



## Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 01:25 AM UTC

PDB ID : 9G9Y / pdb\_00009g9y  
EMDB ID : EMD-51161  
Title : Respiratory supercomplex CI2-CIII2-CIV2 (megacomplex) from alphaproteobacterium  
Authors : Yaikhomba, M.; Hirst, J.; Croll, T.I.; Spikes, T.E.; Agip, A.N.A.  
Deposited on : 2024-07-25  
Resolution : 4.91 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.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : **NOT EXECUTED**  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

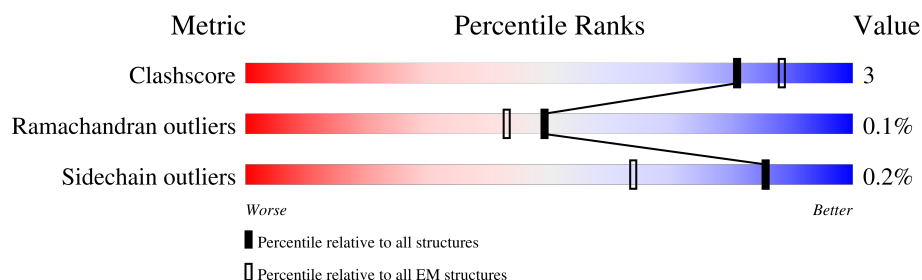
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.91 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.












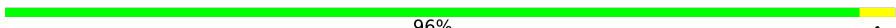
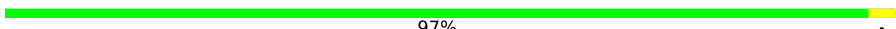








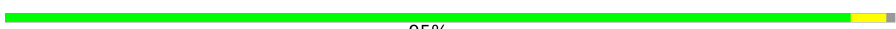
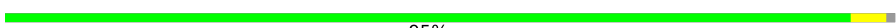

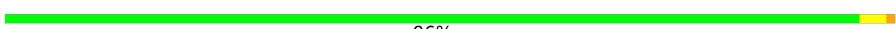


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	121	92% 8%
1	A1	121	95% 5%
2	B	175	82% 11% 7%
2	B1	175	84% 9% 7%
3	C	208	88% 5% 7%
3	C1	208	88% 5% 7%
4	D	412	92% 8%
4	D1	412	91% 9%
5	E	239	90% 9% .

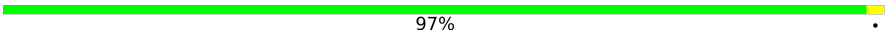
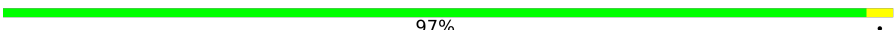


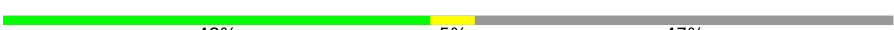





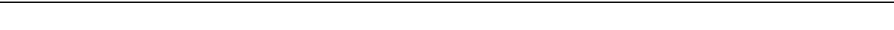

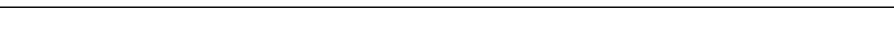
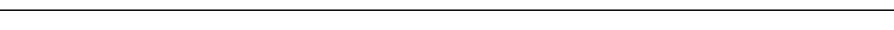
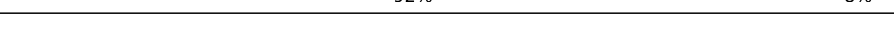




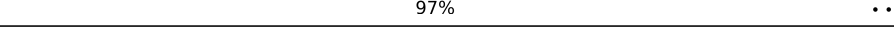
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Mol	Chain	Length	Quality of chain
5	E1	239	 92% 7% .
6	F	431	 88% 10% .
6	F1	431	 88% 10% .
7	G	674	 92% 6% .
7	G1	674	 92% 6% .
8	H	345	 91% 8% .
8	H1	345	 92% 7% .
9	I	163	 91% 8% .
9	I1	163	 93% 7% .
10	J	199	 96% .
10	J1	199	 97% .
11	K	101	 93% 6% .
11	K1	101	 92% 7% .
12	L	703	 88% 6% 6%
12	L1	703	 88% 6% 6%
13	M	513	 89% 8% .
13	M1	513	 89% 8% .
14	N	499	 91% 5% .
14	N1	499	 92% . .
15	P	330	 95% . .
15	P1	330	 95% . .
16	Q	103	 96% . .
16	Q1	103	 96% . .
17	R	62	 92% 6% .
17	R1	62	 92% 6% .

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Mol	Chain	Length	Quality of chain
18	Z	217	 97% .
18	Z1	217	 97% .
19	a	440	 92% 7% .
19	d	440	 91% 7% .
20	b	450	 48% 5% 47%
20	e	450	 48% 5% 47%
21	c	195	 86% 7% 7%
21	f	195	 86% 7% 7%
22	g	558	 88% 9% .
22	k	558	 90% 8% .
23	h	298	 77% 8% 15%
23	l	298	 76% 8% 15%
24	i	274	 91% 9%
24	m	274	 92% 8%
25	j	66	 64% . 35%
25	n	66	 64% . 35%
26	o	176	 23% . 75%
26	p	176	 23% . 75%
27	q	124	 97% ..
27	q1	124	 96% ..

## 2 Entry composition

There are 45 unique types of molecules in this entry. The entry contains 120030 atoms, of which 0 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 NADH-quinone oxidoreductase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	121	Total	C	N	O	S	0	0
			969	658	141	164	6		
1	A1	121	Total	C	N	O	S	0	0
			969	658	141	164	6		

- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	162	Total	C	N	O	S	0	0
			1270	799	227	231	13		
2	B1	162	Total	C	N	O	S	0	0
			1270	799	227	231	13		

- Molecule 3 is a protein called NADH-quinone oxidoreductase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	194	Total	C	N	O	S	0	0
			1586	1020	274	290	2		
3	C1	194	Total	C	N	O	S	0	0
			1586	1020	274	290	2		

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	411	Total	C	N	O	S	0	0
			3277	2072	582	601	22		
4	D1	411	Total	C	N	O	S	0	0
			3277	2072	582	601	22		

- Molecule 5 is a protein called NADH dehydrogenase subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	237	Total	C	N	O	S	0	0
			1822	1155	314	340	13		
5	E1	237	Total	C	N	O	S	0	0
			1822	1155	314	340	13		

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	422	Total	C	N	O	S	0	0
			3241	2027	583	600	31		
6	F1	422	Total	C	N	O	S	0	0
			3241	2027	583	600	31		

- Molecule 7 is a protein called NADH-quinone oxidoreductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	665	Total	C	N	O	S	0	0
			5068	3149	917	969	33		
7	G1	665	Total	C	N	O	S	0	0
			5068	3149	917	969	33		

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	341	Total	C	N	O	S	0	0
			2722	1848	413	439	22		
8	H1	341	Total	C	N	O	S	0	0
			2722	1848	413	439	22		

- Molecule 9 is a protein called NADH-quinone oxidoreductase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	162	Total	C	N	O	S	0	0
			1319	836	230	242	11		
9	I1	162	Total	C	N	O	S	0	0
			1319	836	230	242	11		

- Molecule 10 is a protein called NADH-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	199	Total	C	N	O	S	0	0
			1528	1014	246	257	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	J1	199	Total	C	N	O	S	0	0
			1528	1014	246	257	11		

- Molecule 11 is a protein called NADH-quinone oxidoreductase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			764	508	123	128	5		
11	K1	101	Total	C	N	O	S	0	0
			764	508	123	128	5		

- Molecule 12 is a protein called NADH dehydrogenase subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	661	Total	C	N	O	S	0	0
			5215	3472	853	857	33		
12	L1	661	Total	C	N	O	S	0	0
			5215	3472	853	857	33		

- Molecule 13 is a protein called NADH dehydrogenase subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	503	Total	C	N	O	S	0	0
			3915	2615	610	658	32		
13	M1	503	Total	C	N	O	S	0	0
			3915	2615	610	658	32		

- Molecule 14 is a protein called NADH-quinone oxidoreductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	480	Total	C	N	O	S	0	0
			3556	2342	565	617	32		
14	N1	480	Total	C	N	O	S	0	0
			3556	2342	565	617	32		

- Molecule 15 is a protein called NAD-dependent epimerase/dehydratase.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	328	Total	C	N	O	S	0	0
			2468	1541	463	452	12		
15	P1	328	Total	C	N	O	S	0	0
			2468	1541	463	452	12		

- Molecule 16 is a protein called ETC complex I subunit conserved region.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	103	Total	C	N	O	S	0	0
			849	523	167	156	3		
16	Q1	103	Total	C	N	O	S	0	0
			849	523	167	156	3		

- Molecule 17 is a protein called Zinc finger CHCC-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	61	Total	C	N	O	S	0	0
			488	304	90	91	3		
17	R1	61	Total	C	N	O	S	0	0
			488	304	90	91	3		

- Molecule 18 is a protein called Protein-L-isoaspartate O-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	216	Total	C	N	O	S	0	0
			1642	1033	294	306	9		
18	Z1	216	Total	C	N	O	S	0	0
			1642	1033	294	306	9		

- Molecule 19 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	434	Total	C	N	O	S	0	0
			3513	2378	553	564	18		
19	d	434	Total	C	N	O	S	0	0
			3513	2378	553	564	18		

- Molecule 20 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	239	Total	C	N	O	S	0	0
			1855	1181	311	354	9		
20	e	239	Total	C	N	O	S	0	0
			1855	1181	311	354	9		

- Molecule 21 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.



Mol	Chain	Residues	Atoms					AltConf	Trace
21	c	181	Total	C	N	O	S	0	0
			1361	842	246	266	7		
21	f	181	Total	C	N	O	S	0	0
			1361	842	246	266	7		

- Molecule 22 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	g	544	Total	C	N	O	S	0	0
			4322	2890	684	715	33		
22	k	544	Total	C	N	O	S	0	0
			4322	2890	684	715	33		

- Molecule 23 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	h	252	Total	C	N	O	S	0	0
			1976	1295	319	354	8		
23	l	252	Total	C	N	O	S	0	0
			1976	1295	319	354	8		

- Molecule 24 is a protein called cytochrome-c oxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	i	273	Total	C	N	O	S	0	0
			2183	1483	341	348	11		
24	m	273	Total	C	N	O	S	0	0
			2183	1483	341	348	11		

- Molecule 25 is a protein called Aa3 type cytochrome c oxidase subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	j	43	Total	C	N	O	S	0	0
			332	214	58	59	1		
25	n	43	Total	C	N	O	S	0	0
			332	214	58	59	1		

- Molecule 26 is a protein called Cytochrome c, class I.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	o	44	Total	C	N	O	S	0	0
			324	215	49	58	2		

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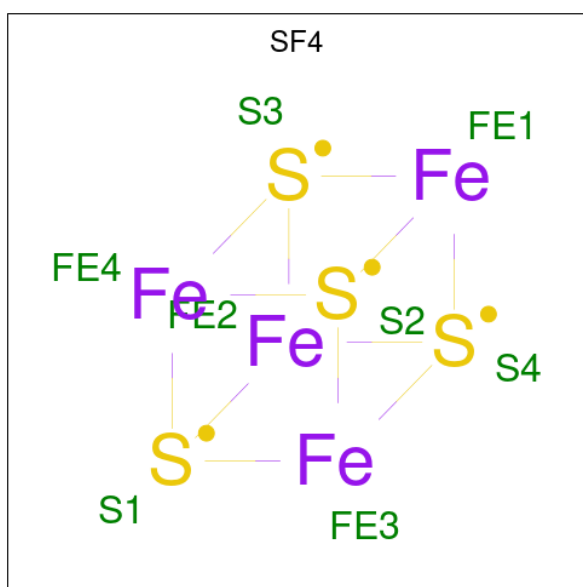
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Mol	Chain	Residues	Atoms					AltConf	Trace
26	p	44	Total	C	N	O	S	0	0
			324	215	49	58	2		

- Molecule 27 is a protein called NADH:ubiquinone oxidoreductase 17.2 kD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	q	123	Total	C	N	O	S	0	0
			1018	651	181	185	1		
27	q1	123	Total	C	N	O	S	0	0
			1018	651	181	185	1		

- Molecule 28 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



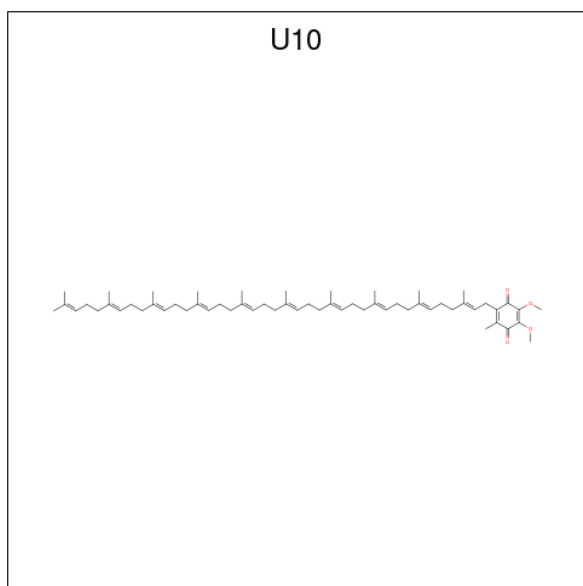
Mol	Chain	Residues	Atoms			AltConf
28	B	1	Total	Fe	S	0
			8	4	4	
28	B1	1	Total	Fe	S	0
			8	4	4	
28	F	1	Total	Fe	S	0
			8	4	4	
28	F1	1	Total	Fe	S	0
			8	4	4	
28	G	1	Total	Fe	S	0
			8	4	4	
28	G	1	Total	Fe	S	0
			8	4	4	

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Mol	Chain	Residues	Atoms			AltConf
28	G1	1	Total	Fe	S	0
			8	4	4	
28	G1	1	Total	Fe	S	0
			8	4	4	
28	I	1	Total	Fe	S	0
			8	4	4	
28	I	1	Total	Fe	S	0
			8	4	4	
28	I1	1	Total	Fe	S	0
			8	4	4	
28	I1	1	Total	Fe	S	0
			8	4	4	

- Molecule 29 is UBIQUINONE-10 (CCD ID: U10) (formula:  $C_{59}H_{90}O_4$ ).



Mol	Chain	Residues	Atoms			AltConf
29	B	1	Total	C	O	0
			63	59	4	
29	B1	1	Total	C	O	0
			63	59	4	
29	a	1	Total	C	O	0
			63	59	4	
29	a	1	Total	C	O	0
			63	59	4	
29	d	1	Total	C	O	0
			63	59	4	

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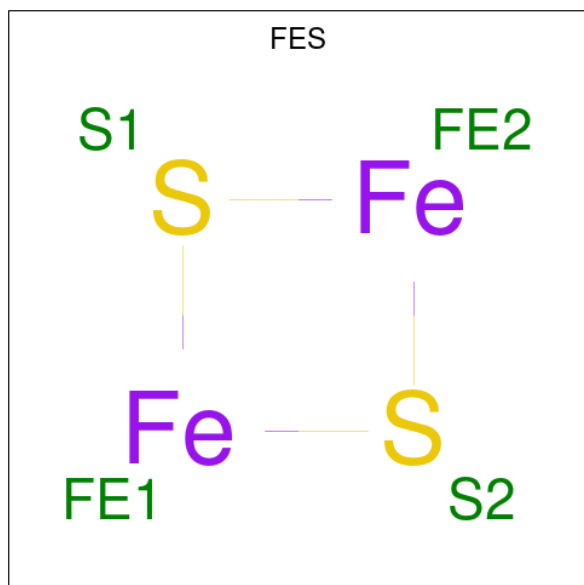
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Mol	Chain	Residues	Atoms			AltConf
29	d	1	Total	C	O	0
			63	59	4	

- Molecule 30 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
30	D	1	Total	Ca	0
			1	1	
30	D1	1	Total	Ca	0
			1	1	
30	b	1	Total	Ca	0
			1	1	
30	e	1	Total	Ca	0
			1	1	
30	g	1	Total	Ca	0
			1	1	
30	k	1	Total	Ca	0
			1	1	

- Molecule 31 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



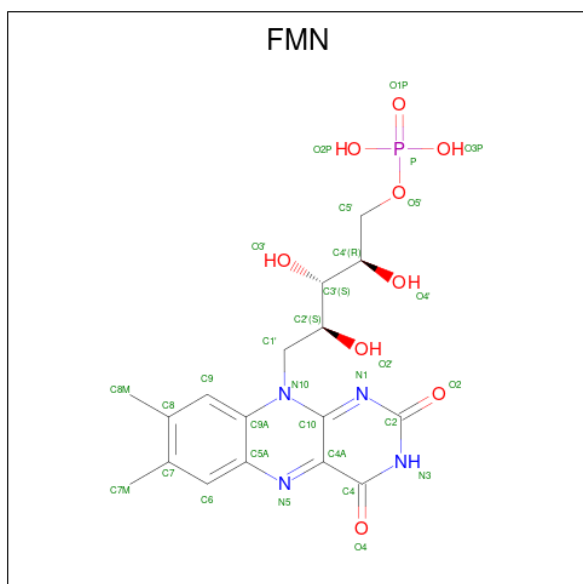
Mol	Chain	Residues	Atoms			AltConf
31	E	1	Total	Fe	S	0
			4	2	2	
31	E1	1	Total	Fe	S	0
			4	2	2	

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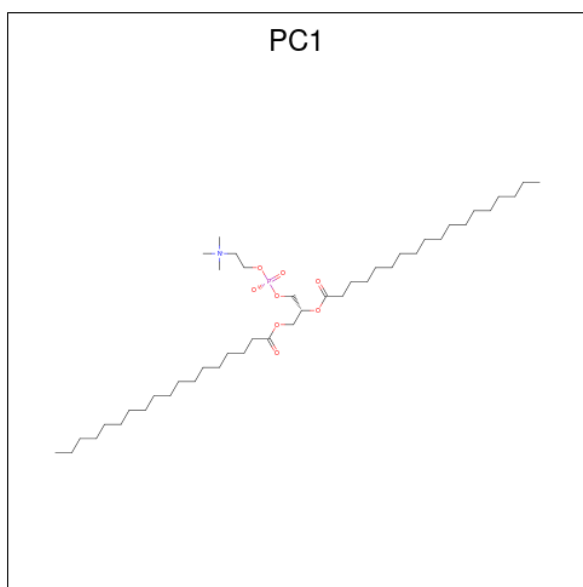
Mol	Chain	Residues	Atoms			AltConf
31	G	1	Total	Fe	S	0
			4	2	2	
31	G1	1	Total	Fe	S	0
			4	2	2	
31	c	1	Total	Fe	S	0
			4	2	2	
31	f	1	Total	Fe	S	0
			4	2	2	

- Molecule 32 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ) (labeled as "Ligand of Interest" by depositor).



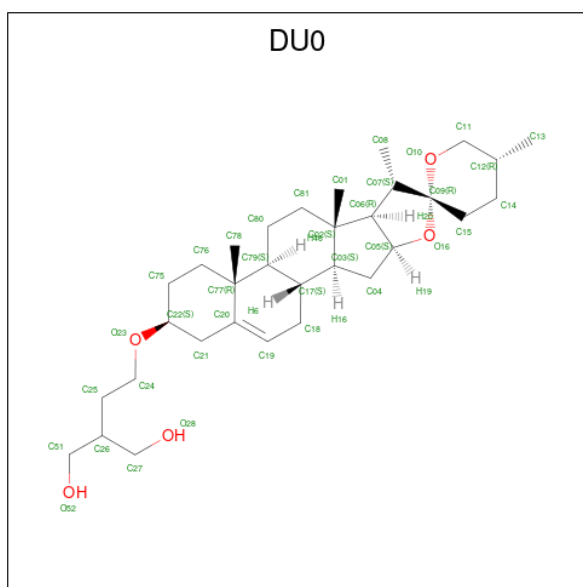
Mol	Chain	Residues	Atoms					AltConf
32	F	1	Total	C	N	O	P	0
			31	17	4	9	1	
32	F1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 33 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).



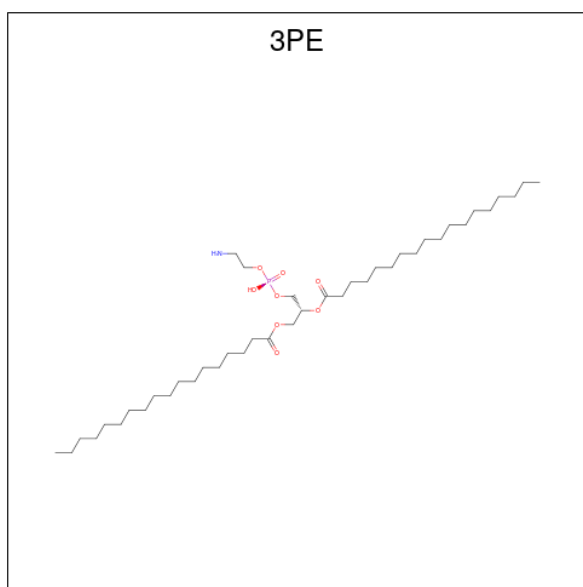
Mol	Chain	Residues	Atoms					AltConf
33	H	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	H1	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	H1	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	L1	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	M	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	M1	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	i	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	i	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	j	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	m	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	m	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	n	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 34 is 2-[2-[(1 {S},2 {S},4 {S},5' {R},6 {R},7 {S},8 {R},9 {S},12 {S},13 {R},16 {S})-5',7,9,13-tetramethylspiro[5-oxapentacyclo[10.8.0.0<sup>2,9</sup>.0<sup>4,8</sup>.0<sup>13,18</sup>]]icos-18-ene-6,2'-oxane]-16-yl]oxyethyl]propane-1,3-diol (CCD ID: DU0) (formula: C<sub>32</sub>H<sub>52</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			AltConf
34	K	1	Total	C	O	0
			37	32	5	
34	M	1	Total	C	O	0
			37	32	5	
34	M1	1	Total	C	O	0
			37	32	5	
34	a	1	Total	C	O	0
			37	32	5	
34	d	1	Total	C	O	0
			37	32	5	

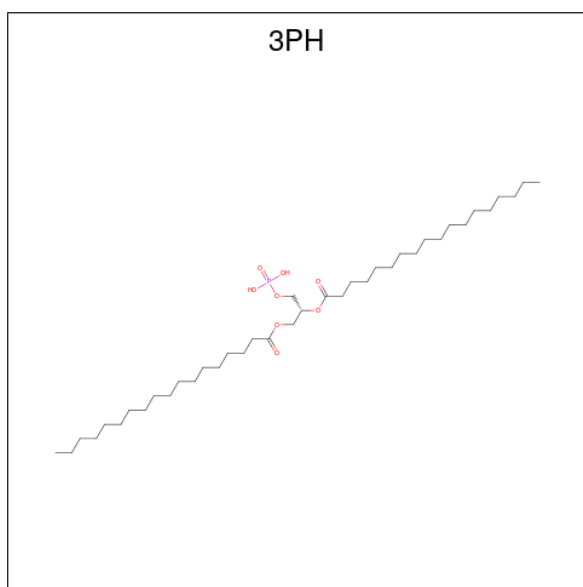
- Molecule 35 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
35	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
35	L1	1	Total	C	N	O	P	0
			51	41	1	8	1	
35	b	1	Total	C	N	O	P	0
			51	41	1	8	1	
35	e	1	Total	C	N	O	P	0
			51	41	1	8	1	
35	g	1	Total	C	N	O	P	0
			51	41	1	8	1	
35	i	1	Total	C	N	O	P	0
			51	41	1	8	1	
35	k	1	Total	C	N	O	P	0
			51	41	1	8	1	
35	m	1	Total	C	N	O	P	0
			51	41	1	8	1	
35	m	1	Total	C	N	O	P	0
			51	41	1	8	1	

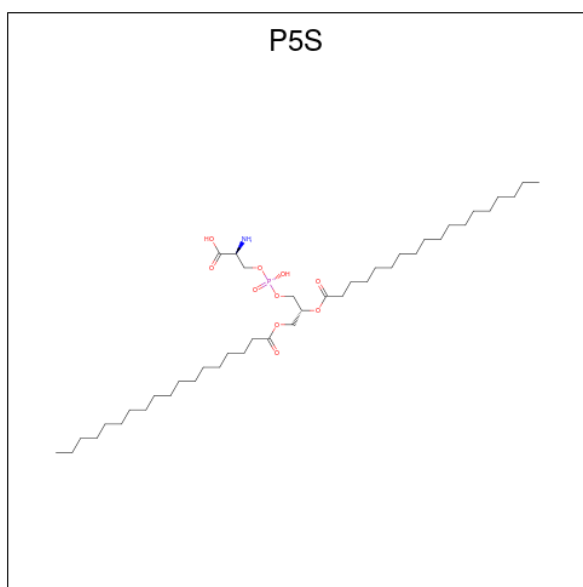
- Molecule 36 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula:  $C_{39}H_{77}O_8P$ ).





Mol	Chain	Residues	Atoms				AltConf
36	L	1	Total	C	O	P	0
			48	39	8	1	
36	L1	1	Total	C	O	P	0
			48	39	8	1	
36	f	1	Total	C	O	P	0
			48	39	8	1	
36	g	1	Total	C	O	P	0
			48	39	8	1	
36	k	1	Total	C	O	P	0
			48	39	8	1	
36	p	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 37 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>10</sub>P).

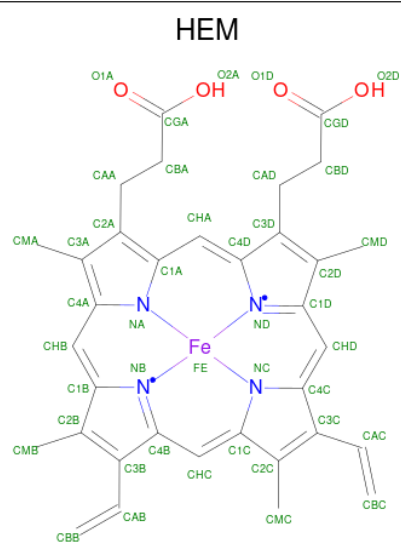


Mol	Chain	Residues	Atoms					AltConf
37	L	1	Total	C	N	O	P	0
			54	42	1	10	1	
37	L1	1	Total	C	N	O	P	0
			54	42	1	10	1	

- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

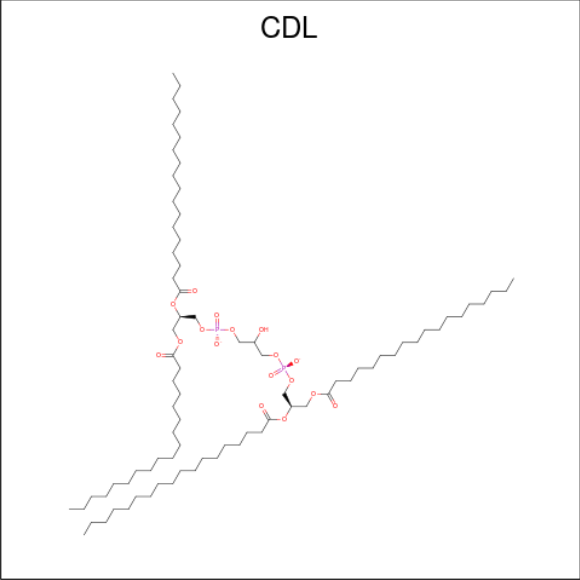
Mol	Chain	Residues	Atoms		AltConf
38	R	1	Total	Zn	0
			1	1	
38	R1	1	Total	Zn	0
			1	1	
38	i	1	Total	Zn	0
			1	1	
38	m	1	Total	Zn	0
			1	1	

- Molecule 39 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



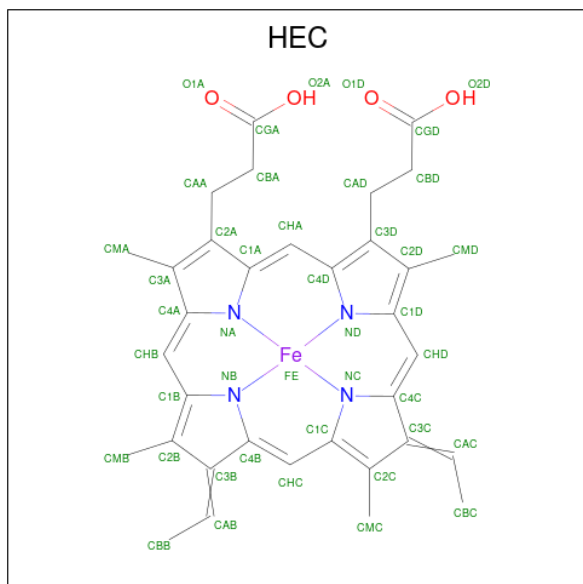
Mol	Chain	Residues	Atoms					AltConf
39	a	1	Total 43	C 34	Fe 1	N 4	O 4	0
39	a	1	Total 43	C 34	Fe 1	N 4	O 4	0
39	d	1	Total 43	C 34	Fe 1	N 4	O 4	0
39	d	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 40 is CARDIOLIPIN (CCD ID: CDL) (formula:  $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$ ).



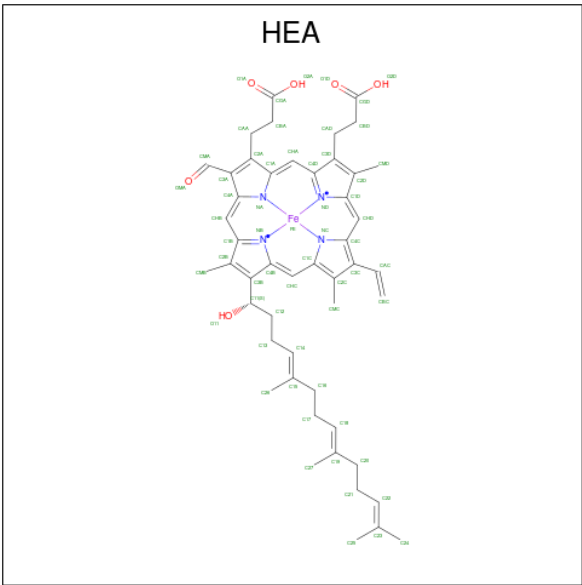
Mol	Chain	Residues	Atoms				AltConf
40	a	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 41 is HEME C (CCD ID: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
41	b	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
41	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 42 is HEME-A (CCD ID: HEA) (formula:  $C_{49}H_{56}FeN_4O_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
42	g	1	Total 60	C 49	Fe 1	N 4	O 6	0
42	g	1	Total 60	C 49	Fe 1	N 4	O 6	0
42	k	1	Total 60	C 49	Fe 1	N 4	O 6	0
42	k	1	Total 60	C 49	Fe 1	N 4	O 6	0

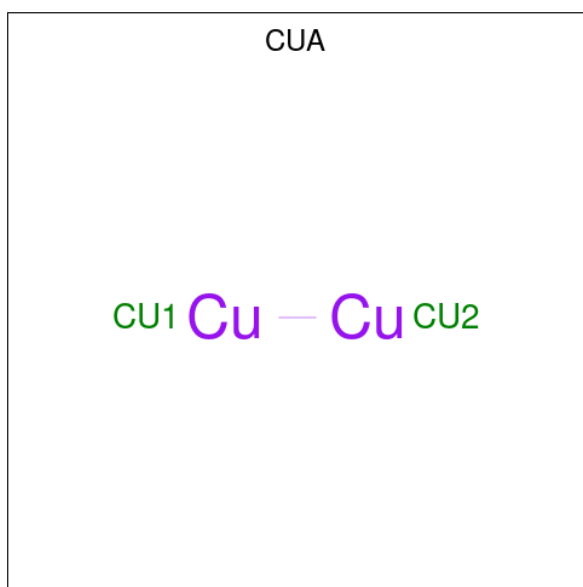
- Molecule 43 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
43	g	1	Total	Cu	0
			1	1	
43	k	1	Total	Cu	0
			1	1	

- Molecule 44 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
44	g	1	Total	Mn	0
			1	1	
44	k	1	Total	Mn	0
			1	1	

- Molecule 45 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu<sub>2</sub>).



Mol	Chain	Residues	Atoms		AltConf
45	h	1	Total 2	Cu 2	0
45	l	1	Total 2	Cu 2	0

### 3 Residue-property plots [i](#)

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

Chain A: 




- Molecule 1: NADH-quinone oxidoreductase subunit A

Chain A1: 




- Molecule 2: NADH-quinone oxidoreductase subunit B

Chain B: 




- Molecule 2: NADH-quinone oxidoreductase subunit B

Chain B1: 



- Molecule 3: NADH-quinone oxidoreductase subunit C

Chain C: 



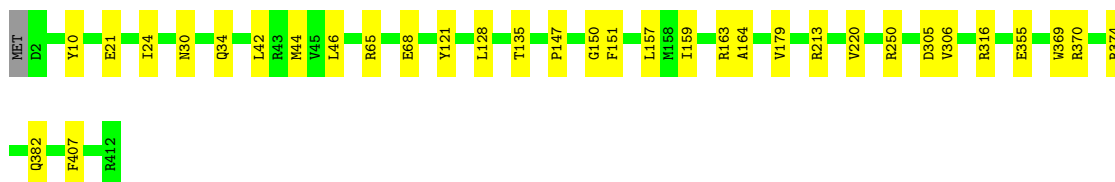
- Molecule 3: NADH-quinone oxidoreductase subunit C

Chain C1: 



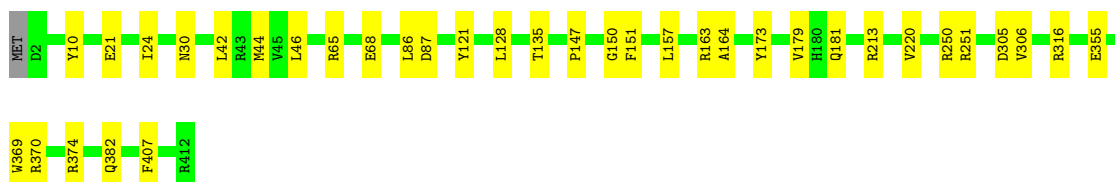
- Molecule 4: NADH-quinone oxidoreductase subunit D

Chain D: 92% 8%



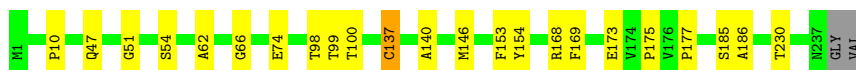
- Molecule 4: NADH-quinone oxidoreductase subunit D

Chain D1: 91% 9%



- Molecule 5: NADH dehydrogenase subunit E

Chain E: 90% 9%



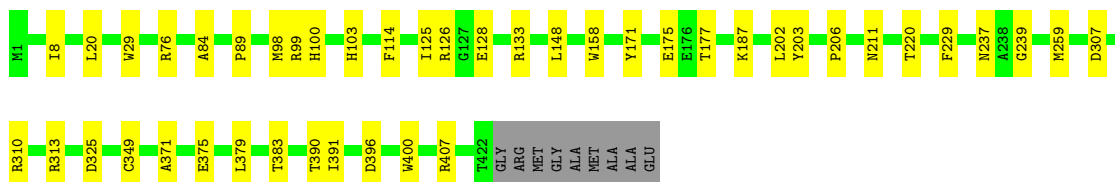
- Molecule 5: NADH dehydrogenase subunit E

Chain E1: 92% 7%




- Molecule 6: NADH-quinone oxidoreductase subunit F

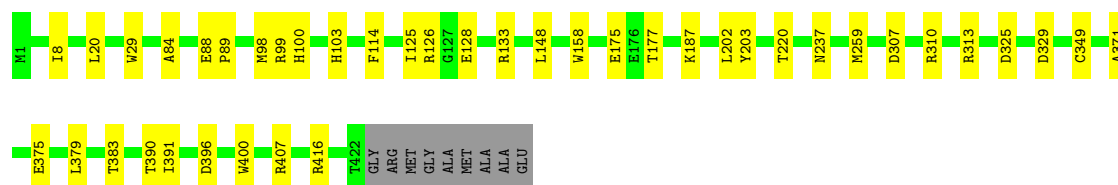
Chain F: 88% 10%



- Molecule 6: NADH-quinone oxidoreductase subunit F

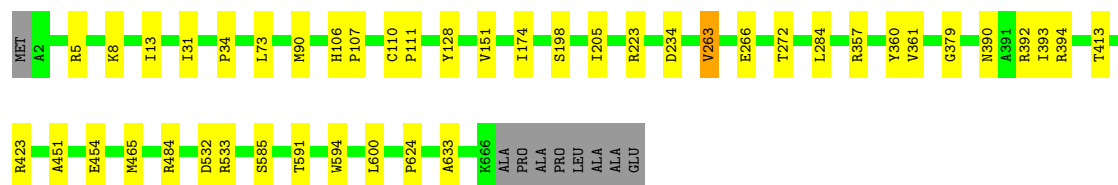


Chain F1:  88% 10% .



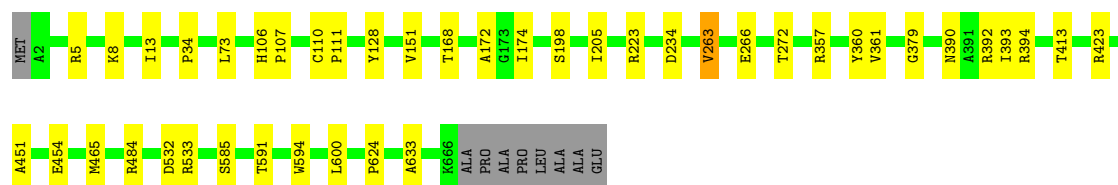
• Molecule 7: NADH-quinone oxidoreductase

Chain G:  92% 6% .



