Atoms						AltConf	Trace
9	G	216	Total	C	H	N	O	S	0	0
			1732	645	640	217	229	1		
9	D	216	Total	C	H	N	O	S	0	0
			1732	645	640	217	229	1		

- Molecule 10 is a protein called Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	O	223	Total	C	H	N	O	S	0	0
			3187	1008	1564	289	314	12		
10	I	223	Total	C	H	N	O	S	0	0
			3186	1008	1563	289	314	12		

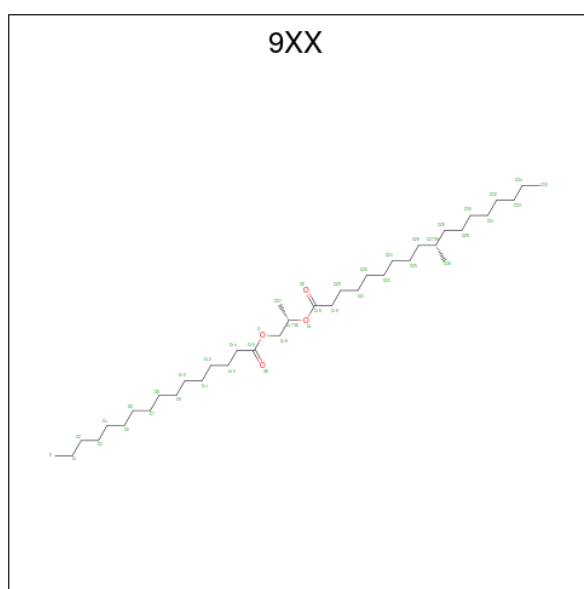
- Molecule 11 is a protein called Cytochrome bc1 complex cytochrome b subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	E	535	Total	C	H	N	O	S	0	0
			8385	2751	4204	711	701	18		
11	F	535	Total	C	H	N	O	S	0	0
			8385	2751	4204	711	701	18		

- Molecule 12 is a protein called Cytochrome bc1 complex Rieske iron-sulfur subunit.

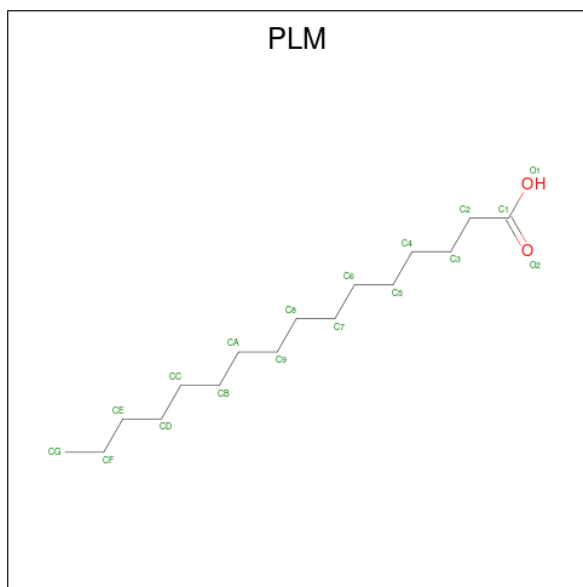
Mol	Chain	Residues	Atoms						AltConf	Trace
12	Y	382	Total	C	H	N	O	S	0	0
			5961	1924	2984	504	538	11		
12	M	382	Total	C	H	N	O	S	0	0
			5961	1924	2984	504	538	11		

- Molecule 13 is (2S)-1-(hexadecanoyloxy)propan-2-yl (10S)-10-methyloctadecanoate (three-letter code: 9XX) (formula: C<sub>38</sub>H<sub>74</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				AltConf
13	W	1	Total	C	H	O	0
			115	38	73	4	
13	G	1	Total	C	H	O	0
			83	28	51	4	
13	D	1	Total	C	H	O	0
			83	28	51	4	
13	c	1	Total	C	H	O	0
			115	38	73	4	

- Molecule 14 is PALMITIC ACID (three-letter code: PLM) (formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>).



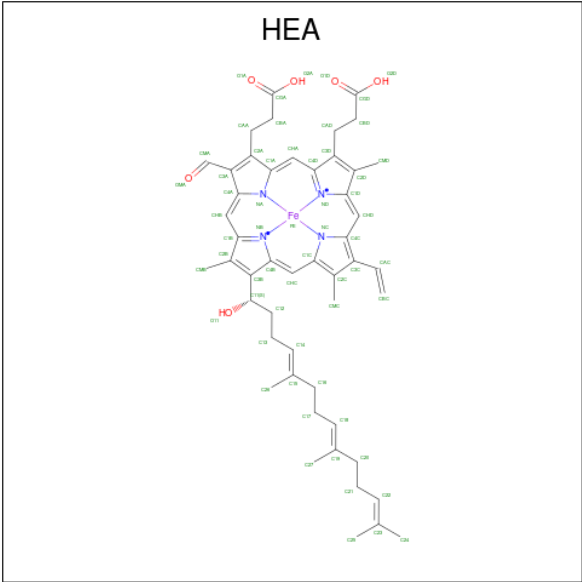
Mol	Chain	Residues	Atoms				AltConf
14	W	1	Total	C	H	O	0
			48	16	31	1	
14	G	1	Total	C	H	O	0
			27	10	16	1	
14	D	1	Total	C	H	O	0
			27	10	16	1	
14	c	1	Total	C	H	O	0
			48	16	31	1	

- Molecule 15 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
15	Q	2	Total	Cu	0
			2	2	
15	R	1	Total	Cu	0
			1	1	
15	K	2	Total	Cu	0
			2	2	
15	L	1	Total	Cu	0
			1	1	

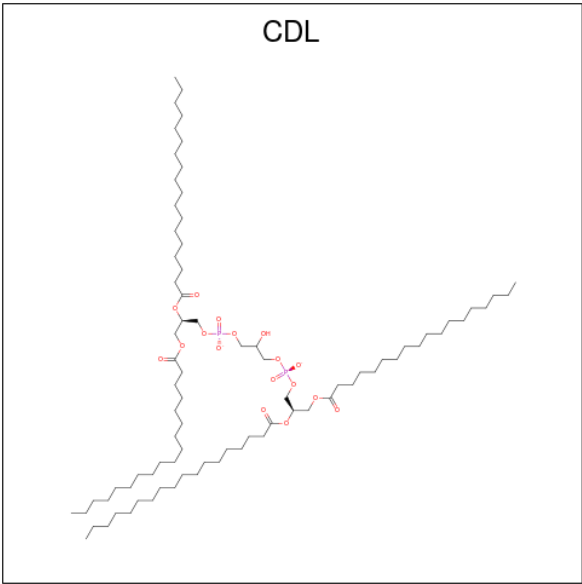
- Molecule 16 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).





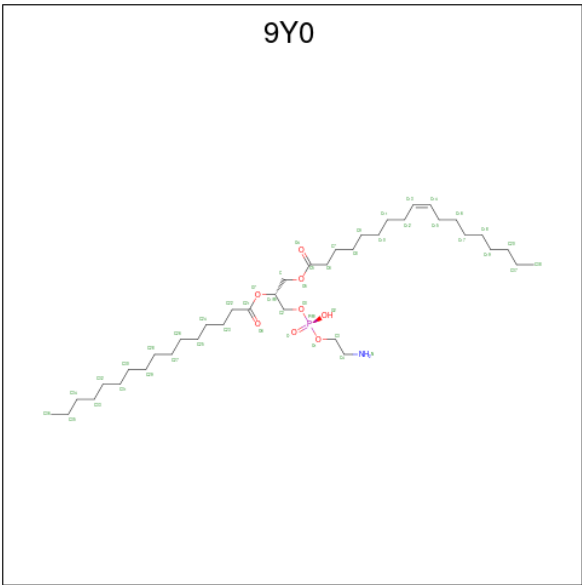
Mol	Chain	Residues	Atoms						AltConf
16	R	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
16	R	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
16	L	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
16	L	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	

- Molecule 17 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



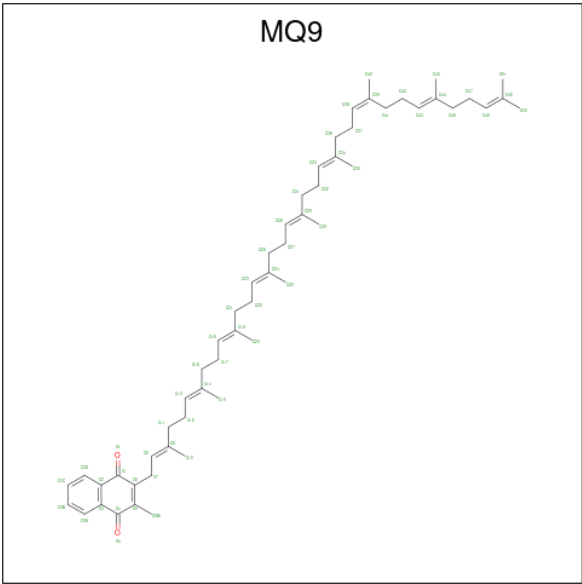
Mol	Chain	Residues	Atoms				AltConf
17	R	1	Total	C	O	P	0
			76	57	17	2	
17	S	1	Total	C	O	P	0
			76	57	17	2	
17	S	1	Total	C	O	P	0
			76	57	17	2	
17	T	1	Total	C	O	P	0
			76	57	17	2	
17	P	1	Total	C	O	P	0
			76	57	17	2	
17	E	1	Total	C	O	P	0
			76	57	17	2	
17	E	1	Total	C	O	P	0
			76	57	17	2	
17	E	1	Total	C	O	P	0
			76	57	17	2	
17	L	1	Total	C	O	P	0
			76	57	17	2	
17	X	1	Total	C	O	P	0
			76	57	17	2	
17	X	1	Total	C	O	P	0
			76	57	17	2	
17	Z	1	Total	C	O	P	0
			76	57	17	2	
17	J	1	Total	C	O	P	0
			76	57	17	2	
17	F	1	Total	C	O	P	0
			76	57	17	2	
17	F	1	Total	C	O	P	0
			76	57	17	2	
17	F	1	Total	C	O	P	0
			76	57	17	2	

- Molecule 18 is (2R)-3-(((2-aminoethoxy)(hydroxy)phosphoryl)oxy)-2-(palmitoyloxy)propyl (E)-octadec-9-enoate (three-letter code: 9Y0) (formula: C<sub>39</sub>H<sub>76</sub>NO<sub>8</sub>P).



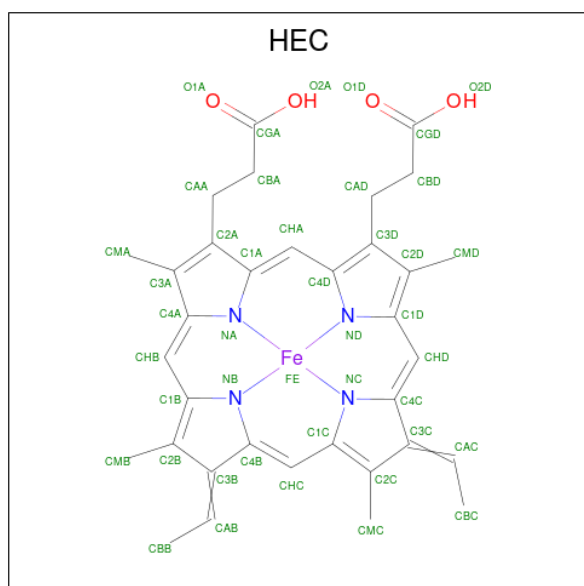
Mol	Chain	Residues	Atoms						AltConf
18	S	1	Total 124	C 39	H 75	N 1	O 8	P 1	0
18	P	1	Total 124	C 39	H 75	N 1	O 8	P 1	0
18	L	1	Total 124	C 39	H 75	N 1	O 8	P 1	0
18	X	1	Total 124	C 39	H 75	N 1	O 8	P 1	0

- Molecule 19 is MENAQUINONE-9 (three-letter code: MQ9) (formula:  $C_{56}H_{80}O_2$ ).



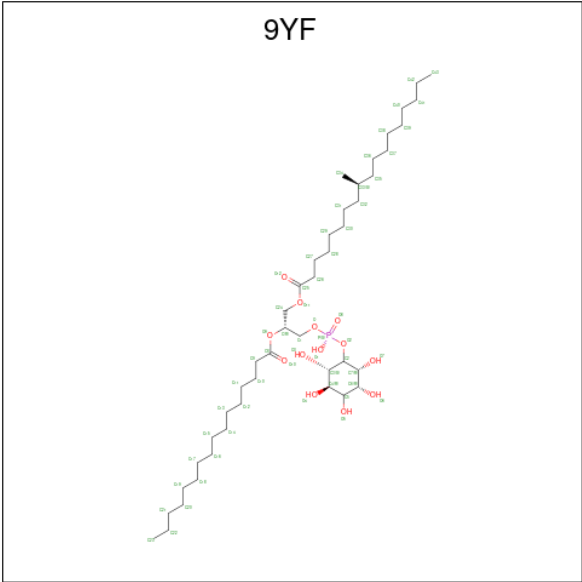
Mol	Chain	Residues	Atoms				AltConf
19	T	1	Total	C	H	O	0
			138	56	80	2	
19	E	1	Total	C	H	O	0
			138	56	80	2	
19	E	1	Total	C	H	O	0
			138	56	80	2	
19	Z	1	Total	C	H	O	0
			138	56	80	2	
19	F	1	Total	C	H	O	0
			138	56	80	2	
19	F	1	Total	C	H	O	0
			138	56	80	2	

- Molecule 20 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



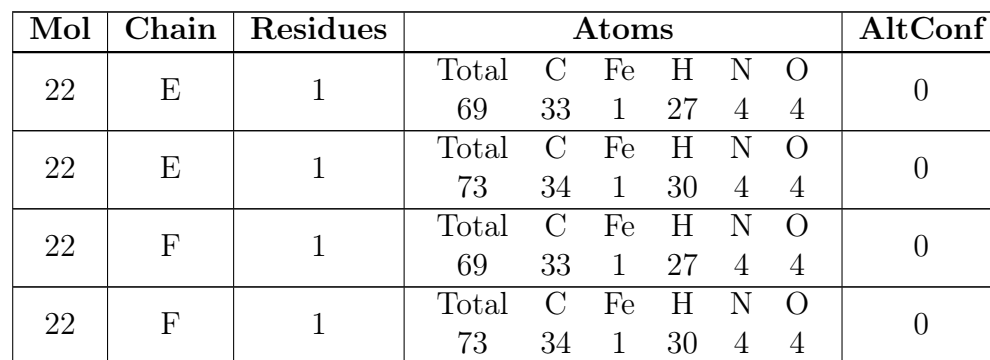
Mol	Chain	Residues	Atoms						AltConf
20	O	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	
20	O	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	
20	I	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	
20	I	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	

- Molecule 21 is (2R)-2-(hexadecanoyloxy)-3-[(S)-hydroxy{[(1R,2R,3R,4R,5R,6S)-2,3,4,5,6-pentahydroxycyclohexyl]oxy}phosphoryl]oxy}propyl (9S)-9-methyloctadecanoate (three-letter code: 9YF) (formula:  $C_{44}H_{85}O_{13}P$ ).

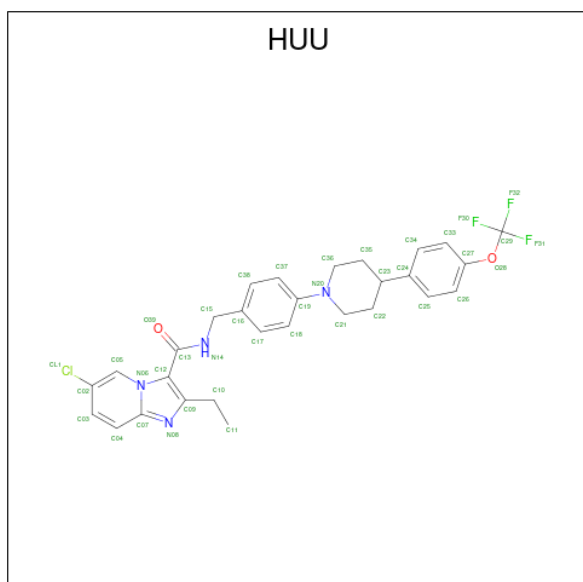


Mol	Chain	Residues	Atoms					AltConf
21	O	1	Total	C	H	O	P	0
			142	44	84	13	1	
21	E	1	Total	C	H	O	P	0
			142	44	84	13	1	
21	I	1	Total	C	H	O	P	0
			142	44	84	13	1	
21	F	1	Total	C	H	O	P	0
			142	44	84	13	1	
21	Y	1	Total	C	H	O	P	0
			142	44	84	13	1	
21	Y	1	Total	C	H	O	P	0
			142	44	84	13	1	
21	M	1	Total	C	H	O	P	0
			142	44	84	13	1	
21	M	1	Total	C	H	O	P	0
			142	44	84	13	1	

- Molecule 22 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).

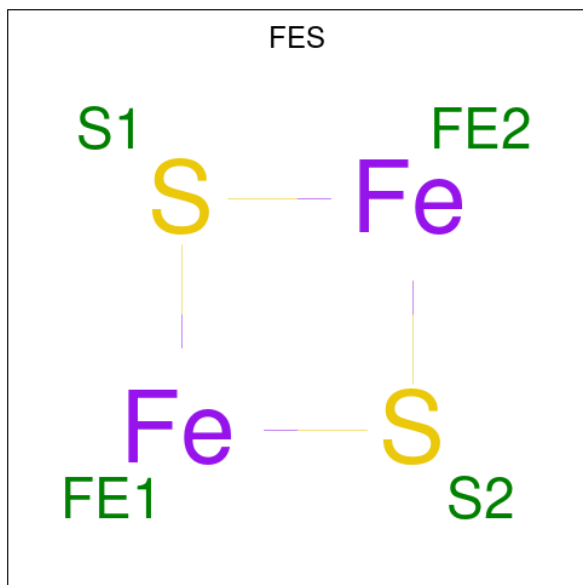


- Molecule 23 is 6-chloranyl-2-ethyl-N-[[4-[4-[4-(trifluoromethoxy)phenyl]piperidin-1-yl]phenyl]methyl]imidazo[1,2-a]pyridine-3-carboxamide (three-letter code: HUU) (formula: C<sub>29</sub>H<sub>28</sub>ClF<sub>3</sub>N<sub>4</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							AltConf
23	E	1	Total	C	Cl	F	H	N	O	0
			67	29	1	3	28	4	2	
23	F	1	Total	C	Cl	F	H	N	O	0
			67	29	1	3	28	4	2	

- Molecule 24 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).

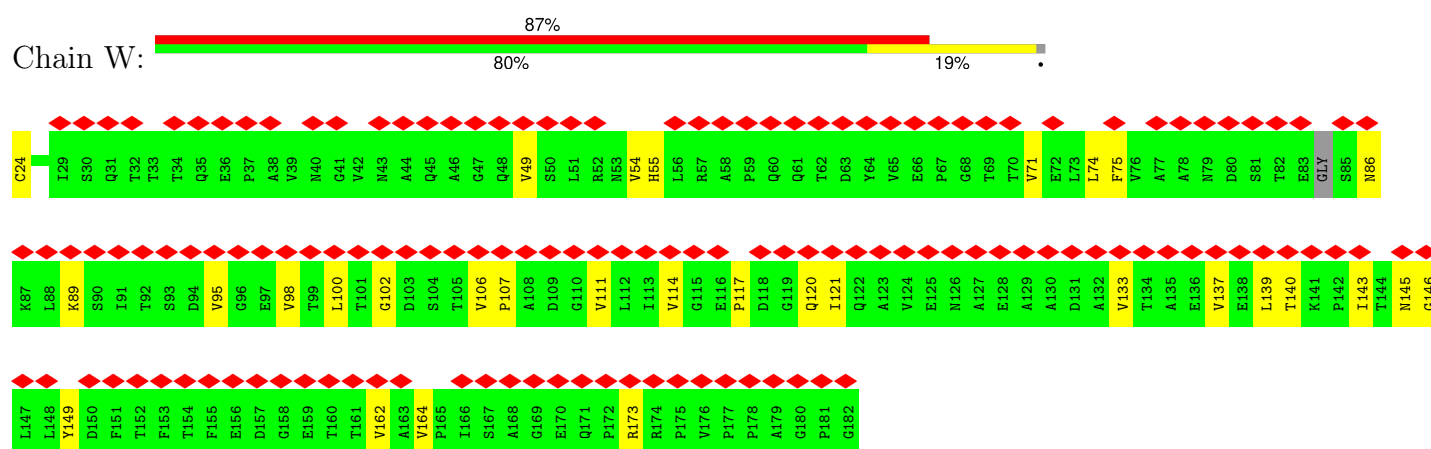


Mol	Chain	Residues	Atoms			AltConf
24	Y	1	Total	Fe	S	0
			4	2	2	
24	M	1	Total	Fe	S	0
			4	2	2	

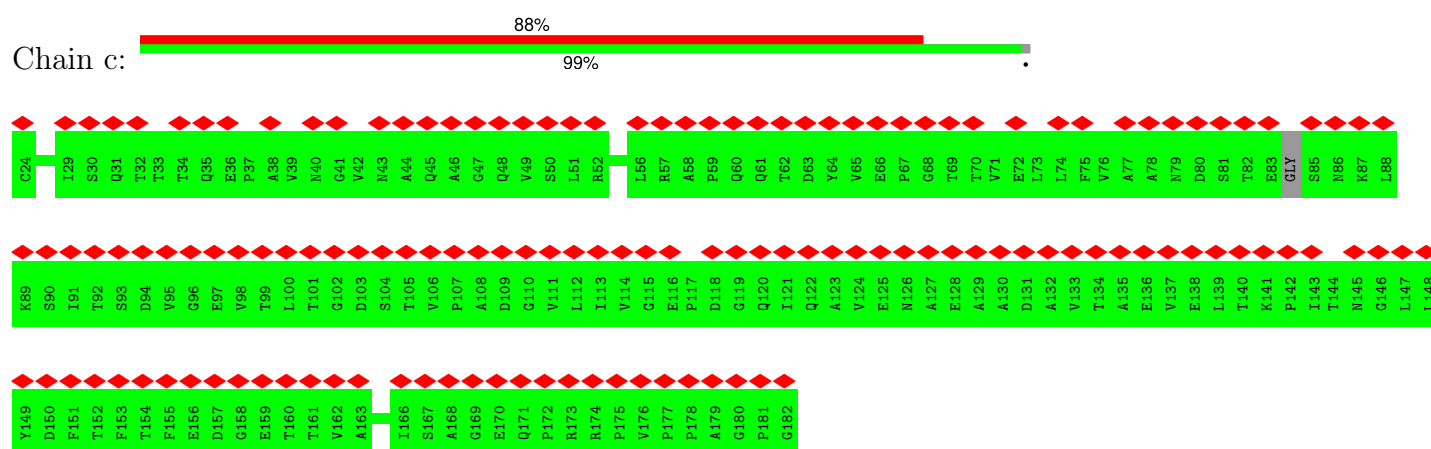
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

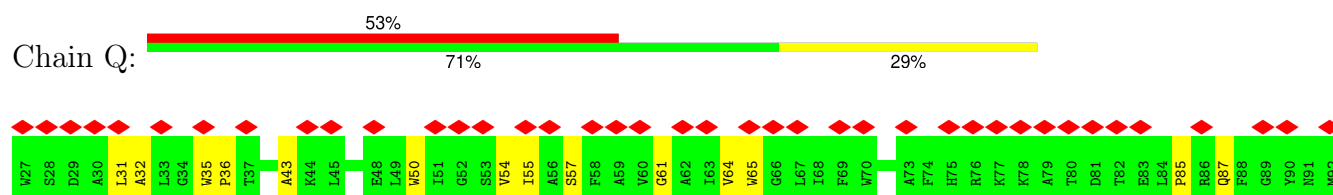
#### • Molecule 1: LpqE protein



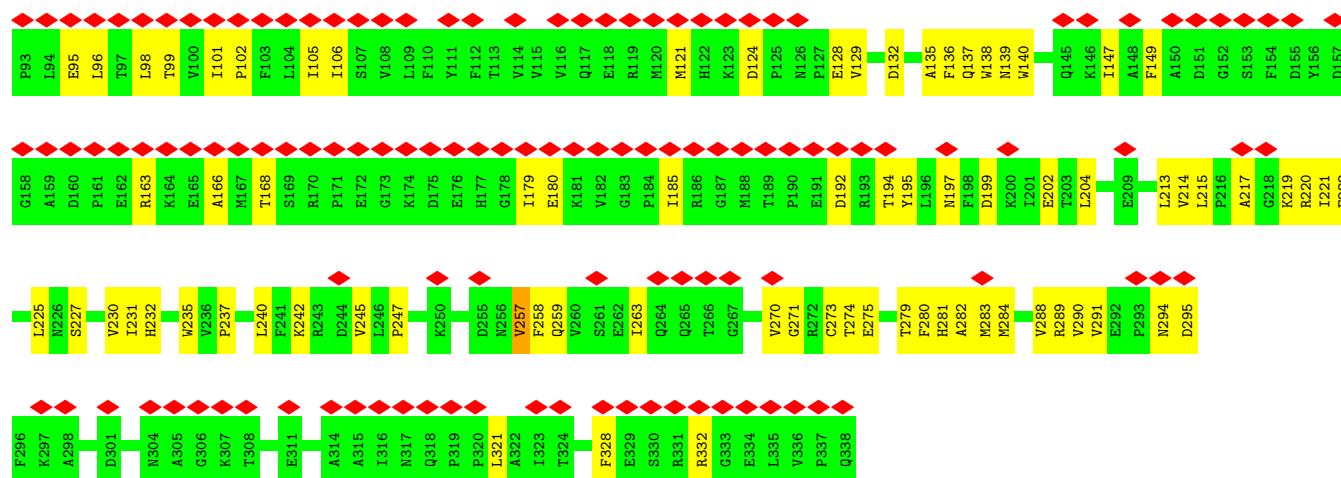
#### • Molecule 1: LpqE protein



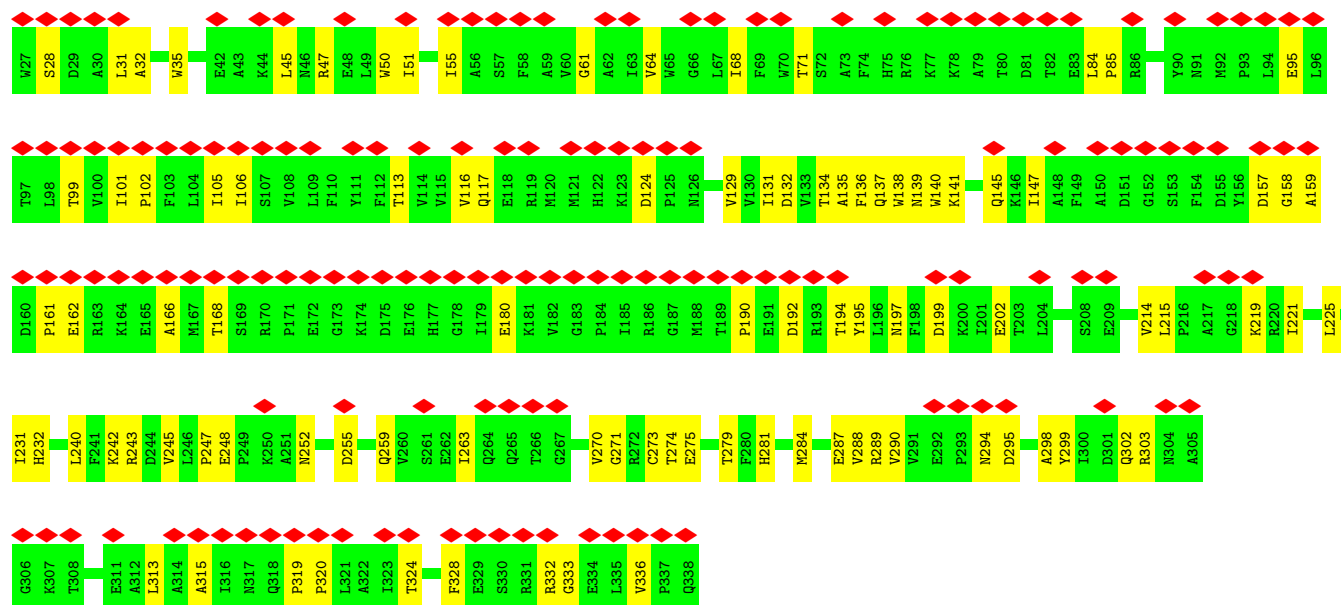
#### • Molecule 2: Cytochrome aa3 subunit 2



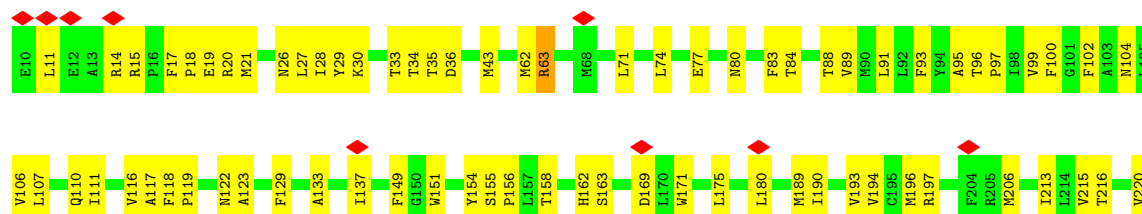


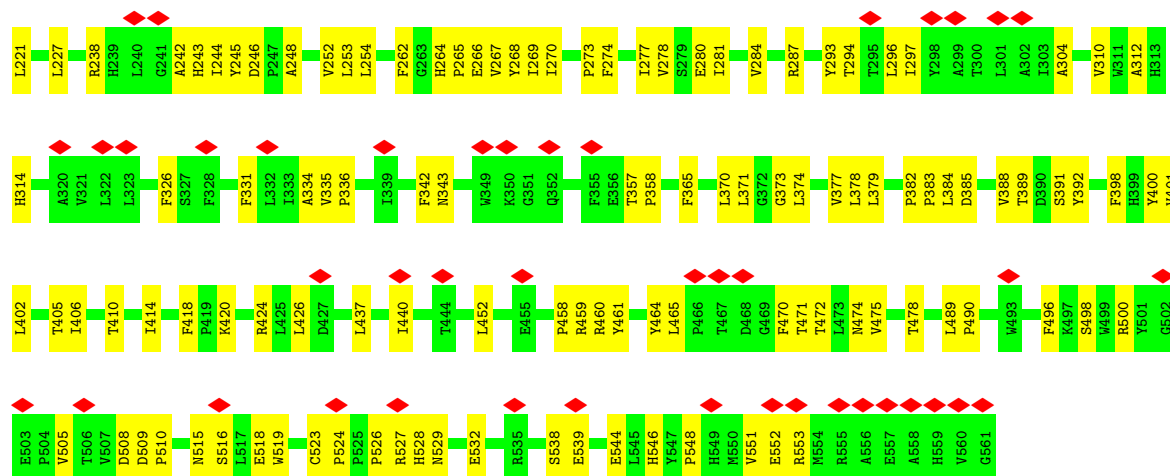


• Molecule 2: Cytochrome aa3 subunit 2

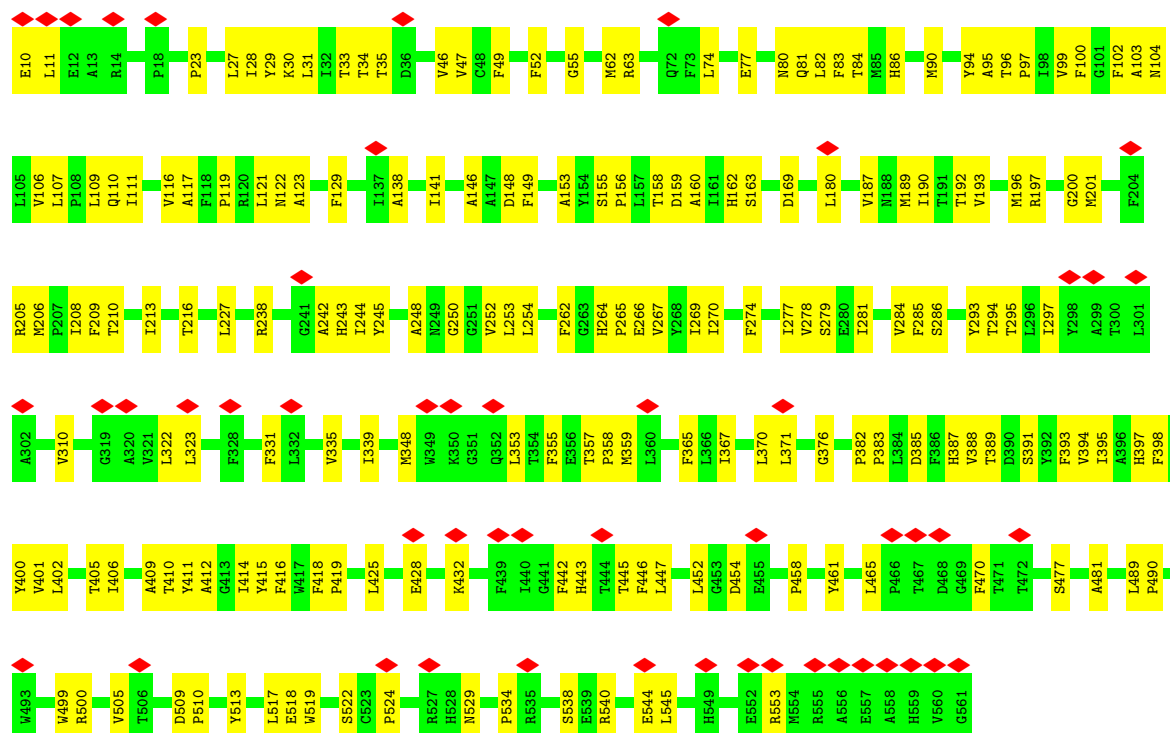


• Molecule 3: Cytochrome c oxidase subunit 1

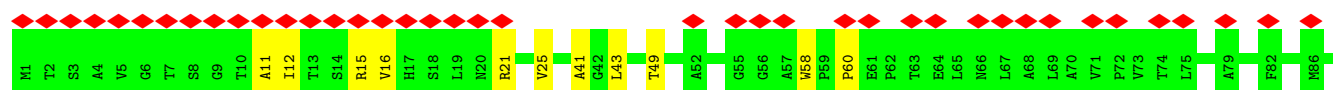


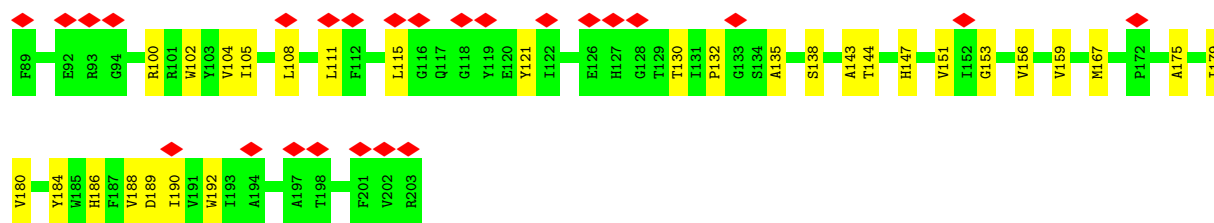


• Molecule 3: Cytochrome c oxidase subunit 1

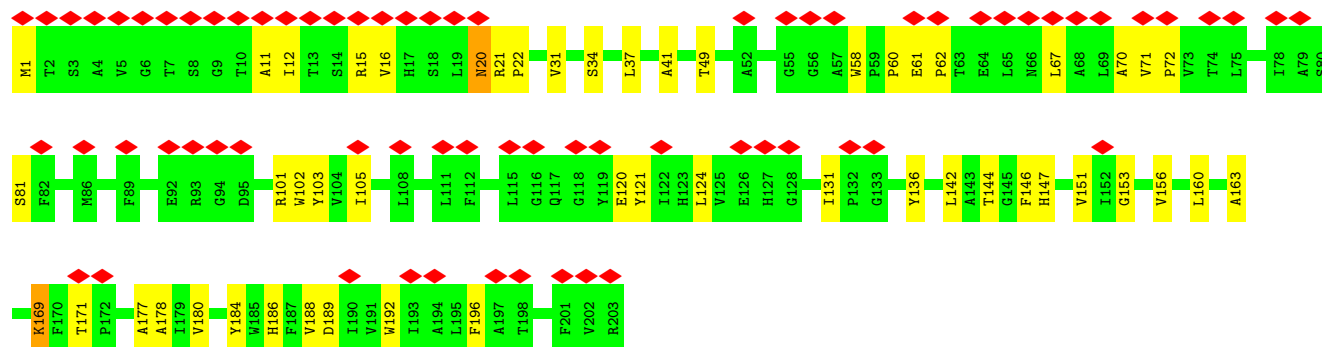
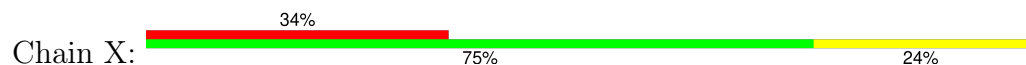


• Molecule 4: Cytochrome aa3 subunit 3

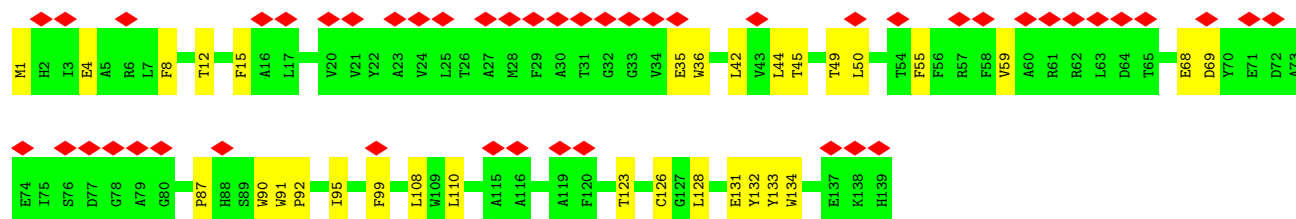
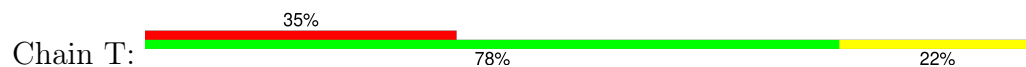




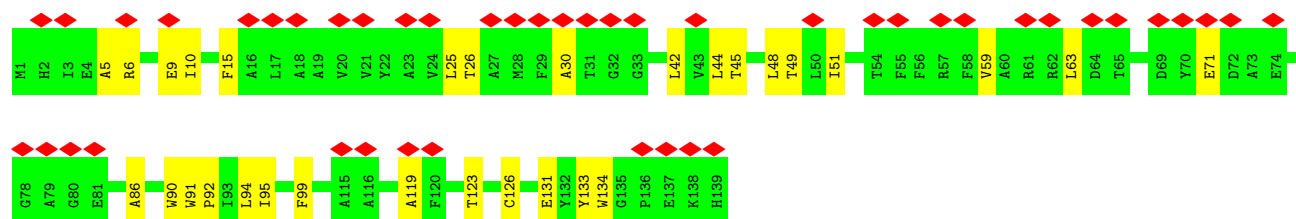
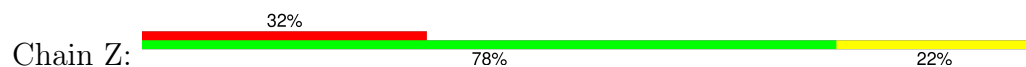
• Molecule 4: Cytochrome aa3 subunit 3



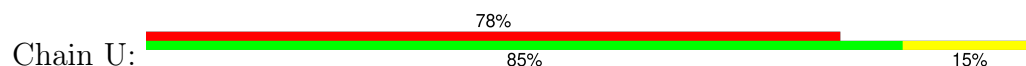
• Molecule 5: Cytochrome c oxidase polypeptide 4

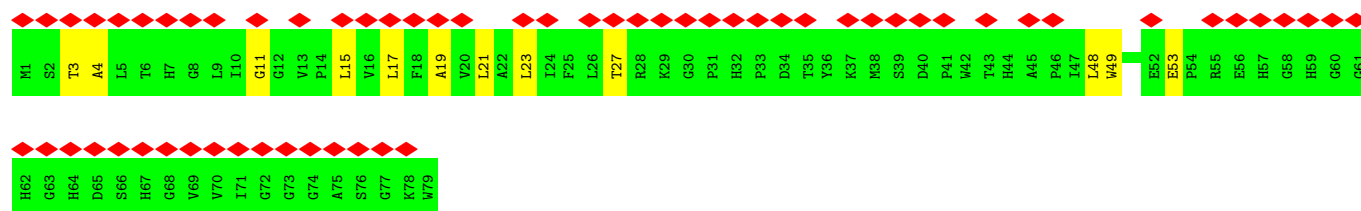


• Molecule 5: Cytochrome c oxidase polypeptide 4

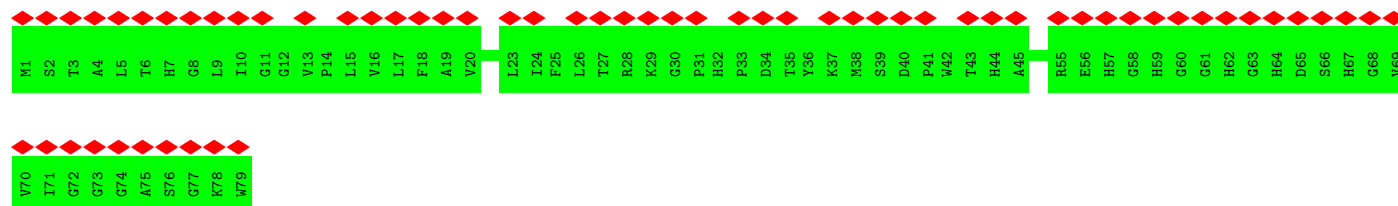
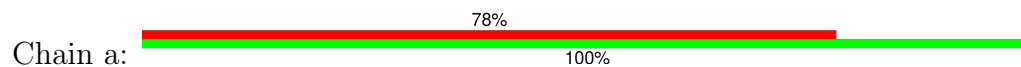


• Molecule 6: Cytochrome c oxidase subunit CtaJ

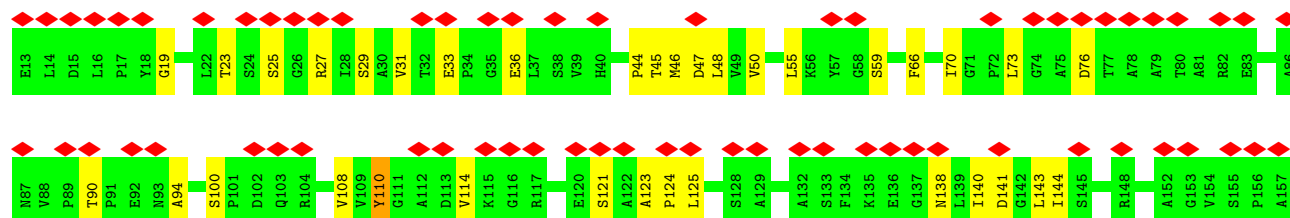
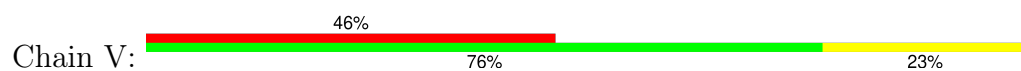




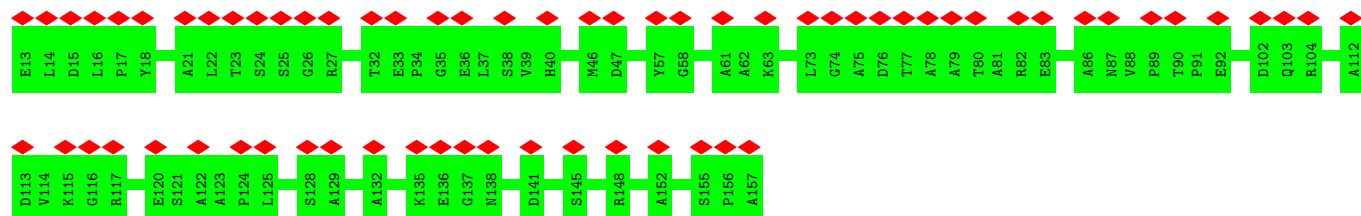
• Molecule 6: Cytochrome c oxidase subunit CtaJ



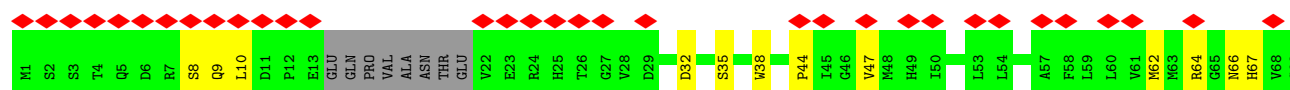
• Molecule 7: Uncharacterized protein MSMEG\_4692/MSMEI\_4575

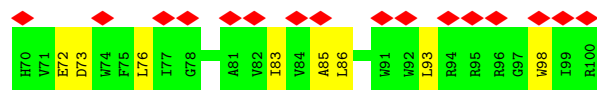


• Molecule 7: Uncharacterized protein MSMEG\_4692/MSMEI\_4575

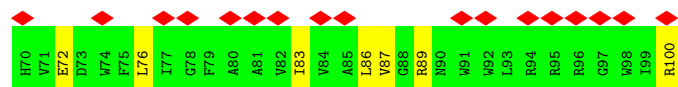
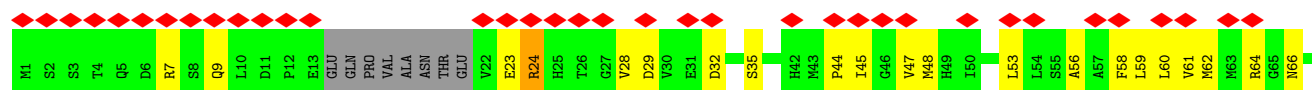


• Molecule 8: Conserved transmembrane protein

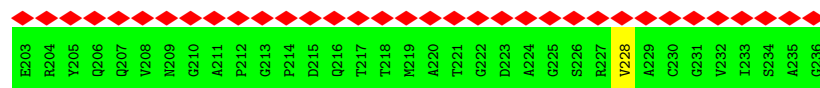
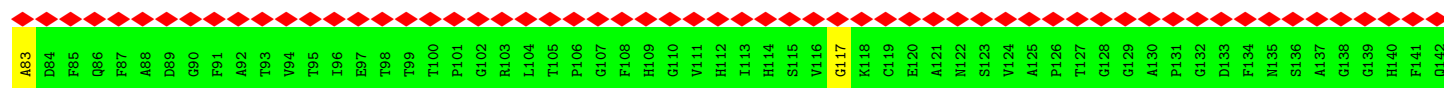
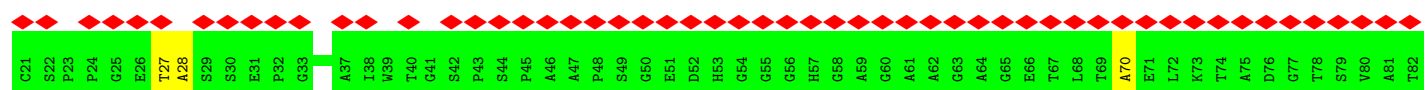




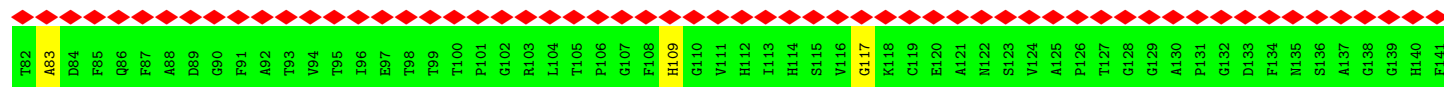
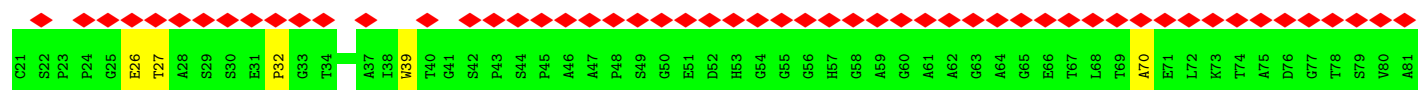
• Molecule 8: Conserved transmembrane protein

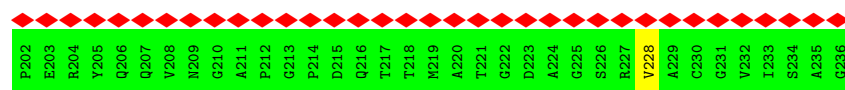


• Molecule 9: Superoxide dismutase [Cu-Zn]

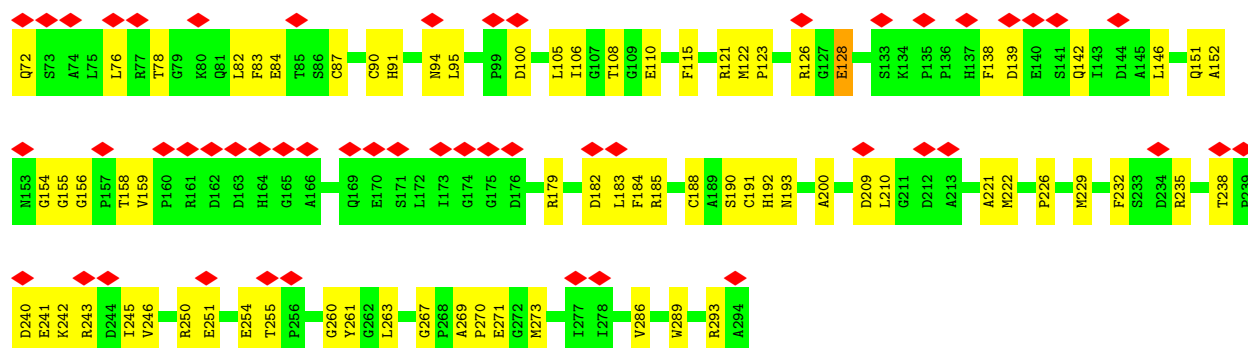


• Molecule 9: Superoxide dismutase [Cu-Zn]

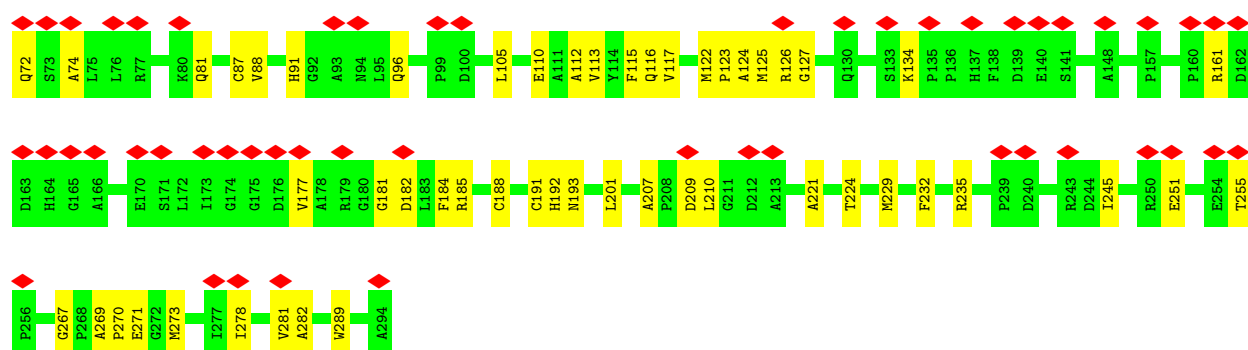
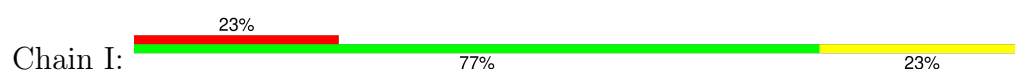




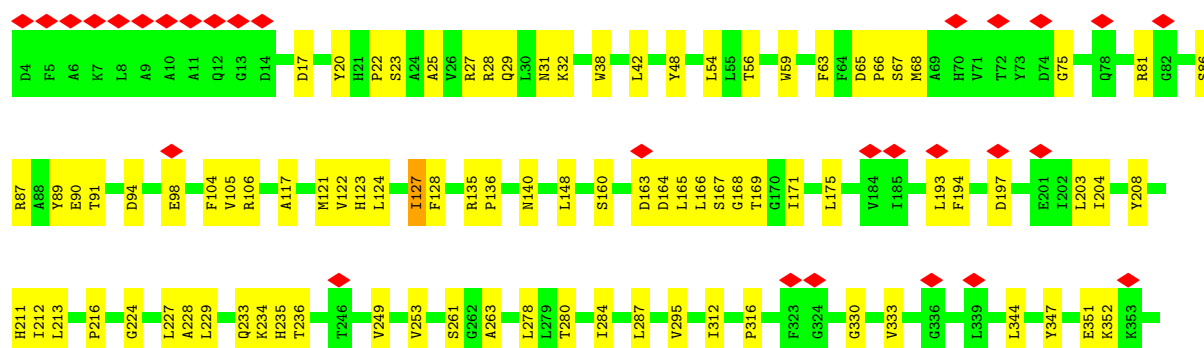
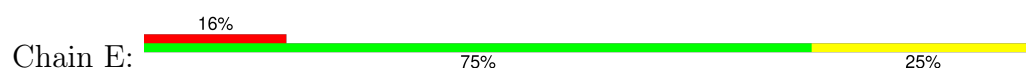
• Molecule 10: Cytochrome bc1 complex cytochrome c subunit

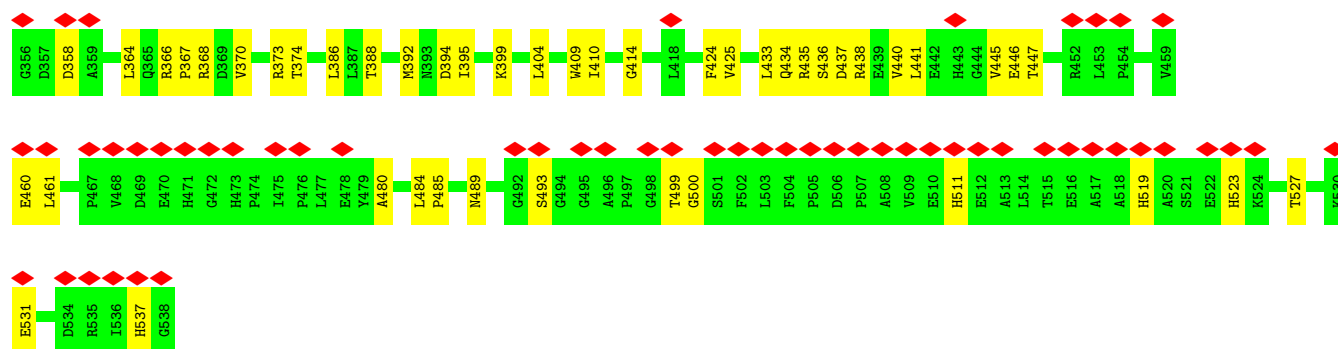


• Molecule 10: Cytochrome bc1 complex cytochrome c subunit



• Molecule 11: Cytochrome bc1 complex cytochrome b subunit

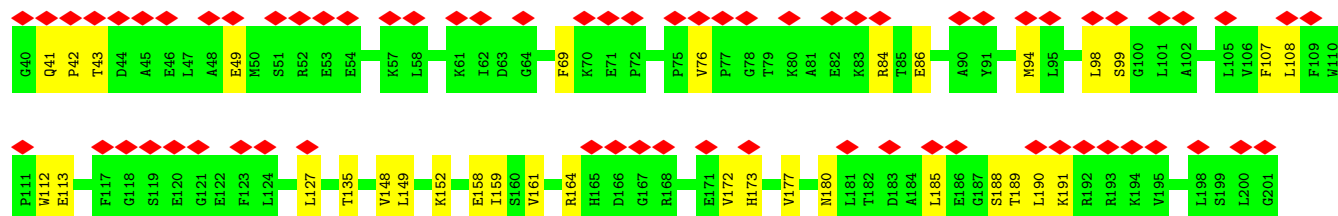


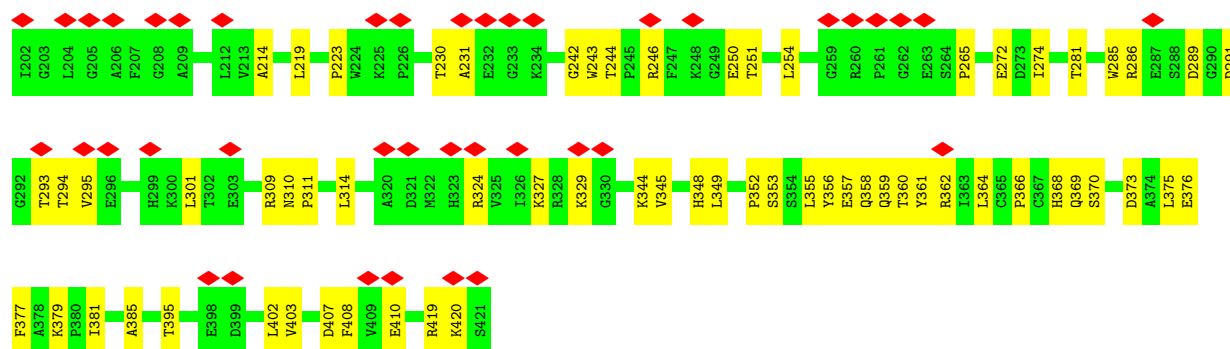


• Molecule 11: Cytochrome bc1 complex cytochrome b subunit

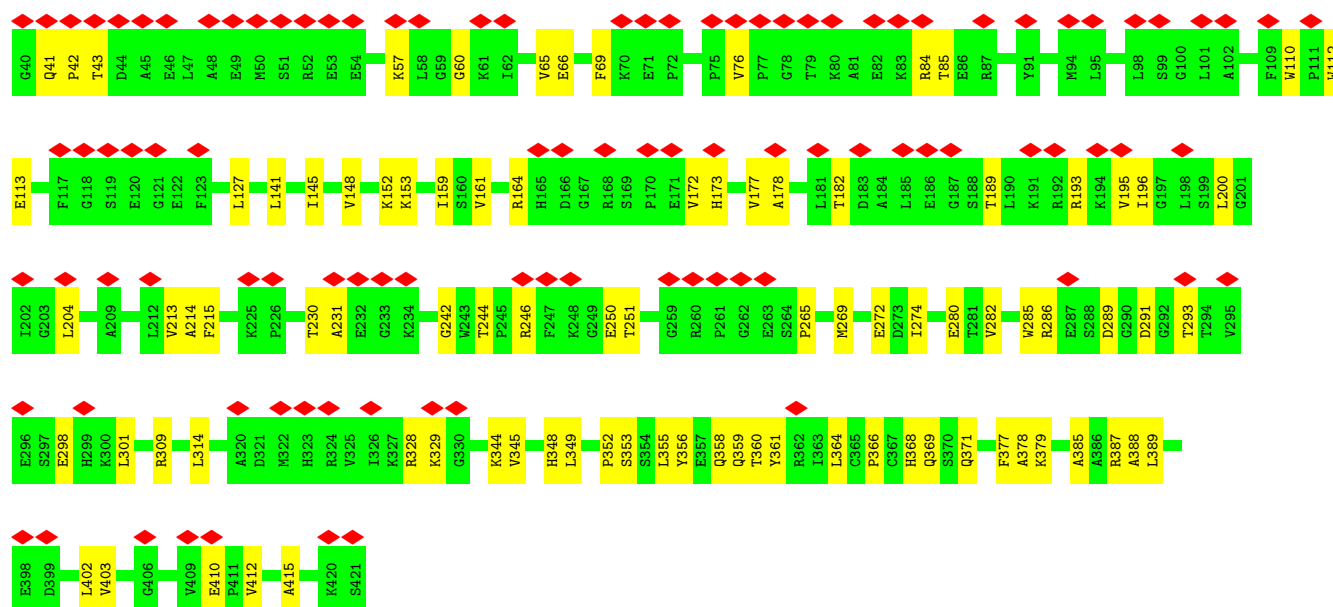
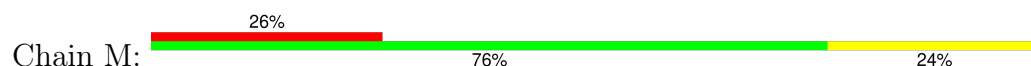


• Molecule 12: Cytochrome bc1 complex Rieske iron-sulfur subunit





• Molecule 12: Cytochrome bc1 complex Rieske iron-sulfur subunit





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70818	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 ( $e^-/\text{\AA}^2$ )	43.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	6.407	Depositor
Minimum map value	-4.052	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.183	Depositor
Recommended contour level	0.82	Depositor
Map size ( $\text{\AA}$ )	339.9, 339.9, 339.9	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.03, 1.03, 1.03	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, 9XX, HEM, FES, CU, 9Y0, 9YF, MQ9, HUU, HEA, PLM, HEC

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	W	0.25	0/1166	0.51	0/1599
1	c	0.25	0/1166	0.50	0/1599
2	K	0.27	0/2534	0.49	0/3451
2	Q	0.31	0/2534	0.54	0/3451
3	L	0.32	0/4530	0.49	0/6188
3	R	0.31	0/4530	0.50	0/6188
4	S	0.29	0/1608	0.47	0/2195
4	X	0.29	0/1608	0.47	0/2195
5	T	0.28	0/1112	0.46	0/1524
5	Z	0.28	0/1112	0.46	0/1524
6	U	0.36	0/613	0.63	0/836
6	a	0.26	0/613	0.45	0/836
7	V	0.30	0/1059	0.55	0/1446
7	b	0.29	0/1059	0.52	0/1446
8	J	0.25	0/757	0.54	0/1027
8	P	0.25	0/757	0.51	0/1027
9	D	0.26	0/1099	0.46	0/1519
9	G	0.26	0/1099	0.47	0/1519
10	I	0.28	0/1660	0.50	0/2250
10	O	0.38	0/1660	0.68	3/2250 (0.1%)
11	E	0.36	0/4314	0.59	2/5882 (0.0%)
11	F	0.29	0/4314	0.49	0/5882
12	M	0.29	0/3056	0.51	0/4142
12	Y	0.28	0/3056	0.50	0/4142
All	All	0.30	0/47016	0.51	5/64118 (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
10	O	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	E	136	PRO	N-CA-C	-7.17	93.45	112.10
11	E	140	ASN	CB-CA-C	6.46	123.31	110.40
10	O	121	ARG	CB-CA-C	-5.09	100.22	110.40
10	O	121	ARG	NE-CZ-NH1	5.06	122.83	120.30
10	O	123	PRO	N-CA-C	-5.03	99.03	112.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	O	128	GLU	Mainchain

## 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	W	1149	1110	1110	26	0
1	c	1149	1110	1110	0	0
2	K	2465	2392	2392	84	0
2	Q	2465	2392	2392	84	0
3	L	4370	4346	4346	172	0
3	R	4370	4347	4345	179	0
4	S	1560	1548	1547	41	0
4	X	1560	1548	1547	50	0
5	T	1077	1058	1058	30	0
5	Z	1077	1058	1058	40	0
6	U	591	576	576	9	0
6	a	591	576	576	0	0
7	V	1041	1052	1052	25	0
7	b	1041	1052	1052	0	0
8	J	736	717	717	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	P	736	716	717	18	0
9	D	1092	640	640	8	0
9	G	1092	640	640	5	0
10	I	1623	1563	1563	52	0
10	O	1623	1564	1564	64	0
11	E	4181	4204	4202	115	0
11	F	4181	4204	4202	122	0
12	M	2977	2984	2984	76	0
12	Y	2977	2984	2984	89	0
13	D	32	51	0	0	0
13	G	32	51	0	0	0
13	W	42	73	0	1	0
13	c	42	73	0	0	0
14	D	11	16	16	1	0
14	G	11	16	16	0	0
14	W	17	31	31	0	0
14	c	17	31	31	0	0
15	K	2	0	0	0	0
15	L	1	0	0	0	0
15	Q	2	0	0	0	0
15	R	1	0	0	0	0
16	L	120	108	108	13	0
16	R	120	108	108	12	0
17	E	228	0	288	17	0
17	F	228	0	288	25	0
17	J	76	0	96	11	0
17	L	76	0	96	14	0
17	P	76	0	96	8	0
17	R	76	0	96	10	0
17	S	152	0	190	34	0
17	T	76	0	96	21	0
17	X	152	0	192	34	0
17	Z	76	0	96	26	0
18	L	49	75	0	0	0
18	P	49	75	0	0	0
18	S	49	75	0	0	0
18	X	49	75	0	1	0
19	E	116	160	160	11	0
19	F	116	160	160	13	0
19	T	58	80	80	5	0
19	Z	58	80	80	3	0
20	I	86	64	64	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	O	86	64	64	21	0
21	E	58	84	0	0	0
21	F	58	84	0	0	0
21	I	58	84	0	1	0
21	M	116	168	0	0	0
21	O	58	84	0	0	0
21	Y	116	168	0	0	0
22	E	85	57	57	14	0
22	F	85	57	57	9	0
23	E	39	28	0	0	0
23	F	39	28	0	0	0
24	M	4	0	0	1	0
24	Y	4	0	0	3	0
All	All	48826	46689	46940	1240	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 14.

