



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 01:01 PM UTC

PDB ID : 8UGN / pdb_00008ugn
EMDB ID : EMD-42230
Title : In-situ structure of typeO supercomplex in respiratory chain (composite)
Authors : Zheng, W.; Zhang, K.; Zhu, J.
Deposited on : 2023-10-05
Resolution : 2.70 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

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>.

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 : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

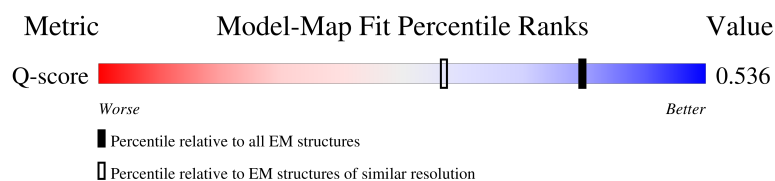
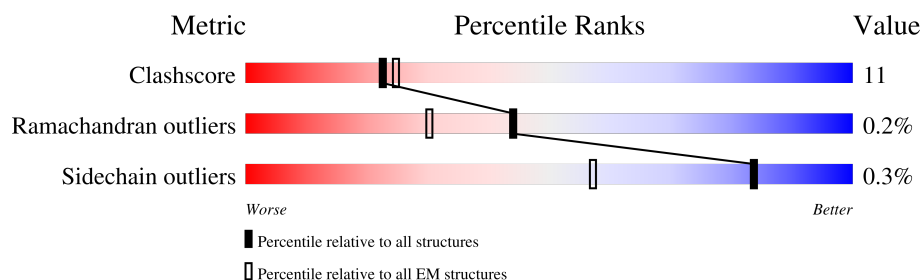
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	115	 63% 37%
1	5A	115	 57% 43%
2	1B	258	 43% 17% 40%
2	5B	258	 40% 20% 40%

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Mol	Chain	Length	Quality of chain
3	1C	264	
3	5C	264	
4	1D	476	
4	5D	476	
5	1E	249	
5	5E	249	
6	1F	464	
6	5F	464	
7	1G	727	
7	5G	727	
8	1H	318	
8	5H	318	
9	1I	239	
9	5I	239	
10	1J	175	
10	5J	175	
11	1K	98	
11	5K	98	
12	1L	606	
12	5L	606	
13	1M	459	
13	5M	459	
14	1N	347	
14	5N	347	
15	1O	357	

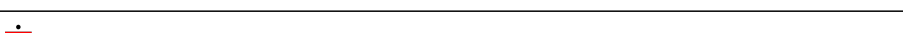
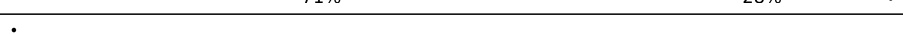
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Mol	Chain	Length	Quality of chain
15	5O	357	
16	1P	377	
16	5P	377	
17	1Q	175	
17	5Q	175	
18	1R	123	
18	5R	123	
19	1S	99	
19	5S	99	
20	1T	156	
20	1U	156	
20	5T	156	
20	5U	156	
21	1V	116	
21	5V	116	
22	1W	128	
22	5W	128	
23	1X	172	
23	5X	172	
24	1Y	141	
24	5Y	141	
25	1Z	144	
25	5Z	144	
26	1a	70	
26	5a	70	

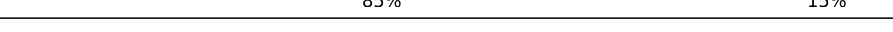
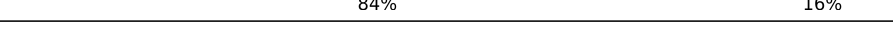
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Mol	Chain	Length	Quality of chain
27	1b	84	
27	5b	84	
28	1c	76	
28	5c	76	
29	1d	122	
29	5d	122	
30	1e	106	
30	5e	106	
31	1f	135	
31	5f	135	
32	1g	154	
32	5g	154	
33	1h	189	
33	5h	189	
34	1i	128	
34	5i	128	
35	1j	105	
35	5j	105	
36	1k	98	
36	5k	98	
37	1l	186	
37	5l	186	
38	1m	129	
38	5m	129	
39	1n	179	

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Mol	Chain	Length	Quality of chain
39	5n	179	
40	1o	137	
40	5o	137	
41	1p	176	
41	5p	176	
42	1q	145	
42	5q	145	
43	1r	113	
43	5r	113	
44	1s	471	
44	5s	471	
45	3A	480	
45	3N	480	
46	3B	453	
46	3O	453	
47	3C	379	
47	3P	379	
48	3D	326	
48	3Q	326	
49	3E	274	
49	3I	274	
49	3R	274	
49	3V	274	
50	3F	111	
50	3S	111	

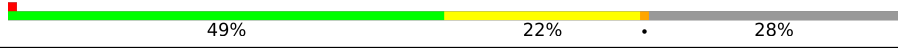
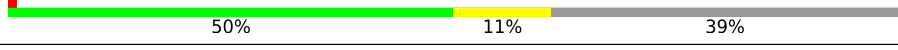
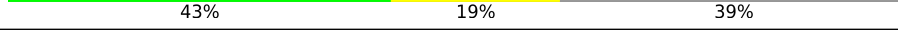
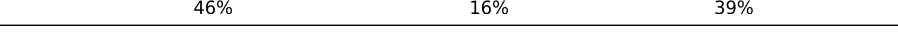
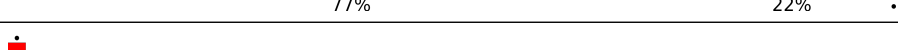
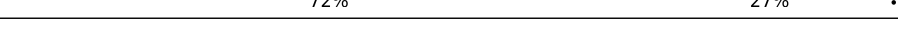
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Mol	Chain	Length	Quality of chain
51	3G	82	
51	3T	82	
52	3H	91	
52	3U	91	
53	3J	64	
53	3W	64	
54	3X	56	
54	3Y	56	
55	4A	514	
55	8A	514	
56	4B	229	
56	8B	229	
57	4C	261	
57	8C	261	
58	4D	169	
58	8D	169	
59	4E	152	
59	8E	152	
60	4F	128	
60	8F	128	
61	4G	97	
61	8G	97	
62	4H	86	
62	8H	86	
63	4I	75	

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Mol	Chain	Length	Quality of chain
63	8I	75	
64	4J	80	
64	8J	80	
65	4K	80	
65	8K	80	
66	4L	63	
66	8L	63	
67	4M	70	
67	8M	70	
68	4N	82	
68	8N	82	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
71	FES	1G	803	-	-	X	-
71	FES	5G	803	-	-	X	-
91	CUA	4B	303	-	-	X	-

2 Entry composition

There are 93 unique types of molecules in this entry. The entry contains 202910 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-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	115	Total	C	N	O	S	0	0
			916	616	134	159	7		
1	5A	115	Total	C	N	O	S	0	0
			916	616	134	159	7		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1B	155	Total	C	N	O	S	0	0
			1242	791	226	211	14		
2	5B	155	Total	C	N	O	S	0	0
			1242	791	226	211	14		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1C	209	Total	C	N	O	S	0	0
			1740	1125	297	316	2		
3	5C	209	Total	C	N	O	S	0	0
			1740	1125	297	316	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1C	104	GLN	ARG	conflict	UNP A0A286ZNN4
1C	154	GLY	ASP	conflict	UNP A0A286ZNN4
5C	104	GLN	ARG	conflict	UNP A0A286ZNN4
5C	154	GLY	ASP	conflict	UNP A0A286ZNN4

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1D	429	Total	C	N	O	S	0	0
			3452	2207	593	628	24		
4	5D	429	Total	C	N	O	S	0	0
			3452	2207	593	628	24		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1D	0	GLY	GLU	conflict	UNP A0A8D0QM68
5D	0	GLY	GLU	conflict	UNP A0A8D0QM68

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1E	214	Total	C	N	O	S	0	0
			1658	1058	278	312	10		
5	5E	214	Total	C	N	O	S	0	0
			1658	1058	278	312	10		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1F	432	Total	C	N	O	S	0	0
			3325	2100	592	613	20		
6	5F	432	Total	C	N	O	S	0	0
			3325	2100	592	613	20		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1G	699	Total	C	N	O	S	0	0
			5362	3360	933	1029	40		
7	5G	699	Total	C	N	O	S	0	0
			5362	3360	933	1029	40		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1H	318	Total	C	N	O	S	0	0
			2504	1673	385	425	21		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	5H	318	Total	C	N	O	S	0	0
			2504	1673	385	425	21		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1I	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		
9	5I	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1J	174	Total	C	N	O	S	0	0
			1329	892	189	236	12		
10	5J	174	Total	C	N	O	S	0	0
			1329	892	189	236	12		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1K	98	Total	C	N	O	S	0	0
			750	494	113	129	14		
11	5K	98	Total	C	N	O	S	0	0
			750	494	113	129	14		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1L	606	Total	C	N	O	S	0	0
			4818	3195	746	826	51		
12	5L	606	Total	C	N	O	S	0	0
			4818	3195	746	826	51		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1M	459	Total	C	N	O	S	0	0
			3632	2411	572	610	39		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	5M	459	Total	C	N	O	S	0	0
			3632	2411	572	610	39		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1N	347	Total	C	N	O	S	0	0
			2712	1783	420	463	46		
14	5N	347	Total	C	N	O	S	0	0
			2712	1783	420	463	46		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1O	320	Total	C	N	O	S	0	0
			2590	1649	440	491	10		
15	5O	320	Total	C	N	O	S	0	0
			2590	1649	440	491	10		

- Molecule 16 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	1P	342	Total	C	N	O	S	0	0
			2751	1783	481	478	9		
16	5P	342	Total	C	N	O	S	0	0
			2751	1783	481	478	9		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	1Q	129	Total	C	N	O	S	0	0
			1047	659	186	199	3		
17	5Q	129	Total	C	N	O	S	0	0
			1047	659	186	199	3		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1R	96	Total	C	N	O	S	0	0
			741	452	140	146	3		
18	5R	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	1S	87	Total	C	N	O	S	0	0
			700	440	131	127	2		
19	5S	87	Total	C	N	O	S	0	0
			700	440	131	127	2		

- Molecule 20 is a protein called NADH:ubiquinone oxidoreductase subunit AB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1T	85	Total	C	N	O	S	0	0
			689	445	101	138	5		
20	1U	86	Total	C	N	O	S	0	0
			694	448	102	139	5		
20	5T	85	Total	C	N	O	S	0	0
			689	445	101	138	5		
20	5U	86	Total	C	N	O	S	0	0
			694	448	102	139	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1V	115	Total	C	N	O	S	0	0
			927	599	157	168	3		
21	5V	115	Total	C	N	O	S	0	0
			927	599	157	168	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1W	115	Total	C	N	O	S	0	0
			971	619	179	168	5		
22	5W	115	Total	C	N	O	S	0	0
			971	619	179	168	5		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1X	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		
23	5X	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1Y	139	Total	C	N	O	S	0	0
			1016	648	173	189	6		
24	5Y	139	Total	C	N	O	S	0	0
			1016	648	173	189	6		

- Molecule 25 is a protein called NADH:ubiquinone oxidoreductase subunit A13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1Z	141	Total	C	N	O	S	0	0
			1168	752	202	205	9		
25	5Z	141	Total	C	N	O	S	0	0
			1168	752	202	205	9		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1a	70	Total	C	N	O	S	0	0
			562	361	101	94	6		
26	5a	70	Total	C	N	O	S	0	0
			562	361	101	94	6		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1b	83	Total	C	N	O	S	0	0
			643	417	110	115	1		
27	5b	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochond-

drial.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	1c	49	Total	C	N	O	0	0
			417	276	71	70		
28	5c	49	Total	C	N	O	0	0
			417	276	71	70		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	1d	119	Total	C	N	O	S	0	0
			985	641	171	168	5		
29	5d	119	Total	C	N	O	S	0	0
			985	641	171	168	5		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	1e	99	Total	C	N	O	S	0	0
			816	519	151	140	6		
30	5e	99	Total	C	N	O	S	0	0
			816	519	151	140	6		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa].

Mol	Chain	Residues	Atoms					AltConf	Trace
31	1f	57	Total	C	N	O	S	0	0
			487	316	89	80	2		
31	5f	57	Total	C	N	O	S	0	0
			487	316	89	80	2		

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1f	-77	MET	-	initiating methionine	UNP A0A8D1IZ33
1f	-76	ALA	-	expression tag	UNP A0A8D1IZ33
1f	-75	ALA	-	expression tag	UNP A0A8D1IZ33
1f	-74	ALA	-	expression tag	UNP A0A8D1IZ33
1f	-73	ILE	-	expression tag	UNP A0A8D1IZ33
1f	-72	LEU	-	expression tag	UNP A0A8D1IZ33
1f	-71	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-70	LEU	-	expression tag	UNP A0A8D1IZ33

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Chain	Residue	Modelled	Actual	Comment	Reference
1f	-69	GLU	-	expression tag	UNP A0A8D1IZ33
1f	-68	GLU	-	expression tag	UNP A0A8D1IZ33
1f	-67	THR	-	expression tag	UNP A0A8D1IZ33
1f	-66	ARG	-	expression tag	UNP A0A8D1IZ33
1f	-65	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-64	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-63	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-62	GLU	-	expression tag	UNP A0A8D1IZ33
1f	-61	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-60	CYS	-	expression tag	UNP A0A8D1IZ33
1f	-59	ASP	-	expression tag	UNP A0A8D1IZ33
1f	-58	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-57	ASN	-	expression tag	UNP A0A8D1IZ33
1f	-56	GLN	-	expression tag	UNP A0A8D1IZ33
1f	-55	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-54	VAL	-	expression tag	UNP A0A8D1IZ33
1f	-53	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-52	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-51	ARG	-	expression tag	UNP A0A8D1IZ33
1f	-50	ARG	-	expression tag	UNP A0A8D1IZ33
1f	-49	PHE	-	expression tag	UNP A0A8D1IZ33
5f	-77	MET	-	initiating methionine	UNP A0A8D1IZ33
5f	-76	ALA	-	expression tag	UNP A0A8D1IZ33
5f	-75	ALA	-	expression tag	UNP A0A8D1IZ33
5f	-74	ALA	-	expression tag	UNP A0A8D1IZ33
5f	-73	ILE	-	expression tag	UNP A0A8D1IZ33
5f	-72	LEU	-	expression tag	UNP A0A8D1IZ33
5f	-71	LYS	-	expression tag	UNP A0A8D1IZ33
5f	-70	LEU	-	expression tag	UNP A0A8D1IZ33
5f	-69	GLU	-	expression tag	UNP A0A8D1IZ33
5f	-68	GLU	-	expression tag	UNP A0A8D1IZ33
5f	-67	THR	-	expression tag	UNP A0A8D1IZ33
5f	-66	ARG	-	expression tag	UNP A0A8D1IZ33
5f	-65	GLY	-	expression tag	UNP A0A8D1IZ33
5f	-64	GLY	-	expression tag	UNP A0A8D1IZ33
5f	-63	GLY	-	expression tag	UNP A0A8D1IZ33
5f	-62	GLU	-	expression tag	UNP A0A8D1IZ33
5f	-61	LYS	-	expression tag	UNP A0A8D1IZ33
5f	-60	CYS	-	expression tag	UNP A0A8D1IZ33
5f	-59	ASP	-	expression tag	UNP A0A8D1IZ33
5f	-58	LYS	-	expression tag	UNP A0A8D1IZ33
5f	-57	ASN	-	expression tag	UNP A0A8D1IZ33

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Chain	Residue	Modelled	Actual	Comment	Reference
5f	-56	GLN	-	expression tag	UNP A0A8D1IZ33
5f	-55	GLY	-	expression tag	UNP A0A8D1IZ33
5f	-54	VAL	-	expression tag	UNP A0A8D1IZ33
5f	-53	LYS	-	expression tag	UNP A0A8D1IZ33
5f	-52	GLY	-	expression tag	UNP A0A8D1IZ33
5f	-51	ARG	-	expression tag	UNP A0A8D1IZ33
5f	-50	ARG	-	expression tag	UNP A0A8D1IZ33
5f	-49	PHE	-	expression tag	UNP A0A8D1IZ33

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	1g	100	Total	C	N	O	S	0	0
			835	535	138	158	4		
32	5g	100	Total	C	N	O	S	0	0
			835	535	138	158	4		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	1h	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		
33	5h	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1i	127	Total	C	N	O	S	0	0
			1100	723	194	181	2		
34	5i	127	Total	C	N	O	S	0	0
			1100	723	194	181	2		

- Molecule 35 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1j	71	Total	C	N	O	S	0	0
			601	394	99	107	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
35	5j	71	Total	C	N	O	S	0	0
			601	394	99	107	1		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1k	81	Total	C	N	O	S	0	0
			649	422	110	116	1		
36	5k	81	Total	C	N	O	S	0	0
			649	422	110	116	1		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	1l	156	Total	C	N	O	S	0	0
			1310	847	213	242	8		
37	5l	156	Total	C	N	O	S	0	0
			1310	847	213	242	8		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	1m	128	Total	C	N	O		0	0
			1062	691	182	189			
38	5m	128	Total	C	N	O		0	0
			1062	691	182	189			

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	1n	172	Total	C	N	O	S	0	0
			1495	956	273	258	8		
39	5n	172	Total	C	N	O	S	0	0
			1495	956	273	258	8		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	1o	122	Total	C	N	O	S	0	0
			1045	650	198	187	10		
40	5o	122	Total	C	N	O	S	0	0
			1045	650	198	187	10		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1o	0	MYR	-	insertion	UNP F1SCH1
5o	0	MYR	-	insertion	UNP F1SCH1

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	1p	173	Total	C	N	O	S	0	0
			1449	908	263	270	8		
41	5p	173	Total	C	N	O	S	0	0
			1449	908	263	270	8		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	1q	145	Total	C	N	O	S	0	0
			1212	775	219	213	5		
42	5q	145	Total	C	N	O	S	0	0
			1212	775	219	213	5		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	1r	94	Total	C	N	O	S	0	0
			759	478	143	135	3		
43	5r	94	Total	C	N	O	S	0	0
			759	478	143	135	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1s	45	Total	C	N	O	S	0	0
			382	238	70	73	1		
44	5s	45	Total	C	N	O	S	0	0
			382	238	70	73	1		

- Molecule 45 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	3A	440	Total	C	N	O	S	0	0
			3411	2131	599	662	19		
45	3N	445	Total	C	N	O	S	1	0
			3424	2162	606	637	19		

- Molecule 46 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	3B	418	Total	C	N	O	S	0	0
			3138	1965	555	610	8		
46	3O	417	Total	C	N	O	S	0	0
			3124	1960	554	602	8		

- Molecule 47 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3C	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		
47	3P	379	Total	C	N	O	S	0	0
			3024	2031	471	501	21		

- Molecule 48 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	3D	237	Total	C	N	O	S	0	0
			1888	1205	325	342	16		
48	3Q	239	Total	C	N	O	S	0	0
			1904	1215	327	346	16		

- Molecule 49 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	3E	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
49	3I	47	Total	C	N	O	S	0	0
			340	211	65	63	1		
49	3R	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
49	3V	31	Total	C	N	O	S	0	0
			224	136	48	39	1		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3E	34	VAL	LEU	conflict	UNP A0A4X1TWD8
3E	45	LEU	ALA	conflict	UNP A0A4X1TWD8
3E	49	VAL	PHE	conflict	UNP A0A4X1TWD8
3E	56	ARG	SER	conflict	UNP A0A4X1TWD8
3I	34	VAL	LEU	conflict	UNP A0A4X1TWD8
3I	45	LEU	ALA	conflict	UNP A0A4X1TWD8
3I	49	VAL	PHE	conflict	UNP A0A4X1TWD8
3I	56	ARG	SER	conflict	UNP A0A4X1TWD8
3R	34	VAL	LEU	conflict	UNP A0A4X1TWD8
3R	45	LEU	ALA	conflict	UNP A0A4X1TWD8
3R	49	VAL	PHE	conflict	UNP A0A4X1TWD8
3R	56	ARG	SER	conflict	UNP A0A4X1TWD8
3V	34	VAL	LEU	conflict	UNP A0A4X1TWD8
3V	45	LEU	ALA	conflict	UNP A0A4X1TWD8
3V	49	VAL	PHE	conflict	UNP A0A4X1TWD8
3V	56	ARG	SER	conflict	UNP A0A4X1TWD8

- Molecule 50 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3F	98	Total	C	N	O	S	0	0
			868	557	152	157	2		
50	3S	98	Total	C	N	O	S	0	0
			868	557	152	157	2		

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3G	74	Total	C	N	O	S	0	0
			628	411	116	99	2		
51	3T	74	Total	C	N	O	S	0	0
			628	411	116	99	2		

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	3H	65	Total	C	N	O	S	0	0
			533	325	97	106	5		
52	3U	65	Total	C	N	O	S	0	0
			533	325	97	106	5		

- Molecule 53 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein 53 complex iii.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	3J	56	Total	C	N	O	0	0
			454	295	81	78		
53	3W	56	Total	C	N	O	0	0
			454	295	81	78		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3J	60	ASN	LYS	conflict	UNP Q2EN79
3J	61	GLN	HIS	conflict	UNP Q2EN79
3J	62	GLY	LYS	conflict	UNP Q2EN79
3J	63	LYS	TYR	conflict	UNP Q2EN79
3W	56	ASN	LYS	conflict	UNP Q2EN79
3W	57	GLN	HIS	conflict	UNP Q2EN79
3W	58	GLY	LYS	conflict	UNP Q2EN79
3W	59	LYS	TYR	conflict	UNP Q2EN79

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3X	52	Total	C	N	O	S	0	0
			429	286	75	66	2		
54	3Y	51	Total	C	N	O	S	0	0
			421	281	74	65	1		

- Molecule 55 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	4A	514	Total	C	N	O	S	0	0
			4026	2693	625	676	32		
55	8A	514	Total	C	N	O	S	0	0
			4026	2693	625	676	32		

- Molecule 56 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	4B	227	Total	C	N	O	S	0	0
			1828	1190	281	339	18		
56	8B	227	Total	C	N	O	S	0	0
			1828	1190	281	339	18		

- Molecule 57 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	4C	259	Total	C	N	O	S	0	0
			2096	1399	336	351	10		
57	8C	259	Total	C	N	O	S	0	0
			2096	1399	336	351	10		

- Molecule 58 is a protein called Cytochrome c oxidase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	4D	139	Total	C	N	O	S	0	0
			1163	757	190	212	4		
58	8D	139	Total	C	N	O	S	0	0
			1163	757	190	212	4		

- Molecule 59 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	4E	105	Total	C	N	O	S	0	0
			852	544	144	162	2		
59	8E	105	Total	C	N	O	S	0	0
			852	544	144	162	2		

- Molecule 60 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	4F	97	Total	C	N	O	S	0	0
			734	455	130	143	6		
60	8F	97	Total	C	N	O	S	0	0
			734	455	130	143	6		

- Molecule 61 is a protein called Cytochrome c oxidase subunit 6A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	4G	75	Total	C	N	O	S	0	0
			617	398	118	100	1		
61	8G	75	Total	C	N	O	S	0	0
			617	398	118	100	1		

- Molecule 62 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	4H	82	Total	C	N	O	S	0	0
			687	434	125	123	5		
62	8H	82	Total	C	N	O	S	0	0
			687	434	125	123	5		

- Molecule 63 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	4I	67	Total	C	N	O	S	0	0
			550	359	97	91	3		
63	8I	67	Total	C	N	O	S	0	0
			550	359	97	91	3		

- Molecule 64 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	4J	58	Total	C	N	O	S	0	0
			456	293	78	82	3		
64	8J	58	Total	C	N	O	S	0	0
			456	293	78	82	3		

- Molecule 65 is a protein called Cytochrome c oxidase subunit 7B.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	4K	49	Total	C	N	O	S	0	0
			383	249	65	68	1		
65	8K	49	Total	C	N	O	S	0	0
			383	249	65	68	1		

- Molecule 66 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	4L	46	Total	C	N	O	S	0	0
			381	254	64	61	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
66	8L	46	Total	C	N	O	S	0	0
			381	254	64	61	2		

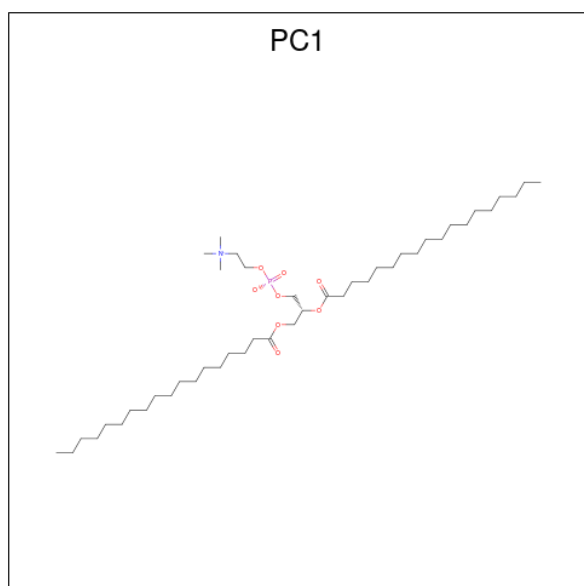
- Molecule 67 is a protein called Cytochrome c oxidase subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
67	4M	43	Total	C	N	O	0	0
			338	222	57	59		
67	8M	43	Total	C	N	O	0	0
			338	222	57	59		

- Molecule 68 is a protein called Cytochrome c oxidase subunit NDUF44.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	4N	82	Total	C	N	O	S	0	0
			660	432	112	114	2		
68	8N	82	Total	C	N	O	S	0	0
			660	432	112	114	2		

- Molecule 69 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
69	1A	1	Total	C	N	O	P	0
			35	25	1	8	1	

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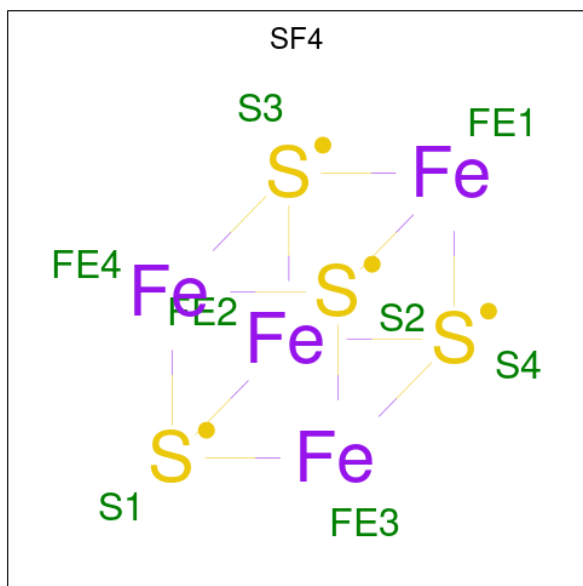
Mol	Chain	Residues	Atoms					AltConf
69	1A	1	Total	C	N	O	P	0
			35	25	1	8	1	
69	1A	1	Total	C	N	O	P	0
			33	23	1	8	1	
69	1B	1	Total	C	N	O	P	0
			46	36	1	8	1	
69	1B	1	Total	C	N	O	P	0
			48	38	1	8	1	
69	1H	1	Total	C	N	O	P	0
			48	38	1	8	1	
69	1I	1	Total	C	N	O	P	0
			54	44	1	8	1	
69	1I	1	Total	C	N	O	P	0
			44	34	1	8	1	
69	1L	1	Total	C	N	O	P	0
			46	36	1	8	1	
69	1M	1	Total	C	N	O	P	0
			35	25	1	8	1	
69	1M	1	Total	C	N	O	P	0
			44	34	1	8	1	
69	1d	1	Total	C	N	O	P	0
			39	29	1	8	1	
69	1h	1	Total	C	N	O	P	0
			47	37	1	8	1	
69	1q	1	Total	C	N	O	P	0
			49	39	1	8	1	
69	3J	1	Total	C	N	O	P	0
			47	37	1	8	1	
69	3R	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	3X	1	Total	C	N	O	P	0
			29	19	1	8	1	
69	5A	1	Total	C	N	O	P	0
			35	25	1	8	1	
69	5A	1	Total	C	N	O	P	0
			35	25	1	8	1	
69	5B	1	Total	C	N	O	P	0
			46	36	1	8	1	
69	5B	1	Total	C	N	O	P	0
			48	38	1	8	1	
69	5H	1	Total	C	N	O	P	0
			48	38	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
69	5I	1	Total	C	N	O	P	0
			54	44	1	8	1	
69	5I	1	Total	C	N	O	P	0
			44	34	1	8	1	
69	5L	1	Total	C	N	O	P	0
			46	36	1	8	1	
69	5M	1	Total	C	N	O	P	0
			35	25	1	8	1	
69	5M	1	Total	C	N	O	P	0
			44	34	1	8	1	
69	5P	1	Total	C	N	O	P	0
			33	23	1	8	1	
69	5d	1	Total	C	N	O	P	0
			39	29	1	8	1	
69	5h	1	Total	C	N	O	P	0
			47	37	1	8	1	
69	5q	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 70 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



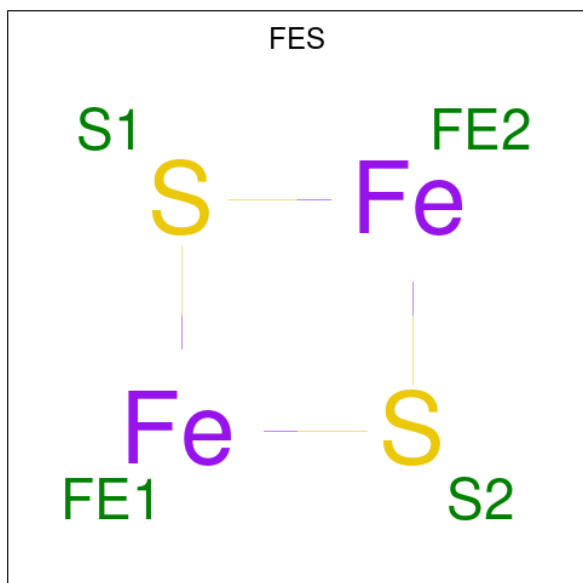
Mol	Chain	Residues	Atoms			AltConf
70	1B	1	Total	Fe	S	0
			8	4	4	
70	1F	1	Total	Fe	S	0
			8	4	4	

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Mol	Chain	Residues	Atoms			AltConf
70	1G	1	Total	Fe	S	0
			8	4	4	
70	1G	1	Total	Fe	S	0
			8	4	4	
70	1I	1	Total	Fe	S	0
			8	4	4	
70	1I	1	Total	Fe	S	0
			8	4	4	
70	5B	1	Total	Fe	S	0
			8	4	4	
70	5F	1	Total	Fe	S	0
			8	4	4	
70	5G	1	Total	Fe	S	0
			8	4	4	
70	5G	1	Total	Fe	S	0
			8	4	4	
70	5I	1	Total	Fe	S	0
			8	4	4	
70	5I	1	Total	Fe	S	0
			8	4	4	

- Molecule 71 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



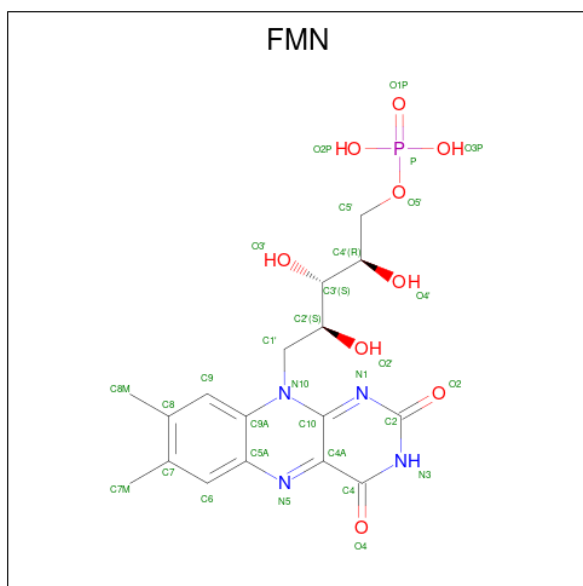
Mol	Chain	Residues	Atoms			AltConf
71	1E	1	Total	Fe	S	0
			4	2	2	

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Mol	Chain	Residues	Atoms			AltConf
71	1G	1	Total	Fe	S	0
			4	2	2	
71	3E	1	Total	Fe	S	0
			4	2	2	
71	3R	1	Total	Fe	S	0
			4	2	2	
71	5E	1	Total	Fe	S	0
			4	2	2	
71	5G	1	Total	Fe	S	0
			4	2	2	

- Molecule 72 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

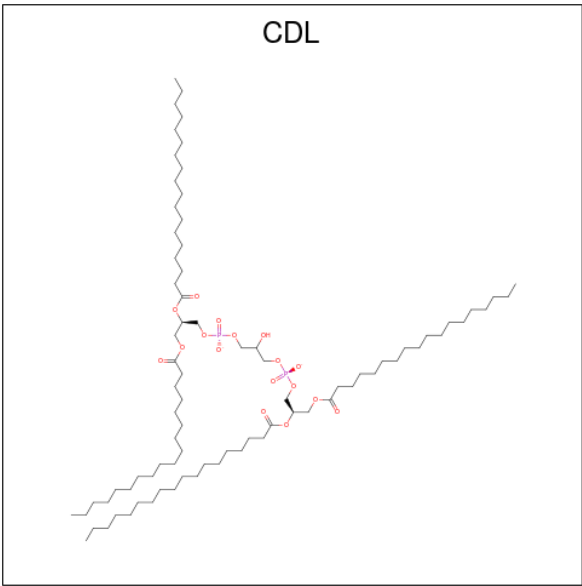


Mol	Chain	Residues	Atoms					AltConf
72	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	
72	5F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 73 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
73	1G	1	Total	K	0
			1	1	
73	5G	1	Total	K	0
			1	1	

- Molecule 74 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



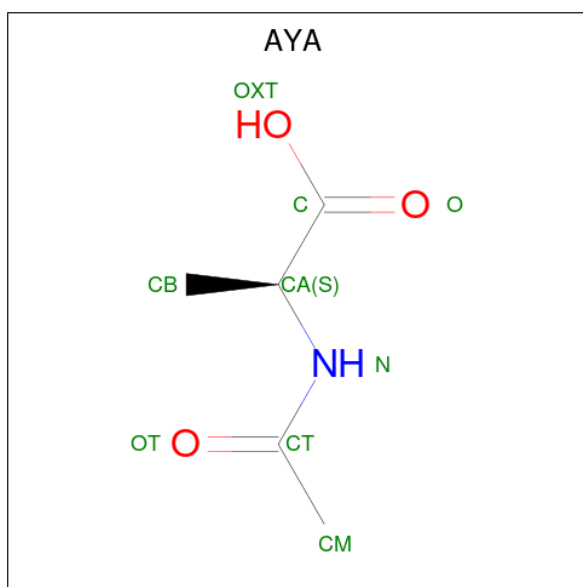
Mol	Chain	Residues	Atoms				AltConf
74	1H	1	Total	C	O	P	0
			51	32	17	2	
74	1L	1	Total	C	O	P	0
			76	57	17	2	
74	1N	1	Total	C	O	P	0
			62	43	17	2	
74	1X	1	Total	C	O	P	0
			86	67	17	2	
74	1d	1	Total	C	O	P	0
			65	46	17	2	
74	1h	1	Total	C	O	P	0
			80	61	17	2	
74	1q	1	Total	C	O	P	0
			61	42	17	2	
74	3A	1	Total	C	O	P	0
			58	39	17	2	
74	3C	1	Total	C	O	P	0
			52	33	17	2	
74	3G	1	Total	C	O	P	0
			56	37	17	2	
74	3N	1	Total	C	O	P	0
			43	24	17	2	
74	3P	1	Total	C	O	P	0
			56	37	17	2	
74	3T	1	Total	C	O	P	0
			57	38	17	2	

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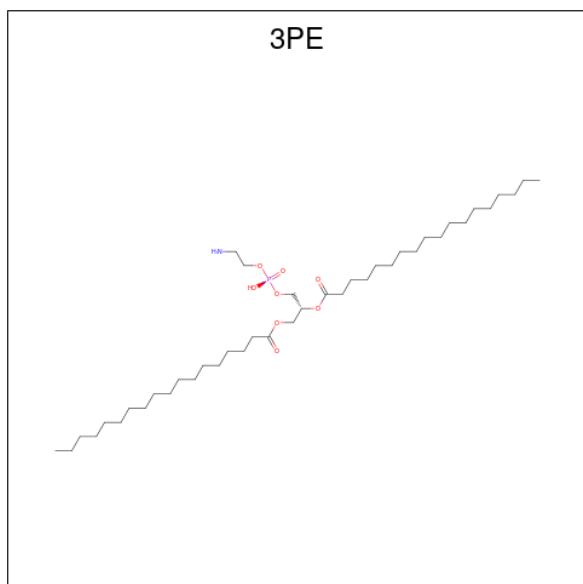
Mol	Chain	Residues	Atoms				AltConf
74	4B	1	Total 100	C 81	O 17	P 2	0
74	4C	1	Total 100	C 81	O 17	P 2	0
74	4D	1	Total 100	C 81	O 17	P 2	0
74	5H	1	Total 51	C 32	O 17	P 2	0
74	5L	1	Total 76	C 57	O 17	P 2	0
74	5N	1	Total 62	C 43	O 17	P 2	0
74	5X	1	Total 86	C 67	O 17	P 2	0
74	5d	1	Total 65	C 46	O 17	P 2	0
74	5h	1	Total 80	C 61	O 17	P 2	0
74	5q	1	Total 61	C 42	O 17	P 2	0
74	8B	1	Total 100	C 81	O 17	P 2	0
74	8C	1	Total 100	C 81	O 17	P 2	0
74	8D	1	Total 100	C 81	O 17	P 2	0

- Molecule 75 is N-ACETYLALANINE (CCD ID: AYA) (formula: C₅H₉NO₃).



Mol	Chain	Residues	Atoms				AltConf
75	1I	1	Total	C	N	O	0
			8	5	1	2	
75	5q	1	Total	C	N	O	0
			8	5	1	2	

- Molecule 76 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
76	1K	1	Total	C	N	O	P	0
			44	34	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
76	1L	1	Total 46	C 36	N 1	O 8	P 1	0
76	1L	1	Total 45	C 35	N 1	O 8	P 1	0
76	1M	1	Total 49	C 39	N 1	O 8	P 1	0
76	1M	1	Total 45	C 35	N 1	O 8	P 1	0
76	1M	1	Total 48	C 38	N 1	O 8	P 1	0
76	1M	1	Total 50	C 40	N 1	O 8	P 1	0
76	1O	1	Total 51	C 41	N 1	O 8	P 1	0
76	1P	1	Total 35	C 25	N 1	O 8	P 1	0
76	1Y	1	Total 31	C 21	N 1	O 8	P 1	0
76	1Y	1	Total 40	C 30	N 1	O 8	P 1	0
76	1Y	1	Total 30	C 20	N 1	O 8	P 1	0
76	1Y	1	Total 33	C 23	N 1	O 8	P 1	0
76	1Y	1	Total 27	C 17	N 1	O 8	P 1	0
76	1Y	1	Total 41	C 31	N 1	O 8	P 1	0
76	1b	1	Total 47	C 37	N 1	O 8	P 1	0
76	1d	1	Total 49	C 39	N 1	O 8	P 1	0
76	1j	1	Total 44	C 34	N 1	O 8	P 1	0
76	3A	1	Total 27	C 17	N 1	O 8	P 1	0
76	3A	1	Total 32	C 22	N 1	O 8	P 1	0
76	3C	1	Total 35	C 25	N 1	O 8	P 1	0
76	3C	1	Total 34	C 24	N 1	O 8	P 1	0

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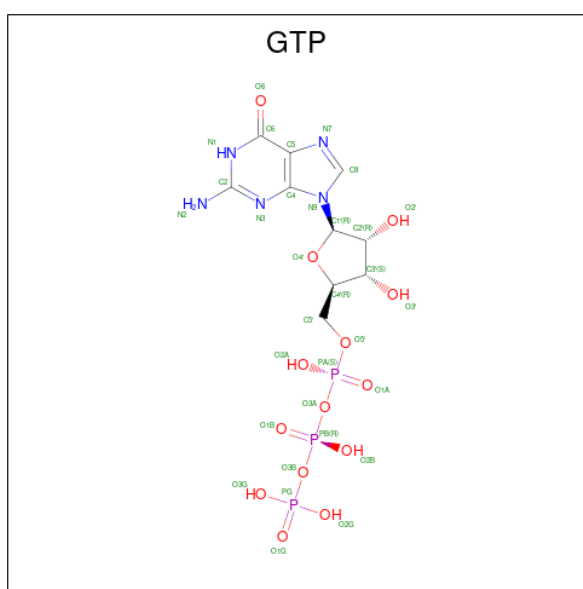
Mol	Chain	Residues	Atoms					AltConf
76	3D	1	Total 33	C 23	N 1	O 8	P 1	0
76	3G	1	Total 29	C 19	N 1	O 8	P 1	0
76	3N	1	Total 33	C 23	N 1	O 8	P 1	0
76	3N	1	Total 25	C 15	N 1	O 8	P 1	0
76	3P	1	Total 33	C 23	N 1	O 8	P 1	0
76	3Q	1	Total 47	C 37	N 1	O 8	P 1	0
76	3Y	1	Total 30	C 20	N 1	O 8	P 1	0
76	5A	1	Total 47	C 37	N 1	O 8	P 1	0
76	5K	1	Total 44	C 34	N 1	O 8	P 1	0
76	5L	1	Total 46	C 36	N 1	O 8	P 1	0
76	5L	1	Total 45	C 35	N 1	O 8	P 1	0
76	5L	1	Total 49	C 39	N 1	O 8	P 1	0
76	5M	1	Total 45	C 35	N 1	O 8	P 1	0
76	5M	1	Total 48	C 38	N 1	O 8	P 1	0
76	5M	1	Total 51	C 41	N 1	O 8	P 1	0
76	5M	1	Total 50	C 40	N 1	O 8	P 1	0
76	5P	1	Total 35	C 25	N 1	O 8	P 1	0
76	5Y	1	Total 31	C 21	N 1	O 8	P 1	0
76	5Y	1	Total 40	C 30	N 1	O 8	P 1	0
76	5Y	1	Total 30	C 20	N 1	O 8	P 1	0
76	5Y	1	Total 33	C 23	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
76	5Y	1	Total	C	N	O	P	0
			27	17	1	8	1	
76	5Y	1	Total	C	N	O	P	0
			41	31	1	8	1	
76	5d	1	Total	C	N	O	P	0
			49	39	1	8	1	
76	5j	1	Total	C	N	O	P	0
			44	34	1	8	1	

- Molecule 77 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
77	1O	1	Total	C	N	O	P	0
			32	10	5	14	3	
77	5O	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 78 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
78	1O	1	Total	Mg	0
			1	1	
78	4A	1	Total	Mg	0
			1	1	
78	5O	1	Total	Mg	0
			1	1	

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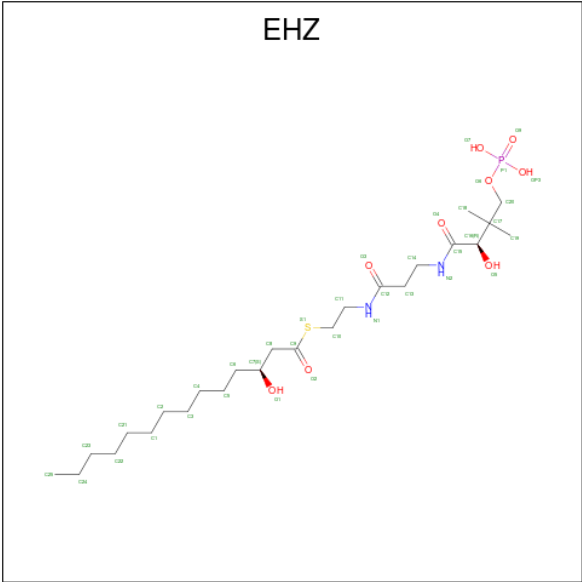
Mol	Chain	Residues	Atoms	AltConf
78	8A	1	Total Mg 1 1	0

- # NDP

Mol	Chain	Residues	Atoms					AltConf
79	1P	1	Total 48	C 21	N 7	O 17	P 3	0
79	5P	1	Total 48	C 21	N 7	O 17	P 3	0

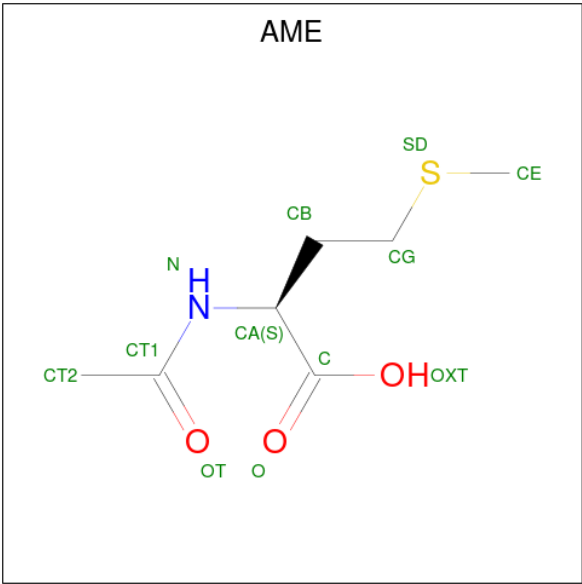
Mol	Chain	Residues	Atoms	AltConf
80	1R	1	Total Zn 1 1	0
80	4F	1	Total Zn 1 1	0
80	5R	1	Total Zn 1 1	0
80	8F	1	Total Zn 1 1	0

- 



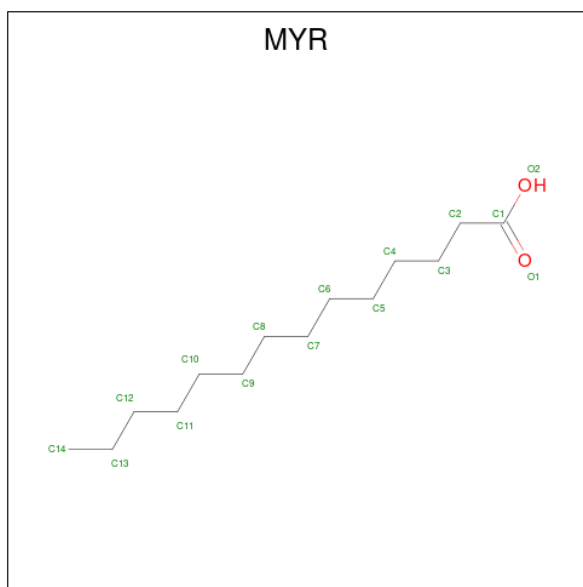
Mol	Chain	Residues	Atoms						AltConf
81	1T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
81	1n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
81	5T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
81	5n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 82 is N-ACETYLMETHIONINE (CCD ID: AME) (formula: C₇H₁₃NO₃S).



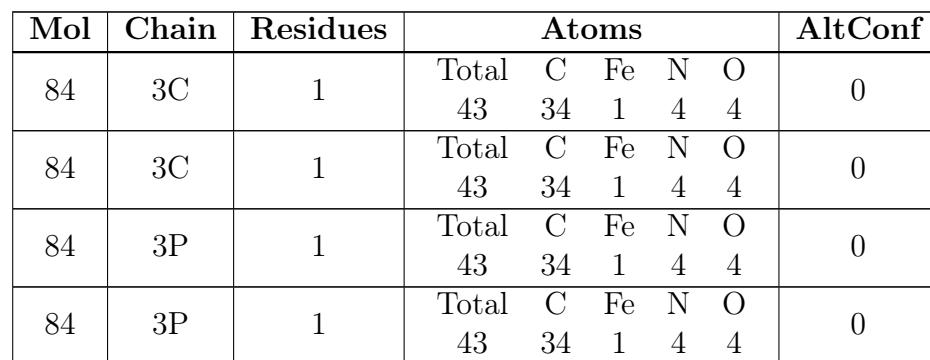
Mol	Chain	Residues	Atoms					AltConf
82	1h	1	Total	C	N	O	S	0
			11	7	1	2	1	
82	5h	1	Total	C	N	O	S	0
			11	7	1	2	1	

- Molecule 83 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			AltConf
83	1o	1	Total	C	O	0
			15	14	1	
83	5o	1	Total	C	O	0
			15	14	1	

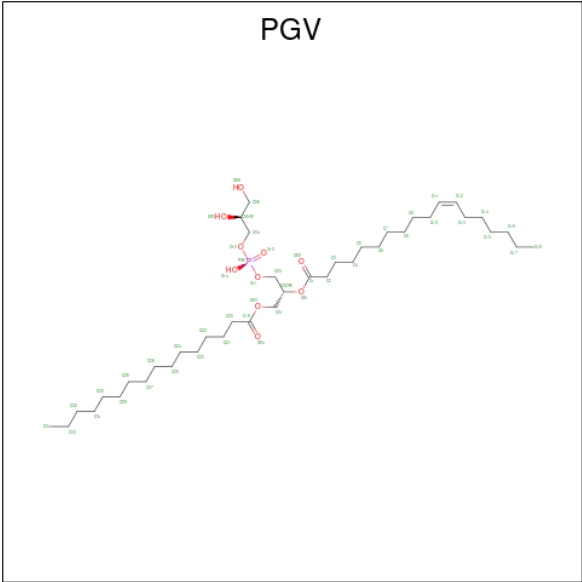
- Molecule 84 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



-
- The chemical structure of HEC (Hydroxyethylchlorin) is shown. It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The structure includes various side chains and a central hydrogen atom (H). The side chains are labeled with green text: CAA, CBA, CAD, CBD, CMA, C3A, C4A, C3B, C4B, CMB, CBB, CAA, CBA, CAD, CBD, CMA, C3A, C4A, C3B, C4B, CMB, CBB. The central hydrogen atom is labeled with red text: H1A, H2A, H1D, H2D. The central iron atom is labeled with purple text: FE. The nitrogen atoms are labeled with blue text: NA, NB, NC, ND. The side chains are labeled with green text: CAA, CBA, CAD, CBD, CMA, C3A, C4A, C3B, C4B, CMB, CBB, CAA, CBA, CAD, CBD, CMA, C3A, C4A, C3B, C4B, CMB, CBB.

Mol	Chain	Residues	Atoms					AltConf
85	3D	1	Total	C	Fe	N	O	0
			42	34	1	4	3	
85	3Q	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 86 is (1R)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



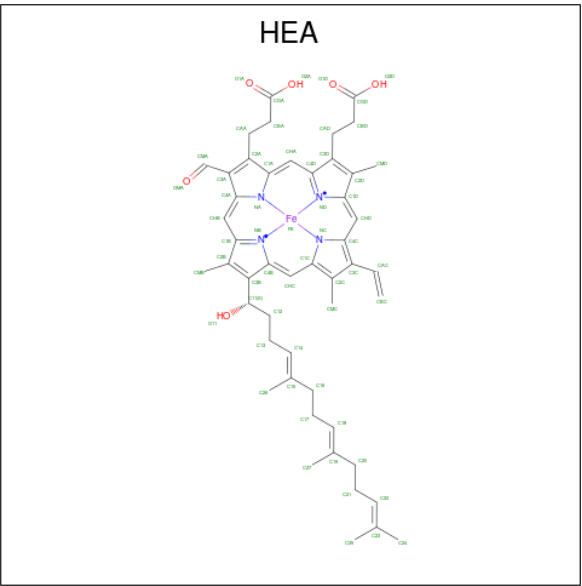
Mol	Chain	Residues	Atoms				AltConf
86	4A	1	Total	C	O	P	0
			51	40	10	1	
86	4A	1	Total	C	O	P	0
			51	40	10	1	
86	4A	1	Total	C	O	P	0
			51	40	10	1	
86	4B	1	Total	C	O	P	0
			51	40	10	1	
86	4C	1	Total	C	O	P	0
			51	40	10	1	
86	4C	1	Total	C	O	P	0
			51	40	10	1	
86	4C	1	Total	C	O	P	0
			51	40	10	1	
86	4C	1	Total	C	O	P	0
			51	40	10	1	
86	4C	1	Total	C	O	P	0
			51	40	10	1	

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Mol	Chain	Residues	Atoms				AltConf
86	4C	1	Total	C	O	P	0
			51	40	10	1	
86	4G	1	Total	C	O	P	0
			51	40	10	1	
86	4J	1	Total	C	O	P	0
			51	40	10	1	
86	4K	1	Total	C	O	P	0
			51	40	10	1	
86	4L	1	Total	C	O	P	0
			51	40	10	1	
86	4M	1	Total	C	O	P	0
			51	40	10	1	
86	8A	1	Total	C	O	P	0
			51	40	10	1	
86	8A	1	Total	C	O	P	0
			51	40	10	1	
86	8B	1	Total	C	O	P	0
			51	40	10	1	
86	8B	1	Total	C	O	P	0
			51	40	10	1	
86	8C	1	Total	C	O	P	0
			51	40	10	1	
86	8C	1	Total	C	O	P	0
			51	40	10	1	
86	8C	1	Total	C	O	P	0
			51	40	10	1	
86	8C	1	Total	C	O	P	0
			51	40	10	1	
86	8C	1	Total	C	O	P	0
			51	40	10	1	
86	8C	1	Total	C	O	P	0
			51	40	10	1	
86	8G	1	Total	C	O	P	0
			51	40	10	1	
86	8J	1	Total	C	O	P	0
			51	40	10	1	
86	8K	1	Total	C	O	P	0
			51	40	10	1	
86	8L	1	Total	C	O	P	0
			51	40	10	1	
86	8M	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 87 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
87	4A	1	Total 60	C 49	Fe 1	N 4	O 6	0
87	4A	1	Total 60	C 49	Fe 1	N 4	O 6	0
87	8A	1	Total 60	C 49	Fe 1	N 4	O 6	0
87	8A	1	Total 60	C 49	Fe 1	N 4	O 6	0

- Molecule 88 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

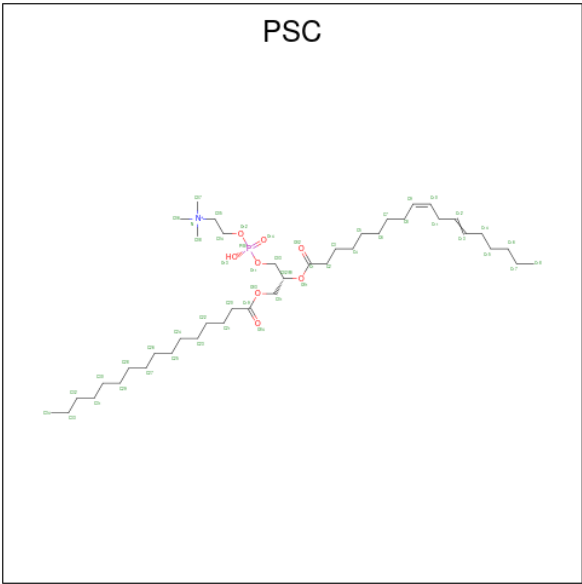
Mol	Chain	Residues	Atoms		AltConf
88	4A	1	Total	Cu	0
			1	1	
88	8A	1	Total	Cu	0
			1	1	

- Molecule 89 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
89	4A	1	Total	Na	0
			1	1	
89	8A	1	Total	Na	0
			1	1	

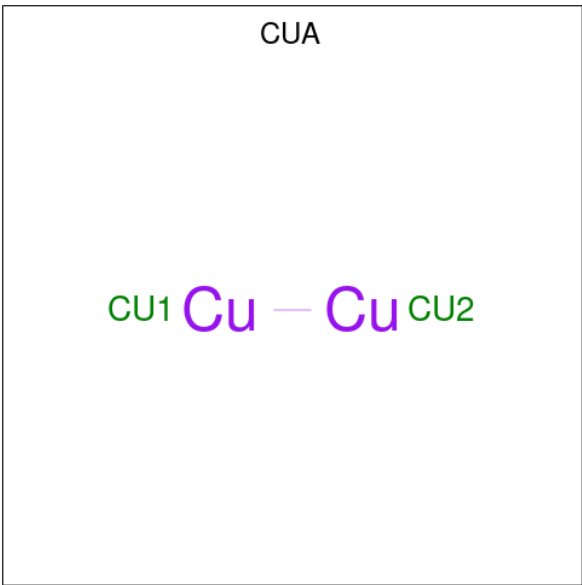
- Molecule 90 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITO

YLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM
4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).



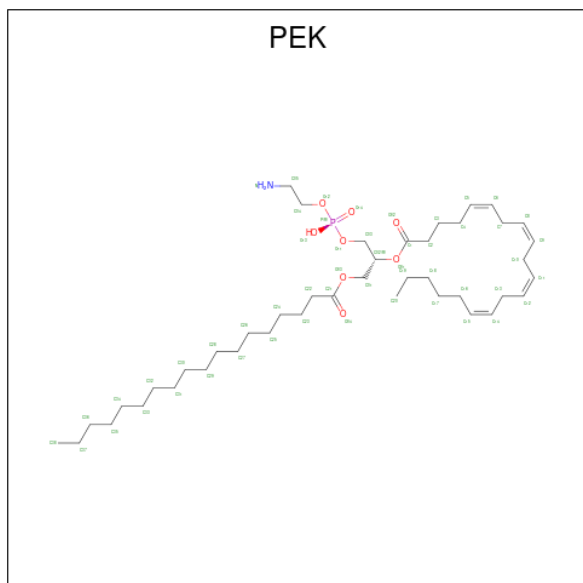
Mol	Chain	Residues	Atoms					AltConf
90	4A	1	Total	C	N	O	P	0
			52	42	1	8	1	
90	8I	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 91 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



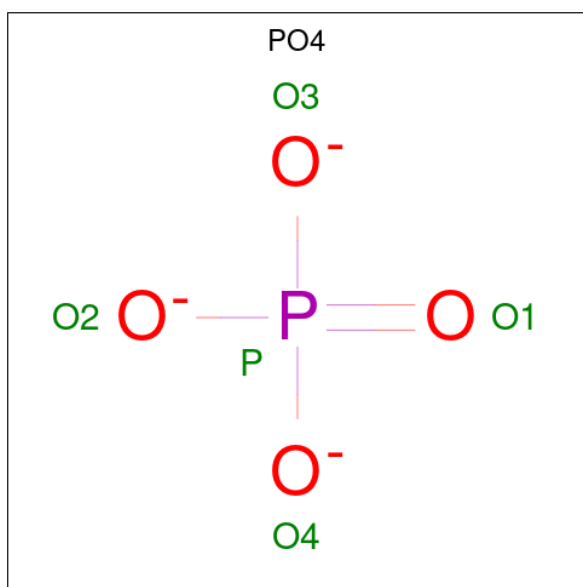
Mol	Chain	Residues	Atoms		AltConf
91	4B	1	Total	Cu	0
			2	2	
91	8B	1	Total	Cu	0
			2	2	

- Molecule 92 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYL)OXY]METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C₄₃H₇₈NO₈P).

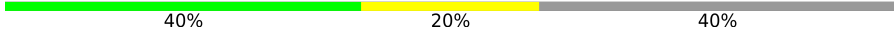


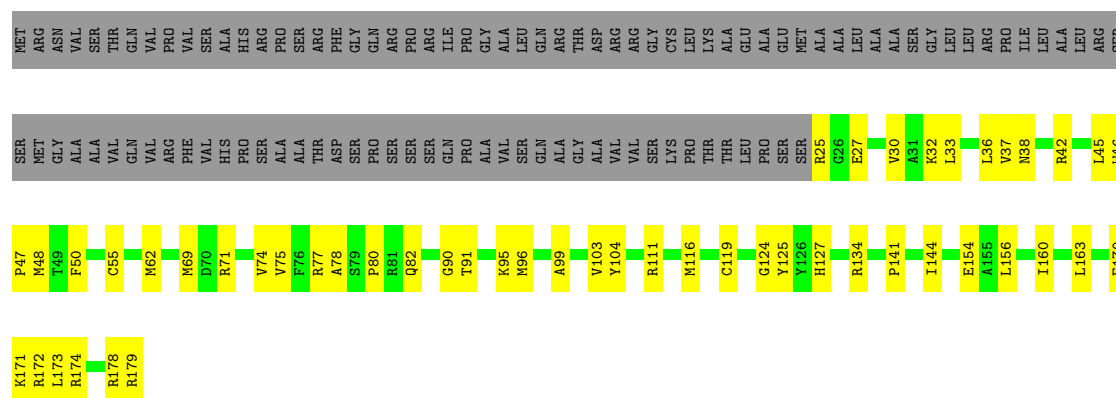
Mol	Chain	Residues	Atoms					AltConf
92	4C	1	Total	C	N	O	P	0
			52	42	1	8	1	
92	4G	1	Total	C	N	O	P	0
			53	43	1	8	1	
92	8C	1	Total	C	N	O	P	0
			52	42	1	8	1	
92	8G	1	Total	C	N	O	P	0
			53	43	1	8	1	

- Molecule 93 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



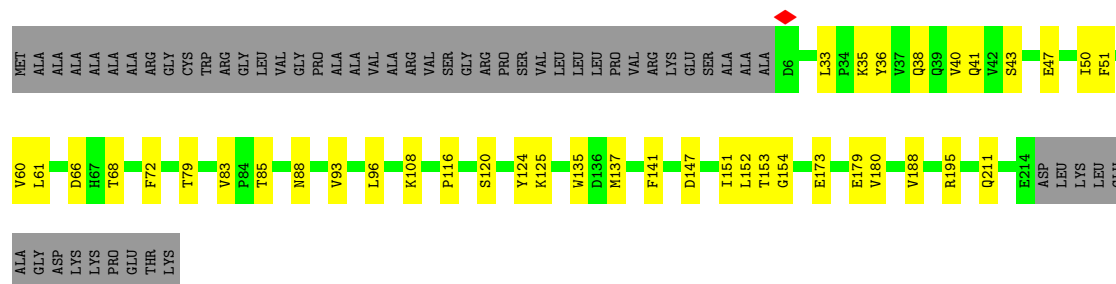
Mol	Chain	Residues	Atoms			AltConf
93	4H	1	Total	O	P	0
			5	4	1	
93	8H	1	Total	O	P	0
			5	4	1	

Chain 5B: 



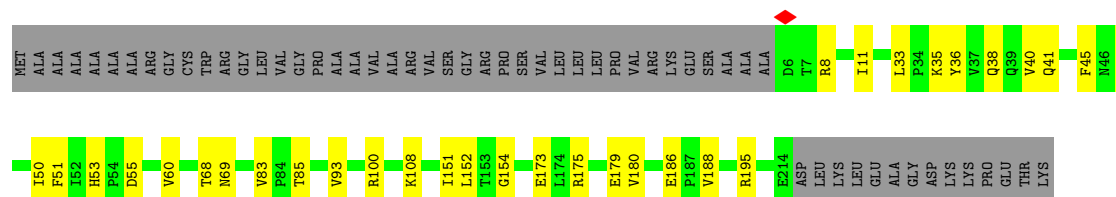
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain 1C: 



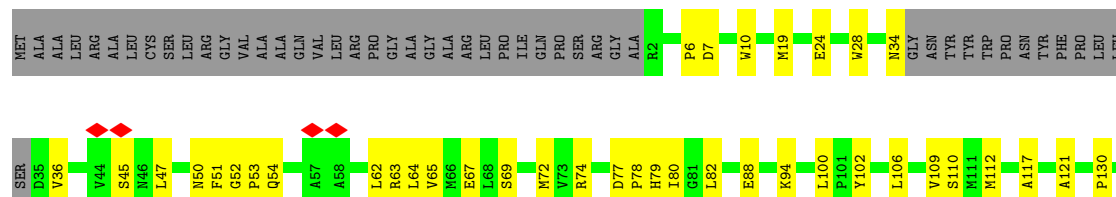
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

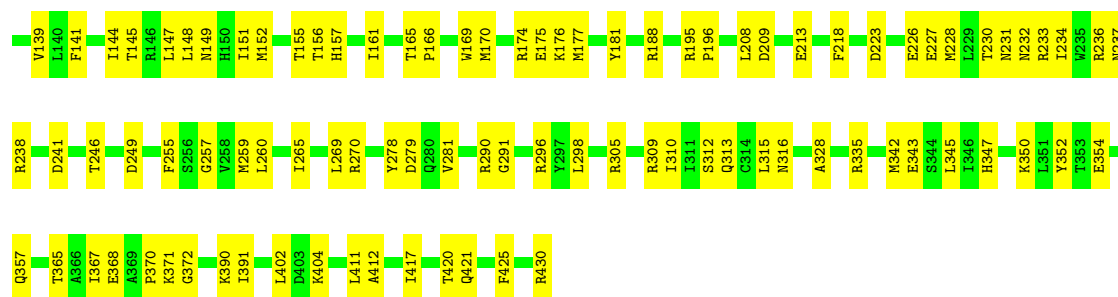
Chain 5C: 



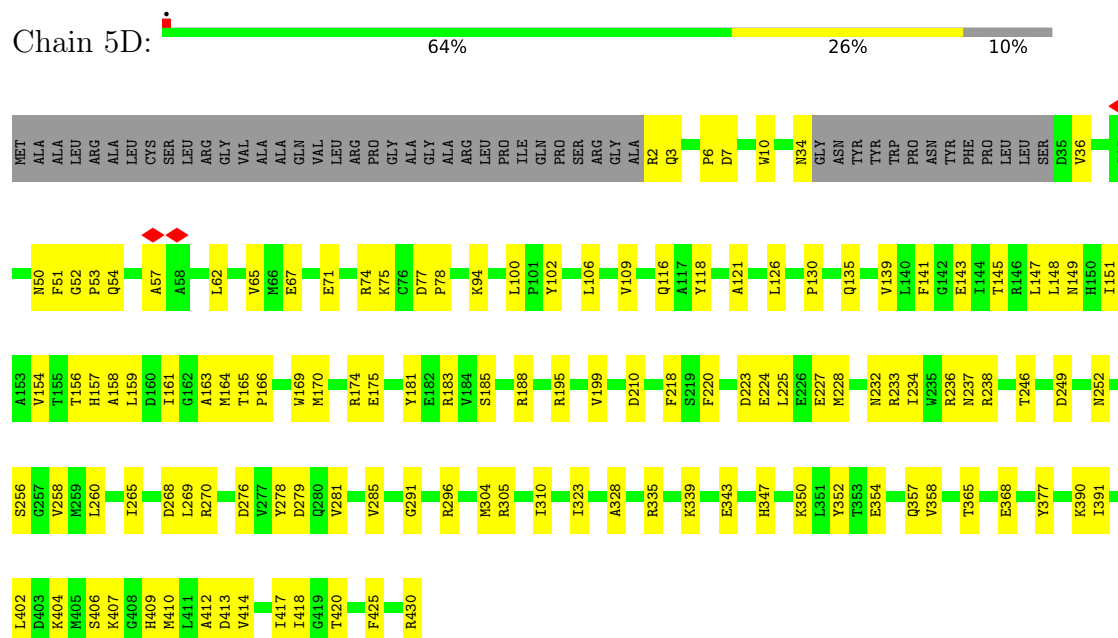
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain 1D: 

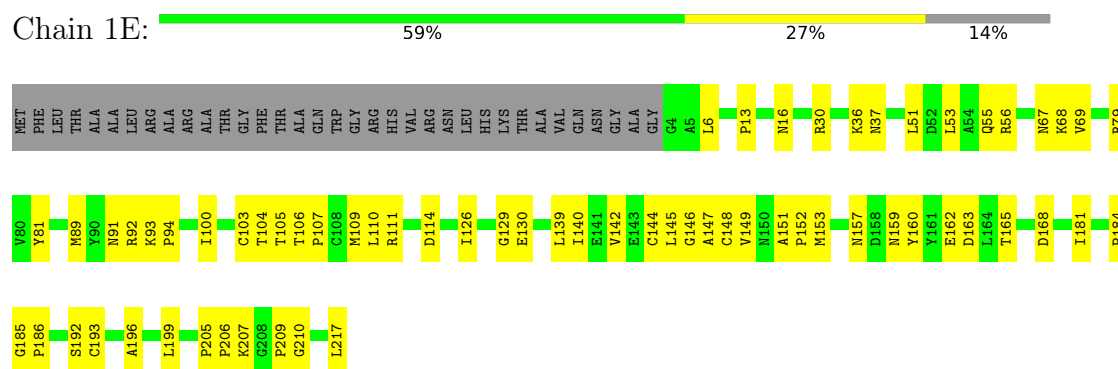




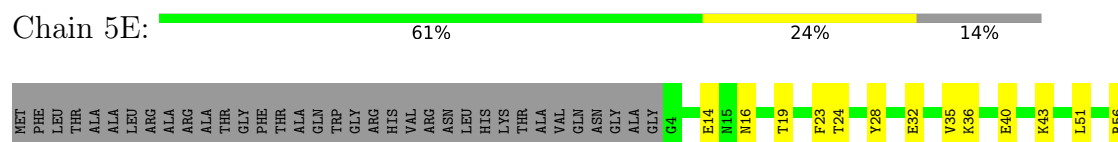
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

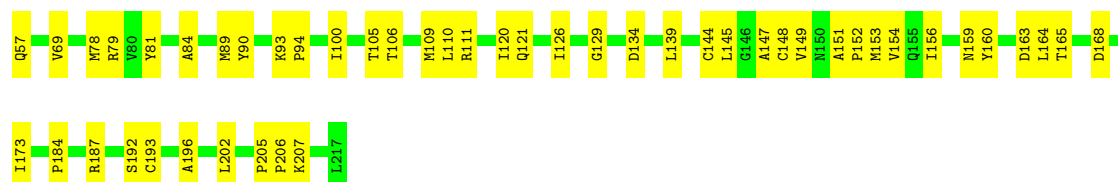


- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



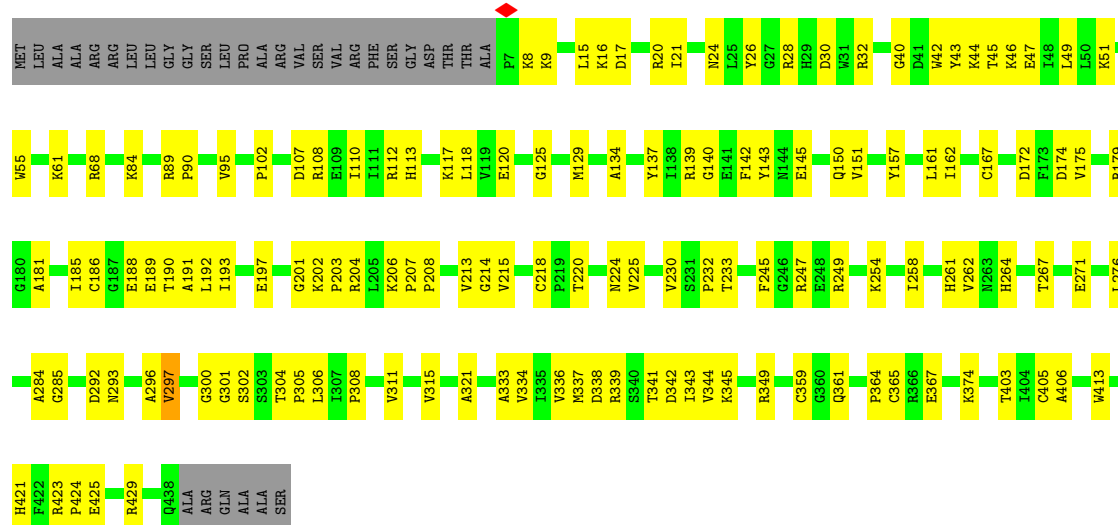
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial





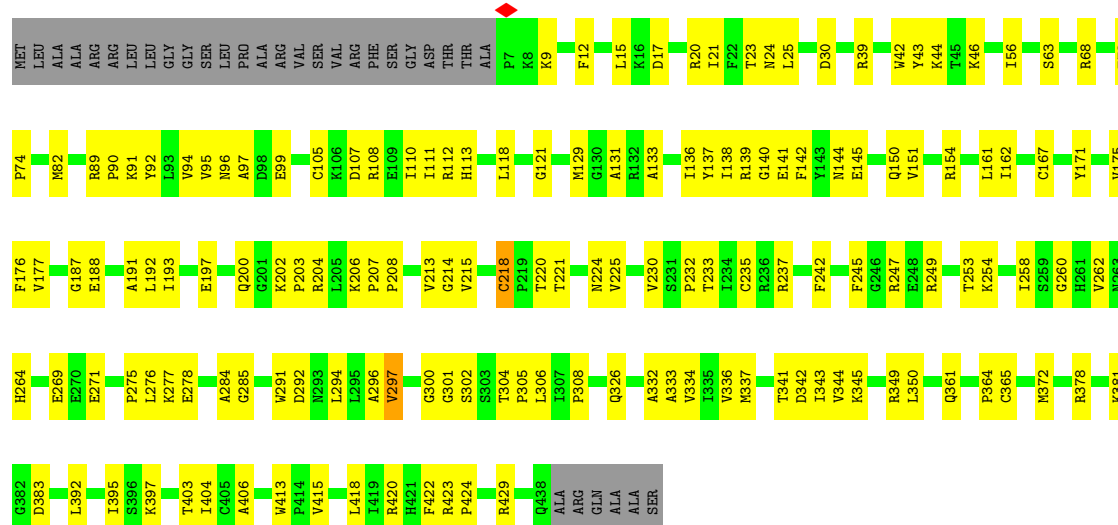
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1F: 64% 29% 7%



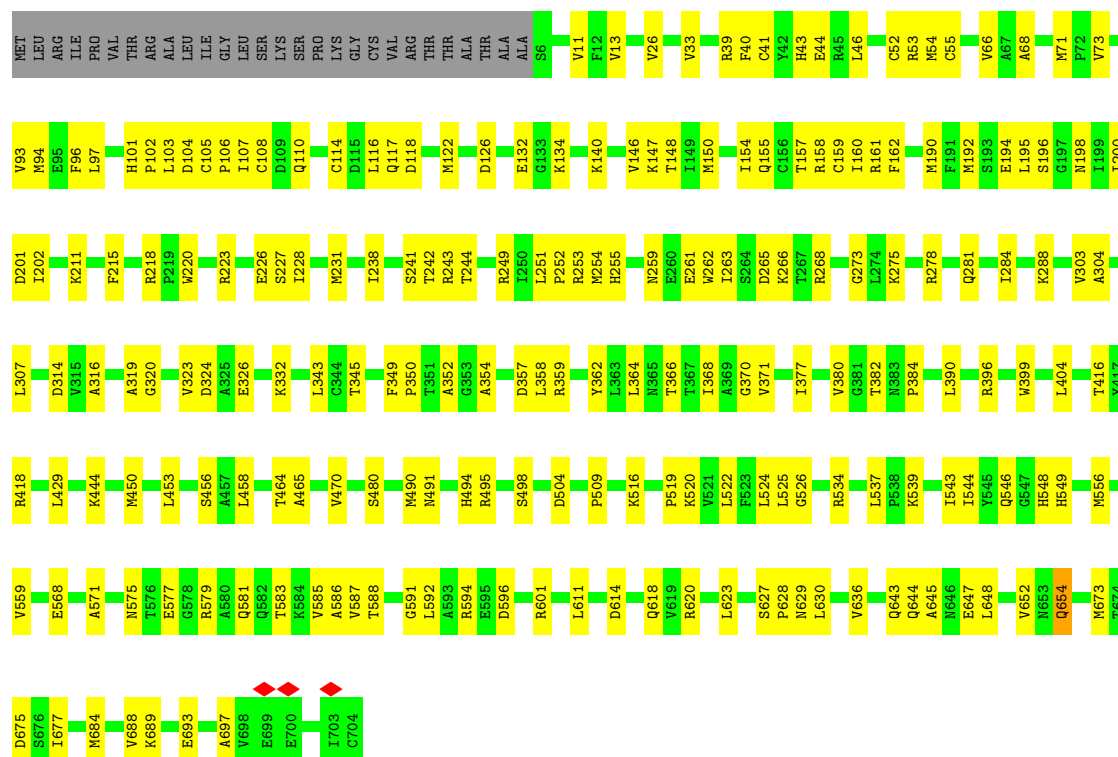
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 5F: 61% 32% 7%



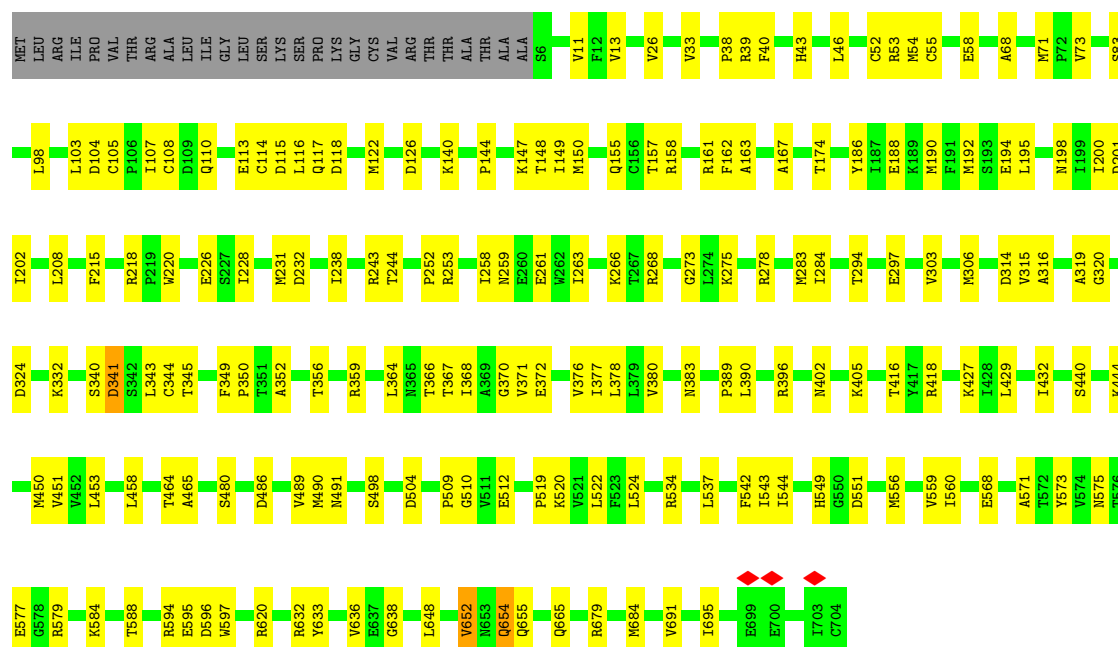
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain 1G: 68% 28% 4%



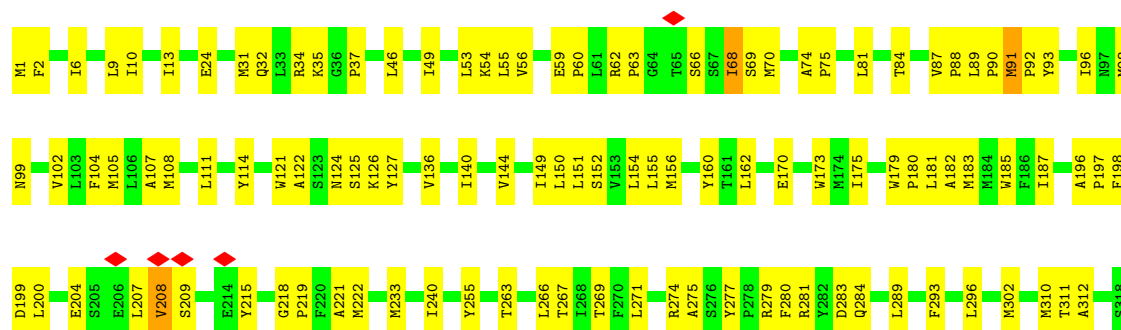
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain 5G: 71% 25% •



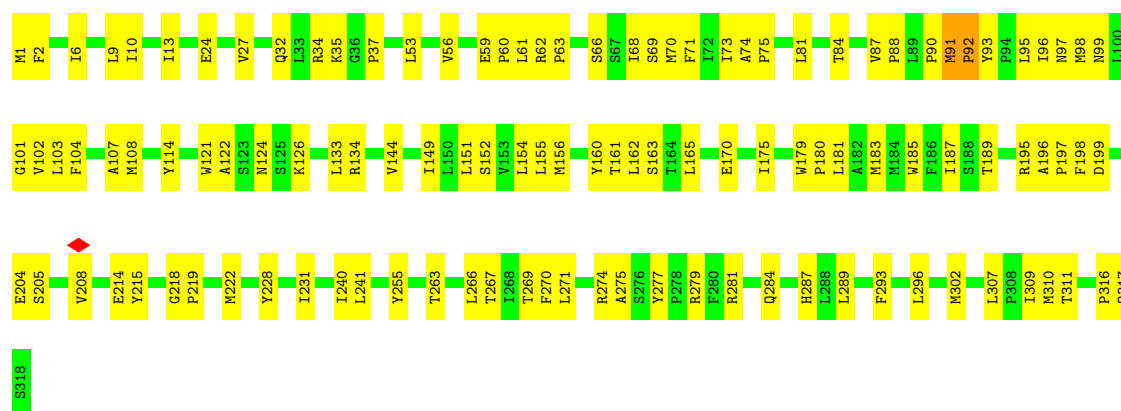
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain 1H: 65% 34% •



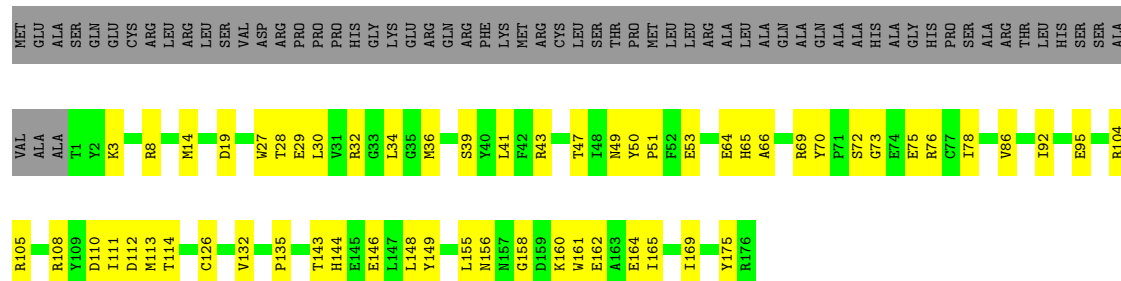
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain 5H: 64% 36%



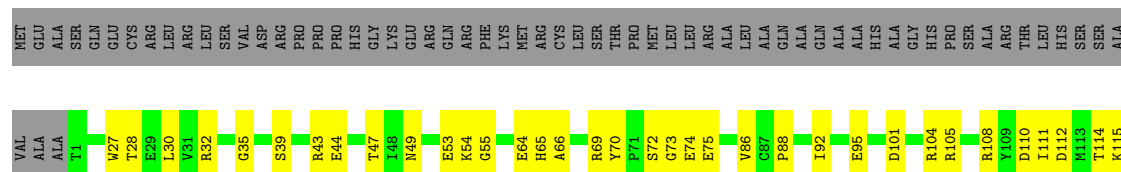
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 1I: 49% 24% 26%



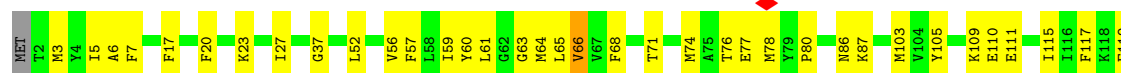
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 5I: 49% 25% 26%

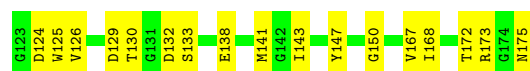
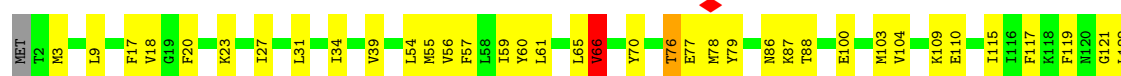




- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

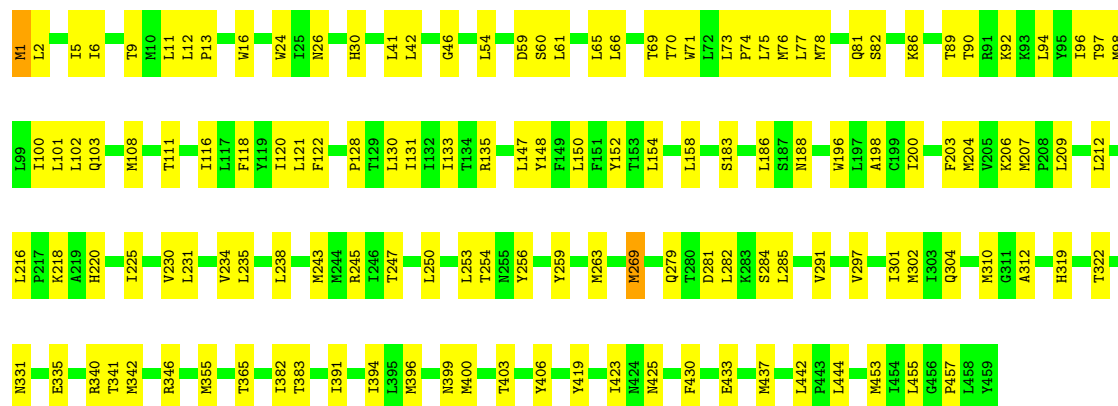


- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

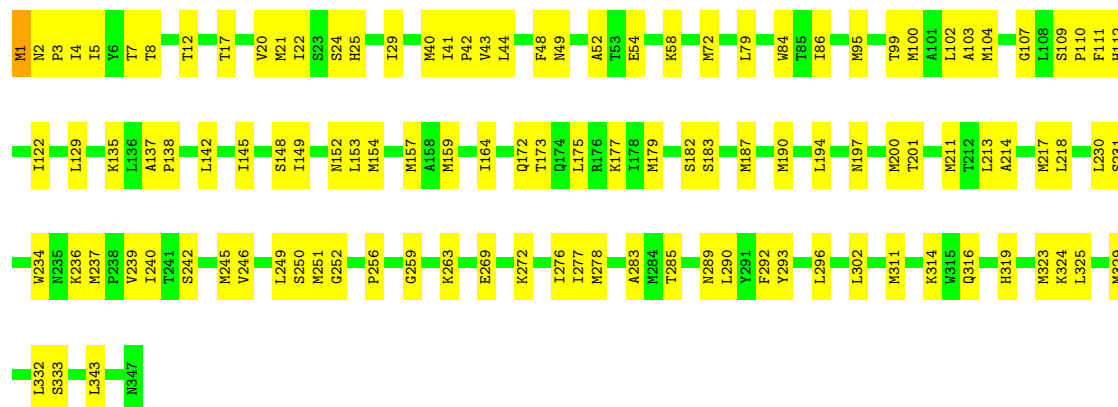




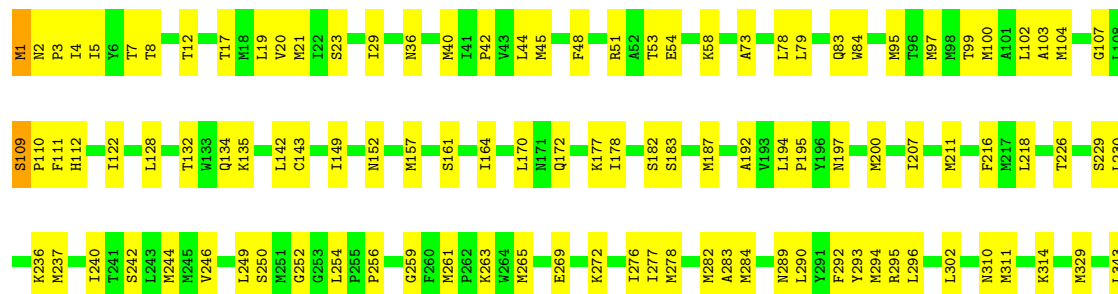
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4



• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

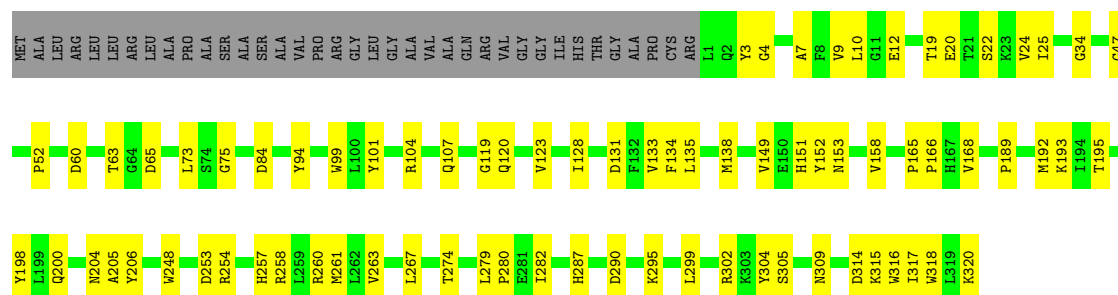


• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

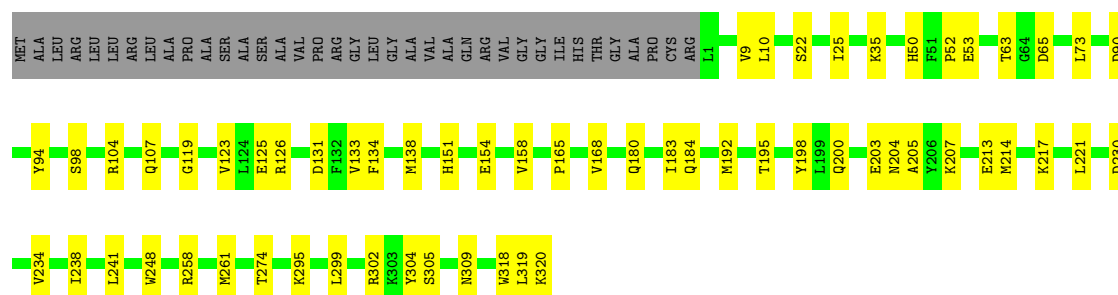


R347

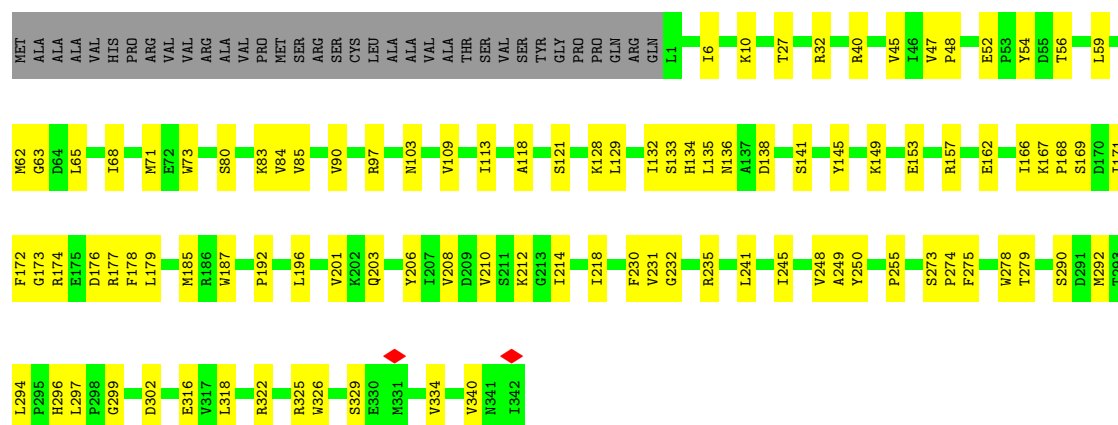
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain 10:  68% 22% 10%

- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

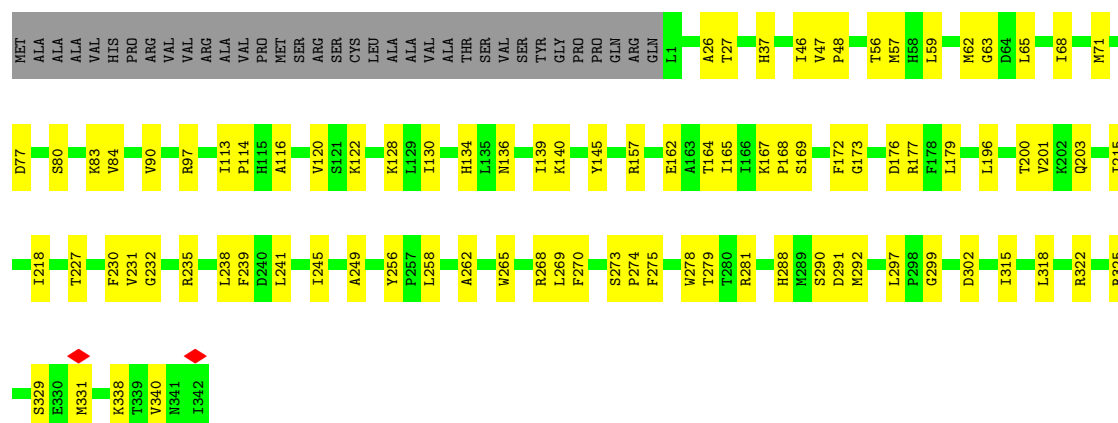
Chain 50:  73% 17% 10%

- Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

Chain 1P:  65% 26% 9%

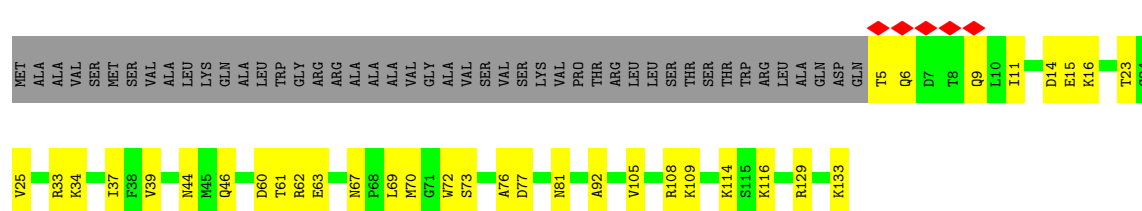
- Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

Chain 5P: 



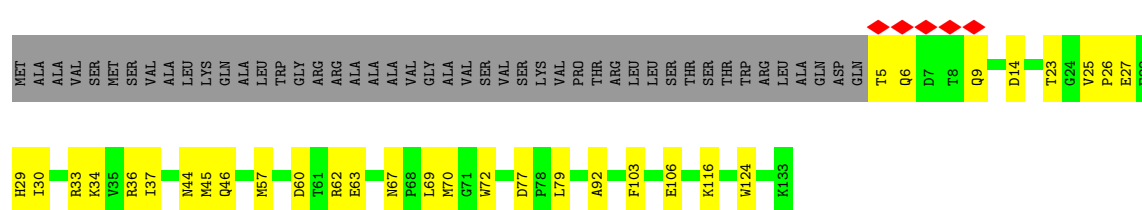
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain 1Q: 



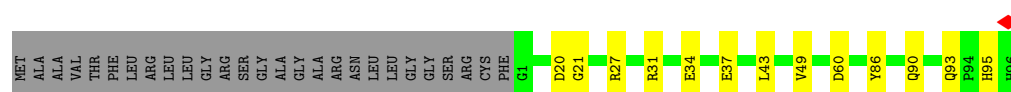
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain 5Q: 



- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain 1R: 



- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

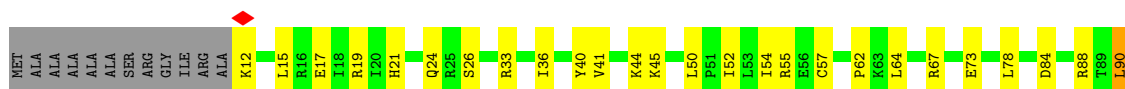
Chain 5R: 



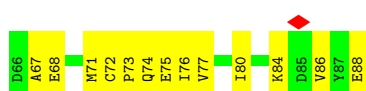
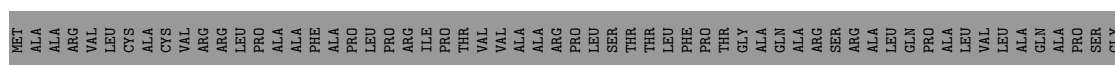
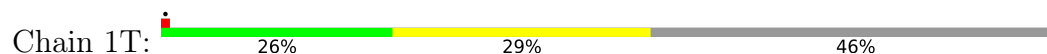
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



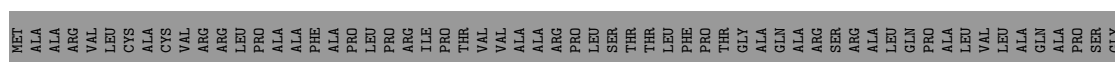
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



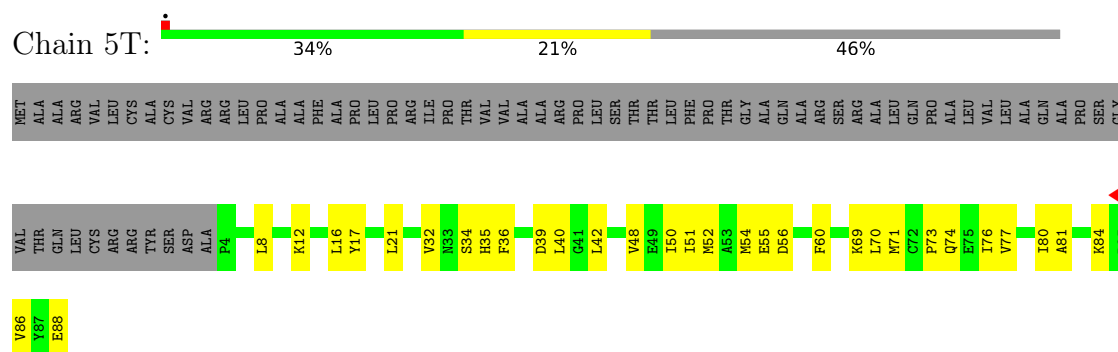
- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



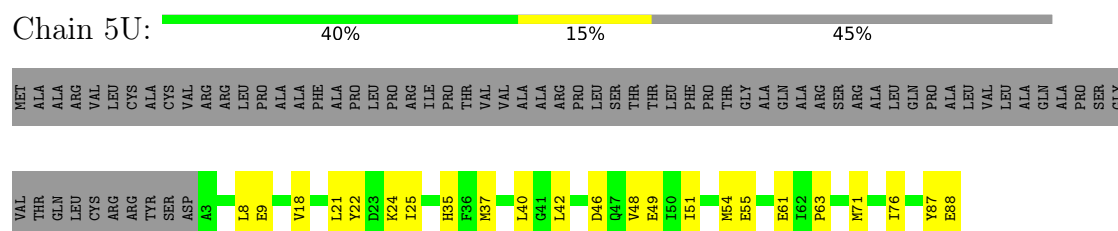
- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



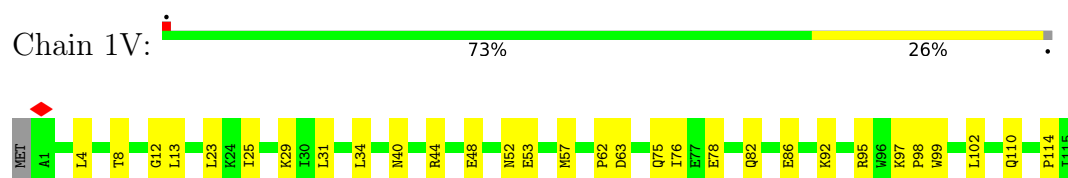
- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



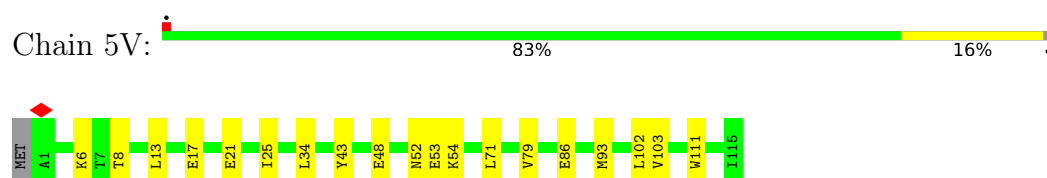
- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



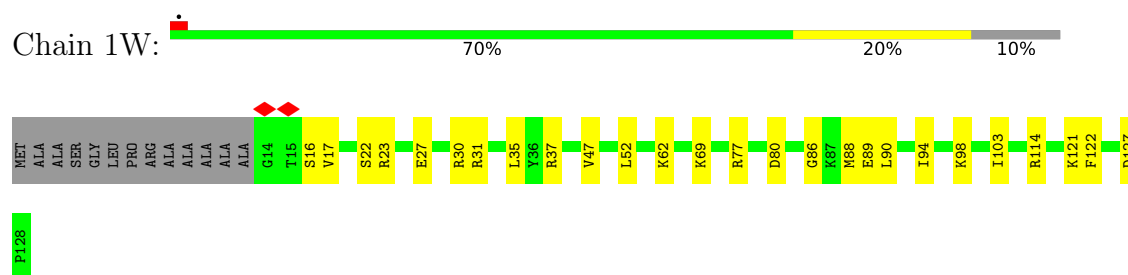
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1



- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1

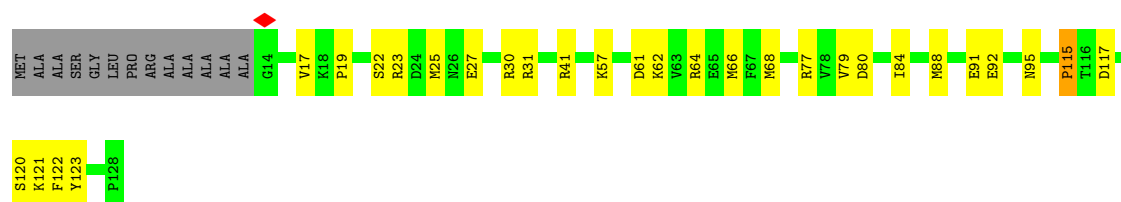


- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



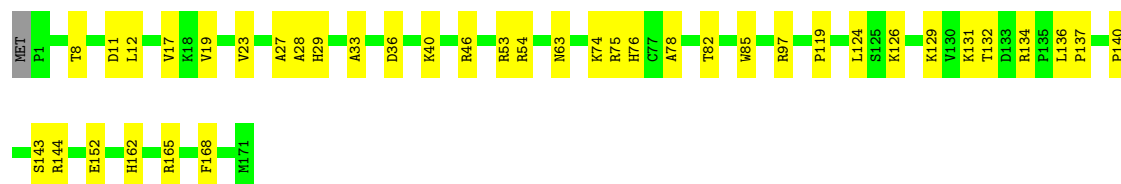
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6





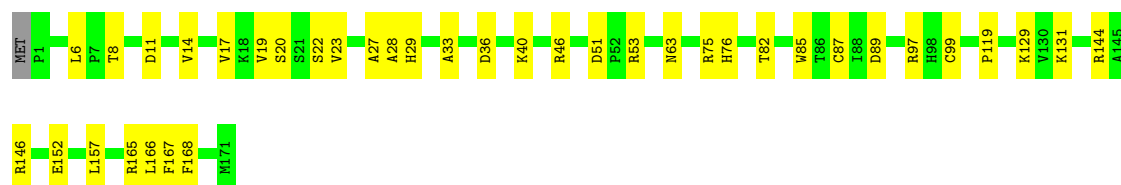
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain 1X: 77% 23%



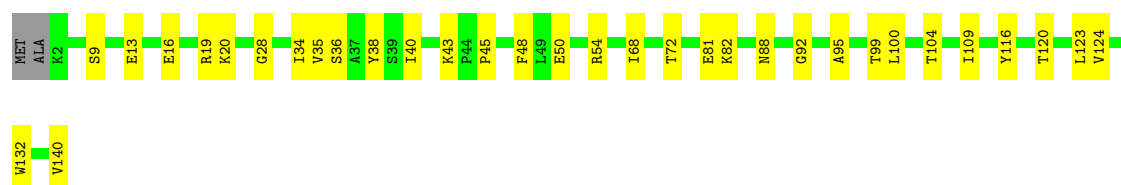
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain 5X: 77% 22%



- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain 1Y: 75% 23%



- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain 5Y: 79% 19%

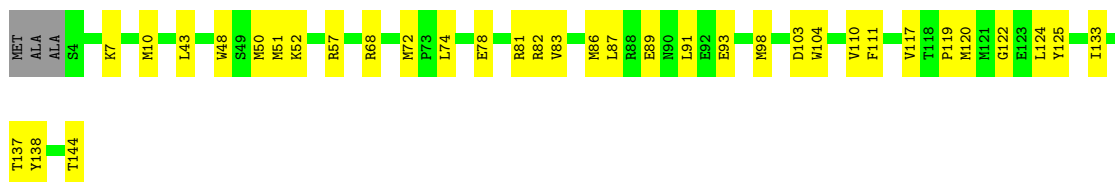


- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13

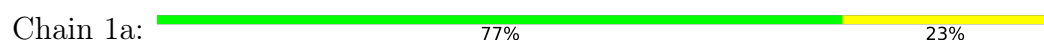
Chain 1Z: 77% 20%



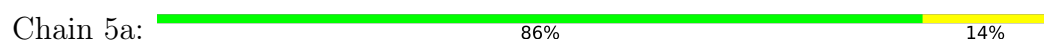
- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13



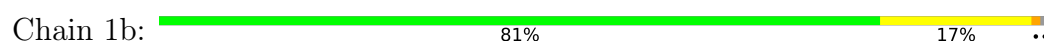
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



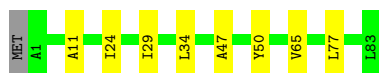
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



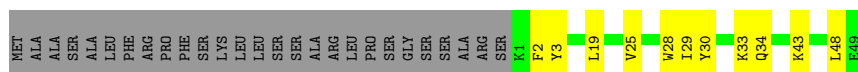
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

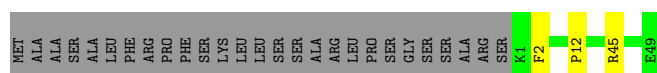


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain 5c:  61% 36%



- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain 1d:  80% 16% ..



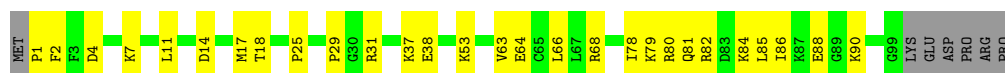
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain 5d:  79% 19%



- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain 1e:  67% 26% 7%



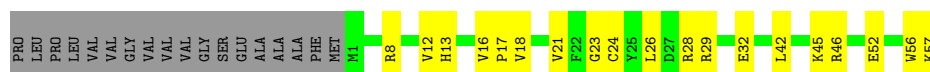
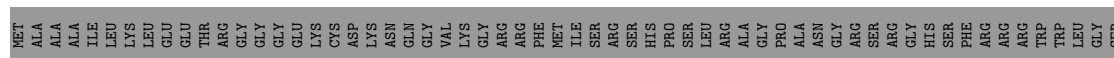
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain 5e:  72% 22% 7%



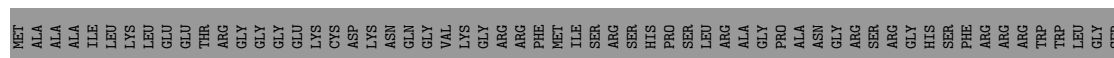
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]

Chain 1f:  28% 14% 58%



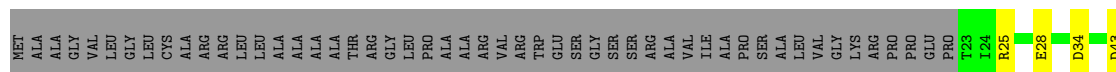
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]

Chain 5f:  32% 10% 58%

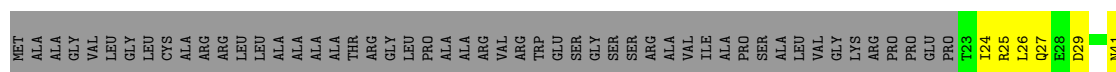




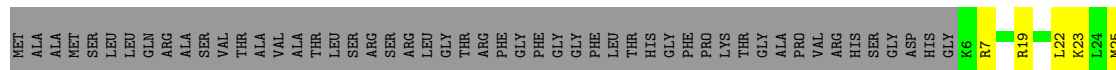
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



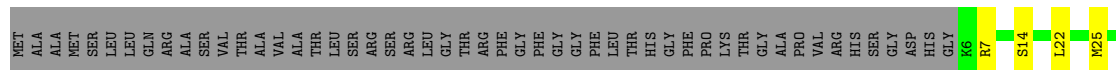
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

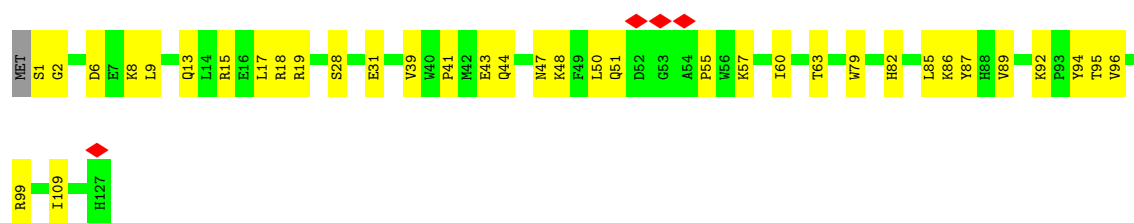


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain 1i: 



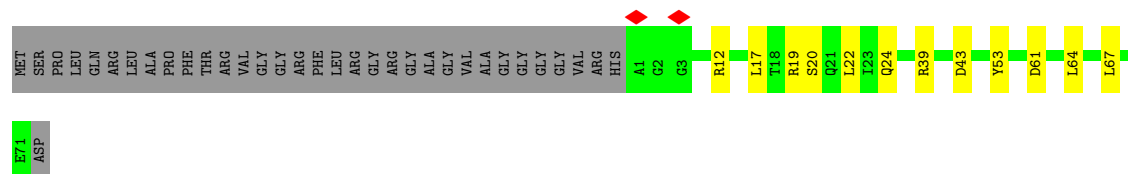
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain 5i: 



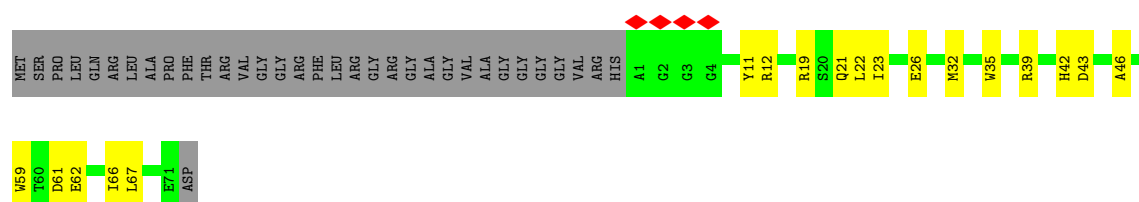
- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

Chain 1j: 



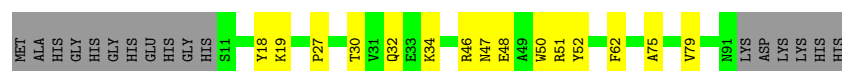
- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

Chain 5j: 



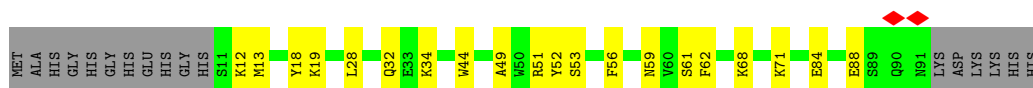
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain 1k: 



- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain 5k: 



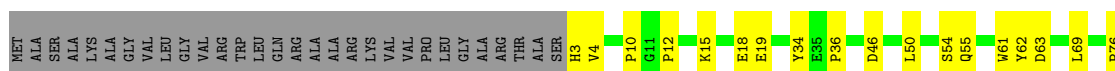
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain 11l: 65% 19% 16%



- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain 5l: 67% 17% 16%



- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain 1m: 78% 22%



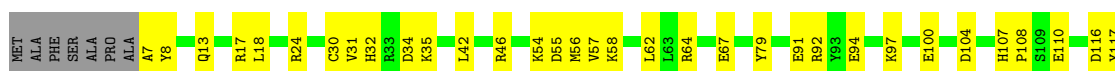
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain 5m: 75% 24%

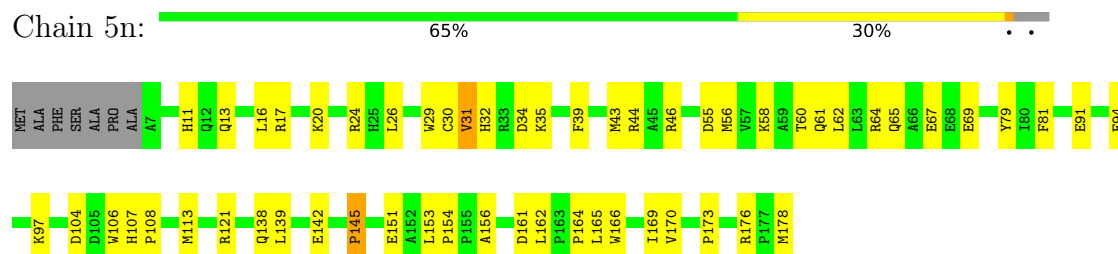


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

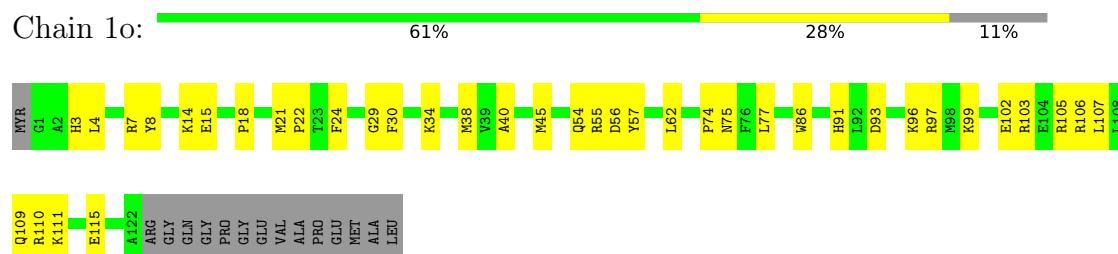
Chain 1n: 68% 28%



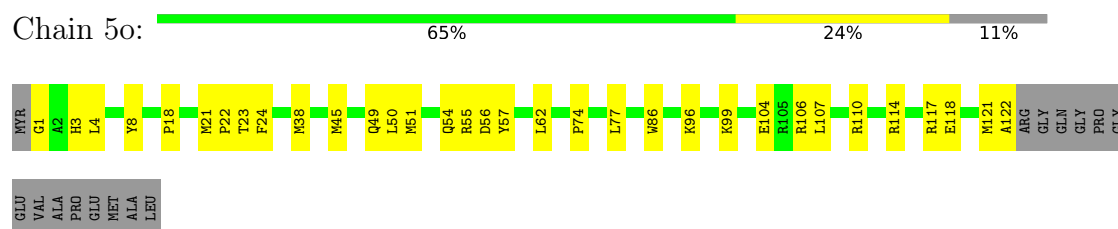
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



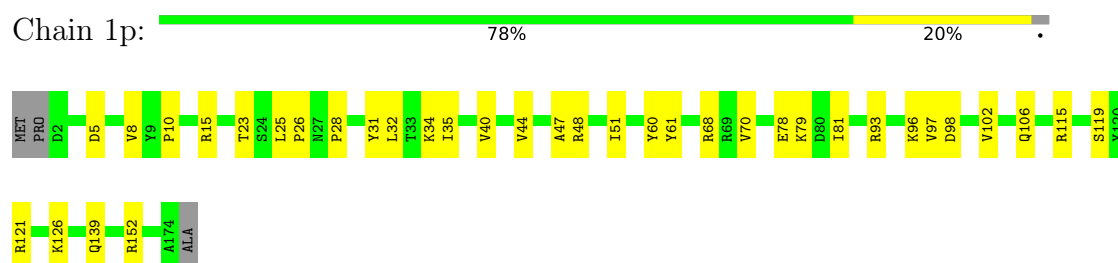
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



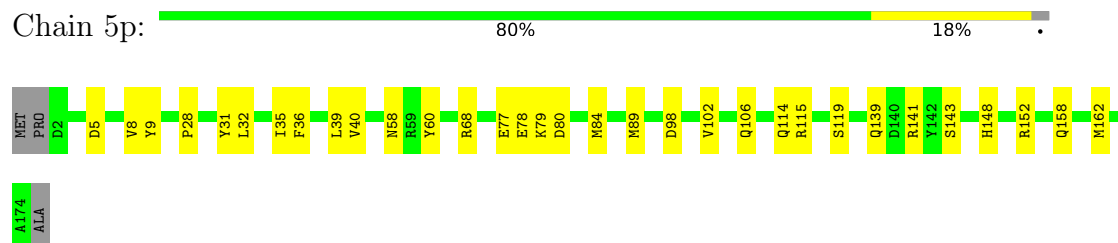
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



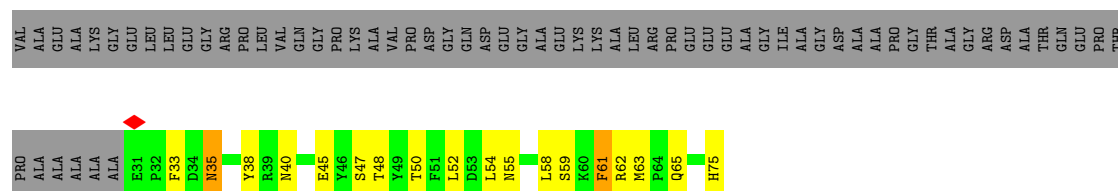
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

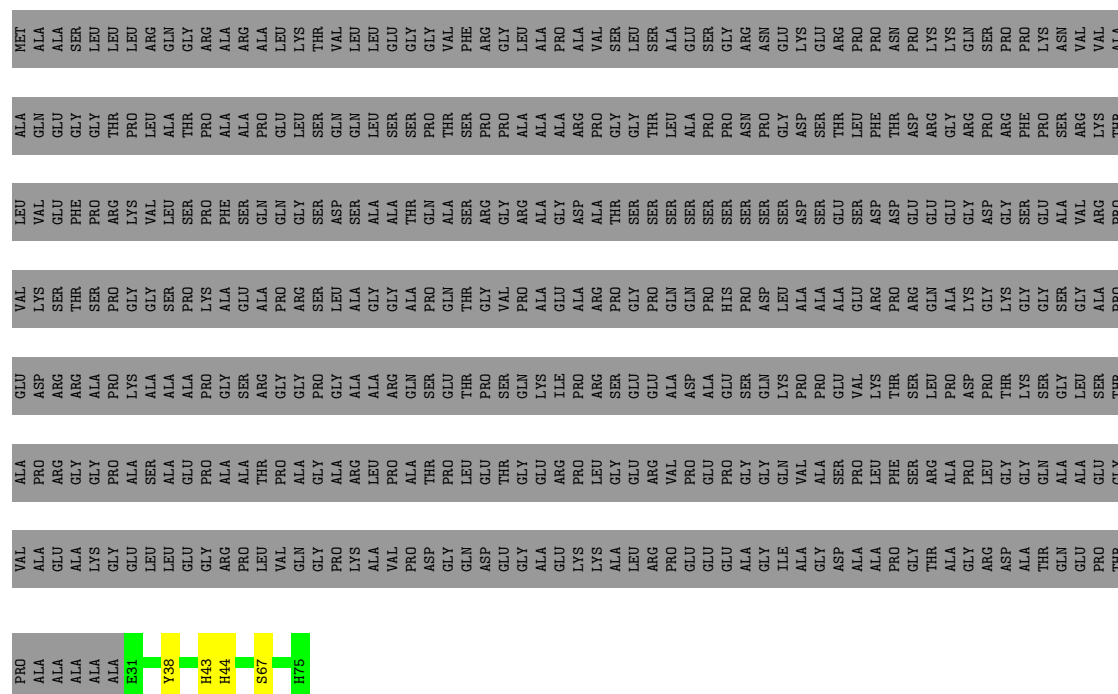


- [illegible]



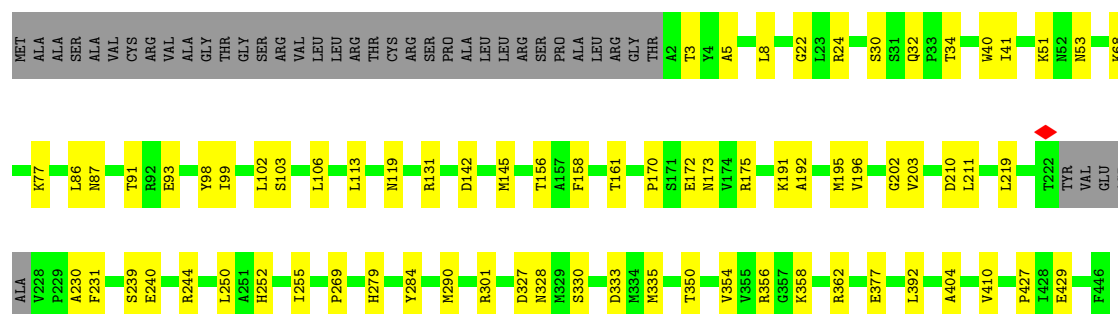
• Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain 5s: 9% 90%



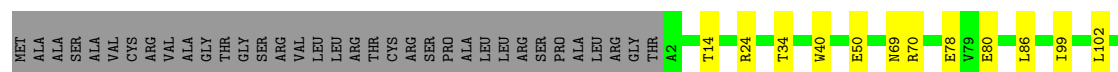
• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

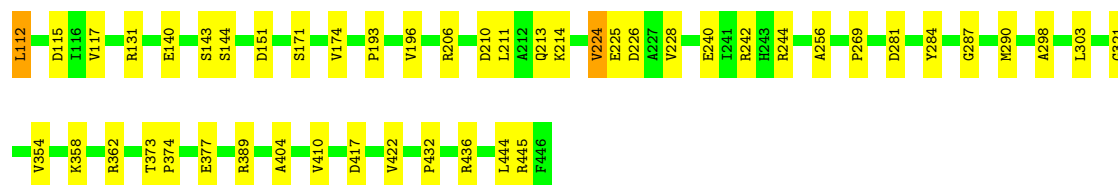
Chain 3A: 76% 15% 8%



• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

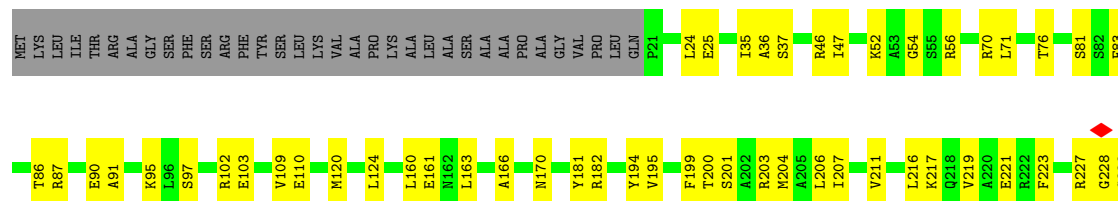
Chain 3N: 80% 12% 7%





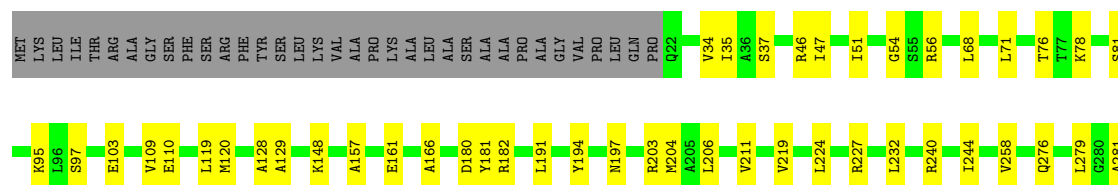
- Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain 3B: 74% 18% 8%



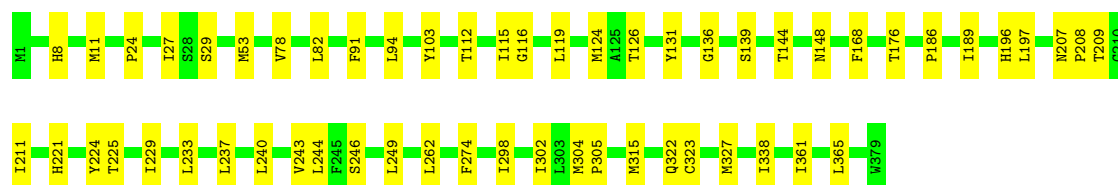
- Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain 3O: 77% 15% 8%



- Molecule 47: Cytochrome b

Chain 3C: 85% 15%



- Molecule 47: Cytochrome b

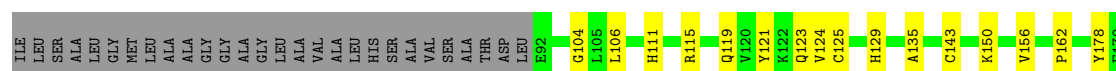
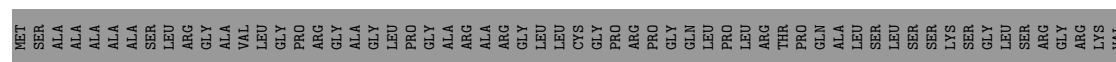
Chain 3P: 84% 16%





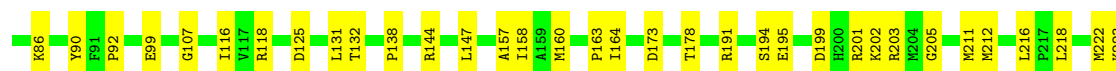
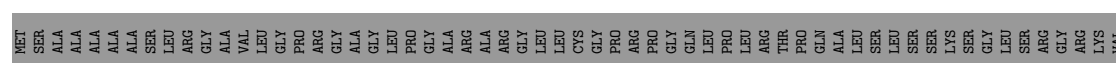
- Molecule 48: Cytochrome c1

Chain 3D: 59% 14% 27%



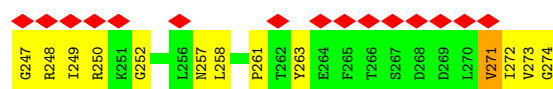
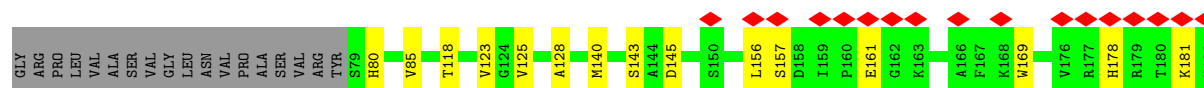
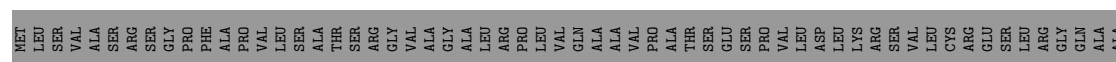
- Molecule 48: Cytochrome c1

Chain 3Q: 56% 17% 27%

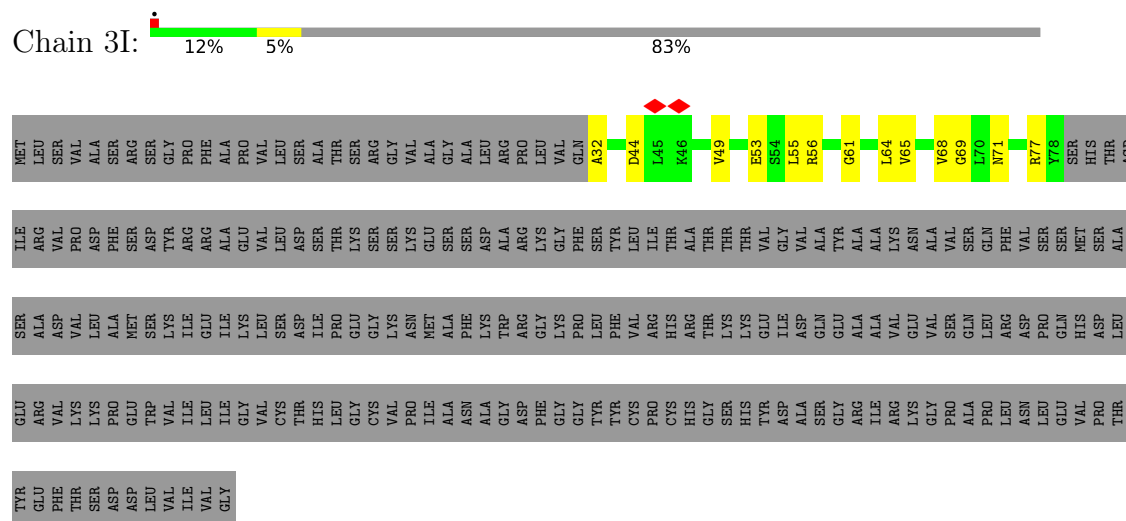


- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

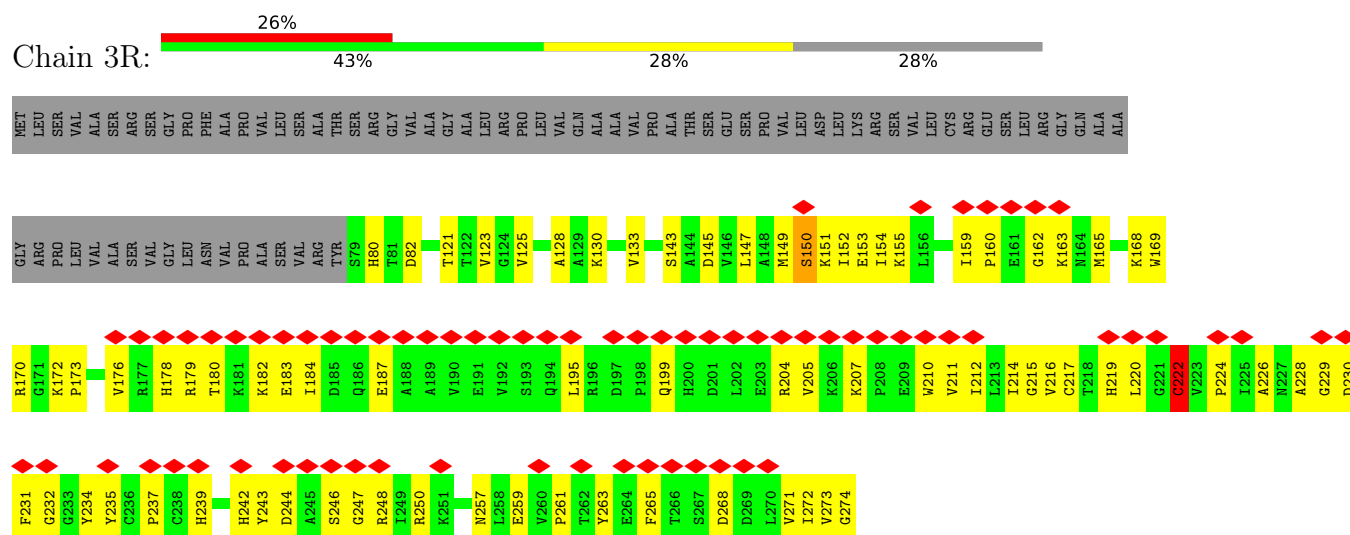
Chain 3E: 28% 54% 18% 28%



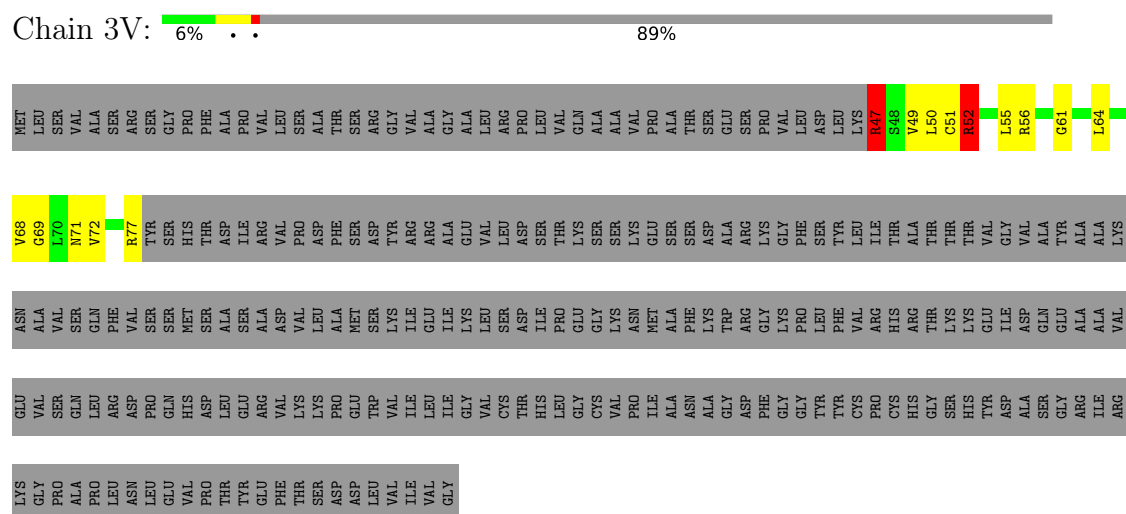
- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial



• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial



• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 50: Cytochrome b-c1 complex subunit 7

Chain 3F:  80% 8% 12%



- Molecule 50: Cytochrome b-c1 complex subunit 7

Chain 3S:  78% 10% 12%



- Molecule 51: Cytochrome b-c1 complex subunit 8

Chain 3G:  82% 9% 10%



- Molecule 51: Cytochrome b-c1 complex subunit 8

Chain 3T:  73% 17% 10%



- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain 3H:  56% 14% 29%



- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain 3U:  57% 14% 29%



- Molecule 53: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein 53 complex iii

Chain 3J:  78% 9% 12%



- Molecule 53: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein 53 complex iii

Chain 3W:  66% 19% 12%



- Molecule 54: Cytochrome b-c1 complex subunit 10

Chain 3X:  82% 11% 7%



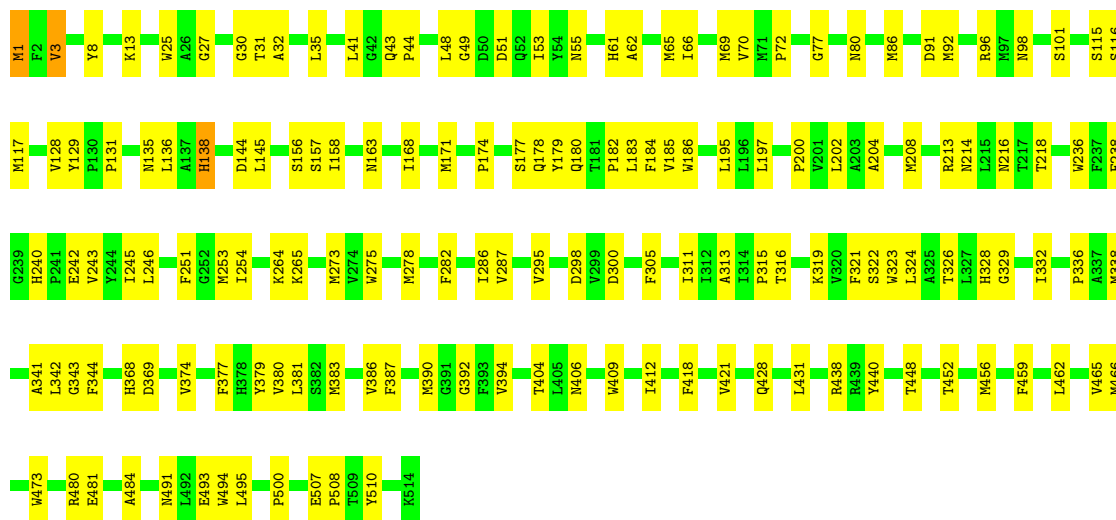
- Molecule 54: Cytochrome b-c1 complex subunit 10

Chain 3Y:  75% 16% 9%



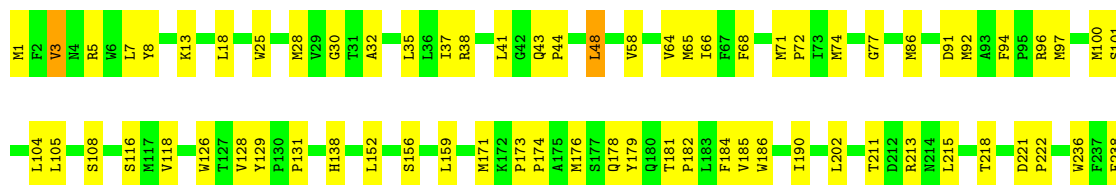
- Molecule 55: Cytochrome c oxidase subunit 1

Chain 4A:  70% 29% 1%



- Molecule 55: Cytochrome c oxidase subunit 1

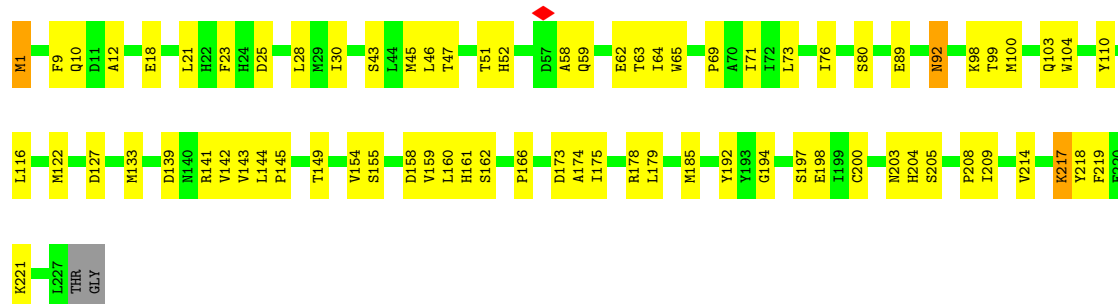
Chain 8A:  69% 30% 1%





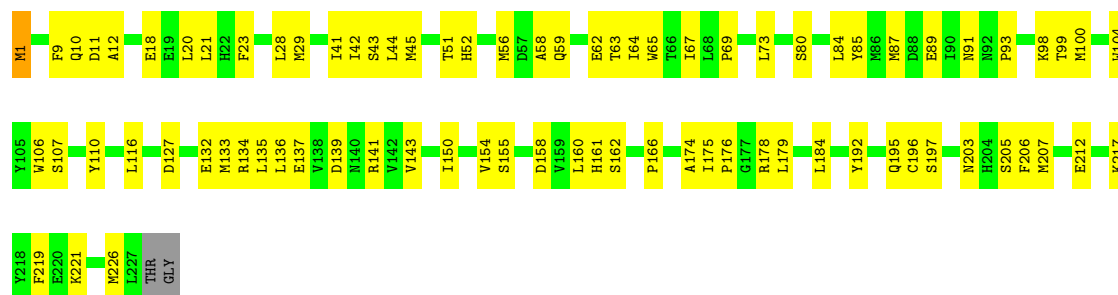
• Molecule 56: Cytochrome c oxidase subunit 2

Chain 4B: 66% 31% ..



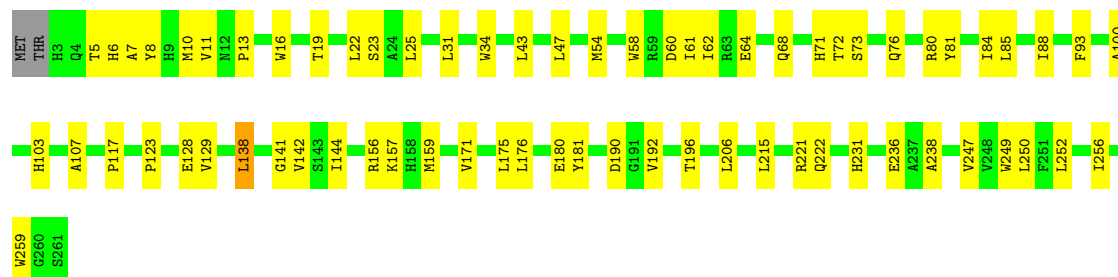
• Molecule 56: Cytochrome c oxidase subunit 2

Chain 8B: 64% 34% .



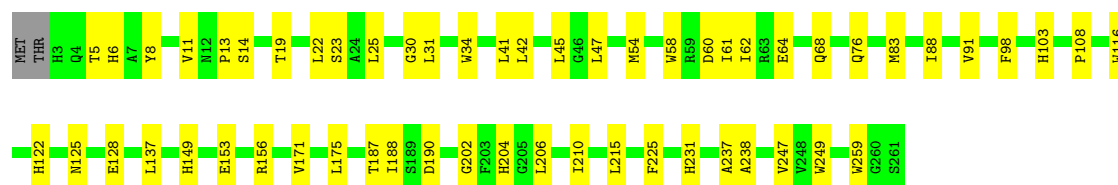
• Molecule 57: Cytochrome c oxidase subunit 3

Chain 4C: 73% 26% .