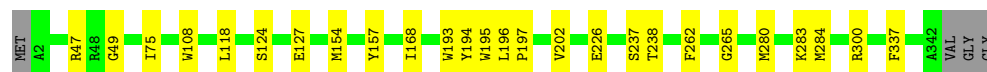
• Molecule 7: NADH-quinone oxidoreductase

Chain G1:  92% 6% .



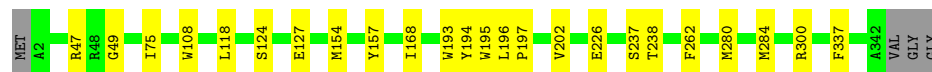
• Molecule 8: NADH-quinone oxidoreductase subunit H

Chain H:  91% 8% .




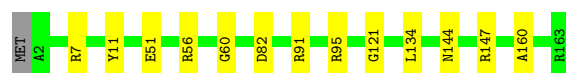
• Molecule 8: NADH-quinone oxidoreductase subunit H

Chain H1:  92% 7% .



• Molecule 9: NADH-quinone oxidoreductase subunit I

Chain I:  91% 8% .



- Molecule 9: NADH-quinone oxidoreductase subunit I

Chain I1:  93% 7%



- Molecule 10: NADH-quinone oxidoreductase subunit J

Chain J:  96%



- Molecule 10: NADH-quinone oxidoreductase subunit J

Chain J1:  97%



- Molecule 11: NADH-quinone oxidoreductase subunit K

Chain K:  93% 6%




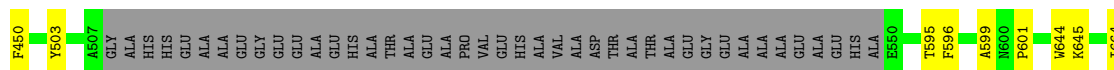
- Molecule 11: NADH-quinone oxidoreductase subunit K

Chain K1:  92% 7%



- Molecule 12: NADH dehydrogenase subunit L

Chain L:  88% 6% 6%



- Molecule 12: NADH dehydrogenase subunit L

W644 K645	F447	M1
I664 P665	F450	R78
H703	Y503	D105
	A507	D106
	GLY	N107
	ALA	S196
	HIS	E201
	HIS	T202
	GLU	F203
	ALA	V206
	GLU	M236
	GLY	Q241
	GLU	V258
	HIS	L262
	ALA	T266
	THR	C276
	ALA	S279
	VAL	P280
	GLU	D312
	HIS	M341
	ALA	F342
	VAL	H343
	ASP	H347
	THR	F350
	ALA	E368
	GLU	Q369
	GLY	Y374
	GLU	R378
	ALA	G399
	ALA	F410
	E550	L411
	T595	S412
	F596	T438
	A599	Y441
	M600	S442
	P601	W443
	L614	

H365	T366	M379	Y382	S430	Y433	T458	P459	M471	A503	ALA	PRO	VAL	VAL	G83	W104	Y137	T145	P146	G152	T153	W154	R159	L178	D200	P234	P237	V238	H239	L257	L261	M276	T277	P278	D308	A309	K310	Y361	M364
------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

M364	M365	T366	M379	Y382	S430	Y433	T458	P459	M471	M503	ALA	PRO	VAL	ALA	THR	ALA	GLN	ALA	SER	HIS															
M1	L11	P12	D27	E28	K35	T45	V66	W71	I72	W79	D82	G83	W104	Y137	I145	P146	I153	W154	L178	D200	P234	P237	V238	H239	L257	L261	M276	P277	P278	V288	D308	K309	K310	F329	Y361

[illegible]

PRO	VAL	GLN	GLY	GLU
#1	T37	V41	A62	G66
			V88	E105
			Y130	L133
			L172	E188
			F216	K217
			W226	L266
			W269	R296
			R347	P383
			F388	M441
			L449	D467
			P480	VAL
				ALA
				ALA
				ILE
				GLU
				GLN
				PRO
				ALA
				GLU
				ALA
				ALA
				GLN
				ALA
				GLU

- Molecule 15: NAD-dependent epimerase/dehydratase

Chain P:  95% ..



- Molecule 15: NAD-dependent epimerase/dehydratase

Chain P1:  95% ..



- Molecule 16: ETC complex I subunit conserved region

Chain Q:  96% ..



- Molecule 16: ETC complex I subunit conserved region

Chain Q1:  96% ..



- Molecule 17: Zinc finger CHCC-type domain-containing protein

Chain R:  92% 6% .



- Molecule 17: Zinc finger CHCC-type domain-containing protein

Chain R1:  92% 6% .

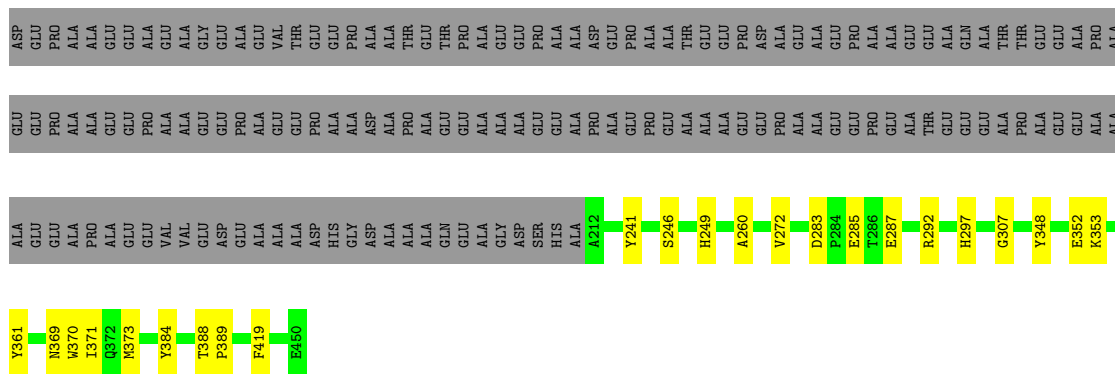


- Molecule 18: Protein-L-isoaspartate O-methyltransferase

Chain Z:  97% .

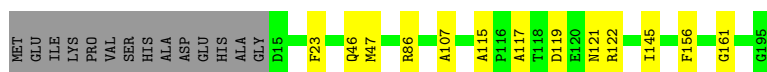


- |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | LEU | ARG | ASN | ALA | SER | LEU | THR | ALA | VAL | ALA | LEU | GLY | GLY | ALA | VAL | VAL | GLN | ASP | SER | THR | ALA | PRO | GLY | GLY | THR | THR | ALA | ALA | PRO | ALA | ALA | ALA | ASP | THR | ALA | PRO | ALA | ALA | GLU | ALA | ALA | PRO | GLU | ALA | ALA |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|



• Molecule 21: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain c: 86% 7% 7%



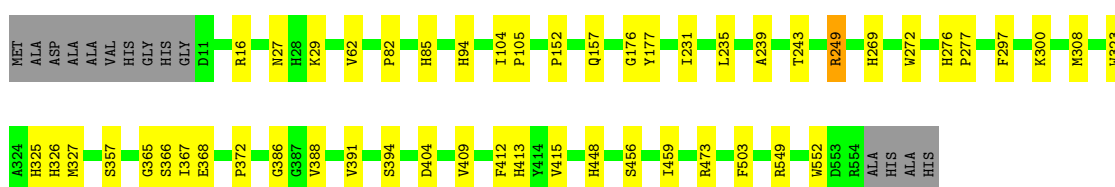
• Molecule 21: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain f: 86% 7% 7%



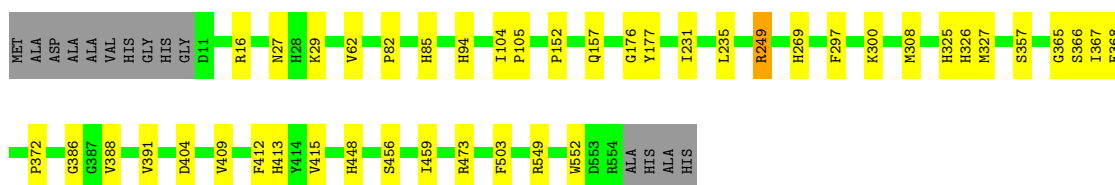
• Molecule 22: Cytochrome c oxidase subunit 1

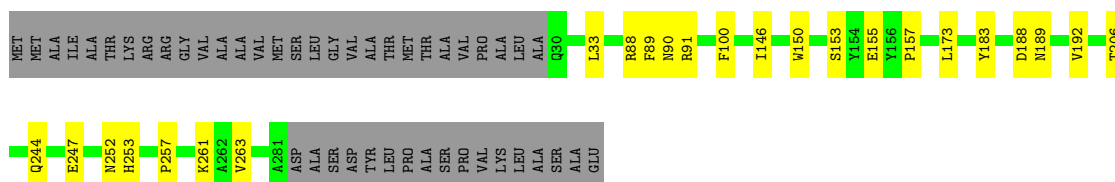
Chain g: 88% 9% 3%



• Molecule 22: Cytochrome c oxidase subunit 1

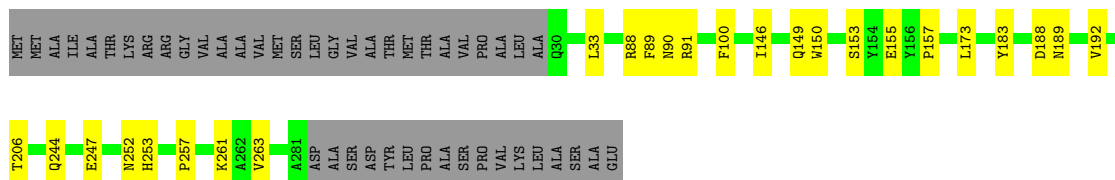
Chain k: 90% 8% 2%





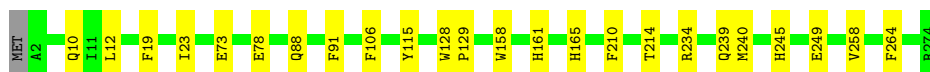
- Molecule 23: Cytochrome c oxidase subunit 2

Chain l:



- Molecule 24: cytochrome-c oxidase

Chain i:



- Molecule 24: cytochrome-c oxidase

Chain m:



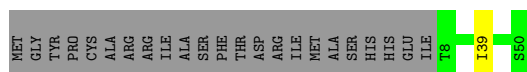
- Molecule 25: Aa3 type cytochrome c oxidase subunit IV

Chain j:



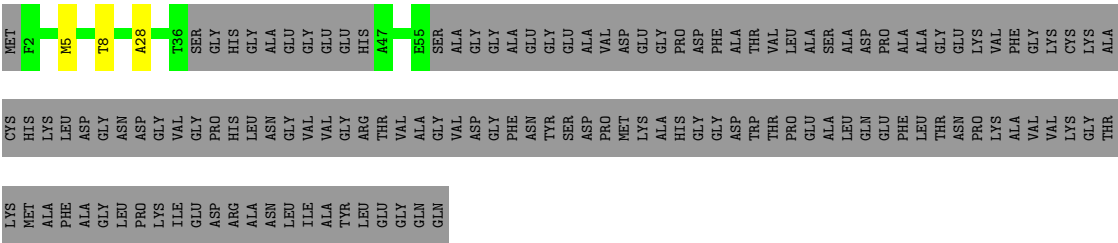
- Molecule 25: Aa3 type cytochrome c oxidase subunit IV

Chain n:

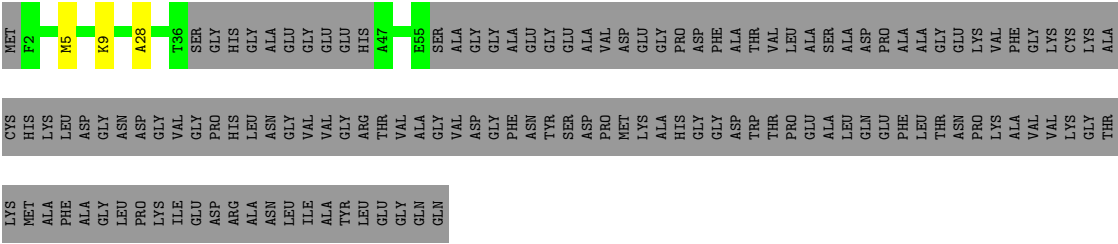


- Molecule 26: Cytochrome c, class I

Chain o:



• Molecule 26: Cytochrome c, class I



• Molecule 27: NADH:ubiquinone oxidoreductase 17.2 kD subunit



• Molecule 27: NADH:ubiquinone oxidoreductase 17.2 kD subunit





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	3002	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	55.2	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, CDL, HEM, 2MR, HEC, FES, ZN, U10, CU, MN, CA, PC1, P5S, FME, 3PH, DU0, CUA, SF4, HEA, FMN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.27	0/988	0.54	0/1345
1	A1	0.27	0/988	0.54	0/1345
2	B	0.33	0/1297	0.66	0/1758
2	B1	0.33	0/1297	0.66	0/1758
3	C	0.29	0/1624	0.68	0/2208
3	C1	0.29	0/1624	0.68	0/2208
4	D	0.28	0/3339	0.60	0/4520
4	D1	0.28	0/3339	0.60	0/4520
5	E	0.23	0/1865	0.61	0/2537
5	E1	0.23	0/1865	0.61	0/2537
6	F	0.23	0/3308	0.62	0/4456
6	F1	0.23	0/3308	0.62	0/4456
7	G	0.24	0/5156	0.64	0/6982
7	G1	0.24	0/5156	0.64	0/6982
8	H	0.30	0/2815	0.61	0/3837
8	H1	0.30	0/2815	0.60	0/3837
9	I	0.29	0/1354	0.59	0/1828
9	I1	0.29	0/1354	0.59	0/1828
10	J	0.29	0/1548	0.59	0/2104
10	J1	0.29	0/1548	0.60	0/2104
11	K	0.33	0/775	0.58	1/1050 (0.1%)
11	K1	0.33	0/775	0.58	1/1050 (0.1%)
12	L	0.27	0/5379	0.56	1/7323 (0.0%)
12	L1	0.27	0/5379	0.56	1/7323 (0.0%)
13	M	0.30	0/4010	0.59	0/5460
13	M1	0.30	0/4010	0.59	0/5460
14	N	0.30	0/3634	0.55	0/4935
14	N1	0.30	0/3634	0.55	0/4935
15	P	0.27	0/2511	0.62	0/3409
15	P1	0.27	0/2511	0.62	0/3409
16	Q	0.26	0/872	0.63	0/1181

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	Q1	0.26	0/872	0.63	0/1181
17	R	0.23	0/503	0.63	0/685
17	R1	0.22	0/503	0.64	0/685
18	Z	0.27	0/1669	0.62	0/2266
18	Z1	0.27	0/1669	0.62	0/2266
19	a	0.40	0/3650	0.59	0/5005
19	d	0.40	0/3650	0.59	0/5005
20	b	0.33	0/1906	0.62	0/2592
20	e	0.33	0/1906	0.62	0/2592
21	c	0.27	0/1390	0.56	0/1891
21	f	0.27	0/1390	0.56	0/1891
22	g	0.30	0/4483	0.63	0/6118
22	k	0.29	0/4483	0.61	0/6118
23	h	0.25	0/2033	0.60	0/2787
23	l	0.25	0/2033	0.60	0/2787
24	i	0.32	0/2270	0.55	0/3107
24	m	0.32	0/2270	0.55	0/3107
25	j	0.27	0/339	0.55	0/457
25	n	0.27	0/339	0.56	0/457
26	o	0.32	0/330	0.51	0/448
26	p	0.32	0/330	0.52	0/448
27	q	0.25	0/1049	0.62	0/1434
27	q1	0.25	0/1049	0.62	0/1434
All	All	0.29	0/120194	0.60	4/163446 (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
2	B	0	1
2	B1	0	1
4	D	0	1
4	D1	0	1
7	G	0	2
7	G1	0	2
9	I	0	2
9	I1	0	1
14	N	0	1
14	N1	0	1
16	Q	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	Q1	0	2
22	g	0	1
22	k	0	1
All	All	0	19

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K1	25	ASN	N-CA-C	5.82	119.56	112.23
11	K	25	ASN	N-CA-C	5.80	119.54	112.23
12	L	266	THR	N-CA-C	5.47	119.52	111.04
12	L1	266	THR	N-CA-C	5.45	119.49	111.04

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	134	ARG	Sidechain
2	B1	134	ARG	Sidechain
4	D	250	ARG	Sidechain
4	D1	250	ARG	Sidechain
7	G	223	ARG	Sidechain
7	G	484	ARG	Sidechain
7	G1	223	ARG	Sidechain
7	G1	484	ARG	Sidechain
9	I	7	ARG	Sidechain
9	I	91	ARG	Sidechain
9	I1	91	ARG	Sidechain
14	N	347	ARG	Sidechain
14	N1	347	ARG	Sidechain
16	Q	33	ARG	Sidechain
16	Q	80	ARG	Sidechain
16	Q1	33	ARG	Sidechain
16	Q1	80	ARG	Sidechain
22	g	249	ARG	Sidechain
22	k	249	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	969	0	970	9	0
1	A1	969	0	970	7	0
2	B	1270	0	1268	10	0
2	B1	1270	0	1268	8	0
3	C	1586	0	1562	9	0
3	C1	1586	0	1562	9	0
4	D	3277	0	3217	23	0
4	D1	3277	0	3217	24	0
5	E	1822	0	1796	14	0
5	E1	1822	0	1796	11	0
6	F	3241	0	3188	26	0
6	F1	3241	0	3188	24	0
7	G	5068	0	5037	21	0
7	G1	5068	0	5037	21	0
8	H	2722	0	2744	17	0
8	H1	2722	0	2744	16	0
9	I	1319	0	1259	7	0
9	I1	1319	0	1259	7	0
10	J	1528	0	1612	7	0
10	J1	1528	0	1612	6	0
11	K	764	0	817	4	0
11	K1	764	0	817	5	0
12	L	5215	0	5174	22	0
12	L1	5215	0	5174	24	0
13	M	3915	0	4024	25	0
13	M1	3915	0	4024	23	0
14	N	3556	0	3656	16	0
14	N1	3556	0	3656	12	0
15	P	2468	0	2498	9	0
15	P1	2468	0	2498	9	0
16	Q	849	0	812	1	0
16	Q1	849	0	812	1	0
17	R	488	0	450	2	0
17	R1	488	0	450	2	0
18	Z	1642	0	1643	3	0
18	Z1	1642	0	1643	4	0
19	a	3513	0	3489	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	d	3513	0	3489	25	0
20	b	1855	0	1773	14	0
20	e	1855	0	1773	15	0
21	c	1361	0	1301	8	0
21	f	1361	0	1301	8	0
22	g	4322	0	4225	31	0
22	k	4322	0	4225	27	0
23	h	1976	0	1960	16	0
23	l	1976	0	1960	17	0
24	i	2183	0	2144	19	0
24	m	2183	0	2144	15	0
25	j	332	0	331	2	0
25	n	332	0	331	1	0
26	o	324	0	330	3	0
26	p	324	0	330	4	0
27	q	1018	0	942	1	0
27	q1	1018	0	942	2	0
28	B	8	0	0	0	0
28	B1	8	0	0	0	0
28	F	8	0	0	1	0
28	F1	8	0	0	1	0
28	G	16	0	0	0	0
28	G1	16	0	0	0	0
28	I	16	0	0	0	0
28	I1	16	0	0	0	0
29	B	63	0	90	1	0
29	B1	63	0	90	0	0
29	a	126	0	180	15	0
29	d	126	0	180	12	0
30	D	1	0	0	0	0
30	D1	1	0	0	0	0
30	b	1	0	0	0	0
30	e	1	0	0	0	0
30	g	1	0	0	0	0
30	k	1	0	0	0	0
31	E	4	0	0	1	0
31	E1	4	0	0	1	0
31	G	4	0	0	0	0
31	G1	4	0	0	0	0
31	c	4	0	0	0	0
31	f	4	0	0	0	0
32	F	31	0	19	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	F1	31	0	19	1	0
33	H	54	0	88	1	0
33	H1	108	0	176	2	0
33	L1	54	0	88	0	0
33	M	54	0	88	0	0
33	M1	54	0	88	0	0
33	i	108	0	176	8	0
33	j	54	0	88	5	0
33	m	108	0	176	3	0
33	n	54	0	88	0	0
34	K	37	0	0	0	0
34	M	37	0	0	0	0
34	M1	37	0	0	0	0
34	a	37	0	0	0	0
34	d	37	0	0	0	0
35	L	51	0	82	0	0
35	L1	51	0	82	0	0
35	b	51	0	82	0	0
35	e	51	0	82	1	0
35	g	51	0	82	2	0
35	i	51	0	82	0	0
35	k	51	0	82	2	0
35	m	102	0	164	0	0
36	L	48	0	75	0	0
36	L1	48	0	75	0	0
36	f	48	0	75	0	0
36	g	48	0	75	0	0
36	k	48	0	75	0	0
36	p	48	0	75	0	0
37	L	54	0	80	0	0
37	L1	54	0	80	0	0
38	R	1	0	0	0	0
38	R1	1	0	0	0	0
38	i	1	0	0	0	0
38	m	1	0	0	0	0
39	a	86	0	60	4	0
39	d	86	0	60	4	0
40	a	100	0	156	1	0
41	b	43	0	30	1	0
41	e	43	0	30	1	0
42	g	120	0	108	2	0
42	k	120	0	108	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	g	1	0	0	0	0
43	k	1	0	0	0	0
44	g	1	0	0	0	0
44	k	1	0	0	0	0
45	h	2	0	0	0	0
45	l	2	0	0	0	0
All	All	120030	0	119978	622	0