All (1240) 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)
17:S:303:CDL:OA9	17:S:303:CDL:H332	1.37	1.14
17:X:302:CDL:HB62	17:X:302:CDL:C51	1.73	1.10
4:S:15:ARG:NH1	17:S:303:CDL:CA2	2.20	1.04
17:L:605:CDL:H512	17:L:605:CDL:H721	1.40	1.04
11:E:425:VAL:HG11	17:E:608:CDL:H371	1.40	1.04
19:F:605:MQ9:H501	12:M:214:ALA:HB1	1.38	1.02
17:X:302:CDL:HB62	17:X:302:CDL:H511	1.38	1.01
17:S:302:CDL:HB21	17:T:202:CDL:HB4	1.40	1.00
17:R:604:CDL:H512	17:R:604:CDL:H732	1.45	0.98
5:Z:119:ALA:HB1	17:Z:202:CDL:H411	1.47	0.95
4:S:15:ARG:NH1	17:S:303:CDL:HA21	1.79	0.94
17:Z:202:CDL:H161	10:I:281:VAL:HG11	1.50	0.92
4:S:15:ARG:NH1	17:S:303:CDL:HA22	1.83	0.92
4:S:15:ARG:CZ	17:S:303:CDL:HA21	2.00	0.91
8:P:66:ASN:ND2	12:M:385:ALA:O	2.05	0.90
11:E:425:VAL:CG1	17:E:608:CDL:H371	2.02	0.89
17:X:302:CDL:HB31	12:Y:149:LEU:HD21	1.55	0.89
3:R:206:MET:O	3:R:293:TYR:OH	1.92	0.88
2:K:243:ARG:NH1	2:K:255:ASP:O	2.07	0.88
17:S:303:CDL:HA32	17:S:303:CDL:OB2	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:L:605:CDL:H771	17:L:605:CDL:H562	1.57	0.87
17:E:607:CDL:H772	17:E:607:CDL:H151	1.57	0.87
11:E:447:THR:OG1	11:E:461:LEU:O	1.93	0.86
17:X:302:CDL:H721	17:Z:202:CDL:H511	1.58	0.86
8:J:61:VAL:HG21	14:D:302:PLM:H71	1.58	0.85
2:K:129:VAL:HG23	2:K:147:ILE:HD13	1.60	0.83
17:S:302:CDL:H751	17:S:302:CDL:H611	1.60	0.83
2:K:332:ARG:NH2	3:L:77:GLU:OE2	2.11	0.83
2:Q:332:ARG:NH2	3:R:77:GLU:OE2	2.12	0.82
10:O:289:TRP:O	12:M:152:LYS:NZ	2.13	0.82
2:Q:192:ASP:OD2	2:Q:194:THR:OG1	1.98	0.82
3:L:206:MET:O	3:L:293:TYR:OH	1.97	0.82
3:R:424:ARG:NH2	3:R:500:ARG:O	2.13	0.81
10:O:151:GLN:OE1	10:O:156:GLY:N	2.12	0.81
9:D:26:GLU:O	9:D:27:THR:OG1	1.97	0.81
3:R:385:ASP:O	3:R:389:THR:OG1	1.99	0.81
2:K:273:CYS:SG	2:K:284:MET:SD	2.79	0.81
17:X:302:CDL:H602	17:X:302:CDL:H751	1.63	0.80
1:W:173:ARG:NE	10:O:235:ARG:O	2.15	0.80
10:O:229:MET:O	12:M:358:GLN:NE2	2.15	0.80
11:E:75:GLY:O	11:E:81:ARG:NH1	2.15	0.80
17:X:302:CDL:HB61	12:Y:149:LEU:HD11	1.63	0.80
10:I:229:MET:O	12:Y:358:GLN:NE2	2.15	0.79
2:Q:85:PRO:O	3:R:553:ARG:NH2	2.15	0.79
5:T:131:GLU:O	11:E:489:ASN:ND2	2.15	0.79
2:K:275:GLU:O	2:K:281:HIS:NE2	2.15	0.78
11:E:89:TYR:OH	11:E:287:LEU:O	2.01	0.78
2:K:242:LYS:NZ	3:L:389:THR:O	2.15	0.78
19:E:605:MQ9:H501	12:Y:214:ALA:HB1	1.66	0.78
3:R:385:ASP:OD2	3:R:389:THR:OG1	2.01	0.77
3:L:110:GLN:HE22	3:L:209:PHE:HD2	1.29	0.77
11:F:500:GLY:O	12:Y:84:ARG:NH1	2.16	0.77
11:F:330:GLY:O	11:F:333:VAL:HG12	1.84	0.77
12:Y:185:LEU:O	12:Y:188:SER:OG	2.01	0.77
17:S:303:CDL:OA9	17:S:303:CDL:C33	2.25	0.77
3:L:355:PHE:O	3:L:432:LYS:NZ	2.18	0.77
20:O:301:HEC:HBC3	20:O:301:HEC:HHD	1.66	0.77
10:I:251:GLU:O	10:I:255:THR:OG1	2.01	0.77
17:X:302:CDL:HB62	17:X:302:CDL:H512	1.63	0.77
3:R:30:LYS:O	3:R:34:THR:N	2.17	0.76
5:Z:131:GLU:O	11:F:489:ASN:ND2	2.17	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:285:TRP:NE1	12:M:289:ASP:O	2.18	0.76
7:V:138:ASN:ND2	7:V:141:ASP:OD2	2.19	0.76
2:Q:273:CYS:O	3:R:461:TYR:OH	2.04	0.76
4:X:81:SER:OG	4:X:189:ASP:OD2	2.03	0.76
17:T:202:CDL:H152	17:T:202:CDL:H722	1.66	0.76
2:K:129:VAL:HG23	2:K:147:ILE:CD1	2.16	0.76
11:F:235:HIS:O	12:Y:164:ARG:NH2	2.18	0.76
11:F:107:GLN:HG3	11:F:281:ILE:HG22	1.69	0.74
17:F:607:CDL:H782	17:F:607:CDL:H151	1.70	0.74
2:K:137:GLN:NE2	10:I:125:MET:SD	2.60	0.74
10:O:251:GLU:O	10:O:255:THR:OG1	2.01	0.74
22:E:602:HEM:HBC1	11:F:213:LEU:HD21	1.69	0.74
17:Z:202:CDL:H161	10:I:281:VAL:CG1	2.18	0.74
7:V:23:THR:OG1	7:V:27:ARG:O	2.06	0.74
11:F:447:THR:OG1	11:F:461:LEU:O	2.04	0.74
12:Y:242:GLY:O	12:Y:286:ARG:NH1	2.21	0.73
3:R:334:ALA:HB1	16:R:602:HEA:H262	1.69	0.73
8:P:32:ASP:O	11:E:435:ARG:NH2	2.21	0.73
3:R:162:HIS:O	3:R:163:SER:OG	2.07	0.73
17:Z:202:CDL:C16	10:I:281:VAL:HG11	2.18	0.73
6:U:23:LEU:O	6:U:27:THR:OG1	2.04	0.73
17:E:607:CDL:H321	17:E:607:CDL:H752	1.69	0.73
17:S:302:CDL:CB2	17:T:202:CDL:HB4	2.18	0.73
11:F:329:GLN:OE1	12:Y:348:HIS:NE2	2.21	0.73
11:F:295:VAL:HG22	12:Y:352:PRO:HG2	1.71	0.73
3:R:36:ASP:OD1	3:R:527:ARG:NH1	2.22	0.72
3:L:443:HIS:O	3:L:447:LEU:HD23	1.89	0.72
3:L:30:LYS:O	3:L:34:THR:N	2.21	0.72
22:F:602:HEM:HHC	22:F:602:HEM:HBB2	1.72	0.72
10:O:191:CYS:CB	20:O:302:HEC:HBC2	2.20	0.71
10:O:191:CYS:HB2	20:O:302:HEC:HBC2	1.72	0.71
11:E:212:ILE:HD11	11:F:212:ILE:HD11	1.72	0.71
2:K:289:ARG:NH1	2:K:319:PRO:O	2.23	0.71
3:L:205:ARG:NH1	5:Z:71:GLU:OE2	2.23	0.71
4:S:121:TYR:OH	4:S:144:THR:OG1	2.06	0.71
3:R:274:PHE:CD2	3:R:406:ILE:HG22	2.25	0.71
16:R:602:HEA:H261	16:R:602:HEA:C18	2.22	0.70
3:R:193:VAL:O	3:R:197:ARG:NH1	2.24	0.70
10:I:191:CYS:HB2	20:I:302:HEC:HBC2	1.72	0.70
12:Y:285:TRP:NE1	12:Y:289:ASP:O	2.24	0.70
3:R:532:GLU:OE2	7:V:25:SER:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:400:TYR:OH	3:L:447:LEU:HD22	1.91	0.70
11:E:235:HIS:O	12:M:164:ARG:NH2	2.24	0.70
17:X:302:CDL:C51	17:X:302:CDL:CB6	2.61	0.70
2:K:287:GLU:OE2	2:K:324:THR:OG1	2.06	0.70
3:L:200:GLY:O	3:L:205:ARG:NH2	2.25	0.70
11:E:499:THR:O	12:M:84:ARG:NH2	2.24	0.69
3:R:392:TYR:CD2	3:R:452:LEU:HD23	2.28	0.69
2:K:71:THR:OG1	3:L:348:MET:O	2.09	0.69
3:R:371:LEU:HD23	3:R:400:TYR:CE2	2.27	0.69
3:R:496:PHE:O	3:R:500:ARG:NH1	2.26	0.69
17:F:607:CDL:H711	17:F:608:CDL:HB4	1.74	0.69
2:Q:227:SER:OG	2:Q:230:VAL:O	2.06	0.69
2:K:45:LEU:HD21	2:K:116:VAL:HG22	1.74	0.69
17:L:605:CDL:H551	17:J:201:CDL:H362	1.73	0.69
3:R:392:TYR:HD2	3:R:452:LEU:HD23	1.56	0.69
4:S:25:VAL:HG12	4:S:180:VAL:HG11	1.73	0.69
11:E:56:THR:HG22	19:E:605:MQ9:H451	1.72	0.69
17:S:302:CDL:H772	17:T:202:CDL:H791	1.74	0.69
2:K:273:CYS:O	3:L:461:TYR:OH	2.06	0.69
3:L:107:LEU:HD11	3:L:210:THR:HG23	1.74	0.69
2:Q:231:ILE:HG22	3:R:156:PRO:HG2	1.74	0.69
1:W:173:ARG:NH2	10:O:241:GLU:OE1	2.25	0.68
3:R:122:ASN:OD1	3:R:123:ALA:N	2.25	0.68
3:R:406:ILE:O	3:R:410:THR:OG1	2.10	0.68
7:V:47:ASP:OD1	7:V:48:LEU:N	2.26	0.68
10:O:269:ALA:HB3	10:O:270:PRO:HD3	1.76	0.68
5:Z:119:ALA:HB1	17:Z:202:CDL:C41	2.23	0.68
11:F:312:ILE:HD11	11:F:333:VAL:HG11	1.75	0.68
20:I:301:HEC:HBC3	20:I:301:HEC:HHD	1.76	0.68
20:O:302:HEC:HHD	20:O:302:HEC:HBC3	1.74	0.67
11:E:330:GLY:O	11:E:333:VAL:HG12	1.94	0.67
3:R:84:THR:O	3:R:88:THR:HG23	1.94	0.67
3:R:515:ASN:O	3:R:516:SER:OG	2.10	0.67
4:X:102:TRP:HE3	4:X:105:ILE:HD11	1.59	0.67
20:I:302:HEC:HBC3	20:I:302:HEC:HHD	1.75	0.67
2:Q:95:GLU:OE2	3:R:343:ASN:ND2	2.27	0.67
3:L:81:GLN:OE1	3:L:146:ALA:N	2.27	0.67
1:W:149:TYR:O	1:W:164:VAL:N	2.28	0.67
2:K:85:PRO:O	3:L:553:ARG:NH2	2.27	0.67
10:I:191:CYS:CB	20:I:302:HEC:HBC2	2.25	0.67
9:G:117:GLY:N	9:G:185:LYS:O	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:192:HIS:CE1	10:O:210:LEU:HD21	2.30	0.67
3:R:88:THR:HG21	3:R:171:TRP:HE1	1.60	0.66
2:K:263:ILE:HG21	2:K:290:VAL:HG21	1.75	0.66
4:X:20:ASN:O	4:X:20:ASN:ND2	2.25	0.66
12:M:195:VAL:HG23	12:M:196:ILE:HD12	1.77	0.66
2:K:192:ASP:OD2	2:K:194:THR:OG1	2.11	0.66
3:R:274:PHE:HD1	3:R:277:ILE:HD12	1.60	0.66
5:T:4:GLU:N	5:T:4:GLU:OE1	2.28	0.66
2:K:101:ILE:O	2:K:105:ILE:HD12	1.96	0.66
3:L:398:PHE:HA	3:L:401:VAL:HG22	1.76	0.66
11:F:42:LEU:HD13	11:F:122:VAL:HG12	1.78	0.66
12:M:200:LEU:HD12	12:M:204:LEU:HD23	1.78	0.66
11:E:65:ASP:HB3	11:E:91:THR:HG21	1.77	0.66
8:J:83:ILE:HG23	17:J:201:CDL:H542	1.77	0.66
10:I:271:GLU:CD	11:F:281:ILE:HD12	2.16	0.65
2:Q:31:LEU:HD21	2:Q:55:ILE:HD11	1.76	0.65
3:L:116:VAL:HG21	3:L:122:ASN:ND2	2.11	0.65
8:J:32:ASP:O	11:F:435:ARG:NH2	2.30	0.65
3:R:548:PRO:O	3:R:551:VAL:HG22	1.96	0.65
2:Q:101:ILE:O	2:Q:105:ILE:HD12	1.97	0.65
2:K:162:GLU:OE1	10:I:81:GLN:NE2	2.29	0.65
11:F:433:LEU:HD22	17:F:607:CDL:HA31	1.79	0.65
9:G:190:ILE:O	9:G:228:VAL:N	2.29	0.65
3:L:33:THR:HG22	5:Z:90:TRP:HB3	1.78	0.65
2:Q:129:VAL:HG23	2:Q:147:ILE:HG13	1.79	0.65
2:Q:166:ALA:N	2:Q:192:ASP:OD1	2.30	0.64
2:K:166:ALA:N	2:K:192:ASP:OD1	2.30	0.64
11:F:227:LEU:HD12	17:F:606:CDL:H782	1.79	0.64
11:E:368:ARG:O	11:E:434:GLN:NE2	2.31	0.64
17:P:202:CDL:HB62	17:P:202:CDL:H632	1.79	0.64
2:K:231:ILE:HG22	3:L:156:PRO:HG2	1.77	0.64
10:I:269:ALA:HB3	10:I:270:PRO:HD3	1.79	0.64
2:Q:242:LYS:NZ	3:R:389:THR:O	2.30	0.64
3:L:10:GLU:N	3:L:10:GLU:OE1	2.32	0.63
3:L:499:TRP:CE3	17:L:605:CDL:H131	2.33	0.63
12:M:159:ILE:O	12:M:159:ILE:HG22	1.98	0.63
12:M:349:LEU:HD12	12:M:368:HIS:CE1	2.33	0.63
2:K:332:ARG:NH2	10:I:127:GLY:O	2.31	0.63
2:Q:163:ARG:NH2	2:Q:194:THR:O	2.31	0.63
3:R:21:MET:O	17:R:604:CDL:HA22	1.98	0.63
11:E:441:LEU:HD21	11:E:484:LEU:HD21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:17:ASP:OD2	11:E:23:SER:OG	2.15	0.63
3:R:89:VAL:CG2	3:R:137:ILE:HD11	2.29	0.63
11:E:89:TYR:OH	11:E:284:ILE:O	2.16	0.63
2:Q:87:GLN:NE2	3:R:287:ARG:O	2.32	0.63
17:Z:202:CDL:H572	10:I:282:ALA:HA	1.80	0.63
3:R:227:LEU:HD22	3:R:262:PHE:CZ	2.34	0.63
17:R:604:CDL:H111	17:P:202:CDL:H312	1.80	0.63
11:E:236:THR:HG21	11:E:364:LEU:HD21	1.80	0.63
2:Q:294:ASN:OD1	2:Q:295:ASP:N	2.32	0.62
2:K:106:ILE:HD13	3:L:335:VAL:HG23	1.80	0.62
4:X:102:TRP:CE3	4:X:105:ILE:HD11	2.34	0.62
12:Y:377:PHE:O	12:Y:379:LYS:N	2.31	0.62
19:F:605:MQ9:H452	12:M:215:PHE:CZ	2.33	0.62
12:M:377:PHE:O	12:M:379:LYS:N	2.32	0.62
17:T:202:CDL:H352	17:T:202:CDL:H162	1.82	0.62
22:E:602:HEM:HBB2	22:E:602:HEM:HHC	1.79	0.62
2:Q:215:LEU:HD13	2:Q:288:VAL:HG23	1.80	0.62
4:S:102:TRP:CE3	4:S:105:ILE:HD11	2.35	0.62
6:U:53:GLU:OE1	7:V:59:SER:OG	2.12	0.62
2:Q:54:VAL:HG22	3:R:378:LEU:HD21	1.81	0.62
12:M:328:ARG:NH1	12:M:410:GLU:OE2	2.32	0.62
11:F:65:ASP:HB3	11:F:91:THR:HG21	1.81	0.62
16:R:602:HEA:HMC1	16:R:602:HEA:HBC1	1.82	0.61
3:R:15:ARG:NH1	3:R:19:GLU:OE2	2.27	0.61
11:E:104:PHE:HD2	19:E:605:MQ9:H502	1.65	0.61
12:M:242:GLY:O	12:M:286:ARG:NH1	2.32	0.61
12:M:291:ASP:OD2	12:M:293:THR:HG23	2.00	0.61
12:M:344:LYS:O	12:M:353:SER:N	2.32	0.61
4:S:15:ARG:HD2	17:S:303:CDL:HB22	1.82	0.61
2:Q:36:PRO:O	2:Q:240:LEU:HD21	2.01	0.61
3:R:385:ASP:O	3:R:389:THR:N	2.32	0.61
17:T:202:CDL:HA22	10:O:293:ARG:NH1	2.14	0.61
16:L:602:HEA:HMC1	16:L:602:HEA:HBC1	1.82	0.61
17:L:605:CDL:HB4	11:F:424:PHE:HE2	1.65	0.61
20:I:301:HEC:HMB1	20:I:301:HEC:HBB3	1.81	0.61
11:F:263:ALA:HB1	12:Y:148:VAL:HG23	1.82	0.61
2:Q:35:TRP:CE3	2:Q:240:LEU:HD22	2.35	0.61
11:F:25:ALA:O	11:F:29:GLN:OE1	2.18	0.61
11:F:27:ARG:HB2	12:M:177:VAL:HG22	1.83	0.61
3:R:406:ILE:HD11	16:R:603:HEA:CBC	2.29	0.61
20:O:301:HEC:HMB1	20:O:301:HEC:HBB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:E:602:HEM:CBC	11:F:213:LEU:HD21	2.31	0.61
3:L:35:THR:HG21	5:Z:86:ALA:O	1.99	0.61
4:S:41:ALA:HA	5:T:44:LEU:HD22	1.82	0.61
3:L:103:ALA:HB1	3:L:189:MET:SD	2.40	0.61
11:F:194:PHE:CE2	11:F:203:LEU:HD22	2.36	0.61
3:L:534:PRO:HB3	3:L:545:LEU:HD12	1.81	0.61
17:L:605:CDL:H572	17:J:201:CDL:H381	1.81	0.61
2:K:219:LYS:O	2:K:221:ILE:HD12	2.01	0.61
8:J:7:ARG:NH1	8:J:9:GLN:OE1	2.33	0.61
2:Q:35:TRP:CZ3	2:Q:240:LEU:HD22	2.36	0.60
3:R:220:VAL:HG22	3:R:269:ILE:HD12	1.82	0.60
3:R:391:SER:HA	3:R:458:PRO:HA	1.83	0.60
8:J:83:ILE:HG12	17:J:201:CDL:H561	1.82	0.60
11:F:66:PRO:O	11:F:67:SER:OG	2.19	0.60
3:R:398:PHE:HA	3:R:401:VAL:HG22	1.83	0.60
17:X:302:CDL:H511	17:X:302:CDL:CB6	2.24	0.60
3:L:227:LEU:HD22	3:L:262:PHE:CZ	2.37	0.60
5:Z:123:THR:CG2	17:Z:202:CDL:H322	2.31	0.60
12:M:265:PRO:CG	12:M:301:LEU:HD23	2.31	0.60
2:Q:237:PRO:O	2:Q:240:LEU:HD23	2.01	0.60
3:L:122:ASN:OD1	3:L:123:ALA:N	2.35	0.60
12:Y:349:LEU:HD12	12:Y:368:HIS:CE1	2.36	0.60
12:M:274:ILE:HD12	12:M:314:LEU:HD23	1.84	0.60
1:W:111:VAL:HG13	10:O:94:ASN:OD1	2.02	0.60
3:R:274:PHE:CE2	3:R:406:ILE:HG22	2.37	0.60
11:E:312:ILE:HD11	11:E:333:VAL:HG11	1.84	0.60
9:D:27:THR:O	12:Y:329:LYS:N	2.33	0.60
7:V:73:LEU:HD23	7:V:100:SER:HB2	1.84	0.60
17:E:608:CDL:H712	17:E:608:CDL:H521	1.84	0.60
3:R:420:LYS:NZ	3:R:518:GLU:O	2.29	0.59
3:L:169:ASP:OD1	3:L:238:ARG:NE	2.35	0.59
3:R:111:ILE:HD12	3:R:196:MET:O	2.02	0.59
9:G:70:ALA:N	9:G:83:ALA:O	2.35	0.59
3:L:406:ILE:HD11	16:L:603:HEA:CBC	2.32	0.59
12:M:246:ARG:N	12:M:250:GLU:OE1	2.35	0.59
11:F:366:ARG:NH1	11:F:437:ASP:OD2	2.35	0.59
4:S:12:ILE:HG21	5:T:133:TYR:CZ	2.37	0.59
10:I:289:TRP:O	12:Y:152:LYS:NZ	2.30	0.59
7:V:46:MET:O	7:V:50:VAL:HG23	2.03	0.59
8:P:76:LEU:HD11	11:E:409:TRP:CZ3	2.37	0.59
3:L:148:ASP:OD2	10:I:126:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:263:ALA:HB1	12:M:148:VAL:HG23	1.84	0.58
3:L:250:GLY:O	3:L:254:LEU:N	2.29	0.58
11:E:48:TYR:OH	11:E:261:SER:OG	2.21	0.58
10:I:122:MET:O	10:I:124:ALA:N	2.36	0.58
2:Q:204:LEU:HD22	10:O:84:GLU:HG3	1.83	0.58
3:R:169:ASP:OD1	3:R:238:ARG:NE	2.37	0.58
11:E:66:PRO:O	11:E:67:SER:OG	2.21	0.58
12:M:127:LEU:HD12	12:M:127:LEU:O	2.03	0.58
7:V:33:GLU:N	7:V:36:GLU:OE2	2.37	0.58
8:P:35:SER:OG	11:E:438:ARG:NH2	2.36	0.58
3:L:274:PHE:CD2	3:L:406:ILE:HG22	2.39	0.58
12:Y:410:GLU:OE1	12:Y:420:LYS:NZ	2.37	0.58
10:O:238:THR:O	10:O:241:GLU:N	2.36	0.58
8:P:9:GLN:OE1	11:E:537:HIS:NE2	2.37	0.58
11:E:208:TYR:CE2	11:E:212:ILE:HD13	2.39	0.58
2:K:101:ILE:HG22	2:K:102:PRO:HD3	1.85	0.58
10:O:235:ARG:NH1	12:M:272:GLU:O	2.37	0.57
12:M:269:MET:HE1	12:M:282:VAL:HG11	1.86	0.57
11:F:236:THR:HG21	11:F:364:LEU:HD21	1.85	0.57
3:R:116:VAL:HG21	3:R:122:ASN:ND2	2.18	0.57
6:U:19:ALA:O	6:U:23:LEU:HD23	2.04	0.57
2:K:31:LEU:HD21	2:K:55:ILE:HD11	1.86	0.57
2:K:157:ASP:OD1	2:K:158:GLY:N	2.37	0.57
11:F:433:LEU:CD1	17:F:608:CDL:HA61	2.33	0.57
12:Y:159:ILE:O	12:Y:159:ILE:HG22	2.04	0.57
2:Q:222:GLU:OE2	2:Q:257:VAL:HG22	2.05	0.57
11:E:56:THR:CG2	19:E:605:MQ9:H451	2.34	0.57
4:X:12:ILE:HG21	5:Z:133:TYR:CE2	2.39	0.57
5:Z:123:THR:HG23	17:Z:202:CDL:H322	1.86	0.57
9:D:190:ILE:O	9:D:228:VAL:N	2.38	0.57
2:Q:50:TRP:O	2:Q:54:VAL:HG23	2.05	0.57
1:W:139:LEU:HD11	1:W:143:ILE:HD13	1.86	0.57
2:K:232:HIS:HA	2:K:275:GLU:HB3	1.87	0.57
11:F:104:PHE:HD2	19:F:605:MQ9:H502	1.68	0.57
8:P:86:LEU:HD23	17:P:202:CDL:H162	1.87	0.57
11:E:347:TYR:OH	11:E:351:GLU:OE1	2.17	0.57
17:L:605:CDL:H111	17:J:201:CDL:HA62	1.85	0.57
10:I:72:GLN:OE1	10:I:74:ALA:N	2.38	0.57
9:D:70:ALA:N	9:D:83:ALA:O	2.38	0.57
10:I:96:GLN:N	10:I:96:GLN:OE1	2.34	0.57
2:K:117:GLN:CD	3:L:323:LEU:HD23	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:270:ILE:CG2	3:R:406:ILE:HG21	2.35	0.56
11:E:32:LYS:O	11:E:253:VAL:HG23	2.05	0.56
4:X:169:LYS:O	4:X:171:THR:HG23	2.05	0.56
17:R:604:CDL:H552	17:P:202:CDL:H362	1.88	0.56
19:T:201:MQ9:H5M1	11:E:395:ILE:CG2	2.36	0.56
11:F:37:HIS:ND1	11:F:39:SER:OG	2.27	0.56
2:K:45:LEU:CD2	2:K:116:VAL:HG22	2.36	0.56
4:X:41:ALA:HA	5:Z:44:LEU:HD22	1.87	0.56
12:Y:230:THR:HG23	12:Y:244:THR:CG2	2.35	0.56
2:K:140:TRP:NE1	2:K:284:MET:O	2.35	0.56
17:L:605:CDL:HB4	11:F:424:PHE:CE2	2.40	0.56
5:Z:126:CYS:HB2	17:Z:202:CDL:H321	1.87	0.56
11:F:56:THR:HA	19:F:605:MQ9:H451	1.87	0.56
19:F:605:MQ9:C50	12:M:214:ALA:HB1	2.25	0.56
12:Y:265:PRO:HG2	12:Y:301:LEU:HD23	1.88	0.56
12:Y:355:LEU:HD22	12:Y:364:LEU:HD23	1.87	0.56
11:E:175:LEU:HD22	11:E:193:LEU:HD21	1.86	0.56
11:F:252:ARG:NH1	12:Y:158:GLU:OE1	2.38	0.56
11:F:499:THR:HG22	11:F:511:HIS:ND1	2.21	0.56
2:Q:328:PHE:CD1	3:R:465:LEU:HD21	2.41	0.56
3:R:538:SER:OG	3:R:544:GLU:OE2	2.22	0.56
17:S:302:CDL:H622	17:S:302:CDL:H771	1.88	0.56
3:L:445:THR:HG23	3:L:446:PHE:CD2	2.41	0.56
3:L:84:THR:OG1	3:L:149:PHE:O	2.16	0.55
16:R:602:HEA:H261	16:R:602:HEA:H18	1.88	0.55
2:K:135:ALA:HB2	2:K:140:TRP:CE3	2.41	0.55
3:L:77:GLU:O	3:L:81:GLN:HG3	2.06	0.55
4:X:70:ALA:HB1	4:X:196:PHE:HE1	1.71	0.55
10:I:110:GLU:OE2	10:I:161:ARG:NH2	2.38	0.55
4:S:16:VAL:HG13	4:S:21:ARG:NH1	2.21	0.55
17:S:302:CDL:H731	17:T:202:CDL:C53	2.35	0.55
2:K:131:ILE:HG13	2:K:215:LEU:HD21	1.89	0.55
3:L:270:ILE:CG2	3:L:406:ILE:HG21	2.36	0.55
5:Z:131:GLU:O	11:F:487:ARG:NH1	2.36	0.55
17:R:604:CDL:H722	11:E:425:VAL:HG22	1.88	0.55
11:F:254:MET:HB3	11:F:255:PRO:HD3	1.87	0.55
12:Y:42:PRO:O	12:Y:43:THR:OG1	2.22	0.55
11:E:499:THR:HG22	11:E:511:HIS:ND1	2.22	0.55
3:R:80:ASN:HA	3:R:83:PHE:CE1	2.41	0.55
17:S:302:CDL:HB21	17:T:202:CDL:CB4	2.26	0.55
16:L:602:HEA:C18	16:L:602:HEA:H261	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:46:MET:SD	7:V:47:ASP:N	2.80	0.55
12:Y:112:TRP:O	12:Y:113:GLU:HB2	2.06	0.55
1:W:139:LEU:O	1:W:140:THR:OG1	2.22	0.55
3:L:401:VAL:HG21	16:L:602:HEA:C4C	2.37	0.55
11:E:20:TYR:HE1	11:F:229:LEU:HD22	1.72	0.54
3:L:419:PRO:HG3	3:L:425:LEU:HD23	1.90	0.54
4:X:12:ILE:HG21	5:Z:133:TYR:CZ	2.42	0.54
17:L:605:CDL:H112	17:L:605:CDL:HA61	1.89	0.54
8:J:66:ASN:ND2	12:Y:385:ALA:O	2.39	0.54
10:I:235:ARG:NH1	12:Y:272:GLU:O	2.40	0.54
12:M:112:TRP:O	12:M:113:GLU:HB2	2.07	0.54
3:R:458:PRO:HB2	3:R:461:TYR:HE2	1.72	0.54
4:S:104:VAL:O	4:S:108:LEU:HD23	2.08	0.54
12:Y:265:PRO:CG	12:Y:301:LEU:HD23	2.37	0.54
5:T:132:TYR:HA	11:E:489:ASN:HD22	1.72	0.54
2:K:138:TRP:HA	2:K:284:MET:HG2	1.90	0.54
5:T:134:TRP:O	11:E:489:ASN:OD1	2.26	0.54
5:Z:119:ALA:CB	17:Z:202:CDL:H411	2.28	0.54
12:Y:344:LYS:O	12:Y:353:SER:N	2.37	0.54
4:S:15:ARG:HH11	17:S:303:CDL:HA22	1.66	0.54
17:S:302:CDL:H731	17:T:202:CDL:H531	1.90	0.54
11:E:65:ASP:CB	11:E:91:THR:HG21	2.37	0.54
11:F:295:VAL:HG22	12:Y:352:PRO:CG	2.35	0.54
3:R:88:THR:HG21	3:R:171:TRP:NE1	2.22	0.54
4:S:21:ARG:NH2	5:T:68:GLU:OE2	2.36	0.54
2:K:190:PRO:HG3	3:L:243:HIS:HE1	1.73	0.54
4:X:1:MET:O	4:X:1:MET:SD	2.65	0.54
2:Q:185:ILE:HG22	4:S:135:ALA:HB2	1.89	0.54
3:R:464:TYR:HE2	3:R:471:THR:HG1	1.56	0.54
3:L:27:LEU:HG	3:L:31:LEU:HD13	1.89	0.54
3:R:102:PHE:O	3:R:106:VAL:HG12	2.07	0.54
5:Z:5:ALA:O	5:Z:9:GLU:OE1	2.26	0.54
12:M:42:PRO:O	12:M:43:THR:OG1	2.23	0.54
3:R:171:TRP:O	3:R:175:LEU:HD23	2.08	0.53
3:L:109:LEU:HD23	3:L:529:ASN:HB3	1.90	0.53
12:M:265:PRO:HG2	12:M:301:LEU:HD23	1.89	0.53
11:F:404:LEU:HD21	12:Y:369:GLN:HB3	1.90	0.53
3:R:18:PRO:O	3:R:20:ARG:NH1	2.41	0.53
3:L:96:THR:HB	3:L:270:ILE:HD11	1.91	0.53
19:T:201:MQ9:H5M1	11:E:395:ILE:HG22	1.90	0.53
10:O:106:ILE:HG23	10:O:154:GLY:HA2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:106:ILE:HD13	3:L:335:VAL:CG2	2.37	0.53
12:M:328:ARG:HH21	12:M:388:ALA:HB3	1.73	0.53
1:W:75:PHE:CZ	1:W:114:VAL:HG11	2.44	0.53
4:S:102:TRP:HE3	4:S:105:ILE:HD11	1.72	0.53
11:E:104:PHE:CD2	19:E:605:MQ9:H502	2.43	0.53
1:W:89:LYS:HD2	1:W:89:LYS:O	2.08	0.53
4:X:153:GLY:HA3	17:X:303:CDL:H772	1.89	0.53
5:Z:123:THR:HG23	17:Z:202:CDL:H331	1.90	0.53
19:Z:201:MQ9:H502	11:F:411:GLY:CA	2.38	0.53
3:L:264:HIS:O	3:L:267:VAL:HG22	2.08	0.53
11:F:59:TRP:CE3	11:F:105:VAL:HG11	2.43	0.53
3:L:371:LEU:HD22	3:L:400:TYR:CE2	2.44	0.53
10:I:115:PHE:CE1	10:I:221:ALA:HB2	2.44	0.53
11:F:346:ALA:O	11:F:350:ILE:HD12	2.09	0.53
11:F:425:VAL:HG11	17:F:608:CDL:H382	1.89	0.53
20:O:301:HEC:HHD	20:O:301:HEC:CBC	2.38	0.53
11:E:370:VAL:O	11:E:370:VAL:HG13	2.09	0.53
11:E:63:PHE:HZ	12:Y:219:LEU:HD22	1.74	0.53
9:D:117:GLY:N	9:D:185:LYS:O	2.41	0.52
11:F:445:VAL:HG22	11:F:485:PRO:O	2.09	0.52
3:R:96:THR:HB	3:R:270:ILE:HD11	1.92	0.52
3:R:470:PHE:O	3:R:474:ASN:ND2	2.41	0.52
2:K:99:THR:OG1	3:L:339:ILE:HD11	2.09	0.52
3:L:104:ASN:OD1	3:L:122:ASN:ND2	2.42	0.52
12:Y:127:LEU:O	12:Y:127:LEU:HD12	2.10	0.52
3:R:296:LEU:HD11	3:R:343:ASN:HB3	1.90	0.52
22:E:601:HEM:HMB1	22:E:601:HEM:HBB2	1.90	0.52
3:L:274:PHE:CE2	3:L:406:ILE:HG22	2.44	0.52
3:L:406:ILE:HD11	16:L:603:HEA:HBC2	1.91	0.52
11:F:295:VAL:HG12	11:F:296:SER:N	2.24	0.52
3:L:35:THR:HG22	3:L:35:THR:O	2.10	0.52
11:E:445:VAL:HG22	11:E:485:PRO:O	2.09	0.52
20:I:302:HEC:HAC	12:Y:356:TYR:O	2.09	0.52
11:E:28:ARG:HH21	17:E:606:CDL:PB2	2.32	0.52
2:K:124:ASP:O	2:K:259:GLN:NE2	2.40	0.52
11:F:58:VAL:O	11:F:61:THR:OG1	2.21	0.52
2:Q:263:ILE:HG21	2:Q:290:VAL:HG21	1.92	0.52
9:G:27:THR:HG22	9:G:28:ALA:N	2.24	0.52
10:O:261:TYR:N	11:E:278:LEU:O	2.41	0.52
7:V:114:VAL:HG23	7:V:114:VAL:O	2.10	0.52
11:F:104:PHE:CD2	19:F:605:MQ9:H502	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:420:LYS:HZ1	3:R:519:TRP:HA	1.75	0.52
17:T:202:CDL:H542	10:O:286:VAL:HG22	1.92	0.52
10:O:90:CYS:HB3	20:O:301:HEC:HBC2	1.91	0.52
2:K:137:GLN:OE1	2:K:138:TRP:NE1	2.42	0.52
11:F:256:VAL:HG12	11:F:260:LYS:HE3	1.92	0.52
12:Y:366:PRO:O	12:Y:369:GLN:NE2	2.43	0.52
2:K:199:ASP:N	2:K:202:GLU:OE2	2.39	0.51
5:T:1:MET:N	5:T:69:ASP:OD2	2.37	0.51
11:E:236:THR:HG22	22:E:601:HEM:O1D	2.11	0.51
3:L:159:ASP:OD1	3:L:160:ALA:N	2.42	0.51
11:F:89:TYR:OH	11:F:287:LEU:O	2.18	0.51
11:F:465:LEU:HD21	11:F:485:PRO:HG2	1.92	0.51
3:R:546:HIS:NE2	7:V:29:SER:OG	2.38	0.51
4:S:153:GLY:HA2	17:S:303:CDL:H602	1.92	0.51
3:L:193:VAL:O	3:L:197:ARG:NH1	2.44	0.51
11:F:249:VAL:HG22	12:Y:161:VAL:HG23	1.92	0.51
2:Q:213:LEU:HG	2:Q:215:LEU:CD1	2.41	0.51
3:L:96:THR:N	3:L:97:PRO:CD	2.74	0.51
4:X:15:ARG:HD2	17:X:303:CDL:H1	1.93	0.51
19:F:605:MQ9:H453	19:F:605:MQ9:H511	1.92	0.51
11:E:65:ASP:OD1	11:F:67:SER:OG	2.27	0.51
3:L:505:VAL:HG21	3:L:510:PRO:HB3	1.92	0.51
12:Y:362:ARG:NH1	12:Y:381:ILE:HD11	2.26	0.51
2:Q:135:ALA:HB1	2:Q:232:HIS:NE2	2.26	0.51
3:R:426:LEU:HD23	3:R:498:SER:HB2	1.91	0.51
2:K:299:TYR:OH	2:K:303:ARG:NH1	2.42	0.51
3:L:80:ASN:HA	3:L:83:PHE:CE1	2.46	0.51
10:I:245:ILE:HG21	20:I:302:HEC:HMB1	1.92	0.51
12:Y:243:TRP:CZ3	12:Y:254:LEU:HD23	2.46	0.51
2:Q:140:TRP:NE1	2:Q:284:MET:O	2.44	0.51
19:E:605:MQ9:C50	12:Y:214:ALA:HB1	2.37	0.51
11:F:161:LEU:HD21	11:F:208:TYR:CA	2.40	0.51
11:E:527:THR:O	11:E:531:GLU:HG2	2.11	0.51
10:I:182:ASP:OD1	10:I:185:ARG:NH2	2.44	0.51
12:M:269:MET:HE3	12:M:402:LEU:HD12	1.93	0.51
3:R:96:THR:N	3:R:97:PRO:HD2	2.26	0.50
3:L:387:HIS:NE2	3:L:454:ASP:O	2.41	0.50
3:R:63:ARG:CG	3:R:478:THR:HA	2.41	0.50
7:V:108:VAL:HG12	7:V:110:TYR:CE1	2.46	0.50
11:E:42:LEU:HD13	11:E:122:VAL:HG12	1.93	0.50
3:L:385:ASP:O	3:L:389:THR:N	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:251:THR:HG23	12:Y:403:VAL:HG11	1.93	0.50
3:R:62:MET:SD	3:R:83:PHE:HB3	2.51	0.50
10:O:184:PHE:O	10:O:188:CYS:N	2.43	0.50
11:E:433:LEU:CD1	17:E:608:CDL:HA61	2.42	0.50
3:L:63:ARG:CD	16:L:603:HEA:OMA	2.59	0.50
3:L:155:SER:OG	3:L:245:TYR:HB3	2.11	0.50
11:E:224:GLY:HA2	17:E:606:CDL:H782	1.93	0.50
2:K:275:GLU:O	2:K:281:HIS:CE1	2.64	0.50
12:M:364:LEU:HD13	12:M:371:GLN:NE2	2.27	0.50
5:T:126:CYS:CB	17:T:202:CDL:H321	2.42	0.50
8:P:72:GLU:HG2	11:E:409:TRP:NE1	2.27	0.50
12:M:355:LEU:HD22	12:M:364:LEU:HD23	1.94	0.50
2:Q:43:ALA:O	2:Q:240:LEU:HD12	2.11	0.50
10:O:240:ASP:OD1	10:O:243:ARG:NH2	2.45	0.50
2:K:135:ALA:HB1	2:K:232:HIS:HE1	1.77	0.50
3:L:111:ILE:HD12	3:L:196:MET:O	2.12	0.50
11:F:124:LEU:HD11	11:F:344:LEU:HD11	1.93	0.50
11:F:135:ARG:NE	11:F:358:ASP:O	2.45	0.50
10:O:245:ILE:HG21	20:O:302:HEC:HMB1	1.94	0.50
11:E:227:LEU:HD22	17:E:606:CDL:H781	1.92	0.50
3:L:63:ARG:HG3	3:L:481:ALA:CB	2.42	0.50
8:J:72:GLU:HG2	11:F:409:TRP:CD1	2.47	0.50
17:F:608:CDL:H771	17:F:608:CDL:H162	1.94	0.50
2:Q:232:HIS:O	2:Q:245:VAL:N	2.44	0.50
3:R:265:PRO:O	3:R:269:ILE:HG23	2.12	0.50
11:E:27:ARG:HB2	12:Y:177:VAL:HG22	1.92	0.50
11:E:235:HIS:ND1	11:E:236:THR:O	2.45	0.50
11:E:249:VAL:HG22	12:M:161:VAL:HG23	1.93	0.50
2:K:28:SER:O	2:K:32:ALA:N	2.44	0.50
3:L:371:LEU:HD23	3:L:371:LEU:O	2.11	0.50
11:F:161:LEU:HD21	11:F:208:TYR:HA	1.93	0.50
3:R:516:SER:OG	3:R:518:GLU:OE1	2.29	0.49
1:W:75:PHE:CE2	1:W:114:VAL:HG11	2.47	0.49
19:T:201:MQ9:O4	11:E:399:LYS:NZ	2.43	0.49
12:M:173:HIS:O	12:M:177:VAL:HG23	2.11	0.49
3:R:266:GLU:O	3:R:269:ILE:HG12	2.12	0.49
4:S:175:ALA:O	4:S:179:ILE:HG13	2.13	0.49
22:F:601:HEM:HMB1	22:F:601:HEM:HBB2	1.94	0.49
12:M:269:MET:CE	12:M:282:VAL:HG11	2.42	0.49
3:R:95:ALA:CB	3:R:270:ILE:HD12	2.42	0.49
3:L:35:THR:HG22	3:L:119:PRO:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:95:ALA:CB	3:L:270:ILE:HD12	2.43	0.49
5:Z:123:THR:HG23	17:Z:202:CDL:C32	2.43	0.49
12:Y:230:THR:HG23	12:Y:244:THR:HG22	1.93	0.49
10:O:267:GLY:O	10:O:271:GLU:HG3	2.12	0.49
11:E:106:ARG:NH2	22:E:602:HEM:O2A	2.46	0.49
3:L:395:ILE:HA	3:L:398:PHE:CE1	2.48	0.49
3:L:538:SER:OG	3:L:544:GLU:OE2	2.30	0.49
17:X:302:CDL:H131	17:Z:202:CDL:OB7	2.13	0.49
11:F:37:HIS:CE1	11:F:39:SER:HG	2.25	0.49
2:Q:50:TRP:CE3	3:R:384:LEU:HD13	2.47	0.49
2:Q:214:VAL:C	2:Q:215:LEU:HD12	2.32	0.49
3:L:95:ALA:HB1	3:L:270:ILE:HG23	1.93	0.49
17:L:605:CDL:H582	17:J:201:CDL:H402	1.95	0.49
12:M:230:THR:HG23	12:M:244:THR:HG22	1.93	0.49
11:E:121:MET:HE3	19:E:604:MQ9:H261	1.94	0.49
8:J:58:PHE:HA	8:J:61:VAL:HG12	1.95	0.49
3:R:71:LEU:HD12	3:R:74:LEU:O	2.12	0.49
10:O:90:CYS:CB	20:O:301:HEC:HBC2	2.43	0.49
2:K:135:ALA:HB1	2:K:232:HIS:CE1	2.48	0.49
1:W:54:VAL:HG22	1:W:75:PHE:HB2	1.94	0.49
4:S:41:ALA:CA	5:T:44:LEU:HD22	2.43	0.49
17:T:202:CDL:H751	17:T:202:CDL:H561	1.94	0.49
19:Z:201:MQ9:H5M1	11:F:395:ILE:CG2	2.43	0.49
1:W:54:VAL:HG11	1:W:162:VAL:HG11	1.95	0.49
9:D:39:TRP:HE1	12:Y:251:THR:HG1	1.59	0.49
2:Q:231:ILE:HG22	3:R:156:PRO:CG	2.43	0.48
2:Q:273:CYS:O	2:Q:281:HIS:CE1	2.65	0.48
4:S:167:MET:CE	17:S:302:CDL:HA31	2.43	0.48
2:K:294:ASN:OD1	2:K:295:ASP:N	2.46	0.48
16:L:603:HEA:HMC1	16:L:603:HEA:HBC1	1.94	0.48
10:I:267:GLY:O	10:I:271:GLU:HG3	2.12	0.48
11:F:76:VAL:HG13	11:F:98:GLU:OE2	2.12	0.48
11:F:192:ALA:O	11:F:206:ARG:NH1	2.46	0.48
2:Q:57:SER:O	3:R:374:LEU:HD13	2.13	0.48
2:Q:279:THR:HG23	2:Q:280:PHE:CD1	2.48	0.48
3:R:14:ARG:O	6:U:49:TRP:HA	2.13	0.48
8:J:76:LEU:HD11	11:F:409:TRP:CZ3	2.47	0.48
2:K:113:THR:HG23	3:L:383:PRO:HD2	1.94	0.48
3:L:505:VAL:HG13	3:L:505:VAL:O	2.13	0.48
4:X:121:TYR:HH	4:X:144:THR:CB	2.24	0.48
11:F:254:MET:HB3	11:F:255:PRO:CD	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:60:GLY:O	12:M:65:VAL:N	2.45	0.48
3:R:84:THR:OG1	3:R:149:PHE:O	2.31	0.48
5:T:108:LEU:O	5:T:110:LEU:N	2.47	0.48
8:P:83:ILE:HG12	17:P:202:CDL:H561	1.95	0.48
11:E:59:TRP:CE3	11:E:105:VAL:HG11	2.48	0.48
2:K:279:THR:HG21	10:I:126:ARG:HA	1.96	0.48
17:X:302:CDL:H731	17:Z:202:CDL:C53	2.43	0.48
17:Z:202:CDL:C57	10:I:282:ALA:HA	2.42	0.48
11:F:71:VAL:HG21	11:F:90:GLU:OE1	2.13	0.48
2:Q:106:ILE:HD13	3:R:335:VAL:HG23	1.95	0.48
8:J:35:SER:OG	11:F:438:ARG:NH2	2.43	0.48
10:I:177:VAL:O	10:I:181:GLY:N	2.43	0.48
2:Q:222:GLU:OE1	2:Q:259:GLN:CG	2.61	0.48
3:R:26:ASN:OD1	17:R:604:CDL:HA21	2.13	0.48
3:R:406:ILE:HD11	16:R:603:HEA:HBC2	1.94	0.48
4:X:11:ALA:N	11:F:493:SER:OG	2.46	0.48
17:X:302:CDL:OB6	17:X:302:CDL:C13	2.61	0.48
3:R:216:THR:HG23	3:R:269:ILE:HB	1.96	0.48
3:R:539:GLU:N	3:R:539:GLU:OE1	2.46	0.48
2:K:159:ALA:C	2:K:161:PRO:HD3	2.34	0.48
5:Z:59:VAL:HG12	5:Z:63:LEU:HD22	1.96	0.48
12:M:76:VAL:O	12:M:76:VAL:HG13	2.13	0.48
2:Q:138:TRP:CZ2	2:Q:279:THR:HG22	2.49	0.48
3:R:97:PRO:HG3	3:R:129:PHE:CZ	2.49	0.48
2:Q:98:LEU:HD13	3:R:342:PHE:HD1	1.79	0.48
3:R:110:GLN:NE2	3:R:280:GLU:OE1	2.46	0.48
7:V:19:GLY:O	7:V:31:VAL:HG22	2.14	0.48
8:P:76:LEU:HD11	11:E:409:TRP:CH2	2.48	0.48
10:O:191:CYS:SG	20:O:302:HEC:HBC2	2.54	0.48
11:E:404:LEU:HD21	12:M:369:GLN:HB3	1.96	0.48
3:L:418:PHE:HB3	3:L:419:PRO:HD3	1.95	0.48
11:F:447:THR:HG22	11:F:488:MET:HG3	1.95	0.48
2:Q:61:GLY:HA2	3:R:370:LEU:HD21	1.96	0.48
3:R:264:HIS:O	3:R:267:VAL:HG22	2.14	0.48
17:S:302:CDL:H551	17:S:302:CDL:H141	1.96	0.48
10:O:72:GLN:O	10:O:76:LEU:HD23	2.14	0.48
2:K:68:ILE:HG21	3:L:367:ILE:HD11	1.96	0.48
2:K:302:GLN:OE1	2:K:315:ALA:HB3	2.14	0.48
17:L:605:CDL:H531	17:L:605:CDL:CB7	2.44	0.48
8:P:10:LEU:HD23	8:P:10:LEU:H	1.79	0.47
2:K:231:ILE:HG22	3:L:156:PRO:CG	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:242:GLY:N	12:Y:310:ASN:OD1	2.47	0.47
3:R:194:VAL:HG13	5:T:4:GLU:HG2	1.95	0.47
4:S:100:ARG:O	4:S:104:VAL:HG23	2.15	0.47
5:T:15:PHE:CE2	5:T:49:THR:HG21	2.48	0.47
8:J:72:GLU:HG2	11:F:409:TRP:NE1	2.28	0.47
2:Q:185:ILE:CD1	3:R:248:ALA:HB3	2.44	0.47
3:R:88:THR:HG22	3:R:151:TRP:HD1	1.80	0.47
11:E:228:ALA:CB	17:E:606:CDL:H321	2.44	0.47
2:K:328:PHE:CD1	3:L:465:LEU:HD21	2.49	0.47
1:W:95:VAL:O	1:W:95:VAL:HG23	2.13	0.47
2:Q:64:VAL:HG11	3:R:370:LEU:HD13	1.96	0.47
2:Q:222:GLU:OE1	2:Q:259:GLN:HG2	2.13	0.47
3:R:264:HIS:CE1	3:R:268:TYR:HE2	2.32	0.47
4:S:11:ALA:N	11:E:493:SER:OG	2.47	0.47
10:O:110:GLU:OE1	10:O:159:VAL:HG12	2.14	0.47
3:L:96:THR:N	3:L:97:PRO:HD3	2.30	0.47
10:I:209:ASP:OD1	10:I:210:LEU:N	2.47	0.47
2:Q:215:LEU:HD13	2:Q:288:VAL:CG2	2.44	0.47
5:T:126:CYS:HB3	17:T:202:CDL:H321	1.96	0.47
11:F:100:ARG:NH1	12:Y:107:PHE:O	2.41	0.47
17:F:607:CDL:H712	17:F:607:CDL:H511	1.96	0.47
3:R:33:THR:HG22	5:T:90:TRP:HB3	1.96	0.47
3:R:216:THR:O	3:R:220:VAL:HG23	2.15	0.47
12:M:356:TYR:HH	12:M:361:TYR:HD1	1.62	0.47
5:T:123:THR:HG23	17:T:202:CDL:H351	1.97	0.47
8:P:44:PRO:O	8:P:47:VAL:HG12	2.14	0.47
11:E:164:ASP:O	11:E:168:GLY:N	2.40	0.47
11:E:445:VAL:HG12	11:E:446:GLU:N	2.28	0.47
11:E:519:HIS:O	11:E:523:HIS:ND1	2.39	0.47
22:E:601:HEM:HBB2	22:E:601:HEM:CMB	2.44	0.47
3:L:163:SER:O	3:L:163:SER:OG	2.32	0.47
3:L:266:GLU:O	3:L:270:ILE:HG12	2.15	0.47
3:L:382:PRO:N	3:L:383:PRO:HD2	2.30	0.47
4:X:151:VAL:HG22	4:X:188:VAL:HG11	1.96	0.47
17:X:302:CDL:C74	17:Z:202:CDL:H532	2.45	0.47
5:Z:94:LEU:HD11	17:F:607:CDL:H752	1.97	0.47
8:J:62:MET:HG2	11:F:316:PRO:HG2	1.96	0.47
11:F:433:LEU:CD2	17:F:607:CDL:HA31	2.45	0.47
12:M:57:LYS:NZ	12:M:66:GLU:OE2	2.35	0.47
2:Q:195:TYR:CE2	2:Q:247:PRO:O	2.68	0.47
3:R:117:ALA:O	4:S:15:ARG:NH2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:401:VAL:HG23	3:L:402:LEU:N	2.29	0.47
17:L:605:CDL:H522	17:L:605:CDL:H552	1.52	0.47
4:X:186:HIS:O	4:X:189:ASP:OD1	2.33	0.47
10:I:123:PRO:O	10:I:134:LYS:NZ	2.37	0.47
11:F:312:ILE:HG21	12:Y:368:HIS:CD2	2.49	0.47
17:T:202:CDL:H571	17:T:202:CDL:H151	1.96	0.47
11:E:31:ASN:OD1	12:Y:180:ASN:ND2	2.46	0.47
11:E:94:ASP:O	11:E:98:GLU:N	2.45	0.47
3:L:52:PHE:O	3:L:55:GLY:O	2.33	0.47
4:X:186:HIS:HA	4:X:189:ASP:OD1	2.14	0.47
12:Y:348:HIS:O	24:Y:501:FES:S2	2.73	0.47
2:Q:31:LEU:HD21	2:Q:55:ILE:CD1	2.43	0.47
5:Z:6:ARG:O	5:Z:10:ILE:HG12	2.15	0.47
11:F:86:SER:OG	11:F:163:ASP:HB3	2.15	0.47
12:Y:291:ASP:OD1	12:Y:293:THR:HG22	2.15	0.47
4:X:58:TRP:O	4:X:60:PRO:HD3	2.16	0.46
4:X:184:TYR:CZ	17:X:303:CDL:H752	2.50	0.46
10:I:87:CYS:HB3	20:I:301:HEC:HAB	1.97	0.46
3:R:107:LEU:HD13	3:R:213:ILE:HG21	1.97	0.46
10:O:209:ASP:OD1	10:O:210:LEU:N	2.48	0.46
2:K:245:VAL:HG23	2:K:245:VAL:O	2.14	0.46
3:L:286:SER:HA	3:L:353:LEU:HD23	1.97	0.46
3:L:445:THR:HA	3:L:477:SER:HA	1.96	0.46
17:X:302:CDL:H121	17:X:302:CDL:CB5	2.45	0.46
5:Z:123:THR:HG23	17:Z:202:CDL:C33	2.45	0.46
8:J:23:GLU:O	8:J:24:ARG:HD3	2.15	0.46
10:I:191:CYS:SG	10:I:207:ALA:HB2	2.55	0.46
2:Q:101:ILE:HG22	2:Q:102:PRO:HD3	1.98	0.46
3:R:374:LEU:O	3:R:378:LEU:HD13	2.15	0.46
6:U:11:GLY:O	6:U:15:LEU:HD23	2.15	0.46
10:O:261:TYR:CE2	10:O:263:LEU:HD23	2.50	0.46
3:L:97:PRO:CG	3:L:129:PHE:CE1	2.97	0.46
11:F:261:SER:OG	19:F:605:MQ9:H5M1	2.15	0.46
12:Y:49:GLU:OE1	12:Y:49:GLU:N	2.47	0.46
2:Q:242:LYS:HD3	2:Q:274:THR:HG21	1.98	0.46
3:R:505:VAL:HG21	3:R:510:PRO:HB3	1.97	0.46
17:S:302:CDL:H731	17:T:202:CDL:H532	1.97	0.46
8:P:8:SER:OG	11:E:480:ALA:O	2.17	0.46
8:P:67:HIS:NE2	8:P:73:ASP:OD1	2.45	0.46
11:F:385:LEU:HD11	17:F:608:CDL:H781	1.96	0.46
3:R:243:HIS:NE2	4:S:132:PRO:O	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:264:HIS:CE1	3:R:310:VAL:HG13	2.50	0.46
7:V:73:LEU:HG	7:V:73:LEU:O	2.16	0.46
10:O:108:THR:HG21	20:O:301:HEC:HBA2	1.97	0.46
11:E:235:HIS:NE2	22:E:601:HEM:O2A	2.39	0.46
3:L:28:ILE:HG23	3:L:29:TYR:N	2.30	0.46
3:L:274:PHE:CB	3:L:405:THR:O	2.63	0.46
12:M:412:VAL:O	12:M:412:VAL:HG22	2.14	0.46
10:O:115:PHE:CE1	10:O:221:ALA:HB2	2.51	0.46
3:L:270:ILE:HG22	3:L:406:ILE:HG21	1.97	0.46
3:L:500:ARG:NH2	8:J:100:ARG:O	2.47	0.46
12:M:85:THR:HG23	12:M:153:LYS:HD3	1.97	0.46
2:Q:179:ILE:HG23	2:Q:180:GLU:N	2.30	0.46
20:O:301:HEC:HBA1	20:O:301:HEC:HHA	1.97	0.46
11:E:123:HIS:NE2	22:E:601:HEM:ND	2.64	0.46
3:L:74:LEU:CD1	3:L:82:LEU:HD12	2.46	0.46
3:L:119:PRO:O	3:L:122:ASN:OD1	2.33	0.46
3:L:376:GLY:CA	3:L:397:HIS:CE1	2.99	0.46
10:I:105:LEU:HD21	20:I:301:HEC:CHB	2.46	0.46
11:F:105:VAL:HG22	19:F:605:MQ9:C51	2.45	0.46
3:R:373:GLY:HA2	16:R:602:HEA:C13	2.46	0.46
10:O:232:PHE:CE1	20:O:302:HEC:HBB2	2.50	0.46
2:K:288:VAL:O	2:K:288:VAL:HG13	2.15	0.46
3:L:201:MET:CE	3:L:517:LEU:HD22	2.45	0.46
12:M:387:ARG:CZ	12:M:415:ALA:HB2	2.46	0.46
3:R:440:ILE:HG21	6:U:17:LEU:HD11	1.96	0.46
19:T:201:MQ9:H471	11:E:410:ILE:HG21	1.98	0.46
11:E:22:PRO:HB3	17:F:606:CDL:HA31	1.97	0.46
11:E:54:LEU:HD23	22:E:602:HEM:HMC3	1.98	0.46
11:E:160:SER:HA	11:E:167:SER:HB2	1.98	0.46
11:F:127:ILE:HD11	22:F:601:HEM:CAC	2.46	0.46
17:F:608:CDL:H761	17:F:608:CDL:H792	1.49	0.46
12:Y:76:VAL:HG13	12:Y:76:VAL:O	2.15	0.46
12:Y:246:ARG:N	12:Y:250:GLU:OE1	2.49	0.46
1:W:120:GLN:NE2	10:O:152:ALA:O	2.44	0.46
2:Q:137:GLN:HE21	2:Q:138:TRP:HE1	1.64	0.46
3:R:156:PRO:HD3	3:R:252:VAL:HG12	1.97	0.46
3:R:310:VAL:HG22	3:R:310:VAL:O	2.16	0.46
10:O:179:ARG:O	10:O:183:LEU:HD23	2.16	0.46
19:Z:201:MQ9:H5M1	11:F:395:ILE:HG21	1.98	0.46
11:F:252:ARG:N	12:Y:158:GLU:OE2	2.49	0.46
7:V:140:ILE:O	7:V:144:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:E:606:CDL:H551	17:E:606:CDL:H581	1.49	0.45
17:X:302:CDL:OB9	17:X:302:CDL:CB4	2.63	0.45
12:Y:99:SER:OG	12:Y:135:THR:O	2.34	0.45
3:R:63:ARG:HG2	3:R:478:THR:HA	1.98	0.45
3:R:312:ALA:HB3	3:R:326:PHE:CZ	2.51	0.45
2:K:45:LEU:CD2	2:K:116:VAL:HG13	2.45	0.45
4:X:22:PRO:N	5:Z:63:LEU:HD21	2.31	0.45
17:J:201:CDL:H722	17:J:201:CDL:H512	1.98	0.45
12:Y:173:HIS:O	12:Y:177:VAL:HG23	2.17	0.45
2:Q:96:LEU:HA	2:Q:99:THR:HG22	1.98	0.45
3:L:180:LEU:HD23	5:Z:99:PHE:CE2	2.51	0.45
3:L:281:ILE:HD13	3:L:412:ALA:HB1	1.99	0.45
3:L:442:PHE:O	3:L:445:THR:HG22	2.15	0.45
4:X:41:ALA:CA	5:Z:44:LEU:HD22	2.46	0.45
8:J:56:ALA:O	8:J:60:LEU:HD23	2.16	0.45
11:F:60:LEU:HD21	11:F:106:ARG:HB3	1.99	0.45
11:F:117:ALA:O	11:F:121:MET:HG3	2.16	0.45
12:M:230:THR:HG22	12:M:231:ALA:N	2.31	0.45
2:Q:128:GLU:OE2	2:Q:149:PHE:HA	2.15	0.45
17:S:303:CDL:H351	17:S:303:CDL:H321	1.68	0.45
5:T:95:ILE:HD11	5:T:128:LEU:HB2	1.96	0.45
11:E:117:ALA:O	11:E:121:MET:HG3	2.16	0.45
22:E:602:HEM:HBC2	22:E:602:HEM:CMC	2.47	0.45
4:X:147:HIS:NE2	4:X:192:TRP:HB2	2.31	0.45
2:Q:282:ALA:HA	3:R:461:TYR:CE1	2.51	0.45
3:R:379:LEU:HD23	3:R:388:VAL:HG23	1.98	0.45
3:R:460:ARG:N	16:R:603:HEA:O2A	2.49	0.45
2:K:134:THR:HG23	2:K:141:LYS:HB3	1.97	0.45
3:L:62:MET:SD	3:L:83:PHE:HB3	2.56	0.45
11:F:193:LEU:O	11:F:206:ARG:NH1	2.50	0.45
10:O:87:CYS:HB3	20:O:301:HEC:HAB	1.98	0.45
10:O:222:MET:HG2	20:O:302:HEC:HBB3	1.98	0.45
11:E:38:TRP:CH2	17:E:608:CDL:H522	2.52	0.45
11:E:228:ALA:HB3	17:E:606:CDL:H321	1.99	0.45
3:L:121:LEU:HD13	17:X:303:CDL:HA31	1.98	0.45
3:L:389:THR:OG1	16:L:602:HEA:O1A	2.33	0.45
3:L:391:SER:HA	3:L:458:PRO:HA	1.99	0.45
4:X:156:VAL:HG22	17:X:302:CDL:H381	1.99	0.45
17:X:302:CDL:HA61	17:X:302:CDL:H312	1.66	0.45
10:I:184:PHE:O	10:I:188:CYS:N	2.46	0.45
3:R:264:HIS:HB3	3:R:265:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:523:CYS:HB3	3:R:524:PRO:HD3	1.98	0.45
17:R:604:CDL:HB4	17:R:604:CDL:H721	1.99	0.45
4:S:159:VAL:HG11	17:S:302:CDL:H392	1.99	0.45
10:O:190:SER:O	12:M:355:LEU:HD11	2.16	0.45
4:X:67:LEU:HA	4:X:70:ALA:HB3	1.99	0.45
11:F:22:PRO:HB3	17:F:606:CDL:H542	1.98	0.45
22:F:601:HEM:HBB2	22:F:601:HEM:CMB	2.47	0.45
3:R:216:THR:HG21	3:R:273:PRO:HG3	1.99	0.45
2:K:61:GLY:HA2	3:L:370:LEU:HD21	1.98	0.45
3:L:190:ILE:HG21	4:X:31:VAL:HG11	1.99	0.45
4:X:21:ARG:NH1	4:X:22:PRO:HD2	2.32	0.45
12:M:309:ARG:HA	12:M:345:VAL:HG21	1.99	0.45
2:Q:135:ALA:HB2	2:Q:140:TRP:CE3	2.51	0.45
2:Q:135:ALA:HB2	2:Q:140:TRP:CZ3	2.52	0.45
2:K:180:GLU:O	2:K:180:GLU:OE1	2.35	0.45
2:K:225:LEU:HB3	2:K:245:VAL:HG12	1.99	0.45
3:L:254:LEU:HD13	4:X:49:THR:HG21	1.99	0.45
3:L:357:THR:N	3:L:428:GLU:OE2	2.41	0.45
16:L:602:HEA:H121	16:L:602:HEA:HHC	1.99	0.45
12:M:358:GLN:O	12:M:359:GLN:HB2	2.17	0.45
2:Q:136:PHE:CZ	2:Q:139:ASN:HB3	2.52	0.45
3:R:35:THR:HG21	5:T:87:PRO:HA	1.98	0.45
17:S:302:CDL:H381	17:S:302:CDL:H412	1.73	0.45
17:S:303:CDL:H771	17:S:303:CDL:H581	1.99	0.45
11:E:87:ARG:NH1	11:E:90:GLU:OE2	2.46	0.45
2:K:248:GLU:OE1	3:L:248:ALA:HA	2.17	0.45
3:L:162:HIS:O	3:L:163:SER:OG	2.35	0.45
4:X:184:TYR:CD1	17:X:303:CDL:H731	2.52	0.45
12:M:378:ALA:HB3	12:M:389:LEU:HB2	1.99	0.45
3:R:35:THR:OG1	3:R:119:PRO:HB2	2.17	0.44
5:T:95:ILE:CD1	5:T:128:LEU:HD22	2.46	0.44
10:O:91:HIS:CE1	10:O:105:LEU:HD21	2.51	0.44
3:L:46:VAL:HG21	17:L:605:CDL:H341	1.98	0.44
4:X:22:PRO:HB3	5:Z:59:VAL:HG11	1.99	0.44
11:F:164:ASP:O	11:F:168:GLY:N	2.41	0.44
11:F:236:THR:HG22	22:F:601:HEM:O1D	2.16	0.44
12:Y:94:MET:O	12:Y:98:LEU:HD23	2.18	0.44
3:R:254:LEU:HD22	4:S:49:THR:HG21	1.99	0.44
4:S:41:ALA:HB2	5:T:44:LEU:CB	2.47	0.44
2:K:47:ARG:O	2:K:51:ILE:HG12	2.18	0.44
4:X:34:SER:HB3	5:Z:48:LEU:HG	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:44:PRO:O	8:J:47:VAL:HG22	2.18	0.44
17:F:606:CDL:H362	17:F:606:CDL:H332	1.77	0.44
3:R:266:GLU:O	3:R:270:ILE:HG12	2.18	0.44
17:E:607:CDL:H371	17:E:607:CDL:H801	1.99	0.44
3:L:406:ILE:O	3:L:410:THR:OG1	2.32	0.44
4:X:15:ARG:O	4:X:16:VAL:HG23	2.16	0.44
4:X:101:ARG:HG2	11:F:503:LEU:HD12	2.00	0.44
12:Y:295:VAL:HG23	12:M:293:THR:O	2.16	0.44
3:R:190:ILE:CD1	3:R:221:LEU:HD11	2.48	0.44
11:E:213:LEU:HD21	22:F:602:HEM:HBC1	2.00	0.44
17:E:608:CDL:H632	17:E:608:CDL:H602	1.42	0.44
2:K:195:TYR:CE2	2:K:247:PRO:O	2.70	0.44
3:L:90:MET:CE	16:L:603:HEA:HMC3	2.47	0.44
3:L:99:VAL:HG12	3:L:274:PHE:CE2	2.53	0.44
3:L:254:LEU:HD22	4:X:49:THR:HG21	2.00	0.44
3:L:394:VAL:O	3:L:398:PHE:CD1	2.71	0.44
11:F:106:ARG:NH2	22:F:602:HEM:O2A	2.51	0.44
11:F:122:VAL:HG13	17:F:608:CDL:H571	1.98	0.44
11:F:237:GLN:NE2	11:F:244:THR:O	2.51	0.44
11:F:386:LEU:HD11	11:F:414:GLY:HA3	2.00	0.44
16:R:603:HEA:HBC1	16:R:603:HEA:HMC1	2.00	0.44
4:S:130:THR:HG22	4:S:132:PRO:HD2	1.99	0.44
6:U:3:THR:HG23	6:U:4:ALA:N	2.33	0.44
10:O:269:ALA:HB3	10:O:270:PRO:CD	2.45	0.44
11:E:366:ARG:NH1	11:E:437:ASP:OD2	2.49	0.44
11:E:436:SER:O	11:E:440:VAL:HG23	2.17	0.44
3:L:99:VAL:HG23	3:L:100:PHE:N	2.33	0.44
3:L:227:LEU:HB2	3:L:262:PHE:CD1	2.52	0.44
10:I:191:CYS:SG	10:I:201:LEU:HD21	2.58	0.44
12:Y:69:PHE:O	12:Y:69:PHE:CG	2.70	0.44
12:Y:368:HIS:CE1	24:Y:501:FES:S2	3.11	0.44
2:Q:32:ALA:HB1	2:Q:35:TRP:HD1	1.83	0.44
3:R:312:ALA:HB3	3:R:326:PHE:CE1	2.53	0.44
3:R:437:LEU:HG	6:U:21:LEU:HD12	1.98	0.44
4:S:43:LEU:HD23	4:S:143:ALA:HA	2.00	0.44
7:V:121:SER:O	7:V:125:LEU:HD13	2.17	0.44
8:P:93:LEU:O	8:P:98:TRP:N	2.38	0.44
17:X:302:CDL:H162	17:Z:202:CDL:C73	2.47	0.44
5:Z:123:THR:HG22	17:Z:202:CDL:H322	1.98	0.44
3:R:29:TYR:CZ	3:R:33:THR:HG21	2.53	0.44
11:E:25:ALA:O	11:E:29:GLN:OE1	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:211:HIS:O	11:E:216:PRO:HG3	2.16	0.44
2:K:132:ASP:OD1	2:K:197:ASN:OD1	2.36	0.44
3:L:90:MET:HE2	16:L:603:HEA:HMC3	1.99	0.44
3:L:97:PRO:HG2	3:L:129:PHE:CZ	2.53	0.44
3:L:322:LEU:HD21	5:Z:25:LEU:HB3	2.00	0.44
3:L:400:TYR:HA	3:L:442:PHE:HZ	1.83	0.44
3:L:522:SER:OG	3:L:524:PRO:O	2.34	0.44
17:L:605:CDL:H591	17:L:605:CDL:H561	1.58	0.44
4:X:156:VAL:HG11	17:X:303:CDL:H572	1.99	0.44
4:X:163:ALA:HB1	17:X:302:CDL:HA61	2.00	0.44
4:S:111:LEU:O	4:S:115:LEU:HD13	2.18	0.44
2:K:68:ILE:O	2:K:71:THR:HG22	2.17	0.44
2:K:129:VAL:HG12	2:K:221:ILE:HG13	2.00	0.44
10:I:116:GLN:HB3	10:I:122:MET:CG	2.48	0.44
11:F:197:ASP:OD2	12:Y:309:ARG:NH2	2.45	0.44
12:Y:395:THR:O	12:Y:402:LEU:HD23	2.18	0.44
3:R:270:ILE:HG22	3:R:406:ILE:HG21	2.00	0.44
3:R:401:VAL:HG23	3:R:402:LEU:N	2.33	0.44
3:R:472:THR:O	3:R:475:VAL:HG22	2.18	0.44
3:R:509:ASP:OD1	3:R:519:TRP:HB3	2.18	0.44
11:E:148:LEU:HD21	19:E:604:MQ9:H301	1.99	0.44
12:M:348:HIS:O	24:M:501:FES:S2	2.76	0.44
3:R:11:LEU:HD13	6:U:48:LEU:CB	2.48	0.43
3:R:89:VAL:HG22	3:R:137:ILE:HD11	1.98	0.43
3:R:104:ASN:ND2	3:R:189:MET:CE	2.81	0.43
9:G:28:ALA:HB2	12:M:329:LYS:CG	2.48	0.43
3:L:11:LEU:HD12	3:L:11:LEU:O	2.17	0.43
3:L:29:TYR:HE1	17:F:607:CDL:HA62	1.84	0.43
3:L:49:PHE:CE2	3:L:414:ILE:HD11	2.52	0.43
3:L:95:ALA:HB2	3:L:406:ILE:HD12	1.99	0.43
3:L:97:PRO:HG3	3:L:129:PHE:CE1	2.53	0.43
9:D:32:PRO:O	12:Y:327:LYS:NZ	2.44	0.43
11:F:235:HIS:NE2	22:F:601:HEM:O2A	2.51	0.43
12:Y:295:VAL:HG21	12:M:298:GLU:HG3	2.00	0.43
3:R:155:SER:OG	3:R:245:TYR:HB3	2.18	0.43
3:R:242:ALA:O	3:R:244:ILE:N	2.51	0.43
4:S:151:VAL:HG22	4:S:188:VAL:HG11	2.00	0.43
12:Y:86:GLU:HG3	12:M:196:ILE:CD1	2.48	0.43
3:R:414:ILE:O	3:R:418:PHE:HB2	2.18	0.43
3:R:420:LYS:O	3:R:420:LYS:HD3	2.19	0.43
4:S:184:TYR:CG	17:S:303:CDL:H731	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:83:PHE:CZ	10:O:95:LEU:HD13	2.53	0.43
10:O:182:ASP:OD1	10:O:185:ARG:NH2	2.51	0.43
20:O:301:HEC:HBD1	20:O:301:HEC:HMD1	2.00	0.43
11:E:229:LEU:HD22	11:F:20:TYR:HE1	1.82	0.43
3:L:96:THR:O	3:L:99:VAL:HG22	2.18	0.43
3:L:285:PHE:HB2	3:L:359:MET:CE	2.48	0.43
4:X:103:TYR:OH	4:X:178:ALA:O	2.32	0.43
17:X:302:CDL:H721	17:Z:202:CDL:C51	2.38	0.43
17:X:302:CDL:HB22	17:Z:202:CDL:CB4	2.49	0.43
3:R:420:LYS:NZ	3:R:519:TRP:HA	2.33	0.43
17:S:302:CDL:H1	17:T:202:CDL:HB4	1.99	0.43
8:P:10:LEU:HD22	8:P:38:TRP:CZ3	2.54	0.43
4:X:163:ALA:CB	17:X:302:CDL:H312	2.49	0.43
9:D:109:HIS:N	9:D:158:LEU:O	2.49	0.43
11:F:110:HIS:HB3	11:F:281:ILE:HG21	1.99	0.43
11:F:265:PHE:HE2	19:F:605:MQ9:C34	2.32	0.43
12:Y:41:GLN:NE2	12:Y:43:THR:HG22	2.33	0.43
5:T:91:TRP:N	5:T:92:PRO:CD	2.81	0.43
7:V:70:ILE:HG12	7:V:143:LEU:HD21	1.99	0.43
10:I:112:ALA:HB2	10:I:224:THR:HG21	1.99	0.43
10:I:229:MET:HE3	20:I:302:HEC:NB	2.34	0.43
11:F:368:ARG:O	11:F:434:GLN:NE2	2.38	0.43
11:F:437:ASP:O	11:F:440:VAL:HG12	2.19	0.43
2:Q:199:ASP:N	2:Q:202:GLU:OE2	2.47	0.43
3:R:99:VAL:HG23	3:R:100:PHE:N	2.34	0.43
11:E:171:ILE:HG21	11:E:203:LEU:HD21	2.00	0.43
2:K:298:ALA:O	2:K:302:GLN:HG3	2.18	0.43
3:L:418:PHE:HE1	3:L:499:TRP:CD1	2.37	0.43
10:I:278:ILE:HD11	21:I:303:9YF:C37	2.49	0.43
11:F:231:TRP:CG	17:F:606:CDL:H721	2.53	0.43
2:Q:168:THR:HG23	2:Q:168:THR:O	2.18	0.43
3:R:374:LEU:O	3:R:377:VAL:HG12	2.18	0.43
3:R:420:LYS:HE2	3:R:523:CYS:HA	2.00	0.43
17:R:604:CDL:HB4	11:E:424:PHE:HE2	1.83	0.43
8:P:83:ILE:HG23	17:P:202:CDL:H542	2.00	0.43
11:E:166:LEU:O	11:E:169:THR:HG22	2.19	0.43
4:X:120:GLU:O	4:X:124:LEU:HD13	2.18	0.43
12:Y:324:ARG:HB2	12:Y:375:LEU:HD13	2.00	0.43
2:Q:132:ASP:OD1	2:Q:197:ASN:ND2	2.51	0.43
2:Q:232:HIS:O	2:Q:245:VAL:HG22	2.18	0.43
2:Q:270:VAL:HG22	2:Q:271:GLY:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:283:MET:SD	2:Q:328:PHE:CE2	3.12	0.43
17:S:302:CDL:H722	12:M:145:ILE:HG23	2.01	0.43
10:O:151:GLN:O	10:O:155:GLY:N	2.52	0.43
2:K:64:VAL:HG11	3:L:370:LEU:HD13	2.01	0.43
4:X:41:ALA:HB2	5:Z:44:LEU:CB	2.49	0.43
5:Z:26:THR:O	5:Z:30:ALA:HB3	2.19	0.43
10:I:273:MET:SD	19:F:604:MQ9:H3D	2.59	0.43
3:R:242:ALA:O	4:S:138:SER:HB2	2.19	0.43
3:R:264:HIS:CE1	3:R:268:TYR:CE2	3.07	0.43
10:O:260:GLY:O	11:E:280:THR:OG1	2.36	0.43
20:O:301:HEC:HBB3	20:O:301:HEC:CMB	2.48	0.43
11:E:20:TYR:CE1	11:F:229:LEU:HD22	2.53	0.43
11:E:519:HIS:NE2	11:E:523:HIS:HE1	2.17	0.43
2:K:270:VAL:HG22	2:K:271:GLY:N	2.34	0.43
3:L:95:ALA:HB1	3:L:270:ILE:HD12	2.01	0.43
2:Q:138:TRP:N	2:Q:138:TRP:CD1	2.86	0.43
3:R:227:LEU:HB2	3:R:262:PHE:CD1	2.54	0.43
4:S:156:VAL:HG22	17:S:302:CDL:H381	2.01	0.43
17:S:303:CDL:H391	17:S:303:CDL:H361	1.87	0.43
8:P:62:MET:HG3	11:E:316:PRO:HG2	2.01	0.43
10:O:192:HIS:ND1	10:O:210:LEU:HD21	2.33	0.43
11:E:29:GLN:OE1	11:E:29:GLN:N	2.52	0.43
11:E:123:HIS:CE1	11:E:127:ILE:HD11	2.54	0.43
11:E:295:VAL:HB	12:M:352:PRO:HG2	2.01	0.43
4:X:58:TRP:CE2	4:X:136:TYR:HD2	2.37	0.43
5:Z:90:TRP:HZ2	17:F:607:CDL:HB4	1.83	0.43
12:Y:376:GLU:O	12:Y:377:PHE:C	2.56	0.43
1:W:74:LEU:HD12	1:W:117:PRO:HG3	2.01	0.42
3:R:93:PHE:CE1	3:R:133:ALA:HA	2.54	0.42
3:L:107:LEU:HD22	3:L:213:ILE:HG21	2.01	0.42
3:L:159:ASP:O	3:L:162:HIS:O	2.37	0.42
11:F:433:LEU:HD12	17:F:608:CDL:HA61	2.01	0.42
11:F:512:GLU:O	11:F:513:ALA:C	2.56	0.42
12:M:274:ILE:HD11	12:M:280:GLU:HB3	2.01	0.42
2:Q:124:ASP:O	2:Q:259:GLN:NE2	2.50	0.42
2:Q:219:LYS:O	2:Q:221:ILE:HD12	2.18	0.42
10:O:87:CYS:HB3	20:O:301:HEC:HHC	2.01	0.42
10:O:250:ARG:NH2	10:O:254:GLU:OE2	2.45	0.42
3:L:138:ALA:O	3:L:141:ILE:HG12	2.19	0.42
3:L:278:VAL:HG21	3:L:365:PHE:CD2	2.54	0.42
17:X:302:CDL:H731	17:Z:202:CDL:H532	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:27:LEU:HD21	17:R:604:CDL:H312	2.01	0.42
17:S:302:CDL:C1	17:T:202:CDL:HB4	2.50	0.42
5:T:1:MET:O	5:T:1:MET:HG2	2.19	0.42
5:T:8:PHE:O	5:T:12:THR:HG23	2.19	0.42
17:T:202:CDL:H772	17:T:202:CDL:H741	1.48	0.42
2:K:145:GLN:O	2:K:158:GLY:N	2.53	0.42
3:L:23:PRO:HB2	11:F:435:ARG:CZ	2.50	0.42
3:L:117:ALA:N	3:L:192:THR:OG1	2.47	0.42
3:L:489:LEU:HB2	3:L:490:PRO:HD3	2.01	0.42
4:X:142:LEU:HD11	4:X:146:PHE:HE2	1.84	0.42
8:J:59:LEU:HD12	8:J:83:ILE:HD12	2.00	0.42
10:I:232:PHE:CE2	20:I:302:HEC:HBB2	2.54	0.42
11:F:94:ASP:O	11:F:98:GLU:N	2.44	0.42
1:W:71:VAL:CG2	1:W:139:LEU:HD21	2.49	0.42
1:W:121:ILE:HD11	10:O:151:GLN:HG2	2.02	0.42
2:Q:106:ILE:HD13	3:R:335:VAL:CG2	2.50	0.42
2:Q:235:TRP:CE3	3:R:458:PRO:HG3	2.54	0.42
2:Q:289:ARG:NH2	2:Q:321:LEU:O	2.52	0.42
3:R:243:HIS:ND1	3:R:246:ASP:OD2	2.52	0.42
3:R:551:VAL:HG23	3:R:552:GLU:N	2.33	0.42
8:P:85:ALA:HB1	17:P:202:CDL:H161	2.02	0.42
10:O:78:THR:O	10:O:82:LEU:HD13	2.19	0.42
11:E:194:PHE:CE2	11:E:203:LEU:HD22	2.54	0.42
11:E:367:PRO:O	11:E:374:THR:OG1	2.27	0.42
3:L:388:VAL:HG13	3:L:393:PHE:HB3	2.01	0.42
17:X:302:CDL:H731	17:Z:202:CDL:H531	2.02	0.42
10:I:267:GLY:O	10:I:271:GLU:CG	2.68	0.42
12:Y:358:GLN:O	12:Y:359:GLN:HB2	2.20	0.42
12:M:250:GLU:OE2	12:M:286:ARG:NE	2.40	0.42
3:R:180:LEU:HD23	5:T:99:PHE:CE2	2.55	0.42
4:S:186:HIS:HA	4:S:189:ASP:OD2	2.19	0.42
10:O:95:LEU:HD12	10:O:105:LEU:HB2	2.01	0.42
10:O:142:GLN:O	10:O:146:LEU:HD23	2.19	0.42
2:K:51:ILE:O	2:K:55:ILE:HG12	2.20	0.42
2:K:106:ILE:HB	3:L:331:PHE:HB3	2.01	0.42
2:K:134:THR:HG23	2:K:134:THR:O	2.20	0.42
3:L:187:VAL:HG22	4:X:31:VAL:HG12	2.01	0.42
3:L:216:THR:HG23	3:L:269:ILE:HB	2.02	0.42
17:X:302:CDL:H791	11:F:271:VAL:HG22	2.01	0.42
10:I:87:CYS:HB3	20:I:301:HEC:HHC	2.02	0.42
11:F:65:ASP:CB	11:F:91:THR:HG21	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:154:GLU:HB2	11:F:215:ILE:HG21	2.01	0.42
12:Y:407:ASP:OD1	12:Y:408:PHE:N	2.51	0.42
1:W:89:LYS:CD	1:W:100:LEU:HD13	2.49	0.42
1:W:102:GLY:O	1:W:133:VAL:HG22	2.20	0.42
2:Q:35:TRP:NE1	2:Q:50:TRP:CD1	2.87	0.42
2:Q:128:GLU:HB3	2:Q:220:ARG:O	2.18	0.42
3:R:95:ALA:HB1	3:R:270:ILE:HG23	2.02	0.42
5:Z:42:LEU:HA	5:Z:45:THR:HG22	2.01	0.42
17:Z:202:CDL:OB4	10:I:289:TRP:HD1	2.03	0.42
8:J:53:LEU:CD1	8:J:87:VAL:HG11	2.49	0.42
11:F:187:THR:HG22	12:Y:223:PRO:CB	2.50	0.42
12:M:110:TRP:HZ2	12:M:127:LEU:HD11	1.83	0.42
1:W:49:VAL:HG23	1:W:86:ASN:ND2	2.35	0.42
1:W:145:ASN:OD1	1:W:146:GLY:N	2.53	0.42
10:O:200:ALA:HB3	11:E:394:ASP:OD1	2.19	0.42
11:E:86:SER:OG	11:E:163:ASP:HB3	2.20	0.42
2:K:84:LEU:HD21	3:L:513:TYR:CE2	2.55	0.42
2:K:168:THR:O	2:K:168:THR:HG23	2.19	0.42
3:L:74:LEU:HD13	3:L:82:LEU:HD12	2.00	0.42
3:L:284:VAL:HG21	3:L:416:PHE:CE1	2.55	0.42
11:F:26:VAL:O	11:F:30:LEU:HG	2.19	0.42
12:M:366:PRO:O	12:M:369:GLN:NE2	2.52	0.42
2:Q:225:LEU:HB3	2:Q:245:VAL:HG12	2.02	0.42
3:R:93:PHE:HA	3:R:129:PHE:CZ	2.55	0.42
3:R:294:THR:HA	3:R:297:ILE:HG12	2.01	0.42
11:E:164:ASP:OD1	11:E:165:LEU:N	2.51	0.42
11:E:233:GLN:O	11:E:234:LYS:C	2.57	0.42
3:L:106:VAL:HG21	3:L:518:GLU:OE1	2.19	0.42
5:Z:15:PHE:CE2	5:Z:49:THR:HG21	2.54	0.42
5:Z:94:LEU:HD22	17:F:607:CDL:H611	2.01	0.42
8:J:86:LEU:HD23	17:J:201:CDL:H152	2.01	0.42
8:J:89:ARG:HD2	17:J:201:CDL:H151	2.02	0.42
11:F:48:TYR:CD1	11:F:265:PHE:HD1	2.38	0.42
17:F:606:CDL:H581	17:F:606:CDL:H552	1.51	0.42
12:Y:357:GLU:O	12:Y:361:TYR:N	2.53	0.42
12:M:69:PHE:O	12:M:69:PHE:CG	2.73	0.42
2:Q:98:LEU:C	2:Q:98:LEU:HD12	2.40	0.42
4:S:15:ARG:HD2	17:S:303:CDL:CB2	2.50	0.42
2:K:95:GLU:OE1	3:L:295:THR:OG1	2.27	0.42
2:K:214:VAL:HG22	2:K:313:LEU:HD21	2.02	0.42
11:F:22:PRO:HB2	11:F:26:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:225:ALA:O	11:F:229:LEU:HG	2.19	0.42
19:F:604:MQ9:H202	17:F:608:CDL:H572	2.01	0.42
5:T:35:GLU:O	5:T:36:TRP:HB2	2.20	0.42
19:T:201:MQ9:H402	19:T:201:MQ9:H203	2.02	0.42
10:O:139:ASP:OD1	10:O:139:ASP:N	2.46	0.42
10:O:192:HIS:O	10:O:193:ASN:HB2	2.19	0.42
11:E:386:LEU:HD11	11:E:414:GLY:HA3	2.02	0.42
22:E:602:HEM:HBA2	22:E:602:HEM:HHA	2.01	0.42
2:K:35:TRP:CE3	2:K:240:LEU:HD13	2.55	0.42
3:L:94:TYR:C	3:L:97:PRO:HD2	2.40	0.42
3:L:252:VAL:HG13	3:L:253:LEU:N	2.35	0.42
3:L:405:THR:O	3:L:409:ALA:HB3	2.20	0.42
11:F:48:TYR:CG	11:F:265:PHE:HD1	2.38	0.42
12:Y:172:VAL:HG13	12:Y:173:HIS:N	2.35	0.42
12:M:193:ARG:HB3	12:M:196:ILE:HD13	2.02	0.42
12:M:269:MET:HE1	12:M:314:LEU:HD22	2.02	0.42
1:W:24:CYS:N	13:W:201:9XX:O2	2.53	0.41
2:Q:101:ILE:N	2:Q:102:PRO:CD	2.83	0.41
3:R:215:VAL:CG1	3:R:304:ALA:HB2	2.50	0.41
3:R:274:PHE:CB	3:R:405:THR:O	2.68	0.41
3:R:335:VAL:HB	3:R:336:PRO:HD3	2.02	0.41
5:T:134:TRP:CE2	17:T:202:CDL:HA32	2.55	0.41
19:E:604:MQ9:C17	17:E:608:CDL:H772	2.50	0.41
3:L:310:VAL:O	3:L:310:VAL:HG22	2.21	0.41
11:F:53:LEU:O	11:F:57:GLY:N	2.40	0.41
1:W:139:LEU:HD11	1:W:143:ILE:CD1	2.50	0.41
2:Q:65:TRP:CD1	3:R:370:LEU:HD23	2.55	0.41
10:O:151:GLN:HE21	10:O:158:THR:HG22	1.85	0.41
11:E:68:MET:SD	11:E:204:ILE:HB	2.59	0.41
3:L:266:GLU:HA	3:L:269:ILE:HG12	2.01	0.41
3:L:458:PRO:HD2	3:L:461:TYR:CE2	2.54	0.41
4:X:160:LEU:HD12	17:X:302:CDL:H341	2.00	0.41
5:Z:134:TRP:O	11:F:489:ASN:OD1	2.38	0.41
11:F:156:PHE:CZ	11:F:171:ILE:HD13	2.55	0.41
11:F:312:ILE:HD13	11:F:333:VAL:HB	2.02	0.41
3:R:122:ASN:OD1	3:R:122:ASN:C	2.58	0.41
3:R:452:LEU:HD11	3:R:470:PHE:HB2	2.02	0.41
3:R:489:LEU:HB2	3:R:490:PRO:HD3	2.02	0.41
5:T:12:THR:HG21	5:T:50:LEU:HA	2.02	0.41
11:E:128:PHE:CZ	11:E:373:ARG:HG2	2.55	0.41
3:L:411:TYR:O	3:L:415:TYR:HD1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:41:ALA:CB	5:Z:44:LEU:HD22	2.50	0.41
20:I:301:HEC:HHD	20:I:301:HEC:CBC	2.49	0.41
12:M:172:VAL:HG13	12:M:173:HIS:N	2.35	0.41
3:R:254:LEU:HD13	4:S:49:THR:HG21	2.03	0.41
17:P:202:CDL:H141	17:P:202:CDL:H112	1.73	0.41
10:O:138:PHE:HB3	10:O:142:GLN:HG3	2.03	0.41
3:L:47:VAL:HG22	17:J:201:CDL:H391	2.02	0.41
3:L:294:THR:HA	3:L:297:ILE:HG12	2.03	0.41
4:X:131:ILE:HD12	18:X:301:9Y0:O4	2.19	0.41
17:X:303:CDL:H742	17:X:303:CDL:H541	2.01	0.41
17:Z:202:CDL:HB32	10:I:289:TRP:CD1	2.56	0.41
8:J:28:VAL:HG22	8:J:29:ASP:N	2.35	0.41
10:I:116:GLN:HE21	10:I:122:MET:CE	2.33	0.41
12:Y:41:GLN:HE22	12:Y:43:THR:HG22	1.85	0.41
12:Y:310:ASN:N	12:Y:311:PRO:HD2	2.34	0.41
3:R:89:VAL:HA	3:R:93:PHE:HB2	2.02	0.41
3:R:93:PHE:CD1	3:R:133:ALA:HB2	2.56	0.41
3:R:252:VAL:HG23	3:R:253:LEU:N	2.35	0.41
4:S:147:HIS:NE2	4:S:192:TRP:HB2	2.35	0.41
5:T:42:LEU:HA	5:T:45:THR:HG22	2.03	0.41
7:V:55:LEU:HD22	7:V:66:PHE:O	2.19	0.41
3:L:419:PRO:HB2	3:L:510:PRO:HG3	2.02	0.41
3:L:509:ASP:OD1	3:L:519:TRP:HB3	2.20	0.41
17:X:303:CDL:H152	5:Z:95:ILE:HG21	2.01	0.41
12:Y:108:LEU:CD2	12:M:213:VAL:HG11	2.51	0.41
12:Y:251:THR:CG2	12:Y:403:VAL:HG11	2.50	0.41
12:Y:358:GLN:C	12:Y:360:THR:H	2.23	0.41
12:Y:419:ARG:HG2	12:Y:420:LYS:N	2.35	0.41
12:M:189:THR:HG22	12:M:189:THR:O	2.20	0.41
2:Q:232:HIS:HA	2:Q:275:GLU:HB3	2.02	0.41
3:R:91:LEU:HD23	16:R:603:HEA:HMD3	2.01	0.41
3:R:93:PHE:HD1	3:R:133:ALA:HB2	1.85	0.41
7:V:36:GLU:OE1	7:V:36:GLU:N	2.42	0.41
7:V:44:PRO:O	7:V:47:ASP:OD1	2.38	0.41
11:E:63:PHE:CZ	12:Y:219:LEU:HD22	2.55	0.41
11:E:121:MET:HE3	19:E:604:MQ9:C26	2.50	0.41
11:E:124:LEU:HD11	11:E:344:LEU:HD11	2.02	0.41
11:E:197:ASP:OD2	12:M:309:ARG:NH2	2.43	0.41
3:L:35:THR:CG2	3:L:119:PRO:HB2	2.51	0.41
3:L:357:THR:CG2	3:L:358:PRO:HD3	2.51	0.41
4:X:151:VAL:HG22	4:X:188:VAL:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:192:HIS:O	10:I:193:ASN:HB2	2.20	0.41
12:Y:293:THR:HG23	12:Y:294:THR:N	2.34	0.41
3:R:278:VAL:HG21	3:R:365:PHE:CD2	2.56	0.41
4:S:58:TRP:O	4:S:60:PRO:HD3	2.21	0.41
7:V:90:THR:O	7:V:94:ALA:HB2	2.21	0.41
11:E:388:THR:HG22	11:E:392:MET:CE	2.51	0.41
3:L:153:ALA:HB1	3:L:158:THR:HG21	2.02	0.41
3:L:398:PHE:HB2	16:L:602:HEA:HMD3	2.02	0.41
5:Z:90:TRP:CE3	17:F:607:CDL:H322	2.56	0.41
10:I:112:ALA:O	10:I:116:GLN:HG2	2.21	0.41
12:Y:189:THR:HG22	12:Y:189:THR:O	2.20	0.41
12:Y:274:ILE:HG13	12:Y:314:LEU:HD23	2.02	0.41
12:Y:370:SER:HB2	24:Y:501:FES:S1	2.61	0.41
12:M:178:ALA:O	12:M:182:THR:HG23	2.21	0.41
2:Q:288:VAL:O	2:Q:288:VAL:HG13	2.20	0.41
3:R:43:MET:HG2	17:R:604:CDL:H331	2.03	0.41
3:R:154:TYR:O	3:R:158:THR:HG23	2.21	0.41
3:R:528:HIS:NE2	11:E:460:GLU:HB2	2.35	0.41
20:O:302:HEC:HAC	12:M:356:TYR:O	2.20	0.41
4:X:71:VAL:HB	4:X:72:PRO:HD3	2.02	0.41
5:Z:91:TRP:N	5:Z:92:PRO:CD	2.83	0.41
10:I:88:VAL:HA	10:I:91:HIS:O	2.21	0.41
10:I:192:HIS:CE1	10:I:210:LEU:HD11	2.56	0.41
11:F:143:ILE:HG13	11:F:144:GLY:N	2.36	0.41
17:F:606:CDL:H311	17:F:606:CDL:H111	2.02	0.41
12:M:251:THR:CG2	12:M:403:VAL:HG21	2.51	0.41
1:W:98:VAL:HG22	1:W:137:VAL:HG22	2.02	0.41
2:Q:35:TRP:HE1	2:Q:50:TRP:HB3	1.86	0.41
3:R:104:ASN:HD22	3:R:104:ASN:H	1.69	0.41
3:R:242:ALA:O	4:S:138:SER:CB	2.69	0.41
3:R:281:ILE:O	3:R:284:VAL:HG22	2.21	0.41
10:O:90:CYS:SG	20:O:301:HEC:HBC2	2.61	0.41
10:O:139:ASP:OD1	10:O:142:GLN:NE2	2.54	0.41
11:E:54:LEU:CD2	22:E:602:HEM:HMC3	2.51	0.41
11:E:229:LEU:HD22	11:F:20:TYR:CE1	2.55	0.41
2:K:32:ALA:O	2:K:50:TRP:NE1	2.50	0.41
2:K:136:PHE:CZ	2:K:139:ASN:HB2	2.56	0.41
2:K:333:GLY:O	2:K:336:VAL:HG12	2.20	0.41
3:L:63:ARG:HD3	16:L:603:HEA:OMA	2.20	0.41
3:L:102:PHE:O	3:L:106:VAL:HG12	2.21	0.41
3:L:264:HIS:HB3	3:L:265:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:452:LEU:HD12	3:L:470:PHE:HB2	2.03	0.41
3:L:540:ARG:O	3:L:540:ARG:HG3	2.21	0.41
11:F:92:ALA:HB1	11:F:284:ILE:CD1	2.51	0.41
11:F:229:LEU:O	11:F:233:GLN:N	2.49	0.41
11:F:337:MET:O	11:F:338:GLY:C	2.60	0.41
19:F:605:MQ9:H452	12:M:215:PHE:CE2	2.55	0.41
12:Y:309:ARG:HA	12:Y:345:VAL:HG21	2.03	0.41
12:Y:324:ARG:CB	12:Y:375:LEU:HD13	2.51	0.41
12:Y:373:ASP:O	12:Y:376:GLU:O	2.39	0.41
1:W:106:VAL:N	1:W:107:PRO:CD	2.83	0.41
3:R:118:PHE:CD1	17:S:303:CDL:HA61	2.56	0.41
4:S:189:ASP:OD1	4:S:190:ILE:N	2.54	0.41
10:O:226:PRO:HD2	10:O:229:MET:HB3	2.03	0.41
4:X:177:ALA:O	4:X:180:VAL:HG22	2.21	0.41
17:J:201:CDL:H621	17:J:201:CDL:H521	2.03	0.41
10:I:113:VAL:O	10:I:117:VAL:HG23	2.21	0.41
12:Y:243:TRP:NE1	12:Y:310:ASN:O	2.43	0.41
3:R:17:PHE:CE1	7:V:45:THR:HG23	2.56	0.40
3:R:155:SER:HB3	3:R:156:PRO:HD3	2.03	0.40
3:R:508:ASP:O	7:V:31:VAL:HA	2.21	0.40
11:E:500:GLY:O	12:M:84:ARG:NE	2.53	0.40
2:K:319:PRO:HA	2:K:320:PRO:HD3	1.96	0.40
12:Y:190:LEU:O	12:Y:191:LYS:CG	2.69	0.40
1:W:111:VAL:N	10:O:94:ASN:OD1	2.54	0.40
2:Q:217:ALA:N	2:Q:291:VAL:O	2.45	0.40
3:R:509:ASP:OD1	3:R:519:TRP:CB	2.69	0.40
5:T:90:TRP:HZ2	17:E:607:CDL:HB4	1.86	0.40
2:K:242:LYS:HD3	2:K:274:THR:HG21	2.03	0.40
3:L:208:ILE:HG21	3:L:279:SER:CB	2.52	0.40
4:X:37:LEU:HD22	5:Z:51:ILE:CD1	2.51	0.40
10:I:201:LEU:HD23	10:I:201:LEU:HA	1.97	0.40
11:F:441:LEU:HG	11:F:484:LEU:HD13	2.02	0.40
12:Y:230:THR:HG22	12:Y:231:ALA:N	2.36	0.40
2:Q:65:TRP:NE1	3:R:370:LEU:HD23	2.36	0.40
2:Q:106:ILE:HB	3:R:331:PHE:HB3	2.04	0.40
3:R:264:HIS:HD2	3:R:314:HIS:NE2	2.18	0.40
17:S:302:CDL:H782	12:M:141:LEU:HD11	2.03	0.40
5:T:55:PHE:O	5:T:59:VAL:HG23	2.22	0.40
17:T:202:CDL:HA22	10:O:293:ARG:HH11	1.86	0.40
10:O:100:ASP:OD1	10:O:100:ASP:O	2.40	0.40
3:L:274:PHE:CD1	3:L:277:ILE:HD12	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:45:ILE:O	8:J:48:MET:HB2	2.22	0.40
11:F:235:HIS:CE1	22:F:601:HEM:O1D	2.74	0.40
12:M:358:GLN:C	12:M:360:THR:H	2.23	0.40
1:W:55:HIS:CE1	1:W:74:LEU:HB2	2.56	0.40
3:R:119:PRO:O	3:R:122:ASN:OD1	2.39	0.40
3:R:190:ILE:O	3:R:194:VAL:HG23	2.21	0.40
3:R:526:PRO:O	3:R:529:ASN:N	2.43	0.40
16:R:603:HEA:HHB	16:R:603:HEA:OMA	2.22	0.40
10:O:222:MET:CG	20:O:302:HEC:HMB2	2.52	0.40
10:O:242:LYS:O	10:O:246:VAL:HG23	2.22	0.40
22:E:602:HEM:HBC2	22:E:602:HEM:HMC2	2.03	0.40
2:K:252:ASN:HB3	3:L:253:LEU:HD23	2.03	0.40
3:L:418:PHE:CE1	3:L:499:TRP:CD1	3.10	0.40
3:L:517:LEU:HD11	3:L:534:PRO:HD2	2.02	0.40
4:X:61:GLU:N	4:X:62:PRO:HD2	2.35	0.40
12:M:41:GLN:HE22	12:M:43:THR:HG22	1.87	0.40
3:R:28:ILE:HG23	3:R:29:TYR:N	2.36	0.40
3:R:96:THR:N	3:R:97:PRO:CD	2.85	0.40
3:R:357:THR:CG2	3:R:358:PRO:HD3	2.51	0.40
3:R:382:PRO:N	3:R:383:PRO:HD2	2.37	0.40
16:R:602:HEA:H121	16:R:602:HEA:HHC	2.03	0.40
7:V:76:ASP:OD1	7:V:76:ASP:N	2.55	0.40
7:V:123:ALA:HB3	7:V:124:PRO:CD	2.51	0.40
10:O:273:MET:SD	19:E:604:MQ9:H3D	2.62	0.40
2:K:214:VAL:CG2	2:K:313:LEU:HD21	2.52	0.40
3:L:86:HIS:CE1	3:L:90:MET:HG3	2.56	0.40
3:L:155:SER:HB3	3:L:156:PRO:HD3	2.03	0.40
3:L:242:ALA:O	3:L:244:ILE:N	2.54	0.40
3:L:419:PRO:HB2	3:L:510:PRO:CG	2.51	0.40
10:I:122:MET:HA	10:I:122:MET:HE2	2.02	0.40
12:Y:281:THR:HG23	12:Y:344:LYS:HD2	2.03	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	W	154/159 (97%)	137 (89%)	17 (11%)	0	100	100
1	c	154/159 (97%)	143 (93%)	11 (7%)	0	100	100
2	K	310/312 (99%)	279 (90%)	31 (10%)	0	100	100
2	Q	310/312 (99%)	279 (90%)	31 (10%)	0	100	100
3	L	550/552 (100%)	512 (93%)	38 (7%)	0	100	100
3	R	550/552 (100%)	512 (93%)	38 (7%)	0	100	100
4	S	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
4	X	201/203 (99%)	195 (97%)	6 (3%)	0	100	100
5	T	137/139 (99%)	128 (93%)	9 (7%)	0	100	100
5	Z	137/139 (99%)	128 (93%)	9 (7%)	0	100	100
6	U	77/79 (98%)	69 (90%)	8 (10%)	0	100	100
6	a	77/79 (98%)	72 (94%)	5 (6%)	0	100	100
7	V	143/145 (99%)	135 (94%)	8 (6%)	0	100	100
7	b	143/145 (99%)	135 (94%)	8 (6%)	0	100	100
8	J	88/100 (88%)	82 (93%)	6 (7%)	0	100	100
8	P	88/100 (88%)	84 (96%)	4 (4%)	0	100	100
9	D	214/216 (99%)	193 (90%)	21 (10%)	0	100	100
9	G	214/216 (99%)	190 (89%)	24 (11%)	0	100	100
10	I	221/223 (99%)	199 (90%)	22 (10%)	0	100	100
10	O	221/223 (99%)	193 (87%)	28 (13%)	0	100	100
11	E	533/535 (100%)	489 (92%)	43 (8%)	1 (0%)	44	77
11	F	533/535 (100%)	486 (91%)	47 (9%)	0	100	100
12	M	380/382 (100%)	348 (92%)	32 (8%)	0	100	100
12	Y	380/382 (100%)	350 (92%)	30 (8%)	0	100	100
All	All	6016/6090 (99%)	5531 (92%)	484 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	E	135	ARG