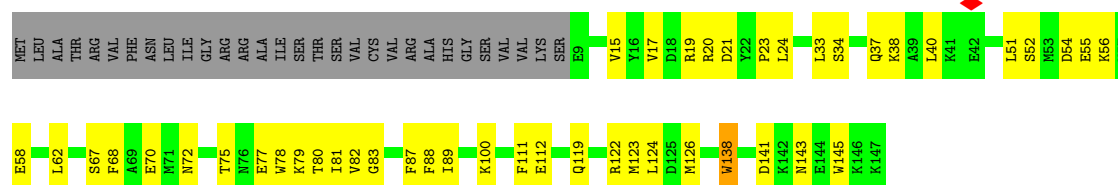
• Molecule 57: Cytochrome c oxidase subunit 3

Chain 8C:  78% 21%



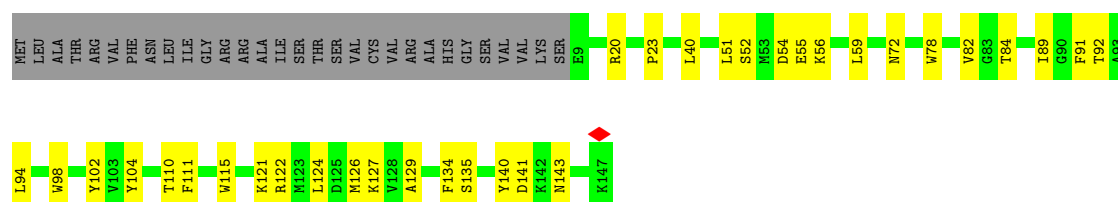
- Molecule 58: Cytochrome c oxidase subunit 4

Chain 4D:  55% 27% 18%



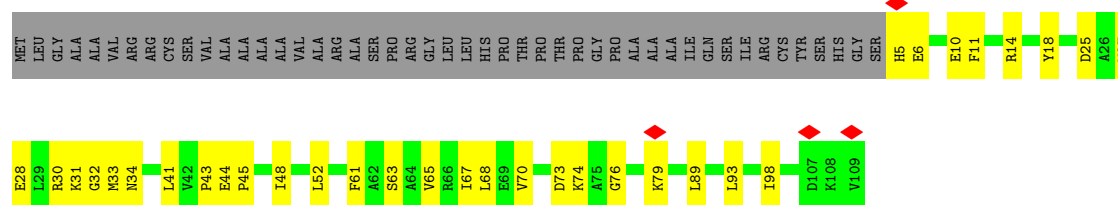
- Molecule 58: Cytochrome c oxidase subunit 4

Chain 8D:  62% 20% 18%



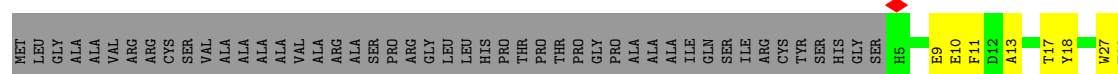
- Molecule 59: Cytochrome c oxidase subunit 5A, mitochondrial

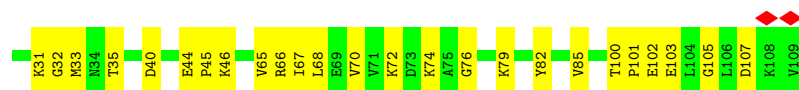
Chain 4E:  47% 22% 31%



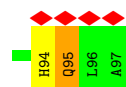
- Molecule 59: Cytochrome c oxidase subunit 5A, mitochondrial

Chain 8E:  47% 22% 31%





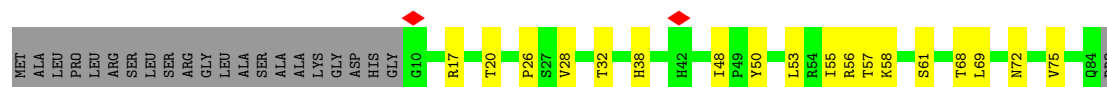
- Molecule 60: Cytochrome c oxidase subunit 5B, mitochondrial



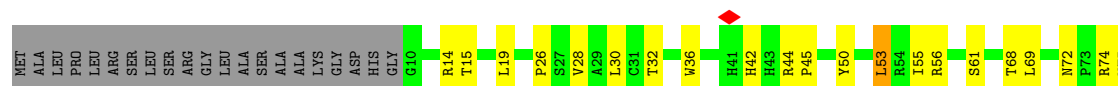
- Molecule 60: Cytochrome c oxidase subunit 5B, mitochondrial



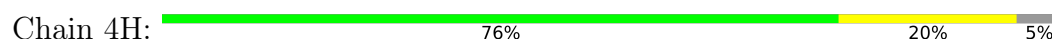
- Molecule 61: Cytochrome c oxidase subunit 6A2



- Molecule 61: Cytochrome c oxidase subunit 6A2



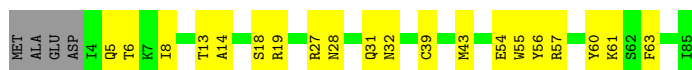
- Molecule 62: Cytochrome c oxidase subunit 6B1





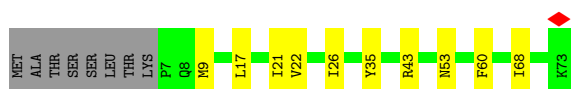
- Molecule 62: Cytochrome c oxidase subunit 6B1

Chain 8H: 72% 23% 5%



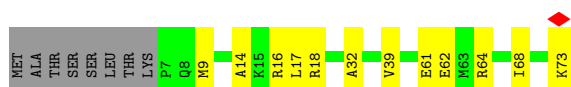
- Molecule 63: Cytochrome c oxidase subunit 6C

Chain 4I: 76% 13% 11%



- Molecule 63: Cytochrome c oxidase subunit 6C

Chain 8I: 73% 16% 11%



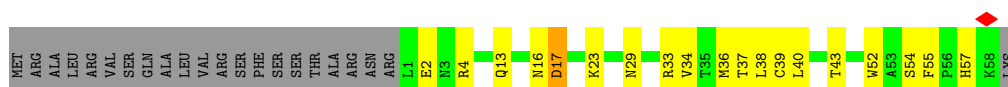
- Molecule 64: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain 4J: 52% 19% 28%



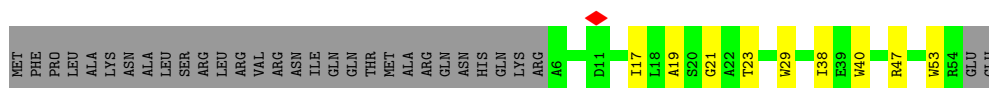
- Molecule 64: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain 8J: 49% 22% 28%

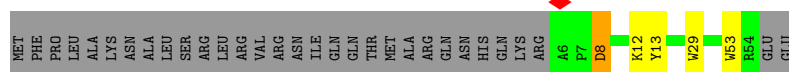


- Molecule 65: Cytochrome c oxidase subunit 7B

Chain 4K: 50% 11% 39%



- Molecule 65: Cytochrome c oxidase subunit 7B



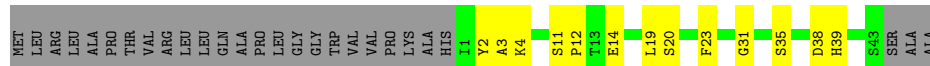
- Molecule 66: Cytochrome c oxidase subunit 7C, mitochondrial



- Molecule 66: Cytochrome c oxidase subunit 7C, mitochondrial



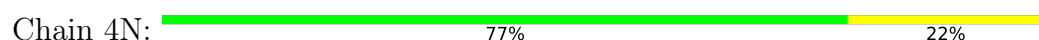
- Molecule 67: Cytochrome c oxidase subunit 8



- Molecule 67: Cytochrome c oxidase subunit 8



- Molecule 68: Cytochrome c oxidase subunit NDUF44



- Molecule 68: Cytochrome c oxidase subunit NDUF44



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.531	Depositor
Minimum map value	0.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	643.50006, 643.50006, 643.50006	wwPDB
Map dimensions	550, 550, 550	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1700001, 1.1700001, 1.1700001	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, ZN, K, NA, 3PE, PO4, HEC, CUA, FMN, CDL, PGV, PSC, HEA, GTP, EHZ, SAC, FES, HEM, CU, AME, PC1, MG, FME, MYR, SF4, AYA, PEK

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	1A	0.14	0/930	0.34	0/1271
1	5A	0.17	0/930	0.40	0/1271
2	1B	0.17	0/1273	0.40	0/1722
2	5B	0.15	0/1273	0.34	0/1722
3	1C	0.13	0/1791	0.29	0/2439
3	5C	0.13	0/1791	0.27	0/2439
4	1D	0.13	0/3545	0.28	0/4806
4	5D	0.14	0/3545	0.29	0/4806
5	1E	0.12	0/1698	0.30	0/2311
5	5E	0.13	0/1698	0.30	0/2311
6	1F	0.11	0/3401	0.28	0/4595
6	5F	0.15	0/3401	0.33	1/4595 (0.0%)
7	1G	0.13	0/5451	0.31	0/7387
7	5G	0.13	0/5451	0.31	1/7387 (0.0%)
8	1H	0.14	0/2566	0.36	0/3509
8	5H	0.14	0/2566	0.35	0/3509
9	1I	0.13	0/1443	0.28	0/1952
9	5I	0.14	0/1443	0.27	0/1952
10	1J	0.13	0/1364	0.39	0/1850
10	5J	0.14	0/1364	0.39	0/1850
11	1K	0.14	0/751	0.31	0/1018
11	5K	0.14	0/751	0.32	0/1018
12	1L	0.13	0/4939	0.31	0/6718
12	5L	0.13	0/4939	0.32	0/6718
13	1M	0.13	0/3713	0.28	0/5063
13	5M	0.13	0/3713	0.28	0/5063
14	1N	0.13	0/2765	0.30	0/3758
14	5N	0.14	0/2765	0.30	0/3758
15	1O	0.11	0/2650	0.26	0/3588
15	5O	0.11	0/2650	0.25	0/3588
16	1P	0.12	0/2828	0.28	0/3834

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	5P	0.12	0/2828	0.28	0/3834
17	1Q	0.15	0/1070	0.32	0/1446
17	5Q	0.15	0/1070	0.34	0/1446
18	1R	0.14	0/755	0.30	0/1018
18	5R	0.14	0/755	0.29	0/1018
19	1S	0.14	0/711	0.37	0/956
19	5S	0.13	0/711	0.35	0/956
20	1T	0.15	0/701	0.44	0/946
20	1U	0.20	0/706	0.47	1/954 (0.1%)
20	5T	0.16	0/701	0.37	0/946
20	5U	0.16	0/706	0.39	0/954
21	1V	0.12	0/946	0.29	0/1281
21	5V	0.11	0/946	0.25	0/1281
22	1W	0.13	0/995	0.30	0/1340
22	5W	0.17	0/995	0.45	1/1340 (0.1%)
23	1X	0.10	0/1436	0.26	0/1938
23	5X	0.11	0/1436	0.28	0/1938
24	1Y	0.14	0/1037	0.32	0/1404
24	5Y	0.13	0/1037	0.28	0/1404
25	1Z	0.16	0/1199	0.40	1/1617 (0.1%)
25	5Z	0.13	0/1199	0.27	0/1617
26	1a	0.13	0/577	0.26	0/777
26	5a	0.11	0/577	0.24	0/777
27	1b	0.13	0/664	0.36	0/912
27	5b	0.13	0/664	0.34	0/912
28	1c	0.14	0/430	0.36	0/581
28	5c	0.13	0/430	0.31	0/581
29	1d	0.12	0/1016	0.26	0/1374
29	5d	0.12	0/1016	0.27	0/1374
30	1e	0.12	0/836	0.31	0/1118
30	5e	0.12	0/836	0.28	0/1118
31	1f	0.11	0/499	0.31	0/673
31	5f	0.12	0/499	0.30	0/673
32	1g	0.14	0/858	0.38	0/1165
32	5g	0.13	0/858	0.35	0/1165
33	1h	0.11	0/1184	0.28	0/1603
33	5h	0.12	0/1184	0.28	0/1603
34	1i	0.17	0/1131	0.42	1/1541 (0.1%)
34	5i	0.12	0/1131	0.32	0/1541
35	1j	0.11	0/627	0.31	0/858
35	5j	0.14	0/627	0.38	0/858
36	1k	0.14	0/668	0.35	0/903
36	5k	0.13	0/668	0.34	0/903

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	1l	0.13	0/1365	0.34	0/1867
37	5l	0.13	0/1365	0.32	0/1867
38	1m	0.12	0/1092	0.35	0/1481
38	5m	0.14	0/1092	0.32	0/1481
39	1n	0.12	0/1549	0.31	0/2098
39	5n	0.21	1/1549 (0.1%)	0.45	3/2098 (0.1%)
40	1o	0.13	0/1069	0.32	0/1430
40	5o	0.12	0/1069	0.34	0/1430
41	1p	0.10	0/1481	0.29	0/1997
41	5p	0.11	0/1481	0.31	0/1997
42	1q	0.11	0/1253	0.29	1/1704 (0.1%)
42	5q	0.13	0/1253	0.30	1/1704 (0.1%)
43	1r	0.11	0/777	0.27	0/1051
43	5r	0.13	0/777	0.32	0/1051
44	1s	0.14	0/394	0.38	0/533
44	5s	0.15	0/394	0.37	0/533
45	3A	0.12	0/3481	0.27	0/4722
45	3N	0.13	0/3496	0.29	0/4723
46	3B	0.12	0/3190	0.26	0/4317
46	3O	0.18	0/3175	0.31	0/4292
47	3C	0.13	0/3123	0.29	0/4269
47	3P	0.13	0/3122	0.29	0/4269
48	3D	0.13	0/1946	0.28	0/2641
48	3Q	0.13	0/1962	0.27	0/2663
49	3E	0.15	0/1551	0.37	0/2098
49	3I	0.14	0/344	0.41	0/468
49	3R	0.18	0/1551	0.44	1/2098 (0.0%)
49	3V	0.63	0/225	0.83	0/303
50	3F	0.11	0/888	0.21	0/1193
50	3S	0.11	0/888	0.21	0/1193
51	3G	0.13	0/649	0.28	0/878
51	3T	0.13	0/649	0.28	0/878
52	3H	0.13	0/539	0.62	2/724 (0.3%)
52	3U	0.12	0/539	0.31	0/724
53	3J	0.11	0/464	0.30	0/625
53	3W	0.31	0/464	0.48	0/625
54	3X	0.10	0/445	0.23	0/608
54	3Y	0.15	0/437	0.37	0/598
55	4A	0.14	0/4156	0.31	0/5679
55	8A	0.14	0/4156	0.29	0/5679
56	4B	0.14	0/1865	0.35	0/2544
56	8B	0.14	0/1865	0.31	0/2544
57	4C	0.12	0/2179	0.27	0/2981

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
57	8C	0.13	0/2179	0.29	2/2981 (0.1%)
58	4D	0.11	0/1197	0.28	0/1617
58	8D	0.12	0/1197	0.33	0/1617
59	4E	0.14	0/871	0.37	0/1182
59	8E	0.15	0/871	0.37	0/1182
60	4F	0.13	0/749	0.32	0/1016
60	8F	0.14	0/749	0.35	0/1016
61	4G	0.11	0/644	0.28	0/881
61	8G	0.13	0/644	0.29	0/881
62	4H	0.13	0/708	0.31	0/956
62	8H	0.12	0/708	0.30	0/956
63	4I	0.10	0/563	0.24	0/748
63	8I	0.10	0/563	0.23	0/748
64	4J	0.13	0/466	0.35	0/631
64	8J	0.13	0/466	0.34	0/631
65	4K	0.17	0/396	0.32	0/543
65	8K	0.13	0/396	0.33	0/543
66	4L	0.12	0/394	0.28	0/528
66	8L	0.11	0/394	0.24	0/528
67	4M	0.13	0/349	0.31	0/477
67	8M	0.09	0/349	0.26	0/477
68	4N	0.13	0/680	0.33	0/921
68	8N	0.16	0/680	0.41	0/921
All	All	0.14	1/199830 (0.0%)	0.31	16/271091 (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
6	1F	0	1
6	5F	0	1
8	1H	0	1
8	5H	0	1
46	3O	0	1
49	3V	0	3
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	5n	145	PRO	CG-CD	-5.54	1.31	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5W	115	PRO	CA-N-CD	-10.69	97.04	112.00
25	1Z	18	PRO	CA-N-CD	-10.18	97.75	112.00
52	3H	77	GLU	CA-C-N	10.17	140.01	121.70
52	3H	77	GLU	C-N-CA	10.17	140.01	121.70
39	5n	145	PRO	N-CD-CG	-9.20	89.40	103.20
34	1i	55	PRO	CA-N-CD	-8.43	100.19	112.00
39	5n	145	PRO	CA-CB-CG	-8.30	88.73	104.50
20	1U	4	PRO	CA-N-CD	-7.65	101.29	112.00
6	5F	308	PRO	CA-N-CD	-7.18	101.95	112.00
57	8C	108	PRO	CA-C-N	5.84	129.56	120.68
57	8C	108	PRO	C-N-CA	5.84	129.56	120.68
49	3R	222	CYS	CA-CB-SG	5.58	127.22	114.40
42	1q	144	TYR	CB-CA-C	-5.17	110.19	117.23
42	5q	144	TYR	CB-CA-C	-5.16	110.21	117.23
39	5n	145	PRO	CA-N-CD	-5.05	104.92	112.00
7	5G	652	VAL	N-CA-C	-5.04	108.92	113.71

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	1F	206	LYS	Peptide
8	1H	91	MET	Peptide
46	3O	287	ARG	Sidechain
49	3V	47	ARG	Sidechain
49	3V	52	ARG	Sidechain
49	3V	56	ARG	Sidechain
6	5F	206	LYS	Peptide
8	5H	91	MET	Peptide

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	1A	916	0	950	47	0
1	5A	916	0	950	48	0
2	1B	1242	0	1249	48	0
2	5B	1242	0	1249	42	0
3	1C	1740	0	1691	33	0
3	5C	1740	0	1691	28	0
4	1D	3452	0	3389	104	0
4	5D	3452	0	3389	87	0
5	1E	1658	0	1662	48	0
5	5E	1658	0	1662	47	0
6	1F	3325	0	3288	100	0
6	5F	3325	0	3288	105	0
7	1G	5362	0	5388	145	0
7	5G	5362	0	5388	131	0
8	1H	2504	0	2602	97	0
8	5H	2504	0	2602	95	0
9	1I	1412	0	1366	53	0
9	5I	1412	0	1366	57	0
10	1J	1329	0	1326	63	0
10	5J	1329	0	1326	56	0
11	1K	750	0	798	34	0
11	5K	750	0	798	30	0
12	1L	4818	0	4956	152	0
12	5L	4818	0	4956	150	0
13	1M	3632	0	3836	99	0
13	5M	3632	0	3836	104	0
14	1N	2712	0	2873	94	0
14	5N	2712	0	2873	88	0
15	1O	2590	0	2556	56	0
15	5O	2590	0	2555	47	0
16	1P	2751	0	2776	72	0
16	5P	2751	0	2776	60	0
17	1Q	1047	0	1042	36	0
17	5Q	1047	0	1042	32	0
18	1R	741	0	704	11	0
18	5R	741	0	704	10	0
19	1S	700	0	719	22	0
19	5S	700	0	719	22	0
20	1T	689	0	687	35	0
20	1U	694	0	691	26	0
20	5T	689	0	687	22	0
20	5U	694	0	691	22	0
21	1V	927	0	972	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	5V	927	0	972	16	0
22	1W	971	0	975	23	0
22	5W	971	0	975	24	0
23	1X	1398	0	1378	34	0
23	5X	1398	0	1378	32	0
24	1Y	1016	0	1020	27	0
24	5Y	1016	0	1020	24	0
25	1Z	1168	0	1161	30	0
25	5Z	1168	0	1161	36	0
26	1a	562	0	557	13	0
26	5a	562	0	557	9	0
27	1b	643	0	645	10	0
27	5b	643	0	645	7	0
28	1c	417	0	425	11	0
28	5c	417	0	425	3	0
29	1d	985	0	978	22	0
29	5d	985	0	978	24	0
30	1e	816	0	823	24	0
30	5e	816	0	823	22	0
31	1f	487	0	498	15	0
31	5f	487	0	498	15	0
32	1g	835	0	795	24	0
32	5g	835	0	795	28	0
33	1h	1151	0	1164	34	0
33	5h	1151	0	1164	31	0
34	1i	1100	0	1107	35	0
34	5i	1100	0	1107	27	0
35	1j	601	0	546	11	0
35	5j	601	0	546	17	0
36	1k	649	0	626	15	0
36	5k	649	0	626	23	0
37	1l	1310	0	1204	30	0
37	5l	1310	0	1204	25	0
38	1m	1062	0	1075	22	0
38	5m	1062	0	1075	29	0
39	1n	1495	0	1434	42	0
39	5n	1495	0	1434	48	0
40	1o	1045	0	1016	39	0
40	5o	1045	0	1016	26	0
41	1p	1449	0	1416	34	0
41	5p	1449	0	1416	29	0
42	1q	1212	0	1174	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	5q	1212	0	1174	30	0
43	1r	759	0	783	15	0
43	5r	759	0	783	21	0
44	1s	382	0	351	21	0
44	5s	382	0	351	4	0
45	3A	3411	0	3308	46	0
45	3N	3424	0	3350	40	0
46	3B	3138	0	3116	51	0
46	3O	3124	0	3108	45	0
47	3C	3025	0	3090	46	0
47	3P	3024	0	3090	40	0
48	3D	1888	0	1834	34	0
48	3Q	1904	0	1849	46	0
49	3E	1518	0	1498	43	0
49	3I	340	0	359	13	0
49	3R	1518	0	1498	74	0
49	3V	224	0	241	11	0
50	3F	868	0	857	6	0
50	3S	868	0	857	8	0
51	3G	628	0	634	7	0
51	3T	628	0	634	12	0
52	3H	533	0	513	9	0
52	3U	533	0	513	9	0
53	3J	454	0	455	4	0
53	3W	454	0	455	10	0
54	3X	429	0	430	5	0
54	3Y	421	0	418	6	0
55	4A	4026	0	4005	127	0
55	8A	4026	0	4005	135	0
56	4B	1828	0	1835	63	0
56	8B	1828	0	1835	62	0
57	4C	2096	0	2027	57	0
57	8C	2096	0	2027	50	0
58	4D	1163	0	1143	40	0
58	8D	1163	0	1143	33	0
59	4E	852	0	845	26	0
59	8E	852	0	845	27	0
60	4F	734	0	718	15	0
60	8F	734	0	718	20	0
61	4G	617	0	585	14	0
61	8G	617	0	585	17	0
62	4H	687	0	645	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	8H	687	0	645	15	0
63	4I	550	0	560	11	0
63	8I	550	0	560	12	0
64	4J	456	0	459	16	0
64	8J	456	0	459	18	0
65	4K	383	0	366	8	0
65	8K	383	0	366	5	0
66	4L	381	0	380	9	0
66	8L	381	0	380	12	0
67	4M	338	0	345	12	0
67	8M	338	0	345	10	0
68	4N	660	0	664	13	0
68	8N	660	0	664	19	0
69	1A	103	0	128	6	0
69	1B	94	0	136	12	0
69	1H	48	0	73	2	0
69	1I	98	0	150	8	0
69	1L	46	0	66	3	0
69	1M	79	0	109	8	0
69	1d	39	0	52	6	0
69	1h	47	0	71	3	0
69	1q	49	0	75	3	0
69	3J	47	0	68	4	0
69	3R	45	0	64	6	0
69	3X	29	0	32	2	0
69	5A	70	0	88	4	0
69	5B	94	0	136	12	0
69	5H	48	0	73	2	0
69	5I	98	0	150	9	0
69	5L	46	0	66	3	0
69	5M	79	0	109	10	0
69	5P	33	0	40	0	0
69	5d	39	0	52	8	0
69	5h	47	0	71	3	0
69	5q	49	0	75	4	0
70	1B	8	0	0	1	0
70	1F	8	0	0	1	0
70	1G	16	0	0	1	0
70	1I	16	0	0	0	0
70	5B	8	0	0	1	0
70	5F	8	0	0	1	0
70	5G	16	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	5I	16	0	0	0	0
71	1E	4	0	0	0	0
71	1G	4	0	0	3	0
71	3E	4	0	0	0	0
71	3R	4	0	0	1	0
71	5E	4	0	0	0	0
71	5G	4	0	0	3	0
72	1F	31	0	19	3	0
72	5F	31	0	19	3	0
73	1G	1	0	0	0	0
73	5G	1	0	0	0	0
74	1H	51	0	46	3	0
74	1L	76	0	99	8	0
74	1N	62	0	68	3	0
74	1X	86	0	125	10	0
74	1d	65	0	77	9	0
74	1h	80	0	104	11	0
74	1q	61	0	66	1	0
74	3A	58	0	60	5	0
74	3C	52	0	48	3	0
74	3G	56	0	56	5	0
74	3N	43	0	30	1	0
74	3P	56	0	56	9	0
74	3T	57	0	58	11	0
74	4B	100	0	156	7	0
74	4C	100	0	156	15	0
74	4D	100	0	156	18	0
74	5H	51	0	46	2	0
74	5L	76	0	99	6	0
74	5N	62	0	68	3	0
74	5X	86	0	125	6	0
74	5d	65	0	77	3	0
74	5h	80	0	104	10	0
74	5q	61	0	66	2	0
74	8B	100	0	156	9	0
74	8C	100	0	156	14	0
74	8D	100	0	156	18	0
75	1I	8	0	8	1	0
75	5q	8	0	8	3	0
76	1K	44	0	62	2	0
76	1L	91	0	136	8	0
76	1M	192	0	289	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
76	1O	51	0	82	10	0
76	1P	35	0	44	3	0
76	1Y	202	0	254	16	0
76	1b	47	0	71	1	0
76	1d	49	0	75	4	0
76	1j	44	0	65	2	0
76	3A	59	0	66	5	0
76	3C	69	0	86	6	0
76	3D	33	0	40	2	0
76	3G	29	0	32	0	0
76	3N	58	0	62	5	0
76	3P	33	0	40	0	0
76	3Q	47	0	71	3	0
76	3Y	30	0	34	2	0
76	5A	47	0	71	3	0
76	5K	44	0	62	3	0
76	5L	140	0	211	8	0
76	5M	194	0	296	22	0
76	5P	35	0	44	1	0
76	5Y	202	0	254	18	0
76	5d	49	0	75	7	0
76	5j	44	0	65	5	0
77	1O	32	0	12	2	0
77	5O	32	0	12	1	0
78	1O	1	0	0	0	0
78	4A	1	0	0	0	0
78	5O	1	0	0	0	0
78	8A	1	0	0	0	0
79	1P	48	0	26	3	0
79	5P	48	0	26	5	0
80	1R	1	0	0	0	0
80	4F	1	0	0	0	0
80	5R	1	0	0	0	0
80	8F	1	0	0	0	0
81	1T	37	0	0	0	0
81	1n	37	0	0	2	0
81	5T	37	0	0	1	0
81	5n	37	0	0	1	0
82	1h	11	0	12	1	0
82	5h	11	0	12	1	0
83	1o	15	0	27	0	0
83	5o	15	0	27	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	3C	86	0	60	4	0
84	3P	86	0	60	3	0
85	3D	42	0	32	3	0
85	3Q	43	0	32	2	0
86	4A	153	0	228	21	0
86	4B	51	0	75	4	0
86	4C	306	0	456	27	0
86	4G	51	0	76	6	0
86	4J	51	0	76	3	0
86	4K	51	0	76	1	0
86	4L	51	0	76	3	0
86	4M	51	0	76	9	0
86	8A	102	0	152	10	0
86	8B	102	0	151	14	0
86	8C	306	0	456	22	0
86	8G	51	0	76	6	0
86	8J	51	0	76	3	0
86	8K	51	0	76	1	0
86	8L	51	0	76	3	0
86	8M	51	0	76	3	0
87	4A	120	0	108	9	0
87	8A	120	0	108	10	0
88	4A	1	0	0	0	0
88	8A	1	0	0	0	0
89	4A	1	0	0	0	0
89	8A	1	0	0	0	0
90	4A	52	0	80	7	0
90	8I	52	0	80	5	0
91	4B	2	0	0	3	0
91	8B	2	0	0	1	0
92	4C	52	0	72	4	0
92	4G	53	0	77	4	0
92	8C	52	0	72	6	0
92	8G	53	0	77	4	0
93	4H	5	0	0	0	0
93	8H	5	0	0	0	0
All	All	202910	0	204833	4594	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 11.