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

All (622) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:HD11	11:K:71:ALA:HB3	1.67	0.76
1:A1:75:LEU:HD11	11:K1:71:ALA:HB3	1.67	0.76
29:a:1002:U10:H301	29:d:504:U10:H351	1.71	0.72
22:k:365:GLY:HA2	23:l:89:PHE:HB3	1.77	0.67
22:g:365:GLY:HA2	23:h:89:PHE:HB3	1.77	0.66
13:M1:430:SER:HA	13:M1:433:TYR:CE2	2.31	0.65
12:L:438:THR:HA	12:L:441:TYR:CE2	2.32	0.65
12:L1:438:THR:HA	12:L1:441:TYR:CE2	2.32	0.65
4:D1:44:MET:HE2	4:D1:46:LEU:HD21	1.79	0.65
22:k:448:HIS:CE1	22:k:503:PHE:HB2	2.32	0.64
35:k:607:3PE:H111	24:m:12:LEU:HD11	1.79	0.64
35:g:607:3PE:H111	24:i:12:LEU:HD11	1.79	0.64
22:g:448:HIS:CE1	22:g:503:PHE:HB2	2.32	0.64
4:D1:42:LEU:HB2	4:D1:407:PHE:CZ	2.33	0.64
13:M:430:SER:HA	13:M:433:TYR:CE2	2.31	0.64
22:k:176:GLY:O	22:k:249:ARG:NH2	2.30	0.64
4:D:42:LEU:HB2	4:D:407:PHE:CZ	2.32	0.64
20:e:353:LYS:HE2	20:e:370:TRP:CD2	2.34	0.63
4:D:44:MET:HE2	4:D:46:LEU:HD21	1.79	0.62
20:b:353:LYS:HE2	20:b:370:TRP:CD2	2.34	0.62
12:L1:347:HIS:HA	12:L1:350:PHE:CZ	2.34	0.62
12:L:347:HIS:HA	12:L:350:PHE:CZ	2.34	0.61
19:a:91:TYR:CE2	19:a:92:MET:HG2	2.35	0.61
22:g:176:GLY:O	22:g:249:ARG:NH2	2.33	0.61
19:d:294:PRO:HB3	29:d:501:U10:H3M1	1.82	0.61
24:i:210:PHE:O	24:i:214:THR:HG22	2.01	0.61
5:E1:98:THR:HG22	5:E1:99:THR:H	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:144:PHE:HB2	29:a:1002:U10:H1M3	1.83	0.61
24:m:210:PHE:O	24:m:214:THR:HG22	2.00	0.61
19:d:91:TYR:CE2	19:d:92:MET:HG2	2.35	0.60
29:a:1002:U10:H563	19:d:204:VAL:HG13	1.82	0.60
22:g:308:MET:HE3	22:g:357:SER:HB2	1.84	0.60
13:M:257:LEU:HA	13:M:261:LEU:HD12	1.84	0.60
22:k:308:MET:HE3	22:k:357:SER:HB2	1.84	0.60
7:G:5:ARG:NH2	7:G:73:LEU:O	2.26	0.60
22:k:62:VAL:HG21	22:k:82:PRO:HB3	1.84	0.59
13:M1:257:LEU:HA	13:M1:261:LEU:HD12	1.84	0.59
5:E:98:THR:HG22	5:E:99:THR:H	1.66	0.59
7:G:585:SER:OG	7:G:591:THR:HA	2.03	0.58
1:A1:115:LYS:NZ	14:N1:105:GLU:OE2	2.34	0.58
12:L:644:TRP:CZ3	12:L:645:LYS:HE2	2.39	0.58
7:G1:585:SER:OG	7:G1:591:THR:HA	2.03	0.58
6:F1:379:LEU:O	6:F1:383:THR:HG23	2.04	0.58
24:i:115:TYR:CE1	33:i:304:PC1:H143	2.38	0.58
1:A:115:LYS:NZ	14:N:105:GLU:OE2	2.34	0.58
6:F:379:LEU:O	6:F:383:THR:HG23	2.04	0.57
19:d:162:ILE:HG13	29:d:501:U10:H3M3	1.85	0.57
3:C1:151:LYS:HE3	4:D1:369:TRP:CZ2	2.39	0.57
3:C:151:LYS:HE3	4:D:369:TRP:CZ2	2.39	0.57
12:L1:644:TRP:CZ3	12:L1:645:LYS:HE2	2.39	0.57
22:g:62:VAL:HG21	22:g:82:PRO:HB3	1.86	0.57
22:g:231:ILE:HG23	22:g:235:LEU:HD12	1.85	0.57
9:I:51:GLU:O	9:I:121:GLY:N	2.36	0.57
21:c:46:GLN:HE22	21:c:47:MET:HG3	1.70	0.57
20:e:292:ARG:NH1	20:e:297:HIS:O	2.36	0.57
3:C:165:ASP:OD1	3:C:168:LYS:NZ	2.34	0.56
3:C1:165:ASP:O	3:C1:168:LYS:NZ	2.35	0.56
21:f:145:ILE:N	21:f:156:PHE:O	2.38	0.56
14:N:441:MET:HE1	14:N:449:LEU:HD22	1.87	0.56
22:g:16:ARG:HH11	22:g:16:ARG:HG3	1.70	0.56
6:F:99:ARG:HG3	6:F:100:HIS:CD2	2.41	0.56
22:g:409:VAL:HA	22:g:412:PHE:CE2	2.41	0.56
9:I1:144:ASN:OD1	9:I1:147:ARG:NH2	2.33	0.56
25:j:49:ASN:HD22	33:j:1001:PC1:C31	2.19	0.56
21:f:46:GLN:HE22	21:f:47:MET:HG3	1.70	0.55
27:q:47:ARG:NH1	27:q:67:TRP:O	2.34	0.55
12:L1:595:THR:HA	12:L1:599:ALA:HB3	1.88	0.55
22:k:16:ARG:HG3	22:k:16:ARG:HH11	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:k:409:VAL:HA	22:k:412:PHE:CE2	2.41	0.55
6:F1:99:ARG:HG3	6:F1:100:HIS:CD2	2.41	0.55
9:I1:51:GLU:O	9:I1:121:GLY:N	2.36	0.55
4:D:163:ARG:HG2	4:D:163:ARG:HH11	1.72	0.55
29:a:1002:U10:H562	19:d:207:ALA:HB3	1.89	0.55
7:G:423:ARG:NH2	7:G:454:GLU:OE1	2.29	0.55
13:M1:71:TRP:CG	13:M1:72:ILE:H	2.25	0.55
14:N1:441:MET:HE1	14:N1:449:LEU:HD22	1.87	0.55
22:k:231:ILE:HG23	22:k:235:LEU:HD12	1.89	0.55
6:F1:29:TRP:CE2	6:F1:148:LEU:HD13	2.42	0.55
2:B1:47:TRP:CZ2	2:B1:76:PRO:HB3	2.42	0.54
8:H:202:VAL:HG22	8:H:262:PHE:CD1	2.42	0.54
12:L:595:THR:HA	12:L:599:ALA:HB3	1.89	0.54
15:P:213:LEU:HB3	15:P:290:PHE:CZ	2.42	0.54
15:P1:213:LEU:HB3	15:P1:290:PHE:CZ	2.42	0.54
3:C:160:GLU:O	3:C:173:GLU:N	2.38	0.54
4:D1:220:VAL:HG11	10:J1:179:GLN:HA	1.90	0.54
20:b:292:ARG:NH1	20:b:297:HIS:O	2.36	0.54
20:b:348:TYR:OH	20:b:373:MET:O	2.25	0.54
8:H1:202:VAL:HG22	8:H1:262:PHE:CD1	2.42	0.54
13:M:71:TRP:CD1	13:M:72:ILE:H	2.26	0.54
21:c:145:ILE:N	21:c:156:PHE:O	2.39	0.54
4:D1:163:ARG:HH11	4:D1:163:ARG:HG2	1.72	0.54
19:a:133:MET:HE1	19:a:343:MET:HE3	1.89	0.54
3:C1:160:GLU:O	3:C1:173:GLU:N	2.38	0.54
2:B:47:TRP:CZ2	2:B:76:PRO:HB3	2.42	0.54
6:F:175:GLU:OE1	6:F:177:THR:N	2.32	0.54
29:a:1002:U10:H411	29:d:504:U10:H251	1.89	0.54
3:C:151:LYS:HE3	4:D:369:TRP:CH2	2.43	0.54
6:F:29:TRP:CE2	6:F:148:LEU:HD13	2.43	0.53
19:d:133:MET:HE1	19:d:343:MET:HE3	1.89	0.53
24:i:115:TYR:CD2	33:i:304:PC1:H122	2.43	0.53
4:D:220:VAL:HG11	10:J:179:GLN:HA	1.90	0.53
12:L:347:HIS:HA	12:L:350:PHE:CE2	2.44	0.53
13:M1:71:TRP:CD1	13:M1:72:ILE:H	2.26	0.53
6:F1:8:ILE:HG12	6:F1:220:THR:HG21	1.90	0.53
9:I:56:ARG:NH1	9:I:60:GLY:O	2.38	0.53
3:C1:151:LYS:HE3	4:D1:369:TRP:CH2	2.44	0.53
13:M:71:TRP:CG	13:M:72:ILE:H	2.25	0.53
19:d:132:GLY:HA3	39:d:502:HEM:HBC2	1.91	0.53
23:l:146:ILE:HD11	23:l:206:THR:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:ARG:HG3	2:B:170:THR:HG23	1.91	0.53
2:B1:169:ARG:HG3	2:B1:170:THR:HG23	1.91	0.53
11:K1:101:GLY:O	14:N1:296:ARG:NH1	2.42	0.53
5:E:74:GLU:HB3	6:F:187:LYS:HE2	1.91	0.53
5:E1:74:GLU:HB3	6:F1:187:LYS:HE2	1.91	0.52
11:K:101:GLY:O	14:N:296:ARG:NH1	2.42	0.52
12:L1:347:HIS:HA	12:L1:350:PHE:CE2	2.43	0.52
19:a:132:GLY:HA3	39:a:1003:HEM:HBC2	1.90	0.52
20:e:348:TYR:OH	20:e:373:MET:O	2.25	0.52
22:g:368:GLU:OE2	23:h:91:ARG:NH1	2.38	0.52
3:C1:165:ASP:OD1	3:C1:168:LYS:NZ	2.34	0.52
12:L1:78:ARG:HD3	12:L1:503:TYR:CE2	2.45	0.52
3:C:165:ASP:O	3:C:168:LYS:NZ	2.34	0.52
9:I:144:ASN:OD1	9:I:147:ARG:NH2	2.33	0.52
23:h:146:ILE:HD11	23:h:206:THR:HG23	1.90	0.52
12:L:78:ARG:HD3	12:L:503:TYR:CE2	2.45	0.52
3:C:59:PHE:CE1	3:C:90:GLN:HG3	2.45	0.51
24:i:10:GLN:HG3	24:i:78:GLU:HG3	1.92	0.51
27:q1:47:ARG:NH1	27:q1:67:TRP:O	2.34	0.51
19:a:162:ILE:HG13	29:a:1002:U10:H3M3	1.92	0.51
1:A1:46:GLU:HG3	4:D1:30:ASN:HD22	1.76	0.51
6:F:8:ILE:HG12	6:F:220:THR:HG21	1.91	0.51
24:i:245:HIS:CD2	24:i:249:GLU:OE1	2.63	0.51
1:A:46:GLU:HG3	4:D:30:ASN:HD22	1.76	0.51
13:M1:82:ASP:OD1	13:M1:83:GLY:N	2.43	0.51
33:i:304:PC1:H141	33:j:1001:PC1:H152	1.92	0.51
21:f:23:PHE:CD1	24:m:158:TRP:HH2	2.29	0.51
24:m:10:GLN:HG3	24:m:78:GLU:HG3	1.92	0.51
11:K1:28:ASN:OD1	11:K1:30:ILE:HG22	2.11	0.51
13:M:82:ASP:OD1	13:M:83:GLY:N	2.43	0.51
13:M:153:ILE:HB	13:M:154:TRP:CE3	2.46	0.51
13:M1:153:ILE:HB	13:M1:154:TRP:CE3	2.46	0.51
7:G1:5:ARG:NH2	7:G1:73:LEU:O	2.26	0.50
17:R:14:TRP:CZ3	17:R:37:ARG:HA	2.46	0.50
21:f:156:PHE:CE1	21:f:161:GLY:HA2	2.46	0.50
3:C1:59:PHE:CE1	3:C1:90:GLN:HG3	2.45	0.50
12:L:312:ASP:CG	12:L:369:GLN:HE21	2.19	0.50
13:M1:27:ASP:OD1	13:M1:28:GLU:N	2.45	0.50
2:B:68:ASP:OD1	8:H:47:ARG:NH1	2.38	0.50
6:F1:175:GLU:OE1	6:F1:177:THR:N	2.32	0.50
11:K:28:ASN:OD1	11:K:30:ILE:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:e:285:GLU:CD	20:e:285:GLU:H	2.20	0.50
10:J:90:PRO:HB3	19:a:366:TRP:CZ3	2.47	0.50
20:b:285:GLU:CD	20:b:285:GLU:H	2.20	0.50
22:g:27:ASN:OD1	22:g:29:LYS:HG2	2.12	0.50
21:f:115:ALA:HB1	21:f:121:ASN:CG	2.37	0.50
22:g:325:HIS:CD2	22:g:326:HIS:CD2	2.99	0.50
29:B:1002:U10:H321	29:B:1002:U10:H552	1.94	0.49
2:B1:58:GLU:O	2:B1:62:THR:HG23	2.12	0.49
10:J1:90:PRO:HB3	19:d:366:TRP:CZ3	2.47	0.49
12:L:236:MET:HG3	12:L:241:GLN:HB2	1.93	0.49
12:L1:312:ASP:CG	12:L1:369:GLN:HE21	2.19	0.49
13:M:27:ASP:OD1	13:M:28:GLU:N	2.45	0.49
17:R1:14:TRP:CZ3	17:R1:37:ARG:HA	2.46	0.49
9:I1:56:ARG:NH1	9:I1:60:GLY:O	2.38	0.49
19:d:244:PHE:CE2	29:d:504:U10:H3M2	2.48	0.49
23:h:150:TRP:CD2	23:h:252:ASN:HB2	2.48	0.49
22:k:368:GLU:OE2	23:l:91:ARG:NH1	2.38	0.49
21:c:156:PHE:CE1	21:c:161:GLY:HA2	2.47	0.49
2:B:58:GLU:O	2:B:62:THR:HG23	2.12	0.49
19:d:403:TYR:HA	19:d:407:ILE:HD12	1.93	0.49
20:e:283:ASP:O	20:e:287:GLU:N	2.45	0.49
12:L:378:ARG:HB3	12:L:450:PHE:HB3	1.94	0.49
12:L1:236:MET:HG3	12:L1:241:GLN:HB2	1.93	0.49
13:M:276:MET:C	13:M:278:PRO:HD3	2.38	0.49
5:E:230:THR:O	5:E:230:THR:HG22	2.13	0.49
23:l:150:TRP:CD2	23:l:252:ASN:HB2	2.48	0.49
33:m:303:PC1:H2G1	25:n:39:ILE:HD11	1.93	0.49
3:C:123:ASP:OD1	3:C:137:ARG:NH1	2.41	0.49
5:E1:100:THR:HB	31:E1:401:FES:S1	2.53	0.49
21:c:115:ALA:HB1	21:c:121:ASN:CG	2.37	0.49
19:a:403:TYR:HA	19:a:407:ILE:HD12	1.94	0.48
14:N1:216:PHE:CE1	14:N1:226:TRP:CD1	3.01	0.48
19:d:121:TYR:OH	19:d:350:ASP:OD2	2.29	0.48
22:g:297:PHE:CE2	22:g:372:PRO:HB2	2.48	0.48
22:k:27:ASN:OD1	22:k:29:LYS:HG2	2.12	0.48
5:E1:230:THR:O	5:E1:230:THR:HG22	2.13	0.48
24:i:115:TYR:CD1	33:i:304:PC1:H132	2.48	0.48
12:L1:378:ARG:HB3	12:L1:450:PHE:HB3	1.94	0.48
13:M:145:ILE:HB	13:M:146:PRO:HD3	1.96	0.48
16:Q:2:ARG:NE	16:Q:73:GLU:OE1	2.40	0.48
19:a:302:TYR:HA	29:a:1002:U10:H4M1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:k:605:HEA:OMA	42:k:605:HEA:HHB	2.13	0.48
26:p:5:MET:HG3	26:p:9:LYS:HE2	1.96	0.48
7:G1:8:LYS:HE2	7:G1:13:ILE:HD11	1.96	0.48
8:H1:154:MET:HA	8:H1:157:TYR:CE2	2.49	0.48
3:C1:123:ASP:OD1	3:C1:137:ARG:NH1	2.41	0.48
8:H:154:MET:HA	8:H:157:TYR:CE2	2.49	0.48
14:N:216:PHE:CE1	14:N:226:TRP:CD1	3.02	0.48
6:F:211:ASN:ND2	32:F:502:FMN:O2	2.45	0.48
13:M1:276:MET:C	13:M1:278:PRO:HD3	2.38	0.48
18:Z1:54:ASP:OD1	18:Z1:54:ASP:N	2.47	0.48
5:E:100:THR:HB	31:E:401:FES:S1	2.53	0.48
7:G1:465:MET:SD	7:G1:624:PRO:HA	2.54	0.48
15:P1:190:TYR:CE2	15:P1:192:GLU:HB3	2.49	0.48
4:D1:305:ASP:OD2	4:D1:316:ARG:NH1	2.47	0.48
22:g:386:GLY:HA3	22:g:415:VAL:HG13	1.95	0.48
22:k:456:SER:HA	22:k:459:ILE:HD12	1.95	0.48
7:G:465:MET:SD	7:G:624:PRO:HA	2.54	0.47
14:N:130:TYR:CZ	14:N:172:LEU:HD11	2.49	0.47
18:Z1:166:ARG:HD2	18:Z1:167:GLU:O	2.13	0.47
24:m:234:ARG:NH2	24:m:240:MET:SD	2.87	0.47
4:D1:21:GLU:HA	4:D1:24:ILE:HD12	1.95	0.47
6:F1:396:ASP:HB3	6:F1:400:TRP:CZ2	2.49	0.47
8:H:280:MET:HG3	8:H:284:MET:HE2	1.96	0.47
19:d:144:PHE:HB2	29:d:501:U10:H1M3	1.96	0.47
22:k:104:ILE:HB	22:k:105:PRO:HD3	1.97	0.47
22:k:269:HIS:HA	22:k:327:MET:HE1	1.96	0.47
13:M1:145:ILE:HB	13:M1:146:PRO:HD3	1.96	0.47
14:N1:130:TYR:CZ	14:N1:172:LEU:HD11	2.49	0.47
18:Z:54:ASP:OD1	18:Z:54:ASP:N	2.46	0.47
22:g:456:SER:HA	22:g:459:ILE:HD12	1.95	0.47
24:m:154:VAL:HG13	26:o:8:THR:HG23	1.97	0.47
24:m:245:HIS:CD2	24:m:249:GLU:OE1	2.67	0.47
4:D:21:GLU:HA	4:D:24:ILE:HD12	1.96	0.47
1:A1:64:TYR:OH	11:K1:86:ARG:NH2	2.45	0.47
24:i:234:ARG:NH2	24:i:240:MET:SD	2.87	0.47
6:F:396:ASP:HB3	6:F:400:TRP:CZ2	2.49	0.47
7:G:8:LYS:HE2	7:G:13:ILE:HD11	1.96	0.47
9:I1:160:ALA:HB1	17:R1:24:ARG:HD3	1.96	0.47
15:P:190:TYR:CE2	15:P:192:GLU:HB3	2.49	0.47
22:k:297:PHE:CE2	22:k:372:PRO:HB2	2.48	0.47
1:A1:81:PHE:CZ	8:H1:118:LEU:HD21	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:305:ASP:OD2	4:D:316:ARG:NH1	2.47	0.47
6:F1:390:THR:HB	28:F1:502:SF4:S4	2.55	0.47
7:G:532:ASP:CG	7:G:533:ARG:H	2.23	0.47
7:G1:423:ARG:NH2	7:G1:454:GLU:OE1	2.29	0.47
14:N:133:LEU:HD21	14:N:217:LYS:HE3	1.96	0.47
24:m:128:TRP:HA	24:m:129:PRO:C	2.39	0.47
6:F:349:CYS:HB3	6:F:391:ILE:HD12	1.97	0.47
6:F1:237:ASN:HB3	6:F1:259:MET:HE2	1.97	0.47
7:G1:532:ASP:CG	7:G1:533:ARG:H	2.23	0.47
9:I:160:ALA:HB1	17:R:24:ARG:HD3	1.96	0.47
18:Z:166:ARG:HD2	18:Z:167:GLU:O	2.13	0.47
19:a:2:ALA:N	40:a:1006:CDL:OA3	2.48	0.47
13:M:237:PRO:C	13:M:239:HIS:H	2.23	0.47
19:a:197:LEU:HD21	29:a:1002:U10:H252	1.96	0.47
20:e:249:HIS:CE1	20:e:307:GLY:HA3	2.50	0.47
42:g:605:HEA:HBB	42:g:605:HEA:OMA	2.13	0.47
24:m:239:GLN:O	33:m:302:PC1:H121	2.15	0.47
6:F1:349:CYS:HB3	6:F1:391:ILE:HD12	1.97	0.47
13:M1:237:PRO:C	13:M1:239:HIS:H	2.23	0.46
4:D1:135:THR:HB	4:D1:147:PRO:HA	1.97	0.46
24:m:158:TRP:CG	26:o:5:MET:HE1	2.50	0.46
6:F1:20:LEU:HD13	6:F1:103:HIS:CE1	2.51	0.46
12:L:203:PHE:HA	12:L:206:VAL:HG23	1.97	0.46
12:L1:203:PHE:HA	12:L1:206:VAL:HG23	1.96	0.46
12:L1:276:CYS:SG	12:L1:341:MET:HE3	2.55	0.46
15:P1:31:ILE:HB	15:P1:53:VAL:HG13	1.97	0.46
24:i:128:TRP:HA	24:i:129:PRO:C	2.39	0.46
24:i:158:TRP:CZ2	26:p:9:LYS:HG2	2.50	0.46
24:i:239:GLN:O	33:i:301:PC1:H121	2.15	0.46
6:F:20:LEU:HD13	6:F:103:HIS:CE1	2.51	0.46
6:F:237:ASN:HB3	6:F:259:MET:HE2	1.97	0.46
14:N:266:ILE:HA	14:N:269:TRP:NE1	2.30	0.46
22:g:388:VAL:O	22:g:391:VAL:HG22	2.15	0.46
12:L:276:CYS:SG	12:L:341:MET:HE3	2.56	0.46
22:k:388:VAL:O	22:k:391:VAL:HG22	2.15	0.46
7:G1:151:VAL:HG22	7:G1:205:ILE:HD11	1.97	0.46
14:N1:266:ILE:HA	14:N1:269:TRP:NE1	2.30	0.46
35:g:607:3PE:N	24:i:73:GLU:OE1	2.42	0.46
23:h:173:LEU:HD11	23:h:183:TYR:HA	1.98	0.46
1:A:81:PHE:CZ	8:H:118:LEU:HD21	2.50	0.46
20:b:283:ASP:O	20:b:287:GLU:N	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N1:133:LEU:HD21	14:N1:217:LYS:HE3	1.97	0.46
22:g:152:PRO:HD2	22:g:177:TYR:CZ	2.50	0.46
24:i:106:PHE:CE2	24:i:264:PHE:HB3	2.51	0.46
35:k:607:3PE:N	24:m:73:GLU:OE1	2.42	0.46
5:E:169:PHE:CZ	5:E:175:PRO:HD2	2.51	0.46
15:P:31:ILE:HB	15:P:53:VAL:HG13	1.97	0.46
20:b:249:HIS:CE1	20:b:307:GLY:HA3	2.50	0.46
24:i:161:HIS:CE1	24:i:165:HIS:CD2	3.04	0.46
22:k:300:LYS:NZ	23:l:100:PHE:O	2.49	0.46
8:H1:280:MET:HG3	8:H1:284:MET:HE2	1.97	0.46
13:M1:234:PRO:HB2	13:M1:239:HIS:HA	1.98	0.46
19:a:162:ILE:CG1	29:a:1002:U10:H3M3	2.46	0.46
2:B1:71:ARG:HA	8:H1:49:GLY:HA3	1.97	0.45
6:F:390:THR:HB	28:F:501:SF4:S2	2.55	0.45
7:G:594:TRP:CZ2	7:G:600:LEU:HD13	2.51	0.45
19:a:212:HIS:CE1	39:a:1003:HEM:NC	2.84	0.45
21:c:23:PHE:CD1	24:i:158:TRP:HH2	2.34	0.45
20:e:419:PHE:CD1	26:o:28:ALA:HB2	2.51	0.45
22:g:404:ASP:HA	22:g:473:ARG:HD3	1.98	0.45
23:l:173:LEU:HD11	23:l:183:TYR:HA	1.98	0.45
7:G:423:ARG:NH1	7:G:633:ALA:O	2.50	0.45
33:H1:1001:PC1:H133	10:J1:180:MET:HE1	1.98	0.45
13:M:308:ASP:OD1	13:M:310:LYS:N	2.49	0.45
4:D:135:THR:HG21	4:D:150:GLY:HA3	1.98	0.45
7:G1:423:ARG:NH1	7:G1:633:ALA:O	2.50	0.45
7:G1:594:TRP:CZ2	7:G1:600:LEU:HD13	2.51	0.45
10:J1:170:ASP:OD1	10:J1:170:ASP:N	2.49	0.45
13:M1:308:ASP:OD1	13:M1:310:LYS:N	2.49	0.45
24:i:88:GLN:HA	24:i:91:PHE:CE2	2.52	0.45
22:k:152:PRO:HD2	22:k:177:TYR:CZ	2.52	0.45
5:E:168:ARG:HE	5:E:173:GLU:CD	2.23	0.45
12:L1:78:ARG:HD3	12:L1:503:TYR:CZ	2.51	0.45
7:G:151:VAL:HG22	7:G:205:ILE:HD11	1.97	0.45
7:G1:263:VAL:O	7:G1:392:ARG:NH1	2.48	0.45
8:H:193:TRP:HB2	8:H:195:TRP:CD1	2.52	0.45
22:k:325:HIS:CD2	22:k:326:HIS:CD2	3.04	0.45
5:E1:168:ARG:HE	5:E1:173:GLU:CD	2.24	0.45
5:E1:169:PHE:CZ	5:E1:175:PRO:HD2	2.51	0.45
8:H:237:SER:OG	8:H:238:THR:N	2.50	0.45
12:L1:399:GLY:HA3	12:L1:410:PHE:CD2	2.52	0.45
13:M:234:PRO:HB2	13:M:239:HIS:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H1:193:TRP:HB2	8:H1:195:TRP:CD1	2.51	0.45
13:M1:458:THR:HB	13:M1:459:PRO:HD2	1.99	0.45
19:a:121:TYR:OH	19:a:350:ASP:OD2	2.29	0.45
19:a:203:PHE:CD1	29:a:1002:U10:H503	2.52	0.45
29:a:1002:U10:H512	29:d:501:U10:H501	1.98	0.45
22:g:104:ILE:HB	22:g:105:PRO:HD3	1.98	0.45
33:H:1001:PC1:H133	10:J:180:MET:HE1	1.98	0.45
22:k:404:ASP:HA	22:k:473:ARG:HD3	1.98	0.45
12:L:78:ARG:HD3	12:L:503:TYR:CZ	2.51	0.45
29:a:1002:U10:H502	19:d:203:PHE:HB3	1.98	0.45
20:e:371:ILE:HG12	20:e:373:MET:H	1.82	0.45
7:G:174:ILE:HG21	7:G:198:SER:HB2	1.98	0.45
7:G:263:VAL:O	7:G:392:ARG:NH1	2.48	0.45
13:M:361:TYR:O	13:M:365:HIS:HA	2.17	0.45
20:b:419:PHE:CD1	26:p:28:ALA:HB2	2.52	0.45
2:B:71:ARG:HA	8:H:49:GLY:HA3	1.98	0.44
22:g:272:TRP:O	22:g:323:TRP:HB2	2.16	0.44
22:g:391:VAL:O	22:g:394:SER:OG	2.33	0.44
4:D1:135:THR:HG21	4:D1:150:GLY:HA3	1.98	0.44
13:M:200:ASP:OD1	13:M:200:ASP:N	2.51	0.44
13:M1:361:TYR:O	13:M1:365:HIS:HA	2.17	0.44
24:m:161:HIS:CE1	24:m:165:HIS:CD2	3.05	0.44
5:E:47:GLN:O	5:E:51:GLY:N	2.48	0.44
7:G:34:PRO:HG3	7:G:128:TYR:CE2	2.52	0.44
8:H1:197:PRO:HG3	8:H1:337:PHE:CZ	2.52	0.44
12:L:399:GLY:HA3	12:L:410:PHE:CD2	2.52	0.44
19:a:294:PRO:HB3	29:a:1002:U10:H3M1	1.98	0.44
20:b:371:ILE:HG12	20:b:373:MET:H	1.82	0.44
22:g:269:HIS:HA	22:g:327:MET:HE1	2.00	0.44
4:D:135:THR:HB	4:D:147:PRO:HA	1.98	0.44
4:D:179:VAL:HG22	4:D:306:VAL:CG1	2.47	0.44
4:D1:179:VAL:HG22	4:D1:306:VAL:CG1	2.47	0.44
7:G:106:HIS:CG	7:G:107:PRO:HD2	2.53	0.44
7:G1:34:PRO:HG3	7:G1:128:TYR:CE2	2.52	0.44
8:H1:237:SER:OG	8:H1:238:THR:N	2.49	0.44
19:d:212:HIS:CE1	39:d:502:HEM:NC	2.86	0.44
23:h:146:ILE:HG23	23:h:153:SER:OG	2.18	0.44
23:l:146:ILE:HG23	23:l:153:SER:HG	1.82	0.44
1:A:45:TYR:OH	4:D:34:GLN:OE1	2.14	0.44
4:D:355:GLU:O	4:D:374:ARG:NH1	2.49	0.44
4:D1:121:TYR:OH	4:D1:164:ALA:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:458:THR:HB	13:M:459:PRO:HD2	1.99	0.44
15:P:182:ALA:HA	15:P:221:MET:HB3	2.00	0.44
20:e:384:TYR:CD2	20:e:388:THR:HB	2.52	0.44
22:g:448:HIS:NE2	22:g:503:PHE:HB2	2.31	0.44
7:G1:106:HIS:CG	7:G1:107:PRO:HD2	2.53	0.44
7:G1:174:ILE:HG21	7:G1:198:SER:HB2	1.98	0.44
14:N1:37:THR:O	14:N1:41:VAL:HG23	2.18	0.44
23:h:192:VAL:HA	23:h:261:LYS:O	2.18	0.44
23:h:244:GLN:HA	23:h:257:PRO:HA	2.00	0.44
24:m:88:GLN:HA	24:m:91:PHE:CE2	2.52	0.44
5:E1:146:MET:HE1	5:E1:153:PHE:CG	2.53	0.44
13:M1:200:ASP:OD1	13:M1:200:ASP:N	2.51	0.44
8:H:168:ILE:HD11	8:H:262:PHE:CE1	2.53	0.43
13:M:35:LYS:HB3	13:M:104:TRP:CZ3	2.53	0.43
15:P:118:SER:O	15:P:153:PRO:HD2	2.18	0.43
19:a:84:MET:SD	19:a:94:ARG:HD3	2.58	0.43
33:i:304:PC1:H142	33:j:1001:PC1:H122	1.99	0.43
22:k:448:HIS:NE2	22:k:503:PHE:HB2	2.32	0.43
8:H1:168:ILE:HD11	8:H1:262:PHE:CE1	2.53	0.43
12:L1:279:SER:N	12:L1:280:PRO:HD2	2.33	0.43
12:L1:664:ILE:HB	12:L1:665:PRO:HD3	2.01	0.43
14:N:37:THR:O	14:N:41:VAL:HG23	2.18	0.43
19:a:59:ILE:HA	39:a:1001:HEM:HAB	2.00	0.43
20:b:352:GLU:HG2	20:b:361:TYR:CD2	2.53	0.43
20:b:384:TYR:CD2	20:b:388:THR:HB	2.52	0.43
4:D:121:TYR:OH	4:D:164:ALA:HB2	2.18	0.43
5:E:137:CYS:SG	6:F:89:PRO:HA	2.58	0.43
7:G:357:ARG:HA	7:G:360:TYR:CE2	2.54	0.43
8:H:124:SER:HA	8:H:127:GLU:OE2	2.19	0.43
12:L1:596:PHE:O	12:L1:601:PRO:HA	2.18	0.43
24:i:115:TYR:CE2	33:i:304:PC1:H122	2.54	0.43
23:l:192:VAL:HA	23:l:261:LYS:O	2.18	0.43
8:H:197:PRO:HG3	8:H:337:PHE:CZ	2.53	0.43
8:H1:196:LEU:HB3	8:H1:197:PRO:HD3	2.00	0.43
12:L:279:SER:N	12:L:280:PRO:HD2	2.33	0.43
13:M1:11:LEU:HD23	13:M1:45:THR:HG23	2.01	0.43
15:P1:330:SER:OG	18:Z1:100:ALA:O	2.33	0.43
29:d:504:U10:C38	29:d:504:U10:H452	2.49	0.43
23:l:146:ILE:HG23	23:l:153:SER:OG	2.18	0.43
5:E1:137:CYS:SG	6:F1:89:PRO:HA	2.59	0.43
13:M:11:LEU:HD23	13:M:45:THR:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:152:GLY:O	13:M:159:ARG:NE	2.50	0.43
13:M1:35:LYS:HB3	13:M1:104:TRP:CZ3	2.53	0.43
15:P1:118:SER:O	15:P1:153:PRO:HD2	2.18	0.43
41:b:503:HEC:HBB3	41:b:503:HEC:HMB3	2.01	0.43
19:d:162:ILE:CG1	29:d:501:U10:H3M3	2.49	0.43
22:g:549:ARG:HA	22:g:552:TRP:CE2	2.53	0.43
33:i:304:PC1:H142	33:j:1001:PC1:O12	2.19	0.43
22:k:386:GLY:HA3	22:k:415:VAL:HG13	1.99	0.43
2:B:62:THR:HG21	2:B:156:LEU:HD23	2.01	0.43
7:G1:357:ARG:HA	7:G1:360:TYR:CE2	2.54	0.43
8:H1:108:TRP:CD1	8:H1:108:TRP:N	2.87	0.43
29:a:1004:U10:H351	29:d:501:U10:H301	1.99	0.43
21:c:107:ALA:O	21:c:122:ARG:NH1	2.40	0.43
20:e:388:THR:HG23	20:e:389:PRO:HD2	2.01	0.43
23:l:155:GLU:O	23:l:157:PRO:HD3	2.19	0.43
23:l:188:ASP:OD1	23:l:189:ASN:N	2.51	0.43
1:A:64:TYR:OH	11:K:86:ARG:NH2	2.45	0.43
4:D1:213:ARG:NH2	9:I1:11:TYR:O	2.48	0.43
19:d:84:MET:SD	19:d:94:ARG:HD3	2.58	0.43
41:e:503:HEC:HBB3	41:e:503:HEC:HMB3	2.00	0.43
22:k:549:ARG:HA	22:k:552:TRP:CE2	2.53	0.43
23:l:244:GLN:HA	23:l:257:PRO:HA	2.00	0.43
7:G1:390:ASN:HA	7:G1:393:ILE:HD12	2.01	0.43
8:H1:75:ILE:HD12	8:H1:75:ILE:H	1.84	0.43
6:F1:126:ARG:HE	6:F1:128:GLU:CD	2.26	0.43
20:e:352:GLU:HG2	20:e:361:TYR:CD2	2.53	0.43
23:h:155:GLU:O	23:h:157:PRO:HD3	2.19	0.43
4:D:213:ARG:NH2	9:I:11:TYR:O	2.48	0.43
6:F:84:ALA:HB1	6:F:98:MET:SD	2.58	0.43
6:F:307:ASP:OD1	6:F:310:ARG:NH1	2.51	0.43
12:L:596:PHE:O	12:L:601:PRO:HA	2.19	0.43
13:M1:379:MET:HE2	13:M1:382:TYR:CG	2.54	0.43
20:b:260:ALA:HB2	20:b:272:VAL:HG21	2.01	0.43
23:h:188:ASP:OD1	23:h:189:ASN:N	2.51	0.43
23:h:247:GLU:C	23:h:253:HIS:CE1	2.97	0.43
24:i:158:TRP:CG	26:p:5:MET:HE1	2.54	0.43
3:C:116:TRP:CH2	4:D:382:GLN:HA	2.54	0.42
3:C1:116:TRP:CH2	4:D1:382:GLN:HA	2.54	0.42
5:E:185:SER:OG	5:E:186:ALA:N	2.52	0.42
6:F1:114:PHE:HD1	6:F1:158:TRP:CD2	2.37	0.42
14:N:62:ALA:HB1	14:N:66:GLY:HA2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:e:260:ALA:HB2	20:e:272:VAL:HG21	2.01	0.42
4:D1:68:GLU:HB3	4:D1:370:ARG:HH12	1.85	0.42
5:E:146:MET:HE1	5:E:153:PHE:CG	2.53	0.42
6:F1:329:ASP:OD1	6:F1:416:ARG:NH2	2.47	0.42
8:H:75:ILE:HD12	8:H:75:ILE:H	1.84	0.42
12:L:196:SER:OG	12:L:201:GLU:OE1	2.34	0.42
12:L1:258:VAL:O	12:L1:262:ILE:HG23	2.20	0.42
15:P1:182:ALA:HA	15:P1:221:MET:HB3	2.00	0.42
15:P1:213:LEU:HB3	15:P1:290:PHE:CE2	2.55	0.42
23:h:146:ILE:HG23	23:h:153:SER:HG	1.84	0.42
6:F1:84:ALA:HB1	6:F1:98:MET:SD	2.59	0.42
8:H:226:GLU:OE2	8:H:300:ARG:NE	2.42	0.42
13:M1:364:MET:HG3	13:M1:366:THR:HG22	2.01	0.42
20:b:388:THR:HG23	20:b:389:PRO:HD2	2.01	0.42
22:g:85:HIS:CD2	22:g:157:GLN:HB2	2.54	0.42
22:g:367:ILE:HB	23:h:90:ASN:HA	2.02	0.42
8:H1:124:SER:HA	8:H1:127:GLU:OE2	2.19	0.42
6:F:125:ILE:HD13	6:F:133:ARG:HB3	2.02	0.42
6:F:325:ASP:OD1	6:F:325:ASP:C	2.63	0.42
6:F1:202:LEU:HG	6:F1:203:TYR:CD2	2.54	0.42
7:G:357:ARG:O	7:G:361:VAL:HG22	2.20	0.42
12:L:79:LEU:HD23	12:L:277:ARG:HE	1.84	0.42
12:L:664:ILE:HB	12:L:665:PRO:HD3	2.00	0.42
15:P:33:VAL:HG21	15:P:44:VAL:HG11	2.01	0.42
29:a:1002:U10:H102	29:a:1002:U10:H1M1	2.01	0.42
22:k:367:ILE:HB	23:l:90:ASN:HA	2.02	0.42
23:l:247:GLU:C	23:l:253:HIS:CE1	2.97	0.42
2:B:64:MET:HG3	4:D:151:PHE:HB3	2.00	0.42
6:F1:307:ASP:OD1	6:F1:310:ARG:NH1	2.52	0.42
6:F1:329:ASP:CG	6:F1:416:ARG:HH22	2.27	0.42
15:P:268:ILE:HD12	15:P:268:ILE:H	1.84	0.42
15:P1:268:ILE:HD12	15:P1:268:ILE:H	1.84	0.42
18:Z1:39:VAL:HG13	18:Z1:40:PRO:HD2	2.02	0.42
22:g:300:LYS:NZ	23:h:100:PHE:O	2.50	0.42
8:H1:194:TYR:C	8:H1:197:PRO:HD2	2.45	0.42
13:M1:12:PRO:HG3	13:M1:45:THR:HG21	2.02	0.42
15:P:213:LEU:HB3	15:P:290:PHE:CE2	2.55	0.42
18:Z:39:VAL:HG13	18:Z:40:PRO:HD2	2.01	0.42
8:H:196:LEU:HB3	8:H:197:PRO:HD3	2.00	0.42
8:H1:226:GLU:OE2	8:H1:300:ARG:NE	2.42	0.42
12:L1:105:ASP:OD1	12:L1:107:ASN:ND2	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N1:467:ASP:OD1	14:N1:467:ASP:N	2.52	0.42
15:P1:33:VAL:HG21	15:P1:44:VAL:HG11	2.01	0.42
19:a:366:TRP:CE3	19:a:407:ILE:HD13	2.54	0.42
25:j:49:ASN:O	33:j:1001:PC1:H121	2.20	0.42
22:k:85:HIS:CD2	22:k:157:GLN:HB2	2.54	0.42
6:F:126:ARG:HE	6:F:128:GLU:CD	2.27	0.42
32:F1:501:FMN:H9	32:F1:501:FMN:H1'1	1.85	0.42
13:M1:137:TYR:CE2	13:M1:178:LEU:HD13	2.55	0.42
16:Q1:2:ARG:NE	16:Q1:73:GLU:OE1	2.40	0.42
21:f:86:ARG:HH22	21:f:119:ASP:CG	2.28	0.42
22:k:366:SER:HA	23:l:91:ARG:HA	2.02	0.42
6:F:171:TYR:CE1	32:F:502:FMN:H6	2.55	0.42
6:F1:313:ARG:HD3	6:F1:407:ARG:NH1	2.35	0.42
14:N:226:TRP:HE3	14:N:230:VAL:HG21	1.85	0.42
21:c:86:ARG:HH22	21:c:119:ASP:CG	2.28	0.42
4:D:68:GLU:HB3	4:D:370:ARG:HH12	1.85	0.41
5:E1:154:TYR:CE2	5:E1:177:PRO:HA	2.56	0.41
6:F1:371:ALA:HB1	6:F1:375:GLU:HG3	2.02	0.41
7:G:390:ASN:HA	7:G:393:ILE:HD12	2.01	0.41
7:G1:357:ARG:O	7:G1:361:VAL:HG22	2.20	0.41
13:M1:66:VAL:HA	13:M1:79:MET:O	2.20	0.41
22:k:412:PHE:CE1	22:k:413:HIS:CE1	3.08	0.41
6:F:202:LEU:HG	6:F:203:TYR:CD2	2.54	0.41
7:G:110:CYS:HB2	7:G:111:PRO:HD3	2.02	0.41
7:G:379:GLY:HA3	7:G:451:ALA:HB2	2.03	0.41
12:L1:443:TRP:HB3	12:L1:447:PHE:CE2	2.56	0.41
19:a:235:GLU:OE2	19:a:236:GLU:HG2	2.20	0.41
19:d:106:LEU:HD22	35:e:501:3PE:H291	2.02	0.41
19:d:119:GLY:HA2	19:d:121:TYR:CE2	2.55	0.41
19:d:235:GLU:OE2	19:d:236:GLU:HG2	2.20	0.41
22:g:94:HIS:CE1	42:g:601:HEA:NC	2.88	0.41
23:l:33:LEU:HD22	23:l:263:VAL:HG11	2.02	0.41
2:B1:62:THR:HG21	2:B1:156:LEU:HD23	2.01	0.41
4:D1:10:TYR:HA	10:J1:168:ARG:HA	2.02	0.41
4:D1:251:ARG:O	10:J1:196:GLY:N	2.47	0.41
6:F:313:ARG:HD3	6:F:407:ARG:NH1	2.35	0.41
6:F1:325:ASP:OD1	6:F1:325:ASP:C	2.63	0.41
8:H:108:TRP:N	8:H:108:TRP:CD1	2.87	0.41
13:M:137:TYR:CE2	13:M:178:LEU:HD13	2.55	0.41
19:d:108:VAL:HG21	19:d:139:MET:HE1	2.03	0.41
2:B:50:PHE:HZ	2:B:96:MET:HE3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:64:MET:HG3	4:D1:151:PHE:HB3	2.01	0.41
5:E:154:TYR:CE2	5:E:177:PRO:HA	2.56	0.41
6:F:371:ALA:HB1	6:F:375:GLU:HG3	2.02	0.41
7:G:234:ASP:CG	7:G:272:THR:HG23	2.45	0.41
12:L:343:HIS:HA	12:L:412:SER:OG	2.20	0.41
20:b:353:LYS:HE2	20:b:370:TRP:CE2	2.55	0.41
19:d:366:TRP:CE3	19:d:407:ILE:HD13	2.54	0.41
22:g:239:ALA:O	22:g:243:THR:OG1	2.36	0.41
23:h:33:LEU:HD22	23:h:263:VAL:HG11	2.02	0.41
5:E1:47:GLN:O	5:E1:51:GLY:N	2.48	0.41
5:E1:140:ALA:HB3	5:E1:146:MET:SD	2.61	0.41
8:H:194:TYR:C	8:H:197:PRO:HD2	2.45	0.41
13:M:364:MET:HG3	13:M:366:THR:HG22	2.01	0.41
7:G:394:ARG:NH1	7:G:413:THR:O	2.54	0.41
12:L1:368:GLU:O	12:L1:374:TYR:OH	2.30	0.41
13:M:66:VAL:HA	13:M:79:MET:O	2.20	0.41
13:M1:288:VAL:HG11	13:M1:329:PHE:CD1	2.56	0.41
14:N1:62:ALA:HB1	14:N1:66:GLY:HA2	2.01	0.41
19:d:45:TRP:HA	19:d:114:ARG:NH1	2.35	0.41
21:f:64:SER:HB3	21:f:190:THR:HB	2.03	0.41
4:D:10:TYR:HA	10:J:168:ARG:HA	2.02	0.41
4:D:159:ILE:HD13	4:D:159:ILE:HA	1.92	0.41
9:I1:82:ASP:HB2	9:I1:95:ARG:HB3	2.02	0.41
14:N:188:GLU:H	14:N:188:GLU:CD	2.29	0.41
14:N:383:PRO:HG3	14:N:388:PHE:CD1	2.56	0.41
14:N1:188:GLU:H	14:N1:188:GLU:CD	2.29	0.41
21:f:193:LYS:NZ	21:f:195:GLY:O	2.49	0.41
2:B1:50:PHE:HZ	2:B1:96:MET:HE3	1.85	0.41
6:F:114:PHE:HD1	6:F:158:TRP:CD2	2.37	0.41
7:G1:110:CYS:HB2	7:G1:111:PRO:HD3	2.02	0.41
33:H1:1002:PC1:H143	27:q1:21:TRP:CE3	2.56	0.41
12:L:258:VAL:O	12:L:262:ILE:HG23	2.20	0.41
12:L1:196:SER:OG	12:L1:201:GLU:OE1	2.34	0.41
13:M:379:MET:HE2	13:M:382:TYR:CG	2.55	0.41
14:N:467:ASP:OD1	14:N:467:ASP:N	2.52	0.41
19:a:119:GLY:HA2	19:a:121:TYR:CE2	2.55	0.41
19:d:62:GLY:HA3	39:d:505:HEM:C2B	2.56	0.41
1:A:46:GLU:CG	4:D:30:ASN:HD22	2.34	0.41
2:B1:68:ASP:OD1	8:H1:47:ARG:NH1	2.40	0.41
4:D1:128:LEU:HD21	4:D1:157:LEU:HB2	2.02	0.41
4:D1:173:TYR:OH	4:D1:181:GLN:O	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:313:ARG:HG2	6:F:313:ARG:HH11	1.86	0.41
6:F1:313:ARG:HG2	6:F1:313:ARG:HH11	1.86	0.41
7:G1:168:THR:HA	7:G1:172:ALA:HB3	2.02	0.41
7:G1:234:ASP:CG	7:G1:272:THR:HG23	2.45	0.41
7:G1:394:ARG:NH1	7:G1:413:THR:O	2.54	0.41
9:I:82:ASP:HB2	9:I:95:ARG:HB3	2.03	0.41
12:L1:343:HIS:HA	12:L1:412:SER:OG	2.20	0.41
19:a:359:TYR:CD2	19:a:420:MET:HG2	2.56	0.41
29:d:501:U10:H421	29:d:501:U10:H401	1.81	0.41
29:d:504:U10:C13	29:d:504:U10:C18	2.96	0.41
20:e:241:TYR:CE2	20:e:246:SER:HB3	2.56	0.41
22:g:366:SER:HA	23:h:91:ARG:HA	2.02	0.41
22:g:412:PHE:CE1	22:g:413:HIS:CE1	3.08	0.41
22:k:94:HIS:CE1	42:k:603:HEA:NC	2.88	0.41
24:m:244:GLN:CD	33:m:302:PC1:H132	2.46	0.41
3:C:57:CYS:HB3	3:C:59:PHE:CD2	2.56	0.41
5:E:140:ALA:HB3	5:E:146:MET:SD	2.61	0.41
6:F1:125:ILE:HD13	6:F1:133:ARG:HB3	2.03	0.41
7:G1:379:GLY:HA3	7:G1:451:ALA:HB2	2.03	0.41
10:J:113:SER:HB3	14:N:181:PHE:CE2	2.56	0.41
12:L:191:TYR:O	12:L:195:GLY:N	2.43	0.41
19:a:45:TRP:HA	19:a:114:ARG:NH1	2.35	0.41
20:b:384:TYR:HD2	20:b:388:THR:HB	1.85	0.41
4:D:128:LEU:HD21	4:D:157:LEU:HB2	2.02	0.40
4:D1:355:GLU:O	4:D1:374:ARG:NH1	2.49	0.40
9:I1:56:ARG:HD3	9:I1:60:GLY:O	2.21	0.40
12:L1:614:LEU:HB2	24:m:61:TYR:OH	2.22	0.40
19:a:62:GLY:HA3	39:a:1001:HEM:C2B	2.56	0.40
21:c:46:GLN:NE2	21:c:47:MET:HG3	2.34	0.40
22:g:276:HIS:HB3	22:g:277:PRO:HD3	2.03	0.40
6:F:76:ARG:CZ	6:F:206:PRO:HD3	2.51	0.40
7:G:284:LEU:HD23	7:G:284:LEU:HA	1.94	0.40
8:H:265:GLY:O	8:H:283:LYS:NZ	2.36	0.40
9:I:134:LEU:HD23	9:I:134:LEU:HA	1.92	0.40
12:L1:644:TRP:CH2	12:L1:645:LYS:HE2	2.57	0.40
20:e:353:LYS:HE2	20:e:370:TRP:CE2	2.55	0.40
1:A:58:LYS:HE2	10:J:73:MET:O	2.22	0.40
1:A1:46:GLU:CG	4:D1:30:ASN:HD22	2.33	0.40
1:A1:75:LEU:HD13	11:K1:68:THR:HA	2.03	0.40
3:C1:57:CYS:HB3	3:C1:59:PHE:CD2	2.56	0.40
4:D1:86:LEU:O	4:D1:87:ASP:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:71:TRP:CG	13:M:72:ILE:N	2.89	0.40
24:i:19:PHE:CZ	24:i:23:ILE:HD11	2.55	0.40
42:k:603:HEA:HMD3	42:k:603:HEA:HHD	1.90	0.40
2:B:52:LEU:HB2	2:B:90:GLY:HA3	2.03	0.40
6:F:229:PHE:CZ	6:F:239:GLY:HA3	2.56	0.40
10:J:132:LEU:HD23	10:J:132:LEU:HA	1.90	0.40
12:L:443:TRP:HB3	12:L:447:PHE:CE2	2.56	0.40
13:M:12:PRO:HG3	13:M:45:THR:HG21	2.02	0.40
13:M:137:TYR:CZ	13:M:178:LEU:HB2	2.56	0.40
14:N:130:TYR:CE2	14:N:134:GLU:HG3	2.57	0.40
19:d:59:ILE:HA	39:d:505:HEM:HAB	2.03	0.40
19:d:359:TYR:CD2	19:d:420:MET:HG2	2.56	0.40
23:l:149:GLN:HA	23:l:150:TRP:HA	1.86	0.40
1:A:53:ASP:OD1	1:A:54:ASP:N	2.53	0.40
2:B:23:LEU:HD21	15:P:69:CYS:HA	2.04	0.40
5:E:10:PRO:HD2	5:E:54:SER:HB2	2.04	0.40
5:E:62:ALA:O	5:E:66:GLY:N	2.54	0.40
14:N:188:GLU:CD	14:N:188:GLU:N	2.80	0.40
14:N1:383:PRO:HG3	14:N1:388:PHE:CD1	2.57	0.40
19:a:145:MET:HE1	19:a:197:LEU:HB3	2.04	0.40
20:e:384:TYR:HD2	20:e:388:THR:HB	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
1	A1	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
2	B	160/175 (91%)	153 (96%)	6 (4%)	1 (1%)	21	58
2	B1	160/175 (91%)	154 (96%)	5 (3%)	1 (1%)	21	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	192/208 (92%)	187 (97%)	5 (3%)	0	100	100
3	C1	192/208 (92%)	187 (97%)	5 (3%)	0	100	100
4	D	408/412 (99%)	398 (98%)	10 (2%)	0	100	100
4	D1	408/412 (99%)	398 (98%)	10 (2%)	0	100	100
5	E	235/239 (98%)	225 (96%)	9 (4%)	1 (0%)	30	67
5	E1	235/239 (98%)	225 (96%)	9 (4%)	1 (0%)	30	67
6	F	420/431 (97%)	404 (96%)	16 (4%)	0	100	100
6	F1	420/431 (97%)	403 (96%)	17 (4%)	0	100	100
7	G	663/674 (98%)	637 (96%)	24 (4%)	2 (0%)	36	71
7	G1	663/674 (98%)	637 (96%)	24 (4%)	2 (0%)	36	71
8	H	339/345 (98%)	329 (97%)	10 (3%)	0	100	100
8	H1	339/345 (98%)	329 (97%)	10 (3%)	0	100	100
9	I	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
9	I1	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
10	J	197/199 (99%)	193 (98%)	4 (2%)	0	100	100
10	J1	197/199 (99%)	193 (98%)	4 (2%)	0	100	100
11	K	99/101 (98%)	98 (99%)	0	1 (1%)	12	47
11	K1	99/101 (98%)	98 (99%)	0	1 (1%)	12	47
12	L	657/703 (94%)	628 (96%)	29 (4%)	0	100	100
12	L1	657/703 (94%)	628 (96%)	29 (4%)	0	100	100
13	M	501/513 (98%)	494 (99%)	6 (1%)	1 (0%)	43	77
13	M1	501/513 (98%)	494 (99%)	6 (1%)	1 (0%)	43	77
14	N	478/499 (96%)	470 (98%)	8 (2%)	0	100	100
14	N1	478/499 (96%)	470 (98%)	8 (2%)	0	100	100
15	P	326/330 (99%)	317 (97%)	9 (3%)	0	100	100
15	P1	326/330 (99%)	315 (97%)	11 (3%)	0	100	100
16	Q	101/103 (98%)	101 (100%)	0	0	100	100
16	Q1	101/103 (98%)	101 (100%)	0	0	100	100
17	R	59/62 (95%)	54 (92%)	4 (7%)	1 (2%)	7	35
17	R1	59/62 (95%)	54 (92%)	4 (7%)	1 (2%)	7	35
18	Z	214/217 (99%)	209 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	Z1	214/217 (99%)	209 (98%)	5 (2%)	0	100	100
19	a	432/440 (98%)	424 (98%)	8 (2%)	0	100	100
19	d	432/440 (98%)	423 (98%)	9 (2%)	0	100	100
20	b	237/450 (53%)	234 (99%)	2 (1%)	1 (0%)	30	67
20	e	237/450 (53%)	233 (98%)	3 (1%)	1 (0%)	30	67
21	c	179/195 (92%)	174 (97%)	4 (2%)	1 (1%)	21	58
21	f	179/195 (92%)	174 (97%)	5 (3%)	0	100	100
22	g	542/558 (97%)	528 (97%)	14 (3%)	0	100	100
22	k	542/558 (97%)	528 (97%)	14 (3%)	0	100	100
23	h	250/298 (84%)	240 (96%)	10 (4%)	0	100	100
23	l	250/298 (84%)	240 (96%)	10 (4%)	0	100	100
24	i	271/274 (99%)	260 (96%)	11 (4%)	0	100	100
24	m	271/274 (99%)	261 (96%)	10 (4%)	0	100	100
25	j	41/66 (62%)	39 (95%)	2 (5%)	0	100	100
25	n	41/66 (62%)	39 (95%)	2 (5%)	0	100	100
26	o	40/176 (23%)	39 (98%)	1 (2%)	0	100	100
26	p	40/176 (23%)	39 (98%)	1 (2%)	0	100	100
27	q	121/124 (98%)	115 (95%)	6 (5%)	0	100	100
27	q1	121/124 (98%)	115 (95%)	6 (5%)	0	100	100
All	All	14882/16152 (92%)	14441 (97%)	424 (3%)	17 (0%)	49	83