### 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	W	127/127 (100%)	127 (100%)	0	100	100
1	c	127/127 (100%)	127 (100%)	0	100	100
2	K	260/266 (98%)	260 (100%)	0	100	100
2	Q	260/266 (98%)	257 (99%)	3 (1%)	67	86
3	L	452/453 (100%)	452 (100%)	0	100	100
3	R	452/453 (100%)	450 (100%)	2 (0%)	89	95
4	S	155/161 (96%)	155 (100%)	0	100	100
4	X	155/161 (96%)	153 (99%)	2 (1%)	65	85
5	T	106/106 (100%)	106 (100%)	0	100	100
5	Z	106/106 (100%)	106 (100%)	0	100	100
6	U	59/59 (100%)	59 (100%)	0	100	100
6	a	59/59 (100%)	59 (100%)	0	100	100
7	V	107/107 (100%)	106 (99%)	1 (1%)	75	89
7	b	107/107 (100%)	107 (100%)	0	100	100
8	J	76/83 (92%)	74 (97%)	2 (3%)	41	72
8	P	76/83 (92%)	75 (99%)	1 (1%)	65	85
9	D	20/151 (13%)	20 (100%)	0	100	100
9	G	20/151 (13%)	20 (100%)	0	100	100
10	I	163/163 (100%)	163 (100%)	0	100	100
10	O	163/163 (100%)	160 (98%)	3 (2%)	54	80
11	E	429/429 (100%)	426 (99%)	3 (1%)	81	91
11	F	429/429 (100%)	428 (100%)	1 (0%)	92	97
12	M	312/312 (100%)	312 (100%)	0	100	100
12	Y	312/312 (100%)	312 (100%)	0	100	100
All	All	4532/4834 (94%)	4514 (100%)	18 (0%)	88	95

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

Mol	Chain	Res	Type
2	Q	121	MET
2	Q	257	VAL
2	Q	258	PHE
3	R	63	ARG
3	R	459	ARG
7	V	110	TYR
8	P	64	ARG
10	O	122	MET
10	O	126	ARG
10	O	128	GLU
11	E	127	ILE
11	E	352	LYS
11	E	358	ASP
4	X	20	ASN
4	X	169	LYS
8	J	24	ARG
8	J	64	ARG
11	F	523	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	R	104	ASN
11	E	325	HIS
10	I	116	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 64 ligands modelled in this entry, 6 are monoatomic - leaving 58 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
23	HUU	E	603	-	39,43,43	2.12	10 (25%)	50,62,62	2.14	6 (12%)
18	9Y0	S	301	-	48,48,48	1.18	3 (6%)	51,53,53	0.86	2 (3%)
17	CDL	T	202	-	75,75,99	0.34	0	81,87,111	0.42	0
18	9Y0	L	604	-	48,48,48	1.18	3 (6%)	51,53,53	0.81	2 (3%)
17	CDL	Z	202	-	75,75,99	1.32	7 (9%)	81,87,111	2.04	9 (11%)
13	9XX	D	301	-	31,31,41	1.10	4 (12%)	34,34,44	1.31	3 (8%)
13	9XX	W	201	-	41,41,41	0.98	4 (9%)	44,44,44	1.26	3 (6%)
14	PLM	G	302	9	9,10,17	0.55	0	8,9,17	0.43	0
21	9YF	E	609	-	58,58,58	1.00	4 (6%)	68,71,71	1.42	8 (11%)
21	9YF	Y	503	-	58,58,58	1.13	7 (12%)	68,71,71	1.49	9 (13%)
17	CDL	P	202	-	75,75,99	0.32	0	81,87,111	0.42	0
21	9YF	O	303	-	58,58,58	1.07	6 (10%)	68,71,71	1.07	4 (5%)
24	FES	M	501	12	0,4,4	-	-	-	-	-
21	9YF	M	503	-	58,58,58	1.12	5 (8%)	68,71,71	1.40	10 (14%)
22	HEM	E	602	11	42,50,50	1.48	4 (9%)	46,82,82	1.34	4 (8%)
14	PLM	D	302	9	9,10,17	0.53	0	8,9,17	0.43	0
13	9XX	c	202	1	41,41,41	0.95	4 (9%)	44,44,44	1.22	3 (6%)
16	HEA	L	603	3	58,67,67	1.54	9 (15%)	63,103,103	2.05	20 (31%)
16	HEA	R	603	3	58,67,67	1.52	9 (15%)	63,103,103	2.04	18 (28%)
22	HEM	F	602	11	42,50,50	1.49	4 (9%)	46,82,82	1.29	6 (13%)
17	CDL	F	606	-	75,75,99	0.36	0	81,87,111	0.61	2 (2%)
17	CDL	L	605	-	75,75,99	0.33	0	81,87,111	0.70	2 (2%)
19	MQ9	F	604	-	59,59,59	2.37	22 (37%)	73,75,75	1.51	19 (26%)
16	HEA	L	602	3	58,67,67	1.58	9 (15%)	63,103,103	2.32	24 (38%)
17	CDL	F	607	-	75,75,99	0.38	0	81,87,111	0.48	0
17	CDL	R	604	-	75,75,99	0.34	0	81,87,111	0.66	2 (2%)
22	HEM	F	601	11	41,49,50	1.22	2 (4%)	47,81,82	1.25	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	HUU	F	603	-	39,43,43	2.11	10 (25%)	50,62,62	2.12	6 (12%)
14	PLM	W	202	1	15,16,17	0.49	0	14,15,17	0.33	0
21	9YF	I	303	-	58,58,58	1.06	6 (10%)	68,71,71	1.18	4 (5%)
17	CDL	J	201	-	75,75,99	0.31	0	81,87,111	0.42	0
19	MQ9	T	201	-	59,59,59	2.36	22 (37%)	73,75,75	1.58	16 (21%)
20	HEC	O	301	10	32,50,50	2.11	3 (9%)	30,82,82	2.44	7 (23%)
18	9Y0	P	201	-	48,48,48	1.16	3 (6%)	51,53,53	0.87	2 (3%)
17	CDL	E	606	-	75,75,99	0.35	0	81,87,111	0.46	0
19	MQ9	Z	201	-	59,59,59	2.36	22 (37%)	73,75,75	1.56	16 (21%)
20	HEC	I	301	10	32,50,50	2.10	3 (9%)	30,82,82	2.16	5 (16%)
17	CDL	X	303	-	75,75,99	0.33	0	81,87,111	0.69	2 (2%)
17	CDL	S	302	-	75,75,99	0.32	0	81,87,111	0.43	0
16	HEA	R	602	3	58,67,67	1.58	9 (15%)	63,103,103	2.25	23 (36%)
21	9YF	F	609	-	58,58,58	1.00	5 (8%)	68,71,71	1.47	8 (11%)
14	PLM	c	201	1	15,16,17	0.45	0	14,15,17	0.34	0
17	CDL	E	608	-	75,75,99	0.36	0	81,87,111	0.45	0
19	MQ9	E	605	-	59,59,59	2.39	22 (37%)	73,75,75	1.53	17 (23%)
20	HEC	I	302	10	32,50,50	2.12	3 (9%)	30,82,82	2.32	5 (16%)
19	MQ9	E	604	-	59,59,59	2.37	22 (37%)	73,75,75	1.50	19 (26%)
13	9XX	G	301	-	31,31,41	1.08	4 (12%)	34,34,44	1.44	3 (8%)
21	9YF	Y	502	-	58,58,58	1.09	6 (10%)	68,71,71	1.35	8 (11%)
17	CDL	E	607	-	75,75,99	0.38	0	81,87,111	0.55	1 (1%)
18	9Y0	X	301	-	48,48,48	1.18	3 (6%)	51,53,53	0.87	2 (3%)
20	HEC	O	302	10	32,50,50	2.11	3 (9%)	30,82,82	2.29	5 (16%)
17	CDL	X	302	-	75,75,99	0.30	0	81,87,111	0.36	0
22	HEM	E	601	11	41,49,50	1.22	2 (4%)	47,81,82	1.31	5 (10%)
17	CDL	S	303	-	75,75,99	0.34	0	81,87,111	0.51	0
17	CDL	F	608	-	75,75,99	0.38	0	81,87,111	0.42	0
21	9YF	M	502	-	58,58,58	1.09	6 (10%)	68,71,71	1.31	7 (10%)
24	FES	Y	501	12	0,4,4	-	-	-	-	-
19	MQ9	F	605	-	59,59,59	2.39	23 (38%)	73,75,75	1.50	18 (24%)

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
23	HUU	E	603	-	-	6/20/34/34	0/5/5/5
18	9Y0	S	301	-	-	20/52/52/52	-
17	CDL	T	202	-	-	41/86/86/110	-
18	9Y0	L	604	-	-	24/52/52/52	-
17	CDL	Z	202	-	-	38/86/86/110	-
13	9XX	D	301	-	-	13/33/33/43	-
13	9XX	W	201	-	-	16/43/43/43	-
14	PLM	G	302	9	-	2/8/8/15	-
21	9YF	E	609	-	-	19/54/78/78	0/1/1/1
21	9YF	Y	503	-	-	26/54/78/78	0/1/1/1
17	CDL	P	202	-	-	46/86/86/110	-
21	9YF	O	303	-	-	30/54/78/78	0/1/1/1
24	FES	M	501	12	-	-	0/1/1/1
21	9YF	M	503	-	-	24/54/78/78	0/1/1/1
22	HEM	E	602	11	-	3/12/54/54	-
14	PLM	D	302	9	-	3/8/8/15	-
13	9XX	c	202	1	-	13/43/43/43	-
16	HEA	L	603	3	-	3/32/76/76	-
16	HEA	R	603	3	-	4/32/76/76	-
22	HEM	F	602	11	-	4/12/54/54	-
17	CDL	F	606	-	-	51/86/86/110	-
17	CDL	L	605	-	-	48/86/86/110	-
19	MQ9	F	604	-	-	9/53/73/73	0/2/2/2
16	HEA	L	602	3	-	9/32/76/76	-
17	CDL	F	607	-	-	40/86/86/110	-
17	CDL	R	604	-	-	39/86/86/110	-
22	HEM	F	601	11	-	2/12/52/54	-
23	HUU	F	603	-	-	2/20/34/34	0/5/5/5
14	PLM	W	202	1	-	4/14/14/15	-
21	9YF	I	303	-	-	25/54/78/78	0/1/1/1
17	CDL	J	201	-	-	55/86/86/110	-
19	MQ9	T	201	-	-	11/53/73/73	0/2/2/2
20	HEC	O	301	10	-	3/10/54/54	-
18	9Y0	P	201	-	-	24/52/52/52	-
17	CDL	E	606	-	-	51/86/86/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	MQ9	Z	201	-	-	14/53/73/73	0/2/2/2
20	HEC	I	301	10	-	1/10/54/54	-
17	CDL	X	303	-	-	44/86/86/110	-
17	CDL	S	302	-	-	52/86/86/110	-
16	HEA	R	602	3	-	8/32/76/76	-
21	9YF	F	609	-	-	22/54/78/78	0/1/1/1
14	PLM	c	201	1	-	3/14/14/15	-
17	CDL	E	608	-	-	45/86/86/110	-
19	MQ9	E	605	-	-	11/53/73/73	0/2/2/2
20	HEC	I	302	10	-	0/10/54/54	-
19	MQ9	E	604	-	-	11/53/73/73	0/2/2/2
13	9XX	G	301	-	-	11/33/33/43	-
21	9YF	Y	502	-	-	23/54/78/78	0/1/1/1
17	CDL	E	607	-	-	47/86/86/110	-
18	9Y0	X	301	-	-	18/52/52/52	-
20	HEC	O	302	10	-	0/10/54/54	-
17	CDL	X	302	-	-	52/86/86/110	-
22	HEM	E	601	11	-	3/12/52/54	-
17	CDL	S	303	-	-	47/86/86/110	-
17	CDL	F	608	-	-	37/86/86/110	-
21	9YF	M	502	-	-	23/54/78/78	0/1/1/1
24	FES	Y	501	12	-	-	0/1/1/1
19	MQ9	F	605	-	-	8/53/73/73	0/2/2/2