All (4594) 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)
2:1B:77:ARG:HD2	2:1B:78:ALA:H	1.28	0.97
56:4B:200:CYS:HG	91:4B:303:CUA:CU2	0.67	0.97
2:1B:77:ARG:HD2	2:1B:78:ALA:N	1.88	0.89
45:3N:444:LEU:HB2	74:3N:502:CDL:HB31	1.59	0.85
12:5L:600:THR:HG22	12:5L:601:LEU:H	1.41	0.84
86:8M:101:PGV:H61	86:8M:101:PGV:H221	1.58	0.83
34:5i:76:ILE:HG13	34:5i:77:PRO:HD3	1.60	0.83
5:5E:151:ALA:HB3	5:5E:163:ASP:HA	1.60	0.83
13:1M:216:LEU:HD23	13:1M:291:VAL:HG22	1.61	0.82
7:1G:41:CYS:SG	7:1G:52:CYS:HB2	2.20	0.81
7:1G:41:CYS:SG	7:1G:52:CYS:CB	2.67	0.81
55:4A:251:PHE:HB3	55:4A:319:LYS:HZ3	1.45	0.81
2:1B:77:ARG:CD	2:1B:78:ALA:H	1.93	0.81
56:8B:196:CYS:SG	91:8B:304:CUA:CU1	1.70	0.81
1:5A:57:LEU:HD21	10:5J:172:THR:HG21	1.62	0.80
35:1j:64:LEU:HD23	40:1o:106:ARG:HD2	1.63	0.80
12:5L:286:LEU:HG	12:5L:411:MET:HE3	1.63	0.80
49:3R:199:GLN:HE22	49:3R:257:ASN:HD22	1.29	0.79
20:1T:72:CYS:HB3	20:1T:75:GLU:HG3	1.62	0.79
8:1H:68:ILE:HD13	74:1H:401:CDL:H332	1.65	0.79
12:5L:217:LEU:HD11	12:5L:277:THR:HB	1.65	0.78
4:5D:165:THR:OG1	8:5H:275:ALA:O	2.01	0.78
58:4D:126:MET:HG3	63:4I:68:ILE:HD13	1.64	0.78
4:1D:281:VAL:HG11	4:1D:310:ILE:HG23	1.65	0.78
42:5q:60:ARG:HH22	42:5q:95:ASP:HA	1.48	0.77
49:3E:237:PRO:HB2	48:3Q:144:ARG:HD2	1.64	0.77
12:5L:2:ASN:HD21	12:5L:53:MET:HE1	1.49	0.77
47:3C:53:MET:HE1	49:3E:140:MET:HG2	1.65	0.77
4:5D:328:ALA:HB3	7:5G:126:ASP:HB2	1.66	0.77
32:1g:108:MET:HE1	41:1p:98:ASP:HB3	1.67	0.77
11:5K:44:SER:HB3	11:5K:59:MET:HE1	1.66	0.77
69:1B:203:PC1:H341	69:1q:201:PC1:H352	1.66	0.77
55:4A:91:ASP:OD1	55:4A:92:MET:N	2.17	0.77
57:4C:157:LYS:HD2	86:4C:302:PGV:H22	1.67	0.77
69:5B:203:PC1:H341	69:5q:201:PC1:H352	1.65	0.77
25:1Z:125:TYR:HB3	25:1Z:133:ILE:HG22	1.66	0.76
47:3C:8:HIS:HB3	47:3C:11:MET:HB2	1.66	0.76
14:5N:236:LYS:HG3	14:5N:237:MET:HG3	1.67	0.76
11:1K:93:LEU:HG	14:1N:54:GLU:HG2	1.66	0.76
76:5j:101:3PE:H32	40:5o:77:LEU:HD11	1.68	0.76
86:4B:301:PGV:H91	86:4B:301:PGV:H251	1.66	0.76
48:3D:267:THR:HG22	52:3H:38:LEU:HD21	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1J:121:GLY:HA2	11:1K:3:LEU:HB2	1.67	0.76
55:8A:96:ARG:NH2	57:8C:64:GLU:OE2	2.18	0.76
8:5H:32:GLN:OE1	8:5H:34:ARG:NH1	2.18	0.76
56:8B:58:ALA:HB2	90:8I:101:PSC:H031	1.68	0.76
56:4B:200:CYS:SG	91:4B:303:CUA:CU1	1.75	0.75
4:1D:328:ALA:HB3	7:1G:126:ASP:HB2	1.67	0.75
55:4A:321:PHE:HA	55:4A:324:LEU:HD12	1.69	0.75
16:1P:249:ALA:HB2	16:1P:318:LEU:HD12	1.66	0.75
8:5H:228:TYR:HA	8:5H:231:ILE:HD12	1.66	0.75
4:1D:149:ASN:HD21	4:1D:371:LYS:HG3	1.51	0.75
14:1N:29:ILE:HG13	14:1N:86:ILE:HD11	1.68	0.75
2:1B:82:GLN:NE2	8:1H:215:TYR:O	2.19	0.74
7:1G:105:CYS:HA	7:1G:108:CYS:HB2	1.68	0.74
13:1M:102:LEU:HD13	13:1M:128:PRO:HG2	1.69	0.74
56:8B:161:HIS:HB2	56:8B:174:ALA:HB3	1.69	0.74
57:8C:83:MET:HE3	57:8C:237:ALA:HB1	1.68	0.74
3:1C:79:THR:HG22	4:1D:390:LYS:HG2	1.68	0.74
23:1X:75:ARG:HG2	23:1X:76:HIS:HD2	1.52	0.74
8:1H:32:GLN:OE1	8:1H:34:ARG:NH1	2.19	0.74
7:1G:52:CYS:HB3	71:1G:803:FES:S1	2.28	0.74
12:5L:346:ILE:HG21	12:5L:359:MET:HE3	1.69	0.74
55:8A:38:ARG:HD3	55:8A:455:SER:HA	1.70	0.74
37:5I:158:ILE:HG12	40:5o:99:LYS:HB3	1.70	0.74
65:8K:12:LYS:HG3	65:8K:13:TYR:HD1	1.53	0.73
5:1E:105:THR:HG23	5:1E:107:PRO:HD2	1.69	0.73
6:5F:21:ILE:HG21	6:5F:230:VAL:HG12	1.68	0.73
7:5G:632:ARG:NH1	19:5S:57:CYS:SG	2.61	0.73
1:1A:70:ALA:HB2	10:1J:59:ILE:HG12	1.70	0.73
12:1L:23:ASN:HD22	74:1L:702:CDL:H321	1.53	0.73
16:5P:249:ALA:HB2	16:5P:318:LEU:HD12	1.71	0.73
2:1B:25:ARG:HG2	2:1B:27:GLU:H	1.53	0.73
5:1E:56:ARG:HD3	44:1s:48:THR:HG22	1.71	0.73
4:1D:34:ASN:HB2	15:1O:158:VAL:HG13	1.70	0.72
23:5X:46:ARG:NH2	33:5h:142:ASP:OD1	2.21	0.72
87:8A:603:HEA:HHC	87:8A:603:HEA:H131	1.71	0.72
1:1A:27:LEU:HD11	8:1H:60:PRO:HD2	1.69	0.72
8:1H:302:MET:HE1	76:1b:201:3PE:H2D1	1.69	0.72
45:3A:250:LEU:HD12	49:3I:44:ASP:HB2	1.71	0.72
47:3C:237:LEU:HD13	48:3D:301:MET:HG3	1.70	0.72
12:5L:23:ASN:HD22	74:5L:702:CDL:H321	1.53	0.72
25:5Z:83:VAL:HG23	25:5Z:124:LEU:HD11	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:50:PRO:HB2	10:1J:74:MET:HA	1.68	0.72
58:4D:75:THR:HG23	58:4D:77:GLU:H	1.53	0.72
5:5E:144:CYS:O	6:5F:139:ARG:NH2	2.22	0.72
34:1i:28:SER:HB3	34:1i:31:GLU:HG3	1.71	0.72
6:5F:224:ASN:ND2	72:5F:501:FMN:O2	2.23	0.72
10:5J:3:MET:HE1	25:5Z:133:ILE:HD11	1.71	0.72
6:1F:343:ILE:HD11	6:1F:425:GLU:HG2	1.71	0.72
13:1M:243:MET:HB3	13:1M:301:ILE:HG21	1.71	0.72
7:5G:283:MET:HE1	42:5q:139:PRO:HG3	1.71	0.72
55:4A:135:ASN:HD21	61:4G:57:THR:HG23	1.54	0.72
55:8A:91:ASP:OD1	55:8A:92:MET:N	2.18	0.72
46:3B:227:ARG:HG3	46:3B:229:GLY:H	1.53	0.71
6:5F:215:VAL:HG23	6:5F:220:THR:HG21	1.72	0.71
7:5G:451:VAL:HG22	7:5G:489:VAL:HG12	1.71	0.71
12:5L:69:MET:HE3	12:5L:71:LEU:HD21	1.72	0.71
34:5i:18:ARG:HA	39:5n:170:VAL:HG23	1.72	0.71
4:1D:175:GLU:OE2	4:1D:188:ARG:NH1	2.23	0.71
8:5H:196:ALA:HB3	8:5H:197:PRO:HD3	1.71	0.71
55:8A:381:LEU:HD13	87:8A:603:HEA:HAC	1.72	0.71
86:8B:302:PGV:H91	86:8B:302:PGV:H251	1.72	0.71
1:1A:57:LEU:HD21	10:1J:172:THR:HG21	1.73	0.71
49:3R:214:ILE:HG12	49:3R:261:PRO:HG3	1.73	0.71
34:5i:13:GLN:HE22	39:5n:156:ALA:H	1.37	0.71
8:1H:196:ALA:HB3	8:1H:197:PRO:HD3	1.71	0.71
55:8A:222:PRO:HG2	56:8B:176:PRO:HB2	1.73	0.71
13:1M:91:ARG:NH2	15:1O:290:ASP:OD2	2.22	0.71
14:1N:211:MET:HG3	14:1N:333:SER:HB2	1.72	0.71
49:3E:242:HIS:O	49:3E:250:ARG:N	2.21	0.71
7:1G:41:CYS:SG	7:1G:52:CYS:HB3	2.31	0.71
16:5P:322:ARG:HH21	16:5P:329:SER:HB3	1.56	0.71
38:5m:24:ILE:H	38:5m:24:ILE:HD12	1.56	0.71
13:5M:216:LEU:HD23	13:5M:291:VAL:HG22	1.71	0.70
2:5B:25:ARG:HG2	2:5B:27:GLU:H	1.54	0.70
5:5E:23:PHE:HA	5:5E:57:GLN:HE22	1.55	0.70
34:1i:18:ARG:HA	39:1n:170:VAL:HG23	1.72	0.70
47:3P:207:ASN:ND2	47:3P:211:ILE:O	2.23	0.70
57:8C:259:TRP:O	68:8N:47:ARG:NH2	2.24	0.70
4:1D:165:THR:OG1	8:1H:275:ALA:O	2.07	0.70
74:3P:504:CDL:HA61	74:3P:504:CDL:H532	1.71	0.70
5:5E:159:ASN:HB3	5:5E:184:PRO:HB3	1.71	0.70
12:5L:9:LEU:HD12	34:5i:85:LEU:HD11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:215:VAL:HG23	6:1F:220:THR:HG21	1.73	0.70
37:1l:5:THR:OG1	37:1l:7:ASP:OD1	2.10	0.70
24:5Y:43:LYS:O	24:5Y:54:ARG:NH2	2.24	0.70
86:4A:603:PGV:H22	74:4D:201:CDL:H312	1.74	0.70
13:1M:282:LEU:HG	13:1M:342:MET:HG3	1.74	0.70
1:5A:70:ALA:HB2	10:5J:59:ILE:HG12	1.74	0.70
33:5h:47:ILE:HA	41:5p:58:ASN:HD21	1.54	0.69
55:4A:273:MET:HE1	55:4A:319:LYS:HA	1.72	0.69
2:1B:95:LYS:HD2	3:1C:154:GLY:HA2	1.73	0.69
12:1L:393:ASP:OD1	12:1L:394:LEU:N	2.25	0.69
52:3H:77:GLU:HA	52:3H:79:ASP:HB2	1.74	0.69
56:4B:200:CYS:SG	91:4B:303:CUA:CU2	1.79	0.69
44:1s:35:ASN:O	44:1s:35:ASN:ND2	2.21	0.69
22:1W:27:GLU:HA	22:1W:30:ARG:HB3	1.74	0.69
47:3P:8:HIS:HB3	47:3P:11:MET:HB2	1.74	0.69
55:8A:264:LYS:NZ	55:8A:326:THR:O	2.25	0.69
49:3R:151:LYS:HE3	49:3R:152:ILE:HB	1.73	0.69
7:5G:372:GLU:O	7:5G:402:ASN:ND2	2.26	0.69
55:8A:343:GLY:HA2	86:8B:301:PGV:H062	1.75	0.69
55:4A:27:GLY:HA2	55:4A:69:MET:HE2	1.73	0.69
58:4D:23:PRO:HB3	59:4E:70:VAL:HG11	1.74	0.69
4:5D:50:ASN:HB2	4:5D:65:VAL:HG22	1.75	0.69
12:5L:188:TRP:HZ3	12:5L:206:ASN:HD22	1.41	0.69
13:5M:220:HIS:CE1	13:5M:231:LEU:HB3	2.28	0.69
55:4A:144:ASP:OD2	55:4A:213:ARG:NH1	2.26	0.69
5:1E:151:ALA:HB3	5:1E:163:ASP:HA	1.75	0.69
19:1S:64:LEU:HB2	19:1S:78:LEU:HD11	1.74	0.69
49:3R:155:LYS:HE2	49:3R:176:VAL:HG21	1.72	0.69
51:3T:40:ARG:NH1	74:3T:101:CDL:OA3	2.26	0.69
48:3D:284:GLU:OE2	48:3D:290:ARG:NH1	2.26	0.68
62:4H:78:GLU:OE1	62:4H:80:THR:OG1	2.10	0.68
7:5G:157:THR:HB	7:5G:161:ARG:HE	1.58	0.68
12:5L:29:THR:HG23	12:5L:31:LEU:H	1.57	0.68
39:1n:64:ARG:NH2	39:1n:67:GLU:OE1	2.26	0.68
12:1L:297:ASP:HB3	12:1L:300:LYS:HB2	1.74	0.68
42:1q:106:ARG:HB2	42:1q:109:ILE:HG13	1.76	0.68
29:5d:111:GLU:N	29:5d:111:GLU:OE1	2.26	0.68
59:8E:10:GLU:OE1	59:8E:10:GLU:N	2.26	0.68
2:1B:42:ARG:HH22	69:1B:203:PC1:H12	1.59	0.68
4:5D:52:GLY:H	4:5D:53:PRO:HD3	1.59	0.68
15:5O:104:ARG:NH2	77:5O:401:GTP:N7	2.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:204:GLU:HG2	8:1H:279:ARG:HH22	1.59	0.68
14:1N:256:PRO:HD2	76:1O:401:3PE:H3I1	1.76	0.68
45:3N:131:ARG:NH1	45:3N:174:VAL:O	2.26	0.68
4:5D:249:ASP:OD2	4:5D:404:LYS:NZ	2.27	0.68
55:8A:66:ILE:HG23	55:8A:246:LEU:HD21	1.76	0.68
55:8A:306:THR:OG1	55:8A:361:SER:OG	2.12	0.68
55:4A:129:TYR:OH	55:4A:236:TRP:NE1	2.27	0.68
76:5M:504:3PE:H3I1	14:5N:256:PRO:HD2	1.73	0.68
74:8B:303:CDL:H661	74:8B:303:CDL:H412	1.74	0.68
12:1L:474:PRO:O	40:1o:54:GLN:NE2	2.24	0.68
49:3R:204:ARG:NH1	49:3R:246:SER:O	2.27	0.68
22:5W:31:ARG:NH2	22:5W:80:ASP:OD2	2.26	0.68
43:1r:45:SER:O	43:1r:51:ASN:ND2	2.25	0.68
2:5B:42:ARG:HH22	69:5B:203:PC1:H12	1.57	0.68
7:5G:324:ASP:HB3	7:5G:571:ALA:HB1	1.76	0.68
10:1J:127:ILE:HG21	11:1K:2:PRO:HG3	1.74	0.67
45:3A:290:MET:SD	49:3I:71:ASN:ND2	2.67	0.67
49:3R:162:GLY:H	49:3R:178:HIS:HB3	1.58	0.67
7:5G:105:CYS:HA	7:5G:108:CYS:HB2	1.74	0.67
31:5f:30:SER:O	31:5f:33:LYS:NZ	2.27	0.67
55:8A:86:MET:HE1	55:8A:184:PHE:HB3	1.74	0.67
8:1H:114:TYR:OH	10:1J:65:LEU:O	2.10	0.67
76:1M:903:3PE:H371	29:1d:43:LEU:HB3	1.76	0.67
6:5F:91:LYS:HB2	6:5F:131:ALA:HA	1.75	0.67
14:5N:170:LEU:O	14:5N:295:ARG:NH2	2.27	0.67
33:5h:63:HIS:NE2	33:5h:76:ALA:O	2.27	0.67
10:1J:111:GLU:OE1	30:1e:80:ARG:NH2	2.27	0.67
19:1S:26:SER:O	19:1S:33:ARG:NH2	2.27	0.67
3:5C:195:ARG:NH2	9:5I:92:ILE:O	2.28	0.67
5:5E:100:ILE:HG12	5:5E:156:ILE:HD12	1.76	0.67
10:5J:130:THR:HG21	25:5Z:124:LEU:HD12	1.75	0.67
35:5j:39:ARG:NH2	35:5j:43:ASP:OD2	2.27	0.67
20:1T:52:MET:HA	20:1T:55:GLU:HG2	1.76	0.67
7:1G:194:GLU:HG2	7:1G:195:LEU:HG	1.76	0.67
22:1W:31:ARG:HH21	22:1W:80:ASP:HB3	1.60	0.67
44:1s:45:GLU:N	44:1s:45:GLU:OE2	2.27	0.67
76:5d:201:3PE:H221	69:5d:202:PC1:H221	1.75	0.67
56:8B:9:PHE:HB2	56:8B:21:LEU:HD21	1.76	0.67
68:8N:32:TYR:O	68:8N:34:THR:N	2.26	0.67
20:1U:8:LEU:HD11	34:1i:19:ARG:HH21	1.59	0.67
16:5P:315:ILE:HG21	16:5P:331:MET:HE3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5G:226:GLU:HG2	7:5G:253:ARG:HD3	1.77	0.67
58:8D:89:ILE:HG22	65:8K:29:TRP:HE1	1.60	0.67
4:1D:52:GLY:H	4:1D:53:PRO:HD3	1.60	0.67
15:1O:73:LEU:HD21	15:1O:295:LYS:HB3	1.76	0.67
59:8E:100:THR:OG1	59:8E:103:GLU:OE1	2.13	0.67
16:1P:118:ALA:HA	16:1P:129:LEU:HD21	1.77	0.67
2:1B:58:GLU:OE2	4:1D:188:ARG:NH2	2.27	0.67
2:1B:63:ALA:HB1	2:1B:76:PHE:HE1	1.59	0.67
3:1C:93:VAL:HG22	3:1C:108:LYS:HE2	1.77	0.67
14:1N:40:MET:HE3	14:1N:44:LEU:HD21	1.76	0.67
46:3B:201:SER:HB2	46:3B:228:GLY:HA2	1.77	0.67
48:3Q:203:ARG:NH2	53:3W:44:GLU:OE2	2.27	0.67
35:5j:39:ARG:NH1	76:5j:101:3PE:O12	2.27	0.67
55:8A:420:GLY:O	55:8A:424:THR:OG1	2.13	0.67
7:1G:364:LEU:HD12	7:1G:491:ASN:HB3	1.76	0.66
12:1L:102:GLU:OE1	12:1L:456:ARG:NH2	2.27	0.66
43:1r:104:GLU:N	43:1r:104:GLU:OE2	2.28	0.66
56:4B:92:ASN:O	56:4B:92:ASN:ND2	2.23	0.66
62:4H:46:LYS:HG2	62:4H:47:GLY:H	1.59	0.66
7:5G:243:ARG:HG2	7:5G:244:THR:HG23	1.76	0.66
1:1A:38:GLU:HB2	1:1A:43:PRO:HG3	1.75	0.66
8:5H:24:GLU:OE2	8:5H:274:ARG:NH1	2.28	0.66
39:5n:94:GLU:HA	39:5n:97:LYS:HG3	1.76	0.66
1:1A:36:PRO:HB2	1:1A:43:PRO:HG2	1.75	0.66
13:5M:365:THR:HG21	13:5M:444:LEU:HD21	1.77	0.66
86:8C:307:PGV:H152	86:8C:307:PGV:H291	1.77	0.66
6:1F:224:ASN:ND2	72:1F:501:FMN:O2	2.28	0.66
39:5n:64:ARG:NH1	39:5n:67:GLU:OE1	2.28	0.66
7:1G:190:MET:HG3	7:1G:192:MET:HG2	1.76	0.66
13:1M:365:THR:HG21	13:1M:444:LEU:HD21	1.77	0.66
24:1Y:68:ILE:HG13	24:1Y:99:THR:HG21	1.76	0.66
40:1o:74:PRO:HG3	41:1p:28:PRO:HD3	1.78	0.66
49:3E:241:SER:H	49:3E:252:GLY:HA3	1.59	0.66
4:5D:152:MET:O	4:5D:156:THR:OG1	2.13	0.66
8:1H:90:PRO:HD2	8:1H:240:ILE:HD13	1.77	0.66
12:5L:562:LEU:HD22	76:5L:704:3PE:H3B2	1.78	0.66
13:5M:108:MET:HB3	13:5M:121:LEU:HD13	1.75	0.66
24:5Y:82:LYS:O	24:5Y:88:ASN:ND2	2.28	0.66
4:1D:50:ASN:HB2	4:1D:65:VAL:HG22	1.76	0.66
7:1G:118:ASP:OD2	17:1Q:46:GLN:NE2	2.28	0.66
12:1L:5:ALA:HB2	12:1L:61:MET:HE1	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:4F:50:PRO:O	60:4F:56:ARG:NH1	2.29	0.66
7:5G:273:GLY:O	7:5G:549:HIS:NE2	2.27	0.66
12:5L:600:THR:CG2	12:5L:601:LEU:H	2.09	0.66
7:1G:228:ILE:HG13	7:1G:581:GLN:HB3	1.76	0.66
33:1h:63:HIS:NE2	33:1h:76:ALA:O	2.29	0.66
1:5A:38:GLU:HB2	1:5A:43:PRO:HG3	1.78	0.66
4:5D:281:VAL:HG11	4:5D:310:ILE:HG23	1.77	0.66
69:5M:505:PC1:H322	74:5h:202:CDL:H111	1.78	0.66
17:5Q:36:ARG:NH1	17:5Q:106:GLU:OE1	2.28	0.66
6:1F:214:GLY:HA3	6:1F:220:THR:HG22	1.77	0.66
7:1G:465:ALA:HB2	7:1G:654:GLN:HG3	1.78	0.66
14:1N:213:LEU:O	14:1N:217:MET:HG3	1.96	0.66
20:5T:17:TYR:CE1	20:5T:21:LEU:HD21	2.31	0.66
21:5V:8:THR:HG21	21:5V:13:LEU:HD23	1.78	0.66
4:1D:269:LEU:HB2	4:1D:368:GLU:HB2	1.78	0.66
13:1M:220:HIS:CE1	13:1M:231:LEU:HB3	2.31	0.66
55:4A:381:LEU:HD13	87:4A:604:HEA:HAC	1.78	0.66
14:5N:272:LYS:HD3	33:5h:108:LEU:HD21	1.76	0.66
15:5O:73:LEU:HD21	15:5O:295:LYS:HB3	1.78	0.66
20:1U:4:PRO:HD2	20:1U:4:PRO:O	1.95	0.65
86:4A:601:PGV:H332	86:4A:601:PGV:H162	1.76	0.65
56:4B:9:PHE:HB2	56:4B:21:LEU:HD21	1.78	0.65
42:1q:60:ARG:HH22	42:1q:95:ASP:HA	1.62	0.65
45:3A:255:ILE:HG21	45:3A:335:MET:HE1	1.78	0.65
86:4M:101:PGV:H61	86:4M:101:PGV:H221	1.78	0.65
20:5U:25:ILE:HD11	20:5U:42:LEU:HD11	1.78	0.65
57:8C:190:ASP:OD1	61:8G:53:LEU:HD22	1.96	0.65
5:1E:159:ASN:HB3	5:1E:184:PRO:HB3	1.78	0.65
55:4A:510:TYR:HB3	60:4F:58:VAL:HG22	1.78	0.65
9:5I:108:ARG:NH1	9:5I:110:ASP:OD2	2.30	0.65
14:5N:109:SER:HB3	14:5N:157:MET:HG2	1.77	0.65
56:4B:92:ASN:HD22	56:4B:92:ASN:C	2.02	0.65
74:4D:201:CDL:H402	74:4D:201:CDL:H592	1.78	0.65
7:5G:43:HIS:HB3	7:5G:46:LEU:HB2	1.78	0.65
13:5M:42:LEU:HD12	13:5M:453:MET:HB3	1.77	0.65
32:5g:48:ASP:OD1	32:5g:49:LYS:N	2.28	0.65
7:1G:55:CYS:HB3	71:1G:803:FES:S2	2.36	0.65
7:1G:579:ARG:HG2	7:1G:636:VAL:HB	1.78	0.65
13:1M:453:MET:HE2	32:1g:77:VAL:HG13	1.77	0.65
57:4C:221:ARG:NH1	86:4C:307:PGV:O13	2.29	0.65
76:5M:502:3PE:H371	29:5d:43:LEU:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:3E:263:TYR:HB2	49:3E:272:ILE:H	1.60	0.65
69:5B:203:PC1:H3C1	8:5H:53:LEU:HD11	1.79	0.65
7:5G:263:ILE:HA	7:5G:390:LEU:HD11	1.79	0.65
7:1G:594:ARG:NH1	22:1W:122:PHE:O	2.30	0.65
76:1d:201:3PE:H221	69:1d:202:PC1:H221	1.78	0.65
33:1h:49:GLU:OE1	33:1h:68:LYS:NZ	2.29	0.65
4:5D:233:ARG:NH1	69:5I:201:PC1:O12	2.29	0.65
8:5H:90:PRO:HD2	8:5H:240:ILE:HD13	1.78	0.65
69:5M:503:PC1:H272	69:5M:503:PC1:H371	1.78	0.65
16:5P:245:ILE:HG23	16:5P:318:LEU:HD11	1.77	0.65
4:1D:65:VAL:HB	4:1D:77:ASP:HB3	1.79	0.65
7:1G:243:ARG:HG2	7:1G:244:THR:HG23	1.79	0.65
86:8A:601:PGV:H332	86:8A:601:PGV:H162	1.78	0.65
3:1C:195:ARG:NH2	9:1I:92:ILE:O	2.30	0.65
7:1G:263:ILE:HA	7:1G:390:LEU:HD11	1.78	0.65
76:3C:505:3PE:H322	69:3X:101:PC1:H252	1.78	0.65
47:3P:221:HIS:O	47:3P:225:THR:OG1	2.15	0.65
57:4C:72:THR:HG22	57:4C:73:SER:H	1.62	0.65
2:5B:71:ARG:NH2	9:5I:49:ASN:OD1	2.29	0.65
7:5G:104:ASP:O	7:5G:108:CYS:N	2.29	0.65
74:1h:202:CDL:H562	34:1i:79:TRP:HB3	1.78	0.64
3:5C:40:VAL:HG23	43:5r:68:VAL:HG23	1.78	0.64
4:5D:65:VAL:HB	4:5D:77:ASP:HB3	1.79	0.64
92:8C:308:PEK:O14	61:8G:68:THR:OG1	2.13	0.64
5:1E:217:LEU:HD21	6:1F:44:LYS:HD3	1.78	0.64
6:5F:162:ILE:HG21	6:5F:175:VAL:HG12	1.78	0.64
14:5N:142:LEU:HB3	14:5N:194:LEU:HD21	1.79	0.64
7:1G:226:GLU:HG2	7:1G:253:ARG:HD3	1.77	0.64
7:1G:273:GLY:O	7:1G:549:HIS:NE2	2.30	0.64
86:4G:101:PGV:H011	86:4G:101:PGV:H51	1.78	0.64
4:1D:78:PRO:HG3	4:1D:402:LEU:HD23	1.78	0.64
55:4A:86:MET:HE1	55:4A:184:PHE:HB3	1.79	0.64
68:4N:32:TYR:O	68:4N:34:THR:N	2.30	0.64
9:5I:49:ASN:ND2	42:5q:30:ALA:O	2.26	0.64
76:5M:502:3PE:H372	76:5M:502:3PE:H272	1.79	0.64
19:5S:26:SER:O	19:5S:33:ARG:NH2	2.30	0.64
33:5h:138:LYS:HB2	33:5h:143:ASN:HD21	1.62	0.64
86:8B:301:PGV:H22	74:8D:201:CDL:H312	1.80	0.64
13:1M:147:LEU:HB3	76:1M:901:3PE:H332	1.80	0.64
47:3C:229:ILE:HG23	69:3J:101:PC1:H3A1	1.78	0.64
48:3Q:68:VAL:HG21	48:3Q:92:PRO:HG2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:5H:114:TYR:OH	10:5J:65:LEU:O	2.14	0.64
12:1L:9:LEU:HD12	34:1i:85:LEU:HD11	1.79	0.64
46:3O:240:ARG:O	46:3O:421:ARG:NH1	2.31	0.64
2:1B:59:MET:HB3	2:1B:116:MET:HE1	1.80	0.64
4:1D:110:SER:OG	4:1D:149:ASN:ND2	2.31	0.64
33:1h:36:VAL:HA	69:1h:203:PC1:H2G2	1.80	0.64
55:4A:246:LEU:HD23	55:4A:381:LEU:HD21	1.78	0.64
4:5D:78:PRO:HG3	4:5D:402:LEU:HD23	1.78	0.64
7:5G:118:ASP:OD2	17:5Q:46:GLN:NE2	2.31	0.64
25:5Z:125:TYR:HB3	25:5Z:133:ILE:HG22	1.78	0.64
12:5L:375:ILE:HD13	12:5L:462:ILE:HD11	1.79	0.64
17:5Q:69:LEU:HD11	42:5q:126:PRO:HG2	1.80	0.64
69:1M:905:PC1:H322	74:1h:202:CDL:H111	1.79	0.64
51:3T:34:ILE:HG12	74:3T:101:CDL:H331	1.79	0.64
55:4A:179:TYR:OH	86:4A:602:PGV:O02	2.11	0.64
57:4C:129:VAL:HG11	57:4C:180:GLU:HG3	1.79	0.64
58:8D:126:MET:HG3	63:8I:68:ILE:HD13	1.79	0.64
14:1N:1:FME:O1	15:1O:258:ARG:NH2	2.28	0.64
45:3N:226:ASP:OD2	39:5n:11:HIS:N	2.28	0.64
49:3R:224:PRO:HA	49:3R:237:PRO:HD3	1.81	0.63
17:1Q:9:GLN:HB3	22:1W:23:ARG:HH12	1.63	0.63
74:1q:202:CDL:H181	74:1q:202:CDL:H331	1.81	0.63
45:3N:224:VAL:HG13	45:3N:225:GLU:H	1.64	0.63
67:4M:19:LEU:HD23	86:4M:101:PGV:H271	1.79	0.63
2:5B:171:LYS:HG2	2:5B:174:ARG:HE	1.63	0.63
14:5N:99:THR:HG22	14:5N:157:MET:HE1	1.80	0.63
58:4D:52:SER:OG	58:4D:54:ASP:OD1	2.16	0.63
2:5B:27:GLU:OE2	2:5B:178:ARG:NH1	2.31	0.63
32:5g:100:ARG:HD2	32:5g:107:LEU:HA	1.78	0.63
9:1I:75:GLU:O	9:1I:105:ARG:NH1	2.31	0.63
49:3R:243:TYR:HB3	49:3R:247:GLY:HA2	1.81	0.63
8:5H:68:ILE:HA	8:5H:71:PHE:HB3	1.79	0.63
74:5h:202:CDL:H562	34:5i:79:TRP:HB3	1.81	0.63
55:8A:510:TYR:HB3	60:8F:58:VAL:HG22	1.81	0.63
7:1G:382:THR:HG23	7:1G:384:PRO:HD3	1.79	0.63
12:1L:596:MET:O	12:1L:600:THR:HG22	1.98	0.63
49:3E:204:ARG:NH1	49:3E:246:SER:O	2.32	0.63
12:5L:188:TRP:CD2	12:5L:212:PRO:HG3	2.33	0.63
2:1B:173:LEU:HD21	69:1B:202:PC1:H341	1.81	0.63
20:1T:71:MET:N	20:1T:71:MET:SD	2.71	0.63
39:1n:55:ASP:OD1	39:1n:56:MET:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:3O:35:ILE:HD13	46:3O:206:LEU:HB3	1.81	0.63
12:5L:191:THR:O	38:5m:125:ASN:ND2	2.32	0.63
55:8A:138:HIS:O	55:8A:213:ARG:NH2	2.32	0.63
1:1A:73:LEU:O	8:1H:160:TYR:OH	2.13	0.63
2:1B:42:ARG:NH1	69:1B:203:PC1:O12	2.32	0.63
6:1F:197:GLU:OE1	6:1F:204:ARG:NH2	2.32	0.63
10:1J:65:LEU:O	10:1J:66:VAL:HG23	1.99	0.63
1:5A:60:ILE:HG21	10:5J:168:ILE:HG21	1.79	0.63
20:5T:56:ASP:OD1	22:5W:41:ARG:NH2	2.31	0.63
43:5r:45:SER:O	43:5r:51:ASN:ND2	2.28	0.63
31:1f:56:TRP:HE1	33:1h:88:GLU:HG3	1.64	0.63
4:1D:354:GLU:OE2	4:1D:357:GLN:NE2	2.32	0.63
7:1G:104:ASP:O	7:1G:108:CYS:N	2.31	0.63
13:1M:325:MET:HE2	13:1M:362:ALA:HB2	1.80	0.63
4:5D:269:LEU:HB2	4:5D:368:GLU:HB2	1.80	0.63
13:5M:281:ASP:HB3	13:5M:284:SER:HB3	1.79	0.63
13:5M:341:THR:HG21	38:5m:64:LEU:HD21	1.80	0.63
56:8B:28:LEU:HD21	74:8B:303:CDL:H561	1.81	0.63
11:5K:23:ARG:HG2	76:5K:101:3PE:H32	1.81	0.62
12:5L:474:PRO:O	40:5o:54:GLN:NE2	2.23	0.62
12:5L:503:GLU:OE2	64:8J:33:ARG:NH2	2.32	0.62
65:8K:12:LYS:HG3	65:8K:13:TYR:CD1	2.34	0.62
1:1A:27:LEU:HD22	69:1A:201:PC1:H122	1.81	0.62
6:1F:185:ILE:HG12	6:1F:359:CYS:HB2	1.81	0.62
47:3P:233:LEU:HD22	48:3Q:212:MET:HE1	1.81	0.62
10:5J:138:GLU:HG3	30:5e:28:ILE:HD13	1.82	0.62
11:5K:93:LEU:HB3	14:5N:54:GLU:HG3	1.81	0.62
76:5L:703:3PE:N	69:5M:505:PC1:O12	2.32	0.62
25:5Z:78:GLU:OE1	26:5a:50:ARG:NH1	2.32	0.62
74:5q:203:CDL:H181	74:5q:203:CDL:H331	1.82	0.62
74:8D:201:CDL:H371	74:8D:201:CDL:H561	1.81	0.62
7:1G:648:LEU:HD21	19:1S:44:LYS:HG2	1.82	0.62
38:1m:7:PRO:HB3	38:1m:13:LEU:HB2	1.80	0.62
47:3C:304:MET:HA	47:3C:304:MET:HE3	1.82	0.62
58:4D:112:GLU:OE2	58:4D:112:GLU:N	2.30	0.62
6:5F:17:ASP:HA	6:5F:20:ARG:HB2	1.79	0.62
12:5L:341:MET:HE3	12:5L:454:ILE:HG12	1.81	0.62
7:1G:623:LEU:HD22	7:1G:630:LEU:HD23	1.81	0.62
8:1H:208:VAL:HG13	8:1H:209:SER:H	1.65	0.62
74:3P:504:CDL:H361	74:3P:504:CDL:H541	1.81	0.62
55:4A:116:SER:O	66:4L:43:GLN:NE2	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5D:116:GLN:NE2	4:5D:276:ASP:OD2	2.33	0.62
40:1o:106:ARG:HA	40:1o:109:GLN:HB2	1.81	0.62
46:3O:37:SER:OG	46:3O:211:VAL:O	2.17	0.62
48:3Q:118:ARG:HG3	48:3Q:194:SER:HB3	1.81	0.62
55:4A:336:PRO:HB2	55:4A:394:VAL:HG11	1.81	0.62
86:4C:303:PGV:H332	92:4C:308:PEK:H322	1.80	0.62
59:4E:76:GLY:O	59:4E:79:LYS:NZ	2.33	0.62
1:5A:3:ILE:HG21	69:5H:402:PC1:H221	1.80	0.62
69:5M:505:PC1:H341	74:5h:202:CDL:H311	1.79	0.62
1:1A:68:GLU:HB2	1:1A:98:LEU:HD11	1.80	0.62
10:1J:122:LEU:HD23	10:1J:126:VAL:HG21	1.82	0.62
21:1V:23:LEU:HD11	21:1V:76:ILE:HD11	1.80	0.62
44:1s:35:ASN:HD22	44:1s:35:ASN:C	2.07	0.62
45:3A:269:PRO:HB2	45:3A:410:VAL:HG11	1.81	0.62
58:4D:34:SER:HB2	58:4D:37:GLN:HG3	1.82	0.62
7:5G:194:GLU:HG2	7:5G:195:LEU:HG	1.81	0.62
8:5H:91:MET:O	8:5H:93:TYR:N	2.32	0.62
34:5i:112:THR:HG22	34:5i:114:GLU:H	1.62	0.62
68:8N:3:ARG:HH21	68:8N:7:THR:HB	1.64	0.62
7:5G:594:ARG:NH1	22:5W:122:PHE:O	2.33	0.62
7:5G:648:LEU:HD21	19:5S:44:LYS:HG2	1.81	0.62
20:5U:46:ASP:OD1	39:5n:44:ARG:NH1	2.33	0.62
24:5Y:38:TYR:HB3	76:5Y:801:3PE:H232	1.80	0.62
6:1F:46:LYS:NZ	6:1F:167:CYS:O	2.30	0.62
46:3B:308:ASP:OD1	49:3I:56:ARG:NH1	2.33	0.62
13:5M:73:LEU:HA	13:5M:76:MET:HE2	1.82	0.62
74:8D:201:CDL:H562	74:8D:201:CDL:H191	1.81	0.62
22:1W:22:SER:OG	22:1W:31:ARG:NH2	2.31	0.62
7:5G:522:LEU:HD22	7:5G:537:LEU:HD21	1.82	0.62
22:5W:25:MET:HE1	22:5W:79:VAL:HG21	1.82	0.62
69:1B:203:PC1:H3C1	8:1H:53:LEU:HD11	1.80	0.62
6:1F:191:ALA:HB2	6:1F:203:PRO:HG3	1.82	0.62
10:1J:86:ASN:OD1	10:1J:87:LYS:N	2.32	0.62
38:1m:24:ILE:HG21	38:1m:29:ARG:HH11	1.65	0.62
1:5A:36:PRO:HB2	1:5A:43:PRO:HG2	1.81	0.62
7:5G:356:THR:O	19:5S:55:ARG:NH2	2.30	0.62
12:5L:136:ASN:HA	12:5L:197:ASP:HA	1.80	0.62
17:5Q:33:ARG:NH2	17:5Q:60:ASP:O	2.33	0.62
12:1L:301:ILE:HD11	12:1L:422:TYR:HB2	1.82	0.61
5:5E:151:ALA:HB1	5:5E:152:PRO:HD2	1.81	0.61
55:8A:251:PHE:HB3	55:8A:319:LYS:HZ3	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:8C:225:PHE:O	60:8F:12:GLN:NE2	2.30	0.61
10:1J:115:ILE:O	10:1J:117:PHE:N	2.32	0.61
76:1j:101:3PE:H32	40:1o:77:LEU:HD11	1.80	0.61
5:5E:35:VAL:HG13	5:5E:43:LYS:HD2	1.82	0.61
6:5F:294:LEU:HD11	6:5F:297:VAL:HG23	1.81	0.61
12:5L:561:ILE:HG23	69:5L:705:PC1:H2B2	1.81	0.61
74:8B:303:CDL:HB21	74:8B:303:CDL:HB61	1.82	0.61
60:8F:93:SER:O	60:8F:94:HIS:ND1	2.32	0.61
66:8L:22:LEU:HD21	67:8M:21:VAL:HG11	1.81	0.61
4:1D:226:GLU:OE1	25:1Z:23:ARG:NH1	2.34	0.61
7:1G:43:HIS:HB3	7:1G:46:LEU:HB2	1.80	0.61
9:1I:156:ASN:ND2	18:1R:34:GLU:OE2	2.33	0.61
14:1N:272:LYS:HD3	33:1h:108:LEU:HD21	1.81	0.61
17:1Q:69:LEU:HD11	42:1q:126:PRO:HG2	1.81	0.61
34:1i:87:TYR:CE2	41:1p:48:ARG:HG2	2.35	0.61
38:1m:27:GLU:HA	38:1m:30:LYS:HD3	1.80	0.61
1:5A:73:LEU:O	8:5H:160:TYR:OH	2.12	0.61
35:5j:11:TYR:HB2	36:5k:13:MET:HE1	1.82	0.61
69:5q:201:PC1:H3B2	69:5q:201:PC1:H2G2	1.82	0.61
4:1D:151:ILE:HG12	4:1D:170:MET:HE3	1.81	0.61
12:1L:600:THR:OG1	12:1L:601:LEU:N	2.32	0.61
45:3A:41:ILE:HG23	45:3A:195:MET:HG2	1.82	0.61
46:3O:47:ILE:HD11	46:3O:211:VAL:HG21	1.81	0.61
55:4A:66:ILE:HG23	55:4A:246:LEU:HD21	1.82	0.61
9:5I:27:TRP:HB3	9:5I:30:LEU:HD12	1.82	0.61
5:1E:36:LYS:O	44:1s:65:GLN:NE2	2.33	0.61
16:1P:52:GLU:HG3	16:1P:54:TYR:H	1.65	0.61
37:5l:124:SER:HA	40:5o:4:LEU:HD21	1.81	0.61
8:1H:88:PRO:HB3	8:1H:98:MET:HE2	1.83	0.61
12:1L:142:ILE:HG21	74:1L:702:CDL:H641	1.81	0.61
12:1L:188:TRP:HZ3	12:1L:206:ASN:HD22	1.48	0.61
16:1P:153:GLU:OE2	16:1P:167:LYS:NZ	2.33	0.61
33:1h:75:ILE:HG23	33:1h:79:PHE:HE1	1.65	0.61
34:1i:79:TRP:HE1	41:1p:40:VAL:HA	1.66	0.61
54:3X:15:ARG:NH2	92:8G:102:PEK:O14	2.29	0.61
6:5F:96:ASN:ND2	6:5F:187:GLY:O	2.32	0.61
43:5r:57:ASP:OD2	43:5r:60:ARG:NH1	2.32	0.61
33:1h:7:ARG:NH2	34:1i:31:GLU:O	2.34	0.61
2:5B:69:MET:HE3	2:5B:74:VAL:HG12	1.82	0.61
2:5B:141:PRO:HB2	16:5P:57:MET:HG3	1.83	0.61
10:5J:55:MET:HE2	10:5J:55:MET:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:5J:86:ASN:OD1	10:5J:87:LYS:N	2.32	0.61
7:1G:275:LYS:HA	42:1q:134:ILE:HD13	1.83	0.61
68:4N:19:PHE:HA	68:4N:22:ILE:HG22	1.82	0.61
6:1F:202:LYS:HE2	6:1F:361:GLN:HB2	1.83	0.61
9:1I:69:ARG:NH1	9:1I:73:GLY:O	2.34	0.61
15:1O:47:GLY:O	15:1O:120:GLN:NE2	2.34	0.61
6:5F:30:ASP:O	6:5F:39:ARG:NH1	2.33	0.61
14:5N:314:LYS:NZ	15:5O:274:THR:OG1	2.33	0.61
55:8A:179:TYR:OH	86:8A:602:PGV:O02	2.16	0.61
6:1F:134:ALA:HB3	6:1F:175:VAL:HG12	1.83	0.61
12:1L:486:MET:HE1	37:1l:126:GLN:HE22	1.66	0.61
40:1o:14:LYS:HE3	40:1o:109:GLN:HG2	1.83	0.61
55:4A:86:MET:HE2	55:4A:185:VAL:HG23	1.83	0.61
3:5C:33:LEU:HD13	3:5C:60:VAL:HG22	1.82	0.61
55:8A:297:MET:O	55:8A:302:ARG:NH1	2.33	0.61
55:8A:406:ASN:HD22	55:8A:409:TRP:HD1	1.49	0.61
58:8D:52:SER:OG	58:8D:54:ASP:OD1	2.16	0.61
7:1G:323:VAL:HG11	7:1G:525:LEU:HG	1.82	0.60
13:1M:73:LEU:HA	13:1M:76:MET:HE3	1.83	0.60
34:1i:17:LEU:HD11	39:1n:162:LEU:HD22	1.83	0.60
49:3R:155:LYS:HD3	49:3R:271:VAL:HG23	1.83	0.60
6:5F:264:HIS:HD2	6:5F:285:GLY:HA3	1.66	0.60
60:8F:14:THR:OG1	64:8J:13:GLN:OE1	2.18	0.60
12:1L:159:HIS:HB2	13:1M:416:ARG:HB3	1.82	0.60
6:5F:200:GLN:HE22	7:5G:174:THR:HG23	1.65	0.60
9:5I:53:GLU:OE2	42:5q:58:ARG:NE	2.34	0.60
62:8H:28:ASN:OD1	62:8H:32:ASN:ND2	2.34	0.60
4:1D:50:ASN:HA	4:1D:65:VAL:HA	1.83	0.60
14:1N:95:MET:SD	14:1N:148:SER:OG	2.57	0.60
21:1V:8:THR:HG21	21:1V:13:LEU:HB3	1.83	0.60
49:3R:234:TYR:HB2	49:3R:243:TYR:HB2	1.83	0.60
3:5C:173:GLU:HG3	3:5C:188:VAL:HA	1.83	0.60
6:5F:110:ILE:HD11	6:5F:225:VAL:HG12	1.82	0.60
30:5e:63:VAL:HA	30:5e:66:LEU:HD12	1.84	0.60
42:5q:34:ARG:NH1	42:5q:54:GLN:OE1	2.34	0.60
15:1O:320:LYS:O	29:1d:60:ARG:NH2	2.35	0.60
37:1l:68:ASP:OD1	37:1l:68:ASP:N	2.34	0.60
46:3B:350:GLY:HA2	46:3B:411:ILE:HD13	1.84	0.60
74:3P:504:CDL:HB22	51:3T:40:ARG:HH21	1.67	0.60
49:3R:176:VAL:HG22	49:3R:212:ILE:HG13	1.83	0.60
90:4A:609:PSC:H031	56:4B:58:ALA:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5E:93:LYS:HG3	5:5E:94:PRO:HD2	1.82	0.60
6:5F:188:GLU:HG2	6:5F:203:PRO:HB3	1.82	0.60
33:5h:44:ASN:ND2	74:5h:202:CDL:OB9	2.34	0.60
42:5q:106:ARG:HB2	42:5q:109:ILE:HG13	1.84	0.60
9:1I:49:ASN:ND2	42:1q:30:ALA:O	2.28	0.60
40:1o:38:MET:HE1	40:1o:57:TYR:HA	1.83	0.60
53:3W:10:TYR:HA	53:3W:14:PHE:HB2	1.84	0.60
55:4A:418:PHE:HE2	74:4D:201:CDL:HB21	1.66	0.60
7:5G:158:ARG:NH1	7:5G:202:ILE:O	2.34	0.60
8:5H:24:GLU:HA	8:5H:271:LEU:HD13	1.83	0.60
8:5H:149:ILE:HG21	8:5H:185:TRP:HB2	1.82	0.60
14:5N:230:LEU:HD11	14:5N:244:MET:HE1	1.83	0.60
59:8E:9:GLU:N	59:8E:9:GLU:OE1	2.34	0.60
2:1B:27:GLU:OE2	2:1B:178:ARG:NH1	2.35	0.60
22:1W:80:ASP:OD1	22:1W:80:ASP:N	2.33	0.60
46:3B:102:ARG:NH2	46:3B:161:GLU:OE1	2.33	0.60
2:5B:170:GLU:OE1	2:5B:172:ARG:NE	2.20	0.60
6:5F:99:GLU:O	6:5F:139:ARG:NH1	2.34	0.60
6:5F:245:PHE:HB3	6:5F:271:GLU:HG3	1.84	0.60
9:5I:75:GLU:O	9:5I:105:ARG:NH1	2.34	0.60
41:5p:5:ASP:HB3	41:5p:8:VAL:HG22	1.83	0.60
55:8A:380:VAL:HG12	87:8A:604:HEA:HBC1	1.84	0.60
55:8A:484:ALA:HB3	67:8M:2:TYR:HB2	1.83	0.60
57:8C:88:ILE:HG12	74:8C:306:CDL:H621	1.84	0.60
3:1C:40:VAL:HG23	43:1r:68:VAL:HG23	1.82	0.60
11:1K:23:ARG:HG2	76:1K:101:3PE:H32	1.84	0.60
12:1L:213:LEU:HB2	12:1L:273:VAL:HG21	1.84	0.60
13:1M:108:MET:HB3	13:1M:121:LEU:HD13	1.84	0.60
13:1M:114:GLU:OE1	23:1X:168:PHE:HB3	2.02	0.60
14:1N:316:GLN:NE2	15:1O:60:ASP:OD1	2.34	0.60
15:1O:104:ARG:NH2	77:1O:402:GTP:N7	2.50	0.60
24:1Y:82:LYS:O	24:1Y:88:ASN:ND2	2.34	0.60
86:4C:307:PGV:H291	86:4C:307:PGV:H152	1.83	0.60
12:5L:526:LEU:HD12	12:5L:530:PRO:HG2	1.84	0.60
14:5N:152:ASN:ND2	76:5Y:804:3PE:O12	2.33	0.60
61:8G:42:HIS:O	61:8G:74:ARG:NH2	2.35	0.60
4:1D:233:ARG:NH1	69:1I:201:PC1:O12	2.34	0.60
20:1U:8:LEU:N	20:1U:88:GLU:OE2	2.33	0.60
3:5C:38:GLN:HG2	21:5V:102:LEU:HD21	1.83	0.60
20:1U:18:VAL:HB	20:1U:54:MET:HE1	1.84	0.60
24:1Y:104:THR:HG22	76:1Y:802:3PE:H11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:3B:279:LEU:HB3	46:3B:295:LEU:HG	1.84	0.60
45:3N:86:LEU:HD13	45:3N:99:ILE:HG12	1.84	0.60
47:3P:246:SER:HB2	47:3P:249:LEU:HB2	1.83	0.60
56:4B:30:ILE:HG21	56:4B:76:ILE:HD11	1.83	0.60
8:5H:9:LEU:HD12	26:5a:19:PRO:HB3	1.84	0.60
29:5d:45:ASP:OD1	29:5d:51:ARG:NH2	2.34	0.60
57:8C:91:VAL:HG13	86:8C:304:PGV:H172	1.84	0.60
86:8C:302:PGV:H162	92:8G:102:PEK:H162	1.83	0.60
12:1L:214:ILE:HD11	12:1L:276:MET:HE1	1.82	0.60
74:4B:302:CDL:H811	74:4B:302:CDL:H262	1.84	0.60
6:5F:301:GLY:H	6:5F:333:ALA:HB3	1.66	0.60
69:5M:503:PC1:H282	76:5M:506:3PE:H262	1.84	0.60
2:1B:71:ARG:NH2	9:1I:49:ASN:OD1	2.34	0.59
12:1L:366:MET:HE3	12:1L:443:ILE:HG23	1.84	0.59
16:1P:245:ILE:HG23	16:1P:318:LEU:HD11	1.84	0.59
39:1n:54:LYS:HE3	45:3A:22:GLY:HA2	1.84	0.59
53:3J:14:TYR:HA	53:3J:18:PHE:HB2	1.84	0.59
86:4A:601:PGV:H341	86:4L:101:PGV:H152	1.84	0.59
59:4E:33:MET:HE2	59:4E:67:ILE:HB	1.84	0.59
1:5A:22:PHE:HZ	8:5H:62:ARG:HD2	1.67	0.59
8:1H:92:PRO:HG3	8:1H:255:TYR:HB3	1.83	0.59
24:1Y:38:TYR:HB3	76:1Y:801:3PE:H232	1.83	0.59
13:5M:61:LEU:HB2	13:5M:457:PRO:HD3	1.83	0.59
13:5M:102:LEU:HD13	13:5M:128:PRO:HG2	1.84	0.59
39:5n:56:MET:HA	39:5n:56:MET:HE3	1.84	0.59
55:8A:72:PRO:O	55:8A:77:GLY:N	2.35	0.59
14:1N:152:ASN:ND2	76:1Y:804:3PE:O12	2.35	0.59
2:5B:125:TYR:HE1	9:5I:88:PRO:HB2	1.67	0.59
2:1B:116:MET:HG3	2:1B:151:PRO:HG2	1.85	0.59
7:1G:359:ARG:NH1	7:1G:504:ASP:OD2	2.34	0.59
45:3A:244:ARG:NH2	45:3A:429:GLU:OE1	2.36	0.59
46:3B:24:LEU:HD11	46:3B:36:ALA:HB1	1.84	0.59
47:3C:262:LEU:HD11	49:3R:172:LYS:HA	1.84	0.59
48:3Q:147:LEU:HD12	48:3Q:157:ALA:HB1	1.84	0.59
56:4B:28:LEU:HD21	74:4B:302:CDL:H561	1.84	0.59
6:5F:142:PHE:HB3	6:5F:145:GLU:HB2	1.84	0.59
6:5F:197:GLU:OE1	6:5F:204:ARG:NH2	2.34	0.59
20:5U:18:VAL:HB	20:5U:54:MET:HE1	1.85	0.59
22:5W:91:GLU:O	22:5W:95:ASN:ND2	2.36	0.59
57:8C:58:TRP:HD1	57:8C:61:ILE:HD12	1.67	0.59
9:1I:53:GLU:OE2	42:1q:58:ARG:NE	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1S:84:ASP:OD1	19:1S:84:ASP:N	2.35	0.59
49:3V:77:ARG:O	49:3V:77:ARG:NE	2.29	0.59
10:5J:9:LEU:HD22	10:5J:39:VAL:HG13	1.85	0.59
25:5Z:87:LEU:HD11	25:5Z:119:PRO:HG3	1.84	0.59
58:8D:127:LYS:NZ	63:8I:62:GLU:OE1	2.34	0.59
62:8H:5:GLN:HG3	62:8H:6:THR:H	1.68	0.59
5:1E:93:LYS:HG3	5:1E:94:PRO:HD2	1.85	0.59
9:1I:95:GLU:HG3	9:1I:108:ARG:HD2	1.83	0.59
7:5G:231:MET:HG3	7:5G:266:LYS:HD2	1.83	0.59
35:5j:26:GLU:OE2	36:5k:68:LYS:NZ	2.35	0.59
5:1E:89:MET:HE2	6:1F:181:ALA:HA	1.83	0.59
12:1L:136:ASN:HA	12:1L:197:ASP:HA	1.85	0.59
13:1M:341:THR:HG21	38:1m:64:LEU:HD21	1.85	0.59
33:1h:69:HIS:NE2	74:1h:202:CDL:OA4	2.33	0.59
7:5G:306:MET:HE3	7:5G:542:PHE:HB2	1.84	0.59
8:5H:152:SER:HA	8:5H:155:LEU:HD12	1.84	0.59
13:5M:282:LEU:HG	13:5M:342:MET:HG3	1.84	0.59
76:5M:502:3PE:H2E2	76:5M:504:3PE:H2C2	1.85	0.59
16:5P:173:GLY:H	16:5P:176:ASP:HB3	1.67	0.59
24:5Y:28:GLY:HA2	76:5Y:802:3PE:H2B2	1.85	0.59
5:1E:142:VAL:HG21	5:1E:145:LEU:HD11	1.83	0.59
9:1I:148:LEU:HD23	17:1Q:70:MET:HG3	1.85	0.59
20:1T:6:LEU:HD12	20:1T:10:ALA:HB1	1.85	0.59
47:3C:176:THR:OG1	47:3P:53:MET:O	2.17	0.59
9:5I:132:VAL:HG21	9:5I:165:ILE:HD12	1.85	0.59
76:5L:704:3PE:H332	13:5M:147:LEU:HB3	1.85	0.59
55:8A:336:PRO:HB2	55:8A:394:VAL:HG11	1.85	0.59
59:8E:76:GLY:O	59:8E:79:LYS:NZ	2.35	0.59
13:1M:61:LEU:HB2	13:1M:457:PRO:HD3	1.83	0.59
49:3E:235:TYR:CE2	49:3E:237:PRO:HB3	2.38	0.59
49:3R:163:LYS:HG3	49:3R:165:MET:HE3	1.85	0.59
10:5J:115:ILE:O	10:5J:117:PHE:N	2.35	0.59
12:5L:6:SER:O	12:5L:10:THR:OG1	2.18	0.59
76:5M:501:3PE:H31	14:5N:276:ILE:HG21	1.85	0.59
4:1D:63:ARG:HB3	4:1D:79:HIS:HB2	1.85	0.59
10:1J:23:LYS:NZ	11:1K:18:GLY:O	2.36	0.59
12:1L:441:VAL:HG13	12:1L:443:ILE:HG12	1.85	0.59
15:1O:287:HIS:ND1	32:1g:28:GLU:OE2	2.31	0.59
45:3N:281:ASP:HB3	45:3N:284:TYR:CE1	2.37	0.59
55:4A:138:HIS:O	55:4A:213:ARG:NH2	2.36	0.59
69:5L:705:PC1:H342	24:5Y:109:ILE:HG23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:5M:505:PC1:H2D2	69:5M:505:PC1:H292	1.85	0.59
8:1H:99:ASN:OD1	26:1a:40:HIS:ND1	2.36	0.58
19:1S:35:PHE:HZ	19:1S:43:LEU:HD12	1.68	0.58
46:3O:97:SER:HA	49:3V:69:GLY:HA2	1.84	0.58
15:5O:214:MET:HE3	15:5O:217:LYS:HE2	1.83	0.58
55:8A:295:VAL:O	56:8B:178:ARG:NH1	2.35	0.58
6:1F:367:GLU:HB2	7:1G:96:PHE:HB3	1.85	0.58
76:1M:903:3PE:H391	76:1M:903:3PE:H291	1.83	0.58
26:1a:1:MET:SD	26:1a:1:MET:N	2.72	0.58
67:4M:38:ASP:OD1	67:4M:39:HIS:N	2.36	0.58
7:5G:43:HIS:NE2	7:5G:261:GLU:OE2	2.28	0.58
9:5I:156:ASN:ND2	18:5R:34:GLU:OE2	2.34	0.58
57:8C:247:VAL:HG21	74:8C:306:CDL:H842	1.84	0.58
16:1P:248:VAL:HG22	16:1P:334:VAL:HG21	1.85	0.58
20:1U:66:ASP:HB3	20:1U:79:TYR:HE2	1.68	0.58
47:3P:315:MET:HE1	47:3P:325:PHE:HB2	1.83	0.58
55:4A:406:ASN:HD22	55:4A:409:TRP:HD1	1.51	0.58
74:4D:201:CDL:H371	74:4D:201:CDL:H561	1.86	0.58
5:5E:16:ASN:OD1	5:5E:19:THR:OG1	2.17	0.58
14:5N:182:SER:OG	14:5N:293:TYR:OH	2.19	0.58
23:5X:129:LYS:HD3	27:5b:65:VAL:HG13	1.85	0.58
61:8G:50:TYR:HB2	61:8G:53:LEU:HB2	1.85	0.58
1:1A:60:ILE:HG21	10:1J:168:ILE:HG21	1.85	0.58
4:1D:88:GLU:OE2	4:1D:430:ARG:NH1	2.36	0.58
7:1G:215:PHE:HB3	9:1I:104:ARG:HG3	1.84	0.58
86:4A:601:PGV:H81	64:4J:40:LEU:HD11	1.85	0.58
59:4E:52:LEU:HD12	59:4E:67:ILE:HD11	1.86	0.58
1:5A:57:LEU:O	1:5A:61:THR:OG1	2.21	0.58
9:5I:69:ARG:NH1	9:5I:73:GLY:O	2.35	0.58
13:5M:54:LEU:HD21	33:5h:96:ILE:HD11	1.84	0.58
16:5P:97:ARG:NH1	79:5P:402:NDP:O3X	2.35	0.58
57:8C:116:TRP:HD1	68:8N:47:ARG:HH12	1.50	0.58
7:1G:534:ARG:NH1	7:1G:556:MET:O	2.35	0.58
12:1L:6:SER:O	12:1L:10:THR:OG1	2.16	0.58
12:1L:366:MET:HB3	12:1L:369:THR:HB	1.84	0.58
22:1W:35:LEU:HD21	22:1W:86:GLY:HA3	1.86	0.58
7:5G:465:ALA:HB2	7:5G:654:GLN:HG3	1.84	0.58
8:5H:99:ASN:OD1	26:5a:40:HIS:ND1	2.37	0.58
12:5L:13:ILE:HD11	34:5i:77:PRO:HB3	1.85	0.58
12:5L:375:ILE:HG12	35:5j:32:MET:HE2	1.84	0.58
23:5X:51:ASP:OD1	23:5X:53:ARG:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:308:PRO:HD3	6:1F:421:HIS:CD2	2.38	0.58
10:1J:130:THR:HG21	25:1Z:124:LEU:HD12	1.85	0.58
14:1N:211:MET:HE3	14:1N:251:MET:HA	1.84	0.58
23:1X:29:HIS:HB3	23:1X:119:PRO:HD2	1.86	0.58
39:1n:57:VAL:HG13	39:1n:58:LYS:HD3	1.83	0.58
49:3E:231:PHE:HE1	49:3E:242:HIS:HB3	1.68	0.58
46:3O:197:ASN:HB3	46:3O:232:LEU:HB2	1.86	0.58
52:3U:50:THR:HG22	52:3U:52:GLU:H	1.68	0.58
12:5L:62:ILE:HG12	41:5p:114:GLN:HG2	1.85	0.58
13:5M:196:TRP:CD1	13:5M:250:LEU:HB3	2.39	0.58
81:5n:201:EHZ:O1	81:5n:201:EHZ:S1	2.62	0.58
49:3V:69:GLY:HA3	49:3V:72:VAL:HG12	1.85	0.58
4:5D:100:LEU:HD22	4:5D:195:ARG:HD3	1.85	0.58
6:5F:46:LYS:NZ	6:5F:167:CYS:O	2.37	0.58
7:5G:110:GLN:HG2	7:5G:114:CYS:HA	1.85	0.58
7:5G:126:ASP:OD1	43:5r:56:ARG:NH1	2.36	0.58
7:5G:188:GLU:HG2	7:5G:695:ILE:HG21	1.84	0.58
69:1M:904:PC1:H272	69:1M:904:PC1:H371	1.86	0.58
42:1q:34:ARG:NH1	42:1q:54:GLN:OE1	2.36	0.58
52:3H:49:CYS:SG	52:3H:98:LYS:NZ	2.74	0.58
51:3T:36:ASN:ND2	74:3T:101:CDL:OA4	2.34	0.58
1:5A:79:SER:HA	1:5A:87:MET:HE2	1.86	0.58
4:5D:228:MET:HE2	4:5D:228:MET:HA	1.86	0.58
23:5X:17:VAL:HG11	25:5Z:74:LEU:HD11	1.85	0.58
33:5h:14:SER:HB2	39:5n:106:TRP:HA	1.85	0.58
1:1A:3:ILE:HG21	69:1H:402:PC1:H221	1.86	0.58
13:1M:183:SER:O	41:1p:152:ARG:NH2	2.33	0.58
49:3R:219:HIS:ND1	49:3R:239:HIS:HE1	2.02	0.58
2:5B:104:TYR:O	2:5B:111:ARG:NH1	2.37	0.58
4:5D:50:ASN:HA	4:5D:65:VAL:HA	1.84	0.58
11:5K:70:GLU:O	11:5K:74:GLY:N	2.27	0.58
12:5L:319:ILE:HD13	12:5L:399:VAL:HG12	1.86	0.58
76:5M:502:3PE:H2B2	76:5M:504:3PE:H252	1.86	0.58
59:8E:100:THR:HB	59:8E:102:GLU:OE1	2.04	0.58
5:1E:6:LEU:O	5:1E:92:ARG:NH2	2.37	0.58
12:1L:209:PRO:HB2	12:1L:213:LEU:HG	1.86	0.58
13:1M:195:MET:HG3	76:1M:902:3PE:H221	1.85	0.58
55:4A:35:LEU:HD12	66:4L:37:PHE:HZ	1.67	0.58
57:4C:80:ARG:O	57:4C:84:ILE:HG13	2.04	0.58
58:4D:20:ARG:HA	58:4D:68:PHE:HE1	1.69	0.58
6:5F:151:VAL:HG23	6:5F:154:ARG:HH21	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:5N:329:MET:HE1	74:5N:401:CDL:H402	1.85	0.58
4:1D:34:ASN:HB3	4:1D:36:VAL:HG22	1.86	0.57
13:1M:198:ALA:HB2	76:1M:902:3PE:H271	1.86	0.57
20:1T:47:GLN:HE22	20:1T:68:GLU:HA	1.69	0.57
76:1d:201:3PE:H2A2	69:1d:202:PC1:H332	1.86	0.57
49:3R:160:PRO:HD2	49:3R:163:LYS:HB3	1.86	0.57
3:5C:93:VAL:HG22	3:5C:108:LYS:HE2	1.85	0.57
9:5I:150:ASN:ND2	42:5q:127:TYR:O	2.37	0.57
13:5M:425:ASN:HB2	38:5m:57:GLY:HA2	1.86	0.57
56:8B:132:GLU:HB3	56:8B:137:GLU:HG3	1.85	0.57
7:1G:157:THR:HG22	7:1G:161:ARG:HG3	1.87	0.57
15:1O:25:ILE:HB	15:1O:123:VAL:HG12	1.85	0.57
16:1P:71:MET:HE3	16:1P:84:VAL:HG12	1.85	0.57
81:1n:201:EHZ:O1	81:1n:201:EHZ:S1	2.61	0.57
67:4M:20:SER:HA	86:4M:101:PGV:H342	1.86	0.57
4:5D:335:ARG:NH2	9:5I:126:CYS:O	2.31	0.57
12:5L:11:THR:HG22	12:5L:46:LEU:HB3	1.87	0.57
24:5Y:140:VAL:O	33:5h:115:ARG:NH1	2.34	0.57
4:1D:237:ASN:O	8:1H:284:GLN:NE2	2.32	0.57
6:1F:197:GLU:OE2	17:1Q:129:ARG:NH2	2.35	0.57
12:1L:561:ILE:HG23	69:1L:704:PC1:H2B2	1.86	0.57
55:4A:459:PHE:HA	55:4A:462:LEU:HB3	1.85	0.57
2:5B:127:HIS:O	2:5B:134:ARG:NH1	2.37	0.57
4:5D:165:THR:HG23	8:5H:32:GLN:HG2	1.86	0.57
32:5g:108:MET:HE1	41:5p:98:ASP:HB3	1.86	0.57
45:3A:240:GLU:HG2	51:3G:19:SER:HB2	1.86	0.57
49:3R:173:PRO:O	49:3R:215:GLY:N	2.29	0.57
3:5C:151:ILE:HG23	3:5C:152:LEU:HG	1.86	0.57
6:5F:95:VAL:HB	6:5F:136:ILE:HG13	1.85	0.57
12:5L:387:THR:HA	12:5L:465:GLY:HA3	1.86	0.57
55:8A:483:SER:HB3	67:8M:4:LYS:HG3	1.86	0.57
86:8B:301:PGV:O05	74:8D:201:CDL:OA7	2.13	0.57
74:8C:306:CDL:H141	74:8C:306:CDL:H541	1.86	0.57
4:1D:342:MET:HE2	7:1G:101:HIS:HB3	1.85	0.57
8:1H:24:GLU:HA	8:1H:271:LEU:HD13	1.87	0.57
10:1J:5:ILE:HG21	25:1Z:142:TRP:HZ2	1.70	0.57
15:1O:165:PRO:O	15:1O:248:TRP:NE1	2.31	0.57
7:5G:105:CYS:HA	7:5G:108:CYS:CB	2.34	0.57
14:5N:265:MET:HE2	14:5N:343:LEU:HD21	1.86	0.57
40:5o:51:MET:HB2	40:5o:54:GLN:HG3	1.86	0.57
74:8C:306:CDL:H191	74:8C:306:CDL:H322	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:207:LEU:O	8:1H:209:SER:N	2.38	0.57
12:1L:319:ILE:HD13	12:1L:399:VAL:HG12	1.86	0.57
69:1q:201:PC1:H2G2	69:1q:201:PC1:H3B2	1.85	0.57
55:4A:298:ASP:OD2	62:4H:22:ASN:ND2	2.37	0.57
3:5C:53:HIS:ND1	3:5C:55:ASP:OD1	2.36	0.57
4:5D:130:PRO:HG2	4:5D:135:GLN:HE21	1.68	0.57
7:5G:11:VAL:HG11	7:5G:73:VAL:HB	1.85	0.57
4:1D:246:THR:HG23	21:1V:12:GLY:HA3	1.86	0.57
7:1G:524:LEU:HD13	7:1G:543:ILE:HG23	1.86	0.57
12:1L:510:TYR:HE2	64:4J:29:ASN:HD21	1.52	0.57
48:3D:214:TYR:OH	85:3D:501:HEC:O2A	2.16	0.57
49:3E:161:GLU:HA	49:3E:178:HIS:HB3	1.85	0.57
45:3N:211:LEU:HD23	45:3N:214:LYS:HZ3	1.70	0.57
55:4A:481:GLU:HB2	67:4M:4:LYS:HE2	1.86	0.57
56:4B:71:ILE:H	56:4B:71:ILE:HD12	1.69	0.57
7:5G:283:MET:HB2	7:5G:560:ILE:HB	1.86	0.57
7:5G:486:ASP:OD1	7:5G:486:ASP:N	2.36	0.57
13:5M:243:MET:HB3	13:5M:301:ILE:HG21	1.87	0.57
38:5m:82:THR:HG22	38:5m:85:THR:HG23	1.85	0.57
61:8G:28:VAL:O	61:8G:32:THR:OG1	2.20	0.57
4:1D:69:SER:OG	4:1D:74:ARG:NH1	2.38	0.57
12:1L:217:LEU:HD11	12:1L:277:THR:HB	1.87	0.57
76:1M:903:3PE:H2E2	76:1O:401:3PE:H2C2	1.87	0.57
15:1O:4:GLY:HA2	15:1O:261:MET:HE1	1.87	0.57
46:3O:54:GLY:O	46:3O:194:TYR:OH	2.22	0.57
48:3Q:178:THR:HG22	52:3U:13:LEU:HD21	1.87	0.57
86:4A:602:PGV:H91	86:4A:602:PGV:H142	1.87	0.57
6:5F:342:ASP:OD1	6:5F:429:ARG:NH2	2.31	0.57
10:5J:23:LYS:HG2	11:5K:28:SER:HB2	1.85	0.57
42:5q:78:ASP:OD2	42:5q:80:SER:OG	2.21	0.57
57:8C:25:LEU:HD23	64:8J:43:THR:HG22	1.87	0.57
12:1L:416:THR:O	12:1L:419:THR:OG1	2.22	0.57
13:1M:71:TRP:CG	69:1M:905:PC1:H2C2	2.40	0.57
14:1N:329:MET:HE1	74:1N:401:CDL:H402	1.87	0.57
21:1V:62:PRO:HD2	21:1V:63:ASP:H	1.70	0.57
49:3E:125:VAL:HG21	69:3J:101:PC1:H362	1.87	0.57
7:5G:201:ASP:OD2	7:5G:268:ARG:NH2	2.38	0.57
13:5M:425:ASN:O	13:5M:425:ASN:ND2	2.29	0.57
13:5M:457:PRO:HA	32:5g:84:ARG:HH21	1.69	0.57
55:8A:32:ALA:HB3	66:8L:36:PRO:HG2	1.87	0.57
1:1A:41:PHE:HE2	4:1D:63:ARG:HG3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:259:MET:HE2	4:1D:421:GLN:HG2	1.86	0.57
5:1E:126:ILE:HG13	5:1E:130:GLU:HG3	1.86	0.57
13:1M:196:TRP:CD1	13:1M:250:LEU:HB3	2.39	0.57
14:1N:142:LEU:HB3	14:1N:194:LEU:HD21	1.86	0.57
15:1O:318:TRP:HB2	29:1d:58:LEU:HD12	1.87	0.57
45:3A:86:LEU:HD13	45:3A:99:ILE:HG13	1.86	0.57
46:3B:71:LEU:HD23	49:3I:68:VAL:HG21	1.86	0.57
48:3D:119:GLN:NE2	48:3D:261:ASP:OD1	2.29	0.57
1:5A:22:PHE:HD1	8:5H:60:PRO:HG2	1.70	0.57
8:5H:35:LYS:HD2	9:5I:47:THR:HB	1.85	0.57
8:5H:317:GLN:HE22	10:5J:141:MET:HE1	1.70	0.57
9:5I:148:LEU:HD23	17:5Q:70:MET:HG3	1.87	0.57
24:5Y:104:THR:HG22	76:5Y:802:3PE:H11	1.87	0.57
34:5i:17:LEU:HD11	39:5n:162:LEU:HD22	1.87	0.57
34:5i:79:TRP:HE1	41:5p:40:VAL:HA	1.70	0.57
40:5o:74:PRO:HG3	41:5p:28:PRO:HD3	1.87	0.57
55:8A:86:MET:HB3	55:8A:182:PRO:HG2	1.87	0.57
86:8A:601:PGV:H81	64:8J:40:LEU:HD11	1.85	0.57
60:8F:50:PRO:O	60:8F:56:ARG:NH1	2.35	0.57
3:1C:151:ILE:HG23	3:1C:152:LEU:HG	1.85	0.56
10:1J:175:ASN:H	14:1N:48:PHE:HD2	1.52	0.56
24:1Y:28:GLY:HA2	76:1Y:802:3PE:H2B2	1.87	0.56
45:3N:171:SER:N	49:3R:82:ASP:OD1	2.38	0.56
4:5D:354:GLU:OE2	4:5D:357:GLN:NE2	2.38	0.56
9:5I:43:ARG:HG3	43:5r:11:ARG:HD2	1.85	0.56
16:5P:145:TYR:HH	79:5P:402:NDP:HO2N	1.53	0.56
23:5X:8:THR:OG1	23:5X:11:ASP:OD1	2.15	0.56
17:1Q:33:ARG:NH1	17:1Q:77:ASP:OD1	2.37	0.56
23:1X:75:ARG:HG2	23:1X:76:HIS:CD2	2.37	0.56
56:4B:161:HIS:HB2	56:4B:174:ALA:HB3	1.86	0.56
6:5F:214:GLY:HA3	6:5F:220:THR:HG22	1.88	0.56
10:5J:23:LYS:NZ	11:5K:18:GLY:O	2.35	0.56
15:5O:22:SER:OG	15:5O:119:GLY:O	2.23	0.56
40:5o:117:ARG:HE	40:5o:118:GLU:HG3	1.70	0.56
4:1D:148:LEU:HD23	4:1D:174:ARG:HG2	1.86	0.56
9:1I:135:PRO:HD3	9:1I:165:ILE:HG22	1.86	0.56
13:1M:26:ASN:OD1	31:1f:13:HIS:NE2	2.38	0.56
21:1V:34:LEU:HD13	21:1V:48:GLU:HG2	1.86	0.56
46:3O:128:ALA:HA	46:3O:227:ARG:HH22	1.71	0.56
46:3O:204:MET:HE1	46:3O:224:LEU:HD22	1.86	0.56
46:3O:279:LEU:HB3	46:3O:295:LEU:HG	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:3R:232:GLY:HA3	49:3R:244:ASP:HA	1.86	0.56
4:5D:166:PRO:HG3	4:5D:228:MET:HG3	1.87	0.56
6:5F:276:LEU:HD21	6:5F:297:VAL:HG11	1.86	0.56
7:5G:228:ILE:HD11	7:5G:573:TYR:HB2	1.88	0.56
7:5G:359:ARG:NH1	7:5G:504:ASP:OD2	2.39	0.56
7:5G:432:ILE:O	7:5G:440:SER:OG	2.23	0.56
12:5L:559:GLU:OE2	13:5M:218:LYS:NZ	2.39	0.56
23:5X:27:ALA:O	23:5X:29:HIS:N	2.39	0.56
24:5Y:34:ILE:HD12	76:5Y:804:3PE:H372	1.87	0.56
56:8B:99:THR:HG23	56:8B:154:VAL:HA	1.87	0.56
74:8C:306:CDL:H581	74:8C:306:CDL:H761	1.86	0.56
2:1B:30:VAL:HG13	2:1B:173:LEU:HB3	1.87	0.56
13:1M:382:ILE:HA	13:1M:396:MET:HE1	1.87	0.56
15:1O:149:VAL:O	15:1O:153:ASN:ND2	2.34	0.56
15:1O:279:LEU:HD13	15:1O:282:ILE:HD11	1.87	0.56
38:1m:16:THR:O	39:1n:64:ARG:NH2	2.36	0.56
57:4C:47:LEU:HD13	86:4C:303:PGV:H12	1.88	0.56
5:5E:78:MET:HE3	5:5E:81:TYR:HB2	1.86	0.56
14:5N:84:TRP:HB2	30:5e:18:THR:HA	1.85	0.56
37:5l:55:GLN:NE2	37:5l:69:LEU:O	2.38	0.56
4:1D:335:ARG:NH2	9:1I:126:CYS:O	2.28	0.56
6:1F:21:ILE:O	6:1F:117:LYS:NZ	2.31	0.56
76:1M:903:3PE:H372	76:1M:903:3PE:H272	1.87	0.56
69:1M:905:PC1:H341	74:1h:202:CDL:H311	1.86	0.56
18:1R:20:ASP:OD1	18:1R:21:GLY:N	2.38	0.56
25:1Z:78:GLU:OE1	26:1a:50:ARG:NH1	2.39	0.56
45:3A:103:SER:OG	45:3A:202:GLY:O	2.23	0.56
49:3R:149:MET:O	49:3R:151:LYS:N	2.39	0.56
55:4A:30:GLY:HA3	55:4A:65:MET:HE2	1.88	0.56
55:4A:368:HIS:ND1	87:4A:605:HEA:O1A	2.36	0.56
57:4C:58:TRP:HD1	57:4C:61:ILE:HD12	1.70	0.56
7:5G:192:MET:HG3	7:5G:691:VAL:HG22	1.88	0.56
37:5l:133:TYR:O	37:5l:155:HIS:NE2	2.39	0.56
55:8A:129:TYR:OH	55:8A:236:TRP:NE1	2.35	0.56
63:8I:17:LEU:HD23	90:8I:101:PSC:H011	1.87	0.56
7:1G:278:ARG:HH21	7:1G:548:HIS:HB2	1.71	0.56
7:1G:371:VAL:HG23	7:1G:377:ILE:HD11	1.87	0.56
37:1l:18:GLU:OE1	37:1l:18:GLU:N	2.27	0.56
4:5D:223:ASP:HB3	4:5D:305:ARG:HH22	1.71	0.56
8:5H:289:LEU:HA	8:5H:293:PHE:HB2	1.87	0.56
10:5J:124:ASP:OD1	25:5Z:138:TYR:OH	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:5f:45:LYS:O	41:5p:68:ARG:NH2	2.39	0.56
65:8K:8:ASP:OD1	65:8K:8:ASP:N	2.35	0.56
2:1B:57:VAL:HB	4:1D:152:MET:HE1	1.87	0.56
6:1F:208:PRO:HG2	6:1F:213:VAL:HG22	1.86	0.56
20:1U:25:ILE:HD11	20:1U:42:LEU:HD11	1.86	0.56
6:5F:262:VAL:HG11	6:5F:284:ALA:HB1	1.86	0.56
6:5F:297:VAL:HG22	6:5F:336:VAL:HG12	1.87	0.56
7:5G:579:ARG:HG2	7:5G:636:VAL:HB	1.87	0.56
9:5I:54:LYS:NZ	9:5I:138:GLU:OE2	2.31	0.56
69:5I:201:PC1:H3C1	27:5b:24:ILE:HD11	1.87	0.56
12:5L:86:SER:O	12:5L:90:ILE:HG12	2.06	0.56
12:5L:459:ILE:HG22	76:5j:101:3PE:H292	1.87	0.56
17:5Q:33:ARG:HH12	17:5Q:77:ASP:HB2	1.70	0.56
14:1N:49:ASN:OD1	14:1N:52:ALA:N	2.37	0.56
14:1N:183:SER:O	14:1N:187:MET:HG2	2.06	0.56
13:5M:355:MET:HE1	13:5M:437:MET:HE3	1.87	0.56
33:5h:69:HIS:NE2	74:5h:202:CDL:OA4	2.32	0.56
43:5r:70:SER:OG	43:5r:72:GLN:NE2	2.34	0.56
13:1M:281:ASP:HB3	13:1M:284:SER:HB3	1.87	0.56
74:1N:401:CDL:OA4	74:1N:401:CDL:O1	2.21	0.56
18:1R:31:ARG:HE	42:1q:125:VAL:HG11	1.71	0.56
46:3B:305:GLN:N	46:3B:305:GLN:OE1	2.39	0.56
49:3E:195:LEU:HD11	49:3E:248:ARG:HD2	1.87	0.56
74:5N:401:CDL:OA4	74:5N:401:CDL:O1	2.22	0.56
7:1G:284:ILE:HG22	7:1G:559:VAL:HG12	1.86	0.56
7:1G:324:ASP:HB3	7:1G:571:ALA:HB1	1.87	0.56
7:1G:352:ALA:HB1	7:1G:652:VAL:HG11	1.89	0.56
9:1I:39:SER:OG	9:1I:43:ARG:NH2	2.32	0.56
47:3C:82:LEU:HD12	47:3C:243:VAL:HG21	1.88	0.56
1:5A:27:LEU:HD22	69:5A:202:PC1:H122	1.87	0.56
7:5G:396:ARG:NH1	7:5G:416:THR:O	2.39	0.56
9:5I:92:ILE:HG12	9:5I:111:ILE:HG12	1.88	0.56
15:5O:52:PRO:O	15:5O:107:GLN:NE2	2.32	0.56
55:8A:463:THR:HA	55:8A:466:MET:HE2	1.87	0.56
10:1J:126:VAL:HG13	25:1Z:122:GLY:HA3	1.88	0.55
13:1M:158:LEU:HD22	14:1N:283:ALA:HB1	1.88	0.55
15:1O:22:SER:OG	15:1O:119:GLY:O	2.24	0.55
16:1P:179:LEU:H	16:1P:179:LEU:HD23	1.71	0.55
23:1X:129:LYS:HD3	27:1b:65:VAL:HG13	1.87	0.55
39:1n:91:GLU:HB2	39:1n:94:GLU:HG3	1.88	0.55
76:3D:502:3PE:H351	49:3E:128:ALA:HB1	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:3R:195:LEU:HB3	49:3R:248:ARG:HH21	1.71	0.55
55:4A:96:ARG:HE	57:4C:11:VAL:HG11	1.70	0.55
6:5F:342:ASP:HB3	6:5F:345:LYS:HB3	1.87	0.55
7:5G:349:PHE:H	7:5G:509:PRO:HB2	1.70	0.55
7:5G:534:ARG:NH1	7:5G:556:MET:O	2.39	0.55
12:5L:209:PRO:HB2	12:5L:213:LEU:HG	1.88	0.55
13:5M:198:ALA:HB2	76:5M:501:3PE:H271	1.86	0.55
55:8A:428:GLN:HA	55:8A:431:LEU:HD12	1.87	0.55
86:8C:304:PGV:H221	86:8C:304:PGV:H31	1.89	0.55
86:8G:101:PGV:H261	86:8G:101:PGV:H92	1.88	0.55
7:1G:575:ASN:ND2	7:1G:577:GLU:OE2	2.39	0.55
69:1M:905:PC1:H292	69:1M:905:PC1:H2D2	1.89	0.55
16:1P:322:ARG:HH21	16:1P:329:SER:HB3	1.71	0.55
24:1Y:36:SER:O	24:1Y:40:ILE:HG13	2.06	0.55
34:1i:47:ASN:O	34:1i:51:GLN:NE2	2.37	0.55
49:3E:197:ASP:N	49:3E:197:ASP:OD1	2.38	0.55
49:3E:261:PRO:HB2	49:3E:273:VAL:HG11	1.86	0.55
56:4B:127:ASP:OD1	56:4B:127:ASP:N	2.38	0.55
86:4G:101:PGV:H162	92:4G:102:PEK:H172	1.87	0.55
2:5B:33:LEU:HD22	69:5B:202:PC1:H381	1.87	0.55
8:5H:204:GLU:HG2	8:5H:279:ARG:HH22	1.71	0.55
57:8C:125:ASN:HB3	57:8C:128:GLU:HG3	1.88	0.55
1:1A:73:LEU:HD23	8:1H:151:LEU:HD12	1.88	0.55
4:1D:100:LEU:HD22	4:1D:195:ARG:HD3	1.88	0.55
6:1F:28:ARG:NH1	44:1s:35:ASN:O	2.39	0.55
12:1L:566:THR:O	12:1L:570:GLN:HG2	2.06	0.55
24:1Y:43:LYS:O	24:1Y:54:ARG:NH2	2.40	0.55
4:5D:377:TYR:HB3	4:5D:390:LYS:HB3	1.88	0.55
5:5E:205:PRO:O	5:5E:207:LYS:NZ	2.33	0.55
7:5G:275:LYS:HA	42:5q:134:ILE:HD13	1.87	0.55
7:5G:638:GLY:O	19:5S:24:GLN:NE2	2.40	0.55
8:5H:98:MET:HG3	8:5H:101:GLY:HA2	1.88	0.55
10:5J:126:VAL:O	25:5Z:120:MET:HE2	2.06	0.55
58:8D:84:THR:HG21	86:8M:101:PGV:H71	1.88	0.55
7:1G:40:PHE:HB2	7:1G:52:CYS:SG	2.47	0.55
12:1L:8:THR:HB	12:1L:82:MET:HE3	1.89	0.55
15:1O:52:PRO:O	15:1O:107:GLN:NE2	2.36	0.55
23:1X:36:ASP:OD1	23:1X:40:LYS:NZ	2.40	0.55
34:1i:92:LYS:HE3	34:1i:95:THR:HG21	1.89	0.55
34:1i:94:TYR:OH	41:1p:10:PRO:O	2.24	0.55
36:1k:32:GLN:NE2	36:1k:32:GLN:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:3R:179:ARG:HB3	49:3R:183:GLU:HB2	1.87	0.55
49:3R:207:LYS:HB2	49:3R:265:PHE:HD2	1.72	0.55
87:4A:604:HEA:H132	87:4A:604:HEA:HHC	1.88	0.55
56:4B:69:PRO:O	56:4B:73:LEU:HD12	2.06	0.55
57:4C:16:TRP:NE1	57:4C:60:ASP:OD2	2.33	0.55
86:4C:304:PGV:H231	86:4C:304:PGV:H271	1.88	0.55
1:5A:13:LEU:HD13	8:5H:10:ILE:HG21	1.87	0.55
6:5F:12:PHE:CE2	6:5F:247:ARG:HG2	2.42	0.55
10:5J:65:LEU:O	10:5J:66:VAL:HG23	2.07	0.55
12:5L:207:GLU:C	12:5L:209:PRO:HD3	2.31	0.55
16:5P:71:MET:HE2	16:5P:83:LYS:HE3	1.89	0.55
55:8A:43:GLN:HG2	55:8A:44:PRO:HD2	1.89	0.55
5:1E:151:ALA:HB1	5:1E:152:PRO:HD2	1.88	0.55
7:1G:396:ARG:NH1	7:1G:416:THR:O	2.39	0.55
11:1K:70:GLU:O	11:1K:74:GLY:N	2.30	0.55
24:1Y:123:LEU:HB3	76:1Y:803:3PE:H261	1.86	0.55
47:3C:196:HIS:HE1	84:3C:502:HEM:ND	2.04	0.55
49:3E:248:ARG:HG3	49:3E:257:ASN:ND2	2.21	0.55
49:3R:205:VAL:HB	49:3R:211:VAL:HG23	1.88	0.55
55:4A:343:GLY:HA2	86:4A:603:PGV:H062	1.87	0.55
55:4A:493:GLU:OE1	55:4A:493:GLU:N	2.21	0.55
60:4F:21:MET:HG3	60:4F:22:MET:HE2	1.88	0.55
14:5N:277:ILE:HD11	24:5Y:132:TRP:HB3	1.86	0.55
16:5P:270:PHE:HD2	16:5P:279:THR:HG22	1.72	0.55
3:1C:33:LEU:HD13	3:1C:60:VAL:HG22	1.88	0.55
4:1D:249:ASP:OD2	4:1D:404:LYS:NZ	2.40	0.55
69:1I:204:PC1:O32	25:1Z:28:ARG:NH1	2.39	0.55
13:1M:203:PHE:O	13:1M:207:MET:HG2	2.06	0.55
20:1T:19:LEU:HB3	20:1T:25:ILE:HG21	1.89	0.55
35:1j:61:ASP:OD1	40:1o:106:ARG:NH1	2.40	0.55
37:1l:124:SER:HA	40:1o:4:LEU:HD21	1.89	0.55
39:1n:56:MET:HA	39:1n:56:MET:HE3	1.88	0.55
46:3O:46:ARG:HG2	46:3O:379:LEU:HD22	1.88	0.55
12:5L:357:ARG:HG2	39:5n:31:VAL:HG22	1.87	0.55
16:5P:97:ARG:NH2	79:5P:402:NDP:O1A	2.36	0.55
16:5P:200:THR:OG1	16:5P:288:HIS:O	2.21	0.55
24:5Y:123:LEU:HB3	76:5Y:803:3PE:H261	1.88	0.55
57:8C:54:MET:HE1	86:8C:307:PGV:H151	1.89	0.55
4:1D:141:PHE:O	4:1D:145:THR:OG1	2.24	0.55
10:1J:132:ASP:N	10:1J:132:ASP:OD1	2.37	0.55
14:1N:153:LEU:O	14:1N:157:MET:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:236:LYS:HD3	14:1N:314:LYS:HB3	1.89	0.55
39:1n:97:LYS:HG2	39:1n:177:PRO:HG3	1.89	0.55
46:3B:86:THR:O	46:3B:90:GLU:HG3	2.07	0.55
47:3C:207:ASN:ND2	47:3C:211:ILE:O	2.32	0.55
51:3T:24:ARG:HG3	51:3T:26:PHE:H	1.71	0.55
86:4C:304:PGV:H221	86:4C:304:PGV:H31	1.89	0.55
5:5E:147:ALA:HB3	5:5E:153:MET:HE3	1.87	0.55
76:5L:704:3PE:H111	76:5L:704:3PE:H2	1.88	0.55
15:5O:25:ILE:HB	15:5O:123:VAL:HG12	1.88	0.55
55:8A:38:ARG:NH1	87:8A:603:HEA:OMA	2.39	0.55
55:8A:477:ALA:HB1	66:8L:18:LYS:HE3	1.88	0.55
5:1E:30:ARG:HG2	44:1s:52:LEU:HB3	1.89	0.55
17:1Q:9:GLN:HB3	22:1W:23:ARG:NH1	2.21	0.55
30:1e:88:GLU:HB2	30:1e:90:LYS:HE2	1.88	0.55
45:3A:24:ARG:HB2	45:3A:196:VAL:HG22	1.89	0.55
47:3P:304:MET:HA	47:3P:304:MET:HE3	1.89	0.55
4:5D:52:GLY:N	4:5D:53:PRO:HD3	2.21	0.55
5:5E:168:ASP:HB3	5:5E:187:ARG:HG2	1.89	0.55
12:5L:584:ILE:HD11	14:5N:58:LYS:HG2	1.88	0.55
14:5N:73:ALA:HB2	14:5N:97:MET:HB3	1.89	0.55
4:1D:352:TYR:HD1	9:1I:86:VAL:HG21	1.72	0.55
7:1G:588:THR:HG21	17:1Q:63:GLU:HA	1.89	0.55
19:1S:82:SER:HB3	19:1S:85:GLN:HG3	1.89	0.55
34:1i:18:ARG:NH1	39:1n:170:VAL:O	2.39	0.55
43:5r:51:ASN:O	43:5r:56:ARG:NH2	2.38	0.55
58:8D:40:LEU:HD21	58:8D:59:LEU:HG	1.88	0.55
1:1A:71:LEU:O	10:1J:147:TYR:OH	2.23	0.55
6:1F:364:PRO:HB2	6:1F:403:THR:HG22	1.88	0.55
8:1H:149:ILE:HG12	8:1H:181:LEU:HD22	1.89	0.55
35:1j:17:LEU:HD23	35:1j:22:LEU:HD21	1.89	0.55
47:3C:229:ILE:HG21	69:3J:101:PC1:H351	1.89	0.55
45:3N:213:GLN:HG3	45:3N:213:GLN:O	2.07	0.55
4:5D:170:MET:HE1	4:5D:304:MET:HE1	1.88	0.55
12:5L:468:ILE:HD11	76:5j:101:3PE:H2I1	1.89	0.55
13:5M:243:MET:O	13:5M:247:THR:HG23	2.06	0.55
76:5d:201:3PE:H2A2	69:5d:202:PC1:H332	1.89	0.55
35:5j:21:GLN:HG3	35:5j:22:LEU:HD12	1.89	0.55
36:5k:32:GLN:NE2	36:5k:32:GLN:O	2.40	0.55
55:8A:418:PHE:HE2	74:8D:201:CDL:HB21	1.71	0.55
56:8B:10:GLN:HE21	56:8B:166:PRO:HB2	1.71	0.55
8:1H:121:TRP:HE1	10:1J:80:PRO:HG2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:430:PHE:HB2	13:1M:433:GLU:HG3	1.88	0.54
46:3B:160:LEU:HD12	49:3I:64:LEU:HD13	1.88	0.54
1:5A:73:LEU:HD23	8:5H:151:LEU:HD12	1.89	0.54
4:5D:352:TYR:HD1	9:5I:86:VAL:HG21	1.72	0.54
5:5E:106:THR:O	5:5E:110:LEU:HG	2.07	0.54
12:5L:193:SER:HB2	12:5L:206:ASN:HD21	1.71	0.54
13:5M:71:TRP:CG	69:5M:505:PC1:H2C2	2.42	0.54
62:8H:27:ARG:NH1	68:8N:42:ASP:OD1	2.40	0.54
8:1H:126:LYS:O	8:1H:126:LYS:HD3	2.08	0.54
49:3E:271:VAL:HG23	49:3E:274:GLY:H	1.71	0.54
11:5K:93:LEU:HD22	14:5N:54:GLU:HB2	1.89	0.54
13:5M:41:LEU:HD13	13:5M:66:LEU:HD13	1.89	0.54
13:5M:442:LEU:HD11	33:5h:25:MET:HE3	1.88	0.54
55:8A:508:PRO:HG3	57:8C:6:HIS:HB3	1.88	0.54
6:1F:202:LYS:HB2	17:1Q:133:LYS:HE3	1.90	0.54
10:1J:170:GLU:OE1	10:1J:173:ARG:NH2	2.41	0.54
74:4D:201:CDL:H171	74:4D:201:CDL:H721	1.90	0.54
86:4M:101:PGV:H321	86:4M:101:PGV:H152	1.88	0.54
8:5H:170:GLU:OE2	23:5X:97:ARG:NH2	2.38	0.54
9:5I:101:ASP:OD1	9:5I:101:ASP:N	2.36	0.54
15:5O:320:LYS:O	29:5d:60:ARG:NH2	2.40	0.54
21:5V:34:LEU:HD13	21:5V:48:GLU:HG2	1.87	0.54
31:5f:49:ARG:HB2	31:5f:52:GLU:HB2	1.89	0.54
57:8C:231:HIS:CD2	86:8C:307:PGV:H042	2.41	0.54
3:1C:120:SER:O	3:1C:120:SER:OG	2.25	0.54
69:1d:202:PC1:H381	30:1e:2:PHE:HE2	1.73	0.54
37:1l:124:SER:O	37:1l:124:SER:OG	2.25	0.54
57:4C:176:LEU:O	57:4C:180:GLU:HG2	2.07	0.54
3:5C:40:VAL:HG22	43:5r:69:MET:HB3	1.88	0.54
10:5J:121:GLY:HA2	11:5K:3:LEU:HD13	1.89	0.54
12:5L:142:ILE:HG21	74:5L:702:CDL:H641	1.89	0.54
12:5L:416:THR:O	12:5L:419:THR:OG1	2.26	0.54
16:5P:63:GLY:HA3	16:5P:68:ILE:HD13	1.90	0.54
57:8C:47:LEU:HD13	86:8C:303:PGV:H12	1.89	0.54
6:1F:68:ARG:HD2	6:1F:254:LYS:HZ3	1.72	0.54
74:1L:702:CDL:H351	33:1h:25:MET:HE2	1.89	0.54
13:1M:382:ILE:HG12	13:1M:396:MET:HE3	1.89	0.54
20:1U:55:GLU:OE1	39:1n:24:ARG:NH1	2.37	0.54
24:1Y:124:VAL:HA	76:1Y:803:3PE:H222	1.89	0.54
51:3T:18:LEU:HD23	51:3T:23:GLN:HB3	1.88	0.54
56:4B:25:ASP:OD2	63:4I:43:ARG:NH1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:5K:1:FME:SD	14:5N:79:LEU:HD21	2.48	0.54
25:5Z:110:VAL:HG13	30:5e:70:LYS:HE2	1.89	0.54
38:5m:7:PRO:HB3	38:5m:13:LEU:HB2	1.90	0.54
57:8C:149:HIS:O	57:8C:153:GLU:HG2	2.08	0.54
58:8D:141:ASP:OD2	58:8D:143:ASN:ND2	2.41	0.54
64:8J:16:ASN:OD1	64:8J:23:LYS:NZ	2.40	0.54
1:1A:18:VAL:HG22	8:1H:222:MET:HE1	1.90	0.54
7:1G:44:GLU:OE1	17:1Q:114:LYS:NZ	2.41	0.54
7:1G:689:LYS:HE2	7:1G:693:GLU:OE2	2.08	0.54
12:1L:73:THR:HG22	41:1p:102:VAL:HG11	1.90	0.54
14:1N:214:ALA:HB2	14:1N:329:MET:HB3	1.89	0.54
14:1N:314:LYS:NZ	15:1O:274:THR:OG1	2.34	0.54
26:1a:64:LYS:HB3	26:1a:68:ASN:HB2	1.89	0.54
45:3N:69:ASN:ND2	45:3N:115:ASP:OD1	2.41	0.54
4:5D:237:ASN:O	8:5H:284:GLN:NE2	2.36	0.54
12:5L:559:GLU:O	12:5L:563:PRO:HD2	2.08	0.54
19:5S:44:LYS:NZ	19:5S:50:LEU:O	2.40	0.54
41:5p:158:GLN:HE21	41:5p:162:MET:HE2	1.73	0.54
4:1D:52:GLY:N	4:1D:53:PRO:HD3	2.22	0.54
5:1E:196:ALA:H	6:1F:264:HIS:HB3	1.72	0.54
14:1N:217:MET:HB3	14:1N:323:MET:HG2	1.90	0.54
15:1O:73:LEU:HD13	15:1O:299:LEU:HD11	1.89	0.54
16:1P:138:ASP:HB3	16:1P:141:SER:HB2	1.90	0.54
2:5B:50:PHE:HE2	2:5B:96:MET:HE2	1.72	0.54
7:5G:364:LEU:HD12	7:5G:491:ASN:HB3	1.90	0.54
15:5O:134:PHE:O	15:5O:138:MET:HG3	2.07	0.54
22:5W:84:ILE:HG22	22:5W:88:MET:HE3	1.88	0.54
29:5d:34:MET:HA	29:5d:34:MET:HE2	1.90	0.54
42:5q:41:GLU:HG3	42:5q:47:LYS:HG3	1.89	0.54
1:1A:79:SER:HA	1:1A:87:MET:HE2	1.90	0.54
13:1M:114:GLU:OE2	13:1M:116:ILE:N	2.41	0.54
36:1k:48:GLU:OE1	36:1k:51:ARG:NH1	2.39	0.54
41:1p:78:GLU:HG2	41:1p:79:LYS:HG2	1.89	0.54
50:3S:35:ASP:OD1	50:3S:89:TYR:OH	2.22	0.54
4:5D:220:PHE:O	4:5D:224:GLU:HG3	2.08	0.54
12:5L:10:THR:HG22	12:5L:14:ILE:HD11	1.90	0.54
21:5V:52:ASN:OD1	21:5V:53:GLU:N	2.41	0.54
24:5Y:40:ILE:HG21	76:5Y:805:3PE:H231	1.90	0.54
40:5o:55:ARG:HH22	41:5p:119:SER:HB3	1.72	0.54
6:1F:247:ARG:HH12	6:1F:321:ALA:HB2	1.72	0.54
13:1M:54:LEU:HD21	33:1h:96:ILE:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:135:LYS:HD2	14:1N:187:MET:SD	2.48	0.54
15:1O:134:PHE:O	15:1O:138:MET:HG3	2.08	0.54
15:1O:280:PRO:HB3	32:1g:25:ARG:HA	1.89	0.54
31:1f:46:ARG:NH2	31:1f:52:GLU:OE1	2.41	0.54
38:1m:41:ARG:O	38:1m:44:ARG:N	2.34	0.54
48:3Q:173:ASP:OD1	48:3Q:173:ASP:N	2.37	0.54
54:3Y:38:TRP:HA	76:3Y:101:3PE:H11	1.90	0.54
57:4C:175:LEU:HD22	86:4C:305:PGV:H221	1.89	0.54
6:5F:17:ASP:N	6:5F:17:ASP:OD1	2.41	0.54
6:5F:191:ALA:HB2	6:5F:203:PRO:HG3	1.88	0.54
19:5S:19:ARG:NH1	19:5S:73:GLU:OE2	2.40	0.54
32:5g:109:GLU:O	41:5p:141:ARG:NH1	2.36	0.54
36:5k:28:LEU:HD11	36:5k:52:TYR:HD2	1.73	0.54
1:1A:41:PHE:HD2	4:1D:51:PHE:HD1	1.56	0.54
4:1D:144:ILE:HG23	4:1D:177:MET:HG2	1.90	0.54
76:1L:703:3PE:H281	74:1h:202:CDL:HB62	1.89	0.54
13:1M:66:LEU:HD11	13:1M:111:THR:HG23	1.89	0.54
23:1X:8:THR:OG1	23:1X:11:ASP:OD1	2.26	0.54
33:1h:41:THR:HG22	74:1h:202:CDL:H711	1.90	0.54
33:1h:84:GLU:O	33:1h:88:GLU:HG2	2.08	0.54
37:1l:127:PRO:HG3	40:1o:3:HIS:CG	2.42	0.54
47:3C:323:CYS:O	47:3C:327:MET:HG3	2.08	0.54
49:3R:180:THR:O	49:3R:182:LYS:N	2.39	0.54
55:4A:72:PRO:O	55:4A:77:GLY:N	2.40	0.54
56:4B:149:THR:HA	56:4B:185:MET:HG2	1.89	0.54
59:4E:70:VAL:HA	59:4E:73:ASP:HB3	1.90	0.54
14:5N:36:ASN:OD1	14:5N:134:GLN:NE2	2.41	0.54
14:5N:44:LEU:HD22	14:5N:122:ILE:HG21	1.89	0.54
55:8A:3:VAL:HA	55:8A:7:LEU:HB2	1.89	0.54
2:1B:49:THR:HG23	2:1B:59:MET:HE3	1.89	0.53
6:1F:193:ILE:HG12	6:1F:215:VAL:HG22	1.90	0.53
20:1U:23:ASP:OD1	36:1k:46:ARG:NH1	2.32	0.53
46:3B:56:ARG:HD2	46:3B:103:GLU:HG2	1.89	0.53
55:4A:32:ALA:HB3	66:4L:36:PRO:HG2	1.90	0.53
74:4B:302:CDL:HB21	74:4B:302:CDL:HB61	1.90	0.53
4:5D:279:ASP:N	4:5D:279:ASP:OD1	2.35	0.53
6:5F:326:GLN:O	6:5F:420:ARG:NH2	2.41	0.53
7:5G:303:VAL:HG22	7:5G:559:VAL:HG21	1.90	0.53
12:5L:213:LEU:HB3	12:5L:273:VAL:HG11	1.90	0.53
12:5L:566:THR:O	12:5L:570:GLN:HG2	2.08	0.53
25:5Z:10:MET:HE2	25:5Z:10:MET:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:126:ASP:OD1	43:1r:56:ARG:NH1	2.38	0.53
7:1G:303:VAL:HG22	7:1G:559:VAL:HG21	1.90	0.53
8:1H:263:THR:O	8:1H:267:THR:OG1	2.22	0.53
74:1L:702:CDL:H311	33:1h:22:LEU:HD22	1.90	0.53
20:1T:12:LYS:NZ	20:1T:74:GLN:OE1	2.41	0.53
46:3B:276:GLN:HG2	46:3B:281:ALA:HB2	1.90	0.53
57:4C:25:LEU:HD23	64:4J:43:THR:HG22	1.90	0.53
74:4C:306:CDL:H322	74:4C:306:CDL:H191	1.89	0.53
60:4F:16:LEU:HD11	60:4F:31:TYR:HE2	1.73	0.53
4:5D:391:ILE:HB	4:5D:430:ARG:HD2	1.90	0.53
13:5M:382:ILE:HA	13:5M:396:MET:HE1	1.91	0.53
76:5M:504:3PE:H3I3	76:5M:504:3PE:H2F2	1.90	0.53
31:5f:31:ASP:HB2	33:5h:89:LYS:HD3	1.88	0.53
32:5g:56:TRP:O	32:5g:60:VAL:HG23	2.09	0.53
4:1D:279:ASP:OD1	4:1D:279:ASP:N	2.40	0.53
7:1G:627:SER:OG	7:1G:629:ASN:ND2	2.42	0.53
9:1I:27:TRP:HB3	9:1I:30:LEU:HD12	1.89	0.53
76:1K:101:3PE:H3C1	76:1K:101:3PE:H2C1	1.90	0.53
24:1Y:16:GLU:HB3	24:1Y:19:ARG:HG3	1.90	0.53
45:3A:279:HIS:ND1	45:3A:284:TYR:OH	2.38	0.53
49:3E:235:TYR:CD1	49:3E:242:HIS:HA	2.43	0.53
57:4C:10:MET:HA	57:4C:10:MET:HE3	1.90	0.53
57:4C:22:LEU:HD22	64:4J:43:THR:HG21	1.90	0.53
86:4C:302:PGV:H162	92:4G:102:PEK:H162	1.89	0.53
1:5A:27:LEU:HD13	69:5A:202:PC1:H132	1.88	0.53
4:5D:181:TYR:O	4:5D:185:SER:OG	2.24	0.53
10:5J:109:LYS:HE2	10:5J:110:GLU:HG2	1.90	0.53
12:5L:25:ASN:H	12:5L:28:LYS:HZ2	1.55	0.53
55:8A:331:ASN:ND2	58:8D:20:ARG:HB2	2.23	0.53
55:8A:338:MET:HE2	55:8A:342:LEU:HG	1.90	0.53
45:3A:131:ARG:HD3	45:3A:175:ARG:HA	1.90	0.53
48:3D:235:LEU:HD13	48:3D:246:ALA:HB1	1.90	0.53
49:3R:219:HIS:O	49:3R:222:CYS:N	2.40	0.53
57:4C:107:ALA:O	86:4C:304:PGV:O05	2.21	0.53
5:5E:51:LEU:HD23	5:5E:69:VAL:HG21	1.89	0.53
12:5L:36:VAL:HG21	12:5L:118:PHE:HB3	1.90	0.53
34:5i:109:ILE:HD11	34:5i:116:ILE:HD11	1.90	0.53
14:1N:239:VAL:HG22	76:1O:401:3PE:H2	1.89	0.53
67:4M:31:GLY:O	67:4M:35:SER:OG	2.19	0.53
1:5A:18:VAL:HG22	8:5H:222:MET:HG3	1.91	0.53
6:5F:208:PRO:HG2	6:5F:213:VAL:HG22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:5H:87:VAL:HG12	8:5H:95:LEU:HD23	1.91	0.53
76:5M:501:3PE:O12	76:5M:501:3PE:N	2.34	0.53
15:5O:94:TYR:OH	15:5O:151:HIS:ND1	2.32	0.53
23:5X:19:VAL:O	26:5a:50:ARG:NH2	2.39	0.53
40:5o:1:GLY:N	83:5o:201:MYR:O1	2.41	0.53
1:1A:92:LEU:O	1:1A:96:ILE:HG12	2.08	0.53
6:1F:21:ILE:HD13	6:1F:230:VAL:HG12	1.91	0.53
6:1F:262:VAL:HG11	6:1F:284:ALA:HB1	1.91	0.53
7:1G:228:ILE:H	7:1G:583:THR:HG22	1.73	0.53
12:1L:203:MET:O	41:1p:121:ARG:NH2	2.31	0.53
12:1L:207:GLU:C	12:1L:209:PRO:HD3	2.33	0.53
74:1L:702:CDL:H562	74:1L:702:CDL:H601	1.89	0.53
14:1N:2:ASN:HB3	14:1N:5:ILE:HD12	1.90	0.53
49:3I:49:VAL:HG21	49:3I:55:LEU:HD13	1.91	0.53
46:3O:51:ILE:HG12	46:3O:204:MET:HG2	1.91	0.53
55:4A:404:THR:O	55:4A:480:ARG:NH1	2.40	0.53
7:5G:105:CYS:N	70:5G:801:SF4:S2	2.81	0.53
14:5N:2:ASN:HB3	14:5N:5:ILE:HD12	1.91	0.53
55:8A:253:MET:HG2	55:8A:396:TRP:HZ3	1.73	0.53
66:8L:14:SER:OG	66:8L:20:ARG:NH1	2.42	0.53
6:1F:102:PRO:HD2	6:1F:302:SER:HB3	1.90	0.53
16:1P:171:ILE:HG12	16:1P:210:VAL:HG21	1.90	0.53
23:1X:12:LEU:HB2	25:1Z:81:ARG:HG2	1.91	0.53
23:1X:27:ALA:O	23:1X:29:HIS:N	2.42	0.53
38:1m:45:GLU:O	38:1m:49:GLN:HG3	2.08	0.53
76:3C:505:3PE:H2A1	49:3R:130:LYS:HA	1.90	0.53
58:4D:122:ARG:HG3	65:4K:53:TRP:CE2	2.44	0.53
3:5C:68:THR:HG21	21:5V:54:LYS:HE3	1.91	0.53
6:5F:297:VAL:HA	6:5F:336:VAL:HA	1.91	0.53
7:5G:278:ARG:NH1	7:5G:568:GLU:OE2	2.42	0.53
12:5L:27:TYR:O	12:5L:115:ASN:ND2	2.40	0.53
15:5O:73:LEU:HD13	15:5O:299:LEU:HD11	1.90	0.53
4:1D:121:ALA:HA	4:1D:365:THR:HG21	1.91	0.53
6:1F:296:ALA:HB1	6:1F:306:LEU:HD12	1.91	0.53
7:1G:110:GLN:HG2	7:1G:114:CYS:HA	1.90	0.53
10:1J:119:PHE:CE1	11:1K:1:FME:HE2	2.44	0.53
16:1P:134:HIS:NE2	16:1P:169:SER:O	2.42	0.53
47:3C:361:ILE:HA	47:3C:365:LEU:HB2	1.91	0.53
45:3N:80:GLU:OE1	46:3O:292:THR:OG1	2.25	0.53
56:4B:1:FME:HE2	56:4B:192:TYR:HA	1.91	0.53
61:4G:61:SER:O	61:4G:61:SER:OG	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5A:49:LEU:HD12	8:5H:126:LYS:HG3	1.91	0.53
4:5D:343:GLU:O	4:5D:347:HIS:ND1	2.39	0.53
12:5L:301:ILE:HD11	12:5L:422:TYR:HB2	1.90	0.53
12:5L:434:LYS:HG3	36:5k:52:TYR:CD1	2.44	0.53
56:8B:143:VAL:HG12	56:8B:219:PHE:HD1	1.72	0.53
86:8C:304:PGV:H231	86:8C:304:PGV:H271	1.90	0.53
4:1D:106:LEU:HD13	4:1D:391:ILE:HG21	1.91	0.53
6:1F:15:LEU:HD13	6:1F:271:GLU:HB2	1.90	0.53
7:1G:320:GLY:O	7:1G:498:SER:OG	2.27	0.53
7:1G:693:GLU:HG3	7:1G:697:ALA:HB2	1.90	0.53
8:1H:99:ASN:N	69:1H:402:PC1:O12	2.38	0.53
13:1M:44:GLN:HB2	32:1g:83:TYR:HE1	1.73	0.53
24:1Y:13:GLU:OE2	24:1Y:20:LYS:NZ	2.42	0.53
24:1Y:35:VAL:HG23	76:1Y:801:3PE:H252	1.91	0.53
24:1Y:40:ILE:HG23	24:1Y:45:PRO:HD3	1.91	0.53
47:3C:246:SER:HB2	47:3C:249:LEU:HB2	1.89	0.53
46:3O:306:PRO:HA	49:3V:52:ARG:HD3	1.90	0.53
57:4C:156:ARG:NH2	57:4C:222:GLN:O	2.41	0.53
86:4G:101:PGV:H261	86:4G:101:PGV:H92	1.91	0.53
8:5H:70:MET:HA	8:5H:73:ILE:HG22	1.89	0.53
8:5H:92:PRO:HD3	8:5H:255:TYR:CD1	2.44	0.53
12:5L:434:LYS:HZ1	36:5k:59:ASN:H	1.56	0.53
74:8D:201:CDL:H171	74:8D:201:CDL:H721	1.91	0.53
7:1G:252:PRO:O	17:1Q:44:ASN:ND2	2.37	0.53
8:1H:91:MET:O	8:1H:93:TYR:N	2.42	0.53
12:1L:584:ILE:HD11	14:1N:58:LYS:HG2	1.89	0.53
13:1M:297:VAL:HG13	13:1M:312:ALA:HB1	1.90	0.53
20:1T:63:PRO:HB2	20:1T:65:ILE:HG22	1.89	0.53
49:3R:143:SER:OG	49:3R:145:ASP:OD1	2.26	0.53
49:3R:235:TYR:HA	49:3R:242:HIS:HA	1.90	0.53
9:5I:54:LYS:HD2	42:5q:90:LEU:HD23	1.91	0.53
13:5M:304:GLN:HE22	41:5p:148:HIS:HD2	1.56	0.53
55:8A:331:ASN:HD22	58:8D:20:ARG:HB2	1.73	0.53
55:8A:336:PRO:HG3	55:8A:411:LYS:HG3	1.90	0.53
90:8I:101:PSC:H261	90:8I:101:PSC:H10	1.90	0.53
6:1F:301:GLY:H	6:1F:333:ALA:HB3	1.74	0.52
12:1L:395:ILE:O	12:1L:399:VAL:HG13	2.09	0.52
24:1Y:140:VAL:O	33:1h:115:ARG:NH1	2.42	0.52
48:3D:247:ILE:HG12	48:3D:249:MET:H	1.73	0.52
49:3R:265:PHE:HA	49:3R:271:VAL:HG12	1.91	0.52
1:5A:24:LEU:HD21	69:5B:202:PC1:H3C2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5D:121:ALA:HA	4:5D:365:THR:HG21	1.91	0.52
7:5G:551:ASP:OD2	7:5G:679:ARG:NE	2.42	0.52
55:8A:243:VAL:HG13	87:8A:604:HEA:C3C	2.39	0.52
59:8E:102:GLU:CD	59:8E:102:GLU:H	2.15	0.52
12:1L:331:MET:HG3	12:1L:391:SER:HB3	1.90	0.52
13:1M:44:GLN:H	32:1g:83:TYR:HD1	1.55	0.52
20:1T:35:HIS:CE1	20:1T:37:MET:HE3	2.44	0.52
47:3P:25:SER:OG	47:3P:216:ASP:OD2	2.22	0.52
47:3P:361:ILE:HA	47:3P:365:LEU:HB2	1.90	0.52
49:3R:219:HIS:ND1	49:3R:239:HIS:CE1	2.77	0.52
56:4B:198:GLU:O	56:4B:204:HIS:CE1	2.62	0.52
57:4C:34:TRP:HZ3	92:4C:308:PEK:H272	1.74	0.52
6:5F:378:ARG:NH1	6:5F:383:ASP:O	2.41	0.52
8:5H:81:LEU:HA	8:5H:84:THR:HG22	1.90	0.52
55:8A:287:VAL:HG21	55:8A:312:ILE:HD11	1.91	0.52
12:1L:142:ILE:HG12	13:1M:370:PRO:HB2	1.92	0.52
12:1L:290:LEU:O	12:1L:523:SER:OG	2.27	0.52
15:1O:133:VAL:HG23	15:1O:205:ALA:HB3	1.91	0.52
29:1d:34:MET:HE2	29:1d:34:MET:HA	1.91	0.52
40:1o:29:GLY:HA3	40:1o:103:ARG:NH2	2.24	0.52
40:1o:75:ASN:HB2	41:1p:23:THR:HG21	1.91	0.52
68:4N:71:ASP:OD2	68:4N:74:LYS:HB2	2.09	0.52
8:5H:266:LEU:O	8:5H:269:THR:OG1	2.25	0.52
56:8B:69:PRO:O	56:8B:73:LEU:HG	2.09	0.52
57:8C:34:TRP:HZ3	92:8C:308:PEK:H272	1.73	0.52
86:8C:303:PGV:H51	61:8G:69:LEU:HD21	1.90	0.52
58:8D:72:ASN:HB2	74:8D:201:CDL:H832	1.91	0.52
1:1A:39:CYS:O	4:1D:53:PRO:HD2	2.10	0.52
3:1C:79:THR:OG1	3:1C:93:VAL:HB	2.09	0.52
6:1F:21:ILE:HG22	6:1F:233:THR:HG21	1.90	0.52
10:1J:130:THR:HG22	25:1Z:121:MET:HE2	1.90	0.52
12:1L:495:ILE:O	12:1L:499:MET:HG3	2.10	0.52
16:1P:97:ARG:NH1	79:1P:501:NDP:O3X	2.40	0.52
39:1n:94:GLU:HA	39:1n:97:LYS:HG3	1.91	0.52
47:3C:24:PRO:HB2	47:3C:27:ILE:HG23	1.90	0.52
12:5L:2:ASN:HB2	12:5L:3:PRO:HD2	1.91	0.52
15:5O:180:GLN:O	15:5O:184:GLN:HG2	2.10	0.52
20:5U:35:HIS:CE1	20:5U:37:MET:HB2	2.45	0.52
57:8C:122:HIS:CE1	61:8G:45:PRO:HB3	2.44	0.52
6:1F:403:THR:OG1	6:1F:405:CYS:O	2.28	0.52
7:1G:198:ASN:OD1	7:1G:268:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1K:48:ILE:HG23	11:1K:53:PHE:HB3	1.92	0.52
13:1M:133:ILE:HD11	13:1M:231:LEU:HD11	1.92	0.52
13:1M:425:ASN:HB2	38:1m:57:GLY:HA2	1.90	0.52
14:1N:104:MET:HG3	14:1N:111:PHE:HB3	1.92	0.52
15:1O:315:LYS:HD3	15:1O:316:TRP:H	1.73	0.52
52:3H:49:CYS:HA	52:3H:52:ILE:HD13	1.92	0.52
67:4M:12:PRO:HG3	86:4M:101:PGV:H202	1.90	0.52
7:5G:352:ALA:HB1	7:5G:652:VAL:HG11	1.90	0.52
12:5L:576:MET:HG2	76:5Y:801:3PE:H32	1.91	0.52
35:5j:42:HIS:NE2	36:5k:84:GLU:OE2	2.35	0.52
56:8B:51:THR:O	59:8E:74:LYS:NZ	2.43	0.52
67:8M:11:SER:HB3	67:8M:14:GLU:HG3	1.91	0.52
68:8N:81:ASP:N	68:8N:81:ASP:OD1	2.40	0.52
6:1F:125:GLY:O	6:1F:129:MET:HG3	2.10	0.52
8:1H:104:PHE:O	8:1H:108:MET:HG2	2.10	0.52
12:1L:345:SER:HB2	12:1L:450:LEU:HD11	1.92	0.52
12:1L:536:LEU:HB3	12:1L:537:PRO:HD3	1.92	0.52
76:1M:902:3PE:H31	14:1N:276:ILE:HG21	1.91	0.52
17:1Q:60:ASP:OD2	17:1Q:62:ARG:NH1	2.42	0.52
25:1Z:27:ARG:NH1	25:1Z:27:ARG:HB2	2.25	0.52
32:1g:25:ARG:NH1	32:1g:25:ARG:HB2	2.25	0.52
39:1n:55:ASP:OD1	39:1n:57:VAL:HG12	2.09	0.52
45:3A:210:ASP:OD1	45:3A:211:LEU:N	2.43	0.52
57:4C:81:TYR:O	57:4C:85:LEU:HD12	2.10	0.52
74:4C:306:CDL:H822	74:4C:306:CDL:H612	1.92	0.52
10:5J:100:GLU:OE1	10:5J:104:VAL:HG13	2.09	0.52
11:5K:48:ILE:HD11	11:5K:59:MET:HE3	1.91	0.52
76:5M:502:3PE:H391	76:5M:502:3PE:H291	1.91	0.52
3:1C:179:GLU:OE1	16:1P:40:ARG:NH2	2.38	0.52
5:1E:146:GLY:HA3	6:1F:142:PHE:HZ	1.74	0.52
15:1O:200:GLN:NE2	15:1O:204:ASN:OD1	2.43	0.52
38:1m:18:ASP:HB3	38:1m:21:GLU:HB2	1.91	0.52
46:3B:37:SER:HB3	46:3B:216:LEU:HD12	1.92	0.52
47:3C:124:MET:HG2	47:3C:274:PHE:HE1	1.73	0.52
74:3C:503:CDL:OA7	74:3C:503:CDL:O1	2.28	0.52
56:4B:158:ASP:OD1	56:4B:159:VAL:N	2.40	0.52
4:5D:34:ASN:HD22	15:5O:158:VAL:HA	1.74	0.52
5:5E:149:VAL:HG23	6:5F:105:CYS:SG	2.50	0.52
13:5M:154:LEU:HD11	14:5N:254:LEU:HD21	1.91	0.52
19:5S:41:VAL:HG12	19:5S:45:LYS:HD2	1.90	0.52
69:5d:202:PC1:H381	30:5e:2:PHE:HE2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:8G:72:ASN:HB3	61:8G:75:VAL:HG12	1.90	0.52
3:1C:83:VAL:HG12	3:1C:85:THR:HG22	1.92	0.52
6:1F:151:VAL:HG13	44:1s:54:LEU:HD11	1.90	0.52
49:3E:241:SER:HA	49:3E:249:ILE:HG13	1.92	0.52
68:4N:44:CYS:HB2	68:4N:53:PRO:HG3	1.92	0.52
4:5D:106:LEU:HD13	4:5D:391:ILE:HG21	1.92	0.52
8:5H:215:TYR:HD1	8:5H:219:PRO:HB2	1.74	0.52
12:5L:600:THR:HG22	12:5L:601:LEU:N	2.18	0.52
16:5P:59:LEU:HD23	16:5P:62:MET:HE3	1.91	0.52
20:5U:22:TYR:CE2	20:5U:24:LYS:HD2	2.45	0.52
1:1A:21:ALA:HB1	8:1H:218:GLY:HA3	1.91	0.52
3:1C:173:GLU:HG3	3:1C:188:VAL:HA	1.91	0.52
7:1G:103:LEU:O	18:1R:86:TYR:OH	2.19	0.52
7:1G:252:PRO:HB3	7:1G:263:ILE:HG23	1.91	0.52
13:1M:283:LYS:HB2	13:1M:340:ARG:HD2	1.92	0.52
74:3A:501:CDL:H151	74:3A:501:CDL:H321	1.91	0.52
49:3E:143:SER:OG	49:3E:145:ASP:OD1	2.27	0.52
47:3P:91:PHE:HA	47:3P:94:LEU:HB2	1.91	0.52
2:5B:30:VAL:HG13	2:5B:173:LEU:HB3	1.91	0.52
4:5D:7:ASP:OD1	4:5D:7:ASP:N	2.41	0.52
6:5F:253:THR:OG1	6:5F:269:GLU:OE2	2.26	0.52
7:5G:524:LEU:HD13	7:5G:543:ILE:HG23	1.92	0.52
57:8C:64:GLU:HA	57:8C:68:GLN:HB2	1.91	0.52
74:8C:306:CDL:H212	74:8C:306:CDL:H311	1.91	0.52
2:1B:68:ASP:O	2:1B:71:ARG:HG2	2.09	0.52
12:1L:357:ARG:HG2	39:1n:31:VAL:HG22	1.92	0.52
14:1N:8:THR:O	14:1N:12:THR:OG1	2.25	0.52
76:1O:401:3PE:H3I3	76:1O:401:3PE:H2F2	1.91	0.52
16:1P:173:GLY:H	16:1P:176:ASP:HB3	1.74	0.52
48:3D:232:ARG:NE	49:3R:237:PRO:O	2.42	0.52
47:3P:24:PRO:HB2	47:3P:27:ILE:HG23	1.92	0.52
49:3R:125:VAL:HG21	69:3R:302:PC1:H361	1.92	0.52
86:4A:603:PGV:H81	74:4D:201:CDL:H361	1.92	0.52
56:4B:89:GLU:OE2	68:4N:68:VAL:N	2.42	0.52
16:5P:165:ILE:HB	16:5P:227:THR:HG23	1.91	0.52
17:5Q:9:GLN:HB3	22:5W:23:ARG:NH1	2.25	0.52
17:5Q:23:THR:HG23	17:5Q:25:VAL:HG23	1.92	0.52
55:8A:459:PHE:HB3	58:8D:92:THR:HG23	1.92	0.52
7:1G:362:TYR:O	7:1G:494:HIS:NE2	2.40	0.51
23:1X:19:VAL:O	26:1a:50:ARG:NH2	2.40	0.51
29:1d:62:LEU:O	29:1d:66:THR:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3C:112:THR:O	47:3C:196:HIS:NE2	2.43	0.51
54:3Y:12:GLU:HA	54:3Y:15:ARG:HG2	1.92	0.51
55:4A:264:LYS:NZ	55:4A:326:THR:O	2.31	0.51
57:4C:80:ARG:NH1	57:4C:236:GLU:OE1	2.42	0.51
3:5C:8:ARG:NH1	43:5r:61:GLU:OE2	2.39	0.51
4:5D:34:ASN:HB3	15:5O:158:VAL:HG13	1.91	0.51
7:5G:319:ALA:HB3	7:5G:345:THR:HG22	1.91	0.51
15:5O:195:THR:HG23	15:5O:198:TYR:H	1.73	0.51
22:5W:22:SER:HB3	22:5W:31:ARG:HH22	1.75	0.51
23:5X:75:ARG:HG2	23:5X:76:HIS:HD2	1.75	0.51
30:5e:43:ALA:O	33:5h:127:THR:OG1	2.23	0.51
34:5i:28:SER:HB2	34:5i:31:GLU:HG3	1.93	0.51
10:1J:52:LEU:N	10:1J:139:GLU:OE2	2.36	0.51
31:1f:32:GLU:OE2	31:1f:57:LYS:NZ	2.43	0.51
39:1n:104:ASP:OD1	39:1n:121:ARG:NH2	2.40	0.51
59:4E:30:ARG:O	59:4E:34:ASN:ND2	2.42	0.51
6:5F:392:LEU:HD12	6:5F:395:ILE:HD11	1.92	0.51
14:5N:95:MET:HE2	14:5N:149:ILE:HG12	1.92	0.51
14:5N:218:LEU:HD22	14:5N:240:ILE:HG23	1.93	0.51
55:8A:240:HIS:CD2	55:8A:244:TYR:HE2	2.28	0.51
55:8A:460:ILE:HG12	58:8D:92:THR:HG21	1.91	0.51
1:1A:13:LEU:HD13	8:1H:10:ILE:HG21	1.90	0.51
2:1B:92:LEU:HD11	2:1B:97:ALA:HA	1.92	0.51
4:1D:227:GLU:OE2	9:1I:32:ARG:NE	2.44	0.51
4:1D:246:THR:HB	4:1D:249:ASP:HB2	1.92	0.51
37:1l:7:ASP:OD1	37:1l:7:ASP:N	2.44	0.51
45:3N:193:PRO:HG2	39:5n:55:ASP:HB2	1.91	0.51
49:3R:179:ARG:HH21	49:3R:184:ILE:HA	1.74	0.51
50:3S:84:GLU:CD	50:3S:84:GLU:H	2.17	0.51
55:4A:117:MET:HG3	64:4J:54:SER:HB2	1.92	0.51
56:4B:25:ASP:OD1	63:4I:35:TYR:OH	2.24	0.51
58:4D:67:SER:N	58:4D:70:GLU:OE2	2.41	0.51
8:5H:197:PRO:HD2	8:5H:198:PHE:CD2	2.45	0.51
12:5L:253:VAL:HB	12:5L:310:LEU:HD11	1.92	0.51
69:5L:705:PC1:H262	24:5Y:112:ALA:HB2	1.92	0.51
20:5T:60:PHE:HE1	20:5T:80:ILE:HG23	1.75	0.51
20:5T:84:LYS:HG3	20:5T:86:VAL:HG23	1.92	0.51
20:5U:48:VAL:HG21	39:5n:16:LEU:HD12	1.92	0.51
32:5g:107:LEU:HD23	32:5g:107:LEU:H	1.74	0.51
37:5l:18:GLU:OE1	37:5l:18:GLU:N	2.27	0.51
3:1C:33:LEU:HD23	21:1V:98:PRO:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1J:109:LYS:NZ	10:1J:110:GLU:OE1	2.42	0.51
76:1M:901:3PE:H111	76:1M:901:3PE:H2	1.92	0.51
37:1L:130:PRO:HG3	40:1o:22:PRO:HD3	1.91	0.51
39:1n:116:ASP:OD1	39:1n:117:TYR:N	2.43	0.51
86:4B:301:PGV:H202	86:4C:304:PGV:H62	1.92	0.51
58:4D:141:ASP:O	58:4D:143:ASN:N	2.43	0.51
6:5F:150:GLN:HE22	6:5F:177:VAL:HB	1.75	0.51
14:5N:278:MET:O	14:5N:282:MET:HG3	2.10	0.51
2:1B:90:GLY:HA2	70:1B:201:SF4:S4	2.51	0.51
7:1G:157:THR:HB	7:1G:161:ARG:HE	1.75	0.51
12:1L:188:TRP:CD2	12:1L:212:PRO:HG3	2.45	0.51
15:1O:34:GLY:N	77:1O:402:GTP:O3G	2.39	0.51
30:1e:4:ASP:OD2	30:1e:7:LYS:HB3	2.11	0.51
38:1m:122:GLN:O	41:1p:139:GLN:NE2	2.27	0.51
48:3Q:33:TYR:CD1	48:3Q:37:CYS:HB2	2.45	0.51
86:4A:603:PGV:H312	74:4D:201:CDL:H462	1.91	0.51
74:4C:306:CDL:H401	74:4C:306:CDL:H342	1.92	0.51
58:4D:23:PRO:HB2	58:4D:24:LEU:HD12	1.92	0.51
58:4D:87:PHE:HD1	65:4K:21:GLY:HA2	1.74	0.51
5:5E:40:GLU:HB2	44:5s:67:SER:HA	1.92	0.51
13:5M:131:ILE:HD12	14:5N:302:LEU:HD21	1.91	0.51
34:5i:18:ARG:NH1	39:5n:170:VAL:O	2.43	0.51
55:8A:176:MET:HE3	55:8A:181:THR:HG22	1.92	0.51
6:1F:297:VAL:HG22	6:1F:336:VAL:HG12	1.92	0.51
7:1G:105:CYS:HA	7:1G:108:CYS:CB	2.37	0.51
76:1L:703:3PE:N	69:1M:905:PC1:O12	2.43	0.51
13:1M:65:LEU:O	13:1M:69:THR:HG23	2.11	0.51
16:1P:166:ILE:HG22	16:1P:168:PRO:HD3	1.92	0.51
25:1Z:86:MET:HB2	25:1Z:124:LEU:HD22	1.92	0.51
45:3A:91:THR:HG23	45:3A:93:GLU:H	1.76	0.51
48:3D:156:VAL:HG21	48:3D:180:PRO:HG2	1.92	0.51
45:3N:210:ASP:OD1	45:3N:211:LEU:N	2.44	0.51
76:3Q:502:3PE:H361	49:3R:128:ALA:HB1	1.92	0.51
74:4B:302:CDL:H412	74:4B:302:CDL:H661	1.91	0.51
4:5D:94:LYS:HD2	4:5D:102:TYR:HE2	1.74	0.51
7:5G:537:LEU:HD13	7:5G:543:ILE:HD11	1.92	0.51
76:5L:703:3PE:H281	74:5h:202:CDL:HB62	1.92	0.51
15:5O:184:GLN:HA	15:5O:192:MET:SD	2.51	0.51
20:5U:55:GLU:OE2	39:5n:20:LYS:NZ	2.42	0.51
32:5g:63:PHE:O	32:5g:67:SER:HB2	2.11	0.51
62:8H:57:ARG:O	62:8H:61:LYS:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:124:ASN:C	8:1H:126:LYS:H	2.18	0.51
8:1H:126:LYS:HA	8:1H:126:LYS:HE3	1.92	0.51
8:1H:197:PRO:HD2	8:1H:198:PHE:CD2	2.46	0.51
34:1i:9:LEU:HG	34:1i:13:GLN:HE21	1.74	0.51
37:1l:54:SER:HA	37:1l:84:TYR:HB3	1.93	0.51
40:1o:24:PHE:HD2	40:1o:107:LEU:HD13	1.75	0.51
52:3H:92:ASP:HA	52:3H:95:VAL:HG12	1.92	0.51
1:5A:11:VAL:O	1:5A:15:SER:OG	2.28	0.51
7:5G:144:PRO:HD2	7:5G:192:MET:HE1	1.90	0.51
13:5M:12:LEU:HB2	13:5M:13:PRO:HD3	1.93	0.51
74:8C:306:CDL:H342	74:8C:306:CDL:H401	1.92	0.51
4:1D:343:GLU:O	4:1D:347:HIS:ND1	2.43	0.51
5:1E:37:ASN:C	44:1s:65:GLN:HE22	2.17	0.51
5:1E:165:THR:OG1	5:1E:168:ASP:OD1	2.24	0.51
6:1F:150:GLN:NE2	44:1s:55:ASN:OD1	2.44	0.51
11:1K:1:FME:SD	14:1N:79:LEU:HD21	2.51	0.51
37:1l:158:ILE:HD12	40:1o:103:ARG:HD2	1.91	0.51
64:4J:52:TRP:O	64:4J:57:HIS:ND1	2.44	0.51
69:5B:202:PC1:H3D2	8:5H:56:VAL:HG21	1.93	0.51
4:5D:2:ARG:NH1	32:5g:29:ASP:O	2.44	0.51
7:5G:366:THR:HG22	7:5G:370:GLY:HA3	1.93	0.51
20:5U:37:MET:HE3	20:5U:71:MET:HE1	1.93	0.51
23:5X:23:VAL:HG21	26:5a:65:GLY:HA2	1.93	0.51
23:5X:82:THR:HA	23:5X:85:TRP:NE1	2.26	0.51
57:8C:175:LEU:HD22	86:8C:305:PGV:H221	1.93	0.51
6:1F:264:HIS:HD2	6:1F:285:GLY:HA3	1.74	0.51
8:1H:81:LEU:HA	8:1H:84:THR:HG22	1.93	0.51
12:1L:261:ILE:HD12	12:1L:326:PHE:HB2	1.92	0.51
19:1S:87:THR:O	19:1S:90:LEU:N	2.39	0.51
20:1U:51:ILE:O	20:1U:55:GLU:HG3	2.10	0.51
23:1X:136:LEU:HD23	23:1X:137:PRO:HD2	1.93	0.51
45:3N:240:GLU:HG3	45:3N:422:VAL:HB	1.92	0.51
45:3N:269:PRO:HB2	45:3N:410:VAL:HG11	1.92	0.51
56:4B:142:VAL:HG12	56:4B:144:LEU:HG	1.92	0.51
56:4B:145:PRO:HA	56:4B:214:VAL:O	2.10	0.51
57:4C:247:VAL:HG21	74:4C:306:CDL:H842	1.93	0.51
58:4D:54:ASP:OD1	58:4D:54:ASP:N	2.43	0.51
59:4E:65:VAL:HA	59:4E:68:LEU:HD12	1.93	0.51
6:5F:193:ILE:HG12	6:5F:215:VAL:HG22	1.93	0.51
9:5I:135:PRO:HD3	9:5I:165:ILE:HG22	1.93	0.51
10:5J:18:VAL:HG22	11:5K:14:ILE:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:5J:86:ASN:OD1	10:5J:88:THR:N	2.33	0.51
12:5L:553:LEU:HD11	38:5m:93:GLY:HA3	1.93	0.51
59:8E:33:MET:HG2	59:8E:67:ILE:HG22	1.93	0.51
2:1B:25:ARG:HD3	2:1B:27:GLU:HB2	1.93	0.51
7:1G:43:HIS:NE2	7:1G:261:GLU:OE2	2.36	0.51
8:1H:24:GLU:OE2	8:1H:274:ARG:NH1	2.44	0.51
21:1V:4:LEU:HD23	21:1V:4:LEU:H	1.76	0.51
26:1a:52:ARG:NH1	26:1a:58:ASN:OD1	2.44	0.51
47:3P:43:LEU:O	47:3P:47:THR:OG1	2.27	0.51
55:4A:386:VAL:O	55:4A:390:MET:HG2	2.11	0.51
1:5A:71:LEU:O	10:5J:147:TYR:OH	2.25	0.51
5:5E:84:ALA:HA	5:5E:90:TYR:CD2	2.46	0.51
74:5L:702:CDL:H601	74:5L:702:CDL:H562	1.93	0.51
13:5M:391:ILE:HG23	13:5M:394:ILE:HD12	1.93	0.51
74:5h:202:CDL:OB3	34:5i:88:HIS:NE2	2.39	0.51
9:1I:112:ASP:OD1	9:1I:114:THR:OG1	2.28	0.50
15:1O:63:THR:OG1	15:1O:302:ARG:NH2	2.43	0.50
20:1T:13:ASP:OD1	20:1T:14:ARG:N	2.43	0.50
20:1T:18:VAL:HA	20:1T:21:LEU:HD12	1.92	0.50
23:1X:126:LYS:HE3	27:1b:66:PRO:HG3	1.92	0.50
74:1X:201:CDL:HA21	74:1X:201:CDL:H541	1.94	0.50
37:1l:158:ILE:HG12	40:1o:99:LYS:HB3	1.94	0.50
41:1p:5:ASP:HB3	41:1p:8:VAL:HG12	1.92	0.50
46:3O:56:ARG:HD2	46:3O:103:GLU:HG2	1.93	0.50
48:3Q:195:GLU:OE2	48:3Q:201:ARG:NE	2.44	0.50
56:4B:143:VAL:HG12	56:4B:219:PHE:HD1	1.75	0.50
58:4D:33:LEU:HB3	58:4D:38:LYS:HG2	1.92	0.50
6:5F:337:MET:HG2	6:5F:341:THR:HG21	1.93	0.50
10:5J:119:PHE:CD1	11:5K:6:MET:HB2	2.46	0.50
12:5L:495:ILE:O	12:5L:499:MET:HG3	2.11	0.50
74:5L:702:CDL:H311	33:5h:22:LEU:HD22	1.93	0.50
19:5S:36:ILE:HA	19:5S:40:TYR:HB2	1.93	0.50
20:5U:54:MET:HG3	20:5U:76:ILE:HG21	1.92	0.50
24:5Y:124:VAL:HA	76:5Y:803:3PE:H222	1.92	0.50
55:8A:25:TRP:HB2	86:8L:101:PGV:H281	1.93	0.50
2:1B:63:ALA:HB1	2:1B:76:PHE:CE1	2.45	0.50
7:1G:470:VAL:HG12	7:1G:490:MET:HE1	1.92	0.50
20:1T:76:ILE:O	20:1T:80:ILE:HG12	2.10	0.50
34:1i:50:LEU:HD12	34:1i:57:LYS:HG2	1.93	0.50
47:3P:344:GLU:OE1	47:3P:344:GLU:HA	2.10	0.50
48:3Q:216:LEU:HB3	74:3T:101:CDL:H562	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:3R:214:ILE:HB	49:3R:259:GLU:HB3	1.92	0.50
55:4A:171:MET:HG2	57:4C:8:TYR:CE2	2.45	0.50
66:4L:22:LEU:O	66:4L:26:THR:HG22	2.11	0.50
7:5G:46:LEU:O	17:5Q:116:LYS:NZ	2.39	0.50
7:5G:103:LEU:O	18:5R:86:TYR:OH	2.22	0.50
16:5P:200:THR:HB	16:5P:238:LEU:HB2	1.92	0.50
18:5R:1:GLY:N	18:5R:42:ASP:OD2	2.32	0.50
76:5Y:806:3PE:O12	76:5Y:806:3PE:N	2.38	0.50
57:8C:45:LEU:HD11	64:8J:38:LEU:HD22	1.92	0.50
58:8D:78:TRP:CD1	74:8D:201:CDL:H202	2.47	0.50
64:8J:33:ARG:O	64:8J:37:THR:HG22	2.10	0.50
1:1A:49:LEU:HB2	8:1H:126:LYS:HD2	1.94	0.50
7:1G:26:VAL:HB	7:1G:68:ALA:HA	1.93	0.50
7:1G:223:ARG:NH2	17:1Q:81:ASN:OD1	2.29	0.50
10:1J:167:VAL:HG22	14:1N:42:PRO:HG2	1.93	0.50
11:1K:47:ILE:HG12	14:1N:79:LEU:HD13	1.92	0.50
45:3N:40:TRP:CZ2	45:3N:377:GLU:HA	2.46	0.50
47:3P:237:LEU:HD22	48:3Q:216:LEU:HD11	1.94	0.50
58:4D:87:PHE:CD2	86:4M:101:PGV:H142	2.46	0.50
59:4E:14:ARG:HG2	59:4E:14:ARG:HH11	1.77	0.50
1:5A:39:CYS:O	4:5D:53:PRO:HD2	2.11	0.50
5:5E:14:GLU:O	5:5E:19:THR:OG1	2.29	0.50
7:5G:13:VAL:HB	7:5G:33:VAL:HG21	1.93	0.50
8:5H:311:THR:HB	25:5Z:51:MET:HE2	1.92	0.50
13:5M:1:FME:HE3	13:5M:111:THR:HG21	1.93	0.50
13:5M:101:LEU:HD13	76:5M:502:3PE:H2H1	1.94	0.50
29:5d:89:ASP:HB2	33:5h:121:PRO:HG2	1.93	0.50
32:5g:67:SER:OG	33:5h:28:TYR:O	2.24	0.50
38:5m:19:PRO:HA	38:5m:22:TYR:CE2	2.46	0.50
43:5r:104:GLU:N	43:5r:104:GLU:OE2	2.45	0.50
55:8A:362:SER:HB2	56:8B:20:LEU:HD21	1.92	0.50
57:8C:202:GLY:HA3	92:8C:308:PEK:H31	1.93	0.50
6:1F:262:VAL:HG23	6:1F:336:VAL:HG21	1.93	0.50
6:1F:300:GLY:O	6:1F:304:THR:OG1	2.28	0.50
12:1L:231:PRO:HB3	12:1L:530:PRO:HG3	1.93	0.50
13:1M:24:TRP:CD2	13:1M:81:GLN:HB3	2.47	0.50
14:1N:217:MET:HE1	14:1N:324:LYS:O	2.12	0.50
39:1n:13:GLN:O	39:1n:17:ARG:HG2	2.11	0.50
46:3B:435:PHE:H	46:3B:438:GLU:HG2	1.76	0.50
49:3E:156:LEU:HG	49:3E:157:SER:H	1.77	0.50
86:4C:301:PGV:H242	86:4C:301:PGV:H22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5B:62:MET:HE1	2:5B:160:ILE:HG13	1.93	0.50
9:5I:164:GLU:HG3	42:5q:88:ARG:HD3	1.94	0.50
10:5J:167:VAL:HG22	14:5N:42:PRO:HG2	1.94	0.50
21:5V:71:LEU:HD13	21:5V:79:VAL:HG11	1.94	0.50
24:5Y:35:VAL:HG23	76:5Y:801:3PE:H252	1.94	0.50
55:8A:64:VAL:HA	55:8A:68:PHE:HD2	1.76	0.50
57:8C:76:GLN:HE21	57:8C:231:HIS:CE1	2.29	0.50
64:8J:2:GLU:OE1	64:8J:4:ARG:NH2	2.44	0.50
69:1L:704:PC1:H342	24:1Y:109:ILE:HG23	1.93	0.50
17:1Q:69:LEU:HG	17:1Q:70:MET:HG2	1.92	0.50
29:1d:99:GLU:OE1	29:1d:99:GLU:N	2.34	0.50
32:1g:50:ASP:HB3	32:1g:53:VAL:HG22	1.94	0.50
34:1i:86:LYS:HE3	34:1i:87:TYR:CE1	2.46	0.50
45:3N:242:ARG:NH2	45:3N:432:PRO:O	2.43	0.50
45:3N:298:ALA:HA	45:3N:303:LEU:HB2	1.92	0.50
56:4B:104:TRP:CG	56:4B:203:ASN:HB2	2.47	0.50
2:5B:90:GLY:HA2	70:5B:201:SF4:S4	2.52	0.50
7:5G:655:GLN:OE1	7:5G:655:GLN:N	2.28	0.50
12:5L:576:MET:HG2	76:5Y:801:3PE:H12	1.94	0.50
15:5O:35:LYS:NZ	15:5O:53:GLU:OE1	2.42	0.50
18:5R:54:SER:OG	18:5R:56:VAL:O	2.29	0.50
55:8A:277:MET:HE2	55:8A:319:LYS:NZ	2.26	0.50
61:8G:36:TRP:CZ3	86:8G:101:PGV:H292	2.47	0.50
6:1F:47:GLU:OE1	6:1F:47:GLU:N	2.40	0.50
7:1G:522:LEU:HD22	7:1G:537:LEU:HD11	1.92	0.50
12:1L:576:MET:HG2	76:1Y:801:3PE:H12	1.94	0.50
13:1M:25:ILE:HG23	32:1g:60:VAL:HG21	1.94	0.50
19:1S:22:LEU:HD23	19:1S:32:VAL:HG22	1.93	0.50
33:1h:19:ARG:O	33:1h:23:LYS:HG3	2.11	0.50
37:1l:82:ASP:OD1	37:1l:82:ASP:N	2.45	0.50
46:3O:350:GLY:HA2	46:3O:411:ILE:HD13	1.93	0.50
52:3U:31:ILE:O	52:3U:35:GLU:HG2	2.11	0.50
55:4A:208:MET:HE1	57:4C:100:ALA:CB	2.42	0.50
56:4B:100:MET:HE2	62:4H:65:PRO:HB3	1.92	0.50
57:4C:252:LEU:HD22	57:4C:256:ILE:HD11	1.94	0.50
74:4C:306:CDL:H141	74:4C:306:CDL:H541	1.93	0.50
4:5D:234:ILE:HD12	8:5H:277:TYR:HB3	1.93	0.50
34:5i:71:VAL:HA	34:5i:75:LEU:HB2	1.94	0.50
43:5r:11:ARG:HB3	43:5r:19:LEU:HD21	1.93	0.50
9:1I:132:VAL:HG11	9:1I:169:ILE:HD11	1.94	0.50
11:1K:55:LEU:HG	30:1e:25:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:510:TYR:HB3	64:4J:18:LEU:HD11	1.94	0.50
12:1L:591:PHE:CE1	14:1N:111:PHE:HA	2.47	0.50
41:1p:26:PRO:HB2	41:1p:31:TYR:HE2	1.77	0.50
55:4A:13:LYS:HE2	55:4A:500:PRO:HB2	1.92	0.50
55:4A:86:MET:HE3	55:4A:182:PRO:HB2	1.93	0.50
68:4N:67:ALA:HB1	68:4N:70:VAL:HG12	1.93	0.50
1:5A:1:FME:HE3	1:5A:4:MET:HE3	1.94	0.50
2:5B:42:ARG:NH1	69:5B:203:PC1:O12	2.45	0.50
6:5F:68:ARG:HD2	6:5F:254:LYS:HE2	1.94	0.50
7:5G:544:ILE:HG23	7:5G:559:VAL:HG23	1.94	0.50
12:5L:536:LEU:HB3	12:5L:537:PRO:HD3	1.93	0.50
17:5Q:60:ASP:OD2	17:5Q:62:ARG:NH1	2.41	0.50
37:5l:63:ASP:OD1	37:5l:63:ASP:N	2.39	0.50
59:8E:18:TYR:HE2	59:8E:32:GLY:HA3	1.77	0.50
3:1C:41:GLN:HG2	3:1C:51:PHE:HE2	1.76	0.50
8:1H:187:ILE:HD11	69:1I:201:PC1:H271	1.94	0.50
14:1N:182:SER:OG	14:1N:293:TYR:OH	2.23	0.50
74:4C:306:CDL:H311	74:4C:306:CDL:H212	1.92	0.50
59:4E:18:TYR:OH	59:4E:28:GLU:O	2.29	0.50
2:5B:38:ASN:ND2	2:5B:170:GLU:O	2.43	0.50
10:5J:20:PHE:HE1	11:5K:32:CYS:HA	1.76	0.50
10:5J:76:THR:OG1	10:5J:77:GLU:N	2.44	0.50
20:5U:21:LEU:HD11	36:5k:18:TYR:OH	2.12	0.50
20:5U:55:GLU:OE1	39:5n:24:ARG:NH1	2.40	0.50
55:8A:251:PHE:HB3	55:8A:319:LYS:NZ	2.26	0.50
55:8A:404:THR:O	55:8A:480:ARG:NH1	2.44	0.50
86:8A:601:PGV:H341	86:8L:101:PGV:H152	1.93	0.50
4:1D:291:GLY:O	4:1D:296:ARG:NH2	2.45	0.50
5:1E:106:THR:O	5:1E:110:LEU:HG	2.11	0.50
12:1L:559:GLU:O	12:1L:563:PRO:HD2	2.12	0.50
12:1L:576:MET:HE3	76:1Y:801:3PE:H32	1.94	0.50
31:1f:29:ARG:HG3	31:1f:29:ARG:HH11	1.77	0.50
40:1o:29:GLY:HA3	40:1o:103:ARG:HH22	1.75	0.50
47:3C:124:MET:HE1	47:3C:298:ILE:HD13	1.92	0.50
46:3O:276:GLN:HG2	46:3O:281:ALA:HB2	1.94	0.50
49:3R:219:HIS:CE1	49:3R:239:HIS:CE1	2.99	0.50
56:4B:194:GLY:O	56:4B:209:ILE:N	2.40	0.50
4:5D:158:ALA:HB1	4:5D:163:ALA:HB3	1.93	0.50
5:5E:105:THR:O	5:5E:109:MET:N	2.45	0.50
6:5F:112:ARG:HB3	6:5F:145:GLU:HG3	1.92	0.50
8:5H:307:LEU:HA	8:5H:310:MET:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:5I:64:GLU:OE2	9:5I:149:TYR:OH	2.26	0.50
12:5L:521:LYS:O	12:5L:525:MET:HG2	2.12	0.50
14:5N:252:GLY:HA3	14:5N:290:LEU:HD13	1.93	0.50
14:5N:289:ASN:HA	14:5N:292:PHE:CE2	2.46	0.50
1:1A:51:PHE:HE2	4:1D:45:SER:HB2	1.77	0.49
8:1H:96:ILE:HG23	25:1Z:144:THR:HG21	1.94	0.49
12:1L:213:LEU:HB3	12:1L:273:VAL:HG11	1.93	0.49
16:1P:90:VAL:HG21	16:1P:218:ILE:HD13	1.94	0.49
17:1Q:39:VAL:HG11	17:1Q:108:ARG:HG3	1.94	0.49
23:1X:137:PRO:HB2	23:1X:140:PRO:HG3	1.94	0.49
45:3A:68:LYS:HD3	45:3A:119:ASN:HB3	1.93	0.49
46:3O:76:THR:HG23	46:3O:81:SER:HA	1.93	0.49
47:3P:108:MET:HA	47:3P:108:MET:HE3	1.93	0.49
55:4A:177:SER:HB3	55:4A:180:GLN:NE2	2.27	0.49
3:5C:40:VAL:HG12	3:5C:50:ILE:HG23	1.94	0.49
6:5F:418:LEU:HD23	6:5F:422:PHE:HB2	1.94	0.49
13:5M:11:LEU:HB3	13:5M:100:ILE:HD13	1.94	0.49
13:5M:183:SER:O	41:5p:152:ARG:NH2	2.37	0.49
13:5M:302:MET:HE2	13:5M:302:MET:HA	1.93	0.49
7:1G:158:ARG:NH1	7:1G:202:ILE:O	2.45	0.49
12:1L:282:ALA:O	12:1L:285:THR:OG1	2.30	0.49
13:1M:5:ILE:HG23	13:1M:104:LEU:HD11	1.93	0.49
16:1P:10:LYS:HE3	17:1Q:76:ALA:HB3	1.93	0.49
17:1Q:11:ILE:O	22:1W:16:SER:OG	2.30	0.49
22:1W:17:VAL:HG21	22:1W:77:ARG:CZ	2.42	0.49
37:1l:10:PRO:HD3	38:1m:66:ARG:HG2	1.94	0.49
50:3F:90:GLU:OE1	50:3F:90:GLU:N	2.43	0.49
47:3P:43:LEU:HD13	47:3P:236:MET:HE1	1.94	0.49
57:4C:231:HIS:CD2	86:4C:307:PGV:H042	2.47	0.49
58:4D:77:GLU:O	58:4D:80:THR:HG22	2.11	0.49
5:5E:129:GLY:N	5:5E:139:LEU:O	2.39	0.49
6:5F:364:PRO:HB2	6:5F:403:THR:HG22	1.95	0.49
15:5O:104:ARG:NE	15:5O:131:ASP:OD1	2.39	0.49
23:5X:36:ASP:OD1	23:5X:40:LYS:NZ	2.45	0.49
74:5h:202:CDL:H761	74:5h:202:CDL:H131	1.94	0.49
34:5i:100:LYS:HG3	40:5o:49:GLN:HE22	1.77	0.49
55:8A:35:LEU:HD21	55:8A:462:LEU:HB2	1.94	0.49
7:1G:544:ILE:HG23	7:1G:559:VAL:HG23	1.93	0.49
8:1H:149:ILE:HG21	8:1H:185:TRP:HB2	1.93	0.49
8:1H:152:SER:HA	8:1H:155:LEU:HD12	1.93	0.49
12:1L:367:PRO:O	12:1L:371:THR:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:54:LEU:HD11	33:1h:96:ILE:HD11	1.94	0.49
14:1N:197:ASN:HB2	14:1N:269:GLU:HG2	1.94	0.49
16:1P:179:LEU:HD12	16:1P:318:LEU:HD21	1.95	0.49
16:1P:278:TRP:CH2	76:1P:502:3PE:H251	2.48	0.49
41:1p:31:TYR:O	41:1p:35:ILE:HD12	2.12	0.49
45:3A:284:TYR:HD2	45:3A:290:MET:HE1	1.76	0.49
47:3C:207:ASN:OD1	47:3C:209:THR:OG1	2.24	0.49
57:4C:71:HIS:NE2	86:4C:301:PGV:O06	2.36	0.49
57:4C:128:GLU:OE2	61:4G:38:HIS:ND1	2.45	0.49
58:4D:52:SER:OG	58:4D:55:GLU:HG3	2.11	0.49
1:5A:68:GLU:HG3	1:5A:98:LEU:HD21	1.93	0.49
5:5E:202:LEU:HD11	6:5F:25:LEU:HB3	1.94	0.49
6:5F:108:ARG:HD2	6:5F:142:PHE:CE1	2.47	0.49
11:5K:80:MET:HA	11:5K:80:MET:HE3	1.94	0.49
12:5L:297:ASP:HB3	12:5L:300:LYS:HB2	1.95	0.49
13:5M:186:LEU:HD22	13:5M:250:LEU:HA	1.94	0.49
29:5d:71:PHE:HD2	74:5d:203:CDL:H422	1.77	0.49
39:5n:176:ARG:HG3	39:5n:178:MET:SD	2.52	0.49
55:8A:509:THR:HG22	60:8F:57:ILE:HB	1.94	0.49
9:1I:92:ILE:HG12	9:1I:111:ILE:HG12	1.94	0.49
10:1J:129:ASP:HB2	30:1e:31:ARG:HE	1.77	0.49
12:1L:86:SER:O	12:1L:90:ILE:HG12	2.12	0.49
12:1L:595:ILE:HA	14:1N:100:MET:HE3	1.94	0.49
13:1M:131:ILE:HD12	14:1N:302:LEU:HD21	1.93	0.49
14:1N:95:MET:HE2	14:1N:149:ILE:HG22	1.94	0.49
14:1N:245:MET:HE1	76:1O:401:3PE:H3D2	1.94	0.49
16:1P:63:GLY:HA3	16:1P:68:ILE:HD13	1.95	0.49
74:1h:202:CDL:H582	34:1i:79:TRP:CD2	2.47	0.49
45:3A:8:LEU:HD22	45:3A:392:LEU:HB3	1.93	0.49
46:3B:207:ILE:HG12	46:3B:382:VAL:HG12	1.93	0.49
52:3H:56:ILE:O	52:3H:60:GLU:HG2	2.12	0.49
86:4A:603:PGV:O05	74:4D:201:CDL:OA7	2.16	0.49
1:5A:95:LEU:HD13	8:5H:302:MET:HG3	1.94	0.49
6:5F:111:ILE:HD13	6:5F:138:ILE:HD13	1.93	0.49
10:5J:129:ASP:HB2	30:5e:31:ARG:HD2	1.93	0.49
10:5J:132:ASP:OD1	10:5J:133:SER:N	2.44	0.49
12:5L:316:THR:HA	12:5L:319:ILE:HG12	1.93	0.49
13:5M:209:LEU:HB3	13:5M:212:LEU:HD12	1.94	0.49
38:5m:41:ARG:O	38:5m:45:GLU:HG3	2.12	0.49
56:8B:116:LEU:HD11	56:8B:226:MET:HB3	1.94	0.49
2:1B:36:LEU:HD22	69:1B:203:PC1:H2C2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1I:28:THR:HG22	69:1I:204:PC1:H221	1.94	0.49
69:1I:204:PC1:H362	69:1I:204:PC1:H3A1	1.94	0.49
35:1j:19:ARG:O	35:1j:19:ARG:HD3	2.12	0.49
45:3A:301:ARG:NH2	45:3A:333:ASP:OD2	2.44	0.49
46:3B:54:GLY:O	46:3B:194:TYR:OH	2.30	0.49
46:3O:78:LYS:HB2	46:3O:129:ALA:HB1	1.94	0.49
55:4A:295:VAL:HA	56:4B:173:ASP:HB2	1.94	0.49
10:5J:119:PHE:CE1	11:5K:1:FME:HE2	2.48	0.49
13:5M:403:THR:HA	13:5M:406:TYR:CE2	2.48	0.49
23:5X:152:GLU:OE1	23:5X:152:GLU:N	2.40	0.49
37:5l:34:TYR:OH	37:5l:46:ASP:O	2.23	0.49
39:5n:104:ASP:OD1	39:5n:121:ARG:NH2	2.42	0.49
41:5p:8:VAL:HG23	41:5p:9:TYR:CD2	2.47	0.49
2:1B:69:MET:HB2	2:1B:74:VAL:HB	1.95	0.49
6:1F:42:TRP:CD2	6:1F:161:LEU:HD13	2.48	0.49
12:1L:291:CYS:SG	12:1L:526:LEU:HA	2.52	0.49
14:1N:200:MET:HE1	14:1N:343:LEU:HD13	1.95	0.49
20:1U:69:LYS:HA	34:1i:2:GLY:HA2	1.93	0.49
21:1V:52:ASN:OD1	21:1V:53:GLU:N	2.45	0.49
23:1X:17:VAL:HG12	23:1X:19:VAL:HG22	1.95	0.49
29:1d:94:VAL:HG11	33:1h:106:LYS:HD2	1.94	0.49
52:3H:53:GLU:HA	52:3H:56:ILE:HD12	1.95	0.49
45:3N:354:VAL:HG21	45:3N:404:ALA:HA	1.95	0.49
6:5F:63:SER:HB2	6:5F:242:PHE:HB3	1.93	0.49
17:5Q:5:THR:HG23	17:5Q:6:GLN:HG2	1.95	0.49
18:5R:51:GLU:OE2	18:5R:92:ARG:NH1	2.36	0.49
25:5Z:68:ARG:NH2	27:5b:50:TYR:O	2.44	0.49
25:5Z:86:MET:HB2	25:5Z:124:LEU:HD22	1.94	0.49
59:8E:18:TYR:OH	59:8E:28:GLU:O	2.31	0.49
2:1B:77:ARG:NH2	2:1B:82:GLN:HB2	2.27	0.49
6:1F:95:VAL:HG11	6:1F:118:LEU:HD11	1.95	0.49
6:1F:365:CYS:HB2	70:1F:502:SF4:S3	2.52	0.49
39:1n:64:ARG:HG2	39:1n:64:ARG:HH11	1.77	0.49
46:3B:312:PHE:HA	49:3l:61:GLY:HA2	1.93	0.49
47:3C:186:PRO:HA	47:3C:189:ILE:HD12	1.94	0.49
49:3E:235:TYR:HA	49:3E:243:TYR:H	1.78	0.49
74:3G:102:CDL:H522	74:3G:102:CDL:H562	1.95	0.49
45:3N:14:THR:HG21	45:3N:389:ARG:HB3	1.94	0.49
48:3Q:31:GLN:O	48:3Q:35:GLN:HG3	2.11	0.49
1:5A:48:ARG:HH11	10:5J:76:THR:HG23	1.76	0.49
3:5C:83:VAL:HG12	3:5C:85:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5D:67:GLU:HG2	4:5D:75:LYS:HB3	1.94	0.49
7:5G:315:VAL:HG13	7:5G:340:SER:HB2	1.94	0.49
9:5I:65:HIS:NE2	9:5I:133:GLU:OE2	2.46	0.49
69:5I:204:PC1:H3A1	69:5I:204:PC1:H362	1.95	0.49
11:5K:14:ILE:HG23	76:5K:101:3PE:H382	1.94	0.49
12:5L:186:MET:HG2	12:5L:196:TRP:NE1	2.27	0.49
12:5L:439:PRO:HB3	35:5j:12:ARG:HG2	1.95	0.49
13:5M:116:ILE:HG21	23:5X:167:PHE:HB3	1.94	0.49
13:5M:430:PHE:HB2	13:5M:433:GLU:HG3	1.94	0.49
20:5T:81:ALA:HA	20:5T:86:VAL:HB	1.93	0.49
29:5d:63:LEU:HD23	74:5d:203:CDL:HA62	1.95	0.49
35:5j:19:ARG:HD3	35:5j:23:ILE:HG12	1.94	0.49
42:5q:75:TRP:NE1	69:5q:201:PC1:O14	2.46	0.49
86:8C:303:PGV:H183	86:8C:307:PGV:H142	1.93	0.49
4:1D:161:ILE:HG23	4:1D:238:ARG:HD3	1.95	0.49
6:1F:258:ILE:HA	6:1F:334:VAL:HG13	1.94	0.49
6:1F:261:HIS:HD2	6:1F:337:MET:HA	1.78	0.49
6:1F:297:VAL:HA	6:1F:336:VAL:HA	1.95	0.49
8:1H:68:ILE:HD12	8:1H:69:SER:N	2.28	0.49
14:1N:246:VAL:HG11	76:1O:401:3PE:H281	1.93	0.49
15:1O:135:LEU:HD22	15:1O:152:TYR:CD1	2.48	0.49
23:1X:74:LYS:HD2	26:1a:69:ILE:HD11	1.93	0.49
32:1g:63:PHE:O	32:1g:67:SER:HB2	2.12	0.49
48:3D:119:GLN:O	48:3D:123:GLN:HG3	2.13	0.49
49:3R:230:ASP:OD1	49:3R:231:PHE:N	2.46	0.49
55:4A:329:GLY:O	56:4B:52:HIS:N	2.42	0.49
64:4J:7:GLU:OE1	64:4J:7:GLU:N	2.42	0.49
69:5B:202:PC1:H221	16:5P:275:PHE:CE1	2.47	0.49
7:5G:297:GLU:HG3	22:5W:123:TYR:CZ	2.48	0.49
7:5G:383:ASN:ND2	7:5G:665:GLN:O	2.42	0.49
12:5L:435:PRO:HB3	12:5L:437:PHE:CZ	2.48	0.49
13:5M:76:MET:SD	13:5M:230:VAL:HB	2.52	0.49
76:5M:504:3PE:H272	14:5N:246:VAL:HG21	1.95	0.49
55:8A:43:GLN:HB2	58:8D:104:TYR:CE2	2.48	0.49
56:8B:41:ILE:HG23	56:8B:45:MET:HE3	1.95	0.49
67:8M:33:VAL:HG13	67:8M:40:TYR:HE2	1.76	0.49
2:1B:71:ARG:HA	8:1H:37:PRO:HA	1.93	0.49
12:1L:429:PHE:O	12:1L:436:ARG:NH2	2.46	0.49
14:1N:277:ILE:HD11	24:1Y:132:TRP:HB3	1.95	0.49
31:1f:24:CYS:O	31:1f:28:ARG:HG2	2.12	0.49
37:1l:18:GLU:H	37:1l:18:GLU:CD	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1L:50:LEU:HD11	37:1L:76:PRO:HB2	1.94	0.49
46:3B:166:ALA:HB2	46:3B:244:ILE:HG13	1.93	0.49
76:3N:503:3PE:H221	76:3N:503:3PE:H2	1.47	0.49
48:3Q:158:ILE:HG12	48:3Q:160:MET:HB2	1.95	0.49
86:4B:301:PGV:H202	86:4C:304:PGV:H32	1.95	0.49
1:5A:69:ILE:HD11	8:5H:144:VAL:HG13	1.94	0.49
4:5D:109:VAL:HG12	4:5D:149:ASN:HA	1.95	0.49
6:5F:296:ALA:HB1	6:5F:306:LEU:HD12	1.95	0.49
7:5G:194:GLU:HG3	7:5G:389:PRO:HB3	1.94	0.49
12:5L:503:GLU:O	12:5L:507:THR:OG1	2.28	0.49
12:5L:591:PHE:CE1	14:5N:111:PHE:HA	2.48	0.49
16:5P:177:ARG:NH2	79:5P:402:NDP:O2N	2.41	0.49
38:5m:117:GLU:OE2	38:5m:119:LYS:NZ	2.37	0.49
86:8B:301:PGV:H312	74:8D:201:CDL:H462	1.95	0.49
67:8M:19:LEU:HD23	86:8M:101:PGV:H271	1.95	0.49
67:8M:42:ARG:HH11	67:8M:42:ARG:HG3	1.78	0.49
4:1D:166:PRO:HG3	4:1D:228:MET:HG3	1.95	0.49
6:1F:162:ILE:HG21	6:1F:175:VAL:HG22	1.94	0.49
9:1I:66:ALA:HB1	9:1I:158:GLY:HA2	1.95	0.49
10:1J:3:MET:HE1	25:1Z:133:ILE:HD11	1.95	0.49
12:1L:149:ILE:HG21	13:1M:369:LEU:HD21	1.95	0.49
13:1M:263:MET:HE2	13:1M:263:MET:N	2.28	0.49
19:1S:19:ARG:NH1	19:1S:73:GLU:OE2	2.44	0.49
33:1h:50:ALA:HB2	41:1p:60:TYR:CE1	2.48	0.49
48:3D:299:MET:HE1	53:3J:43:ALA:HA	1.95	0.49
49:3R:199:GLN:HE22	49:3R:257:ASN:ND2	2.04	0.49
50:3S:45:GLU:OE2	50:3S:48:ARG:NH2	2.35	0.49
50:3S:52:GLU:OE1	51:3T:11:ARG:NH1	2.46	0.49
55:4A:332:ILE:HG23	55:4A:338:MET:HE3	1.95	0.49
60:4F:16:LEU:HD11	60:4F:31:TYR:CE2	2.48	0.49
6:5F:131:ALA:O	6:5F:171:TYR:OH	2.26	0.49
29:5d:114:GLU:OE1	41:5p:152:ARG:NH1	2.46	0.49
40:5o:21:MET:HG2	40:5o:22:PRO:HA	1.94	0.49
56:8B:104:TRP:CG	56:8B:203:ASN:HB2	2.48	0.49
86:8C:304:PGV:H201	68:8N:36:LEU:HD13	1.94	0.49
62:8H:8:ILE:HD11	62:8H:55:TRP:HB2	1.93	0.49
86:8K:101:PGV:H62	86:8K:101:PGV:H21	1.95	0.49
4:1D:109:VAL:HG12	4:1D:149:ASN:HA	1.94	0.48
7:1G:11:VAL:HG11	7:1G:73:VAL:HB	1.94	0.48
8:1H:179:TRP:N	8:1H:180:PRO:HD2	2.28	0.48
13:1M:60:SER:HB2	13:1M:457:PRO:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:3D:253:ILE:HG22	48:3D:268:MET:HG3	1.95	0.48
48:3Q:47:ALA:HA	48:3Q:90:TYR:HA	1.94	0.48
49:3R:248:ARG:HH11	49:3R:257:ASN:HB3	1.78	0.48
2:5B:50:PHE:CE2	2:5B:96:MET:HE2	2.48	0.48
6:5F:89:ARG:HB3	6:5F:218:CYS:HB3	1.94	0.48
7:5G:320:GLY:O	7:5G:498:SER:OG	2.31	0.48
12:5L:136:ASN:OD1	12:5L:139:GLN:HB2	2.13	0.48
13:5M:158:LEU:HD22	14:5N:283:ALA:HB1	1.94	0.48
29:5d:94:VAL:HG21	33:5h:106:LYS:HD2	1.94	0.48
55:8A:65:MET:HB3	87:8A:603:HEA:HBC1	1.95	0.48
86:8B:301:PGV:H12	74:8D:201:CDL:H382	1.93	0.48
6:1F:120:GLU:HG3	6:1F:232:PRO:HG2	1.95	0.48
8:1H:170:GLU:CD	23:1X:97:ARG:HH22	2.21	0.48
9:1I:14:MET:HG3	25:1Z:33:TYR:OH	2.13	0.48
10:1J:20:PHE:HE1	11:1K:32:CYS:HA	1.77	0.48
16:1P:177:ARG:NH1	79:1P:501:NDP:O2N	2.36	0.48
20:1T:80:ILE:O	20:1T:84:LYS:HG2	2.12	0.48
40:1o:38:MET:HG3	40:1o:40:ALA:O	2.13	0.48
49:3R:172:LYS:HB3	49:3R:214:ILE:HG23	1.95	0.48
57:4C:54:MET:HG2	86:4C:301:PGV:H61	1.95	0.48
2:5B:154:GLU:OE2	9:5I:55:GLY:N	2.38	0.48
3:5C:8:ARG:HB3	3:5C:11:ILE:HD12	1.94	0.48
5:5E:134:ASP:OD1	5:5E:134:ASP:N	2.44	0.48
9:5I:35:GLY:HA3	69:5I:204:PC1:H342	1.94	0.48
10:5J:86:ASN:OD1	10:5J:88:THR:HG22	2.13	0.48
13:5M:457:PRO:HA	32:5g:84:ARG:NH2	2.28	0.48
14:5N:249:LEU:HD22	14:5N:254:LEU:HD12	1.95	0.48
15:5O:305:SER:H	15:5O:309:ASN:HD21	1.61	0.48
76:5d:201:3PE:H252	76:5d:201:3PE:H362	1.94	0.48
34:5i:40:TRP:HB2	34:5i:42:MET:HE3	1.95	0.48
36:5k:49:ALA:O	36:5k:53:SER:OG	2.27	0.48
7:1G:107:ILE:HG23	9:1I:78:ILE:HD12	1.94	0.48
12:1L:375:ILE:HD12	12:1L:458:LEU:HD11	1.94	0.48
14:1N:250:SER:O	14:1N:259:GLY:HA3	2.13	0.48
20:1T:17:TYR:O	20:1T:20:LYS:HG3	2.14	0.48
21:1V:40:ASN:OD1	21:1V:40:ASN:N	2.46	0.48
32:1g:116:ASN:OD1	32:1g:117:LYS:N	2.46	0.48
48:3D:297:MET:HE3	48:3D:297:MET:HB3	1.78	0.48
45:3N:140:GLU:O	45:3N:143:SER:OG	2.29	0.48
57:4C:142:VAL:HG13	61:4G:20:THR:HG22	1.96	0.48
62:4H:57:ARG:O	62:4H:61:LYS:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5E:145:LEU:HD22	6:5F:141:GLU:HG2	1.94	0.48
6:5F:277:LYS:HD3	6:5F:291:TRP:CE2	2.48	0.48
8:5H:170:GLU:CD	23:5X:97:ARG:HH22	2.21	0.48
9:5I:54:LYS:HD3	42:5q:91:HIS:NE2	2.29	0.48
12:5L:395:ILE:O	12:5L:399:VAL:HG13	2.13	0.48
13:5M:133:ILE:HD11	13:5M:231:LEU:HD11	1.94	0.48
76:5M:504:3PE:H281	14:5N:246:VAL:HG11	1.95	0.48
24:5Y:125:LYS:HE3	24:5Y:129:LEU:HD13	1.93	0.48
37:5l:138:LEU:HB3	37:5l:141:GLU:HB2	1.95	0.48
38:5m:47:LEU:HB3	39:5n:165:LEU:HD13	1.95	0.48
55:8A:265:LYS:HB3	55:8A:490:THR:HG21	1.95	0.48
2:1B:104:TYR:O	2:1B:111:ARG:NH1	2.46	0.48
4:1D:149:ASN:ND2	4:1D:370:PRO:HB2	2.28	0.48
4:1D:176:LYS:HD3	43:1r:26:ARG:HE	1.77	0.48
7:1G:46:LEU:O	17:1Q:116:LYS:NZ	2.35	0.48
9:1I:132:VAL:HG21	9:1I:165:ILE:HD12	1.95	0.48
10:1J:60:TYR:CE2	11:1K:38:LEU:HD13	2.48	0.48
76:1L:701:3PE:H242	76:1L:701:3PE:H322	1.94	0.48
13:1M:12:LEU:HB2	13:1M:13:PRO:HD3	1.94	0.48
19:1S:90:LEU:O	19:1S:94:LEU:HG	2.14	0.48
23:1X:46:ARG:NH1	25:1Z:80:ASP:OD2	2.47	0.48
74:1X:201:CDL:H452	74:1X:201:CDL:H251	1.95	0.48
39:1n:176:ARG:HG3	39:1n:178:MET:HE3	1.94	0.48
50:3S:72:GLN:HB2	74:3T:101:CDL:HA21	1.95	0.48
55:4A:342:LEU:HD22	56:4B:46:LEU:HD11	1.93	0.48
4:5D:143:GLU:OE2	4:5D:278:TYR:OH	2.26	0.48
5:5E:89:MET:HE1	6:5F:140:GLY:C	2.38	0.48
14:5N:143:CYS:HA	14:5N:194:LEU:HD11	1.96	0.48
15:5O:154:GLU:O	15:5O:158:VAL:HG23	2.13	0.48
20:5U:9:GLU:OE1	20:5U:9:GLU:HA	2.13	0.48
41:5p:80:ASP:O	41:5p:84:MET:HG3	2.14	0.48
55:8A:28:MET:HG3	66:8L:29:PHE:HD1	1.77	0.48
90:8I:101:PSC:H02	90:8I:101:PSC:H21	1.55	0.48
64:8J:52:TRP:O	64:8J:57:HIS:ND1	2.47	0.48
7:1G:316:ALA:HB3	7:1G:519:PRO:HG3	1.96	0.48
10:1J:7:PHE:CE1	11:1K:3:LEU:HG	2.49	0.48
14:1N:289:ASN:HA	14:1N:292:PHE:CE2	2.47	0.48
15:1O:305:SER:H	15:1O:309:ASN:HD21	1.61	0.48
24:1Y:50:GLU:OE2	24:1Y:50:GLU:N	2.45	0.48
35:1j:39:ARG:NH2	35:1j:43:ASP:OD2	2.47	0.48
40:1o:4:LEU:HG	40:1o:8:TYR:HE2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1o:7:ARG:HG3	40:1o:15:GLU:HB2	1.95	0.48
49:3R:155:LYS:HZ2	49:3R:155:LYS:HB3	1.79	0.48
55:4A:377:PHE:O	55:4A:381:LEU:HB2	2.13	0.48
55:4A:428:GLN:HA	55:4A:431:LEU:HD12	1.95	0.48
61:4G:28:VAL:O	61:4G:32:THR:HG23	2.13	0.48
1:5A:84:LEU:HD13	8:5H:309:ILE:HG23	1.96	0.48
4:5D:141:PHE:O	4:5D:145:THR:OG1	2.27	0.48
4:5D:260:LEU:HD22	4:5D:265:ILE:HD13	1.93	0.48
4:5D:270:ARG:HG3	4:5D:368:GLU:HB3	1.96	0.48
6:5F:90:PRO:O	6:5F:218:CYS:HB2	2.14	0.48
6:5F:292:ASP:OD1	6:5F:292:ASP:N	2.47	0.48
8:5H:24:GLU:OE1	8:5H:228:TYR:OH	2.25	0.48
18:5R:11:VAL:HG22	18:5R:17:ALA:HB2	1.96	0.48
20:5T:17:TYR:HE1	20:5T:21:LEU:HD21	1.76	0.48
25:5Z:82:ARG:O	25:5Z:86:MET:HG3	2.13	0.48
74:8C:306:CDL:HB61	74:8C:306:CDL:H542	1.96	0.48
62:8H:39:CYS:O	62:8H:43:MET:HB2	2.14	0.48
4:1D:151:ILE:O	4:1D:155:THR:OG1	2.24	0.48
4:1D:238:ARG:HH22	4:1D:412:ALA:HB1	1.79	0.48
6:1F:140:GLY:O	6:1F:179:ARG:NH2	2.46	0.48
14:1N:237:MET:HE1	14:1N:319:HIS:HE2	1.78	0.48
34:1i:43:GLU:O	34:1i:47:ASN:ND2	2.46	0.48
76:3A:503:3PE:H332	47:3C:11:MET:SD	2.53	0.48
47:3C:91:PHE:HA	47:3C:94:LEU:HB2	1.95	0.48
48:3D:121:TYR:HA	48:3D:125:CYS:SG	2.53	0.48
48:3D:309:TYR:OH	74:3G:102:CDL:OB3	2.24	0.48
46:3O:319:SER:OG	46:3O:320:GLY:N	2.46	0.48
55:4A:265:LYS:NZ	60:4F:84:SER:OG	2.39	0.48
67:4M:11:SER:OG	67:4M:14:GLU:HG3	2.13	0.48
1:5A:92:LEU:HD13	27:5b:29:ILE:HG12	1.95	0.48
8:5H:104:PHE:O	8:5H:108:MET:HG2	2.14	0.48
8:5H:199:ASP:OD1	8:5H:279:ARG:NE	2.40	0.48
14:5N:200:MET:HE1	14:5N:343:LEU:HD13	1.95	0.48
16:5P:116:ALA:O	16:5P:120:VAL:HG23	2.13	0.48
37:5l:62:TYR:OH	39:5n:151:GLU:OE1	2.23	0.48
55:8A:240:HIS:O	55:8A:243:VAL:HB	2.13	0.48
57:8C:156:ARG:NH1	86:8C:302:PGV:O13	2.46	0.48
3:1C:211:GLN:NE2	21:1V:114:PRO:O	2.46	0.48
6:1F:110:ILE:HD11	6:1F:225:VAL:HG12	1.96	0.48
8:1H:170:GLU:OE2	23:1X:97:ARG:NH2	2.46	0.48
12:1L:10:THR:HA	12:1L:13:ILE:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:97:THR:HG21	76:1M:903:3PE:H2C2	1.94	0.48
16:1P:32:ARG:HB3	16:1P:62:MET:HE1	1.96	0.48
17:1Q:14:ASP:HB2	17:1Q:16:LYS:HE2	1.94	0.48
47:3C:103:TYR:HA	47:3C:315:MET:HE3	1.94	0.48
57:4C:117:PRO:HG2	57:4C:123:PRO:HG3	1.95	0.48
62:4H:56:TYR:CE2	68:4N:80:PRO:HD2	2.48	0.48
12:5L:2:ASN:ND2	12:5L:53:MET:HE1	2.22	0.48
12:5L:147:VAL:CG1	12:5L:252:MET:HG3	2.44	0.48
13:5M:231:LEU:HA	13:5M:235:LEU:HB2	1.95	0.48
14:5N:103:ALA:O	14:5N:107:GLY:N	2.44	0.48
37:5l:54:SER:HA	37:5l:84:TYR:HB3	1.95	0.48
37:5l:62:TYR:HD1	37:5l:63:ASP:N	2.11	0.48
39:5n:26:LEU:HD22	39:5n:43:MET:HE2	1.96	0.48
56:8B:43:SER:OG	86:8B:301:PGV:O02	2.31	0.48
6:1F:89:ARG:HB3	6:1F:218:CYS:HB3	1.95	0.48
8:1H:55:LEU:HD13	8:1H:221:ALA:HB2	1.95	0.48
12:1L:387:THR:HA	12:1L:465:GLY:HA3	1.94	0.48
13:1M:78:MET:HE1	13:1M:439:LEU:HD12	1.96	0.48
14:1N:332:LEU:HD21	74:1d:203:CDL:H431	1.96	0.48
55:4A:51:ASP:O	55:4A:55:ASN:ND2	2.47	0.48
58:4D:78:TRP:CG	74:4D:201:CDL:H202	2.49	0.48
86:4G:101:PGV:H02	86:4G:101:PGV:H21	1.45	0.48
2:5B:48:MET:HE2	2:5B:80:PRO:HB3	1.94	0.48
62:8H:28:ASN:O	62:8H:32:ASN:ND2	2.41	0.48
2:1B:63:ALA:HB2	2:1B:69:MET:HE2	1.95	0.48
10:1J:6:ALA:HB3	10:1J:124:ASP:OD2	2.14	0.48
10:1J:173:ARG:NH1	10:1J:174:GLY:O	2.46	0.48
13:1M:2:LEU:HD21	74:1X:201:CDL:H552	1.96	0.48
14:1N:107:GLY:HA2	14:1N:111:PHE:O	2.14	0.48
17:1Q:37:ILE:HB	17:1Q:105:VAL:HG22	1.95	0.48
24:1Y:34:ILE:HD12	76:1Y:804:3PE:H372	1.94	0.48
26:1a:59:ARG:HD2	26:1a:61:HIS:NE2	2.28	0.48
48:3Q:15:ARG:NH2	48:3Q:125:ASP:OD2	2.46	0.48
58:4D:78:TRP:CE2	58:4D:79:LYS:HG3	2.49	0.48
2:5B:47:PRO:HD2	2:5B:75:VAL:O	2.12	0.48
6:5F:300:GLY:O	6:5F:304:THR:OG1	2.26	0.48
16:5P:122:LYS:NZ	16:5P:162:GLU:OE2	2.46	0.48
20:5U:25:ILE:HG13	20:5U:40:LEU:HD13	1.96	0.48
23:5X:20:SER:HB2	26:5a:63:THR:HG23	1.95	0.48
25:5Z:68:ARG:NH1	25:5Z:72:MET:SD	2.86	0.48
36:5k:34:LYS:HZ3	64:8J:17:ASP:CG	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8A:94:PHE:HB2	55:8A:97:MET:HG2	1.96	0.48
2:1B:95:LYS:HG2	4:1D:82:LEU:HD23	1.95	0.48
4:1D:309:ARG:HG2	4:1D:313:GLN:HE21	1.79	0.48
6:1F:84:LYS:HB2	6:1F:84:LYS:HE3	1.63	0.48
8:1H:310:MET:O	27:1b:37:TYR:HB2	2.14	0.48
13:1M:403:THR:HA	13:1M:406:TYR:CE2	2.49	0.48
15:1O:9:VAL:HG12	15:1O:10:LEU:HD23	1.96	0.48
16:1P:172:PHE:HB2	16:1P:179:LEU:CD2	2.44	0.48
20:1T:36:PHE:HA	20:1T:40:LEU:HD23	1.95	0.48
20:1U:36:PHE:HD1	20:1U:40:LEU:HD12	1.78	0.48
74:1d:203:CDL:HA4	74:1d:203:CDL:H512	1.95	0.48
49:3R:154:ILE:HG22	49:3R:272:ILE:HG22	1.96	0.48
12:5L:102:GLU:OE1	12:5L:456:ARG:NH2	2.42	0.48
13:5M:122:PHE:HE1	13:5M:206:LYS:HD3	1.79	0.48
13:5M:188:ASN:OD1	13:5M:256:TYR:OH	2.30	0.48
15:5O:168:VAL:HG11	15:5O:238:ILE:HD12	1.94	0.48
19:5S:64:LEU:HB2	19:5S:78:LEU:HD11	1.94	0.48
57:8C:210:ILE:HD13	86:8C:307:PGV:H302	1.96	0.48
4:1D:165:THR:HG23	8:1H:32:GLN:HG2	1.96	0.47
4:1D:174:ARG:HA	4:1D:177:MET:HE3	1.96	0.47
6:1F:17:ASP:HA	6:1F:20:ARG:HB2	1.96	0.47
12:1L:310:LEU:HA	12:1L:313:MET:HE3	1.95	0.47
39:1n:34:ASP:OD1	39:1n:35:LYS:N	2.47	0.47
39:1n:107:HIS:CD2	39:1n:108:PRO:HD2	2.49	0.47
41:1p:93:ARG:O	41:1p:97:VAL:HG23	2.14	0.47
46:3B:46:ARG:NH2	46:3B:110:GLU:OE2	2.47	0.47
55:4A:218:THR:HG21	61:4G:55:ILE:HD13	1.94	0.47
65:4K:47:ARG:HH22	86:4K:101:PGV:H221	1.78	0.47
8:5H:2:PHE:O	8:5H:6:ILE:HG13	2.14	0.47
20:5T:48:VAL:O	20:5T:52:MET:HG3	2.14	0.47
74:5d:203:CDL:H512	74:5d:203:CDL:HA4	1.96	0.47
35:5j:62:GLU:OE1	35:5j:62:GLU:N	2.47	0.47
35:5j:67:LEU:O	40:5o:110:ARG:HD2	2.14	0.47
39:5n:65:GLN:O	39:5n:69:GLU:HB2	2.14	0.47
59:8E:107:ASP:N	59:8E:107:ASP:OD1	2.46	0.47
62:8H:31:GLN:HE21	68:8N:55:ASN:HD21	1.61	0.47
3:1C:72:PHE:O	3:1C:124:TYR:OH	2.24	0.47
10:1J:60:TYR:CD1	10:1J:64:MET:HE3	2.49	0.47
13:1M:456:GLY:O	32:1g:84:ARG:NH1	2.42	0.47
15:1O:314:ASP:HB3	15:1O:317:ILE:HD11	1.96	0.47
16:1P:45:VAL:HG12	16:1P:47:VAL:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1U:48:VAL:O	20:1U:52:MET:HG3	2.13	0.47
45:3N:358:LYS:O	45:3N:362:ARG:HG3	2.14	0.47
55:4A:43:GLN:HG2	55:4A:44:PRO:HD2	1.96	0.47
55:4A:381:LEU:HB3	87:4A:604:HEA:HAC	1.96	0.47
68:4N:7:THR:HA	68:4N:10:LYS:HD3	1.96	0.47
7:5G:115:ASP:OD1	17:5Q:46:GLN:HG3	2.14	0.47
7:5G:215:PHE:HB3	9:5I:104:ARG:HG3	1.96	0.47
7:5G:418:ARG:HE	7:5G:418:ARG:HB2	1.47	0.47
10:5J:138:GLU:OE1	10:5J:138:GLU:N	2.47	0.47
12:5L:90:ILE:HB	12:5L:91:PRO:HD3	1.96	0.47
12:5L:375:ILE:HD12	12:5L:458:LEU:HD11	1.96	0.47
13:5M:16:TRP:CE2	76:5M:502:3PE:H281	2.49	0.47
13:5M:65:LEU:O	13:5M:69:THR:HG23	2.15	0.47
13:5M:74:PRO:O	13:5M:78:MET:HG3	2.14	0.47
13:5M:196:TRP:HB2	13:5M:253:LEU:HD23	1.94	0.47
20:5T:60:PHE:CE1	20:5T:80:ILE:HG23	2.49	0.47
20:5U:49:GLU:HB3	36:5k:44:TRP:HE1	1.77	0.47
20:5U:51:ILE:O	20:5U:55:GLU:HG3	2.14	0.47
63:8I:14:ALA:O	63:8I:18:ARG:HG3	2.14	0.47
6:1F:90:PRO:O	6:1F:218:CYS:HB2	2.14	0.47
6:1F:143:TYR:HB2	6:1F:179:ARG:HH21	1.79	0.47
7:1G:380:VAL:HG11	7:1G:429:LEU:HD11	1.96	0.47
8:1H:173:TRP:HB3	8:1H:175:ILE:HG22	1.96	0.47
12:1L:151:SER:HB2	12:1L:248:HIS:NE2	2.29	0.47
13:1M:6:ILE:HG12	74:1X:201:CDL:H652	1.95	0.47
15:1O:84:ASP:HA	15:1O:193:LYS:HE2	1.97	0.47
16:1P:176:ASP:OD1	16:1P:178:PHE:N	2.37	0.47
39:1n:18:LEU:HD22	39:1n:67:GLU:HG3	1.97	0.47
45:3A:34:THR:HG22	45:3A:102:LEU:HD23	1.96	0.47
57:4C:159:MET:SD	57:4C:222:GLN:HG2	2.55	0.47
61:4G:72:ASN:HB3	61:4G:75:VAL:HG12	1.95	0.47
4:5D:147:LEU:HD22	4:5D:218:PHE:HE2	1.79	0.47
7:5G:252:PRO:HB3	7:5G:263:ILE:HG23	1.97	0.47
7:5G:444:LYS:NZ	7:5G:480:SER:HB2	2.30	0.47
11:5K:40:LEU:O	11:5K:44:SER:OG	2.26	0.47
11:5K:95:LEU:HD11	14:5N:51:ARG:HA	1.96	0.47
13:5M:269:MET:HE2	13:5M:399:ASN:HD22	1.79	0.47
32:5g:24:ILE:C	32:5g:25:ARG:HG2	2.39	0.47
38:5m:22:TYR:HB3	39:5n:64:ARG:HE	1.79	0.47
55:8A:131:PRO:HD3	56:8B:160:LEU:HD13	1.95	0.47
55:8A:277:MET:HE2	55:8A:319:LYS:HZ1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:8B:52:HIS:CE1	56:8B:56:MET:HG2	2.49	0.47
56:8B:85:TYR:O	56:8B:89:GLU:HG3	2.14	0.47
74:8D:201:CDL:HB4	74:8D:201:CDL:H512	1.40	0.47
74:8D:201:CDL:H402	74:8D:201:CDL:H592	1.97	0.47
62:8H:57:ARG:HA	62:8H:60:TYR:CE2	2.49	0.47
6:1F:305:PRO:HD3	6:1F:413:TRP:HB3	1.94	0.47
10:1J:103:MET:HE1	10:1J:115:ILE:HG21	1.96	0.47
13:1M:306:PRO:HA	13:1M:458:LEU:HD22	1.97	0.47
19:1S:90:LEU:O	19:1S:93:VAL:HG12	2.14	0.47
20:1U:36:PHE:HB3	20:1U:42:LEU:HD12	1.97	0.47
37:1I:34:TYR:OH	37:1I:46:ASP:O	2.23	0.47
48:3D:135:ALA:HA	48:3D:178:TYR:HA	1.95	0.47
45:3N:287:GLY:O	45:3N:290:MET:HG3	2.14	0.47
74:3P:504:CDL:HB61	74:3P:504:CDL:H712	1.55	0.47
49:3R:123:VAL:HG13	53:3W:28:ALA:HA	1.95	0.47
49:3R:226:ALA:HA	49:3R:234:TYR:HD1	1.79	0.47
55:4A:86:MET:HB3	55:4A:182:PRO:HG2	1.97	0.47
57:4C:190:ASP:OD1	61:4G:53:LEU:HD13	2.14	0.47
62:4H:71:ALA:O	62:4H:75:ARG:HG3	2.14	0.47
7:5G:39:ARG:HB2	71:5G:803:FES:S2	2.54	0.47
7:5G:40:PHE:HB2	7:5G:52:CYS:SG	2.54	0.47
9:5I:160:LYS:HD2	9:5I:161:TRP:NE1	2.29	0.47
12:5L:233:LEU:HB3	12:5L:234:PRO:HD3	1.97	0.47
12:5L:480:THR:OG1	12:5L:481:THR:N	2.47	0.47
14:5N:8:THR:O	14:5N:12:THR:OG1	2.30	0.47
26:5a:55:SER:HB2	26:5a:62:VAL:HG13	1.96	0.47
31:5f:49:ARG:HH11	31:5f:49:ARG:HG3	1.79	0.47
31:5f:56:TRP:HE1	33:5h:88:GLU:HG3	1.79	0.47
33:5h:84:GLU:O	33:5h:88:GLU:HG2	2.14	0.47
39:5n:91:GLU:HB2	39:5n:94:GLU:HG3	1.97	0.47
55:8A:374:VAL:HG12	55:8A:428:GLN:HE22	1.80	0.47
69:1B:203:PC1:H221	69:1B:203:PC1:H2	1.36	0.47
4:1D:208:LEU:HD22	4:1D:315:LEU:HD23	1.96	0.47
5:1E:129:GLY:HA2	5:1E:140:ILE:HG22	1.96	0.47
5:1E:205:PRO:O	5:1E:207:LYS:NZ	2.47	0.47
6:1F:45:THR:HG22	6:1F:49:LEU:HD23	1.95	0.47
7:1G:218:ARG:HD2	7:1G:220:TRP:CH2	2.49	0.47
8:1H:289:LEU:HA	8:1H:293:PHE:HB2	1.96	0.47
13:1M:423:ILE:HG23	38:1m:58:VAL:HG12	1.96	0.47
14:1N:252:GLY:HA3	14:1N:290:LEU:HD13	1.95	0.47
24:1Y:40:ILE:HG21	76:1Y:805:3PE:H231	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1b:14:LYS:C	27:1b:16:PRO:HD3	2.39	0.47
33:1h:138:LYS:HB2	33:1h:143:ASN:HD21	1.80	0.47
38:1m:45:GLU:OE2	38:1m:45:GLU:N	2.43	0.47
46:3B:46:ARG:HD3	46:3B:379:LEU:HD22	1.95	0.47
48:3D:121:TYR:CD1	48:3D:125:CYS:HB2	2.49	0.47
49:3R:159:ILE:HD13	49:3R:268:ASP:HB2	1.97	0.47
49:3R:222:CYS:O	71:3R:301:FES:S2	2.73	0.47
55:4A:275:TRP:CE3	86:4A:602:PGV:H12	2.49	0.47
55:4A:377:PHE:HA	55:4A:380:VAL:HG22	1.96	0.47
58:4D:40:LEU:HD22	58:4D:58:GLU:OE1	2.15	0.47
60:4F:14:THR:OG1	64:4J:13:GLN:OE1	2.23	0.47
6:5F:258:ILE:HA	6:5F:334:VAL:HG13	1.97	0.47
11:5K:59:MET:HE2	14:5N:84:TRP:CH2	2.50	0.47
13:5M:116:ILE:O	13:5M:120:ILE:HG12	2.15	0.47
15:5O:53:GLU:OE2	15:5O:126:ARG:NH1	2.47	0.47
16:5P:27:THR:HG21	16:5P:56:THR:HG22	1.96	0.47
19:5S:88:ARG:HH21	19:5S:92:ASN:HD21	1.63	0.47
37:5l:82:ASP:OD1	37:5l:82:ASP:N	2.44	0.47
55:8A:273:MET:HE1	55:8A:323:TRP:CD1	2.49	0.47
61:8G:15:THR:O	61:8G:19:LEU:HD12	2.15	0.47
68:8N:68:VAL:HG12	68:8N:69:ASN:OD1	2.14	0.47
2:1B:50:PHE:CE1	2:1B:103:VAL:HG21	2.48	0.47
4:1D:19:MET:HG2	14:1N:173:THR:HG22	1.96	0.47
6:1F:51:LYS:HD3	6:1F:55:TRP:CD2	2.50	0.47
7:1G:238:ILE:HG22	7:1G:263:ILE:HG21	1.97	0.47
74:1H:401:CDL:HB4	74:1H:401:CDL:H511	1.44	0.47
12:1L:63:ILE:HG23	34:1i:96:VAL:HG22	1.97	0.47
12:1L:521:LYS:O	12:1L:525:MET:HE3	2.15	0.47
16:1P:169:SER:HB3	16:1P:231:VAL:HG23	1.97	0.47
37:1l:132:GLN:OE1	37:1l:155:HIS:HB3	2.15	0.47
45:3N:436:ARG:HD3	47:3P:222:PRO:HD3	1.97	0.47
57:4C:58:TRP:CZ3	86:4C:307:PGV:H71	2.49	0.47
59:4E:89:LEU:O	59:4E:93:LEU:HD23	2.14	0.47
4:5D:343:GLU:HG3	7:5G:98:LEU:HD12	1.96	0.47
6:5F:302:SER:HB2	6:5F:350:LEU:HD12	1.97	0.47
8:5H:316:PRO:HG3	25:5Z:57:ARG:HB3	1.96	0.47
12:5L:371:THR:HG22	36:5k:68:LYS:HE3	1.95	0.47
25:5Z:89:GLU:O	25:5Z:93:GLU:HG2	2.13	0.47
31:5f:8:ARG:HD2	31:5f:8:ARG:HA	1.61	0.47
55:8A:348:PHE:CD1	55:8A:380:VAL:HG13	2.49	0.47
60:8F:17:GLU:O	60:8F:21:MET:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:57:LEU:O	1:1A:61:THR:OG1	2.29	0.47
5:1E:210:GLY:HA2	6:1F:43:TYR:CZ	2.49	0.47
7:1G:684:MET:HE2	7:1G:684:MET:HA	1.95	0.47
8:1H:2:PHE:O	8:1H:6:ILE:HG13	2.15	0.47
11:1K:96:LEU:HD12	14:1N:54:GLU:OE2	2.14	0.47
12:1L:260:LEU:HD22	12:1L:267:MET:HE1	1.96	0.47
12:1L:291:CYS:O	12:1L:295:GLN:HG2	2.15	0.47
12:1L:401:MET:SD	12:1L:482:MET:HB3	2.55	0.47
12:1L:572:LYS:HZ3	76:1Y:802:3PE:H332	1.79	0.47
13:1M:92:LYS:O	13:1M:96:ILE:HG12	2.14	0.47
13:1M:101:LEU:HD13	76:1M:903:3PE:H2H1	1.97	0.47
13:1M:279:GLN:HB2	13:1M:285:LEU:HD12	1.97	0.47
76:1M:901:3PE:H2F2	14:1N:285:THR:HA	1.97	0.47
15:1O:3:TYR:OH	15:1O:257:HIS:ND1	2.41	0.47
16:1P:145:TYR:CE1	16:1P:149:LYS:HD2	2.49	0.47
16:1P:196:LEU:HD21	16:1P:255:PRO:HB2	1.97	0.47
22:1W:89:GLU:HG2	22:1W:98:LYS:NZ	2.29	0.47
74:1X:201:CDL:H273	74:1X:201:CDL:H322	1.96	0.47
24:1Y:81:GLU:O	24:1Y:81:GLU:CD	2.58	0.47
34:1i:44:GLN:HA	34:1i:47:ASN:HD21	1.80	0.47
45:3A:354:VAL:HG21	45:3A:404:ALA:HA	1.96	0.47
46:3B:36:ALA:HB3	46:3B:207:ILE:HG13	1.97	0.47
46:3B:76:THR:HG23	46:3B:81:SER:HA	1.96	0.47
46:3B:120:MET:SD	46:3B:219:VAL:HG21	2.54	0.47
47:3C:240:LEU:HD21	76:3D:502:3PE:H242	1.97	0.47
48:3D:111:HIS:NE2	48:3D:288:ASP:OD2	2.40	0.47
48:3D:124:VAL:HG12	85:3D:501:HEC:HAB	1.97	0.47
48:3D:162:PRO:HB2	48:3Q:99:GLU:HG3	1.97	0.47
55:4A:31:THR:HG21	55:4A:465:VAL:HG11	1.95	0.47
57:4C:54:MET:HB3	57:4C:58:TRP:CZ3	2.49	0.47
57:4C:249:TRP:HA	57:4C:252:LEU:HB2	1.95	0.47
1:5A:53:MET:HE1	11:5K:79:VAL:HG13	1.96	0.47
4:5D:151:ILE:HD11	4:5D:218:PHE:CZ	2.50	0.47
5:5E:84:ALA:HA	5:5E:90:TYR:HD2	1.80	0.47
6:5F:275:PRO:HB2	6:5F:278:GLU:HG2	1.97	0.47
7:5G:26:VAL:HB	7:5G:68:ALA:HA	1.97	0.47
7:5G:157:THR:HG22	7:5G:161:ARG:HG3	1.96	0.47
8:5H:63:PRO:HB2	8:5H:66:SER:HB3	1.97	0.47
8:5H:179:TRP:N	8:5H:180:PRO:HD2	2.30	0.47
12:5L:49:VAL:HG22	41:5p:32:LEU:HD13	1.97	0.47
12:5L:487:LYS:NZ	35:5j:46:ALA:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:5N:310:ASN:HD21	15:5O:98:SER:HG	1.59	0.47
18:5R:14:THR:O	42:5q:131:ARG:NH2	2.48	0.47
25:5Z:103:ASP:OD1	25:5Z:103:ASP:N	2.43	0.47
36:5k:84:GLU:O	36:5k:88:GLU:HG2	2.15	0.47
39:5n:26:LEU:HD21	39:5n:39:PHE:HB3	1.95	0.47
55:8A:44:PRO:HG3	58:8D:111:PHE:CZ	2.49	0.47
57:8C:30:GLY:HA2	57:8C:42:LEU:HB3	1.97	0.47
74:8C:306:CDL:HB61	74:8C:306:CDL:H712	1.77	0.47
74:8D:201:CDL:H711	74:8D:201:CDL:HB61	1.46	0.47
1:1A:27:LEU:HG	8:1H:59:GLU:HB2	1.96	0.47
7:1G:13:VAL:HB	7:1G:33:VAL:HG21	1.96	0.47
7:1G:114:CYS:C	7:1G:116:LEU:H	2.23	0.47
7:1G:118:ASP:O	7:1G:122:MET:HG2	2.15	0.47
7:1G:366:THR:HG22	7:1G:370:GLY:HA3	1.96	0.47
12:1L:136:ASN:OD1	12:1L:139:GLN:HB2	2.15	0.47
13:1M:371:PRO:HG2	13:1M:448:THR:HG21	1.97	0.47
16:1P:171:ILE:HD12	79:1P:501:NDP:C3N	2.45	0.47
49:3E:223:VAL:HB	48:3Q:107:GLY:HA3	1.97	0.47
86:4A:603:PGV:H031	74:4D:201:CDL:HA31	1.97	0.47
58:4D:51:LEU:O	58:4D:56:LYS:NZ	2.47	0.47
5:5E:206:PRO:HB3	6:5F:23:THR:HG21	1.96	0.47
6:5F:56:ILE:HG23	6:5F:235:CYS:SG	2.55	0.47
6:5F:202:LYS:HE2	6:5F:361:GLN:HB2	1.96	0.47
9:5I:132:VAL:HG11	9:5I:169:ILE:HD11	1.96	0.47
10:5J:103:MET:HE2	10:5J:103:MET:HB2	1.81	0.47
38:5m:127:SER:O	38:5m:127:SER:OG	2.32	0.47
1:1A:48:ARG:HE	10:1J:78:MET:HA	1.80	0.47
6:1F:343:ILE:HD12	6:1F:344:VAL:N	2.30	0.47
7:1G:54:MET:HE1	7:1G:94:MET:HE2	1.95	0.47
12:1L:188:TRP:CE3	12:1L:212:PRO:HG3	2.50	0.47
12:1L:384:PRO:HA	12:1L:389:PHE:CD1	2.49	0.47
13:1M:16:TRP:CE2	76:1M:903:3PE:H281	2.50	0.47
30:1e:37:LYS:HG3	33:1h:133:ILE:HG21	1.97	0.47
76:3A:502:3PE:H32	76:3A:502:3PE:H322	1.66	0.47
49:3E:233:GLY:HA3	49:3E:245:ALA:HA	1.96	0.47
54:3X:4:ARG:HG2	54:3X:5:PHE:CD1	2.50	0.47
2:5B:95:LYS:HD2	3:5C:154:GLY:HA2	1.97	0.47
4:5D:246:THR:HB	4:5D:249:ASP:HB2	1.97	0.47
20:5T:54:MET:HE2	20:5T:54:MET:HB3	1.77	0.47
22:5W:57:LYS:HE2	22:5W:57:LYS:HA	1.97	0.47
22:5W:117:ASP:OD1	22:5W:120:SER:OG	2.16	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:5k:71:LYS:HA	36:5k:71:LYS:HD3	1.74	0.47
55:8A:13:LYS:HE2	55:8A:500:PRO:HB2	1.97	0.47
57:8C:19:THR:O	57:8C:23:SER:OG	2.28	0.47
10:1J:60:TYR:HE2	11:1K:38:LEU:HD13	1.79	0.47
12:1L:316:THR:HA	12:1L:319:ILE:HG12	1.97	0.47
23:1X:152:GLU:OE1	23:1X:152:GLU:N	2.45	0.47
74:1X:201:CDL:H531	74:1X:201:CDL:H352	1.97	0.47
34:1i:60:ILE:HA	34:1i:63:THR:HB	1.97	0.47
46:3O:180:ASP:N	46:3O:180:ASP:OD1	2.47	0.47
47:3P:24:PRO:O	47:3P:224:TYR:OH	2.22	0.47
49:3R:219:HIS:CE1	49:3R:239:HIS:HE1	2.33	0.47
55:4A:383:MET:HE2	55:4A:421:VAL:HG13	1.95	0.47
58:4D:78:TRP:CD1	74:4D:201:CDL:H202	2.50	0.47
63:4I:22:VAL:O	63:4I:26:ILE:HG12	2.15	0.47
5:5E:192:SER:HB3	44:5s:38:TYR:CE1	2.50	0.47
7:5G:378:LEU:HB3	7:5G:451:VAL:HG12	1.97	0.47
7:5G:575:ASN:ND2	7:5G:577:GLU:OE2	2.48	0.47
12:5L:121:LEU:HD22	12:5L:246:LEU:HD23	1.96	0.47
15:5O:203:GLU:O	15:5O:207:LYS:HG2	2.15	0.47
37:5l:132:GLN:NE2	37:5l:155:HIS:HB3	2.29	0.47
39:5n:65:GLN:OE1	39:5n:65:GLN:N	2.45	0.47
67:8M:39:HIS:HD1	67:8M:39:HIS:C	2.22	0.47
15:1O:309:ASN:OD1	28:1c:3:TYR:OH	2.33	0.46
16:1P:109:VAL:HA	16:1P:113:ILE:HD12	1.97	0.46
31:1f:18:VAL:HA	31:1f:21:VAL:HG22	1.96	0.46
36:1k:18:TYR:HH	36:1k:46:ARG:HB3	1.79	0.46
37:1l:128:VAL:HG12	37:1l:129:GLY:O	2.15	0.46
46:3B:195:VAL:O	46:3B:199:PHE:HB2	2.15	0.46
48:3D:104:GLY:O	48:3D:291:LYS:NZ	2.41	0.46
48:3Q:27:ARG:HB2	48:3Q:55:CYS:HB2	1.98	0.46
57:4C:7:ALA:HB1	57:4C:72:THR:HG21	1.97	0.46
59:4E:18:TYR:HE2	59:4E:32:GLY:HA3	1.80	0.46
62:4H:57:ARG:HA	62:4H:60:TYR:CD2	2.50	0.46
6:5F:365:CYS:HB2	70:5F:502:SF4:S3	2.55	0.46
9:5I:70:TYR:C	9:5I:72:SER:H	2.23	0.46
11:5K:47:ILE:HG12	14:5N:79:LEU:HD13	1.96	0.46
76:5K:101:3PE:H3C1	76:5K:101:3PE:H2C1	1.97	0.46
14:5N:107:GLY:HA2	14:5N:111:PHE:O	2.15	0.46
21:5V:21:GLU:O	21:5V:25:ILE:HG13	2.15	0.46
55:8A:171:MET:HG2	57:8C:8:TYR:CE1	2.50	0.46
55:8A:218:THR:HG21	61:8G:55:ILE:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:8B:29:MET:HE3	63:8I:32:ALA:HB1	1.96	0.46
57:8C:62:ILE:HG13	86:8C:307:PGV:H21	1.96	0.46
58:8D:110:THR:HG23	58:8D:115:TRP:CD1	2.51	0.46
59:8E:44:GLU:OE1	59:8E:46:LYS:HG2	2.14	0.46
11:1K:95:LEU:HD23	11:1K:95:LEU:H	1.80	0.46
12:1L:478:PRO:HD3	40:1o:86:TRP:CH2	2.50	0.46
12:1L:546:GLN:HA	12:1L:550:SER:HB3	1.96	0.46
13:1M:186:LEU:HD23	13:1M:253:LEU:HD22	1.97	0.46
19:1S:17:GLU:HG2	19:1S:67:ARG:HH21	1.80	0.46
20:1T:56:ASP:N	20:1T:56:ASP:OD1	2.47	0.46
20:1U:54:MET:HG3	20:1U:76:ILE:HG21	1.97	0.46
23:1X:78:ALA:O	23:1X:82:THR:HG23	2.15	0.46
24:1Y:50:GLU:H	24:1Y:50:GLU:CD	2.23	0.46
30:1e:82:ARG:O	30:1e:86:ILE:HG13	2.15	0.46
45:3A:328:ASN:HB3	45:3A:427:PRO:HB2	1.97	0.46
49:3R:195:LEU:HD13	49:3R:248:ARG:HE	1.81	0.46
49:3R:199:GLN:NE2	49:3R:257:ASN:HD22	2.05	0.46
55:4A:204:ALA:O	55:4A:208:MET:HG3	2.14	0.46
90:4A:609:PSC:H02	90:4A:609:PSC:H21	1.49	0.46
56:4B:59:GLN:O	56:4B:63:THR:OG1	2.30	0.46
60:4F:76:LYS:HE3	60:4F:76:LYS:HB2	1.76	0.46
1:5A:33:LYS:HG2	8:5H:61:LEU:HD11	1.97	0.46
2:5B:32:LYS:HD3	2:5B:32:LYS:HA	1.72	0.46
5:5E:148:CYS:N	6:5F:105:CYS:SG	2.88	0.46
8:5H:183:MET:HE3	69:5I:204:PC1:H272	1.97	0.46
12:5L:264:TYR:CD2	12:5L:265:PRO:HD3	2.51	0.46
12:5L:367:PRO:O	12:5L:371:THR:HG23	2.15	0.46
14:5N:104:MET:HG3	14:5N:111:PHE:HB3	1.96	0.46
20:5U:63:PRO:HB3	37:5l:61:TRP:CD2	2.50	0.46
33:5h:7:ARG:NH2	34:5i:31:GLU:O	2.48	0.46
33:5h:50:ALA:HB2	41:5p:60:TYR:CE1	2.51	0.46
62:8H:14:ALA:HB3	62:8H:63:PHE:CE1	2.51	0.46
2:1B:95:LYS:NZ	4:1D:80:ILE:O	2.48	0.46
7:1G:366:THR:HG21	7:1G:450:MET:SD	2.55	0.46
8:1H:70:MET:HB2	8:1H:122:ALA:HB2	1.97	0.46
12:1L:128:MET:HE2	12:1L:147:VAL:HG21	1.98	0.46
12:1L:147:VAL:CG1	12:1L:252:MET:HG3	2.45	0.46
15:1O:189:PRO:HA	15:1O:192:MET:HE2	1.97	0.46
34:1i:41:PRO:HA	34:1i:44:GLN:HG2	1.97	0.46
48:3D:262:ASP:OD2	48:3D:264:THR:OG1	2.31	0.46
49:3E:169:TRP:HD1	49:3E:214:ILE:HD11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:3G:102:CDL:H121	74:3G:102:CDL:H512	1.96	0.46
45:3N:151:ASP:OD2	49:3R:80:HIS:NE2	2.48	0.46
55:4A:174:PRO:HB2	60:4F:35:ALA:HB2	1.97	0.46
56:4B:64:ILE:HG13	56:4B:65:TRP:N	2.30	0.46
68:4N:81:ASP:OD1	68:4N:81:ASP:N	2.48	0.46
4:5D:135:GLN:O	4:5D:139:VAL:HG23	2.14	0.46
4:5D:238:ARG:HE	4:5D:238:ARG:HB3	1.58	0.46
5:5E:184:PRO:HG2	44:5s:44:HIS:HD2	1.79	0.46
7:5G:259:ASN:HB2	7:5G:390:LEU:HD13	1.97	0.46
8:5H:189:THR:HG22	8:5H:270:PHE:HZ	1.80	0.46
12:5L:288:THR:HG21	12:5L:307:SER:HB3	1.96	0.46
13:5M:70:THR:HA	13:5M:103:GLN:NE2	2.30	0.46
76:5M:501:3PE:H3A1	14:5N:284:MET:HG3	1.97	0.46
39:5n:13:GLN:O	39:5n:17:ARG:HG2	2.15	0.46
42:5q:25:ARG:HD2	42:5q:74:PHE:HZ	1.79	0.46
55:8A:469:ILE:HD11	66:8L:25:MET:HG2	1.97	0.46
58:8D:52:SER:OG	58:8D:55:GLU:HG3	2.15	0.46
4:1D:223:ASP:HB3	4:1D:305:ARG:HH22	1.80	0.46
6:1F:157:TYR:OH	6:1F:174:ASP:OD1	2.23	0.46
7:1G:196:SER:OG	7:1G:265:ASP:OD2	2.27	0.46
9:1I:8:ARG:NH2	43:1r:111:TYR:O	2.48	0.46
12:1L:4:PHE:HZ	12:1L:87:VAL:HG11	1.81	0.46
12:1L:481:THR:OG1	40:1o:91:HIS:ND1	2.27	0.46
16:1P:136:ASN:ND2	16:1P:292:MET:H	2.13	0.46
16:1P:322:ARG:NH2	16:1P:329:SER:HB3	2.30	0.46
23:1X:165:ARG:HH12	29:1d:87:ASP:CG	2.23	0.46
44:1s:35:ASN:ND2	44:1s:35:ASN:C	2.70	0.46
47:3C:29:SER:HB2	74:3G:102:CDL:H731	1.97	0.46
47:3P:186:PRO:HA	47:3P:189:ILE:HD12	1.98	0.46
48:3Q:23:HIS:NE2	48:3Q:199:ASP:OD2	2.39	0.46
54:3Y:14:ALA:O	54:3Y:18:ILE:HG12	2.15	0.46
55:4A:157:SER:HB2	55:4A:195:LEU:HD22	1.98	0.46
55:4A:383:MET:HE3	55:4A:421:VAL:HG22	1.96	0.46
4:5D:34:ASN:ND2	15:5O:158:VAL:HG22	2.31	0.46
7:5G:38:PRO:HB2	7:5G:54:MET:HG2	1.97	0.46
7:5G:350:PRO:HB3	7:5G:464:THR:HG22	1.98	0.46
11:5K:33:LEU:HD12	11:5K:36:MET:HE2	1.98	0.46
12:5L:400:ASN:ND2	12:5L:489:THR:HG21	2.30	0.46
13:5M:71:TRP:NE1	13:5M:75:LEU:HD11	2.31	0.46
34:5i:99:ARG:HA	41:5p:115:ARG:HA	1.96	0.46
55:8A:425:PHE:HD1	55:8A:428:GLN:NE2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:8B:303:CDL:H811	74:8B:303:CDL:H262	1.97	0.46
74:8C:306:CDL:H822	74:8C:306:CDL:H612	1.98	0.46
58:8D:78:TRP:O	58:8D:82:VAL:HG23	2.16	0.46
86:8G:101:PGV:H51	86:8G:101:PGV:H011	1.96	0.46
3:1C:38:GLN:HG2	21:1V:102:LEU:HD21	1.98	0.46
6:1F:112:ARG:HB3	6:1F:145:GLU:HG3	1.98	0.46
12:1L:375:ILE:HD13	12:1L:462:ILE:HD11	1.96	0.46
13:1M:122:PHE:HE1	13:1M:206:LYS:HD3	1.81	0.46
23:1X:82:THR:HA	23:1X:85:TRP:NE1	2.30	0.46
24:1Y:72:THR:HB	24:1Y:92:GLY:HA2	1.97	0.46
28:1c:33:LYS:O	28:1c:33:LYS:HD3	2.15	0.46
45:3A:77:LYS:HE3	45:3A:77:LYS:HB2	1.69	0.46
47:3P:318:ARG:O	47:3P:322:GLN:HG3	2.15	0.46
74:4B:302:CDL:H442	74:4B:302:CDL:H182	1.96	0.46
61:4G:68:THR:OG1	61:4G:69:LEU:N	2.49	0.46
6:5F:42:TRP:CD2	6:5F:161:LEU:HD13	2.51	0.46
12:5L:194:ASN:ND2	41:5p:106:GLN:OE1	2.49	0.46
13:5M:24:TRP:CD2	13:5M:81:GLN:HB3	2.51	0.46
13:5M:269:MET:HE2	13:5M:399:ASN:ND2	2.31	0.46
15:5O:165:PRO:O	15:5O:248:TRP:NE1	2.38	0.46
16:5P:262:ALA:HA	16:5P:265:TRP:CD1	2.50	0.46
23:5X:168:PHE:CE1	74:5X:201:CDL:H172	2.51	0.46
32:5g:58:MET:HE2	32:5g:59:ARG:HG2	1.97	0.46
63:8I:61:GLU:OE2	63:8I:64:ARG:NH1	2.49	0.46
64:8J:36:MET:HA	64:8J:36:MET:HE3	1.96	0.46
66:8L:35:ALA:O	66:8L:39:ILE:HG13	2.15	0.46
3:1C:88:ASN:HB2	21:1V:110:GLN:NE2	2.31	0.46
10:1J:163:ILE:HG21	14:1N:12:THR:HG21	1.97	0.46
76:1M:902:3PE:O12	76:1M:902:3PE:N	2.35	0.46
16:1P:299:GLY:N	16:1P:302:ASP:OD2	2.48	0.46
19:1S:91:GLU:OE1	19:1S:91:GLU:N	2.37	0.46
21:1V:98:PRO:HD2	21:1V:99:TRP:CZ3	2.50	0.46
30:1e:1:PRO:HG2	30:1e:4:ASP:HA	1.97	0.46
46:3B:35:ILE:HD13	46:3B:206:LEU:HB3	1.98	0.46
50:3F:57:GLU:OE2	50:3F:60:ARG:NH2	2.38	0.46
54:3X:48:ILE:O	54:3X:51:LYS:HG2	2.16	0.46
76:5A:201:3PE:H2E1	76:5A:201:3PE:H2A2	1.98	0.46
3:5C:179:GLU:OE1	16:5P:37:HIS:NE2	2.48	0.46
7:5G:200:ILE:HG22	17:5Q:45:MET:HE1	1.96	0.46
8:5H:263:THR:O	8:5H:267:THR:OG1	2.26	0.46
17:5Q:33:ARG:HD3	17:5Q:79:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:5S:84:ASP:OD1	19:5S:84:ASP:N	2.49	0.46
69:5d:202:PC1:H321	69:5d:202:PC1:H112	1.97	0.46
58:8D:124:LEU:O	58:8D:140:TYR:OH	2.32	0.46
59:8E:46:LYS:HD3	59:8E:46:LYS:N	2.30	0.46
2:1B:37:VAL:HG21	69:1B:202:PC1:H342	1.96	0.46
8:1H:35:LYS:HD2	9:1I:47:THR:HB	1.97	0.46
12:1L:562:LEU:HB2	12:1L:563:PRO:HD3	1.97	0.46
15:1O:135:LEU:HD21	15:1O:149:VAL:HG23	1.98	0.46
16:1P:59:LEU:HA	16:1P:62:MET:HG3	1.97	0.46
38:1m:112:GLU:O	38:1m:116:GLN:HG2	2.15	0.46
47:3C:221:HIS:O	47:3C:225:THR:OG1	2.17	0.46
48:3D:125:CYS:SG	85:3D:501:HEC:HBB3	2.56	0.46
49:3E:183:GLU:O	49:3E:187:GLU:HG2	2.15	0.46
45:3N:34:THR:HG22	45:3N:102:LEU:HD23	1.96	0.46
47:3P:116:GLY:C	84:3P:502:HEM:HBC2	2.40	0.46
55:4A:101:SER:O	55:4A:156:SER:HB2	2.16	0.46
55:4A:286:ILE:HG13	55:4A:287:VAL:HG13	1.98	0.46
55:4A:379:TYR:HA	55:4A:383:MET:SD	2.56	0.46
12:5L:336:LYS:HD3	12:5L:336:LYS:HA	1.71	0.46
22:5W:19:PRO:HG3	22:5W:23:ARG:HH12	1.80	0.46
22:5W:64:ARG:O	22:5W:68:MET:HG2	2.16	0.46
74:5X:201:CDL:H452	74:5X:201:CDL:H251	1.97	0.46
55:8A:348:PHE:HD1	55:8A:380:VAL:HG13	1.80	0.46
58:8D:122:ARG:HG3	65:8K:53:TRP:CD2	2.50	0.46
60:8F:1:ALA:HB1	61:8G:14:ARG:HH12	1.80	0.46
61:8G:61:SER:O	61:8G:61:SER:OG	2.30	0.46
2:1B:77:ARG:CZ	2:1B:82:GLN:HB2	2.46	0.46
8:1H:125:SER:C	8:1H:127:TYR:H	2.23	0.46
10:1J:57:PHE:HA	10:1J:61:LEU:HB2	1.97	0.46
15:1O:94:TYR:OH	15:1O:151:HIS:ND1	2.42	0.46
17:1Q:23:THR:HG23	17:1Q:25:VAL:HG23	1.96	0.46
38:1m:47:LEU:HB3	39:1n:165:LEU:HD13	1.96	0.46
45:3A:99:ILE:HD12	45:3A:113:LEU:HG	1.97	0.46
47:3C:144:THR:O	47:3C:148:ASN:HB2	2.16	0.46
48:3Q:132:THR:O	52:3U:21:ARG:NH2	2.37	0.46
55:4A:49:GLY:HA3	55:4A:53:ILE:HG21	1.98	0.46
55:4A:158:ILE:HD13	86:4C:301:PGV:H331	1.98	0.46
55:4A:186:TRP:HZ3	55:4A:278:MET:HE3	1.80	0.46
56:4B:133:MET:HE3	56:4B:133:MET:HB3	1.74	0.46
1:5A:73:LEU:HD23	1:5A:73:LEU:HA	1.76	0.46
5:5E:145:LEU:O	5:5E:160:TYR:OH	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5G:284:ILE:HG23	7:5G:294:THR:HG21	1.98	0.46
7:5G:344:CYS:HB3	7:5G:510:GLY:O	2.15	0.46
7:5G:371:VAL:HG23	7:5G:377:ILE:HD11	1.97	0.46
8:5H:70:MET:HE3	10:5J:27:ILE:HD12	1.97	0.46
11:5K:2:PRO:HG3	30:5e:72:MET:HE1	1.98	0.46
14:5N:3:PRO:O	14:5N:7:THR:HG23	2.16	0.46
14:5N:236:LYS:HD3	14:5N:314:LYS:HB3	1.97	0.46
15:5O:230:ASP:OD1	15:5O:230:ASP:N	2.37	0.46
16:5P:136:ASN:ND2	16:5P:292:MET:H	2.13	0.46
20:5T:35:HIS:N	20:5T:39:ASP:OD2	2.48	0.46
22:5W:115:PRO:HB2	22:5W:121:LYS:HG2	1.98	0.46
55:8A:254:ILE:HD12	55:8A:341:ALA:HA	1.98	0.46
56:8B:110:TYR:HB2	56:8B:116:LEU:HB3	1.97	0.46
57:8C:60:ASP:O	57:8C:64:GLU:HG3	2.16	0.46
58:8D:23:PRO:O	59:8E:66:ARG:NH1	2.48	0.46
60:8F:16:LEU:HD11	60:8F:31:TYR:HE2	1.81	0.46
2:1B:80:PRO:HD3	4:1D:54:GLN:NE2	2.31	0.46
5:1E:114:ASP:OD1	5:1E:114:ASP:N	2.48	0.46
12:1L:128:MET:HE2	12:1L:128:MET:HB2	1.83	0.46
12:1L:128:MET:HE3	12:1L:251:THR:HG22	1.97	0.46
12:1L:359:MET:HB3	12:1L:430:ALA:HA	1.98	0.46
12:1L:561:ILE:HD12	69:1L:704:PC1:H291	1.98	0.46
14:1N:3:PRO:O	14:1N:7:THR:HG23	2.15	0.46
24:1Y:48:PHE:HA	76:1Y:805:3PE:H222	1.98	0.46
39:1n:156:ALA:HB1	39:1n:161:ASP:OD1	2.16	0.46
41:1p:35:ILE:HD12	41:1p:35:ILE:H	1.80	0.46
48:3D:129:HIS:HE1	48:3D:199:PRO:HD2	1.81	0.46
47:3P:89:MET:HE2	47:3P:235:MET:HG2	1.98	0.46
74:3P:504:CDL:H312	74:3T:101:CDL:H731	1.98	0.46
69:5B:203:PC1:H221	69:5B:203:PC1:H2	1.36	0.46
3:5C:41:GLN:HG2	3:5C:51:PHE:HE2	1.80	0.46
6:5F:404:ILE:HG22	7:5G:53:ARG:NH1	2.31	0.46
7:5G:314:ASP:O	7:5G:520:LYS:N	2.47	0.46
10:5J:173:ARG:CZ	10:5J:173:ARG:HB3	2.45	0.46
12:5L:100:ILE:O	12:5L:104:SER:OG	2.30	0.46
15:5O:9:VAL:HG12	15:5O:10:LEU:HD23	1.97	0.46
16:5P:203:GLN:NE2	16:5P:232:GLY:O	2.47	0.46
17:5Q:116:LYS:HD3	17:5Q:116:LYS:HA	1.74	0.46
74:5X:201:CDL:HA21	74:5X:201:CDL:H541	1.97	0.46
55:8A:276:ALA:O	55:8A:280:ILE:HG13	2.15	0.46
55:8A:507:GLU:HA	57:8C:5:THR:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:44:SER:OG	8:1H:54:LYS:HD3	2.16	0.46
6:1F:338:ASP:OD1	6:1F:341:THR:OG1	2.34	0.46
7:1G:349:PHE:H	7:1G:509:PRO:HB2	1.81	0.46
12:1L:403:TYR:HE2	40:1o:18:PRO:HG2	1.81	0.46
13:1M:225:ILE:HD13	13:1M:331:ASN:HB2	1.98	0.46
16:1P:10:LYS:HD2	22:1W:127:ASP:OD2	2.16	0.46
16:1P:206:TYR:OH	16:1P:316:GLU:OE1	2.33	0.46
23:1X:162:HIS:NE2	33:1h:99:GLU:OE1	2.46	0.46
29:1d:86:ARG:HD3	82:1h:201:AME:HE1	1.97	0.46
46:3B:207:ILE:HD13	46:3B:383:GLY:HA2	1.97	0.46
45:3N:244:ARG:HG2	51:3T:10:MET:HG2	1.98	0.46
47:3P:89:MET:HE1	74:3T:101:CDL:H792	1.98	0.46
55:4A:253:MET:HE3	55:4A:392:GLY:HA3	1.98	0.46
56:4B:98:LYS:HE3	56:4B:98:LYS:HB2	1.65	0.46
56:4B:110:TYR:HB2	56:4B:116:LEU:HB3	1.98	0.46
4:5D:350:LYS:HD2	7:5G:117:GLN:HB3	1.98	0.46
7:5G:110:GLN:HG3	7:5G:113:GLU:HG3	1.98	0.46
7:5G:218:ARG:HD2	7:5G:220:TRP:CH2	2.51	0.46
12:5L:23:ASN:ND2	74:5L:702:CDL:H321	2.27	0.46
12:5L:73:THR:HG22	41:5p:102:VAL:HG11	1.98	0.46
13:5M:46:GLY:HA2	32:5g:84:ARG:HH11	1.81	0.46
16:5P:278:TRP:CH2	76:5P:403:3PE:H251	2.51	0.46
22:5W:66:MET:HE2	22:5W:66:MET:HA	1.98	0.46
28:5c:45:ARG:NH2	29:5d:19:ARG:HB2	2.31	0.46
29:5d:8:ARG:HH22	29:5d:82:MET:HE1	1.80	0.46
39:5n:153:LEU:HD13	39:5n:165:LEU:HB2	1.98	0.46
39:5n:166:TRP:O	39:5n:170:VAL:HG12	2.16	0.46
56:8B:150:ILE:HB	56:8B:184:LEU:HB3	1.98	0.46
59:8E:13:ALA:O	59:8E:17:THR:HG23	2.15	0.46
4:1D:94:LYS:HD2	4:1D:102:TYR:HE2	1.81	0.45
4:1D:230:THR:HG23	4:1D:298:LEU:HD21	1.96	0.45
10:1J:17:PHE:HA	10:1J:20:PHE:CE2	2.51	0.45
14:1N:246:VAL:HG21	76:1O:401:3PE:H272	1.97	0.45
15:1O:253:ASP:N	15:1O:253:ASP:OD1	2.49	0.45
30:1e:63:VAL:HA	30:1e:66:LEU:HD12	1.98	0.45
74:1h:202:CDL:HB62	74:1h:202:CDL:H712	1.60	0.45
34:1i:6:ASP:N	34:1i:6:ASP:OD1	2.49	0.45
39:1n:30:CYS:O	39:1n:32:HIS:N	2.47	0.45
42:1q:66:THR:HG23	42:1q:74:PHE:HD1	1.80	0.45
48:3D:313:ARG:HD3	51:3G:28:PHE:CE2	2.50	0.45
55:4A:328:HIS:HB2	56:4B:45:MET:HE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:4B:103:GLN:HA	56:4B:104:TRP:HA	1.69	0.45
57:4C:138:LEU:HD21	57:4C:250:LEU:HD21	1.97	0.45
59:4E:25:ASP:C	59:4E:25:ASP:OD1	2.59	0.45
2:5B:80:PRO:HD3	4:5D:54:GLN:NE2	2.31	0.45
11:5K:6:MET:O	11:5K:10:MET:HG3	2.16	0.45
12:5L:355:ASP:OD2	12:5L:357:ARG:NH2	2.47	0.45
14:5N:102:LEU:HD13	14:5N:142:LEU:HG	1.97	0.45
20:5T:34:SER:HB3	20:5T:40:LEU:HD11	1.99	0.45
20:5U:87:TYR:HA	34:5i:19:ARG:HD3	1.98	0.45
23:5X:144:ARG:HD2	30:5e:57:ILE:HD11	1.98	0.45
29:5d:99:GLU:H	29:5d:99:GLU:CD	2.22	0.45
40:5o:96:LYS:HE3	40:5o:96:LYS:HB2	1.81	0.45
56:8B:160:LEU:HD11	56:8B:175:ILE:HG23	1.98	0.45
62:8H:19:ARG:NH1	68:8N:55:ASN:OD1	2.48	0.45
1:1A:90:MET:SD	69:1A:202:PC1:H322	2.56	0.45
12:1L:336:LYS:HD3	12:1L:336:LYS:HA	1.75	0.45
76:1M:903:3PE:H2B2	76:1O:401:3PE:H252	1.98	0.45
17:1Q:34:LYS:HE2	17:1Q:34:LYS:HB2	1.79	0.45
25:1Z:94:GLU:O	25:1Z:98:MET:HB2	2.17	0.45
45:3A:358:LYS:O	45:3A:362:ARG:HG3	2.16	0.45
47:3C:119:LEU:HD22	84:3C:502:HEM:HBB2	1.98	0.45
47:3C:126:THR:HG21	47:3C:186:PRO:HG3	1.97	0.45
49:3E:140:MET:HE2	49:3E:140:MET:HB3	1.87	0.45
46:3O:334:GLY:HA2	46:3O:434:PRO:HD3	1.97	0.45
56:4B:12:ALA:HB3	56:4B:18:GLU:HG3	1.98	0.45
6:5F:89:ARG:HG2	17:5Q:124:TRP:CD1	2.50	0.45
7:5G:107:ILE:HG22	9:5I:104:ARG:HD3	1.98	0.45
16:5P:59:LEU:HA	16:5P:62:MET:HG3	1.98	0.45
23:5X:146:ARG:NH2	30:5e:38:GLU:OE1	2.47	0.45
55:8A:474:GLU:OE1	55:8A:480:ARG:NH2	2.49	0.45
57:8C:41:LEU:HD21	86:8J:101:PGV:H211	1.98	0.45
57:8C:171:VAL:HG23	86:8G:101:PGV:H181	1.98	0.45
74:8C:306:CDL:H822	74:8C:306:CDL:H591	1.96	0.45
59:8E:101:PRO:O	59:8E:105:GLY:N	2.46	0.45
64:8J:34:VAL:O	64:8J:38:LEU:HB2	2.16	0.45
1:1A:94:LEU:HD12	10:1J:147:TYR:HE1	1.81	0.45
3:1C:35:LYS:HD3	3:1C:36:TYR:CZ	2.52	0.45
3:1C:66:ASP:O	21:1V:82:GLN:NE2	2.48	0.45
4:1D:157:HIS:O	4:1D:161:ILE:HG12	2.16	0.45
8:1H:296:LEU:HD13	69:1I:201:PC1:H351	1.98	0.45
12:1L:154:LEU:HD13	12:1L:243:VAL:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:264:TYR:CD2	12:1L:265:PRO:HD3	2.52	0.45
13:1M:123:GLU:OE2	13:1M:157:SER:OG	2.25	0.45
15:1O:195:THR:HG23	15:1O:198:TYR:H	1.80	0.45
16:1P:85:VAL:HG11	16:1P:121:SER:HA	1.98	0.45
23:1X:46:ARG:NH2	33:1h:142:ASP:OD1	2.49	0.45
23:1X:168:PHE:CE1	74:1X:201:CDL:H172	2.50	0.45
76:1Y:802:3PE:H2	76:1Y:802:3PE:H221	1.35	0.45
33:1h:142:ASP:N	33:1h:142:ASP:OD1	2.49	0.45
37:1l:62:TYR:HD1	37:1l:63:ASP:N	2.13	0.45
45:3A:30:SER:HB2	45:3A:32:GLN:HG3	1.98	0.45
74:3C:503:CDL:OB2	76:3C:504:3PE:H2	2.16	0.45
76:3C:504:3PE:H281	76:3C:504:3PE:H242	1.97	0.45
49:3E:263:TYR:HB3	49:3E:273:VAL:HG22	1.98	0.45
46:3O:109:VAL:HB	46:3O:119:LEU:HD23	1.99	0.45
48:3Q:34:LYS:O	48:3Q:38:SER:OG	2.33	0.45
50:3S:67:ASP:OD2	50:3S:71:ARG:NH1	2.50	0.45
55:4A:374:VAL:HG23	55:4A:438:ARG:HD2	1.97	0.45
61:4G:17:ARG:HH22	92:4G:102:PEK:H011	1.81	0.45
12:5L:513:PHE:HE1	39:5n:29:TRP:HB3	1.81	0.45
15:5O:320:LYS:HB2	28:5c:12:PRO:HG3	1.99	0.45
32:5g:114:ASP:OD1	32:5g:116:ASN:ND2	2.49	0.45
34:5i:13:GLN:HE22	39:5n:156:ALA:N	2.10	0.45
37:5l:50:LEU:HD11	37:5l:76:PRO:HB2	1.99	0.45
37:5l:127:PRO:HG3	40:5o:3:HIS:CG	2.50	0.45
55:8A:239:GLY:O	55:8A:243:VAL:HG23	2.15	0.45
55:8A:440:TYR:CZ	56:8B:205:SER:HA	2.51	0.45
56:8B:162:SER:HB3	56:8B:197:SER:H	1.82	0.45
4:1D:350:LYS:HD2	7:1G:117:GLN:HB3	1.98	0.45
5:1E:206:PRO:HD2	44:1s:33:PHE:CZ	2.51	0.45
6:1F:61:LYS:HB2	6:1F:61:LYS:HE2	1.78	0.45
6:1F:142:PHE:HB3	6:1F:145:GLU:HB2	1.97	0.45
12:1L:49:VAL:HG22	41:1p:32:LEU:HD13	1.98	0.45
16:1P:48:PRO:HB3	16:1P:84:VAL:HG11	1.97	0.45
16:1P:168:PRO:HA	16:1P:230:PHE:O	2.17	0.45
20:1U:51:ILE:HG21	20:1U:67:ALA:HB1	1.98	0.45
31:1f:45:LYS:O	41:1p:68:ARG:NH2	2.49	0.45
34:1i:15:ARG:HG3	34:1i:19:ARG:HD2	1.97	0.45
35:1j:67:LEU:HB2	40:1o:110:ARG:NH2	2.31	0.45
45:3A:142:ASP:OD1	49:3E:80:HIS:ND1	2.50	0.45
47:3C:244:LEU:HD13	48:3D:294:GLY:HA2	1.96	0.45
47:3C:302:ILE:O	47:3C:305:PRO:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:3O:157:ALA:O	46:3O:161:GLU:HG2	2.16	0.45
46:3O:307:PHE:CD2	49:3V:52:ARG:HD2	2.52	0.45
49:3R:229:GLY:HA2	49:3R:235:TYR:HD1	1.81	0.45
55:4A:254:ILE:HG13	55:4A:344:PHE:CD2	2.52	0.45
74:4D:201:CDL:H512	74:4D:201:CDL:HB4	1.41	0.45
59:4E:6:GLU:HB3	59:4E:10:GLU:OE2	2.15	0.45
7:5G:684:MET:HE2	7:5G:684:MET:HA	1.98	0.45
8:5H:99:ASN:N	69:5H:402:PC1:O12	2.30	0.45
10:5J:126:VAL:HG23	25:5Z:122:GLY:HA3	1.98	0.45
12:5L:173:LEU:HD22	76:5L:701:3PE:H332	1.99	0.45
12:5L:207:GLU:HG2	12:5L:269:THR:HG21	1.97	0.45
12:5L:271:LYS:HE3	12:5L:271:LYS:HB3	1.73	0.45
12:5L:291:CYS:O	12:5L:295:GLN:HG2	2.17	0.45
13:5M:70:THR:HA	13:5M:103:GLN:HE21	1.81	0.45
13:5M:71:TRP:CD1	69:5M:505:PC1:H2C2	2.51	0.45
14:5N:207:ILE:O	14:5N:211:MET:HG3	2.17	0.45
16:5P:83:LYS:HE2	16:5P:83:LYS:HB3	1.68	0.45
23:5X:29:HIS:HB3	23:5X:119:PRO:HD2	1.99	0.45
34:5i:64:TYR:O	34:5i:68:ILE:HG12	2.17	0.45
55:8A:71:MET:HB2	55:8A:72:PRO:HD3	1.98	0.45
55:8A:96:ARG:HE	57:8C:11:VAL:HG11	1.80	0.45
56:8B:59:GLN:O	56:8B:63:THR:OG1	2.29	0.45
60:8F:25:ARG:HH11	60:8F:25:ARG:HG3	1.80	0.45
4:1D:257:GLY:HA3	4:1D:372:GLY:HA2	1.99	0.45
6:1F:16:LYS:HE2	6:1F:16:LYS:HB2	1.72	0.45
8:1H:31:MET:HG2	9:1I:41:LEU:HB2	1.98	0.45
8:1H:208:VAL:HG13	8:1H:209:SER:N	2.30	0.45
12:1L:49:VAL:O	12:1L:53:MET:HG3	2.17	0.45
12:1L:467:ILE:O	12:1L:471:ASN:ND2	2.32	0.45
13:1M:325:MET:HB2	13:1M:440:HIS:HB3	1.99	0.45
15:1O:267:LEU:HD23	15:1O:267:LEU:HA	1.80	0.45
16:1P:208:VAL:O	16:1P:212:LYS:HG3	2.16	0.45
19:1S:21:HIS:O	19:1S:62:PRO:HA	2.16	0.45
20:1T:33:ASN:HA	20:1T:72:CYS:SG	2.57	0.45
20:1U:83:LYS:HA	20:1U:83:LYS:HD2	1.77	0.45
74:1X:201:CDL:H671	74:1X:201:CDL:H392	1.98	0.45
49:3E:237:PRO:CB	48:3Q:144:ARG:HD2	2.42	0.45
47:3P:244:LEU:HD13	48:3Q:205:GLY:HA2	1.98	0.45
55:4A:61:HIS:HE1	87:4A:604:HEA:NB	2.14	0.45
55:4A:243:VAL:HG13	87:4A:605:HEA:C3C	2.46	0.45
55:4A:406:ASN:HB3	55:4A:409:TRP:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:4C:43:LEU:HD21	86:4C:303:PGV:H262	1.98	0.45
74:4C:306:CDL:H222	74:4C:306:CDL:H372	1.99	0.45
60:4F:74:VAL:HG13	60:4F:91:LEU:HD13	1.98	0.45
4:5D:3:GLN:NE2	13:5M:135:ARG:O	2.35	0.45
7:5G:148:THR:HG22	7:5G:208:LEU:HD22	1.99	0.45
12:5L:49:VAL:HB	12:5L:50:PRO:HD3	1.98	0.45
12:5L:213:LEU:HB2	12:5L:273:VAL:HG21	1.99	0.45
69:5d:202:PC1:H222	69:5d:202:PC1:H2	1.59	0.45
34:5i:14:LEU:HD13	39:5n:169:ILE:HG21	1.96	0.45
55:8A:74:MET:HE3	55:8A:389:ILE:HG13	1.97	0.45
2:1B:144:ILE:HG13	2:1B:163:LEU:HB2	1.98	0.45
3:1C:68:THR:HA	21:1V:82:GLN:HE21	1.81	0.45
4:1D:112:MET:HG3	4:1D:181:TYR:CZ	2.52	0.45
5:1E:145:LEU:O	5:1E:160:TYR:OH	2.33	0.45
7:1G:147:LYS:HB2	7:1G:211:LYS:HG3	1.99	0.45
7:1G:326:GLU:OE2	7:1G:620:ARG:NH1	2.50	0.45
10:1J:68:PHE:HE1	11:1K:71:ALA:HB1	1.82	0.45
11:1K:34:GLU:OE2	11:1K:71:ALA:HB2	2.16	0.45
12:1L:358:LYS:HG3	39:1n:79:TYR:CE1	2.52	0.45
13:1M:188:ASN:OD1	13:1M:256:TYR:OH	2.32	0.45
14:1N:242:SER:O	14:1N:246:VAL:HG23	2.15	0.45
15:1O:75:GLY:HA2	15:1O:99:TRP:CD2	2.51	0.45
15:1O:260:ARG:HA	15:1O:263:VAL:HB	1.98	0.45
16:1P:297:LEU:HD23	16:1P:297:LEU:HA	1.84	0.45
17:1Q:37:ILE:HG12	17:1Q:92:ALA:HB1	1.99	0.45
34:1i:82:HIS:HD2	41:1p:44:VAL:HG21	1.80	0.45
40:1o:102:GLU:O	40:1o:106:ARG:HG2	2.16	0.45
45:3A:172:GLU:HG2	45:3A:173:ASN:N	2.32	0.45
46:3B:217:LYS:O	46:3B:221:GLU:HG2	2.17	0.45
46:3B:290:ASN:O	46:3B:297:GLN:NE2	2.47	0.45
47:3C:24:PRO:O	47:3C:224:TYR:OH	2.28	0.45
46:3O:95:LYS:HE3	49:3V:71:ASN:OD1	2.16	0.45
47:3P:377:LEU:HG	50:3S:20:TYR:HE2	1.82	0.45
66:4L:38:PHE:HD1	66:4L:41:ARG:HD3	1.82	0.45
1:5A:41:PHE:CE1	2:5B:99:ALA:HB2	2.51	0.45
7:5G:278:ARG:HH12	7:5G:568:GLU:CD	2.25	0.45
7:5G:534:ARG:HH22	42:5q:145:LYS:HE3	1.80	0.45
7:5G:620:ARG:NH1	7:5G:633:TYR:OH	2.50	0.45
8:5H:195:ARG:HD3	8:5H:231:ILE:HG12	1.98	0.45
12:5L:301:ILE:HD13	12:5L:426:ILE:HG13	1.99	0.45
14:5N:265:MET:HE1	23:5X:166:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5O:50:HIS:NE2	15:5O:125:GLU:OE1	2.49	0.45
20:5T:51:ILE:O	20:5T:54:MET:HG2	2.16	0.45
23:5X:165:ARG:HH12	29:5d:87:ASP:CG	2.24	0.45
24:5Y:89:TYR:CD2	24:5Y:125:LYS:HB2	2.51	0.45
40:5o:18:PRO:HA	40:5o:21:MET:HE3	1.98	0.45
56:8B:12:ALA:HB3	56:8B:18:GLU:HG3	1.98	0.45
56:8B:139:ASP:N	56:8B:139:ASP:OD1	2.47	0.45
59:8E:31:LYS:O	59:8E:35:THR:HG22	2.17	0.45
1:1A:18:VAL:CG2	8:1H:222:MET:HE1	2.46	0.45
4:1D:209:ASP:O	4:1D:213:GLU:HG2	2.17	0.45
7:1G:628:PRO:HG2	19:1S:57:CYS:HB2	1.97	0.45
8:1H:310:MET:HG3	8:1H:311:THR:HG23	1.99	0.45
12:1L:484:LEU:HD12	12:1L:484:LEU:HA	1.77	0.45
14:1N:84:TRP:HB2	30:1e:18:THR:HA	1.98	0.45
15:1O:7:ALA:HB1	15:1O:12:GLU:HG2	1.98	0.45
23:1X:132:THR:HG22	23:1X:134:ARG:H	1.82	0.45
25:1Z:68:ARG:NH1	25:1Z:72:MET:SD	2.89	0.45
32:1g:62:PHE:HA	32:1g:66:PHE:HD2	1.82	0.45
35:1j:20:SER:O	35:1j:24:GLN:HG3	2.17	0.45
49:3E:261:PRO:HG2	49:3E:273:VAL:HG21	1.99	0.45
46:3O:148:LYS:NZ	46:3O:180:ASP:OD1	2.39	0.45
48:3Q:224:ARG:NH1	74:3T:101:CDL:OB3	2.49	0.45
52:3U:32:LYS:HB2	52:3U:32:LYS:HE3	1.57	0.45
56:4B:160:LEU:HD11	56:4B:175:ILE:HG23	1.99	0.45
56:4B:217:LYS:HG2	56:4B:221:LYS:HE3	1.98	0.45
65:4K:19:ALA:O	65:4K:23:THR:OG1	2.20	0.45
5:5E:56:ARG:HD2	5:5E:56:ARG:HA	1.71	0.45
7:5G:596:ASP:N	7:5G:596:ASP:OD1	2.50	0.45
9:5I:74:GLU:HA	18:5R:40:ALA:HB1	1.98	0.45
12:5L:66:TRP:HZ3	76:5L:703:3PE:H3D1	1.81	0.45
12:5L:332:HIS:HA	12:5L:335:PHE:CZ	2.52	0.45
13:5M:60:SER:HB2	13:5M:457:PRO:HA	1.98	0.45
16:5P:26:ALA:HB3	16:5P:47:VAL:HG13	1.99	0.45
20:5T:73:PRO:O	20:5T:77:VAL:HG23	2.16	0.45
33:5h:73:ARG:NE	69:5h:203:PC1:O14	2.39	0.45
42:5q:6:VAL:HG11	74:5q:203:CDL:HB32	1.99	0.45
42:5q:25:ARG:HD2	42:5q:74:PHE:CZ	2.52	0.45
56:8B:28:LEU:HD11	74:8B:303:CDL:H592	1.98	0.45
62:8H:56:TYR:CZ	68:8N:80:PRO:HD2	2.52	0.45
4:1D:28:TRP:NE1	11:1K:97:GLN:OE1	2.50	0.45
9:1I:30:LEU:HD13	69:1I:201:PC1:H261	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1I:143:THR:OG1	9:1I:146:GLU:HG3	2.17	0.45
12:1L:503:GLU:O	12:1L:507:THR:OG1	2.34	0.45
12:1L:526:LEU:HD12	12:1L:530:PRO:HG2	1.98	0.45
30:1e:53:LYS:HE2	30:1e:53:LYS:HB3	1.68	0.45
32:1g:84:ARG:O	32:1g:86:GLN:NE2	2.50	0.45
34:1i:9:LEU:O	34:1i:13:GLN:HG3	2.17	0.45
36:1k:19:LYS:HA	36:1k:19:LYS:HD3	1.66	0.45
38:1m:24:ILE:HB	38:1m:29:ARG:HD3	1.99	0.45
45:3A:156:THR:HA	49:3E:85:VAL:HG21	1.98	0.45
51:3G:66:GLN:O	51:3G:70:LYS:HG3	2.16	0.45
55:4A:62:ALA:HB2	87:4A:604:HEA:HBD1	1.98	0.45
55:4A:328:HIS:CE1	63:4I:17:LEU:HD22	2.52	0.45
58:4D:78:TRP:CZ2	58:4D:79:LYS:HG3	2.52	0.45
21:5V:93:MET:HE3	21:5V:93:MET:HB3	1.88	0.45
33:5h:75:ILE:HG23	33:5h:79:PHE:HE1	1.82	0.45
36:5k:13:MET:HG3	36:5k:13:MET:O	2.17	0.45
55:8A:97:MET:HE2	55:8A:159:LEU:HB3	1.99	0.45
55:8A:254:ILE:HG13	55:8A:344:PHE:CD2	2.51	0.45
4:1D:117:ALA:HB2	4:1D:367:ILE:HG12	1.98	0.45
8:1H:266:LEU:O	8:1H:269:THR:OG1	2.27	0.45
9:1I:14:MET:HE2	9:1I:14:MET:HA	1.98	0.45
12:1L:22:SER:HA	12:1L:27:TYR:HB2	1.99	0.45
12:1L:78:LEU:HD11	74:1L:702:CDL:H662	1.99	0.45
14:1N:316:GLN:HA	15:1O:302:ARG:HH12	1.81	0.45
39:1n:138:GLN:NE2	39:1n:142:GLU:OE1	2.49	0.45
41:1p:47:ALA:O	41:1p:51:ILE:HG13	2.16	0.45
45:3A:34:THR:OG1	46:3B:373:GLU:OE2	2.29	0.45
47:3C:27:ILE:HA	47:3C:208:PRO:HD3	1.99	0.45
48:3D:106:LEU:HD22	48:3D:295:LEU:HB2	1.97	0.45
45:3N:50:GLU:OE1	45:3N:50:GLU:N	2.50	0.45
48:3Q:212:MET:SD	76:3Q:502:3PE:H352	2.56	0.45
49:3R:147:LEU:O	49:3R:151:LYS:HD3	2.17	0.45
60:4F:94:HIS:ND1	60:4F:95:GLN:HG3	2.32	0.45
76:5A:201:3PE:H362	27:5b:11:ALA:HB1	1.99	0.45
3:5C:45:PHE:CD1	3:5C:47:GLU:HG3	2.52	0.45
4:5D:409:HIS:HB3	4:5D:413:ASP:HB2	1.99	0.45
6:5F:21:ILE:HB	6:5F:269:GLU:OE2	2.17	0.45
7:5G:366:THR:O	7:5G:367:THR:OG1	2.30	0.45
7:5G:366:THR:HG21	7:5G:450:MET:SD	2.57	0.45
8:5H:61:LEU:HD23	8:5H:61:LEU:HA	1.83	0.45
8:5H:121:TRP:C	8:5H:121:TRP:CD1	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:5H:401:CDL:H511	74:5H:401:CDL:HB4	1.44	0.45
9:5I:28:THR:HG22	69:5I:204:PC1:H221	1.98	0.45
9:5I:158:GLY:O	9:5I:162:GLU:HB2	2.17	0.45
10:5J:175:ASN:H	14:5N:48:PHE:HD2	1.64	0.45
19:5S:64:LEU:HD21	19:5S:90:LEU:HD12	1.98	0.45
23:5X:22:SER:OG	23:5X:89:ASP:OD1	2.18	0.45
31:5f:31:ASP:C	31:5f:31:ASP:OD1	2.60	0.45
35:5j:35:TRP:CH2	35:5j:39:ARG:HD3	2.51	0.45
55:8A:406:ASN:HD22	55:8A:409:TRP:CD1	2.32	0.45
58:8D:51:LEU:O	58:8D:56:LYS:NZ	2.50	0.45
4:1D:149:ASN:HD22	4:1D:370:PRO:HB2	1.82	0.45
74:1H:401:CDL:HA32	16:1P:187:TRP:CZ3	2.52	0.45
10:1J:5:ILE:HG21	25:1Z:142:TRP:CZ2	2.51	0.45
12:1L:66:TRP:HZ3	76:1L:703:3PE:H3D1	1.82	0.45
76:1L:701:3PE:H321	76:1L:701:3PE:H32	1.20	0.45
13:1M:297:VAL:O	13:1M:301:ILE:HG13	2.17	0.45
76:1M:903:3PE:H321	76:1M:903:3PE:H31	1.25	0.45
14:1N:24:SER:HB3	30:1e:1:PRO:HD3	1.99	0.45
14:1N:332:LEU:HD22	74:1d:203:CDL:H451	1.99	0.45
16:1P:172:PHE:HB2	16:1P:179:LEU:HD22	1.99	0.45
17:1Q:5:THR:HG23	17:1Q:6:GLN:HG2	1.99	0.45
17:1Q:33:ARG:NH2	17:1Q:60:ASP:O	2.50	0.45
31:1f:42:LEU:HB3	41:1p:70:VAL:HG12	1.99	0.45
39:1n:57:VAL:HG21	45:3A:230:ALA:HB3	1.99	0.45
48:3Q:116:ILE:HG12	85:3Q:501:HEC:HMA3	1.99	0.45
49:3R:242:HIS:HB2	49:3R:250:ARG:HG2	1.99	0.45
57:4C:171:VAL:HG23	86:4G:101:PGV:H181	1.99	0.45
1:5A:92:LEU:O	1:5A:96:ILE:HD12	2.17	0.45
5:5E:106:THR:HA	5:5E:109:MET:HB3	1.99	0.45
6:5F:215:VAL:H	6:5F:220:THR:HG21	1.82	0.45
8:5H:281:ARG:HB3	8:5H:284:GLN:HG3	1.97	0.45
12:5L:433:GLY:O	36:5k:59:ASN:ND2	2.46	0.45
19:5S:50:LEU:HD23	19:5S:52:ILE:HG13	1.99	0.45
19:5S:91:GLU:O	19:5S:95:SER:HB3	2.17	0.45
22:5W:62:LYS:HD3	22:5W:62:LYS:HA	1.68	0.45
39:5n:107:HIS:CD2	39:5n:108:PRO:HD2	2.52	0.45
55:8A:288:TRP:HH2	86:8B:302:PGV:H222	1.81	0.45
68:8N:11:LYS:HA	68:8N:11:LYS:HD2	1.83	0.45
1:1A:40:GLY:HA2	2:1B:103:VAL:HG13	1.99	0.44
3:1C:125:LYS:HB3	3:1C:125:LYS:HE3	1.80	0.44
7:1G:399:TRP:HA	7:1G:404:LEU:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:473:PRO:HG2	12:1L:475:MET:SD	2.57	0.44
12:1L:562:LEU:HD11	76:1M:906:3PE:H3I3	1.99	0.44
20:1T:60:PHE:HE1	20:1T:80:ILE:HG23	1.82	0.44
23:1X:131:LYS:HD3	23:1X:131:LYS:HA	1.82	0.44
47:3C:233:LEU:HD21	48:3D:304:LEU:HB3	1.98	0.44
46:3O:120:MET:HE3	46:3O:219:VAL:HG11	1.99	0.44
47:3P:132:VAL:HA	47:3P:139:SER:HB3	1.99	0.44
55:4A:8:TYR:O	57:4C:13:PRO:HB3	2.17	0.44
55:4A:168:ILE:HG22	55:4A:178:GLN:HE22	1.82	0.44
55:4A:202:LEU:HD22	55:4A:238:PHE:CE2	2.52	0.44
55:4A:466:MET:HB3	67:4M:23:PHE:CE1	2.52	0.44
7:5G:332:LYS:HG3	7:5G:343:LEU:HD13	1.99	0.44
9:5I:175:TYR:CE1	43:5r:38:PRO:HG3	2.52	0.44
13:5M:97:THR:HG21	76:5M:502:3PE:H2C2	1.99	0.44
15:5O:25:ILE:HG23	15:5O:168:VAL:HB	1.99	0.44
33:5h:108:LEU:HD23	33:5h:108:LEU:HA	1.75	0.44
42:5q:66:THR:HG23	42:5q:74:PHE:HD1	1.82	0.44
58:8D:135:SER:OG	58:8D:140:TYR:OH	2.28	0.44
5:1E:53:LEU:HD13	44:1s:52:LEU:HD12	1.99	0.44
5:1E:67:ASN:OD1	5:1E:81:TYR:OH	2.21	0.44
5:1E:105:THR:O	5:1E:109:MET:N	2.49	0.44
7:1G:227:SER:HB2	7:1G:583:THR:HB	1.99	0.44
7:1G:242:THR:HG21	7:1G:586:ALA:HB1	1.99	0.44
9:1I:175:TYR:CZ	43:1r:38:PRO:HG3	2.52	0.44
12:1L:439:PRO:HB3	35:1j:12:ARG:HG2	1.99	0.44
13:1M:59:ASP:OD2	13:1M:245:ARG:NH1	2.43	0.44
14:1N:159:MET:HG2	14:1N:278:MET:HE1	1.97	0.44
20:1T:8:LEU:N	20:1T:88:GLU:OE1	2.50	0.44
45:3A:40:TRP:CZ2	45:3A:377:GLU:HA	2.52	0.44
50:3F:84:GLN:HB2	74:3G:102:CDL:HA22	1.99	0.44
49:3R:163:LYS:HA	49:3R:163:LYS:HD2	1.79	0.44
55:4A:1:FME:HE3	86:4A:601:PGV:H251	1.98	0.44
55:4A:177:SER:OG	55:4A:178:GLN:N	2.50	0.44
64:4J:41:GLY:HA2	86:4J:101:PGV:H92	1.99	0.44
68:4N:32:TYR:O	68:4N:33:VAL:HG12	2.17	0.44
2:5B:50:PHE:CE1	2:5B:103:VAL:HG21	2.52	0.44
2:5B:55:CYS:HB3	2:5B:116:MET:HE2	1.99	0.44
69:5B:202:PC1:H3G1	69:5B:203:PC1:H3E1	1.99	0.44
7:5G:163:ALA:HA	7:5G:167:ALA:HB3	2.00	0.44
12:5L:11:THR:HA	12:5L:14:ILE:HD12	1.99	0.44
13:5M:86:LYS:HB2	13:5M:86:LYS:HE3	1.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:5M:89:THR:HA	13:5M:92:LYS:HE2	1.99	0.44
13:5M:130:LEU:HD13	13:5M:150:LEU:HD13	1.99	0.44
14:5N:78:LEU:HD22	14:5N:84:TRP:CZ2	2.53	0.44
16:5P:168:PRO:HA	16:5P:230:PHE:O	2.17	0.44
20:5T:12:LYS:NZ	20:5T:16:LEU:HB2	2.32	0.44
37:5l:129:GLY:HA2	40:5o:21:MET:HE1	1.98	0.44
41:5p:78:GLU:HG2	41:5p:79:LYS:HG2	2.00	0.44
55:8A:126:TRP:HZ3	87:8A:604:HEA:HBD2	1.83	0.44
57:8C:137:LEU:HD23	57:8C:137:LEU:HA	1.84	0.44
60:8F:49:VAL:HB	60:8F:91:LEU:HD12	1.99	0.44
68:8N:40:ASN:HB3	68:8N:43:VAL:HG22	2.00	0.44
3:1C:68:THR:N	21:1V:86:GLU:OE1	2.50	0.44
6:1F:8:LYS:HE2	6:1F:8:LYS:HB2	1.75	0.44
6:1F:137:TYR:HB3	6:1F:192:LEU:HD11	2.00	0.44
6:1F:188:GLU:HA	72:1F:501:FMN:O2'	2.17	0.44
8:1H:215:TYR:HD1	8:1H:219:PRO:HB2	1.81	0.44
12:1L:233:LEU:HB3	12:1L:234:PRO:HD3	1.98	0.44
14:1N:99:THR:HG23	14:1N:154:MET:HE1	1.98	0.44
37:1l:21:ALA:HA	37:1l:31:VAL:HG22	2.00	0.44
41:1p:96:LYS:HE3	41:1p:96:LYS:HB3	1.68	0.44
46:3B:97:SER:HA	49:3I:69:GLY:HA3	1.99	0.44
48:3Q:160:MET:HE1	48:3Q:163:PRO:HG3	2.00	0.44
53:3W:44:GLU:HG3	53:3W:51:LEU:HD12	1.98	0.44
55:4A:240:HIS:O	55:4A:243:VAL:HB	2.18	0.44
56:4B:43:SER:O	56:4B:47:THR:OG1	2.21	0.44
86:4M:101:PGV:H152	86:4M:101:PGV:H292	2.00	0.44
1:5A:90:MET:SD	69:5A:203:PC1:H322	2.56	0.44
4:5D:238:ARG:NH2	4:5D:412:ALA:HB1	2.33	0.44
6:5F:254:LYS:HD3	6:5F:332:ALA:HB2	1.98	0.44
7:5G:114:CYS:C	7:5G:116:LEU:H	2.25	0.44
7:5G:324:ASP:OD1	7:5G:324:ASP:N	2.39	0.44
12:5L:338:MET:HB2	12:5L:338:MET:HE3	1.73	0.44
13:5M:94:LEU:O	13:5M:98:MET:HG2	2.17	0.44
13:5M:263:MET:HE3	38:5m:101:TYR:HD1	1.83	0.44
30:5e:50:ARG:HE	30:5e:50:ARG:HB3	1.70	0.44
40:5o:24:PHE:CE2	40:5o:107:LEU:HB3	2.52	0.44
55:8A:8:TYR:O	57:8C:13:PRO:HB3	2.18	0.44
74:8C:306:CDL:H512	74:8C:306:CDL:HB4	1.43	0.44
61:8G:44:ARG:HH12	61:8G:84:GLN:HG3	1.82	0.44
63:8I:17:LEU:HD21	90:8I:101:PSC:H52	1.99	0.44
5:1E:199:LEU:HD23	6:1F:26:TYR:HD2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:105:CYS:N	70:1G:801:SF4:S4	2.91	0.44
8:1H:312:ALA:HA	27:1b:41:ALA:HB2	1.99	0.44
9:1I:105:ARG:NH2	18:1R:86:TYR:O	2.47	0.44
10:1J:124:ASP:OD1	10:1J:125:TRP:N	2.50	0.44
11:1K:16:LEU:HA	11:1K:36:MET:HE2	1.99	0.44
12:1L:186:MET:HG3	12:1L:196:TRP:NE1	2.32	0.44
20:1U:21:LEU:HD11	36:1k:18:TYR:CE2	2.52	0.44
25:1Z:69:ILE:HD11	27:1b:49:PRO:HB2	2.00	0.44
38:1m:29:ARG:O	39:1n:8:TYR:OH	2.25	0.44
46:3O:258:VAL:HA	46:3O:323:GLY:HA3	1.99	0.44
48:3Q:158:ILE:HG12	48:3Q:160:MET:H	1.83	0.44
48:3Q:160:MET:HE2	48:3Q:160:MET:HB3	1.90	0.44
48:3Q:211:MET:HG2	53:3W:35:PHE:CZ	2.53	0.44
55:4A:316:THR:HA	55:4A:319:LYS:HG3	1.99	0.44
55:4A:473:TRP:NE1	66:4L:22:LEU:HB2	2.33	0.44
86:4L:101:PGV:H211	86:4L:101:PGV:H251	1.98	0.44
1:5A:68:GLU:H	1:5A:68:GLU:HG2	1.65	0.44
3:5C:100:ARG:O	43:5r:100:ILE:HG22	2.18	0.44
6:5F:144:ASN:ND2	44:5s:43:HIS:HD2	2.15	0.44
9:5I:43:ARG:CZ	43:5r:19:LEU:HD22	2.48	0.44
9:5I:114:THR:HG21	9:5I:144:HIS:CE1	2.52	0.44
10:5J:103:MET:HG3	11:5K:6:MET:HE3	1.99	0.44
12:5L:356:ILE:HA	12:5L:359:MET:SD	2.57	0.44
14:5N:183:SER:O	14:5N:187:MET:HG2	2.18	0.44
23:5X:33:ALA:HB2	23:5X:119:PRO:HG3	2.00	0.44
23:5X:63:ASN:OD1	25:5Z:81:ARG:NH2	2.48	0.44
34:5i:89:VAL:O	34:5i:95:THR:OG1	2.33	0.44
55:8A:116:SER:O	66:8L:43:GLN:NE2	2.51	0.44
55:8A:473:TRP:HB2	66:8L:25:MET:HE1	1.99	0.44
56:8B:110:TYR:CD1	56:8B:116:LEU:HD23	2.53	0.44
58:8D:82:VAL:HG22	74:8D:201:CDL:OB7	2.18	0.44
58:8D:129:ALA:HB3	58:8D:134:PHE:H	1.82	0.44
8:1H:24:GLU:HB2	8:1H:271:LEU:HD22	1.98	0.44
13:1M:231:LEU:HA	13:1M:235:LEU:HB2	1.99	0.44
14:1N:40:MET:O	14:1N:43:VAL:HG22	2.17	0.44
25:1Z:98:MET:HG3	25:1Z:104:TRP:CE2	2.52	0.44
33:1h:40:ILE:HG22	74:1h:202:CDL:OB9	2.18	0.44
38:1m:36:LEU:HG	39:1n:7:ALA:HA	1.99	0.44
48:3D:150:LYS:HB2	48:3D:150:LYS:HE3	1.69	0.44
45:3N:144:SER:HB2	49:3V:47:ARG:HG3	2.00	0.44
45:3N:445:ARG:NH2	76:3N:501:3PE:O12	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:4A:183:LEU:HD11	55:4A:273:MET:HG2	1.99	0.44
1:5A:1:FME:O1	1:5A:2:ASN:N	2.51	0.44
2:5B:71:ARG:HA	8:5H:37:PRO:HA	1.98	0.44
4:5D:268:ASP:HB2	4:5D:285:VAL:HG11	2.00	0.44
7:5G:584:LYS:HE2	17:5Q:36:ARG:HD2	2.00	0.44
8:5H:179:TRP:O	8:5H:183:MET:HG3	2.18	0.44
8:5H:296:LEU:HD13	69:5I:201:PC1:H351	2.00	0.44
10:5J:122:LEU:HD23	10:5J:126:VAL:HG21	2.00	0.44
12:5L:161:ARG:NH2	12:5L:238:GLU:OE2	2.33	0.44
12:5L:297:ASP:O	12:5L:301:ILE:HG22	2.18	0.44
13:5M:26:ASN:OD1	31:5f:13:HIS:NE2	2.50	0.44
13:5M:69:THR:HG22	13:5M:234:VAL:HG11	1.98	0.44
13:5M:319:HIS:HA	13:5M:322:THR:HG22	1.99	0.44
16:5P:169:SER:HB3	16:5P:231:VAL:HG23	1.99	0.44
76:5Y:806:3PE:H2F1	38:5m:93:GLY:HA3	1.99	0.44
25:5Z:68:ARG:O	25:5Z:72:MET:HG3	2.17	0.44
34:5i:74:VAL:C	34:5i:77:PRO:HD2	2.43	0.44
56:8B:98:LYS:HB2	56:8B:98:LYS:HE3	1.61	0.44
56:8B:106:TRP:CD1	56:8B:207:MET:HG2	2.52	0.44
59:8E:82:TYR:HA	59:8E:85:VAL:HG22	1.99	0.44
1:1A:1:FME:O1	1:1A:2:ASN:N	2.51	0.44
4:1D:234:ILE:HD12	8:1H:277:TYR:HB3	2.00	0.44
5:1E:192:SER:OG	5:1E:193:CYS:N	2.51	0.44
6:1F:245:PHE:HB3	6:1F:271:GLU:HG3	2.00	0.44
6:1F:349:ARG:O	6:1F:349:ARG:NH1	2.51	0.44
7:1G:140:LYS:HG2	7:1G:150:MET:HG3	1.99	0.44
9:1I:70:TYR:C	9:1I:72:SER:H	2.26	0.44
12:1L:253:VAL:HB	12:1L:310:LEU:HD11	2.00	0.44
12:1L:596:MET:O	12:1L:599:MET:N	2.47	0.44
13:1M:459:TYR:HD2	32:1g:84:ARG:HD3	1.82	0.44
20:1T:55:GLU:OE2	20:1T:61:GLU:HA	2.17	0.44
20:1U:21:LEU:HD11	36:1k:18:TYR:CZ	2.52	0.44
21:1V:34:LEU:HD22	21:1V:44:ARG:HA	1.98	0.44
21:1V:92:LYS:HA	21:1V:95:ARG:NH1	2.33	0.44
25:1Z:98:MET:HG3	25:1Z:104:TRP:NE1	2.32	0.44
26:1a:69:ILE:C	26:1a:69:ILE:HD12	2.42	0.44
39:1n:100:GLU:H	39:1n:100:GLU:HG3	1.68	0.44
40:1o:96:LYS:O	40:1o:99:LYS:HB2	2.17	0.44
47:3P:28:SER:HB2	74:3P:504:CDL:HA22	2.00	0.44
47:3P:126:THR:HG21	84:3P:501:HEM:HBB2	1.99	0.44
76:3Q:502:3PE:H3B1	69:3R:302:PC1:H3F1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:3S:85:GLU:O	50:3S:85:GLU:HG2	2.18	0.44
54:3X:38:TRP:HA	69:3X:101:PC1:H32	1.99	0.44
54:3Y:45:VAL:HG23	54:3Y:48:ILE:HB	2.00	0.44
55:4A:25:TRP:HB2	86:4L:101:PGV:H281	1.98	0.44
57:4C:19:THR:O	57:4C:23:SER:OG	2.31	0.44
60:4F:16:LEU:HD12	60:4F:16:LEU:HA	1.71	0.44
1:5A:5:LEU:HD23	8:5H:2:PHE:HD2	1.83	0.44
2:5B:46:TRP:HB3	2:5B:77:ARG:HG2	2.00	0.44
2:5B:77:ARG:NH2	2:5B:82:GLN:HE21	2.15	0.44
7:5G:453:LEU:HD21	7:5G:458:LEU:HD21	1.99	0.44
10:5J:78:MET:HE2	10:5J:78:MET:HA	1.98	0.44
12:5L:435:PRO:HG2	36:5k:56:PHE:CG	2.52	0.44
13:5M:225:ILE:HD13	13:5M:331:ASN:HB2	2.00	0.44
14:5N:172:GLN:NE2	14:5N:177:LYS:HD3	2.33	0.44
19:5S:21:HIS:O	19:5S:62:PRO:HA	2.17	0.44
22:5W:22:SER:HB3	22:5W:31:ARG:HH12	1.83	0.44
56:8B:23:PHE:CZ	56:8B:80:SER:HB2	2.52	0.44
56:8B:106:TRP:NE1	56:8B:207:MET:HG2	2.33	0.44
2:1B:179:ARG:O	16:1P:103:ASN:ND2	2.33	0.44
4:1D:6:PRO:HB3	4:1D:10:TRP:CD1	2.53	0.44
4:1D:231:ASN:O	9:1I:29:GLU:HG3	2.18	0.44
7:1G:281:GLN:HG2	7:1G:592:LEU:HD12	1.99	0.44
12:1L:139:GLN:HG3	76:1L:703:3PE:H3H1	2.00	0.44
12:1L:385:TYR:OH	35:1j:43:ASP:O	2.24	0.44
12:1L:529:TYR:HB3	12:1L:530:PRO:HD3	2.00	0.44
69:1M:904:PC1:H221	69:1M:904:PC1:H2	1.44	0.44
14:1N:44:LEU:HD22	14:1N:122:ILE:HG21	1.99	0.44
14:1N:325:LEU:N	74:1d:203:CDL:OB3	2.47	0.44
15:1O:65:ASP:HB3	28:1c:2:PHE:CE1	2.52	0.44
16:1P:73:TRP:HA	16:1P:80:SER:HB2	1.98	0.44
22:1W:62:LYS:HD3	22:1W:62:LYS:HA	1.73	0.44
41:1p:126:LYS:HA	41:1p:126:LYS:HD2	1.59	0.44
45:3A:53:ASN:HB3	45:3A:173:ASN:HD22	1.82	0.44
45:3A:191:LYS:O	45:3A:195:MET:HG3	2.17	0.44
53:3W:57:GLN:HE21	53:3W:57:GLN:HB3	1.64	0.44
55:4A:452:THR:O	55:4A:456:MET:HG2	2.18	0.44
63:4I:9:MET:HE3	63:4I:9:MET:HB2	1.90	0.44
4:5D:148:LEU:HD23	4:5D:174:ARG:HG2	1.99	0.44
4:5D:339:LYS:NZ	9:5I:129:ASP:OD1	2.48	0.44
12:5L:9:LEU:HD23	12:5L:9:LEU:HA	1.87	0.44
14:5N:135:LYS:HD2	14:5N:187:MET:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:5P:172:PHE:HB2	16:5P:179:LEU:HD23	1.99	0.44
16:5P:256:TYR:HE1	16:5P:258:LEU:HD12	1.81	0.44
30:5e:37:LYS:HG3	33:5h:133:ILE:HG21	2.00	0.44
36:5k:61:SER:OG	36:5k:62:PHE:N	2.51	0.44
55:8A:211:THR:HG22	55:8A:215:LEU:HD12	1.99	0.44
55:8A:467:LEU:O	55:8A:471:ILE:HG13	2.18	0.44
55:8A:512:ASN:HD21	60:8F:38:ALA:HA	1.83	0.44
86:8A:601:PGV:H142	57:8C:22:LEU:HD21	2.00	0.44
86:8C:303:PGV:H202	86:8C:303:PGV:H011	1.25	0.44
4:1D:260:LEU:HD22	4:1D:265:ILE:HD13	1.99	0.44
6:1F:374:LYS:HB3	7:1G:132:GLU:HG2	2.00	0.44
7:1G:350:PRO:HB3	7:1G:464:THR:HG22	2.00	0.44
8:1H:150:LEU:HG	8:1H:185:TRP:CZ3	2.53	0.44
10:1J:60:TYR:HE2	11:1K:38:LEU:HB2	1.83	0.44
13:1M:6:ILE:HD12	31:1f:23:GLY:HA2	2.00	0.44
13:1M:76:MET:SD	13:1M:230:VAL:HB	2.58	0.44
13:1M:457:PRO:HA	32:1g:84:ARG:HH22	1.82	0.44
17:1Q:70:MET:HE3	17:1Q:70:MET:HB3	1.80	0.44
36:1k:18:TYR:OH	36:1k:46:ARG:HB3	2.17	0.44
37:1l:3:HIS:ND1	37:1l:4:VAL:HG22	2.33	0.44
47:3C:168:PHE:CZ	49:3R:151:LYS:HB2	2.53	0.44
46:3O:34:VAL:HG11	46:3O:386:ALA:HB1	2.00	0.44
46:3O:284:HIS:NE2	46:3O:363:LYS:HD2	2.32	0.44
46:3O:369:LEU:HD11	46:3O:399:LEU:HD11	1.99	0.44
47:3P:35:SER:OG	47:3P:228:ASP:OD2	2.25	0.44
48:3Q:27:ARG:NH2	53:3W:59:LYS:HG2	2.33	0.44
55:4A:44:PRO:HG3	58:4D:111:PHE:CZ	2.53	0.44
56:4B:62:GLU:HA	56:4B:65:TRP:CE2	2.52	0.44
74:4B:302:CDL:H631	74:4B:302:CDL:H141	1.99	0.44
74:4B:302:CDL:HA61	74:4B:302:CDL:H311	1.64	0.44
57:4C:88:ILE:HG12	74:4C:306:CDL:H621	2.00	0.44
74:4C:306:CDL:H541	74:4C:306:CDL:H162	1.98	0.44
67:4M:11:SER:HG	67:4M:14:GLU:HG3	1.82	0.44
2:5B:125:TYR:CE1	9:5I:88:PRO:HB2	2.49	0.44
3:5C:45:PHE:HD1	3:5C:47:GLU:HG3	1.82	0.44
3:5C:175:ARG:NH1	3:5C:186:GLU:OE2	2.51	0.44
6:5F:343:ILE:HD12	6:5F:344:VAL:N	2.33	0.44
6:5F:381:LYS:HB3	6:5F:381:LYS:HE2	1.85	0.44
7:5G:595:GLU:OE1	7:5G:597:TRP:NE1	2.51	0.44
13:5M:2:LEU:HD21	74:5X:201:CDL:H552	1.99	0.44
14:5N:19:LEU:O	14:5N:23:SER:OG	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:5N:157:MET:O	14:5N:161:SER:OG	2.34	0.44
14:5N:250:SER:O	14:5N:259:GLY:HA3	2.17	0.44
15:5O:25:ILE:O	15:5O:123:VAL:HA	2.18	0.44
20:5U:18:VAL:O	20:5U:21:LEU:HB2	2.18	0.44
22:5W:27:GLU:HA	22:5W:30:ARG:HB3	1.99	0.44
24:5Y:139:LYS:HE3	24:5Y:140:VAL:HG13	2.00	0.44
87:8A:603:HEA:HHC	87:8A:603:HEA:C13	2.43	0.44
74:8B:303:CDL:HB31	63:8I:39:VAL:HG22	1.99	0.44
1:1A:24:LEU:HD21	69:1B:202:PC1:H3C2	2.00	0.44
2:1B:77:ARG:CG	2:1B:78:ALA:H	2.31	0.44
5:1E:104:THR:O	5:1E:104:THR:OG1	2.28	0.44
5:1E:107:PRO:HG2	5:1E:148:CYS:SG	2.58	0.44
7:1G:456:SER:HB3	7:1G:495:ARG:HD3	2.00	0.44
18:1R:27:ARG:HE	18:1R:27:ARG:HB3	1.63	0.44
46:3O:95:LYS:HB2	46:3O:110:GLU:OE2	2.18	0.44
47:3P:227:LYS:HG3	48:3Q:223:LYS:HE2	2.00	0.44
48:3Q:224:ARG:HD3	51:3T:26:PHE:CE2	2.52	0.44
49:3R:150:SER:HB3	49:3R:170:ARG:H	1.83	0.44
49:3R:207:LYS:HE3	49:3R:210:TRP:HZ3	1.83	0.44
55:4A:92:MET:HE3	55:4A:163:ASN:ND2	2.33	0.44
55:4A:507:GLU:HA	57:4C:5:THR:HG22	2.00	0.44
56:4B:139:ASP:OD1	56:4B:139:ASP:N	2.48	0.44
61:4G:26:PRO:HB2	92:4G:102:PEK:H383	1.99	0.44
5:5E:196:ALA:H	6:5F:264:HIS:HB3	1.81	0.44
7:5G:58:GLU:OE1	7:5G:83:SER:OG	2.32	0.44
12:5L:118:PHE:O	12:5L:122:VAL:HG23	2.18	0.44
12:5L:429:PHE:O	12:5L:436:ARG:NH2	2.51	0.44
12:5L:546:GLN:HA	12:5L:550:SER:HB3	2.00	0.44
22:5W:61:ASP:OD1	22:5W:61:ASP:N	2.51	0.44
76:5Y:806:3PE:H31	76:5Y:806:3PE:H321	1.63	0.44
27:5b:34:LEU:HD12	27:5b:34:LEU:O	2.18	0.44
39:5n:58:LYS:HA	39:5n:61:GLN:HB3	1.99	0.44
55:8A:270:TYR:CD1	60:8F:67:SER:HB2	2.52	0.44
56:8B:127:ASP:N	56:8B:127:ASP:OD1	2.51	0.44
86:8B:301:PGV:H281	74:8D:201:CDL:H261	2.00	0.44
58:8D:98:TRP:HD1	58:8D:102:TYR:CD2	2.35	0.44
59:8E:11:PHE:CD1	59:8E:11:PHE:C	2.96	0.44
62:8H:54:GLU:OE1	62:8H:57:ARG:NE	2.39	0.44
5:1E:13:PRO:O	5:1E:16:ASN:ND2	2.50	0.43
7:1G:162:PHE:CZ	7:1G:198:ASN:HB2	2.53	0.43
7:1G:304:ALA:HA	7:1G:307:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:94:LEU:HD23	12:1L:125:LEU:HD21	2.00	0.43
14:1N:231:SER:O	14:1N:234:TRP:HD1	2.00	0.43
19:1S:19:ARG:HB2	19:1S:65:TRP:HB2	2.00	0.43
32:1g:34:ASP:OD1	32:1g:34:ASP:N	2.49	0.43
33:1h:114:MET:HE2	33:1h:120:GLY:HA3	2.00	0.43
34:1i:109:ILE:HG13	41:1p:15:ARG:HD2	2.00	0.43
39:1n:166:TRP:O	39:1n:170:VAL:HG12	2.18	0.43
49:3R:165:MET:HE2	49:3R:165:MET:HA	1.99	0.43
55:4A:92:MET:HE3	55:4A:163:ASN:HD22	1.83	0.43
55:4A:404:THR:HG21	67:4M:3:ALA:HB2	2.00	0.43
56:4B:23:PHE:CZ	56:4B:80:SER:HB2	2.53	0.43
86:4M:101:PGV:H81	86:4M:101:PGV:H242	2.00	0.43
2:5B:36:LEU:HD22	69:5B:203:PC1:H2C2	2.00	0.43
6:5F:92:TYR:HD1	6:5F:133:ALA:HB3	1.83	0.43
7:5G:140:LYS:O	7:5G:148:THR:OG1	2.35	0.43
10:5J:56:VAL:O	10:5J:61:LEU:N	2.51	0.43
12:5L:3:PRO:HB3	41:5p:36:PHE:CD2	2.53	0.43
12:5L:510:TYR:HE2	64:8J:29:ASN:HD21	1.66	0.43
15:5O:133:VAL:HG23	15:5O:205:ALA:HB3	2.00	0.43
16:5P:134:HIS:NE2	16:5P:169:SER:O	2.51	0.43
16:5P:273:SER:HA	16:5P:274:PRO:HD3	1.89	0.43
20:5T:69:LYS:HG3	20:5T:70:LEU:HD23	2.00	0.43
20:5U:21:LEU:HD21	36:5k:18:TYR:CE2	2.53	0.43
22:5W:23:ARG:HG2	22:5W:23:ARG:HH11	1.82	0.43
25:5Z:98:MET:HG3	25:5Z:104:TRP:NE1	2.33	0.43
25:5Z:98:MET:HE1	30:5e:81:GLN:HB3	1.99	0.43
29:5d:71:PHE:HE2	76:5d:201:3PE:H3E2	1.83	0.43
55:8A:30:GLY:HA3	55:8A:65:MET:HE2	2.00	0.43
57:8C:58:TRP:CZ3	86:8C:307:PGV:H71	2.53	0.43
1:1A:25:PRO:HG2	8:1H:60:PRO:HD3	1.99	0.43
69:1B:202:PC1:H3D2	8:1H:56:VAL:HG21	2.00	0.43
4:1D:169:TRP:HH2	4:1D:228:MET:HE3	1.81	0.43
5:1E:145:LEU:HA	6:1F:139:ARG:HH22	1.83	0.43
8:1H:66:SER:HA	8:1H:122:ALA:O	2.19	0.43
10:1J:52:LEU:HD13	11:1K:45:THR:HG23	2.00	0.43
10:1J:103:MET:HE3	10:1J:103:MET:HB2	1.90	0.43
12:1L:593:ILE:O	12:1L:597:ILE:HG13	2.18	0.43
13:1M:6:ILE:HD11	31:1f:26:LEU:HD12	2.00	0.43
16:1P:250:TYR:HE2	16:1P:322:ARG:HH21	1.66	0.43
17:1Q:116:LYS:HD3	17:1Q:116:LYS:HA	1.80	0.43
19:1S:16:ARG:HD2	19:1S:16:ARG:HA	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1T:60:PHE:CE1	20:1T:80:ILE:HG23	2.53	0.43
36:1k:27:PRO:HG2	36:1k:52:TYR:CD2	2.53	0.43
40:1o:62:LEU:HD12	40:1o:86:TRP:CZ2	2.52	0.43
46:3B:47:ILE:HD11	46:3B:211:VAL:HG11	1.99	0.43
55:4A:383:MET:O	55:4A:387:PHE:HB2	2.18	0.43
4:5D:6:PRO:HB3	4:5D:10:TRP:CD1	2.54	0.43
4:5D:291:GLY:O	4:5D:296:ARG:NH2	2.51	0.43
10:5J:17:PHE:HA	10:5J:20:PHE:CE2	2.53	0.43
12:5L:9:LEU:O	12:5L:13:ILE:HG23	2.18	0.43
17:5Q:37:ILE:HG12	17:5Q:92:ALA:HB1	2.00	0.43
32:5g:26:LEU:HA	32:5g:26:LEU:HD12	1.78	0.43
37:5l:134:PRO:HD3	40:5o:56:ASP:HA	1.99	0.43
38:5m:30:LYS:O	38:5m:34:GLU:HG3	2.17	0.43
55:8A:381:LEU:HB3	87:8A:603:HEA:HAC	2.00	0.43
86:8G:101:PGV:H171	92:8G:102:PEK:H15	2.00	0.43
7:1G:444:LYS:NZ	7:1G:480:SER:HB2	2.34	0.43
15:1O:101:TYR:CE1	15:1O:128:ILE:HG23	2.53	0.43
22:1W:121:LYS:HE2	22:1W:121:LYS:HB2	1.76	0.43
32:1g:43:ASP:N	32:1g:43:ASP:OD1	2.51	0.43
34:1i:48:LYS:HA	34:1i:51:GLN:HE21	1.81	0.43
38:1m:114:LEU:HD23	38:1m:119:LYS:HD2	2.00	0.43
40:1o:45:MET:HE3	40:1o:55:ARG:HD3	1.99	0.43
43:1r:11:ARG:HD3	43:1r:19:LEU:HD11	2.00	0.43
44:1s:59:SER:HA	44:1s:62:ARG:HG3	2.00	0.43
46:3B:369:LEU:HD11	46:3B:399:LEU:HD11	1.98	0.43
48:3D:308:VAL:HA	48:3D:311:MET:HG3	2.00	0.43
49:3I:65:VAL:HG22	49:3I:77:ARG:HB3	2.00	0.43
51:3T:68:LYS:HA	51:3T:71:ARG:HG3	1.99	0.43
55:4A:374:VAL:HA	55:4A:377:PHE:CE2	2.53	0.43
74:4C:306:CDL:HB4	74:4C:306:CDL:H512	1.44	0.43
58:4D:15:VAL:HG12	58:4D:17:VAL:HG23	2.00	0.43
6:5F:343:ILE:HD12	6:5F:344:VAL:HG23	2.00	0.43
8:5H:101:GLY:HA3	8:5H:162:LEU:HD12	2.01	0.43
8:5H:124:ASN:C	8:5H:126:LYS:H	2.27	0.43
8:5H:149:ILE:HG12	8:5H:181:LEU:HD22	2.01	0.43
12:5L:434:LYS:HG3	36:5k:52:TYR:HD1	1.83	0.43
13:5M:238:LEU:HD23	13:5M:238:LEU:HA	1.91	0.43
14:5N:197:ASN:HD22	14:5N:269:GLU:CD	2.26	0.43
16:5P:90:VAL:HG23	16:5P:128:LYS:HB2	1.99	0.43
16:5P:215:ILE:O	16:5P:218:ILE:HB	2.18	0.43
20:5T:35:HIS:CD2	20:5T:71:MET:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:5d:108:THR:O	29:5d:112:ILE:HG13	2.18	0.43
55:8A:86:MET:HE3	55:8A:182:PRO:HB2	1.99	0.43
55:8A:507:GLU:HG3	57:8C:5:THR:HG21	1.99	0.43
61:8G:56:ARG:HA	61:8G:56:ARG:HD3	1.71	0.43
2:1B:48:MET:HE2	2:1B:80:PRO:HG3	2.00	0.43
3:1C:88:ASN:HB2	21:1V:110:GLN:HE22	1.84	0.43
6:1F:423:ARG:N	6:1F:424:PRO:HD2	2.33	0.43
7:1G:241:SER:HB2	7:1G:249:ARG:HG3	2.00	0.43
7:1G:418:ARG:HD2	44:1s:75:HIS:HA	2.00	0.43
8:1H:9:LEU:HD12	26:1a:19:PRO:HB3	2.00	0.43
8:1H:102:VAL:HG21	8:1H:154:LEU:CD1	2.48	0.43
9:1I:65:HIS:ND1	9:1I:113:MET:HE1	2.33	0.43
13:1M:14:MET:HG3	31:1f:12:VAL:HB	2.01	0.43
19:1S:19:ARG:HB3	19:1S:21:HIS:CE1	2.53	0.43
19:1S:82:SER:O	19:1S:86:VAL:HG13	2.17	0.43
20:1T:58:PHE:CD1	20:1T:80:ILE:HG21	2.53	0.43
22:1W:52:LEU:HD11	22:1W:103:ILE:HG21	2.00	0.43
29:1d:63:LEU:HD23	74:1d:203:CDL:HA62	2.00	0.43
34:1i:8:LYS:HE2	34:1i:8:LYS:HB2	1.77	0.43
40:1o:107:LEU:HD23	40:1o:107:LEU:HA	1.89	0.43
45:3A:156:THR:O	45:3A:239:SER:OG	2.36	0.43
46:3O:68:LEU:HD23	46:3O:191:LEU:HD11	2.00	0.43
46:3O:203:ARG:NH1	46:3O:232:LEU:O	2.52	0.43
49:3R:263:TYR:CD1	49:3R:265:PHE:CD1	3.07	0.43
86:4C:303:PGV:H011	86:4C:303:PGV:H202	1.25	0.43
58:4D:82:VAL:HG22	74:4D:201:CDL:OB7	2.17	0.43
6:5F:9:LYS:HE2	6:5F:9:LYS:HB3	1.81	0.43
6:5F:73:PHE:CD1	6:5F:74:PRO:HD2	2.53	0.43
6:5F:372:MET:HE3	6:5F:415:VAL:HG21	2.00	0.43
7:5G:55:CYS:HB3	71:5G:803:FES:S2	2.58	0.43
8:5H:27:VAL:HG23	26:5a:5:ILE:HG21	2.01	0.43
8:5H:187:ILE:HD11	69:5I:201:PC1:H271	2.01	0.43
76:5M:502:3PE:H271	76:5M:502:3PE:H222	2.00	0.43
76:5Y:802:3PE:H221	76:5Y:802:3PE:H2	1.36	0.43
31:5f:34:LEU:HD22	33:5h:93:ILE:HG13	2.00	0.43
33:5h:47:ILE:HD13	41:5p:58:ASN:ND2	2.32	0.43
55:8A:246:LEU:HD23	55:8A:381:LEU:HD21	1.99	0.43
56:8B:44:LEU:HG	63:8I:16:ARG:HH12	1.83	0.43
86:8J:101:PGV:H302	86:8J:101:PGV:H343	2.01	0.43
3:1C:179:GLU:HG2	3:1C:180:VAL:HG13	2.00	0.43
6:1F:189:GLU:HG2	6:1F:190:THR:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:644:GLN:NE2	19:1S:37:GLU:O	2.52	0.43
8:1H:105:MET:HE1	8:1H:233:MET:SD	2.58	0.43
11:1K:10:MET:HE2	11:1K:10:MET:HB3	1.78	0.43
11:1K:40:LEU:HD21	14:1N:72:MET:HB2	2.00	0.43
12:1L:23:ASN:ND2	74:1L:702:CDL:H321	2.28	0.43
14:1N:103:ALA:O	14:1N:107:GLY:N	2.41	0.43
26:1a:27:HIS:O	26:1a:31:ASN:ND2	2.46	0.43
40:1o:18:PRO:HA	40:1o:21:MET:HG3	2.00	0.43
74:3A:501:CDL:H132	76:3A:503:3PE:H342	2.00	0.43
48:3D:311:MET:HE3	49:3E:118:THR:HA	1.99	0.43
50:3F:103:GLU:HG2	50:3F:107:LYS:HE2	2.00	0.43
45:3N:206:ARG:O	45:3N:206:ARG:HD3	2.19	0.43
49:3R:204:ARG:HE	49:3R:257:ASN:ND2	2.16	0.43
54:3X:4:ARG:HG2	54:3X:5:PHE:CE1	2.53	0.43
86:4A:602:PGV:H211	74:4C:306:CDL:H331	2.01	0.43
57:4C:192:VAL:HG12	57:4C:196:THR:HG23	2.00	0.43
68:4N:57:LEU:HD23	68:4N:57:LEU:HA	1.89	0.43
6:5F:305:PRO:HD3	6:5F:413:TRP:HB3	2.01	0.43
8:5H:175:ILE:O	8:5H:179:TRP:HB3	2.19	0.43
76:5L:701:3PE:H322	76:5L:701:3PE:H242	2.01	0.43
15:5O:261:MET:HE3	15:5O:261:MET:HB3	1.74	0.43
17:5Q:67:ASN:HB2	17:5Q:72:TRP:HB2	2.00	0.43
20:5T:54:MET:HE1	20:5T:76:ILE:HD13	2.00	0.43
21:5V:25:ILE:HG13	21:5V:25:ILE:H	1.64	0.43
25:5Z:111:PHE:CZ	25:5Z:117:VAL:HG11	2.53	0.43
29:5d:11:LEU:C	69:5d:202:PC1:H232	2.43	0.43
55:8A:86:MET:HE2	55:8A:185:VAL:HG23	2.01	0.43
55:8A:100:MET:HE1	86:8C:301:PGV:H71	2.01	0.43
55:8A:282:PHE:HA	86:8A:602:PGV:H292	2.00	0.43
55:8A:510:TYR:CG	60:8F:49:VAL:HG13	2.53	0.43
74:8B:303:CDL:HA61	74:8B:303:CDL:H311	1.62	0.43
86:8C:305:PGV:H21	86:8C:305:PGV:H222	2.01	0.43
58:8D:51:LEU:HD22	58:8D:55:GLU:HB2	2.01	0.43
60:8F:70:ILE:HG13	60:8F:84:SER:HB3	2.01	0.43
9:1I:144:HIS:CE1	16:1P:65:LEU:HD21	2.53	0.43
75:1I:205:AYA:OT	42:1q:55:PHE:HB3	2.18	0.43
12:1L:27:TYR:O	12:1L:115:ASN:ND2	2.42	0.43
12:1L:362:LEU:HA	12:1L:365:ALA:HB3	2.00	0.43
12:1L:481:THR:HG22	35:1j:53:TYR:HD1	1.84	0.43
76:1M:902:3PE:H332	76:1M:902:3PE:H291	2.01	0.43
16:1P:203:GLN:NE2	16:1P:232:GLY:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:1X:201:CDL:H221	74:1X:201:CDL:H472	2.01	0.43
76:1Y:803:3PE:H2	76:1Y:803:3PE:H221	1.74	0.43
29:1d:60:ARG:HD3	74:1d:203:CDL:OA2	2.19	0.43
33:1h:51:GLU:N	33:1h:51:GLU:OE1	2.52	0.43
36:1k:30:THR:O	36:1k:34:LYS:HG2	2.19	0.43
45:3A:192:ALA:HB2	45:3A:219:LEU:HB3	2.00	0.43
50:3F:30:LYS:HE3	50:3F:30:LYS:HB3	1.79	0.43
45:3N:256:ALA:HA	45:3N:321:GLY:HA3	2.01	0.43
46:3O:166:ALA:HB2	46:3O:244:ILE:HG13	2.00	0.43
59:4E:10:GLU:O	59:4E:14:ARG:N	2.50	0.43
6:5F:24:ASN:O	6:5F:113:HIS:HB3	2.18	0.43
7:5G:444:LYS:HA	7:5G:444:LYS:HD2	1.83	0.43
9:5I:66:ALA:HB1	9:5I:158:GLY:HA2	2.01	0.43
11:5K:37:MET:HG3	11:5K:67:ALA:CB	2.48	0.43
12:5L:214:ILE:HD11	12:5L:276:MET:SD	2.59	0.43
13:5M:391:ILE:HD12	13:5M:391:ILE:H	1.84	0.43
14:5N:294:MET:HE2	14:5N:294:MET:HB2	1.75	0.43
16:5P:268:ARG:HG2	16:5P:281:ARG:HD2	1.99	0.43
17:5Q:26:PRO:O	17:5Q:30:ILE:HG22	2.18	0.43
22:5W:88:MET:O	22:5W:92:GLU:HG3	2.19	0.43
55:8A:37:ILE:HD11	55:8A:58:VAL:HA	2.00	0.43
55:8A:48:LEU:HD12	55:8A:48:LEU:O	2.17	0.43
55:8A:275:TRP:CE3	86:8A:602:PGV:H12	2.54	0.43
60:8F:8:THR:HG22	60:8F:9:ASP:H	1.82	0.43
4:1D:130:PRO:HG2	4:1D:135:GLN:HE21	1.82	0.43
7:1G:244:THR:HB	17:1Q:73:SER:HB2	2.00	0.43
7:1G:614:ASP:OD1	7:1G:618:GLN:NE2	2.51	0.43
8:1H:277:TYR:OH	9:1I:34:LEU:HD13	2.19	0.43
9:1I:73:GLY:HA3	18:1R:43:LEU:HD23	2.01	0.43
12:1L:118:PHE:O	12:1L:122:VAL:HG23	2.19	0.43
12:1L:257:VAL:HG23	12:1L:329:ILE:HD11	2.00	0.43
13:1M:196:TRP:HZ2	13:1M:254:THR:HG23	1.82	0.43
14:1N:172:GLN:NE2	14:1N:177:LYS:HD3	2.33	0.43
14:1N:245:MET:HE3	14:1N:249:LEU:HD12	2.00	0.43
16:1P:132:ILE:HD11	16:1P:214:ILE:HD11	2.00	0.43
17:1Q:16:LYS:N	17:1Q:16:LYS:HD3	2.33	0.43
24:1Y:81:GLU:O	24:1Y:82:LYS:HG2	2.19	0.43
39:1n:153:LEU:HD13	39:1n:165:LEU:HB2	2.00	0.43
42:1q:144:TYR:HB3	42:1q:145:LYS:H	1.58	0.43
46:3B:258:VAL:HA	46:3B:323:GLY:HA3	2.00	0.43
45:3N:417:ASP:OD2	53:3W:10:TYR:OH	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:3N:503:3PE:H322	69:3R:302:PC1:H31	2.01	0.43
49:3R:214:ILE:HD13	49:3R:214:ILE:HA	1.94	0.43
52:3U:32:LYS:O	52:3U:36:ARG:HG3	2.19	0.43
74:4C:306:CDL:H822	74:4C:306:CDL:H591	2.00	0.43
2:5B:77:ARG:HG3	2:5B:78:ALA:H	1.83	0.43
3:5C:51:PHE:HB3	21:5V:111:TRP:CE2	2.54	0.43
6:5F:94:VAL:HG21	6:5F:215:VAL:HG21	2.01	0.43
12:5L:117:PHE:HE1	12:5L:240:PRO:HG2	1.84	0.43
12:5L:268:GLU:HA	12:5L:274:GLN:NE2	2.34	0.43
12:5L:468:ILE:O	12:5L:472:ILE:HG12	2.19	0.43
13:5M:196:TRP:HZ2	13:5M:254:THR:HG23	1.83	0.43
23:5X:6:LEU:HD12	25:5Z:91:LEU:HD22	2.01	0.43
40:5o:114:ARG:O	40:5o:117:ARG:HG3	2.18	0.43
55:8A:178:GLN:HG2	86:8A:602:PGV:H011	2.00	0.43
55:8A:361:SER:HB2	56:8B:84:LEU:HD13	2.00	0.43
57:8C:103:HIS:HA	86:8C:304:PGV:O02	2.19	0.43
61:8G:30:LEU:HD12	61:8G:30:LEU:HA	1.86	0.43
68:8N:32:TYR:O	68:8N:33:VAL:HG12	2.19	0.43
3:1C:137:MET:HE1	3:1C:153:THR:HG23	2.00	0.43
4:1D:147:LEU:HD22	4:1D:218:PHE:HE2	1.83	0.43
4:1D:411:LEU:HD23	4:1D:411:LEU:HA	1.87	0.43
6:1F:107:ASP:OD1	6:1F:108:ARG:N	2.52	0.43
7:1G:444:LYS:HA	7:1G:444:LYS:HD2	1.81	0.43
10:1J:76:THR:OG1	10:1J:77:GLU:N	2.51	0.43
15:1O:3:TYR:CZ	15:1O:260:ARG:HD3	2.54	0.43
37:1l:134:PRO:HD3	40:1o:56:ASP:HA	2.01	0.43
44:1s:38:TYR:CE2	44:1s:40:ASN:HB3	2.54	0.43
57:4C:206:LEU:HD23	57:4C:206:LEU:HA	1.85	0.43
57:4C:215:LEU:HD23	57:4C:238:ALA:HB1	2.01	0.43
74:4C:306:CDL:H251	74:4C:306:CDL:H371	1.99	0.43
6:5F:97:ALA:HB3	6:5F:138:ILE:HA	2.00	0.43
13:5M:150:LEU:HG	13:5M:154:LEU:HD12	2.01	0.43
20:5U:8:LEU:HD23	20:5U:88:GLU:OE2	2.19	0.43
24:5Y:11:ILE:H	24:5Y:11:ILE:HG13	1.72	0.43
32:5g:92:GLU:CD	32:5g:95:ARG:HH21	2.27	0.43
55:8A:3:VAL:HG22	55:8A:7:LEU:HD12	2.00	0.43
55:8A:344:PHE:O	55:8A:348:PHE:HB3	2.19	0.43
56:8B:62:GLU:HA	56:8B:65:TRP:CE2	2.54	0.43
2:1B:166:LYS:HE2	2:1B:166:LYS:HB3	1.78	0.43
2:1B:179:ARG:HH21	69:1B:202:PC1:H111	1.84	0.43
5:1E:79:ARG:HA	5:1E:79:ARG:HD3	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:172:ASP:HB3	44:1s:63:MET:HE3	2.01	0.43
7:1G:332:LYS:HG3	7:1G:343:LEU:HD13	2.01	0.43
7:1G:673:MET:HG2	7:1G:688:VAL:HG21	2.00	0.43
12:1L:49:VAL:HB	12:1L:50:PRO:HD3	2.01	0.43
12:1L:489:THR:O	12:1L:493:VAL:HG22	2.19	0.43
15:1O:25:ILE:O	15:1O:123:VAL:HA	2.17	0.43
20:1U:6:LEU:HD23	20:1U:6:LEU:HA	1.79	0.43
23:1X:17:VAL:HG23	23:1X:63:ASN:HD22	1.83	0.43
25:1Z:6:VAL:HG11	43:1r:41:PRO:HB3	2.00	0.43
25:1Z:98:MET:HE3	30:1e:78:ILE:HA	2.01	0.43
32:1g:49:LYS:HA	32:1g:49:LYS:HD2	1.81	0.43
32:1g:56:TRP:O	32:1g:60:VAL:HG23	2.18	0.43
36:1k:75:ALA:O	36:1k:79:VAL:HG23	2.19	0.43
40:1o:55:ARG:HH22	41:1p:119:SER:HB3	1.84	0.43
45:3N:70:ARG:HD3	45:3N:78:GLU:OE1	2.19	0.43
74:3P:504:CDL:H721	51:3T:41:THR:OG1	2.19	0.43
49:3R:150:SER:HA	49:3R:153:GLU:OE2	2.19	0.43
49:3R:217:CYS:SG	49:3R:219:HIS:N	2.92	0.43
55:4A:456:MET:HE2	65:4K:40:TRP:HH2	1.84	0.43
55:4A:484:ALA:HB3	67:4M:2:TYR:HD2	1.83	0.43
86:4A:601:PGV:H22	86:4J:101:PGV:H183	2.00	0.43
57:4C:31:LEU:HD12	86:4C:301:PGV:H181	2.01	0.43
57:4C:62:ILE:HG13	86:4C:307:PGV:H21	2.00	0.43
58:4D:119:GLN:O	58:4D:123:MET:HG3	2.19	0.43
63:4I:53:ASN:OD1	63:4I:53:ASN:N	2.51	0.43
4:5D:256:SER:HA	4:5D:260:LEU:HG	2.01	0.43
10:5J:60:TYR:CE2	11:5K:38:LEU:HD13	2.53	0.43
14:5N:4:ILE:O	14:5N:7:THR:OG1	2.37	0.43
14:5N:134:GLN:O	14:5N:135:LYS:HD3	2.19	0.43
74:5N:401:CDL:H111	74:5N:401:CDL:H141	1.84	0.43
76:5d:201:3PE:H3F1	76:5d:201:3PE:H2D2	2.01	0.43
34:5i:41:PRO:HA	34:5i:44:GLN:HB2	2.00	0.43
55:8A:190:ILE:HD12	55:8A:277:MET:HB3	2.01	0.43
57:8C:204:HIS:NE2	57:8C:249:TRP:HB2	2.34	0.43
1:1A:41:PHE:CE1	2:1B:99:ALA:HB2	2.54	0.43
6:1F:342:ASP:HB3	6:1F:345:LYS:HB3	2.01	0.43
7:1G:262:TRP:HB2	7:1G:390:LEU:HD21	2.01	0.43
7:1G:314:ASP:O	7:1G:520:LYS:N	2.49	0.43
7:1G:453:LEU:HD21	7:1G:458:LEU:HD21	2.00	0.43
8:1H:90:PRO:HG3	8:1H:162:LEU:HB3	2.01	0.43
11:1K:73:LEU:HD21	14:1N:41:ILE:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:435:PRO:HB3	12:1L:437:PHE:CZ	2.53	0.43
16:1P:27:THR:HG21	16:1P:56:THR:HG22	2.01	0.43
28:1c:25:VAL:HG12	28:1c:29:ILE:HD12	2.01	0.43
30:1e:64:GLU:O	30:1e:68:ARG:HD2	2.18	0.43
30:1e:81:GLN:O	30:1e:84:LYS:HG3	2.19	0.43
31:1f:57:LYS:HE2	31:1f:57:LYS:HB2	1.83	0.43
39:1n:107:HIS:HB3	39:1n:110:GLU:HG3	2.01	0.43
40:1o:15:GLU:HG3	40:1o:105:ARG:HD2	2.00	0.43
40:1o:54:GLN:HB3	40:1o:62:LEU:HD13	2.01	0.43
45:3A:327:ASP:OD1	45:3A:330:SER:OG	2.30	0.43
46:3B:47:ILE:HB	46:3B:109:VAL:HG23	2.01	0.43
49:3E:185:ASP:OD1	49:3E:186:GLN:N	2.52	0.43
46:3O:71:LEU:HD12	49:3V:68:VAL:HG11	2.01	0.43
48:3Q:37:CYS:SG	85:3Q:501:HEC:HBB3	2.59	0.43
49:3R:169:TRP:HB3	49:3R:274:GLY:O	2.18	0.43
52:3U:38:GLU:O	52:3U:42:GLN:HG3	2.19	0.43
55:4A:131:PRO:HD3	56:4B:160:LEU:HD13	2.00	0.43
55:4A:412:ILE:HA	58:4D:81:ILE:HG23	2.01	0.43
55:4A:440:TYR:CZ	56:4B:205:SER:HA	2.54	0.43
57:4C:103:HIS:HA	86:4C:304:PGV:O02	2.17	0.43
57:4C:181:TYR:HE2	92:4C:308:PEK:H191	1.84	0.43
74:4D:201:CDL:HB61	74:4D:201:CDL:H711	1.47	0.43
59:4E:11:PHE:CE2	59:4E:41:LEU:HD21	2.54	0.43
61:4G:48:ILE:O	61:4G:50:TYR:N	2.51	0.43
66:4L:39:ILE:HD13	66:4L:39:ILE:HA	1.87	0.43
2:5B:124:GLY:HA2	9:5I:115:LYS:HA	2.00	0.43
4:5D:139:VAL:HG13	4:5D:278:TYR:CZ	2.54	0.43
5:5E:111:ARG:CB	5:5E:152:PRO:HD3	2.49	0.43
6:5F:406:ALA:HB3	72:5F:501:FMN:HM82	2.00	0.43
7:5G:405:LYS:HE3	7:5G:405:LYS:HB2	1.90	0.43
9:5I:54:LYS:HD3	42:5q:91:HIS:CE1	2.54	0.43
10:5J:167:VAL:HG13	14:5N:42:PRO:HG3	2.00	0.43
12:5L:358:LYS:HG3	39:5n:79:TYR:CE1	2.54	0.43
12:5L:400:ASN:HD21	12:5L:489:THR:HG21	1.84	0.43
76:5M:502:3PE:H292	76:5M:502:3PE:H2C1	1.90	0.43
16:5P:201:VAL:HG12	16:5P:290:SER:HB3	2.00	0.43
16:5P:235:ARG:NH2	16:5P:291:ASP:OD1	2.52	0.43
17:5Q:37:ILE:HD12	17:5Q:103:PHE:HB2	2.00	0.43
21:5V:43:TYR:CG	21:5V:93:MET:HE2	2.54	0.43
27:5b:47:ALA:HB1	27:5b:77:LEU:HD11	2.00	0.43
38:5m:30:LYS:H	38:5m:30:LYS:HG2	1.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:5p:39:LEU:HD23	41:5p:39:LEU:HA	1.86	0.43
56:8B:52:HIS:CD2	59:8E:40:ASP:HB2	2.54	0.43
56:8B:63:THR:O	56:8B:67:ILE:HD12	2.19	0.43
86:8B:302:PGV:H62	68:8N:29:ALA:HB1	2.01	0.43
58:8D:121:LYS:HB2	58:8D:121:LYS:HE2	1.77	0.43
59:8E:65:VAL:HA	59:8E:68:LEU:HD12	2.01	0.43
69:1B:203:PC1:H381	69:1q:201:PC1:H362	2.00	0.42
8:1H:107:ALA:HB1	10:1J:57:PHE:HB3	2.01	0.42
9:1I:64:GLU:OE2	9:1I:149:TYR:OH	2.26	0.42
11:1K:37:MET:HE3	11:1K:37:MET:HB3	1.91	0.42
13:1M:90:THR:HG21	76:1O:401:3PE:H12	2.01	0.42
13:1M:277:LEU:HD23	13:1M:406:TYR:HB3	2.01	0.42
14:1N:190:MET:HB3	14:1N:201:THR:HG23	2.01	0.42
15:1O:24:VAL:HB	15:1O:166:PRO:HA	2.01	0.42
16:1P:162:GLU:N	16:1P:162:GLU:OE1	2.52	0.42
20:1U:21:LEU:HD23	36:1k:47:ASN:OD1	2.19	0.42
21:1V:25:ILE:HG22	21:1V:29:LYS:HD2	2.00	0.42
22:1W:90:LEU:O	22:1W:94:ILE:HD12	2.19	0.42
23:1X:33:ALA:HB2	23:1X:119:PRO:HG3	2.00	0.42
28:1c:43:LYS:HE2	28:1c:43:LYS:HB2	1.74	0.42
34:1i:39:VAL:HB	34:1i:44:GLN:OE1	2.19	0.42
41:1p:23:THR:HG22	41:1p:25:LEU:H	1.83	0.42
47:3C:322:GLN:HE22	76:3C:504:3PE:H111	1.84	0.42
55:4A:322:SER:O	55:4A:326:THR:OG1	2.30	0.42
59:4E:27:TRP:CZ3	59:4E:31:LYS:HD3	2.53	0.42
3:5C:179:GLU:HG2	3:5C:180:VAL:HG13	2.00	0.42
5:5E:154:VAL:HG12	5:5E:164:LEU:HD11	2.00	0.42
6:5F:43:TYR:CE1	6:5F:44:LYS:HG3	2.54	0.42
6:5F:82:MET:HG3	6:5F:129:MET:HB3	2.01	0.42
6:5F:258:ILE:HD13	6:5F:284:ALA:HB2	2.01	0.42
8:5H:156:MET:HE2	25:5Z:50:MET:HB3	1.99	0.42
9:5I:175:TYR:CZ	43:5r:38:PRO:HG3	2.53	0.42
10:5J:31:LEU:HA	10:5J:34:ILE:HD12	2.01	0.42
12:5L:384:PRO:HA	12:5L:389:PHE:CD1	2.54	0.42
13:5M:118:PHE:O	13:5M:122:PHE:HB3	2.19	0.42
14:5N:45:MET:HE2	14:5N:45:MET:HB3	1.87	0.42
14:5N:100:MET:HE3	14:5N:100:MET:HB2	1.81	0.42
16:5P:46:ILE:HD12	18:5R:26:VAL:HG21	2.01	0.42
76:5Y:803:3PE:H2	76:5Y:803:3PE:H221	1.72	0.42
39:5n:178:MET:SD	39:5n:178:MET:N	2.92	0.42
56:8B:133:MET:HE3	56:8B:133:MET:HB3	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:8C:206:LEU:HD12	92:8C:308:PEK:H11	2.01	0.42
3:1C:147:ASP:N	3:1C:147:ASP:OD1	2.50	0.42
5:1E:51:LEU:HD23	5:1E:69:VAL:HG21	2.01	0.42
7:1G:358:LEU:HD12	7:1G:645:ALA:HB2	2.01	0.42
7:1G:516:LYS:HE2	7:1G:516:LYS:HB3	1.92	0.42
8:1H:182:ALA:HB1	69:1I:201:PC1:H2I3	2.01	0.42
12:1L:564:LYS:HG3	38:1m:76:TYR:CZ	2.54	0.42
13:1M:44:GLN:HB2	32:1g:83:TYR:CE1	2.52	0.42
14:1N:311:MET:HE2	14:1N:311:MET:HB2	1.77	0.42
22:1W:47:VAL:HA	22:1W:52:LEU:HD12	2.02	0.42
37:1l:158:ILE:CD1	40:1o:103:ARG:HD2	2.49	0.42
39:1n:170:VAL:HG13	39:1n:171:THR:HG23	2.00	0.42
46:3B:24:LEU:HD12	46:3B:25:GLU:N	2.34	0.42
46:3B:163:LEU:HD11	46:3B:258:VAL:HG22	2.01	0.42
48:3Q:8:PRO:HG3	52:3U:66:ASP:HB3	2.01	0.42
53:3W:4:THR:O	53:3W:8:ARG:HG2	2.19	0.42
56:4B:162:SER:HB3	56:4B:197:SER:H	1.85	0.42
59:4E:44:GLU:HG2	59:4E:45:PRO:HD2	2.01	0.42
3:5C:35:LYS:HD3	3:5C:36:TYR:CZ	2.54	0.42
3:5C:68:THR:N	21:5V:86:GLU:OE1	2.51	0.42
7:5G:162:PHE:CZ	7:5G:198:ASN:HB2	2.54	0.42
9:5I:112:ASP:OD1	9:5I:114:THR:OG1	2.33	0.42
10:5J:23:LYS:HE3	11:5K:21:MET:O	2.19	0.42
10:5J:78:MET:HG3	10:5J:79:TYR:CD1	2.54	0.42
12:5L:2:ASN:HD21	12:5L:53:MET:CE	2.27	0.42
12:5L:128:MET:HE3	12:5L:131:LEU:HD22	2.01	0.42
12:5L:187:ALA:HA	13:5M:383:THR:HG22	2.00	0.42
12:5L:503:GLU:OE1	64:8J:29:ASN:HB3	2.19	0.42
13:5M:259:TYR:O	13:5M:263:MET:HE2	2.18	0.42
69:5M:503:PC1:H2	69:5M:503:PC1:H221	1.45	0.42
15:5O:90:ASP:O	32:5g:27:GLN:NE2	2.52	0.42
15:5O:318:TRP:HB2	29:5d:58:LEU:HD12	2.01	0.42
17:5Q:34:LYS:HE2	17:5Q:34:LYS:HB2	1.79	0.42
20:5T:32:VAL:HG13	20:5T:74:GLN:HB2	2.00	0.42
38:5m:82:THR:OG1	38:5m:83:PRO:HD2	2.19	0.42
39:5n:30:CYS:O	39:5n:32:HIS:N	2.50	0.42
41:5p:89:MET:HE2	41:5p:89:MET:HA	2.01	0.42
55:8A:101:SER:O	55:8A:156:SER:HB2	2.18	0.42
56:8B:203:ASN:HB3	56:8B:206:PHE:HB2	2.01	0.42
56:8B:217:LYS:O	56:8B:221:LYS:HG2	2.19	0.42
6:1F:113:HIS:NE2	44:1s:38:TYR:OH	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:146:VAL:HG22	7:1G:200:ILE:HD11	2.00	0.42
7:1G:534:ARG:HH22	42:1q:145:LYS:HE3	1.84	0.42
7:1G:601:ARG:HA	7:1G:611:LEU:HD12	2.00	0.42
10:1J:64:MET:HE2	10:1J:64:MET:HB3	1.89	0.42
13:1M:11:LEU:HB3	13:1M:100:ILE:HD13	1.99	0.42
13:1M:339:SER:HB3	13:1M:344:LEU:HD22	2.01	0.42
14:1N:25:HIS:HB2	30:1e:14:ASP:HB2	2.01	0.42
23:1X:23:VAL:HG21	26:1a:65:GLY:HA2	2.01	0.42
45:3N:373:THR:HB	45:3N:374:PRO:HD3	2.02	0.42
76:3Y:101:3PE:H252	76:3Y:101:3PE:H362	2.00	0.42
55:4A:242:GLU:HA	55:4A:245:ILE:HD12	2.00	0.42
55:4A:313:ALA:HB3	56:4B:73:LEU:HD21	2.01	0.42
56:4B:10:GLN:HE21	56:4B:166:PRO:HB2	1.84	0.42
4:5D:71:GLU:HG2	4:5D:410:MET:SD	2.59	0.42
4:5D:227:GLU:OE2	9:5I:32:ARG:NE	2.52	0.42
5:5E:28:TYR:O	5:5E:32:GLU:HG2	2.19	0.42
6:5F:233:THR:HG22	6:5F:237:ARG:HG3	2.01	0.42
14:5N:20:VAL:HG13	14:5N:29:ILE:HG23	2.01	0.42
14:5N:128:LEU:HD12	14:5N:216:PHE:HB3	2.02	0.42
15:5O:200:GLN:NE2	15:5O:204:ASN:OD1	2.50	0.42
40:5o:45:MET:HG3	40:5o:50:LEU:HD22	2.01	0.42
55:8A:456:MET:O	55:8A:460:ILE:HG13	2.19	0.42
74:8D:201:CDL:HA4	74:8D:201:CDL:OB4	2.19	0.42
66:8L:20:ARG:HG2	66:8L:24:MET:HE3	2.01	0.42
2:1B:92:LEU:HD13	2:1B:100:LEU:HD12	2.02	0.42
10:1J:125:TRP:HB2	25:1Z:137:THR:HG21	2.00	0.42
12:1L:90:ILE:HB	12:1L:91:PRO:HD3	2.02	0.42
17:1Q:15:GLU:N	17:1Q:15:GLU:OE1	2.52	0.42
32:1g:80:LEU:HD23	32:1g:80:LEU:HA	1.86	0.42
48:3Q:218:LEU:HB3	49:3R:121:THR:OG1	2.18	0.42
48:3Q:222:MET:HE1	69:3R:302:PC1:H331	2.00	0.42
69:3R:302:PC1:H32	69:3R:302:PC1:H321	1.26	0.42
55:4A:491:ASN:HB3	55:4A:494:TRP:HD1	1.84	0.42
58:4D:88:PHE:HZ	67:4M:19:LEU:HD21	1.85	0.42
59:4E:25:ASP:OD1	59:4E:27:TRP:N	2.52	0.42
4:5D:199:VAL:HG23	4:5D:323:ILE:HB	2.01	0.42
7:5G:278:ARG:HE	7:5G:278:ARG:HB3	1.60	0.42
8:5H:161:THR:HG22	8:5H:163:SER:H	1.84	0.42
12:5L:89:PHE:CD2	12:5L:132:VAL:HG21	2.54	0.42
12:5L:261:ILE:HD12	12:5L:326:PHE:HB2	1.99	0.42
13:5M:148:TYR:O	13:5M:152:TYR:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:5M:423:ILE:HG23	38:5m:58:VAL:HG12	2.01	0.42
15:5O:180:GLN:O	15:5O:183:ILE:HG13	2.18	0.42
17:5Q:9:GLN:HB3	22:5W:23:ARG:HH12	1.85	0.42
29:5d:11:LEU:HA	69:5d:202:PC1:H12	2.01	0.42
36:5k:19:LYS:HD3	36:5k:19:LYS:HA	1.81	0.42
43:5r:5:ARG:HH21	43:5r:9:LEU:HD21	1.84	0.42
55:8A:18:LEU:HD22	86:8L:101:PGV:H62	2.01	0.42
55:8A:41:LEU:HD21	55:8A:440:TYR:O	2.19	0.42
55:8A:338:MET:HE3	55:8A:341:ALA:HB3	2.00	0.42
86:8B:301:PGV:H302	86:8B:301:PGV:H342	2.01	0.42
74:8C:306:CDL:O1	74:8C:306:CDL:OA7	2.36	0.42
58:8D:91:PHE:HA	58:8D:94:LEU:HD12	2.02	0.42
59:8E:72:LYS:HB2	59:8E:82:TYR:CE1	2.55	0.42
7:1G:53:ARG:HA	7:1G:53:ARG:HD2	1.87	0.42
7:1G:549:HIS:CE1	7:1G:677:ILE:HG22	2.55	0.42
7:1G:591:GLY:HA2	16:1P:6:ILE:HG21	2.01	0.42
8:1H:111:LEU:HD11	10:1J:57:PHE:CD1	2.54	0.42
8:1H:281:ARG:HB3	8:1H:284:GLN:HG3	2.01	0.42
12:1L:327:LEU:O	12:1L:331:MET:HG2	2.19	0.42
12:1L:502:LEU:HD22	36:1k:62:PHE:HD2	1.83	0.42
14:1N:4:ILE:HG13	15:1O:9:VAL:HG22	2.01	0.42
14:1N:237:MET:O	14:1N:237:MET:HG2	2.19	0.42
15:1O:19:THR:HG22	15:1O:20:GLU:H	1.84	0.42
29:1d:11:LEU:C	69:1d:202:PC1:H232	2.44	0.42
30:1e:79:LYS:HB2	30:1e:79:LYS:HE3	1.82	0.42
33:1h:108:LEU:HD23	33:1h:108:LEU:HA	1.83	0.42
37:1l:6:LYS:HD3	37:1l:6:LYS:N	2.34	0.42
37:1l:12:PRO:O	37:1l:46:ASP:HB3	2.18	0.42
46:3B:181:TYR:CZ	46:3B:182:ARG:HG2	2.55	0.42
49:3R:226:ALA:HA	49:3R:234:TYR:CD1	2.54	0.42
74:3T:101:CDL:HB61	74:3T:101:CDL:H711	1.62	0.42
55:4A:254:ILE:HD12	55:4A:341:ALA:HA	2.02	0.42
90:4A:609:PSC:H261	90:4A:609:PSC:H10	2.02	0.42
90:4A:609:PSC:H292	63:4I:21:ILE:HG21	2.02	0.42
56:4B:141:ARG:H	56:4B:141:ARG:HG2	1.68	0.42
56:4B:155:SER:HB2	56:4B:179:LEU:HD12	2.02	0.42
86:4C:302:PGV:H012	86:4C:302:PGV:H21	2.01	0.42
74:4C:306:CDL:H581	74:4C:306:CDL:H761	2.01	0.42
59:4E:63:SER:O	59:4E:67:ILE:HG23	2.20	0.42
6:5F:397:LYS:HA	6:5F:397:LYS:HD2	1.86	0.42
7:5G:368:ILE:O	7:5G:371:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:5N:112:HIS:NE2	14:5N:164:ILE:HG21	2.35	0.42
14:5N:263:LYS:HE3	14:5N:263:LYS:HB3	1.74	0.42
14:5N:311:MET:HE2	14:5N:311:MET:HB2	1.91	0.42
15:5O:63:THR:OG1	15:5O:302:ARG:NH2	2.47	0.42
15:5O:221:LEU:HD11	15:5O:241:LEU:HD11	2.02	0.42
16:5P:77:ASP:OD1	16:5P:80:SER:N	2.42	0.42
20:5T:8:LEU:HD23	20:5T:88:GLU:HB3	2.01	0.42
24:5Y:105:ARG:HA	24:5Y:105:ARG:HD2	1.79	0.42
33:5h:36:VAL:HA	69:5h:203:PC1:H2G2	2.00	0.42
74:5h:202:CDL:H511	74:5h:202:CDL:HB4	1.71	0.42
40:5o:121:MET:SD	40:5o:122:ALA:N	2.93	0.42
55:8A:202:LEU:HB2	55:8A:238:PHE:CG	2.54	0.42
56:8B:11:ASP:HB2	58:8D:129:ALA:HA	2.01	0.42
74:8B:303:CDL:H861	74:8B:303:CDL:H202	2.01	0.42
60:8F:52:ILE:HG13	60:8F:53:THR:HG23	2.02	0.42
68:8N:36:LEU:O	68:8N:40:ASN:HB2	2.20	0.42
1:1A:22:PHE:HZ	8:1H:62:ARG:HD3	1.84	0.42
3:1C:61:LEU:HD22	3:1C:96:LEU:HD21	2.01	0.42
4:1D:100:LEU:HD13	4:1D:196:PRO:HD3	2.01	0.42
4:1D:152:MET:O	4:1D:156:THR:OG1	2.21	0.42
5:1E:111:ARG:CB	5:1E:152:PRO:HD3	2.50	0.42
7:1G:354:ALA:O	7:1G:357:ASP:HB2	2.19	0.42
9:1I:164:GLU:OE2	42:1q:87:HIS:ND1	2.49	0.42
11:1K:12:PHE:CD2	11:1K:36:MET:HG2	2.54	0.42
12:1L:355:ASP:OD2	12:1L:357:ARG:NH2	2.52	0.42
12:1L:558:LEU:HD23	12:1L:558:LEU:HA	1.84	0.42
13:1M:148:TYR:O	13:1M:152:TYR:HB2	2.19	0.42
13:1M:196:TRP:HB2	13:1M:253:LEU:HD23	2.01	0.42
20:1T:64:ASP:OD2	22:1W:37:ARG:NH1	2.47	0.42
33:1h:38:ILE:O	33:1h:41:THR:OG1	2.34	0.42
49:3E:195:LEU:HD12	49:3E:249:ILE:O	2.19	0.42
48:3Q:16:GLY:O	48:3Q:202:LYS:NZ	2.46	0.42
49:3R:172:LYS:HD3	49:3R:214:ILE:HG21	2.01	0.42
1:5A:42:ASP:OD1	1:5A:42:ASP:N	2.44	0.42
1:5A:74:PRO:HB3	10:5J:143:ILE:HG22	2.02	0.42
2:5B:37:VAL:HG21	69:5B:202:PC1:H342	2.01	0.42
5:5E:36:LYS:HE3	5:5E:36:LYS:HB3	1.87	0.42
7:5G:150:MET:HE1	7:5G:208:LEU:HD21	2.01	0.42
7:5G:238:ILE:HG22	7:5G:263:ILE:HG21	2.01	0.42
8:5H:102:VAL:HG21	8:5H:154:LEU:CD1	2.49	0.42
8:5H:107:ALA:HB1	10:5J:57:PHE:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:5M:5:ILE:O	13:5M:9:THR:HG23	2.20	0.42
16:5P:235:ARG:HB2	16:5P:340:VAL:O	2.19	0.42
21:5V:17:GLU:H	21:5V:17:GLU:HG2	1.59	0.42
76:5j:101:3PE:H221	76:5j:101:3PE:O31	2.19	0.42
39:5n:46:ARG:HE	39:5n:46:ARG:HB3	1.68	0.42
55:8A:186:TRP:CZ3	55:8A:278:MET:HE2	2.55	0.42
55:8A:511:ILE:HD11	60:8F:71:TRP:CH2	2.55	0.42
56:8B:42:ILE:HG21	86:8B:301:PGV:O14	2.20	0.42
56:8B:136:LEU:HD23	56:8B:136:LEU:HA	1.92	0.42
56:8B:155:SER:HB2	56:8B:179:LEU:HD12	2.00	0.42
58:8D:98:TRP:HZ2	67:8M:31:GLY:HA2	1.83	0.42
59:8E:10:GLU:H	59:8E:10:GLU:CD	2.23	0.42
1:1A:67:LEU:HD23	1:1A:67:LEU:HA	1.89	0.42
4:1D:7:ASP:OD1	4:1D:7:ASP:N	2.46	0.42
6:1F:17:ASP:HA	6:1F:20:ARG:HD3	2.01	0.42
7:1G:368:ILE:O	7:1G:371:VAL:HG12	2.19	0.42
8:1H:136:VAL:O	8:1H:140:ILE:HG12	2.19	0.42
9:1I:110:ASP:HB2	17:1Q:72:TRP:HH2	1.83	0.42
12:1L:89:PHE:CD2	12:1L:132:VAL:HG21	2.55	0.42
74:1L:702:CDL:H341	74:1L:702:CDL:H312	1.87	0.42
14:1N:112:HIS:NE2	14:1N:164:ILE:HG21	2.35	0.42
19:1S:78:LEU:HD12	19:1S:78:LEU:H	1.84	0.42
20:1T:36:PHE:HD1	20:1T:40:LEU:HD23	1.83	0.42
20:1U:36:PHE:HA	20:1U:40:LEU:HB2	2.02	0.42
22:1W:69:LYS:HB2	22:1W:69:LYS:NZ	2.33	0.42
25:1Z:98:MET:HE1	30:1e:81:GLN:HB3	2.02	0.42
45:3A:170:PRO:HB2	45:3A:172:GLU:OE2	2.19	0.42
46:3B:95:LYS:HB2	49:3I:32:ALA:HA	2.01	0.42
46:3B:342:ASP:O	46:3B:346:THR:HG23	2.19	0.42
49:3I:56:ARG:HA	49:3I:56:ARG:HD2	1.81	0.42
47:3P:361:ILE:O	47:3P:366:MET:HG3	2.20	0.42
48:3Q:131:LEU:HB3	48:3Q:164:ILE:HD11	2.02	0.42
54:3Y:18:ILE:HD13	54:3Y:18:ILE:HA	1.92	0.42
55:4A:1:FME:SD	86:4A:601:PGV:H211	2.59	0.42
55:4A:70:VAL:HG21	87:4A:604:HEA:HBC2	2.02	0.42
56:4B:21:LEU:HD23	56:4B:21:LEU:HA	1.90	0.42
56:4B:73:LEU:HA	56:4B:76:ILE:HD12	2.01	0.42
56:4B:122:MET:HB2	56:4B:208:PRO:HD3	2.01	0.42
1:5A:55:PHE:HZ	8:5H:134:ARG:HD3	1.83	0.42
3:5C:35:LYS:O	21:5V:103:VAL:HG23	2.20	0.42
4:5D:175:GLU:OE2	4:5D:188:ARG:NH1	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5G:53:ARG:N	71:5G:803:FES:S1	2.80	0.42
12:5L:267:MET:HE2	12:5L:267:MET:HB2	1.89	0.42
12:5L:316:THR:HG23	12:5L:325:ALA:HB2	2.02	0.42
14:5N:296:LEU:HD23	14:5N:296:LEU:HA	1.83	0.42
17:5Q:14:ASP:OD1	17:5Q:14:ASP:N	2.50	0.42
23:5X:87:CYS:SG	23:5X:99:CYS:HB3	2.59	0.42
29:5d:108:THR:HA	41:5p:77:GLU:HA	2.01	0.42
32:5g:41:ASN:HB3	32:5g:44:SER:HB2	2.02	0.42
32:5g:97:VAL:O	32:5g:101:GLU:HB2	2.20	0.42
41:5p:31:TYR:O	41:5p:35:ILE:HG13	2.20	0.42
56:8B:20:LEU:HD23	56:8B:20:LEU:HA	1.88	0.42
56:8B:64:ILE:HD12	56:8B:64:ILE:HA	1.89	0.42
56:8B:141:ARG:HD2	56:8B:212:GLU:HB2	2.01	0.42
86:8B:302:PGV:H242	86:8B:302:PGV:H282	2.02	0.42
57:8C:187:THR:HG22	57:8C:188:ILE:H	1.85	0.42
2:1B:62:MET:O	2:1B:67:TYR:HB2	2.20	0.42
4:1D:62:LEU:HD22	4:1D:425:PHE:HZ	1.84	0.42
5:1E:147:ALA:HB3	5:1E:153:MET:HG2	2.01	0.42
6:1F:292:ASP:OD1	6:1F:292:ASP:N	2.50	0.42
7:1G:66:VAL:HB	7:1G:71:MET:HE3	2.02	0.42
12:1L:236:ALA:HB1	12:1L:248:HIS:HD1	1.84	0.42
12:1L:512:LYS:HE3	12:1L:512:LYS:HB3	1.73	0.42
13:1M:71:TRP:CD1	69:1M:905:PC1:H2C2	2.55	0.42
15:1O:318:TRP:CD1	15:1O:318:TRP:H	2.38	0.42
20:1U:21:LEU:HD12	20:1U:21:LEU:HA	1.43	0.42
23:1X:53:ARG:HG3	23:1X:54:ARG:HG2	2.00	0.42
26:1a:55:SER:HB2	26:1a:62:VAL:HG13	2.02	0.42
28:1c:28:TRP:HE1	29:1d:66:THR:HG22	1.84	0.42
37:1l:97:SER:OG	38:1m:6:LYS:HG2	2.20	0.42
39:1n:62:LEU:HD23	39:1n:62:LEU:HA	1.79	0.42
46:3B:70:ARG:HG2	49:3I:68:VAL:HG22	2.02	0.42
46:3B:203:ARG:HD2	46:3B:230:LEU:O	2.20	0.42
47:3C:78:VAL:O	47:3C:82:LEU:HB2	2.19	0.42
46:3O:341:TYR:O	46:3O:345:LYS:HG3	2.20	0.42
48:3Q:86:LYS:HE2	48:3Q:86:LYS:HB2	1.88	0.42
55:4A:295:VAL:O	56:4B:178:ARG:NH1	2.49	0.42
87:4A:604:HEA:H202	87:4A:604:HEA:H171	1.74	0.42
58:4D:72:ASN:HB2	74:4D:201:CDL:H832	2.01	0.42
58:4D:89:ILE:HG22	65:4K:29:TRP:HE1	1.83	0.42
64:4J:42:GLY:O	64:4J:46:SER:N	2.43	0.42
1:5A:105:GLU:HB3	1:5A:111:LEU:HG	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5C:41:GLN:HG2	3:5C:51:PHE:CE2	2.55	0.42
5:5E:79:ARG:HA	5:5E:79:ARG:HD3	1.83	0.42
6:5F:15:LEU:HD13	6:5F:271:GLU:HB2	2.02	0.42
7:5G:190:MET:HE3	7:5G:190:MET:HB2	1.81	0.42
7:5G:490:MET:HE2	7:5G:490:MET:HA	2.02	0.42
10:5J:57:PHE:HA	10:5J:61:LEU:HB2	2.01	0.42
12:5L:205:ASN:HB2	12:5L:207:GLU:CD	2.44	0.42
12:5L:529:TYR:CE2	12:5L:533:MET:HG3	2.54	0.42
14:5N:242:SER:O	14:5N:246:VAL:HG23	2.19	0.42
16:5P:331:MET:SD	16:5P:331:MET:N	2.87	0.42
20:5U:61:GLU:HB2	39:5n:81:PHE:CD2	2.55	0.42
23:5X:131:LYS:HA	23:5X:131:LYS:HD2	1.65	0.42
69:5h:203:PC1:O32	69:5h:203:PC1:H352	2.20	0.42
39:5n:97:LYS:HD2	39:5n:173:PRO:HB2	2.02	0.42
42:5q:55:PHE:HB3	75:5q:202:AYA:OT	2.20	0.42
55:8A:43:GLN:HB2	58:8D:104:TYR:HE2	1.84	0.42
55:8A:104:LEU:HD22	55:8A:152:LEU:HD22	2.01	0.42
59:8E:45:PRO:HD2	63:8I:9:MET:HE1	2.01	0.42
1:1A:27:LEU:HD13	69:1A:201:PC1:H132	2.02	0.42
1:1A:51:PHE:CE2	4:1D:45:SER:HB2	2.54	0.42
4:1D:151:ILE:HD11	4:1D:218:PHE:CZ	2.55	0.42
5:1E:55:GLN:OE1	5:1E:91:ASN:N	2.39	0.42
5:1E:181:ILE:C	5:1E:181:ILE:HD12	2.45	0.42
9:1I:114:THR:HG21	9:1I:144:HIS:CE1	2.55	0.42
9:1I:158:GLY:O	9:1I:162:GLU:HB2	2.20	0.42
12:1L:292:ALA:HB2	12:1L:304:PHE:HB2	2.02	0.42
13:1M:442:LEU:HD11	33:1h:25:MET:HE3	2.01	0.42
14:1N:20:VAL:HG13	14:1N:29:ILE:HG23	2.01	0.42
16:1P:90:VAL:HG23	16:1P:128:LYS:HB2	2.02	0.42
20:1T:84:LYS:HG3	20:1T:86:VAL:HG23	2.02	0.42
38:1m:82:THR:OG1	38:1m:83:PRO:HD2	2.19	0.42
45:3A:158:PHE:HB3	45:3A:161:THR:OG1	2.20	0.42
48:3D:121:TYR:HD1	48:3D:125:CYS:HB2	1.84	0.42
49:3E:123:VAL:HG13	53:3J:32:ALA:HA	2.00	0.42
45:3N:445:ARG:HG2	76:3N:501:3PE:H252	2.02	0.42
47:3P:27:ILE:HA	47:3P:208:PRO:HD3	2.01	0.42
47:3P:138:MET:HG3	47:3P:252:ASP:HB3	2.01	0.42
55:4A:41:LEU:HD21	55:4A:440:TYR:O	2.20	0.42
1:5A:27:LEU:HG	8:5H:59:GLU:HB2	2.01	0.42
2:5B:45:LEU:HD23	2:5B:45:LEU:HA	1.88	0.42
4:5D:57:ALA:HB2	8:5H:205:SER:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:5I:143:THR:OG1	9:5I:146:GLU:HG3	2.20	0.42
12:5L:5:ALA:HB2	12:5L:61:MET:HE1	2.02	0.42
12:5L:587:TYR:O	12:5L:590:SER:OG	2.34	0.42
13:5M:6:ILE:HD12	31:5f:23:GLY:HA2	2.01	0.42
13:5M:203:PHE:O	13:5M:207:MET:HG2	2.20	0.42
13:5M:279:GLN:HB2	13:5M:285:LEU:HD12	2.01	0.42
16:5P:268:ARG:HA	16:5P:268:ARG:HD2	1.75	0.42
23:5X:75:ARG:HG2	23:5X:76:HIS:CD2	2.53	0.42
29:5d:85:LEU:HD23	29:5d:85:LEU:HA	1.84	0.42
29:5d:86:ARG:HD3	82:5h:201:AME:HE1	2.01	0.42
32:5g:83:TYR:CE1	32:5g:84:ARG:HG3	2.54	0.42
37:5l:10:PRO:HD3	38:5m:66:ARG:HG2	2.00	0.42
37:5l:15:LYS:N	37:5l:19:GLU:OE2	2.44	0.42
39:5n:34:ASP:OD1	39:5n:35:LYS:N	2.53	0.42
56:8B:1:FME:HG2	56:8B:10:GLN:OE1	2.20	0.42
6:1F:186:CYS:SG	6:1F:201:GLY:HA3	2.59	0.42
6:1F:293:ASN:OD1	6:1F:339:ARG:HB2	2.20	0.42
7:1G:643:GLN:O	7:1G:647:GLU:HG2	2.19	0.42
8:1H:46:LEU:HD23	8:1H:49:ILE:HD12	2.02	0.42
8:1H:200:LEU:HD21	8:1H:280:PHE:O	2.20	0.42
12:1L:356:ILE:HA	12:1L:359:MET:HE3	2.01	0.42
13:1M:116:ILE:O	13:1M:120:ILE:HG12	2.19	0.42
14:1N:175:LEU:HD11	14:1N:230:LEU:HB2	2.02	0.42
15:1O:133:VAL:HG11	15:1O:206:TYR:CZ	2.55	0.42
16:1P:136:ASN:HD21	16:1P:292:MET:H	1.67	0.42
19:1S:64:LEU:HB3	19:1S:76:VAL:HG22	2.01	0.42
33:1h:73:ARG:NE	69:1h:203:PC1:O14	2.37	0.42
74:3A:501:CDL:H722	69:3J:101:PC1:H232	2.02	0.42
45:3N:228:VAL:HG21	39:5n:60:THR:HG21	2.02	0.42
74:3P:504:CDL:OA7	74:3P:504:CDL:H512	2.20	0.42
48:3Q:230:LEU:O	48:3Q:233:ARG:HG2	2.20	0.42
90:4A:609:PSC:H083	59:4E:5:HIS:CD2	2.54	0.42
90:4A:609:PSC:H251	63:4I:21:ILE:HG13	2.02	0.42
56:4B:218:TYR:HE2	63:4I:60:PHE:CE2	2.38	0.42
86:4J:101:PGV:H302	86:4J:101:PGV:H343	2.01	0.42
4:5D:62:LEU:HD13	4:5D:425:PHE:CE1	2.55	0.42
4:5D:183:ARG:NH1	4:5D:210:ASP:OD2	2.29	0.42
4:5D:258:VAL:HG12	4:5D:296:ARG:HG2	2.02	0.42
5:5E:111:ARG:HD3	6:5F:260:GLY:O	2.19	0.42
6:5F:137:TYR:HB3	6:5F:192:LEU:HD11	2.01	0.42
7:5G:519:PRO:HD2	7:5G:537:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:5H:87:VAL:HG23	8:5H:88:PRO:HD3	2.02	0.42
16:5P:48:PRO:HB3	16:5P:84:VAL:HG11	2.02	0.42
16:5P:338:LYS:HB2	16:5P:338:LYS:HE2	1.82	0.42
29:5d:71:PHE:CE1	76:5d:201:3PE:H351	2.54	0.42
30:5e:64:GLU:O	30:5e:68:ARG:HD2	2.20	0.42
39:5n:138:GLN:NE2	39:5n:142:GLU:OE1	2.52	0.42
40:5o:62:LEU:HB2	40:5o:86:TRP:NE1	2.34	0.42
1:1A:49:LEU:N	1:1A:50:PRO:HD2	2.35	0.41
4:1D:255:PHE:HB3	4:1D:259:MET:HB3	2.02	0.41
5:1E:103:CYS:SG	5:1E:144:CYS:HA	2.60	0.41
6:1F:276:LEU:HD21	6:1F:297:VAL:HG11	2.01	0.41
7:1G:159:CYS:SG	7:1G:160:ILE:HD12	2.59	0.41
12:1L:206:ASN:OD1	12:1L:206:ASN:N	2.53	0.41
12:1L:237:MET:SD	12:1L:244:SER:HB2	2.60	0.41
12:1L:438:PRO:HA	12:1L:439:PRO:HD3	1.96	0.41
13:1M:8:THR:O	13:1M:11:LEU:HB2	2.20	0.41
13:1M:122:PHE:CE1	13:1M:206:LYS:HD3	2.55	0.41
14:1N:109:SER:O	14:1N:111:PHE:N	2.53	0.41
14:1N:218:LEU:HD22	14:1N:240:ILE:HG23	2.02	0.41
16:1P:235:ARG:HB2	16:1P:340:VAL:O	2.20	0.41
69:1d:202:PC1:H112	69:1d:202:PC1:H321	2.02	0.41
74:1h:202:CDL:H511	74:1h:202:CDL:HB4	1.70	0.41
40:1o:93:ASP:O	40:1o:97:ARG:HG3	2.20	0.41
43:1r:110:PRO:HB2	43:1r:111:TYR:CD1	2.55	0.41
47:3C:116:GLY:C	84:3C:502:HEM:HBC2	2.45	0.41
49:3E:235:TYR:HD1	49:3E:242:HIS:HA	1.84	0.41
55:4A:3:VAL:HG21	86:4A:601:PGV:H02	2.01	0.41
55:4A:311:ILE:O	55:4A:315:PRO:HD2	2.20	0.41
55:4A:319:LYS:HE2	55:4A:319:LYS:HB3	1.77	0.41
1:5A:41:PHE:HB2	4:5D:51:PHE:CD1	2.55	0.41
1:5A:49:LEU:N	1:5A:50:PRO:HD2	2.35	0.41
4:5D:100:LEU:HD12	4:5D:118:TYR:HD2	1.85	0.41
4:5D:406:SER:HB2	4:5D:414:VAL:HG22	2.02	0.41
6:5F:95:VAL:HG11	6:5F:118:LEU:HD11	2.00	0.41
6:5F:133:ALA:HB1	6:5F:176:PHE:HE1	1.85	0.41
7:5G:588:THR:HG21	17:5Q:63:GLU:HA	2.02	0.41
8:5H:9:LEU:O	8:5H:13:ILE:HD12	2.20	0.41
8:5H:74:ALA:HB3	8:5H:75:PRO:HD3	2.02	0.41
8:5H:93:TYR:OH	26:5a:35:GLU:OE2	2.37	0.41
13:5M:200:ILE:O	13:5M:204:MET:HG2	2.20	0.41
14:5N:128:LEU:O	14:5N:132:THR:OG1	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:5R:43:LEU:HD23	42:5q:107:LYS:HD2	2.02	0.41
20:5U:21:LEU:HD23	20:5U:21:LEU:HA	1.57	0.41
36:5k:51:ARG:H	36:5k:51:ARG:HG3	1.70	0.41
55:8A:291:HIS:HD2	87:8A:604:HEA:HAA2	1.85	0.41
56:8B:65:TRP:CD1	56:8B:65:TRP:C	2.98	0.41
74:8C:306:CDL:H541	74:8C:306:CDL:H162	2.02	0.41
92:8C:308:PEK:H72	92:8C:308:PEK:H42	1.87	0.41
3:1C:51:PHE:CE1	3:1C:108:LYS:HD2	2.54	0.41
4:1D:417:ILE:O	4:1D:420:THR:HG22	2.19	0.41
7:1G:39:ARG:HB2	71:1G:803:FES:S2	2.60	0.41
7:1G:97:LEU:HD22	7:1G:154:ILE:HB	2.02	0.41
7:1G:201:ASP:OD2	7:1G:268:ARG:NH1	2.54	0.41
7:1G:255:HIS:CD2	17:1Q:109:LYS:HE2	2.55	0.41
7:1G:568:GLU:HA	7:1G:587:VAL:O	2.20	0.41
8:1H:204:GLU:HG2	8:1H:279:ARG:NH2	2.30	0.41
10:1J:175:ASN:O	15:1O:254:ARG:NH2	2.48	0.41
16:1P:201:VAL:HG12	16:1P:290:SER:OG	2.20	0.41
20:1U:43:ASP:HB2	81:1n:201:EHZ:P1	2.60	0.41
21:1V:31:LEU:HD23	21:1V:31:LEU:HA	1.95	0.41
21:1V:75:GLN:O	21:1V:78:GLU:HG2	2.20	0.41
23:1X:143:SER:OG	30:1e:38:GLU:OE1	2.25	0.41
29:1d:100:ASP:OD2	33:1h:117:ARG:NH2	2.47	0.41
76:1d:201:3PE:H2I2	74:1d:203:CDL:H473	2.01	0.41
34:1i:89:VAL:O	34:1i:95:THR:OG1	2.24	0.41
76:1j:101:3PE:O31	76:1j:101:3PE:H221	2.20	0.41
46:3B:52:LYS:O	46:3B:203:ARG:NH2	2.38	0.41
46:3B:170:ASN:OD1	46:3B:170:ASN:N	2.52	0.41
46:3B:286:LYS:HG2	46:3B:287:ARG:HG3	2.02	0.41
47:3C:338:ILE:HD13	47:3C:338:ILE:HA	1.90	0.41
52:3H:47:GLU:HA	52:3H:50:GLU:HG3	2.01	0.41
46:3O:78:LYS:HD3	46:3O:129:ALA:HB1	2.01	0.41
48:3Q:72:ASP:HB2	48:3Q:83:ARG:HG2	2.02	0.41
48:3Q:138:PRO:HB2	52:3U:54:CYS:HB2	2.02	0.41
53:3W:11:SER:O	53:3W:15:ARG:NH2	2.53	0.41
57:4C:259:TRP:O	68:4N:47:ARG:NH2	2.44	0.41
59:4E:14:ARG:HG2	59:4E:14:ARG:NH1	2.34	0.41
2:5B:116:MET:SD	2:5B:156:LEU:HD22	2.60	0.41
13:5M:310:MET:HG2	13:5M:455:LEU:O	2.20	0.41
14:5N:17:THR:O	14:5N:21:MET:HG3	2.20	0.41
14:5N:109:SER:C	14:5N:111:PHE:N	2.78	0.41
19:5S:97:LYS:HE3	19:5S:97:LYS:HB3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:5Y:801:3PE:H242	76:5Y:801:3PE:H31	2.01	0.41
30:5e:93:PRO:HB2	30:5e:98:LEU:HG	2.02	0.41
31:5f:56:TRP:CE3	33:5h:85:LYS:HG3	2.55	0.41
42:5q:55:PHE:CD2	75:5q:202:AYA:HM1	2.55	0.41
55:8A:5:ARG:NH2	66:8L:10:ASN:OD1	2.48	0.41
55:8A:319:LYS:HB3	55:8A:319:LYS:HE2	1.83	0.41
56:8B:91:ASN:O	56:8B:93:PRO:HD3	2.20	0.41
86:8B:302:PGV:H102	86:8B:302:PGV:H271	2.01	0.41
57:8C:34:TRP:CZ3	92:8C:308:PEK:H272	2.54	0.41
62:8H:57:ARG:HA	62:8H:60:TYR:CD2	2.55	0.41
63:8I:73:LYS:HD2	63:8I:73:LYS:HA	1.82	0.41
68:8N:52:GLU:HA	68:8N:53:PRO:HD3	1.85	0.41
1:1A:30:TYR:OH	16:1P:174:ARG:HD3	2.20	0.41
69:1A:203:PC1:H153	16:1P:275:PHE:CZ	2.55	0.41
5:1E:162:GLU:O	5:1E:186:PRO:HA	2.21	0.41
6:1F:342:ASP:OD1	6:1F:429:ARG:NH2	2.41	0.41
7:1G:259:ASN:HB2	7:1G:390:LEU:HD13	2.03	0.41
12:1L:194:ASN:ND2	41:1p:106:GLN:OE1	2.53	0.41
14:1N:263:LYS:HE3	14:1N:263:LYS:HB3	1.70	0.41
16:1P:294:LEU:HB3	16:1P:296:HIS:CE1	2.55	0.41
17:1Q:9:GLN:CB	22:1W:23:ARG:HH12	2.32	0.41
17:1Q:70:MET:SD	42:1q:126:PRO:HB2	2.60	0.41
20:1T:52:MET:SD	22:1W:37:ARG:HG2	2.59	0.41
20:1U:4:PRO:O	20:1U:4:PRO:CD	2.68	0.41
28:1c:30:TYR:O	28:1c:34:GLN:HB2	2.20	0.41
29:1d:45:ASP:OD1	29:1d:51:ARG:NH2	2.54	0.41
36:1k:50:TRP:CE2	36:1k:51:ARG:HG2	2.55	0.41
37:1l:121:ILE:HG13	37:1l:122:TYR:CD1	2.54	0.41
39:1n:137:LYS:HE2	39:1n:137:LYS:HB3	1.68	0.41
43:1r:105:LEU:HD12	43:1r:105:LEU:HA	1.85	0.41
45:3A:3:THR:C	45:3A:5:ALA:H	2.27	0.41
45:3A:106:LEU:HD22	45:3A:203:VAL:HG23	2.01	0.41
45:3A:145:MET:HE2	45:3A:252:HIS:CD2	2.55	0.41
46:3O:181:TYR:CZ	46:3O:182:ARG:HG2	2.55	0.41
55:4A:242:GLU:HA	55:4A:245:ILE:HB	2.02	0.41
55:4A:495:LEU:HA	55:4A:495:LEU:HD23	1.81	0.41
56:4B:1:FME:HG2	56:4B:10:GLN:OE1	2.19	0.41
56:4B:65:TRP:CD1	56:4B:65:TRP:C	2.98	0.41
57:4C:64:GLU:HA	57:4C:68:GLN:HB2	2.02	0.41
62:4H:49:ASP:O	62:4H:52:VAL:HG22	2.19	0.41
64:4J:55:PHE:HB2	64:4J:57:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5D:154:VAL:HG11	4:5D:225:LEU:HD21	2.01	0.41
6:5F:92:TYR:CD1	6:5F:133:ALA:HB3	2.56	0.41
12:5L:40:VAL:HG11	12:5L:97:THR:HG23	2.01	0.41
12:5L:529:TYR:HB3	12:5L:530:PRO:HD3	2.01	0.41
14:5N:4:ILE:HG13	15:5O:9:VAL:HG22	2.03	0.41
16:5P:139:ILE:HG23	16:5P:140:LYS:HG2	2.02	0.41
16:5P:196:LEU:O	16:5P:239:PHE:HB2	2.20	0.41
19:5S:12:LYS:HD2	19:5S:12:LYS:HA	1.83	0.41
25:5Z:43:LEU:HD23	25:5Z:43:LEU:HA	1.87	0.41
32:5g:96:LEU:HD12	32:5g:100:ARG:NH2	2.35	0.41
38:5m:45:GLU:O	38:5m:49:GLN:HG3	2.19	0.41
38:5m:113:LYS:HB3	38:5m:113:LYS:HE3	1.76	0.41
39:5n:62:LEU:HD23	39:5n:62:LEU:HA	1.94	0.41
42:5q:138:VAL:HA	42:5q:139:PRO:HD3	1.96	0.41
42:5q:144:TYR:HB3	42:5q:145:LYS:H	1.62	0.41
58:8D:141:ASP:O	58:8D:143:ASN:N	2.53	0.41
59:8E:10:GLU:HA	59:8E:13:ALA:HB3	2.03	0.41
1:1A:49:LEU:HA	1:1A:51:PHE:CE2	2.55	0.41
69:1A:201:PC1:H261	69:1A:201:PC1:H222	2.02	0.41
4:1D:139:VAL:HG23	4:1D:278:TYR:CZ	2.55	0.41
8:1H:183:MET:HB3	9:1I:27:TRP:CH2	2.56	0.41
8:1H:283:ASP:OD1	8:1H:283:ASP:N	2.50	0.41
12:1L:158:TRP:CD2	39:1n:92:ARG:HG3	2.56	0.41
14:1N:256:PRO:HG2	76:1O:401:3PE:H2H2	2.02	0.41
16:1P:325:ARG:HD3	16:1P:326:TRP:CD1	2.55	0.41
20:1T:19:LEU:HD13	20:1T:50:ILE:HD12	2.02	0.41
25:1Z:124:LEU:HD23	25:1Z:124:LEU:HA	1.94	0.41
31:1f:16:VAL:HB	31:1f:17:PRO:HD3	2.02	0.41
34:1i:87:TYR:CD2	41:1p:48:ARG:HG2	2.54	0.41
44:1s:58:LEU:HD22	44:1s:61:PHE:HE1	1.85	0.41
74:3A:501:CDL:H132	76:3A:503:3PE:H372	2.01	0.41
46:3B:124:LEU:HB3	46:3B:223:PHE:CD2	2.56	0.41
47:3C:262:LEU:HD12	49:3R:216:VAL:HB	2.01	0.41
49:3E:181:LYS:HA	49:3E:181:LYS:HD3	1.81	0.41
49:3E:218:THR:OG1	49:3E:257:ASN:O	2.37	0.41
49:3E:263:TYR:HB3	49:3E:273:VAL:HG13	2.03	0.41
47:3P:197:LEU:HD21	84:3P:502:HEM:HMA3	2.01	0.41
55:4A:44:PRO:HD3	55:4A:448:THR:HG23	2.02	0.41
1:5A:113:TRP:HD1	8:5H:287:HIS:CE1	2.39	0.41
6:5F:107:ASP:OD1	6:5F:108:ARG:N	2.54	0.41
6:5F:423:ARG:N	6:5F:424:PRO:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:5H:66:SER:HA	8:5H:122:ALA:O	2.21	0.41
16:5P:241:LEU:HD12	16:5P:241:LEU:HA	1.90	0.41
17:5Q:33:ARG:NH1	17:5Q:77:ASP:HB2	2.34	0.41
17:5Q:37:ILE:HG13	17:5Q:57:MET:HG3	2.01	0.41
19:5S:36:ILE:HD13	19:5S:54:ILE:HD13	2.02	0.41
22:5W:17:VAL:HG21	22:5W:77:ARG:CZ	2.50	0.41
25:5Z:7:LYS:HB2	25:5Z:7:LYS:HE3	1.82	0.41
25:5Z:48:TRP:CZ2	25:5Z:52:LYS:HD3	2.55	0.41
25:5Z:98:MET:CE	30:5e:78:ILE:HA	2.50	0.41
35:5j:61:ASP:OD2	35:5j:66:ILE:HB	2.21	0.41
55:8A:118:VAL:HA	64:8J:54:SER:HA	2.01	0.41
67:8M:42:ARG:HG3	67:8M:42:ARG:NH1	2.36	0.41
5:1E:160:TYR:O	5:1E:185:GLY:N	2.45	0.41
5:1E:217:LEU:O	6:1F:51:LYS:HD2	2.20	0.41
6:1F:429:ARG:HE	6:1F:429:ARG:HB2	1.61	0.41
12:1L:245:ALA:HB2	12:1L:340:PHE:HB3	2.03	0.41
12:1L:553:LEU:HD11	76:1Y:806:3PE:H2F1	2.01	0.41
13:1M:252:PRO:HG3	29:1d:117:HIS:CE1	2.56	0.41
13:1M:346:ARG:O	13:1M:419:TYR:HA	2.20	0.41
14:1N:25:HIS:O	14:1N:29:ILE:HG12	2.21	0.41
14:1N:129:LEU:HD12	14:1N:129:LEU:HA	1.86	0.41
18:1R:37:GLU:OE1	18:1R:37:GLU:HA	2.21	0.41
18:1R:60:ASP:OD1	18:1R:60:ASP:C	2.64	0.41
18:1R:93:GLN:O	18:1R:95:HIS:N	2.53	0.41
20:1T:35:HIS:HB3	20:1T:38:LYS:HG2	2.01	0.41
23:1X:12:LEU:HD12	23:1X:12:LEU:O	2.20	0.41
43:1r:8:GLN:HA	43:1r:11:ARG:HG2	2.01	0.41
45:3A:356:ARG:HG3	46:3B:91:ALA:HA	2.02	0.41
76:3A:503:3PE:H2	76:3A:503:3PE:O14	2.21	0.41
48:3D:115:ARG:HB2	48:3D:143:CYS:HB2	2.01	0.41
47:3P:59:THR:HG23	47:3P:135:TRP:NE1	2.36	0.41
49:3R:219:HIS:CD2	49:3R:220:LEU:HB2	2.56	0.41
49:3V:64:LEU:HA	49:3V:77:ARG:O	2.21	0.41
55:4A:115:SER:HB2	55:4A:145:LEU:HB2	2.01	0.41
86:4C:301:PGV:H281	86:4C:307:PGV:H312	2.02	0.41
74:4C:306:CDL:H542	74:4C:306:CDL:HB61	2.02	0.41
58:4D:87:PHE:HD2	86:4M:101:PGV:H142	1.85	0.41
60:4F:14:THR:HG21	64:4J:9:GLN:HG2	2.01	0.41
5:5E:24:THR:HG23	5:5E:57:GLN:HE21	1.86	0.41
5:5E:111:ARG:HB2	5:5E:152:PRO:HD3	2.01	0.41
5:5E:165:THR:OG1	5:5E:168:ASP:OD1	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5G:258:ILE:HD11	7:5G:579:ARG:HD3	2.01	0.41
7:5G:341:ASP:CG	19:5S:67:ARG:HH22	2.28	0.41
7:5G:380:VAL:HG11	7:5G:429:LEU:HD11	2.02	0.41
8:5H:165:LEU:HD13	8:5H:241:LEU:HA	2.03	0.41
9:5I:144:HIS:CE1	16:5P:65:LEU:HD21	2.56	0.41
12:5L:154:LEU:HD13	12:5L:243:VAL:HG22	2.03	0.41
12:5L:373:LEU:HD13	12:5L:431:PHE:CE2	2.55	0.41
13:5M:74:PRO:HA	13:5M:77:LEU:HD12	2.03	0.41
13:5M:206:LYS:HE3	13:5M:206:LYS:HB3	1.90	0.41
15:5O:319:LEU:HD12	15:5O:319:LEU:HA	1.83	0.41
16:5P:157:ARG:HA	16:5P:157:ARG:HD3	1.90	0.41
16:5P:269:LEU:HD13	16:5P:269:LEU:HA	1.93	0.41
17:5Q:9:GLN:O	22:5W:19:PRO:HD3	2.20	0.41
76:5d:201:3PE:H232	69:5d:202:PC1:H251	2.02	0.41
37:5l:12:PRO:O	37:5l:46:ASP:HB3	2.20	0.41
55:8A:105:LEU:HD23	55:8A:105:LEU:HA	1.95	0.41
55:8A:218:THR:HG22	55:8A:221:ASP:HB3	2.01	0.41
86:8C:301:PGV:H242	86:8C:301:PGV:H22	2.01	0.41
63:8I:18:ARG:HG3	63:8I:18:ARG:H	1.71	0.41
3:1C:43:SER:OG	3:1C:47:GLU:HB2	2.21	0.41
4:1D:165:THR:HG22	4:1D:169:TRP:CE2	2.55	0.41
4:1D:342:MET:HB2	7:1G:134:LYS:NZ	2.36	0.41
7:1G:226:GLU:HB3	7:1G:253:ARG:CZ	2.51	0.41
10:1J:63:GLY:O	10:1J:66:VAL:HB	2.21	0.41
10:1J:71:THR:HG21	11:1K:75:LEU:HD22	2.01	0.41
12:1L:297:ASP:O	12:1L:301:ILE:HG22	2.19	0.41
13:1M:16:TRP:HB3	76:1M:903:3PE:H221	2.02	0.41
15:1O:104:ARG:NE	15:1O:131:ASP:OD1	2.43	0.41
16:1P:83:LYS:HB3	16:1P:83:LYS:HE2	1.71	0.41
16:1P:273:SER:HA	16:1P:274:PRO:HD3	1.89	0.41
17:1Q:67:ASN:HB3	17:1Q:72:TRP:H	1.85	0.41
30:1e:85:LEU:HD23	30:1e:85:LEU:HA	1.86	0.41
31:1f:8:ARG:HA	31:1f:8:ARG:HD2	1.60	0.41
33:1h:49:GLU:OE1	33:1h:68:LYS:HG2	2.21	0.41
35:1j:64:LEU:C	40:1o:30:PHE:HE1	2.29	0.41
41:1p:31:TYR:O	41:1p:34:LYS:N	2.53	0.41
41:1p:81:ILE:HD12	41:1p:81:ILE:HA	1.88	0.41
46:3B:238:LYS:HB2	46:3B:238:LYS:HE3	1.90	0.41
48:3D:198:PRO:HA	48:3D:199:PRO:HD3	1.95	0.41
53:3J:60:ASN:C	53:3J:60:ASN:OD1	2.63	0.41
46:3O:128:ALA:HA	46:3O:227:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:3R:187:GLU:OE1	49:3R:244:ASP:HB2	2.20	0.41
55:4A:305:PHE:CE2	86:4B:301:PGV:H21	2.55	0.41
56:4B:99:THR:HG23	56:4B:154:VAL:HA	2.02	0.41
58:4D:83:GLY:HA3	65:4K:17:ILE:HG22	2.01	0.41
2:5B:91:THR:HA	2:5B:119:CYS:HB3	2.02	0.41
12:5L:589:LEU:HD23	24:5Y:41:ALA:HA	2.03	0.41
76:5M:506:3PE:H292	38:5m:101:TYR:HB2	2.02	0.41
14:5N:40:MET:HE2	14:5N:44:LEU:HD21	2.02	0.41
14:5N:83:GLN:HE21	30:5e:62:PHE:HE2	1.69	0.41
17:5Q:67:ASN:HB3	17:5Q:72:TRP:H	1.86	0.41
32:5g:90:ARG:HD3	32:5g:90:ARG:HA	1.77	0.41
38:5m:116:GLN:OE1	38:5m:116:GLN:HA	2.19	0.41
39:5n:156:ALA:HB1	39:5n:161:ASP:OD1	2.20	0.41
56:8B:1:FME:HE2	56:8B:192:TYR:HA	2.03	0.41
1:1A:19:LEU:HD13	1:1A:23:TRP:CD1	2.56	0.41
1:1A:69:ILE:HD11	8:1H:144:VAL:HG13	2.01	0.41
2:1B:77:ARG:NH1	2:1B:78:ALA:HB3	2.35	0.41
3:1C:135:TRP:CZ2	22:1W:88:MET:HE1	2.56	0.41
5:1E:209:PRO:HA	6:1F:40:GLY:HA2	2.03	0.41
6:1F:108:ARG:HD2	6:1F:142:PHE:CE1	2.56	0.41
7:1G:364:LEU:HB3	7:1G:577:GLU:HA	2.02	0.41
8:1H:89:LEU:HD23	8:1H:89:LEU:HA	1.83	0.41
12:1L:99:SER:HA	12:1L:456:ARG:HH22	1.86	0.41
13:1M:206:LYS:HE3	13:1M:206:LYS:HB3	1.87	0.41
13:1M:211:GLY:HA3	76:1M:906:3PE:H3G1	2.02	0.41
76:1M:903:3PE:H362	29:1d:44:ILE:HG12	2.03	0.41
16:1P:10:LYS:O	22:1W:114:ARG:NH2	2.49	0.41
16:1P:135:LEU:HA	16:1P:167:LYS:HB2	2.03	0.41
20:1T:29:LYS:O	20:1T:29:LYS:NZ	2.37	0.41
20:1U:29:LYS:HE3	20:1U:29:LYS:HB3	1.83	0.41
28:1c:43:LYS:HG3	28:1c:48:LEU:HB3	2.02	0.41
32:1g:90:ARG:HA	32:1g:90:ARG:HD3	1.78	0.41
39:1n:154:PRO:O	39:1n:164:PRO:HD2	2.20	0.41
43:1r:30:ILE:H	43:1r:30:ILE:HG12	1.69	0.41
46:3B:424:MET:HB2	46:3B:436:VAL:HG22	2.01	0.41
49:3R:179:ARG:H	49:3R:179:ARG:HG3	1.74	0.41
55:4A:369:ASP:HB3	56:4B:197:SER:HB3	2.01	0.41
55:4A:508:PRO:HG3	57:4C:6:HIS:HB3	2.01	0.41
86:4A:603:PGV:O02	56:4B:43:SER:OG	2.37	0.41
58:4D:62:LEU:HD23	58:4D:62:LEU:HA	1.96	0.41
2:5B:179:ARG:HH12	79:5P:402:NDP:P2B	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5C:69:ASN:O	43:5r:96:PRO:HD3	2.20	0.41
4:5D:34:ASN:HB2	4:5D:36:VAL:HG22	2.02	0.41
4:5D:157:HIS:O	4:5D:161:ILE:HG12	2.21	0.41
4:5D:165:THR:HG22	4:5D:169:TRP:CE2	2.56	0.41
7:5G:147:LYS:HE3	7:5G:149:ILE:HD11	2.03	0.41
8:5H:68:ILE:HD11	74:5H:401:CDL:OA5	2.19	0.41
9:5I:64:GLU:O	9:5I:134:GLY:N	2.49	0.41
9:5I:155:LEU:HD23	9:5I:155:LEU:HA	1.93	0.41
12:5L:385:TYR:OH	35:5j:43:ASP:O	2.29	0.41
14:5N:261:MET:O	14:5N:265:MET:HG2	2.21	0.41
16:5P:297:LEU:HD23	16:5P:297:LEU:HA	1.85	0.41
17:5Q:27:GLU:OE1	17:5Q:27:GLU:N	2.50	0.41
21:5V:6:LYS:HB2	21:5V:6:LYS:HE3	1.87	0.41
24:5Y:72:THR:OG1	24:5Y:92:GLY:HA2	2.20	0.41
34:5i:76:ILE:HG13	34:5i:77:PRO:CD	2.40	0.41
38:5m:126:ILE:HG22	41:5p:139:GLN:HB2	2.02	0.41
74:8D:201:CDL:H662	74:8D:201:CDL:H622	2.02	0.41
2:1B:121:ASN:HB3	9:1I:114:THR:HG22	2.03	0.41
4:1D:24:GLU:OE2	4:1D:24:GLU:N	2.41	0.41
4:1D:64:LEU:HD23	4:1D:64:LEU:HA	1.96	0.41
4:1D:232:ASN:O	4:1D:236:ARG:HG3	2.21	0.41
5:1E:100:ILE:HB	5:1E:139:LEU:HA	2.02	0.41
6:1F:311:VAL:O	6:1F:315:VAL:HG13	2.21	0.41
7:1G:116:LEU:HD23	7:1G:116:LEU:HA	1.92	0.41
7:1G:147:LYS:HB3	7:1G:147:LYS:HE2	1.90	0.41
8:1H:102:VAL:HA	8:1H:105:MET:HB2	2.02	0.41
9:1I:155:LEU:HD23	9:1I:155:LEU:HA	1.93	0.41
9:1I:175:TYR:CE1	43:1r:38:PRO:HG3	2.55	0.41
10:1J:20:PHE:CZ	11:1K:35:GLY:HA3	2.56	0.41
11:1K:3:LEU:HD12	11:1K:3:LEU:O	2.21	0.41
11:1K:75:LEU:HD23	11:1K:78:LEU:HD23	2.02	0.41
12:1L:2:ASN:HB2	12:1L:3:PRO:HD2	2.02	0.41
12:1L:503:GLU:OE2	64:4J:33:ARG:NH2	2.53	0.41
14:1N:145:ILE:O	14:1N:149:ILE:HG23	2.21	0.41
24:1Y:100:LEU:O	24:1Y:104:THR:HG23	2.20	0.41
29:1d:95:LYS:HB2	29:1d:95:LYS:HE3	1.70	0.41
32:1g:92:GLU:OE2	41:1p:97:VAL:HG22	2.20	0.41
45:3A:87:ASN:HB3	45:3A:98:TYR:CZ	2.56	0.41
51:3G:66:GLN:OE1	51:3G:66:GLN:HA	2.20	0.41
47:3P:63:PHE:O	47:3P:67:THR:HG23	2.20	0.41
55:4A:216:ASN:ND2	61:4G:56:ARG:HD3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:4A:275:TRP:CZ3	86:4A:602:PGV:H12	2.56	0.41
55:4A:495:LEU:HD22	60:4F:73:TRP:CD1	2.55	0.41
57:4C:73:SER:HA	57:4C:76:GLN:OE1	2.21	0.41
62:4H:5:GLN:HG2	62:4H:6:THR:N	2.36	0.41
4:5D:232:ASN:O	4:5D:236:ARG:HG3	2.21	0.41
5:5E:121:GLN:HG2	5:5E:126:ILE:O	2.20	0.41
6:5F:254:LYS:HE2	6:5F:254:LYS:HB2	1.91	0.41
7:5G:427:LYS:HE2	7:5G:427:LYS:HB3	1.75	0.41
8:5H:63:PRO:HG3	8:5H:214:GLU:HB3	2.01	0.41
8:5H:90:PRO:HG3	8:5H:162:LEU:HB3	2.02	0.41
12:5L:441:VAL:HG13	12:5L:443:ILE:HG12	2.02	0.41
14:5N:1:FME:O1	15:5O:258:ARG:NH2	2.41	0.41
16:5P:113:ILE:HB	16:5P:114:PRO:HD3	2.03	0.41
21:5V:54:LYS:HG2	21:5V:71:LEU:HD22	2.01	0.41
32:5g:43:ASP:OD1	32:5g:43:ASP:N	2.54	0.41
33:5h:60:VAL:HA	33:5h:61:PRO:HD3	1.92	0.41
37:5l:81:LEU:O	37:5l:85:ILE:HG23	2.21	0.41
55:8A:449:ALA:O	55:8A:453:ILE:HG12	2.21	0.41
57:8C:31:LEU:HD23	57:8C:31:LEU:HA	1.95	0.41
3:1C:116:PRO:HB3	3:1C:141:PHE:HD2	1.86	0.41
5:1E:210:GLY:HA2	6:1F:43:TYR:CE2	2.56	0.41
6:1F:9:LYS:HE2	6:1F:9:LYS:HB3	1.85	0.41
7:1G:53:ARG:O	7:1G:93:VAL:HG21	2.21	0.41
7:1G:140:LYS:O	7:1G:148:THR:OG1	2.39	0.41
7:1G:288:LYS:HB3	7:1G:288:LYS:HE3	1.72	0.41
7:1G:319:ALA:HB3	7:1G:345:THR:HG22	2.01	0.41
7:1G:596:ASP:OD1	7:1G:596:ASP:N	2.52	0.41
8:1H:63:PRO:HB2	8:1H:66:SER:HB3	2.03	0.41
8:1H:121:TRP:CZ3	10:1J:27:ILE:HD13	2.56	0.41
10:1J:143:ILE:HG13	11:1K:57:ASN:HB3	2.03	0.41
11:1K:26:LEU:O	11:1K:30:LEU:HD12	2.21	0.41
12:1L:54:PHE:CZ	12:1L:84:TYR:HB2	2.56	0.41
12:1L:214:ILE:HD13	12:1L:214:ILE:HA	1.89	0.41
12:1L:486:MET:HA	12:1L:489:THR:OG1	2.21	0.41
12:1L:560:THR:HA	12:1L:564:LYS:HB2	2.03	0.41
13:1M:262:LEU:HD23	13:1M:299:VAL:HG22	2.02	0.41
14:1N:137:ALA:HB3	14:1N:138:PRO:HD3	2.03	0.41
14:1N:296:LEU:HA	14:1N:296:LEU:HD23	1.80	0.41
16:1P:157:ARG:HD3	16:1P:157:ARG:HA	1.89	0.41
16:1P:241:LEU:HD12	16:1P:241:LEU:HA	1.85	0.41
20:1T:18:VAL:HG21	20:1T:54:MET:SD	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1T:34:SER:O	20:1T:73:PRO:HD3	2.21	0.41
20:1U:25:ILE:HG13	20:1U:40:LEU:HD13	2.03	0.41
21:1V:97:LYS:HD3	21:1V:97:LYS:HA	1.72	0.41
23:1X:124:LEU:HD21	25:1Z:70:ALA:HB2	2.03	0.41
24:1Y:116:TYR:O	24:1Y:120:THR:OG1	2.32	0.41
27:1b:68:HIS:CD2	27:1b:69:PRO:HD2	2.56	0.41
34:1i:99:ARG:HA	41:1p:115:ARG:HA	2.02	0.41
37:1l:16:THR:OG1	37:1l:19:GLU:HG2	2.20	0.41
39:1n:163:PRO:HA	39:1n:164:PRO:HD3	1.96	0.41
74:3A:501:CDL:H352	47:3C:225:THR:HG21	2.02	0.41
46:3B:83:PHE:CZ	46:3B:87:ARG:HG3	2.56	0.41
76:3C:505:3PE:H291	49:3R:133:VAL:HG11	2.02	0.41
49:3E:211:VAL:HG21	49:3E:246:SER:HA	2.03	0.41
49:3E:235:TYR:N	49:3E:243:TYR:HB2	2.35	0.41
52:3H:57:LYS:HB2	52:3H:57:LYS:HE3	1.70	0.41
49:3I:53:GLU:CD	49:3I:53:GLU:H	2.29	0.41
47:3P:1:MET:HE3	47:3P:1:MET:HB3	1.98	0.41
55:4A:48:LEU:HD12	55:4A:48:LEU:O	2.21	0.41
90:4A:609:PSC:H011	63:4I:17:LEU:HD23	2.01	0.41
57:4C:141:GLY:O	57:4C:144:ILE:HG22	2.20	0.41
86:4C:303:PGV:H62	92:4C:308:PEK:H15	2.03	0.41
59:4E:61:PHE:HE1	59:4E:98:ILE:HA	1.86	0.41
68:4N:55:ASN:OD1	68:4N:55:ASN:N	2.53	0.41
4:5D:74:ARG:O	4:5D:407:LYS:NZ	2.54	0.41
4:5D:402:LEU:HD22	4:5D:418:ILE:HD11	2.02	0.41
5:5E:43:LYS:HD3	5:5E:43:LYS:HA	1.67	0.41
5:5E:120:ILE:HG12	5:5E:173:ILE:HD11	2.03	0.41
5:5E:192:SER:OG	5:5E:193:CYS:N	2.52	0.41
6:5F:429:ARG:HE	6:5F:429:ARG:HB2	1.62	0.41
72:5F:501:FMN:HM73	72:5F:501:FMN:HM81	1.90	0.41
7:5G:118:ASP:O	7:5G:122:MET:HG2	2.21	0.41
7:5G:232:ASP:OD1	7:5G:232:ASP:N	2.53	0.41
7:5G:316:ALA:HB3	7:5G:519:PRO:HG3	2.03	0.41
7:5G:376:VAL:HG12	7:5G:405:LYS:HB3	2.03	0.41
9:5I:39:SER:OG	9:5I:43:ARG:NH2	2.43	0.41
12:5L:2:ASN:CB	12:5L:3:PRO:HD2	2.51	0.41
12:5L:49:VAL:O	12:5L:53:MET:HG3	2.21	0.41
12:5L:291:CYS:SG	12:5L:526:LEU:HA	2.61	0.41
12:5L:378:LEU:HD22	12:5L:383:MET:HE2	2.03	0.41
13:5M:30:HIS:CD2	31:5f:16:VAL:HB	2.56	0.41
13:5M:59:ASP:OD2	13:5M:245:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:5M:92:LYS:O	13:5M:96:ILE:HG12	2.21	0.41
76:5M:502:3PE:H321	76:5M:502:3PE:H31	1.22	0.41
15:5O:65:ASP:HB3	28:5c:2:PHE:CE1	2.55	0.41
17:5Q:70:MET:SD	42:5q:126:PRO:HB2	2.61	0.41
23:5X:14:VAL:HG11	25:5Z:81:ARG:CZ	2.51	0.41
32:5g:70:LEU:O	32:5g:74:SER:OG	2.24	0.41
35:5j:61:ASP:OD1	35:5j:66:ILE:N	2.46	0.41
36:5k:12:LYS:HA	36:5k:12:LYS:HD2	1.97	0.41
69:5q:201:PC1:H351	69:5q:201:PC1:H322	1.99	0.41
55:8A:108:SER:HB3	55:8A:152:LEU:HB2	2.01	0.41
55:8A:173:PRO:HA	55:8A:174:PRO:HD3	1.95	0.41
55:8A:417:MET:O	55:8A:421:VAL:HG22	2.21	0.41
56:8B:93:PRO:HG2	62:8H:13:THR:HG21	2.01	0.41
74:8B:303:CDL:H182	74:8B:303:CDL:H442	2.03	0.41
59:8E:27:TRP:CZ3	59:8E:31:LYS:HD3	2.56	0.41
59:8E:67:ILE:HA	59:8E:70:VAL:HG12	2.03	0.41
60:8F:61:ILE:HG23	60:8F:66:ASN:HB2	2.02	0.41
61:8G:26:PRO:HB2	92:8G:102:PEK:H383	2.03	0.41
3:1C:40:VAL:HG12	3:1C:50:ILE:HG23	2.03	0.41
4:1D:270:ARG:HG3	4:1D:368:GLU:HB3	2.02	0.41
8:1H:105:MET:HB3	8:1H:105:MET:HE2	1.85	0.41
9:1I:70:TYR:CE2	9:1I:76:ARG:HA	2.55	0.41
10:1J:37:GLY:HA3	10:1J:61:LEU:HD11	2.02	0.41
12:1L:173:LEU:HD22	76:1L:701:3PE:H332	2.03	0.41
12:1L:503:GLU:HG3	64:4J:33:ARG:HB2	2.02	0.41
14:1N:17:THR:O	14:1N:21:MET:HG3	2.21	0.41
16:1P:185:MET:HE3	16:1P:185:MET:HB3	1.95	0.41
28:1c:19:LEU:C	74:1d:203:CDL:H122	2.46	0.41
34:1i:85:LEU:HD23	34:1i:89:VAL:HG21	2.02	0.41
37:1l:57:GLU:N	37:1l:57:GLU:OE1	2.54	0.41
39:1n:42:LEU:O	39:1n:46:ARG:HG3	2.21	0.41
40:1o:111:LYS:O	40:1o:115:GLU:HG2	2.21	0.41
45:3A:210:ASP:OD1	45:3A:210:ASP:C	2.63	0.41
47:3C:115:ILE:HB	47:3C:196:HIS:HD2	1.86	0.41
49:3E:236:CYS:HB3	49:3E:241:SER:HB3	2.01	0.41
47:3P:143:ALA:O	47:3P:147:THR:OG1	2.27	0.41
74:3P:504:CDL:H131	74:3T:101:CDL:H521	2.02	0.41
57:4C:54:MET:HE1	86:4C:307:PGV:H131	2.02	0.41
58:4D:124:LEU:HD23	58:4D:124:LEU:HA	1.88	0.41
74:4D:201:CDL:H562	74:4D:201:CDL:H191	2.03	0.41
66:4L:38:PHE:CD1	66:4L:41:ARG:HD3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5A:16:LEU:O	1:5A:20:ILE:HG23	2.20	0.41
76:5A:201:3PE:H361	76:5A:201:3PE:H3A2	2.03	0.41
8:5H:97:ASN:O	25:5Z:144:THR:HG23	2.21	0.41
8:5H:133:LEU:HD22	10:5J:70:TYR:CE1	2.56	0.41
9:5I:30:LEU:HD13	69:5I:201:PC1:H261	2.03	0.41
9:5I:44:GLU:OE2	75:5q:202:AYA:N	2.54	0.41
9:5I:152:GLU:HG3	42:5q:127:TYR:OH	2.21	0.41
11:5K:10:MET:HE2	11:5K:10:MET:HB3	1.76	0.41
12:5L:63:ILE:O	12:5L:79:SER:HA	2.21	0.41
13:5M:116:ILE:HG21	23:5X:167:PHE:CD1	2.56	0.41
13:5M:297:VAL:HG13	13:5M:312:ALA:HB1	2.01	0.41
19:5S:17:GLU:OE1	19:5S:67:ARG:NE	2.50	0.41
20:5T:36:PHE:HB3	20:5T:42:LEU:HD12	2.03	0.41
74:5X:201:CDL:H241	74:5X:201:CDL:H612	2.03	0.41
74:5X:201:CDL:H531	74:5X:201:CDL:H352	2.03	0.41
38:5m:4:LYS:HE2	38:5m:4:LYS:HB2	1.86	0.41
39:5n:113:MET:HE3	39:5n:113:MET:HB3	1.87	0.41
55:8A:362:SER:HA	56:8B:87:MET:HE2	2.02	0.41
57:8C:98:PHE:CD2	86:8C:304:PGV:H132	2.56	0.41
74:8D:201:CDL:H741	74:8D:201:CDL:H772	1.94	0.41
64:8J:55:PHE:HB2	64:8J:57:HIS:CE1	2.55	0.41
1:1A:115:GLU:HA	4:1D:72:MET:SD	2.61	0.40
4:1D:52:GLY:H	4:1D:53:PRO:CD	2.32	0.40
4:1D:228:MET:CE	9:1I:36:MET:HB3	2.51	0.40
7:1G:231:MET:HG3	7:1G:266:LYS:HD2	2.02	0.40
7:1G:526:GLY:N	7:1G:546:GLN:O	2.54	0.40
8:1H:9:LEU:O	8:1H:13:ILE:HD12	2.21	0.40
8:1H:199:ASP:OD1	8:1H:279:ARG:NE	2.45	0.40
10:1J:56:VAL:O	10:1J:60:TYR:HB3	2.21	0.40
12:1L:480:THR:OG1	12:1L:481:THR:N	2.55	0.40
16:1P:133:SER:HA	16:1P:149:LYS:HE3	2.03	0.40
27:1b:34:LEU:O	27:1b:34:LEU:HD12	2.21	0.40
30:1e:29:PRO:HB3	33:1h:143:ASN:HD22	1.87	0.40
69:1h:203:PC1:H2	69:1h:203:PC1:O13	2.21	0.40
40:1o:34:LYS:HE2	40:1o:34:LYS:HB2	1.88	0.40
51:3G:47:ILE:HD12	51:3G:47:ILE:HA	1.94	0.40
45:3N:284:TYR:CD2	49:3V:71:ASN:HA	2.55	0.40
76:3N:503:3PE:H332	69:3R:302:PC1:H342	2.03	0.40
46:3O:51:ILE:HG23	46:3O:204:MET:HG2	2.03	0.40
46:3O:232:LEU:HD12	46:3O:232:LEU:HA	1.96	0.40
51:3T:29:TYR:CE1	74:3T:101:CDL:HA61	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:4A:200:PRO:HB3	57:4C:93:PHE:HB2	2.03	0.40
86:4A:603:PGV:H221	74:4D:201:CDL:H152	2.03	0.40
58:4D:24:LEU:HB3	59:4E:30:ARG:HG2	2.03	0.40
59:4E:43:PRO:HB2	59:4E:48:ILE:HG12	2.02	0.40
60:4F:54:ASN:OD1	60:4F:54:ASN:N	2.53	0.40
86:4G:101:PGV:H202	86:4G:101:PGV:H012	1.47	0.40
62:4H:5:GLN:HG2	62:4H:6:THR:H	1.86	0.40
66:4L:16:GLU:OE1	66:4L:16:GLU:N	2.52	0.40
6:5F:349:ARG:O	6:5F:349:ARG:NH1	2.54	0.40
8:5H:2:PHE:HZ	8:5H:96:ILE:HD11	1.86	0.40
8:5H:92:PRO:HD3	8:5H:255:TYR:HD1	1.83	0.40
9:5I:95:GLU:HB2	9:5I:108:ARG:HB3	2.02	0.40
9:5I:161:TRP:CE3	42:5q:84:PRO:HB3	2.56	0.40
10:5J:79:TYR:HB2	16:5P:325:ARG:NH1	2.36	0.40
10:5J:150:GLY:HA2	30:5e:16:TRP:CZ2	2.56	0.40
12:5L:137:LEU:HD23	12:5L:137:LEU:HA	1.82	0.40
12:5L:183:VAL:HG21	13:5M:400:MET:HE1	2.02	0.40
12:5L:401:MET:HE1	12:5L:481:THR:O	2.21	0.40
13:5M:30:HIS:HB3	31:5f:16:VAL:HG11	2.03	0.40
13:5M:90:THR:HG21	76:5M:504:3PE:H12	2.03	0.40
13:5M:297:VAL:O	13:5M:301:ILE:HG13	2.20	0.40
13:5M:346:ARG:O	13:5M:419:TYR:HA	2.21	0.40
14:5N:230:LEU:HD23	14:5N:296:LEU:HD22	2.04	0.40
15:5O:318:TRP:H	15:5O:318:TRP:CD1	2.39	0.40
16:5P:299:GLY:N	16:5P:302:ASP:OD2	2.54	0.40
17:5Q:29:HIS:ND1	17:5Q:33:ARG:HD2	2.36	0.40
20:5T:50:ILE:HA	20:5T:50:ILE:HD13	1.82	0.40
24:5Y:123:LEU:HD12	24:5Y:126:MET:HE3	2.02	0.40
25:5Z:98:MET:HE3	30:5e:78:ILE:HA	2.02	0.40
37:5l:3:HIS:HB2	38:5m:60:GLU:OE1	2.21	0.40
37:5l:34:TYR:CZ	37:5l:36:PRO:HG3	2.56	0.40
43:5r:102:ARG:HB3	43:5r:102:ARG:NH1	2.36	0.40
60:8F:18:ARG:O	60:8F:22:MET:HG2	2.21	0.40
64:8J:36:MET:HB3	86:8J:101:PGV:H182	2.03	0.40
1:1A:27:LEU:HB2	69:1A:201:PC1:H143	2.02	0.40
1:1A:84:LEU:HB2	27:1b:42:ILE:HG12	2.03	0.40
1:1A:96:ILE:HG12	1:1A:96:ILE:H	1.74	0.40
4:1D:237:ASN:C	8:1H:284:GLN:HE22	2.26	0.40
9:1I:3:LYS:HE2	43:1r:112:LEU:HB2	2.03	0.40
9:1I:19:ASP:OD1	25:1Z:32:GLY:N	2.44	0.40
10:1J:115:ILE:O	10:1J:115:ILE:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1J:167:VAL:HG13	14:1N:42:PRO:HG3	2.02	0.40
76:1P:502:3PE:H112	76:1P:502:3PE:H11	2.03	0.40
18:1R:49:VAL:HG22	18:1R:90:GLN:HB2	2.02	0.40
20:1T:73:PRO:O	20:1T:77:VAL:HG23	2.20	0.40
33:1h:53:ALA:HB2	41:1p:61:TYR:HD2	1.86	0.40
45:3A:51:LYS:HB3	45:3A:51:LYS:HE2	1.90	0.40
55:4A:251:PHE:CD1	55:4A:323:TRP:HH2	2.38	0.40
56:4B:51:THR:O	59:4E:74:LYS:NZ	2.54	0.40
56:4B:217:LYS:HE3	56:4B:218:TYR:CE1	2.55	0.40
74:4D:201:CDL:H581	74:4D:201:CDL:H621	2.02	0.40
12:5L:174:TYR:CD2	12:5L:232:TRP:HB3	2.56	0.40
69:5M:503:PC1:O32	24:5Y:87:LEU:HB2	2.21	0.40
14:5N:192:ALA:O	14:5N:195:PRO:HD2	2.21	0.40
20:5T:52:MET:HA	20:5T:55:GLU:HG3	2.04	0.40
23:5X:157:LEU:HD23	23:5X:157:LEU:HA	1.95	0.40
31:5f:18:VAL:HA	31:5f:21:VAL:HG22	2.02	0.40
38:5m:110:LYS:HE3	38:5m:110:LYS:HB2	1.84	0.40
40:5o:4:LEU:HG	40:5o:8:TYR:HE2	1.86	0.40
40:5o:38:MET:HE2	40:5o:57:TYR:HA	2.02	0.40
41:5p:139:GLN:O	41:5p:143:SER:HB2	2.21	0.40
43:5r:35:GLN:HE21	43:5r:35:GLN:HB3	1.63	0.40
55:8A:374:VAL:HG12	55:8A:428:GLN:NE2	2.37	0.40
56:8B:158:ASP:OD1	56:8B:161:HIS:HE1	2.04	0.40
57:8C:22:LEU:HD12	64:8J:39:CYS:SG	2.61	0.40
68:8N:46:ASP:C	68:8N:48:LYS:H	2.29	0.40
5:1E:68:LYS:HE3	5:1E:68:LYS:HB2	1.87	0.40
5:1E:149:VAL:HG21	6:1F:267:THR:HG22	2.02	0.40
6:1F:143:TYR:HB2	6:1F:179:ARG:NH2	2.37	0.40
6:1F:406:ALA:HB3	72:1F:501:FMN:HM82	2.04	0.40
7:1G:102:PRO:HB2	7:1G:104:ASP:OD2	2.21	0.40
7:1G:675:ASP:OD1	7:1G:675:ASP:N	2.54	0.40
8:1H:87:VAL:HG22	8:1H:88:PRO:HD3	2.04	0.40
9:1I:160:LYS:HD2	9:1I:161:TRP:NE1	2.36	0.40
12:1L:583:LEU:HD12	12:1L:586:LEU:HD22	2.04	0.40
76:1L:703:3PE:H282	74:1h:202:CDL:OA9	2.21	0.40
13:1M:72:LEU:HD23	13:1M:76:MET:HE2	2.02	0.40
14:1N:179:MET:HE3	14:1N:179:MET:HB3	1.94	0.40
74:1N:401:CDL:H221	74:1N:401:CDL:H371	2.02	0.40
15:1O:304:TYR:O	29:1d:50:ARG:HB3	2.21	0.40
16:1P:59:LEU:HD23	16:1P:62:MET:HE3	2.03	0.40
16:1P:185:MET:HE3	16:1P:192:PRO:HD2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:1X:201:CDL:H382	29:1d:32:VAL:HG12	2.04	0.40
27:1b:15:GLU:O	27:1b:19:VAL:HG12	2.21	0.40
47:3C:197:LEU:HD21	84:3C:502:HEM:HMA3	2.02	0.40
47:3P:112:THR:HG22	47:3P:199:PHE:HB3	2.03	0.40
48:3Q:191:ARG:NH2	48:3Q:195:GLU:OE1	2.55	0.40
55:4A:80:ASN:OD1	55:4A:98:ASN:ND2	2.39	0.40
55:4A:214:ASN:HA	61:4G:58:LYS:HD3	2.04	0.40
58:4D:24:LEU:HD11	59:4E:67:ILE:HG22	2.03	0.40
1:5A:23:TRP:HE1	69:5A:202:PC1:H31	1.86	0.40
2:5B:45:LEU:O	2:5B:47:PRO:HD3	2.21	0.40
2:5B:144:ILE:HG13	2:5B:163:LEU:HB2	2.02	0.40
4:5D:159:LEU:HD12	4:5D:164:MET:HA	2.03	0.40
6:5F:121:GLY:HA2	6:5F:232:PRO:HG3	2.03	0.40
7:5G:26:VAL:HG23	7:5G:71:MET:O	2.22	0.40
8:5H:103:LEU:HB3	10:5J:54:LEU:HD13	2.03	0.40
11:5K:56:ALA:HA	30:5e:17:MET:SD	2.62	0.40
12:5L:419:THR:HA	12:5L:422:TYR:CE2	2.55	0.40
74:5L:702:CDL:H351	33:5h:25:MET:HE2	2.03	0.40
14:5N:45:MET:HE3	14:5N:53:THR:HG22	2.03	0.40
14:5N:226:THR:HG23	14:5N:229:SER:H	1.87	0.40
16:5P:130:ILE:HG23	16:5P:164:THR:HB	2.03	0.40
16:5P:130:ILE:HD11	16:5P:218:ILE:HD13	2.02	0.40
19:5S:15:LEU:HB3	19:5S:50:LEU:HD11	2.03	0.40
30:5e:16:TRP:CE3	30:5e:17:MET:HB2	2.56	0.40
30:5e:85:LEU:HA	30:5e:85:LEU:HD12	1.80	0.40
74:5h:202:CDL:H582	34:5i:79:TRP:CD2	2.57	0.40
39:5n:64:ARG:HA	39:5n:64:ARG:HD3	1.89	0.40
43:5r:42:VAL:HB	43:5r:46:HIS:CG	2.56	0.40
55:8A:393:PHE:O	55:8A:397:PHE:HB2	2.22	0.40
55:8A:445:ASP:OD1	56:8B:134:ARG:NE	2.41	0.40
56:8B:135:LEU:HD21	56:8B:206:PHE:HE1	1.85	0.40
86:8G:101:PGV:H02	86:8G:101:PGV:H21	1.57	0.40
4:1D:241:ASP:OD1	4:1D:290:ARG:NH2	2.53	0.40
4:1D:312:SER:O	4:1D:316:ASN:ND2	2.54	0.40
6:1F:24:ASN:O	6:1F:113:HIS:HB3	2.21	0.40
6:1F:203:PRO:HG2	6:1F:405:CYS:SG	2.62	0.40
7:1G:251:LEU:HD23	7:1G:251:LEU:HA	1.90	0.40
7:1G:585:VAL:HG13	17:1Q:61:THR:OG1	2.21	0.40
10:1J:105:TYR:O	10:1J:109:LYS:HG2	2.22	0.40
12:1L:155:ILE:HD11	12:1L:248:HIS:HE1	1.86	0.40
12:1L:459:ILE:HG23	12:1L:463:PHE:HD2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:86:LYS:H	13:1M:86:LYS:HG2	1.61	0.40
13:1M:367:LEU:HD12	13:1M:407:SER:HB2	2.03	0.40
14:1N:25:HIS:HE2	30:1e:17:MET:HG2	1.87	0.40
14:1N:102:LEU:HD13	14:1N:142:LEU:HG	2.04	0.40
20:1T:14:ARG:HA	20:1T:17:TYR:CZ	2.57	0.40
20:1T:55:GLU:OE2	20:1T:55:GLU:HA	2.21	0.40
20:1T:64:ASP:HA	20:1T:67:ALA:HB3	2.02	0.40
24:1Y:95:ALA:O	24:1Y:99:THR:HG23	2.21	0.40
25:1Z:48:TRP:CZ2	25:1Z:52:LYS:HE2	2.57	0.40
25:1Z:51:MET:SD	25:1Z:55:ARG:NH1	2.94	0.40
28:1c:19:LEU:HB3	74:1d:203:CDL:H122	2.03	0.40
28:1c:28:TRP:NE1	29:1d:66:THR:HG22	2.37	0.40
29:1d:3:SER:HB2	69:1d:202:PC1:H131	2.03	0.40
76:1d:201:3PE:H271	76:1d:201:3PE:H3B2	2.03	0.40
30:1e:11:LEU:HD23	30:1e:11:LEU:HA	1.83	0.40
36:1k:18:TYR:CD1	36:1k:18:TYR:C	2.99	0.40
44:1s:45:GLU:H	44:1s:45:GLU:CD	2.26	0.40
44:1s:47:SER:H	44:1s:50:THR:HG1	1.67	0.40
46:3B:200:THR:O	46:3B:204:MET:HG3	2.21	0.40
47:3C:131:TYR:O	47:3C:139:SER:OG	2.35	0.40
47:3C:262:LEU:HD13	49:3R:172:LYS:HG2	2.03	0.40
74:3C:503:CDL:OB3	51:3G:42:ARG:HD2	2.21	0.40
49:3E:247:GLY:HA2	49:3E:258:LEU:HD12	2.02	0.40
50:3F:110:ILE:HD13	50:3F:113:ARG:HH21	1.86	0.40
46:3O:47:ILE:HD13	46:3O:120:MET:HG3	2.03	0.40
46:3O:312:PHE:HA	49:3V:61:GLY:HA2	2.02	0.40
48:3Q:56:TYR:HD2	48:3Q:60:GLU:HB3	1.86	0.40
55:4A:282:PHE:HA	86:4A:602:PGV:H292	2.03	0.40
57:4C:16:TRP:HZ2	64:4J:21:HIS:HB2	1.86	0.40
58:4D:19:ARG:NH1	58:4D:21:ASP:OD1	2.55	0.40
1:5A:21:ALA:HB1	8:5H:218:GLY:HA3	2.02	0.40
4:5D:417:ILE:O	4:5D:420:THR:HG22	2.21	0.40
6:5F:129:MET:HE3	6:5F:221:THR:HB	2.03	0.40
6:5F:302:SER:HB2	6:5F:350:LEU:CD1	2.52	0.40
12:5L:556:ILE:HD12	38:5m:79:PHE:CD1	2.56	0.40
13:5M:82:SER:OG	13:5M:335:GLU:OE2	2.33	0.40
13:5M:204:MET:HE3	13:5M:204:MET:HB3	1.91	0.40
15:5O:234:VAL:O	15:5O:238:ILE:HG12	2.21	0.40
24:5Y:43:LYS:HG3	76:5Y:801:3PE:O11	2.20	0.40
32:5g:109:GLU:OE2	32:5g:110:SER:N	2.50	0.40
35:5j:66:ILE:HG13	40:5o:106:ARG:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:5n:139:LEU:HD11	39:5n:165:LEU:HG	2.03	0.40
55:8A:96:ARG:HD3	57:8C:14:SER:HB2	2.03	0.40
55:8A:476:PHE:HB3	66:8L:21:LEU:HD21	2.03	0.40
86:8A:601:PGV:H232	86:8A:601:PGV:H82	2.03	0.40
86:8A:602:PGV:H141	86:8A:602:PGV:H182	2.02	0.40
56:8B:100:MET:HB2	56:8B:107:SER:OG	2.21	0.40
68:8N:6:ILE:HG22	68:8N:10:LYS:NZ	2.37	0.40
4:1D:47:LEU:O	4:1D:67:GLU:HA	2.21	0.40
4:1D:345:LEU:HD21	7:1G:106:PRO:HD3	2.02	0.40
6:1F:30:ASP:OD1	6:1F:32:ARG:NE	2.43	0.40
7:1G:539:LYS:HA	7:1G:539:LYS:HD3	1.73	0.40
8:1H:74:ALA:HB3	8:1H:75:PRO:HD3	2.04	0.40
9:1I:50:TYR:CD1	9:1I:51:PRO:HA	2.56	0.40
12:1L:316:THR:HG23	12:1L:325:ALA:HB2	2.02	0.40
13:1M:212:LEU:HD22	76:1M:901:3PE:H3E2	2.03	0.40
15:1O:25:ILE:HG23	15:1O:168:VAL:HB	2.04	0.40
16:1P:279:THR:HG21	76:1P:502:3PE:H372	2.03	0.40
47:3C:136:GLY:H	47:3C:139:SER:HB2	1.87	0.40
51:3G:12:MET:HB2	51:3G:12:MET:HE3	1.90	0.40
45:3N:24:ARG:HB2	45:3N:196:VAL:HG22	2.04	0.40
45:3N:112:LEU:HD12	45:3N:112:LEU:HA	1.93	0.40
49:3R:168:LYS:HB3	49:3R:168:LYS:HE3	1.78	0.40
54:3Y:7:GLY:O	54:3Y:11:ARG:HG3	2.22	0.40
56:4B:92:ASN:ND2	56:4B:92:ASN:C	2.72	0.40
58:4D:100:LYS:HD3	65:4K:38:ILE:HG13	2.04	0.40
58:4D:138:TRP:HB2	58:4D:145:TRP:CE3	2.55	0.40
62:4H:22:ASN:O	62:4H:25:GLN:NE2	2.55	0.40
4:5D:126:LEU:HG	4:5D:358:VAL:HG22	2.02	0.40
7:5G:512:GLU:OE1	7:5G:512:GLU:N	2.52	0.40
10:5J:125:TRP:HB2	25:5Z:137:THR:HG21	2.04	0.40
13:5M:245:ARG:HA	13:5M:245:ARG:HD2	1.90	0.40
14:5N:172:GLN:HB2	14:5N:178:ILE:HG13	2.03	0.40
15:5O:304:TYR:H	15:5O:309:ASN:ND2	2.20	0.40
16:5P:196:LEU:HD23	16:5P:196:LEU:HA	1.90	0.40
81:5T:101:EHZ:O3	81:5T:101:EHZ:N2	2.53	0.40
25:5Z:7:LYS:NZ	43:5r:37:PRO:O	2.44	0.40
29:5d:113:LEU:HD22	32:5g:121:PRO:HG3	2.02	0.40
32:5g:68:ILE:O	32:5g:72:LEU:HB2	2.22	0.40
37:5l:3:HIS:ND1	37:5l:4:VAL:HG22	2.36	0.40
39:5n:154:PRO:O	39:5n:164:PRO:HD2	2.22	0.40
40:5o:23:THR:N	40:5o:104:GLU:OE2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:8C:215:LEU:HD23	57:8C:238:ALA:HB1	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	113/115 (98%)	100 (88%)	12 (11%)	1 (1%)	14	35
1	5A	113/115 (98%)	104 (92%)	7 (6%)	2 (2%)	6	18
2	1B	153/258 (59%)	145 (95%)	8 (5%)	0	100	100
2	5B	153/258 (59%)	141 (92%)	12 (8%)	0	100	100
3	1C	207/264 (78%)	200 (97%)	7 (3%)	0	100	100
3	5C	207/264 (78%)	200 (97%)	7 (3%)	0	100	100
4	1D	427/476 (90%)	411 (96%)	16 (4%)	0	100	100
4	5D	427/476 (90%)	408 (96%)	19 (4%)	0	100	100
5	1E	212/249 (85%)	201 (95%)	10 (5%)	1 (0%)	24	48
5	5E	212/249 (85%)	199 (94%)	13 (6%)	0	100	100
6	1F	430/464 (93%)	409 (95%)	18 (4%)	3 (1%)	18	41
6	5F	430/464 (93%)	403 (94%)	24 (6%)	3 (1%)	18	41
7	1G	697/727 (96%)	666 (96%)	29 (4%)	2 (0%)	36	60
7	5G	697/727 (96%)	669 (96%)	25 (4%)	3 (0%)	30	54
8	1H	316/318 (99%)	297 (94%)	18 (6%)	1 (0%)	36	60
8	5H	316/318 (99%)	300 (95%)	14 (4%)	2 (1%)	21	44
9	1I	174/239 (73%)	168 (97%)	6 (3%)	0	100	100
9	5I	174/239 (73%)	167 (96%)	7 (4%)	0	100	100
10	1J	172/175 (98%)	161 (94%)	10 (6%)	1 (1%)	21	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	5J	172/175 (98%)	161 (94%)	10 (6%)	1 (1%)	21	44
11	1K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
11	5K	96/98 (98%)	92 (96%)	3 (3%)	1 (1%)	12	32
12	1L	604/606 (100%)	562 (93%)	42 (7%)	0	100	100
12	5L	604/606 (100%)	562 (93%)	41 (7%)	1 (0%)	43	68
13	1M	457/459 (100%)	448 (98%)	9 (2%)	0	100	100
13	5M	457/459 (100%)	447 (98%)	10 (2%)	0	100	100
14	1N	345/347 (99%)	333 (96%)	11 (3%)	1 (0%)	36	60
14	5N	345/347 (99%)	333 (96%)	11 (3%)	1 (0%)	36	60
15	1O	318/357 (89%)	307 (96%)	11 (4%)	0	100	100
15	5O	318/357 (89%)	308 (97%)	10 (3%)	0	100	100
16	1P	340/377 (90%)	328 (96%)	12 (4%)	0	100	100
16	5P	340/377 (90%)	330 (97%)	10 (3%)	0	100	100
17	1Q	127/175 (73%)	116 (91%)	11 (9%)	0	100	100
17	5Q	127/175 (73%)	115 (91%)	12 (9%)	0	100	100
18	1R	94/123 (76%)	90 (96%)	4 (4%)	0	100	100
18	5R	94/123 (76%)	91 (97%)	3 (3%)	0	100	100
19	1S	85/99 (86%)	78 (92%)	7 (8%)	0	100	100
19	5S	85/99 (86%)	79 (93%)	6 (7%)	0	100	100
20	1T	83/156 (53%)	83 (100%)	0	0	100	100
20	1U	84/156 (54%)	80 (95%)	4 (5%)	0	100	100
20	5T	83/156 (53%)	82 (99%)	1 (1%)	0	100	100
20	5U	84/156 (54%)	82 (98%)	2 (2%)	0	100	100
21	1V	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
21	5V	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
22	1W	113/128 (88%)	108 (96%)	5 (4%)	0	100	100
22	5W	113/128 (88%)	109 (96%)	4 (4%)	0	100	100
23	1X	169/172 (98%)	162 (96%)	6 (4%)	1 (1%)	21	44
23	5X	169/172 (98%)	162 (96%)	6 (4%)	1 (1%)	21	44
24	1Y	137/141 (97%)	135 (98%)	2 (2%)	0	100	100
24	5Y	137/141 (97%)	135 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	1Z	139/144 (96%)	136 (98%)	3 (2%)	0	100	100
25	5Z	139/144 (96%)	135 (97%)	4 (3%)	0	100	100
26	1a	68/70 (97%)	68 (100%)	0	0	100	100
26	5a	68/70 (97%)	68 (100%)	0	0	100	100
27	1b	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
27	5b	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
28	1c	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
28	5c	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
29	1d	117/122 (96%)	114 (97%)	3 (3%)	0	100	100
29	5d	117/122 (96%)	115 (98%)	2 (2%)	0	100	100
30	1e	97/106 (92%)	93 (96%)	4 (4%)	0	100	100
30	5e	97/106 (92%)	92 (95%)	5 (5%)	0	100	100
31	1f	55/135 (41%)	51 (93%)	4 (7%)	0	100	100
31	5f	55/135 (41%)	52 (94%)	3 (6%)	0	100	100
32	1g	98/154 (64%)	89 (91%)	9 (9%)	0	100	100
32	5g	98/154 (64%)	91 (93%)	7 (7%)	0	100	100
33	1h	136/189 (72%)	134 (98%)	2 (2%)	0	100	100
33	5h	136/189 (72%)	131 (96%)	5 (4%)	0	100	100
34	1i	125/128 (98%)	120 (96%)	5 (4%)	0	100	100
34	5i	125/128 (98%)	117 (94%)	8 (6%)	0	100	100
35	1j	69/105 (66%)	67 (97%)	2 (3%)	0	100	100
35	5j	69/105 (66%)	66 (96%)	3 (4%)	0	100	100
36	1k	79/98 (81%)	75 (95%)	4 (5%)	0	100	100
36	5k	79/98 (81%)	76 (96%)	3 (4%)	0	100	100
37	1l	154/186 (83%)	148 (96%)	6 (4%)	0	100	100
37	5l	154/186 (83%)	144 (94%)	10 (6%)	0	100	100
38	1m	126/129 (98%)	120 (95%)	6 (5%)	0	100	100
38	5m	126/129 (98%)	120 (95%)	6 (5%)	0	100	100
39	1n	170/179 (95%)	165 (97%)	5 (3%)	0	100	100
39	5n	170/179 (95%)	160 (94%)	9 (5%)	1 (1%)	21	44
40	1o	120/137 (88%)	113 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	5o	120/137 (88%)	115 (96%)	5 (4%)	0	100	100
41	1p	171/176 (97%)	167 (98%)	4 (2%)	0	100	100
41	5p	171/176 (97%)	168 (98%)	3 (2%)	0	100	100
42	1q	143/145 (99%)	138 (96%)	5 (4%)	0	100	100
42	5q	143/145 (99%)	139 (97%)	4 (3%)	0	100	100
43	1r	90/113 (80%)	86 (96%)	4 (4%)	0	100	100
43	5r	90/113 (80%)	86 (96%)	4 (4%)	0	100	100
44	1s	43/471 (9%)	41 (95%)	2 (5%)	0	100	100
44	5s	43/471 (9%)	39 (91%)	4 (9%)	0	100	100
45	3A	436/480 (91%)	429 (98%)	5 (1%)	2 (0%)	24	48
45	3N	444/480 (92%)	425 (96%)	18 (4%)	1 (0%)	43	68
46	3B	414/453 (91%)	405 (98%)	9 (2%)	0	100	100
46	3O	413/453 (91%)	406 (98%)	7 (2%)	0	100	100
47	3C	377/379 (100%)	371 (98%)	6 (2%)	0	100	100
47	3P	377/379 (100%)	372 (99%)	5 (1%)	0	100	100
48	3D	235/326 (72%)	229 (97%)	6 (3%)	0	100	100
48	3Q	237/326 (73%)	230 (97%)	7 (3%)	0	100	100
49	3E	194/274 (71%)	176 (91%)	17 (9%)	1 (0%)	24	48
49	3I	45/274 (16%)	43 (96%)	2 (4%)	0	100	100
49	3R	194/274 (71%)	175 (90%)	16 (8%)	3 (2%)	8	22
49	3V	29/274 (11%)	28 (97%)	1 (3%)	0	100	100
50	3F	96/111 (86%)	96 (100%)	0	0	100	100
50	3S	96/111 (86%)	95 (99%)	1 (1%)	0	100	100
51	3G	72/82 (88%)	71 (99%)	1 (1%)	0	100	100
51	3T	72/82 (88%)	71 (99%)	1 (1%)	0	100	100
52	3H	63/91 (69%)	61 (97%)	2 (3%)	0	100	100
52	3U	63/91 (69%)	63 (100%)	0	0	100	100
53	3J	54/64 (84%)	53 (98%)	0	1 (2%)	6	17
53	3W	54/64 (84%)	54 (100%)	0	0	100	100
54	3X	50/56 (89%)	48 (96%)	2 (4%)	0	100	100
54	3Y	49/56 (88%)	45 (92%)	4 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	4A	512/514 (100%)	492 (96%)	18 (4%)	2 (0%)	30	54
55	8A	512/514 (100%)	489 (96%)	21 (4%)	2 (0%)	30	54
56	4B	225/229 (98%)	219 (97%)	6 (3%)	0	100	100
56	8B	225/229 (98%)	216 (96%)	9 (4%)	0	100	100
57	4C	257/261 (98%)	250 (97%)	7 (3%)	0	100	100
57	8C	257/261 (98%)	248 (96%)	9 (4%)	0	100	100
58	4D	137/169 (81%)	129 (94%)	8 (6%)	0	100	100
58	8D	137/169 (81%)	129 (94%)	8 (6%)	0	100	100
59	4E	103/152 (68%)	101 (98%)	2 (2%)	0	100	100
59	8E	103/152 (68%)	100 (97%)	3 (3%)	0	100	100
60	4F	95/128 (74%)	91 (96%)	3 (3%)	1 (1%)	11	29
60	8F	95/128 (74%)	89 (94%)	5 (5%)	1 (1%)	11	29
61	4G	73/97 (75%)	70 (96%)	3 (4%)	0	100	100
61	8G	73/97 (75%)	71 (97%)	2 (3%)	0	100	100
62	4H	80/86 (93%)	76 (95%)	4 (5%)	0	100	100
62	8H	80/86 (93%)	75 (94%)	5 (6%)	0	100	100
63	4I	65/75 (87%)	65 (100%)	0	0	100	100
63	8I	65/75 (87%)	63 (97%)	2 (3%)	0	100	100
64	4J	56/80 (70%)	52 (93%)	4 (7%)	0	100	100
64	8J	56/80 (70%)	54 (96%)	2 (4%)	0	100	100
65	4K	47/80 (59%)	47 (100%)	0	0	100	100
65	8K	47/80 (59%)	45 (96%)	2 (4%)	0	100	100
66	4L	44/63 (70%)	42 (96%)	2 (4%)	0	100	100
66	8L	44/63 (70%)	43 (98%)	1 (2%)	0	100	100
67	4M	41/70 (59%)	40 (98%)	1 (2%)	0	100	100
67	8M	41/70 (59%)	41 (100%)	0	0	100	100
68	4N	80/82 (98%)	70 (88%)	9 (11%)	1 (1%)	9	25
68	8N	80/82 (98%)	70 (88%)	9 (11%)	1 (1%)	9	25
All	All	24082/28836 (84%)	23087 (96%)	952 (4%)	43 (0%)	44	68