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	137	CYS
5	E1	137	CYS
13	M	238	VAL
13	M1	238	VAL
20	b	369	ASN
20	e	369	ASN
7	G	266	GLU
7	G1	266	GLU
17	R	55	ARG
17	R1	55	ARG
21	c	117	ALA

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Mol	Chain	Res	Type
7	G	263	VAL
7	G1	263	VAL
2	B	122	GLY
2	B1	122	GLY
11	K	96	VAL
11	K1	96	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	97/97 (100%)	97 (100%)	0	100	100
1	A1	97/97 (100%)	97 (100%)	0	100	100
2	B	136/145 (94%)	134 (98%)	2 (2%)	57	71
2	B1	136/145 (94%)	135 (99%)	1 (1%)	76	79
3	C	172/183 (94%)	172 (100%)	0	100	100
3	C1	172/183 (94%)	172 (100%)	0	100	100
4	D	341/342 (100%)	341 (100%)	0	100	100
4	D1	341/342 (100%)	341 (100%)	0	100	100
5	E	189/190 (100%)	189 (100%)	0	100	100
5	E1	189/190 (100%)	189 (100%)	0	100	100
6	F	331/335 (99%)	331 (100%)	0	100	100
6	F1	331/335 (99%)	330 (100%)	1 (0%)	86	84
7	G	530/535 (99%)	528 (100%)	2 (0%)	84	83
7	G1	530/535 (99%)	530 (100%)	0	100	100
8	H	277/279 (99%)	277 (100%)	0	100	100
8	H1	277/279 (99%)	277 (100%)	0	100	100
9	I	136/137 (99%)	136 (100%)	0	100	100
9	I1	136/137 (99%)	136 (100%)	0	100	100
10	J	158/158 (100%)	158 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J1	158/158 (100%)	158 (100%)	0	100	100
11	K	81/81 (100%)	80 (99%)	1 (1%)	63	74
11	K1	81/81 (100%)	80 (99%)	1 (1%)	63	74
12	L	520/543 (96%)	520 (100%)	0	100	100
12	L1	520/543 (96%)	520 (100%)	0	100	100
13	M	410/416 (99%)	408 (100%)	2 (0%)	81	82
13	M1	410/416 (99%)	408 (100%)	2 (0%)	81	82
14	N	357/369 (97%)	356 (100%)	1 (0%)	86	84
14	N1	357/369 (97%)	355 (99%)	2 (1%)	78	81
15	P	248/250 (99%)	248 (100%)	0	100	100
15	P1	248/250 (99%)	248 (100%)	0	100	100
16	Q	87/87 (100%)	86 (99%)	1 (1%)	65	74
16	Q1	87/87 (100%)	86 (99%)	1 (1%)	65	74
17	R	51/52 (98%)	51 (100%)	0	100	100
17	R1	51/52 (98%)	51 (100%)	0	100	100
18	Z	167/168 (99%)	167 (100%)	0	100	100
18	Z1	167/168 (99%)	167 (100%)	0	100	100
19	a	361/366 (99%)	361 (100%)	0	100	100
19	d	361/366 (99%)	361 (100%)	0	100	100
20	b	192/319 (60%)	192 (100%)	0	100	100
20	e	192/319 (60%)	192 (100%)	0	100	100
21	c	140/151 (93%)	140 (100%)	0	100	100
21	f	140/151 (93%)	140 (100%)	0	100	100
22	g	447/454 (98%)	447 (100%)	0	100	100
22	k	447/454 (98%)	447 (100%)	0	100	100
23	h	211/243 (87%)	210 (100%)	1 (0%)	81	82
23	l	211/243 (87%)	210 (100%)	1 (0%)	81	82
24	i	220/221 (100%)	219 (100%)	1 (0%)	81	82
24	m	220/221 (100%)	219 (100%)	1 (0%)	81	82
25	j	34/53 (64%)	34 (100%)	0	100	100
25	n	34/53 (64%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	o	33/126 (26%)	33 (100%)	0	100	100
26	p	33/126 (26%)	33 (100%)	0	100	100
27	q	103/104 (99%)	103 (100%)	0	100	100
27	q1	103/104 (99%)	103 (100%)	0	100	100
All	All	12058/12808 (94%)	12037 (100%)	21 (0%)	85	86

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	54	CYS
2	B	91	THR
2	B1	91	THR
6	F1	88	GLU
7	G	31	ILE
7	G	90	MET
11	K	25	ASN
11	K1	25	ASN
13	M	365	HIS
13	M	471	MET
13	M1	365	HIS
13	M1	471	MET
14	N	188	GLU
14	N1	88	VAL
14	N1	188	GLU
16	Q	73	GLU
16	Q1	73	GLU
23	h	88	ARG
24	i	258	VAL
23	l	88	ARG
24	m	258	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	29	GLN
3	C	38	ASN
3	C	179	GLN
3	C1	29	GLN
3	C1	38	ASN
3	C1	179	GLN

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Mol	Chain	Res	Type
4	D	28	ASN
4	D	94	GLN
4	D	170	HIS
4	D	329	HIS
4	D1	28	ASN
4	D1	94	GLN
4	D1	329	HIS
5	E	85	GLN
5	E1	85	GLN
6	F	83	ASN
6	F	137	GLN
6	F1	83	ASN
7	G	592	GLN
7	G	619	GLN
7	G1	592	GLN
7	G1	619	GLN
9	I	39	HIS
9	I1	39	HIS
12	L	205	GLN
12	L	208	GLN
12	L	225	ASN
12	L	347	HIS
12	L	369	GLN
12	L1	205	GLN
12	L1	208	GLN
12	L1	225	ASN
12	L1	369	GLN
13	M	69	HIS
13	M	248	GLN
13	M	495	GLN
13	M	498	ASN
13	M	499	GLN
13	M1	69	HIS
13	M1	248	GLN
13	M1	495	GLN
13	M1	498	ASN
13	M1	499	GLN
14	N	198	HIS
14	N	323	ASN
14	N1	198	HIS
14	N1	271	GLN
14	N1	323	ASN

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Mol	Chain	Res	Type
15	P	27	GLN
15	P	95	HIS
15	P	243	HIS
15	P1	27	GLN
15	P1	95	HIS
15	P1	243	HIS
16	Q	48	GLN
16	Q1	48	GLN
18	Z	6	GLN
18	Z1	6	GLN
19	a	8	HIS
19	a	99	ASN
19	a	358	GLN
20	b	372	GLN
20	b	436	ASN
21	c	46	GLN
21	c	92	GLN
21	c	121	ASN
19	d	8	HIS
19	d	358	GLN
20	e	372	GLN
20	e	436	ASN
21	f	92	GLN
21	f	121	ASN
22	g	59	HIS
22	g	206	ASN
22	g	269	HIS
23	h	94	ASN
23	h	158	ASN
23	h	230	GLN
23	h	252	ASN
24	i	79	HIS
24	i	161	HIS
24	i	165	HIS
24	i	196	HIS
25	j	21	GLN
25	j	49	ASN
22	k	59	HIS
22	k	206	ASN
22	k	269	HIS
23	l	158	ASN
23	l	252	ASN

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Mol	Chain	Res	Type
24	m	79	HIS
24	m	165	HIS
24	m	196	HIS
26	o	33	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
27	FME	q1	1	27	8,9,10	0.96	0	8,9,11	1.10	1 (12%)
13	FME	M1	1	13	8,9,10	0.97	0	8,9,11	1.13	1 (12%)
4	2MR	D	65	4	10,12,13	2.49	3 (30%)	5,13,15	1.12	0
1	FME	A1	1	1	8,9,10	0.94	0	8,9,11	1.07	1 (12%)
10	FME	J	1	10	8,9,10	0.99	0	8,9,11	0.71	0
12	FME	L1	1	12	8,9,10	0.93	0	8,9,11	1.26	1 (12%)
27	FME	q	1	27	8,9,10	0.96	0	8,9,11	1.10	1 (12%)
4	2MR	D1	65	4	10,12,13	2.49	3 (30%)	5,13,15	1.13	1 (20%)
10	FME	J1	1	10	8,9,10	1.03	0	8,9,11	0.71	0
13	FME	M	1	13	8,9,10	0.96	0	8,9,11	1.13	1 (12%)
1	FME	A	1	1	8,9,10	0.96	0	8,9,11	1.08	1 (12%)
12	FME	L	1	12	8,9,10	0.95	0	8,9,11	1.27	1 (12%)

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
27	FME	q1	1	27	-	0/7/9/11	-
13	FME	M1	1	13	-	3/7/9/11	-
4	2MR	D	65	4	-	0/10/13/15	-
1	FME	A1	1	1	-	1/7/9/11	-
10	FME	J	1	10	-	0/7/9/11	-
12	FME	L1	1	12	-	1/7/9/11	-
27	FME	q	1	27	-	0/7/9/11	-
4	2MR	D1	65	4	-	0/10/13/15	-
10	FME	J1	1	10	-	1/7/9/11	-
13	FME	M	1	13	-	3/7/9/11	-
1	FME	A	1	1	-	1/7/9/11	-
12	FME	L	1	12	-	1/7/9/11	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D1	65	2MR	CZ-NH2	5.23	1.44	1.33
4	D	65	2MR	CZ-NH2	5.22	1.44	1.33
4	D	65	2MR	CZ-NE	5.05	1.45	1.34
4	D1	65	2MR	CZ-NE	5.05	1.45	1.34
4	D	65	2MR	CQ1-NH1	-2.08	1.42	1.46
4	D1	65	2MR	CQ1-NH1	-2.07	1.42	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	1	FME	C-CA-N	2.78	114.86	109.50
12	L	1	FME	C-CA-N	2.76	114.83	109.50
12	L1	1	FME	C-CA-N	2.76	114.83	109.50
13	M1	1	FME	C-CA-N	2.76	114.82	109.50
27	q1	1	FME	C-CA-N	2.57	114.46	109.50
27	q	1	FME	C-CA-N	2.52	114.36	109.50
1	A	1	FME	C-CA-N	2.40	114.14	109.50
1	A1	1	FME	C-CA-N	2.39	114.12	109.50
4	D1	65	2MR	NE-CZ-NH2	-2.02	117.62	119.48

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	J1	1	FME	O-C-CA-CB
12	L	1	FME	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
12	L1	1	FME	O-C-CA-CB
13	M	1	FME	N-CA-CB-CG
13	M1	1	FME	N-CA-CB-CG
13	M	1	FME	C-CA-CB-CG
13	M1	1	FME	C-CA-CB-CG
1	A	1	FME	CB-CG-SD-CE
1	A1	1	FME	CB-CG-SD-CE
13	M	1	FME	CB-CA-N-CN
13	M1	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 87 ligands modelled in this entry, 14 are monoatomic - leaving 73 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	$\# Z  > 2$
28	SF4	I1	201	9	0,12,12	-	-	-		
28	SF4	G	701	7	0,12,12	-	-	-		
35	3PE	m	304	-	50,50,50	0.97	4 (8%)	53,55,55	0.97	2 (3%)
29	U10	B	1002	-	63,63,63	0.69	0	78,79,79	1.27	6 (7%)
31	FES	E	401	5	0,4,4	-	-	-		
28	SF4	G	702	7	0,12,12	-	-	-		
32	FMN	F1	501	-	33,33,33	1.06	3 (9%)	48,50,50	1.27	6 (12%)
45	CUA	h	301	23	0,1,1	-	-	-		
28	SF4	F	501	6	0,12,12	-	-	-		
33	PC1	H1	1002	-	53,53,53	0.97	3 (5%)	59,61,61	0.86	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	3PH	L	802	-	47,47,47	1.37	5 (10%)	50,52,52	1.04	4 (8%)
33	PC1	M	601	-	53,53,53	0.97	3 (5%)	59,61,61	0.87	2 (3%)
36	3PH	L1	804	-	47,47,47	1.37	5 (10%)	50,52,52	1.04	4 (8%)
36	3PH	p	201	-	47,47,47	1.37	5 (10%)	50,52,52	0.98	4 (8%)
37	P5S	L	803	-	52,53,53	0.94	3 (5%)	54,60,60	0.83	3 (5%)
32	FMN	F	502	-	33,33,33	1.05	3 (9%)	48,50,50	1.27	6 (12%)
33	PC1	L1	801	-	53,53,53	0.98	3 (5%)	59,61,61	0.93	2 (3%)
35	3PE	e	501	-	50,50,50	0.95	4 (8%)	53,55,55	1.00	3 (5%)
33	PC1	H	1001	-	53,53,53	0.97	3 (5%)	59,61,61	0.83	1 (1%)
31	FES	G	703	7	0,4,4	-	-	-	-	-
31	FES	c	1000	21	0,4,4	-	-	-	-	-
33	PC1	i	304	-	53,53,53	0.96	3 (5%)	59,61,61	0.87	2 (3%)
34	DU0	M	602	-	42,42,42	0.70	0	64,66,66	0.91	2 (3%)
39	HEM	a	1001	19	50,50,50	1.52	8 (16%)	67,82,82	1.06	2 (2%)
28	SF4	G1	703	7	0,12,12	-	-	-	-	-
28	SF4	I	201	9	0,12,12	-	-	-	-	-
34	DU0	a	1005	-	42,42,42	0.73	0	64,66,66	0.82	1 (1%)
35	3PE	L1	802	-	50,50,50	0.96	4 (8%)	53,55,55	0.99	4 (7%)
34	DU0	M1	602	-	42,42,42	0.68	0	64,66,66	0.94	4 (6%)
42	HEA	g	605	22	67,67,67	1.39	8 (11%)	81,103,103	2.28	33 (40%)
29	U10	d	501	-	63,63,63	0.68	0	78,79,79	1.07	4 (5%)
33	PC1	m	302	-	53,53,53	0.97	3 (5%)	59,61,61	0.84	2 (3%)
34	DU0	d	503	-	42,42,42	0.73	0	64,66,66	0.82	1 (1%)
35	3PE	i	303	-	50,50,50	0.97	4 (8%)	53,55,55	1.03	2 (3%)
37	P5S	L1	803	-	52,53,53	0.94	3 (5%)	54,60,60	0.83	3 (5%)
35	3PE	m	301	-	50,50,50	0.97	4 (8%)	53,55,55	0.99	4 (7%)
33	PC1	i	301	-	53,53,53	0.97	3 (5%)	59,61,61	0.84	1 (1%)
39	HEM	a	1003	19	50,50,50	1.46	6 (12%)	67,82,82	0.99	3 (4%)
29	U10	d	504	-	63,63,63	0.73	0	78,79,79	1.05	4 (5%)
36	3PH	f	201	-	47,47,47	1.39	5 (10%)	50,52,52	1.02	4 (8%)
35	3PE	L	801	-	50,50,50	0.95	4 (8%)	53,55,55	0.99	4 (7%)
28	SF4	B	1001	2	0,12,12	-	-	-	-	-
28	SF4	G1	702	7	0,12,12	-	-	-	-	-
33	PC1	j	1001	-	53,53,53	0.97	3 (5%)	59,61,61	0.88	3 (5%)
40	CDL	a	1006	-	99,99,99	0.92	6 (6%)	105,111,111	0.89	4 (3%)
36	3PH	k	602	-	47,47,47	1.40	6 (12%)	50,52,52	1.02	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	FES	G1	701	7	0,4,4	-	-	-		
33	PC1	n	1001	-	53,53,53	0.96	3 (5%)	59,61,61	0.89	3 (5%)
28	SF4	I1	202	9	0,12,12	-	-	-		
45	CUA	l	301	23	0,1,1	-	-	-		
28	SF4	B1	1001	2	0,12,12	-	-	-		
31	FES	f	202	21	0,4,4	-	-	-		
33	PC1	m	303	-	53,53,53	0.95	3 (5%)	59,61,61	0.91	3 (5%)
34	DU0	K	1000	-	42,42,42	0.73	0	64,66,66	0.84	1 (1%)
33	PC1	M1	601	-	53,53,53	0.97	3 (5%)	59,61,61	0.87	2 (3%)
35	3PE	b	502	-	50,50,50	0.95	4 (8%)	53,55,55	1.00	4 (7%)
29	U10	B1	1002	-	63,63,63	0.69	0	78,79,79	1.23	6 (7%)
29	U10	a	1004	-	63,63,63	0.69	0	78,79,79	1.09	5 (6%)
35	3PE	g	607	-	50,50,50	0.95	4 (8%)	53,55,55	1.01	3 (5%)
33	PC1	H1	1001	-	53,53,53	0.97	3 (5%)	59,61,61	0.83	1 (1%)
31	FES	E1	401	5	0,4,4	-	-	-		
39	HEM	d	505	19	50,50,50	1.52	8 (16%)	67,82,82	1.07	2 (2%)
41	HEC	e	503	20	46,50,50	2.01	10 (21%)	58,82,82	1.83	9 (15%)
28	SF4	I	202	9	0,12,12	-	-	-		
42	HEA	k	603	22	67,67,67	1.40	8 (11%)	81,103,103	2.29	31 (38%)
35	3PE	k	607	-	50,50,50	0.94	4 (8%)	53,55,55	1.01	3 (5%)
36	3PH	g	602	-	47,47,47	1.39	5 (10%)	50,52,52	1.04	5 (10%)
42	HEA	k	605	22	67,67,67	1.39	9 (13%)	81,103,103	2.28	32 (39%)
29	U10	a	1002	-	63,63,63	0.68	0	78,79,79	1.06	2 (2%)
39	HEM	d	502	19	50,50,50	1.47	7 (14%)	67,82,82	0.99	3 (4%)
28	SF4	F1	502	6	0,12,12	-	-	-		
42	HEA	g	601	22	67,67,67	1.40	7 (10%)	81,103,103	2.28	30 (37%)
41	HEC	b	503	20	46,50,50	2.00	10 (21%)	58,82,82	1.82	10 (17%)

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
28	SF4	I1	201	9	-	-	0/6/5/5
28	SF4	G	701	7	-	-	0/6/5/5
35	3PE	m	304	-	-	7/54/54/54	-
29	U10	B	1002	-	-	13/63/87/87	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	FES	E	401	5	-	-	0/1/1/1
32	FMN	F1	501	-	-	9/18/18/18	0/3/3/3
28	SF4	G	702	7	-	-	0/6/5/5
28	SF4	F	501	6	-	-	0/6/5/5
33	PC1	H1	1002	-	-	5/57/57/57	-
36	3PH	L	802	-	-	5/49/49/49	-
33	PC1	M	601	-	-	11/57/57/57	-
36	3PH	L1	804	-	-	6/49/49/49	-
36	3PH	p	201	-	-	9/49/49/49	-
37	P5S	L	803	-	-	3/59/59/59	-
32	FMN	F	502	-	-	1/18/18/18	0/3/3/3
33	PC1	L1	801	-	-	18/57/57/57	-
35	3PE	e	501	-	-	11/54/54/54	-
33	PC1	H	1001	-	-	11/57/57/57	-
34	DU0	M	602	-	-	0/10/98/98	0/6/6/6
39	HEM	a	1001	19	-	8/14/54/54	-
33	PC1	i	304	-	-	10/57/57/57	-
42	HEA	g	605	22	-	5/36/76/76	-
42	HEA	k	603	22	-	7/36/76/76	-
28	SF4	G1	703	7	-	-	0/6/5/5
28	SF4	I	201	9	-	-	0/6/5/5
31	FES	G	703	7	-	-	0/1/1/1
35	3PE	L1	802	-	-	7/54/54/54	-
34	DU0	M1	602	-	-	0/10/98/98	0/6/6/6
31	FES	c	1000	21	-	-	0/1/1/1
29	U10	d	501	-	-	9/63/87/87	0/1/1/1
33	PC1	m	302	-	-	6/57/57/57	-
34	DU0	d	503	-	-	0/10/98/98	0/6/6/6
35	3PE	i	303	-	-	12/54/54/54	-
37	P5S	L1	803	-	-	4/59/59/59	-
35	3PE	m	301	-	-	10/54/54/54	-
28	SF4	F1	502	6	-	-	0/6/5/5
33	PC1	i	301	-	-	6/57/57/57	-
39	HEM	a	1003	19	-	9/14/54/54	-
29	U10	d	504	-	-	15/63/87/87	0/1/1/1
36	3PH	f	201	-	-	8/49/49/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	3PE	L	801	-	-	7/54/54/54	-
33	PC1	j	1001	-	-	13/57/57/57	-
28	SF4	B	1001	2	-	-	0/6/5/5
28	SF4	G1	702	7	-	-	0/6/5/5
40	CDL	a	1006	-	-	21/110/110/110	-
36	3PH	k	602	-	-	7/49/49/49	-
31	FES	G1	701	7	-	-	0/1/1/1
33	PC1	n	1001	-	-	18/57/57/57	-
28	SF4	I1	202	9	-	-	0/6/5/5
33	PC1	m	303	-	-	12/57/57/57	-
28	SF4	B1	1001	2	-	-	0/6/5/5
31	FES	f	202	21	-	-	0/1/1/1
34	DU0	K	1000	-	-	0/10/98/98	0/6/6/6
33	PC1	M1	601	-	-	10/57/57/57	-
35	3PE	b	502	-	-	13/54/54/54	-
29	U10	a	1004	-	-	13/63/87/87	0/1/1/1
29	U10	B1	1002	-	-	8/63/87/87	0/1/1/1
35	3PE	g	607	-	-	10/54/54/54	-
33	PC1	H1	1001	-	-	11/57/57/57	-
39	HEM	d	505	19	-	8/14/54/54	-
41	HEC	e	503	20	-	7/14/54/54	-
31	FES	E1	401	5	-	-	0/1/1/1
28	SF4	I	202	9	-	-	0/6/5/5
35	3PE	k	607	-	-	11/54/54/54	-
36	3PH	g	602	-	-	5/49/49/49	-
42	HEA	k	605	22	-	5/36/76/76	-
29	U10	a	1002	-	-	8/63/87/87	0/1/1/1
39	HEM	d	502	19	-	9/14/54/54	-
34	DU0	a	1005	-	-	0/10/98/98	0/6/6/6
42	HEA	g	601	22	-	7/36/76/76	-
41	HEC	b	503	20	-	7/14/54/54	-

All (202) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	f	201	3PH	P-O11	7.45	1.83	1.60
36	k	602	3PH	P-O11	7.41	1.83	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	g	602	3PH	P-O11	7.34	1.83	1.60
36	p	201	3PH	P-O11	7.29	1.83	1.60
36	L1	804	3PH	P-O11	7.28	1.83	1.60
36	L	802	3PH	P-O11	7.26	1.83	1.60
41	e	503	HEC	CAC-C3C	6.07	1.54	1.35
41	b	503	HEC	CAC-C3C	6.06	1.54	1.35
41	e	503	HEC	CAB-C3B	6.02	1.54	1.35
41	b	503	HEC	CAB-C3B	6.00	1.54	1.35
41	e	503	HEC	C3D-C2D	4.57	1.50	1.38
41	b	503	HEC	C3D-C2D	4.54	1.50	1.38
42	g	601	HEA	C3B-C2B	4.08	1.44	1.34
42	k	603	HEA	C3B-C2B	4.07	1.44	1.34
42	g	605	HEA	C3B-C2B	3.88	1.43	1.34
42	k	605	HEA	C3B-C2B	3.88	1.43	1.34
35	b	502	3PE	P-O14	-3.61	1.38	1.50
35	m	304	3PE	P-O14	-3.61	1.38	1.50
35	e	501	3PE	P-O14	-3.60	1.38	1.50
33	j	1001	PC1	P-O14	-3.58	1.38	1.50
35	i	303	3PE	P-O14	-3.57	1.38	1.50
33	H1	1002	PC1	P-O14	-3.57	1.38	1.50
35	k	607	3PE	P-O14	-3.55	1.38	1.50
35	g	607	3PE	P-O14	-3.55	1.38	1.50
33	i	304	PC1	P-O14	-3.55	1.38	1.50
42	g	605	HEA	C3D-C2D	3.54	1.44	1.36
33	m	303	PC1	P-O14	-3.54	1.38	1.50
42	k	605	HEA	C3D-C2D	3.53	1.44	1.36
33	i	301	PC1	P-O14	-3.51	1.38	1.50
35	L1	802	3PE	P-O14	-3.51	1.38	1.50
35	L	801	3PE	P-O14	-3.51	1.38	1.50
33	m	302	PC1	P-O14	-3.50	1.38	1.50
33	n	1001	PC1	P-O14	-3.47	1.38	1.50
42	k	603	HEA	C3D-C2D	3.46	1.44	1.36
42	g	601	HEA	C3D-C2D	3.45	1.44	1.36
33	M1	601	PC1	P-O14	-3.45	1.38	1.50
33	L1	801	PC1	P-O14	-3.43	1.38	1.50
33	H1	1001	PC1	P-O14	-3.42	1.39	1.50
33	M	601	PC1	P-O14	-3.42	1.39	1.50
35	m	301	3PE	P-O14	-3.41	1.39	1.50
33	H	1001	PC1	P-O14	-3.40	1.39	1.50
33	i	304	PC1	P-O13	3.31	1.72	1.59
33	n	1001	PC1	P-O13	3.26	1.72	1.59
33	j	1001	PC1	P-O13	3.25	1.72	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	F1	501	FMN	C4A-N5	3.24	1.37	1.30
33	L1	801	PC1	P-O13	3.22	1.72	1.59
33	H1	1001	PC1	P-O12	-3.21	1.40	1.55
37	L	803	P5S	P12-O15	-3.21	1.40	1.55
37	L1	803	P5S	P12-O15	-3.21	1.40	1.55
33	M1	601	PC1	P-O13	3.19	1.71	1.59
33	H	1001	PC1	P-O12	-3.19	1.40	1.55
33	M	601	PC1	P-O13	3.18	1.71	1.59
33	L1	801	PC1	P-O12	-3.17	1.40	1.55
33	M	601	PC1	P-O12	-3.16	1.40	1.55
33	m	302	PC1	P-O12	-3.16	1.40	1.55
33	i	301	PC1	P-O12	-3.16	1.40	1.55
33	M1	601	PC1	P-O12	-3.14	1.40	1.55
33	m	302	PC1	P-O13	3.14	1.71	1.59
33	j	1001	PC1	P-O12	-3.13	1.40	1.55
33	i	301	PC1	P-O13	3.13	1.71	1.59
32	F	502	FMN	C4A-N5	3.13	1.37	1.30
33	H1	1001	PC1	P-O13	3.13	1.71	1.59
33	H1	1002	PC1	P-O13	3.11	1.71	1.59
33	H	1001	PC1	P-O13	3.10	1.71	1.59
33	H1	1002	PC1	P-O12	-3.09	1.41	1.55
33	i	304	PC1	P-O12	-3.09	1.41	1.55
33	m	303	PC1	P-O12	-3.08	1.41	1.55
33	n	1001	PC1	P-O12	-3.06	1.41	1.55
42	k	603	HEA	C1D-ND	-3.06	1.34	1.40
33	m	303	PC1	P-O13	3.05	1.71	1.59
42	g	601	HEA	C1D-ND	-3.05	1.35	1.40
42	g	601	HEA	C3A-C2A	2.98	1.43	1.37
42	g	605	HEA	C3A-C2A	2.98	1.43	1.37
42	k	605	HEA	C3A-C2A	2.96	1.43	1.37
42	k	603	HEA	C3A-C2A	2.94	1.43	1.37
39	a	1001	HEM	C3B-C2B	-2.94	1.31	1.37
42	g	605	HEA	C1D-ND	-2.94	1.35	1.40
39	a	1001	HEM	C3C-C2C	-2.93	1.31	1.37
42	k	605	HEA	C1D-ND	-2.93	1.35	1.40
39	d	505	HEM	C3B-C2B	-2.91	1.31	1.37
39	d	505	HEM	C3C-C2C	-2.91	1.31	1.37
35	b	502	3PE	P-O12	-2.89	1.42	1.55
35	e	501	3PE	P-O12	-2.86	1.42	1.55
35	g	607	3PE	P-O12	-2.85	1.42	1.55
35	k	607	3PE	P-O12	-2.84	1.42	1.55
35	m	304	3PE	P-O12	-2.84	1.42	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	L	801	3PE	P-O12	-2.82	1.42	1.55
35	i	303	3PE	P-O12	-2.81	1.42	1.55
35	L1	802	3PE	P-O12	-2.81	1.42	1.55
42	g	601	HEA	C11-C3B	-2.79	1.48	1.51
35	m	301	3PE	P-O12	-2.75	1.42	1.55
39	d	505	HEM	C2A-C3A	-2.75	1.31	1.38
40	a	1006	CDL	OB6-CB4	-2.74	1.40	1.46
42	k	603	HEA	C11-C3B	-2.74	1.48	1.51
39	a	1001	HEM	C2A-C3A	-2.72	1.31	1.38
39	d	502	HEM	C2A-C3A	-2.69	1.31	1.38
37	L	803	P5S	P12-O13	-2.68	1.41	1.50
42	g	605	HEA	C4A-NA	-2.68	1.34	1.39
36	g	602	3PH	P-O14	-2.67	1.44	1.54
39	d	502	HEM	C3C-C2C	-2.65	1.31	1.37
42	k	605	HEA	C4A-NA	-2.65	1.34	1.39
39	a	1001	HEM	C3D-C2D	-2.65	1.31	1.36
37	L1	803	P5S	P12-O13	-2.65	1.41	1.50
39	a	1003	HEM	C3C-C2C	-2.64	1.31	1.37
39	d	505	HEM	C3D-C2D	-2.64	1.31	1.36
39	a	1003	HEM	C2A-C3A	-2.64	1.32	1.38
36	k	602	3PH	P-O14	-2.64	1.45	1.54
36	L	802	3PH	P-O13	-2.63	1.45	1.54
36	L1	804	3PH	P-O13	-2.63	1.45	1.54
36	p	201	3PH	P-O14	-2.61	1.45	1.54
37	L	803	P5S	P12-O16	2.60	1.69	1.59
36	g	602	3PH	P-O13	-2.60	1.45	1.54
36	k	602	3PH	P-O13	-2.59	1.45	1.54
36	p	201	3PH	P-O13	-2.58	1.45	1.54
36	L1	804	3PH	P-O14	-2.58	1.45	1.54
36	f	201	3PH	P-O14	-2.58	1.45	1.54
37	L1	803	P5S	P12-O16	2.58	1.69	1.59
36	L	802	3PH	P-O14	-2.56	1.45	1.54
40	a	1006	CDL	OB8-CB7	2.56	1.40	1.33
35	m	301	3PE	P-O11	2.52	1.69	1.59
36	f	201	3PH	P-O13	-2.50	1.45	1.54
35	m	301	3PE	P-O13	2.50	1.69	1.59
40	a	1006	CDL	OA8-CA7	2.47	1.40	1.33
35	i	303	3PE	P-O13	2.46	1.69	1.59
35	m	304	3PE	P-O11	2.45	1.69	1.59
41	e	503	HEC	C3B-C2B	-2.42	1.33	1.41
41	b	503	HEC	C3B-C2B	-2.41	1.33	1.41
35	L1	802	3PE	P-O13	2.41	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	g	601	HEA	C4A-NA	-2.40	1.35	1.39
35	L	801	3PE	P-O13	2.40	1.68	1.59
39	d	502	HEM	C3B-C2B	-2.40	1.32	1.37
42	k	603	HEA	C4A-NA	-2.39	1.35	1.39
40	a	1006	CDL	OA6-CA4	-2.39	1.41	1.46
39	a	1003	HEM	C3B-C2B	-2.39	1.32	1.37
40	a	1006	CDL	OA6-CA5	2.38	1.41	1.34
41	e	503	HEC	C3B-C4B	-2.38	1.41	1.46
39	a	1001	HEM	CAB-C3B	2.37	1.53	1.47
41	b	503	HEC	CHC-C1C	-2.37	1.34	1.39
35	m	304	3PE	P-O13	2.37	1.68	1.59
36	g	602	3PH	O11-C1	-2.37	1.35	1.44
35	L1	802	3PE	P-O11	2.36	1.68	1.59
35	L	801	3PE	P-O11	2.36	1.68	1.59
39	d	505	HEM	CAB-C3B	2.36	1.53	1.47
41	e	503	HEC	CHC-C1C	-2.35	1.34	1.39
41	e	503	HEC	CHC-C4B	-2.35	1.33	1.38
41	b	503	HEC	C3B-C4B	-2.34	1.41	1.46
36	L	802	3PH	O11-C1	-2.33	1.35	1.44
39	a	1003	HEM	CAB-C3B	2.32	1.53	1.47
39	d	502	HEM	C3D-C2D	-2.32	1.31	1.36
41	b	503	HEC	CHC-C4B	-2.32	1.33	1.38
39	d	502	HEM	CAB-C3B	2.31	1.53	1.47
36	p	201	3PH	P-O12	-2.31	1.43	1.50
36	L1	804	3PH	O11-C1	-2.31	1.35	1.44
36	p	201	3PH	O11-C1	-2.30	1.35	1.44
36	k	602	3PH	O11-C1	-2.30	1.35	1.44
35	i	303	3PE	P-O11	2.29	1.68	1.59
36	k	602	3PH	P-O12	-2.29	1.43	1.50
42	k	605	HEA	C4B-C3B	2.28	1.48	1.44
36	g	602	3PH	P-O12	-2.28	1.43	1.50
42	g	605	HEA	C4B-C3B	2.28	1.48	1.44
35	g	607	3PE	P-O11	2.28	1.68	1.59
39	a	1003	HEM	CAC-C3C	2.28	1.53	1.47
39	a	1003	HEM	C3D-C2D	-2.27	1.31	1.36
42	g	601	HEA	C4B-NB	-2.27	1.36	1.40
39	d	505	HEM	CAC-C3C	2.27	1.53	1.47
39	a	1001	HEM	CAC-C3C	2.27	1.53	1.47
39	d	502	HEM	CAC-C3C	2.27	1.53	1.47
40	a	1006	CDL	OB8-CB6	-2.26	1.40	1.45
35	k	607	3PE	P-O11	2.25	1.68	1.59
35	e	501	3PE	P-O13	2.25	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	f	201	3PH	O11-C1	-2.25	1.36	1.44
36	L1	804	3PH	P-O12	-2.23	1.43	1.50
32	F	502	FMN	C10-N1	2.22	1.37	1.33
36	L	802	3PH	P-O12	-2.21	1.43	1.50
42	k	603	HEA	C4B-NB	-2.20	1.36	1.40
35	e	501	3PE	P-O11	2.20	1.68	1.59
42	g	605	HEA	C4B-NB	-2.19	1.36	1.40
36	f	201	3PH	P-O12	-2.19	1.43	1.50
42	k	605	HEA	C4B-NB	-2.18	1.36	1.40
41	e	503	HEC	C3C-C2C	-2.18	1.33	1.41
41	b	503	HEC	C3C-C2C	-2.17	1.33	1.41
35	b	502	3PE	P-O13	2.15	1.67	1.59
35	g	607	3PE	P-O13	2.14	1.67	1.59
32	F1	501	FMN	C10-N1	2.13	1.37	1.33
35	k	607	3PE	P-O13	2.13	1.67	1.59
35	b	502	3PE	P-O11	2.13	1.67	1.59
42	k	605	HEA	C1B-NB	-2.13	1.34	1.38
42	g	605	HEA	C1B-NB	-2.12	1.34	1.38
32	F1	501	FMN	C9A-N10	-2.11	1.37	1.41
32	F	502	FMN	C9A-N10	-2.08	1.37	1.41
41	e	503	HEC	C2A-C3A	-2.05	1.32	1.36
41	e	503	HEC	CMC-C2C	2.04	1.55	1.50
36	k	602	3PH	O31-C31	2.04	1.39	1.33
39	d	505	HEM	CHB-C4A	-2.04	1.34	1.39
41	b	503	HEC	CMC-C2C	2.03	1.54	1.50
39	d	502	HEM	FE-ND	-2.02	1.88	1.94
39	a	1001	HEM	CHA-C1A	-2.02	1.34	1.39
39	d	505	HEM	CHA-C1A	-2.02	1.34	1.39
42	k	603	HEA	C4C-NC	-2.01	1.35	1.39
42	k	605	HEA	C1A-NA	-2.01	1.35	1.39
41	b	503	HEC	C2A-C3A	-2.00	1.32	1.36
39	a	1001	HEM	CHB-C4A	-2.00	1.34	1.39