All (293) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	F	605	MQ9	C6-C5	8.56	1.50	1.35
19	E	604	MQ9	C6-C5	8.53	1.50	1.35
19	E	605	MQ9	C6-C5	8.50	1.50	1.35
19	F	604	MQ9	C6-C5	8.43	1.50	1.35
19	Z	201	MQ9	C6-C5	8.37	1.50	1.35
19	T	201	MQ9	C6-C5	8.36	1.50	1.35
20	O	301	HEC	C2B-C3B	-6.40	1.33	1.40
23	F	603	HUU	C07-N08	6.21	1.39	1.33
23	E	603	HUU	C07-N08	6.17	1.39	1.33
20	I	302	HEC	C3C-C2C	-6.15	1.33	1.40
20	I	301	HEC	C2B-C3B	-6.09	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	I	302	HEC	C2B-C3B	-6.05	1.34	1.40
20	O	302	HEC	C2B-C3B	-6.04	1.34	1.40
20	O	302	HEC	C3C-C2C	-6.02	1.34	1.40
23	F	603	HUU	C13-N14	5.91	1.46	1.33
23	E	603	HUU	C13-N14	5.91	1.46	1.33
20	I	301	HEC	C3C-C2C	-5.71	1.34	1.40
20	O	301	HEC	C3C-C2C	-5.52	1.34	1.40
20	O	301	HEC	C3D-C2D	5.47	1.53	1.37
20	O	302	HEC	C3D-C2D	5.40	1.53	1.37
20	I	301	HEC	C3D-C2D	5.37	1.53	1.37
20	I	302	HEC	C3D-C2D	5.34	1.53	1.37
19	F	604	MQ9	C2-C1	4.95	1.57	1.48
19	Z	201	MQ9	C2-C1	4.94	1.57	1.48
19	E	604	MQ9	C2-C1	4.94	1.57	1.48
19	E	605	MQ9	C2-C1	4.93	1.57	1.48
19	F	605	MQ9	C2-C1	4.90	1.57	1.48
22	F	602	HEM	C3C-C2C	-4.89	1.33	1.40
19	T	201	MQ9	C2-C1	4.87	1.57	1.48
16	L	603	HEA	C3A-C4A	4.84	1.48	1.41
16	R	603	HEA	C3A-C4A	4.81	1.48	1.41
22	E	602	HEM	C3C-C2C	-4.77	1.33	1.40
16	L	602	HEA	C3A-C4A	4.65	1.48	1.41
19	F	604	MQ9	C3-C4	4.62	1.57	1.48
19	E	605	MQ9	C26-C24	4.62	1.60	1.51
19	E	605	MQ9	C3-C4	4.61	1.57	1.48
19	F	605	MQ9	C26-C24	4.61	1.60	1.51
19	T	201	MQ9	C3-C4	4.59	1.57	1.48
19	F	605	MQ9	C3-C4	4.59	1.57	1.48
19	E	604	MQ9	C3-C4	4.58	1.57	1.48
19	F	604	MQ9	C26-C24	4.53	1.60	1.51
19	Z	201	MQ9	C26-C24	4.50	1.60	1.51
19	Z	201	MQ9	C3-C4	4.49	1.56	1.48
19	T	201	MQ9	C26-C24	4.47	1.60	1.51
16	R	602	HEA	C3A-C4A	4.45	1.47	1.41
19	E	604	MQ9	C26-C24	4.42	1.60	1.51
16	R	602	HEA	C3B-C2B	4.42	1.44	1.34
16	R	603	HEA	C3B-C2B	4.34	1.44	1.34
16	L	602	HEA	C3B-C2B	4.33	1.44	1.34
16	L	603	HEA	C3B-C2B	4.30	1.44	1.34
23	F	603	HUU	C21-N20	4.24	1.54	1.46
23	E	603	HUU	C21-N20	4.18	1.53	1.46
23	E	603	HUU	C36-N20	4.14	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	E	605	MQ9	C31-C29	4.00	1.59	1.51
19	F	605	MQ9	C31-C29	4.00	1.59	1.51
19	F	604	MQ9	C31-C29	3.99	1.59	1.51
19	Z	201	MQ9	C31-C29	3.97	1.59	1.51
19	T	201	MQ9	C31-C29	3.94	1.59	1.51
13	W	201	9XX	O1-C17	-3.94	1.40	1.47
19	E	604	MQ9	C31-C29	3.93	1.59	1.51
19	F	604	MQ9	C11-C9	3.85	1.59	1.51
19	F	605	MQ9	C11-C9	3.83	1.59	1.51
19	E	605	MQ9	C11-C9	3.81	1.59	1.51
13	D	301	9XX	O1-C17	-3.81	1.40	1.47
16	R	602	HEA	C3D-C2D	3.80	1.45	1.36
19	Z	201	MQ9	C11-C9	3.79	1.59	1.51
19	T	201	MQ9	C11-C9	3.79	1.59	1.51
19	E	604	MQ9	C11-C9	3.78	1.59	1.51
23	F	603	HUU	C36-N20	3.77	1.53	1.46
13	G	301	9XX	O1-C17	-3.76	1.40	1.47
16	L	602	HEA	C3D-C2D	3.72	1.44	1.36
16	L	603	HEA	C3D-C2D	3.70	1.44	1.36
13	c	202	9XX	O1-C17	-3.66	1.40	1.47
16	R	603	HEA	C3D-C2D	3.58	1.44	1.36
16	R	602	HEA	C4D-C3D	3.48	1.50	1.45
16	R	602	HEA	C3A-C2A	3.45	1.45	1.40
16	L	603	HEA	C3C-C2C	3.45	1.45	1.40
16	L	602	HEA	C4B-C3B	3.44	1.50	1.44
23	F	603	HUU	C19-N20	3.43	1.48	1.38
23	E	603	HUU	C19-N20	3.43	1.48	1.38
16	L	602	HEA	C3A-C2A	3.42	1.45	1.40
16	L	602	HEA	C4D-C3D	3.31	1.50	1.45
16	R	603	HEA	C3C-C2C	3.31	1.44	1.40
19	F	605	MQ9	C22-C23	3.30	1.60	1.50
16	R	602	HEA	C3C-C2C	3.28	1.44	1.40
19	E	605	MQ9	C22-C23	3.27	1.60	1.50
16	L	602	HEA	C3C-C2C	3.24	1.44	1.40
18	S	301	9Y0	O7-C1	-3.21	1.39	1.46
22	E	602	HEM	C3C-CAC	3.20	1.54	1.47
19	F	605	MQ9	C21-C19	3.20	1.57	1.51
18	X	301	9Y0	O7-C1	-3.19	1.39	1.46
19	F	605	MQ9	C16-C14	3.17	1.57	1.51
19	F	604	MQ9	C22-C23	3.15	1.60	1.50
19	E	605	MQ9	C21-C19	3.15	1.57	1.51
19	E	604	MQ9	C22-C23	3.15	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	E	604	MQ9	C27-C28	3.15	1.60	1.50
19	Z	201	MQ9	C21-C19	3.14	1.57	1.51
18	P	201	9Y0	O7-C1	-3.13	1.39	1.46
19	E	604	MQ9	C21-C19	3.12	1.57	1.51
19	T	201	MQ9	C21-C19	3.12	1.57	1.51
19	Z	201	MQ9	C22-C23	3.10	1.59	1.50
19	T	201	MQ9	C22-C23	3.09	1.59	1.50
19	F	604	MQ9	C16-C14	3.09	1.57	1.51
19	E	604	MQ9	C16-C14	3.08	1.57	1.51
19	F	604	MQ9	C27-C28	3.07	1.59	1.50
17	Z	202	CDL	OB8-CB7	3.07	1.42	1.33
19	E	605	MQ9	C16-C14	3.07	1.57	1.51
22	F	602	HEM	C3C-CAC	3.07	1.54	1.47
19	F	604	MQ9	C21-C19	3.06	1.57	1.51
19	Z	201	MQ9	C27-C28	3.06	1.59	1.50
19	Z	201	MQ9	C16-C14	3.06	1.57	1.51
19	F	605	MQ9	C27-C28	3.04	1.59	1.50
21	Y	503	9YF	O9-C8	3.04	1.42	1.34
18	L	604	9Y0	O7-C1	-3.04	1.39	1.46
19	E	605	MQ9	C27-C28	3.04	1.59	1.50
19	T	201	MQ9	C27-C28	3.03	1.59	1.50
19	T	201	MQ9	C16-C14	3.00	1.57	1.51
16	R	602	HEA	C2A-C1A	2.98	1.49	1.42
18	L	604	9Y0	O5-C5	2.94	1.41	1.33
23	F	603	HUU	C35-C23	-2.93	1.45	1.53
16	R	602	HEA	C4B-C3B	2.93	1.49	1.44
17	Z	202	CDL	OA6-CA5	2.91	1.42	1.34
21	M	503	9YF	O9-C8	2.91	1.42	1.34
22	F	602	HEM	CAB-C3B	2.90	1.55	1.47
19	E	605	MQ9	C7-C8	2.90	1.55	1.50
18	X	301	9Y0	O5-C5	2.90	1.41	1.33
21	Y	502	9YF	O11-C25	2.89	1.41	1.33
19	E	604	MQ9	C7-C8	2.89	1.55	1.50
22	E	602	HEM	CAB-C3B	2.88	1.55	1.47
16	L	602	HEA	C2A-C1A	2.88	1.49	1.42
18	P	201	9Y0	O5-C5	2.88	1.41	1.33
19	F	604	MQ9	C7-C8	2.87	1.55	1.50
18	L	604	9Y0	O7-C21	2.86	1.42	1.34
17	Z	202	CDL	OB6-CB5	2.86	1.42	1.34
23	E	603	HUU	C35-C23	-2.86	1.45	1.53
21	M	502	9YF	O9-C8	2.85	1.42	1.34
19	F	605	MQ9	C7-C8	2.85	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	S	301	9Y0	O5-C5	2.84	1.41	1.33
21	Y	502	9YF	O9-C8	2.84	1.42	1.34
22	F	601	HEM	CAB-C3B	2.84	1.55	1.47
16	L	603	HEA	C3A-C2A	2.83	1.44	1.40
18	X	301	9Y0	O7-C21	2.81	1.42	1.34
19	E	605	MQ9	C20-C19	2.81	1.57	1.50
21	M	502	9YF	O11-C25	2.81	1.41	1.33
17	Z	202	CDL	OA8-CA7	2.81	1.41	1.33
18	S	301	9Y0	O7-C21	2.80	1.42	1.34
16	R	603	HEA	C3A-C2A	2.80	1.44	1.40
19	T	201	MQ9	C7-C8	2.79	1.55	1.50
19	Z	201	MQ9	C7-C6	2.78	1.56	1.51
19	T	201	MQ9	C20-C19	2.78	1.57	1.50
19	F	605	MQ9	C20-C19	2.78	1.57	1.50
22	E	601	HEM	CAB-C3B	2.78	1.54	1.47
19	F	604	MQ9	C7-C6	2.77	1.56	1.51
17	Z	202	CDL	CB6-CB4	2.76	1.59	1.50
19	Z	201	MQ9	C20-C19	2.76	1.57	1.50
19	E	604	MQ9	C7-C6	2.74	1.56	1.51
19	F	605	MQ9	C7-C6	2.74	1.56	1.51
19	E	604	MQ9	C20-C19	2.73	1.57	1.50
19	E	604	MQ9	C5M-C5	2.73	1.56	1.50
17	Z	202	CDL	CB3-CB4	2.73	1.59	1.50
19	E	605	MQ9	C5M-C5	2.72	1.56	1.50
18	P	201	9Y0	O7-C21	2.72	1.42	1.34
21	F	609	9YF	O11-C25	2.72	1.41	1.33
19	E	605	MQ9	C7-C6	2.71	1.56	1.51
21	E	609	9YF	O11-C25	2.71	1.41	1.33
21	F	609	9YF	O9-C	-2.70	1.40	1.46
19	F	604	MQ9	C5M-C5	2.69	1.56	1.50
19	F	605	MQ9	C5M-C5	2.68	1.56	1.50
19	T	201	MQ9	C7-C6	2.67	1.56	1.51
19	F	604	MQ9	C20-C19	2.66	1.57	1.50
19	Z	201	MQ9	C7-C8	2.66	1.54	1.50
21	M	503	9YF	O9-C	-2.64	1.40	1.46
17	Z	202	CDL	OA6-CA4	-2.64	1.40	1.46
19	E	605	MQ9	C41-C39	2.63	1.56	1.51
21	E	609	9YF	O9-C	-2.62	1.40	1.46
21	E	609	9YF	O9-C8	2.62	1.41	1.34
19	T	201	MQ9	C5M-C5	2.62	1.56	1.50
16	L	603	HEA	C2A-C1A	2.60	1.48	1.42
21	F	609	9YF	O9-C8	2.60	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Y	503	9YF	O11-C24	-2.59	1.39	1.45
19	Z	201	MQ9	C5M-C5	2.59	1.56	1.50
21	I	303	9YF	O11-C25	2.56	1.40	1.33
21	I	303	9YF	O9-C8	2.53	1.41	1.34
19	F	604	MQ9	C41-C39	2.53	1.56	1.51
16	R	603	HEA	C2A-C1A	2.53	1.48	1.42
19	E	605	MQ9	C46-C44	2.53	1.56	1.51
16	L	603	HEA	C4B-C3B	2.52	1.49	1.44
21	O	303	9YF	O9-C	-2.52	1.40	1.46
19	F	605	MQ9	C46-C44	2.51	1.56	1.51
19	E	604	MQ9	C41-C39	2.50	1.56	1.51
21	M	503	9YF	O11-C25	2.50	1.40	1.33
21	Y	503	9YF	O6-C6	-2.50	1.36	1.43
23	E	603	HUU	C24-C23	2.48	1.57	1.52
21	M	503	9YF	O11-C24	-2.47	1.39	1.45
19	T	201	MQ9	C41-C39	2.47	1.56	1.51
21	O	303	9YF	O11-C24	-2.46	1.39	1.45
21	I	303	9YF	O11-C24	-2.45	1.39	1.45
21	Y	503	9YF	O4-C4	-2.45	1.36	1.43
19	Z	201	MQ9	C41-C39	2.45	1.56	1.51
21	O	303	9YF	O9-C8	2.45	1.41	1.34
16	R	603	HEA	C4B-C3B	2.44	1.49	1.44
13	W	201	9XX	O-C15	2.44	1.40	1.33
19	Z	201	MQ9	C42-C43	2.44	1.57	1.50
19	T	201	MQ9	C42-C43	2.43	1.57	1.50
23	E	603	HUU	C22-C23	-2.43	1.46	1.53
19	F	605	MQ9	C41-C39	2.43	1.56	1.51
19	E	605	MQ9	C42-C43	2.43	1.57	1.50
21	O	303	9YF	O11-C25	2.43	1.40	1.33
19	F	605	MQ9	C42-C43	2.42	1.57	1.50
23	F	603	HUU	C24-C23	2.42	1.57	1.52
19	Z	201	MQ9	C12-C13	2.41	1.57	1.50
21	Y	502	9YF	P-O2	2.41	1.66	1.59
22	F	601	HEM	C2C-C3C	-2.41	1.33	1.41
21	I	303	9YF	O9-C	-2.41	1.40	1.46
13	G	301	9XX	O-C15	2.41	1.40	1.33
21	E	609	9YF	O11-C24	-2.40	1.39	1.45
13	D	301	9XX	O-C15	2.40	1.40	1.33
19	F	604	MQ9	C42-C43	2.38	1.57	1.50
13	c	202	9XX	O-C15	2.38	1.40	1.33
19	F	605	MQ9	C12-C13	2.38	1.57	1.50
19	E	604	MQ9	C42-C43	2.37	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	E	601	HEM	C2C-C3C	-2.37	1.33	1.41
19	E	604	MQ9	C12-C13	2.37	1.57	1.50
19	F	604	MQ9	C12-C13	2.37	1.57	1.50
21	Y	503	9YF	O9-C	-2.36	1.41	1.46
16	L	603	HEA	C1D-ND	-2.36	1.36	1.40
16	L	602	HEA	C1D-ND	-2.35	1.36	1.40
21	Y	503	9YF	O11-C25	2.34	1.40	1.33
16	R	603	HEA	C1D-ND	-2.34	1.36	1.40
19	E	605	MQ9	C43-C44	2.32	1.38	1.33
19	T	201	MQ9	O4-C4	-2.32	1.18	1.23
19	E	605	MQ9	C12-C13	2.31	1.57	1.50
21	M	502	9YF	P-O2	2.31	1.66	1.59
19	E	604	MQ9	O4-C4	-2.31	1.18	1.23
19	F	604	MQ9	O4-C4	-2.31	1.18	1.23
19	F	605	MQ9	C43-C44	2.30	1.38	1.33
19	T	201	MQ9	C46-C44	2.30	1.56	1.51
19	Z	201	MQ9	O4-C4	-2.30	1.18	1.23
19	T	201	MQ9	C12-C13	2.29	1.57	1.50
19	E	604	MQ9	C46-C44	2.29	1.56	1.51
19	Z	201	MQ9	C46-C44	2.29	1.56	1.51
19	E	604	MQ9	C28-C29	2.28	1.38	1.33
19	F	605	MQ9	O4-C4	-2.27	1.18	1.23
16	R	602	HEA	C1D-ND	-2.27	1.36	1.40
19	F	604	MQ9	C46-C44	2.27	1.56	1.51
21	Y	502	9YF	O11-C24	-2.25	1.40	1.45
23	F	603	HUU	C22-C23	-2.24	1.47	1.53
19	E	605	MQ9	O4-C4	-2.23	1.18	1.23
19	F	604	MQ9	C28-C29	2.23	1.38	1.33
21	F	609	9YF	P-O2	2.22	1.66	1.59
21	O	303	9YF	P-O2	2.22	1.66	1.59
21	M	502	9YF	O11-C24	-2.21	1.40	1.45
23	F	603	HUU	C10-C09	2.21	1.55	1.51
13	W	201	9XX	O-C16	-2.20	1.40	1.45
19	T	201	MQ9	C28-C29	2.20	1.38	1.33
22	E	602	HEM	C3C-C4C	2.19	1.44	1.41
19	Z	201	MQ9	C3C-C3B	2.18	1.43	1.38
19	Z	201	MQ9	C28-C29	2.18	1.38	1.33
13	D	301	9XX	O1-C18	2.17	1.40	1.34
16	L	603	HEA	C11-C3B	-2.16	1.48	1.51
13	W	201	9XX	O1-C18	2.16	1.40	1.34
19	T	201	MQ9	C43-C44	2.16	1.38	1.33
13	c	202	9XX	O-C16	-2.16	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	I	303	9YF	P-O2	2.15	1.65	1.59
21	Y	502	9YF	O9-C	-2.15	1.41	1.46
19	T	201	MQ9	C3C-C3B	2.15	1.43	1.38
19	Z	201	MQ9	C43-C44	2.14	1.38	1.33
19	E	605	MQ9	C28-C29	2.14	1.38	1.33
19	E	604	MQ9	C43-C44	2.14	1.38	1.33
19	F	605	MQ9	C28-C29	2.14	1.38	1.33
13	c	202	9XX	O1-C18	2.13	1.40	1.34
19	E	605	MQ9	C3C-C3B	2.13	1.42	1.38
21	O	303	9YF	O4-C4	-2.11	1.37	1.43
19	F	604	MQ9	C43-C44	2.11	1.37	1.33
13	G	301	9XX	O1-C18	2.10	1.40	1.34
19	F	605	MQ9	C3C-C3B	2.10	1.42	1.38
19	F	604	MQ9	C3C-C3B	2.10	1.42	1.38
21	F	609	9YF	O11-C24	-2.09	1.40	1.45
13	G	301	9XX	O-C16	-2.09	1.40	1.45
13	D	301	9XX	O-C16	-2.09	1.40	1.45
21	M	502	9YF	P-O	2.07	1.67	1.59
21	Y	502	9YF	P-O	2.06	1.67	1.59
21	I	303	9YF	O4-C4	-2.06	1.37	1.43
19	E	604	MQ9	C3C-C3B	2.06	1.42	1.38
23	E	603	HUU	C02-CL1	2.05	1.79	1.74
23	E	603	HUU	C10-C09	2.05	1.54	1.51
21	M	503	9YF	O4-C4	-2.04	1.37	1.43
21	Y	503	9YF	P-O2	2.02	1.65	1.59
21	M	502	9YF	O4-C4	-2.02	1.38	1.43
22	F	602	HEM	C3C-C4C	2.02	1.44	1.41
23	F	603	HUU	C02-CL1	2.01	1.79	1.74
16	R	603	HEA	C1B-C2B	2.00	1.48	1.44
19	F	605	MQ9	C18-C19	2.00	1.37	1.33

All (340) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	E	603	HUU	C22-C23-C24	-10.69	87.34	112.67
23	F	603	HUU	C22-C23-C24	-10.13	88.69	112.67
17	Z	202	CDL	CB6-CB4-CB3	-9.90	88.70	111.78
17	Z	202	CDL	OB6-CB4-CB3	-8.35	78.39	108.34
23	E	603	HUU	C35-C23-C24	8.29	132.31	112.67
20	O	301	HEC	CBB-CAB-C3B	-8.18	108.34	127.49
20	I	302	HEC	CBB-CAB-C3B	-8.00	108.77	127.49
20	O	302	HEC	CBB-CAB-C3B	-7.90	109.01	127.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	F	603	HUU	C35-C23-C24	7.78	131.09	112.67
20	I	301	HEC	CBB-CAB-C3B	-7.75	109.36	127.49
16	R	602	HEA	CAD-C3D-C4D	7.10	137.07	124.70
16	L	602	HEA	CAD-C3D-C4D	7.01	136.91	124.70
17	Z	202	CDL	OB6-CB4-CB6	6.87	132.98	108.34
16	L	602	HEA	C12-C11-C3B	6.77	122.71	112.12
20	I	302	HEC	CBC-CAC-C3C	-6.68	111.85	127.49
20	O	301	HEC	CBC-CAC-C3C	-6.23	112.90	127.49
20	O	302	HEC	CBC-CAC-C3C	-6.18	113.03	127.49
21	F	609	9YF	O9-C8-C9	6.05	124.57	111.48
16	R	603	HEA	CMC-C2C-C3C	6.00	136.66	124.68
21	E	609	9YF	O9-C8-C9	5.63	123.67	111.48
16	R	603	HEA	CMC-C2C-C1C	-5.59	120.26	128.46
21	M	502	9YF	O9-C8-C9	5.51	123.39	111.48
16	L	603	HEA	CMC-C2C-C3C	5.44	135.55	124.68
21	Y	502	9YF	O9-C8-C9	5.28	122.90	111.48
21	M	503	9YF	O9-C8-C9	5.10	122.51	111.48
20	I	301	HEC	CBC-CAC-C3C	-5.07	115.64	127.49
21	Y	503	9YF	O6-C6-C7	-5.04	98.50	110.38
16	L	603	HEA	CMC-C2C-C1C	-5.03	121.08	128.46
21	Y	503	9YF	C7-C6-C5	4.89	119.41	110.83
19	T	201	MQ9	C7-C8-C9	-4.74	118.67	126.83
16	L	603	HEA	C12-C11-C3B	-4.74	104.72	112.12
16	L	602	HEA	C26-C15-C16	4.69	123.38	115.23
19	Z	201	MQ9	C7-C8-C9	-4.68	118.77	126.83
16	R	603	HEA	C3D-C4D-ND	4.65	114.84	110.35
16	R	602	HEA	C12-C11-C3B	4.59	119.29	112.12
21	Y	503	9YF	O9-C8-C9	4.55	121.32	111.48
17	Z	202	CDL	OA6-CA5-C11	4.52	121.25	111.48
16	R	602	HEA	CMC-C2C-C3C	4.49	133.65	124.68
21	O	303	9YF	O9-C8-C9	4.41	121.02	111.48
21	I	303	9YF	O9-C8-C9	4.35	120.88	111.48
16	L	603	HEA	C3D-C4D-ND	4.21	114.42	110.35
13	W	201	9XX	O1-C18-C19	4.18	120.53	111.48
16	L	602	HEA	CMC-C2C-C3C	4.10	132.87	124.68
20	O	301	HEC	CMC-C2C-C1C	-4.08	122.48	128.46
13	c	202	9XX	O1-C18-C19	4.07	120.29	111.48
13	G	301	9XX	O1-C18-C19	4.05	120.25	111.48
16	R	602	HEA	C4D-C3D-C2D	-4.02	101.05	106.89
18	X	301	9Y0	O7-C21-C22	3.99	120.11	111.48
13	D	301	9XX	O1-C18-C19	3.97	120.07	111.48
16	R	603	HEA	CHA-C4D-C3D	-3.96	119.00	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	G	301	9XX	C17-O1-C18	-3.96	112.07	117.78
18	S	301	9Y0	O7-C21-C22	3.90	119.91	111.48
16	R	602	HEA	C3D-C4D-ND	3.88	114.10	110.35
16	R	602	HEA	CMC-C2C-C1C	-3.84	122.83	128.46
18	P	201	9Y0	O7-C21-C22	3.83	119.78	111.48
17	Z	202	CDL	OB6-CB5-C51	3.78	119.65	111.48
16	L	602	HEA	C3D-C4D-ND	3.77	114.00	110.35
16	L	602	HEA	C4D-C3D-C2D	-3.76	101.42	106.89
18	L	604	9Y0	O7-C21-C22	3.63	119.33	111.48
16	R	603	HEA	C4D-C3D-C2D	-3.62	101.62	106.89
17	X	303	CDL	OA4-PA1-OA5	-3.61	91.21	107.57
21	Y	503	9YF	O11-C25-C26	3.57	122.70	111.83
16	L	603	HEA	CHA-C4D-C3D	-3.56	119.58	124.77
19	T	201	MQ9	C40-C39-C41	-3.56	109.05	115.23
16	R	602	HEA	CMD-C2D-C1D	-3.55	119.49	125.03
16	L	602	HEA	CMC-C2C-C1C	-3.53	123.28	128.46
23	F	603	HUU	C37-C19-N20	-3.53	116.48	121.39
16	R	603	HEA	C12-C11-C3B	-3.52	106.63	112.12
16	L	603	HEA	CMD-C2D-C1D	-3.50	119.56	125.03
21	I	303	9YF	O11-C25-C26	3.50	122.51	111.83
21	M	503	9YF	O11-C25-C26	3.47	122.40	111.83
20	I	301	HEC	CMC-C2C-C1C	-3.44	123.42	128.46
19	Z	201	MQ9	C40-C39-C41	-3.40	109.33	115.23
16	L	603	HEA	C4D-C3D-C2D	-3.40	101.95	106.89
21	M	503	9YF	C7-C6-C5	3.39	116.79	110.83
20	I	302	HEC	CMC-C2C-C1C	-3.36	123.53	128.46
16	R	603	HEA	CAD-C3D-C4D	3.30	130.46	124.70
16	L	602	HEA	CAD-C3D-C2D	-3.30	121.68	127.87
21	Y	502	9YF	C30-C31-C32	3.29	126.04	113.62
21	M	502	9YF	O11-C25-C26	3.26	121.78	111.83
20	O	302	HEC	CMC-C2C-C1C	-3.26	123.68	128.46
21	Y	502	9YF	O11-C25-C26	3.25	121.74	111.83
16	L	602	HEA	C26-C15-C14	-3.24	115.30	123.63
21	F	609	9YF	C6-C7-C2	3.23	117.01	109.68
19	E	605	MQ9	C12-C13-C14	-3.23	120.24	127.62
16	R	602	HEA	C27-C19-C20	3.21	120.80	115.23
19	F	605	MQ9	C30-C29-C31	3.21	120.80	115.23
19	E	605	MQ9	C17-C18-C19	-3.20	120.30	127.62
16	R	602	HEA	CAD-C3D-C2D	-3.20	121.88	127.87
19	E	605	MQ9	C32-C33-C34	-3.18	120.34	127.62
19	F	605	MQ9	C32-C33-C34	-3.18	120.34	127.62
21	O	303	9YF	O11-C25-C26	3.17	121.50	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	E	604	MQ9	C45-C44-C46	3.17	120.72	115.23
21	F	609	9YF	O11-C25-C26	3.12	121.34	111.83
20	O	301	HEC	C1D-C2D-C3D	-3.11	104.83	107.00
16	L	602	HEA	C17-C18-C19	-3.10	120.53	127.62
23	E	603	HUU	C12-C13-N14	3.10	122.92	115.86
19	E	604	MQ9	C17-C18-C19	-3.09	120.56	127.62
21	E	609	9YF	O11-C25-C26	3.09	121.24	111.83
16	R	602	HEA	CMB-C2B-C1B	-3.07	120.23	125.03
16	R	603	HEA	CAA-CBA-CGA	-3.06	105.58	113.83
16	L	602	HEA	CMD-C2D-C1D	-3.05	120.27	125.03
17	L	605	CDL	OA6-CA5-C11	3.05	118.08	111.48
21	F	609	9YF	O2-C2-C7	-3.04	102.30	108.73
19	Z	201	MQ9	C42-C43-C44	-3.04	120.67	127.62
19	E	605	MQ9	C30-C29-C31	3.02	120.47	115.23
22	E	601	HEM	CBD-CAD-C3D	-3.02	104.19	112.53
21	Y	503	9YF	O6-C6-C5	-3.01	103.27	110.38
16	L	603	HEA	CAD-C3D-C4D	3.01	129.94	124.70
21	Y	502	9YF	O11-C24-C	3.01	117.07	108.40
19	F	604	MQ9	C17-C18-C19	-3.00	120.76	127.62
19	F	604	MQ9	C45-C44-C46	3.00	120.43	115.23
19	F	605	MQ9	C17-C18-C19	-2.99	120.78	127.62
16	R	603	HEA	CMB-C2B-C1B	-2.98	120.38	125.03
19	E	605	MQ9	C27-C28-C29	-2.97	120.83	127.62
19	F	605	MQ9	C7-C8-C9	-2.97	121.72	126.83
17	R	604	CDL	OA2-PA1-OA3	2.96	120.68	108.94
16	R	602	HEA	C26-C15-C14	-2.95	116.04	123.63
16	L	603	HEA	CMB-C2B-C1B	-2.95	120.42	125.03
16	L	603	HEA	CMD-C2D-C3D	2.95	134.12	126.15
19	F	605	MQ9	C40-C39-C41	-2.92	110.15	115.23
19	T	201	MQ9	C12-C13-C14	-2.92	120.94	127.62
19	E	605	MQ9	C7-C8-C9	-2.92	121.81	126.83
21	M	502	9YF	C30-C31-C32	2.91	124.58	113.62
19	E	604	MQ9	C25-C24-C26	2.89	120.25	115.23
19	Z	201	MQ9	C17-C18-C19	-2.89	121.01	127.62
23	F	603	HUU	C12-C13-N14	2.89	122.44	115.86
19	T	201	MQ9	C17-C18-C19	-2.88	121.04	127.62
19	E	604	MQ9	C12-C13-C14	-2.88	121.04	127.62
19	E	605	MQ9	C15-C14-C16	2.87	120.21	115.23
19	Z	201	MQ9	C12-C13-C14	-2.86	121.07	127.62
17	Z	202	CDL	OB8-CB7-C71	2.86	120.55	111.83
16	L	602	HEA	C27-C19-C20	2.86	120.19	115.23
21	M	503	9YF	C6-C5-C4	2.86	115.84	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	602	HEA	CAA-CBA-CGA	-2.85	106.15	113.83
21	E	609	9YF	C6-C5-C4	2.85	115.83	110.83
19	E	604	MQ9	C42-C43-C44	-2.85	121.11	127.62
19	F	604	MQ9	C42-C43-C44	-2.85	121.11	127.62
19	F	604	MQ9	C25-C24-C26	2.84	120.16	115.23
19	T	201	MQ9	C22-C23-C24	-2.84	121.13	127.62
19	F	605	MQ9	C12-C13-C14	-2.83	121.15	127.62
19	Z	201	MQ9	C22-C23-C24	-2.83	121.15	127.62
16	R	602	HEA	OMA-CMA-C3A	-2.83	118.10	124.80
19	F	604	MQ9	C40-C39-C41	-2.81	110.34	115.23
19	E	605	MQ9	C35-C34-C36	2.80	120.10	115.23
19	T	201	MQ9	C32-C33-C34	-2.80	121.22	127.62
19	F	605	MQ9	C27-C28-C29	-2.80	121.23	127.62
19	T	201	MQ9	C5M-C5-C6	-2.79	119.87	124.45
19	F	605	MQ9	C15-C14-C16	2.77	120.04	115.23
22	E	602	HEM	C4B-CHC-C1C	2.77	126.21	122.56
23	F	603	HUU	C21-N20-C19	2.76	125.64	118.11
21	M	503	9YF	O9-C8-O10	-2.74	117.30	123.70
17	Z	202	CDL	OA8-CA7-C31	2.74	120.19	111.83
16	R	603	HEA	CMD-C2D-C1D	-2.74	120.76	125.03
18	L	604	9Y0	O5-C5-C6	2.74	120.18	111.83
18	X	301	9Y0	O5-C5-C6	2.73	120.17	111.83
19	T	201	MQ9	C7-C6-C5	-2.73	120.21	124.89
19	F	604	MQ9	C12-C13-C14	-2.72	121.39	127.62
16	L	602	HEA	OMA-CMA-C3A	-2.72	118.34	124.80
19	Z	201	MQ9	C32-C33-C34	-2.72	121.40	127.62
19	F	604	MQ9	C32-C33-C34	-2.71	121.42	127.62
19	E	604	MQ9	C40-C39-C41	-2.71	110.53	115.23
19	Z	201	MQ9	C45-C44-C46	2.70	119.91	115.23
22	F	602	HEM	C3B-C2B-C1B	2.69	108.43	106.41
16	R	602	HEA	CAA-CBA-CGA	-2.69	106.59	113.83
13	G	301	9XX	O-C15-C14	2.69	120.02	111.83
19	T	201	MQ9	C20-C19-C21	2.68	119.88	115.23
16	R	602	HEA	C17-C18-C19	-2.68	121.49	127.62
21	M	503	9YF	O2-P-O8	-2.68	101.25	109.81
19	F	604	MQ9	C35-C34-C36	2.67	119.87	115.23
19	E	604	MQ9	C32-C33-C34	-2.67	121.52	127.62
13	D	301	9XX	O-C15-C14	2.67	119.96	111.83
18	S	301	9Y0	O5-C5-C6	2.65	119.91	111.83
22	E	602	HEM	C3B-C4B-NB	-2.64	107.57	109.47
19	E	604	MQ9	C35-C34-C36	2.63	119.79	115.23
19	F	604	MQ9	C7-C8-C9	-2.62	122.31	126.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	R	602	HEA	C26-C15-C16	2.61	119.77	115.23
16	R	602	HEA	C3B-C4B-NB	2.61	112.84	109.84
19	E	605	MQ9	C20-C19-C21	2.58	119.70	115.23
16	L	602	HEA	C4B-C3B-C2B	-2.57	103.11	107.44
18	P	201	9Y0	O5-C5-C6	2.57	119.68	111.83
19	E	604	MQ9	C7-C8-C9	-2.57	122.40	126.83
19	T	201	MQ9	C42-C43-C44	-2.57	121.74	127.62
19	Z	201	MQ9	C7-C6-C5	-2.57	120.49	124.89
19	F	604	MQ9	C22-C23-C24	-2.57	121.75	127.62
16	R	602	HEA	CMD-C2D-C3D	2.57	133.09	126.15
19	E	604	MQ9	C15-C14-C16	2.55	119.66	115.23
17	Z	202	CDL	OA4-PA1-OA3	-2.54	100.62	112.44
19	T	201	MQ9	C25-C24-C26	2.53	119.62	115.23
22	E	602	HEM	C3B-C2B-C1B	2.53	108.31	106.41
19	E	605	MQ9	C40-C39-C41	-2.53	110.84	115.23
13	c	202	9XX	O-C15-C14	2.52	119.52	111.83
19	F	604	MQ9	C15-C14-C16	2.51	119.59	115.23
19	T	201	MQ9	C35-C34-C36	2.51	119.58	115.23
19	E	604	MQ9	C22-C23-C24	-2.51	121.89	127.62
21	Y	502	9YF	O9-C8-O10	-2.50	117.86	123.70
13	W	201	9XX	O-C15-C14	2.49	119.43	111.83
19	Z	201	MQ9	C35-C34-C36	2.48	119.54	115.23
17	L	605	CDL	OB4-PB2-OB5	-2.48	96.31	107.57
19	F	604	MQ9	C20-C19-C21	2.48	119.54	115.23
19	T	201	MQ9	C45-C44-C46	2.47	119.52	115.23
16	R	602	HEA	C4B-C3B-C2B	-2.47	103.29	107.44
22	E	602	HEM	C1B-NB-C4B	2.47	108.13	105.21
21	E	609	9YF	C7-C6-C5	2.46	115.15	110.83
16	R	603	HEA	C26-C15-C16	2.46	119.50	115.23
21	E	609	9YF	O11-C24-C	2.46	115.48	108.40
19	Z	201	MQ9	C20-C19-C21	2.46	119.50	115.23
17	Z	202	CDL	OB4-PB2-OB3	-2.46	101.01	112.44
21	E	609	9YF	O5-C5-C4	-2.46	104.58	110.38
19	Z	201	MQ9	C25-C24-C26	2.45	119.48	115.23
16	L	602	HEA	CMD-C2D-C3D	2.43	132.73	126.15
19	E	604	MQ9	C7-C6-C5	-2.42	120.75	124.89
21	M	502	9YF	O11-C24-C	2.41	115.36	108.40
20	I	301	HEC	C1D-C2D-C3D	-2.41	105.32	107.00
21	Y	502	9YF	C31-C32-C33	-2.40	107.98	115.97
16	L	602	HEA	CMB-C2B-C1B	-2.40	121.28	125.03
16	R	603	HEA	CBD-CAD-C3D	-2.40	105.90	112.53
19	E	605	MQ9	C22-C23-C24	-2.39	122.14	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	F	604	MQ9	C7-C6-C5	-2.39	120.78	124.89
19	Z	201	MQ9	C5M-C5-C6	-2.39	120.52	124.45
19	F	605	MQ9	C20-C19-C21	2.39	119.37	115.23
22	E	601	HEM	CBA-CAA-C2A	-2.39	108.53	112.54
16	R	603	HEA	CMD-C2D-C3D	2.38	132.60	126.15
19	Z	201	MQ9	C30-C29-C31	2.38	119.37	115.23
19	F	605	MQ9	C22-C23-C24	-2.38	122.17	127.62
19	E	604	MQ9	C20-C19-C21	2.37	119.35	115.23
19	T	201	MQ9	C30-C29-C31	2.37	119.34	115.23
21	M	502	9YF	O9-C8-O10	-2.37	118.17	123.70
17	F	606	CDL	OB6-CB4-CB3	2.36	116.82	108.34
23	E	603	HUU	O39-C13-N14	-2.36	117.99	122.59
19	F	604	MQ9	C5M-C5-C6	-2.36	120.57	124.45
21	F	609	9YF	O5-C5-C4	-2.36	104.81	110.38
19	F	605	MQ9	C7-C6-C5	-2.36	120.85	124.89
21	E	609	9YF	C6-C7-C2	2.35	115.01	109.68
16	L	602	HEA	C3C-C4C-NC	2.34	112.24	109.21
17	R	604	CDL	OA5-PA1-OA3	-2.34	99.67	108.94
22	E	601	HEM	C4B-CHC-C1C	2.34	125.64	122.56
22	F	601	HEM	C3C-C2C-C1C	2.33	108.46	106.85
19	E	605	MQ9	C5M-C5-C6	-2.33	120.62	124.45
16	L	603	HEA	CBD-CAD-C3D	-2.33	106.10	112.53
20	I	302	HEC	CMB-C2B-C1B	-2.33	125.05	128.46
19	E	604	MQ9	C10-C9-C11	2.33	119.26	115.23
16	L	603	HEA	CHB-C1B-C2B	-2.32	121.36	125.03
13	W	201	9XX	C25-C26-C27	-2.32	108.24	115.97
20	O	301	HEC	CBD-CAD-C3D	-2.32	108.64	112.54
19	F	604	MQ9	C10-C9-C11	2.31	119.24	115.23
16	L	603	HEA	CBA-CAA-C2A	-2.31	108.74	112.55
19	E	605	MQ9	C42-C43-C44	-2.31	122.34	127.62
19	E	605	MQ9	C7-C6-C5	-2.31	120.94	124.89
16	L	603	HEA	CAA-CBA-CGA	-2.30	107.63	113.83
21	M	502	9YF	C31-C32-C33	-2.30	108.31	115.97
21	I	303	9YF	C40-C39-C38	-2.30	102.73	114.37
16	L	602	HEA	C3B-C4B-NB	2.30	112.48	109.84
20	I	302	HEC	C1D-C2D-C3D	-2.30	105.40	107.00
19	E	605	MQ9	C10-C9-C11	2.29	119.21	115.23
13	c	202	9XX	C25-C26-C27	-2.29	108.34	115.97
21	M	502	9YF	C7-C2-C3	-2.29	107.68	110.86
22	F	601	HEM	C3D-C4D-ND	-2.28	107.67	110.17
21	M	503	9YF	O6-C6-C5	-2.28	105.01	110.38
19	E	604	MQ9	C5M-C5-C6	-2.27	120.71	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Y	502	9YF	O3-C3-C4	-2.27	105.02	110.38
21	O	303	9YF	C43-C42-C41	2.27	128.71	113.36
19	F	604	MQ9	C30-C29-C28	-2.27	117.80	123.63
22	F	602	HEM	C1B-NB-C4B	2.27	107.89	105.21
19	Z	201	MQ9	C15-C14-C16	2.27	119.16	115.23
21	Y	503	9YF	O3-C3-C4	-2.26	105.04	110.38
16	R	603	HEA	C3B-C4B-NB	2.26	112.44	109.84
21	E	609	9YF	O2-C2-C7	-2.25	103.96	108.73
19	F	605	MQ9	C35-C34-C36	2.25	119.14	115.23
16	R	602	HEA	CHB-C1B-C2B	-2.25	121.47	125.03
19	F	605	MQ9	C5M-C5-C6	-2.24	120.77	124.45
21	M	503	9YF	O5-C5-C4	-2.24	105.09	110.38
16	L	602	HEA	CHB-C1B-C2B	-2.23	121.50	125.03
22	F	602	HEM	C4C-CHD-C1D	2.23	125.50	122.56
19	T	201	MQ9	C15-C14-C16	2.23	119.09	115.23
23	F	603	HUU	O39-C13-N14	-2.23	118.25	122.59
19	E	604	MQ9	C30-C29-C28	-2.23	117.91	123.63
21	F	609	9YF	C6-C5-C4	2.22	114.73	110.83
17	E	607	CDL	OA4-PA1-OA5	-2.22	97.49	107.57
23	E	603	HUU	C10-C09-C12	-2.22	127.52	130.39
16	L	602	HEA	O11-C11-C3B	-2.21	107.20	111.26
19	F	604	MQ9	C47-C48-C49	-2.21	120.27	127.64
22	E	601	HEM	C3D-C4D-ND	-2.20	107.76	110.17
19	F	605	MQ9	C10-C9-C11	2.19	119.04	115.23
16	L	602	HEA	C25-C23-C24	2.19	119.64	114.59
16	L	603	HEA	CMB-C2B-C3B	2.19	134.52	130.28
20	O	302	HEC	CMB-C2B-C1B	-2.19	125.25	128.46
21	F	609	9YF	O9-C8-O10	-2.18	118.60	123.70
19	F	604	MQ9	C51-C49-C50	2.18	119.61	114.59
20	O	301	HEC	CAA-CBA-CGA	-2.18	107.96	113.83
16	R	603	HEA	CMB-C2B-C3B	2.18	134.49	130.28
16	L	603	HEA	C25-C23-C24	2.17	119.59	114.59
16	R	603	HEA	C25-C23-C24	2.17	119.58	114.59
16	R	602	HEA	C3C-C4C-NC	2.16	112.00	109.21
22	F	602	HEM	C3B-C4B-NB	-2.16	107.92	109.47
19	F	605	MQ9	C42-C43-C44	-2.16	122.69	127.62
22	F	602	HEM	C4B-CHC-C1C	2.15	125.40	122.56
16	L	602	HEA	C2D-C1D-ND	2.15	112.31	109.84
16	L	602	HEA	CHD-C1D-C2D	-2.15	120.85	126.94
21	M	503	9YF	O12-C25-C26	-2.15	115.38	123.78
17	X	303	CDL	OA4-PA1-OA2	2.15	117.30	107.57
19	Z	201	MQ9	C27-C28-C29	-2.14	122.72	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	F	609	9YF	C7-C2-C3	2.14	113.83	110.86
16	R	602	HEA	C25-C23-C24	2.14	119.51	114.59
16	R	603	HEA	CHB-C1B-C2B	-2.14	121.65	125.03
19	T	201	MQ9	C27-C28-C29	-2.14	122.73	127.62
21	I	303	9YF	O11-C25-O12	-2.14	118.29	123.63
17	F	606	CDL	OB4-PB2-OB3	2.13	122.35	112.44
16	L	603	HEA	C3C-C4C-NC	2.12	111.95	109.21
22	F	601	HEM	C4D-ND-C1D	2.10	107.69	105.21
20	I	301	HEC	CMB-C2B-C1B	-2.10	125.39	128.46
16	L	603	HEA	C26-C15-C16	2.09	118.86	115.23
20	O	302	HEC	C1D-C2D-C3D	-2.08	105.55	107.00
19	E	604	MQ9	C47-C48-C49	-2.07	120.72	127.64
22	F	602	HEM	CMA-C3A-C4A	-2.07	125.42	128.46
19	E	605	MQ9	C25-C24-C26	2.07	118.83	115.23
21	Y	503	9YF	O7-C7-C6	-2.06	105.52	110.38
22	F	601	HEM	CAD-CBD-CGD	-2.06	108.21	113.67
19	F	605	MQ9	C25-C24-C26	2.06	118.80	115.23
13	D	301	9XX	C25-C26-C27	-2.05	109.14	115.97
16	R	602	HEA	CHD-C1D-C2D	-2.05	121.14	126.94
21	O	303	9YF	O11-C25-O12	-2.05	118.51	123.63
19	E	604	MQ9	C51-C49-C50	2.04	119.29	114.59
21	Y	502	9YF	C7-C2-C3	-2.04	108.02	110.86
19	F	604	MQ9	C32-C31-C29	-2.04	106.42	113.19
16	R	602	HEA	CHD-C1D-ND	2.03	126.89	124.37
16	L	603	HEA	C3B-C4B-NB	2.03	112.17	109.84
20	O	301	HEC	CMB-C2B-C1B	-2.03	125.49	128.46
16	R	603	HEA	C4B-C3B-C2B	-2.02	104.04	107.44
23	E	603	HUU	C09-C12-C13	-2.02	127.60	131.32
22	F	601	HEM	C4B-CHC-C1C	2.02	125.22	122.56
21	Y	503	9YF	O2-P-O8	-2.01	103.37	109.81
22	E	601	HEM	O1D-CGD-CBD	-2.01	116.70	123.09
19	F	605	MQ9	C45-C44-C46	2.01	118.71	115.23
21	M	503	9YF	C6-C7-C2	2.01	114.23	109.68
21	Y	503	9YF	O9-C8-O10	-2.01	119.02	123.70
16	L	603	HEA	C13-C14-C15	-2.00	123.04	127.62
19	E	604	MQ9	C32-C31-C29	-2.00	106.55	113.19
19	F	605	MQ9	C51-C49-C50	2.00	119.20	114.59
19	E	605	MQ9	C45-C44-C43	-2.00	118.49	123.63

There are no chirality outliers.

All (1188) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	D	301	9XX	O2-C18-O1-C17
13	c	202	9XX	O-C16-C17-O1
13	c	202	9XX	C37-C17-O1-C18
13	c	202	9XX	C19-C18-O1-C17
16	R	602	HEA	C2D-C3D-CAD-CBD
16	R	602	HEA	C4D-C3D-CAD-CBD
16	L	602	HEA	C2D-C3D-CAD-CBD
16	L	602	HEA	C4D-C3D-CAD-CBD
17	R	604	CDL	CA2-OA2-PA1-OA4
17	R	604	CDL	CA2-OA2-PA1-OA5
17	R	604	CDL	OA7-CA5-OA6-CA4
17	R	604	CDL	CB2-OB2-PB2-OB3
17	R	604	CDL	C51-CB5-OB6-CB4
17	S	302	CDL	O1-C1-CB2-OB2
17	S	302	CDL	CA2-C1-CB2-OB2
17	S	302	CDL	CA2-OA2-PA1-OA3
17	S	302	CDL	CA2-OA2-PA1-OA4
17	S	302	CDL	CA2-OA2-PA1-OA5
17	S	302	CDL	CA3-OA5-PA1-OA2
17	S	302	CDL	CA3-OA5-PA1-OA3
17	S	302	CDL	CA3-OA5-PA1-OA4
17	S	302	CDL	CB2-OB2-PB2-OB4
17	S	302	CDL	CB2-OB2-PB2-OB5
17	S	302	CDL	CB3-OB5-PB2-OB2
17	S	302	CDL	CB3-OB5-PB2-OB4
17	S	302	CDL	C51-CB5-OB6-CB4
17	S	303	CDL	C1-CA2-OA2-PA1
17	S	303	CDL	CA2-OA2-PA1-OA4
17	S	303	CDL	CA3-OA5-PA1-OA4
17	S	303	CDL	C11-CA5-OA6-CA4
17	S	303	CDL	CB2-OB2-PB2-OB4
17	S	303	CDL	CB2-OB2-PB2-OB5
17	S	303	CDL	CB3-OB5-PB2-OB2
17	S	303	CDL	CB3-OB5-PB2-OB4
17	S	303	CDL	C51-CB5-OB6-CB4
17	T	202	CDL	CA2-C1-CB2-OB2
17	T	202	CDL	CA2-OA2-PA1-OA3
17	T	202	CDL	C11-CA5-OA6-CA4
17	T	202	CDL	OA9-CA7-OA8-CA6
17	T	202	CDL	C31-CA7-OA8-CA6
17	T	202	CDL	CB3-OB5-PB2-OB2
17	T	202	CDL	CB3-OB5-PB2-OB4
17	P	202	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
17	P	202	CDL	CA2-OA2-PA1-OA3
17	P	202	CDL	CA2-OA2-PA1-OA4
17	P	202	CDL	CA2-OA2-PA1-OA5
17	P	202	CDL	CB2-OB2-PB2-OB4
17	P	202	CDL	CB2-OB2-PB2-OB5
17	P	202	CDL	C51-CB5-OB6-CB4
17	E	606	CDL	CA2-OA2-PA1-OA3
17	E	606	CDL	CA2-OA2-PA1-OA5
17	E	606	CDL	CA3-OA5-PA1-OA2
17	E	606	CDL	CA3-OA5-PA1-OA3
17	E	606	CDL	CA3-OA5-PA1-OA4
17	E	606	CDL	C1-CB2-OB2-PB2
17	E	606	CDL	CB2-OB2-PB2-OB4
17	E	606	CDL	CB2-OB2-PB2-OB5
17	E	606	CDL	CB3-OB5-PB2-OB2
17	E	606	CDL	CB3-OB5-PB2-OB3
17	E	607	CDL	CA2-OA2-PA1-OA3
17	E	607	CDL	CA2-OA2-PA1-OA5
17	E	607	CDL	CB2-OB2-PB2-OB4
17	E	607	CDL	CB3-OB5-PB2-OB2
17	E	608	CDL	CA2-OA2-PA1-OA3
17	E	608	CDL	CA2-OA2-PA1-OA4
17	E	608	CDL	CA2-OA2-PA1-OA5
17	E	608	CDL	CA3-OA5-PA1-OA2
17	E	608	CDL	CA3-OA5-PA1-OA3
17	E	608	CDL	CB3-OB5-PB2-OB2
17	E	608	CDL	CB3-OB5-PB2-OB4
17	E	608	CDL	C51-CB5-OB6-CB4
17	L	605	CDL	CA2-C1-CB2-OB2
17	L	605	CDL	CA2-OA2-PA1-OA3
17	L	605	CDL	CA2-OA2-PA1-OA4
17	L	605	CDL	CA2-OA2-PA1-OA5
17	L	605	CDL	OA7-CA5-OA6-CA4
17	L	605	CDL	C11-CA5-OA6-CA4
17	L	605	CDL	CB2-OB2-PB2-OB5
17	L	605	CDL	CB3-OB5-PB2-OB4
17	L	605	CDL	C51-CB5-OB6-CB4
17	X	302	CDL	CB2-C1-CA2-OA2
17	X	302	CDL	CA2-C1-CB2-OB2
17	X	302	CDL	CA2-OA2-PA1-OA3
17	X	302	CDL	OA6-CA4-CA6-OA8
17	X	302	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
17	X	302	CDL	C1-CB2-OB2-PB2
17	X	302	CDL	CB2-OB2-PB2-OB3
17	X	302	CDL	CB3-OB5-PB2-OB2
17	X	302	CDL	CB3-OB5-PB2-OB4
17	X	302	CDL	OB7-CB5-OB6-CB4
17	X	302	CDL	C51-CB5-OB6-CB4
17	X	303	CDL	O1-C1-CB2-OB2
17	X	303	CDL	CA3-OA5-PA1-OA2
17	X	303	CDL	CA3-OA5-PA1-OA3
17	X	303	CDL	CA3-OA5-PA1-OA4
17	X	303	CDL	CB2-OB2-PB2-OB3
17	X	303	CDL	CB2-OB2-PB2-OB4
17	X	303	CDL	CB2-OB2-PB2-OB5
17	X	303	CDL	C51-CB5-OB6-CB4
17	Z	202	CDL	O1-C1-CB2-OB2
17	Z	202	CDL	CA2-OA2-PA1-OA3
17	Z	202	CDL	CA2-OA2-PA1-OA4
17	Z	202	CDL	CA2-OA2-PA1-OA5
17	Z	202	CDL	OA7-CA5-OA6-CA4
17	Z	202	CDL	C11-CA5-OA6-CA4
17	J	201	CDL	O1-C1-CB2-OB2
17	J	201	CDL	CA3-OA5-PA1-OA3
17	J	201	CDL	C11-CA5-OA6-CA4
17	J	201	CDL	CB2-OB2-PB2-OB3
17	J	201	CDL	CB2-OB2-PB2-OB4
17	J	201	CDL	CB2-OB2-PB2-OB5
17	J	201	CDL	CB3-OB5-PB2-OB2
17	J	201	CDL	CB3-OB5-PB2-OB3
17	F	606	CDL	O1-C1-CB2-OB2
17	F	606	CDL	CA2-C1-CB2-OB2
17	F	606	CDL	CA2-OA2-PA1-OA3
17	F	606	CDL	CA3-OA5-PA1-OA2
17	F	606	CDL	CA3-OA5-PA1-OA4
17	F	606	CDL	CB2-OB2-PB2-OB3
17	F	606	CDL	CB2-OB2-PB2-OB4
17	F	606	CDL	CB2-OB2-PB2-OB5
17	F	606	CDL	CB3-OB5-PB2-OB2
17	F	606	CDL	CB3-OB5-PB2-OB3
17	F	607	CDL	CB2-C1-CA2-OA2
17	F	607	CDL	CB2-OB2-PB2-OB3
17	F	607	CDL	CB3-OB5-PB2-OB2
17	F	607	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
17	F	608	CDL	CA2-OA2-PA1-OA5
17	F	608	CDL	OA5-CA3-CA4-OA6
17	F	608	CDL	C51-CB5-OB6-CB4
18	S	301	9Y0	C22-C21-O7-C1
18	S	301	9Y0	O6-C21-O7-C1
18	S	301	9Y0	O1-C3-C4-N
18	P	201	9Y0	O5-C-C1-O7
18	P	201	9Y0	O1-C3-C4-N
18	P	201	9Y0	C3-O1-P-O
18	P	201	9Y0	C3-O1-P-O2
18	P	201	9Y0	C3-O1-P-O3
18	P	201	9Y0	C2-O3-P-O1
18	P	201	9Y0	C2-O3-P-O2
18	L	604	9Y0	O1-C3-C4-N
18	L	604	9Y0	C2-O3-P-O
18	L	604	9Y0	C2-O3-P-O1
18	X	301	9Y0	C22-C21-O7-C1
18	X	301	9Y0	O1-C3-C4-N
19	T	201	MQ9	C44-C46-C47-C48
19	E	605	MQ9	C29-C31-C32-C33
20	O	301	HEC	C2D-C3D-CAD-CBD
20	O	301	HEC	C4D-C3D-CAD-CBD
21	O	303	9YF	C-C1-O-P
21	O	303	9YF	C9-C8-O9-C
21	E	609	9YF	C1-O-P-O1
21	E	609	9YF	C1-O-P-O8
21	E	609	9YF	C9-C8-O9-C
21	I	303	9YF	C-C1-O-P
21	I	303	9YF	C9-C8-O9-C
21	F	609	9YF	C2-O2-P-O1
21	F	609	9YF	C2-O2-P-O
21	F	609	9YF	C9-C8-O9-C
21	Y	502	9YF	C9-C8-O9-C
21	Y	503	9YF	C1-O-P-O1
21	Y	503	9YF	C1-O-P-O2
21	Y	503	9YF	C1-O-P-O8
21	Y	503	9YF	C9-C8-O9-C
21	M	502	9YF	C1-O-P-O1
21	M	502	9YF	C1-O-P-O2
21	M	502	9YF	C9-C8-O9-C
21	M	503	9YF	C1-O-P-O1
21	M	503	9YF	C1-O-P-O2

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Mol	Chain	Res	Type	Atoms
21	M	503	9YF	C1-O-P-O8
21	M	503	9YF	C9-C8-O9-C
22	E	602	HEM	C1A-C2A-CAA-CBA
22	E	602	HEM	C3A-C2A-CAA-CBA
17	R	604	CDL	OA9-CA7-OA8-CA6
17	L	605	CDL	OA9-CA7-OA8-CA6
17	R	604	CDL	C31-CA7-OA8-CA6
17	L	605	CDL	C31-CA7-OA8-CA6
17	T	202	CDL	OB9-CB7-OB8-CB6
17	Z	202	CDL	OA9-CA7-OA8-CA6
17	Z	202	CDL	OB9-CB7-OB8-CB6
18	S	301	9Y0	O4-C5-O5-C
21	O	303	9YF	O12-C25-O11-C24
21	I	303	9YF	O12-C25-O11-C24
21	Y	502	9YF	O12-C25-O11-C24
21	Y	503	9YF	O12-C25-O11-C24
21	M	502	9YF	O12-C25-O11-C24
13	c	202	9XX	O2-C18-O1-C17
17	R	604	CDL	OB7-CB5-OB6-CB4
17	S	303	CDL	OA7-CA5-OA6-CA4
17	S	303	CDL	OB7-CB5-OB6-CB4
17	T	202	CDL	OA7-CA5-OA6-CA4
17	P	202	CDL	OB7-CB5-OB6-CB4
17	E	608	CDL	OB7-CB5-OB6-CB4
17	L	605	CDL	OB7-CB5-OB6-CB4
17	X	303	CDL	OB7-CB5-OB6-CB4
17	F	608	CDL	OB7-CB5-OB6-CB4
18	X	301	9Y0	O6-C21-O7-C1
21	E	609	9YF	O10-C8-O9-C
21	I	303	9YF	O10-C8-O9-C
21	F	609	9YF	O10-C8-O9-C
21	Y	503	9YF	O10-C8-O9-C
21	M	502	9YF	O10-C8-O9-C
21	M	503	9YF	O10-C8-O9-C
17	X	302	CDL	C31-CA7-OA8-CA6
17	Z	202	CDL	C71-CB7-OB8-CB6
21	O	303	9YF	C26-C25-O11-C24
21	I	303	9YF	C26-C25-O11-C24
21	Y	502	9YF	C26-C25-O11-C24
21	M	502	9YF	C26-C25-O11-C24
13	D	301	9XX	C19-C18-O1-C17
17	R	604	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
18	X	301	9Y0	O4-C5-O5-C
17	T	202	CDL	C71-CB7-OB8-CB6
17	Z	202	CDL	C31-CA7-OA8-CA6
18	S	301	9Y0	C6-C5-O5-C
21	Y	503	9YF	C26-C25-O11-C24
17	S	302	CDL	OA9-CA7-OA8-CA6
21	M	503	9YF	O12-C25-O11-C24
17	S	302	CDL	OB7-CB5-OB6-CB4
17	J	201	CDL	OA7-CA5-OA6-CA4
21	O	303	9YF	O10-C8-O9-C
21	Y	502	9YF	O10-C8-O9-C
17	S	302	CDL	C71-C72-C73-C74
17	R	604	CDL	C74-C75-C76-C77
17	S	303	CDL	O1-C1-CA2-OA2
17	T	202	CDL	O1-C1-CB2-OB2
17	P	202	CDL	O1-C1-CA2-OA2
17	E	606	CDL	O1-C1-CB2-OB2
17	E	608	CDL	O1-C1-CA2-OA2
17	L	605	CDL	O1-C1-CB2-OB2
17	X	302	CDL	O1-C1-CB2-OB2
17	F	607	CDL	O1-C1-CA2-OA2
21	M	503	9YF	C26-C25-O11-C24
13	W	201	9XX	C19-C18-O1-C17
13	G	301	9XX	C19-C18-O1-C17
17	P	202	CDL	C11-CA5-OA6-CA4
17	S	303	CDL	CA7-C31-C32-C33
17	S	302	CDL	C31-CA7-OA8-CA6
18	X	301	9Y0	C6-C5-O5-C
16	L	602	HEA	C14-C15-C16-C17
16	L	603	HEA	C15-C16-C17-C18
19	T	201	MQ9	C14-C16-C17-C18
19	T	201	MQ9	C29-C31-C32-C33
19	T	201	MQ9	C39-C41-C42-C43
19	E	604	MQ9	C14-C16-C17-C18
19	E	605	MQ9	C44-C46-C47-C48
19	Z	201	MQ9	C29-C31-C32-C33
19	Z	201	MQ9	C39-C41-C42-C43
19	F	604	MQ9	C14-C16-C17-C18
19	F	605	MQ9	C29-C31-C32-C33
19	F	605	MQ9	C39-C41-C42-C43
17	E	606	CDL	C55-C56-C57-C58
17	L	605	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
17	F	608	CDL	C76-C77-C78-C79
22	E	602	HEM	C3D-CAD-CBD-CGD
22	F	602	HEM	C3D-CAD-CBD-CGD
17	E	608	CDL	C60-C61-C62-C63
17	T	202	CDL	C11-C12-C13-C14
17	E	606	CDL	C35-C36-C37-C38
17	R	604	CDL	C71-CB7-OB8-CB6
17	S	302	CDL	C58-C59-C60-C61
17	S	302	CDL	C73-C74-C75-C76
21	Y	502	9YF	C11-C10-C9-C8
17	F	606	CDL	C59-C60-C61-C62
17	S	303	CDL	C32-C33-C34-C35
17	P	202	CDL	C72-C73-C74-C75
17	P	202	CDL	C11-C12-C13-C14
17	L	605	CDL	C76-C77-C78-C79
17	F	606	CDL	C35-C36-C37-C38
21	M	502	9YF	C11-C10-C9-C8
17	R	604	CDL	OB9-CB7-OB8-CB6
13	W	201	9XX	O2-C18-O1-C17
17	Z	202	CDL	CA2-C1-CB2-OB2
17	J	201	CDL	CA2-C1-CB2-OB2
13	W	201	9XX	C14-C15-O-C16
17	E	606	CDL	C31-CA7-OA8-CA6
17	E	608	CDL	C31-CA7-OA8-CA6
17	F	606	CDL	C31-CA7-OA8-CA6
18	L	604	9Y0	C6-C5-O5-C
17	S	303	CDL	C36-C37-C38-C39
17	T	202	CDL	C74-C75-C76-C77
17	E	606	CDL	C33-C34-C35-C36
17	E	607	CDL	C36-C37-C38-C39
17	L	605	CDL	C56-C57-C58-C59
17	X	302	CDL	C73-C74-C75-C76
21	O	303	9YF	C39-C40-C41-C42
17	X	302	CDL	C71-C72-C73-C74
17	S	302	CDL	C38-C39-C40-C41
17	P	202	CDL	C55-C56-C57-C58
17	E	608	CDL	C57-C58-C59-C60
16	L	602	HEA	C26-C15-C16-C17
17	L	605	CDL	C52-C53-C54-C55
13	G	301	9XX	C14-C15-O-C16
17	E	606	CDL	C59-C60-C61-C62
17	X	302	CDL	C75-C76-C77-C78