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	1H	208	VAL
10	1J	66	VAL
23	1X	28	ALA
49	3E	271	VAL
53	3J	57	LYS
45	3N	224	VAL
8	5H	92	PRO
10	5J	66	VAL
23	5X	28	ALA
49	3R	150	SER
49	3R	273	VAL
6	5F	297	VAL
8	5H	208	VAL
5	1E	157	ASN
6	1F	249	ARG
6	1F	297	VAL
49	3R	228	ALA
12	5L	72	GLN
7	1G	654	GLN
1	5A	52	SER
6	5F	249	ARG
7	5G	654	GLN
68	8N	33	VAL
1	1A	52	SER
14	1N	110	PRO
45	3A	231	PHE
45	3A	350	THR
60	4F	95	GLN
7	5G	155	GLN
14	5N	110	PRO
6	1F	207	PRO
7	1G	155	GLN
68	4N	33	VAL
1	5A	109	LYS
6	5F	207	PRO
7	5G	186	TYR
60	8F	95	GLN
55	4A	3	VAL
11	5K	2	PRO
55	8A	3	VAL
55	8A	128	VAL
55	4A	128	VAL
39	5n	31	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	1A	99/99 (100%)	98 (99%)	1 (1%)	68	86
1	5A	99/99 (100%)	99 (100%)	0	100	100
2	1B	131/212 (62%)	131 (100%)	0	100	100
2	5B	131/212 (62%)	131 (100%)	0	100	100
3	1C	190/227 (84%)	190 (100%)	0	100	100
3	5C	190/227 (84%)	190 (100%)	0	100	100
4	1D	371/405 (92%)	371 (100%)	0	100	100
4	5D	371/405 (92%)	370 (100%)	1 (0%)	86	94
5	1E	183/207 (88%)	183 (100%)	0	100	100
5	5E	183/207 (88%)	183 (100%)	0	100	100
6	1F	346/368 (94%)	346 (100%)	0	100	100
6	5F	346/368 (94%)	345 (100%)	1 (0%)	86	94
7	1G	588/610 (96%)	587 (100%)	1 (0%)	87	95
7	5G	588/610 (96%)	587 (100%)	1 (0%)	87	95
8	1H	274/274 (100%)	272 (99%)	2 (1%)	76	90
8	5H	274/274 (100%)	273 (100%)	1 (0%)	84	93
9	1I	151/201 (75%)	151 (100%)	0	100	100
9	5I	151/201 (75%)	151 (100%)	0	100	100
10	1J	140/141 (99%)	140 (100%)	0	100	100
10	5J	140/141 (99%)	138 (99%)	2 (1%)	59	82
11	1K	84/84 (100%)	84 (100%)	0	100	100
11	5K	84/84 (100%)	84 (100%)	0	100	100
12	1L	539/539 (100%)	537 (100%)	2 (0%)	84	93
12	5L	539/539 (100%)	539 (100%)	0	100	100
13	1M	408/408 (100%)	407 (100%)	1 (0%)	87	95
13	5M	408/408 (100%)	406 (100%)	2 (0%)	81	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	1N	310/310 (100%)	309 (100%)	1 (0%)	86	94
14	5N	310/310 (100%)	309 (100%)	1 (0%)	86	94
15	1O	283/307 (92%)	283 (100%)	0	100	100
15	5O	283/307 (92%)	282 (100%)	1 (0%)	84	93
16	1P	296/323 (92%)	296 (100%)	0	100	100
16	5P	296/323 (92%)	295 (100%)	1 (0%)	86	94
17	1Q	117/152 (77%)	117 (100%)	0	100	100
17	5Q	117/152 (77%)	116 (99%)	1 (1%)	70	87
18	1R	79/97 (81%)	79 (100%)	0	100	100
18	5R	79/97 (81%)	79 (100%)	0	100	100
19	1S	77/82 (94%)	77 (100%)	0	100	100
19	5S	77/82 (94%)	76 (99%)	1 (1%)	61	83
20	1T	79/133 (59%)	79 (100%)	0	100	100
20	1U	79/133 (59%)	77 (98%)	2 (2%)	42	71
20	5T	79/133 (59%)	79 (100%)	0	100	100
20	5U	79/133 (59%)	79 (100%)	0	100	100
21	1V	100/101 (99%)	99 (99%)	1 (1%)	68	86
21	5V	100/101 (99%)	100 (100%)	0	100	100
22	1W	107/112 (96%)	107 (100%)	0	100	100
22	5W	107/112 (96%)	107 (100%)	0	100	100
23	1X	153/154 (99%)	152 (99%)	1 (1%)	76	90
23	5X	153/154 (99%)	153 (100%)	0	100	100
24	1Y	101/102 (99%)	100 (99%)	1 (1%)	68	86
24	5Y	101/102 (99%)	101 (100%)	0	100	100
25	1Z	123/124 (99%)	122 (99%)	1 (1%)	73	88
25	5Z	123/124 (99%)	123 (100%)	0	100	100
26	1a	58/58 (100%)	58 (100%)	0	100	100
26	5a	58/58 (100%)	57 (98%)	1 (2%)	53	79
27	1b	69/70 (99%)	66 (96%)	3 (4%)	26	54
27	5b	69/70 (99%)	69 (100%)	0	100	100
28	1c	45/66 (68%)	45 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	5c	45/66 (68%)	45 (100%)	0	100	100
29	1d	106/109 (97%)	105 (99%)	1 (1%)	70	87
29	5d	106/109 (97%)	106 (100%)	0	100	100
30	1e	87/94 (93%)	87 (100%)	0	100	100
30	5e	87/94 (93%)	87 (100%)	0	100	100
31	1f	54/113 (48%)	54 (100%)	0	100	100
31	5f	54/113 (48%)	54 (100%)	0	100	100
32	1g	92/129 (71%)	92 (100%)	0	100	100
32	5g	92/129 (71%)	92 (100%)	0	100	100
33	1h	121/158 (77%)	121 (100%)	0	100	100
33	5h	121/158 (77%)	121 (100%)	0	100	100
34	1i	119/120 (99%)	119 (100%)	0	100	100
34	5i	119/120 (99%)	119 (100%)	0	100	100
35	1j	62/84 (74%)	62 (100%)	0	100	100
35	5j	62/84 (74%)	61 (98%)	1 (2%)	55	80
36	1k	63/76 (83%)	63 (100%)	0	100	100
36	5k	63/76 (83%)	63 (100%)	0	100	100
37	1l	141/161 (88%)	141 (100%)	0	100	100
37	5l	141/161 (88%)	141 (100%)	0	100	100
38	1m	113/114 (99%)	113 (100%)	0	100	100
38	5m	113/114 (99%)	113 (100%)	0	100	100
39	1n	156/160 (98%)	156 (100%)	0	100	100
39	5n	156/160 (98%)	155 (99%)	1 (1%)	78	91
40	1o	110/119 (92%)	110 (100%)	0	100	100
40	5o	110/119 (92%)	110 (100%)	0	100	100
41	1p	154/156 (99%)	154 (100%)	0	100	100
41	5p	154/156 (99%)	154 (100%)	0	100	100
42	1q	131/131 (100%)	131 (100%)	0	100	100
42	5q	131/131 (100%)	131 (100%)	0	100	100
43	1r	85/98 (87%)	85 (100%)	0	100	100
43	5r	85/98 (87%)	85 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	1s	44/351 (12%)	42 (96%)	2 (4%)	24	52
44	5s	44/351 (12%)	44 (100%)	0	100	100
45	3A	367/397 (92%)	367 (100%)	0	100	100
45	3N	372/397 (94%)	370 (100%)	2 (0%)	81	92
46	3B	328/355 (92%)	328 (100%)	0	100	100
46	3O	327/355 (92%)	327 (100%)	0	100	100
47	3C	332/332 (100%)	332 (100%)	0	100	100
47	3P	332/332 (100%)	332 (100%)	0	100	100
48	3D	202/259 (78%)	201 (100%)	1 (0%)	81	92
48	3Q	204/259 (79%)	203 (100%)	1 (0%)	81	92
49	3E	166/226 (74%)	166 (100%)	0	100	100
49	3I	37/226 (16%)	37 (100%)	0	100	100
49	3R	166/226 (74%)	165 (99%)	1 (1%)	78	91
49	3V	24/226 (11%)	18 (75%)	6 (25%)	0	2
50	3F	90/99 (91%)	90 (100%)	0	100	100
50	3S	90/99 (91%)	90 (100%)	0	100	100
51	3G	67/73 (92%)	67 (100%)	0	100	100
51	3T	67/73 (92%)	66 (98%)	1 (2%)	57	81
52	3H	62/85 (73%)	62 (100%)	0	100	100
52	3U	62/85 (73%)	61 (98%)	1 (2%)	55	80
53	3J	45/51 (88%)	45 (100%)	0	100	100
53	3W	45/51 (88%)	41 (91%)	4 (9%)	9	23
54	3X	42/46 (91%)	42 (100%)	0	100	100
54	3Y	41/46 (89%)	41 (100%)	0	100	100
55	4A	424/424 (100%)	420 (99%)	4 (1%)	70	87
55	8A	424/424 (100%)	423 (100%)	1 (0%)	87	95
56	4B	210/211 (100%)	208 (99%)	2 (1%)	68	86
56	8B	210/211 (100%)	209 (100%)	1 (0%)	81	92
57	4C	223/225 (99%)	222 (100%)	1 (0%)	84	93
57	8C	223/225 (99%)	223 (100%)	0	100	100
58	4D	124/149 (83%)	123 (99%)	1 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	8D	124/149 (83%)	124 (100%)	0	100	100
59	4E	92/124 (74%)	92 (100%)	0	100	100
59	8E	92/124 (74%)	92 (100%)	0	100	100
60	4F	80/100 (80%)	80 (100%)	0	100	100
60	8F	80/100 (80%)	79 (99%)	1 (1%)	61	83
61	4G	65/80 (81%)	65 (100%)	0	100	100
61	8G	65/80 (81%)	64 (98%)	1 (2%)	57	81
62	4H	73/76 (96%)	73 (100%)	0	100	100
62	8H	73/76 (96%)	72 (99%)	1 (1%)	59	82
63	4I	54/61 (88%)	54 (100%)	0	100	100
63	8I	54/61 (88%)	54 (100%)	0	100	100
64	4J	49/68 (72%)	48 (98%)	1 (2%)	48	76
64	8J	49/68 (72%)	48 (98%)	1 (2%)	48	76
65	4K	38/66 (58%)	38 (100%)	0	100	100
65	8K	38/66 (58%)	37 (97%)	1 (3%)	40	70
66	4L	39/55 (71%)	39 (100%)	0	100	100
66	8L	39/55 (71%)	39 (100%)	0	100	100
67	4M	37/57 (65%)	37 (100%)	0	100	100
67	8M	37/57 (65%)	37 (100%)	0	100	100
68	4N	70/70 (100%)	70 (100%)	0	100	100
68	8N	70/70 (100%)	70 (100%)	0	100	100
All	All	21060/24374 (86%)	20991 (100%)	69 (0%)	84	94

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	4	MET
7	1G	254	MET
8	1H	68	ILE
8	1H	156	MET
12	1L	267	MET
12	1L	482	MET
13	1M	47	GLU
14	1N	22	ILE
20	1U	21	LEU

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Mol	Chain	Res	Type
20	1U	24	LYS
21	1V	57	MET
23	1X	144	ARG
24	1Y	9	SER
25	1Z	28	ARG
27	1b	4	ILE
27	1b	19	VAL
27	1b	67	SER
29	1d	34	MET
44	1s	35	ASN
44	1s	61	PHE
48	3D	280	ARG
45	3N	112	LEU
45	3N	117	VAL
48	3Q	43	MET
49	3R	222	CYS
51	3T	6	HIS
52	3U	68	CYS
49	3V	47	ARG
49	3V	49	VAL
49	3V	50	LEU
49	3V	51	CYS
49	3V	52	ARG
49	3V	55	LEU
53	3W	53	LYS
53	3W	56	ASN
53	3W	57	GLN
53	3W	59	LYS
55	4A	136	LEU
55	4A	138	HIS
55	4A	197	LEU
55	4A	300	ASP
56	4B	92	ASN
56	4B	217	LYS
57	4C	138	LEU
58	4D	138	TRP
64	4J	40	LEU
4	5D	252	ASN
6	5F	218	CYS
7	5G	341	ASP
8	5H	69	SER
10	5J	66	VAL

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Mol	Chain	Res	Type
10	5J	76	THR
13	5M	269	MET
13	5M	340	ARG
14	5N	109	SER
15	5O	213	GLU
16	5P	167	LYS
17	5Q	44	ASN
19	5S	90	LEU
26	5a	1	MET
35	5j	59	TRP
39	5n	145	PRO
55	8A	48	LEU
56	8B	195	GLN
60	8F	54	ASN
61	8G	53	LEU
62	8H	18	SER
64	8J	17	ASP
65	8K	8	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (215) such sidechains are listed below:

Mol	Chain	Res	Type
2	1B	162	GLN
2	1B	164	GLN
3	1C	19	HIS
3	1C	41	GLN
3	1C	46	ASN
3	1C	144	ASN
5	1E	16	ASN
5	1E	58	ASN
6	1F	96	ASN
6	1F	356	HIS
7	1G	51	ASN
7	1G	101	HIS
7	1G	237	ASN
7	1G	255	HIS
7	1G	277	GLN
7	1G	402	ASN
7	1G	629	ASN
8	1H	235	ASN
8	1H	284	GLN
12	1L	23	ASN

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Mol	Chain	Res	Type
12	1L	30	ASN
12	1L	194	ASN
12	1L	323	HIS
12	1L	506	ASN
12	1L	546	GLN
12	1L	603	ASN
13	1M	144	ASN
13	1M	184	HIS
13	1M	220	HIS
13	1M	304	GLN
13	1M	331	ASN
14	1N	204	ASN
15	1O	57	HIS
15	1O	114	HIS
15	1O	251	GLN
15	1O	309	ASN
16	1P	67	GLN
16	1P	87	HIS
16	1P	296	HIS
17	1Q	43	ASN
17	1Q	67	ASN
17	1Q	99	ASN
18	1R	93	GLN
19	1S	24	GLN
20	1T	33	ASN
21	1V	36	GLN
21	1V	75	GLN
21	1V	110	GLN
22	1W	58	GLN
22	1W	70	ASN
25	1Z	112	HIS
26	1a	68	ASN
28	1c	34	GLN
29	1d	46	ASN
29	1d	61	GLN
29	1d	97	HIS
32	1g	86	GLN
33	1h	143	ASN
34	1i	25	GLN
34	1i	47	ASN
35	1j	24	GLN
35	1j	42	HIS

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Mol	Chain	Res	Type
37	1l	66	HIS
37	1l	126	GLN
38	1m	32	GLN
38	1m	78	ASN
39	1n	61	GLN
39	1n	123	GLN
41	1p	106	GLN
41	1p	148	HIS
43	1r	12	ASN
43	1r	24	GLN
43	1r	28	GLN
43	1r	35	GLN
43	1r	109	GLN
44	1s	43	HIS
44	1s	65	GLN
45	3A	6	GLN
45	3A	118	GLN
45	3A	159	GLN
45	3A	252	HIS
46	3B	143	GLN
46	3B	156	GLN
46	3B	254	HIS
46	3B	429	ASN
47	3C	322	GLN
47	3C	345	HIS
48	3D	270	GLN
49	3E	186	GLN
49	3E	257	ASN
50	3F	34	ASN
52	3H	67	GLN
49	3I	58	GLN
45	3N	9	GLN
45	3N	87	ASN
45	3N	139	GLN
45	3N	159	GLN
46	3O	143	GLN
46	3O	254	HIS
46	3O	432	HIS
47	3P	68	HIS
47	3P	85	ASN
47	3P	341	GLN
47	3P	375	ASN

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Mol	Chain	Res	Type
48	3Q	71	GLN
49	3R	199	GLN
49	3R	239	HIS
49	3R	257	ASN
49	3V	58	GLN
53	3W	48	GLN
53	3W	57	GLN
54	3Y	16	ASN
55	4A	178	GLN
55	4A	451	ASN
55	4A	491	ASN
56	4B	24	HIS
56	4B	26	HIS
57	4C	76	GLN
57	4C	133	ASN
58	4D	29	HIS
61	4G	51	HIS
62	4H	37	HIS
63	4I	20	HIS
65	4K	35	GLN
65	4K	41	ASN
2	5B	82	GLN
3	5C	39	GLN
4	5D	34	ASN
4	5D	135	GLN
4	5D	232	ASN
5	5E	57	GLN
6	5F	148	ASN
6	5F	150	GLN
6	5F	224	ASN
6	5F	264	HIS
7	5G	101	HIS
8	5H	235	ASN
12	5L	2	ASN
12	5L	23	ASN
12	5L	194	ASN
12	5L	206	ASN
12	5L	309	GLN
12	5L	348	HIS
12	5L	400	ASN
12	5L	452	ASN
12	5L	506	ASN

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Mol	Chain	Res	Type
12	5L	540	HIS
12	5L	546	GLN
13	5M	44	GLN
13	5M	144	ASN
13	5M	175	ASN
13	5M	220	HIS
13	5M	331	ASN
14	5N	63	GLN
14	5N	77	ASN
14	5N	174	GLN
14	5N	197	ASN
14	5N	309	ASN
15	5O	120	GLN
15	5O	251	GLN
15	5O	309	ASN
16	5P	67	GLN
16	5P	74	ASN
16	5P	131	HIS
16	5P	321	HIS
16	5P	341	ASN
17	5Q	67	ASN
17	5Q	99	ASN
19	5S	72	GLN
20	5U	33	ASN
20	5U	74	GLN
21	5V	110	GLN
22	5W	70	ASN
23	5X	64	GLN
23	5X	94	GLN
25	5Z	8	GLN
25	5Z	61	GLN
27	5b	73	GLN
29	5d	16	ASN
29	5d	46	ASN
29	5d	61	GLN
34	5i	13	GLN
37	5l	136	ASN
38	5m	32	GLN
39	5n	11	HIS
39	5n	61	GLN
40	5o	49	GLN
40	5o	75	ASN

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Mol	Chain	Res	Type
41	5p	58	ASN
41	5p	90	GLN
41	5p	106	GLN
42	5q	87	HIS
42	5q	112	ASN
43	5r	12	ASN
43	5r	35	GLN
43	5r	72	GLN
44	5s	43	HIS
44	5s	44	HIS
55	8A	11	ASN
55	8A	291	HIS
55	8A	428	GLN
56	8B	52	HIS
56	8B	161	HIS
57	8C	76	GLN
57	8C	125	ASN
58	8D	65	ASN
60	8F	32	ASN
61	8G	38	HIS
62	8H	12	GLN
62	8H	31	GLN
62	8H	37	HIS
63	8I	20	HIS
65	8K	41	ASN
66	8L	42	HIS
66	8L	43	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

18 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	$\# Z > 2$
13	FME	1M	1	13	8,9,10	0.54	0	8,9,11	0.99	1 (12%)
34	SAC	1i	1	34	7,8,9	0.58	0	7,9,11	0.93	1 (14%)
8	FME	5H	1	8	8,9,10	0.55	0	8,9,11	1.05	1 (12%)
34	SAC	5i	1	34	7,8,9	0.57	0	7,9,11	0.91	1 (14%)
56	FME	4B	1	56	8,9,10	0.57	0	8,9,11	0.96	1 (12%)
56	FME	8B	1	56	8,9,10	0.56	0	8,9,11	1.04	1 (12%)
13	FME	5M	1	13	8,9,10	0.55	0	8,9,11	1.00	1 (12%)
55	FME	4A	1	55	8,9,10	0.56	0	8,9,11	0.96	1 (12%)
11	FME	5K	1	11	8,9,10	0.55	0	8,9,11	1.00	1 (12%)
55	FME	8A	1	55	8,9,10	0.55	0	8,9,11	0.99	1 (12%)
1	FME	1A	1	1	8,9,10	0.53	0	8,9,11	1.07	1 (12%)
8	FME	1H	1	8	8,9,10	0.55	0	8,9,11	1.04	1 (12%)
1	FME	5A	1	1	8,9,10	0.53	0	8,9,11	1.06	1 (12%)
11	FME	1K	1	11	8,9,10	0.54	0	8,9,11	0.97	1 (12%)
12	FME	5L	1	12	8,9,10	0.55	0	8,9,11	0.88	1 (12%)
12	FME	1L	1	12	8,9,10	0.56	0	8,9,11	0.86	1 (12%)
14	FME	5N	1	14	8,9,10	0.56	0	8,9,11	1.00	1 (12%)
14	FME	1N	1	14	8,9,10	0.54	0	8,9,11	0.98	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
13	FME	1M	1	13	-	0/7/9/11	-
34	SAC	1i	1	34	-	0/7/8/10	-
8	FME	5H	1	8	-	1/7/9/11	-
34	SAC	5i	1	34	-	0/7/8/10	-
56	FME	4B	1	56	-	3/7/9/11	-
56	FME	8B	1	56	-	2/7/9/11	-
13	FME	5M	1	13	-	0/7/9/11	-
55	FME	4A	1	55	-	2/7/9/11	-
11	FME	5K	1	11	-	3/7/9/11	-
55	FME	8A	1	55	-	1/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	1A	1	1	-	0/7/9/11	-
8	FME	1H	1	8	-	1/7/9/11	-
1	FME	5A	1	1	-	1/7/9/11	-
11	FME	1K	1	11	-	0/7/9/11	-
12	FME	5L	1	12	-	0/7/9/11	-
12	FME	1L	1	12	-	0/7/9/11	-
14	FME	5N	1	14	-	1/7/9/11	-
14	FME	1N	1	14	-	1/7/9/11	-

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	5H	1	FME	O-C-CA	-2.69	117.86	124.77
8	1H	1	FME	O-C-CA	-2.67	117.90	124.77
11	1K	1	FME	O-C-CA	-2.67	117.92	124.77
1	1A	1	FME	O-C-CA	-2.62	118.02	124.77
11	5K	1	FME	O-C-CA	-2.61	118.05	124.77
13	5M	1	FME	O-C-CA	-2.57	118.16	124.77
56	8B	1	FME	O-C-CA	-2.56	118.19	124.77
13	1M	1	FME	O-C-CA	-2.56	118.19	124.77
56	4B	1	FME	O-C-CA	-2.52	118.30	124.77
14	1N	1	FME	O-C-CA	-2.51	118.31	124.77
1	5A	1	FME	O-C-CA	-2.51	118.31	124.77
14	5N	1	FME	O-C-CA	-2.51	118.32	124.77
55	8A	1	FME	O-C-CA	-2.46	118.44	124.77
55	4A	1	FME	O-C-CA	-2.44	118.49	124.77
34	1i	1	SAC	O-C-CA	-2.38	118.65	124.77
12	5L	1	FME	O-C-CA	-2.38	118.65	124.77
34	5i	1	SAC	O-C-CA	-2.35	118.73	124.77
12	1L	1	FME	O-C-CA	-2.27	118.93	124.77

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	1H	1	FME	O1-CN-N-CA
14	1N	1	FME	O1-CN-N-CA
56	4B	1	FME	O1-CN-N-CA
56	4B	1	FME	CB-CA-N-CN
56	4B	1	FME	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
8	5H	1	FME	O1-CN-N-CA
14	5N	1	FME	O1-CN-N-CA
56	8B	1	FME	O1-CN-N-CA
56	8B	1	FME	O-C-CA-CB
55	4A	1	FME	CA-CB-CG-SD
55	8A	1	FME	CA-CB-CG-SD
1	5A	1	FME	CB-CG-SD-CE
11	5K	1	FME	CB-CG-SD-CE
11	5K	1	FME	N-CA-CB-CG
11	5K	1	FME	C-CA-CB-CG
55	4A	1	FME	N-CA-CB-CG

There are no ring outliers.