All (291) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	k	603	HEA	C3A-C2A-C1A	-6.83	100.59	107.05
42	g	601	HEA	C3A-C2A-C1A	-6.77	100.64	107.05
42	k	605	HEA	C3A-C2A-C1A	-6.63	100.77	107.05
42	g	605	HEA	C3A-C2A-C1A	-6.58	100.82	107.05
41	e	503	HEC	CBB-CAB-C3B	-6.41	114.62	127.43
41	b	503	HEC	CBB-CAB-C3B	-6.39	114.66	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	e	503	HEC	CBC-CAC-C3C	-5.72	116.00	127.43
41	b	503	HEC	CBC-CAC-C3C	-5.72	116.01	127.43
41	b	503	HEC	CMC-C2C-C1C	-5.68	116.76	125.42
41	e	503	HEC	CMC-C2C-C1C	-5.68	116.78	125.42
29	a	1002	U10	C6-C1-C2	5.55	123.55	119.17
29	d	501	U10	C6-C1-C2	5.17	123.25	119.17
29	B	1002	U10	C8-C7-C6	5.07	124.58	112.08
29	B1	1002	U10	C8-C7-C6	5.04	124.49	112.08
42	g	601	HEA	C2A-C1A-NA	4.97	115.12	110.32
42	k	603	HEA	C2A-C1A-NA	4.92	115.07	110.32
42	k	603	HEA	CMD-C2D-C1D	-4.59	117.86	125.03
42	g	601	HEA	CMD-C2D-C1D	-4.58	117.87	125.03
42	g	601	HEA	CMC-C2C-C3C	4.58	137.32	126.55
42	k	603	HEA	CMC-C2C-C3C	4.56	137.28	126.55
33	m	303	PC1	O12-P-O14	4.56	133.66	112.44
29	a	1004	U10	C6-C1-C2	4.54	122.75	119.17
35	b	502	3PE	O12-P-O14	4.50	133.37	112.44
33	H1	1002	PC1	O12-P-O14	4.48	133.29	112.44
33	i	304	PC1	O12-P-O14	4.47	133.24	112.44
42	k	605	HEA	CAD-CBD-CGD	-4.45	101.85	113.67
42	k	605	HEA	C2A-C1A-NA	4.45	114.62	110.32
42	g	605	HEA	CAD-CBD-CGD	-4.44	101.89	113.67
33	H1	1001	PC1	O12-P-O14	4.44	133.09	112.44
33	H	1001	PC1	O12-P-O14	4.44	133.08	112.44
33	M1	601	PC1	O12-P-O14	4.42	133.00	112.44
33	M	601	PC1	O12-P-O14	4.41	132.96	112.44
42	g	605	HEA	C2A-C1A-NA	4.40	114.56	110.32
42	g	605	HEA	CMC-C2C-C3C	4.40	136.89	126.55
35	g	607	3PE	O12-P-O14	4.39	132.84	112.44
35	k	607	3PE	O12-P-O14	4.38	132.84	112.44
42	g	601	HEA	CMB-C2B-C1B	-4.37	118.21	125.03
42	k	603	HEA	CMB-C2B-C1B	-4.35	118.23	125.03
42	k	605	HEA	CMC-C2C-C3C	4.35	136.77	126.55
42	k	605	HEA	CMD-C2D-C1D	-4.35	118.24	125.03
42	k	603	HEA	C3D-C4D-ND	4.33	114.54	110.35
35	e	501	3PE	O12-P-O14	4.31	132.52	112.44
42	g	605	HEA	CMD-C2D-C1D	-4.28	118.35	125.03
42	g	601	HEA	C3D-C4D-ND	4.28	114.48	110.35
35	m	301	3PE	O12-P-O14	4.28	132.33	112.44
35	L1	802	3PE	O12-P-O14	4.27	132.31	112.44
35	i	303	3PE	O12-P-O14	4.26	132.27	112.44
35	L	801	3PE	O12-P-O14	4.26	132.27	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	1002	U10	C7-C8-C9	-4.23	119.54	126.83
29	B1	1002	U10	C7-C8-C9	-4.22	119.56	126.83
33	n	1001	PC1	O12-P-O14	4.22	132.08	112.44
35	m	304	3PE	O12-P-O14	4.21	132.01	112.44
29	d	504	U10	C6-C1-C2	4.19	122.47	119.17
33	j	1001	PC1	O12-P-O14	4.15	131.74	112.44
33	m	302	PC1	O12-P-O14	4.13	131.65	112.44
33	i	301	PC1	O12-P-O14	4.12	131.63	112.44
42	k	605	HEA	C3D-C4D-ND	4.07	114.28	110.35
42	g	605	HEA	C3D-C4D-ND	4.05	114.26	110.35
33	L1	801	PC1	O12-P-O14	4.05	131.27	112.44
42	k	603	HEA	CAD-C3D-C4D	3.99	131.65	124.70
42	g	601	HEA	CAD-C3D-C4D	3.98	131.63	124.70
42	g	601	HEA	CMC-C2C-C1C	-3.98	119.36	125.42
42	g	605	HEA	CAA-CBA-CGA	-3.97	103.14	113.67
42	k	605	HEA	CAA-CBA-CGA	-3.96	103.16	113.67
42	k	603	HEA	CMC-C2C-C1C	-3.95	119.40	125.42
42	g	605	HEA	CMC-C2C-C1C	-3.95	119.41	125.42
42	k	603	HEA	C4D-C3D-C2D	-3.94	101.15	106.89
42	k	605	HEA	CHA-C4D-C3D	-3.94	119.03	124.77
42	g	601	HEA	C4D-C3D-C2D	-3.93	101.18	106.89
42	g	605	HEA	CHA-C4D-C3D	-3.92	119.05	124.77
29	B1	1002	U10	C6-C1-C2	3.91	122.26	119.17
42	k	605	HEA	CMC-C2C-C1C	-3.91	119.47	125.42
29	B	1002	U10	C7-C6-C5	-3.90	113.98	118.52
29	B1	1002	U10	C7-C6-C5	-3.87	114.02	118.52
29	B	1002	U10	C6-C1-C2	3.86	122.22	119.17
42	g	601	HEA	CHA-C1A-C2A	-3.76	118.92	124.86
42	k	603	HEA	CHA-C1A-C2A	-3.74	118.96	124.86
42	k	605	HEA	CMB-C2B-C1B	-3.64	119.34	125.03
42	g	605	HEA	CMB-C2B-C1B	-3.64	119.34	125.03
29	d	504	U10	C7-C6-C5	-3.59	114.35	118.52
42	k	605	HEA	CMD-C2D-C3D	3.50	135.62	126.15
42	g	605	HEA	CMD-C2D-C3D	3.49	135.58	126.15
42	k	605	HEA	CHA-C1A-C2A	-3.48	119.37	124.86
42	g	605	HEA	CHA-C1A-C2A	-3.47	119.39	124.86
42	k	605	HEA	C4D-C3D-C2D	-3.42	101.92	106.89
42	g	605	HEA	C4D-C3D-C2D	-3.39	101.95	106.89
36	L1	804	3PH	O13-P-O11	-3.38	97.84	106.67
36	L	802	3PH	O13-P-O11	-3.38	97.84	106.67
42	k	603	HEA	CMD-C2D-C3D	3.34	135.19	126.15
42	g	601	HEA	CMD-C2D-C3D	3.33	135.17	126.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	k	605	HEA	CAA-C2A-C1A	3.28	131.52	124.85
42	g	601	HEA	C3C-C2C-C1C	-3.28	103.31	107.17
32	F1	501	FMN	C4-N3-C2	-3.27	119.84	125.64
42	k	603	HEA	C3C-C2C-C1C	-3.27	103.32	107.17
42	g	605	HEA	CAA-C2A-C1A	3.27	131.49	124.85
32	F	502	FMN	C4-N3-C2	-3.25	119.87	125.64
35	i	303	3PE	C2-O21-C21	3.24	125.55	117.80
32	F1	501	FMN	C4A-C10-N10	3.23	121.10	116.48
42	g	601	HEA	CHA-C4D-C3D	-3.20	120.11	124.77
42	g	601	HEA	CMB-C2B-C3B	3.20	136.46	130.28
33	L1	801	PC1	C2-O21-C21	3.20	125.44	117.80
42	k	603	HEA	CHA-C4D-C3D	-3.18	120.14	124.77
42	k	603	HEA	CMB-C2B-C3B	3.17	136.41	130.28
42	g	605	HEA	C26-C15-C16	3.17	120.72	115.23
32	F	502	FMN	C4A-C10-N10	3.16	121.01	116.48
42	k	605	HEA	C26-C15-C16	3.16	120.71	115.23
36	f	201	3PH	O13-P-O11	-3.15	98.45	106.67
35	m	301	3PE	C2-O21-C21	3.07	125.14	117.80
33	n	1001	PC1	C2-O21-C21	2.96	124.88	117.80
39	d	505	HEM	CBD-CAD-C3D	-2.94	104.39	112.53
42	g	605	HEA	C3C-C2C-C1C	-2.94	103.70	107.17
29	d	504	U10	C22-C21-C19	-2.94	103.45	113.19
42	g	601	HEA	C26-C15-C16	2.93	120.31	115.23
39	a	1001	HEM	CBD-CAD-C3D	-2.93	104.44	112.53
42	k	603	HEA	CAA-C2A-C1A	2.92	130.79	124.85
42	g	601	HEA	CAA-C2A-C1A	2.92	130.78	124.85
33	j	1001	PC1	C2-O21-C21	2.91	124.76	117.80
42	k	605	HEA	C3C-C2C-C1C	-2.90	103.76	107.17
40	a	1006	CDL	OA6-CA5-C11	2.89	117.74	111.48
36	p	201	3PH	O13-P-O11	-2.89	99.14	106.67
42	k	603	HEA	C26-C15-C16	2.88	120.23	115.23
40	a	1006	CDL	OA8-CA6-CA4	2.86	116.64	108.40
39	d	502	HEM	CAD-CBD-CGD	-2.85	106.11	113.67
36	g	602	3PH	O13-P-O11	-2.83	99.29	106.67
39	a	1003	HEM	CAD-CBD-CGD	-2.83	106.16	113.67
41	b	503	HEC	CBD-CAD-C3D	-2.80	104.78	112.53
41	e	503	HEC	CBD-CAD-C3D	-2.79	104.81	112.53
37	L	803	P5S	O15-P12-O13	2.79	125.41	112.44
42	g	601	HEA	CAA-CBA-CGA	-2.79	106.27	113.67
42	k	603	HEA	CAA-CBA-CGA	-2.79	106.28	113.67
42	k	605	HEA	C17-C18-C19	-2.78	121.27	127.62
29	d	504	U10	C1-C6-C5	2.77	122.32	119.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	L1	803	P5S	O15-P12-O13	2.77	125.32	112.44
42	g	605	HEA	CHB-C1B-C2B	-2.77	120.66	125.03
42	g	605	HEA	C17-C18-C19	-2.76	121.30	127.62
36	p	201	3PH	O31-C31-O32	-2.76	116.72	123.63
42	k	605	HEA	CHB-C1B-C2B	-2.75	120.69	125.03
34	M1	602	DU0	C04-C03-C02	-2.71	100.63	103.85
29	B	1002	U10	C20-C19-C21	-2.71	110.52	115.23
36	k	602	3PH	O13-P-O11	-2.71	99.60	106.67
29	B1	1002	U10	C20-C19-C21	-2.68	110.58	115.23
42	g	605	HEA	C13-C12-C11	-2.66	110.14	114.39
42	k	605	HEA	C13-C12-C11	-2.65	110.17	114.39
42	g	601	HEA	CBD-CAD-C3D	-2.64	105.22	112.53
42	g	601	HEA	CHC-C1C-C2C	-2.63	119.80	127.43
42	k	605	HEA	CMB-C2B-C3B	2.61	135.33	130.28
42	k	603	HEA	CHC-C1C-C2C	-2.61	119.86	127.43
42	k	603	HEA	C12-C13-C14	2.61	119.02	112.16
42	g	605	HEA	CMB-C2B-C3B	2.61	135.32	130.28
42	k	603	HEA	CBA-CAA-C2A	2.59	119.68	112.53
41	e	503	HEC	CHC-C4B-NB	2.58	127.26	124.45
34	M	602	DU0	C04-C03-C02	-2.56	100.81	103.85
42	g	601	HEA	C12-C13-C14	2.56	118.89	112.16
41	b	503	HEC	CHC-C4B-NB	2.56	127.24	124.45
42	k	603	HEA	CHB-C1B-NB	2.54	127.16	124.42
42	k	603	HEA	CBD-CAD-C3D	-2.53	105.53	112.53
42	k	603	HEA	CHB-C1B-C2B	-2.53	121.03	125.03
36	L1	804	3PH	O31-C31-O32	-2.52	117.31	123.63
42	g	601	HEA	CBA-CAA-C2A	2.52	119.50	112.53
42	g	601	HEA	CHB-C1B-NB	2.52	127.13	124.42
36	L	802	3PH	O31-C31-O32	-2.52	117.34	123.63
36	k	602	3PH	O21-C21-O22	-2.51	117.83	123.70
32	F	502	FMN	C5A-C9A-N10	2.51	120.24	117.97
41	b	503	HEC	CHC-C4B-C3B	-2.51	120.97	125.21
29	a	1004	U10	C7-C6-C5	-2.51	115.60	118.52
42	g	605	HEA	C4B-C3B-C2B	-2.51	103.22	107.44
32	F	502	FMN	C4A-C4-N3	2.51	119.64	113.25
35	m	304	3PE	O31-C31-O32	-2.51	117.36	123.63
42	g	601	HEA	CHB-C1B-C2B	-2.51	121.07	125.03
42	k	605	HEA	C4B-C3B-C2B	-2.50	103.23	107.44
32	F1	501	FMN	C4A-C4-N3	2.50	119.62	113.25
39	d	502	HEM	C1C-CHC-C4B	-2.49	120.72	126.02
41	e	503	HEC	CHC-C4B-C3B	-2.49	121.01	125.21
36	g	602	3PH	O31-C31-O32	-2.49	117.40	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	g	601	HEA	C25-C23-C24	2.49	120.31	114.59
42	k	603	HEA	C25-C23-C24	2.48	120.31	114.59
42	k	605	HEA	C2B-C1B-NB	2.48	112.77	109.90
42	g	605	HEA	C3B-C4B-NB	2.48	112.69	109.84
39	a	1003	HEM	C1C-CHC-C4B	-2.48	120.75	126.02
29	a	1004	U10	C1-C6-C5	2.48	122.03	119.62
37	L1	803	P5S	O19-C17-O18	-2.47	117.44	123.63
42	g	605	HEA	CAD-C3D-C4D	2.47	129.00	124.70
32	F1	501	FMN	C5A-C9A-N10	2.47	120.20	117.97
42	k	605	HEA	CBA-CAA-C2A	2.47	119.35	112.53
35	g	607	3PE	O31-C31-O32	-2.46	117.46	123.63
42	g	605	HEA	CBA-CAA-C2A	2.46	119.34	112.53
42	k	605	HEA	C3B-C4B-NB	2.46	112.67	109.84
35	k	607	3PE	O31-C31-O32	-2.46	117.48	123.63
42	g	605	HEA	C27-C19-C20	2.45	119.48	115.23
37	L	803	P5S	O19-C17-O18	-2.45	117.50	123.63
32	F	502	FMN	O4-C4-C4A	-2.45	120.07	126.53
42	g	605	HEA	C2B-C1B-NB	2.45	112.73	109.90
42	k	605	HEA	CAD-C3D-C4D	2.43	128.93	124.70
29	d	501	U10	C7-C8-C9	-2.42	122.67	126.83
42	k	605	HEA	C27-C19-C20	2.41	119.41	115.23
40	a	1006	CDL	OB6-CB5-C51	2.40	116.68	111.48
42	g	605	HEA	CHC-C1C-C2C	-2.39	120.49	127.43
36	k	602	3PH	O31-C31-O32	-2.38	117.67	123.63
36	p	201	3PH	O14-P-O13	2.38	116.72	107.80
32	F1	501	FMN	O4-C4-C4A	-2.38	120.26	126.53
42	k	605	HEA	CHC-C1C-C2C	-2.37	120.55	127.43
42	g	601	HEA	C3B-C4B-NB	2.37	112.56	109.84
32	F1	501	FMN	C10-C4A-N5	-2.36	120.00	124.81
36	g	602	3PH	O21-C21-O22	-2.35	118.21	123.70
34	M1	602	DU0	O10-C09-C15	2.33	112.79	110.76
32	F	502	FMN	C10-C4A-N5	-2.31	120.10	124.81
42	k	603	HEA	O11-C11-C3B	-2.31	107.03	111.26
42	g	601	HEA	O11-C11-C3B	-2.30	107.04	111.26
42	k	603	HEA	C3B-C4B-NB	2.30	112.48	109.84
42	k	605	HEA	CBD-CAD-C3D	2.29	118.88	112.53
33	j	1001	PC1	O31-C31-O32	-2.29	117.89	123.63
33	n	1001	PC1	O31-C31-O32	-2.29	117.91	123.63
33	m	303	PC1	O12-P-O13	-2.27	97.28	107.57
42	g	605	HEA	CBD-CAD-C3D	2.26	118.78	112.53
35	e	501	3PE	O12-P-O11	-2.26	97.34	107.57
35	b	502	3PE	O31-C31-O32	-2.26	117.99	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	K	1000	DU0	C22-C21-C20	2.24	114.77	111.45
34	a	1005	DU0	O10-C09-O16	-2.24	104.56	109.88
35	L1	802	3PE	O31-C31-O32	-2.23	118.05	123.63
35	e	501	3PE	O31-C31-O32	-2.22	118.06	123.63
42	g	605	HEA	C12-C11-C3B	2.22	115.59	112.12
34	d	503	DU0	O10-C09-O16	-2.22	104.60	109.88
40	a	1006	CDL	OA8-CA7-C31	2.22	118.59	111.83
35	L	801	3PE	O31-C31-O32	-2.21	118.09	123.63
42	g	601	HEA	C4B-C3B-C2B	-2.21	103.72	107.44
42	k	603	HEA	C4B-C3B-C2B	-2.21	103.73	107.44
35	m	301	3PE	O31-C31-O32	-2.20	118.13	123.63
37	L1	803	P5S	OG-CB-CA	2.19	109.97	108.06
33	H1	1002	PC1	O31-C31-O32	-2.19	118.16	123.63
34	M	602	DU0	O10-C09-C15	2.19	112.66	110.76
33	i	304	PC1	O31-C31-O32	-2.18	118.18	123.63
36	f	201	3PH	O31-C31-O32	-2.18	118.19	123.63
33	m	303	PC1	O31-C31-O32	-2.16	118.21	123.63
36	g	602	3PH	O14-P-O11	-2.16	101.03	106.67
41	b	503	HEC	C1D-C2D-C3D	-2.16	104.34	106.82
41	e	503	HEC	C1D-C2D-C3D	-2.16	104.34	106.82
36	f	201	3PH	O14-P-O13	2.16	115.88	107.80
35	b	502	3PE	O12-P-O11	-2.16	97.80	107.57
29	a	1002	U10	C41-C39-C38	2.14	125.98	121.17
41	e	503	HEC	CAA-CBA-CGA	-2.14	107.98	113.67
41	b	503	HEC	CAA-CBA-CGA	-2.14	108.00	113.67
29	B1	1002	U10	C47-C48-C49	-2.14	122.73	127.62
42	k	603	HEA	C27-C19-C20	2.14	118.94	115.23
33	M	601	PC1	O31-C31-O32	-2.14	118.29	123.63
35	L	801	3PE	O21-C21-O22	-2.13	118.72	123.70
36	L	802	3PH	O14-P-O13	2.13	115.79	107.80
36	L1	804	3PH	O14-P-O13	2.12	115.76	107.80
35	L1	802	3PE	O21-C21-O22	-2.12	118.75	123.70
33	M1	601	PC1	O31-C31-O32	-2.12	118.34	123.63
39	a	1003	HEM	C4C-CHD-C1D	-2.12	121.52	126.02
29	a	1004	U10	C42-C41-C39	2.11	120.17	113.19
39	a	1001	HEM	CAA-CBA-CGA	-2.11	108.07	113.67
42	k	605	HEA	CHA-C4D-ND	2.11	126.69	124.42
39	d	505	HEM	CAA-CBA-CGA	-2.10	108.09	113.67
42	g	605	HEA	CHA-C4D-ND	2.10	126.68	124.42
29	d	501	U10	C7-C6-C5	-2.10	116.08	118.52
37	L	803	P5S	OG-CB-CA	2.10	109.89	108.06
36	k	602	3PH	O14-P-O11	-2.10	101.20	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	1002	U10	C47-C48-C49	-2.10	122.83	127.62
41	b	503	HEC	CMD-C2D-C1D	2.10	128.61	125.42
29	d	501	U10	C1M-C1-C2	-2.09	109.77	116.93
35	g	607	3PE	O12-P-O11	-2.09	98.08	107.57
35	k	607	3PE	O12-P-O11	-2.09	98.08	107.57
41	e	503	HEC	CMD-C2D-C1D	2.09	128.60	125.42
42	k	605	HEA	CHD-C1D-ND	2.09	126.95	124.37
42	k	605	HEA	C12-C11-C3B	2.09	115.39	112.12
39	d	502	HEM	C4C-CHD-C1D	-2.08	121.60	126.02
36	p	201	3PH	O14-P-O11	-2.07	101.27	106.67
36	L	802	3PH	O14-P-O11	-2.07	101.28	106.67
42	k	603	HEA	CBC-CAC-C3C	-2.07	117.19	127.53
42	g	605	HEA	CHD-C1D-C2D	-2.07	121.08	126.95
42	g	605	HEA	CHD-C1D-ND	2.06	126.92	124.37
42	k	605	HEA	CHD-C1D-C2D	-2.06	121.10	126.95
34	M1	602	DU0	C08-C07-C09	-2.06	111.62	114.94
42	g	601	HEA	CHC-C4B-C3B	-2.05	120.62	125.80
33	m	302	PC1	O21-C21-O22	-2.05	118.91	123.70
35	m	301	3PE	O12-P-O11	-2.05	98.28	107.57
42	g	601	HEA	C27-C19-C20	2.05	118.78	115.23
34	M1	602	DU0	C15-C09-C07	-2.05	111.95	115.66
36	L1	804	3PH	O14-P-O11	-2.04	101.34	106.67
42	k	603	HEA	CHD-C1D-ND	2.04	126.89	124.37
35	L1	802	3PE	O12-P-O11	-2.04	98.33	107.57
29	a	1004	U10	C37-C38-C39	-2.04	122.96	127.62
42	g	601	HEA	CBC-CAC-C3C	-2.03	117.36	127.53
35	L	801	3PE	O12-P-O11	-2.03	98.35	107.57
42	g	605	HEA	CHB-C1B-NB	2.03	126.61	124.42
42	k	603	HEA	CHC-C4B-C3B	-2.03	120.68	125.80
36	f	201	3PH	O31-C3-C2	2.03	114.24	108.40
35	b	502	3PE	O21-C21-O22	-2.03	118.97	123.70
36	g	602	3PH	O32-C31-C32	2.00	131.61	123.78
41	b	503	HEC	CHC-C1C-C2C	-2.00	121.62	127.43

There are no chirality outliers.

All (435) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	B	1002	U10	C1-C6-C7-C8
29	B	1002	U10	C5-C6-C7-C8
29	B	1002	U10	C16-C17-C18-C19
29	B1	1002	U10	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	B1	1002	U10	C5-C6-C7-C8
29	B1	1002	U10	C16-C17-C18-C19
33	H	1001	PC1	C11-O13-P-O11
33	H	1001	PC1	C12-C11-O13-P
33	H	1001	PC1	O13-C11-C12-N
33	H1	1001	PC1	C11-O13-P-O11
33	H1	1001	PC1	C12-C11-O13-P
33	H1	1001	PC1	O13-C11-C12-N
33	H1	1002	PC1	C11-O13-P-O12
33	H1	1002	PC1	C1-O11-P-O12
33	L1	801	PC1	C11-O13-P-O14
33	L1	801	PC1	C1-O11-P-O12
33	L1	801	PC1	C12-C11-O13-P
33	L1	801	PC1	C2-C1-O11-P
33	L1	801	PC1	O21-C2-C3-O31
33	M	601	PC1	C11-O13-P-O12
33	M	601	PC1	C11-O13-P-O11
33	M1	601	PC1	C11-O13-P-O12
33	M1	601	PC1	C11-O13-P-O11
33	i	301	PC1	C1-O11-P-O14
33	i	301	PC1	C1-O11-P-O13
33	i	304	PC1	C1-O11-P-O12
33	i	304	PC1	C2-C1-O11-P
33	j	1001	PC1	C1-O11-P-O14
33	j	1001	PC1	C12-C11-O13-P
33	m	302	PC1	C1-O11-P-O14
33	m	302	PC1	C1-O11-P-O13
33	m	303	PC1	C2-C1-O11-P
33	m	303	PC1	O21-C2-C3-O31
33	n	1001	PC1	C11-O13-P-O12
33	n	1001	PC1	C1-O11-P-O13
33	n	1001	PC1	C12-C11-O13-P
33	n	1001	PC1	C2-C1-O11-P
35	L	801	3PE	C1-O11-P-O13
35	L	801	3PE	C1-O11-P-O14
35	L	801	3PE	C12-C11-O13-P
35	L1	802	3PE	C1-O11-P-O13
35	L1	802	3PE	C1-O11-P-O14
35	L1	802	3PE	C12-C11-O13-P
35	b	502	3PE	C1-O11-P-O13
35	b	502	3PE	C2-C1-O11-P
35	e	501	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
35	e	501	3PE	C1-O11-P-O13
35	e	501	3PE	C1-O11-P-O14
35	e	501	3PE	C12-C11-O13-P
35	g	607	3PE	C11-O13-P-O11
35	g	607	3PE	C11-O13-P-O12
35	g	607	3PE	C11-O13-P-O14
35	g	607	3PE	O13-C11-C12-N
35	i	303	3PE	C11-O13-P-O12
35	i	303	3PE	C12-C11-O13-P
35	k	607	3PE	C11-O13-P-O11
35	k	607	3PE	C11-O13-P-O12
35	k	607	3PE	C11-O13-P-O14
35	k	607	3PE	O13-C11-C12-N
35	m	301	3PE	C11-O13-P-O12
35	m	304	3PE	C12-C11-O13-P
36	f	201	3PH	C1-O11-P-O13
36	f	201	3PH	C1-O11-P-O14
36	f	201	3PH	C1-O11-P-O12
36	p	201	3PH	C2-C1-O11-P
37	L1	803	P5S	CB-OG-P12-O13
39	a	1001	HEM	C2B-C3B-CAB-CBB
39	a	1001	HEM	C4B-C3B-CAB-CBB
39	a	1001	HEM	C2C-C3C-CAC-CBC
39	a	1003	HEM	C2C-C3C-CAC-CBC
39	a	1003	HEM	C4C-C3C-CAC-CBC
39	d	502	HEM	C2C-C3C-CAC-CBC
39	d	502	HEM	C4C-C3C-CAC-CBC
39	d	505	HEM	C2B-C3B-CAB-CBB
39	d	505	HEM	C4B-C3B-CAB-CBB
39	d	505	HEM	C2C-C3C-CAC-CBC
40	a	1006	CDL	CB3-OB5-PB2-OB2
40	a	1006	CDL	CB3-OB5-PB2-OB3
40	a	1006	CDL	CB3-OB5-PB2-OB4
40	a	1006	CDL	CB4-CB3-OB5-PB2
41	b	503	HEC	C2B-C3B-CAB-CBB
41	b	503	HEC	C4B-C3B-CAB-CBB
41	b	503	HEC	C4C-C3C-CAC-CBC
41	e	503	HEC	C2B-C3B-CAB-CBB
41	e	503	HEC	C4B-C3B-CAB-CBB
41	e	503	HEC	C4C-C3C-CAC-CBC
29	a	1004	U10	C25-C24-C26-C27
29	a	1004	U10	C23-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
29	d	501	U10	C38-C39-C41-C42
29	a	1002	U10	C44-C46-C47-C48
36	f	201	3PH	C2-C1-O11-P
29	d	501	U10	C40-C39-C41-C42
32	F1	501	FMN	C2'-C3'-C4'-C5'
35	k	607	3PE	C21-C22-C23-C24
35	g	607	3PE	C21-C22-C23-C24
33	j	1001	PC1	C2-C1-O11-P
33	M	601	PC1	C23-C24-C25-C26
33	M1	601	PC1	C23-C24-C25-C26
32	F1	501	FMN	O3'-C3'-C4'-C5'
36	L	802	3PH	C28-C29-C2A-C2B
33	M	601	PC1	C31-C32-C33-C34
33	M1	601	PC1	C31-C32-C33-C34
33	i	304	PC1	C3C-C3D-C3E-C3F
36	p	201	3PH	C29-C2A-C2B-C2C
37	L	803	P5S	C42-C43-C44-C45
36	p	201	3PH	C2D-C2E-C2F-C2G
33	H	1001	PC1	C3B-C3C-C3D-C3E
33	H1	1001	PC1	C3B-C3C-C3D-C3E
33	m	303	PC1	C3C-C3D-C3E-C3F
35	L	801	3PE	C2A-C2B-C2C-C2D
35	L1	802	3PE	C2A-C2B-C2C-C2D
37	L1	803	P5S	C42-C43-C44-C45
33	n	1001	PC1	C33-C34-C35-C36
35	L	801	3PE	C35-C36-C37-C38
35	L1	802	3PE	C35-C36-C37-C38
33	m	302	PC1	C2E-C2F-C2G-C2H
36	k	602	3PH	C34-C35-C36-C37
39	a	1001	HEM	C4C-C3C-CAC-CBC
39	d	505	HEM	C4C-C3C-CAC-CBC
35	m	301	3PE	C3E-C3F-C3G-C3H
35	i	303	3PE	O21-C2-C3-O31
40	a	1006	CDL	OA6-CA4-CA6-OA8
33	L1	801	PC1	C39-C3A-C3B-C3C
33	i	301	PC1	C2D-C2E-C2F-C2G
36	p	201	3PH	C38-C39-C3A-C3B
35	i	303	3PE	C3E-C3F-C3G-C3H
33	H1	1002	PC1	O11-C1-C2-C3
40	a	1006	CDL	OB5-CB3-CB4-CB6
32	F1	501	FMN	O3'-C3'-C4'-O4'
36	f	201	3PH	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
29	d	504	U10	C25-C24-C26-C27
29	d	504	U10	C23-C24-C26-C27
35	i	303	3PE	C1-C2-C3-O31
35	m	304	3PE	C1-C2-C3-O31
35	k	607	3PE	C39-C3A-C3B-C3C
29	d	504	U10	C48-C49-C51-C52
36	L1	804	3PH	C28-C29-C2A-C2B
32	F1	501	FMN	C5'-O5'-P-O1P
35	i	303	3PE	C3A-C3B-C3C-C3D
33	L1	801	PC1	O11-C1-C2-O21
32	F1	501	FMN	C2'-C3'-C4'-O4'
29	d	504	U10	C50-C49-C51-C52
29	B	1002	U10	C43-C44-C46-C47
33	H1	1001	PC1	C2A-C2B-C2C-C2D
33	H	1001	PC1	C2A-C2B-C2C-C2D
33	H	1001	PC1	O21-C2-C3-O31
33	H1	1001	PC1	O21-C2-C3-O31
42	g	605	HEA	C3B-C11-C12-C13
42	k	605	HEA	C3B-C11-C12-C13
40	a	1006	CDL	C17-C18-C19-C20
29	d	504	U10	C15-C14-C16-C17
35	b	502	3PE	C28-C29-C2A-C2B
35	g	607	3PE	C39-C3A-C3B-C3C
35	e	501	3PE	C2-C1-O11-P
35	m	304	3PE	C2-C1-O11-P
39	a	1003	HEM	C2A-CAA-CBA-CGA
35	e	501	3PE	C28-C29-C2A-C2B
29	B	1002	U10	C45-C44-C46-C47
29	a	1004	U10	C35-C34-C36-C37
40	a	1006	CDL	C32-C33-C34-C35
33	L1	801	PC1	C1-C2-C3-O31
40	a	1006	CDL	CA3-CA4-CA6-OA8
33	H1	1002	PC1	O11-C1-C2-O21
36	f	201	3PH	O11-C1-C2-O21
40	a	1006	CDL	C1-CA2-OA2-PA1
39	d	502	HEM	C2A-CAA-CBA-CGA
40	a	1006	CDL	OB6-CB4-CB6-OB8
29	B	1002	U10	C50-C49-C51-C52
33	n	1001	PC1	C32-C33-C34-C35
37	L	803	P5S	OXT-C-CA-N
37	L1	803	P5S	OXT-C-CA-N
36	g	602	3PH	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
29	B	1002	U10	C14-C16-C17-C18
35	k	607	3PE	C28-C29-C2A-C2B
29	B	1002	U10	C48-C49-C51-C52
29	a	1004	U10	C13-C14-C16-C17
29	d	504	U10	C12-C11-C9-C8
29	d	504	U10	C13-C14-C16-C17
29	d	501	U10	C1-C6-C7-C8
35	e	501	3PE	C29-C2A-C2B-C2C
35	m	301	3PE	O11-C1-C2-O21
40	a	1006	CDL	OB5-CB3-CB4-OB6
29	B1	1002	U10	C14-C16-C17-C18
29	a	1004	U10	C15-C14-C16-C17
29	d	504	U10	C12-C11-C9-C10
29	d	501	U10	C5-C6-C7-C8
33	M	601	PC1	C12-C11-O13-P
33	M1	601	PC1	C12-C11-O13-P
33	i	301	PC1	C12-C11-O13-P
33	i	304	PC1	C12-C11-O13-P
33	m	302	PC1	C12-C11-O13-P
35	b	502	3PE	C12-C11-O13-P
35	m	301	3PE	C12-C11-O13-P
35	m	301	3PE	O21-C2-C3-O31
35	m	304	3PE	O21-C2-C3-O31
35	b	502	3PE	C26-C27-C28-C29
35	e	501	3PE	C26-C27-C28-C29
35	g	607	3PE	C28-C29-C2A-C2B
40	a	1006	CDL	C1-CB2-OB2-PB2
33	L1	801	PC1	O13-C11-C12-N
33	i	301	PC1	O13-C11-C12-N
33	i	304	PC1	O13-C11-C12-N
33	j	1001	PC1	O13-C11-C12-N
33	m	302	PC1	O13-C11-C12-N
33	m	303	PC1	O13-C11-C12-N
33	n	1001	PC1	O13-C11-C12-N
29	a	1004	U10	C45-C44-C46-C47
29	a	1004	U10	C33-C34-C36-C37
33	M	601	PC1	C3A-C3B-C3C-C3D
33	M1	601	PC1	C3A-C3B-C3C-C3D
29	a	1002	U10	C45-C44-C46-C47
42	g	601	HEA	C26-C15-C16-C17
42	k	603	HEA	C26-C15-C16-C17
35	e	501	3PE	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
33	L1	801	PC1	O11-C1-C2-C3
35	b	502	3PE	C29-C2A-C2B-C2C
36	g	602	3PH	C34-C35-C36-C37
33	n	1001	PC1	O21-C2-C3-O31
33	H	1001	PC1	C1-C2-C3-O31
33	m	303	PC1	C1-C2-C3-O31
29	B	1002	U10	C35-C34-C36-C37
33	H	1001	PC1	C11-O13-P-O14
33	H	1001	PC1	C1-O11-P-O12
33	H	1001	PC1	C1-O11-P-O14
33	H1	1001	PC1	C11-O13-P-O14
33	H1	1001	PC1	C1-O11-P-O12
33	H1	1001	PC1	C1-O11-P-O14
33	L1	801	PC1	C11-O13-P-O11
33	M	601	PC1	C11-O13-P-O14
33	M1	601	PC1	C11-O13-P-O14
33	m	303	PC1	C1-O11-P-O14
33	n	1001	PC1	C1-O11-P-O14
35	b	502	3PE	C1-O11-P-O14
35	m	304	3PE	C1-O11-P-O14
32	F	502	FMN	C4'-C5'-O5'-P
32	F1	501	FMN	C4'-C5'-O5'-P
33	i	301	PC1	C2-C1-O11-P
33	m	302	PC1	C2-C1-O11-P
35	i	303	3PE	C2-C1-O11-P
33	i	304	PC1	C3A-C3B-C3C-C3D
33	n	1001	PC1	C1-C2-O21-C21
29	a	1002	U10	C9-C11-C12-C13
36	f	201	3PH	O11-C1-C2-C3
33	L1	801	PC1	C21-C22-C23-C24
42	g	605	HEA	C27-C19-C20-C21
29	a	1004	U10	C43-C44-C46-C47
35	m	304	3PE	C2C-C2D-C2E-C2F
29	B	1002	U10	C5-C4-O4-C4M
29	B1	1002	U10	C5-C4-O4-C4M
42	k	605	HEA	C27-C19-C20-C21
29	a	1004	U10	C44-C46-C47-C48
33	H1	1001	PC1	C1-C2-C3-O31
33	n	1001	PC1	C1-C2-C3-O31
33	H1	1001	PC1	C23-C24-C25-C26
35	L	801	3PE	C36-C37-C38-C39
33	L1	801	PC1	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
33	H	1001	PC1	C23-C24-C25-C26
29	a	1002	U10	C43-C44-C46-C47
39	a	1003	HEM	C2B-C3B-CAB-CBB
39	d	502	HEM	C2B-C3B-CAB-CBB
35	L1	802	3PE	C36-C37-C38-C39
36	g	602	3PH	C21-C22-C23-C24
42	k	605	HEA	C18-C19-C20-C21
33	M1	601	PC1	O11-C1-C2-C3
33	H1	1002	PC1	C39-C3A-C3B-C3C
35	b	502	3PE	C3A-C3B-C3C-C3D
36	p	201	3PH	C34-C35-C36-C37
33	i	304	PC1	O21-C2-C3-O31
33	j	1001	PC1	O21-C2-C3-O31
33	j	1001	PC1	C23-C24-C25-C26
29	d	504	U10	C35-C34-C36-C37
42	g	605	HEA	C18-C19-C20-C21
35	b	502	3PE	C23-C24-C25-C26
29	a	1004	U10	C20-C19-C21-C22
29	d	504	U10	C40-C39-C41-C42
42	g	601	HEA	C14-C15-C16-C17
42	k	603	HEA	C14-C15-C16-C17
36	k	602	3PH	C21-C22-C23-C24
33	i	304	PC1	C1-C2-C3-O31
36	L1	804	3PH	C37-C38-C39-C3A
36	g	602	3PH	C27-C28-C29-C2A
33	j	1001	PC1	C1-C2-O21-C21
35	i	303	3PE	C3-C2-O21-C21
35	m	301	3PE	C3-C2-O21-C21
40	a	1006	CDL	CA3-CA4-OA6-CA5
41	e	503	HEC	CAA-CBA-CGA-O1A
29	d	501	U10	C50-C49-C51-C52
29	d	504	U10	C38-C39-C41-C42
35	e	501	3PE	C3A-C3B-C3C-C3D
41	b	503	HEC	CAA-CBA-CGA-O1A
42	g	605	HEA	CAD-CBD-CGD-O1D
29	d	504	U10	C4-C3-O3-C3M
39	a	1001	HEM	CAD-CBD-CGD-O1D
40	a	1006	CDL	C37-C38-C39-C40
36	k	602	3PH	C2-C1-O11-P
40	a	1006	CDL	CA4-CA3-OA5-PA1
39	a	1003	HEM	CAA-CBA-CGA-O2A
39	d	502	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
39	d	505	HEM	CAD-CBD-CGD-O1D
29	d	504	U10	C30-C29-C31-C32
33	M	601	PC1	O11-C1-C2-C3
35	m	301	3PE	O11-C1-C2-C3
35	m	304	3PE	O11-C1-C2-C3
29	d	504	U10	C33-C34-C36-C37
42	g	605	HEA	CAD-CBD-CGD-O2D
33	n	1001	PC1	C3A-C3B-C3C-C3D
36	L	802	3PH	C37-C38-C39-C3A
33	j	1001	PC1	C32-C33-C34-C35
33	n	1001	PC1	C36-C37-C38-C39
39	a	1003	HEM	CAA-CBA-CGA-O1A
39	d	502	HEM	CAA-CBA-CGA-O1A
33	j	1001	PC1	C3A-C3B-C3C-C3D
33	i	304	PC1	C31-C32-C33-C34
35	m	301	3PE	C3B-C3C-C3D-C3E
35	i	303	3PE	C2-C3-O31-C31
35	i	303	3PE	C31-C32-C33-C34
42	k	605	HEA	CAD-CBD-CGD-O1D
35	m	301	3PE	C39-C3A-C3B-C3C
36	f	201	3PH	C3C-C3D-C3E-C3F
42	k	605	HEA	CAD-CBD-CGD-O2D
33	n	1001	PC1	C23-C24-C25-C26
33	m	303	PC1	C36-C37-C38-C39
29	d	501	U10	C45-C44-C46-C47
39	a	1001	HEM	CAD-CBD-CGD-O2D
29	a	1004	U10	C18-C19-C21-C22
39	d	505	HEM	CAD-CBD-CGD-O2D
42	g	601	HEA	CAD-CBD-CGD-O2D
40	a	1006	CDL	C81-C82-C83-C84
40	a	1006	CDL	C44-C45-C46-C47
29	a	1004	U10	C39-C41-C42-C43
39	d	505	HEM	CAA-CBA-CGA-O2A
41	b	503	HEC	CAA-CBA-CGA-O2A
42	k	603	HEA	CAD-CBD-CGD-O2D
33	M	601	PC1	O11-C1-C2-O21
33	M1	601	PC1	O11-C1-C2-O21
39	a	1001	HEM	CAA-CBA-CGA-O2A
41	e	503	HEC	CAA-CBA-CGA-O2A
35	b	502	3PE	C24-C25-C26-C27
42	g	601	HEA	CAA-CBA-CGA-O2A
42	k	603	HEA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
36	L	802	3PH	O11-C1-C2-C3
36	L1	804	3PH	O11-C1-C2-C3
36	k	602	3PH	O21-C2-C3-O31
39	a	1003	HEM	CAD-CBD-CGD-O2D
29	d	501	U10	C48-C49-C51-C52
39	d	502	HEM	CAD-CBD-CGD-O2D
33	i	304	PC1	C3D-C3E-C3F-C3G
39	a	1003	HEM	CAD-CBD-CGD-O1D
39	d	502	HEM	CAD-CBD-CGD-O1D
33	j	1001	PC1	C33-C34-C35-C36
32	F1	501	FMN	C5'-O5'-P-O3P
36	L	802	3PH	C1-O11-P-O14
36	L1	804	3PH	C1-O11-P-O14
36	p	201	3PH	C1-O11-P-O14
36	p	201	3PH	C1-O11-P-O12
39	d	505	HEM	CAA-CBA-CGA-O1A
29	d	504	U10	C28-C29-C31-C32
33	m	303	PC1	C2A-C2B-C2C-C2D
39	a	1001	HEM	CAA-CBA-CGA-O1A
33	m	303	PC1	O31-C31-C32-C33
33	L1	801	PC1	C3-C2-O21-C21
42	k	603	HEA	CAD-CBD-CGD-O1D
33	n	1001	PC1	C3C-C3D-C3E-C3F
29	B	1002	U10	C33-C34-C36-C37
42	g	601	HEA	CAD-CBD-CGD-O1D
36	L	802	3PH	O11-C1-C2-O21
36	L1	804	3PH	O11-C1-C2-O21
40	a	1006	CDL	CB3-CB4-CB6-OB8
39	a	1003	HEM	C4B-C3B-CAB-CBB
39	d	502	HEM	C4B-C3B-CAB-CBB
42	k	603	HEA	CAA-CBA-CGA-O1A
33	M	601	PC1	C2E-C2F-C2G-C2H
33	m	303	PC1	C3D-C3E-C3F-C3G
35	b	502	3PE	O21-C21-C22-C23
42	g	601	HEA	CAA-CBA-CGA-O1A
35	i	303	3PE	C23-C24-C25-C26
36	g	602	3PH	C3B-C3C-C3D-C3E
29	a	1002	U10	C4-C3-O3-C3M
29	d	501	U10	C3-C4-O4-C4M
33	M	601	PC1	C2A-C2B-C2C-C2D
33	M1	601	PC1	C2A-C2B-C2C-C2D
35	e	501	3PE	C2F-C2G-C2H-C2I