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Mol	Chain	Res	Type	Atoms
17	J	201	CDL	C55-C56-C57-C58
17	E	608	CDL	OA9-CA7-OA8-CA6
13	G	301	9XX	O2-C18-O1-C17
13	D	301	9XX	C14-C15-O-C16
17	S	303	CDL	C31-CA7-OA8-CA6
21	F	609	9YF	C30-C31-C32-C33
17	Z	202	CDL	CB7-C71-C72-C73
17	J	201	CDL	CA7-C31-C32-C33
17	F	606	CDL	C33-C34-C35-C36
17	J	201	CDL	C11-C12-C13-C14
17	F	606	CDL	C55-C56-C57-C58
17	F	608	CDL	C58-C59-C60-C61
21	F	609	9YF	C33-C35-C36-C37
17	E	608	CDL	C76-C77-C78-C79
17	E	606	CDL	CB7-C71-C72-C73
17	F	607	CDL	CB5-C51-C52-C53
17	R	604	CDL	C56-C57-C58-C59
17	P	202	CDL	OA7-CA5-OA6-CA4
16	R	603	HEA	C15-C16-C17-C18
19	E	604	MQ9	C24-C26-C27-C28
19	E	605	MQ9	C9-C11-C12-C13
19	E	605	MQ9	C39-C41-C42-C43
19	Z	201	MQ9	C14-C16-C17-C18
19	Z	201	MQ9	C44-C46-C47-C48
19	F	604	MQ9	C24-C26-C27-C28
19	F	605	MQ9	C9-C11-C12-C13
19	F	605	MQ9	C44-C46-C47-C48
17	S	303	CDL	CA5-C11-C12-C13
17	E	607	CDL	CB5-C51-C52-C53
17	E	608	CDL	CB7-C71-C72-C73
21	M	503	9YF	C25-C26-C27-C28
17	E	606	CDL	OA9-CA7-OA8-CA6
17	J	201	CDL	C51-CB5-OB6-CB4
17	P	202	CDL	C1-CA2-OA2-PA1
17	S	302	CDL	CB5-C51-C52-C53
17	S	303	CDL	CB5-C51-C52-C53
17	J	201	CDL	CA5-C11-C12-C13
17	F	606	CDL	CB7-C71-C72-C73
17	F	607	CDL	CA5-C11-C12-C13
17	F	608	CDL	CB5-C51-C52-C53
18	S	301	9Y0	C5-C6-C7-C8
21	Y	503	9YF	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
17	X	302	CDL	O1-C1-CA2-OA2
13	W	201	9XX	O6-C15-O-C16
18	L	604	9Y0	O4-C5-O5-C
17	P	202	CDL	CB7-C71-C72-C73
17	J	201	CDL	CB7-C71-C72-C73
18	L	604	9Y0	C21-C22-C23-C24
17	F	606	CDL	OA9-CA7-OA8-CA6
17	R	604	CDL	CB5-C51-C52-C53
21	E	609	9YF	C26-C25-O11-C24
17	E	608	CDL	C11-CA5-OA6-CA4
17	X	302	CDL	C11-CA5-OA6-CA4
13	G	301	9XX	O6-C15-O-C16
13	D	301	9XX	O6-C15-O-C16
21	E	609	9YF	C30-C31-C32-C33
17	J	201	CDL	C73-C74-C75-C76
17	X	302	CDL	CB5-C51-C52-C53
17	F	606	CDL	CB5-C51-C52-C53
17	E	608	CDL	OA7-CA5-OA6-CA4
17	X	302	CDL	OA7-CA5-OA6-CA4
17	J	201	CDL	OB7-CB5-OB6-CB4
17	S	303	CDL	CB2-C1-CA2-OA2
17	X	303	CDL	CA2-C1-CB2-OB2
18	P	201	9Y0	C6-C5-O5-C
17	L	605	CDL	C61-C62-C63-C64
17	Z	202	CDL	CB5-C51-C52-C53
17	R	604	CDL	C38-C39-C40-C41
21	Y	502	9YF	C33-C35-C36-C37
17	F	608	CDL	C11-CA5-OA6-CA4
17	F	606	CDL	OB7-CB5-OB6-CB4
17	F	608	CDL	OA7-CA5-OA6-CA4
19	E	604	MQ9	C34-C36-C37-C38
19	F	604	MQ9	C34-C36-C37-C38
17	J	201	CDL	O1-C1-CA2-OA2
21	E	609	9YF	C33-C35-C36-C37
17	L	605	CDL	C38-C39-C40-C41
23	E	603	HUU	C37-C19-N20-C36
21	M	502	9YF	C33-C35-C36-C37
18	S	301	9Y0	C21-C22-C23-C24
17	T	202	CDL	C60-C61-C62-C63
17	S	303	CDL	OA9-CA7-OA8-CA6
17	X	302	CDL	CB4-CB6-OB8-CB7
17	L	605	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
17	T	202	CDL	CA7-C31-C32-C33
21	E	609	9YF	O12-C25-O11-C24
17	T	202	CDL	C32-C33-C34-C35
17	E	607	CDL	C60-C61-C62-C63
17	F	606	CDL	C11-C12-C13-C14
21	M	503	9YF	C26-C27-C28-C29
23	E	603	HUU	C18-C19-N20-C36
17	R	604	CDL	C32-C33-C34-C35
17	R	604	CDL	C58-C59-C60-C61
17	L	605	CDL	C75-C76-C77-C78
17	F	608	CDL	C72-C73-C74-C75
21	M	503	9YF	C37-C38-C39-C40
20	I	301	HEC	C3D-CAD-CBD-CGD
17	R	604	CDL	C77-C78-C79-C80
17	T	202	CDL	C57-C58-C59-C60
17	T	202	CDL	C75-C76-C77-C78
17	E	606	CDL	C38-C39-C40-C41
17	E	607	CDL	C57-C58-C59-C60
17	J	201	CDL	C59-C60-C61-C62
18	X	301	9Y0	C27-C28-C29-C30
21	Y	503	9YF	C35-C36-C37-C38
13	W	201	9XX	C28-C29-C30-C31
13	c	202	9XX	C1-C2-C3-C4
17	J	201	CDL	C72-C73-C74-C75
17	F	607	CDL	C58-C59-C60-C61
18	X	301	9Y0	C9-C10-C11-C12
21	O	303	9YF	C26-C27-C28-C29
13	c	202	9XX	C28-C29-C30-C31
17	S	303	CDL	C72-C73-C74-C75
17	E	607	CDL	C58-C59-C60-C61
17	X	303	CDL	C57-C58-C59-C60
17	F	607	CDL	C60-C61-C62-C63
21	I	303	9YF	C26-C27-C28-C29
21	M	503	9YF	C35-C36-C37-C38
17	Z	202	CDL	C37-C38-C39-C40
17	J	201	CDL	C56-C57-C58-C59
17	F	608	CDL	C53-C54-C55-C56
21	F	609	9YF	C9-C10-C11-C12
17	X	303	CDL	C59-C60-C61-C62
18	P	201	9Y0	C9-C10-C11-C12
17	X	303	CDL	C11-CA5-OA6-CA4
17	F	606	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
17	S	302	CDL	C36-C37-C38-C39
17	Z	202	CDL	C52-C53-C54-C55
17	S	302	CDL	C52-C53-C54-C55
17	T	202	CDL	C52-C53-C54-C55
17	E	607	CDL	C77-C78-C79-C80
17	X	302	CDL	C76-C77-C78-C79
17	X	303	CDL	C60-C61-C62-C63
17	X	303	CDL	C72-C73-C74-C75
17	Z	202	CDL	C31-C32-C33-C34
17	F	606	CDL	C12-C13-C14-C15
18	P	201	9Y0	O4-C5-O5-C
17	E	607	CDL	C11-C12-C13-C14
17	J	201	CDL	C52-C53-C54-C55
17	R	604	CDL	C53-C54-C55-C56
18	S	301	9Y0	C27-C28-C29-C30
17	E	608	CDL	CA5-C11-C12-C13
17	X	302	CDL	CA7-C31-C32-C33
17	P	202	CDL	C37-C38-C39-C40
17	F	608	CDL	C52-C53-C54-C55
17	J	201	CDL	C37-C38-C39-C40
21	O	303	9YF	C35-C36-C37-C38
17	P	202	CDL	C31-C32-C33-C34
17	J	201	CDL	CB3-CB4-CB6-OB8
17	S	303	CDL	C31-C32-C33-C34
17	T	202	CDL	C72-C73-C74-C75
17	F	608	CDL	C59-C60-C61-C62
21	Y	503	9YF	C37-C38-C39-C40
17	R	604	CDL	CB7-C71-C72-C73
17	E	607	CDL	CA5-C11-C12-C13
17	S	302	CDL	C35-C36-C37-C38
17	P	202	CDL	C52-C53-C54-C55
17	P	202	CDL	C54-C55-C56-C57
17	P	202	CDL	C56-C57-C58-C59
17	E	606	CDL	C77-C78-C79-C80
17	E	608	CDL	C38-C39-C40-C41
17	L	605	CDL	C37-C38-C39-C40
17	X	302	CDL	C12-C13-C14-C15
17	Z	202	CDL	C32-C33-C34-C35
17	F	606	CDL	C57-C58-C59-C60
17	R	604	CDL	C31-C32-C33-C34
17	S	303	CDL	C71-C72-C73-C74
17	E	606	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
17	X	303	CDL	C32-C33-C34-C35
17	Z	202	CDL	C35-C36-C37-C38
17	J	201	CDL	C54-C55-C56-C57
17	F	607	CDL	C35-C36-C37-C38
18	P	201	9Y0	C6-C7-C8-C9
17	F	606	CDL	C38-C39-C40-C41
21	Y	503	9YF	C26-C27-C28-C29
17	E	606	CDL	C11-C12-C13-C14
21	Y	503	9YF	C9-C10-C11-C12
17	F	607	CDL	C57-C58-C59-C60
21	F	609	9YF	C15-C16-C17-C18
21	Y	503	9YF	C12-C13-C14-C15
17	E	606	CDL	C11-CA5-OA6-CA4
17	S	303	CDL	C38-C39-C40-C41
17	J	201	CDL	C75-C76-C77-C78
17	F	608	CDL	C36-C37-C38-C39
17	F	608	CDL	C77-C78-C79-C80
17	F	606	CDL	CA7-C31-C32-C33
18	P	201	9Y0	C21-C22-C23-C24
17	T	202	CDL	C12-C13-C14-C15
17	Z	202	CDL	C11-C12-C13-C14
17	Z	202	CDL	C59-C60-C61-C62
18	L	604	9Y0	C9-C10-C11-C12
21	I	303	9YF	C18-C19-C20-C21
21	M	502	9YF	C10-C11-C12-C13
17	E	606	CDL	C32-C33-C34-C35
17	E	606	CDL	C71-C72-C73-C74
17	T	202	CDL	C36-C37-C38-C39
17	P	202	CDL	C32-C33-C34-C35
17	E	608	CDL	C54-C55-C56-C57
21	F	609	9YF	C19-C20-C21-C22
21	M	502	9YF	C28-C29-C30-C31
17	S	302	CDL	CB7-C71-C72-C73
17	J	201	CDL	C13-C14-C15-C16
18	S	301	9Y0	C9-C10-C11-C12
18	L	604	9Y0	C24-C25-C26-C27
21	E	609	9YF	C9-C10-C11-C12
21	M	503	9YF	C19-C20-C21-C22
17	F	606	CDL	C37-C38-C39-C40
17	F	606	CDL	C54-C55-C56-C57
21	I	303	9YF	C35-C36-C37-C38
13	c	202	9XX	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
17	X	303	CDL	C38-C39-C40-C41
17	X	303	CDL	C55-C56-C57-C58
18	X	301	9Y0	C6-C7-C8-C9
17	S	303	CDL	C75-C76-C77-C78
17	E	607	CDL	C34-C35-C36-C37
17	L	605	CDL	C51-C52-C53-C54
18	X	301	9Y0	C21-C22-C23-C24
17	R	604	CDL	C71-C72-C73-C74
17	S	303	CDL	C59-C60-C61-C62
17	T	202	CDL	C37-C38-C39-C40
17	X	303	CDL	C35-C36-C37-C38
17	P	202	CDL	C71-C72-C73-C74
17	F	606	CDL	C71-C72-C73-C74
17	E	606	CDL	C51-CB5-OB6-CB4
17	E	607	CDL	C11-CA5-OA6-CA4
17	E	607	CDL	C51-CB5-OB6-CB4
17	F	606	CDL	C11-CA5-OA6-CA4
17	T	202	CDL	C53-C54-C55-C56
18	L	604	9Y0	C6-C7-C8-C9
17	E	606	CDL	OA7-CA5-OA6-CA4
17	E	607	CDL	OA7-CA5-OA6-CA4
17	E	607	CDL	OB7-CB5-OB6-CB4
17	X	303	CDL	OA7-CA5-OA6-CA4
17	F	606	CDL	OA7-CA5-OA6-CA4
17	E	606	CDL	C37-C38-C39-C40
17	J	201	CDL	C77-C78-C79-C80
18	L	604	9Y0	C14-C15-C16-C17
17	Z	202	CDL	C73-C74-C75-C76
18	L	604	9Y0	C26-C27-C28-C29
17	X	303	CDL	C34-C35-C36-C37
18	L	604	9Y0	C16-C17-C18-C19
21	M	502	9YF	C19-C20-C21-C22
17	S	302	CDL	C59-C60-C61-C62
17	P	202	CDL	C60-C61-C62-C63
17	X	302	CDL	C38-C39-C40-C41
18	S	301	9Y0	C18-C19-C20-C37
21	I	303	9YF	C39-C40-C41-C42
21	Y	503	9YF	C15-C16-C17-C18
22	F	602	HEM	C1A-C2A-CAA-CBA
17	E	606	CDL	OB7-CB5-OB6-CB4
17	F	608	CDL	OB5-CB3-CB4-OB6
17	F	608	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
17	X	303	CDL	C11-C12-C13-C14
17	X	303	CDL	C75-C76-C77-C78
17	L	605	CDL	C73-C74-C75-C76
17	J	201	CDL	C57-C58-C59-C60
17	R	604	CDL	CA7-C31-C32-C33
17	X	303	CDL	CA5-C11-C12-C13
17	T	202	CDL	OA6-CA4-CA6-OA8
17	J	201	CDL	OB6-CB4-CB6-OB8
13	W	201	9XX	C10-C11-C12-C13
17	S	302	CDL	C11-C12-C13-C14
17	X	302	CDL	C36-C37-C38-C39
17	Z	202	CDL	C56-C57-C58-C59
17	F	607	CDL	C11-C12-C13-C14
21	F	609	9YF	C27-C28-C29-C30
14	W	202	PLM	C2-C3-C4-C5
13	W	201	9XX	C19-C20-C21-C22
17	P	202	CDL	C38-C39-C40-C41
17	E	607	CDL	C56-C57-C58-C59
17	L	605	CDL	C11-C12-C13-C14
17	J	201	CDL	C34-C35-C36-C37
21	Y	502	9YF	C28-C29-C30-C31
17	J	201	CDL	C12-C13-C14-C15
17	E	608	CDL	CB2-C1-CA2-OA2
17	F	608	CDL	O1-C1-CA2-OA2
17	E	607	CDL	C76-C77-C78-C79
17	E	608	CDL	C74-C75-C76-C77
17	P	202	CDL	C59-C60-C61-C62
17	F	608	CDL	C35-C36-C37-C38
17	X	302	CDL	C56-C57-C58-C59
17	F	607	CDL	CA7-C31-C32-C33
17	S	302	CDL	C11-CA5-OA6-CA4
13	c	202	9XX	C10-C11-C12-C13
17	S	302	CDL	C55-C56-C57-C58
21	Y	502	9YF	C19-C20-C21-C22
17	X	303	CDL	C73-C74-C75-C76
17	E	607	CDL	C72-C73-C74-C75
17	X	303	CDL	C31-C32-C33-C34
17	F	607	CDL	C56-C57-C58-C59
18	X	301	9Y0	C18-C19-C20-C37
18	X	301	9Y0	C14-C15-C16-C17
17	E	606	CDL	OB5-CB3-CB4-CB6
17	X	302	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
17	F	606	CDL	OB5-CB3-CB4-CB6
17	F	608	CDL	OA5-CA3-CA4-CA6
21	O	303	9YF	C24-C-C1-O
21	I	303	9YF	C24-C-C1-O
17	X	302	CDL	C52-C53-C54-C55
17	L	605	CDL	CB5-C51-C52-C53
13	G	301	9XX	C26-C27-C28-C29
17	F	608	CDL	C33-C34-C35-C36
13	G	301	9XX	C18-C19-C20-C21
18	X	301	9Y0	C5-C6-C7-C8
13	D	301	9XX	C20-C21-C22-C23
21	M	503	9YF	C13-C14-C15-C16
17	E	606	CDL	C78-C79-C80-C81
13	W	201	9XX	C1-C2-C3-C4
18	L	604	9Y0	C7-C8-C9-C10
13	G	301	9XX	C36-C27-C28-C29
21	M	503	9YF	C34-C33-C35-C36
17	T	202	CDL	C14-C15-C16-C17
21	M	502	9YF	C26-C27-C28-C29
17	R	604	CDL	C13-C14-C15-C16
17	E	606	CDL	C57-C58-C59-C60
17	P	202	CDL	CA5-C11-C12-C13
17	S	303	CDL	CA3-CA4-CA6-OA8
17	T	202	CDL	CA3-CA4-CA6-OA8
17	E	606	CDL	CB3-CB4-CB6-OB8
17	E	607	CDL	CA3-CA4-CA6-OA8
17	L	605	CDL	CB3-CB4-CB6-OB8
17	X	303	CDL	CB3-CB4-CB6-OB8
17	J	201	CDL	CA3-CA4-CA6-OA8
17	F	606	CDL	CB3-CB4-CB6-OB8
18	P	201	9Y0	O5-C-C1-C2
18	X	301	9Y0	O5-C-C1-C2
21	I	303	9YF	C1-C-C24-O11
17	P	202	CDL	C76-C77-C78-C79
18	P	201	9Y0	C14-C15-C16-C17
17	F	608	CDL	C74-C75-C76-C77
18	L	604	9Y0	C30-C31-C32-C33
17	R	604	CDL	C73-C74-C75-C76
17	S	303	CDL	C61-C62-C63-C64
17	X	302	CDL	C58-C59-C60-C61
17	F	606	CDL	C52-C53-C54-C55
17	F	607	CDL	C75-C76-C77-C78

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Mol	Chain	Res	Type	Atoms
17	Z	202	CDL	C72-C73-C74-C75
21	F	609	9YF	C38-C39-C40-C41
17	S	302	CDL	C12-C13-C14-C15
17	Z	202	CDL	CA7-C31-C32-C33
17	F	607	CDL	C51-CB5-OB6-CB4
17	P	202	CDL	C31-CA7-OA8-CA6
17	S	302	CDL	C53-C54-C55-C56
21	Y	502	9YF	C25-C26-C27-C28
17	E	606	CDL	C56-C57-C58-C59
17	L	605	CDL	C13-C14-C15-C16
17	X	303	CDL	C71-C72-C73-C74
17	F	606	CDL	C72-C73-C74-C75
17	E	607	CDL	C31-CA7-OA8-CA6
17	R	604	CDL	C61-C62-C63-C64
18	S	301	9Y0	C10-C11-C12-C13
17	S	303	CDL	C54-C55-C56-C57
17	E	606	CDL	C75-C76-C77-C78
17	E	607	CDL	C59-C60-C61-C62
18	X	301	9Y0	C32-C33-C34-C35
17	P	202	CDL	C74-C75-C76-C77
17	E	607	CDL	C33-C34-C35-C36
17	T	202	CDL	OB5-CB3-CB4-OB6
17	X	303	CDL	OB5-CB3-CB4-OB6
17	F	607	CDL	OA5-CA3-CA4-OA6
18	L	604	9Y0	O7-C1-C2-O3
17	E	607	CDL	C73-C74-C75-C76
19	T	201	MQ9	C12-C11-C9-C8
17	F	607	CDL	C52-C53-C54-C55
17	F	607	CDL	C72-C73-C74-C75
17	S	302	CDL	C31-C32-C33-C34
17	E	608	CDL	C56-C57-C58-C59
21	E	609	9YF	C38-C39-C40-C41
17	S	302	CDL	C39-C40-C41-C42
17	P	202	CDL	C34-C35-C36-C37
17	L	605	CDL	C32-C33-C34-C35
17	X	302	CDL	C53-C54-C55-C56
21	Y	502	9YF	C10-C11-C12-C13
17	Z	202	CDL	OB6-CB4-CB6-OB8
18	L	604	9Y0	O5-C-C1-O7
17	E	608	CDL	C59-C60-C61-C62
18	P	201	9Y0	C16-C17-C18-C19
17	S	303	CDL	C60-C61-C62-C63

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Mol	Chain	Res	Type	Atoms
17	X	302	CDL	C33-C34-C35-C36
14	G	302	PLM	C4-C5-C6-C7
21	Y	503	9YF	C11-C12-C13-C14
21	O	303	9YF	C20-C21-C22-C23
17	T	202	CDL	C71-C72-C73-C74
21	Y	503	9YF	C27-C28-C29-C30
17	E	608	CDL	CB5-C51-C52-C53
17	E	607	CDL	C52-C53-C54-C55
17	S	302	CDL	C71-CB7-OB8-CB6
21	F	609	9YF	C26-C25-O11-C24
17	P	202	CDL	C61-C62-C63-C64
13	G	301	9XX	C9-C10-C11-C12
17	R	604	CDL	C76-C77-C78-C79
17	E	608	CDL	C71-C72-C73-C74
17	R	604	CDL	C51-C52-C53-C54
17	S	302	CDL	CA5-C11-C12-C13
17	S	303	CDL	C39-C40-C41-C42
19	T	201	MQ9	C12-C11-C9-C10
19	Z	201	MQ9	C12-C11-C9-C10
17	J	201	CDL	C31-CA7-OA8-CA6
17	S	302	CDL	C33-C34-C35-C36
21	Y	503	9YF	C34-C33-C35-C36
17	R	604	CDL	C37-C38-C39-C40
17	E	606	CDL	C72-C73-C74-C75
17	F	606	CDL	C32-C33-C34-C35
17	F	608	CDL	C1-CA2-OA2-PA1
21	M	502	9YF	C-C1-O-P
17	X	303	CDL	C39-C40-C41-C42
14	W	202	PLM	C9-CA-CB-CC
17	S	302	CDL	C34-C35-C36-C37
17	F	607	CDL	C78-C79-C80-C81
21	M	503	9YF	C40-C41-C42-C43
17	F	607	CDL	C77-C78-C79-C80
17	J	201	CDL	C39-C40-C41-C42
17	T	202	CDL	C56-C57-C58-C59
17	E	608	CDL	C58-C59-C60-C61
17	F	608	CDL	OB5-CB3-CB4-CB6
21	Y	503	9YF	C32-C33-C35-C36
21	M	503	9YF	C32-C33-C35-C36
21	F	609	9YF	O12-C25-O11-C24
17	Z	202	CDL	C38-C39-C40-C41
21	O	303	9YF	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
13	W	201	9XX	O-C16-C17-C37
13	G	301	9XX	O-C16-C17-C37
13	c	202	9XX	O-C16-C17-C37
17	E	607	CDL	C78-C79-C80-C81
17	E	607	CDL	OA9-CA7-OA8-CA6
17	L	605	CDL	C57-C58-C59-C60
21	M	503	9YF	C15-C16-C17-C18
18	X	301	9Y0	C10-C11-C12-C13
17	F	608	CDL	CA7-C31-C32-C33
17	E	608	CDL	C37-C38-C39-C40
17	R	604	CDL	CB3-CB4-CB6-OB8
17	X	302	CDL	CA3-CA4-CA6-OA8
17	X	302	CDL	CB3-CB4-CB6-OB8
18	L	604	9Y0	O5-C-C1-C2
21	O	303	9YF	C1-C-C24-O11
17	F	606	CDL	C56-C57-C58-C59
17	E	608	CDL	C32-C33-C34-C35
21	E	609	9YF	C27-C28-C29-C30
19	Z	201	MQ9	C12-C11-C9-C8
21	M	503	9YF	C27-C28-C29-C30
13	W	201	9XX	O-C16-C17-O1
13	G	301	9XX	O-C16-C17-O1
17	S	303	CDL	C57-C58-C59-C60
17	L	605	CDL	C77-C78-C79-C80
17	F	608	CDL	C31-C32-C33-C34
17	S	303	CDL	CB7-C71-C72-C73
17	R	604	CDL	OA5-CA3-CA4-OA6
17	J	201	CDL	OA5-CA3-CA4-OA6
17	F	607	CDL	OB5-CB3-CB4-OB6
21	M	502	9YF	O9-C-C1-O
17	S	303	CDL	C51-C52-C53-C54
17	E	607	CDL	C32-C33-C34-C35
17	E	607	CDL	C37-C38-C39-C40
21	M	502	9YF	C12-C13-C14-C15
17	E	606	CDL	CB4-CB3-OB5-PB2
17	E	607	CDL	C1-CA2-OA2-PA1
17	E	608	CDL	C1-CA2-OA2-PA1
17	L	605	CDL	C35-C36-C37-C38
17	F	606	CDL	C78-C79-C80-C81
17	T	202	CDL	C13-C14-C15-C16
17	F	607	CDL	C59-C60-C61-C62
18	S	301	9Y0	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
17	S	303	CDL	OA6-CA4-CA6-OA8
17	E	608	CDL	OB6-CB4-CB6-OB8
17	X	302	CDL	OB6-CB4-CB6-OB8
17	J	201	CDL	OA6-CA4-CA6-OA8
17	F	608	CDL	OB6-CB4-CB6-OB8
18	S	301	9Y0	O5-C-C1-O7
18	X	301	9Y0	O5-C-C1-O7
21	E	609	9YF	O9-C-C24-O11
13	c	202	9XX	C7-C8-C9-C10
17	F	607	CDL	OB7-CB5-OB6-CB4
17	X	302	CDL	CA5-C11-C12-C13
21	Y	503	9YF	C18-C19-C20-C21
21	M	503	9YF	C17-C18-C19-C20
21	M	503	9YF	C30-C31-C32-C33
18	X	301	9Y0	C29-C30-C31-C32
23	E	603	HUU	C37-C19-N20-C21
21	E	609	9YF	C26-C27-C28-C29
21	M	502	9YF	C35-C36-C37-C38
17	S	302	CDL	C37-C38-C39-C40
17	P	202	CDL	C57-C58-C59-C60
17	S	303	CDL	C13-C14-C15-C16
17	F	606	CDL	C76-C77-C78-C79
18	P	201	9Y0	C7-C8-C9-C10
18	P	201	9Y0	C30-C31-C32-C33
17	P	202	CDL	C39-C40-C41-C42
17	P	202	CDL	CA7-C31-C32-C33
13	W	201	9XX	C3-C4-C5-C6
17	S	302	CDL	OA7-CA5-OA6-CA4
17	E	606	CDL	CA2-C1-CB2-OB2
17	S	303	CDL	C58-C59-C60-C61
17	F	607	CDL	C31-C32-C33-C34
18	S	301	9Y0	C29-C30-C31-C32
17	S	302	CDL	C13-C14-C15-C16
17	R	604	CDL	OA5-CA3-CA4-CA6
17	X	303	CDL	OB5-CB3-CB4-CB6
18	L	604	9Y0	C-C1-C2-O3
17	P	202	CDL	OA9-CA7-OA8-CA6
17	E	607	CDL	C39-C40-C41-C42
17	X	303	CDL	C78-C79-C80-C81
17	T	202	CDL	C61-C62-C63-C64
17	F	606	CDL	C36-C37-C38-C39
17	S	302	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
22	F	602	HEM	C3A-C2A-CAA-CBA
17	E	607	CDL	C74-C75-C76-C77
17	Z	202	CDL	C54-C55-C56-C57
17	J	201	CDL	C60-C61-C62-C63
19	E	604	MQ9	C15-C14-C16-C17
19	Z	201	MQ9	C30-C29-C31-C32
19	F	604	MQ9	C15-C14-C16-C17
17	J	201	CDL	OA9-CA7-OA8-CA6
18	L	604	9Y0	C32-C33-C34-C35
18	L	604	9Y0	C23-C24-C25-C26
21	Y	502	9YF	C35-C36-C37-C38
21	Y	503	9YF	C17-C18-C19-C20
17	F	606	CDL	C34-C35-C36-C37
14	D	302	PLM	C4-C5-C6-C7
21	Y	502	9YF	C26-C27-C28-C29
17	S	302	CDL	OB5-CB3-CB4-OB6
17	E	607	CDL	OB5-CB3-CB4-OB6
17	S	302	CDL	CB3-CB4-CB6-OB8
17	S	303	CDL	CB3-CB4-CB6-OB8
17	P	202	CDL	CA3-CA4-CA6-OA8
17	E	606	CDL	CA3-CA4-CA6-OA8
18	S	301	9Y0	O5-C-C1-C2
21	E	609	9YF	C1-C-C24-O11
21	F	609	9YF	C1-C-C24-O11
22	F	602	HEM	C4B-C3B-CAB-CBB
17	X	302	CDL	C57-C58-C59-C60
21	O	303	9YF	C37-C38-C39-C40
19	T	201	MQ9	C30-C29-C31-C32
21	O	303	9YF	C33-C35-C36-C37
17	R	604	CDL	OB6-CB4-CB6-OB8
17	S	303	CDL	OB6-CB4-CB6-OB8
17	E	607	CDL	OA6-CA4-CA6-OA8
17	L	605	CDL	OB6-CB4-CB6-OB8
21	O	303	9YF	O9-C-C24-O11
21	I	303	9YF	O9-C-C24-O11
17	Z	202	CDL	C78-C79-C80-C81
17	E	608	CDL	C51-C52-C53-C54
21	Y	502	9YF	C18-C19-C20-C21
17	L	605	CDL	C55-C56-C57-C58
21	E	609	9YF	C2-O2-P-O8
18	P	201	9Y0	C23-C24-C25-C26
14	c	201	PLM	C9-CA-CB-CC

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Mol	Chain	Res	Type	Atoms
21	Y	503	9YF	C19-C20-C21-C22
21	M	502	9YF	C18-C19-C20-C21
17	F	606	CDL	C39-C40-C41-C42
21	Y	503	9YF	C10-C11-C12-C13
17	F	607	CDL	C11-CA5-OA6-CA4
17	L	605	CDL	C58-C59-C60-C61
19	E	604	MQ9	C9-C11-C12-C13
19	Z	201	MQ9	C20-C19-C21-C22
18	S	301	9Y0	C14-C15-C16-C17
17	S	302	CDL	OB5-CB3-CB4-CB6
17	T	202	CDL	OB5-CB3-CB4-CB6
17	E	607	CDL	OB5-CB3-CB4-CB6
17	X	302	CDL	OB5-CB3-CB4-CB6
17	F	607	CDL	OA5-CA3-CA4-CA6
17	F	607	CDL	OB5-CB3-CB4-CB6
17	F	608	CDL	C75-C76-C77-C78
21	I	303	9YF	C32-C33-C35-C36
17	R	604	CDL	C55-C56-C57-C58
21	O	303	9YF	C29-C30-C31-C32
17	E	606	CDL	C14-C15-C16-C17
17	E	607	CDL	C1-CB2-OB2-PB2
17	J	201	CDL	C1-CA2-OA2-PA1
17	F	606	CDL	C1-CB2-OB2-PB2
17	F	606	CDL	CB4-CB3-OB5-PB2
21	Y	502	9YF	C-C1-O-P
17	P	202	CDL	OB5-CB3-CB4-OB6
17	E	606	CDL	OA5-CA3-CA4-OA6
17	E	606	CDL	OB5-CB3-CB4-OB6
17	X	302	CDL	OA5-CA3-CA4-OA6
17	X	302	CDL	OB5-CB3-CB4-OB6
17	J	201	CDL	OB5-CB3-CB4-OB6
17	F	606	CDL	OB5-CB3-CB4-OB6
21	O	303	9YF	O9-C-C1-O
21	I	303	9YF	O9-C-C1-O
21	O	303	9YF	C16-C17-C18-C19
17	R	604	CDL	C52-C53-C54-C55
21	M	502	9YF	C37-C38-C39-C40
17	E	608	CDL	C61-C62-C63-C64
17	P	202	CDL	OA6-CA4-CA6-OA8
17	X	303	CDL	OB6-CB4-CB6-OB8
21	F	609	9YF	O9-C-C24-O11
17	X	302	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
17	E	608	CDL	CB3-CB4-CB6-OB8
14	G	302	PLM	C7-C8-C9-CA
19	E	604	MQ9	C13-C14-C16-C17
17	F	606	CDL	C14-C15-C16-C17
21	Y	503	9YF	C40-C41-C42-C43
17	X	303	CDL	C51-C52-C53-C54
21	M	502	9YF	C25-C26-C27-C28
21	Y	503	9YF	C30-C31-C32-C33
21	Y	502	9YF	C11-C12-C13-C14
17	S	303	CDL	C35-C36-C37-C38
18	S	301	9Y0	C32-C33-C34-C35
13	D	301	9XX	C16-C17-O1-C18
17	S	302	CDL	CB3-OB5-PB2-OB3
17	S	303	CDL	CA2-OA2-PA1-OA3
17	S	303	CDL	CA2-OA2-PA1-OA5
17	S	303	CDL	CA3-OA5-PA1-OA2
17	S	303	CDL	CA3-OA5-PA1-OA3
17	T	202	CDL	CA3-OA5-PA1-OA2
17	T	202	CDL	CA3-OA5-PA1-OA3
17	T	202	CDL	CA3-OA5-PA1-OA4
17	T	202	CDL	CB2-OB2-PB2-OB3
17	P	202	CDL	CB2-OB2-PB2-OB3
17	P	202	CDL	CB3-OB5-PB2-OB3
17	E	606	CDL	CB2-OB2-PB2-OB3
17	E	607	CDL	CB2-OB2-PB2-OB3
17	E	607	CDL	CB2-OB2-PB2-OB5
17	E	607	CDL	CB3-OB5-PB2-OB3
17	E	608	CDL	CA3-OA5-PA1-OA4
17	E	608	CDL	CB2-OB2-PB2-OB3
17	E	608	CDL	CB3-OB5-PB2-OB3
17	L	605	CDL	CB2-OB2-PB2-OB3
17	X	302	CDL	CB3-OB5-PB2-OB3
17	Z	202	CDL	CA3-OA5-PA1-OA2
17	Z	202	CDL	CA3-OA5-PA1-OA3
17	Z	202	CDL	CA3-OA5-PA1-OA4
17	J	201	CDL	CA3-OA5-PA1-OA2
17	J	201	CDL	CA3-OA5-PA1-OA4
17	J	201	CDL	CB3-OB5-PB2-OB4
17	F	606	CDL	CA3-OA5-PA1-OA3
17	F	606	CDL	CB3-OB5-PB2-OB4
17	F	607	CDL	CA2-OA2-PA1-OA3
17	F	608	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
21	E	609	9YF	C2-O2-P-O
21	E	609	9YF	C1-O-P-O2
21	F	609	9YF	C1-O-P-O1
21	F	609	9YF	C1-O-P-O2
21	F	609	9YF	C1-O-P-O8
21	Y	502	9YF	C1-O-P-O2
17	E	608	CDL	C39-C40-C41-C42
18	P	201	9Y0	C24-C25-C26-C27
21	O	303	9YF	C27-C28-C29-C30
19	T	201	MQ9	C28-C29-C31-C32
19	F	604	MQ9	C13-C14-C16-C17
17	L	605	CDL	C53-C54-C55-C56
17	S	302	CDL	CA4-CA3-OA5-PA1
17	S	302	CDL	C1-CB2-OB2-PB2
17	E	606	CDL	C1-CA2-OA2-PA1
17	E	608	CDL	C1-CB2-OB2-PB2
17	X	303	CDL	C1-CB2-OB2-PB2
17	Z	202	CDL	C1-CA2-OA2-PA1
17	F	606	CDL	C1-CA2-OA2-PA1
17	F	607	CDL	C1-CB2-OB2-PB2
17	F	608	CDL	C1-CB2-OB2-PB2
17	E	607	CDL	CA7-C31-C32-C33
17	L	605	CDL	C39-C40-C41-C42
23	E	603	HUU	C18-C19-N20-C21
18	L	604	9Y0	C11-C12-C13-C14
17	L	605	CDL	C78-C79-C80-C81
17	E	606	CDL	CB6-CB4-OB6-CB5
17	X	302	CDL	CB6-CB4-OB6-CB5
17	F	606	CDL	CB3-CB4-OB6-CB5
17	E	608	CDL	C77-C78-C79-C80
17	F	607	CDL	C14-C15-C16-C17
19	Z	201	MQ9	C28-C29-C31-C32
17	L	605	CDL	C72-C73-C74-C75
18	P	201	9Y0	C22-C23-C24-C25
17	J	201	CDL	C14-C15-C16-C17
17	X	303	CDL	C33-C34-C35-C36
21	M	503	9YF	C16-C17-C18-C19
18	P	201	9Y0	C32-C33-C34-C35
17	R	604	CDL	C39-C40-C41-C42
17	E	607	CDL	C71-C72-C73-C74
18	S	301	9Y0	C13-C14-C15-C16
17	X	302	CDL	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
17	X	302	CDL	C78-C79-C80-C81
17	J	201	CDL	C38-C39-C40-C41
17	F	607	CDL	OA7-CA5-OA6-CA4
17	X	302	CDL	C11-C12-C13-C14
21	I	303	9YF	C29-C30-C31-C32
17	X	302	CDL	C51-C52-C53-C54
14	D	302	PLM	C7-C8-C9-CA
17	X	302	CDL	C77-C78-C79-C80
17	S	302	CDL	C14-C15-C16-C17
17	J	201	CDL	C32-C31-CA7-OA8
17	F	608	CDL	C51-C52-C53-C54
17	E	608	CDL	C34-C35-C36-C37
17	F	607	CDL	C39-C40-C41-C42
18	P	201	9Y0	C11-C12-C13-C14
19	T	201	MQ9	C20-C19-C21-C22
23	F	603	HUU	C18-C19-N20-C36
17	F	606	CDL	CA4-CA3-OA5-PA1
20	O	301	HEC	C1A-C2A-CAA-CBA
19	E	605	MQ9	C35-C34-C36-C37
17	X	303	CDL	OA5-CA3-CA4-OA6
21	Y	502	9YF	O9-C-C1-O
16	L	602	HEA	C12-C11-C3B-C2B
14	c	201	PLM	CA-CB-CC-CD
17	Z	202	CDL	C57-C58-C59-C60
21	F	609	9YF	C28-C29-C30-C31
21	Y	502	9YF	C37-C38-C39-C40
13	D	301	9XX	C10-C11-C12-C13
18	L	604	9Y0	C22-C23-C24-C25
17	L	605	CDL	OB9-CB7-OB8-CB6
17	F	606	CDL	C75-C76-C77-C78
17	T	202	CDL	C55-C56-C57-C58
17	F	607	CDL	C36-C37-C38-C39
21	O	303	9YF	C12-C13-C14-C15
21	M	502	9YF	C16-C17-C18-C19
21	Y	502	9YF	C12-C13-C14-C15
17	X	303	CDL	C58-C59-C60-C61
19	Z	201	MQ9	C18-C19-C21-C22
17	F	608	CDL	CB3-CB4-CB6-OB8
19	F	604	MQ9	C19-C21-C22-C23
21	Y	502	9YF	C16-C17-C18-C19
17	T	202	CDL	C73-C74-C75-C76
17	L	605	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
21	O	303	9YF	C15-C16-C17-C18
21	Y	502	9YF	C17-C18-C19-C20
19	E	605	MQ9	C40-C39-C41-C42
19	T	201	MQ9	C18-C19-C21-C22
19	E	605	MQ9	C38-C39-C41-C42
17	S	303	CDL	C14-C15-C16-C17
13	D	301	9XX	O-C16-C17-O1
17	P	202	CDL	C75-C76-C77-C78
16	R	602	HEA	CAA-CBA-CGA-O1A
18	X	301	9Y0	C13-C14-C15-C16
17	L	605	CDL	C71-CB7-OB8-CB6
17	S	303	CDL	CA4-CA3-OA5-PA1
17	L	605	CDL	C1-CB2-OB2-PB2
17	X	303	CDL	CB4-CB3-OB5-PB2
16	L	602	HEA	CAA-CBA-CGA-O1A
19	E	604	MQ9	C20-C19-C21-C22
19	F	605	MQ9	C30-C29-C31-C32
17	E	607	CDL	C55-C56-C57-C58
17	E	606	CDL	OA5-CA3-CA4-CA6
17	X	303	CDL	C76-C77-C78-C79
19	Z	201	MQ9	C31-C32-C33-C34
16	R	603	HEA	CAA-CBA-CGA-O1A
16	L	603	HEA	CAA-CBA-CGA-O2A
21	E	609	9YF	C20-C21-C22-C23
17	E	606	CDL	OA6-CA4-CA6-OA8
17	F	607	CDL	OB6-CB4-CB6-OB8
21	Y	503	9YF	C13-C14-C15-C16
17	F	608	CDL	CA5-C11-C12-C13
16	R	602	HEA	CAD-CBD-CGD-O1D
16	L	603	HEA	CAA-CBA-CGA-O1A
17	F	608	CDL	CB2-C1-CA2-OA2
14	D	302	PLM	C2-C3-C4-C5
19	F	604	MQ9	C12-C11-C9-C10
17	R	604	CDL	C72-C71-CB7-OB8
19	E	605	MQ9	C33-C34-C36-C37
17	F	607	CDL	C71-CB7-OB8-CB6
17	E	606	CDL	C52-C53-C54-C55
17	Z	202	CDL	C14-C15-C16-C17
13	G	301	9XX	C20-C21-C22-C23
17	P	202	CDL	C51-C52-C53-C54
16	R	603	HEA	CAA-CBA-CGA-O2A
19	E	605	MQ9	C12-C11-C9-C10

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Mol	Chain	Res	Type	Atoms
19	Z	201	MQ9	C45-C44-C46-C47
19	F	604	MQ9	C20-C19-C21-C22
19	F	605	MQ9	C20-C19-C21-C22
17	E	606	CDL	CA4-CA3-OA5-PA1
19	Z	201	MQ9	C19-C21-C22-C23
14	W	202	PLM	CC-CD-CE-CF
16	R	602	HEA	CAD-CBD-CGD-O2D
16	L	602	HEA	CAA-CBA-CGA-O2A
17	X	303	CDL	C36-C37-C38-C39
16	R	602	HEA	C26-C15-C16-C17
19	E	604	MQ9	C12-C11-C9-C10
17	E	606	CDL	C54-C55-C56-C57
16	R	602	HEA	CAA-CBA-CGA-O2A
17	J	201	CDL	C72-C71-CB7-OB8
19	E	604	MQ9	C12-C11-C9-C8
17	S	302	CDL	C32-C33-C34-C35
22	F	601	HEM	CAA-CBA-CGA-O1A
13	c	202	9XX	O1-C18-C19-C20
17	T	202	CDL	C52-C51-CB5-OB6
17	J	201	CDL	C58-C59-C60-C61
17	E	607	CDL	CA2-C1-CB2-OB2
17	Z	202	CDL	C13-C14-C15-C16
17	L	605	CDL	C71-C72-C73-C74
17	P	202	CDL	OB5-CB3-CB4-CB6
17	J	201	CDL	OA5-CA3-CA4-CA6
17	J	201	CDL	OB5-CB3-CB4-CB6
19	E	604	MQ9	C19-C21-C22-C23
21	I	303	9YF	C34-C33-C35-C36
14	W	202	PLM	C7-C8-C9-CA
17	X	303	CDL	C52-C51-CB5-OB6
17	E	607	CDL	CB4-CB6-OB8-CB7
13	c	202	9XX	C19-C20-C21-C22
17	X	302	CDL	CB7-C71-C72-C73
17	S	302	CDL	CB6-CB4-OB6-CB5
17	X	303	CDL	C53-C54-C55-C56
21	M	503	9YF	C36-C37-C38-C39
21	Y	503	9YF	C-C1-O-P
19	F	604	MQ9	C9-C11-C12-C13
21	F	609	9YF	C26-C27-C28-C29
21	M	503	9YF	C38-C39-C40-C41
19	E	605	MQ9	C20-C19-C21-C22
19	F	605	MQ9	C12-C11-C9-C10

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Mol	Chain	Res	Type	Atoms
17	F	608	CDL	C73-C74-C75-C76
17	F	607	CDL	OB9-CB7-OB8-CB6
21	M	503	9YF	C9-C10-C11-C12
17	X	302	CDL	C39-C40-C41-C42
17	F	607	CDL	C73-C74-C75-C76
17	X	303	CDL	OA5-CA3-CA4-CA6
22	E	601	HEM	CAA-CBA-CGA-O1A
17	F	608	CDL	CB7-C71-C72-C73
21	I	303	9YF	C17-C18-C19-C20
13	D	301	9XX	C13-C14-C15-O
16	R	602	HEA	C14-C15-C16-C17
19	E	604	MQ9	C18-C19-C21-C22
13	W	201	9XX	C25-C26-C27-C28
13	D	301	9XX	C26-C27-C28-C29
21	F	609	9YF	C31-C32-C33-C35
21	O	303	9YF	C11-C12-C13-C14
21	O	303	9YF	O11-C25-C26-C27
21	I	303	9YF	O11-C25-C26-C27
17	S	302	CDL	CB4-CB3-OB5-PB2
21	I	303	9YF	C11-C12-C13-C14
21	O	303	9YF	C2-O2-P-O8
21	F	609	9YF	C2-O2-P-O8
17	Z	202	CDL	C58-C59-C60-C61
21	I	303	9YF	O9-C8-C9-C10
17	S	303	CDL	C73-C74-C75-C76
13	c	202	9XX	C5-C6-C7-C8
22	F	601	HEM	CAA-CBA-CGA-O2A
21	M	502	9YF	O9-C8-C9-C10
17	Z	202	CDL	C71-C72-C73-C74
21	O	303	9YF	O9-C8-C9-C10
21	I	303	9YF	C12-C13-C14-C15
17	E	608	CDL	C52-C53-C54-C55
13	W	201	9XX	C25-C26-C27-C36
21	I	303	9YF	C33-C35-C36-C37
18	L	604	9Y0	C1-C2-O3-P
17	J	201	CDL	C12-C11-CA5-OA6
18	S	301	9Y0	O7-C21-C22-C23
17	E	608	CDL	OA6-CA4-CA6-OA8
13	W	201	9XX	C13-C14-C15-O
21	Y	502	9YF	O9-C8-C9-C10
17	F	607	CDL	CB7-C71-C72-C73
21	O	303	9YF	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
17	R	604	CDL	C33-C34-C35-C36
19	E	605	MQ9	C41-C42-C43-C44
19	Z	201	MQ9	C16-C17-C18-C19
17	E	607	CDL	C71-CB7-OB8-CB6
23	E	603	HUU	C26-C27-O28-C29
21	E	609	9YF	C39-C40-C41-C42
19	T	201	MQ9	C31-C32-C33-C34
21	M	502	9YF	C17-C18-C19-C20
21	I	303	9YF	O12-C25-C26-C27
17	R	604	CDL	CB4-CB3-OB5-PB2
17	L	605	CDL	CB4-CB3-OB5-PB2
17	J	201	CDL	CA4-CA3-OA5-PA1
16	R	603	HEA	C14-C15-C16-C17
19	F	605	MQ9	C28-C29-C31-C32
21	I	303	9YF	O10-C8-C9-C10
18	L	604	9Y0	O5-C5-C6-C7
23	F	603	HUU	C37-C19-N20-C36
13	D	301	9XX	C36-C27-C28-C29
17	E	608	CDL	C35-C36-C37-C38
22	E	601	HEM	CAD-CBD-CGD-O2D
13	D	301	9XX	C13-C14-C15-O6
21	O	303	9YF	C14-C15-C16-C17
14	c	201	PLM	C5-C6-C7-C8
18	S	301	9Y0	O6-C21-C22-C23
21	O	303	9YF	O12-C25-C26-C27
18	P	201	9Y0	C18-C19-C20-C37
17	Z	202	CDL	CB4-CB6-OB8-CB7
17	P	202	CDL	C77-C78-C79-C80
13	W	201	9XX	C20-C21-C22-C23
17	E	607	CDL	OB9-CB7-OB8-CB6
17	P	202	CDL	C12-C11-CA5-OA6
22	E	601	HEM	CAA-CBA-CGA-O2A
13	W	201	9XX	C13-C14-C15-O6
21	M	502	9YF	O10-C8-C9-C10
17	X	302	CDL	C72-C71-CB7-OB8
17	L	605	CDL	CB7-C71-C72-C73
21	O	303	9YF	O10-C8-C9-C10
16	L	602	HEA	C16-C17-C18-C19
17	X	302	CDL	CB4-CB3-OB5-PB2
13	D	301	9XX	O1-C18-C19-C20
17	S	302	CDL	C52-C51-CB5-OB6
17	F	608	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
21	O	303	9YF	C40-C41-C42-C43
16	L	602	HEA	O11-C11-C3B-C4B
21	I	303	9YF	C10-C11-C12-C13
21	Y	502	9YF	O10-C8-C9-C10
17	J	201	CDL	C12-C11-CA5-OA7
17	T	202	CDL	C12-C11-CA5-OA6
17	E	606	CDL	CB5-C51-C52-C53
18	P	201	9Y0	C5-C6-C7-C8
17	L	605	CDL	C72-C71-CB7-OB8
23	E	603	HUU	C33-C27-O28-C29
17	F	607	CDL	C54-C55-C56-C57

There are no ring outliers.

40 monomers are involved in 296 short contacts:

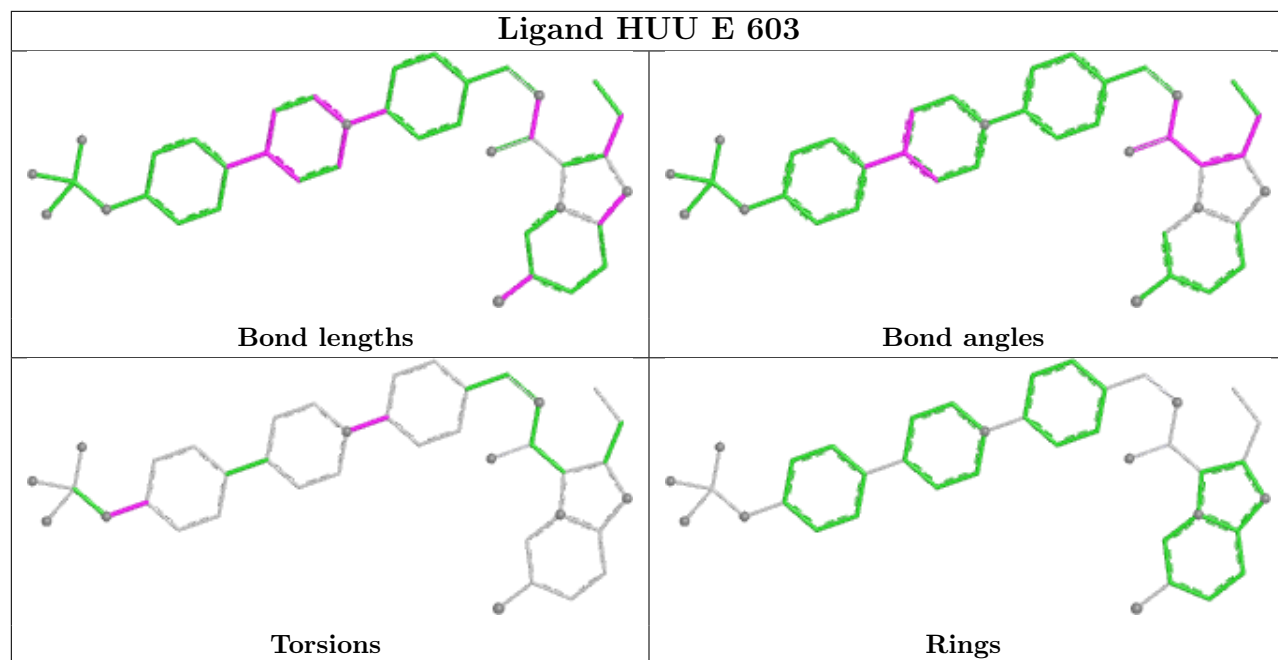
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	T	202	CDL	21	0
17	Z	202	CDL	26	0
13	W	201	9XX	1	0
17	P	202	CDL	8	0
24	M	501	FES	1	0
22	E	602	HEM	9	0
14	D	302	PLM	1	0
16	L	603	HEA	7	0
16	R	603	HEA	6	0
22	F	602	HEM	3	0
17	F	606	CDL	7	0
17	L	605	CDL	14	0
19	F	604	MQ9	2	0
16	L	602	HEA	6	0
17	F	607	CDL	10	0
17	R	604	CDL	10	0
22	F	601	HEM	6	0
21	I	303	9YF	1	0
17	J	201	CDL	11	0
19	T	201	MQ9	5	0
20	O	301	HEC	12	0
17	E	606	CDL	6	0
19	Z	201	MQ9	3	0
20	I	301	HEC	6	0
17	X	303	CDL	8	0
17	S	302	CDL	18	0

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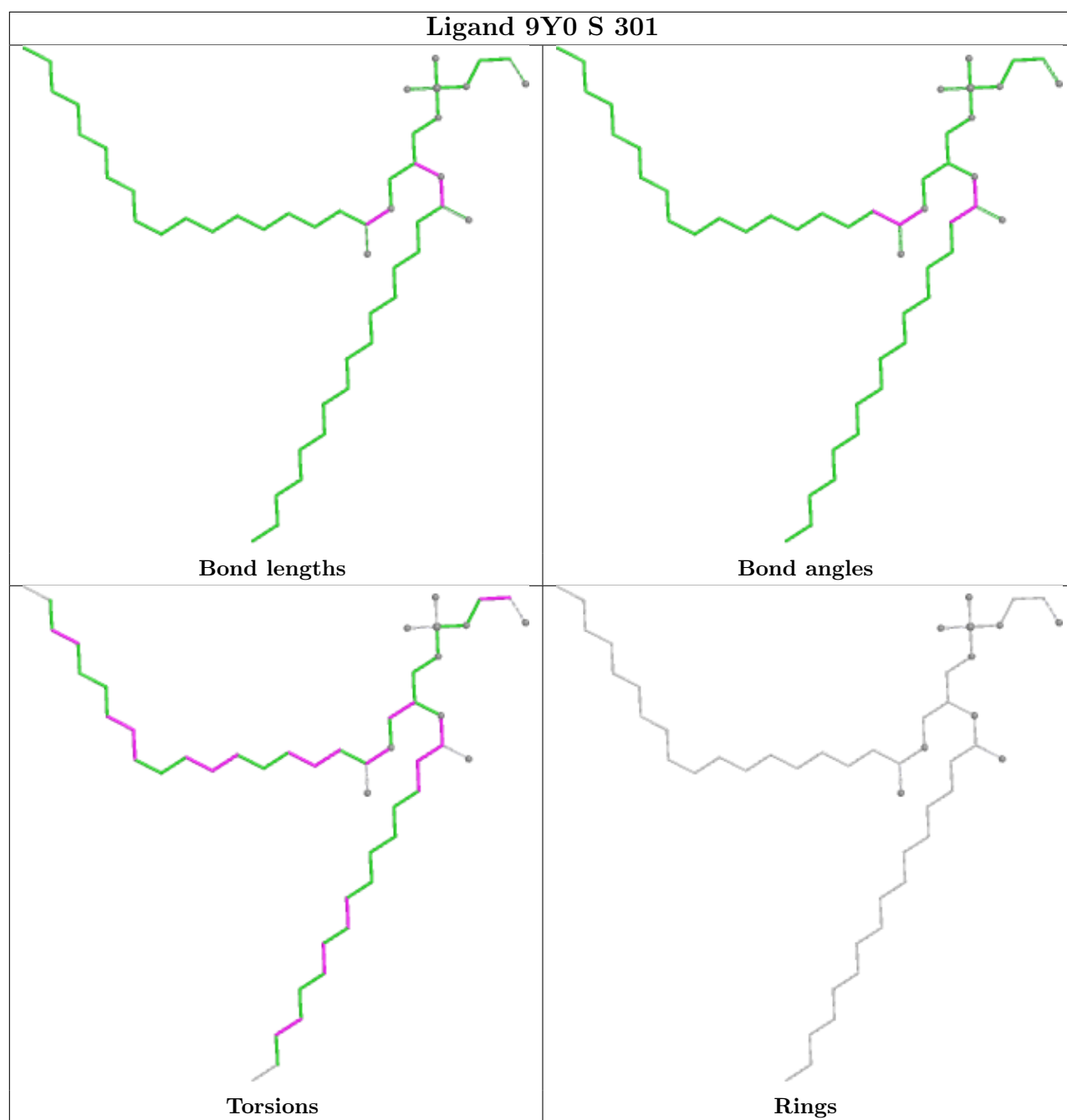
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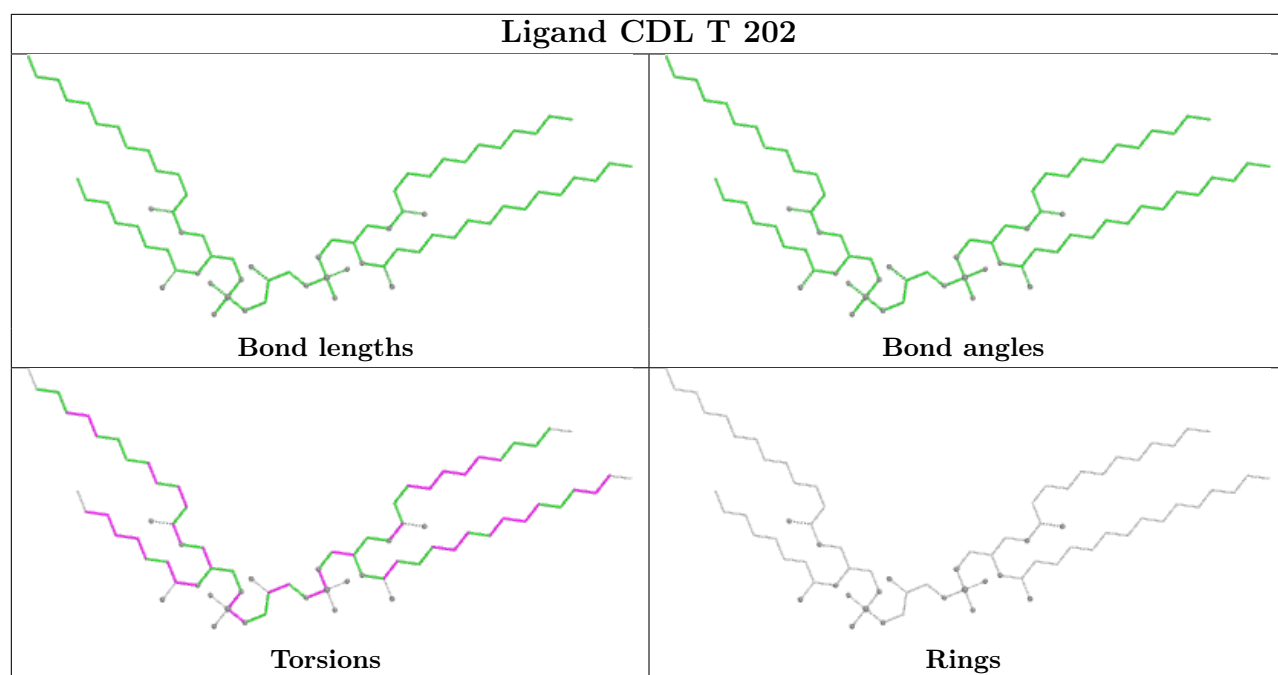
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	R	602	HEA	6	0
17	E	608	CDL	7	0
19	E	605	MQ9	6	0
20	I	302	HEC	7	0
19	E	604	MQ9	5	0
17	E	607	CDL	4	0
18	X	301	9Y0	1	0
20	O	302	HEC	9	0
17	X	302	CDL	26	0
22	E	601	HEM	5	0
17	S	303	CDL	16	0
17	F	608	CDL	9	0
24	Y	501	FES	3	0
19	F	605	MQ9	11	0