10 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	4B	1	FME	2	0
56	8B	1	FME	2	0
13	5M	1	FME	1	0
55	4A	1	FME	2	0
11	5K	1	FME	2	0
1	1A	1	FME	1	0
1	5A	1	FME	2	0
11	1K	1	FME	2	0
14	5N	1	FME	1	0
14	1N	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 202 ligands modelled in this entry, 14 are monoatomic - leaving 188 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	$\# Z > 2$
86	PGV	4C	302	-	50,50,50	0.29	0	53,56,56	0.69	1 (1%)
74	CDL	1d	203	-	64,64,99	0.32	0	70,76,111	0.42	0
86	PGV	8A	602	-	50,50,50	0.29	0	53,56,56	0.36	0
69	PC1	1I	204	-	43,43,53	0.29	0	49,51,61	0.33	0
86	PGV	4M	101	-	50,50,50	0.29	0	53,56,56	0.33	0
74	CDL	8D	201	-	99,99,99	0.27	0	105,111,111	0.41	0
71	FES	5G	803	7	0,4,4	-	-	-		
86	PGV	8B	302	-	50,50,50	0.28	0	53,56,56	0.36	0
69	PC1	5B	202	-	45,45,53	0.29	0	51,53,61	0.36	0
91	CUA	4B	303	56	0,1,1	-	-	-		
74	CDL	1h	202	-	79,79,99	0.31	0	85,91,111	0.40	0
86	PGV	4L	101	-	50,50,50	0.29	0	53,56,56	0.38	0
76	3PE	5M	504	-	50,50,50	0.29	0	53,55,55	0.46	0
74	CDL	3C	503	-	51,51,99	0.35	0	57,63,111	0.54	1 (1%)
86	PGV	8J	101	-	50,50,50	0.28	0	53,56,56	0.40	0
74	CDL	1L	702	-	75,75,99	0.30	0	81,87,111	0.38	0
92	PEK	8C	308	-	51,51,52	0.26	0	54,56,57	0.44	0
86	PGV	4C	307	-	50,50,50	0.29	0	53,56,56	0.37	0
70	SF4	1G	801	7	0,12,12	-	-	-		
76	3PE	1d	201	-	48,48,50	0.27	0	51,53,55	0.33	0
76	3PE	3N	501	-	31,31,50	0.33	0	34,36,55	0.46	0
86	PGV	8C	307	-	50,50,50	0.28	0	53,56,56	0.38	0
69	PC1	5P	401	-	32,32,53	0.33	0	38,40,61	0.37	0
85	HEC	3D	501	48	44,49,50	2.63	23 (52%)	56,80,82	2.09	18 (32%)
70	SF4	5I	203	9	0,12,12	-	-	-		
70	SF4	1I	203	9	0,12,12	-	-	-		
76	3PE	3C	505	-	33,33,50	0.34	0	36,38,55	0.40	0
76	3PE	1K	101	-	43,43,50	0.30	0	46,48,55	0.35	0
81	EHZ	1T	101	20	31,36,37	0.19	0	36,44,47	1.07	1 (2%)
76	3PE	1M	906	-	49,49,50	0.28	0	52,54,55	0.33	0
76	3PE	5M	501	-	44,44,50	0.30	0	47,49,55	0.36	0
76	3PE	5Y	802	-	39,39,50	0.31	0	42,44,55	0.46	0
76	3PE	1O	401	-	50,50,50	0.28	0	53,55,55	0.46	0
76	3PE	1Y	802	-	39,39,50	0.32	0	42,44,55	0.44	0
76	3PE	3A	503	-	31,31,50	0.34	0	34,36,55	0.38	0
76	3PE	3P	503	-	32,32,50	0.34	0	35,37,55	0.37	0
76	3PE	5Y	801	-	30,30,50	0.33	0	33,35,55	0.50	0
74	CDL	5X	201	-	85,85,99	0.29	0	91,97,111	0.38	0
70	SF4	1I	202	9	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
69	PC1	5A	203	-	34,34,53	0.33	0	40,42,61	0.39	0
76	3PE	1Y	801	-	30,30,50	0.33	0	33,35,55	0.51	0
76	3PE	3Q	502	-	46,46,50	0.28	0	49,51,55	0.38	0
74	CDL	8B	303	-	99,99,99	0.26	0	105,111,111	0.31	0
86	PGV	4K	101	-	50,50,50	0.28	0	53,56,56	0.31	0
90	PSC	4A	609	-	51,51,51	0.29	0	57,59,59	0.46	1 (1%)
74	CDL	5L	702	-	75,75,99	0.29	0	81,87,111	0.38	0
86	PGV	8B	301	-	50,50,50	0.27	0	53,56,56	0.33	0
76	3PE	5L	704	-	48,48,50	0.28	0	51,53,55	0.36	0
86	PGV	8A	601	-	50,50,50	0.28	0	53,56,56	0.41	0
69	PC1	1H	402	-	47,47,53	0.29	0	53,55,61	0.34	0
69	PC1	1B	203	-	47,47,53	0.29	0	53,55,61	0.44	0
76	3PE	1P	502	-	34,34,50	0.32	0	37,39,55	0.37	0
93	PO4	8H	101	-	4,4,4	0.96	0	6,6,6	0.48	0
74	CDL	5h	202	-	79,79,99	0.31	0	85,91,111	0.41	0
69	PC1	5I	204	-	43,43,53	0.29	0	49,51,61	0.32	0
76	3PE	1Y	804	-	32,32,50	0.33	0	35,37,55	0.49	0
76	3PE	1M	902	-	44,44,50	0.30	0	47,49,55	0.35	0
86	PGV	8C	302	-	50,50,50	0.29	0	53,56,56	0.70	1 (1%)
74	CDL	3G	102	-	55,55,99	0.34	0	61,67,111	0.48	0
82	AME	5h	201	-	9,10,11	0.52	0	9,11,13	1.01	1 (11%)
74	CDL	3A	501	-	57,57,99	0.34	0	63,69,111	0.42	0
76	3PE	3D	502	-	32,32,50	0.33	0	35,37,55	0.50	0
79	NDP	1P	501	-	51,52,52	0.52	0	71,80,80	0.80	2 (2%)
72	FMN	1F	501	-	33,33,33	0.61	0	48,50,50	0.67	1 (2%)
83	MYR	1o	201	-	13,14,15	0.32	0	12,13,15	0.30	0
81	EHZ	5T	101	20	31,36,37	0.20	0	36,44,47	1.06	1 (2%)
76	3PE	1Y	806	-	40,40,50	0.29	0	43,45,55	0.41	0
70	SF4	5B	201	2	0,12,12	-	-	-	-	-
87	HEA	8A	603	55	67,67,67	2.42	24 (35%)	81,103,103	2.58	37 (45%)
70	SF4	5G	802	7	0,12,12	-	-	-	-	-
84	HEM	3P	501	47	50,50,50	1.57	8 (16%)	67,82,82	1.63	11 (16%)
76	3PE	3Y	101	-	29,29,50	0.34	0	32,34,55	0.41	0
76	3PE	1M	901	-	48,48,50	0.28	0	51,53,55	0.35	0
69	PC1	1A	202	-	34,34,53	0.33	0	40,42,61	0.39	0
76	3PE	5M	502	-	47,47,50	0.28	0	50,52,55	0.34	0
76	3PE	1j	101	-	43,43,50	0.29	0	46,48,55	0.45	0
76	3PE	3G	101	-	28,28,50	0.33	0	31,33,55	0.38	0
76	3PE	5Y	804	-	32,32,50	0.33	0	35,37,55	0.49	0
85	HEC	3Q	501	48	46,50,50	2.59	25 (54%)	58,82,82	2.01	18 (31%)
70	SF4	1B	201	2	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
83	MYR	5o	201	-	13,14,15	0.32	0	12,13,15	0.29	0
86	PGV	8C	304	-	50,50,50	0.27	0	53,56,56	0.38	0
86	PGV	8C	301	-	50,50,50	0.28	0	53,56,56	0.32	0
92	PEK	8G	102	-	52,52,52	0.26	0	55,57,57	0.40	0
74	CDL	5d	203	-	64,64,99	0.32	0	70,76,111	0.42	0
69	PC1	3J	101	-	46,46,53	0.29	0	52,54,61	0.33	0
86	PGV	8M	101	-	50,50,50	0.29	0	53,56,56	0.30	0
69	PC1	5h	203	-	46,46,53	0.28	0	52,54,61	0.30	0
87	HEA	4A	605	55	67,67,67	2.44	24 (35%)	81,103,103	2.51	35 (43%)
74	CDL	3P	504	-	55,55,99	0.36	0	61,67,111	0.52	0
87	HEA	4A	604	55	67,67,67	2.44	25 (37%)	81,103,103	2.57	36 (44%)
69	PC1	5A	202	-	34,34,53	0.33	0	40,42,61	0.41	0
69	PC1	3X	101	-	28,28,53	0.36	0	34,36,61	0.51	0
81	EHZ	5n	201	-	31,36,37	0.18	0	36,44,47	1.09	1 (2%)
86	PGV	8K	101	-	50,50,50	0.29	0	53,56,56	0.32	0
71	FES	1E	301	5	0,4,4	-	-	-	-	-
82	AME	1h	201	-	9,10,11	0.51	0	9,11,13	1.00	1 (11%)
76	3PE	5M	506	-	49,49,50	0.27	0	52,54,55	0.33	0
76	3PE	3C	504	-	34,34,50	0.33	0	37,39,55	0.47	0
76	3PE	5d	201	-	48,48,50	0.27	0	51,53,55	0.33	0
86	PGV	4G	101	-	50,50,50	0.29	0	53,56,56	0.43	0
76	3PE	1L	701	-	45,45,50	0.28	0	48,50,55	0.31	0
84	HEM	3C	502	-	50,50,50	1.57	8 (16%)	67,82,82	1.57	11 (16%)
69	PC1	5L	705	-	45,45,53	0.30	0	51,53,61	0.37	0
92	PEK	4C	308	-	51,51,52	0.26	0	54,56,57	0.44	0
76	3PE	5K	101	-	43,43,50	0.30	0	46,48,55	0.35	0
69	PC1	3R	302	-	44,44,53	0.29	0	50,52,61	0.36	0
74	CDL	1q	202	-	60,60,99	0.34	0	66,72,111	0.43	0
69	PC1	1M	905	-	43,43,53	0.30	0	49,51,61	0.37	0
76	3PE	1Y	805	-	26,26,50	0.34	0	29,31,55	0.55	0
71	FES	5E	301	5	0,4,4	-	-	-	-	-
76	3PE	3A	502	-	26,26,50	0.36	0	29,31,55	0.66	1 (3%)
74	CDL	4B	302	-	99,99,99	0.27	0	105,111,111	0.30	0
86	PGV	4C	301	-	50,50,50	0.28	0	53,56,56	0.31	0
75	AYA	1I	205	-	6,7,8	0.65	0	6,8,10	0.94	1 (16%)
71	FES	3E	301	49	0,4,4	-	-	-	-	-
69	PC1	5M	503	-	34,34,53	0.32	0	40,42,61	0.47	0
74	CDL	1H	401	-	50,50,99	0.36	0	56,62,111	0.61	1 (1%)
69	PC1	1B	202	-	45,45,53	0.28	0	51,53,61	0.37	0
76	3PE	5L	701	-	45,45,50	0.29	0	48,50,55	0.32	0
77	GTP	1O	402	78	33,34,34	0.57	0	50,54,54	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	EHZ	1n	201	-	31,36,37	0.18	0	36,44,47	1.05	1 (2%)
86	PGV	8L	101	-	50,50,50	0.29	0	53,56,56	0.37	0
69	PC1	5I	201	-	53,53,53	0.27	0	59,61,61	0.34	0
76	3PE	5Y	806	-	40,40,50	0.29	0	43,45,55	0.40	0
76	3PE	5Y	803	-	29,29,50	0.34	0	32,34,55	0.77	1 (3%)
90	PSC	8I	101	-	51,51,51	0.30	0	57,59,59	0.48	1 (1%)
69	PC1	5M	505	-	43,43,53	0.30	0	49,51,61	0.38	0
69	PC1	1M	904	-	34,34,53	0.33	0	40,42,61	0.47	0
79	NDP	5P	402	-	51,52,52	0.52	0	71,80,80	0.78	2 (2%)
69	PC1	1q	201	-	48,48,53	0.28	0	54,56,61	0.33	0
74	CDL	4D	201	-	99,99,99	0.27	0	105,111,111	0.42	0
76	3PE	1L	703	-	44,44,50	0.29	0	47,49,55	0.34	0
69	PC1	1A	201	-	34,34,53	0.32	0	40,42,61	0.39	0
76	3PE	5L	703	-	44,44,50	0.29	0	47,49,55	0.33	0
76	3PE	5A	201	-	46,46,50	0.28	0	49,51,55	0.36	0
74	CDL	1N	401	-	61,61,99	0.31	0	67,73,111	0.63	1 (1%)
86	PGV	8C	305	-	50,50,50	0.29	0	53,56,56	0.46	1 (1%)
84	HEM	3C	501	47	50,50,50	1.57	8 (16%)	67,82,82	1.63	11 (16%)
75	AYA	5q	202	-	6,7,8	0.65	0	6,8,10	0.93	1 (16%)
76	3PE	3N	503	-	24,24,50	0.37	0	27,29,55	0.62	0
86	PGV	8C	303	-	50,50,50	0.29	0	53,56,56	0.32	0
74	CDL	3T	101	-	56,56,99	0.34	0	62,68,111	0.44	0
77	GTP	5O	401	78	33,34,34	0.56	0	50,54,54	0.58	0
76	3PE	1b	201	-	46,46,50	0.28	0	49,51,55	0.36	0
86	PGV	4A	601	-	50,50,50	0.28	0	53,56,56	0.42	0
86	PGV	4C	304	-	50,50,50	0.28	0	53,56,56	0.39	0
76	3PE	1M	903	-	47,47,50	0.28	0	50,52,55	0.35	0
76	3PE	5P	403	-	34,34,50	0.32	0	37,39,55	0.38	0
70	SF4	1G	802	7	0,12,12	-	-	-	-	-
74	CDL	1X	201	-	85,85,99	0.29	0	91,97,111	0.40	0
69	PC1	1I	201	-	53,53,53	0.27	0	59,61,61	0.34	0
74	CDL	5N	401	-	61,61,99	0.31	0	67,73,111	0.62	1 (1%)
92	PEK	4G	102	-	52,52,52	0.27	0	55,57,57	0.41	0
70	SF4	5I	202	9	0,12,12	-	-	-	-	-
91	CUA	8B	304	56	0,1,1	-	-	-	-	-
76	3PE	5Y	805	-	26,26,50	0.34	0	29,31,55	0.55	0
74	CDL	5H	401	-	50,50,99	0.36	0	56,62,111	0.61	1 (1%)
74	CDL	3N	502	-	42,42,99	0.38	0	48,54,111	0.52	0
93	PO4	4H	101	-	4,4,4	0.96	0	6,6,6	0.47	0
86	PGV	4A	603	-	50,50,50	0.27	0	53,56,56	0.32	0
69	PC1	5q	201	-	48,48,53	0.28	0	54,56,61	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	PGV	4B	301	-	50,50,50	0.28	0	53,56,56	0.33	0
86	PGV	8G	101	-	50,50,50	0.28	0	53,56,56	0.47	1 (1%)
86	PGV	4C	305	-	50,50,50	0.29	0	53,56,56	0.49	1 (1%)
87	HEA	8A	604	55	67,67,67	2.43	25 (37%)	81,103,103	2.54	34 (41%)
69	PC1	5d	202	-	38,38,53	0.30	0	44,46,61	0.49	1 (2%)
72	FMN	5F	501	-	33,33,33	0.61	0	48,50,50	0.67	1 (2%)
69	PC1	1d	202	-	38,38,53	0.30	0	44,46,61	0.48	0
76	3PE	5j	101	-	43,43,50	0.29	0	46,48,55	0.46	0
69	PC1	1h	203	-	46,46,53	0.28	0	52,54,61	0.30	0
74	CDL	4C	306	-	99,99,99	0.27	0	105,111,111	0.41	1 (0%)
70	SF4	5G	801	7	0,12,12	-	-	-		
70	SF4	1F	502	6	0,12,12	-	-	-		
74	CDL	8C	306	-	99,99,99	0.27	0	105,111,111	0.40	0
71	FES	1G	803	7	0,4,4	-	-	-		
86	PGV	4A	602	-	50,50,50	0.29	0	53,56,56	0.35	0
86	PGV	4J	101	-	50,50,50	0.28	0	53,56,56	0.39	0
76	3PE	1Y	803	-	29,29,50	0.34	0	32,34,55	0.80	1 (3%)
69	PC1	1L	704	-	45,45,53	0.30	0	51,53,61	0.37	0
69	PC1	1A	203	-	32,32,53	0.34	0	38,40,61	0.35	0
69	PC1	5B	203	-	47,47,53	0.30	0	53,55,61	0.44	0
70	SF4	5F	502	6	0,12,12	-	-	-		
69	PC1	5H	402	-	47,47,53	0.28	0	53,55,61	0.34	0
71	FES	3R	301	49	0,4,4	-	-	-		
86	PGV	4C	303	-	50,50,50	0.29	0	53,56,56	0.31	0
74	CDL	5q	203	-	60,60,99	0.34	0	66,72,111	0.42	0
84	HEM	3P	502	47	50,50,50	1.57	9 (18%)	67,82,82	1.59	12 (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
86	PGV	4C	302	-	-	12/55/55/55	-
74	CDL	1d	203	-	-	13/75/75/110	-
86	PGV	8A	602	-	-	3/55/55/55	-
69	PC1	1I	204	-	-	3/47/47/57	-
86	PGV	4M	101	-	-	4/55/55/55	-
74	CDL	8D	201	-	-	14/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
71	FES	5G	803	7	-	-	0/1/1/1
86	PGV	8B	302	-	-	5/55/55/55	-
69	PC1	5B	202	-	-	3/49/49/57	-
74	CDL	1h	202	-	-	18/90/90/110	-
86	PGV	4L	101	-	-	5/55/55/55	-
76	3PE	5M	504	-	-	9/54/54/54	-
74	CDL	3C	503	-	-	9/62/62/110	-
86	PGV	8J	101	-	-	6/55/55/55	-
74	CDL	1L	702	-	-	15/86/86/110	-
92	PEK	8C	308	-	-	4/55/55/56	-
86	PGV	4C	307	-	-	3/55/55/55	-
76	3PE	1d	201	-	-	2/52/52/54	-
70	SF4	1G	801	7	-	-	0/6/5/5
76	3PE	3N	501	-	-	9/35/35/54	-
86	PGV	8C	307	-	-	2/55/55/55	-
69	PC1	5P	401	-	-	3/36/36/57	-
85	HEC	3D	501	48	-	3/13/53/54	-
70	SF4	5I	203	9	-	-	0/6/5/5
70	SF4	1I	203	9	-	-	0/6/5/5
76	3PE	3C	505	-	-	5/37/37/54	-
76	3PE	1K	101	-	-	8/47/47/54	-
81	EHZ	1T	101	20	-	7/42/44/45	-
76	3PE	1M	906	-	-	7/53/53/54	-
76	3PE	5M	501	-	-	9/48/48/54	-
76	3PE	5Y	802	-	-	13/43/43/54	-
76	3PE	1O	401	-	-	8/54/54/54	-
76	3PE	1Y	802	-	-	15/43/43/54	-
76	3PE	3A	503	-	-	5/35/35/54	-
76	3PE	3P	503	-	-	6/36/36/54	-
76	3PE	5Y	801	-	-	9/34/34/54	-
74	CDL	5X	201	-	-	17/96/96/110	-
70	SF4	1I	202	9	-	-	0/6/5/5
69	PC1	5A	203	-	-	2/38/38/57	-
76	3PE	1Y	801	-	-	7/34/34/54	-
76	3PE	3Q	502	-	-	4/50/50/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	CDL	8B	303	-	-	13/110/110/110	-
86	PGV	4K	101	-	-	10/55/55/55	-
90	PSC	4A	609	-	-	10/55/55/55	-
74	CDL	5L	702	-	-	14/86/86/110	-
86	PGV	8B	301	-	-	3/55/55/55	-
76	3PE	5L	704	-	-	12/52/52/54	-
86	PGV	8A	601	-	-	14/55/55/55	-
69	PC1	1H	402	-	-	3/51/51/57	-
76	3PE	1P	502	-	-	1/38/38/54	-
69	PC1	1B	203	-	-	11/51/51/57	-
74	CDL	5h	202	-	-	16/90/90/110	-
69	PC1	5I	204	-	-	5/47/47/57	-
76	3PE	1Y	804	-	-	5/36/36/54	-
76	3PE	1M	902	-	-	9/48/48/54	-
86	PGV	8C	302	-	-	10/55/55/55	-
74	CDL	3G	102	-	-	7/66/66/110	-
82	AME	5h	201	-	-	2/9/10/12	-
74	CDL	3A	501	-	-	2/68/68/110	-
76	3PE	3D	502	-	-	2/36/36/54	-
79	NDP	1P	501	-	-	2/34/77/77	0/5/5/5
72	FMN	1F	501	-	-	2/18/18/18	0/3/3/3
83	MYR	1o	201	-	-	1/12/12/13	-
81	EHZ	5T	101	20	-	8/42/44/45	-
76	3PE	1Y	806	-	-	10/44/44/54	-
70	SF4	5B	201	2	-	-	0/6/5/5
87	HEA	8A	603	55	-	12/36/76/76	-
84	HEM	3P	501	47	-	9/14/54/54	-
70	SF4	5G	802	7	-	-	0/6/5/5
76	3PE	3Y	101	-	-	5/33/33/54	-
76	3PE	1M	901	-	-	14/52/52/54	-
69	PC1	1A	202	-	-	2/38/38/57	-
76	3PE	5M	502	-	-	16/51/51/54	-
76	3PE	1j	101	-	-	5/47/47/54	-
76	3PE	3G	101	-	-	4/32/32/54	-
76	3PE	5Y	804	-	-	5/36/36/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	HEC	3Q	501	48	-	2/14/54/54	-
70	SF4	1B	201	2	-	-	0/6/5/5
83	MYR	5o	201	-	-	2/12/12/13	-
86	PGV	8C	304	-	-	9/55/55/55	-
86	PGV	8C	301	-	-	2/55/55/55	-
92	PEK	8G	102	-	-	7/56/56/56	-
74	CDL	5d	203	-	-	13/75/75/110	-
69	PC1	3J	101	-	-	1/50/50/57	-
86	PGV	8M	101	-	-	6/55/55/55	-
69	PC1	5h	203	-	-	10/50/50/57	-
87	HEA	4A	605	55	-	6/36/76/76	-
74	CDL	3P	504	-	-	13/66/66/110	-
87	HEA	4A	604	55	-	8/36/76/76	-
69	PC1	5A	202	-	-	2/38/38/57	-
69	PC1	3X	101	-	-	2/32/32/57	-
81	EHZ	5n	201	-	-	3/42/44/45	-
86	PGV	8K	101	-	-	12/55/55/55	-
71	FES	1E	301	5	-	-	0/1/1/1
82	AME	1h	201	-	-	2/9/10/12	-
76	3PE	5M	506	-	-	6/53/53/54	-
76	3PE	3C	504	-	-	11/38/38/54	-
76	3PE	5d	201	-	-	3/52/52/54	-
86	PGV	4G	101	-	-	9/55/55/55	-
76	3PE	1L	701	-	-	5/49/49/54	-
84	HEM	3C	502	-	-	6/14/54/54	-
69	PC1	5L	705	-	-	6/49/49/57	-
92	PEK	4C	308	-	-	4/55/55/56	-
76	3PE	5K	101	-	-	9/47/47/54	-
69	PC1	3R	302	-	-	3/48/48/57	-
74	CDL	1q	202	-	-	5/71/71/110	-
69	PC1	1M	905	-	-	14/47/47/57	-
76	3PE	1Y	805	-	-	7/30/30/54	-
71	FES	5E	301	5	-	-	0/1/1/1
76	3PE	3A	502	-	-	7/30/30/54	-
74	CDL	4B	302	-	-	13/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	PGV	4C	301	-	-	2/55/55/55	-
75	AYA	1I	205	-	-	0/5/6/8	-
77	GTP	1O	402	78	-	3/22/38/38	0/3/3/3
69	PC1	5M	503	-	-	5/38/38/57	-
74	CDL	1H	401	-	-	4/61/61/110	-
69	PC1	1B	202	-	-	4/49/49/57	-
76	3PE	5L	701	-	-	4/49/49/54	-
81	EHZ	1n	201	-	-	4/42/44/45	-
71	FES	3E	301	49	-	-	0/1/1/1
86	PGV	8L	101	-	-	5/55/55/55	-
69	PC1	5I	201	-	-	7/57/57/57	-
76	3PE	5Y	806	-	-	9/44/44/54	-
76	3PE	5Y	803	-	-	9/33/33/54	-
90	PSC	8I	101	-	-	12/55/55/55	-
69	PC1	5M	505	-	-	9/47/47/57	-
69	PC1	1M	904	-	-	5/38/38/57	-
79	NDP	5P	402	-	-	2/34/77/77	0/5/5/5
69	PC1	1q	201	-	-	2/52/52/57	-
74	CDL	4D	201	-	-	15/110/110/110	-
76	3PE	1L	703	-	-	6/48/48/54	-
69	PC1	1A	201	-	-	6/38/38/57	-
76	3PE	5L	703	-	-	6/48/48/54	-
76	3PE	5A	201	-	-	6/50/50/54	-
74	CDL	1N	401	-	-	16/71/71/110	-
86	PGV	8C	305	-	-	6/55/55/55	-
84	HEM	3C	501	47	-	7/14/54/54	-
75	AYA	5q	202	-	-	0/5/6/8	-
76	3PE	3N	503	-	-	6/28/28/54	-
86	PGV	8C	303	-	-	12/55/55/55	-
74	CDL	3T	101	-	-	7/67/67/110	-
77	GTP	5O	401	78	-	1/22/38/38	0/3/3/3
76	3PE	1b	201	-	-	8/50/50/54	-
86	PGV	4A	601	-	-	13/55/55/55	-
86	PGV	4C	304	-	-	10/55/55/55	-
76	3PE	1M	903	-	-	16/51/51/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
76	3PE	5P	403	-	-	2/38/38/54	-
70	SF4	1G	802	7	-	-	0/6/5/5
74	CDL	1X	201	-	-	15/96/96/110	-
69	PC1	1I	201	-	-	6/57/57/57	-
74	CDL	5N	401	-	-	14/71/71/110	-
92	PEK	4G	102	-	-	7/56/56/56	-
70	SF4	5I	202	9	-	-	0/6/5/5
76	3PE	5Y	805	-	-	5/30/30/54	-
74	CDL	5H	401	-	-	5/61/61/110	-
74	CDL	3N	502	-	-	5/53/53/110	-
86	PGV	4A	603	-	-	2/55/55/55	-
69	PC1	5q	201	-	-	2/52/52/57	-
86	PGV	4B	301	-	-	5/55/55/55	-
86	PGV	8G	101	-	-	9/55/55/55	-
86	PGV	4C	305	-	-	5/55/55/55	-
87	HEA	8A	604	55	-	6/36/76/76	-
69	PC1	5d	202	-	-	6/42/42/57	-
72	FMN	5F	501	-	-	1/18/18/18	0/3/3/3
69	PC1	1d	202	-	-	6/42/42/57	-
76	3PE	5j	101	-	-	6/47/47/54	-
69	PC1	1h	203	-	-	11/50/50/57	-
74	CDL	4C	306	-	-	19/110/110/110	-
74	CDL	8C	306	-	-	20/110/110/110	-
70	SF4	1F	502	6	-	-	0/6/5/5
70	SF4	5G	801	7	-	-	0/6/5/5
86	PGV	4A	602	-	-	4/55/55/55	-
71	FES	1G	803	7	-	-	0/1/1/1
86	PGV	4J	101	-	-	5/55/55/55	-
76	3PE	1Y	803	-	-	8/33/33/54	-
69	PC1	1L	704	-	-	6/49/49/57	-
69	PC1	1A	203	-	-	3/36/36/57	-
69	PC1	5B	203	-	-	10/51/51/57	-
70	SF4	5F	502	6	-	-	0/6/5/5
69	PC1	5H	402	-	-	2/51/51/57	-
86	PGV	4C	303	-	-	8/55/55/55	-
71	FES	3R	301	49	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
74	CDL	5q	203	-	-	6/71/71/110	-
84	HEM	3P	502	47	-	8/14/54/54	-

All (179) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	4A	604	HEA	FE-ND	5.64	2.12	1.94
87	4A	604	HEA	FE-NB	5.62	2.12	1.94
87	8A	603	HEA	FE-NB	5.61	2.12	1.94
87	8A	603	HEA	FE-ND	5.58	2.12	1.94
87	4A	605	HEA	FE-ND	5.55	2.12	1.94
87	8A	604	HEA	FE-ND	5.53	2.11	1.94
87	8A	604	HEA	FE-NB	5.52	2.11	1.94
87	4A	604	HEA	C3B-C2B	5.48	1.47	1.34
87	4A	605	HEA	C3B-C2B	5.47	1.47	1.34
87	4A	605	HEA	FE-NB	5.46	2.11	1.94
87	8A	604	HEA	C3B-C2B	5.43	1.47	1.34
87	8A	603	HEA	C3B-C2B	5.41	1.47	1.34
84	3C	501	HEM	FE-NB	5.30	2.11	1.94
84	3P	501	HEM	FE-NB	5.29	2.11	1.94
84	3C	502	HEM	FE-NB	5.20	2.10	1.94
84	3P	502	HEM	FE-NB	5.19	2.10	1.94
85	3D	501	HEC	C2A-C3A	4.90	1.47	1.36
85	3Q	501	HEC	C2A-C3A	4.90	1.47	1.36
85	3Q	501	HEC	CHA-C1A	4.87	1.47	1.38
87	8A	604	HEA	FE-NC	4.86	2.11	1.95
87	4A	604	HEA	FE-NC	4.85	2.11	1.95
87	4A	605	HEA	FE-NC	4.84	2.11	1.95
87	8A	603	HEA	FE-NC	4.82	2.11	1.95
87	4A	605	HEA	C3D-C2D	4.82	1.47	1.36
87	8A	604	HEA	C3D-C2D	4.80	1.47	1.36
85	3D	501	HEC	CHB-C4A	4.79	1.47	1.38
87	8A	603	HEA	C3D-C2D	4.79	1.47	1.36
85	3D	501	HEC	CHD-C4C	4.77	1.47	1.38
85	3Q	501	HEC	CHD-C4C	4.77	1.47	1.38
87	4A	604	HEA	C3D-C2D	4.76	1.47	1.36
85	3D	501	HEC	CHA-C1A	4.69	1.47	1.38
85	3Q	501	HEC	CHC-C4B	4.68	1.47	1.38
85	3D	501	HEC	CHC-C4B	4.67	1.47	1.38
85	3Q	501	HEC	CHB-C4A	4.66	1.47	1.38
87	4A	604	HEA	C3A-C2A	4.61	1.47	1.37
87	4A	605	HEA	C3A-C2A	4.55	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	8A	603	HEA	C3A-C2A	4.53	1.47	1.37
87	8A	604	HEA	C3A-C2A	4.49	1.47	1.37
85	3D	501	HEC	CAC-C3C	4.43	1.49	1.35
87	4A	605	HEA	CHD-C1D	4.42	1.47	1.38
87	4A	605	HEA	CHC-C4B	4.41	1.47	1.38
85	3Q	501	HEC	CAB-C3B	4.38	1.49	1.35
87	4A	604	HEA	CHC-C4B	4.38	1.47	1.38
87	4A	604	HEA	CHB-C4A	4.37	1.46	1.38
85	3Q	501	HEC	CAC-C3C	4.36	1.49	1.35
87	8A	604	HEA	CHD-C1D	4.35	1.47	1.38
87	8A	603	HEA	CHC-C4B	4.34	1.47	1.38
87	4A	605	HEA	CHB-C4A	4.32	1.46	1.38
85	3D	501	HEC	CAB-C3B	4.31	1.49	1.35
87	8A	603	HEA	CHD-C1D	4.30	1.47	1.38
87	8A	604	HEA	CHC-C4B	4.28	1.47	1.38
87	4A	604	HEA	CHD-C1D	4.27	1.47	1.38
84	3C	501	HEM	FE-NC	4.26	2.09	1.95
87	8A	603	HEA	CHB-C4A	4.25	1.46	1.38
87	8A	604	HEA	C1A-NA	4.20	1.47	1.39
84	3P	501	HEM	FE-NC	4.19	2.09	1.95
84	3P	502	HEM	FE-NC	4.19	2.09	1.95
87	4A	604	HEA	CHA-C1A	4.18	1.46	1.38
87	4A	605	HEA	C1A-NA	4.17	1.47	1.39
87	8A	604	HEA	CHB-C4A	4.16	1.46	1.38
84	3C	502	HEM	FE-NC	4.13	2.08	1.95
87	8A	604	HEA	CHA-C1A	4.11	1.46	1.38
87	4A	605	HEA	C4A-NA	4.09	1.47	1.39
87	8A	603	HEA	CHA-C1A	4.09	1.46	1.38
87	4A	604	HEA	C1A-NA	4.07	1.47	1.39
87	4A	605	HEA	CHA-C1A	4.07	1.46	1.38
87	8A	604	HEA	C4A-NA	4.07	1.47	1.39
87	8A	603	HEA	C1A-NA	4.06	1.47	1.39
87	4A	604	HEA	C4A-NA	3.94	1.47	1.39
87	8A	603	HEA	C4A-NA	3.93	1.47	1.39
85	3Q	501	HEC	CHA-C4D	3.81	1.48	1.39
85	3D	501	HEC	CHA-C4D	3.71	1.47	1.39
85	3D	501	HEC	CHB-C1B	3.68	1.47	1.39
85	3D	501	HEC	CHD-C1D	3.67	1.47	1.39
85	3Q	501	HEC	CHC-C1C	3.65	1.47	1.39
85	3Q	501	HEC	CHD-C1D	3.63	1.47	1.39
85	3Q	501	HEC	CHB-C1B	3.63	1.47	1.39
85	3D	501	HEC	CHC-C1C	3.59	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	4A	605	HEA	CHD-C4C	3.56	1.47	1.39
87	8A	604	HEA	CHD-C4C	3.51	1.47	1.39
87	4A	605	HEA	CHC-C1C	3.47	1.47	1.39
87	4A	604	HEA	CHC-C1C	3.45	1.47	1.39
84	3C	502	HEM	C1B-NB	-3.44	1.34	1.40
87	8A	604	HEA	CHC-C1C	3.44	1.47	1.39
87	8A	603	HEA	CHC-C1C	3.40	1.47	1.39
87	8A	603	HEA	CHD-C4C	3.40	1.47	1.39
87	4A	605	HEA	CHB-C1B	3.34	1.46	1.39
87	4A	604	HEA	CHD-C4C	3.34	1.46	1.39
84	3P	502	HEM	C1B-NB	-3.33	1.34	1.40
87	4A	604	HEA	CHA-C4D	3.30	1.46	1.39
87	4A	604	HEA	CHB-C1B	3.30	1.46	1.39
84	3P	501	HEM	C1B-NB	-3.28	1.34	1.40
87	8A	604	HEA	CHA-C4D	3.27	1.46	1.39
87	4A	605	HEA	CHA-C4D	3.27	1.46	1.39
85	3Q	501	HEC	C3D-C2D	3.27	1.47	1.38
87	8A	603	HEA	CHA-C4D	3.25	1.46	1.39
84	3C	501	HEM	C1B-NB	-3.24	1.34	1.40
85	3D	501	HEC	C3D-C2D	3.24	1.47	1.38
87	8A	604	HEA	CHB-C1B	3.22	1.46	1.39
87	8A	603	HEA	CHB-C1B	3.22	1.46	1.39
84	3P	501	HEM	C4D-ND	-3.21	1.34	1.40
84	3C	502	HEM	C4D-ND	-3.21	1.34	1.40
84	3P	502	HEM	C4D-ND	-3.20	1.34	1.40
84	3C	501	HEM	C4D-ND	-3.17	1.34	1.40
87	8A	603	HEA	C4B-C3B	2.81	1.49	1.44
87	4A	604	HEA	C4B-C3B	2.75	1.49	1.44
87	8A	604	HEA	C4B-NB	-2.75	1.35	1.40
87	4A	605	HEA	C1D-ND	-2.74	1.35	1.40
87	4A	604	HEA	C1D-ND	-2.74	1.35	1.40
87	8A	603	HEA	C1D-ND	-2.71	1.35	1.40
87	4A	605	HEA	C4B-NB	-2.69	1.35	1.40
87	8A	603	HEA	C4B-NB	-2.68	1.35	1.40
87	8A	604	HEA	C1D-ND	-2.67	1.35	1.40
87	4A	604	HEA	C4B-NB	-2.61	1.35	1.40
87	4A	604	HEA	C4D-C3D	2.60	1.49	1.45
85	3D	501	HEC	C1B-C2B	2.59	1.49	1.43
85	3Q	501	HEC	C1C-C2C	2.55	1.49	1.43
87	4A	605	HEA	C4B-C3B	2.54	1.49	1.44
87	4A	605	HEA	C1C-C2C	2.54	1.49	1.43
85	3Q	501	HEC	C1B-C2B	2.53	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	8A	604	HEA	C1C-C2C	2.52	1.49	1.43
85	3D	501	HEC	C1C-C2C	2.52	1.49	1.43
87	4A	604	HEA	C1C-C2C	2.51	1.49	1.43
85	3D	501	HEC	C4B-NB	-2.50	1.34	1.39
87	8A	603	HEA	C1C-C2C	2.49	1.49	1.43
85	3Q	501	HEC	C4B-NB	-2.49	1.34	1.39
84	3P	502	HEM	FE-ND	-2.47	1.87	1.94
84	3C	502	HEM	FE-ND	-2.47	1.87	1.94
87	8A	603	HEA	C4D-C3D	2.46	1.49	1.45
84	3P	501	HEM	FE-ND	-2.45	1.87	1.94
84	3C	502	HEM	C1C-C2C	-2.45	1.40	1.45
84	3C	501	HEM	FE-ND	-2.44	1.87	1.94
87	8A	604	HEA	C4B-C3B	2.43	1.49	1.44
84	3P	502	HEM	C1C-C2C	-2.43	1.40	1.45
84	3P	501	HEM	C1C-C2C	-2.41	1.40	1.45
87	8A	604	HEA	C11-C3B	-2.39	1.48	1.51
85	3D	501	HEC	C1A-NA	-2.37	1.35	1.39
85	3Q	501	HEC	C4C-NC	-2.37	1.35	1.39
85	3Q	501	HEC	C4A-NA	-2.37	1.35	1.39
84	3C	501	HEM	C1C-C2C	-2.36	1.40	1.45
85	3Q	501	HEC	C1A-NA	-2.34	1.35	1.39
85	3D	501	HEC	C4C-NC	-2.33	1.35	1.39
85	3D	501	HEC	C1D-ND	-2.32	1.35	1.39
85	3D	501	HEC	C1D-C2D	2.31	1.48	1.43
85	3Q	501	HEC	C1D-ND	-2.31	1.35	1.39
85	3Q	501	HEC	C1D-C2D	2.30	1.48	1.43
87	4A	604	HEA	C4C-NC	-2.30	1.35	1.39
87	4A	605	HEA	C4D-C3D	2.29	1.48	1.45
85	3D	501	HEC	C4D-ND	-2.27	1.35	1.39
87	8A	603	HEA	C4C-NC	-2.25	1.35	1.39
85	3D	501	HEC	C4A-NA	-2.24	1.35	1.39
87	4A	605	HEA	C4C-NC	-2.24	1.35	1.39
87	4A	605	HEA	C11-C3B	-2.22	1.48	1.51
87	8A	604	HEA	C4C-NC	-2.22	1.35	1.39
87	8A	604	HEA	C1D-C2D	2.21	1.49	1.44
85	3Q	501	HEC	C1C-NC	-2.18	1.35	1.39
85	3Q	501	HEC	C4D-ND	-2.18	1.35	1.39
85	3D	501	HEC	C4D-C3D	2.18	1.48	1.44
85	3Q	501	HEC	C4D-C3D	2.18	1.48	1.44
85	3D	501	HEC	C1C-NC	-2.17	1.35	1.39
87	4A	605	HEA	C1D-C2D	2.16	1.48	1.44
87	4A	604	HEA	C1A-C2A	2.15	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	3C	501	HEM	C1D-ND	-2.15	1.34	1.38
84	3P	502	HEM	C1D-ND	-2.14	1.34	1.38
84	3C	502	HEM	C1D-ND	-2.14	1.34	1.38
87	8A	603	HEA	C1D-C2D	2.12	1.48	1.44
84	3C	501	HEM	C3C-C4C	-2.11	1.42	1.46
87	8A	604	HEA	C4D-C3D	2.11	1.48	1.45
85	3Q	501	HEC	C1A-C2A	2.11	1.48	1.45
84	3P	501	HEM	C1D-ND	-2.09	1.34	1.38
84	3P	502	HEM	C3C-C4C	-2.07	1.42	1.46
84	3P	501	HEM	C3C-C4C	-2.05	1.42	1.46
84	3C	502	HEM	C4B-NB	-2.05	1.34	1.38
87	8A	603	HEA	C1A-C2A	2.04	1.48	1.45
84	3P	502	HEM	C4B-NB	-2.03	1.34	1.38
85	3Q	501	HEC	C3B-C2B	2.03	1.48	1.41
87	8A	604	HEA	C1A-C2A	2.01	1.48	1.45
87	4A	604	HEA	C1B-C2B	2.00	1.48	1.44
87	4A	604	HEA	C1D-C2D	2.00	1.48	1.44

All (254) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	8A	604	HEA	C3D-C4D-ND	6.64	116.77	110.35
87	8A	603	HEA	C3D-C4D-ND	6.61	116.74	110.35
87	4A	605	HEA	C3D-C4D-ND	6.50	116.63	110.35
87	4A	604	HEA	C3D-C4D-ND	6.45	116.59	110.35
81	5n	201	EHZ	C10-S1-C9	5.97	119.50	101.84
81	1T	101	EHZ	C10-S1-C9	5.86	119.17	101.84
87	8A	603	HEA	C2B-C1B-NB	5.85	116.67	109.90
81	1n	201	EHZ	C10-S1-C9	5.82	119.03	101.84
87	4A	604	HEA	C2B-C1B-NB	5.81	116.61	109.90
87	8A	604	HEA	C2B-C1B-NB	5.79	116.60	109.90
81	5T	101	EHZ	C10-S1-C9	5.73	118.78	101.84
87	4A	604	HEA	C2D-C1D-ND	5.66	116.35	109.84
87	4A	604	HEA	C3B-C4B-NB	5.64	116.33	109.84
87	4A	605	HEA	C2B-C1B-NB	5.62	116.40	109.90
87	8A	604	HEA	C3C-C2C-C1C	-5.61	100.55	107.17
87	4A	605	HEA	C2D-C1D-ND	5.61	116.29	109.84
87	8A	604	HEA	C2D-C1D-ND	5.61	116.29	109.84
87	8A	603	HEA	C3B-C4B-NB	5.61	116.28	109.84
87	4A	604	HEA	C3C-C2C-C1C	-5.59	100.58	107.17
87	8A	604	HEA	C3B-C4B-NB	5.57	116.24	109.84
87	8A	603	HEA	C3C-C2C-C1C	-5.56	100.61	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	4A	605	HEA	C3C-C2C-C1C	-5.54	100.63	107.17
85	3D	501	HEC	C2A-C1A-NA	5.54	115.67	110.32
87	8A	603	HEA	C2D-C1D-ND	5.52	116.19	109.84
87	8A	604	HEA	C3C-C4C-NC	5.46	114.39	109.80
87	4A	604	HEA	C3C-C4C-NC	5.39	114.33	109.80
87	8A	603	HEA	C2A-C1A-NA	5.38	115.51	110.32
87	8A	604	HEA	C2A-C1A-NA	5.35	115.49	110.32
87	4A	604	HEA	C2A-C1A-NA	5.35	115.48	110.32
87	4A	605	HEA	C2A-C1A-NA	5.34	115.48	110.32
87	4A	605	HEA	C3B-C4B-NB	5.32	115.95	109.84
87	8A	603	HEA	C3C-C4C-NC	5.29	114.25	109.80
87	4A	605	HEA	C3C-C4C-NC	5.18	114.16	109.80
84	3C	501	HEM	CHC-C4B-NB	5.15	129.96	124.42
84	3P	501	HEM	CHC-C4B-NB	5.13	129.95	124.42
85	3Q	501	HEC	C2A-C1A-NA	4.92	115.07	110.32
84	3C	502	HEM	CHC-C4B-NB	4.87	129.66	124.42
85	3D	501	HEC	C3D-C4D-ND	4.84	115.52	110.15
84	3P	502	HEM	CHC-C4B-NB	4.80	129.59	124.42
87	4A	604	HEA	CHA-C4D-ND	-4.65	119.42	124.42
79	1P	501	NDP	P2B-O2B-C2B	-4.55	111.27	123.43
85	3Q	501	HEC	C3D-C4D-ND	4.48	115.13	110.15
79	5P	402	NDP	P2B-O2B-C2B	-4.46	111.53	123.43
84	3P	501	HEM	CHD-C1D-ND	4.45	129.22	124.42
84	3C	501	HEM	CHD-C1D-ND	4.33	129.09	124.42
87	8A	603	HEA	CHA-C4D-ND	-4.28	119.82	124.42
87	8A	604	HEA	C2C-C1C-NC	4.27	116.99	110.14
84	3P	502	HEM	CHD-C1D-ND	4.27	129.02	124.42
87	8A	604	HEA	C1D-C2D-C3D	-4.26	102.50	106.98
84	3C	502	HEM	CHD-C1D-ND	4.19	128.93	124.42
87	4A	605	HEA	C1D-C2D-C3D	-4.18	102.59	106.98
87	4A	605	HEA	C2C-C1C-NC	4.11	116.73	110.14
87	8A	603	HEA	C2C-C1C-NC	4.10	116.72	110.14
87	4A	604	HEA	C2C-C1C-NC	4.10	116.71	110.14
87	8A	603	HEA	C3A-C2A-C1A	-4.01	103.25	107.05
87	4A	604	HEA	C3A-C2A-C1A	-4.00	103.26	107.05
85	3D	501	HEC	C2C-C1C-NC	3.99	116.54	110.14
87	4A	605	HEA	C3A-C2A-C1A	-3.93	103.33	107.05
87	8A	603	HEA	C1D-C2D-C3D	-3.88	102.90	106.98
87	4A	604	HEA	C1D-C2D-C3D	-3.86	102.92	106.98
87	8A	604	HEA	C1B-C2B-C3B	-3.85	102.34	106.80
87	4A	604	HEA	CAD-C3D-C4D	3.85	131.40	124.70
85	3Q	501	HEC	C2B-C1B-NB	3.82	116.27	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	3Q	501	HEC	C2C-C1C-NC	3.82	116.27	110.14
87	8A	604	HEA	C3A-C2A-C1A	-3.81	103.44	107.05
87	4A	605	HEA	C1B-C2B-C3B	-3.75	102.46	106.80
87	8A	603	HEA	C13-C14-C15	-3.75	119.05	127.62
85	3D	501	HEC	C2B-C1B-NB	3.73	116.12	110.14
85	3Q	501	HEC	C1D-C2D-C3D	-3.65	102.64	106.82
87	8A	604	HEA	C13-C12-C11	-3.63	108.59	114.39
87	4A	605	HEA	C13-C12-C11	-3.61	108.63	114.39
87	4A	605	HEA	CHA-C4D-ND	-3.60	120.55	124.42
87	4A	604	HEA	C1B-C2B-C3B	-3.58	102.65	106.80
87	8A	603	HEA	C1B-C2B-C3B	-3.55	102.68	106.80
84	3C	501	HEM	CHA-C4D-ND	3.54	128.75	124.37
74	1N	401	CDL	OB6-CB5-C51	3.54	117.40	111.09
86	8C	302	PGV	O01-C1-C2	3.53	119.13	111.48
84	3P	501	HEM	CHA-C4D-ND	3.51	128.71	124.37
85	3D	501	HEC	C1D-C2D-C3D	-3.48	102.83	106.82
74	5N	401	CDL	OB6-CB5-C51	3.46	117.26	111.09
87	8A	603	HEA	C4D-C3D-C2D	-3.45	101.86	106.89
87	4A	604	HEA	C4D-C3D-C2D	-3.45	101.87	106.89
84	3P	502	HEM	CHA-C4D-ND	3.44	128.63	124.37
87	8A	603	HEA	CAD-C3D-C4D	3.43	130.67	124.70
85	3D	501	HEC	C1A-C2A-C3A	-3.39	102.65	107.11
84	3C	502	HEM	CHA-C4D-ND	3.38	128.55	124.37
85	3Q	501	HEC	C2D-C1D-ND	3.38	115.56	110.14
86	4C	302	PGV	O01-C1-C2	3.37	118.77	111.48
84	3P	501	HEM	CHB-C1B-NB	3.36	128.53	124.37
85	3D	501	HEC	C2D-C1D-ND	3.36	115.52	110.14
84	3P	502	HEM	CHB-C1B-NB	3.35	128.51	124.37
84	3C	501	HEM	CHB-C1B-NB	3.34	128.50	124.37
87	8A	604	HEA	C4A-NA-C1A	-3.34	100.37	105.82
84	3P	502	HEM	C1B-NB-C4B	3.33	109.16	105.21
87	8A	604	HEA	C13-C14-C15	-3.30	120.08	127.62
87	4A	605	HEA	C13-C14-C15	-3.29	120.10	127.62
84	3C	502	HEM	C1B-NB-C4B	3.28	109.09	105.21
87	4A	605	HEA	C4D-C3D-C2D	-3.26	102.15	106.89
87	8A	603	HEA	C4A-NA-C1A	-3.22	100.57	105.82
84	3P	501	HEM	C1B-NB-C4B	3.22	109.02	105.21
87	8A	603	HEA	C4B-C3B-C2B	-3.21	102.04	107.44
85	3Q	501	HEC	C3A-C4A-NA	3.21	115.57	109.64
87	8A	604	HEA	C4D-C3D-C2D	-3.21	102.22	106.89
85	3Q	501	HEC	C1A-C2A-C3A	-3.20	102.89	107.11
84	3C	501	HEM	C1B-NB-C4B	3.20	109.00	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	4A	604	HEA	C4B-C3B-C2B	-3.19	102.08	107.44
87	4A	605	HEA	C4A-NA-C1A	-3.18	100.63	105.82
87	4A	604	HEA	C13-C14-C15	-3.18	120.34	127.62
87	4A	604	HEA	C4A-NA-C1A	-3.16	100.67	105.82
84	3C	502	HEM	CHB-C1B-NB	3.16	128.27	124.37
76	1Y	803	3PE	O21-C21-C22	3.14	118.27	111.48
85	3D	501	HEC	C3A-C4A-NA	3.08	115.34	109.64
87	4A	604	HEA	CHB-C1B-NB	-3.02	121.18	124.42
87	8A	604	HEA	CHA-C4D-ND	-3.01	121.18	124.42
87	4A	604	HEA	C26-C15-C16	3.00	120.43	115.23
76	5Y	803	3PE	O21-C21-C22	2.97	117.91	111.48
85	3Q	501	HEC	C4A-C3A-C2A	-2.97	102.57	106.97
87	8A	604	HEA	C4B-C3B-C2B	-2.96	102.46	107.44
87	8A	603	HEA	C13-C12-C11	-2.95	109.67	114.39
87	8A	603	HEA	C26-C15-C16	2.95	120.35	115.23
87	4A	604	HEA	CHA-C1A-NA	-2.94	121.25	124.45
87	4A	605	HEA	C4B-C3B-C2B	-2.92	102.52	107.44
85	3D	501	HEC	C4A-C3A-C2A	-2.88	102.70	106.97
87	4A	605	HEA	C26-C15-C16	2.86	120.19	115.23
82	5h	201	AME	O-C-CA	-2.84	117.45	124.77
85	3D	501	HEC	CAA-CBA-CGA	-2.83	106.15	113.67
85	3D	501	HEC	C4D-C3D-C2D	-2.82	102.50	106.87
87	8A	603	HEA	C17-C18-C19	-2.81	121.19	127.62
82	1h	201	AME	O-C-CA	-2.81	117.55	124.77
87	8A	604	HEA	C26-C15-C16	2.78	120.06	115.23
84	3P	501	HEM	CHD-C1D-C2D	-2.75	120.69	125.03
87	8A	604	HEA	C27-C19-C20	2.75	119.99	115.23
84	3C	501	HEM	CHD-C1D-C2D	-2.74	120.71	125.03
87	8A	603	HEA	CHA-C1A-NA	-2.73	121.48	124.45
84	3P	502	HEM	C3B-C4B-NB	-2.72	107.51	109.47
87	4A	605	HEA	C27-C19-C20	2.70	119.92	115.23
87	8A	603	HEA	CHB-C1B-NB	-2.70	121.52	124.42
87	4A	604	HEA	CMC-C2C-C1C	2.69	129.51	125.42
85	3Q	501	HEC	CAA-CBA-CGA	-2.67	106.57	113.67
87	4A	605	HEA	C17-C18-C19	-2.67	121.52	127.62
79	1P	501	NDP	O4D-C1D-C2D	-2.66	100.93	106.62
84	3C	501	HEM	CHD-C4C-NC	2.63	127.31	124.45
84	3P	501	HEM	CHD-C4C-NC	2.61	127.29	124.45
85	3Q	501	HEC	C4D-C3D-C2D	-2.60	102.85	106.87
87	8A	603	HEA	C27-C19-C20	2.59	119.72	115.23
87	8A	604	HEA	C17-C18-C19	-2.57	121.74	127.62
79	5P	402	NDP	O4D-C1D-C2D	-2.56	101.14	106.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	4A	604	HEA	C17-C18-C19	-2.55	121.79	127.62
87	4A	604	HEA	C1A-CHA-C4D	-2.54	120.61	126.02
87	8A	604	HEA	C1D-ND-C4D	-2.53	102.21	105.21
87	8A	604	HEA	CHC-C1C-C2C	-2.53	120.09	127.43
87	4A	604	HEA	C27-C19-C20	2.51	119.59	115.23
84	3C	502	HEM	C3B-C4B-NB	-2.50	107.67	109.47
87	4A	604	HEA	C1D-ND-C4D	-2.48	102.27	105.21
84	3C	501	HEM	C3B-C4B-NB	-2.48	107.69	109.47
87	8A	604	HEA	CHB-C1B-NB	-2.48	121.75	124.42
87	4A	605	HEA	CMC-C2C-C1C	2.48	129.19	125.42
87	4A	605	HEA	C1A-CHA-C4D	-2.45	120.81	126.02
87	8A	603	HEA	C1D-ND-C4D	-2.45	102.30	105.21
84	3P	501	HEM	C3B-C4B-NB	-2.45	107.71	109.47
87	8A	603	HEA	C4B-NB-C1B	-2.44	102.32	105.21
84	3P	502	HEM	CHD-C1D-C2D	-2.43	121.19	125.03
84	3C	502	HEM	CHD-C1D-C2D	-2.43	121.19	125.03
87	4A	604	HEA	C4B-NB-C1B	-2.43	102.33	105.21
87	4A	605	HEA	CHB-C1B-NB	-2.43	121.81	124.42
87	4A	605	HEA	CAD-C3D-C4D	2.42	128.92	124.70
87	8A	603	HEA	CHC-C1C-C2C	-2.42	120.41	127.43
87	4A	605	HEA	C1D-ND-C4D	-2.42	102.35	105.21
87	8A	604	HEA	C4B-NB-C1B	-2.41	102.35	105.21
76	3A	502	3PE	O21-C21-C22	2.41	116.69	111.48
87	4A	604	HEA	CHC-C1C-C2C	-2.39	120.47	127.43
85	3D	501	HEC	CMC-C2C-C3C	2.39	132.17	126.55
87	4A	604	HEA	CHD-C1D-C2D	-2.37	120.21	126.95
87	8A	604	HEA	C25-C23-C24	2.37	120.04	114.59
87	8A	603	HEA	CMC-C2C-C1C	2.37	129.03	125.42
87	4A	605	HEA	CHC-C1C-C2C	-2.36	120.59	127.43
86	4C	305	PGV	O01-C1-C2	2.35	116.57	111.48
90	8I	101	PSC	O01-C1-C2	2.35	116.56	111.48
87	8A	604	HEA	CMB-C2B-C1B	2.34	128.68	125.03
87	4A	605	HEA	C25-C23-C24	2.33	119.95	114.59
87	4A	604	HEA	CAD-CBD-CGD	-2.33	107.50	113.67
87	4A	605	HEA	CMB-C2B-C1B	2.32	128.66	125.03
85	3Q	501	HEC	CMB-C2B-C3B	2.31	132.00	126.55
87	8A	603	HEA	CBA-CAA-C2A	-2.31	106.14	112.53
87	4A	605	HEA	CHA-C1A-NA	-2.31	121.94	124.45
87	8A	603	HEA	CHD-C1D-C2D	-2.30	120.40	126.95
86	8G	101	PGV	O01-C1-C2	2.30	116.46	111.48
85	3D	501	HEC	CMB-C2B-C3B	2.29	131.93	126.55
84	3C	502	HEM	C1A-CHA-C4D	-2.28	120.88	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	3P	501	HEM	C1A-CHA-C4D	-2.28	120.88	126.25
87	8A	603	HEA	C1A-CHA-C4D	-2.28	121.17	126.02
84	3P	502	HEM	CHD-C4C-NC	2.26	126.92	124.45
84	3P	502	HEM	C1A-CHA-C4D	-2.25	120.96	126.25
84	3P	502	HEM	C4C-CHD-C1D	-2.24	121.25	126.02
87	8A	604	HEA	CAD-C3D-C4D	2.24	128.61	124.70
87	8A	604	HEA	CMD-C2D-C1D	2.24	128.54	125.03
87	8A	603	HEA	CMD-C2D-C1D	2.24	128.54	125.03
85	3D	501	HEC	CHC-C1C-C2C	-2.24	120.92	127.43
87	4A	604	HEA	CMB-C2B-C1B	2.24	128.53	125.03
85	3D	501	HEC	CMA-C3A-C4A	2.24	128.67	124.73
87	4A	604	HEA	C25-C23-C24	2.24	119.74	114.59
85	3Q	501	HEC	CMC-C2C-C3C	2.23	131.80	126.55
85	3D	501	HEC	CHA-C1A-C2A	-2.23	121.35	124.86
87	8A	603	HEA	C25-C23-C24	2.22	119.71	114.59
87	8A	603	HEA	OMA-CMA-C3A	-2.21	120.64	125.62
87	4A	605	HEA	CHD-C1D-C2D	-2.21	120.67	126.95
87	8A	604	HEA	CHD-C1D-C2D	-2.20	120.69	126.95
87	4A	604	HEA	CMD-C2D-C1D	2.20	128.48	125.03
87	8A	603	HEA	CMB-C2B-C1B	2.20	128.47	125.03
84	3C	502	HEM	C4C-CHD-C1D	-2.20	121.35	126.02
74	1H	401	CDL	OB6-CB5-C51	2.19	116.22	111.48
87	4A	605	HEA	CMD-C2D-C1D	2.19	128.46	125.03
84	3C	501	HEM	C1A-CHA-C4D	-2.19	121.10	126.25
84	3C	501	HEM	CHA-C4D-C3D	-2.18	121.21	125.23
87	8A	604	HEA	CBA-CAA-C2A	-2.17	106.53	112.53
87	8A	603	HEA	CAD-CBD-CGD	-2.16	107.95	113.67
87	8A	604	HEA	CHB-C1B-C2B	-2.15	121.64	125.03
87	4A	605	HEA	C4B-NB-C1B	-2.15	102.67	105.21
72	1F	501	FMN	C4-N3-C2	-2.14	121.85	125.64
74	5H	401	CDL	OB6-CB5-C51	2.14	116.10	111.48
75	1I	205	AYA	O-C-CA	-2.13	117.32	123.94
90	4A	609	PSC	O01-C1-C2	2.12	116.08	111.48
85	3Q	501	HEC	CHC-C1C-C2C	-2.12	121.28	127.43
74	3C	503	CDL	OA6-CA5-C11	2.12	116.06	111.48
72	5F	501	FMN	C4-N3-C2	-2.11	121.89	125.64
84	3P	501	HEM	CHA-C4D-C3D	-2.11	121.34	125.23
84	3C	501	HEM	CHA-C1A-NA	2.11	127.68	123.86
85	3D	501	HEC	CHB-C1B-C2B	-2.11	121.31	127.43
84	3C	502	HEM	C4A-CHB-C1B	-2.10	121.30	126.25
87	4A	605	HEA	C21-C22-C23	-2.10	120.65	127.64
75	5q	202	AYA	O-C-CA	-2.09	117.43	123.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	4A	604	HEA	C21-C22-C23	-2.08	120.69	127.64
87	8A	604	HEA	CMC-C2C-C1C	2.08	128.58	125.42
84	3P	502	HEM	C4D-ND-C1D	2.07	107.66	105.21
85	3Q	501	HEC	CAD-C3D-C4D	2.07	128.99	124.94
87	4A	604	HEA	CBA-CAA-C2A	-2.07	106.81	112.53
84	3C	502	HEM	C4D-ND-C1D	2.07	107.66	105.21
84	3P	501	HEM	CHA-C1A-NA	2.07	127.61	123.86
87	8A	603	HEA	CHC-C4B-NB	-2.06	121.81	124.37
87	4A	605	HEA	CHB-C1B-C2B	-2.06	121.78	125.03
87	4A	604	HEA	CHC-C4B-NB	-2.05	121.83	124.37
85	3Q	501	HEC	CMD-C2D-C1D	2.05	128.54	125.42
87	8A	603	HEA	CHB-C1B-C2B	-2.04	121.81	125.03
86	8C	305	PGV	O01-C1-C2	2.04	115.88	111.48
87	8A	604	HEA	CHA-C1A-NA	-2.03	122.24	124.45
87	4A	605	HEA	CBA-CAA-C2A	-2.03	106.92	112.53
85	3Q	501	HEC	CHB-C1B-C2B	-2.03	121.54	127.43
74	4C	306	CDL	OB6-CB5-C51	2.03	115.86	111.48
84	3P	502	HEM	C4A-CHB-C1B	-2.02	121.49	126.25
85	3Q	501	HEC	CHB-C4A-C3A	-2.02	121.29	125.49
87	4A	604	HEA	OMA-CMA-C3A	-2.02	121.07	125.62
85	3D	501	HEC	CAD-C3D-C4D	2.01	128.87	124.94
87	8A	604	HEA	C21-C22-C23	-2.01	120.95	127.64
69	5d	202	PC1	O21-C21-C22	2.00	115.82	111.48

There are no chirality outliers.

All (1163) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	1B	203	PC1	O22-C21-O21-C2
69	1B	203	PC1	C22-C21-O21-C2
69	1I	204	PC1	C1-O11-P-O14
69	1M	904	PC1	O22-C21-O21-C2
69	1M	904	PC1	C22-C21-O21-C2
69	1M	905	PC1	C11-O13-P-O12
69	1M	905	PC1	C11-O13-P-O11
69	1d	202	PC1	O22-C21-O21-C2
69	1d	202	PC1	C22-C21-O21-C2
69	1h	203	PC1	C11-O13-P-O14
69	1h	203	PC1	O32-C31-O31-C3
69	1h	203	PC1	C32-C31-O31-C3
69	3R	302	PC1	O32-C31-O31-C3
69	3R	302	PC1	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
69	3X	101	PC1	C1-O11-P-O14
69	5B	203	PC1	O22-C21-O21-C2
69	5B	203	PC1	C22-C21-O21-C2
69	5I	204	PC1	C1-O11-P-O14
69	5M	503	PC1	C11-O13-P-O11
69	5M	503	PC1	O22-C21-O21-C2
69	5M	503	PC1	C22-C21-O21-C2
69	5M	505	PC1	C1-O11-P-O13
69	5d	202	PC1	O22-C21-O21-C2
69	5d	202	PC1	C22-C21-O21-C2
69	5h	203	PC1	C11-O13-P-O14
69	5h	203	PC1	O32-C31-O31-C3
69	5h	203	PC1	C32-C31-O31-C3
74	1H	401	CDL	CA4-CA3-OA5-PA1
74	1H	401	CDL	OB7-CB5-OB6-CB4
74	1H	401	CDL	C51-CB5-OB6-CB4
74	1L	702	CDL	OA6-CA4-CA6-OA8
74	1N	401	CDL	CB3-OB5-PB2-OB3
74	1X	201	CDL	C1-CA2-OA2-PA1
74	1X	201	CDL	C1-CB2-OB2-PB2
74	1d	203	CDL	CB2-OB2-PB2-OB3
74	1h	202	CDL	CA2-OA2-PA1-OA4
74	1h	202	CDL	CA2-OA2-PA1-OA5
74	1h	202	CDL	C1-CB2-OB2-PB2
74	1h	202	CDL	CB2-OB2-PB2-OB3
74	1h	202	CDL	CB2-OB2-PB2-OB5
74	1h	202	CDL	OB7-CB5-OB6-CB4
74	1h	202	CDL	C51-CB5-OB6-CB4
74	1h	202	CDL	OB9-CB7-OB8-CB6
74	1h	202	CDL	C71-CB7-OB8-CB6
74	3C	503	CDL	CB2-OB2-PB2-OB3
74	3C	503	CDL	CB2-OB2-PB2-OB5
74	3N	502	CDL	CB3-OB5-PB2-OB2
74	3P	504	CDL	OB9-CB7-OB8-CB6
74	3P	504	CDL	C71-CB7-OB8-CB6
74	3T	101	CDL	CA3-OA5-PA1-OA2
74	3T	101	CDL	OB9-CB7-OB8-CB6
74	3T	101	CDL	C71-CB7-OB8-CB6
74	4B	302	CDL	OA9-CA7-OA8-CA6
74	4B	302	CDL	C31-CA7-OA8-CA6
74	4B	302	CDL	CB3-OB5-PB2-OB2
74	4B	302	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
74	4C	306	CDL	C1-CA2-OA2-PA1
74	4C	306	CDL	OB7-CB5-OB6-CB4
74	4C	306	CDL	C51-CB5-OB6-CB4
74	4C	306	CDL	OB9-CB7-OB8-CB6
74	4C	306	CDL	C71-CB7-OB8-CB6
74	4D	201	CDL	C1-CA2-OA2-PA1
74	4D	201	CDL	CA3-OA5-PA1-OA3
74	4D	201	CDL	CB3-OB5-PB2-OB3
74	4D	201	CDL	OB7-CB5-OB6-CB4
74	4D	201	CDL	C51-CB5-OB6-CB4
74	4D	201	CDL	OB9-CB7-OB8-CB6
74	4D	201	CDL	C71-CB7-OB8-CB6
74	5H	401	CDL	CA3-OA5-PA1-OA4
74	5H	401	CDL	CA4-CA3-OA5-PA1
74	5H	401	CDL	OB7-CB5-OB6-CB4
74	5H	401	CDL	C51-CB5-OB6-CB4
74	5L	702	CDL	OA6-CA4-CA6-OA8
74	5N	401	CDL	CB3-OB5-PB2-OB3
74	5X	201	CDL	C1-CA2-OA2-PA1
74	5X	201	CDL	C1-CB2-OB2-PB2
74	5d	203	CDL	CB2-OB2-PB2-OB3
74	5h	202	CDL	CA2-OA2-PA1-OA4
74	5h	202	CDL	CA2-OA2-PA1-OA5
74	5h	202	CDL	C1-CB2-OB2-PB2
74	5h	202	CDL	CB2-OB2-PB2-OB3
74	5h	202	CDL	CB2-OB2-PB2-OB5
74	5h	202	CDL	OB7-CB5-OB6-CB4
74	5h	202	CDL	C51-CB5-OB6-CB4
74	5h	202	CDL	OB9-CB7-OB8-CB6
74	5h	202	CDL	C71-CB7-OB8-CB6
74	8B	303	CDL	OA9-CA7-OA8-CA6
74	8B	303	CDL	C31-CA7-OA8-CA6
74	8B	303	CDL	CB3-OB5-PB2-OB2
74	8B	303	CDL	CB3-OB5-PB2-OB3
74	8C	306	CDL	C1-CA2-OA2-PA1
74	8C	306	CDL	OB7-CB5-OB6-CB4
74	8C	306	CDL	C51-CB5-OB6-CB4
74	8C	306	CDL	OB9-CB7-OB8-CB6
74	8C	306	CDL	C71-CB7-OB8-CB6
74	8D	201	CDL	C1-CA2-OA2-PA1
74	8D	201	CDL	CA3-OA5-PA1-OA3
74	8D	201	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
74	8D	201	CDL	OB7-CB5-OB6-CB4
74	8D	201	CDL	C51-CB5-OB6-CB4
74	8D	201	CDL	OB9-CB7-OB8-CB6
74	8D	201	CDL	C71-CB7-OB8-CB6
76	1K	101	3PE	C1-O11-P-O13
76	1K	101	3PE	C1-O11-P-O14
76	1L	701	3PE	O32-C31-O31-C3
76	1L	701	3PE	C32-C31-O31-C3
76	1L	703	3PE	C2-C1-O11-P
76	1M	901	3PE	C1-O11-P-O12
76	1M	901	3PE	C1-O11-P-O13
76	1M	901	3PE	C1-O11-P-O14
76	1M	903	3PE	C1-O11-P-O12
76	1M	903	3PE	C1-O11-P-O13
76	1M	903	3PE	C1-O11-P-O14
76	1M	903	3PE	C2-C1-O11-P
76	1M	903	3PE	O32-C31-O31-C3
76	1M	903	3PE	C32-C31-O31-C3
76	1M	906	3PE	C1-O11-P-O14
76	1O	401	3PE	C2-C1-O11-P
76	1Y	802	3PE	C1-O11-P-O13
76	1Y	802	3PE	C1-O11-P-O14
76	1Y	802	3PE	C2-C1-O11-P
76	1Y	802	3PE	O22-C21-O21-C2
76	1Y	802	3PE	C22-C21-O21-C2
76	1Y	803	3PE	O22-C21-O21-C2
76	1Y	803	3PE	C22-C21-O21-C2
76	1Y	805	3PE	C11-O13-P-O14
76	1Y	806	3PE	O32-C31-O31-C3
76	1Y	806	3PE	C32-C31-O31-C3
76	1b	201	3PE	C11-O13-P-O12
76	1j	101	3PE	O22-C21-O21-C2
76	1j	101	3PE	C22-C21-O21-C2
76	3A	502	3PE	O32-C31-O31-C3
76	3A	502	3PE	C32-C31-O31-C3
76	3A	502	3PE	O22-C21-O21-C2
76	3A	502	3PE	C22-C21-O21-C2
76	3A	503	3PE	C2-C1-O11-P
76	3C	504	3PE	C11-O13-P-O11
76	3C	504	3PE	C11-O13-P-O12
76	3C	504	3PE	C11-O13-P-O14
76	3C	505	3PE	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
76	3G	101	3PE	O32-C31-O31-C3
76	3G	101	3PE	C32-C31-O31-C3
76	3N	501	3PE	C1-O11-P-O14
76	3N	503	3PE	O22-C21-O21-C2
76	3N	503	3PE	C22-C21-O21-C2
76	3P	503	3PE	C11-O13-P-O11
76	3P	503	3PE	C11-O13-P-O12
76	3P	503	3PE	C11-O13-P-O14
76	5A	201	3PE	C11-O13-P-O12
76	5K	101	3PE	C1-O11-P-O13
76	5K	101	3PE	C1-O11-P-O14
76	5L	701	3PE	O32-C31-O31-C3
76	5L	701	3PE	C32-C31-O31-C3
76	5L	703	3PE	C2-C1-O11-P
76	5L	704	3PE	C1-O11-P-O12
76	5L	704	3PE	C1-O11-P-O13
76	5L	704	3PE	C1-O11-P-O14
76	5M	502	3PE	C1-O11-P-O12
76	5M	502	3PE	C1-O11-P-O13
76	5M	502	3PE	C2-C1-O11-P
76	5M	502	3PE	O32-C31-O31-C3
76	5M	502	3PE	C32-C31-O31-C3
76	5M	504	3PE	C2-C1-O11-P
76	5M	506	3PE	C1-O11-P-O14
76	5Y	801	3PE	C1-O11-P-O13
76	5Y	801	3PE	C2-C1-O11-P
76	5Y	802	3PE	C1-O11-P-O13
76	5Y	802	3PE	C1-O11-P-O14
76	5Y	802	3PE	C2-C1-O11-P
76	5Y	802	3PE	O22-C21-O21-C2
76	5Y	802	3PE	C22-C21-O21-C2
76	5Y	803	3PE	O22-C21-O21-C2
76	5Y	803	3PE	C22-C21-O21-C2
76	5Y	805	3PE	C11-O13-P-O14
76	5Y	805	3PE	C12-C11-O13-P
76	5Y	806	3PE	O32-C31-O31-C3
76	5Y	806	3PE	C32-C31-O31-C3
76	5j	101	3PE	C1-O11-P-O14
76	5j	101	3PE	C11-O13-P-O14
76	5j	101	3PE	O22-C21-O21-C2
76	5j	101	3PE	C22-C21-O21-C2
77	5O	401	GTP	PB-O3A-PA-O5'

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Mol	Chain	Res	Type	Atoms
81	1T	101	EHZ	N2-C15-C16-O5
81	5T	101	EHZ	N2-C15-C16-O5
83	1o	201	MYR	O1-C1-C2-C3
83	5o	201	MYR	O1-C1-C2-C3
84	3C	501	HEM	C2B-C3B-CAB-CBB
84	3C	502	HEM	C2B-C3B-CAB-CBB
84	3C	502	HEM	C2C-C3C-CAC-CBC
84	3P	501	HEM	C2B-C3B-CAB-CBB
84	3P	502	HEM	C2B-C3B-CAB-CBB
84	3P	502	HEM	C2C-C3C-CAC-CBC
86	4A	601	PGV	O04-C19-O03-C01
86	4A	601	PGV	C20-C19-O03-C01
86	4A	602	PGV	C02-C03-O11-P
86	4C	302	PGV	C05-C04-O12-P
86	4C	302	PGV	O02-C1-O01-C02
86	4C	302	PGV	C2-C1-O01-C02
86	4C	303	PGV	O04-C19-O03-C01
86	4C	303	PGV	C20-C19-O03-C01
86	4C	304	PGV	C03-O11-P-O13
86	4C	305	PGV	O02-C1-O01-C02
86	4C	305	PGV	C2-C1-O01-C02
86	4G	101	PGV	O02-C1-O01-C02
86	4G	101	PGV	C2-C1-O01-C02
86	4G	101	PGV	O04-C19-O03-C01
86	4G	101	PGV	C20-C19-O03-C01
86	4K	101	PGV	O04-C19-O03-C01
86	4K	101	PGV	C20-C19-O03-C01
86	8A	601	PGV	O04-C19-O03-C01
86	8A	601	PGV	C20-C19-O03-C01
86	8A	602	PGV	C02-C03-O11-P
86	8C	302	PGV	C05-C04-O12-P
86	8C	302	PGV	O02-C1-O01-C02
86	8C	302	PGV	C2-C1-O01-C02
86	8C	303	PGV	O04-C19-O03-C01
86	8C	303	PGV	C20-C19-O03-C01
86	8C	304	PGV	C03-O11-P-O13
86	8C	305	PGV	O02-C1-O01-C02
86	8C	305	PGV	C2-C1-O01-C02
86	8G	101	PGV	O02-C1-O01-C02
86	8G	101	PGV	C2-C1-O01-C02
86	8G	101	PGV	O04-C19-O03-C01
86	8G	101	PGV	C20-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
86	8K	101	PGV	C03-O11-P-O12
86	8K	101	PGV	C03-O11-P-O14
86	8K	101	PGV	O04-C19-O03-C01
86	8K	101	PGV	C20-C19-O03-C01
87	8A	603	HEA	C3B-C11-C12-C13
87	8A	603	HEA	O11-C11-C12-C13
90	4A	609	PSC	C03-O11-P-O12
90	4A	609	PSC	C03-O11-P-O13
90	4A	609	PSC	O02-C1-O01-C02
90	4A	609	PSC	C2-C1-O01-C02
90	8I	101	PSC	C03-O11-P-O12
90	8I	101	PSC	C03-O11-P-O13
90	8I	101	PSC	O02-C1-O01-C02
90	8I	101	PSC	C2-C1-O01-C02
81	1T	101	EHZ	C13-C12-N1-C11
81	5T	101	EHZ	C13-C12-N1-C11
74	1N	401	CDL	C51-CB5-OB6-CB4
74	5N	401	CDL	C51-CB5-OB6-CB4
74	4D	201	CDL	O1-C1-CB2-OB2
74	8C	306	CDL	O1-C1-CA2-OA2
74	8D	201	CDL	O1-C1-CB2-OB2
74	1N	401	CDL	OB7-CB5-OB6-CB4
74	5N	401	CDL	OB7-CB5-OB6-CB4
85	3D	501	HEC	C3D-CAD-CBD-CGD
87	8A	603	HEA	C19-C20-C21-C22
69	1L	704	PC1	C2-C1-O11-P
69	5L	705	PC1	C2-C1-O11-P
76	1Y	801	3PE	C2-C1-O11-P
76	3Y	101	3PE	C2-C1-O11-P
90	8I	101	PSC	C02-C03-O11-P
81	1T	101	EHZ	O3-C12-N1-C11
81	5T	101	EHZ	O3-C12-N1-C11
74	8C	306	CDL	CB2-C1-CA2-OA2
74	5X	201	CDL	CA7-C31-C32-C33
74	4C	306	CDL	O1-C1-CA2-OA2
76	1O	401	3PE	C31-C32-C33-C34
74	5N	401	CDL	OA6-CA4-CA6-OA8
86	8J	101	PGV	C19-C20-C21-C22
86	4C	307	PGV	C02-C03-O11-P
90	4A	609	PSC	C02-C03-O11-P
86	8B	302	PGV	C1-C2-C3-C4
69	1L	704	PC1	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
76	1Y	806	3PE	C31-C32-C33-C34
76	3C	504	3PE	C21-C22-C23-C24
69	5q	201	PC1	C31-C32-C33-C34
76	3Q	502	3PE	C21-C22-C23-C24
79	1P	501	NDP	O4D-C1D-N1N-C6N
74	5N	401	CDL	O1-C1-CB2-OB2
69	1h	203	PC1	C2-C1-O11-P
69	5h	203	PC1	C2-C1-O11-P
72	5F	501	FMN	C4'-C5'-O5'-P
74	5N	401	CDL	C1-CA2-OA2-PA1
76	3C	505	3PE	C2-C1-O11-P
86	8C	307	PGV	C02-C03-O11-P
69	5L	705	PC1	C24-C25-C26-C27
74	1N	401	CDL	OA6-CA4-CA6-OA8
76	1M	901	3PE	C32-C33-C34-C35
76	5d	201	3PE	C3C-C3D-C3E-C3F
86	4A	603	PGV	C22-C23-C24-C25
86	4J	101	PGV	C19-C20-C21-C22
76	5Y	806	3PE	C31-C32-C33-C34
74	8B	303	CDL	C59-C60-C61-C62
76	5L	703	3PE	C39-C3A-C3B-C3C
86	8B	301	PGV	C22-C23-C24-C25
74	5d	203	CDL	C32-C33-C34-C35
76	3Q	502	3PE	C35-C36-C37-C38
74	4C	306	CDL	CB2-C1-CA2-OA2
74	1d	203	CDL	CA5-C11-C12-C13
74	5d	203	CDL	CA5-C11-C12-C13
76	1M	902	3PE	C21-C22-C23-C24
76	1L	703	3PE	C39-C3A-C3B-C3C
76	5Y	803	3PE	C23-C24-C25-C26
69	1q	201	PC1	C2A-C2B-C2C-C2D
74	1q	202	CDL	C16-C17-C18-C19
74	4B	302	CDL	C59-C60-C61-C62
74	1d	203	CDL	C32-C33-C34-C35
76	5L	704	3PE	C32-C33-C34-C35
69	5M	505	PC1	C23-C24-C25-C26
76	3Q	502	3PE	C27-C28-C29-C2A
86	4C	302	PGV	C26-C27-C28-C29
76	5M	504	3PE	C31-C32-C33-C34
74	8C	306	CDL	C79-C80-C81-C82
76	3A	503	3PE	C32-C33-C34-C35
69	1q	201	PC1	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
74	5h	202	CDL	C60-C61-C62-C63
76	1Y	803	3PE	C23-C24-C25-C26
69	5q	201	PC1	C2A-C2B-C2C-C2D
86	8C	302	PGV	C28-C29-C30-C31
86	4B	301	PGV	C1-C2-C3-C4
74	4C	306	CDL	C79-C80-C81-C82
74	1h	202	CDL	C60-C61-C62-C63
74	5q	203	CDL	C16-C17-C18-C19
69	1h	203	PC1	C2B-C2C-C2D-C2E
86	4C	302	PGV	C27-C28-C29-C30
76	1b	201	3PE	C36-C37-C38-C39
84	3C	501	HEM	C4B-C3B-CAB-CBB
84	3C	502	HEM	C4B-C3B-CAB-CBB
84	3C	502	HEM	C4C-C3C-CAC-CBC
84	3P	501	HEM	C4B-C3B-CAB-CBB
84	3P	502	HEM	C4B-C3B-CAB-CBB
84	3P	502	HEM	C4C-C3C-CAC-CBC
76	5Y	802	3PE	C22-C23-C24-C25
76	1Y	802	3PE	C22-C23-C24-C25
86	4C	302	PGV	C7-C8-C9-C10
76	1M	903	3PE	C22-C23-C24-C25
74	5X	201	CDL	C61-C62-C63-C64
76	5M	502	3PE	C3B-C3C-C3D-C3E
79	5P	402	NDP	O4D-C1D-N1N-C6N
72	1F	501	FMN	C4'-C5'-O5'-P
74	1N	401	CDL	C1-CA2-OA2-PA1
76	3N	501	3PE	C2-C1-O11-P
87	8A	604	HEA	C2A-CAA-CBA-CGA
76	1M	906	3PE	C23-C24-C25-C26
74	5L	702	CDL	C58-C59-C60-C61
76	5M	502	3PE	C22-C23-C24-C25
76	3D	502	3PE	C31-C32-C33-C34
86	4B	301	PGV	C24-C25-C26-C27
69	1M	905	PC1	C32-C33-C34-C35
86	4L	101	PGV	C6-C7-C8-C9
69	5M	505	PC1	C32-C33-C34-C35
74	5d	203	CDL	C42-C43-C44-C45
76	1M	903	3PE	C3B-C3C-C3D-C3E
86	4K	101	PGV	C2-C3-C4-C5
81	1T	101	EHZ	O4-C15-C16-O5
81	5T	101	EHZ	O4-C15-C16-O5
76	5L	704	3PE	C2E-C2F-C2G-C2H

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Mol	Chain	Res	Type	Atoms
74	1d	203	CDL	OA5-CA3-CA4-CA6
74	5d	203	CDL	OA5-CA3-CA4-CA6
76	1M	901	3PE	C2E-C2F-C2G-C2H
86	4K	101	PGV	C22-C23-C24-C25
76	5M	504	3PE	C38-C39-C3A-C3B
76	1L	703	3PE	C33-C34-C35-C36
76	3Y	101	3PE	C31-C32-C33-C34
74	5N	401	CDL	C12-C13-C14-C15
69	1h	203	PC1	C32-C33-C34-C35
74	1X	201	CDL	C36-C37-C38-C39
74	1L	702	CDL	CA3-CA4-CA6-OA8
74	5L	702	CDL	CA3-CA4-CA6-OA8
74	8B	303	CDL	CB3-CB4-CB6-OB8
76	1L	703	3PE	C1-C2-C3-O31
76	1Y	803	3PE	C1-C2-C3-O31
76	5L	703	3PE	C1-C2-C3-O31
76	5M	501	3PE	C1-C2-C3-O31
76	5Y	801	3PE	C1-C2-C3-O31
76	5Y	803	3PE	C1-C2-C3-O31
86	4J	101	PGV	O03-C01-C02-C03
86	4J	101	PGV	C21-C22-C23-C24
74	1L	702	CDL	C33-C34-C35-C36
74	4C	306	CDL	C36-C37-C38-C39
86	8L	101	PGV	C6-C7-C8-C9
74	5L	702	CDL	O1-C1-CB2-OB2
74	1N	401	CDL	C12-C13-C14-C15
74	8C	306	CDL	C36-C37-C38-C39
76	5A	201	3PE	C36-C37-C38-C39
74	5L	702	CDL	C37-C38-C39-C40
69	1B	203	PC1	C28-C29-C2A-C2B
74	1d	203	CDL	C1-CA2-OA2-PA1
76	5L	704	3PE	C2-C1-O11-P
76	1M	903	3PE	C34-C35-C36-C37
76	5L	703	3PE	C33-C34-C35-C36
76	1M	906	3PE	C27-C28-C29-C2A
76	1M	902	3PE	C26-C27-C28-C29
86	4C	303	PGV	C5-C6-C7-C8
87	8A	603	HEA	C2A-C3A-CMA-OMA
87	4A	604	HEA	C4D-C3D-CAD-CBD
74	5N	401	CDL	CA2-C1-CB2-OB2
69	1I	201	PC1	O11-C1-C2-O21
69	5I	201	PC1	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
74	1L	702	CDL	OA5-CA3-CA4-OA6
74	3T	101	CDL	OA5-CA3-CA4-OA6
74	5L	702	CDL	OA5-CA3-CA4-OA6
90	8I	101	PSC	C25-C26-C27-C28
92	4C	308	PEK	C21-C22-C23-C24
92	8C	308	PEK	C21-C22-C23-C24
76	5M	502	3PE	C34-C35-C36-C37
69	1d	202	PC1	C37-C38-C39-C3A
76	1O	401	3PE	C38-C39-C3A-C3B
76	5M	506	3PE	C25-C26-C27-C28
74	1h	202	CDL	C34-C35-C36-C37
74	5L	702	CDL	C33-C34-C35-C36
86	8C	302	PGV	C7-C8-C9-C10
69	1M	905	PC1	O21-C2-C3-O31
74	8B	303	CDL	OB6-CB4-CB6-OB8
74	1N	401	CDL	O1-C1-CB2-OB2
86	8B	302	PGV	C24-C25-C26-C27
90	4A	609	PSC	C25-C26-C27-C28
69	5h	203	PC1	C32-C33-C34-C35
74	1X	201	CDL	C61-C62-C63-C64
74	3C	503	CDL	C72-C71-CB7-OB8
69	1M	905	PC1	C2A-C2B-C2C-C2D
69	5B	203	PC1	C28-C29-C2A-C2B
86	8L	101	PGV	C21-C22-C23-C24
74	1d	203	CDL	C71-C72-C73-C74
74	4B	302	CDL	C1-CA2-OA2-PA1
74	5d	203	CDL	C1-CA2-OA2-PA1
74	8B	303	CDL	C1-CA2-OA2-PA1
76	1M	901	3PE	C2-C1-O11-P
86	4C	305	PGV	C02-C03-O11-P
86	4K	101	PGV	C02-C03-O11-P
86	8C	305	PGV	C02-C03-O11-P
86	8K	101	PGV	C02-C03-O11-P
86	8K	101	PGV	C05-C04-O12-P
74	3P	504	CDL	C31-C32-C33-C34
76	3N	501	3PE	O21-C21-C22-C23
76	1Y	801	3PE	C33-C34-C35-C36
74	4C	306	CDL	C75-C76-C77-C78
69	1M	905	PC1	O11-C1-C2-C3
74	1L	702	CDL	OA5-CA3-CA4-CA6
74	3T	101	CDL	OA5-CA3-CA4-CA6
74	5L	702	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
76	1M	901	3PE	O11-C1-C2-C3
76	1O	401	3PE	O11-C1-C2-C3
76	1Y	803	3PE	O31-C31-C32-C33
76	5Y	803	3PE	O31-C31-C32-C33
74	1L	702	CDL	C37-C38-C39-C40
74	1N	401	CDL	C32-C31-CA7-OA8
69	5d	202	PC1	C37-C38-C39-C3A
76	1M	906	3PE	C21-C22-C23-C24
74	8D	201	CDL	C59-C60-C61-C62
74	8C	306	CDL	C75-C76-C77-C78
76	5M	506	3PE	C21-C22-C23-C24
86	4C	302	PGV	C1-C2-C3-C4
74	5h	202	CDL	C34-C35-C36-C37
74	8D	201	CDL	CA2-C1-CB2-OB2
74	1N	401	CDL	CA3-CA4-CA6-OA8
74	4B	302	CDL	CB3-CB4-CB6-OB8
76	1M	902	3PE	C1-C2-C3-O31
76	1M	903	3PE	C1-C2-C3-O31
76	3C	505	3PE	C1-C2-C3-O31
76	3P	503	3PE	C1-C2-C3-O31
76	5M	502	3PE	C1-C2-C3-O31
86	8J	101	PGV	O03-C01-C02-C03
86	8L	101	PGV	C3-C4-C5-C6
76	5M	501	3PE	C21-C22-C23-C24
76	5M	506	3PE	C27-C28-C29-C2A
74	4D	201	CDL	C59-C60-C61-C62
74	5d	203	CDL	C71-C72-C73-C74
76	5M	501	3PE	C26-C27-C28-C29
74	4D	201	CDL	C62-C63-C64-C65
86	8A	601	PGV	C21-C22-C23-C24
69	5M	505	PC1	C2A-C2B-C2C-C2D
74	1d	203	CDL	OA5-CA3-CA4-OA6
76	3A	502	3PE	O11-C1-C2-O21
86	8C	303	PGV	O01-C02-C03-O11
69	1H	402	PC1	C39-C3A-C3B-C3C
76	1d	201	3PE	C28-C29-C2A-C2B
69	5H	402	PC1	C39-C3A-C3B-C3C
74	5q	203	CDL	C52-C51-CB5-OB6
86	4K	101	PGV	C05-C04-O12-P
86	8C	304	PGV	C02-C03-O11-P
92	8G	102	PEK	C21-C22-C23-C24
81	1n	201	EHZ	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
82	1h	201	AME	C-CA-N-CT1
84	3P	501	HEM	C3D-CAD-CBD-CGD
86	4L	101	PGV	C3-C4-C5-C6
76	3C	504	3PE	C29-C2A-C2B-C2C
74	3N	502	CDL	OA6-CA4-CA6-OA8
74	3P	504	CDL	OB6-CB4-CB6-OB8
76	1M	901	3PE	O21-C2-C3-O31
76	1Y	803	3PE	O21-C2-C3-O31
76	5L	704	3PE	O21-C2-C3-O31
76	5M	502	3PE	O21-C2-C3-O31
76	5Y	803	3PE	O21-C2-C3-O31
86	4C	304	PGV	O03-C01-C02-O01
86	8C	304	PGV	O03-C01-C02-O01
90	4A	609	PSC	C9-C10-C11-C12
90	4A	609	PSC	C10-C11-C12-C13
90	8I	101	PSC	C9-C10-C11-C12
90	8I	101	PSC	C10-C11-C12-C13
92	4G	102	PEK	C5-C6-C7-C8
92	4G	102	PEK	C9-C10-C11-C12
92	8G	102	PEK	C5-C6-C7-C8
92	8G	102	PEK	C9-C10-C11-C12
74	1X	201	CDL	C23-C24-C25-C26
69	1M	905	PC1	C23-C24-C25-C26
74	1X	201	CDL	C58-C59-C60-C61
86	8C	303	PGV	C5-C6-C7-C8
77	1O	402	GTP	PB-O3A-PA-O5'
76	1Y	801	3PE	C32-C33-C34-C35
74	5X	201	CDL	C32-C31-CA7-OA8
86	4A	602	PGV	C14-C15-C16-C17
74	1L	702	CDL	C58-C59-C60-C61
86	8B	302	PGV	C20-C21-C22-C23
74	1q	202	CDL	C52-C51-CB5-OB6
74	3C	503	CDL	C12-C11-CA5-OA6
74	5N	401	CDL	C32-C31-CA7-OA8
76	1b	201	3PE	O21-C21-C22-C23
76	3G	101	3PE	O21-C21-C22-C23
76	5A	201	3PE	O21-C21-C22-C23
74	8C	306	CDL	C59-C60-C61-C62
74	3P	504	CDL	C13-C14-C15-C16
74	4D	201	CDL	CA2-C1-CB2-OB2
69	5B	202	PC1	C36-C37-C38-C39
92	4G	102	PEK	O03-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
69	5I	201	PC1	O11-C1-C2-C3
74	3P	504	CDL	OB5-CB3-CB4-CB6
74	8B	303	CDL	OA5-CA3-CA4-CA6
76	5L	704	3PE	O11-C1-C2-C3
76	5M	504	3PE	O11-C1-C2-C3
74	5d	203	CDL	C1-CB2-OB2-PB2
69	5I	204	PC1	C37-C38-C39-C3A
87	4A	604	HEA	C2D-C3D-CAD-CBD
69	5h	203	PC1	C2B-C2C-C2D-C2E
74	4C	306	CDL	C59-C60-C61-C62
84	3C	501	HEM	C3D-CAD-CBD-CGD
74	1L	702	CDL	CA7-C31-C32-C33
76	1P	502	3PE	C37-C38-C39-C3A
69	5h	203	PC1	C2A-C2B-C2C-C2D
84	3C	501	HEM	C2C-C3C-CAC-CBC
84	3P	501	HEM	C2C-C3C-CAC-CBC
86	4C	304	PGV	C5-C6-C7-C8
92	8G	102	PEK	O03-C21-C22-C23
74	1h	202	CDL	C76-C77-C78-C79
82	1h	201	AME	CB-CA-N-CT1
69	5A	202	PC1	C22-C23-C24-C25
69	1M	905	PC1	O11-C1-C2-O21
74	1X	201	CDL	OB5-CB3-CB4-OB6
74	3P	504	CDL	OB5-CB3-CB4-OB6
74	8B	303	CDL	OA5-CA3-CA4-OA6
76	1Y	802	3PE	O11-C1-C2-O21
76	5L	704	3PE	O11-C1-C2-O21
76	5Y	802	3PE	O11-C1-C2-O21
76	5Y	806	3PE	O11-C1-C2-O21
86	4C	303	PGV	O01-C02-C03-O11
69	1B	203	PC1	C35-C36-C37-C38
81	5T	101	EHZ	C21-C22-C23-C24
86	4L	101	PGV	C21-C22-C23-C24
69	1B	203	PC1	C1-C2-C3-O31
69	1h	203	PC1	C1-C2-C3-O31
69	5B	203	PC1	C1-C2-C3-O31
74	3P	504	CDL	CB3-CB4-CB6-OB8
74	5N	401	CDL	CA3-CA4-CA6-OA8
76	3N	501	3PE	C1-C2-C3-O31
76	3N	503	3PE	C1-C2-C3-O31
87	4A	604	HEA	O11-C11-C12-C13
74	8C	306	CDL	C52-C53-C54-C55

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Mol	Chain	Res	Type	Atoms
69	1A	202	PC1	C12-C11-O13-P
69	1A	203	PC1	C12-C11-O13-P
69	1B	203	PC1	C12-C11-O13-P
69	5A	203	PC1	C12-C11-O13-P
69	5B	203	PC1	C12-C11-O13-P
69	5P	401	PC1	C12-C11-O13-P
76	1K	101	3PE	C12-C11-O13-P
76	1L	701	3PE	C12-C11-O13-P
76	1O	401	3PE	C12-C11-O13-P
76	1Y	802	3PE	C12-C11-O13-P
76	1Y	804	3PE	C12-C11-O13-P
76	1Y	805	3PE	C12-C11-O13-P
76	1Y	806	3PE	C12-C11-O13-P
76	1j	101	3PE	C12-C11-O13-P
76	3C	504	3PE	C12-C11-O13-P
76	3C	505	3PE	C12-C11-O13-P
76	3P	503	3PE	C12-C11-O13-P
76	5K	101	3PE	C12-C11-O13-P
76	5L	701	3PE	C12-C11-O13-P
76	5M	504	3PE	C12-C11-O13-P
76	5Y	802	3PE	C12-C11-O13-P
76	5Y	804	3PE	C12-C11-O13-P
76	5j	101	3PE	C12-C11-O13-P
92	4C	308	PEK	C05-C04-O12-P
92	4G	102	PEK	C05-C04-O12-P
92	8C	308	PEK	C05-C04-O12-P
92	8G	102	PEK	C05-C04-O12-P
69	5B	203	PC1	O21-C2-C3-O31
74	4B	302	CDL	OB6-CB4-CB6-OB8
76	1M	902	3PE	O21-C2-C3-O31
76	1M	903	3PE	O21-C2-C3-O31
76	5M	501	3PE	O21-C2-C3-O31
76	5Y	801	3PE	O21-C2-C3-O31
86	8C	302	PGV	C6-C7-C8-C9
74	5X	201	CDL	C58-C59-C60-C61
74	5L	702	CDL	CA7-C31-C32-C33
92	4G	102	PEK	C21-C22-C23-C24
69	5B	203	PC1	C35-C36-C37-C38
74	4C	306	CDL	C16-C17-C18-C19
74	1h	202	CDL	CB4-CB3-OB5-PB2
76	5Y	803	3PE	C2-C1-O11-P
69	1A	201	PC1	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
69	1A	203	PC1	O13-C11-C12-N
69	1B	203	PC1	O13-C11-C12-N
69	1L	704	PC1	O13-C11-C12-N
69	1h	203	PC1	O13-C11-C12-N
69	5A	202	PC1	O13-C11-C12-N
69	5B	203	PC1	O13-C11-C12-N
69	5L	705	PC1	O13-C11-C12-N
69	5P	401	PC1	O13-C11-C12-N
69	5h	203	PC1	O13-C11-C12-N
74	1L	702	CDL	C57-C58-C59-C60
74	1N	401	CDL	CA2-C1-CB2-OB2
74	1L	702	CDL	O1-C1-CB2-OB2
74	4D	201	CDL	C71-C72-C73-C74
74	4C	306	CDL	C52-C53-C54-C55
74	5X	201	CDL	C23-C24-C25-C26
86	4C	304	PGV	C24-C25-C26-C27
74	5L	702	CDL	C57-C58-C59-C60
74	8D	201	CDL	C71-C72-C73-C74
76	5M	502	3PE	C24-C25-C26-C27
76	1M	903	3PE	C24-C25-C26-C27
69	1I	204	PC1	C37-C38-C39-C3A
74	8C	306	CDL	C16-C17-C18-C19
86	8C	304	PGV	C24-C25-C26-C27
69	1I	201	PC1	O11-C1-C2-C3
69	5M	505	PC1	O11-C1-C2-C3
74	4B	302	CDL	OA5-CA3-CA4-CA6
76	3A	503	3PE	O11-C1-C2-C3
76	5Y	801	3PE	O11-C1-C2-C3
86	4A	601	PGV	C01-C02-C03-O11
86	8A	601	PGV	C01-C02-C03-O11
86	8C	304	PGV	C5-C6-C7-C8
74	8B	303	CDL	C38-C39-C40-C41
86	8C	303	PGV	C9-C10-C11-C12
86	4C	302	PGV	C3-C4-C5-C6
90	8I	101	PSC	C19-C20-C21-C22
69	1M	905	PC1	C2-C1-O11-P
74	1N	401	CDL	C1-CB2-OB2-PB2
74	5N	401	CDL	C1-CB2-OB2-PB2
74	5h	202	CDL	CB4-CB3-OB5-PB2
86	4G	101	PGV	C02-C03-O11-P
74	1X	201	CDL	C35-C36-C37-C38
74	4C	306	CDL	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
81	1n	201	EHZ	C11-C10-S1-C9
81	5n	201	EHZ	C11-C10-S1-C9
86	8K	101	PGV	C2-C3-C4-C5
69	5M	505	PC1	O11-C1-C2-O21
74	4B	302	CDL	OA5-CA3-CA4-OA6
74	5d	203	CDL	OA5-CA3-CA4-OA6
76	1M	901	3PE	O11-C1-C2-O21
86	4A	601	PGV	O01-C02-C03-O11
86	8A	601	PGV	O01-C02-C03-O11
86	8K	101	PGV	C22-C23-C24-C25
74	4C	306	CDL	C11-C12-C13-C14
87	8A	603	HEA	C4A-C3A-CMA-OMA
74	4B	302	CDL	C38-C39-C40-C41
74	3G	102	CDL	C52-C53-C54-C55
69	1B	203	PC1	O21-C2-C3-O31
76	1L	703	3PE	O21-C2-C3-O31
76	3N	501	3PE	O21-C2-C3-O31
76	3N	503	3PE	O21-C2-C3-O31
76	5L	703	3PE	O21-C2-C3-O31
86	4J	101	PGV	O03-C01-C02-O01
86	8J	101	PGV	O03-C01-C02-O01
92	4C	308	PEK	O03-C01-C02-O01
69	1A	201	PC1	C1-C2-C3-O31
69	5I	201	PC1	C1-C2-C3-O31
81	1T	101	EHZ	C10-C11-N1-C12
81	1n	201	EHZ	C10-C11-N1-C12
81	5T	101	EHZ	C10-C11-N1-C12
74	5h	202	CDL	C76-C77-C78-C79
86	8L	101	PGV	C9-C10-C11-C12
74	1X	201	CDL	C55-C56-C57-C58
86	4C	302	PGV	C6-C7-C8-C9
74	8C	306	CDL	C51-C52-C53-C54
69	1A	202	PC1	C1-O11-P-O14
69	1B	202	PC1	C11-O13-P-O14
69	1M	904	PC1	C11-O13-P-O11
69	1M	904	PC1	C1-O11-P-O14
69	1d	202	PC1	C1-O11-P-O14
69	5A	203	PC1	C1-O11-P-O14
69	5B	202	PC1	C11-O13-P-O14
69	5I	204	PC1	C1-O11-P-O13
69	5M	503	PC1	C1-O11-P-O14
69	5d	202	PC1	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
74	1N	401	CDL	CA3-OA5-PA1-OA3
74	1X	201	CDL	CB2-OB2-PB2-OB3
74	1h	202	CDL	CB2-OB2-PB2-OB4
74	3C	503	CDL	CB2-OB2-PB2-OB4
74	3G	102	CDL	CA2-OA2-PA1-OA3
74	3G	102	CDL	CB2-OB2-PB2-OB4
74	3G	102	CDL	CB2-OB2-PB2-OB5
74	3G	102	CDL	CB3-OB5-PB2-OB3
74	3N	502	CDL	CB3-OB5-PB2-OB3
74	3P	504	CDL	CA3-OA5-PA1-OA3
74	4B	302	CDL	CB3-OB5-PB2-OB4
74	4D	201	CDL	CB2-OB2-PB2-OB3
74	5N	401	CDL	CA3-OA5-PA1-OA3
74	5X	201	CDL	CB2-OB2-PB2-OB3
74	8B	303	CDL	CB3-OB5-PB2-OB4
74	8D	201	CDL	CB2-OB2-PB2-OB3
76	1K	101	3PE	C1-O11-P-O12
76	1K	101	3PE	C11-O13-P-O14
76	1M	902	3PE	C11-O13-P-O14
76	1M	906	3PE	C11-O13-P-O14
76	1Y	801	3PE	C11-O13-P-O14
76	1Y	802	3PE	C11-O13-P-O14
76	1Y	804	3PE	C1-O11-P-O14
76	1Y	806	3PE	C11-O13-P-O14
76	1b	201	3PE	C11-O13-P-O11
76	1j	101	3PE	C1-O11-P-O14
76	1j	101	3PE	C11-O13-P-O14
76	3C	504	3PE	C1-O11-P-O14
76	3N	501	3PE	C1-O11-P-O13
76	3N	501	3PE	C11-O13-P-O14
76	3N	503	3PE	C11-O13-P-O14
76	5A	201	3PE	C11-O13-P-O11
76	5K	101	3PE	C1-O11-P-O12
76	5K	101	3PE	C11-O13-P-O14
76	5M	501	3PE	C11-O13-P-O14
76	5M	502	3PE	C1-O11-P-O14
76	5M	506	3PE	C11-O13-P-O14
76	5Y	801	3PE	C11-O13-P-O14
76	5Y	802	3PE	C11-O13-P-O14
76	5Y	804	3PE	C1-O11-P-O14
76	5Y	806	3PE	C11-O13-P-O14
77	1O	402	GTP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
86	4A	601	PGV	C04-O12-P-O13
86	4C	304	PGV	C03-O11-P-O12
86	4C	304	PGV	C03-O11-P-O14
86	4G	101	PGV	C04-O12-P-O13
86	4K	101	PGV	C04-O12-P-O13
86	8A	601	PGV	C04-O12-P-O13
86	8B	301	PGV	C04-O12-P-O13
86	8C	303	PGV	C03-O11-P-O14
86	8C	304	PGV	C03-O11-P-O12
86	8C	304	PGV	C03-O11-P-O14
86	8C	305	PGV	C03-O11-P-O14
86	8G	101	PGV	C04-O12-P-O13
86	8K	101	PGV	C04-O12-P-O13
81	1T	101	EHZ	C21-C22-C23-C24
69	5B	202	PC1	C3D-C3E-C3F-C3G
69	1I	201	PC1	C2-C1-O11-P
69	5M	505	PC1	C2-C1-O11-P
74	1d	203	CDL	C1-CB2-OB2-PB2
74	3T	101	CDL	CA4-CA3-OA5-PA1
74	5L	702	CDL	CA4-CA3-OA5-PA1
76	1Y	803	3PE	C2-C1-O11-P
86	4A	601	PGV	C02-C03-O11-P
86	4C	304	PGV	C02-C03-O11-P
86	8A	601	PGV	C02-C03-O11-P
86	8G	101	PGV	C02-C03-O11-P
76	1M	906	3PE	C28-C29-C2A-C2B
86	4C	303	PGV	C9-C10-C11-C12
86	4L	101	PGV	C9-C10-C11-C12
86	8C	305	PGV	C9-C10-C11-C12
90	8I	101	PSC	C12-C13-C14-C15
69	1M	905	PC1	C21-C22-C23-C24
74	1H	401	CDL	CA3-CA4-OA6-CA5
74	5H	401	CDL	CA3-CA4-OA6-CA5
74	5X	201	CDL	C35-C36-C37-C38
69	1L	704	PC1	O31-C31-C32-C33
74	8C	306	CDL	C11-C12-C13-C14
69	5H	402	PC1	O11-C1-C2-C3
74	8C	306	CDL	OB5-CB3-CB4-CB6
76	5A	201	3PE	C2A-C2B-C2C-C2D
76	1M	901	3PE	C33-C34-C35-C36
86	4M	101	PGV	C11-C12-C13-C14
86	8M	101	PGV	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
90	4A	609	PSC	C12-C13-C14-C15
76	5Y	802	3PE	C27-C28-C29-C2A
76	1O	401	3PE	O11-C1-C2-O21
76	5M	504	3PE	O11-C1-C2-O21
69	5L	705	PC1	O31-C31-C32-C33
69	5L	705	PC1	C23-C24-C25-C26
76	1K	101	3PE	O21-C21-C22-C23
69	1M	905	PC1	C2D-C2E-C2F-C2G
86	8K	101	PGV	C9-C10-C11-C12
69	1L	704	PC1	C3A-C3B-C3C-C3D
69	5I	201	PC1	C2-C1-O11-P
74	1L	702	CDL	CA4-CA3-OA5-PA1
74	8D	201	CDL	C62-C63-C64-C65
86	8C	303	PGV	C26-C27-C28-C29
76	3P	503	3PE	O21-C2-C3-O31
76	5K	101	3PE	O21-C21-C22-C23
87	4A	605	HEA	C2A-CAA-CBA-CGA
76	1Y	806	3PE	O21-C21-C22-C23
76	5Y	806	3PE	O21-C21-C22-C23
69	1M	905	PC1	C1-C2-C3-O31
81	1n	201	EHZ	C7-C8-C9-O2
81	5n	201	EHZ	C7-C8-C9-O2
69	5M	505	PC1	C2D-C2E-C2F-C2G
86	4K	101	PGV	C9-C10-C11-C12
86	8M	101	PGV	C11-C12-C13-C14
86	8C	302	PGV	C1-C2-C3-C4
86	4A	601	PGV	C29-C30-C31-C32
74	5X	201	CDL	CB2-C1-CA2-OA2
87	4A	604	HEA	C4C-C3C-CAC-CBC
76	5M	504	3PE	C24-C25-C26-C27
74	5X	201	CDL	OB5-CB3-CB4-OB6
76	1Y	806	3PE	O11-C1-C2-O21
86	4C	305	PGV	C9-C10-C11-C12
86	4M	101	PGV	C9-C10-C11-C12
86	8C	304	PGV	C9-C10-C11-C12
74	1X	201	CDL	C31-C32-C33-C34
76	5d	201	3PE	C28-C29-C2A-C2B
84	3C	501	HEM	C4C-C3C-CAC-CBC
69	5I	204	PC1	C24-C25-C26-C27
76	1M	901	3PE	C23-C24-C25-C26
86	4C	301	PGV	C11-C12-C13-C14
69	1h	203	PC1	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
74	3G	102	CDL	OB6-CB4-CB6-OB8
74	5q	203	CDL	OB6-CB4-CB6-OB8
76	1Y	802	3PE	C27-C28-C29-C2A
86	4B	301	PGV	C20-C21-C22-C23
74	3C	503	CDL	C11-C12-C13-C14
69	1A	201	PC1	C23-C24-C25-C26
74	1X	201	CDL	C34-C35-C36-C37
86	4M	101	PGV	C3-C4-C5-C6
76	5M	501	3PE	C25-C26-C27-C28
92	4C	308	PEK	C02-C03-O11-P
84	3P	501	HEM	CAA-CBA-CGA-O2A
87	4A	605	HEA	CAD-CBD-CGD-O1D
87	8A	603	HEA	CAD-CBD-CGD-O1D
69	5L	705	PC1	C3A-C3B-C3C-C3D
69	1B	202	PC1	C36-C37-C38-C39
69	3X	101	PC1	O21-C21-C22-C23
76	1L	703	3PE	C29-C2A-C2B-C2C
76	1M	902	3PE	C23-C24-C25-C26
86	4B	301	PGV	C27-C28-C29-C30
84	3C	501	HEM	CAA-CBA-CGA-O2A
87	8A	604	HEA	CAD-CBD-CGD-O1D
86	8M	101	PGV	C3-C4-C5-C6
74	1N	401	CDL	CB3-CB4-CB6-OB8
76	1M	901	3PE	C1-C2-C3-O31
76	5j	101	3PE	C1-C2-C3-O31
81	5n	201	EHZ	C10-C11-N1-C12
86	4C	302	PGV	C11-C12-C13-C14
86	8J	101	PGV	C9-C10-C11-C12
74	4B	302	CDL	C13-C14-C15-C16
69	1A	203	PC1	C24-C25-C26-C27
69	5M	503	PC1	C22-C23-C24-C25
86	8A	601	PGV	C22-C23-C24-C25
86	8B	302	PGV	C27-C28-C29-C30
84	3C	501	HEM	CAA-CBA-CGA-O1A
86	4A	603	PGV	C1-C2-C3-C4
74	5X	201	CDL	C36-C37-C38-C39
76	1Y	806	3PE	C23-C24-C25-C26
84	3P	501	HEM	CAD-CBD-CGD-O1D
76	1O	401	3PE	C1-C2-O21-C21
76	1Y	804	3PE	C1-C2-O21-C21
76	3C	504	3PE	C1-C2-O21-C21
76	5M	504	3PE	C1-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
76	5Y	805	3PE	C3-C2-O21-C21
86	4C	304	PGV	C01-C02-O01-C1
87	4A	605	HEA	CAD-CBD-CGD-O2D
76	5K	101	3PE	C26-C27-C28-C29
74	1h	202	CDL	CB7-C71-C72-C73
69	5M	505	PC1	C28-C29-C2A-C2B
76	5Y	804	3PE	C33-C34-C35-C36
87	8A	603	HEA	C4D-C3D-CAD-CBD
74	5d	203	CDL	OB5-CB3-CB4-OB6
74	5h	202	CDL	OB5-CB3-CB4-OB6
76	1K	101	3PE	C26-C27-C28-C29
87	8A	603	HEA	CAD-CBD-CGD-O2D
87	8A	604	HEA	CAD-CBD-CGD-O2D
86	4C	304	PGV	C9-C10-C11-C12
86	8A	602	PGV	C11-C12-C13-C14
76	1O	401	3PE	C24-C25-C26-C27
82	5h	201	AME	C-CA-N-CT1
84	3P	502	HEM	CAD-CBD-CGD-O1D
76	1Y	801	3PE	O11-C1-C2-C3
76	3C	505	3PE	O11-C1-C2-C3
76	3Y	101	3PE	O11-C1-C2-C3
76	3D	502	3PE	C24-C25-C26-C27
86	4A	601	PGV	C11-C12-C13-C14
86	4C	307	PGV	C11-C12-C13-C14
86	4J	101	PGV	C9-C10-C11-C12
86	8C	302	PGV	C9-C10-C11-C12
69	5I	201	PC1	O21-C2-C3-O31
74	1N	401	CDL	OB6-CB4-CB6-OB8
76	3Y	101	3PE	O21-C2-C3-O31
92	8C	308	PEK	O03-C01-C02-O01
79	1P	501	NDP	C2N-C3N-C7N-N7N
79	5P	402	NDP	C2N-C3N-C7N-N7N
86	4K	101	PGV	C19-C20-C21-C22
84	3C	502	HEM	CAA-CBA-CGA-O1A
84	3P	502	HEM	CAA-CBA-CGA-O1A
74	5X	201	CDL	C55-C56-C57-C58
74	8B	303	CDL	C13-C14-C15-C16
87	4A	605	HEA	C26-C15-C16-C17
87	8A	603	HEA	C2D-C3D-CAD-CBD
74	3A	501	CDL	O1-C1-CA2-OA2
90	4A	609	PSC	C19-C20-C21-C22
84	3P	502	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
92	4G	102	PEK	O04-C21-C22-C23
76	1d	201	3PE	C2-C1-O11-P
69	1I	204	PC1	C24-C25-C26-C27
69	1H	402	PC1	C21-C22-C23-C24
69	5h	203	PC1	C1-C2-C3-O31
76	5L	704	3PE	C1-C2-C3-O31
74	3C	503	CDL	C12-C13-C14-C15
76	5L	703	3PE	C29-C2A-C2B-C2C
84	3P	502	HEM	CAA-CBA-CGA-O2A
74	3C	503	CDL	C72-C71-CB7-OB9
76	1M	903	3PE	C2A-C2B-C2C-C2D
84	3C	502	HEM	CAA-CBA-CGA-O2A
84	3P	501	HEM	CAA-CBA-CGA-O1A
74	1d	203	CDL	OB5-CB3-CB4-OB6
74	1h	202	CDL	OB5-CB3-CB4-OB6
76	1Y	805	3PE	O11-C1-C2-O21
76	3A	503	3PE	O11-C1-C2-O21
90	8I	101	PSC	O01-C02-C03-O11
74	1N	401	CDL	C32-C31-CA7-OA9
76	3Q	502	3PE	C34-C35-C36-C37
76	3C	504	3PE	C2C-C2D-C2E-C2F
69	1B	202	PC1	C3D-C3E-C3F-C3G
74	8C	306	CDL	C71-C72-C73-C74
76	5L	704	3PE	C23-C24-C25-C26
86	8A	601	PGV	C11-C12-C13-C14
86	8C	307	PGV	C11-C12-C13-C14
87	8A	603	HEA	C11-C12-C13-C14
76	5P	403	3PE	C36-C37-C38-C39
74	1d	203	CDL	C72-C73-C74-C75
69	1H	402	PC1	O11-C1-C2-C3
74	1X	201	CDL	OB5-CB3-CB4-CB6
74	1h	202	CDL	OB5-CB3-CB4-CB6
74	4C	306	CDL	OB5-CB3-CB4-CB6
74	5h	202	CDL	OB5-CB3-CB4-CB6
76	1Y	802	3PE	O11-C1-C2-C3
76	1Y	806	3PE	O11-C1-C2-C3
76	3A	502	3PE	O11-C1-C2-C3
76	5Y	802	3PE	O11-C1-C2-C3
76	5Y	806	3PE	O11-C1-C2-C3
86	8C	303	PGV	C01-C02-C03-O11
86	8M	101	PGV	C01-C02-C03-O11
87	8A	604	HEA	C26-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
74	4D	201	CDL	OB6-CB4-CB6-OB8
76	3A	502	3PE	O21-C2-C3-O31
76	5Y	805	3PE	O21-C2-C3-O31
86	4G	101	PGV	C1-C2-C3-C4
86	8B	301	PGV	C1-C2-C3-C4
84	3P	501	HEM	CAD-CBD-CGD-O2D
76	5Y	803	3PE	O32-C31-C32-C33
86	8A	601	PGV	C9-C10-C11-C12
86	8C	301	PGV	C11-C12-C13-C14
86	8A	601	PGV	C29-C30-C31-C32
76	5L	701	3PE	C28-C29-C2A-C2B
81	5T	101	EHZ	C1-C21-C22-C23
87	4A	604	HEA	CAD-CBD-CGD-O2D
74	5d	203	CDL	C72-C73-C74-C75
76	5M	506	3PE	C23-C24-C25-C26
76	5K	101	3PE	C24-C25-C26-C27
76	1Y	803	3PE	O32-C31-C32-C33
87	4A	604	HEA	CAD-CBD-CGD-O1D
86	4C	302	PGV	C9-C10-C11-C12
86	4G	101	PGV	C9-C10-C11-C12
86	4K	101	PGV	C11-C12-C13-C14
86	8G	101	PGV	C9-C10-C11-C12
86	4A	601	PGV	C24-C25-C26-C27
86	8A	602	PGV	C6-C7-C8-C9
69	1B	202	PC1	C3C-C3D-C3E-C3F
74	5q	203	CDL	CA5-C11-C12-C13
81	1T	101	EHZ	C1-C21-C22-C23
92	8G	102	PEK	O04-C21-C22-C23
74	4C	306	CDL	C72-C73-C74-C75
74	5X	201	CDL	C31-C32-C33-C34
76	1Y	801	3PE	C1-C2-O21-C21
76	1Y	805	3PE	C3-C2-O21-C21
76	5Y	801	3PE	C1-C2-O21-C21
76	5Y	804	3PE	C1-C2-O21-C21
86	8C	304	PGV	C01-C02-O01-C1
86	8K	101	PGV	C11-C12-C13-C14
86	8L	101	PGV	C11-C12-C13-C14
86	8A	601	PGV	C11-C10-C9-C8
74	5h	202	CDL	C74-C75-C76-C77
76	1Y	804	3PE	C33-C34-C35-C36
69	5I	201	PC1	C36-C37-C38-C39
76	1M	903	3PE	C29-C2A-C2B-C2C

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Mol	Chain	Res	Type	Atoms
86	8C	305	PGV	C7-C8-C9-C10
82	5h	201	AME	CB-CA-N-CT1
76	5d	201	3PE	C2-C1-O11-P
76	1b	201	3PE	C2B-C2C-C2D-C2E
81	5T	101	EHZ	C1-C2-C3-C4
76	5M	501	3PE	C29-C2A-C2B-C2C
69	1I	201	PC1	C1-C2-C3-O31
84	3P	501	HEM	C4C-C3C-CAC-CBC
74	4C	306	CDL	C71-C72-C73-C74
76	1M	902	3PE	C25-C26-C27-C28
76	3N	501	3PE	O22-C21-C22-C23
74	1L	702	CDL	C11-C12-C13-C14
76	5M	502	3PE	C2A-C2B-C2C-C2D
86	4A	602	PGV	C11-C12-C13-C14
69	1M	904	PC1	C22-C23-C24-C25
76	1M	902	3PE	C12-C11-O13-P
76	5Y	806	3PE	C12-C11-O13-P
76	1b	201	3PE	C27-C28-C29-C2A
76	5M	501	3PE	C22-C23-C24-C25
86	8C	303	PGV	C2-C3-C4-C5
76	5K	101	3PE	C34-C35-C36-C37
74	5L	702	CDL	C11-C12-C13-C14
86	4C	302	PGV	C20-C21-C22-C23
74	5X	201	CDL	C32-C31-CA7-OA9
74	1q	202	CDL	OB6-CB4-CB6-OB8
76	1Y	805	3PE	O21-C2-C3-O31
86	4A	601	PGV	C9-C10-C11-C12
76	5M	502	3PE	C29-C2A-C2B-C2C
69	1L	704	PC1	C28-C29-C2A-C2B
74	3C	503	CDL	C12-C11-CA5-OA7
69	1B	203	PC1	O11-C1-C2-C3
69	5B	203	PC1	O11-C1-C2-C3
74	5X	201	CDL	OB5-CB3-CB4-CB6
86	4C	303	PGV	C01-C02-C03-O11
76	5Y	806	3PE	C23-C24-C25-C26
86	8J	101	PGV	C21-C22-C23-C24
86	8G	101	PGV	C27-C28-C29-C30
87	4A	604	HEA	C2C-C3C-CAC-CBC
86	4L	101	PGV	C11-C12-C13-C14
69	1h	203	PC1	C22-C23-C24-C25
86	8C	302	PGV	C3-C4-C5-C6
87	4A	605	HEA	C3B-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
87	8A	604	HEA	C3B-C11-C12-C13
92	8G	102	PEK	C22-C23-C24-C25
76	5Y	802	3PE	C2D-C2E-C2F-C2G
69	1A	201	PC1	C22-C23-C24-C25
86	4C	303	PGV	C2-C3-C4-C5
69	3R	302	PC1	C27-C28-C29-C2A
69	1B	203	PC1	O11-C1-C2-O21
74	3T	101	CDL	OB5-CB3-CB4-OB6
76	3C	504	3PE	O11-C1-C2-O21
76	5Y	801	3PE	O11-C1-C2-O21
87	8A	603	HEA	CAA-CBA-CGA-O2A
86	4A	601	PGV	O03-C19-C20-C21
85	3D	501	HEC	CAA-CBA-CGA-O2A
76	1M	906	3PE	C25-C26-C27-C28
74	5N	401	CDL	C32-C31-CA7-OA9
69	5I	204	PC1	C25-C26-C27-C28
74	5q	203	CDL	C52-C51-CB5-OB7
76	5M	501	3PE	C23-C24-C25-C26
92	8C	308	PEK	C02-C03-O11-P
69	5d	202	PC1	O21-C21-C22-C23
74	5d	203	CDL	C32-C31-CA7-OA8
86	8K	101	PGV	C3-C4-C5-C6
69	5h	203	PC1	C22-C23-C24-C25
86	4G	101	PGV	C7-C8-C9-C10
74	1X	201	CDL	CA7-C31-C32-C33
69	1d	202	PC1	O21-C21-C22-C23
74	3P	504	CDL	C32-C31-CA7-OA8
74	4D	201	CDL	C37-C38-C39-C40
87	4A	605	HEA	C14-C15-C16-C17
74	3N	502	CDL	CA4-CA6-OA8-CA7
87	8A	603	HEA	CAA-CBA-CGA-O1A
69	1A	201	PC1	O31-C31-C32-C33
74	1d	203	CDL	C32-C31-CA7-OA8
76	1Y	804	3PE	C21-C22-C23-C24
86	4C	305	PGV	C3-C4-C5-C6
72	1F	501	FMN	N10-C1'-C2'-O2'
74	1L	702	CDL	C38-C39-C40-C41
76	3Y	101	3PE	C2-C3-O31-C31
86	4C	303	PGV	C6-C7-C8-C9
76	3A	503	3PE	C34-C35-C36-C37
76	5L	704	3PE	C33-C34-C35-C36
86	8C	303	PGV	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
74	3N	502	CDL	CB6-CB4-OB6-CB5
76	1Y	801	3PE	C3-C2-O21-C21
76	5Y	801	3PE	C3-C2-O21-C21
74	8C	306	CDL	C72-C73-C74-C75
86	4A	601	PGV	C11-C10-C9-C8
86	8B	302	PGV	C11-C10-C9-C8
74	1d	203	CDL	C38-C39-C40-C41
76	1Y	802	3PE	C2D-C2E-C2F-C2G
86	4C	304	PGV	C13-C14-C15-C16
76	3G	101	3PE	O22-C21-C22-C23
76	1b	201	3PE	C2A-C2B-C2C-C2D
74	1q	202	CDL	CA5-C11-C12-C13
76	3C	504	3PE	C23-C24-C25-C26
76	1Y	805	3PE	O21-C21-C22-C23
76	1K	101	3PE	C24-C25-C26-C27
86	4A	602	PGV	C6-C7-C8-C9
86	8C	301	PGV	C26-C27-C28-C29
76	1Y	802	3PE	C34-C35-C36-C37
74	1N	401	CDL	C32-C33-C34-C35
74	5N	401	CDL	C32-C33-C34-C35
86	8G	101	PGV	C7-C8-C9-C10
87	8A	604	HEA	CAA-CBA-CGA-O1A
76	5M	504	3PE	C33-C34-C35-C36
76	1M	903	3PE	C2D-C2E-C2F-C2G
86	4M	101	PGV	C15-C16-C17-C18
74	1X	201	CDL	C63-C64-C65-C66
74	3P	504	CDL	C52-C51-CB5-OB6
87	4A	604	HEA	CAA-CBA-CGA-O1A
76	1b	201	3PE	O22-C21-C22-C23
76	5A	201	3PE	O22-C21-C22-C23
69	3J	101	PC1	C22-C23-C24-C25
76	3N	501	3PE	C22-C23-C24-C25
74	5X	201	CDL	C63-C64-C65-C66
76	1M	901	3PE	C38-C39-C3A-C3B
86	8C	303	PGV	C6-C7-C8-C9
69	5P	401	PC1	C24-C25-C26-C27
74	3A	501	CDL	C31-C32-C33-C34
76	1Y	802	3PE	C33-C34-C35-C36
76	1L	701	3PE	C28-C29-C2A-C2B
69	5d	202	PC1	O22-C21-C22-C23
69	1A	201	PC1	O32-C31-C32-C33
69	1M	905	PC1	O22-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
69	1d	202	PC1	O22-C21-C22-C23
76	5Y	804	3PE	C21-C22-C23-C24
69	1I	201	PC1	C36-C37-C38-C39
86	8C	303	PGV	C30-C31-C32-C33
92	4G	102	PEK	C22-C23-C24-C25
85	3Q	501	HEC	CAA-CBA-CGA-O2A
74	5d	203	CDL	C32-C31-CA7-OA9
90	8I	101	PSC	C2-C3-C4-C5
74	8C	306	CDL	C18-C19-C20-C21
76	1L	701	3PE	C2A-C2B-C2C-C2D
76	1M	902	3PE	C22-C23-C24-C25
74	3P	504	CDL	C32-C31-CA7-OA9
69	1I	201	PC1	C38-C39-C3A-C3B
69	1h	203	PC1	O31-C31-C32-C33
76	5P	403	3PE	C37-C38-C39-C3A
74	8C	306	CDL	C22-C23-C24-C25
85	3D	501	HEC	CAA-CBA-CGA-O1A
85	3Q	501	HEC	CAD-CBD-CGD-O2D
74	1L	702	CDL	C52-C51-CB5-OB7
76	1Y	805	3PE	O22-C21-C22-C23
86	4A	601	PGV	O04-C19-C20-C21
76	5Y	805	3PE	O21-C21-C22-C23
83	5o	201	MYR	C3-C4-C5-C6
69	1M	905	PC1	O21-C21-C22-C23
76	1Y	802	3PE	O21-C21-C22-C23
86	8J	101	PGV	C30-C31-C32-C33
86	8M	101	PGV	C21-C22-C23-C24
86	4C	301	PGV	C26-C27-C28-C29
74	1d	203	CDL	C32-C31-CA7-OA9
74	1q	202	CDL	C52-C51-CB5-OB7
74	1h	202	CDL	C74-C75-C76-C77
74	1L	702	CDL	C52-C51-CB5-OB6
74	3G	102	CDL	C12-C11-CA5-OA6
74	3P	504	CDL	C72-C71-CB7-OB8
74	5L	702	CDL	C52-C51-CB5-OB6
74	5q	203	CDL	C12-C11-CA5-OA6
76	1M	903	3PE	O21-C21-C22-C23
76	3N	503	3PE	O21-C21-C22-C23
76	5M	502	3PE	O21-C21-C22-C23
76	5Y	802	3PE	O21-C21-C22-C23
86	8A	601	PGV	O03-C19-C20-C21
86	8C	302	PGV	O03-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
86	8M	101	PGV	O01-C1-C2-C3
86	4C	307	PGV	C5-C6-C7-C8
69	5B	203	PC1	C34-C35-C36-C37
77	1O	402	GTP	PA-O3A-PB-O2B
74	5L	702	CDL	C52-C51-CB5-OB7
69	5I	201	PC1	C34-C35-C36-C37
86	4B	301	PGV	C11-C10-C9-C8
69	1B	203	PC1	O21-C21-C22-C23
74	8D	201	CDL	C32-C31-CA7-OA8
76	1Y	806	3PE	O31-C31-C32-C33
76	5M	502	3PE	O31-C31-C32-C33
76	5Y	803	3PE	O21-C21-C22-C23
74	4C	306	CDL	C18-C19-C20-C21
86	8A	601	PGV	O04-C19-C20-C21
76	1M	901	3PE	C35-C36-C37-C38

There are no ring outliers.