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Mol	Chain	Res	Type	Atoms
36	p	201	3PH	C3C-C3D-C3E-C3F
32	F1	501	FMN	O2'-C2'-C3'-O3'
32	F1	501	FMN	O2'-C2'-C3'-C4'
35	b	502	3PE	C2F-C2G-C2H-C2I
37	L	803	P5S	C29-C30-C31-C32
29	a	1002	U10	C29-C31-C32-C33
41	b	503	HEC	CAD-CBD-CGD-O1D
29	B	1002	U10	C25-C24-C26-C27
29	B1	1002	U10	C25-C24-C26-C27
37	L1	803	P5S	C29-C30-C31-C32
41	e	503	HEC	CAD-CBD-CGD-O1D
29	d	501	U10	C30-C29-C31-C32
29	B1	1002	U10	C12-C11-C9-C8
36	k	602	3PH	O21-C21-C22-C23
36	k	602	3PH	C39-C3A-C3B-C3C
33	j	1001	PC1	C1-C2-C3-O31
33	n	1001	PC1	C22-C23-C24-C25
42	g	601	HEA	C20-C21-C22-C23
40	a	1006	CDL	C15-C16-C17-C18
29	a	1004	U10	C41-C42-C43-C44
33	L1	801	PC1	C1-C2-O21-C21
35	m	301	3PE	C1-C2-O21-C21
33	m	303	PC1	C3A-C3B-C3C-C3D
33	L1	801	PC1	C29-C2A-C2B-C2C
42	k	603	HEA	C20-C21-C22-C23
36	L1	804	3PH	C2-C1-O11-P
33	n	1001	PC1	O31-C31-C32-C33
35	g	607	3PE	O31-C31-C32-C33
35	k	607	3PE	O31-C31-C32-C33
35	k	607	3PE	C36-C37-C38-C39
33	m	303	PC1	C3B-C3C-C3D-C3E
33	L1	801	PC1	O21-C21-C22-C23
41	e	503	HEC	CAD-CBD-CGD-O2D
33	j	1001	PC1	C3C-C3D-C3E-C3F
40	a	1006	CDL	C78-C79-C80-C81
33	n	1001	PC1	O32-C31-C32-C33
35	L1	802	3PE	O21-C21-C22-C23
29	B	1002	U10	C12-C11-C9-C8
29	B1	1002	U10	C23-C24-C26-C27
41	b	503	HEC	CAD-CBD-CGD-O2D
35	g	607	3PE	O32-C31-C32-C33
35	L	801	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
35	b	502	3PE	O22-C21-C22-C23
36	k	602	3PH	O22-C21-C22-C23
29	a	1002	U10	C1-C6-C7-C8
33	L1	801	PC1	O22-C21-C22-C23
35	k	607	3PE	O32-C31-C32-C33
29	a	1002	U10	C24-C26-C27-C28
35	i	303	3PE	C29-C2A-C2B-C2C
36	p	201	3PH	C26-C27-C28-C29
35	g	607	3PE	O21-C21-C22-C23
35	k	607	3PE	O21-C21-C22-C23
33	j	1001	PC1	O32-C31-C32-C33

There are no ring outliers.

33 monomers are involved in 68 short contacts:

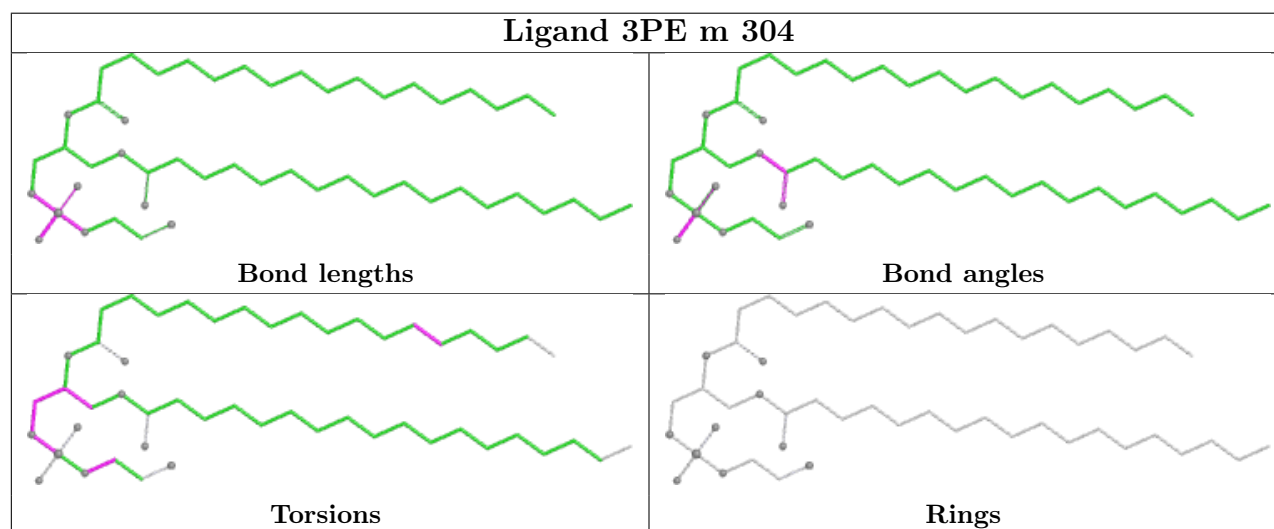
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	B	1002	U10	1	0
31	E	401	FES	1	0
32	F1	501	FMN	1	0
28	F	501	SF4	1	0
33	H1	1002	PC1	1	0
32	F	502	FMN	2	0
35	e	501	3PE	1	0
33	H	1001	PC1	1	0
33	i	304	PC1	7	0
39	a	1001	HEM	2	0
42	g	605	HEA	1	0
29	d	501	U10	7	0
33	m	302	PC1	2	0
33	i	301	PC1	1	0
39	a	1003	HEM	2	0
29	d	504	U10	5	0
33	j	1001	PC1	5	0
40	a	1006	CDL	1	0
33	m	303	PC1	1	0
29	a	1004	U10	1	0
35	g	607	3PE	2	0
33	H1	1001	PC1	1	0
31	E1	401	FES	1	0
39	d	505	HEM	2	0
41	e	503	HEC	1	0
42	k	603	HEA	2	0

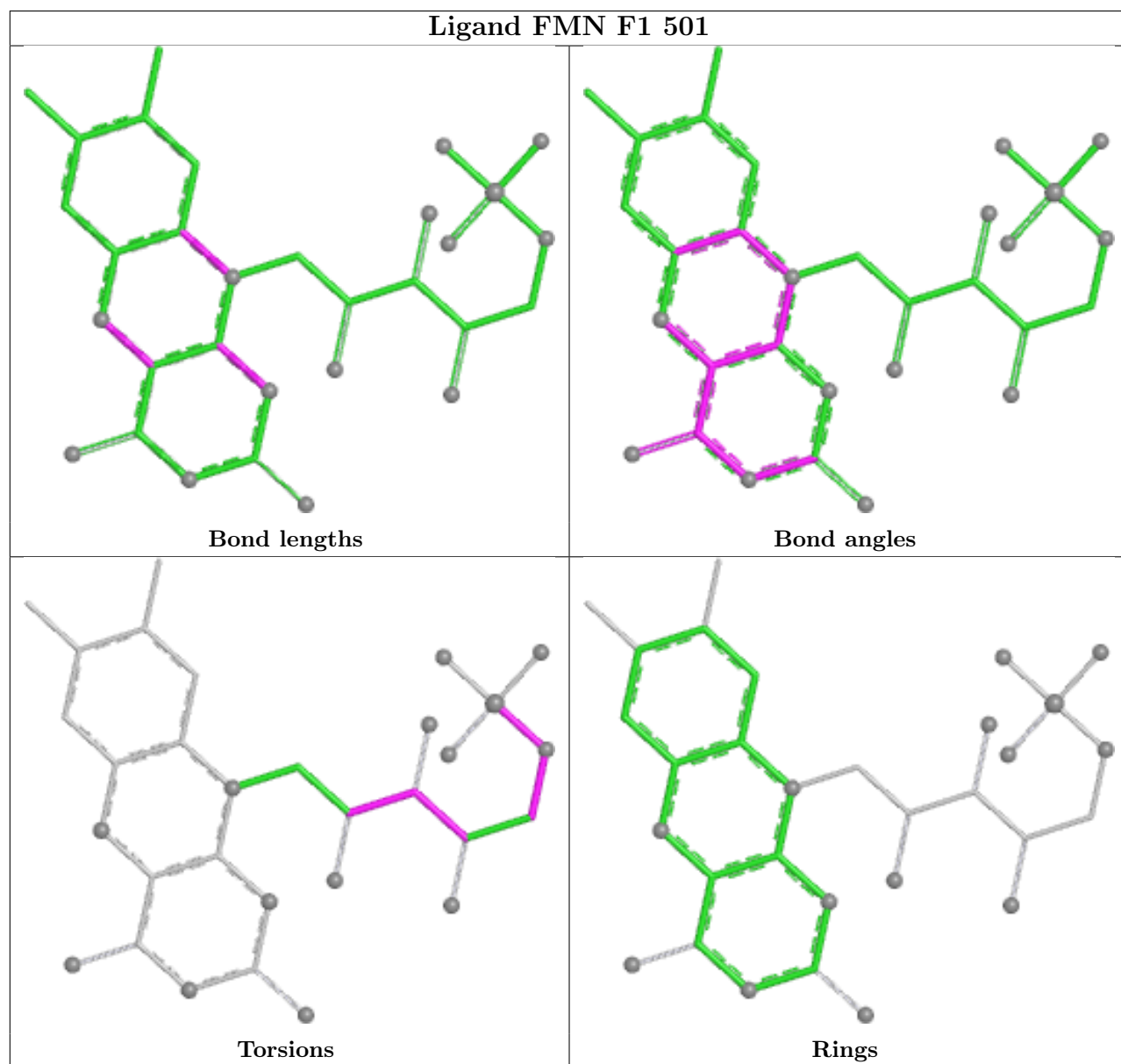
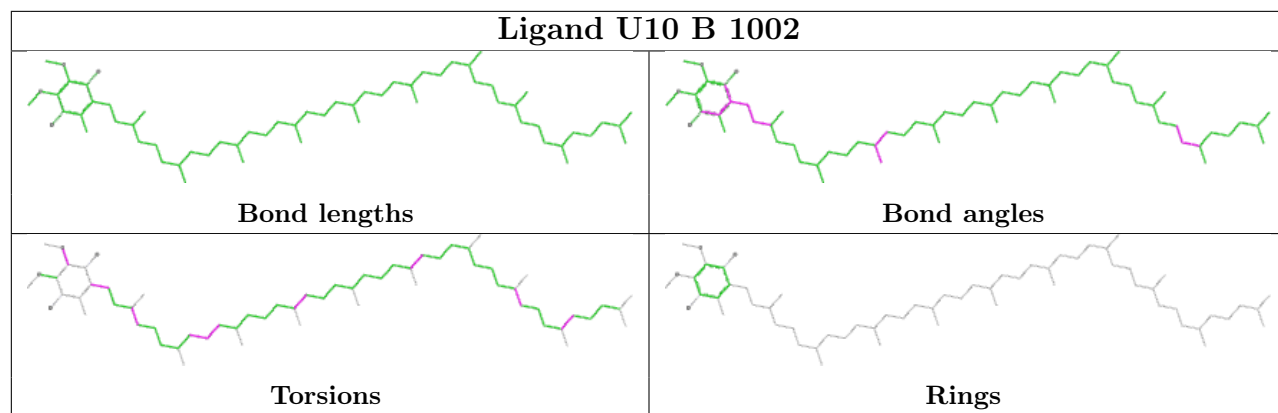
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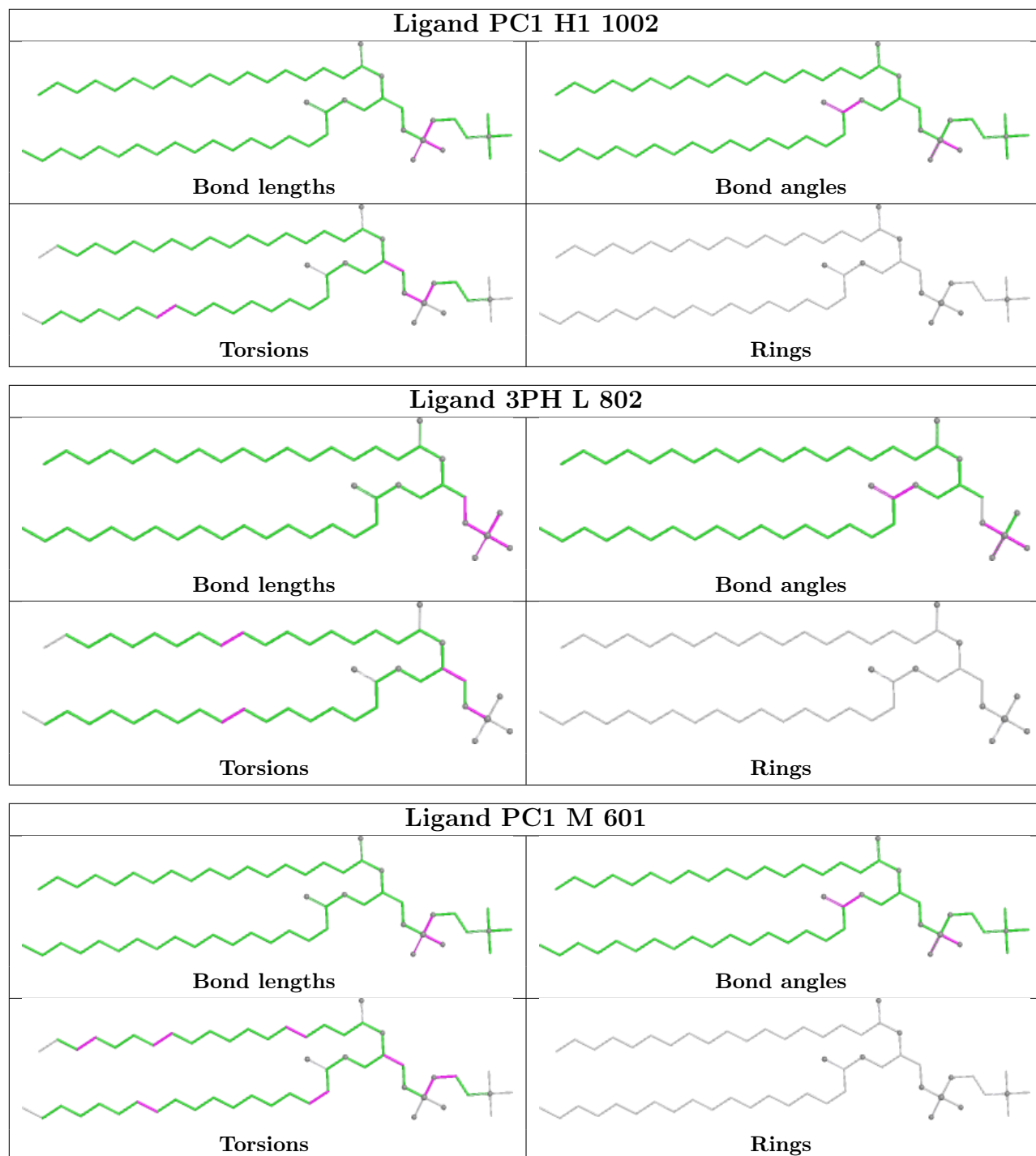
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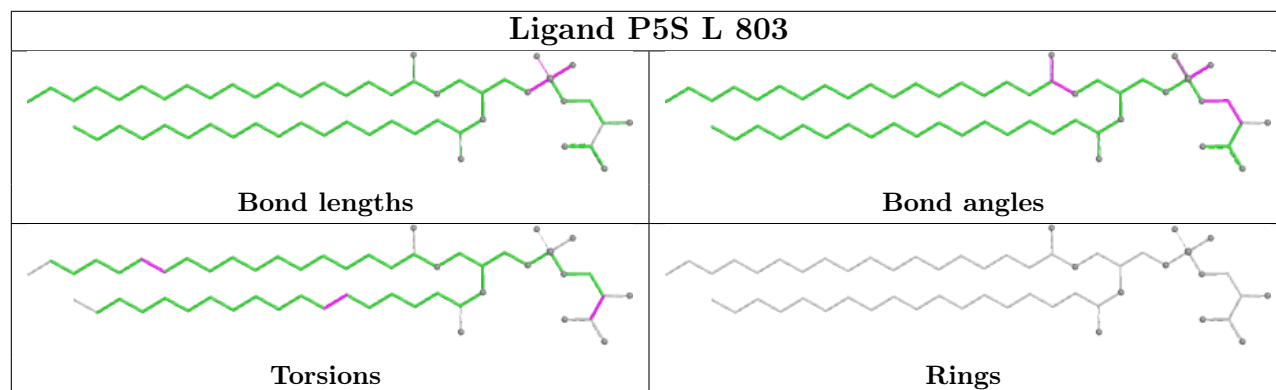
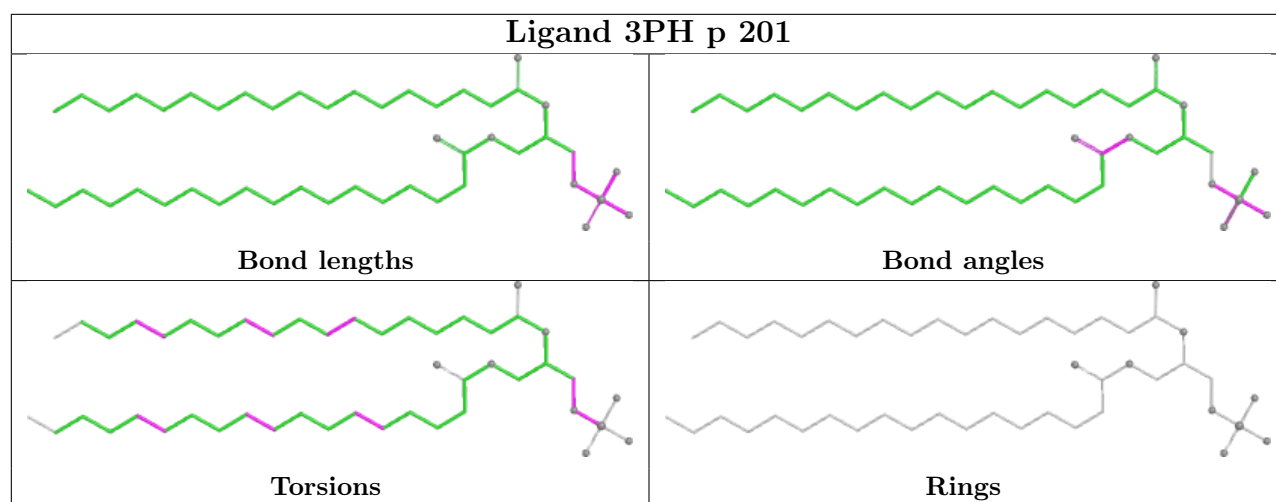
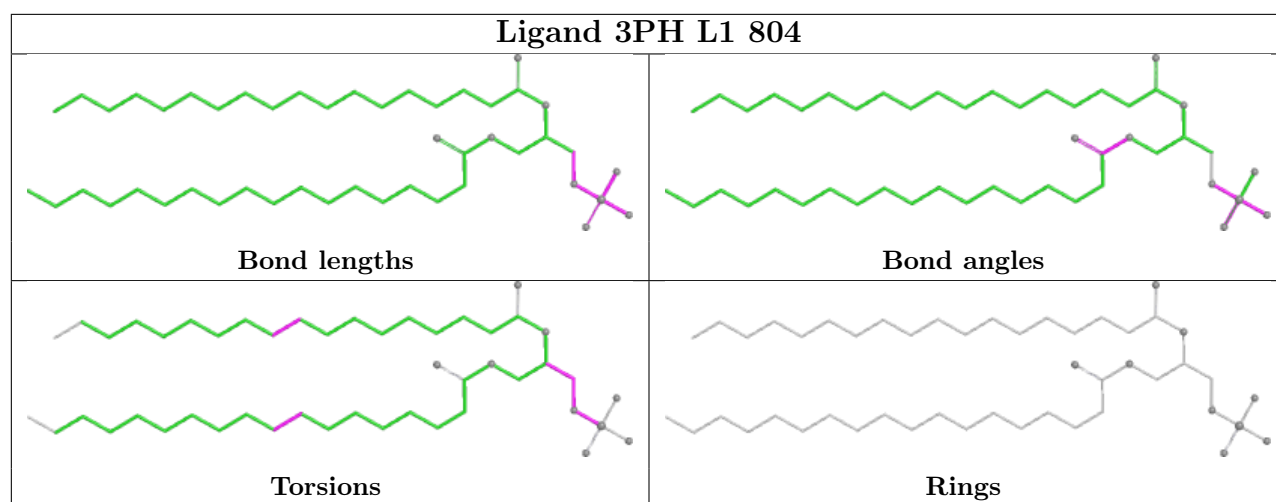
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	k	607	3PE	2	0
42	k	605	HEA	1	0
29	a	1002	U10	14	0
39	d	502	HEM	2	0
28	F1	502	SF4	1	0
42	g	601	HEA	1	0
41	b	503	HEC	1	0

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

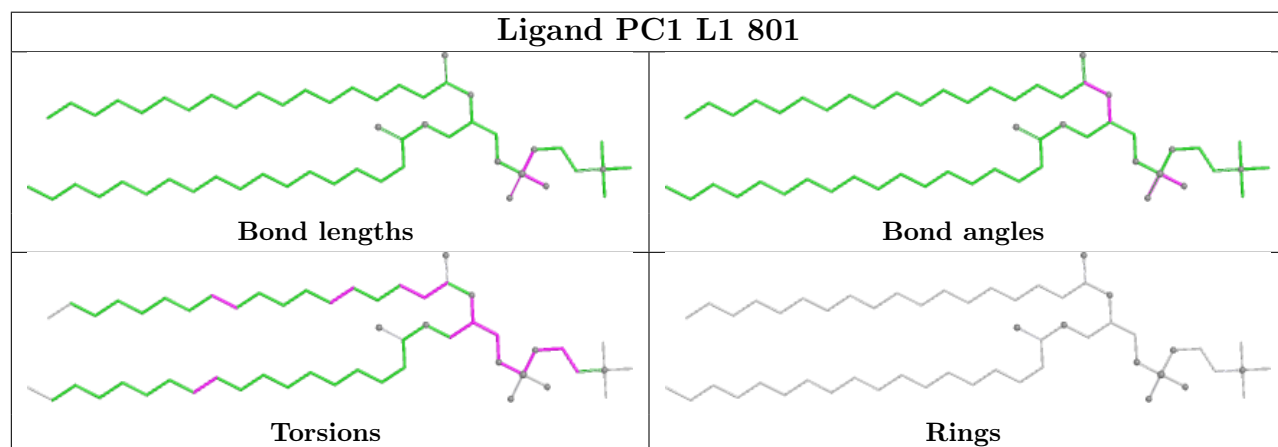
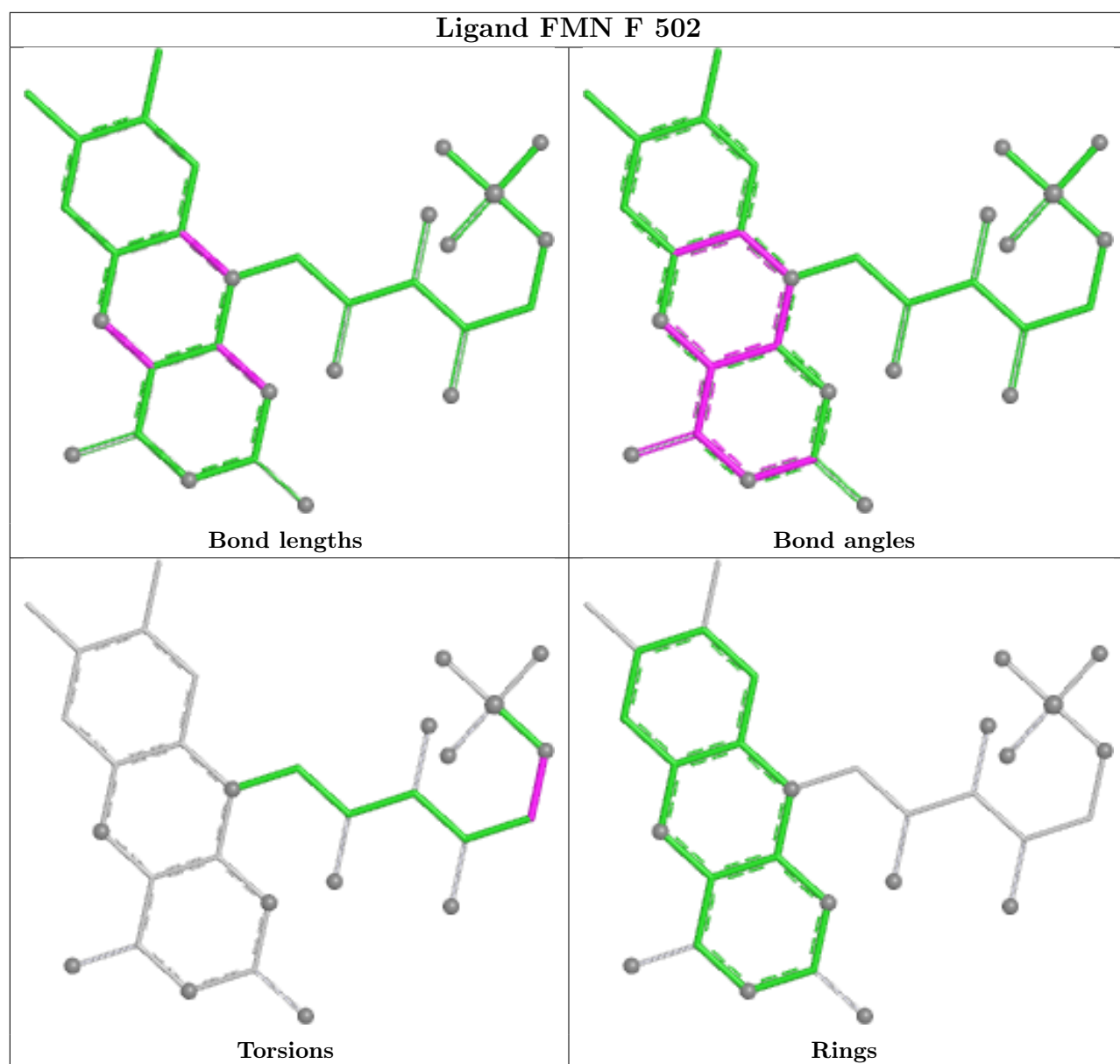