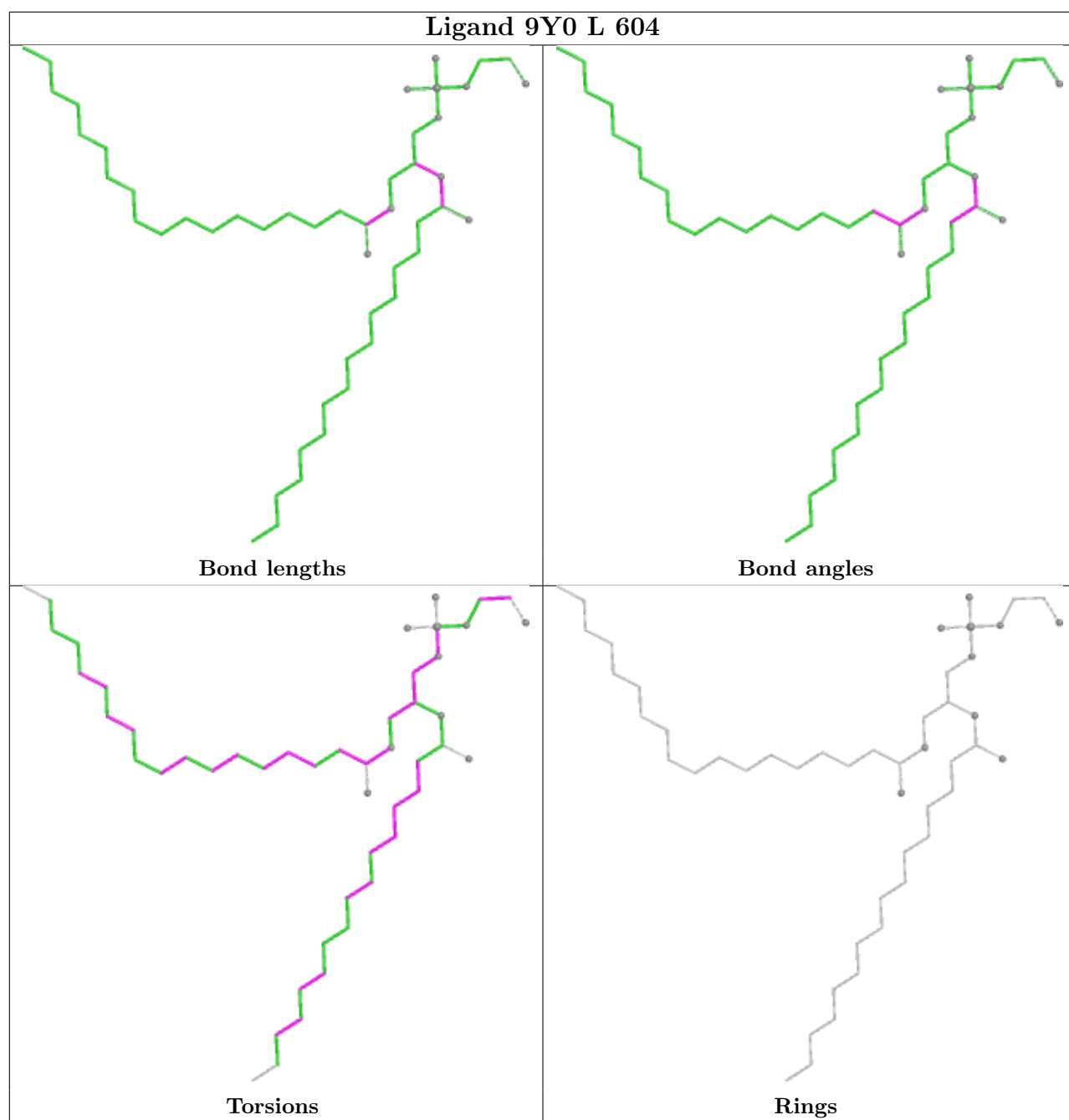
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



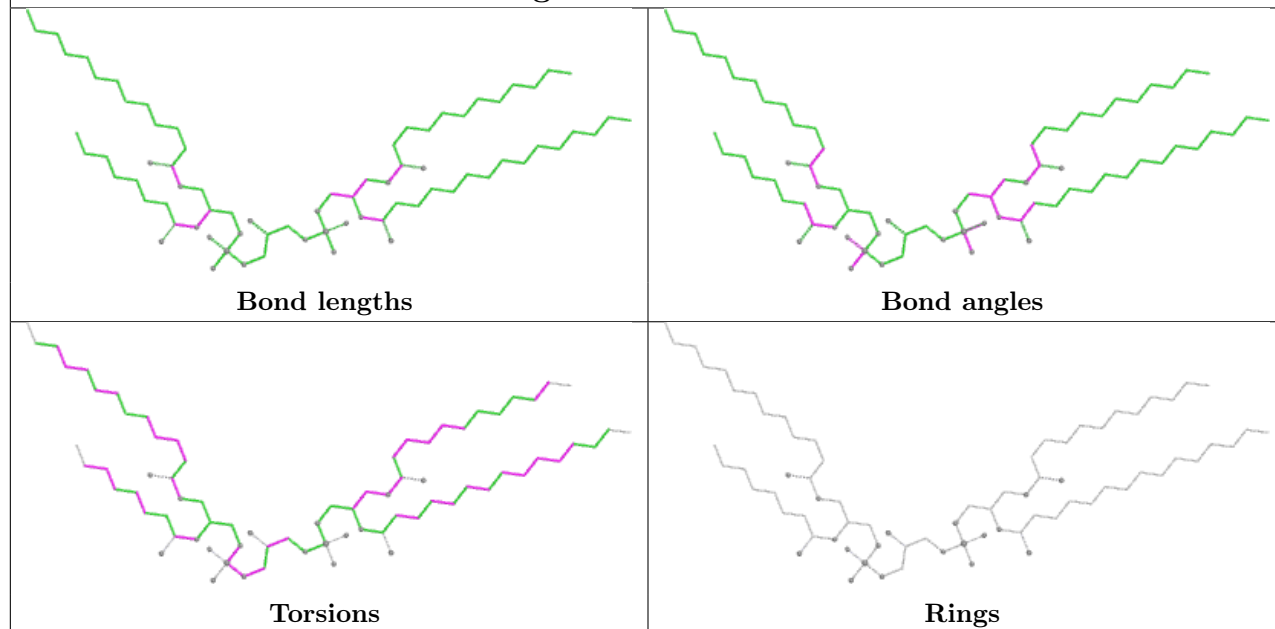




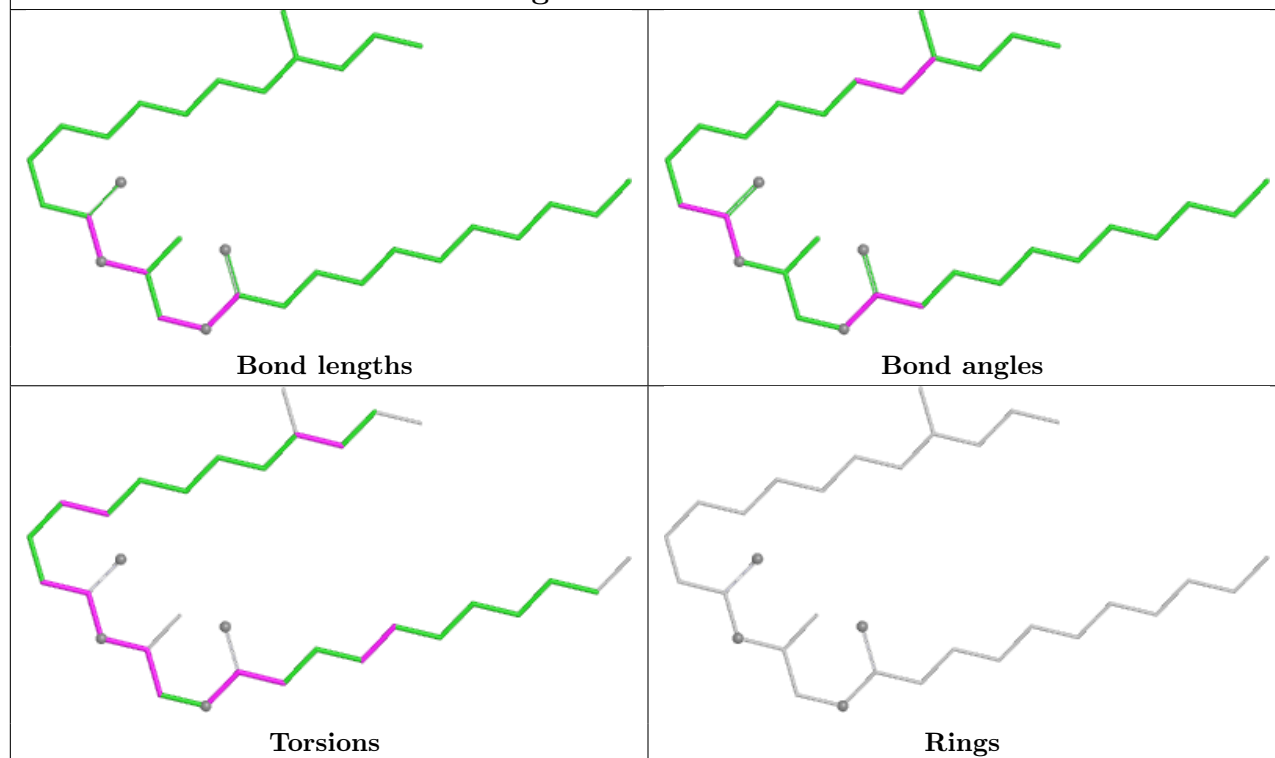


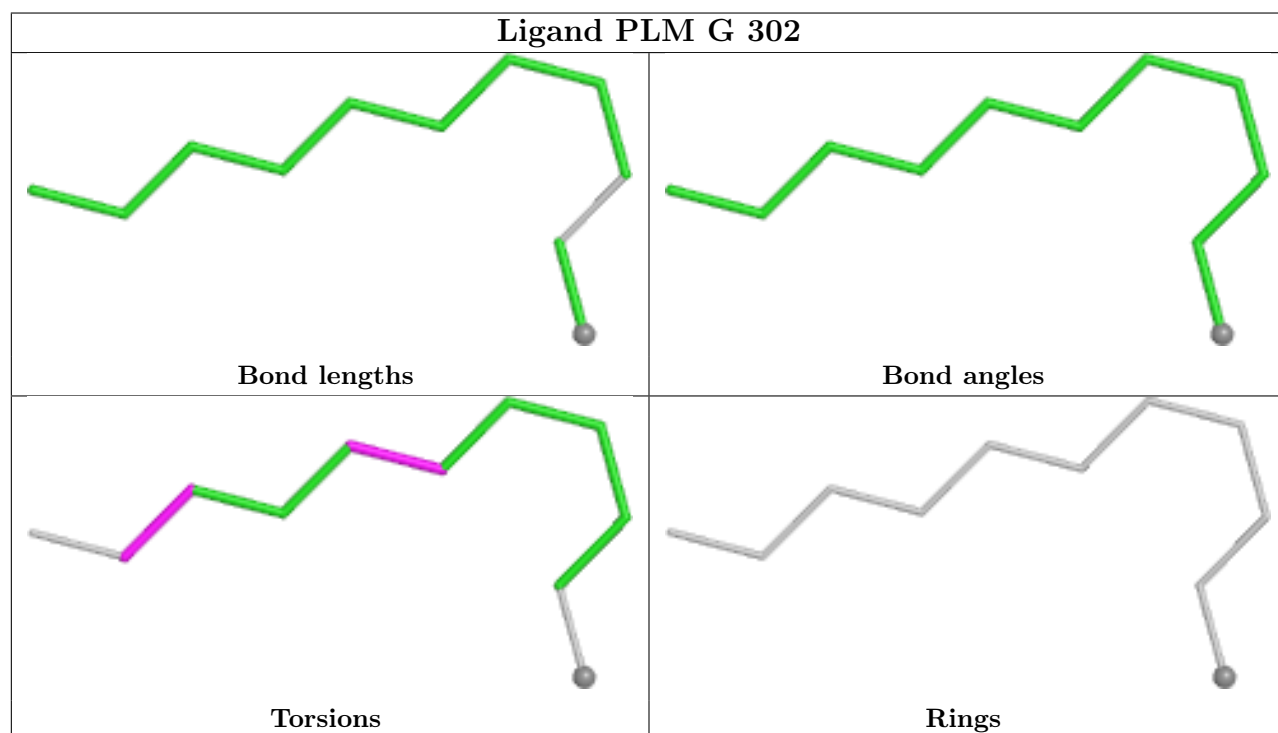
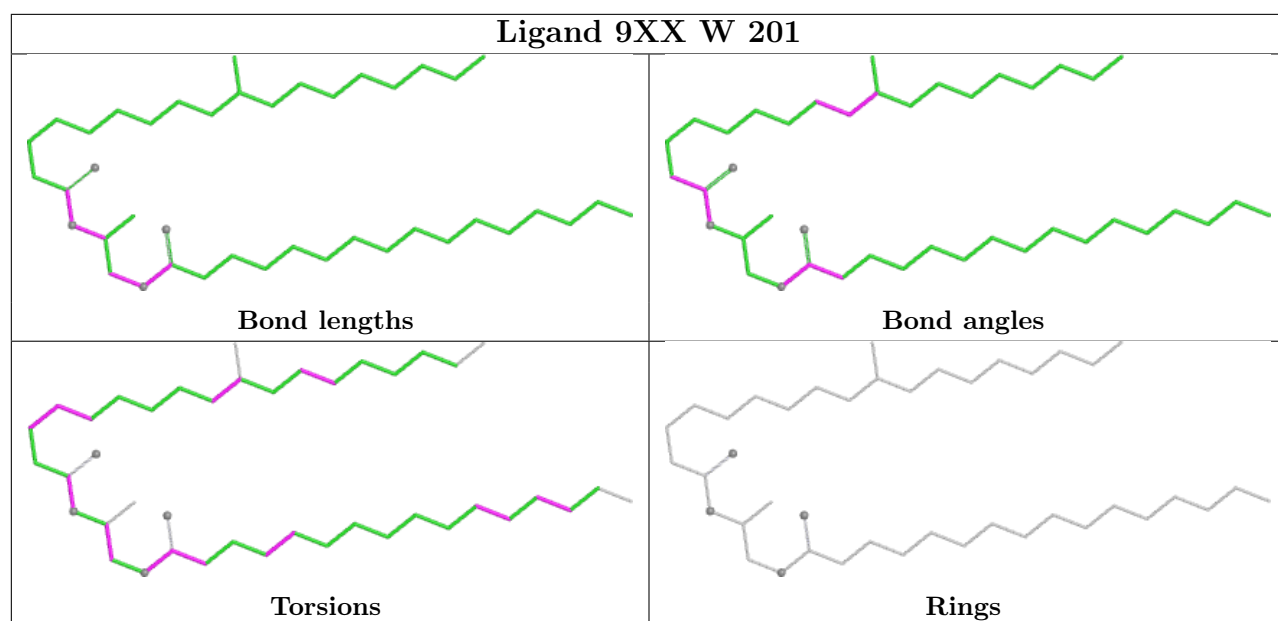


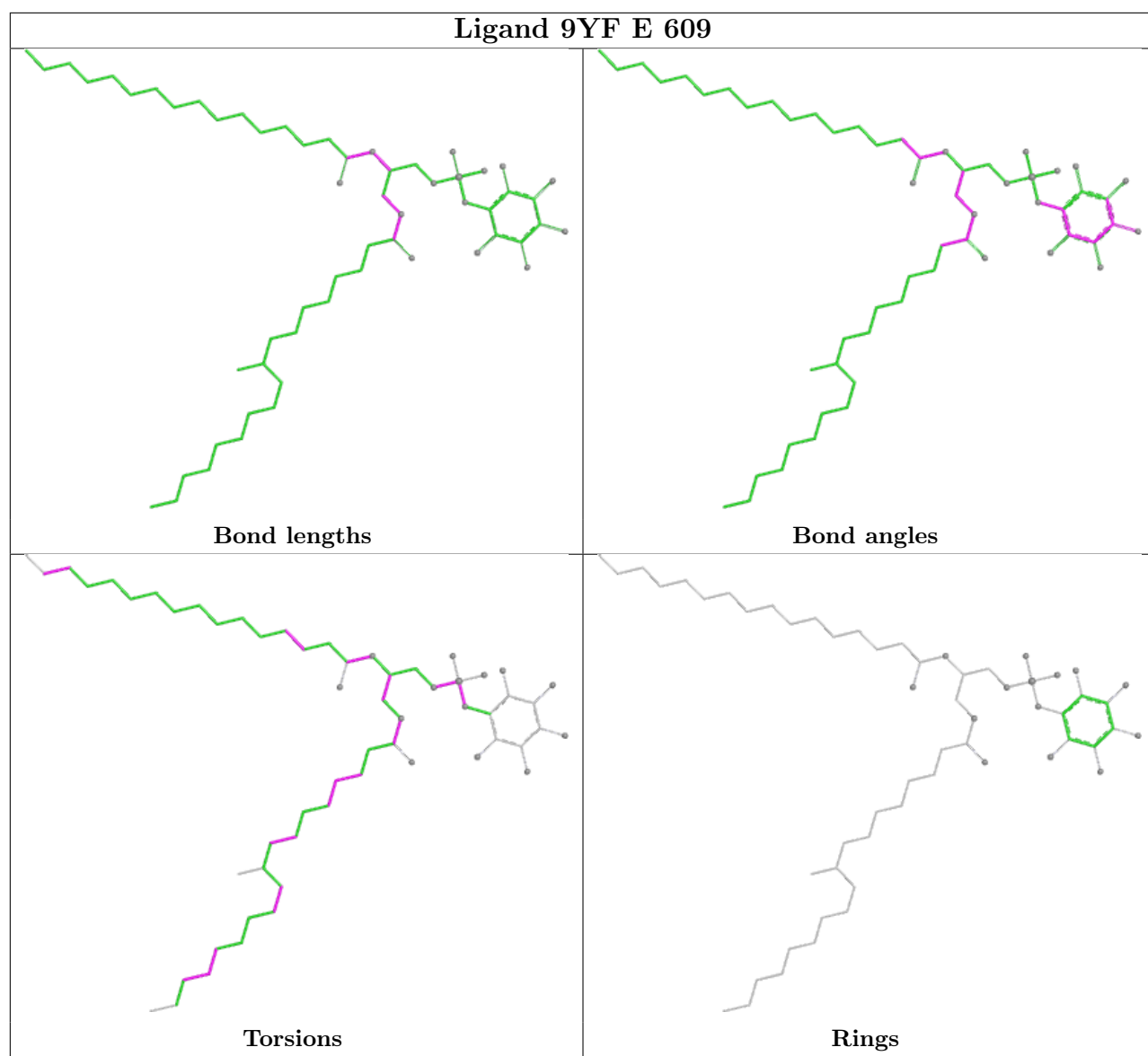
## Ligand CDL Z 202

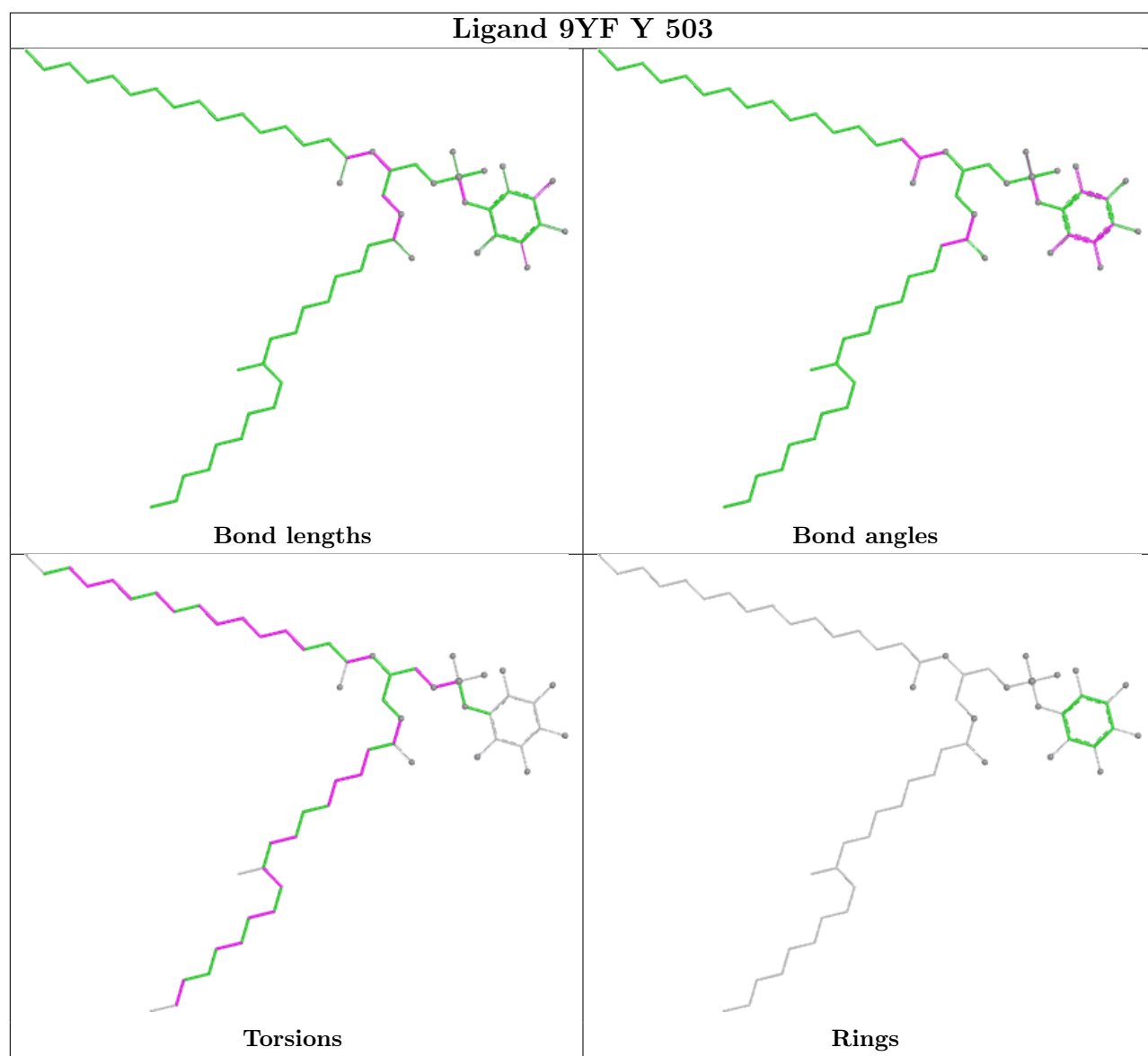


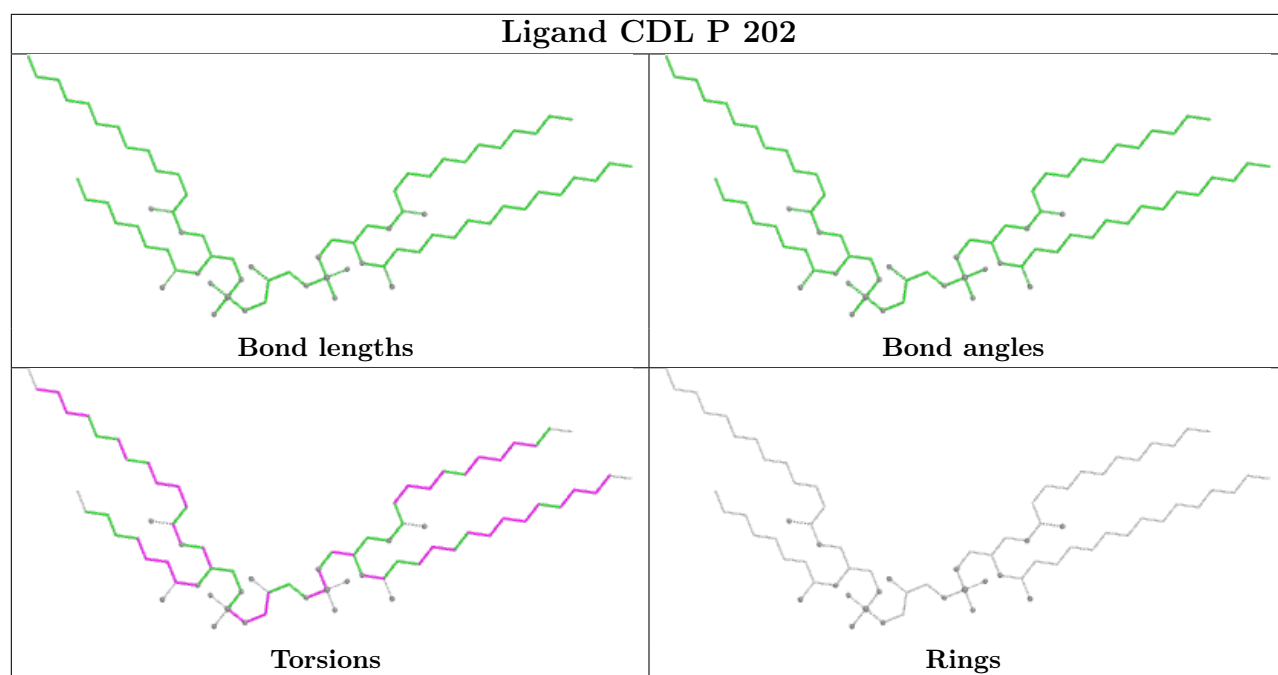
## Ligand 9XX D 301



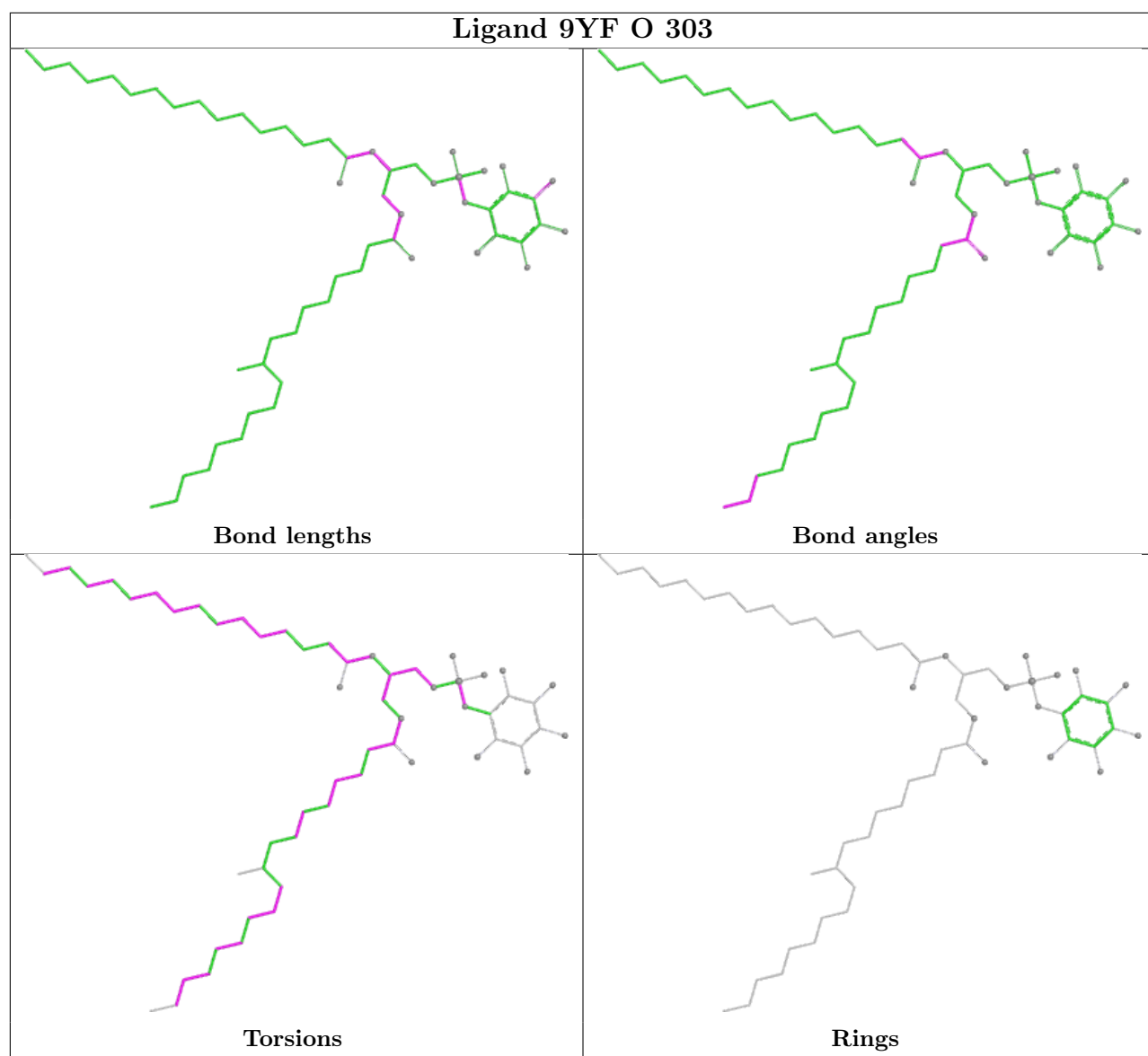


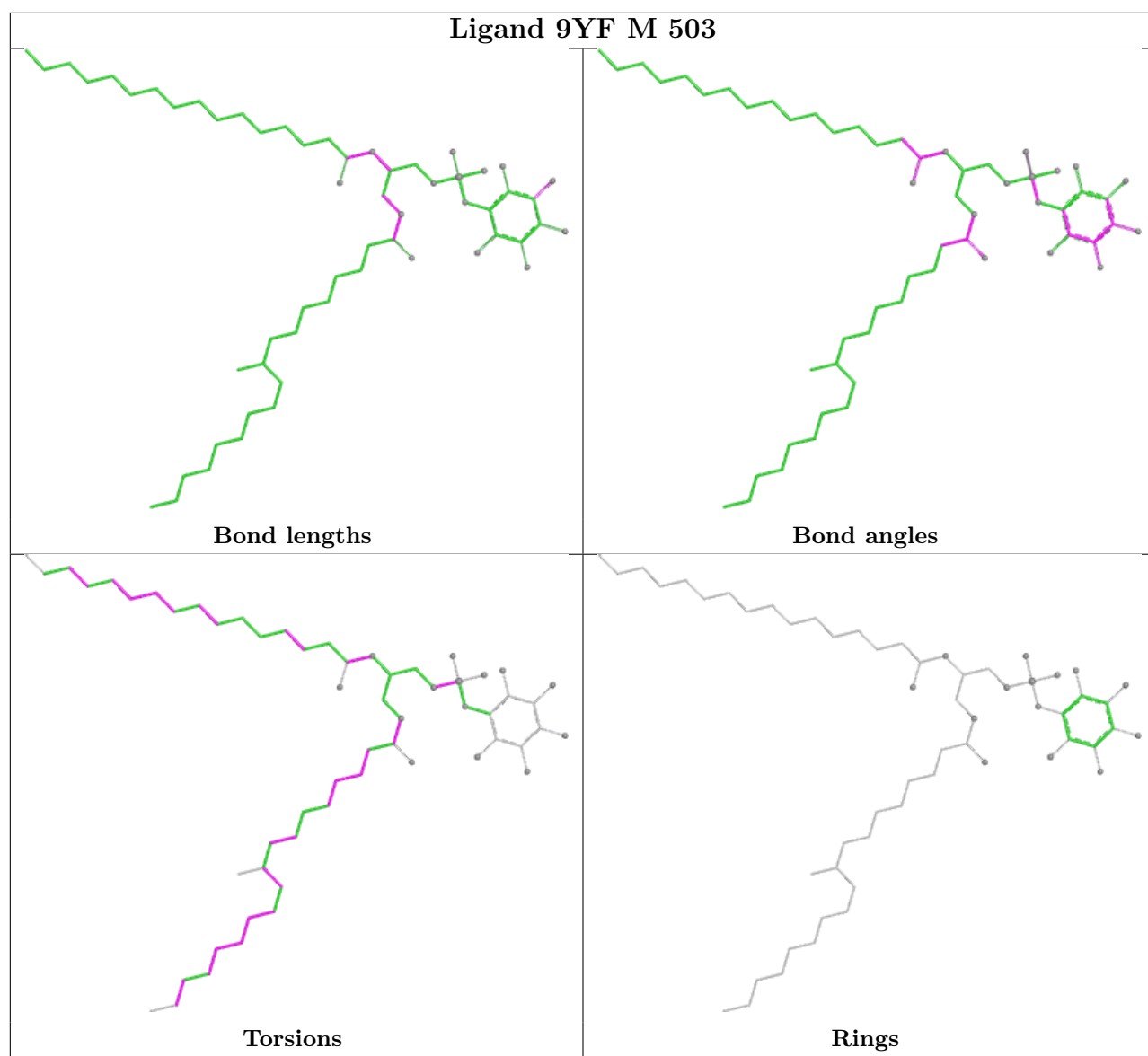


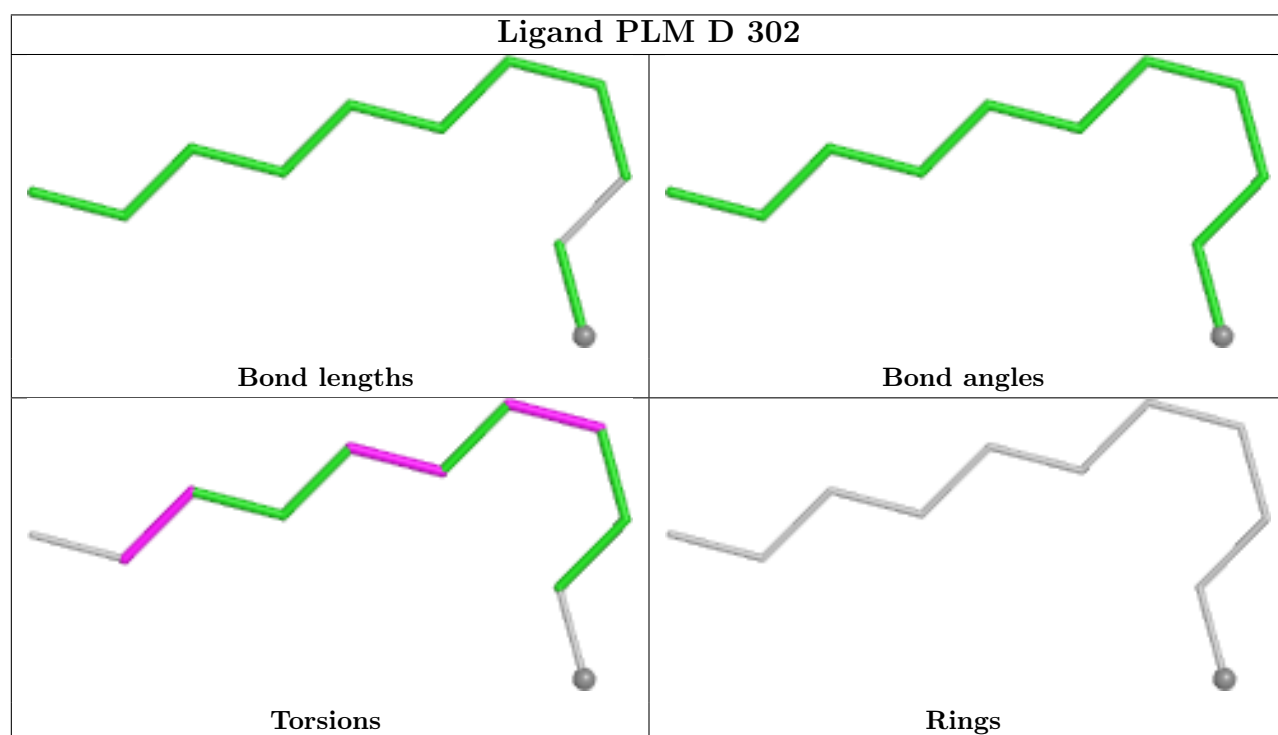
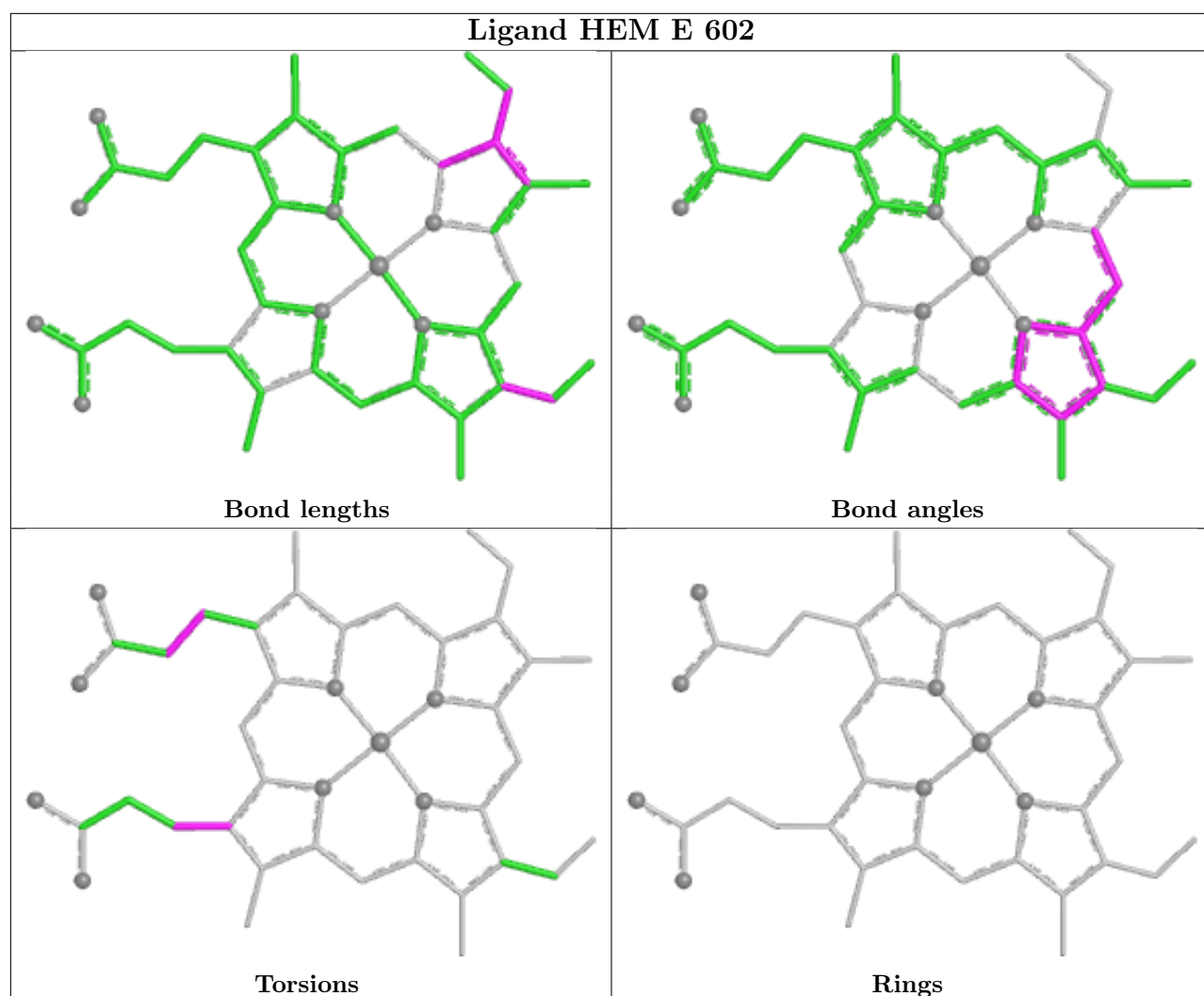


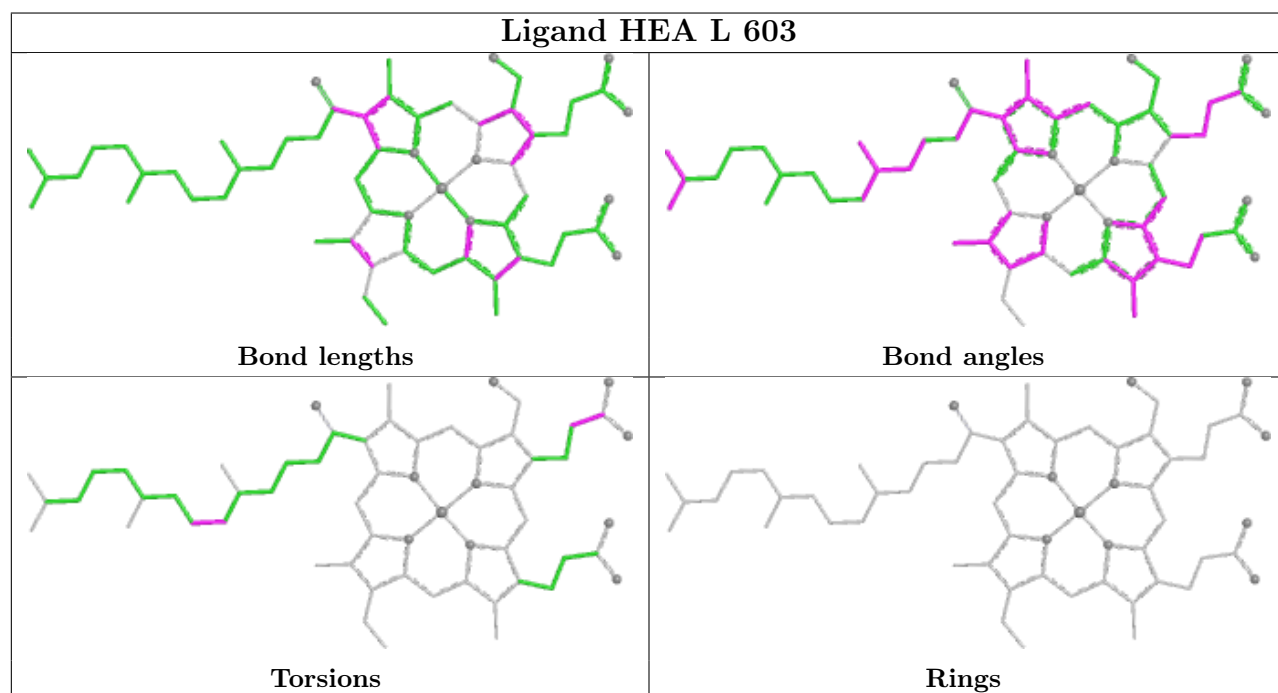
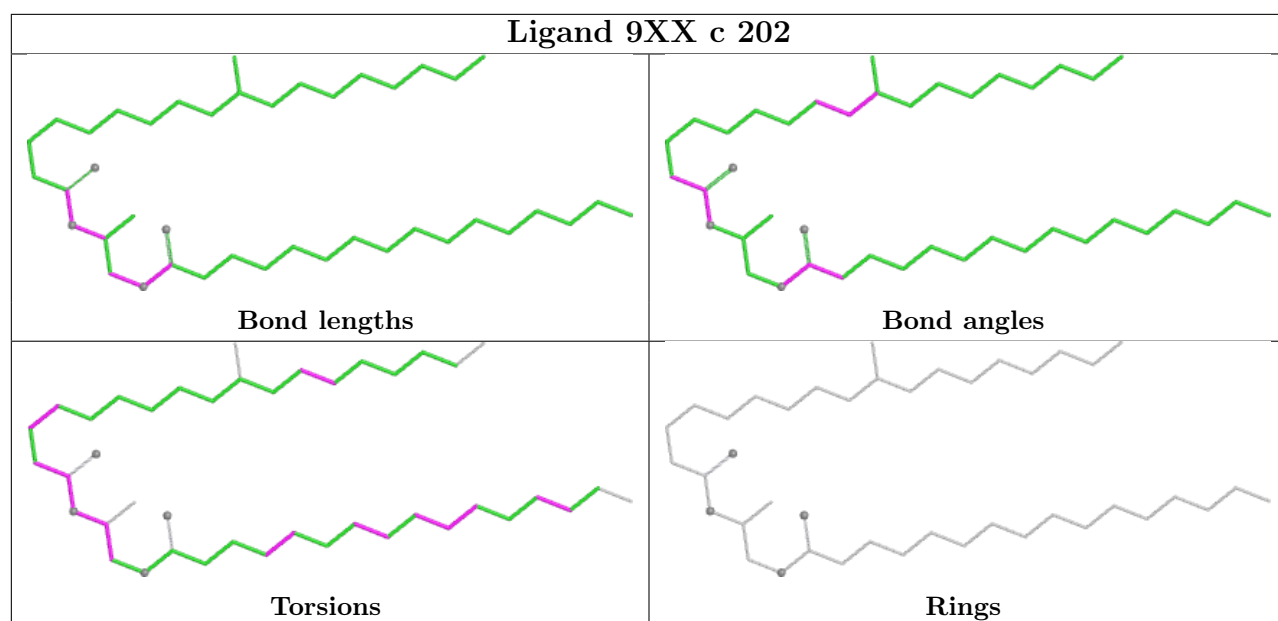


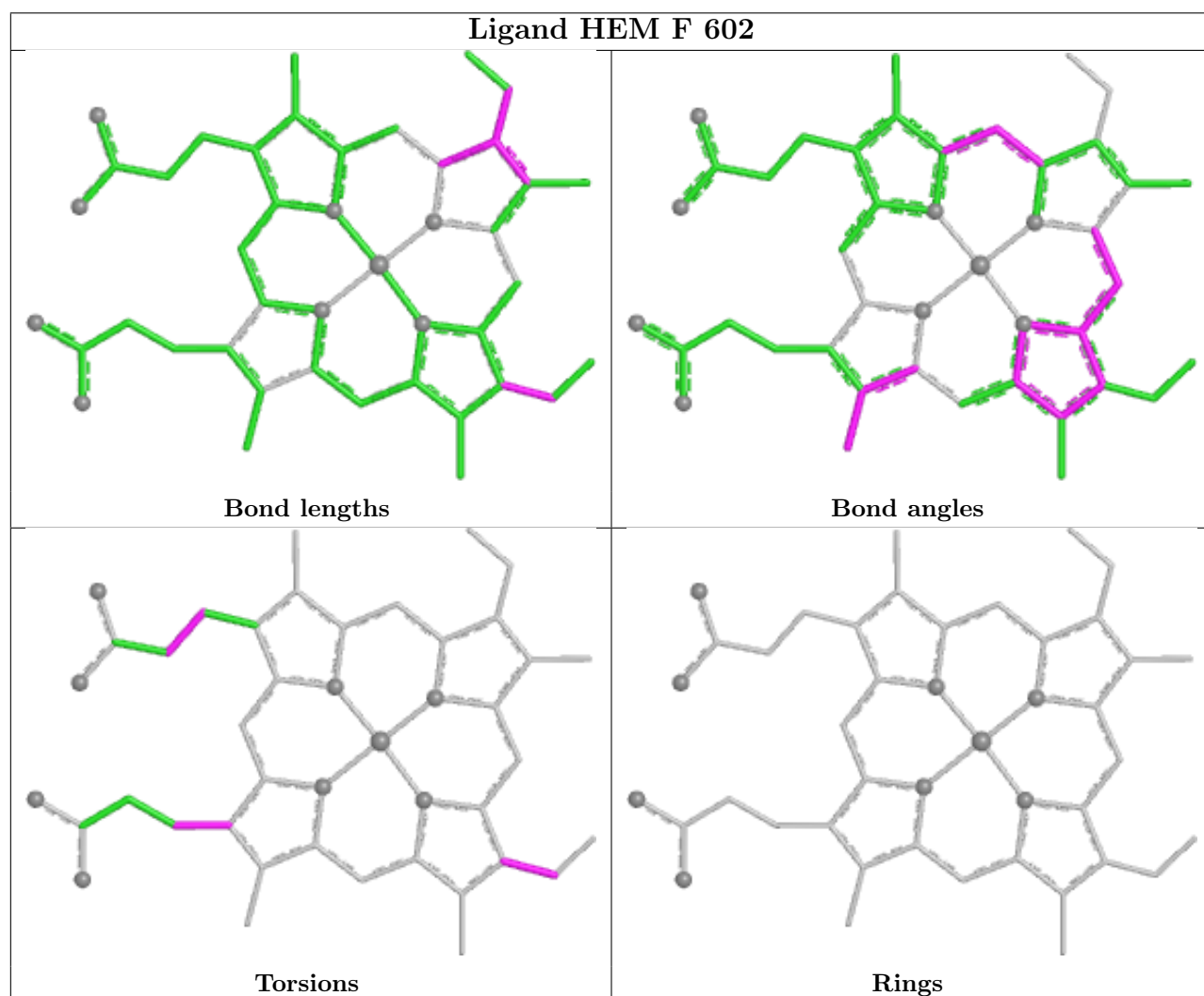
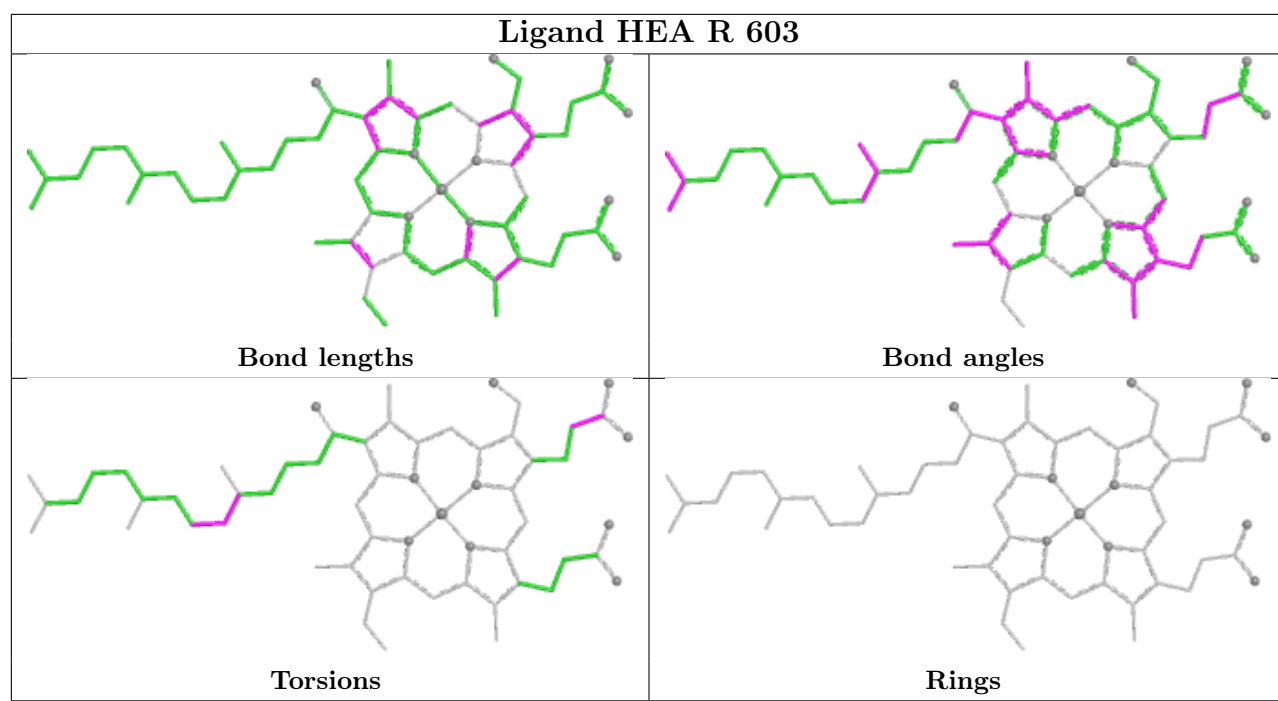


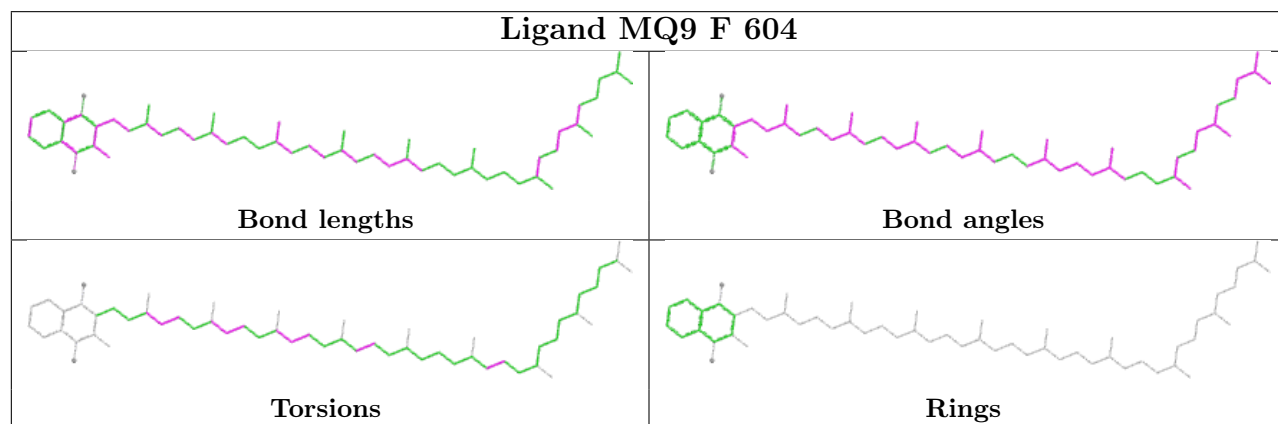
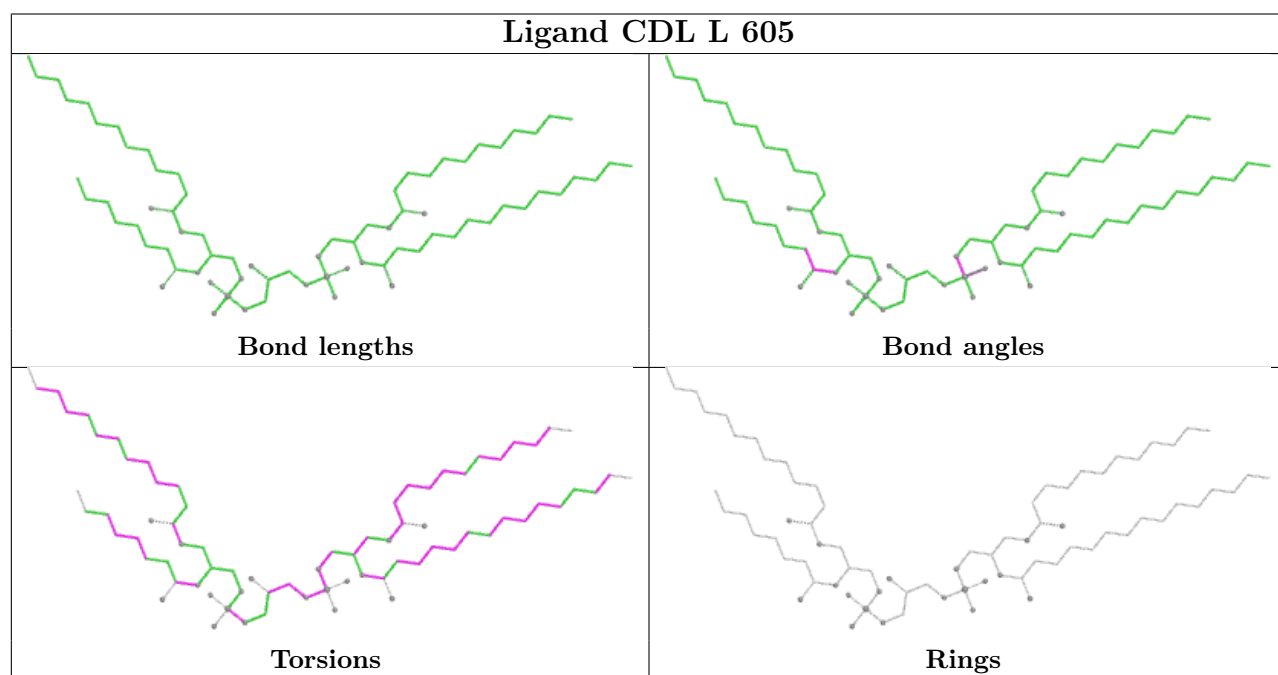
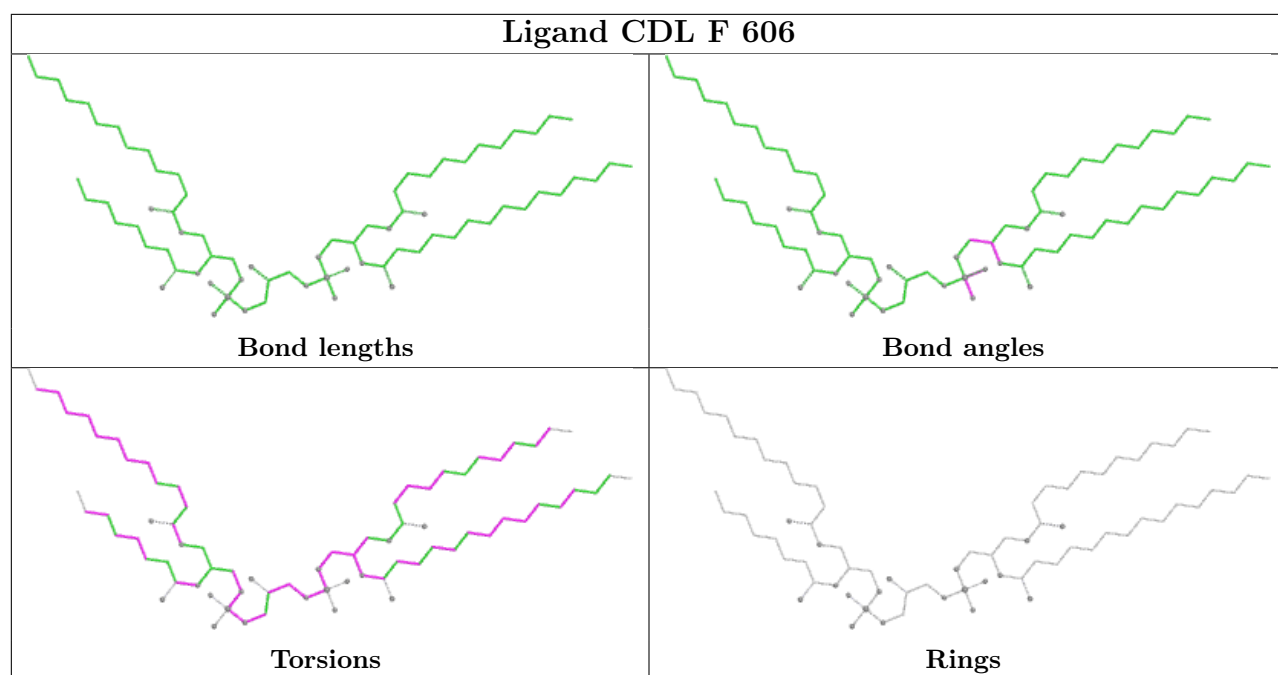