171 monomers are involved in 656 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	4C	302	PGV	3	0
74	1d	203	CDL	9	0
86	8A	602	PGV	5	0
69	1I	204	PC1	3	0
86	4M	101	PGV	9	0
74	8D	201	CDL	18	0
71	5G	803	FES	3	0
86	8B	302	PGV	5	0
69	5B	202	PC1	6	0
91	4B	303	CUA	3	0
74	1h	202	CDL	11	0
86	4L	101	PGV	3	0
76	5M	504	3PE	7	0
74	3C	503	CDL	3	0
86	8J	101	PGV	3	0
74	1L	702	CDL	8	0
92	8C	308	PEK	6	0
86	4C	307	PGV	7	0
70	1G	801	SF4	1	0
76	1d	201	3PE	4	0
76	3N	501	3PE	2	0
86	8C	307	PGV	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	3D	501	HEC	3	0
76	3C	505	3PE	3	0
76	1K	101	3PE	2	0
76	1M	906	3PE	2	0
76	5M	501	3PE	4	0
76	5Y	802	3PE	3	0
76	1O	401	3PE	10	0
76	1Y	802	3PE	4	0
76	3A	503	3PE	4	0
76	5Y	801	3PE	6	0
74	5X	201	CDL	6	0
69	5A	203	PC1	1	0
76	1Y	801	3PE	4	0
76	3Q	502	3PE	3	0
74	8B	303	CDL	9	0
86	4K	101	PGV	1	0
90	4A	609	PSC	7	0
74	5L	702	CDL	6	0
86	8B	301	PGV	9	0
76	5L	704	3PE	3	0
86	8A	601	PGV	5	0
69	1H	402	PC1	2	0
69	1B	203	PC1	7	0
76	1P	502	3PE	3	0
74	5h	202	CDL	10	0
69	5I	204	PC1	4	0
76	1Y	804	3PE	2	0
76	1M	902	3PE	5	0
86	8C	302	PGV	2	0
74	3G	102	CDL	5	0
82	5h	201	AME	1	0
74	3A	501	CDL	5	0
76	3D	502	3PE	2	0
79	1P	501	NDP	3	0
72	1F	501	FMN	3	0
81	5T	101	EHZ	1	0
76	1Y	806	3PE	1	0
70	5B	201	SF4	1	0
87	8A	603	HEA	6	0
84	3P	501	HEM	1	0
76	3Y	101	3PE	2	0
76	1M	901	3PE	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
69	1A	202	PC1	1	0
76	5M	502	3PE	11	0
76	1j	101	3PE	2	0
76	5Y	804	3PE	2	0
85	3Q	501	HEC	2	0
70	1B	201	SF4	1	0
83	5o	201	MYR	1	0
86	8C	304	PGV	6	0
86	8C	301	PGV	2	0
92	8G	102	PEK	4	0
74	5d	203	CDL	3	0
69	3J	101	PC1	4	0
86	8M	101	PGV	3	0
69	5h	203	PC1	3	0
87	4A	605	HEA	2	0
74	3P	504	CDL	9	0
87	4A	604	HEA	7	0
69	5A	202	PC1	3	0
69	3X	101	PC1	2	0
81	5n	201	EHZ	1	0
86	8K	101	PGV	1	0
82	1h	201	AME	1	0
76	5M	506	3PE	2	0
76	3C	504	3PE	3	0
76	5d	201	3PE	7	0
86	4G	101	PGV	6	0
76	1L	701	3PE	3	0
84	3C	502	HEM	4	0
69	5L	705	PC1	3	0
92	4C	308	PEK	4	0
76	5K	101	3PE	3	0
69	3R	302	PC1	6	0
74	1q	202	CDL	1	0
69	1M	905	PC1	6	0
76	1Y	805	3PE	2	0
76	3A	502	3PE	1	0
74	4B	302	CDL	7	0
86	4C	301	PGV	6	0
75	1I	205	AYA	1	0
69	5M	503	PC1	4	0
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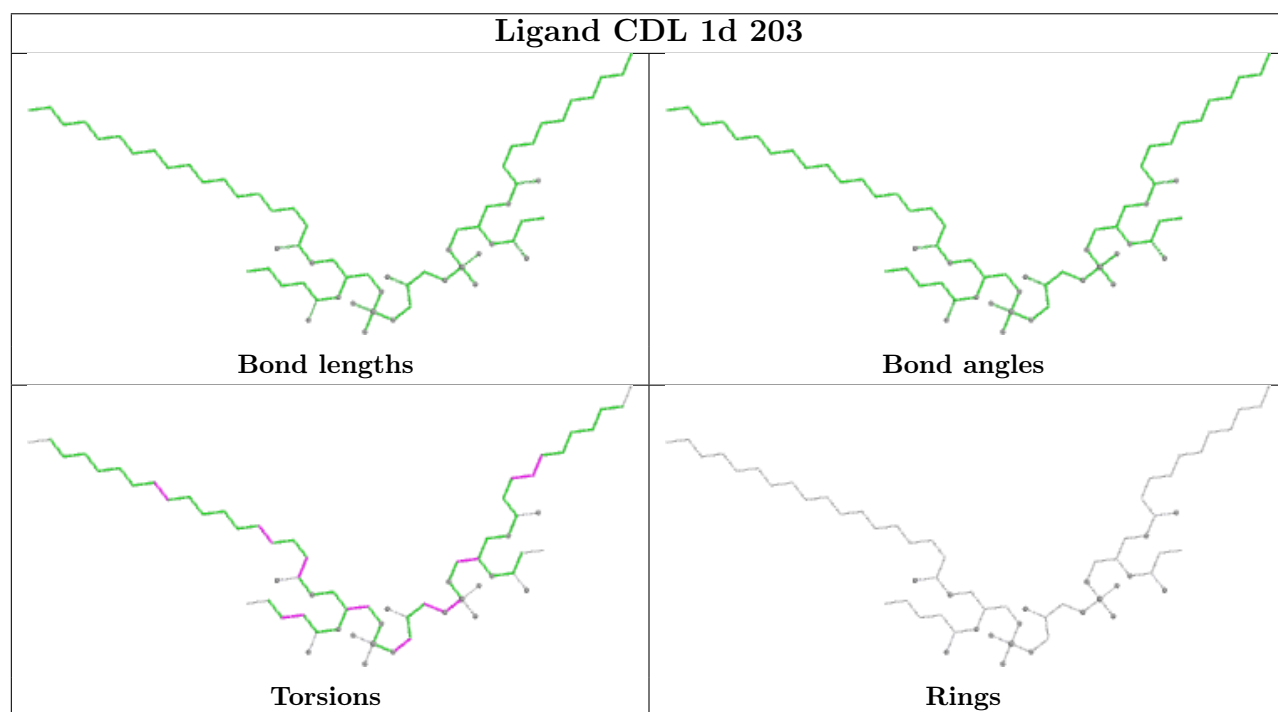
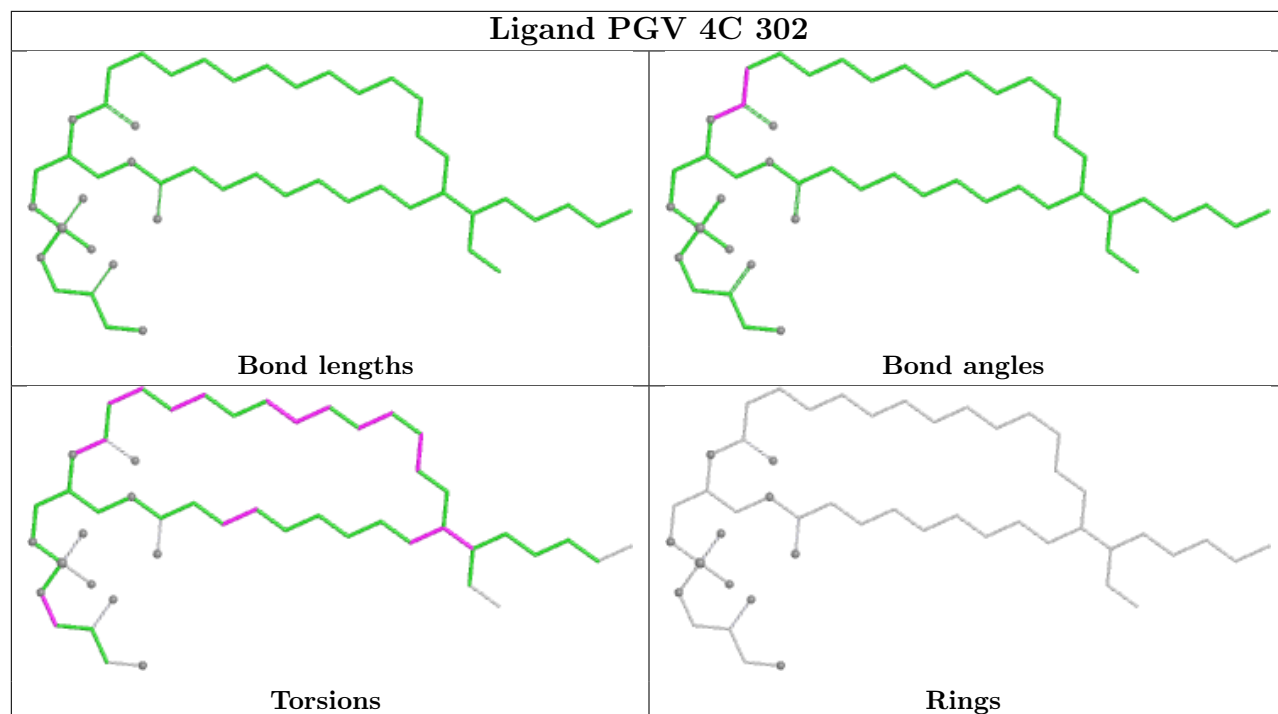
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81	1n	201	EHZ	2	0
86	8L	101	PGV	3	0
69	5I	201	PC1	5	0
76	5Y	806	3PE	3	0
76	5Y	803	3PE	3	0
90	8I	101	PSC	5	0
69	5M	505	PC1	6	0
69	1M	904	PC1	2	0
79	5P	402	NDP	5	0
69	1q	201	PC1	3	0
74	4D	201	CDL	18	0
76	1L	703	3PE	5	0
69	1A	201	PC1	4	0
76	5L	703	3PE	3	0
76	5A	201	3PE	3	0
74	1N	401	CDL	3	0
86	8C	305	PGV	2	0
75	5q	202	AYA	3	0
76	3N	503	3PE	3	0
86	8C	303	PGV	4	0
74	3T	101	CDL	11	0
77	5O	401	GTP	1	0
76	1b	201	3PE	1	0
86	4A	601	PGV	7	0
86	4C	304	PGV	6	0
76	1M	903	3PE	11	0
76	5P	403	3PE	1	0
74	1X	201	CDL	10	0
69	1I	201	PC1	5	0
74	5N	401	CDL	3	0
92	4G	102	PEK	4	0
91	8B	304	CUA	1	0
76	5Y	805	3PE	1	0
74	5H	401	CDL	2	0
74	3N	502	CDL	1	0
86	4A	603	PGV	8	0
69	5q	201	PC1	4	0
86	4B	301	PGV	4	0
86	8G	101	PGV	6	0
86	4C	305	PGV	1	0

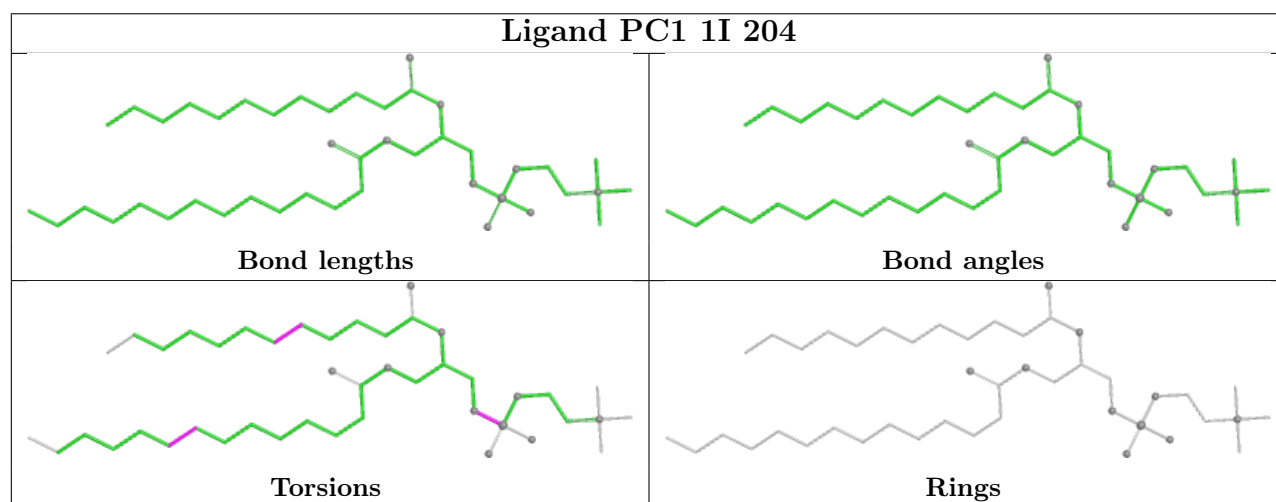
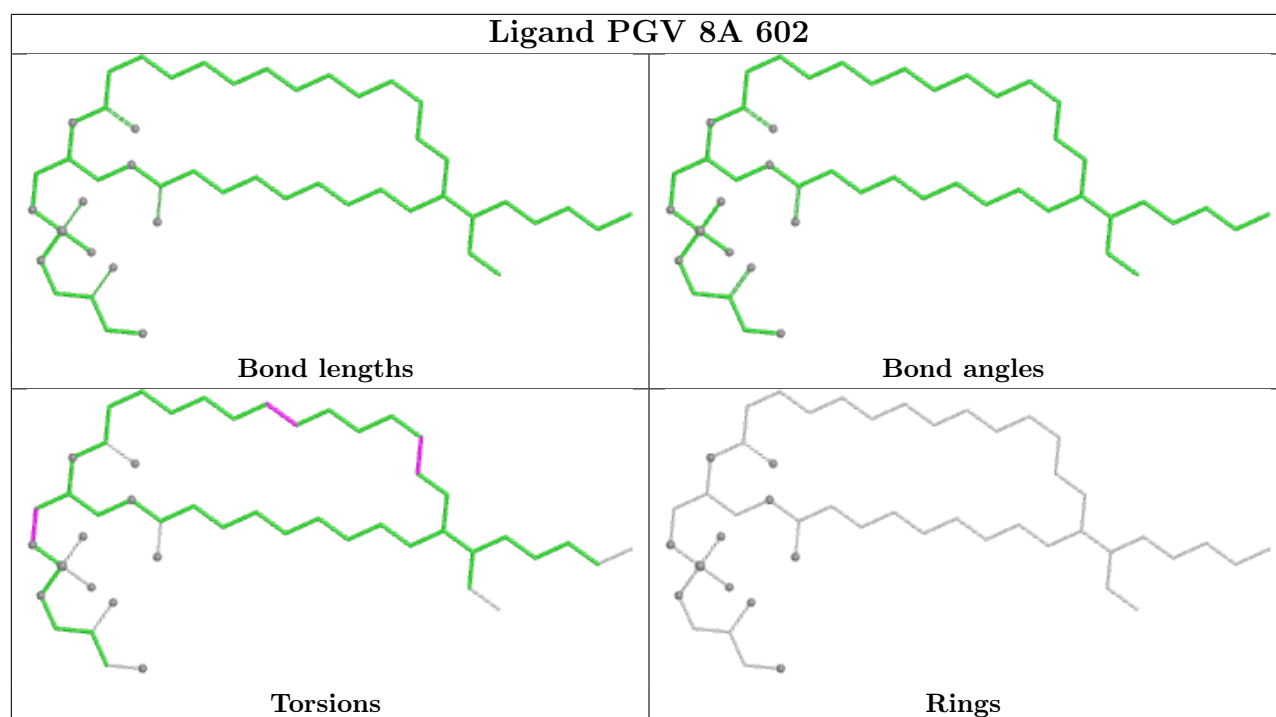
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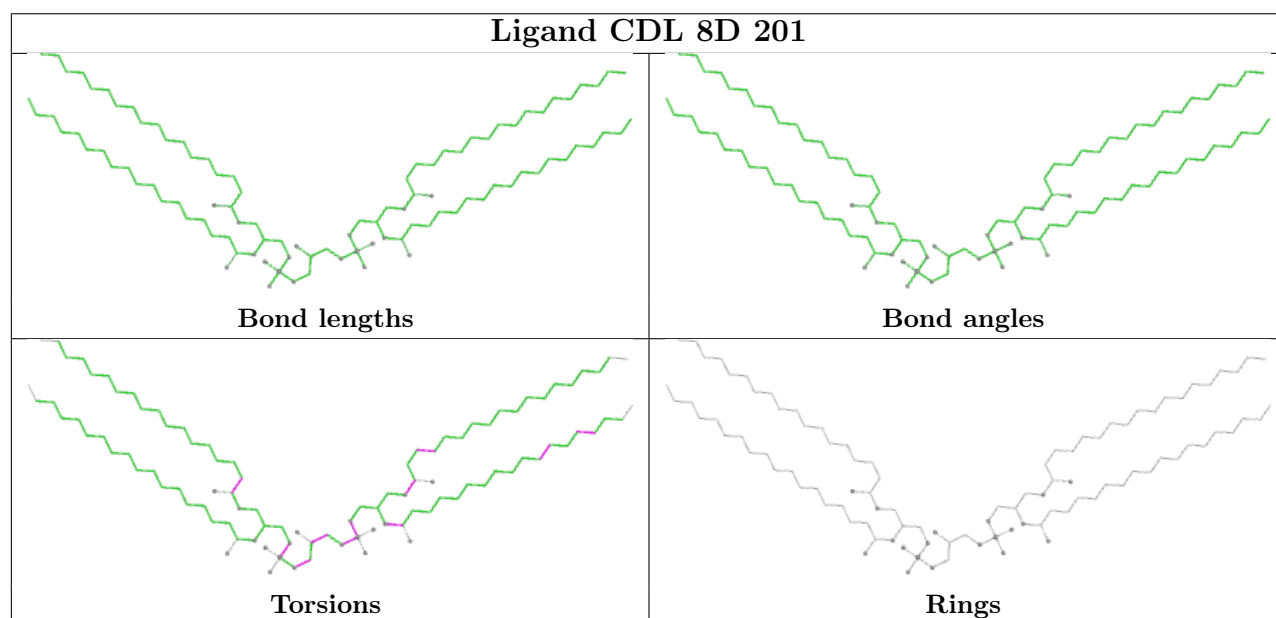
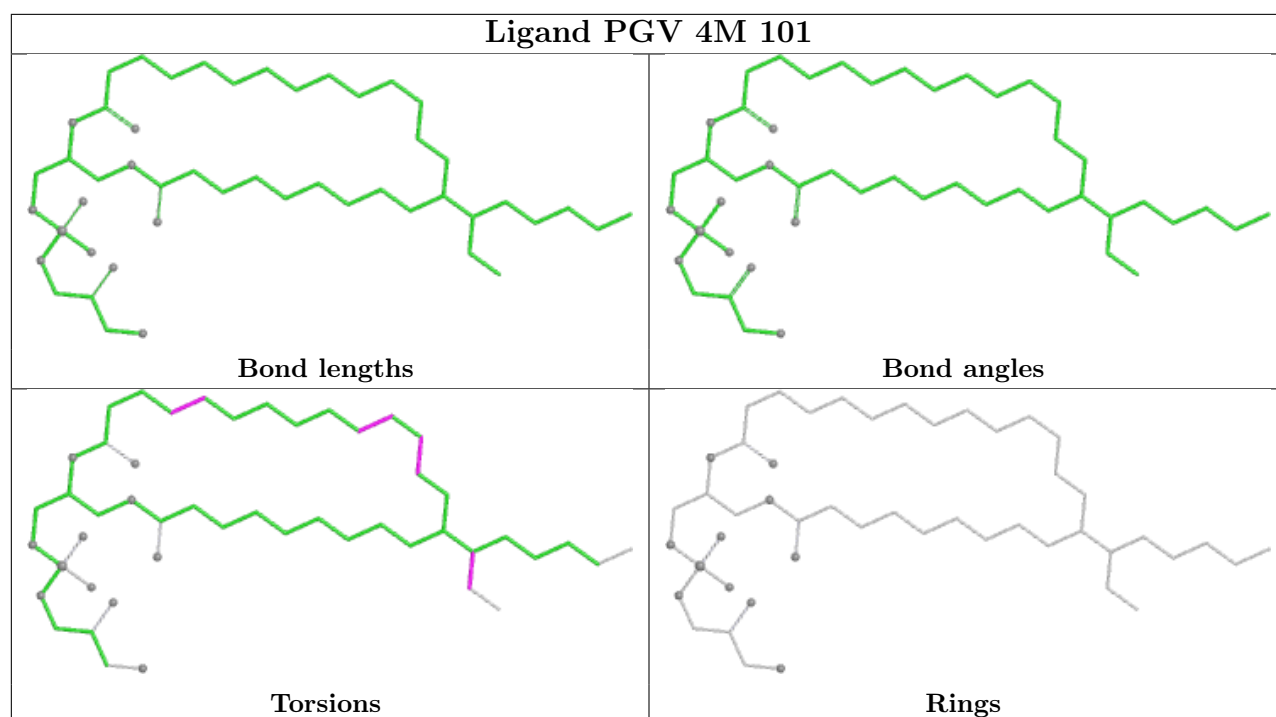
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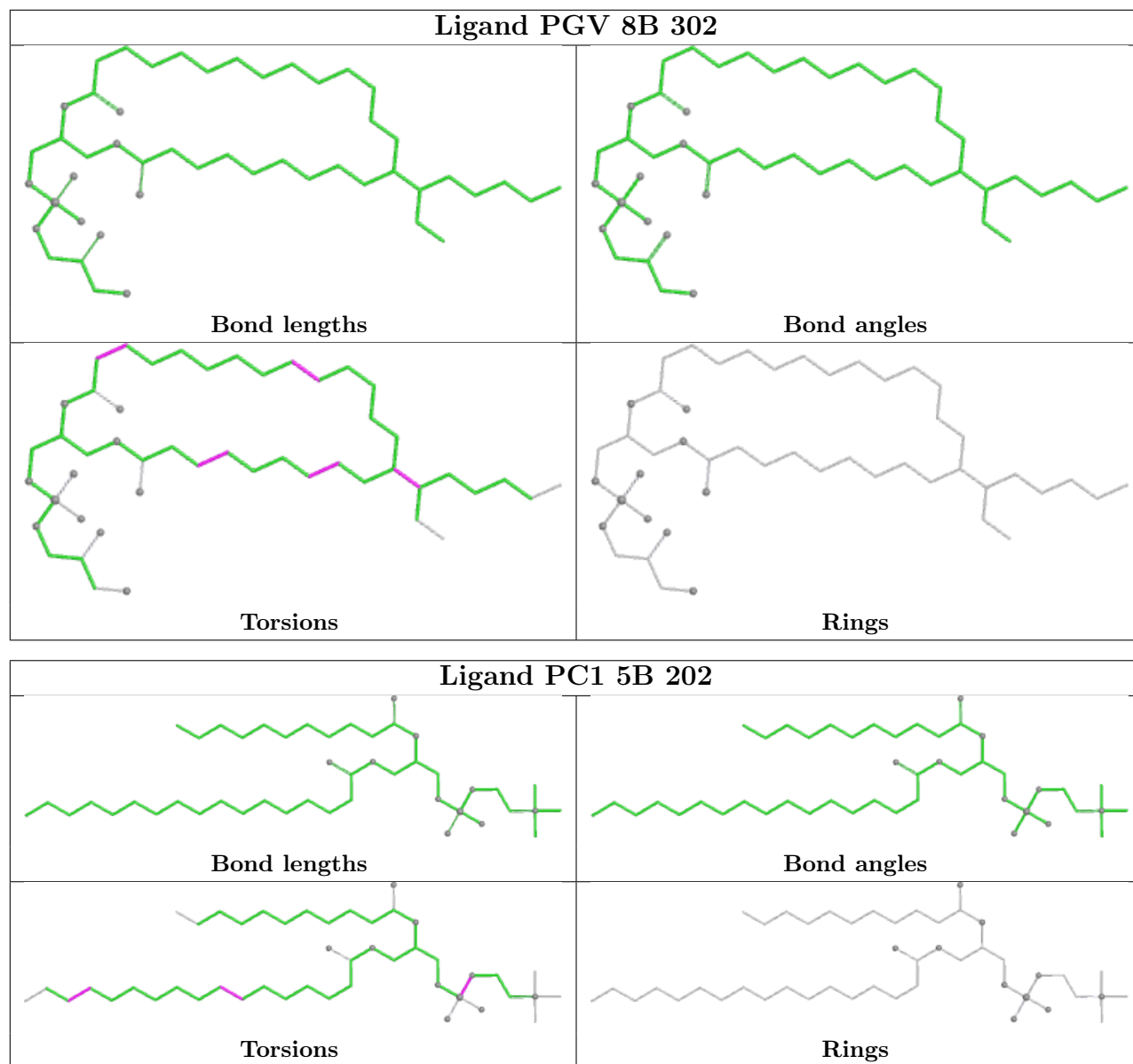
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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69	5d	202	PC1	8	0
72	5F	501	FMN	3	0
69	1d	202	PC1	6	0
76	5j	101	3PE	5	0
69	1h	203	PC1	3	0
74	4C	306	CDL	15	0
70	5G	801	SF4	1	0
70	1F	502	SF4	1	0
74	8C	306	CDL	14	0
71	1G	803	FES	3	0
86	4A	602	PGV	6	0
86	4J	101	PGV	3	0
76	1Y	803	3PE	3	0
69	1L	704	PC1	3	0
69	1A	203	PC1	1	0
69	5B	203	PC1	7	0
70	5F	502	SF4	1	0
69	5H	402	PC1	2	0
71	3R	301	FES	1	0
86	4C	303	PGV	5	0
74	5q	203	CDL	2	0
84	3P	502	HEM	2	0

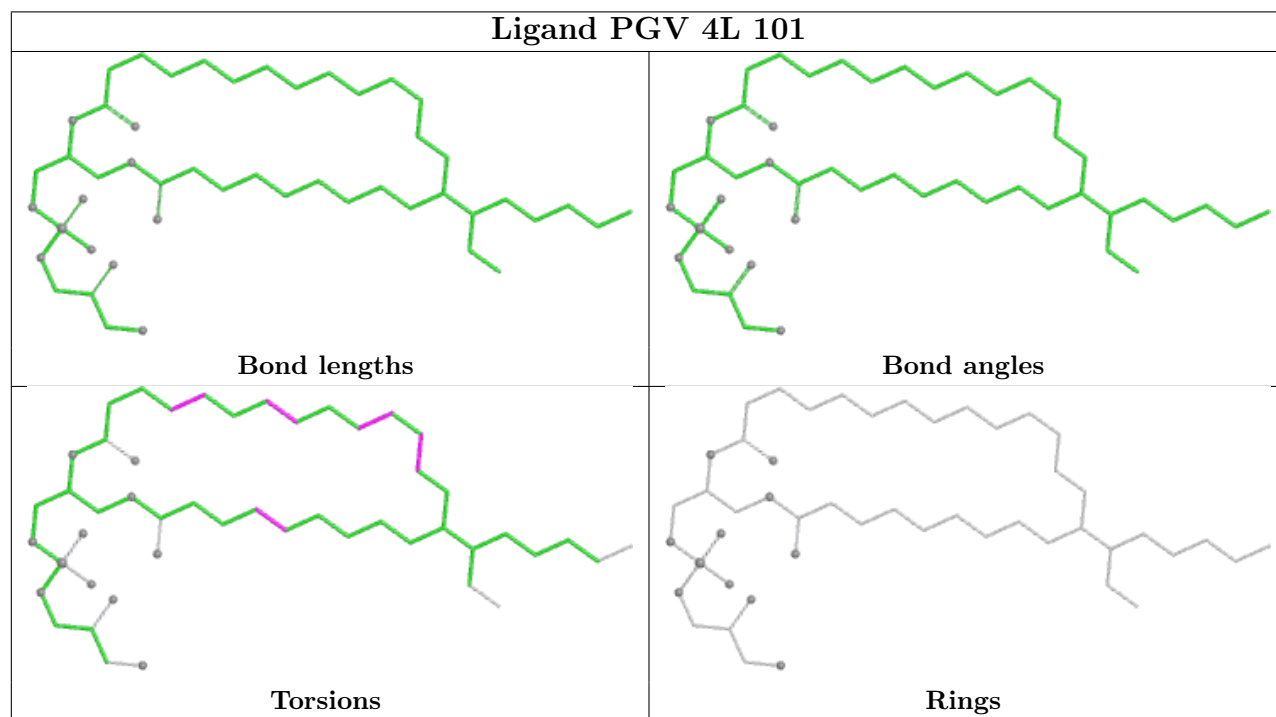
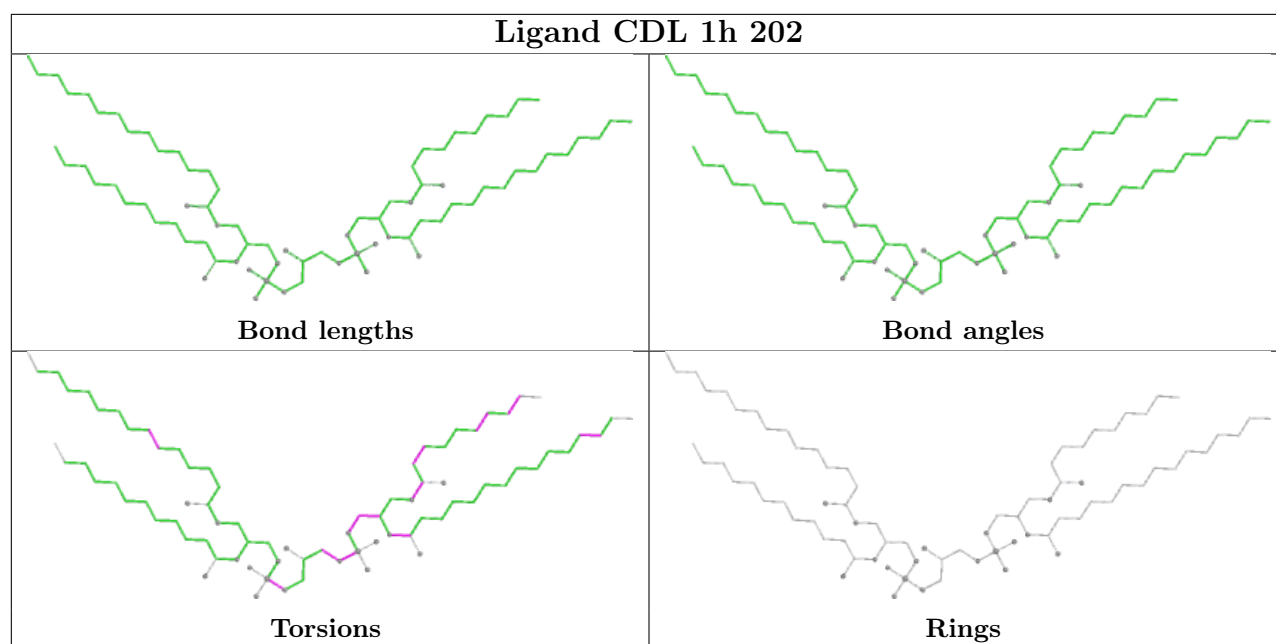
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

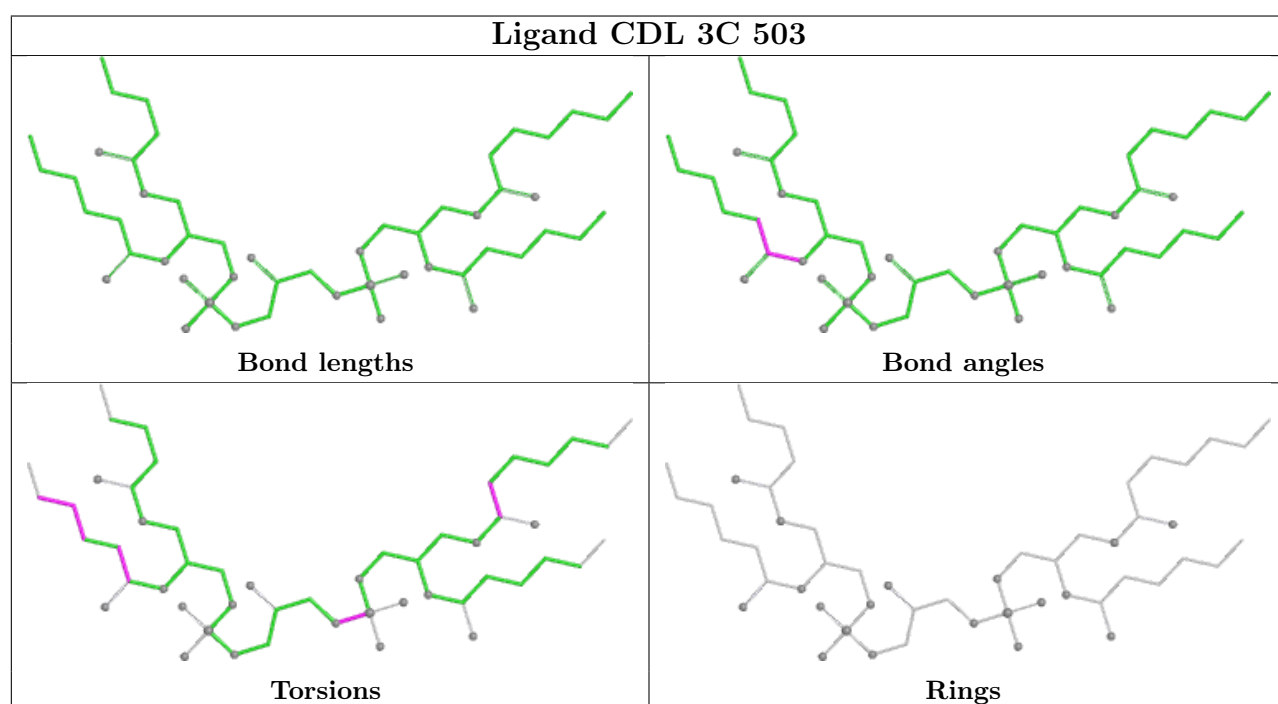
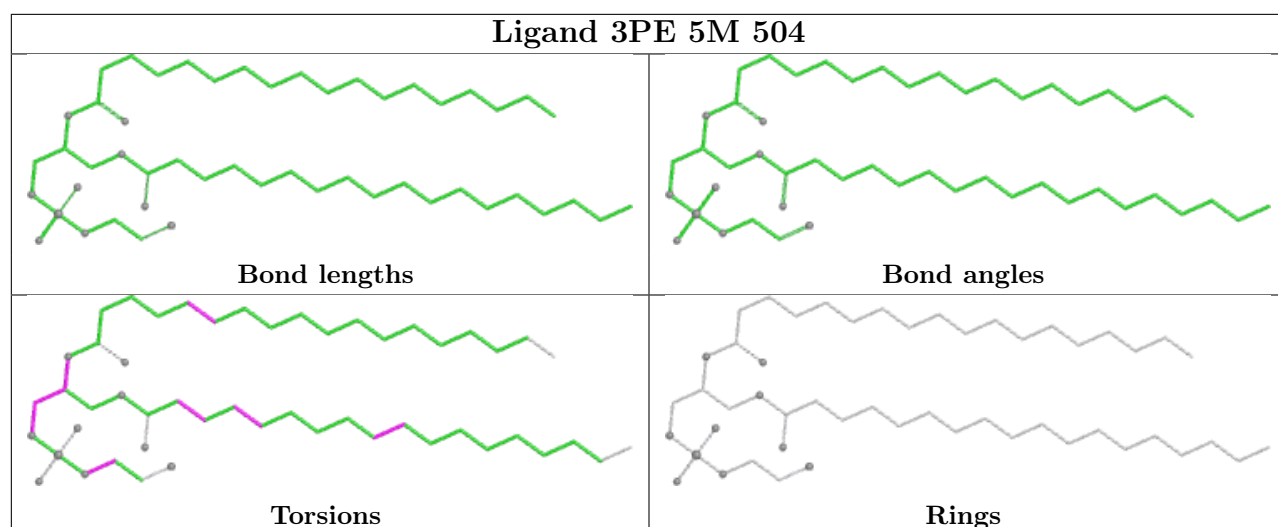


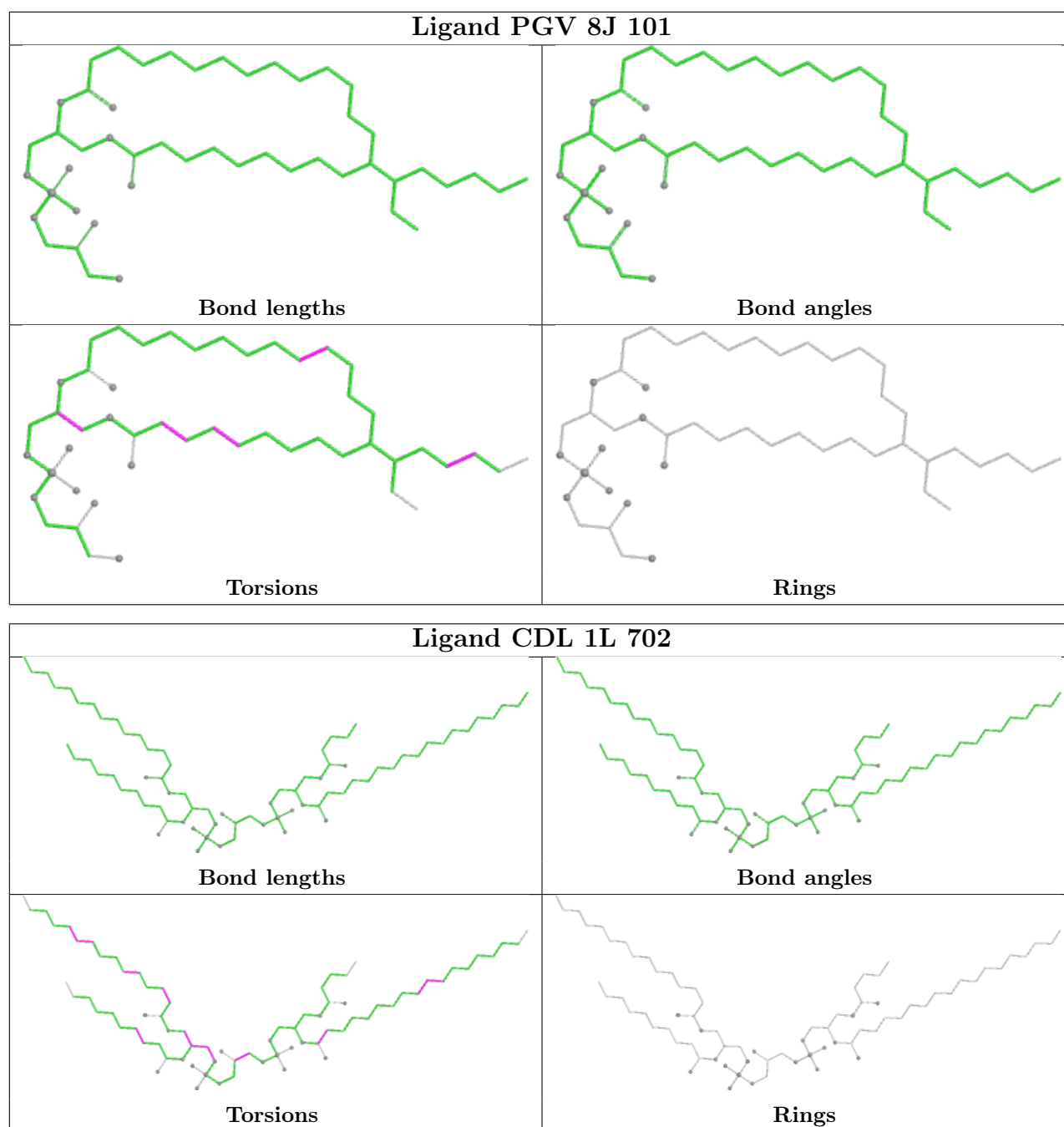


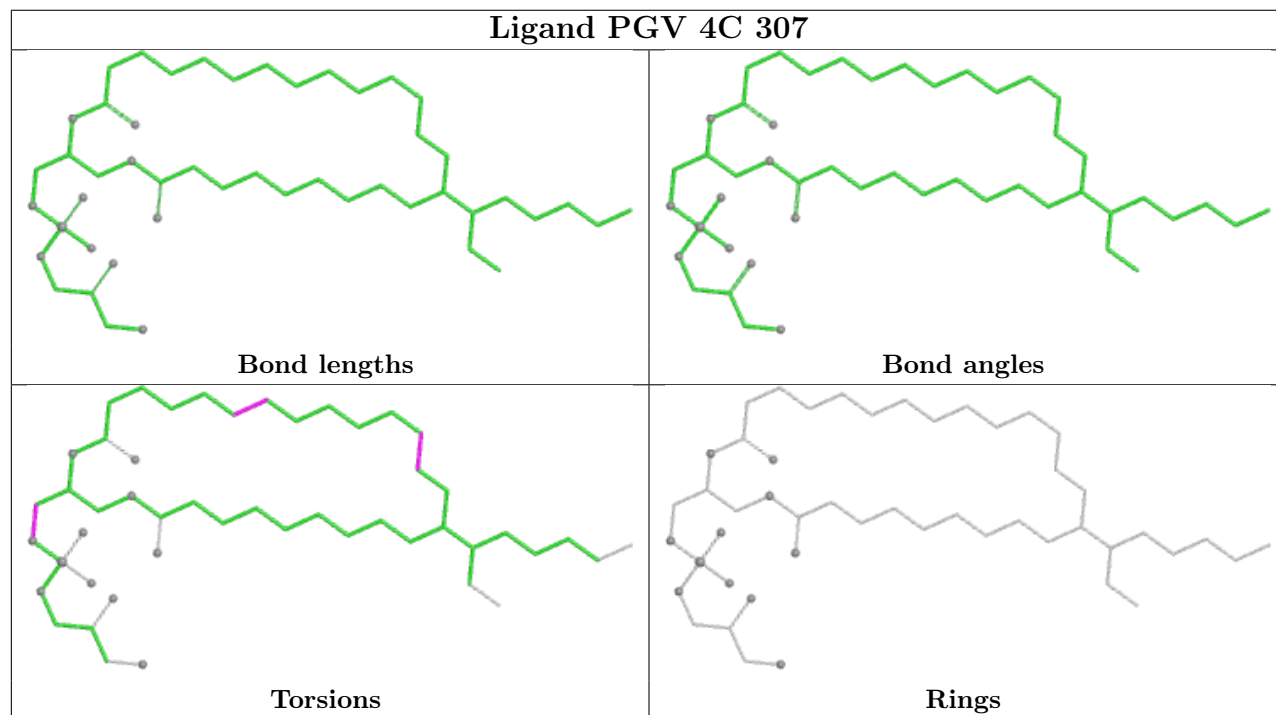
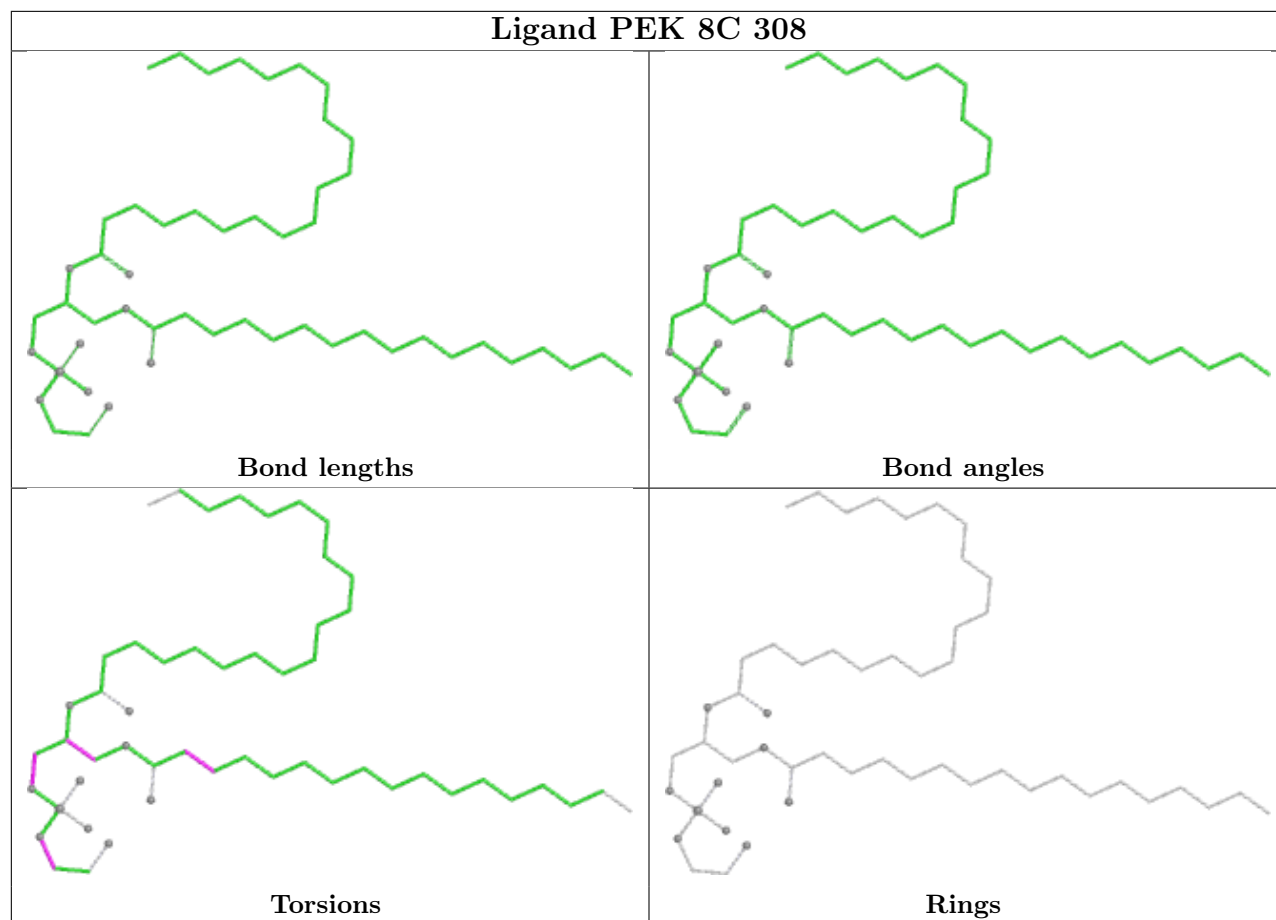


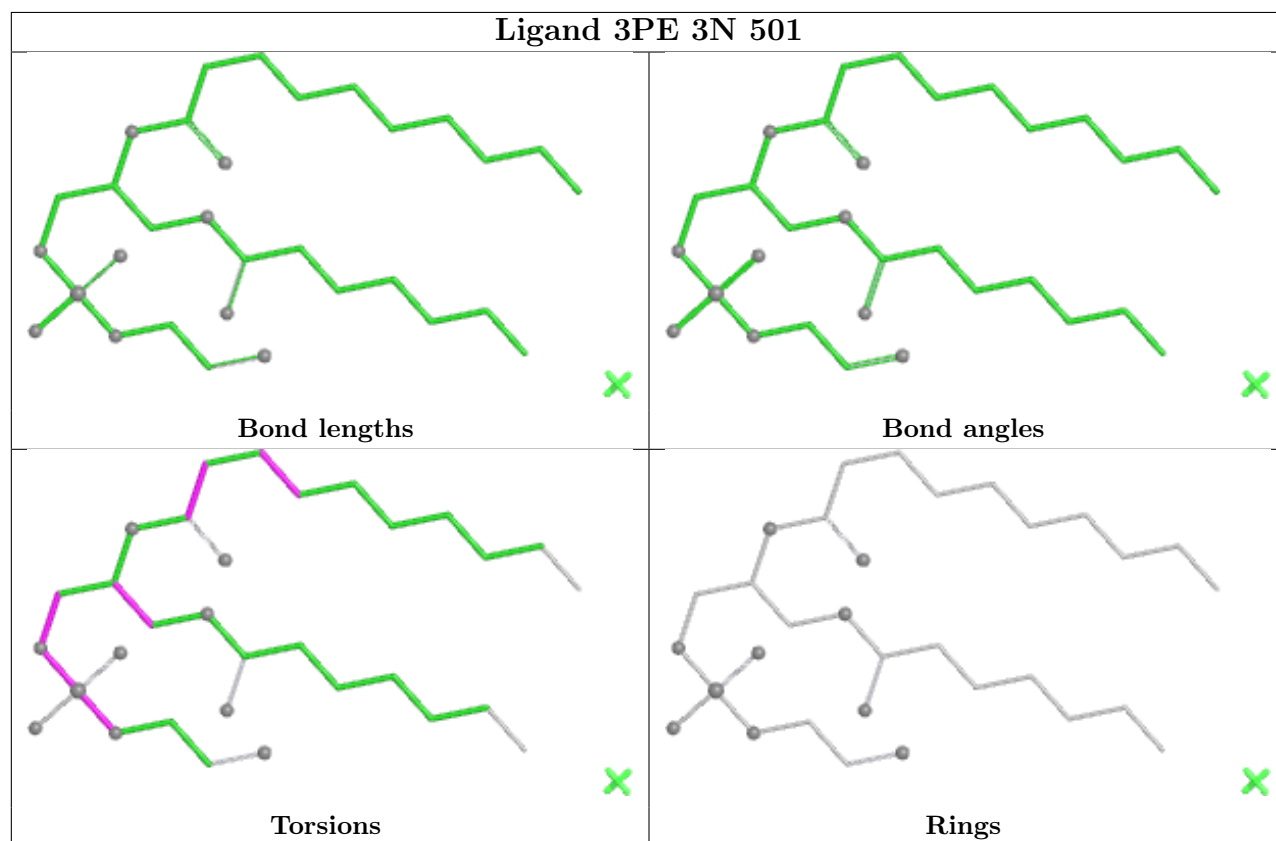
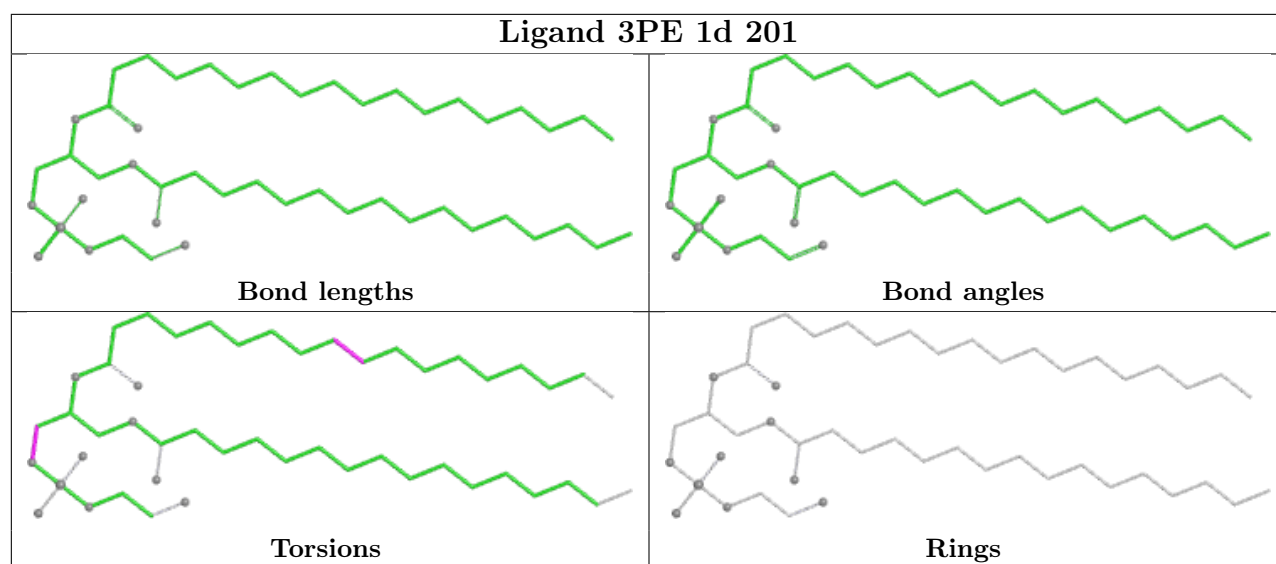


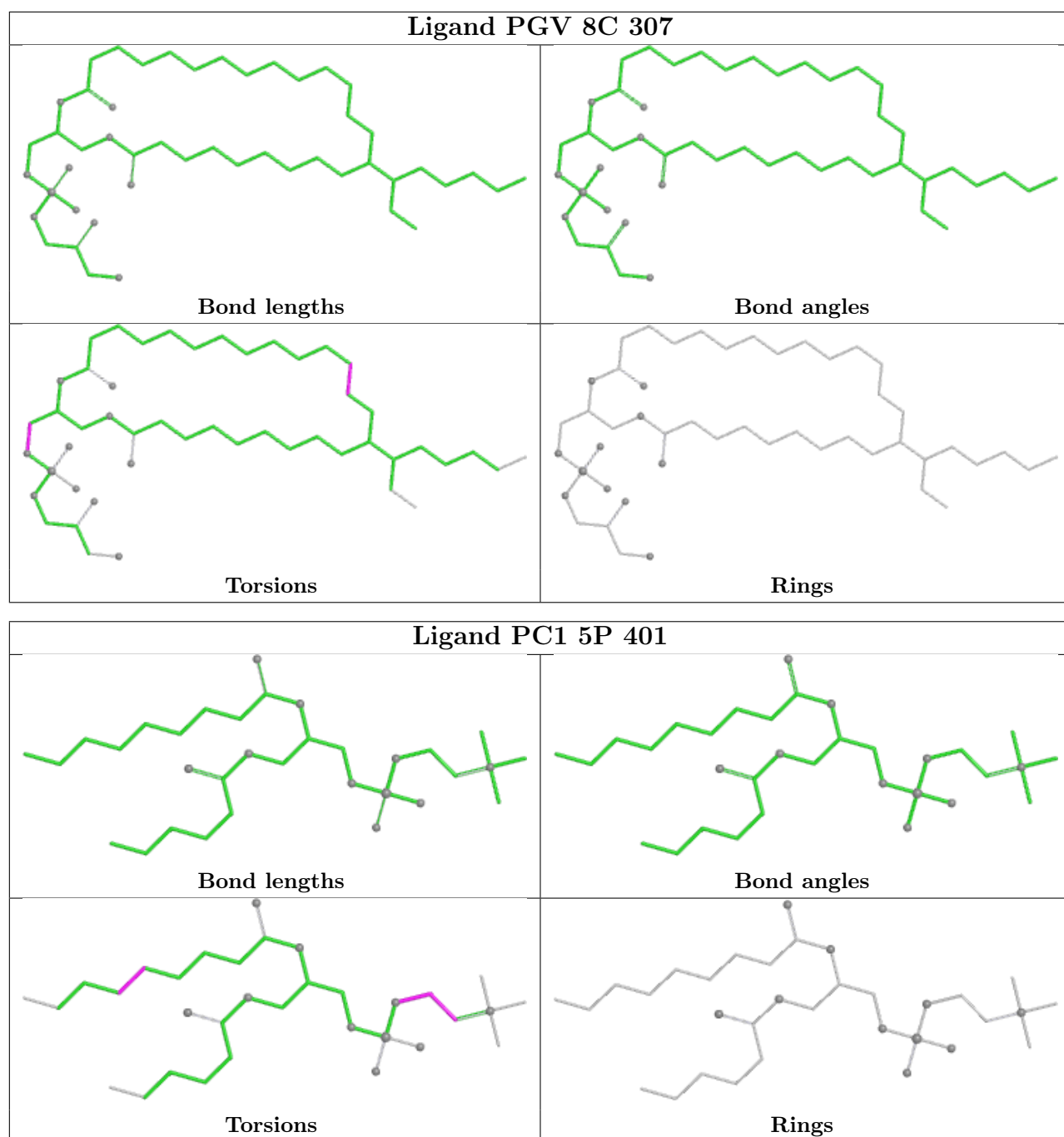




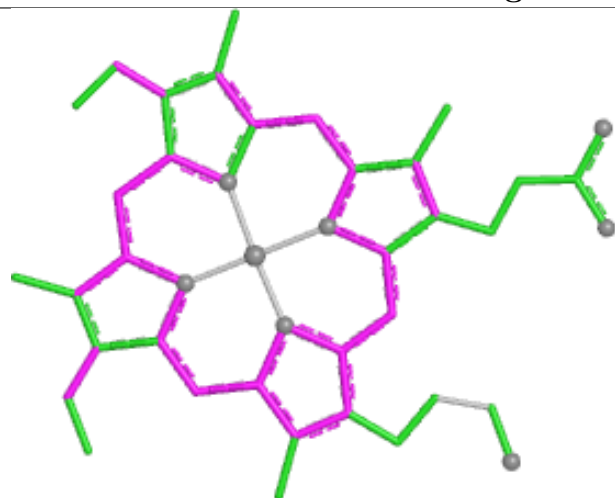




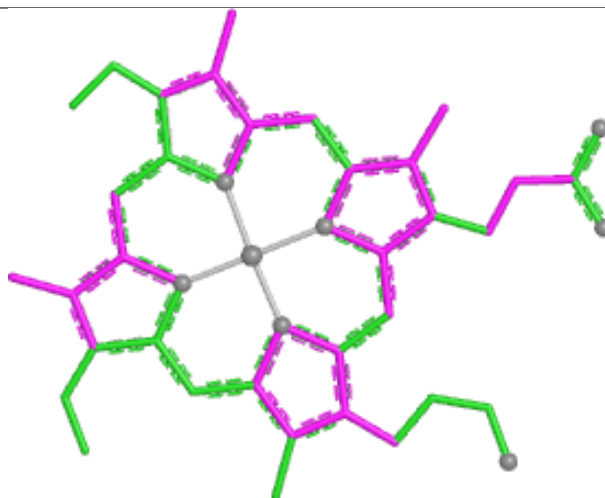




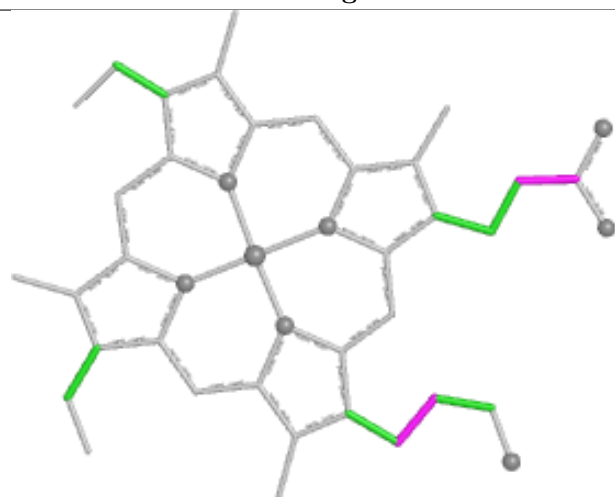
Ligand HEC 3D 501



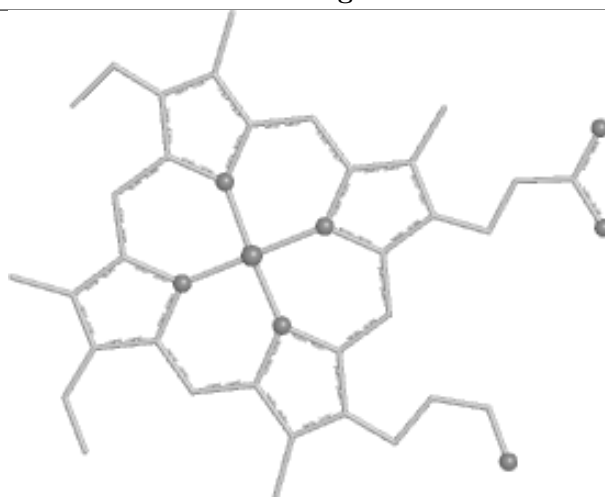
Bond lengths



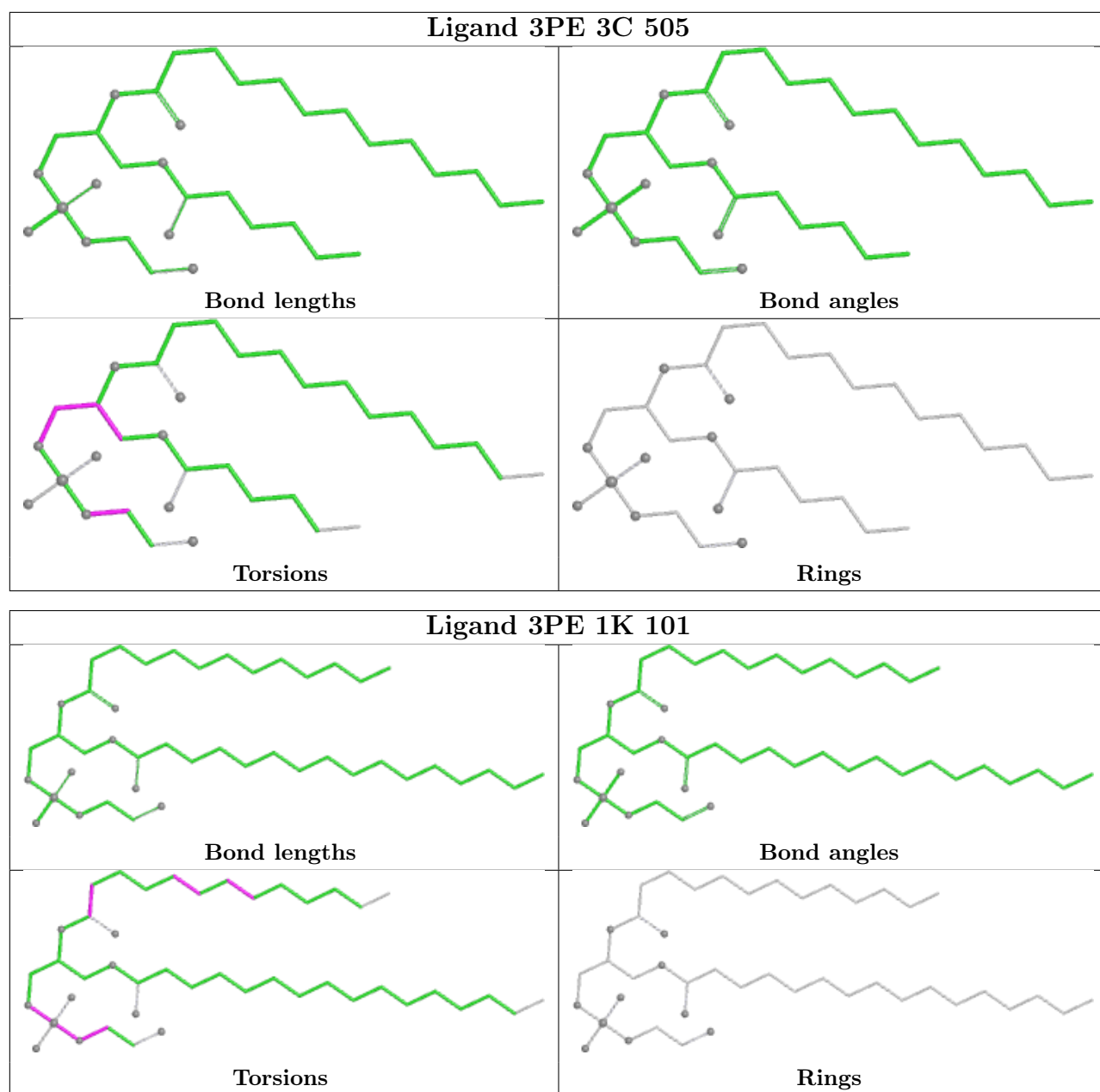
Bond angles

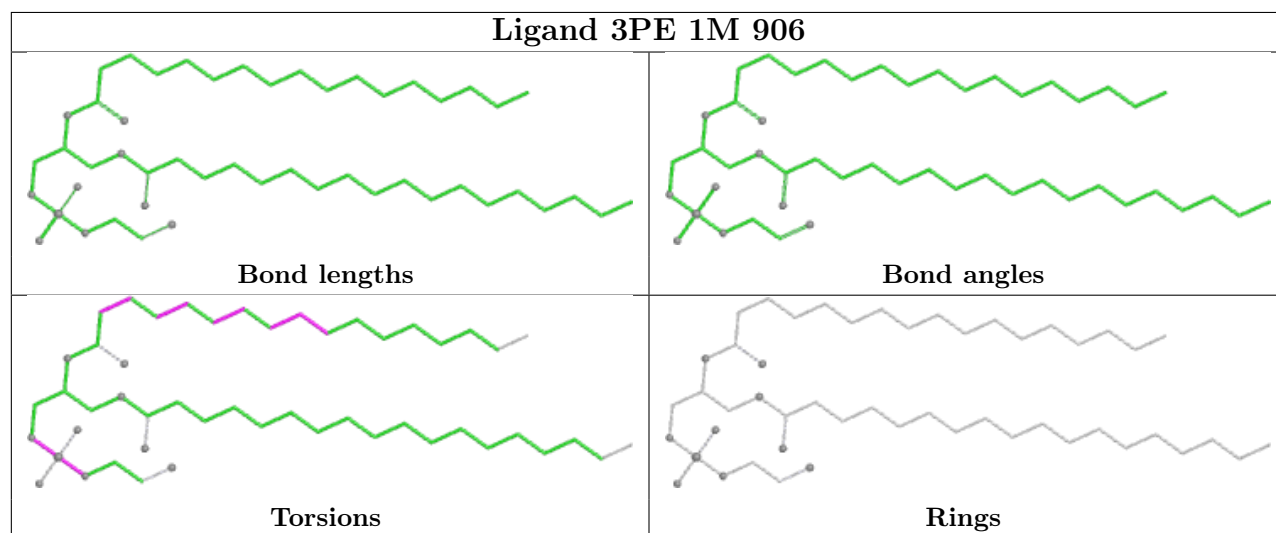
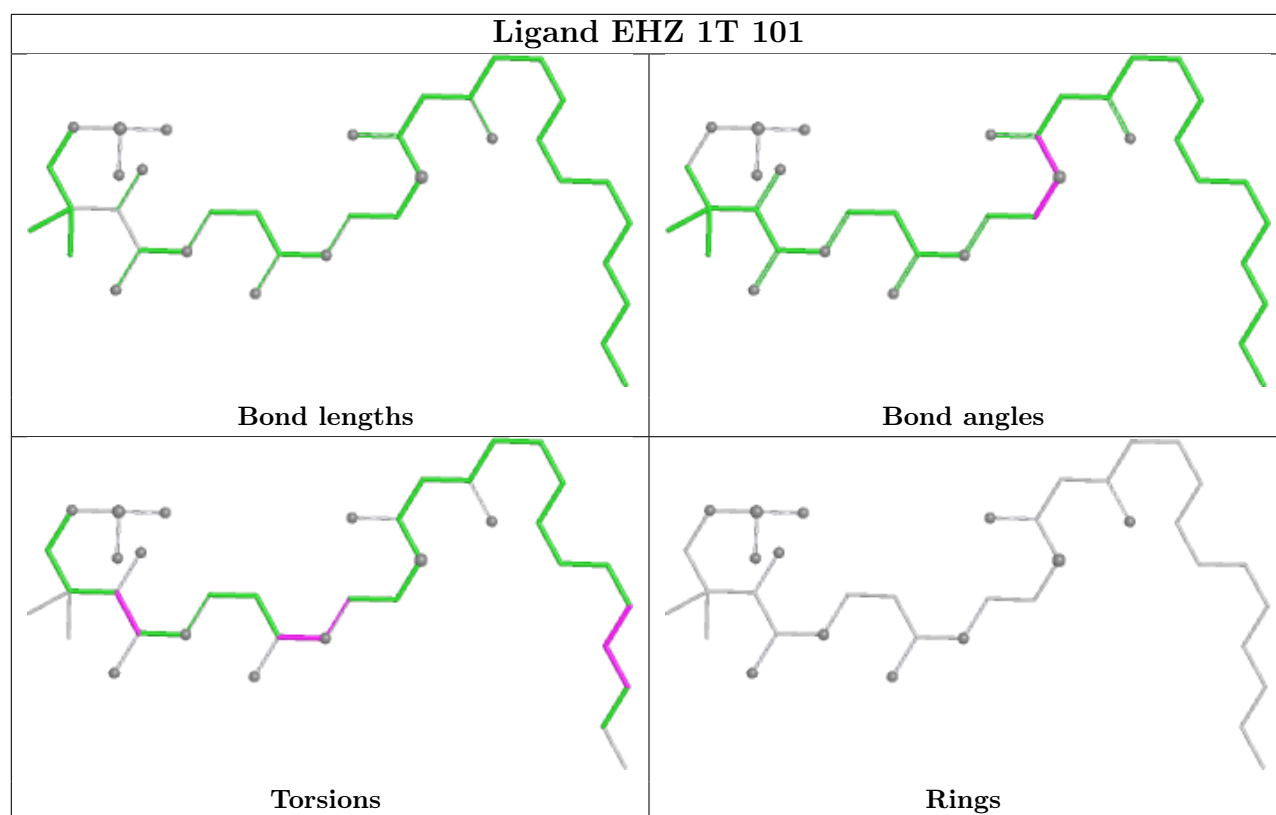


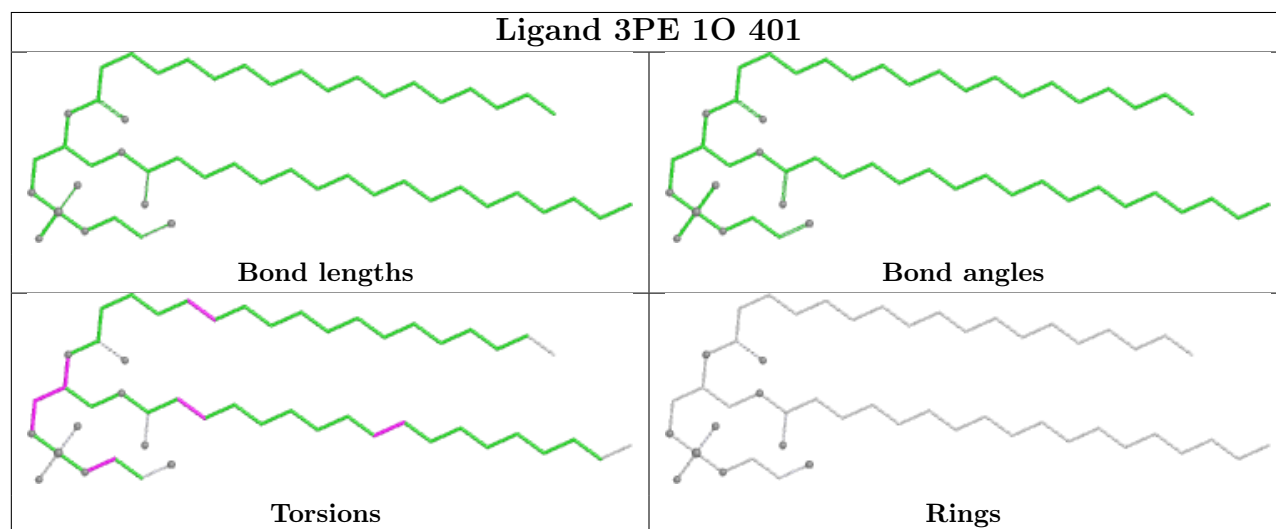
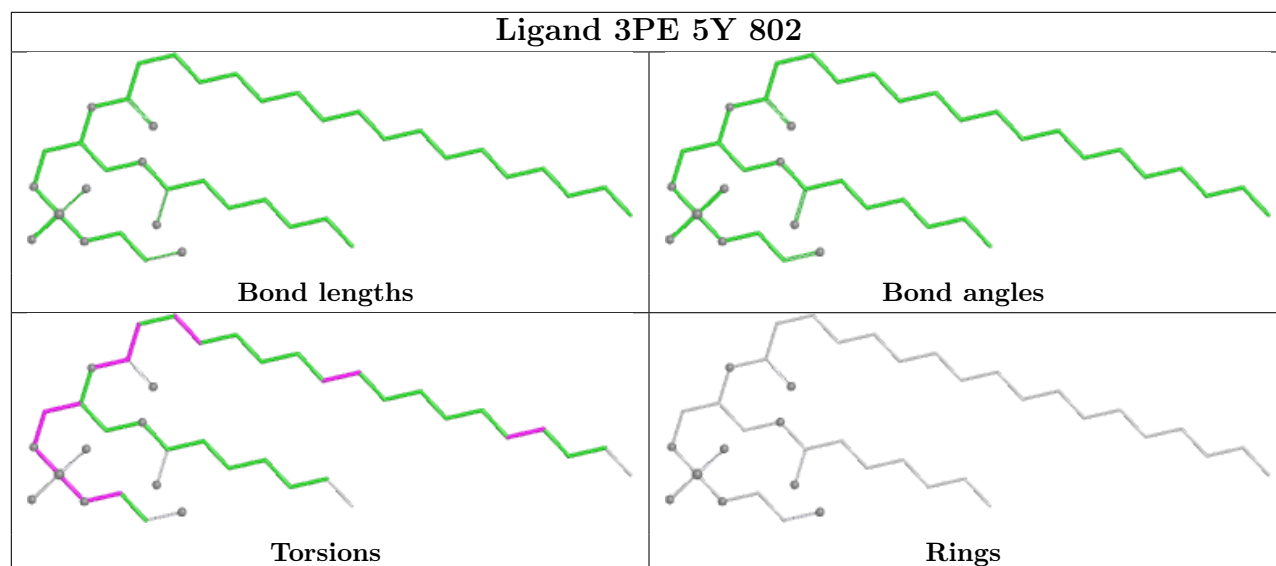
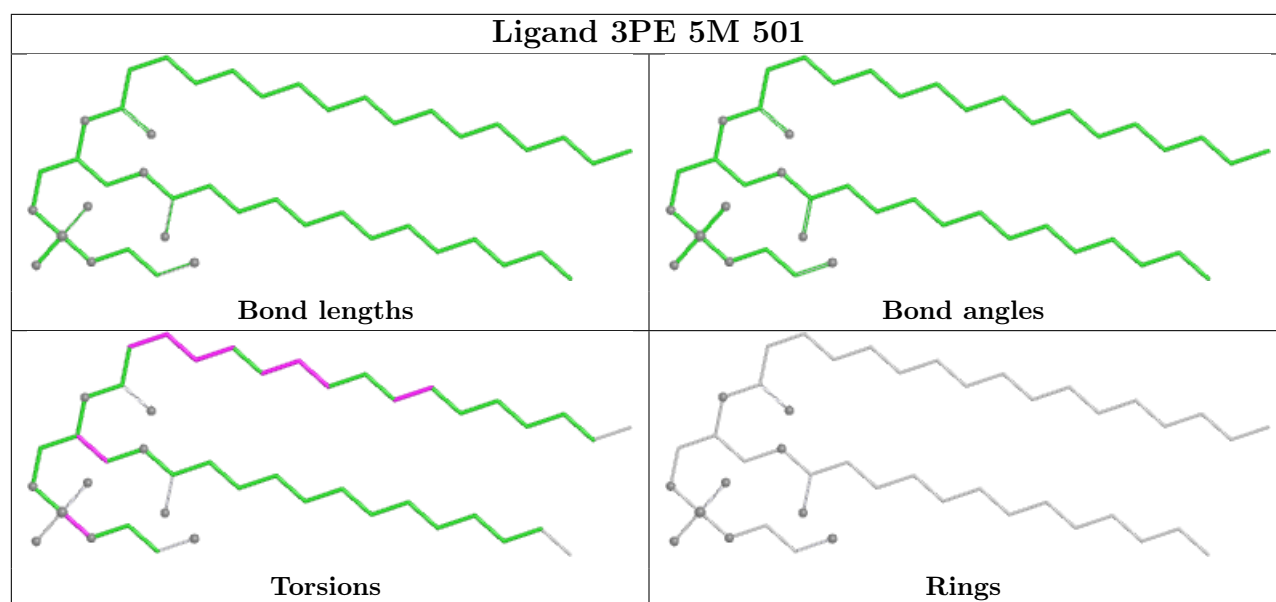
Torsions

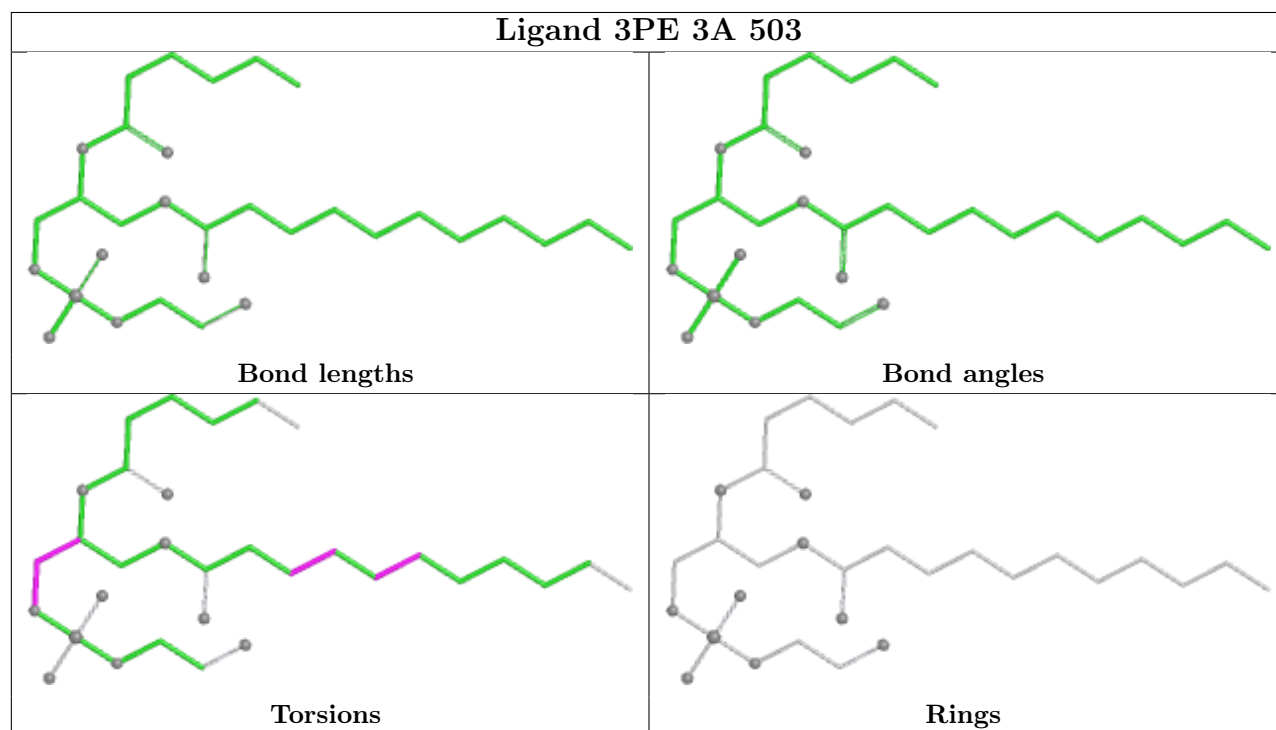
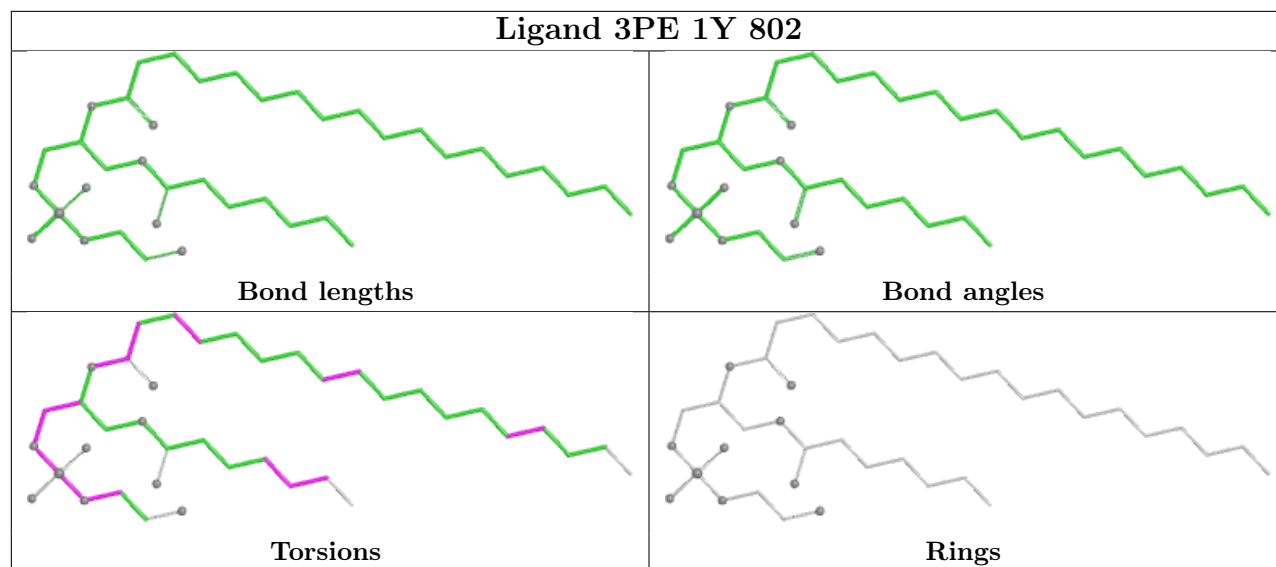


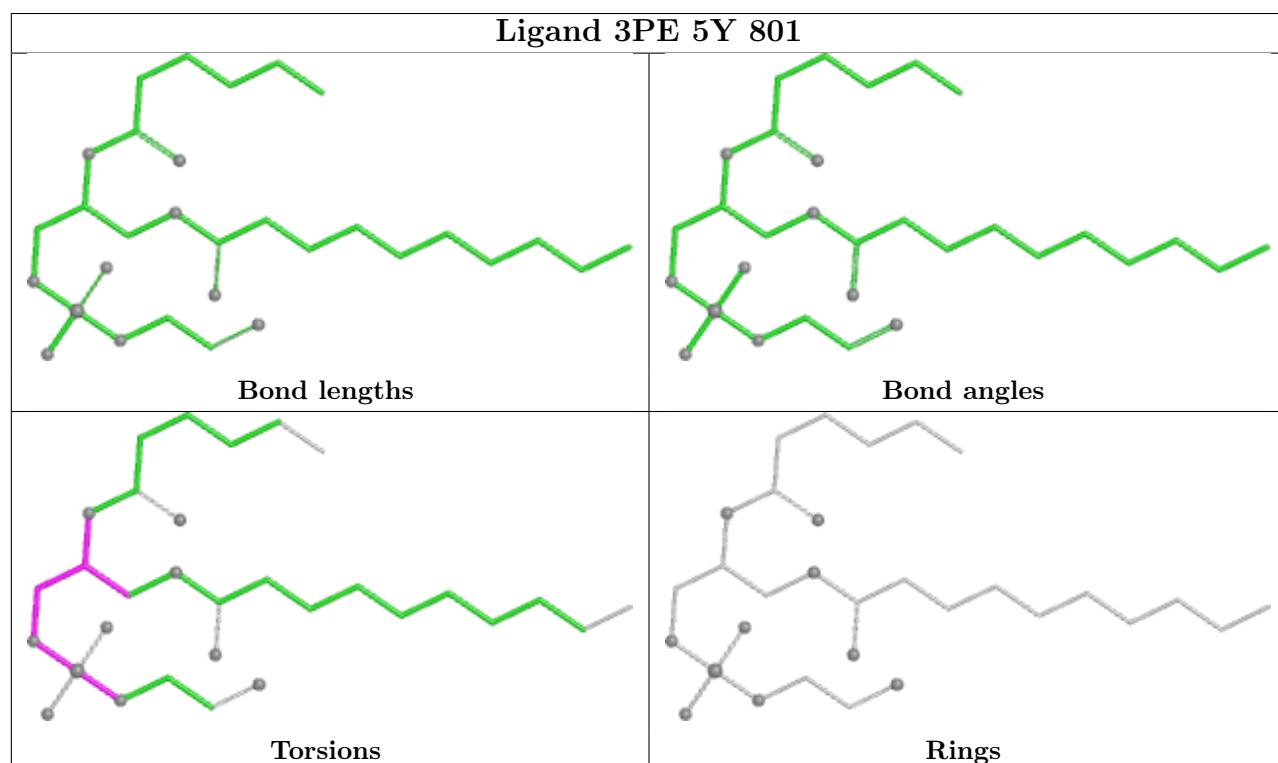
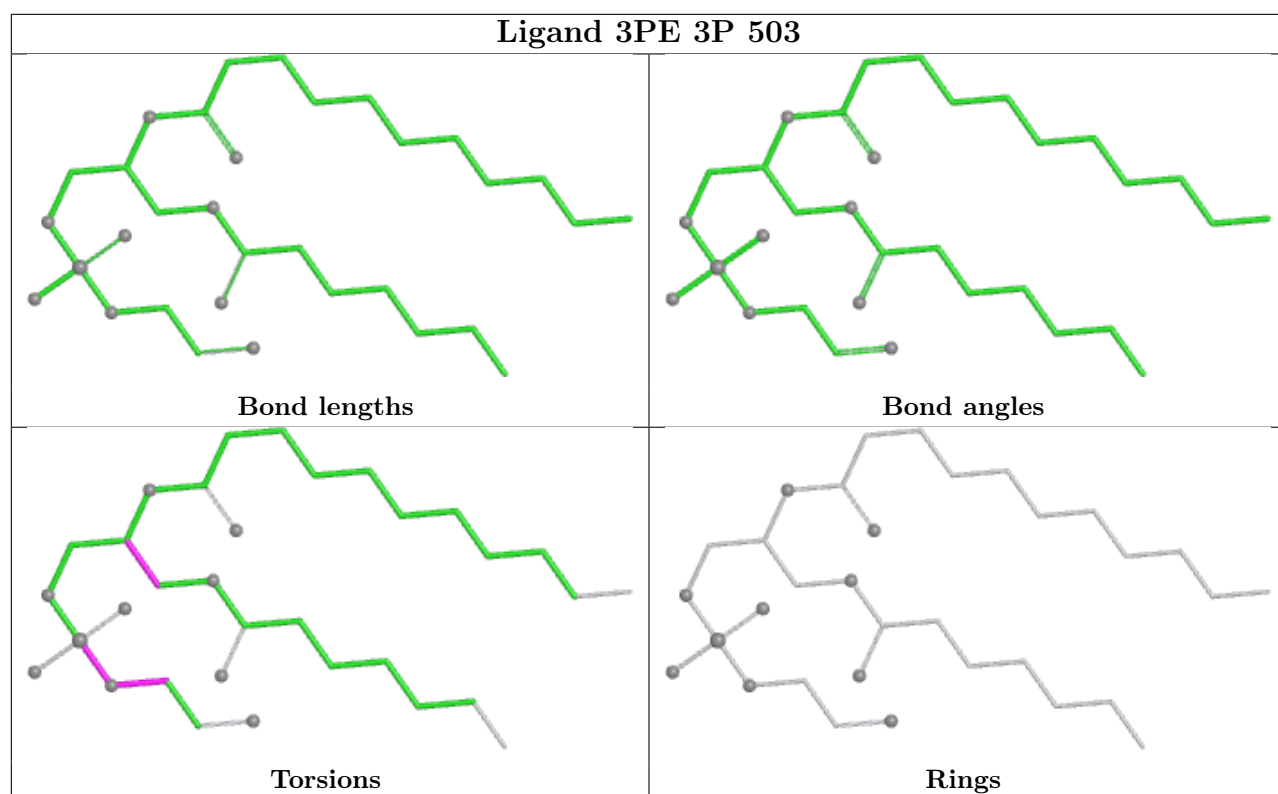
Rings

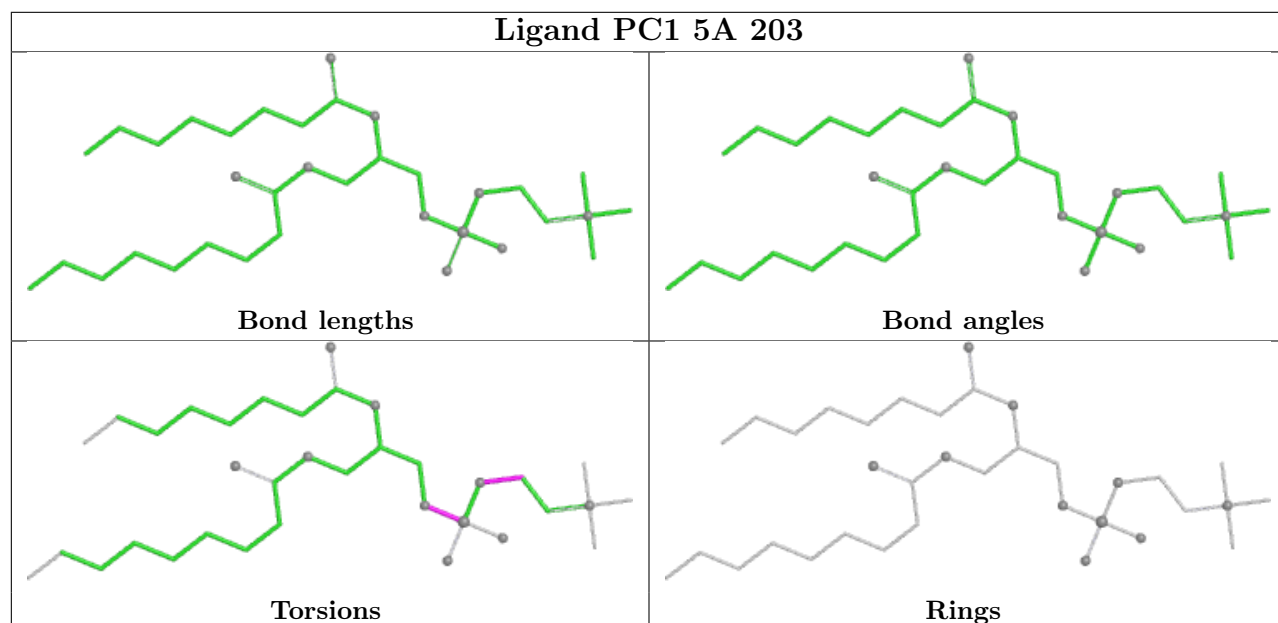
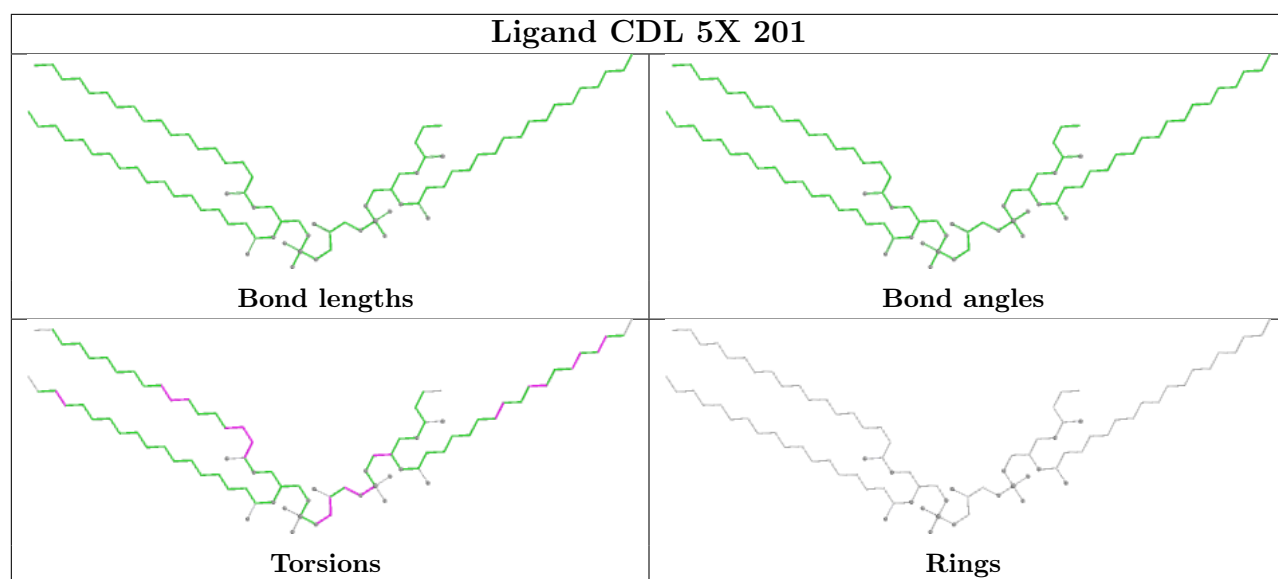


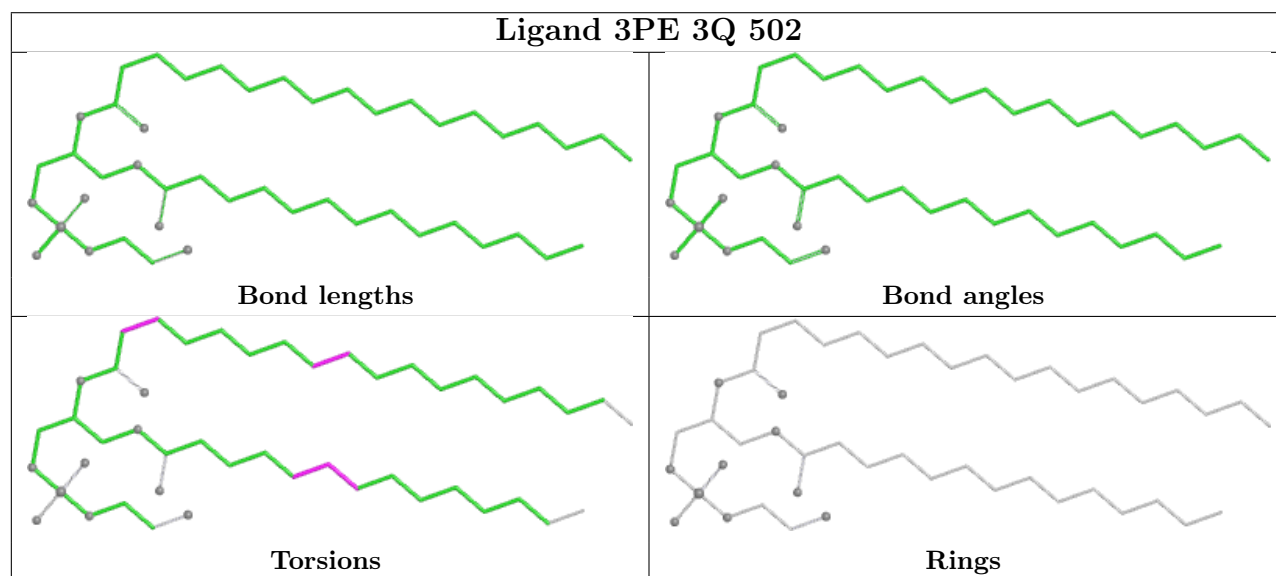
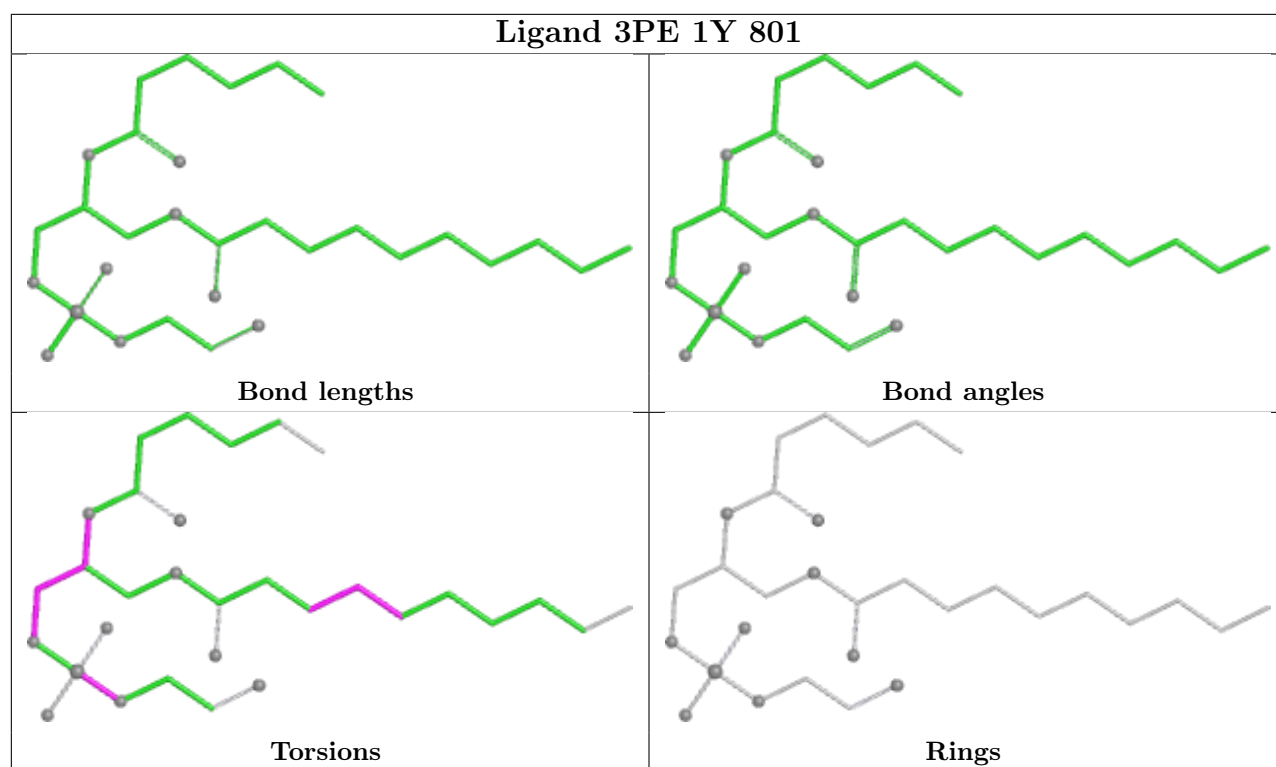


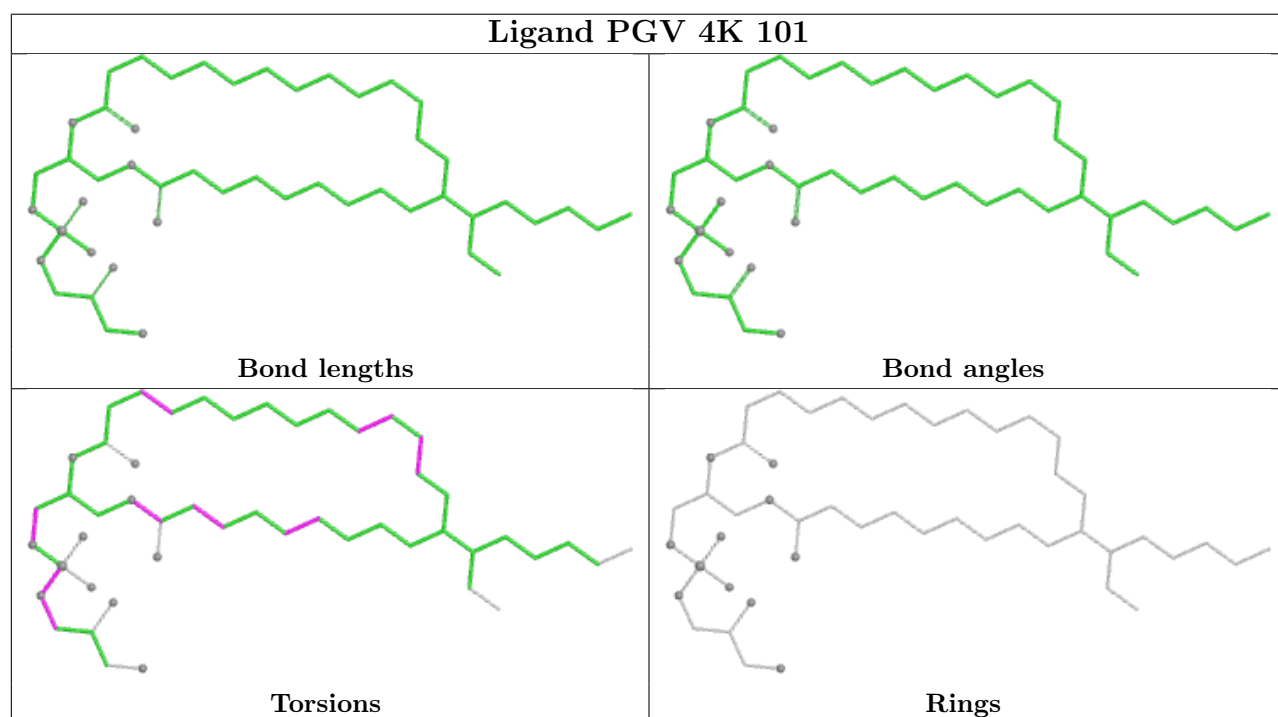
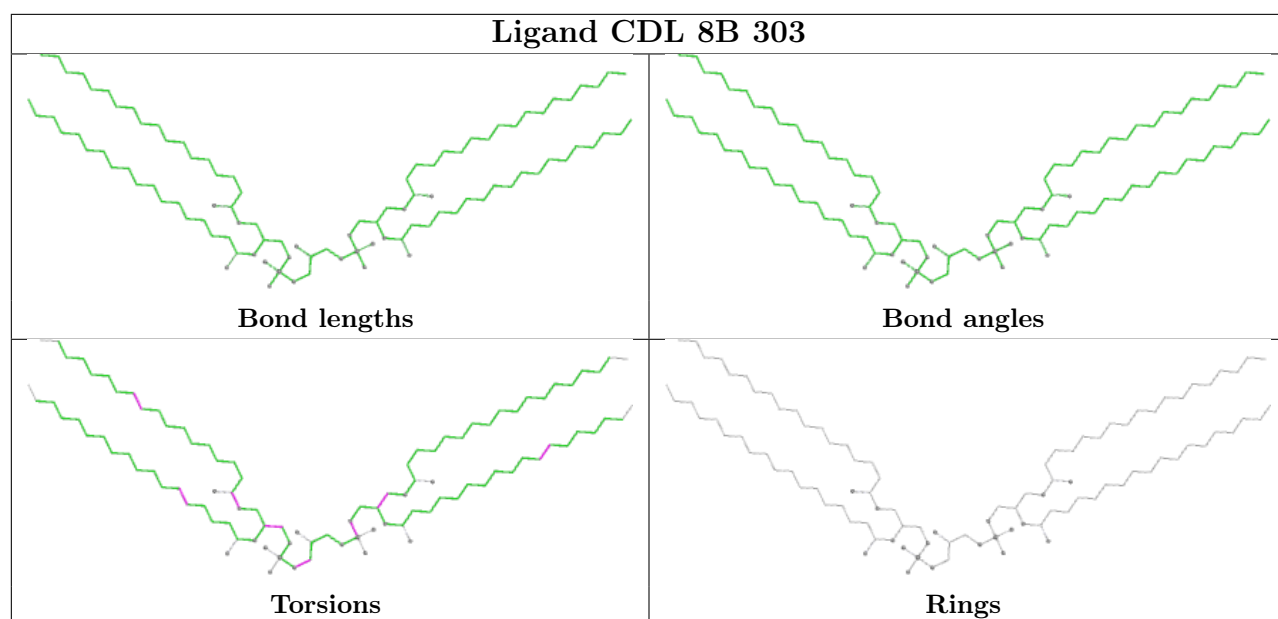


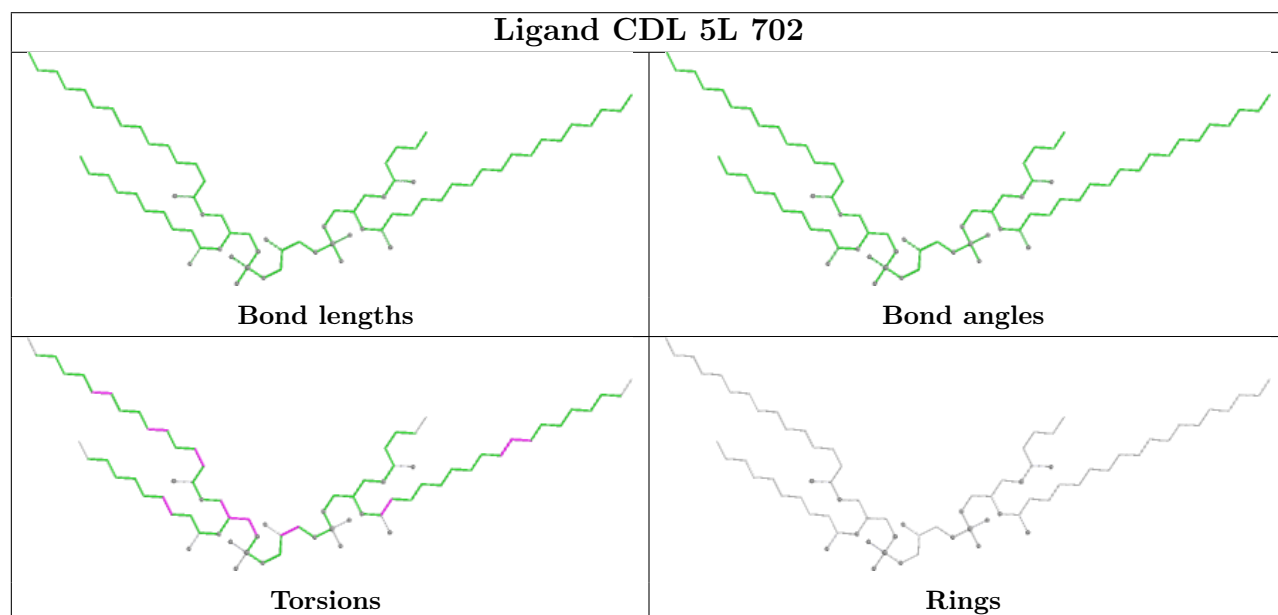
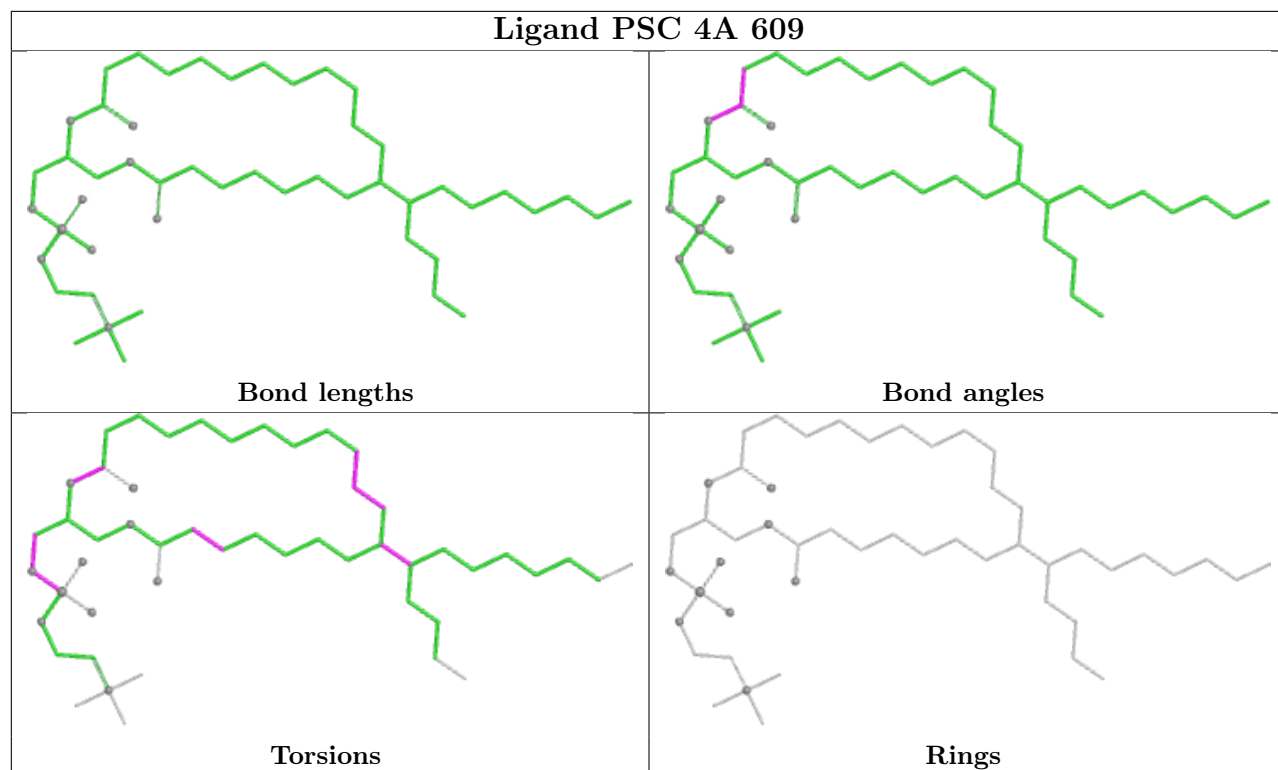


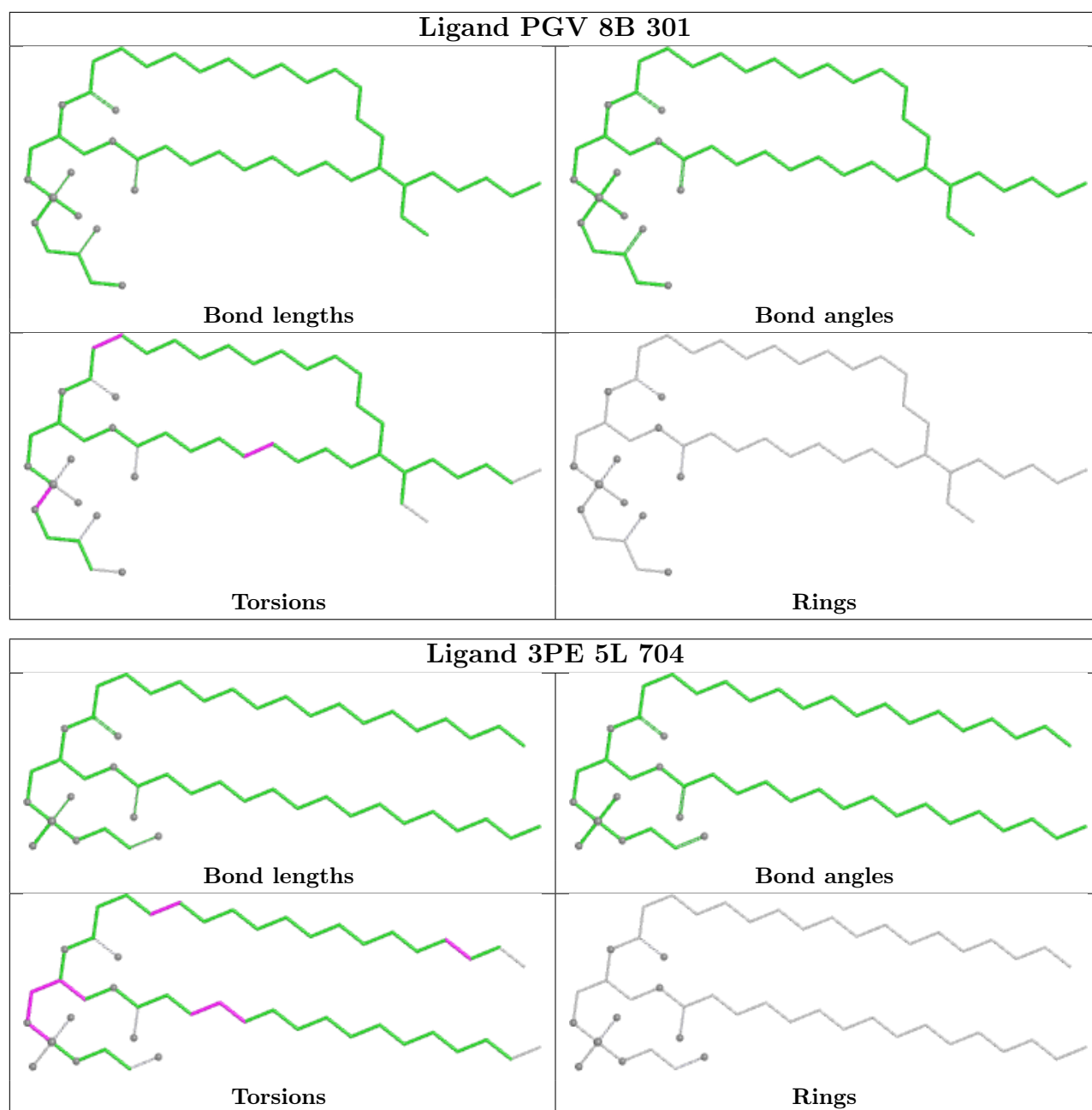


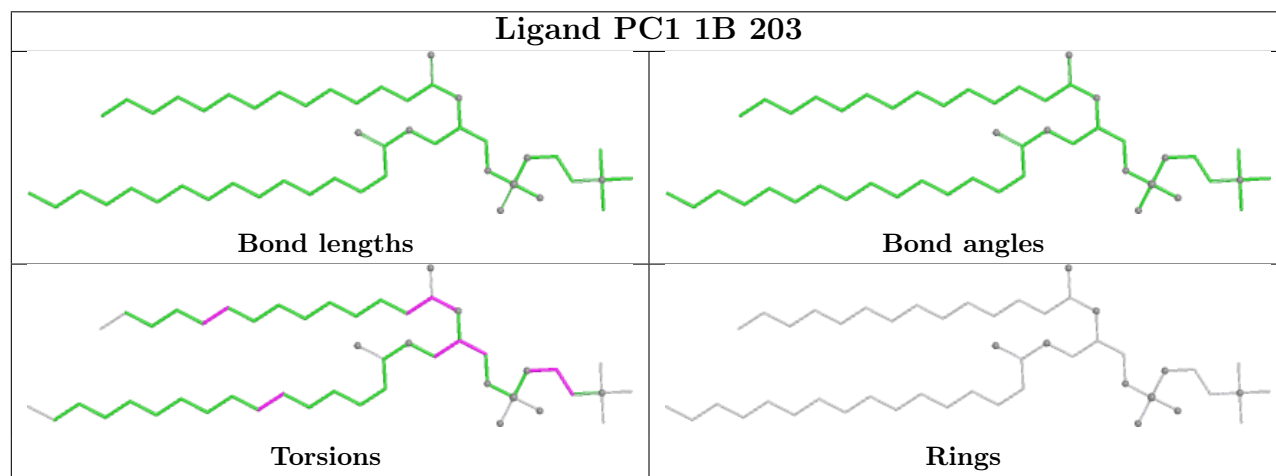
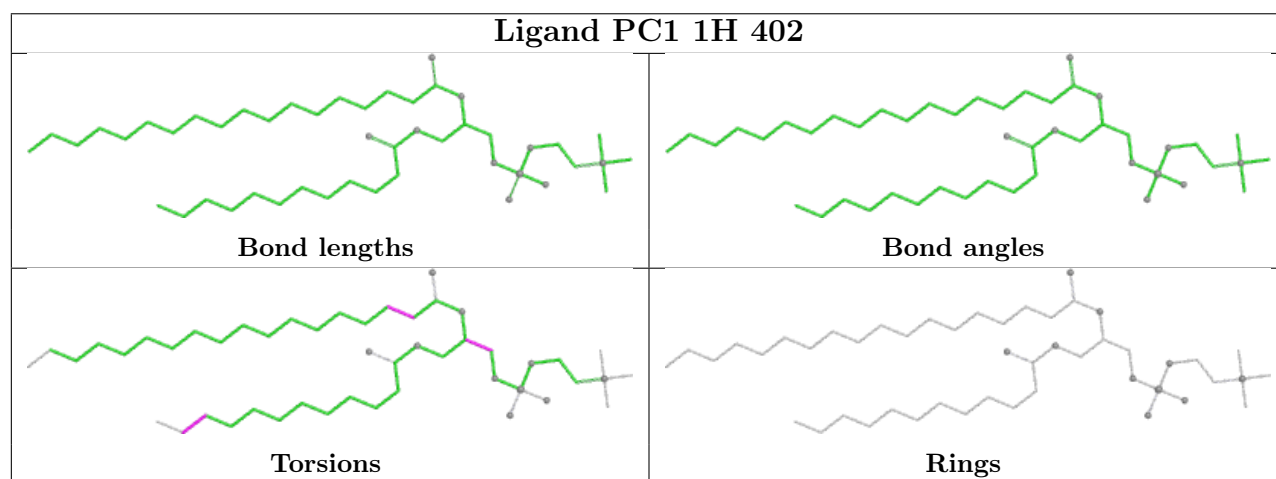
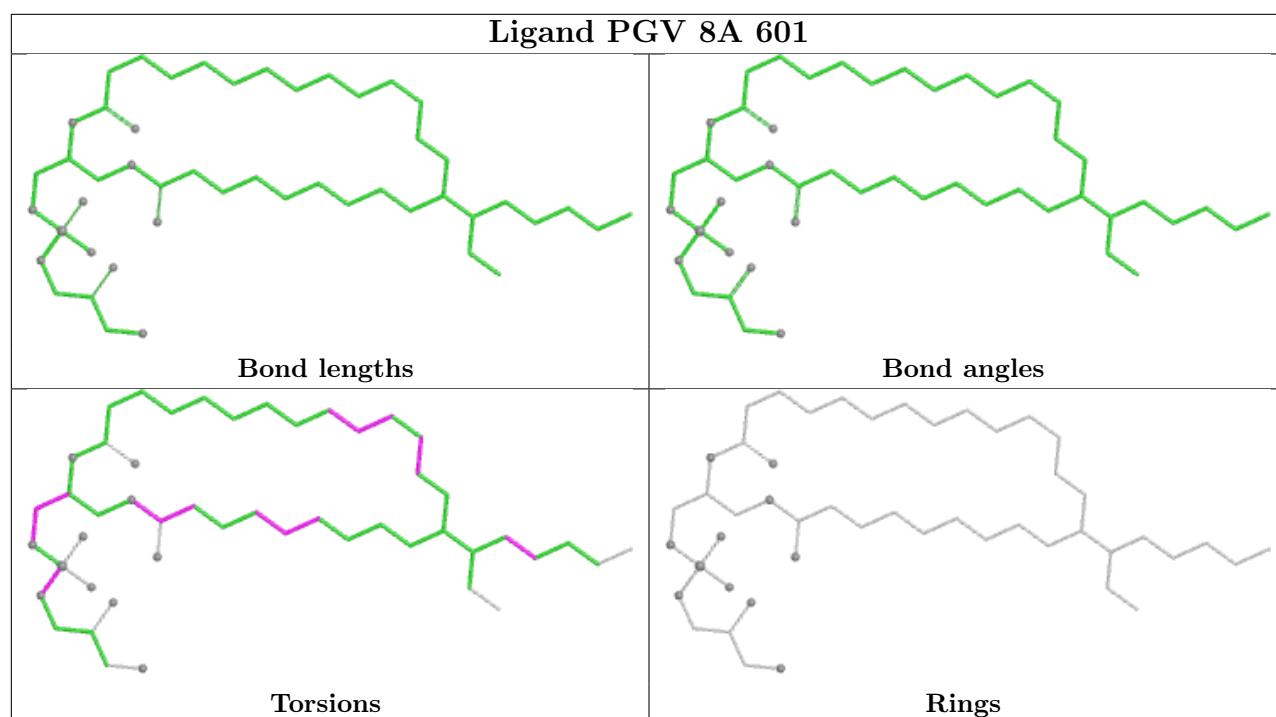


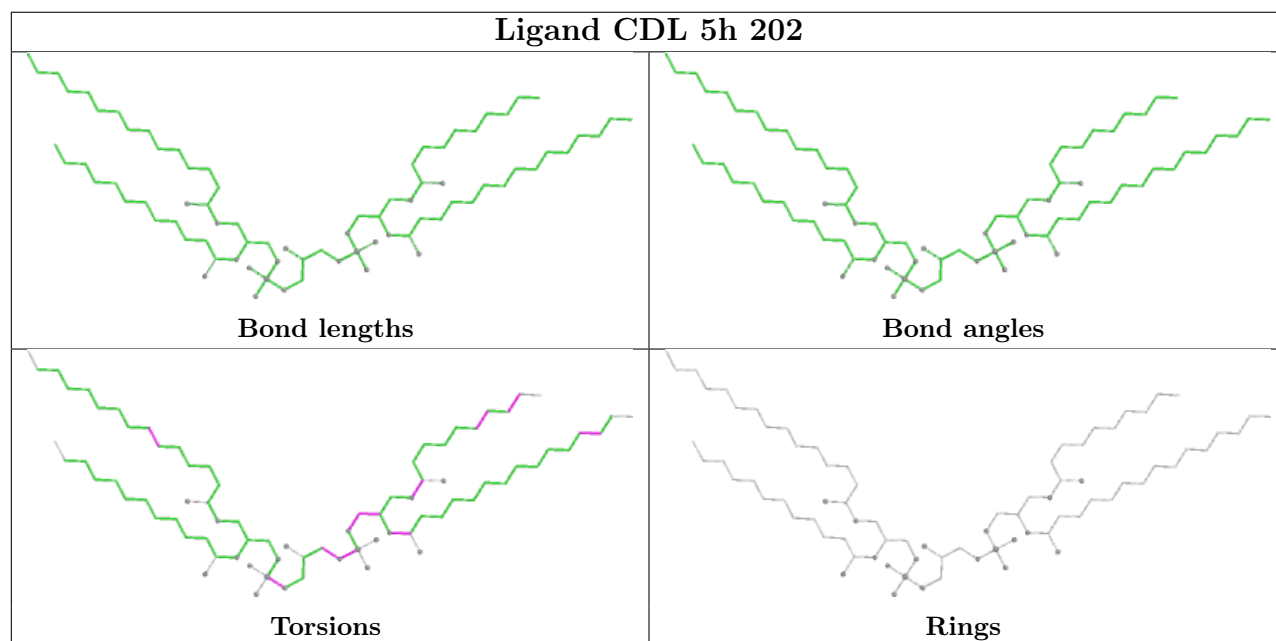
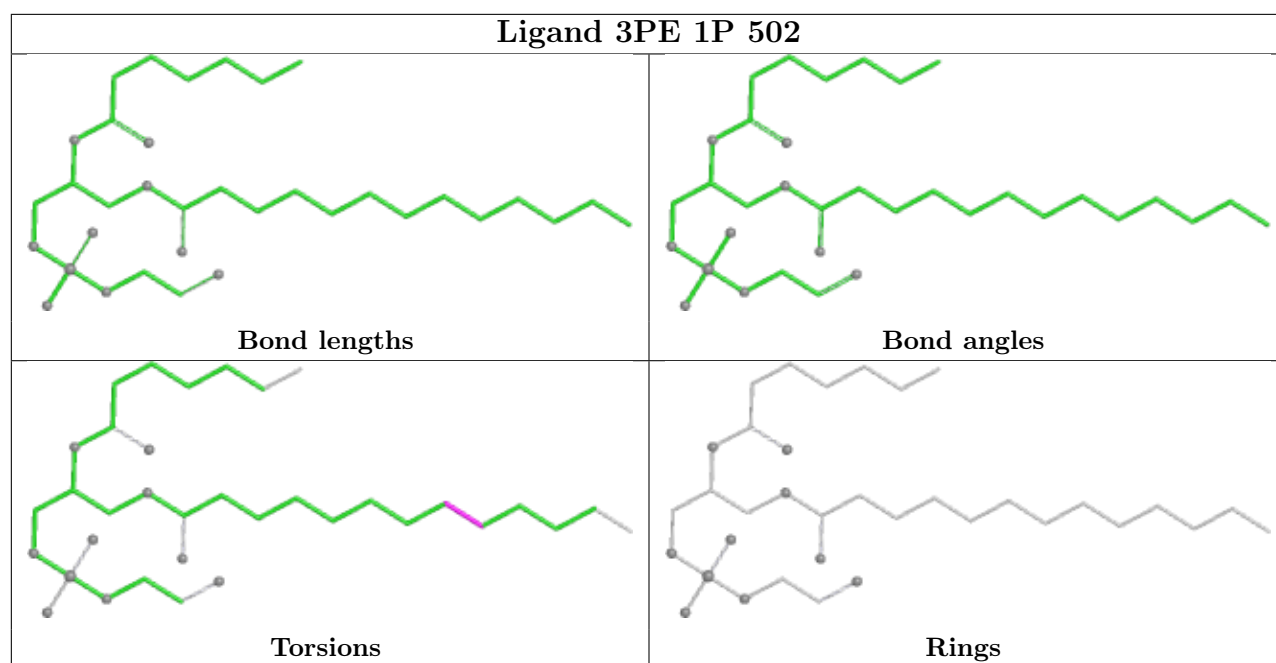


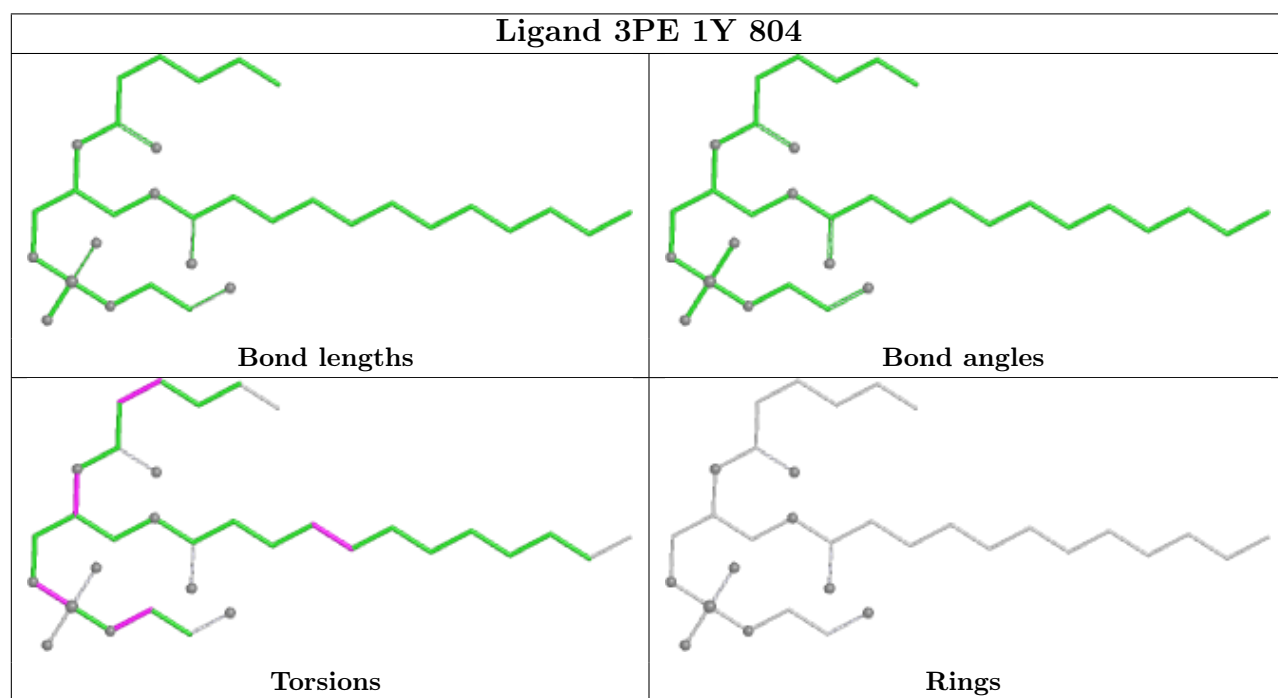
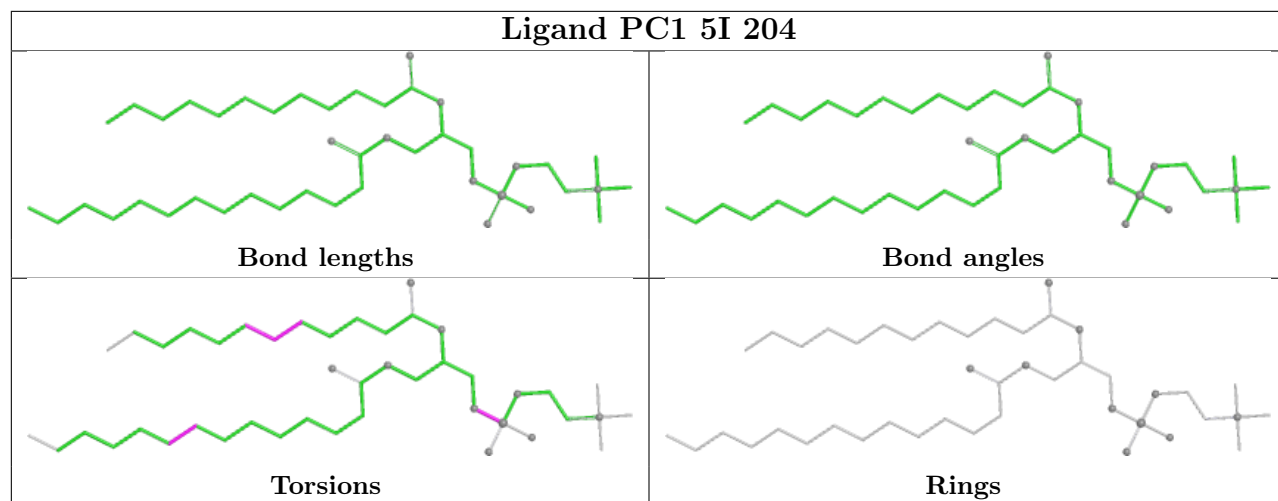


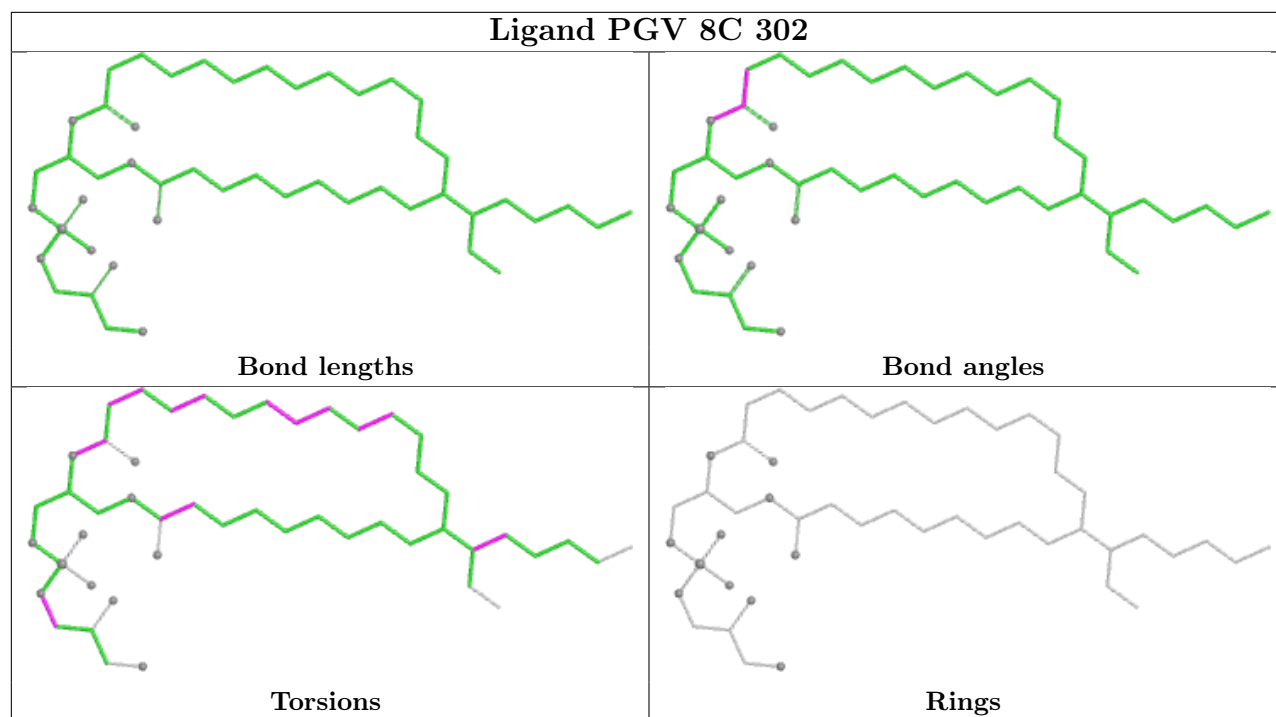
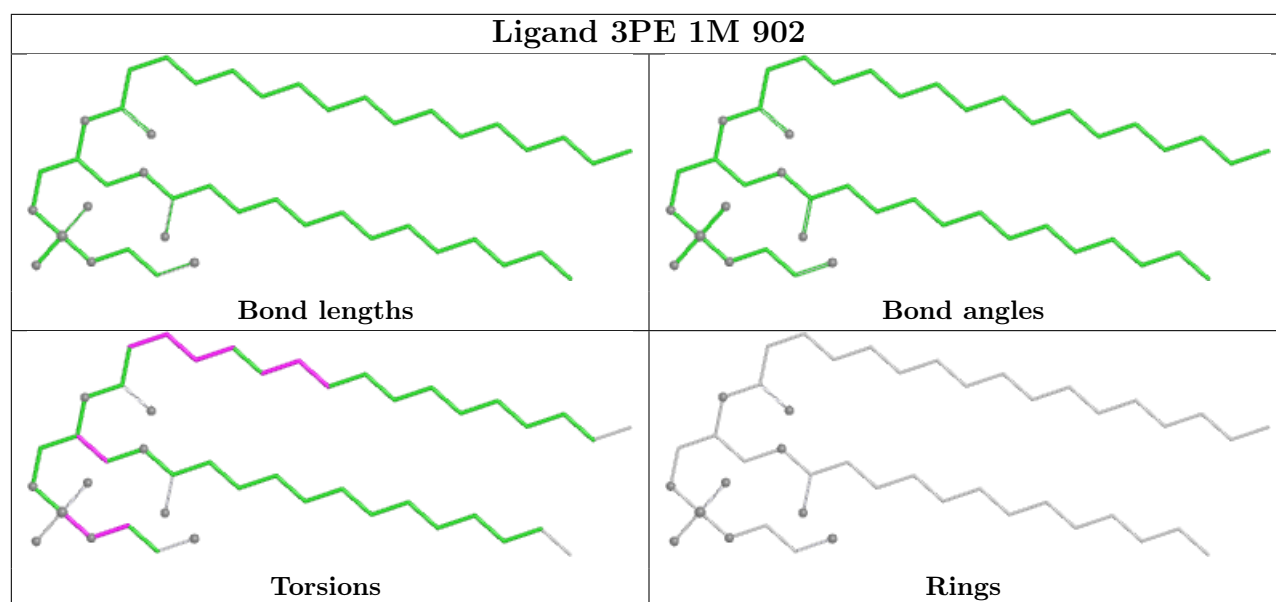


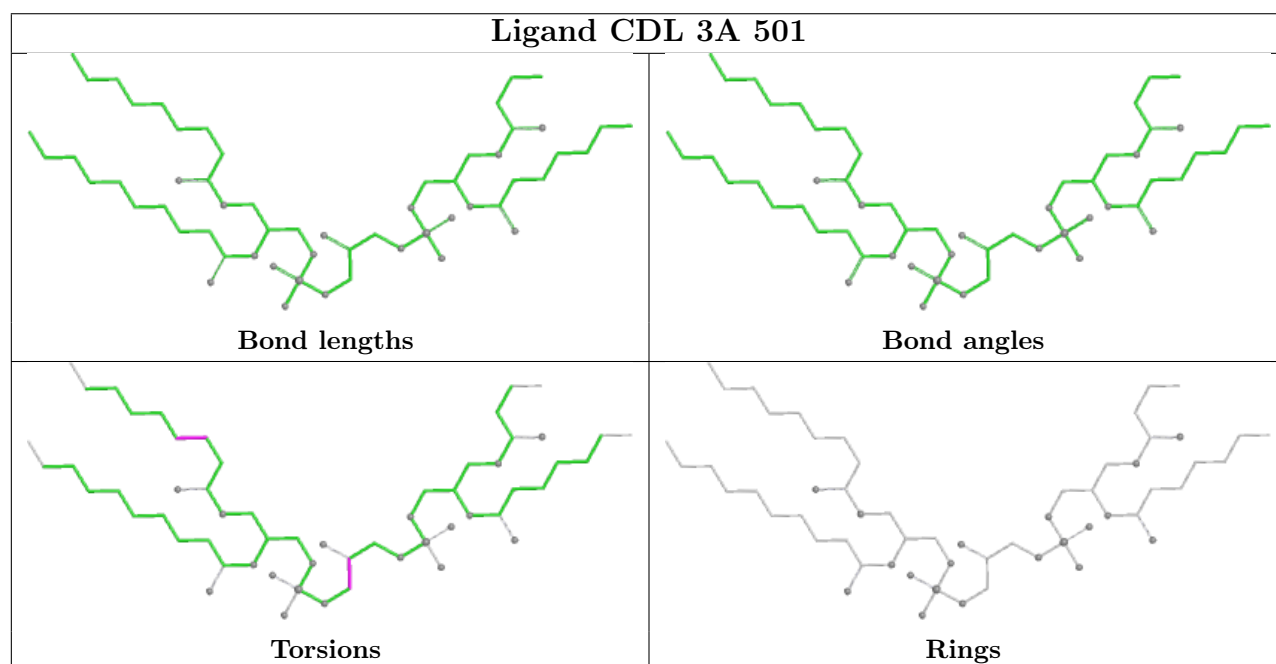
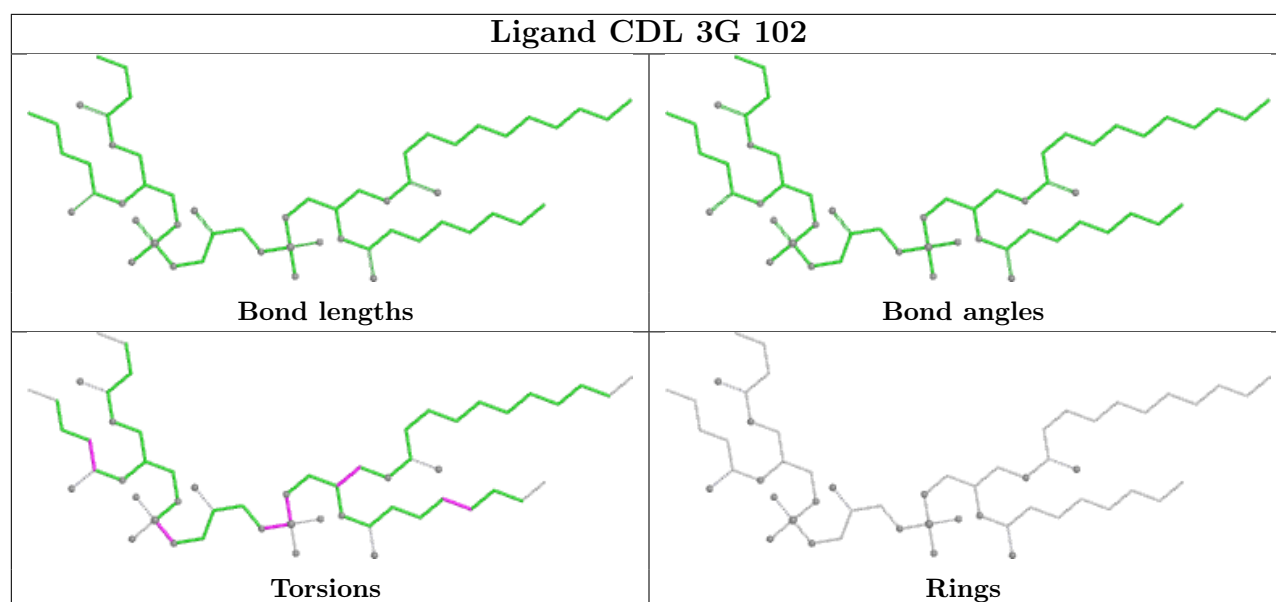


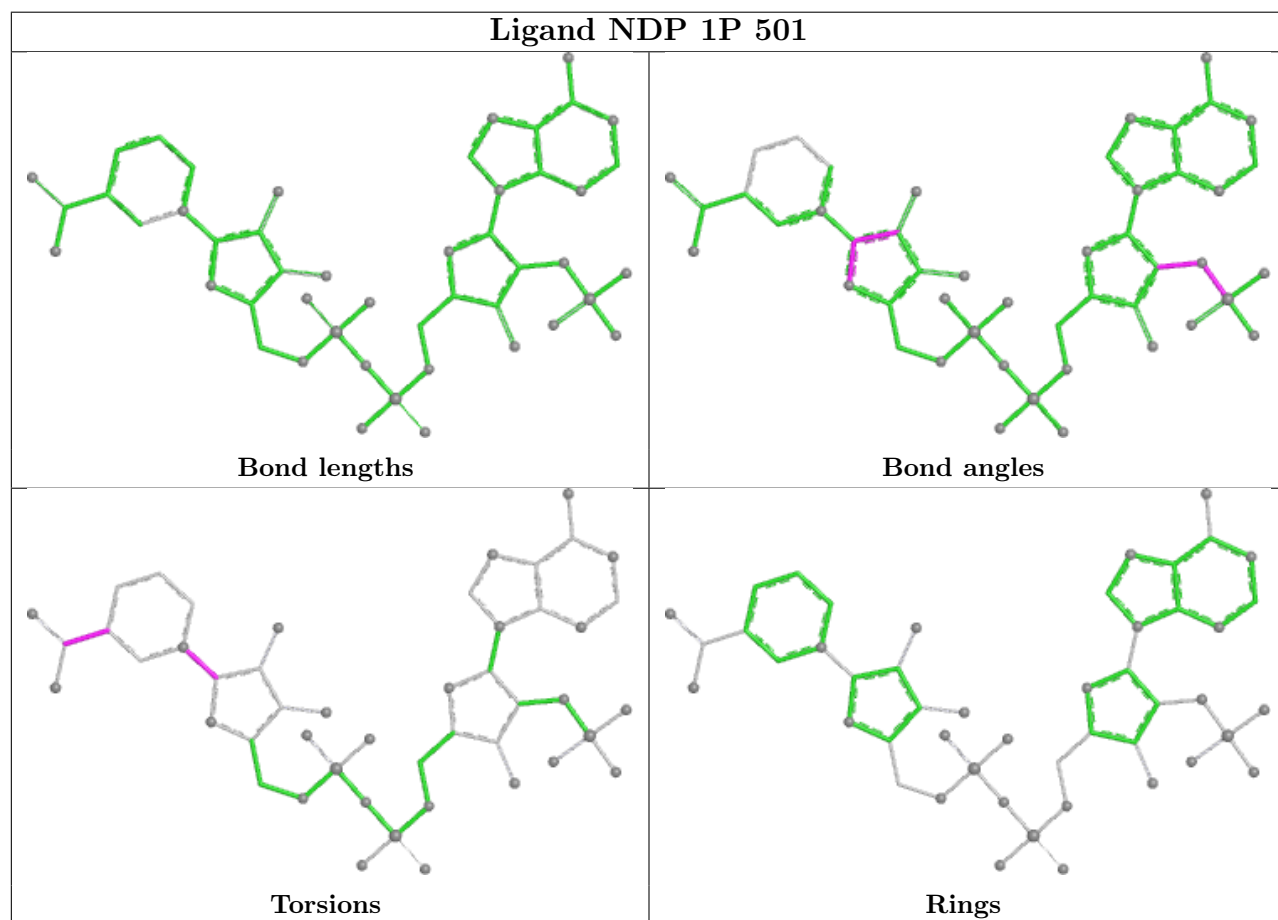
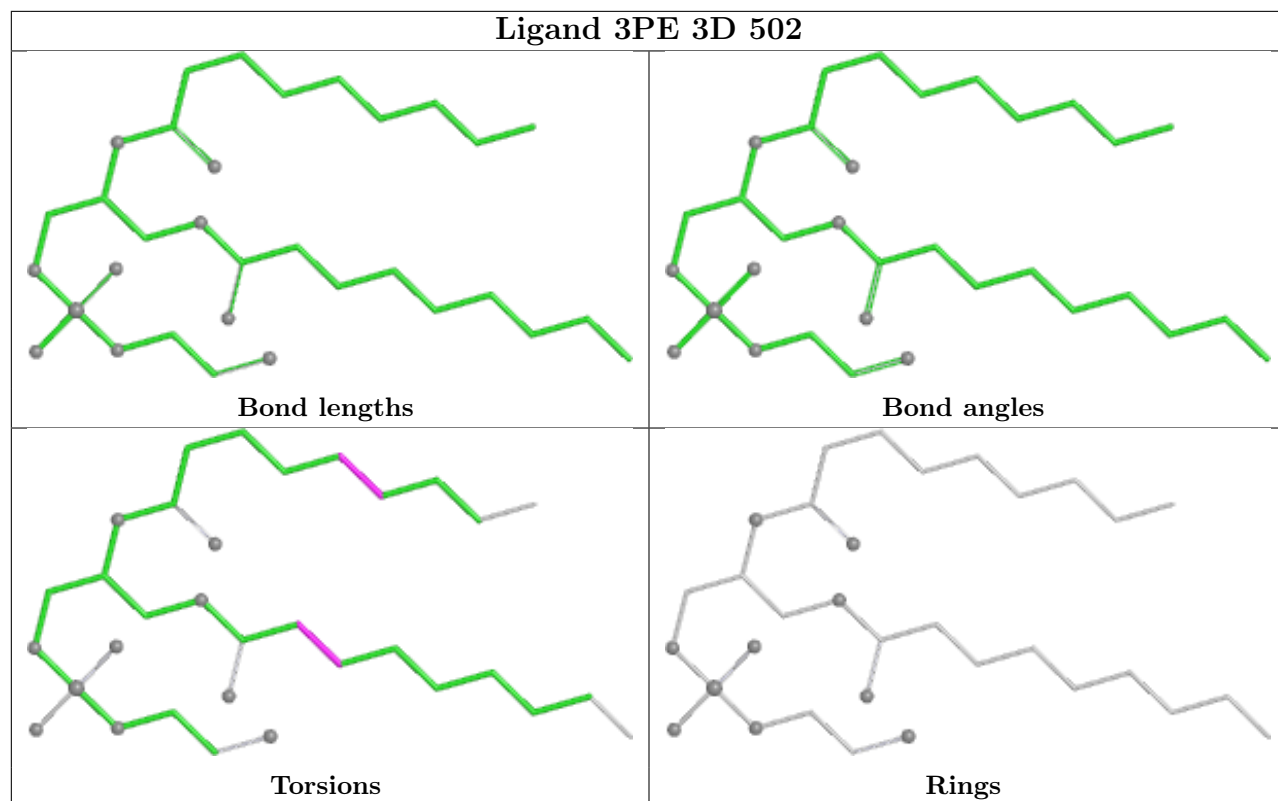