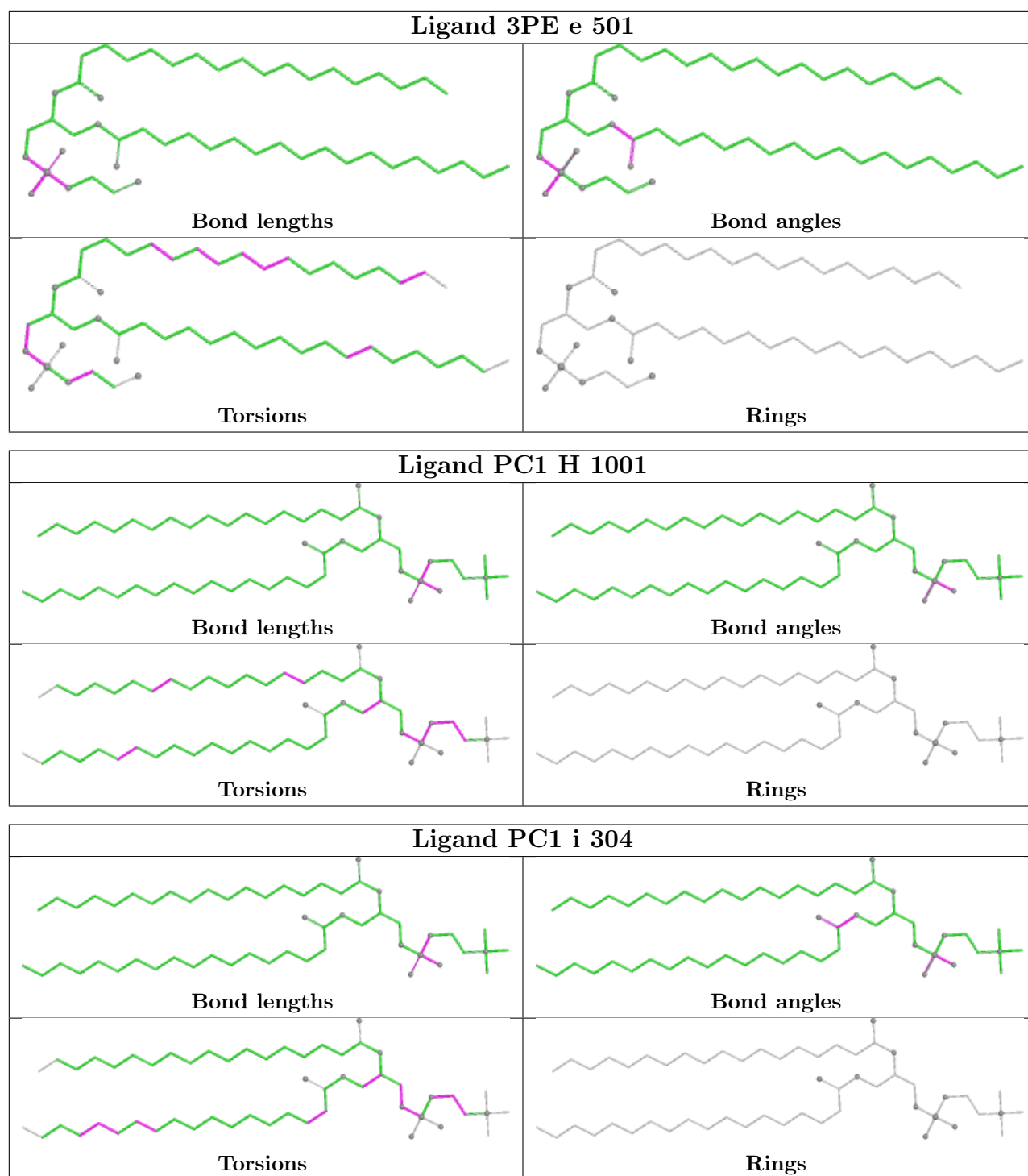


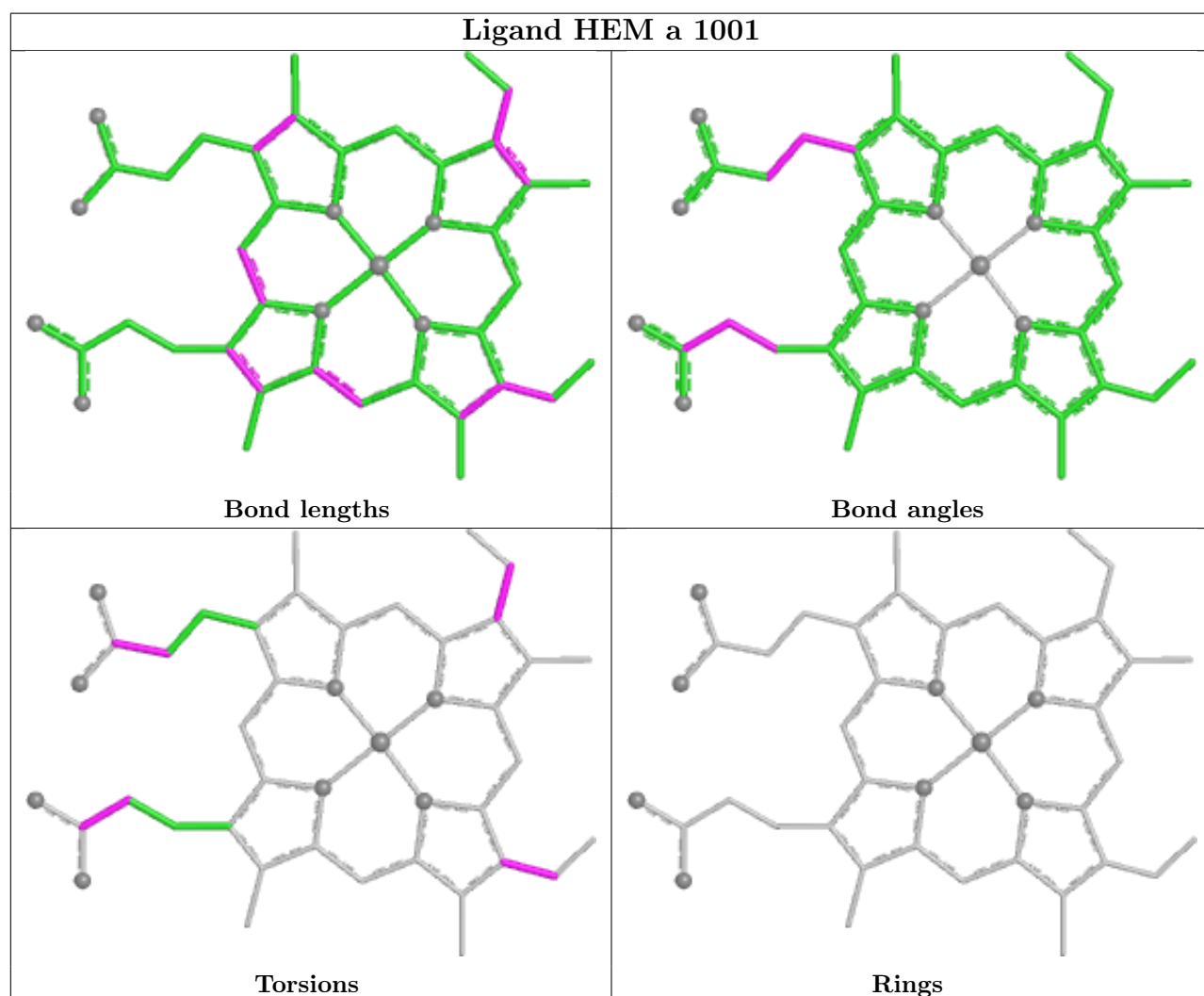
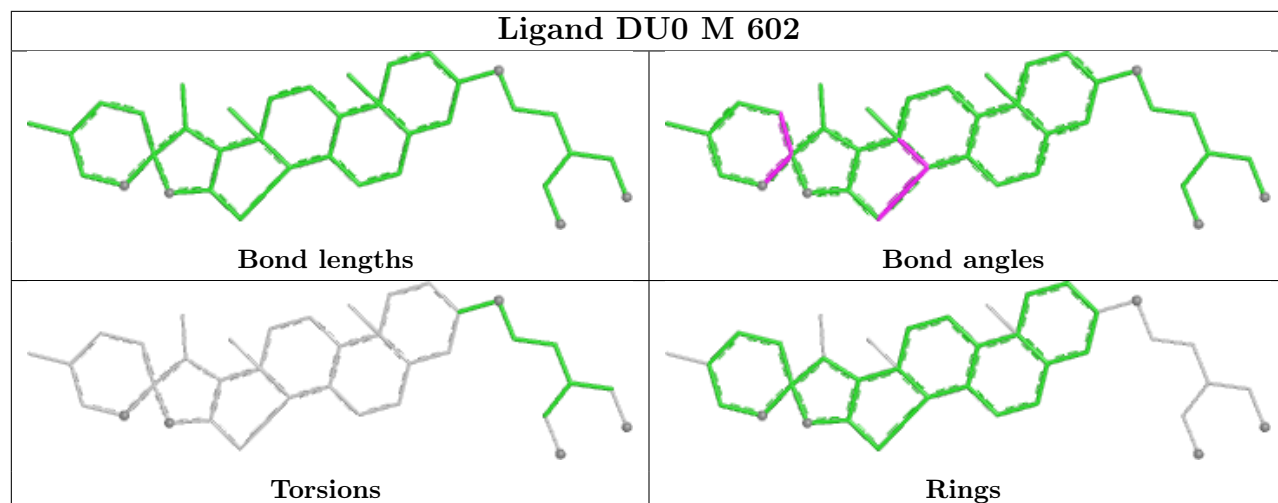


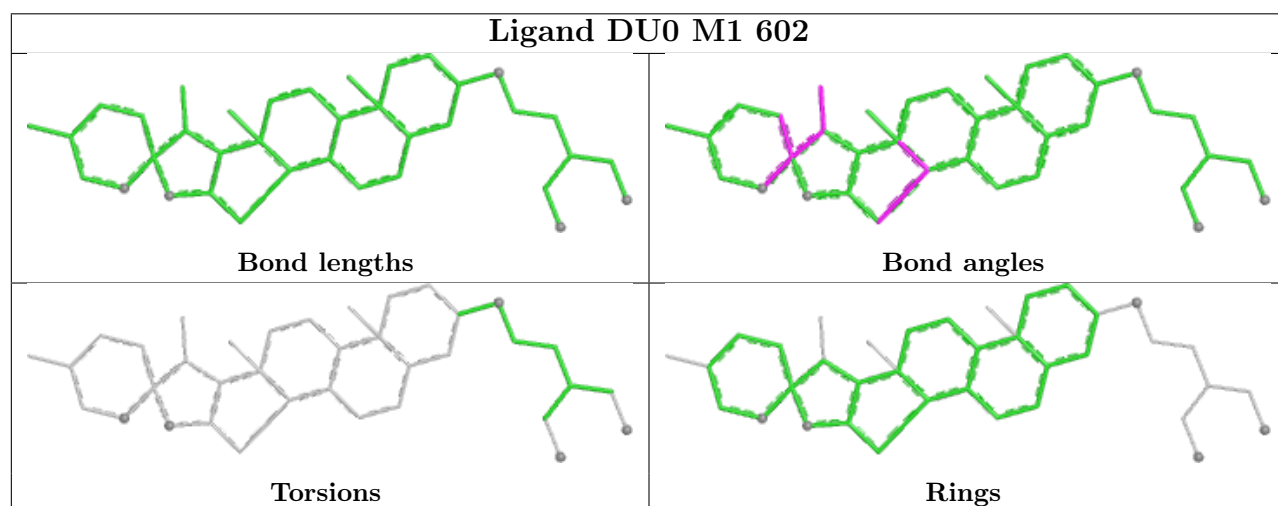
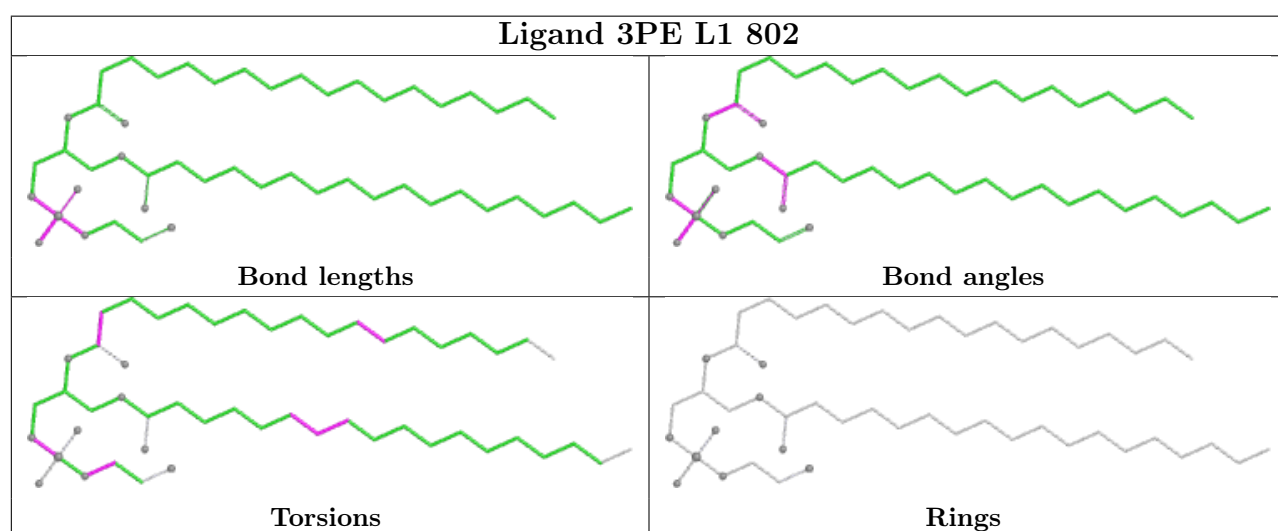
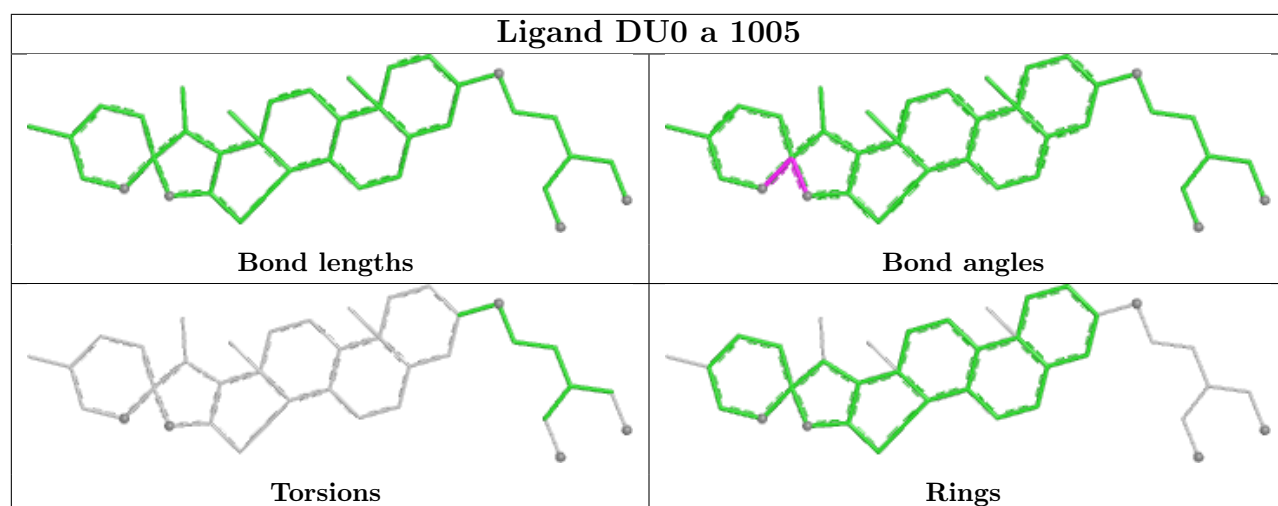


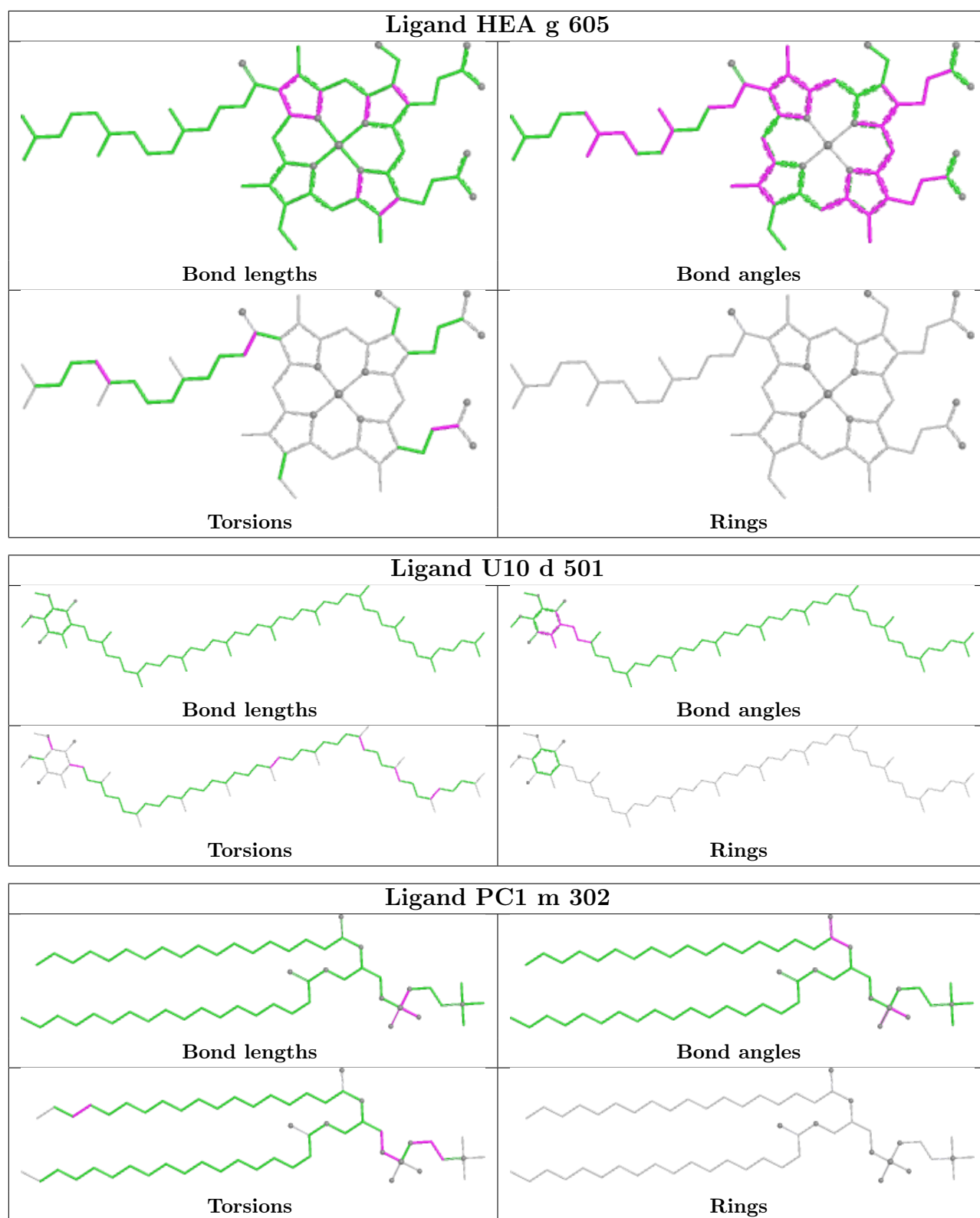


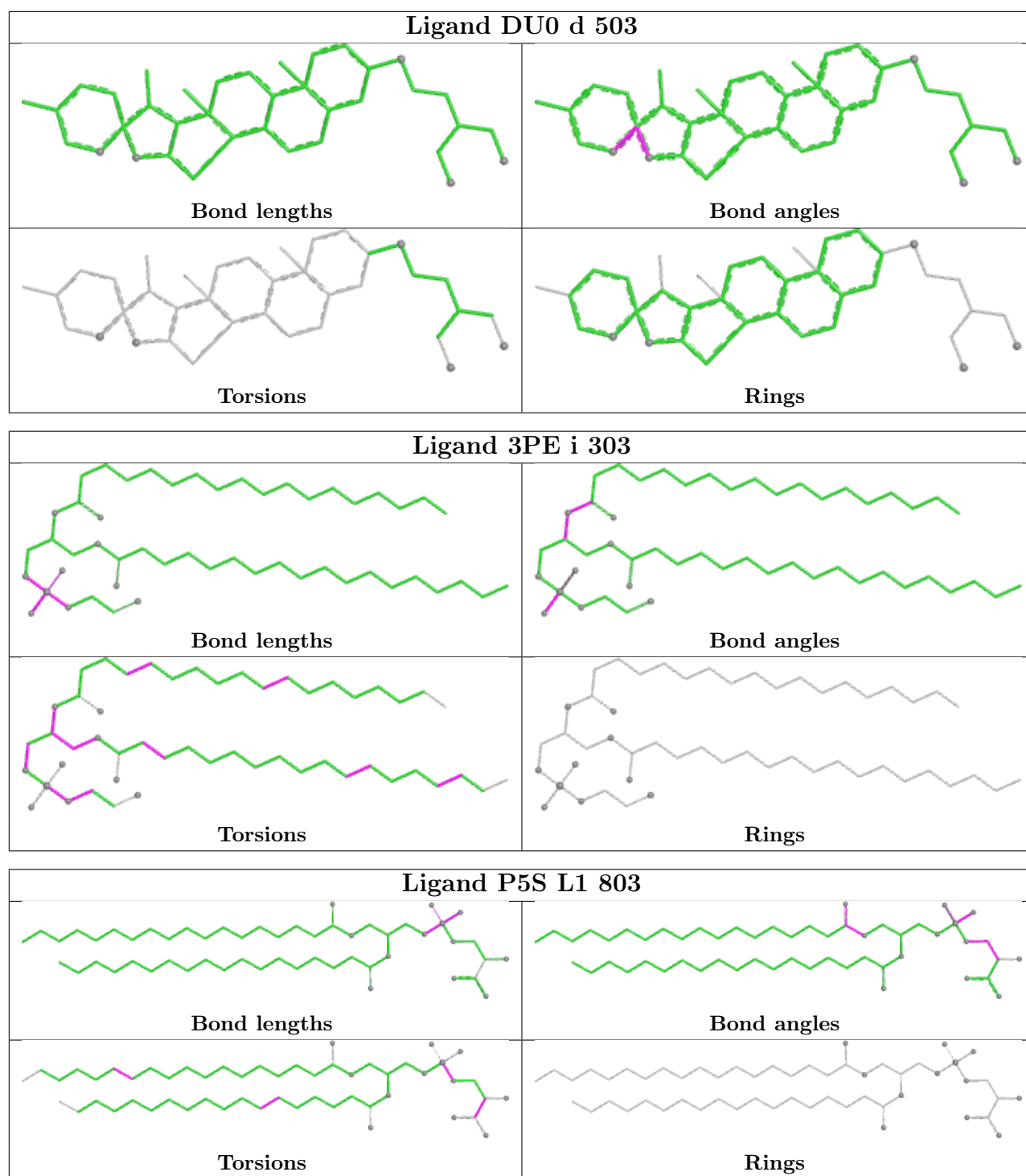


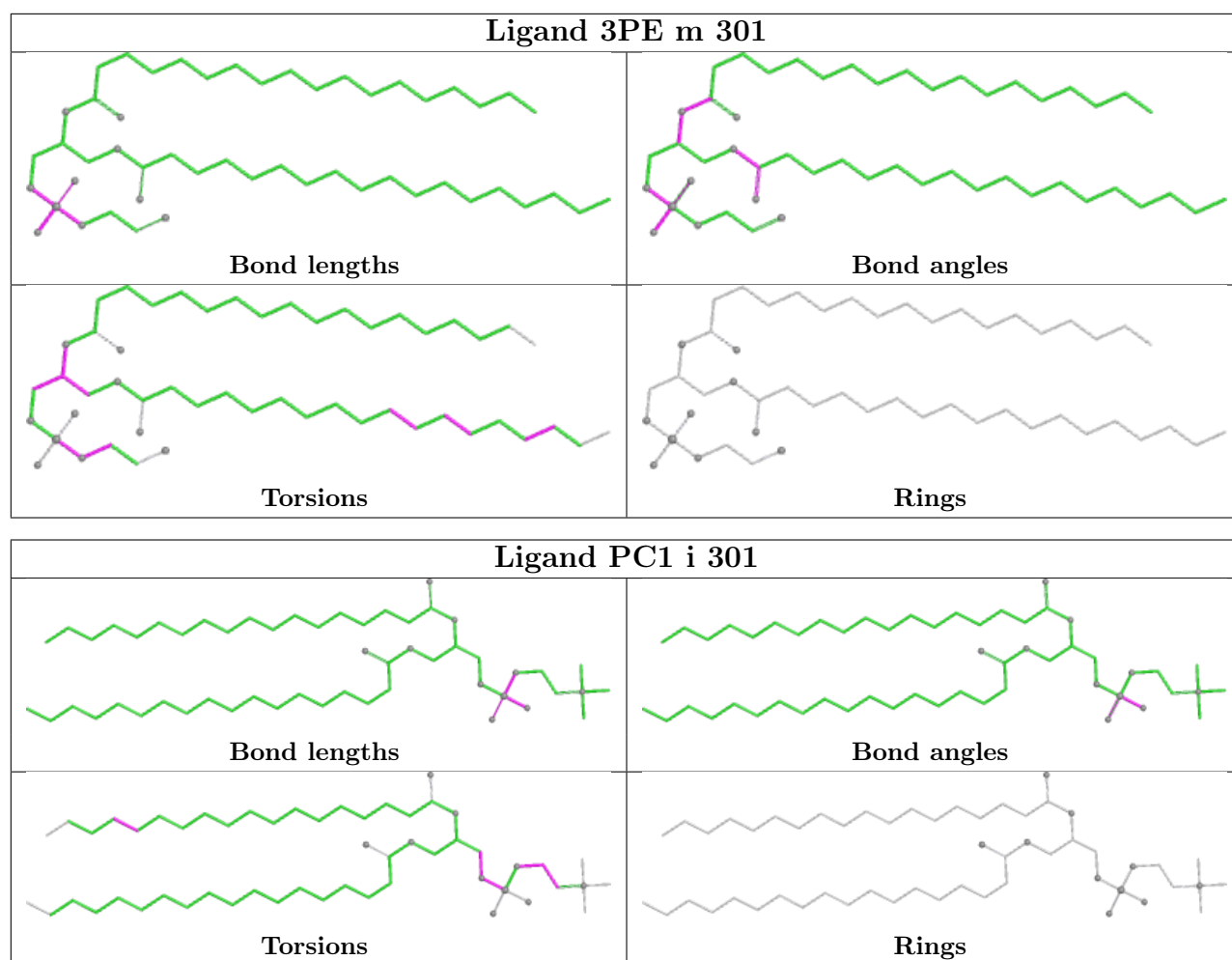




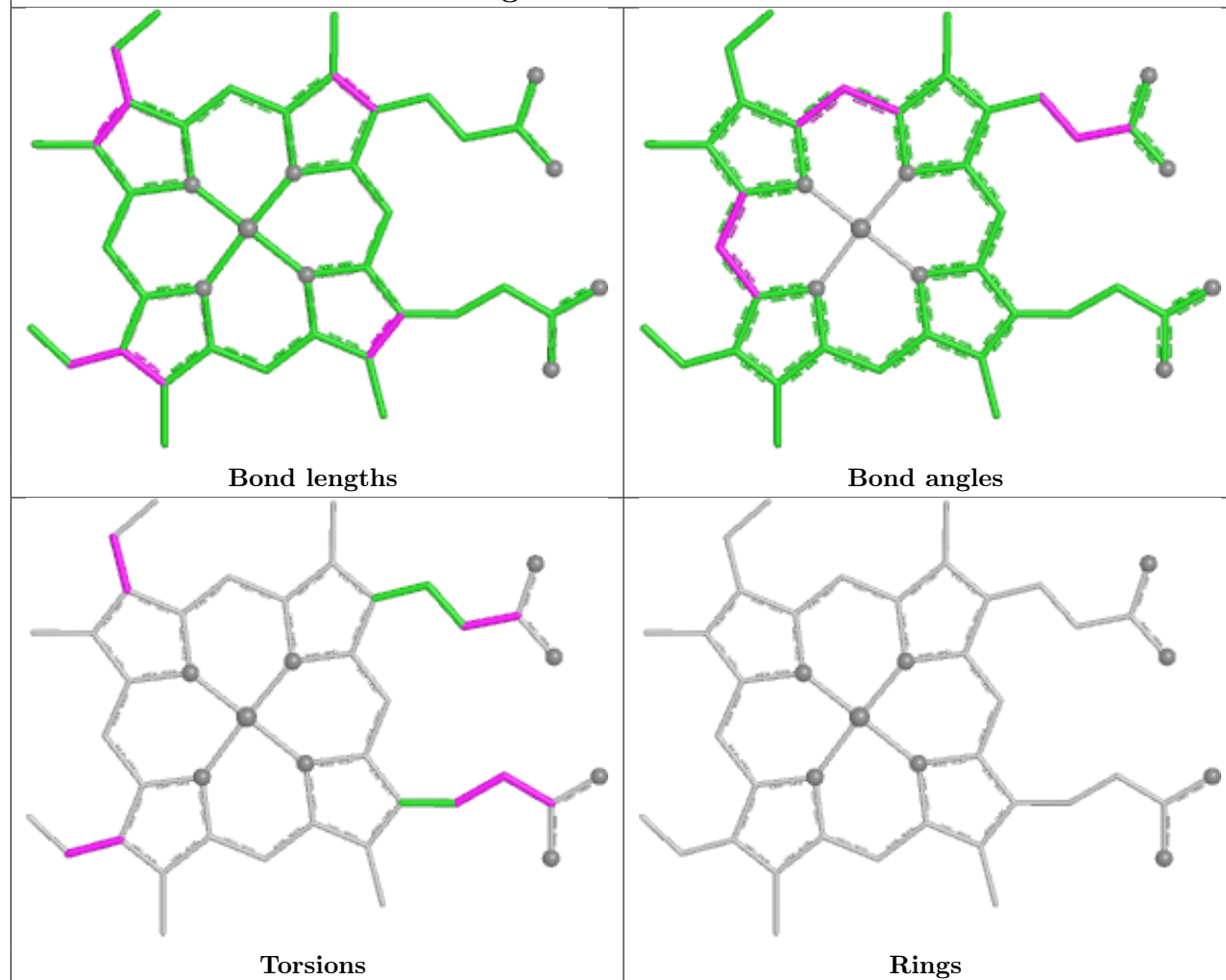




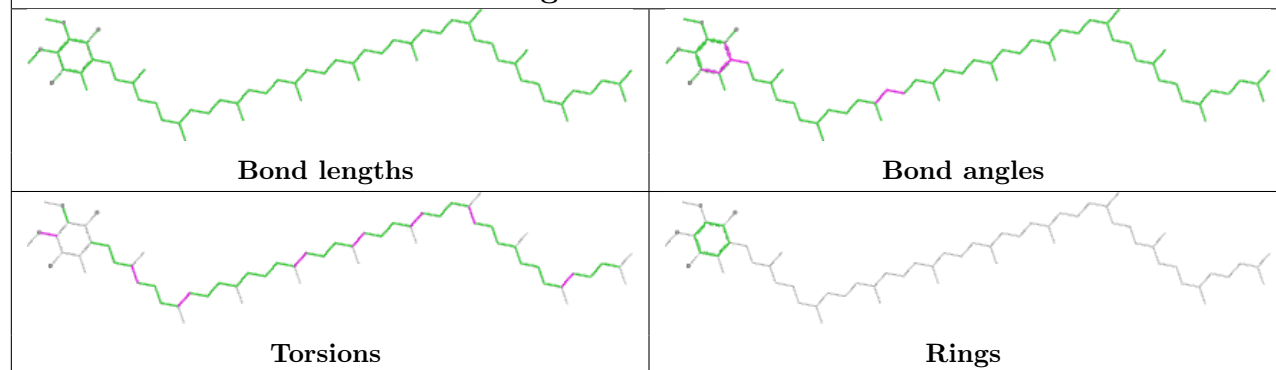




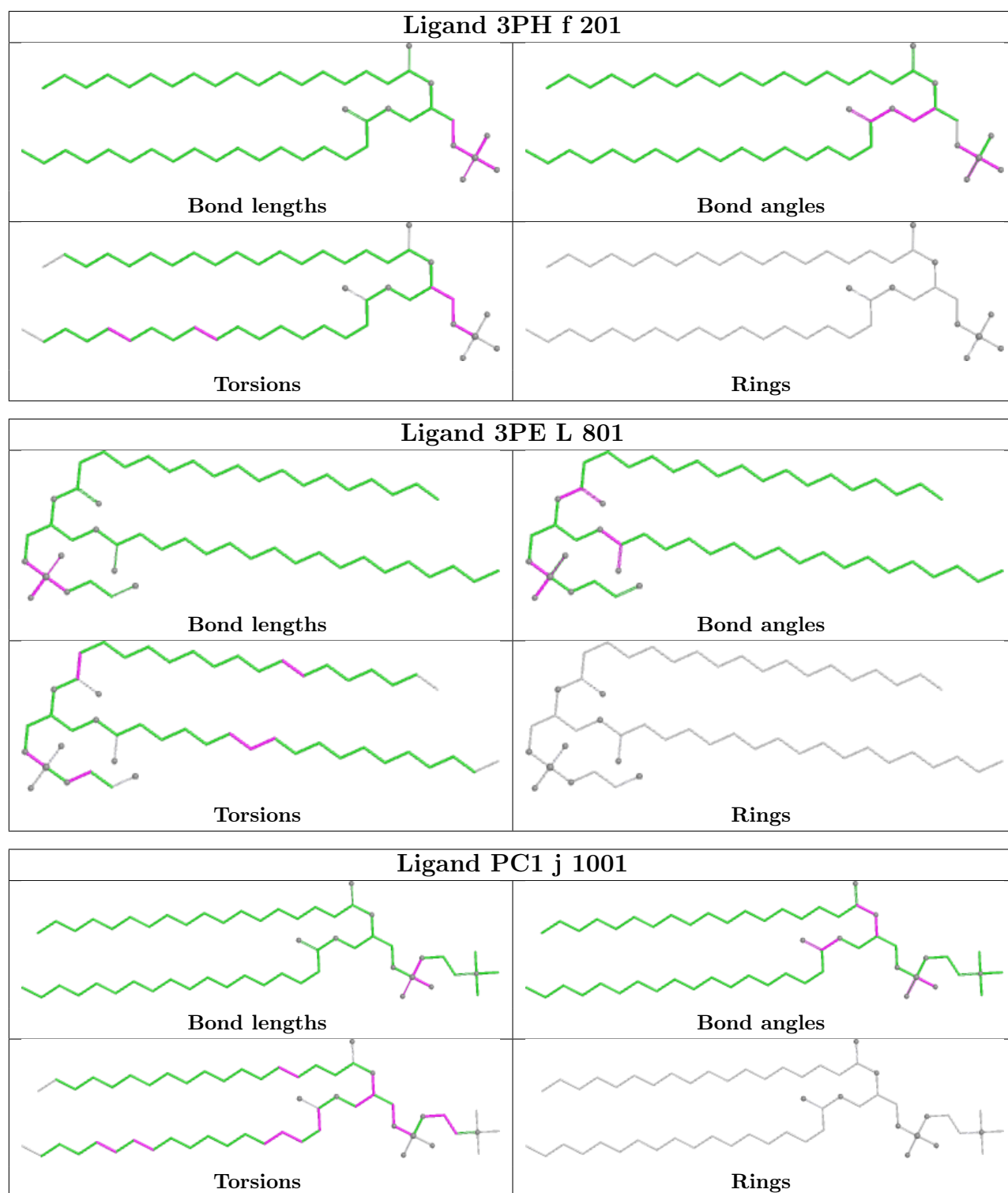
## Ligand HEM a 1003

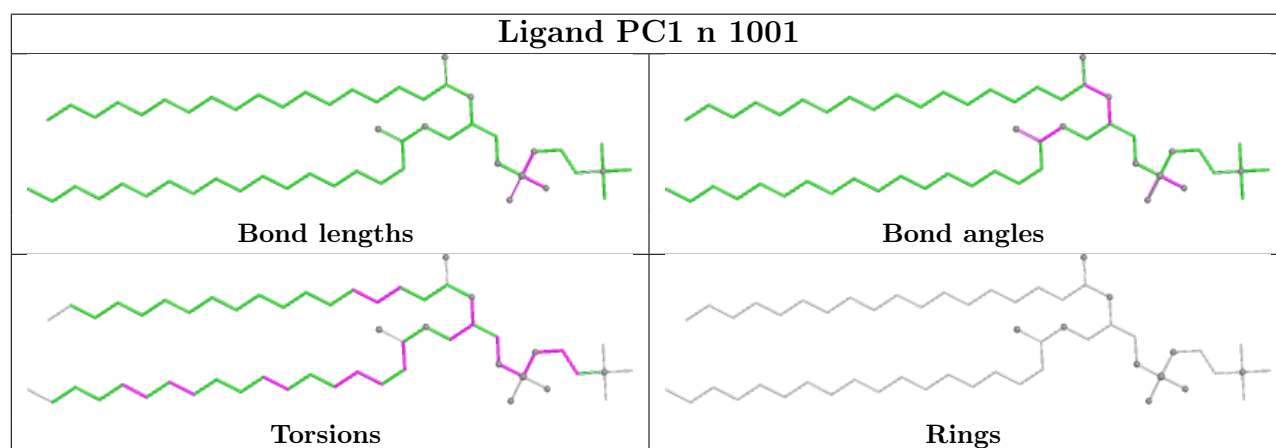
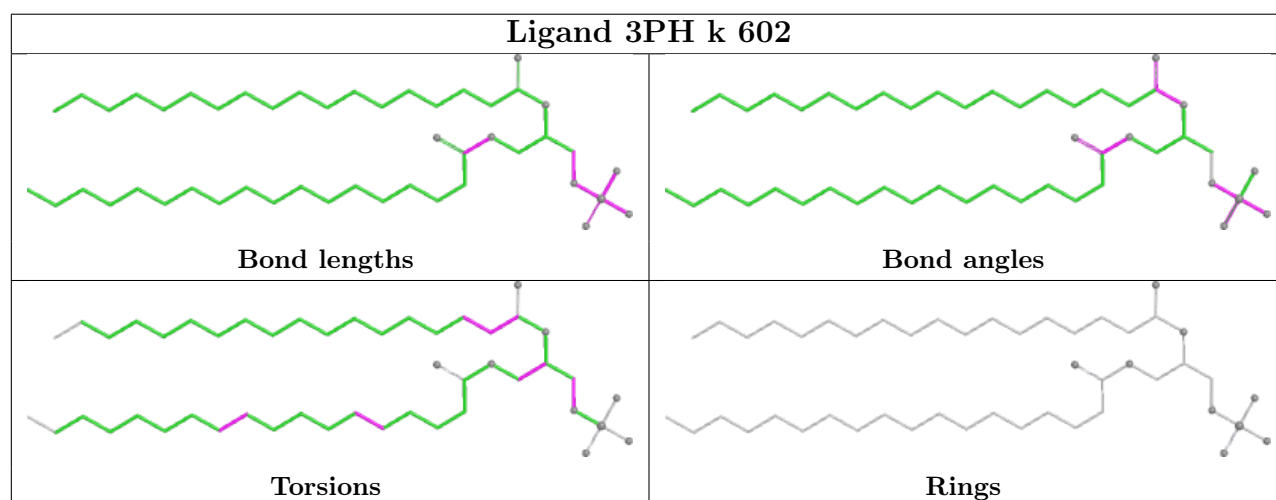
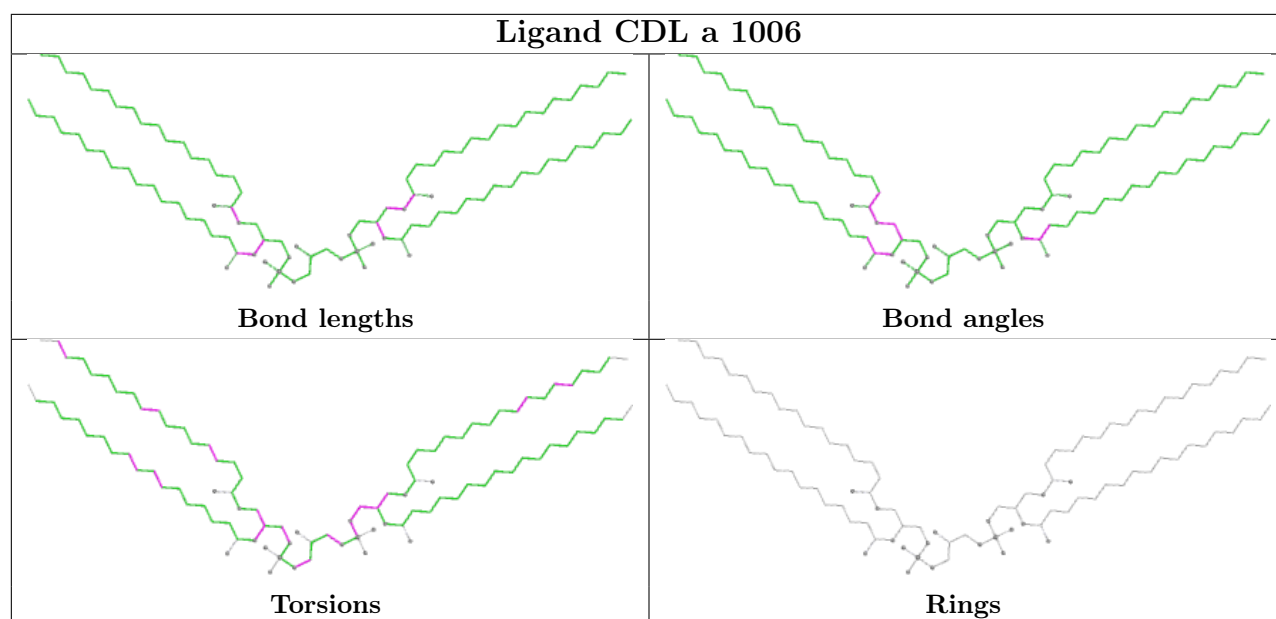