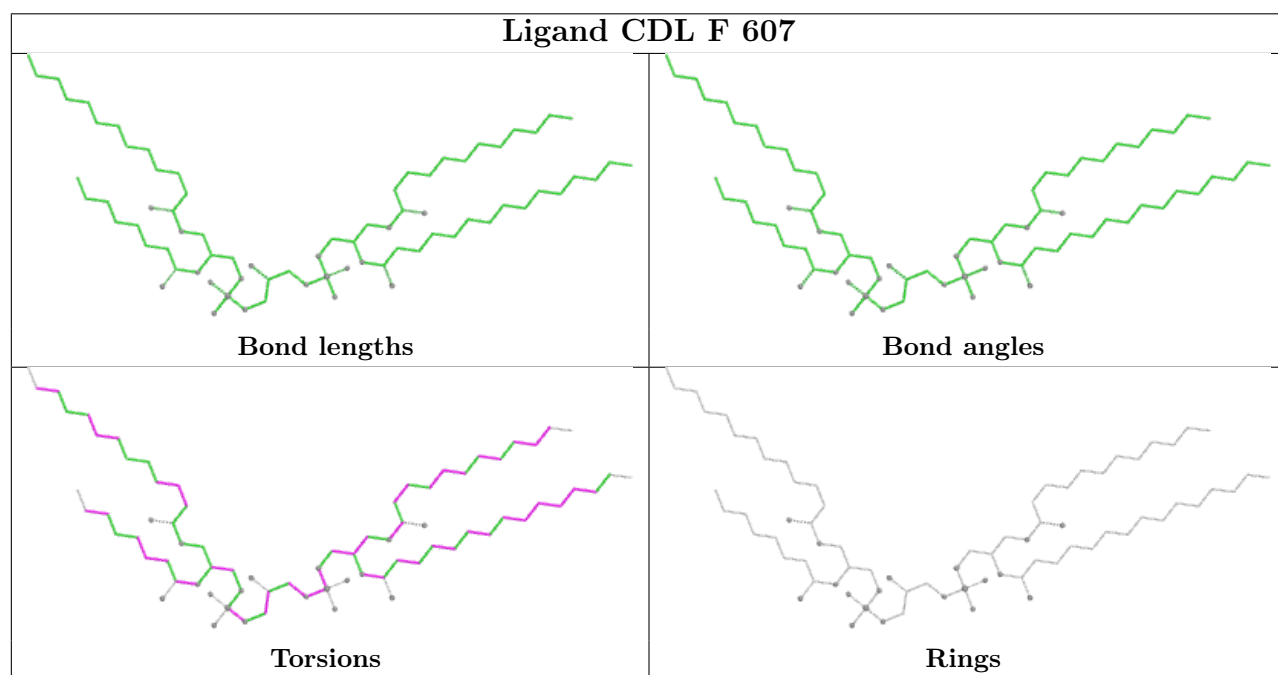
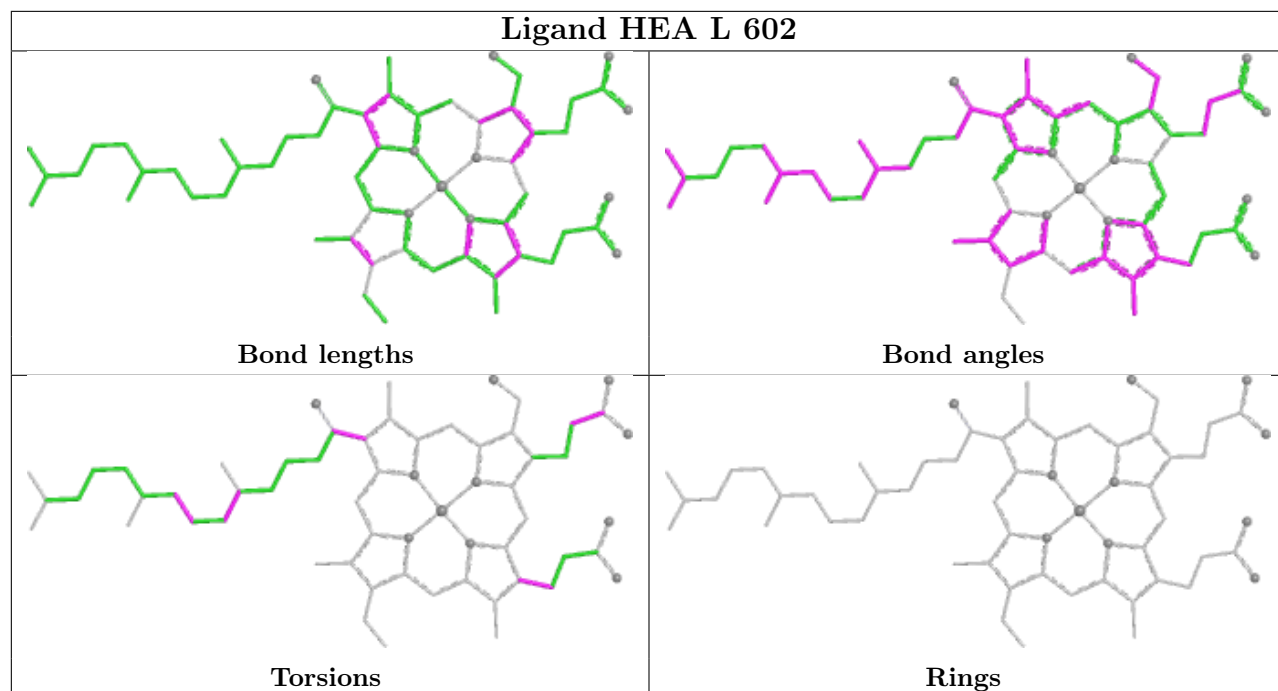


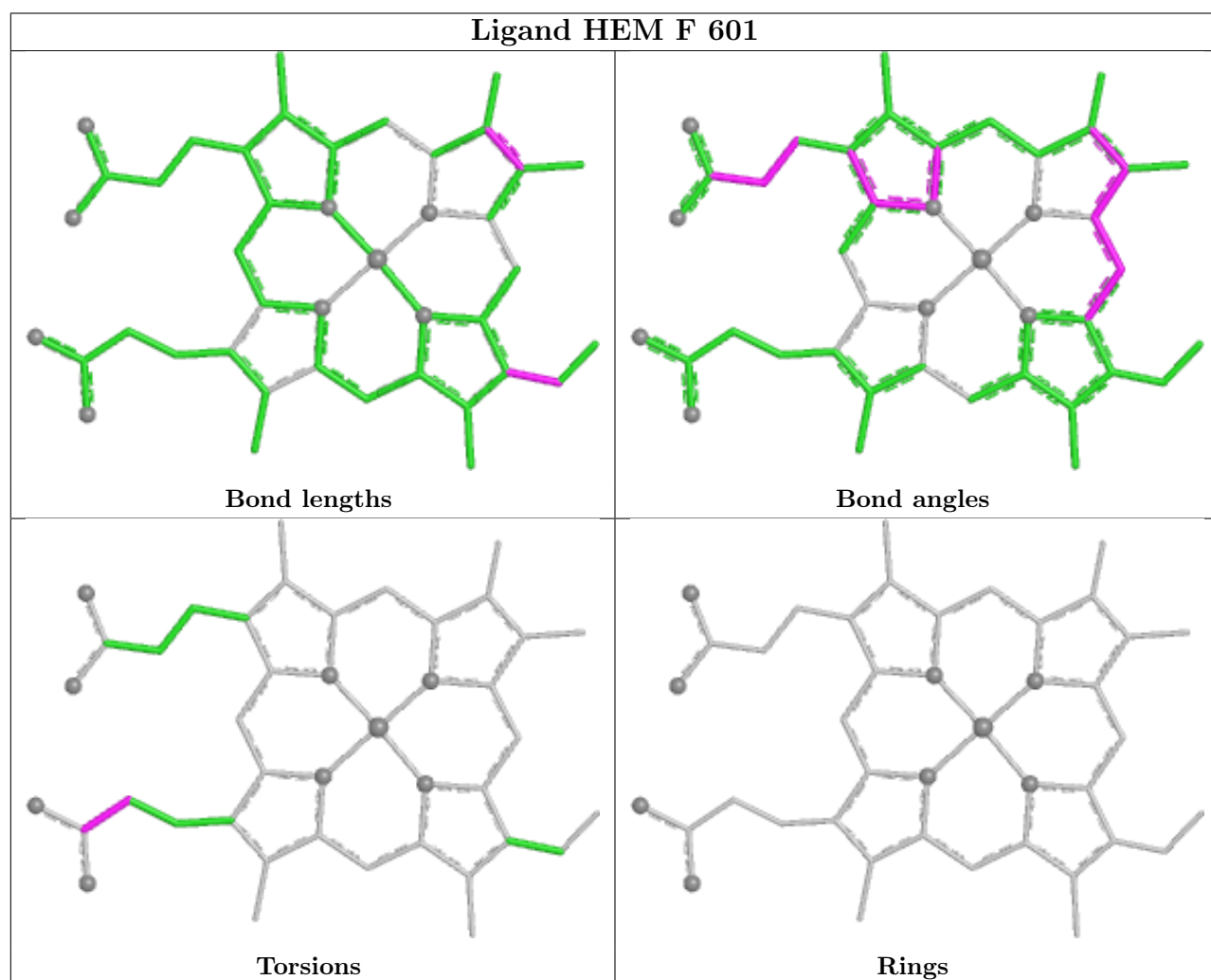
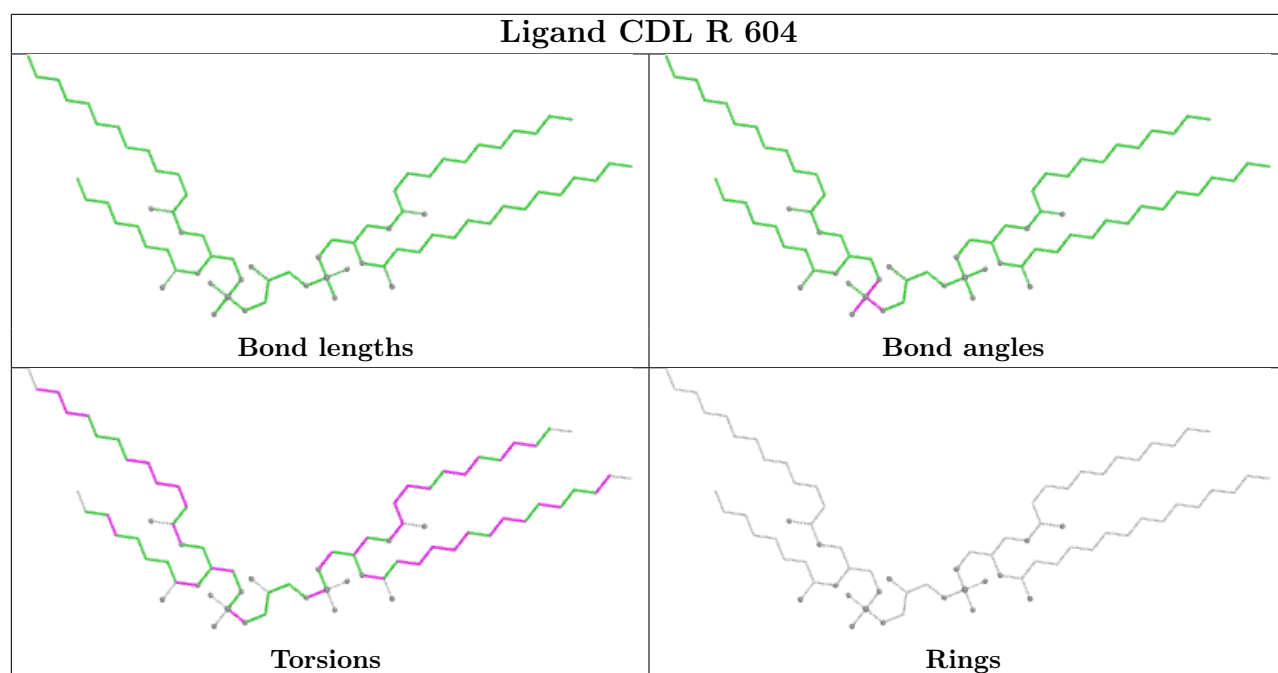




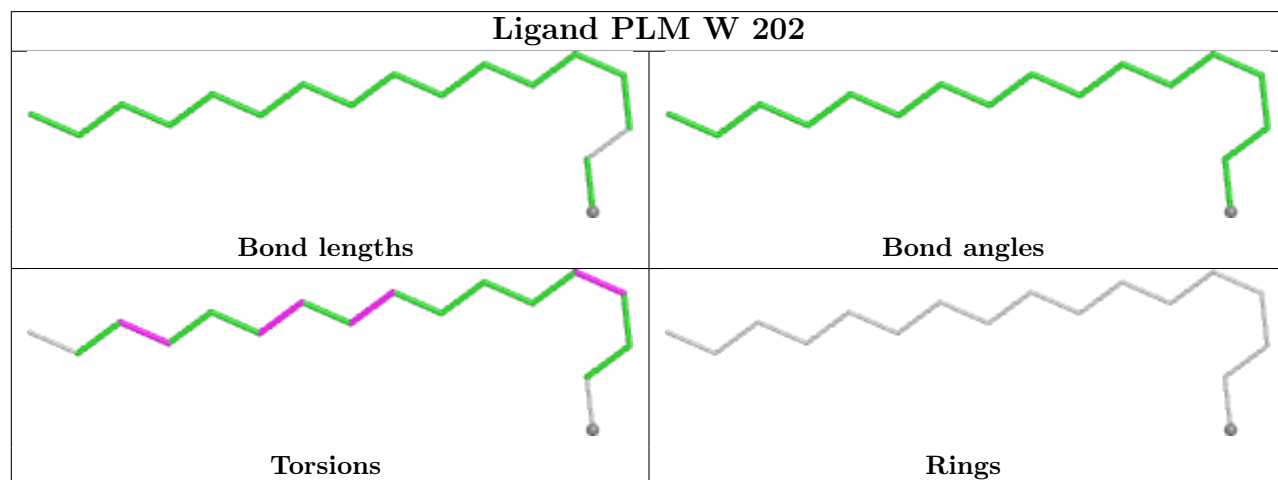
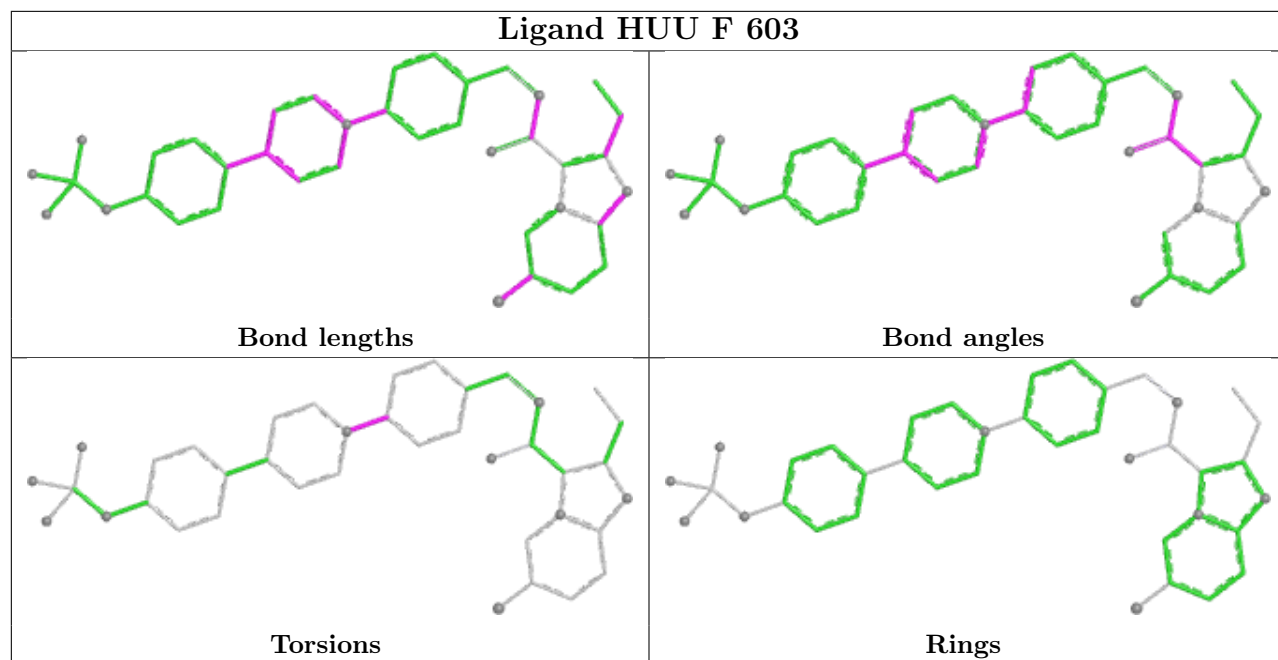


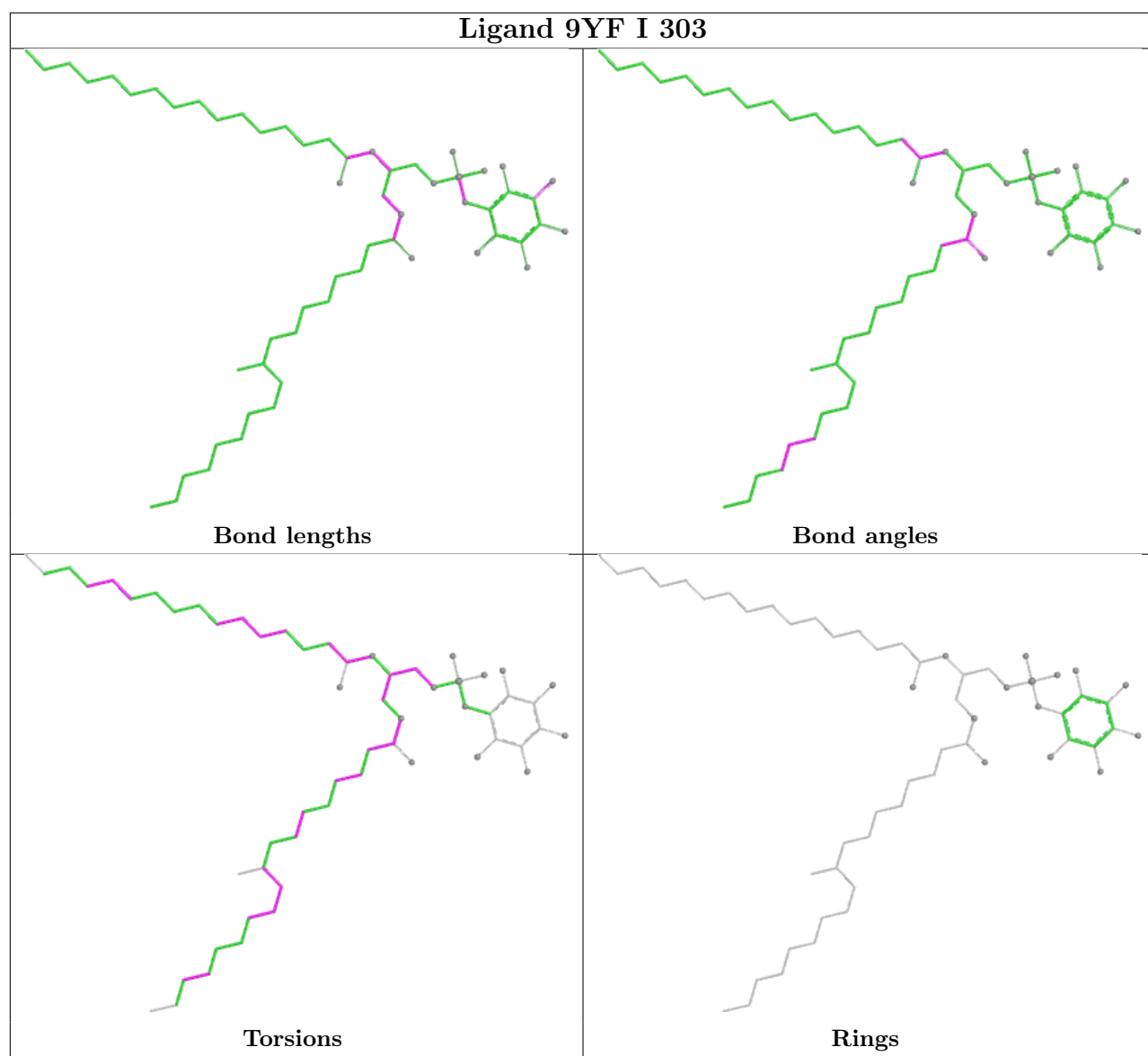


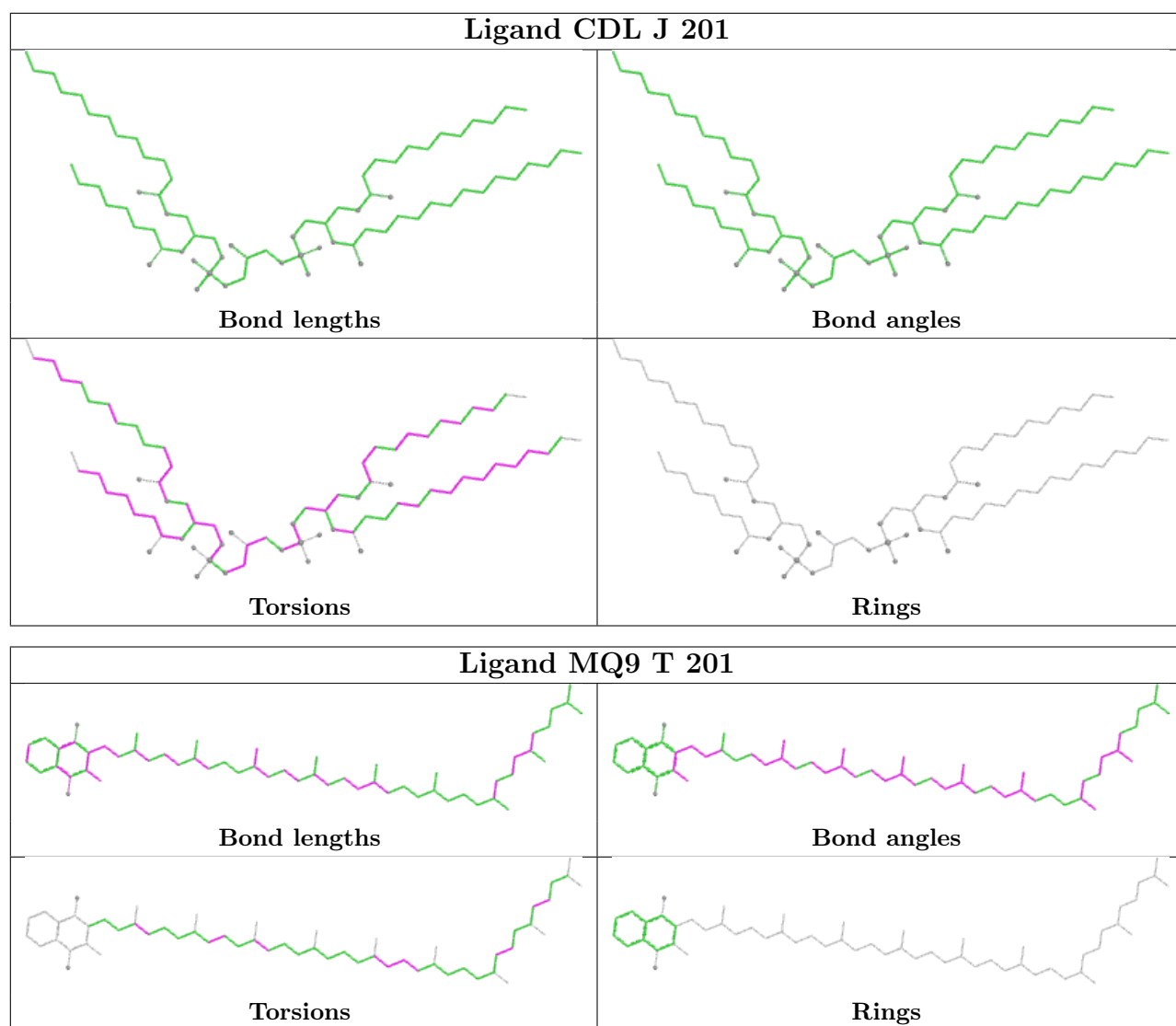


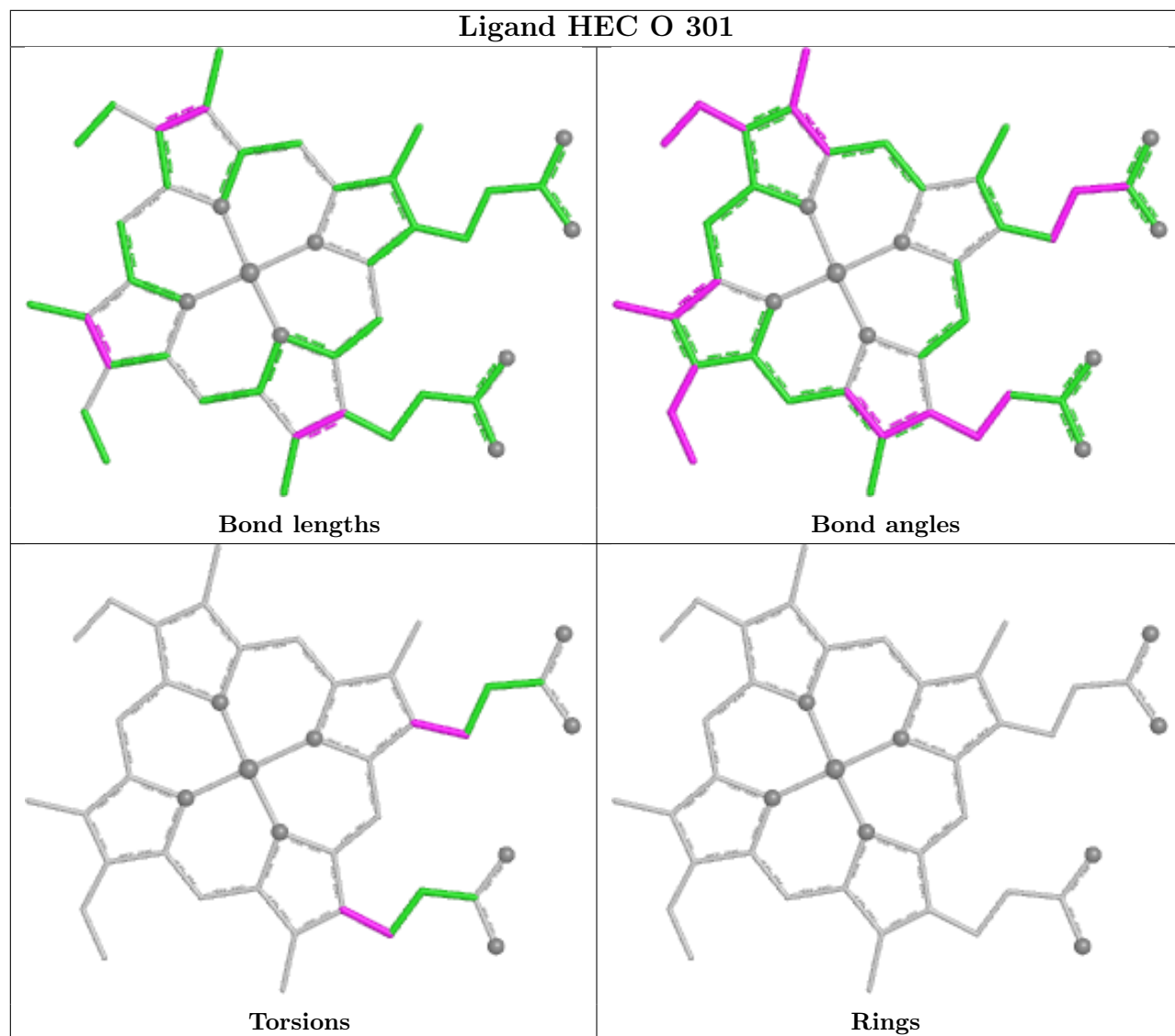


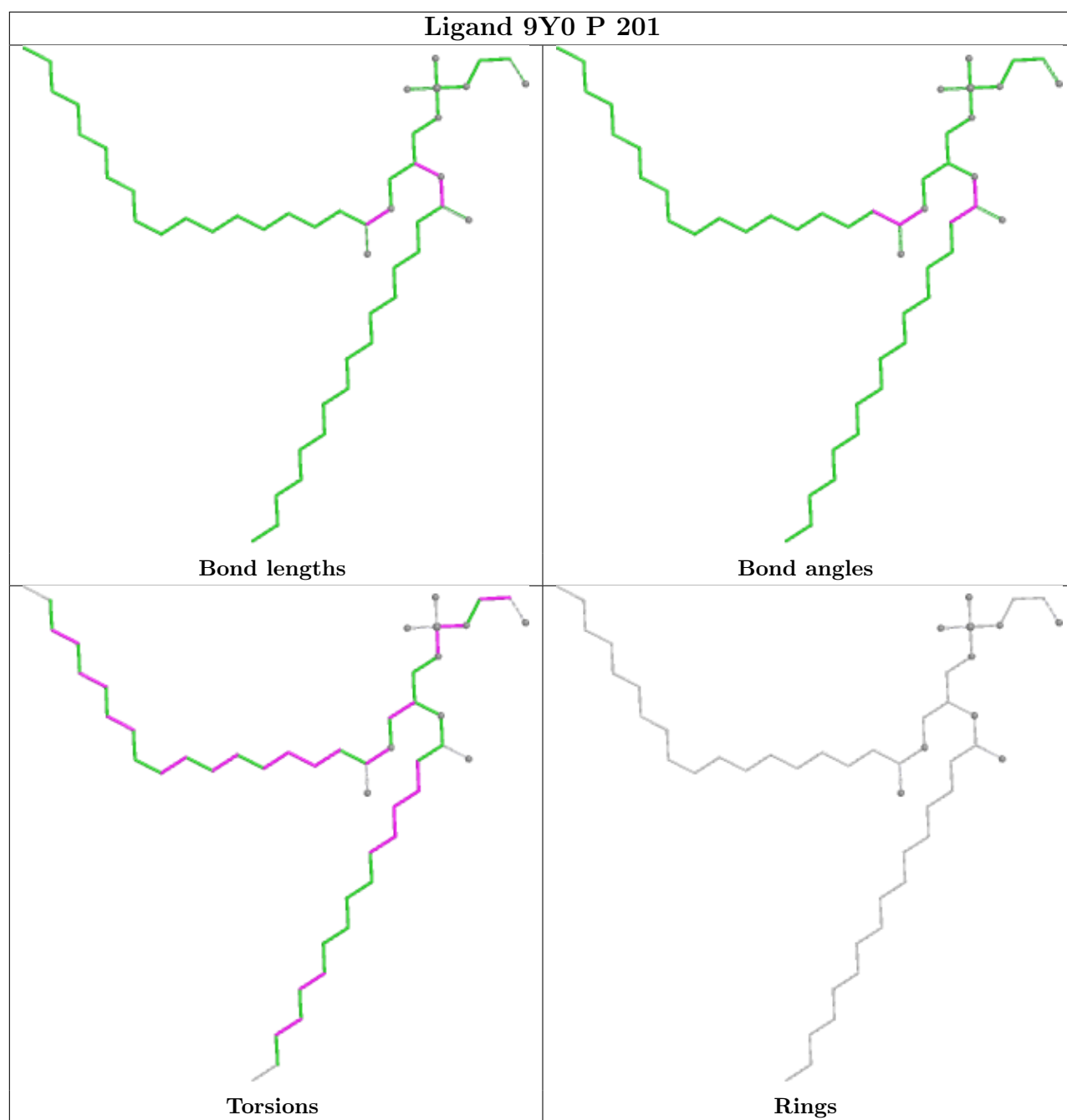


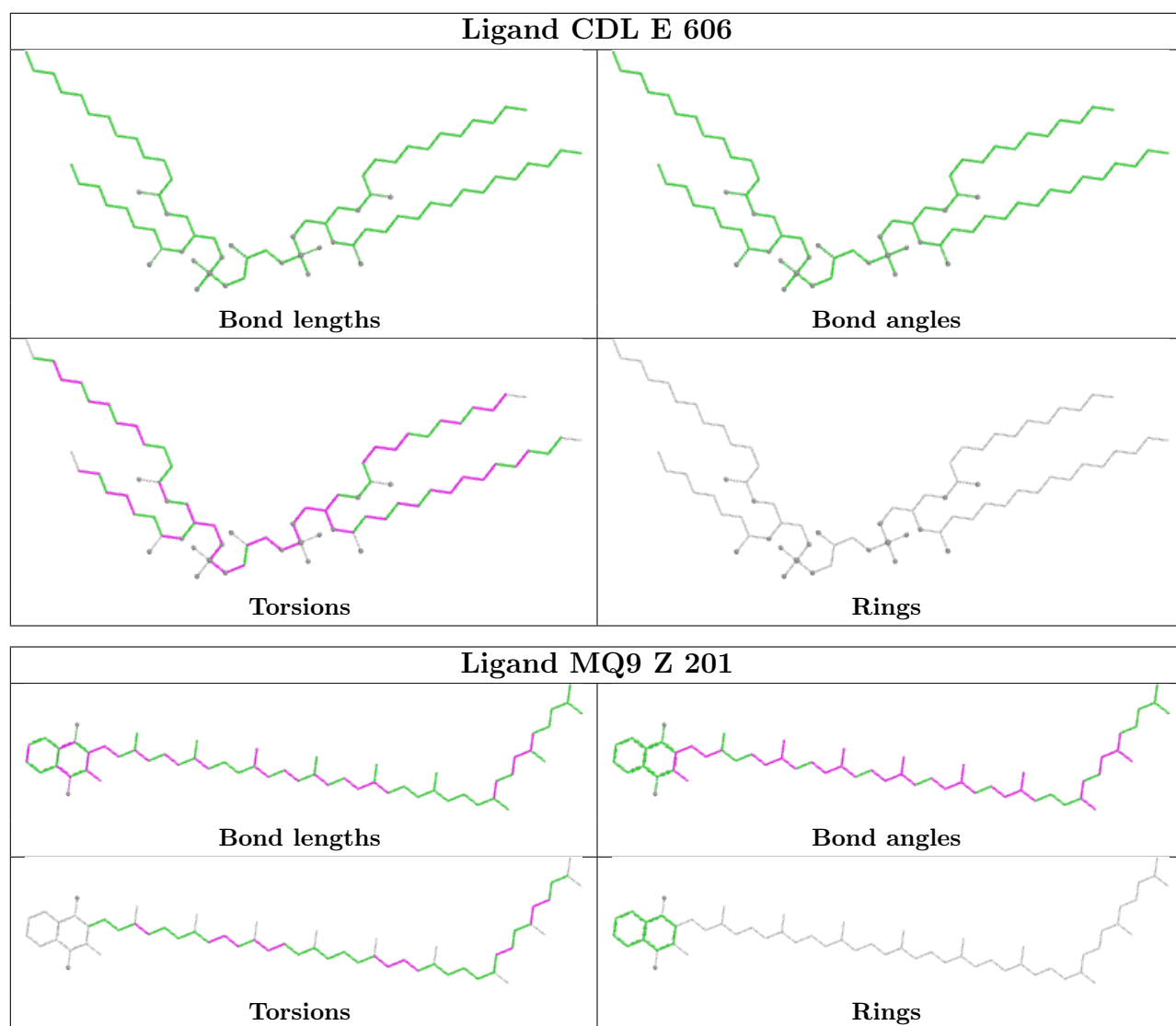




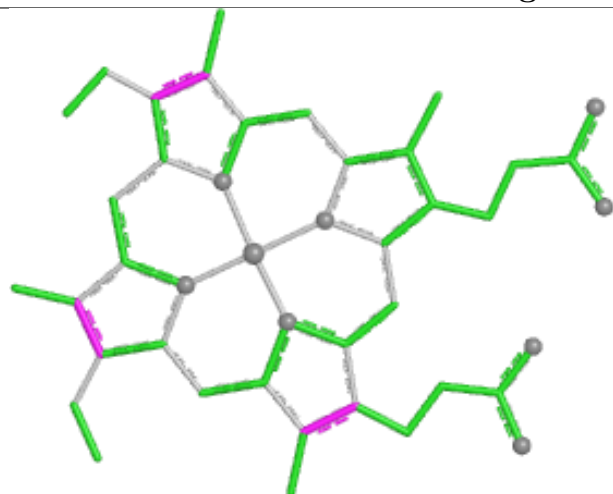




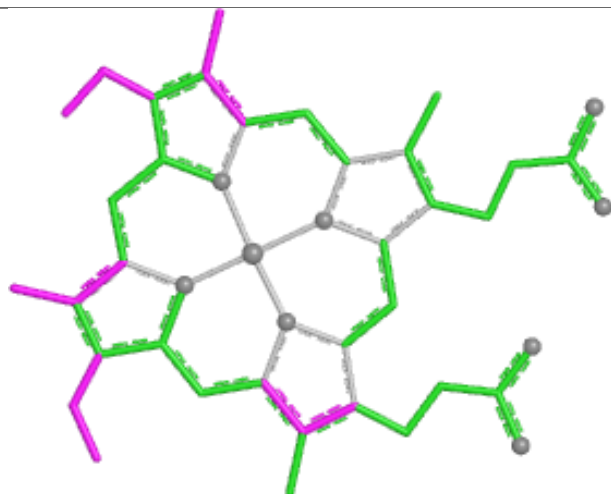




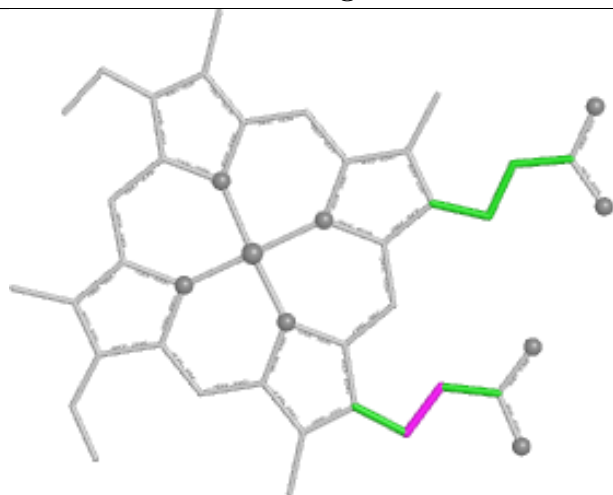
## Ligand HEC I 301



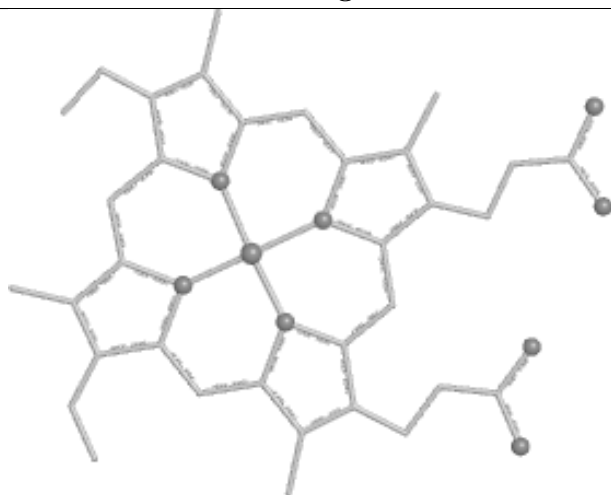
Bond lengths



Bond angles

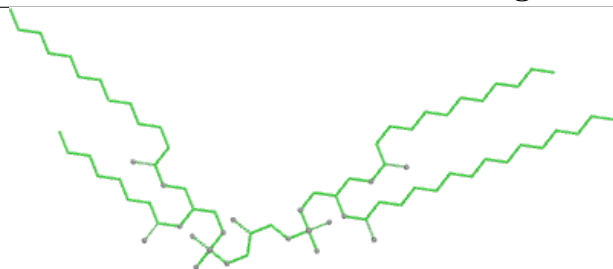


Torsions

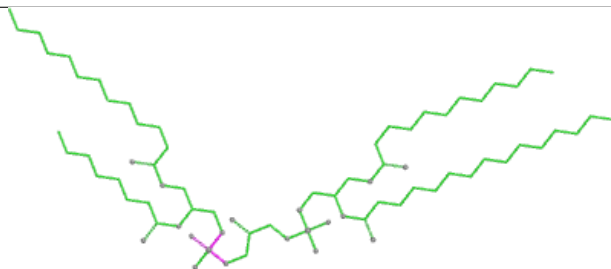


Rings

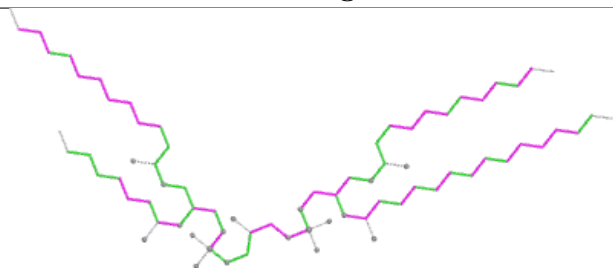
## Ligand CDL X 303



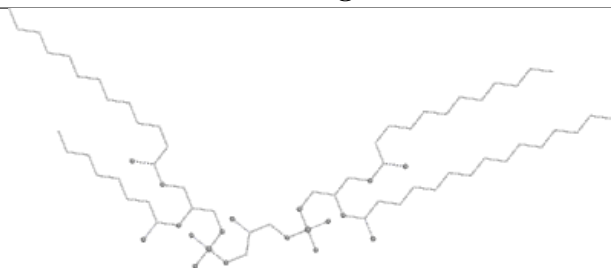
Bond lengths



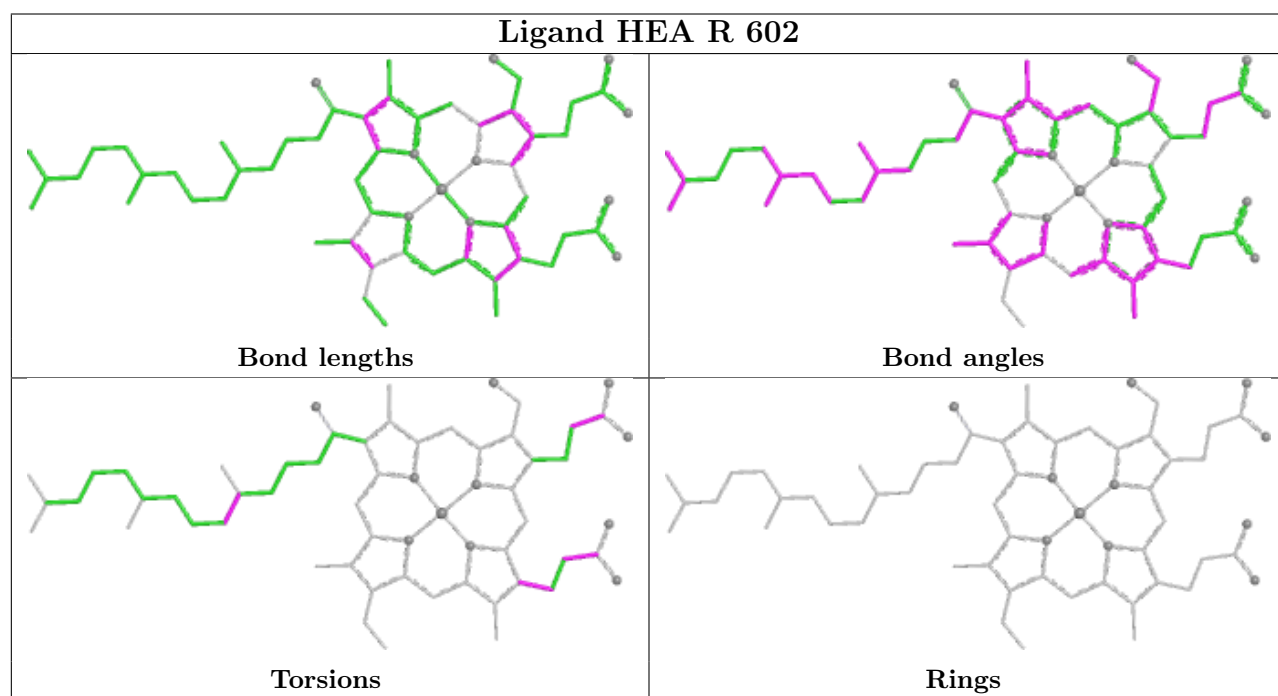
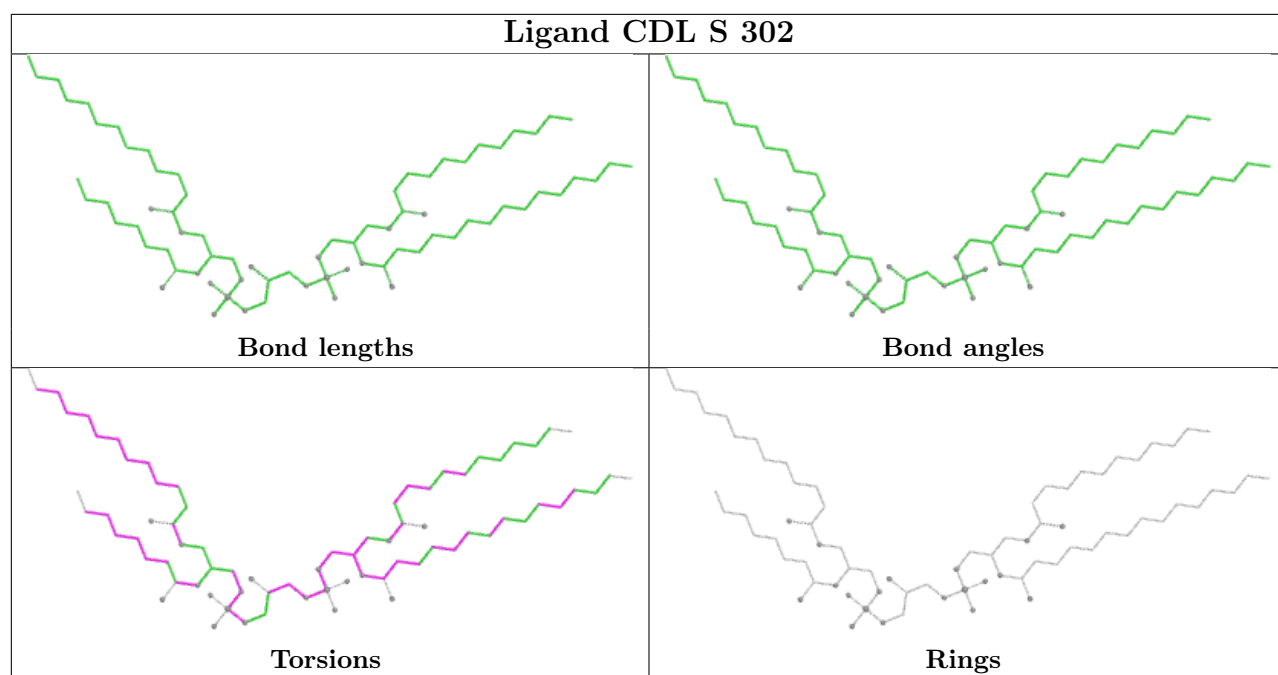
Bond angles



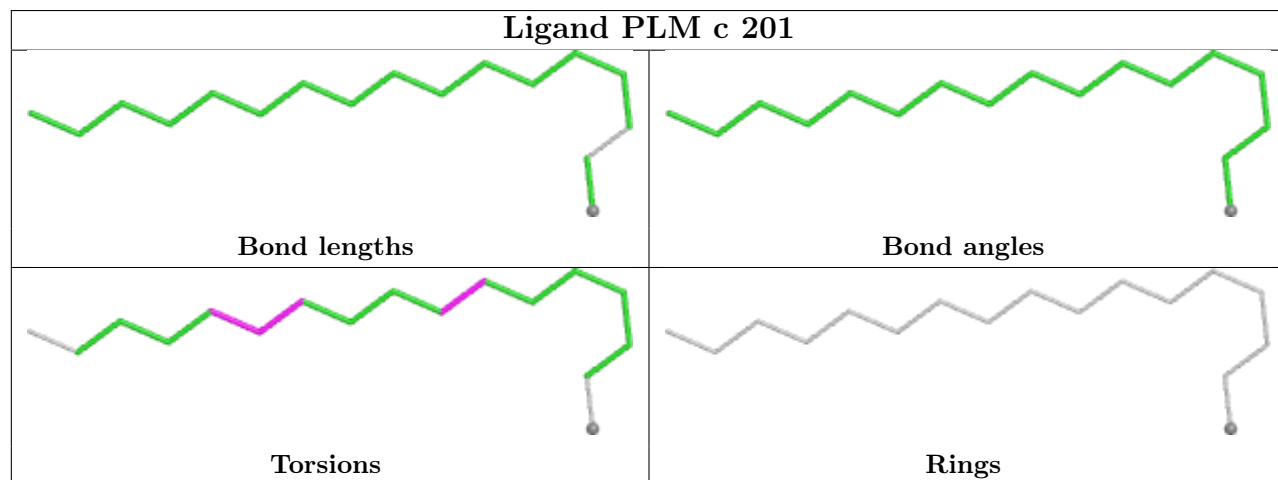
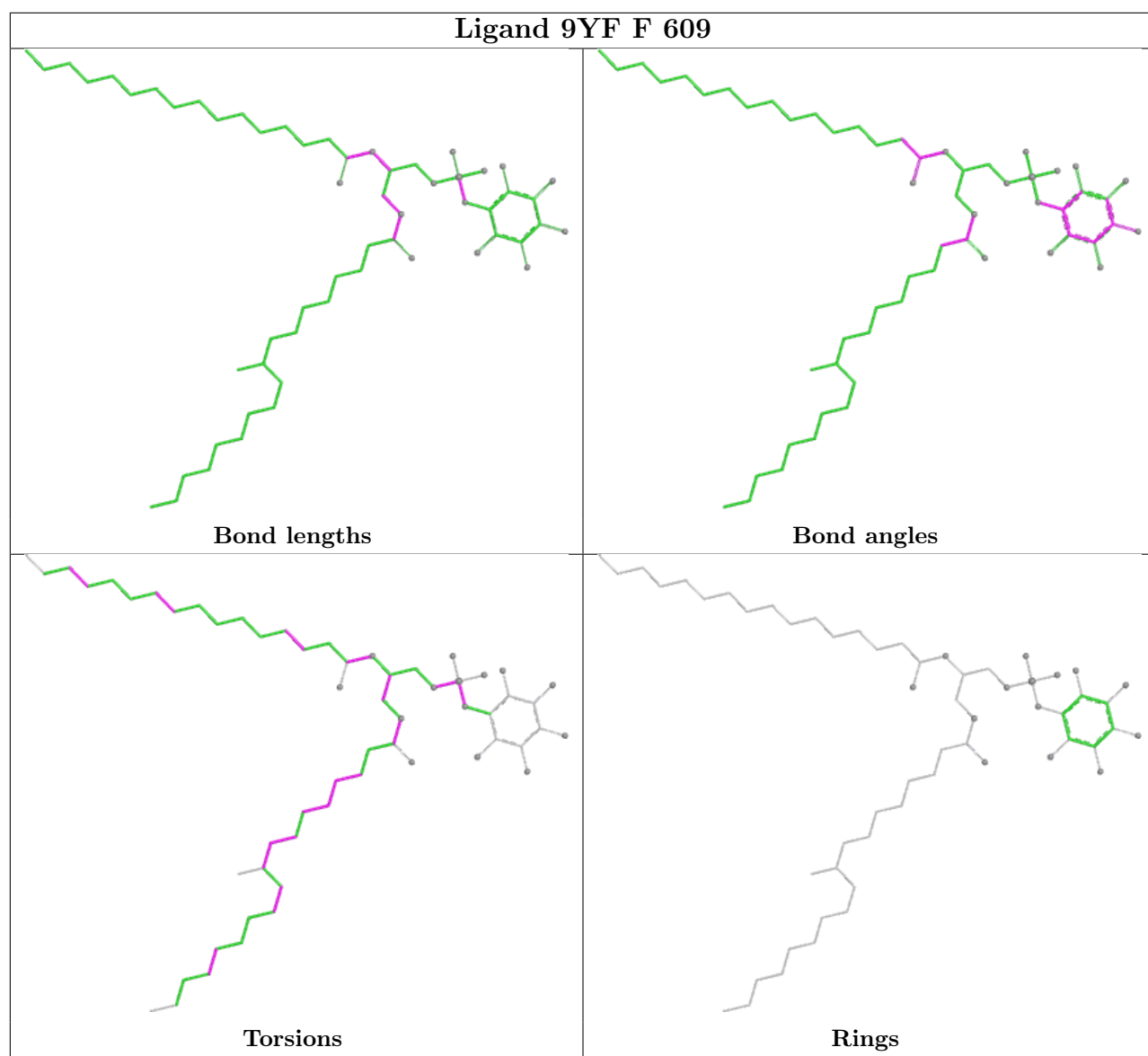
Torsions

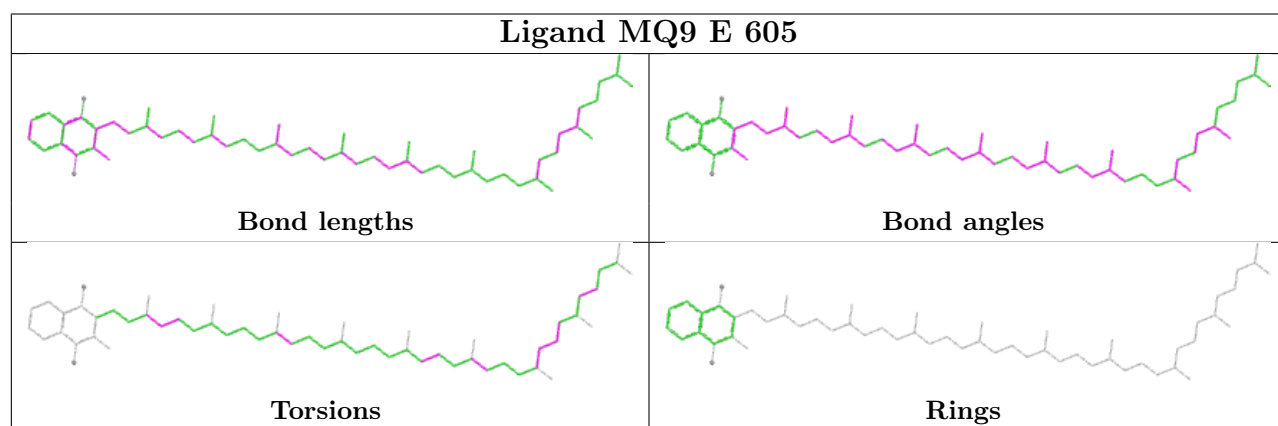
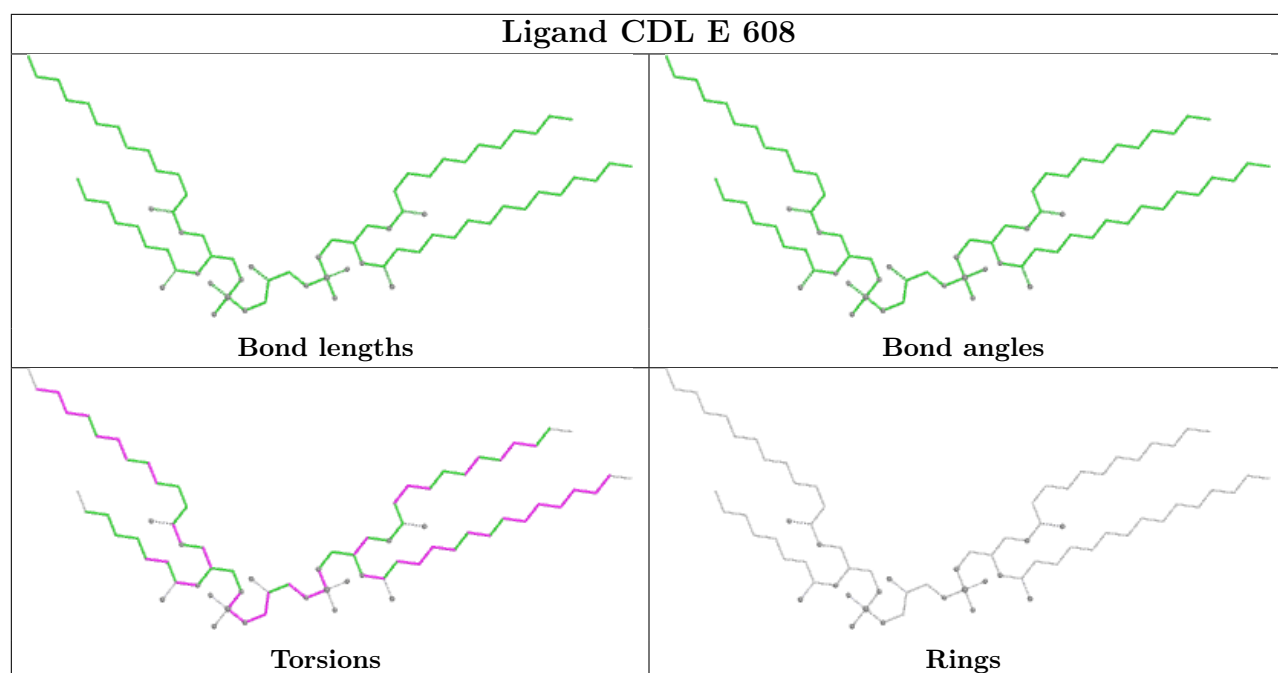