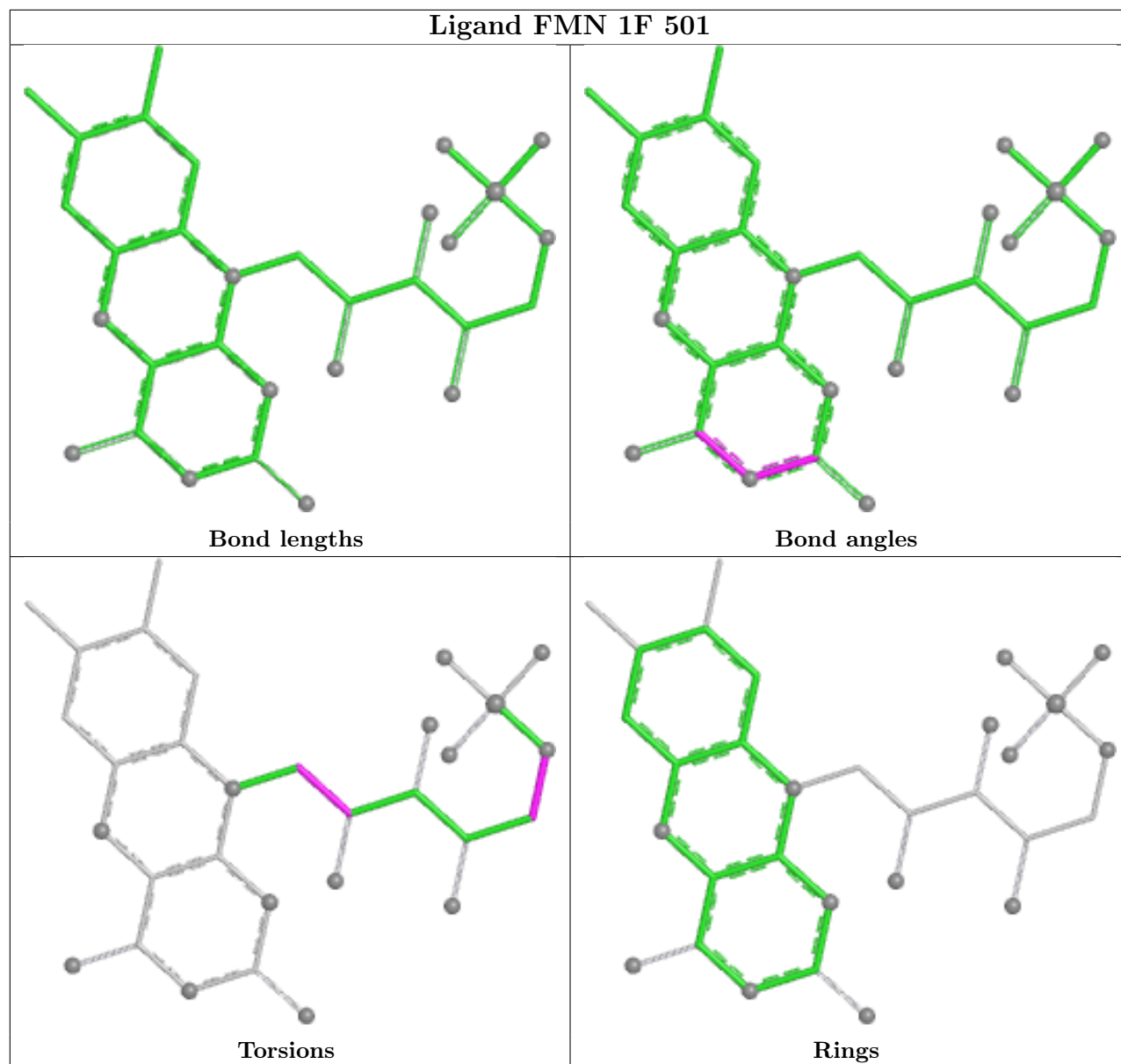


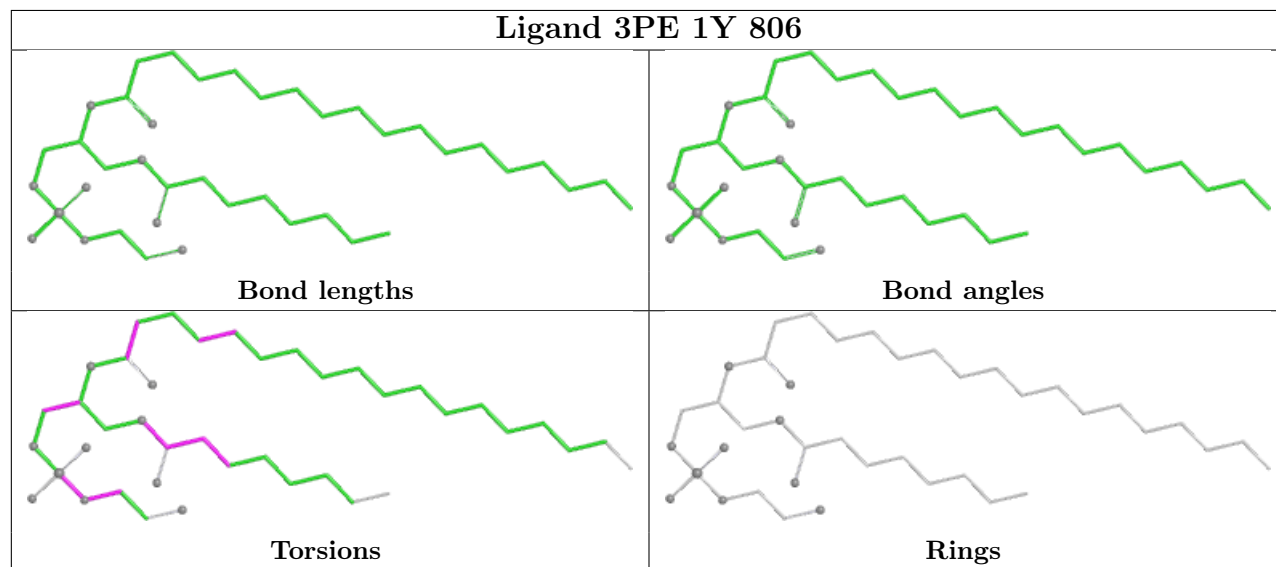
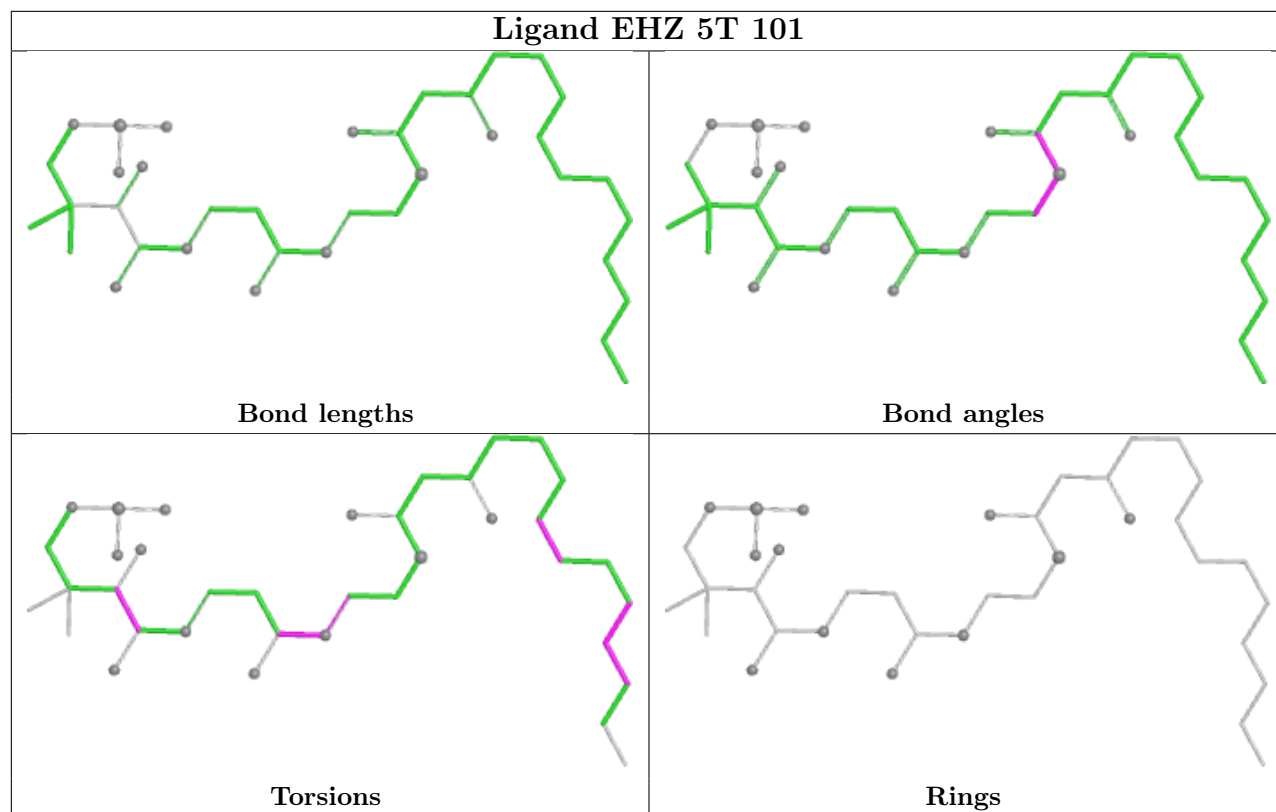




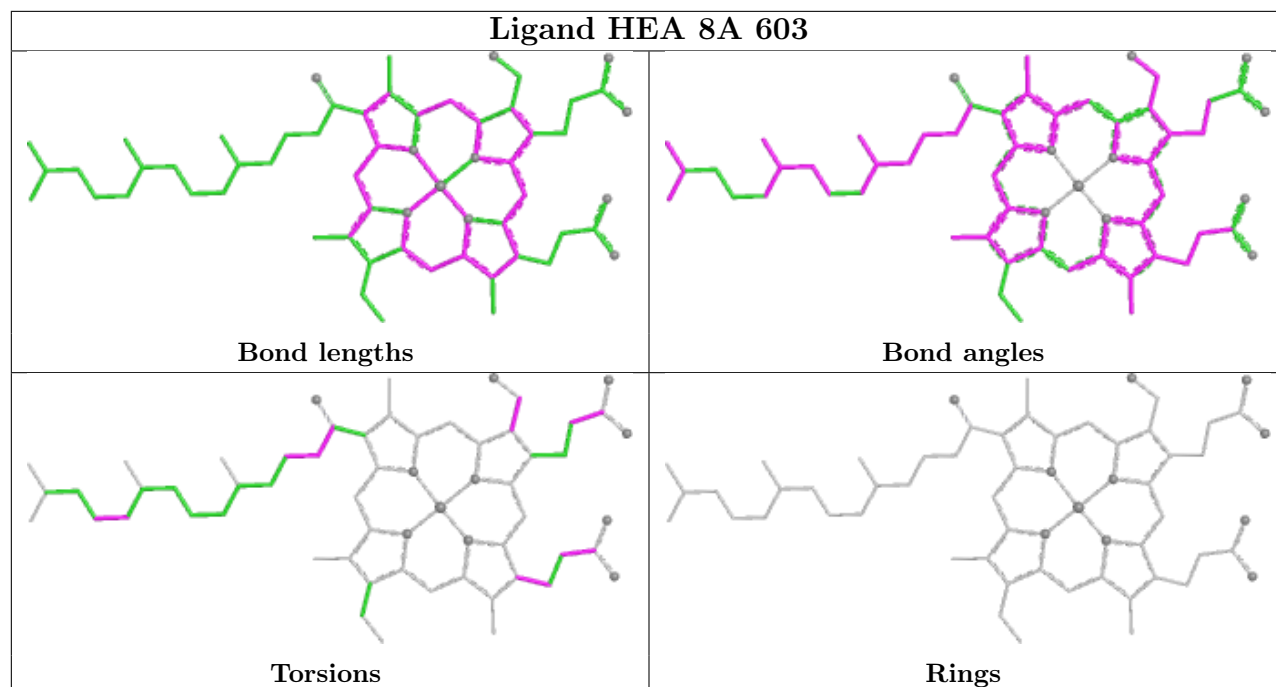


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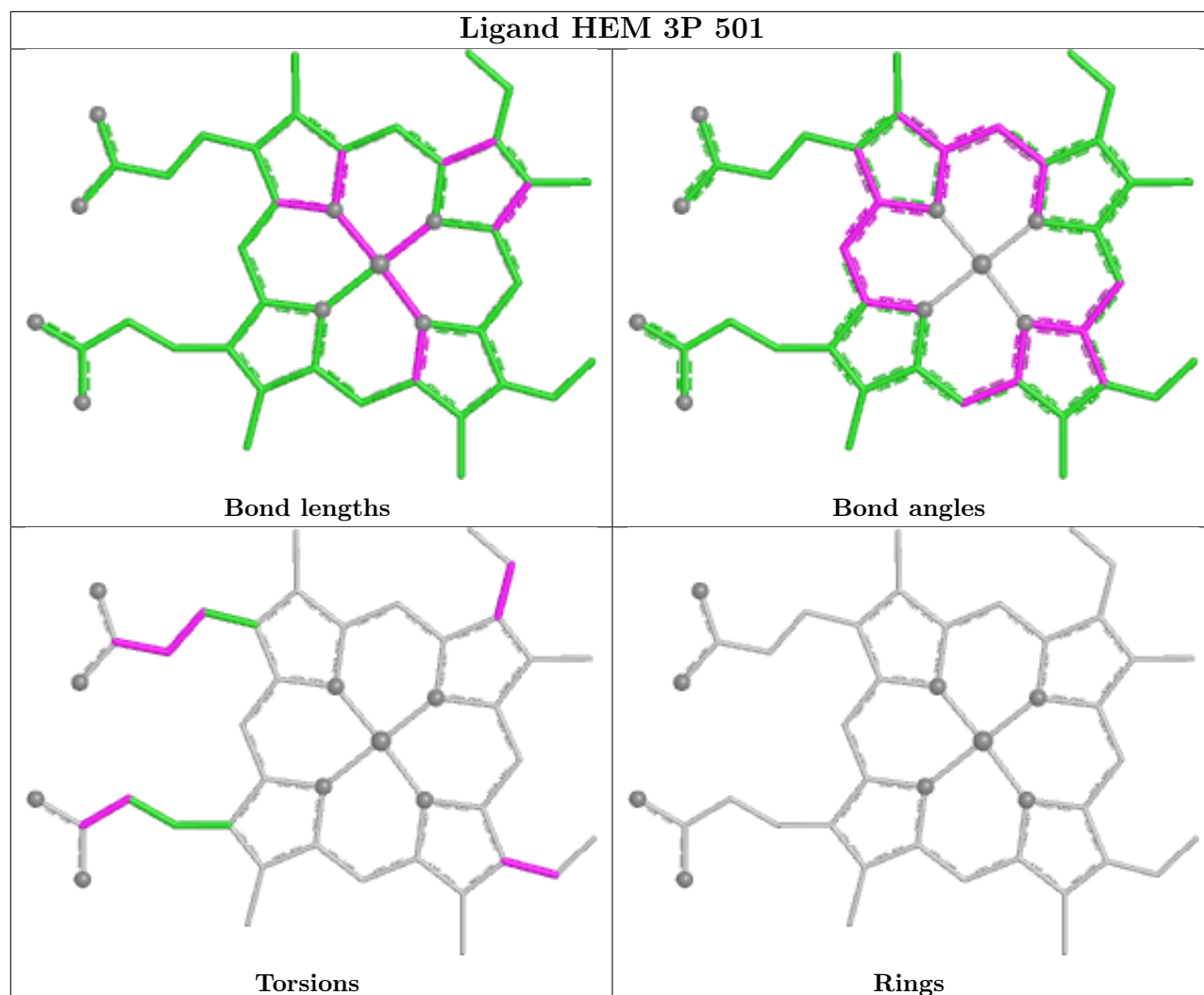


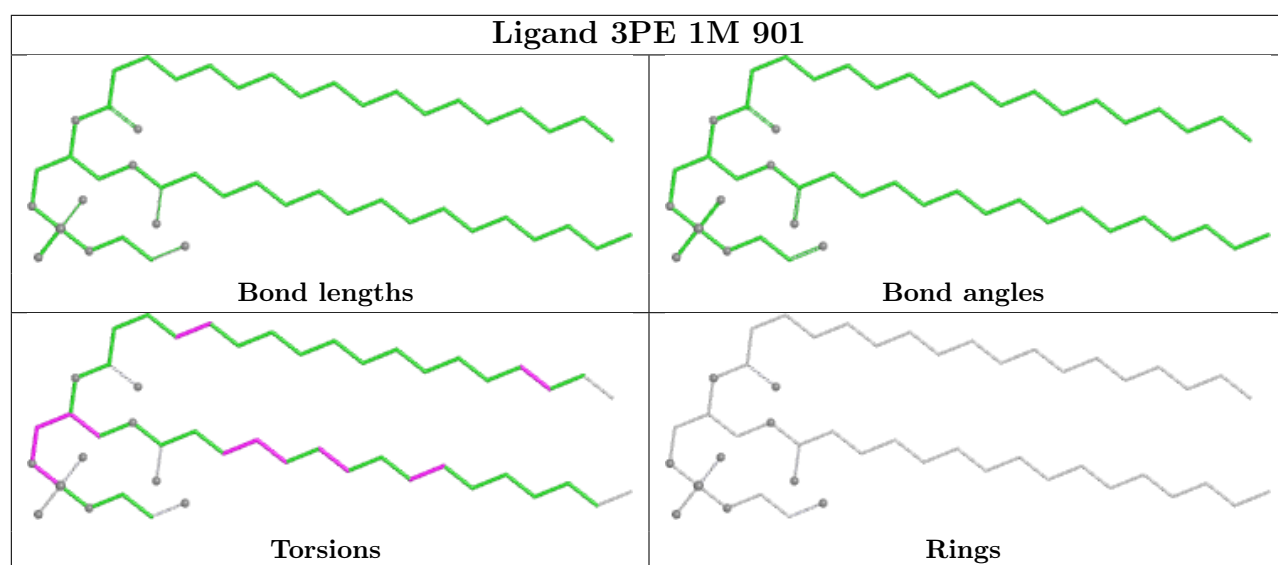
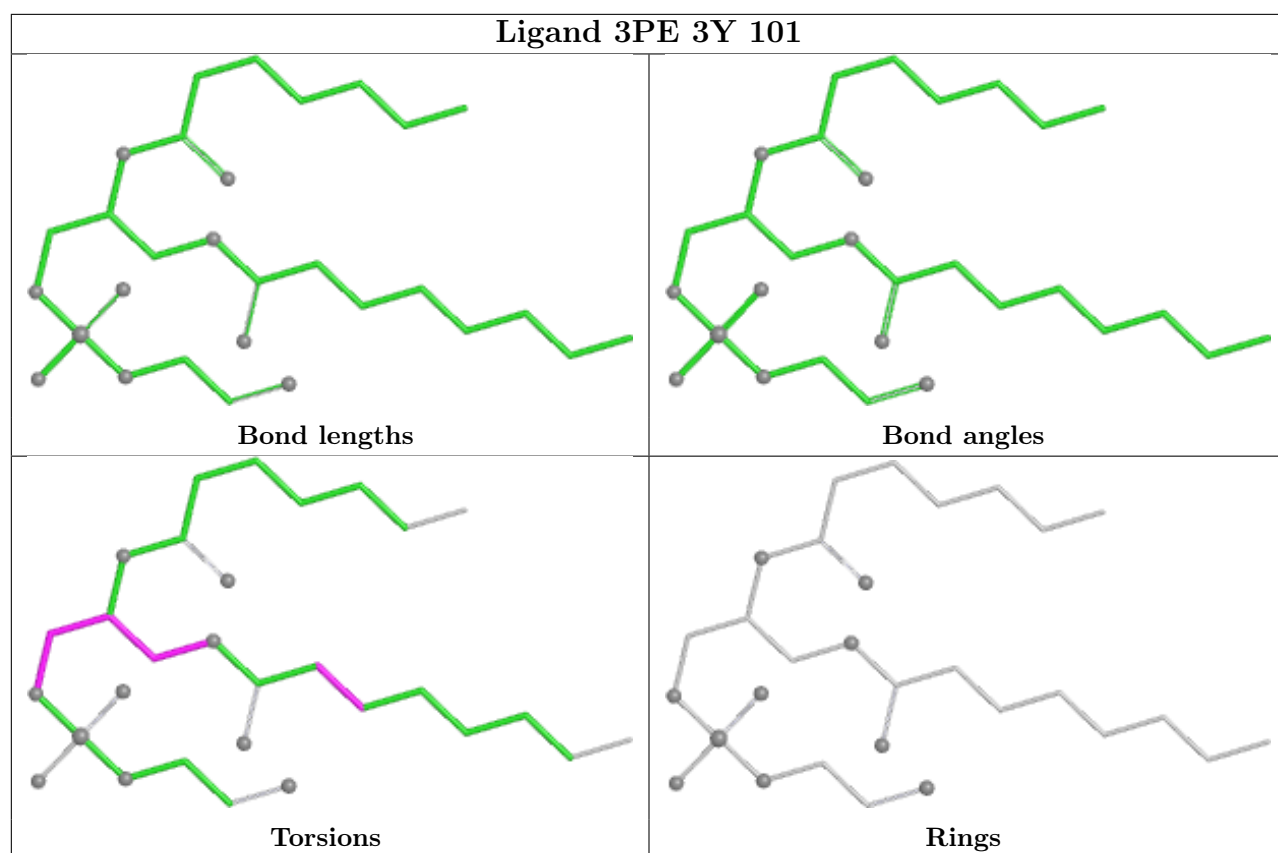


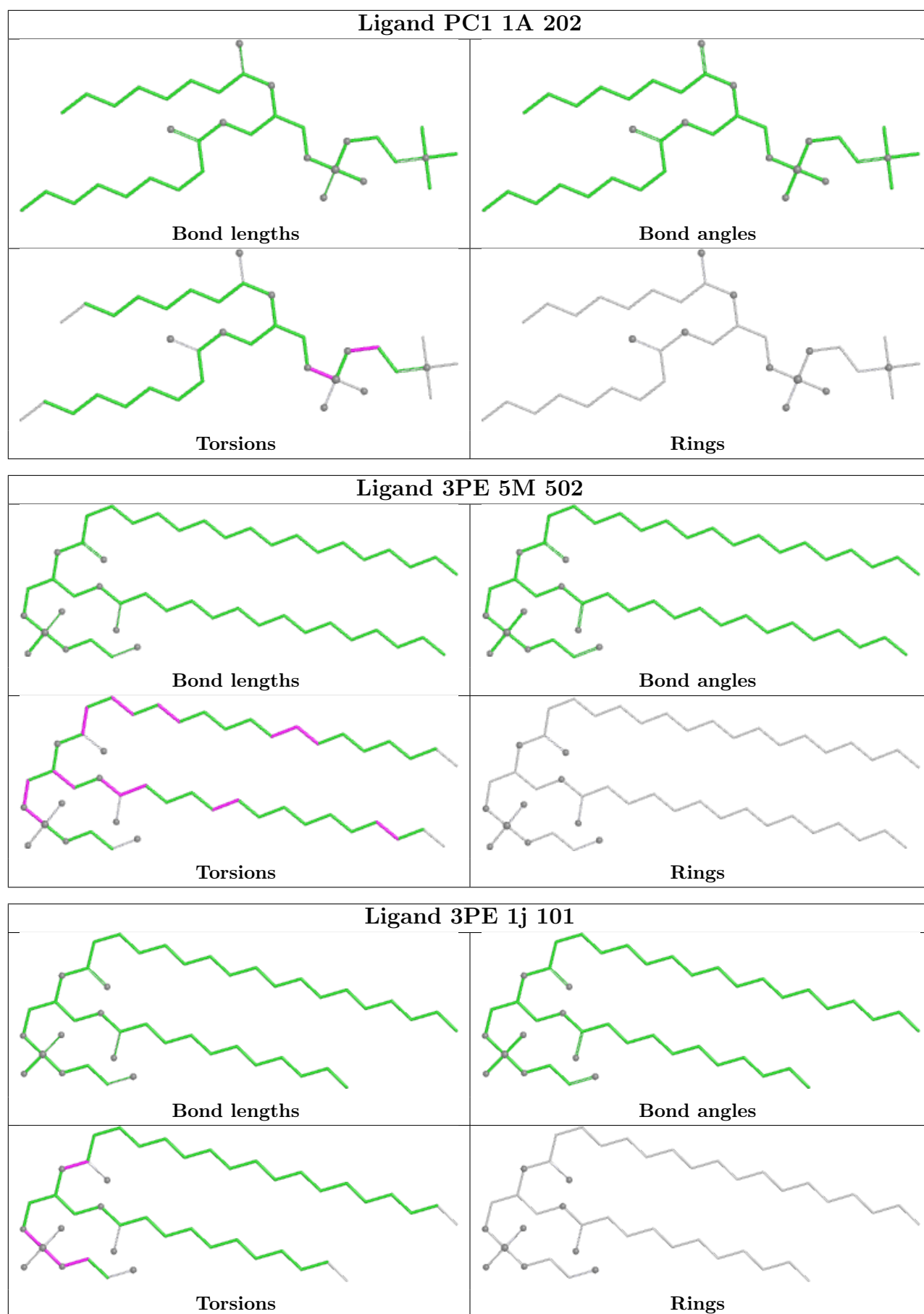
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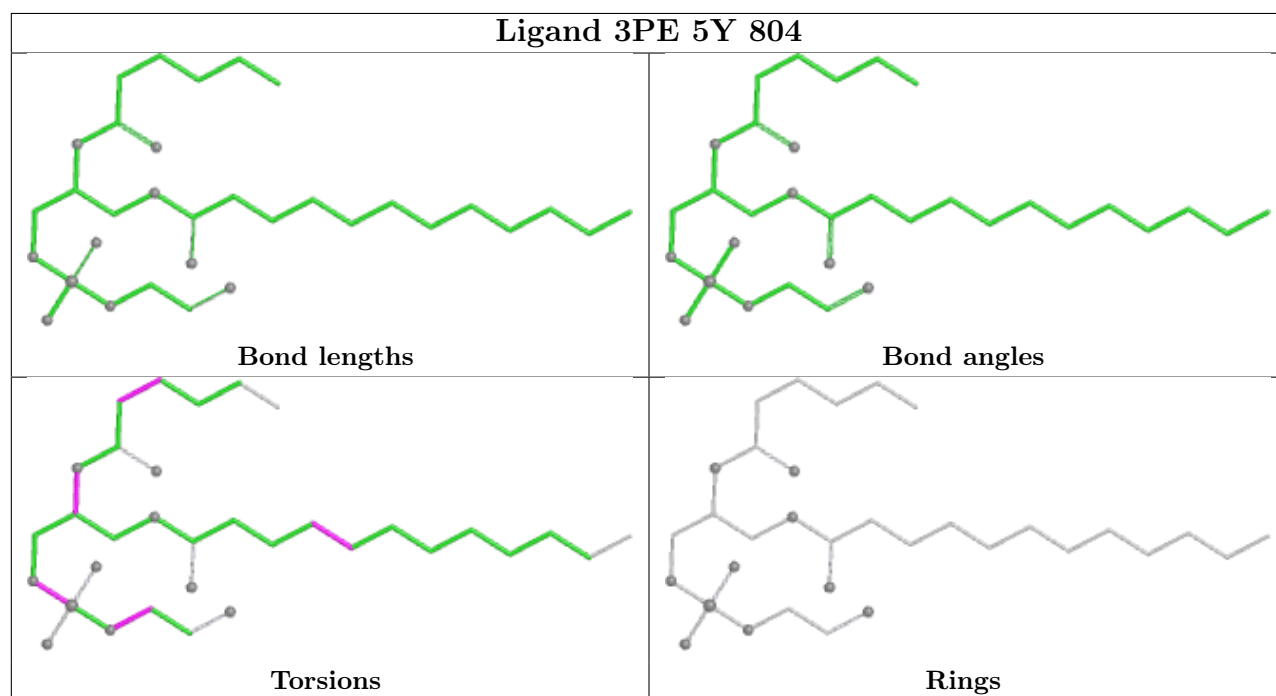
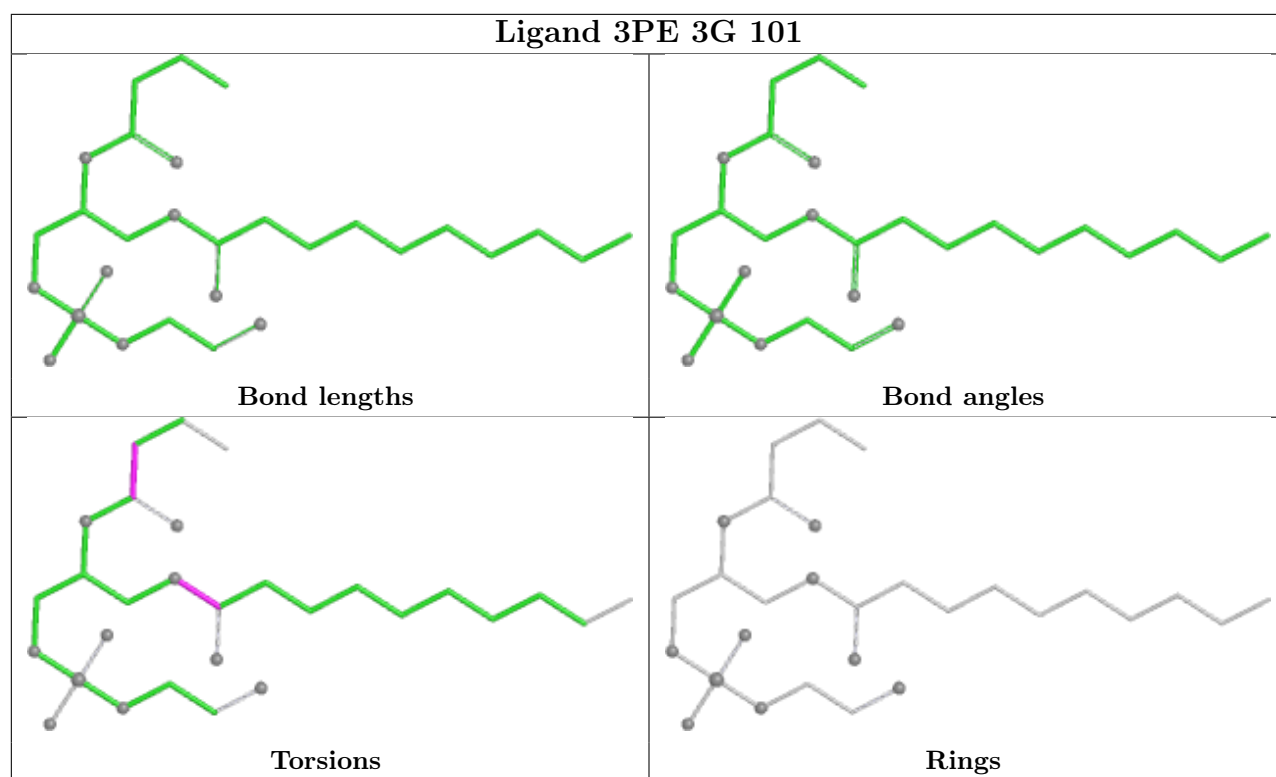


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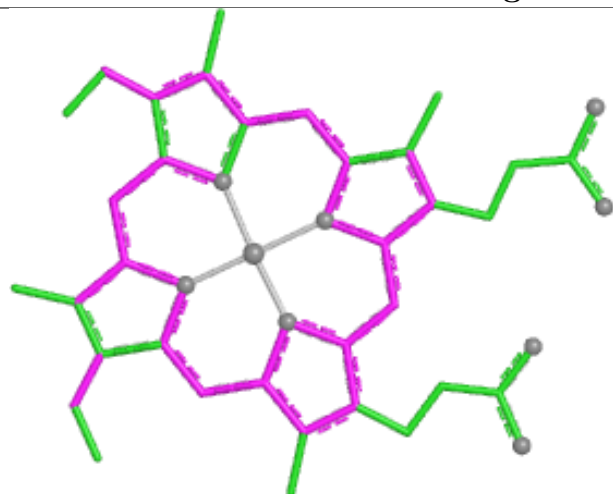




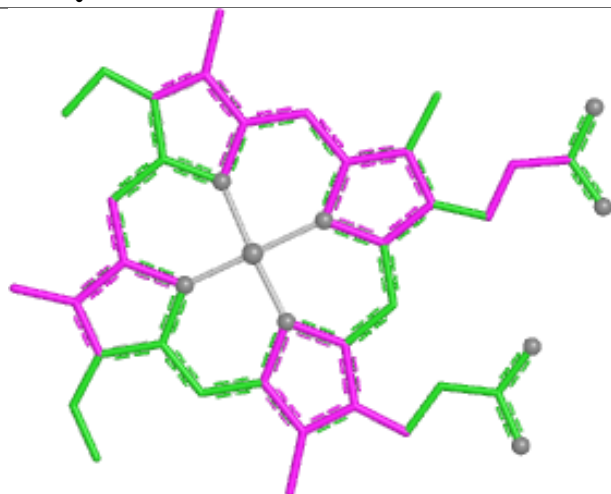




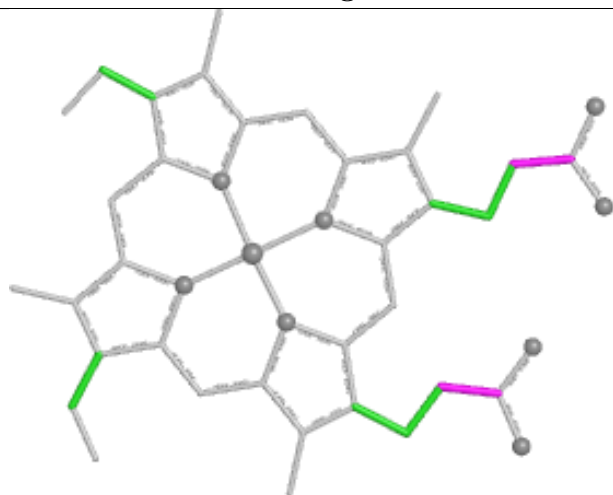
Ligand HEC 3Q 501



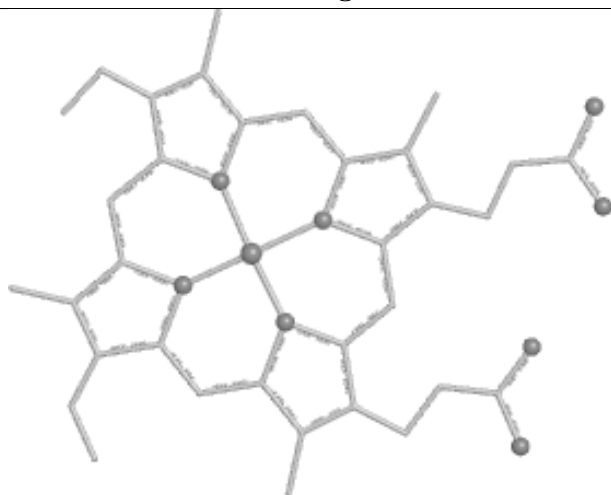
Bond lengths



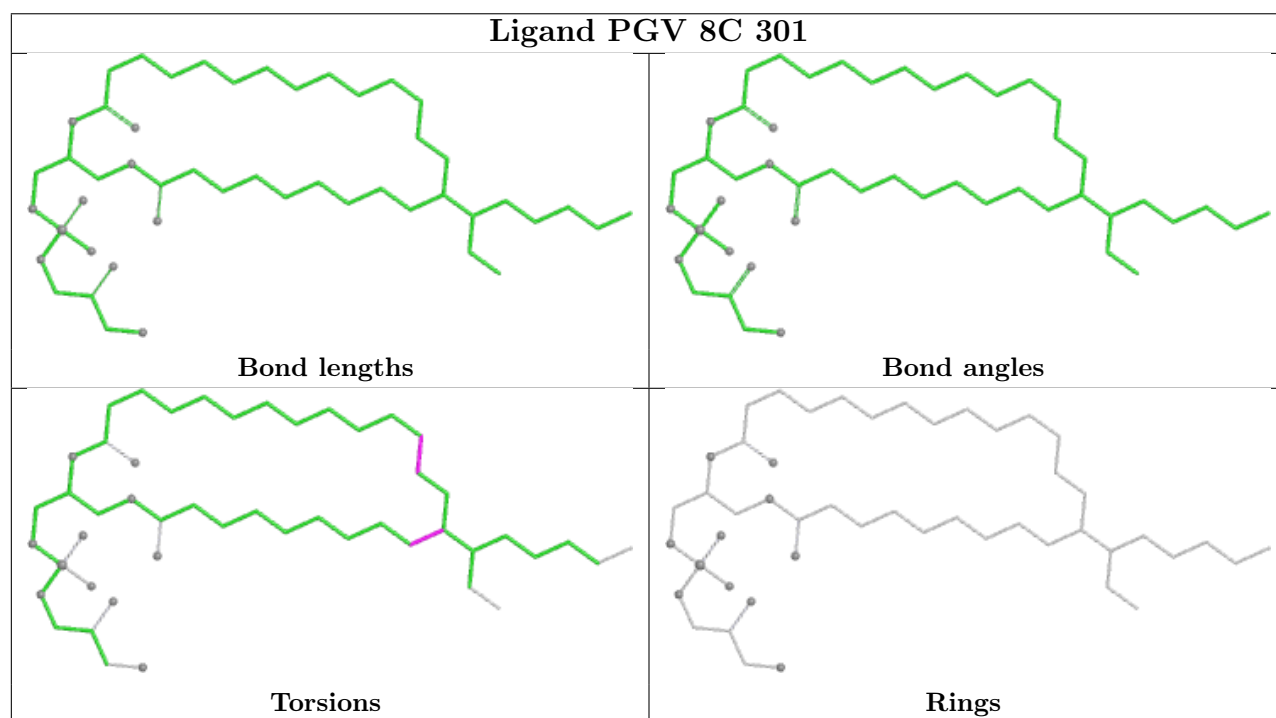
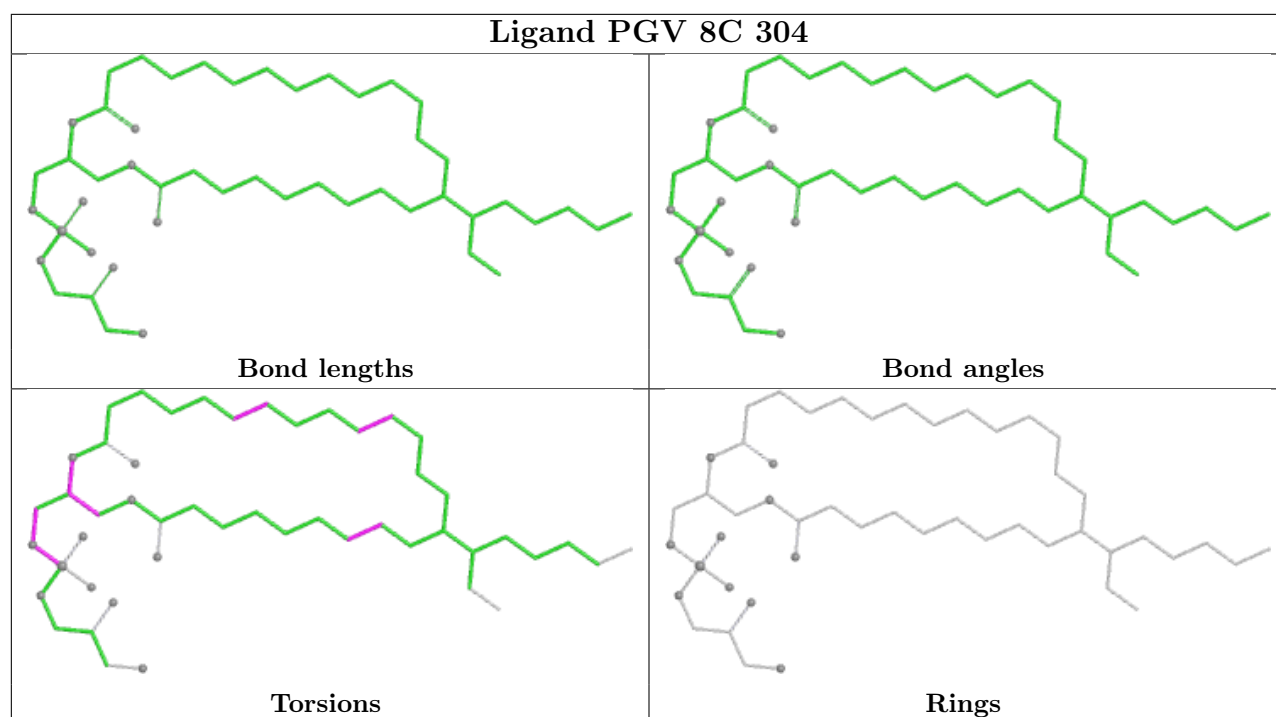
Bond angles

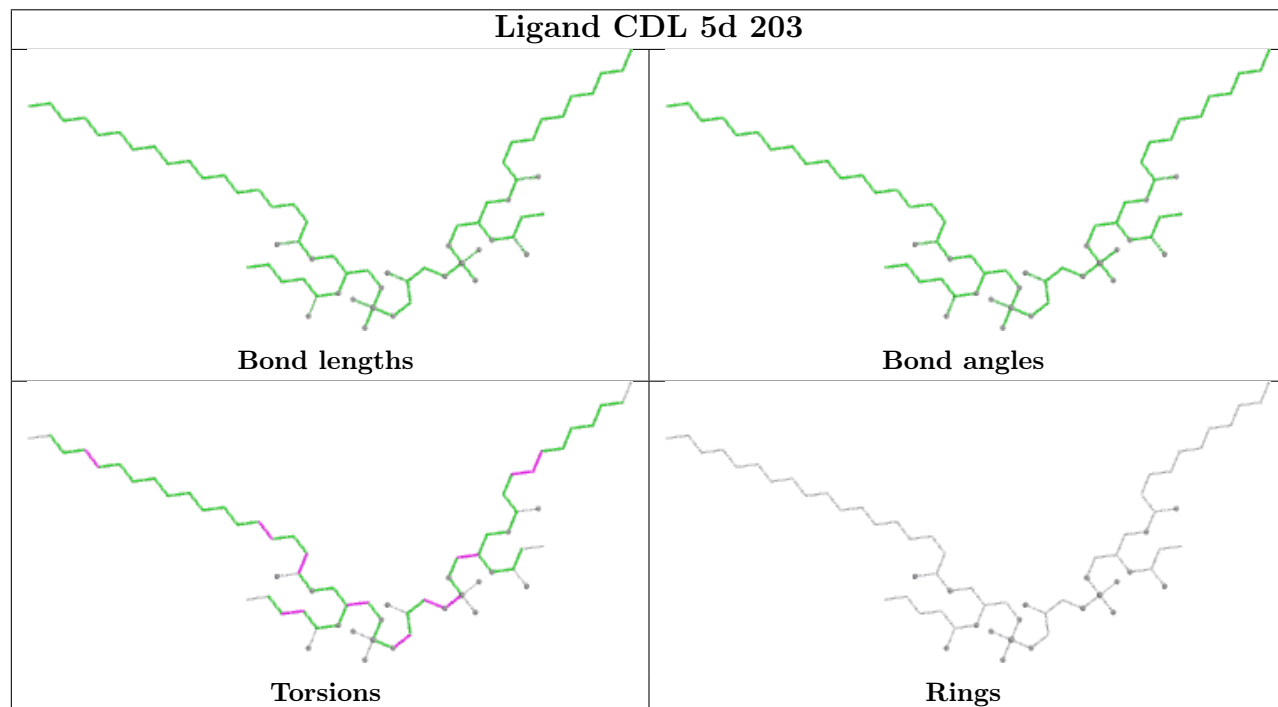
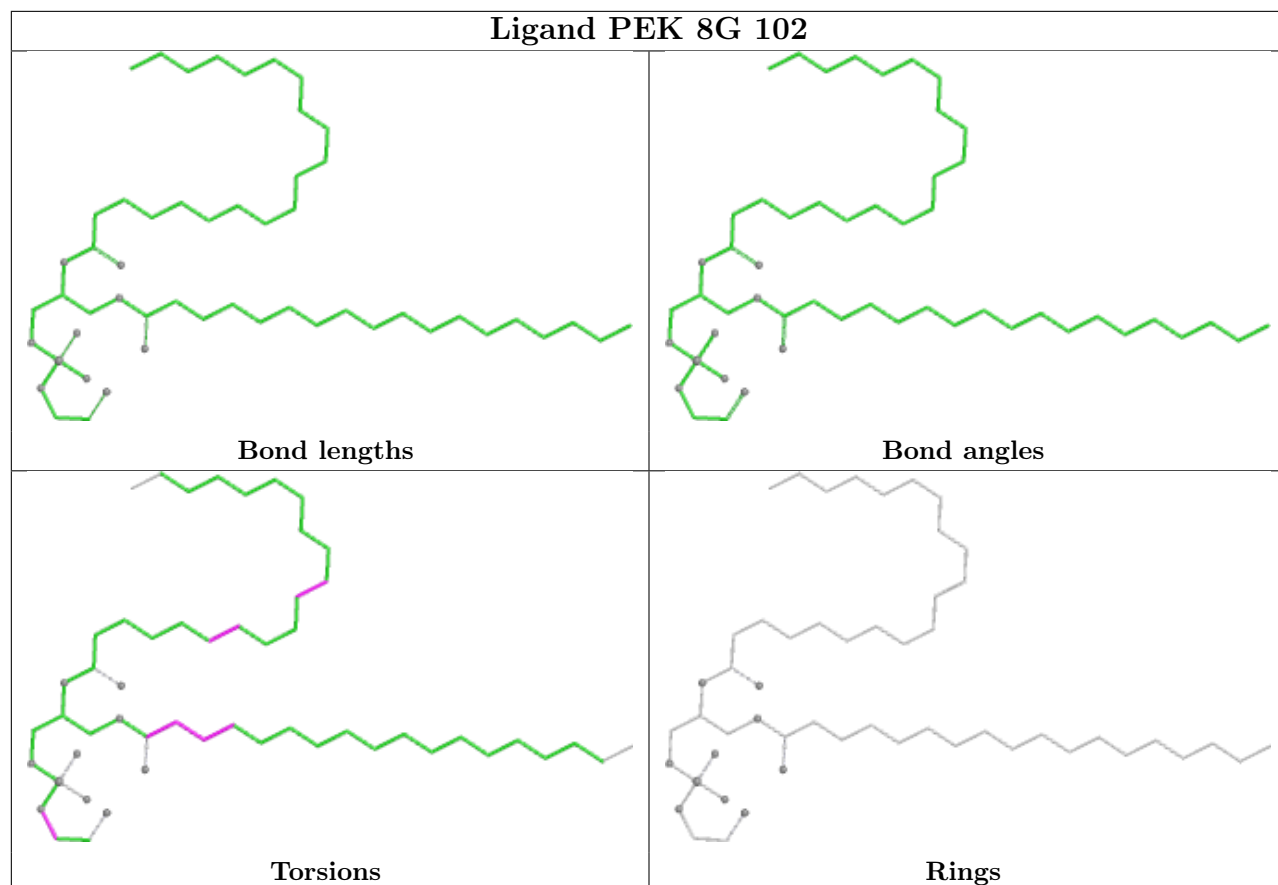


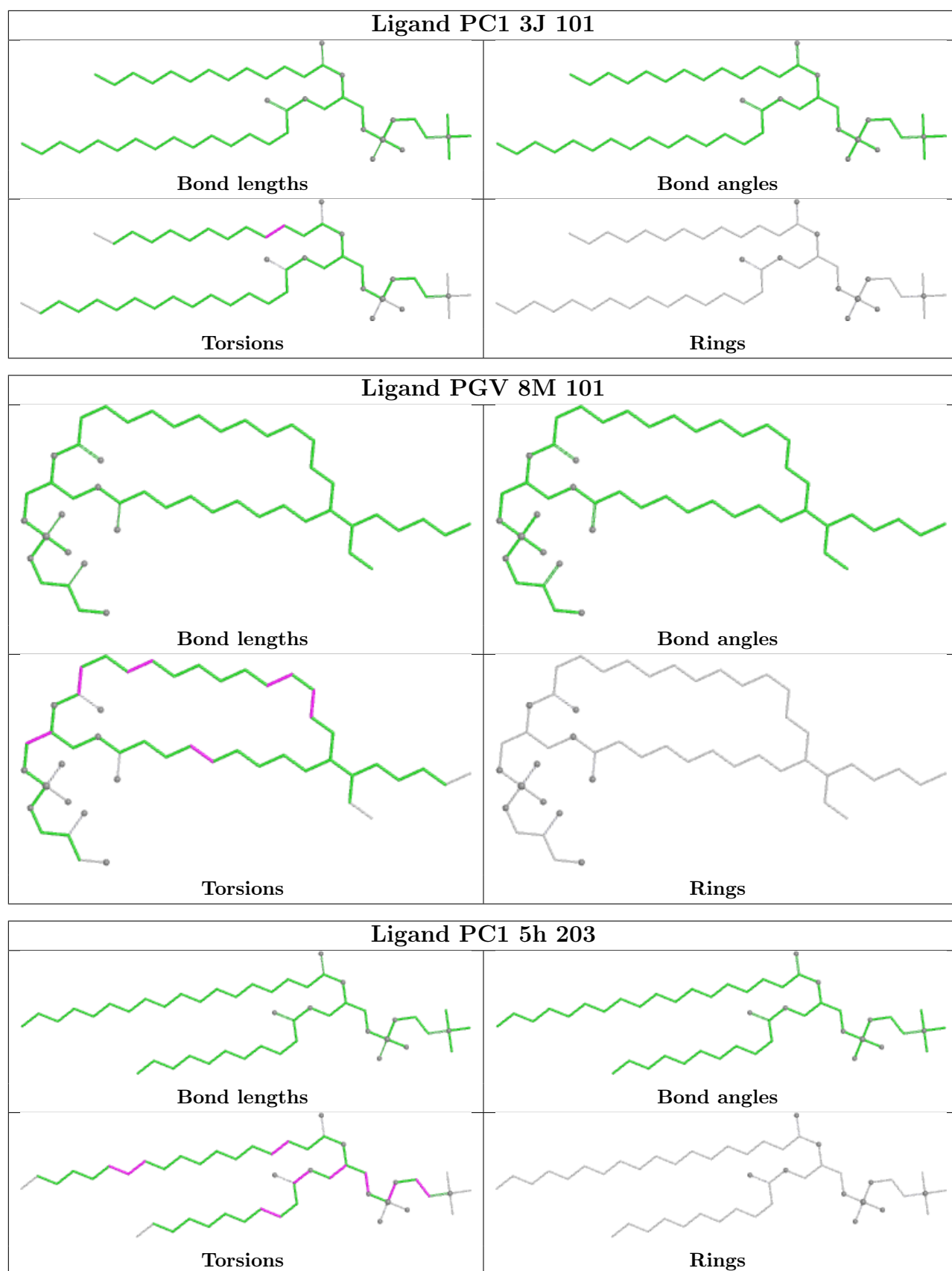
Torsions

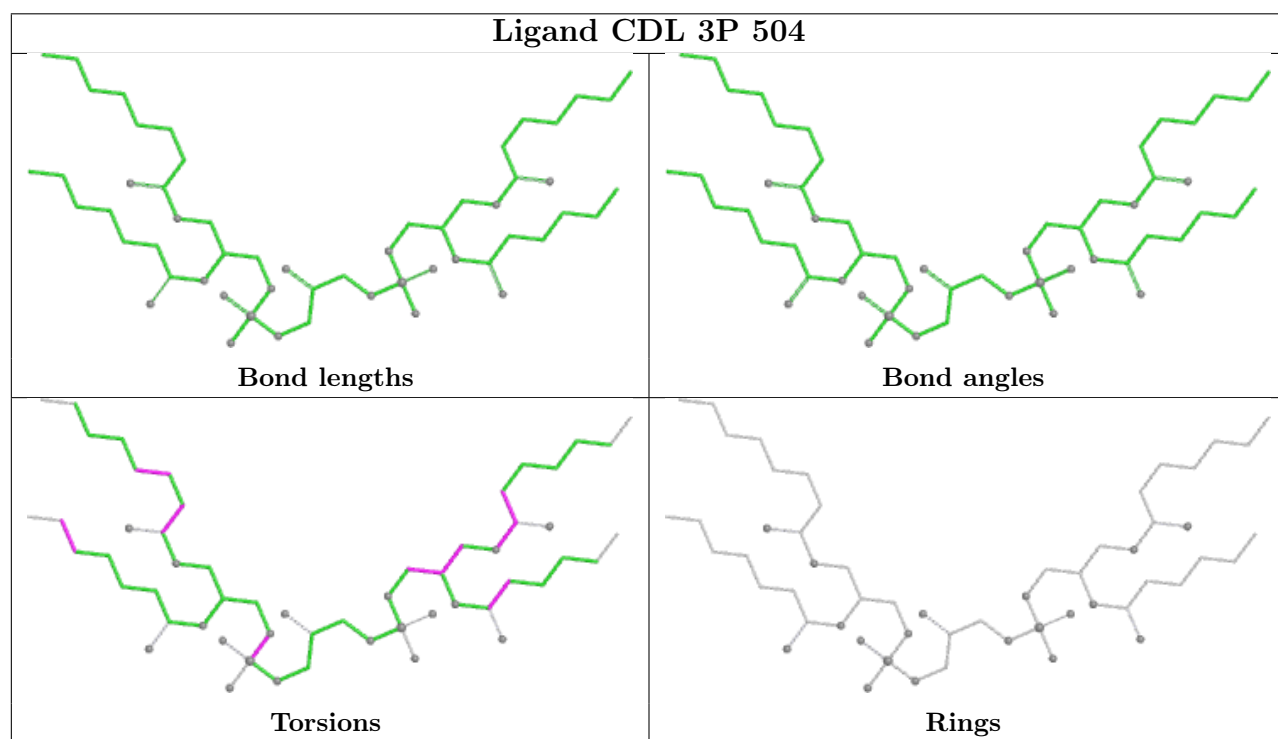
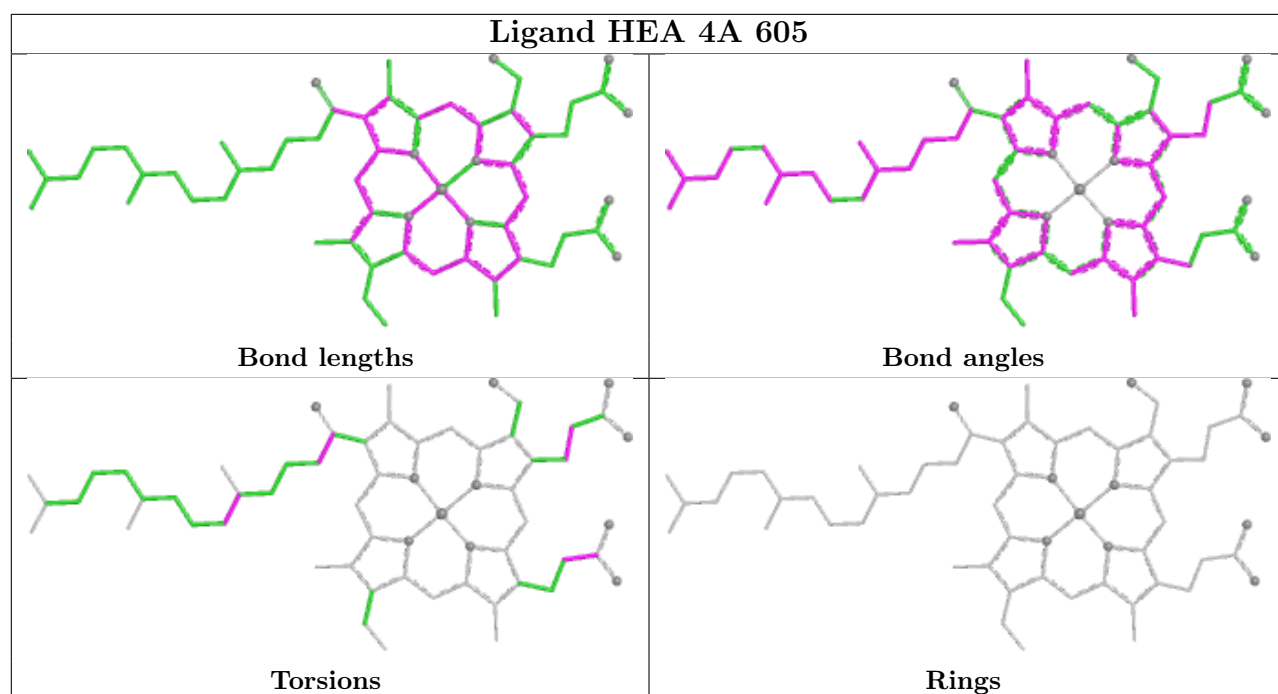


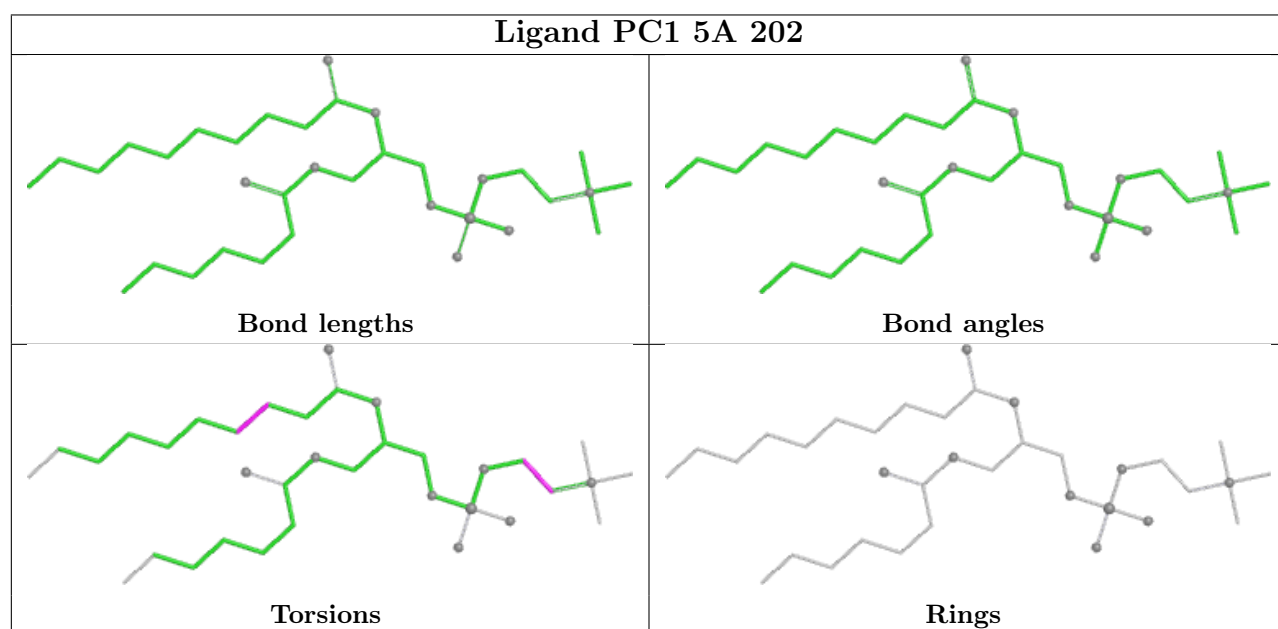
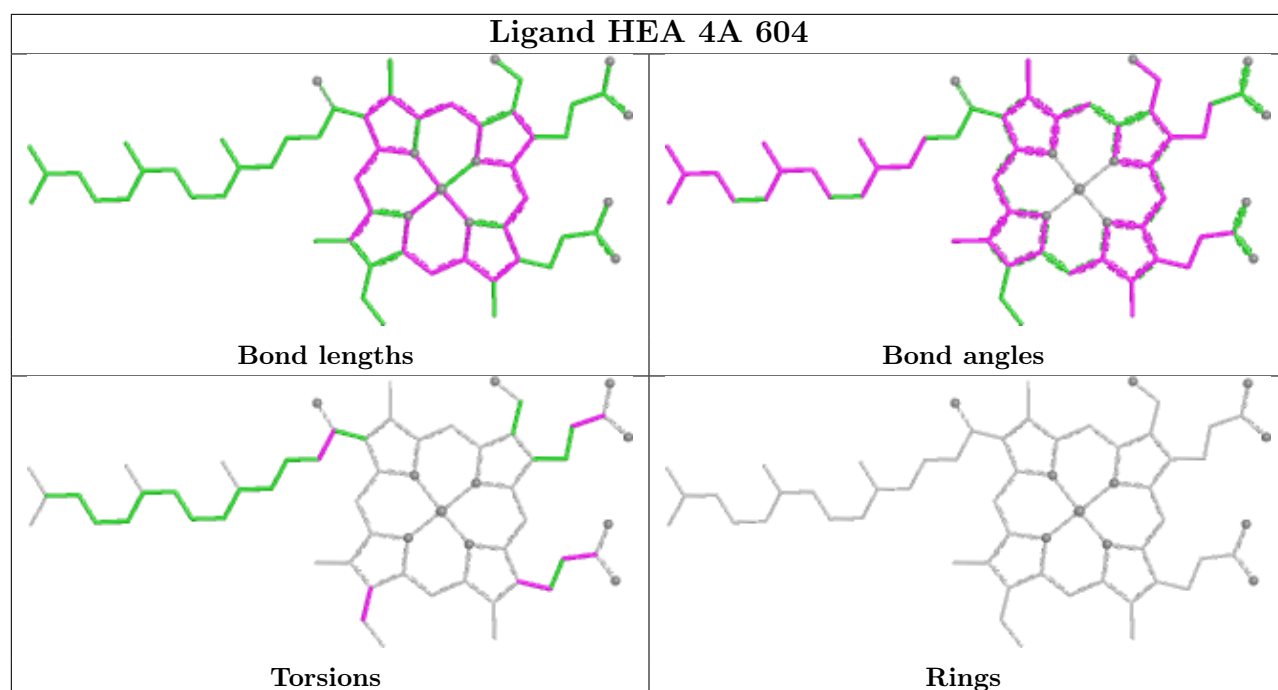
Rings

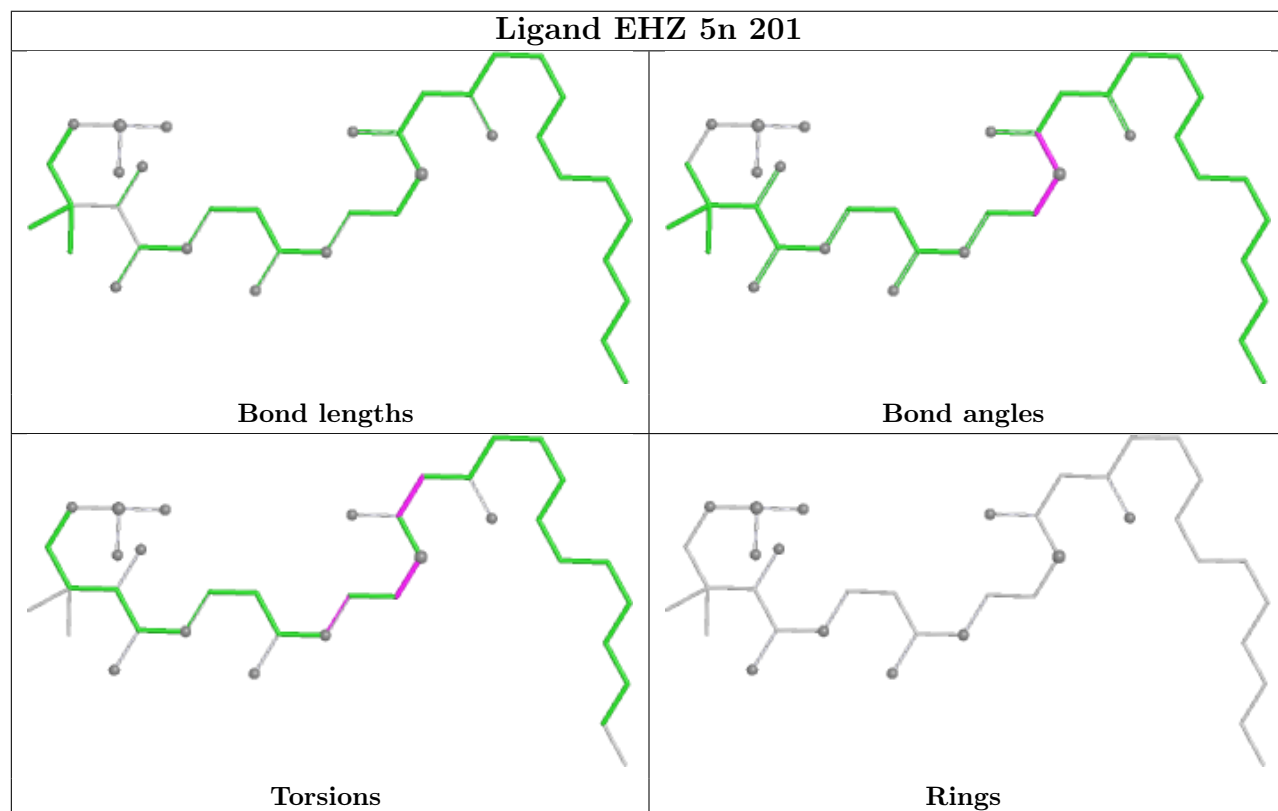
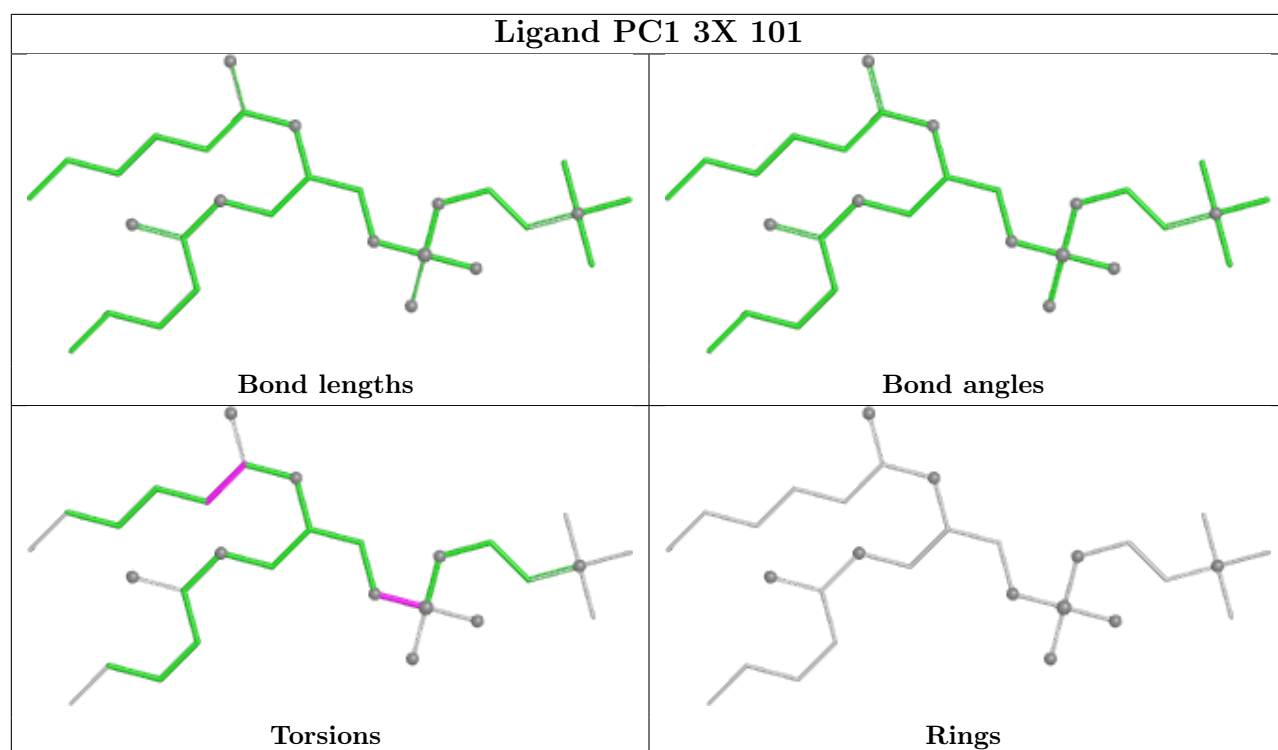


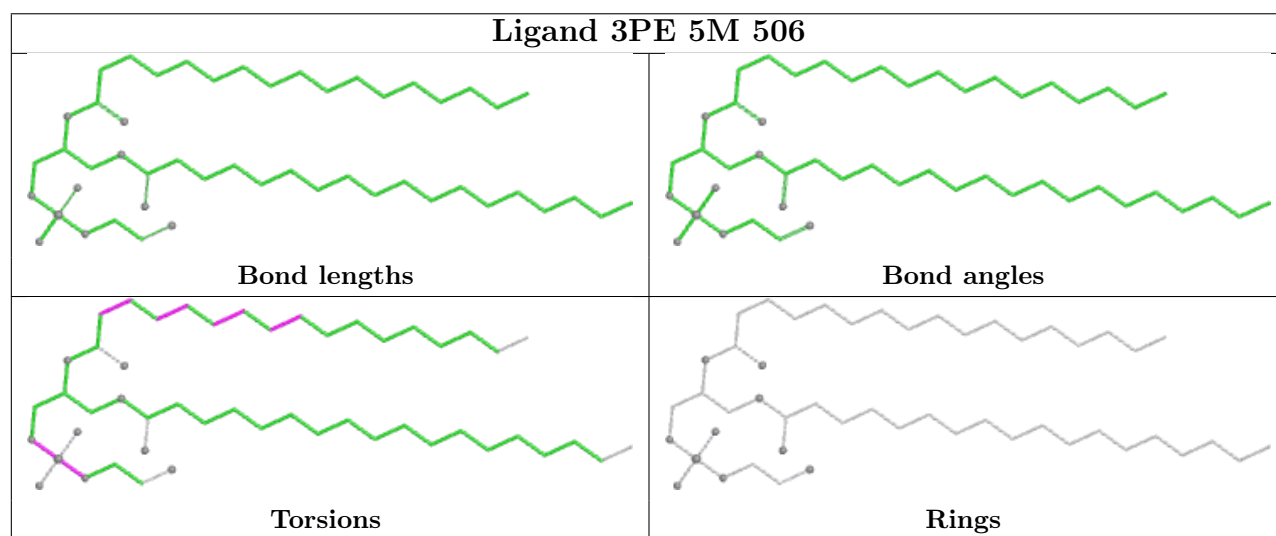
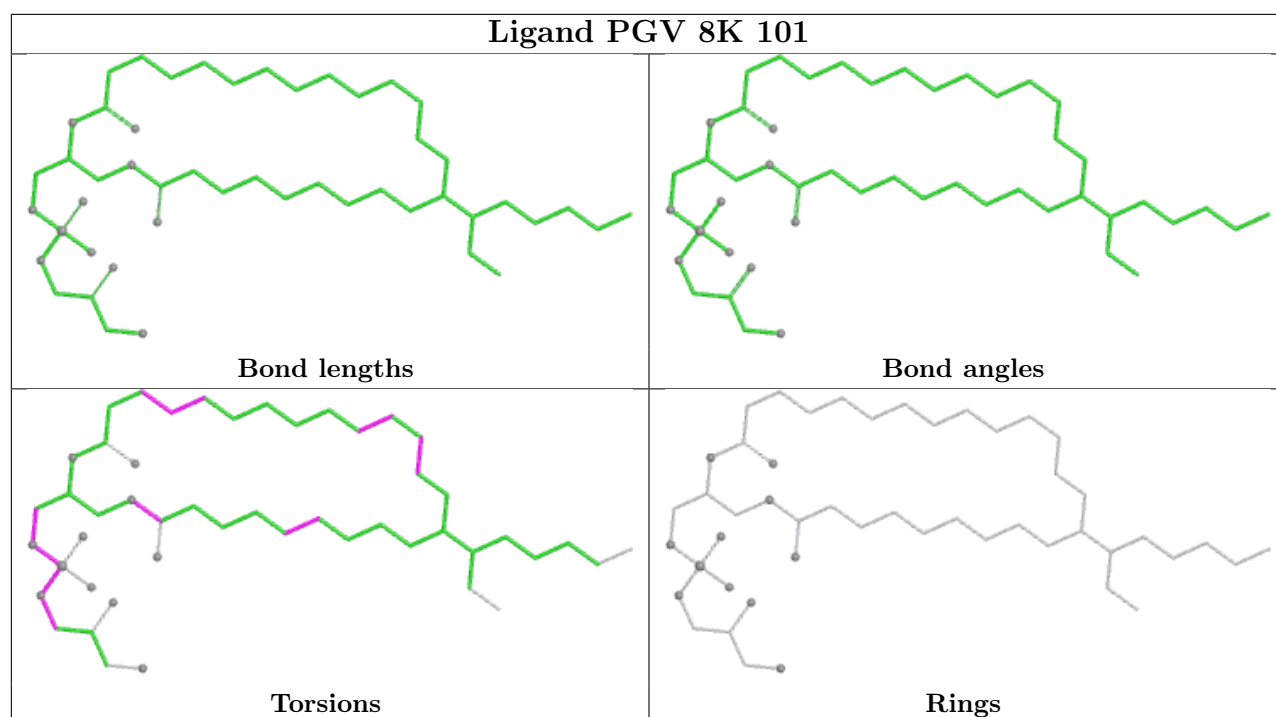


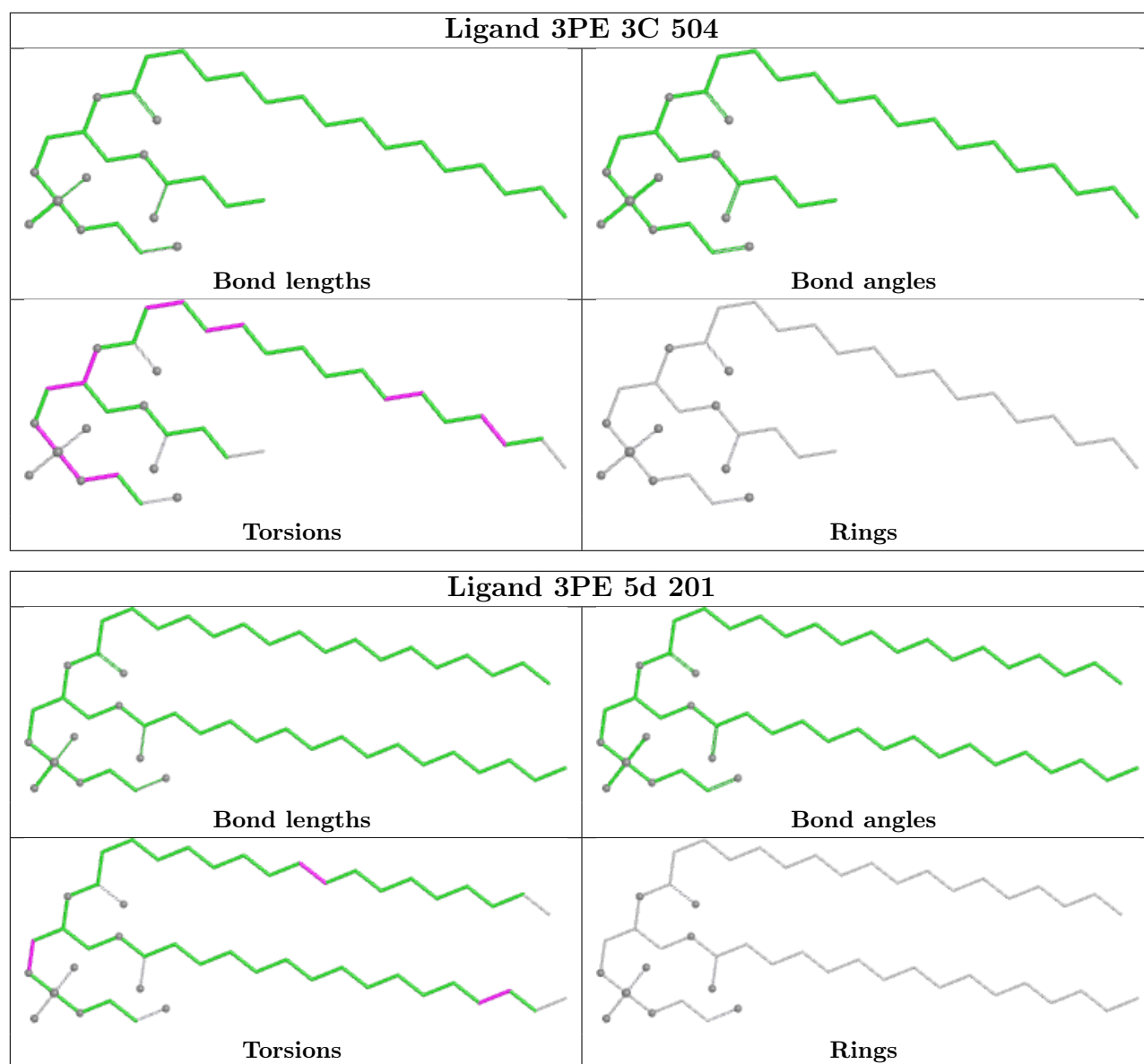


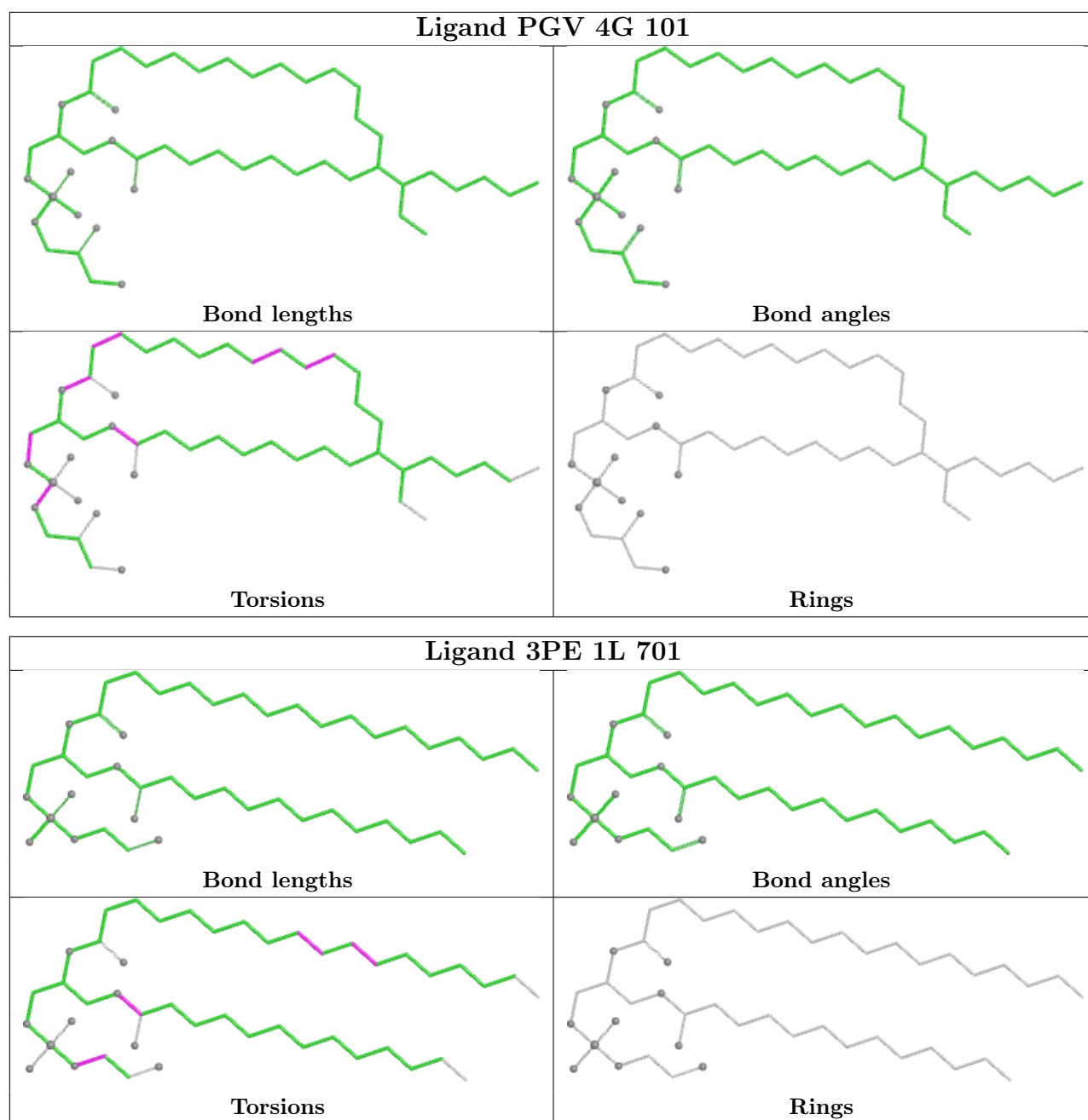




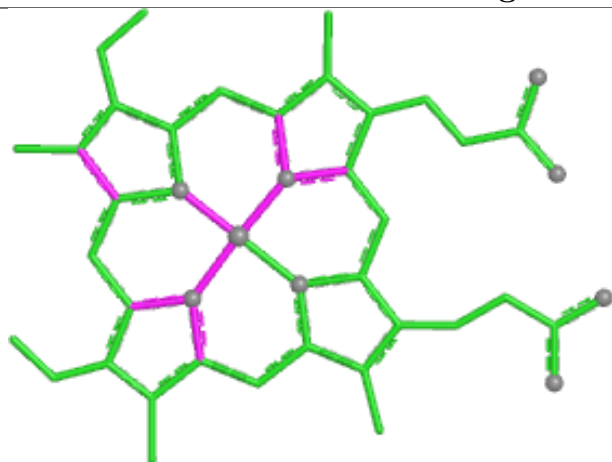




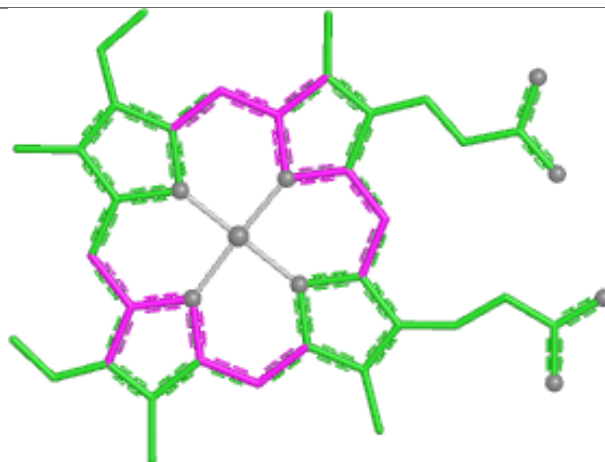




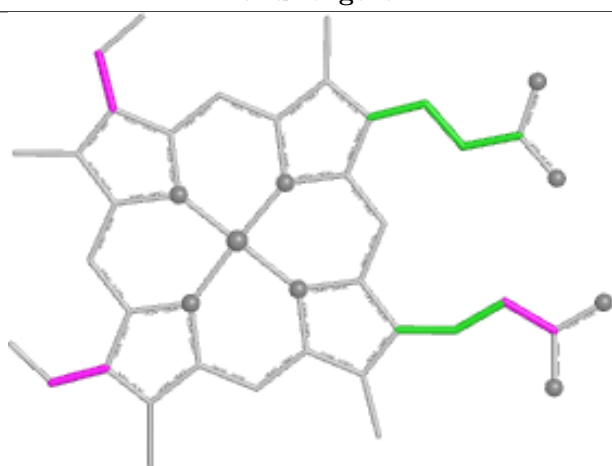
Ligand HEM 3C 502



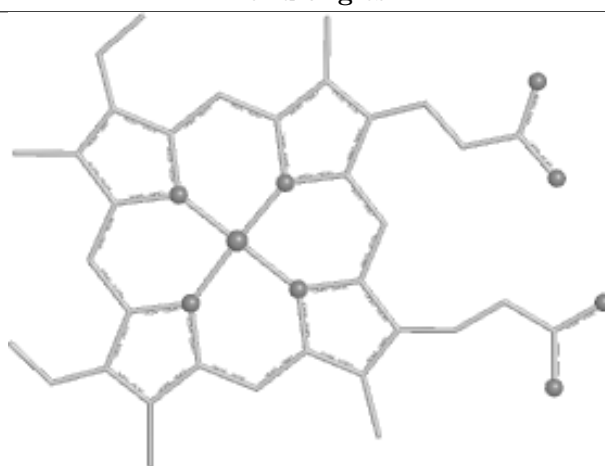
Bond lengths



Bond angles

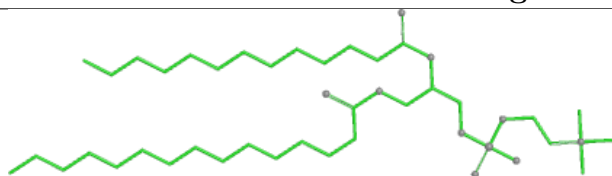


Torsions

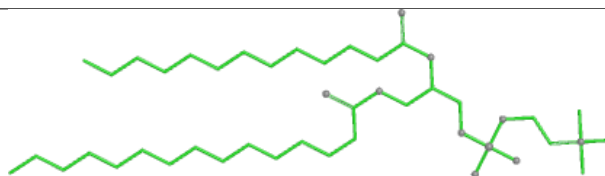


Rings

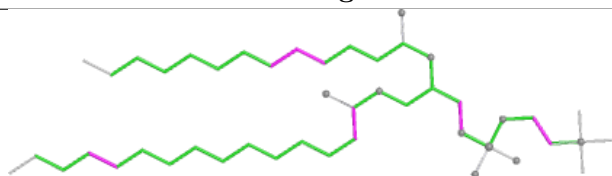
Ligand PC1 5L 705



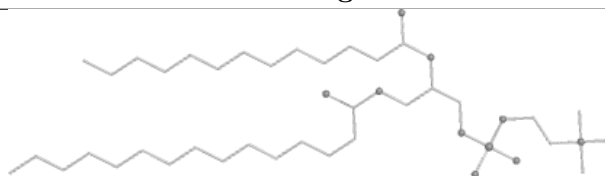
Bond lengths



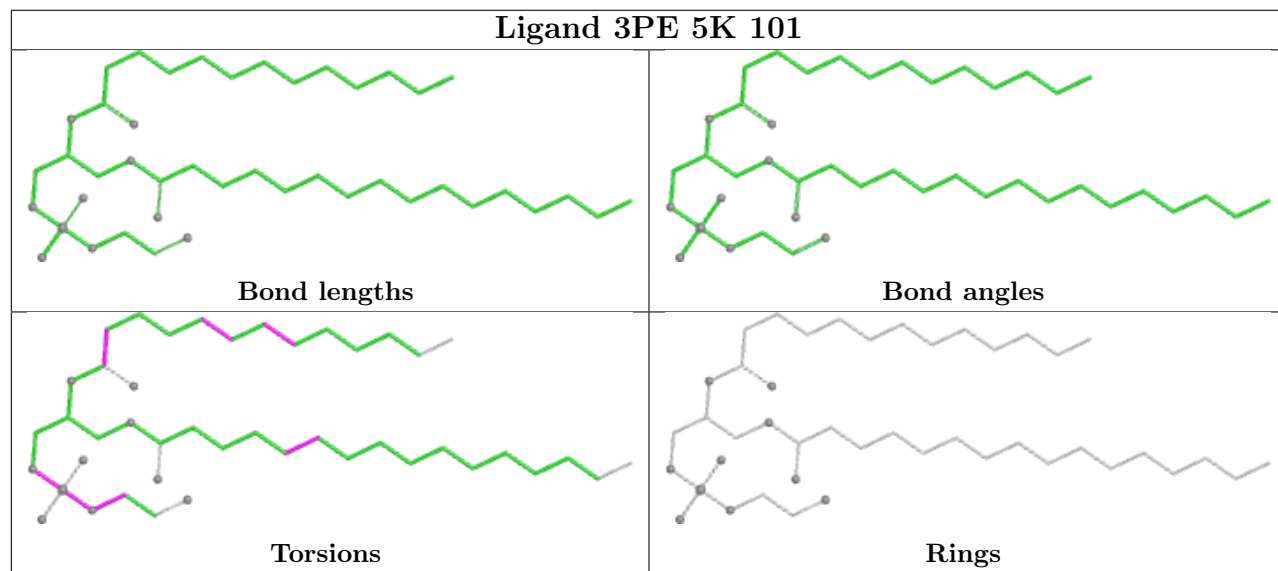
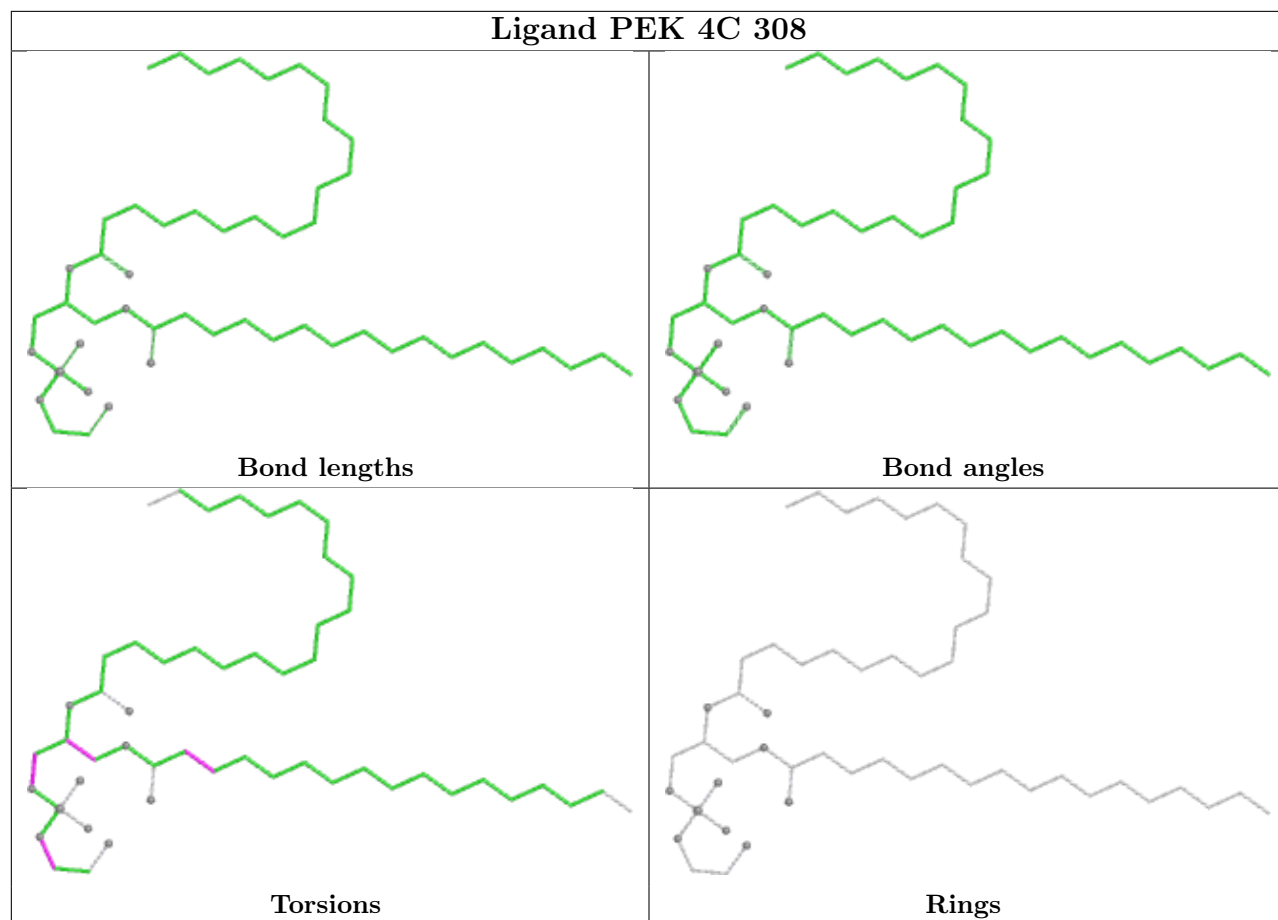
Bond angles

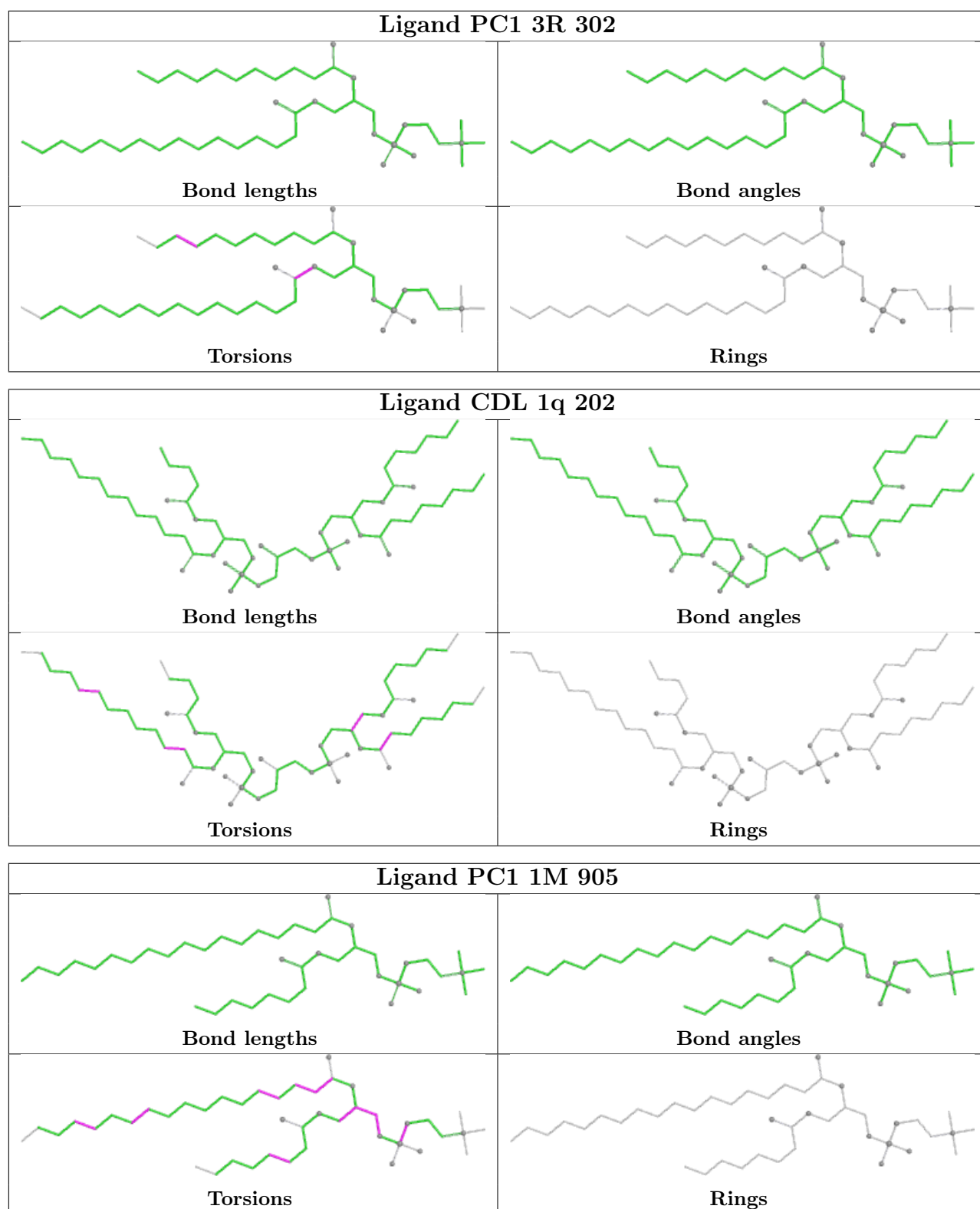


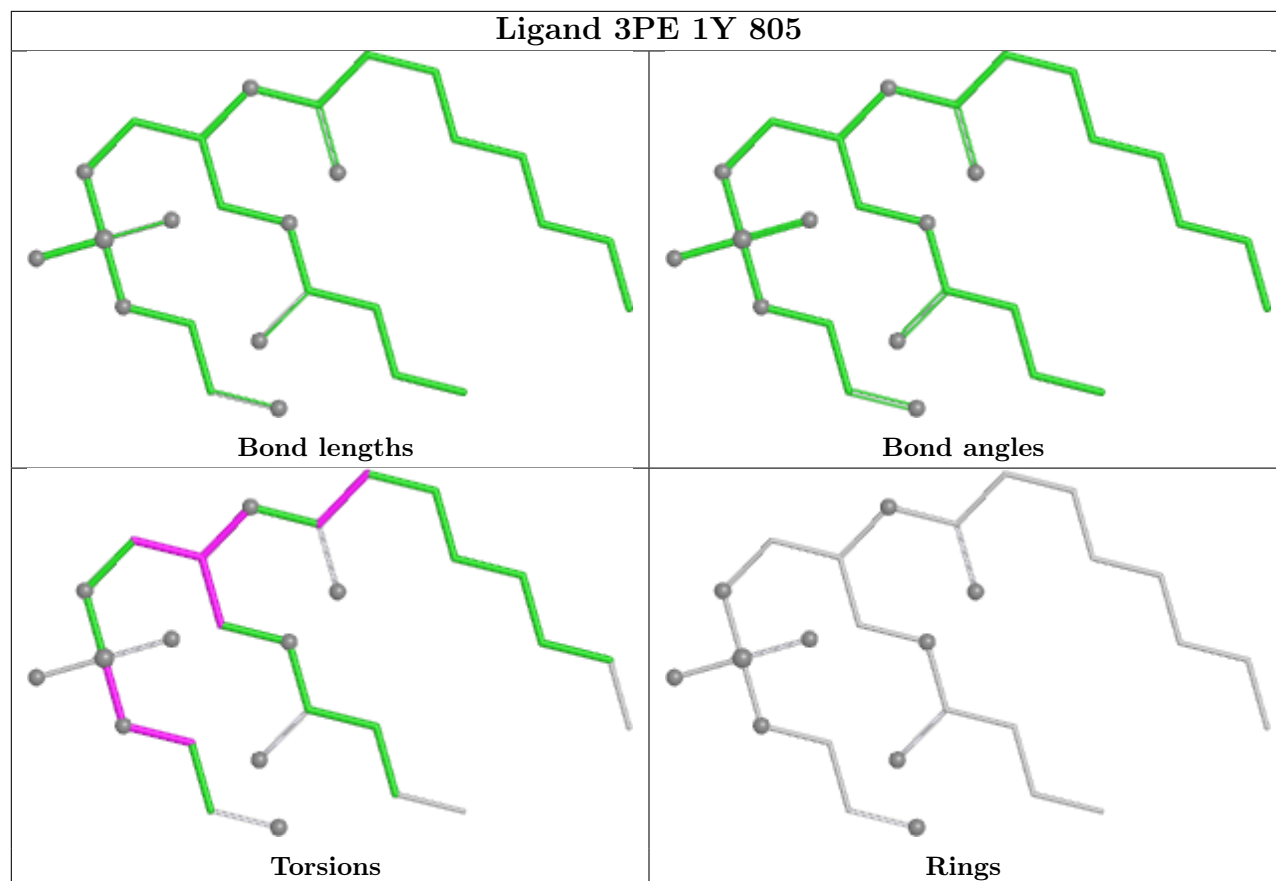
Torsions

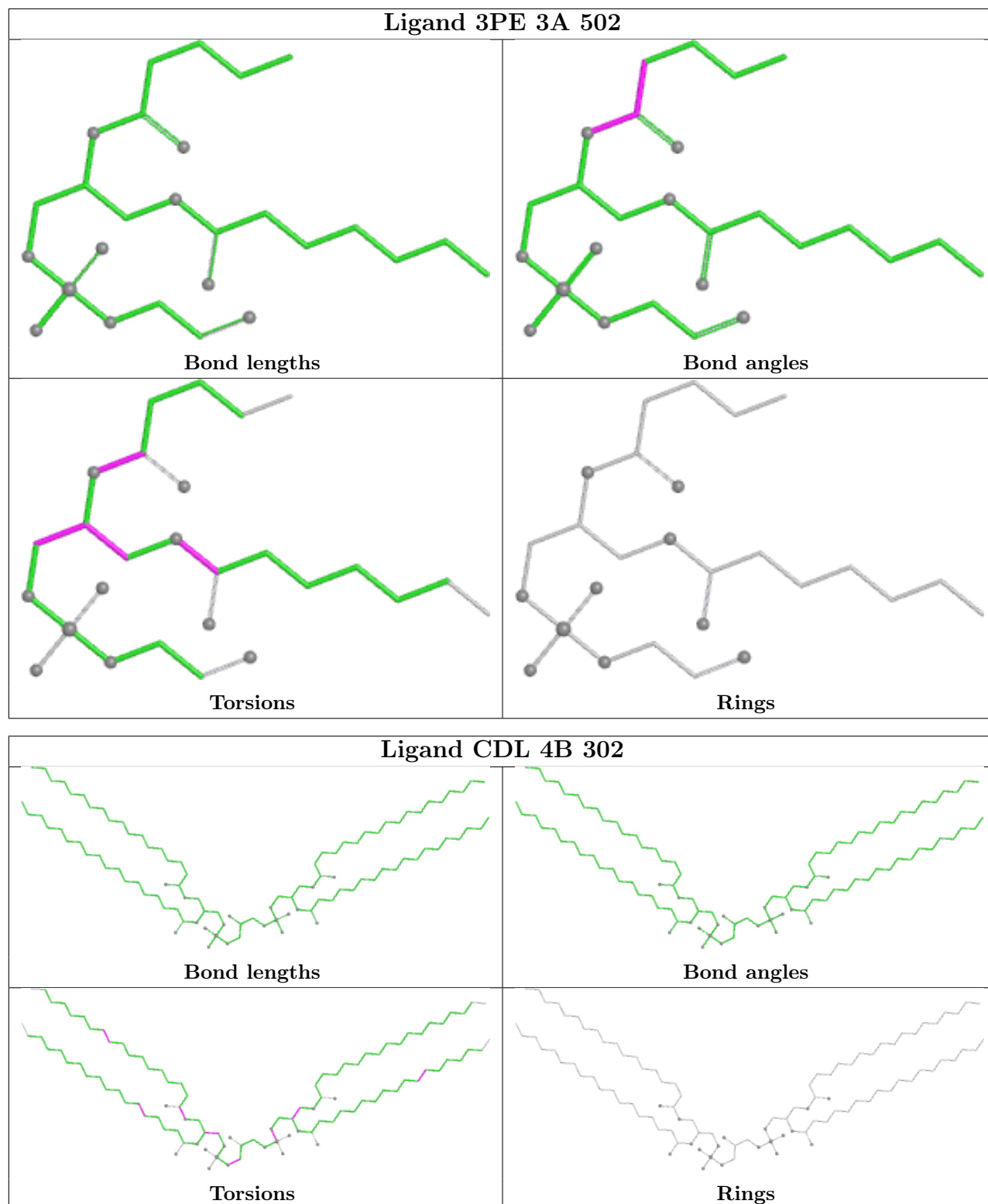


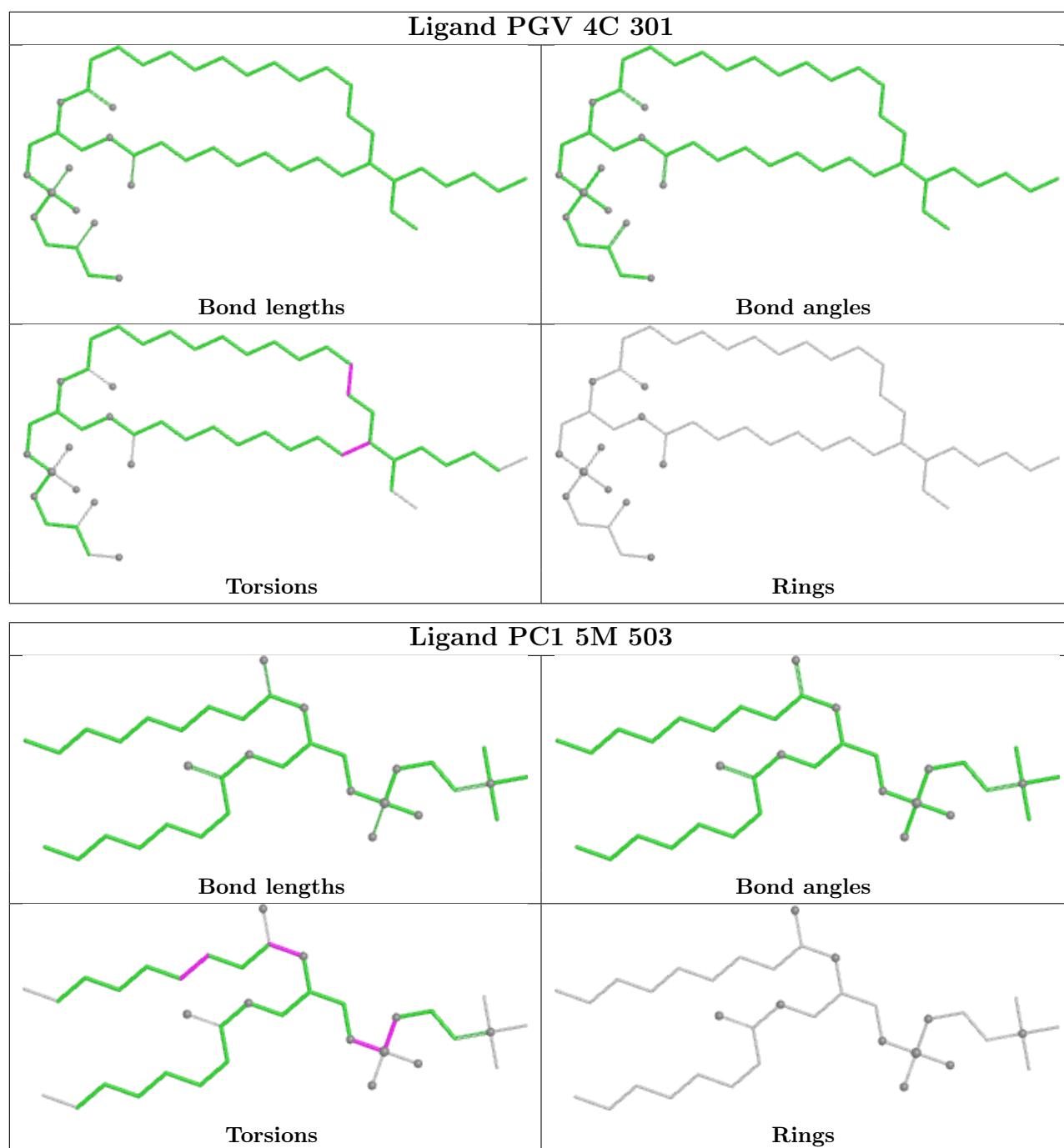
Rings

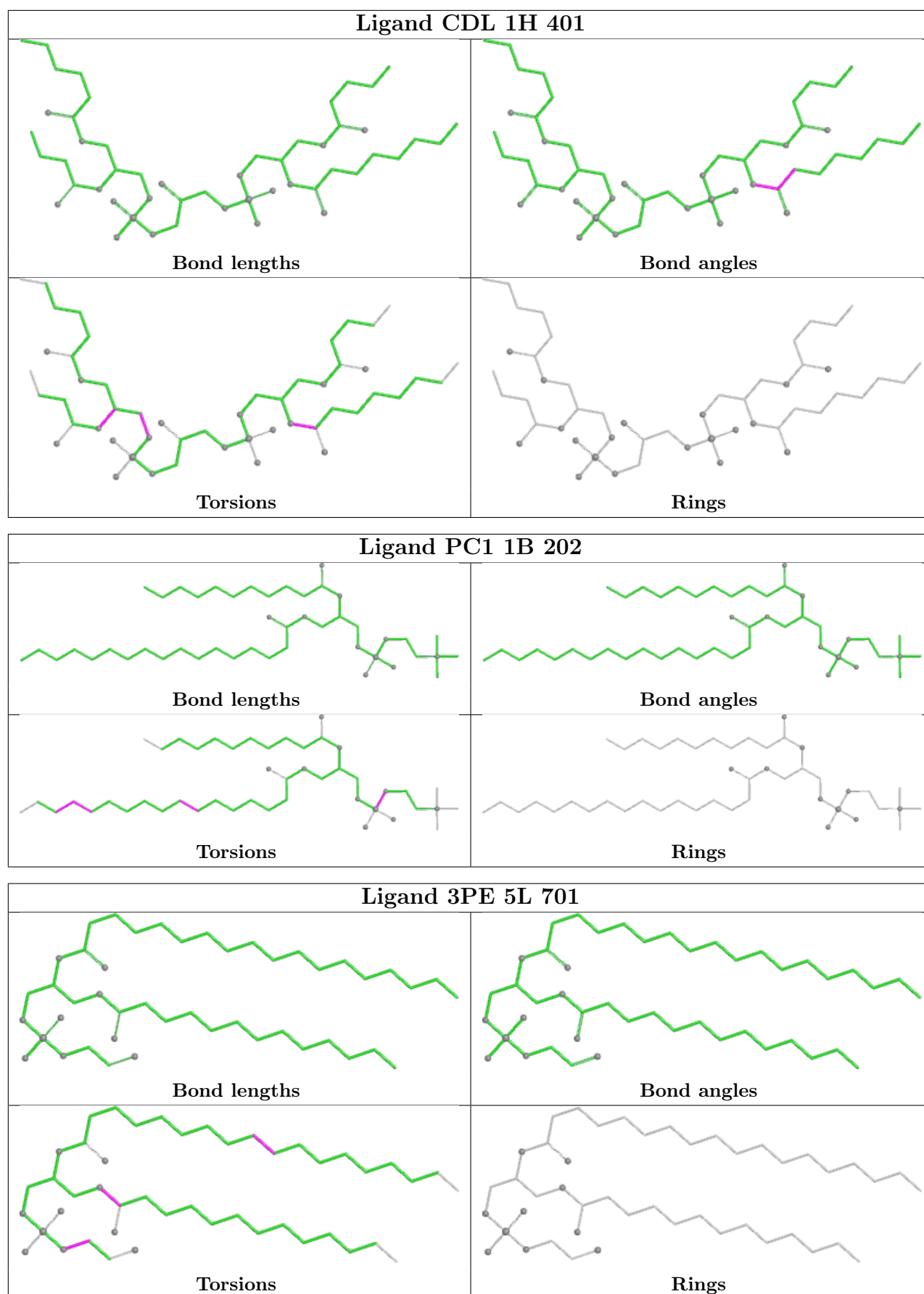




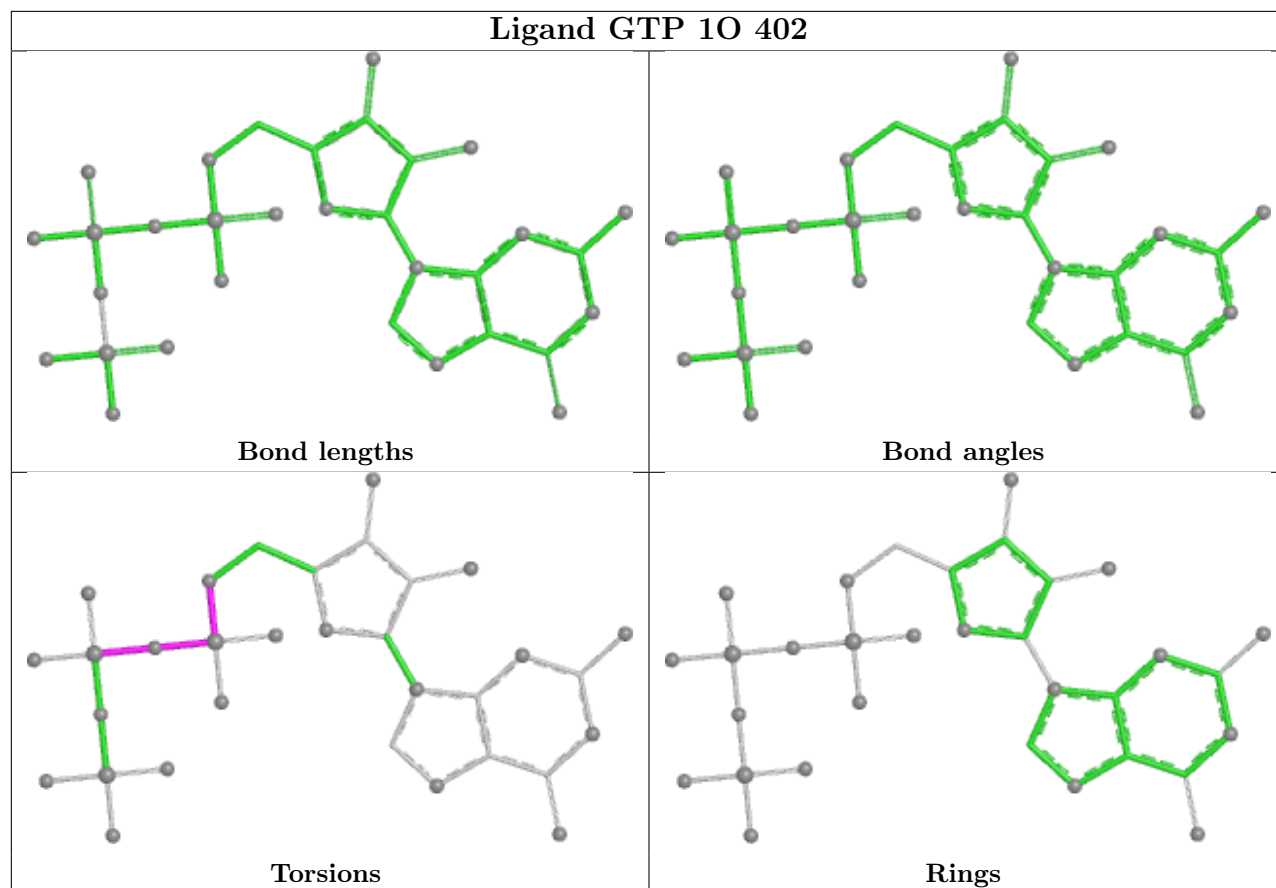




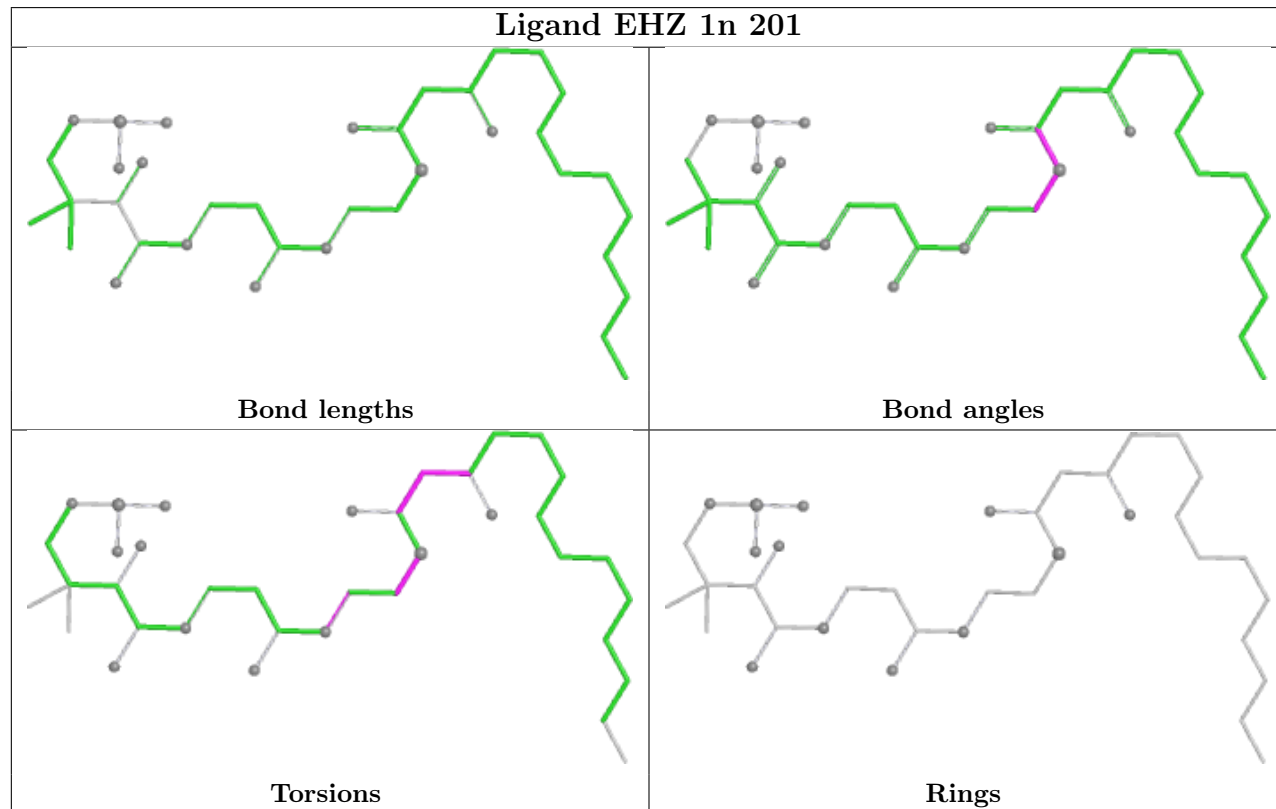


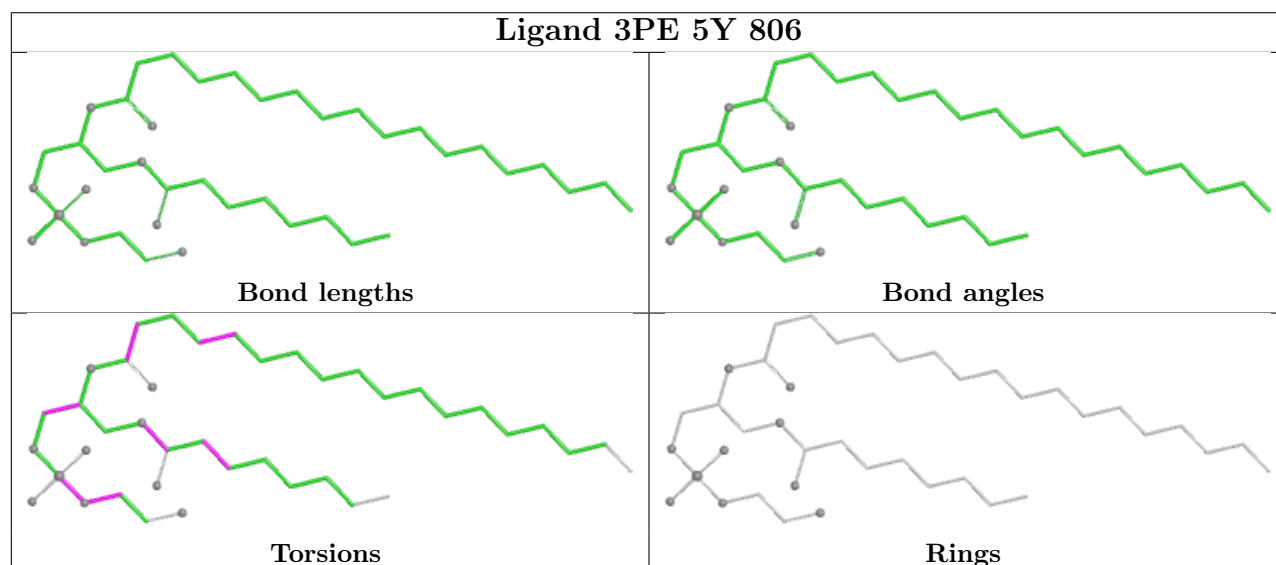
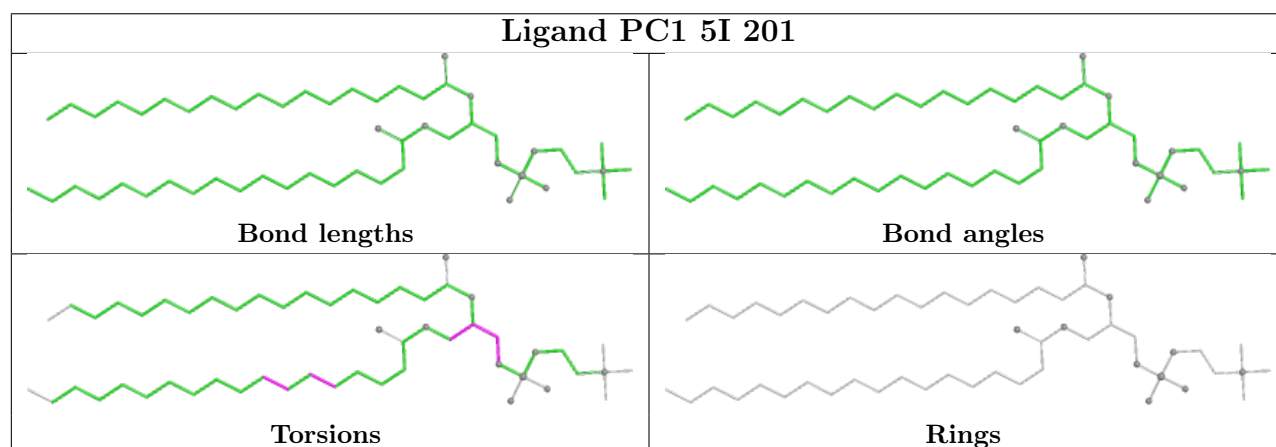
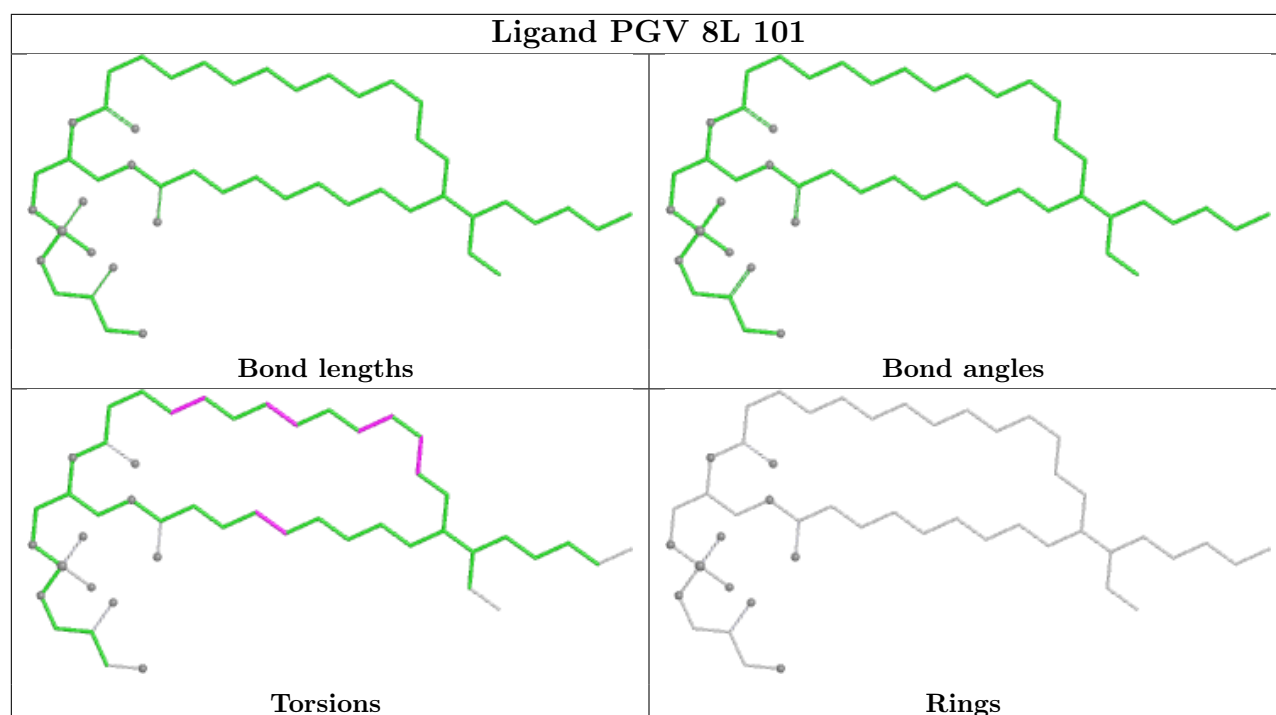


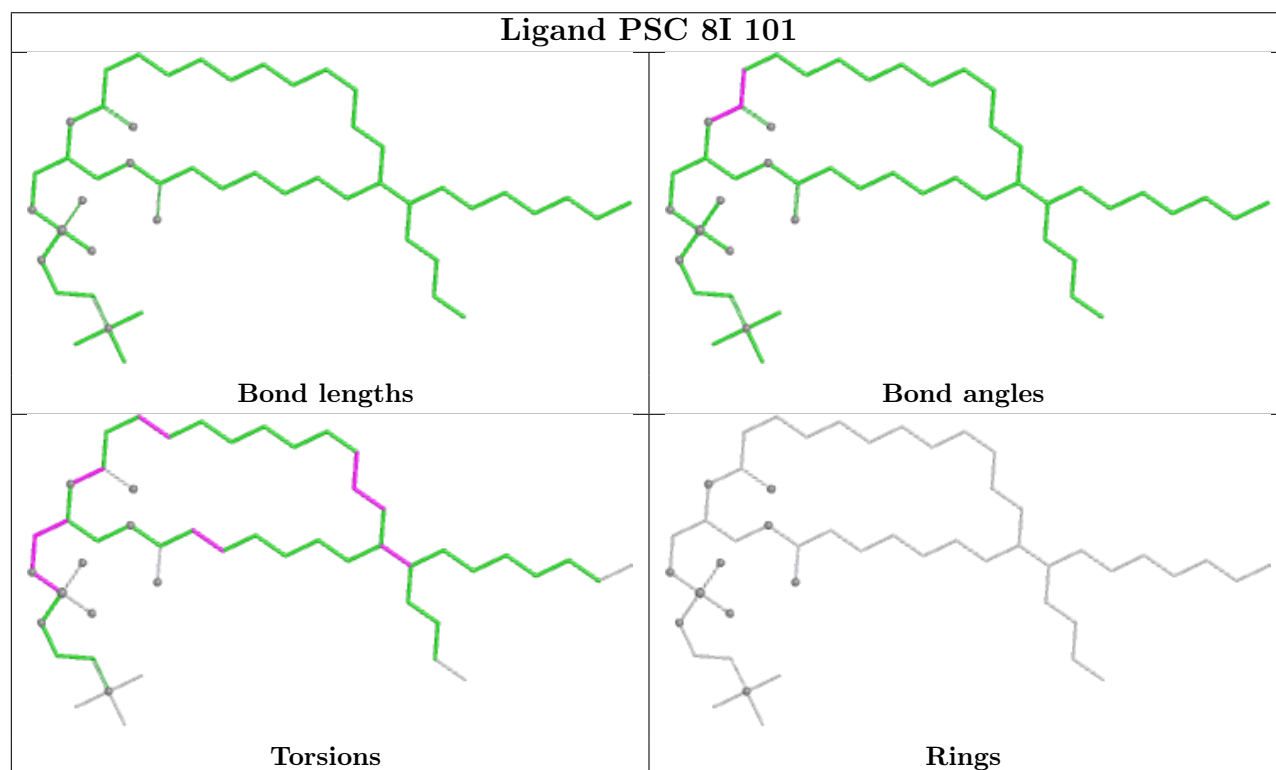
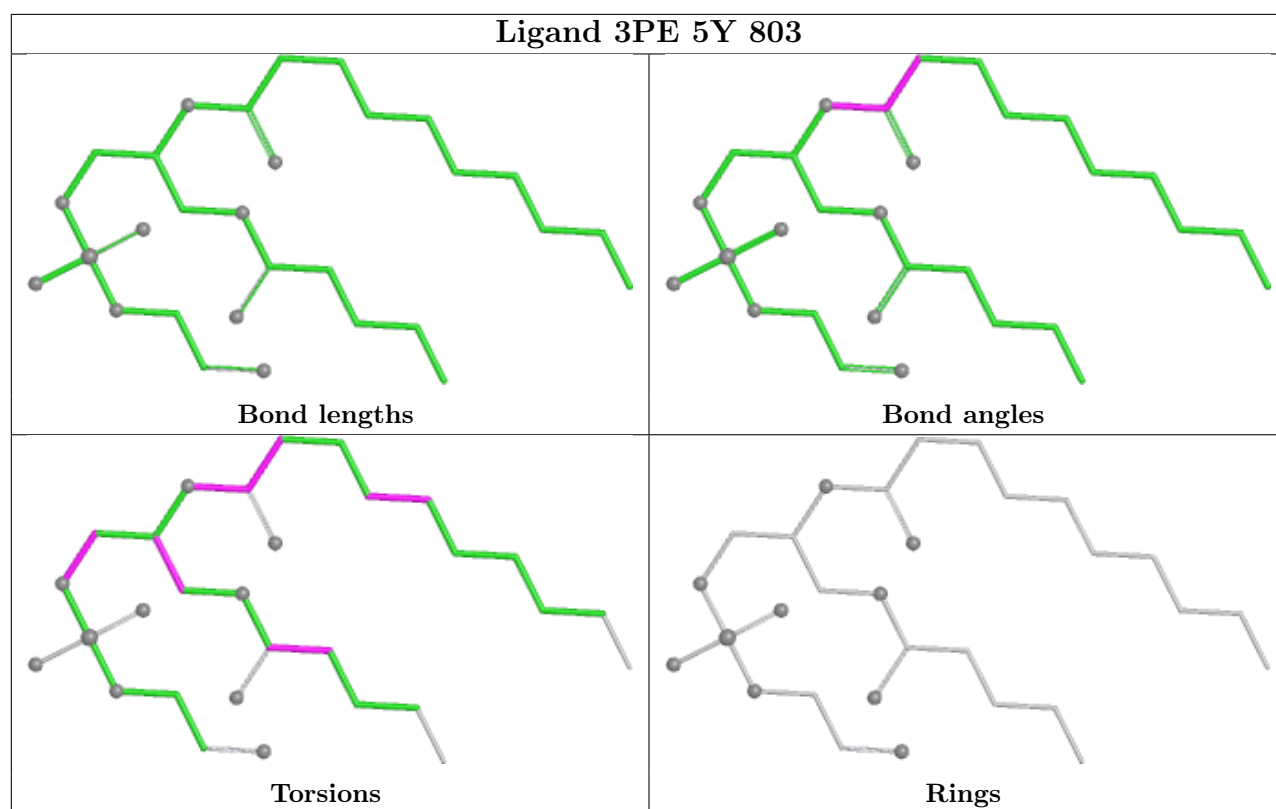
Ligand GTP 1O 402

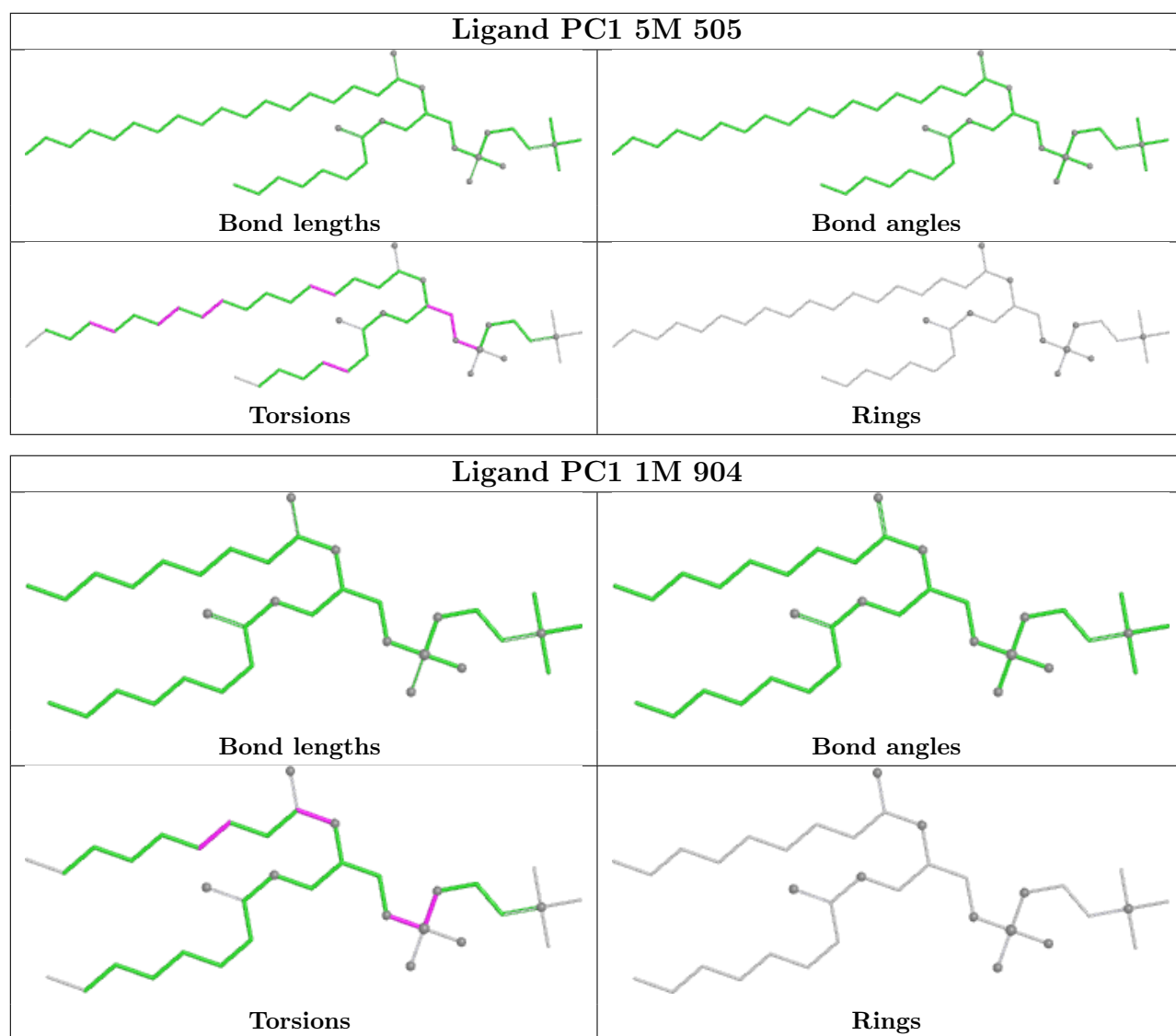


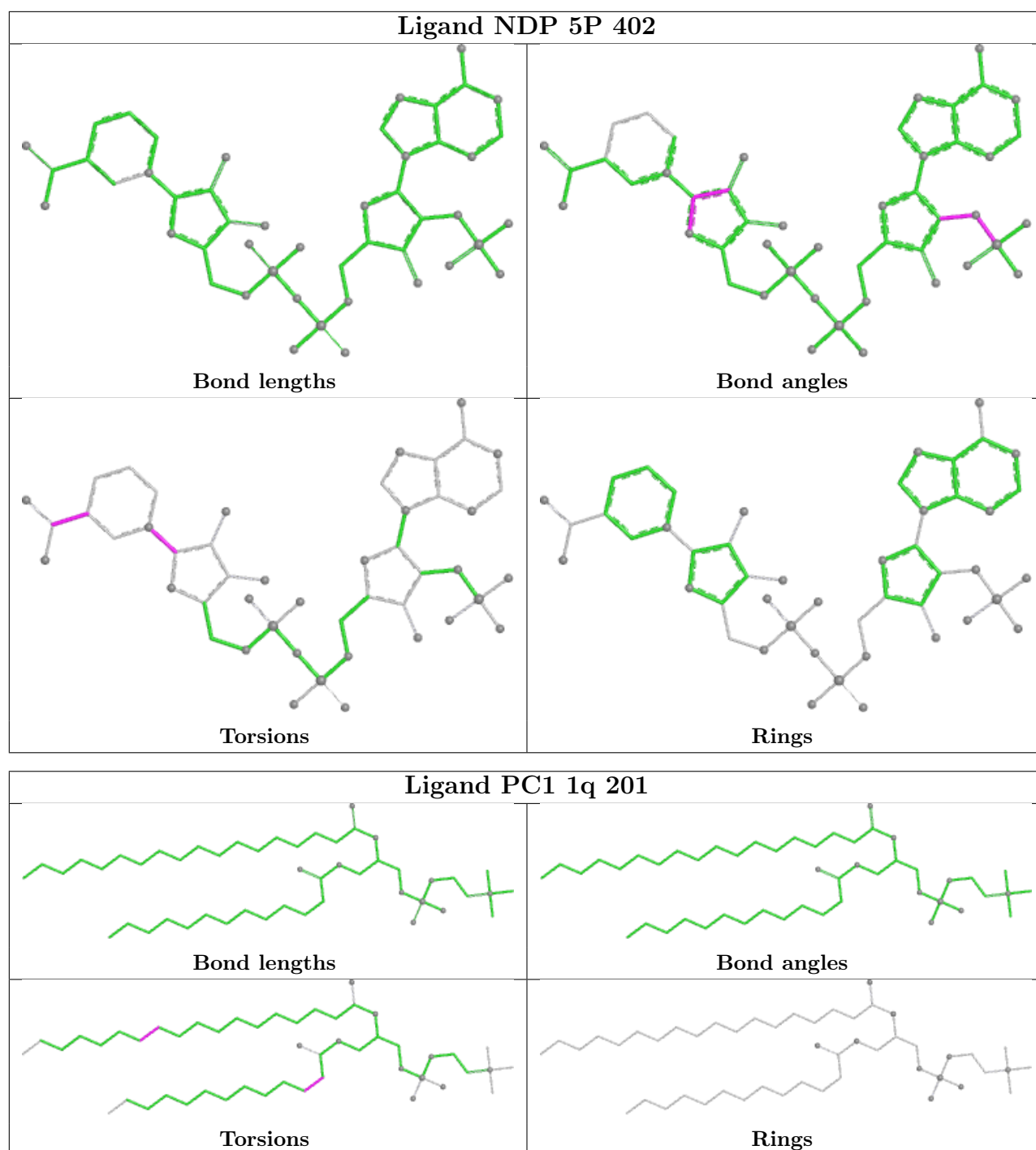
Ligand EHZ 1n 201

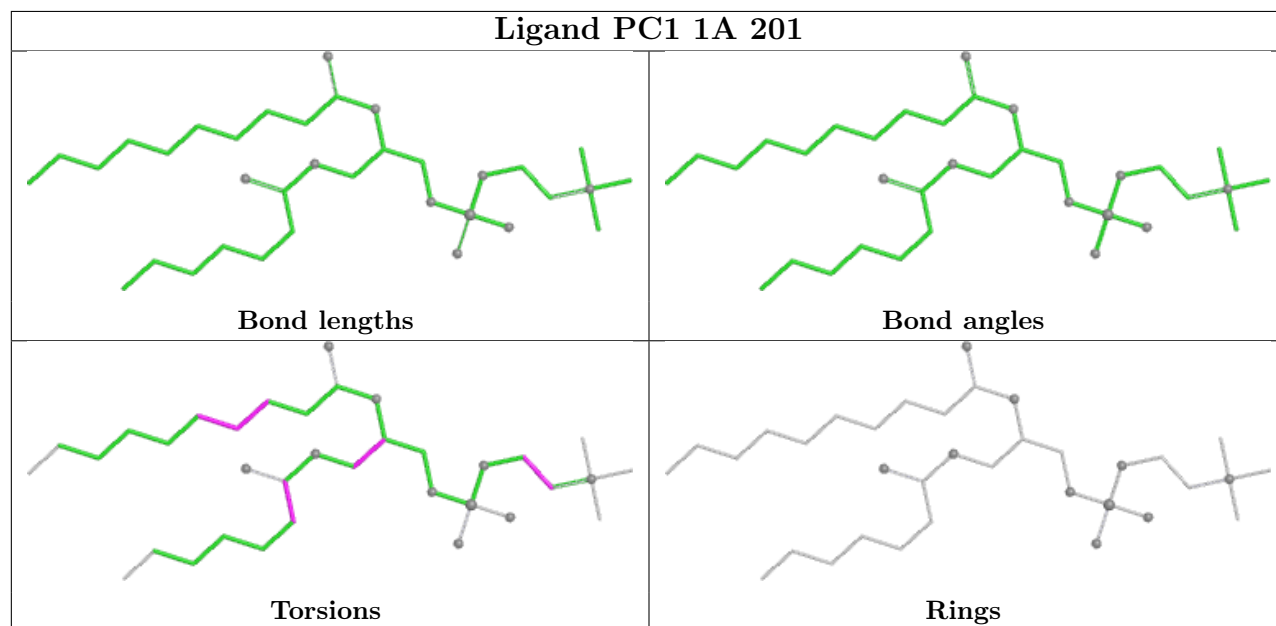
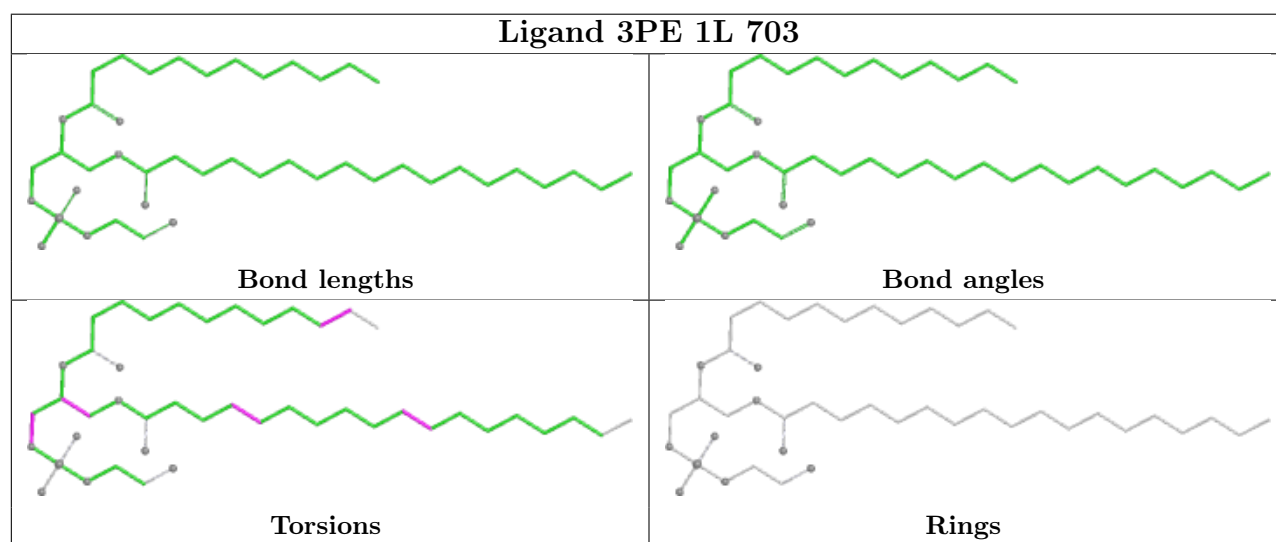
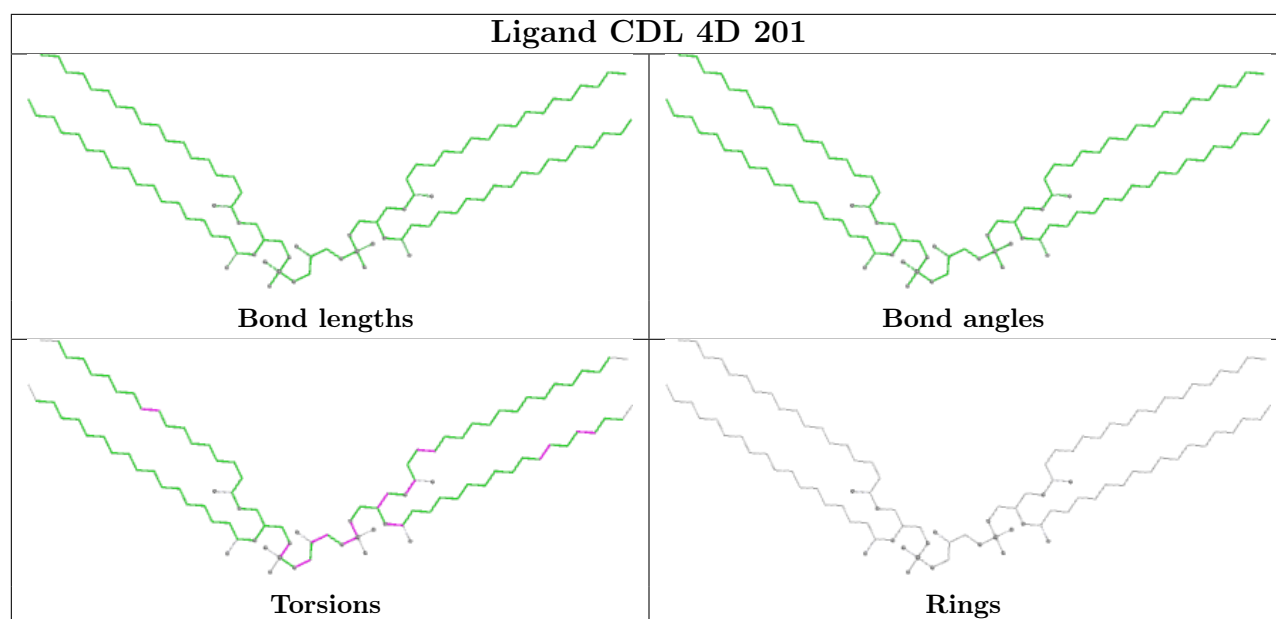