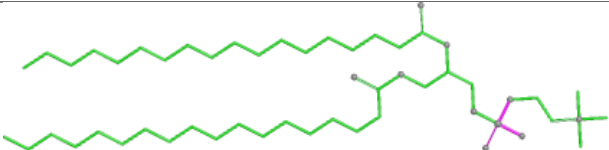
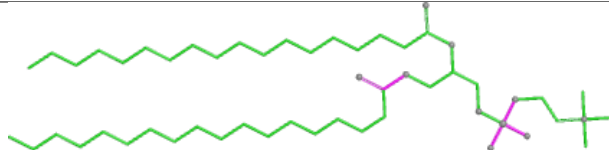
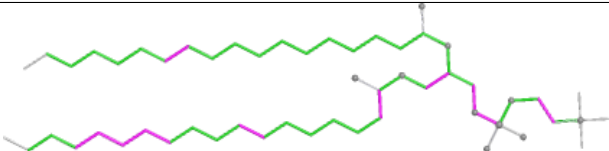
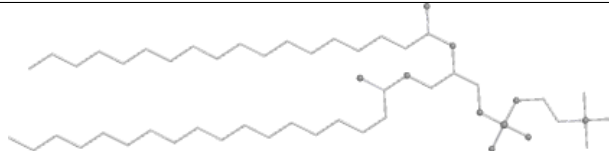
## Ligand U10 d 504

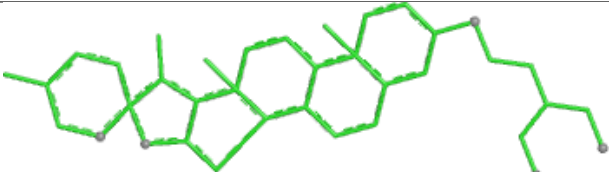
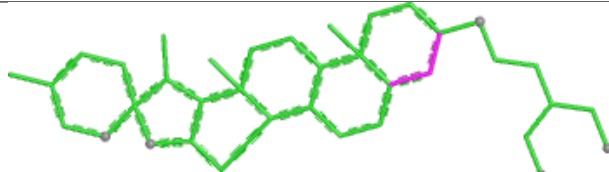
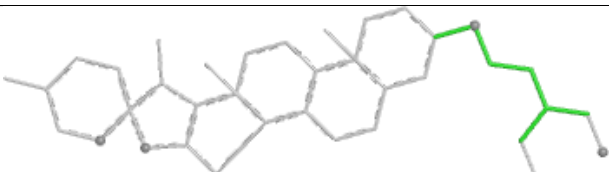
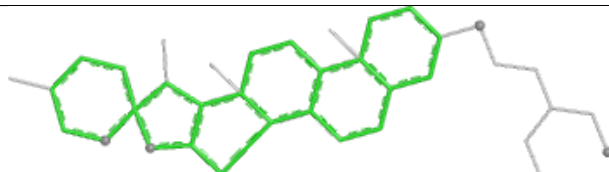


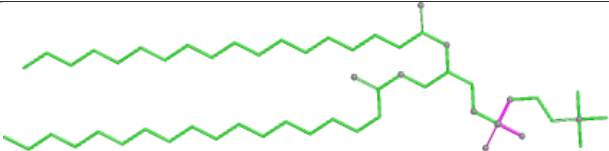
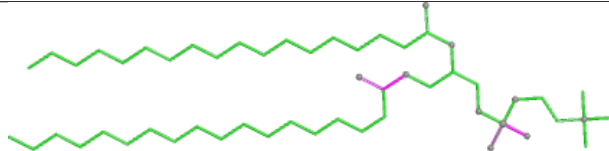
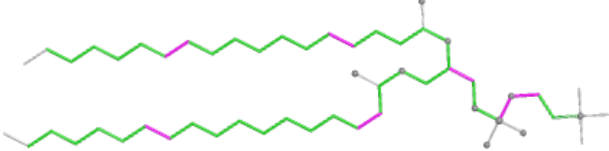
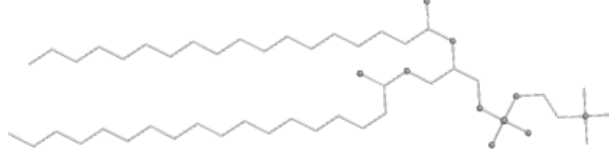


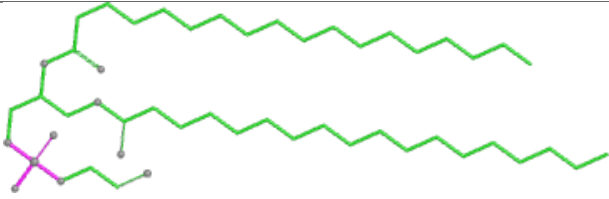
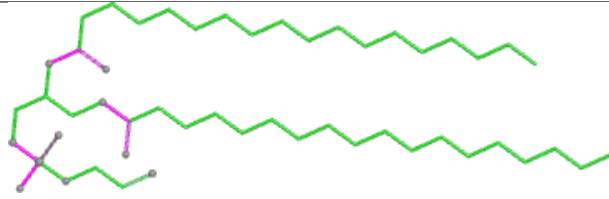
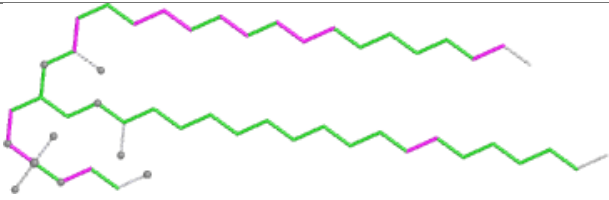
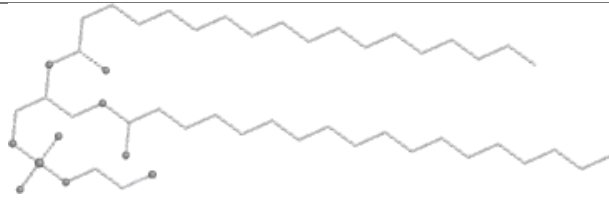




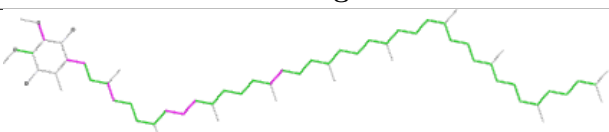



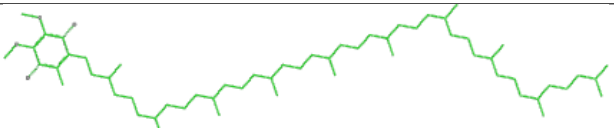
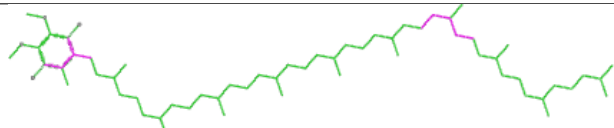
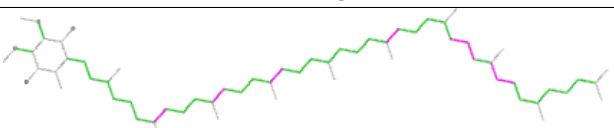

Ligand PC1 m 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

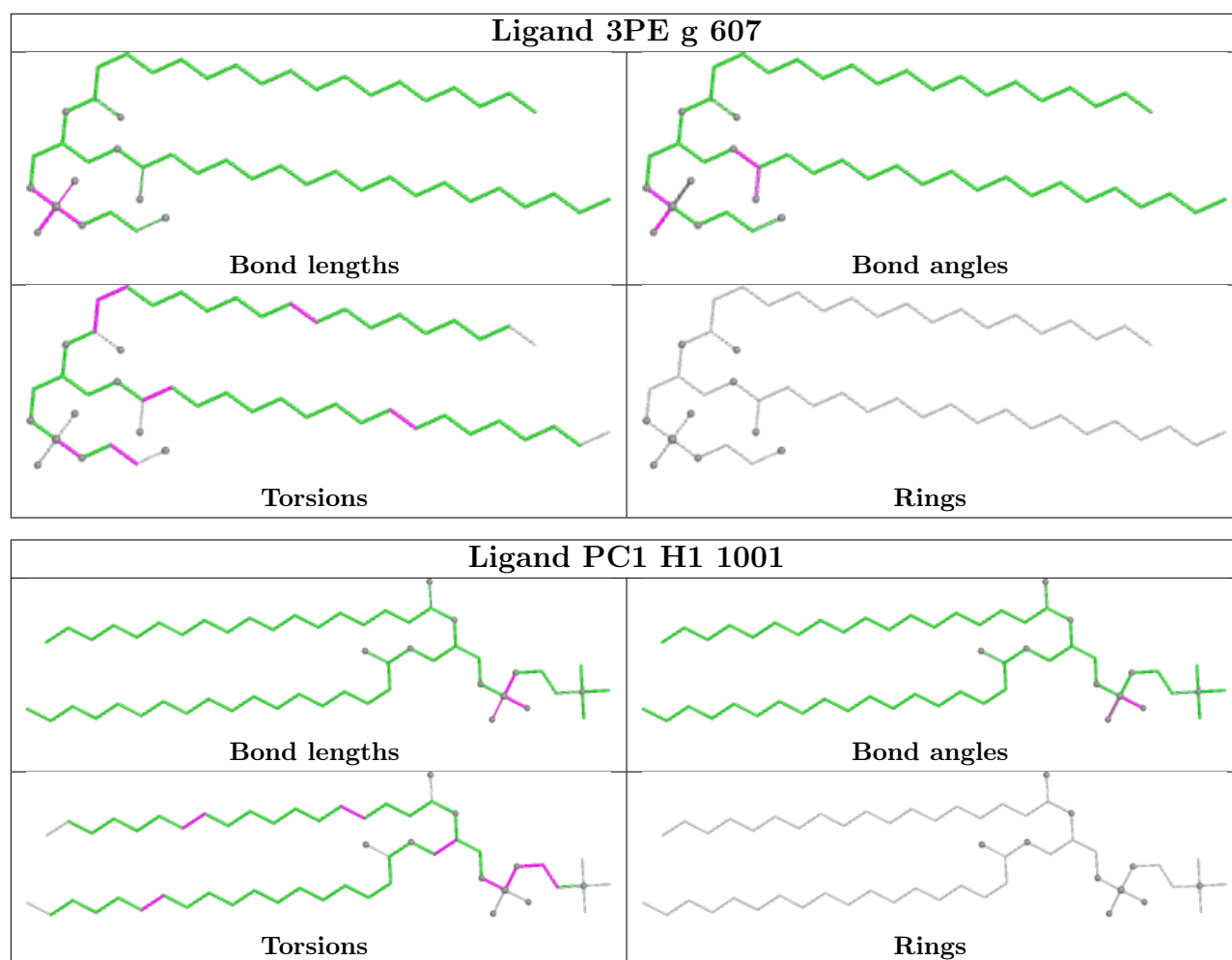
Ligand DU0 K 1000	
	
Bond lengths	Bond angles
	
Torsions	Rings

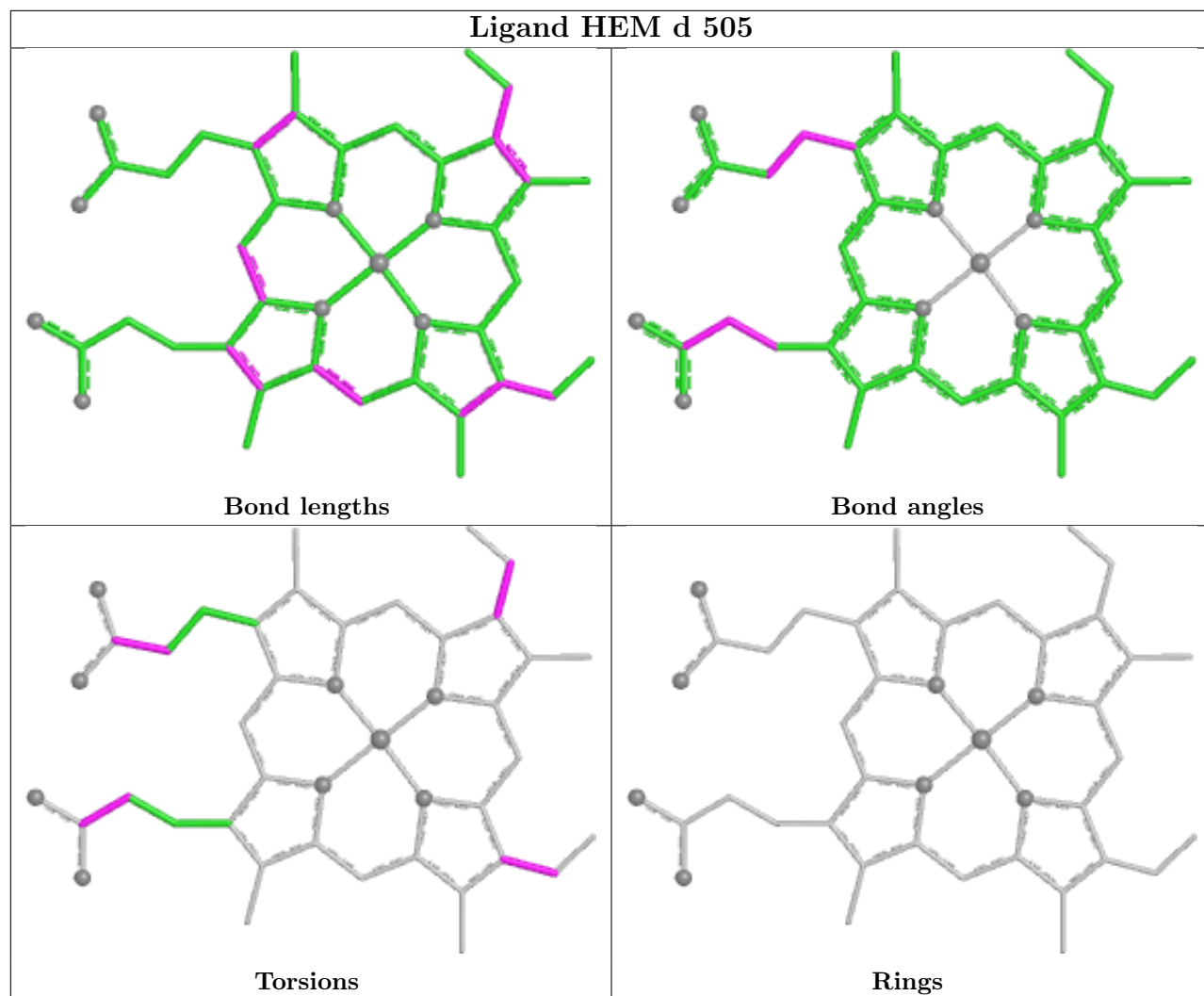
Ligand PC1 M1 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 3PE b 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

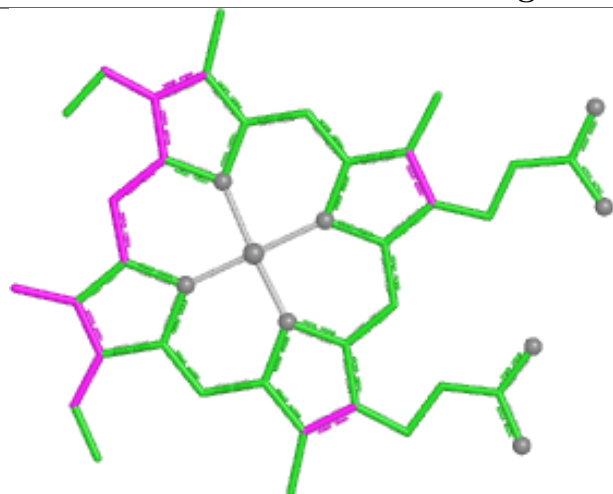
Ligand U10 B1 1002	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand U10 a 1004	
	
Bond lengths	Bond angles
	
Torsions	Rings

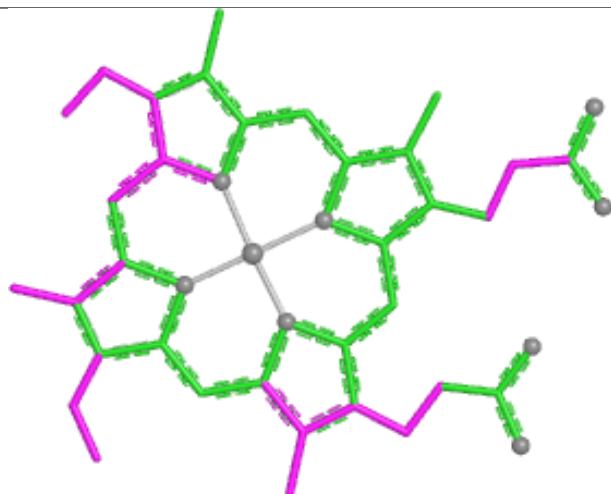




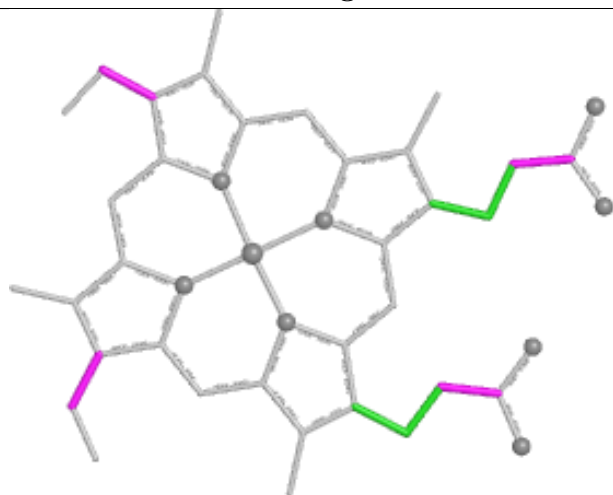
## Ligand HEC e 503



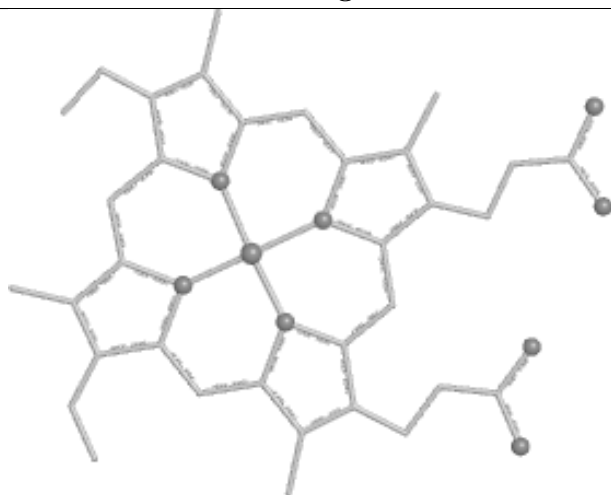
Bond lengths



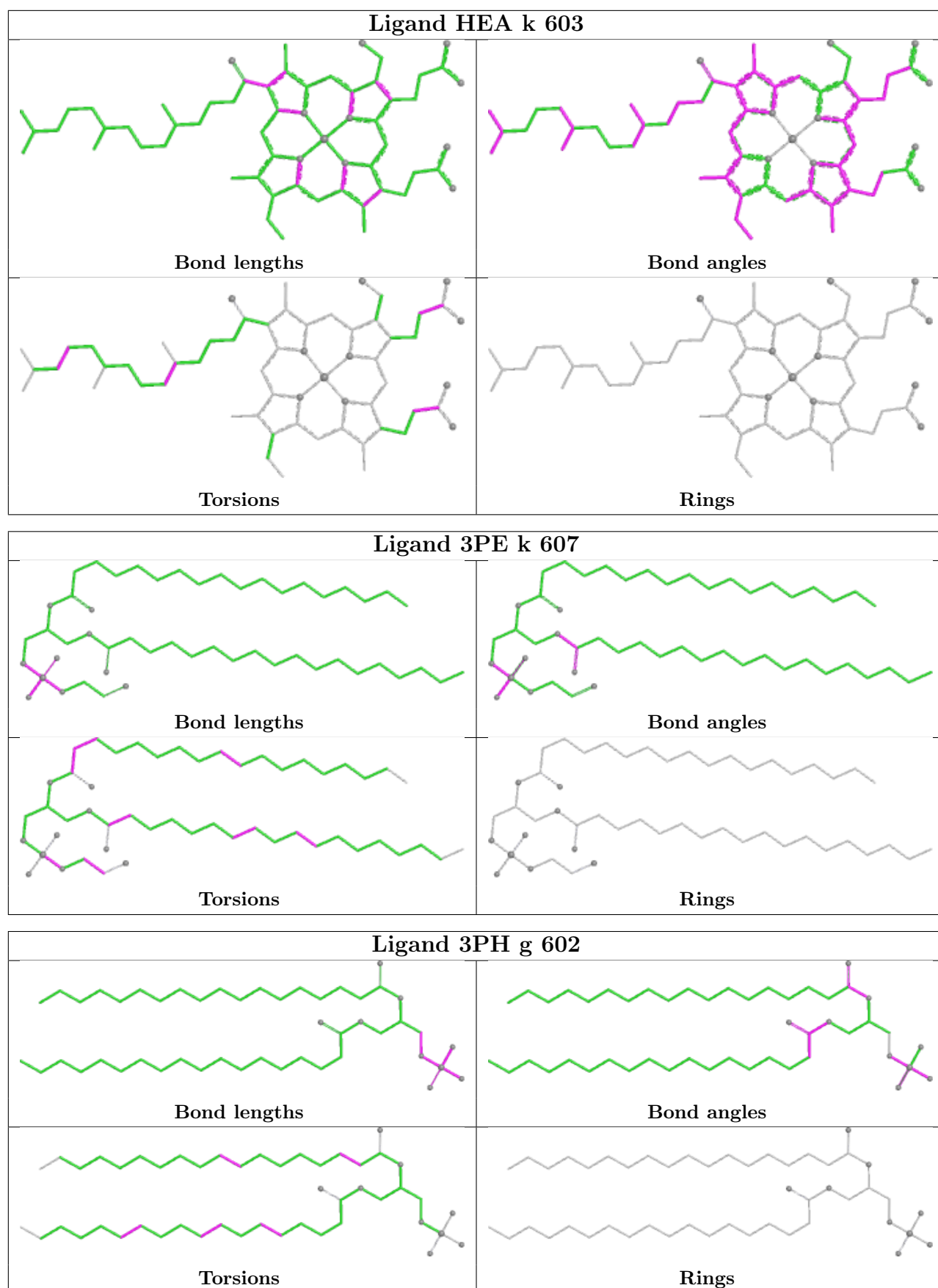
Bond angles



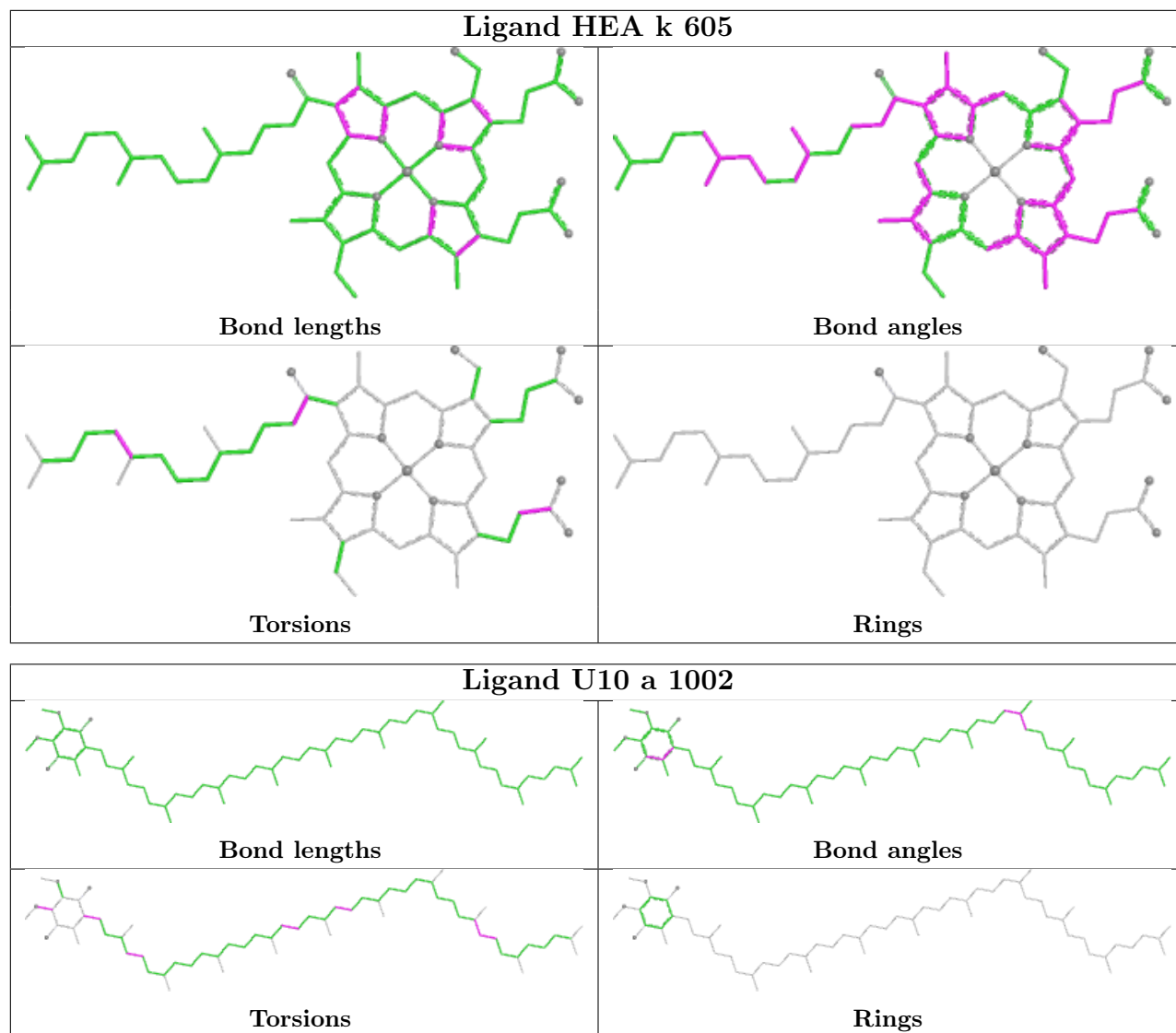
Torsions

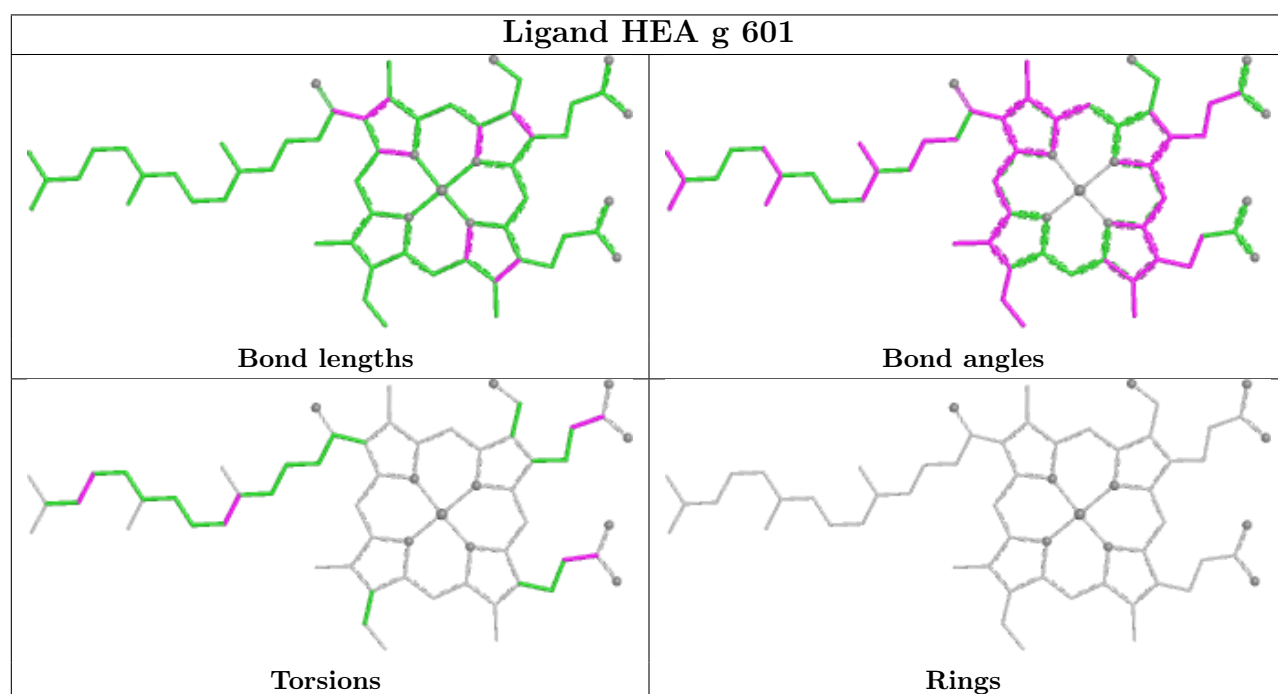
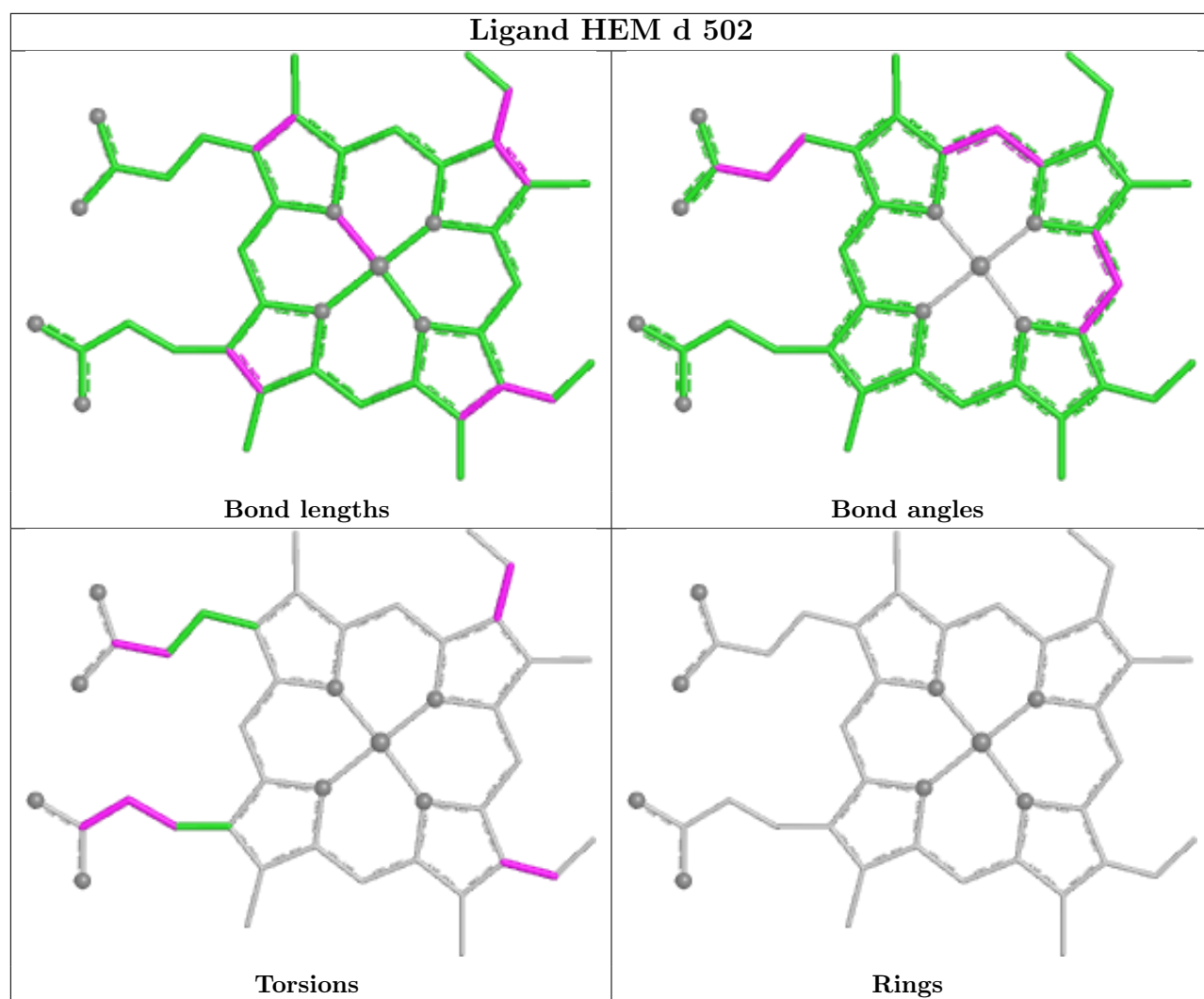


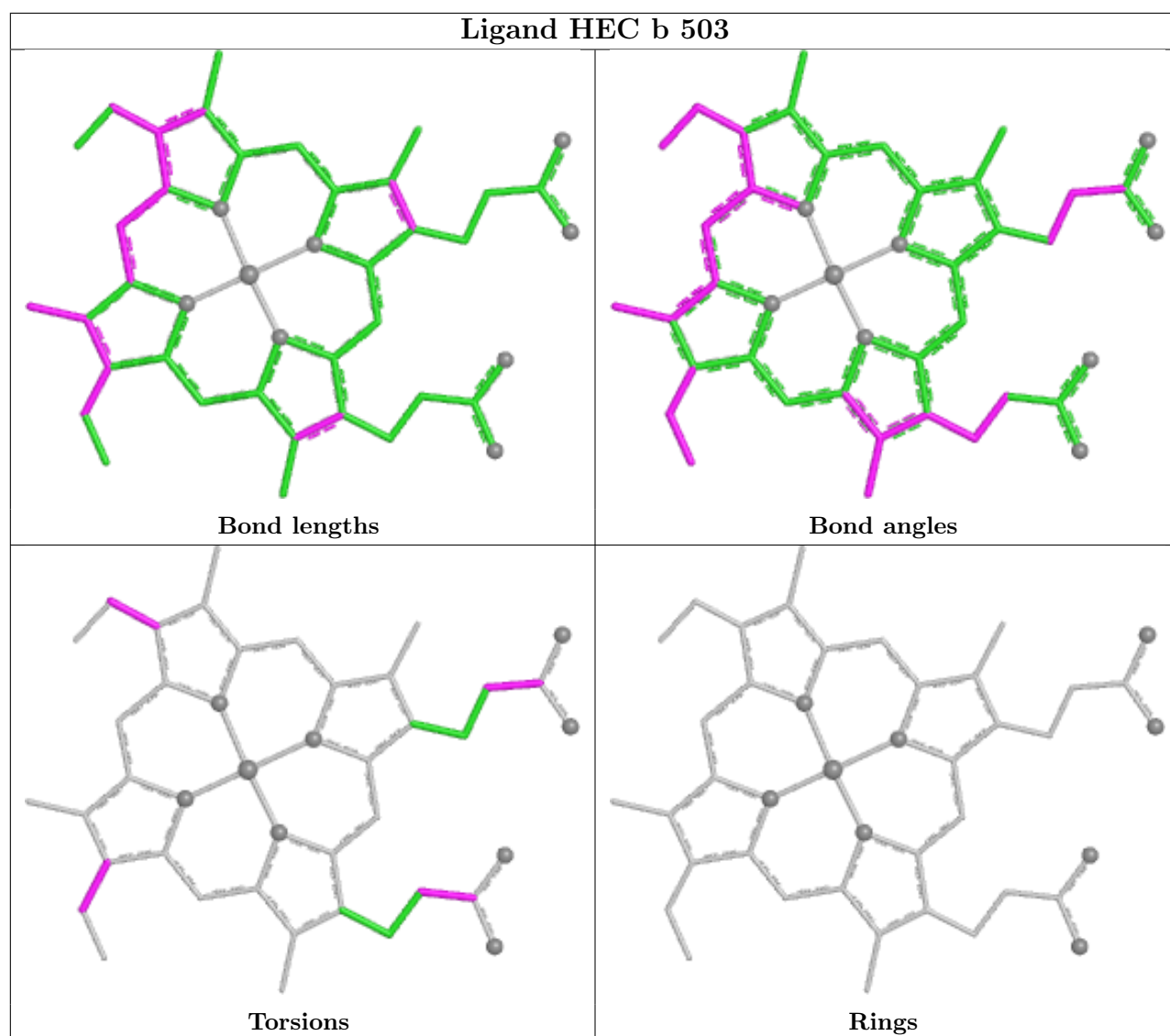
Rings











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51161. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 6.1 Orthogonal projections

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

### 6.5 Orthogonal surface views

This section was not generated.

### 6.6 Mask visualisation

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

## 7 Map analysis ⓘ

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

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation

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

## 9 Map-model fit

This section was not generated.