Rings

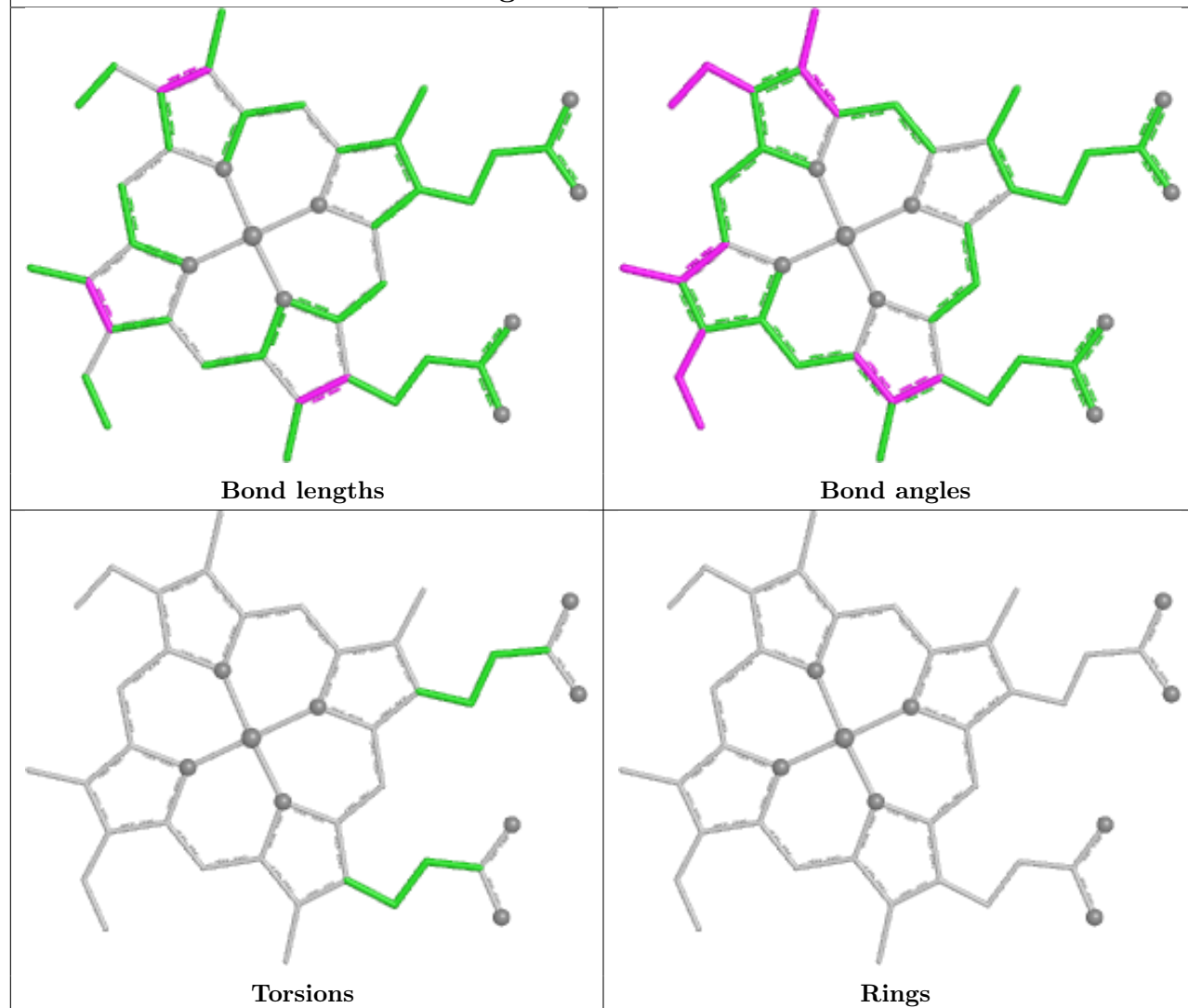




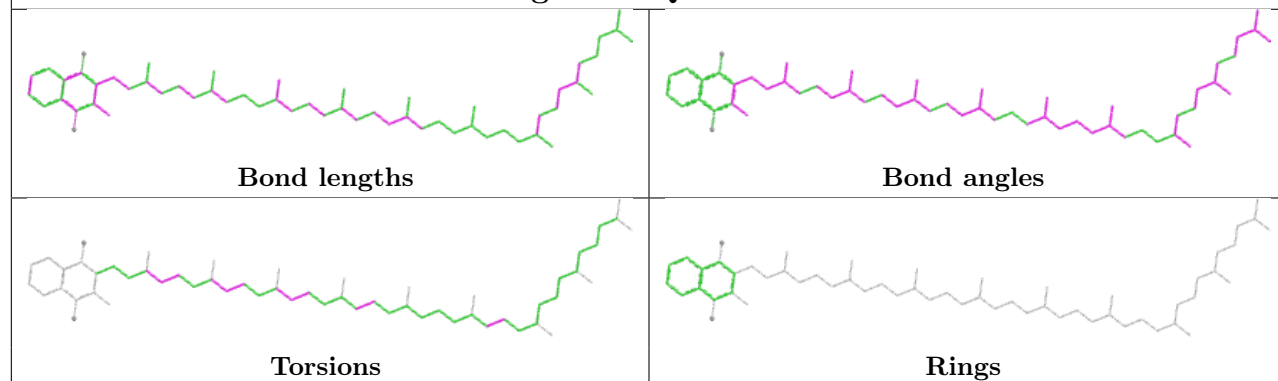


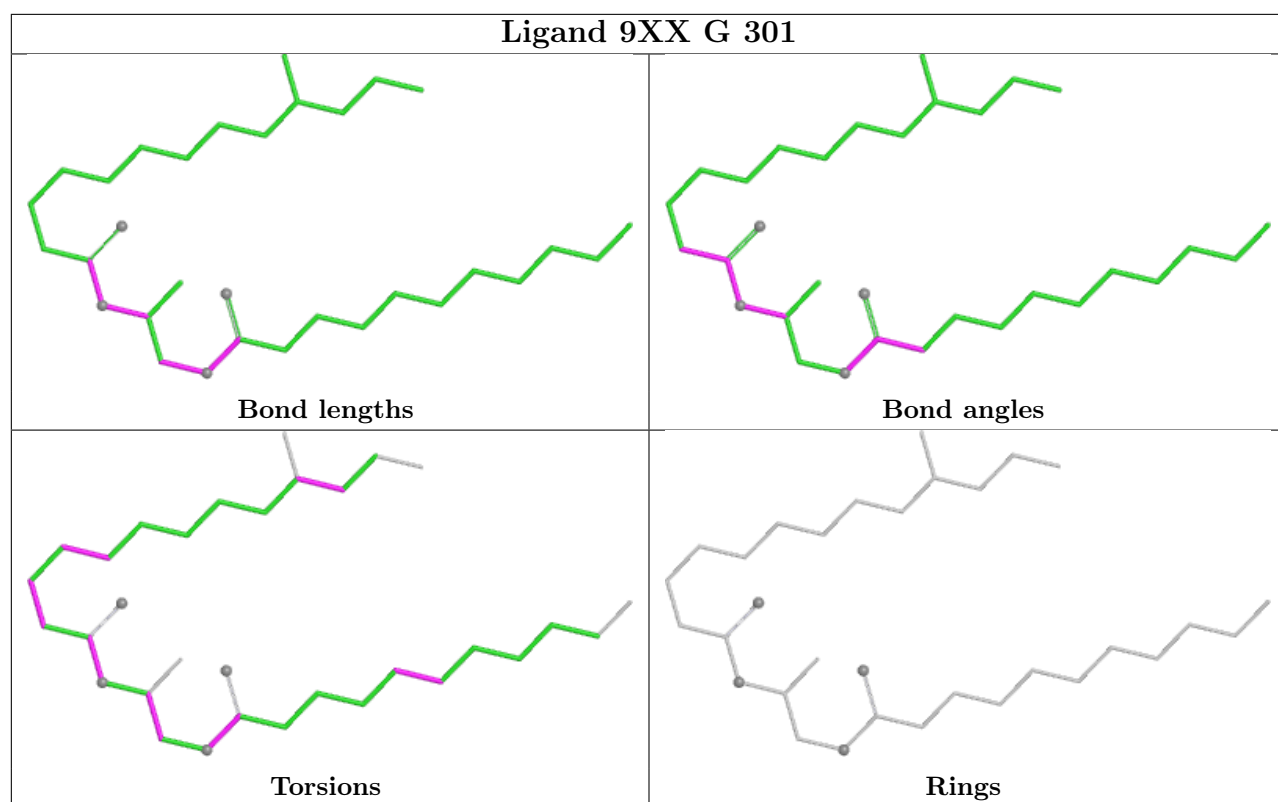


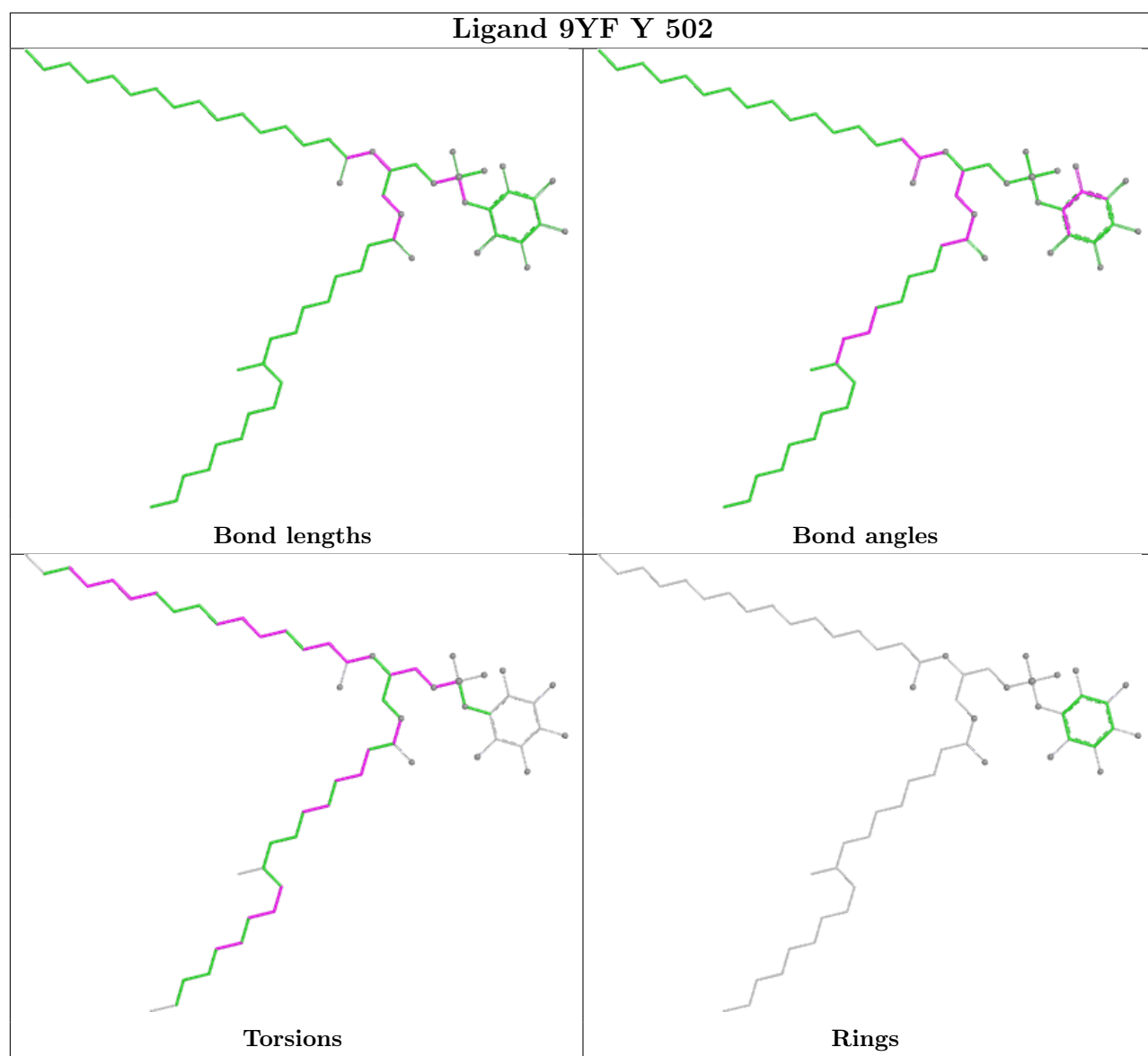
## Ligand HEC I 302

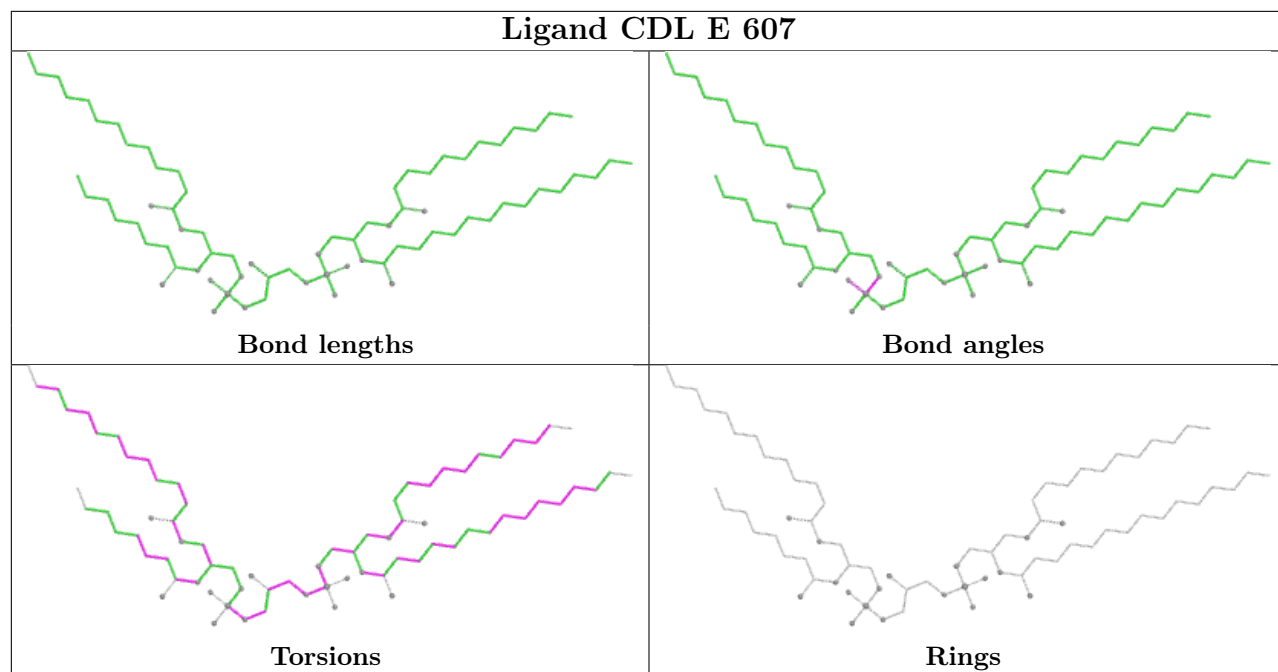


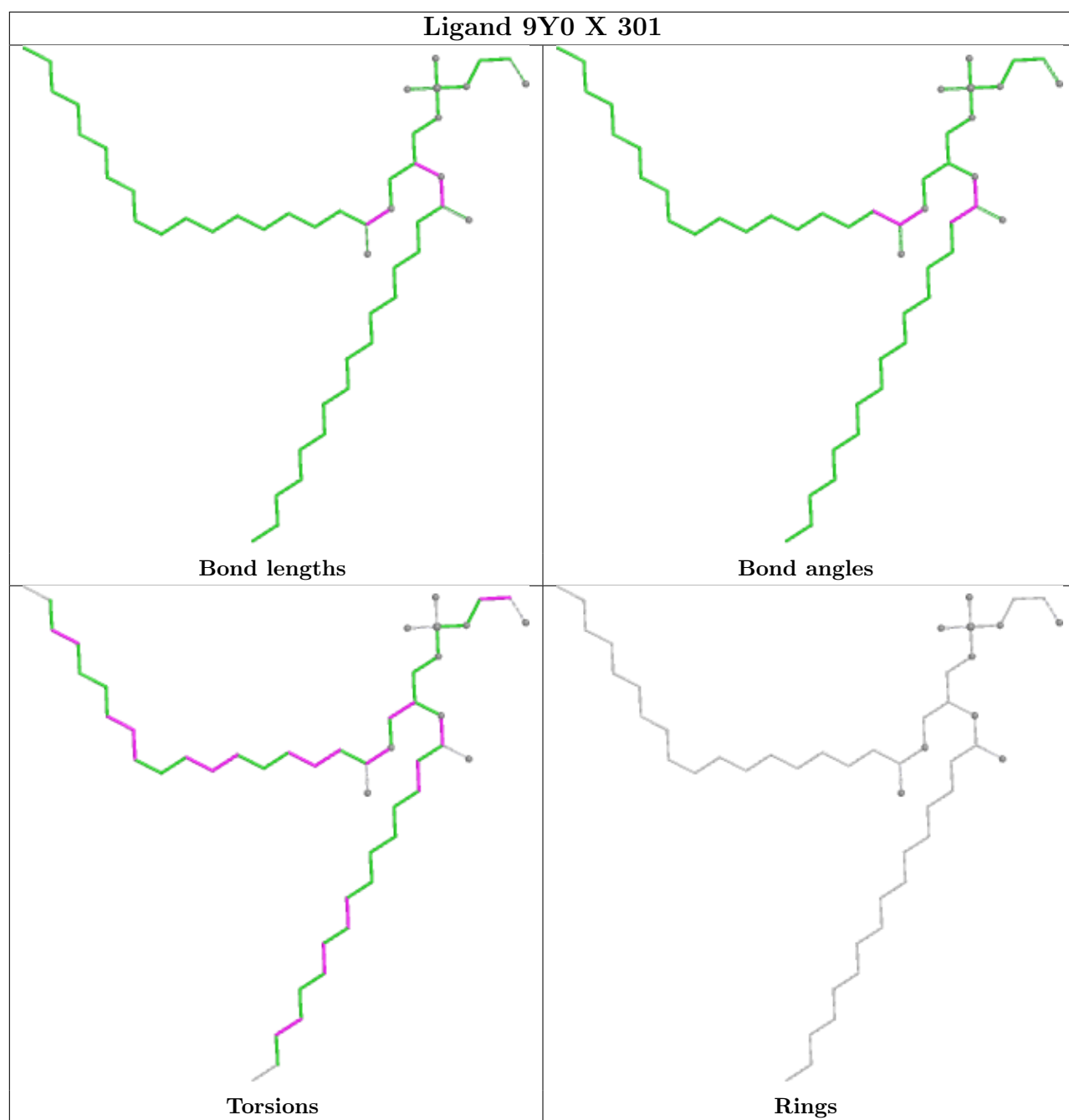
## Ligand MQ9 E 604

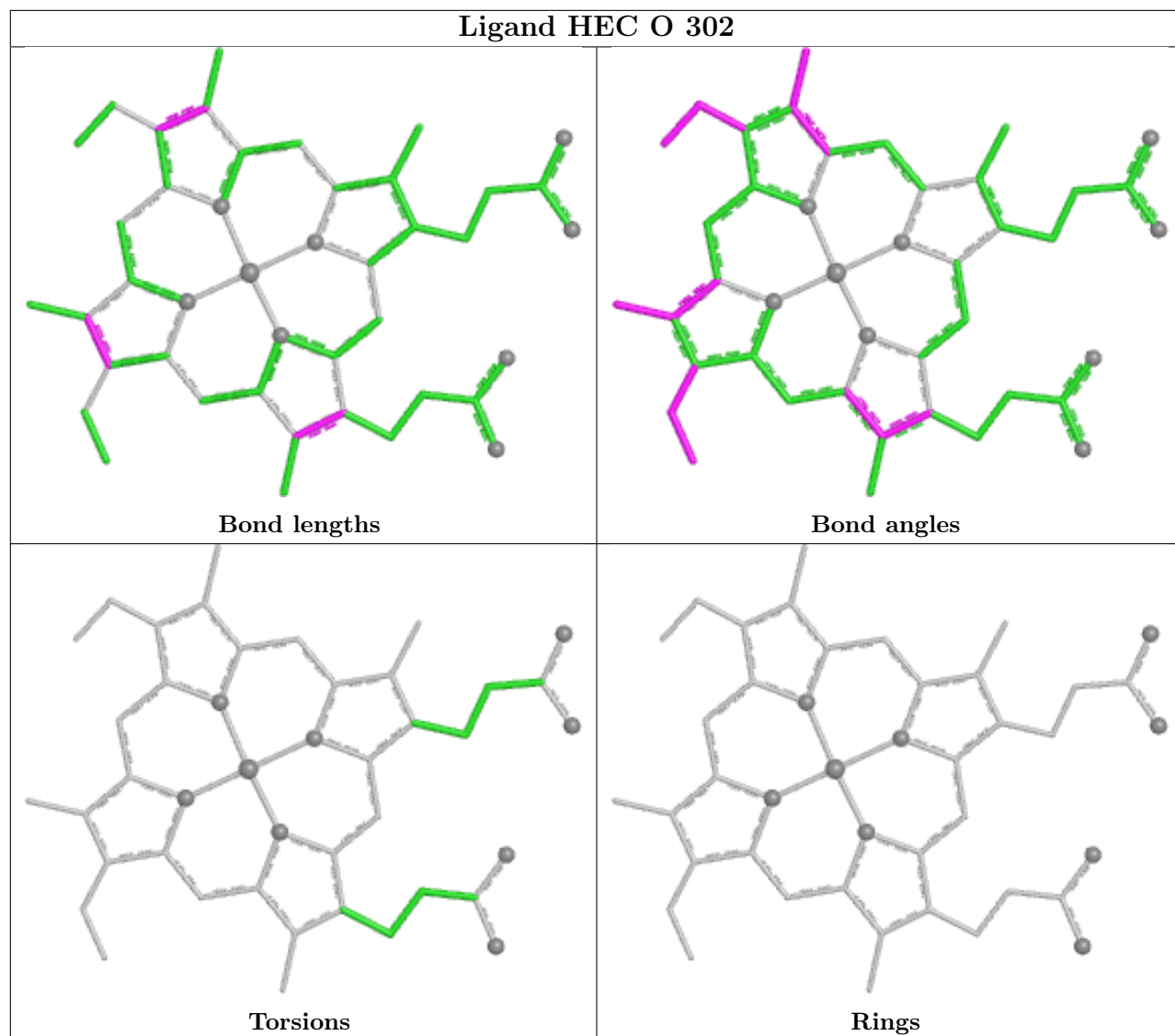




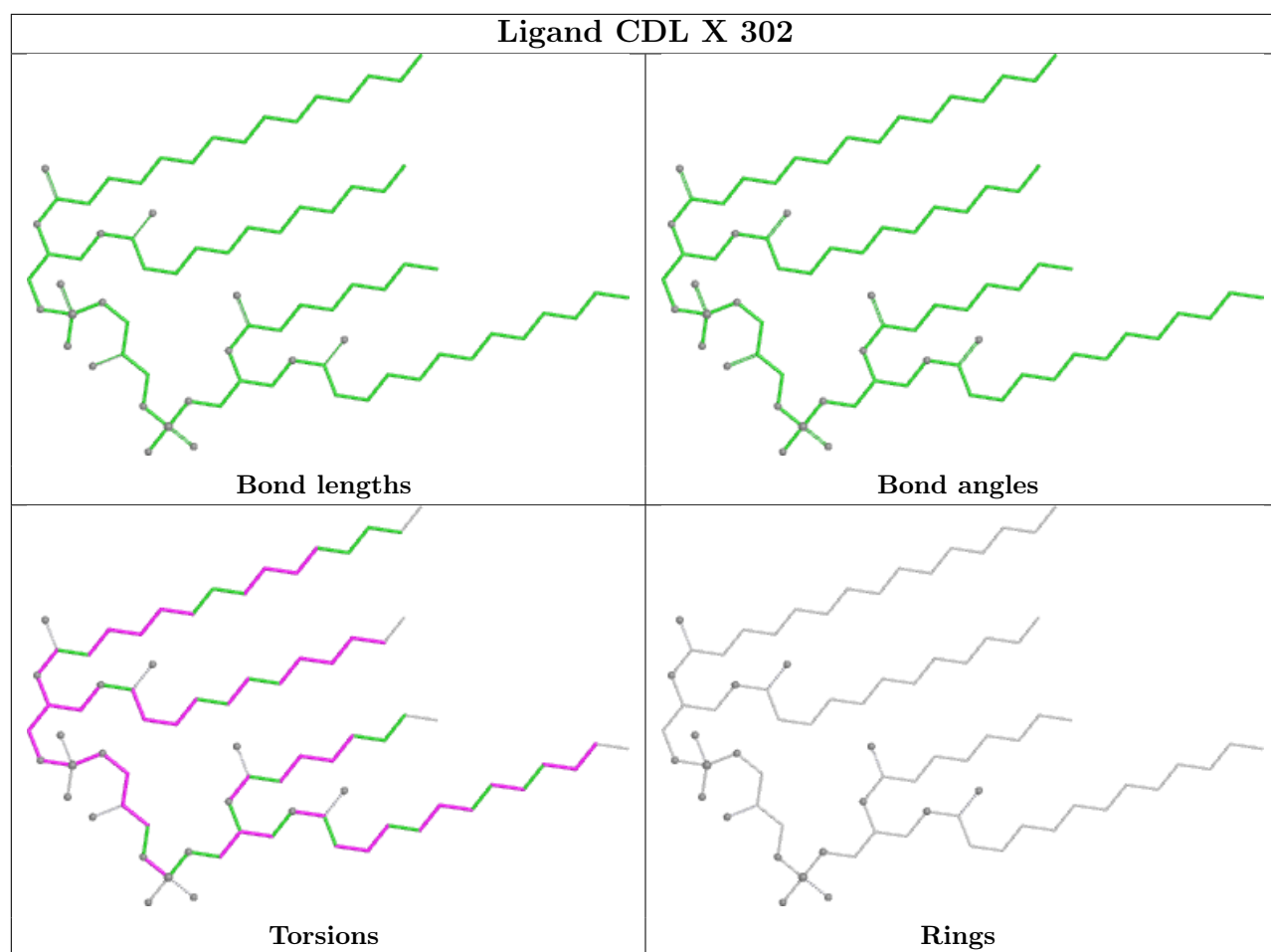


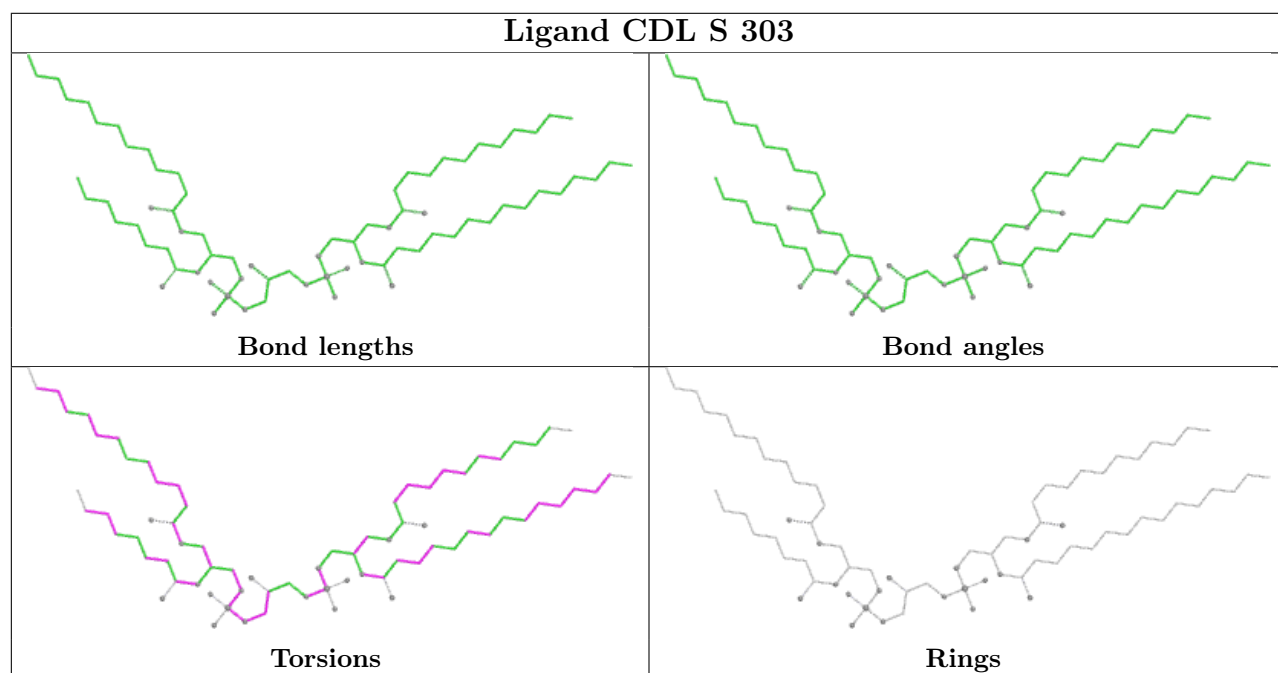
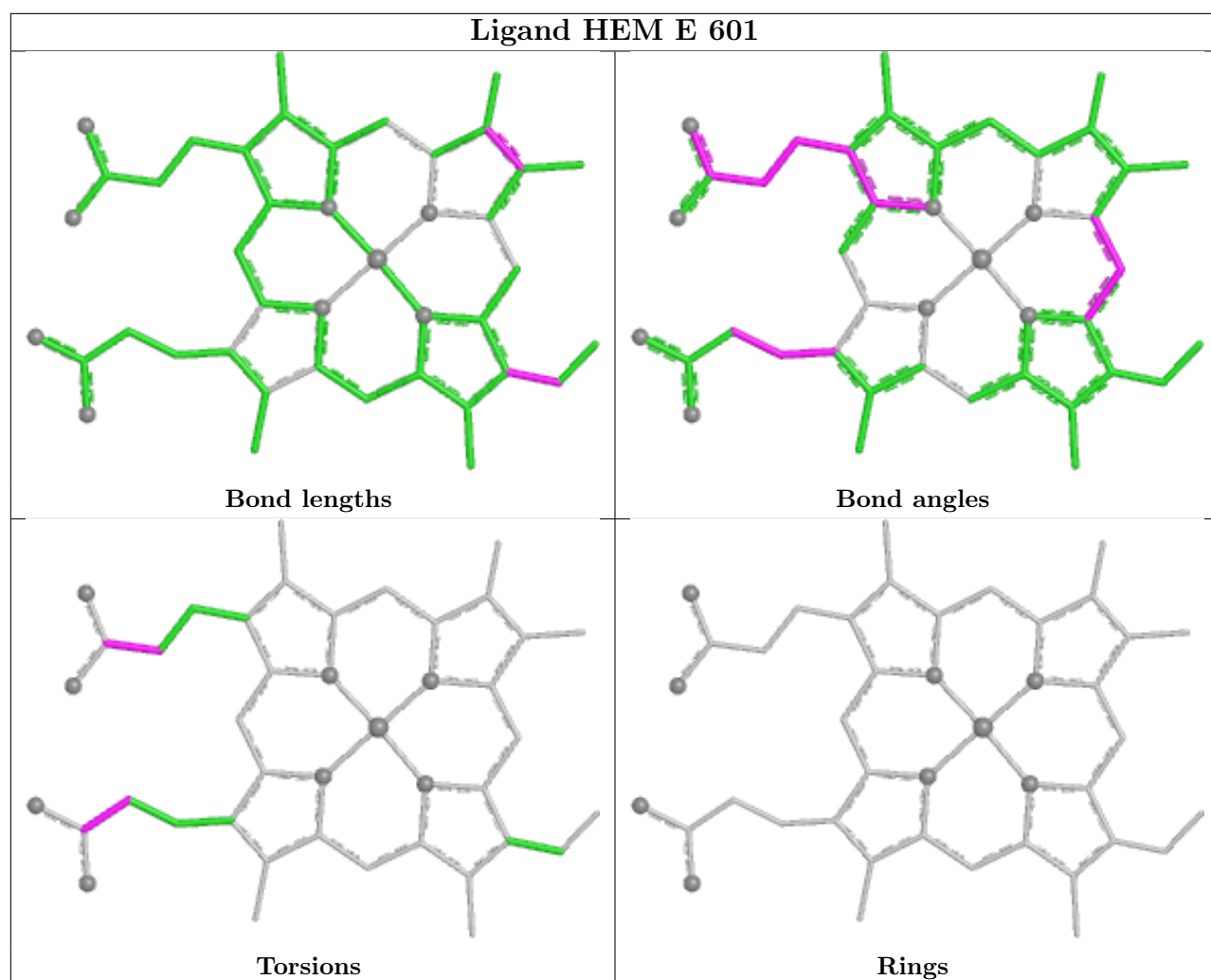


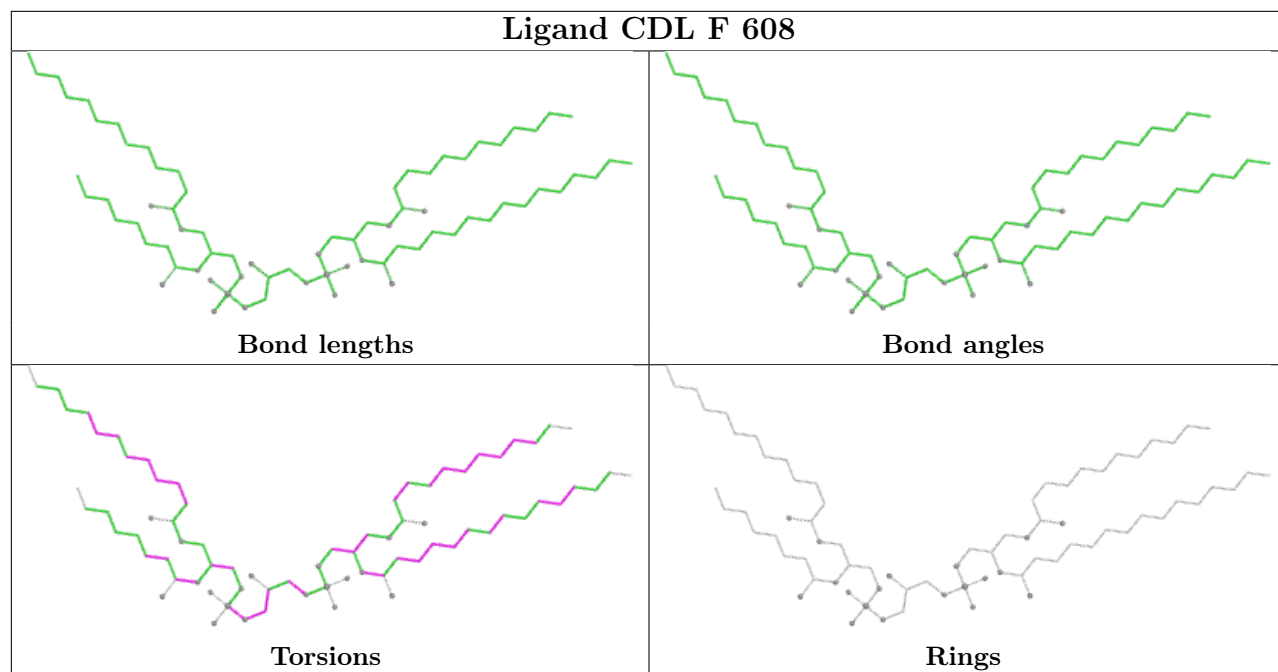


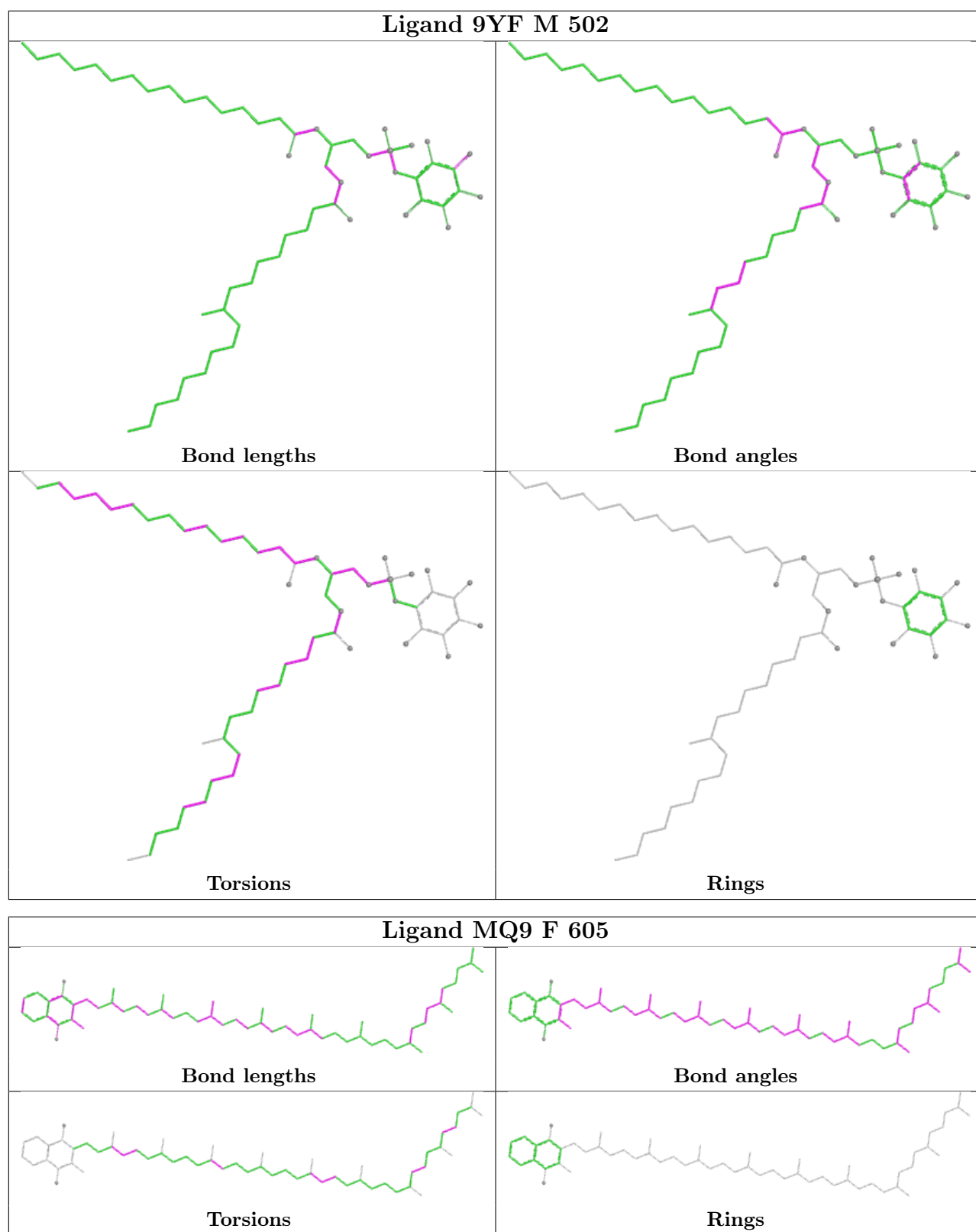












## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

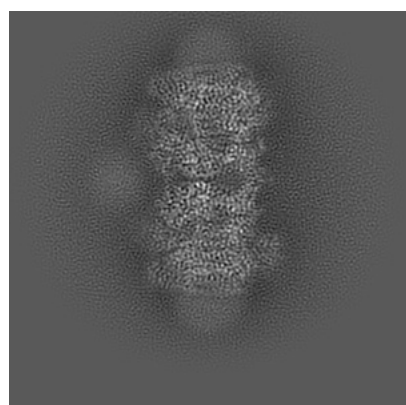
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24457. These allow visual inspection of the internal detail of the map and identification of artifacts.

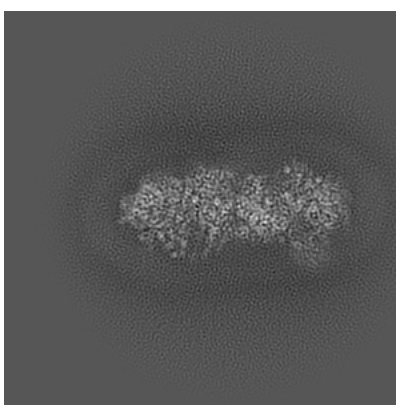
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

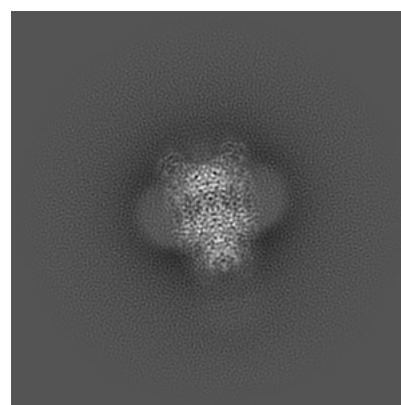
#### 6.1.1 Primary map



X



Y

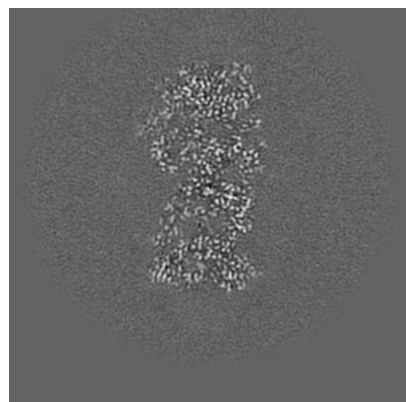


Z

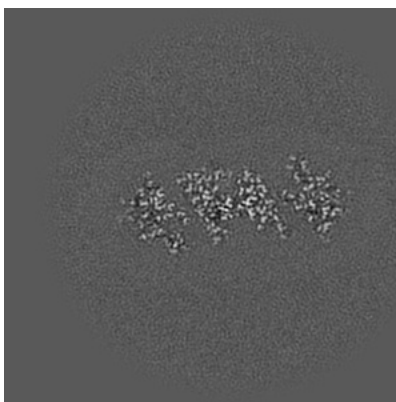
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

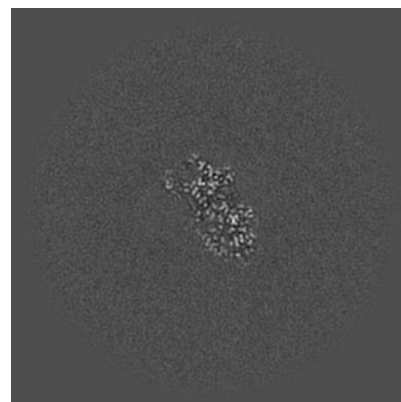
#### 6.2.1 Primary map



X Index: 165



Y Index: 165

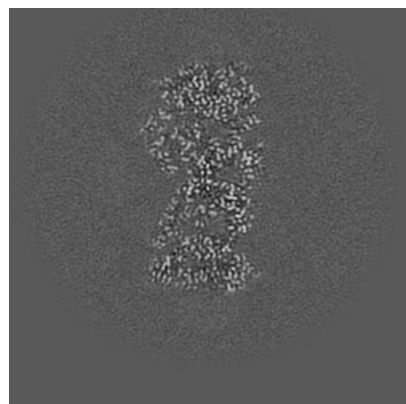


Z Index: 165

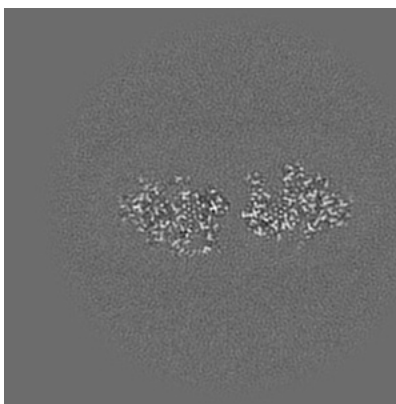
The images above show central slices of the map in three orthogonal directions.

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

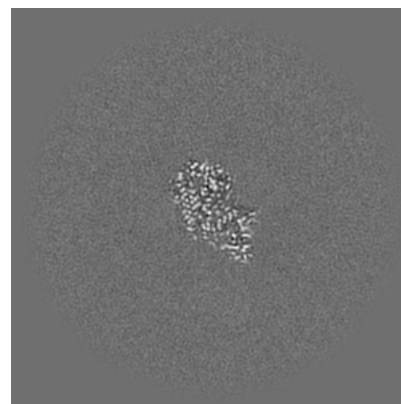
### 6.3.1 Primary map



X Index: 166



Y Index: 182

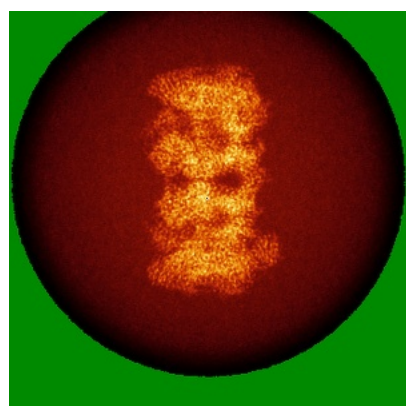


Z Index: 172

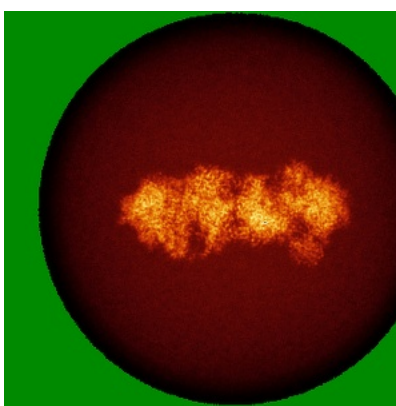
The images above show the largest variance slices of the map in three orthogonal directions.

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

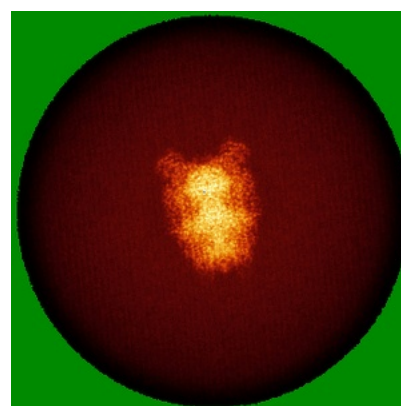
### 6.4.1 Primary map



X



Y

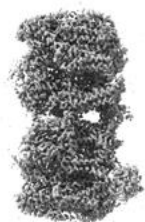


Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.82. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation [i](#)

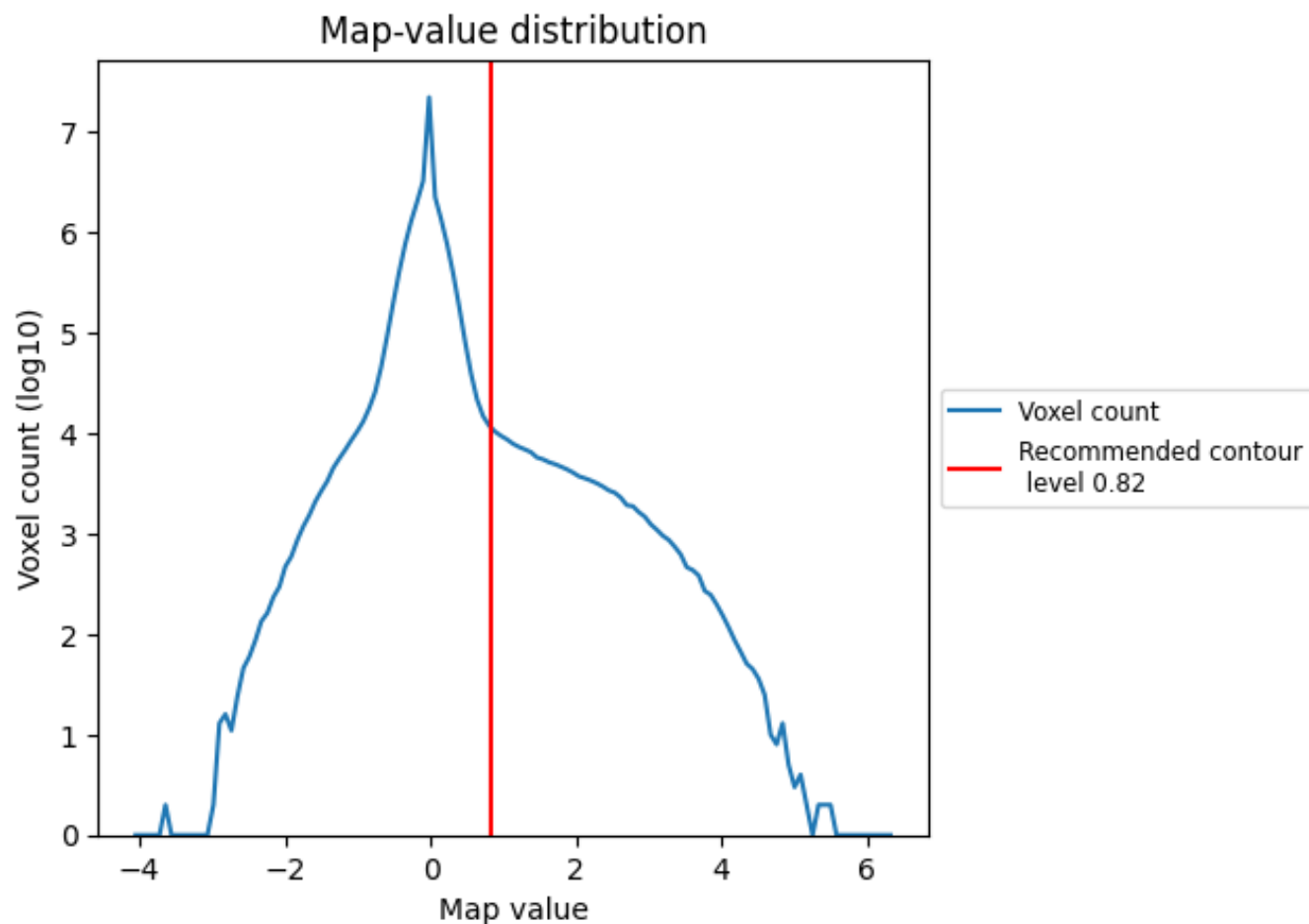
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

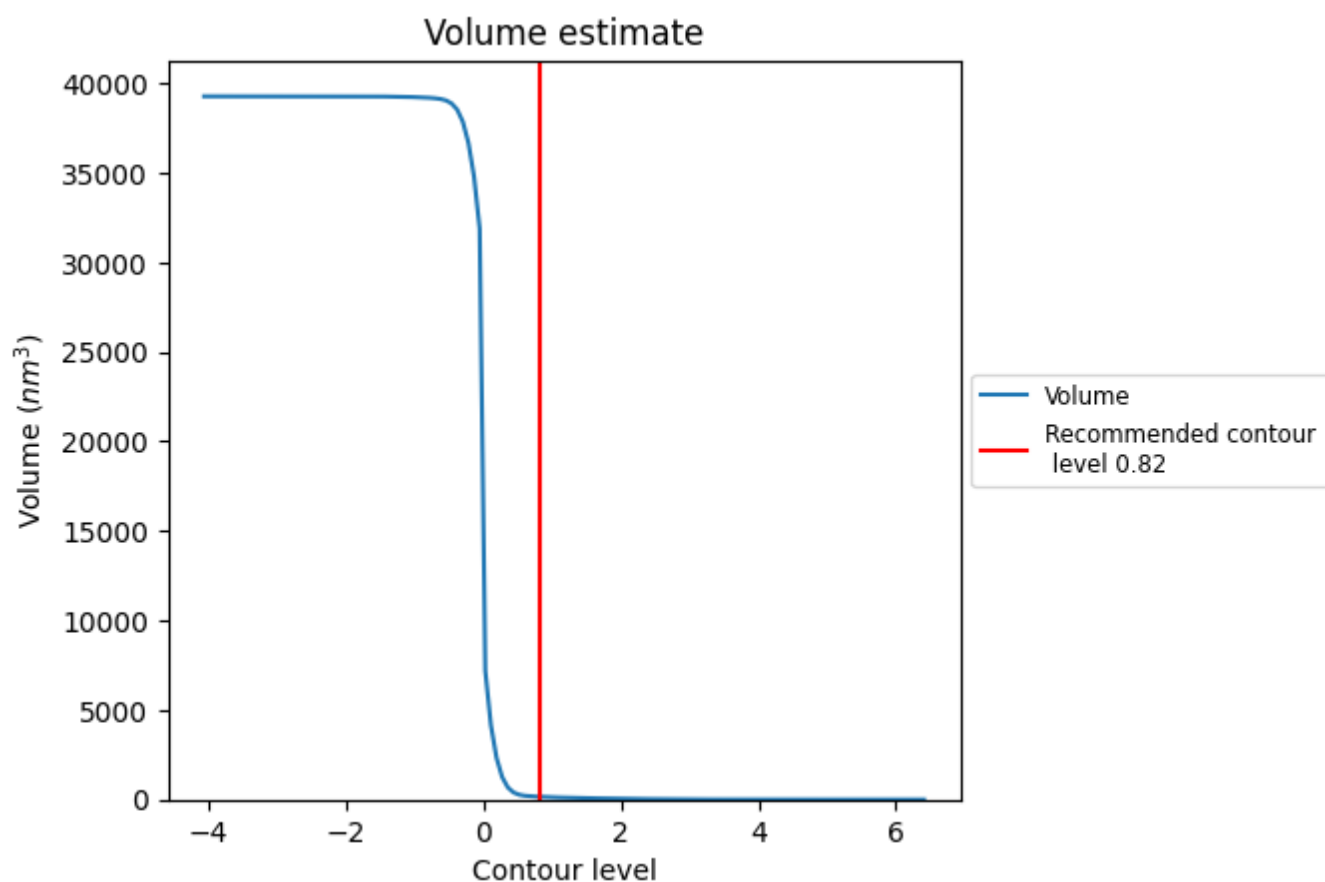
This section contains the results of statistical analysis of the map.

### 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.

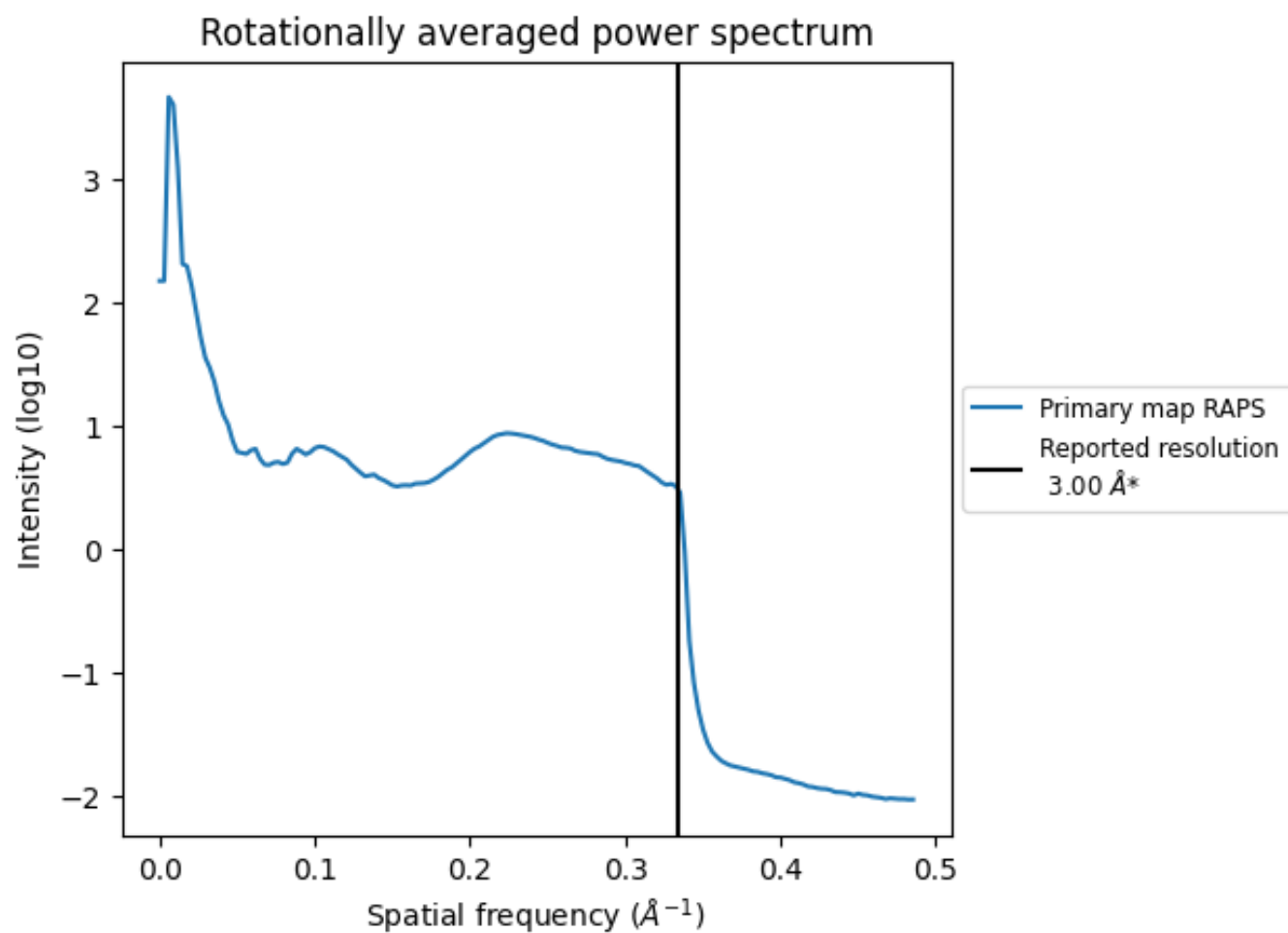
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 155 nm<sup>3</sup>; this corresponds to an approximate mass of 140 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 0.333 Å<sup>-1</sup>

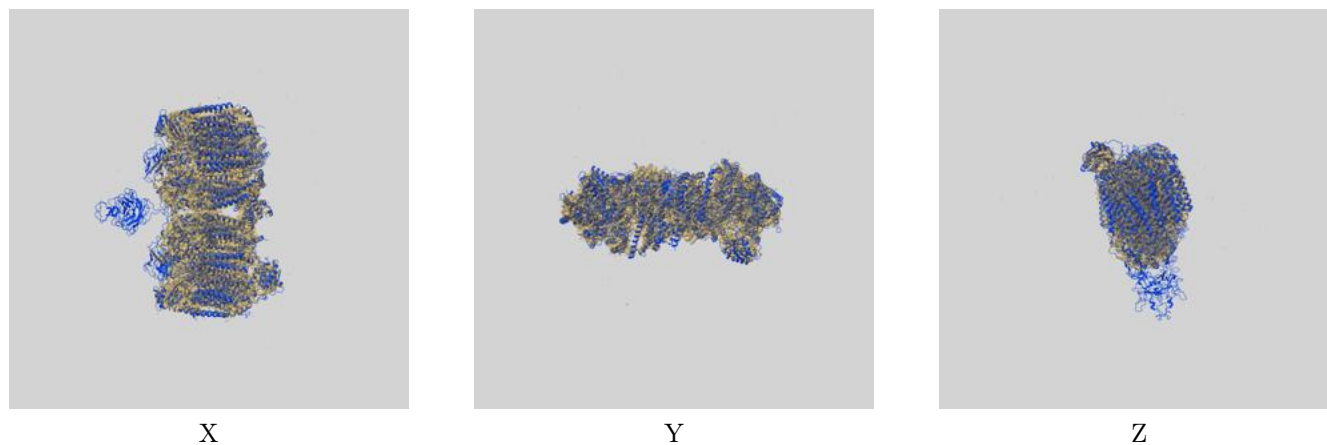
## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

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

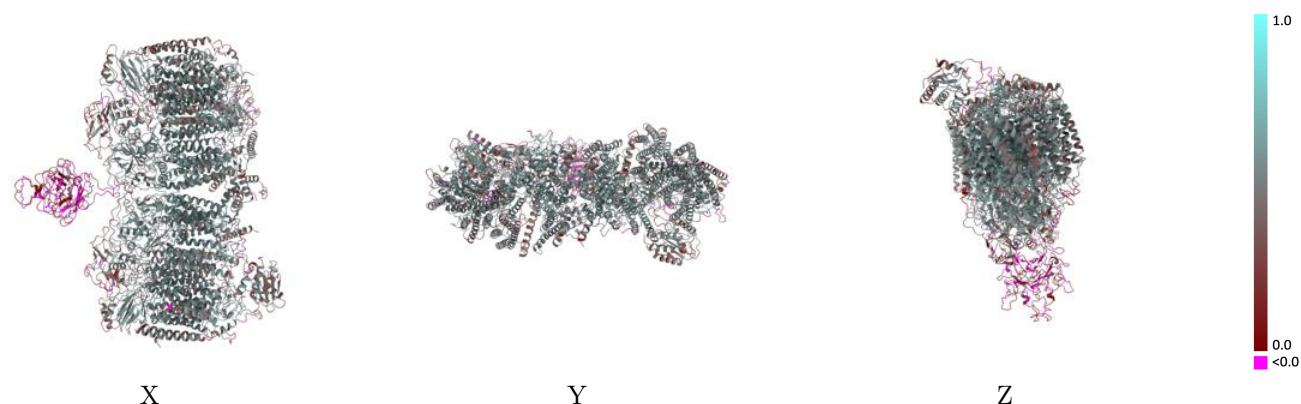
This section contains information regarding the fit between EMDB map EMD-24457 and PDB model 7RH7. Per-residue inclusion information can be found in section [3](#) on page [16](#).

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



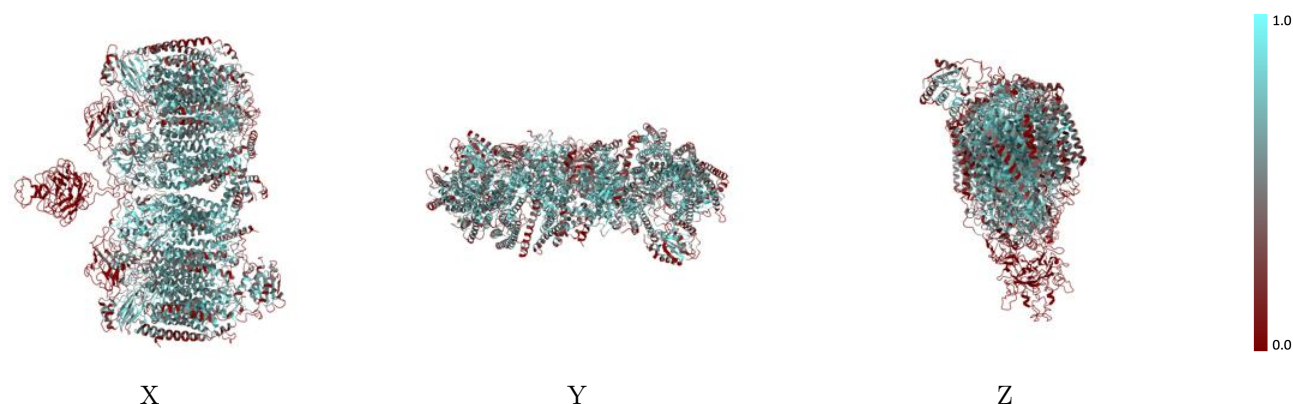
The images above show the 3D surface view of the map at the recommended contour level 0.82 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



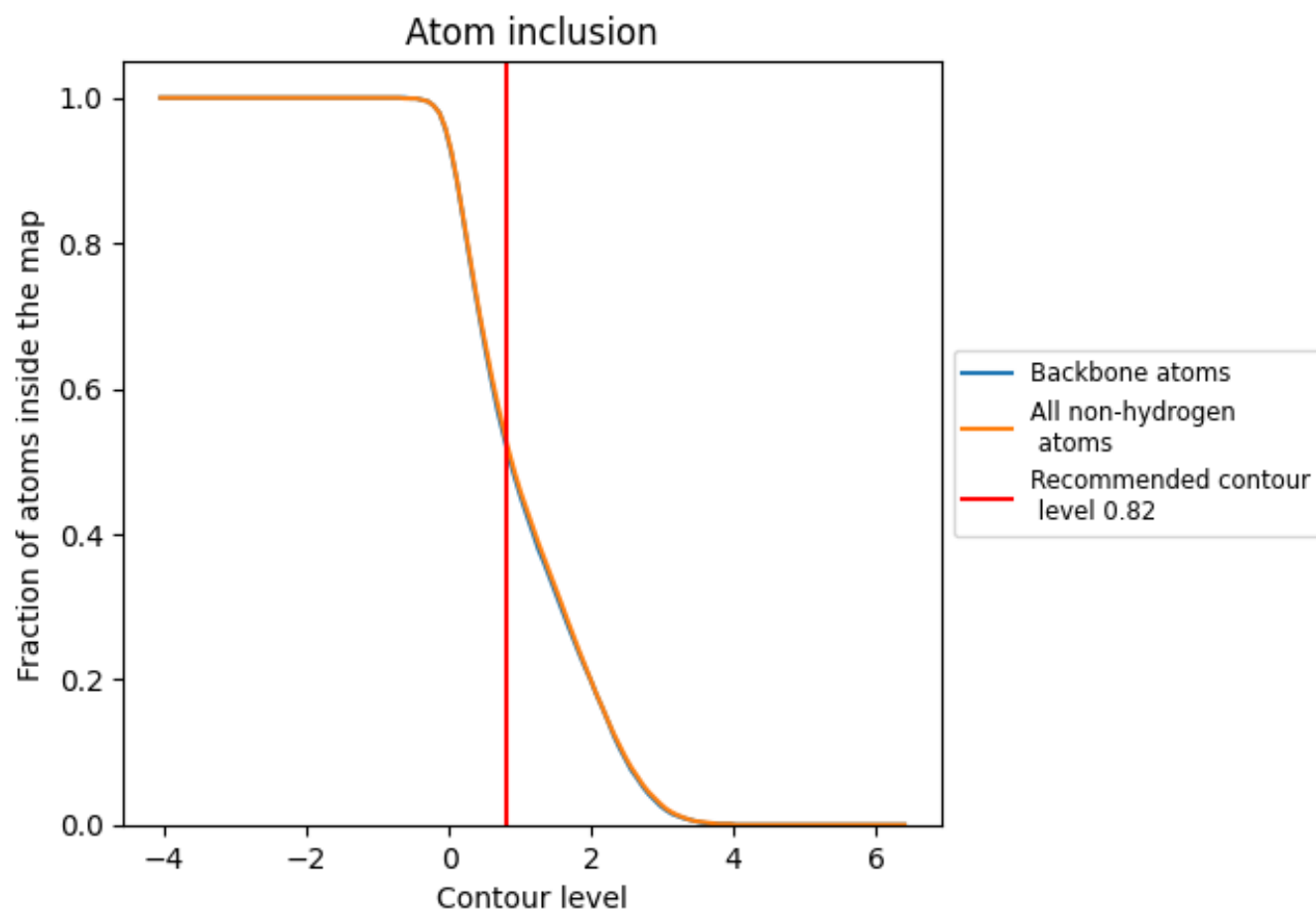
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.82).



















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 52% of all backbone atoms, 52% 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 (0.82) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5230	 0.4770
D	 0.0440	 0.1470
E	 0.6830	 0.5400
F	 0.6730	 0.5350
G	 0.0400	 0.1360
I	 0.5800	 0.5070
J	 0.3510	 0.4360
K	 0.4340	 0.4440
L	 0.6830	 0.5360
M	 0.5960	 0.5090
O	 0.5830	 0.5100
P	 0.3280	 0.4570
Q	 0.4100	 0.4320
R	 0.6900	 0.5350
S	 0.5000	 0.4820
T	 0.5300	 0.5100
U	 0.2280	 0.3790
V	 0.4510	 0.4300
W	 0.1200	 0.3510
X	 0.5070	 0.4940
Y	 0.5840	 0.5080
Z	 0.5140	 0.4870
a	 0.2330	 0.3590
b	 0.4430	 0.4220
c	 0.1110	 0.3700