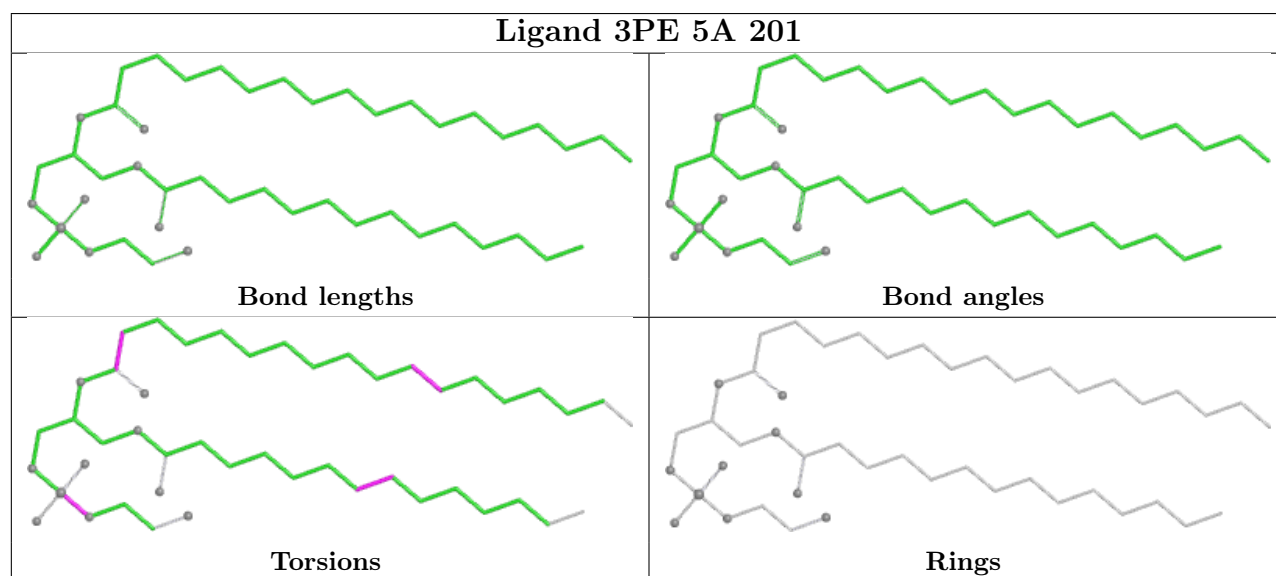
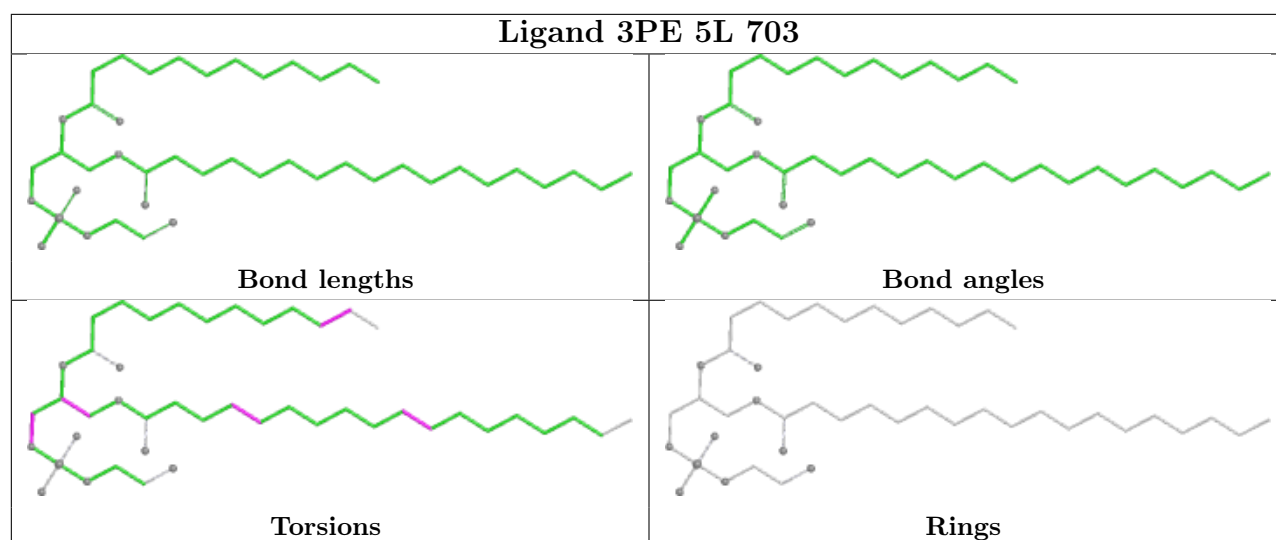


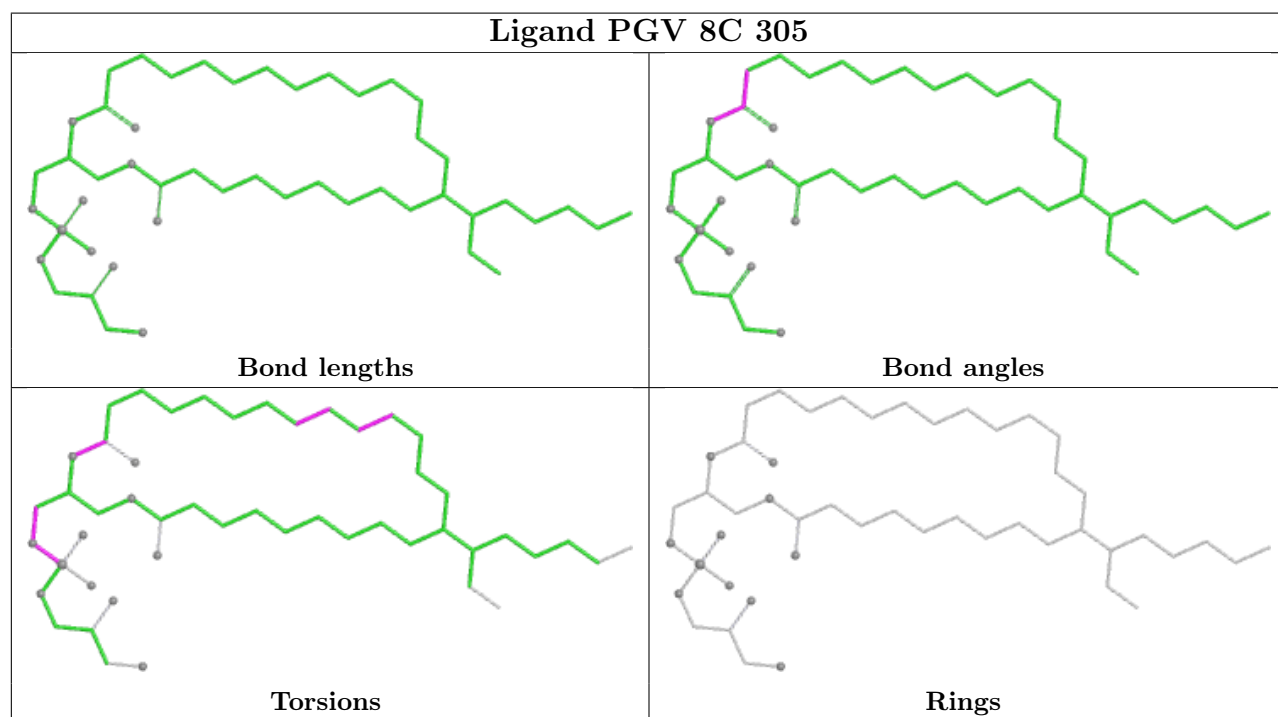
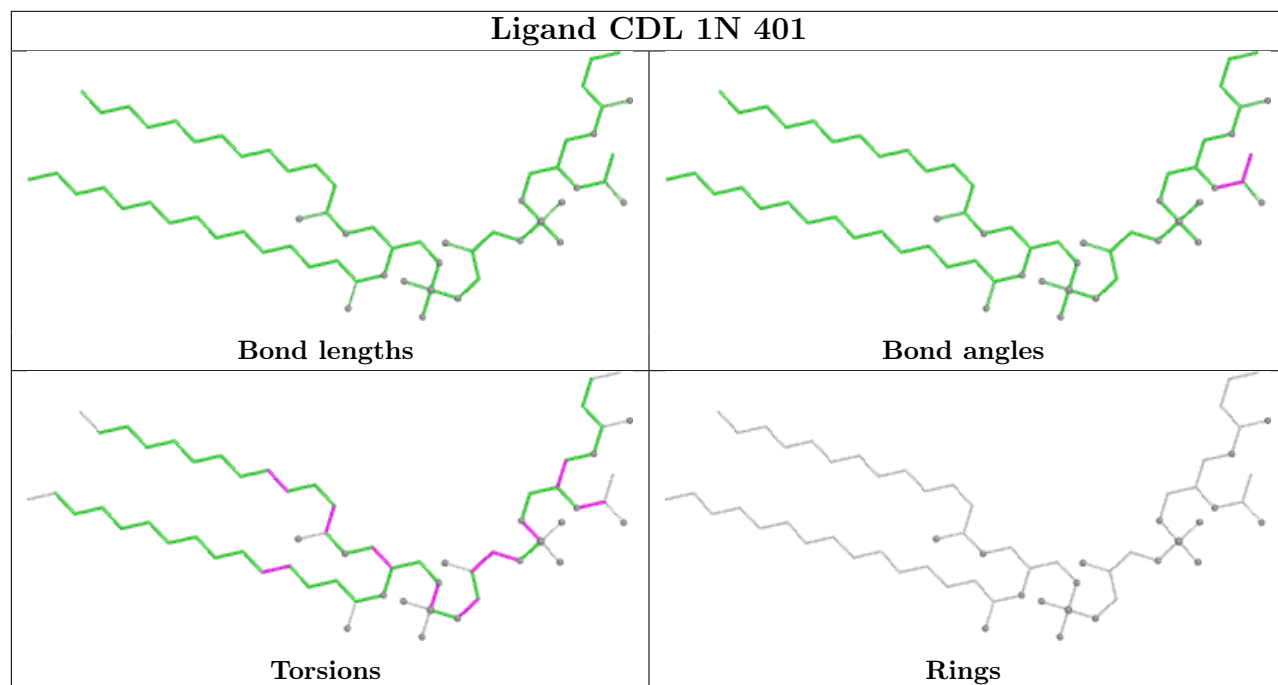


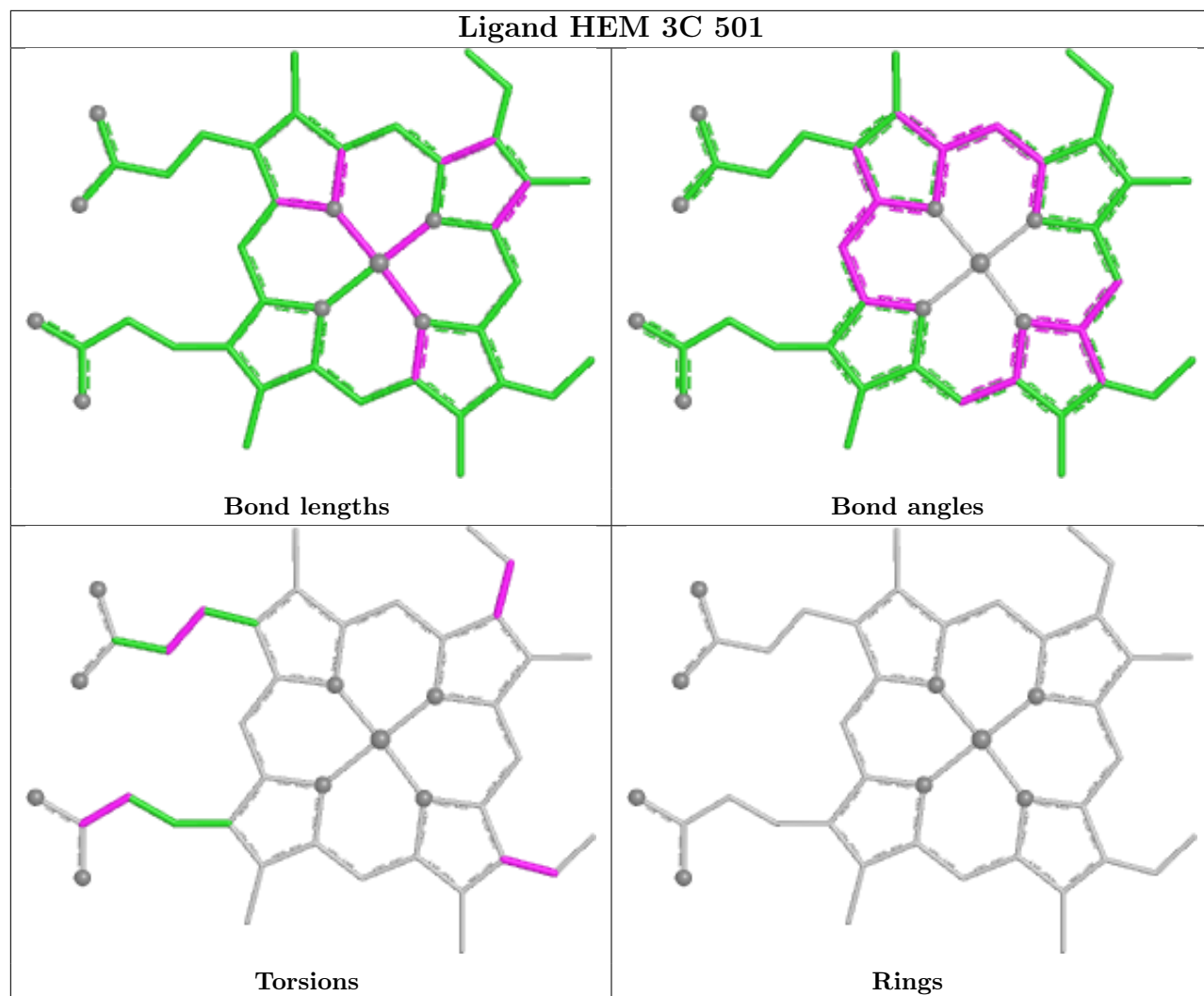


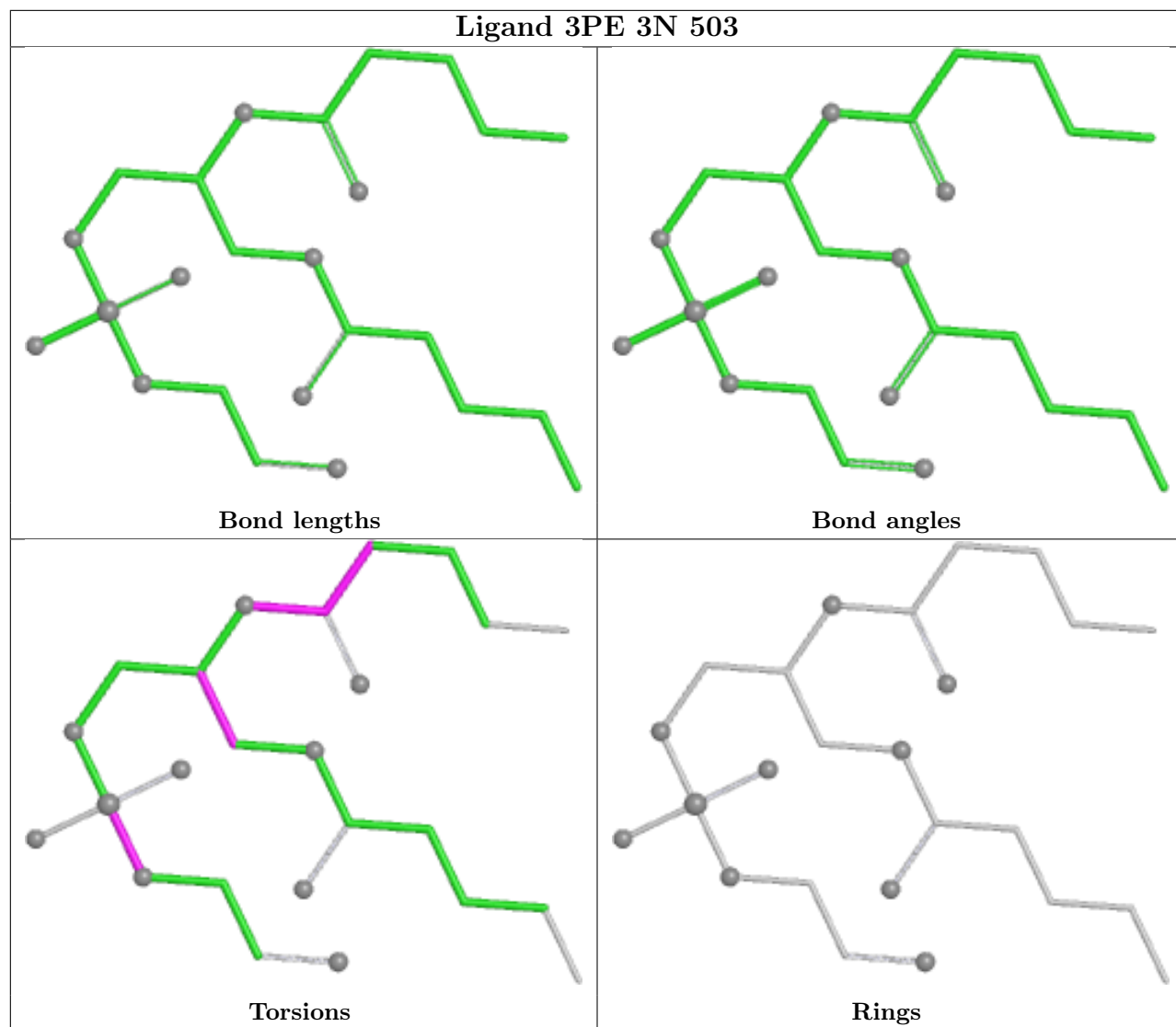


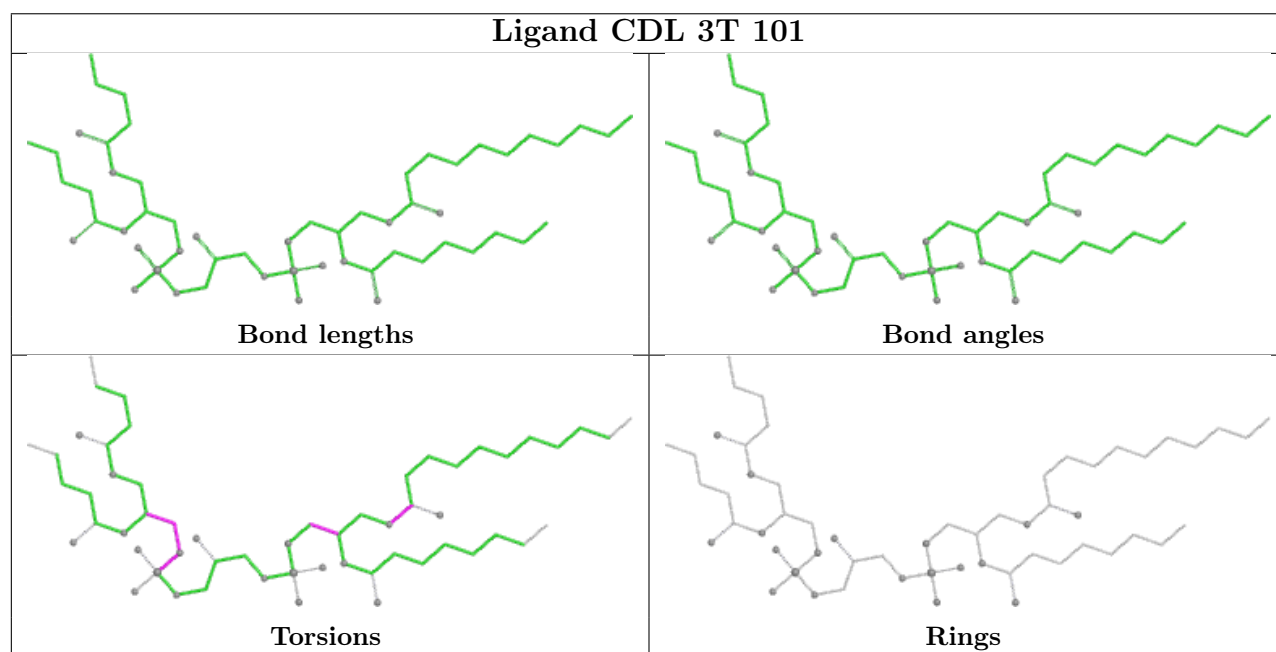
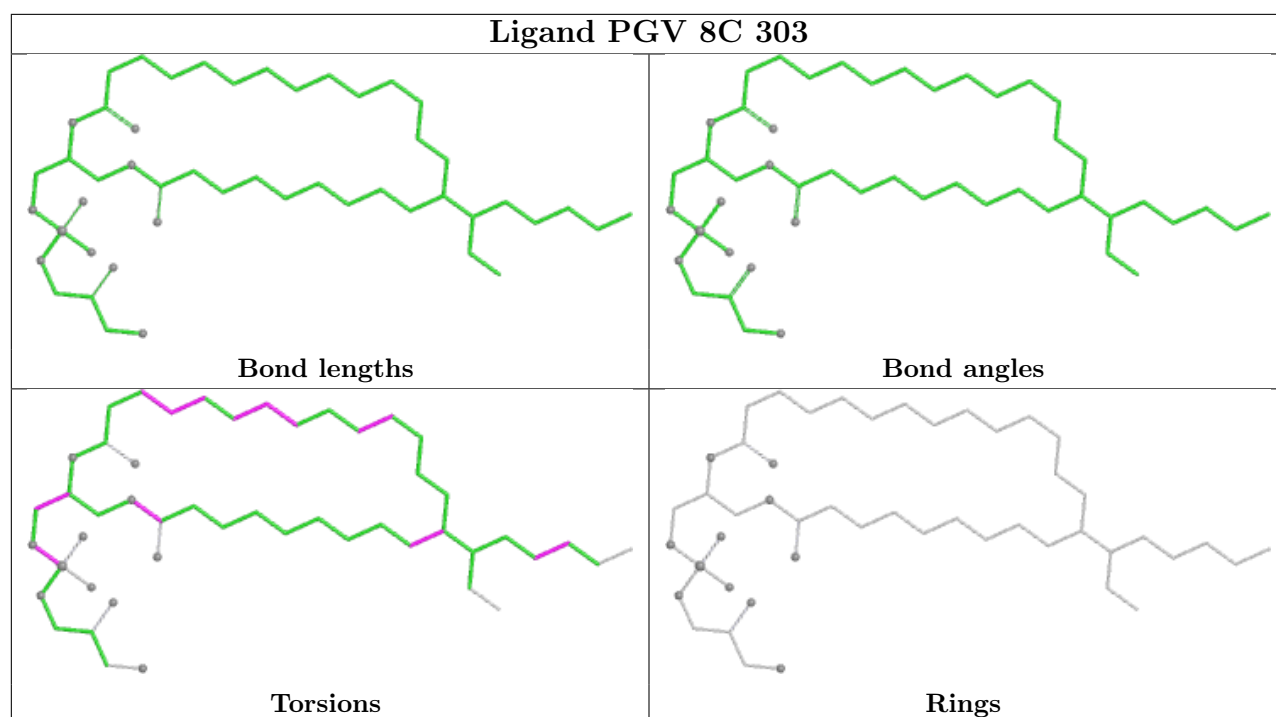


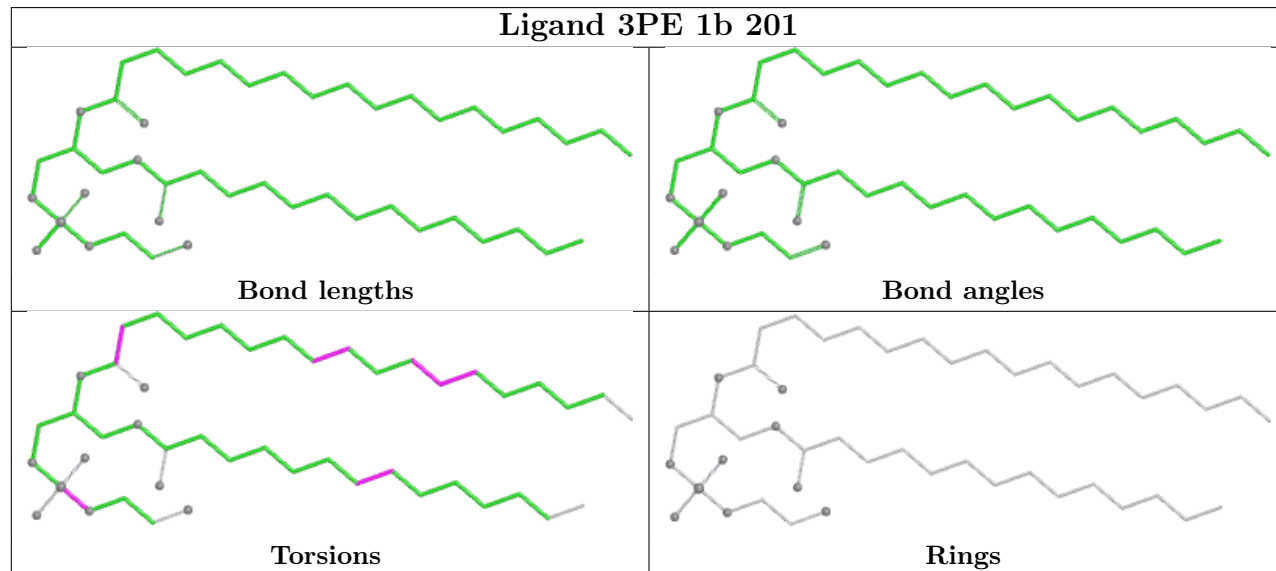
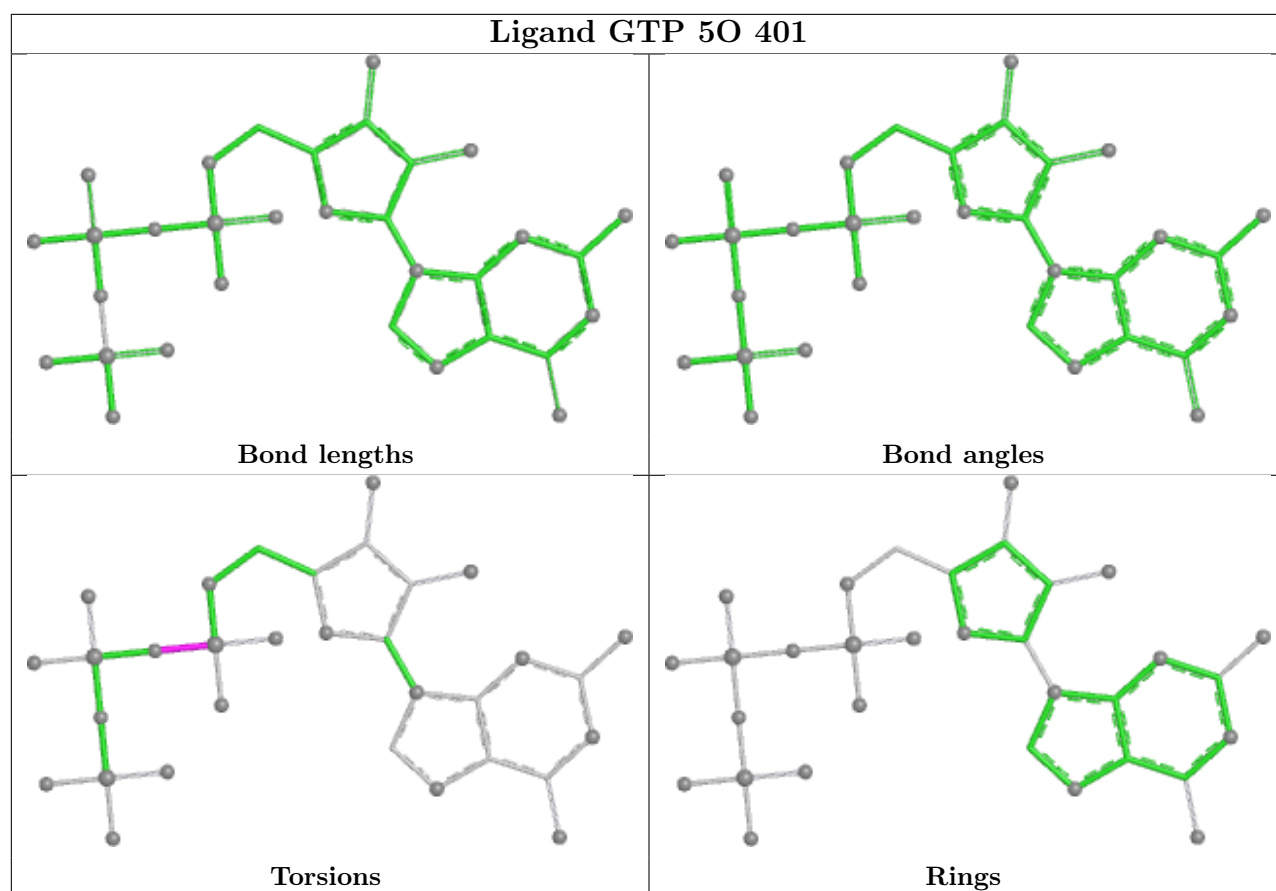


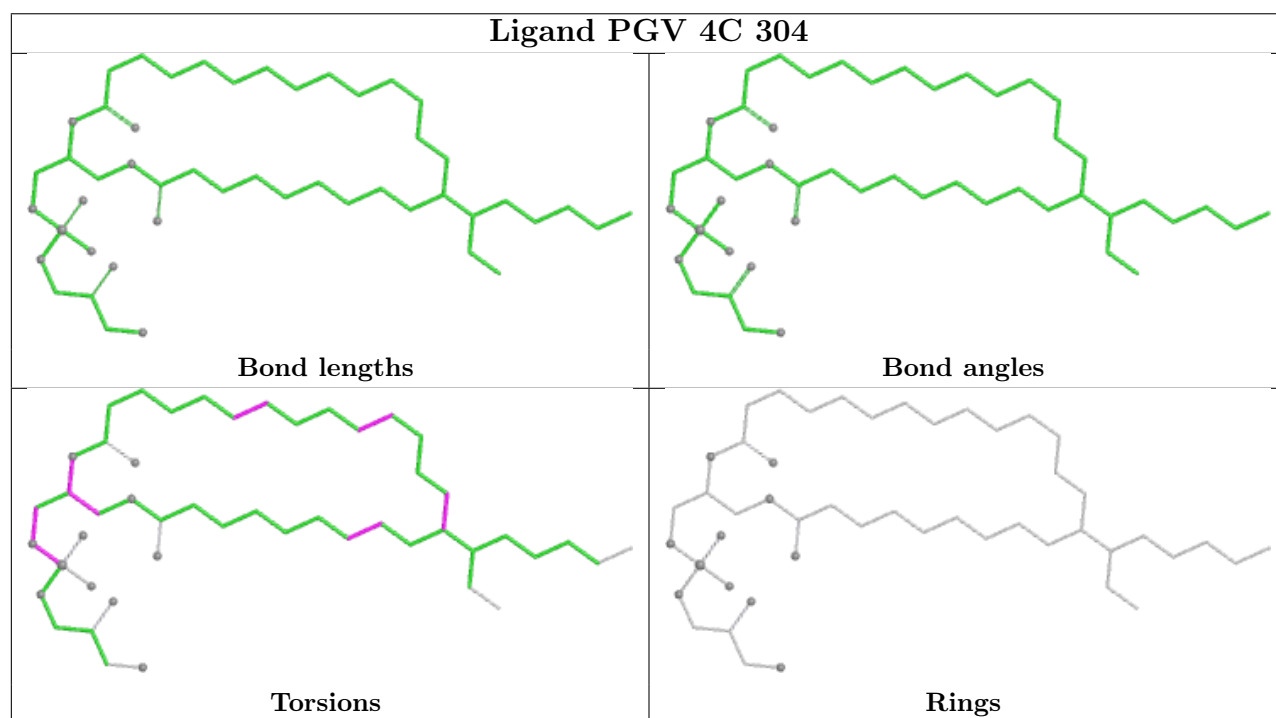
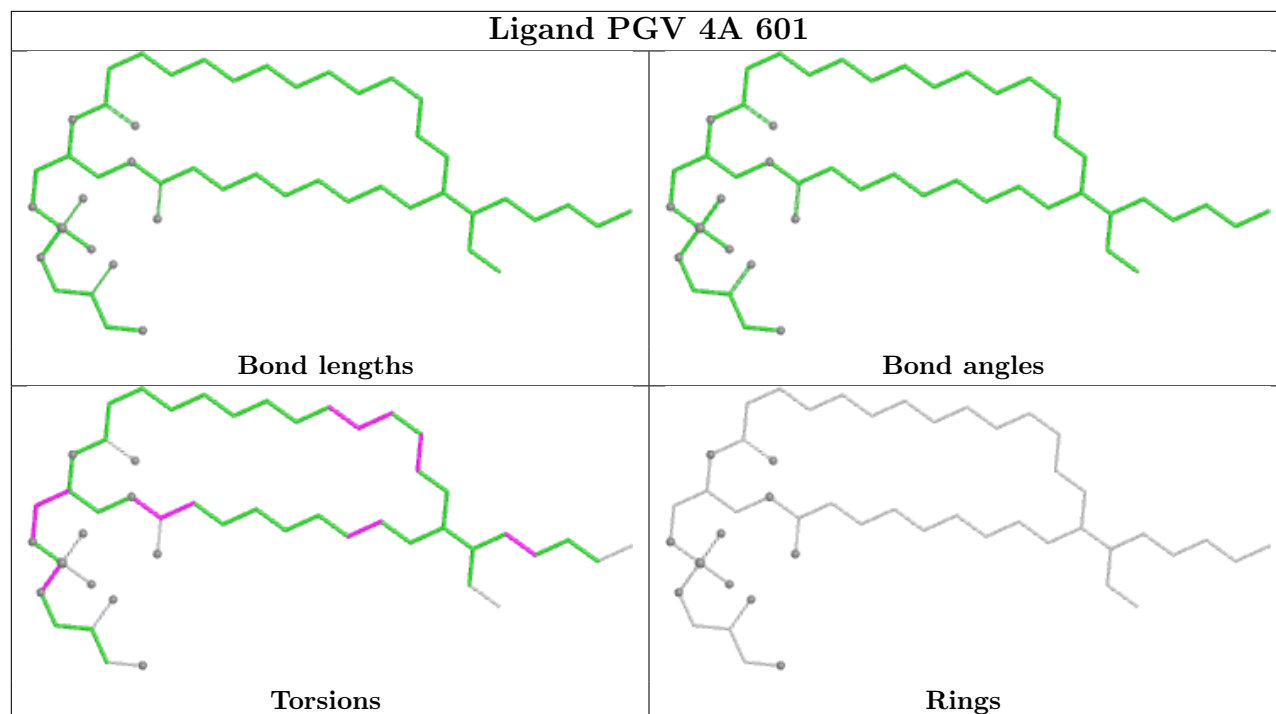


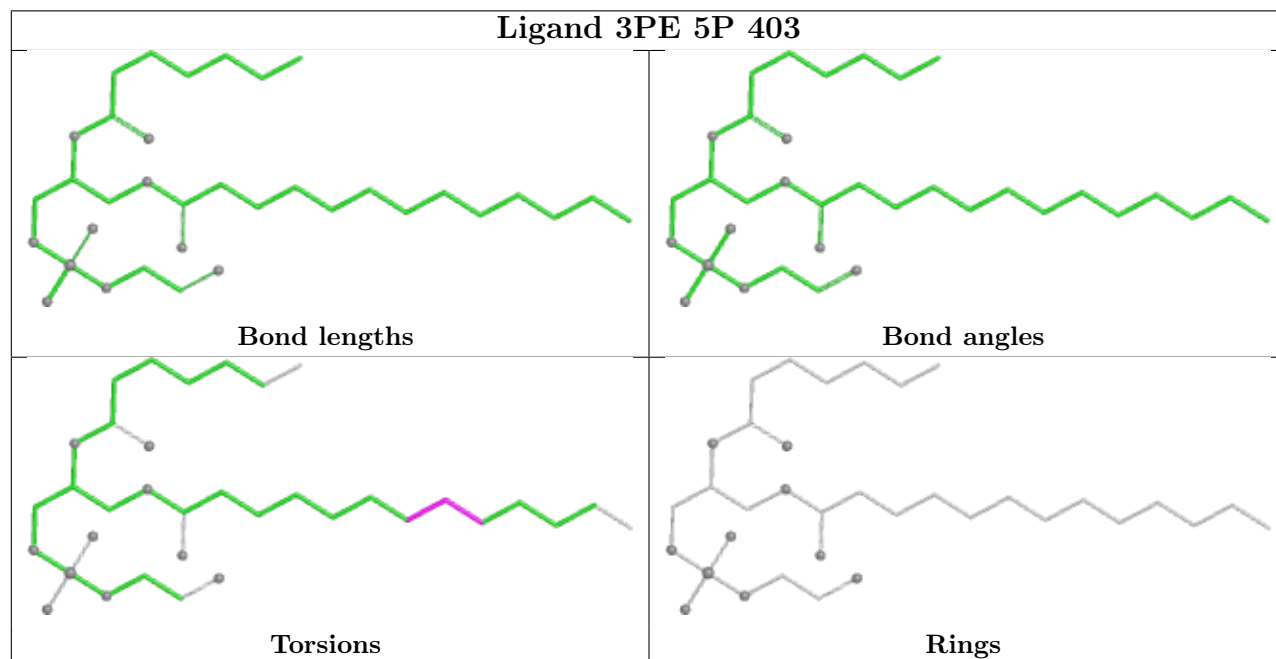
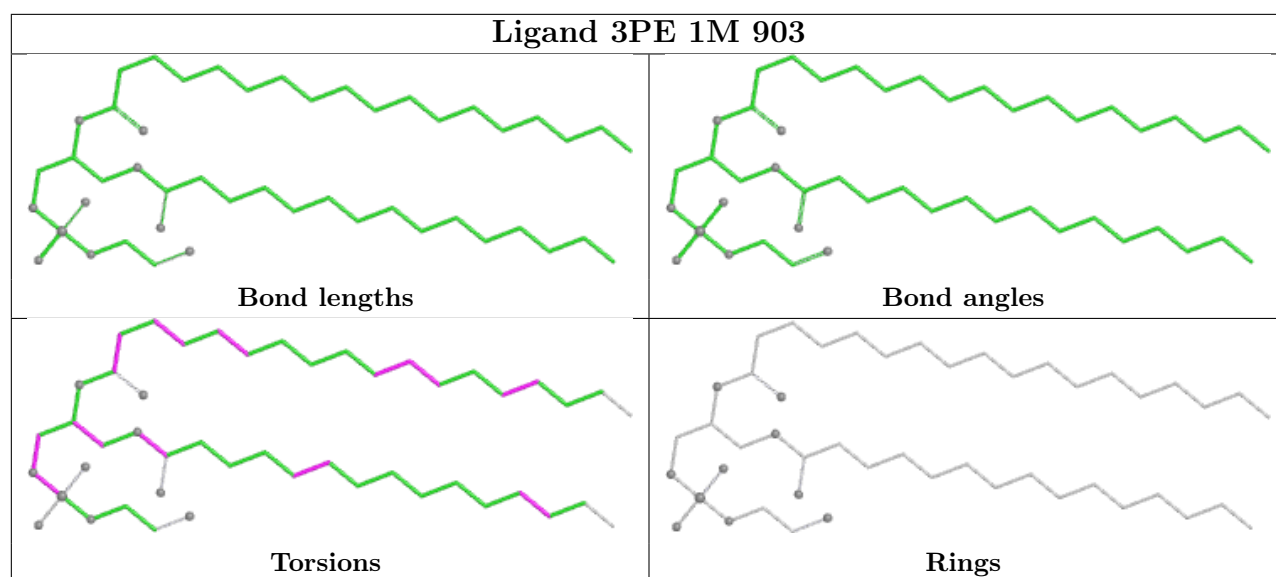


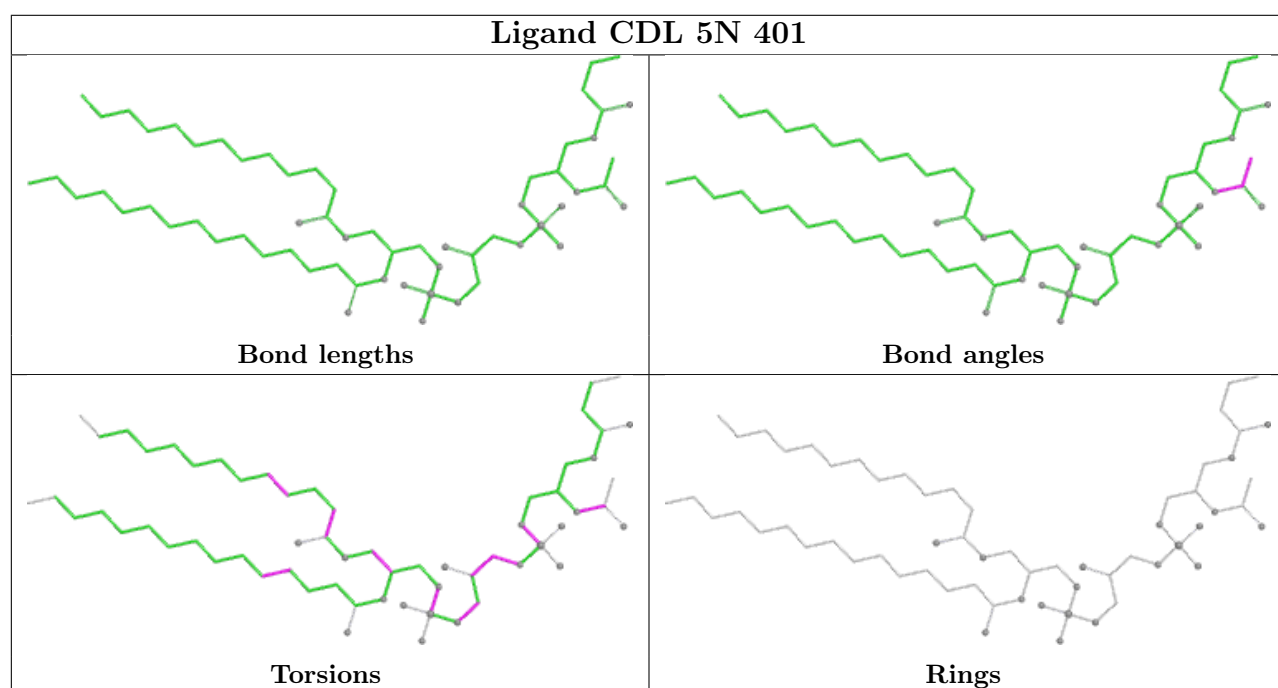
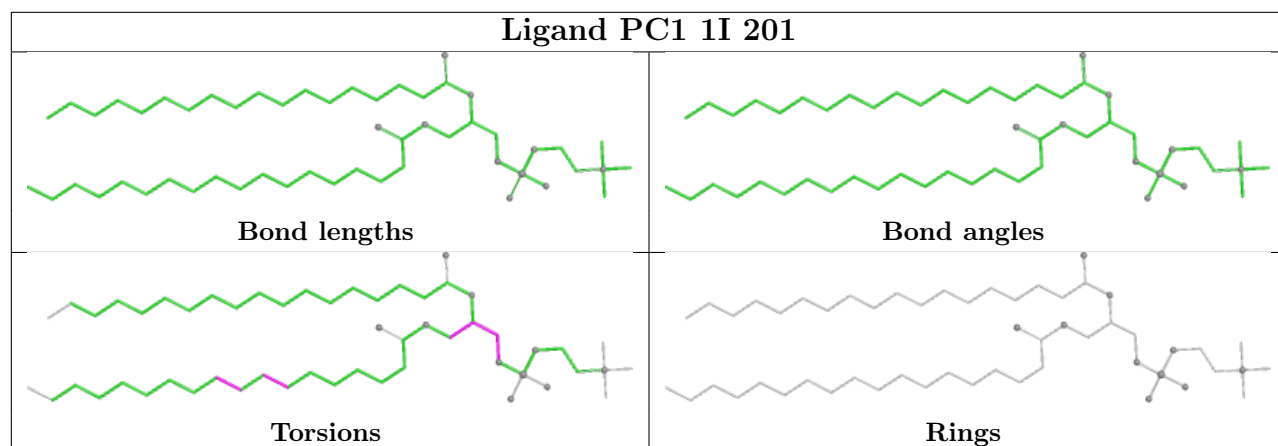
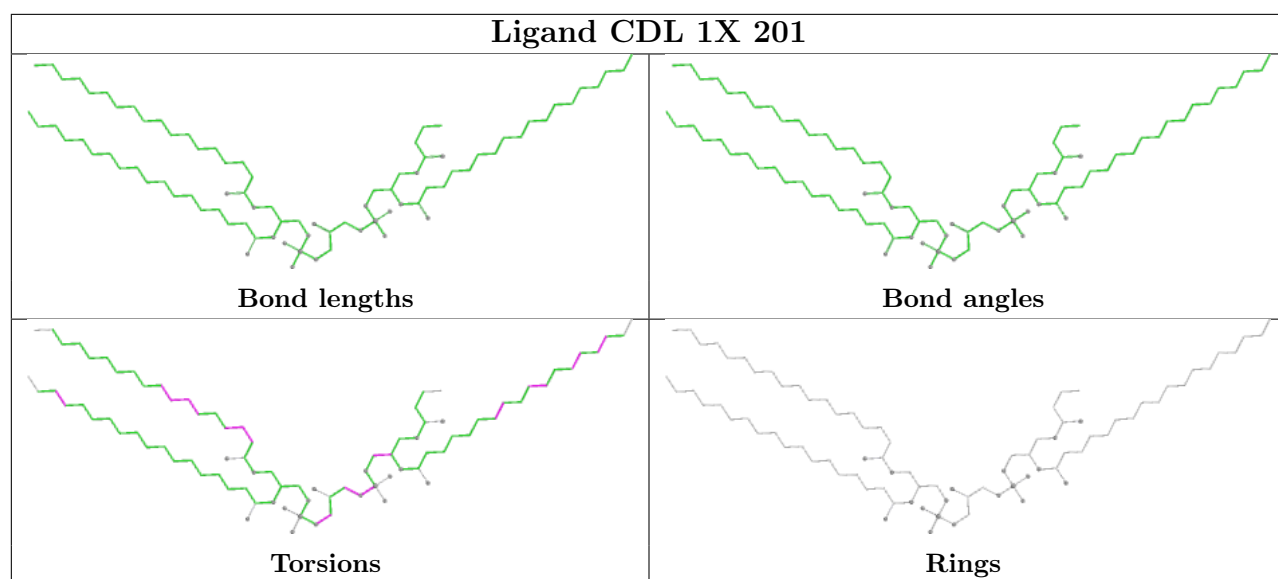


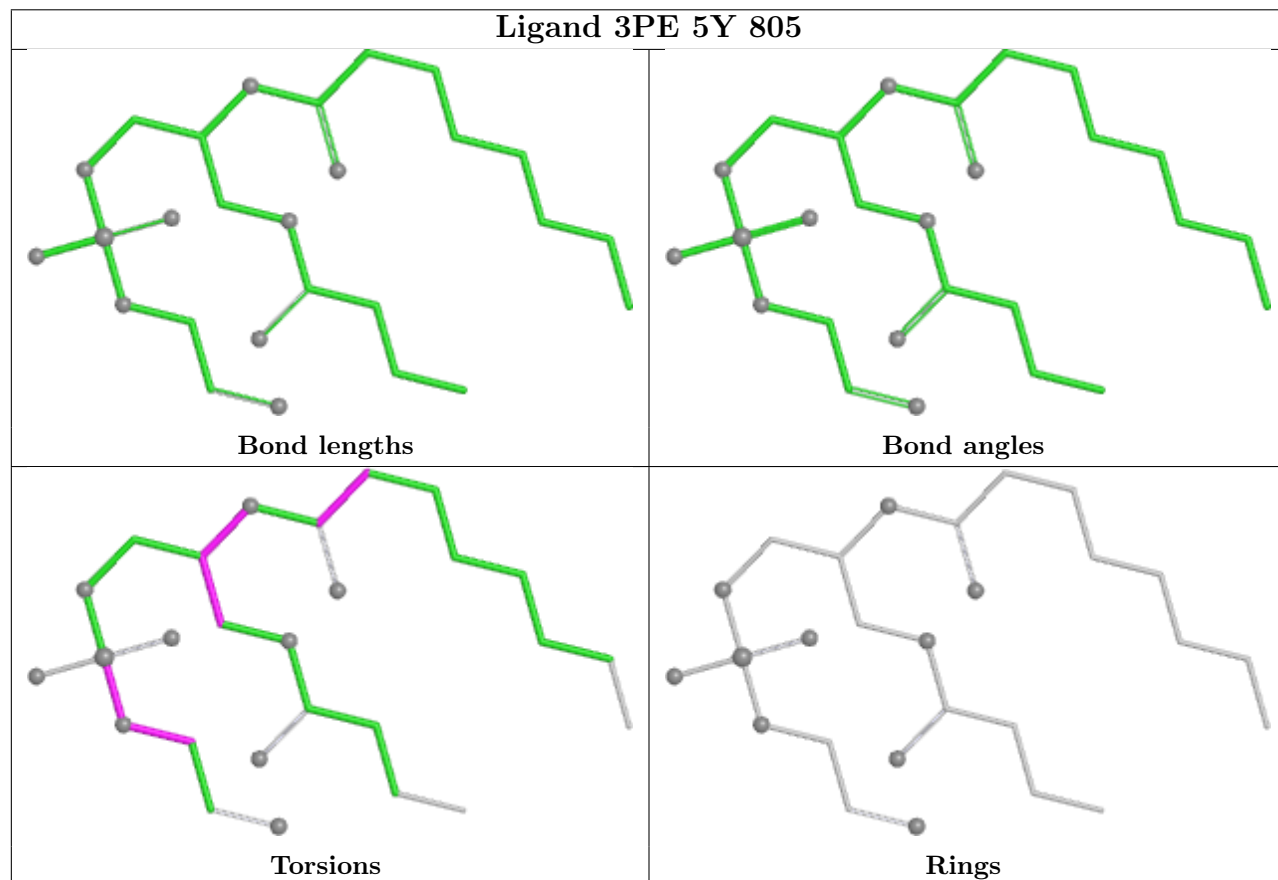
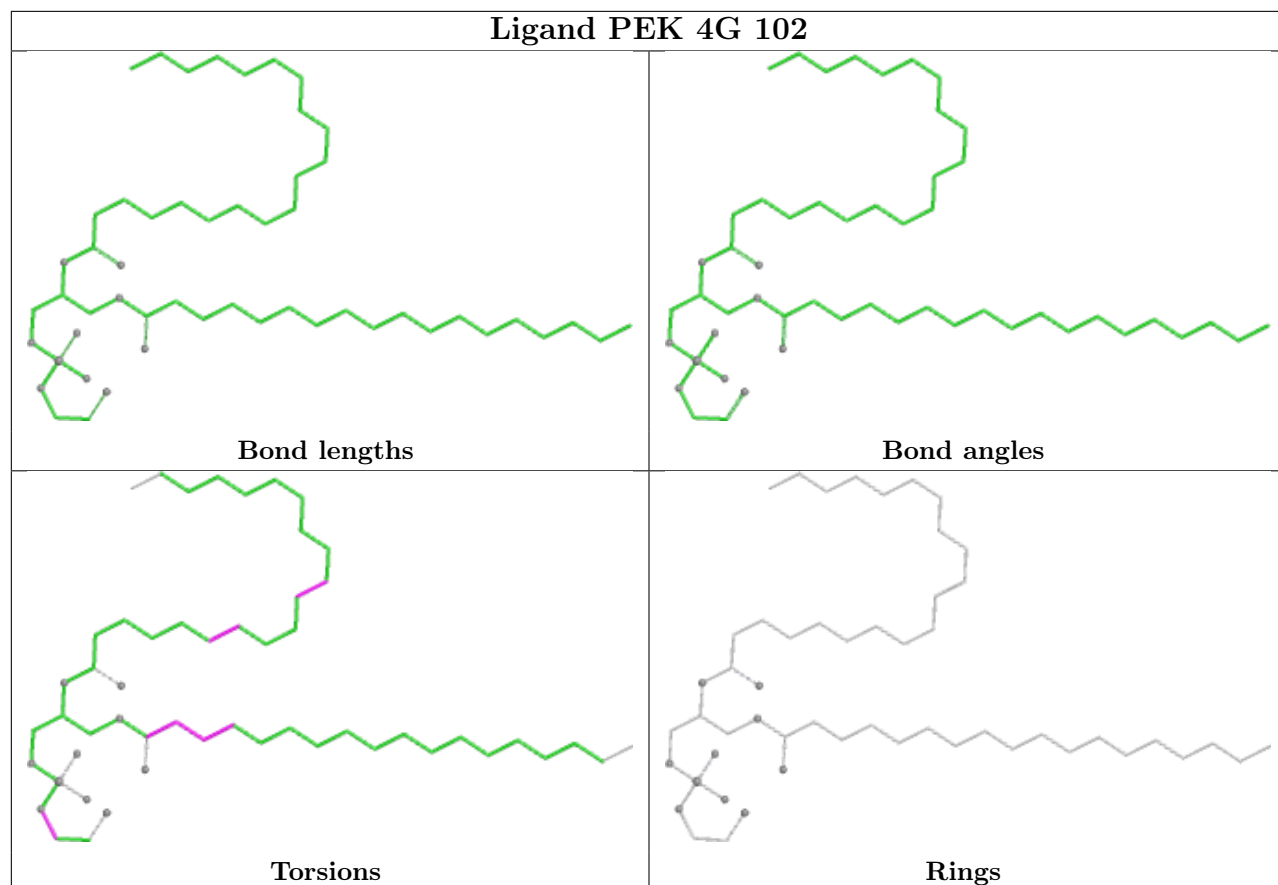


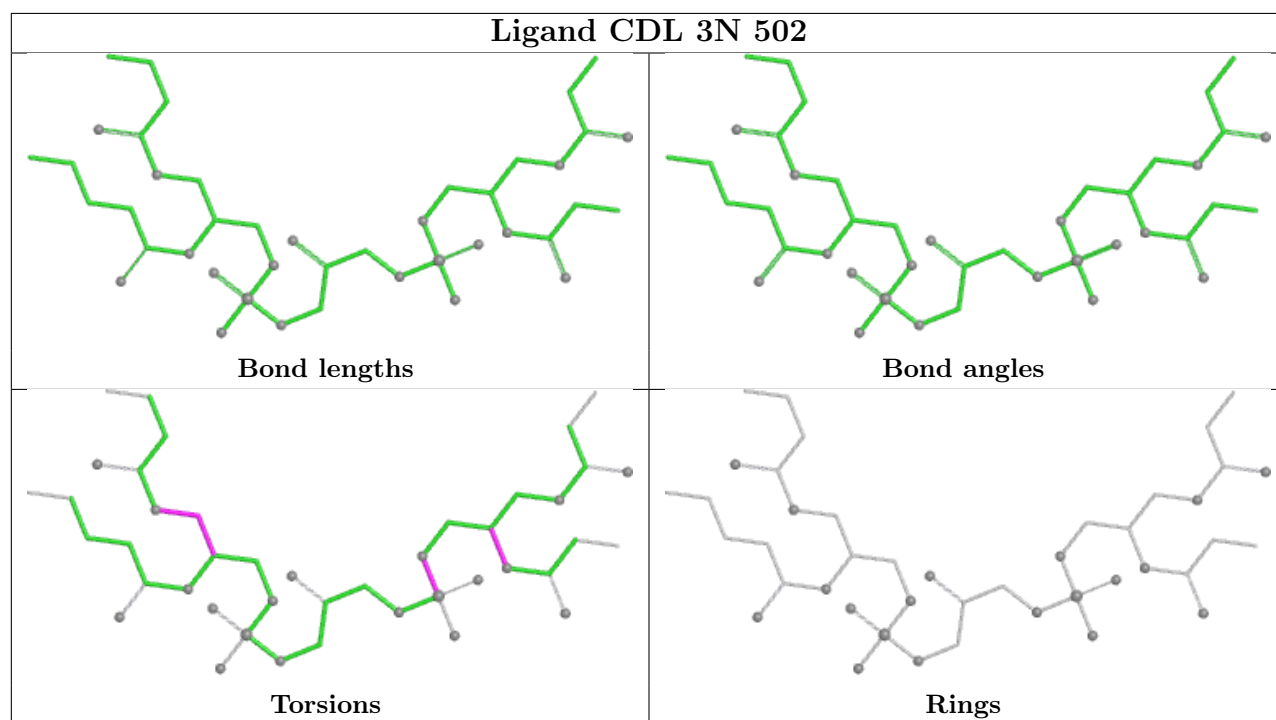
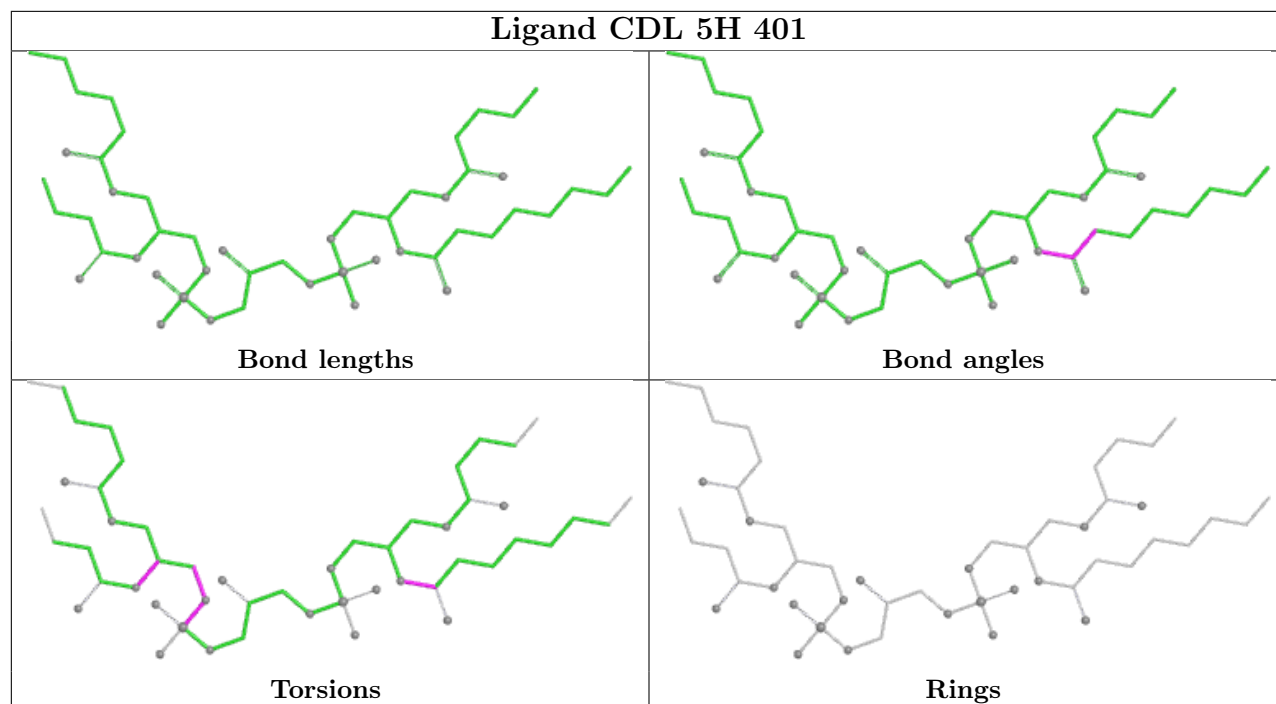


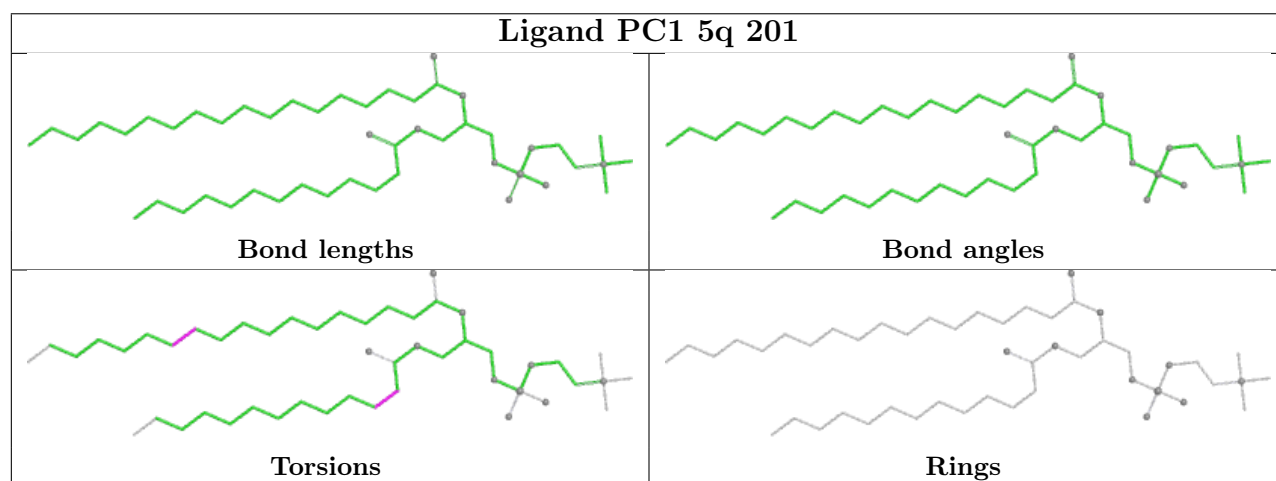
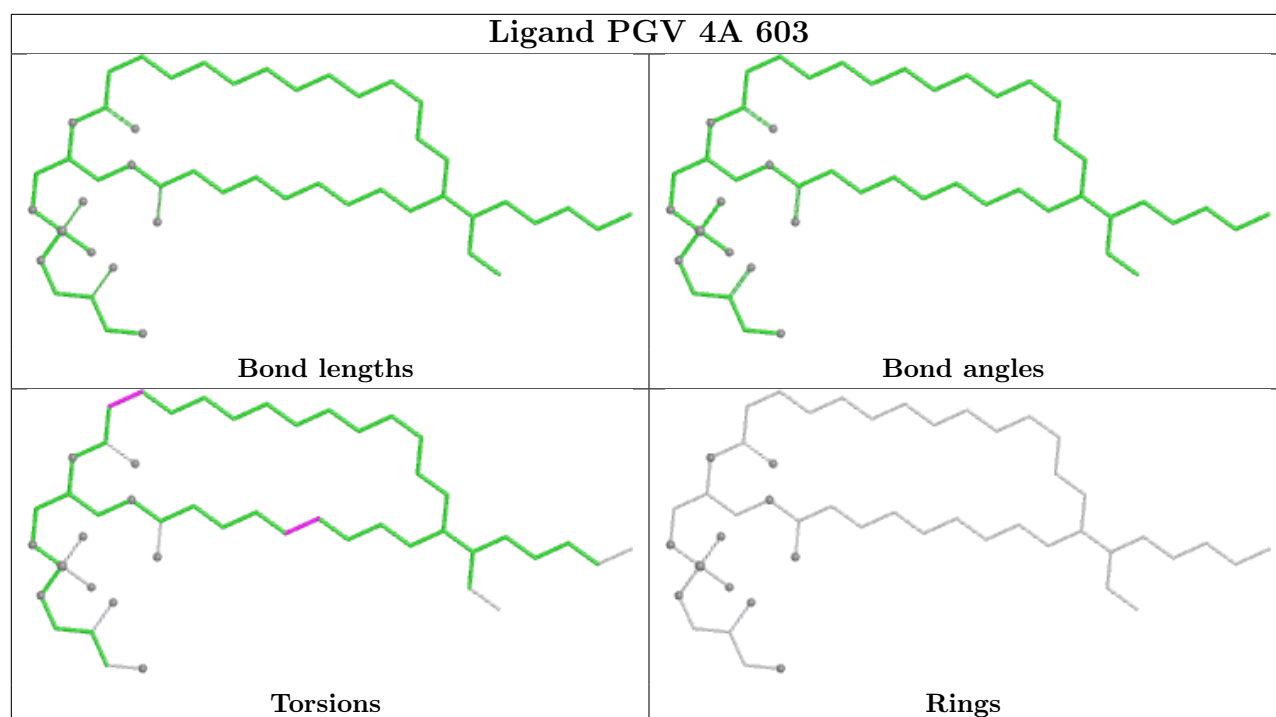


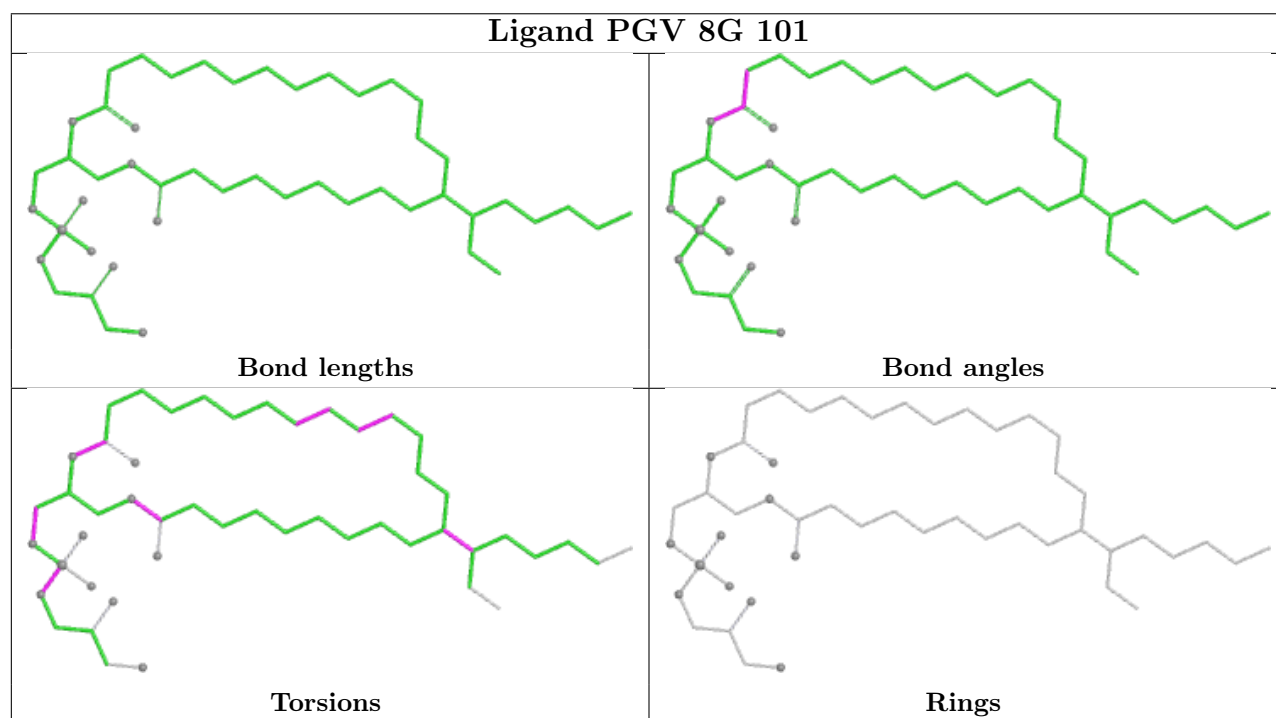
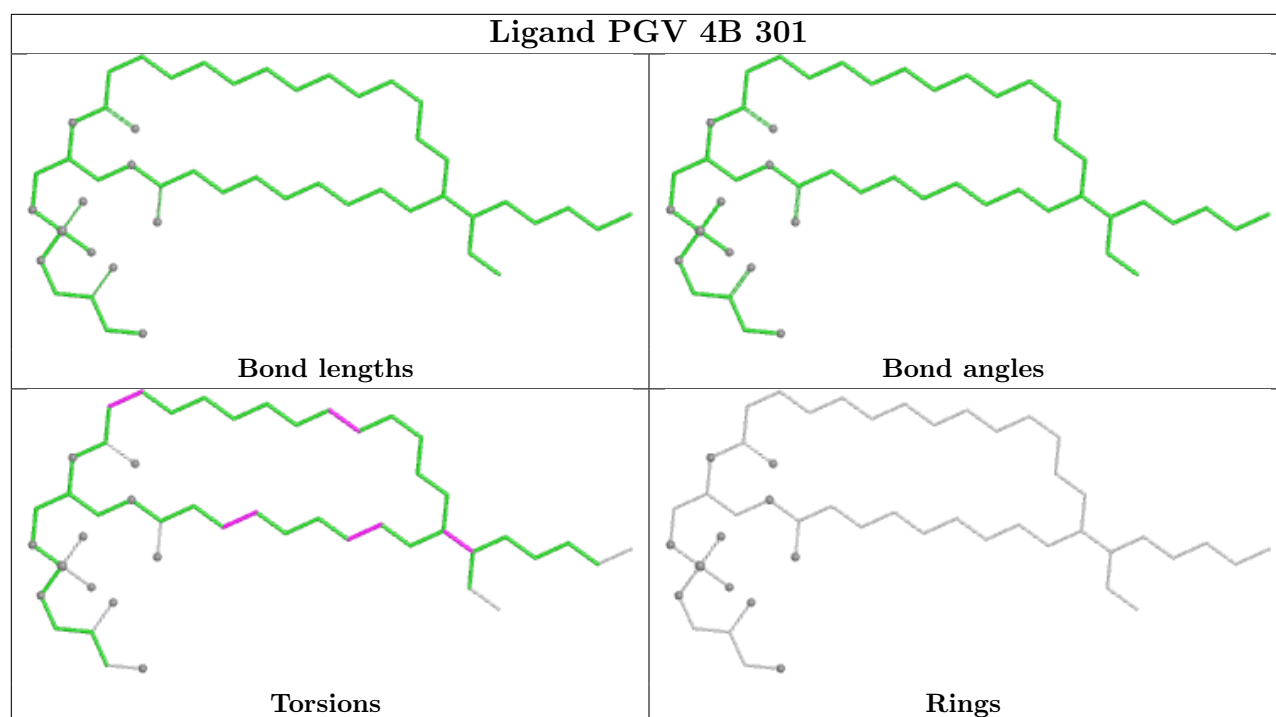


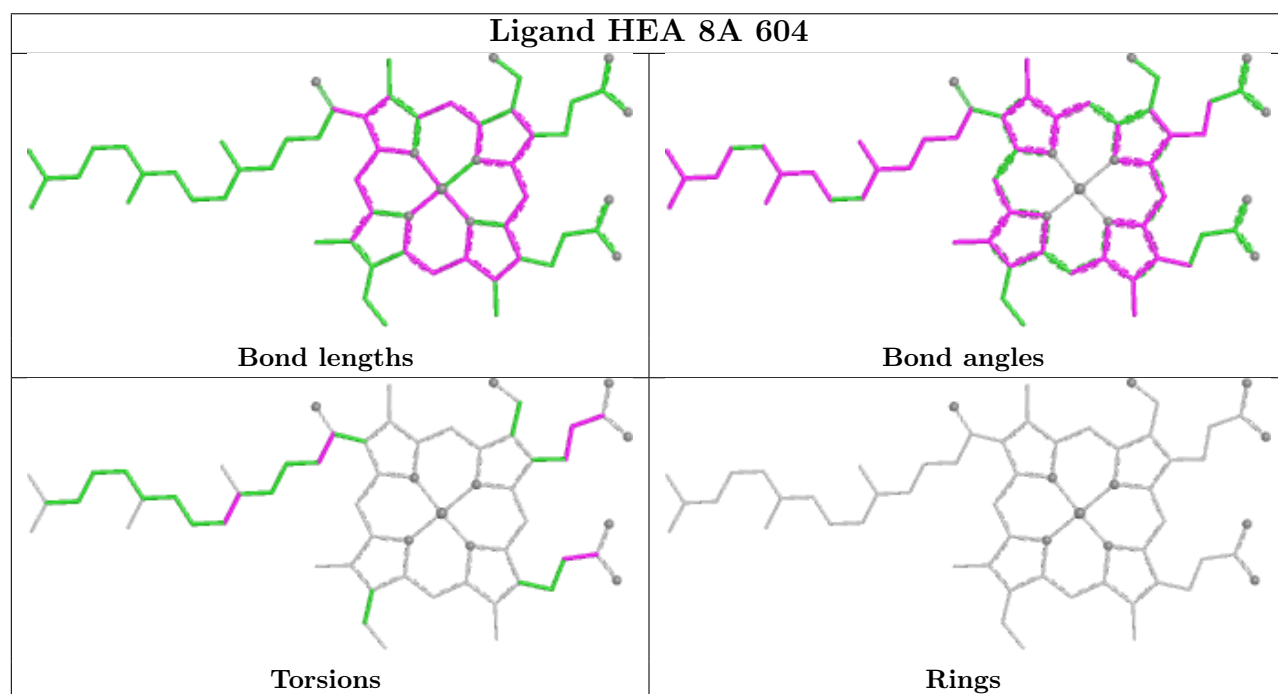
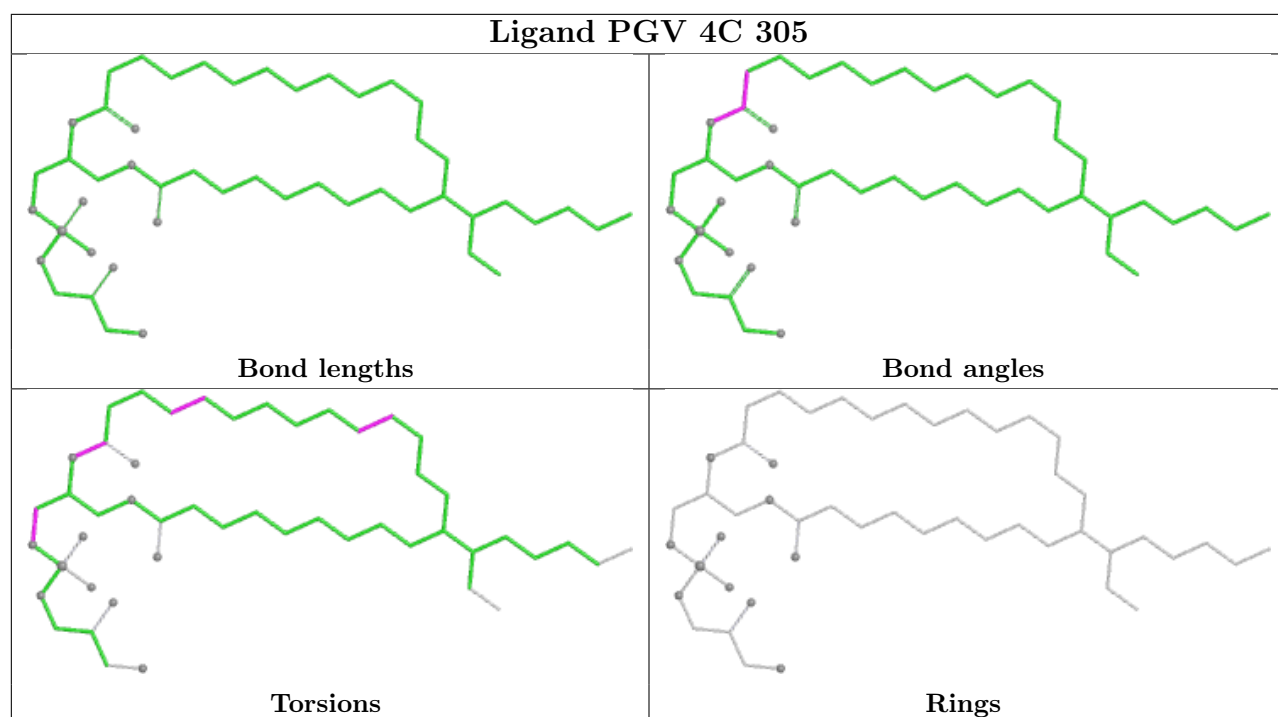


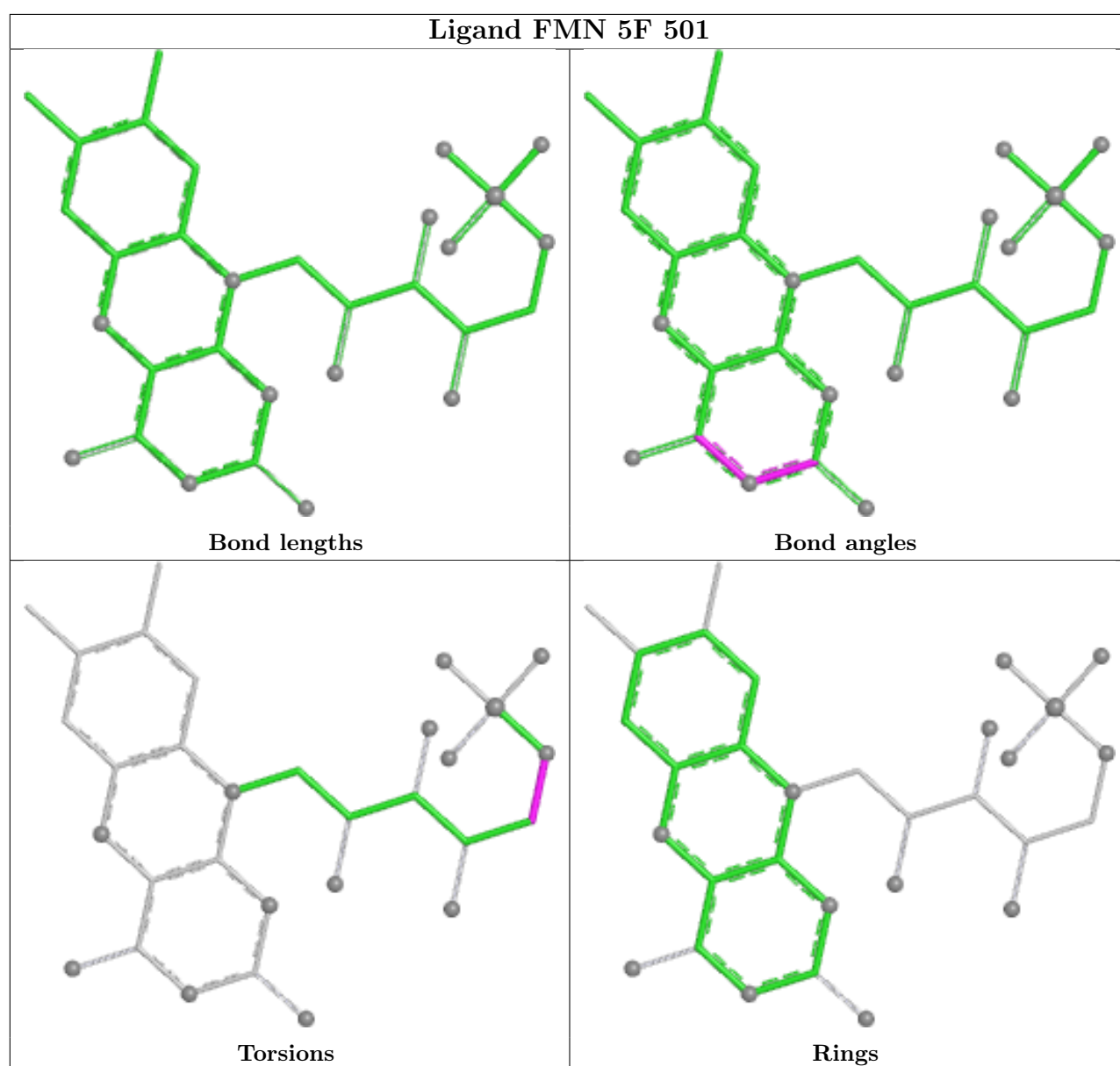
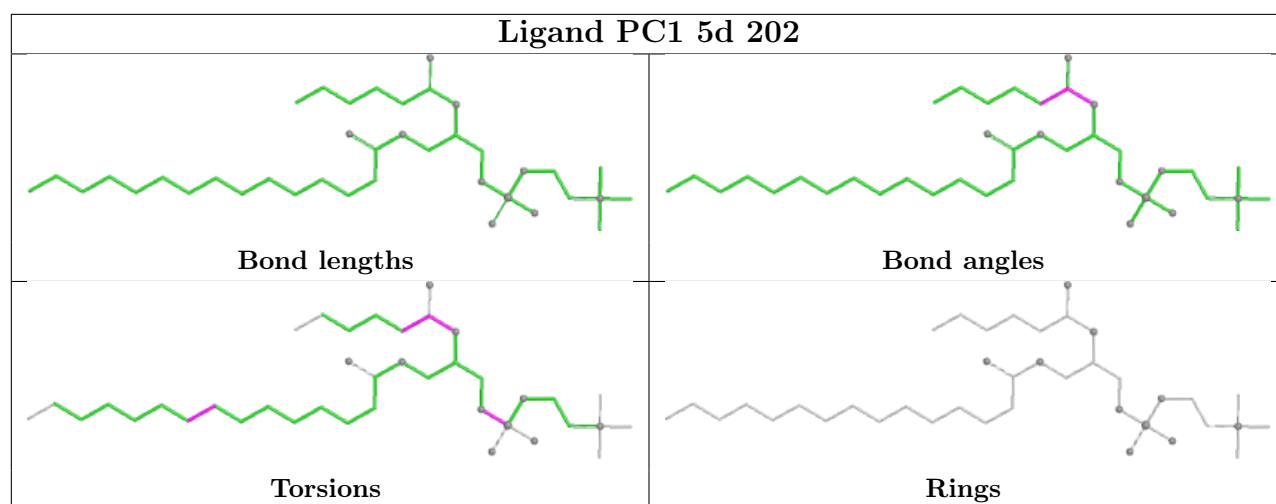


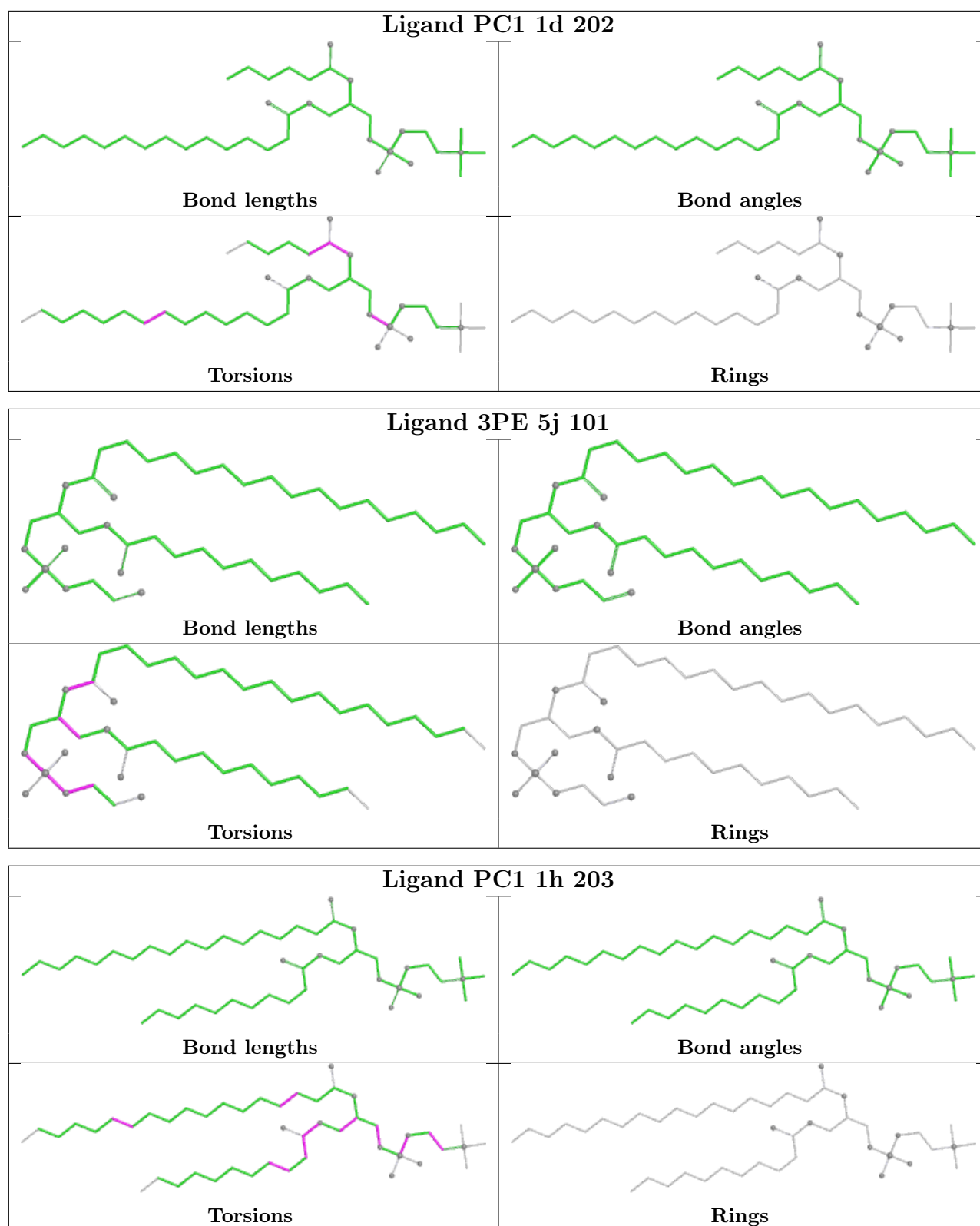


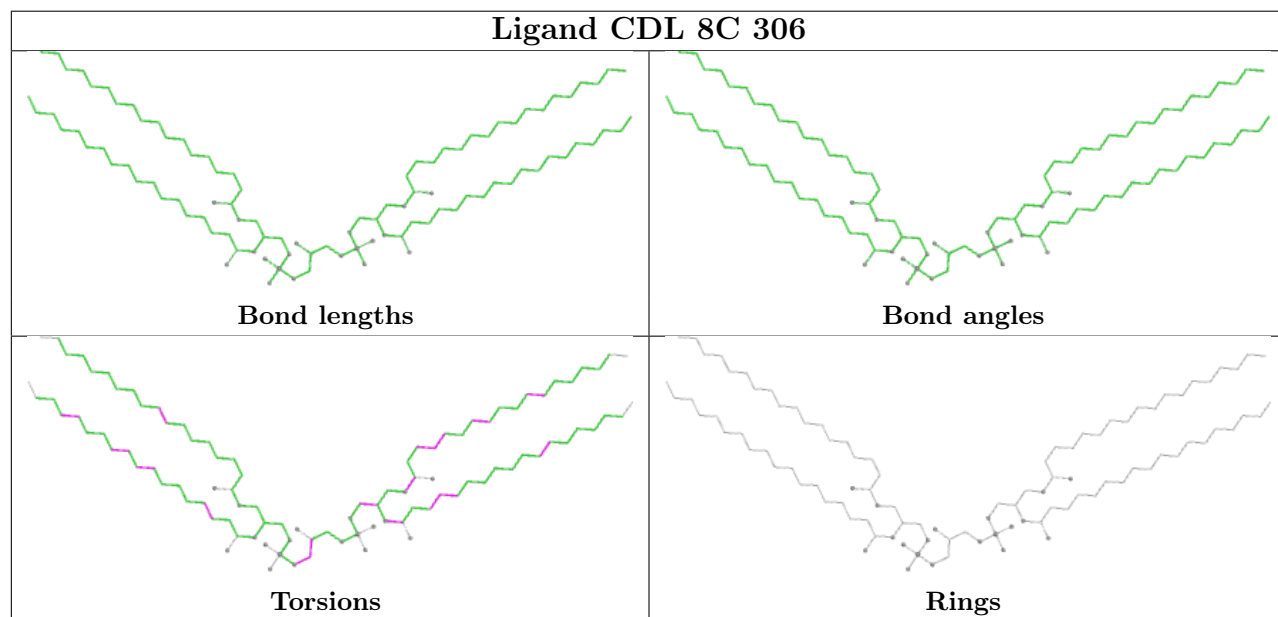
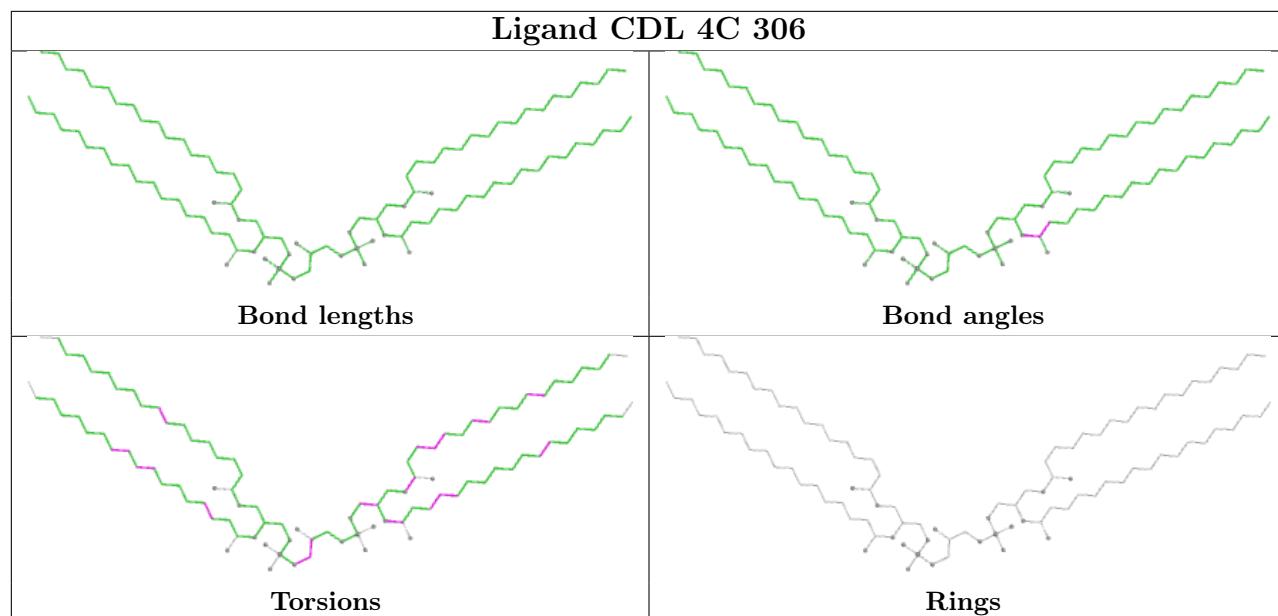


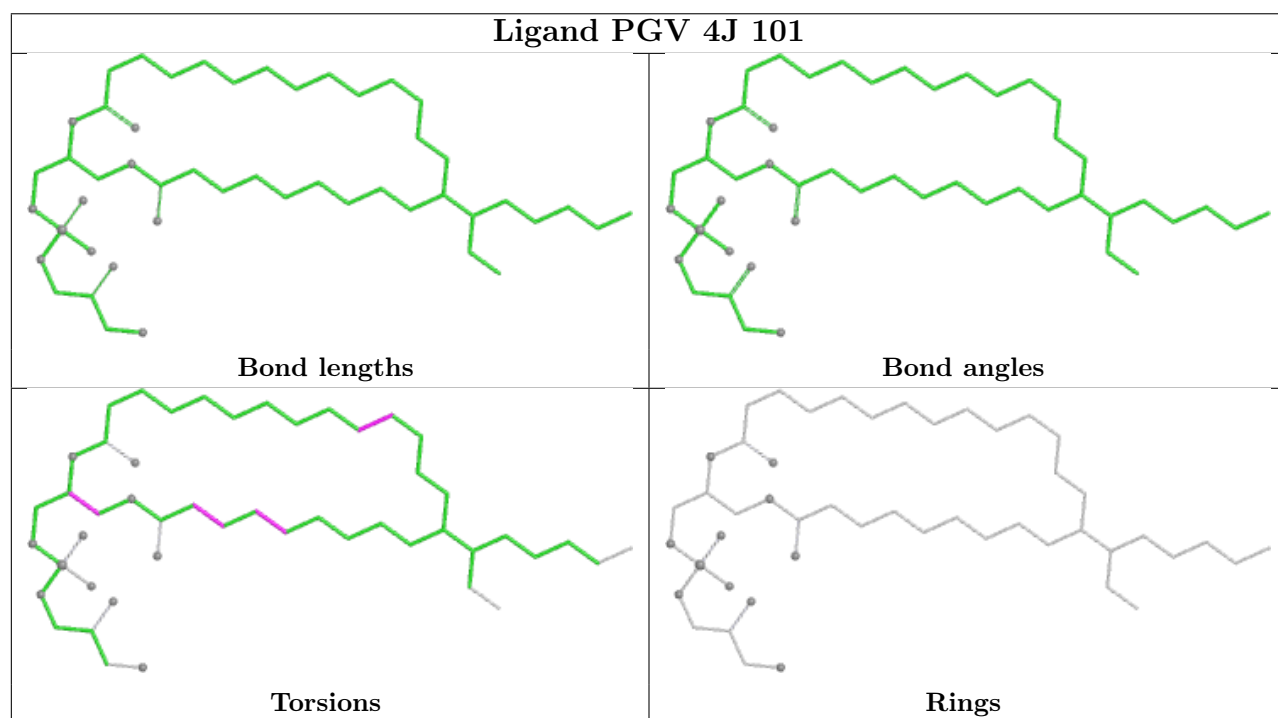
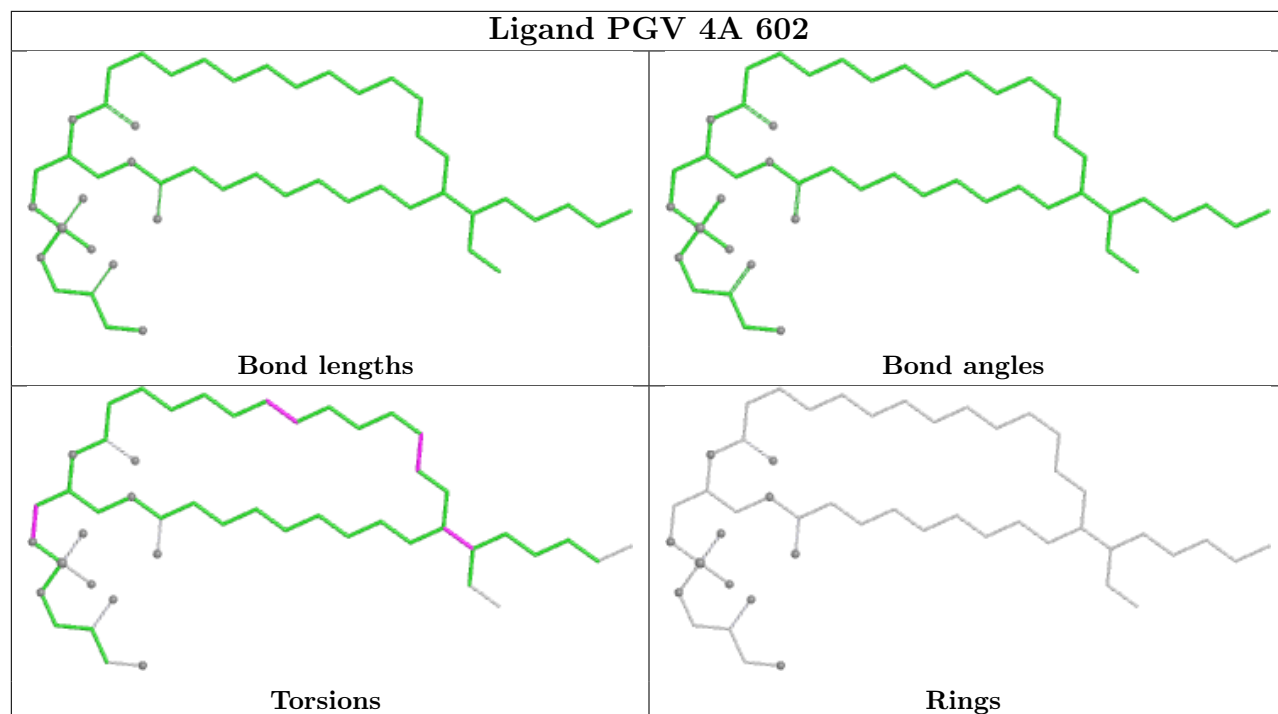


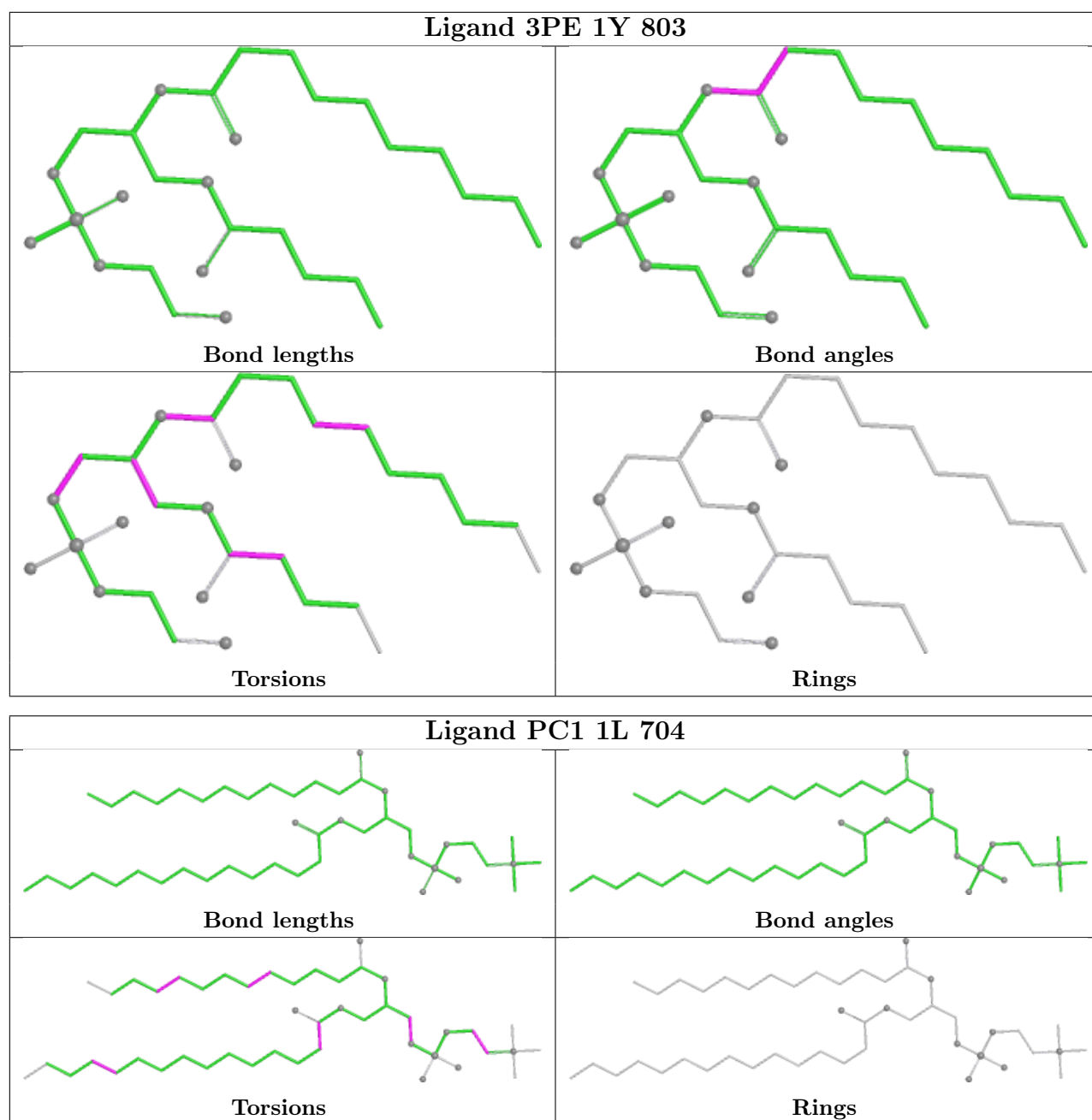


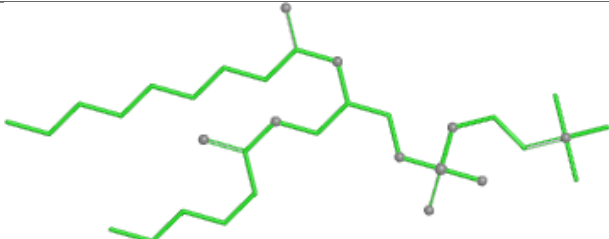
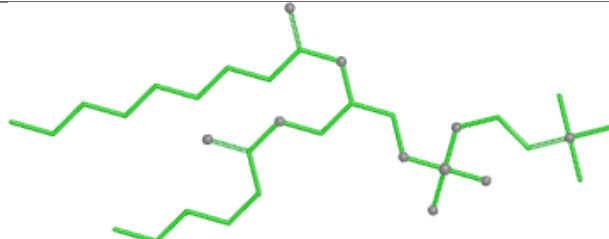
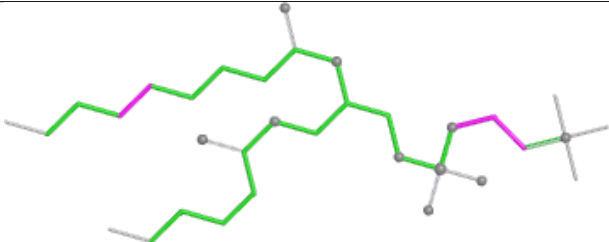
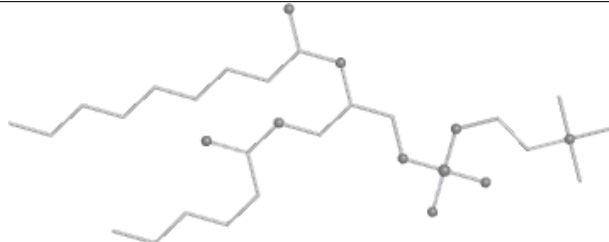
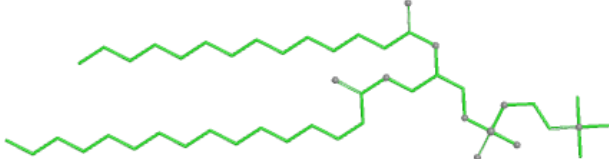
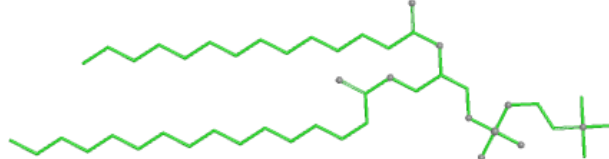
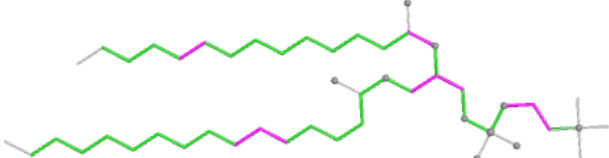
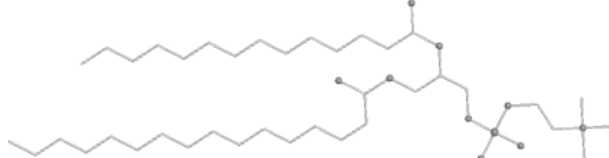
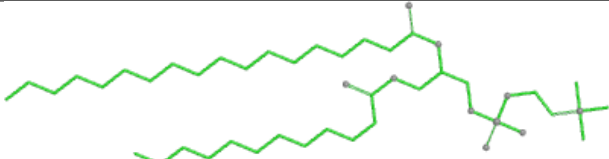
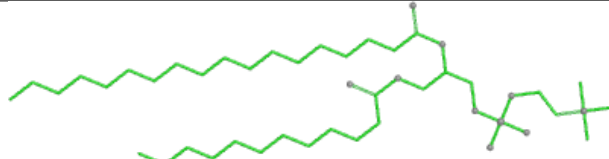
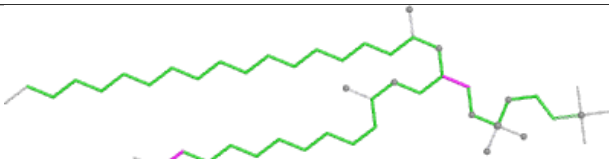
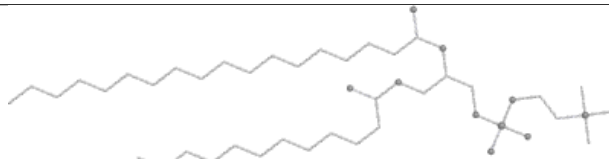


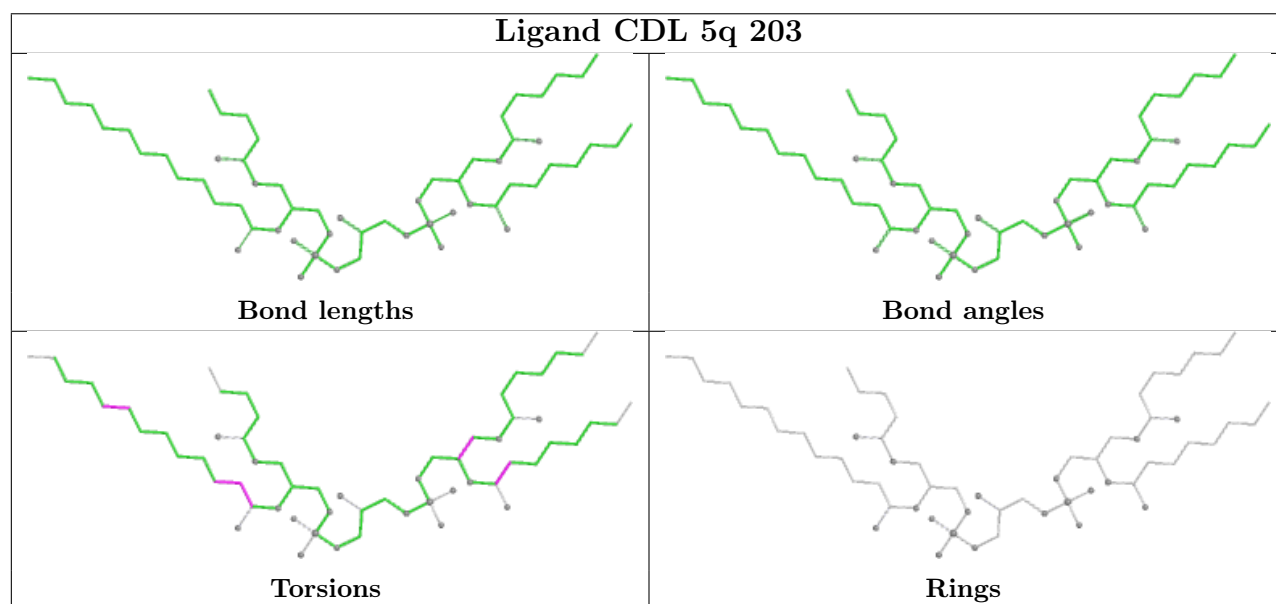
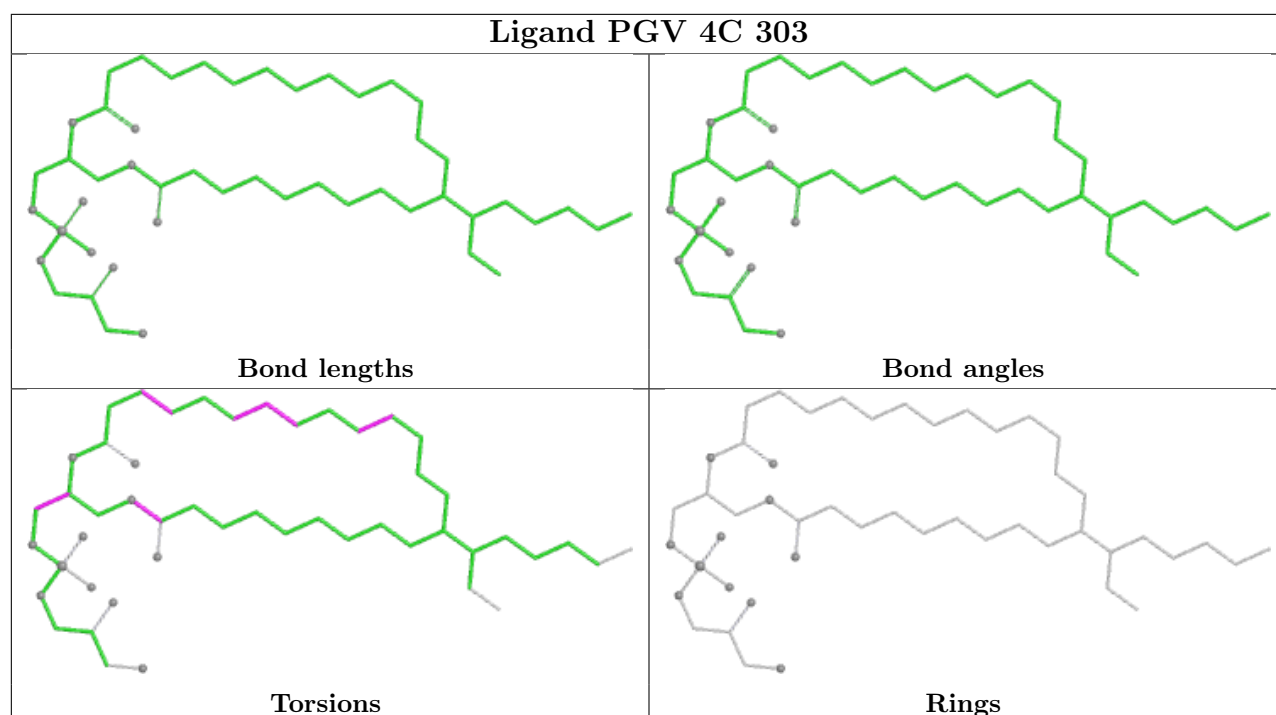


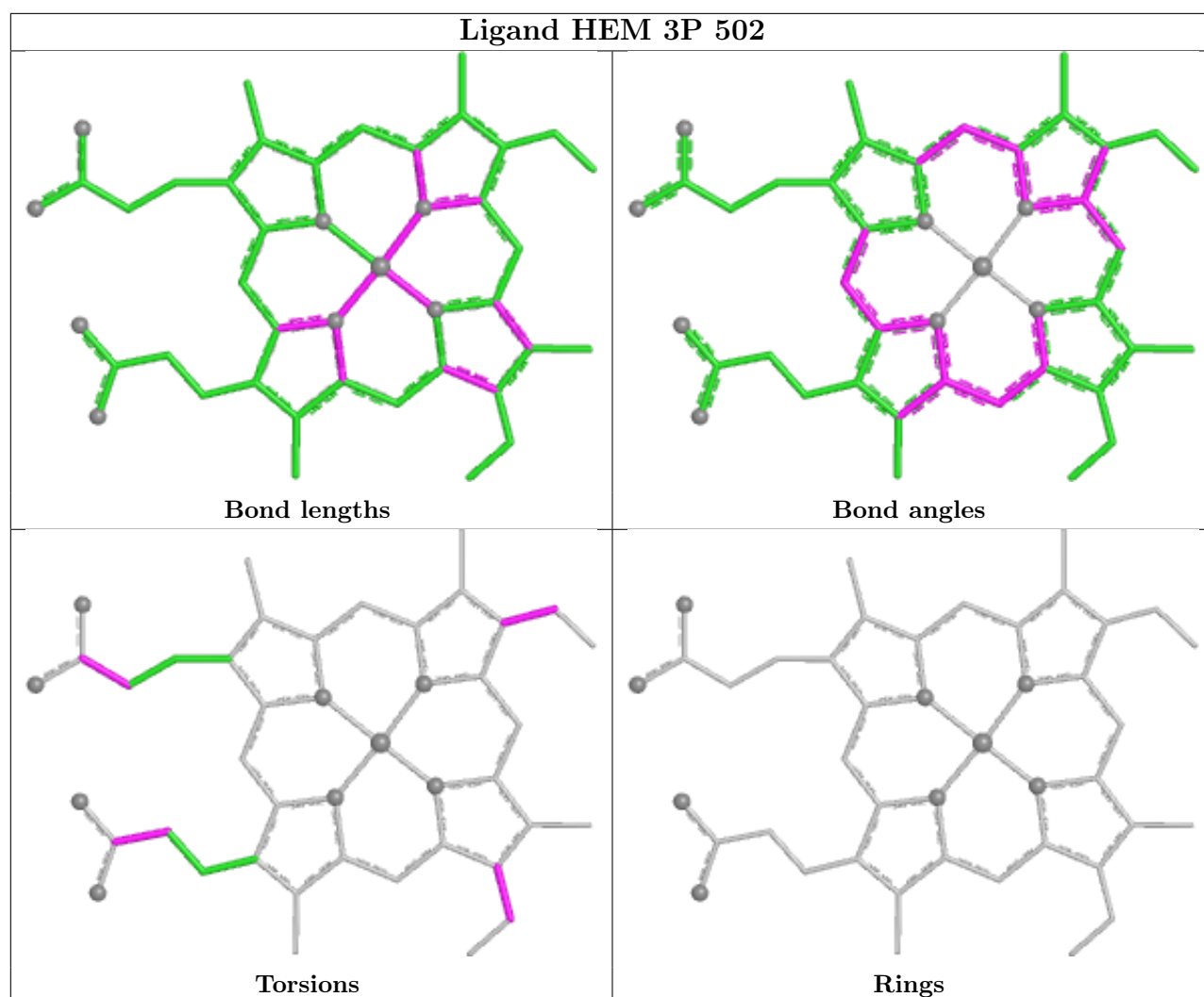






Ligand PC1 1A 203	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PC1 5B 203	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PC1 5H 402	
 Bond lengths	 Bond angles
 Torsions	 Rings





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.

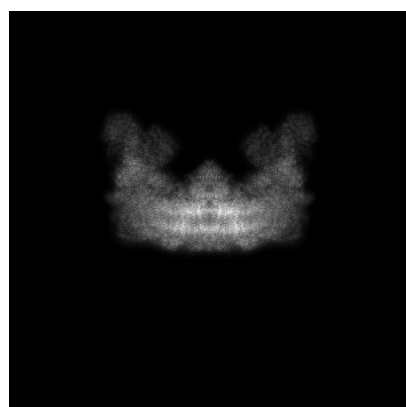
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42230. These allow visual inspection of the internal detail of the map and identification of artifacts.

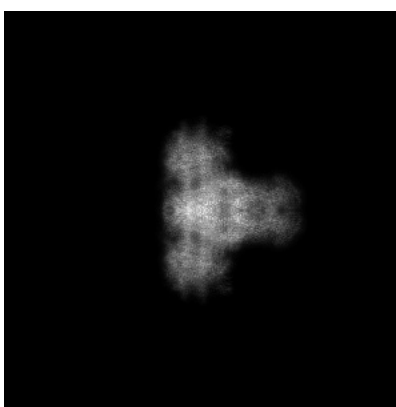
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

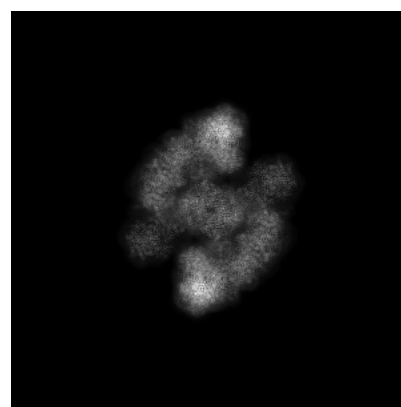
6.1.1 Primary map



X



Y

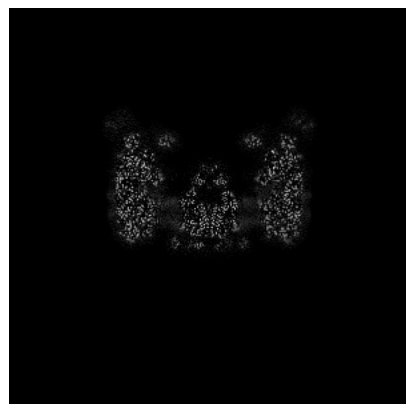


Z

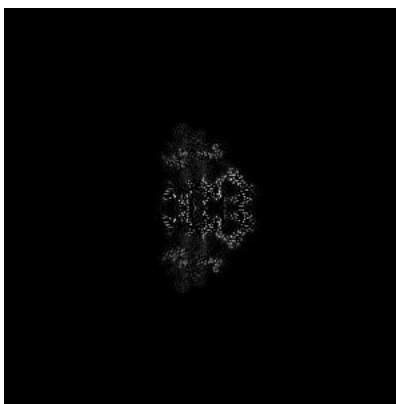
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

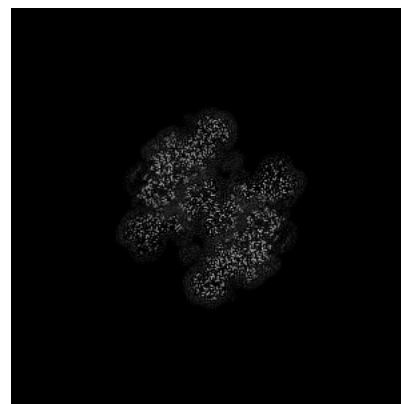
6.2.1 Primary map



X Index: 275



Y Index: 275

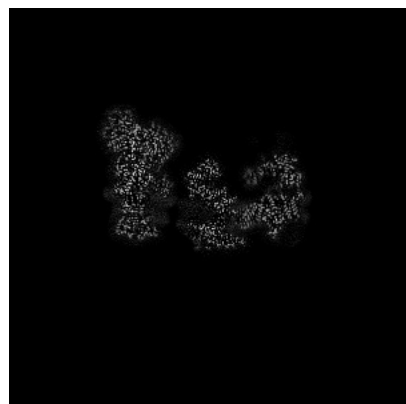


Z Index: 275

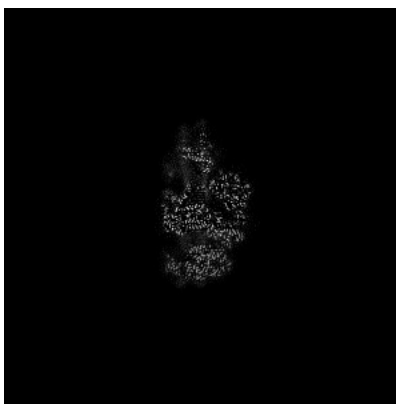
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

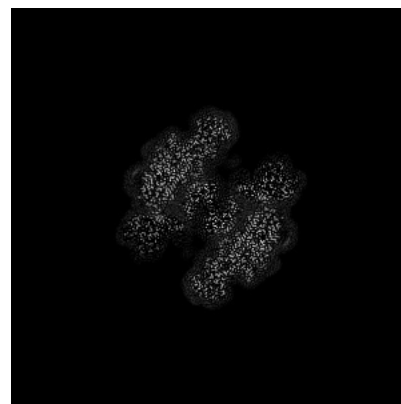
6.3.1 Primary map



X Index: 260



Y Index: 288

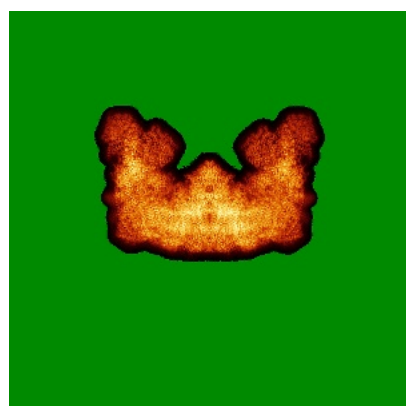


Z Index: 271

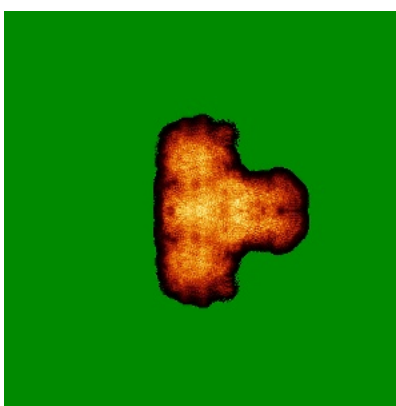
The images above show the largest variance slices of the map in three orthogonal directions.

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

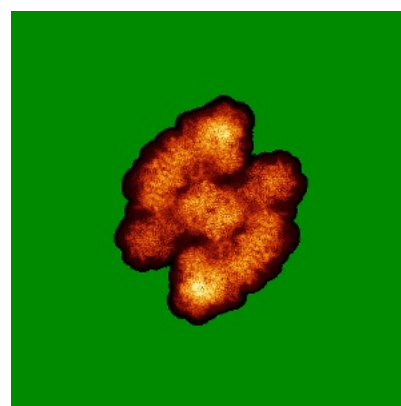
6.4.1 Primary map



X



Y

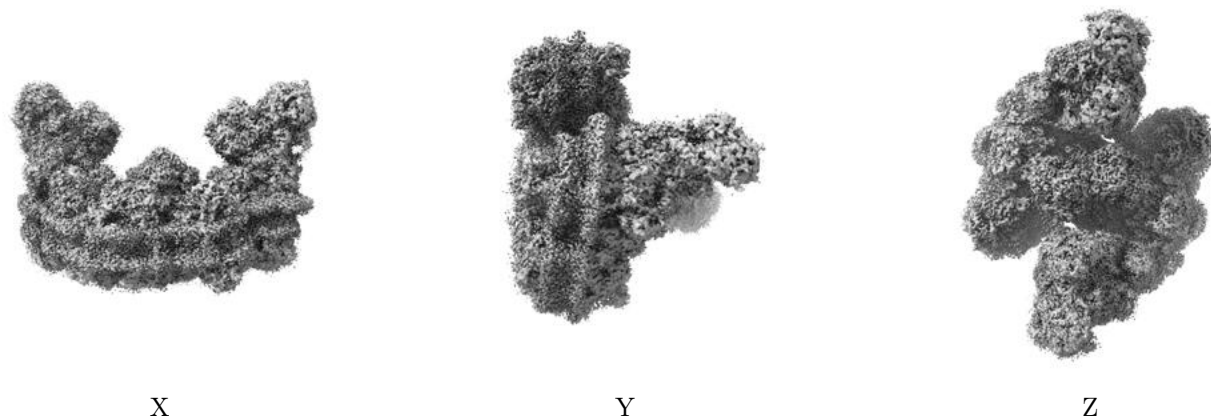


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

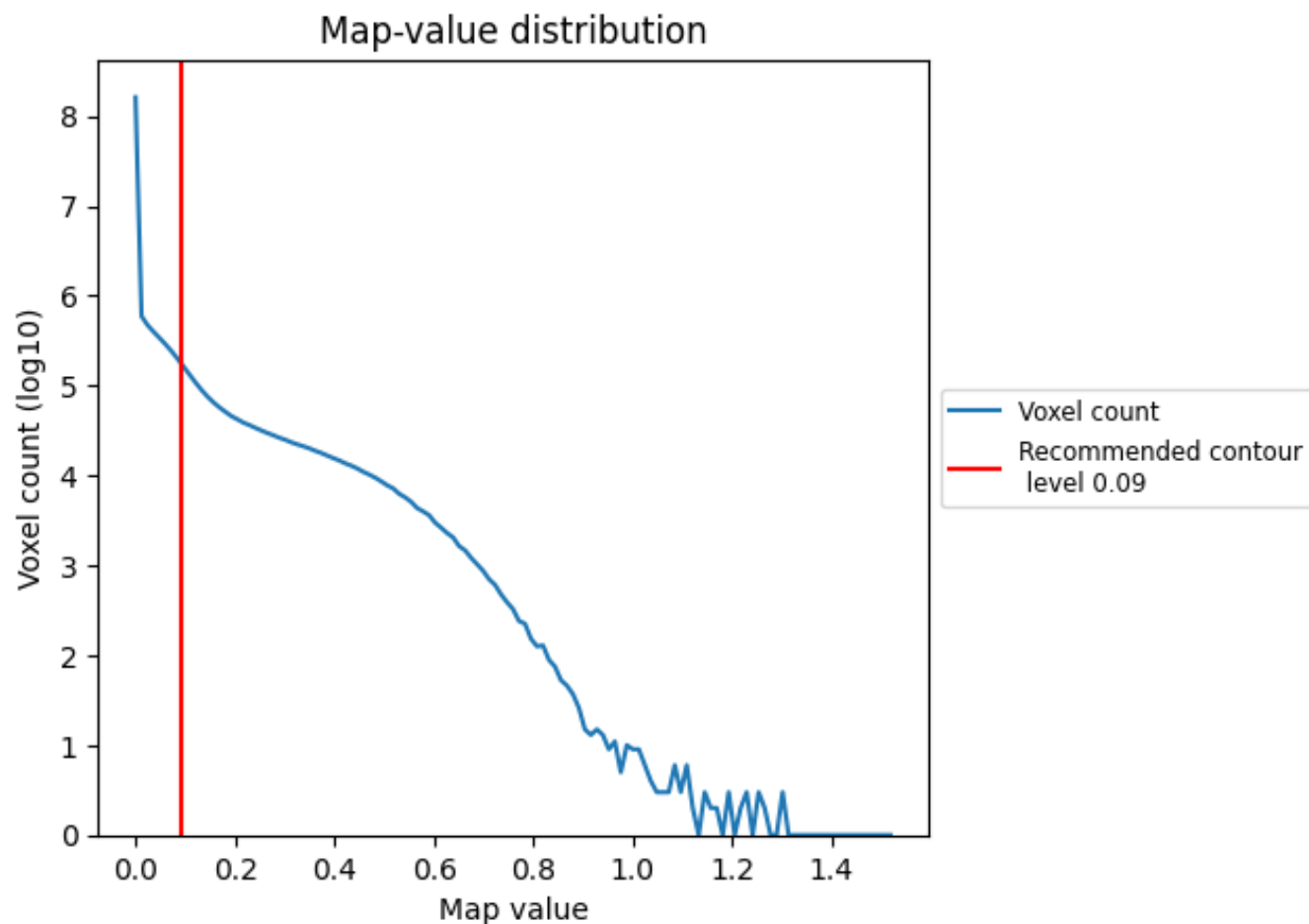
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

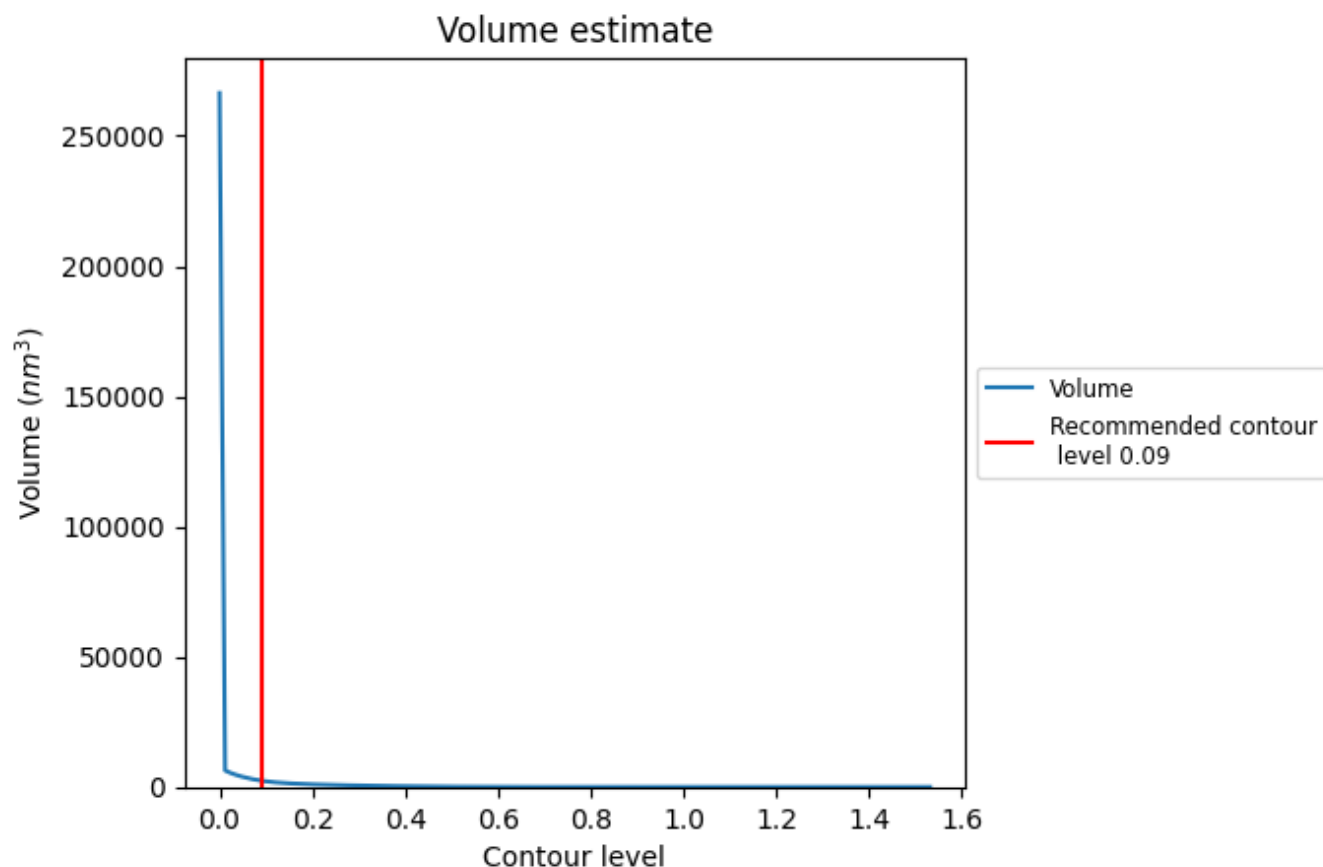
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

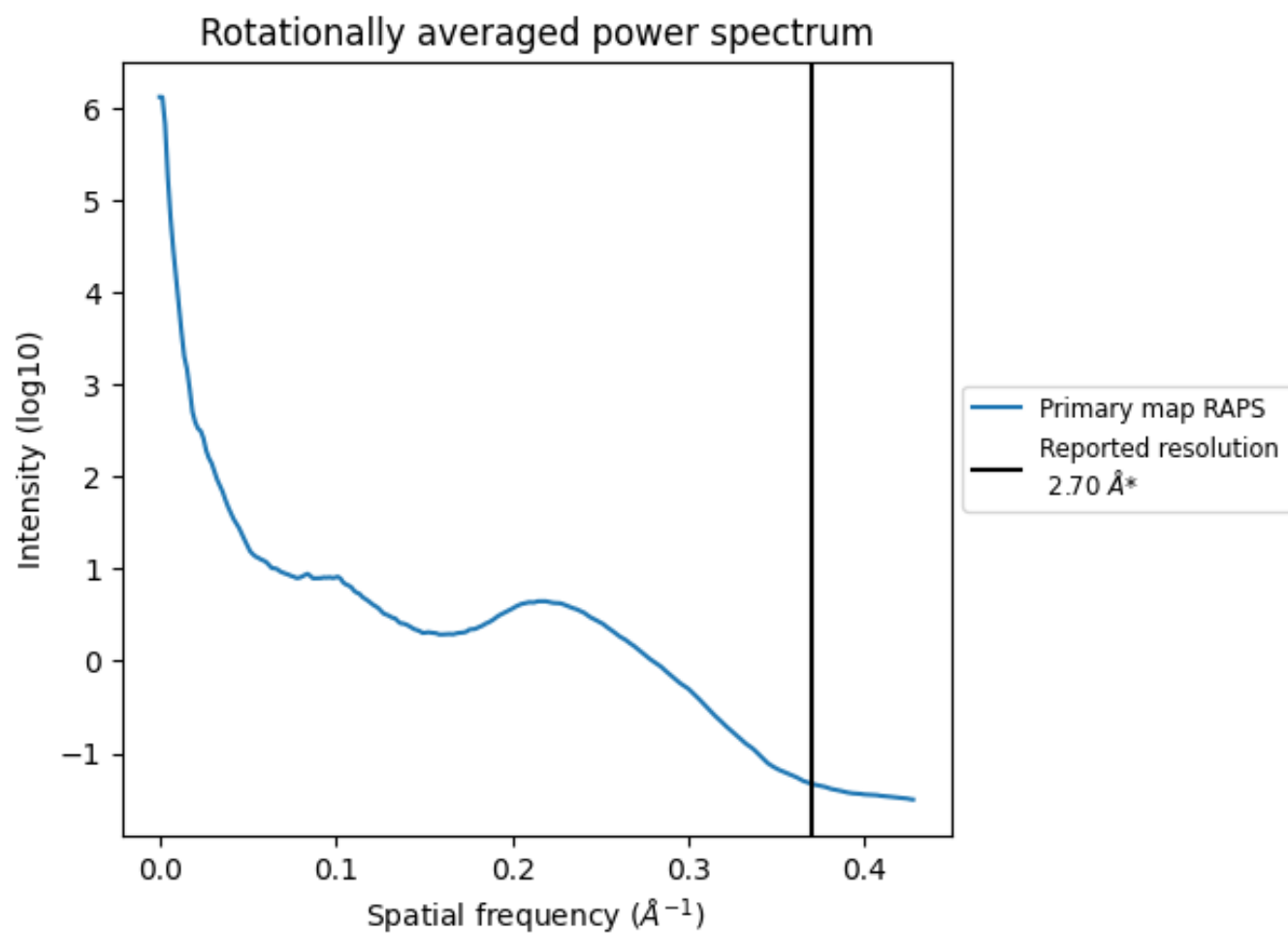
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2412 nm^3 ; this corresponds to an approximate mass of 2179 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

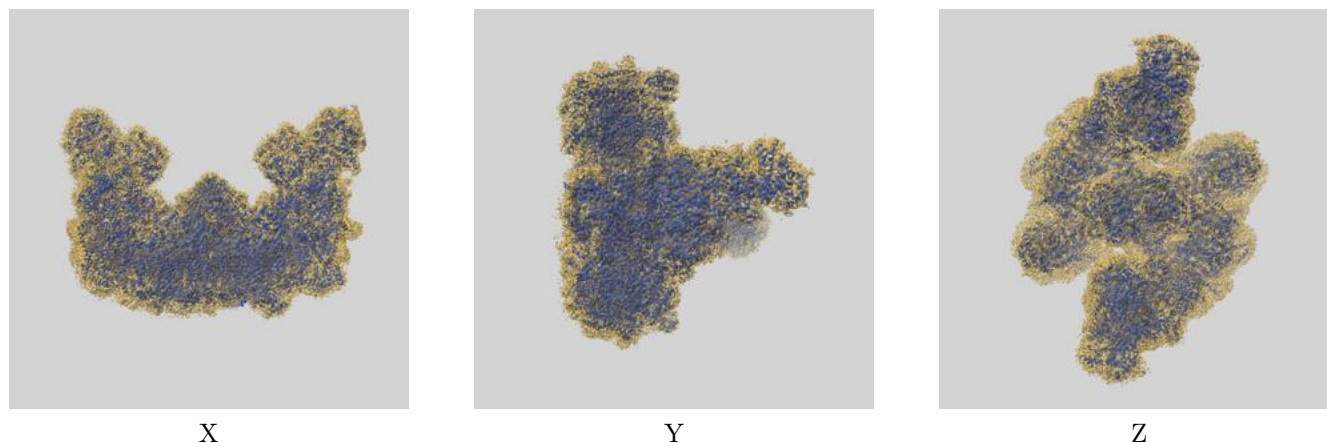
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

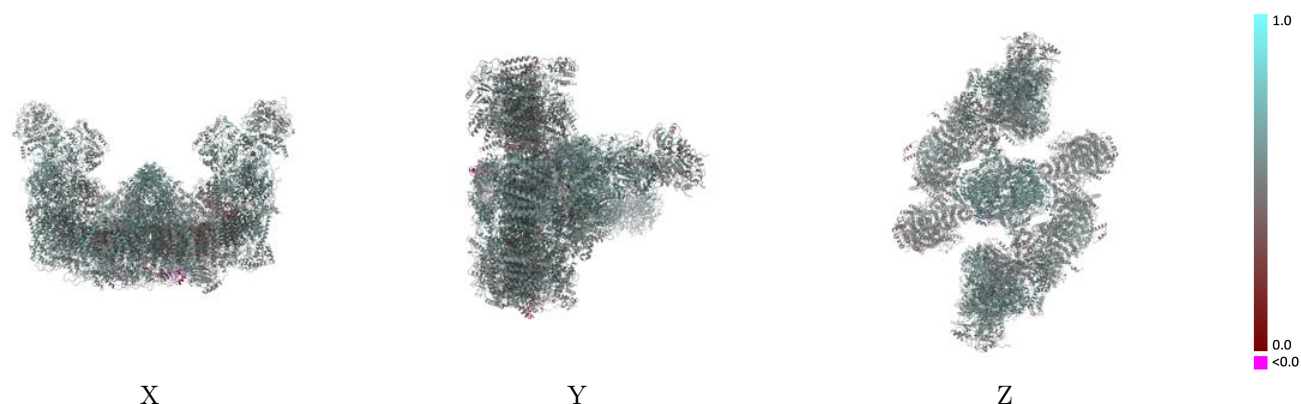
This section contains information regarding the fit between EMDB map EMD-42230 and PDB model 8UGN. Per-residue inclusion information can be found in section [3](#) on page [46](#).

9.1 Map-model overlay [i](#)



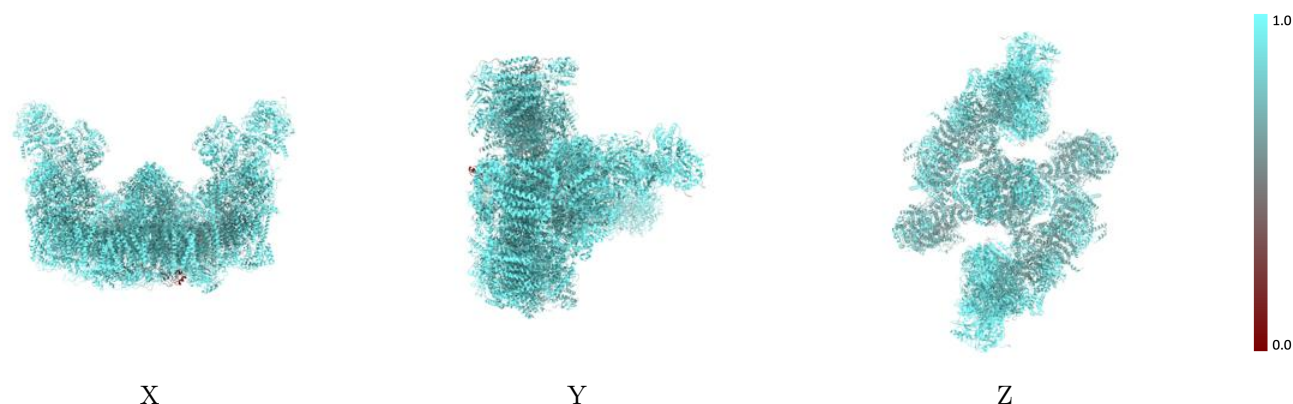
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



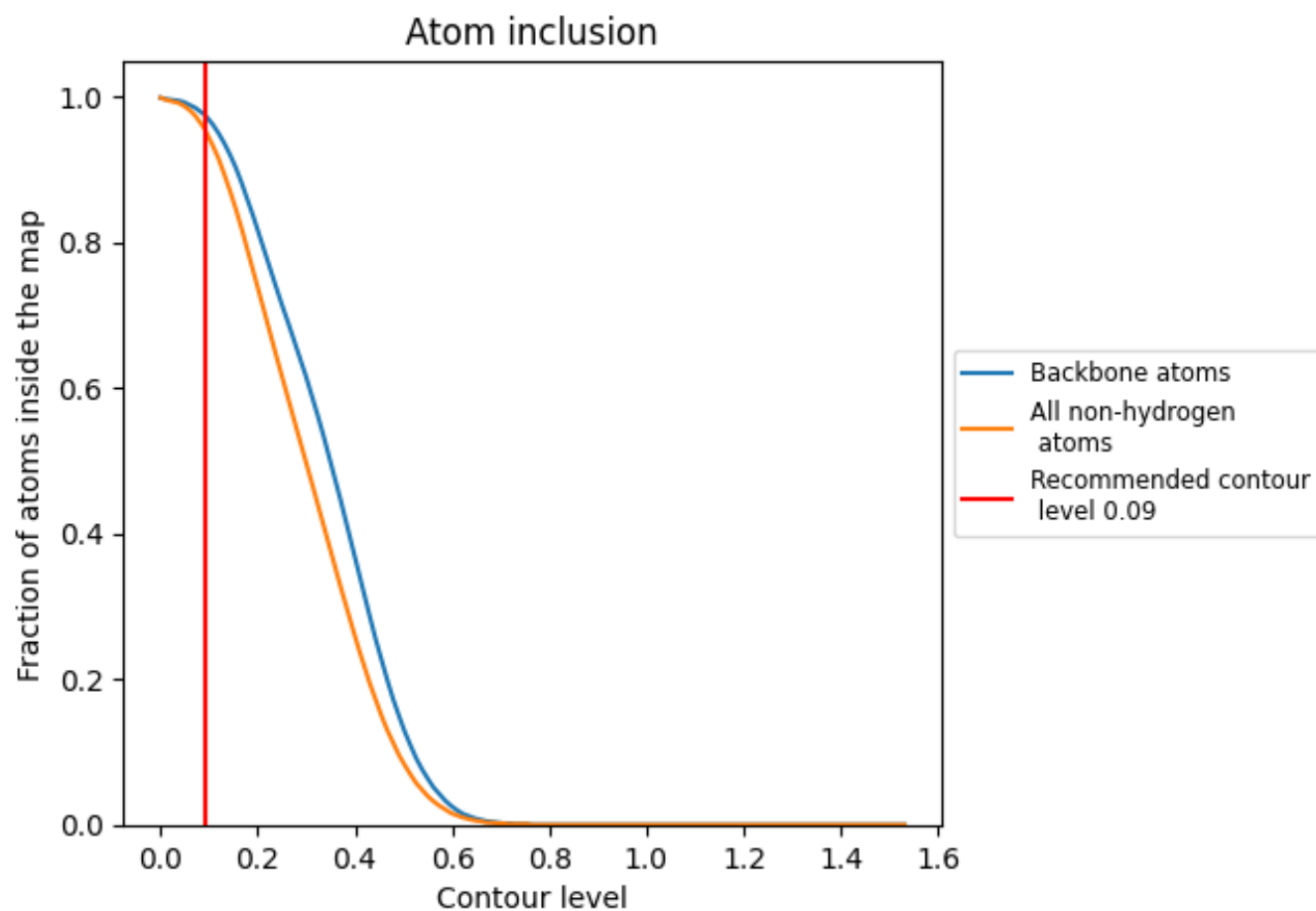
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.09).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9560	 0.5360
1A	 0.8920	 0.4560
1B	 0.9780	 0.5530
1C	 0.9800	 0.5790
1D	 0.9800	 0.5660
1E	 0.9490	 0.5020
1F	 0.9610	 0.5120
1G	 0.9700	 0.5520
1H	 0.9670	 0.5310
1I	 0.9850	 0.5740
1J	 0.9700	 0.4990
1K	 0.9910	 0.5510
1L	 0.9880	 0.5300
1M	 0.9950	 0.5540
1N	 0.9940	 0.5590
1O	 0.9710	 0.5250
1P	 0.9560	 0.5220
1Q	 0.9240	 0.5440
1R	 0.9710	 0.5620
1S	 0.9460	 0.5180
1T	 0.9040	 0.4060
1U	 0.9680	 0.5060
1V	 0.9610	 0.5260
1W	 0.9610	 0.5360
1X	 0.9880	 0.5310
1Y	 0.9790	 0.5110
1Z	 0.9840	 0.5400
1a	 0.9910	 0.5540
1b	 0.9720	 0.5250
1c	 0.9630	 0.5050
1d	 0.9740	 0.5350
1e	 0.9860	 0.5420
1f	 0.9750	 0.5110
1g	 0.9850	 0.5220
1h	 0.9810	 0.5310



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Chain	Atom inclusion	Q-score
1i	 0.9200	 0.4570
1j	 0.9440	 0.4770
1k	 0.9420	 0.4800
1l	 0.9800	 0.5360
1m	 0.9790	 0.5360
1n	 0.9870	 0.5360
1o	 0.9740	 0.4870
1p	 0.9770	 0.5160
1q	 0.9760	 0.5580
1r	 0.9860	 0.5610
1s	 0.9570	 0.4960
3A	 0.9750	 0.5960
3B	 0.9760	 0.6000
3C	 0.9890	 0.6140
3D	 0.9900	 0.6130
3E	 0.5600	 0.2830
3F	 0.9840	 0.6070
3G	 0.9800	 0.5740
3H	 0.9690	 0.5670
3I	 0.8390	 0.5010
3J	 0.9880	 0.6000
3N	 0.9830	 0.6030
3O	 0.9790	 0.6080
3P	 0.9870	 0.6170
3Q	 0.9860	 0.6100
3R	 0.5850	 0.3000
3S	 0.9760	 0.6160
3T	 0.9860	 0.5870
3U	 0.9660	 0.5740
3V	 0.9210	 0.5550
3W	 0.9890	 0.6060
3X	 0.9750	 0.5710
3Y	 0.9820	 0.5570
4A	 0.9080	 0.5130
4B	 0.8720	 0.4950
4C	 0.8940	 0.4810
4D	 0.8400	 0.4430
4E	 0.8260	 0.4260
4F	 0.8240	 0.4660
4G	 0.8620	 0.4220
4H	 0.8810	 0.4700
4I	 0.8840	 0.4820

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Chain	Atom inclusion	Q-score
4J	 0.9500	 0.4730
4K	 0.8240	 0.4480
4L	 0.8660	 0.4790
4M	 0.8670	 0.4620
4N	 0.8690	 0.4730
5A	 0.9110	 0.4750
5B	 0.9820	 0.5650
5C	 0.9860	 0.5890
5D	 0.9830	 0.5780
5E	 0.9700	 0.5140
5F	 0.9820	 0.5290
5G	 0.9790	 0.5620
5H	 0.9710	 0.5410
5I	 0.9940	 0.5910
5J	 0.9720	 0.5190
5K	 0.9920	 0.5750
5L	 0.9880	 0.5450
5M	 0.9930	 0.5620
5N	 0.9930	 0.5730
5O	 0.9800	 0.5430
5P	 0.9600	 0.5250
5Q	 0.9330	 0.5480
5R	 0.9780	 0.5720
5S	 0.9570	 0.5110
5T	 0.9110	 0.4100
5U	 0.9750	 0.5210
5V	 0.9740	 0.5510
5W	 0.9580	 0.5460
5X	 0.9890	 0.5430
5Y	 0.9770	 0.5200
5Z	 0.9920	 0.5650
5a	 0.9930	 0.5720
5b	 0.9840	 0.5360
5c	 0.9750	 0.5250
5d	 0.9790	 0.5430
5e	 0.9760	 0.5430
5f	 0.9700	 0.5050
5g	 0.9940	 0.5250
5h	 0.9800	 0.5430
5i	 0.9180	 0.4640
5j	 0.9300	 0.4760
5k	 0.9400	 0.4780

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Chain	Atom inclusion	Q-score
5l	 0.9780	 0.5400
5m	 0.9780	 0.5480
5n	 0.9860	 0.5430
5o	 0.9770	 0.4840
5p	 0.9780	 0.5290
5q	 0.9750	 0.5570
5r	 0.9890	 0.5700
5s	 0.9650	 0.5040
8A	 0.9440	 0.5410
8B	 0.8840	 0.5050
8C	 0.9230	 0.5040
8D	 0.8560	 0.4650
8E	 0.8640	 0.4650
8F	 0.8590	 0.4940
8G	 0.8790	 0.4460
8H	 0.9070	 0.4890
8I	 0.8750	 0.4840
8J	 0.9460	 0.4890
8K	 0.8540	 0.4790
8L	 0.8850	 0.4830
8M	 0.8670	 0.4850
8N	 0.8720	 0.4830